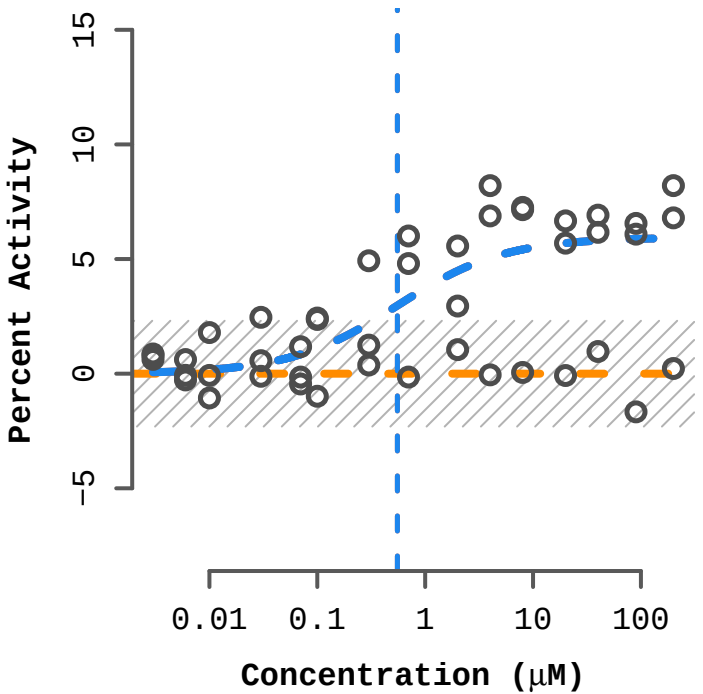
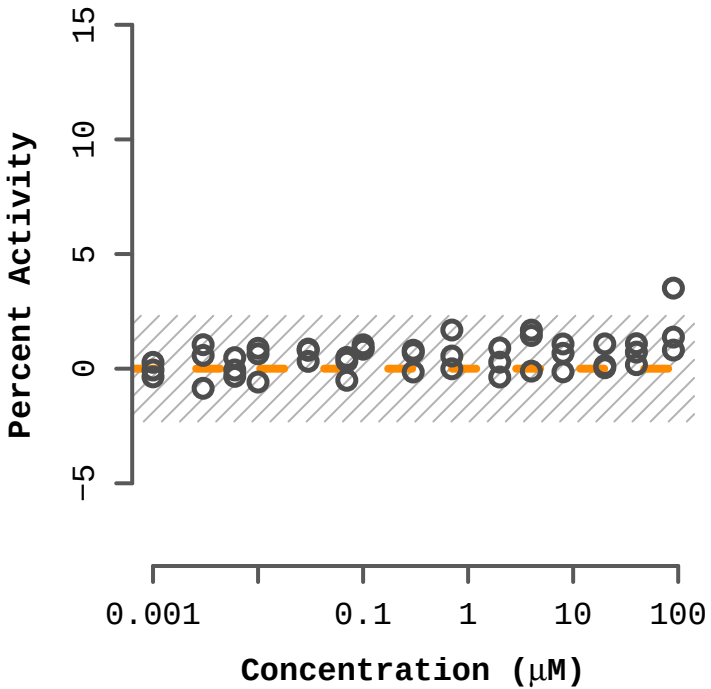



```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Acetamide
CHID:    20005   CASRN: 60-35-5
SPID(S): Tox21_300776
M4ID:    12478357

HILL MODEL (in red):
      tp       ga       gw
val:  5.94     -0.257   0.872
sd:   0.848    0.351    0.465

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.94     -0.257   0.872    3.34     7.92
sd:   0.848    0.351    0.465    1740     13300

      CNST       HILL       GNLS
AIC:  256.46     217.82     221.82
PROB: 0          0.88       0.12
RMSE: 4.03       2.58       2.58

MAX_MEAN: 5.08      MAX_MED: 7.16      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

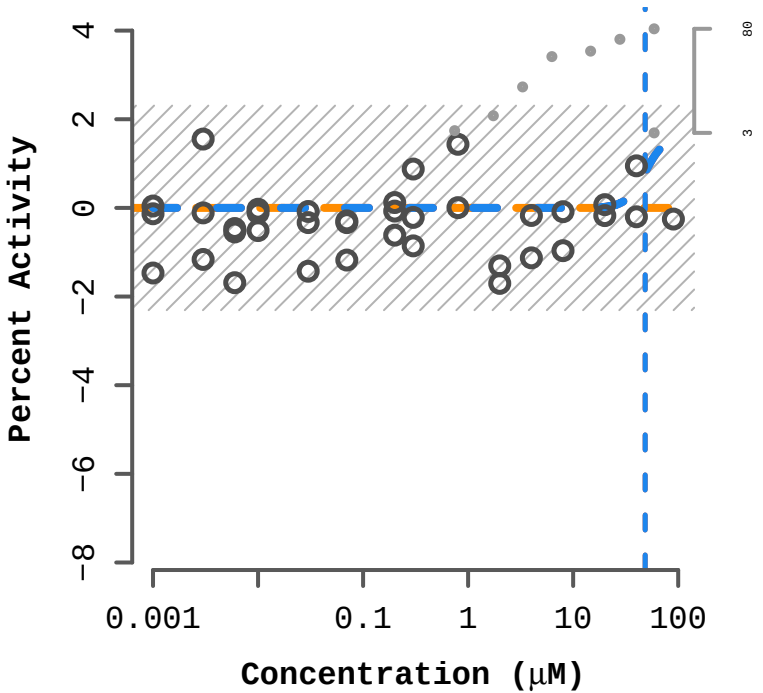
NAME: Acetaminophen
CHID: 20006 **CASRN:** 103-90-2
SPID(S): Tox21_300100
M4ID: 12479030

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acetaminophen
CHID: 20006 CASRN: 103-90-2
SPID(S): Tox21_201930
M4ID: 12480322 BRK

HILL MODEL (in red):

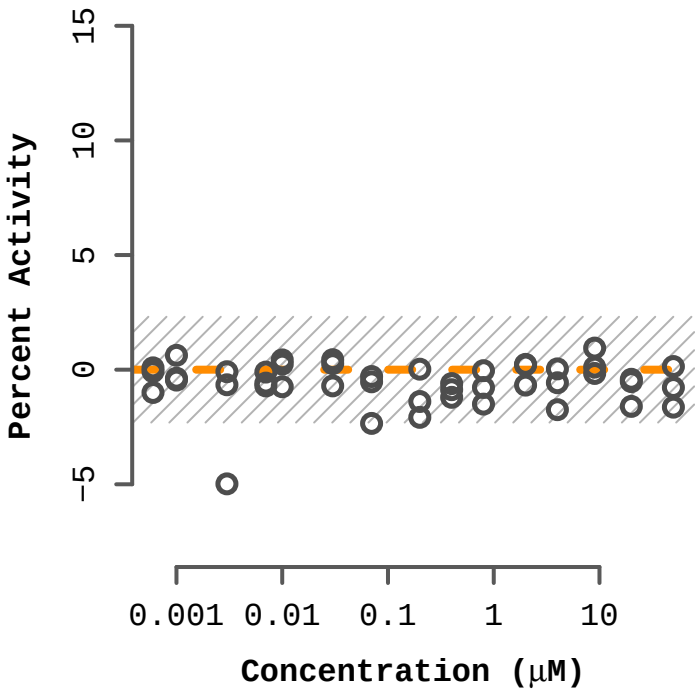
	tp	ga	gw
val:	1.6	1.69	4.81
sd:	3.89	1.23	51.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.61	1.69	4.81	3.4	1.62
sd:	19.6	1.63	51.6	1010	1240

	CNST	HILL	GNLS
AIC:	316.21	320.98	324.98
PROB:	0.91	0.08	0.01
RMSE:	21.65	21.48	21.48

MAX_MEAN: 27.7 MAX_MED: 3.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

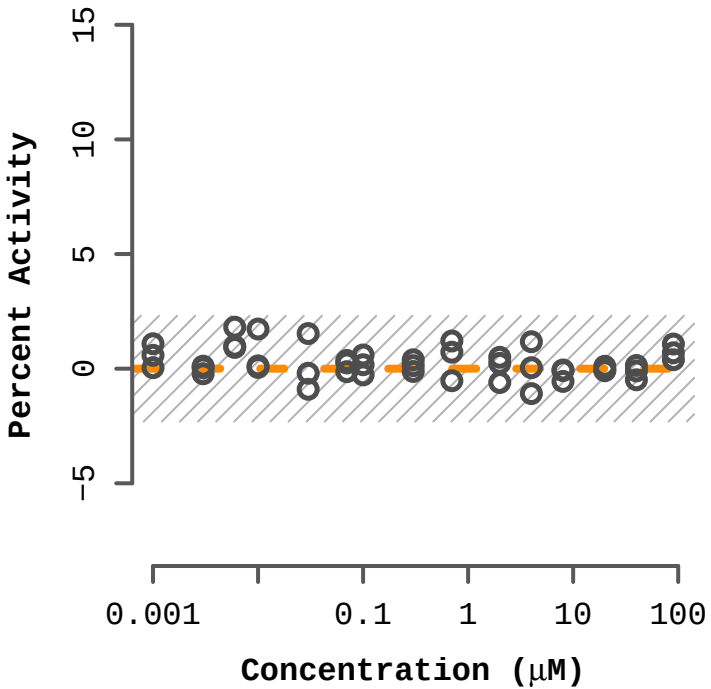
NAME: Acetaminophen
CHID: 20006 **CASRN:** 103-90-2
SPID(S): Tox21_110397_1
M4ID: 12484394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.298 **MAX_MED:** 0.264 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

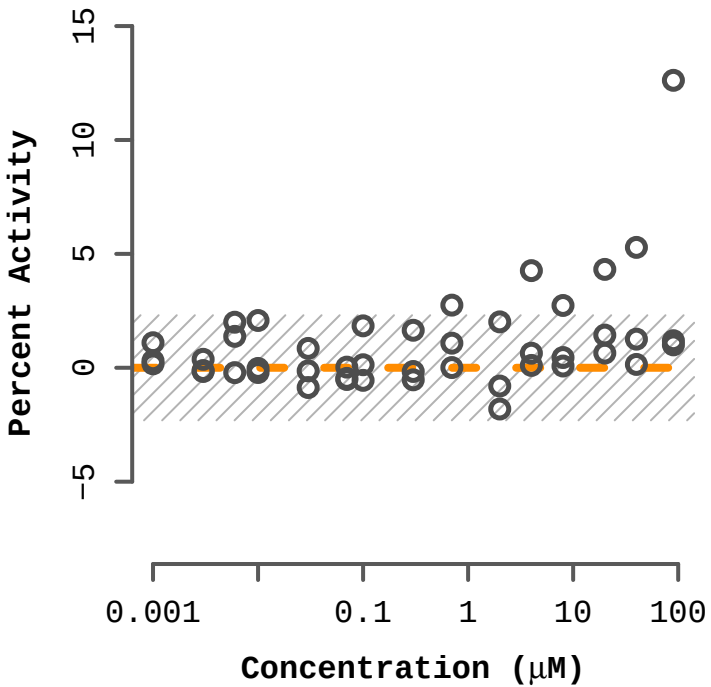
NAME: Acetohexamide
CHID: 20007 **CASRN:** 968-81-0
SPID(S): Tox21_302735
M4ID: 12476398

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

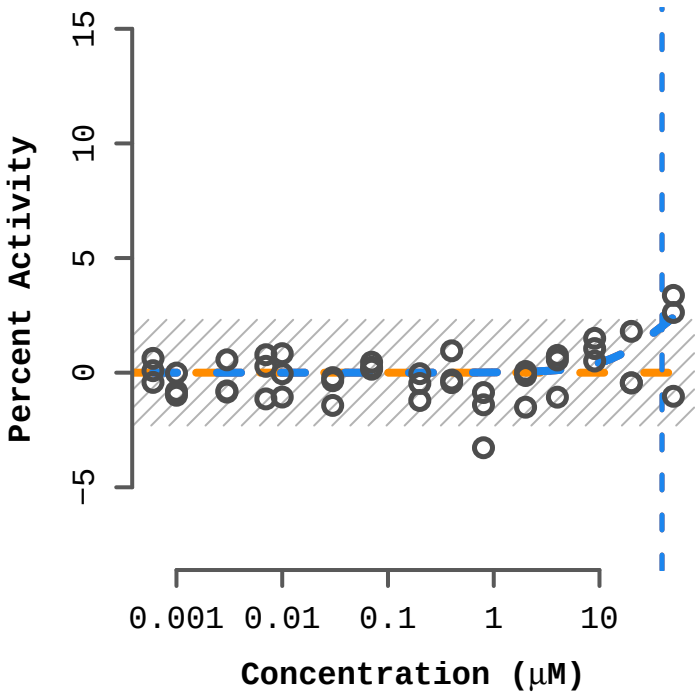
NAME: Acetohexamide
CHID: 20007 CASRN: 968-81-0
SPID(S): Tox21_202022
M4ID: 12480230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.48	NA	NA

MAX_MEAN: 4.94 MAX_MED: 1.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acetohexamide
CHID: 20007 **CASRN:** 968-81-0
SPID(S): Tox21_110067_1
M4ID: 12484683

HILL MODEL (in red):

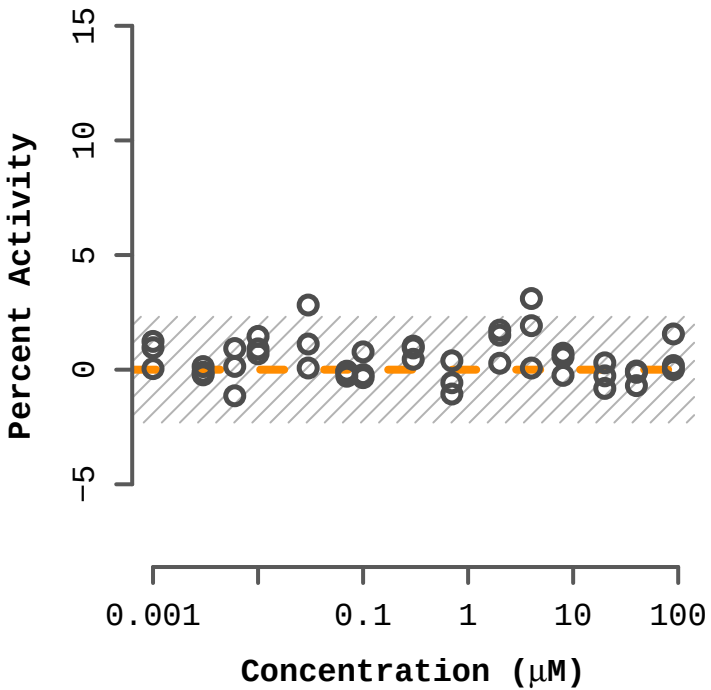
	tp	ga	gw
val:	4.05	1.59	1.56
sd:	3.31	0.48	0.928

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.05	1.59	1.56	3.58	3.86
sd:	3.32	0.48	0.929	1200	2490

	CNST	HILL	GNLS
AIC:	137.58	137.3	141.3
PROB:	0.43	0.5	0.07
RMSE:	1.13	1.06	1.06

MAX_MEAN: 1.66 **MAX_MED:** 2.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

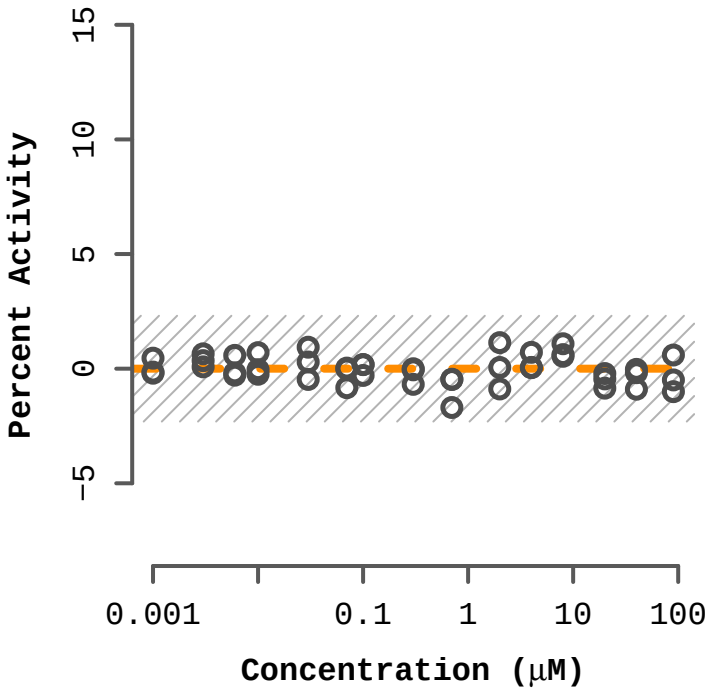
NAME: Acetonitrile
CHID: 20009 CASRN: 75-05-8
SPID(S): Tox21_202481
M4ID: 12479771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.54	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.7 MAX_MED: 1.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

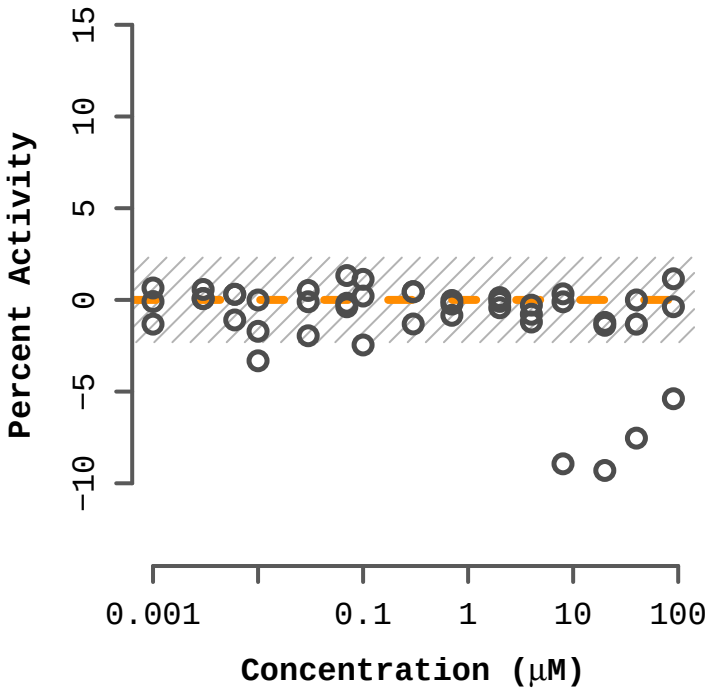
NAME: Dehydroacetic acid
CHID: 20014 CASRN: 520-45-6
SPID(S): Tox21_302764
M4ID: 12476369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	83.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.59	NA	NA

MAX_MEAN: 0.748 MAX_MED: 0.616 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

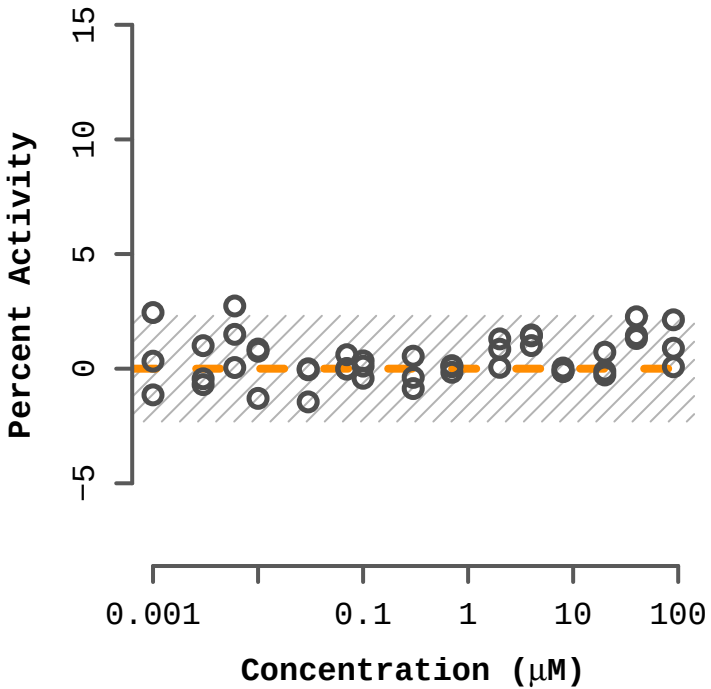
NAME: 1-Acetyl-2-phenylhydrazine
CHID: 20015 **CASRN:** 114-83-0
SPID(S): Tox21_200069
M4ID: 12482183

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.56	NA	NA

MAX_MEAN: 0.259 **MAX_MED:** 0.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

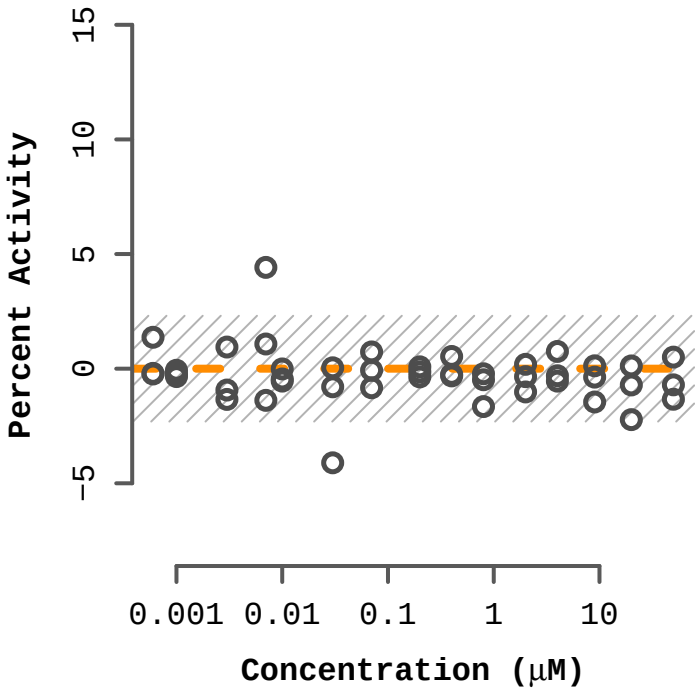
NAME: 4-Acetylaminophenylacetic acid
CHID: 20020 **CASRN:** 18699-02-0
SPID(S): Tox21_301197
M4ID: 12477936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

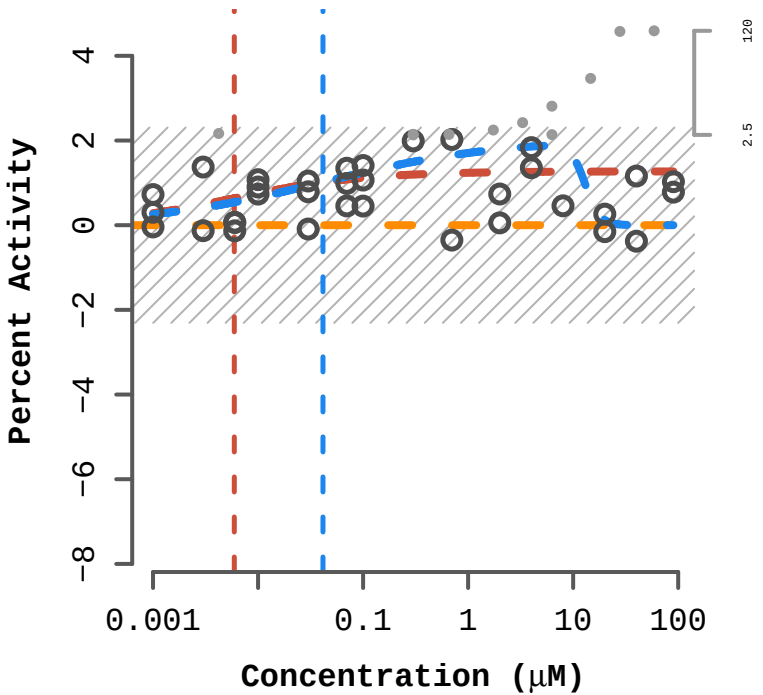
NAME: 4-Acetylaminophenylacetic acid
CHID: 20020 **CASRN:** 18699-02-0
SPID(S): Tox21_111820_1
M4ID: 12483459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Acetyl-L-cysteine
CHID: 20021 **CASRN:** 616-91-1
SPID(S): Tox21_201078
M4ID: 12481174 **BRK**

HILL MODEL (in red):

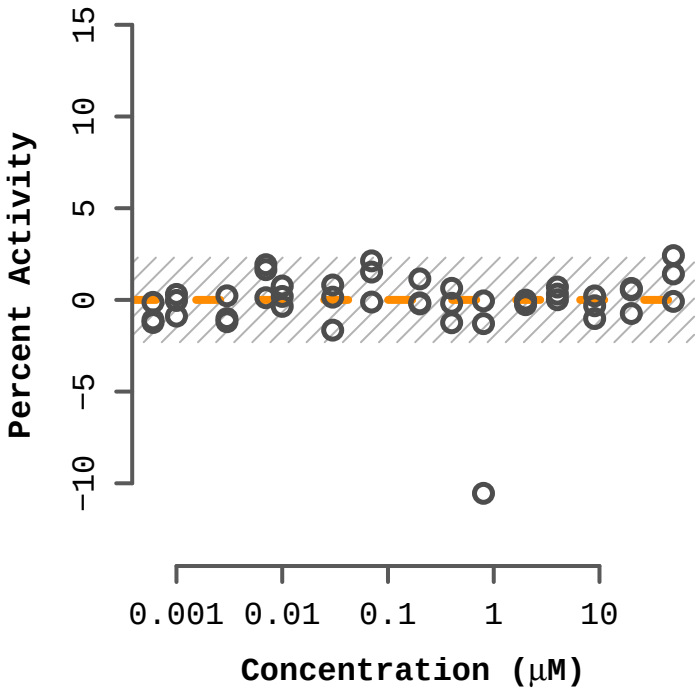
	tp	ga	gw
val:	1.27	−2.23	0.704
sd:	0.388	1.09	0.722

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.03	−1.38	0.52	1.11	6.24
sd:	1.19	1.23	0.624	0.585	20.9

	CNST	HILL	GNLS
AIC:	315.38	307.3	309.01
PROB:	0.01	0.69	0.29
RMSE:	28.66	28.27	28.55

MAX_MEAN: 41.9 **MAX_MED:** 2.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

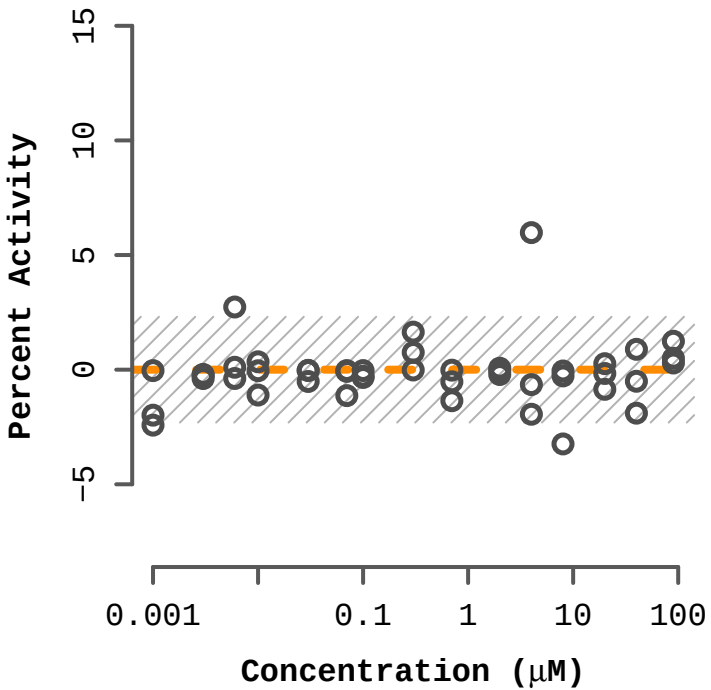
NAME: N-Acetyl-L-cysteine
CHID: 20021 **CASRN:** 616-91-1
SPID(S): Tox21_110877_1
M4ID: 12484050

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

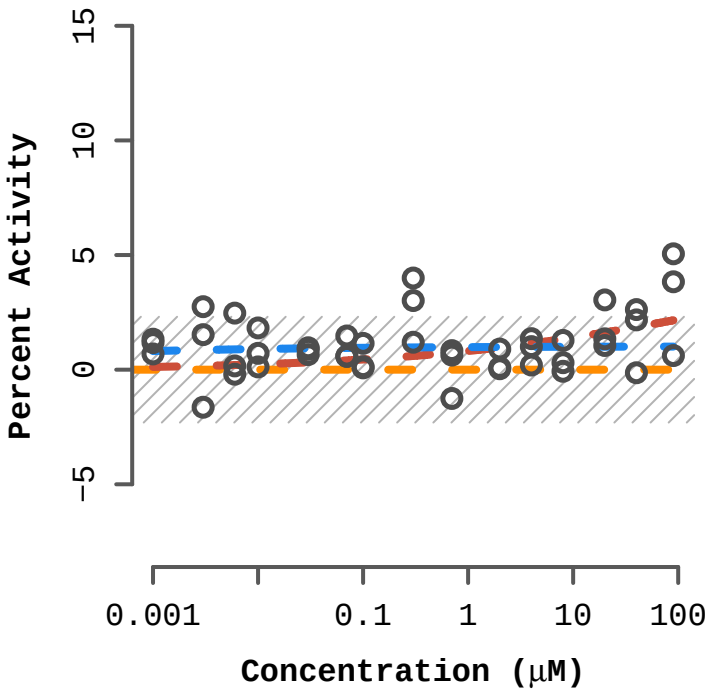
NAME: Acifluorfen
CHID: 20022 CASRN: 50594-66-6
SPID(S): Tox21_300760
M4ID: 12478373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.13 MAX_MED: 0.753 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acifluorfen
CHID: 20022 CASRN: 50594-66-6
SPID(S): Tox21_201839
M4ID: 12480413

HILL MODEL (in red):

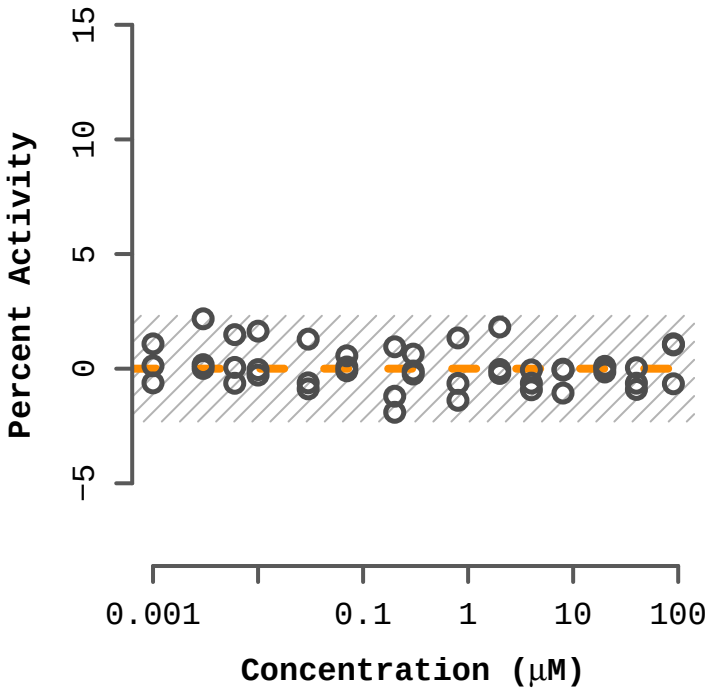
	tp	ga	gw
val:	5.06	2.39	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.01	−5	0.3	3.95	17.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	176.27	158.32	159.01
PROB:	0	0.59	0.41
RMSE:	1.71	1.28	1.29

MAX_MEAN: 3.17 **MAX_MED:** 3.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

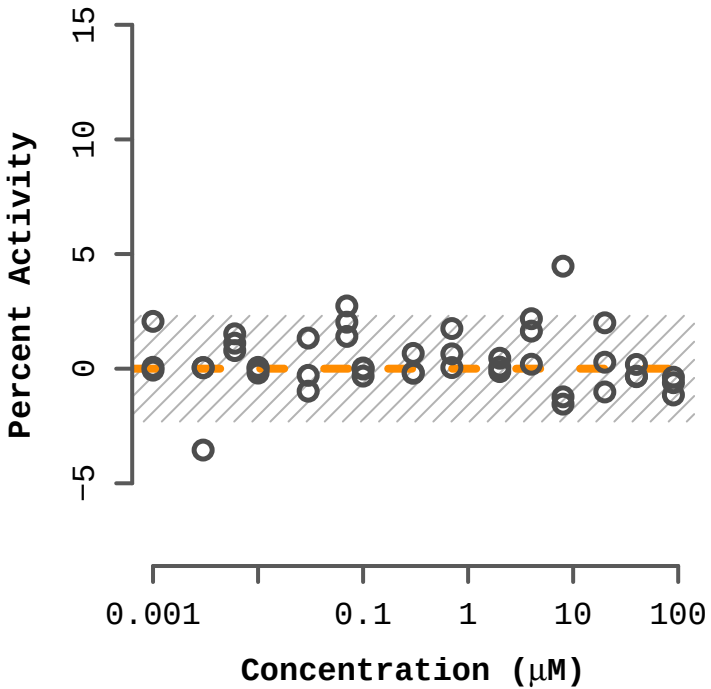
NAME: Acrolein
CHID: 20023 CASRN: 107-02-8
SPID(S): Tox21_200984
M4ID: 12481268

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.789 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

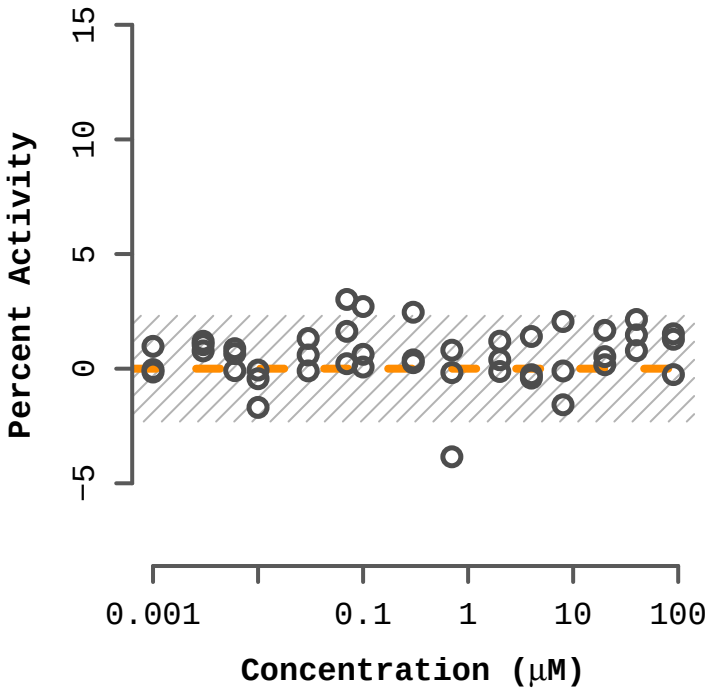
NAME: Acrolein diethylacetal
CHID: 20024 **CASRN:** 3054-95-3
SPID(S): Tox21_200229
M4ID: 12482023

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

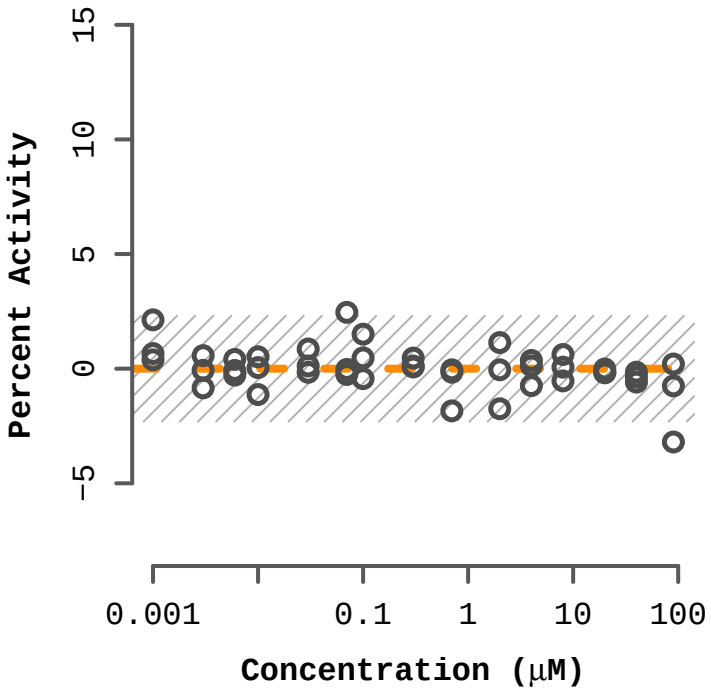
NAME: Acrylamide
CHID: 20027 **CASRN:** 79-06-1
SPID(S): Tox21_300145
M4ID: 12478985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

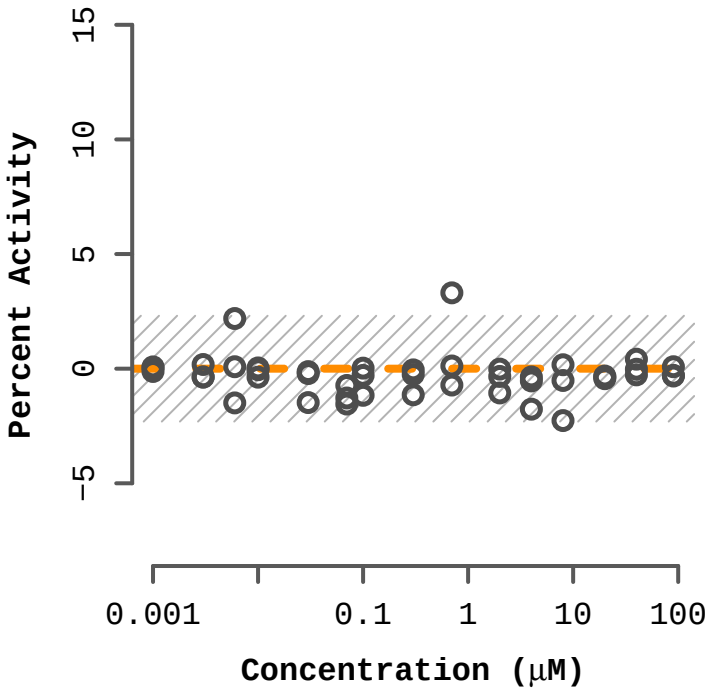
NAME: Acrylamide
CHID: 20027 **CASRN:** 79-06-1
SPID(S): Tox21_201526
M4ID: 12480726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.662 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

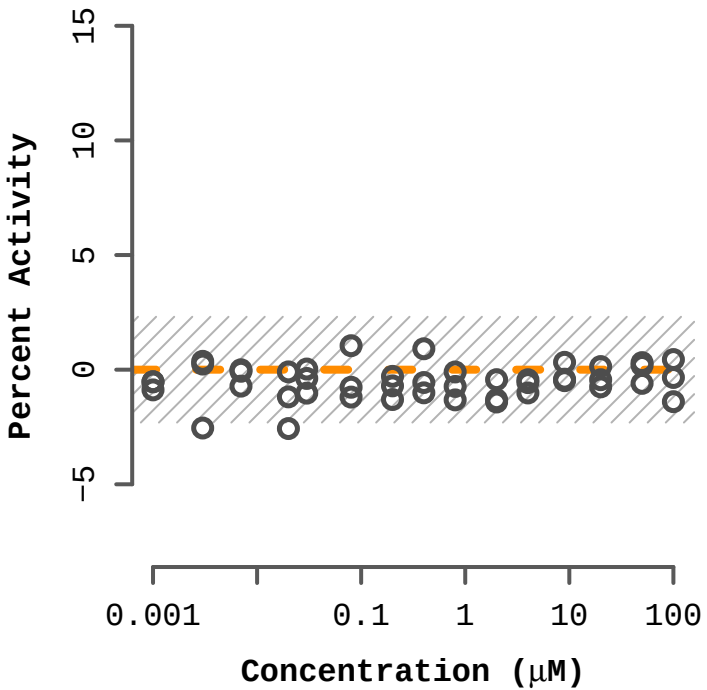
NAME: Acrylonitrile
CHID: 20029 CASRN: 107-13-1
SPID(S): Tox21_302951
M4ID: 12476182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.906 MAX_MED: 0.119 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

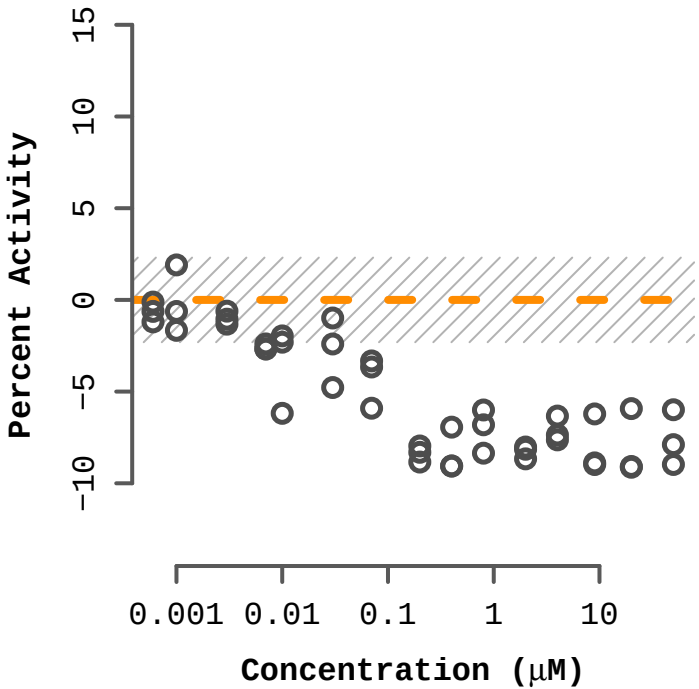
NAME: Acrylonitrile
CHID: 20029 **CASRN:** 107-13-1
SPID(S): Tox21_202076
M4ID: 12480176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: −0.0332 **MAX_MED:** 0.246 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

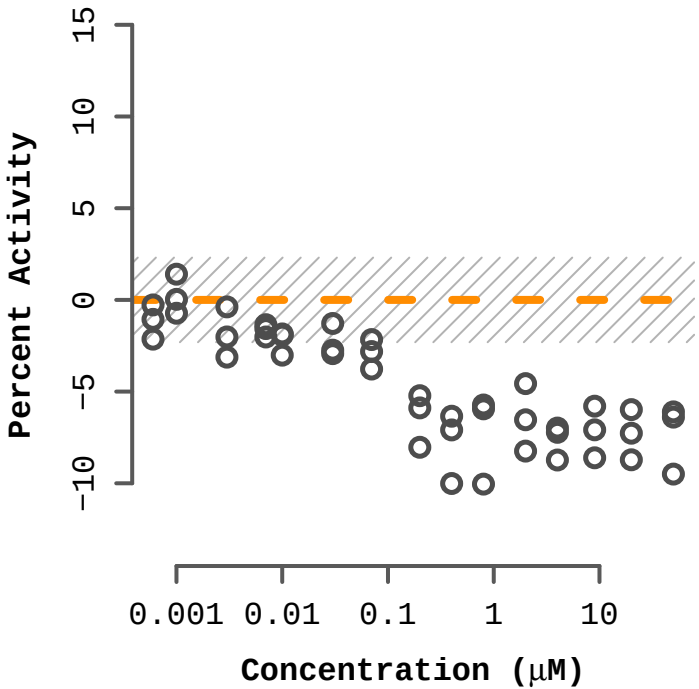
NAME: Actinomycin D
CHID: 20031 **CASRN:** 50-76-0
SPID(S): Tox21_202482
M4ID: 12479770

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	299.82	NA	NA
PROB:	1	NA	NA
RMSE:	6.11	NA	NA

MAX_MEAN: −0.126 **MAX_MED:** −0.625 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

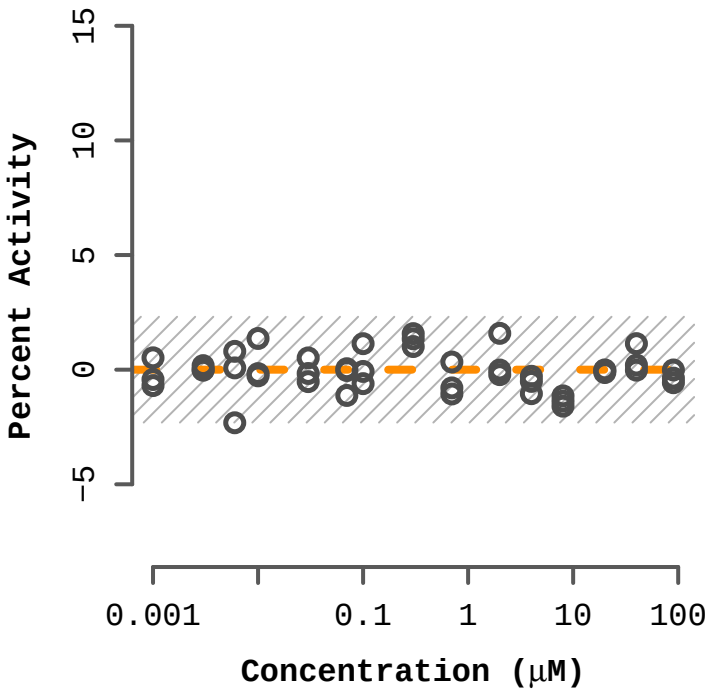
NAME: Actinomycin D
CHID: 20031 **CASRN:** 50-76-0
SPID(S): Tox21_111997_1
M4ID: 12483382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.78	NA	NA
PROB:	1	NA	NA
RMSE:	5.53	NA	NA

MAX_MEAN: 0.236 **MAX_MED:** 0.0326 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

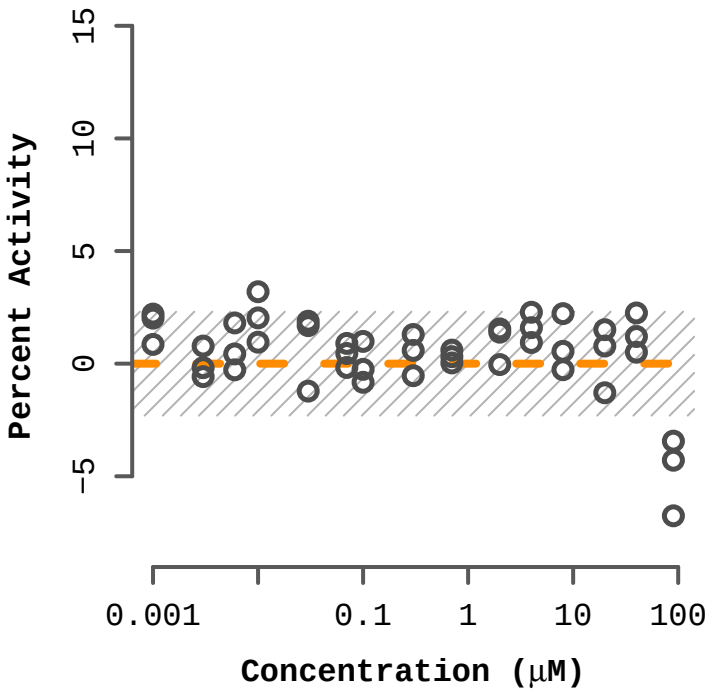
NAME: Adipamide
CHID: 20032 CASRN: 628-94-4
SPID(S): Tox21_200347
M4ID: 12481905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

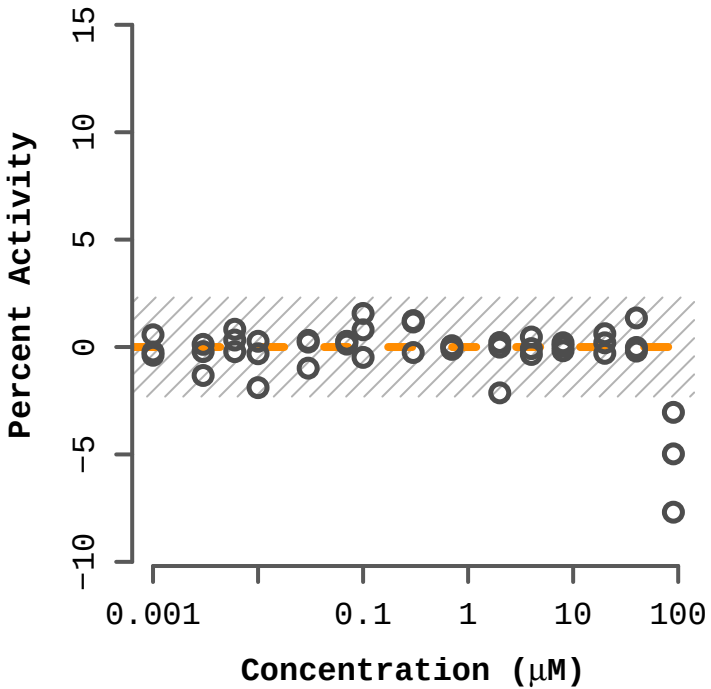
NAME: Aldrin
CHID: 20040 CASRN: 309-00-2
SPID(S): Tox21_300172
M4ID: 12478958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

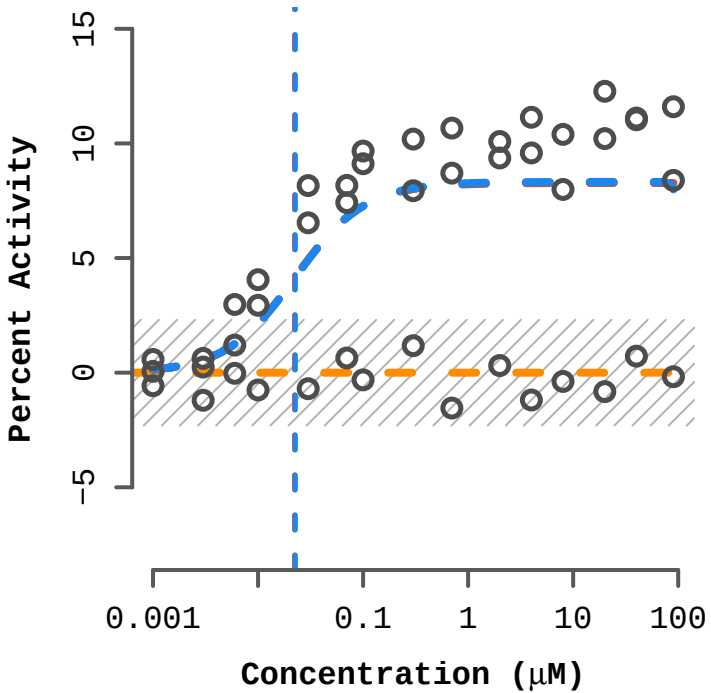
NAME: Aldrin
CHID: 20040 CASRN: 309-00-2
SPID(S): Tox21_202072
M4ID: 12480180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 0.716 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Allantoin
CHID: 20043 CASRN: 97-59-6
SPID(S): Tox21_302912
M4ID: 12476221

HILL MODEL (in red):

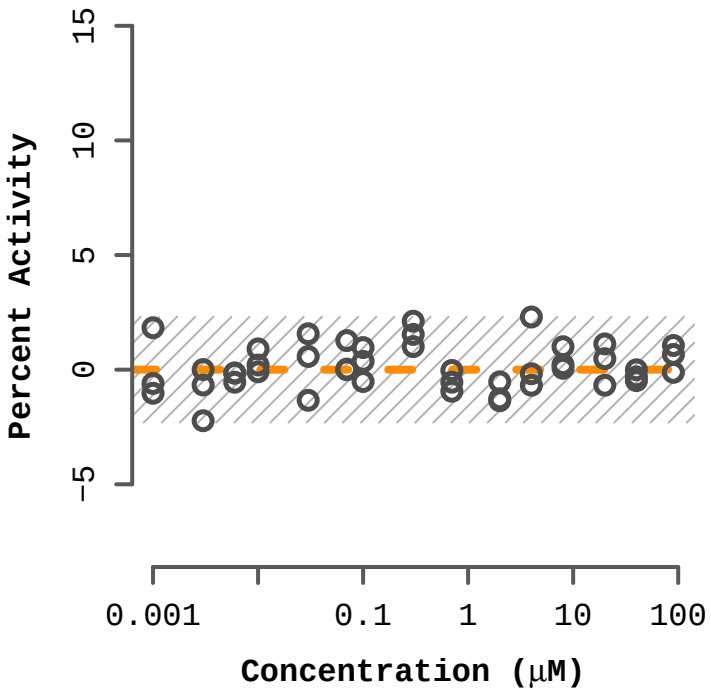
	tp	ga	gw
val:	8.27	−1.65	1.32
sd:	1.01	0.272	0.758

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.32	−1.65	1.3	2.04	15.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	307.14	265.58	269.56
PROB:	0	0.88	0.12
RMSE:	6.82	4.29	4.29

MAX_MEAN: 7.62 **MAX_MED:** 11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

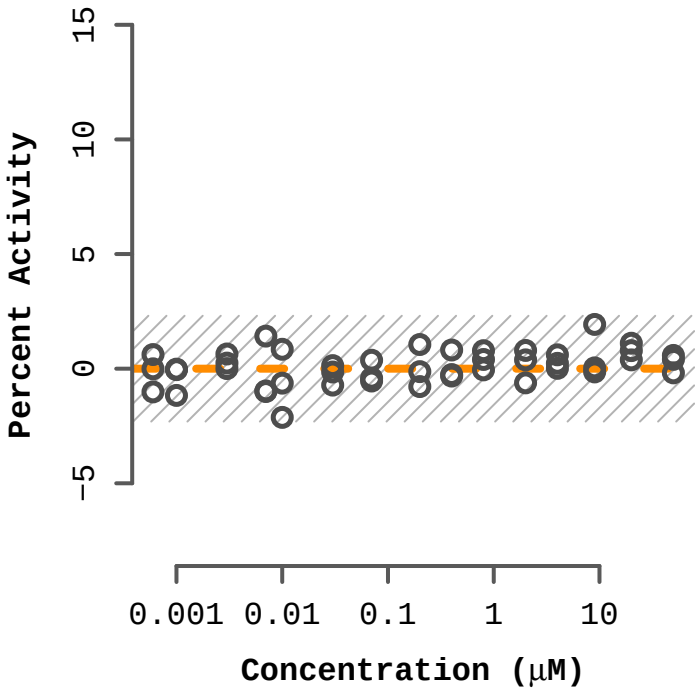
NAME: Allantoin
CHID: 20043 CASRN: 97-59-6
SPID(S): Tox21_202087
M4ID: 12480165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.55 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

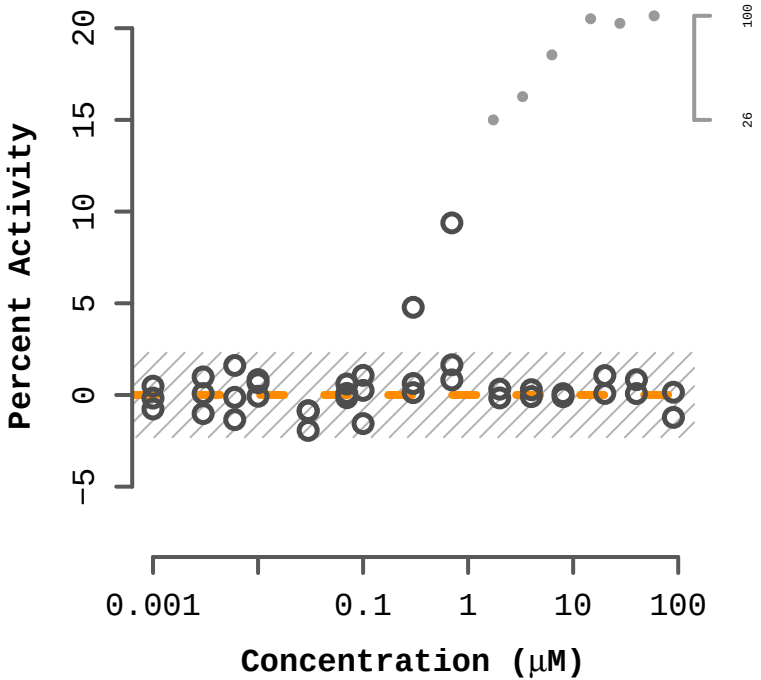
NAME: Allantoin
CHID: 20043 **CASRN:** 97-59-6
SPID(S): Tox21_110395_1
M4ID: 12484396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.762 **MAX_MED:** 0.788 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

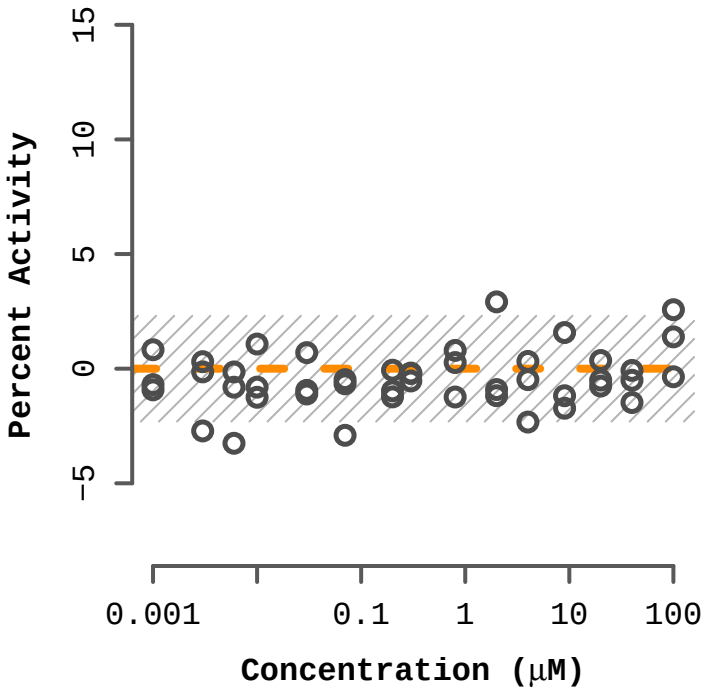
NAME: Allyl alcohol
CHID: 20044 CASRN: 107-18-6
SPID(S): Tox21_303507
M4ID: 12475635 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	341.66	NA	NA
PROB:	1	NA	NA
RMSE:	28.65	NA	NA

MAX_MEAN: 33.3 MAX_MED: 1.65 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

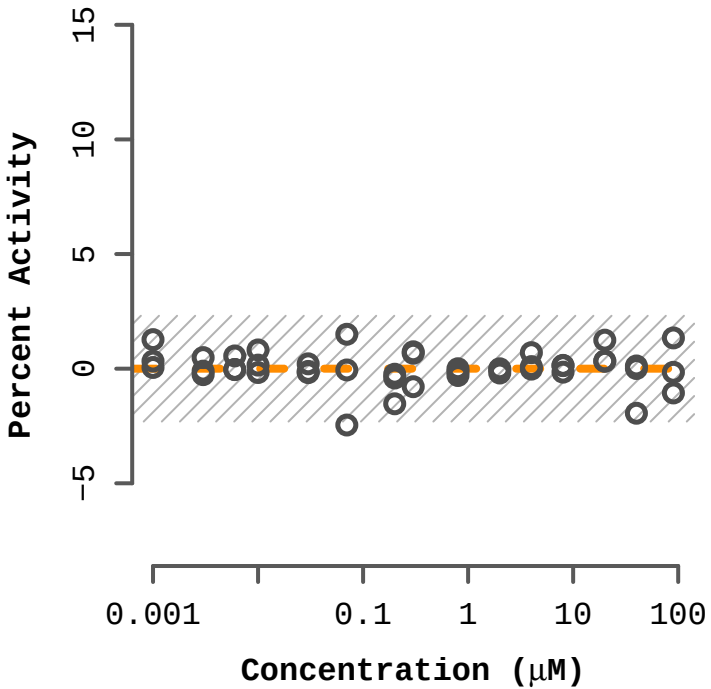
NAME: Allyl alcohol
CHID: 20044 **CASRN:** 107-18-6
SPID(S): Tox21_200200
M4ID: 12482052

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

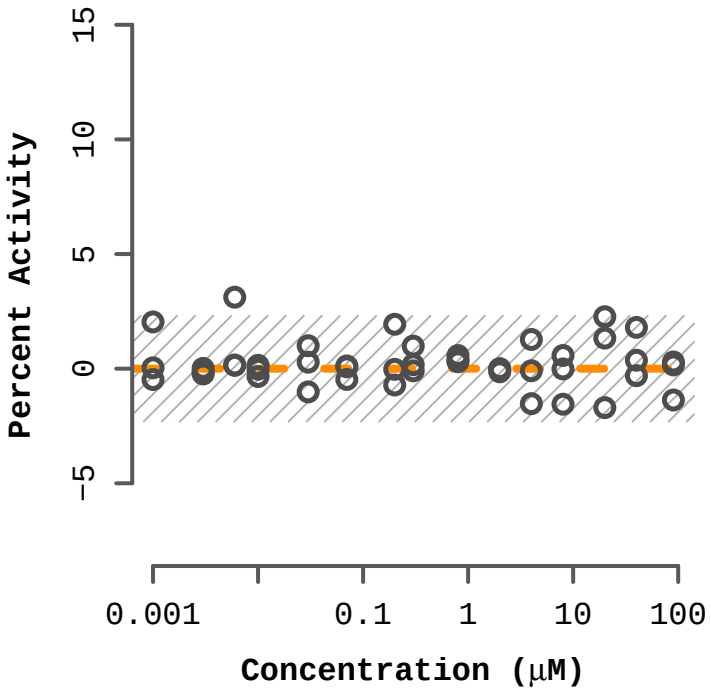
NAME: Allyl isothiocyanate
CHID: 20047 CASRN: 57-06-7
SPID(S): Tox21_302890
M4ID: 12476243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.637 MAX_MED: 0.673 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

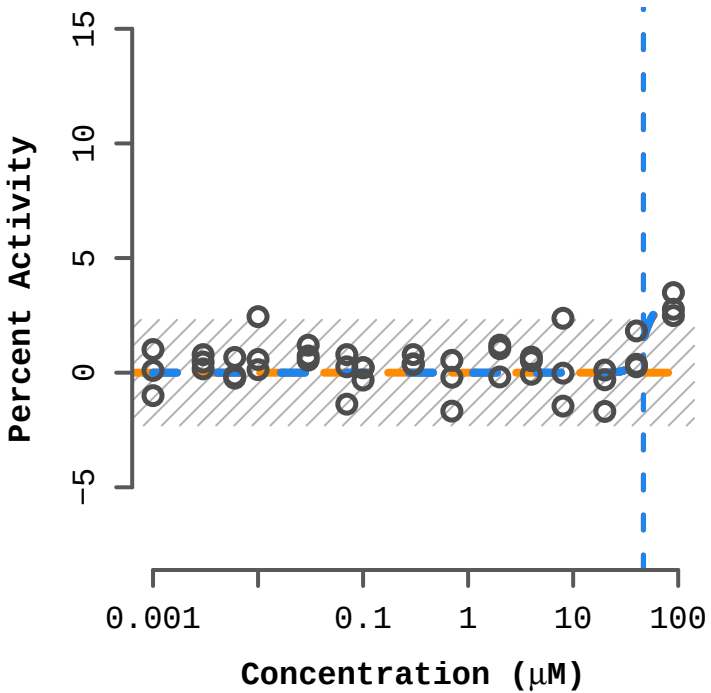
NAME: Allyl isothiocyanate
CHID: 20047 **CASRN:** 57-06-7
SPID(S): Tox21_202249
M4ID: 12480003

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.97	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Amino-4-ethoxyacetanilide
CHID: 20053 CASRN: 17026-81-2
SPID(S): Tox21_200653
M4ID: 12481599

HILL MODEL (in red):

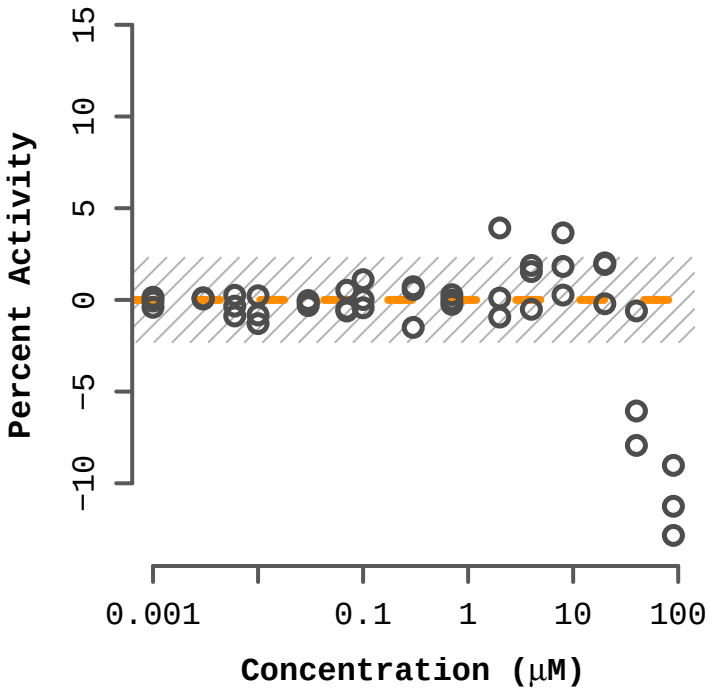
	tp	ga	gw
val:	2.91	1.67	8
sd:	0.448	0.146	15.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3	1.67	8	2.2	6.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	141.12	123.29	127.29
PROB:	0	0.88	0.12
RMSE:	1.18	0.88	0.88

MAX_MEAN: 2.92 MAX_MED: 2.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

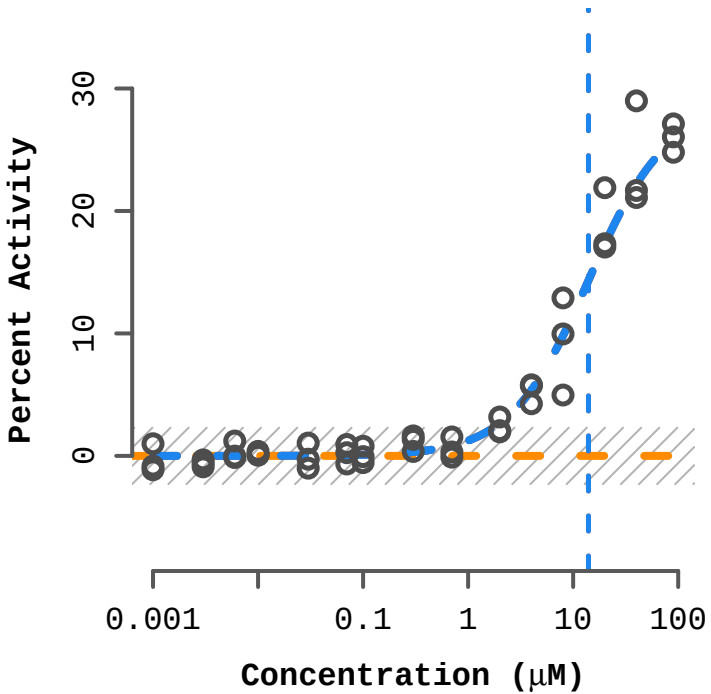
NAME: 3-Amino-9-ethylcarbazole hydrochloride
CHID: 20054 CASRN: 6109-97-3
SPID(S): Tox21_200486
M4ID: 12481766

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.75	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 1.92 MAX_MED: 1.93 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Amino-2-methylanthraquinone
CHID: 20057 CASRN: 82-28-0
SPID(S): Tox21_302964
M4ID: 12476169

HILL MODEL (in red):

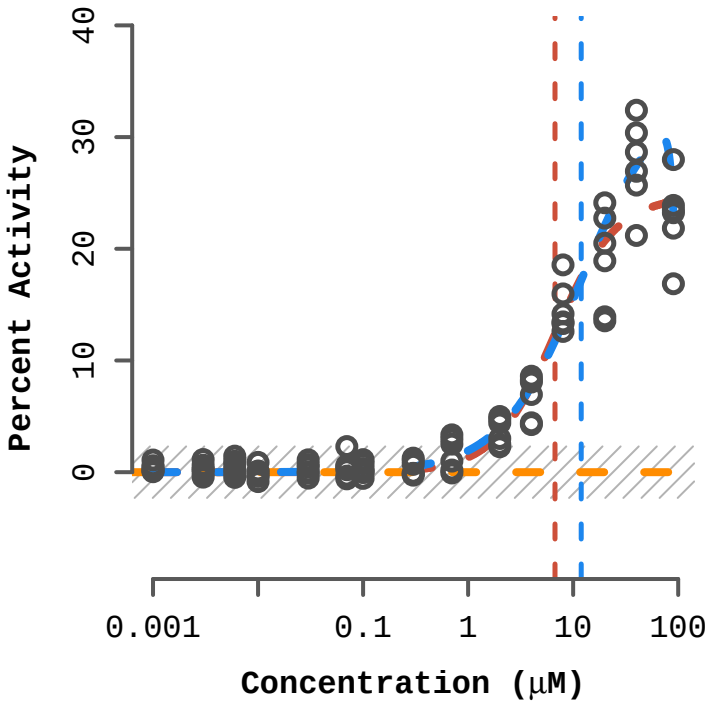
	tp	ga	gw
val:	28.7	1.15	1.17
sd:	1.37	0.053	0.0918

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	28.7	1.15	1.17	2.7	9.91
sd:	1.37	0.053	0.0918	143	1920

	CNST	HILL	GNLS
AIC:	331.11	157.17	161.17
PROB:	0	0.88	0.12
RMSE:	10.82	1.65	1.65

MAX_MEAN: 26 MAX_MED: 26.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Amino-2-methylanthraquinone
CHID: 20057 CASRN: 82-28-0
SPID(S): Tox21_201681
M4ID: 12480571

HILL MODEL (in red):

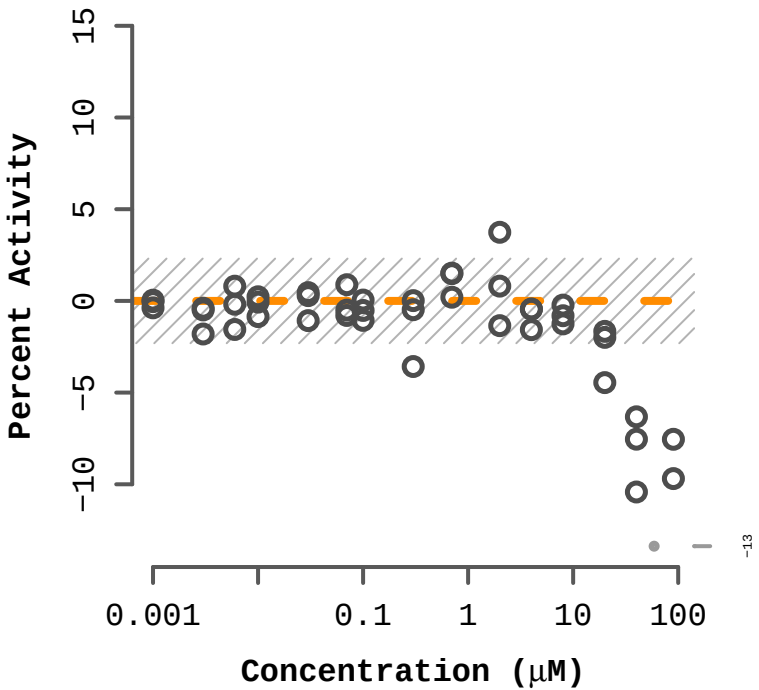
	tp	ga	gw
val:	24.7	0.827	1.51
sd:	0.872	0.0327	0.142

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	34.4	1.08	1.14	1.99	14.2
sd:	3.36	0.0929	0.121	0.00447	3.32

	CNST	HILL	GNLS
AIC:	678.08	377.42	359.96
PROB:	0	0	1
RMSE:	11.47	2.32	2.11

MAX_MEAN: 27.5 MAX_MED: 27.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

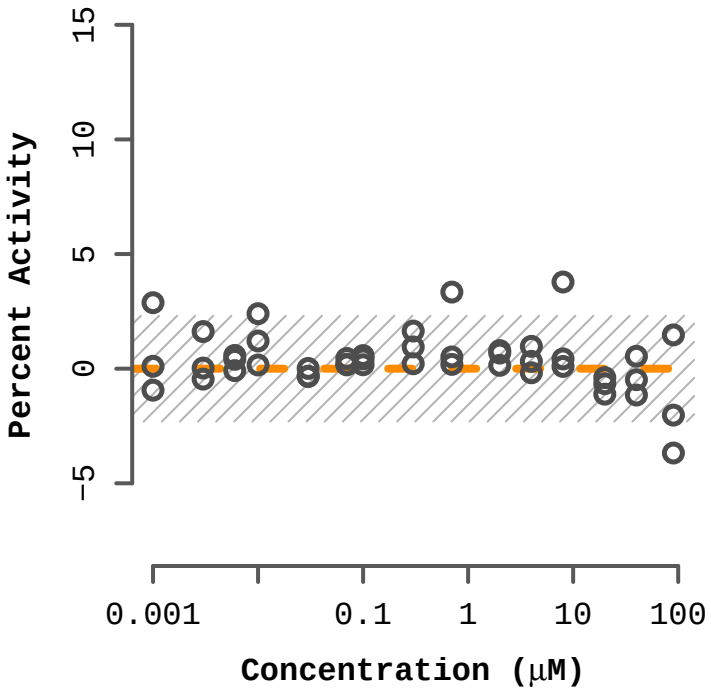
NAME: 2-Amino-5-(5-nitro-2-furyl)-1,3,4-oxadiazole
CHID: 20058 **CASRN:** 3775-55-1
SPID(S): Tox21_300647
M4ID: 12478486 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.2	NA	NA
PROB:	1	NA	NA
RMSE:	3.7	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

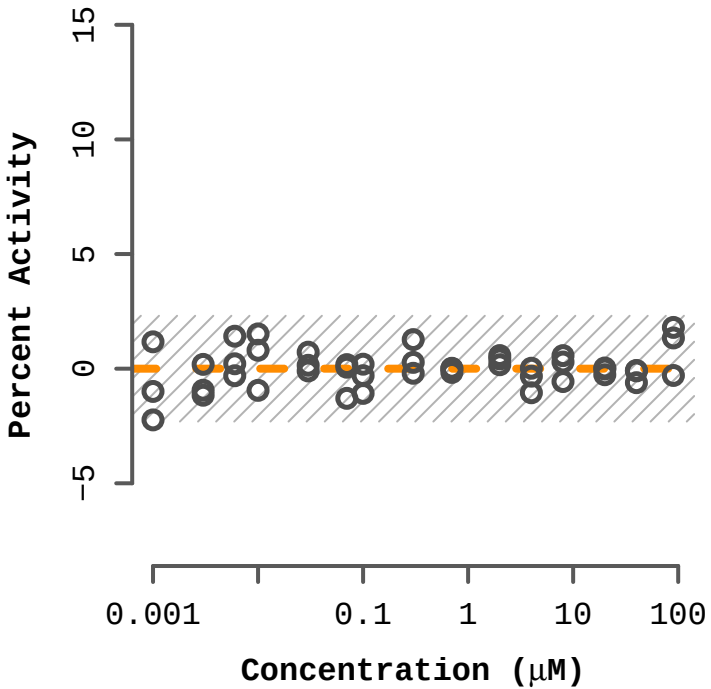
NAME: 2-Amino-4-nitrophenol
CHID: 20062 **CASRN:** 99-57-0
SPID(S): Tox21_302788
M4ID: 12476345

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

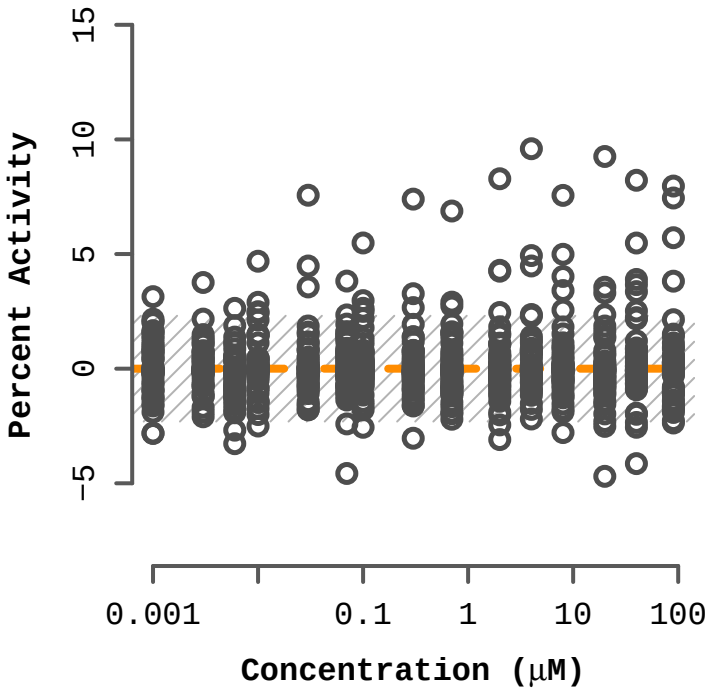
NAME: 2-Amino-4-nitrophenol
CHID: 20062 **CASRN:** 99-57-0
SPID(S): Tox21_201351
M4ID: 12480901

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.949 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

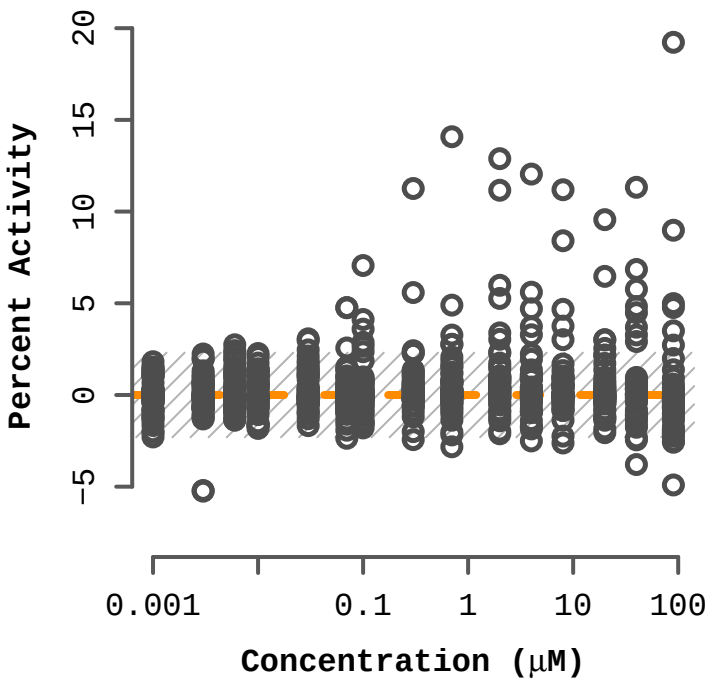
NAME: 2-Amino-5-nitrophenol
CHID: 20063 **CASRN:** 121-88-0
SPID(S): Tox21_400036
M4ID: 12475101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2418.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 0.454 **MAX_MED:** 0.105 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

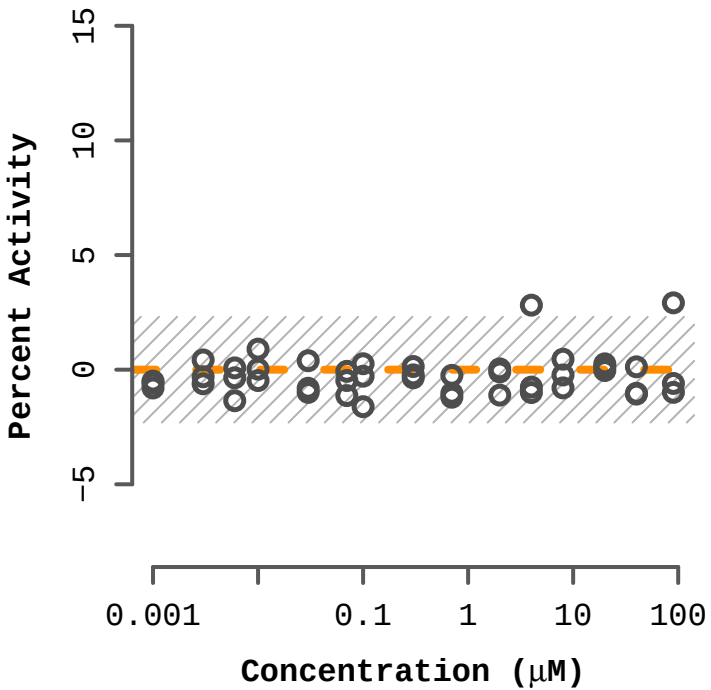
NAME: 4-Amino-2-nitrophenol
CHID: 20064 CASRN: 119-34-6
SPID(S): Tox21_400027
M4ID: 12475110

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2540.7	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 1.06 MAX_MED: 0.367 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

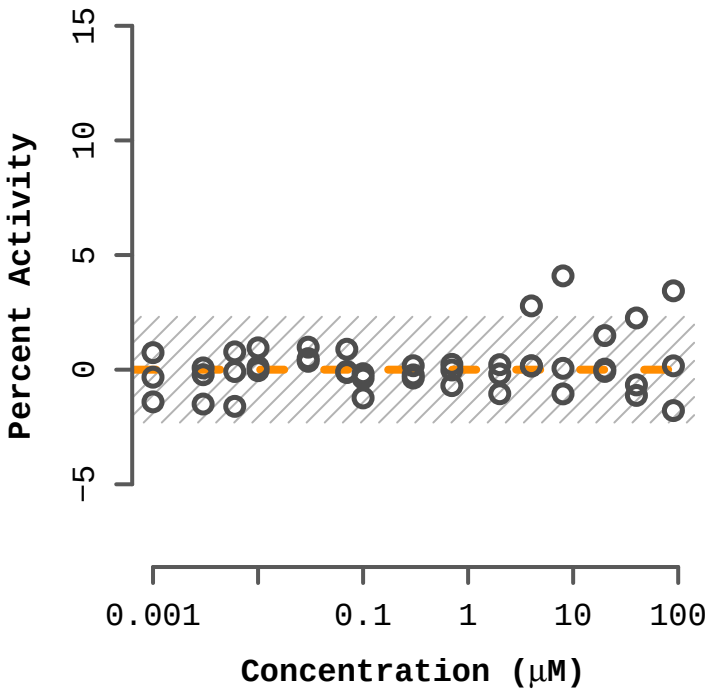
NAME: 2-Amino-5-nitrothiazole
CHID: 20066 **CASRN:** 121-66-4
SPID(S): Tox21_303575
M4ID: 12475570

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.443 **MAX_MED:** 0.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

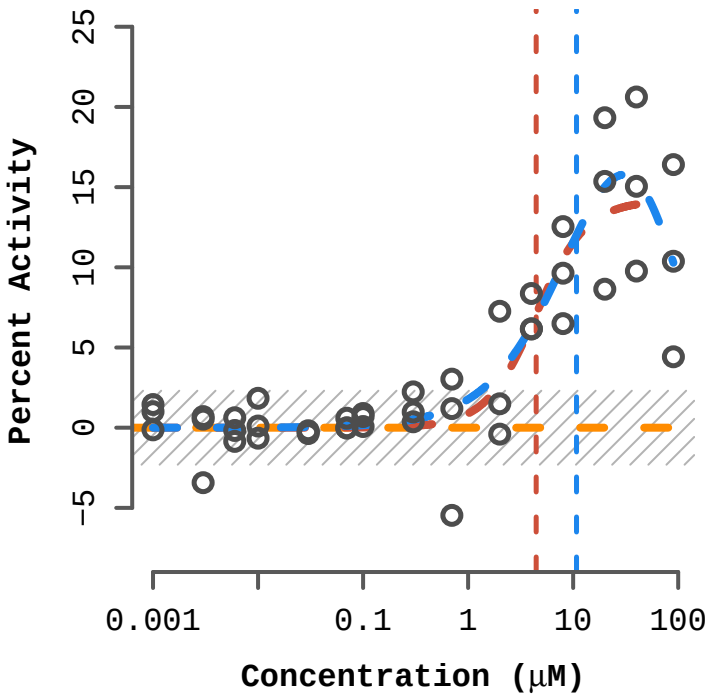
NAME: 2-Amino-5-nitrothiazole
CHID: 20066 **CASRN:** 121-66-4
SPID(S): Tox21_202377
M4ID: 12479875

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.482 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminoanthraquinone
CHID: 20068 CASRN: 117-79-3
SPID(S): Tox21_300101
M4ID: 12479029

HILL MODEL (in red):

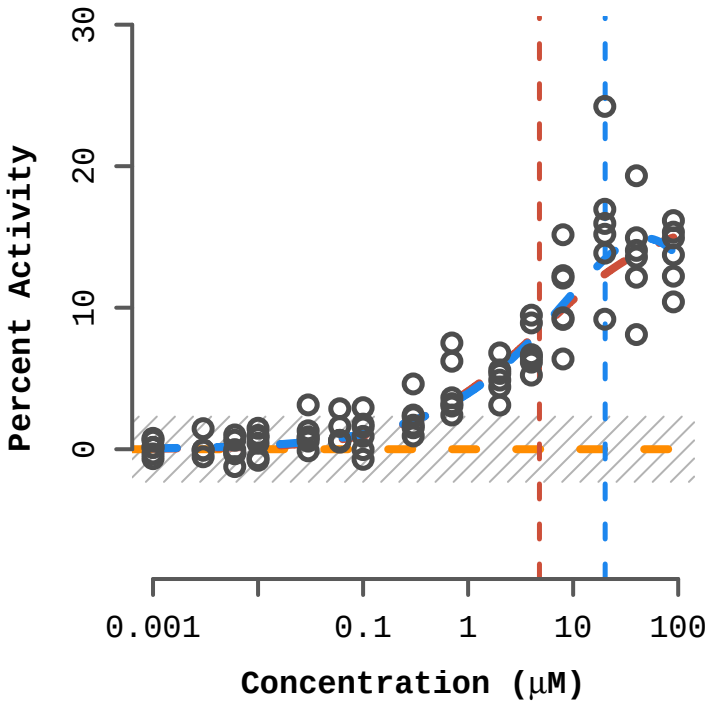
	tp	ga	gw
val:	14.2	0.648	1.82
sd:	1.92	0.0971	0.766

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.7	1.03	1.08	1.91	1.72
sd:	19.9	0.583	0.465	0.324	1.39

	CNST	HILL	GNLS
AIC:	301.38	222.96	222.42
PROB:	0	0.43	0.57
RMSE:	7.29	2.85	2.67

MAX_MEAN: 15.1 MAX_MED: 15.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminoanthraquinone
CHID: 20068 CASRN: 117-79-3
SPID(S): Tox21_201521
M4ID: 12480731

HILL MODEL (in red):

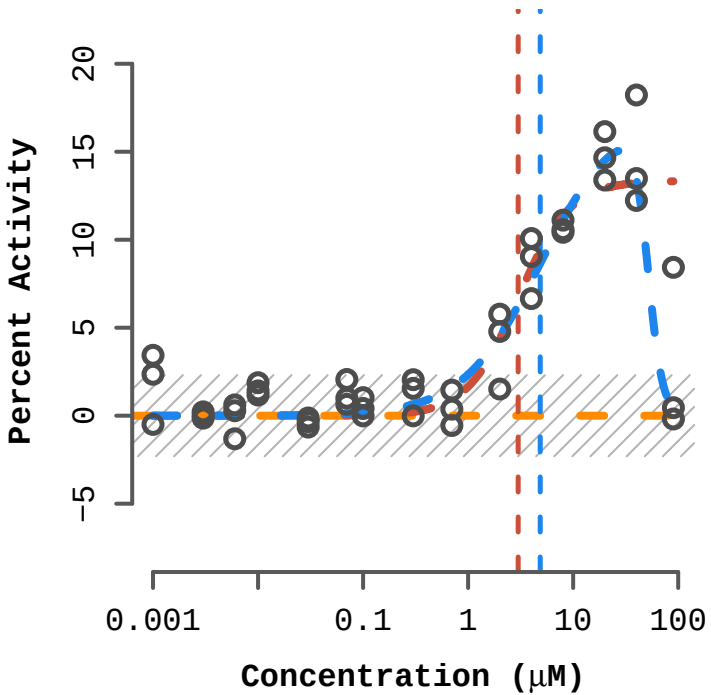
	tp	ga	gw
val:	16.8	0.679	0.722
sd:	1.28	0.136	0.0995

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29.1	1.3	0.615	2.21	1.21
sd:	12.2	0.475	0.0856	0.219	0.58

	CNST	HILL	GNLS
AIC:	609.28	370.06	367.23
PROB:	0	0.2	0.8
RMSE:	7.86	2.24	2.13

MAX_MEAN: 15.9 MAX_MED: 15.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-5-azotoluene
CHID: 20069 CASRN: 97-56-3
SPID(S): Tox21_300300
M4ID: 12478830

HILL MODEL (in red):

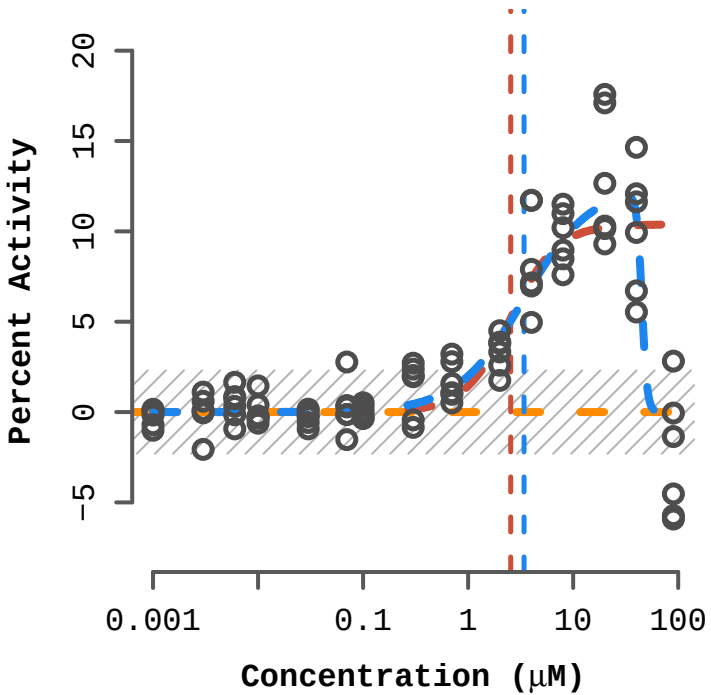
	tp	ga	gw
val:	13.4	0.476	1.79
sd:	0.959	0.0721	0.425

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.3	0.686	1.17	1.71	6.48
sd:	3.05	0.169	0.298	0.0545	2.37

	CNST	HILL	GNLS
AIC:	296.24	208.93	180.88
PROB:	0	0	1
RMSE:	6.77	3.24	1.86

MAX_MEAN: 14.7 **MAX_MED:** 14.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-5-azotoluene
CHID: 20069 CASRN: 97-56-3
SPID(S): Tox21_202261
M4ID: 12479991

HILL MODEL (in red):

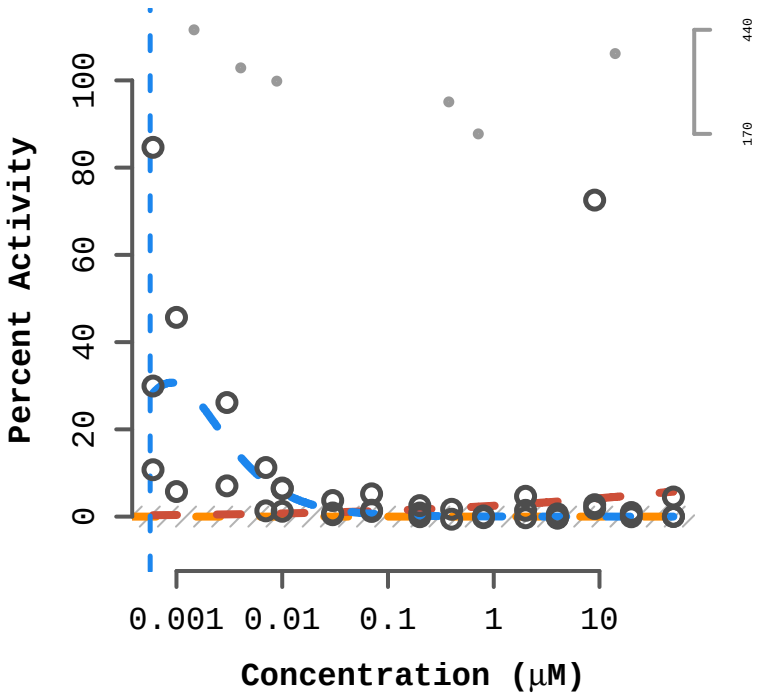
	tp	ga	gw
val:	10.4	0.405	1.95
sd:	0.686	0.0563	0.59

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.5	0.532	1.36	1.65	17.5
sd:	1.68	0.113	0.335	0.0927	34.2

	CNST	HILL	GNLS
AIC:	559.61	435.56	372.28
PROB:	0	0	1
RMSE:	5.77	3.86	2

MAX_MEAN: 12.9 **MAX_MED:** 11.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Aminocaproic acid
CHID: 20070 CASRN: 60-32-2
SPID(S): Tox21_110081_1
M4ID: 12484671 BRK

HILL MODEL (in red):

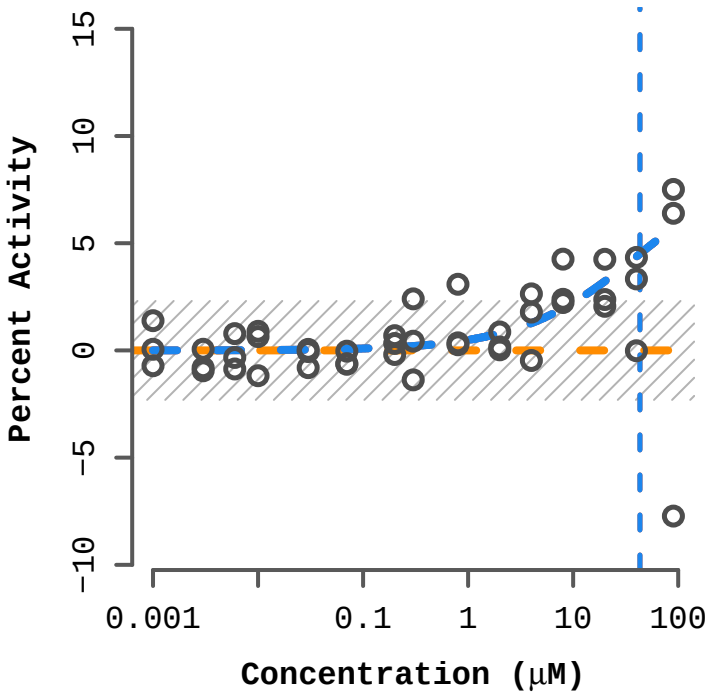
	tp	ga	gw
val:	13.8	2.2	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

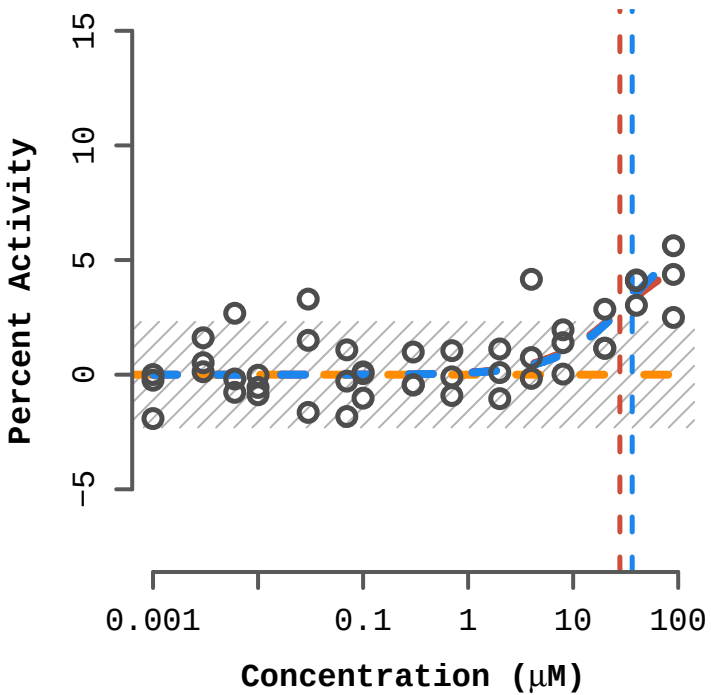
	tp	ga	gw	la	lw
val:	83.6	-3.25	1.73	-3	1.15
sd:	904	2.84	8.22	5.82	2.43

	CNST	HILL	GNLS
AIC:	506.95	512.1	505.18
PROB:	0.29	0.02	0.69
RMSE:	120.38	119.72	115.76

MAX_MEAN: 164 MAX_MED: 45.7 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Biphenylamine
CHID:    20071   CASRN: 92-67-1
SPID(S): Tox21_200376
M4ID:    12481876

HILL MODEL (in red):
      tp       ga       gw
val:  9.01     1.64     0.759
sd:   4.12     0.512    0.188

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.01     1.64     0.759    3.77     4.26
sd:   4.12     0.512    0.188    706      1670

      CNST        HILL        GNLS
AIC:  202.5       166.04      170.04
PROB: 0           0.88        0.12
RMSE: 2.51        2.33        2.33

MAX_MEAN: 2.96      MAX_MED: 6.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Biphenylamine hydrochloride
CHID: 20072 CASRN: 2113-61-3
SPID(S): Tox21_300973
M4ID: 12478160

HILL MODEL (in red):

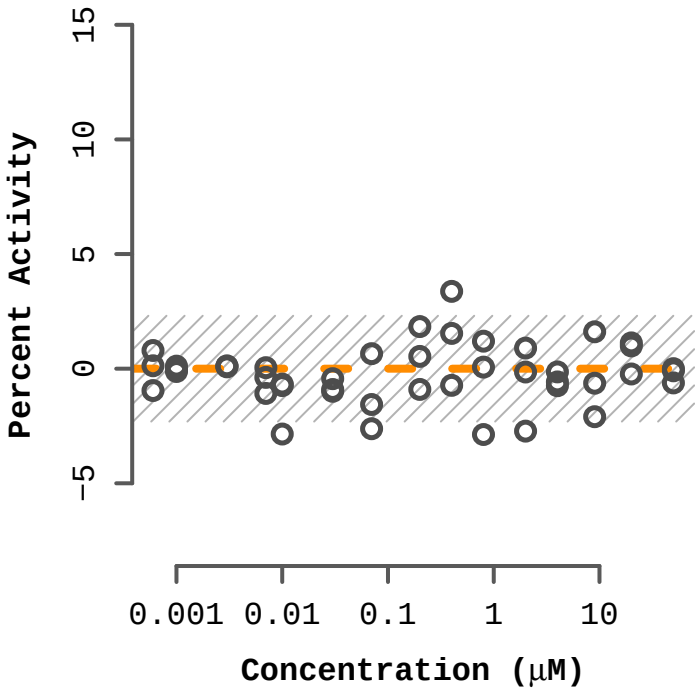
	tp	ga	gw
val:	5.58	1.44	1.24
sd:	2.22	0.345	0.619

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.75	1.56	1.23	2	18
sd:	5.9	0.594	0.566	0.185	98.3

	CNST	HILL	GNLS
AIC:	188.94	152.26	155.89
PROB:	0	0.86	0.14
RMSE:	1.98	1.23	1.23

MAX_MEAN: 4.17 MAX_MED: 4.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

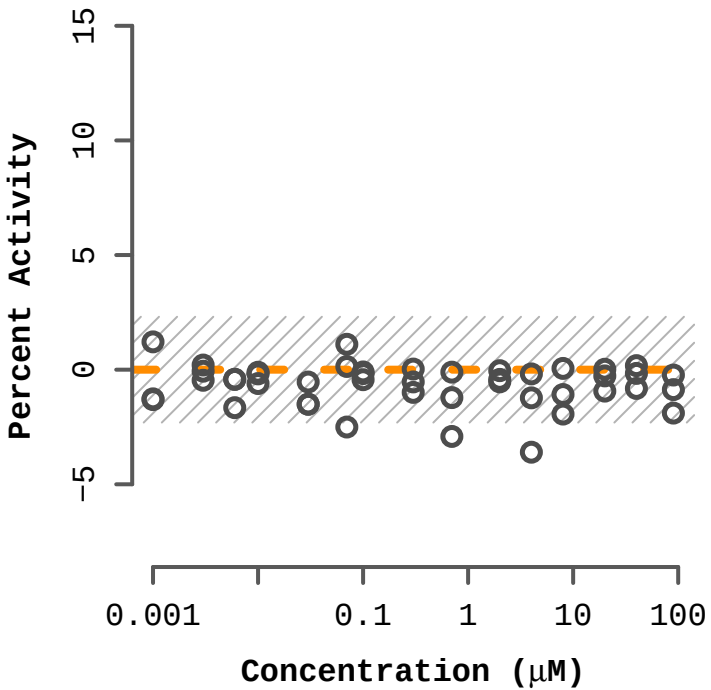
NAME: Gabapentin
CHID: 20074 CASRN: 60142-96-3
SPID(S): Tox21_110157_1
M4ID: 12484600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.4 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

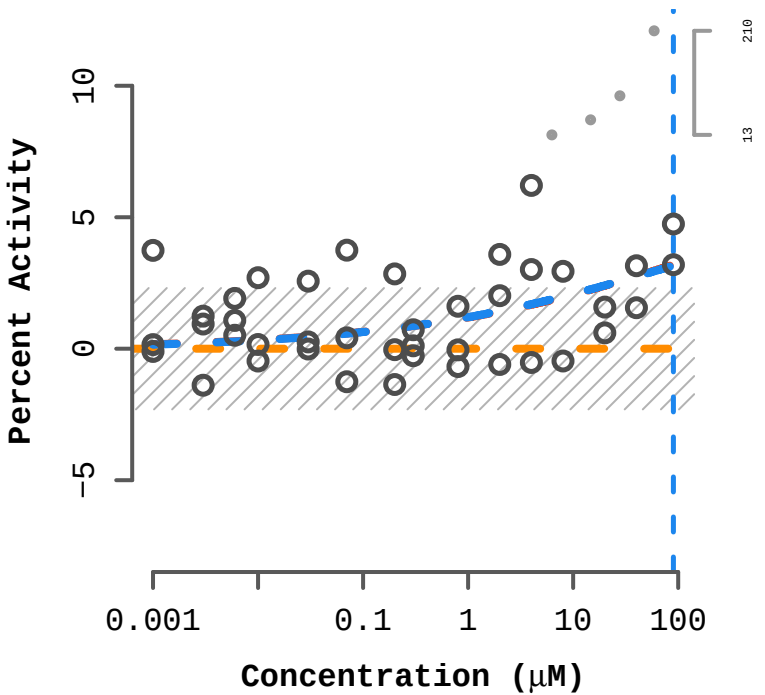
NAME: Amitrole
CHID: 20076 CASRN: 61-82-5
SPID(S): Tox21_302991
M4ID: 12476142

HILL MODEL: Not applicable.

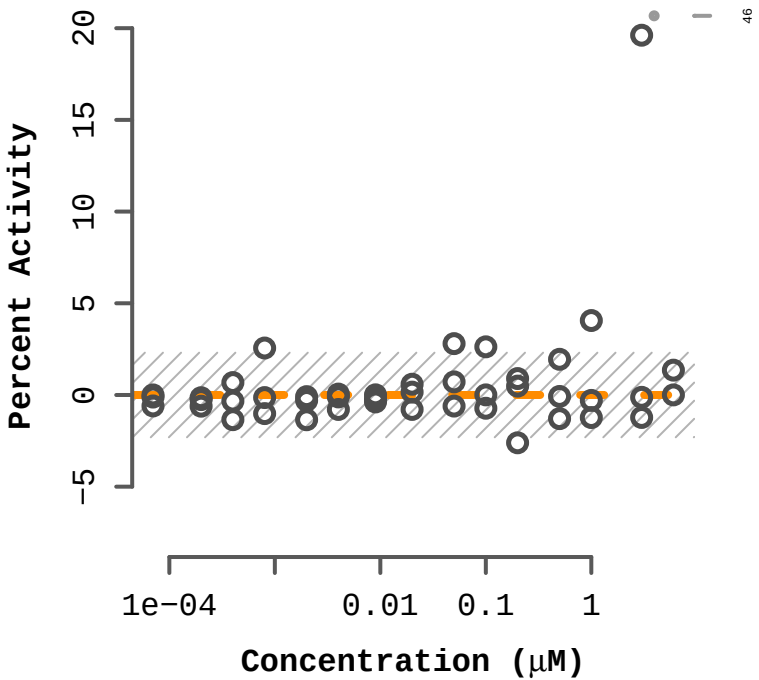
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: −0.108 **MAX_MED:** 0.141 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Amitrole
CHID:    20076   CASRN: 61-82-5
SPID(S): Tox21_201782
M4ID:    12480470  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  7.74     2.45     0.303
sd:   14.6     4.46     0.207

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.31     1.95     0.322    3.22     8.07
sd:   9.56     3.61     0.229    18900    121000

      CNST        HILL        GNLS
AIC:  299.92      290.88      294.97
PROB: 0.01        0.88        0.11
RMSE: 34.47       33.78       33.78

MAX_MEAN: 72.5      MAX_MED: 4.75      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

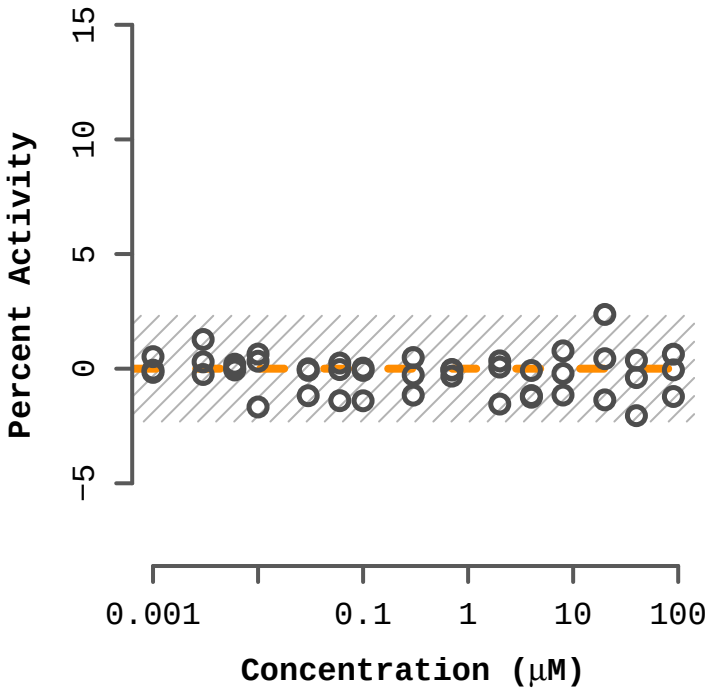
NAME: Ammonium citrate (2:1)
CHID: 20079 **CASRN:** 3012-65-5
SPID(S): Tox21_202778
M4ID: 12479474 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.98	NA	NA
PROB:	1	NA	NA
RMSE:	7.59	NA	NA

MAX_MEAN: 15.9 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

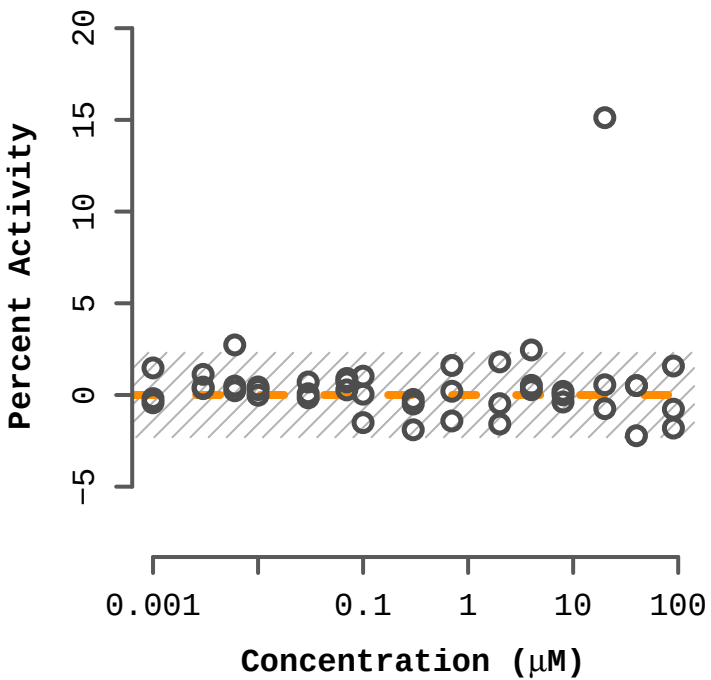
NAME: Amobarbital
CHID: 20081 CASRN: 57-43-2
SPID(S): Tox21_112866
M4ID: 12482912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.482 **MAX_MED:** 0.438 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

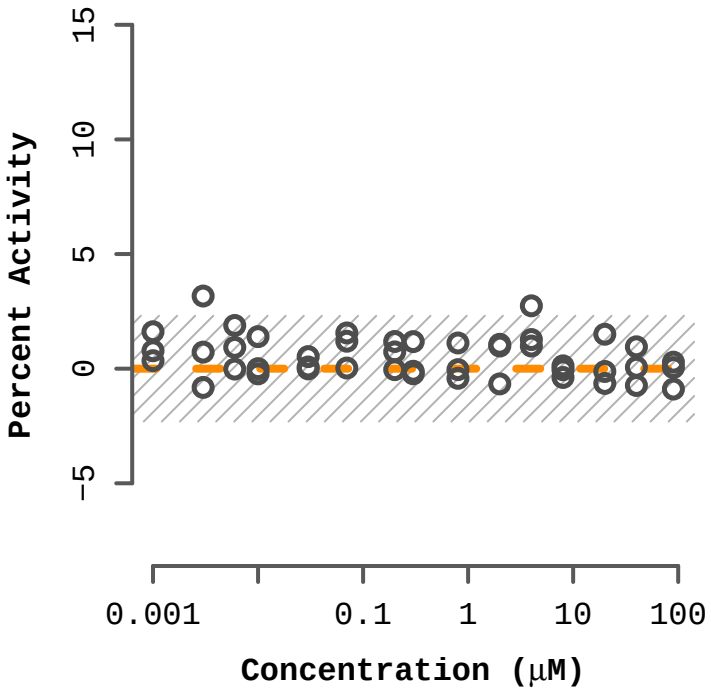
NAME: Ampicillin trihydrate
CHID: 20083 CASRN: 7177-48-2
SPID(S): Tox21_201148
M4ID: 12481104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 4.98 MAX_MED: 0.714 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

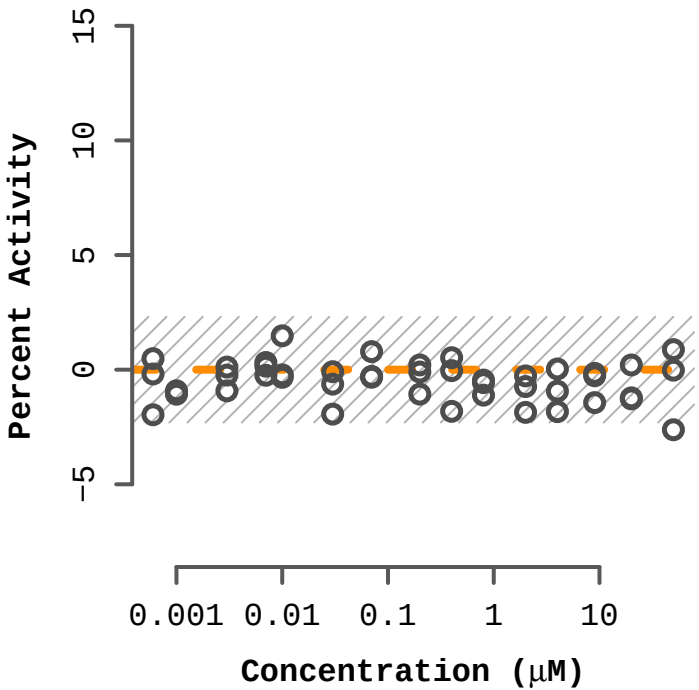
NAME: Anethole
CHID: 20086 **CASRN:** 104-46-1
SPID(S): Tox21_202001
M4ID: 12480251

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

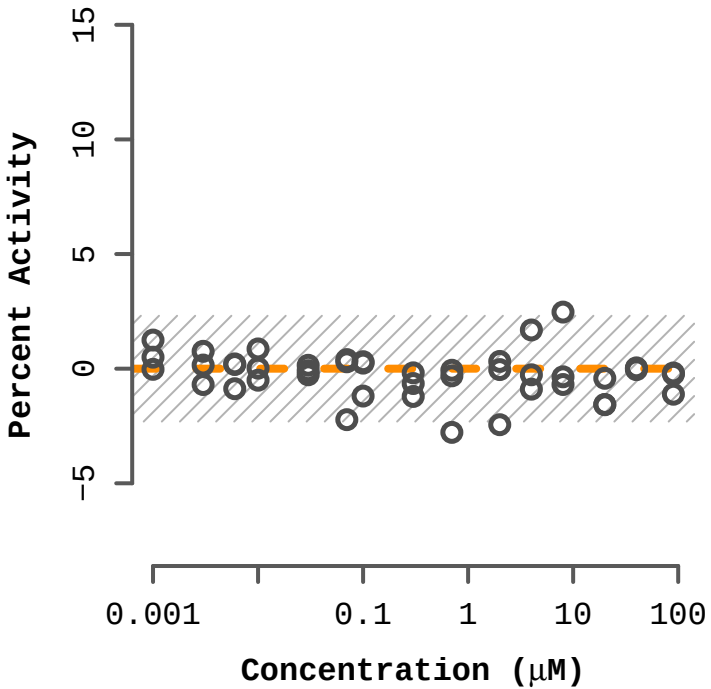
NAME: Anethole
CHID: 20086 **CASRN:** 104-46-1
SPID(S): Tox21_111139_1
M4ID: 12483883

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.308 **MAX_MED:** 0.153 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

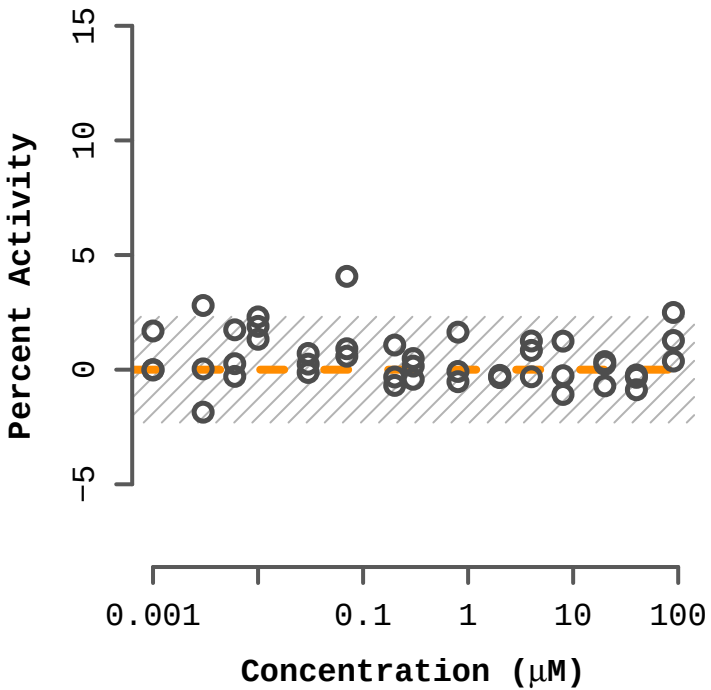
NAME: (E)−Anethole
CHID: 20087 CASRN: 4180−23−8
SPID(S): Tox21_300132
M4ID: 12478998

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.575 **MAX_MED:** 0.503 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

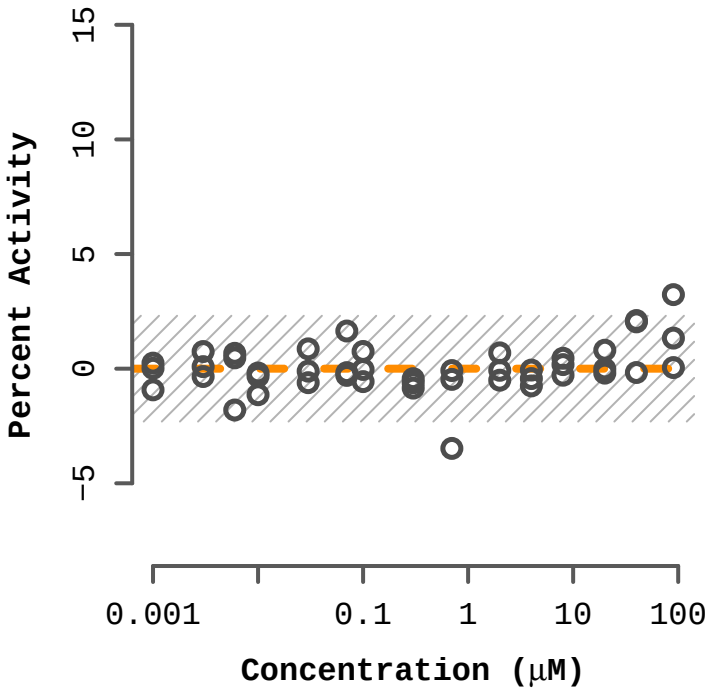
NAME: (E)−Anethole
CHID: 20087 CASRN: 4180−23−8
SPID(S): Tox21_202282
M4ID: 12479970

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.86 MAX_MED: 1.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

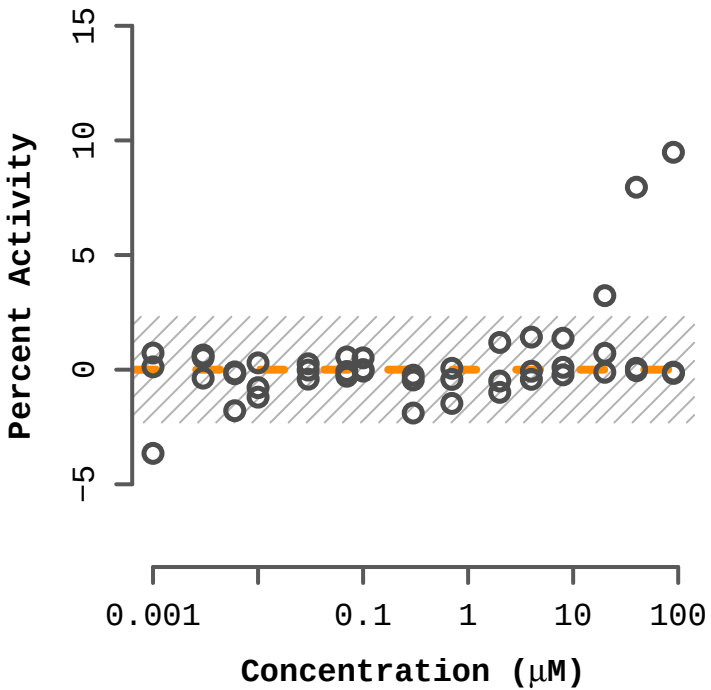
NAME: Chloralose
CHID: 20088 **CASRN:** 15879-93-3
SPID(S): Tox21_302997
M4ID: 12476136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

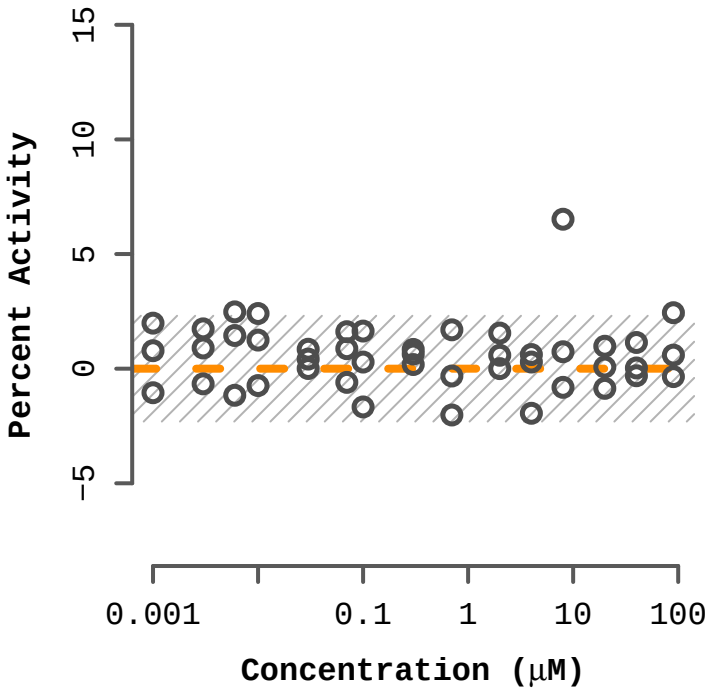
NAME: Chloralose
CHID: 20088 **CASRN:** 15879-93-3
SPID(S): Tox21_201447
M4ID: 12480805

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.96	NA	NA
PROB:	1	NA	NA
RMSE:	2.1	NA	NA

MAX_MEAN: 3.07 **MAX_MED:** 0.715 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

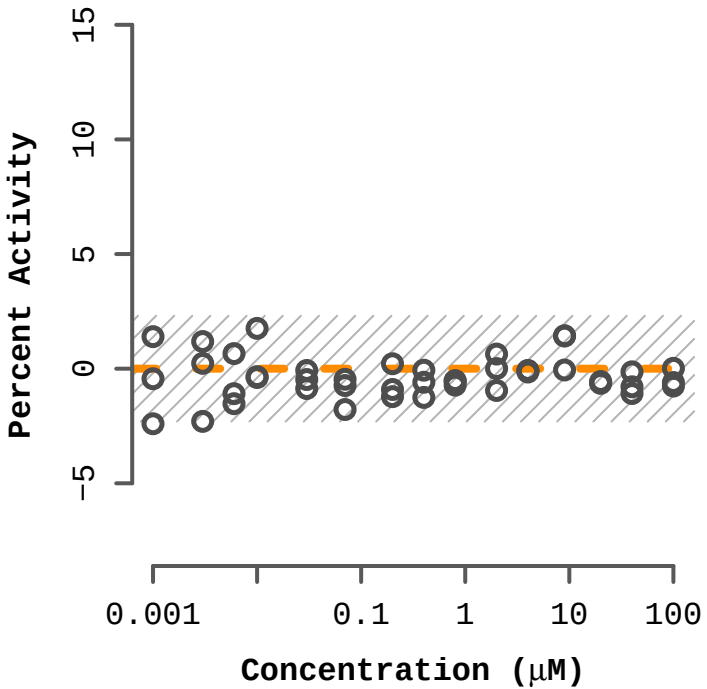
NAME: Anilazine
CHID: 20089 **CASRN:** 101-05-3
SPID(S): Tox21_301181
M4ID: 12477952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

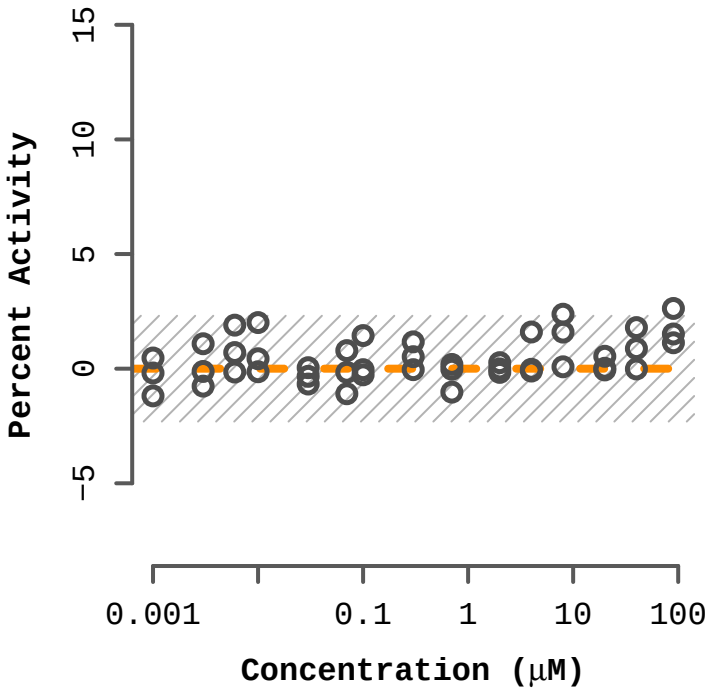
NAME: Aniline
CHID: 20090 CASRN: 62-53-3
SPID(S): Tox21_200345
M4ID: 12481907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.936 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

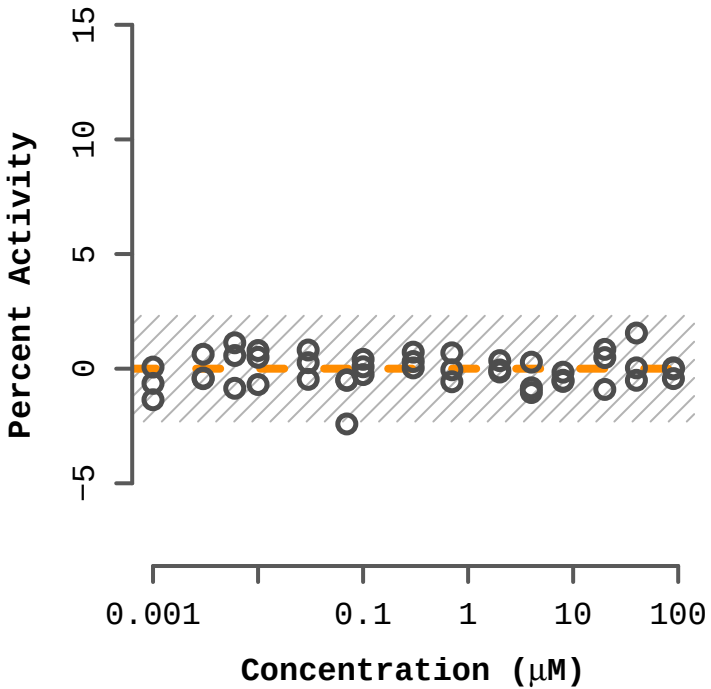
NAME: Aniline hydrochloride
CHID: 20091 **CASRN:** 142-04-1
SPID(S): Tox21_302869
M4ID: 12476264

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.44	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

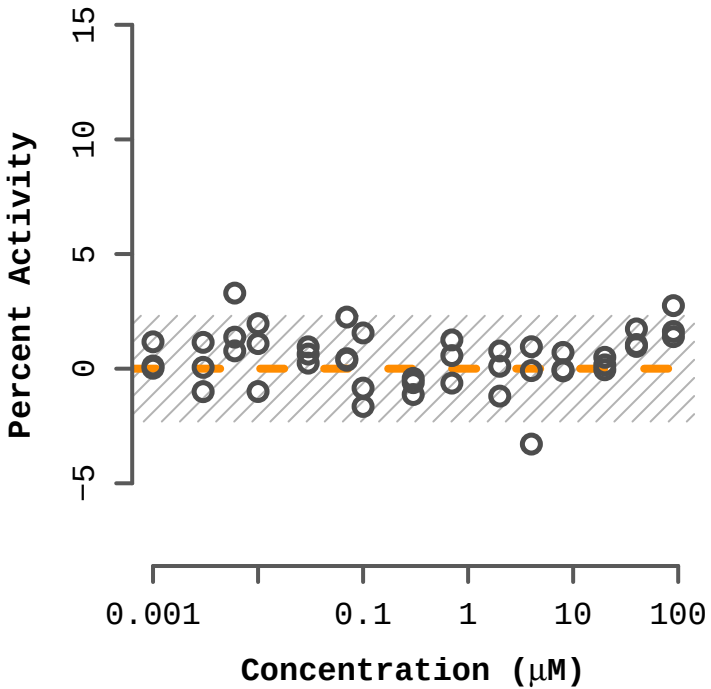
NAME: Aniline hydrochloride
CHID: 20091 **CASRN:** 142-04-1
SPID(S): Tox21_202304
M4ID: 12479948

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.363 **MAX_MED:** 0.576 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

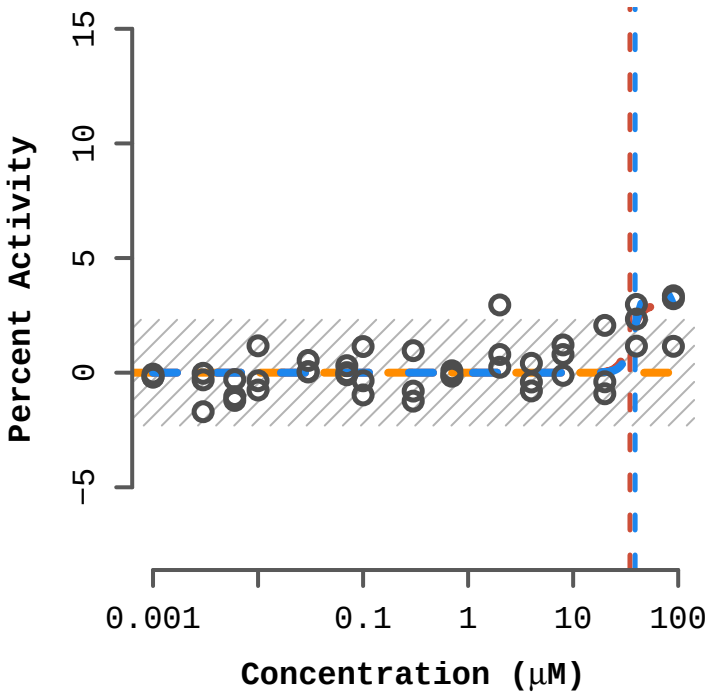
NAME: 2-Methoxyaniline hydrochloride
CHID: 20092 **CASRN:** 134-29-2
SPID(S): Tox21_302807
M4ID: 12476326

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methoxyaniline hydrochloride
CHID: 20092 CASRN: 134-29-2
SPID(S): Tox21_201358
M4ID: 12480894

HILL MODEL (in red):

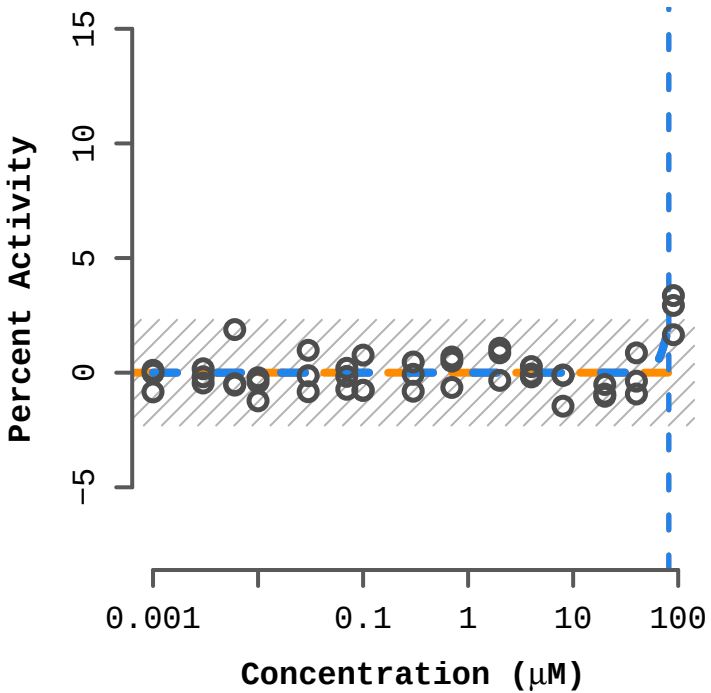
	tp	ga	gw
val:	2.95	1.54	8
sd:	0.494	0.0748	7.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.03	1.59	8	2.02	6.69
sd:	27.2	0.789	13.3	0.548	119

	CNST	HILL	GNLS
AIC:	145.3	124.22	128.18
PROB:	0	0.88	0.12
RMSE:	1.25	0.9	0.9

MAX_MEAN: 2.58 **MAX_MED:** 3.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methoxyaniline hydrochloride
CHID: 20093 CASRN: 20265-97-8
SPID(S): Tox21_302909
M4ID: 12476224

HILL MODEL (in red):

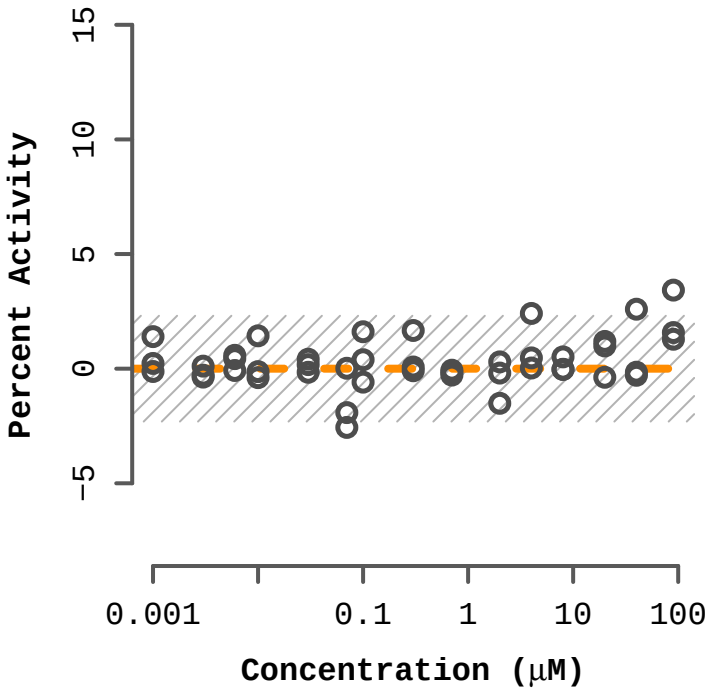
	tp	ga	gw
val:	4.04	1.91	8
sd:	4.85	0.189	10.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.04	1.91	8	2.54	5.99
sd:	4.83	0.188	10.2	36.8	376

	CNST	HILL	GNLS
AIC:	122.58	108.45	112.45
PROB:	0	0.88	0.12
RMSE:	0.99	0.71	0.71

MAX_MEAN: 2.65 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

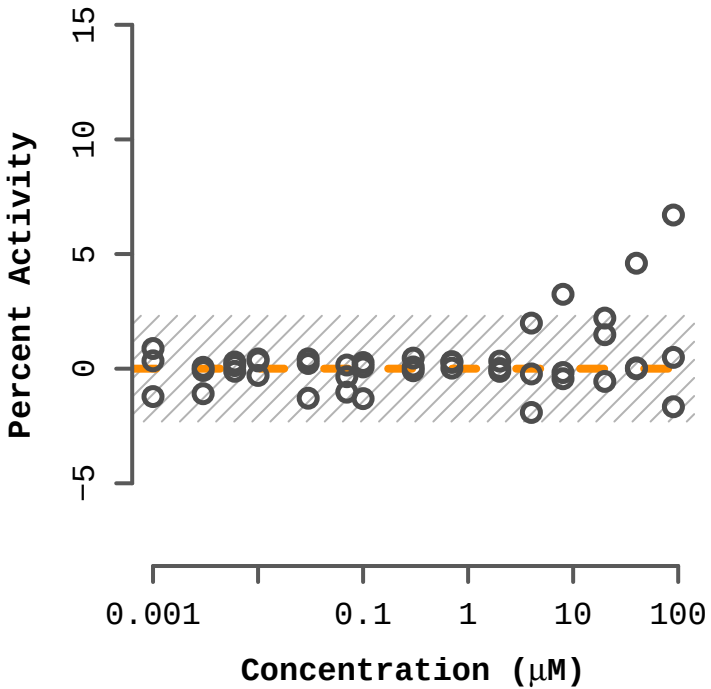
NAME: 4-Methoxyaniline hydrochloride
CHID: 20093 **CASRN:** 20265-97-8
SPID(S): Tox21_201498
M4ID: 12480754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

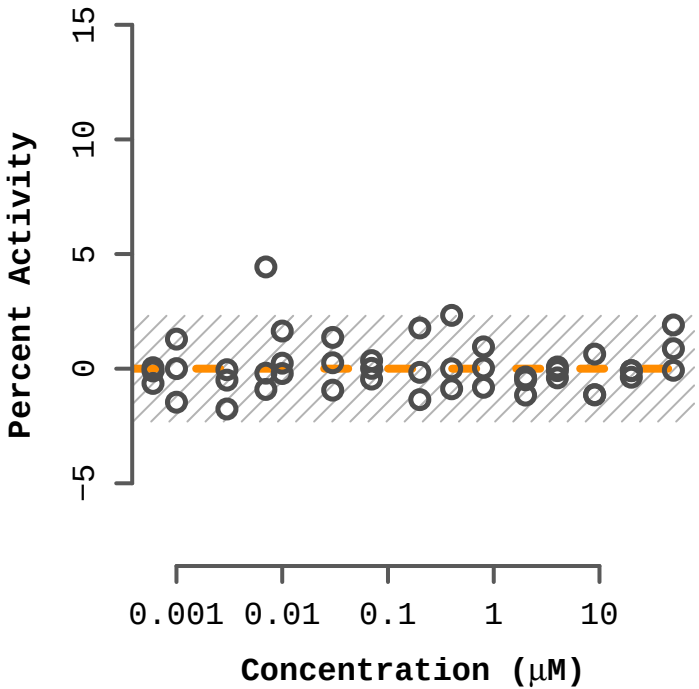
NAME: Anthranilic acid
CHID: 20094 **CASRN:** 118-92-3
SPID(S): Tox21_200703
M4ID: 12481549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

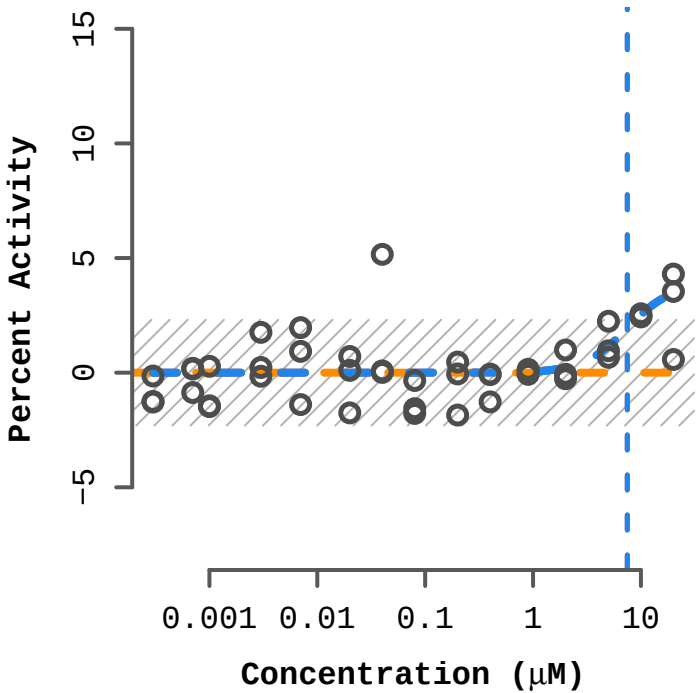
NAME: Anthranilic acid
CHID: 20094 **CASRN:** 118-92-3
SPID(S): Tox21_111095_1
M4ID: 12483910

HILL MODEL: Not applicable.

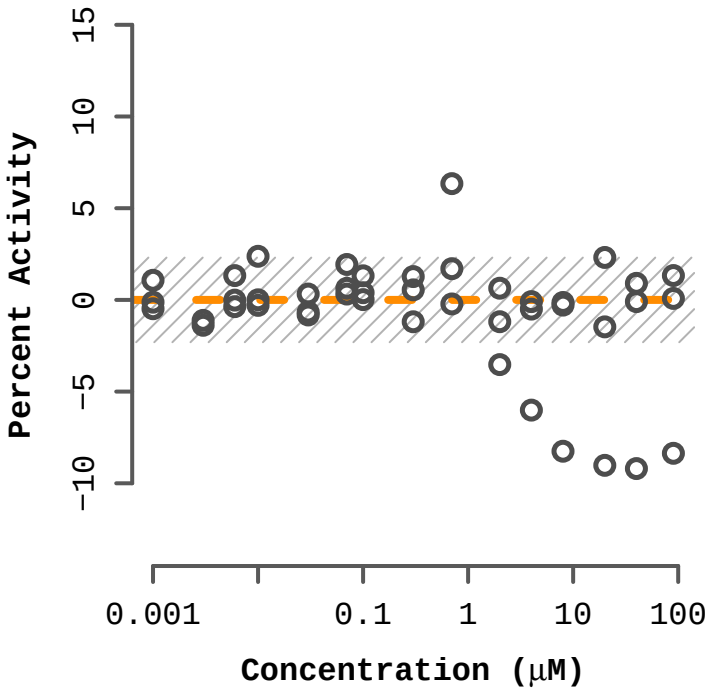
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.873 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Anthraquinone
CHID:    20095   CASRN: 84-65-1
SPID(S): Tox21_111369_1
M4ID:    12483735

HILL MODEL (in red):
      tp       ga       gw
val:  3.88     0.874    2.14
sd:   1.4      0.201    1.22

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.88     0.874    2.14     2.74     4.8
sd:   1.4      0.201    1.22     1540     5200

      CNST        HILL        GNLS
AIC:  168.32      146.05      150.05
PROB: 0           0.88        0.12
RMSE: 1.61        1.26        1.26

MAX_MEAN: 2.81      MAX_MED: 3.54      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

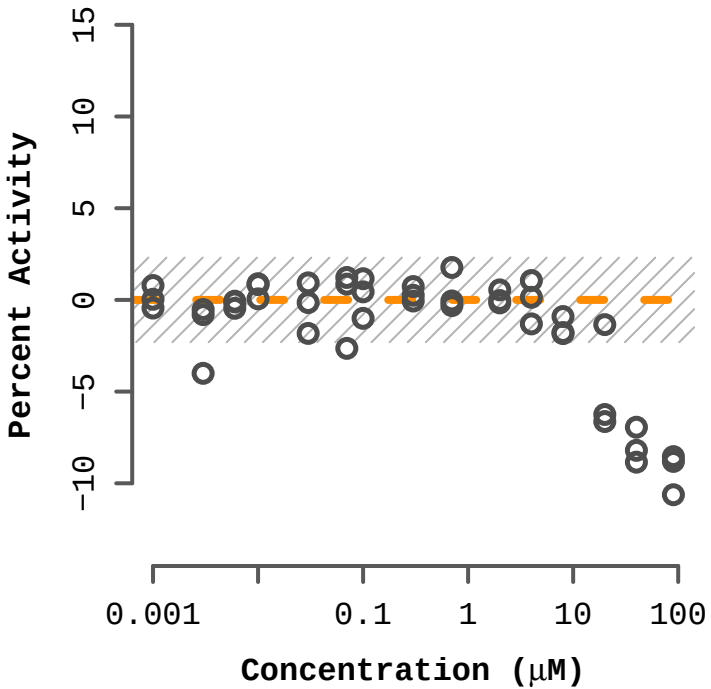
NAME: Aramite
CHID: 20097 **CASRN:** 140-57-8
SPID(S): Tox21_200398
M4ID: 12481854

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.16	NA	NA
PROB:	1	NA	NA
RMSE:	3.13	NA	NA

MAX_MEAN: 2.61 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

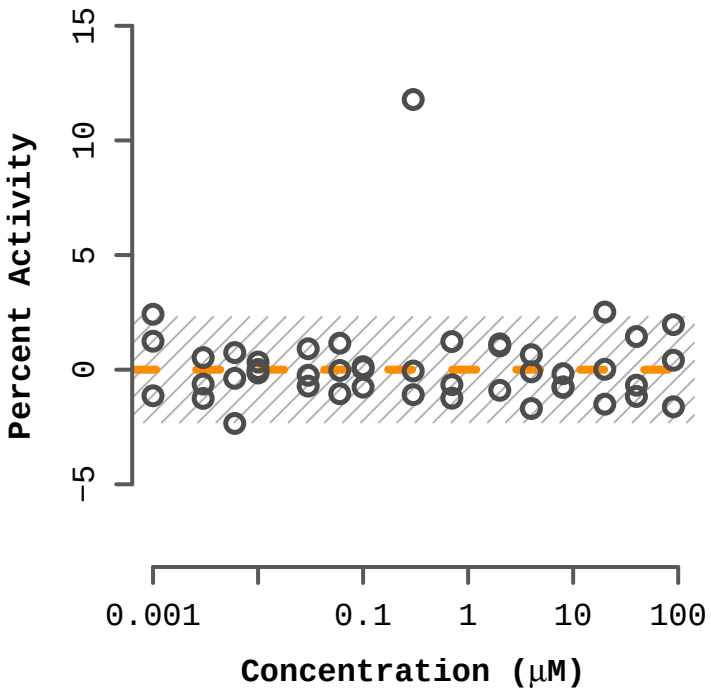
NAME: Sodium aristolochate-I
CHID: 20099 CASRN: 10190-99-5
SPID(S): Tox21_200026
M4ID: 12482226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.99	NA	NA
PROB:	1	NA	NA
RMSE:	3.63	NA	NA

MAX_MEAN: 0.594 **MAX_MED:** 0.862 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

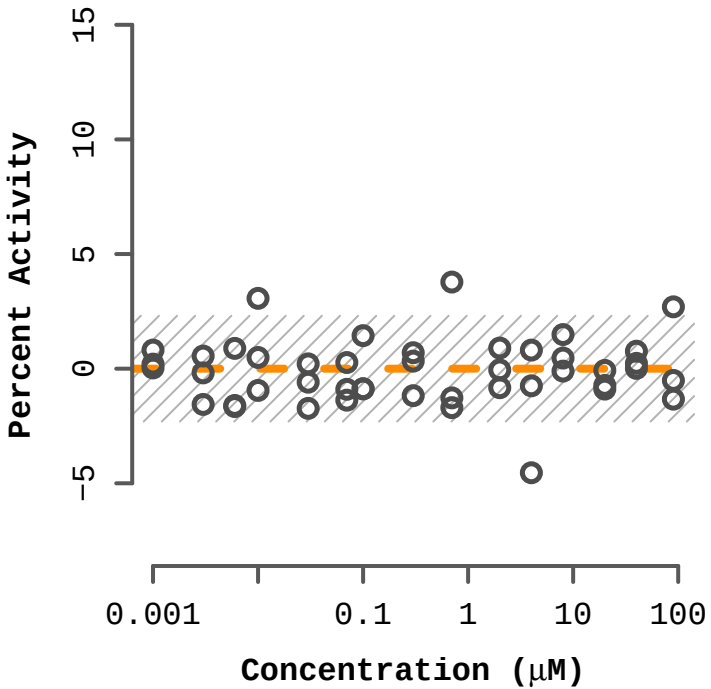
NAME: Aroclor 1260
CHID: 20101 **CASRN:** 11096-82-5
SPID(S): Tox21_200183
M4ID: 12482069

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 3.55 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

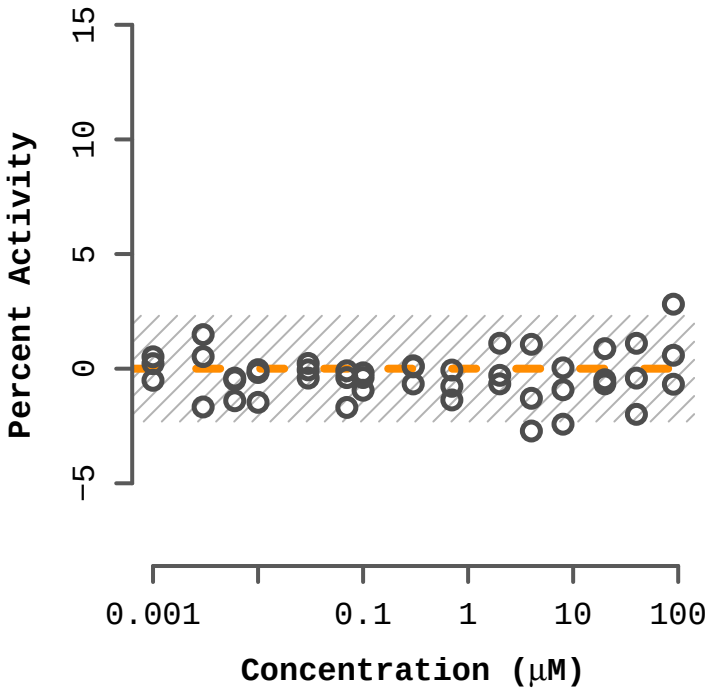
NAME: Sodium L-ascorbate
CHID: 20105 **CASRN:** 134-03-2
SPID(S): Tox21_300556
M4ID: 12478577

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.87 **MAX_MED:** 0.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

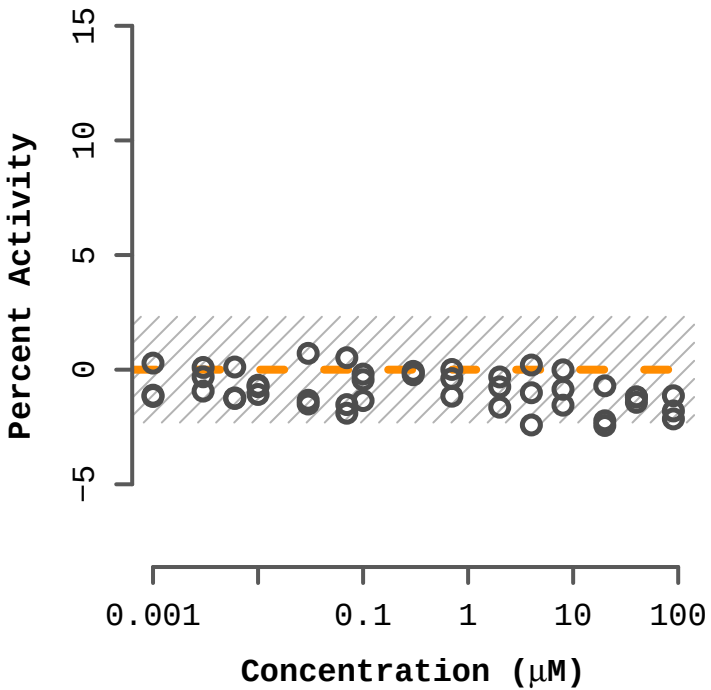
NAME: L-Ascorbic acid
CHID: 20106 **CASRN:** 50-81-7
SPID(S): Tox21_302958
M4ID: 12476175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.907 **MAX_MED:** 0.585 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

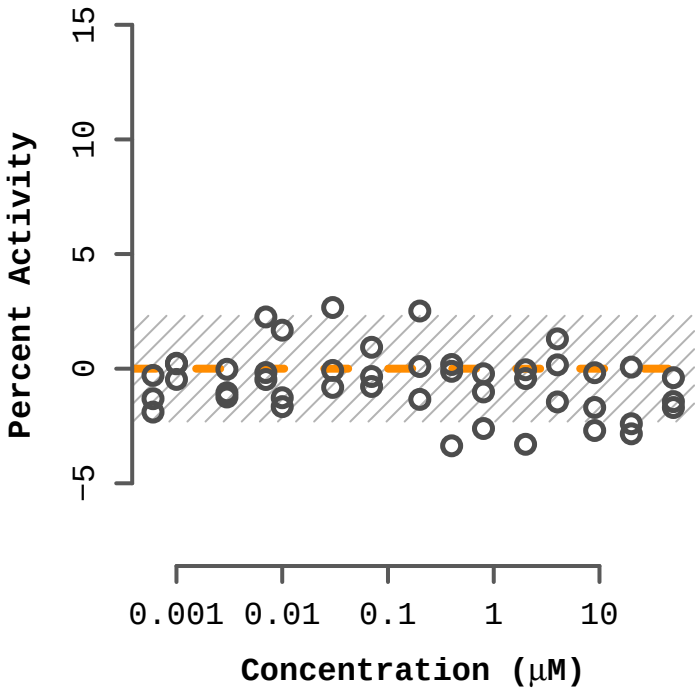
NAME: L−Ascorbic acid
CHID: 20106 **CASRN:** 50−81−7
SPID(S): Tox21_202127
M4ID: 12480125

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: −0.142 **MAX_MED:** −0.136 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

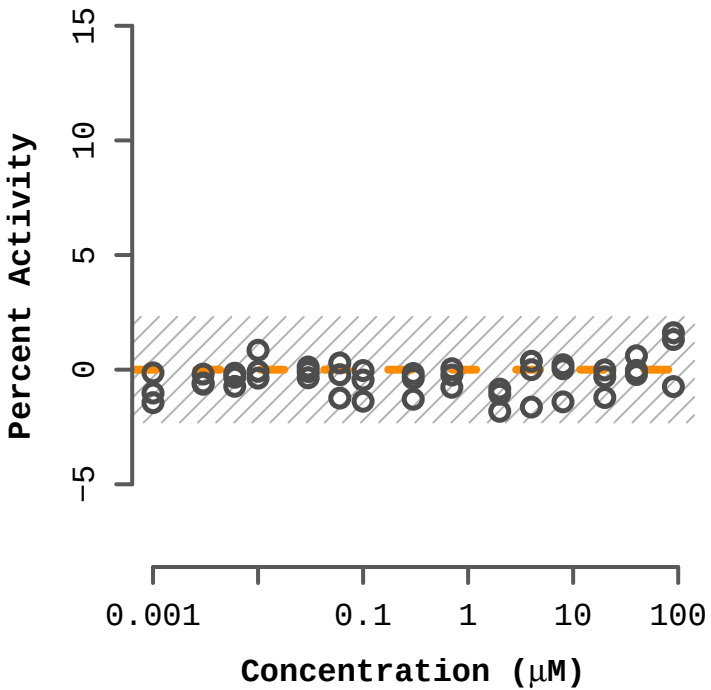
NAME: L−Ascorbic acid
CHID: 20106 CASRN: 50−81−7
SPID(S): Tox21_112104_1
M4ID: 12483317

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.592 **MAX_MED:** 0.215 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

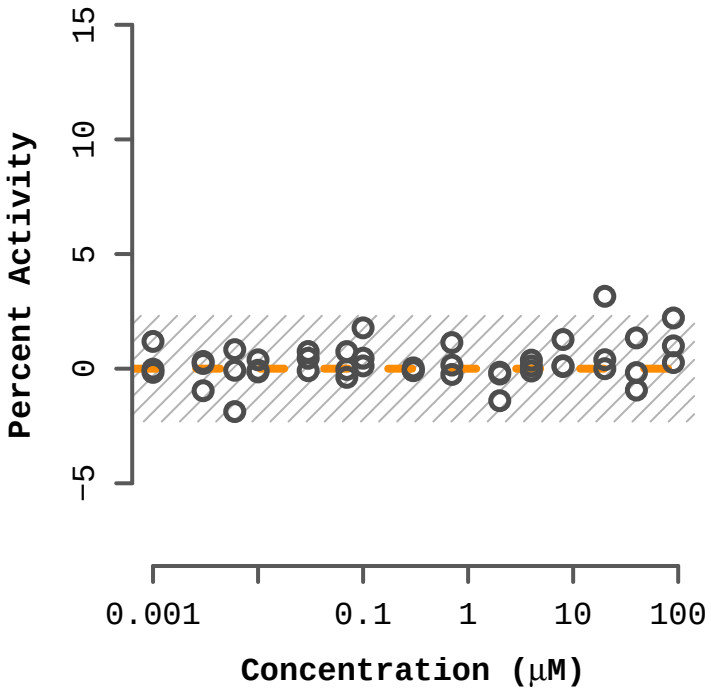
NAME: Aspartame
CHID: 20107 **CASRN:** 22839-47-0
SPID(S): Tox21_302965
M4ID: 12476168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.732 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

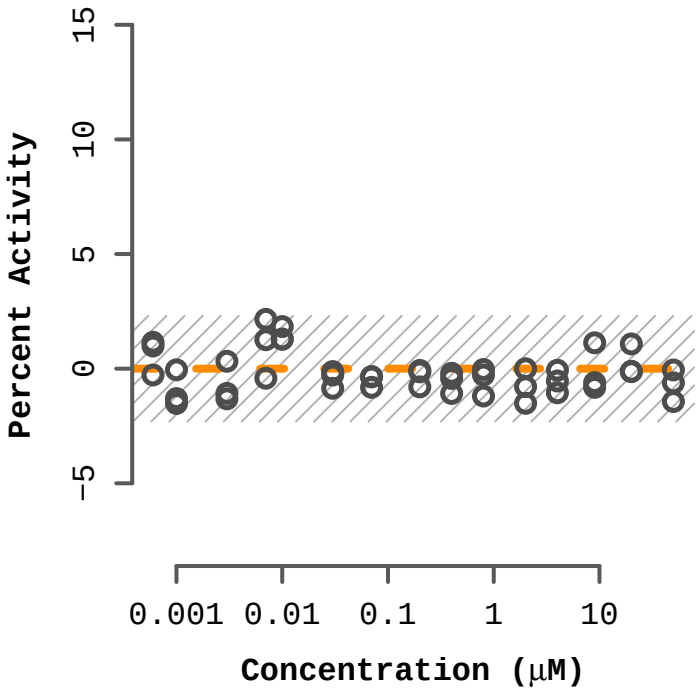
NAME: Aspartame
CHID: 20107 **CASRN:** 22839-47-0
SPID(S): Tox21_202315
M4ID: 12479937

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.996 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

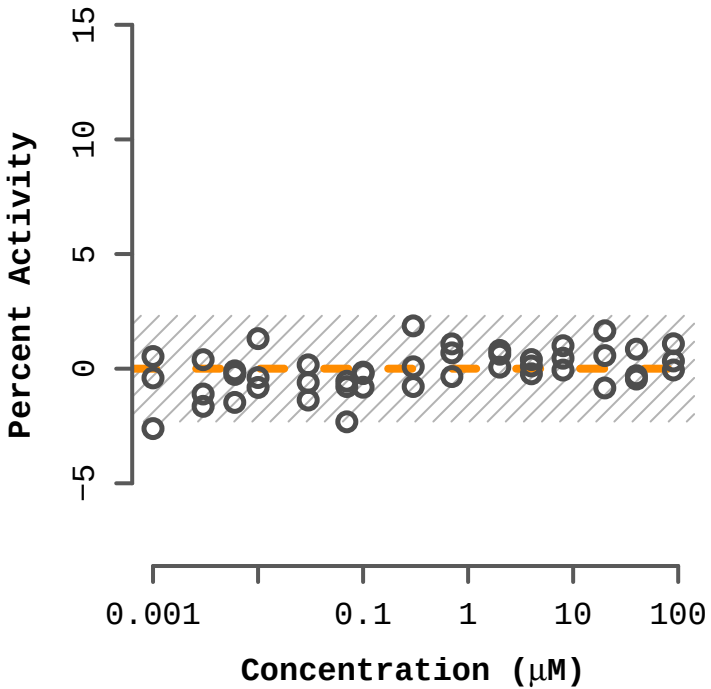
NAME: Aspartame
CHID: 20107 **CASRN:** 22839-47-0
SPID(S): Tox21_111080_1
M4ID: 12483918

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

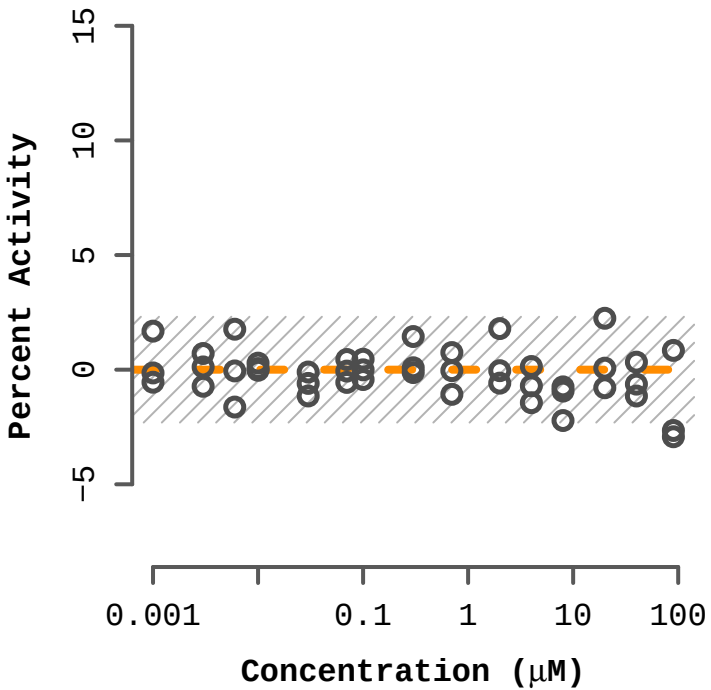
NAME: Aspirin
CHID: 20108 CASRN: 50-78-2
SPID(S): Tox21_300146
M4ID: 12478984

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.499 **MAX_MED:** 0.692 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

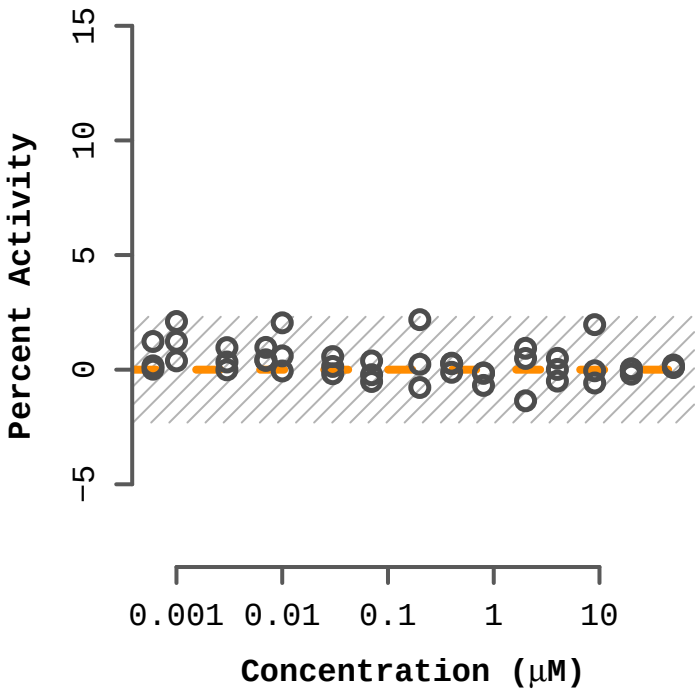
NAME: Aspirin
CHID: 20108 CASRN: 50-78-2
SPID(S): Tox21_202117
M4ID: 12480135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.507 MAX_MED: 0.121 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

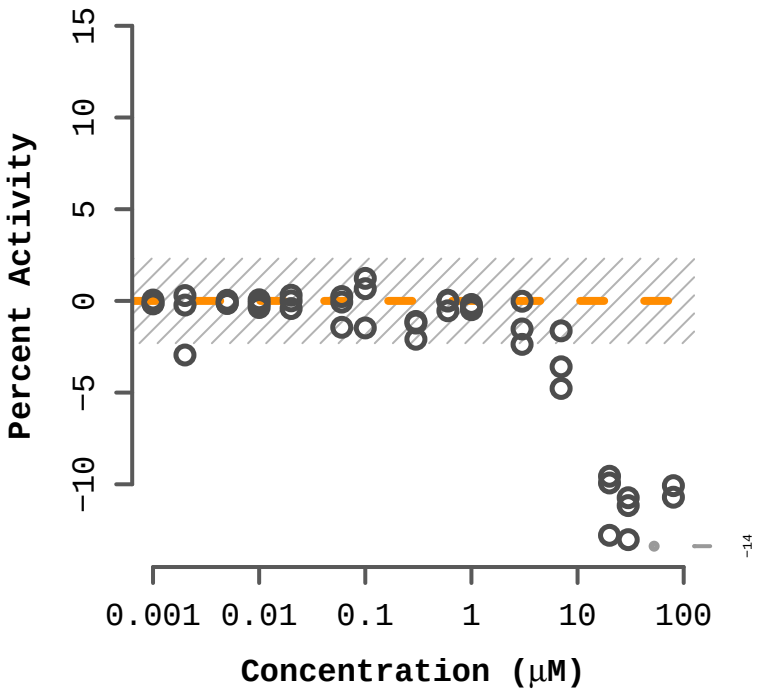
NAME: Aspirin
CHID: 20108 CASRN: 50-78-2
SPID(S): Tox21_110076_1
M4ID: 12484676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

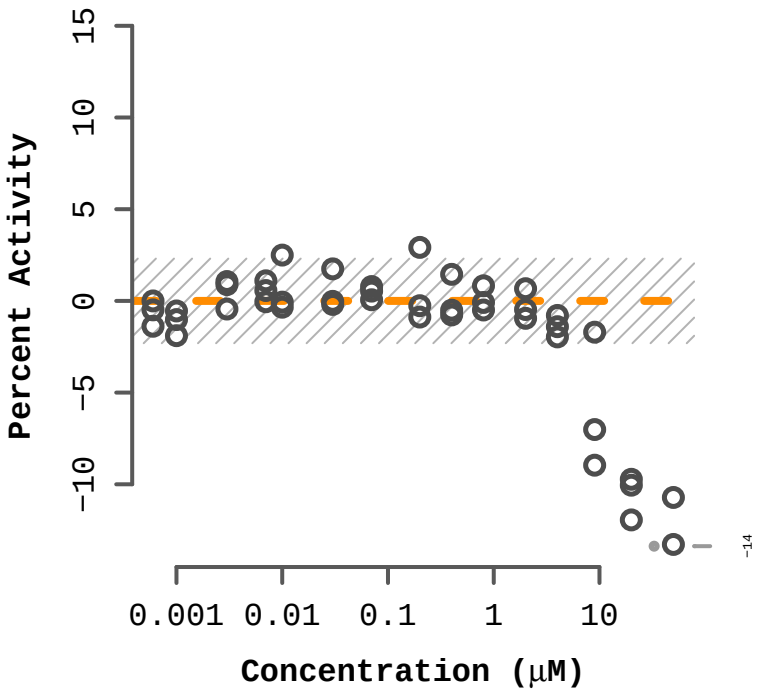
NAME: Astemizole
CHID: 20110 CASRN: 68844-77-9
SPID(S): Tox21_200095
M4ID: 12482157 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.01	NA	NA
PROB:	1	NA	NA
RMSE:	5.23	NA	NA

MAX_MEAN: 0.142 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

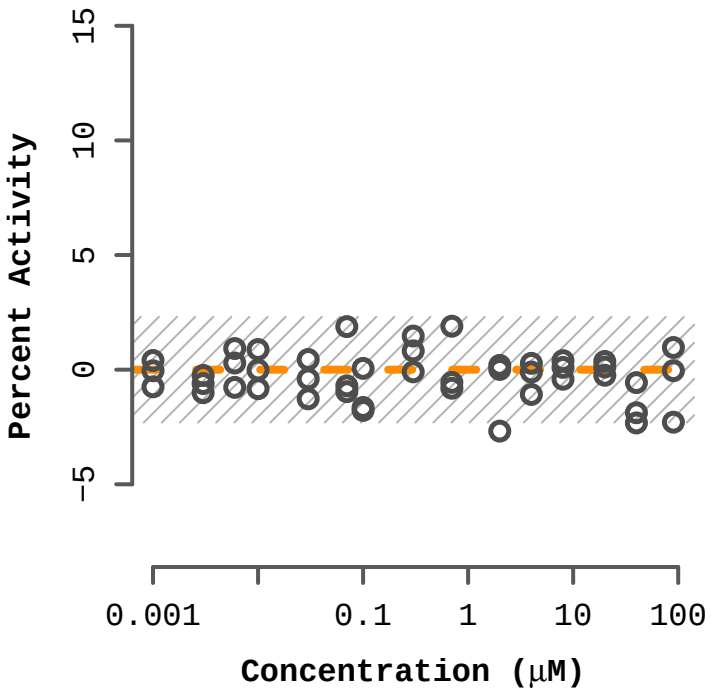
NAME: Astemizole
CHID: 20110 CASRN: 68844-77-9
SPID(S): Tox21_110680_1
M4ID: 12484183 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.14	NA	NA
PROB:	1	NA	NA
RMSE:	4.7	NA	NA

MAX_MEAN: 0.697 **MAX_MED:** 0.891 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

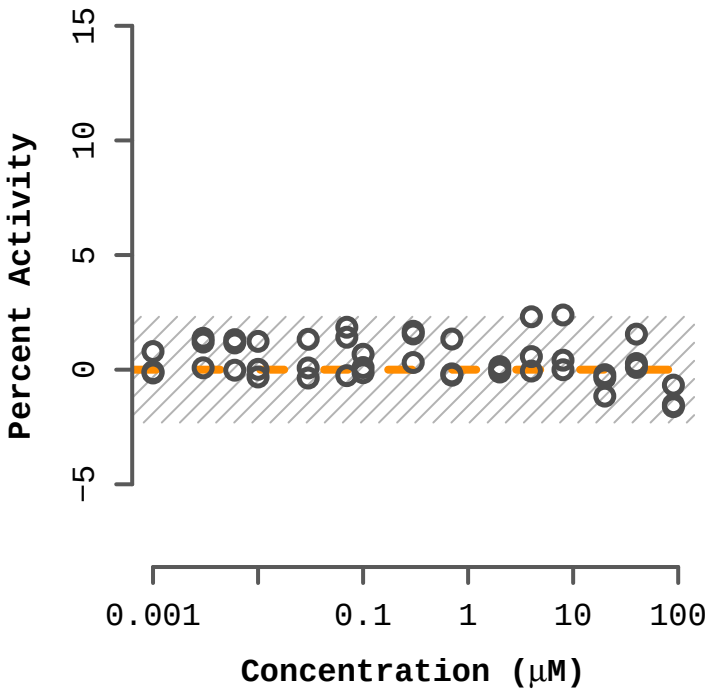
NAME: Atrazine
CHID: 20112 CASRN: 1912-24-9
SPID(S): Tox21_301021
M4ID: 12478112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.733 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

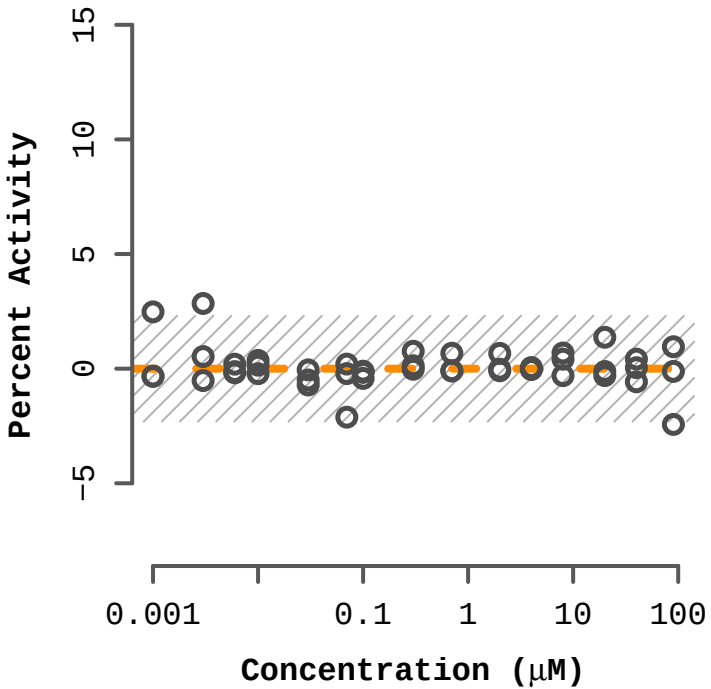
NAME: Atrazine
CHID: 20112 **CASRN:** 1912-24-9
SPID(S): Tox21_201986
M4ID: 12480266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.58	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

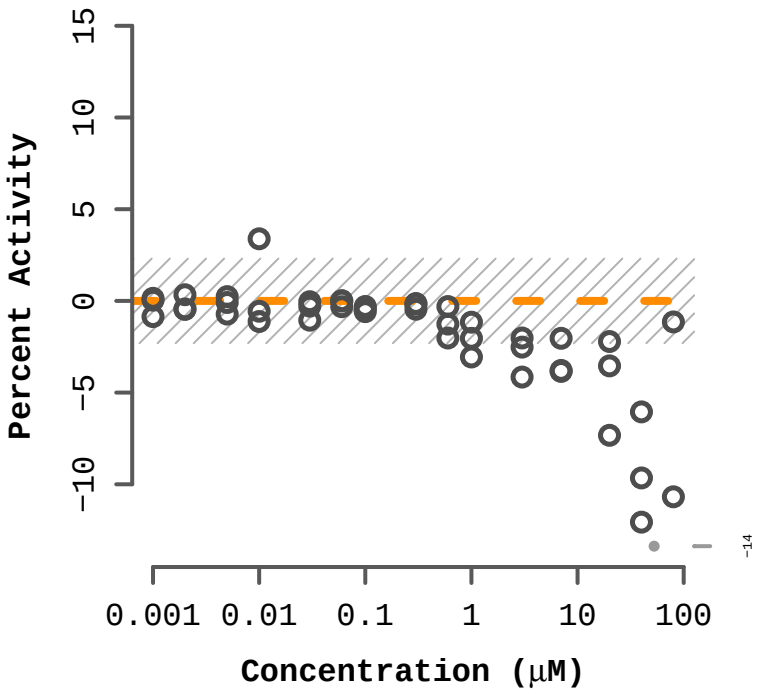
NAME: Atropine
CHID: 20113 CASRN: 51-55-8
SPID(S): Tox21_200487
M4ID: 12481765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.953 **MAX_MED:** 0.529 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

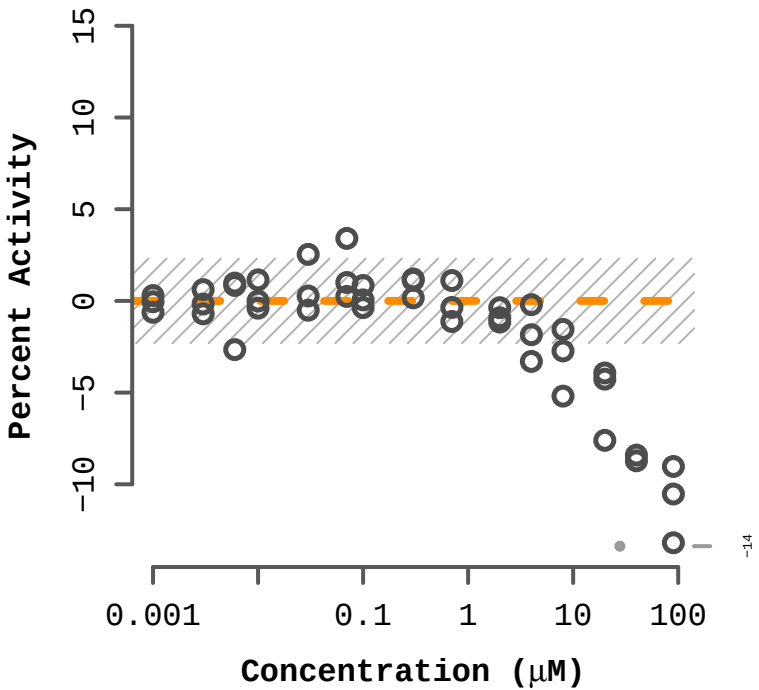
NAME: Auramine hydrochloride
CHID: 20114 **CASRN:** 2465-27-2
SPID(S): Tox21_303002
M4ID: 12476131 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	238.76	NA	NA
PROB:	1	NA	NA
RMSE:	4.09	NA	NA

MAX_MEAN: 0.568 **MAX_MED:** 0.0406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

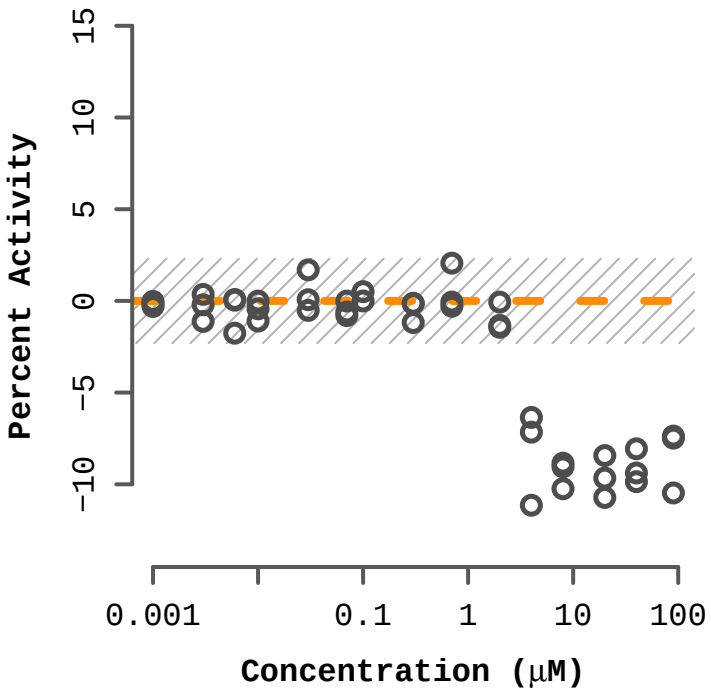
NAME: Auramine hydrochloride
CHID: 20114 **CASRN:** 2465-27-2
SPID(S): Tox21_202337
M4ID: 12479915 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.22	NA	NA
PROB:	1	NA	NA
RMSE:	4.42	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

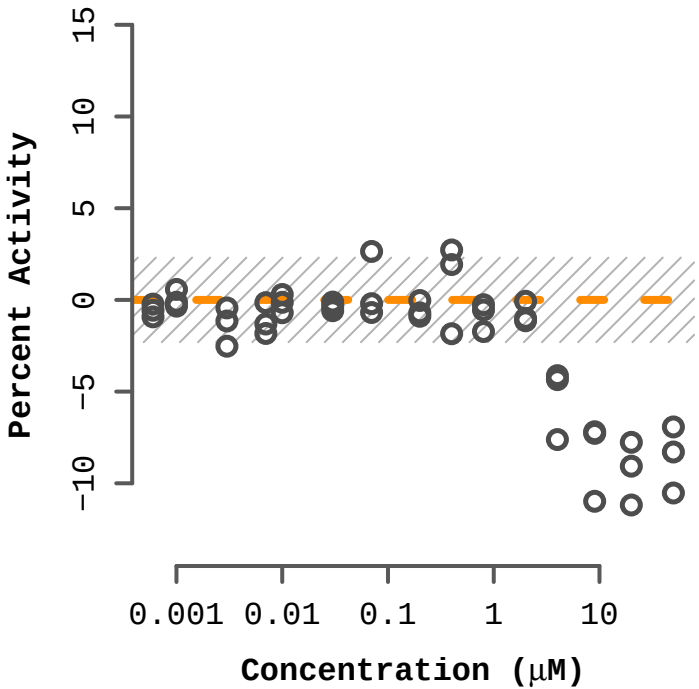
NAME: 5-Azacytidine
CHID: 20116 **CASRN:** 320-67-2
SPID(S): Tox21_302985
M4ID: 12476148

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	272.56	NA	NA
PROB:	1	NA	NA
RMSE:	5.33	NA	NA

MAX_MEAN: 0.568 **MAX_MED:** 0.251 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

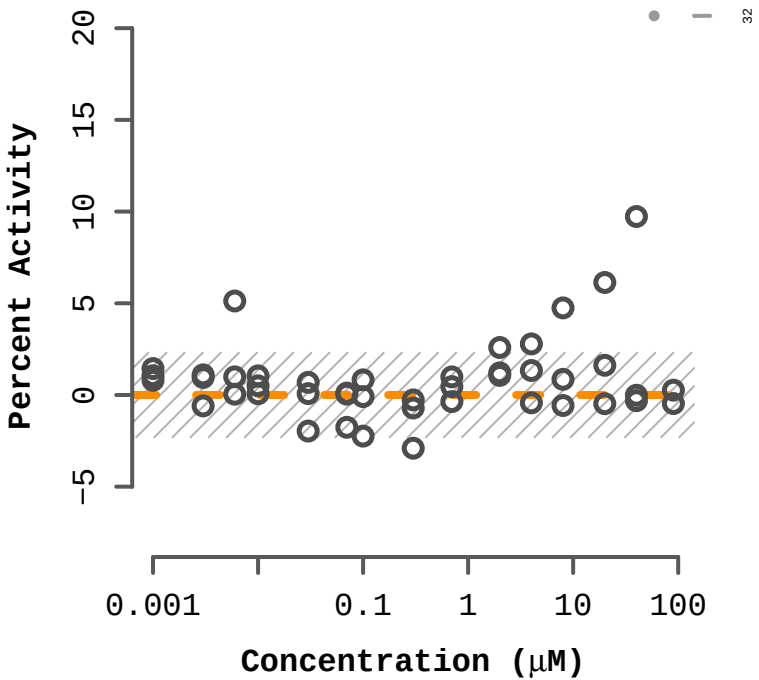
NAME: 5-Azacytidine
CHID: 20116 **CASRN:** 320-67-2
SPID(S): Tox21_111032_1
M4ID: 12483940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.9	NA	NA
PROB:	1	NA	NA
RMSE:	4.37	NA	NA

MAX_MEAN: 0.937 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

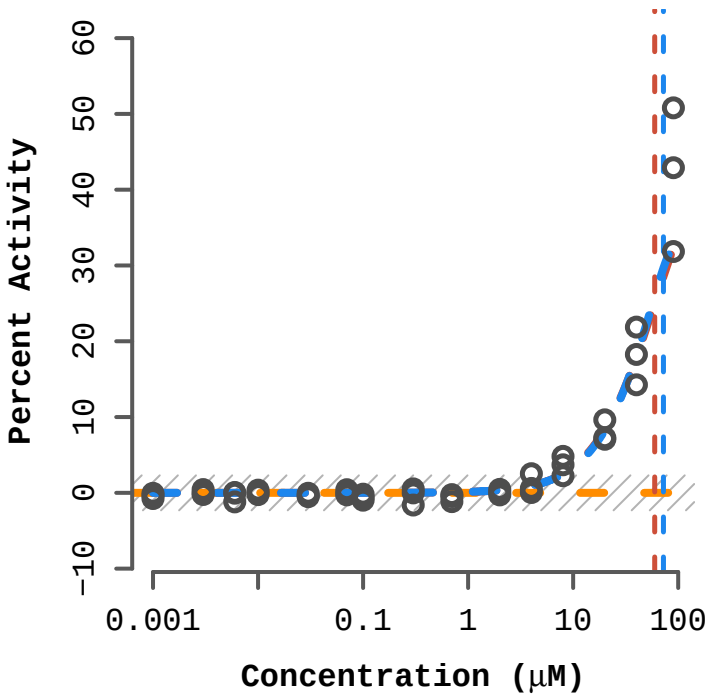
NAME: 6-Azacytidine
CHID: 20117 CASRN: 3131-60-0
SPID(S): Tox21_201231
M4ID: 12481021 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.31	NA	NA
PROB:	1	NA	NA
RMSE:	5.34	NA	NA

MAX_MEAN: 10.7 MAX_MED: 1.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Azaserine
CHID: 20118 **CASRN:** 115-02-6
SPID(S): Tox21_302892
M4ID: 12476241

HILL MODEL (in red):

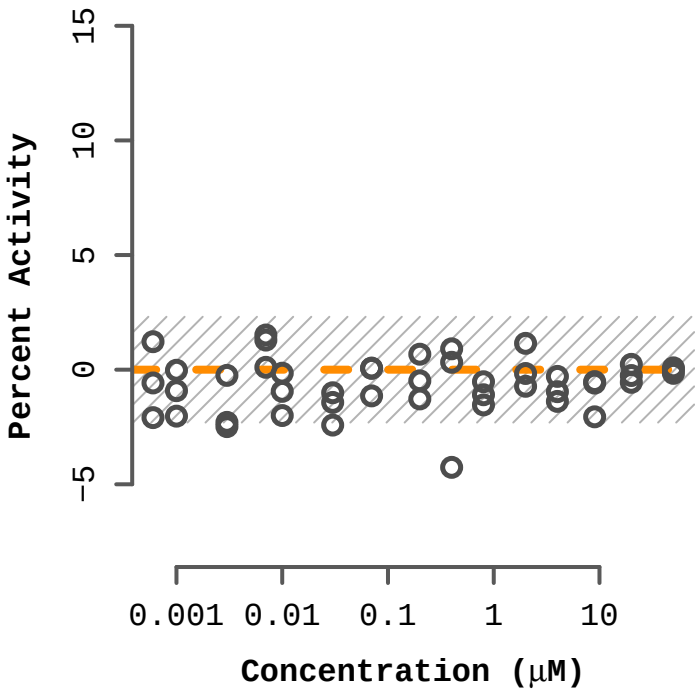
	tp	ga	gw
val:	50.1	1.78	1.46
sd:	7.12	0.0947	0.154

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	60.3	1.86	1.43	2.11	7.08
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	303.67	174.85	178.53
PROB:	0	0.86	0.14
RMSE:	12.21	3.35	3.37

MAX_MEAN: 41.9 **MAX_MED:** 42.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

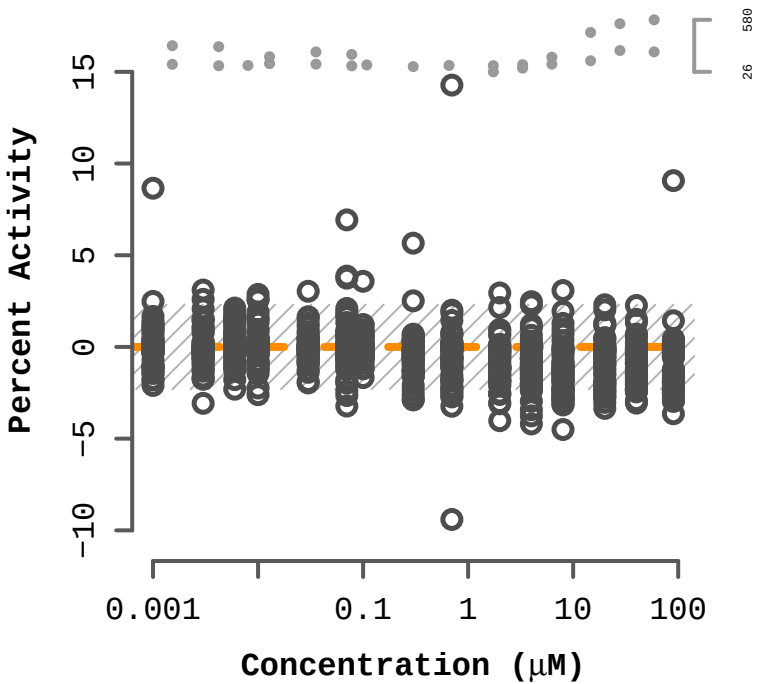
NAME: Azaserine
CHID: 20118 **CASRN:** 115-02-6
SPID(S): Tox21_110833_1
M4ID: 12484083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.97 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

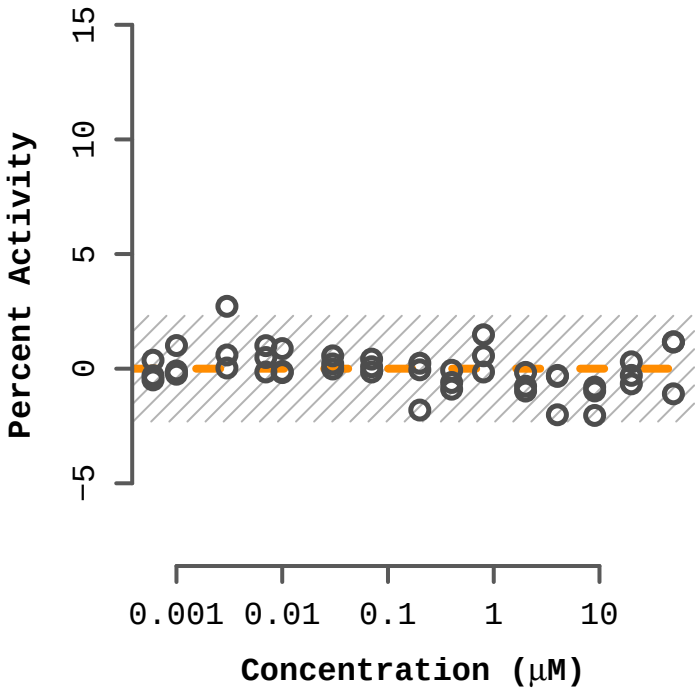
NAME: Azathioprine
CHID: 20119 **CASRN:** 446-86-6
SPID(S): Tox21_400024
M4ID: 12475113 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3733.34	NA	NA
PROB:	1	NA	NA
RMSE:	43.46	NA	NA

MAX_MEAN: 15.2 **MAX_MED:** 0.00304 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

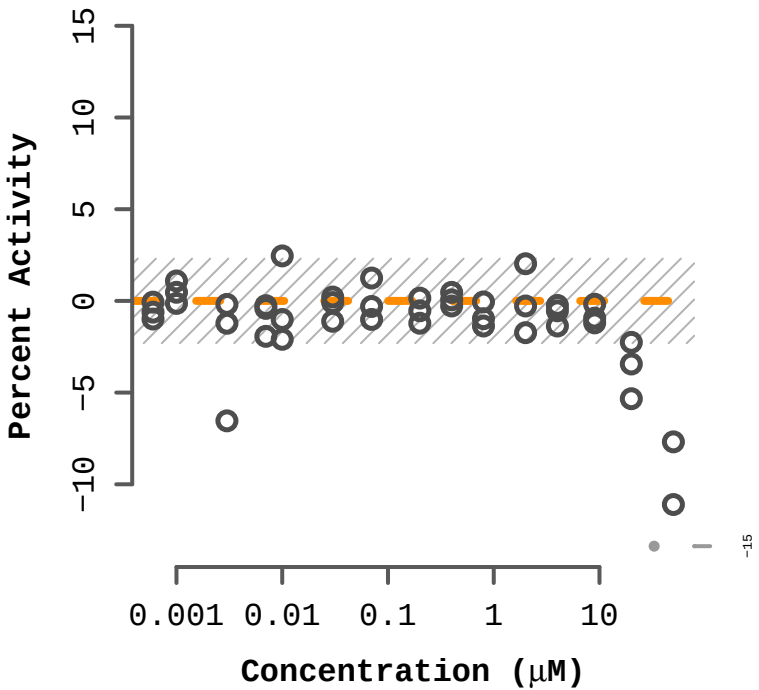
NAME: Azathioprine
CHID: 20119 **CASRN:** 446-86-6
SPID(S): Tox21_110074_1
M4ID: 12484678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

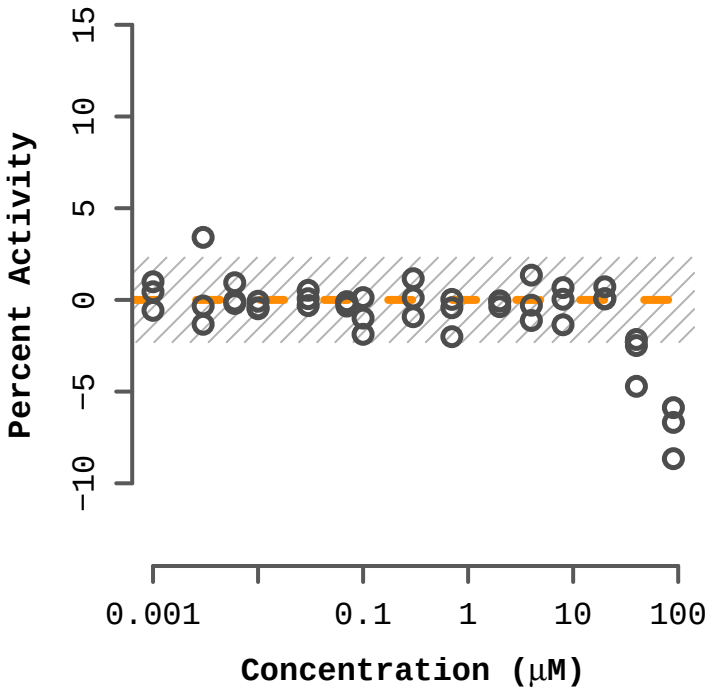
NAME: Azelnidipine
CHID: 20120 **CASRN:** 123524-52-7
SPID(S): Tox21_112440_1
M4ID: 12483102 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.28	NA	NA
PROB:	1	NA	NA
RMSE:	3.44	NA	NA

MAX_MEAN: 0.475 **MAX_MED:** 0.471 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

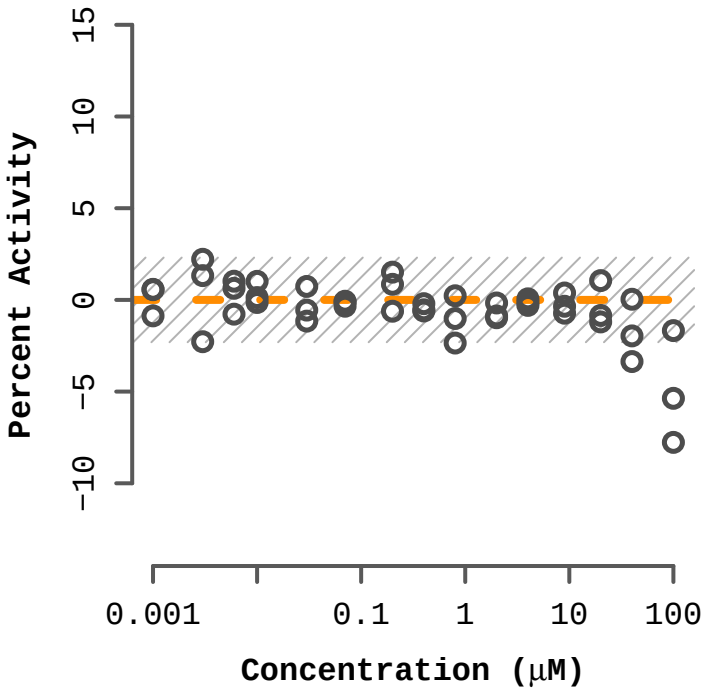
NAME: Sodium azide
CHID: 20121 **CASRN:** 26628-22-8
SPID(S): Tox21_300024
M4ID: 12479106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.446 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

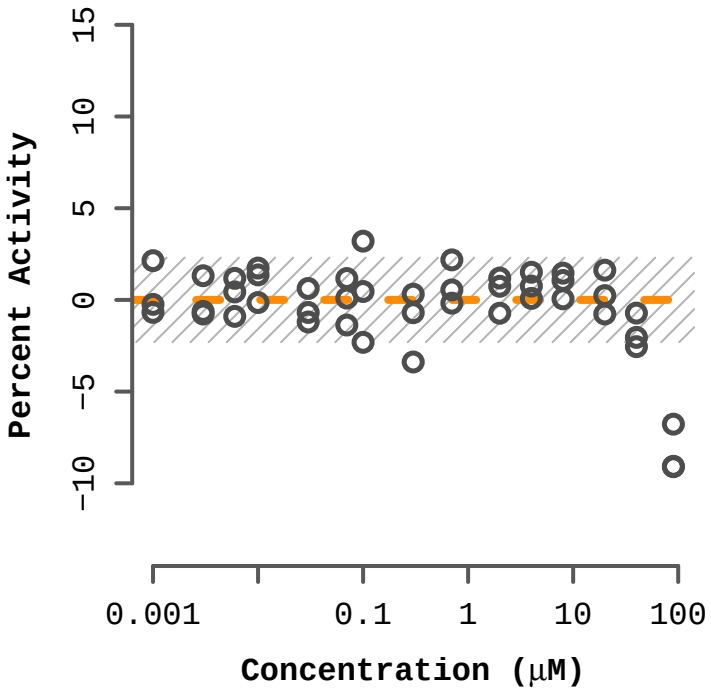
NAME: Sodium azide
CHID: 20121 CASRN: 26628-22-8
SPID(S): Tox21_202461
M4ID: 12479791

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.78	NA	NA

MAX_MEAN: 0.584 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

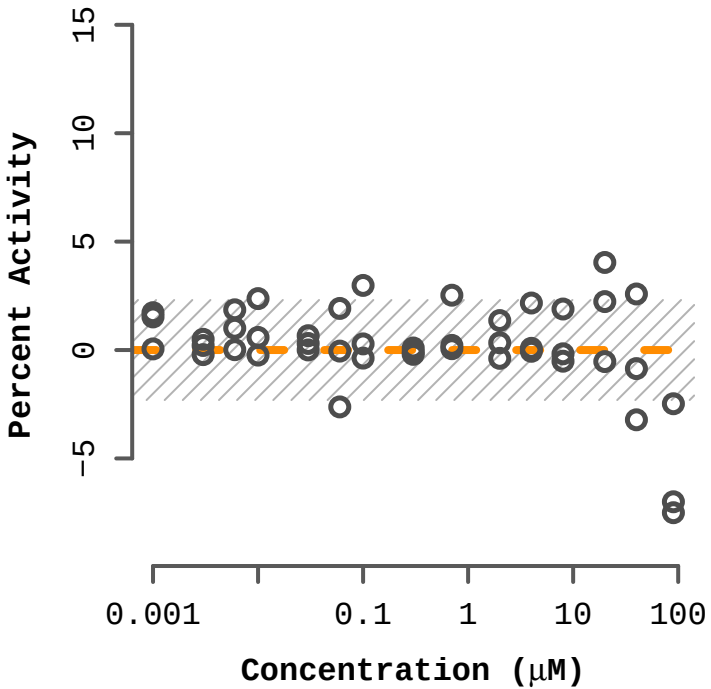
NAME: Azinphos-methyl
CHID: 20122 **CASRN:** 86-50-0
SPID(S): Tox21_300929
M4ID: 12478204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.53	NA	NA

MAX_MEAN: 0.987 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

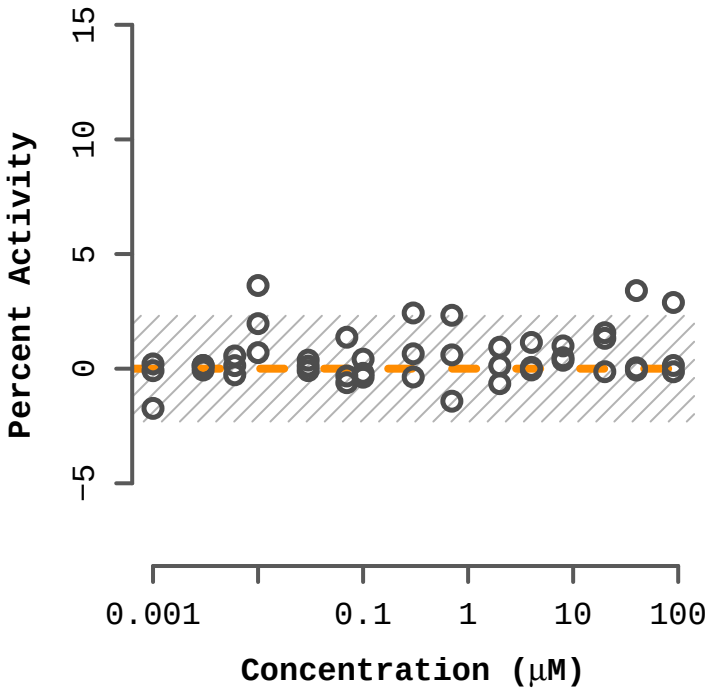
NAME: Azinphos-methyl
CHID: 20122 **CASRN:** 86-50-0
SPID(S): Tox21_201965
M4ID: 12480287

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

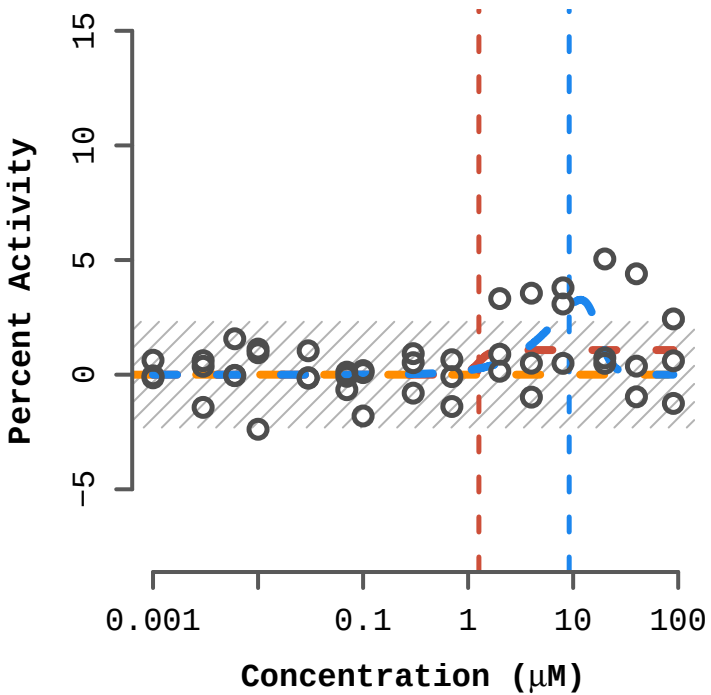
NAME: Azobenzene
CHID: 20123 **CASRN:** 103-33-3
SPID(S): Tox21_300495
M4ID: 12478637

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Azobenzene
CHID: 20123 CASRN: 103-33-3
SPID(S): Tox21_201458
M4ID: 12480794

HILL MODEL (in red):

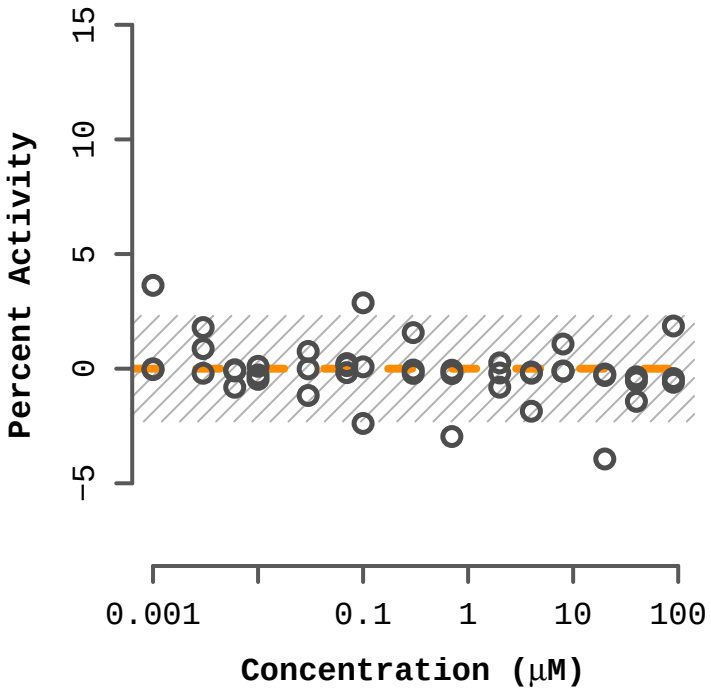
	tp	ga	gw
val:	1.07	0.102	8
sd:	0.402	0.541	19.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.06	0.962	1.55	1.22	6.54
sd:	10.5	0.869	1.23	0.36	27.9

	CNST	HILL	GNLS
AIC:	169.03	166.21	167.5
PROB:	0.14	0.57	0.3
RMSE:	1.68	1.42	1.43

MAX_MEAN: 2.46 MAX_MED: 3.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

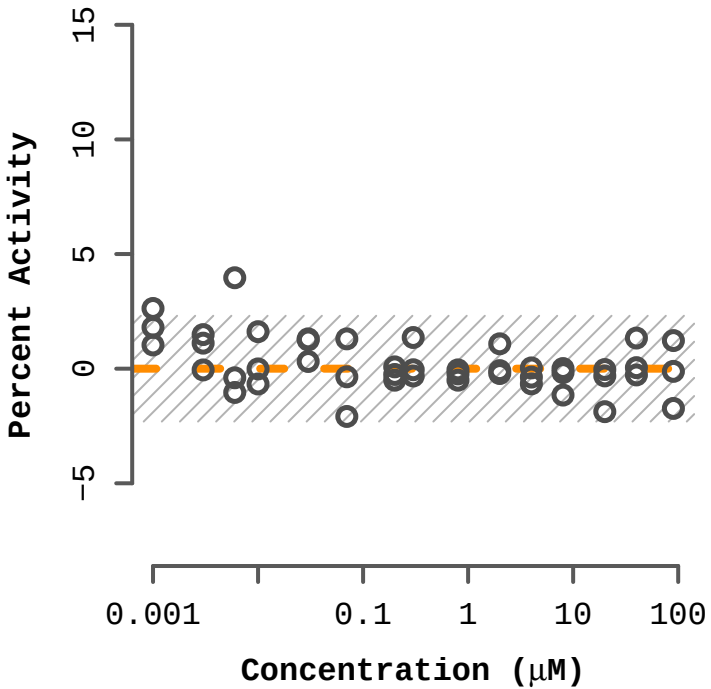
NAME: 3'−Azido−3'−deoxythymidine
CHID: 20127 **CASRN:** 30516−87−1
SPID(S): Tox21_300578
M4ID: 12478555

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.877 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

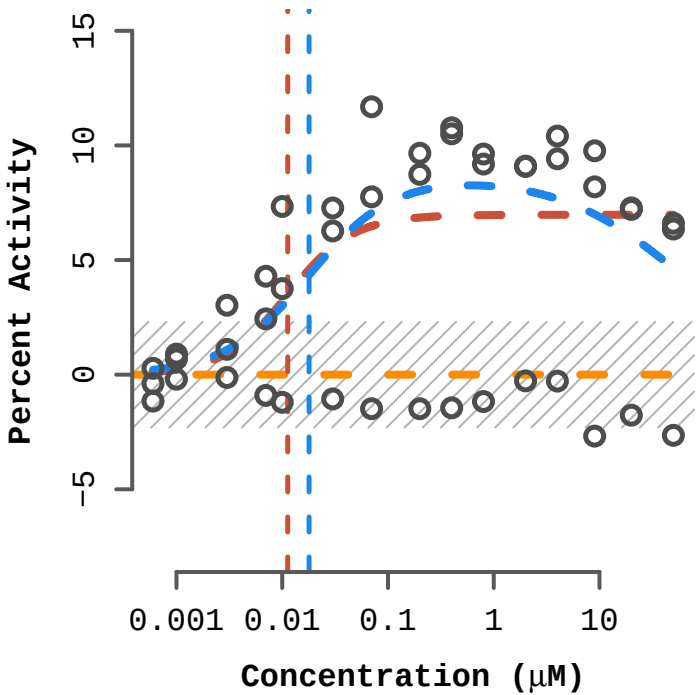
NAME: 3'−Azido−3'−deoxythymidine
CHID: 20127 **CASRN:** 30516−87−1
SPID(S): Tox21_202203
M4ID: 12480049

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3'−Azido−3'−deoxythymidine
CHID: 20127 CASRN: 30516−87−1
SPID(S): Tox21_110062_1
M4ID: 12484688

HILL MODEL (in red):

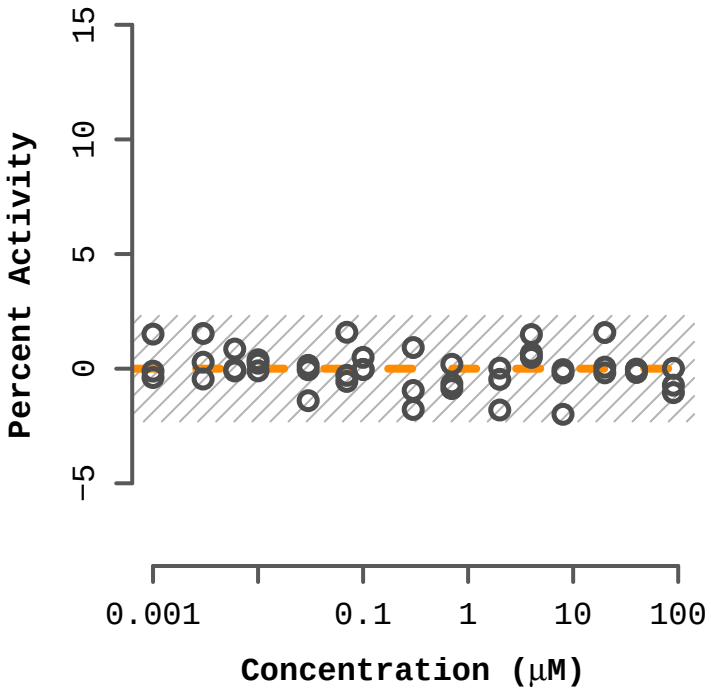
	tp	ga	gw
val:	6.97	−1.95	1.41
sd:	0.959	0.27	0.927

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.71	−1.75	1.09	1.78	0.748
sd:	2.98	0.428	0.702	0.608	1.34

	CNST	HILL	GNLS
AIC:	297.93	268.35	270.05
PROB:	0	0.7	0.3
RMSE:	6.17	4.37	4.38

MAX_MEAN: 6.61 MAX_MED: 10.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

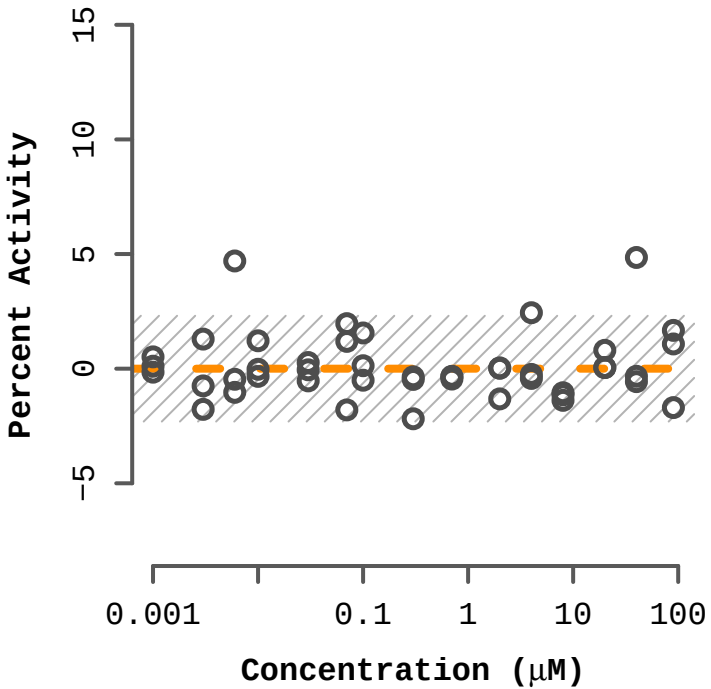
NAME: Sodium barbital
CHID: 20128 CASRN: 144-02-5
SPID(S): Tox21_200862
M4ID: 12481390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 0.669 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

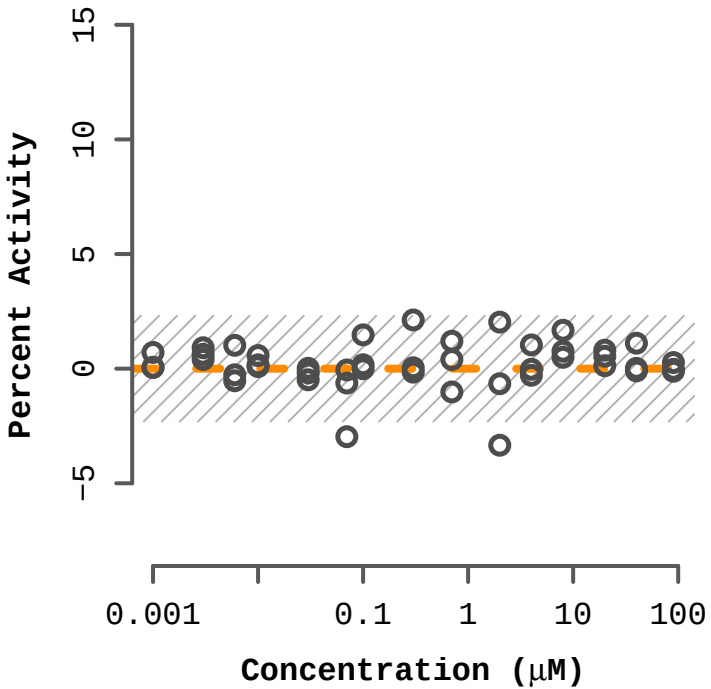
NAME: Barbituric acid
CHID: 20129 CASRN: 67-52-7
SPID(S): Tox21_200924
M4ID: 12481328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.32 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

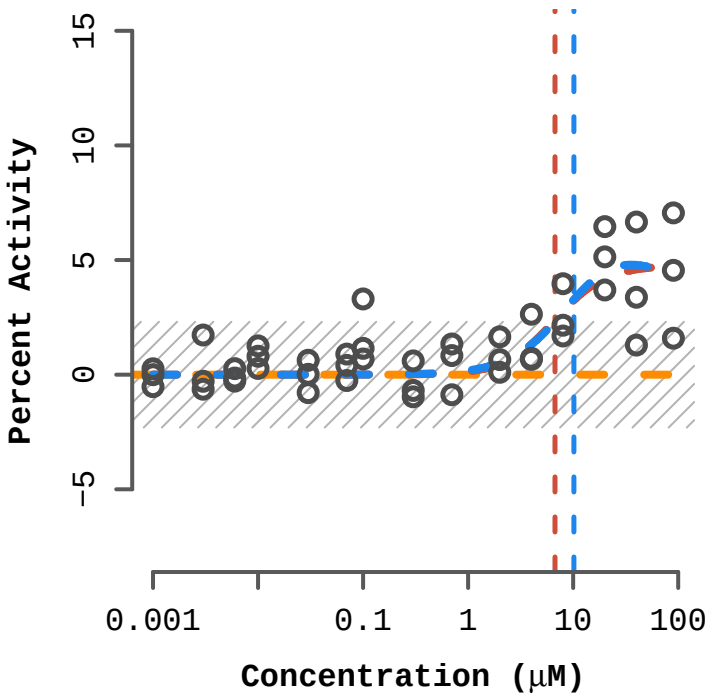
NAME: Barium chloride dihydrate
CHID: 20131 CASRN: 10326-27-9
SPID(S): Tox21_200488
M4ID: 12481764

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.08	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 0.762 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzidine
CHID: 20137 CASRN: 92-87-5
SPID(S): Tox21_300405
M4ID: 12478727

HILL MODEL (in red):

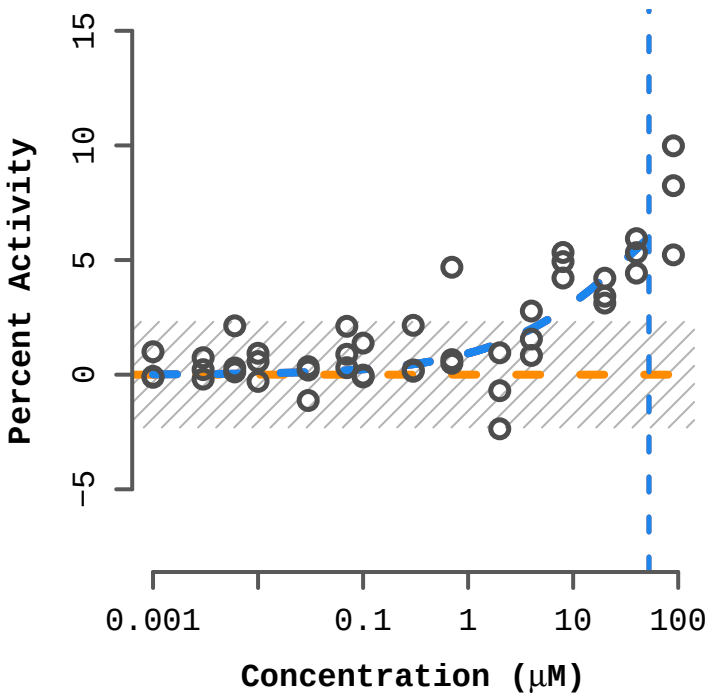
	tp	ga	gw
val:	4.77	0.827	1.83
sd:	0.788	0.134	0.918

GAIN-LOSS MODEL (in blue):

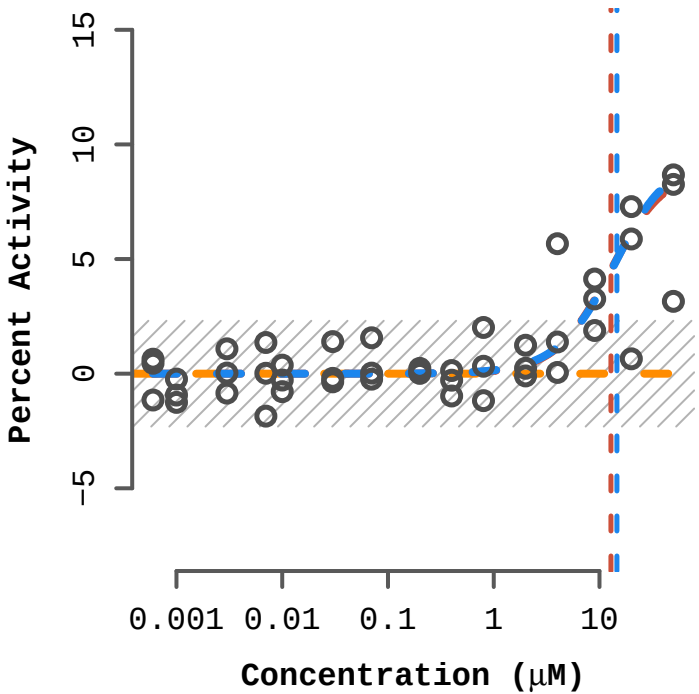
	tp	ga	gw	la	lw
val:	8.47	1.01	1.61	2.03	0.524
sd:	13.9	0.397	0.907	2.79	1.23

	CNST	HILL	GNLS
AIC:	202.46	154.53	158.01
PROB:	0	0.85	0.15
RMSE:	2.46	1.26	1.25

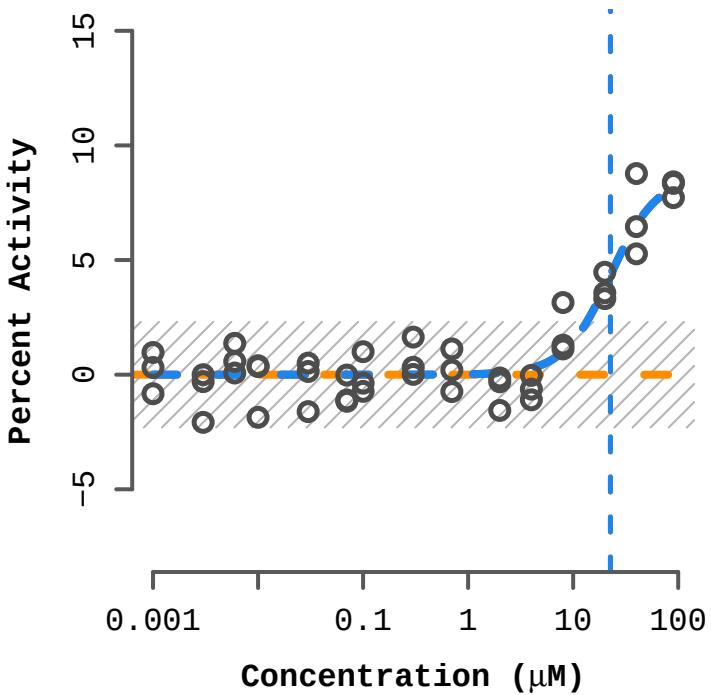
MAX_MEAN: 5.1 MAX_MED: 5.14 BMAD: 0.769



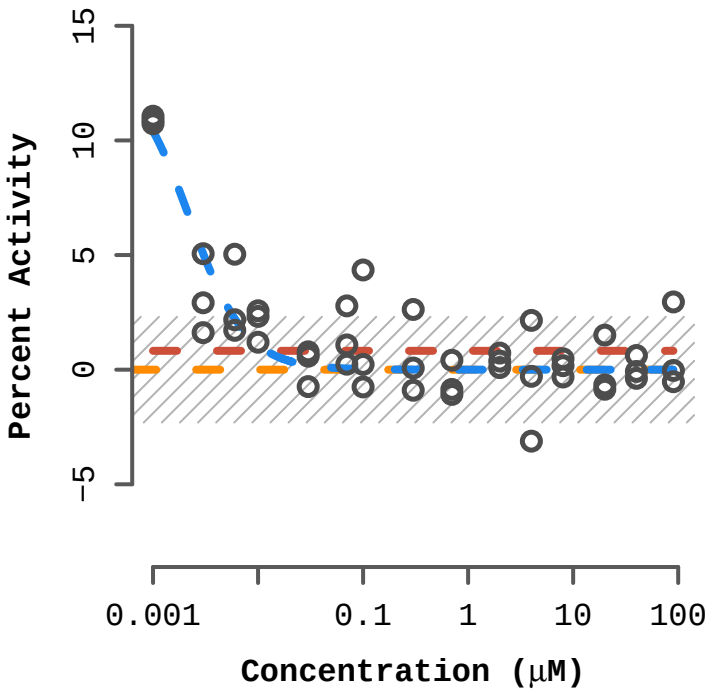

```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzidine
CHID:    20137   CASRN: 92-87-5
SPID(S): Tox21_202359
M4ID:    12479893

HILL MODEL (in red):
      tp       ga       gw
val:  12       1.72     0.624
sd:   6.48     0.704    0.178

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12       1.72     0.624    2.99     13
sd:   6.47     0.703    0.178    83600    995000

      CNST        HILL        GNLS
AIC:  227.99      159.58      163.58
PROB: 0           0.88        0.12
RMSE: 3.16        1.36        1.36

MAX_MEAN: 7.82      MAX_MED: 8.25      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzidine dihydrochloride
CHID:    20138   CASRN: 531-85-1
SPID(S): Tox21_202584
M4ID:    12479668

HILL MODEL (in red):
      tp       ga       gw
val:  9.04     1.11     1.66
sd:   1.33     0.123    0.52

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.96     1.16     1.57     1.96     4.57
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  202.26      156.3       160.28
PROB: 0           0.88        0.12
RMSE: 2.72        1.53        1.54

MAX_MEAN: 6.7       MAX_MED: 8.26      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzo(a)pyrene
CHID:    20139   CASRN: 50-32-8
SPID(S): Tox21_200710
M4ID:    12481542

HILL MODEL (in red):
      tp       ga       gw
val:  8.68     1.35     1.96
sd:   0.731    0.0684   0.432

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.68     1.35     1.96     3.12     6.75
sd:   0.731    0.0684   0.432    1410     8130

      CNST        HILL        GNLS
AIC:  218.02      133.49      137.49
PROB: 0           0.88        0.12
RMSE: 3.1         0.96        0.96

MAX_MEAN: 8.16      MAX_MED: 8.34      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium benzoate
CHID: 20140 CASRN: 532-32-1
SPID(S): Tox21_300125
M4ID: 12479005

HILL MODEL (in red):

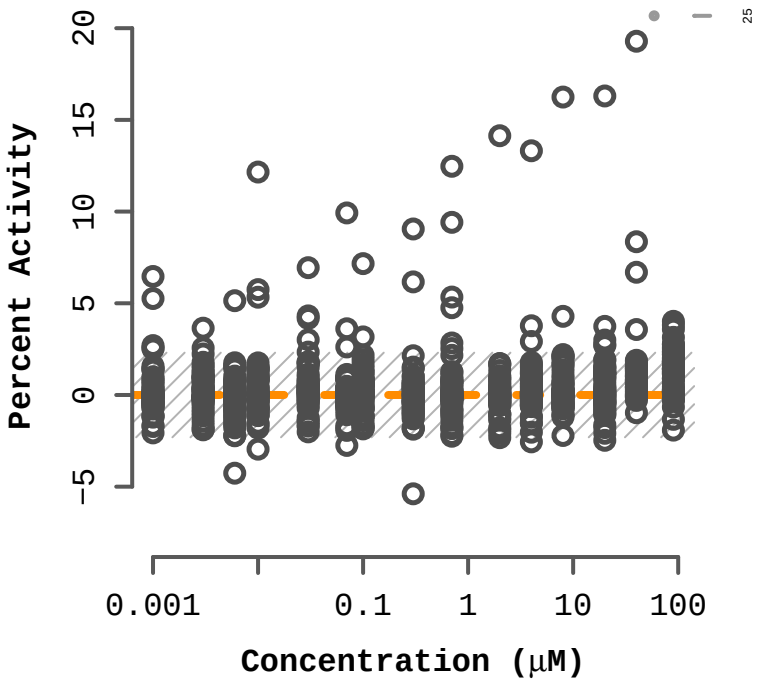
	tp	ga	gw
val:	0.823	−4.83	5.56
sd:	0.297	32300	98100

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.3	−4.54	5.31	−2.65	1.61
sd:	1.92	770	2650	0.108	0.343

	CNST	HILL	GNLS
AIC:	219.37	217.49	169.03
PROB:	0	0	1
RMSE:	3.36	3.07	1.47

MAX_MEAN: 10.9 **MAX_MED:** 10.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

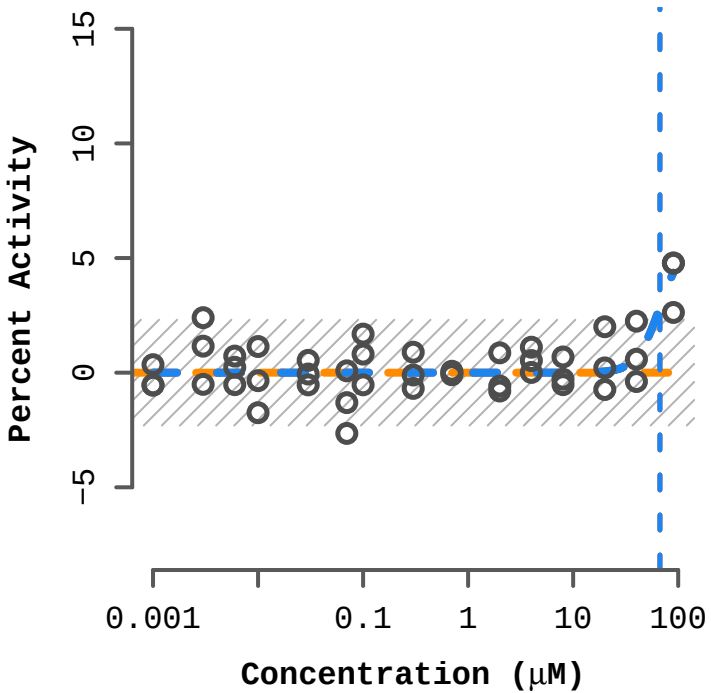
NAME: 2,3-Benzofuran
CHID: 20141 CASRN: 271-89-6
SPID(S): Tox21_400054
M4ID: 12475083 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2681.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.26	NA	NA

MAX_MEAN: 1.73 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Phenyl-1,3,5-triazine-2,4-diamine
CHID: 20142 **CASRN:** 91-76-9
SPID(S): Tox21_302969
M4ID: 12476164

HILL MODEL (in red):

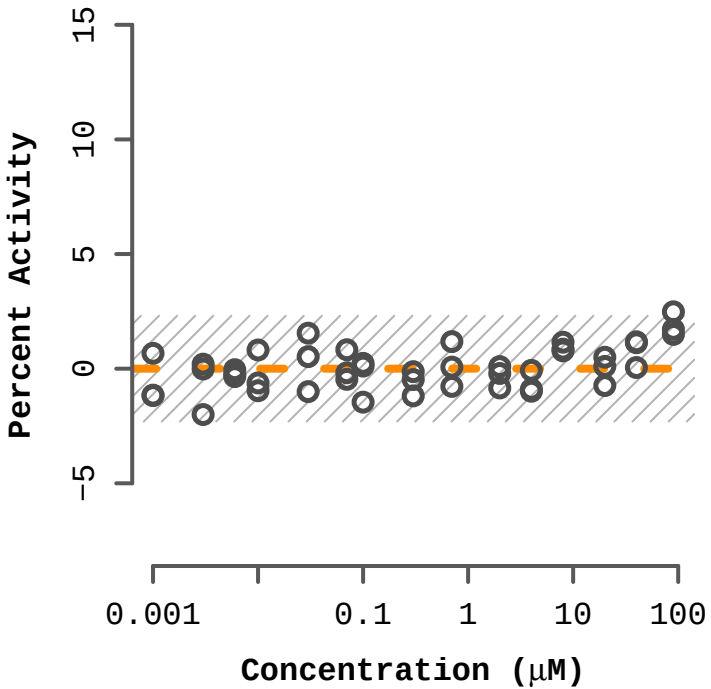
	tp	ga	gw
val:	5.75	1.83	3.88
sd:	11.5	0.674	7.82

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.75	1.83	3.88	3.94	2.57
sd:	11.6	0.684	7.93	476	625

	CNST	HILL	GNLS
AIC:	152.97	134.01	138.01
PROB:	0	0.88	0.12
RMSE:	1.45	0.98	0.98

MAX_MEAN: 4.06 **MAX_MED:** 4.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

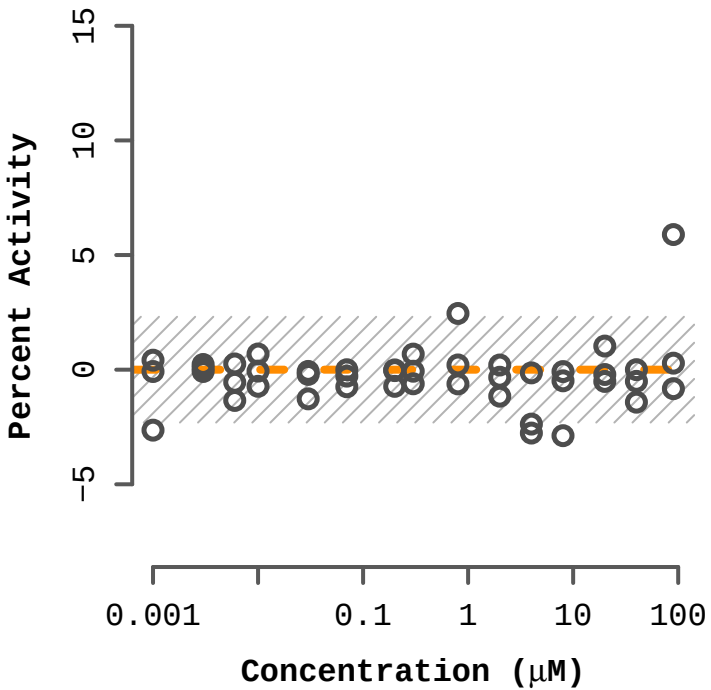
NAME: 6-Phenyl-1,3,5-triazine-2,4-diamine
CHID: 20142 **CASRN:** 91-76-9
SPID(S): Tox21_201624
M4ID: 12480628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

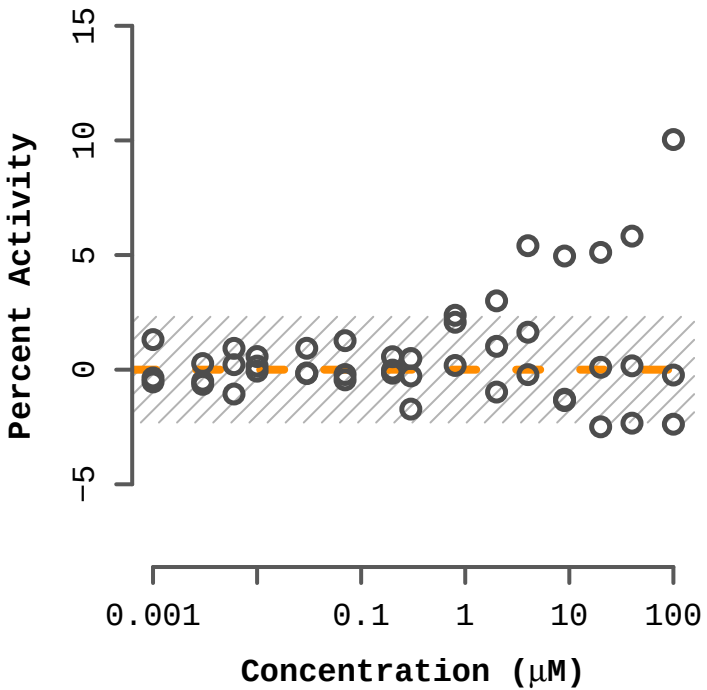
NAME: Benzoic acid
CHID: 20143 **CASRN:** 65-85-0
SPID(S): Tox21_300180
M4ID: 12478950

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

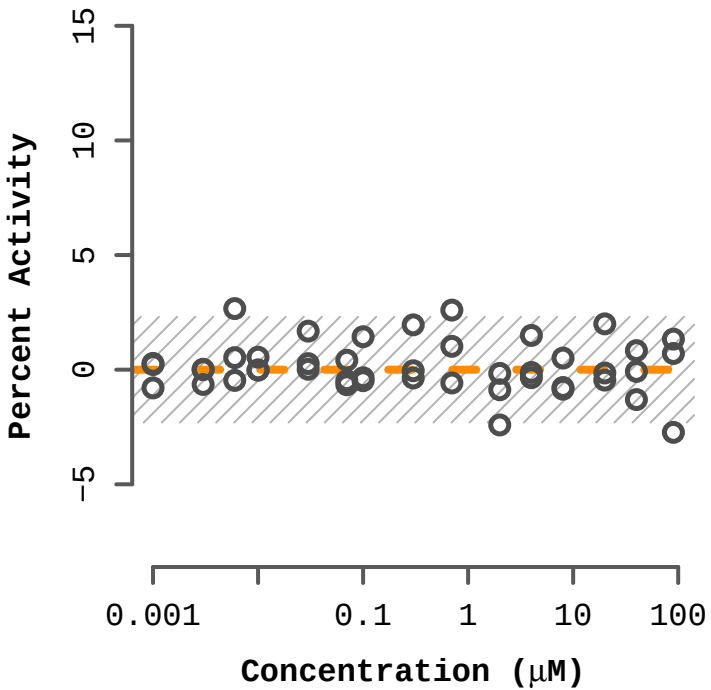
NAME: Benzoic acid
CHID: 20143 **CASRN:** 65-85-0
SPID(S): Tox21_202403
M4ID: 12479849

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.81	NA	NA
PROB:	1	NA	NA
RMSE:	2.45	NA	NA

MAX_MEAN: 2.48 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

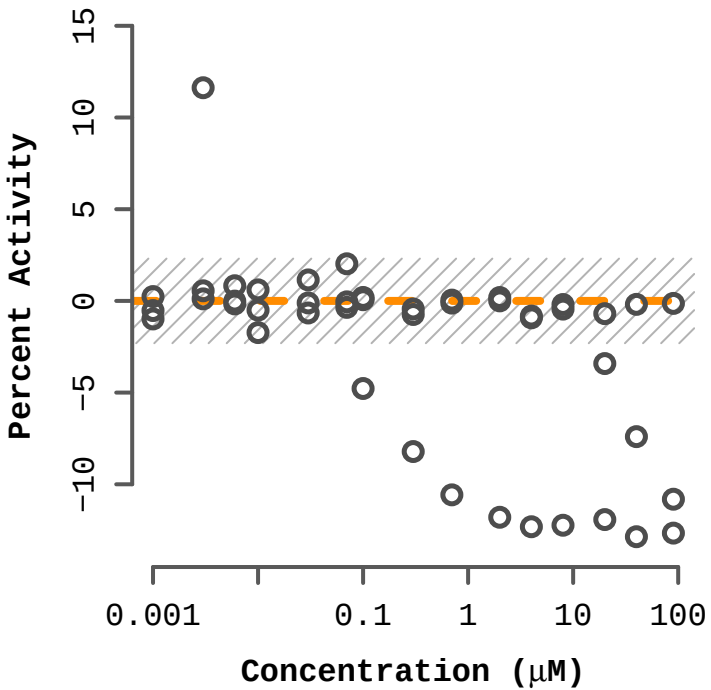
NAME: Benzoin
CHID: 20144 CASRN: 119-53-9
SPID(S): Tox21_302790
M4ID: 12476343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

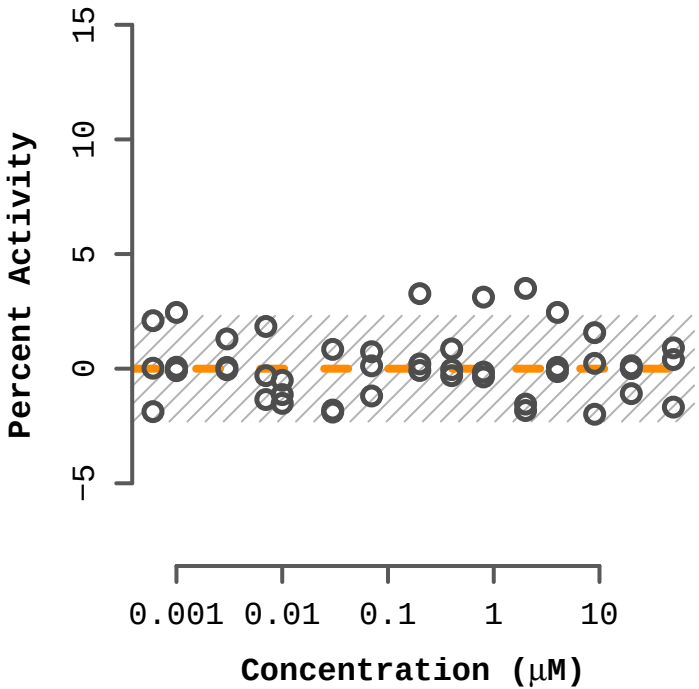
NAME: Benzoin
CHID: 20144 **CASRN:** 119-53-9
SPID(S): Tox21_201888
M4ID: 12480364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.3	NA	NA
PROB:	1	NA	NA
RMSE:	5.66	NA	NA

MAX_MEAN: 4.1 **MAX_MED:** 0.553 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

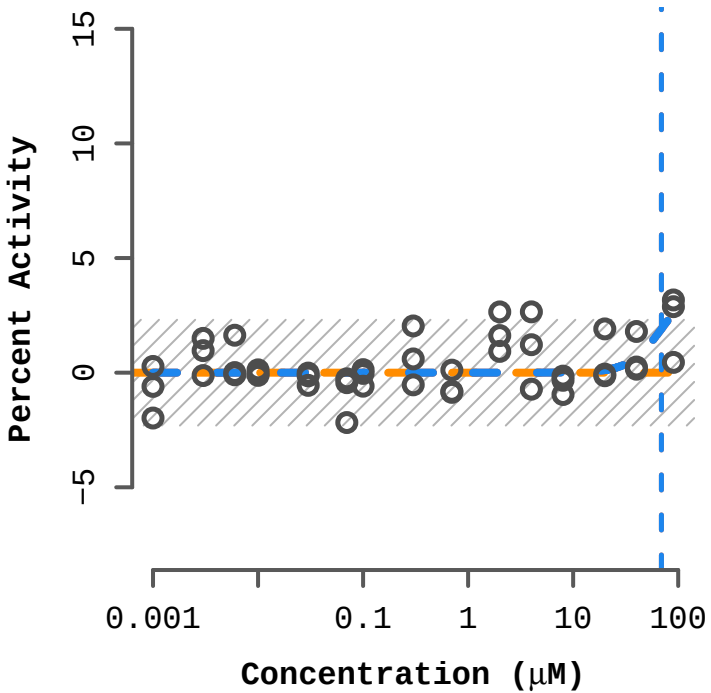
NAME: Benzoin
CHID: 20144 **CASRN:** 119-53-9
SPID(S): Tox21_111126_1
M4ID: 12483892

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Benzoquinone
CHID: 20145 CASRN: 106−51−4
SPID(S): Tox21_302970
M4ID: 12476163

HILL MODEL (in red):

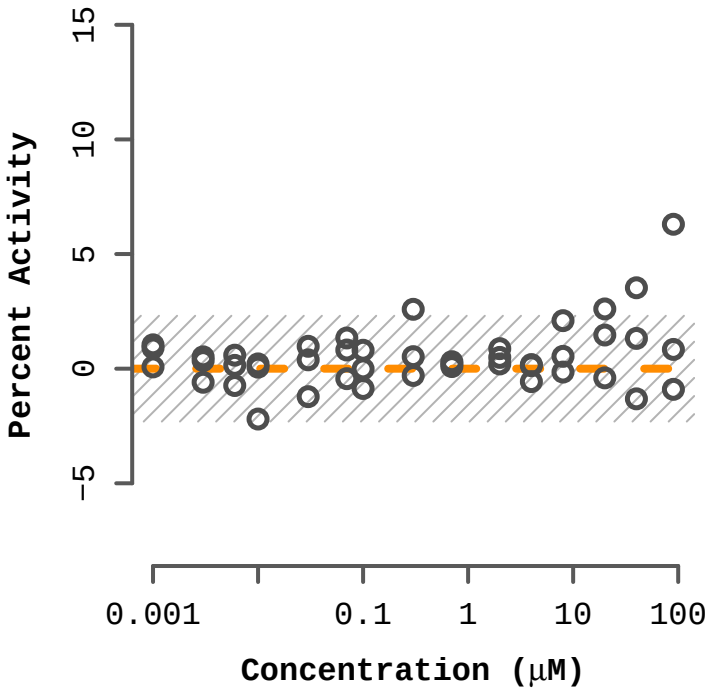
	tp	ga	gw
val:	3.81	1.84	2.81
sd:	6.3	0.635	3.88

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.81	1.84	2.81	3.55	4.07
sd:	6.3	0.635	3.88	1530	3950

	CNST	HILL	GNLS
AIC:	146.19	141.64	145.64
PROB:	0.08	0.81	0.11
RMSE:	1.23	1.08	1.08

MAX_MEAN: 2.17 **MAX_MED:** 2.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

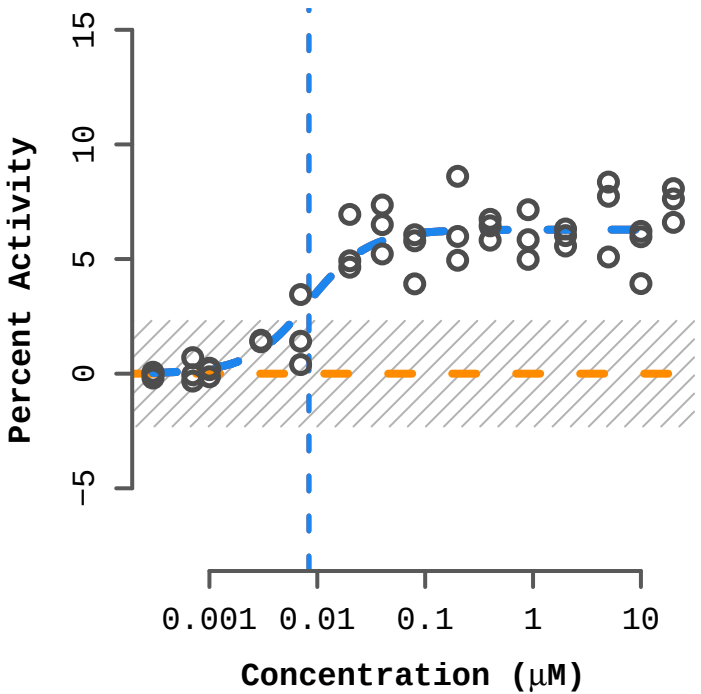
NAME: 1,4−Benzoquinone
CHID: 20145 **CASRN:** 106−51−4
SPID(S): Tox21_202020
M4ID: 12480232

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'−Dithiobisbenzothiazole
CHID: 20146 CASRN: 120−78−5
SPID(S): Tox21_111106_1
M4ID: 12483904

HILL MODEL (in red):

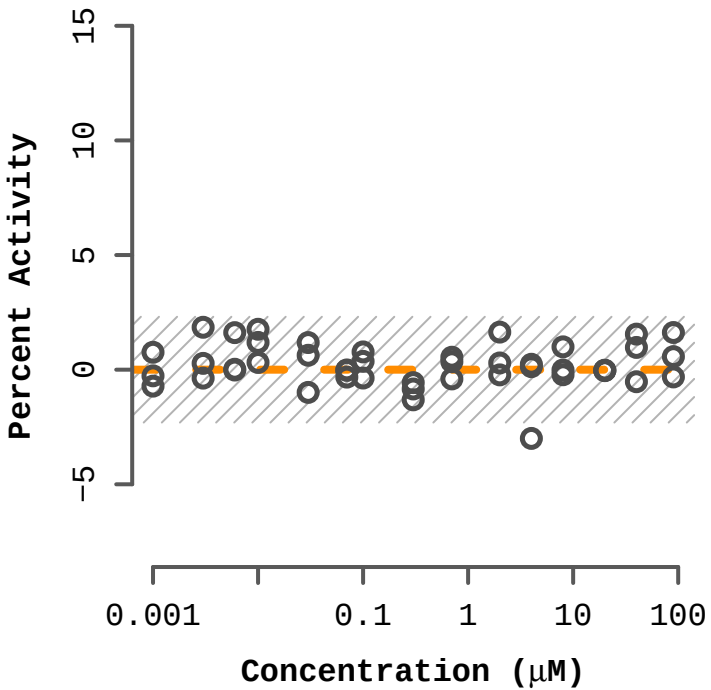
	tp	ga	gw
val:	6.28	−2.08	1.57
sd:	0.215	0.0907	0.341

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.28	−2.08	1.57	3.3	4.21
sd:	0.215	0.0907	0.341	1100	2320

	CNST	HILL	GNLS
AIC:	285.24	140.12	144.12
PROB:	0	0.88	0.12
RMSE:	5.18	1.06	1.06

MAX_MEAN: 7.43 MAX_MED: 7.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

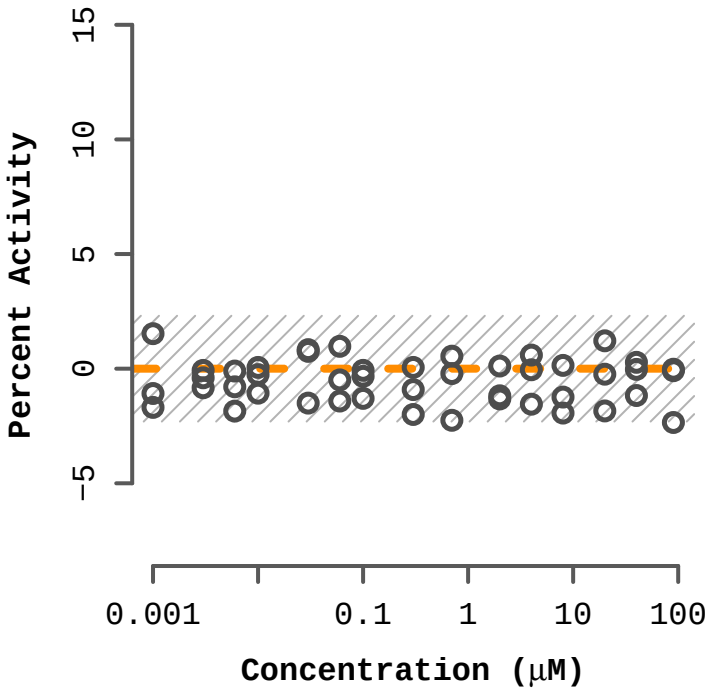
NAME: 1,2,3-Benzotriazole
CHID: 20147 **CASRN:** 95-14-7
SPID(S): Tox21_302934
M4ID: 12476199

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

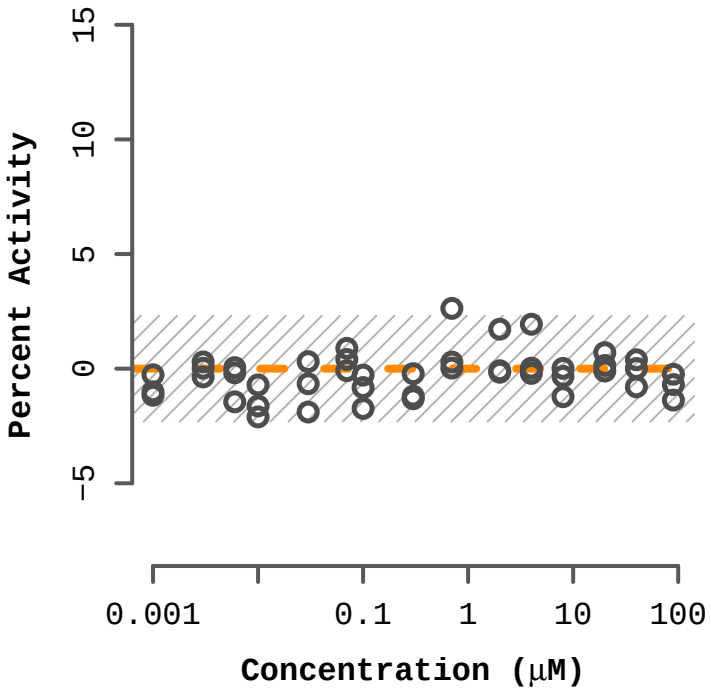
NAME: 1,2,3-Benzotriazole
CHID: 20147 **CASRN:** 95-14-7
SPID(S): Tox21_201501
M4ID: 12480751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.0291 **MAX_MED:** 0.756 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

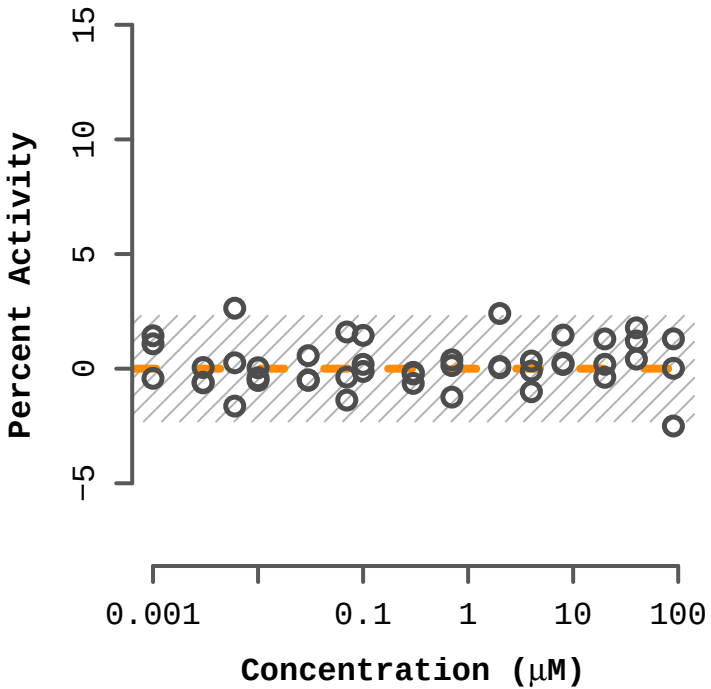
NAME: Benzotrichloride
CHID: 20148 **CASRN:** 98-07-7
SPID(S): Tox21_300181
M4ID: 12478949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.402 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

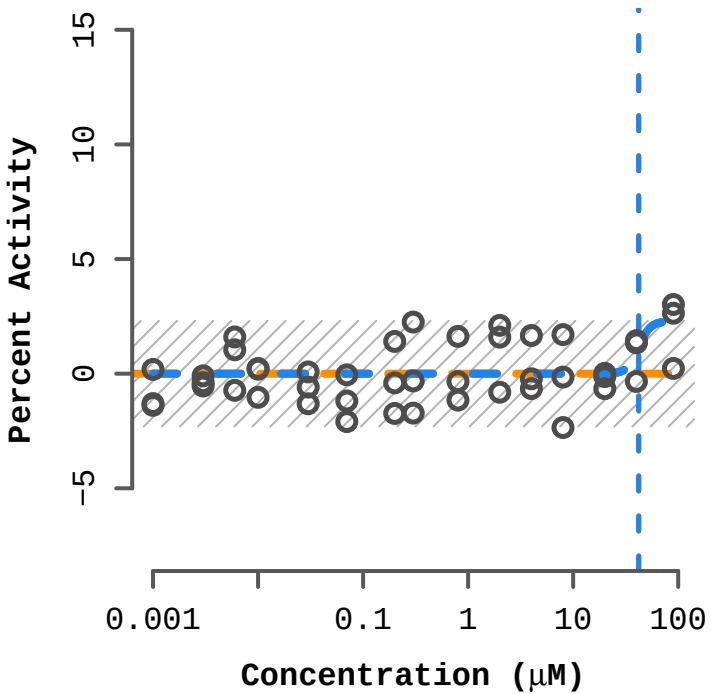
NAME: Benzotrichloride
CHID: 20148 **CASRN:** 98-07-7
SPID(S): Tox21_201290
M4ID: 12480962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzoyl hydrazine
CHID: 20149 CASRN: 613-94-5
SPID(S): Tox21_200878
M4ID: 12481374

HILL MODEL (in red):

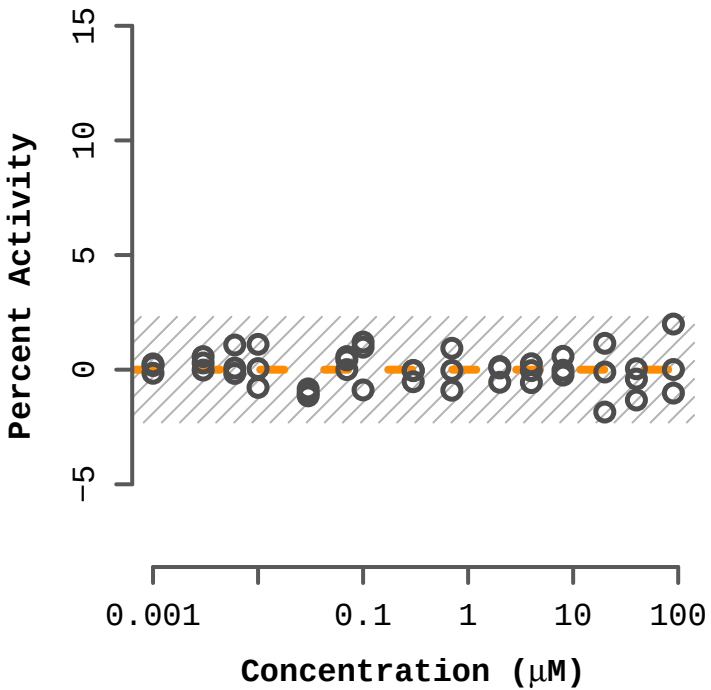
	tp	ga	gw
val:	2.28	1.62	8
sd:	0.732	0.0938	19.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.28	1.62	8	2.36	7.75
sd:	4.56	0.204	19.8	208	3170

	CNST	HILL	GNLS
AIC:	156.15	154.08	158.08
PROB:	0.24	0.67	0.09
RMSE:	1.29	1.17	1.17

MAX_MEAN: 1.96 MAX_MED: 2.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

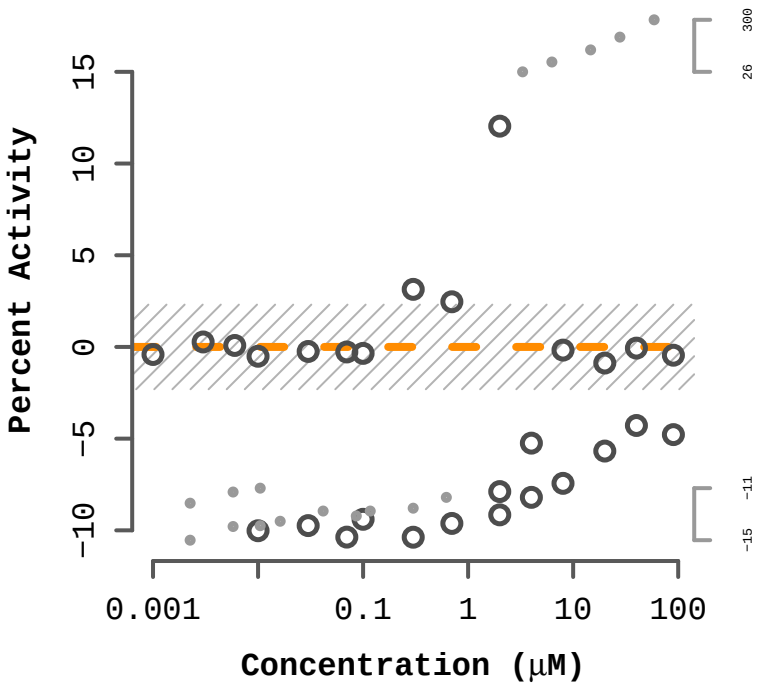
NAME: Benzyl acetate
CHID: 20151 CASRN: 140-11-4
SPID(S): Tox21_302841
M4ID: 12476292

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.435 **MAX_MED:** 0.983 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

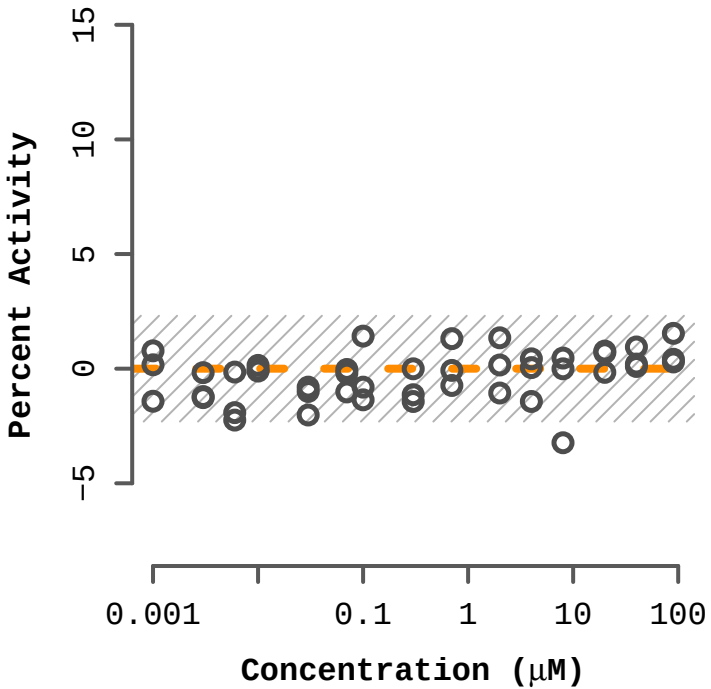
NAME: Benzyl acetate
CHID: 20151 **CASRN:** 140-11-4
SPID(S): Tox21_201826
M4ID: 12480426 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	418.55	NA	NA
PROB:	1	NA	NA
RMSE:	59.54	NA	NA

MAX_MEAN: 96.9 **MAX_MED:** −0.0627 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

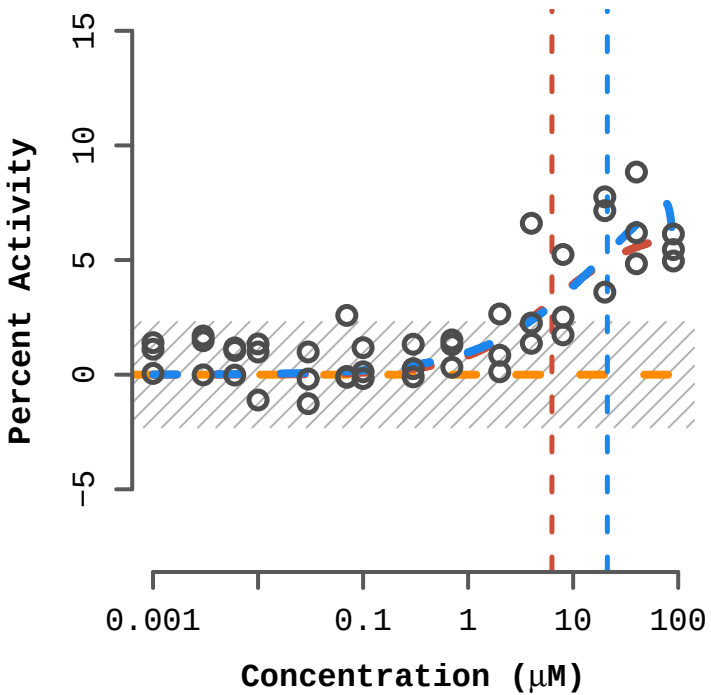
NAME: Benzyl alcohol
CHID: 20152 **CASRN:** 100-51-6
SPID(S): Tox21_300044
M4ID: 12479086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.75 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzyl alcohol
CHID: 20152 CASRN: 100-51-6
SPID(S): Tox21_202447
M4ID: 12479805

HILL MODEL (in red):

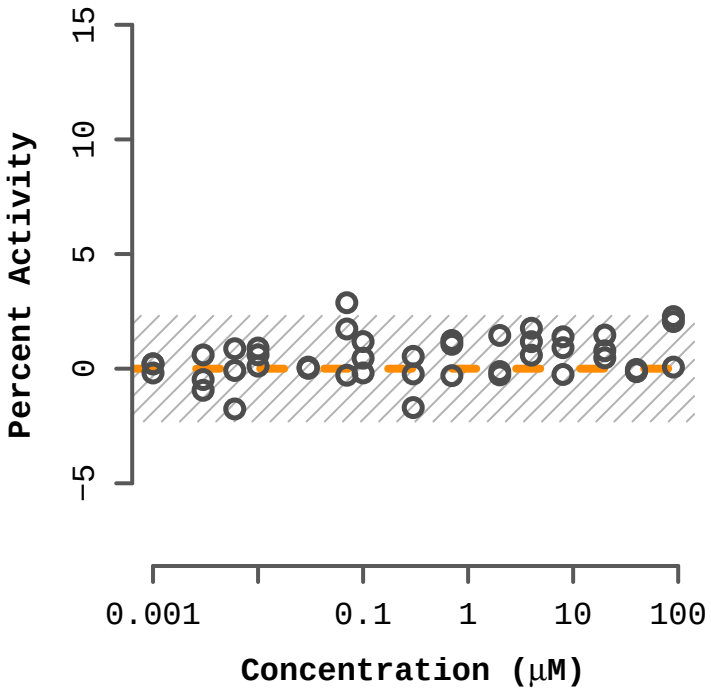
	tp	ga	gw
val:	6.39	0.798	1.03
sd:	1.02	0.232	0.552

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.6	1.33	0.75	1.97	18
sd:	8.2	0.942	0.384	0.0133	18.9

	CNST	HILL	GNLS
AIC:	232.33	164.22	165.27
PROB:	0	0.63	0.37
RMSE:	3.28	1.37	1.32

MAX_MEAN: 6.62 MAX_MED: 7.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

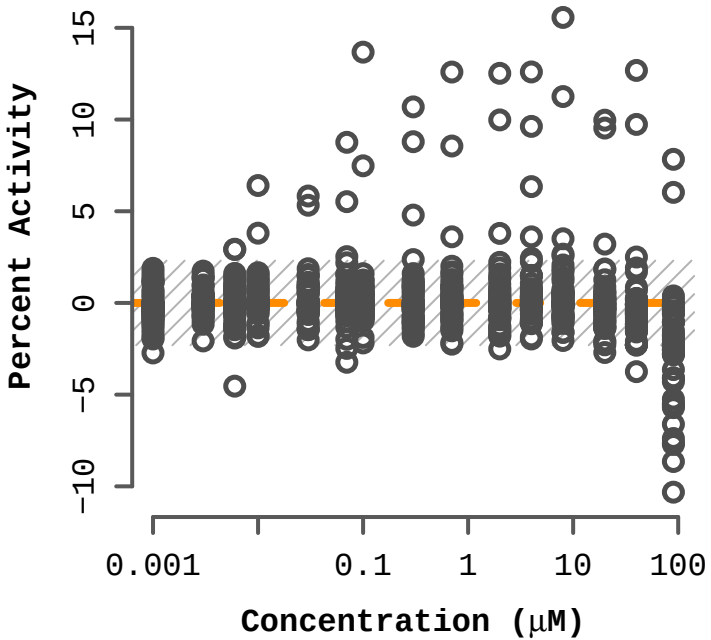
NAME: Benzyl chloride
CHID: 20153 CASRN: 100-44-7
SPID(S): Tox21_200266
M4ID: 12481986

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.47 MAX_MED: 2.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

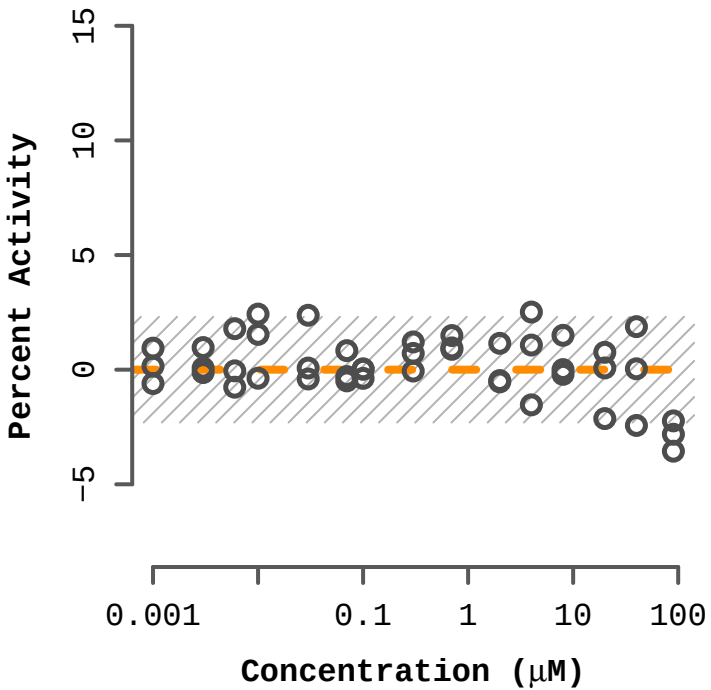
NAME: Clorophene
CHID: 20154 **CASRN:** 120-32-1
SPID(S): Tox21_400046
M4ID: 12475091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2629.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.28	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** 0.0373 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

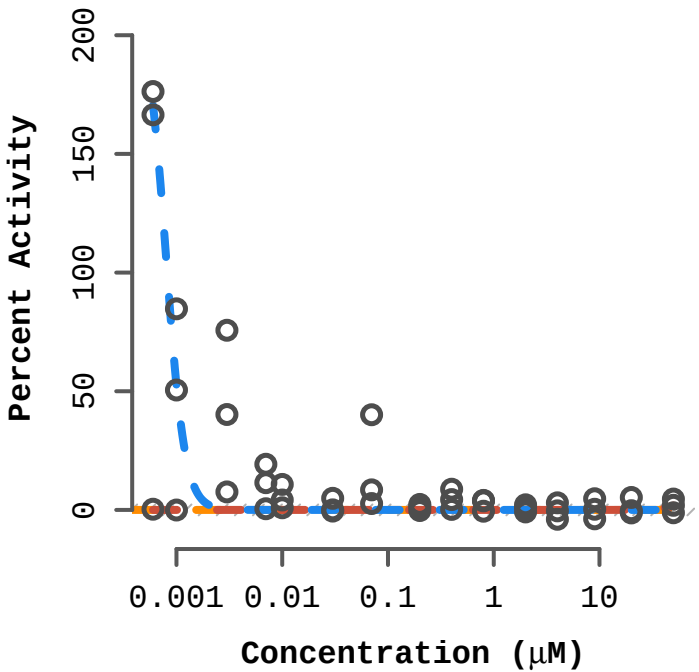
NAME: Clorophene
CHID: 20154 **CASRN:** 120-32-1
SPID(S): Tox21_202985
M4ID: 12479267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clorophene
CHID: 20154 CASRN: 120-32-1
SPID(S): Tox21_111146_1
M4ID: 12483879

HILL MODEL (in red):

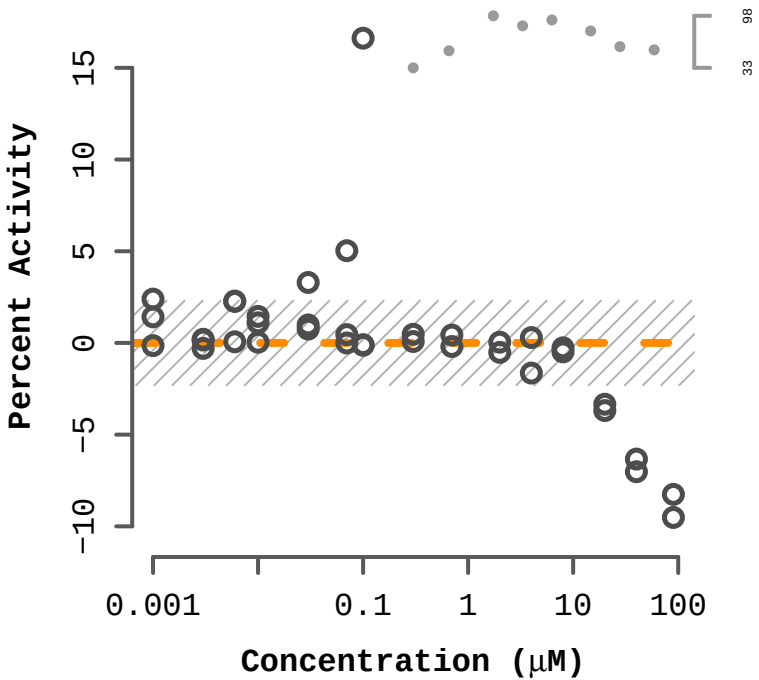
	tp	ga	gw
val:	129	2.2	3.68
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	212	-4.57	5.14	-3.1	4.95
sd:	10.8	664	2550	0.0154	0.653

	CNST	HILL	GNLS
AIC:	405.66	411.49	383.88
PROB:	0	0	1
RMSE:	41.78	41.78	30.81

MAX_MEAN: 114 MAX_MED: 166 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

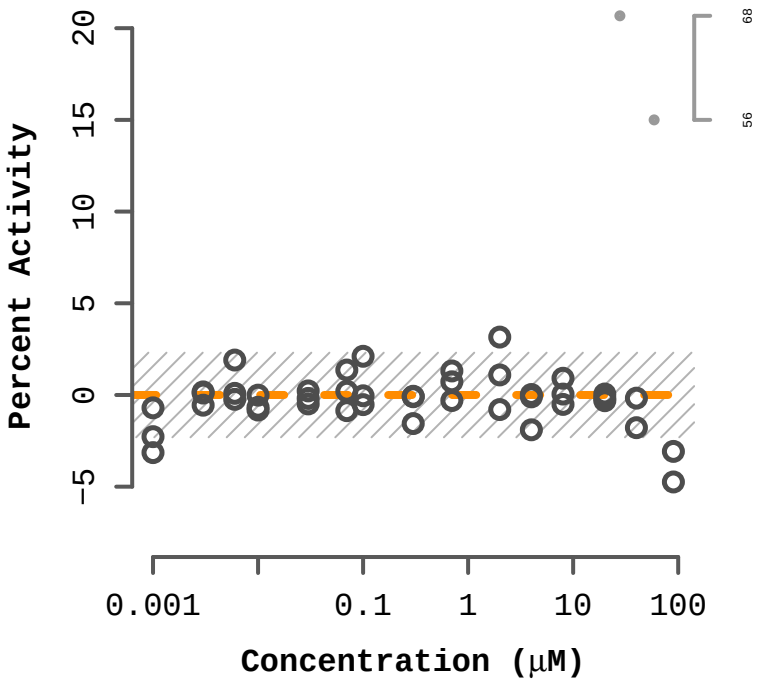
NAME: Benzyl isothiocyanate
CHID: 20155 CASRN: 622-78-6
SPID(S): Tox21_201191
M4ID: 12481061 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	403.1	NA	NA
PROB:	1	NA	NA
RMSE:	30.87	NA	NA

MAX_MEAN: 32.5 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

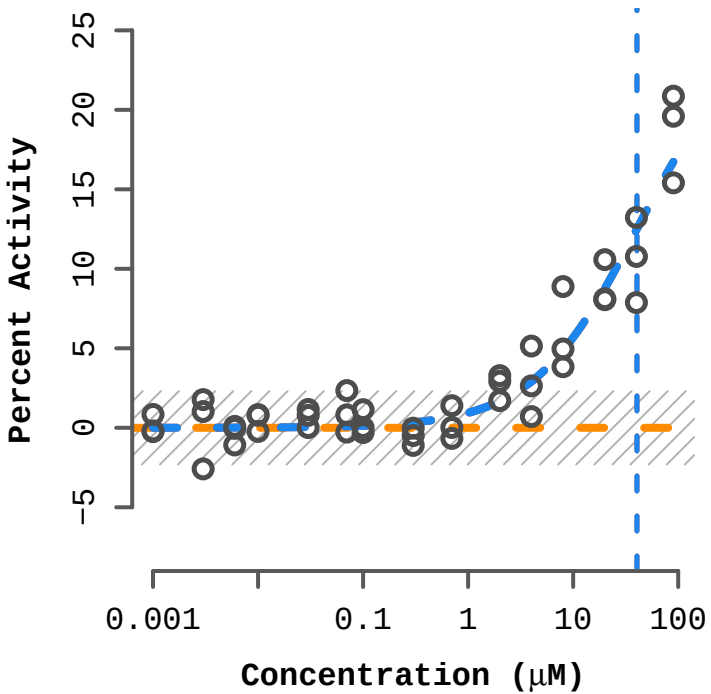
NAME: Benzyl thiocyanate
CHID: 20156 CASRN: 3012-37-1
SPID(S): Tox21_200015
M4ID: 12482237 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.83	NA	NA
PROB:	1	NA	NA
RMSE:	13.2	NA	NA

MAX_MEAN: 21.9 MAX_MED: 1.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzylhydrazine dihydrochloride
CHID: 20157 CASRN: 20570-96-1
SPID(S): Tox21_200489
M4ID: 12481763

HILL MODEL (in red):

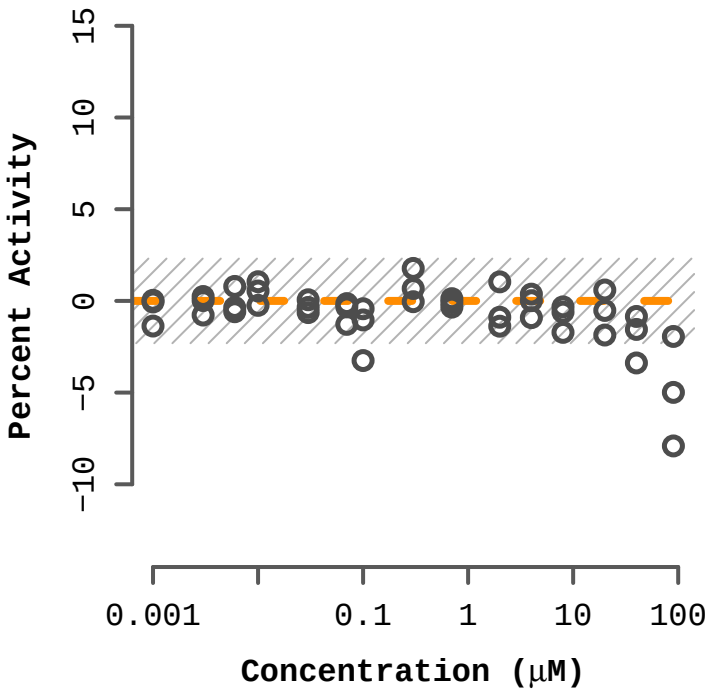
	tp	ga	gw
val:	25	1.61	0.877
sd:	6.9	0.261	0.136

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	25	1.61	0.877	3.81	4.81
sd:	6.9	0.261	0.136	2010	5240

	CNST	HILL	GNLS
AIC:	282.24	175.4	179.4
PROB:	0	0.88	0.12
RMSE:	6.42	1.6	1.6

MAX_MEAN: 18.6 MAX_MED: 19.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

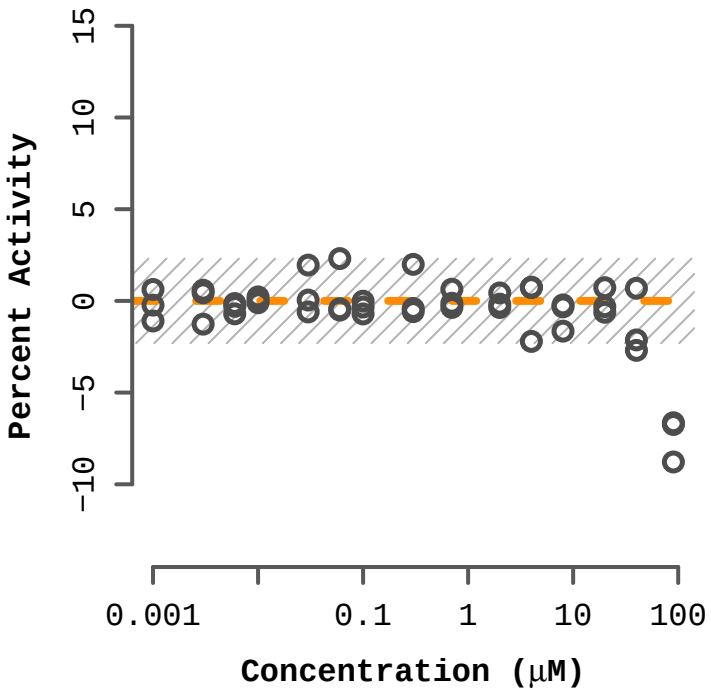
NAME: Bifenthrin
CHID: 20160 **CASRN:** 82657-04-3
SPID(S): Tox21_301064
M4ID: 12478069

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 0.803 **MAX_MED:** 0.678 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

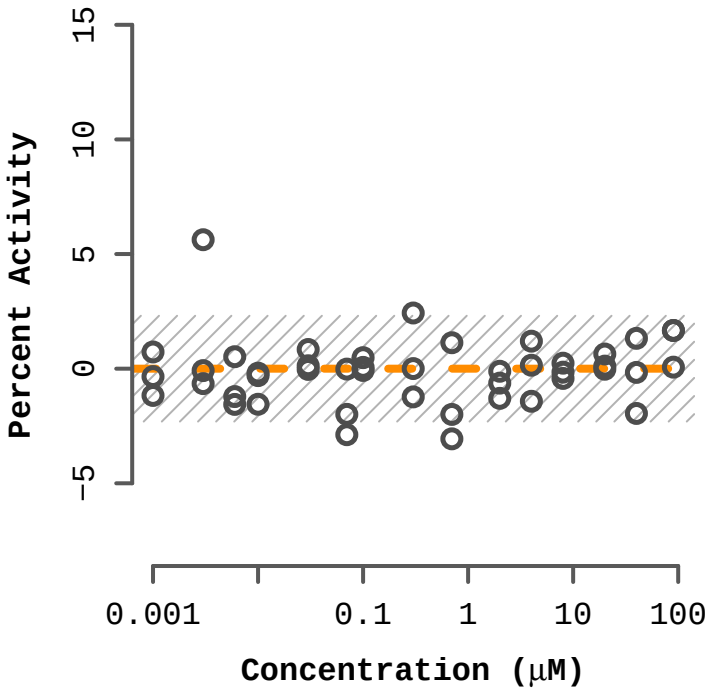
NAME: Bifenthrin
CHID: 20160 CASRN: 82657-04-3
SPID(S): Tox21_201530
M4ID: 12480722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.38	NA	NA
PROB:	1	NA	NA
RMSE:	2.16	NA	NA

MAX_MEAN: 0.468 **MAX_MED:** 0.726 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

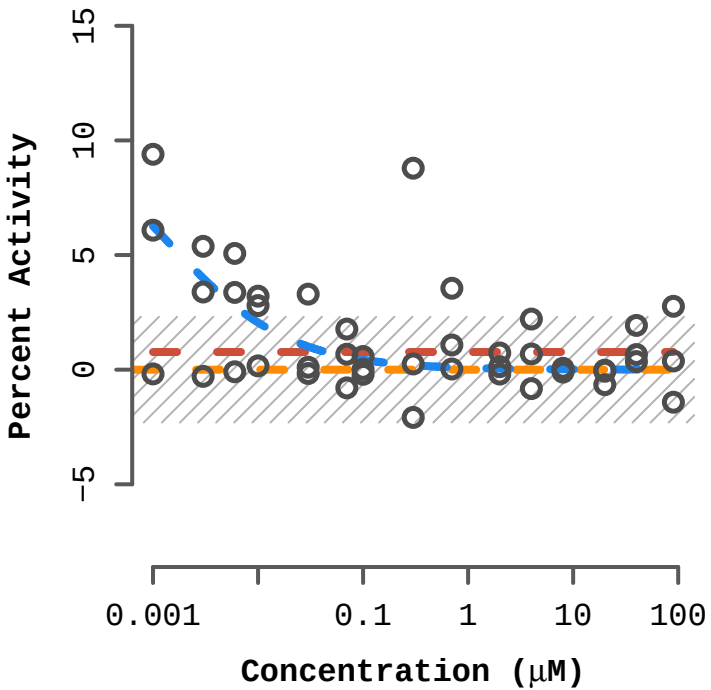
NAME: Biphenyl
CHID: 20161 CASRN: 92-52-4
SPID(S): Tox21_300167
M4ID: 12478963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.63 MAX_MED: 1.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Biphenyl
CHID: 20161 CASRN: 92-52-4
SPID(S): Tox21_202108
M4ID: 12480144

HILL MODEL (in red):

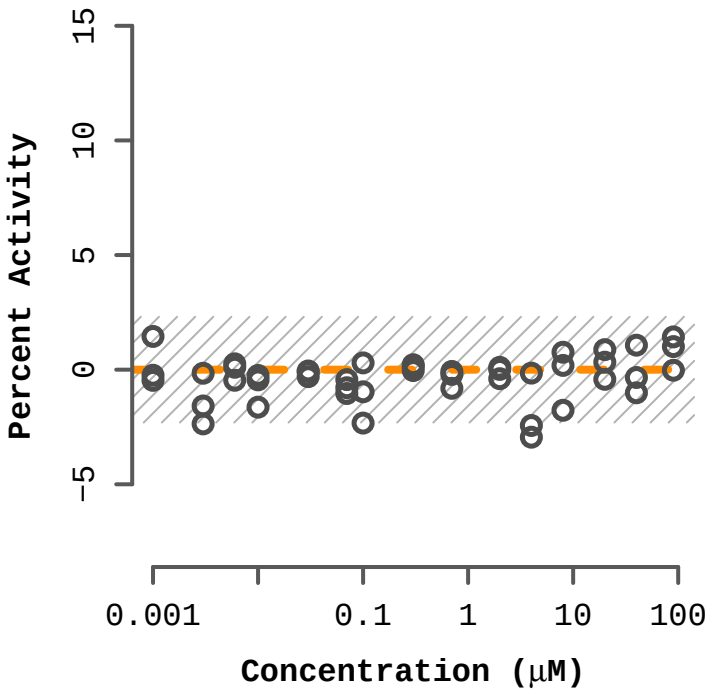
	tp	ga	gw
val:	0.77	−5	3.11
sd:	0.29	613	940

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.3	−5	4.15	−2.87	0.748
sd:	13.9	4980	10400	1.41	0.468

	CNST	HILL	GNLS
AIC:	209.67	207.92	196.72
PROB:	0	0	0.99
RMSE:	2.8	2.52	2.19

MAX_MEAN: 5.1 **MAX_MED:** 6.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

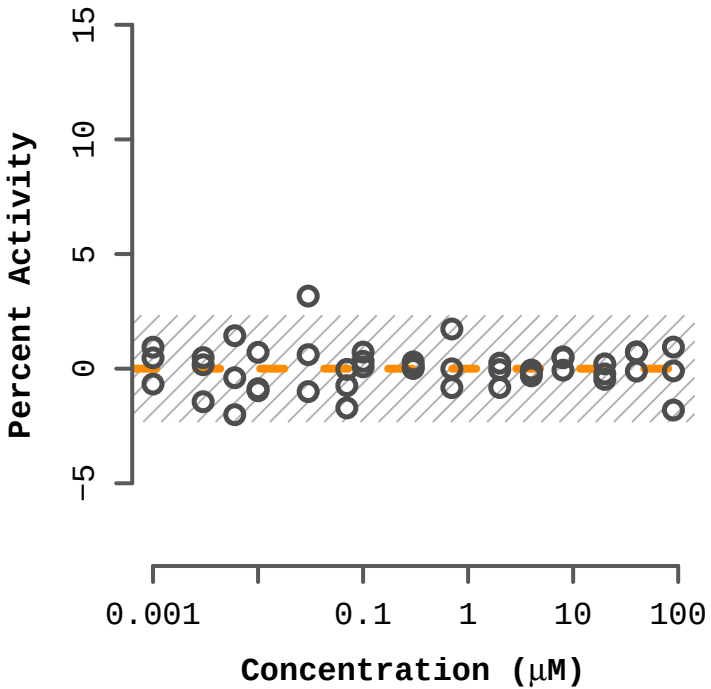
NAME: 2,2-Bis(bromomethyl)-1,3-propanediol
CHID: 20164 **CASRN:** 3296-90-0
SPID(S): Tox21_300296
M4ID: 12478834

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

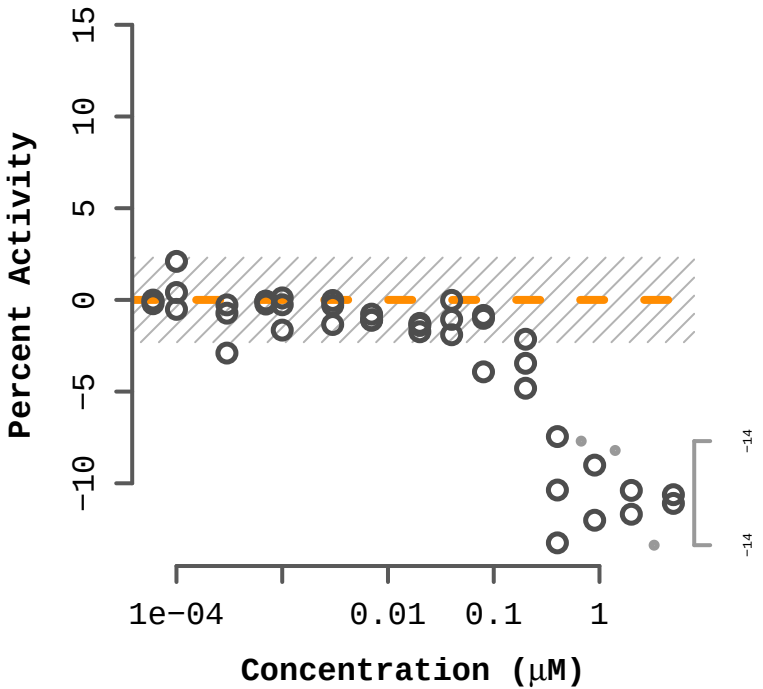
NAME: 2,2-Bis(bromomethyl)-1,3-propanediol
CHID: 20164 **CASRN:** 3296-90-0
SPID(S): Tox21_201856
M4ID: 12480396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.927 **MAX_MED:** 0.717 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

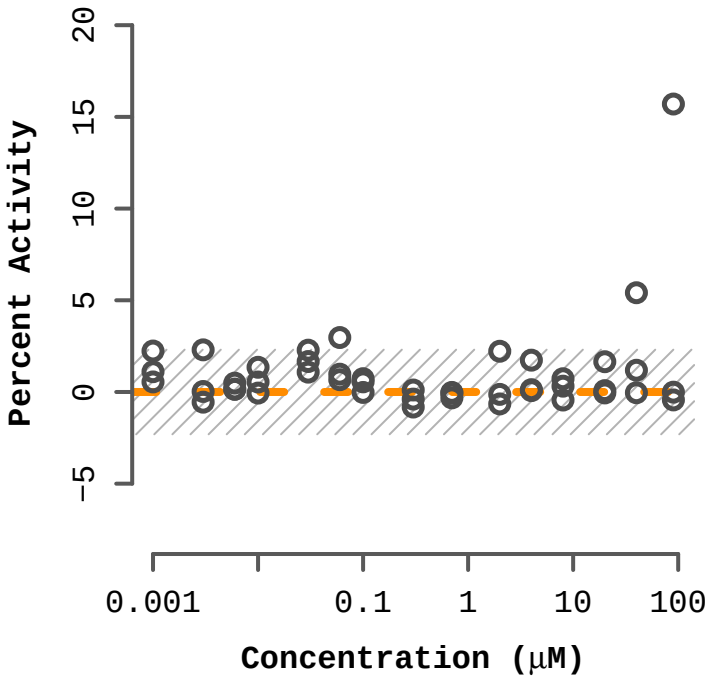
NAME: Bis(tributyltin)oxide
CHID: 20166 **CASRN:** 56-35-9
SPID(S): Tox21_203001
M4ID: 12479251 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	288.29	NA	NA
PROB:	1	NA	NA
RMSE:	6.19	NA	NA

MAX_MEAN: 0.665 **MAX_MED:** 0.406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

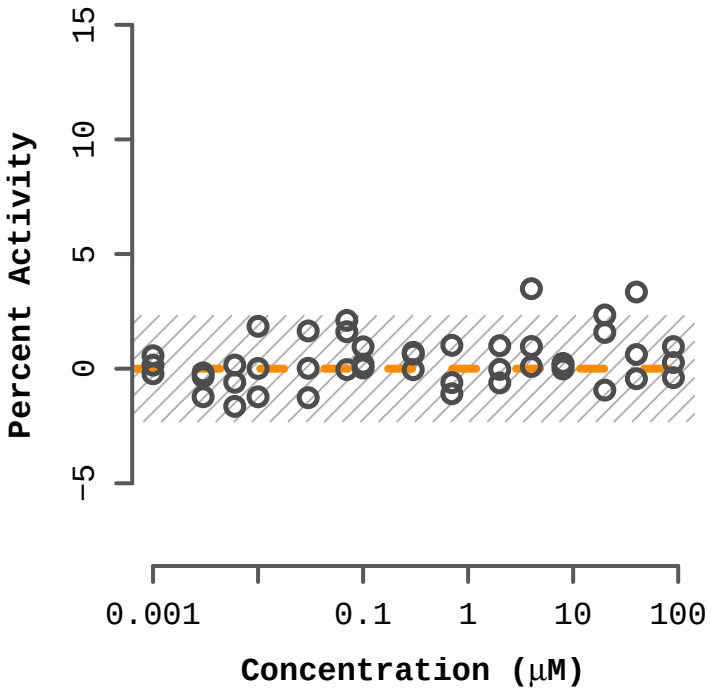
NAME: bis(2-Chloro-1-methylethyl) ether
CHID: 20167 CASRN: 108-60-1
SPID(S): Tox21_201201
M4ID: 12481051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.69	NA	NA

MAX_MEAN: 5.09 MAX_MED: 1.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

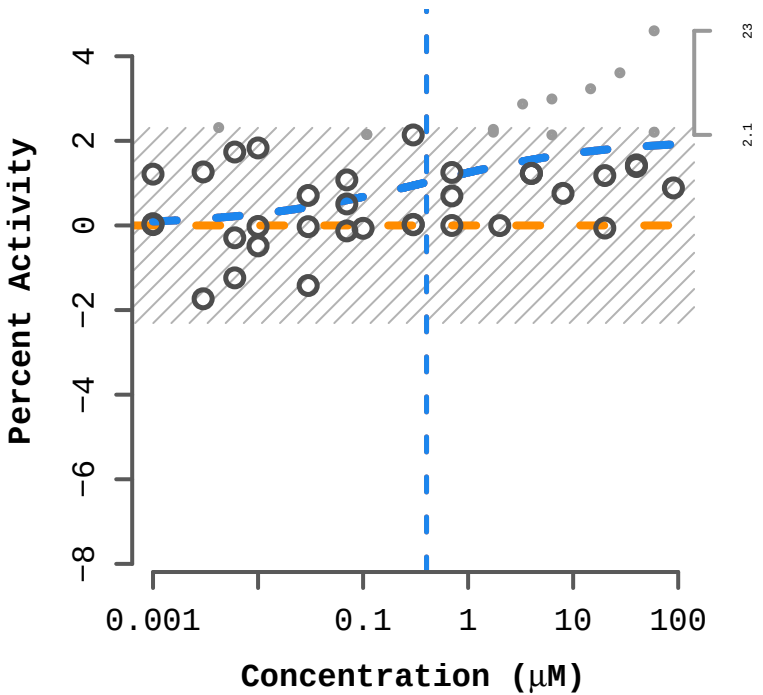
NAME: Bis(2-chloroethyl) ether
CHID: 20168 **CASRN:** 111-44-4
SPID(S): Tox21_300514
M4ID: 12478618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(2-chloroethyl) ether
CHID: 20168 CASRN: 111-44-4
SPID(S): Tox21_202074
M4ID: 12480178 BRK

HILL MODEL (in red):

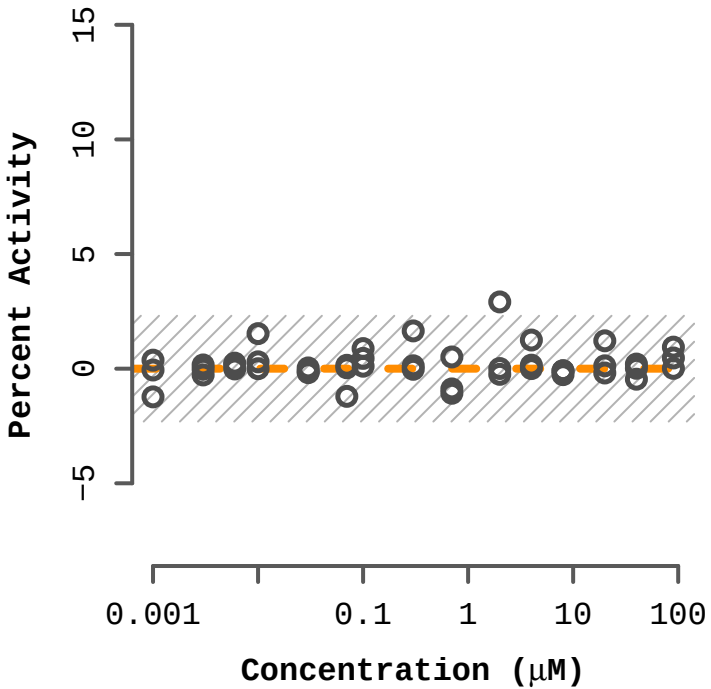
	tp	ga	gw
val:	2.04	−0.396	0.506
sd:	1.21	1.43	0.697

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.04	−0.396	0.506	2.97	7.33
sd:	1.21	1.43	0.697	1820	13200

	CNST	HILL	GNLS
AIC:	236.39	224.75	228.75
PROB:	0	0.88	0.12
RMSE:	5.06	4.45	4.45

MAX_MEAN: 9 MAX_MED: 2.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

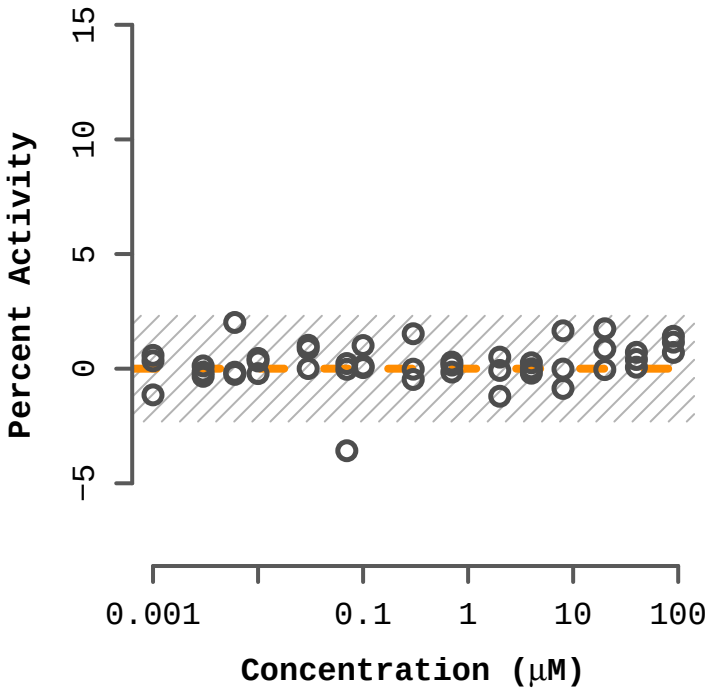
NAME: Bis(chloromethyl) ether
CHID: 20173 **CASRN:** 542-88-1
SPID(S): Tox21_200840
M4ID: 12481412

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 0.468 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

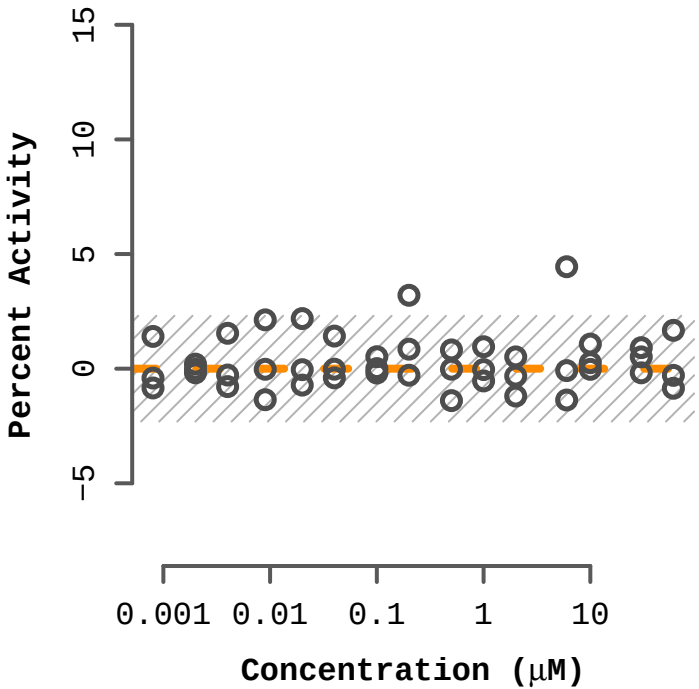
NAME: 1,4-Bis[2-(3,5-dichloropyridyloxy)]benzene
CHID: 20175 **CASRN:** 76150-91-9
SPID(S): Tox21_302870
M4ID: 12476263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

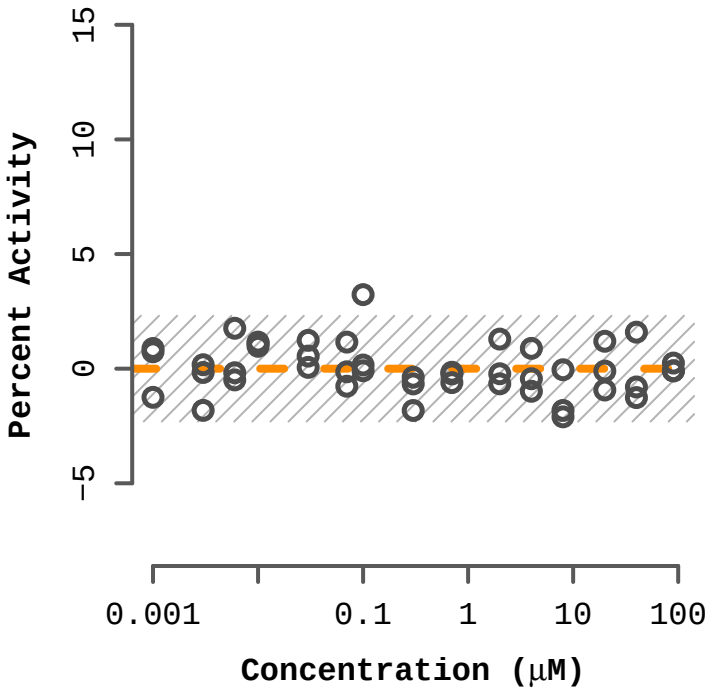
NAME: 1,4-Bis[2-(3,5-dichloropyridyloxy)]benzene
CHID: 20175 **CASRN:** 76150-91-9
SPID(S): Tox21_200168
M4ID: 12482084

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.853 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

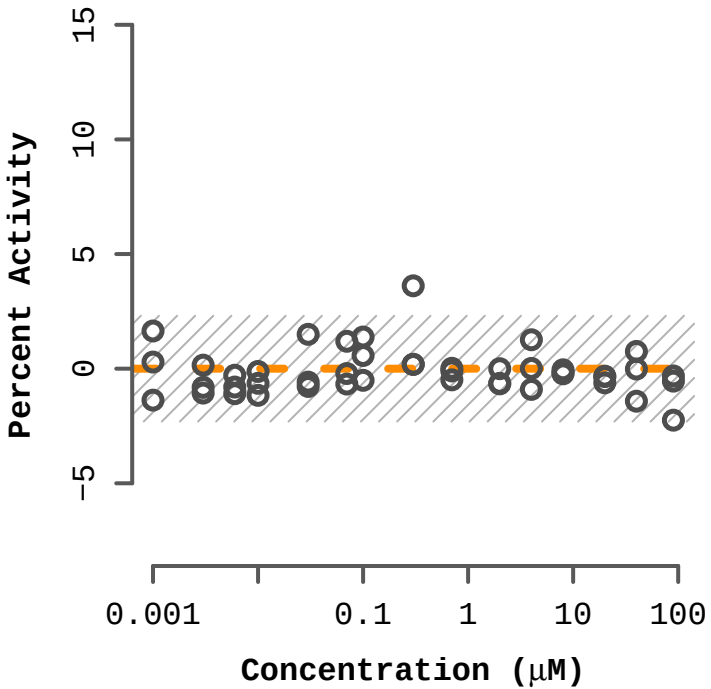
NAME: Diisopropanolamine
CHID: 20179 **CASRN:** 110-97-4
SPID(S): Tox21_302859
M4ID: 12476274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

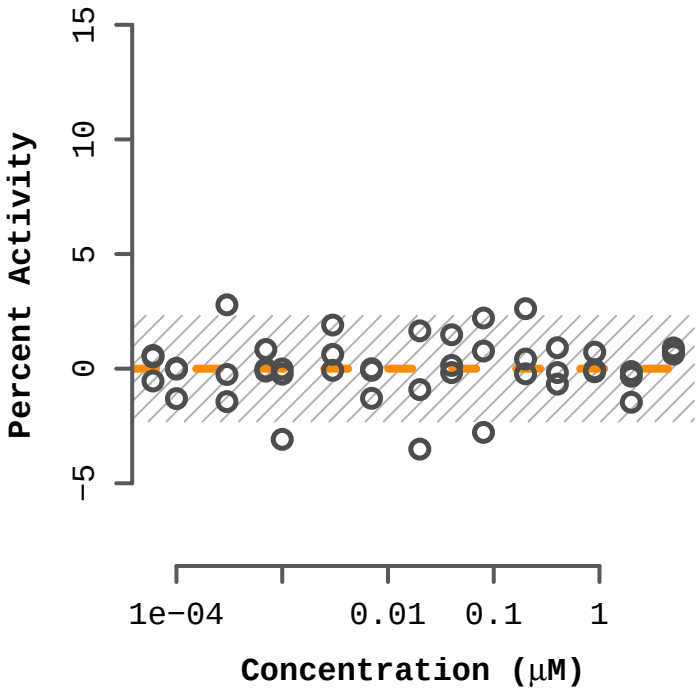
NAME: Diisopropanolamine
CHID: 20179 **CASRN:** 110-97-4
SPID(S): Tox21_201602
M4ID: 12480650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

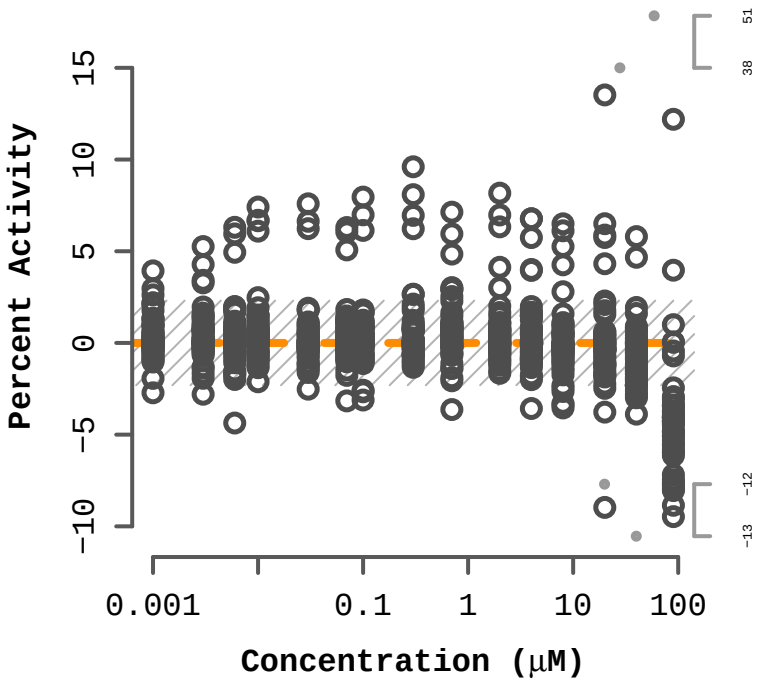
NAME: Bismuth oxychloride
CHID: 20181 **CASRN:** 7787-59-9
SPID(S): Tox21_202779
M4ID: 12479473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.94 **MAX_MED:** 0.771 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

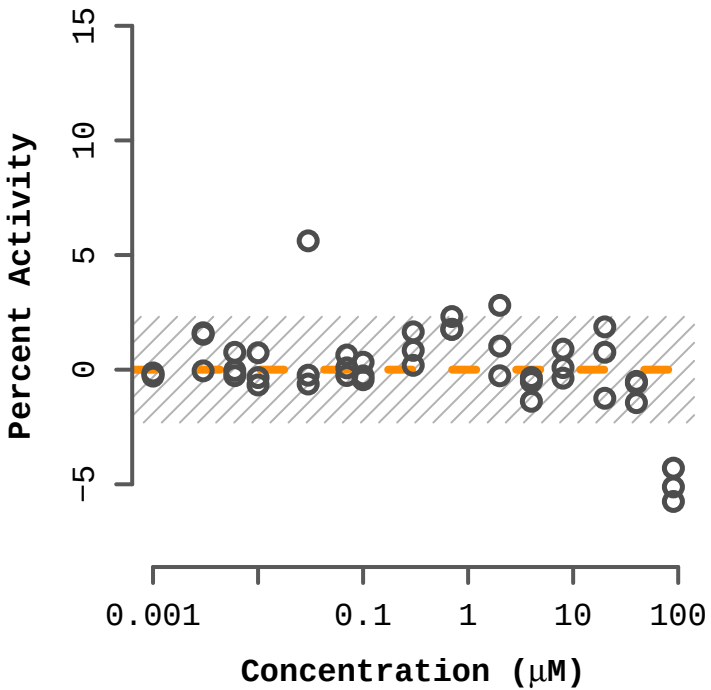
NAME: Bisphenol A
CHID: 20182 CASRN: 80-05-7
SPID(S): Tox21_400088
M4ID: 12475049 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3258.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.35	NA	NA

MAX_MEAN: 0.831 **MAX_MED:** 0.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

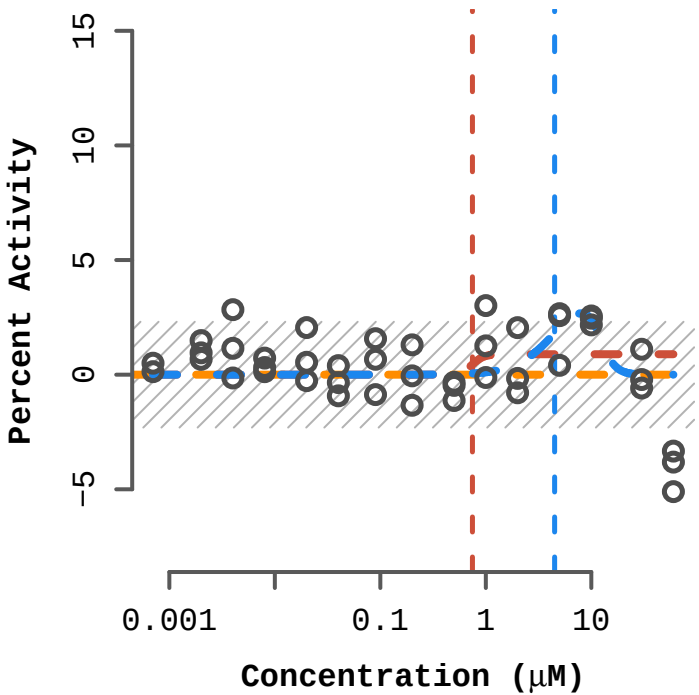
NAME: Bisphenol A
CHID: 20182 CASRN: 80-05-7
SPID(S): Tox21_202992
M4ID: 12479260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 1.95 MAX_MED: 1.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Direct Black 38
CHID: 20184 CASRN: 1937-37-7
SPID(S): Tox21_302342
M4ID: 12476791

HILL MODEL (in red):

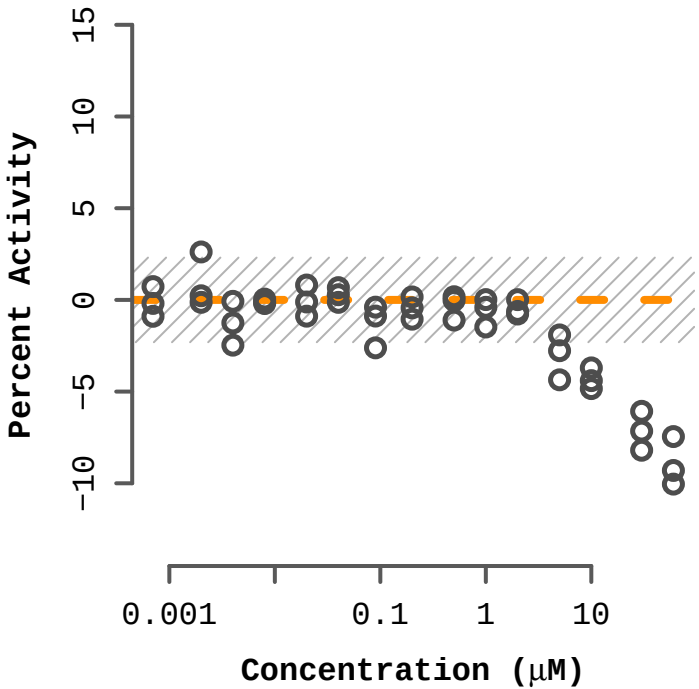
	tp	ga	gw
val:	0.892	−0.127	8
sd:	0.435	0.18	9.48

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.62	0.652	2.35	1.08	6.31
sd:	7.03	0.756	4	0.612	37.9

	CNST	HILL	GNLS
AIC:	172.73	174.72	166.1
PROB:	0.03	0.01	0.95
RMSE:	1.71	1.73	1.5

MAX_MEAN: 2.4 MAX_MED: 2.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

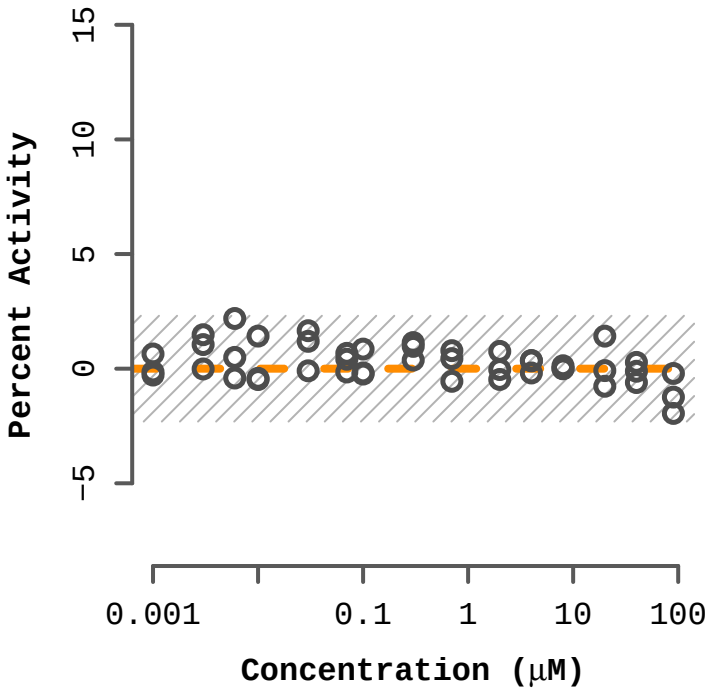
NAME: FD&C Blue No. 1
CHID: 20189 **CASRN:** 3844-45-9
SPID(S): Tox21_300516
M4ID: 12478616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.97	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 0.904 **MAX_MED:** 0.284 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

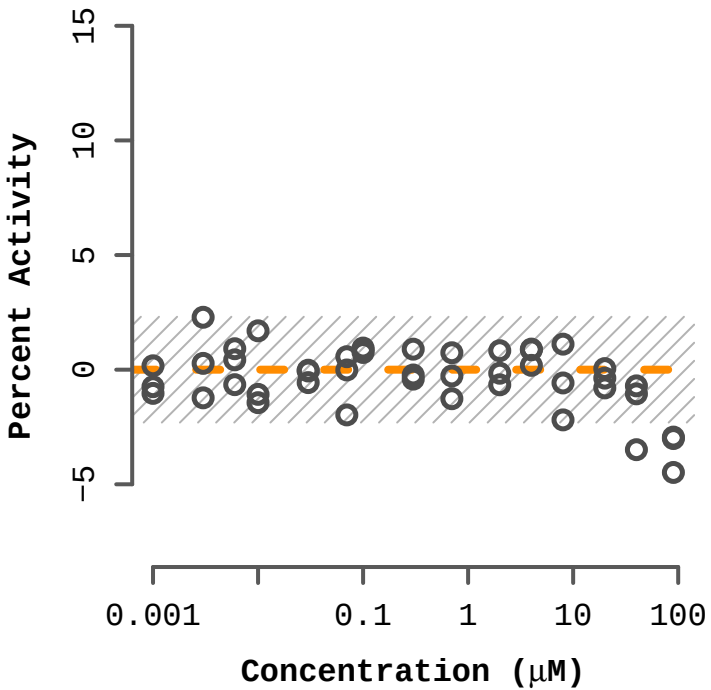
NAME: C.I. Acid Blue 74
CHID: 20190 **CASRN:** 860-22-0
SPID(S): Tox21_302732
M4ID: 12476401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.92 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

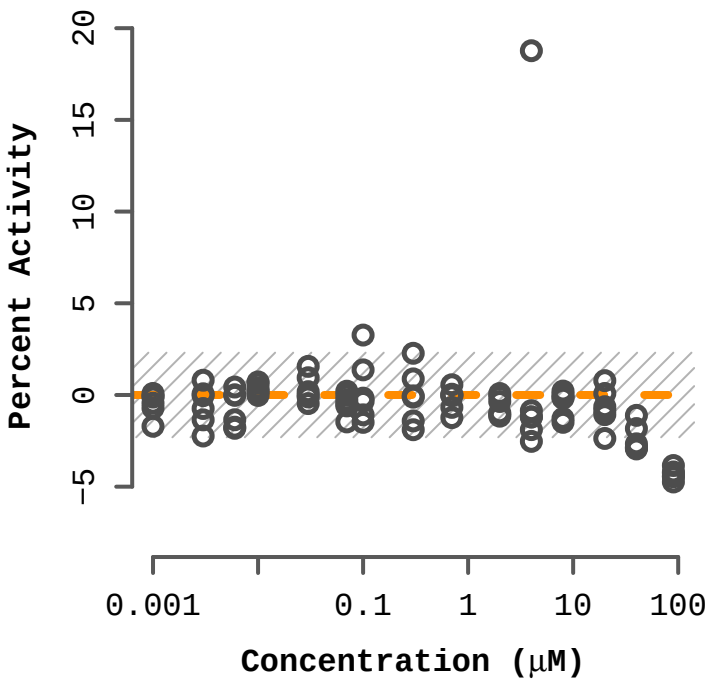
NAME: HC Blue 2
CHID: 20193 CASRN: 33229-34-4
SPID(S): Tox21_302947
M4ID: 12476186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.853 MAX_MED: 0.869 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

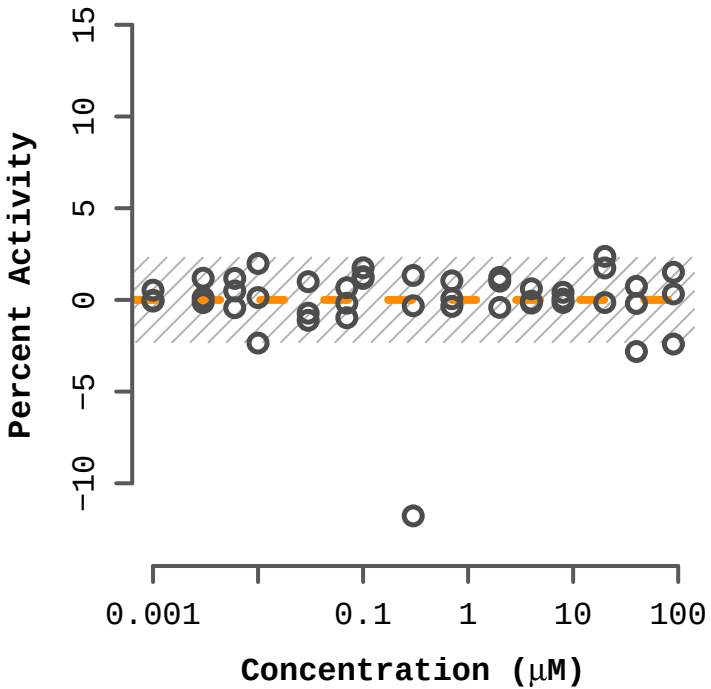
NAME: HC Blue 2
CHID: 20193 CASRN: 33229-34-4
SPID(S): Tox21_202257
M4ID: 12479995

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	355.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.56	NA	NA

MAX_MEAN: 1.85 MAX_MED: 0.302 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

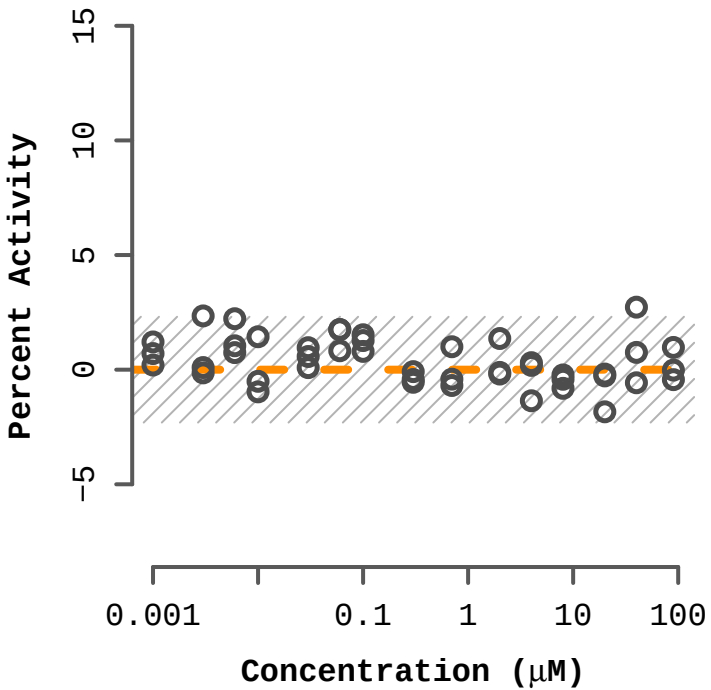
NAME: Boric acid
CHID: 20194 **CASRN:** 10043-35-3
SPID(S): Tox21_301000
M4ID: 12478133

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

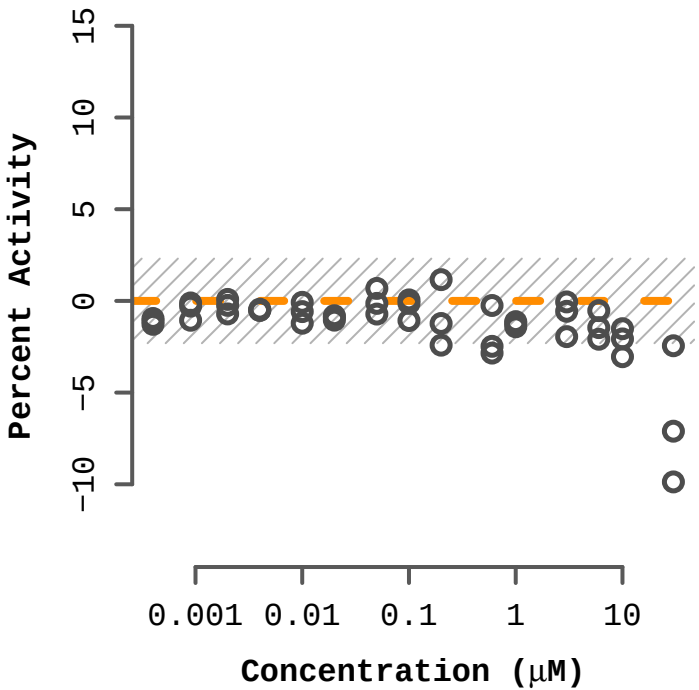
NAME: Boric acid
CHID: 20194 CASRN: 10043-35-3
SPID(S): Tox21_202185
M4ID: 12480067

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.44 MAX_MED: 1.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

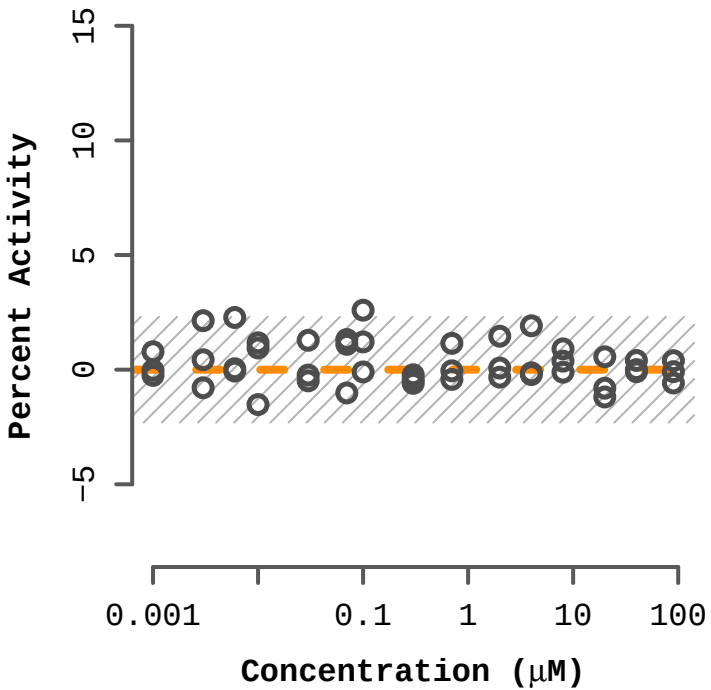
NAME: Bromocriptine mesylate
CHID: 20197 **CASRN:** 22260-51-1
SPID(S): Tox21_303597
M4ID: 12475548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: −0.0558 **MAX_MED:** −0.133 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

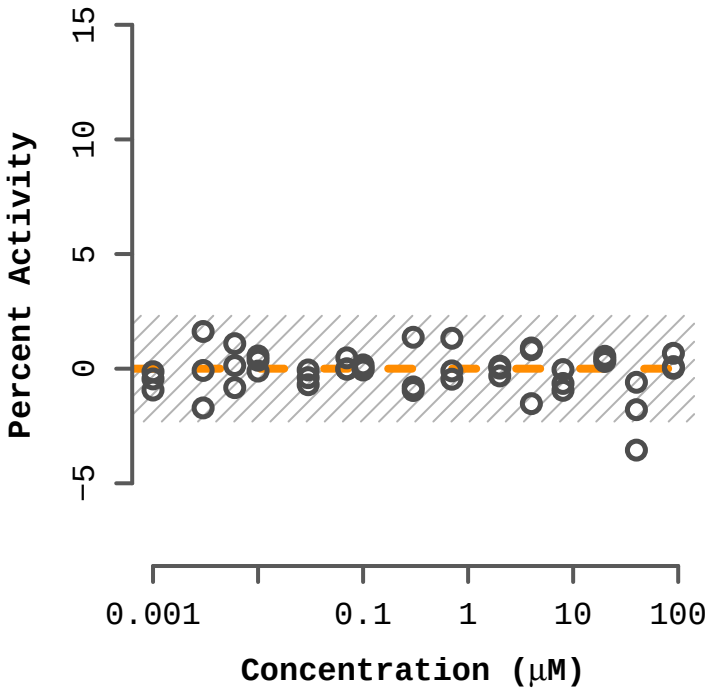
NAME: Bromodichloromethane
CHID: 20198 CASRN: 75-27-4
SPID(S): Tox21_200806
M4ID: 12481446

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

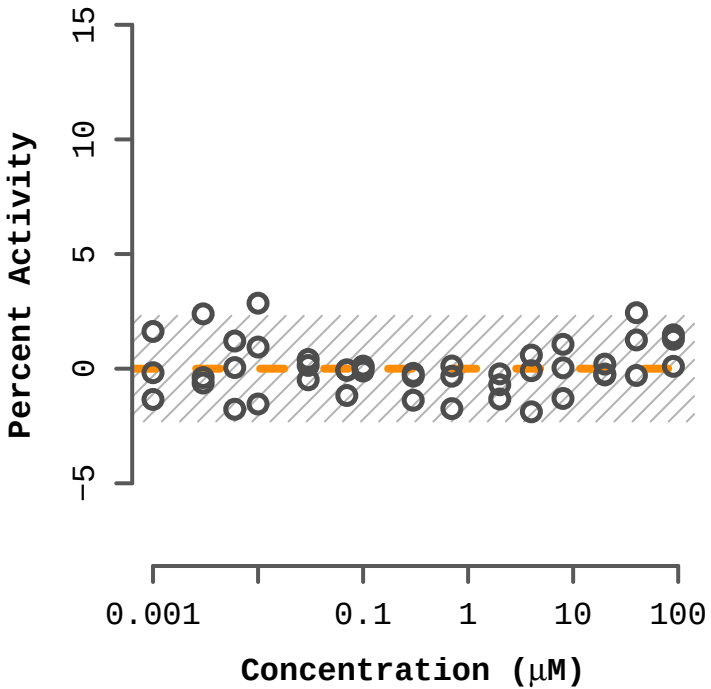
NAME: Bromoethane
CHID: 20199 **CASRN:** 74-96-4
SPID(S): Tox21_200355
M4ID: 12481897

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.424 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

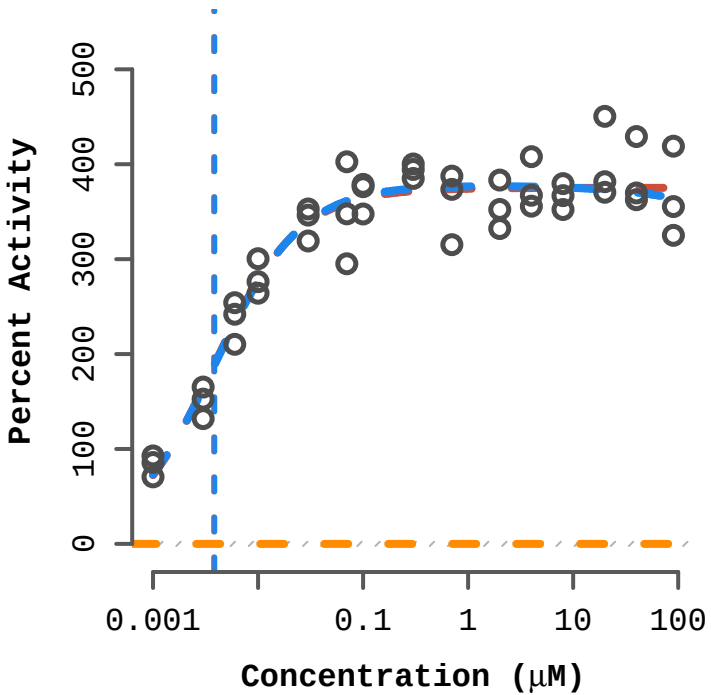
NAME: 2-Bromo-1-ethanol
CHID: 20200 **CASRN:** 540-51-2
SPID(S): Tox21_201036
M4ID: 12481216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Budesonide
CHID: 20202 CASRN: 51333-22-3
SPID(S): Tox21_302815
M4ID: 12476318

HILL MODEL (in red):

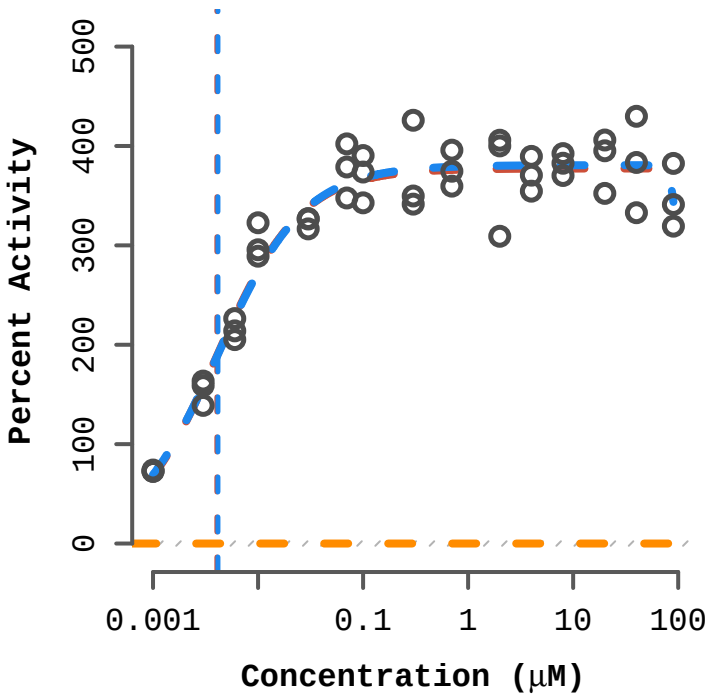
	tp	ga	gw
val:	375	-2.42	1.07
sd:	5.23	0.0376	0.101

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	378	-2.41	1.06	3.95	0.708
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	662.57	433.75	437.27
PROB:	0	0.85	0.15
RMSE:	334.23	27.58	27.88

MAX_MEAN: 401 MAX_MED: 395 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Budesonide
CHID: 20202 CASRN: 51333-22-3
SPID(S): Tox21_201827
M4ID: 12480425

HILL MODEL (in red):

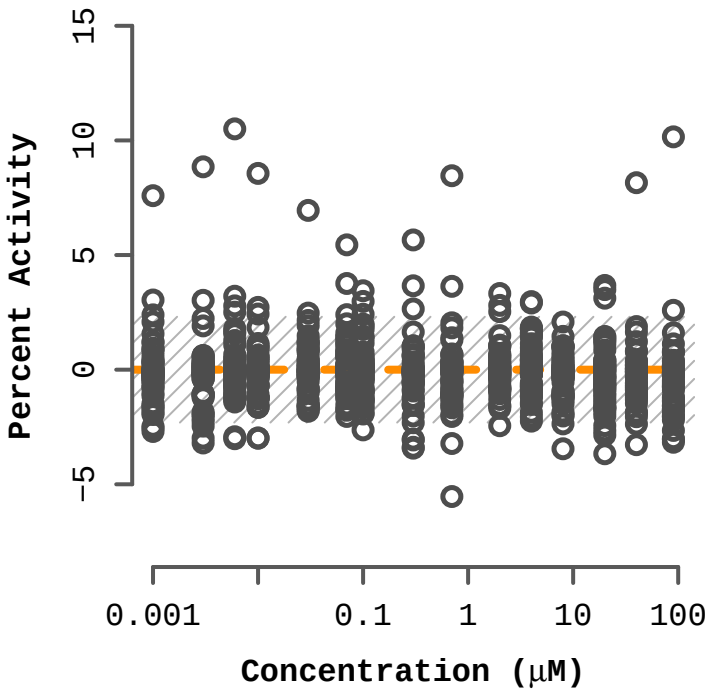
	tp	ga	gw
val:	377	-2.39	1.08
sd:	5.54	0.0362	0.104

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	381	-2.38	1.05	2.04	11.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	662.54	432.41	432.48
PROB:	0	0.51	0.49
RMSE:	334.13	26.52	25.43

MAX_MEAN: 385 MAX_MED: 400 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

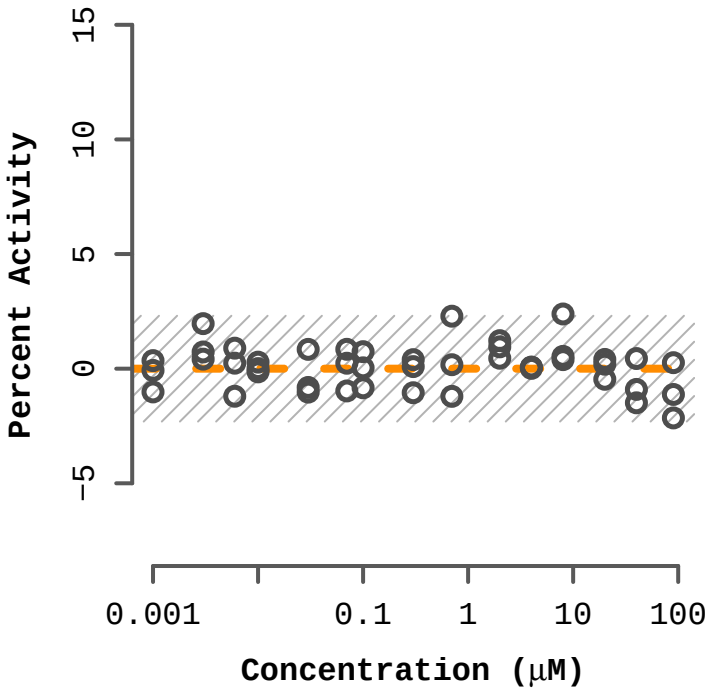
NAME: Benzyl butyl phthalate
CHID: 20205 CASRN: 85-68-7
SPID(S): Tox21_400057
M4ID: 12475080

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2538.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.176 **MAX_MED:** 0.134 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

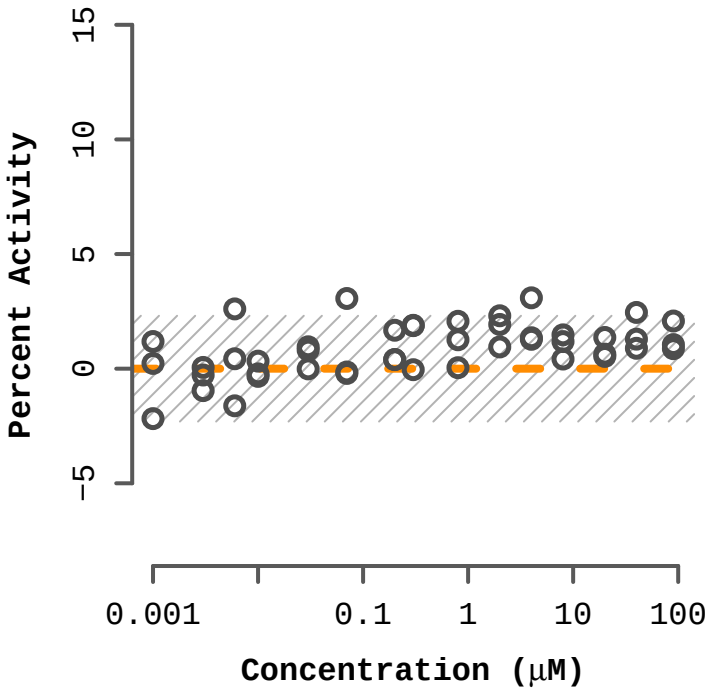
NAME: Benzyl butyl phthalate
CHID: 20205 CASRN: 85-68-7
SPID(S): Tox21_202991
M4ID: 12479261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.954 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

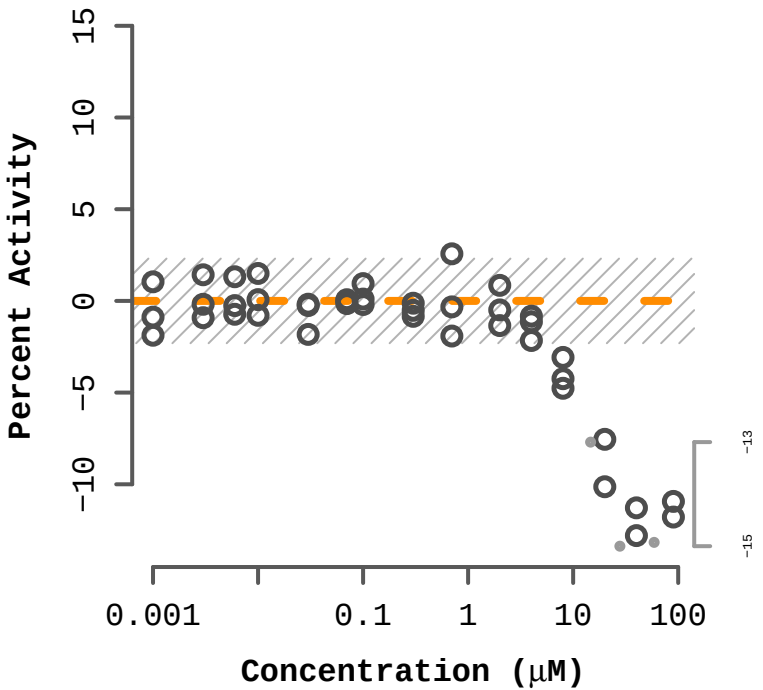
NAME: 1-Chlorobutane
CHID: 20206 **CASRN:** 109-69-3
SPID(S): Tox21_200865
M4ID: 12481387

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

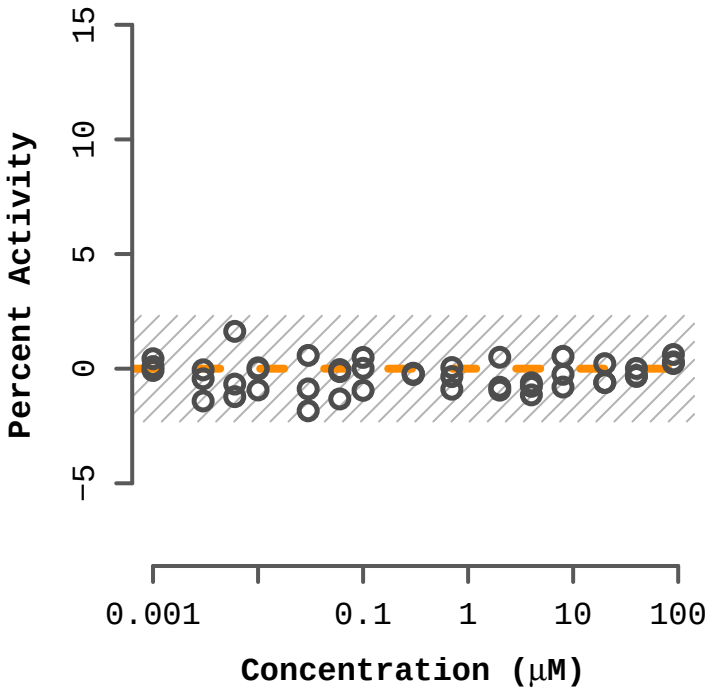
NAME: Dinoseb
CHID: 20207 CASRN: 88-85-7
SPID(S): Tox21_300421
M4ID: 12478711 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.98	NA	NA
PROB:	1	NA	NA
RMSE:	5.58	NA	NA

MAX_MEAN: 0.284 **MAX_MED:** 0.101 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

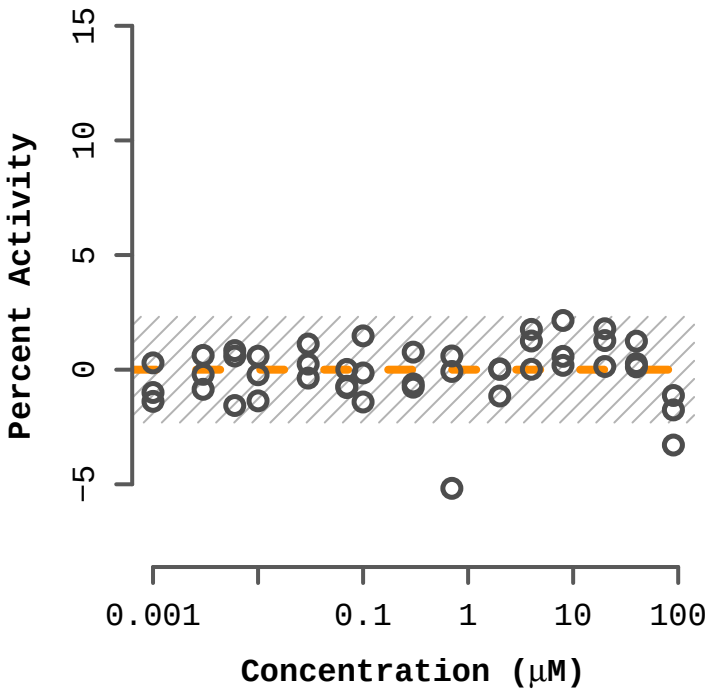
NAME: Dinoseb
CHID: 20207 CASRN: 88-85-7
SPID(S): Tox21_201878
M4ID: 12480374

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.381 **MAX_MED:** 0.298 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

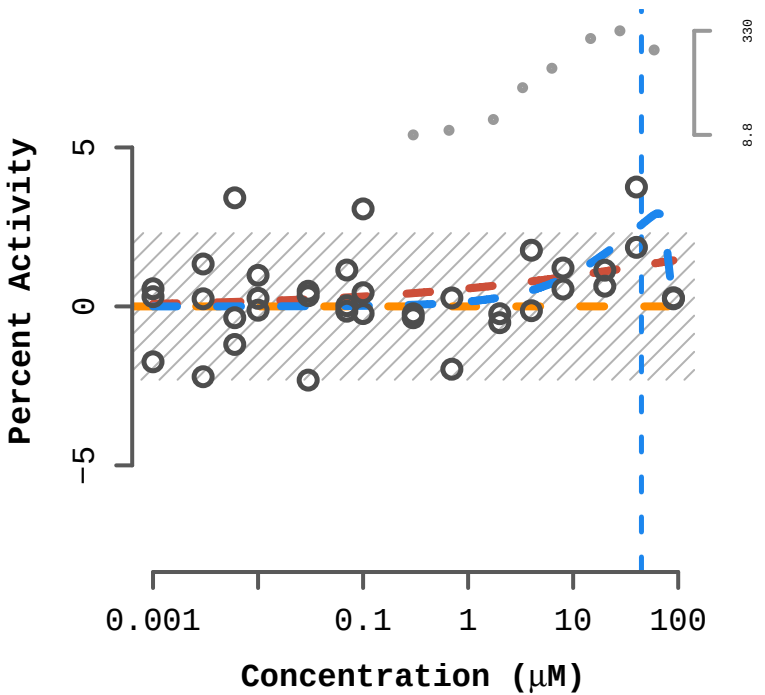
NAME: Butylparaben
CHID: 20209 **CASRN:** 94-26-8
SPID(S): Tox21_300332
M4ID: 12478800

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butylparaben
CHID: 20209 CASRN: 94-26-8
SPID(S): Tox21_201785
M4ID: 12480467 BRK

HILL MODEL (in red):

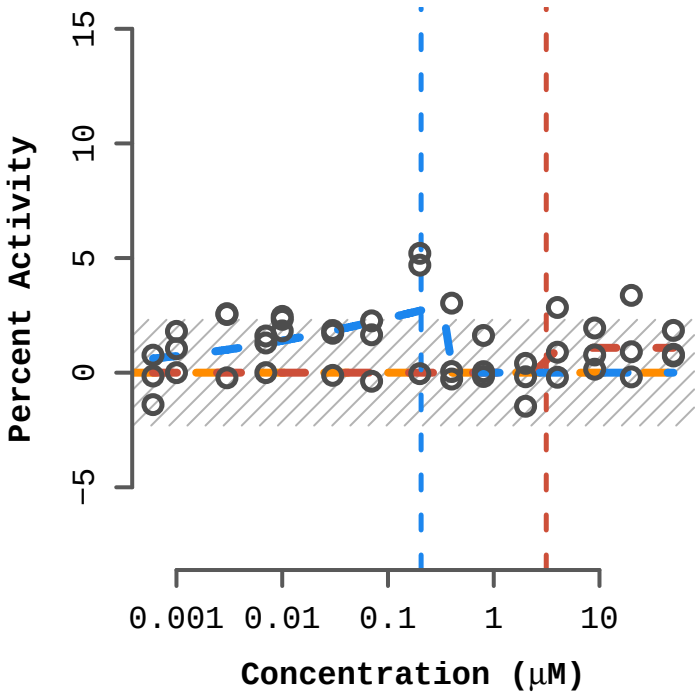
	tp	ga	gw
val:	3.2	2.22	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

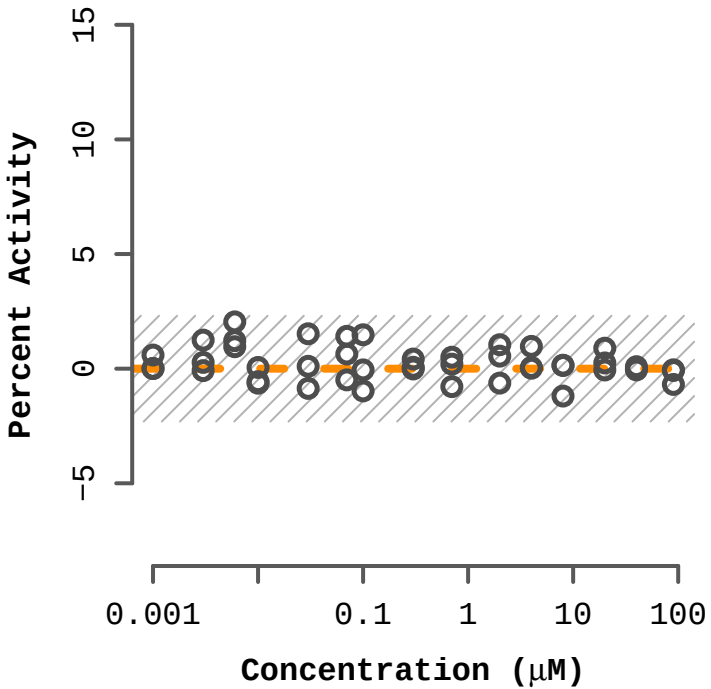
	tp	ga	gw	la	lw
val:	5.14	1.65	0.918	1.9	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	424.85	429.03	432.39
PROB:	0.87	0.11	0.02
RMSE:	87.2	86.82	86.77

MAX_MEAN: 111 **MAX_MED:** 3.76 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Butylparaben
CHID:    20209   CASRN: 94-26-8
SPID(S): Tox21_110393_1
M4ID:    12484398

HILL MODEL (in red):
      tp       ga       gw
val:  1.08     0.497    8
sd:   0.431    0.244    13.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.43     -0.687   0.352    -0.437   18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  182.51      182.06      171.67
PROB: 0           0.01        0.99
RMSE: 1.81        1.71        1.4

MAX_MEAN: 3.29      MAX_MED: 4.69      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

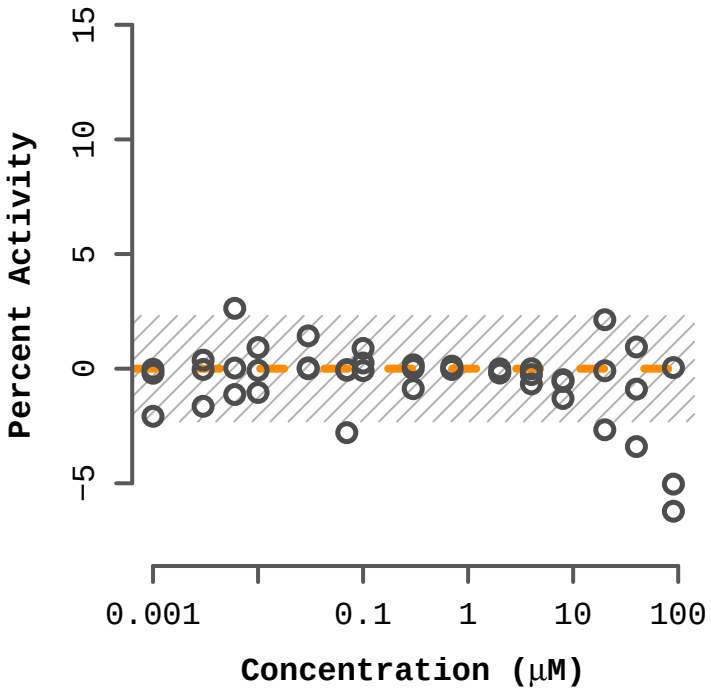
NAME: Butyl−N−(4−hydroxybutyl)nitrosamine
CHID: 20210 **CASRN:** 3817−11−6
SPID(S): Tox21_301263
M4ID: 12477870

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

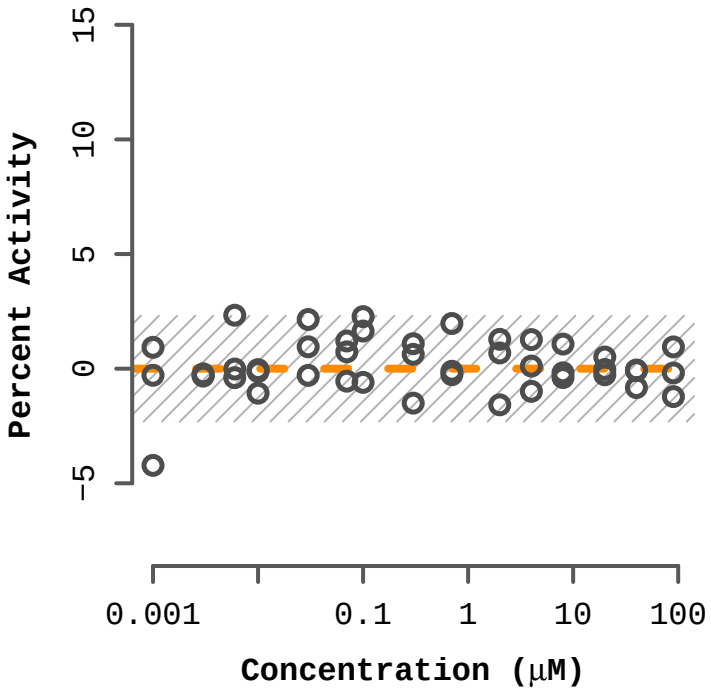
NAME: di-tert-Butyl-4-hydroxymethyl phenol
CHID: 20211 CASRN: 88-26-6
SPID(S): Tox21_200631
M4ID: 12481621

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 0.512 MAX_MED: 0.248 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

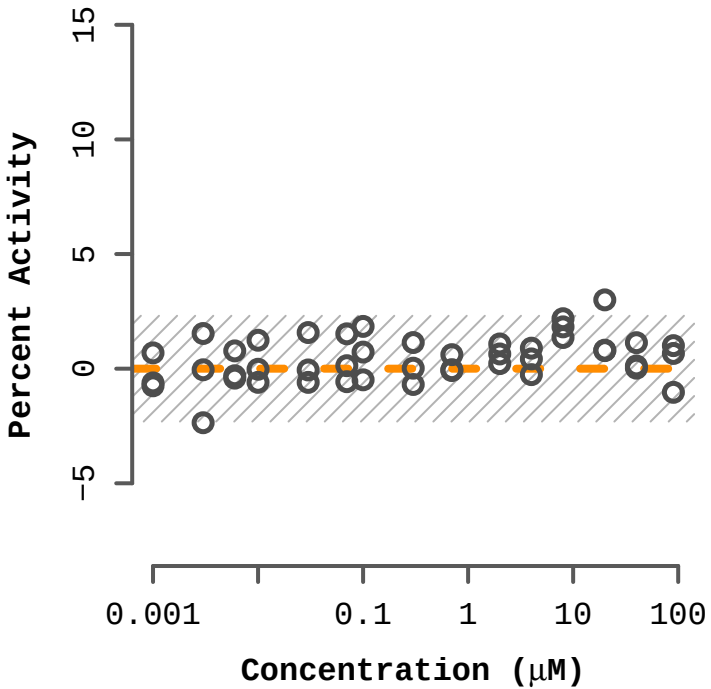
NAME: 2-tert-Butyl-4-methylphenol
CHID: 20212 **CASRN:** 2409-55-4
SPID(S): Tox21_303003
M4ID: 12476130

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

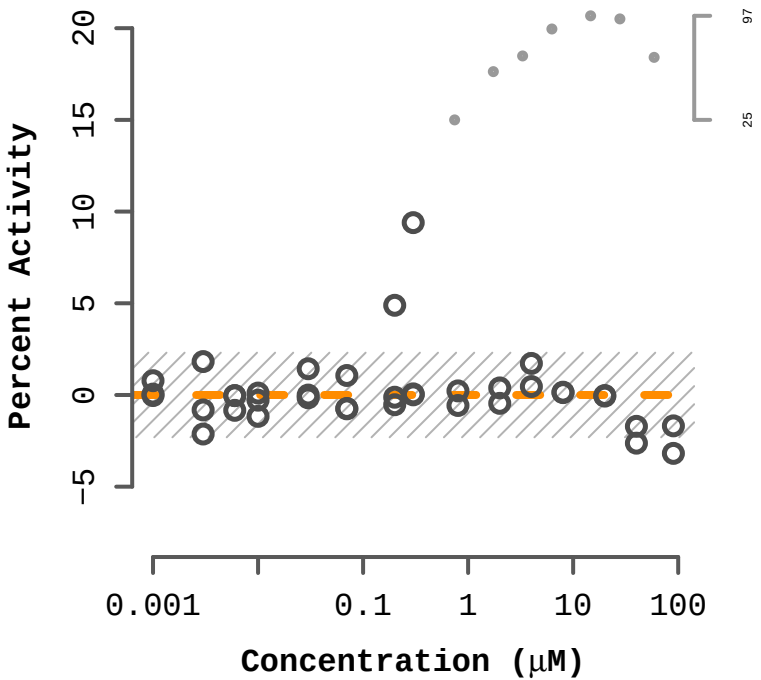
NAME: 2-tert-Butyl-4-methylphenol
CHID: 20212 **CASRN:** 2409-55-4
SPID(S): Tox21_201938
M4ID: 12480314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

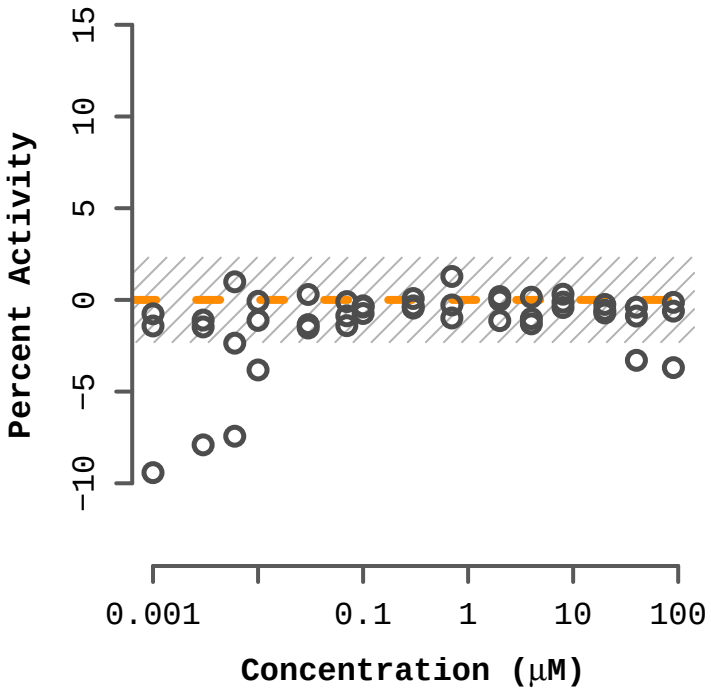
NAME: N-Butyl-N'-nitro-N-nitrosoguanidine
CHID: 20213 CASRN: 13010-08-7
SPID(S): Tox21_201172
M4ID: 12481080 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	371.91	NA	NA
PROB:	1	NA	NA
RMSE:	29.62	NA	NA

MAX_MEAN: 32.1 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

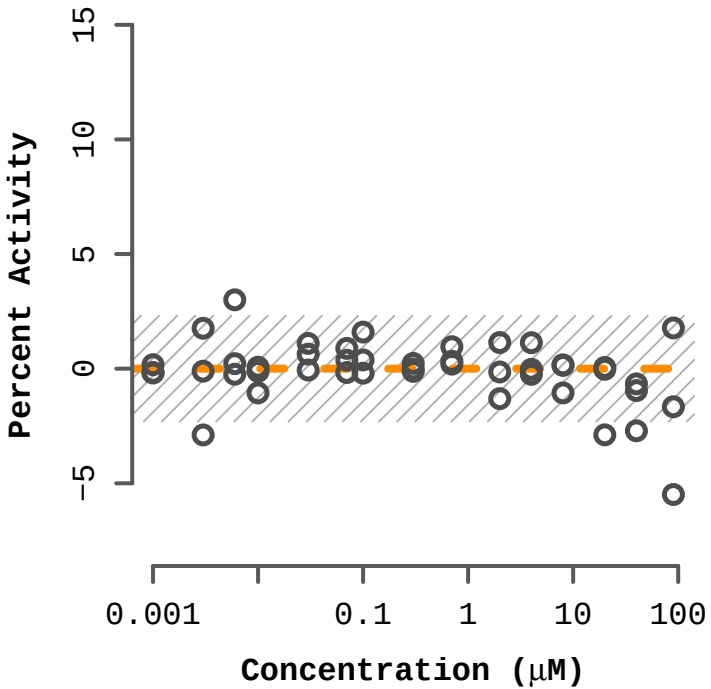
NAME: Butylated hydroxyanisole
CHID: 20215 **CASRN:** 25013-16-5
SPID(S): Tox21_201822
M4ID: 12480430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.48	NA	NA

MAX_MEAN: 0.00741 **MAX_MED:** −0.00732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

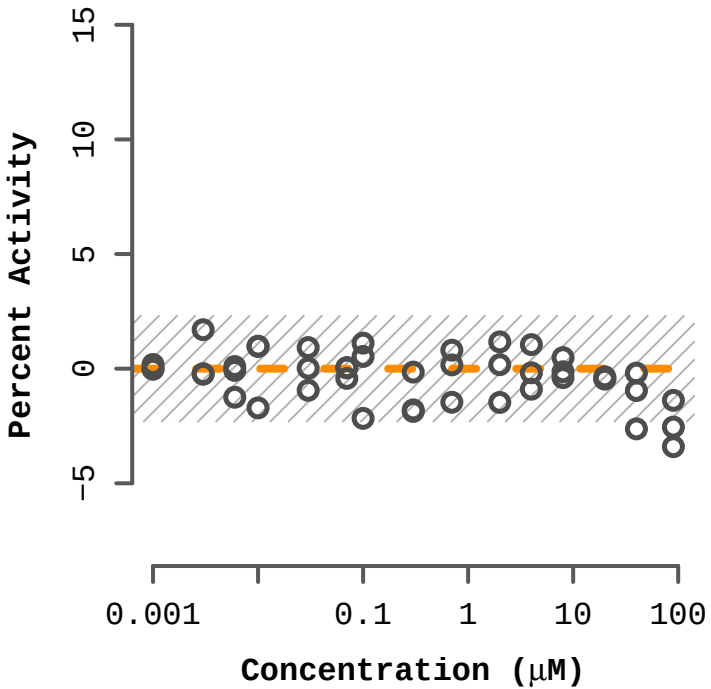
NAME: Butylated hydroxytoluene
CHID: 20216 **CASRN:** 128-37-0
SPID(S): Tox21_303408
M4ID: 12475731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.995 **MAX_MED:** 0.636 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

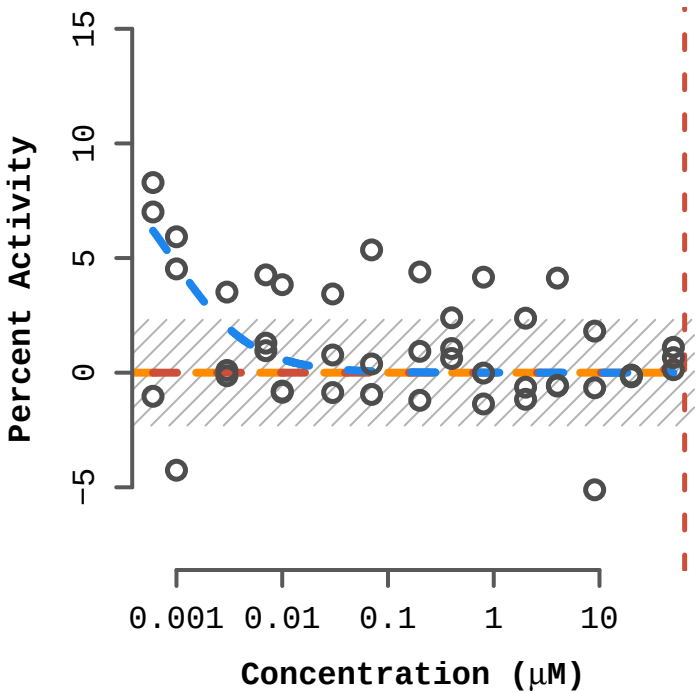
NAME: Butylated hydroxytoluene
CHID: 20216 **CASRN:** 128-37-0
SPID(S): Tox21_201093
M4ID: 12481159

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.415 **MAX_MED:** 0.974 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butylated hydroxytoluene
CHID: 20216 CASRN: 128-37-0
SPID(S): Tox21_113537_1
M4ID: 12482617

HILL MODEL (in red):

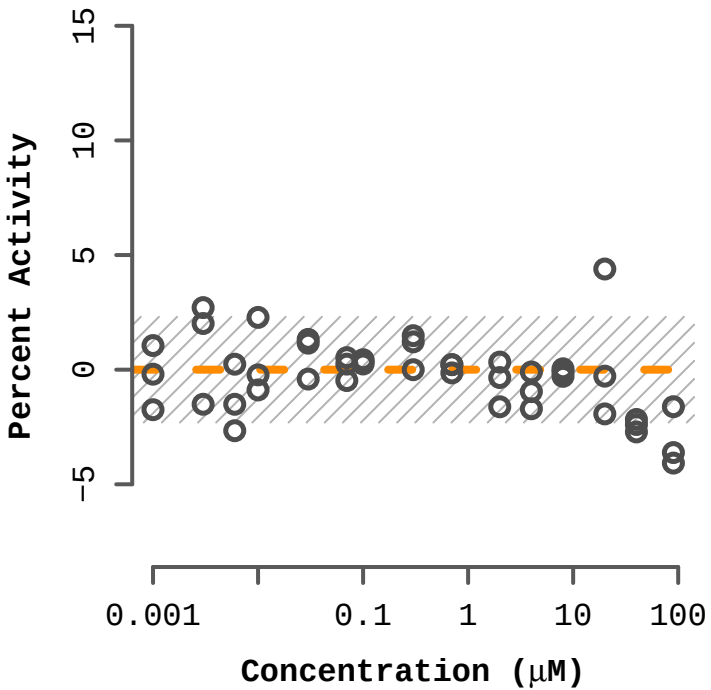
	tp	ga	gw
val:	5.12	1.81	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.95	−3.92	8	−3.04	1.16
sd:	6.79	60.8	698	0.529	0.857

	CNST	HILL	GNLS
AIC:	224.64	230.33	221.39
PROB:	0.16	0.01	0.83
RMSE:	2.94	2.94	2.68

MAX_MEAN: 4.76 **MAX_MED:** 7.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

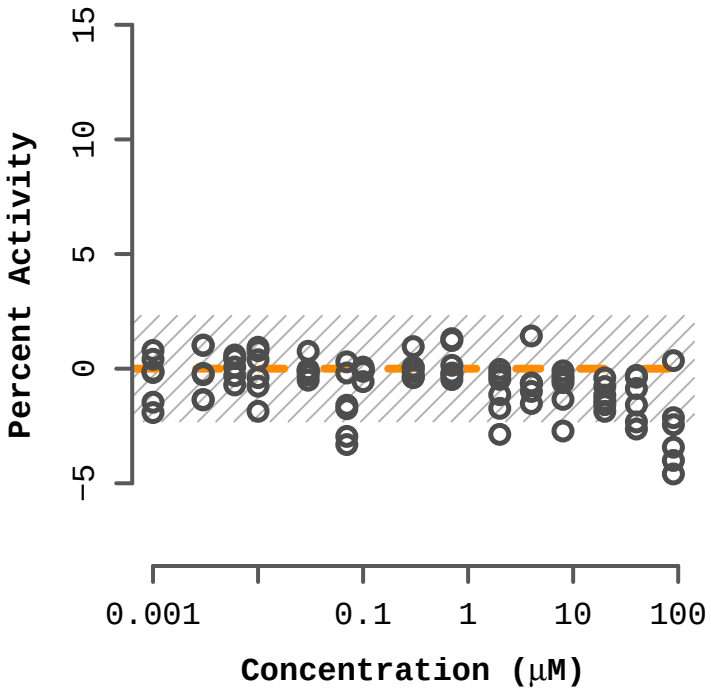
NAME: tert-Butylhydroquinone
CHID: 20220 **CASRN:** 1948-33-0
SPID(S): Tox21_300081
M4ID: 12479049

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

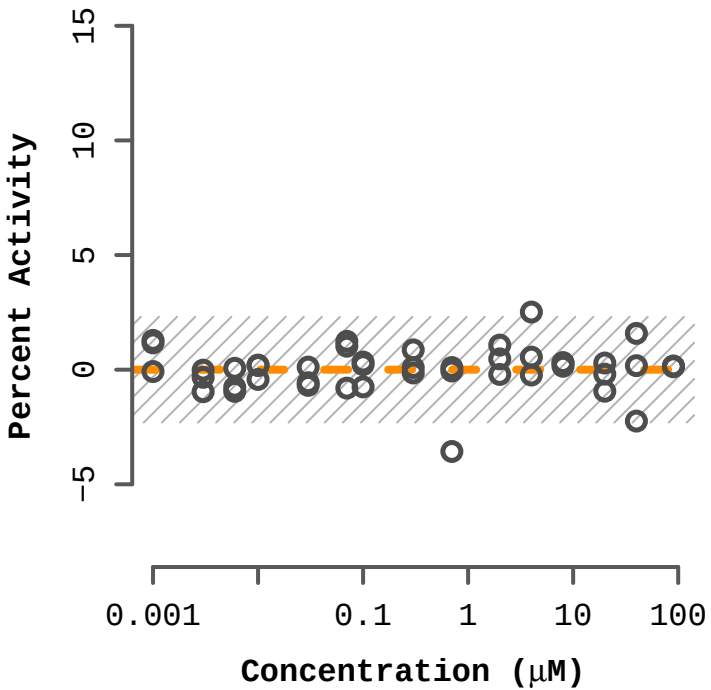
NAME: tert-Butylhydroquinone
CHID: 20220 CASRN: 1948-33-0
SPID(S): Tox21_202309
M4ID: 12479943

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.292 MAX_MED: 0.257 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

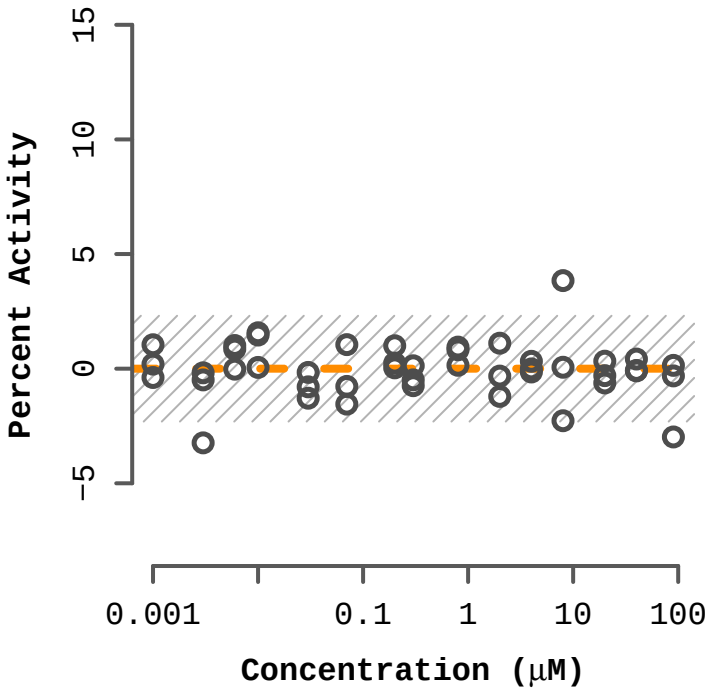
NAME: 4-tert-Butylphenol
CHID: 20221 CASRN: 98-54-4
SPID(S): Tox21_300103
M4ID: 12479027

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.944 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

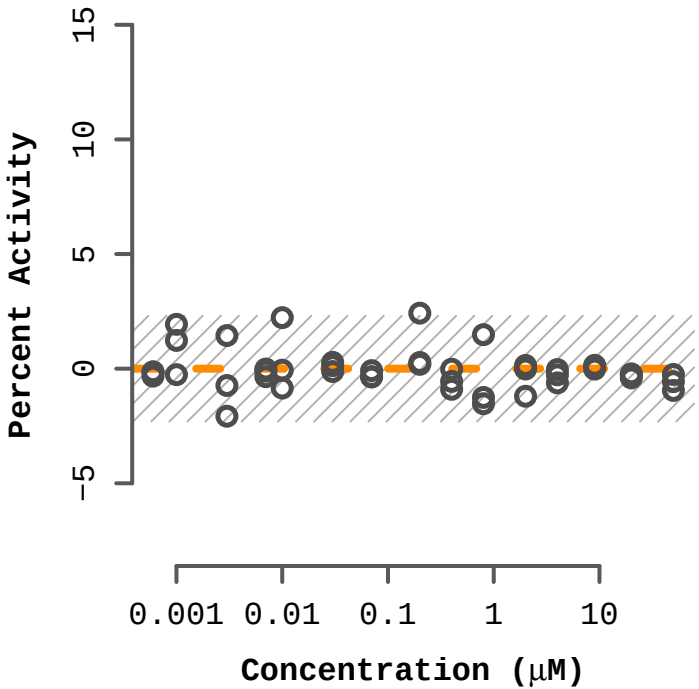
NAME: 4-tert-Butylphenol
CHID: 20221 **CASRN:** 98-54-4
SPID(S): Tox21_202326
M4ID: 12479926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

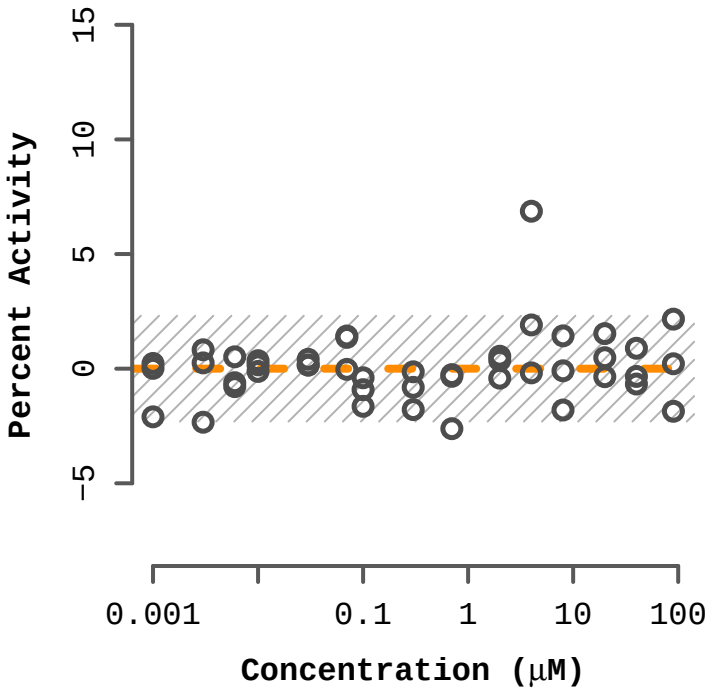
NAME: 4-tert-Butylphenol
CHID: 20221 CASRN: 98-54-4
SPID(S): Tox21_111617_1
M4ID: 12483583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.97 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

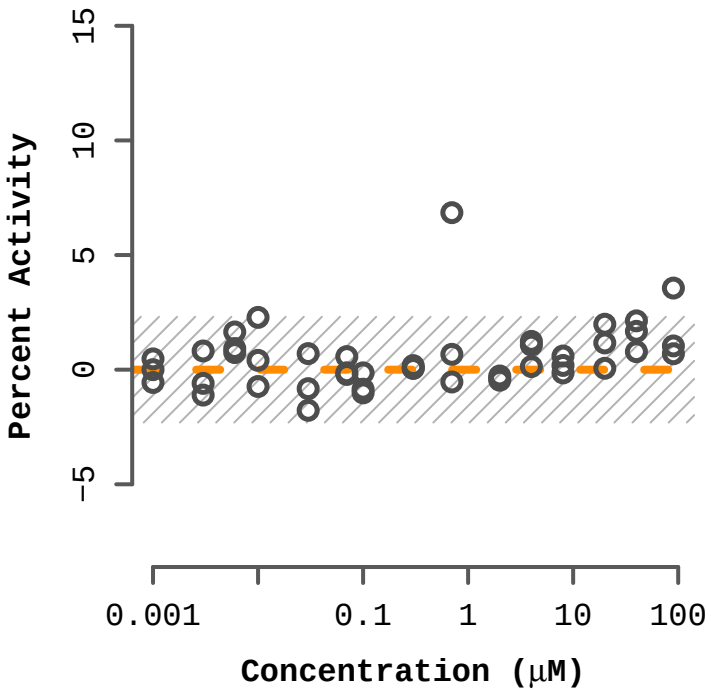
NAME: N-Butylurea
CHID: 20222 CASRN: 592-31-4
SPID(S): Tox21_302837
M4ID: 12476296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.87 MAX_MED: 1.91 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

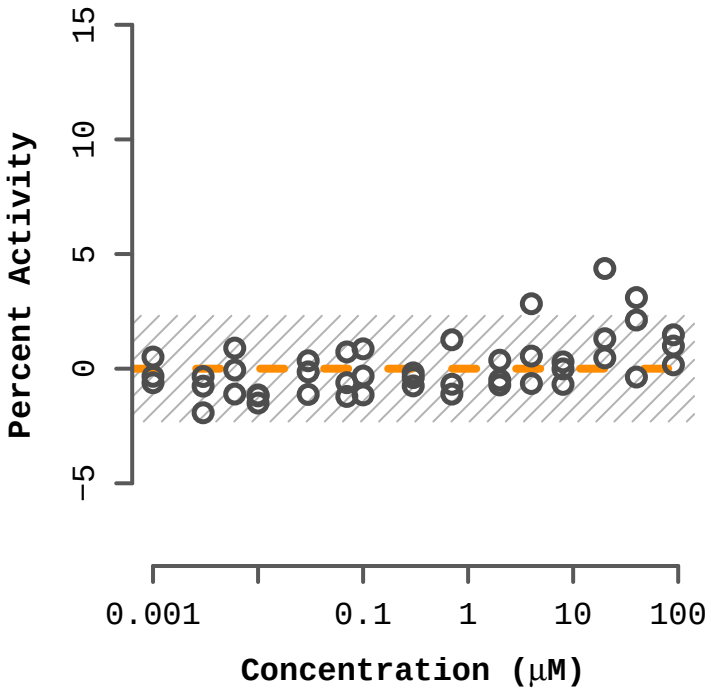
NAME: N-Butylurea
CHID: 20222 **CASRN:** 592-31-4
SPID(S): Tox21_202015
M4ID: 12480237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

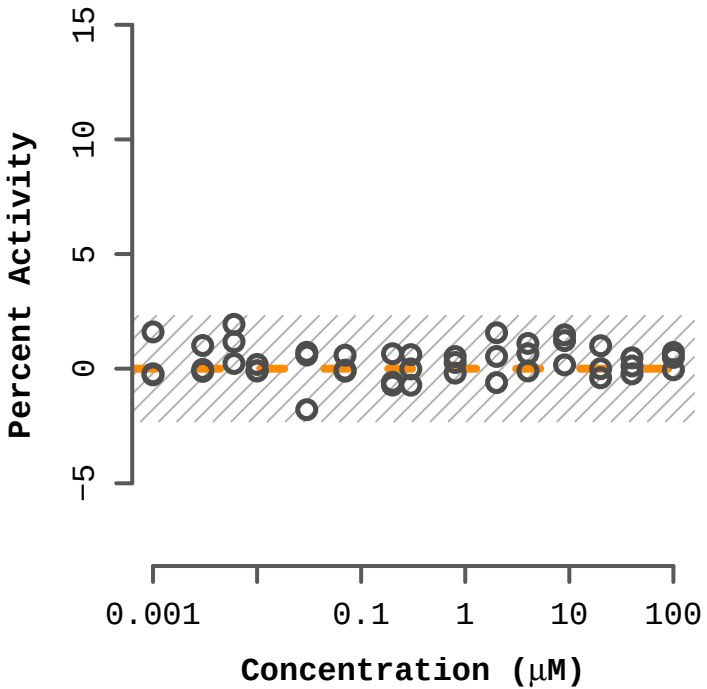
NAME: beta-Butyrolactone
CHID: 20223 **CASRN:** 3068-88-0
SPID(S): Tox21_302988
M4ID: 12476145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

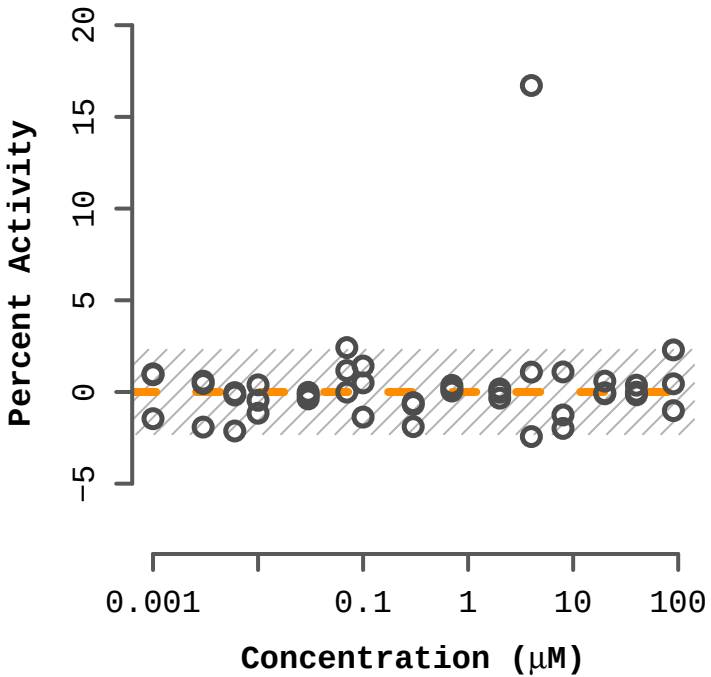
NAME: beta-Butyrolactone
CHID: 20223 **CASRN:** 3068-88-0
SPID(S): Tox21_201253
M4ID: 12480999

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

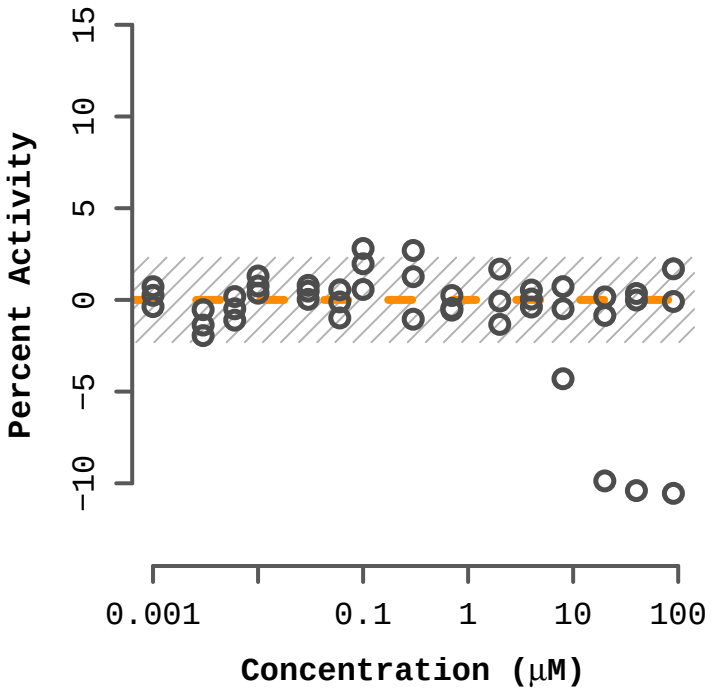
NAME: 4-Butyrolactone
CHID: 20224 CASRN: 96-48-0
SPID(S): Tox21_300188
M4ID: 12478942

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.57	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 5.12 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

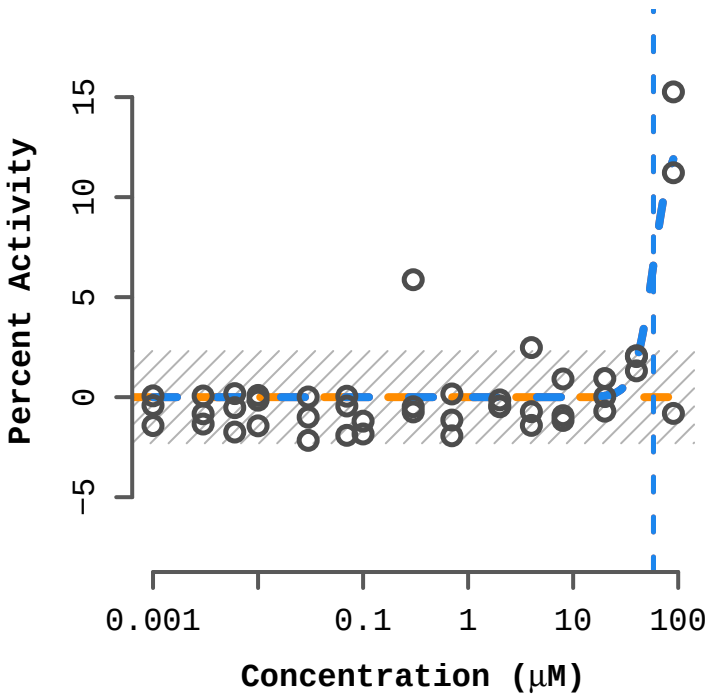
NAME: 4-Butyrolactone
CHID: 20224 **CASRN:** 96-48-0
SPID(S): Tox21_200490
M4ID: 12481762

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.74	NA	NA
PROB:	1	NA	NA
RMSE:	2.91	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cadmium chloride
CHID: 20226 CASRN: 10108-64-2
SPID(S): Tox21_303000
M4ID: 12476133

HILL MODEL (in red):

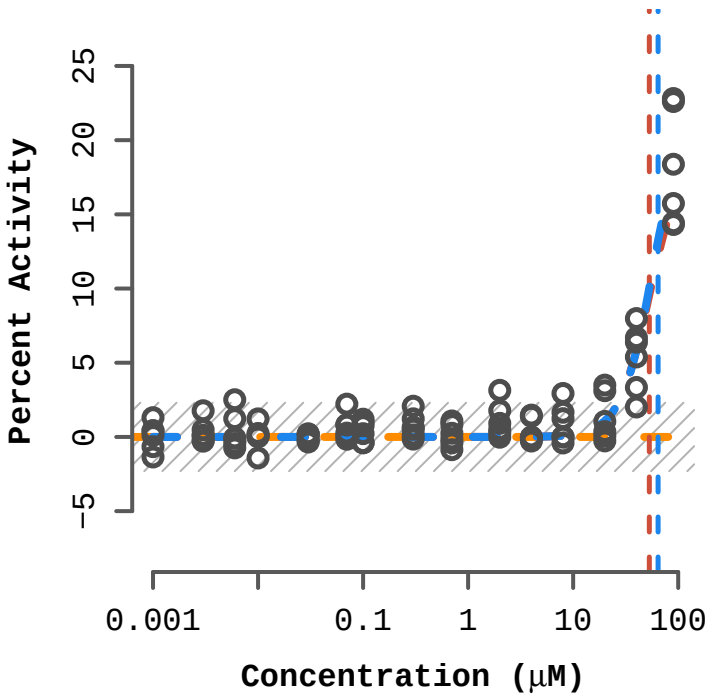
	tp	ga	gw
val:	13.3	1.76	4.93
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.3	1.76	4.93	3.17	3.53
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	186.57	173.38	177.38
PROB:	0	0.88	0.12
RMSE:	3.19	2.39	2.39

MAX_MEAN: 8.56 MAX_MED: 11.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cadmium chloride
CHID: 20226 CASRN: 10108-64-2
SPID(S): Tox21_202229
M4ID: 12480023

HILL MODEL (in red):

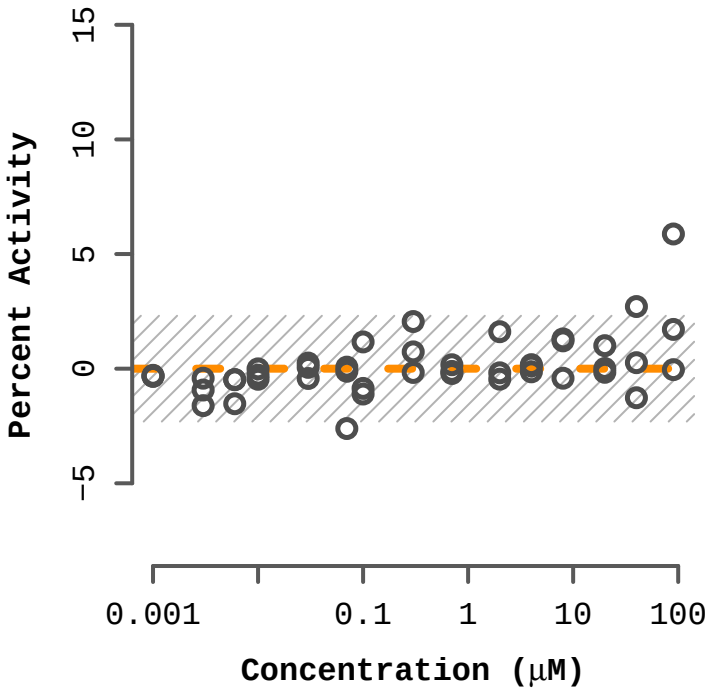
	tp	ga	gw
val:	19.2	1.72	2.91
sd:	5.56	0.13	1.33

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27.4	1.81	2.74	2.06	5.93
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	440.64	310.47	314.4
PROB:	0	0.88	0.12
RMSE:	5.07	1.55	1.55

MAX_MEAN: 18 **MAX_MED:** 17.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

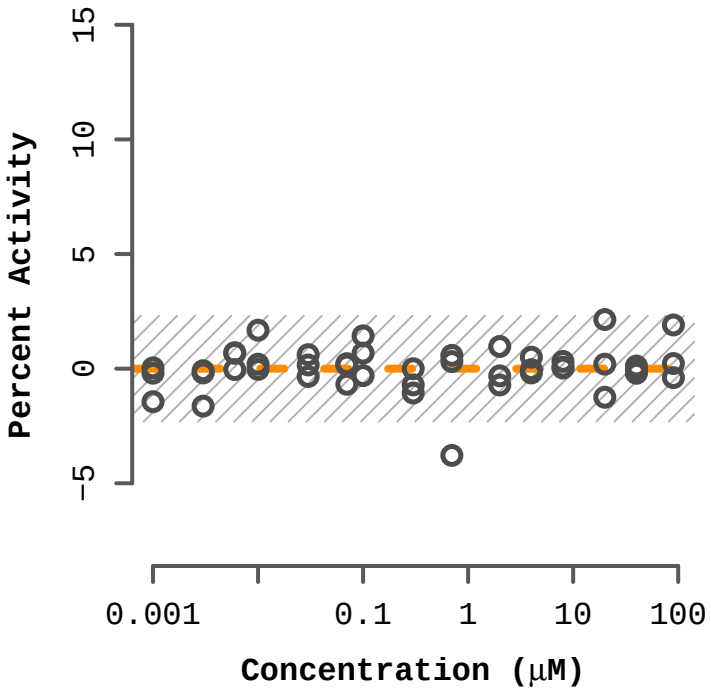
NAME: Caffeic acid
CHID: 20231 **CASRN:** 331-39-5
SPID(S): Tox21_200648
M4ID: 12481604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.52 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

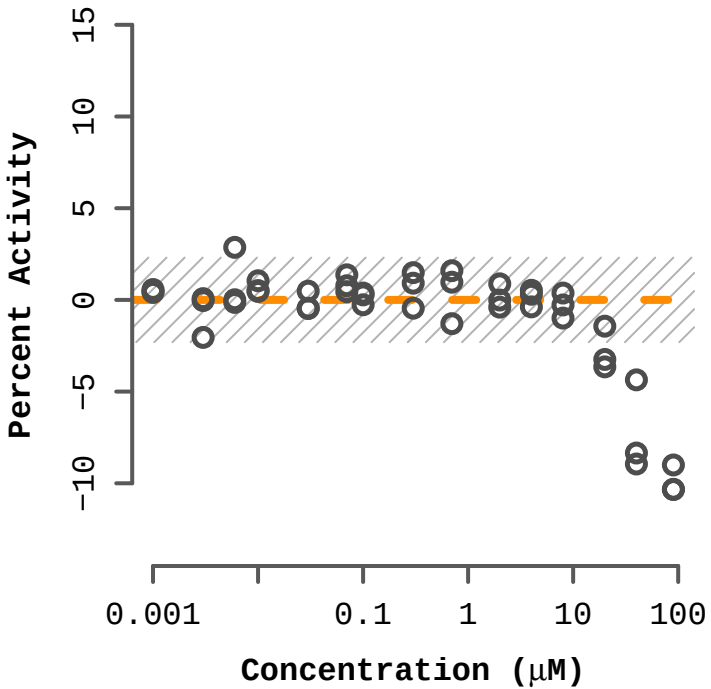
NAME: Caffeine
CHID: 20232 CASRN: 58-08-2
SPID(S): Tox21_300010
M4ID: 12479120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.616 **MAX_MED:** 0.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

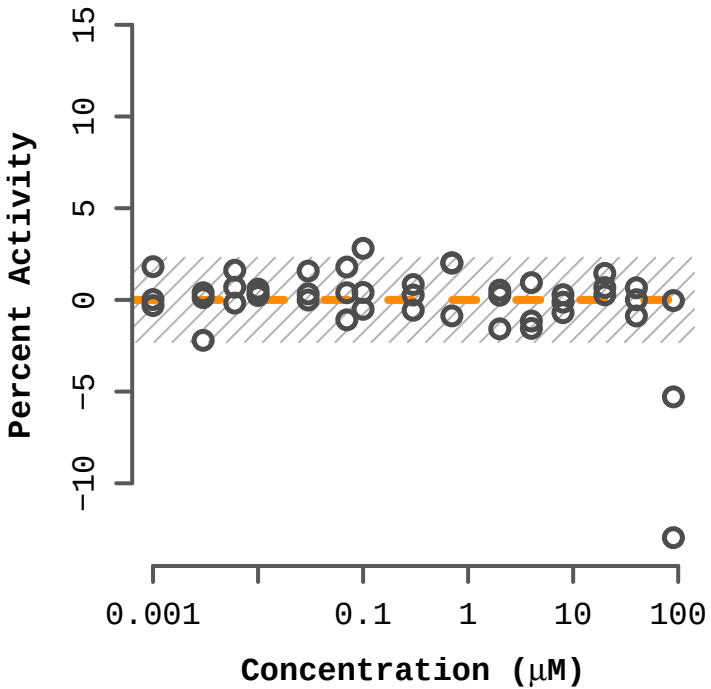
NAME: Caffeine
CHID: 20232 CASRN: 58-08-2
SPID(S): Tox21_201685
M4ID: 12480567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 0.914 **MAX_MED:** 0.967 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

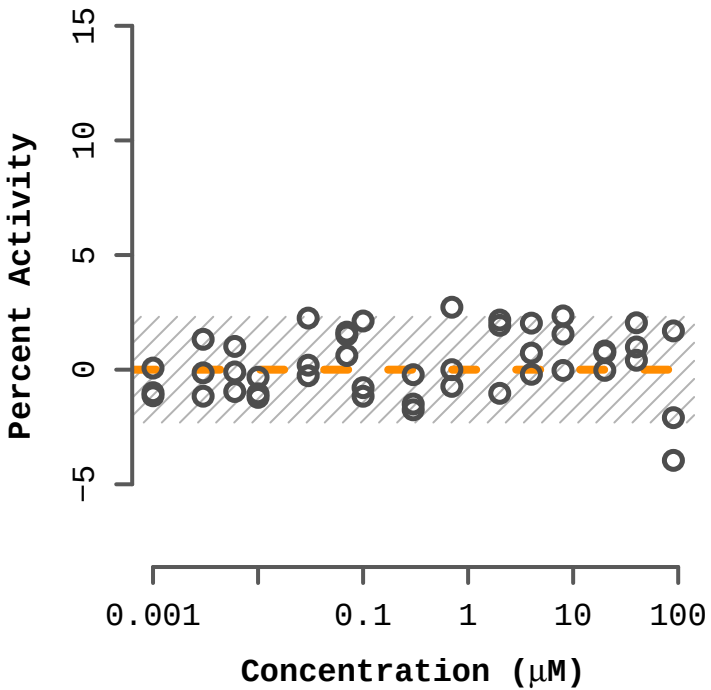
NAME: Ergocalciferol
CHID: 20233 **CASRN:** 50-14-6
SPID(S): Tox21_302752
M4ID: 12476381

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.13	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

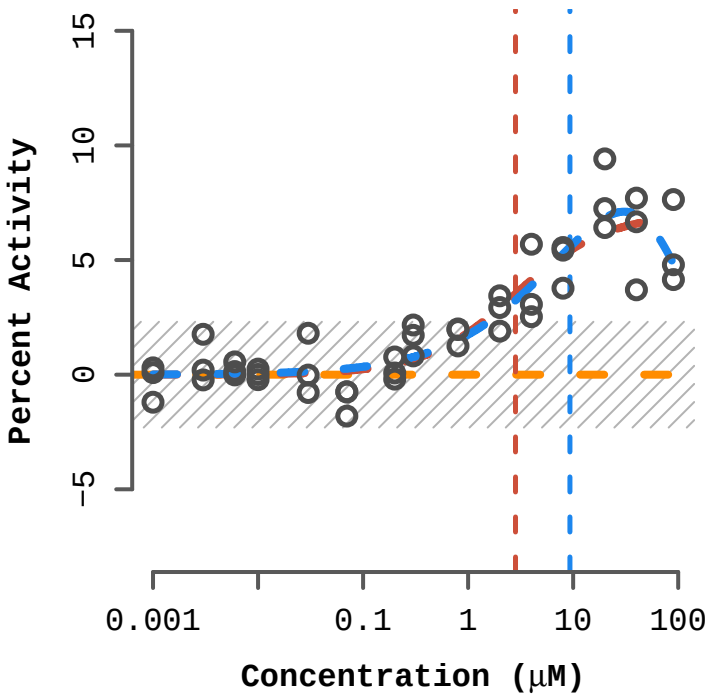
NAME: Ergocalciferol
CHID: 20233 **CASRN:** 50-14-6
SPID(S): Tox21_202348
M4ID: 12479904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Calcium chloride
CHID: 20235 CASRN: 10043-52-4
SPID(S): Tox21_202585
M4ID: 12479667

HILL MODEL (in red):

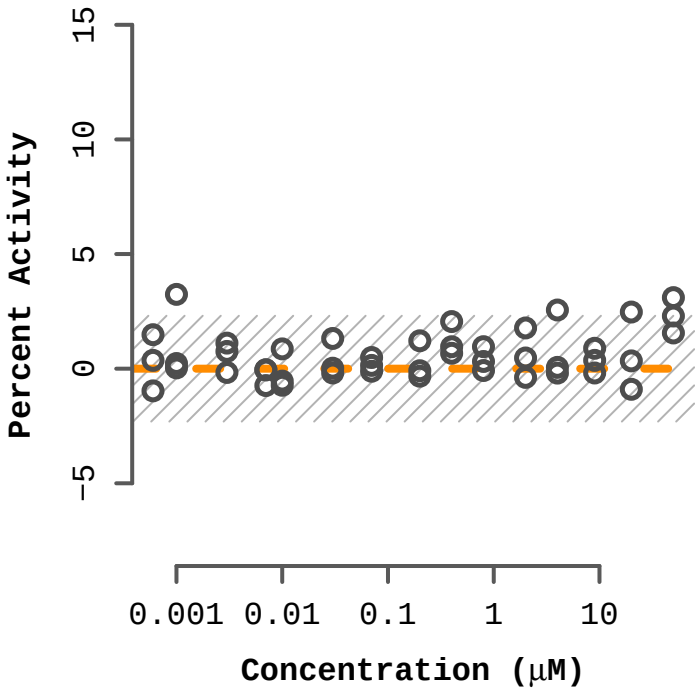
	tp	ga	gw
val:	7.05	0.451	1
sd:	0.779	0.153	0.209

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.3	0.969	0.762	1.96	1.86
sd:	6.37	0.604	0.192	0.179	1.13

	CNST	HILL	GNLS
AIC:	243.02	148.68	145.55
PROB:	0	0.17	0.83
RMSE:	3.58	1.17	1.11

MAX_MEAN: 7.69 MAX_MED: 7.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

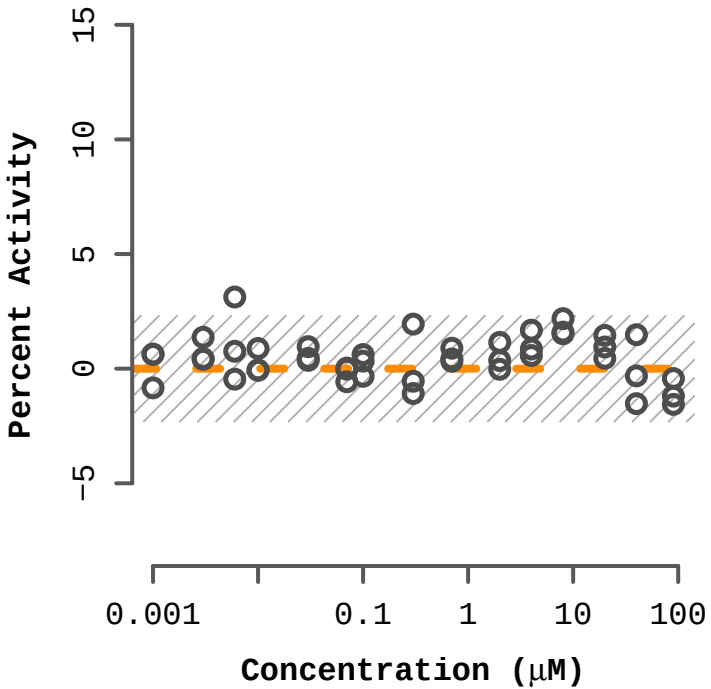
NAME: Calcium lactate
CHID: 20236 **CASRN:** 814-80-2
SPID(S): Tox21_302896
M4ID: 12476237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

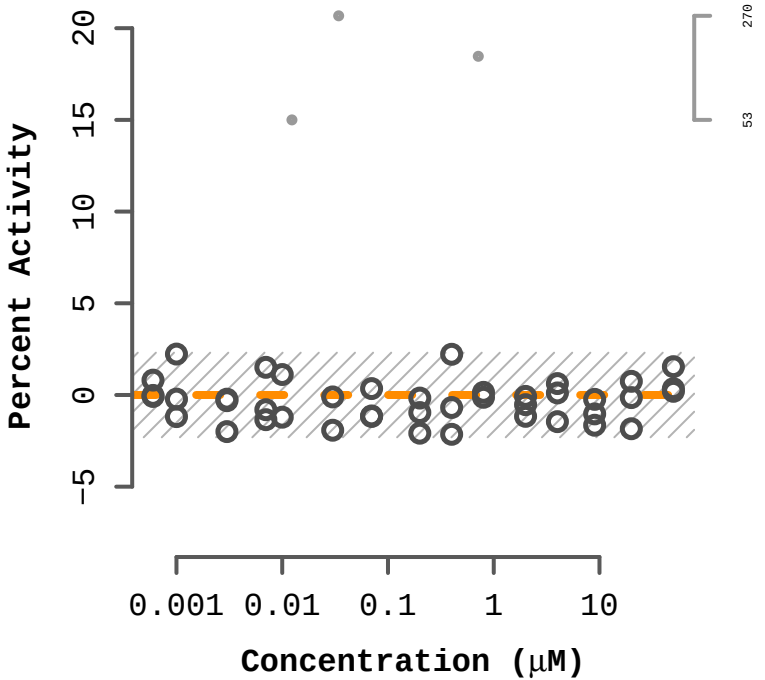
NAME: Calcium lactate
CHID: 20236 **CASRN:** 814-80-2
SPID(S): Tox21_201378
M4ID: 12480874

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

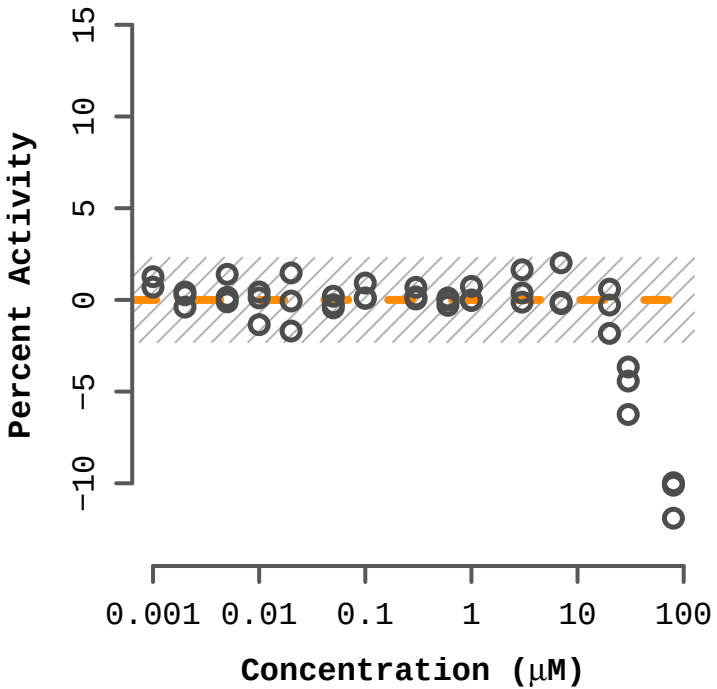
NAME: Camostat mesylate
CHID: 20238 **CASRN:** 59721-29-8
SPID(S): Tox21_112523_1
M4ID: 12483050 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	266.72	NA	NA
PROB:	1	NA	NA
RMSE:	49.16	NA	NA

MAX_MEAN: 88.7 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

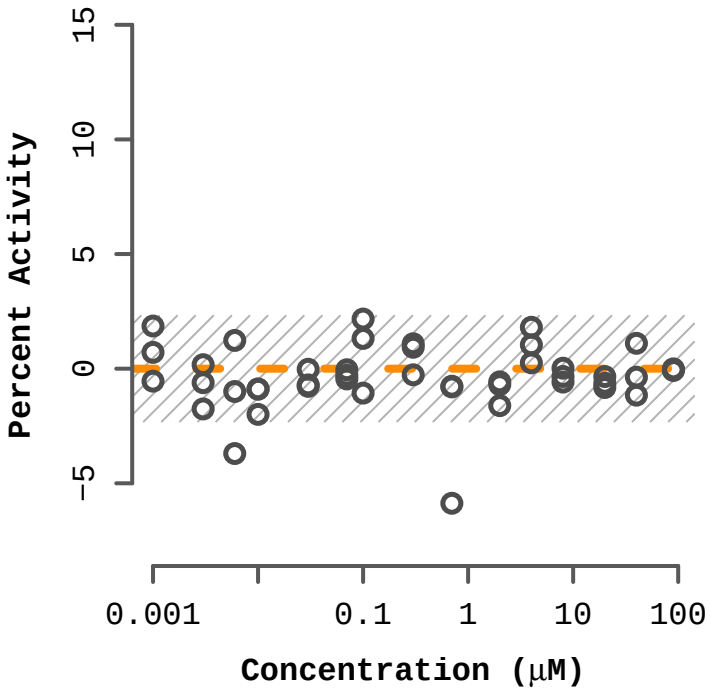
NAME: Candesartan cilexetil
CHID: 20239 **CASRN:** 145040-37-5
SPID(S): Tox21_302202
M4ID: 12476931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.16	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

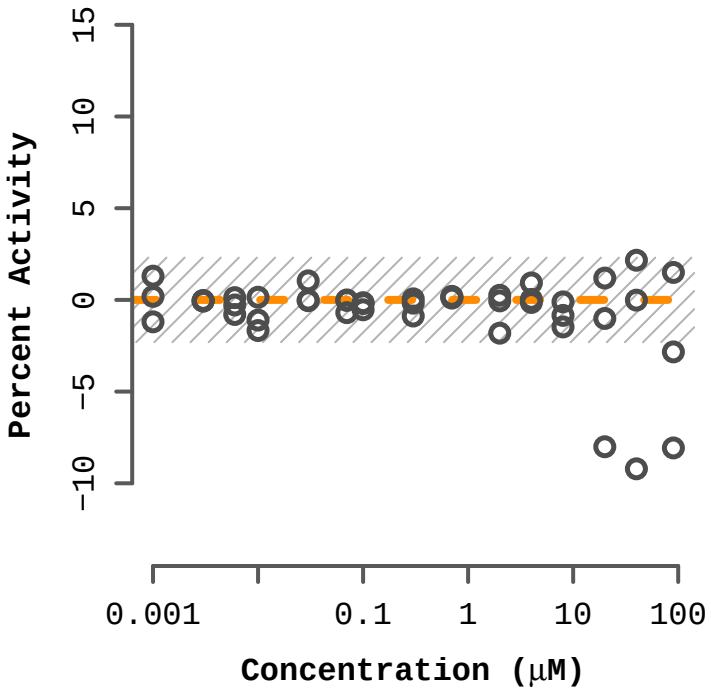
NAME: Caprolactam
CHID: 20240 **CASRN:** 105-60-2
SPID(S): Tox21_300163
M4ID: 12478967

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

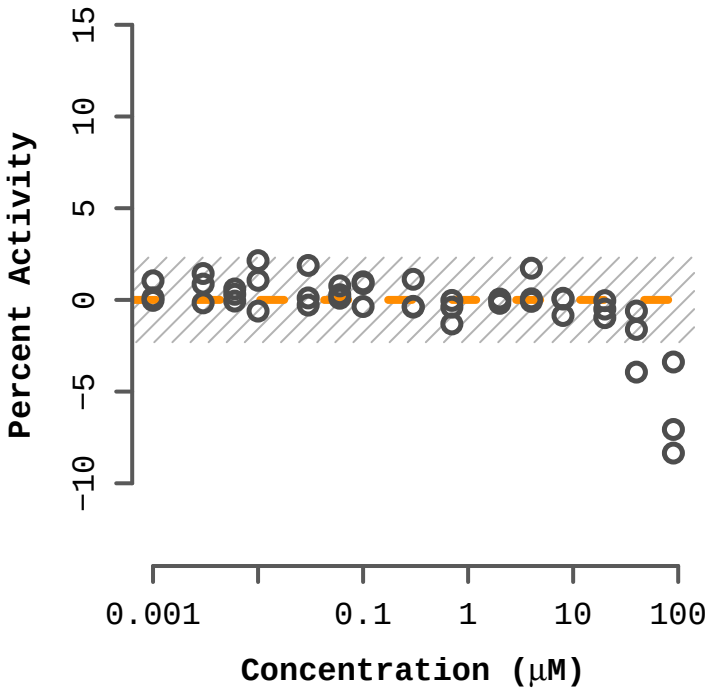
NAME: Caprolactam
CHID: 20240 **CASRN:** 105-60-2
SPID(S): Tox21_202202
M4ID: 12480050

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.22	NA	NA
PROB:	1	NA	NA
RMSE:	2.35	NA	NA

MAX_MEAN: 0.329 **MAX_MED:** 0.192 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

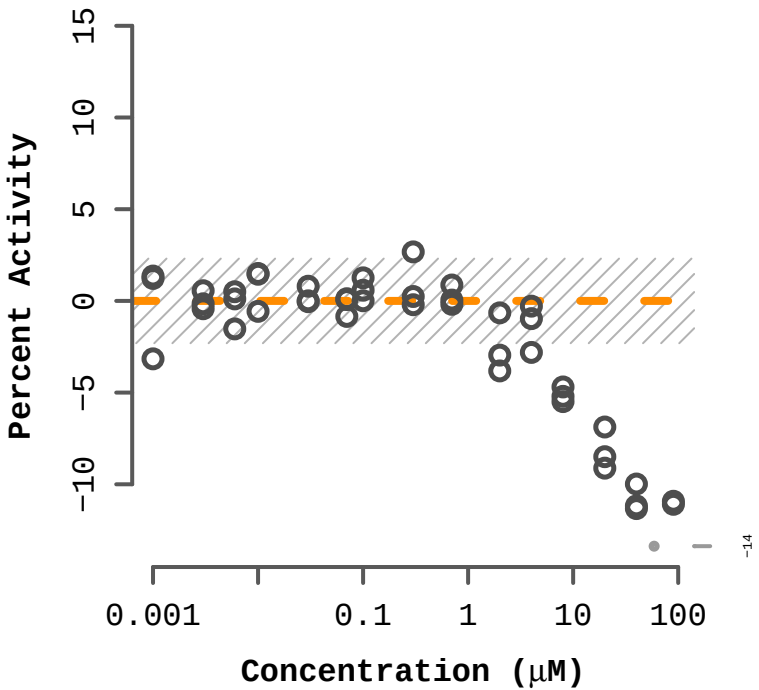
NAME: Capsaicin
CHID: 20241 CASRN: 404-86-4
SPID(S): Tox21_200315
M4ID: 12481937

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 0.868 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

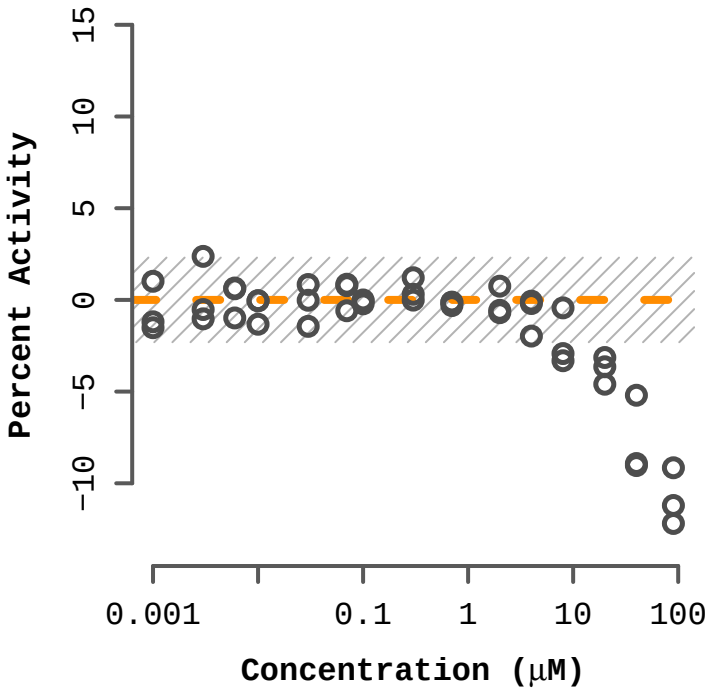
NAME: Captafol
CHID: 20242 CASRN: 2425-06-1
SPID(S): Tox21_300801
M4ID: 12478332 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.03	NA	NA
PROB:	1	NA	NA
RMSE:	5.04	NA	NA

MAX_MEAN: 0.903 MAX_MED: 1.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

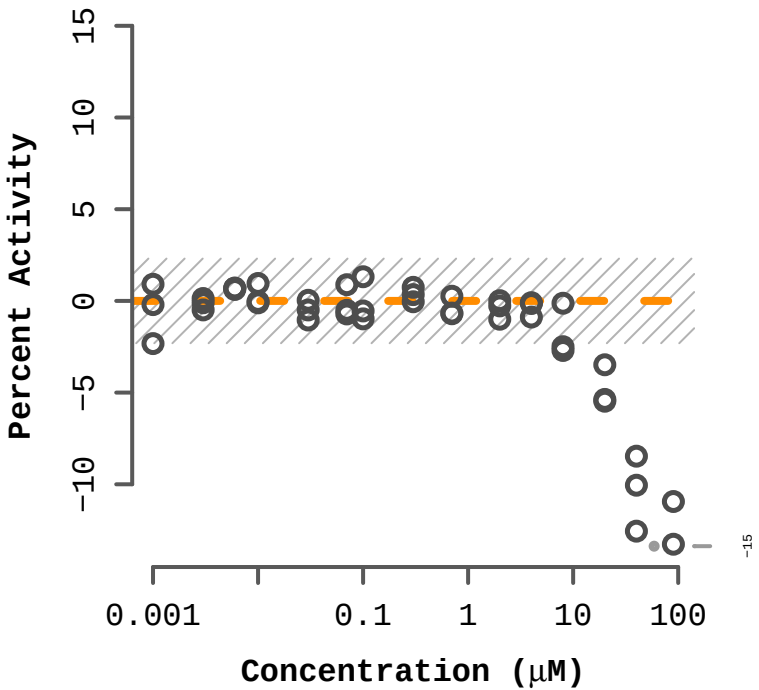
NAME: Captafol
CHID: 20242 **CASRN:** 2425-06-1
SPID(S): Tox21_201709
M4ID: 12480543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.35	NA	NA
PROB:	1	NA	NA
RMSE:	3.76	NA	NA

MAX_MEAN: 0.502 **MAX_MED:** 0.778 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

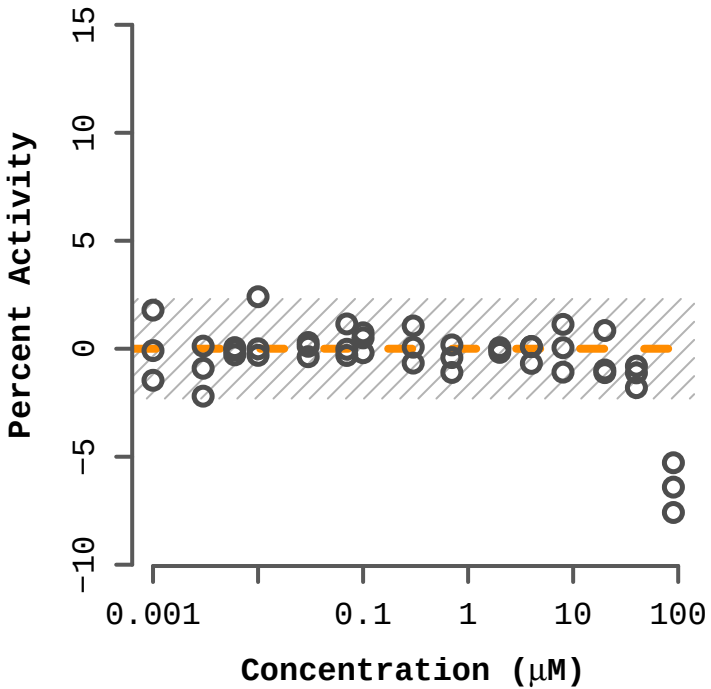
NAME: Captan
CHID: 20243 CASRN: 133-06-2
SPID(S): Tox21_300772
M4ID: 12478361 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.62	NA	NA
PROB:	1	NA	NA
RMSE:	4.59	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 0.692 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

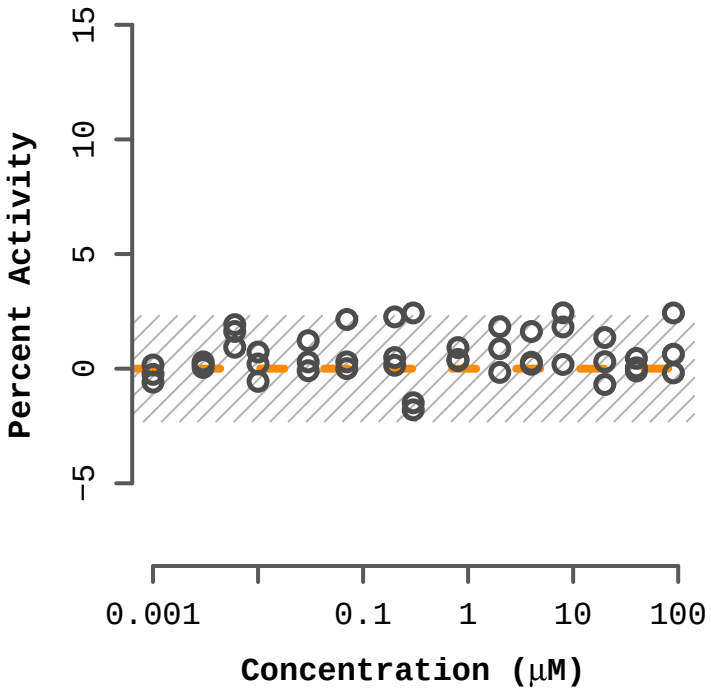
NAME: Captan
CHID: 20243 CASRN: 133-06-2
SPID(S): Tox21_201276
M4ID: 12480976

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 0.701 MAX_MED: 0.504 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

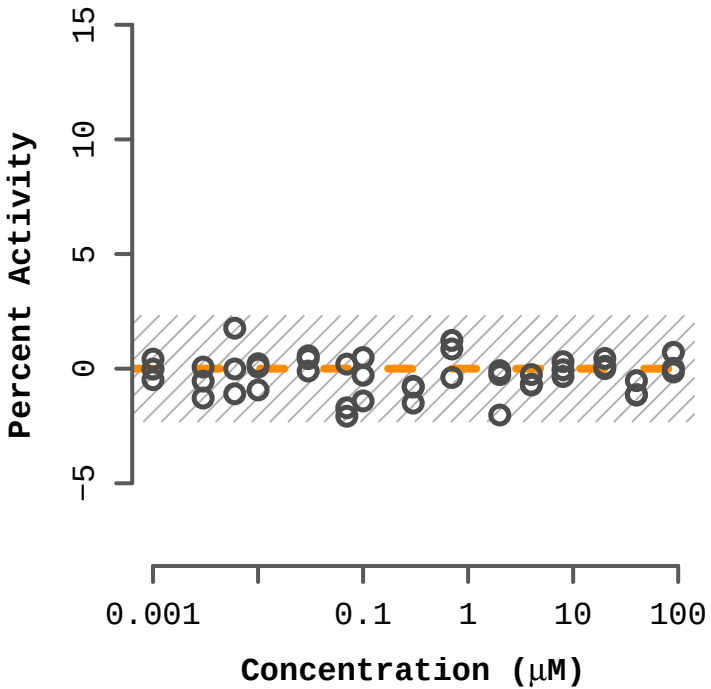
NAME: Semicarbazide hydrochloride
CHID: 20244 **CASRN:** 563-41-7
SPID(S): Tox21_200950
M4ID: 12481302

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

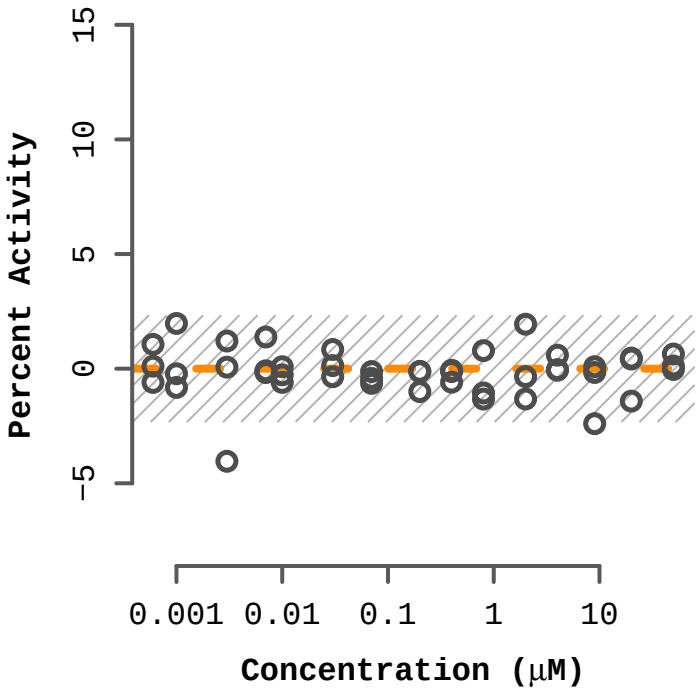
NAME: Phenicarbazide
CHID: 20245 **CASRN:** 103-03-7
SPID(S): Tox21_200048
M4ID: 12482204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.57 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

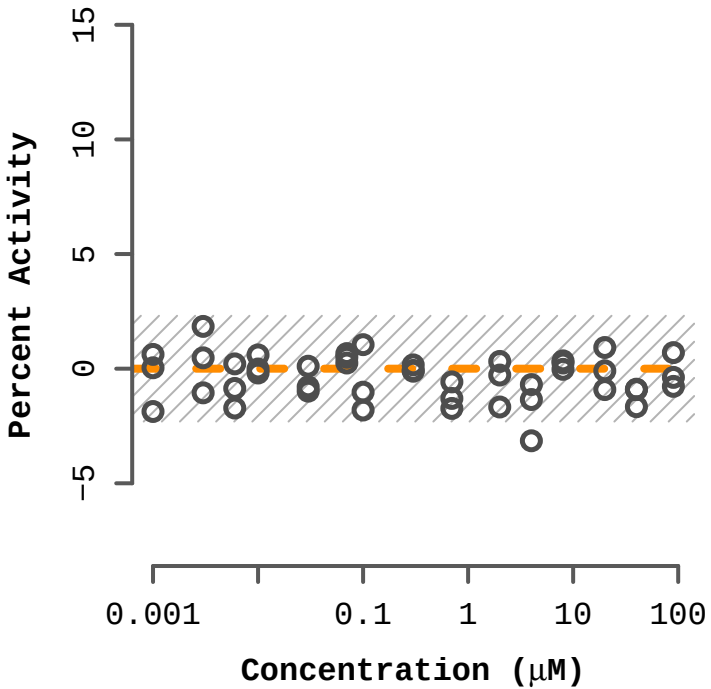
NAME: Phenicarbazide
CHID: 20245 **CASRN:** 103-03-7
SPID(S): Tox21_111632_1
M4ID: 12483573

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.375 **MAX_MED:** 0.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

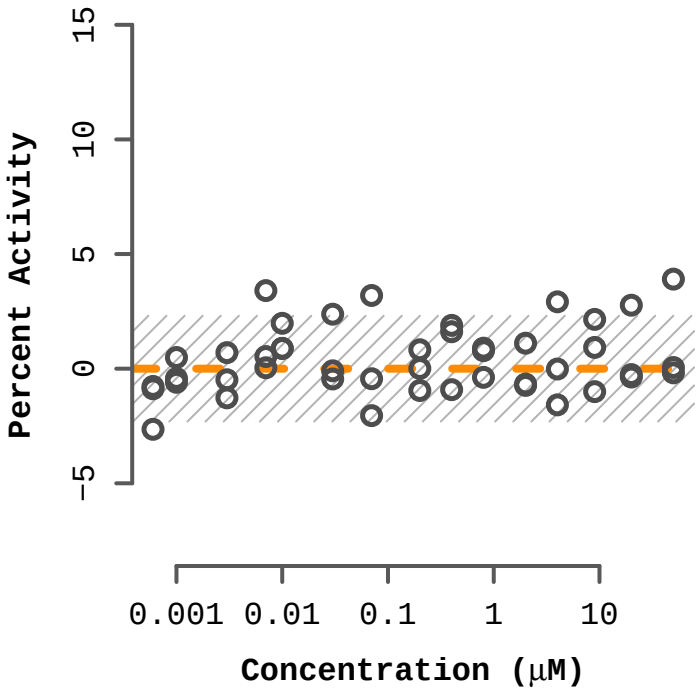
NAME: Carbarsone
CHID: 20246 **CASRN:** 121-59-5
SPID(S): Tox21_201049
M4ID: 12481203

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.468 **MAX_MED:** 0.497 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

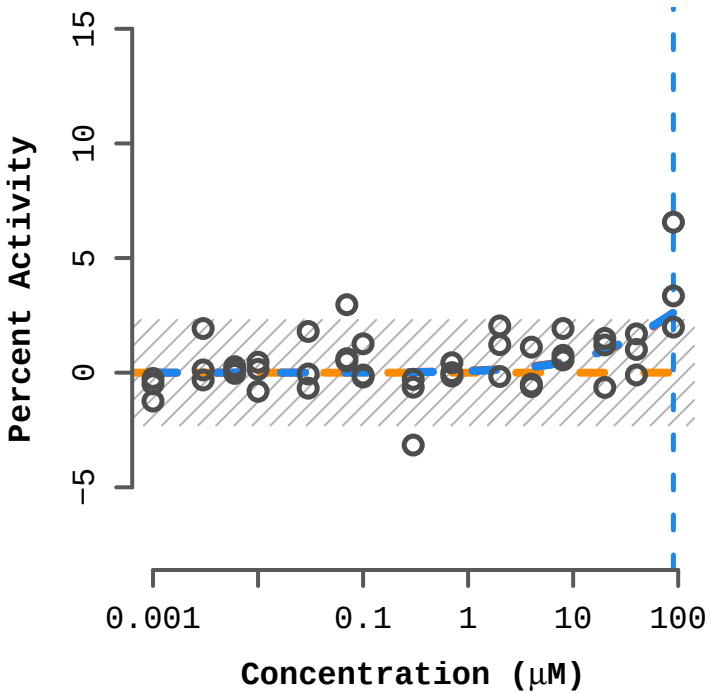
NAME: Carbarsone
CHID: 20246 **CASRN:** 121-59-5
SPID(S): Tox21_110404_1
M4ID: 12484388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carbaryl
CHID: 20247 CASRN: 63-25-2
SPID(S): Tox21_300854
M4ID: 12478279

HILL MODEL (in red):

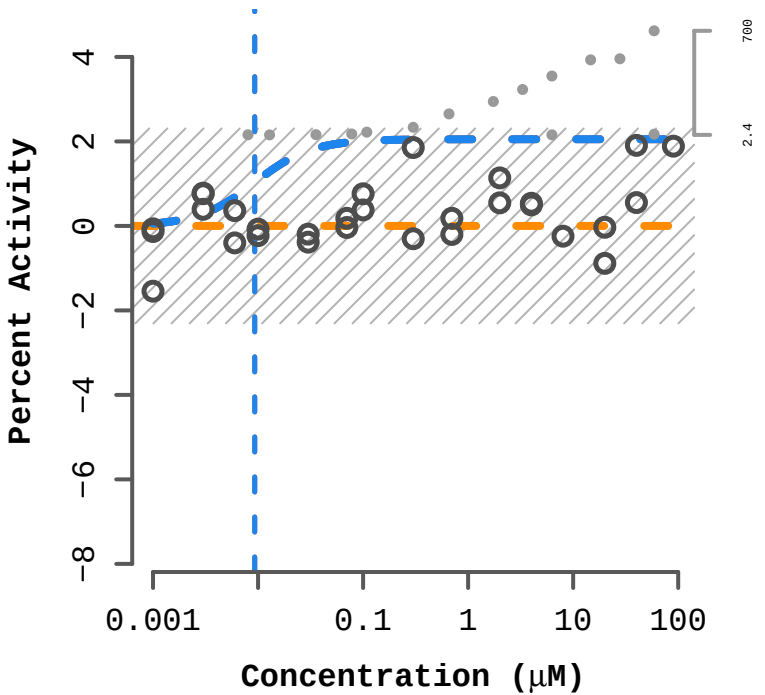
	tp	ga	gw
val:	7.88	2.31	0.847
sd:	8.71	0.9	0.472

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.22	1.95	0.973	3.95	2.64
sd:	5.95	0.815	0.534	110	150

	CNST	HILL	GNLS
AIC:	157.94	143.91	148.33
PROB:	0	0.9	0.1
RMSE:	1.57	1.19	1.2

MAX_MEAN: 3.97 MAX_MED: 3.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carbaryl
CHID: 20247 CASRN: 63-25-2
SPID(S): Tox21_201836
M4ID: 12480416 BRK

HILL MODEL (in red):

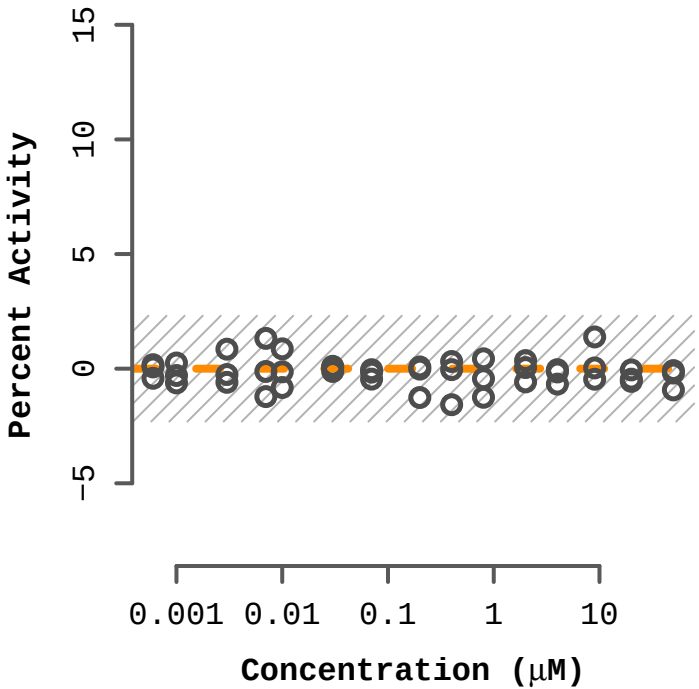
	tp	ga	gw
val:	2.05	-2.03	1.6
sd:	1.74	1.77	4.85

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.05	-2.03	1.6	3.71	5.16
sd:	1.74	1.77	4.84	22000	64900

	CNST	HILL	GNLS
AIC:	515.66	519.86	523.86
PROB:	0.88	0.11	0.01
RMSE:	173.29	172.53	172.53

MAX_MEAN: 238 MAX_MED: 6.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

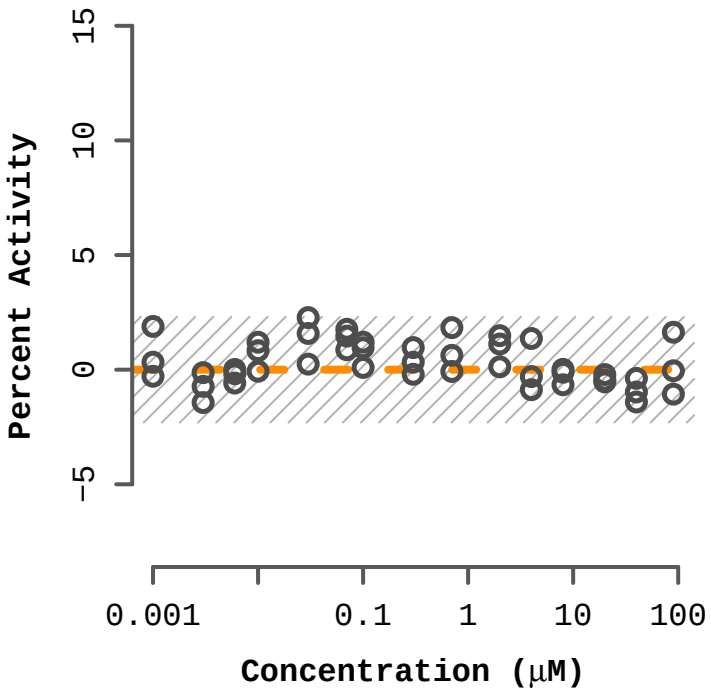
NAME: Carbaryl
CHID: 20247 CASRN: 63-25-2
SPID(S): Tox21_110994_1
M4ID: 12483959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	85.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.62	NA	NA

MAX_MEAN: 0.32 **MAX_MED:** 0.0769 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

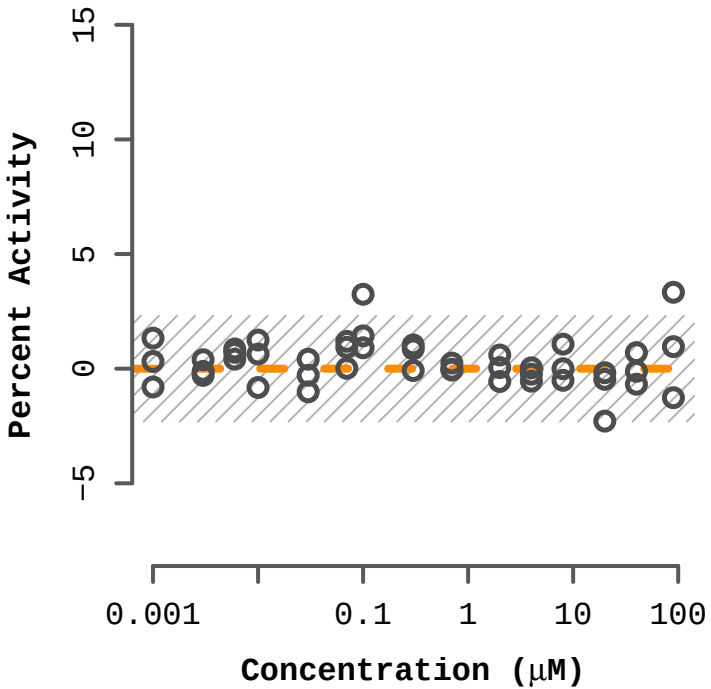
NAME: Carbazole
CHID: 20248 **CASRN:** 86-74-8
SPID(S): Tox21_302847
M4ID: 12476286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

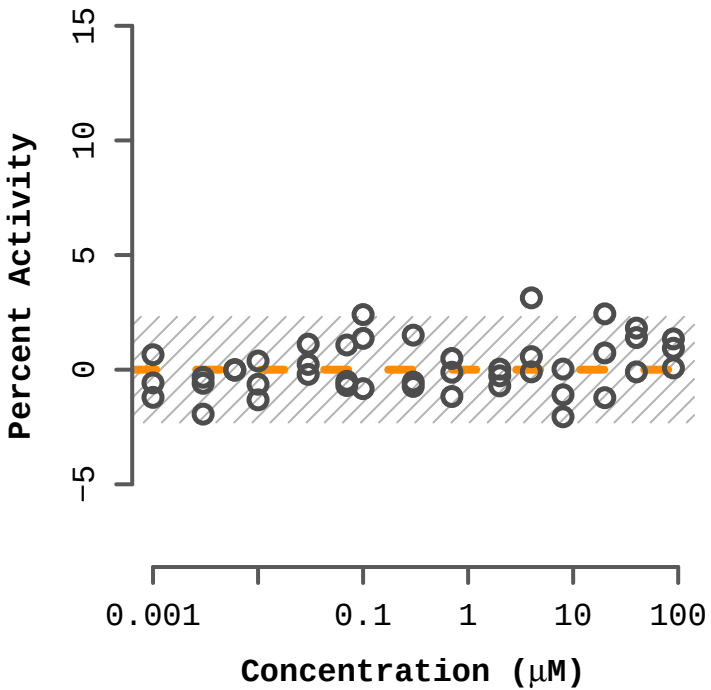
NAME: Carbazole
CHID: 20248 **CASRN:** 86-74-8
SPID(S): Tox21_201703
M4ID: 12480549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

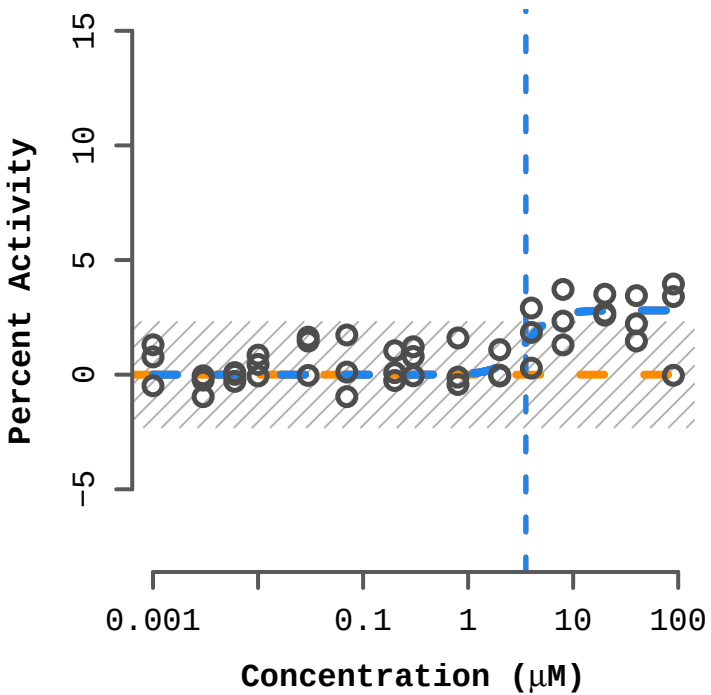
NAME: Carbofuran
CHID: 20249 **CASRN:** 1563-66-2
SPID(S): Tox21_300623
M4ID: 12478510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carbofuran
CHID: 20249 CASRN: 1563-66-2
SPID(S): Tox21_201955
M4ID: 12480297

HILL MODEL (in red):

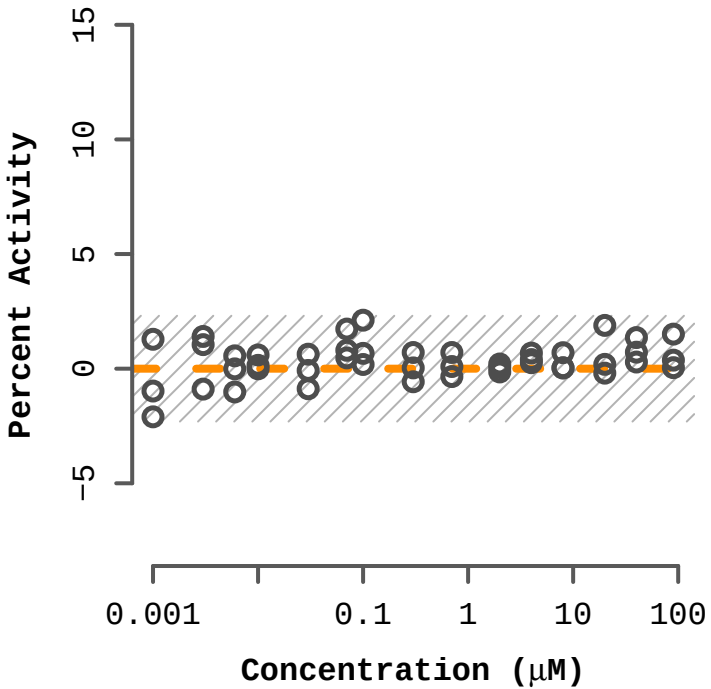
	tp	ga	gw
val:	2.8	0.55	3.24
sd:	0.341	0.126	2.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.8	0.55	3.24	2.67	12.4
sd:	0.341	0.126	2.9	1340	23200

	CNST	HILL	GNLS
AIC:	175.66	131.08	135.08
PROB:	0	0.88	0.12
RMSE:	1.67	0.94	0.94

MAX_MEAN: 2.93 MAX_MED: 3.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

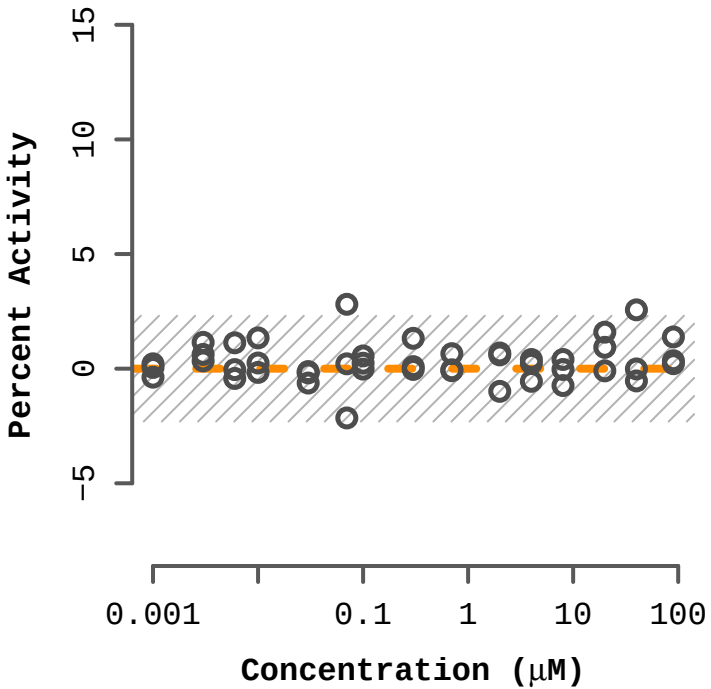
NAME: Carbon tetrachloride
CHID: 20250 **CASRN:** 56-23-5
SPID(S): Tox21_200039
M4ID: 12482213

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

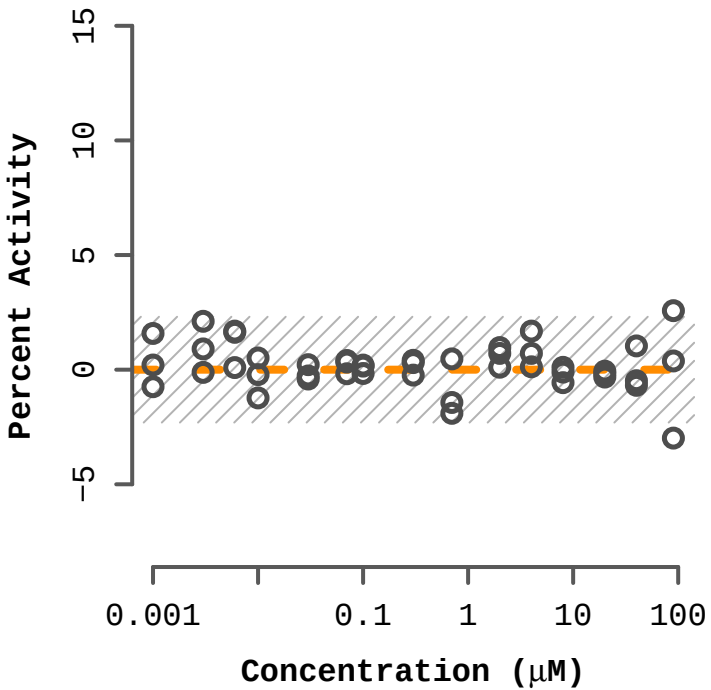
NAME: Carbromal
CHID: 20252 CASRN: 77-65-6
SPID(S): Tox21_302247
M4ID: 12476886

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.811 **MAX_MED:** 0.934 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

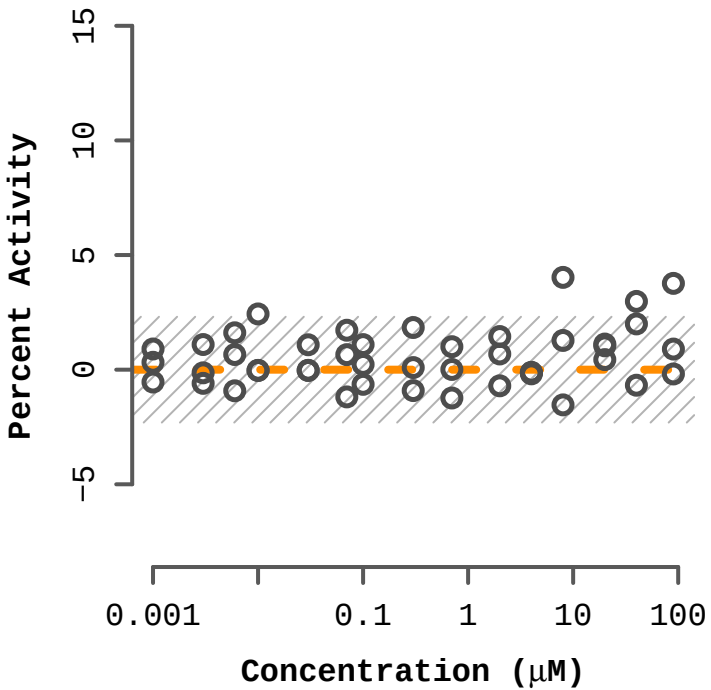
NAME: d-Carvone
CHID: 20256 **CASRN:** 2244-16-8
SPID(S): Tox21_302743
M4ID: 12476390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.61	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

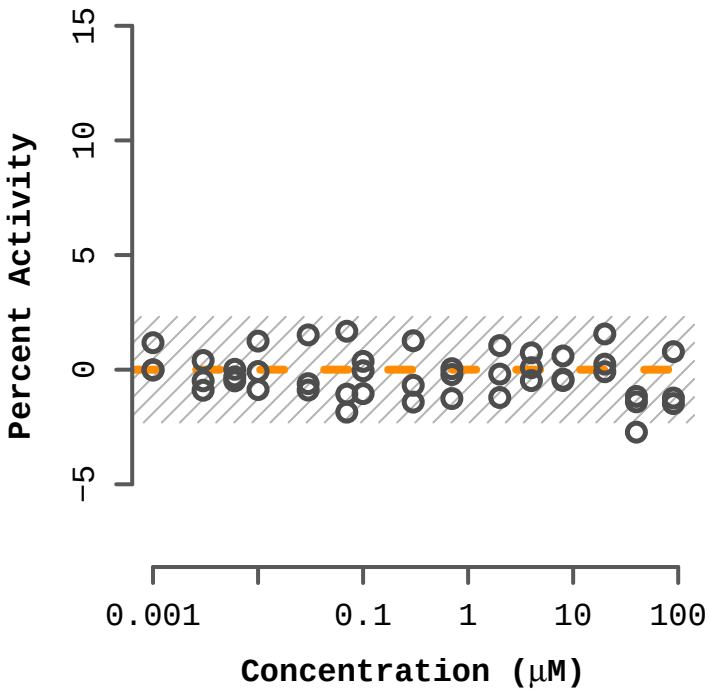
NAME: d−Carvone
CHID: 20256 **CASRN:** 2244−16−8
SPID(S): Tox21_201441
M4ID: 12480811

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

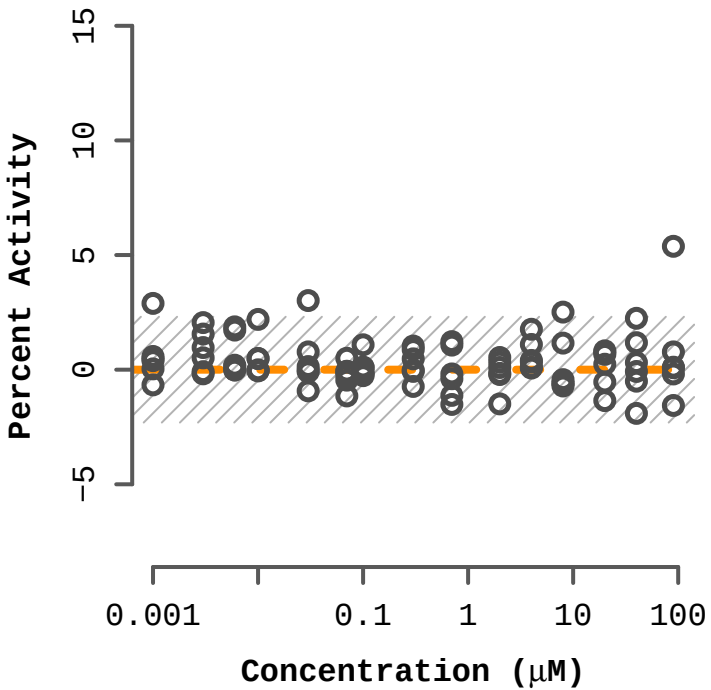
NAME: Catechol
CHID: 20257 CASRN: 120-80-9
SPID(S): Tox21_300153
M4ID: 12478977

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.94	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.571 MAX_MED: 0.243 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

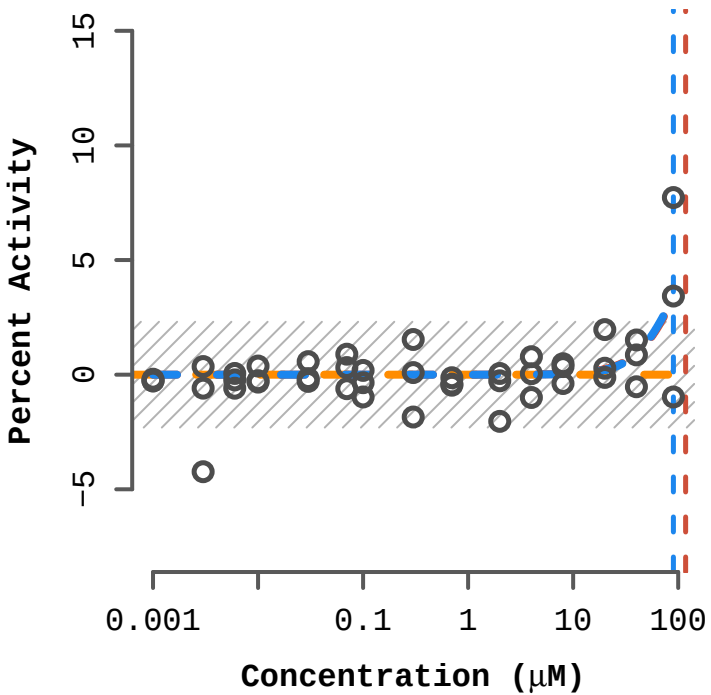
NAME: Catechol
CHID: 20257 **CASRN:** 120-80-9
SPID(S): Tox21_202317
M4ID: 12479935

HILL MODEL: Not applicable.

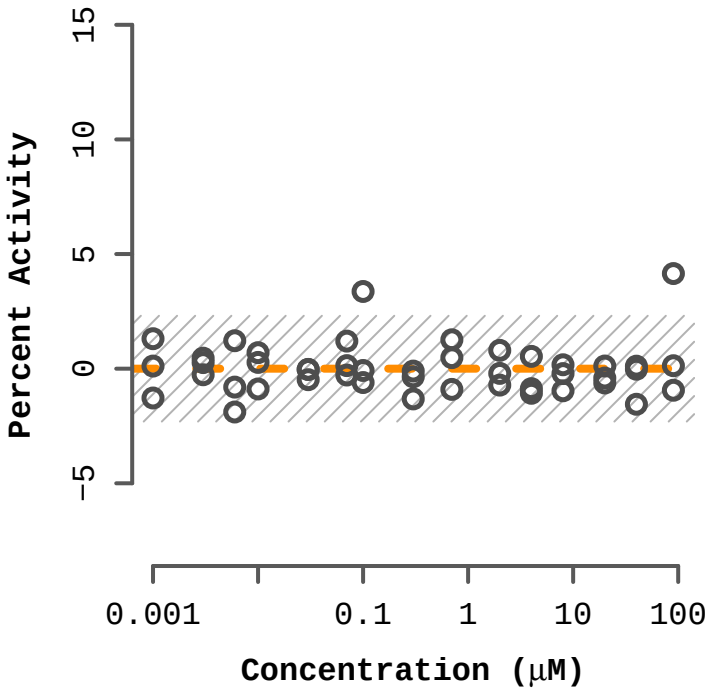
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 0.742 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Chenodeoxycholic acid
CHID:    20260   CASRN: 474-25-9
SPID(S): Tox21_200491
M4ID:    12481761

HILL MODEL (in red):
      tp       ga       gw
val:  9.27     2.07     2.05
sd:   16.9     0.662    1.23

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.07     1.95     2.32     3.95     0.697
sd:   12.6     0.59     1.84     11.9     5.6

      CNST        HILL        GNLS
AIC:  140.51      138.74      142.82
PROB: 0.27        0.65        0.08
RMSE: 1.59        1.32        1.32

MAX_MEAN: 3.4       MAX_MED: 3.43      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

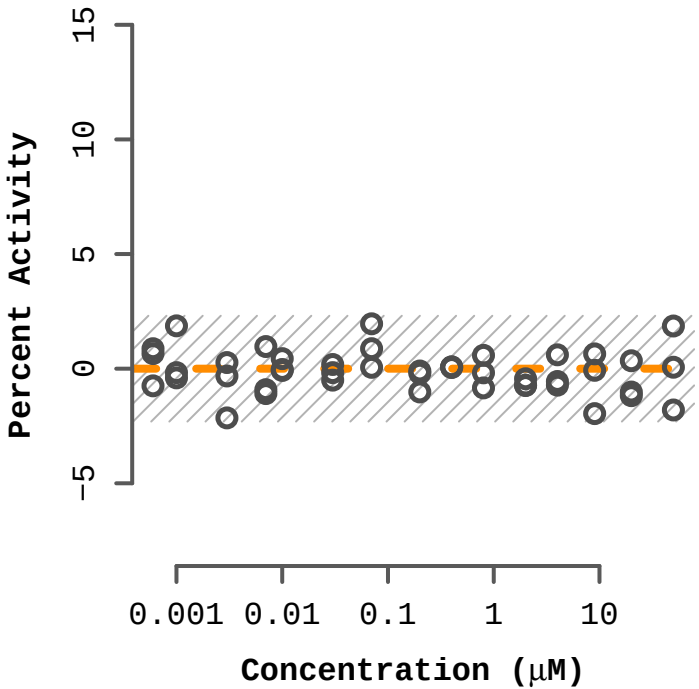
NAME: Chloral hydrate
CHID: 20261 **CASRN:** 302-17-0
SPID(S): Tox21_200110
M4ID: 12482142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.483 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

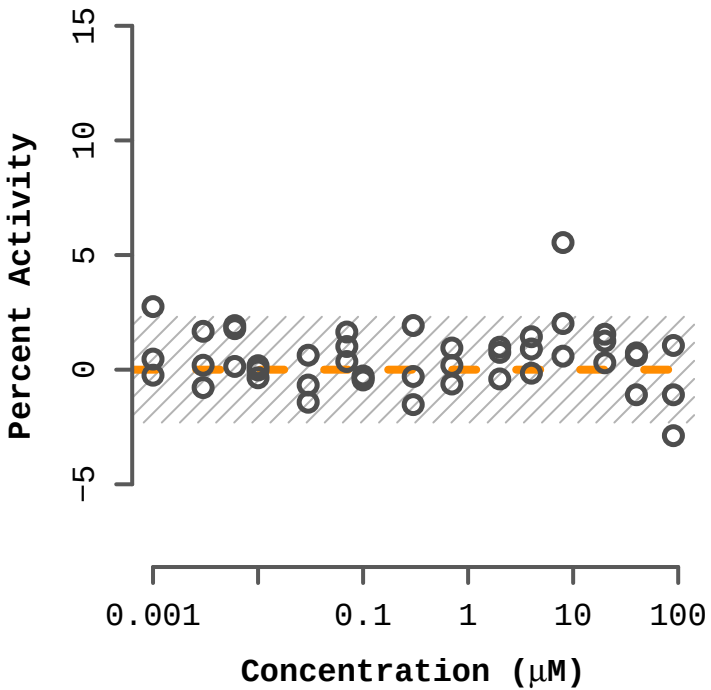
NAME: Chloral hydrate
CHID: 20261 **CASRN:** 302-17-0
SPID(S): Tox21_111614_1
M4ID: 12483586

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.964 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

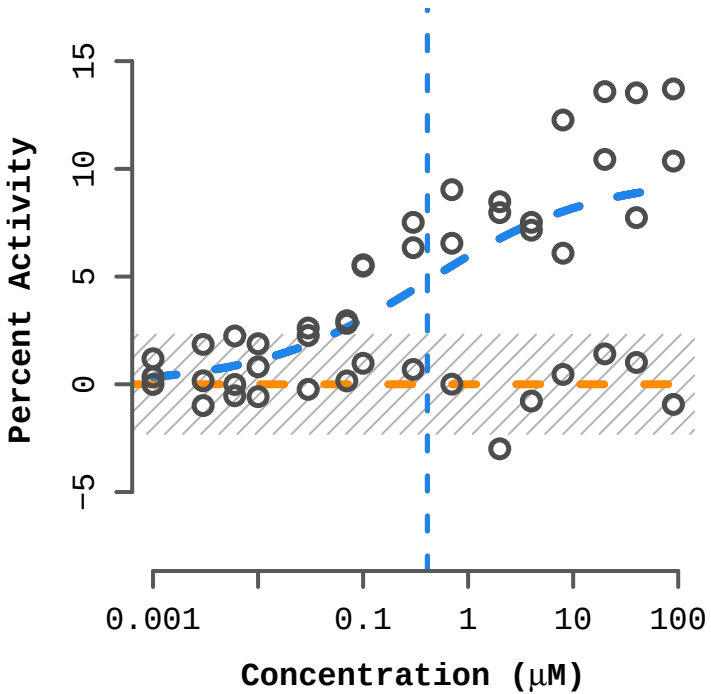
NAME: Chloramben
CHID: 20262 **CASRN:** 133-90-4
SPID(S): Tox21_300588
M4ID: 12478545

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 2.72 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloramben
CHID: 20262 CASRN: 133-90-4
SPID(S): Tox21_201368
M4ID: 12480884

HILL MODEL (in red):

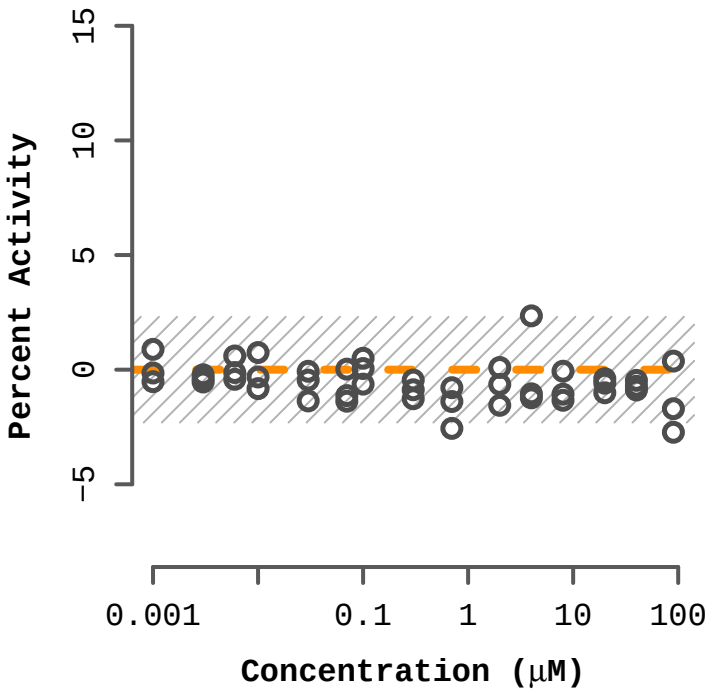
	tp	ga	gw
val:	9.6	−0.388	0.548
sd:	3.51	0.924	0.331

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.6	−0.388	0.548	3.58	9.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	290.06	252.09	256.09
PROB:	0	0.88	0.12
RMSE:	5.97	3.79	3.79

MAX_MEAN: 8.48 MAX_MED: 10.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

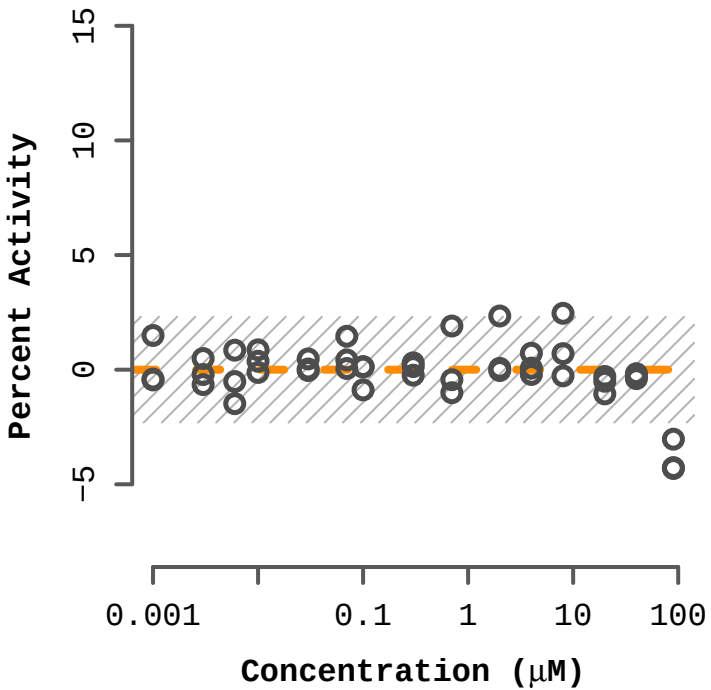
NAME: Chlorambucil
CHID: 20263 CASRN: 305-03-3
SPID(S): Tox21_302996
M4ID: 12476137

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.0745 **MAX_MED:** 0.0512 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

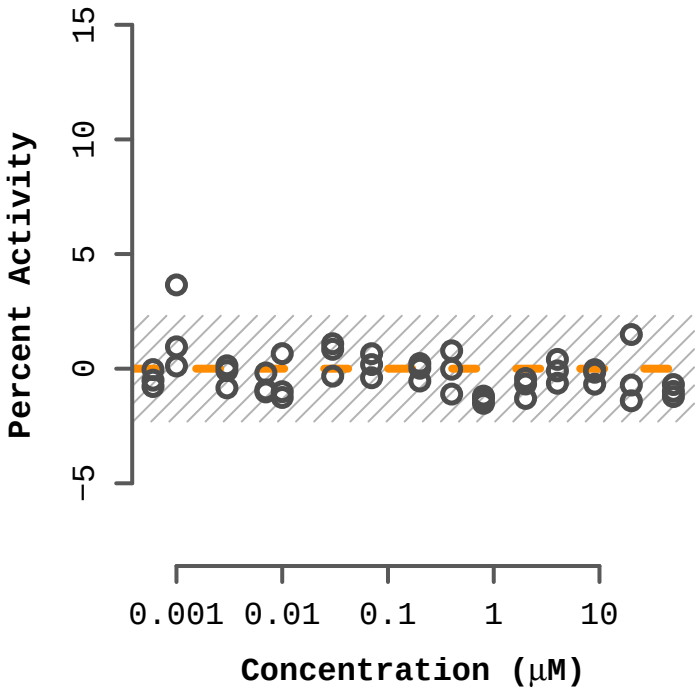
NAME: Chlorambucil
CHID: 20263 CASRN: 305-03-3
SPID(S): Tox21_201390
M4ID: 12480862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.964 MAX_MED: 0.702 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

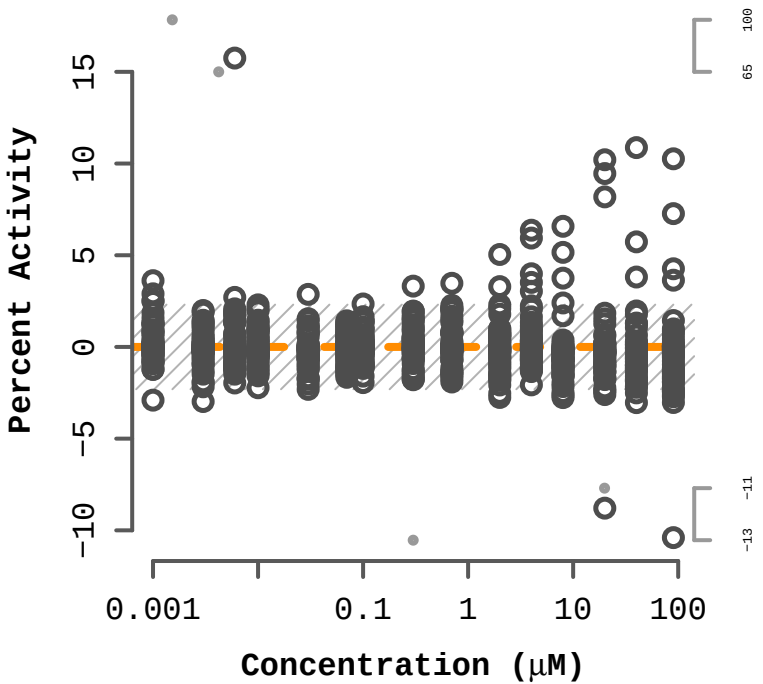
NAME: Chlorambucil
CHID: 20263 **CASRN:** 305-03-3
SPID(S): Tox21_110096_1
M4ID: 12484657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.955 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

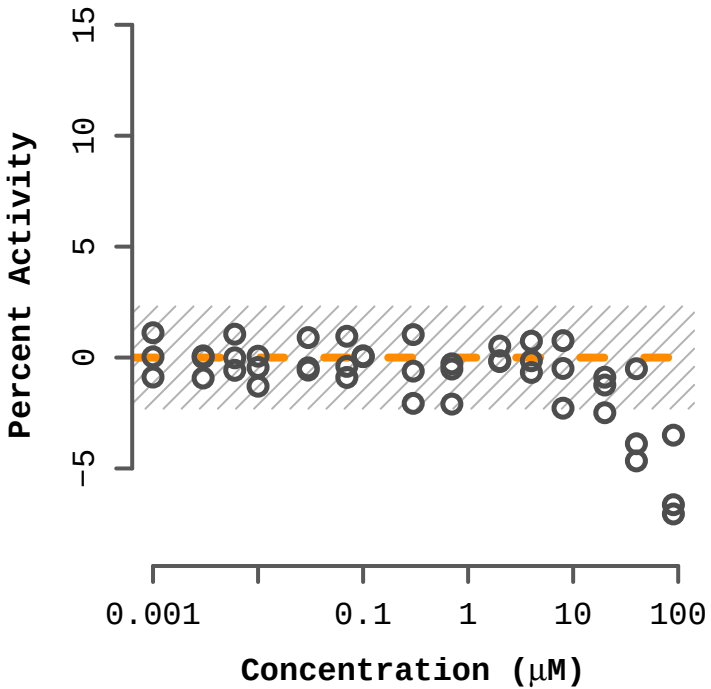
NAME: Chloramphenicol
CHID: 20265 **CASRN:** 56-75-7
SPID(S): Tox21_400061
M4ID: 12475076 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2523.02	NA	NA
PROB:	1	NA	NA
RMSE:	4.91	NA	NA

MAX_MEAN: 2.45 **MAX_MED:** 0.0536 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

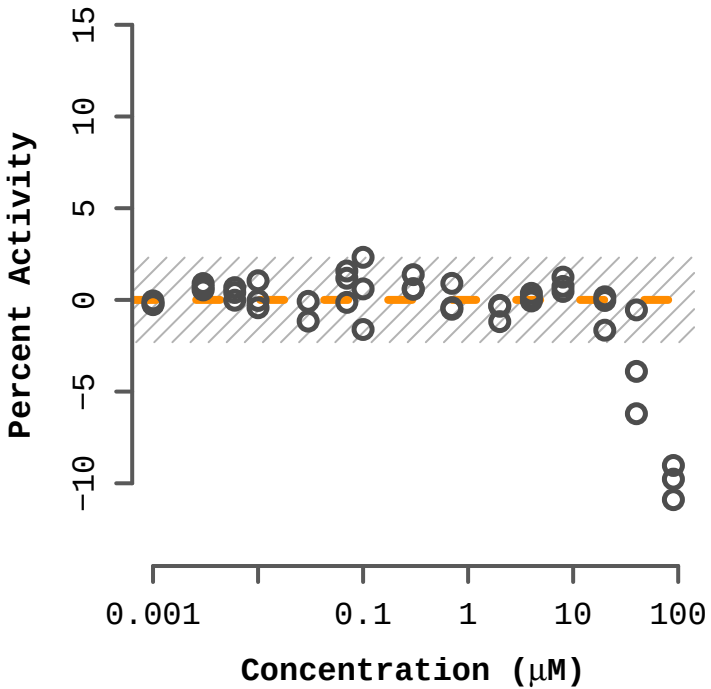
NAME: Chloranil
CHID: 20266 **CASRN:** 118-75-2
SPID(S): Tox21_303021
M4ID: 12476112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 0.157 **MAX_MED:** 0.0476 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

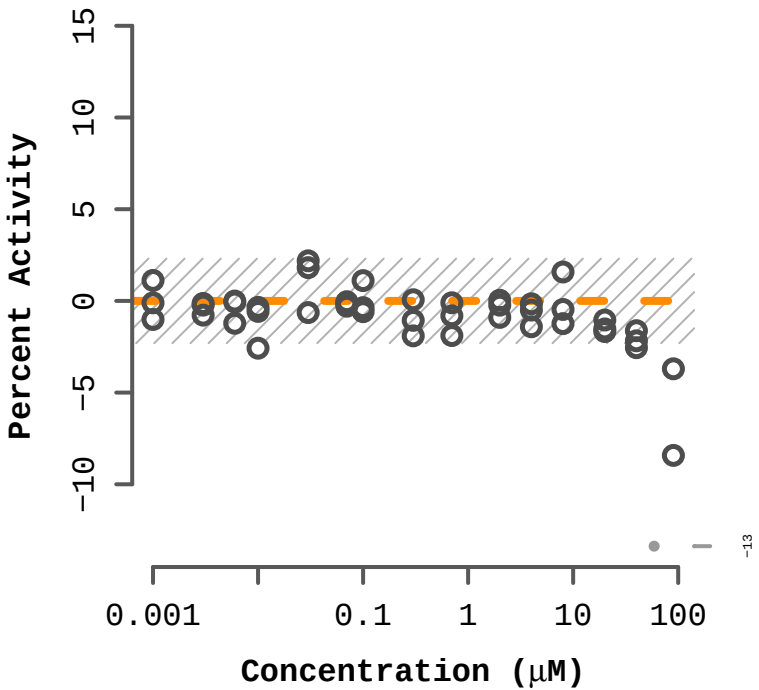
NAME: Chloranil
CHID: 20266 **CASRN:** 118-75-2
SPID(S): Tox21_201656
M4ID: 12480596

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

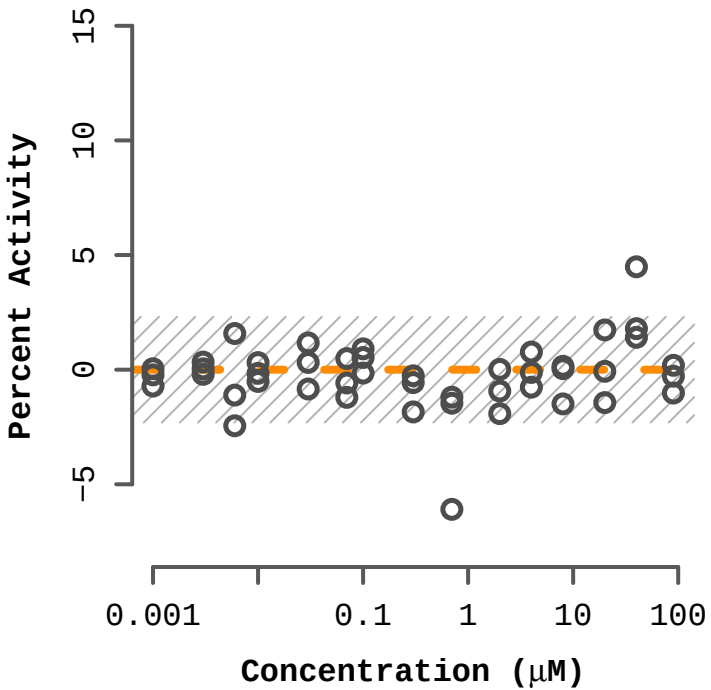
NAME: Chlordane
CHID: 20267 **CASRN:** 57-74-9
SPID(S): Tox21_300586
M4ID: 12478547 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

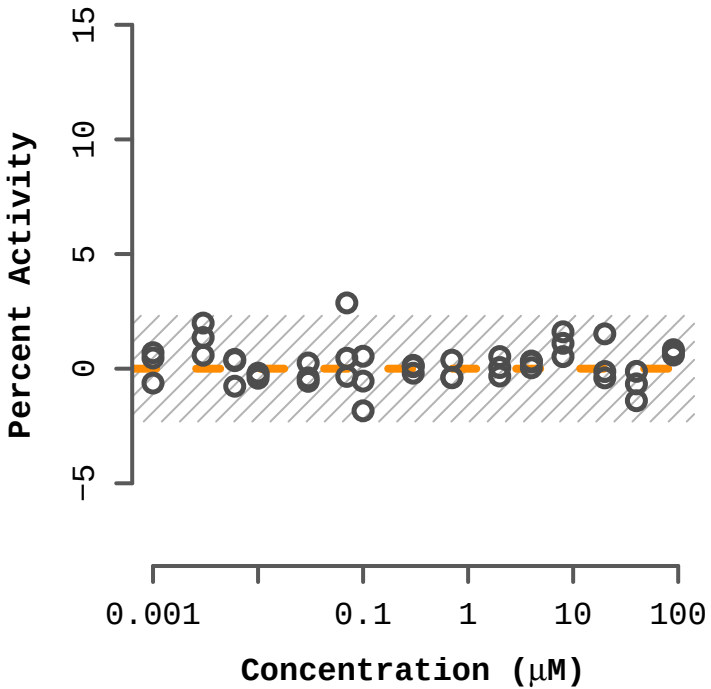
NAME: Chlorendic acid
CHID: 20268 CASRN: 115-28-6
SPID(S): Tox21_300190
M4ID: 12478940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.56 MAX_MED: 1.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

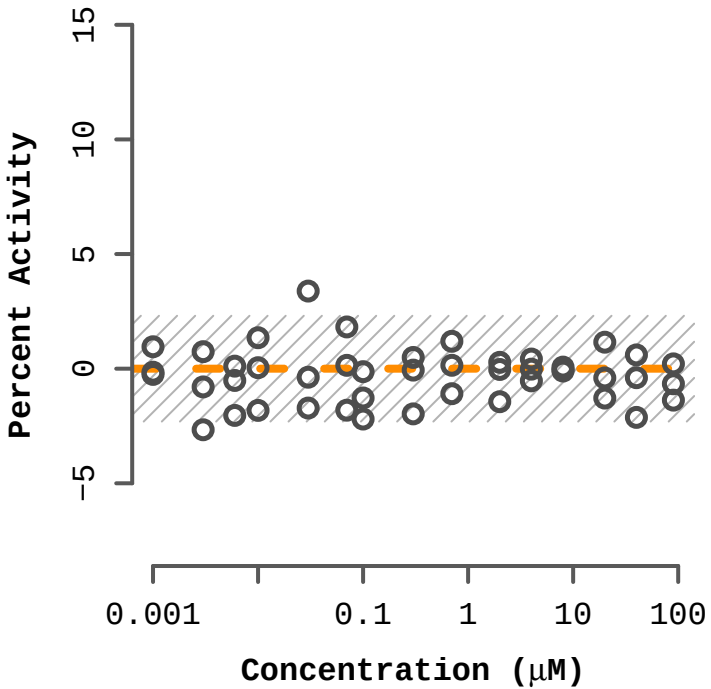
NAME: Chlorendic acid
CHID: 20268 **CASRN:** 115-28-6
SPID(S): Tox21_202339
M4ID: 12479913

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

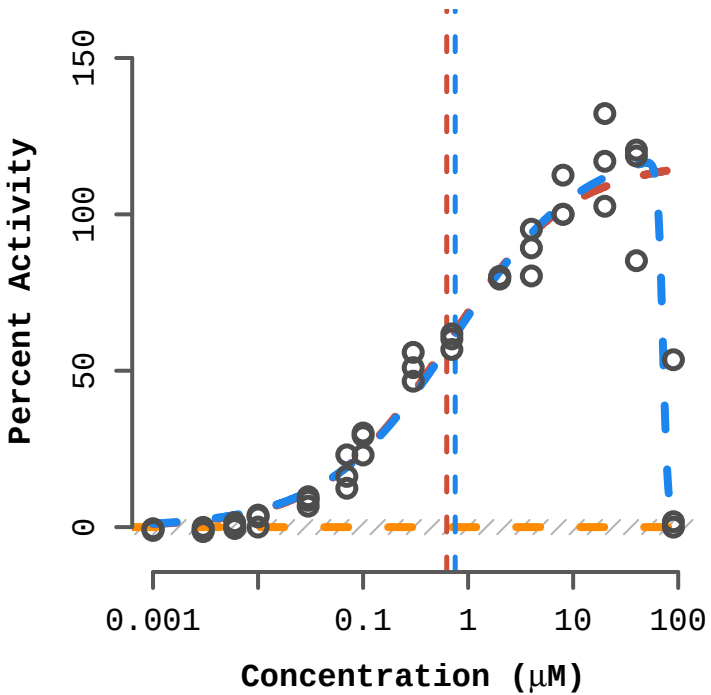
NAME: Chlorinated paraffins (C12, 60% chlorine)
CHID: 20269 **CASRN:** NOCAS_20269
SPID(S): Tox21_202496
M4ID: 12479756

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.433 **MAX_MED:** 0.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlormadinone acetate
CHID: 20274 CASRN: 302-22-7
SPID(S): Tox21_200665
M4ID: 12481587

HILL MODEL (in red):

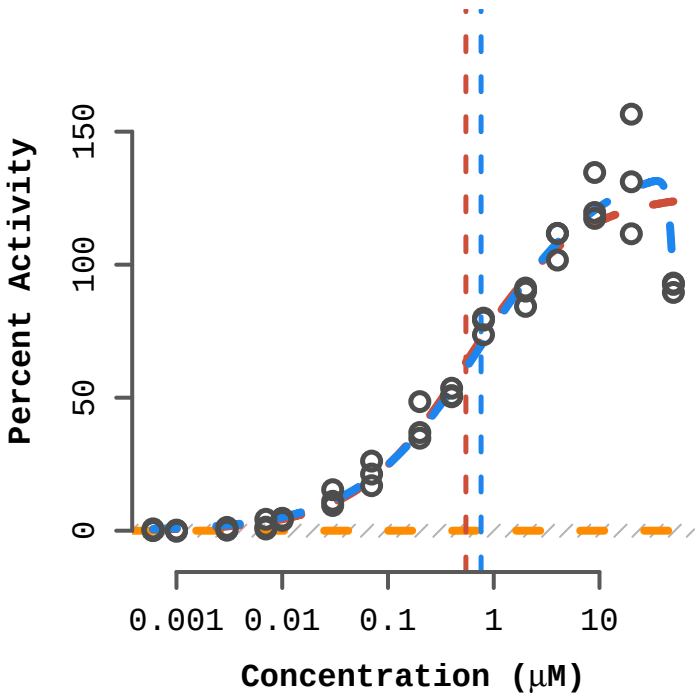
	tp	ga	gw
val:	117	-0.204	0.743
sd:	6.66	0.102	0.0666

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	123	-0.123	0.709	1.85	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	504.97	365.93	321.56
PROB:	0	0	1
RMSE:	62.86	26.57	10.65

MAX_MEAN: 117 MAX_MED: 119 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlormadinone acetate
CHID: 20274 CASRN: 302-22-7
SPID(S): Tox21_110881_1
M4ID: 12484046

HILL MODEL (in red):

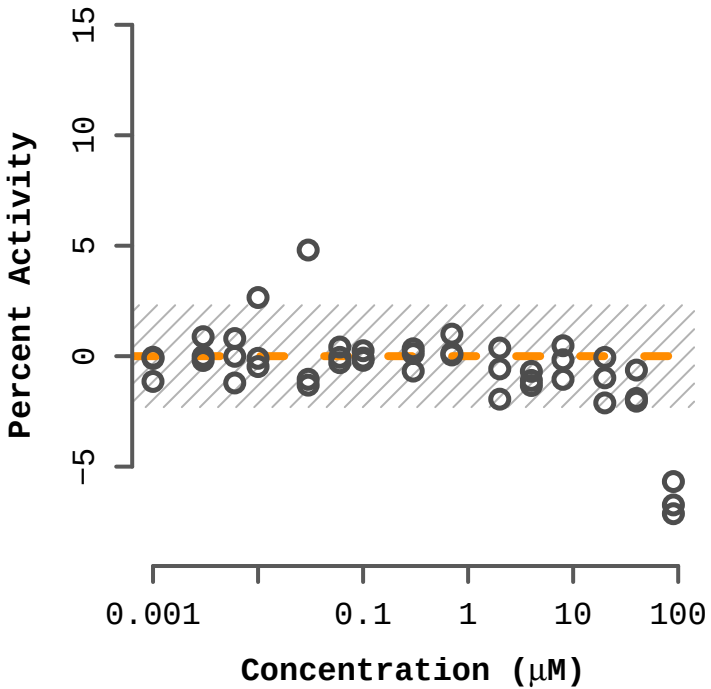
	tp	ga	gw
val:	127	-0.263	0.834
sd:	7.05	0.0817	0.0716

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	139	-0.12	0.753	1.72	13.9
sd:	5.2	0.0634	0.0439	0.00348	1.96

	CNST	HILL	GNLS
AIC:	513.99	328.47	286.96
PROB:	0	0	1
RMSE:	69.53	11.07	6.48

MAX_MEAN: 133 MAX_MED: 131 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

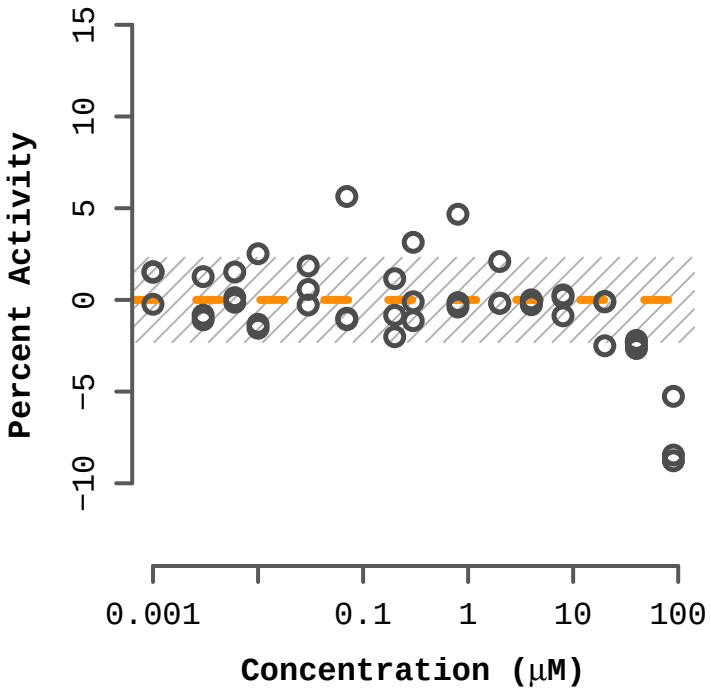
NAME: 4-Chloro-4'-aminodiphenyl ether
CHID: 20275 **CASRN:** 101-79-1
SPID(S): Tox21_200985
M4ID: 12481267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 0.139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

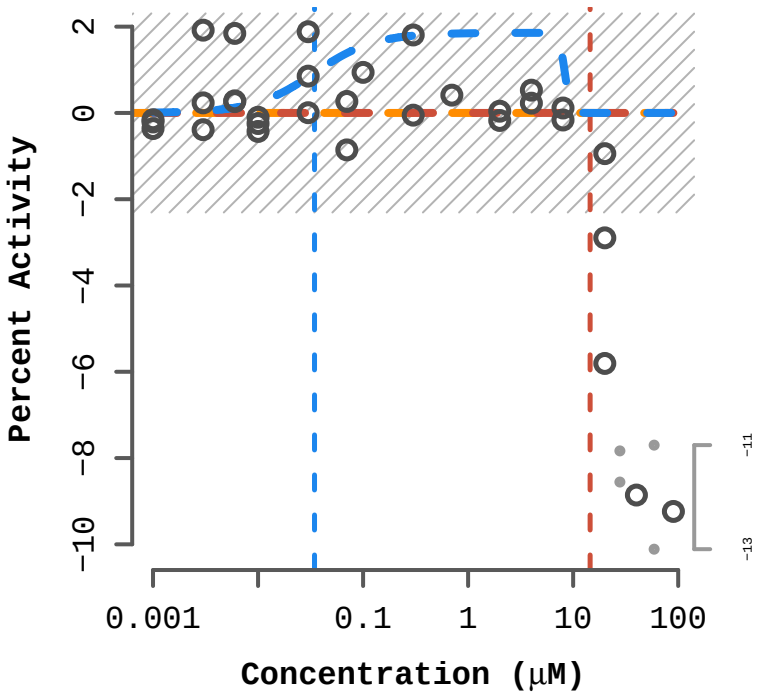
NAME: 3-Chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-fu
CHID: 20276 CASRN: 77439-76-0
SPID(S): Tox21_201209
M4ID: 12481043

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.74	NA	NA
PROB:	1	NA	NA
RMSE:	2.6	NA	NA

MAX_MEAN: 1.38 MAX_MED: 1.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Chloro-2,4-dinitrobenzene
CHID: 20278 CASRN: 97-00-7
SPID(S): Tox21_302802
M4ID: 12476331 BRK

HILL MODEL (in red):

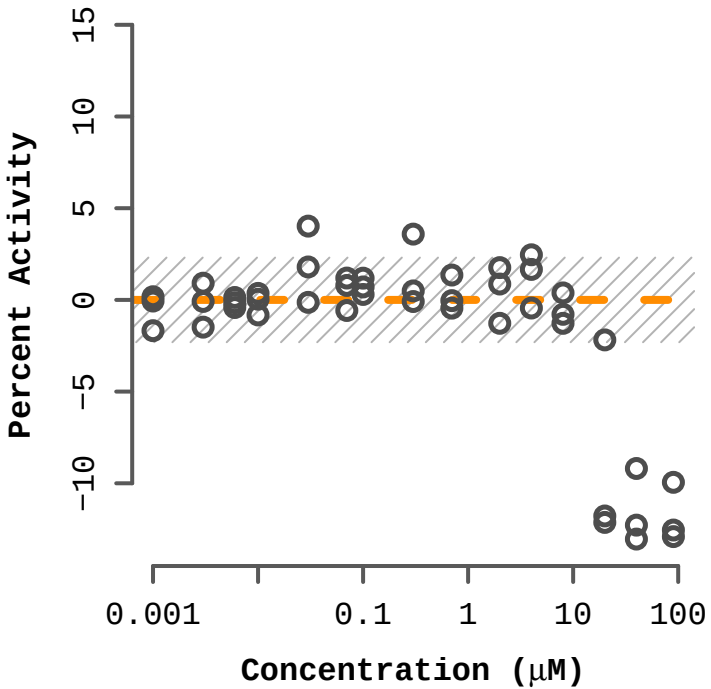
	tp	ga	gw
val:	4.04e-10	1.16	0.372
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.86	-1.46	1.52	0.921	15.6
sd:	0.804	0.666	3.37	0.639	553

	CNST	HILL	GNLS
AIC:	255.04	261.04	256.69
PROB:	0.67	0.03	0.29
RMSE:	4.55	4.55	4.38

MAX_MEAN: 2.84 MAX_MED: 3.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

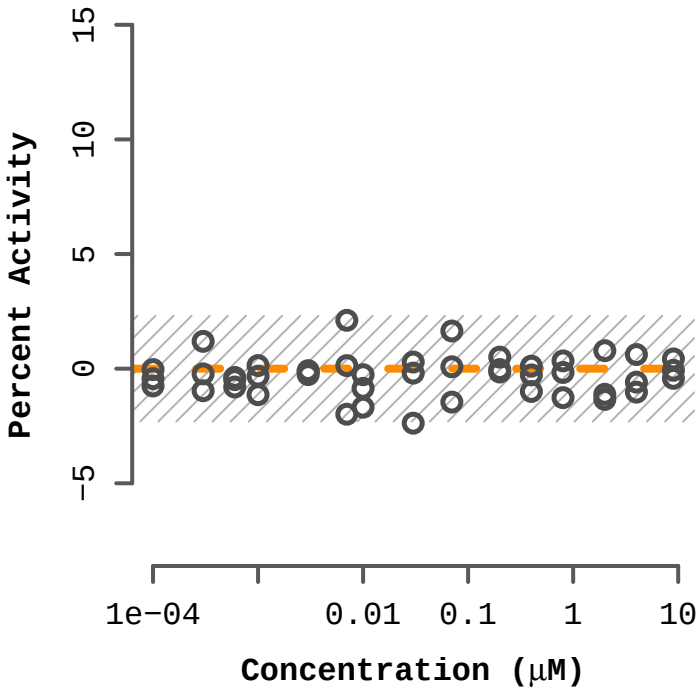
NAME: 1-Chloro-2,4-dinitrobenzene
CHID: 20278 **CASRN:** 97-00-7
SPID(S): Tox21_201956
M4ID: 12480296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	259.14	NA	NA
PROB:	1	NA	NA
RMSE:	5.12	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

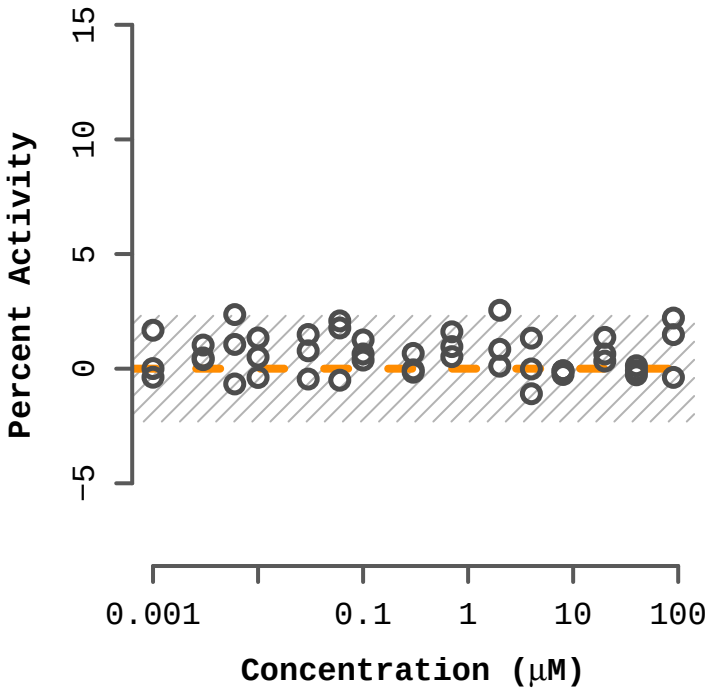
NAME: 3-Chloro-2-methylpropene
CHID: 20279 **CASRN:** 563-47-3
SPID(S): Tox21_303609
M4ID: 12475536

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.108 **MAX_MED:** 0.136 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

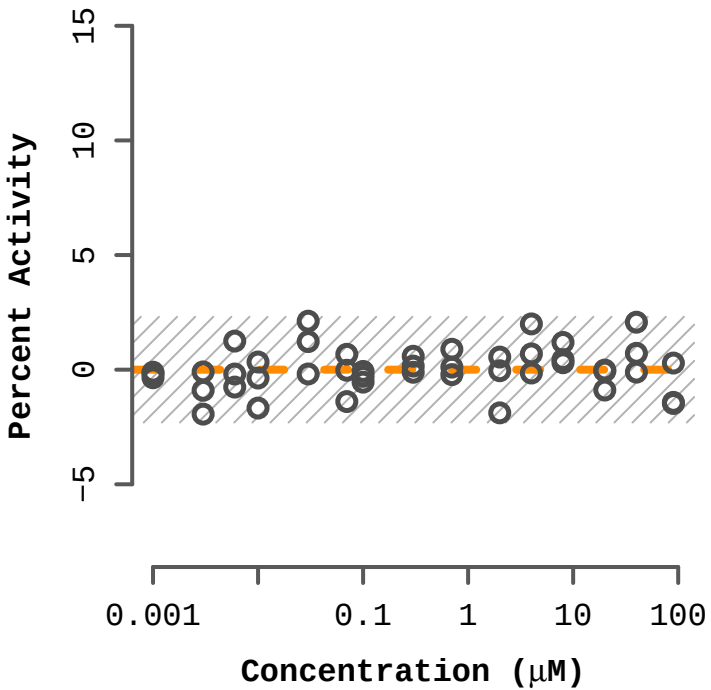
NAME: 3-Chloro-2-methylpropene
CHID: 20279 **CASRN:** 563-47-3
SPID(S): Tox21_201640
M4ID: 12480612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

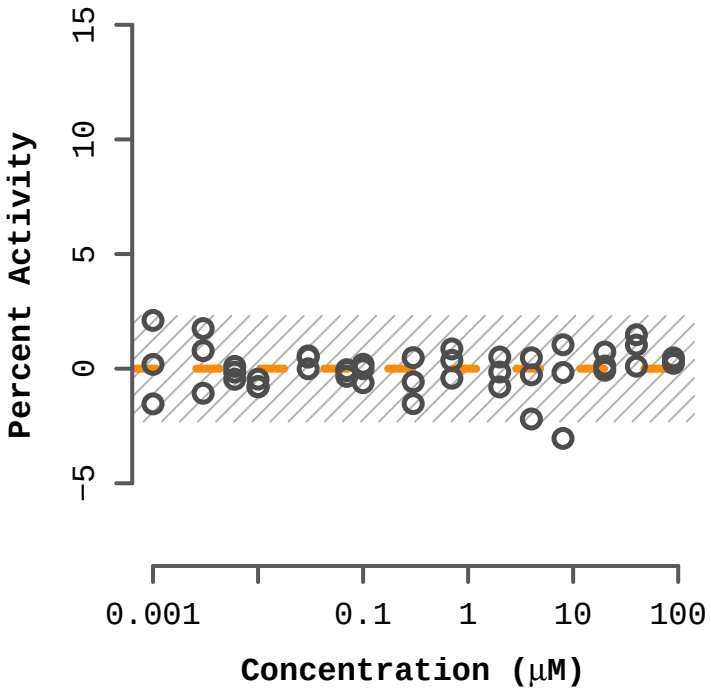
NAME: 1-Chloro-2-nitrobenzene
CHID: 20280 **CASRN:** 88-73-3
SPID(S): Tox21_200791
M4ID: 12481461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

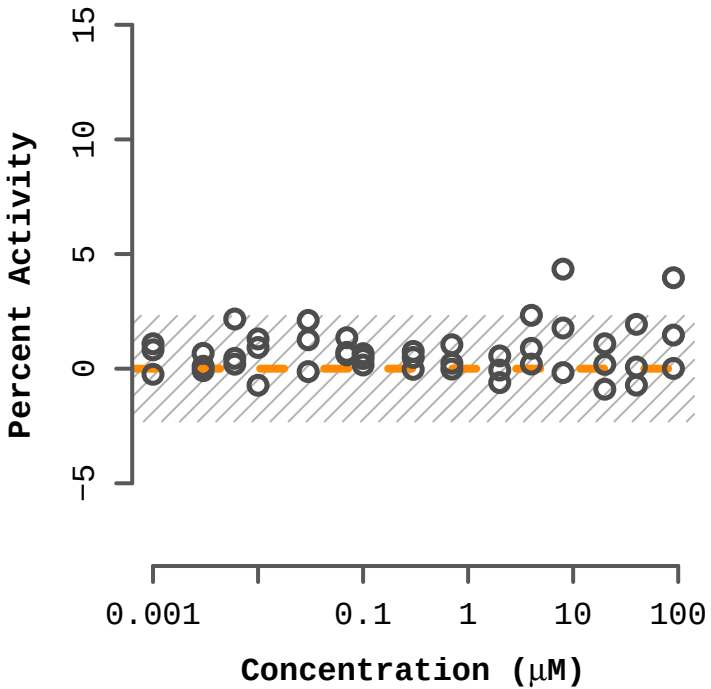
NAME: 1-Chloro-4-nitrobenzene
CHID: 20281 CASRN: 100-00-5
SPID(S): Tox21_300033
M4ID: 12479097

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.874 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

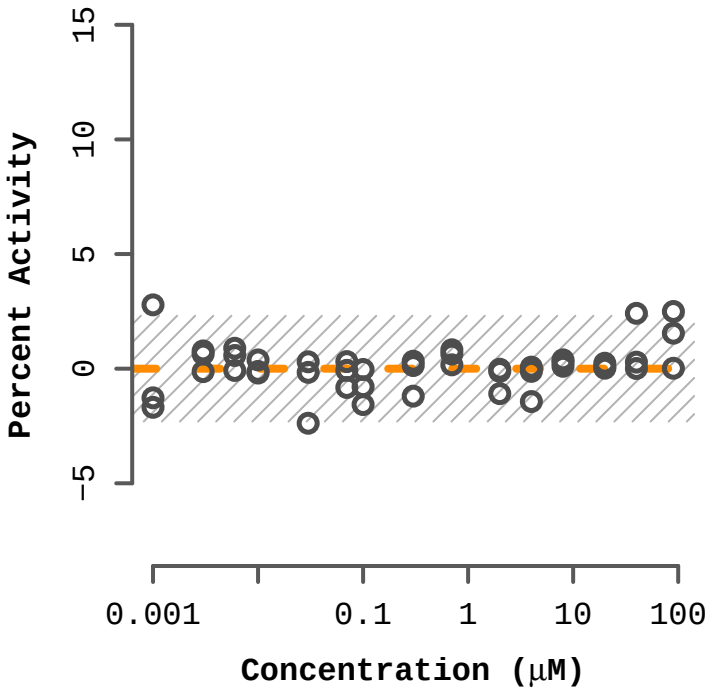
NAME: 1-Chloro-4-nitrobenzene
CHID: 20281 **CASRN:** 100-00-5
SPID(S): Tox21_202291
M4ID: 12479961

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.98 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

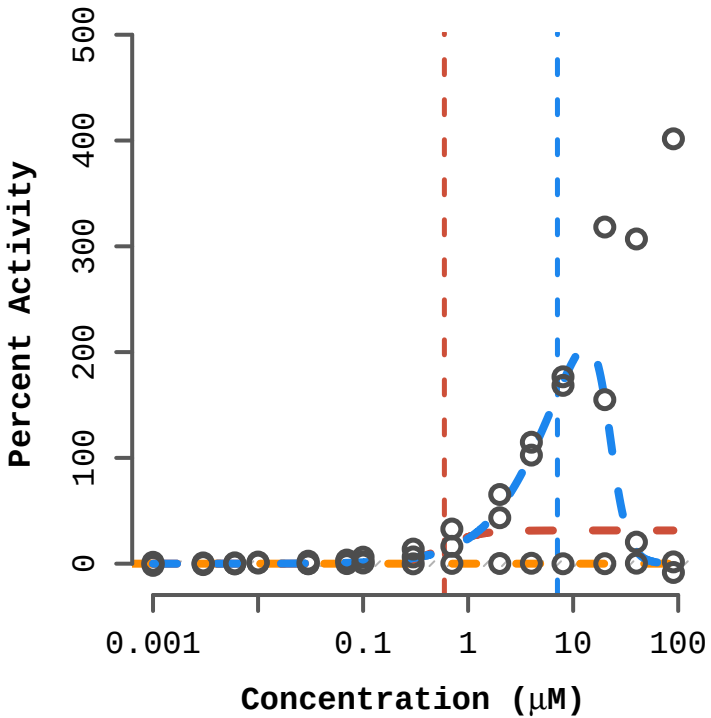
NAME: 4-Chloro-1,3-diaminobenzene
CHID: 20282 **CASRN:** 5131-60-2
SPID(S): Tox21_302821
M4ID: 12476312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.77	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chloro-1,3-diaminobenzene
CHID: 20282 CASRN: 5131-60-2
SPID(S): Tox21_201696
M4ID: 12480556

HILL MODEL (in red):

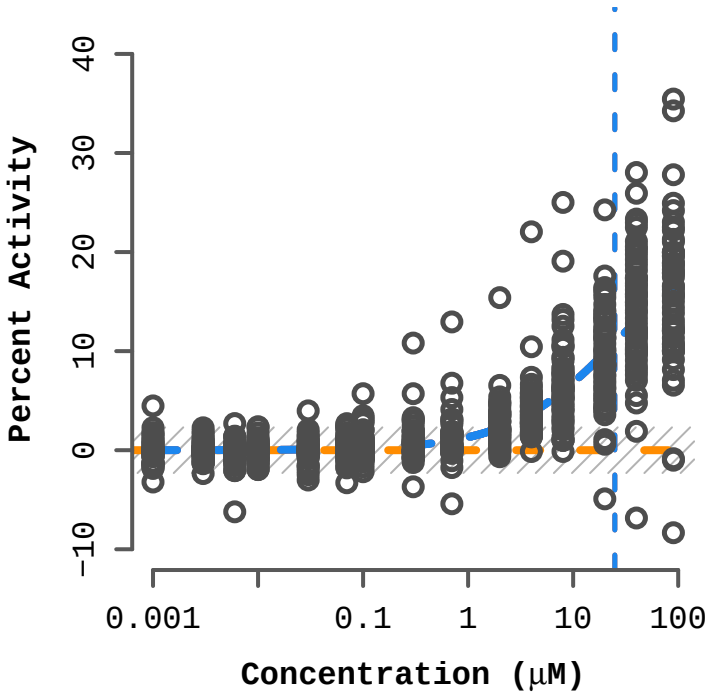
	tp	ga	gw
val:	31.4	-0.226	2.7
sd:	16.8	0.428	3.97

GAIN-LOSS MODEL (in blue):

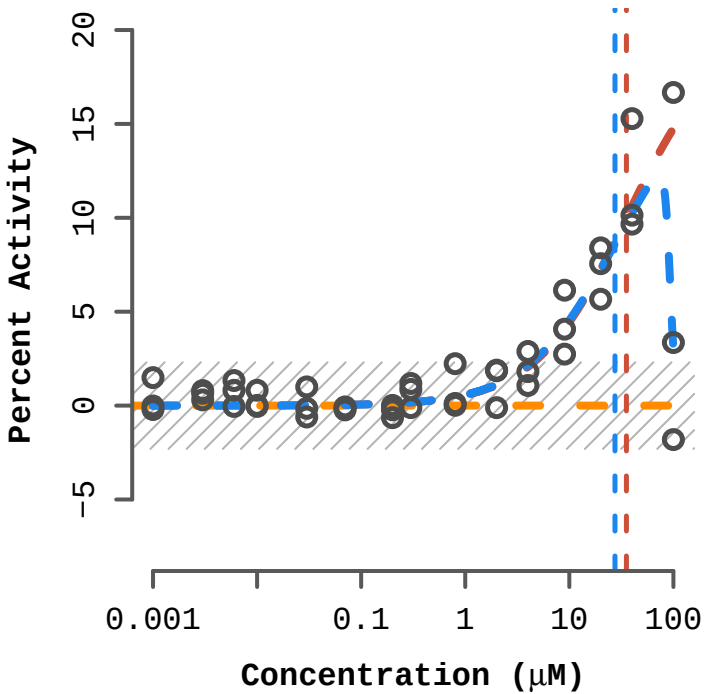
	tp	ga	gw	la	lw
val:	320	0.85	1.29	1.34	5.2
sd:	75.9	0.166	0.226	0.0218	1.25

	CNST	HILL	GNLS
AIC:	507.87	500.5	468.9
PROB:	0	0	1
RMSE:	102.48	90.93	87.32

MAX_MEAN: 158 MAX_MED: 169 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Chloro-1,2-diaminobenzene
CHID:    20283   CASRN: 95-83-0
SPID(S): Tox21_400037
M4ID:    12475100

HILL MODEL (in red):
      tp       ga       gw
val:  21.7     1.4      0.853
sd:   2.19     0.118    0.0665

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  21.7     1.4      0.853    3.04     10.7
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  4905.85     3614.32     3618.32
PROB: 0           0.88        0.12
RMSE: 7.17        3.45        3.45

MAX_MEAN: 15.5      MAX_MED: 15.8      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chloro-1,2-diaminobenzene
CHID: 20283 **CASRN:** 95-83-0
SPID(S): Tox21_202984
M4ID: 12479268

HILL MODEL (in red):

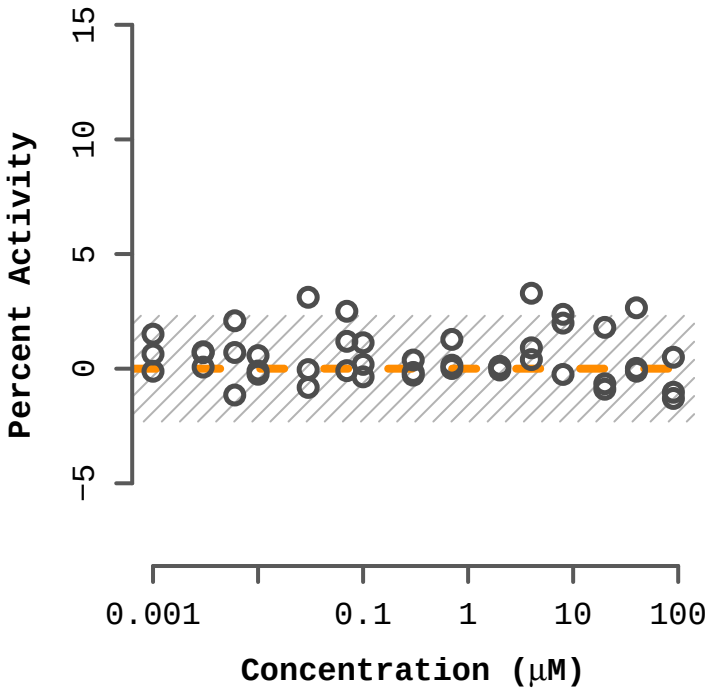
	tp	ga	gw
val:	20	1.55	0.993
sd:	10.5	0.43	0.212

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.2	1.44	1.02	1.97	16.5
sd:	8.71	0.457	0.309	0.0118	5.99

	CNST	HILL	GNLS
AIC:	246.76	177.7	167.75
PROB:	0	0.01	0.99
RMSE:	4.67	3.19	2.42

MAX_MEAN: 11.7 **MAX_MED:** 10.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

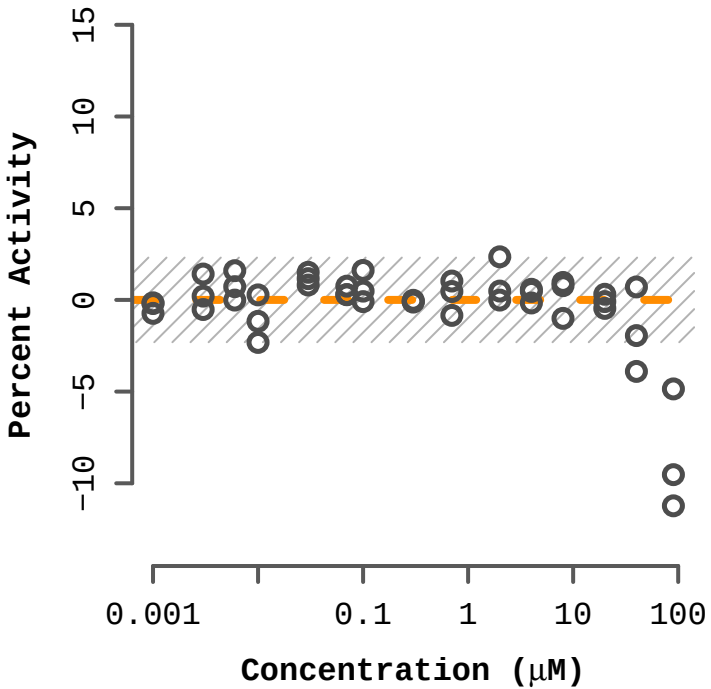
NAME: 2-Chloro-1,4-diaminobenzene sulfate
CHID: 20284 **CASRN:** 61702-44-1
SPID(S): Tox21_302907
M4ID: 12476226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

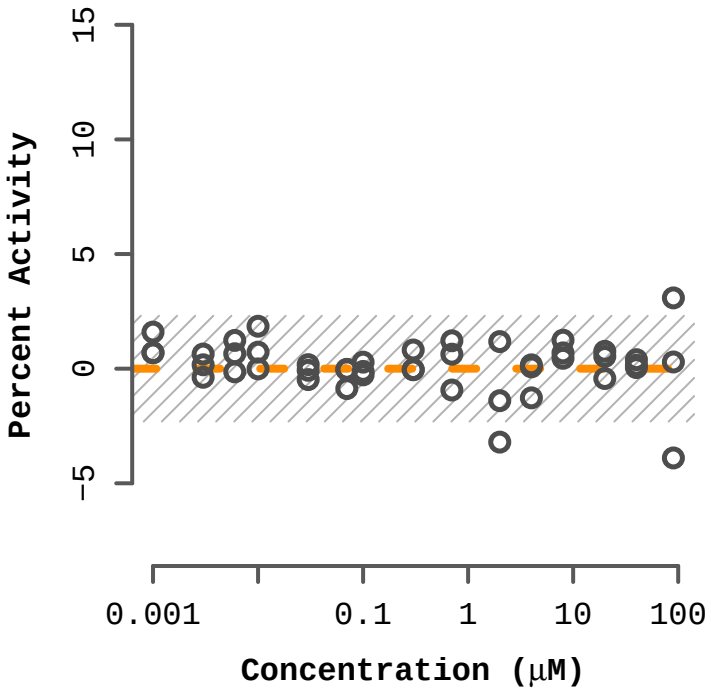
NAME: 2-Chloro-1,4-diaminobenzene sulfate
CHID: 20284 **CASRN:** 61702-44-1
SPID(S): Tox21_201310
M4ID: 12480942

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.85	NA	NA
PROB:	1	NA	NA
RMSE:	2.55	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

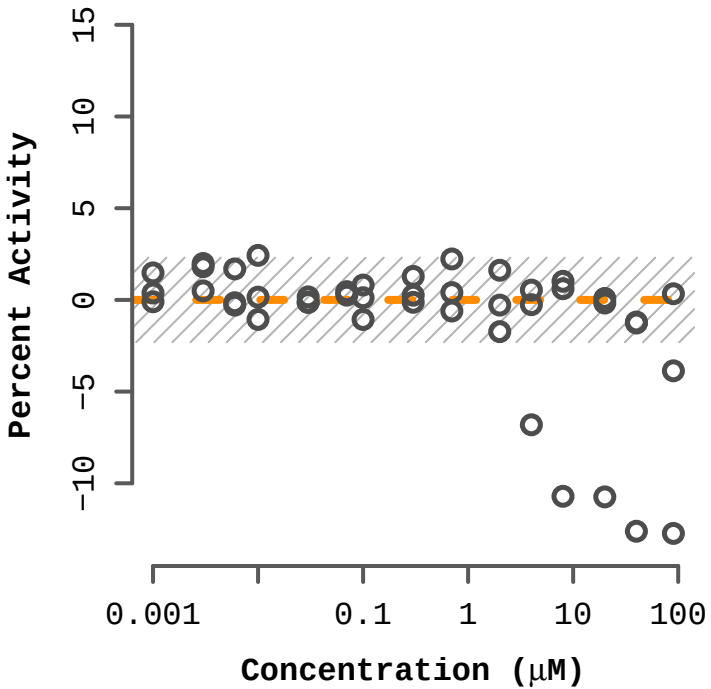
NAME: 3-Chloro-4-methylaniline
CHID: 20286 **CASRN:** 95-74-9
SPID(S): Tox21_302755
M4ID: 12476378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.997 **MAX_MED:** 0.723 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

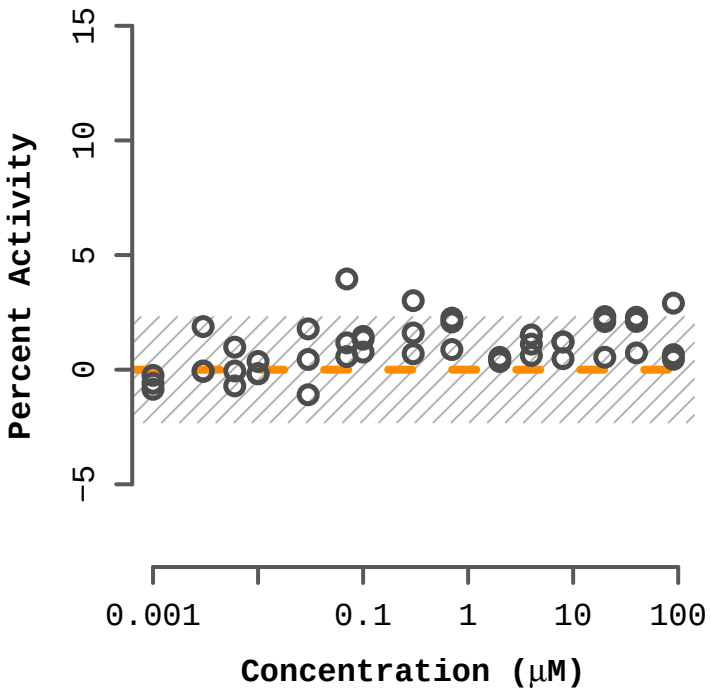
NAME: 3-Chloro-4-methylaniline
CHID: 20286 **CASRN:** 95-74-9
SPID(S): Tox21_201871
M4ID: 12480381

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.81	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

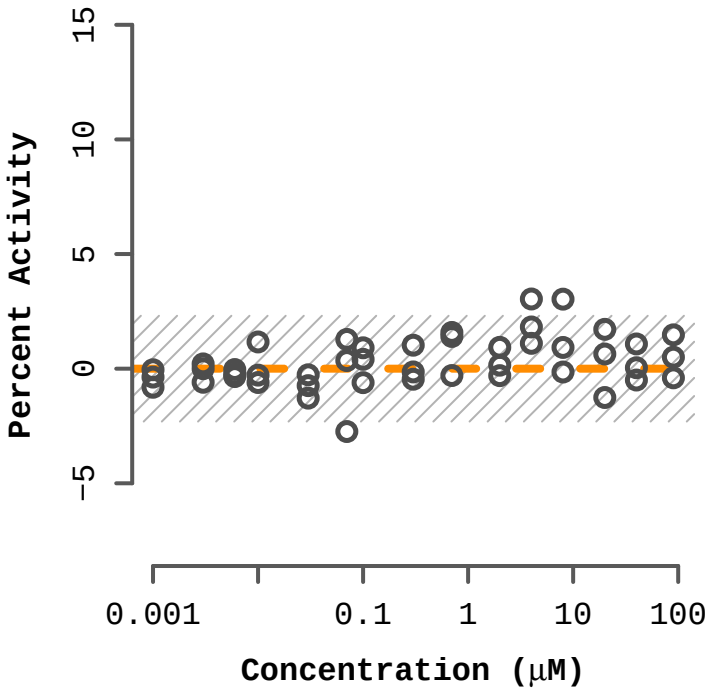
NAME: 5-Chloro-2-methylaniline
CHID: 20287 **CASRN:** 95-79-4
SPID(S): Tox21_200075
M4ID: 12482177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

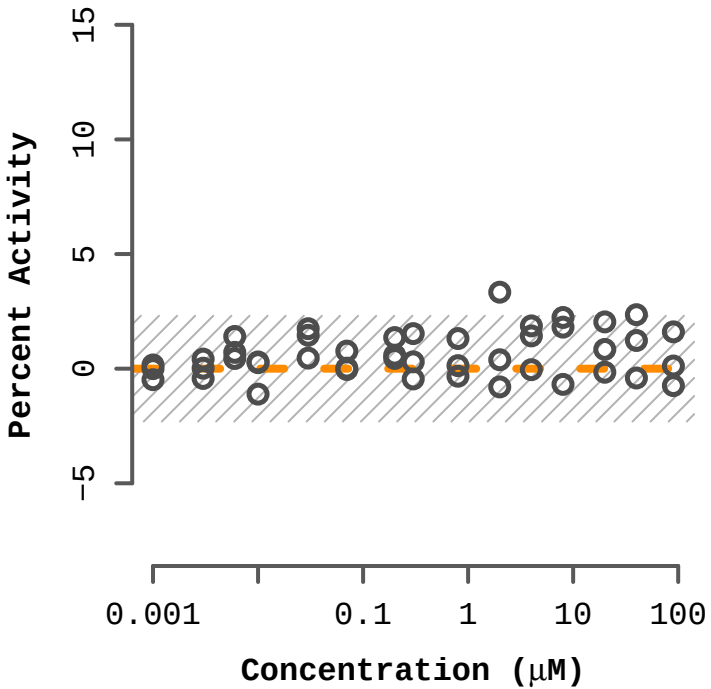
NAME: 4-Chloro-2-methylaniline hydrochloride
CHID: 20288 **CASRN:** 3165-93-3
SPID(S): Tox21_302920
M4ID: 12476213

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

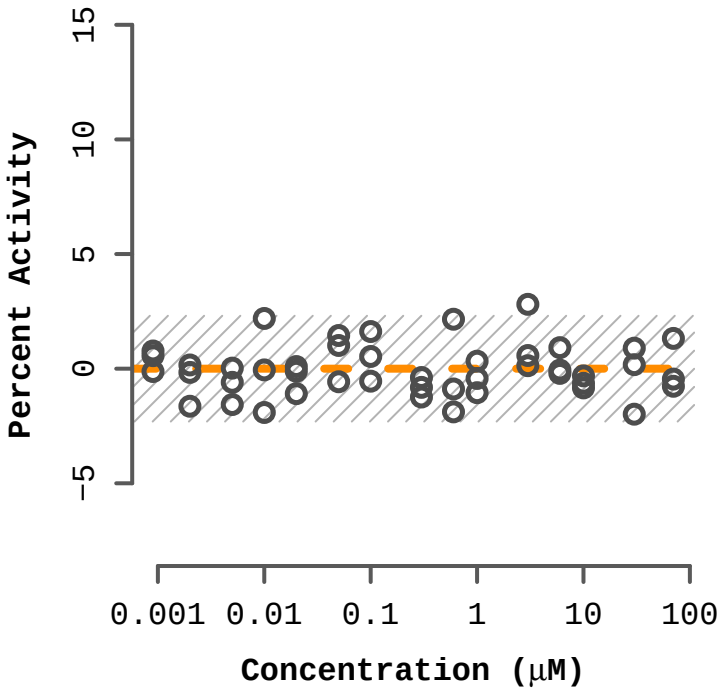
NAME: 4-Chloro-2-methylaniline hydrochloride
CHID: 20288 **CASRN:** 3165-93-3
SPID(S): Tox21_201283
M4ID: 12480969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

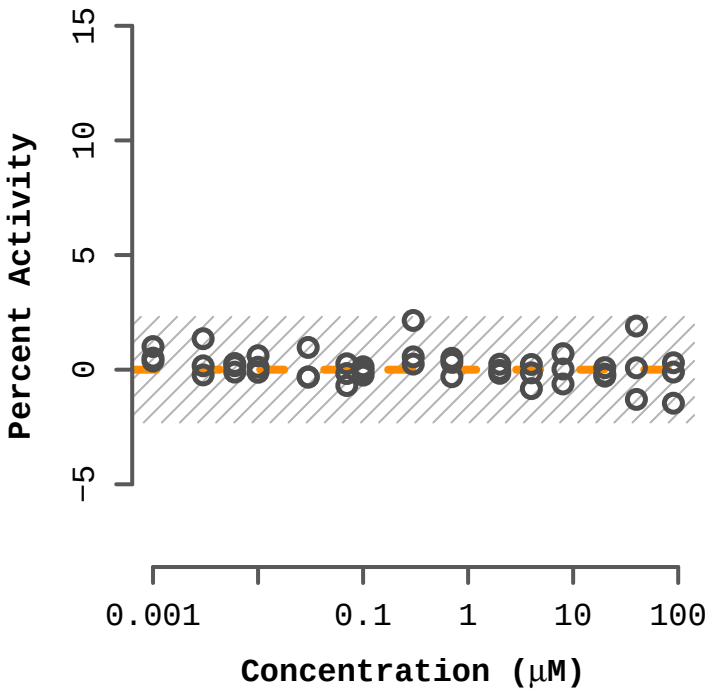
NAME: Pirinixic acid
CHID: 20290 CASRN: 50892-23-4
SPID(S): Tox21_300634
M4ID: 12478499

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.17 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

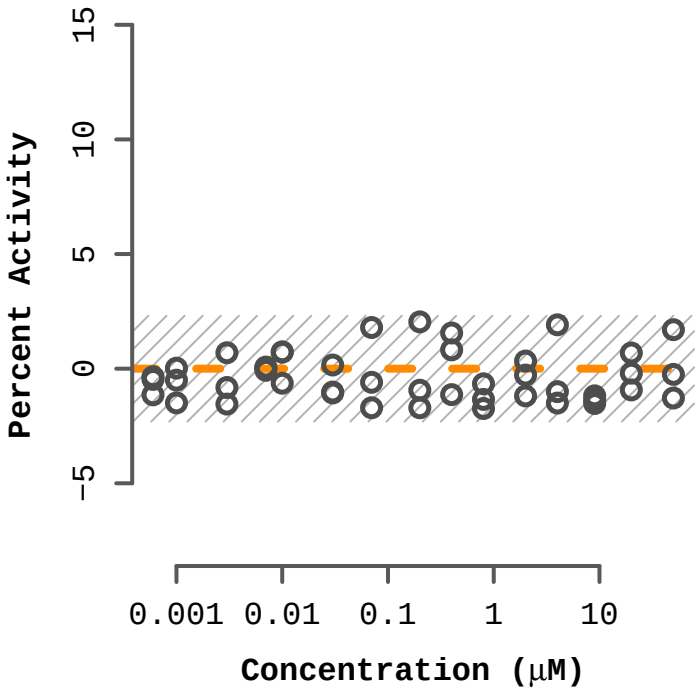
NAME: Pirinixic acid
CHID: 20290 CASRN: 50892-23-4
SPID(S): Tox21_201609
M4ID: 12480643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	86.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.985 MAX_MED: 0.561 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

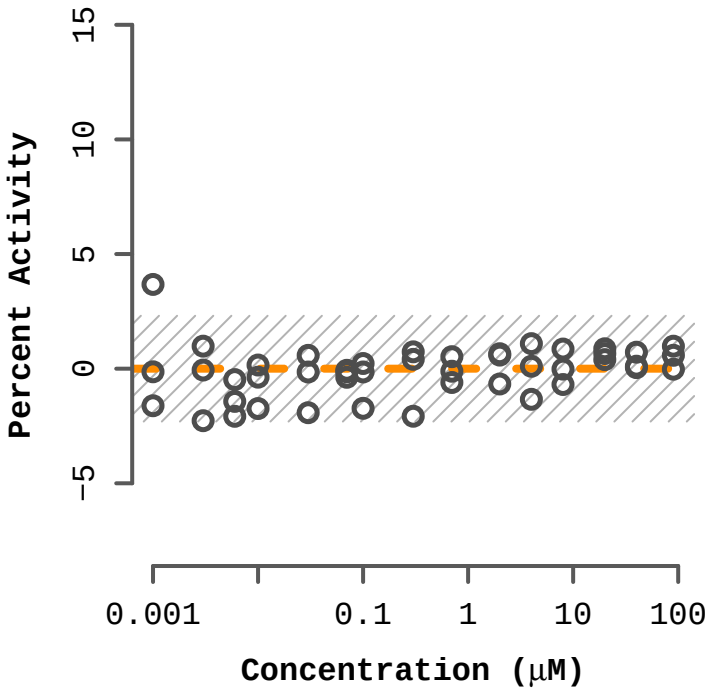
NAME: Pirinixic acid
CHID: 20290 **CASRN:** 50892-23-4
SPID(S): Tox21_110058_1
M4ID: 12484691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.821 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

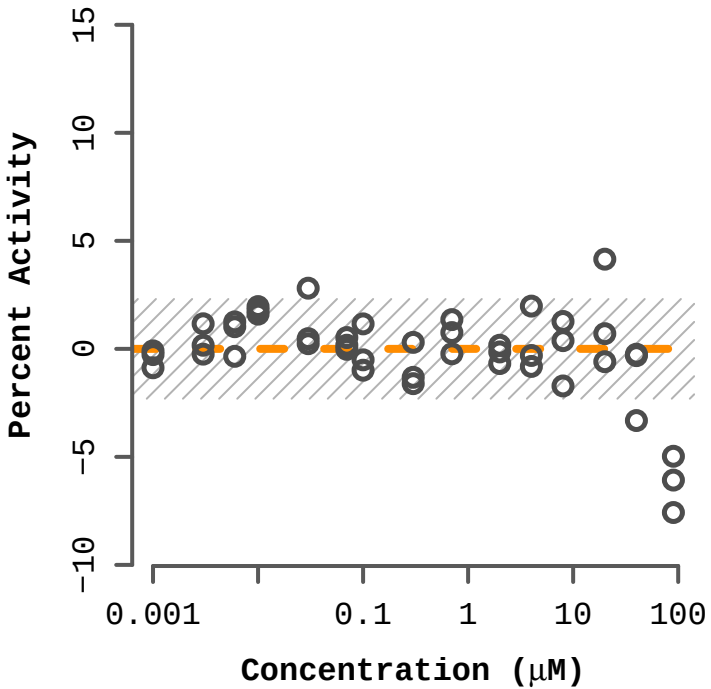
NAME: Chloroacetaldehyde
CHID: 20292 **CASRN:** 107-20-0
SPID(S): Tox21_301152
M4ID: 12477981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.643 **MAX_MED:** 0.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

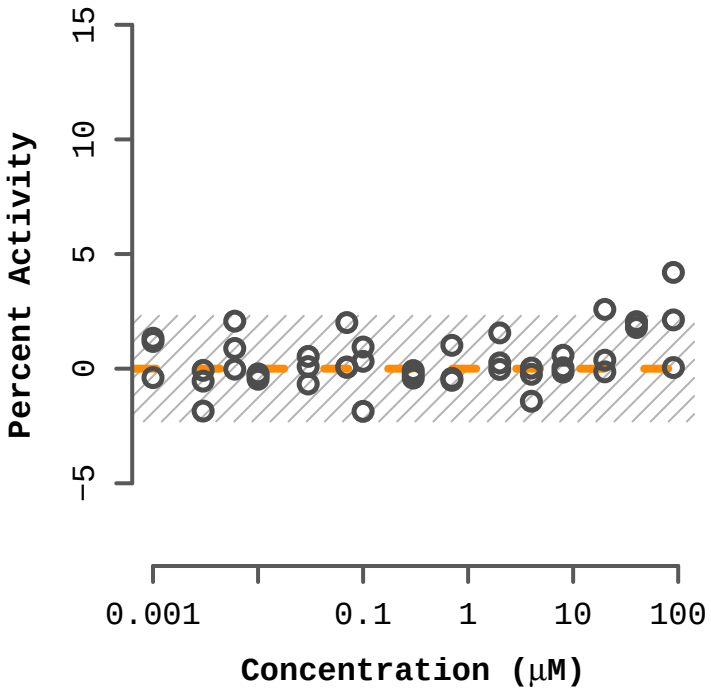
NAME: 2-Chloroacetophenone
CHID: 20293 **CASRN:** 532-27-4
SPID(S): Tox21_300045
M4ID: 12479085

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.75	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

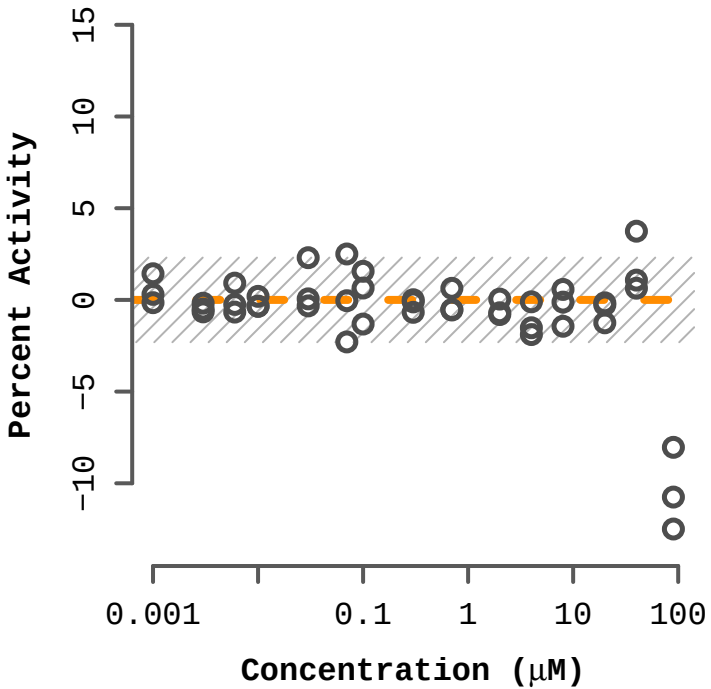
NAME: 2-Chloroacetophenone
CHID: 20293 **CASRN:** 532-27-4
SPID(S): Tox21_202075
M4ID: 12480177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

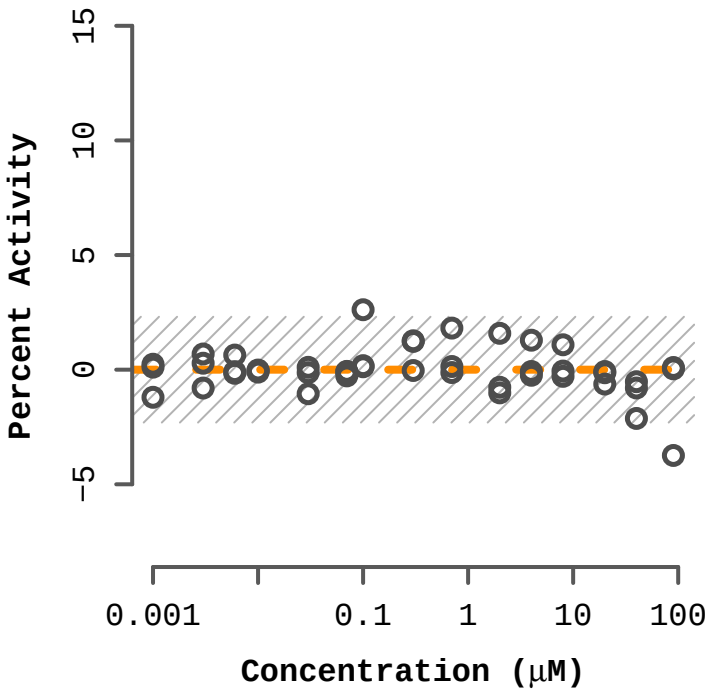
NAME: 4'−(Chloroacetyl)acetanilide
CHID: 20294 **CASRN:** 140−49−8
SPID(S): Tox21_302954
M4ID: 12476179

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.95	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

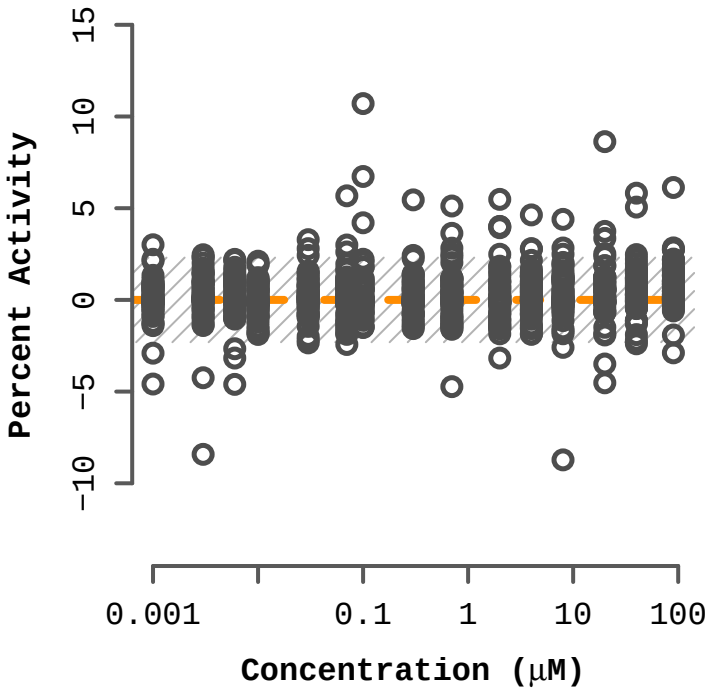
NAME: 4'−(Chloroacetyl)acetanilide
CHID: 20294 **CASRN:** 140−49−8
SPID(S): Tox21_201314
M4ID: 12480938

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.19	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.974 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

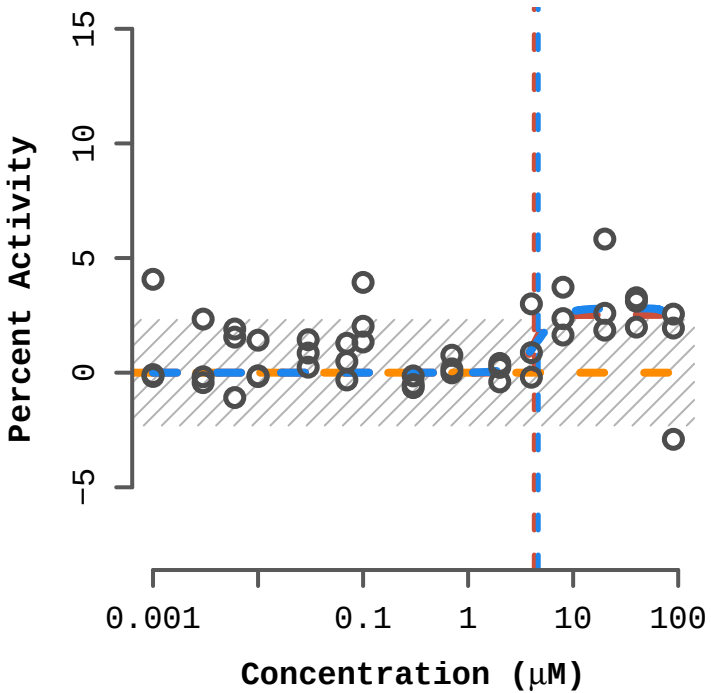
NAME: 4-Chloroaniline
CHID: 20295 **CASRN:** 106-47-8
SPID(S): Tox21_400030
M4ID: 12475107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2511.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.828 **MAX_MED:** 0.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chloroaniline hydrochloride
CHID: 20296 CASRN: 20265-96-7
SPID(S): Tox21_302915
M4ID: 12476218

HILL MODEL (in red):

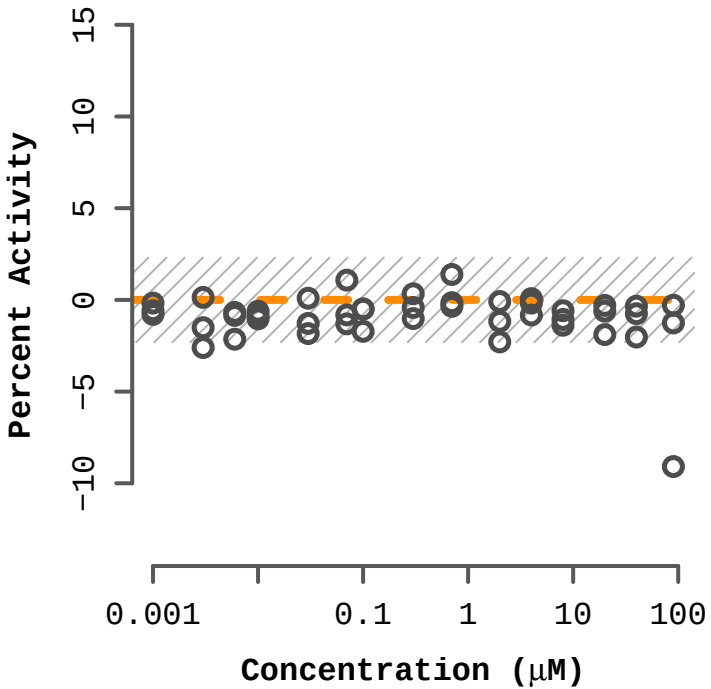
	tp	ga	gw
val:	2.52	0.63	6.36
sd:	0.365	0.12	20.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.8	0.667	3.97	1.98	10.7
sd:	0.47	0.135	3.99	0.124	48.9

	CNST	HILL	GNLS
AIC:	191.85	165.58	168.25
PROB:	0	0.79	0.21
RMSE:	1.99	1.56	1.5

MAX_MEAN: 3.43 MAX_MED: 3.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

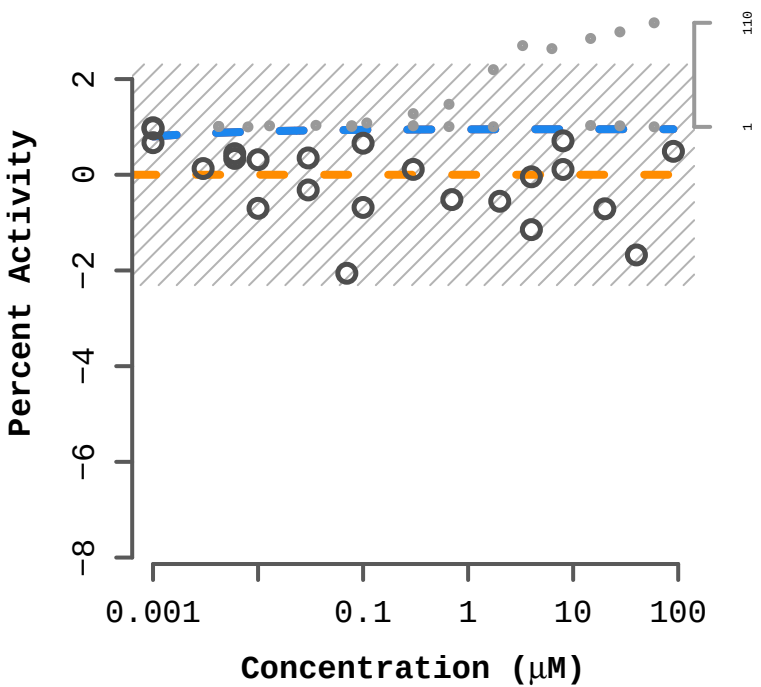
NAME: 4-Chloroaniline hydrochloride
CHID: 20296 **CASRN:** 20265-96-7
SPID(S): Tox21_201627
M4ID: 12480625

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 0.297 **MAX_MED:** −0.149 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorobenzene
CHID: 20298 **CASRN:** 108-90-7
SPID(S): Tox21_201223
M4ID: 12481029 **BRK**

HILL MODEL (in red):

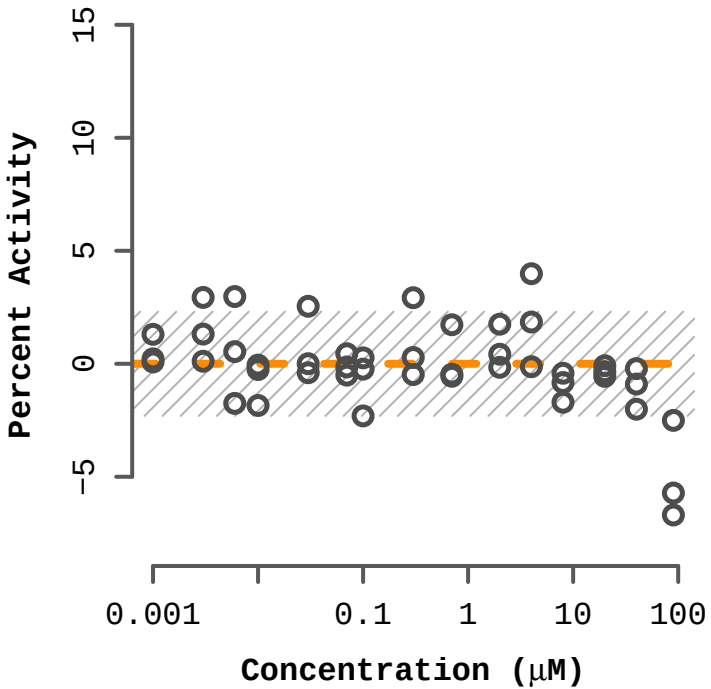
	tp	ga	gw
val:	0.953	-4.32	0.547
sd:	0.763	17.3	4.74

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.953	-4.32	0.546	3.93	2.81
sd:	0.763	17.3	4.75	3950	7240

	CNST	HILL	GNLS
AIC:	387.72	390.91	394.91
PROB:	0.81	0.16	0.02
RMSE:	34.76	34.39	34.39

MAX_MEAN: 38.8 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

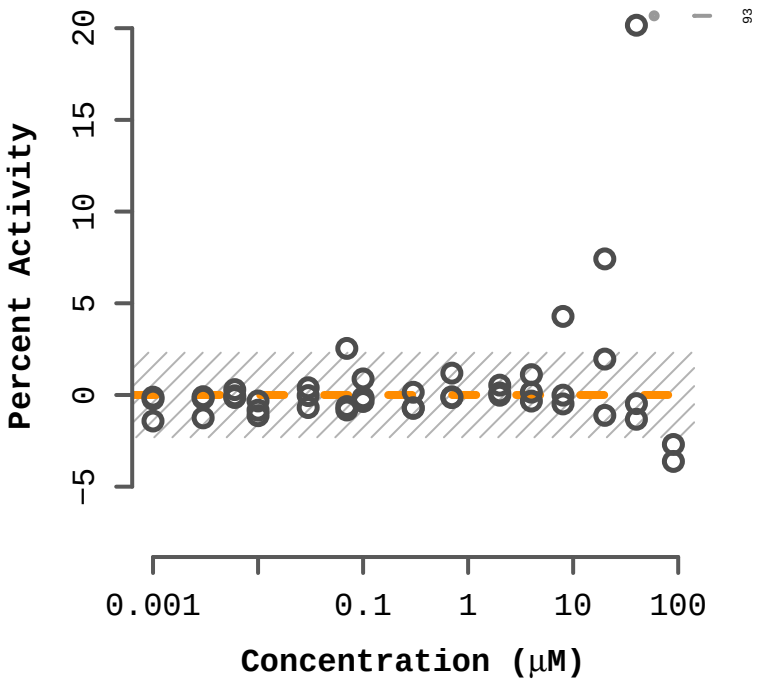
NAME: Chlorobenzilate
CHID: 20299 CASRN: 510-15-6
SPID(S): Tox21_300594
M4ID: 12478539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 1.9 MAX_MED: 1.85 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

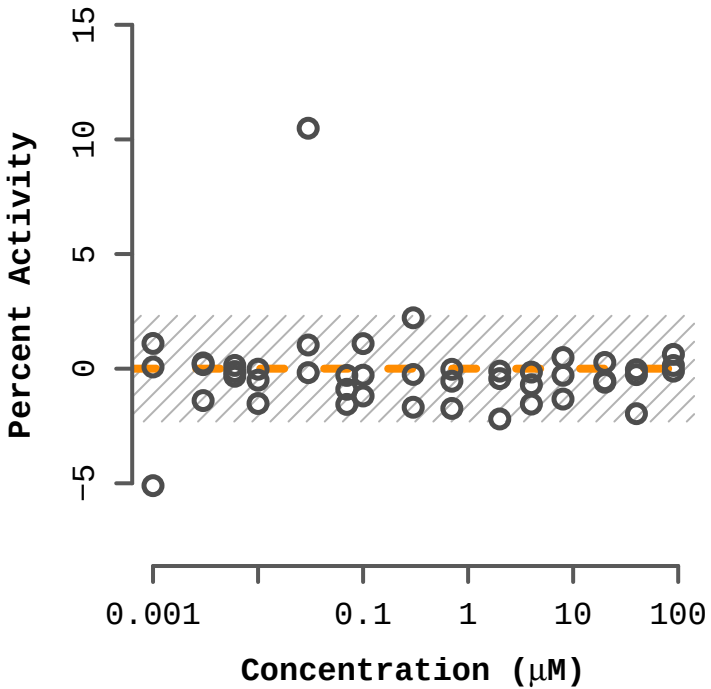
NAME: Chlorobenzilate
CHID: 20299 CASRN: 510-15-6
SPID(S): Tox21_201753
M4ID: 12480499 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.09	NA	NA
PROB:	1	NA	NA
RMSE:	14.33	NA	NA

MAX_MEAN: 29 MAX_MED: 1.96 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

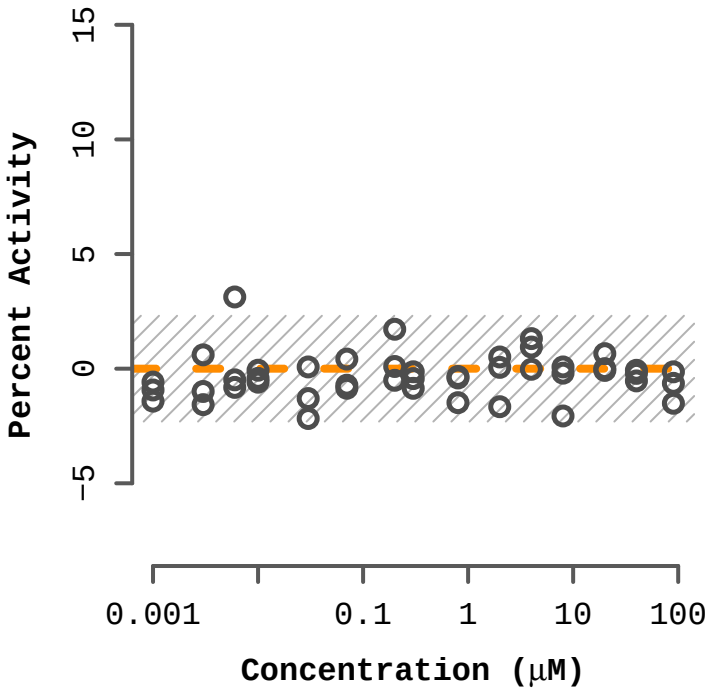
NAME: Chlorodibromomethane
CHID: 20300 CASRN: 124-48-1
SPID(S): Tox21_200153
M4ID: 12482099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 3.78 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

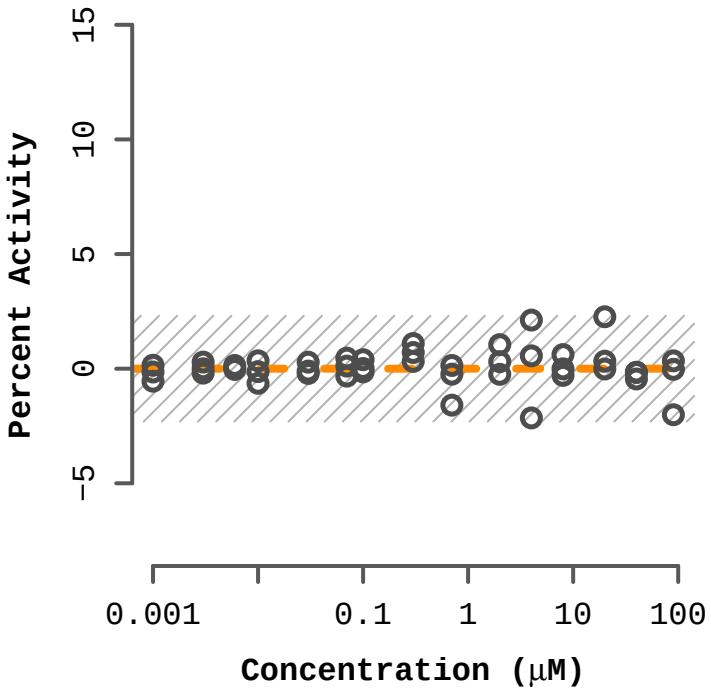
NAME: Chlormequat chloride
CHID: 20303 CASRN: 999-81-5
SPID(S): Tox21_200065
M4ID: 12482187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.744 **MAX_MED:** 0.944 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

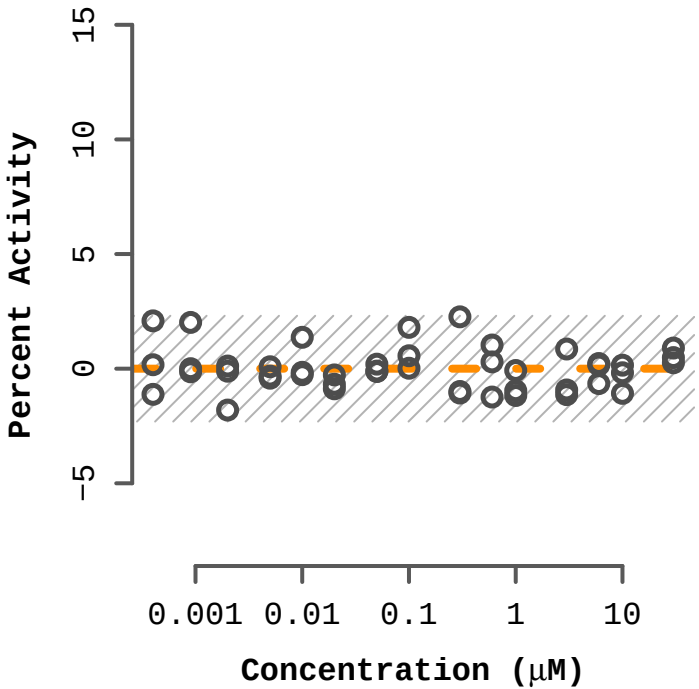
NAME: Chloroform
CHID: 20306 **CASRN:** 67-66-3
SPID(S): Tox21_202494
M4ID: 12479758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 0.707 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

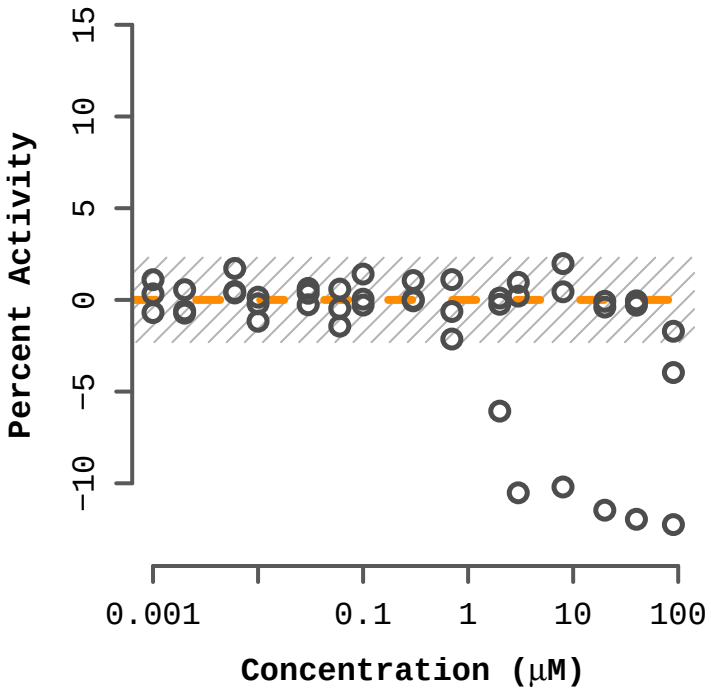
NAME: Chloromethyl methyl ether
CHID: 20307 **CASRN:** 107-30-2
SPID(S): Tox21_302939
M4ID: 12476194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.796 **MAX_MED:** 0.566 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

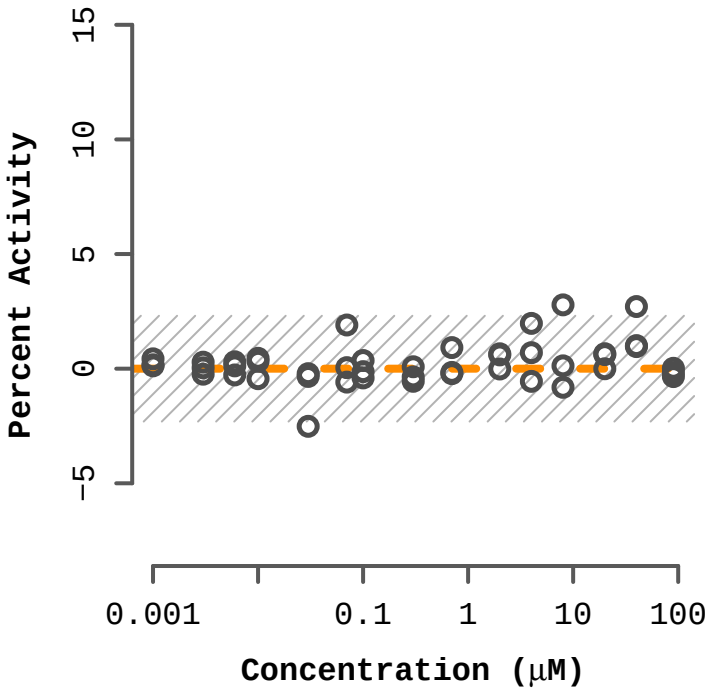
NAME: Chloromethyl methyl ether
CHID: 20307 **CASRN:** 107-30-2
SPID(S): Tox21_201575
M4ID: 12480677

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.8	NA	NA
PROB:	1	NA	NA
RMSE:	4	NA	NA

MAX_MEAN: 0.853 **MAX_MED:** 0.461 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

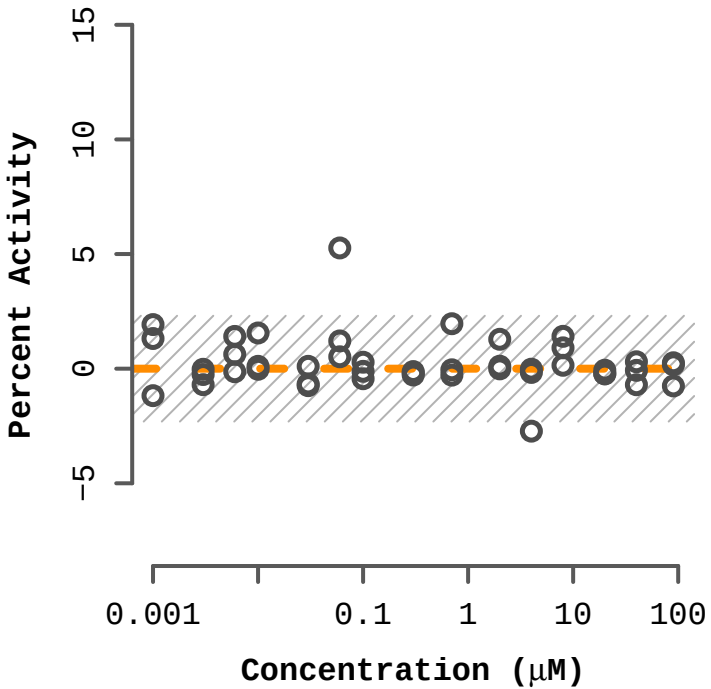
NAME: 2-(Chloromethyl)pyridine hydrochloride
CHID: 20308 **CASRN:** 6959-47-3
SPID(S): Tox21_302733
M4ID: 12476400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

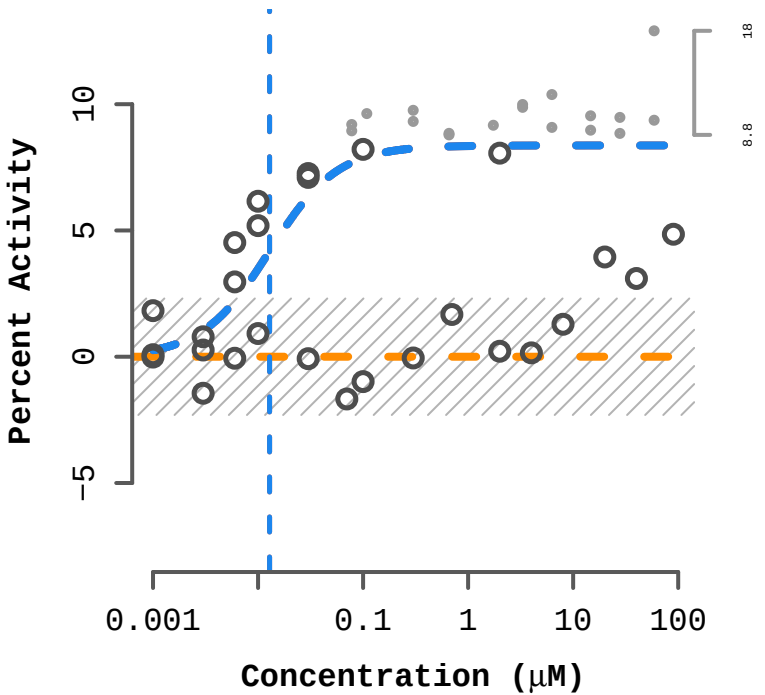
NAME: 2-(Chloromethyl)pyridine hydrochloride
CHID: 20308 CASRN: 6959-47-3
SPID(S): Tox21_201329
M4ID: 12480923

HILL MODEL: Not applicable.

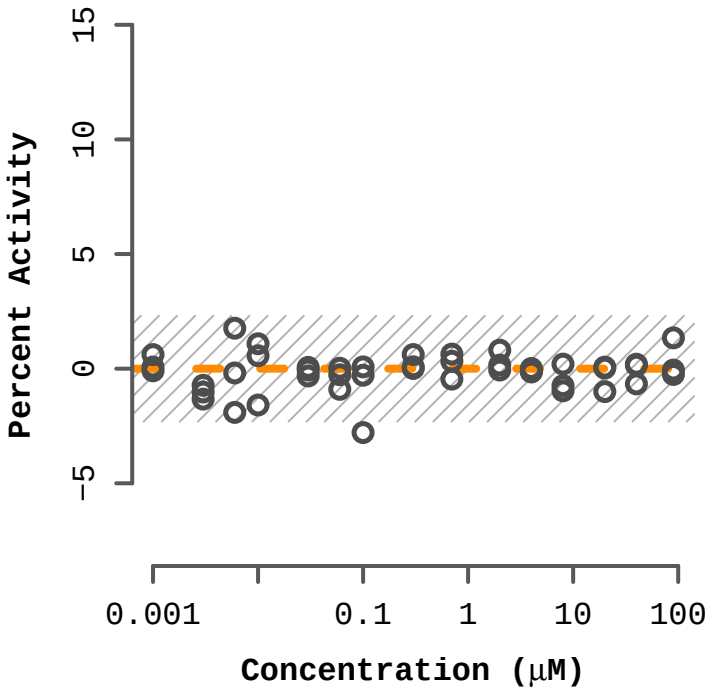
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.33 MAX_MED: 1.32 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-(Chloromethyl)pyridine hydrochloride
CHID:    20309   CASRN: 6959-48-4
SPID(S): Tox21_302887
M4ID:    12476246  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  8.37     -1.89    1.34
sd:   0.866    0.243    0.79

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.37     -1.89    1.34     3.92     3.55
sd:   0.866    0.243    0.79     805      1460

      CNST        HILL        GNLS
AIC:  314.91      262.79      266.79
PROB: 0           0.88        0.12
RMSE: 7.43        4.15        4.15

MAX_MEAN: 11.1      MAX_MED: 11.3      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

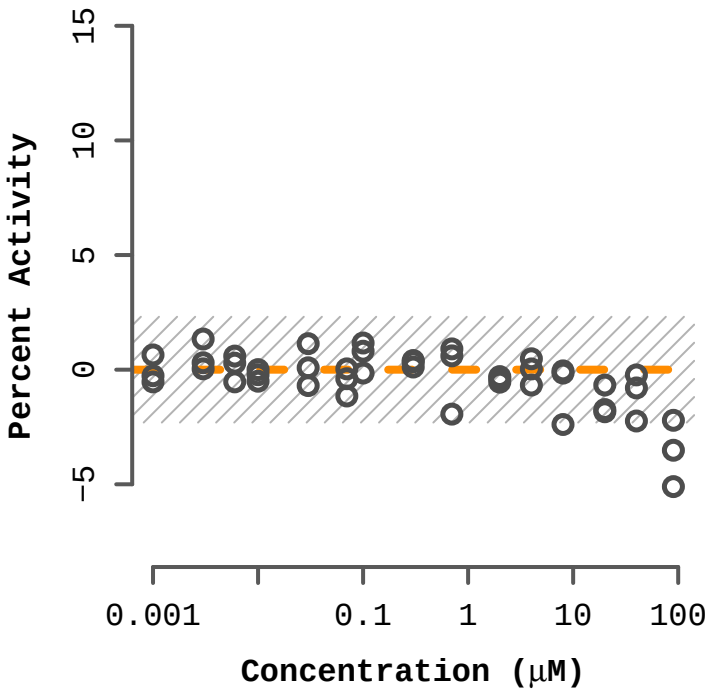
NAME: 3-(Chloromethyl)pyridine hydrochloride
CHID: 20309 **CASRN:** 6959-48-4
SPID(S): Tox21_202370
M4ID: 12479882

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.346 **MAX_MED:** 0.566 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

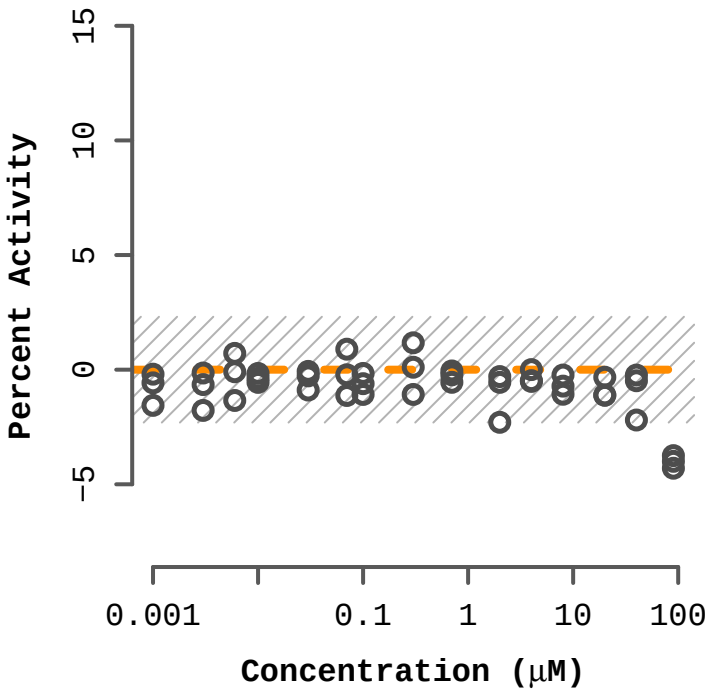
NAME: Chlorfenson
CHID: 20310 **CASRN:** 80-33-1
SPID(S): Tox21_302742
M4ID: 12476391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.807 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

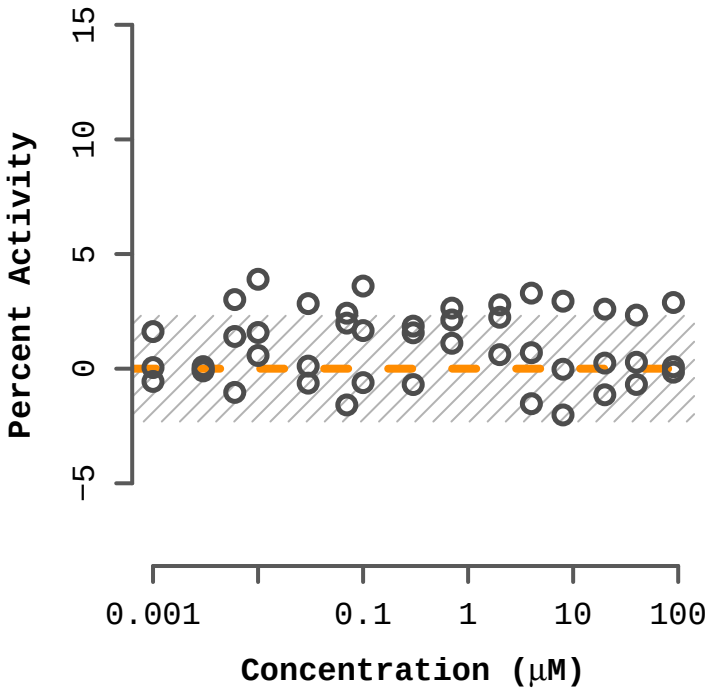
NAME: Chlorfenson
CHID: 20310 CASRN: 80-33-1
SPID(S): Tox21_201263
M4ID: 12480989

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.0672 MAX_MED: 0.107 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

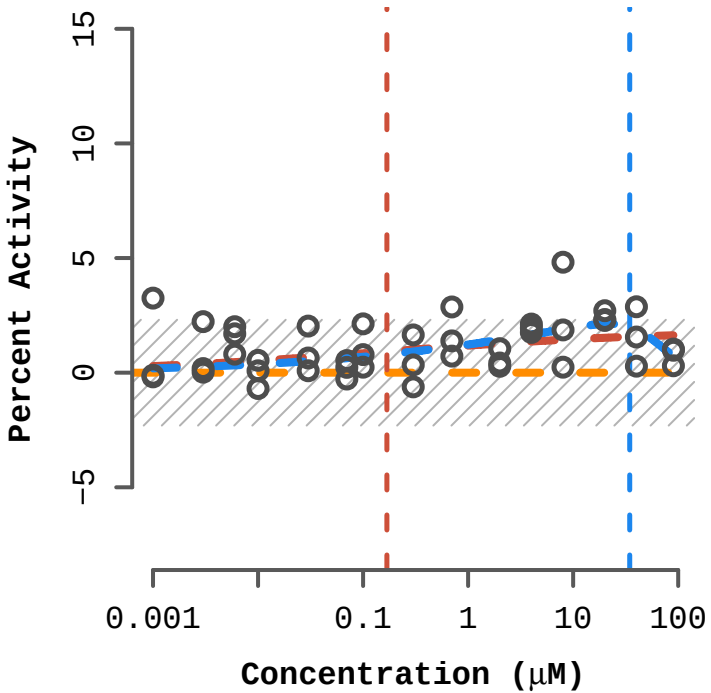
NAME: Monuron
CHID: 20311 CASRN: 150-68-5
SPID(S): Tox21_300367
M4ID: 12478765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 2.02 MAX_MED: 2.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Monuron
CHID: 20311 CASRN: 150-68-5
SPID(S): Tox21_201439
M4ID: 12480813

HILL MODEL (in red):

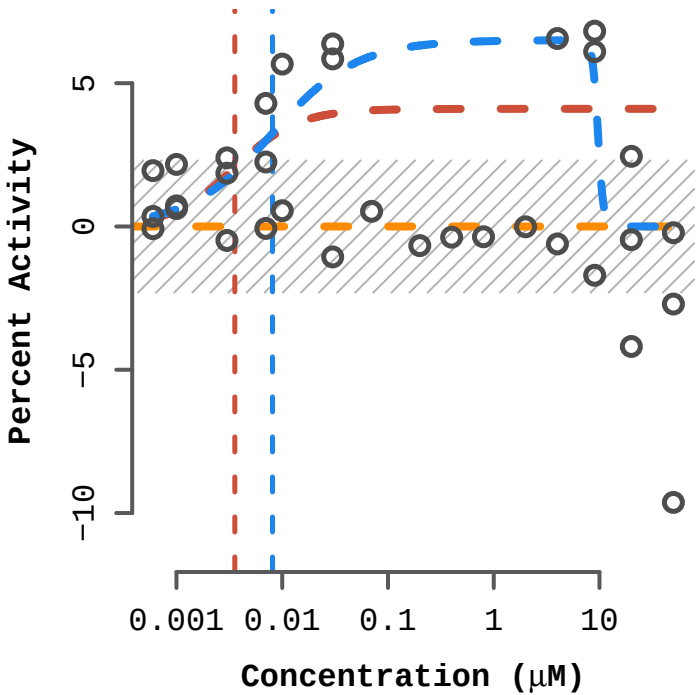
	tp	ga	gw
val:	1.84	−0.773	0.329
sd:	0.75	1.36	0.259

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.87	1.54	0.307	1.79	2.65
sd:	5.52	2.69	0.133	0.184	1.58

	CNST	HILL	GNLS
AIC:	173.91	144.73	142.18
PROB:	0	0.22	0.78
RMSE:	1.62	1.11	1.06

MAX_MEAN: 2.44 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Israpafant
CHID: 20312 CASRN: 117279-73-9
SPID(S): Tox21_113300
M4ID: 12482725

HILL MODEL (in red):

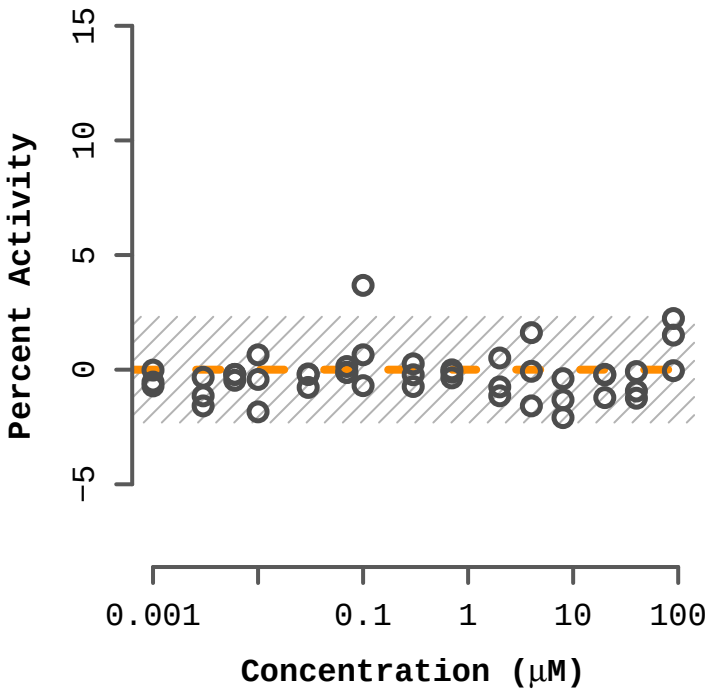
	tp	ga	gw
val:	4.11	−2.45	1.46
sd:	0.941	0.503	1.66

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.5	−2.09	1.1	0.986	16.8
sd:	0.96	0.277	0.709	0.356	189

	CNST	HILL	GNLS
AIC:	281.43	266.7	253.41
PROB:	0	0	1
RMSE:	5.18	4.2	3.58

MAX_MEAN: 5.89 **MAX_MED:** 8.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

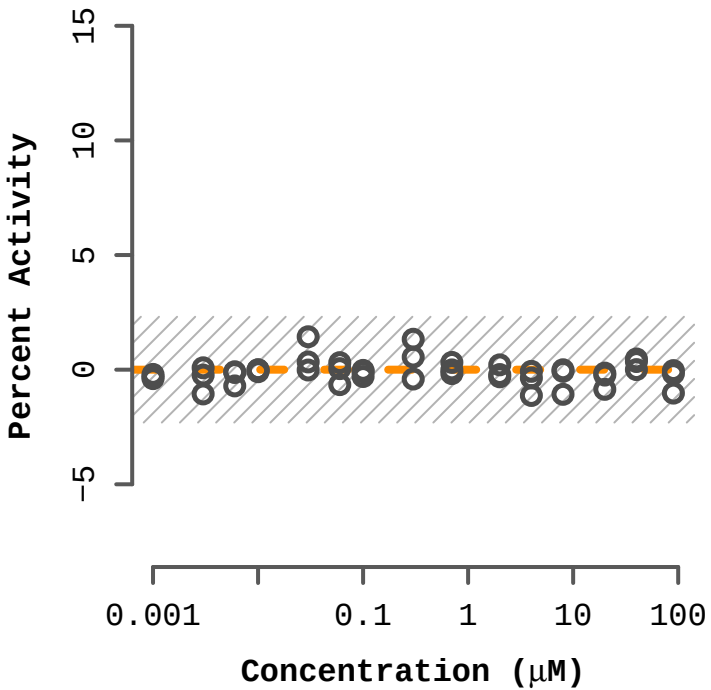
NAME: Tetrasul
CHID: 20314 **CASRN:** 2227-13-6
SPID(S): Tox21_302984
M4ID: 12476149

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

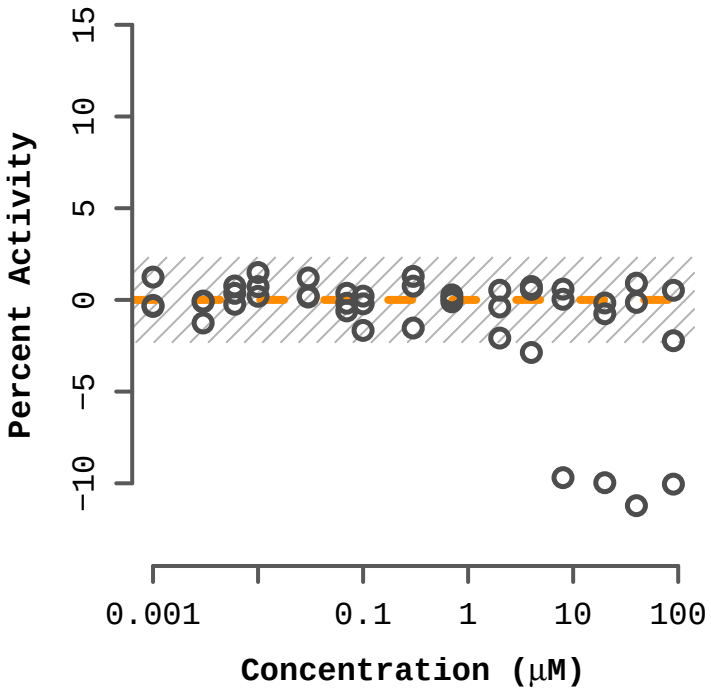
NAME: Tetrasul
CHID: 20314 CASRN: 2227-13-6
SPID(S): Tox21_202392
M4ID: 12479860

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	65.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.52	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 0.551 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

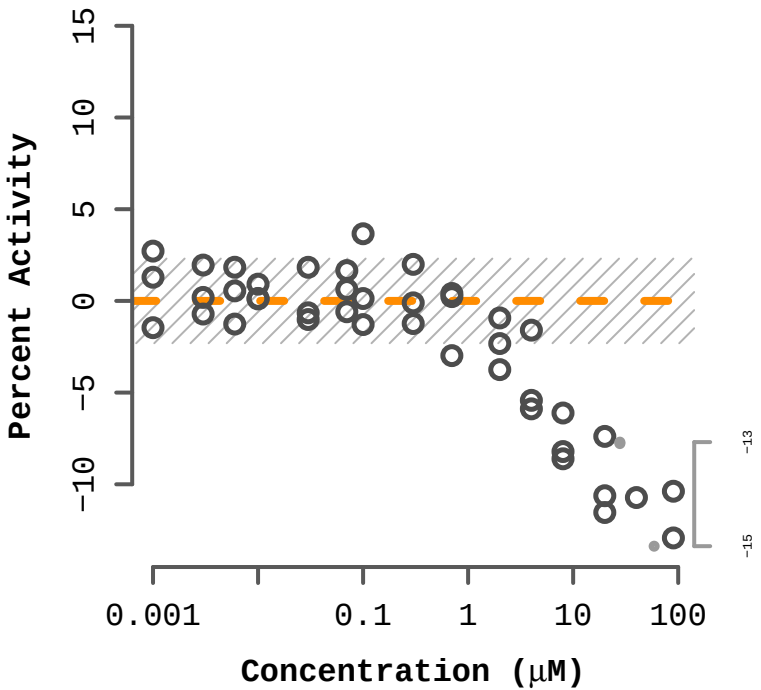
NAME: Chloropicrin
CHID: 20315 **CASRN:** 76-06-2
SPID(S): Tox21_201570
M4ID: 12480682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.61	NA	NA
PROB:	1	NA	NA
RMSE:	3.19	NA	NA

MAX_MEAN: 0.806 **MAX_MED:** 0.753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

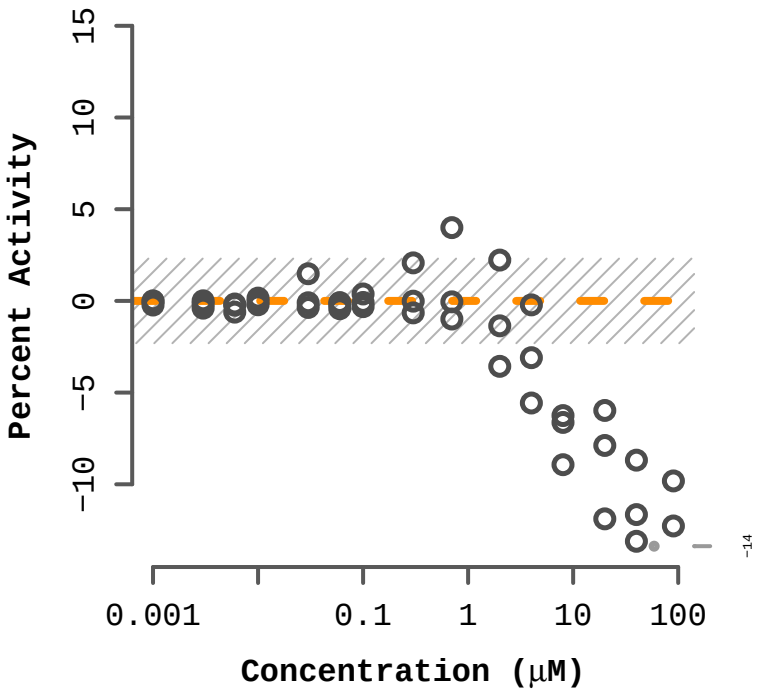
NAME: Chlorothalonil
CHID: 20319 **CASRN:** 1897-45-6
SPID(S): Tox21_300862
M4ID: 12478271 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.08	NA	NA
PROB:	1	NA	NA
RMSE:	5.96	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

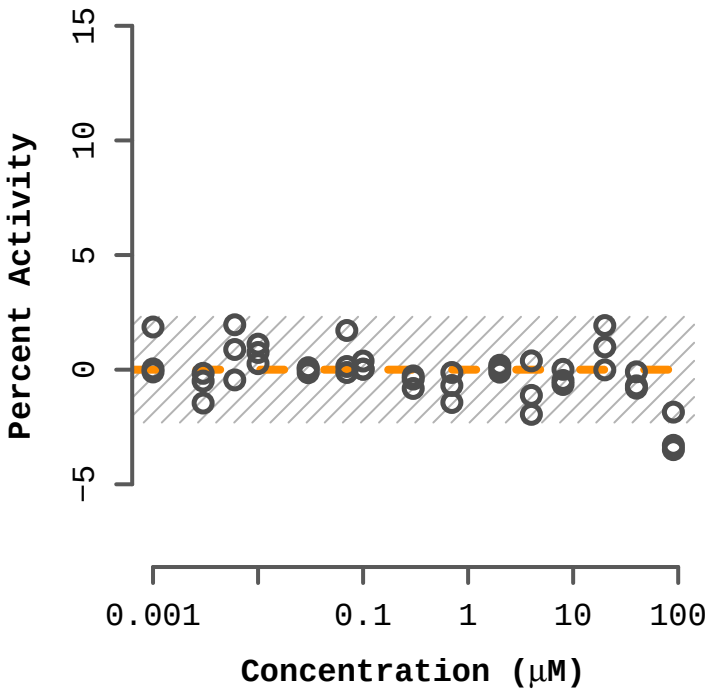
NAME: Chlorothalonil
CHID: 20319 CASRN: 1897-45-6
SPID(S): Tox21_201687
M4ID: 12480565 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	274.21	NA	NA
PROB:	1	NA	NA
RMSE:	5.38	NA	NA

MAX_MEAN: 0.987 MAX_MED: -0.0121 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

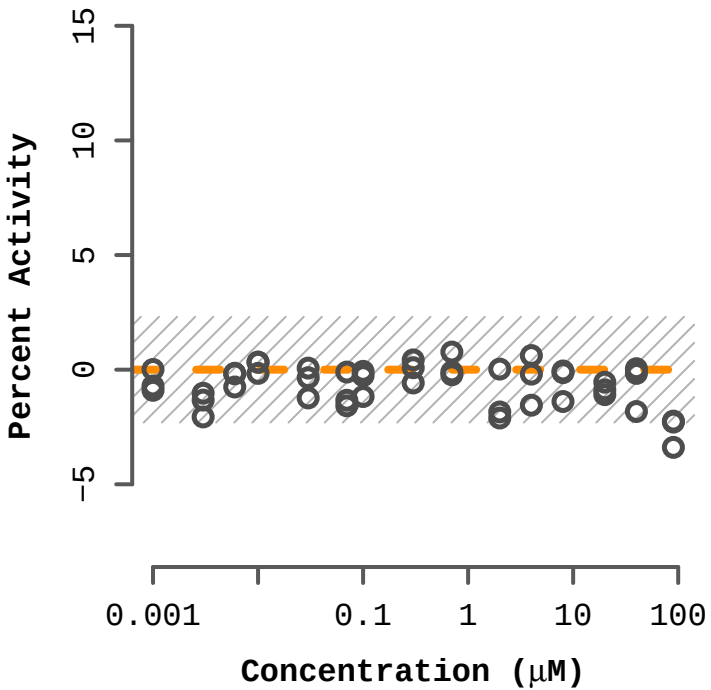
NAME: Chlorpheniramine maleate
CHID: 20321 CASRN: 113-92-8
SPID(S): Tox21_303456
M4ID: 12475684

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.971 MAX_MED: 0.995 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

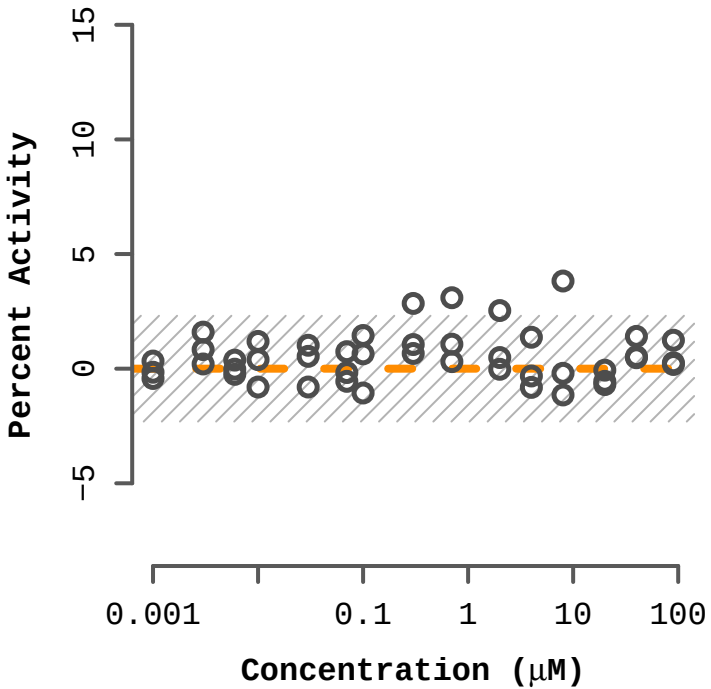
NAME: Chlorpheniramine maleate
CHID: 20321 CASRN: 113-92-8
SPID(S): Tox21_202092
M4ID: 12480160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.166 **MAX_MED:** 0.328 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

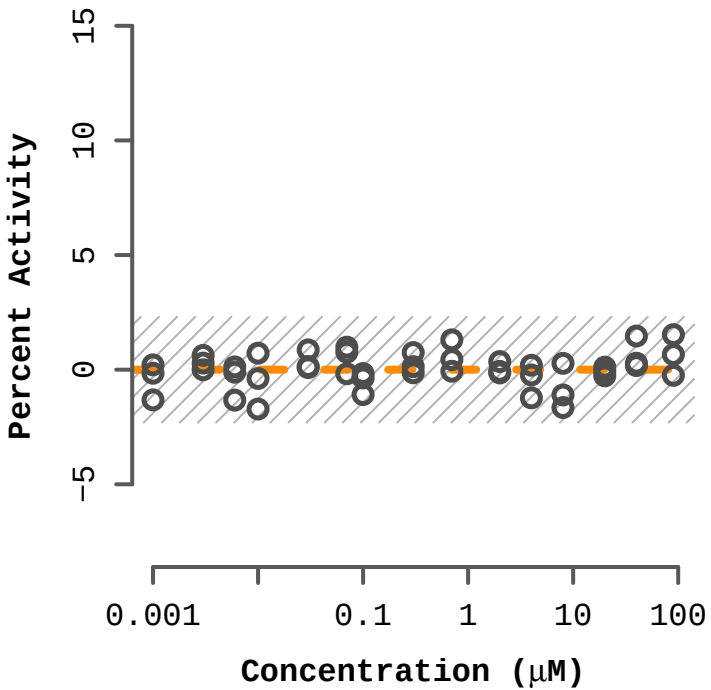
NAME: Chlorpropamide
CHID: 20322 **CASRN:** 94-20-2
SPID(S): Tox21_302789
M4ID: 12476344

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

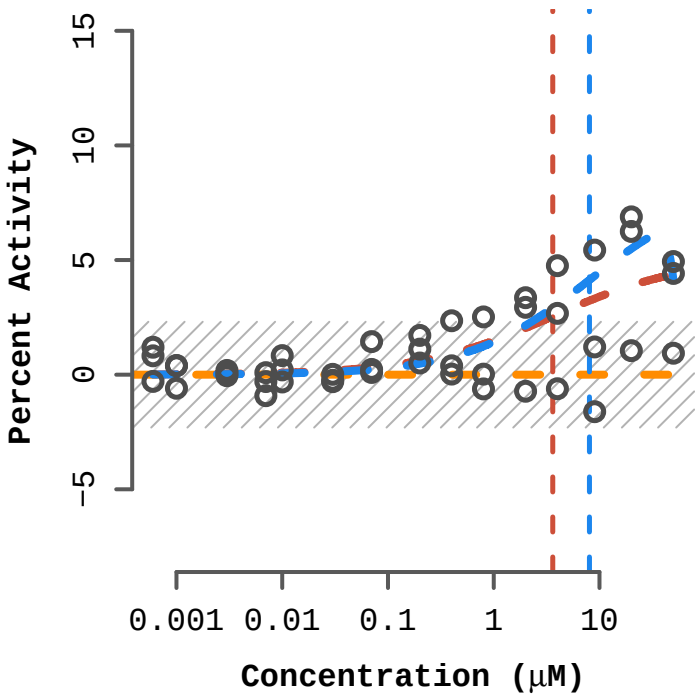
NAME: Chlorpropamide
CHID: 20322 CASRN: 94-20-2
SPID(S): Tox21_201391
M4ID: 12480861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.648 MAX_MED: 0.766 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorpropamide
CHID: 20322 **CASRN:** 94-20-2
SPID(S): Tox21_110102_1
M4ID: 12484651

HILL MODEL (in red):

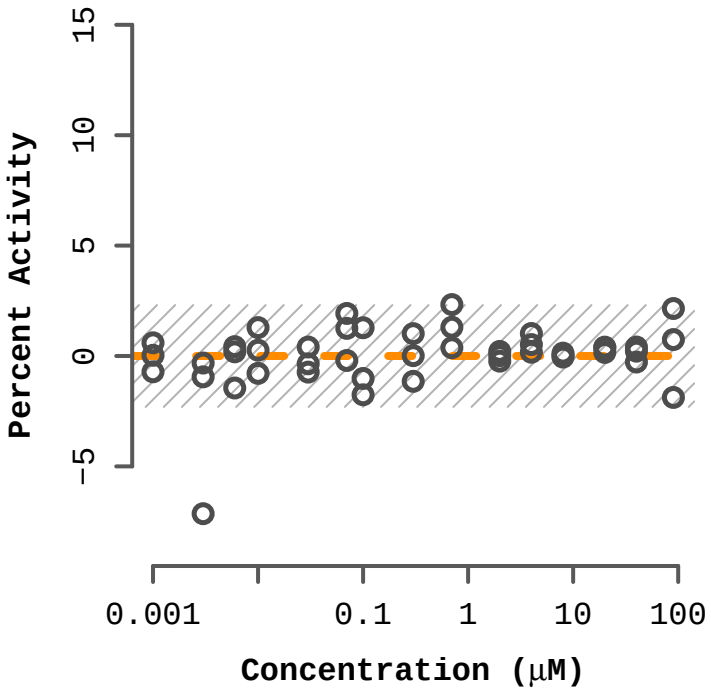
	tp	ga	gw
val:	5.09	0.558	0.69
sd:	1.9	0.724	0.391

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.26	0.905	0.752	1.72	10.7
sd:	3.97	0.581	0.262	0.121	61.4

	CNST	HILL	GNLS
AIC:	195.23	172.93	174.94
PROB:	0	0.73	0.27
RMSE:	2.31	1.57	1.66

MAX_MEAN: 4.73 **MAX_MED:** 6.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

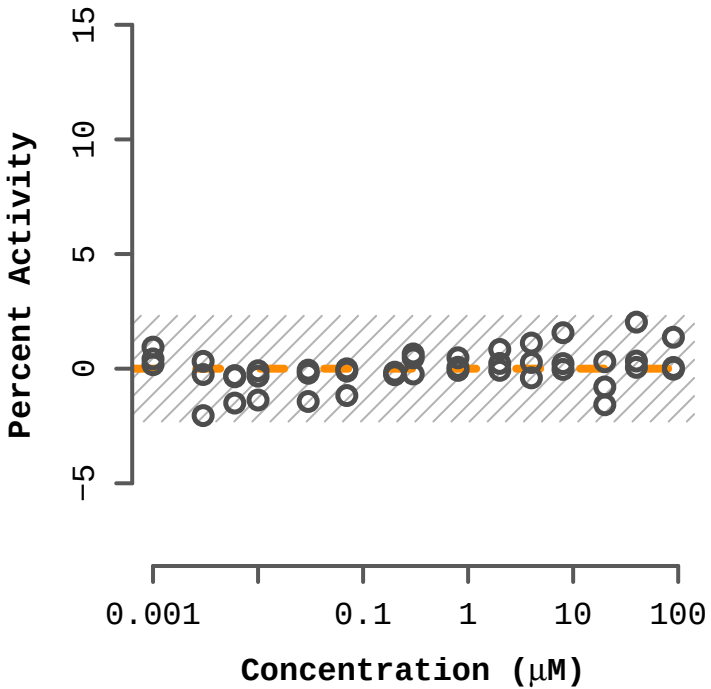
NAME: Choline chloride
CHID: 20325 CASRN: 67-48-1
SPID(S): Tox21_200492
M4ID: 12481760

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.34 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

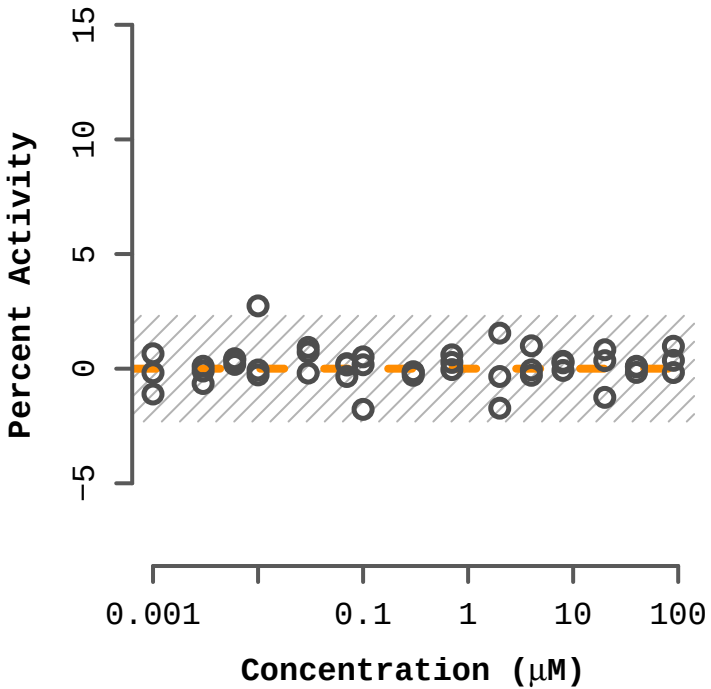
NAME: Chromic oxide pigment
CHID: 20326 **CASRN:** NOCAS_20326
SPID(S): Tox21_200784
M4ID: 12481468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.808 **MAX_MED:** 0.474 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

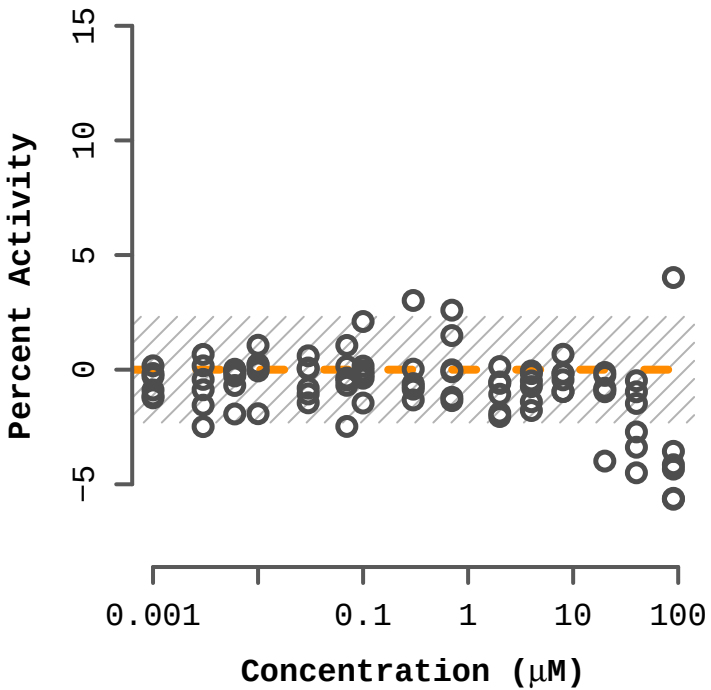
NAME: Chromium(III) acetate
CHID: 20327 **CASRN:** 1066-30-4
SPID(S): Tox21_202498
M4ID: 12479754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 0.725 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

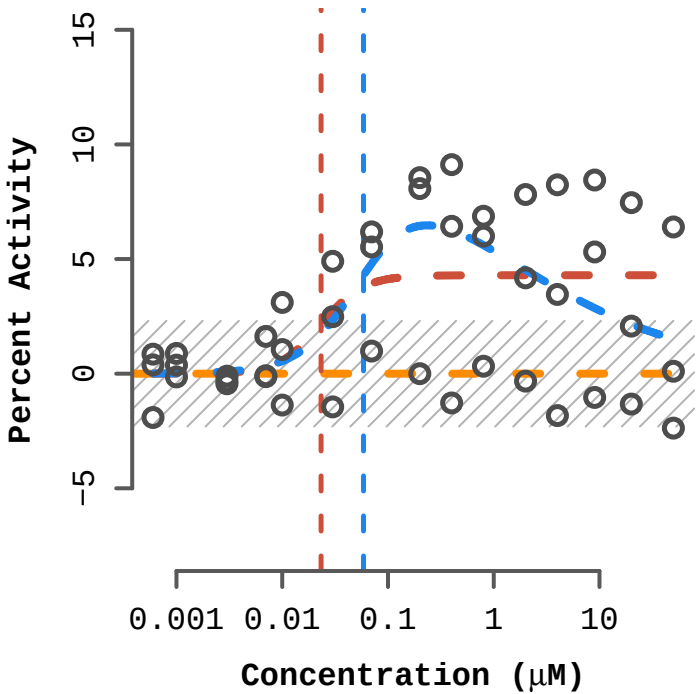
NAME: Danthron
CHID: 20328 CASRN: 117-10-2
SPID(S): Tox21_200986
M4ID: 12481266

HILL MODEL: Not applicable.

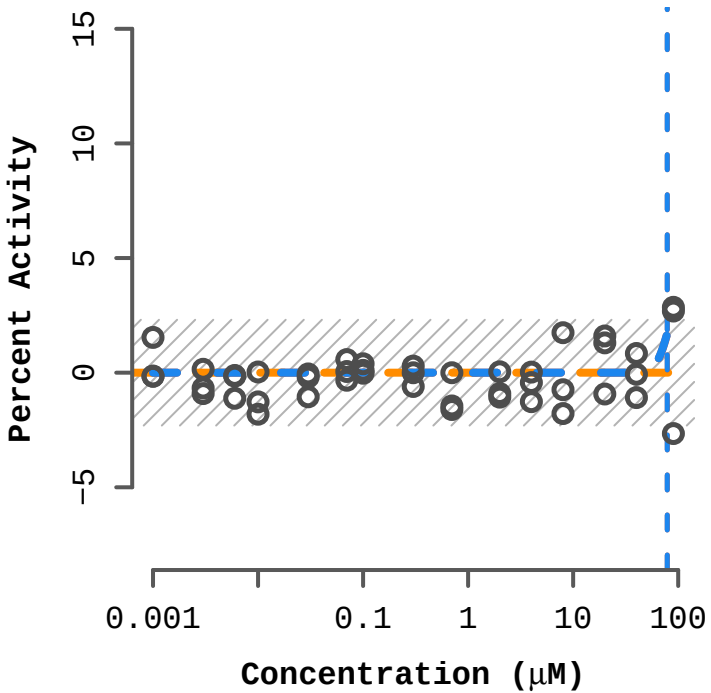
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	342.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 0.24 MAX_MED: 0.108 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Danthron
CHID:    20328   CASRN: 117-10-2
SPID(S): Tox21_111122_1
M4ID:    12483894

HILL MODEL (in red):
      tp       ga       gw
val:  4.29     -1.63    2.19
sd:   0.832    0.344    1.92

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.9     -1.23    1.59     -0.0214  0.462
sd:   22.9     0.524    1.05     4        0.619

      CNST        HILL        GNLS
AIC:  262.57      242.52      241.5
PROB: 0           0.38        0.62
RMSE: 4.33        3.12        3.05

MAX_MEAN: 5.54      MAX_MED: 8.08      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cimetidine
CHID: 20329 **CASRN:** 51481-61-9
SPID(S): Tox21_201160
M4ID: 12481092

HILL MODEL (in red):

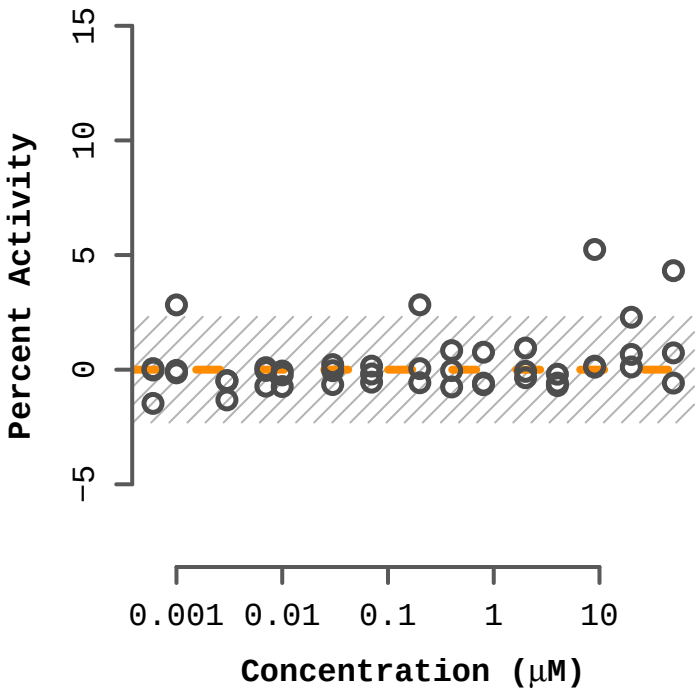
	tp	ga	gw
val:	3.42	1.9	8
sd:	9.21	0.463	22.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.42	1.9	7.93	3.95	3.92
sd:	9.46	0.484	22	21300	41900

	CNST	HILL	GNLS
AIC:	140.23	138.7	142.7
PROB:	0.29	0.62	0.08
RMSE:	1.12	1.17	1.17

MAX_MEAN: 0.962 **MAX_MED:** 2.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

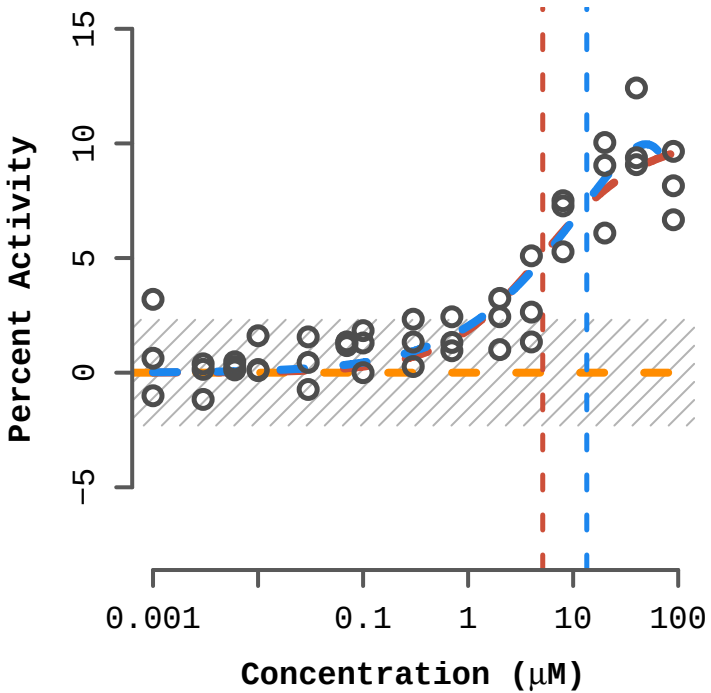
NAME: Cimetidine
CHID: 20329 **CASRN:** 51481-61-9
SPID(S): Tox21_110106_1
M4ID: 12484647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 0.734 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cinnamyl anthranilate
CHID: 20330 CASRN: 87-29-6
SPID(S): Tox21_200682
M4ID: 12481570

HILL MODEL (in red):

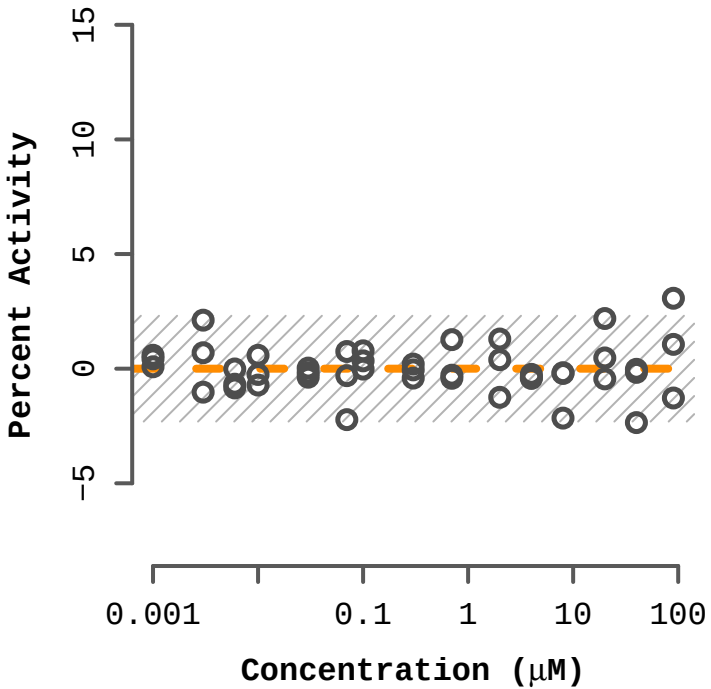
	tp	ga	gw
val:	10.3	0.71	0.92
sd:	1.32	0.171	0.341

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.9	1.13	0.71	2.07	3.1
sd:	4.93	0.409	0.182	0.117	4.16

	CNST	HILL	GNLS
AIC:	265.01	164.76	160.99
PROB:	0	0.13	0.87
RMSE:	4.67	1.37	1.25

MAX_MEAN: 10.3 **MAX_MED:** 9.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

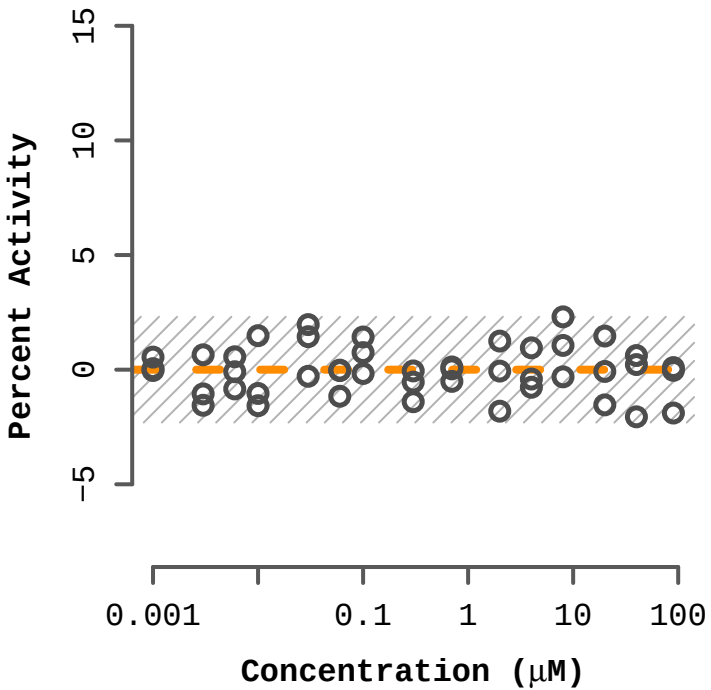
NAME: Ciprofibrate
CHID: 20331 CASRN: 52214-84-3
SPID(S): Tox21_302840
M4ID: 12476293

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.952 MAX_MED: 1.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

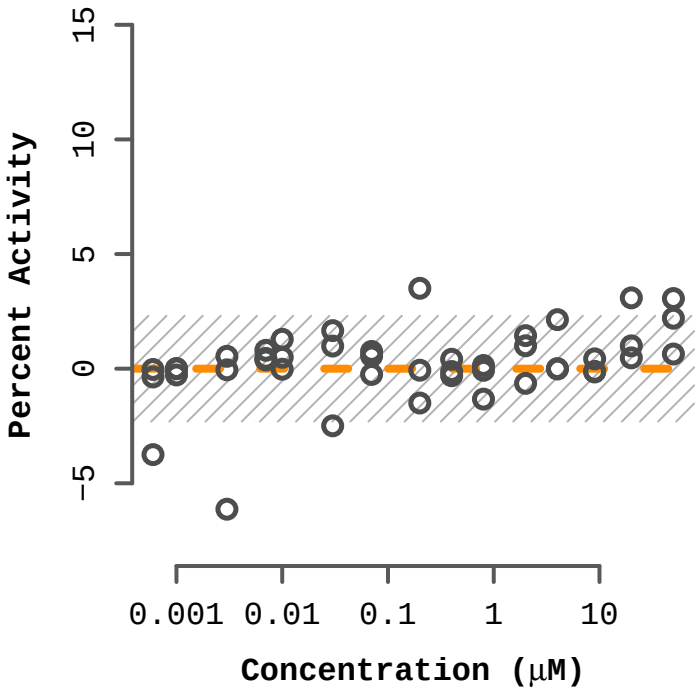
NAME: Ciprofibrate
CHID: 20331 **CASRN:** 52214-84-3
SPID(S): Tox21_201359
M4ID: 12480893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

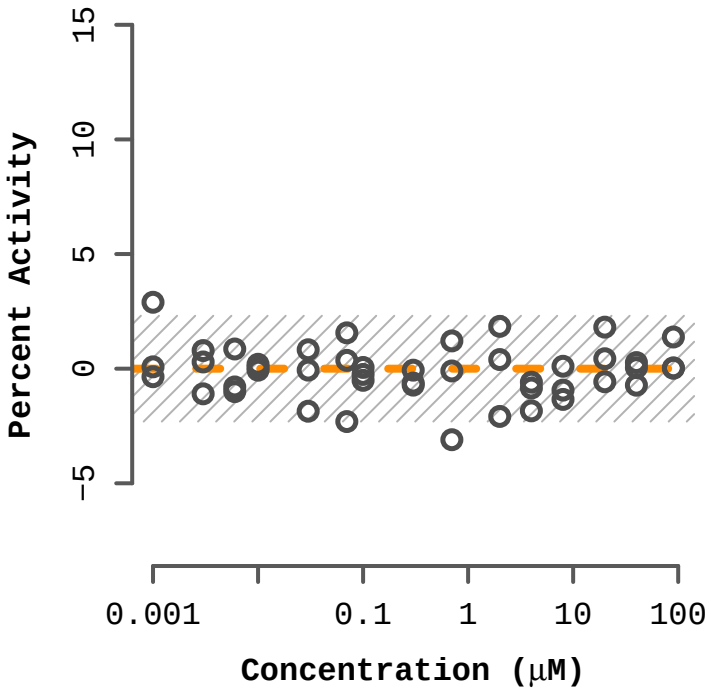
NAME: Ciprofibrate
CHID: 20331 **CASRN:** 52214-84-3
SPID(S): Tox21_112121_1
M4ID: 12483305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 2.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

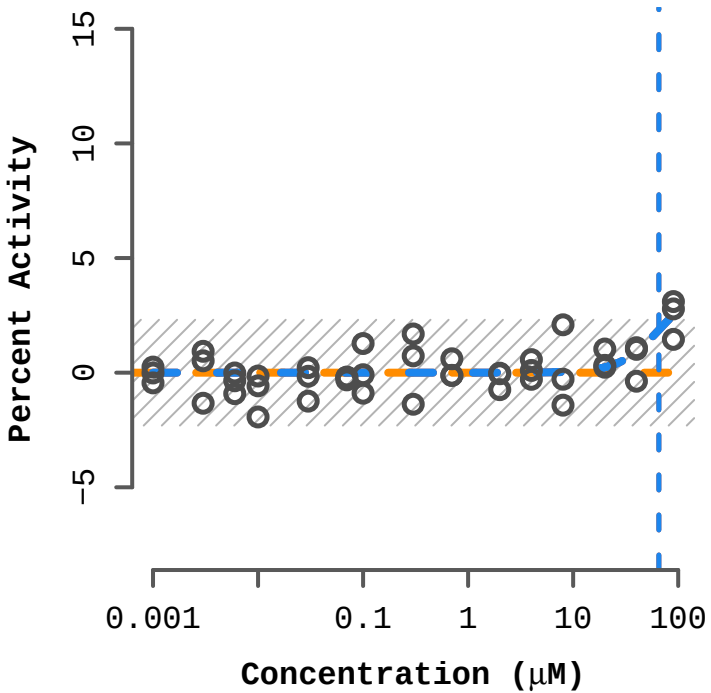
NAME: Citric acid
CHID: 20332 **CASRN:** 77-92-9
SPID(S): Tox21_300124
M4ID: 12479006

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.877 **MAX_MED:** 0.435 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Citric acid
CHID: 20332 CASRN: 77-92-9
SPID(S): Tox21_202405
M4ID: 12479847

HILL MODEL (in red):

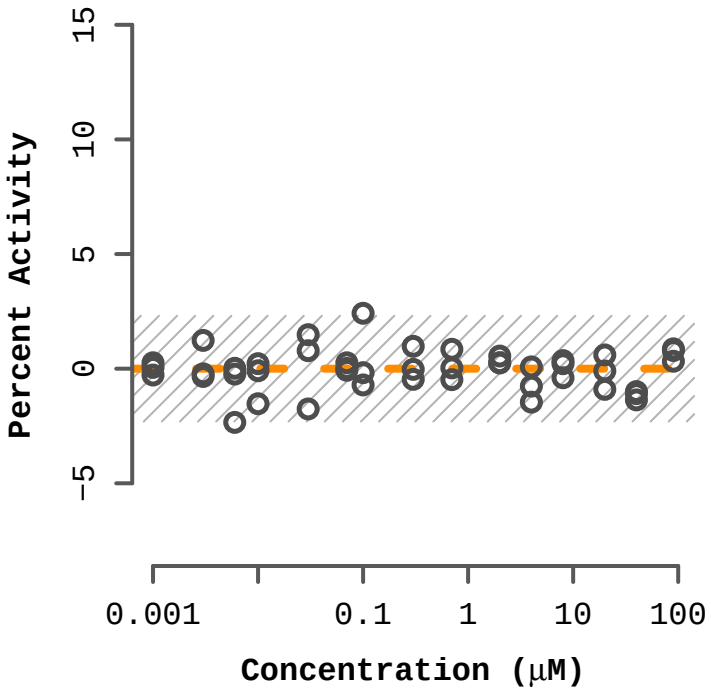
	tp	ga	gw
val:	3.72	1.82	2.28
sd:	2.5	0.3	1.49

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.72	1.82	2.28	2.99	7.56
sd:	2.5	0.301	1.49	1440	10500

	CNST	HILL	GNLS
AIC:	130.33	116.13	120.13
PROB:	0	0.88	0.12
RMSE:	1.04	0.81	0.81

MAX_MEAN: 2.45 MAX_MED: 2.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

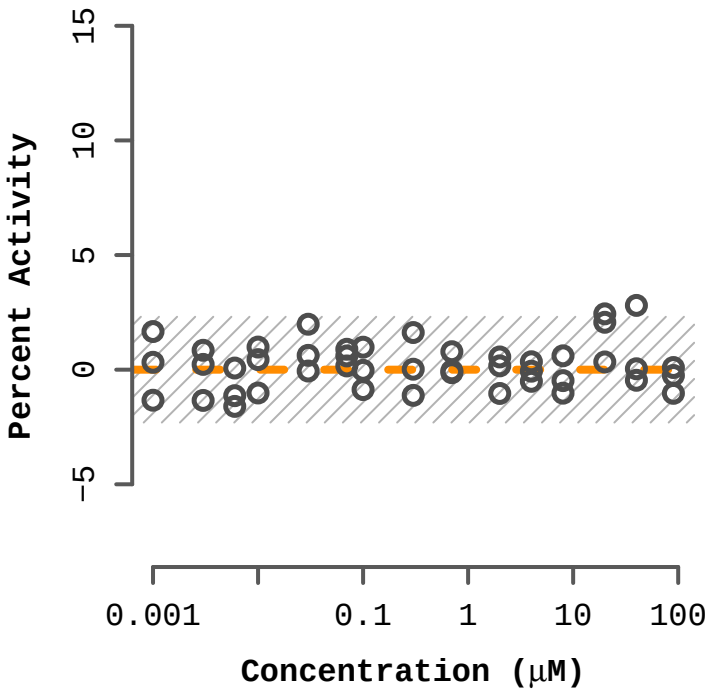
NAME: Clofibrate
CHID: 20336 CASRN: 637-07-0
SPID(S): Tox21_300277
M4ID: 12478853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.662 MAX_MED: 0.793 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

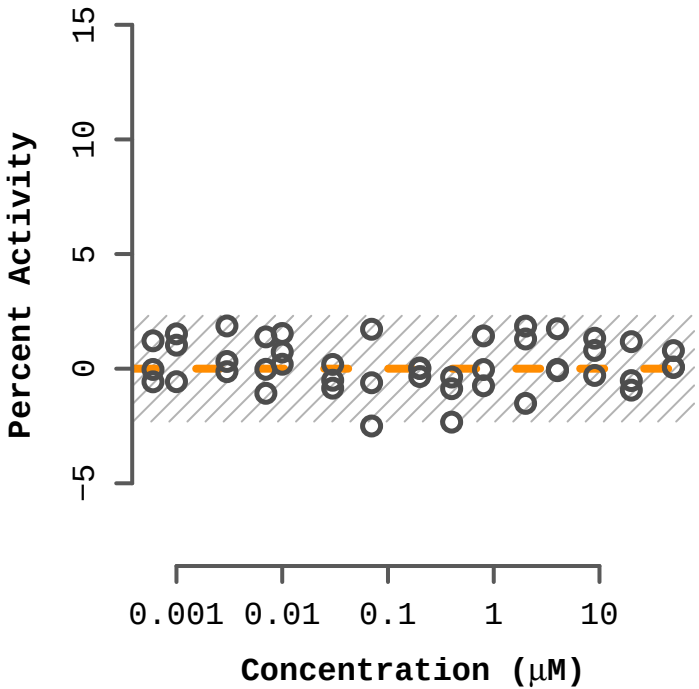
NAME: Clofibrate
CHID: 20336 CASRN: 637-07-0
SPID(S): Tox21_202414
M4ID: 12479838

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.61 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

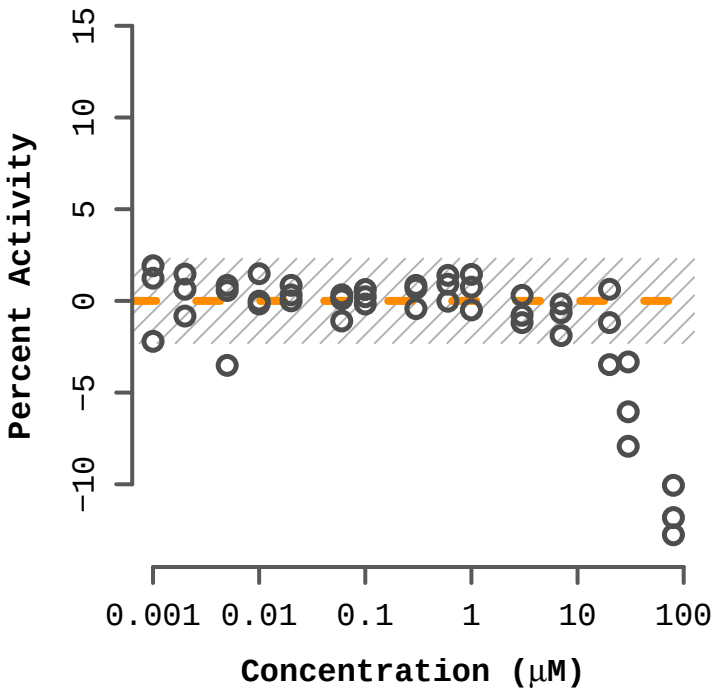
NAME: Clofibrate
CHID: 20336 CASRN: 637-07-0
SPID(S): Tox21_110116_1
M4ID: 12484637

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.821 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

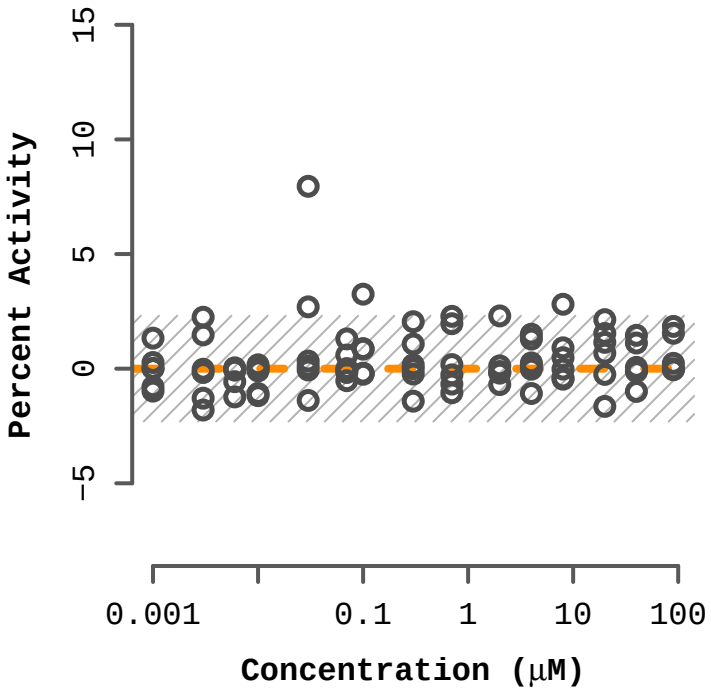
NAME: Clomiphene citrate (1:1)
CHID: 20337 **CASRN:** 50-41-9
SPID(S): Tox21_301875
M4ID: 12477258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.04	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 0.764 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

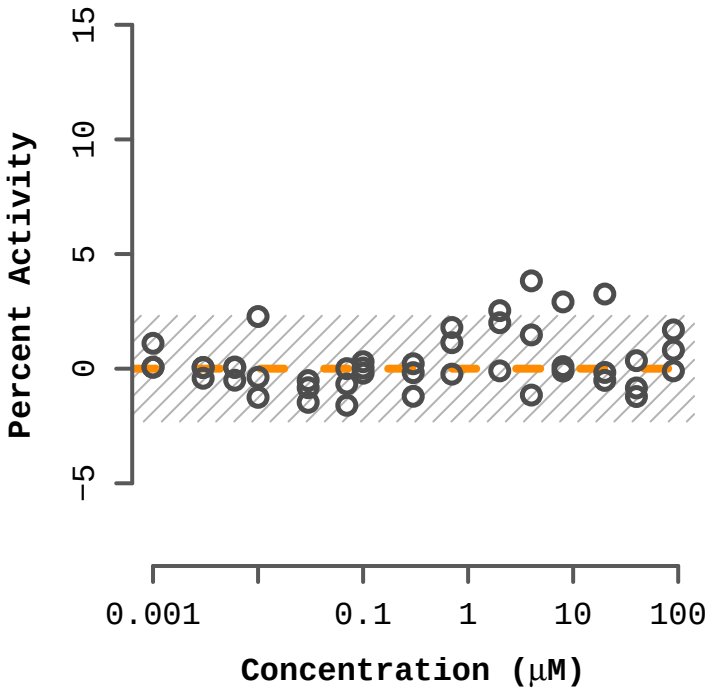
NAME: Cobalt sulfate heptahydrate
CHID: 20340 CASRN: 10026-24-1
SPID(S): Tox21_202501
M4ID: 12479751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.61 MAX_MED: 0.913 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

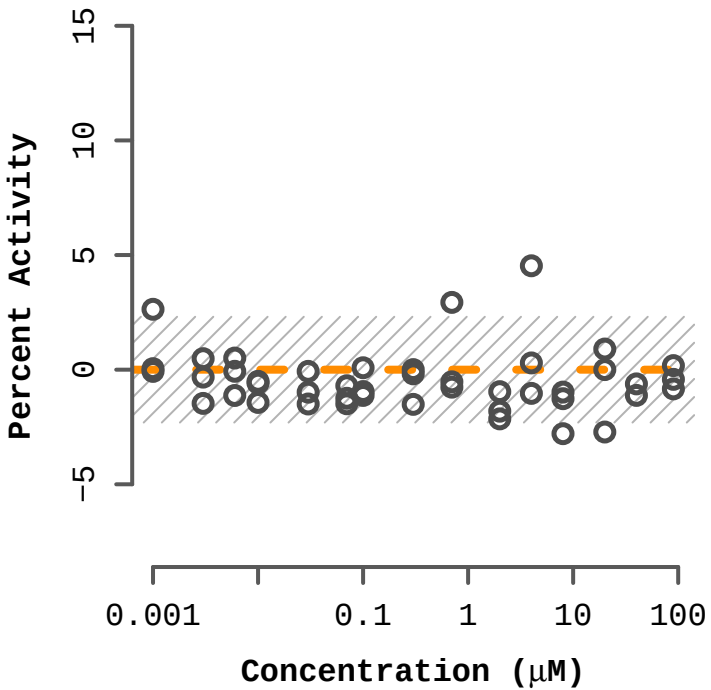
NAME: Codeine
CHID: 20341 CASRN: 76-57-3
SPID(S): Tox21_200082
M4ID: 12482170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

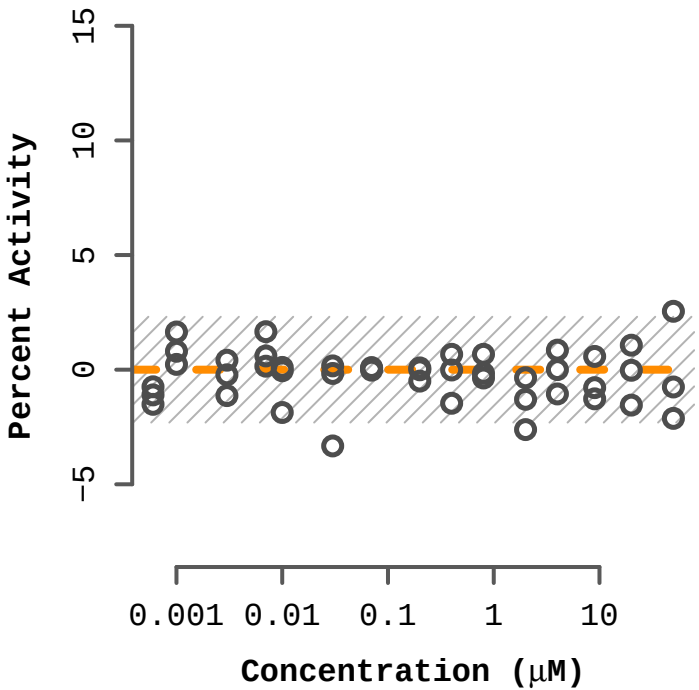
NAME: Tomelukast
CHID: 20344 **CASRN:** 88107-10-2
SPID(S): Tox21_302412
M4ID: 12476721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.296 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

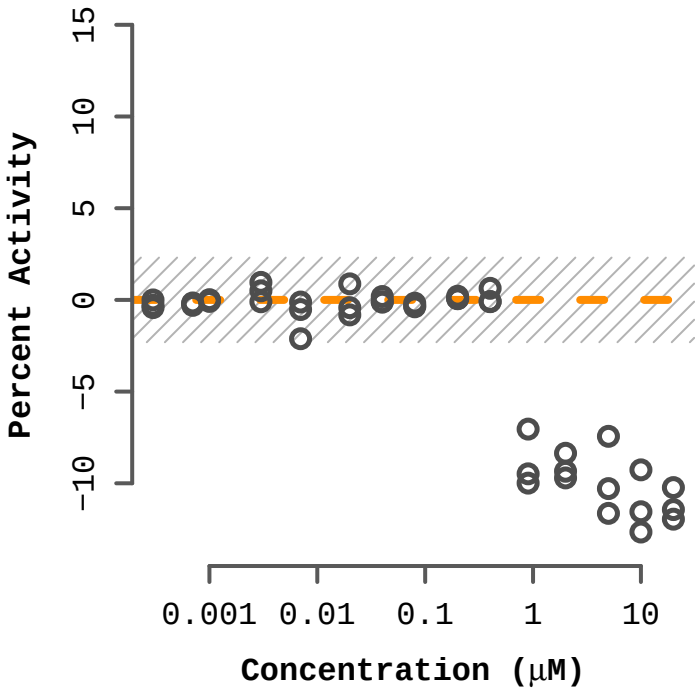
NAME: Tomelukast
CHID: 20344 **CASRN:** 88107-10-2
SPID(S): Tox21_110828_1
M4ID: 12484088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

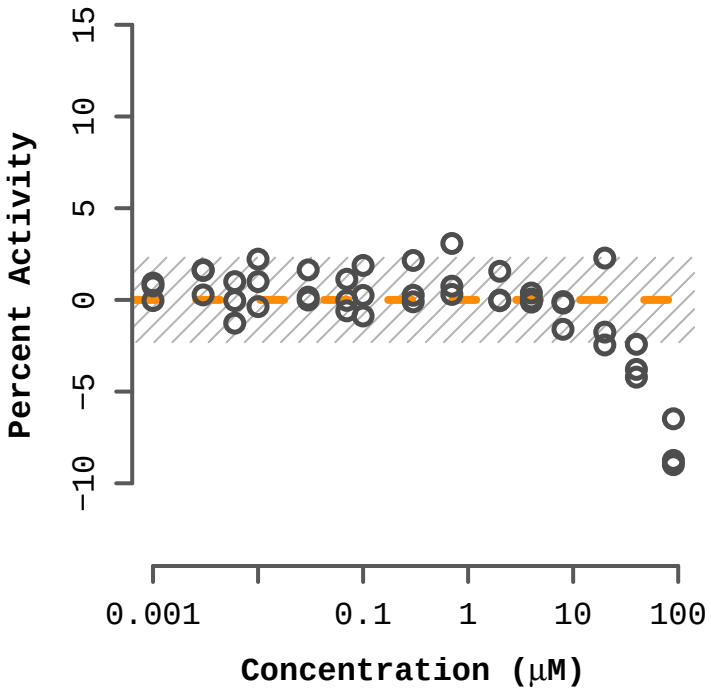
NAME: Copper dimethyldithiocarbamate
CHID: 20345 CASRN: 137-29-1
SPID(S): Tox21_202780
M4ID: 12479472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.27	NA	NA
PROB:	1	NA	NA
RMSE:	5.88	NA	NA

MAX_MEAN: 0.452 **MAX_MED:** 0.498 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

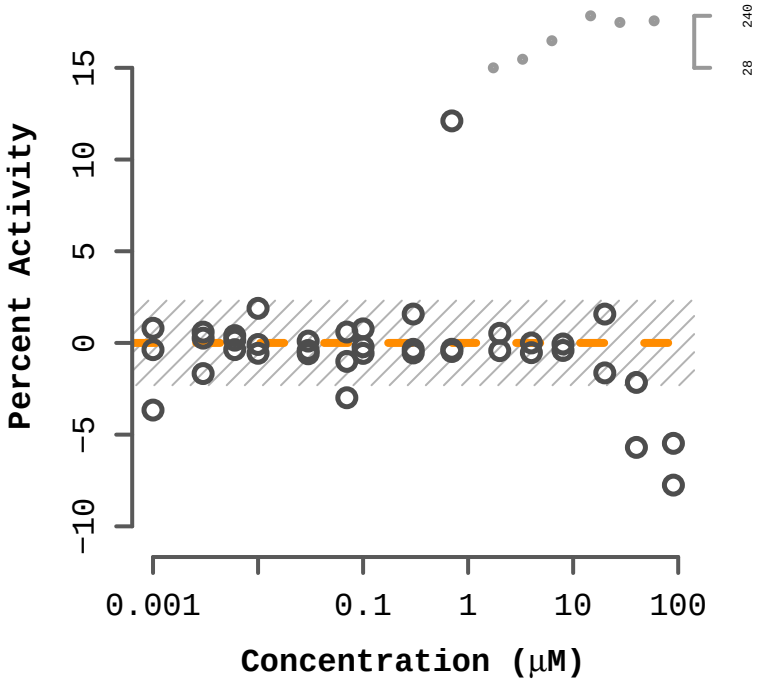
NAME: Coumaphos
CHID: 20347 CASRN: 56-72-4
SPID(S): Tox21_300769
M4ID: 12478364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.56	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

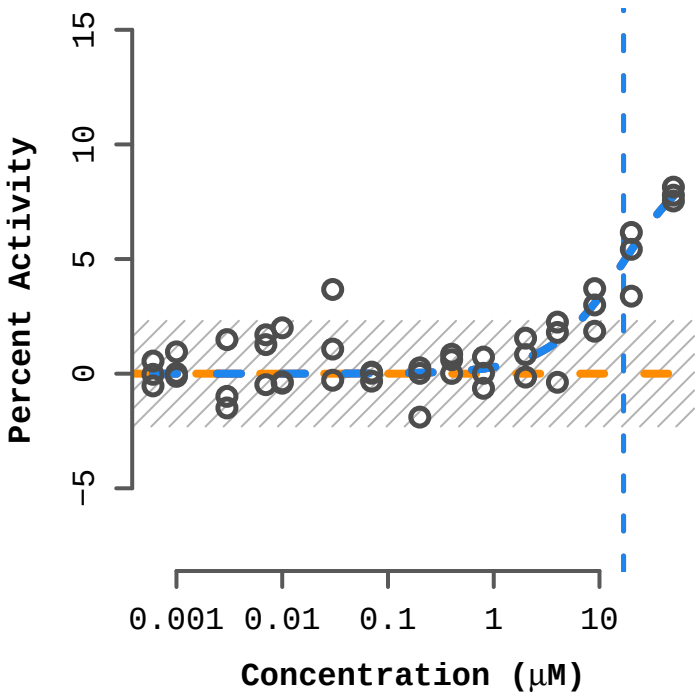
NAME: Coumaphos
CHID: 20347 **CASRN:** 56-72-4
SPID(S): Tox21_201841
M4ID: 12480411 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	393.98	NA	NA
PROB:	1	NA	NA
RMSE:	63.37	NA	NA

MAX_MEAN: 81.2 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Coumaphos
CHID: 20347 **CASRN:** 56-72-4
SPID(S): Tox21_111290_1
M4ID: 12483788

HILL MODEL (in red):

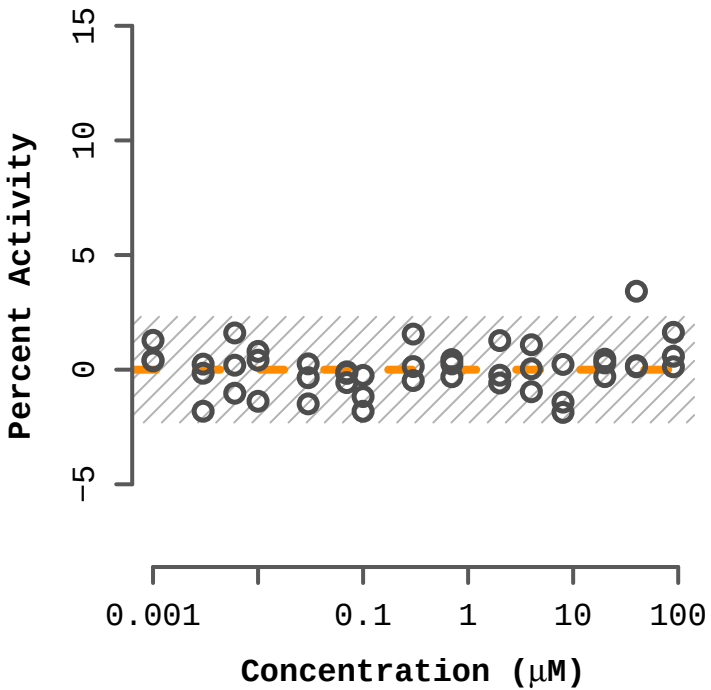
	tp	ga	gw
val:	9.77	1.23	1.23
sd:	1.81	0.174	0.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.77	1.23	1.23	3.38	4.69
sd:	1.81	0.174	0.31	1280	3570

	CNST	HILL	GNLS
AIC:	207.99	135.11	139.11
PROB:	0	0.88	0.12
RMSE:	2.74	1.04	1.04

MAX_MEAN: 7.82 **MAX_MED:** 7.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

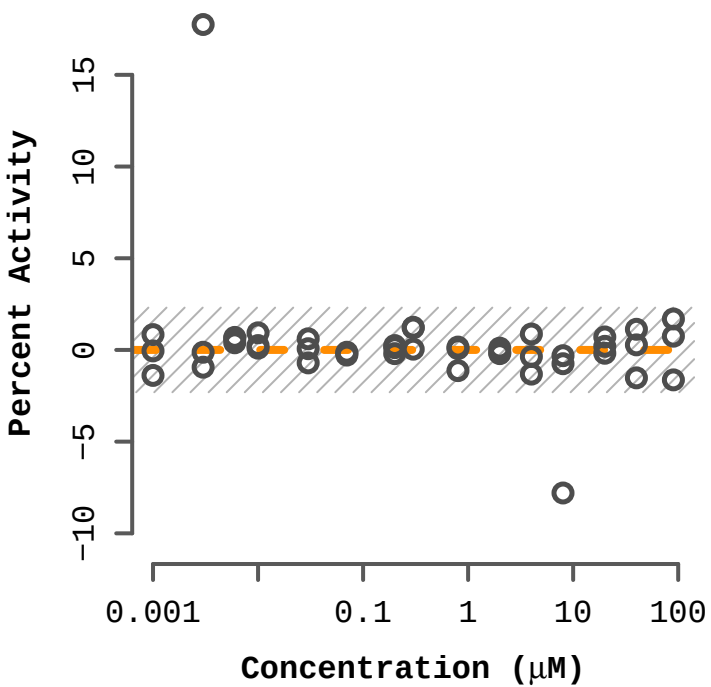
NAME: Coumarin
CHID: 20348 CASRN: 91-64-5
SPID(S): Tox21_300057
M4ID: 12479073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.585 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

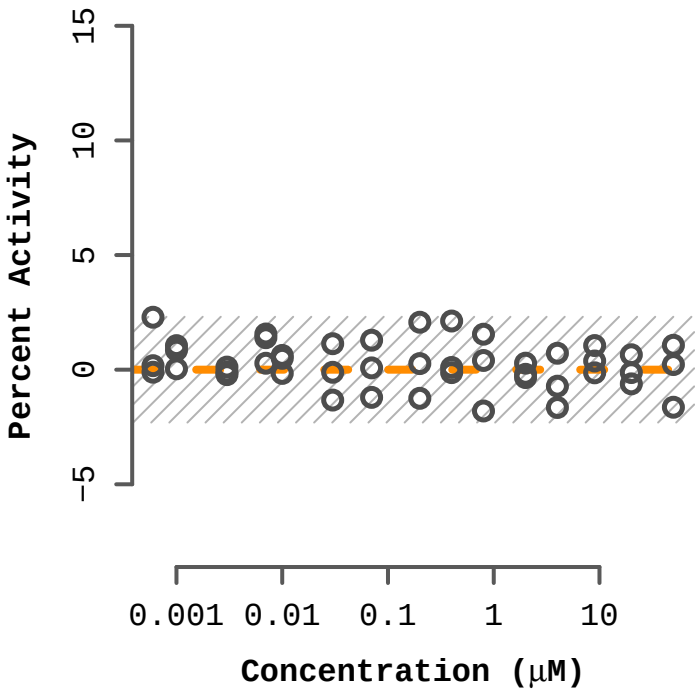
NAME: Coumarin
CHID: 20348 CASRN: 91-64-5
SPID(S): Tox21_202427
M4ID: 12479825

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.69	NA	NA
PROB:	1	NA	NA
RMSE:	2.98	NA	NA

MAX_MEAN: 5.56 MAX_MED: 1.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

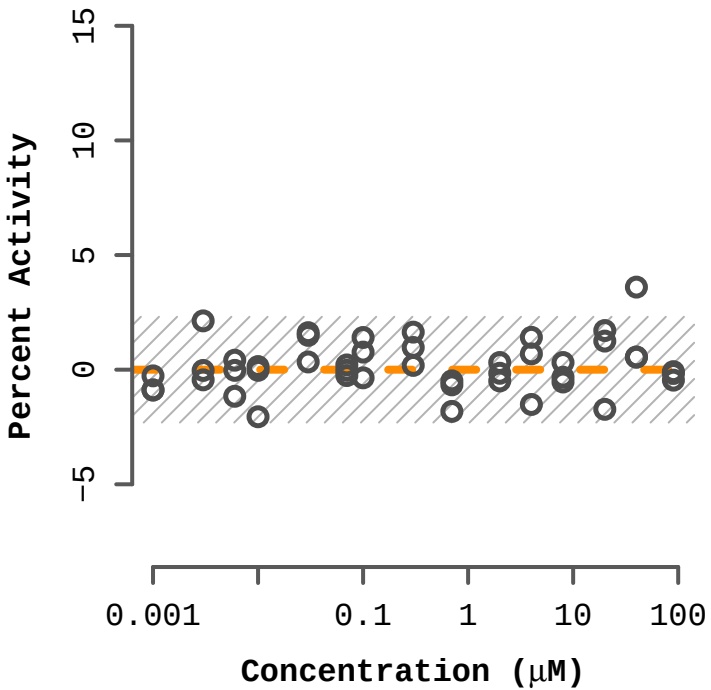
NAME: Coumarin
CHID: 20348 **CASRN:** 91-64-5
SPID(S): Tox21_111141_1
M4ID: 12483881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.28	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

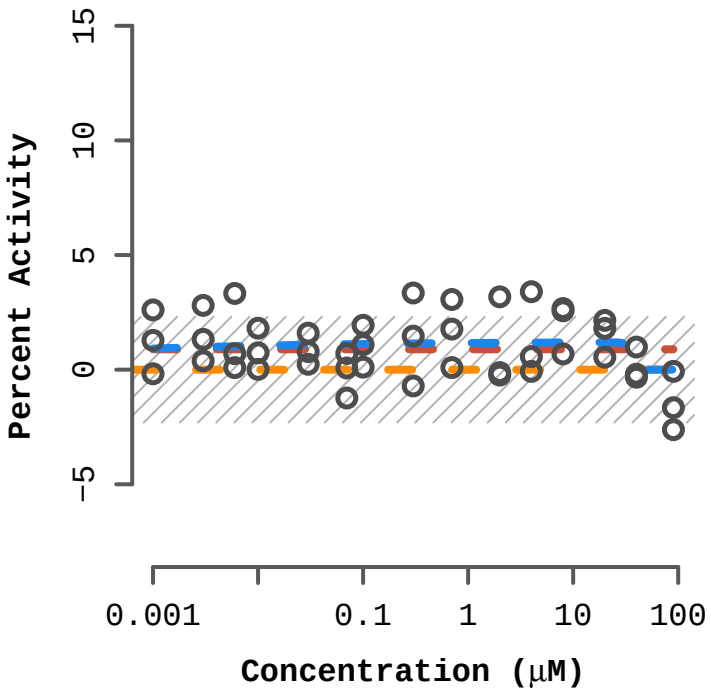
NAME: 4-Methoxy-2-methylaniline
CHID: 20349 **CASRN:** 102-50-1
SPID(S): Tox21_303531
M4ID: 12475612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methoxy-2-methylaniline
CHID: 20349 CASRN: 102-50-1
SPID(S): Tox21_201440
M4ID: 12480812

HILL MODEL (in red):

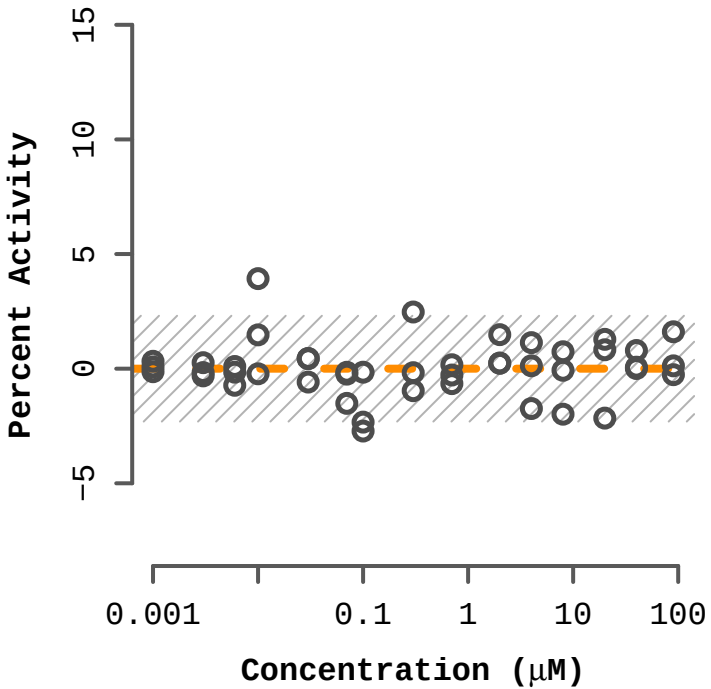
	tp	ga	gw
val:	0.889	-4.55	4.7
sd:	0.209	1640	4950

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.21	-4.67	0.3	1.55	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	178.35	167.61	164.54
PROB:	0	0.18	0.82
RMSE:	1.67	1.38	1.25

MAX_MEAN: 1.98 **MAX_MED:** 2.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

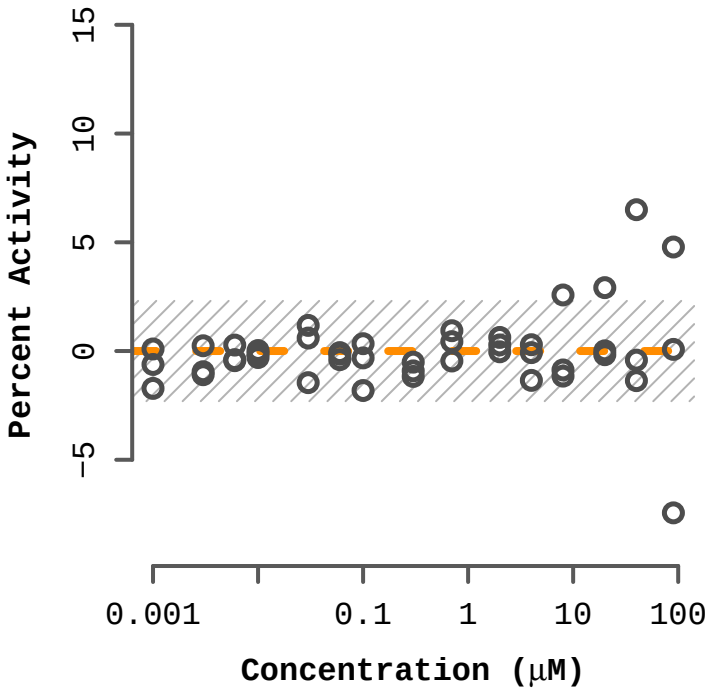
NAME: 2-Methoxy-5-methylaniline
CHID: 20350 **CASRN:** 120-71-8
SPID(S): Tox21_300012
M4ID: 12479118

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

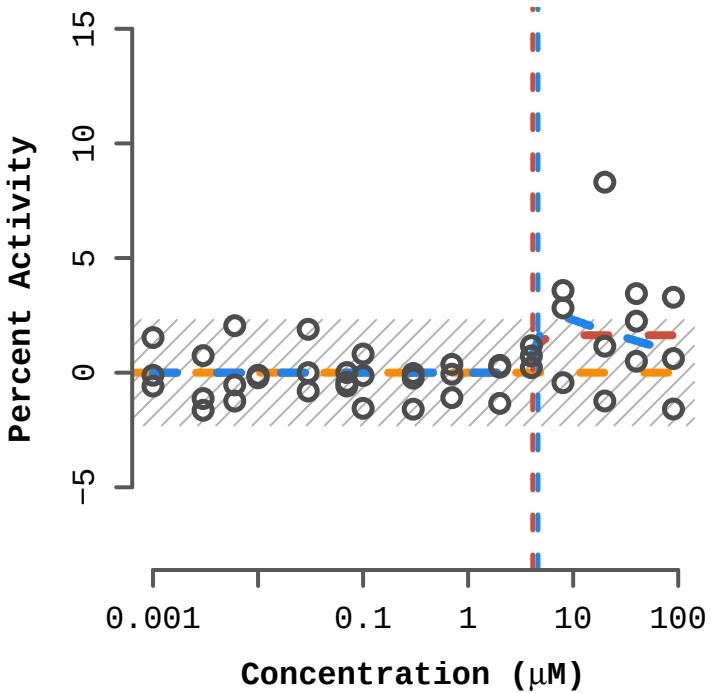
NAME: 2-Methoxy-5-methylaniline
CHID: 20350 **CASRN:** 120-71-8
SPID(S): Tox21_201907
M4ID: 12480345

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 0.599 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cupferron
CHID: 20352 **CASRN:** 135-20-6
SPID(S): Tox21_302952
M4ID: 12476181

HILL MODEL (in red):

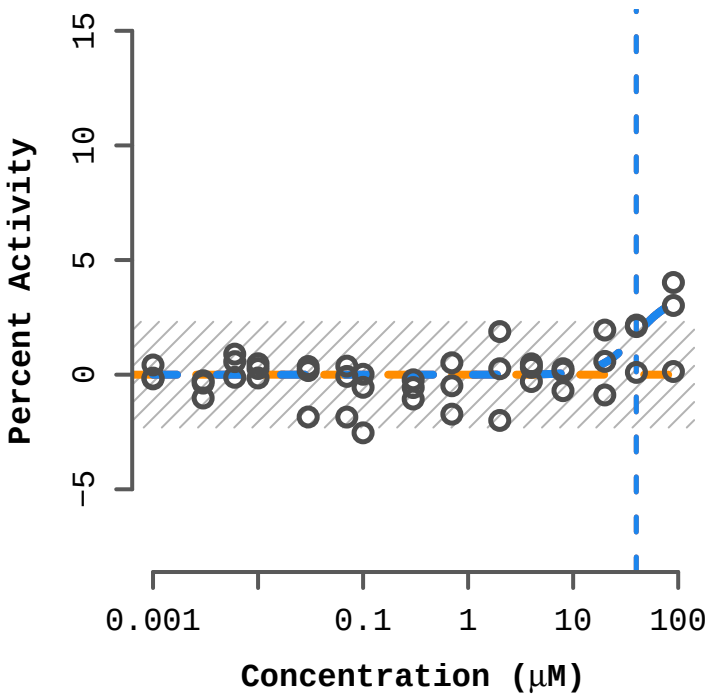
	tp	ga	gw
val:	1.63	0.616	8
sd:	0.551	0.0842	14.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.9	0.664	7.94	0.914	0.588
sd:	16.9	0.127	12.7	4.91	1.1

	CNST	HILL	GNLS
AIC:	169.61	165.33	168.17
PROB:	0.09	0.74	0.18
RMSE:	1.84	1.56	1.54

MAX_MEAN: 2.74 **MAX_MED:** 2.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cupferron
CHID: 20352 CASRN: 135-20-6
SPID(S): Tox21_201493
M4ID: 12480759

HILL MODEL (in red):

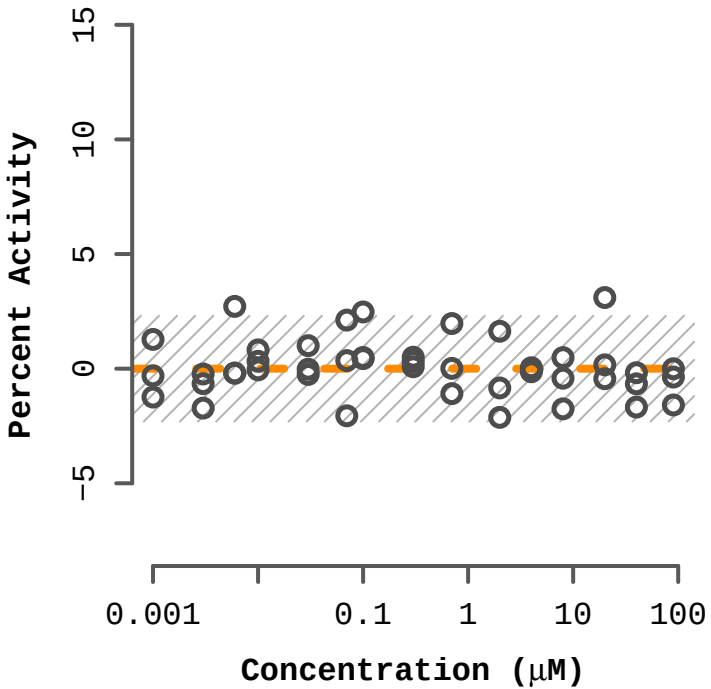
	tp	ga	gw
val:	3.49	1.6	2.52
sd:	1.5	0.215	2.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.49	1.6	2.52	3.36	3.51
sd:	1.51	0.215	2.3	553	1440

	CNST	HILL	GNLS
AIC:	143.61	134.07	138.07
PROB:	0.01	0.87	0.12
RMSE:	1.24	1.02	1.02

MAX_MEAN: 2.39 MAX_MED: 3.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

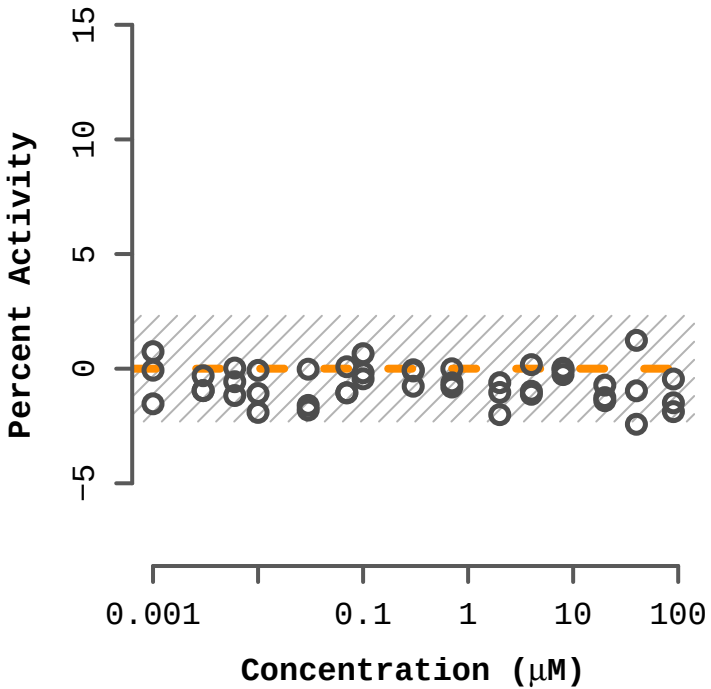
NAME: Cyanoguanidine
CHID: 20354 CASRN: 461-58-5
SPID(S): Tox21_302730
M4ID: 12476403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.14 MAX_MED: 0.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

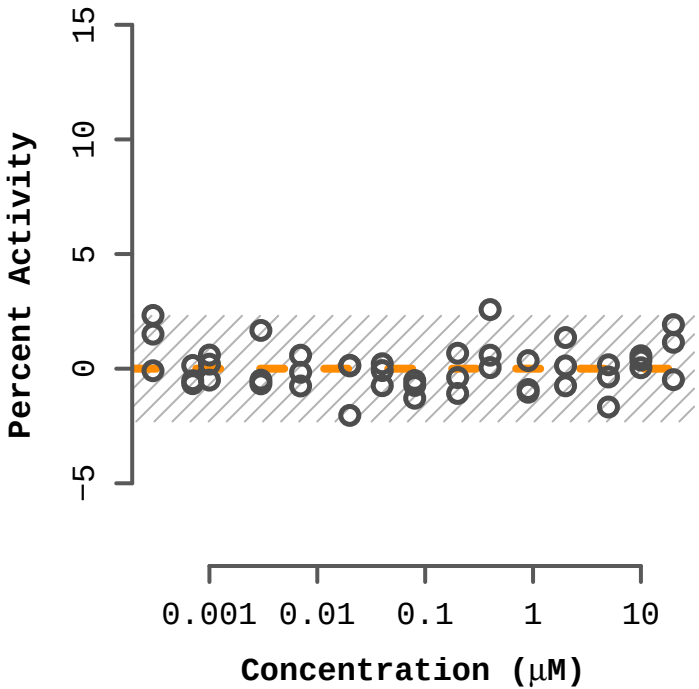
NAME: Cyanoguanidine
CHID: 20354 CASRN: 461-58-5
SPID(S): Tox21_201513
M4ID: 12480739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.0129 MAX_MED: −0.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

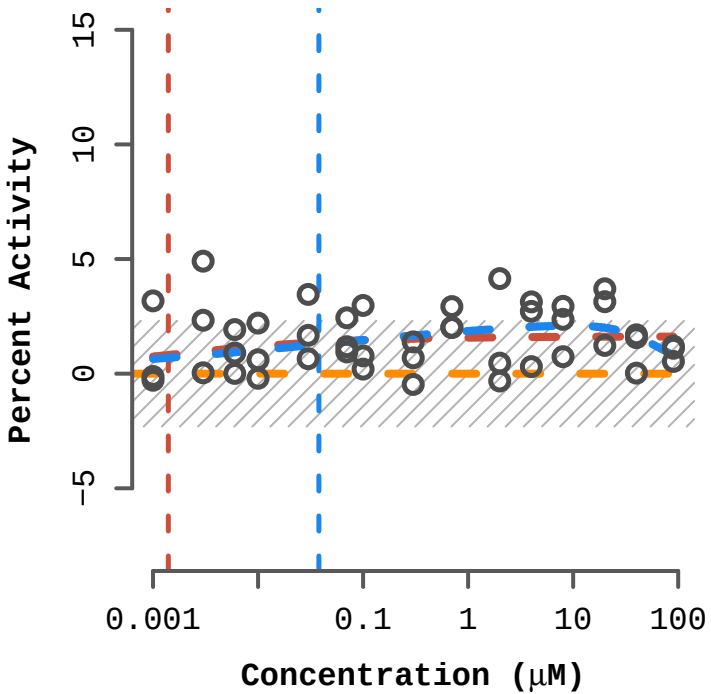
NAME: Sodium cyclamate
CHID: 20355 CASRN: 139-05-9
SPID(S): Tox21_202781
M4ID: 12479471

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclocytidine
CHID: 20357 CASRN: 31698-14-3
SPID(S): Tox21_301815
M4ID: 12477318

HILL MODEL (in red):

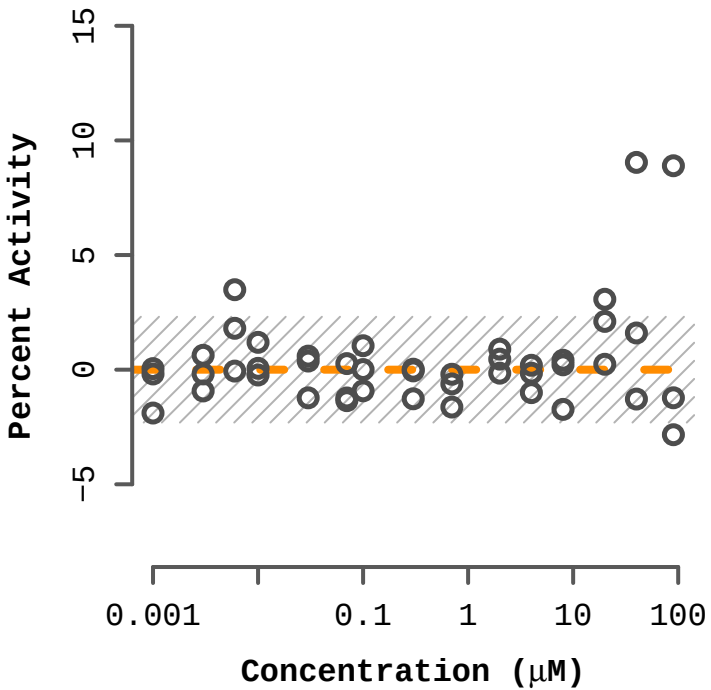
	tp	ga	gw
val:	1.62	−2.85	0.51
sd:	0.365	1.21	0.75

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.56	−1.42	0.3	1.81	1.91
sd:	4.68	6.23	0.775	0.528	1.65

	CNST	HILL	GNLS
AIC:	196.45	164.29	165.54
PROB:	0	0.65	0.35
RMSE:	2.03	1.33	1.31

MAX_MEAN: 2.69 MAX_MED: 3.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

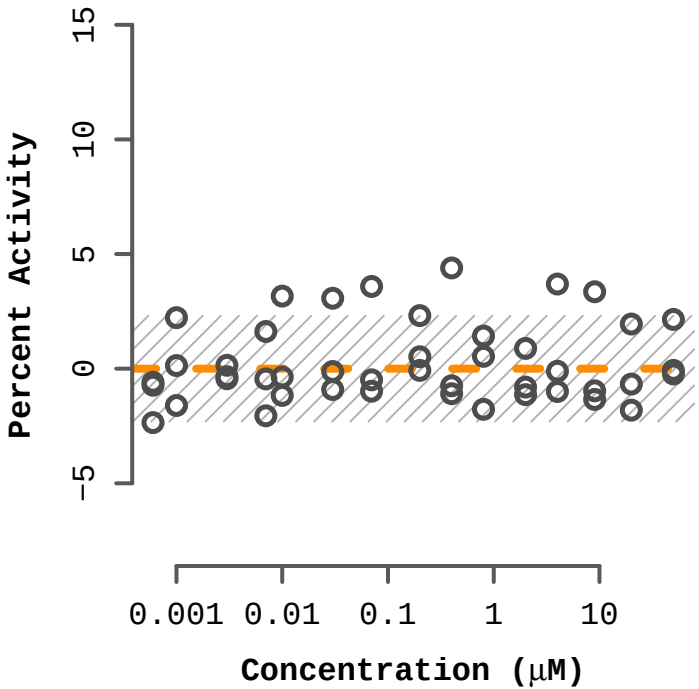
NAME: beta-Cyclodextrin
CHID: 20358 **CASRN:** 7585-39-9
SPID(S): Tox21_201006
M4ID: 12481246

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.25	NA	NA

MAX_MEAN: 3.12 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

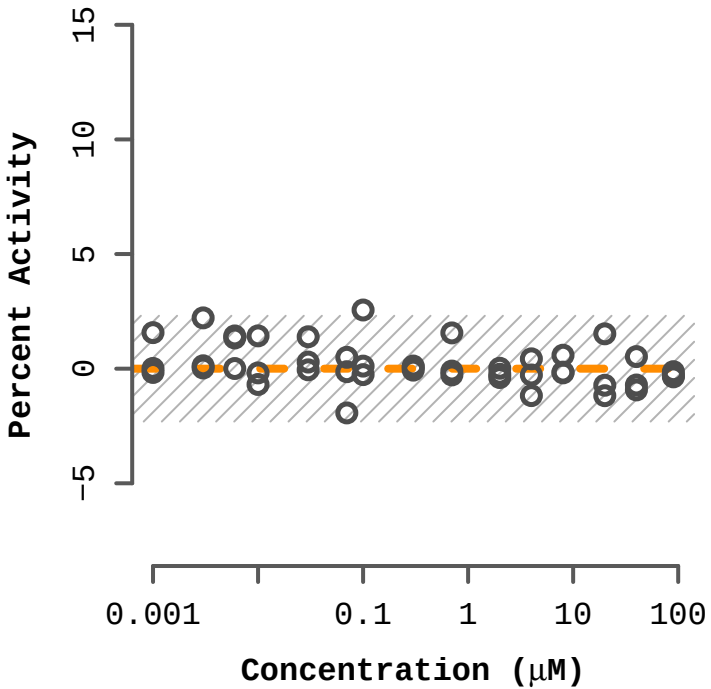
NAME: beta-Cyclodextrin
CHID: 20358 **CASRN:** 7585-39-9
SPID(S): Tox21_111017_1
M4ID: 12483946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 0.921 **MAX_MED:** 0.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

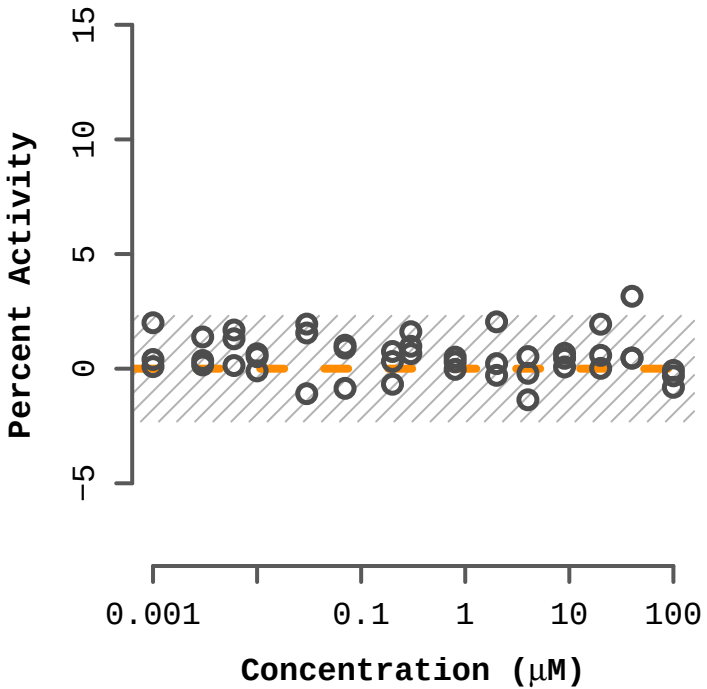
NAME: Cyclohexanone
CHID: 20359 CASRN: 108-94-1
SPID(S): Tox21_302750
M4ID: 12476383

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.926 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

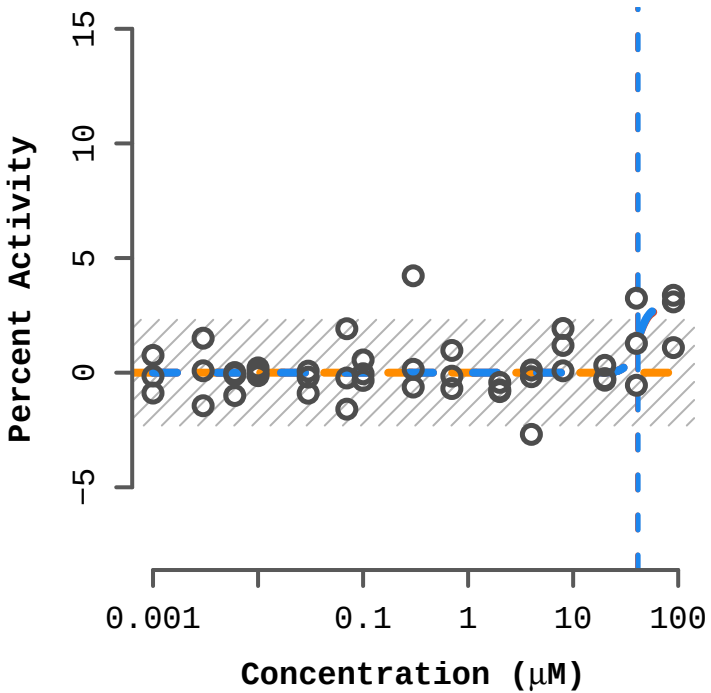
NAME: Cyclohexanone
CHID: 20359 **CASRN:** 108-94-1
SPID(S): Tox21_202121
M4ID: 12480131

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Cyclohexyl-2-benzothiazolesulfenamide
CHID: 20360 CASRN: 95-33-0
SPID(S): Tox21_302924
M4ID: 12476209

HILL MODEL (in red):

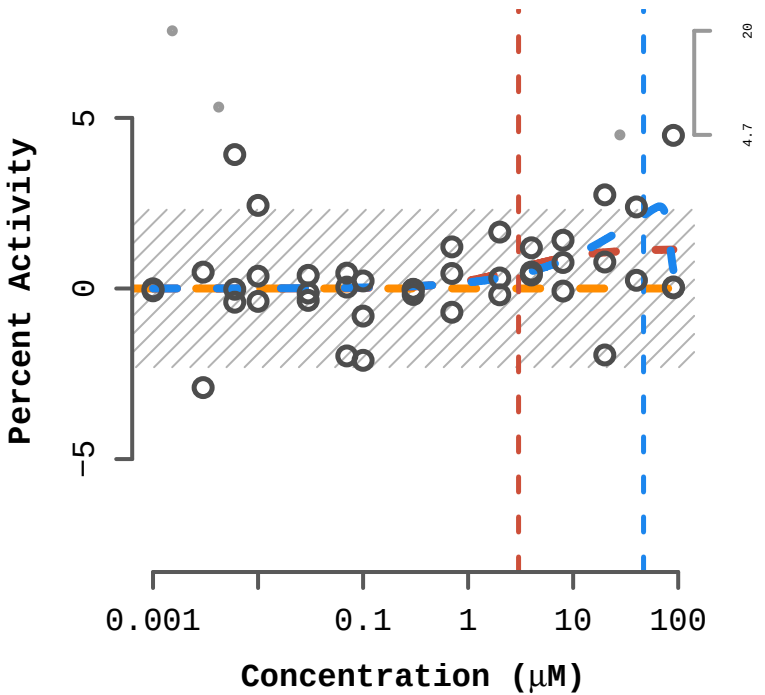
	tp	ga	gw
val:	2.81	1.61	8
sd:	0.574	0.0717	19.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.03	1.62	8	2.83	1.28
sd:	18.2	0.384	19.8	47.5	53.8

	CNST	HILL	GNLS
AIC:	149.57	140.2	144.2
PROB:	0.01	0.87	0.12
RMSE:	1.36	1.14	1.14

MAX_MEAN: 2.52 MAX_MED: 3.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Cyclohexyl-2-benzothiazolesulfenamide
CHID: 20360 CASRN: 95-33-0
SPID(S): Tox21_202436
M4ID: 12479816 BRK

HILL MODEL (in red):

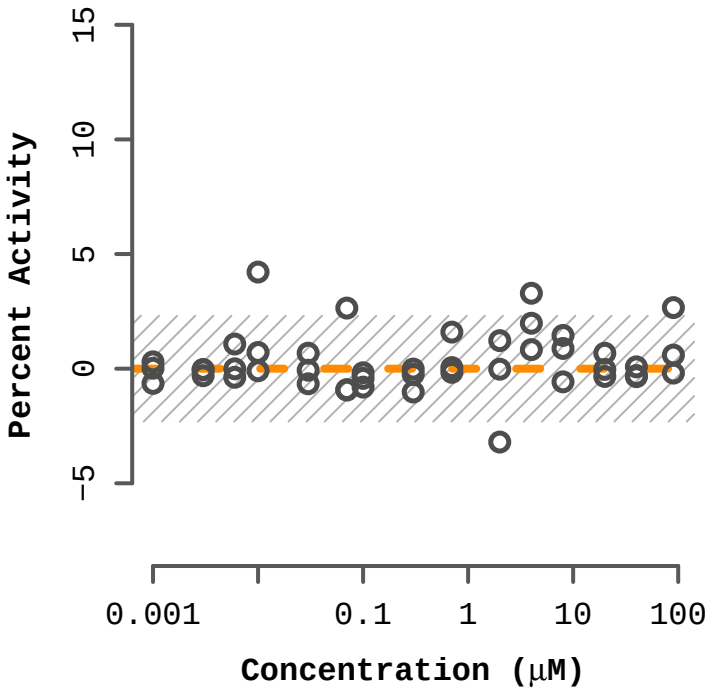
	tp	ga	gw
val:	1.15	0.48	1.27
sd:	0.863	0.924	1.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.29	1.67	0.817	1.92	17.7
sd:	12	2.47	0.64	0.0836	41.5

	CNST	HILL	GNLS
AIC:	196.29	195.33	197.99
PROB:	0.33	0.53	0.14
RMSE:	3.63	3.56	3.56

MAX_MEAN: 6.7 MAX_MED: 2.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

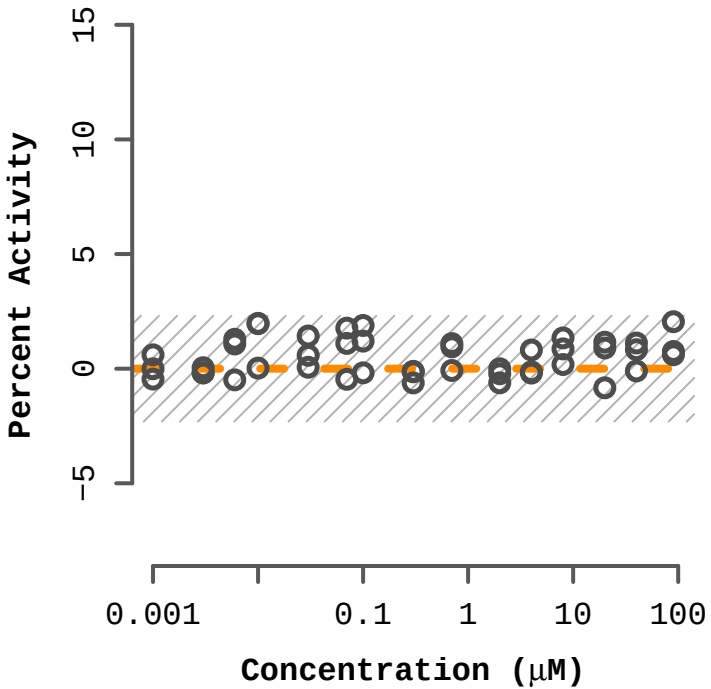
NAME: Cyclohexylamine hydrochloride
CHID: 20361 **CASRN:** 4998-76-9
SPID(S): Tox21_302760
M4ID: 12476373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

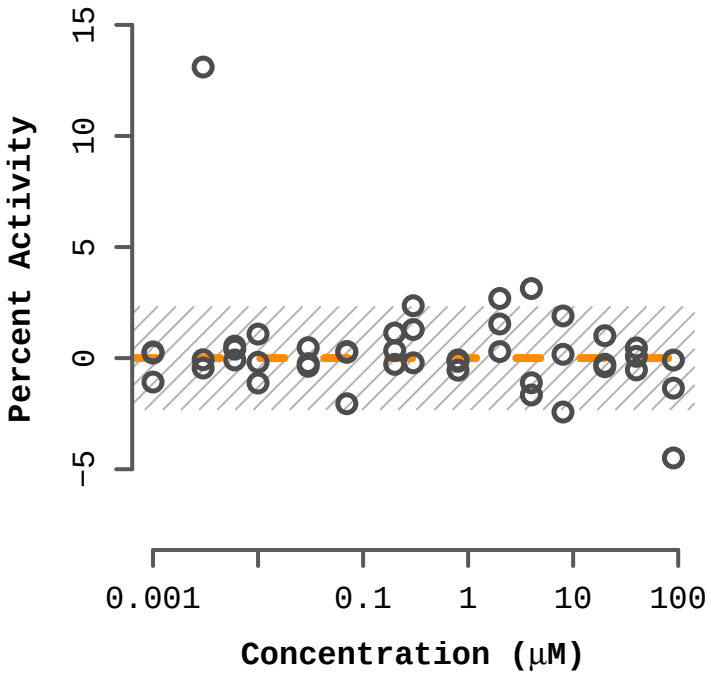
NAME: Cyclohexylamine hydrochloride
CHID: 20361 **CASRN:** 4998-76-9
SPID(S): Tox21_201289
M4ID: 12480963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

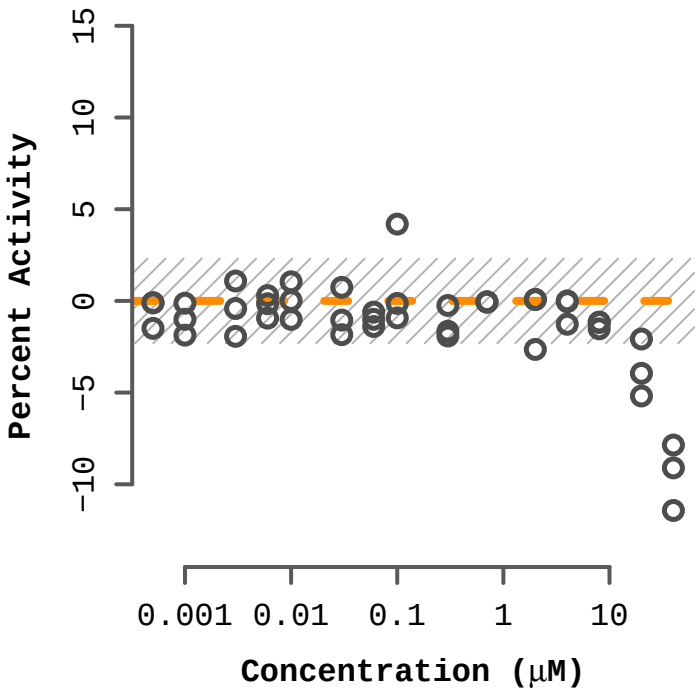
NAME: Cyclopentanone oxime
CHID: 20363 CASRN: 1192-28-5
SPID(S): Tox21_200493
M4ID: 12481759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 4.2 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

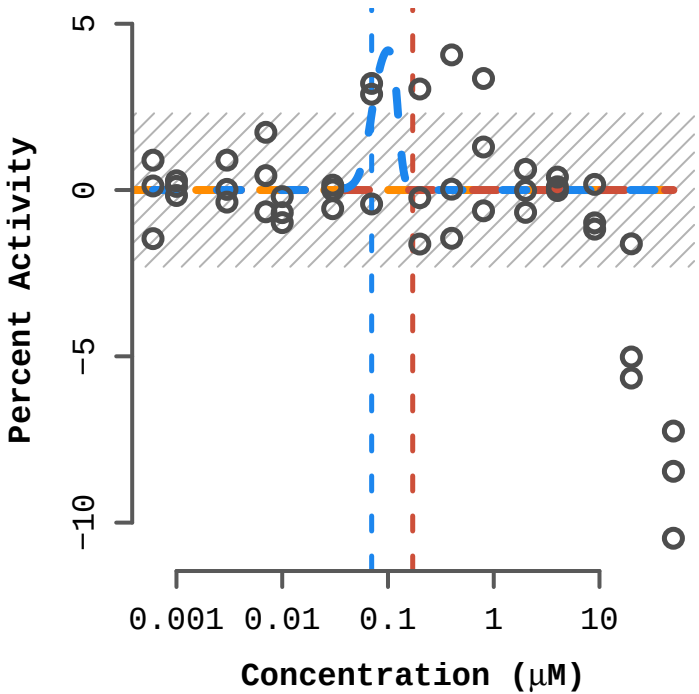
NAME: Cyclosporin A
CHID: 20365 **CASRN:** 59865-13-3
SPID(S): Tox21_301849
M4ID: 12477284

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.92	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.0732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclosporin A
CHID: 20365 CASRN: 59865-13-3
SPID(S): Tox21_110667_1
M4ID: 12484192

HILL MODEL (in red):

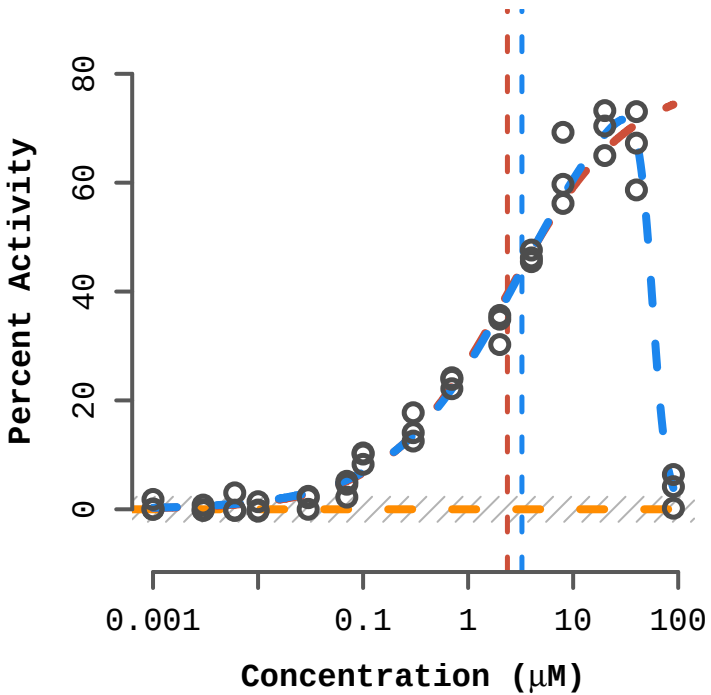
	tp	ga	gw
val:	3.84e-10	-0.766	1.86
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.59	-1.15	7.81	-0.904	16.2
sd:	73	1.76	33.7	6.56	516

	CNST	HILL	GNLS
AIC:	205.75	211.75	212.04
PROB:	0.92	0.05	0.04
RMSE:	2.86	2.86	2.82

MAX_MEAN: 1.89 MAX_MED: 2.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyproterone acetate
CHID: 20366 CASRN: 427-51-0
SPID(S): Tox21_302941
M4ID: 12476192

HILL MODEL (in red):

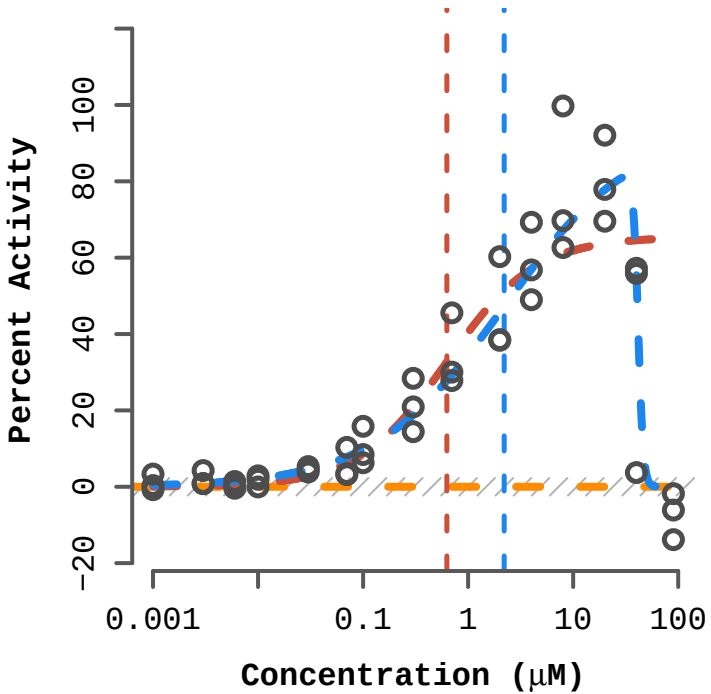
	tp	ga	gw
val:	79.1	0.374	0.755
sd:	4.27	0.0815	0.0545

GAIN-LOSS MODEL (in blue):

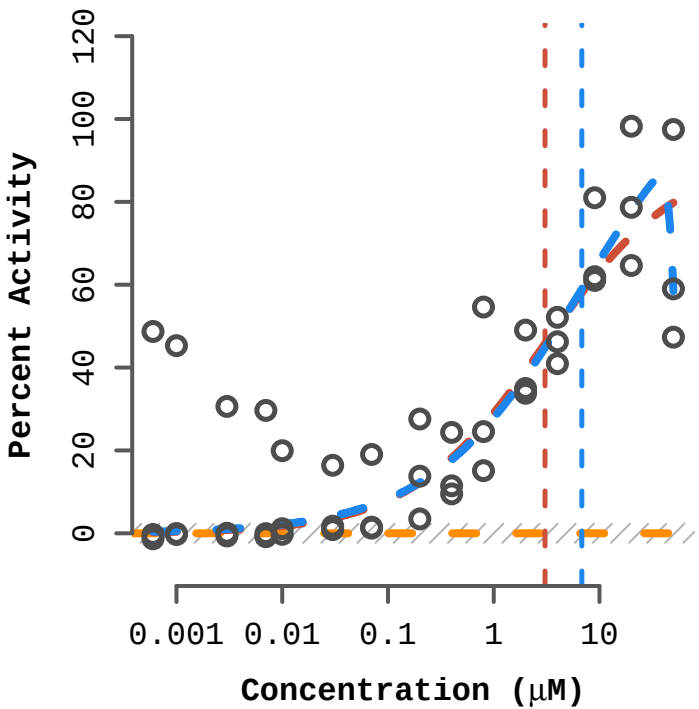
	tp	ga	gw	la	lw
val:	87.9	0.512	0.71	1.75	6.39
sd:	5.3	0.085	0.0399	0.0199	0.752

	CNST	HILL	GNLS
AIC:	445.19	311.97	232.9
PROB:	0	0	1
RMSE:	33.99	18.61	3.14

MAX_MEAN: 69.6 MAX_MED: 70.4 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cyproterone acetate
CHID:    20366   CASRN: 427-51-0
SPID(S): Tox21_201686
M4ID:    12480566

HILL MODEL (in red):
      tp       ga       gw
val:  65.5     -0.202   1.03
sd:   5.33     0.131    0.201

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  94.5     0.343    0.698    1.62     17.8
sd:   12.9     0.226    0.0972   0.00618  7.39

      CNST        HILL        GNLS
AIC:  456.76      383.59      324.47
PROB: 0           0           1
RMSE: 38.76       22.72       10.88

MAX_MEAN: 79.8      MAX_MED: 77.9      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyproterone acetate
CHID: 20366 CASRN: 427-51-0
SPID(S): Tox21_111064_1
M4ID: 12483926

HILL MODEL (in red):

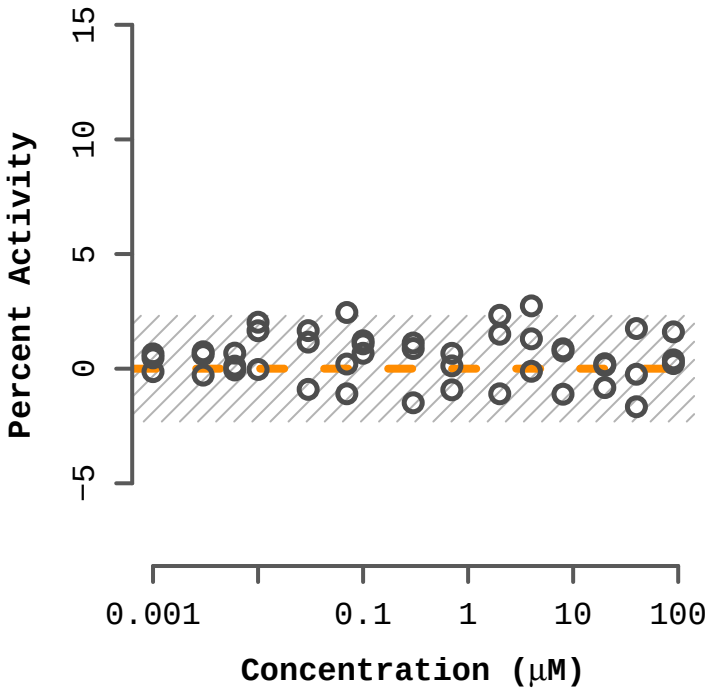
	tp	ga	gw
val:	91.6	0.485	0.686
sd:	24.7	0.4	0.213

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	118	0.833	0.611	1.72	12.7
sd:	41.7	0.524	0.154	0.0174	12.2

	CNST	HILL	GNLS
AIC:	463.44	377.92	376.7
PROB:	0	0.35	0.65
RMSE:	40.43	15.92	15.59

MAX_MEAN: 80.5 MAX_MED: 78.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

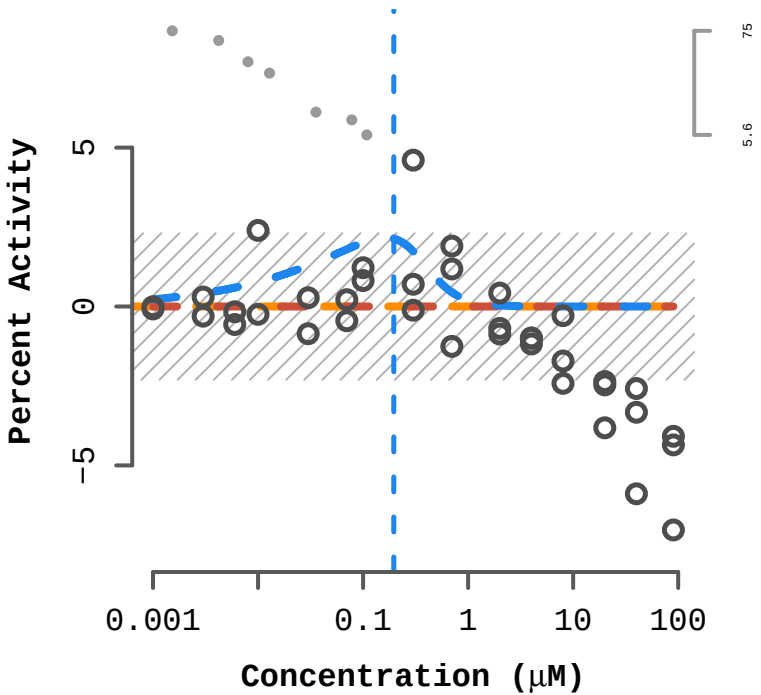
NAME: l-Cysteine hydrochloride
CHID: 20367 **CASRN:** 52-89-1
SPID(S): Tox21_200699
M4ID: 12481553

HILL MODEL: Not applicable.

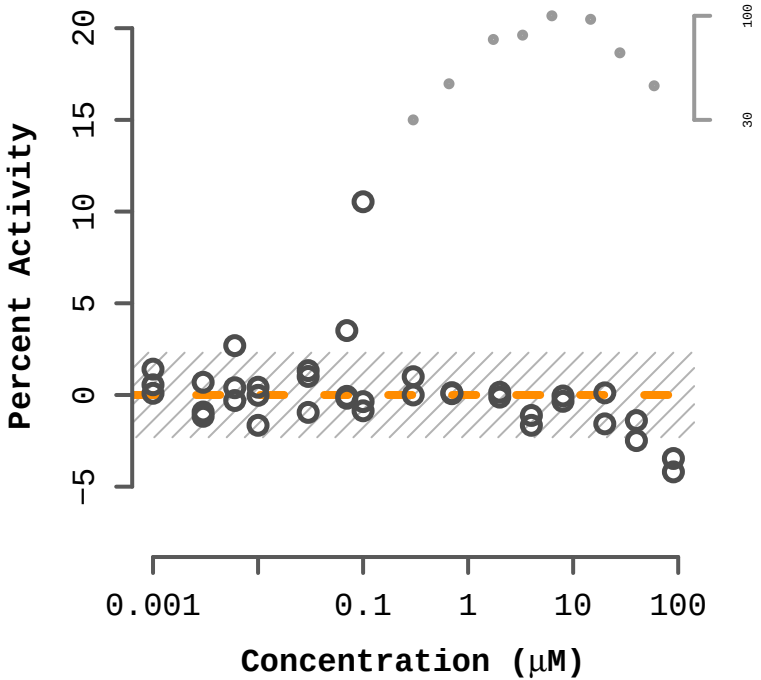
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.66 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cytembena
CHID:    20368   CASRN: 21739-91-3
SPID(S): Tox21_301889
M4ID:    12477244  BRK

HILL MODEL (in red):
      tp        ga        gw
val:  1.62e-09 -4.02     2.49
sd:   0.0046   144000    335000

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  5.14      -0.708    0.584     -0.458    2.75
sd:   82        20        2.58      1.64      4.89

      CNST         HILL         GNLS
AIC:  330.3        336.3        337.55
PROB: 0.93         0.05         0.02
RMSE: 19.1         19.1         18.9

MAX_MEAN: 25        MAX_MED: 2.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

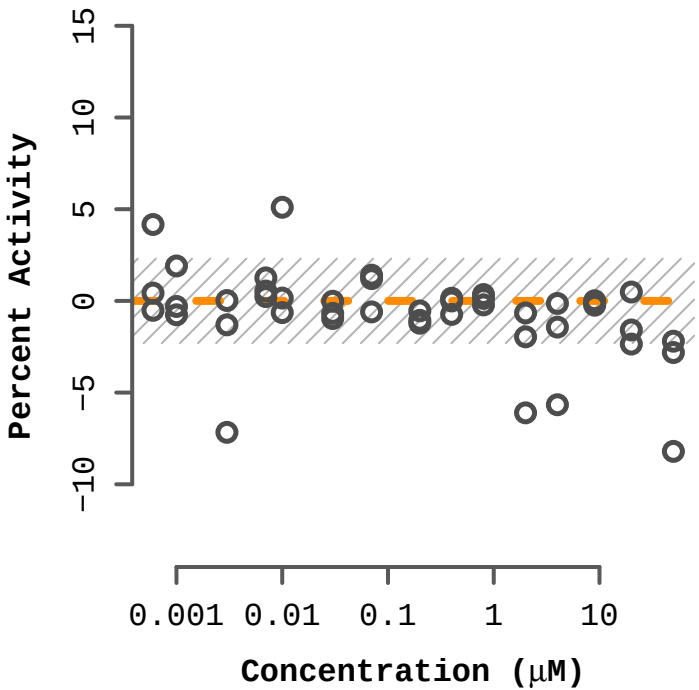
NAME: Dacarbazine
CHID: 20369 CASRN: 4342-03-4
SPID(S): Tox21_201010
M4ID: 12481242 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	398.48	NA	NA
PROB:	1	NA	NA
RMSE:	32.88	NA	NA

MAX_MEAN: 34 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

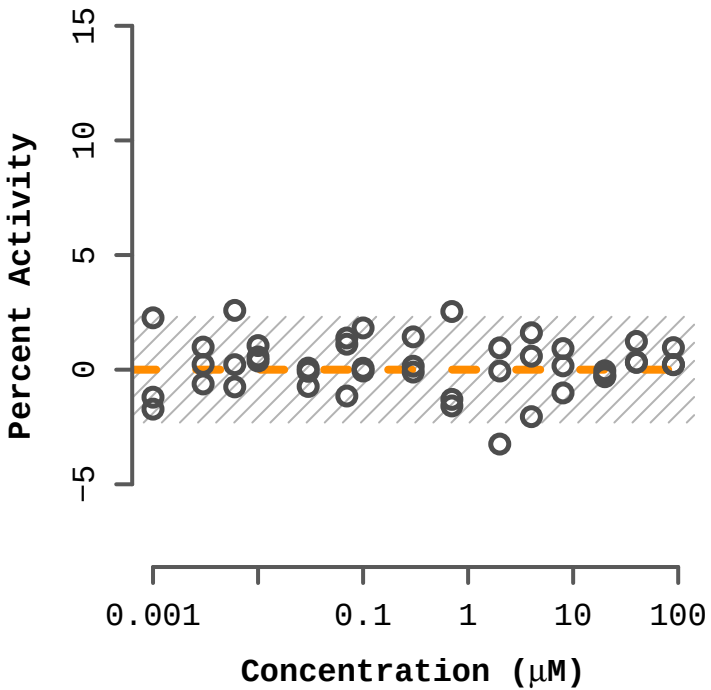
NAME: Dacarbazine
CHID: 20369 **CASRN:** 4342-03-4
SPID(S): Tox21_111171_1
M4ID: 12483864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.76	NA	NA
PROB:	1	NA	NA
RMSE:	2.48	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

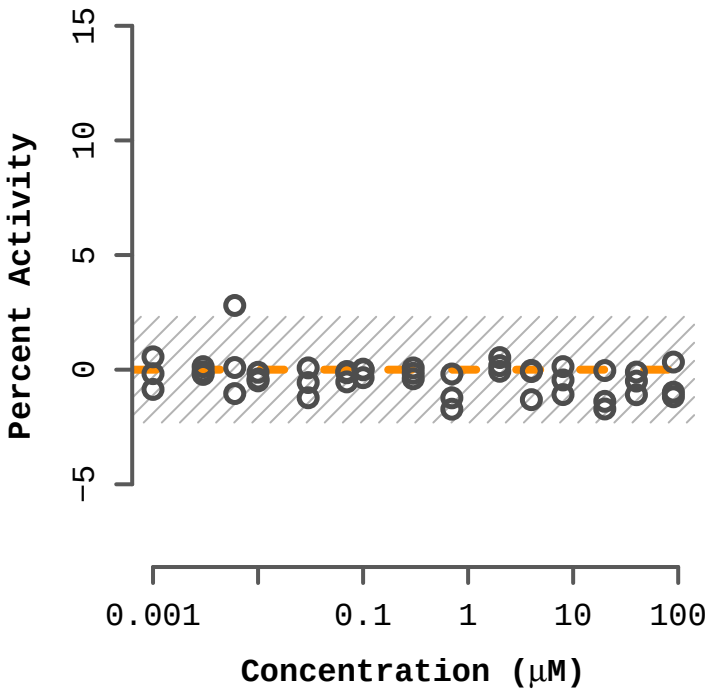
NAME: Daminozide
CHID: 20370 **CASRN:** 1596-84-5
SPID(S): Tox21_300919
M4ID: 12478214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

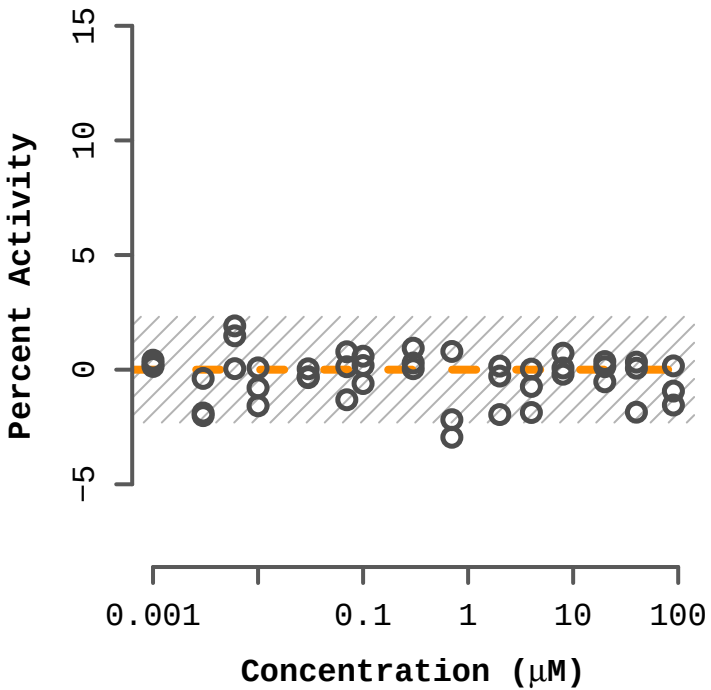
NAME: Daminozide
CHID: 20370 CASRN: 1596-84-5
SPID(S): Tox21_202199
M4ID: 12480053

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.619 MAX_MED: 0.179 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

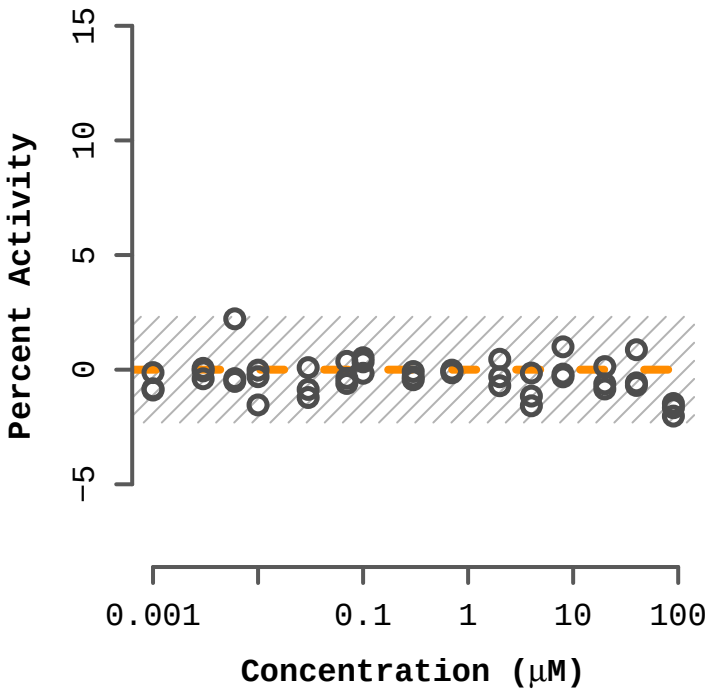
NAME: Dapsone
CHID: 20371 CASRN: 80-08-0
SPID(S): Tox21_300558
M4ID: 12478575

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.15 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

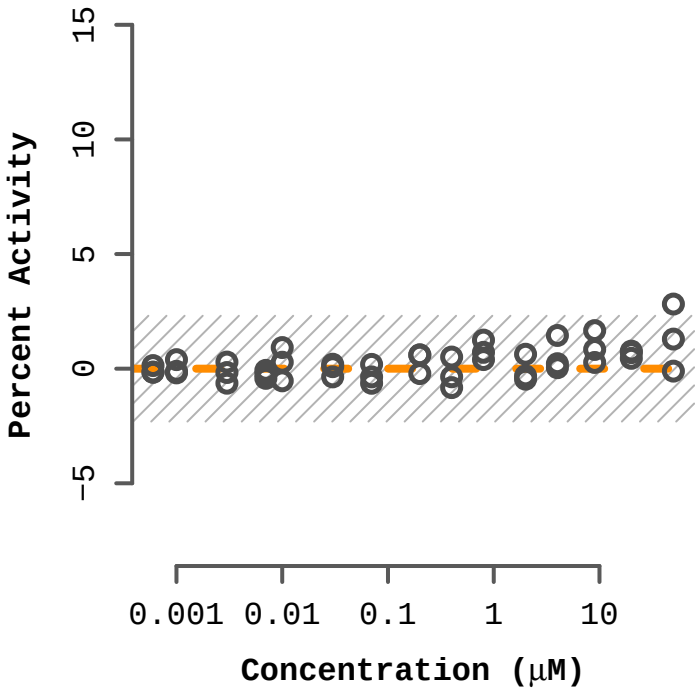
NAME: Dapsone
CHID: 20371 CASRN: 80-08-0
SPID(S): Tox21_201347
M4ID: 12480905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.44 MAX_MED: 0.342 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

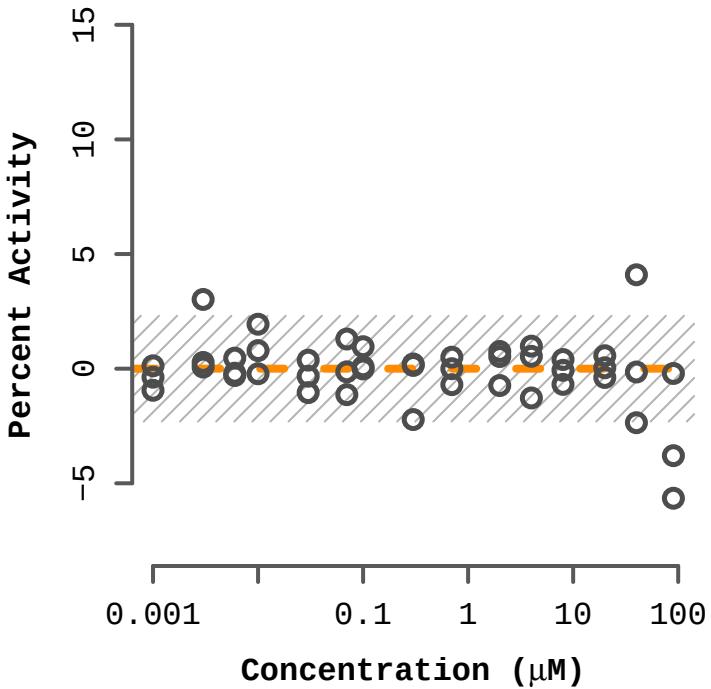
NAME: Dapsone
CHID: 20371 CASRN: 80-08-0
SPID(S): Tox21_110371_1
M4ID: 12484417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

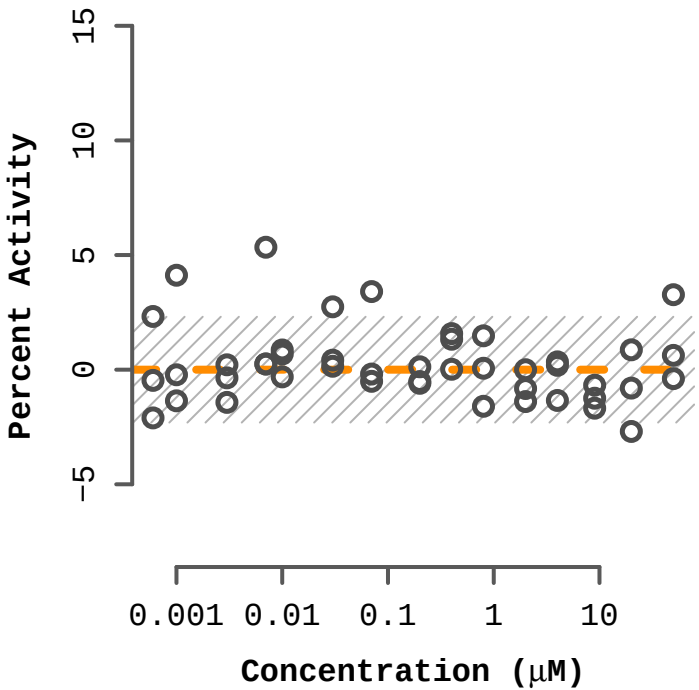
NAME: o,p'−DDD
CHID: 20372 CASRN: 53−19−0
SPID(S): Tox21_302804
M4ID: 12476329

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.12 MAX_MED: 0.791 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

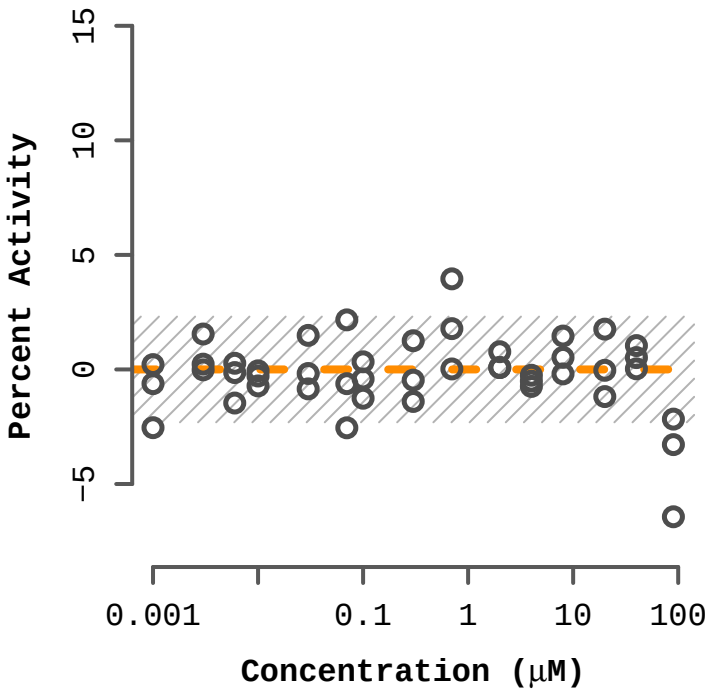
NAME: o,p'−DDD
CHID: 20372 CASRN: 53−19−0
SPID(S): Tox21_110103_1
M4ID: 12484650

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

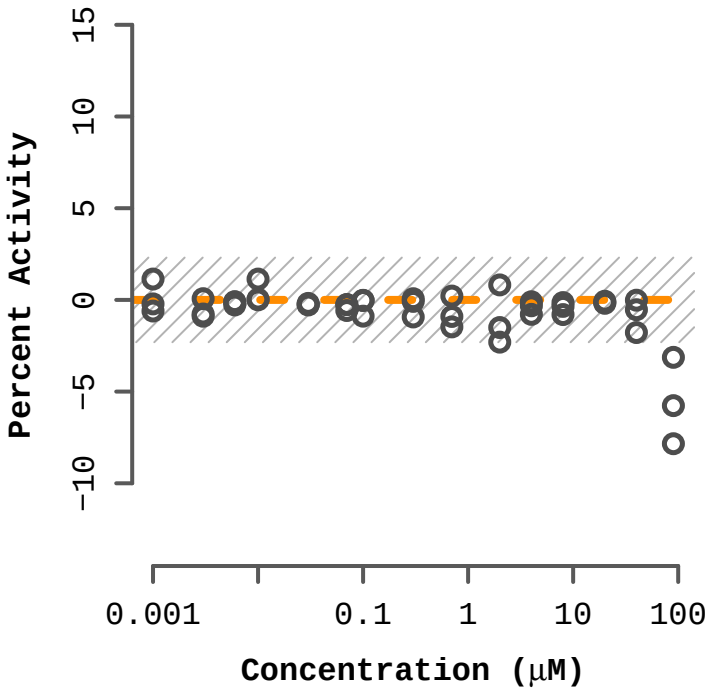
NAME: p,p'−DDD
CHID: 20373 CASRN: 72−54−8
SPID(S): Tox21_300191
M4ID: 12478939

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.92 MAX_MED: 1.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

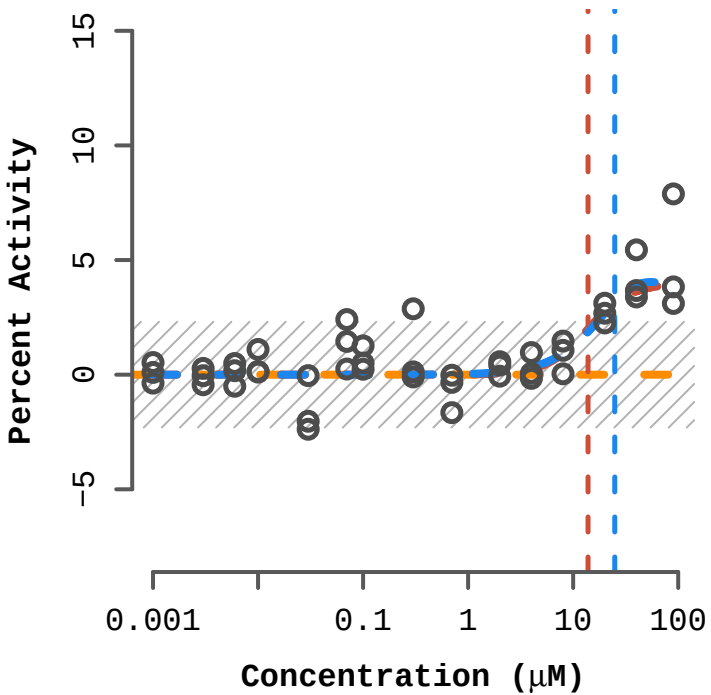
NAME: p,p'−DDD
CHID: 20373 CASRN: 72−54−8
SPID(S): Tox21_201296
M4ID: 12480956

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 0.396 **MAX_MED:** 0.0458 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: p,p'−DDE
CHID: 20374 CASRN: 72−55−9
SPID(S): Tox21_300109
M4ID: 12479021

HILL MODEL (in red):

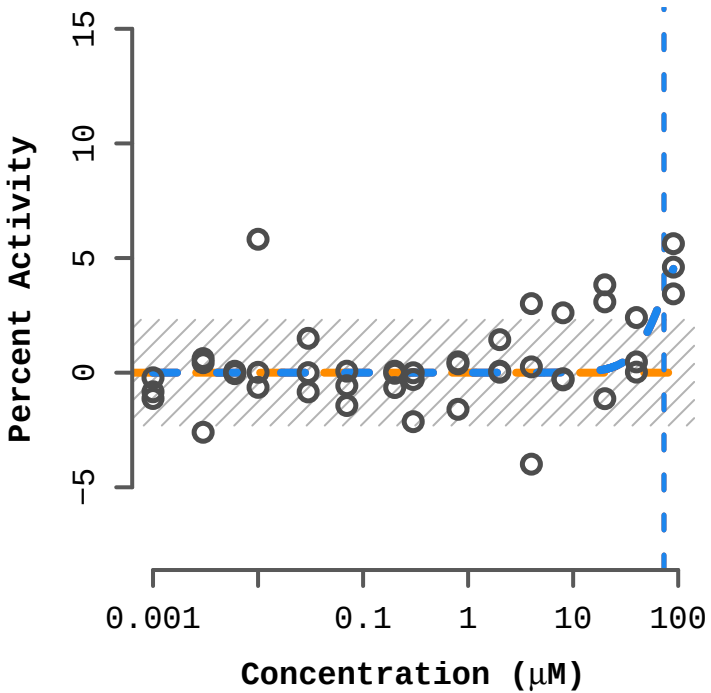
	tp	ga	gw
val:	3.99	1.14	2.2
sd:	0.509	0.0984	0.777

GAIN−LOSS MODEL (in blue):

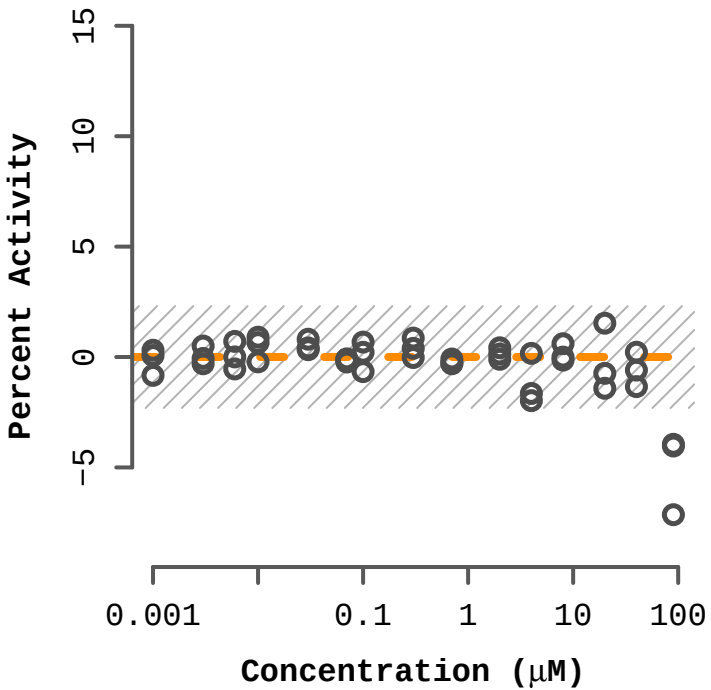
	tp	ga	gw	la	lw
val:	7.63	1.4	1.68	2.02	1.09
sd:	27.6	0.811	0.912	2.67	4.55

	CNST	HILL	GNLS
AIC:	187.31	132.97	136.37
PROB:	0	0.85	0.15
RMSE:	2.11	1.11	1.12

MAX_MEAN: 4.94 MAX_MED: 3.83 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    p,p'-DDE
CHID:    20374   CASRN: 72-55-9
SPID(S): Tox21_201260
M4ID:    12480992

HILL MODEL (in red):
      tp       ga       gw
val:  6.99     1.86     2.96
sd:   10.2     0.5      3.97

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.99     1.86     2.96     3.89     3.27
sd:   10.2     0.502    3.98     869      1490

      CNST       HILL       GNLS
AIC:  187.12     170.79     174.79
PROB: 0          0.88       0.12
RMSE: 2.04       1.64       1.64

MAX_MEAN: 4.56      MAX_MED: 4.61      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

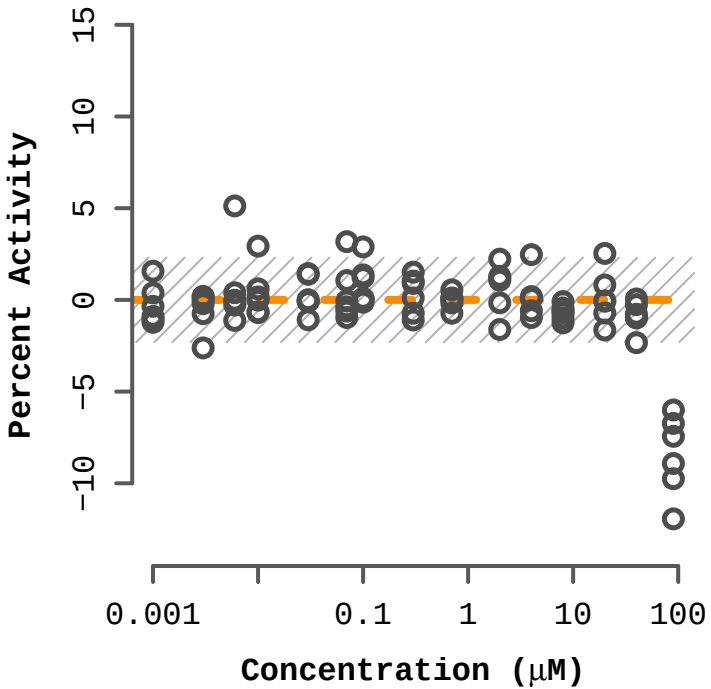
NAME: p,p'−DDT
CHID: 20375 CASRN: 50−29−3
SPID(S): Tox21_300067
M4ID: 12479063

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.519 **MAX_MED:** 0.655 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

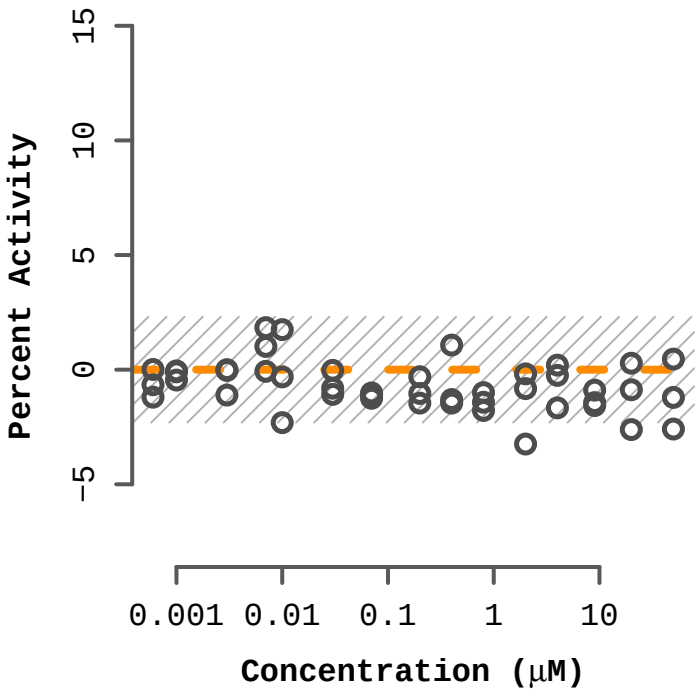
NAME: p,p'−DDT
CHID: 20375 CASRN: 50−29−3
SPID(S): Tox21_201495
M4ID: 12480757

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	363.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 0.908 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

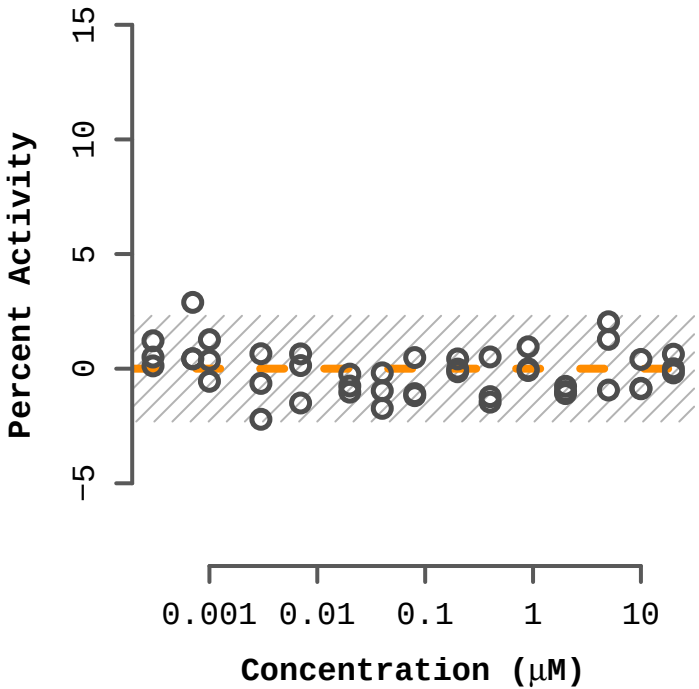
NAME: p,p'−DDT
CHID: 20375 CASRN: 50−29−3
SPID(S): Tox21_111076_1
M4ID: 12483920

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.927 MAX_MED: 1.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

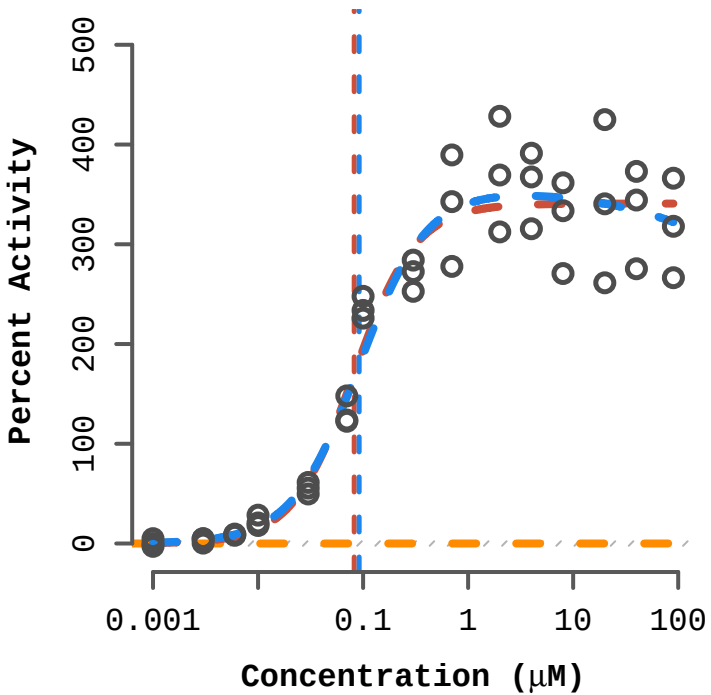
NAME: Decabromodiphenyl oxide
CHID: 20376 **CASRN:** 1163-19-5
SPID(S): Tox21_303970
M4ID: 12475218

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Deflazacort
CHID: 20378 **CASRN:** 14484-47-0
SPID(S): Tox21_301415
M4ID: 12477718

HILL MODEL (in red):

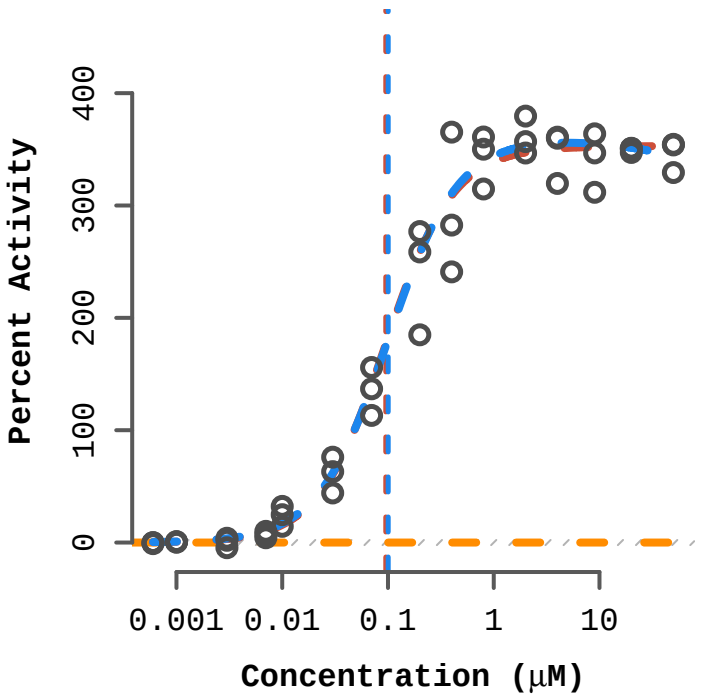
	tp	ga	gw
val:	341	-1.08	1.48
sd:	9.86	0.0549	0.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	358	-1.04	1.34	3.75	0.53
sd:	68.9	0.141	0.325	7.14	2.36

	CNST	HILL	GNLS
AIC:	635.01	459.57	462.33
PROB:	0	0.8	0.2
RMSE:	254.82	36.88	36.07

MAX_MEAN: 370 **MAX_MED:** 369 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Deflazacort
CHID: 20378 CASRN: 14484-47-0
SPID(S): Tox21_112506_1
M4ID: 12483062

HILL MODEL (in red):

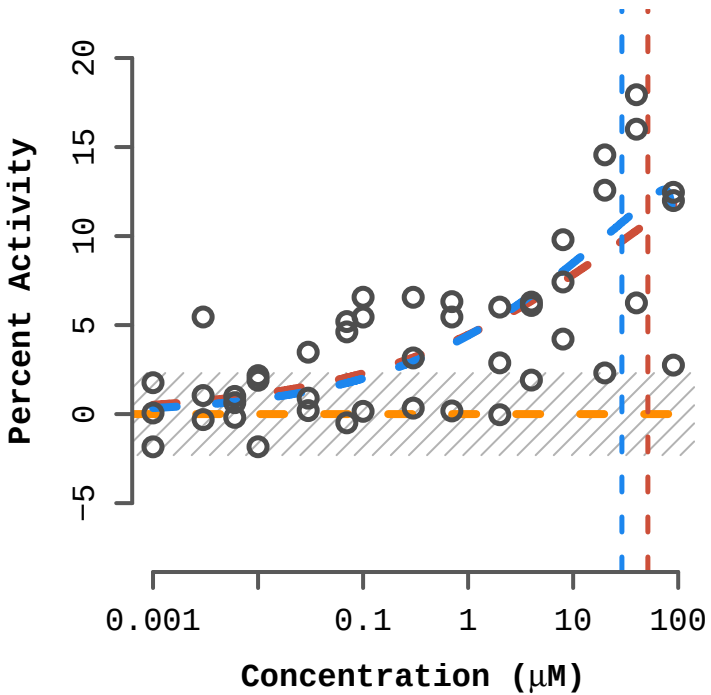
	tp	ga	gw
val:	353	-1.02	1.36
sd:	4.13	0.0309	0.106

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	363	-0.998	1.31	3.7	0.631
sd:	17.6	0.0471	0.116	2.34	0.916

	CNST	HILL	GNLS
AIC:	630.74	403.04	405.37
PROB:	0	0.76	0.24
RMSE:	244.98	22.21	22.08

MAX_MEAN: 361 MAX_MED: 360 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dehydroepiandrosterone
CHID: 20379 CASRN: 53-43-0
SPID(S): Tox21_302761
M4ID: 12476372

HILL MODEL (in red):

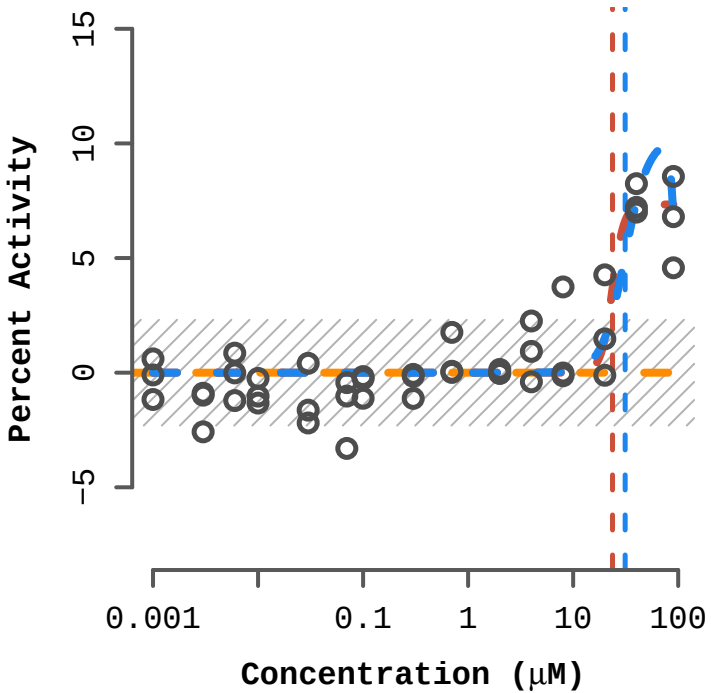
	tp	ga	gw
val:	21.5	1.71	0.341
sd:	13.3	1.51	0.111

GAIN-LOSS MODEL (in blue):

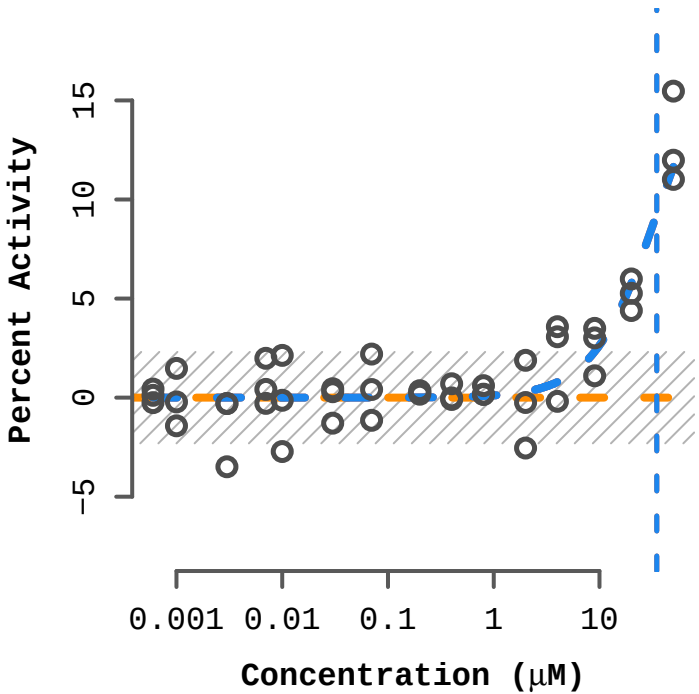
	tp	ga	gw	la	lw
val:	21.5	1.46	0.402	2	14.6
sd:	13	0.956	0.13	0.063	24.2

	CNST	HILL	GNLS
AIC:	295.68	244.6	248.01
PROB:	0	0.85	0.15
RMSE:	6.5	3.32	3.26

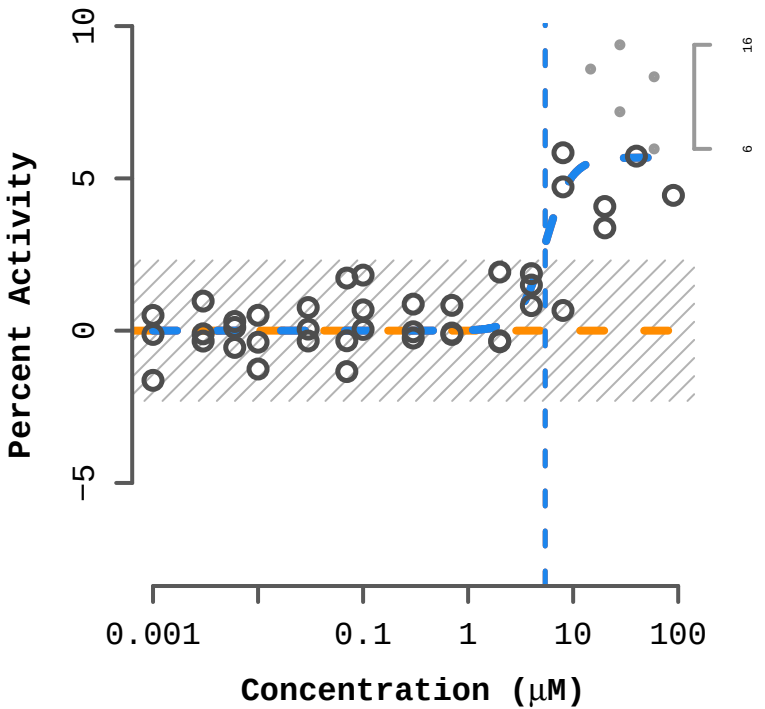
MAX_MEAN: 13.4 MAX_MED: 16 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dehydroepiandrosterone
CHID:    20379   CASRN: 53-43-0
SPID(S): Tox21_201996
M4ID:    12480256

HILL MODEL (in red):
      tp       ga       gw
val:  7.34     1.37     8
sd:   0.548    0.0557   4.99

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.3     1.49     3.94     1.97     17.1
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  214.26      160.13      163.51
PROB: 0           0.84        0.16
RMSE: 2.95        1.35        1.33

MAX_MEAN: 7.49      MAX_MED: 7.21      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dehydroepiandrosterone
CHID:    20379   CASRN: 53-43-0
SPID(S): Tox21_111222_1
M4ID:    12483833

HILL MODEL (in red):
      tp       ga       gw
val:  18.6     1.54     1.44
sd:   5.22     0.185    0.362

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  18.6     1.54     1.44     3.65     7.96
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  228.29      162.91      166.91
PROB: 0           0.88        0.12
RMSE: 3.9         1.4         1.4

MAX_MEAN: 12.8      MAX_MED: 12        BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dehydroepiandrosterone acetate
CHID: 20380 CASRN: 853-23-6
SPID(S): Tox21_200963
M4ID: 12481289 BRK

HILL MODEL (in red):

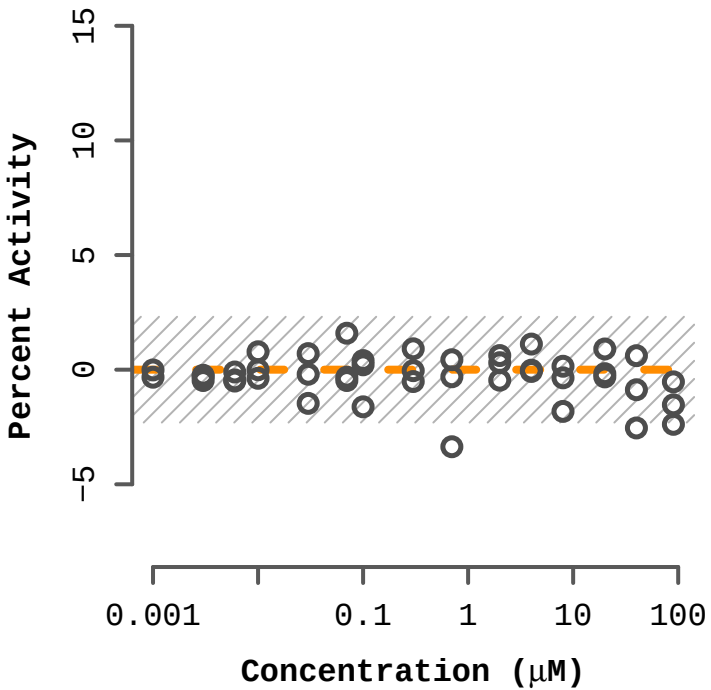
	tp	ga	gw
val:	5.68	0.734	3.53
sd:	0.721	0.0887	2.21

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.68	0.734	3.53	3.08	5.89
sd:	0.721	0.0887	2.21	2090	8130

	CNST	HILL	GNLS
AIC:	241.25	187.63	191.63
PROB:	0	0.88	0.12
RMSE:	4.48	2.52	2.52

MAX_MEAN: 10.4 MAX_MED: 9.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

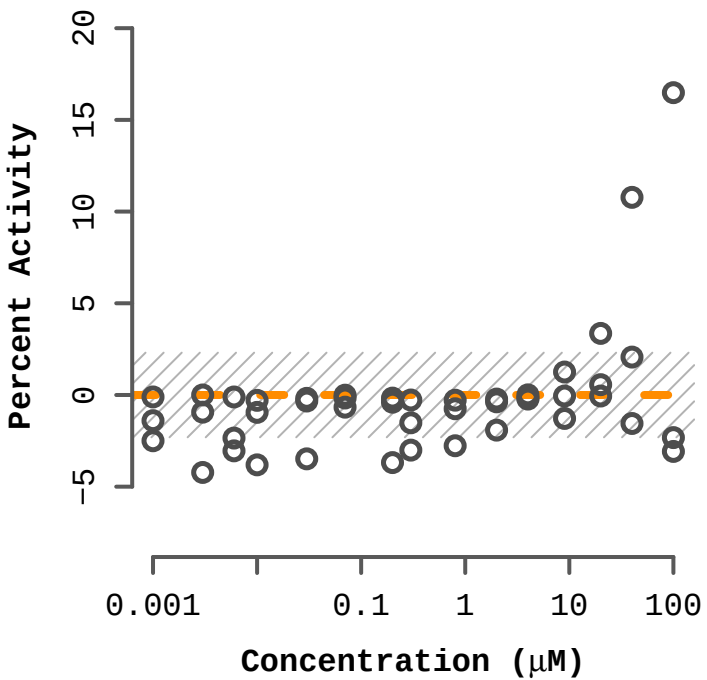
NAME: Deltamethrin
CHID: 20381 CASRN: 52918-63-5
SPID(S): Tox21_303009
M4ID: 12476124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.341 MAX_MED: 0.307 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

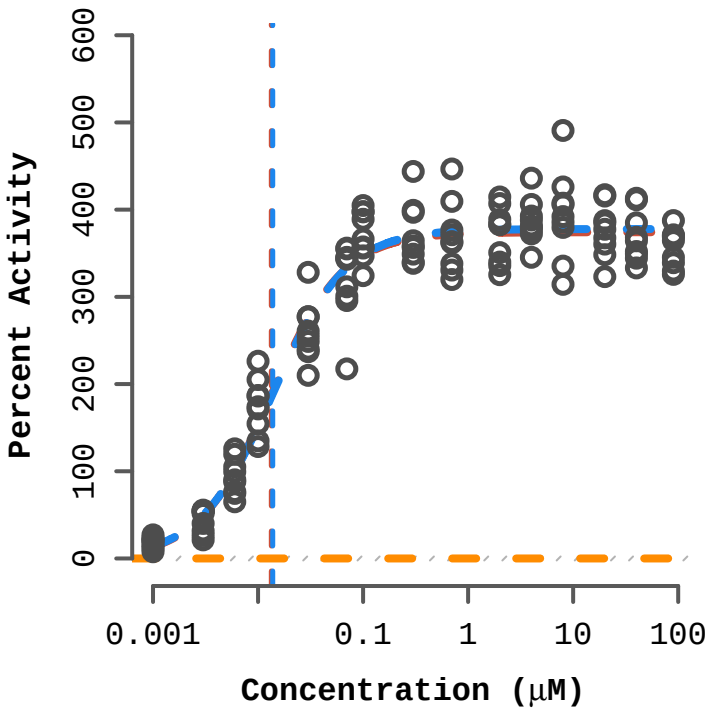
NAME: Deltamethrin
CHID: 20381 CASRN: 52918-63-5
SPID(S): Tox21_201432
M4ID: 12480820

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.57	NA	NA
PROB:	1	NA	NA
RMSE:	3.44	NA	NA

MAX_MEAN: 3.76 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexamethasone
CHID: 20384 CASRN: 50-02-2
SPID(S): Tox21_200122
M4ID: 12482130

HILL MODEL (in red):

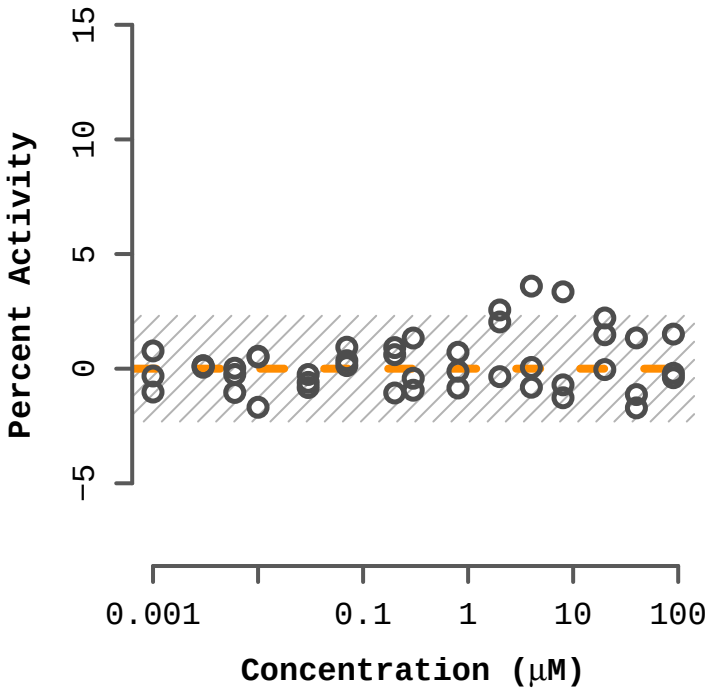
	tp	ga	gw
val:	374	-1.87	1.27
sd:	3.77	0.0268	0.0738

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	378	-1.86	1.24	2.02	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	1964.11	1325.93	1325.5
PROB:	0	0.45	0.55
RMSE:	314.12	32.27	31.77

MAX_MEAN: 393 MAX_MED: 392 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

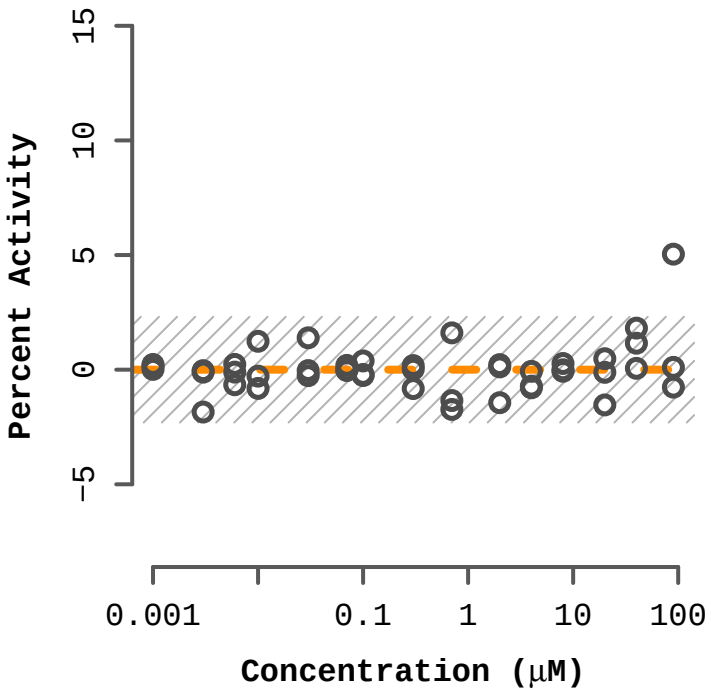
NAME: Diacetyl hydrazine
CHID: 20390 **CASRN:** 3148-73-0
SPID(S): Tox21_200099
M4ID: 12482153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

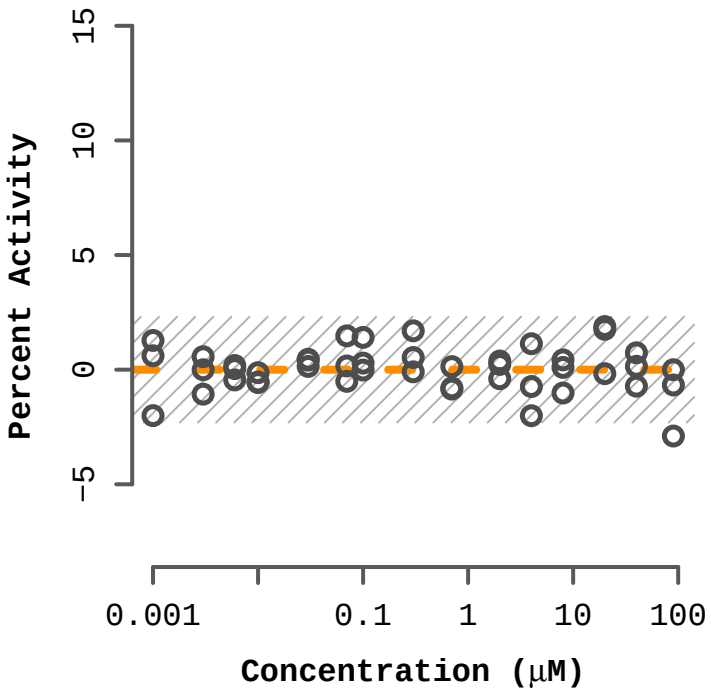
NAME: Diallate
CHID: 20391 CASRN: 2303-16-4
SPID(S): Tox21_200642
M4ID: 12481610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.46 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

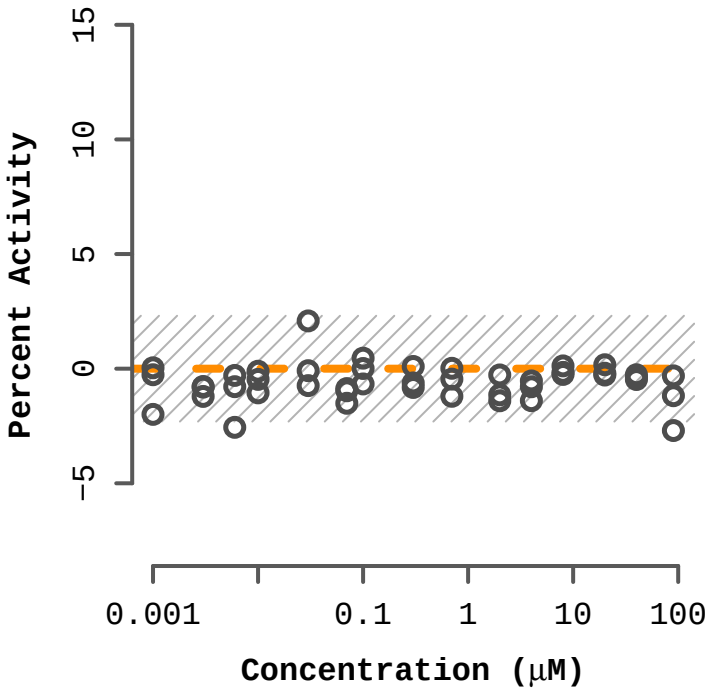
NAME: Diallyl phthalate
CHID: 20392 **CASRN:** 131-17-9
SPID(S): Tox21_300135
M4ID: 12478995

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

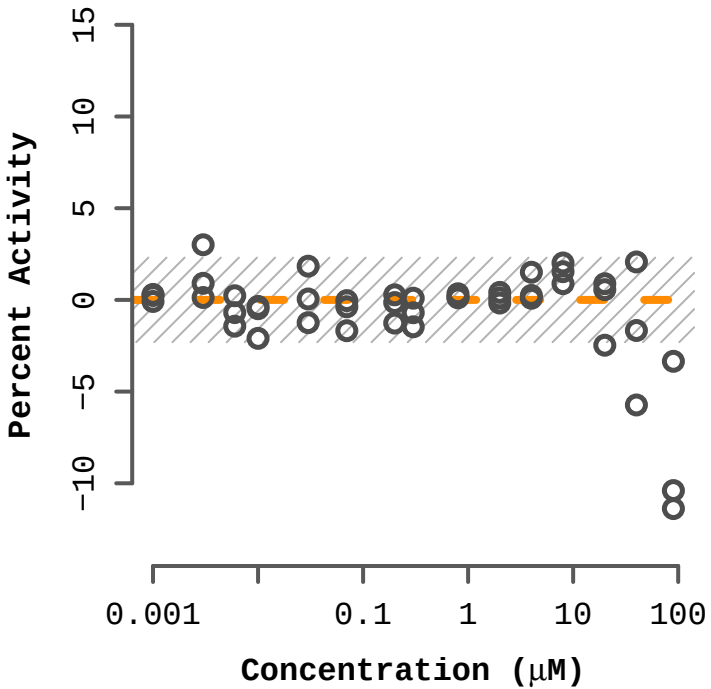
NAME: Diallyl phthalate
CHID: 20392 **CASRN:** 131-17-9
SPID(S): Tox21_201961
M4ID: 12480291

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.421 **MAX_MED:** 0.00915 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

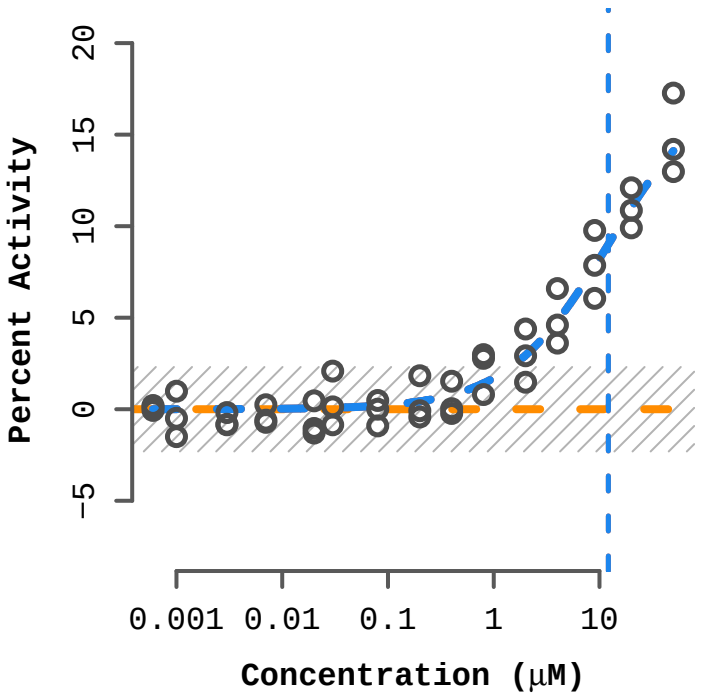
NAME: 2,4-Diaminoanisole sulfate
CHID: 20398 **CASRN:** 39156-41-7
SPID(S): Tox21_200494
M4ID: 12481758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Diaminoazobenzene
CHID: 20399 CASRN: 538−41−0
SPID(S): Tox21_202586
M4ID: 12479666

HILL MODEL (in red):

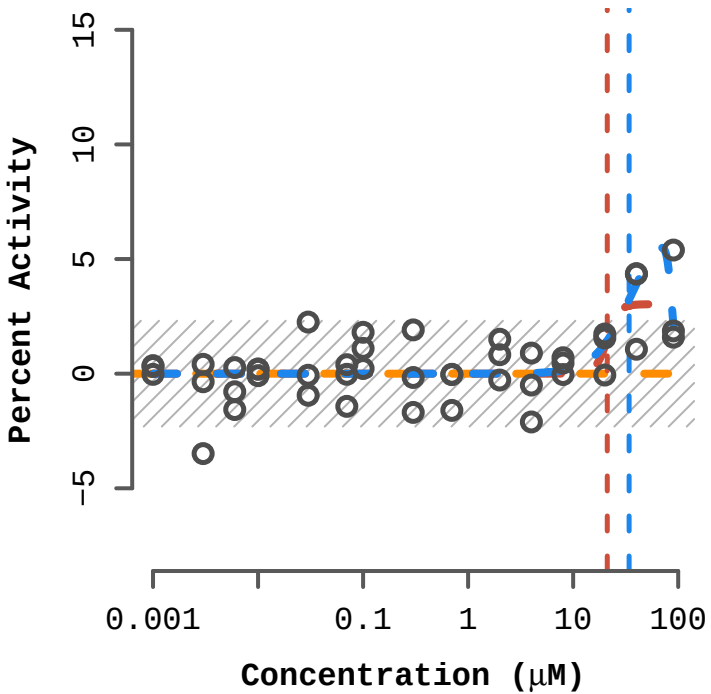
	tp	ga	gw
val:	18	1.08	0.905
sd:	2.98	0.195	0.152

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18	1.08	0.905	3.6	16.1
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	271.53	147.48	151.48
PROB:	0	0.88	0.12
RMSE:	5.52	1.1	1.1

MAX_MEAN: 14.8 **MAX_MED:** 14.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Diaminobenzanilide
CHID: 20400 CASRN: 785−30−8
SPID(S): Tox21_200716
M4ID: 12481536

HILL MODEL (in red):

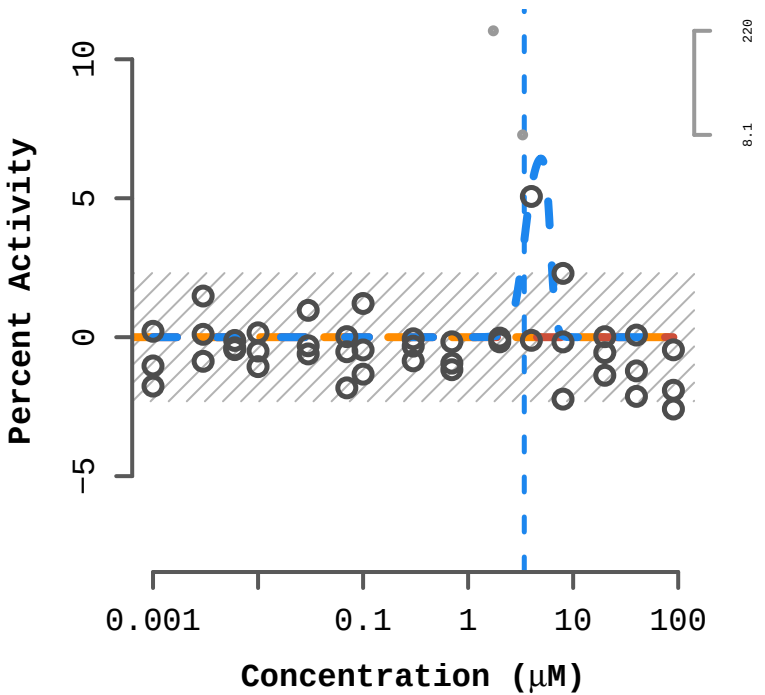
	tp	ga	gw
val:	3.03	1.32	8
sd:	0.91	0.0586	11.1

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.47	1.53	2.61	1.94	17.6
sd:	10.1	0.57	2.93	0.0263	68.6

	CNST	HILL	GNLS
AIC:	169.35	153.32	154.4
PROB:	0	0.63	0.37
RMSE:	1.68	1.2	1.23

MAX_MEAN: 3.26 MAX_MED: 4.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4−Diaminophenol dihydrochloride
CHID: 20401 CASRN: 137−09−7
SPID(S): Tox21_303017
M4ID: 12476116 BRK

HILL MODEL (in red):

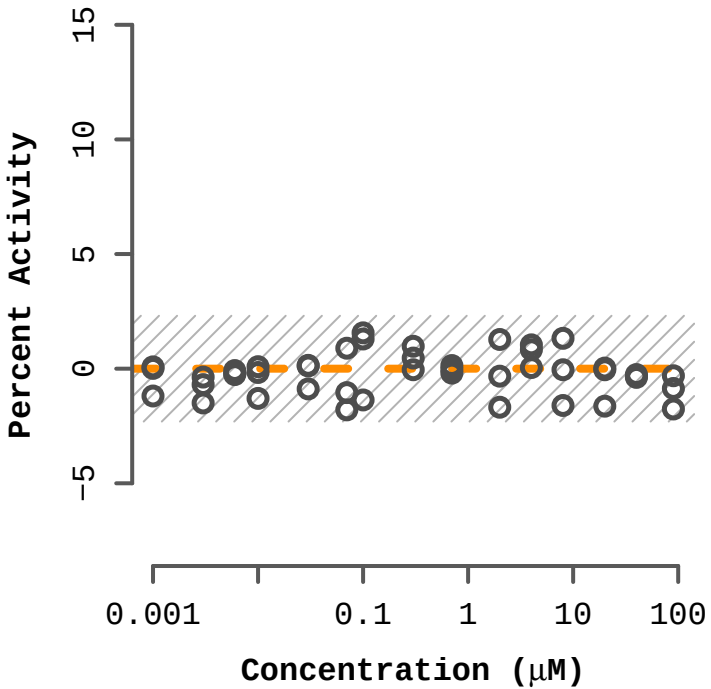
	tp	ga	gw
val:	4.83e−11	2.35	0.763
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.93	0.534	7.96	0.784	17.9
sd:	13.1	0.388	10.7	0.359	54.1

	CNST	HILL	GNLS
AIC:	206.81	212.81	208.94
PROB:	0.72	0.04	0.25
RMSE:	32.94	32.94	32.91

MAX_MEAN: 73.5 MAX_MED: 5.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

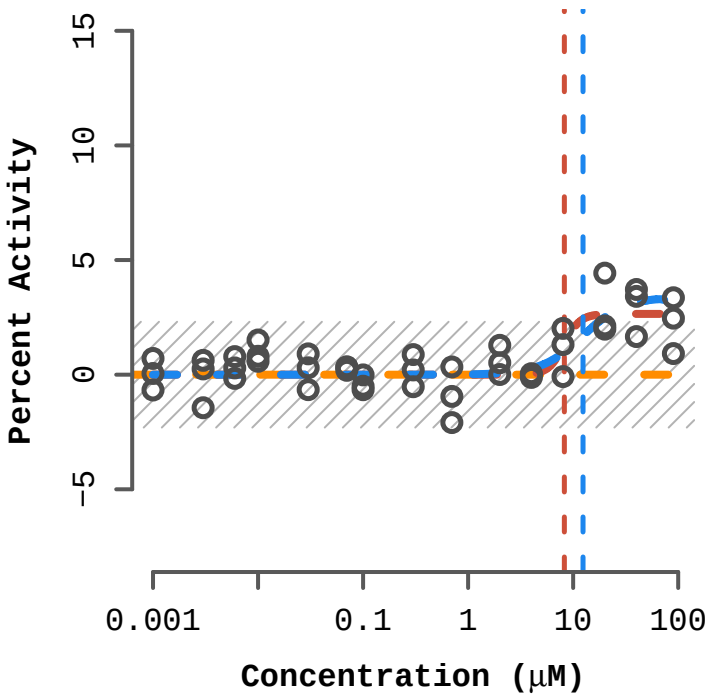
NAME: 2,4−Diaminophenol dihydrochloride
CHID: 20401 CASRN: 137−09−7
SPID(S): Tox21_201248
M4ID: 12481004

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.641 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4−Diaminotoluene
CHID: 20402 CASRN: 95−80−7
SPID(S): Tox21_300143
M4ID: 12478987

HILL MODEL (in red):

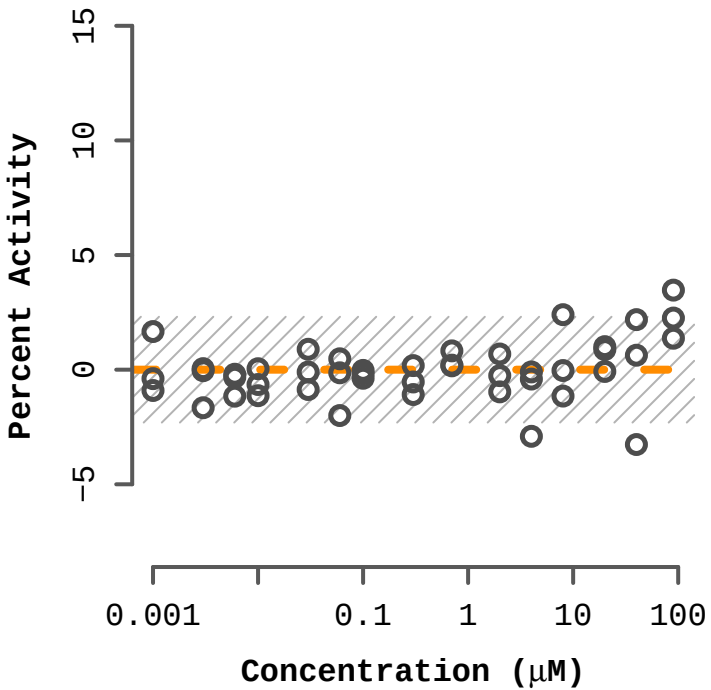
	tp	ga	gw
val:	2.65	0.916	5.77
sd:	0.406	0.133	29

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.39	1.09	2.17	1.98	14.8
sd:	1.17	0.262	1.43	0.0462	25.8

	CNST	HILL	GNLS
AIC:	159.77	120.66	123.93
PROB:	0	0.84	0.16
RMSE:	1.48	0.83	0.82

MAX_MEAN: 2.93 MAX_MED: 3.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

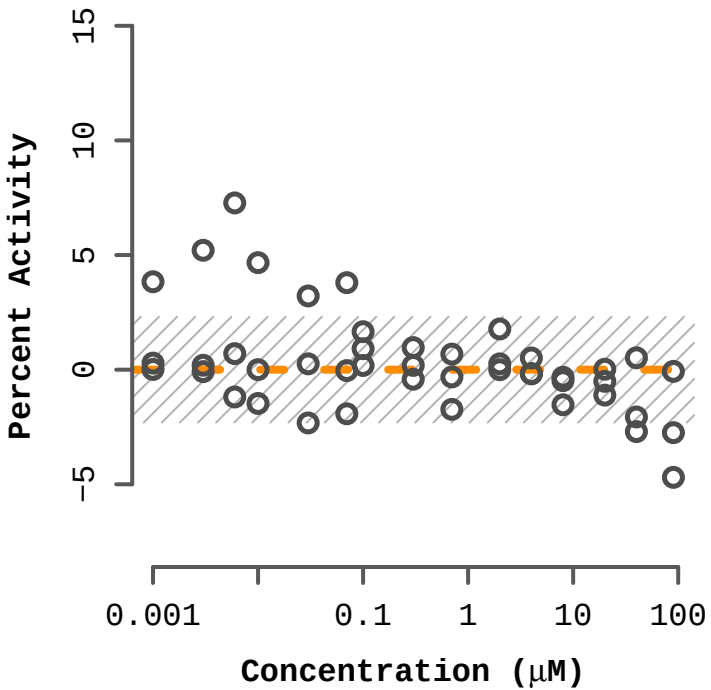
NAME: 2,4−Diaminotoluene
CHID: 20402 **CASRN:** 95−80−7
SPID(S): Tox21_201411
M4ID: 12480841

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 2.37 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

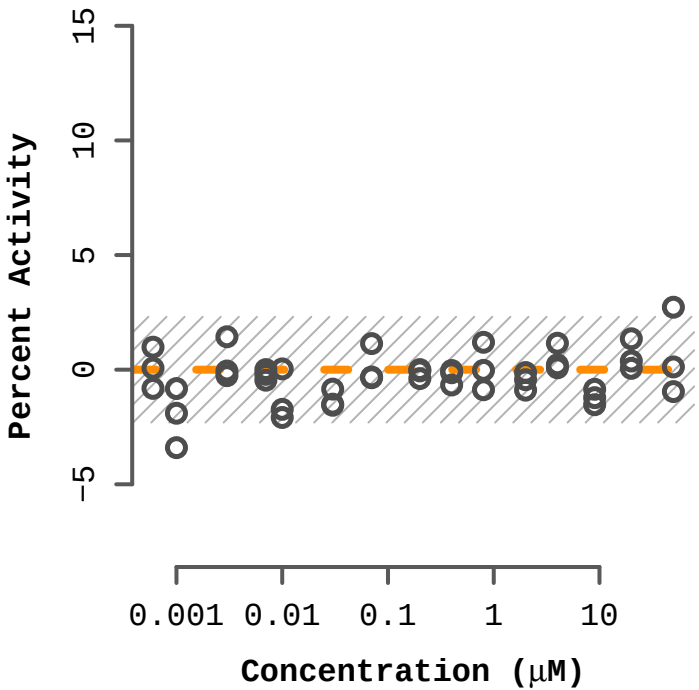
NAME: Diazepam
CHID: 20406 CASRN: 439-14-5
SPID(S): Tox21_202458
M4ID: 12479794

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 2.26 **MAX_MED:** 0.916 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

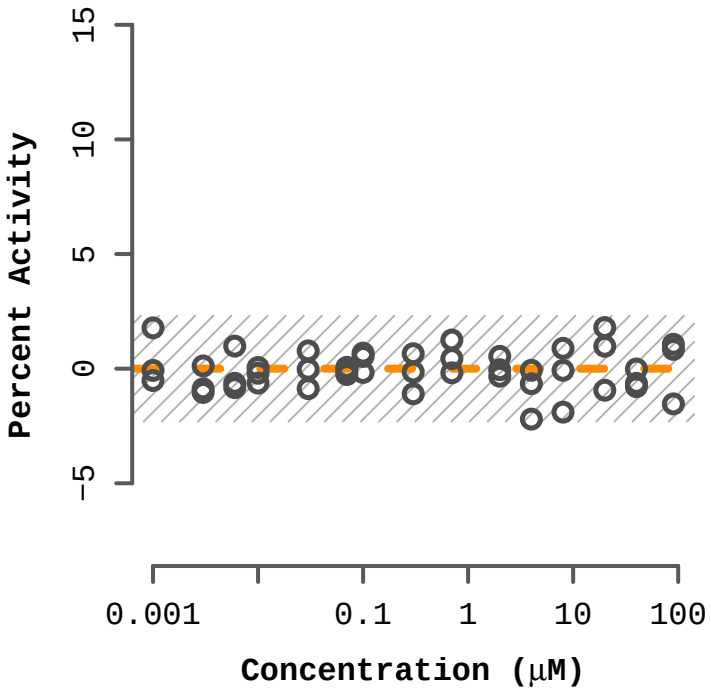
NAME: Diazepam
CHID: 20406 CASRN: 439-14-5
SPID(S): Tox21_113071_1
M4ID: 12482821

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.631 **MAX_MED:** 0.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

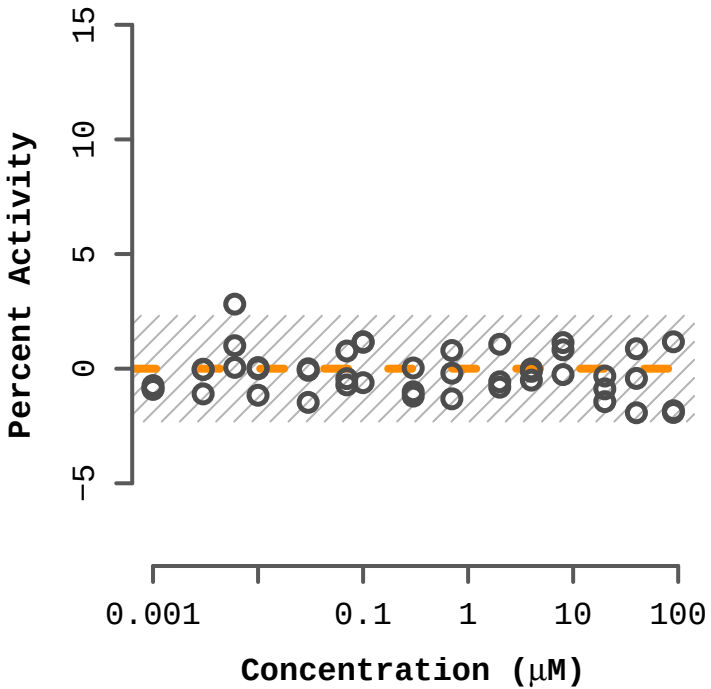
NAME: Diazinon
CHID: 20407 CASRN: 333-41-5
SPID(S): Tox21_300730
M4ID: 12478403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.612 MAX_MED: 0.978 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

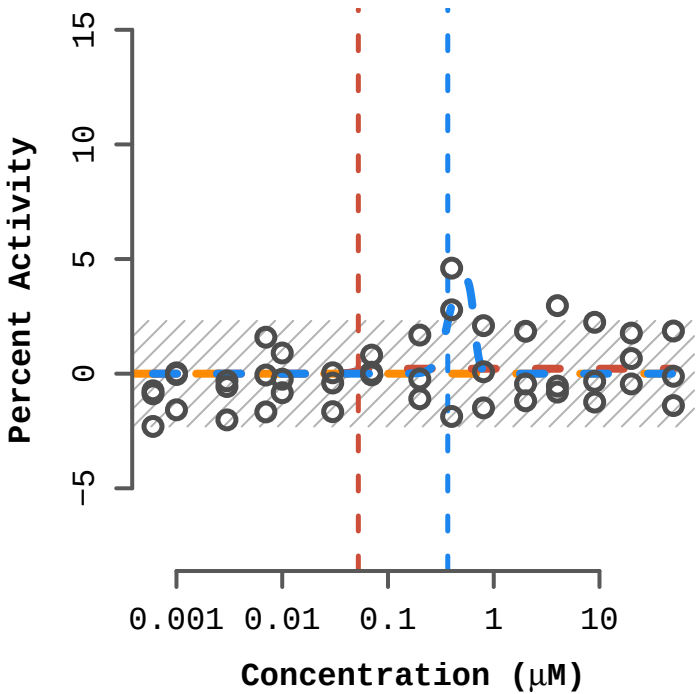
NAME: Diazinon
CHID: 20407 CASRN: 333-41-5
SPID(S): Tox21_201409
M4ID: 12480843

HILL MODEL: Not applicable.

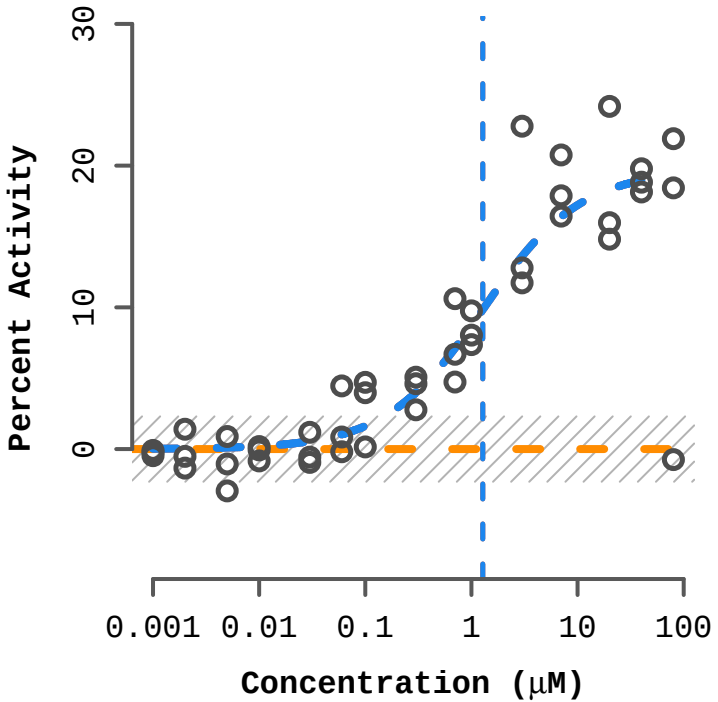
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.06	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

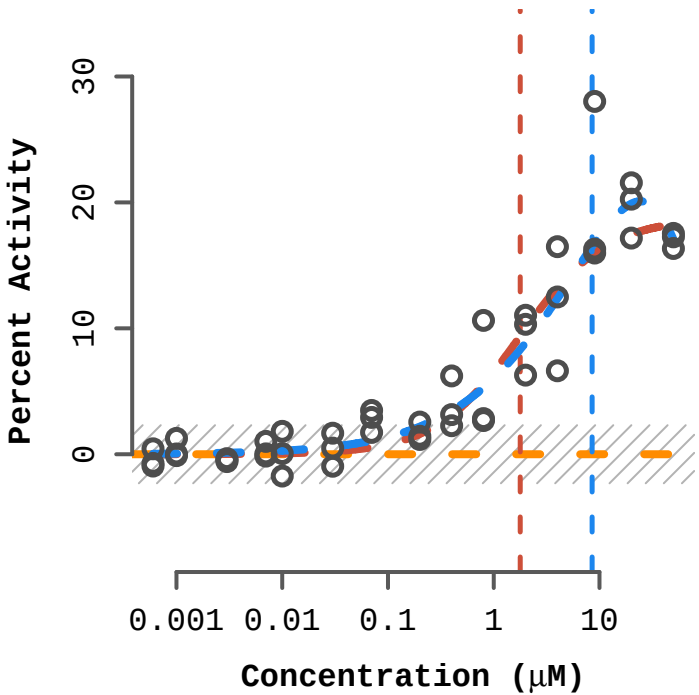
MAX_MEAN: 1.29 MAX_MED: 1.15 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diazinon
CHID:    20407   CASRN: 333-41-5
SPID(S): Tox21_111077_1
M4ID:    12483919

HILL MODEL (in red):
      tp       ga       gw
val:  0.217    -1.28    8
sd:   0.308    0.714    29.6

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.53     -0.435   7.97     -0.185   17.4
sd:   41.8     1.38     31.6     17.8     3520

      CNST        HILL        GNLS
AIC:  165.28      170.76      170.71
PROB: 0.88        0.06        0.06
RMSE: 1.47        1.44        1.43

MAX_MEAN: 1.84      MAX_MED: 2.79      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dibenz(a,h)anthracene
CHID:    20409   CASRN: 53-70-3
SPID(S): Tox21_303587
M4ID:    12475558

HILL MODEL (in red):
      tp       ga       gw
val:  19.7     0.107    0.944
sd:   1.04     0.0928   0.152

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  19.7     0.107    0.944    3.13     5.9
sd:   1.04     0.0928   0.152    635      3050

      CNST        HILL        GNLS
AIC:  344.42      221.26      225.26
PROB: 0           0.88        0.12
RMSE: 10.87       3.79        3.79

MAX_MEAN: 18.9      MAX_MED: 18.8      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dibenz(a,h)anthracene
CHID: 20409 CASRN: 53-70-3
SPID(S): Tox21_202505
M4ID: 12479747

HILL MODEL (in red):

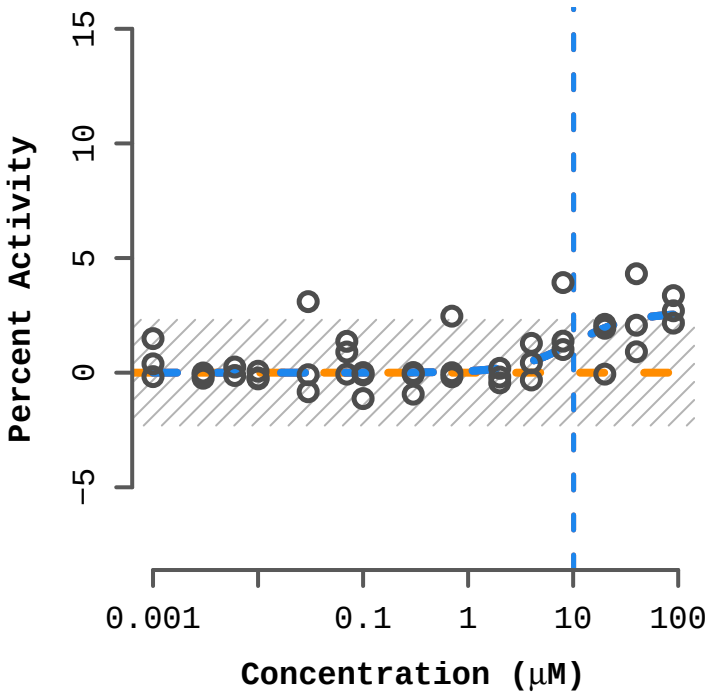
	tp	ga	gw
val:	18.8	0.251	1.08
sd:	1.07	0.0897	0.191

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	33.6	0.93	0.71	1.84	1.91
sd:	72.1	2.21	0.395	0.283	6.82

	CNST	HILL	GNLS
AIC:	330.79	207.66	203.71
PROB:	0	0.12	0.88
RMSE:	9.8	2.7	2.49

MAX_MEAN: 20.1 MAX_MED: 20.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dibenzo-p-dioxin
CHID: 20410 CASRN: 262-12-4
SPID(S): Tox21_302831
M4ID: 12476302

HILL MODEL (in red):

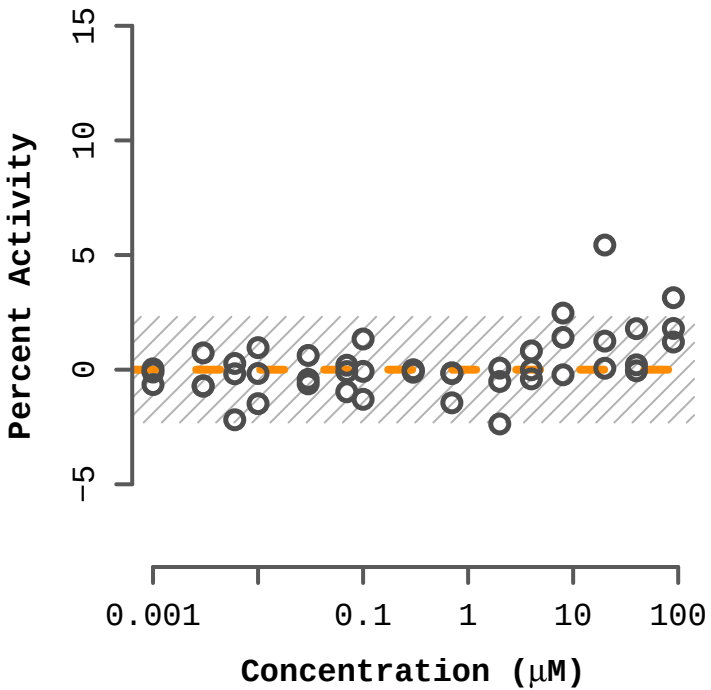
	tp	ga	gw
val:	2.62	1	1.56
sd:	0.665	0.294	0.937

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.62	1	1.56	3.54	5.11
sd:	0.665	0.294	0.937	1660	5350

	CNST	HILL	GNLS
AIC:	157.34	123.74	127.74
PROB:	0	0.88	0.12
RMSE:	1.51	1.01	1.01

MAX_MEAN: 2.74 MAX_MED: 2.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

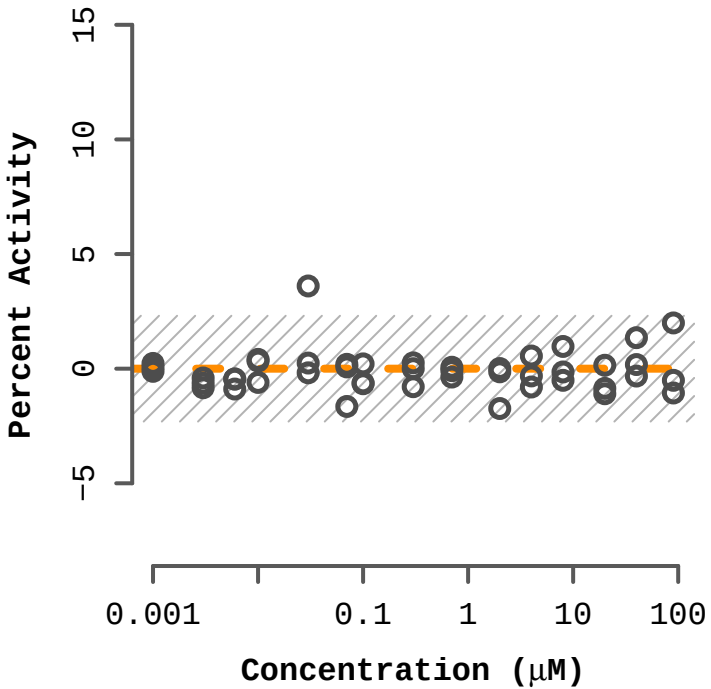
NAME: Dibenzo-p-dioxin
CHID: 20410 **CASRN:** 262-12-4
SPID(S): Tox21_202045
M4ID: 12480207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

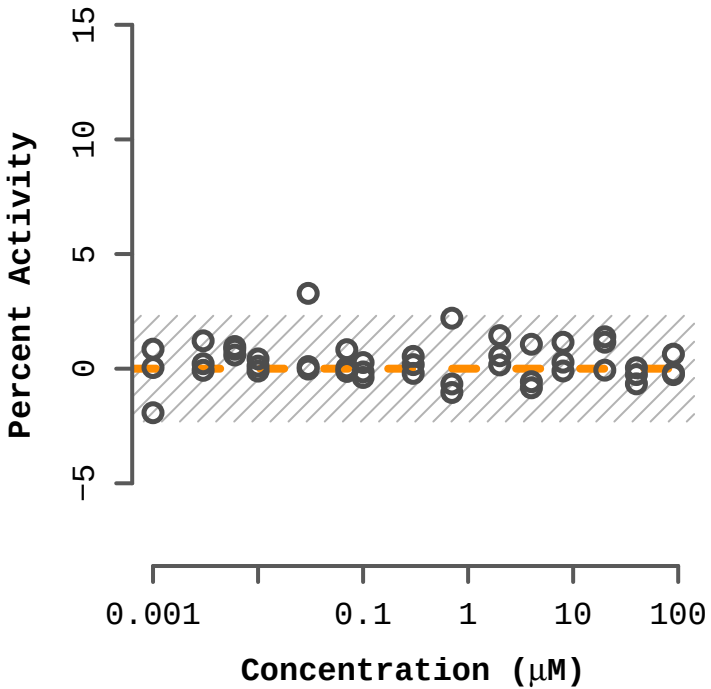
NAME: 1,2-Dibromo-3-chloropropane
CHID: 20413 **CASRN:** 96-12-8
SPID(S): Tox21_200382
M4ID: 12481870

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.333 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

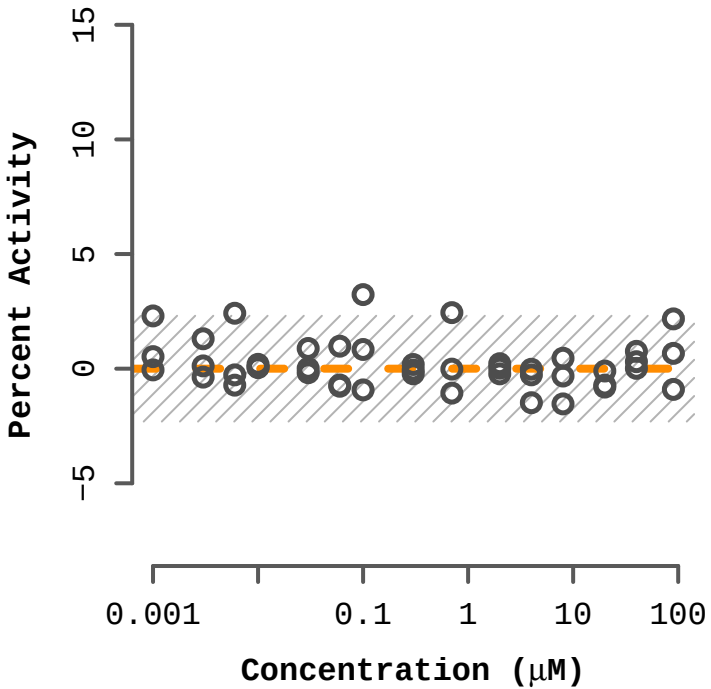
NAME: 1,2-Dibromoethane
CHID: 20415 **CASRN:** 106-93-4
SPID(S): Tox21_302879
M4ID: 12476254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

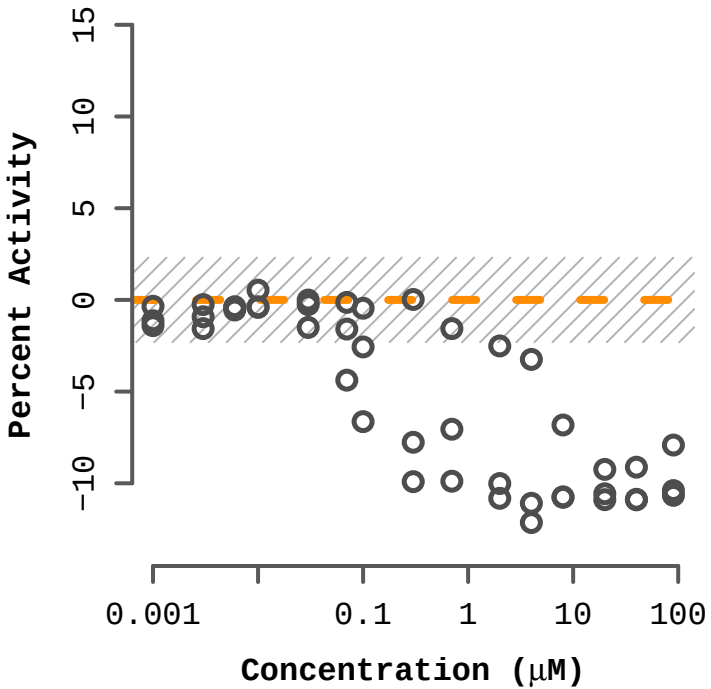
NAME: 1,2−Dibromoethane
CHID: 20415 **CASRN:** 106−93−4
SPID(S): Tox21_201427
M4ID: 12480825

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.839 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

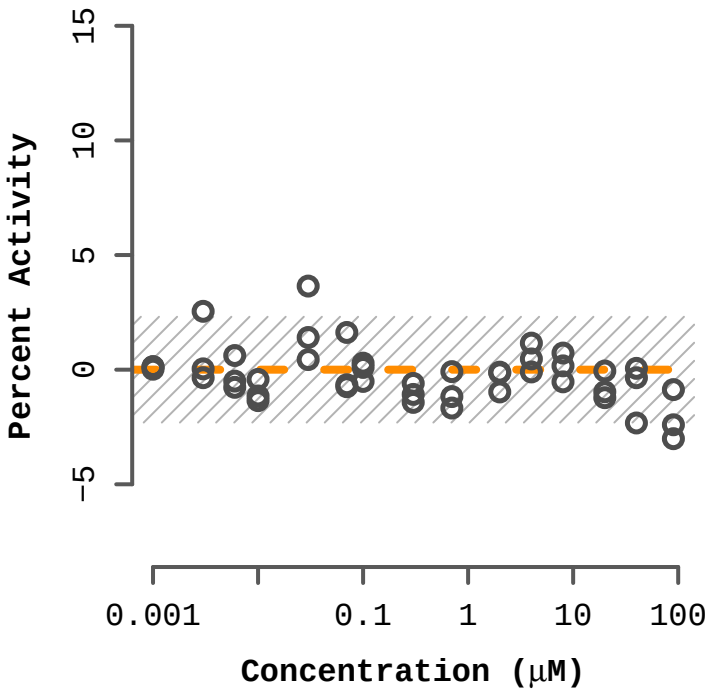
NAME: Dibutyltin diacetate
CHID: 20419 **CASRN:** 1067-33-0
SPID(S): Tox21_200116
M4ID: 12482136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	306.68	NA	NA
PROB:	1	NA	NA
RMSE:	6.82	NA	NA

MAX_MEAN: −0.082 **MAX_MED:** −0.254 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

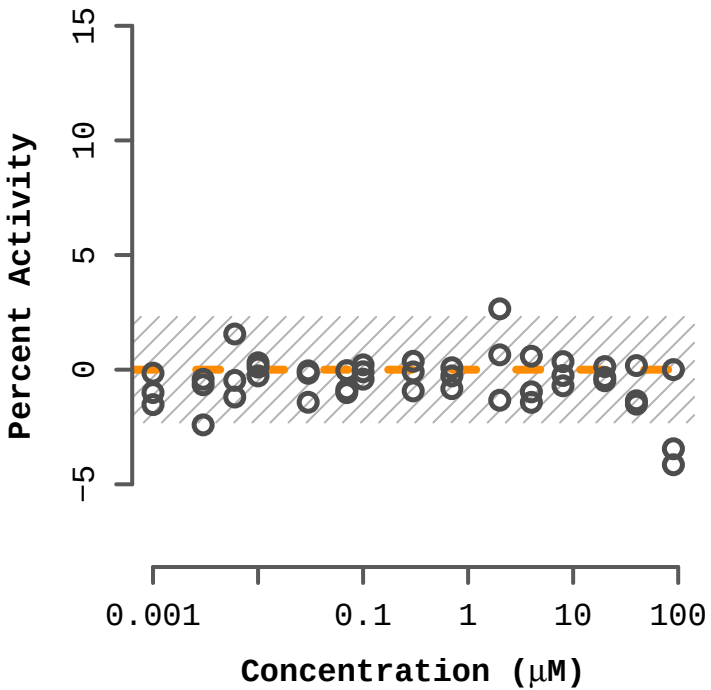
NAME: Propyzamide
CHID: 20420 **CASRN:** 23950-58-5
SPID(S): Tox21_301164
M4ID: 12477969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

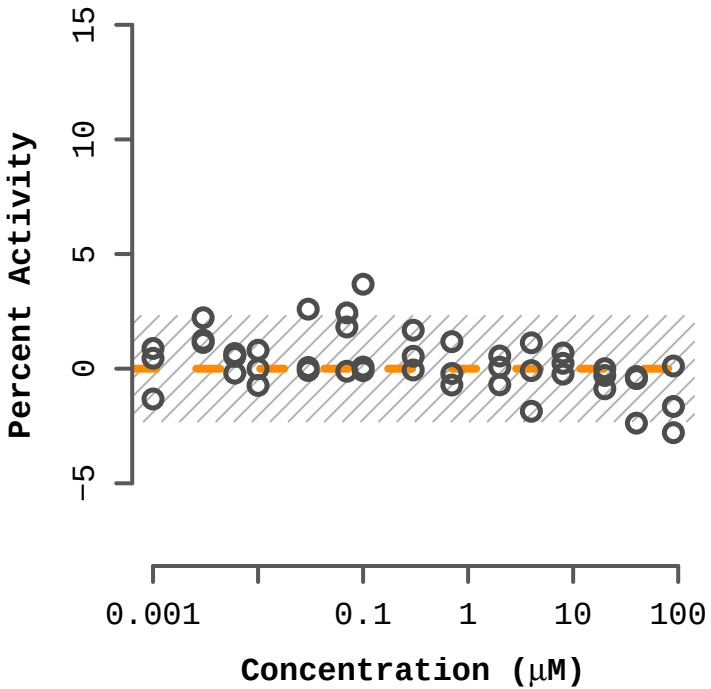
NAME: Propyzamide
CHID: 20420 CASRN: 23950-58-5
SPID(S): Tox21_201413
M4ID: 12480839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.658 MAX_MED: 0.648 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

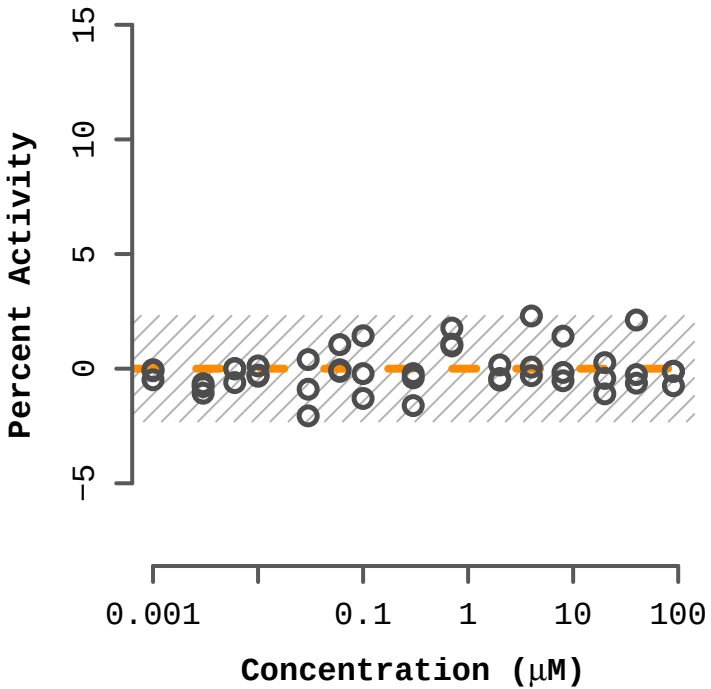
NAME: 2,3-Dichloro-p-dioxane
CHID: 20421 **CASRN:** 3883-43-0
SPID(S): Tox21_302806
M4ID: 12476327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

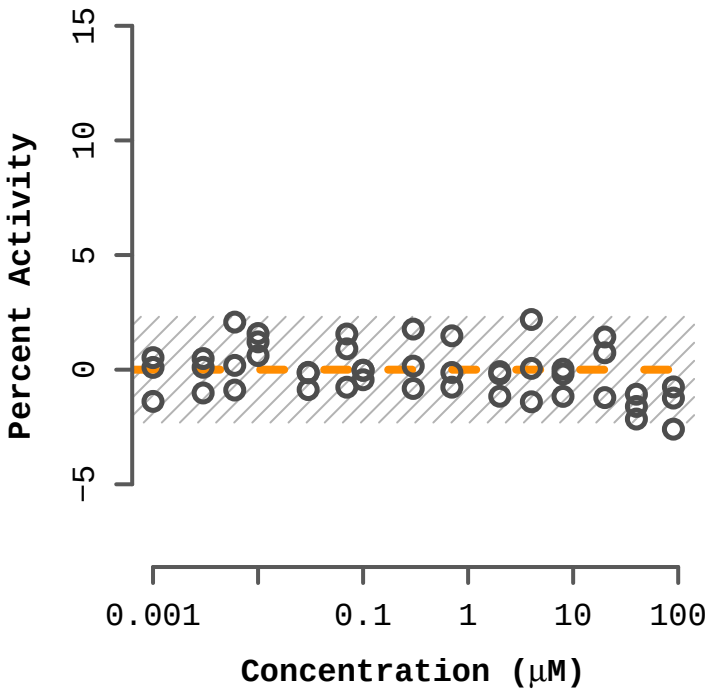
NAME: 2,3-Dichloro-p-dioxane
CHID: 20421 CASRN: 3883-43-0
SPID(S): Tox21_202130
M4ID: 12480122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.28 MAX_MED: 1.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

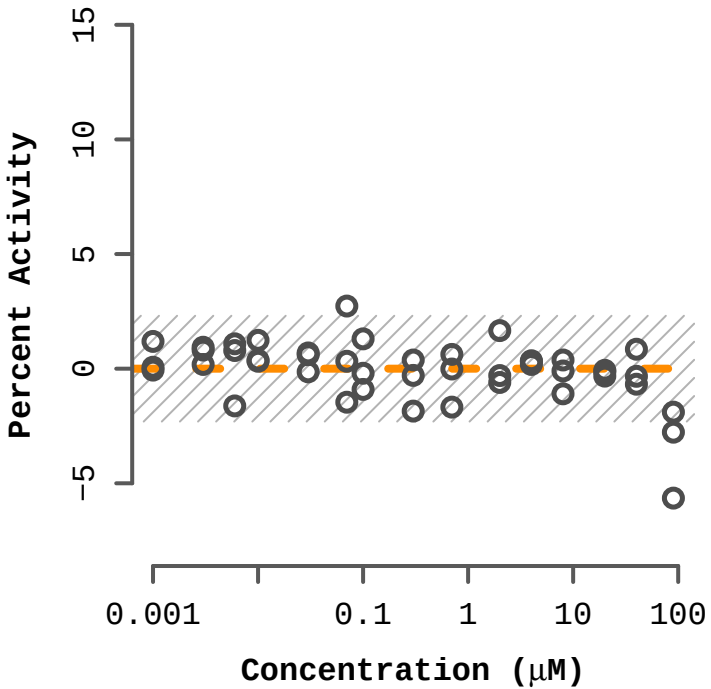
NAME: (2Z)-2,3-Dichloro-4-oxobut-2-enoic acid
CHID: 20423 **CASRN:** 87-56-9
SPID(S): Tox21_302857
M4ID: 12476276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

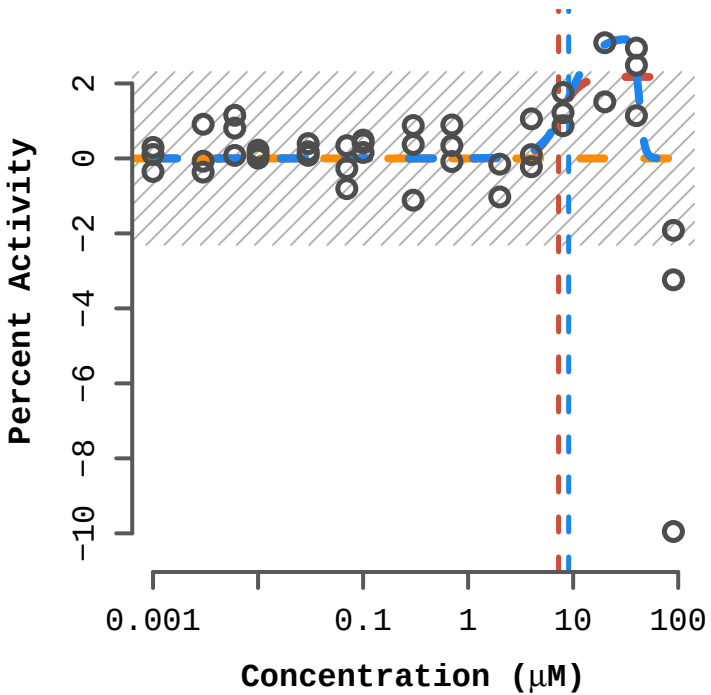
NAME: (2Z)-2,3-Dichloro-4-oxobut-2-enoic acid
CHID: 20423 **CASRN:** 87-56-9
SPID(S): Tox21_201305
M4ID: 12480947

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.646 **MAX_MED:** 0.812 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloranocryl
CHID: 20424 CASRN: 2164-09-2
SPID(S): Tox21_302753
M4ID: 12476380

HILL MODEL (in red):

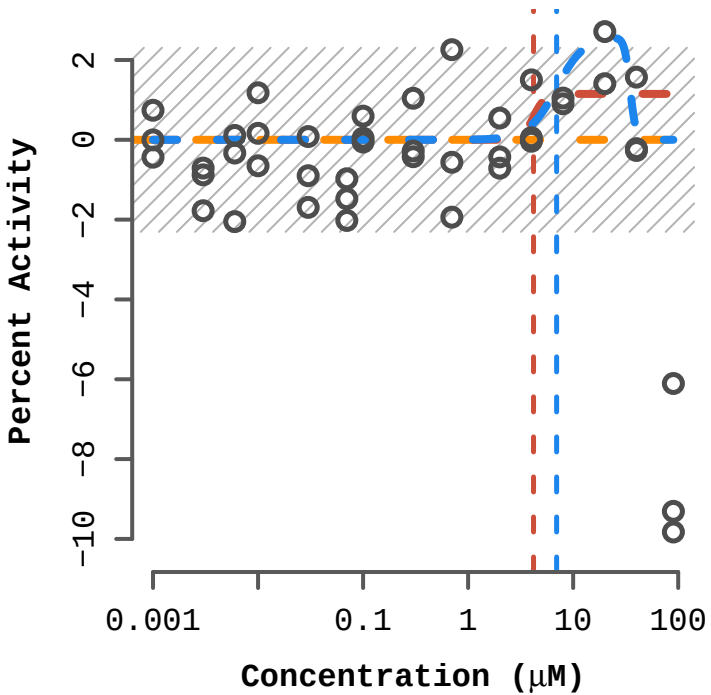
	tp	ga	gw
val:	2.18	0.861	4.44
sd:	0.458	0.102	3.79

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.24	0.957	3.37	1.63	16.8
sd:	0.995	0.138	3.06	0.0425	29.8

	CNST	HILL	GNLS
AIC:	180.68	167.6	157
PROB:	0	0	1
RMSE:	2.9	3.04	2.73

MAX_MEAN: 4.41 MAX_MED: 3.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloranocryl
CHID: 20424 CASRN: 2164-09-2
SPID(S): Tox21_201516
M4ID: 12480736

HILL MODEL (in red):

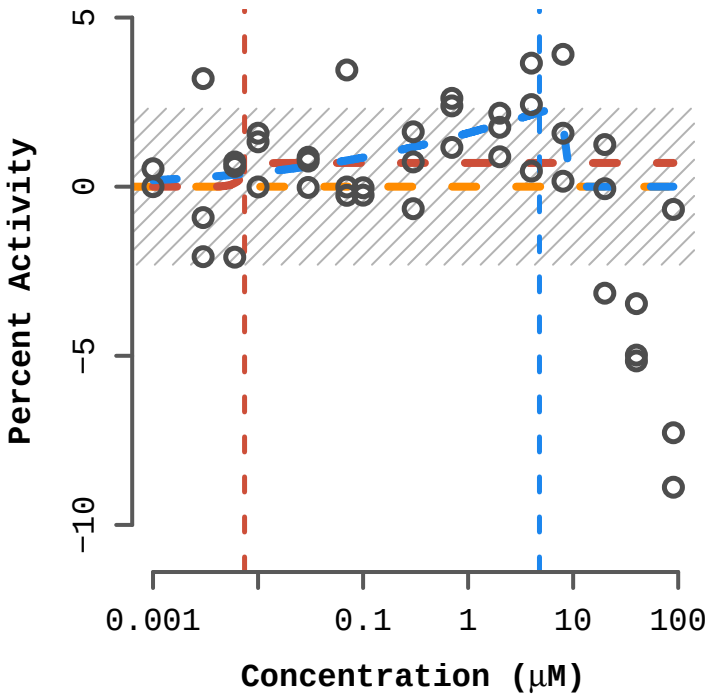
	tp	ga	gw
val:	1.15	0.623	8
sd:	0.492	0.141	18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.6	0.842	3.25	1.54	15.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	190.69	191.56	186.57
PROB:	0.11	0.07	0.83
RMSE:	2.56	2.73	2.43

MAX_MEAN: 2.48 MAX_MED: 2.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dichlone
CHID: 20425 CASRN: 117-80-6
SPID(S): Tox21_303031
M4ID: 12476102

HILL MODEL (in red):

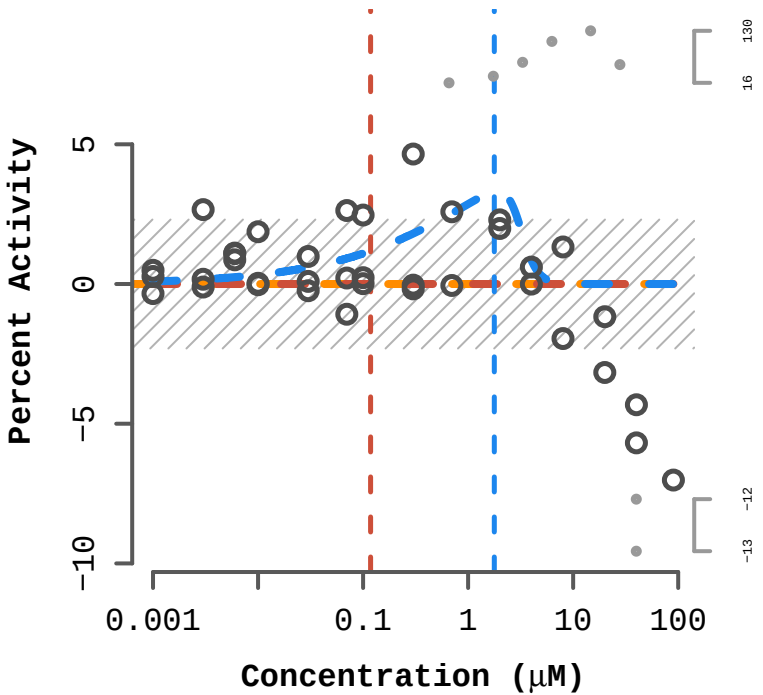
	tp	ga	gw
val:	0.701	−2.13	8
sd:	0.376	0.293	20.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.39	0.679	0.365	0.929	17.9
sd:	14.4	7.22	0.525	3.95	2710

	CNST	HILL	GNLS
AIC:	221.27	224.11	218.33
PROB:	0.18	0.04	0.78
RMSE:	2.9	2.94	2.67

MAX_MEAN: 2.39 MAX_MED: 2.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dichlone
CHID: 20425 CASRN: 117-80-6
SPID(S): Tox21_201652
M4ID: 12480600 BRK

HILL MODEL (in red):

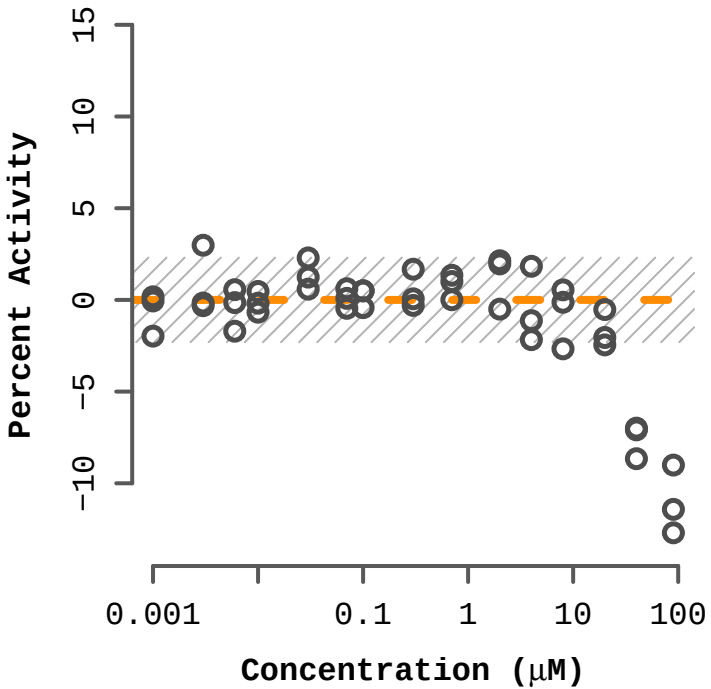
	tp	ga	gw
val:	1.66e-09	-0.929	1.58
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.86	0.249	0.578	0.499	5.76
sd:	44.4	6.33	1.4	1.52	64.5

	CNST	HILL	GNLS
AIC:	353.21	359.21	359.48
PROB:	0.91	0.05	0.04
RMSE:	27.68	27.68	27.53

MAX_MEAN: 40.4 MAX_MED: 2.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

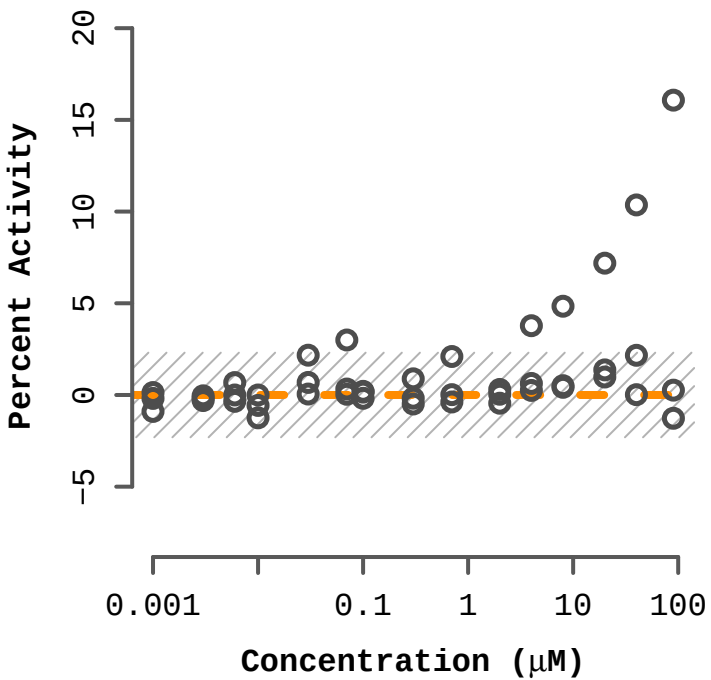
NAME: Dicloran
CHID: 20426 **CASRN:** 99-30-9
SPID(S): Tox21_300838
M4ID: 12478295

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.69	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

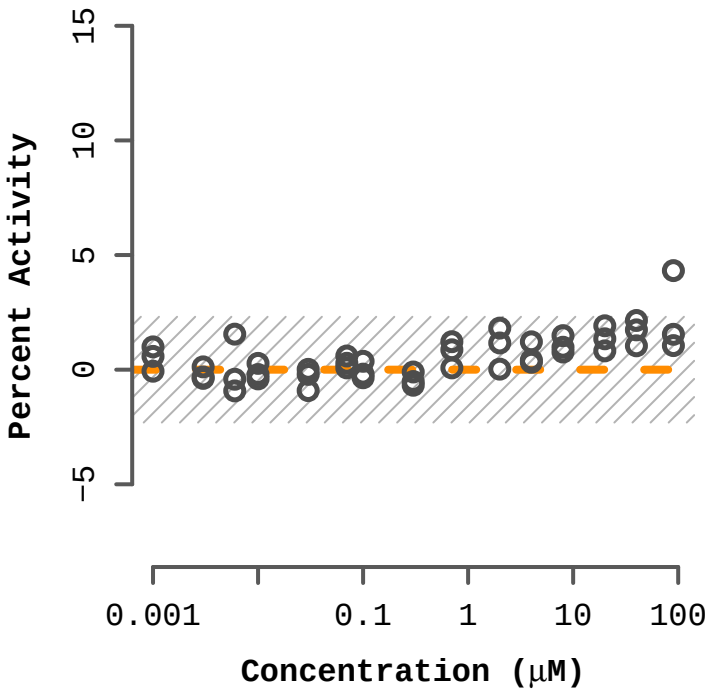
NAME: Dicloran
CHID: 20426 CASRN: 99-30-9
SPID(S): Tox21_202341
M4ID: 12479911

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.89	NA	NA
PROB:	1	NA	NA
RMSE:	3.3	NA	NA

MAX_MEAN: 5.02 MAX_MED: 2.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

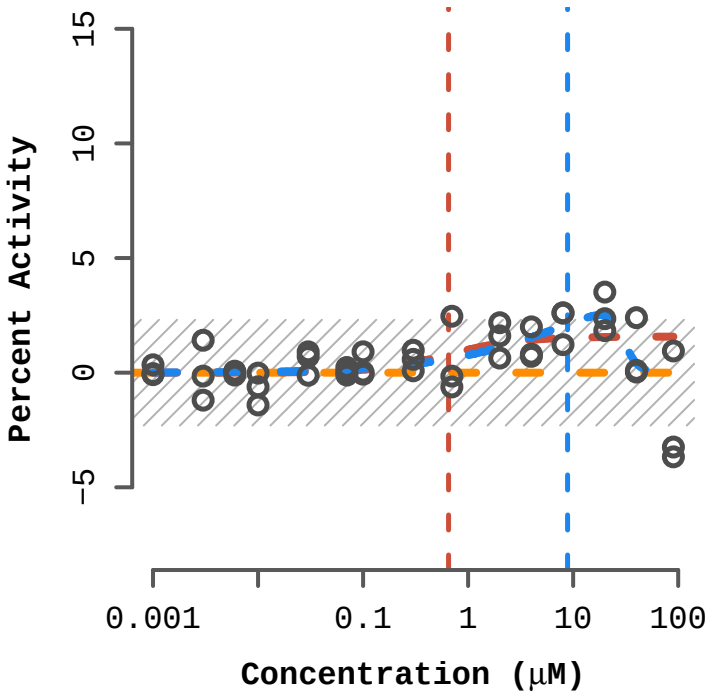
NAME: 2,6-Dichloro-1,4-benzenediamine
CHID: 20427 **CASRN:** 609-20-1
SPID(S): Tox21_302916
M4ID: 12476217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 2.31 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6-Dichloro-1,4-benzenediamine
CHID: 20427 CASRN: 609-20-1
SPID(S): Tox21_201908
M4ID: 12480344

HILL MODEL (in red):

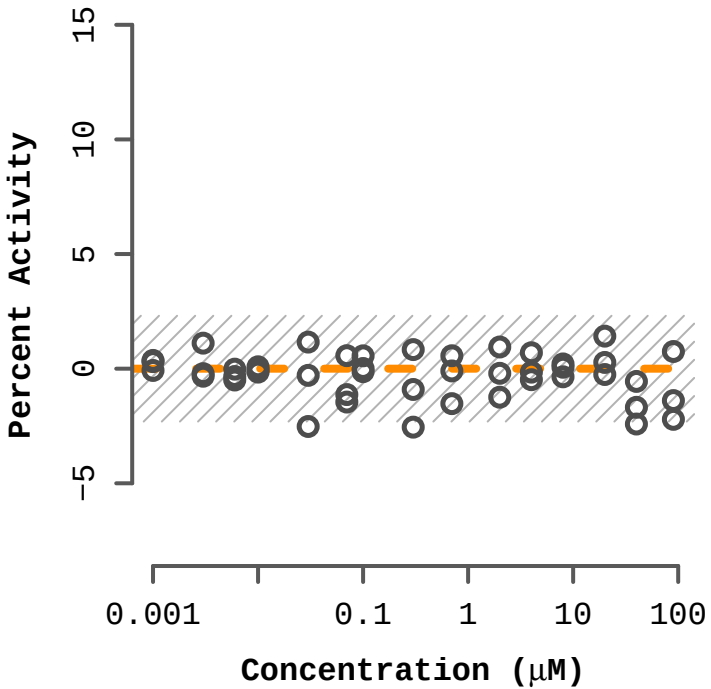
	tp	ga	gw
val:	1.57	-0.186	1.28
sd:	0.347	0.425	0.837

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.22	0.947	0.692	1.47	6.38
sd:	5.18	1.42	0.376	0.208	7.92

	CNST	HILL	GNLS
AIC:	162.27	144.16	134.48
PROB:	0	0.01	0.99
RMSE:	1.46	1.33	1.04

MAX_MEAN: 2.57 **MAX_MED:** 2.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

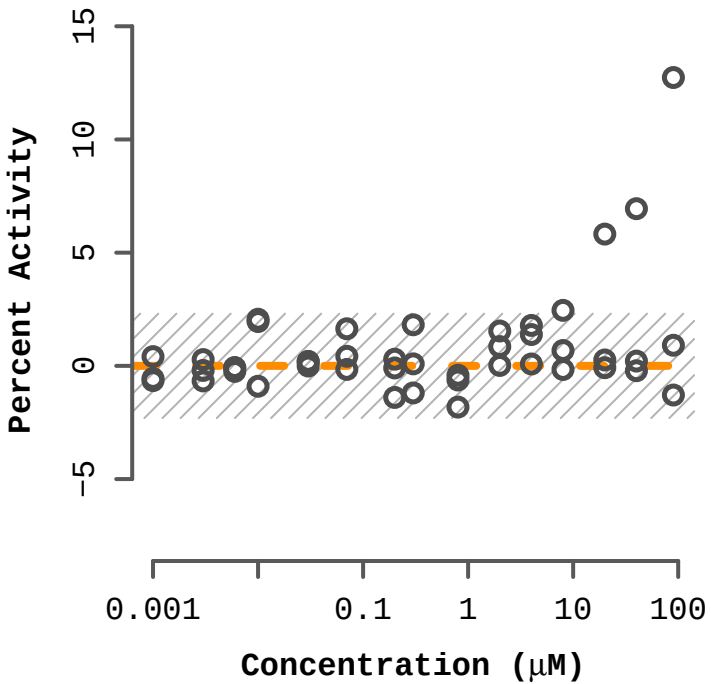
NAME: Dichloroacetic acid
CHID: 20428 **CASRN:** 79-43-6
SPID(S): Tox21_300419
M4ID: 12478713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.48 **MAX_MED:** 0.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

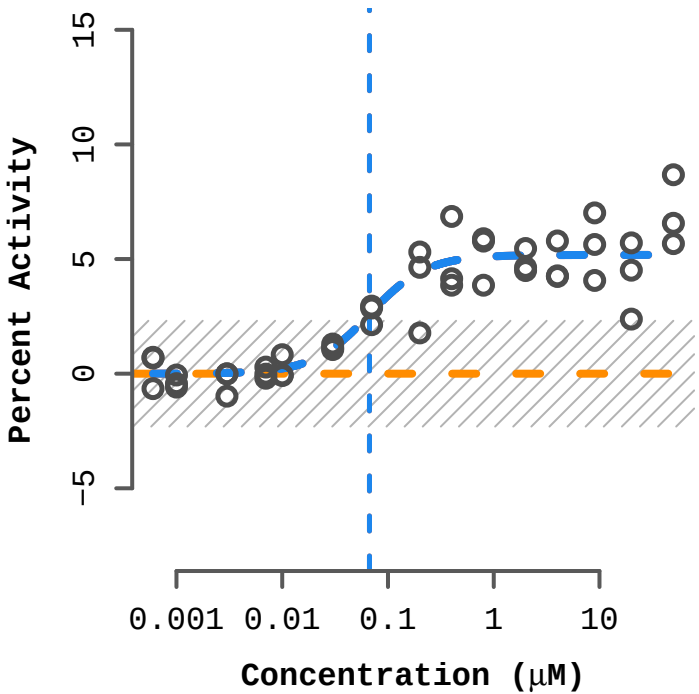
NAME: Dichloroacetic acid
CHID: 20428 CASRN: 79-43-6
SPID(S): Tox21_202363
M4ID: 12479889

HILL MODEL: Not applicable.

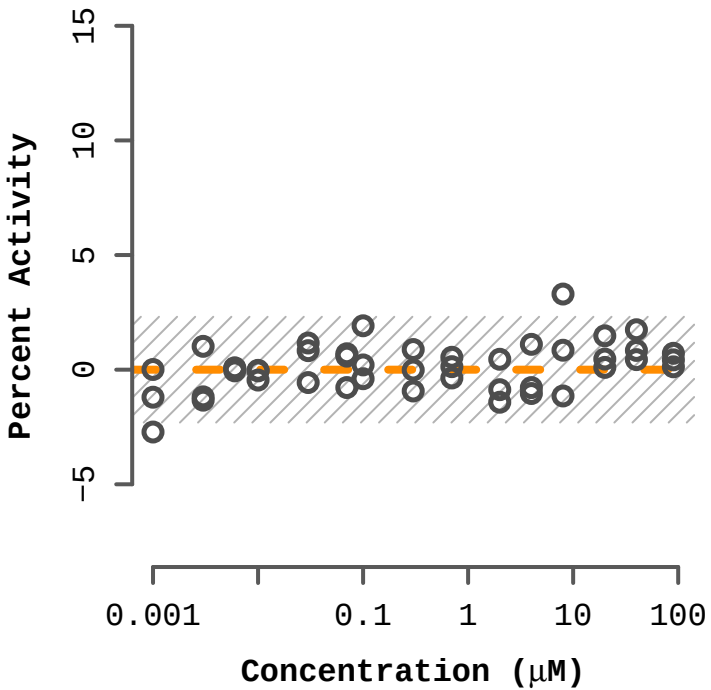
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.1	NA	NA
PROB:	1	NA	NA
RMSE:	2.52	NA	NA

MAX_MEAN: 4.12 **MAX_MED:** 1.96 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dichloroacetic acid
CHID:    20428   CASRN: 79-43-6
SPID(S): Tox21_111133_1
M4ID:    12483887

HILL MODEL (in red):
      tp       ga       gw
val:  5.18     -1.17    1.62
sd:   0.256    0.0815   0.438

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.18     -1.17    1.62     3.42     9.26
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  257.27      134.9       138.9
PROB: 0           0.88        0.12
RMSE: 3.92        1.06        1.06

MAX_MEAN: 6.97      MAX_MED: 6.56      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

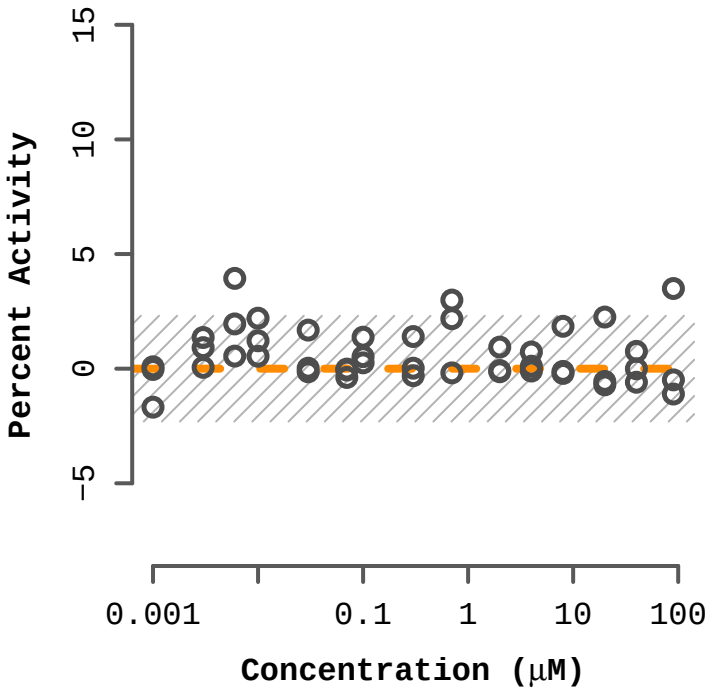
NAME: 1,2-Dichlorobenzene
CHID: 20430 **CASRN:** 95-50-1
SPID(S): Tox21_300046
M4ID: 12479084

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

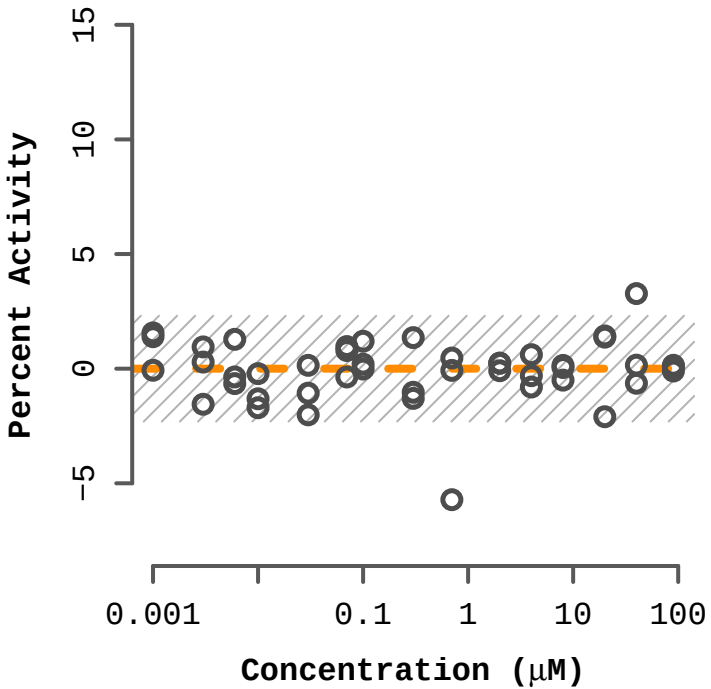
NAME: 1,2-Dichlorobenzene
CHID: 20430 **CASRN:** 95-50-1
SPID(S): Tox21_202157
M4ID: 12480095

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

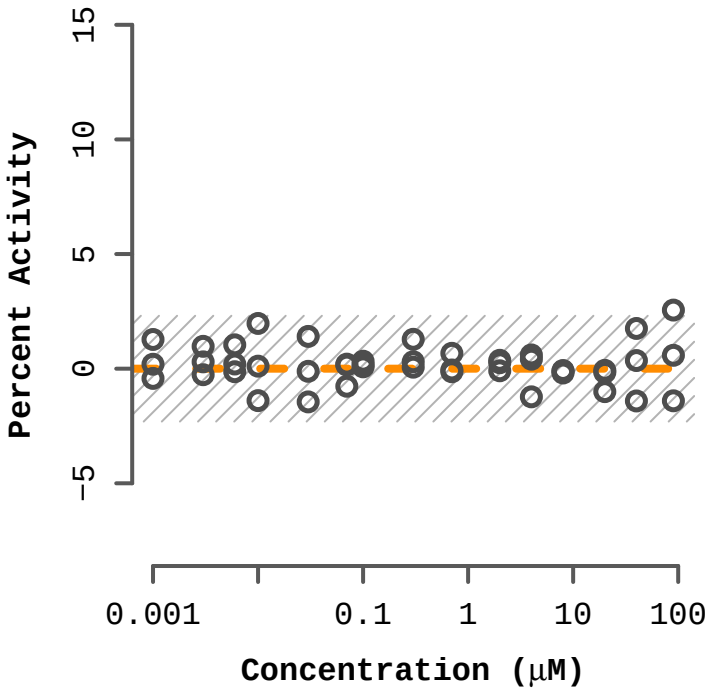
NAME: 1,4-Dichlorobenzene
CHID: 20431 **CASRN:** 106-46-7
SPID(S): Tox21_300018
M4ID: 12479112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

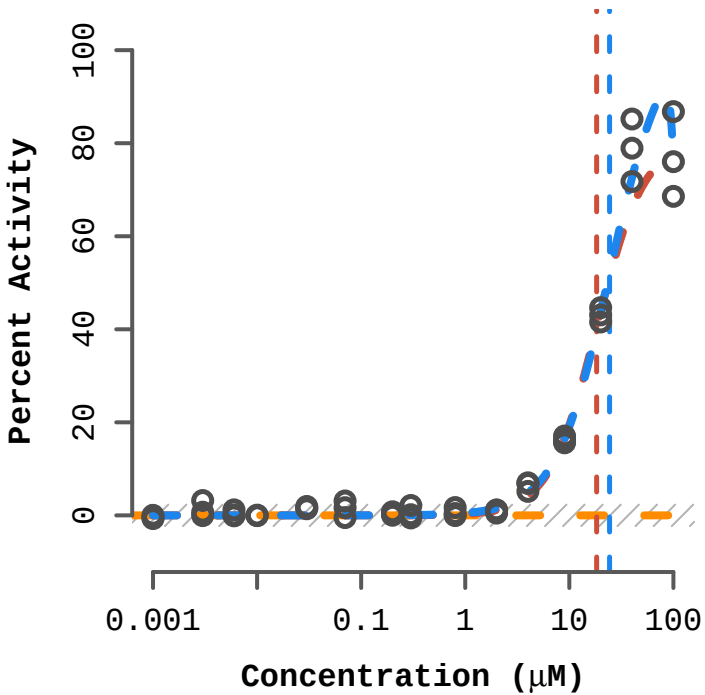
NAME: 1,4-Dichlorobenzene
CHID: 20431 **CASRN:** 106-46-7
SPID(S): Tox21_200399
M4ID: 12481853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.581 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'-Dichlorobenzidine
CHID: 20432 CASRN: 91-94-1
SPID(S): Tox21_202224
M4ID: 12480028

HILL MODEL (in red):

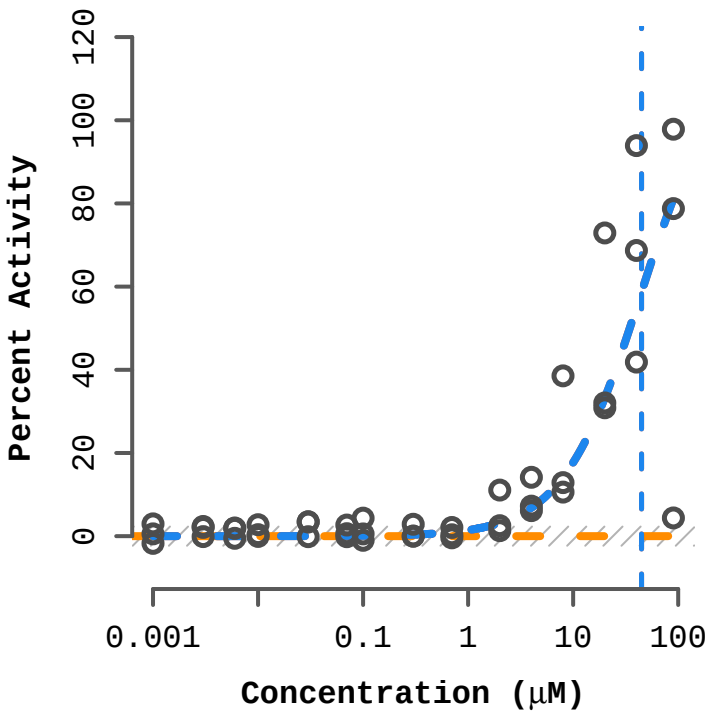
	tp	ga	gw
val:	81	1.26	1.91
sd:	4.74	0.0268	0.113

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	104	1.39	1.68	2.04	16.1
sd:	5.15	0.0289	0.0752	0.00517	2.1

	CNST	HILL	GNLS
AIC:	415.82	227.11	208.4
PROB:	0	0	1
RMSE:	30.99	4.21	3.1

MAX_MEAN: 78.6 MAX_MED: 78.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'-Dichlorobenzidine dihydrochloride
CHID: 20433 CASRN: 612-83-9
SPID(S): Tox21_302894
M4ID: 12476239

HILL MODEL (in red):

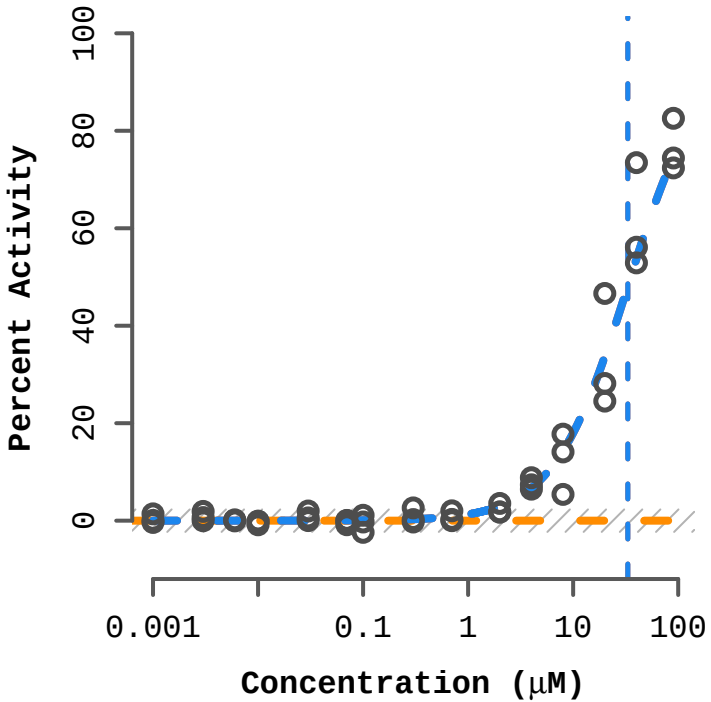
	tp	ga	gw
val:	117	1.65	1.15
sd:	27.7	0.222	0.231

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	117	1.65	1.15	2.31	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	406.85	325.3	329.3
PROB:	0	0.88	0.12
RMSE:	30.06	15.25	15.25

MAX_MEAN: 68.2 MAX_MED: 78.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'-Dichlorobenzidine dihydrochloride
CHID: 20433 CASRN: 612-83-9
SPID(S): Tox21_201906
M4ID: 12480346

HILL MODEL (in red):

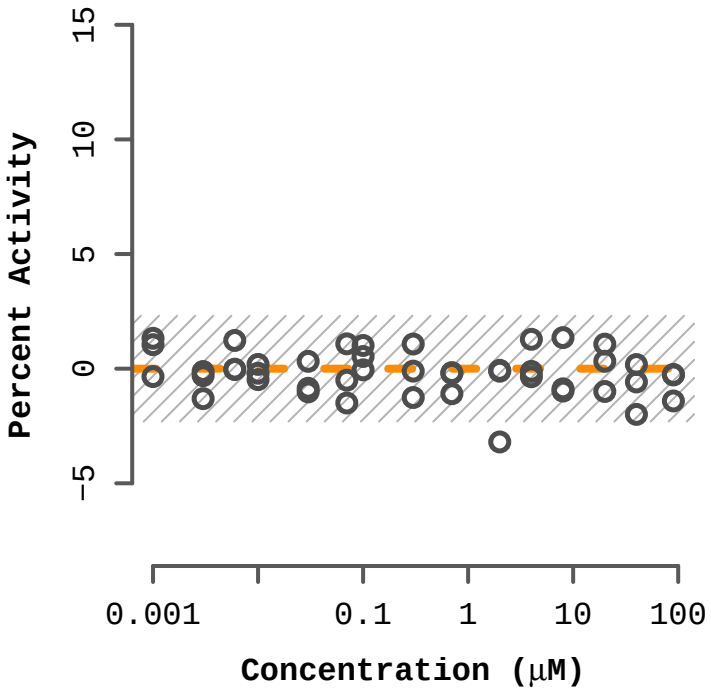
	tp	ga	gw
val:	96.3	1.52	1.23
sd:	6.83	0.0699	0.0816

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	96.3	1.52	1.23	3.15	7.51
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	400.64	233.22	237.22
PROB:	0	0.88	0.12
RMSE:	27.19	4.41	4.41

MAX_MEAN: 76.5 MAX_MED: 74.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

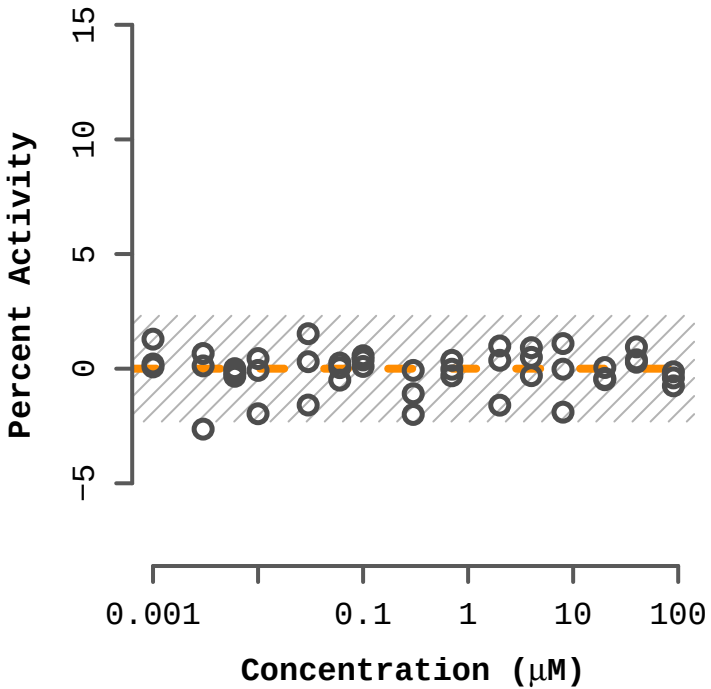
NAME: (2E)−1,4−Dichlorobut−2−ene
CHID: 20434 **CASRN:** 110−57−6
SPID(S): Tox21_200019
M4ID: 12482233

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.678 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

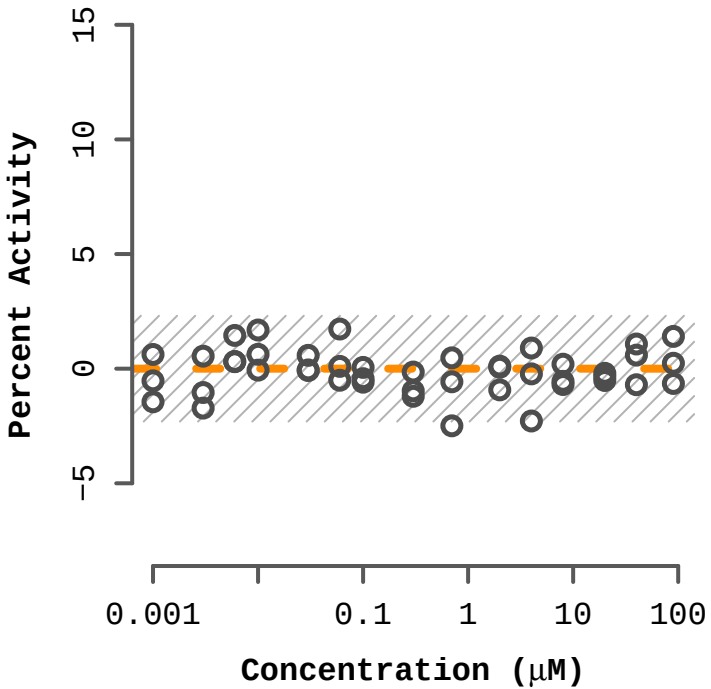
NAME: 1,1-Dichloroethane
CHID: 20437 **CASRN:** 75-34-3
SPID(S): Tox21_200205
M4ID: 12482047

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.541 **MAX_MED:** 0.496 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

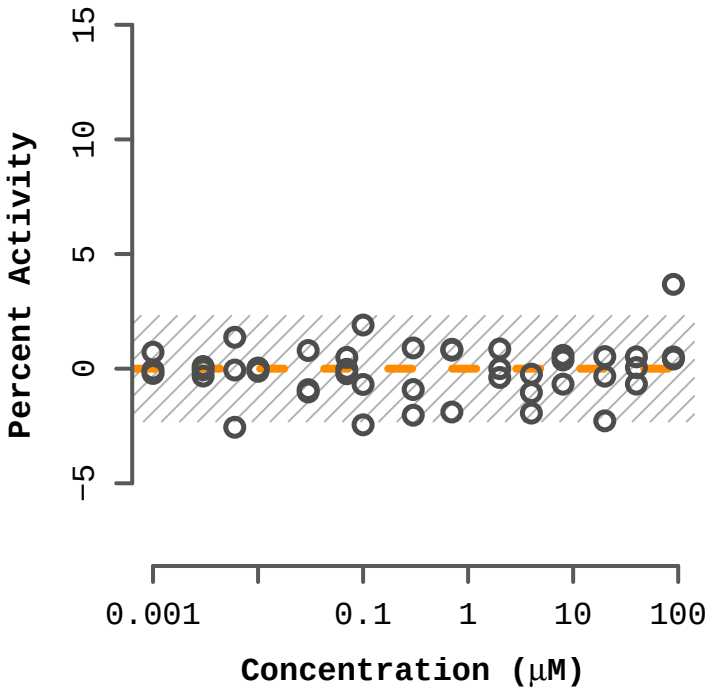
NAME: 1,2-Dichloroethane
CHID: 20438 **CASRN:** 107-06-2
SPID(S): Tox21_202466
M4ID: 12479786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.751 **MAX_MED:** 0.629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

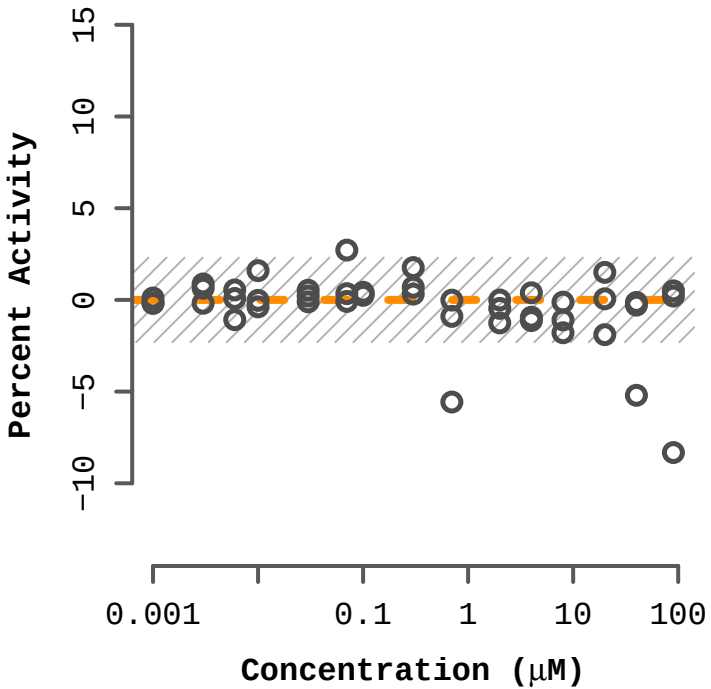
NAME: 2,4-Dichlorophenol
CHID: 20439 **CASRN:** 120-83-2
SPID(S): Tox21_300040
M4ID: 12479090

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.807 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

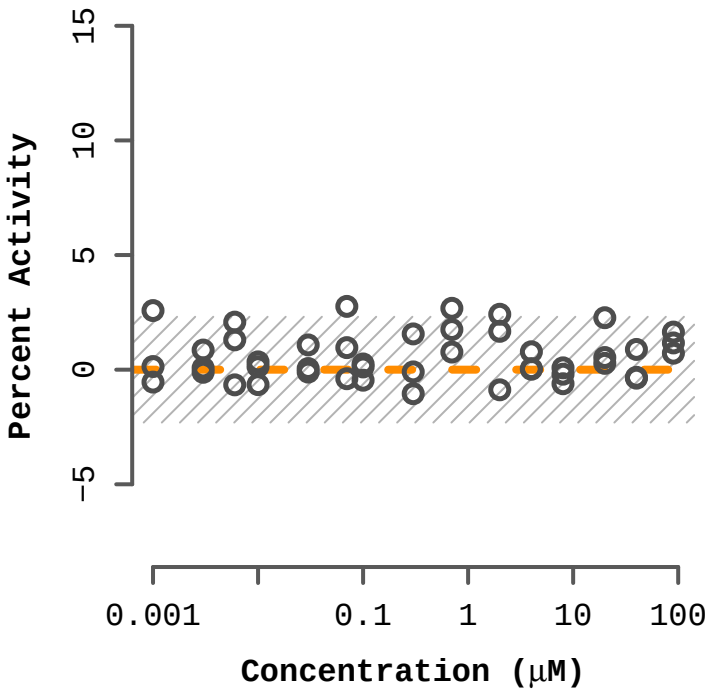
NAME: 2,4-Dichlorophenol
CHID: 20439 **CASRN:** 120-83-2
SPID(S): Tox21_201589
M4ID: 12480663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.994 **MAX_MED:** 0.696 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

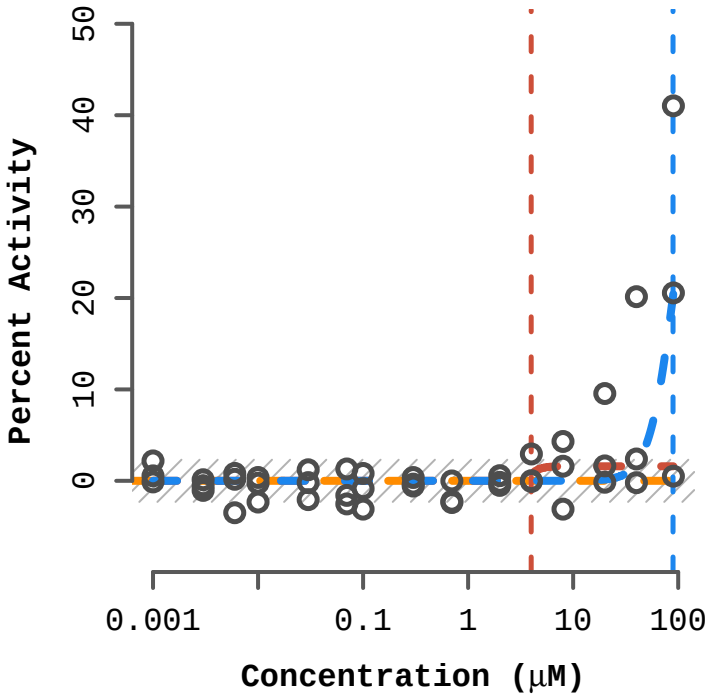
NAME: Dichlorprop
CHID: 20440 CASRN: 120-36-5
SPID(S): Tox21_301143
M4ID: 12477990

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.73 MAX_MED: 1.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dichlorprop
CHID: 20440 CASRN: 120-36-5
SPID(S): Tox21_201847
M4ID: 12480405

HILL MODEL (in red):

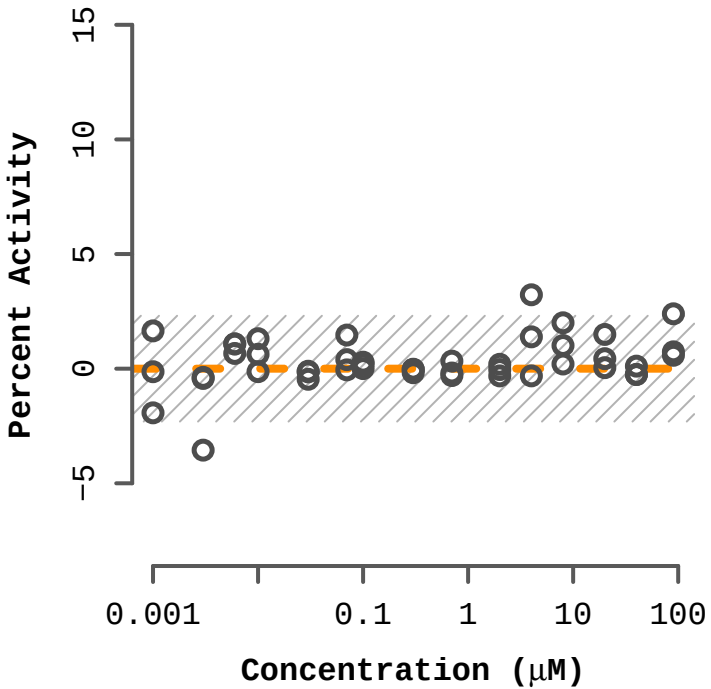
	tp	ga	gw
val:	1.59	0.6	8
sd:	0.776	0.162	76.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	40.4	1.95	3.78	3.95	1.56
sd:	9.35	0.0513	1.14	50.9	42.1

	CNST	HILL	GNLS
AIC:	246.66	247.7	248
PROB:	0.47	0.28	0.24
RMSE:	7.77	7.35	5.49

MAX_MEAN: 20.7 MAX_MED: 20.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

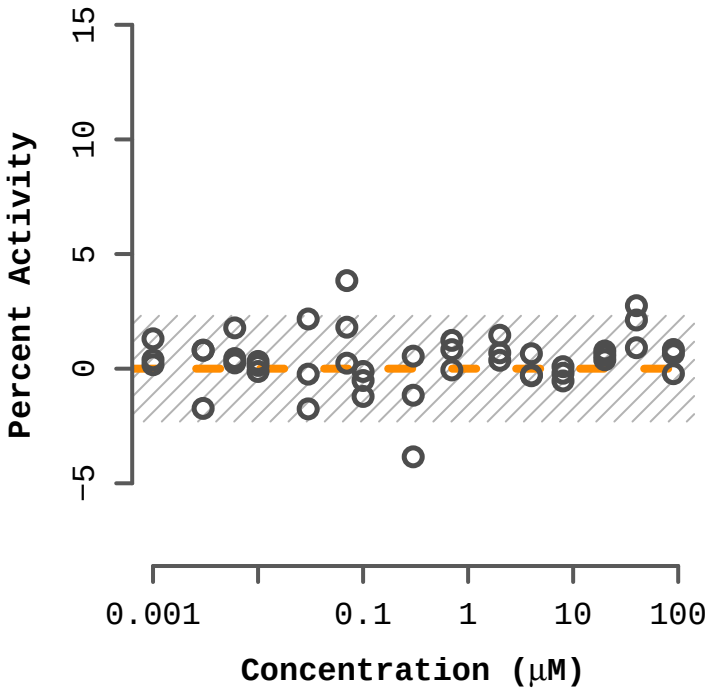
NAME: alpha−(2,5−Dichlorophenoxy)propionic acid
CHID: 20441 CASRN: 6965−71−5
SPID(S): Tox21_301882
M4ID: 12477251

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

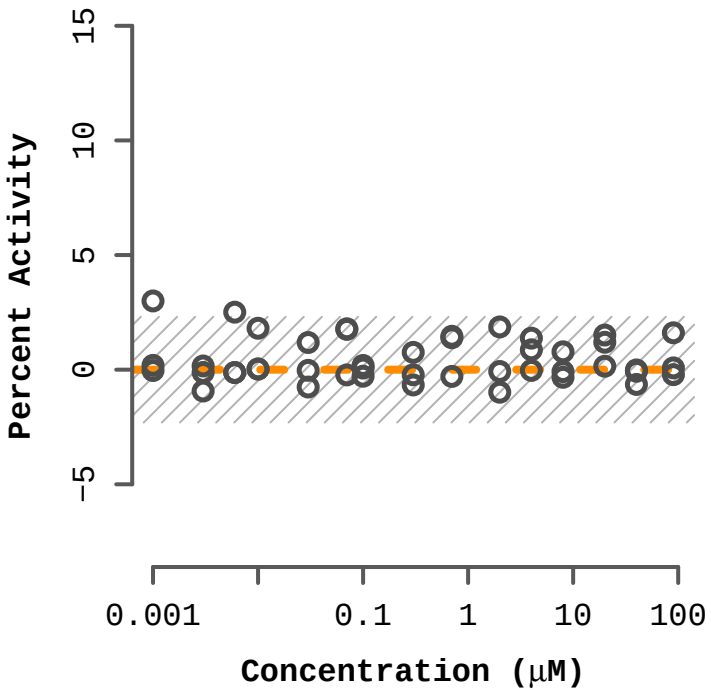
NAME: 2,4-Dichlorophenoxyacetic acid
CHID: 20442 **CASRN:** 94-75-7
SPID(S): Tox21_300890
M4ID: 12478243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

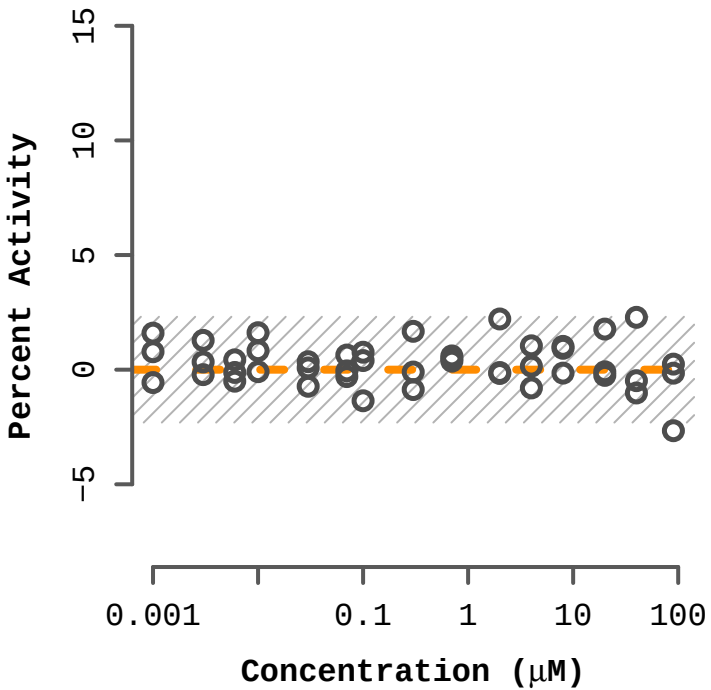
NAME: 2,4−Dichlorophenoxyacetic acid
CHID: 20442 CASRN: 94−75−7
SPID(S): Tox21_201751
M4ID: 12480501

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

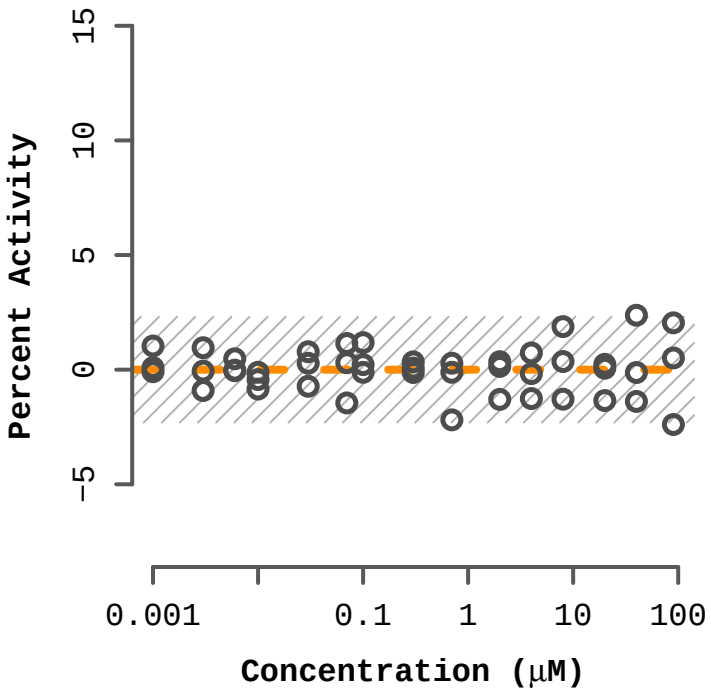
NAME: 2,4-D 1-butyl ester
CHID: 20443 **CASRN:** 94-80-4
SPID(S): Tox21_302757
M4ID: 12476376

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.786 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

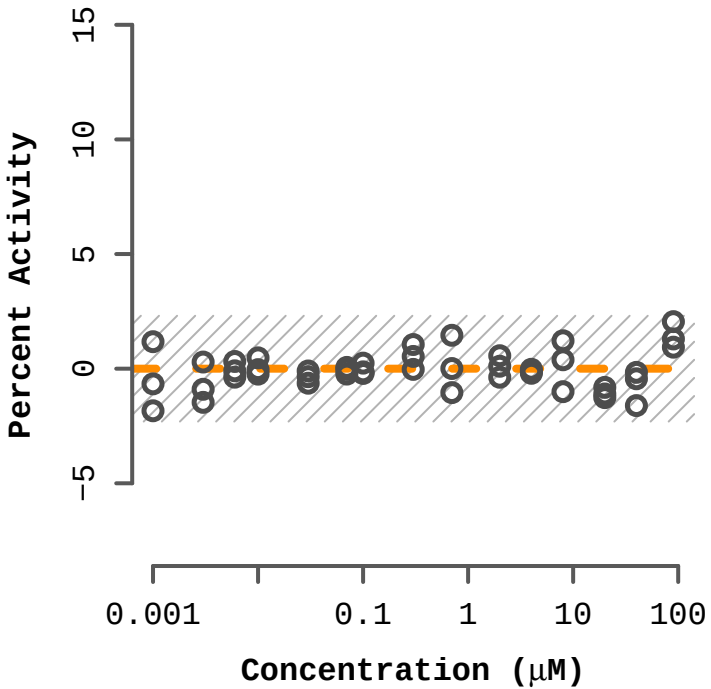
NAME: 2,4-D 1-butyl ester
CHID: 20443 CASRN: 94-80-4
SPID(S): Tox21_201237
M4ID: 12481015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.43 **MAX_MED:** 0.512 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

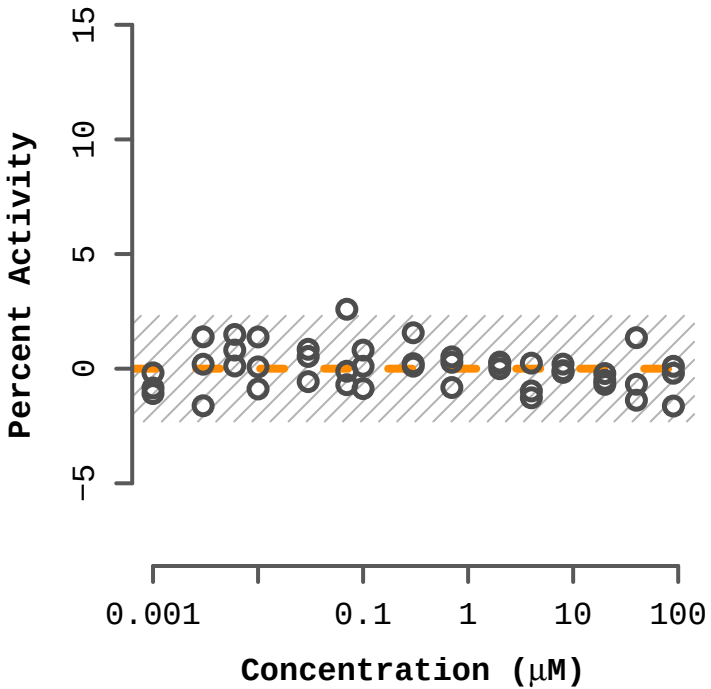
NAME: 2,4-D isooctyl ester
CHID: 20444 **CASRN:** 25168-26-7
SPID(S): Tox21_200926
M4ID: 12481326

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

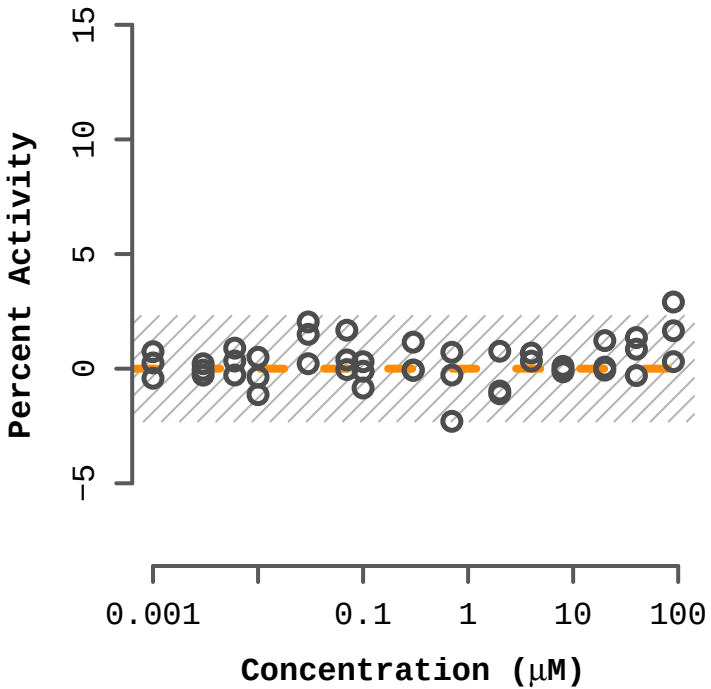
NAME: 2,4−D isopropyl ester
CHID: 20445 CASRN: 94−11−1
SPID(S): Tox21_302786
M4ID: 12476347

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.808 **MAX_MED:** 0.813 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

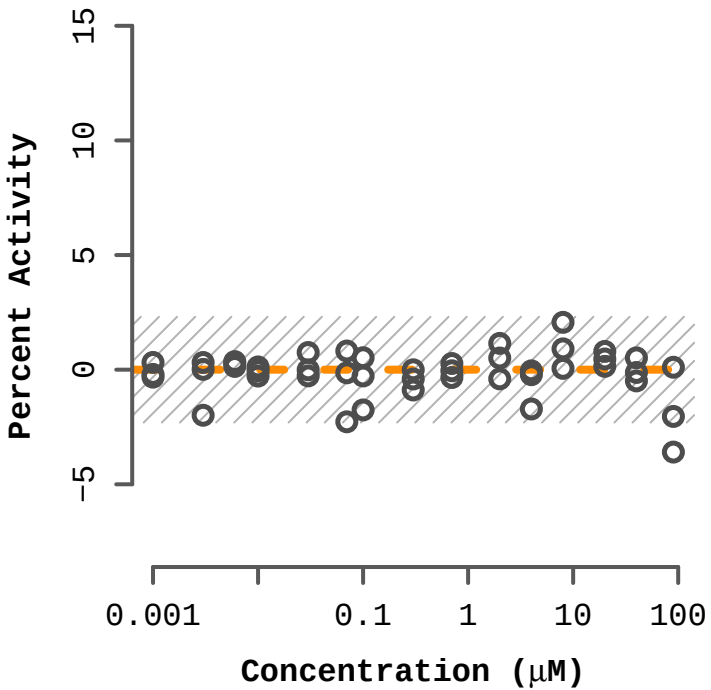
NAME: 2,4−D isopropyl ester
CHID: 20445 CASRN: 94−11−1
SPID(S): Tox21_201563
M4ID: 12480689

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

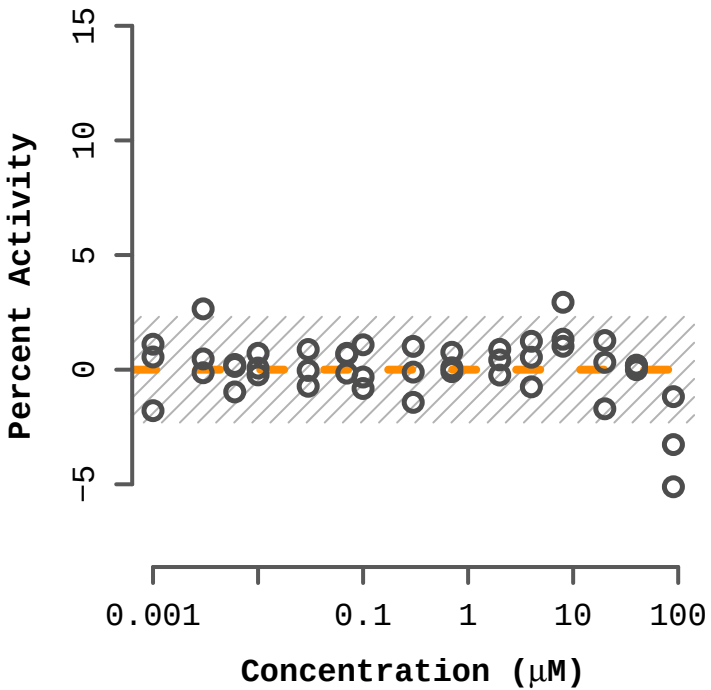
NAME: Diuron
CHID: 20446 CASRN: 330-54-1
SPID(S): Tox21_301016
M4ID: 12478117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.01 MAX_MED: 0.908 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

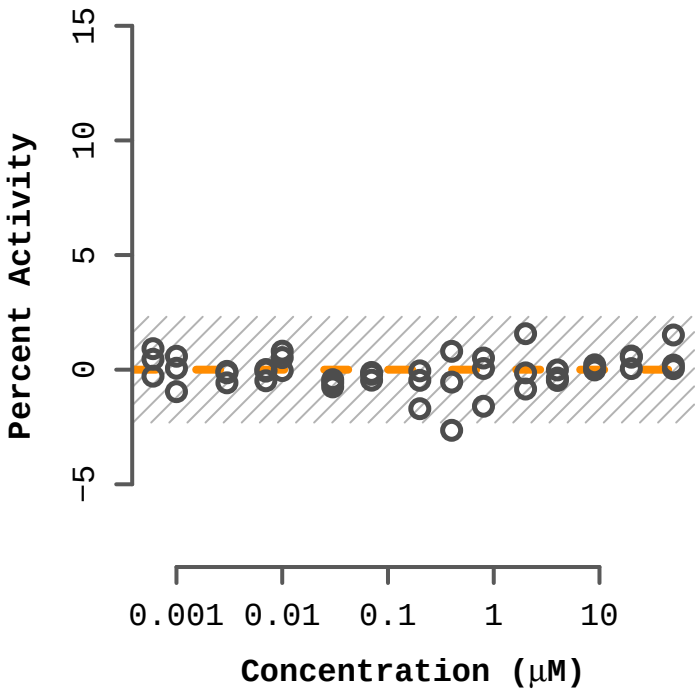
NAME: Diuron
CHID: 20446 CASRN: 330-54-1
SPID(S): Tox21_201438
M4ID: 12480814

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

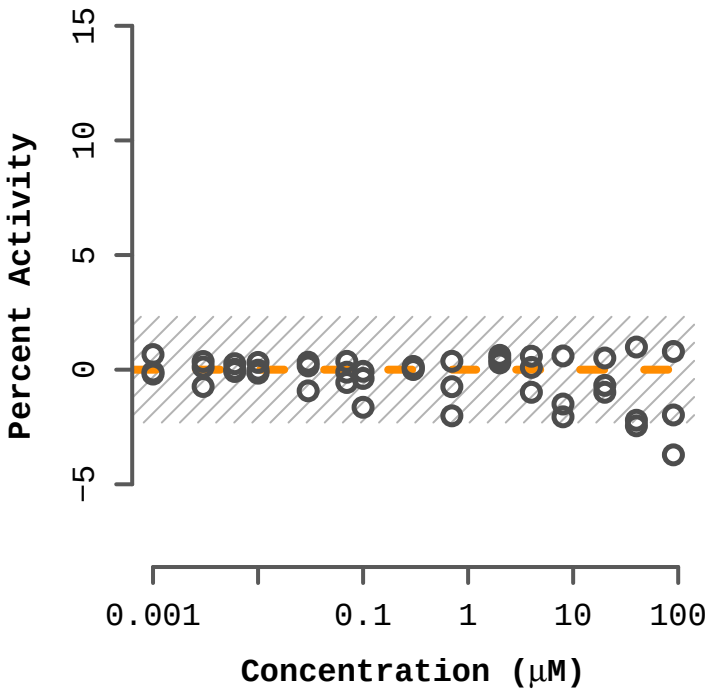
NAME: Diuron
CHID: 20446 CASRN: 330-54-1
SPID(S): Tox21_111292_1
M4ID: 12483786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 0.545 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

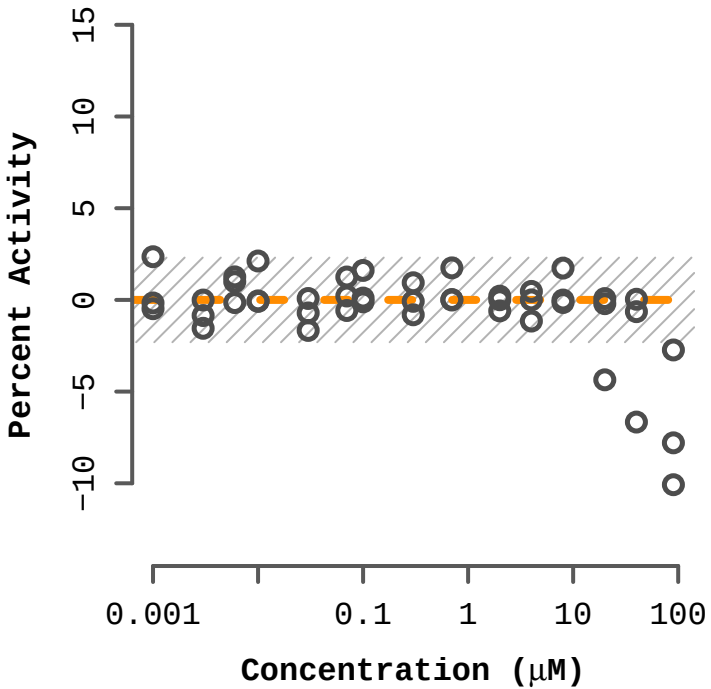
NAME: 2,4−Dichlorophenyl benzenesulfonate
CHID: 20447 CASRN: 97−16−5
SPID(S): Tox21_302810
M4ID: 12476323

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.462 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

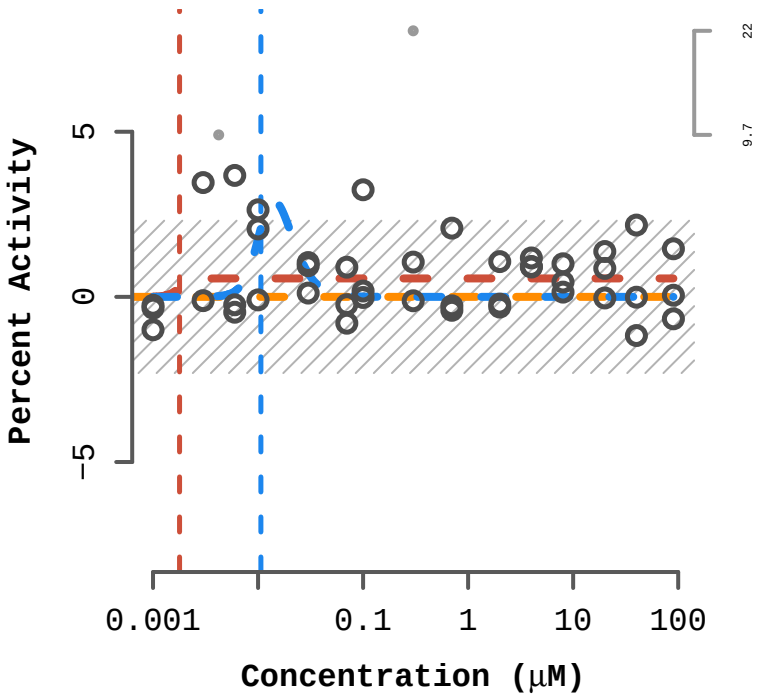
NAME: 2,4-Dichlorophenyl benzenesulfonate
CHID: 20447 **CASRN:** 97-16-5
SPID(S): Tox21_201552
M4ID: 12480700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.44	NA	NA

MAX_MEAN: 0.703 **MAX_MED:** 0.995 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2−Dichloropropane
CHID: 20448 CASRN: 78−87−5
SPID(S): Tox21_200362
M4ID: 12481890 BRK

HILL MODEL (in red):

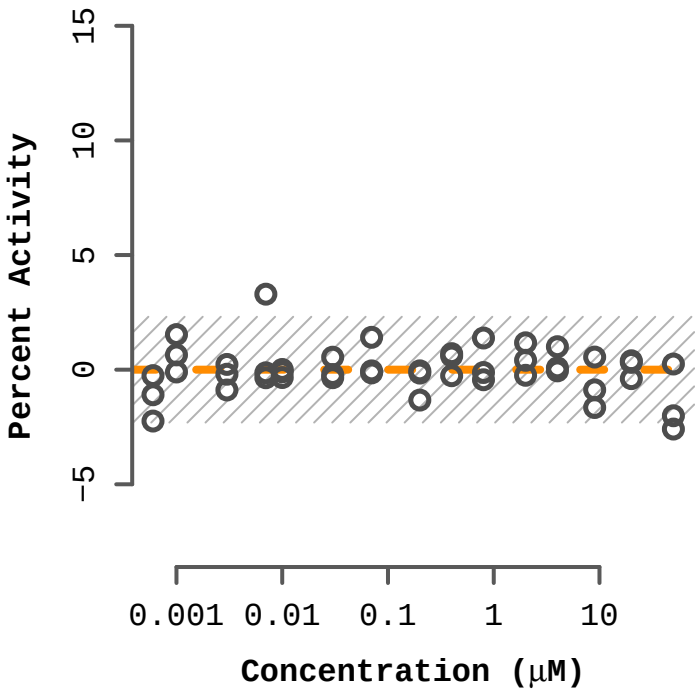
	tp	ga	gw
val:	0.558	−2.75	8
sd:	0.193	0.426	14.3

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.67	−1.97	5.71	−1.72	3.69
sd:	77.8	1.71	18.2	3.46	18.4

	CNST	HILL	GNLS
AIC:	187.1	184.55	191.45
PROB:	0.21	0.76	0.02
RMSE:	3.83	3.67	3.8

MAX_MEAN: 7.7 MAX_MED: 3.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

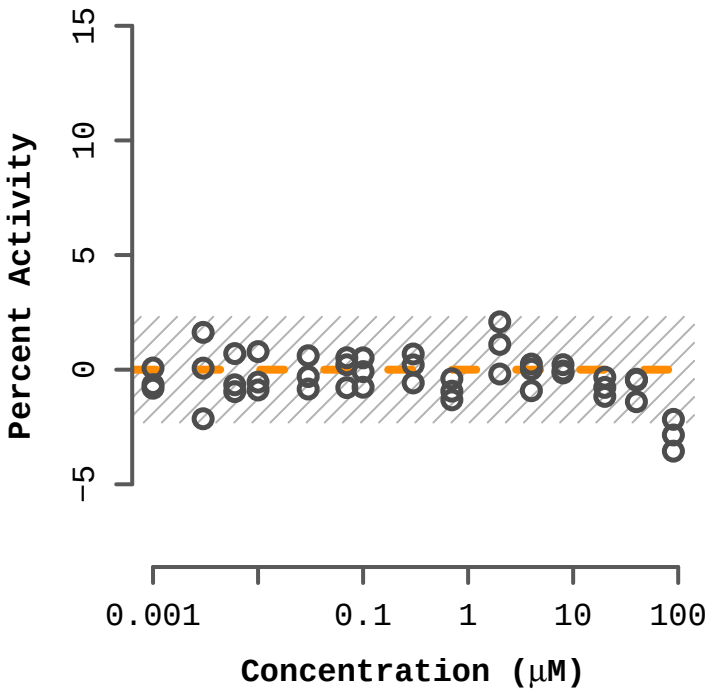
NAME: Dichlorvos
CHID: 20449 **CASRN:** 62-73-7
SPID(S): Tox21_300840
M4ID: 12478293

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.936 **MAX_MED:** 0.646 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

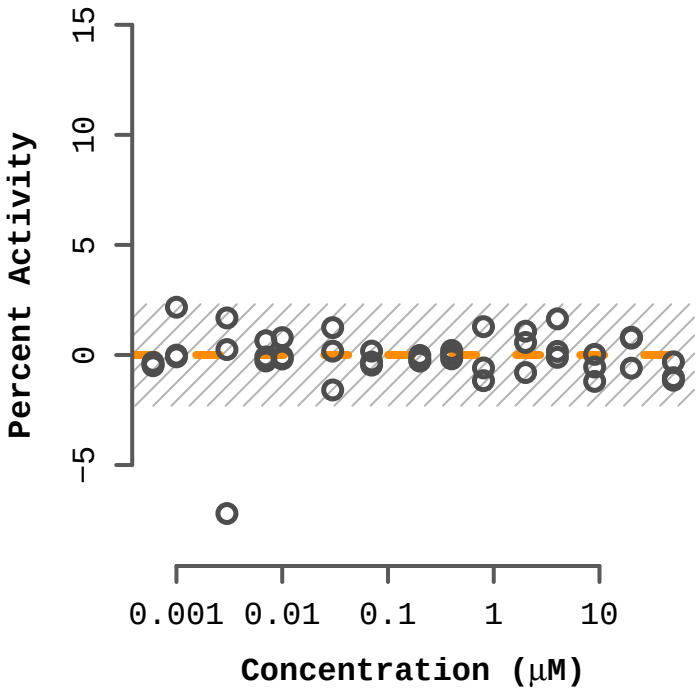
NAME: Dichlorvos
CHID: 20449 CASRN: 62-73-7
SPID(S): Tox21_201617
M4ID: 12480635

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1 MAX_MED: 1.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

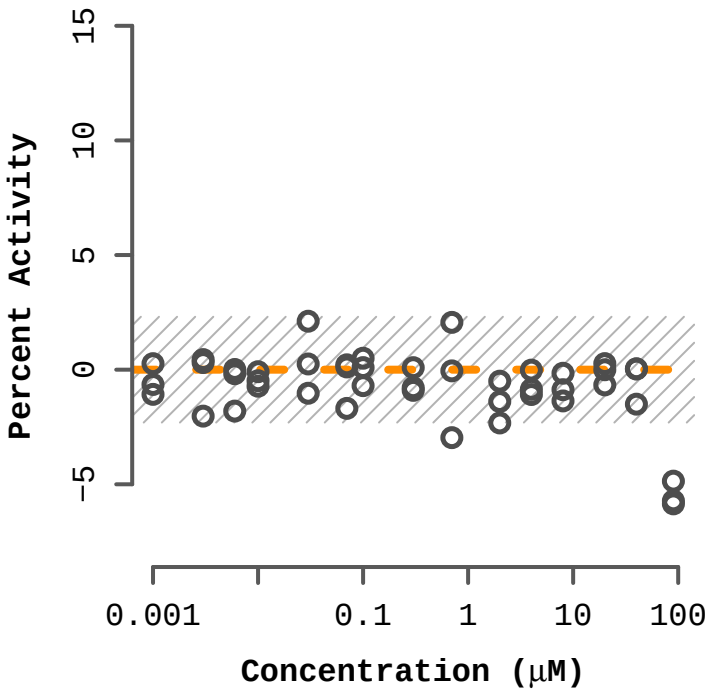
NAME: Dichlorvos
CHID: 20449 **CASRN:** 62-73-7
SPID(S): Tox21_111052_1
M4ID: 12483930

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.693 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

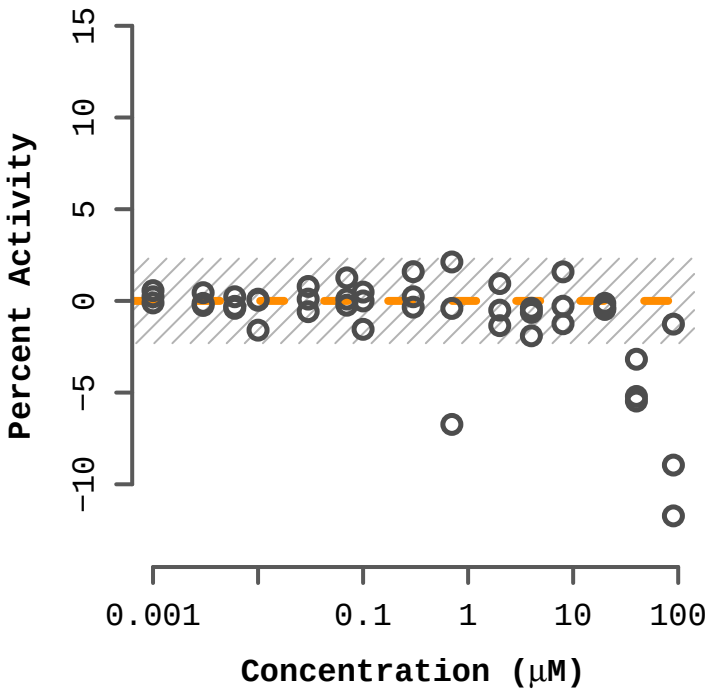
NAME: Dicofol
CHID: 20450 CASRN: 115-32-2
SPID(S): Tox21_300988
M4ID: 12478145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 0.446 MAX_MED: 0.312 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

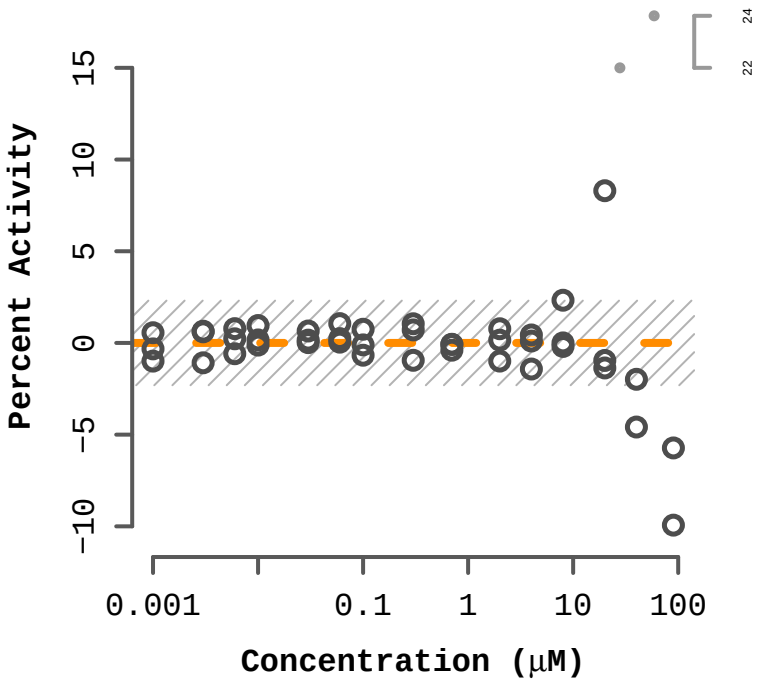
NAME: N,N'−Dicyclohexylthiourea
CHID: 20451 **CASRN:** 1212−29−9
SPID(S): Tox21_302838
M4ID: 12476295

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.83	NA	NA

MAX_MEAN: 0.495 **MAX_MED:** 0.228 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

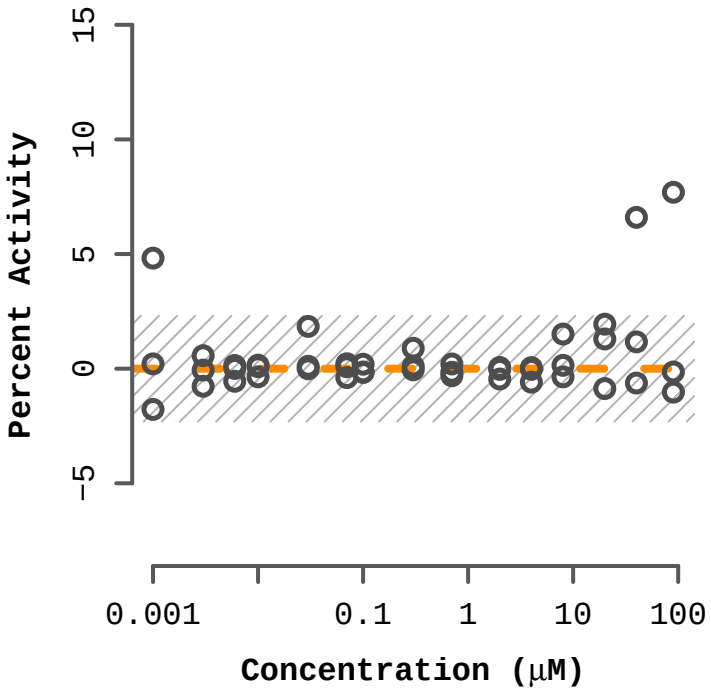
NAME: N,N'−Dicyclohexylthiourea
CHID: 20451 **CASRN:** 1212−29−9
SPID(S): Tox21_201806
M4ID: 12480446 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.18	NA	NA
PROB:	1	NA	NA
RMSE:	5.4	NA	NA

MAX_MEAN: 5.18 **MAX_MED:** 0.712 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

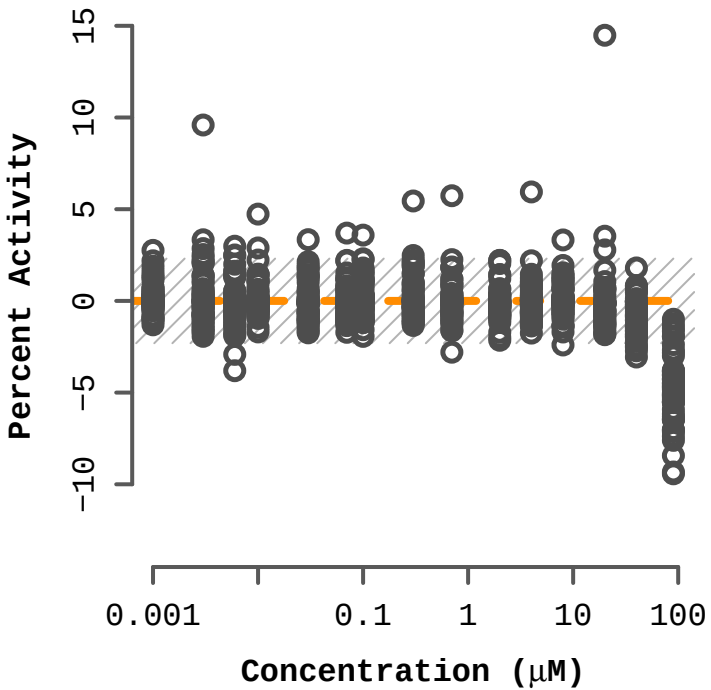
NAME: Dicyclopentadiene dioxide
CHID: 20452 **CASRN:** 81-21-0
SPID(S): Tox21_200495
M4ID: 12481757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

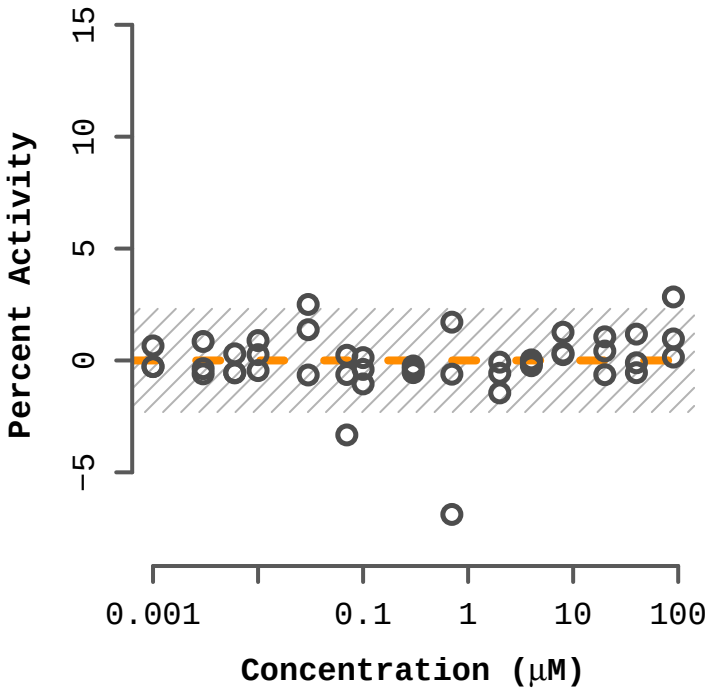
NAME: Dieldrin
CHID: 20453 **CASRN:** 60-57-1
SPID(S): Tox21_400029
M4ID: 12475108

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2731.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 0.321 **MAX_MED:** 0.00936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

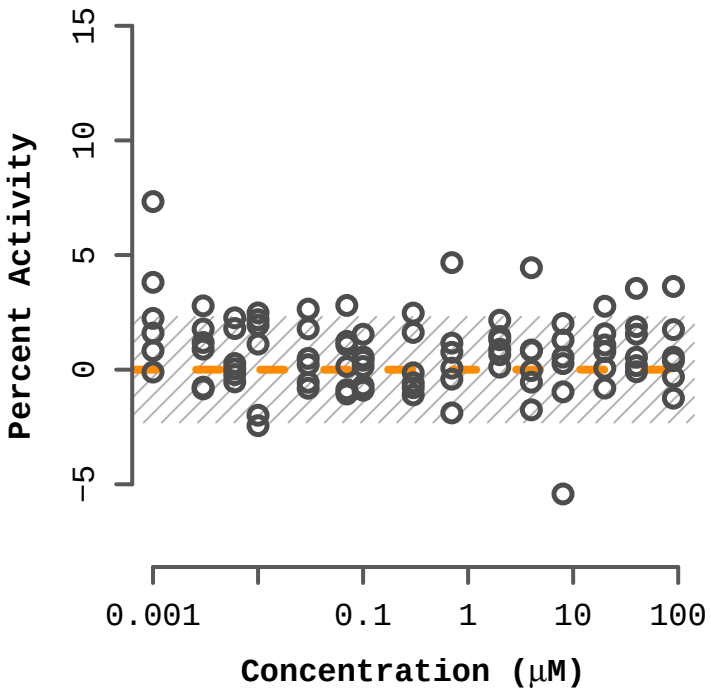
NAME: Chlorpyrifos
CHID: 20458 **CASRN:** 2921-88-2
SPID(S): Tox21_300148
M4ID: 12478982

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

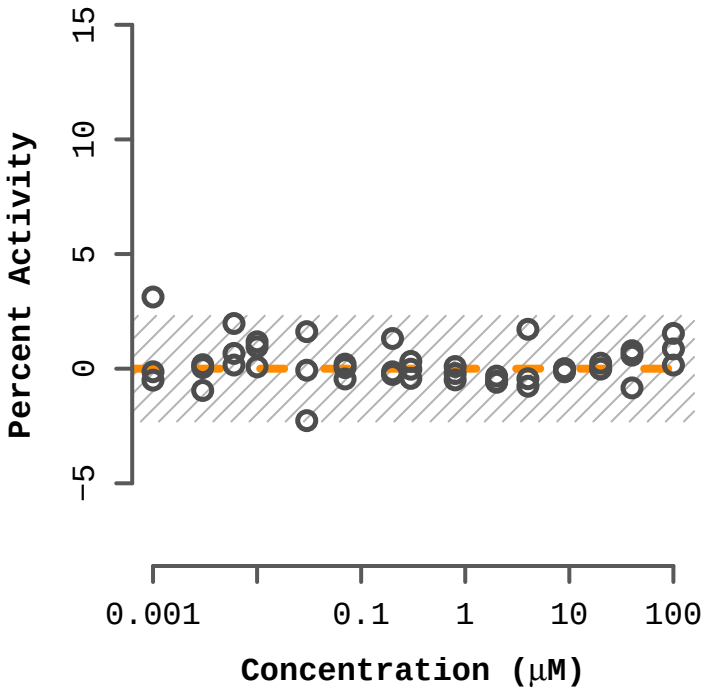
NAME: Chlorpyrifos
CHID: 20458 CASRN: 2921-88-2
SPID(S): Tox21_202383
M4ID: 12479869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	361.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 2.62 MAX_MED: 1.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

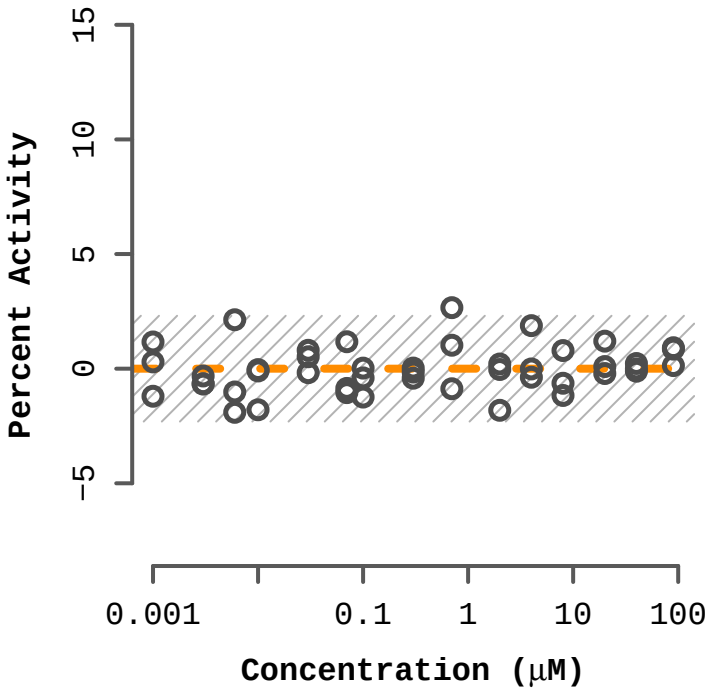
NAME: Diethylacetamide
CHID: 20459 **CASRN:** 685-91-6
SPID(S): Tox21_200733
M4ID: 12481519

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.933 **MAX_MED:** 0.956 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

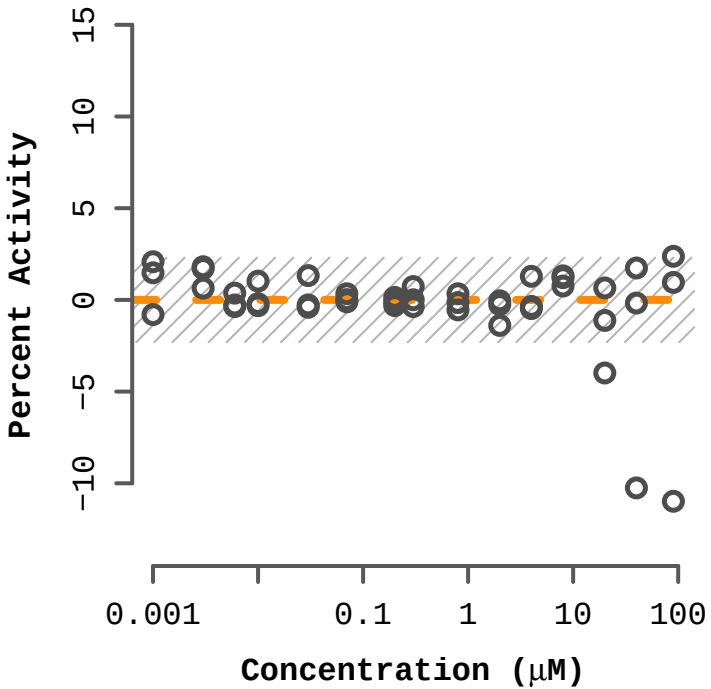
NAME: Diethylene glycol
CHID: 20462 **CASRN:** 111-46-6
SPID(S): Tox21_300064
M4ID: 12479066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.938 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

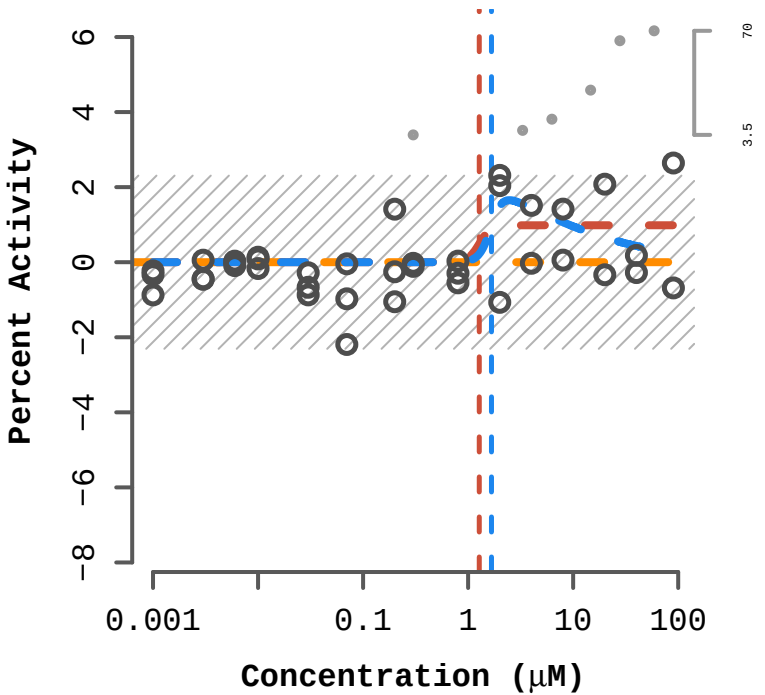
NAME: Diethylene glycol
CHID: 20462 **CASRN:** 111-46-6
SPID(S): Tox21_201616
M4ID: 12480636

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethylformamide
CHID: 20463 **CASRN:** 617-84-5
SPID(S): Tox21_200919
M4ID: 12481333 **BRK**

HILL MODEL (in red):

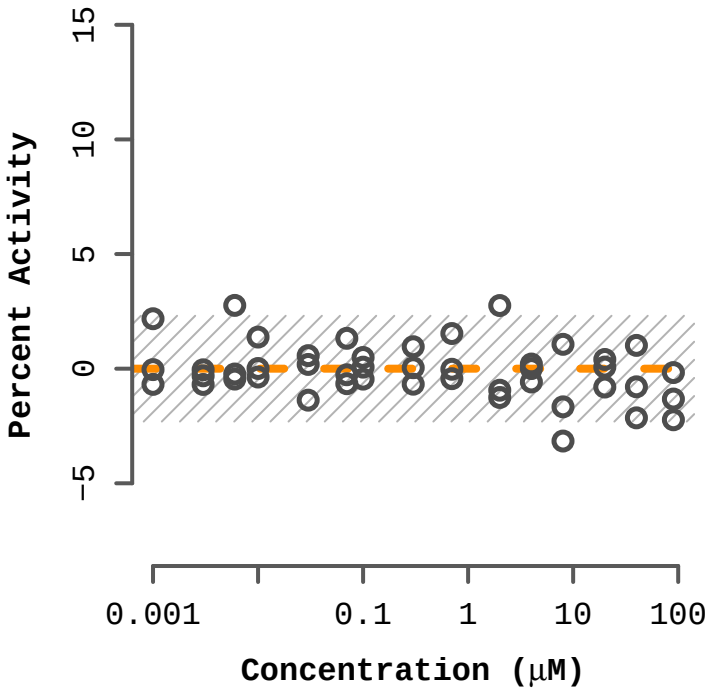
	tp	ga	gw
val:	0.984	0.106	8
sd:	0.444	0.325	13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.23	0.222	8	0.474	0.718
sd:	30.2	0.441	18	10.5	3

	CNST	HILL	GNLS
AIC:	258.39	259.28	262.14
PROB:	0.56	0.36	0.09
RMSE:	15.05	14.77	14.91

MAX_MEAN: 23.9 **MAX_MED:** 2.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

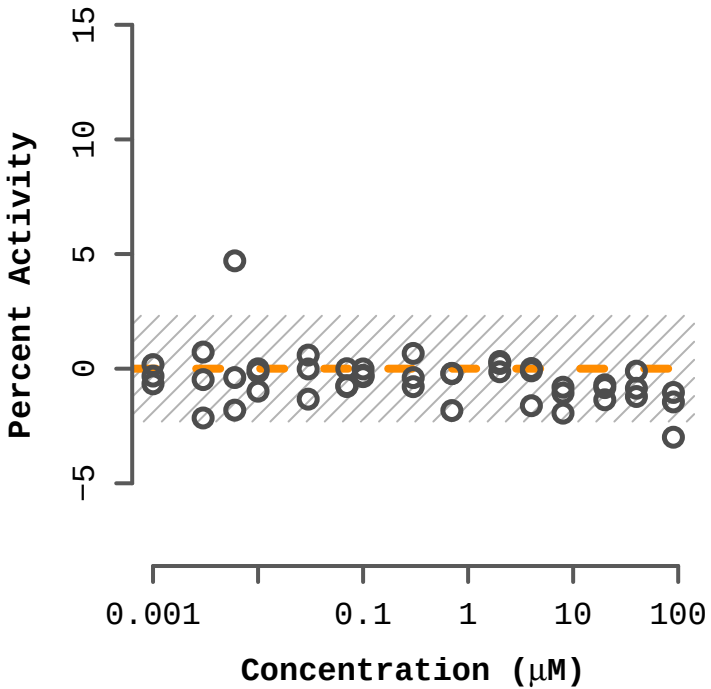
NAME: Diethyl maleate
CHID: 20464 CASRN: 141-05-9
SPID(S): Tox21_303020
M4ID: 12476113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.692 MAX_MED: 0.186 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

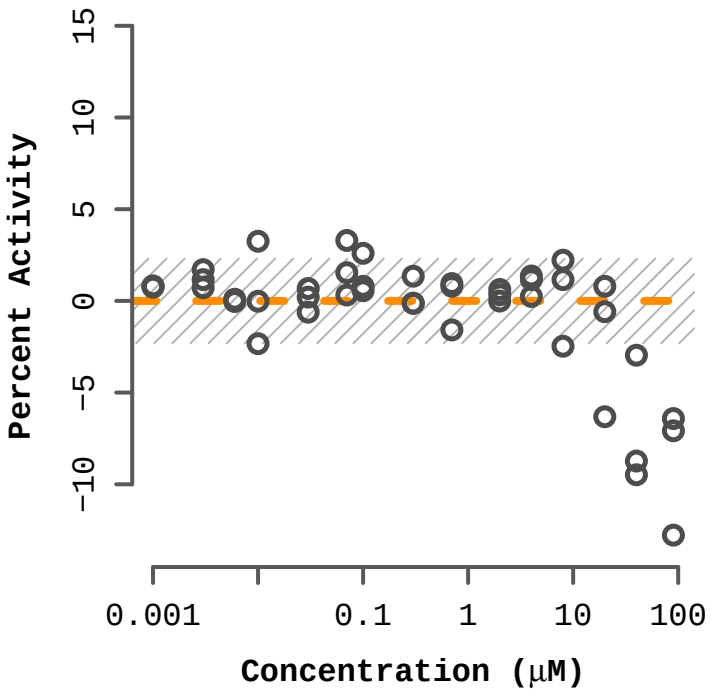
NAME: Diethyl maleate
CHID: 20464 CASRN: 141-05-9
SPID(S): Tox21_201512
M4ID: 12480740

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.837 MAX_MED: 0.227 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

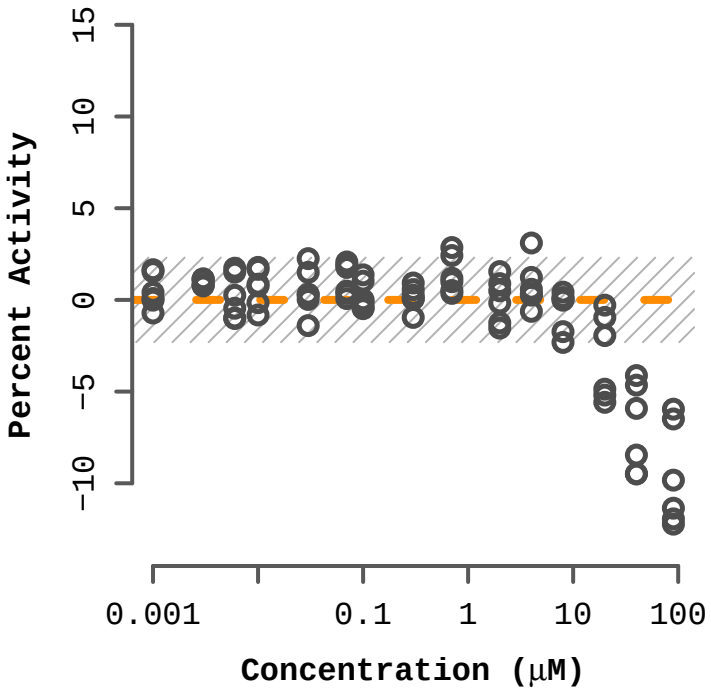
NAME: Diethylstilbestrol
CHID: 20465 **CASRN:** 56-53-1
SPID(S): Tox21_300526
M4ID: 12478606

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.66	NA	NA
PROB:	1	NA	NA
RMSE:	3.45	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

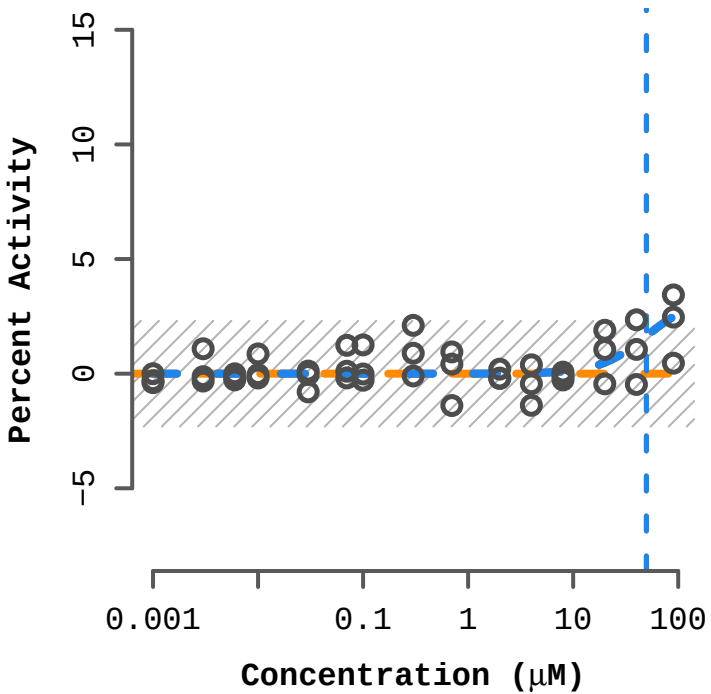
NAME: Diethylstilbestrol
CHID: 20465 **CASRN:** 56-53-1
SPID(S): Tox21_202407
M4ID: 12479845

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	443.57	NA	NA
PROB:	1	NA	NA
RMSE:	3.5	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N,N'−Diethylthiourea
CHID: 20466 CASRN: 105−55−5
SPID(S): Tox21_302956
M4ID: 12476177

HILL MODEL (in red):

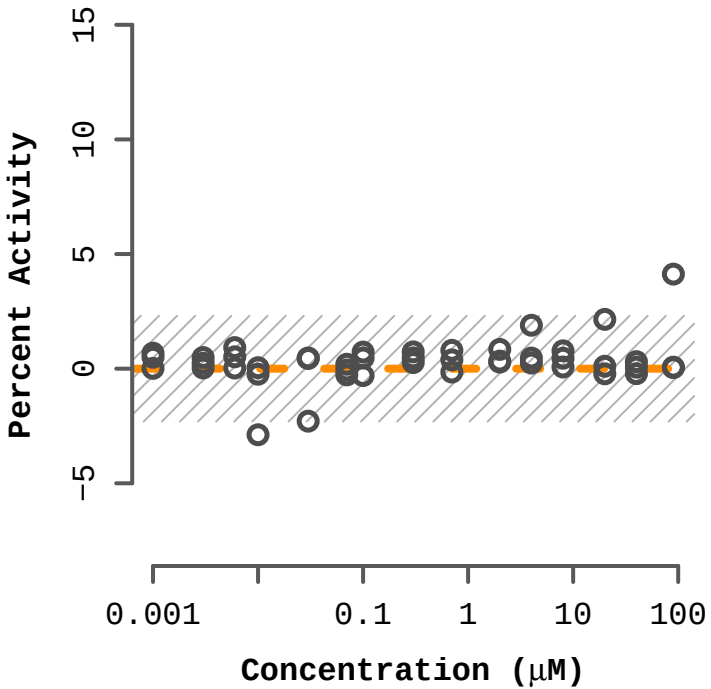
	tp	ga	gw
val:	3.28	1.7	1.93
sd:	2.55	0.476	1.32

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.28	1.7	1.93	3.63	3.67
sd:	2.55	0.476	1.32	754	1700

	CNST	HILL	GNLS
AIC:	123.84	115.32	119.32
PROB:	0.01	0.87	0.12
RMSE:	1.02	0.81	0.81

MAX_MEAN: 2.12 MAX_MED: 2.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

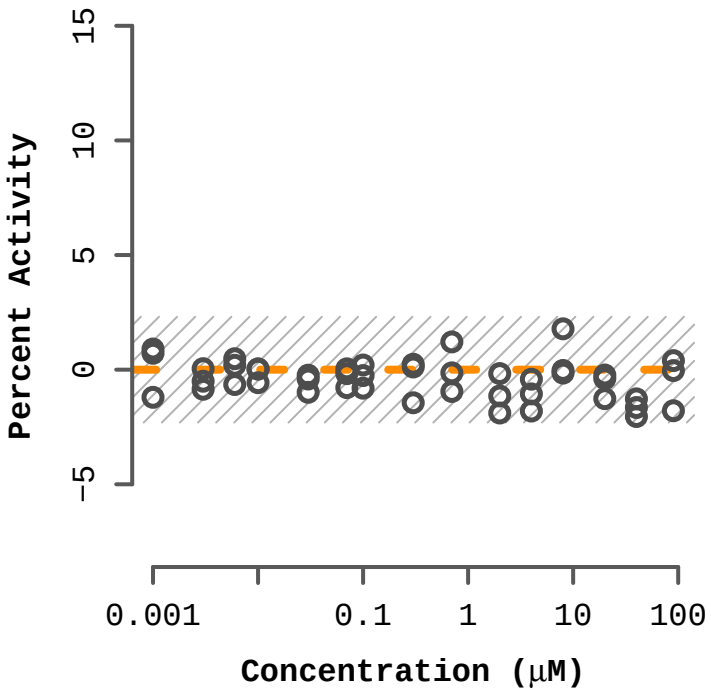
NAME: N,N'−Diethylthiourea
CHID: 20466 **CASRN:** 105−55−5
SPID(S): Tox21_201476
M4ID: 12480776

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 0.519 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

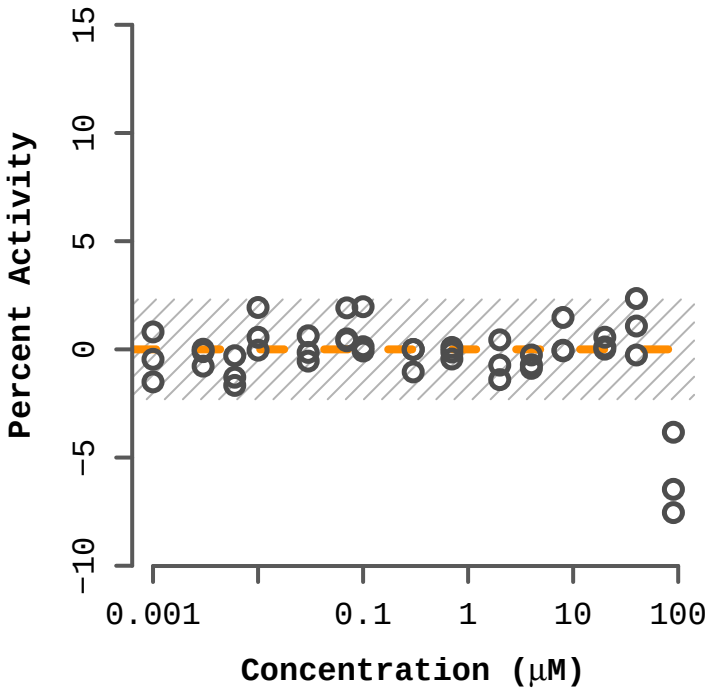
NAME: 1,2-Diformylhydrazine
CHID: 20468 **CASRN:** 628-36-4
SPID(S): Tox21_200133
M4ID: 12482119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.535 **MAX_MED:** 0.716 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

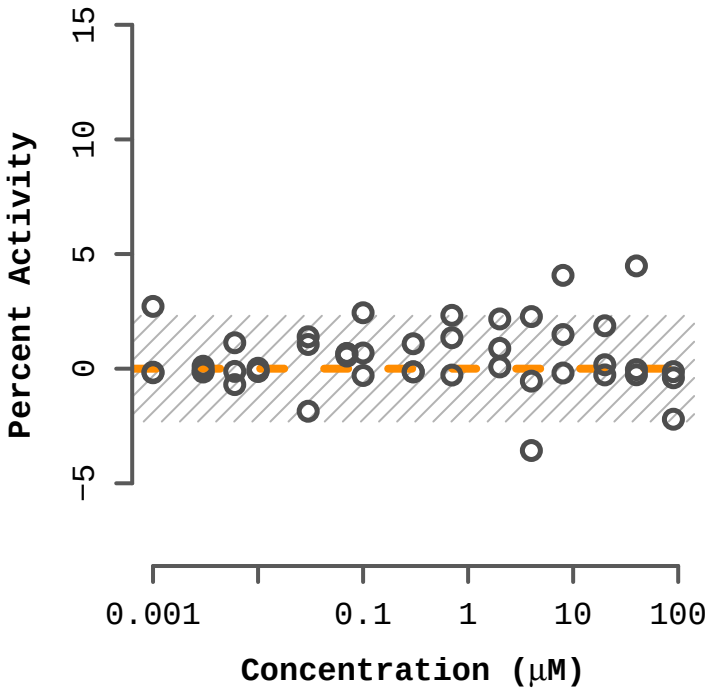
NAME: Diglycidyl resorcinol ether
CHID: 20470 **CASRN:** 101-90-6
SPID(S): Tox21_200668
M4ID: 12481584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

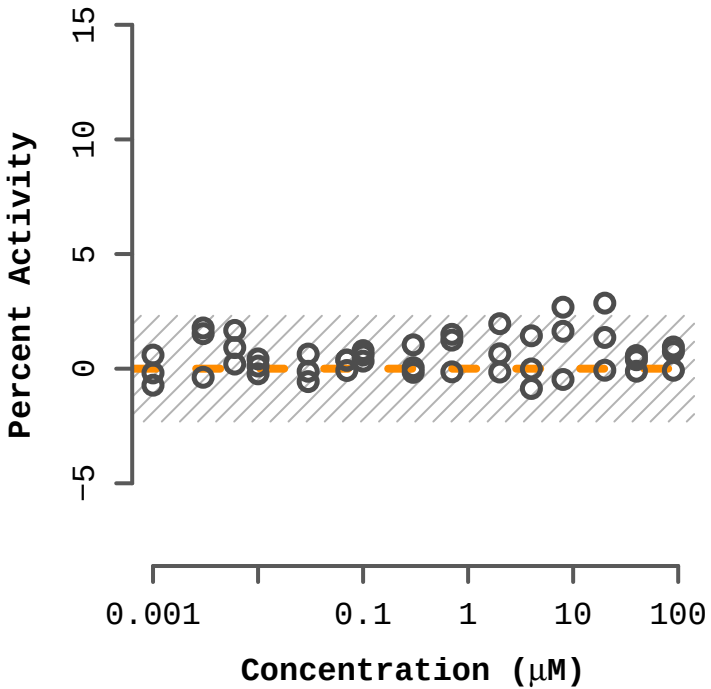
NAME: 3,4−Dihydrocoumarin
CHID: 20474 **CASRN:** 119−84−6
SPID(S): Tox21_302745
M4ID: 12476388

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

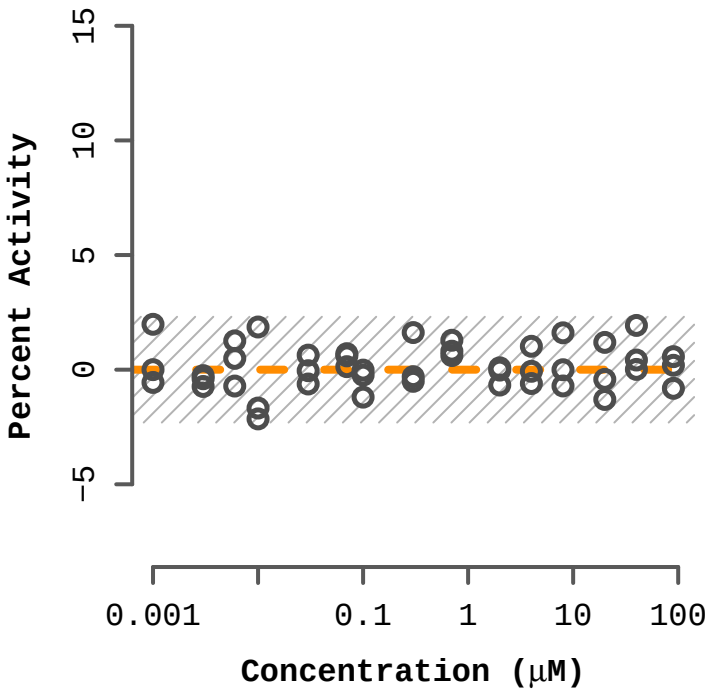
NAME: 3,4−Dihydrocoumarin
CHID: 20474 **CASRN:** 119−84−6
SPID(S): Tox21_202137
M4ID: 12480115

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

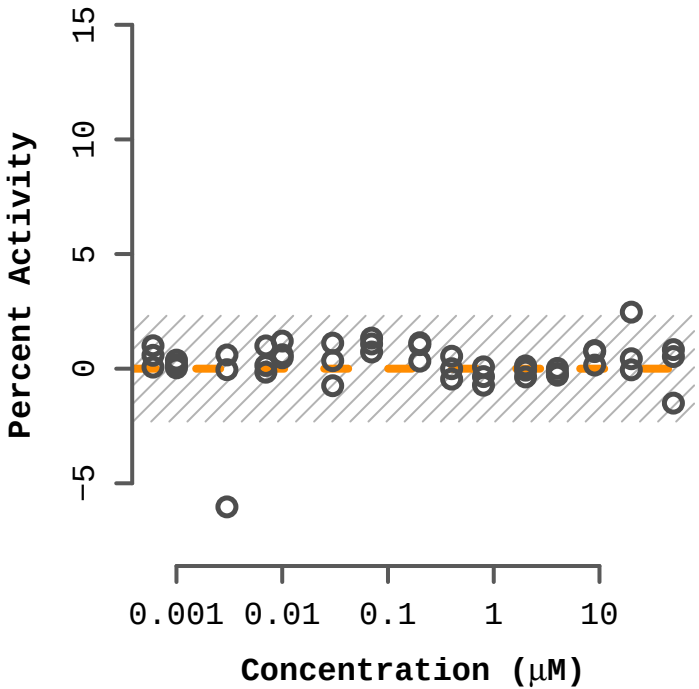
NAME: Dimethadione
CHID: 20478 **CASRN:** 695-53-4
SPID(S): Tox21_200496
M4ID: 12481756

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.903 **MAX_MED:** 0.808 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

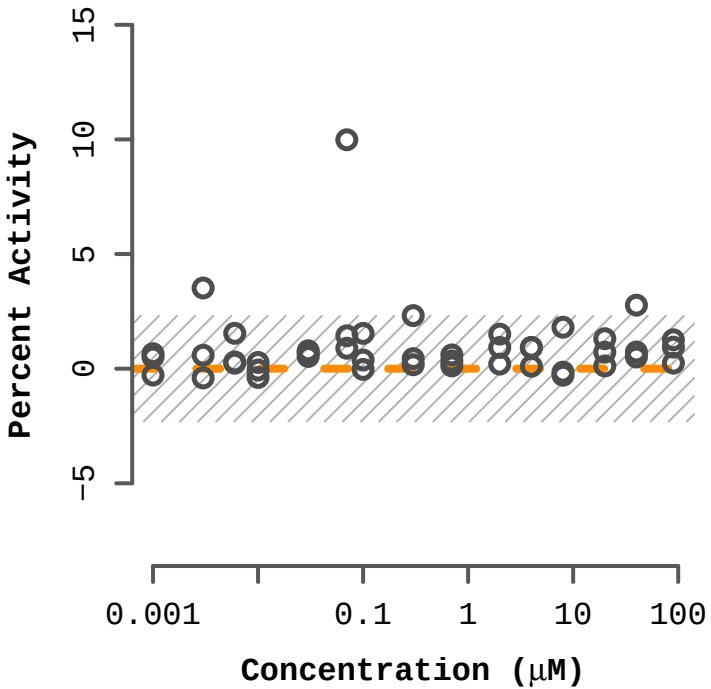
NAME: Dimethadione
CHID: 20478 **CASRN:** 695-53-4
SPID(S): Tox21_110479_1
M4ID: 12484324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

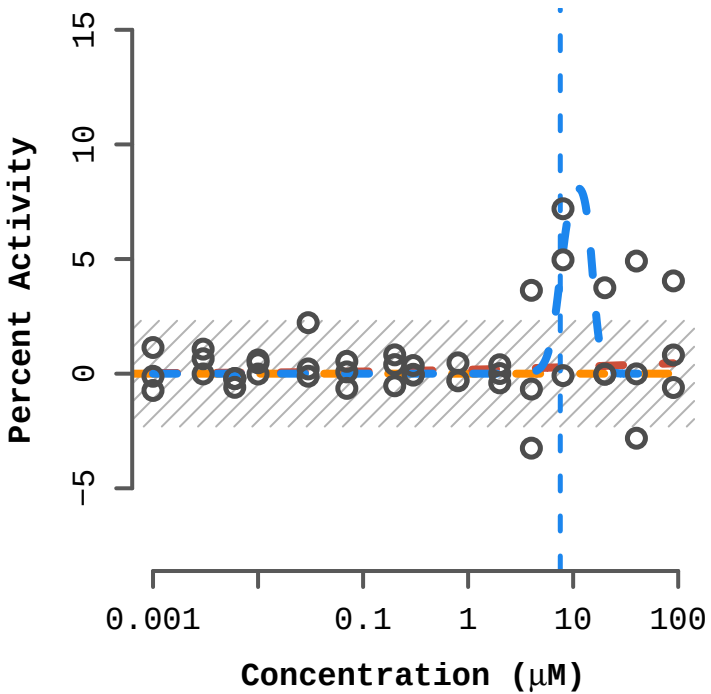
NAME: Dimethoate
CHID: 20479 **CASRN:** 60-51-5
SPID(S): Tox21_301161
M4ID: 12477972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 4.11 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethoate
CHID: 20479 **CASRN:** 60-51-5
SPID(S): Tox21_202246
M4ID: 12480006

HILL MODEL (in red):

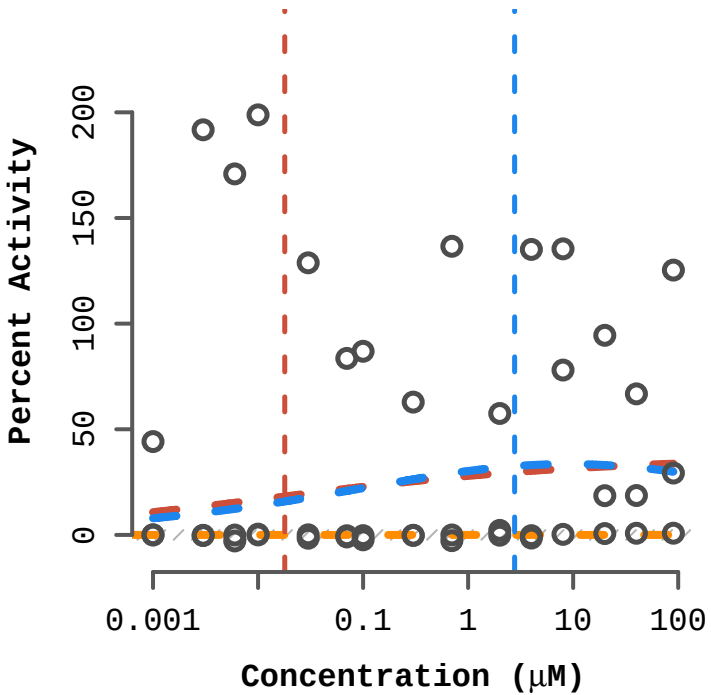
	tp	ga	gw
val:	1.06	2.38	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.64	0.877	8	1.19	11.5
sd:	15.7	0.244	7.82	1.71	173

	CNST	HILL	GNLS
AIC:	172.05	176.87	172.39
PROB:	0.52	0.05	0.44
RMSE:	1.98	1.9	1.7

MAX_MEAN: 4.03 **MAX_MED:** 4.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethoxane
CHID: 20480 CASRN: 828-00-2
SPID(S): Tox21_300414
M4ID: 12478718

HILL MODEL (in red):

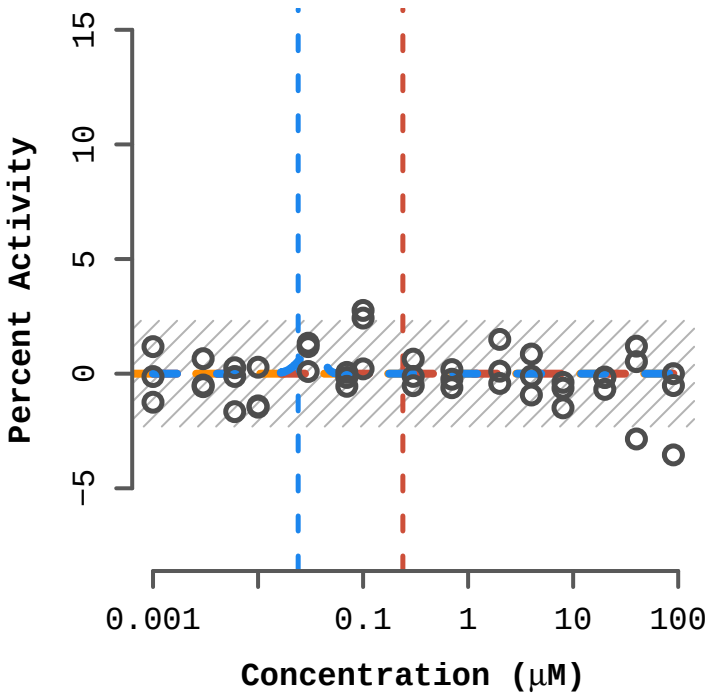
	tp	ga	gw
val:	36.3	-1.75	0.3
sd:	64.2	6.76	1.15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	97.2	0.443	0.3	1.47	0.3
sd:	286	8.11	0.332	1.51	0.424

	CNST	HILL	GNLS
AIC:	520.62	501.97	506.21
PROB:	0	0.89	0.11
RMSE:	72.7	62.8	63.26

MAX_MEAN: 71.2 MAX_MED: 78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethoxane
CHID: 20480 CASRN: 828-00-2
SPID(S): Tox21_202123
M4ID: 12480129

HILL MODEL (in red):

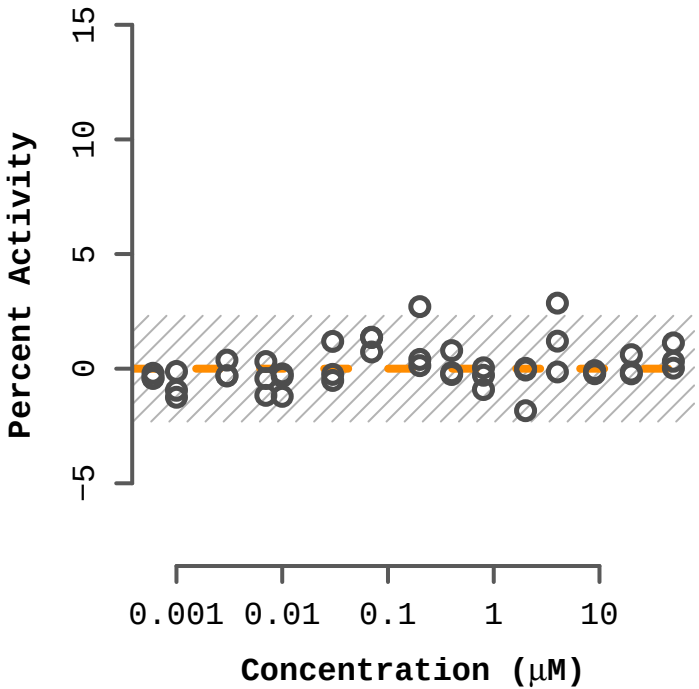
	tp	ga	gw
val:	6.11e-10	-0.621	1.68
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.08	-1.62	8	-1.37	16.1
sd:	5.64	1.62	31	2.24	170

	CNST	HILL	GNLS
AIC:	137.44	143.44	144.27
PROB:	0.92	0.05	0.03
RMSE:	1.15	1.15	1.12

MAX_MEAN: 1.8 **MAX_MED:** 2.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

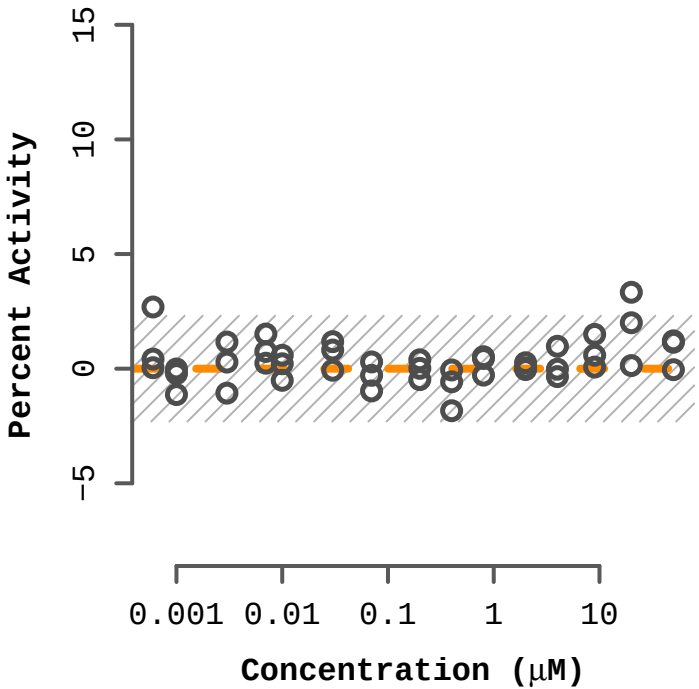
NAME: 2,4−Dimethoxyaniline hydrochloride
CHID: 20483 **CASRN:** 54150−69−5
SPID(S): Tox21_201230
M4ID: 12481022

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

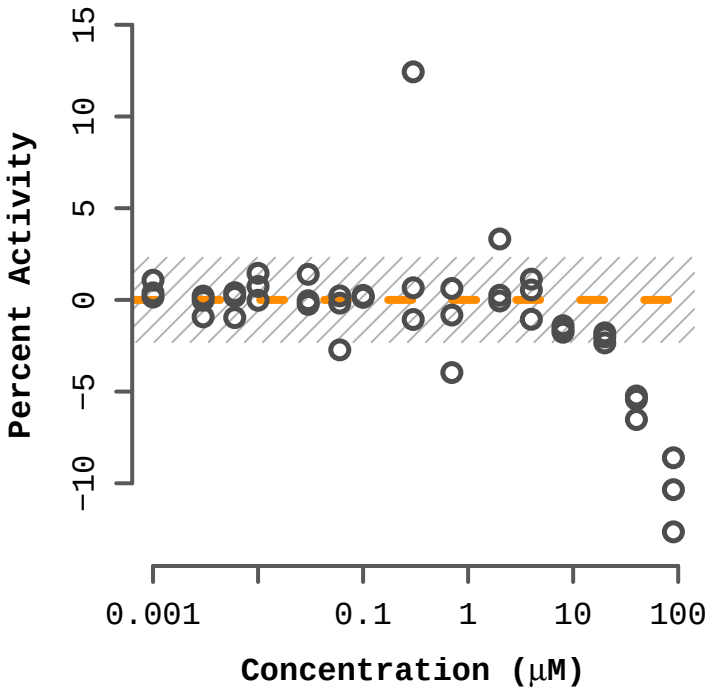
NAME: 3,3'−Dimethoxybenzidine−4,4'−diisocyanate
CHID: 20484 **CASRN:** 91−93−0
SPID(S): Tox21_202477
M4ID: 12479775

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

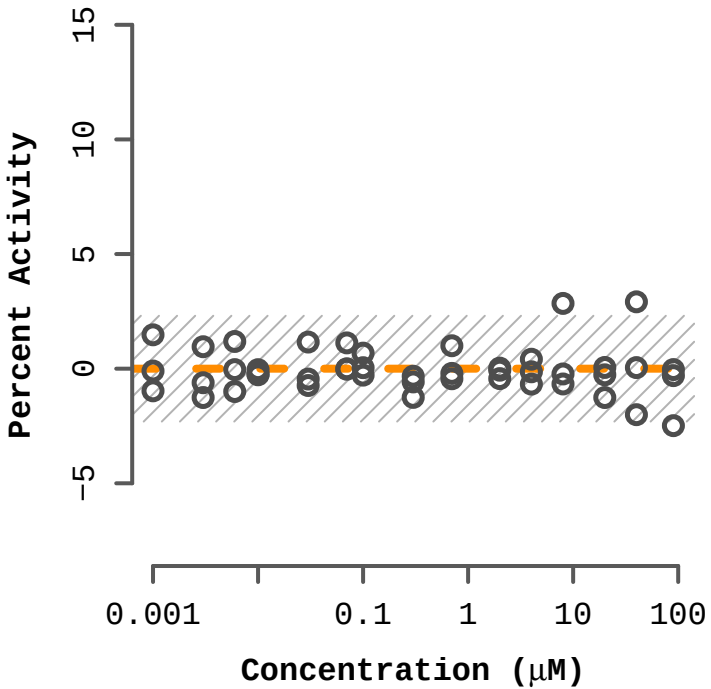
NAME: 3,3'−Dimethoxybenzidine dihydrochloride
CHID: 20485 CASRN: 20325−40−0
SPID(S): Tox21_300315
M4ID: 12478816

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.65	NA	NA
PROB:	1	NA	NA
RMSE:	3.84	NA	NA

MAX_MEAN: 4.01 MAX_MED: 0.736 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

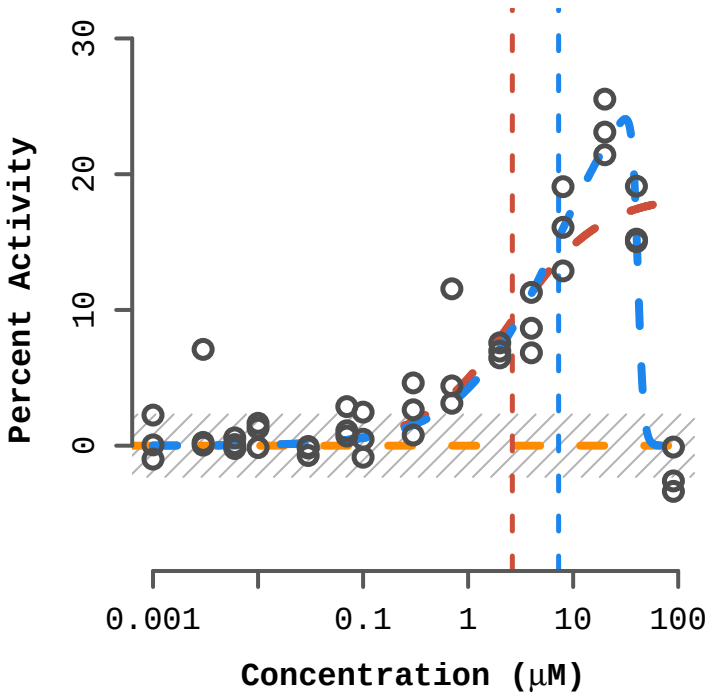
NAME: 3,3'−Dimethoxybenzidine dihydrochloride
CHID: 20485 CASRN: 20325−40−0
SPID(S): Tox21_202152
M4ID: 12480100

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.651 **MAX_MED:** 0.0486 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(Dimethylamino)azobenzene
CHID: 20491 CASRN: 60-11-7
SPID(S): Tox21_200757
M4ID: 12481495

HILL MODEL (in red):

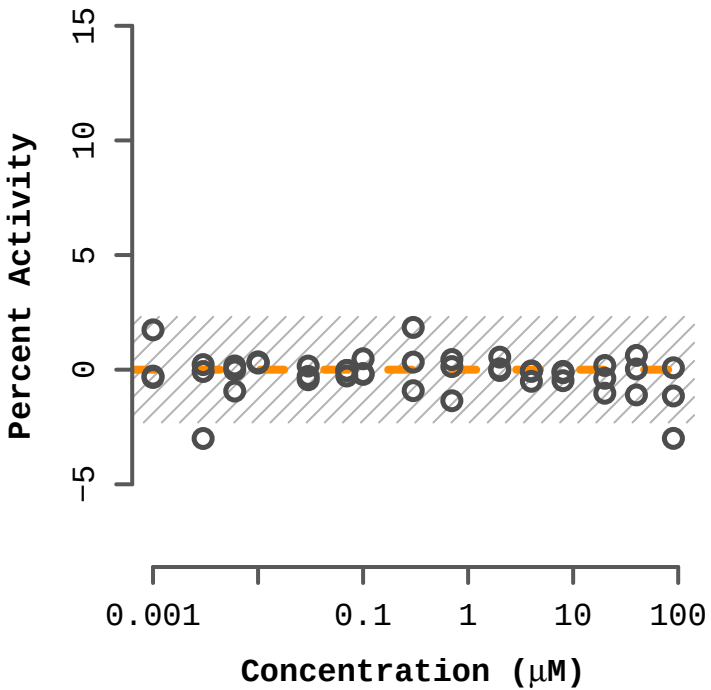
	tp	ga	gw
val:	18.5	0.421	1.03
sd:	2.2	0.142	0.272

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	30.6	0.861	0.925	1.62	16.1
sd:	4.32	0.152	0.131	0.00619	8.16

	CNST	HILL	GNLS
AIC:	325.34	266.68	206.08
PROB:	0	0	1
RMSE:	9.36	5.93	2.34

MAX_MEAN: 23.4 MAX_MED: 23.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

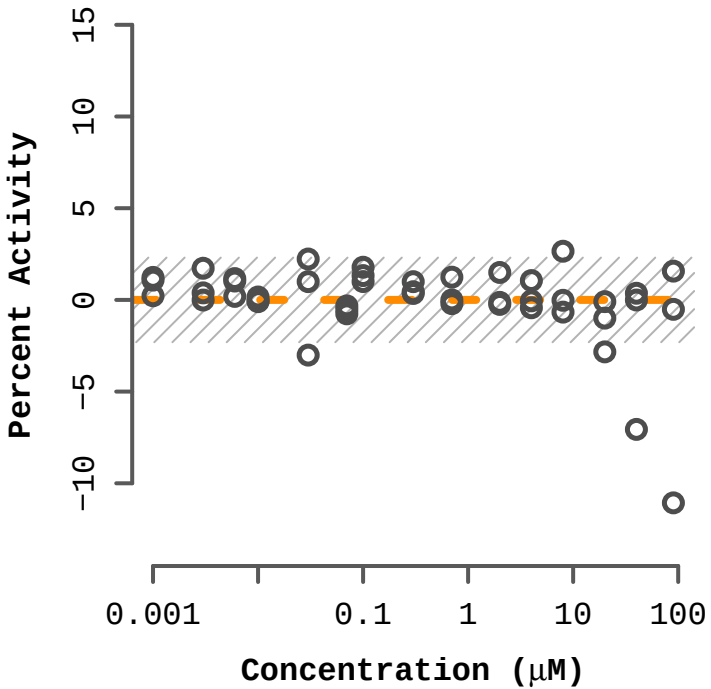
NAME: Dimethyl hydrogen phosphite
CHID: 20493 **CASRN:** 868-85-9
SPID(S): Tox21_302799
M4ID: 12476334

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.42 **MAX_MED:** 0.332 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

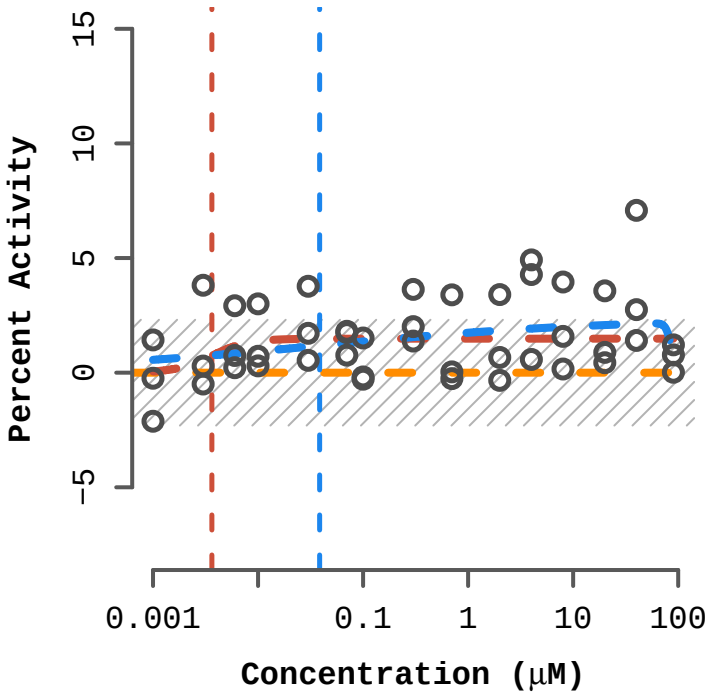
NAME: Dimethyl hydrogen phosphite
CHID: 20493 **CASRN:** 868-85-9
SPID(S): Tox21_201901
M4ID: 12480351

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.29	NA	NA
PROB:	1	NA	NA
RMSE:	2.25	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethyl methylphosphonate
CHID: 20494 CASRN: 756-79-6
SPID(S): Tox21_303029
M4ID: 12476104

HILL MODEL (in red):

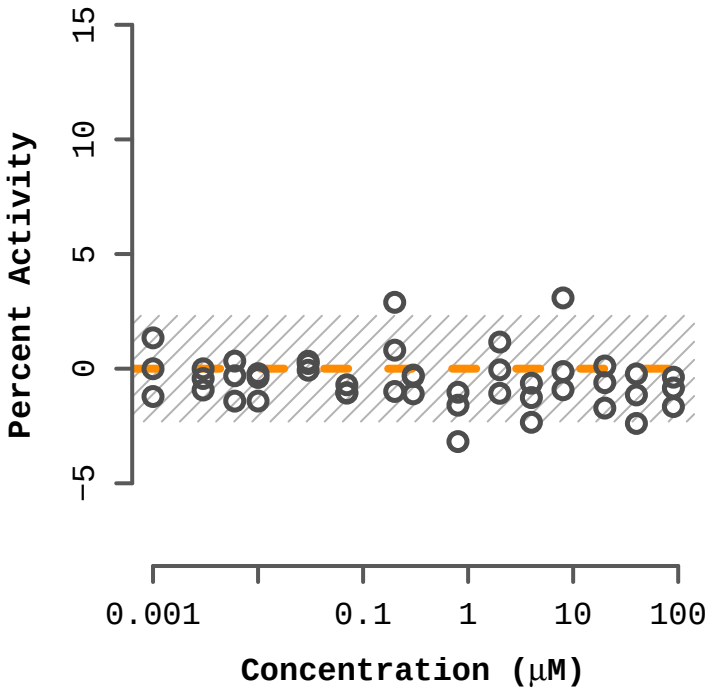
	tp	ga	gw
val:	1.48	−2.44	2.53
sd:	0.297	0.393	4.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.36	−1.41	0.319	1.93	17.2
sd:	2.44	3.53	0.623	0.0572	48.1

	CNST	HILL	GNLS
AIC:	205.36	183.92	186.43
PROB:	0	0.78	0.22
RMSE:	2.34	1.71	1.64

MAX_MEAN: 3.75 **MAX_MED:** 4.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

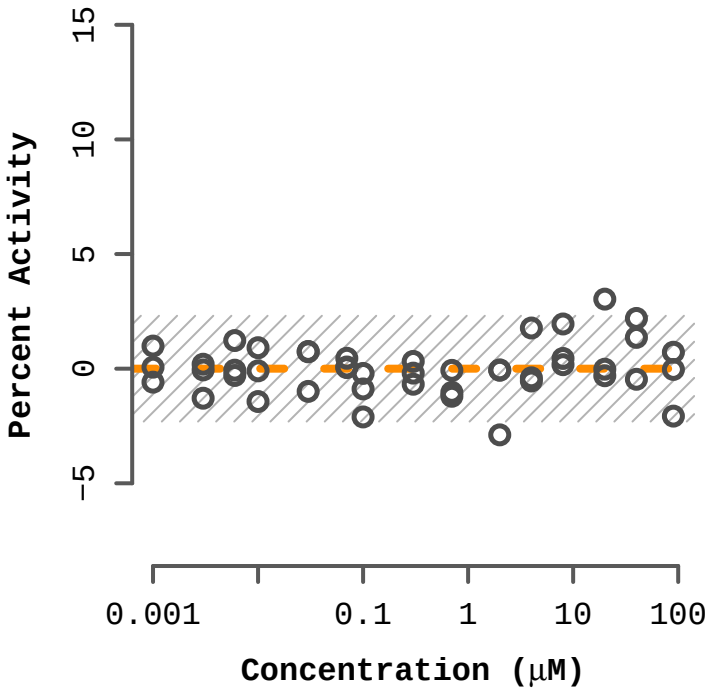
NAME: Dimethyl methylphosphonate
CHID: 20494 **CASRN:** 756-79-6
SPID(S): Tox21_201534
M4ID: 12480718

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.904 **MAX_MED:** 0.809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

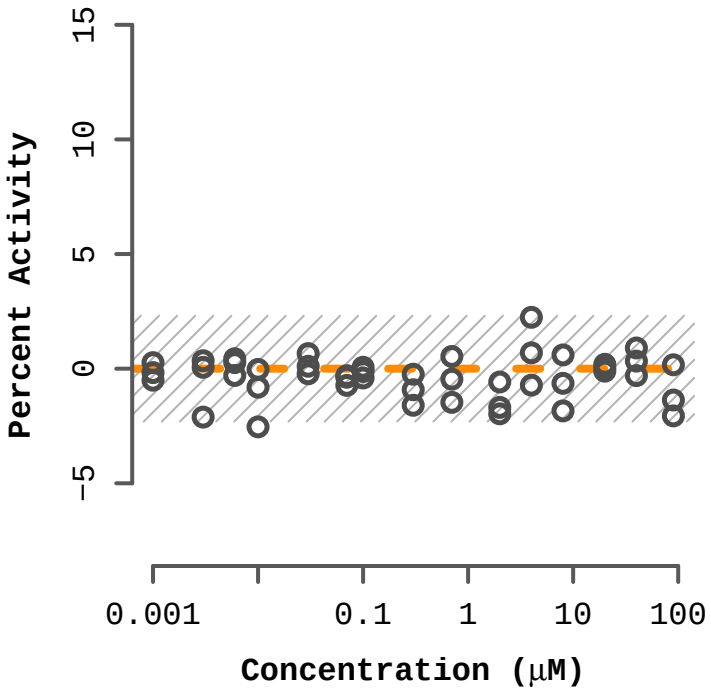
NAME: 1,2-Dimethyl-5-nitroimidazole
CHID: 20497 **CASRN:** 551-92-8
SPID(S): Tox21_302989
M4ID: 12476144

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

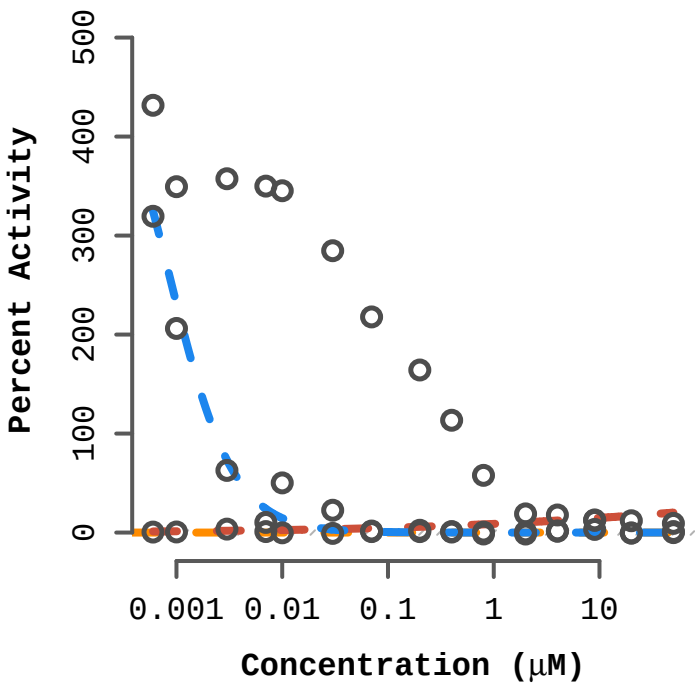
NAME: 1,2-Dimethyl-5-nitroimidazole
CHID: 20497 **CASRN:** 551-92-8
SPID(S): Tox21_201618
M4ID: 12480634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** 0.693 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Dimethyl-5-nitroimidazole
CHID: 20497 CASRN: 551-92-8
SPID(S): Tox21_113657
M4ID: 12482556

HILL MODEL (in red):

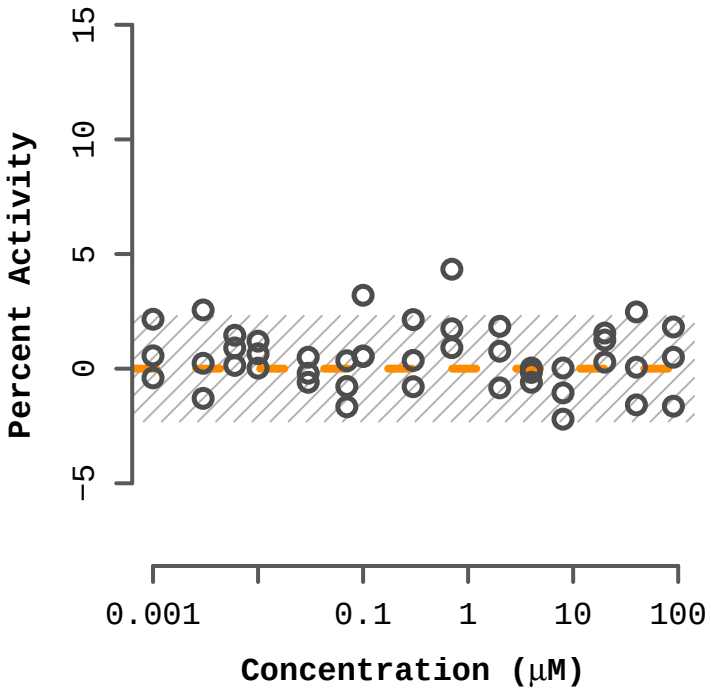
	tp	ga	gw
val:	48.2	2.18	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	518	-4.03	7.86	-3.07	1.44
sd:	323	165	1600	0.408	0.807

	CNST	HILL	GNLS
AIC:	563.95	567.9	553.27
PROB:	0	0	0.99
RMSE:	149.26	148.11	121.01

MAX_MEAN: 251 **MAX_MED:** 320 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

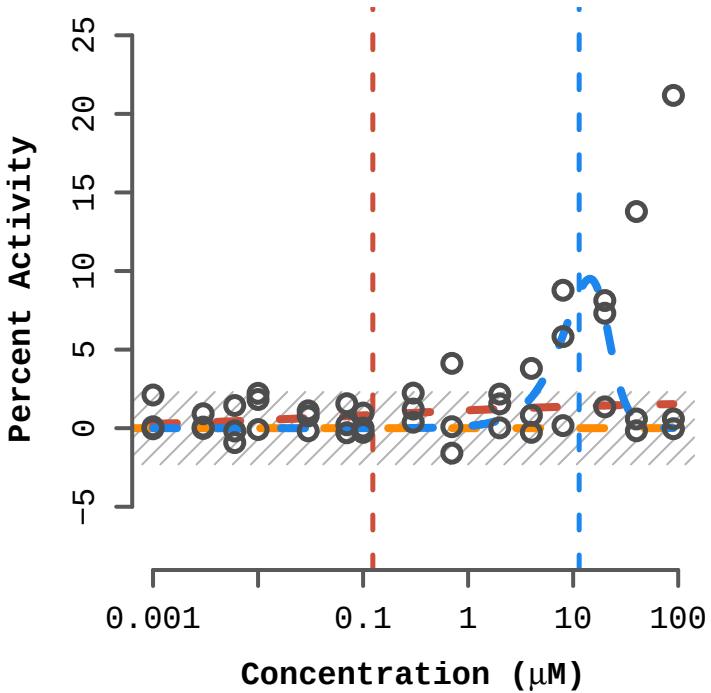
NAME: Dimethyl terephthalate
CHID: 20498 **CASRN:** 120-61-6
SPID(S): Tox21_300139
M4ID: 12478991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethyl terephthalate
CHID: 20498 CASRN: 120-61-6
SPID(S): Tox21_202268
M4ID: 12479984

HILL MODEL (in red):

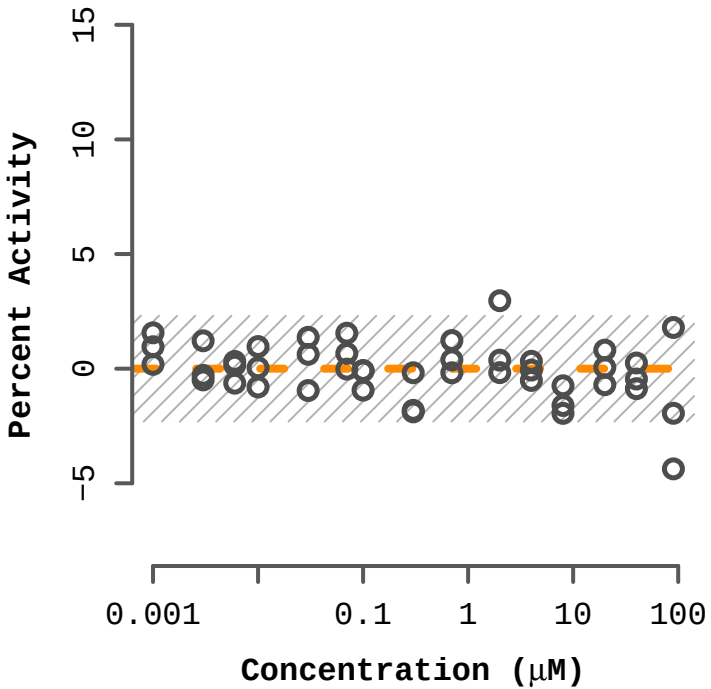
	tp	ga	gw
val:	1.69	−0.907	0.342
sd:	1.26	2.3	0.46

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.2	1.06	2.02	1.31	5.06
sd:	44.2	0.867	1.81	0.241	2.97

	CNST	HILL	GNLS
AIC:	230.42	224.42	217.58
PROB:	0	0.03	0.97
RMSE:	4.58	4.08	4.11

MAX_MEAN: 7.25 MAX_MED: 7.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

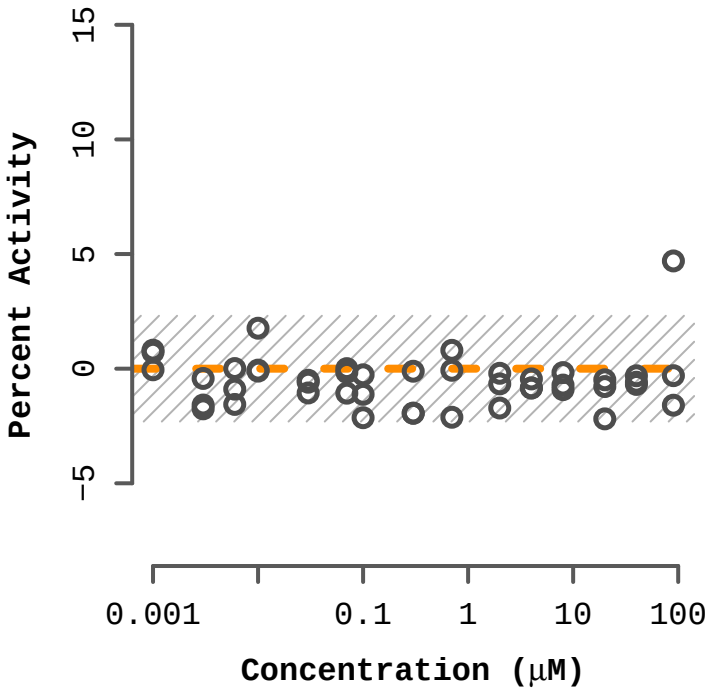
NAME: N,N−Dimethylacetamide
CHID: 20499 **CASRN:** 127−19−5
SPID(S): Tox21_302787
M4ID: 12476346

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.959 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

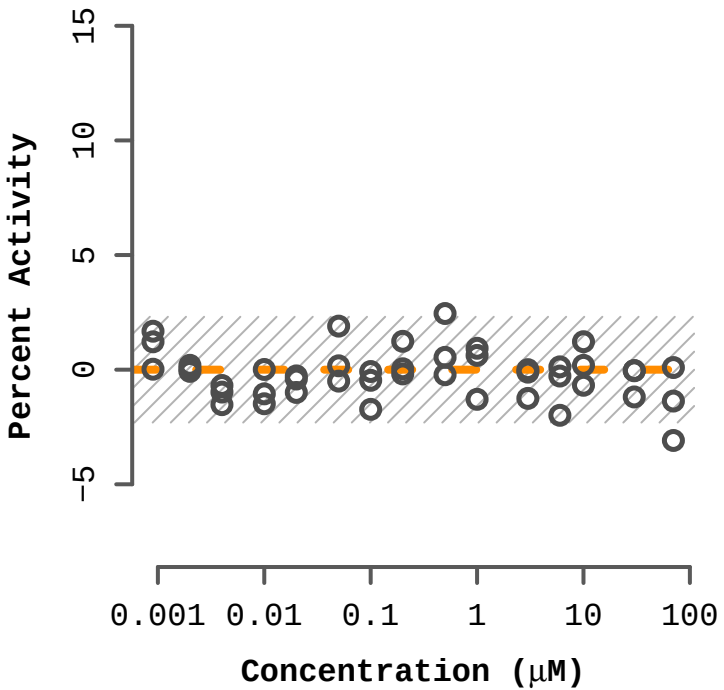
NAME: N,N−Dimethylacetamide
CHID: 20499 **CASRN:** 127−19−5
SPID(S): Tox21_202174
M4ID: 12480078

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.716 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

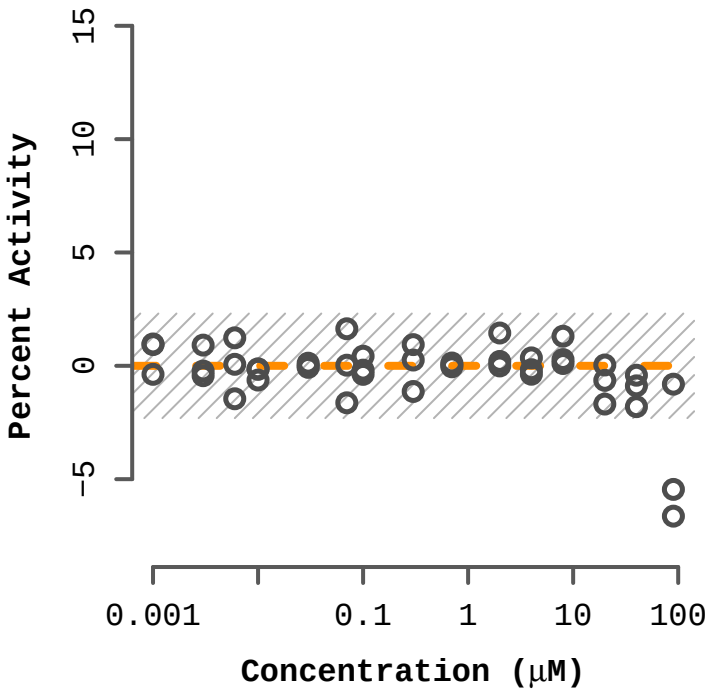
NAME: Methadone hydrochloride
CHID: 20501 **CASRN:** 1095-90-5
SPID(S): Tox21_300633
M4ID: 12478500

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

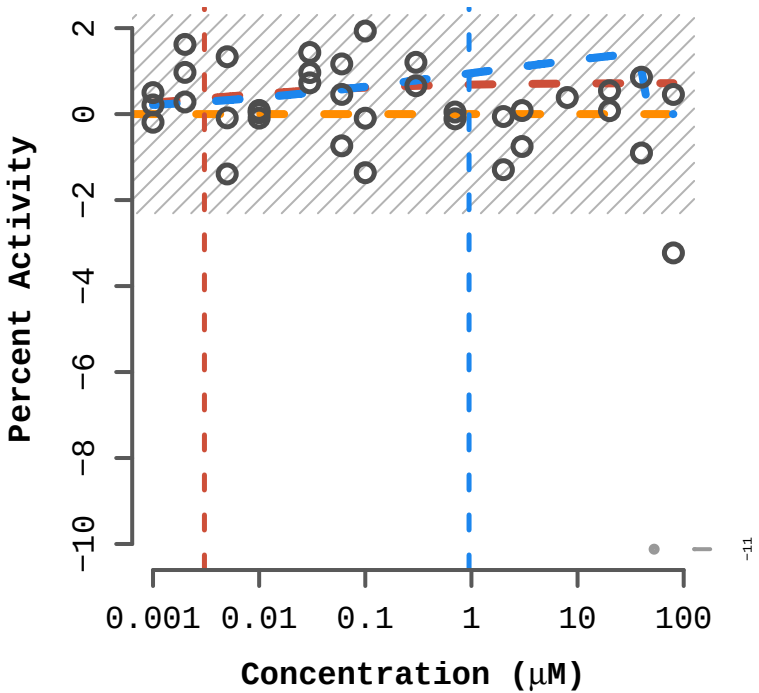
NAME: Methadone hydrochloride
CHID: 20501 CASRN: 1095-90-5
SPID(S): Tox21_202026
M4ID: 12480226

HILL MODEL: Not applicable.

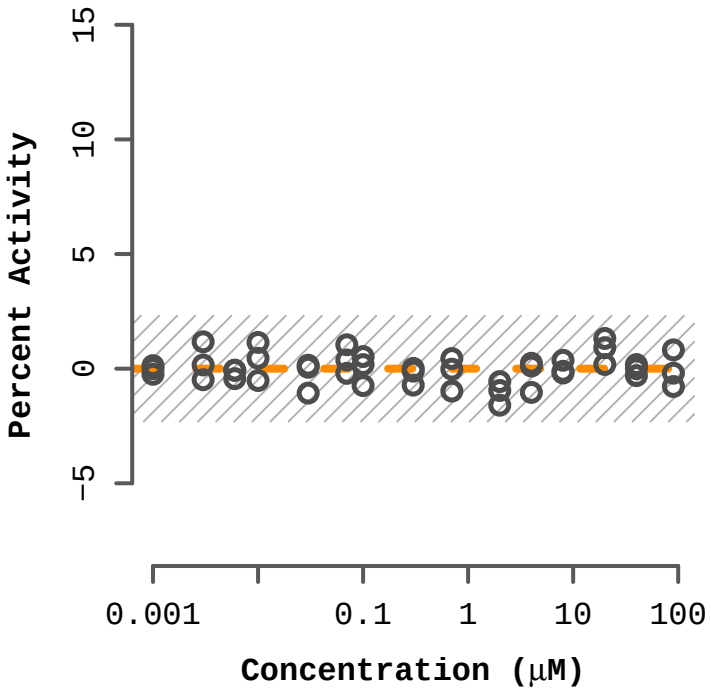
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.563 **MAX_MED:** 0.938 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Methadone hydrochloride
CHID:    20501   CASRN: 1095-90-5
SPID(S): Tox21_112895
M4ID:    12482890  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  0.724    -2.52    0.497
sd:   0.494    2.85     1.08

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.89     -0.0222  0.3      1.62     18
sd:   9.53     16       1.21     0.199    161

      CNST        HILL        GNLS
AIC:  212.54      213.76      215.43
PROB: 0.56        0.31        0.13
RMSE: 3.04        2.91        2.74

MAX_MEAN: 3.53      MAX_MED: 3.01      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

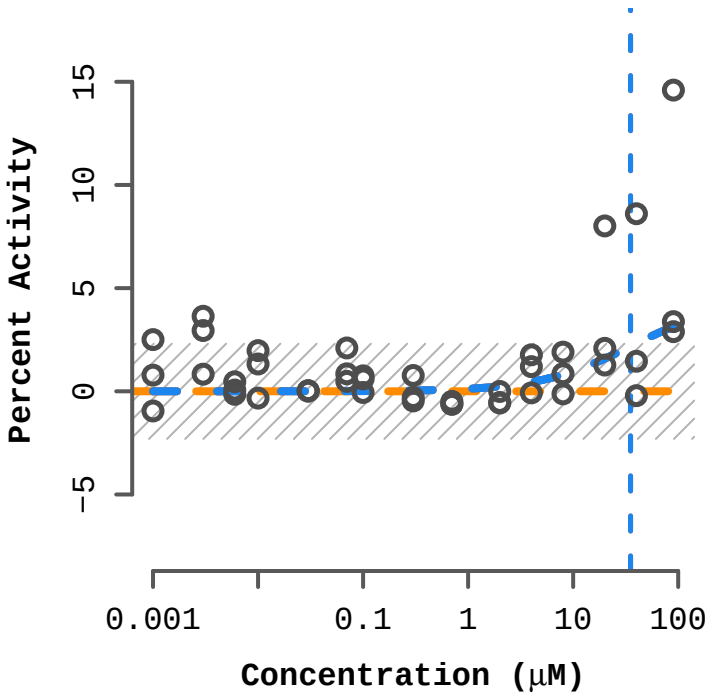
NAME: 4-Dimethylaminoantipyrine
CHID: 20504 **CASRN:** 58-15-1
SPID(S): Tox21_302830
M4ID: 12476303

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 0.918 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Dimethylaminoantipyrine
CHID: 20504 CASRN: 58-15-1
SPID(S): Tox21_201544
M4ID: 12480708

HILL MODEL (in red):

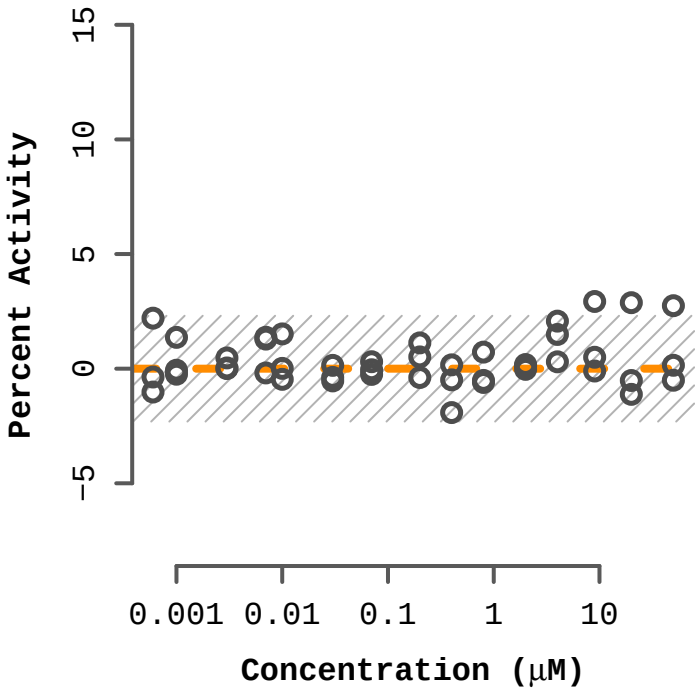
	tp	ga	gw
val:	4.37	1.55	0.998
sd:	6.61	1.63	1.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.36	1.55	0.998	3.3	5.7
sd:	6.6	1.63	1.13	1390	5900

	CNST	HILL	GNLS
AIC:	198.59	184.95	188.95
PROB:	0	0.88	0.12
RMSE:	3.1	2.45	2.45

MAX_MEAN: 6.96 MAX_MED: 3.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

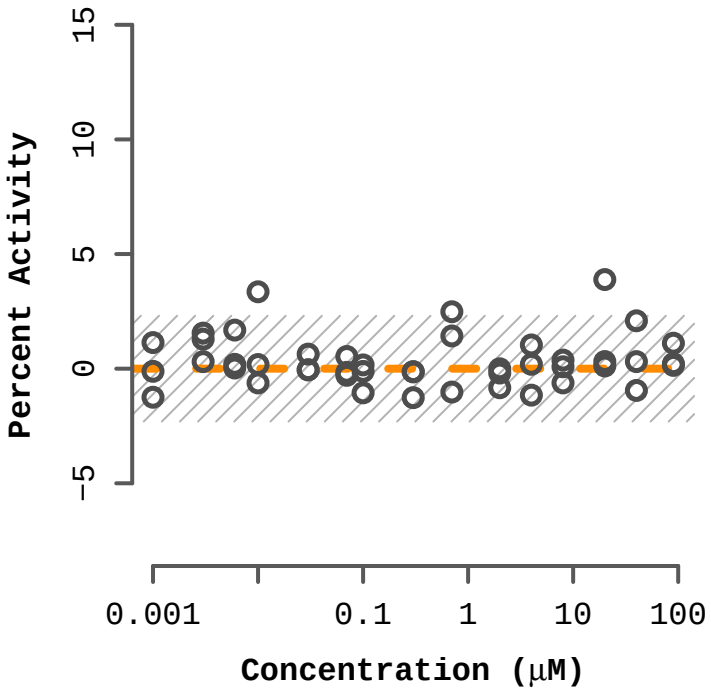
NAME: 4-Dimethylaminoantipyrine
CHID: 20504 **CASRN:** 58-15-1
SPID(S): Tox21_110333_1
M4ID: 12484447

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

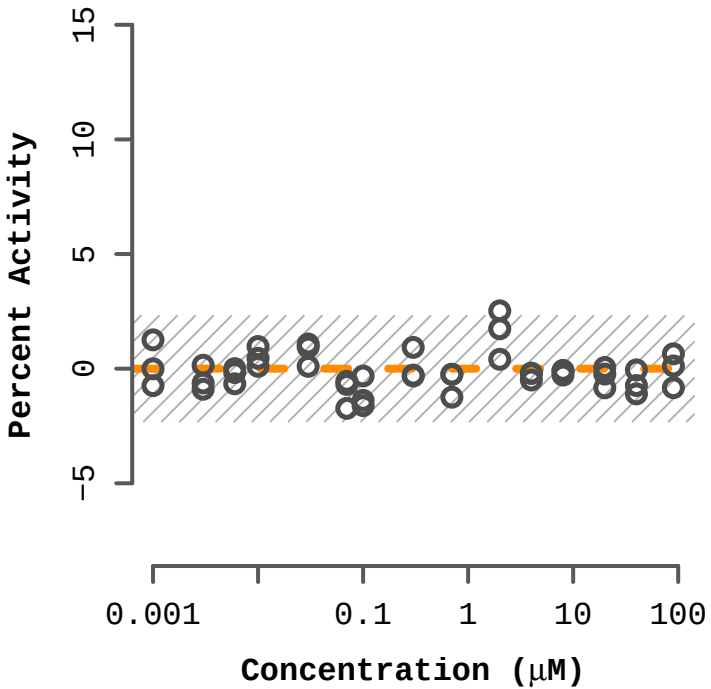
NAME: Dimethylaminoethanol
CHID: 20505 **CASRN:** 108-01-0
SPID(S): Tox21_302844
M4ID: 12476289

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

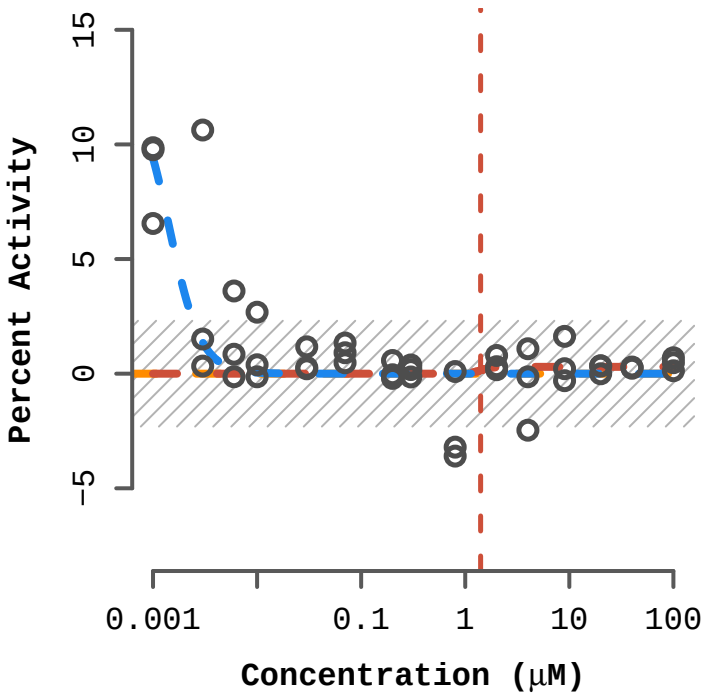
NAME: Dimethylaminoethanol
CHID: 20505 **CASRN:** 108-01-0
SPID(S): Tox21_201821
M4ID: 12480431

HILL MODEL: Not applicable.

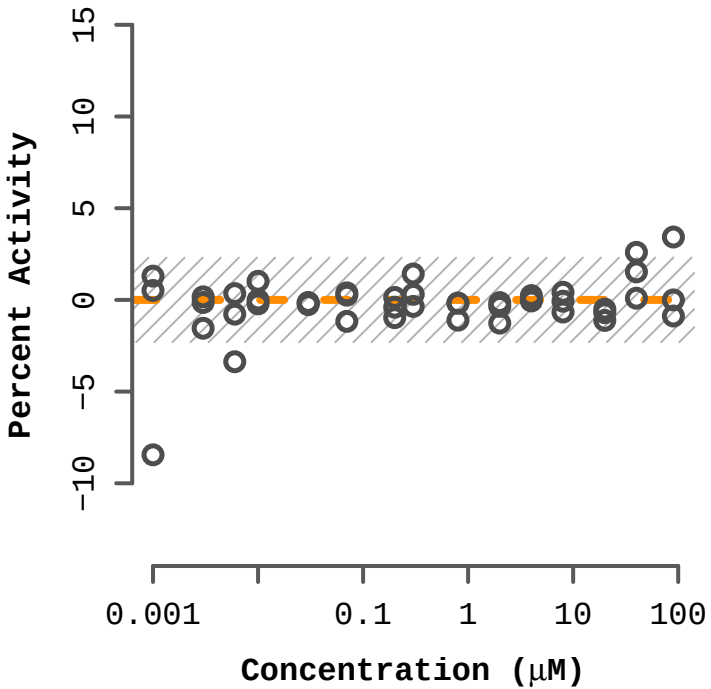
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.74 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N,N-Dimethylaniline
CHID:    20507   CASRN: 121-69-7
SPID(S): Tox21_300036
M4ID:    12479094

HILL MODEL (in red):
      tp       ga       gw
val:  0.298    0.148    8
sd:   0.258    0.498    19.7

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.8     -4.32    7.96     -2.84    2.87
sd:   5.08     30400    184000   0.171    1.27

      CNST        HILL        GNLS
AIC:  196.78      201.51      164.21
PROB: 0           0           1
RMSE: 3.03        3.02        1.85

MAX_MEAN: 8.73      MAX_MED: 9.77      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

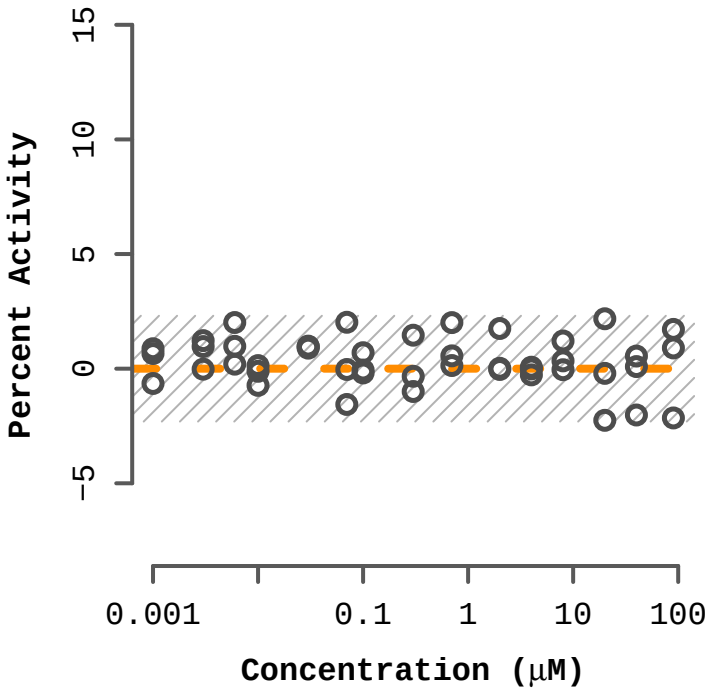
NAME: N,N−Dimethylaniline
CHID: 20507 **CASRN:** 121−69−7
SPID(S): Tox21_201813
M4ID: 12480439

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

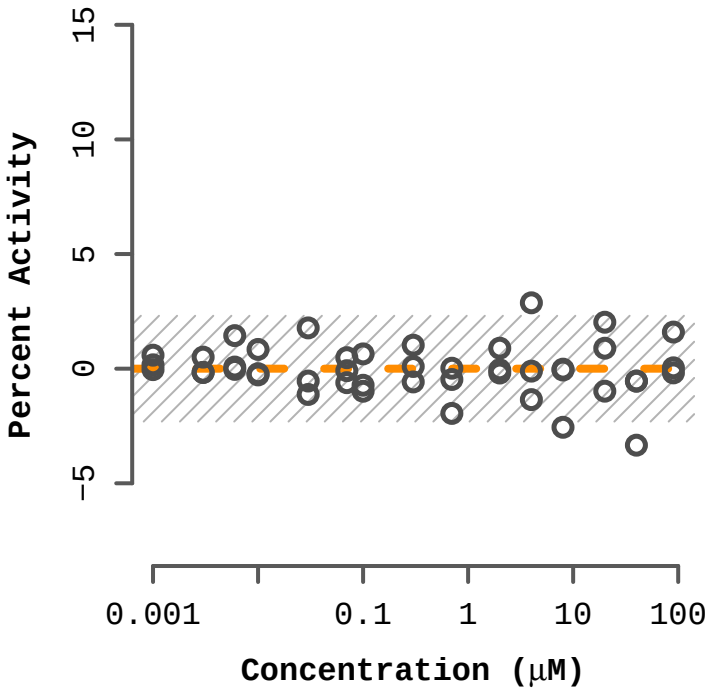
NAME: Dimethylarsinic acid
CHID: 20508 **CASRN:** 75-60-5
SPID(S): Tox21_300767
M4ID: 12478366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

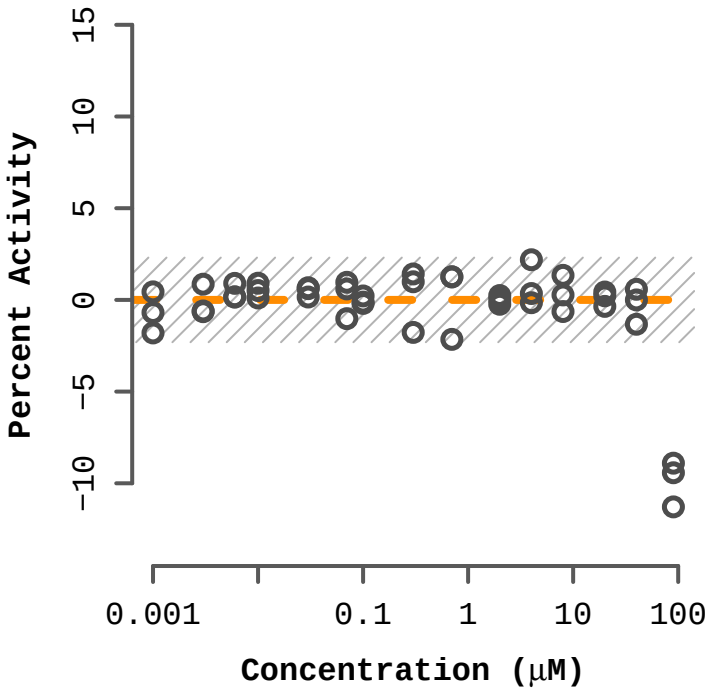
NAME: 5,5-Dimethylbarbituric acid
CHID: 20509 **CASRN:** 24448-94-0
SPID(S): Tox21_301237
M4ID: 12477896

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.647 **MAX_MED:** 0.894 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

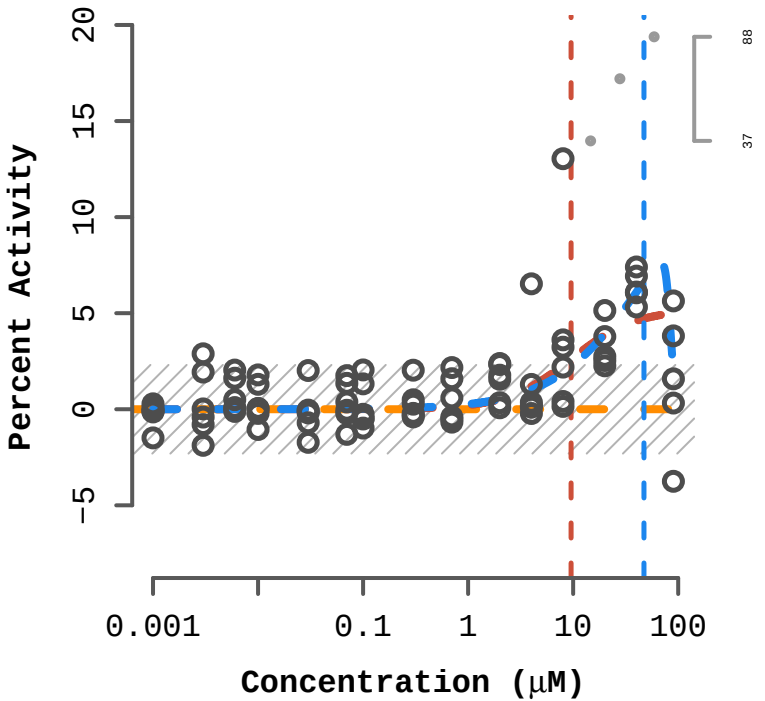
NAME: 7,12-Dimethylbenz(a)anthracene
CHID: 20510 **CASRN:** 57-97-6
SPID(S): Tox21_300500
M4ID: 12478632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 0.797 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 7,12-Dimethylbenz(a)anthracene
CHID: 20510 CASRN: 57-97-6
SPID(S): Tox21_201805
M4ID: 12480447 BRK

HILL MODEL (in red):

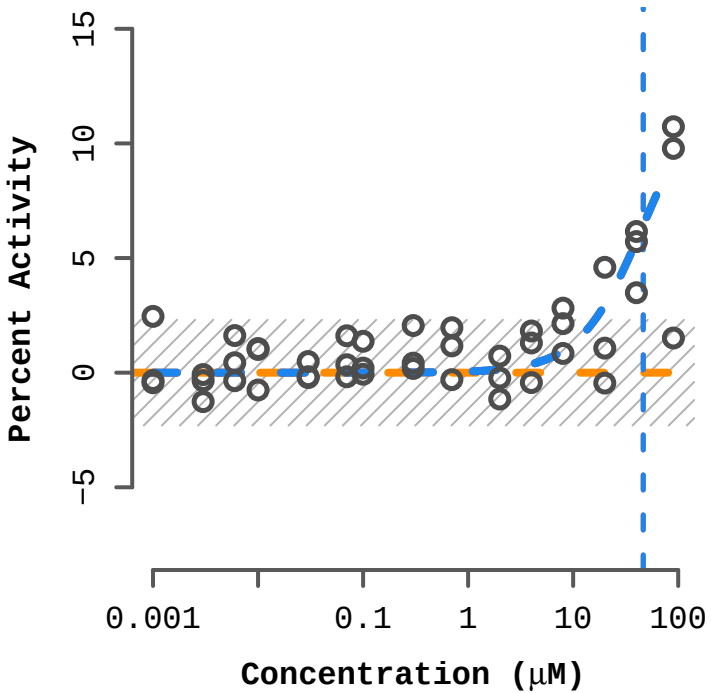
	tp	ga	gw
val:	5.22	0.98	1.4
sd:	0.986	0.174	0.671

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.3	1.67	1.01	1.92	17.6
sd:	9.04	0.531	0.299	0.0369	21.4

	CNST	HILL	GNLS
AIC:	491.55	442.32	430.45
PROB:	0	0	1
RMSE:	12.59	11.67	11.79

MAX_MEAN: 16.5 MAX_MED: 6.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−Dimethylbenzidine dihydrochloride
CHID: 20511 CASRN: 612−82−8
SPID(S): Tox21_302798
M4ID: 12476335

HILL MODEL (in red):

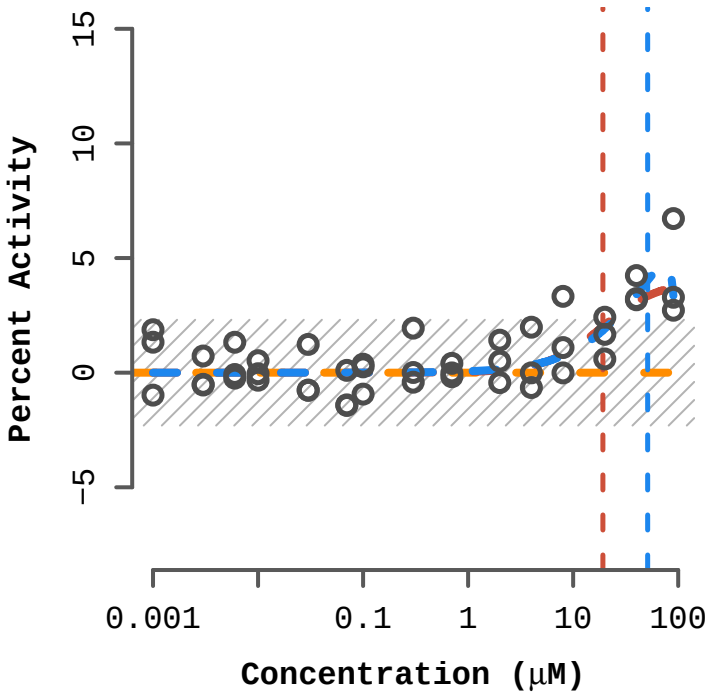
	tp	ga	gw
val:	12.9	1.67	1.44
sd:	3.13	0.159	0.624

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.9	1.67	1.44	2.85	14.6
sd:	3.13	0.159	0.623	48400	862000

	CNST	HILL	GNLS
AIC:	202.95	166.58	170.58
PROB:	0	0.88	0.12
RMSE:	2.86	1.66	1.66

MAX_MEAN: 7.34 **MAX_MED:** 9.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−Dimethylbenzidine dihydrochloride
CHID: 20511 CASRN: 612−82−8
SPID(S): Tox21_202196
M4ID: 12480056

HILL MODEL (in red):

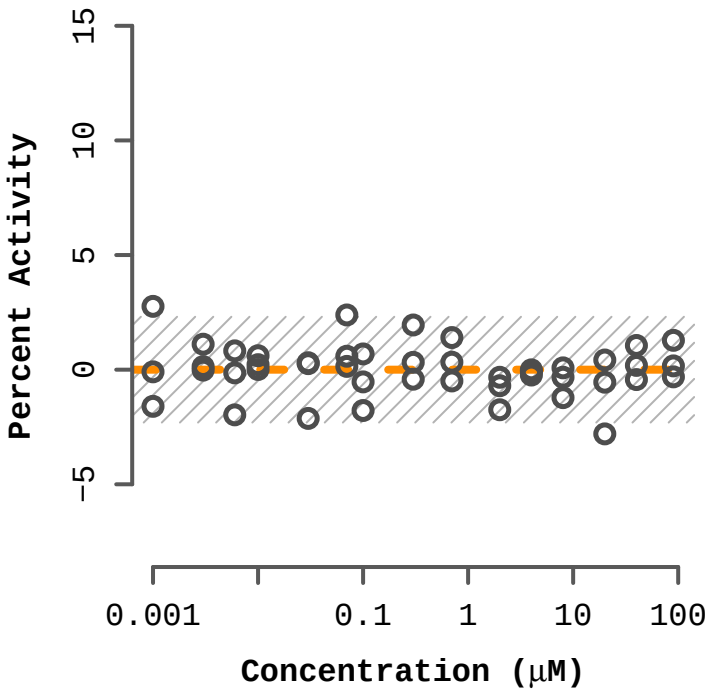
	tp	ga	gw
val:	4.03	1.28	1.61
sd:	1.09	0.199	1.03

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.03	1.71	1.23	1.97	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	177.12	139.1	141.52
PROB:	0	0.77	0.23
RMSE:	1.84	1.04	1.05

MAX_MEAN: 4.25 MAX_MED: 3.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

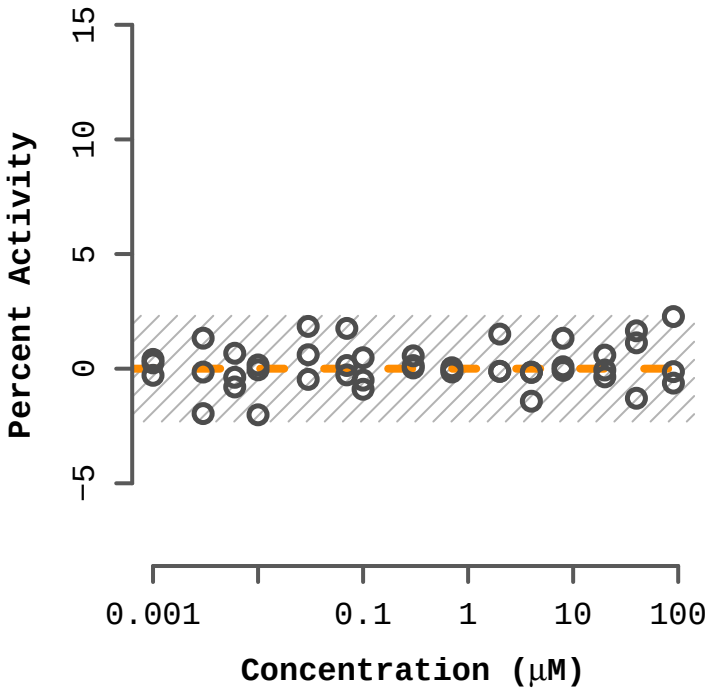
NAME: Dimethylcarbamoyl chloride
CHID: 20512 CASRN: 79-44-7
SPID(S): Tox21_300116
M4ID: 12479014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.587 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

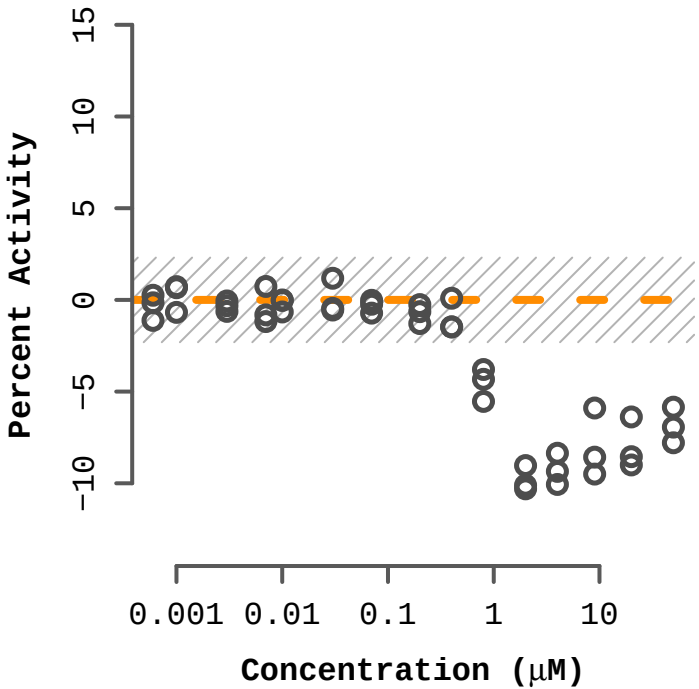
NAME: Dimethylcarbamoyl chloride
CHID: 20512 **CASRN:** 79-44-7
SPID(S): Tox21_201334
M4ID: 12480918

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.663 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

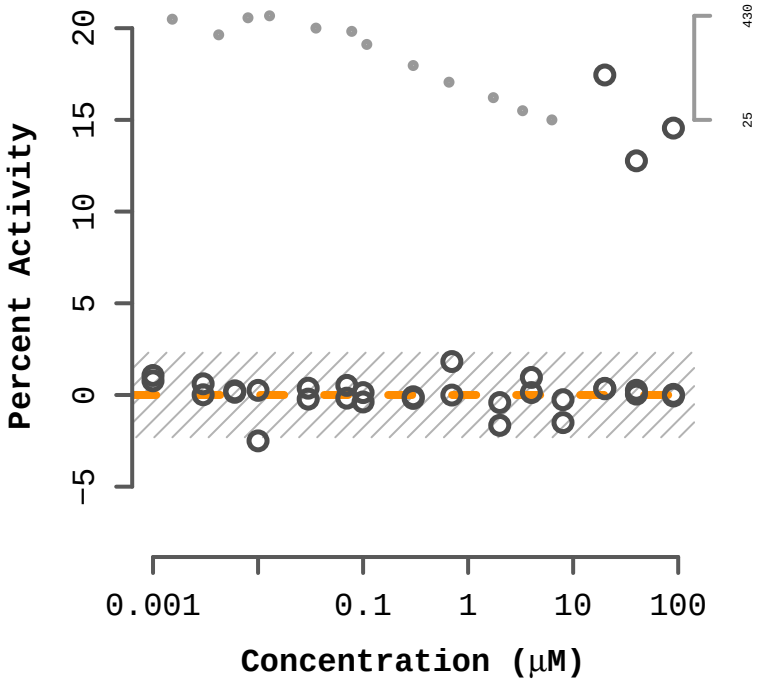
NAME: Dimethyldithiocarbamic acid, dimethylamine
CHID: 20513 **CASRN:** 598-64-1
SPID(S): Tox21_202587
M4ID: 12479665

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	275.94	NA	NA
PROB:	1	NA	NA
RMSE:	5.08	NA	NA

MAX_MEAN: 0.237 **MAX_MED:** 0.664 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

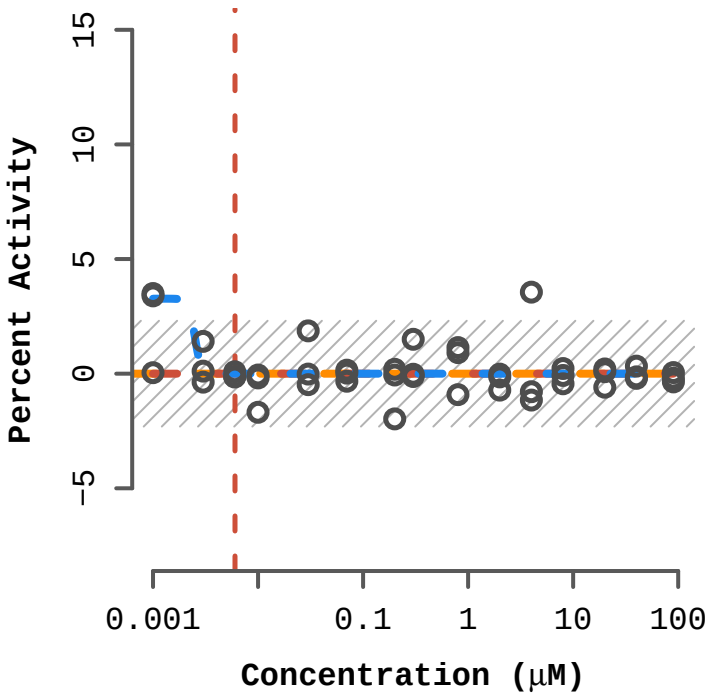
NAME: N,N−Dimethylformamide
CHID: 20515 **CASRN:** 68−12−2
SPID(S): Tox21_300039
M4ID: 12479091 **BRK**

HILL MODEL: Not applicable.

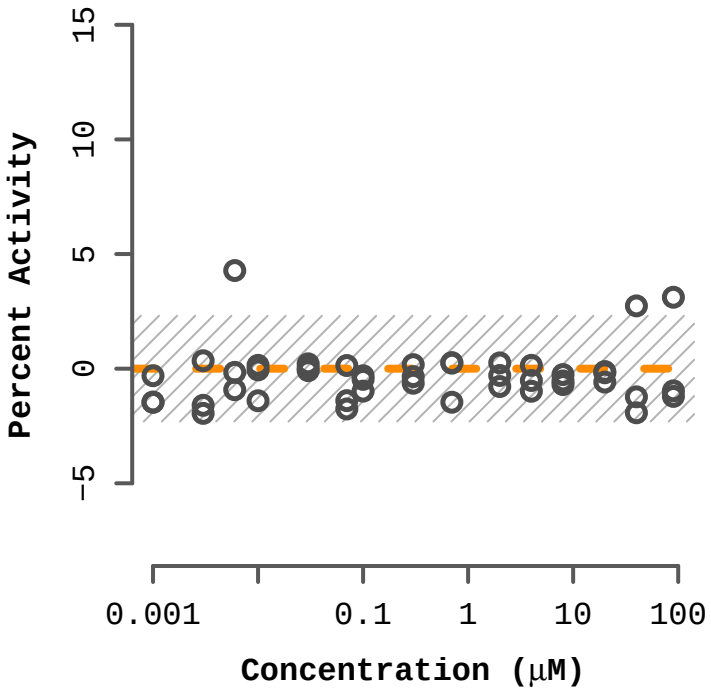
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	606.24	NA	NA
PROB:	1	NA	NA
RMSE:	158.96	NA	NA

MAX_MEAN: 142 **MAX_MED:** 1.83 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N,N-Dimethylformamide
CHID:    20515   CASRN: 68-12-2
SPID(S): Tox21_201259
M4ID:    12480993

HILL MODEL (in red):
      tp        ga        gw
val:  2.35e-10 -2.22     0.514
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.27      -3.47     7.33      -2.6      14.5
sd:   NaN       NaN       NaN       NaN       NaN

      CNST         HILL         GNLS
AIC:  124.89       130.89       122.94
PROB: 0.27         0.01         0.72
RMSE: 1.13         1.13         0.99

MAX_MEAN: 2.31      MAX_MED: 3.39      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

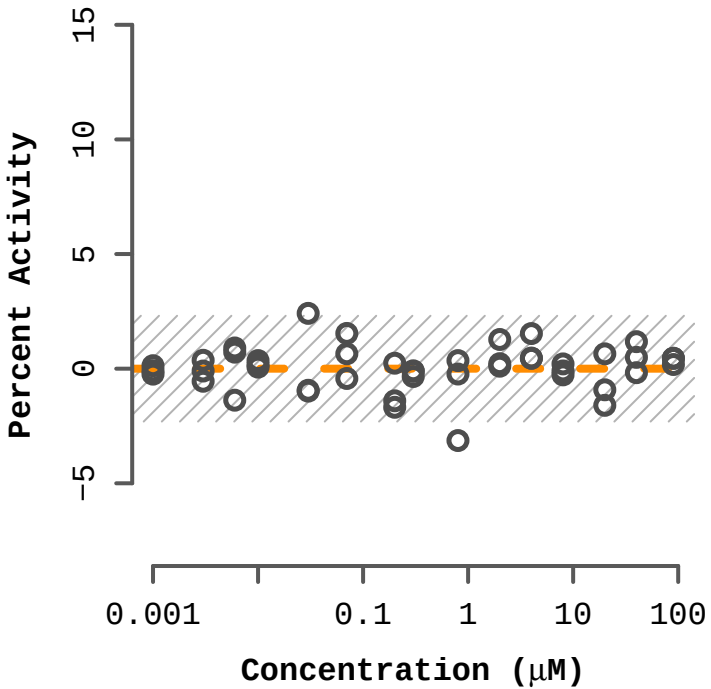
NAME: 1,1−Dimethylhydrazine
CHID: 20516 **CASRN:** 57−14−7
SPID(S): Tox21_302358
M4ID: 12476775

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.242 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

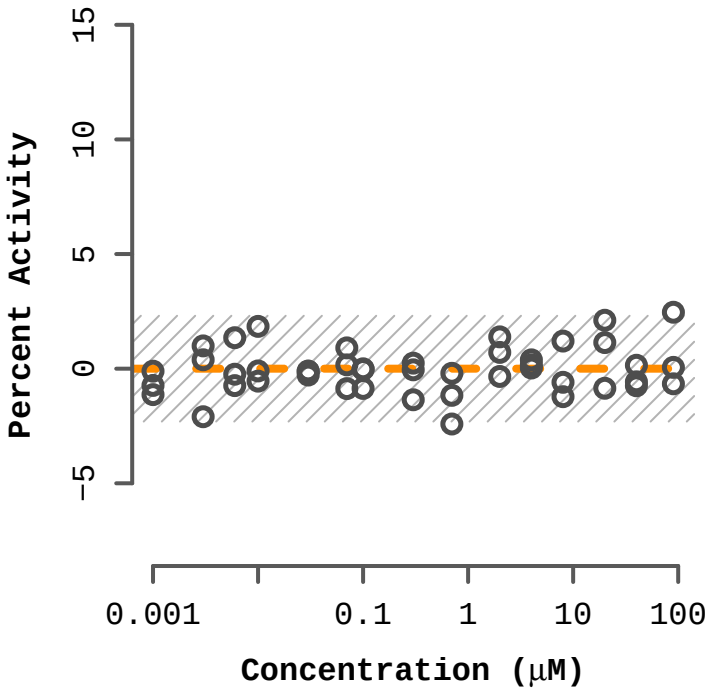
NAME: 1,2−Dimethylhydrazine dihydrochloride
CHID: 20517 **CASRN:** 306−37−6
SPID(S): Tox21_201194
M4ID: 12481058

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.816 **MAX_MED:** 0.721 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

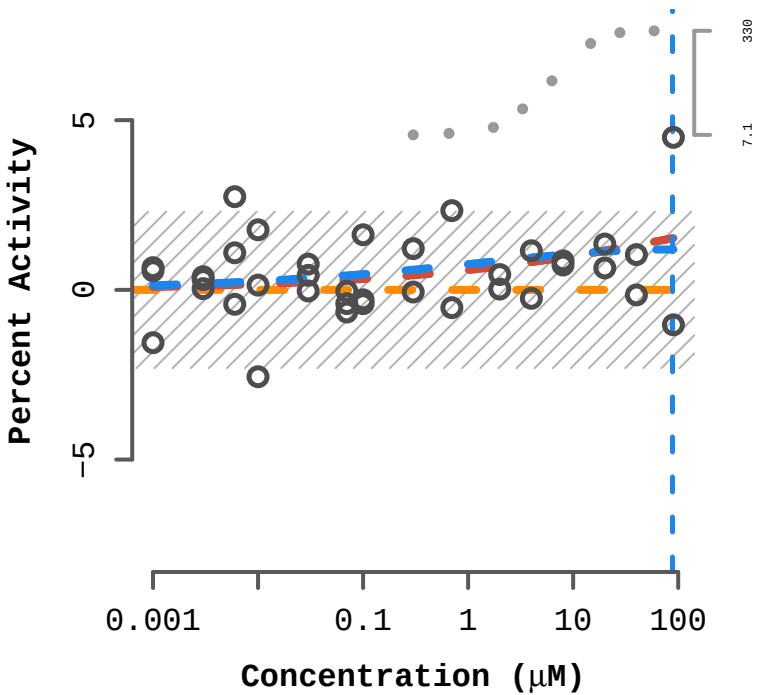
NAME: 2,2−Dimethylvinyl chloride
CHID: 20520 **CASRN:** 513−37−1
SPID(S): Tox21_302858
M4ID: 12476275

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.1	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.8 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2-Dimethylvinyl chloride
CHID: 20520 **CASRN:** 513-37-1
SPID(S): Tox21_201770
M4ID: 12480482 **BRK**

HILL MODEL (in red):

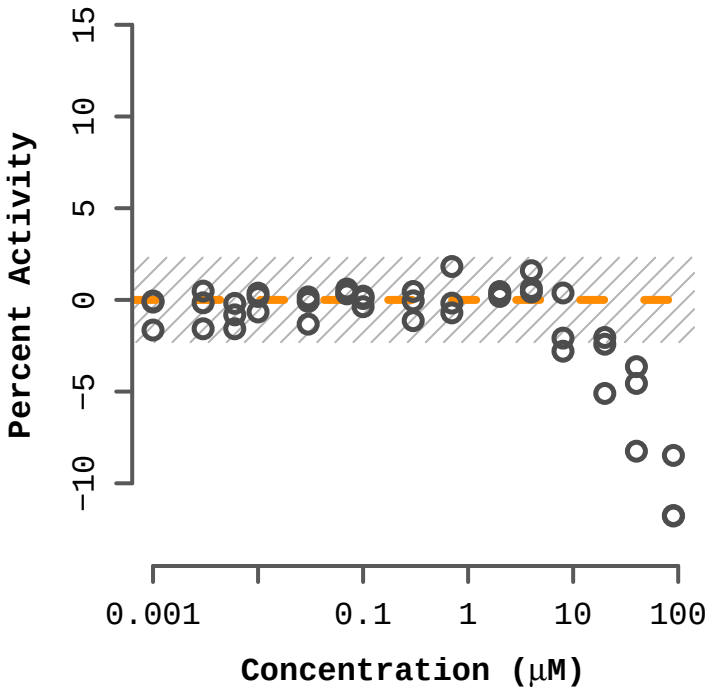
	tp	ga	gw
val:	3.48	2.32	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.35	1.95	0.3	2.2	0.33
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	404.47	408.03	411.79
PROB:	0.84	0.14	0.02
RMSE:	86.33	85.93	85.97

MAX_MEAN: 111 **MAX_MED:** 4.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

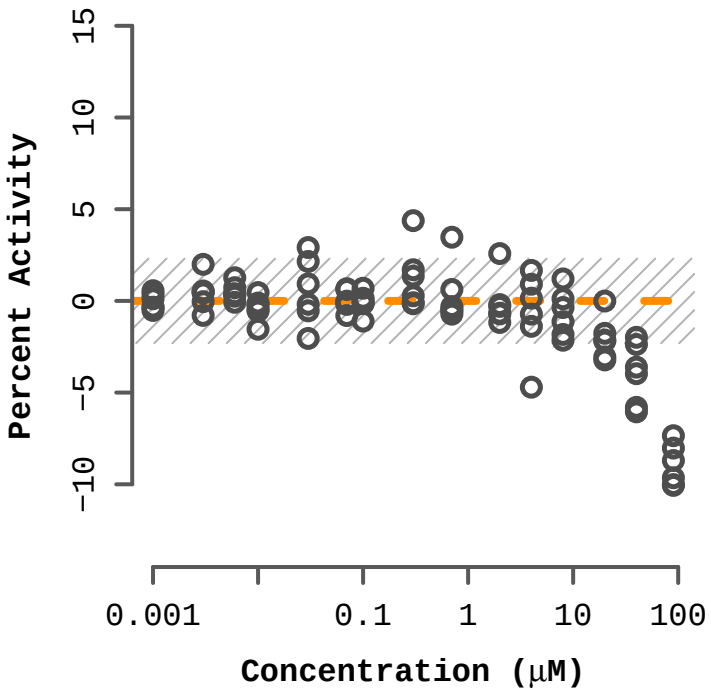
NAME: 2,4-Dinitrophenol
CHID: 20523 **CASRN:** 51-28-5
SPID(S): Tox21_300030
M4ID: 12479100

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.63	NA	NA
PROB:	1	NA	NA
RMSE:	3.4	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 0.626 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

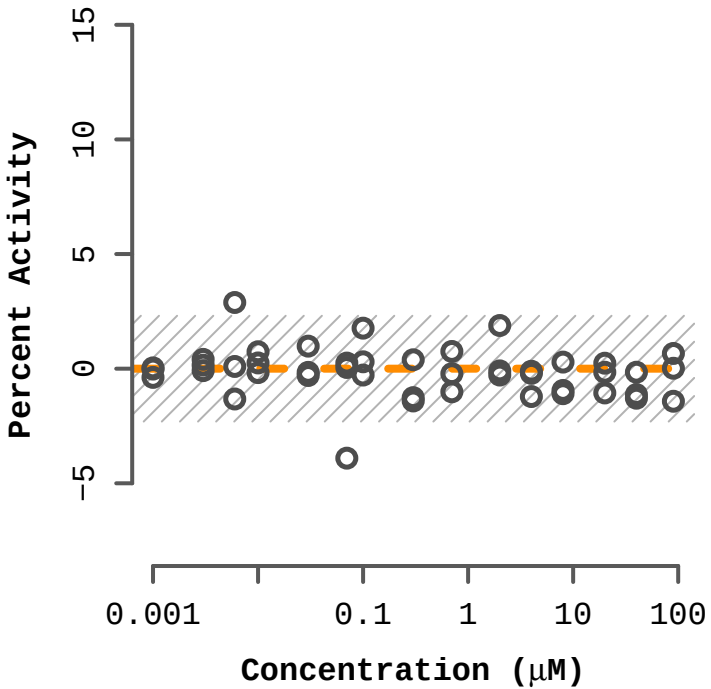
NAME: 2,4-Dinitrophenol
CHID: 20523 **CASRN:** 51-28-5
SPID(S): Tox21_201462
M4ID: 12480790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	410.1	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.816 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

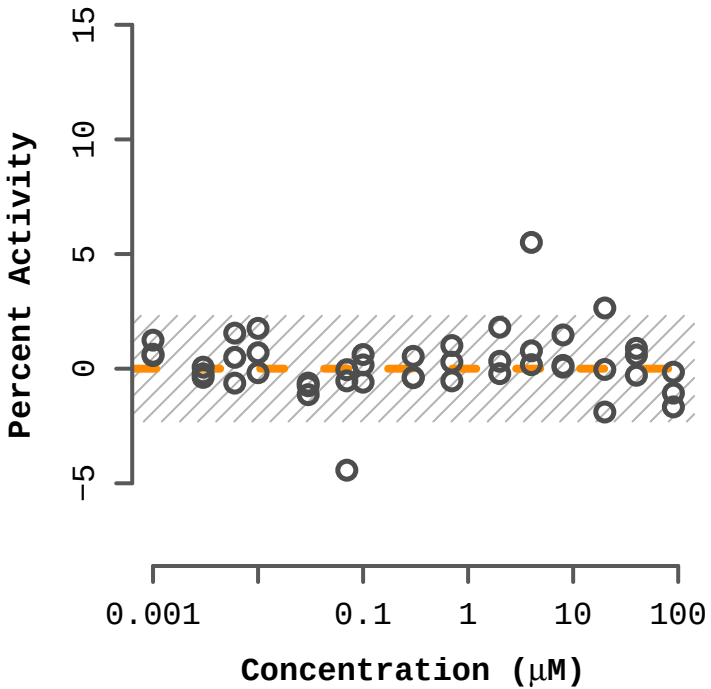
NAME: Dinitrosopiperazine
CHID: 20527 CASRN: 140-79-4
SPID(S): Tox21_202782
M4ID: 12479470

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.598 **MAX_MED:** 0.302 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

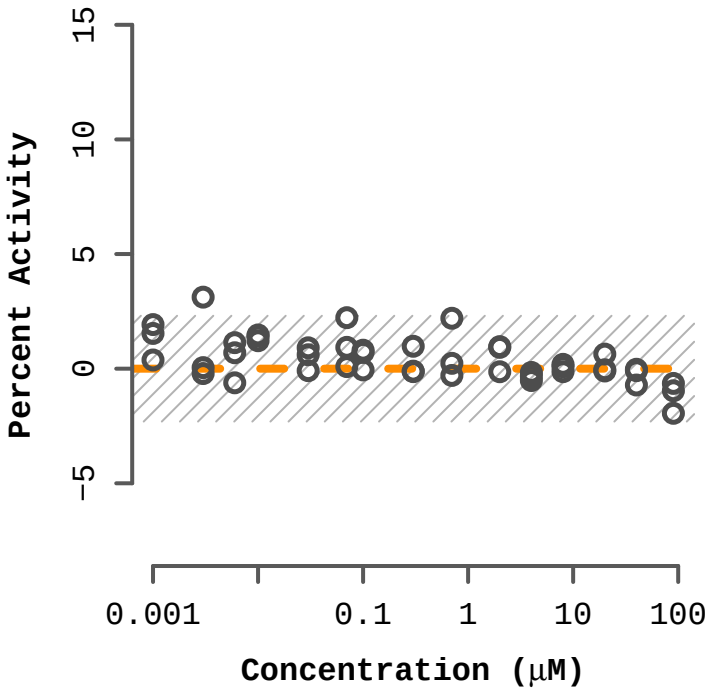
NAME: 2,6-Dinitrotoluene
CHID: 20528 **CASRN:** 606-20-2
SPID(S): Tox21_300479
M4ID: 12478653

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 0.779 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

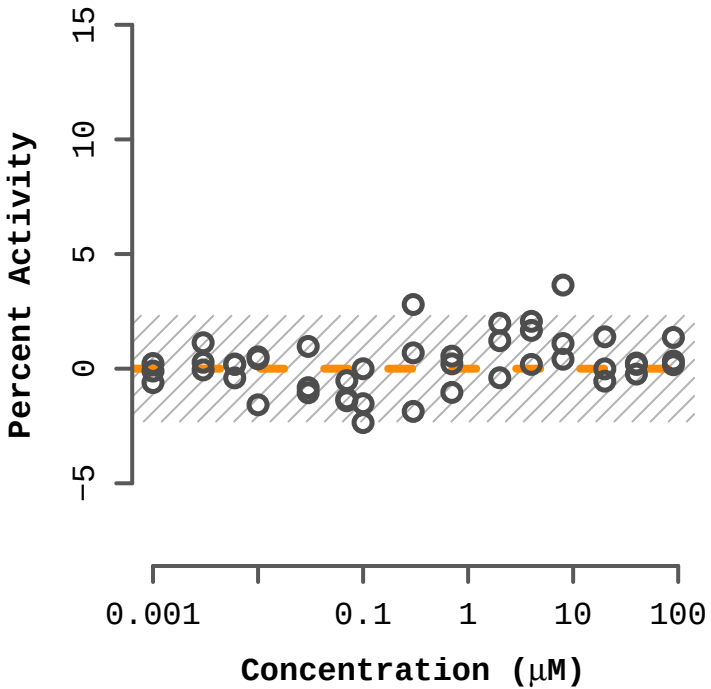
NAME: 2,6-Dinitrotoluene
CHID: 20528 **CASRN:** 606-20-2
SPID(S): Tox21_201855
M4ID: 12480397

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

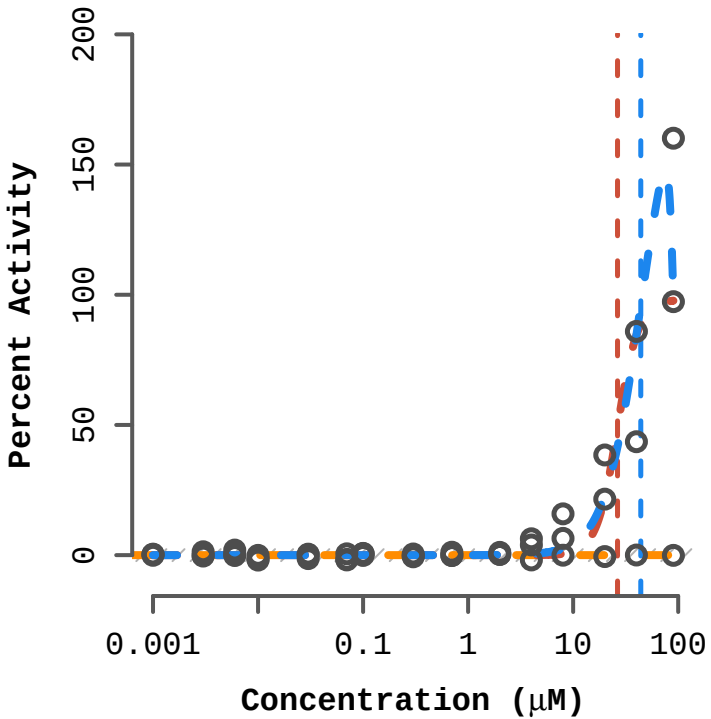
NAME: 2,4-Dinitrotoluene
CHID: 20529 **CASRN:** 121-14-2
SPID(S): Tox21_300493
M4ID: 12478639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-Dinitrotoluene
CHID: 20529 CASRN: 121-14-2
SPID(S): Tox21_201784
M4ID: 12480468

HILL MODEL (in red):

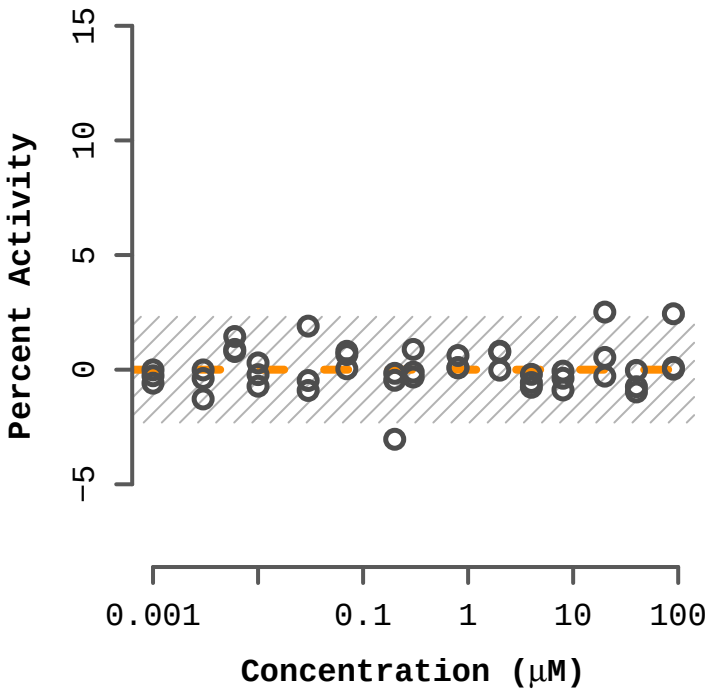
	tp	ga	gw
val:	98.2	1.42	4.39
sd:	2.64	0.0165	0.51

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	192	1.64	2.52	1.96	17.2
sd:	13.1	0.0203	0.231	0.00525	8.18

	CNST	HILL	GNLS
AIC:	351.69	339.58	341.07
PROB:	0	0.68	0.32
RMSE:	32.22	22.8	22.77

MAX_MEAN: 85.8 MAX_MED: 97.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

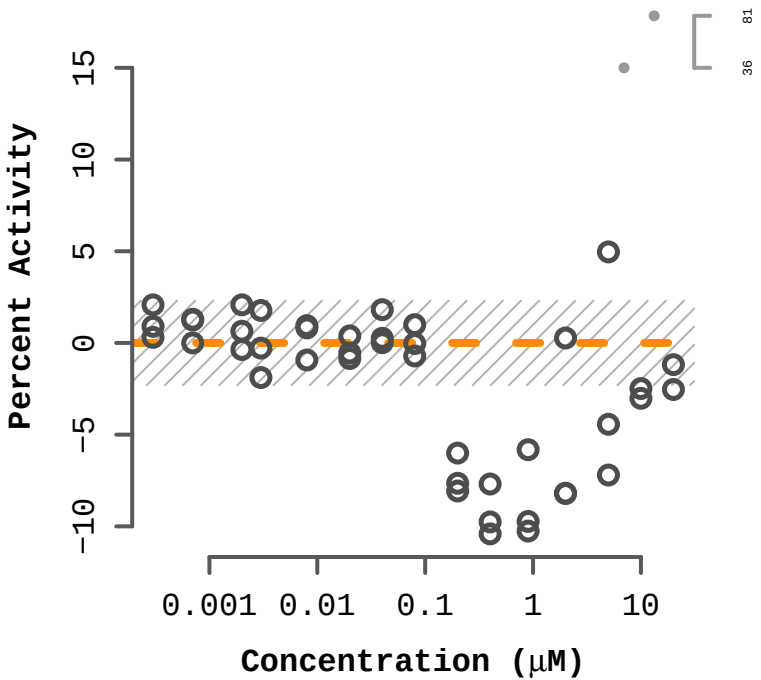
NAME: 1,4-Dioxane
CHID: 20533 **CASRN:** 123-91-1
SPID(S): Tox21_200971
M4ID: 12481281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.885 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

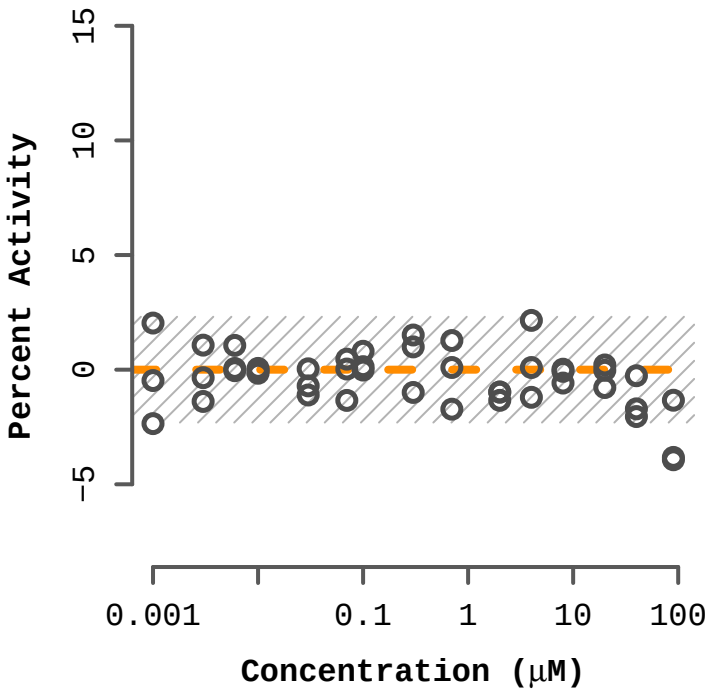
NAME: Bis(1-piperidinylthioxomethyl)hexasulfide
CHID: 20535 **CASRN:** 971-15-3
SPID(S): Tox21_202783
M4ID: 12479469 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.87	NA	NA
PROB:	1	NA	NA
RMSE:	14.02	NA	NA

MAX_MEAN: 25.8 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

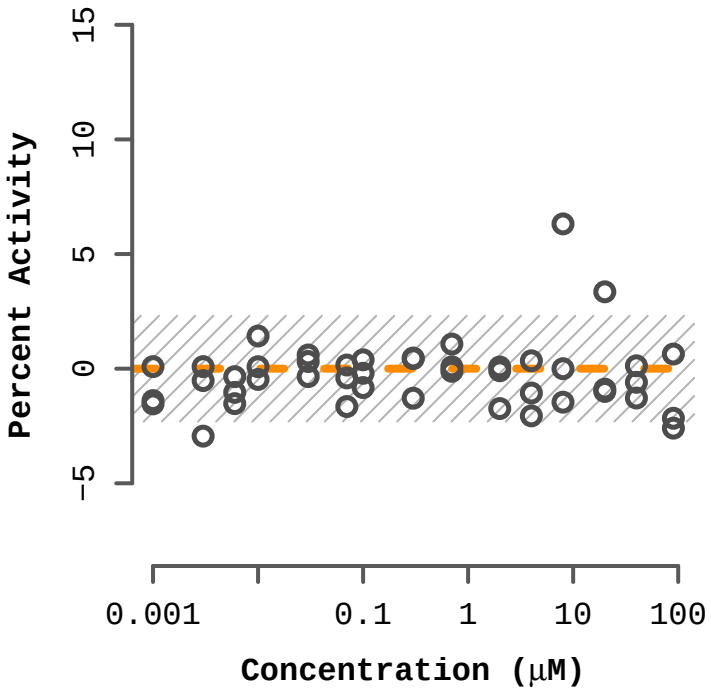
NAME: Diphenhydramine hydrochloride
CHID: 20537 CASRN: 147-24-0
SPID(S): Tox21_300611
M4ID: 12478522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.506 **MAX_MED:** 0.994 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

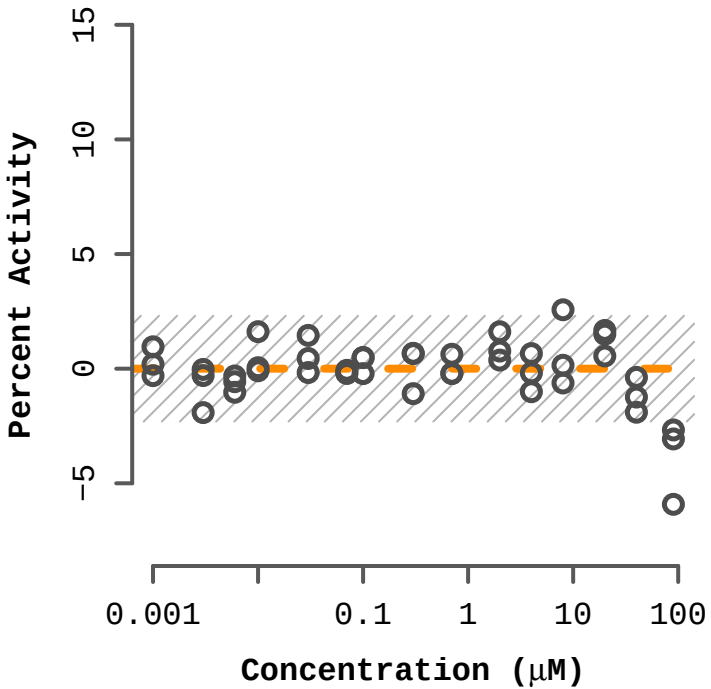
NAME: Diphenhydramine hydrochloride
CHID: 20537 CASRN: 147-24-0
SPID(S): Tox21_201472
M4ID: 12480780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 0.437 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

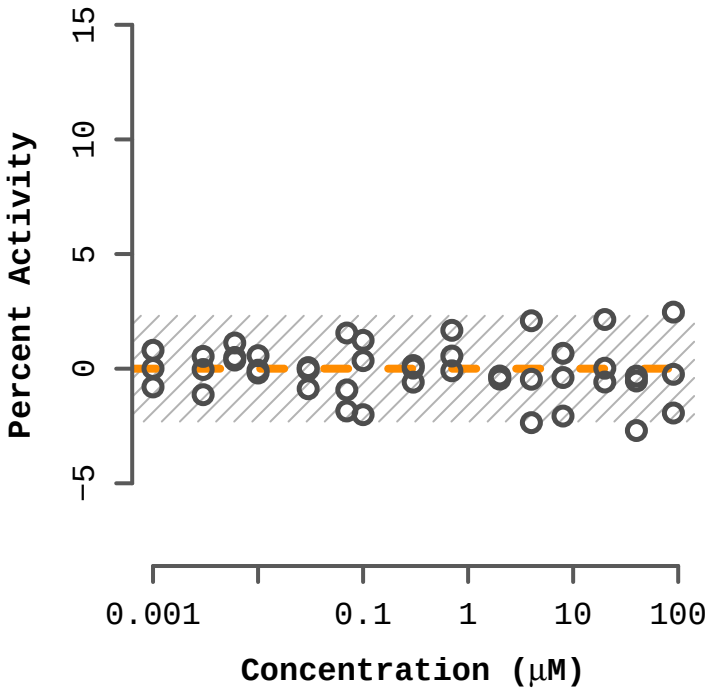
NAME: N,N'−Diphenyl−p−phenylenediamine
CHID: 20538 **CASRN:** 74−31−7
SPID(S): Tox21_200354
M4ID: 12481898

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

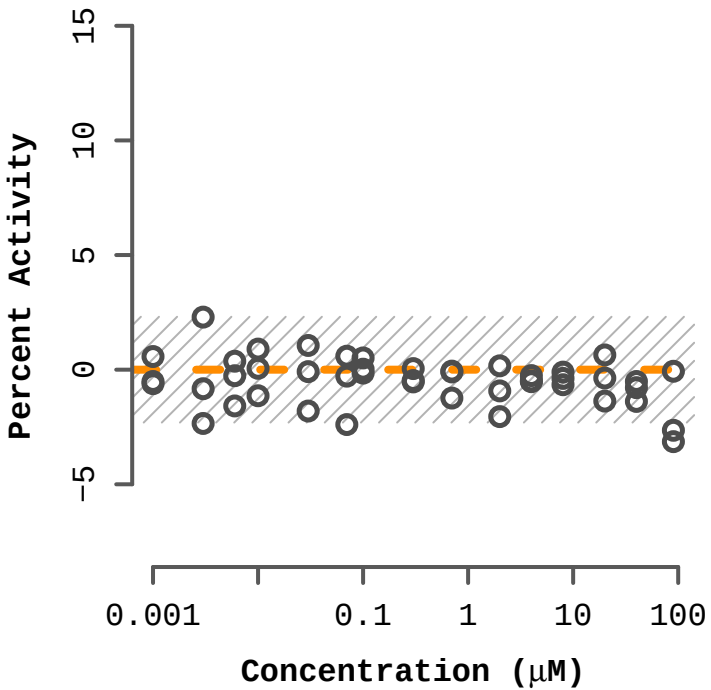
NAME: Diphenylacetonitrile
CHID: 20539 **CASRN:** 86-29-3
SPID(S): Tox21_302854
M4ID: 12476279

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.712 **MAX_MED:** 0.553 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

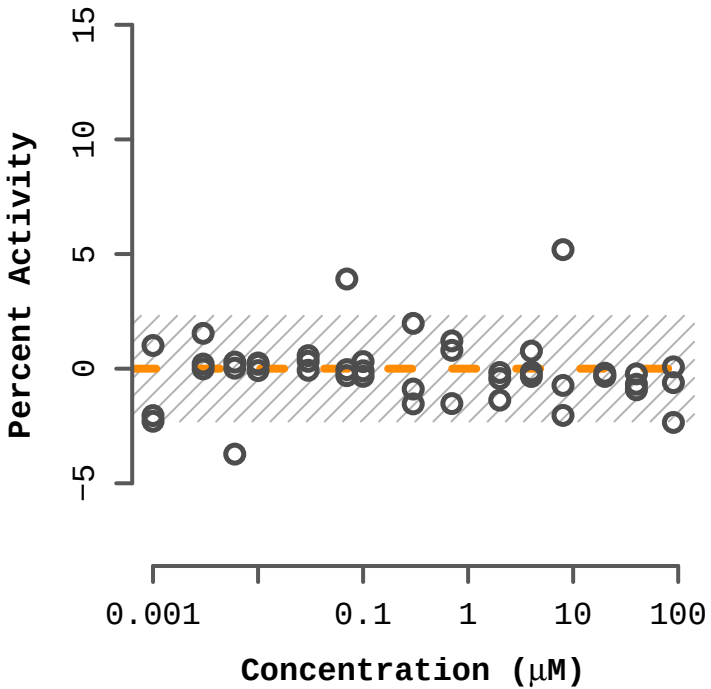
NAME: Diphenylacetonitrile
CHID: 20539 CASRN: 86-29-3
SPID(S): Tox21_201556
M4ID: 12480696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.129 MAX_MED: 0.0612 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

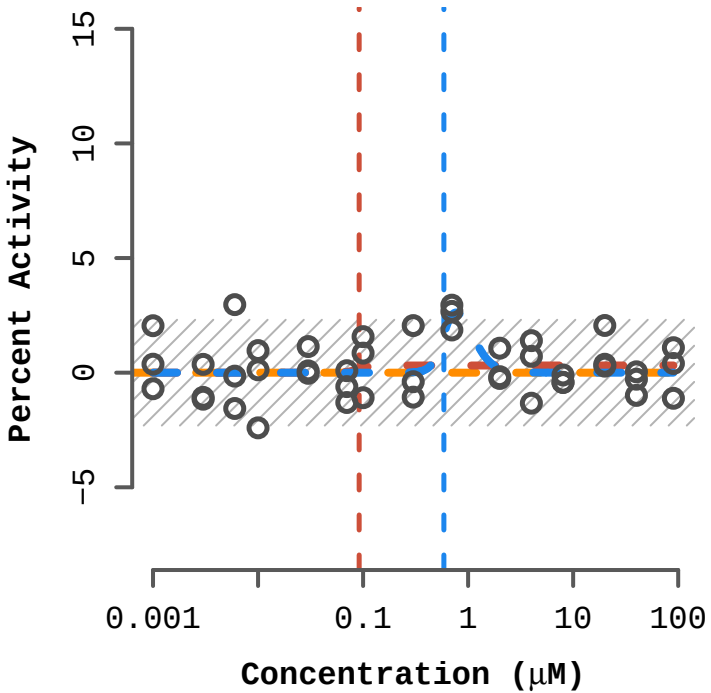
NAME: Diphenylcarbonate
CHID: 20540 **CASRN:** 102-09-0
SPID(S): Tox21_200150
M4ID: 12482102

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5,5−Diphenylhydantoin
CHID: 20541 CASRN: 57−41−0
SPID(S): Tox21_300281
M4ID: 12478849

HILL MODEL (in red):

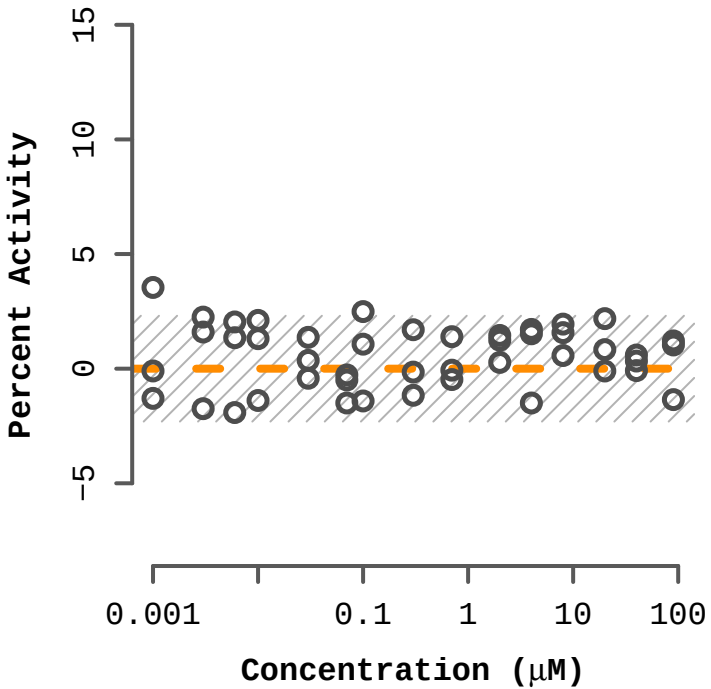
	tp	ga	gw
val:	0.312	−1.04	8
sd:	0.257	0.277	23.9

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.56	−0.231	8	0.0287	4.66
sd:	11.3	0.585	18.7	1.33	21.8

	CNST	HILL	GNLS
AIC:	152.63	157.01	148.51
PROB:	0.11	0.01	0.88
RMSE:	1.27	1.23	1.09

MAX_MEAN: 2.5 **MAX_MED:** 2.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

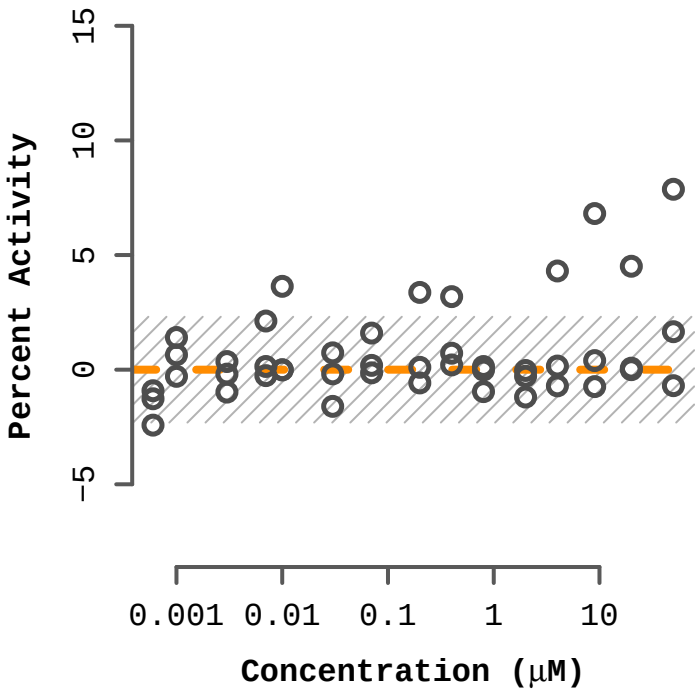
NAME: 5,5-Diphenylhydantoin
CHID: 20541 **CASRN:** 57-41-0
SPID(S): Tox21_202299
M4ID: 12479953

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

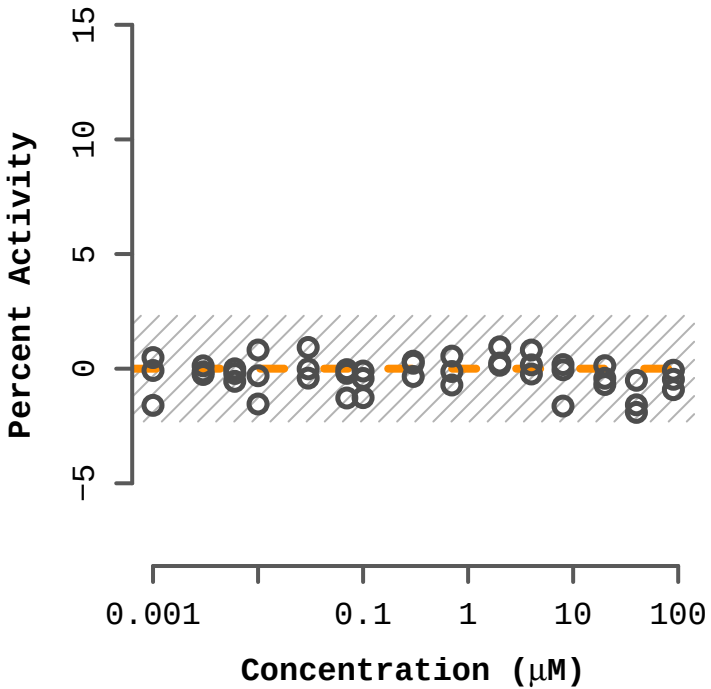
NAME: 5,5-Diphenylhydantoin
CHID: 20541 **CASRN:** 57-41-0
SPID(S): Tox21_110861_1
M4ID: 12484061

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 2.94 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

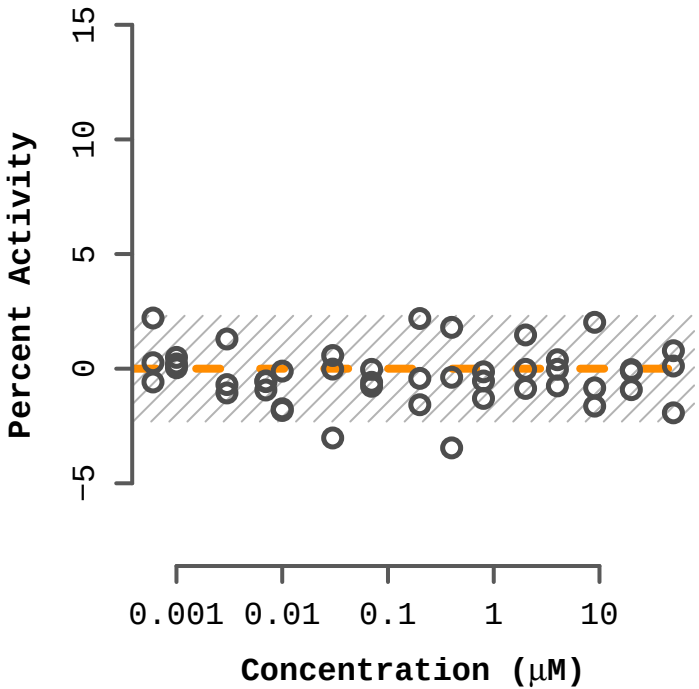
NAME: Dipyrone
CHID: 20543 CASRN: 68-89-3
SPID(S): Tox21_200497
M4ID: 12481755

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.451 **MAX_MED:** 0.248 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

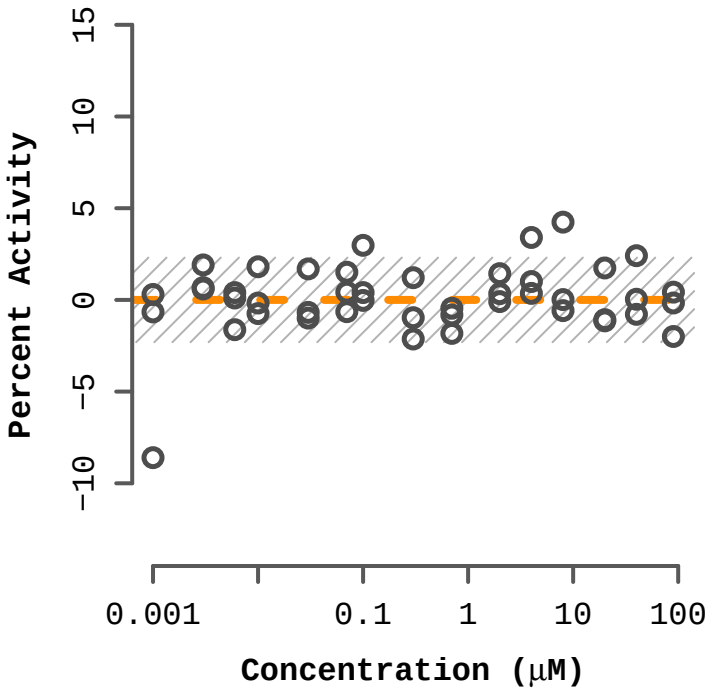
NAME: Dipyrone
CHID: 20543 CASRN: 68-89-3
SPID(S): Tox21_110759_1
M4ID: 12484130

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.632 **MAX_MED:** 0.262 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

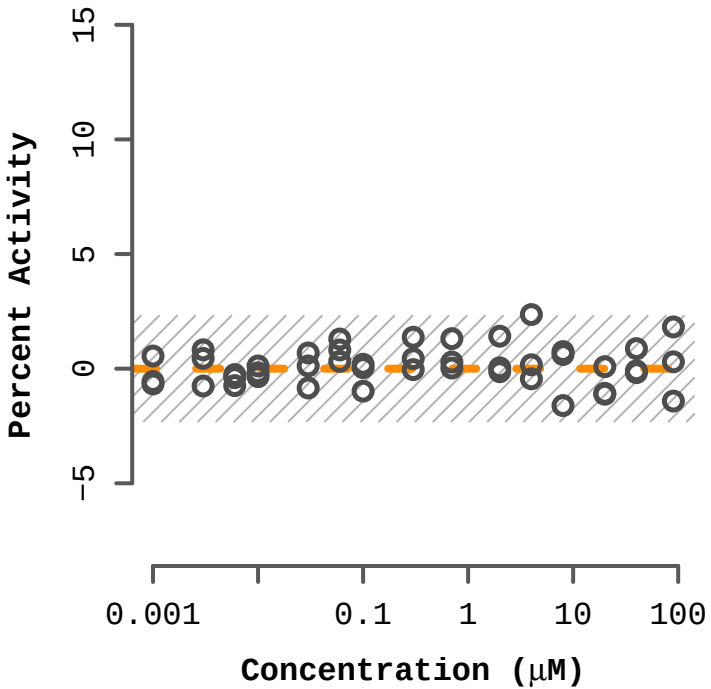
NAME: 2,5-Dithiobiurea
CHID: 20545 **CASRN:** 142-46-1
SPID(S): Tox21_303027
M4ID: 12476106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

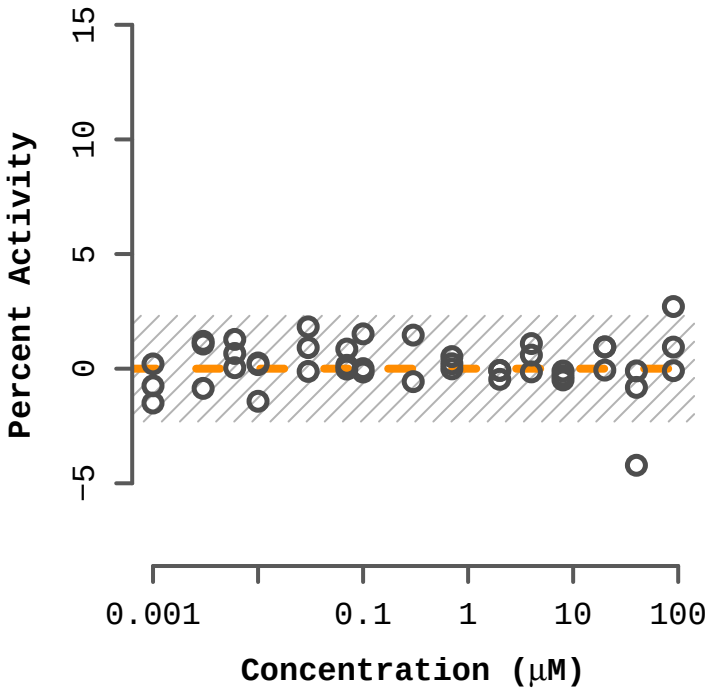
NAME: 2,5−Dithiobiurea
CHID: 20545 CASRN: 142−46−1
SPID(S): Tox21_202355
M4ID: 12479897

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.81 MAX_MED: 0.818 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

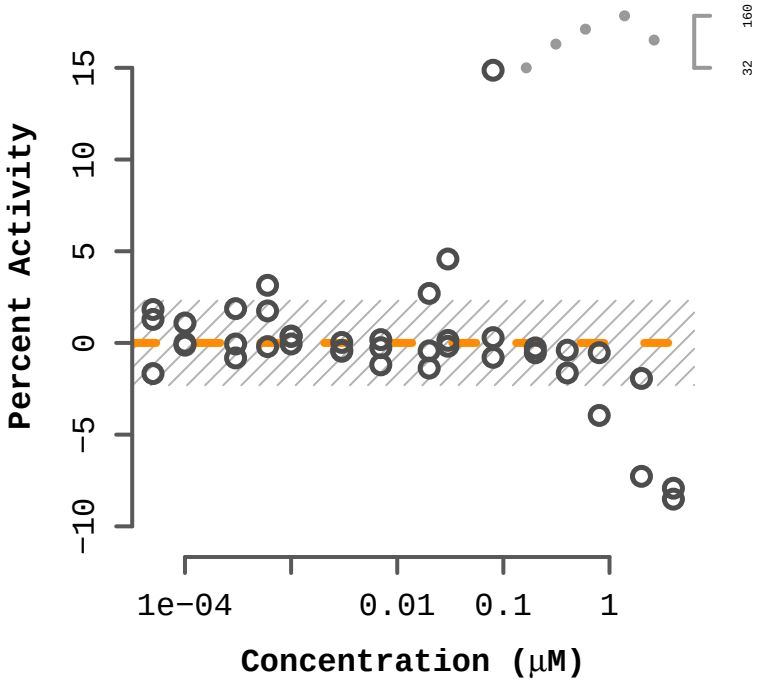
NAME: Dithiooxamide
CHID: 20546 CASRN: 79-40-3
SPID(S): Tox21_200767
M4ID: 12481485

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.19 MAX_MED: 1.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

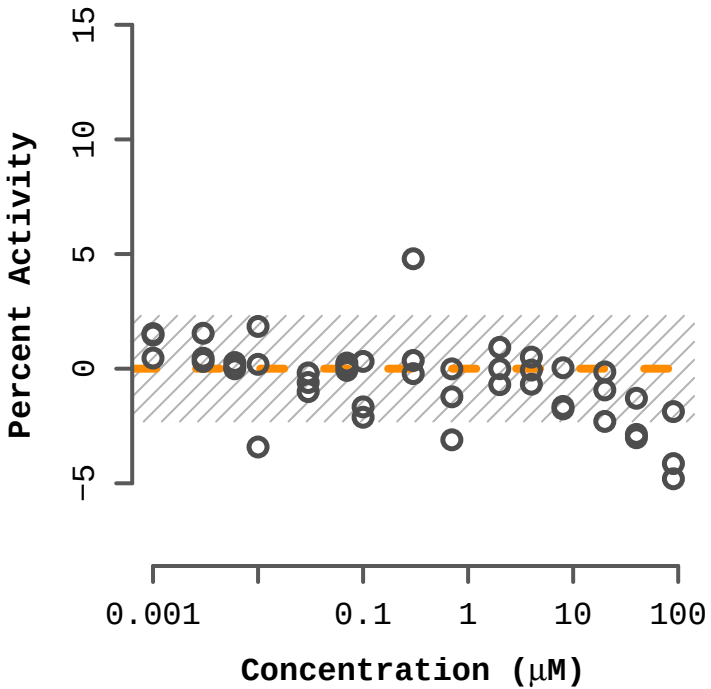
NAME: Dodine
CHID: 20548 **CASRN:** 2439-10-3
SPID(S): Tox21_202731
M4ID: 12479521 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	360.71	NA	NA
PROB:	1	NA	NA
RMSE:	38.02	NA	NA

MAX_MEAN: 51.8 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

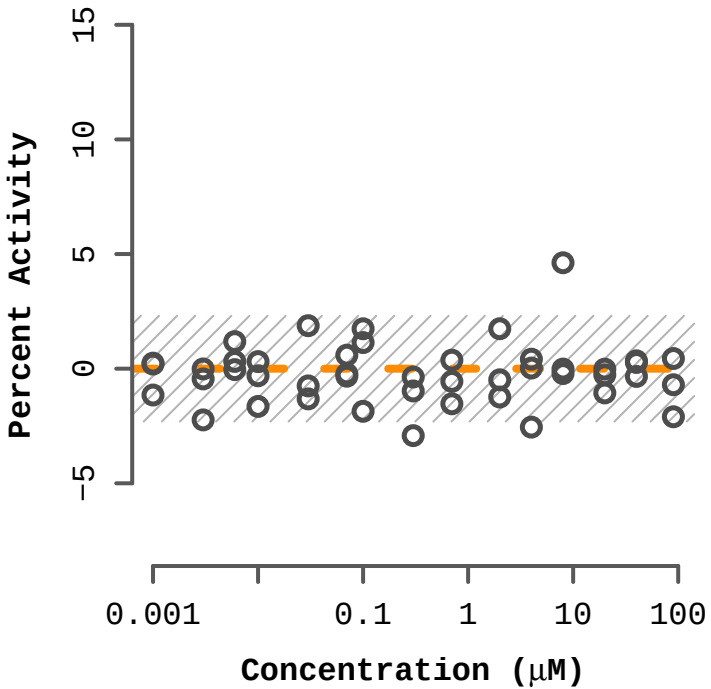
NAME: Dopamine hydrochloride
CHID: 20550 CASRN: 62-31-7
SPID(S): Tox21_201018
M4ID: 12481234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.78	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

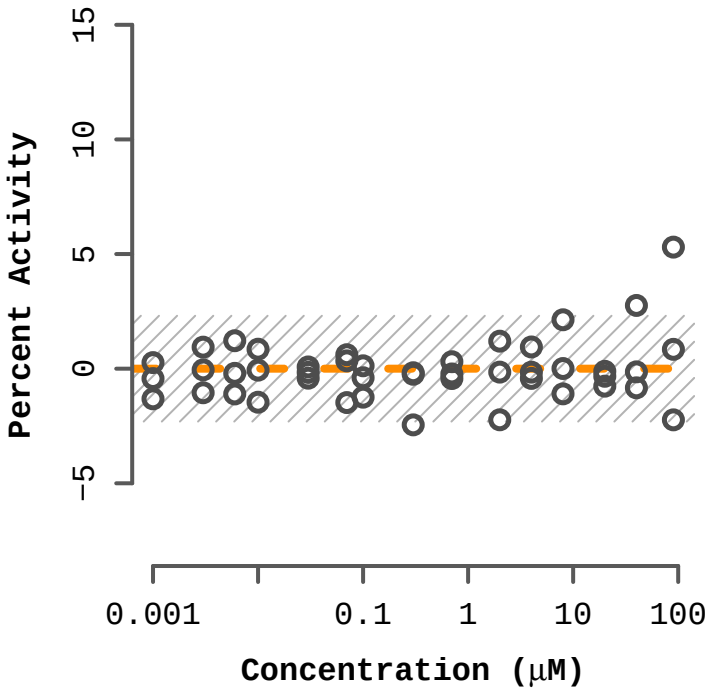
NAME: Doxylamine succinate
CHID: 20552 CASRN: 562-10-7
SPID(S): Tox21_302861
M4ID: 12476272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

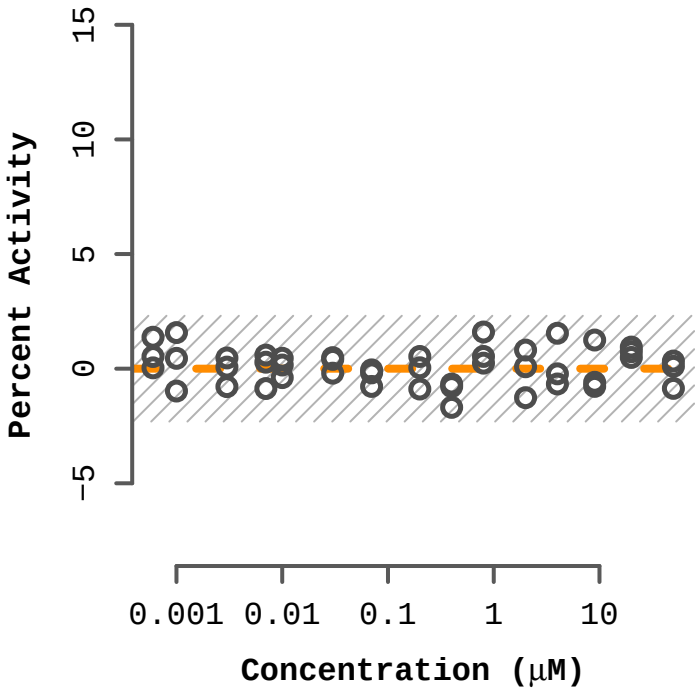
NAME: Doxylamine succinate
CHID: 20552 CASRN: 562-10-7
SPID(S): Tox21_202078
M4ID: 12480174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.31 MAX_MED: 0.844 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

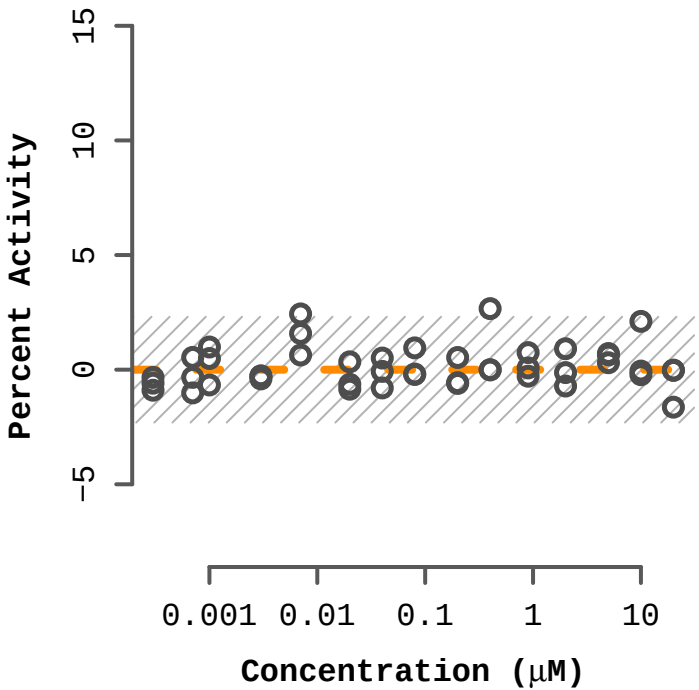
NAME: Doxylamine succinate
CHID: 20552 **CASRN:** 562-10-7
SPID(S): Tox21_113515_1
M4ID: 12482623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 0.741 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

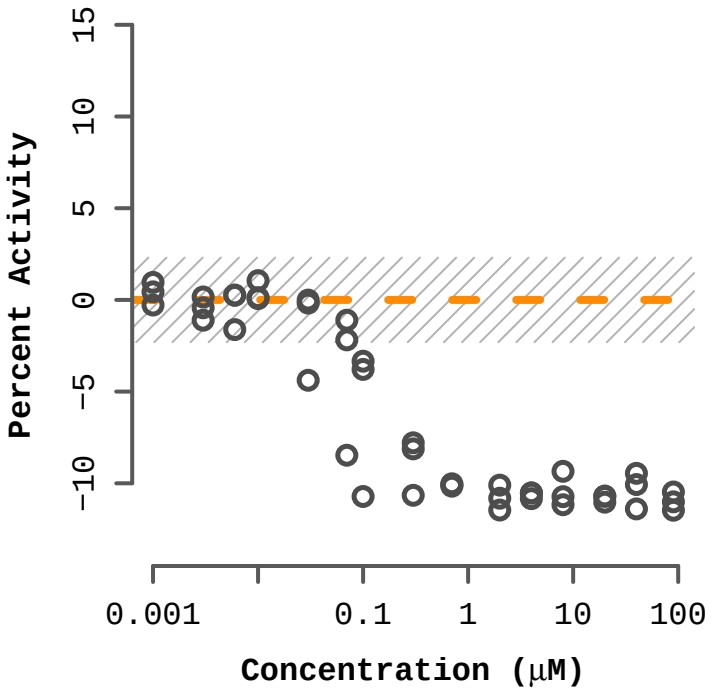
NAME: Ellagic acid
CHID: 20557 **CASRN:** 476-66-4
SPID(S): Tox21_110805_1
M4ID: 12484104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

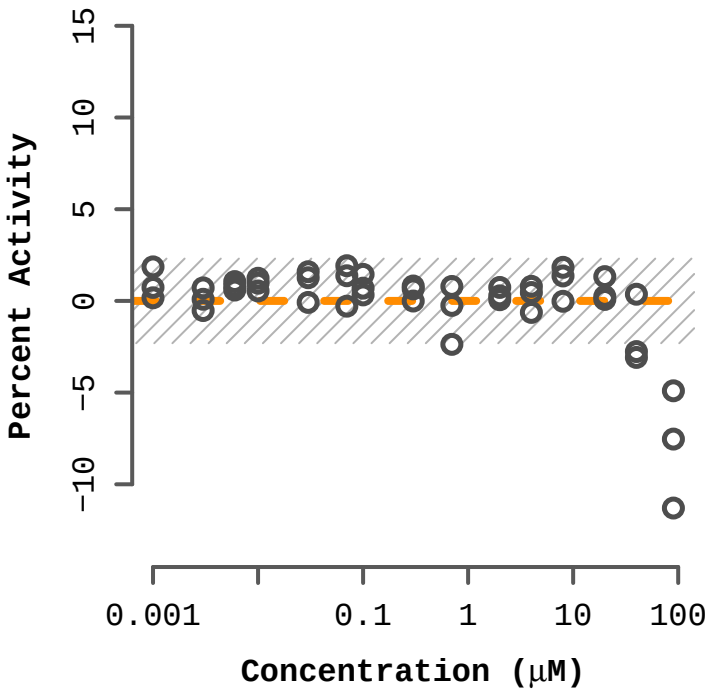
NAME: Emetine dihydrochloride
CHID: 20558 **CASRN:** 316-42-7
SPID(S): Tox21_200397
M4ID: 12481855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	323.13	NA	NA
PROB:	1	NA	NA
RMSE:	7.94	NA	NA

MAX_MEAN: 0.417 **MAX_MED:** 0.441 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

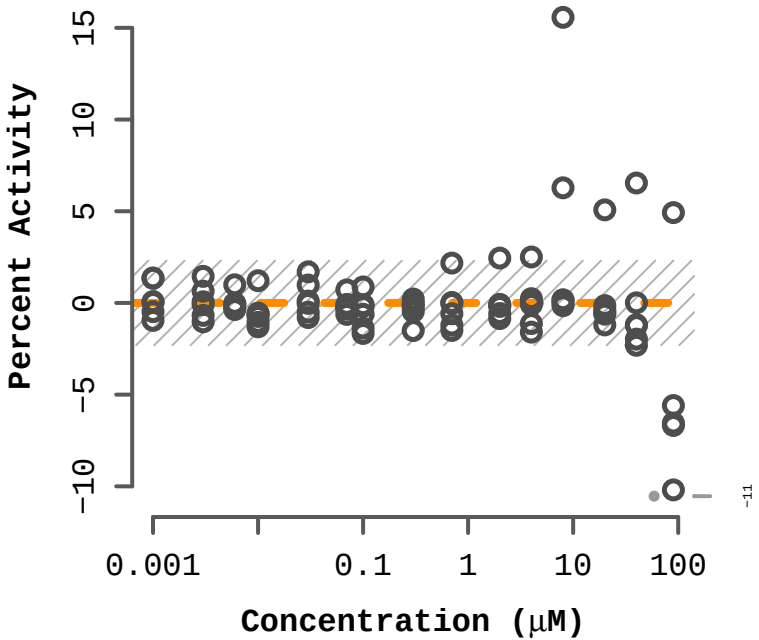
NAME: Endosulfan
CHID: 20560 **CASRN:** 115-29-7
SPID(S): Tox21_300657
M4ID: 12478476

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.42	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

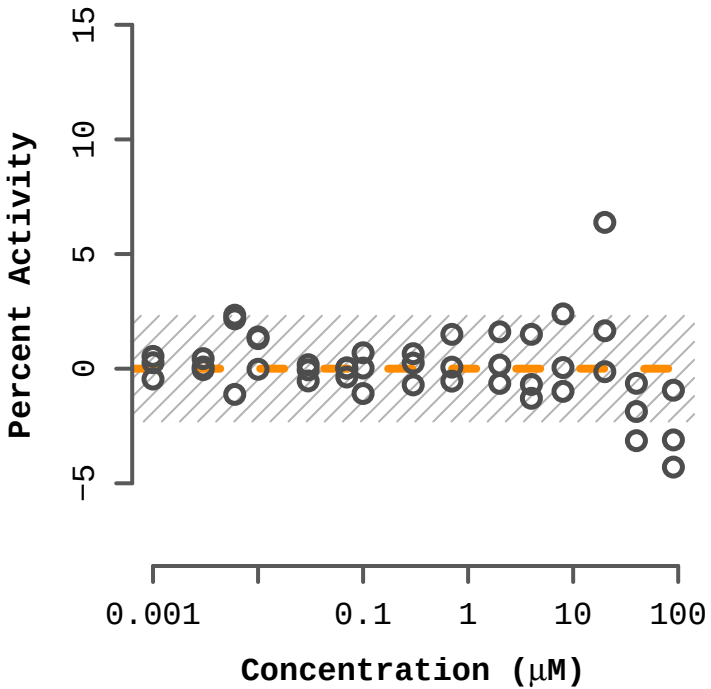
NAME: Endosulfan
CHID: 20560 **CASRN:** 115-29-7
SPID(S): Tox21_202365
M4ID: 12479887 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	378.72	NA	NA
PROB:	1	NA	NA
RMSE:	2.96	NA	NA

MAX_MEAN: 3.67 **MAX_MED:** 0.161 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

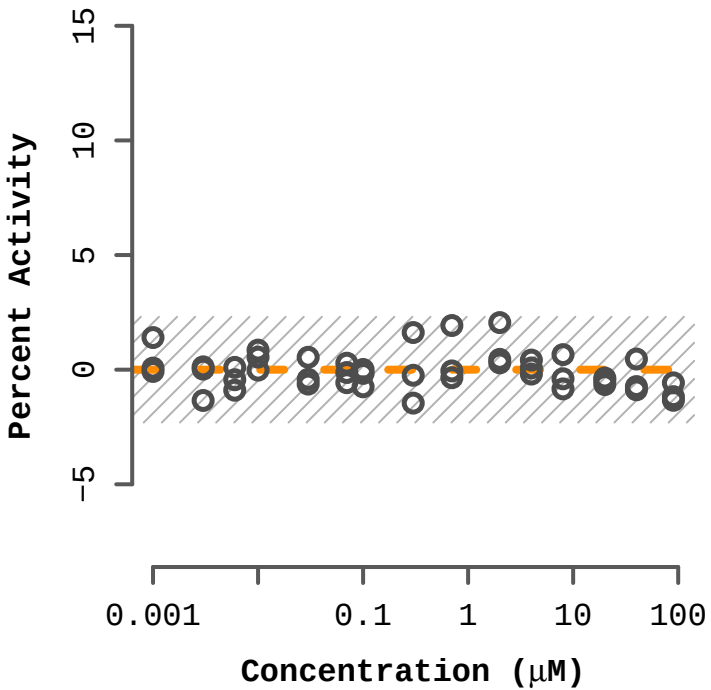
NAME: Endrin
CHID: 20561 CASRN: 72-20-8
SPID(S): Tox21_300613
M4ID: 12478520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 2.64 MAX_MED: 2.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

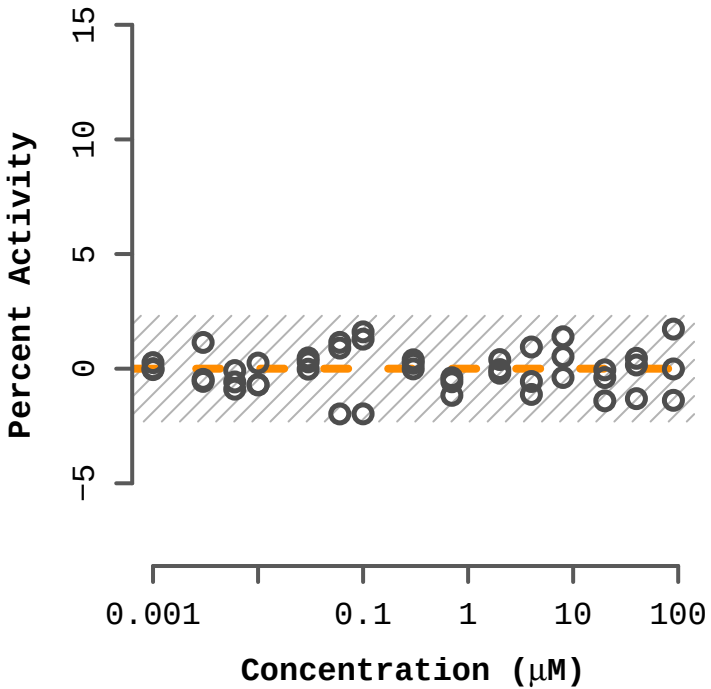
NAME: Enflurane
CHID: 20562 **CASRN:** 13838-16-9
SPID(S): Tox21_200166
M4ID: 12482086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.549 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

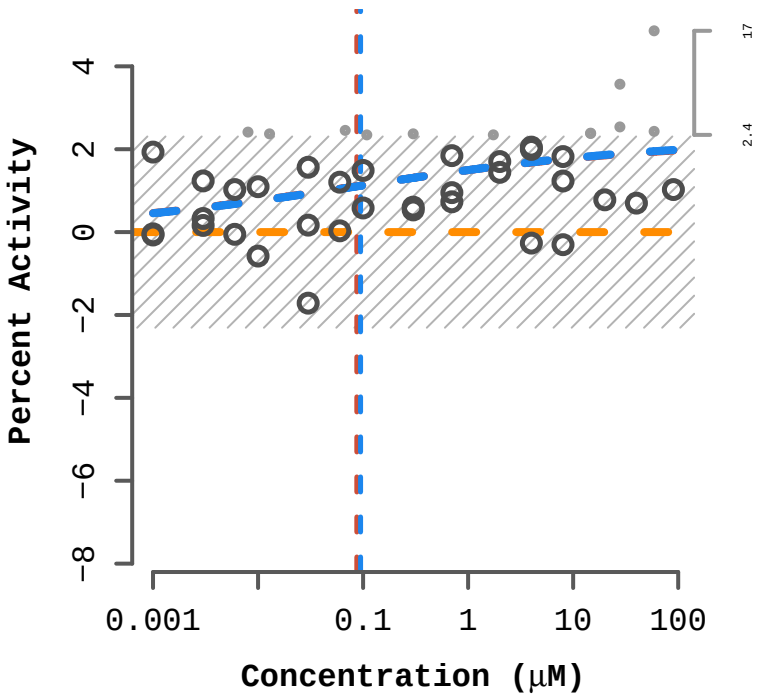
NAME: Epichlorohydrin
CHID: 20566 **CASRN:** 106-89-8
SPID(S): Tox21_200276
M4ID: 12481976

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.513 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Epoxybutane
CHID: 20569 CASRN: 106-88-7
SPID(S): Tox21_200207
M4ID: 12482045 BRK

HILL MODEL (in red):

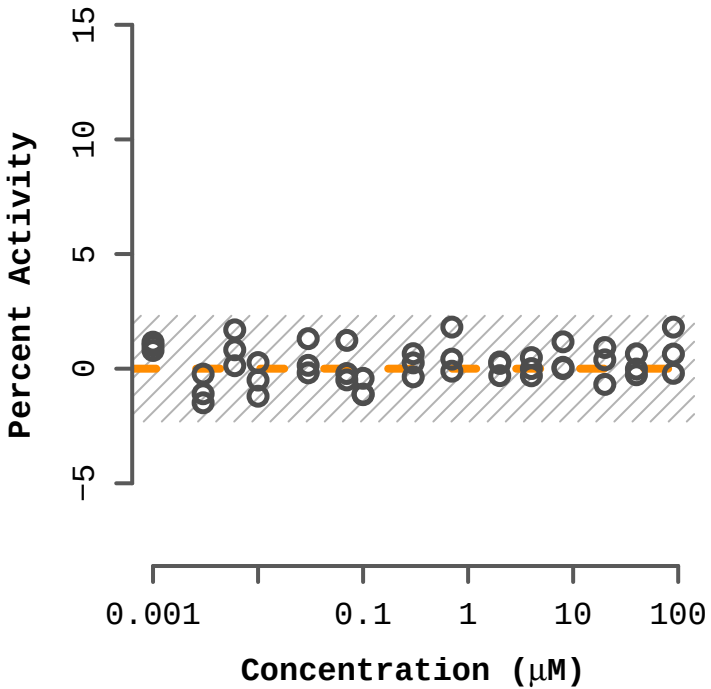
	tp	ga	gw
val:	2.21	−1.06	0.3
sd:	2.35	3.85	0.479

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.23	−1.02	0.3	3.22	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	206.98	177.09	181.09
PROB:	0	0.88	0.12
RMSE:	3.3	2.68	2.68

MAX_MEAN: 6.89 MAX_MED: 3.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

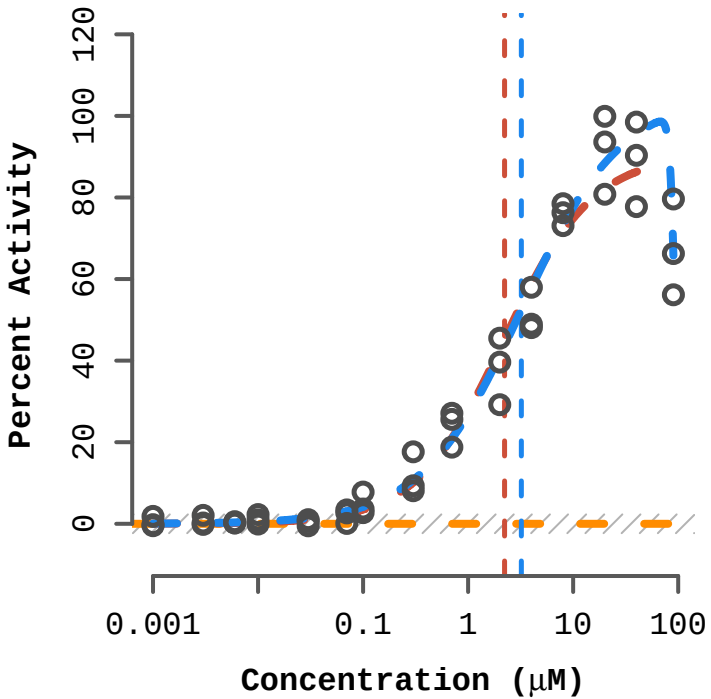
NAME: Sodium erythorbate (1:1)
CHID: 20570 CASRN: 6381-77-7
SPID(S): Tox21_300159
M4ID: 12478971

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.986 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17beta-Estradiol
CHID: 20573 CASRN: 50-28-2
SPID(S): Tox21_300288
M4ID: 12478842

HILL MODEL (in red):

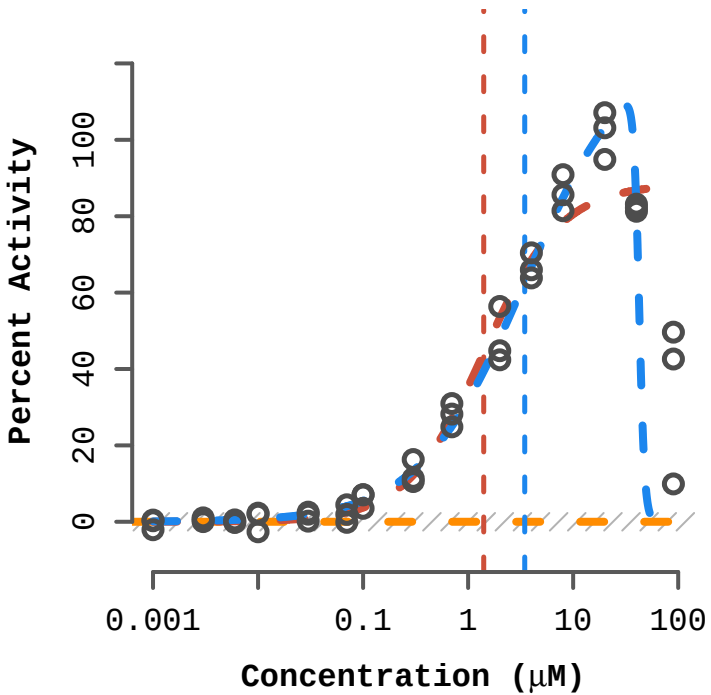
	tp	ga	gw
val:	90.6	0.347	1.04
sd:	5.55	0.0764	0.103

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	105	0.507	0.917	1.97	17.9
sd:	6.18	0.0759	0.0756	0.00567	6.05

	CNST	HILL	GNLS
AIC:	473.81	307.86	287.02
PROB:	0	0	1
RMSE:	46.02	8.13	5.56

MAX_MEAN: 91.4 MAX_MED: 93.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17beta-Estradiol
CHID: 20573 CASRN: 50-28-2
SPID(S): Tox21_202057
M4ID: 12480195

HILL MODEL (in red):

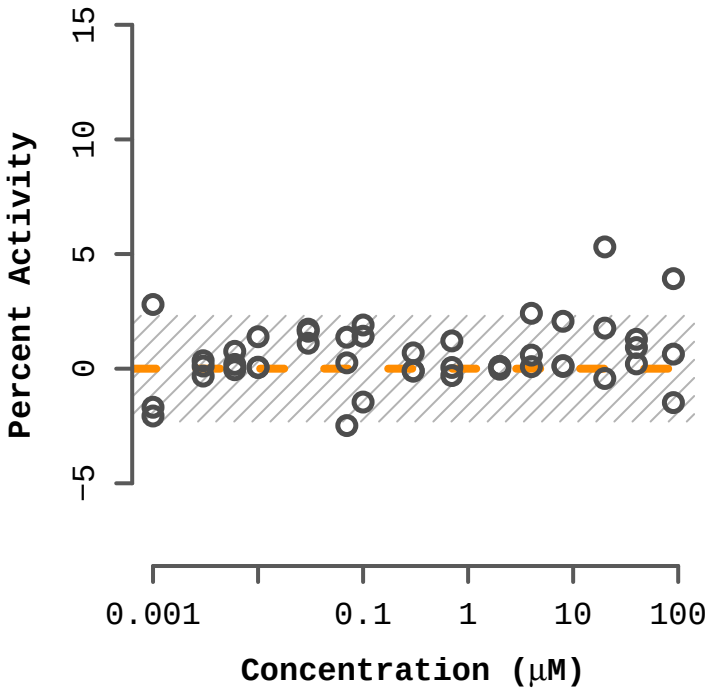
	tp	ga	gw
val:	88.4	0.148	1.18
sd:	3.83	0.0558	0.107

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	126	0.539	0.871	1.63	16.8
sd:	7.24	0.0746	0.055	0.0032	2.34

	CNST	HILL	GNLS
AIC:	476.18	334.14	285.85
PROB:	0	0	1
RMSE:	47.48	15.72	10.3

MAX_MEAN: 102 MAX_MED: 103 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

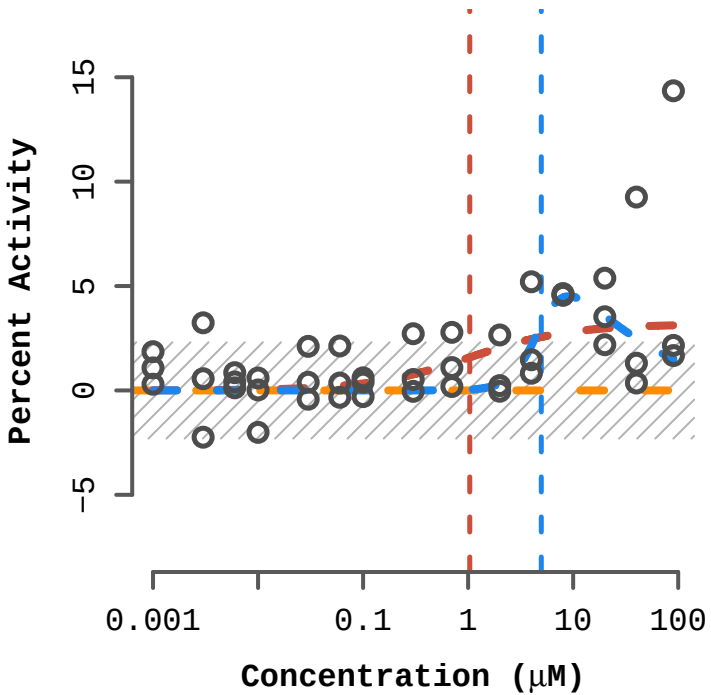
NAME: Estragole
CHID: 20575 **CASRN:** 140-67-0
SPID(S): Tox21_302930
M4ID: 12476203

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estragole
CHID: 20575 CASRN: 140-67-0
SPID(S): Tox21_202387
M4ID: 12479865

HILL MODEL (in red):

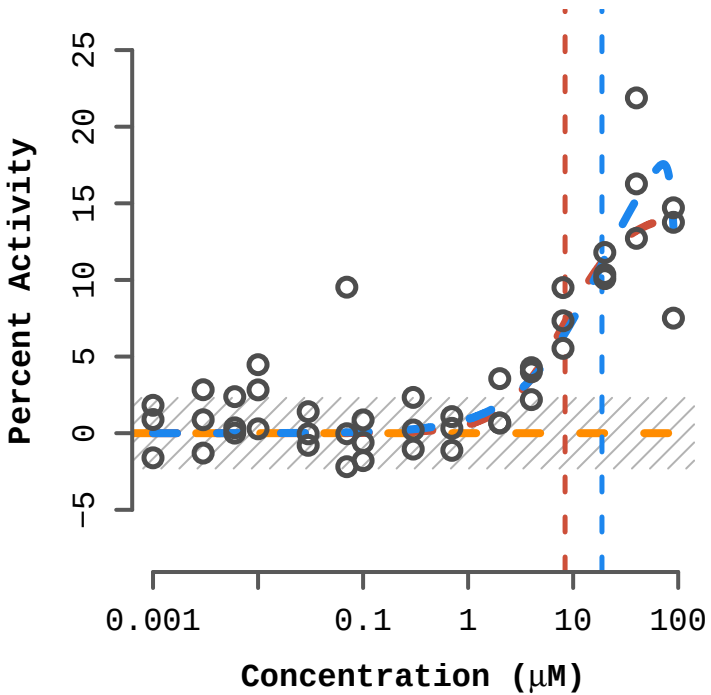
	tp	ga	gw
val:	3.17	0.0153	0.916
sd:	0.771	0.432	0.677

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.3	0.697	3.41	0.947	0.757
sd:	16.9	0.191	3.19	1.59	0.529

	CNST	HILL	GNLS
AIC:	221.3	196.05	194.53
PROB:	0	0.32	0.68
RMSE:	3.33	2.39	2.55

MAX_MEAN: 6.06 MAX_MED: 4.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Ethinylestradiol
CHID: 20576 CASRN: 57-63-6
SPID(S): Tox21_300413
M4ID: 12478719

HILL MODEL (in red):

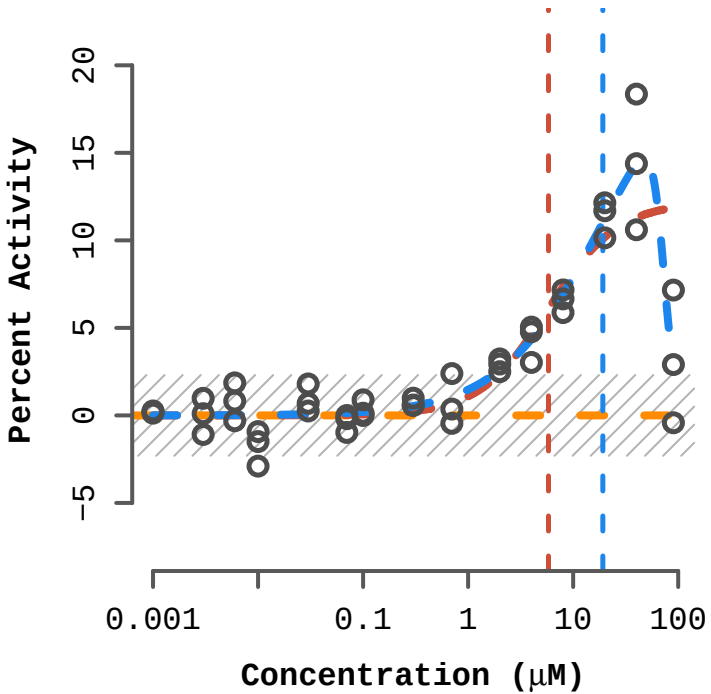
	tp	ga	gw
val:	14.5	0.923	1.51
sd:	1.24	0.0915	0.325

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22	1.27	1.07	1.98	14.8
sd:	10.9	0.436	0.34	0.0159	15.9

	CNST	HILL	GNLS
AIC:	295.38	207.13	209.37
PROB:	0	0.75	0.25
RMSE:	6.84	2.63	2.47

MAX_MEAN: 17 MAX_MED: 16.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Ethinylestradiol
CHID: 20576 **CASRN:** 57-63-6
SPID(S): Tox21_201291
M4ID: 12480961

HILL MODEL (in red):

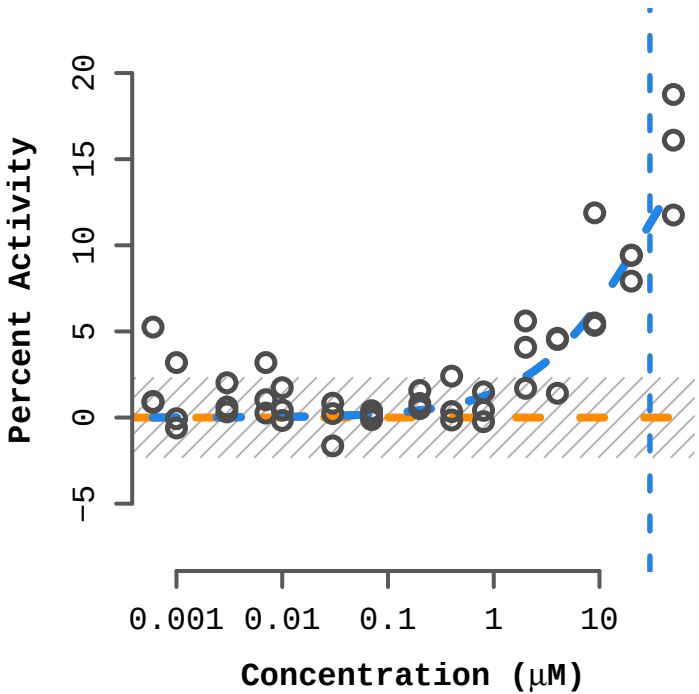
	tp	ga	gw
val:	12.2	0.765	1.32
sd:	1.66	0.117	0.282

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22	1.28	0.893	1.86	7.68
sd:	6	0.274	0.153	0.0583	4.44

	CNST	HILL	GNLS
AIC:	270.8	195.84	163.94
PROB:	0	0	1
RMSE:	5.47	2.81	1.45

MAX_MEAN: 14.4 **MAX_MED:** 14.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Ethinylestradiol
CHID: 20576 CASRN: 57-63-6
SPID(S): Tox21_111147_1
M4ID: 12483878

HILL MODEL (in red):

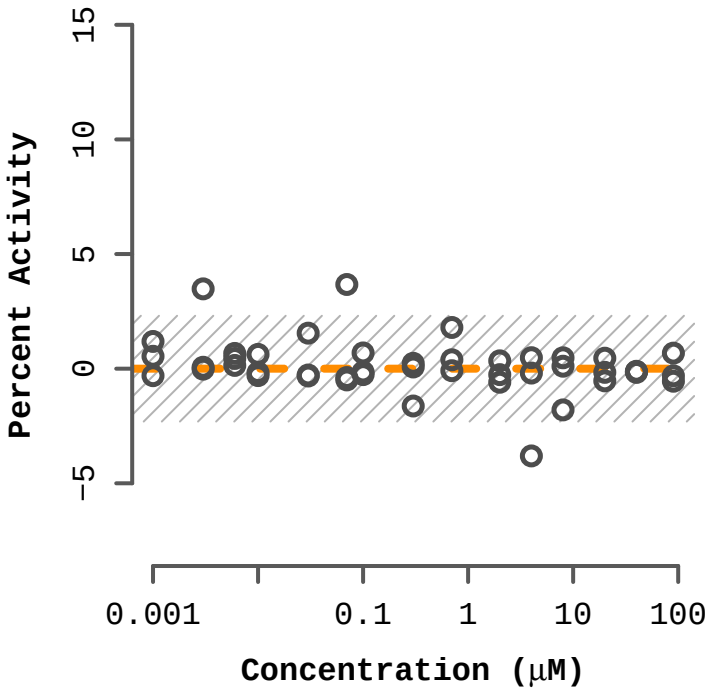
	tp	ga	gw
val:	22.5	1.48	0.789
sd:	8.72	0.381	0.147

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.5	1.48	0.789	3	10.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	269.82	186.86	190.86
PROB:	0	0.88	0.12
RMSE:	5.5	1.91	1.91

MAX_MEAN: 15.5 MAX_MED: 16.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

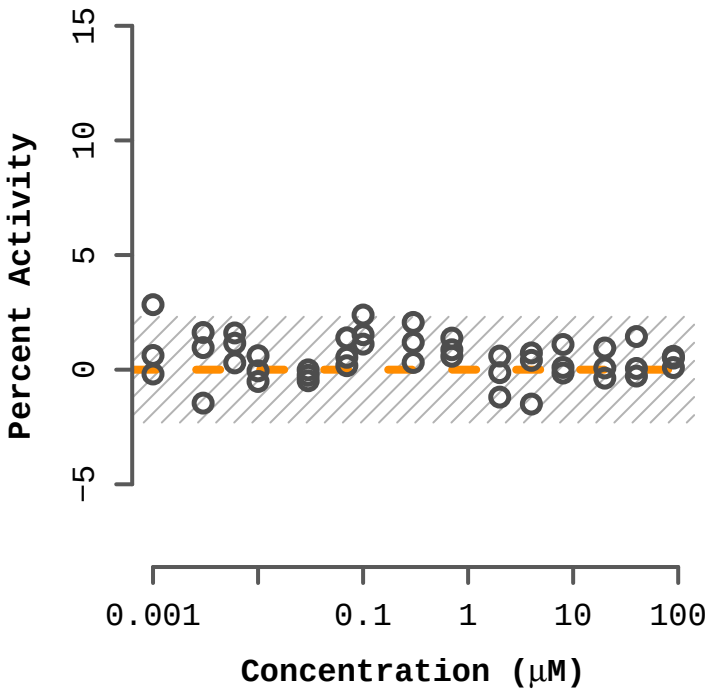
NAME: Ethionamide
CHID: 20577 **CASRN:** 536-33-4
SPID(S): Tox21_302769
M4ID: 12476364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.542 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

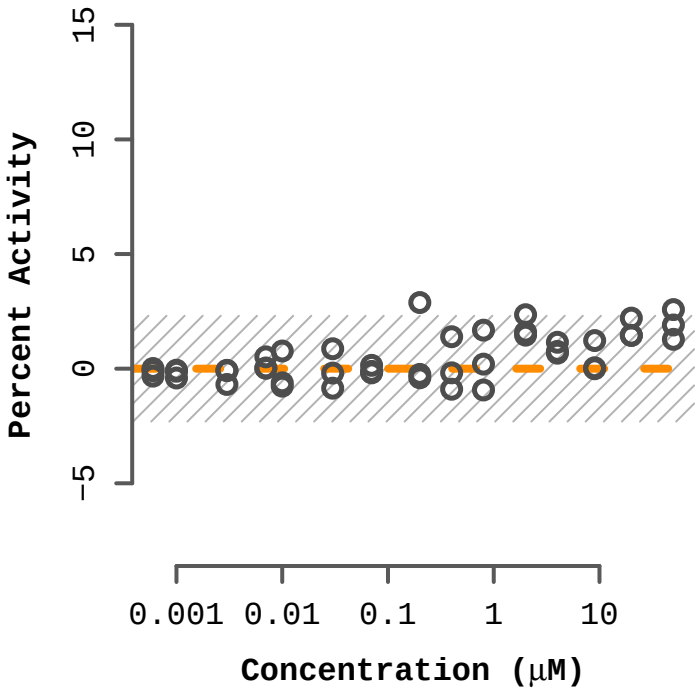
NAME: Ethionamide
CHID: 20577 **CASRN:** 536-33-4
SPID(S): Tox21_202409
M4ID: 12479843

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

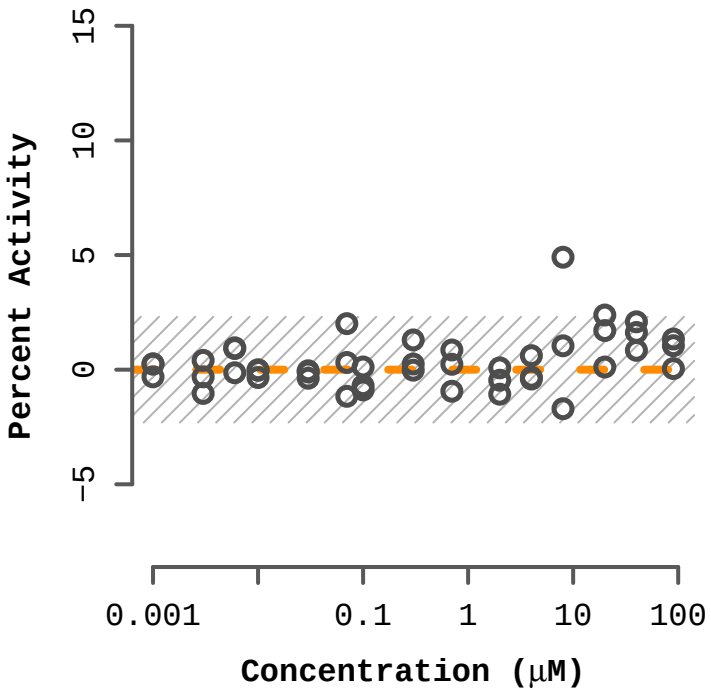
NAME: Ethionamide
CHID: 20577 **CASRN:** 536-33-4
SPID(S): Tox21_110458_1
M4ID: 12484340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

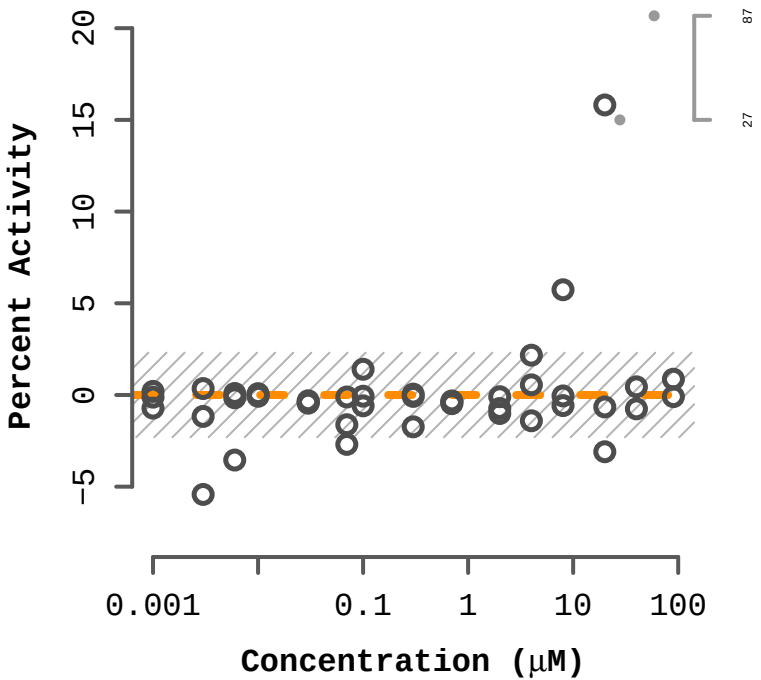
NAME: Dulcin
CHID: 20580 **CASRN:** 150-69-6
SPID(S): Tox21_301340
M4ID: 12477793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

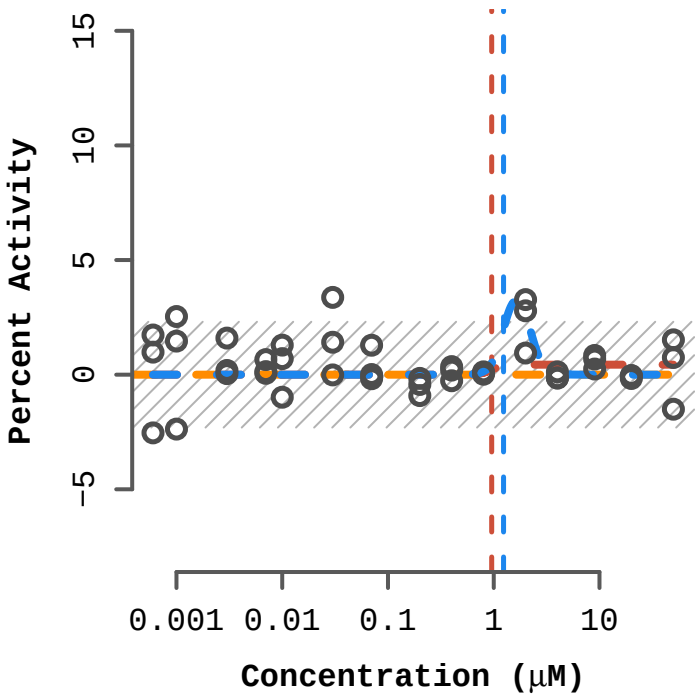
NAME: 2-Ethoxybenzamide
CHID: 20581 **CASRN:** 938-73-8
SPID(S): Tox21_200025
M4ID: 12482227 **BRK**

HILL MODEL: Not applicable.

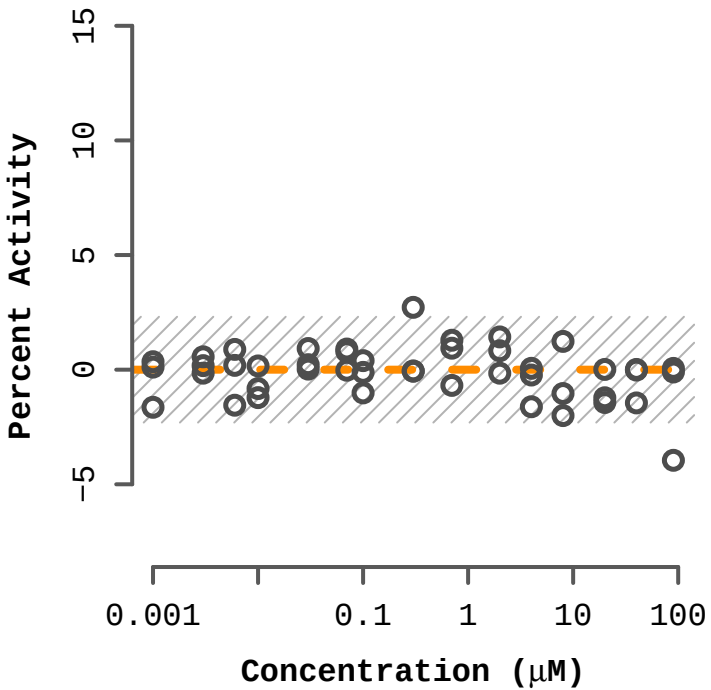
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	235.12	NA	NA
PROB:	1	NA	NA
RMSE:	13.83	NA	NA

MAX_MEAN: 29.2 **MAX_MED:** 0.862 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Ethoxybenzamide
CHID:    20581   CASRN: 938-73-8
SPID(S): Tox21_111156_1
M4ID:    12483872

HILL MODEL (in red):
      tp       ga       gw
val:  0.436    -0.0193  8
sd:   0.265    0.331    19.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.05     0.0928   7.57     0.343    7.28
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  148.15      151.39      146.94
PROB: 0.33        0.07        0.6
RMSE: 1.27        1.23        1.12

MAX_MEAN: 2.34      MAX_MED: 2.79      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

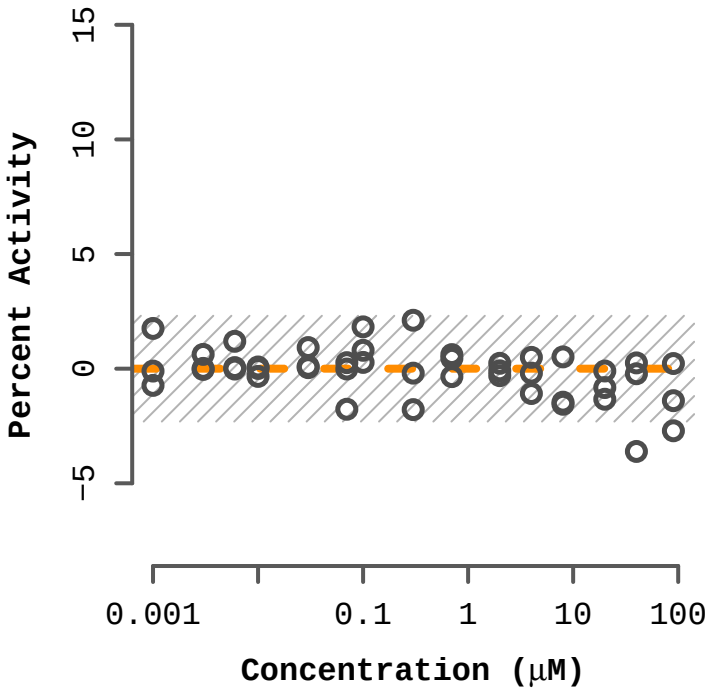
NAME: Ethoxyquin
CHID: 20582 CASRN: 91-53-2
SPID(S): Tox21_300328
M4ID: 12478804

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.867 **MAX_MED:** 0.938 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

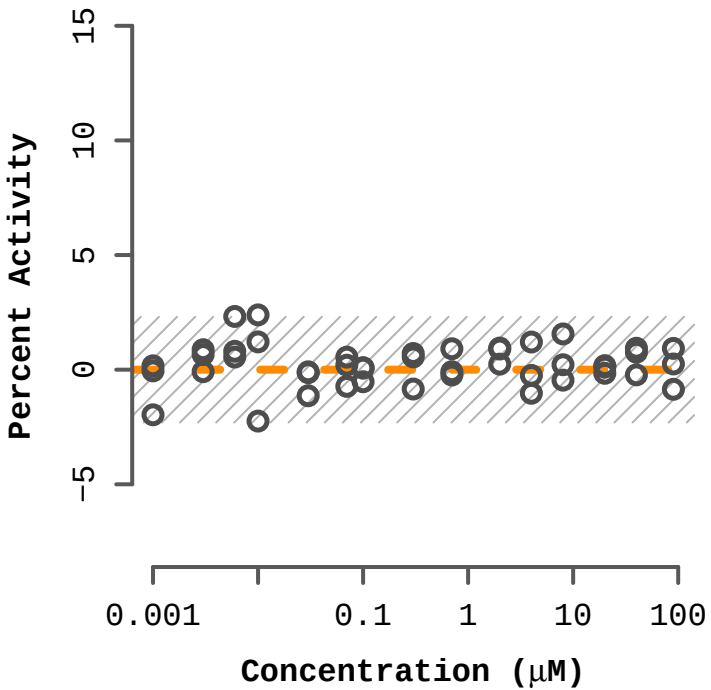
NAME: Ethoxyquin
CHID: 20582 CASRN: 91-53-2
SPID(S): Tox21_201336
M4ID: 12480916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.968 MAX_MED: 0.803 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

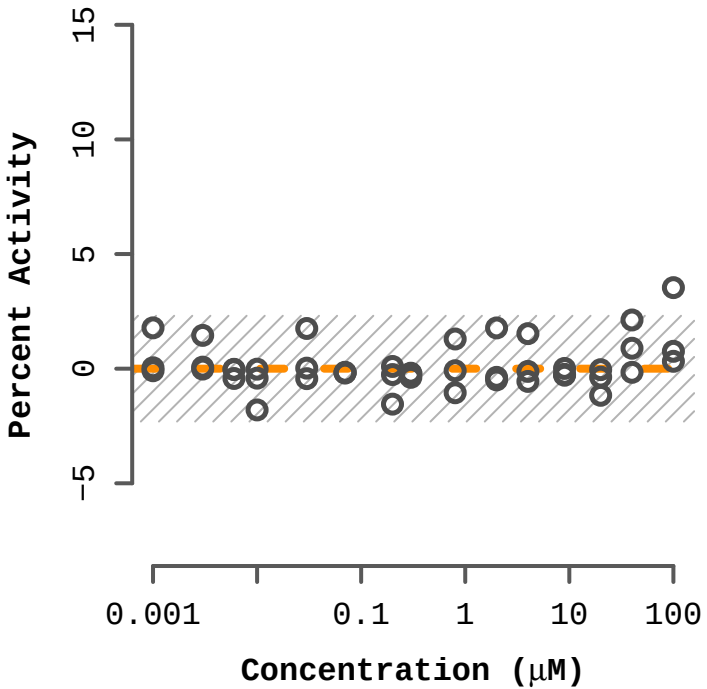
NAME: Ethyl acrylate
CHID: 20583 **CASRN:** 140-88-5
SPID(S): Tox21_202513
M4ID: 12479739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

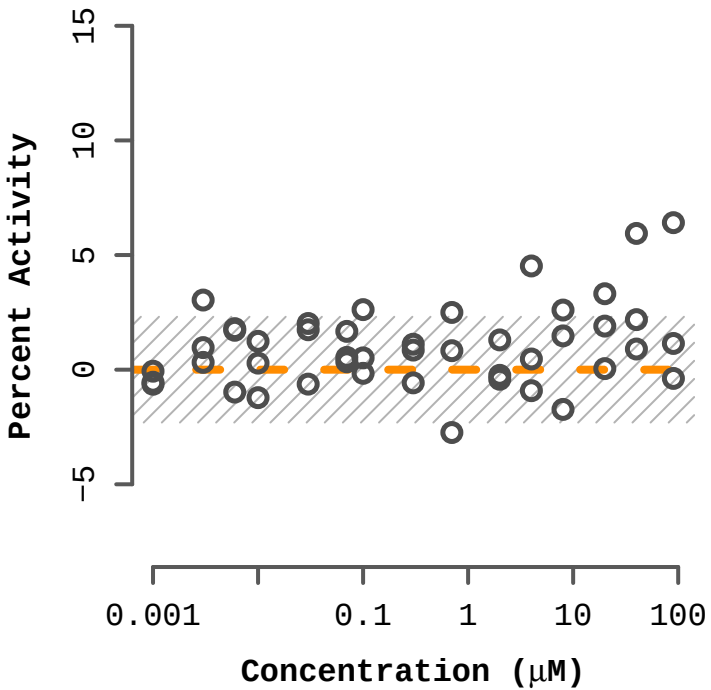
NAME: Ethanol
CHID: 20584 **CASRN:** 64-17-5
SPID(S): Tox21_202510
M4ID: 12479742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.893 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

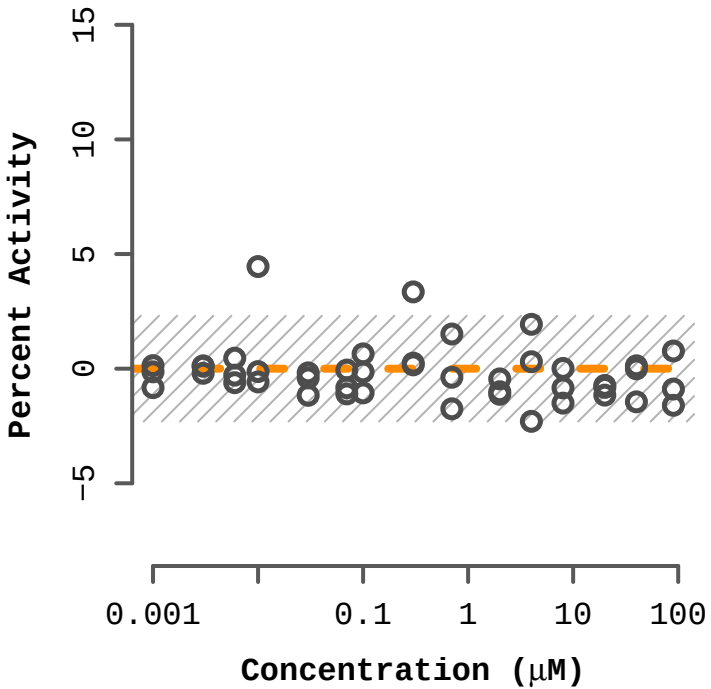
NAME: Ethyl bromoacetate
CHID: 20587 **CASRN:** 105-36-2
SPID(S): Tox21_200152
M4ID: 12482100

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 3.01 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

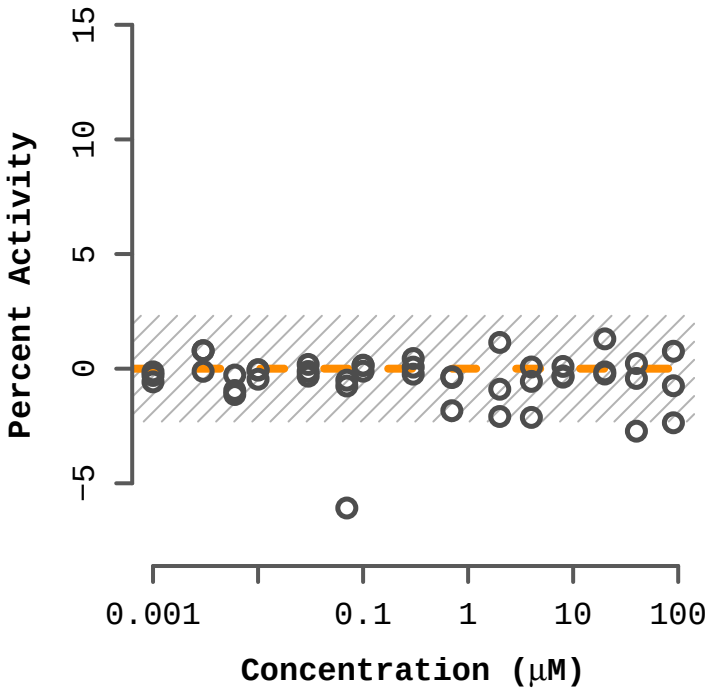
NAME: p,p'−Ethyl−DDD
CHID: 20589 CASRN: 72−56−0
SPID(S): Tox21_302883
M4ID: 12476250

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.25 MAX_MED: 0.305 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

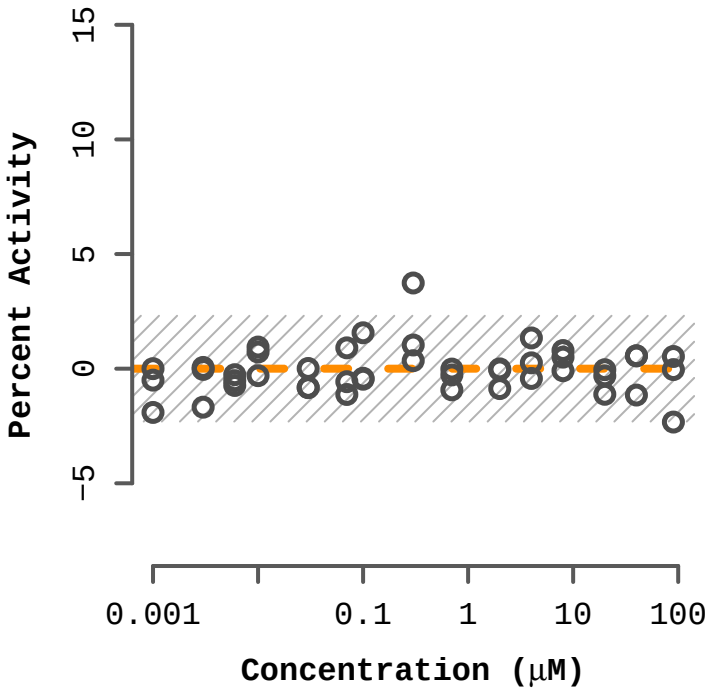
NAME: p,p'−Ethyl−DDD
CHID: 20589 CASRN: 72−56−0
SPID(S): Tox21_201635
M4ID: 12480617

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.485 MAX_MED: 0.784 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

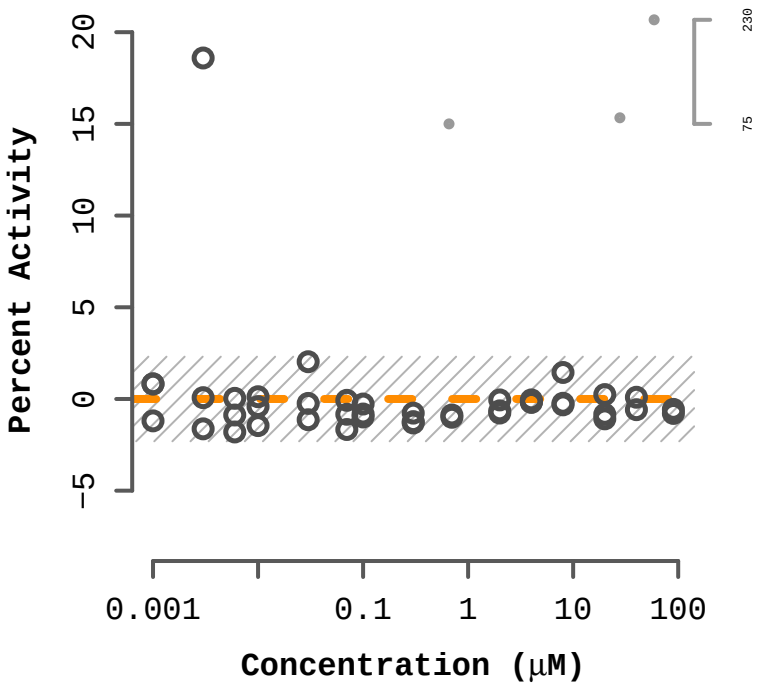
NAME: Ethyl methylphenylglycidate
CHID: 20591 CASRN: 77-83-8
SPID(S): Tox21_302960
M4ID: 12476173

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

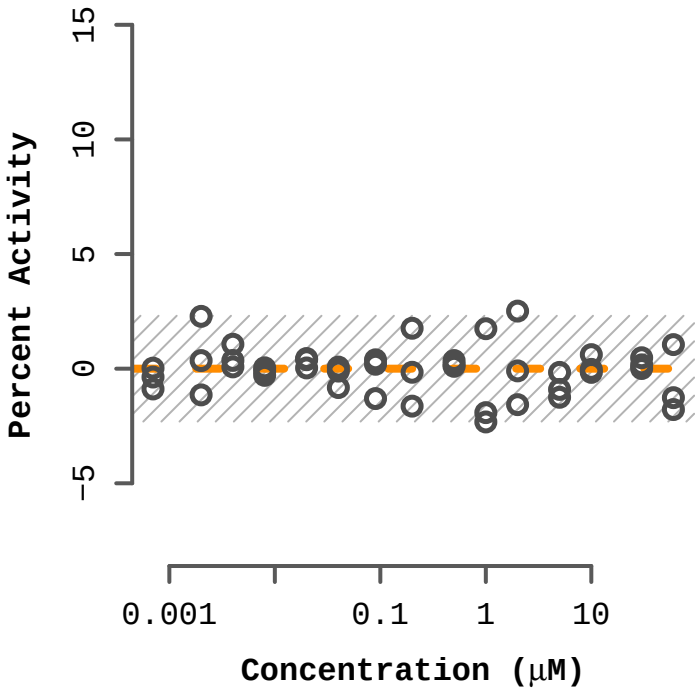
NAME: Ethyl methylphenylglycidate
CHID: 20591 CASRN: 77-83-8
SPID(S): Tox21_201315
M4ID: 12480937 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	268.45	NA	NA
PROB:	1	NA	NA
RMSE:	37.65	NA	NA

MAX_MEAN: 74.6 **MAX_MED:** 0.813 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

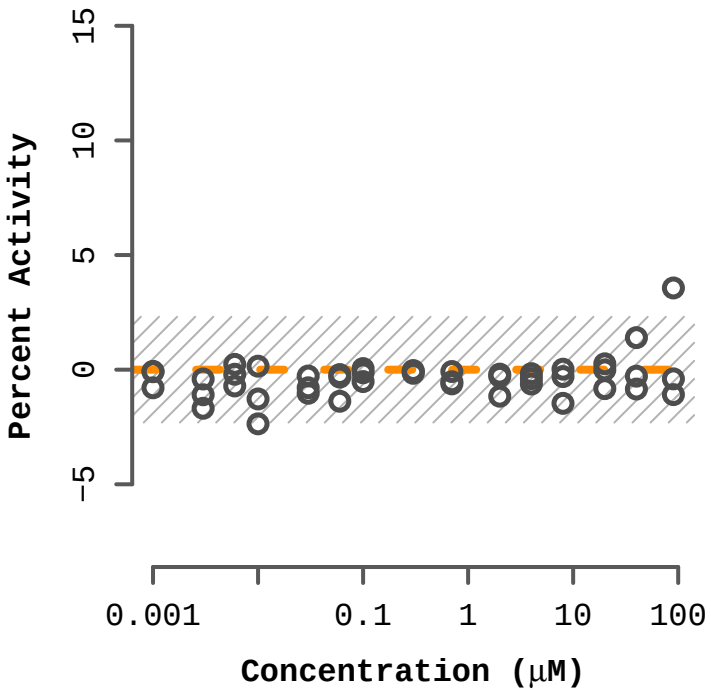
NAME: 1-Ethyl-1-nitrosourea
CHID: 20593 **CASRN:** 759-73-9
SPID(S): Tox21_302749
M4ID: 12476384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.502 **MAX_MED:** 0.393 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

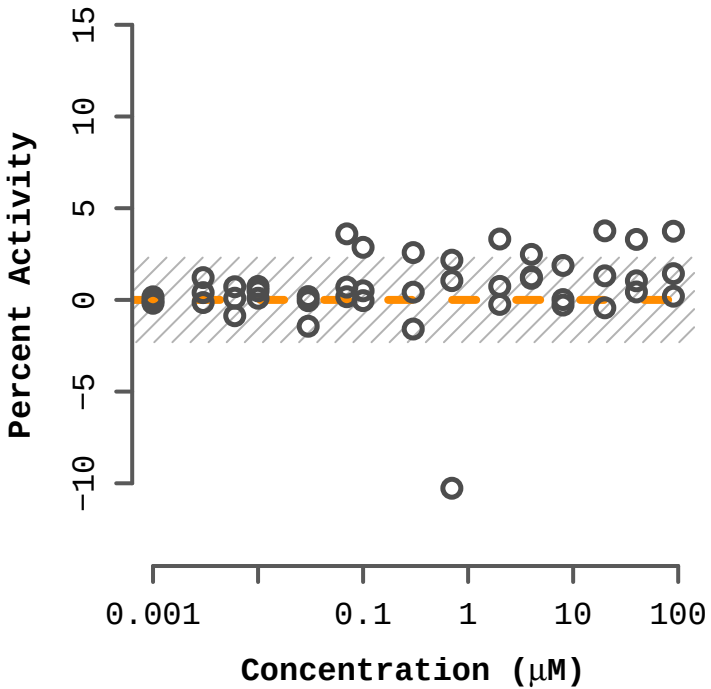
NAME: 1-Ethyl-1-nitrosourea
CHID: 20593 CASRN: 759-73-9
SPID(S): Tox21_202151
M4ID: 12480101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.693 MAX_MED: −0.00755 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

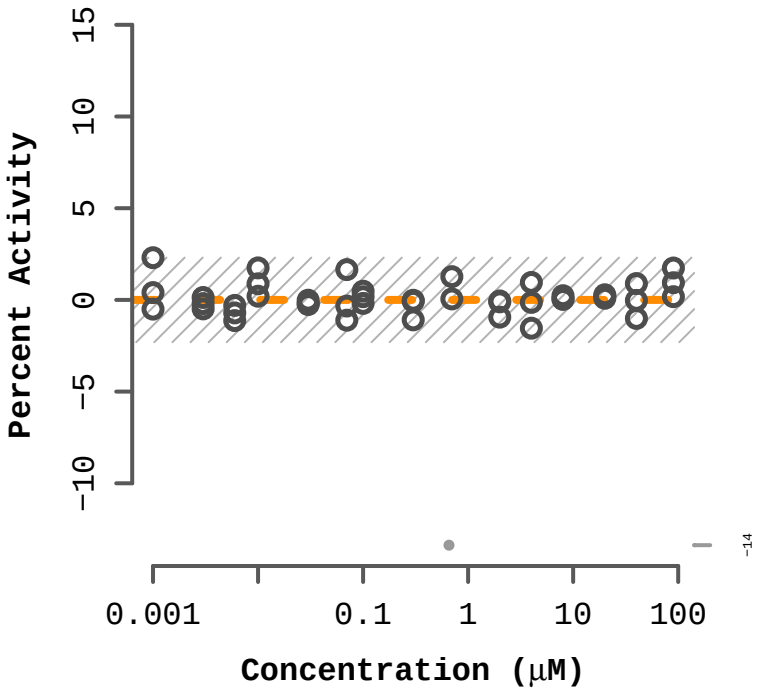
NAME: Ethylbenzene
CHID: 20596 **CASRN:** 100-41-4
SPID(S): Tox21_201064
M4ID: 12481188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

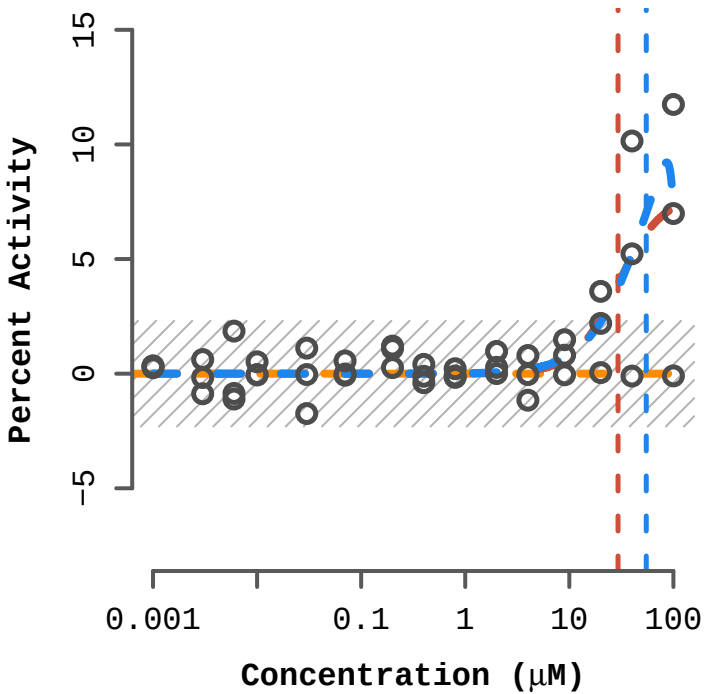
NAME: Ethylene glycol
CHID: 20597 **CASRN:** 107-21-1
SPID(S): Tox21_300637
M4ID: 12478496 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.56	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 0.952 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethylene glycol
CHID: 20597 CASRN: 107-21-1
SPID(S): Tox21_202038
M4ID: 12480214

HILL MODEL (in red):

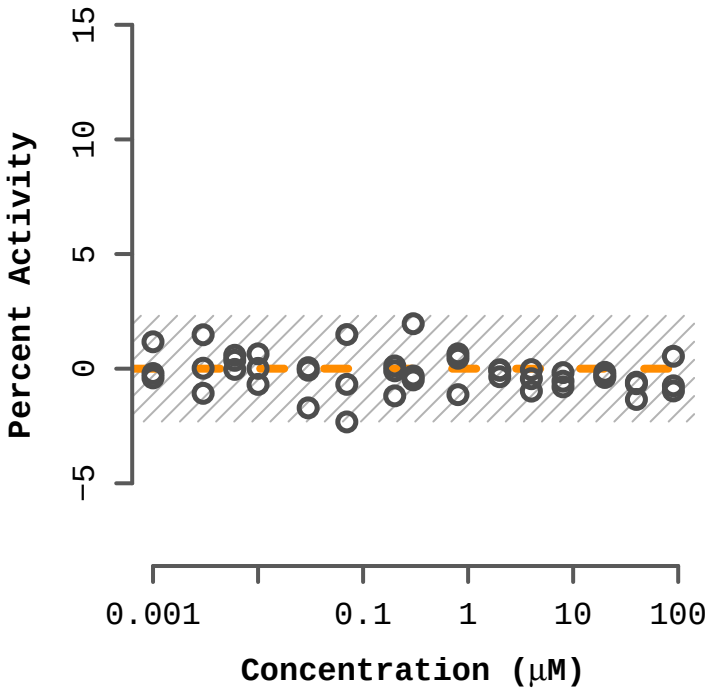
	tp	ga	gw
val:	7.79	1.47	2.08
sd:	1.46	0.126	0.832

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14	1.74	1.64	2.02	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	180.53	164.13	167.95
PROB:	0	0.87	0.13
RMSE:	2.81	1.84	1.84

MAX_MEAN: 6.21 MAX_MED: 6.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

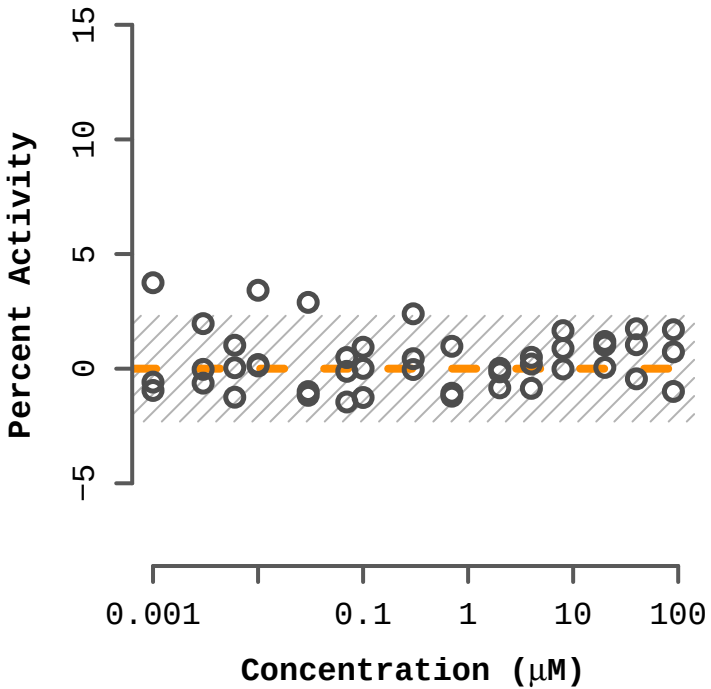
NAME: Ethylene glycol, cyclic sulfate
CHID: 20598 CASRN: 1072-53-3
SPID(S): Tox21_200498
M4ID: 12481754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.386 MAX_MED: 0.455 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

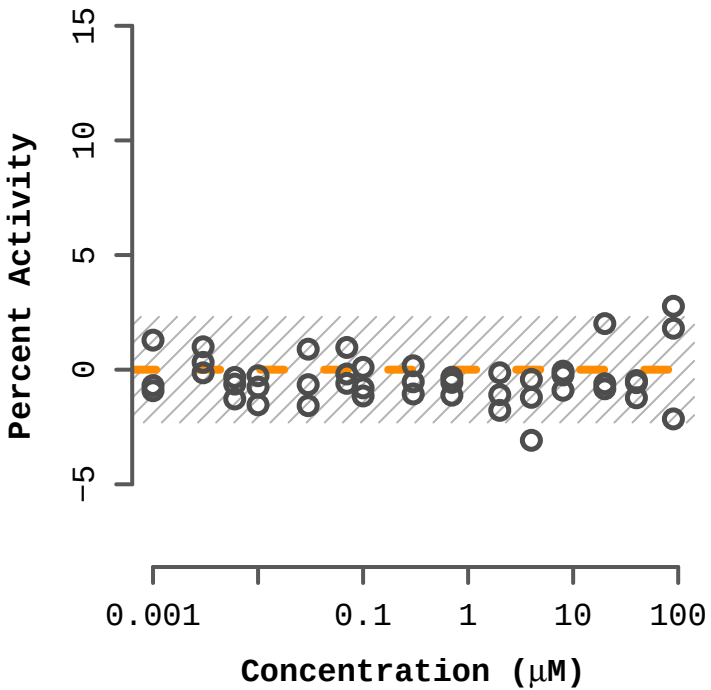
NAME: Ethylene thiourea
CHID: 20601 CASRN: 96-45-7
SPID(S): Tox21_301034
M4ID: 12478099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.24 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

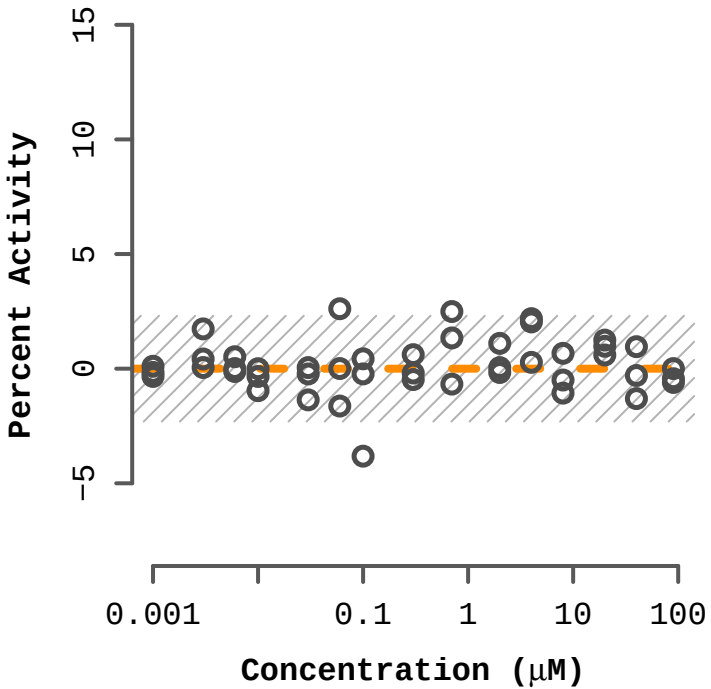
NAME: Ethylene thiourea
CHID: 20601 CASRN: 96-45-7
SPID(S): Tox21_201294
M4ID: 12480958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.809 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

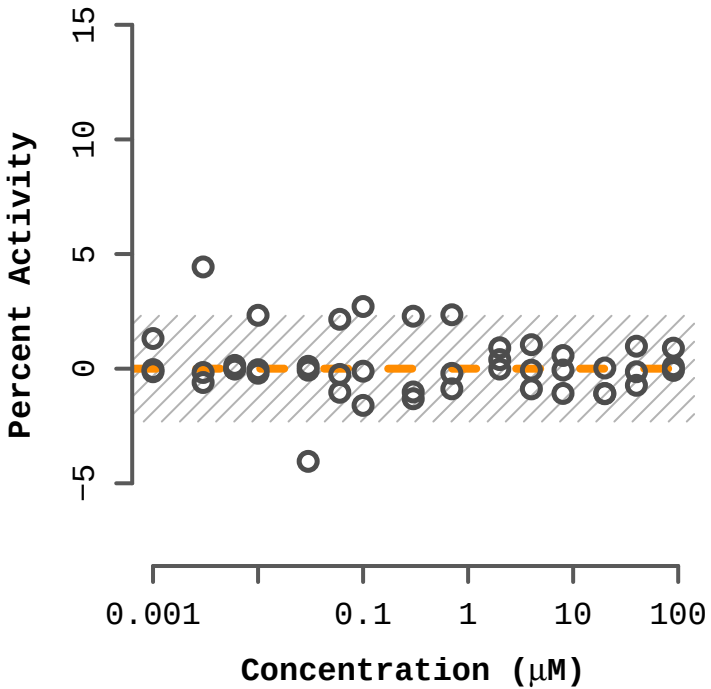
NAME: Ethylene urea
CHID: 20602 CASRN: 120-93-4
SPID(S): Tox21_200783
M4ID: 12481469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.5 MAX_MED: 2.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

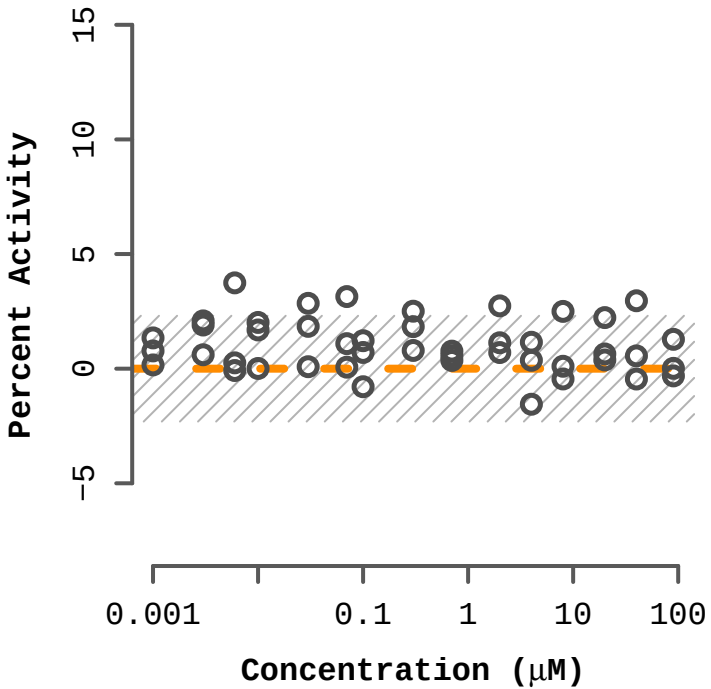
NAME: Nabam−sodium
CHID: 20603 **CASRN:** 142−59−6
SPID(S): Tox21_202588
M4ID: 12479664

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 0.398 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

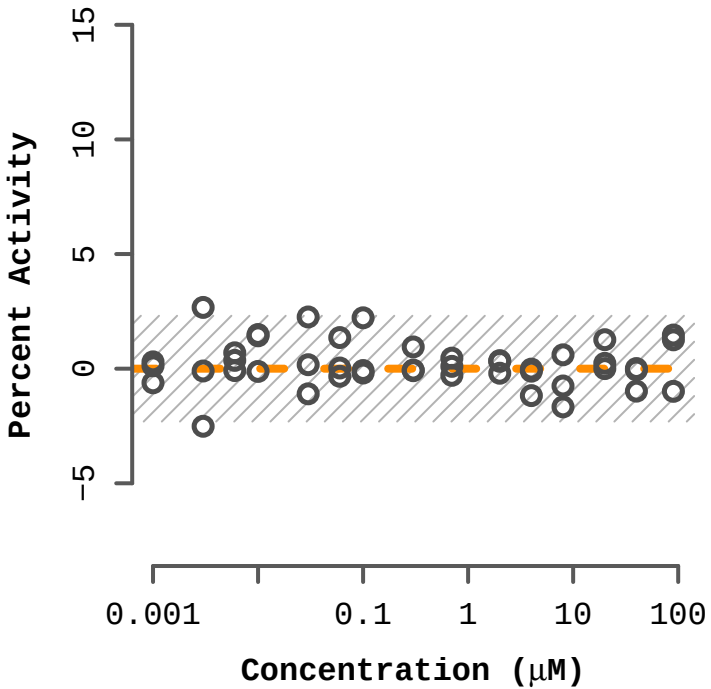
NAME: 4-Vinyl-1-cyclohexene dioxide
CHID: 20604 **CASRN:** 106-87-6
SPID(S): Tox21_300311
M4ID: 12478819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

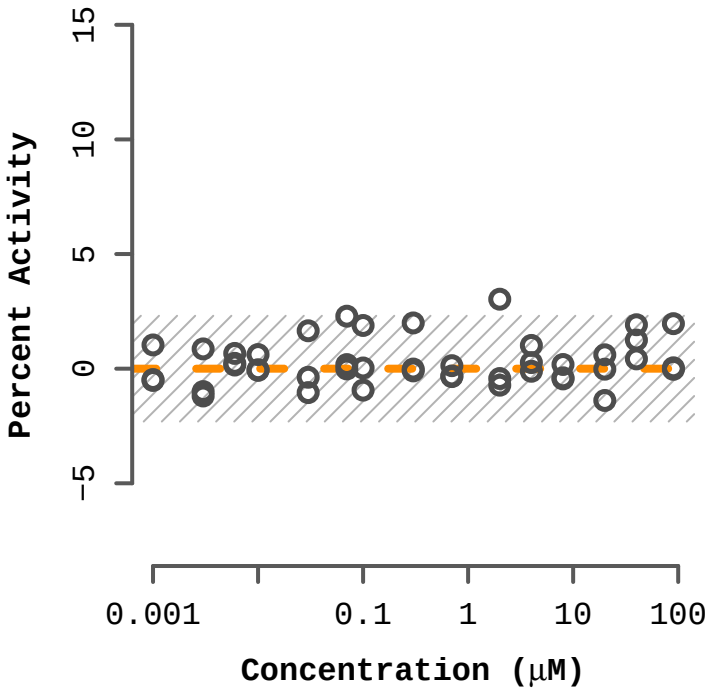
NAME: 4-Vinyl-1-cyclohexene dioxide
CHID: 20604 **CASRN:** 106-87-6
SPID(S): Tox21_201505
M4ID: 12480747

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.936 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

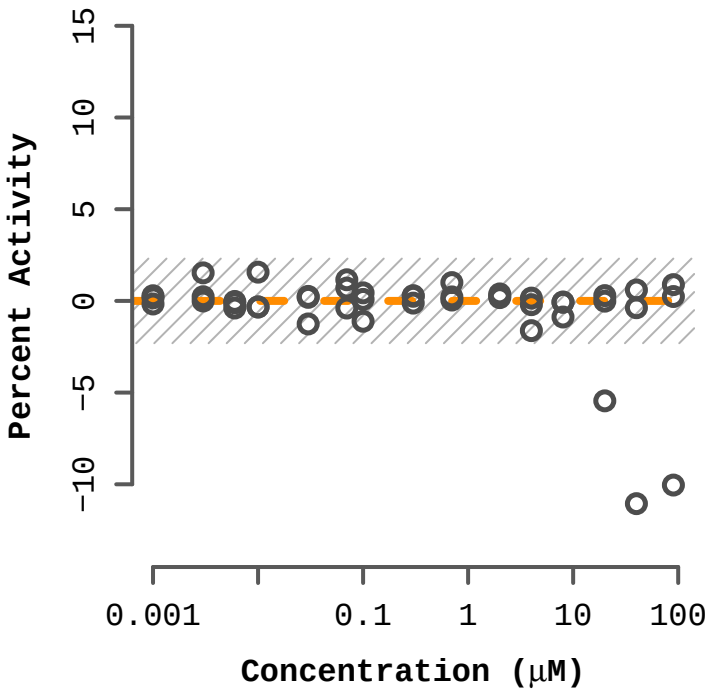
NAME: 2-Ethyl-1-hexanol
CHID: 20605 **CASRN:** 104-76-7
SPID(S): Tox21_300019
M4ID: 12479111

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

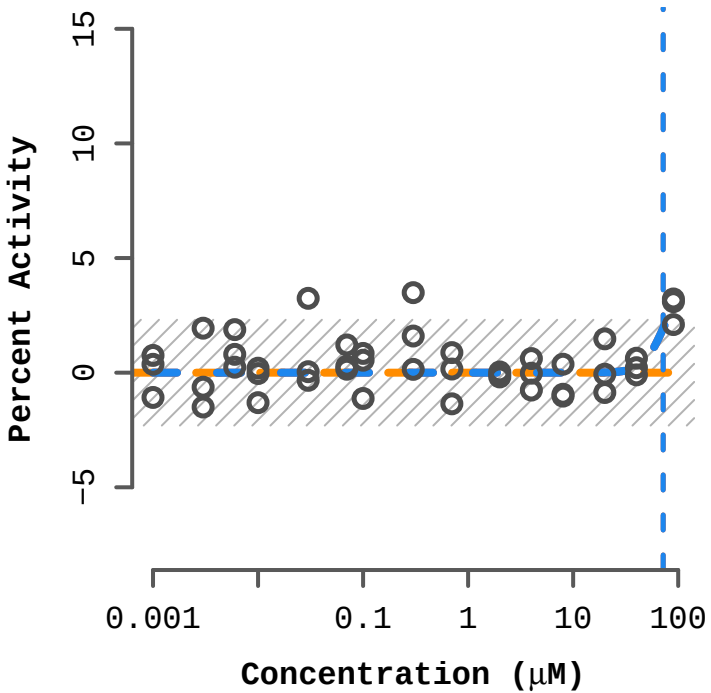
NAME: 2-Ethyl-1-hexanol
CHID: 20605 **CASRN:** 104-76-7
SPID(S): Tox21_202071
M4ID: 12480181

HILL MODEL: Not applicable.

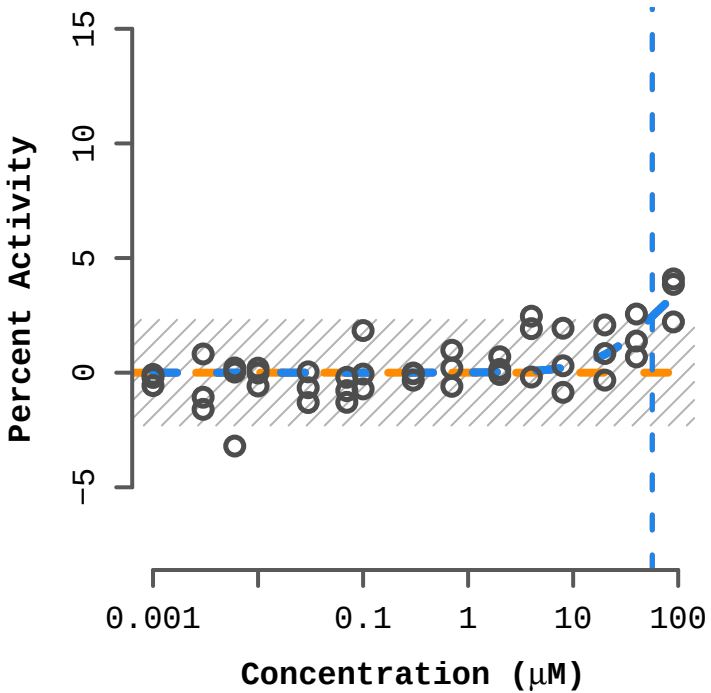
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144	NA	NA
PROB:	1	NA	NA
RMSE:	2.45	NA	NA

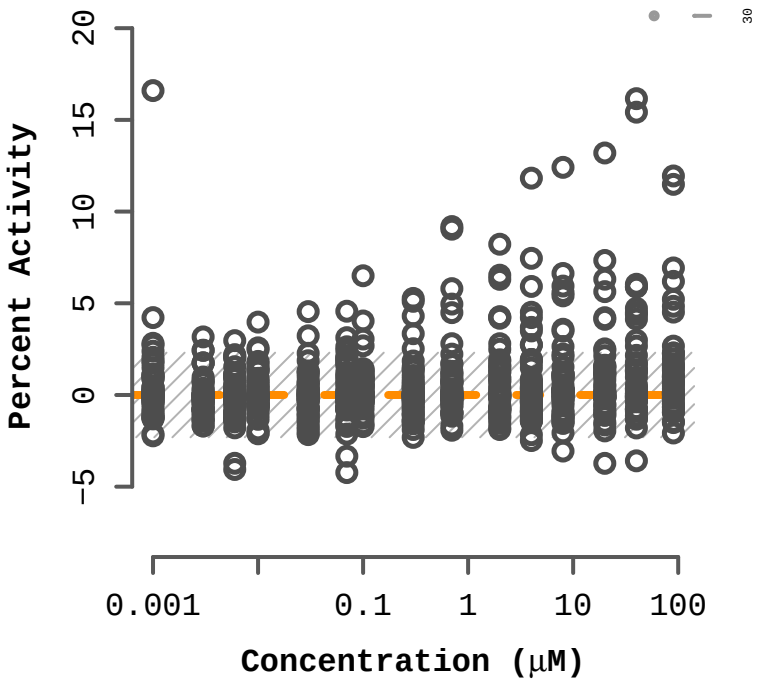
MAX_MEAN: 0.586 **MAX_MED:** 0.701 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Di(2-ethylhexyl) adipate
CHID:    20606   CASRN: 103-23-1
SPID(S): Tox21_300564
M4ID:    12478569

HILL MODEL (in red):
      tp       ga       gw
val:  3.87     1.86     4.55
sd:   33.9     2.53     29.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.87     1.86     4.55     3.04     2.81
sd:   37.7     2.59     29.6     888      2620

      CNST        HILL        GNLS
AIC:  150.55      138.33      142.33
PROB: 0           0.88        0.12
RMSE: 1.31        1.09        1.09

MAX_MEAN: 2.81      MAX_MED: 3.1       BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Di(2-ethylhexyl) adipate
CHID:    20606   CASRN: 103-23-1
SPID(S): Tox21_202231
M4ID:    12480021

HILL MODEL (in red):
      tp       ga       gw
val:  4.91     1.75     1.58
sd:   2.67     0.332    1.28

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.91     1.75     1.58     3.63     3.93
sd:   2.66     0.331    1.27     383      904

      CNST        HILL        GNLS
AIC:  156.95      134.86      138.86
PROB: 0           0.88        0.12
RMSE: 1.42        1.01        1.01

MAX_MEAN: 3.39      MAX_MED: 3.85      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

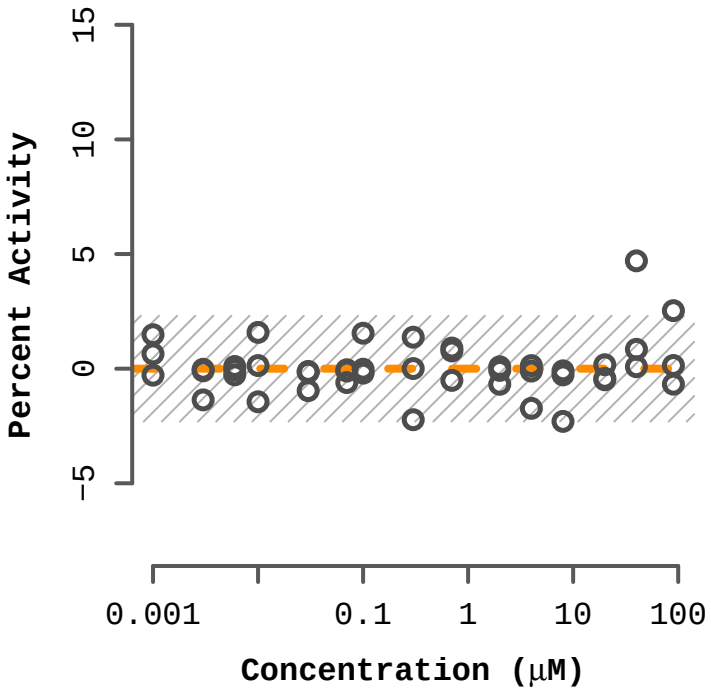
NAME: Di(2-ethylhexyl) phthalate
CHID: 20607 CASRN: 117-81-7
SPID(S): Tox21_400084
M4ID: 12475053 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2841.53	NA	NA
PROB:	1	NA	NA
RMSE:	2.57	NA	NA

MAX_MEAN: 2.04 MAX_MED: 0.751 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

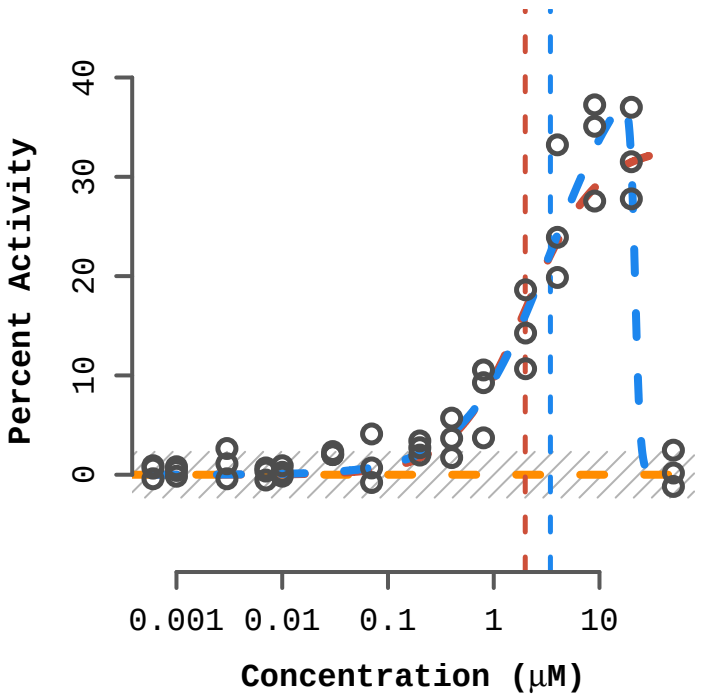
NAME: Ethylphenylacetylurea
CHID: 20612 **CASRN:** 90-49-3
SPID(S): Tox21_302208
M4ID: 12476925

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 0.846 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethynodiol diacetate
CHID: 20614 CASRN: 297-76-7
SPID(S): Tox21_112333_1
M4ID: 12483155

HILL MODEL (in red):

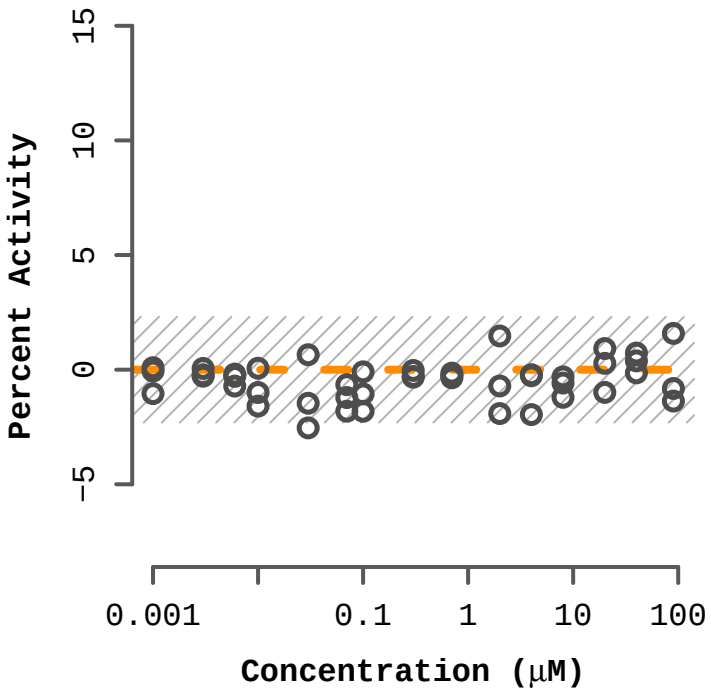
	tp	ga	gw
val:	33.1	0.298	1.27
sd:	2.76	0.0921	0.231

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	44.7	0.536	1.06	1.34	17.9
sd:	9.17	0.174	0.148	0.013	10.9

	CNST	HILL	GNLS
AIC:	360.24	281.95	222.88
PROB:	0	0	1
RMSE:	14.59	8.8	2.66

MAX_MEAN: 33.3 MAX_MED: 35.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

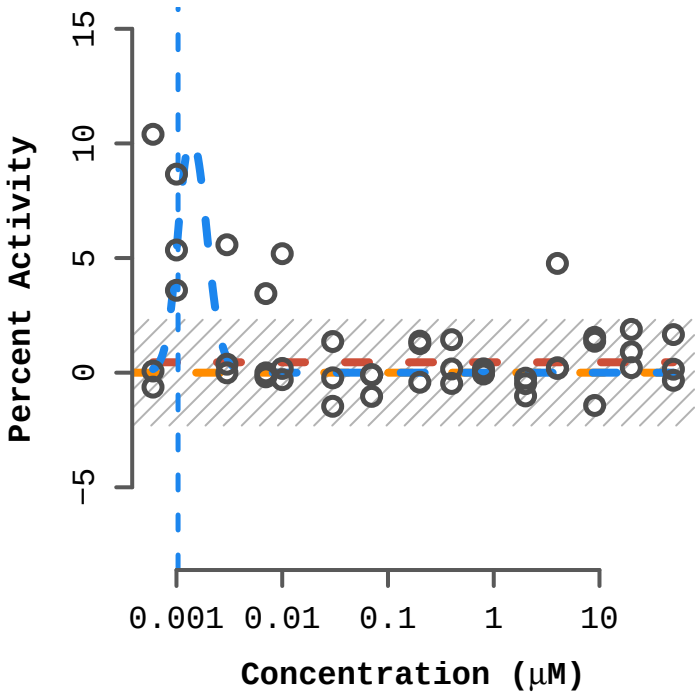
NAME: Etodolac
CHID: 20615 CASRN: 41340-25-4
SPID(S): Tox21_202218
M4ID: 12480034

HILL MODEL: Not applicable.

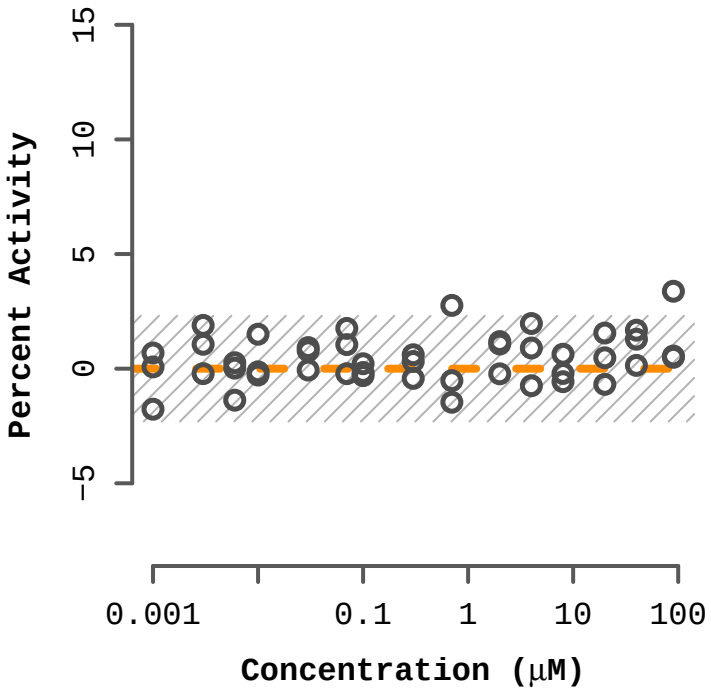
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.324 **MAX_MED:** 0.385 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Etodolac
CHID:    20615   CASRN: 41340-25-4
SPID(S): Tox21_110644_1
M4ID:    12484211

HILL MODEL (in red):
      tp       ga       gw
val:  0.454    -5.17    3.22
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.5     -2.98    8        -2.71    6.56
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  200.54      202.73      189.94
PROB: 0           0           0.99
RMSE: 2.77        2.61        2.27

MAX_MEAN: 5.87      MAX_MED: 5.35      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

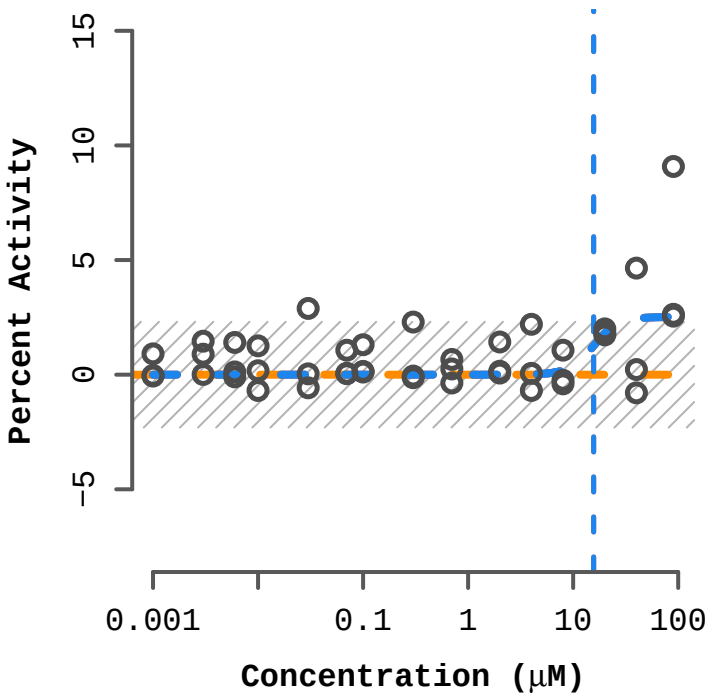
NAME: 1,8-Cineol
CHID: 20616 **CASRN:** 470-82-6
SPID(S): Tox21_302902
M4ID: 12476231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,8-Cineol
CHID: 20616 CASRN: 470-82-6
SPID(S): Tox21_202090
M4ID: 12480162

HILL MODEL (in red):

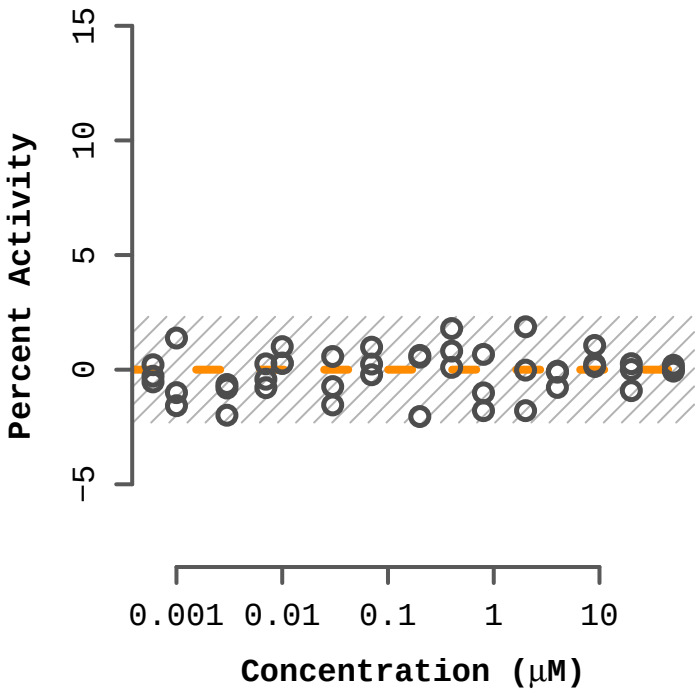
	tp	ga	gw
val:	2.52	1.2	3.74
sd:	0.621	0.125	4.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.52	1.2	3.74	3.54	4.38
sd:	0.621	0.125	4.53	556	1550

	CNST	HILL	GNLS
AIC:	165.39	152.12	156.12
PROB:	0	0.88	0.12
RMSE:	1.9	1.47	1.47

MAX_MEAN: 4.76 MAX_MED: 2.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

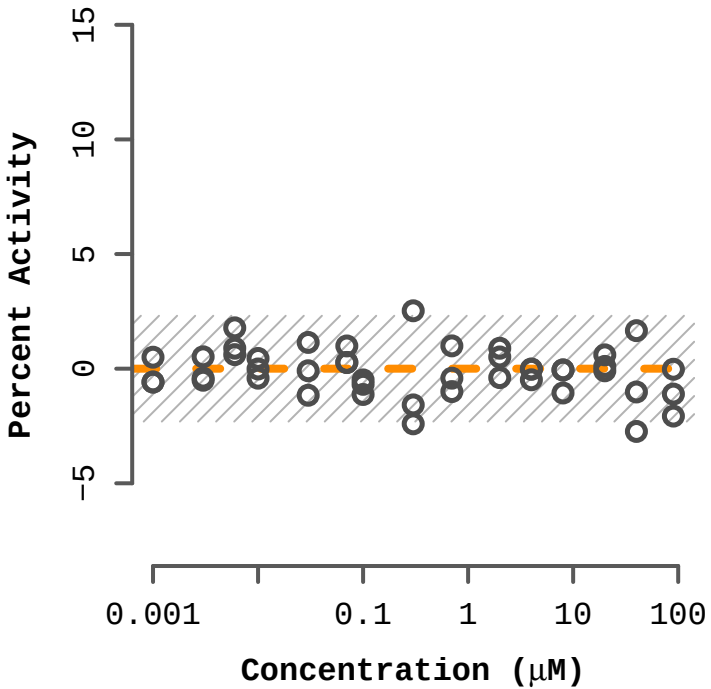
NAME: 1,8-Cineol
CHID: 20616 **CASRN:** 470-82-6
SPID(S): Tox21_111161_1
M4ID: 12483868

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.903 **MAX_MED:** 0.811 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

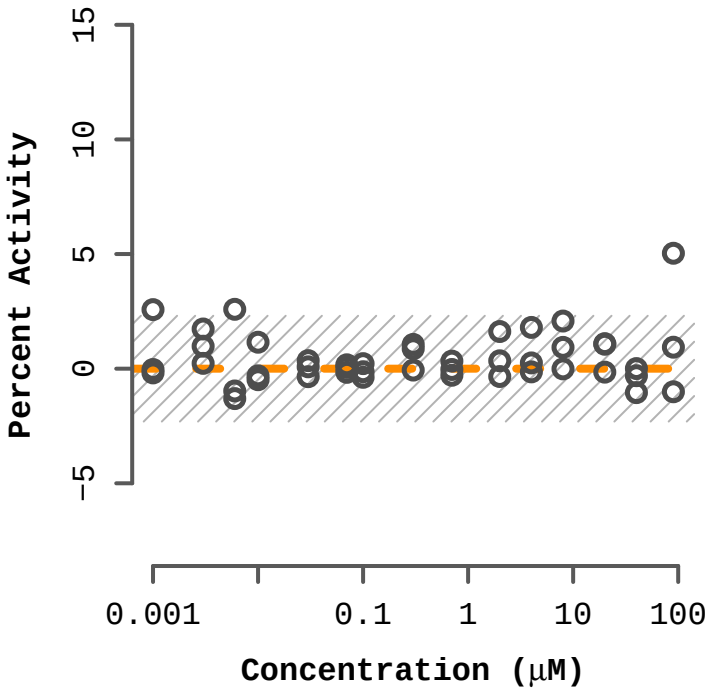
NAME: Eugenol
CHID: 20617 CASRN: 97-53-0
SPID(S): Tox21_300105
M4ID: 12479025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.1 MAX_MED: 0.893 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

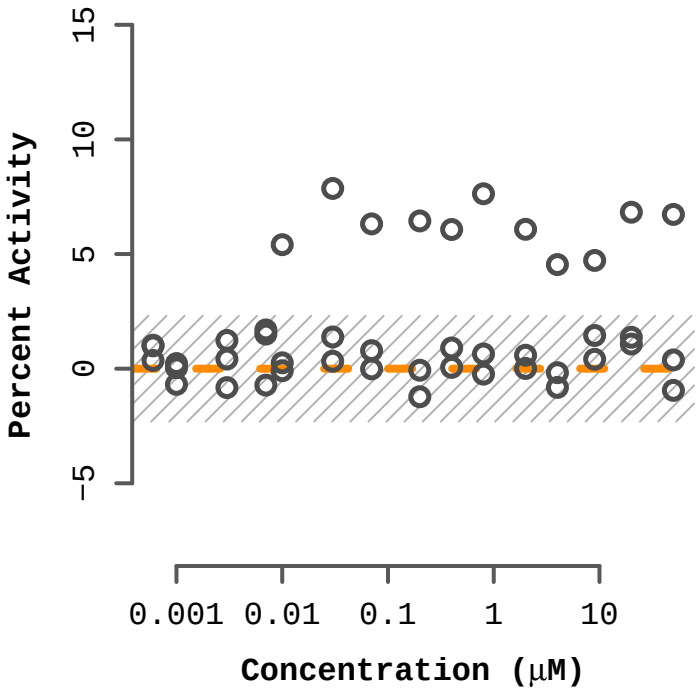
NAME: Eugenol
CHID: 20617 CASRN: 97-53-0
SPID(S): Tox21_202040
M4ID: 12480212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.66 MAX_MED: 1.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

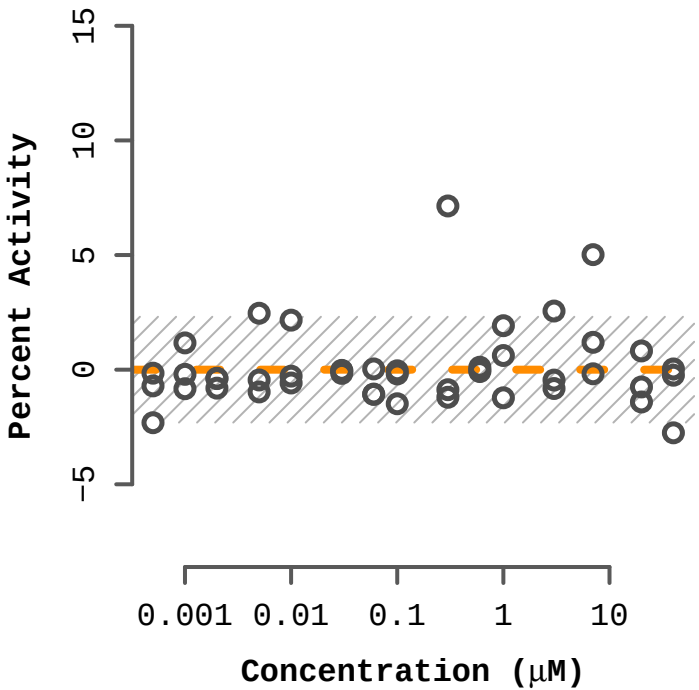
NAME: Eugenol
CHID: 20617 CASRN: 97-53-0
SPID(S): Tox21_111134_1
M4ID: 12483886

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 3.19 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

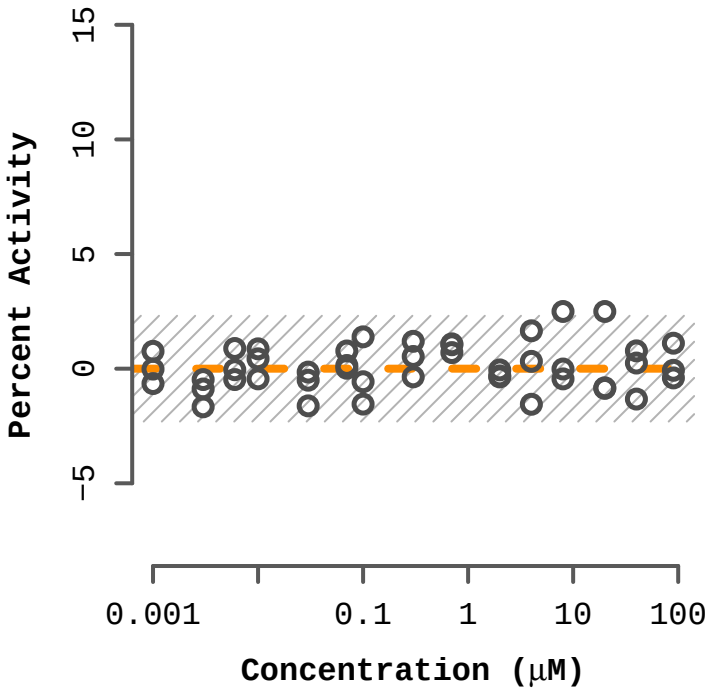
NAME: Fadrozole hydrochloride
CHID: 20618 **CASRN:** 102676-31-3
SPID(S): Tox21_303613
M4ID: 12475532

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

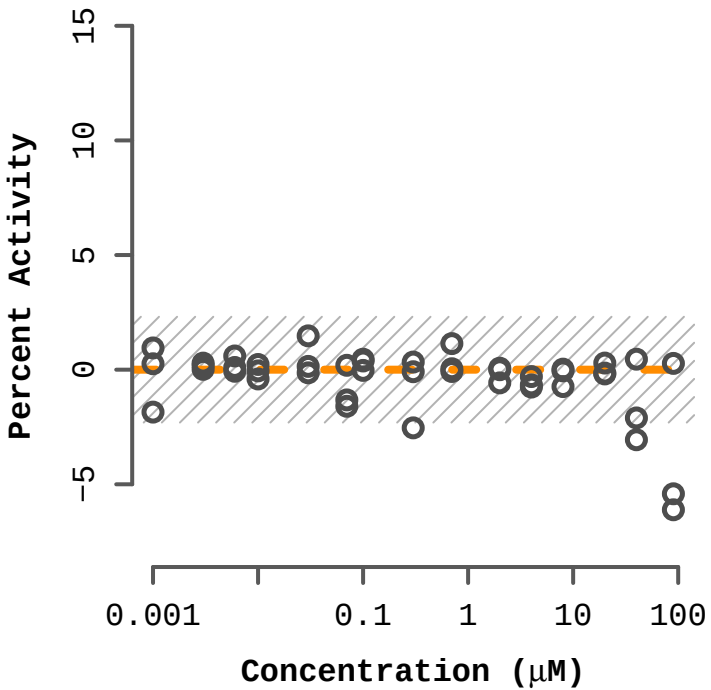
NAME: Fenthion
CHID: 20620 CASRN: 55-38-9
SPID(S): Tox21_300658
M4ID: 12478475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

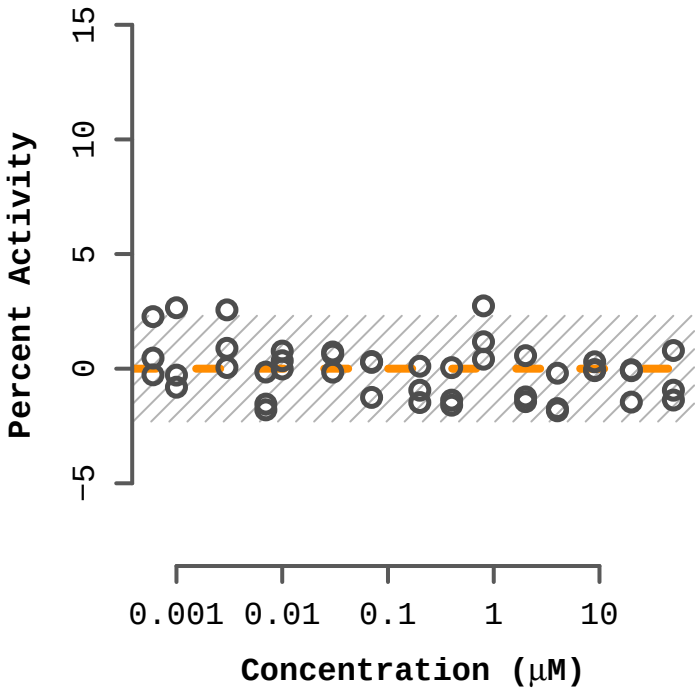
NAME: Fenthion
CHID: 20620 CASRN: 55-38-9
SPID(S): Tox21_201595
M4ID: 12480657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 0.495 **MAX_MED:** 0.381 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

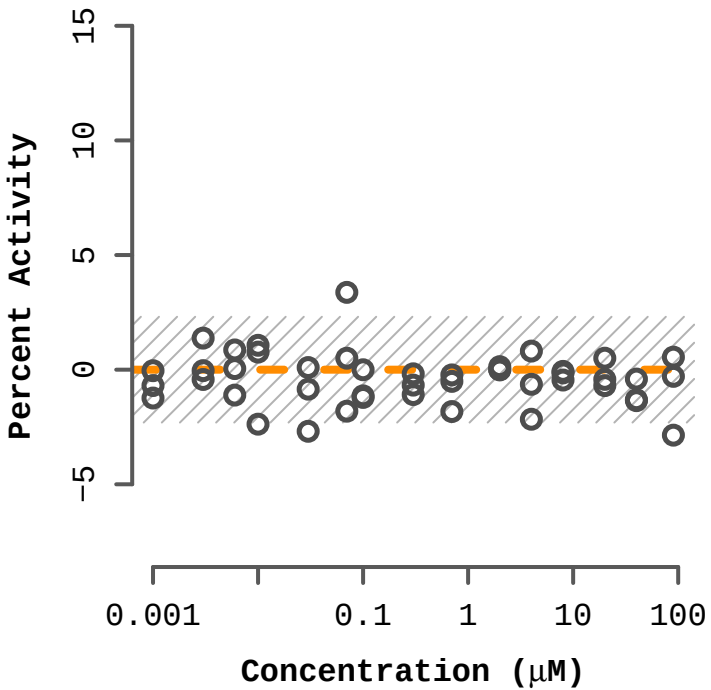
NAME: Fenthion
CHID: 20620 **CASRN:** 55-38-9
SPID(S): Tox21_111157_1
M4ID: 12483871

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

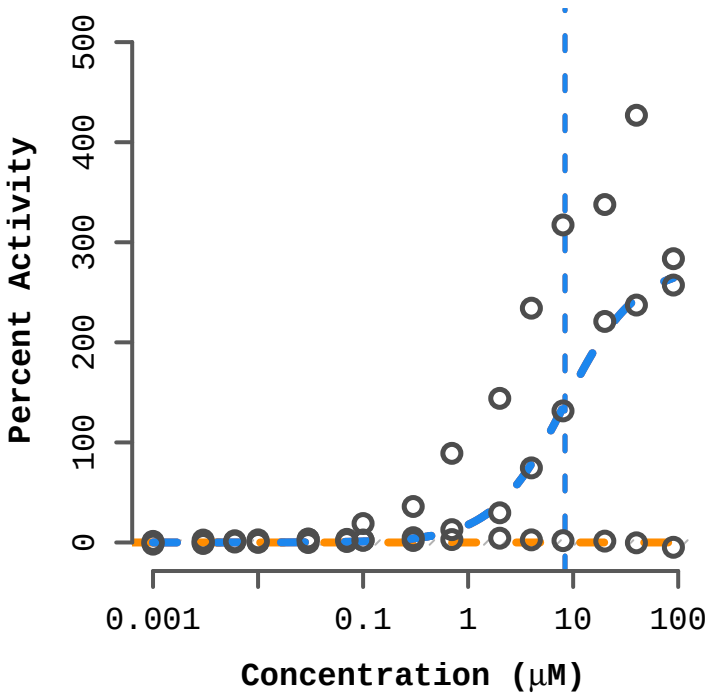
NAME: Fenvalerate
CHID: 20621 CASRN: 51630-58-1
SPID(S): Tox21_302957
M4ID: 12476176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.768 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenvalerate
CHID: 20621 **CASRN:** 51630-58-1
SPID(S): Tox21_201838
M4ID: 12480414

HILL MODEL (in red):

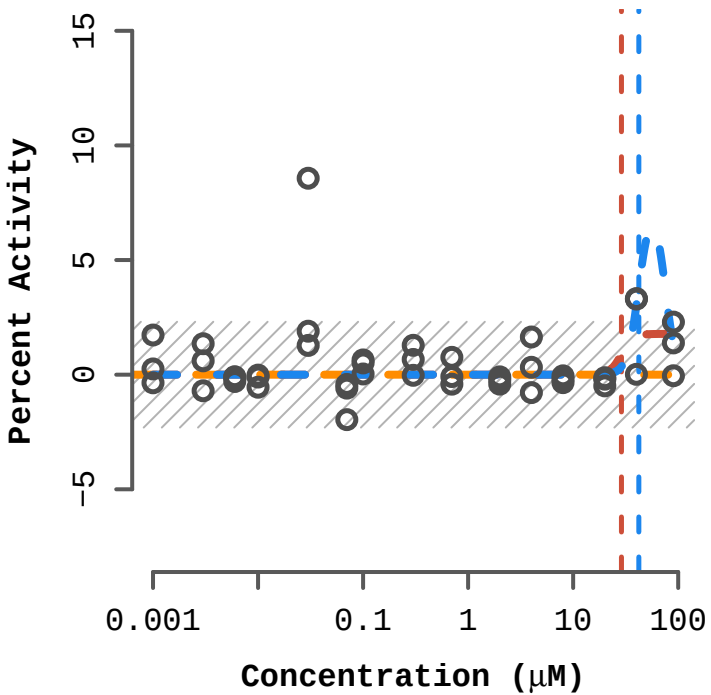
	tp	ga	gw
val:	278	0.922	1.26
sd:	39.8	0.182	0.593

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	278	0.922	1.26	3.79	8.77
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	555.6	515.79	519.79
PROB:	0	0.88	0.12
RMSE:	129.79	85.2	85.2

MAX_MEAN: 221 **MAX_MED:** 257 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ferric chloride
CHID: 20622 CASRN: 7705-08-0
SPID(S): Tox21_302918
M4ID: 12476215

HILL MODEL (in red):

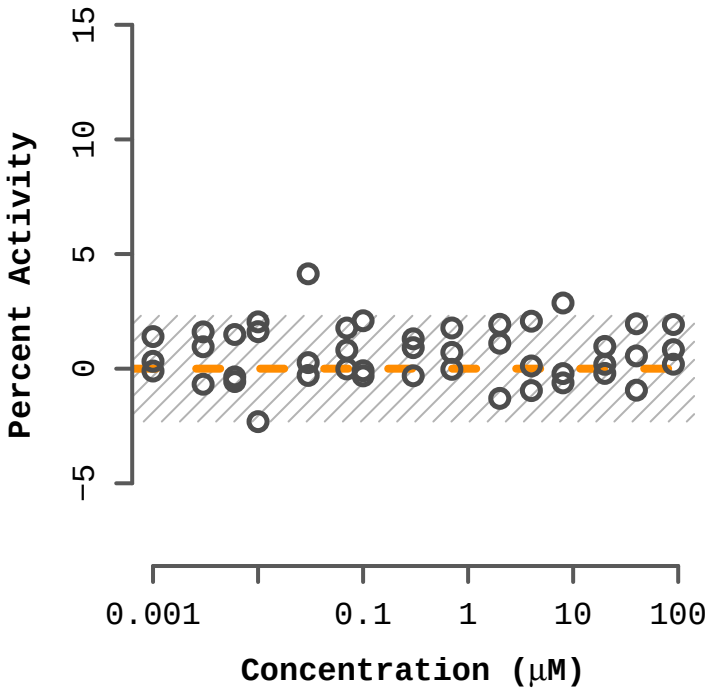
	tp	ga	gw
val:	1.78	1.46	8
sd:	0.601	0.0919	5.05

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.71	1.63	8	1.88	8.48
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	145.87	142.83	142.15
PROB:	0.08	0.38	0.54
RMSE:	1.67	1.56	1.56

MAX_MEAN: 3.91 MAX_MED: 3.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

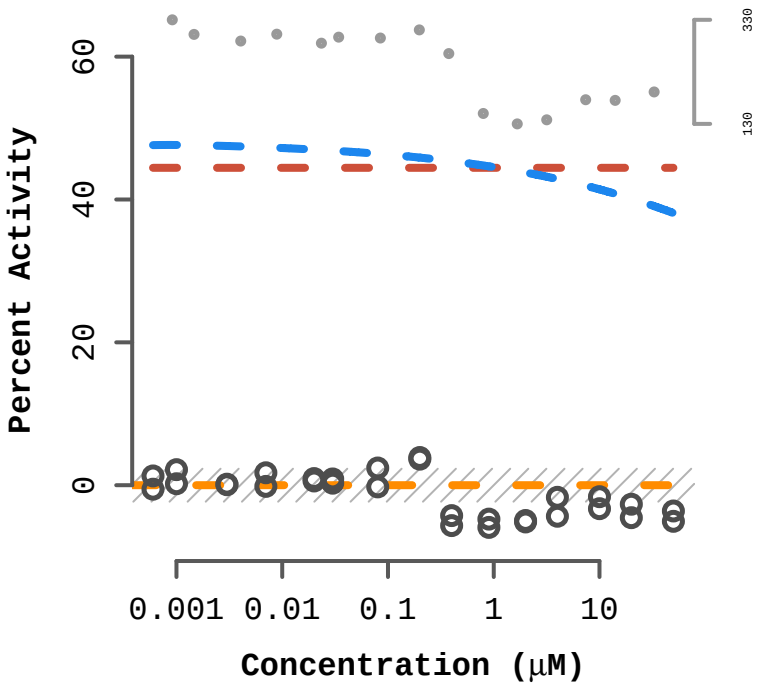
NAME: Ferric chloride
CHID: 20622 **CASRN:** 7705-08-0
SPID(S): Tox21_201882
M4ID: 12480370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ferbam
CHID: 20624 CASRN: 14484-64-1
SPID(S): Tox21_202589
M4ID: 12479663 BRK

HILL MODEL (in red):

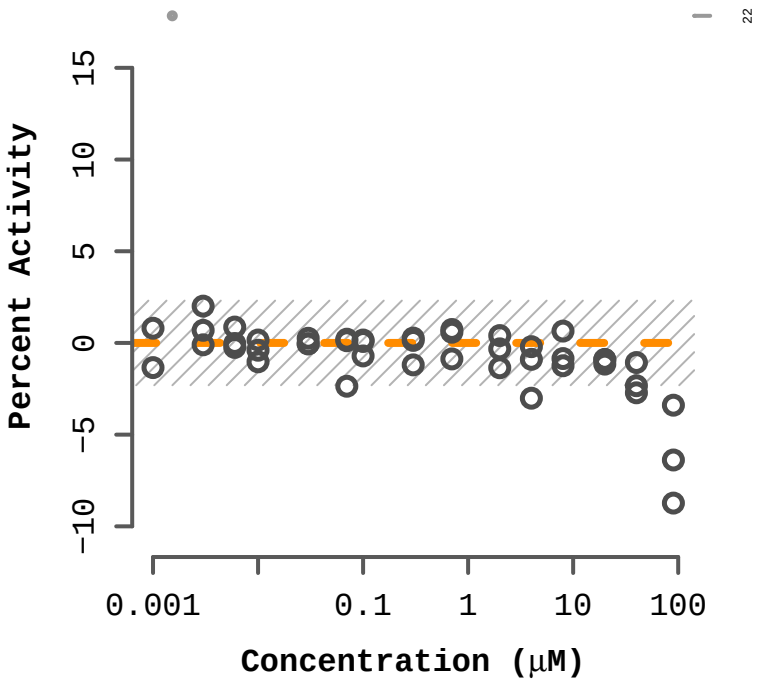
	tp	ga	gw
val:	44.4	-4.04	7.79
sd:	17.7	1600	15100

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	48.2	-4.58	1.85	3.63	0.3
sd:	665	577	859	174	42.5

	CNST	HILL	GNLS
AIC:	576.99	568.51	572.48
PROB:	0.01	0.87	0.12
RMSE:	143.29	124.61	124.1

MAX_MEAN: 109 **MAX_MED:** 3.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

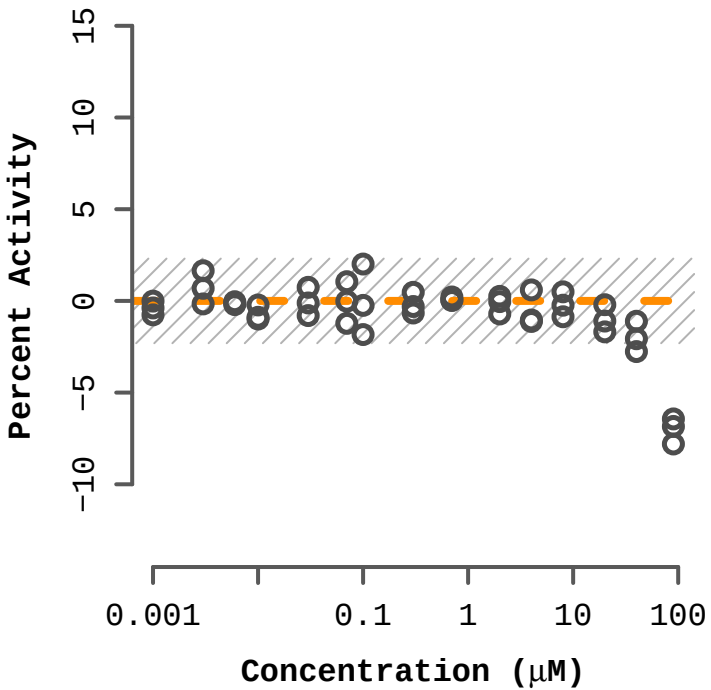
NAME: Finasteride
CHID: 20625 **CASRN:** 98319-26-7
SPID(S): Tox21_302744
M4ID: 12476389 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.89	NA	NA
PROB:	1	NA	NA
RMSE:	3.8	NA	NA

MAX_MEAN: 7.05 **MAX_MED:** 0.803 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

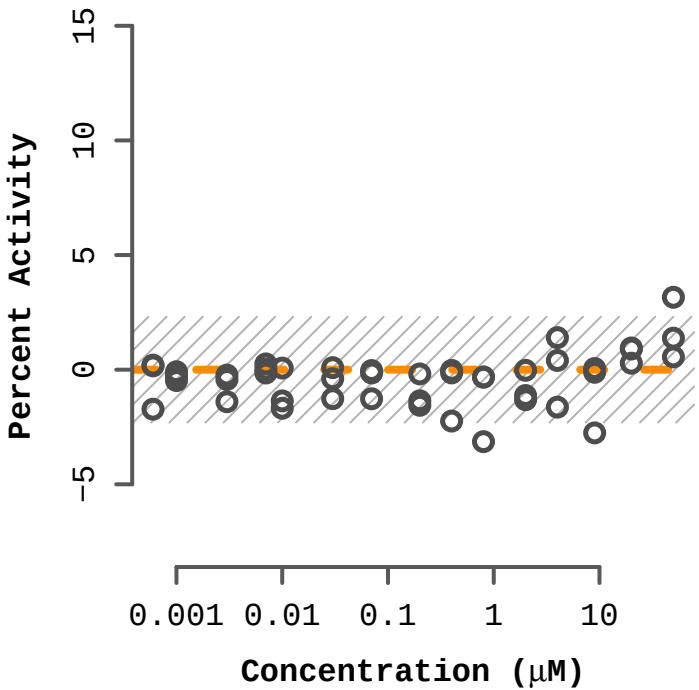
NAME: Finasteride
CHID: 20625 **CASRN:** 98319-26-7
SPID(S): Tox21_201506
M4ID: 12480746

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 0.688 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

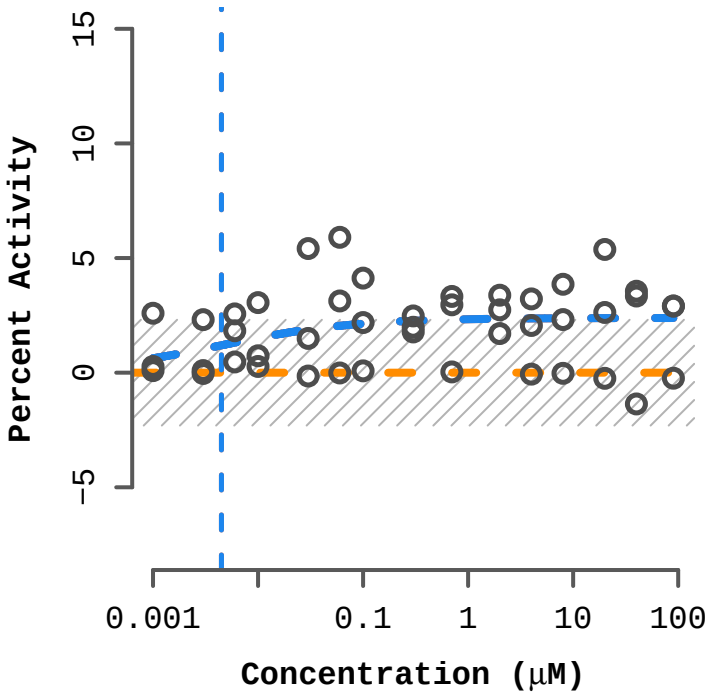
NAME: Finasteride
CHID: 20625 **CASRN:** 98319-26-7
SPID(S): Tox21_110717_1
M4ID: 12484151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flecainide acetate
CHID: 20626 CASRN: 54143-56-5
SPID(S): Tox21_200208
M4ID: 12482044

HILL MODEL (in red):

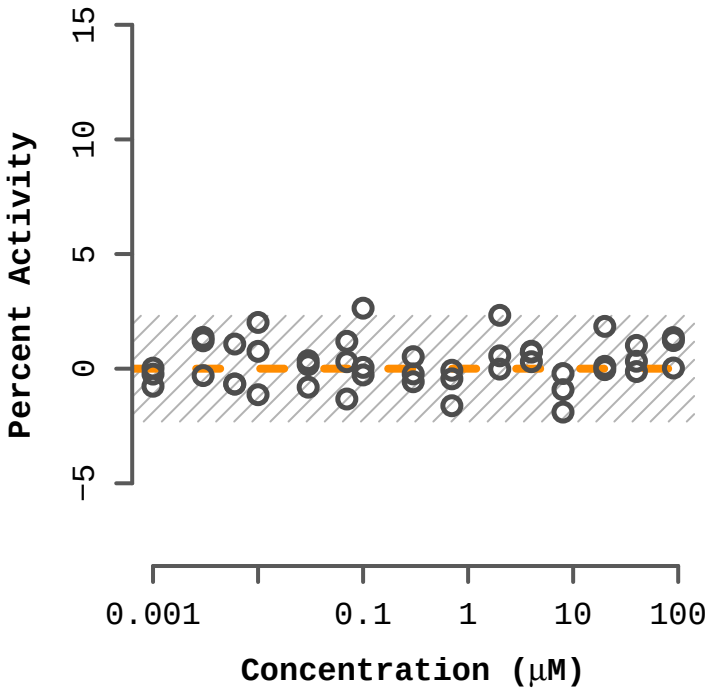
	tp	ga	gw
val:	2.39	−2.35	0.687
sd:	0.398	0.543	0.719

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.39	−2.35	0.687	3.86	6.61
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	219.1	183.34	187.34
PROB:	0	0.88	0.12
RMSE:	2.58	1.66	1.66

MAX_MEAN: 3.01 **MAX_MED:** 3.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

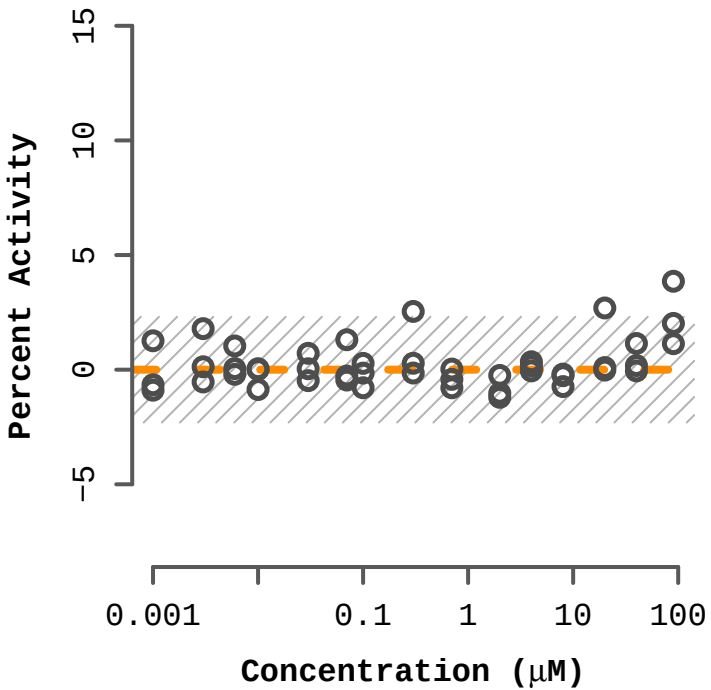
NAME: Fluconazole
CHID: 20627 CASRN: 86386-73-4
SPID(S): Tox21_300581
M4ID: 12478552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

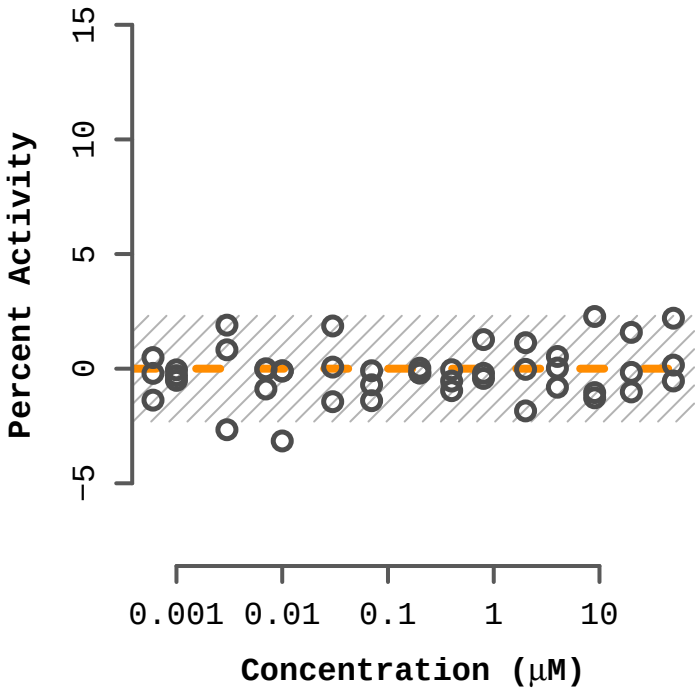
NAME: Fluconazole
CHID: 20627 CASRN: 86386-73-4
SPID(S): Tox21_202240
M4ID: 12480012

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 2.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

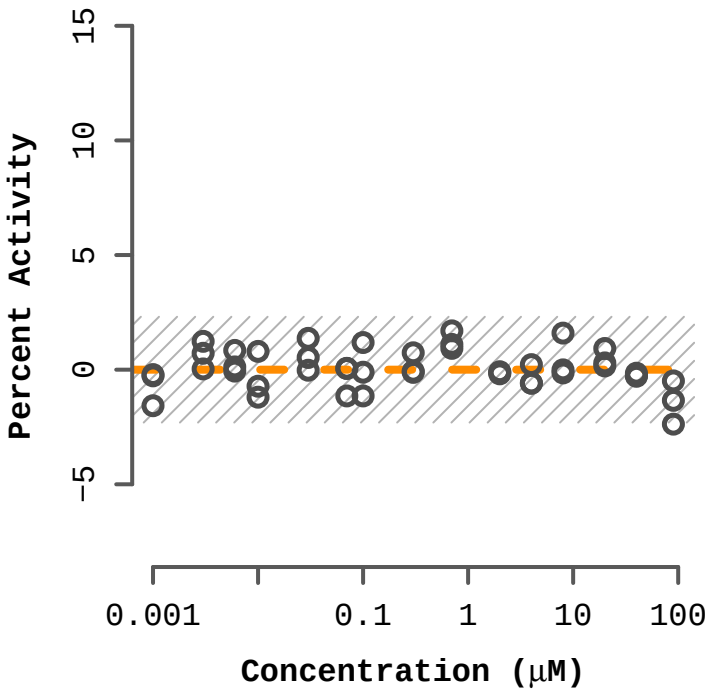
NAME: Fluconazole
CHID: 20627 **CASRN:** 86386-73-4
SPID(S): Tox21_111419_1
M4ID: 12483700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.826 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

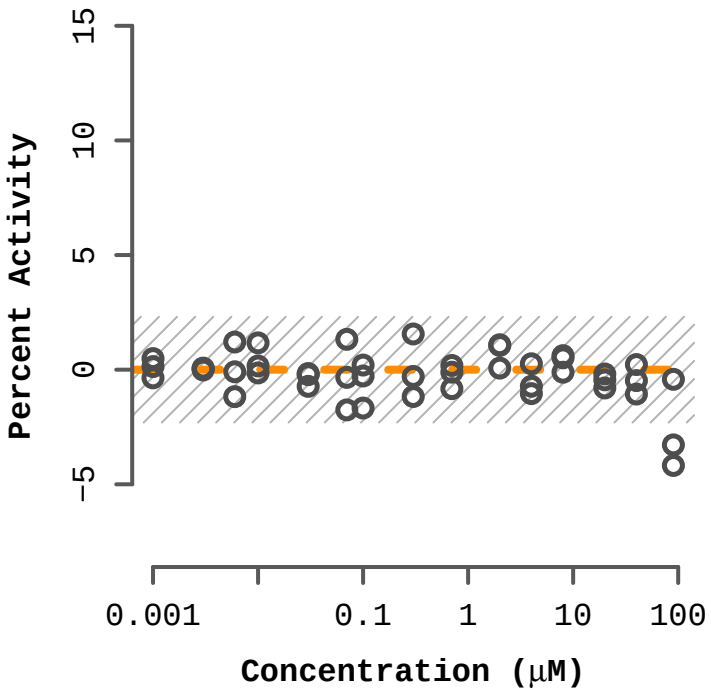
NAME: Fluometuron
CHID: 20628 **CASRN:** 2164-17-2
SPID(S): Tox21_300715
M4ID: 12478418

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

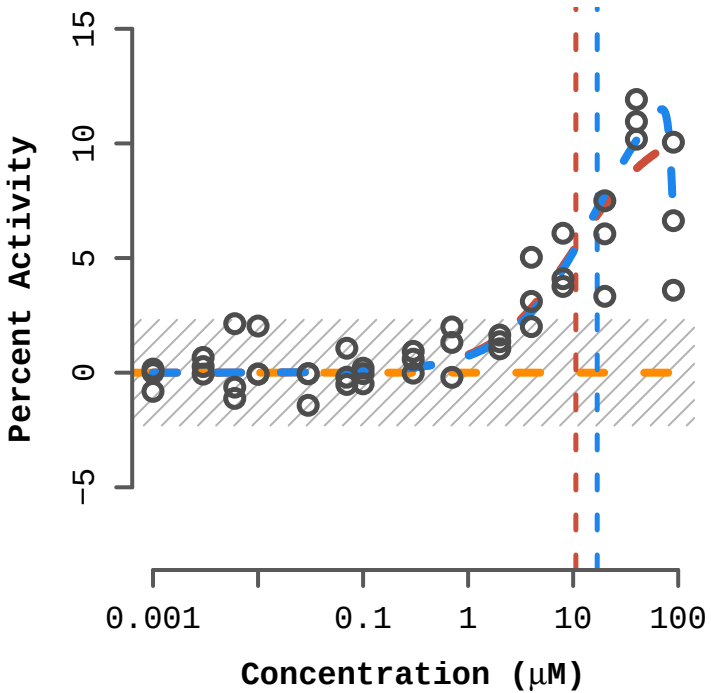
NAME: Fluometuron
CHID: 20628 **CASRN:** 2164-17-2
SPID(S): Tox21_201875
M4ID: 12480377

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(2-Fluorenyl)-2,2,2-trifluoroacetamide
CHID: 20629 CASRN: 363-17-7
SPID(S): Tox21_301891
M4ID: 12477242

HILL MODEL (in red):

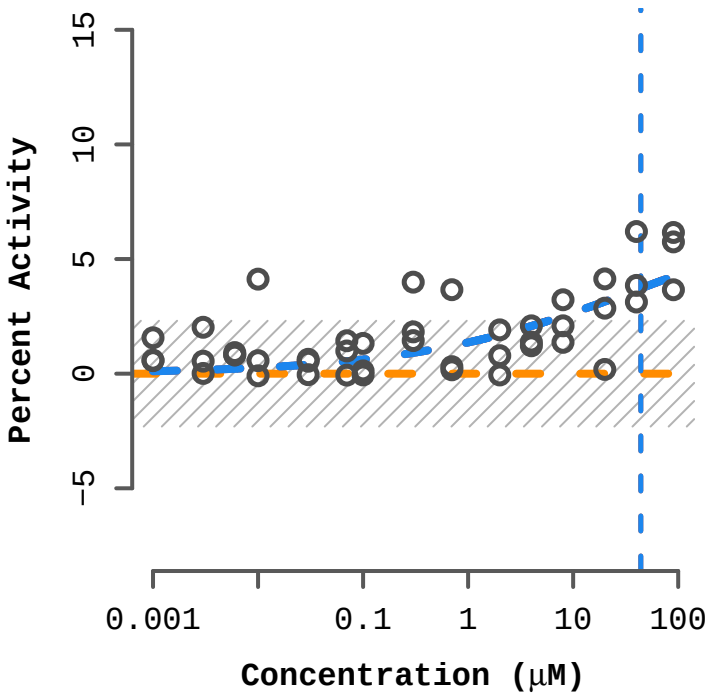
	tp	ga	gw
val:	11	1.03	1.09
sd:	1.49	0.148	0.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.3	1.23	1.03	1.96	17.2
sd:	4.12	0.265	0.186	0.0208	69.7

	CNST	HILL	GNLS
AIC:	247.24	163.75	155.43
PROB:	0	0.02	0.98
RMSE:	4.12	1.59	1.31

MAX_MEAN: 11 MAX_MED: 11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4'-Fluoro-4-aminodiphenyl
CHID: 20631 CASRN: 324-93-6
SPID(S): Tox21_302275
M4ID: 12476858

HILL MODEL (in red):

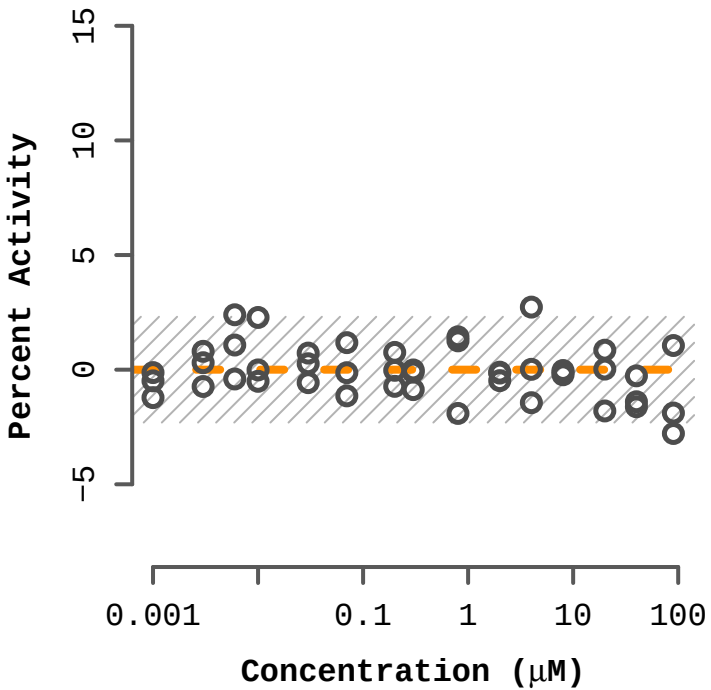
	tp	ga	gw
val:	7.44	1.64	0.395
sd:	2.66	0.72	0.128

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.44	1.64	0.395	3.21	6.05
sd:	2.66	0.721	0.128	479	2300

	CNST	HILL	GNLS
AIC:	208.56	154.7	158.7
PROB:	0	0.88	0.12
RMSE:	2.44	1.28	1.28

MAX_MEAN: 5.19 MAX_MED: 5.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

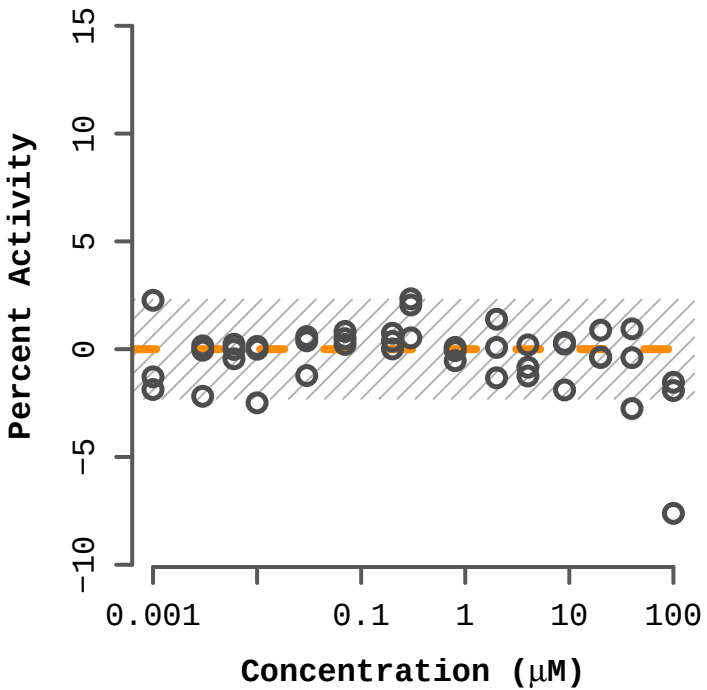
NAME: 5-Fluorouracil
CHID: 20634 CASRN: 51-21-8
SPID(S): Tox21_300112
M4ID: 12479018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.02 MAX_MED: 1.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

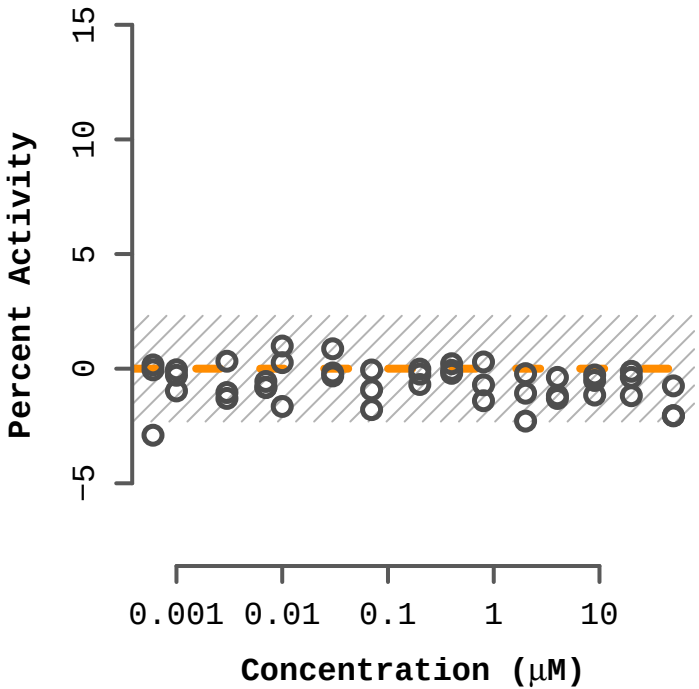
NAME: 5-Fluorouracil
CHID: 20634 CASRN: 51-21-8
SPID(S): Tox21_202335
M4ID: 12479917

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.64 MAX_MED: 2.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

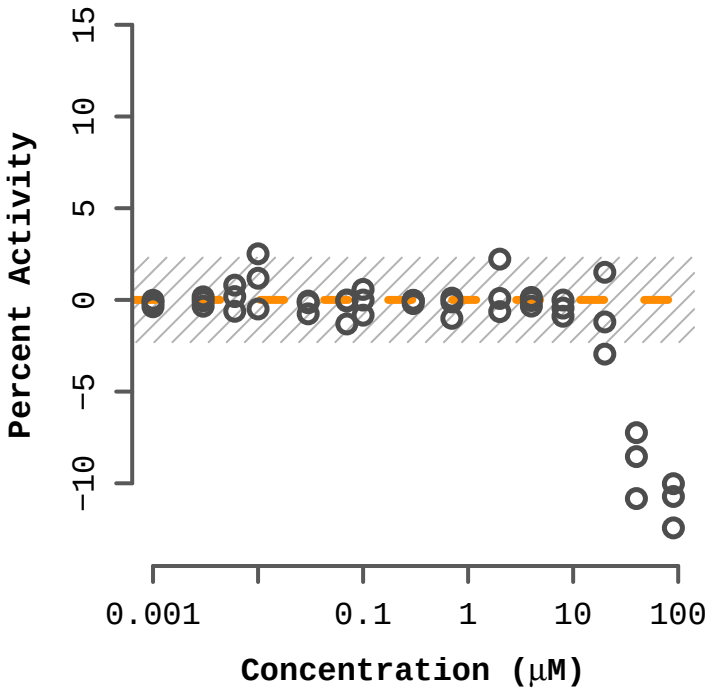
NAME: 5-Fluorouracil
CHID: 20634 **CASRN:** 51-21-8
SPID(S): Tox21_110150_1
M4ID: 12484607

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.124 **MAX_MED:** 0.266 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

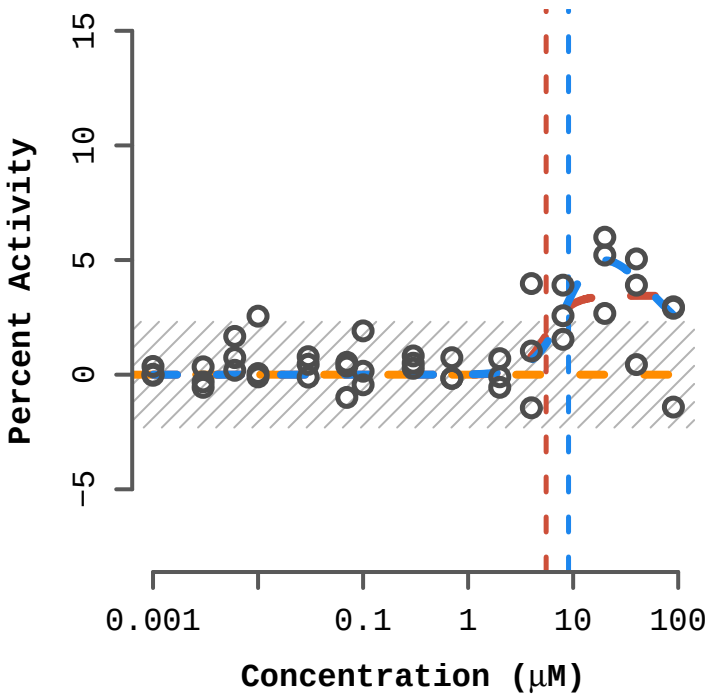
NAME: Fluoxetine hydrochloride
CHID: 20635 CASRN: 56296-78-7
SPID(S): Tox21_200182
M4ID: 12482070

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.45	NA	NA
PROB:	1	NA	NA
RMSE:	3.79	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluvastatin
CHID: 20636 **CASRN:** 93957-54-1
SPID(S): Tox21_302765
M4ID: 12476368

HILL MODEL (in red):

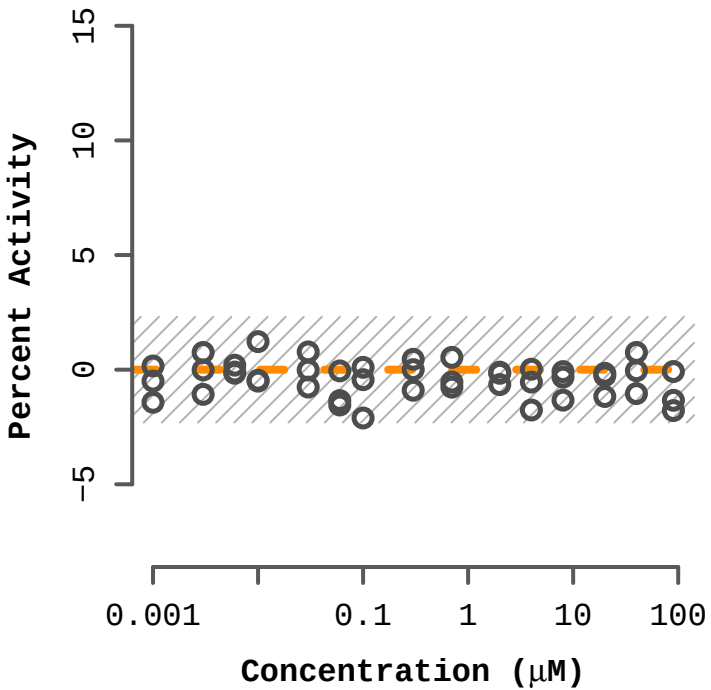
	tp	ga	gw
val:	3.44	0.743	3.66
sd:	0.485	0.128	2.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.2	0.956	2.82	1.74	1.17
sd:	5.86	0.164	1.69	0.645	1.1

	CNST	HILL	GNLS
AIC:	188.54	154.57	152.21
PROB:	0	0.23	0.77
RMSE:	2.07	1.36	1.29

MAX_MEAN: 4.63 **MAX_MED:** 5.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

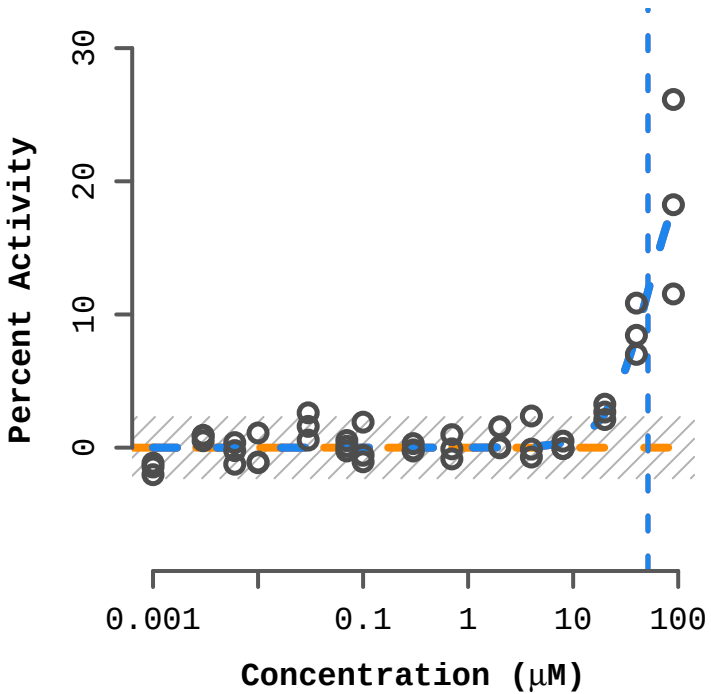
NAME: Furan
CHID: 20646 **CASRN:** 110-00-9
SPID(S): Tox21_200920
M4ID: 12481332

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.089 **MAX_MED:** 0.00415 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Furfural
CHID: 20647 CASRN: 98-01-1
SPID(S): Tox21_300170
M4ID: 12478960

HILL MODEL (in red):

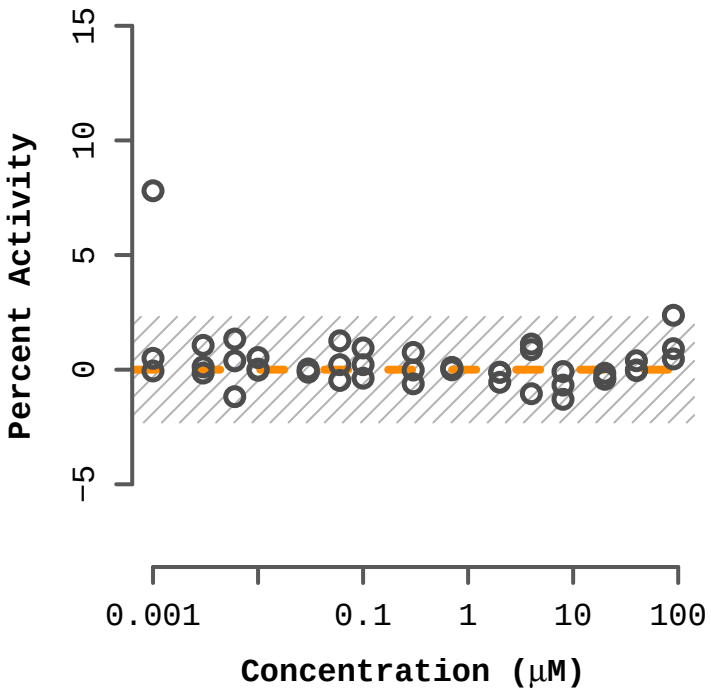
	tp	ga	gw
val:	23.5	1.71	2.21
sd:	4.44	0.101	0.457

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.5	1.71	2.21	3.88	3.23
sd:	4.44	0.101	0.457	1090	1920

	CNST	HILL	GNLS
AIC:	241.13	168.53	172.53
PROB:	0	0.88	0.12
RMSE:	5.68	1.87	1.87

MAX_MEAN: 18.6 MAX_MED: 18.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

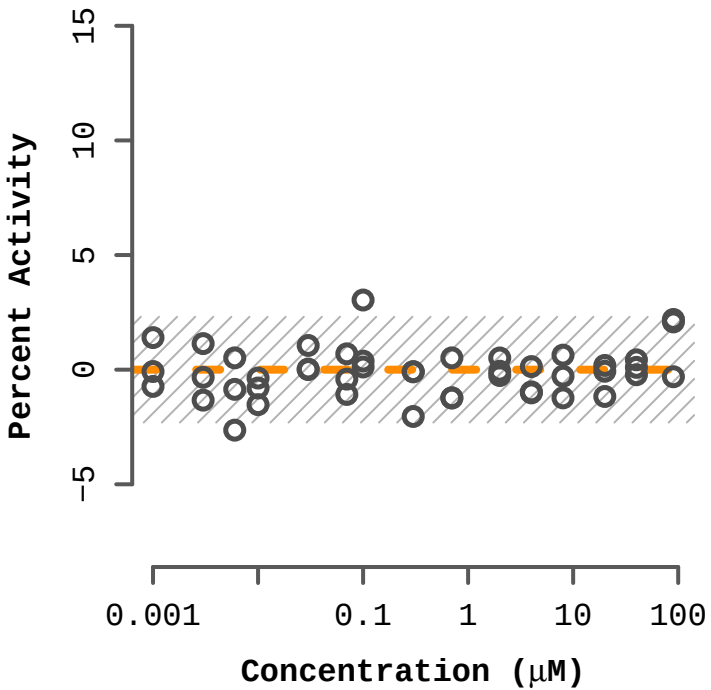
NAME: Furfural
CHID: 20647 CASRN: 98-01-1
SPID(S): Tox21_202191
M4ID: 12480061

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 2.75 MAX_MED: 0.918 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

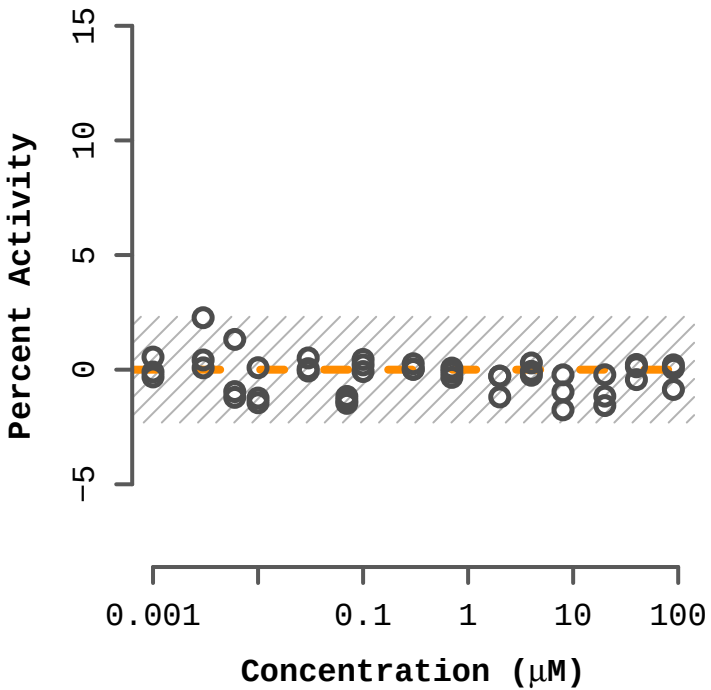
NAME: Furosemide
CHID: 20648 **CASRN:** 54-31-9
SPID(S): Tox21_302971
M4ID: 12476162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

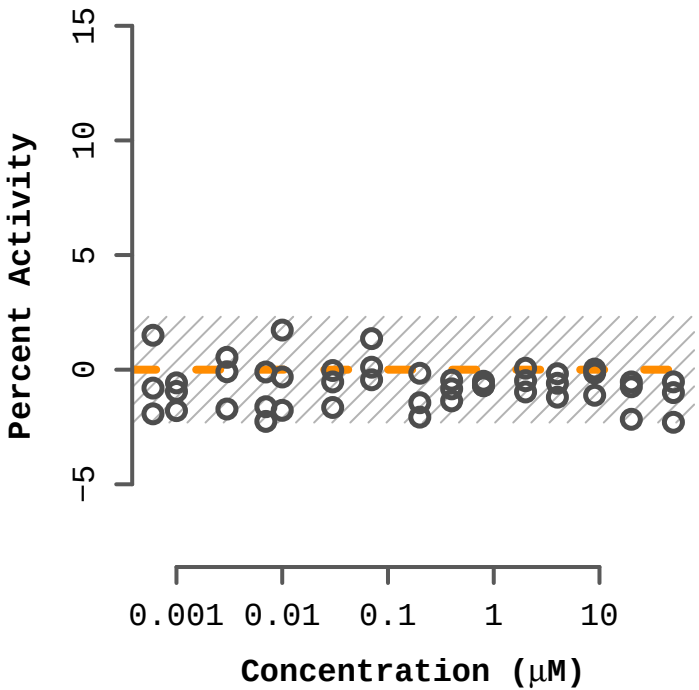
NAME: Furosemide
CHID: 20648 CASRN: 54-31-9
SPID(S): Tox21_202213
M4ID: 12480039

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.926 MAX_MED: 0.426 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

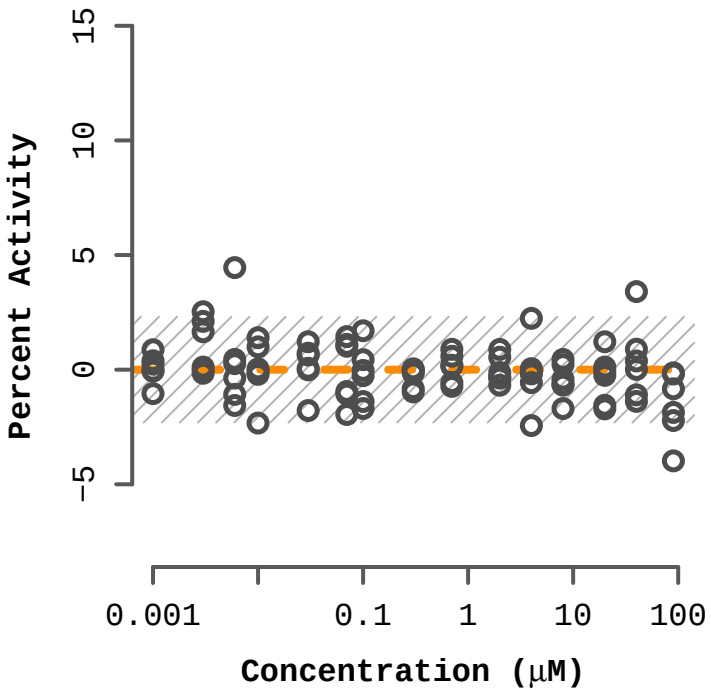
NAME: Furosemide
CHID: 20648 **CASRN:** 54-31-9
SPID(S): Tox21_110322_1
M4ID: 12484457

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.341 **MAX_MED:** 0.109 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

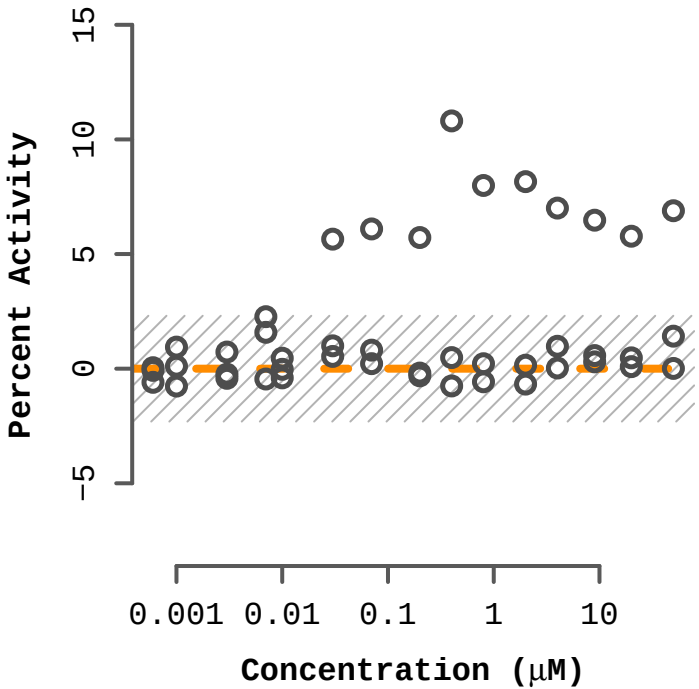
NAME: Gallic acid
CHID: 20650 **CASRN:** 149-91-7
SPID(S): Tox21_202515
M4ID: 12479737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	288.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.885 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

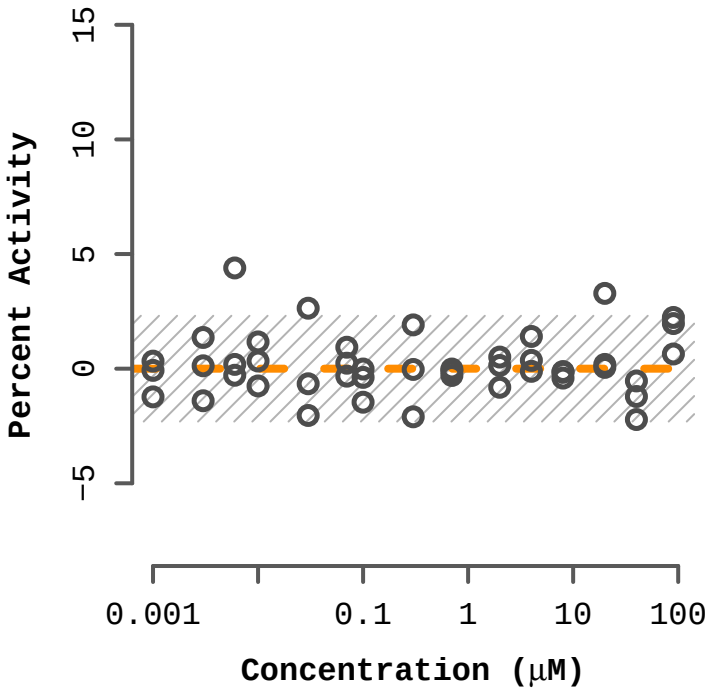
NAME: Gallic acid
CHID: 20650 CASRN: 149-91-7
SPID(S): Tox21_111089_1
M4ID: 12483914

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.58	NA	NA
PROB:	1	NA	NA
RMSE:	3.46	NA	NA

MAX_MEAN: 3.51 MAX_MED: 1.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

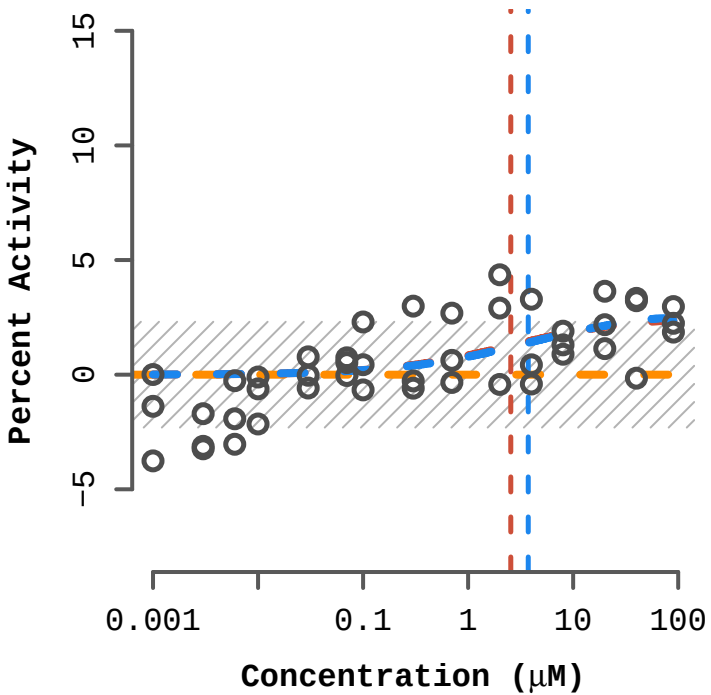
NAME: Gemfibrozil
CHID: 20652 **CASRN:** 25812-30-0
SPID(S): Tox21_302784
M4ID: 12476349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Gemfibrozil
CHID: 20652 CASRN: 25812-30-0
SPID(S): Tox21_201997
M4ID: 12480255

HILL MODEL (in red):

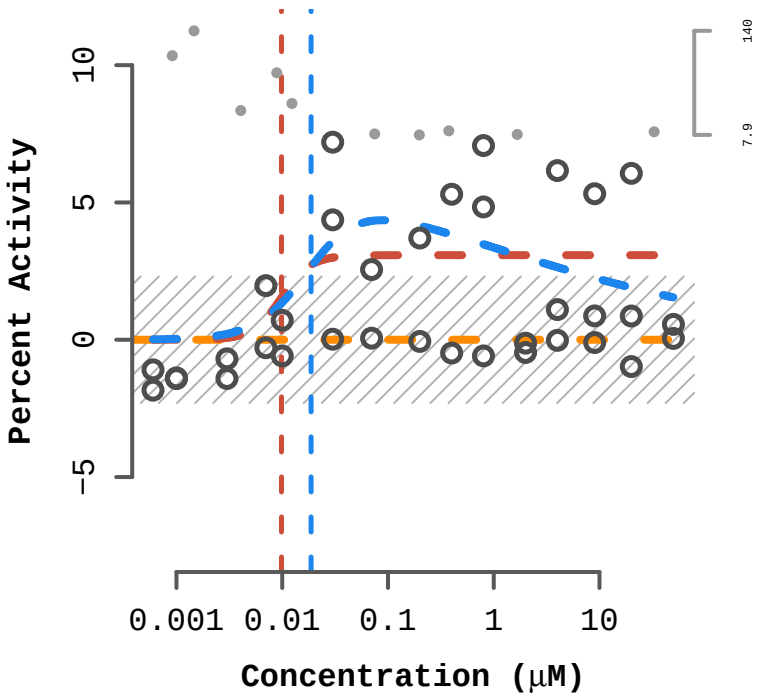
	tp	ga	gw
val:	2.54	0.406	0.754
sd:	1.1	1	0.448

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.78	0.572	0.711	2.07	10.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	197.08	179.84	183.84
PROB:	0	0.88	0.12
RMSE:	2.03	1.59	1.6

MAX_MEAN: 2.36 MAX_MED: 3.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Gemfibrozil
CHID: 20652 CASRN: 25812-30-0
SPID(S): Tox21_110613_1
M4ID: 12484232 BRK

HILL MODEL (in red):

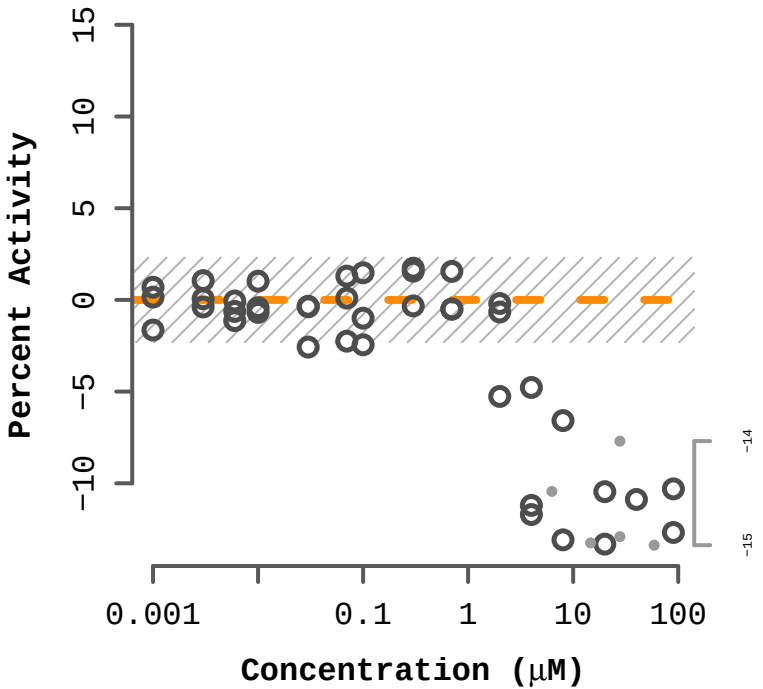
	tp	ga	gw
val:	3.08	−2.01	3.16
sd:	0.942	0.473	7.08

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.11	−1.73	1.8	−0.157	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	366.57	362.28	365.46
PROB:	0.09	0.76	0.15
RMSE:	30.51	30.27	30.27

MAX_MEAN: 44.8 **MAX_MED:** 5.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

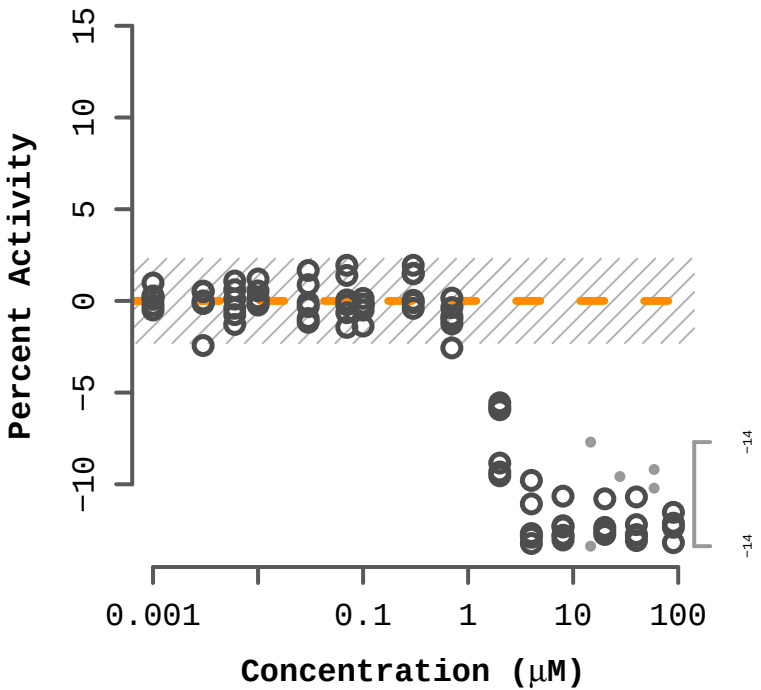
NAME: Gentian Violet
CHID: 20653 **CASRN:** 548-62-9
SPID(S): Tox21_300571
M4ID: 12478562 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	304.35	NA	NA
PROB:	1	NA	NA
RMSE:	7.18	NA	NA

MAX_MEAN: 0.991 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

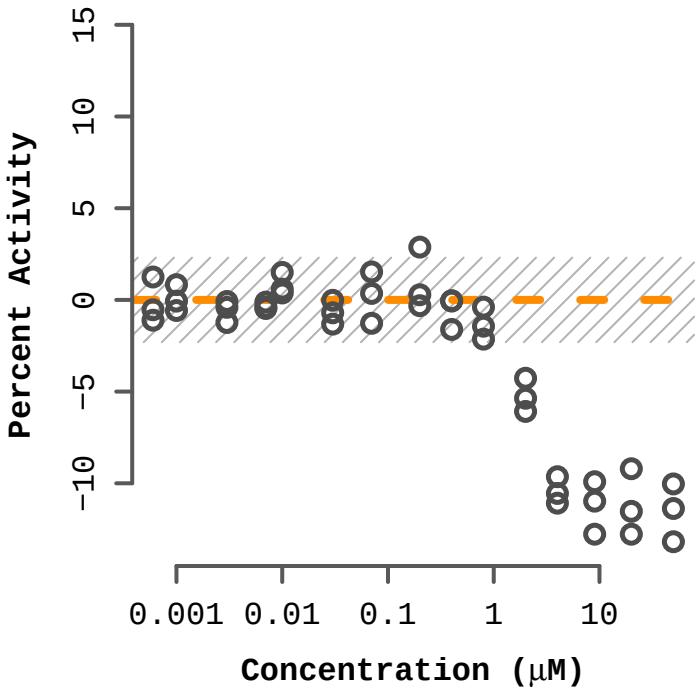
NAME: Gentian Violet
CHID: 20653 **CASRN:** 548-62-9
SPID(S): Tox21_201762
M4ID: 12480490 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	622.77	NA	NA
PROB:	1	NA	NA
RMSE:	7.54	NA	NA

MAX_MEAN: 0.744 **MAX_MED:** 0.755 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

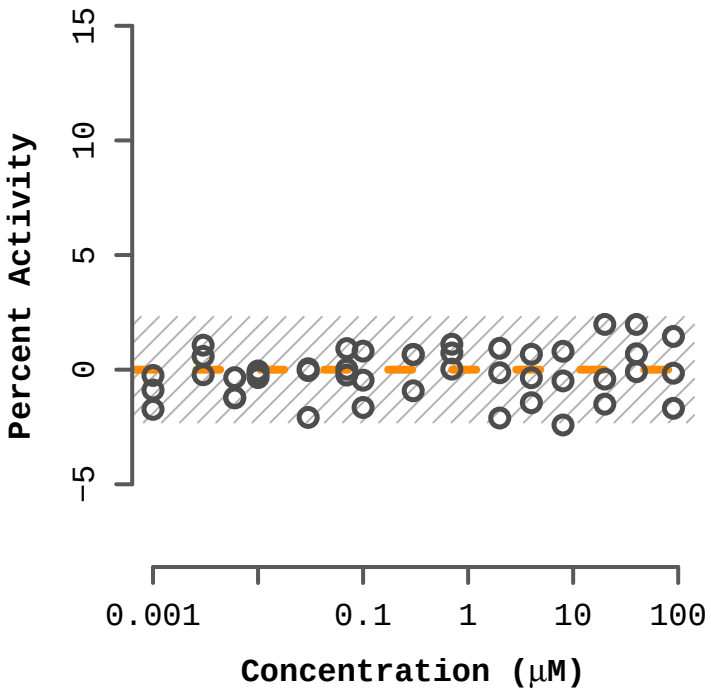
NAME: Gentian Violet
CHID: 20653 **CASRN:** 548-62-9
SPID(S): Tox21_111084_1
M4ID: 12483917

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	287.05	NA	NA
PROB:	1	NA	NA
RMSE:	5.98	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 0.588 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

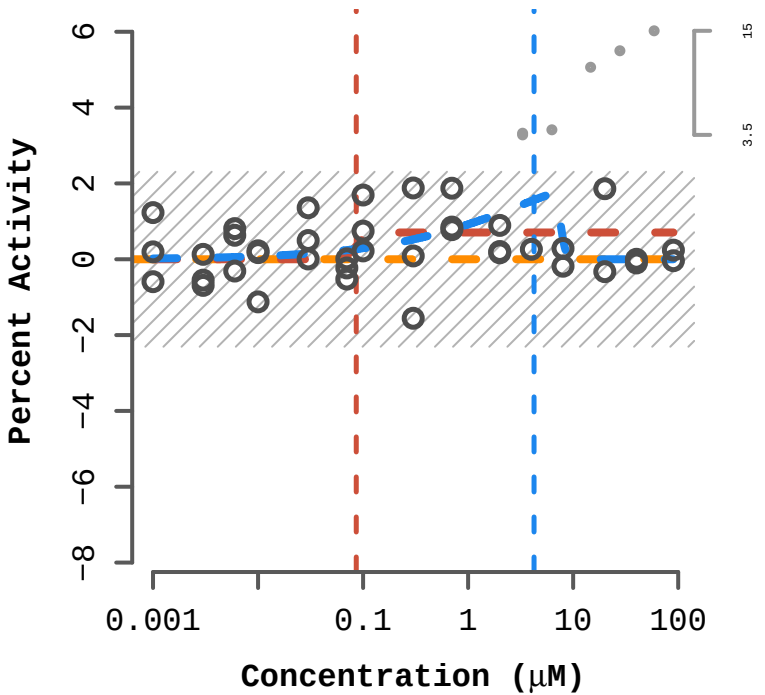
NAME: Geranyl acetate
CHID: 20654 **CASRN:** 105-87-3
SPID(S): Tox21_300355
M4ID: 12478777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.862 **MAX_MED:** 0.731 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Geranyl acetate
CHID: 20654 **CASRN:** 105-87-3
SPID(S): Tox21_202089
M4ID: 12480163 **BRK**

HILL MODEL (in red):

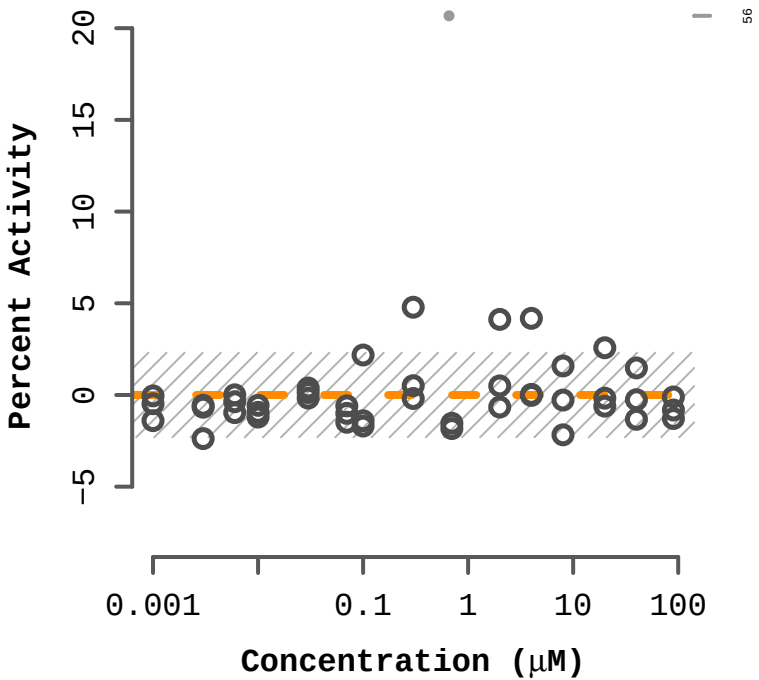
	tp	ga	gw
val:	0.706	−1.07	8
sd:	0.267	0.123	12.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.12	0.627	0.605	0.881	17.9
sd:	22.6	7.57	0.456	0.264	205

	CNST	HILL	GNLS
AIC:	195.66	193.74	197.17
PROB:	0.25	0.64	0.12
RMSE:	3.62	3.39	3.55

MAX_MEAN: 5.13 **MAX_MED:** 3.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

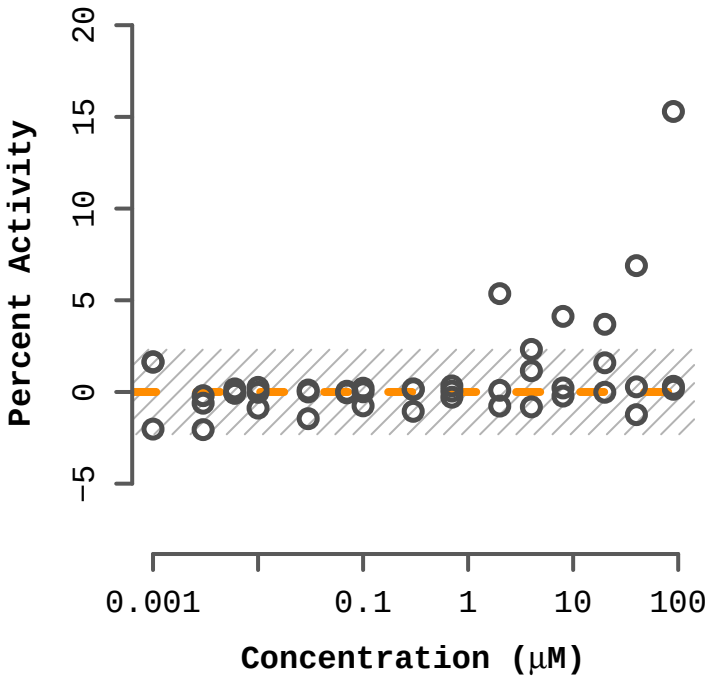
NAME: Gibberellic acid
CHID: 20656 CASRN: 77-06-5
SPID(S): Tox21_303023
M4ID: 12476110 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.78	NA	NA
PROB:	1	NA	NA
RMSE:	8.54	NA	NA

MAX_MEAN: 17.6 MAX_MED: 0.507 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

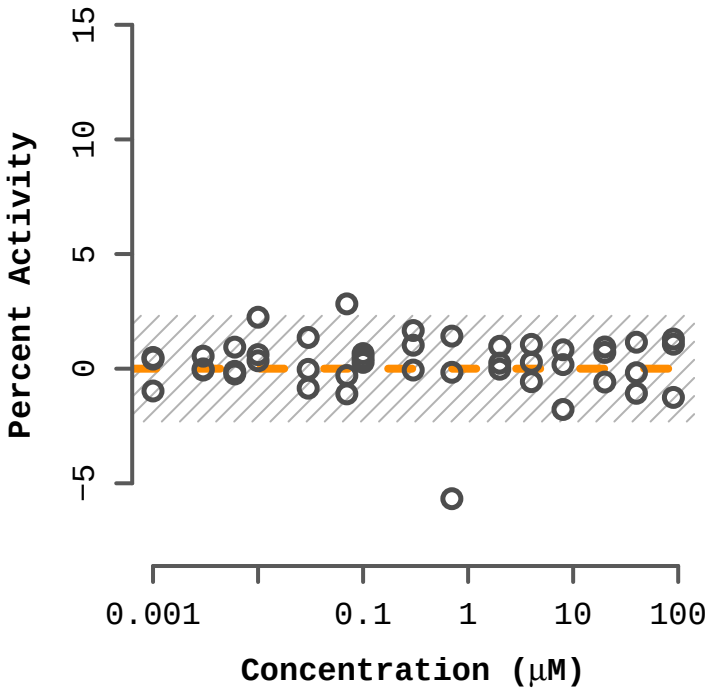
NAME: Gibberellic acid
CHID: 20656 CASRN: 77-06-5
SPID(S): Tox21_202052
M4ID: 12480200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 5.25 MAX_MED: 1.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

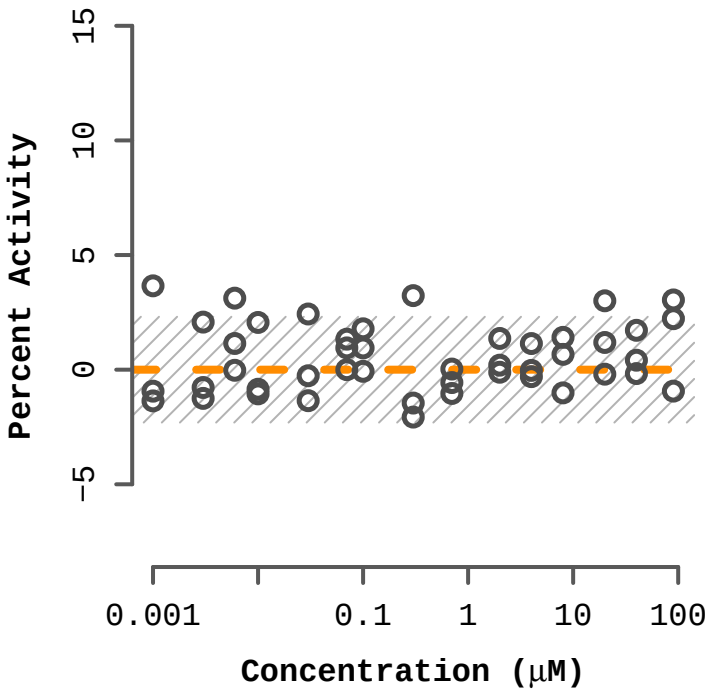
NAME: Glycerol
CHID: 20663 CASRN: 56-81-5
SPID(S): Tox21_300144
M4ID: 12478986

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.07 MAX_MED: 1.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

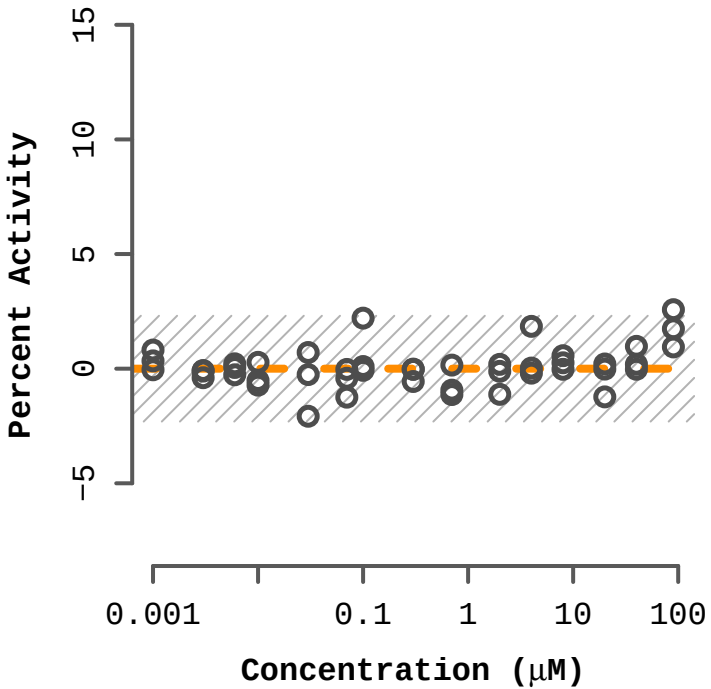
NAME: Glycerol
CHID: 20663 CASRN: 56-81-5
SPID(S): Tox21_202077
M4ID: 12480175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

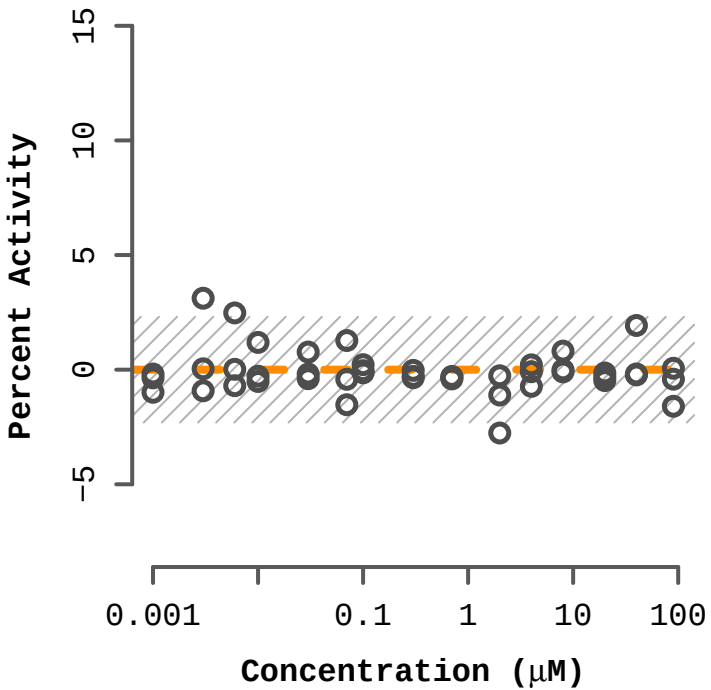
NAME: 3-Chloro-1,2-propanediol
CHID: 20664 **CASRN:** 96-24-2
SPID(S): Tox21_302959
M4ID: 12476174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

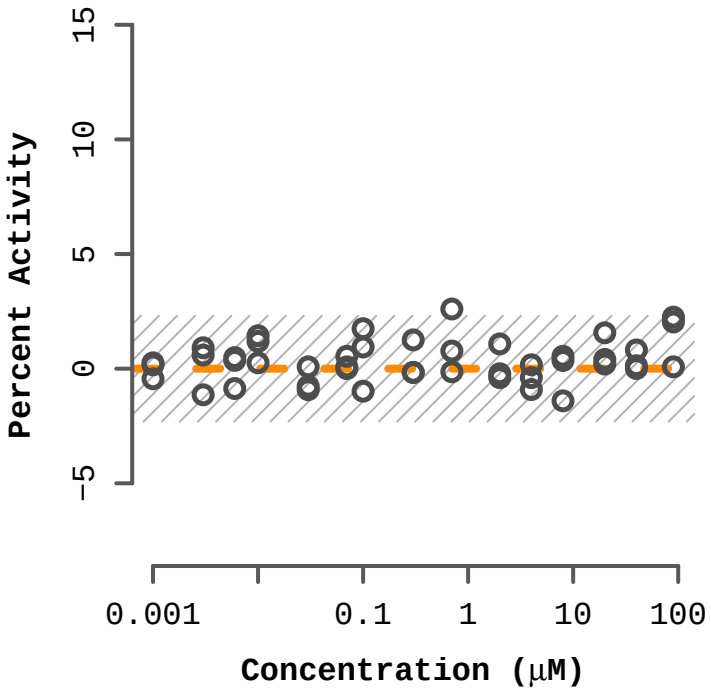
NAME: 3-Chloro-1,2-propanediol
CHID: 20664 **CASRN:** 96-24-2
SPID(S): Tox21_202262
M4ID: 12479990

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.746 **MAX_MED:** 0.0397 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

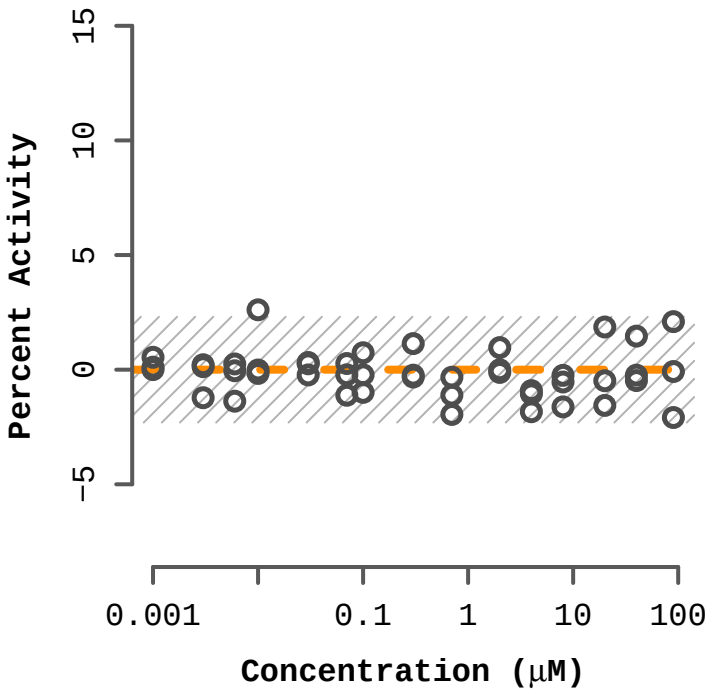
NAME: Glycidol
CHID: 20666 **CASRN:** 556-52-5
SPID(S): Tox21_300301
M4ID: 12478829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

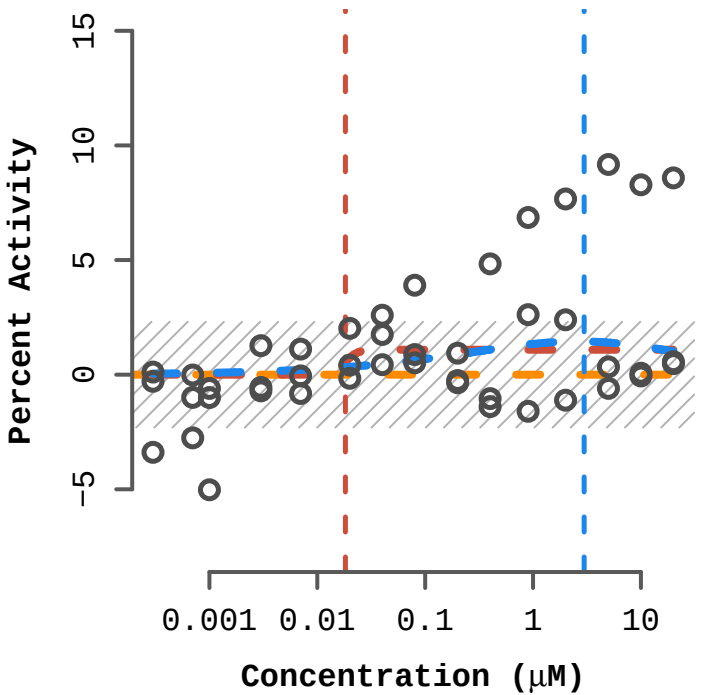
NAME: Glycidol
CHID: 20666 **CASRN:** 556-52-5
SPID(S): Tox21_201309
M4ID: 12480943

HILL MODEL: Not applicable.

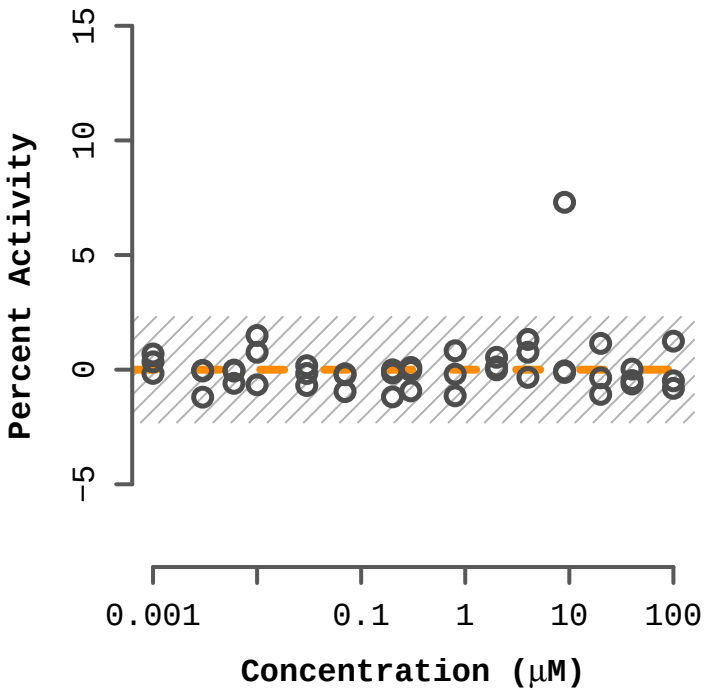
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.813 **MAX_MED:** 0.257 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Glycine
CHID:    20667   CASRN: 56-40-6
SPID(S): Tox21_113575_1
M4ID:    12482602

HILL MODEL (in red):
      tp       ga       gw
val:  1.09     -1.74    8
sd:   0.472    0.38     49.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.85     0.474    0.511    0.724    0.683
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  222.72      222.24      227.65
PROB: 0.43        0.54        0.04
RMSE: 3.19        2.85        2.84

MAX_MEAN: 3.21      MAX_MED: 2.62      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

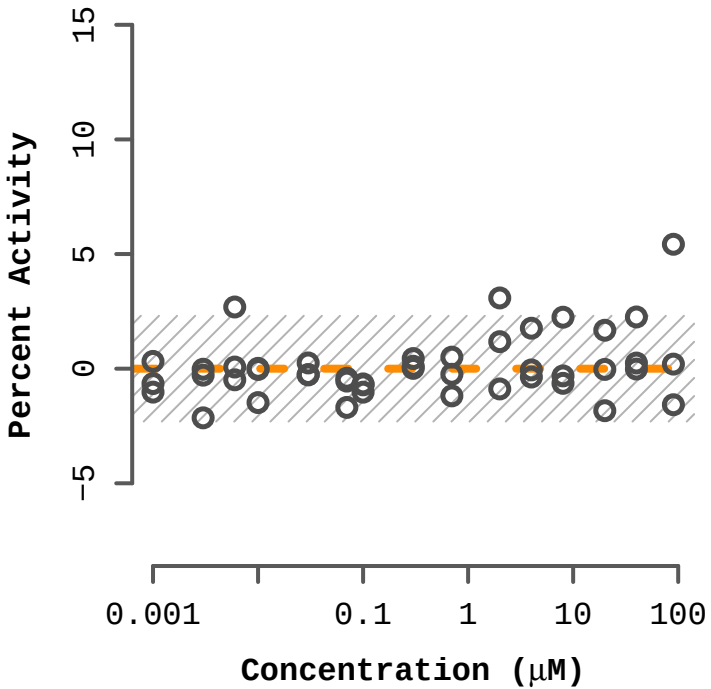
NAME: Glycol sulfite
CHID: 20668 **CASRN:** 3741-38-6
SPID(S): Tox21_200499
M4ID: 12481753

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 0.762 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

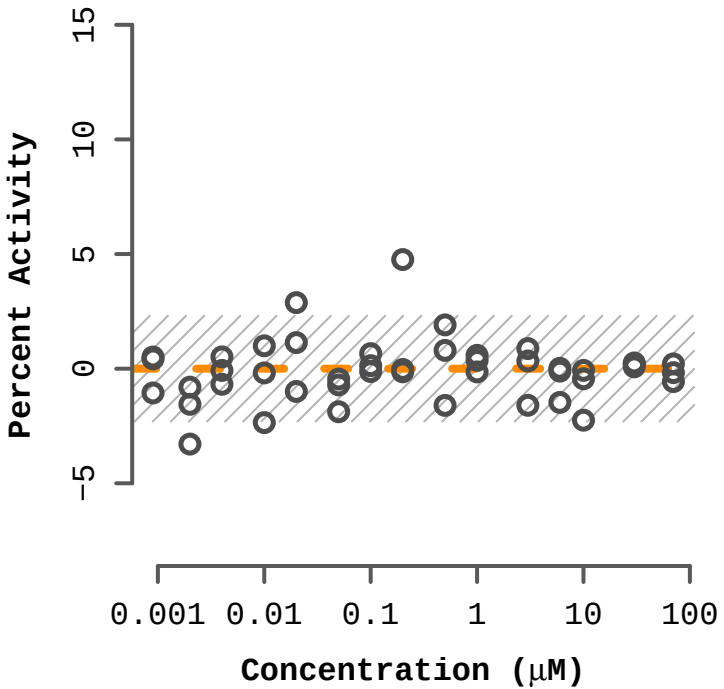
NAME: Glycyrrhetinic acid
CHID: 20669 **CASRN:** 471-53-4
SPID(S): Tox21_200799
M4ID: 12481453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

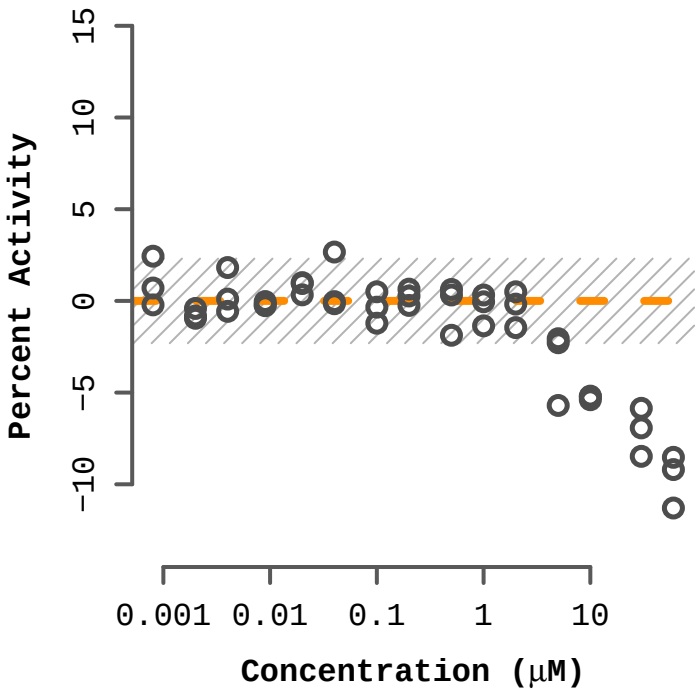
NAME: FD&C Green No. 1
CHID: 20671 **CASRN:** 4680-78-8
SPID(S): Tox21_301679
M4ID: 12477454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

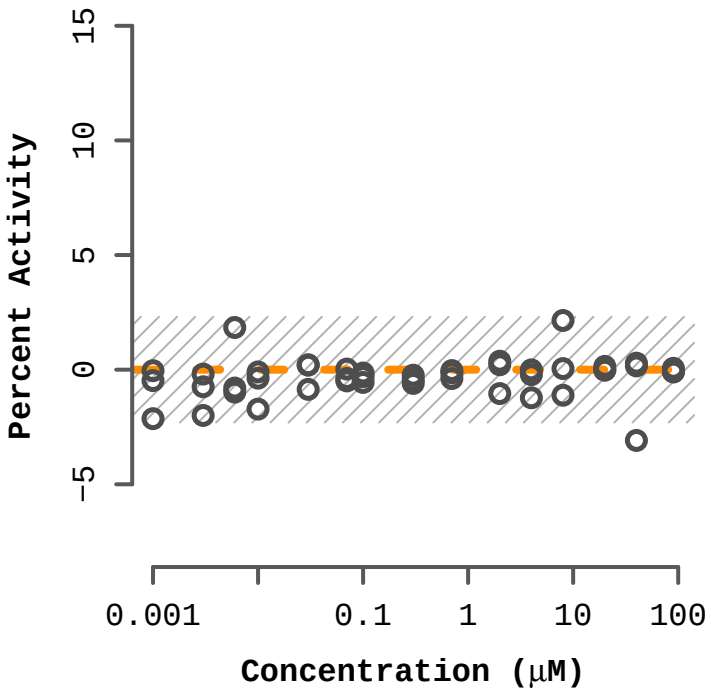
NAME: FD&C Green No. 3
CHID: 20673 **CASRN:** 2353-45-9
SPID(S): Tox21_302086
M4ID: 12477047

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.57	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 0.949 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

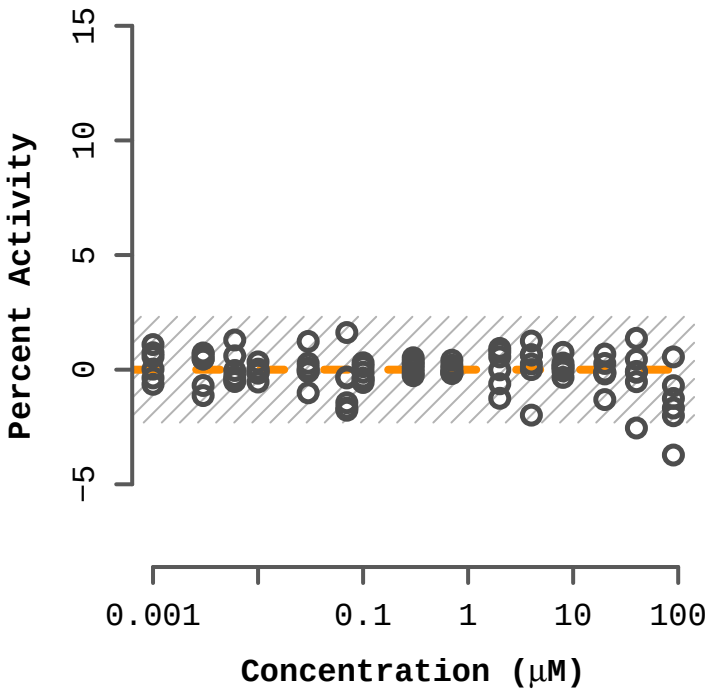
NAME: Griseofulvin
CHID: 20674 CASRN: 126-07-8
SPID(S): Tox21_303005
M4ID: 12476128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.361 MAX_MED: 0.215 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

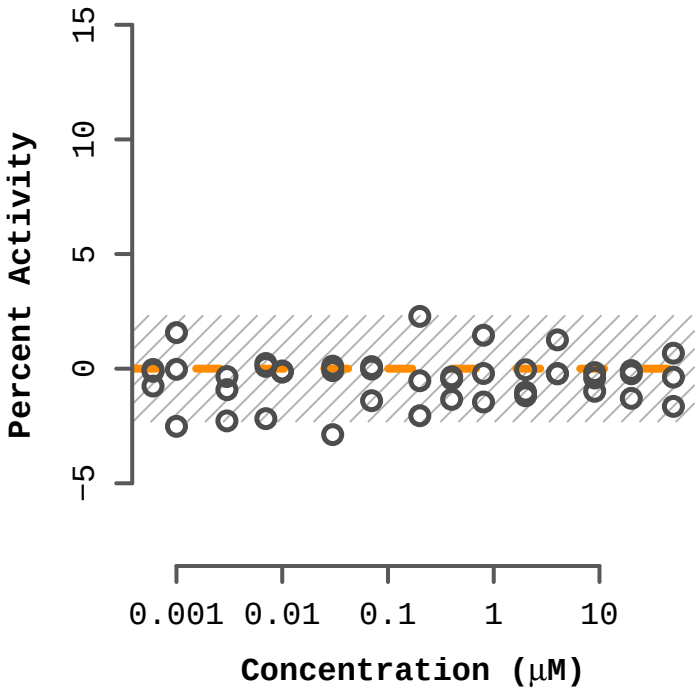
NAME: Griseofulvin
CHID: 20674 CASRN: 126-07-8
SPID(S): Tox21_202235
M4ID: 12480017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.238 MAX_MED: 0.468 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

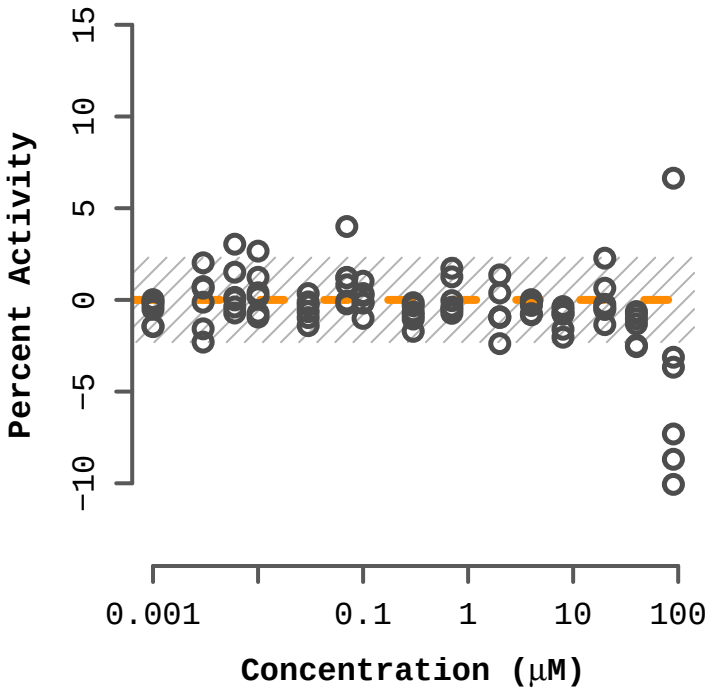
NAME: Griseofulvin
CHID: 20674 **CASRN:** 126-07-8
SPID(S): Tox21_111087_1
M4ID: 12483916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.274 **MAX_MED:** 0.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

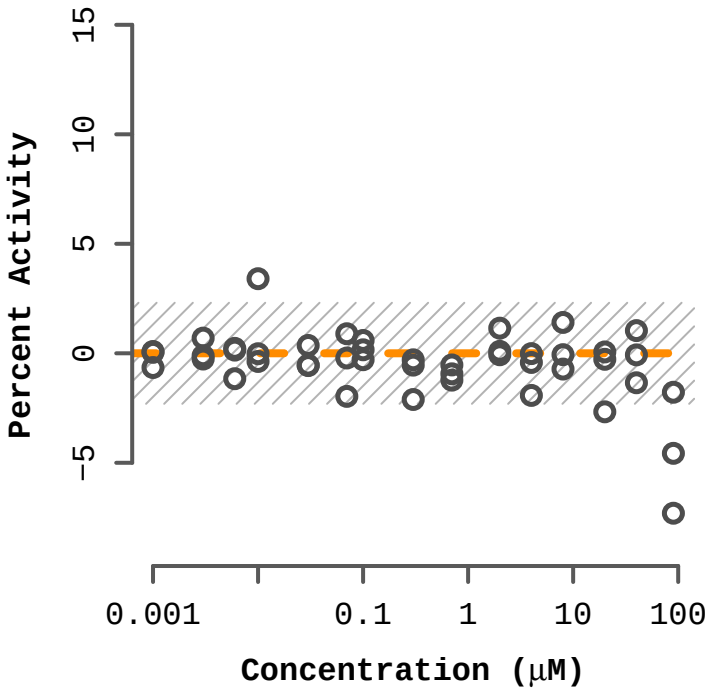
NAME: Hematoxylin
CHID: 20678 **CASRN:** 517-28-2
SPID(S): Tox21_201186
M4ID: 12481066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	349.86	NA	NA
PROB:	1	NA	NA
RMSE:	2.15	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

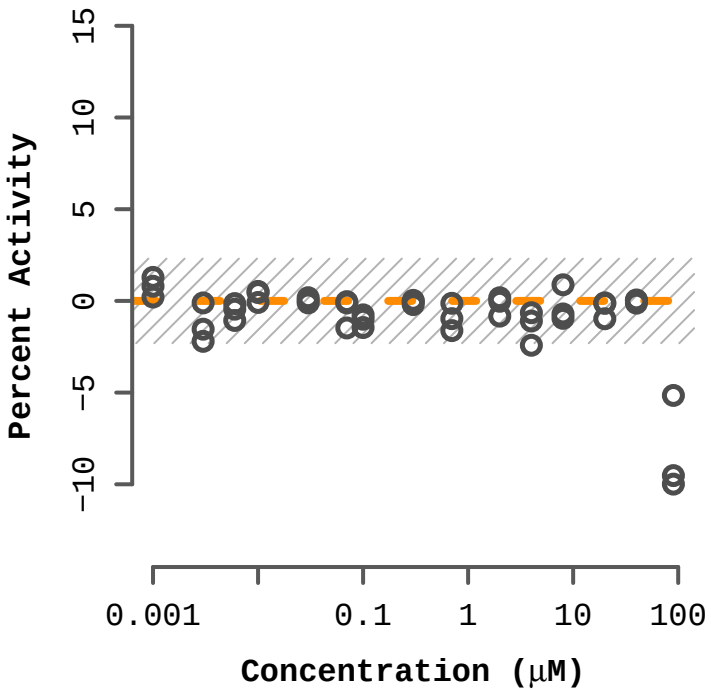
NAME: Heptachlor
CHID: 20679 **CASRN:** 76-44-8
SPID(S): Tox21_300534
M4ID: 12478598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.161 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

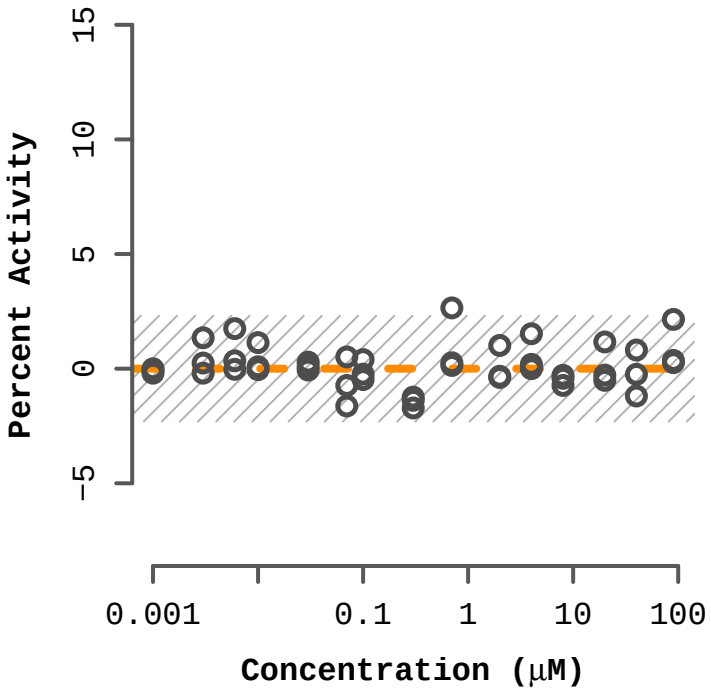
NAME: Heptachlor
CHID: 20679 **CASRN:** 76-44-8
SPID(S): Tox21_201911
M4ID: 12480341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.24	NA	NA
PROB:	1	NA	NA
RMSE:	2.35	NA	NA

MAX_MEAN: 0.765 **MAX_MED:** 0.801 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

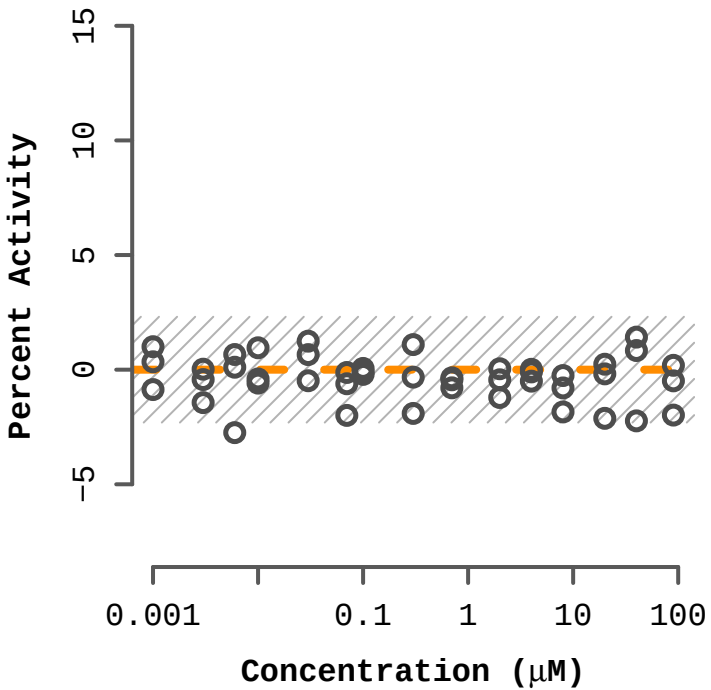
NAME: Heptamethyleneimine
CHID: 20680 **CASRN:** 1121-92-2
SPID(S): Tox21_202590
M4ID: 12479662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.361 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

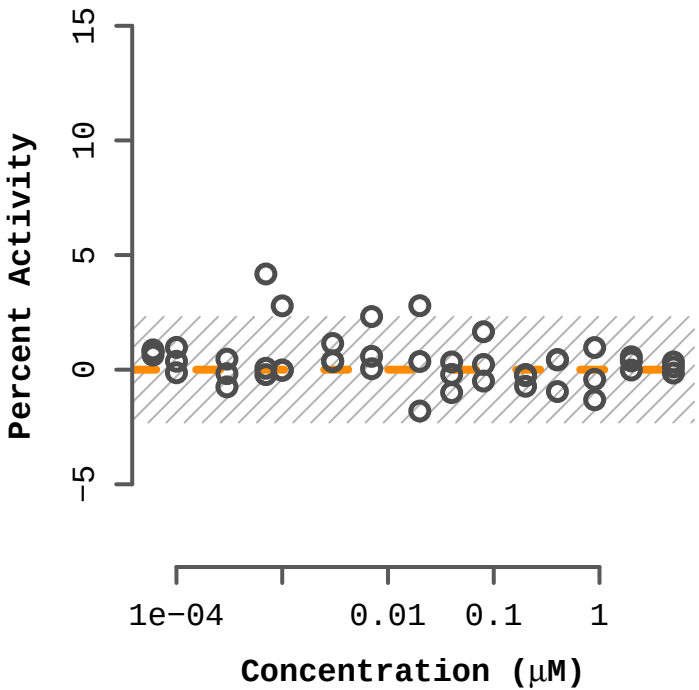
NAME: Heptylamine
CHID: 20681 **CASRN:** 111-68-2
SPID(S): Tox21_201004
M4ID: 12481248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.475 **MAX_MED:** 0.836 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

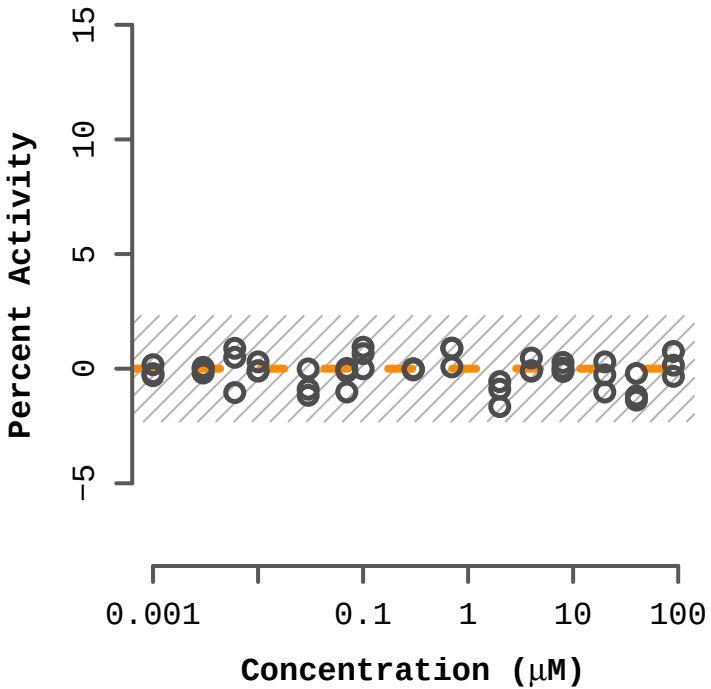
NAME: Hexachlorobenzene
CHID: 20682 **CASRN:** 118-74-1
SPID(S): Tox21_202995
M4ID: 12479257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

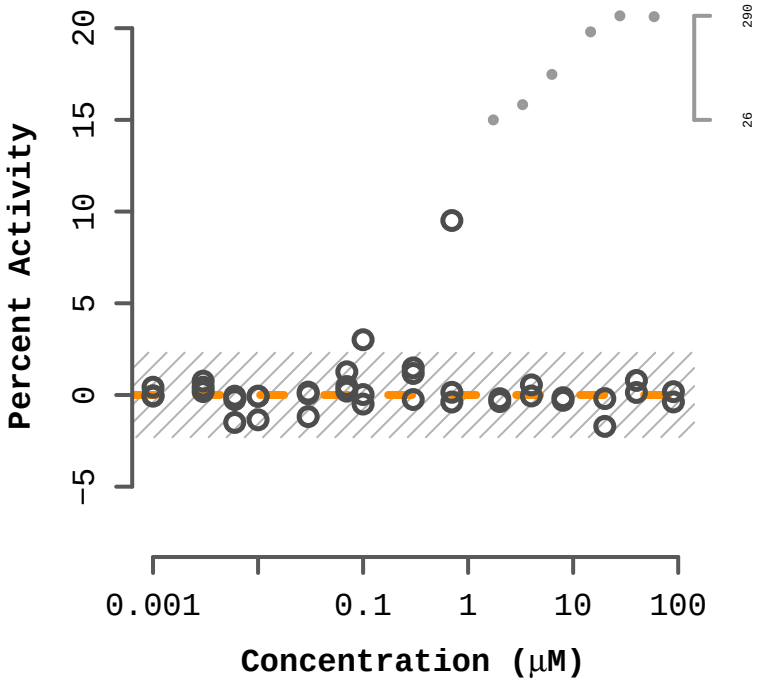
NAME: Hexachloro−1,3−butadiene
CHID: 20683 **CASRN:** 87−68−3
SPID(S): Tox21_302736
M4ID: 12476397

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 0.622 **MAX_MED:** 0.891 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

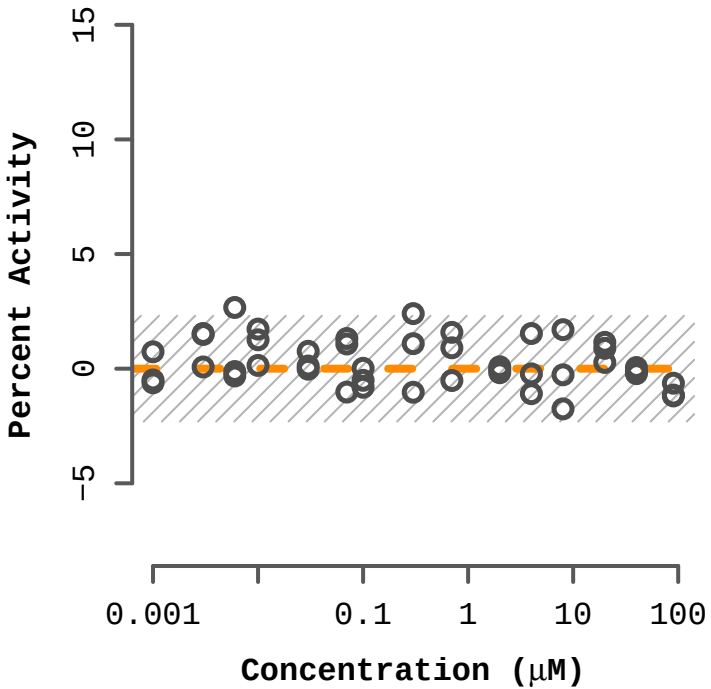
NAME: Hexachloro−1,3−butadiene
CHID: 20683 **CASRN:** 87−68−3
SPID(S): Tox21_201725
M4ID: 12480527 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	377.1	NA	NA
PROB:	1	NA	NA
RMSE:	74.52	NA	NA

MAX_MEAN: 96.1 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

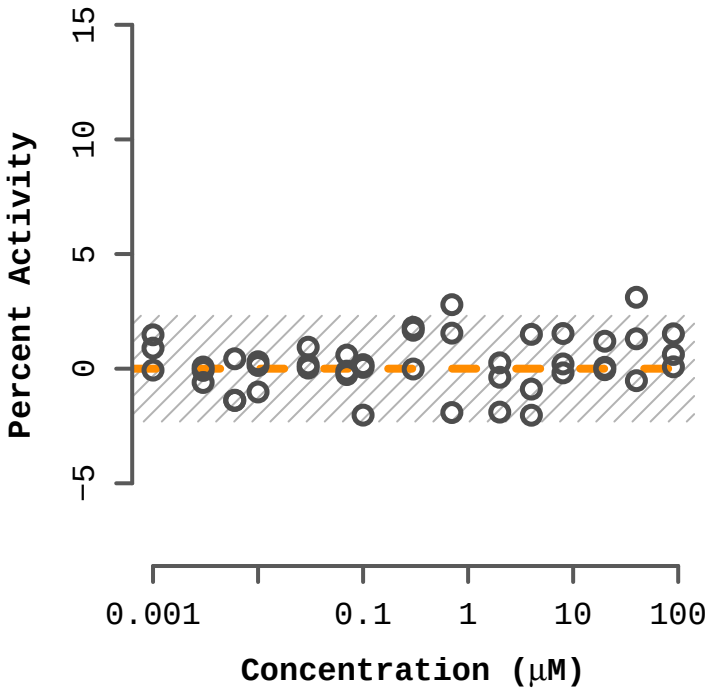
NAME: alpha−1,2,3,4,5,6−Hexachlorocyclohexane
CHID: 20684 **CASRN:** 319−84−6
SPID(S): Tox21_200676
M4ID: 12481576

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

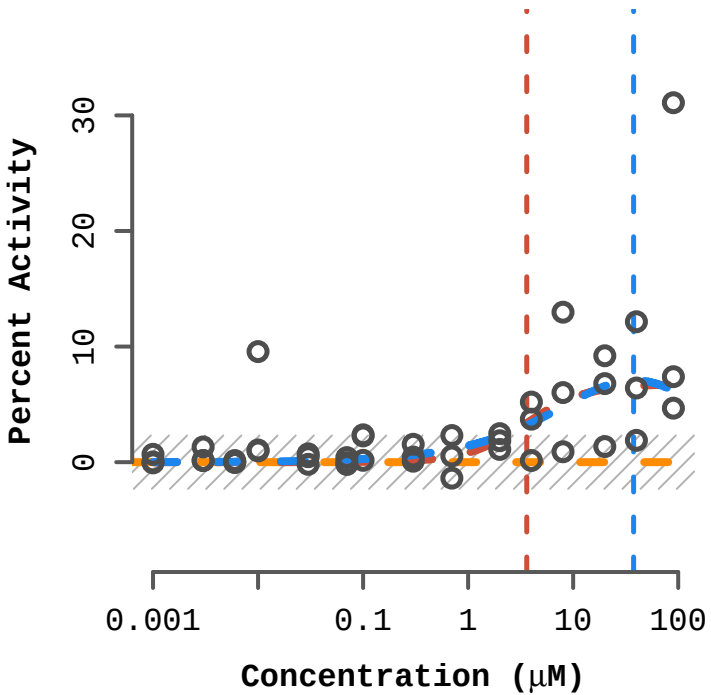
NAME: beta-Hexachlorocyclohexane
CHID: 20685 **CASRN:** 319-85-7
SPID(S): Tox21_300624
M4ID: 12478509

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: beta-Hexachlorocyclohexane
CHID: 20685 CASRN: 319-85-7
SPID(S): Tox21_202290
M4ID: 12479962

HILL MODEL (in red):

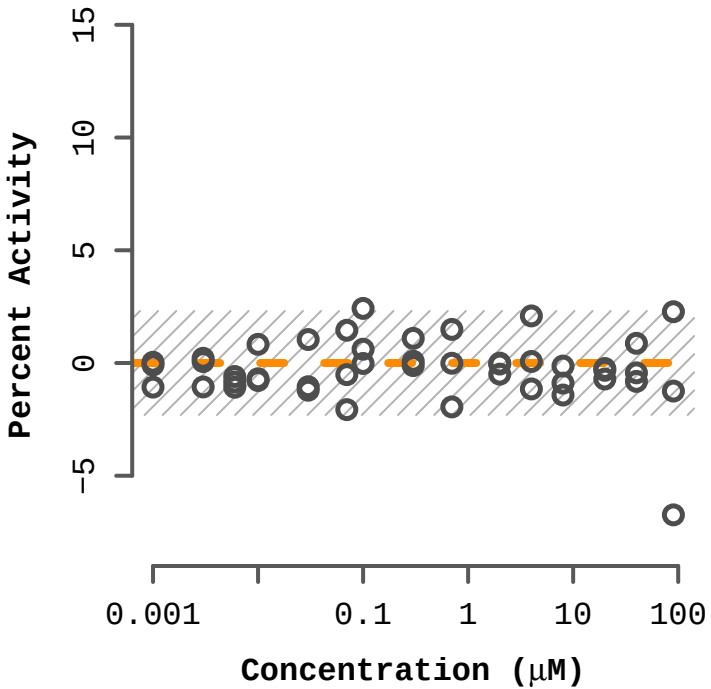
	tp	ga	gw
val:	6.76	0.558	1.53
sd:	1.09	0.175	1.17

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.1	1.58	0.734	1.83	0.997
sd:	135	5.69	1.1	1.96	1.72

	CNST	HILL	GNLS
AIC:	263.3	225.35	228.76
PROB:	0	0.85	0.15
RMSE:	6.23	4.46	4.53

MAX_MEAN: 14.4 MAX_MED: 7.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

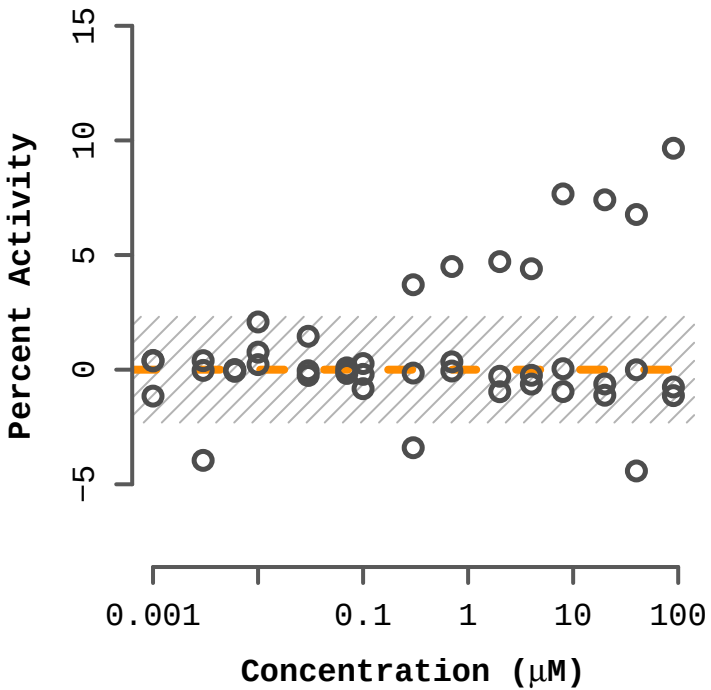
NAME: Lindane
CHID: 20686 **CASRN:** 58-89-9
SPID(S): Tox21_300953
M4ID: 12478180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.613 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

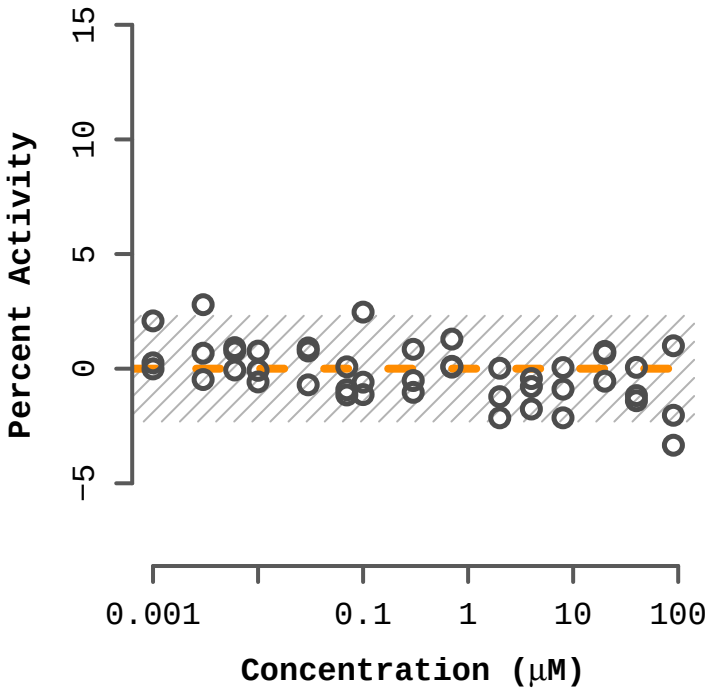
NAME: Lindane
CHID: 20686 **CASRN:** 58-89-9
SPID(S): Tox21_202069
M4ID: 12480183

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.05	NA	NA
PROB:	1	NA	NA
RMSE:	2.95	NA	NA

MAX_MEAN: 2.59 **MAX_MED:** 0.767 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

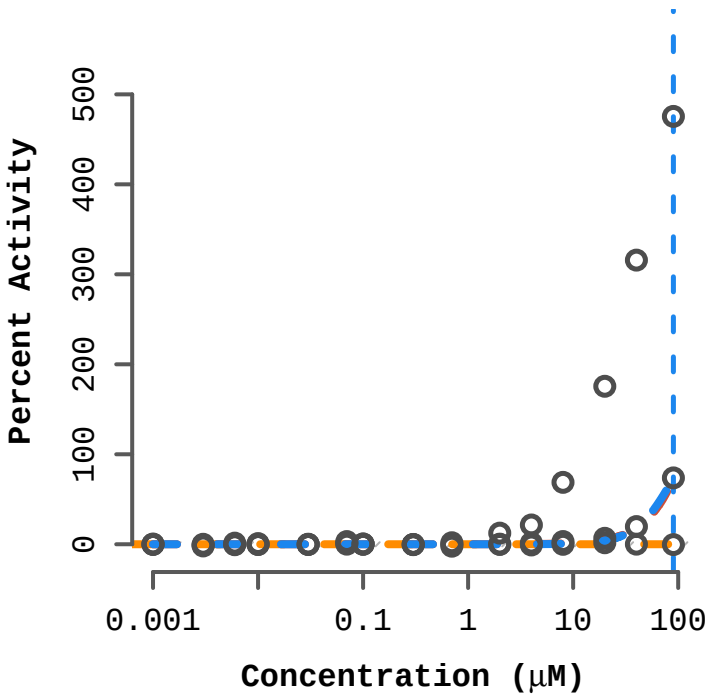
NAME: 1,2,3,4,5,6-Hexachlorocyclohexane
CHID: 20687 **CASRN:** 608-73-1
SPID(S): Tox21_302925
M4ID: 12476208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.999 **MAX_MED:** 0.774 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2,3,4,5,6-Hexachlorocyclohexane
CHID: 20687 CASRN: 608-73-1
SPID(S): Tox21_201777
M4ID: 12480475

HILL MODEL (in red):

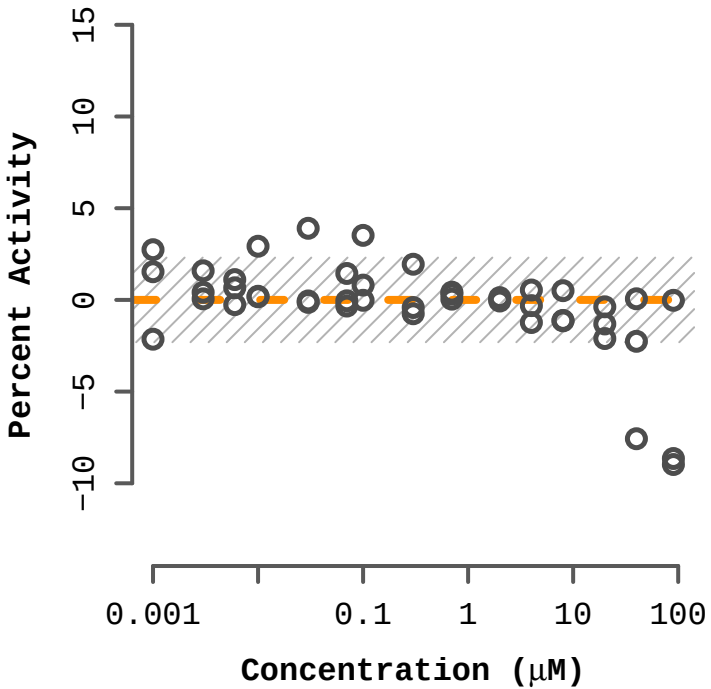
	tp	ga	gw
val:	571	2.4	1.87
sd:	214	0.0294	0.347

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	147	1.95	2.38	3.65	8.94
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	398.82	398.28	402.62
PROB:	0.41	0.53	0.06
RMSE:	90.43	80.35	80.36

MAX_MEAN: 183 MAX_MED: 73.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

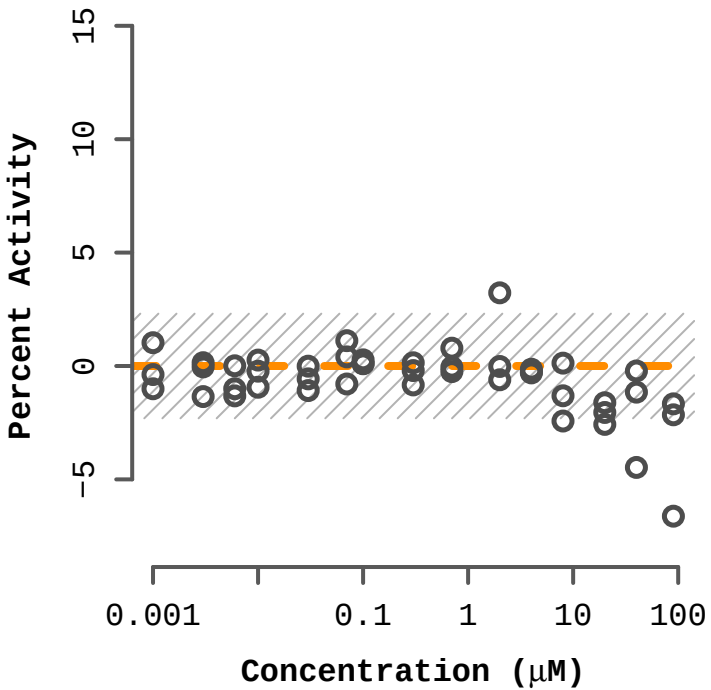
NAME: Hexachlorocyclopentadiene
CHID: 20688 CASRN: 77-47-4
SPID(S): Tox21_302780
M4ID: 12476353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.99	NA	NA
PROB:	1	NA	NA
RMSE:	2.55	NA	NA

MAX_MEAN: 1.44 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

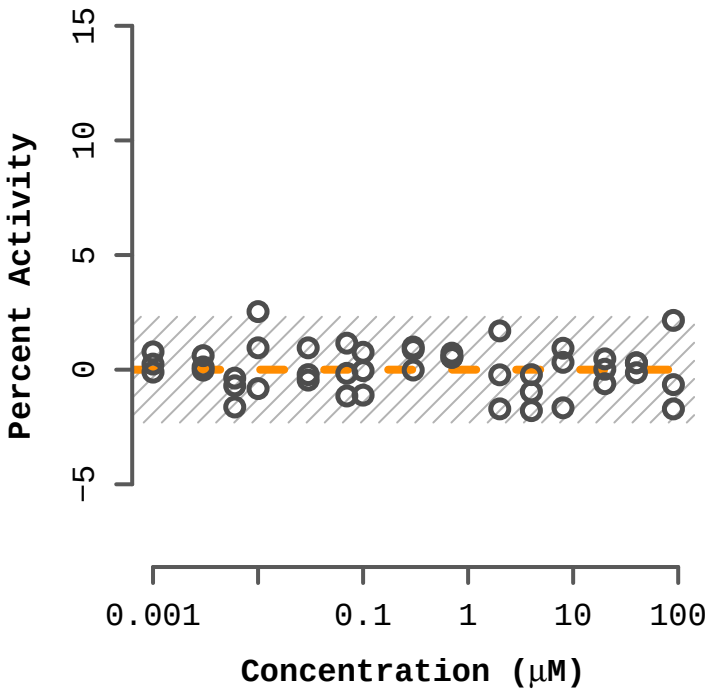
NAME: Hexachlorocyclopentadiene
CHID: 20688 CASRN: 77-47-4
SPID(S): Tox21_202279
M4ID: 12479973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 0.867 MAX_MED: 0.403 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

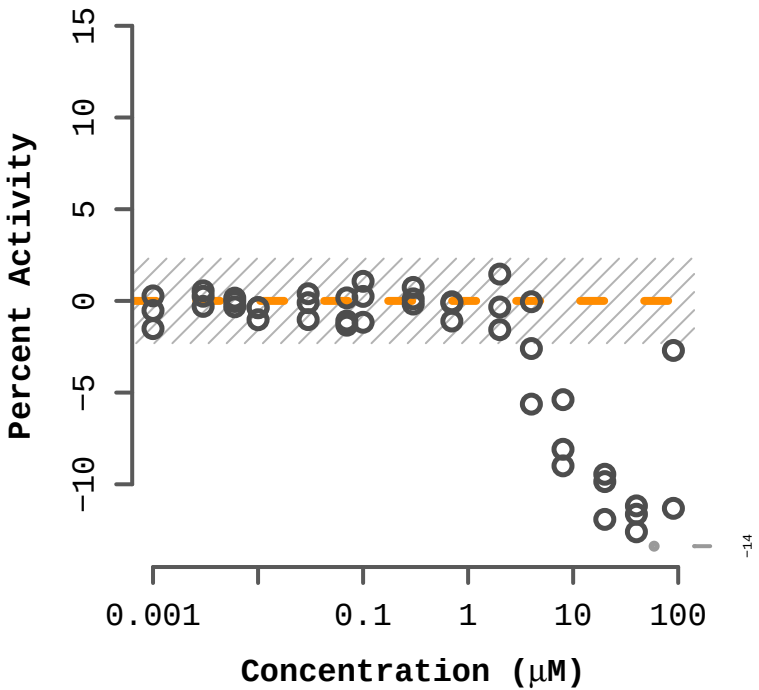
NAME: Hexachloroethane
CHID: 20689 CASRN: 67-72-1
SPID(S): Tox21_200724
M4ID: 12481528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.889 **MAX_MED:** 0.956 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

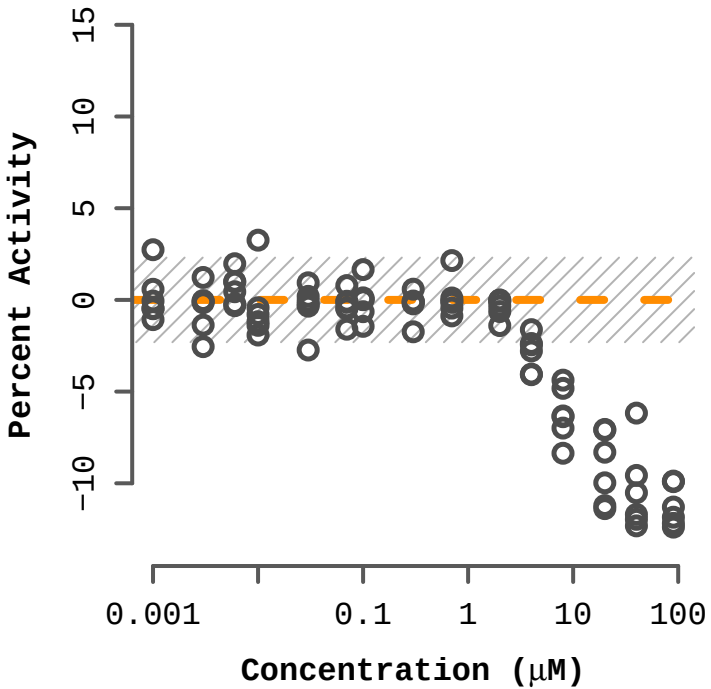
NAME: Hexachlorophene
CHID: 20690 **CASRN:** 70-30-4
SPID(S): Tox21_302741
M4ID: 12476392 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	271.68	NA	NA
PROB:	1	NA	NA
RMSE:	5.38	NA	NA

MAX_MEAN: 0.227 **MAX_MED:** 0.255 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

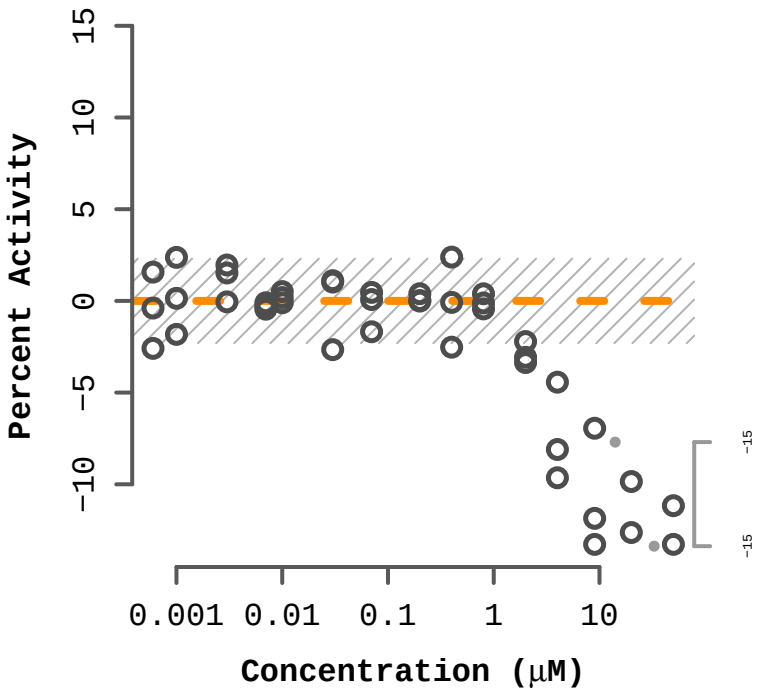
NAME: Hexachlorophene
CHID: 20690 **CASRN:** 70-30-4
SPID(S): Tox21_201350
M4ID: 12480902

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	535.81	NA	NA
PROB:	1	NA	NA
RMSE:	5.09	NA	NA

MAX_MEAN: 0.649 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

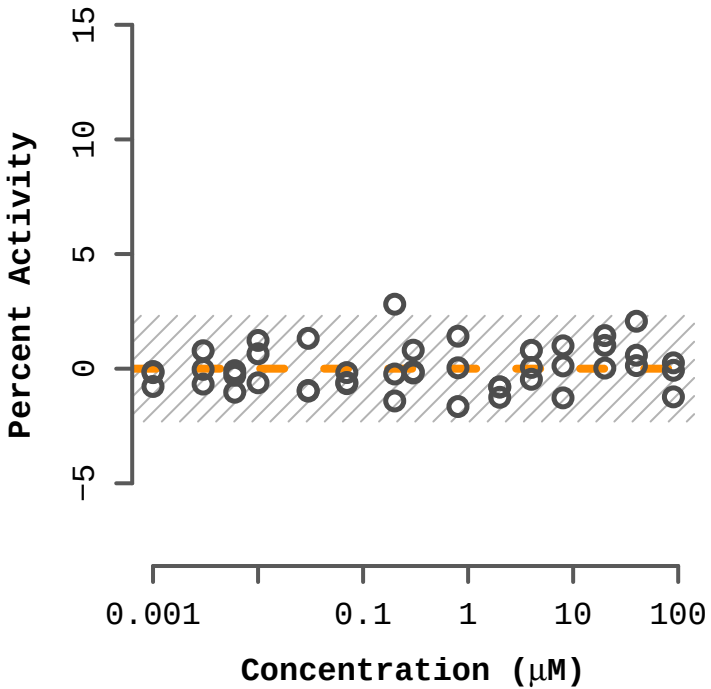
NAME: Hexachlorophene
CHID: 20690 CASRN: 70-30-4
SPID(S): Tox21_111099_1
M4ID: 12483908 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.88	NA	NA
PROB:	1	NA	NA
RMSE:	5.99	NA	NA

MAX_MEAN: 1.15 MAX_MED: 1.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

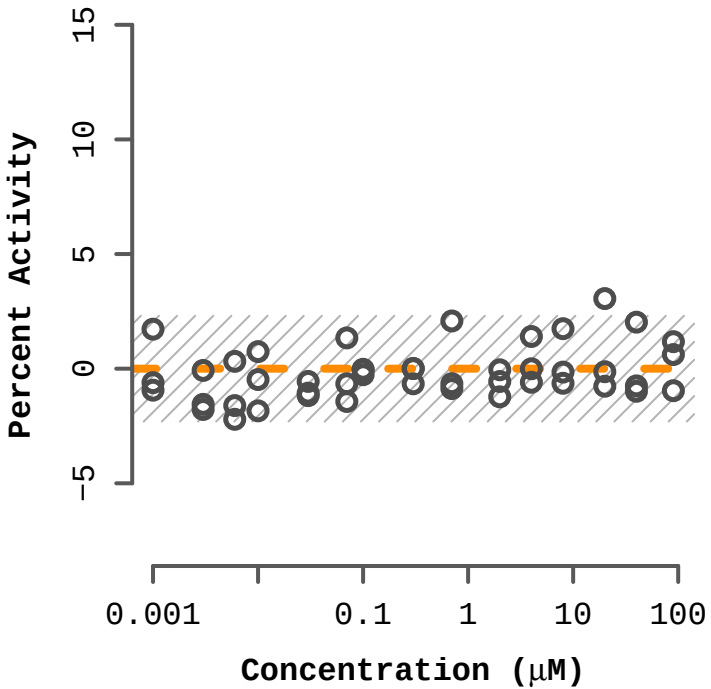
NAME: Methenamine
CHID: 20692 **CASRN:** 100-97-0
SPID(S): Tox21_300502
M4ID: 12478630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.931 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

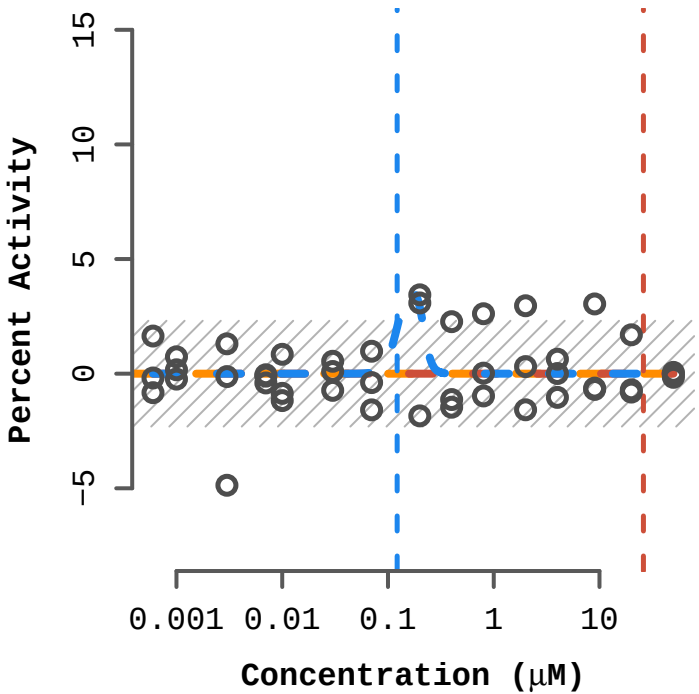
NAME: Methenamine
CHID: 20692 **CASRN:** 100-97-0
SPID(S): Tox21_201606
M4ID: 12480646

HILL MODEL: Not applicable.

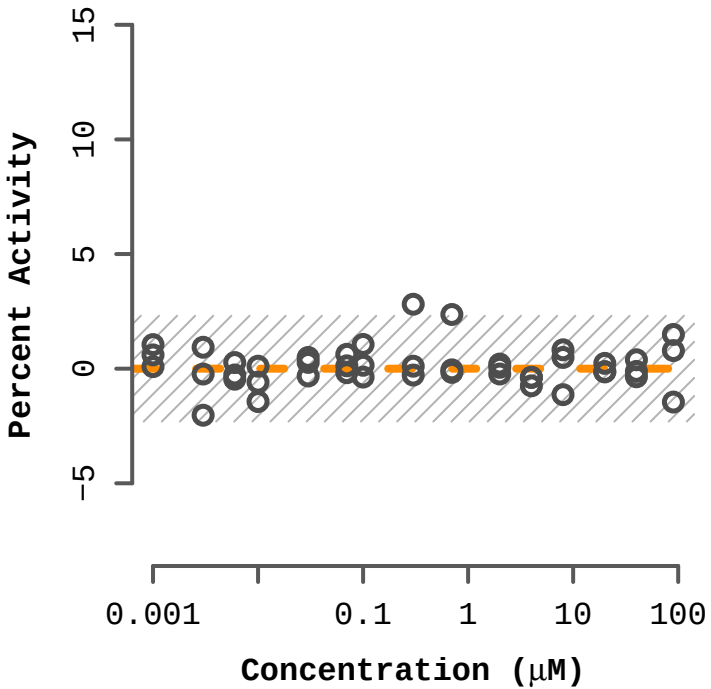
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 0.618 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Methenamine
CHID:    20692   CASRN: 100-97-0
SPID(S): Tox21_113455_1
M4ID:    12482648

HILL MODEL (in red):
      tp        ga        gw
val:  6.38e-10  1.42      1.76
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  4.08      -0.913    7.9       -0.663    11.6
sd:   NaN       NaN       NaN       NaN       NaN

      CNST        HILL        GNLS
AIC:  164.14      170.14      168.62
PROB: 0.86        0.04        0.09
RMSE: 1.53        1.53        1.51

MAX_MEAN: 1.56      MAX_MED: 3.09      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

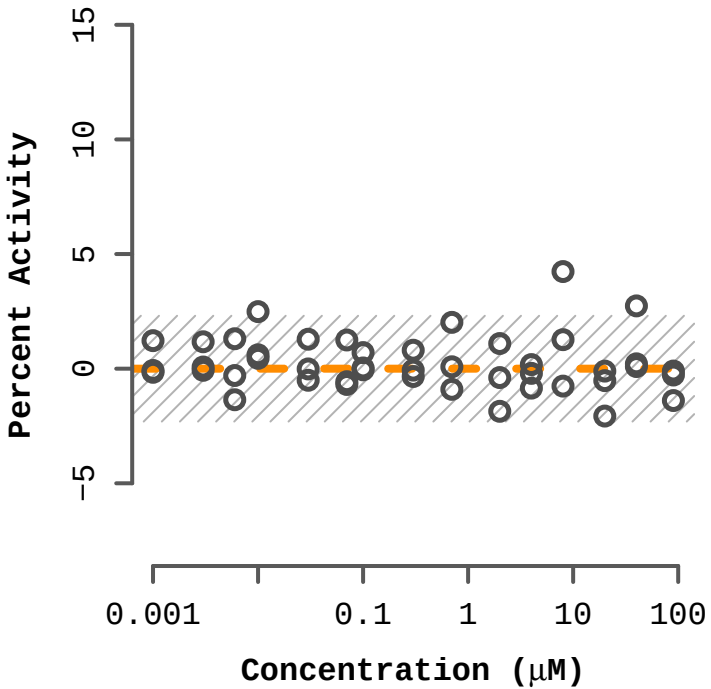
NAME: Hexamethylphosphoramide
CHID: 20694 **CASRN:** 680-31-9
SPID(S): Tox21_302785
M4ID: 12476348

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.882 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

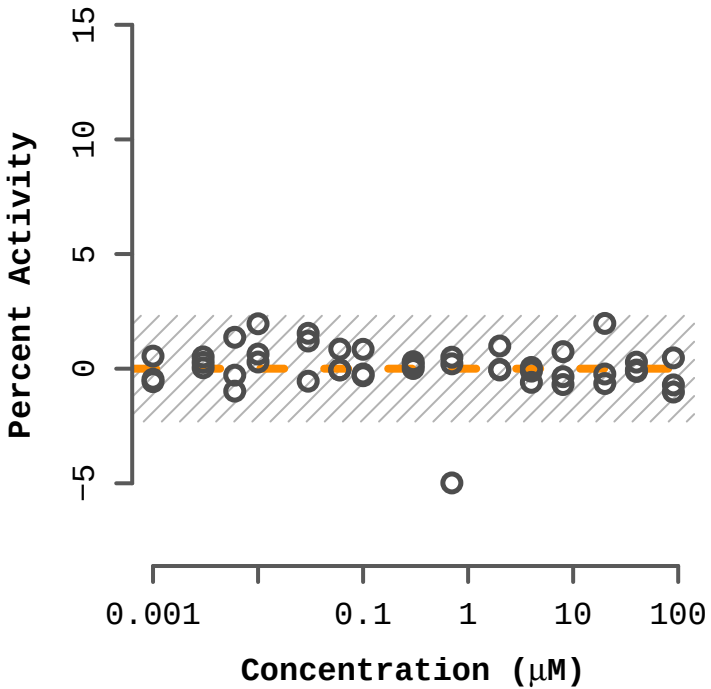
NAME: Hexamethylphosphoramide
CHID: 20694 **CASRN:** 680-31-9
SPID(S): Tox21_201837
M4ID: 12480415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

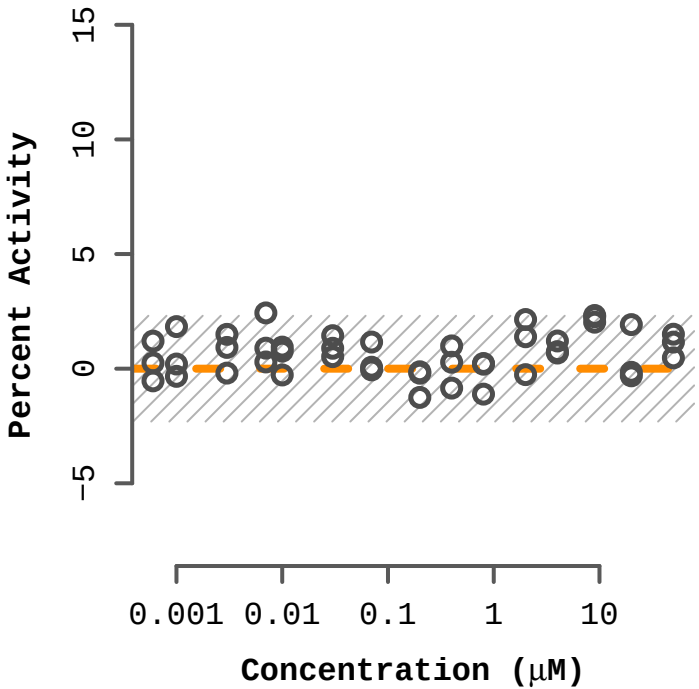
NAME: Hexanamide
CHID: 20696 **CASRN:** 628-02-4
SPID(S): Tox21_201019
M4ID: 12481233

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.964 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

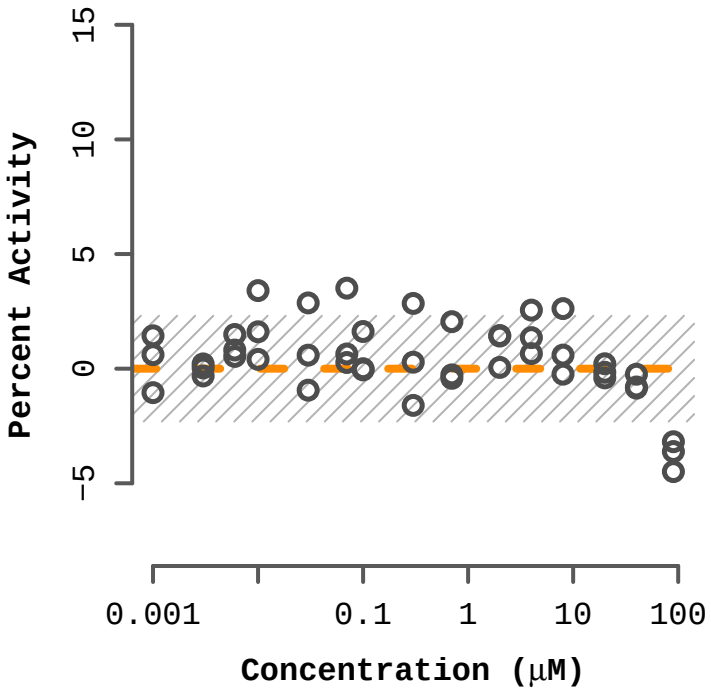
NAME: Hexanamide
CHID: 20696 **CASRN:** 628-02-4
SPID(S): Tox21_111111_1
M4ID: 12483901

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

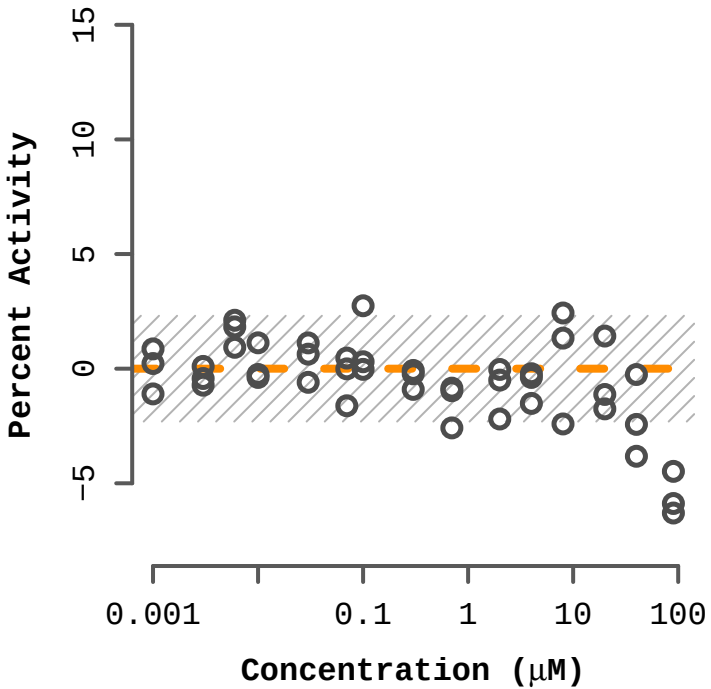
NAME: 1-O-Hexyl-2,3,5-trimethylhydroquinone
CHID: 20697 **CASRN:** 148081-72-5
SPID(S): Tox21_301245
M4ID: 12477888

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

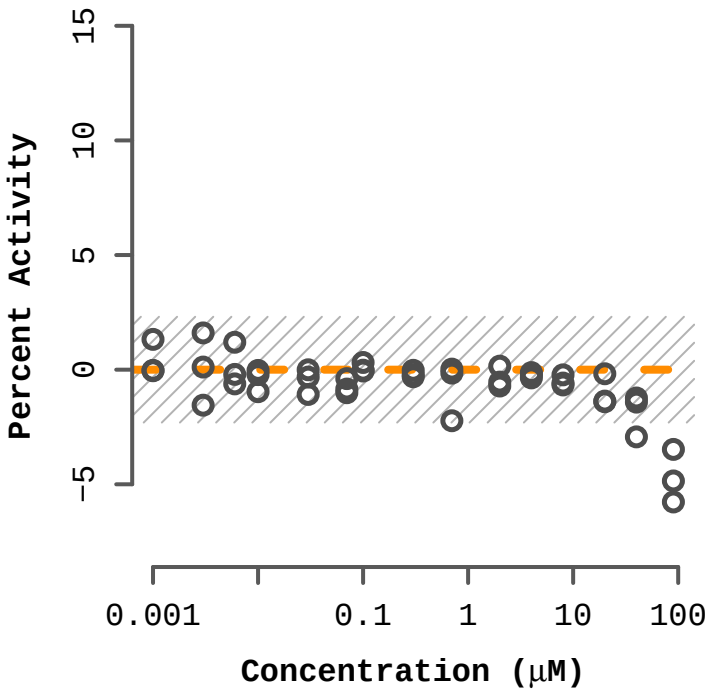
NAME: 4-Hexylresorcinol
CHID: 20699 **CASRN:** 136-77-6
SPID(S): Tox21_300357
M4ID: 12478775

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

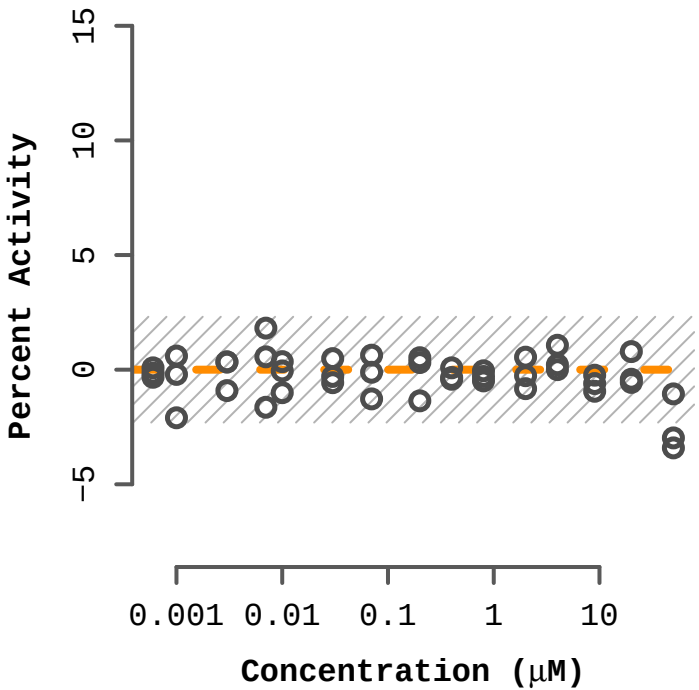
NAME: 4-Hexylresorcinol
CHID: 20699 **CASRN:** 136-77-6
SPID(S): Tox21_202263
M4ID: 12479989

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.115 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

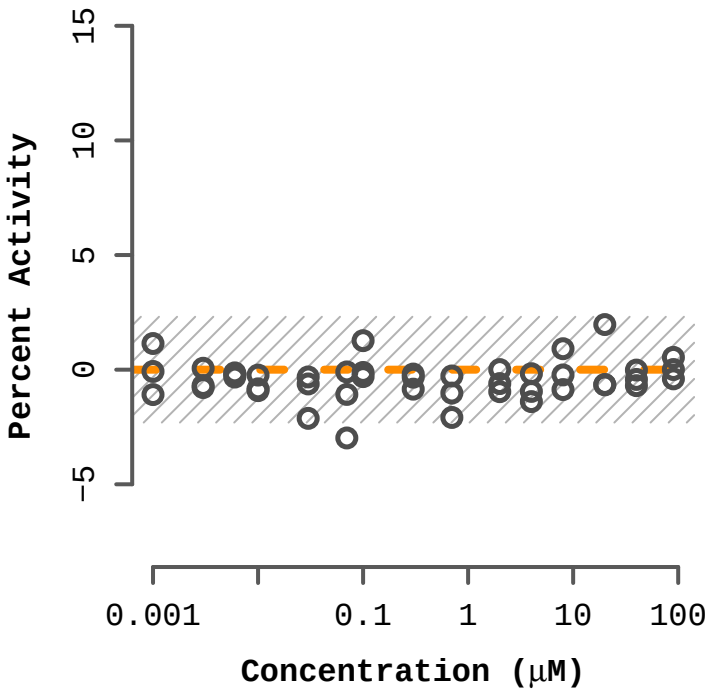
NAME: 4-Hexylresorcinol
CHID: 20699 **CASRN:** 136-77-6
SPID(S): Tox21_111102_1
M4ID: 12483907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.93	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.429 **MAX_MED:** 0.562 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

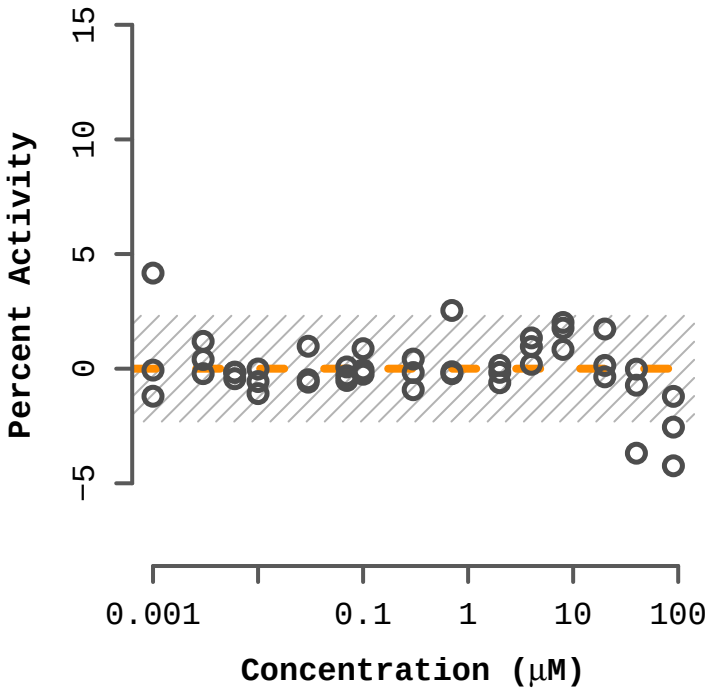
NAME: Hydrazine sulfate
CHID: 20703 CASRN: 10034-93-2
SPID(S): Tox21_302995
M4ID: 12476138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.282 **MAX_MED:** 0.00809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

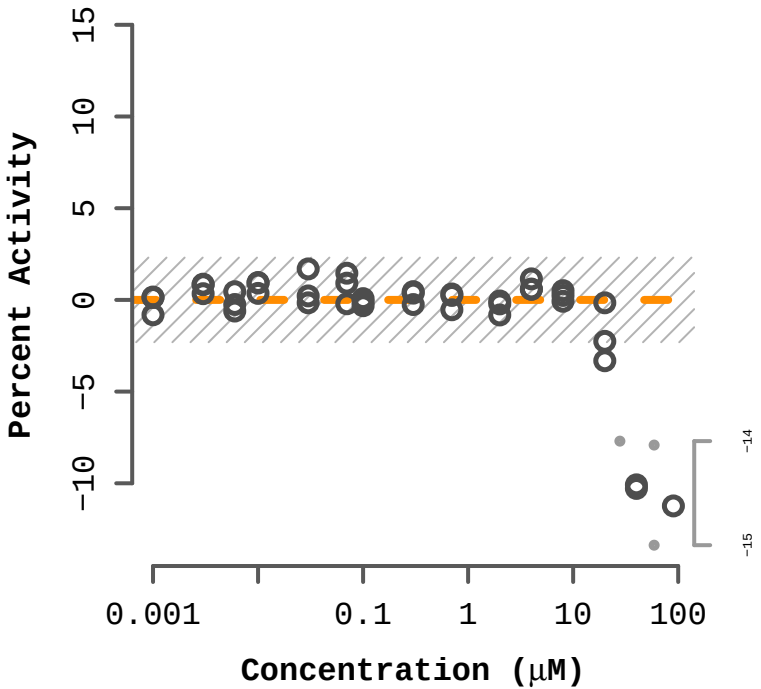
NAME: 2-Hydrazino-4-(4-aminophenyl) thiazole
CHID: 20704 **CASRN:** 26049-71-8
SPID(S): Tox21_301743
M4ID: 12477390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

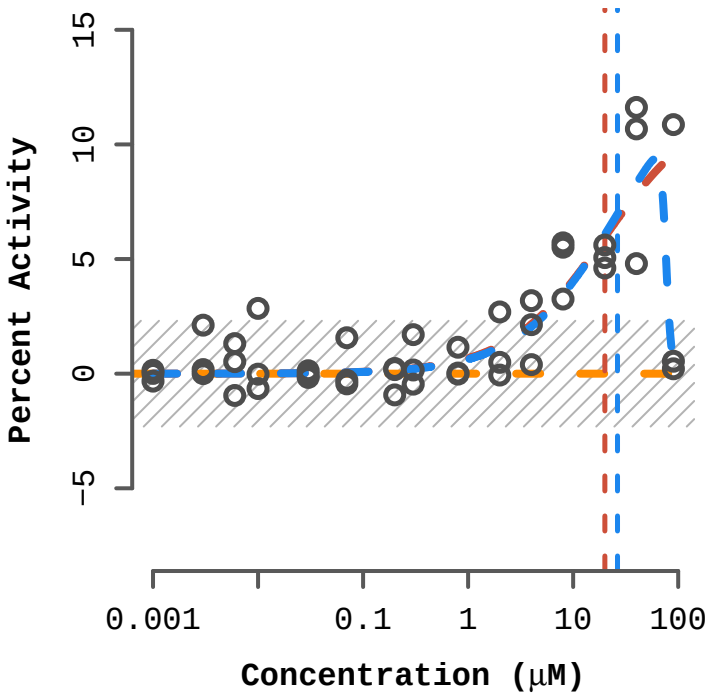
NAME: 2-Hydrazino-4-(4-nitrophenyl)thiazole
CHID: 20706 **CASRN:** 26049-70-7
SPID(S): Tox21_301760
M4ID: 12477373 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.13	NA	NA
PROB:	1	NA	NA
RMSE:	4.69	NA	NA

MAX_MEAN: 0.773 **MAX_MED:** 0.923 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydrazino-4-phenylthiazole
CHID: 20707 CASRN: 34176-52-8
SPID(S): Tox21_200897
M4ID: 12481355

HILL MODEL (in red):

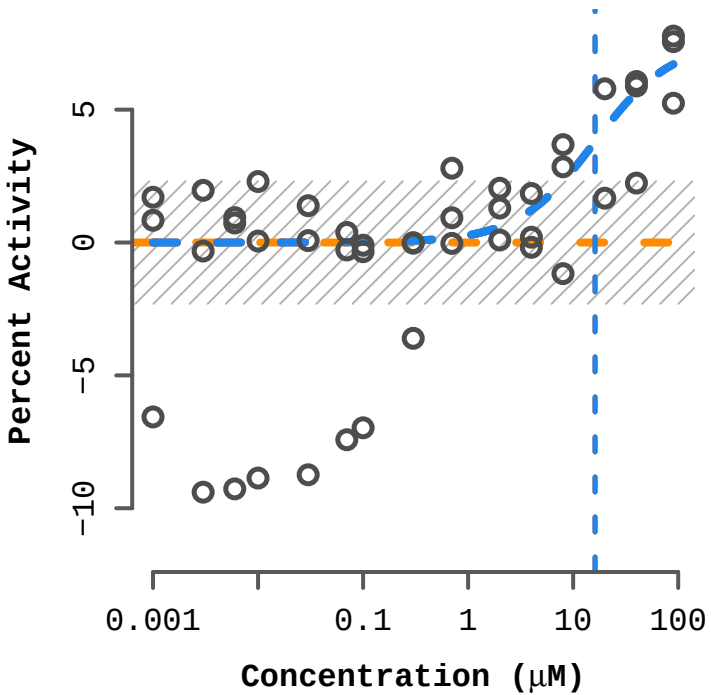
	tp	ga	gw
val:	11.9	1.3	0.94
sd:	5.71	0.474	0.306

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.9	1.42	0.932	1.88	17.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	229.89	186.7	175.7
PROB:	0	0	1
RMSE:	3.62	2.34	2

MAX_MEAN: 9.03 MAX_MED: 10.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydrazinobenzoic acid
CHID: 20708 CASRN: 619-67-0
SPID(S): Tox21_200198
M4ID: 12482054

HILL MODEL (in red):

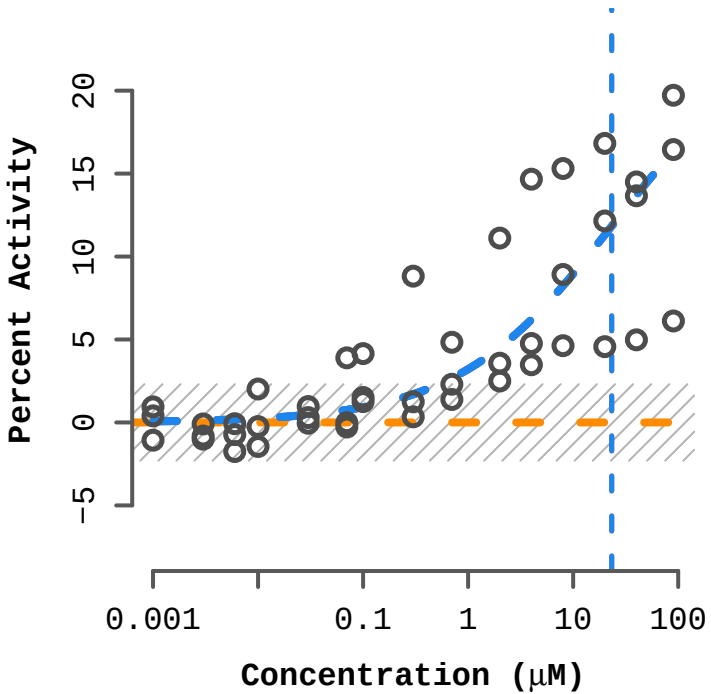
	tp	ga	gw
val:	7.59	1.21	1.18
sd:	3.64	0.549	0.948

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.59	1.21	1.18	3.32	5.19
sd:	3.64	0.549	0.948	969	3720

	CNST	HILL	GNLS
AIC:	264.02	242.09	246.09
PROB:	0	0.88	0.12
RMSE:	4.47	3.62	3.62

MAX_MEAN: 6.86 MAX_MED: 7.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydrazinobenzoic acid hydrochloride
CHID: 20709 **CASRN:** 24589-77-3
SPID(S): Tox21_200500
M4ID: 12481752

HILL MODEL (in red):

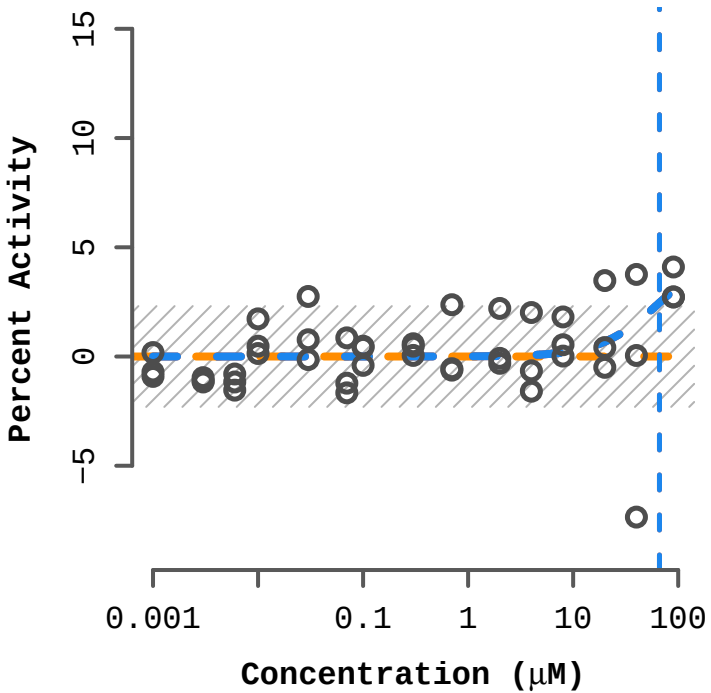
	tp	ga	gw
val:	23.7	1.37	0.588
sd:	9.57	0.662	0.166

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.7	1.37	0.588	3.72	9.07
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	304.41	240.96	244.96
PROB:	0	0.88	0.12
RMSE:	7.39	3.53	3.53

MAX_MEAN: 14.1 **MAX_MED:** 16.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Diphenylhydrazine
CHID: 20710 CASRN: 122-66-7
SPID(S): Tox21_300492
M4ID: 12478640

HILL MODEL (in red):

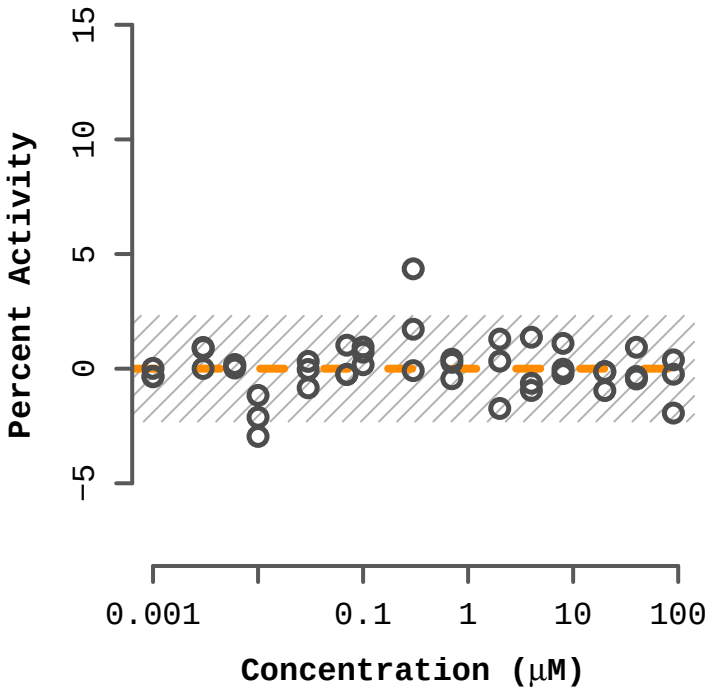
	tp	ga	gw
val:	4.92	1.82	1.53
sd:	4.57	0.589	1.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.92	1.82	1.53	3.72	4.46
sd:	4.57	0.589	1.6	2700	6870

	CNST	HILL	GNLS
AIC:	178.81	169.78	173.78
PROB:	0.01	0.87	0.12
RMSE:	1.89	1.79	1.79

MAX_MEAN: 3.18 **MAX_MED:** 2.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

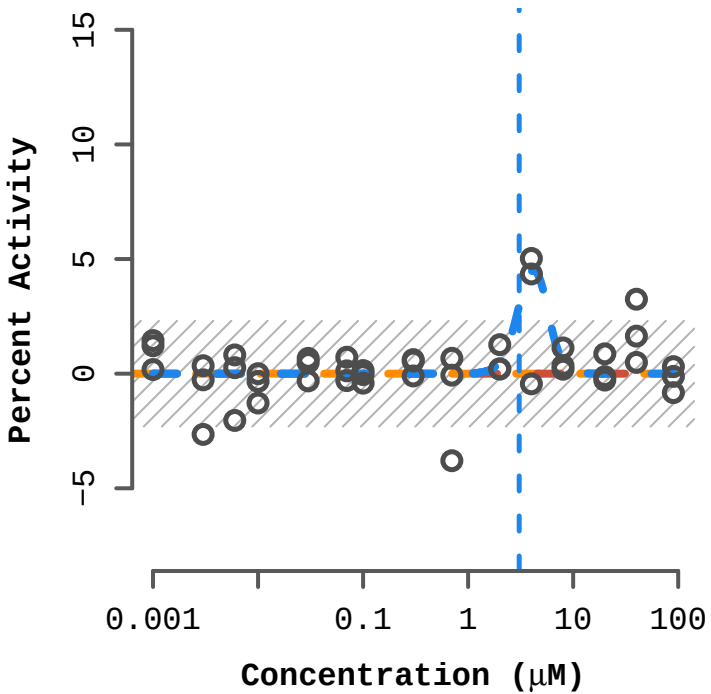
NAME: 1,2-Diphenylhydrazine
CHID: 20710 CASRN: 122-66-7
SPID(S): Tox21_202323
M4ID: 12479929

HILL MODEL: Not applicable.

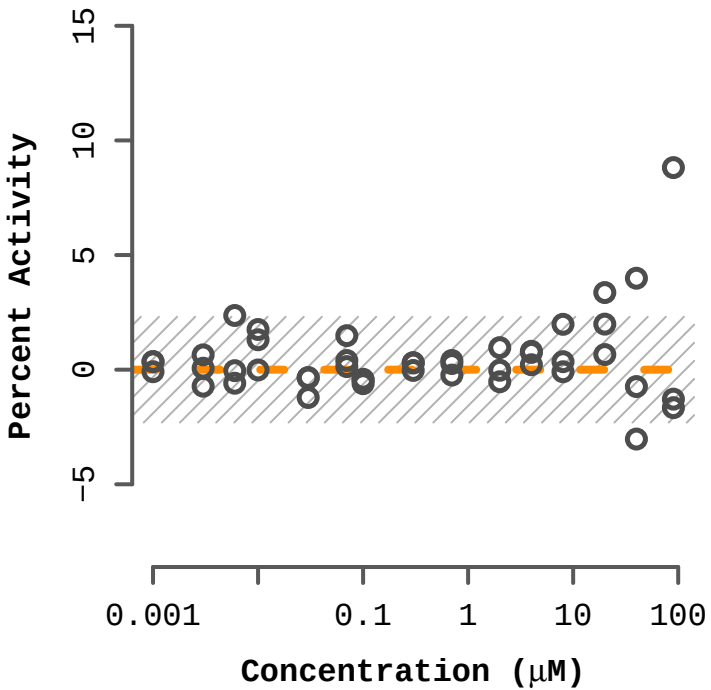
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.72 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hydrochlorothiazide
CHID:    20713   CASRN: 58-93-5
SPID(S): Tox21_300292
M4ID:    12478838

HILL MODEL (in red):
      tp        ga        gw
val:  2.02e-08  2.39      2.49
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  6.03      0.486     5.57      0.751     6.62
sd:   NaN       NaN       NaN       NaN       NaN

      CNST          HILL          GNLS
AIC:  148.63        154.63        144.89
PROB: 0.13          0.01          0.86
RMSE: 1.47          1.47          1.29

MAX_MEAN: 2.98      MAX_MED: 4.35      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

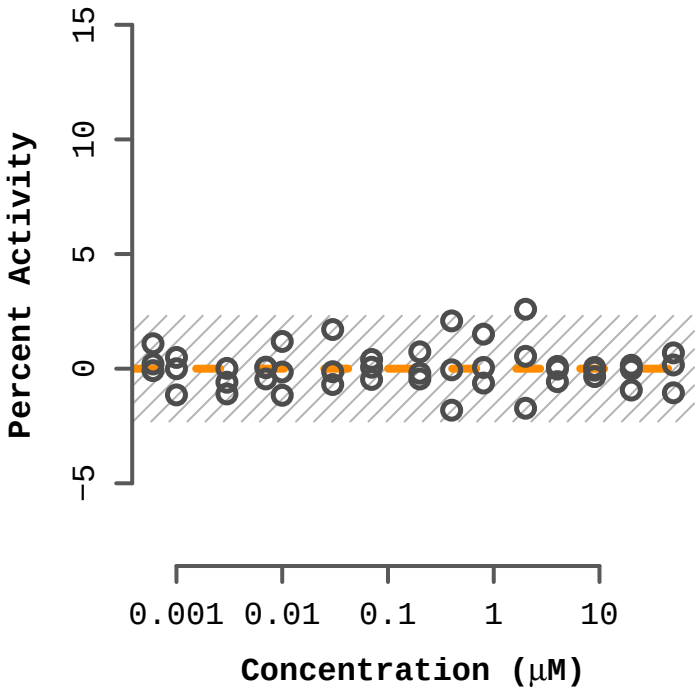
NAME: Hydrochlorothiazide
CHID: 20713 CASRN: 58-93-5
SPID(S): Tox21_201565
M4ID: 12480687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

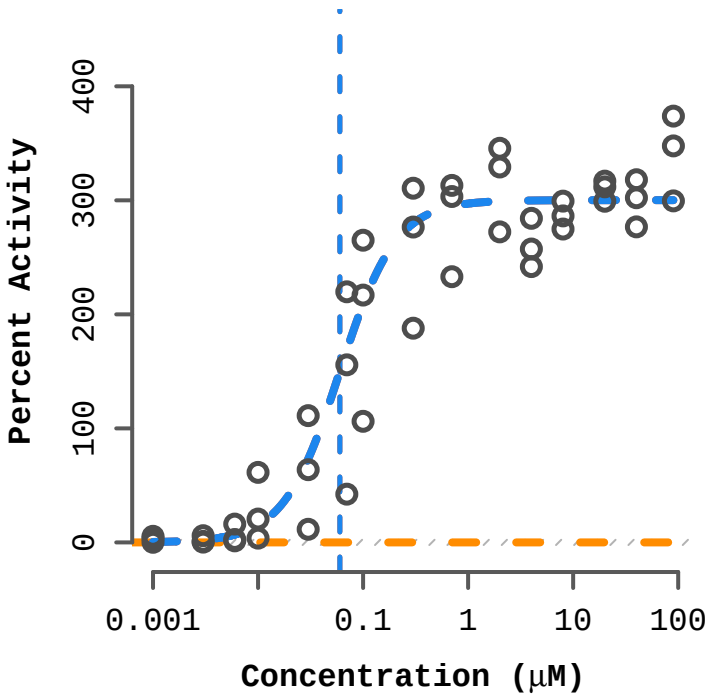
NAME: Hydrochlorothiazide
CHID: 20713 **CASRN:** 58-93-5
SPID(S): Tox21_110165_1
M4ID: 12484592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.47 **MAX_MED:** 0.541 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone
CHID: 20714 **CASRN:** 50-23-7
SPID(S): Tox21_200815
M4ID: 12481437

HILL MODEL (in red):

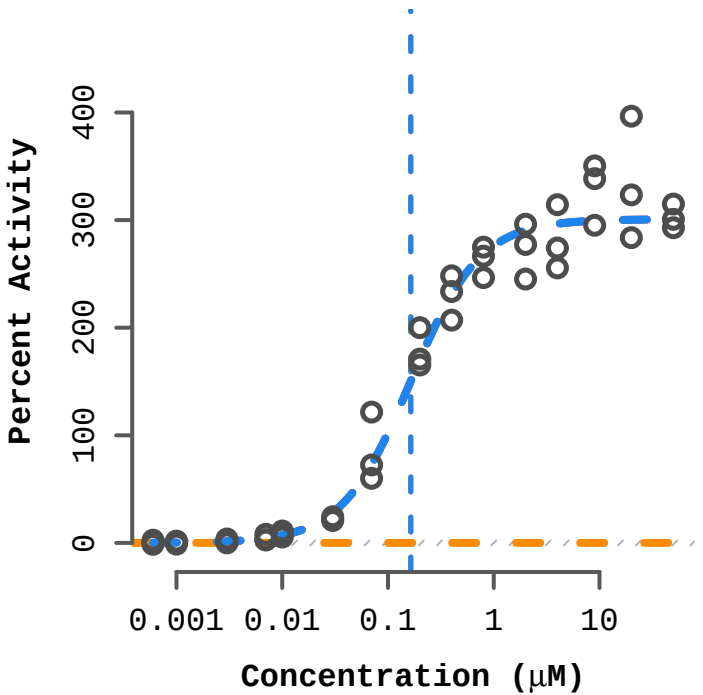
	tp	ga	gw
val:	300	-1.22	1.63
sd:	7.41	0.0639	0.369

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	300	-1.22	1.63	3.53	17
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	625.35	463.16	467.16
PROB:	0	0.88	0.12
RMSE:	227.96	40.26	40.26

MAX_MEAN: 340 **MAX_MED:** 348 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone
CHID: 20714 CASRN: 50-23-7
SPID(S): Tox21_110883_1
M4ID: 12484044

HILL MODEL (in red):

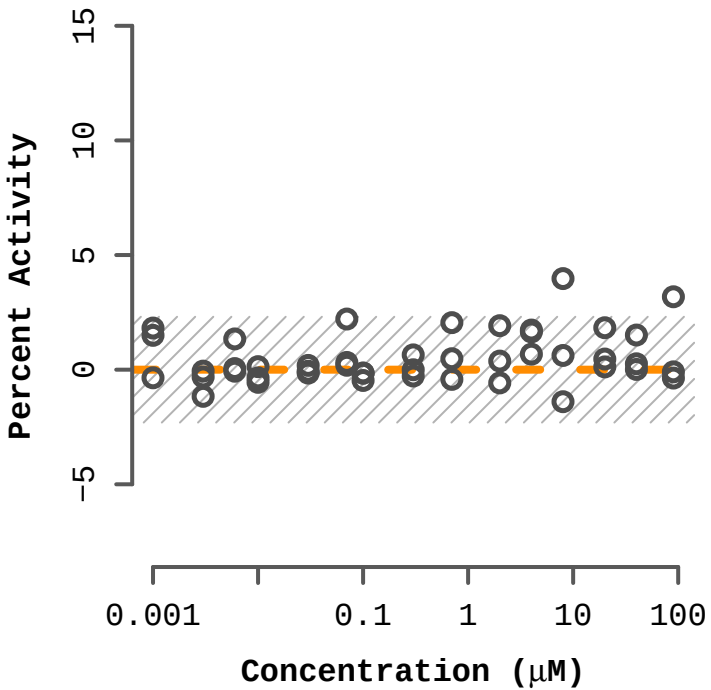
	tp	ga	gw
val:	301	-0.784	1.34
sd:	5.91	0.0322	0.105

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	301	-0.784	1.34	2.87	7.08
sd:	5.91	0.0322	0.105	928	5580

	CNST	HILL	GNLS
AIC:	613.88	402.37	406.37
PROB:	0	0.88	0.12
RMSE:	205.23	23.23	23.23

MAX_MEAN: 335 MAX_MED: 339 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

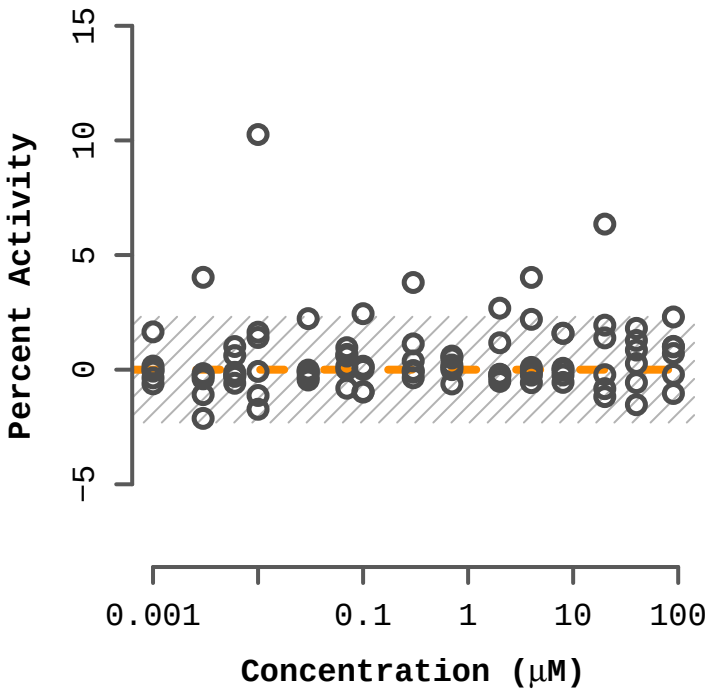
NAME: Hydroquinone
CHID: 20716 **CASRN:** 123-31-9
SPID(S): Tox21_300015
M4ID: 12479115

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

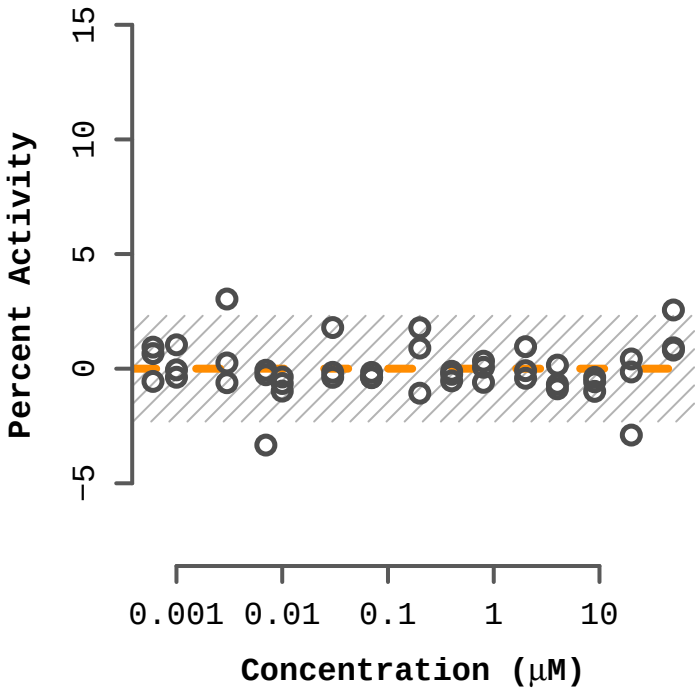
NAME: Hydroquinone
CHID: 20716 CASRN: 123-31-9
SPID(S): Tox21_202345
M4ID: 12479907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	307.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 1.73 MAX_MED: 0.849 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

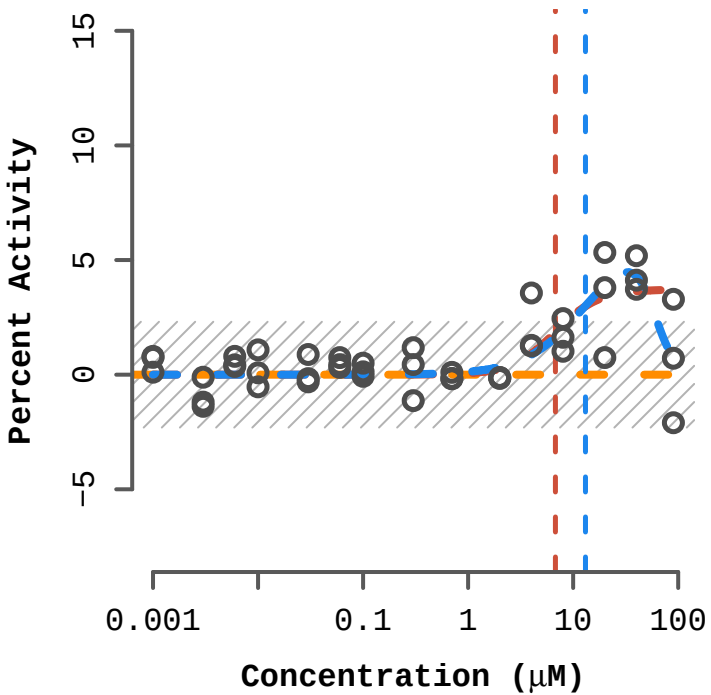
NAME: Hydroquinone
CHID: 20716 **CASRN:** 123-31-9
SPID(S): Tox21_110169_1
M4ID: 12484588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.911 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(Benzyloxyl)phenol
CHID: 20717 **CASRN:** 103-16-2
SPID(S): Tox21_201147
M4ID: 12481105

HILL MODEL (in red):

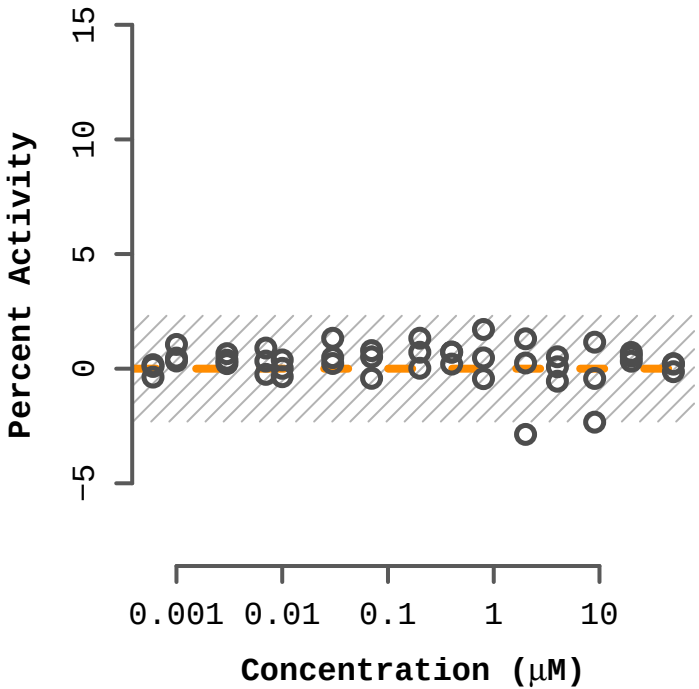
	tp	ga	gw
val:	3.72	0.831	2.13
sd:	0.467	0.116	0.674

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.02	1.12	1.5	1.77	4.42
sd:	5.87	0.598	0.873	0.229	3.55

	CNST	HILL	GNLS
AIC:	176.71	142.82	136.25
PROB:	0	0.04	0.96
RMSE:	1.85	1.31	1.05

MAX_MEAN: 4.35 **MAX_MED:** 4.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

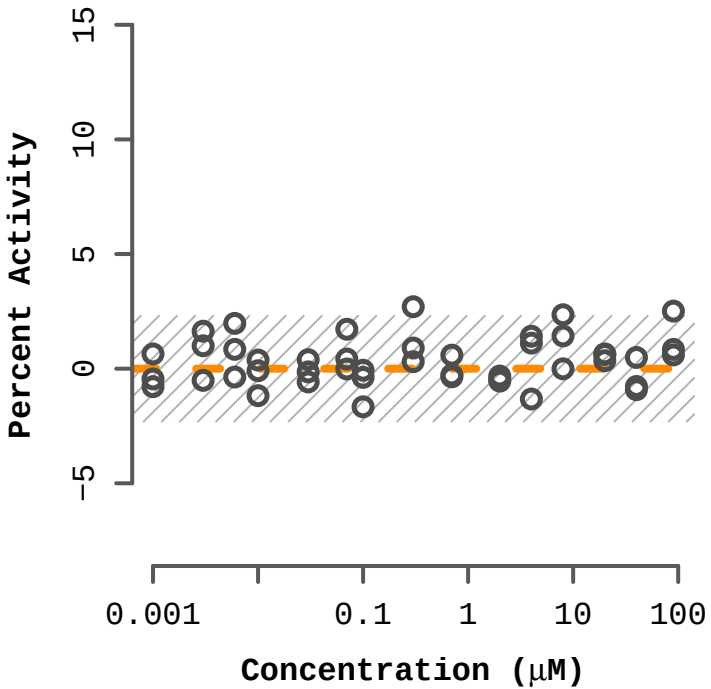
NAME: 4-(Benzyloxyl)phenol
CHID: 20717 **CASRN:** 103-16-2
SPID(S): Tox21_110396_1
M4ID: 12484395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.689 **MAX_MED:** 0.724 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

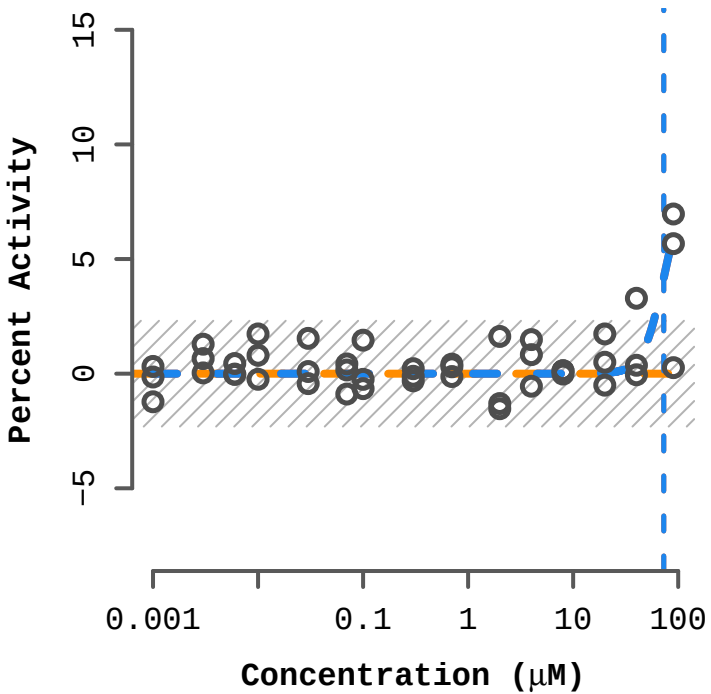
NAME: 3-Hydroxy-4-butyrophenetidide
CHID: 20721 **CASRN:** 1083-57-4
SPID(S): Tox21_302889
M4ID: 12476244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Hydroxy-4-butyrophenetidide
CHID: 20721 CASRN: 1083-57-4
SPID(S): Tox21_201816
M4ID: 12480436

HILL MODEL (in red):

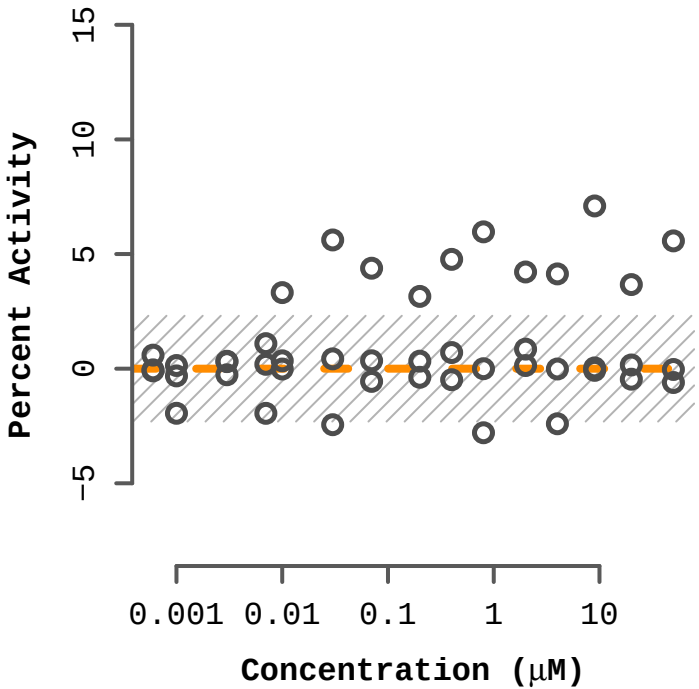
	tp	ga	gw
val:	8.36	1.86	4.4
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.36	1.86	4.39	3.8	5.48
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	147.4	138.94	142.94
PROB:	0.01	0.87	0.12
RMSE:	1.63	1.24	1.24

MAX_MEAN: 4.3 **MAX_MED:** 5.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

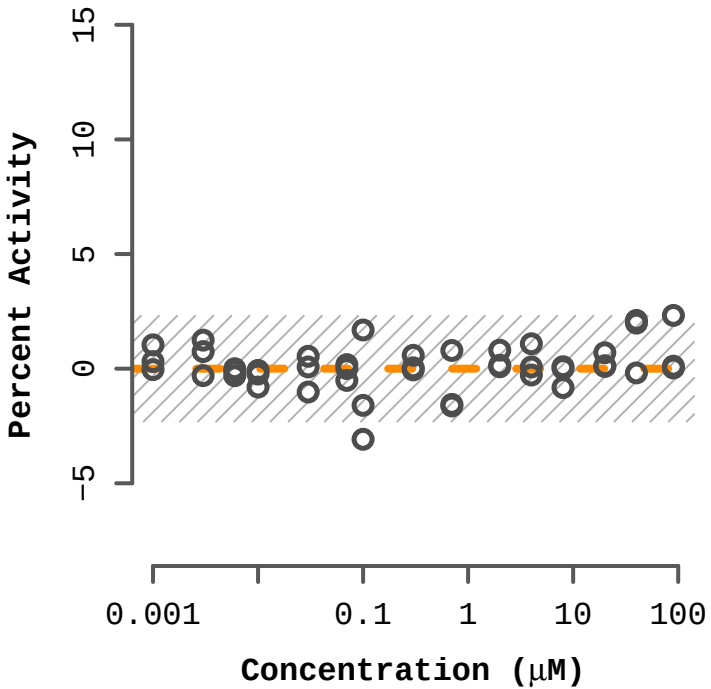
NAME: 3-Hydroxy-4-butyrophenetidide
CHID: 20721 **CASRN:** 1083-57-4
SPID(S): Tox21_112334_1
M4ID: 12483154

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.55	NA	NA

MAX_MEAN: 2.35 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

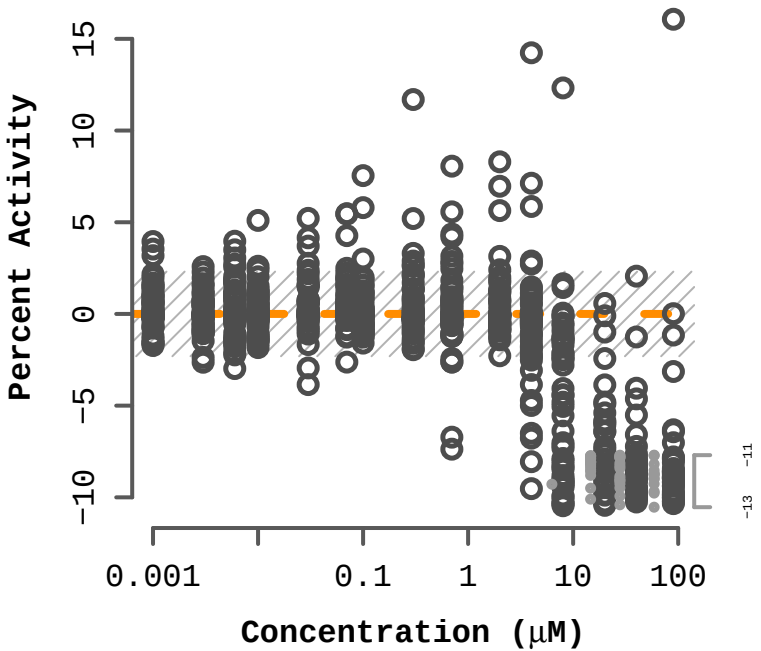
NAME: 2-Hydroxyethylhydrazine
CHID: 20728 CASRN: 109-84-2
SPID(S): Tox21_301204
M4ID: 12477929

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.3 MAX_MED: 1.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

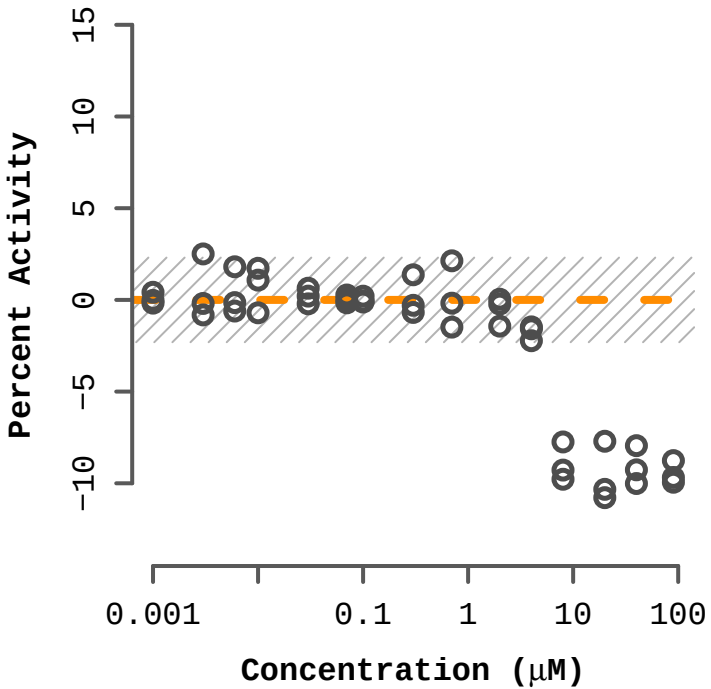
NAME: 8-Hydroxyquinoline
CHID: 20730 **CASRN:** 148-24-3
SPID(S): Tox21_400006
M4ID: 12475131 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	4455.4	NA	NA
PROB:	1	NA	NA
RMSE:	4.84	NA	NA

MAX_MEAN: 0.581 **MAX_MED:** 0.274 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

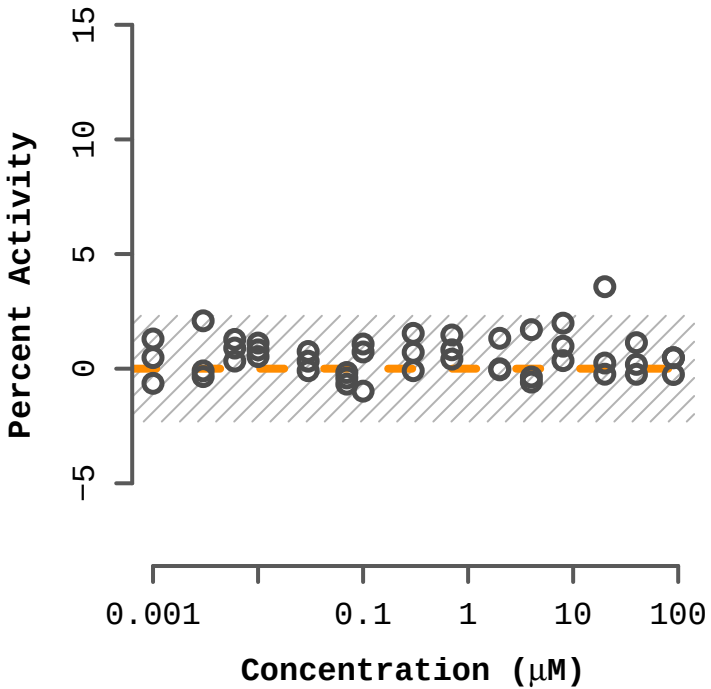
NAME: 8-Hydroxyquinoline
CHID: 20730 **CASRN:** 148-24-3
SPID(S): Tox21_202986
M4ID: 12479266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	266.96	NA	NA
PROB:	1	NA	NA
RMSE:	4.9	NA	NA

MAX_MEAN: 0.7 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

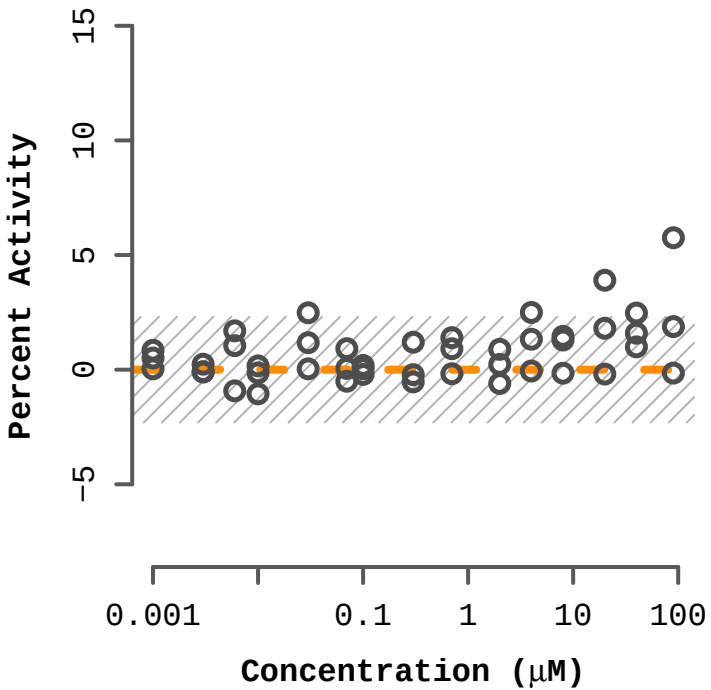
NAME: Ibuprofen
CHID: 20732 CASRN: 15687-27-1
SPID(S): Tox21_302829
M4ID: 12476304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

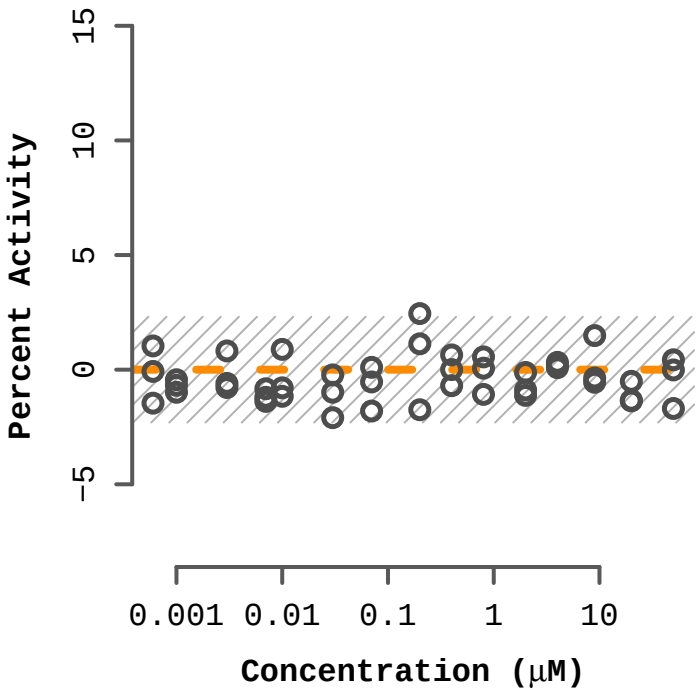
NAME: Ibuprofen
CHID: 20732 CASRN: 15687-27-1
SPID(S): Tox21_201384
M4ID: 12480868

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.5 MAX_MED: 1.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

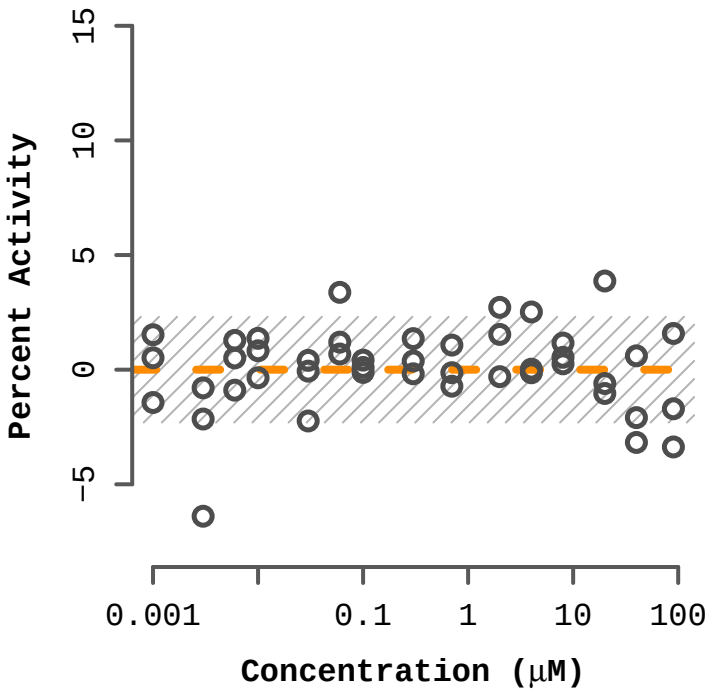
NAME: Ibuprofen
CHID: 20732 CASRN: 15687-27-1
SPID(S): Tox21_110170_1
M4ID: 12484587

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.611 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

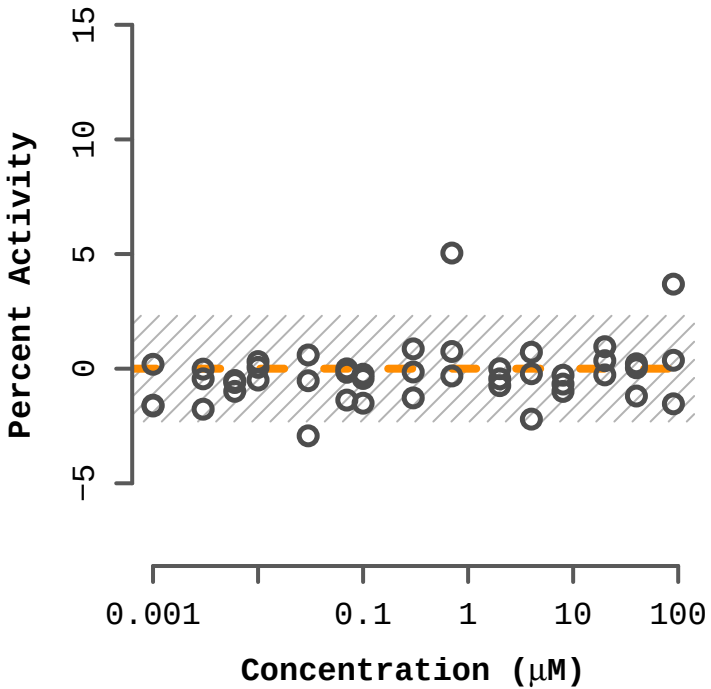
NAME: ICRF−159
CHID: 20733 CASRN: 21416−67−1
SPID(S): Tox21_200258
M4ID: 12481994

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

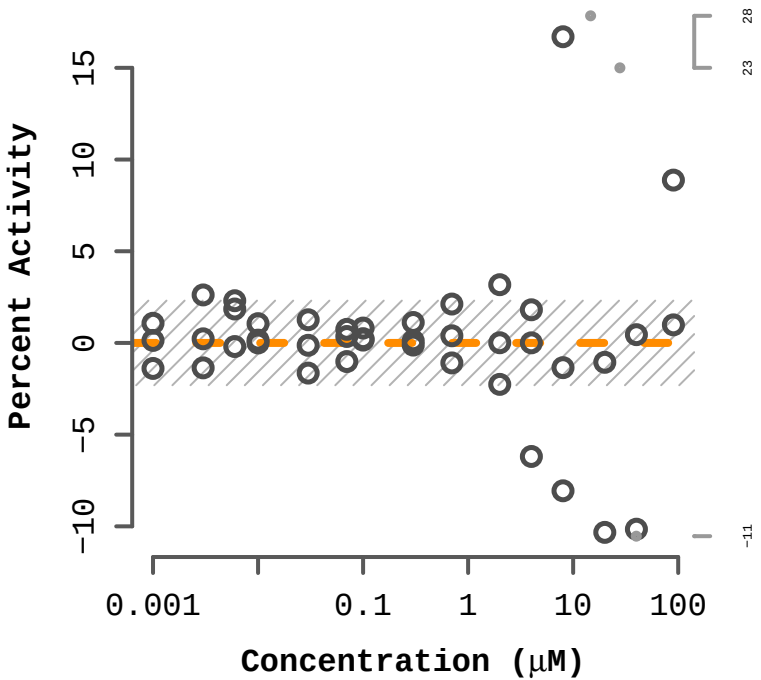
NAME: Indole
CHID: 20737 **CASRN:** 120-72-9
SPID(S): Tox21_302937
M4ID: 12476196

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 0.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

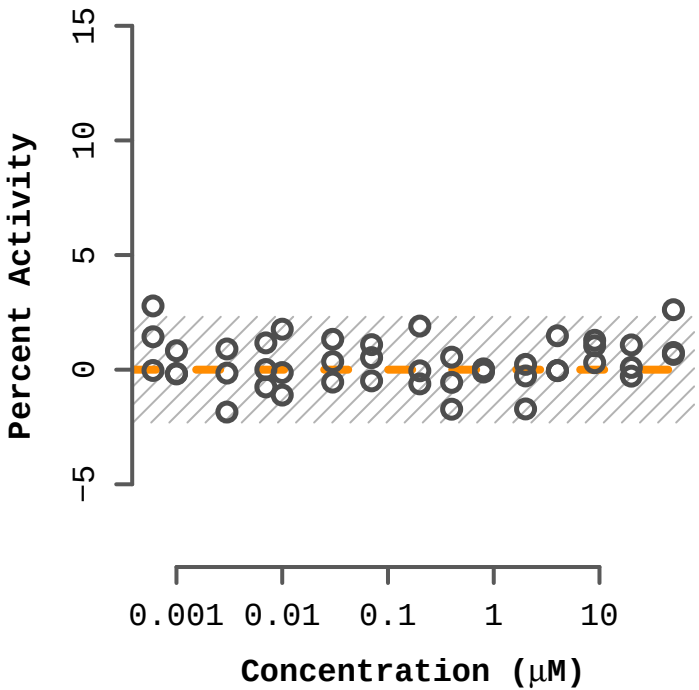
NAME: Indole
CHID: 20737 **CASRN:** 120-72-9
SPID(S): Tox21_201677
M4ID: 12480575 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	271.99	NA	NA
PROB:	1	NA	NA
RMSE:	6.91	NA	NA

MAX_MEAN: 5.59 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

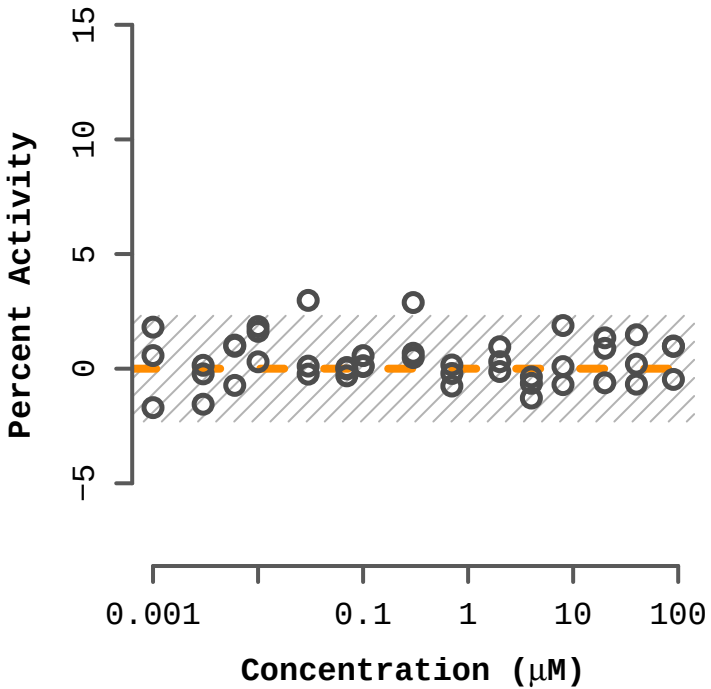
NAME: Indole
CHID: 20737 **CASRN:** 120-72-9
SPID(S): Tox21_112536_1
M4ID: 12483039

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

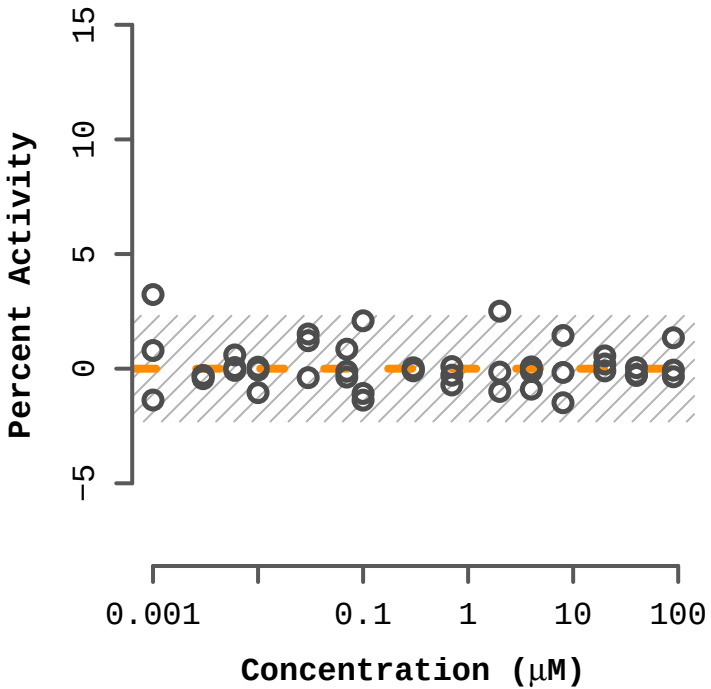
NAME: Indole-3-acetic acid
CHID: 20738 **CASRN:** 87-51-4
SPID(S): Tox21_302731
M4ID: 12476402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

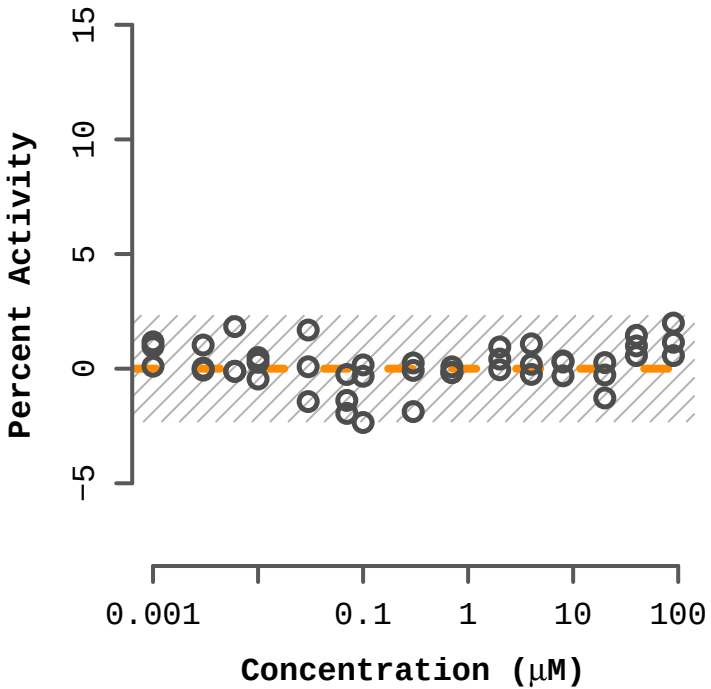
NAME: Indole-3-acetic acid
CHID: 20738 **CASRN:** 87-51-4
SPID(S): Tox21_202284
M4ID: 12479968

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.888 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

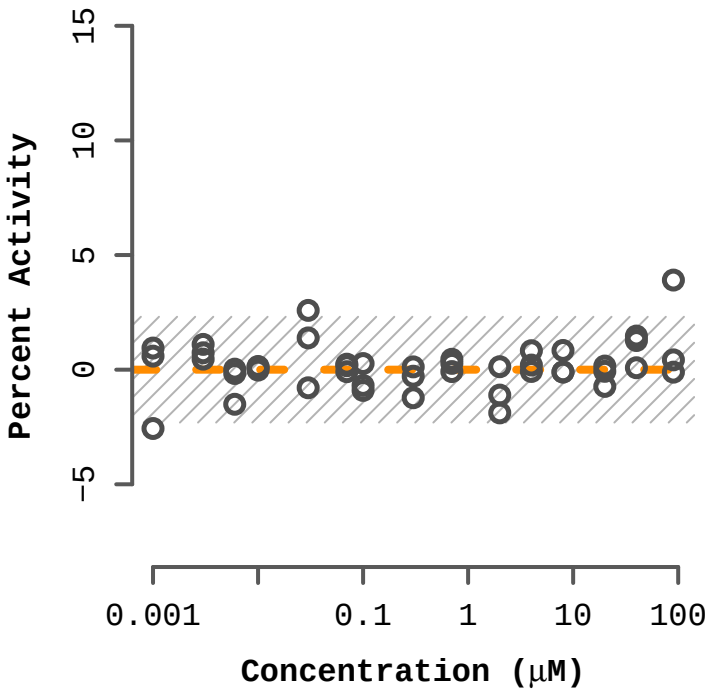
NAME: Indomethacin
CHID: 20740 **CASRN:** 53-86-1
SPID(S): Tox21_300266
M4ID: 12478864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

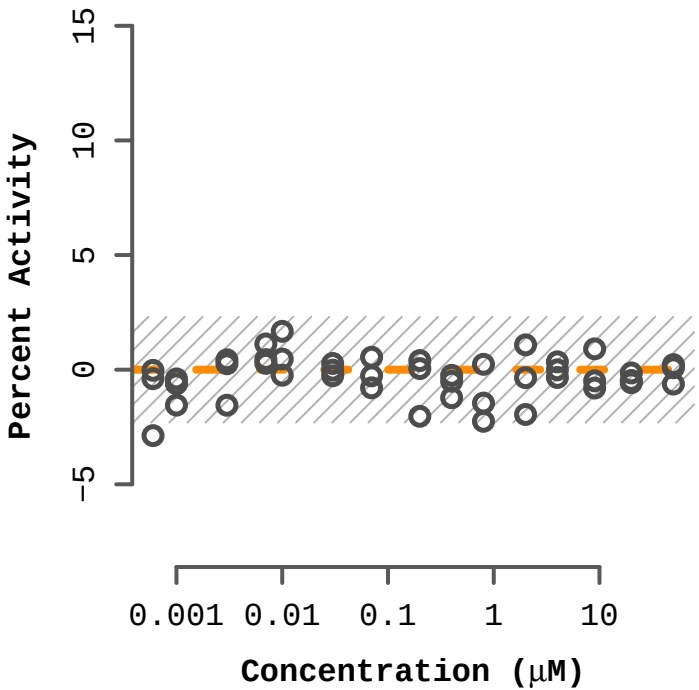
NAME: Indomethacin
CHID: 20740 **CASRN:** 53-86-1
SPID(S): Tox21_201791
M4ID: 12480461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

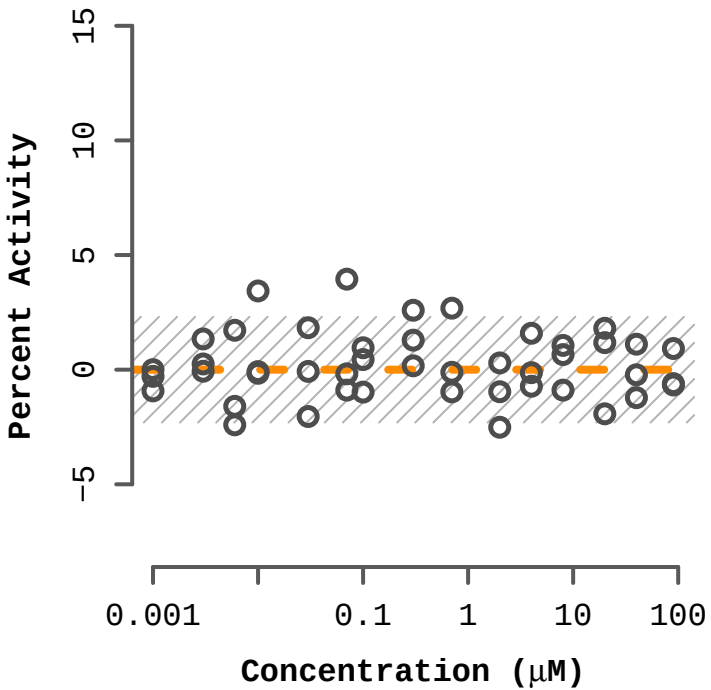
NAME: Indomethacin
CHID: 20740 **CASRN:** 53-86-1
SPID(S): Tox21_113109_1
M4ID: 12482804

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.633 **MAX_MED:** 0.465 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

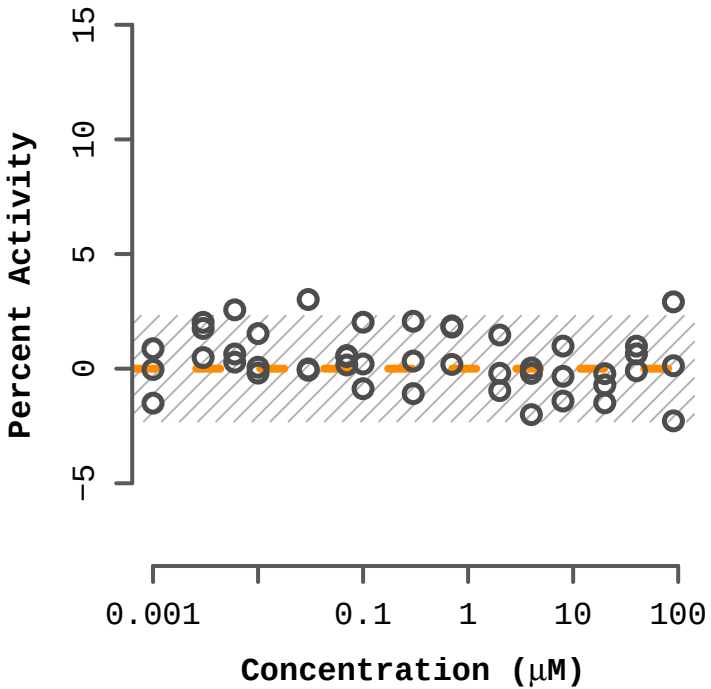
NAME: Iodoacetamide
CHID: 20742 **CASRN:** 144-48-9
SPID(S): Tox21_200214
M4ID: 12482038

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

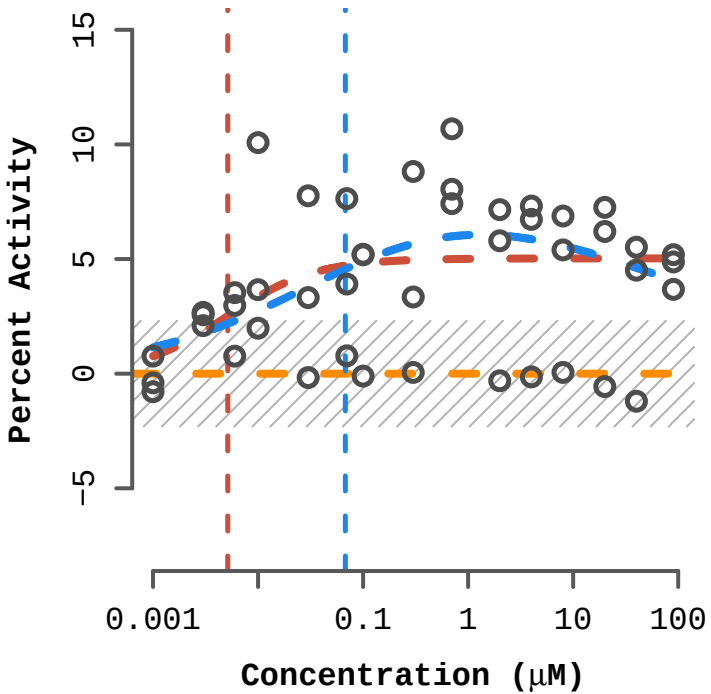
NAME: Iodoform
CHID: 20743 CASRN: 75-47-8
SPID(S): Tox21_302774
M4ID: 12476359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.42 MAX_MED: 1.82 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iodoform
CHID: 20743 CASRN: 75-47-8
SPID(S): Tox21_202389
M4ID: 12479863

HILL MODEL (in red):

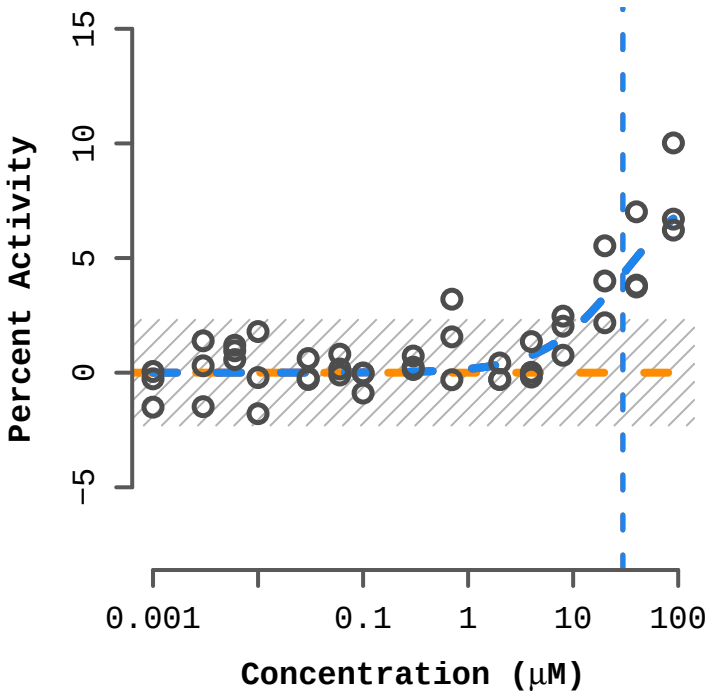
	tp	ga	gw
val:	5.03	−2.29	1.04
sd:	0.697	0.363	1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.8	−1.17	0.492	1.29	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	280.54	235.96	238.69
PROB:	0	0.8	0.2
RMSE:	5.06	2.99	3.02

MAX_MEAN: 8.72 MAX_MED: 8.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: IQ
CHID: 20745 CASRN: 76180-96-6
SPID(S): Tox21_200693
M4ID: 12481559

HILL MODEL (in red):

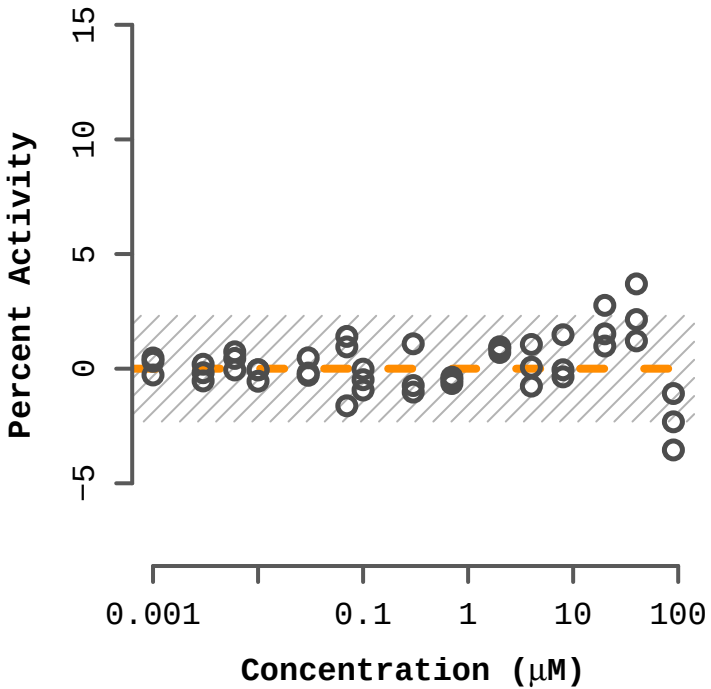
	tp	ga	gw
val:	8.57	1.47	1.16
sd:	4.06	0.499	0.59

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.57	1.47	1.16	2.44	17.6
sd:	4.06	0.499	0.59	479	17000

	CNST	HILL	GNLS
AIC:	209.78	147.18	151.18
PROB:	0	0.88	0.12
RMSE:	2.82	1.15	1.15

MAX_MEAN: 7.65 MAX_MED: 6.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

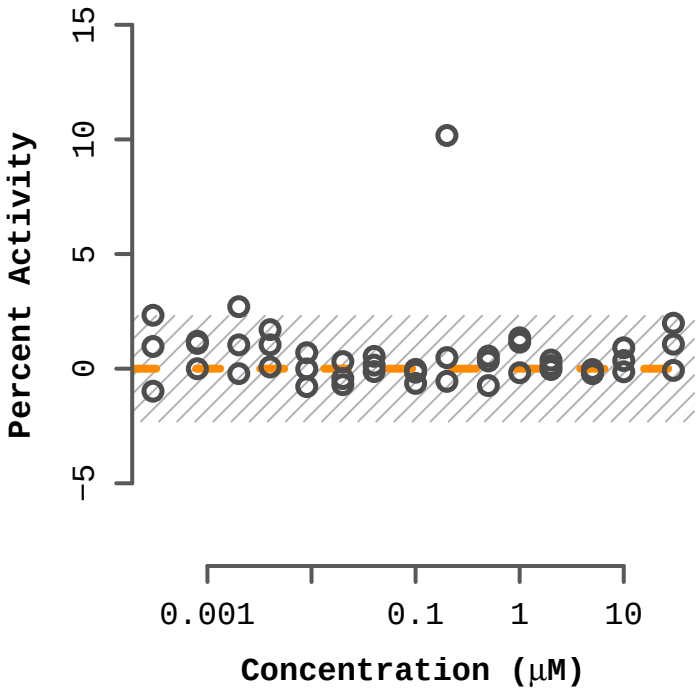
NAME: Isobutylparaben
CHID: 20749 **CASRN:** 4247-02-3
SPID(S): Tox21_200501
M4ID: 12481751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 2.35 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

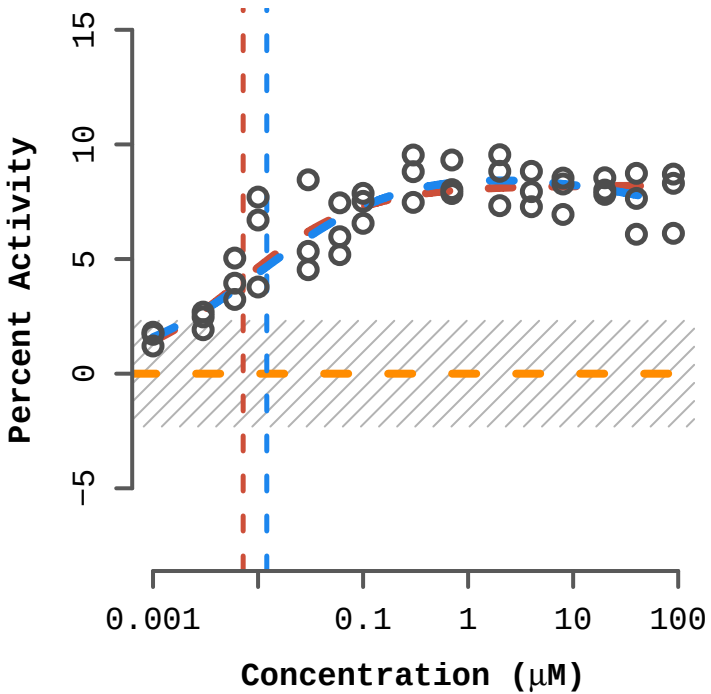
NAME: Isobutyl nitrite
CHID: 20750 **CASRN:** 542-56-3
SPID(S): Tox21_302863
M4ID: 12476270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 3.37 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isobutyl nitrite
CHID: 20750 CASRN: 542-56-3
SPID(S): Tox21_202411
M4ID: 12479841

HILL MODEL (in red):

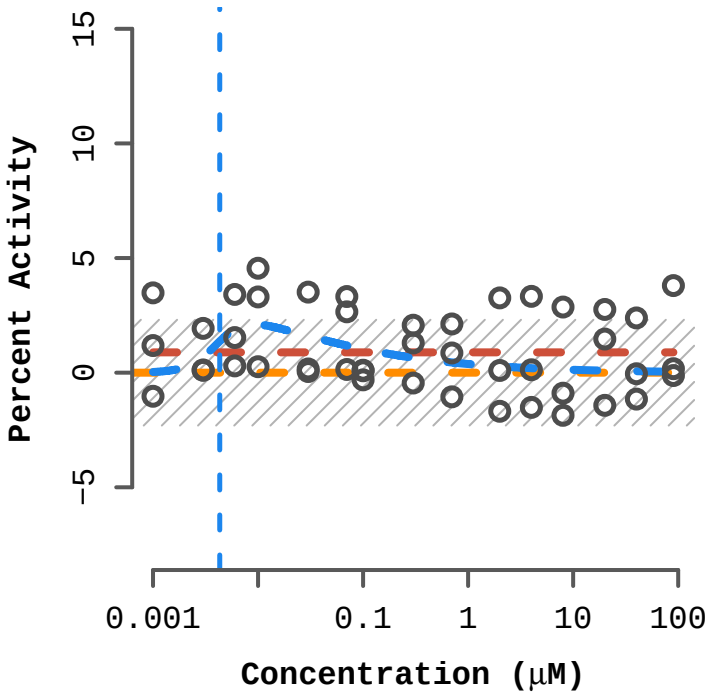
	tp	ga	gw
val:	8.2	−2.14	0.788
sd:	0.224	0.1	0.124

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.51	−1.92	0.639	3.84	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	313.88	142.96	145.42
PROB:	0	0.77	0.23
RMSE:	6.98	1.09	1.07

MAX_MEAN: 8.61 **MAX_MED:** 8.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoflurane
CHID: 20752 CASRN: 26675-46-7
SPID(S): Tox21_200831
M4ID: 12481421

HILL MODEL (in red):

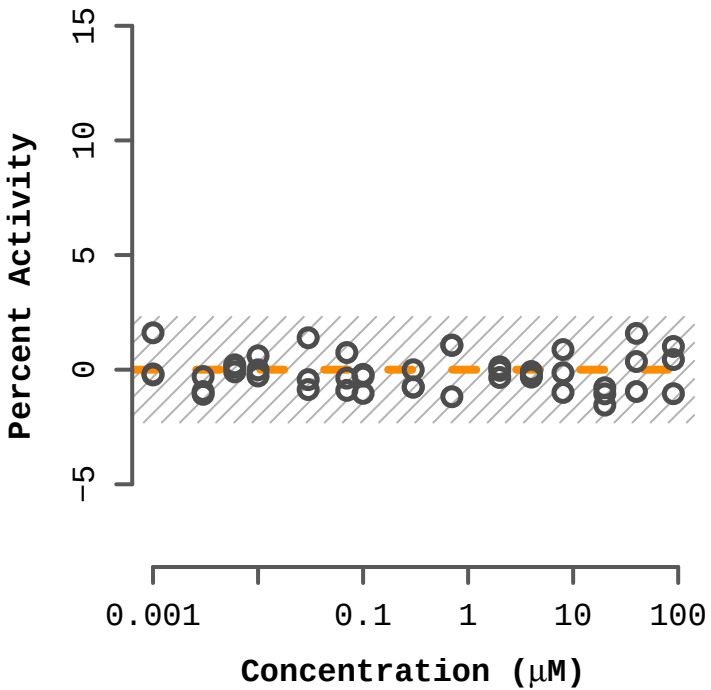
	tp	ga	gw
val:	0.886	−4.22	5.65
sd:	0.287	1390	6420

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.8	−2.36	3.26	−2.11	0.505
sd:	11.2	0.391	4.4	3.05	0.609

	CNST	HILL	GNLS
AIC:	194.95	191.31	193.31
PROB:	0.11	0.65	0.24
RMSE:	2	1.73	1.71

MAX_MEAN: 2.71 MAX_MED: 3.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

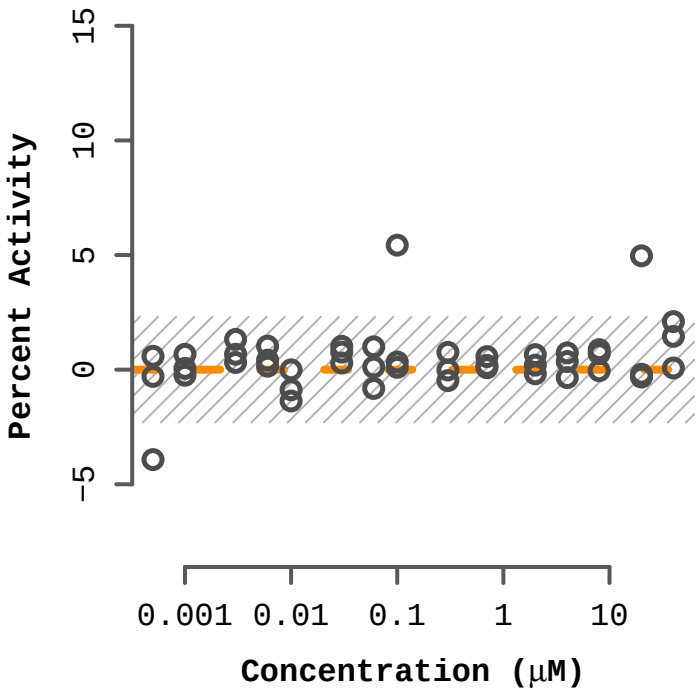
NAME: Isomalt
CHID: 20753 CASRN: 64519-82-0
SPID(S): Tox21_200914
M4ID: 12481338

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.4 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

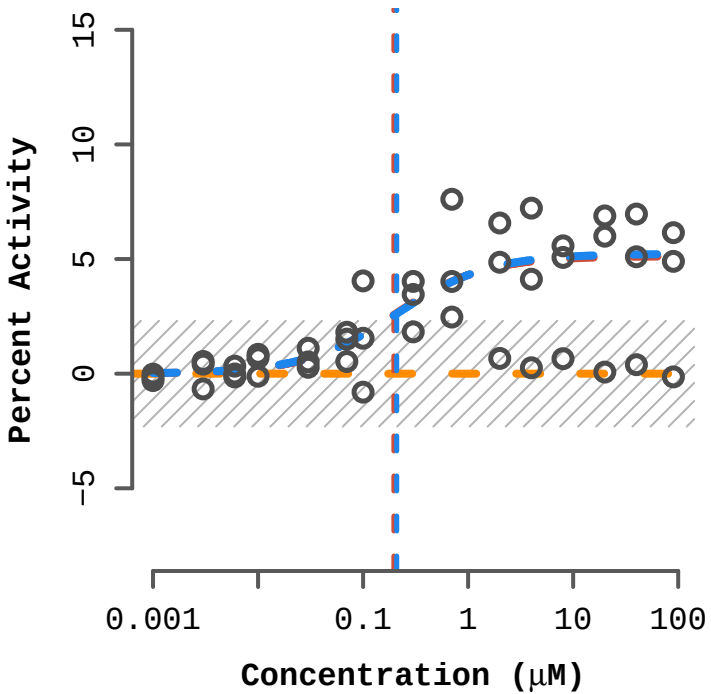
NAME: Isoniazid
CHID: 20755 CASRN: 54-85-3
SPID(S): Tox21_300193
M4ID: 12478937

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoniazid
CHID: 20755 CASRN: 54-85-3
SPID(S): Tox21_201367
M4ID: 12480885

HILL MODEL (in red):

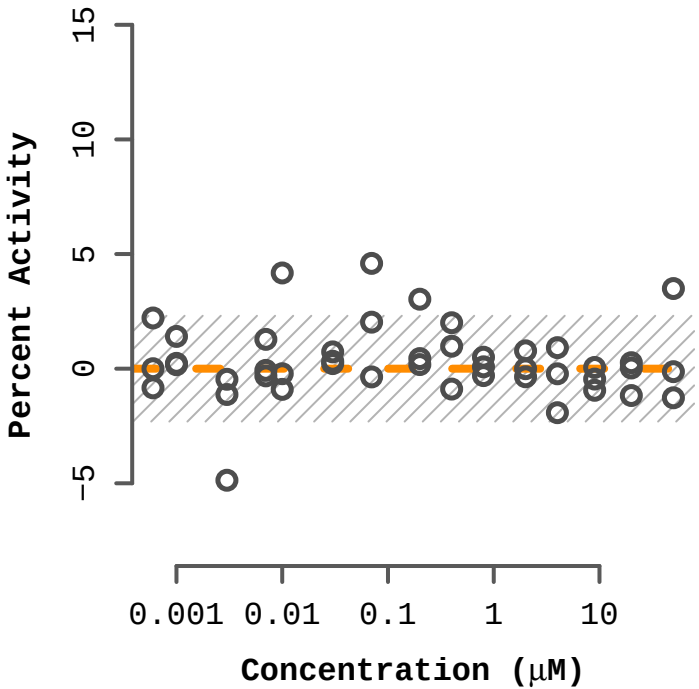
	tp	ga	gw
val:	5.12	−0.707	1.02
sd:	0.56	0.218	0.41

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.23	−0.68	0.982	2.03	15.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	243.13	191.28	195.19
PROB:	0	0.88	0.12
RMSE:	3.51	2.02	2.02

MAX_MEAN: 4.7 MAX_MED: 6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

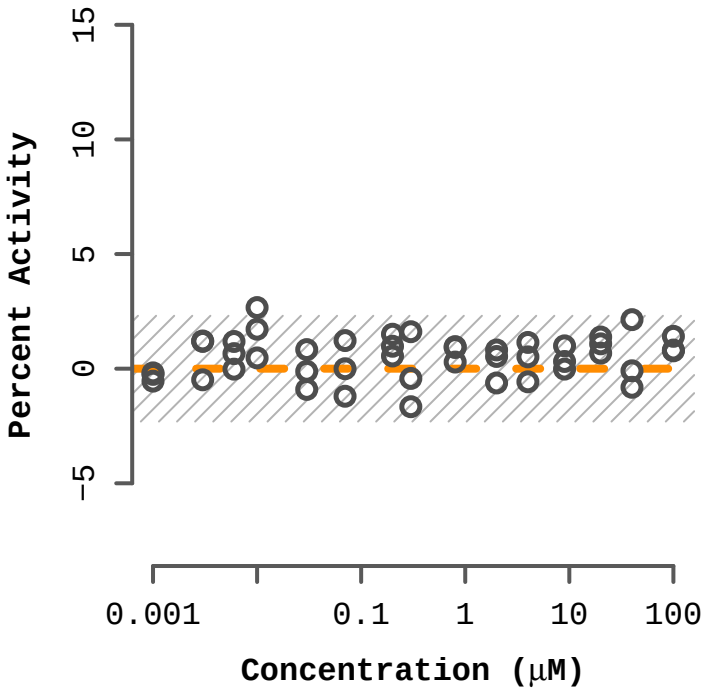
NAME: Isoniazid
CHID: 20755 CASRN: 54-85-3
SPID(S): Tox21_113640_1
M4ID: 12482569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

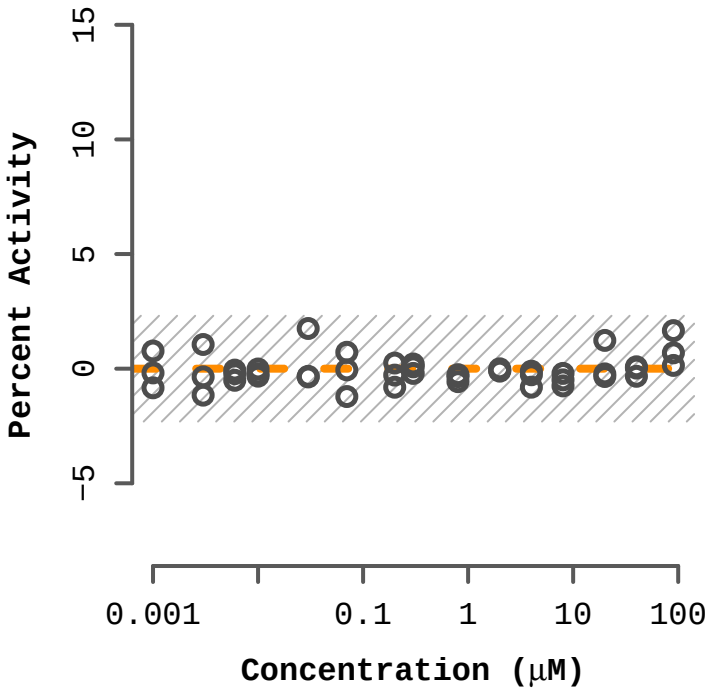
NAME: Isonicotinamide
CHID: 20756 **CASRN:** 1453-82-3
SPID(S): Tox21_200230
M4ID: 12482022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

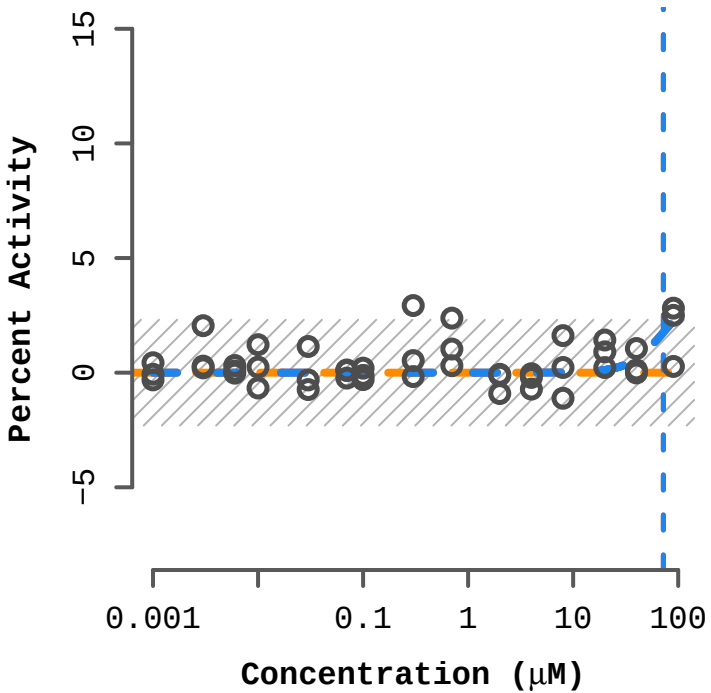
NAME: Isonicotinic acid
CHID: 20757 CASRN: 55-22-1
SPID(S): Tox21_200502
M4ID: 12481750

HILL MODEL: Not applicable.

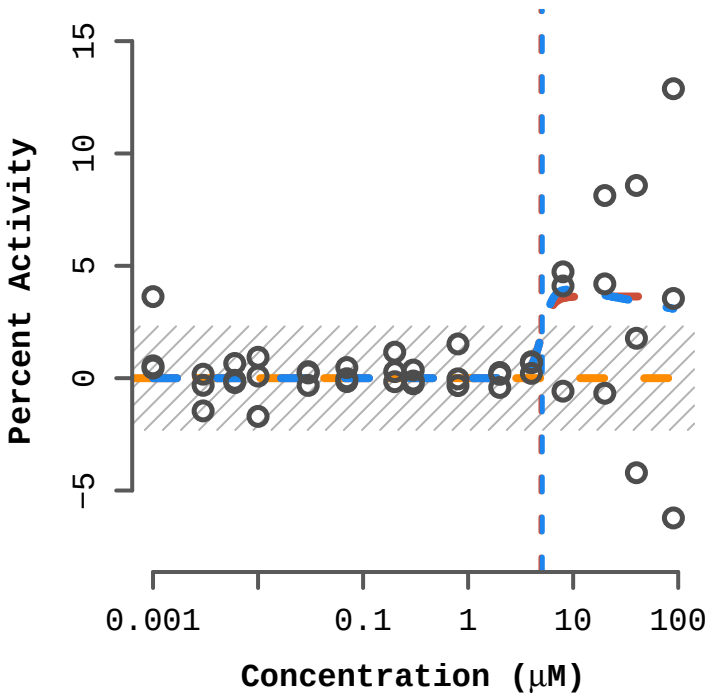
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	85.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 0.833 MAX_MED: 0.693 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Isophorone
CHID:    20759   CASRN: 78-59-1
SPID(S): Tox21_300050
M4ID:    12479080

HILL MODEL (in red):
      tp       ga       gw
val:  3.51     1.86     2.63
sd:   3.18     0.331    3.59

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.51     1.86     2.63     3.51     4.7
sd:   3.18     0.332    3.59     1160     3520

      CNST        HILL        GNLS
AIC:  125.2       120.26      124.26
PROB: 0.07        0.82        0.11
RMSE: 1.04        0.91        0.91

MAX_MEAN: 1.86      MAX_MED: 2.5       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isophorone
CHID: 20759 CASRN: 78-59-1
SPID(S): Tox21_202312
M4ID: 12479940

HILL MODEL (in red):

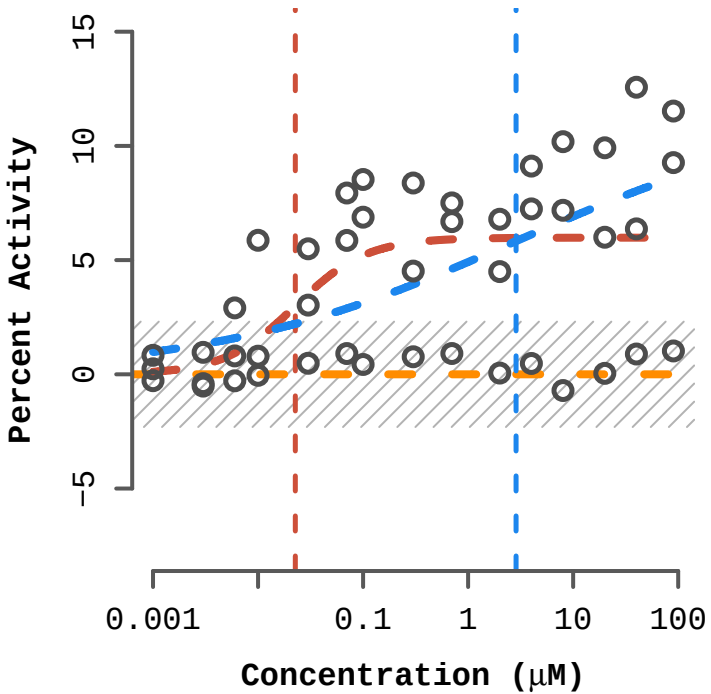
	tp	ga	gw
val:	3.64	0.693	8
sd:	0.68	0.106	8.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.54	0.706	8	2.28	0.306
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	211.41	202.14	205.79
PROB:	0.01	0.85	0.14
RMSE:	3.2	2.81	2.81

MAX_MEAN: 3.89 **MAX_MED:** 4.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ifosfamide
CHID: 20760 CASRN: 3778-73-2
SPID(S): Tox21_302775
M4ID: 12476358

HILL MODEL (in red):

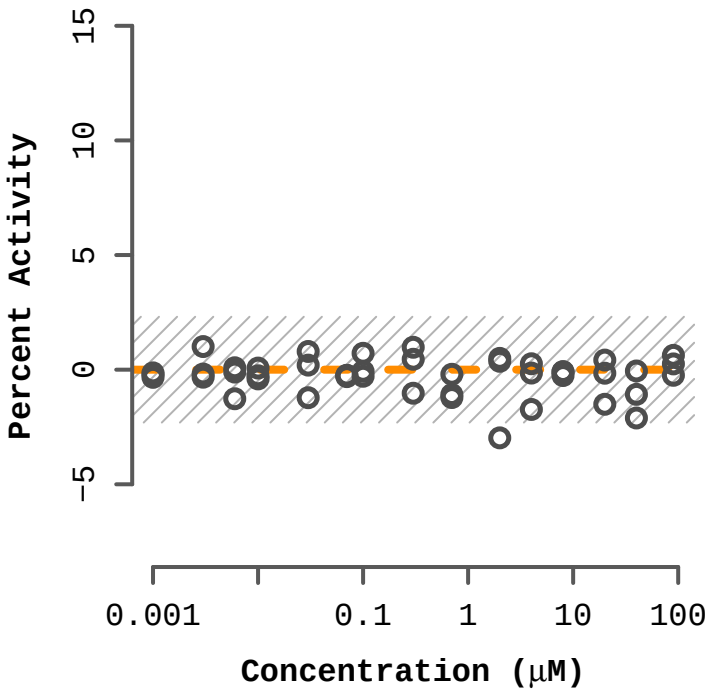
	tp	ga	gw
val:	5.98	-1.65	1.28
sd:	0.873	0.302	0.937

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.7	0.456	0.3	2.5	14.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	287.48	247.64	254.36
PROB:	0	0.97	0.03
RMSE:	5.6	3.32	3.47

MAX_MEAN: 7.27 MAX_MED: 9.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

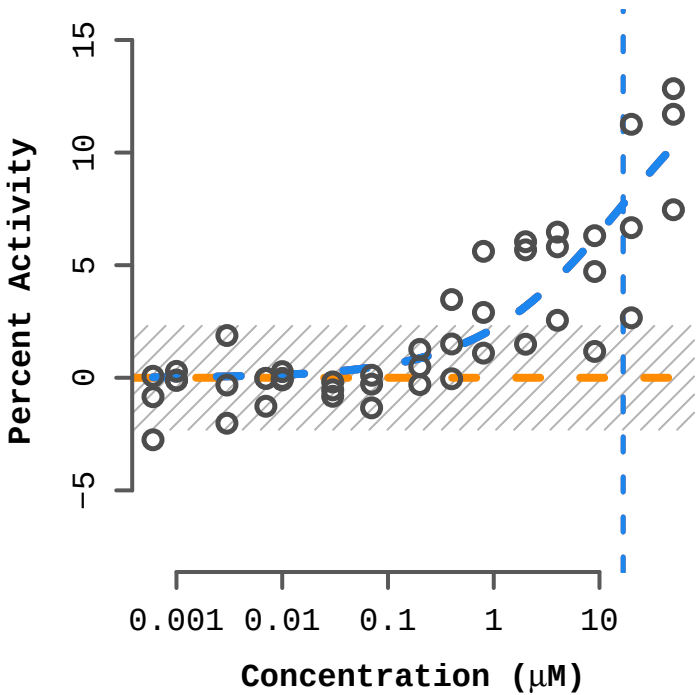
NAME: Ifosfamide
CHID: 20760 CASRN: 3778-73-2
SPID(S): Tox21_201815
M4ID: 12480437

HILL MODEL: Not applicable.

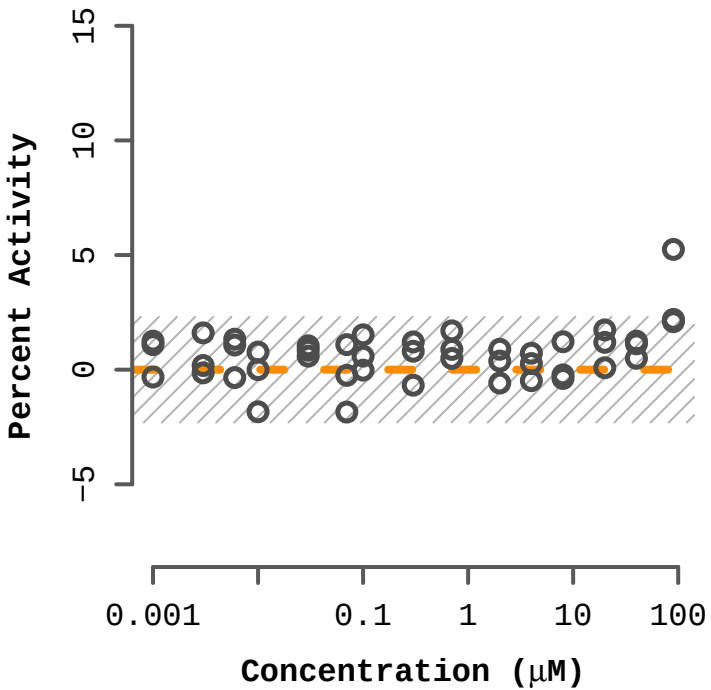
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.212 **MAX_MED:** 0.455 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ifosfamide
CHID:    20760   CASRN: 3778-73-2
SPID(S): Tox21_110539_1
M4ID:    12484281

HILL MODEL (in red):
      tp       ga       gw
val:  15.4     1.22     0.636
sd:   9.15     0.827    0.171

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  15.4     1.22     0.636    3.68     9.72
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  252.93      191.79      195.79
PROB: 0           0.88        0.12
RMSE: 4.3         1.89        1.89

MAX_MEAN: 10.7      MAX_MED: 11.7      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

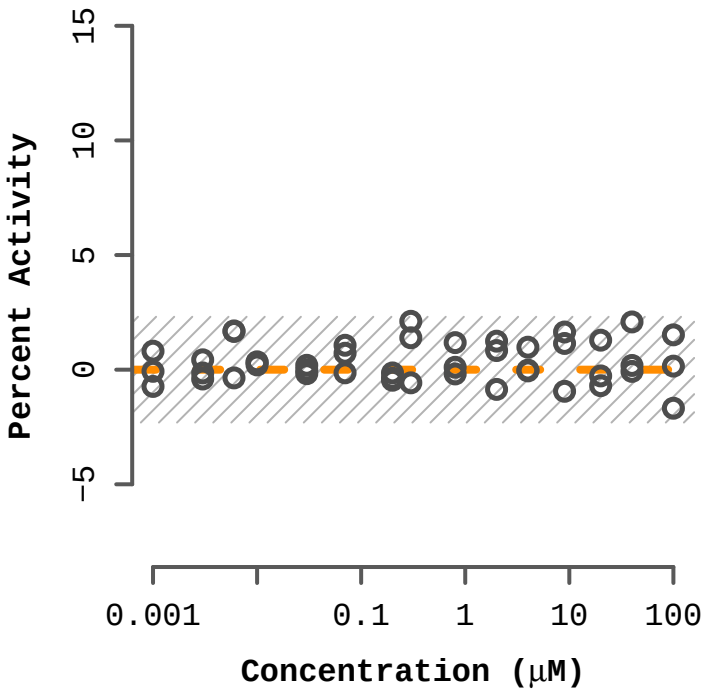
NAME: Isoprene
CHID: 20761 **CASRN:** 78-79-5
SPID(S): Tox21_200067
M4ID: 12482185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 3.18 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

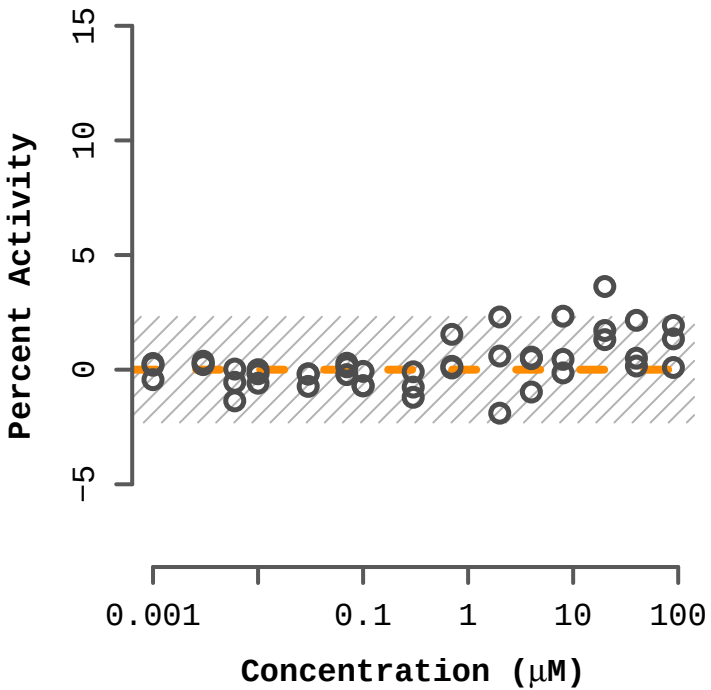
NAME: Isopropanol
CHID: 20762 CASRN: 67-63-0
SPID(S): Tox21_202475
M4ID: 12479777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1 MAX_MED: 1.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

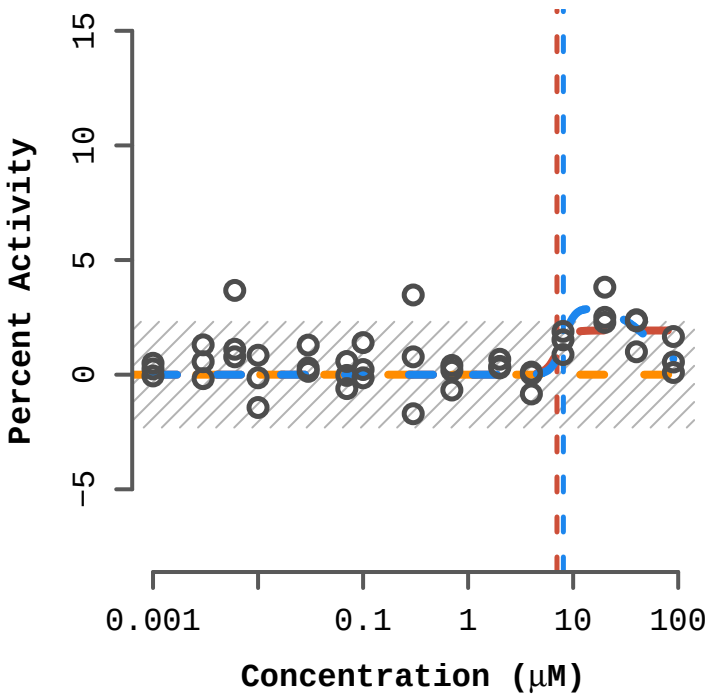
NAME: Chlorpropham
CHID: 20764 **CASRN:** 101-21-3
SPID(S): Tox21_301139
M4ID: 12477994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorpropham
CHID: 20764 **CASRN:** 101-21-3
SPID(S): Tox21_201866
M4ID: 12480386

HILL MODEL (in red):

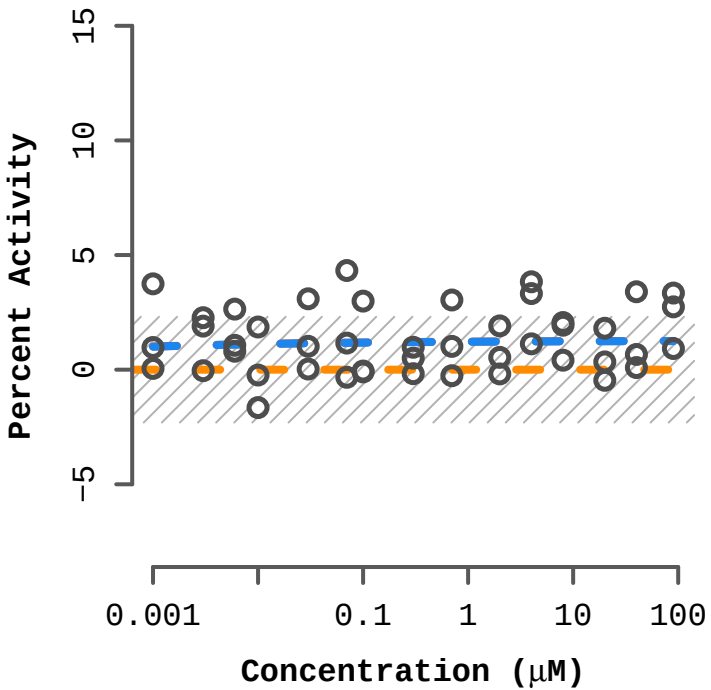
	tp	ga	gw
val:	1.93	0.846	8
sd:	0.328	0.0856	8.57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.01	0.907	8	1.73	2.37
sd:	1.04	0.0442	12	0.198	1.87

	CNST	HILL	GNLS
AIC:	158.51	135.93	131.05
PROB:	0	0.08	0.92
RMSE:	1.42	1.09	1.02

MAX_MEAN: 2.87 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propham
CHID: 20766 CASRN: 122-42-9
SPID(S): Tox21_302973
M4ID: 12476160

HILL MODEL (in red):

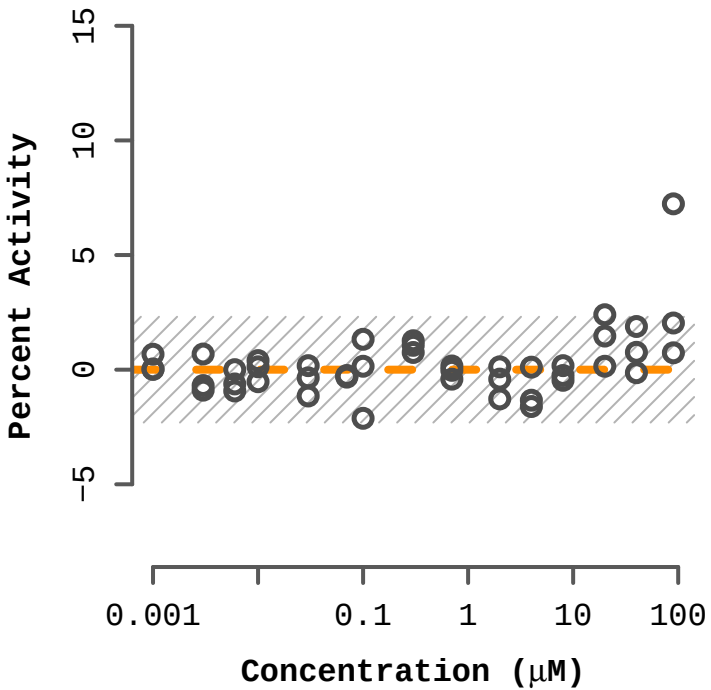
	tp	ga	gw
val:	1.26	−5	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.25	−5	0.3	3.93	5.12
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	190.2	171.08	175.08
PROB:	0	0.88	0.12
RMSE:	1.91	1.41	1.41

MAX_MEAN: 2.76 **MAX_MED:** 3.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

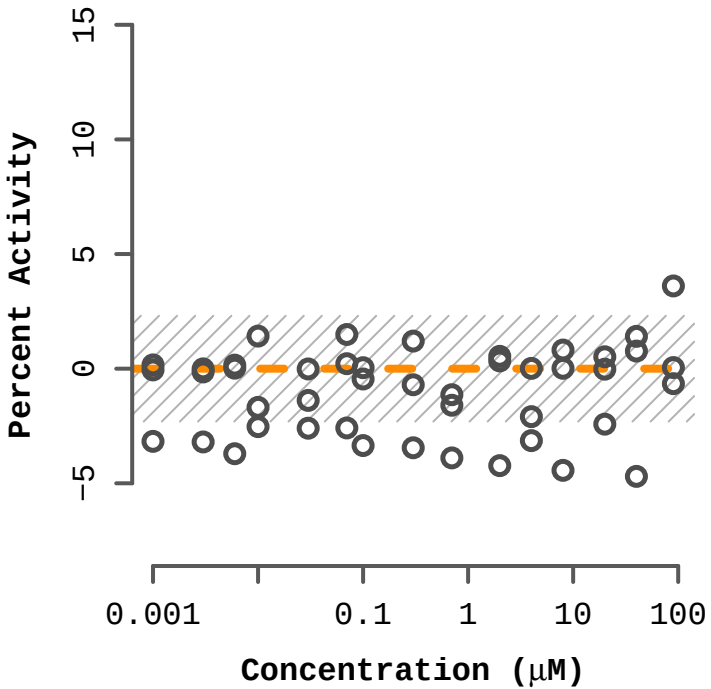
NAME: Propham
CHID: 20766 **CASRN:** 122-42-9
SPID(S): Tox21_201664
M4ID: 12480588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 3.34 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

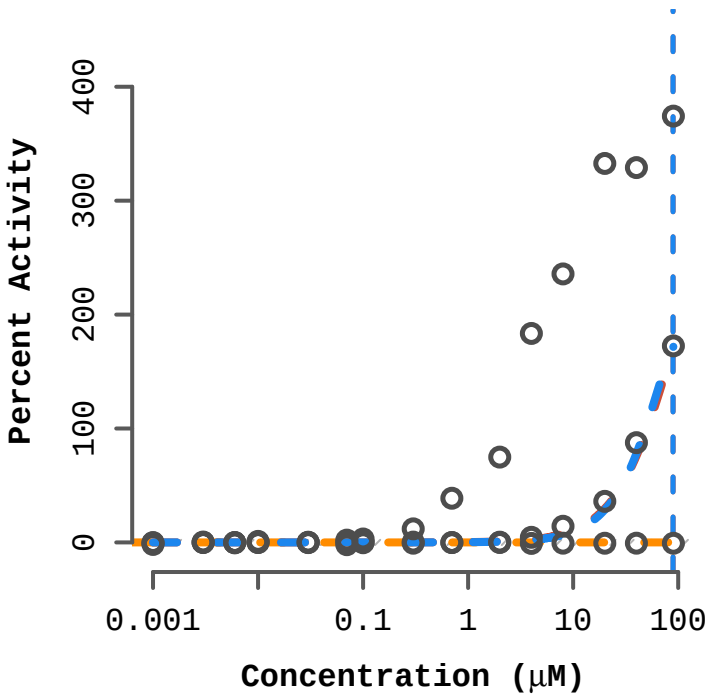
NAME: Isosafrole
CHID: 20767 CASRN: 120-58-1
SPID(S): Tox21_302946
M4ID: 12476187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 1 MAX_MED: 0.769 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isosafrole
CHID: 20767 CASRN: 120-58-1
SPID(S): Tox21_201783
M4ID: 12480469

HILL MODEL (in red):

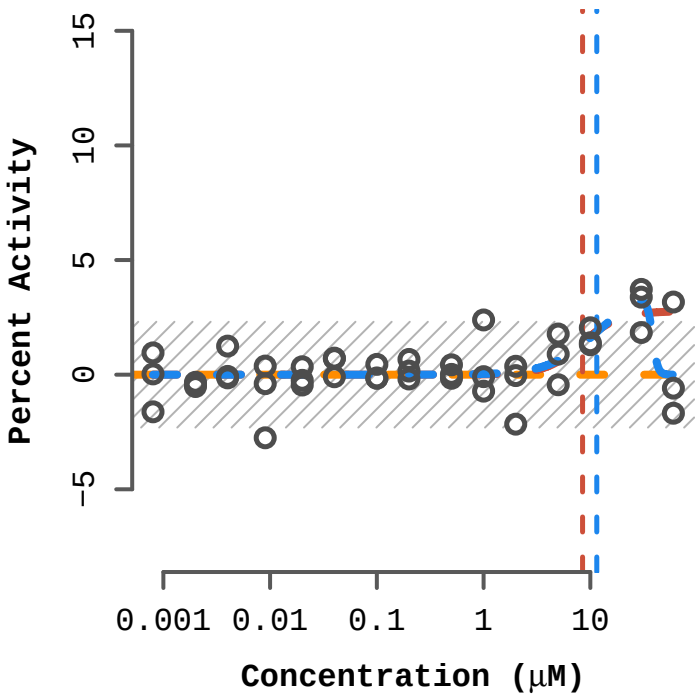
	tp	ga	gw
val:	342	1.95	1.57
sd:	502	0.811	1.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	379	1.95	1.67	2.2	3.87
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	502.35	490.6	494.57
PROB:	0	0.88	0.12
RMSE:	104.83	85.06	85.13

MAX_MEAN: 182 MAX_MED: 173 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Kaempferol
CHID: 20768 **CASRN:** 520-18-3
SPID(S): Tox21_303363
M4ID: 12475772

HILL MODEL (in red):

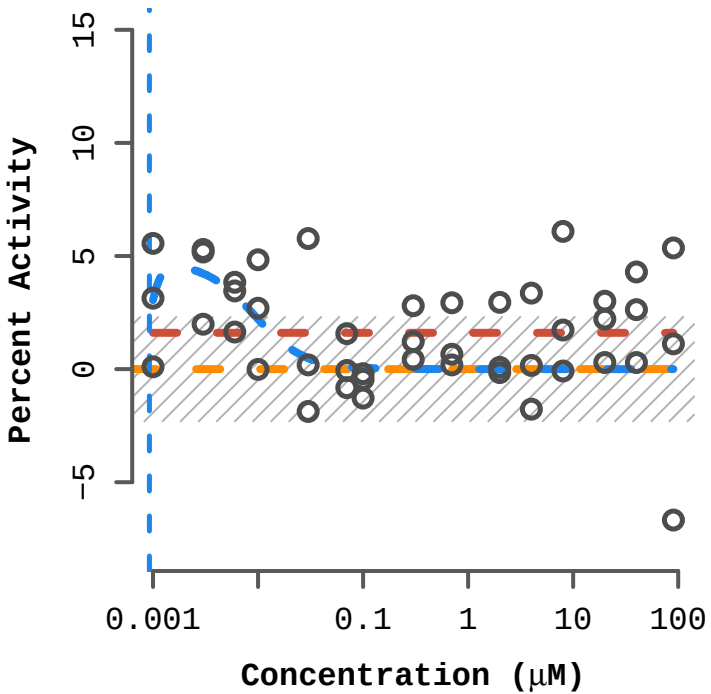
	tp	ga	gw
val:	2.77	0.927	2.53
sd:	0.584	0.13	1.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.71	1.06	1.94	1.58	18
sd:	2.41	0.324	1.36	0.448	51.2

	CNST	HILL	GNLS
AIC:	151.68	136.24	131.62
PROB:	0	0.09	0.91
RMSE:	1.34	1.19	1.01

MAX_MEAN: 2.98 **MAX_MED:** 3.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Kaempferol
CHID: 20768 CASRN: 520-18-3
SPID(S): Tox21_201165
M4ID: 12481087

HILL MODEL (in red):

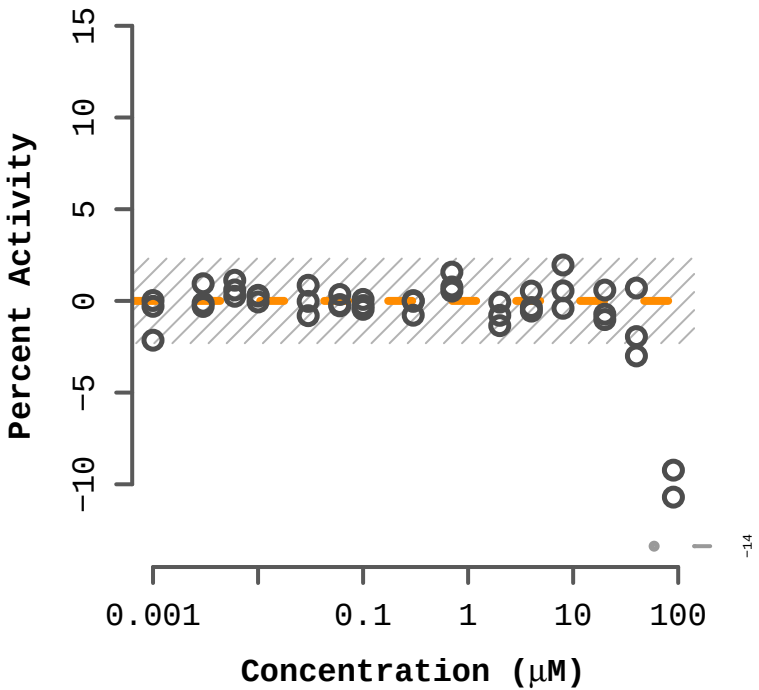
	tp	ga	gw
val:	1.6	-5	3.66
sd:	0.365	1540	2800

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.75	-3.03	7.99	-2.03	1.84
sd:	3.34	0.169	39.9	0.471	2.31

	CNST	HILL	GNLS
AIC:	229.71	217.94	219.28
PROB:	0	0.66	0.34
RMSE:	2.97	2.48	2.46

MAX_MEAN: 4.15 MAX_MED: 5.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

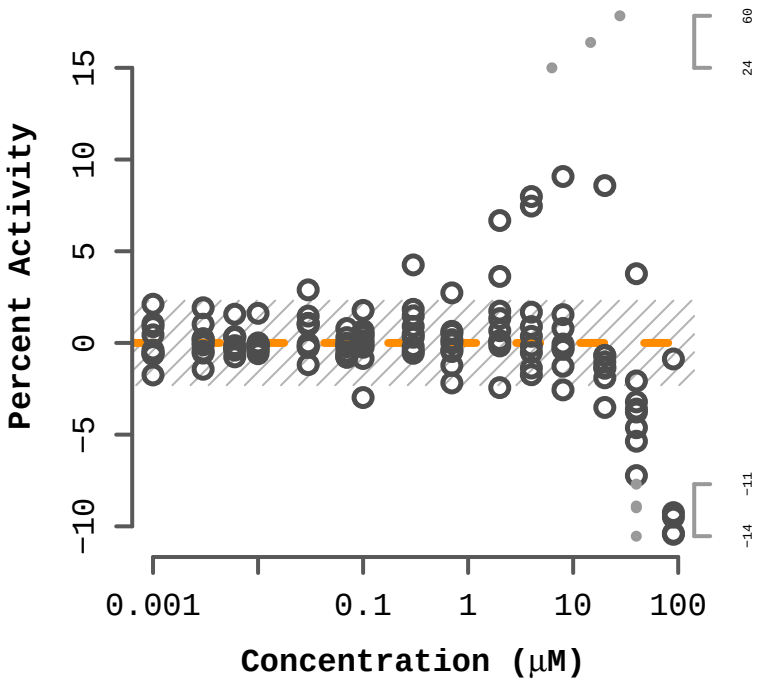
NAME: Kepone
CHID: 20770 **CASRN:** 143-50-0
SPID(S): Tox21_300098
M4ID: 12479032 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.52	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 0.763 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

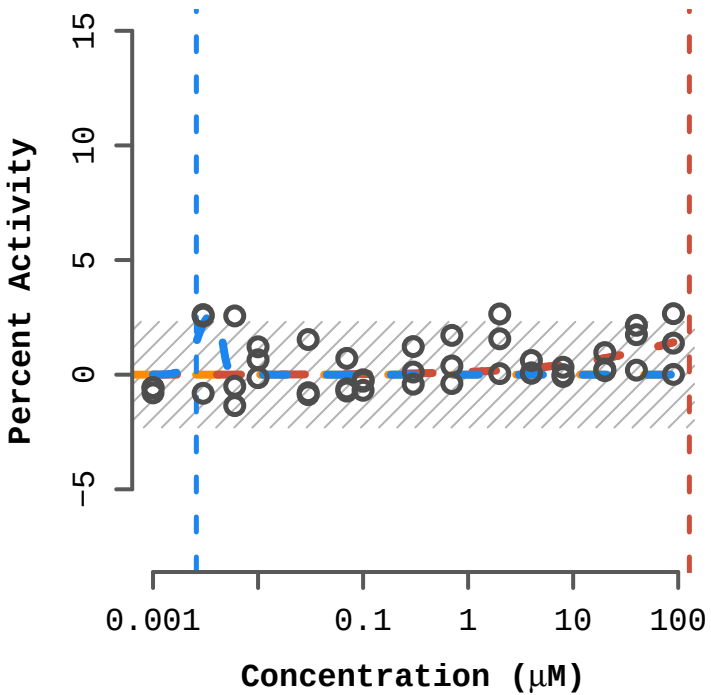
NAME: Kepone
CHID: 20770 **CASRN:** 143-50-0
SPID(S): Tox21_201592
M4ID: 12480660 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	721.49	NA	NA
PROB:	1	NA	NA
RMSE:	7.46	NA	NA

MAX_MEAN: 4.38 **MAX_MED:** 0.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ketoprofen
CHID: 20771 CASRN: 22071-15-4
SPID(S): Tox21_200847
M4ID: 12481405

HILL MODEL (in red):

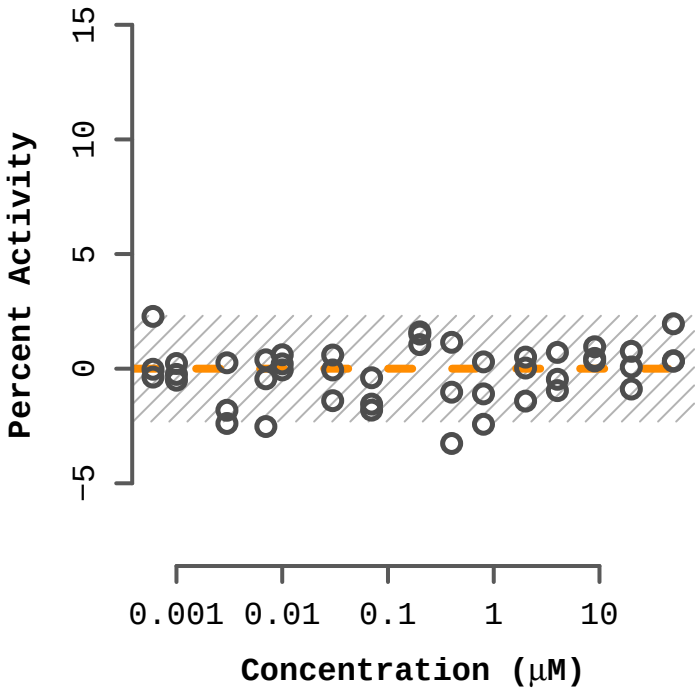
	tp	ga	gw
val:	3.2	2.11	0.669
sd:	5.82	2.11	0.628

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.87	−2.59	8	−2.34	18
sd:	9.85	0.65	23.6	0.258	40.1

	CNST	HILL	GNLS
AIC:	145.41	141.58	150.41
PROB:	0.13	0.86	0.01
RMSE:	1.19	1.07	1.15

MAX_MEAN: 1.46 **MAX_MED:** 2.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

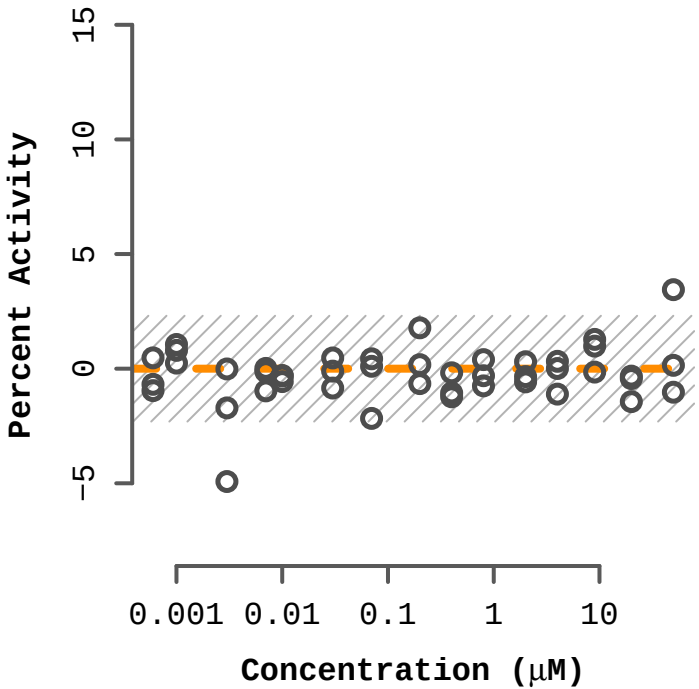
NAME: Ketoprofen
CHID: 20771 CASRN: 22071-15-4
SPID(S): Tox21_110594_1
M4ID: 12484243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

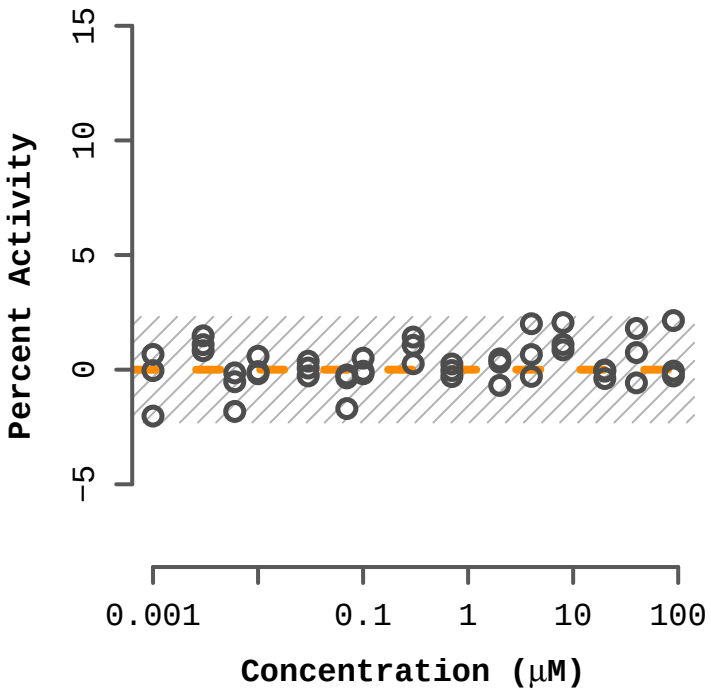
NAME: Levobunolol hydrochloride
CHID: 20777 CASRN: 27912-14-7
SPID(S): Tox21_110617_1
M4ID: 12484228

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.856 **MAX_MED:** 0.984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

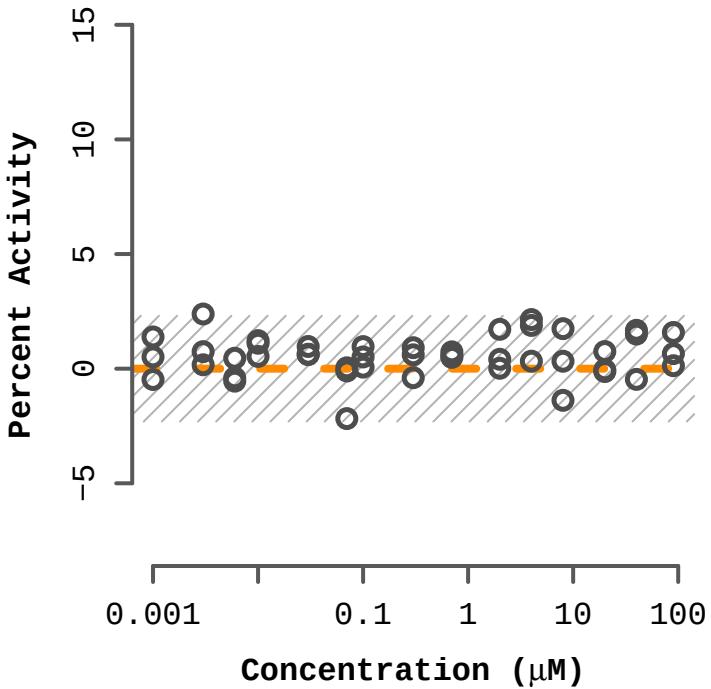
NAME: D−Limonene
CHID: 20778 **CASRN:** 5989−27−5
SPID(S): Tox21_200400
M4ID: 12481852

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

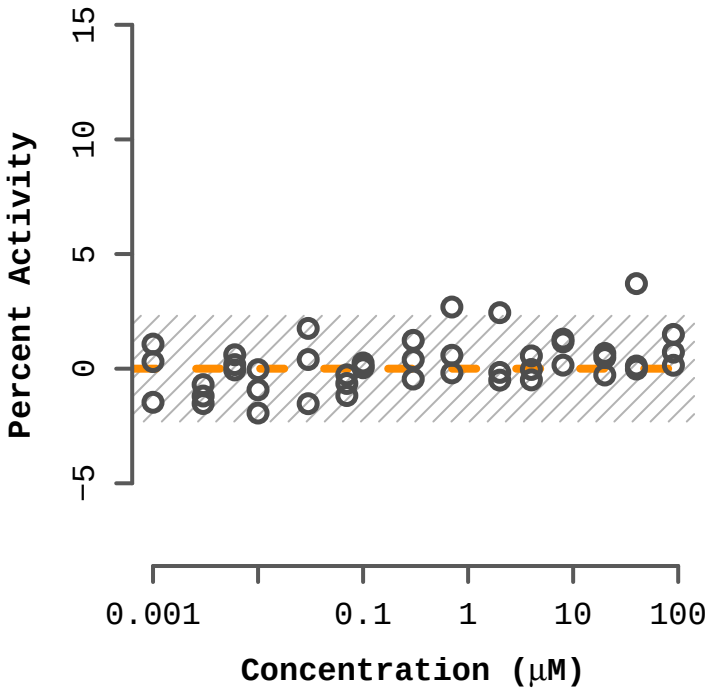
NAME: Lithocholic acid
CHID: 20779 CASRN: 434-13-9
SPID(S): Tox21_302791
M4ID: 12476342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

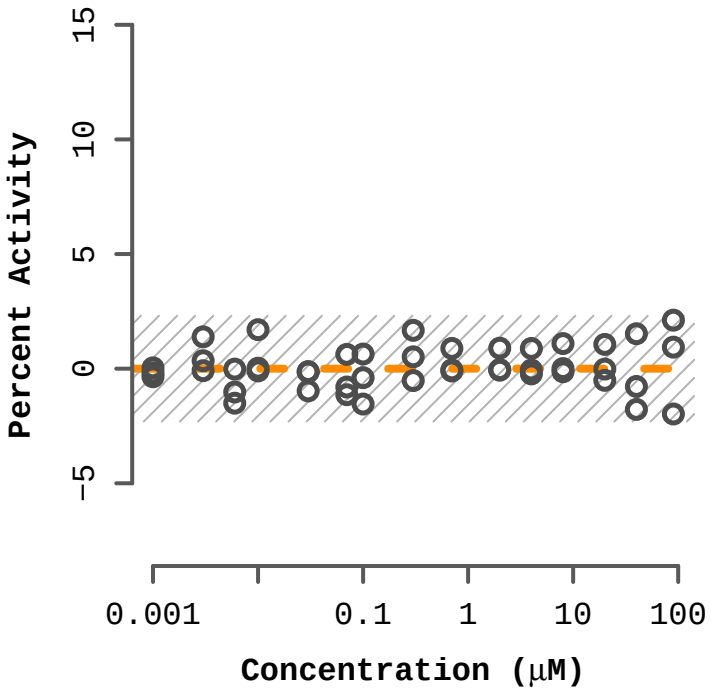
NAME: Lithocholic acid
CHID: 20779 CASRN: 434-13-9
SPID(S): Tox21_201868
M4ID: 12480384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

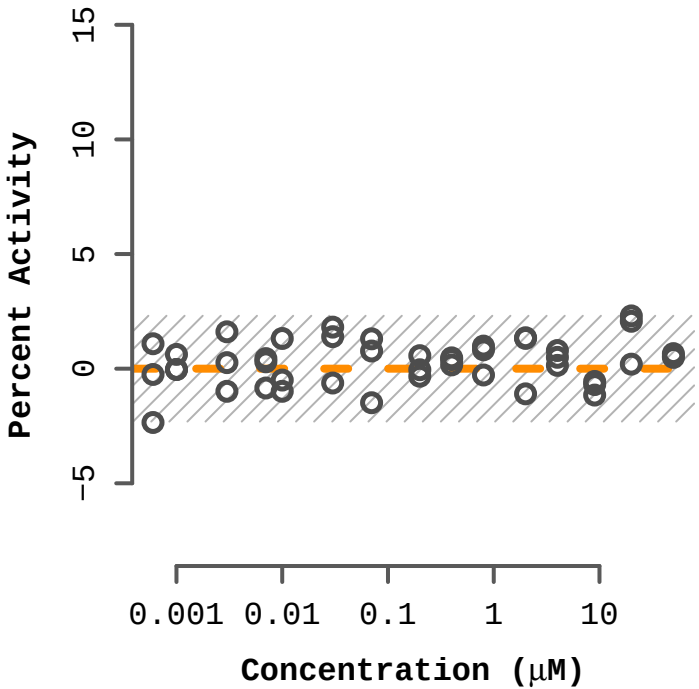
NAME: Lonidamine
CHID: 20782 CASRN: 50264-69-2
SPID(S): Tox21_202306
M4ID: 12479946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.558 MAX_MED: 0.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

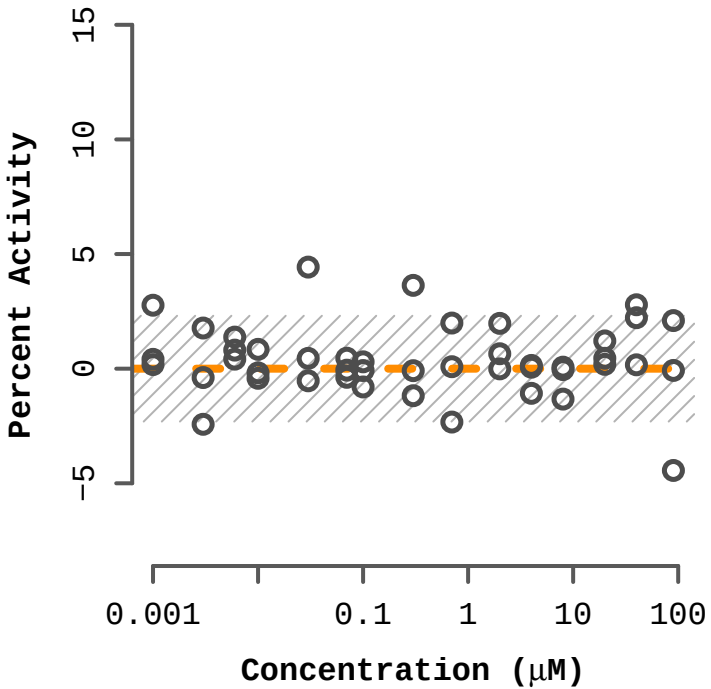
NAME: Lonidamine
CHID: 20782 **CASRN:** 50264-69-2
SPID(S): Tox21_110181_1
M4ID: 12484577

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

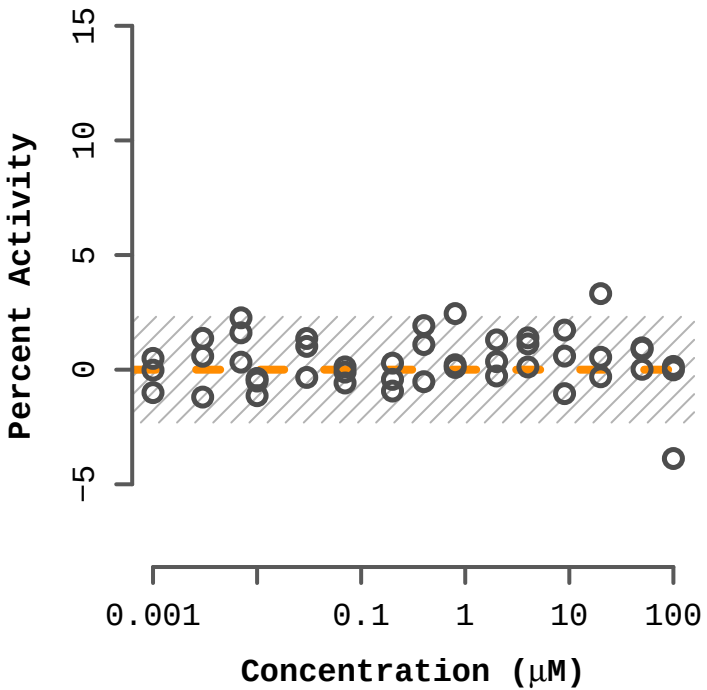
NAME: Lovastatin
CHID: 20784 CASRN: 75330-75-5
SPID(S): Tox21_300268
M4ID: 12478862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

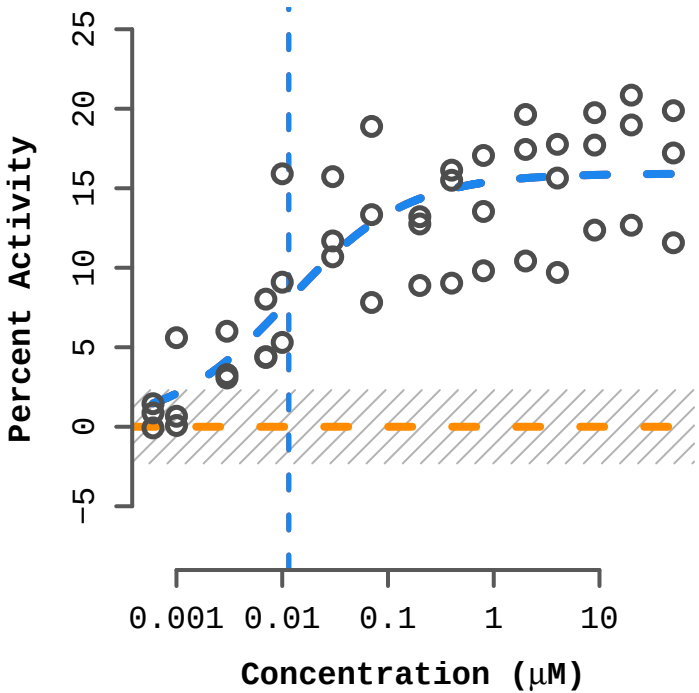
NAME: Lovastatin
CHID: 20784 CASRN: 75330-75-5
SPID(S): Tox21_201475
M4ID: 12480777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.4 MAX_MED: 1.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lovastatin
CHID: 20784 CASRN: 75330-75-5
SPID(S): Tox21_110888_1
M4ID: 12484039

HILL MODEL (in red):

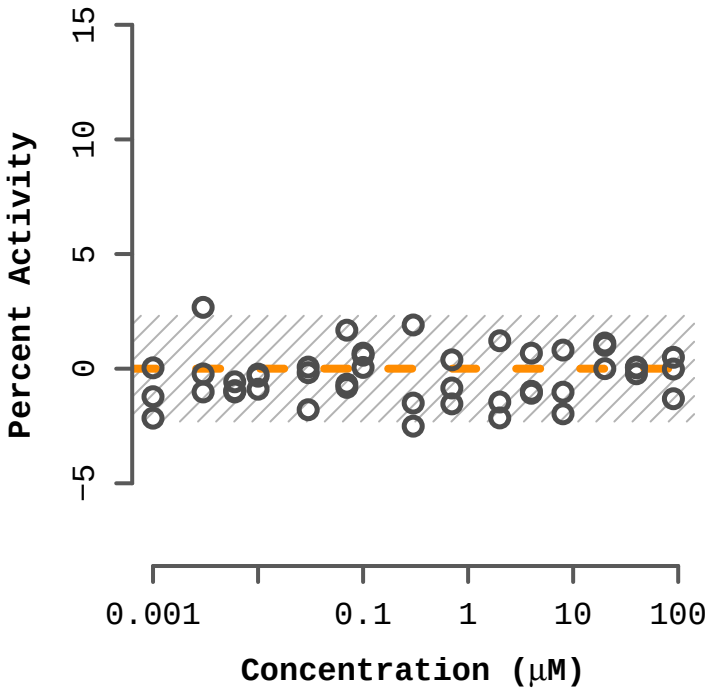
	tp	ga	gw
val:	15.9	−1.94	0.774
sd:	1.24	0.217	0.288

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.9	−1.94	0.774	2.12	16.4
sd:	1.24	0.217	0.288	113	4390

	CNST	HILL	GNLS
AIC:	366.37	248.21	252.21
PROB:	0	0.88	0.12
RMSE:	12.75	3.36	3.36

MAX_MEAN: 17.5 **MAX_MED:** 19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

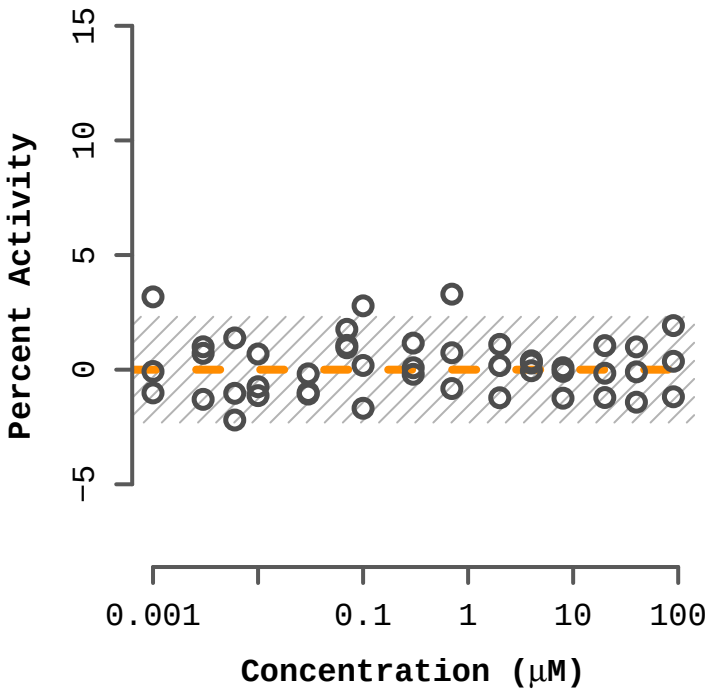
NAME: Magnesium chloride hexahydrate
CHID: 20789 **CASRN:** 7791-18-6
SPID(S): Tox21_200246
M4ID: 12482006

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.714 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

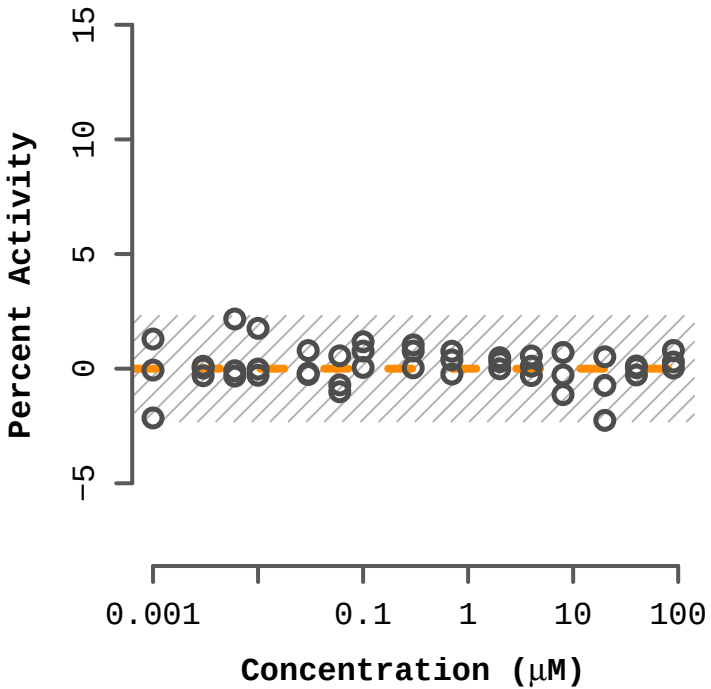
NAME: Malaoxon
CHID: 20790 CASRN: 1634-78-2
SPID(S): Tox21_301103
M4ID: 12478030

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.26 MAX_MED: 1.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

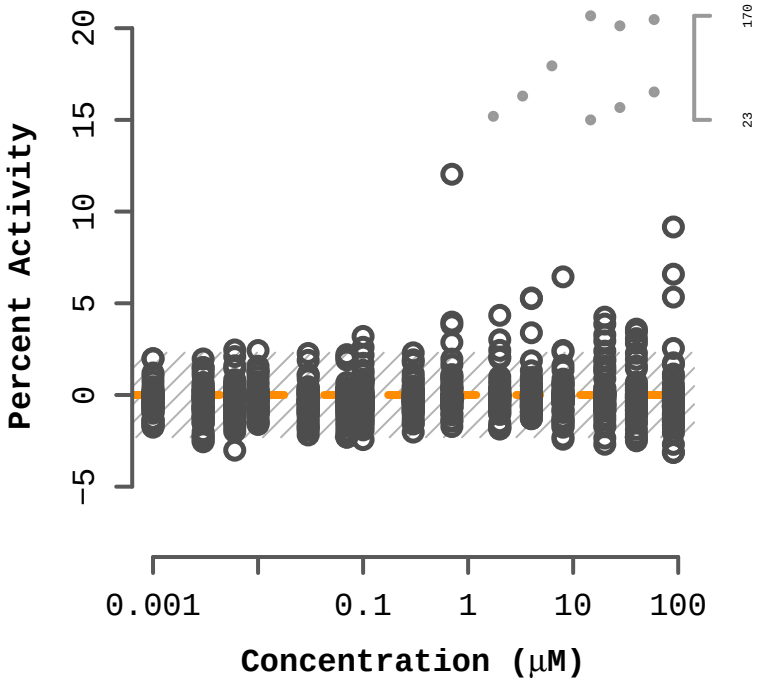
NAME: Malaoxon
CHID: 20790 CASRN: 1634-78-2
SPID(S): Tox21_202017
M4ID: 12480235

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.667 MAX_MED: 0.772 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

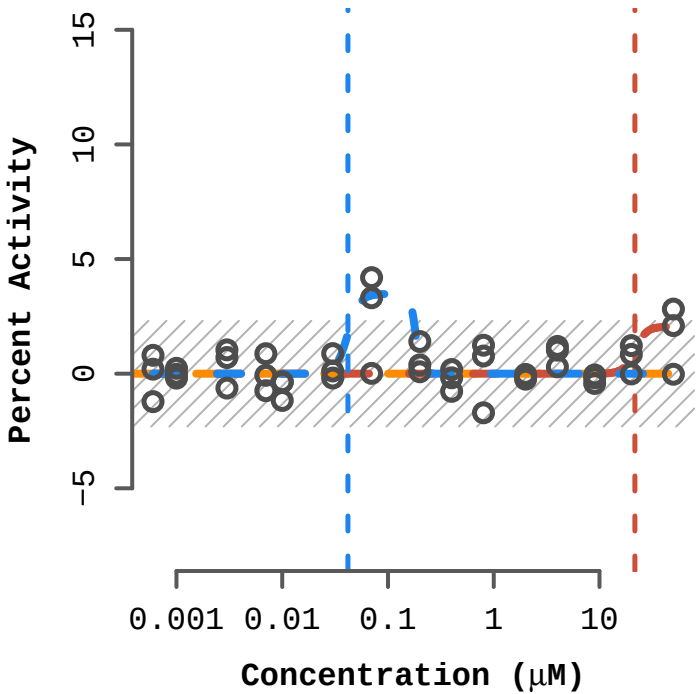
NAME: Malathion
CHID: 20791 **CASRN:** 121-75-5
SPID(S): Tox21_400048
M4ID: 12475089 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2521.48	NA	NA
PROB:	1	NA	NA
RMSE:	12.19	NA	NA

MAX_MEAN: 4.8 **MAX_MED:** 0.00443 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Malathion
CHID: 20791 CASRN: 121-75-5
SPID(S): Tox21_111175_1
M4ID: 12483862

HILL MODEL (in red):

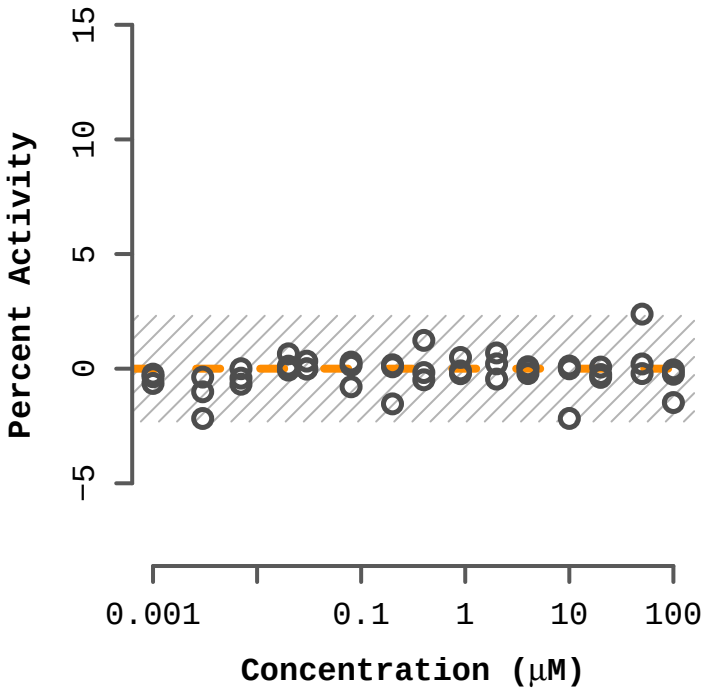
	tp	ga	gw
val:	2.05	1.33	8
sd:	0.555	0.114	22.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.48	−1.38	7.76	−0.739	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	133.84	130.78	132.23
PROB:	0.13	0.59	0.29
RMSE:	1.17	1.08	0.99

MAX_MEAN: 2.51 MAX_MED: 3.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

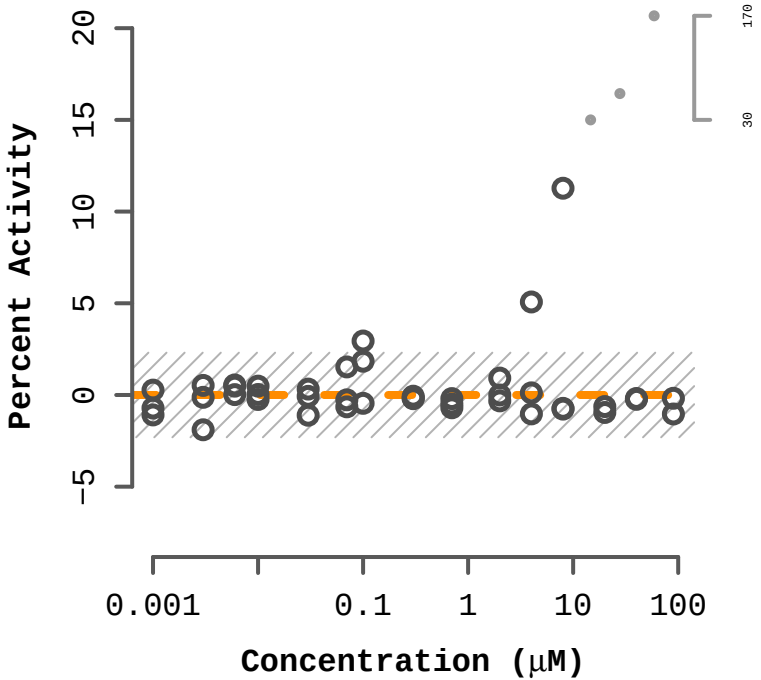
NAME: Maleic hydrazide
CHID: 20792 **CASRN:** 123-33-1
SPID(S): Tox21_300662
M4ID: 12478471

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 0.212 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

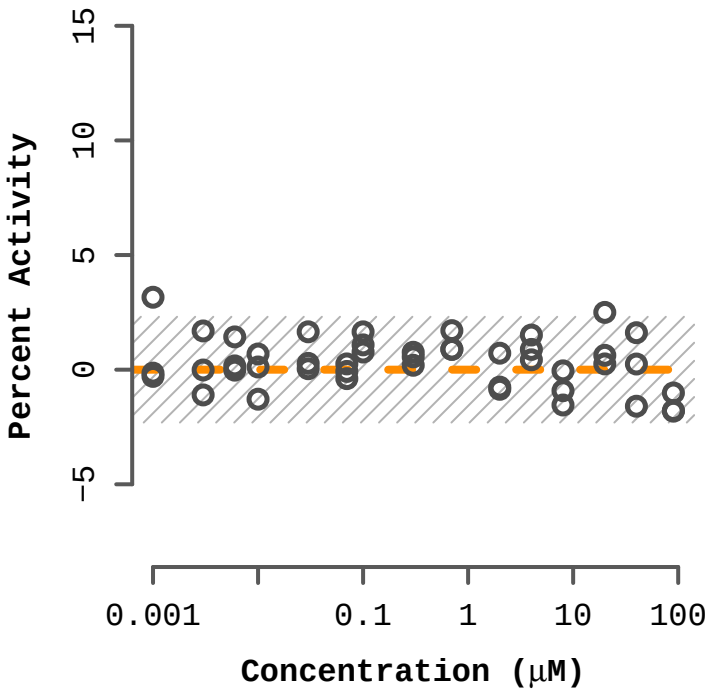
NAME: Maleic hydrazide
CHID: 20792 **CASRN:** 123-33-1
SPID(S): Tox21_201829
M4ID: 12480423 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.68	NA	NA
PROB:	1	NA	NA
RMSE:	27.73	NA	NA

MAX_MEAN: 56.6 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

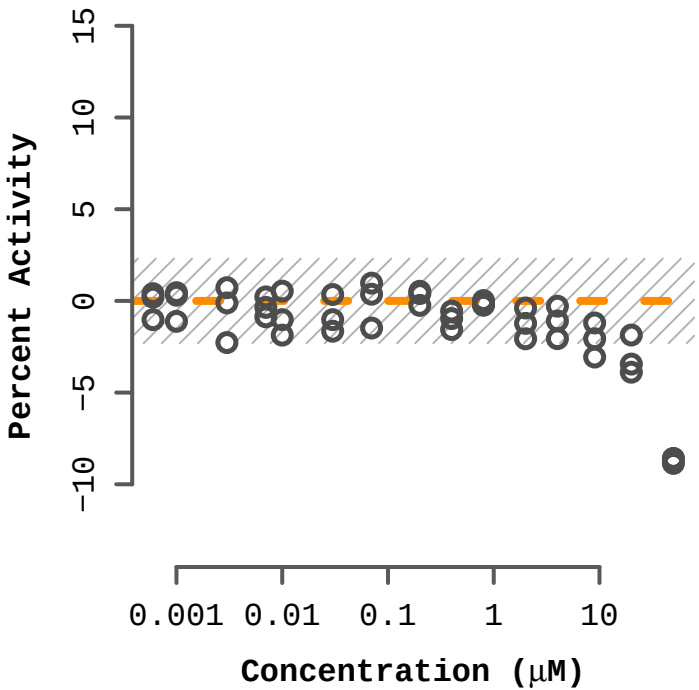
NAME: Maneb
CHID: 20794 CASRN: 12427-38-2
SPID(S): Tox21_300826
M4ID: 12478307

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

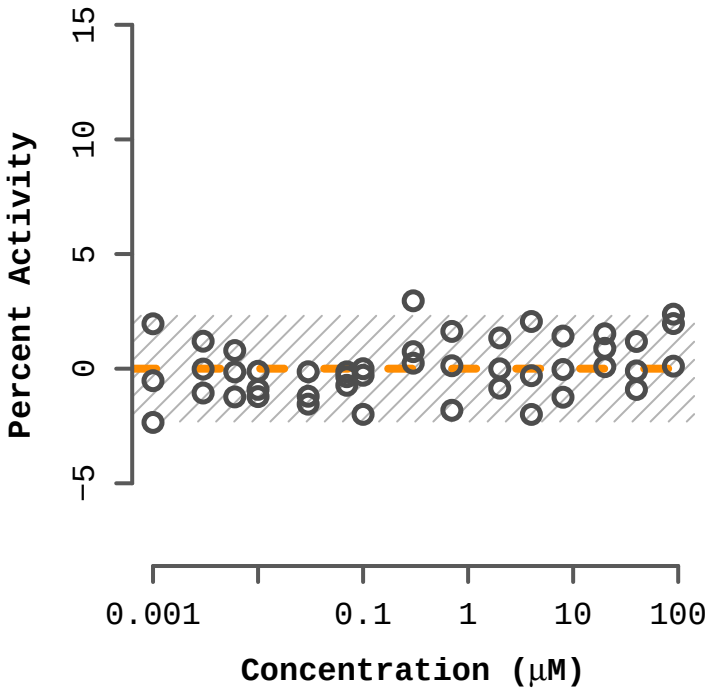
NAME: Manidipine dihydrochloride
CHID: 20796 **CASRN:** 89226-75-5
SPID(S): Tox21_112494_1
M4ID: 12483069

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 0.23 **MAX_MED:** 0.404 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

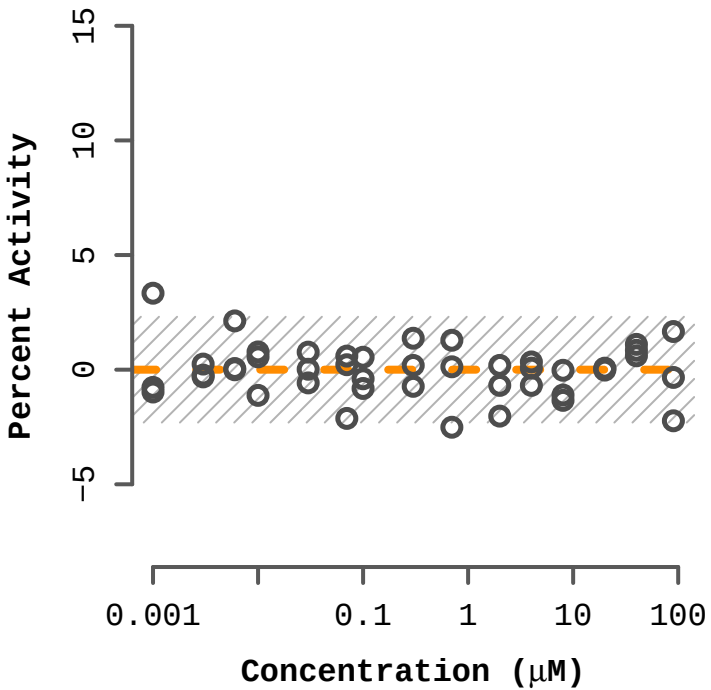
NAME: Melamine
CHID: 20802 CASRN: 108-78-1
SPID(S): Tox21_200503
M4ID: 12481749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.49 MAX_MED: 1.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

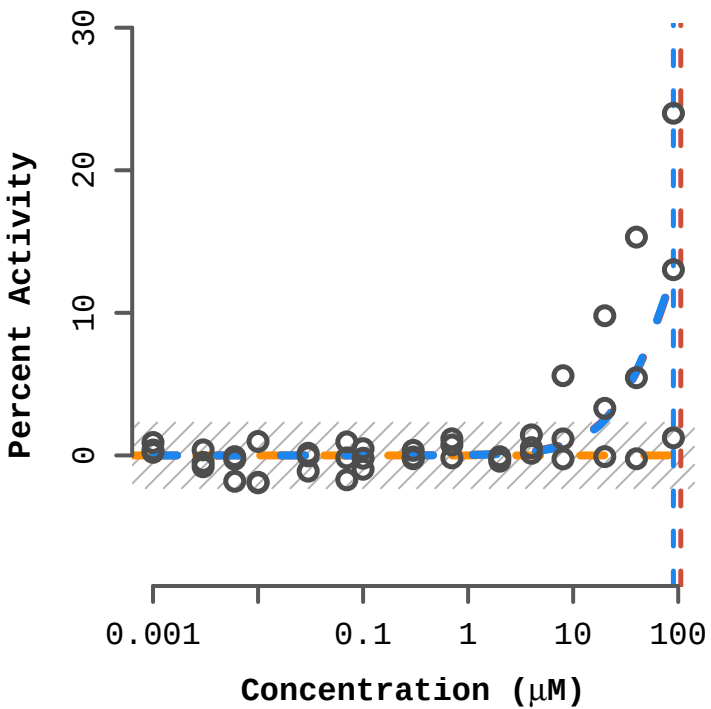
NAME: Meloxicam
CHID: 20803 CASRN: 71125-38-7
SPID(S): Tox21_302756
M4ID: 12476377

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.853 **MAX_MED:** 0.848 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Meloxicam
CHID: 20803 CASRN: 71125-38-7
SPID(S): Tox21_201689
M4ID: 12480563

HILL MODEL (in red):

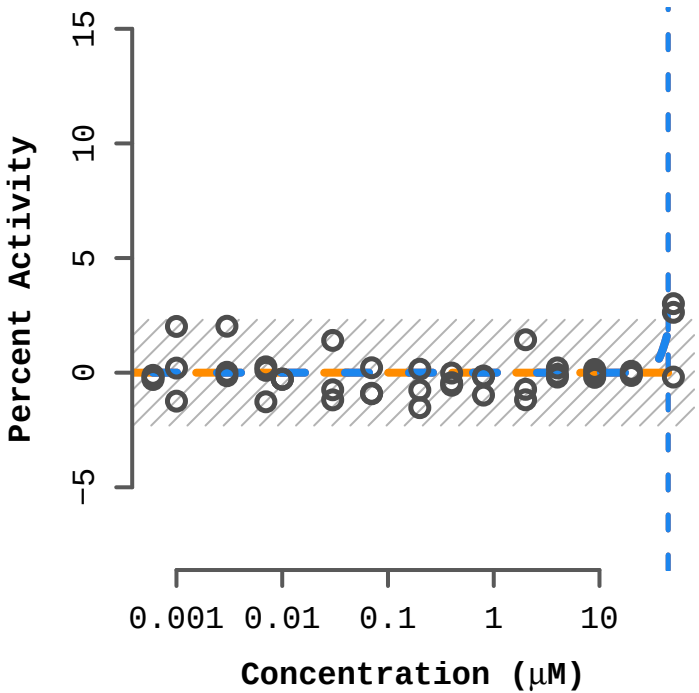
	tp	ga	gw
val:	28.8	2.02	1.4
sd:	18.7	0.37	0.423

GAIN-LOSS MODEL (in blue):

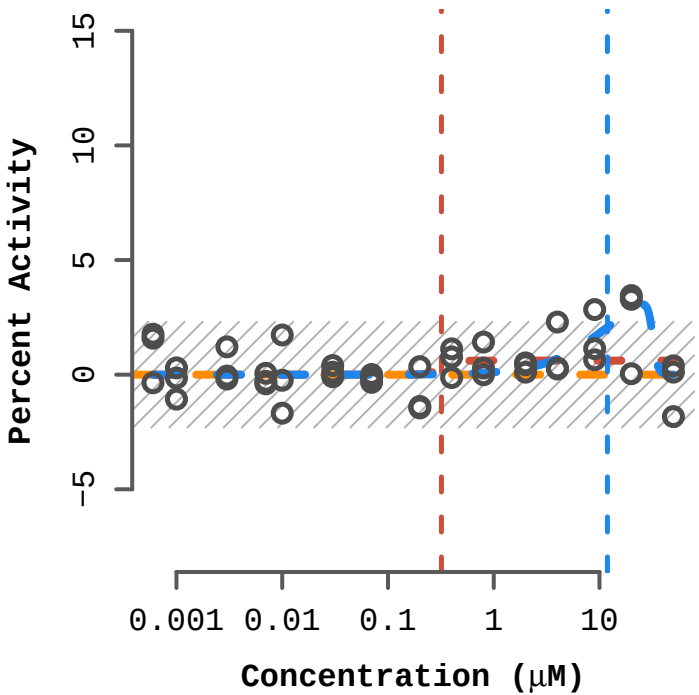
	tp	ga	gw	la	lw
val:	25.6	1.95	1.48	3.72	4.09
sd:	17.2	0.381	0.503	856	2010

	CNST	HILL	GNLS
AIC:	223.6	211.02	215.2
PROB:	0	0.89	0.11
RMSE:	5.11	3.32	3.32

MAX_MEAN: 12.8 MAX_MED: 13 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Meloxicam
CHID:    20803   CASRN: 71125-38-7
SPID(S): Tox21_111734_1
M4ID:    12483514

HILL MODEL (in red):
      tp       ga       gw
val:  3.61     1.65     8
sd:   9.65     0.379    28.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.62     1.65     8        3.62     1.58
sd:   9.96     0.39     28.5     195      162

      CNST        HILL        GNLS
AIC:  120.31      117.65      121.65
PROB: 0.19        0.71        0.1
RMSE: 0.97        0.87        0.87

MAX_MEAN: 1.82      MAX_MED: 2.63      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Melphalan
CHID: 20804 **CASRN:** 148-82-3
SPID(S): Tox21_202522
M4ID: 12479730

HILL MODEL (in red):

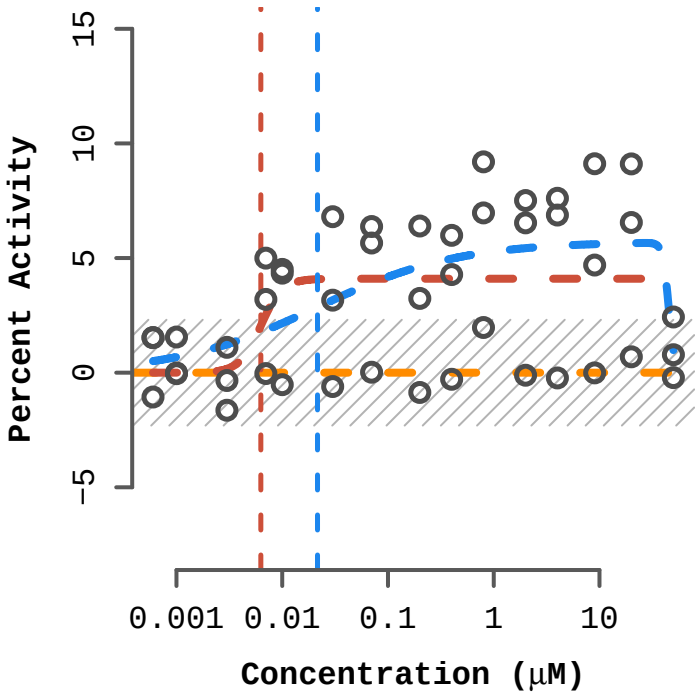
	tp	ga	gw
val:	0.613	−0.495	8
sd:	0.212	0.194	10.3

GAIN-LOSS MODEL (in blue):

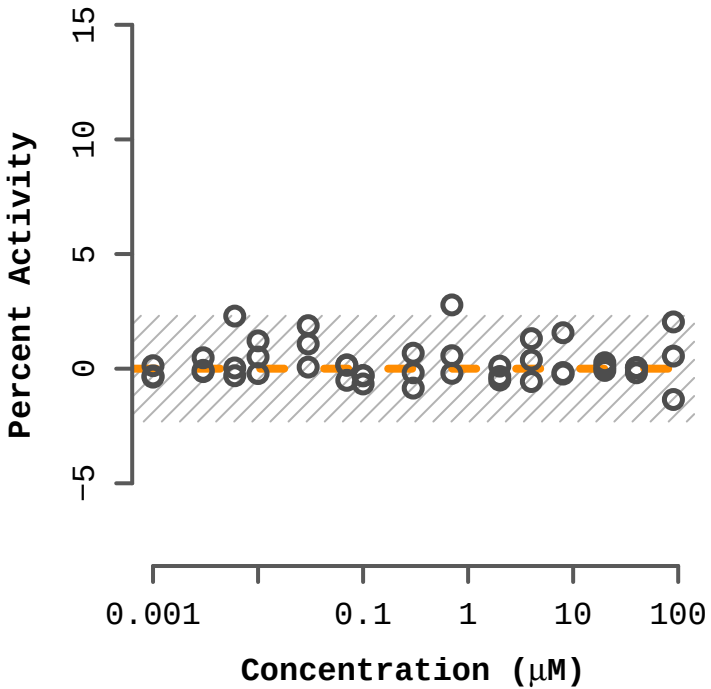
	tp	ga	gw	la	lw
val:	4.14	1.08	1.47	1.5	18
sd:	2.19	0.349	0.816	0.701	63.2

	CNST	HILL	GNLS
AIC:	141.26	138.23	133.59
PROB:	0.02	0.09	0.89
RMSE:	1.2	1.07	0.95

MAX_MEAN: 2.26 **MAX_MED:** 3.29 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Melphalan
CHID:    20804   CASRN: 148-82-3
SPID(S): Tox21_111010_1
M4ID:    12483951

HILL MODEL (in red):
      tp       ga       gw
val:  4.1      -2.2     4.29
sd:   0.694    0.167    6.59

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.71     -1.67    0.652    1.65     15.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  267.43      238.22      236.63
PROB: 0           0.31        0.69
RMSE: 4.48        2.92        2.81

MAX_MEAN: 6.05      MAX_MED: 6.97      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

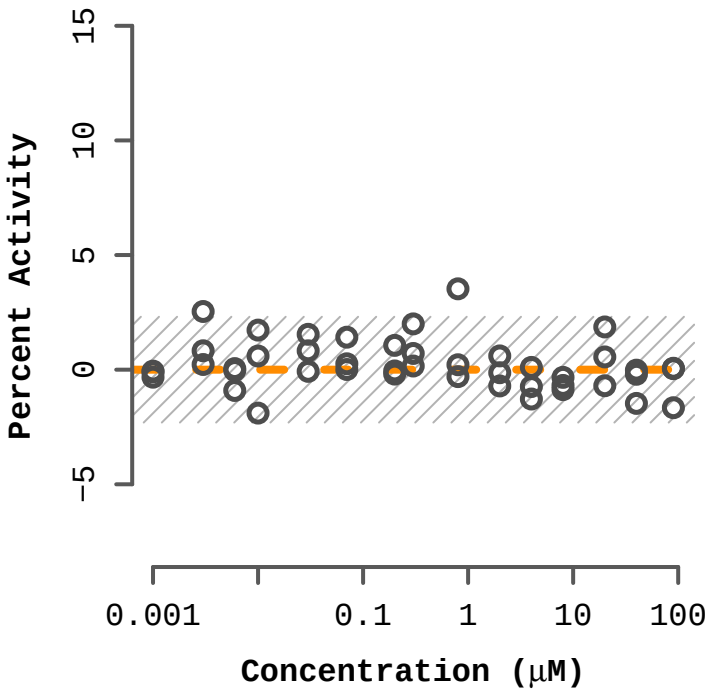
NAME: dl-Menthol
CHID: 20805 CASRN: 89-78-1
SPID(S): Tox21_302999
M4ID: 12476134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.05 MAX_MED: 1.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

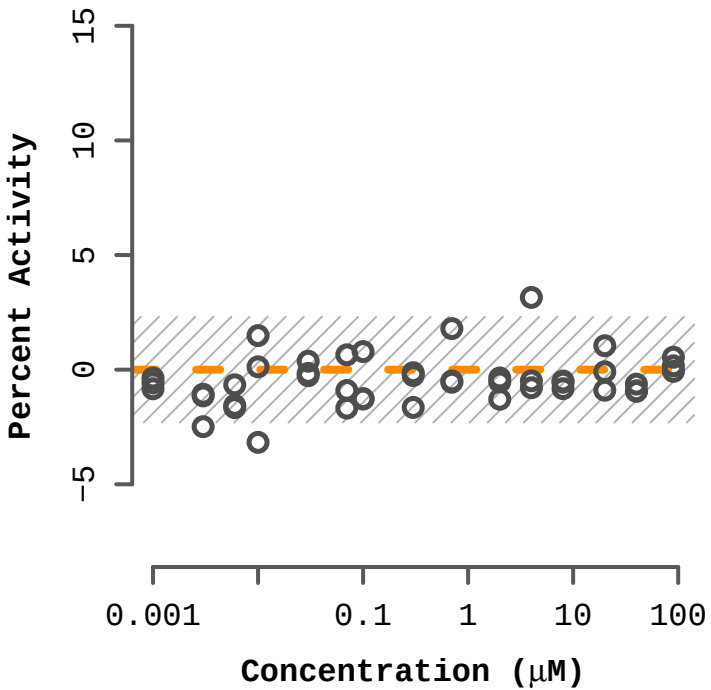
NAME: dl−Menthol
CHID: 20805 **CASRN:** 89−78−1
SPID(S): Tox21_202608
M4ID: 12479644

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.826 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

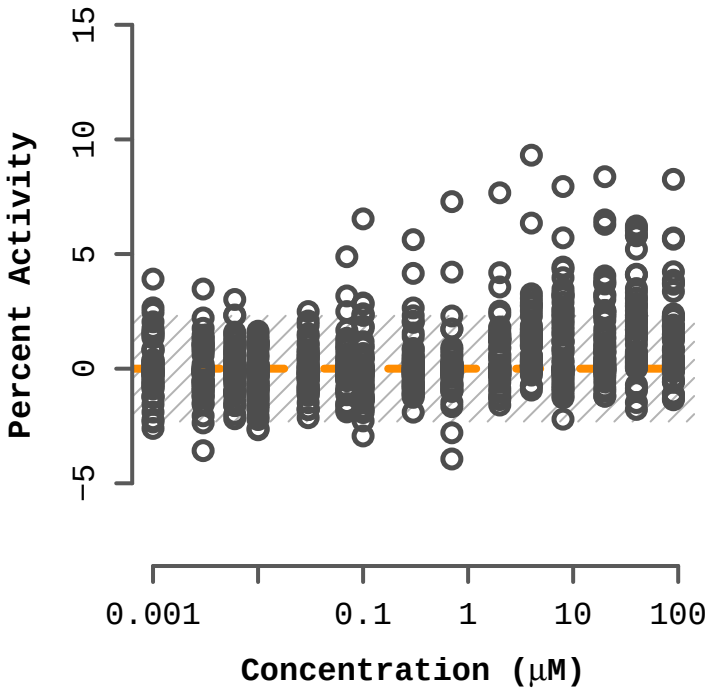
NAME: dl−Menthol
CHID: 20805 **CASRN:** 89−78−1
SPID(S): Tox21_201823
M4ID: 12480429

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.627 **MAX_MED:** 0.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

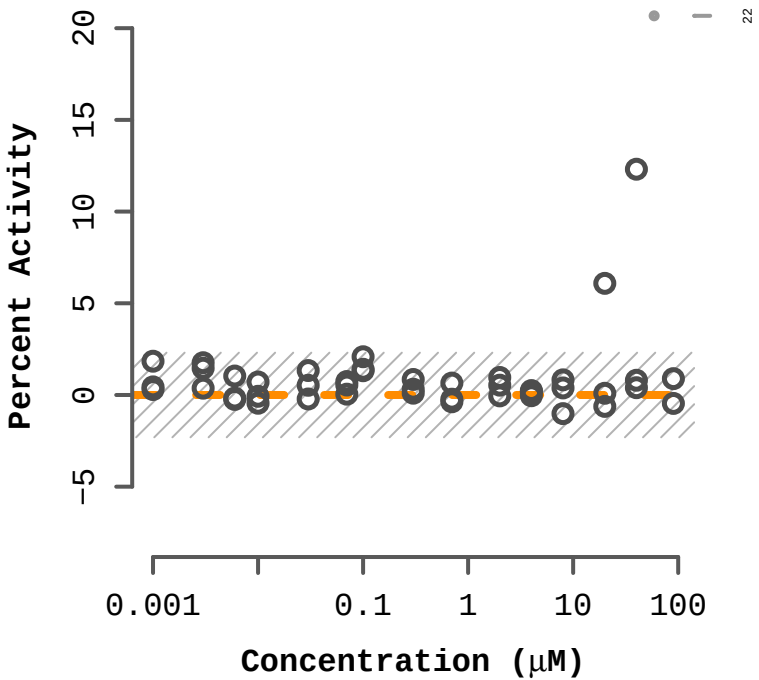
NAME: 2-Mercaptobenzothiazole
CHID: 20807 CASRN: 149-30-4
SPID(S): Tox21_400016
M4ID: 12475121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2827.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 1.83 MAX_MED: 1.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

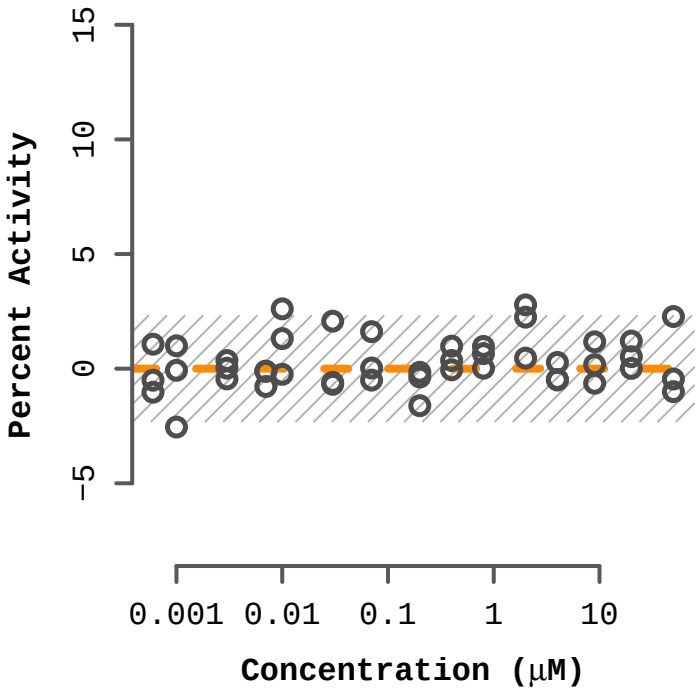
NAME: Sodium 2-mercaptoethanesulfonate
CHID: 20809 CASRN: 19767-45-4
SPID(S): Tox21_200863
M4ID: 12481389 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.92	NA	NA
PROB:	1	NA	NA
RMSE:	4.01	NA	NA

MAX_MEAN: 7.64 MAX_MED: 1.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

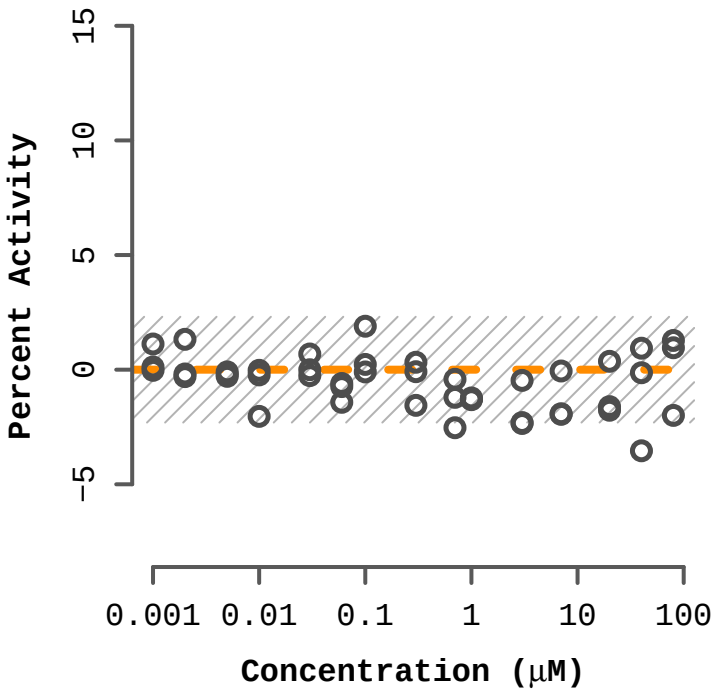
NAME: Sodium 2-mercaptoethanesulfonate
CHID: 20809 CASRN: 19767-45-4
SPID(S): Tox21_112767_1
M4ID: 12482964

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

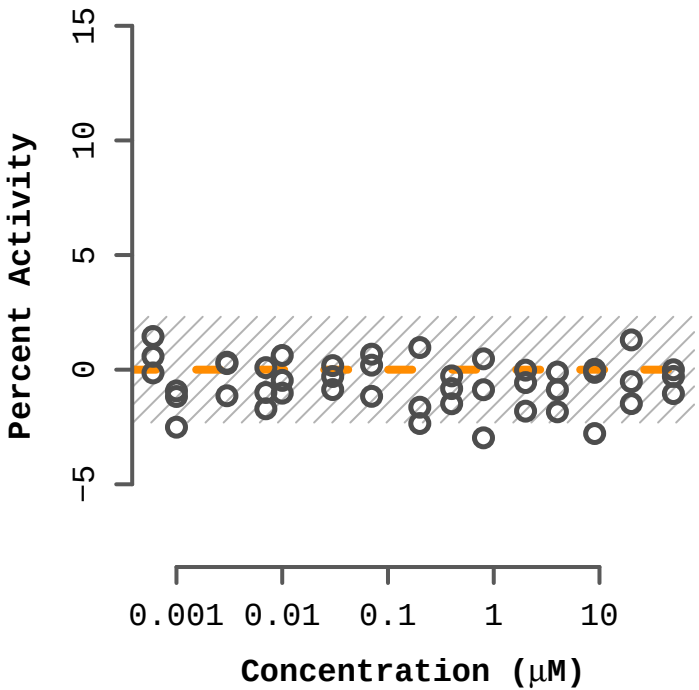
NAME: 6-Mercaptopurine
CHID: 20810 **CASRN:** 50-44-2
SPID(S): Tox21_202591
M4ID: 12479661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.676 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

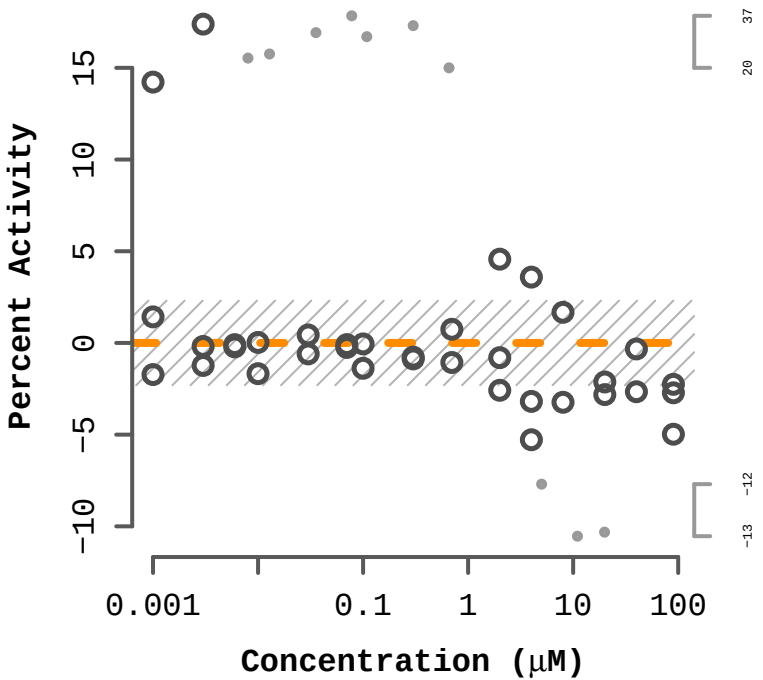
NAME: 6-Mercaptopurine
CHID: 20810 **CASRN:** 50-44-2
SPID(S): Tox21_111158_1
M4ID: 12483870

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.631 **MAX_MED:** 0.583 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

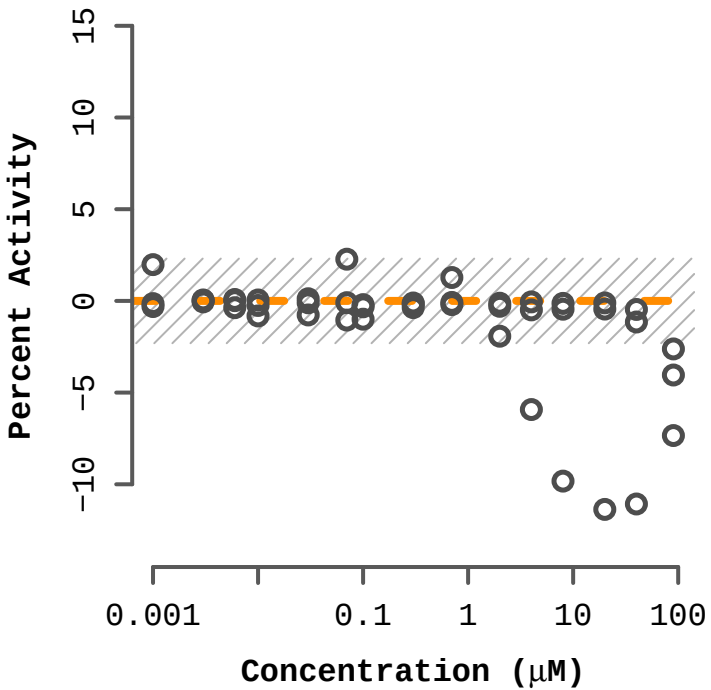
NAME: Mercuric chloride
CHID: 20811 **CASRN:** 7487-94-7
SPID(S): Tox21_300491
M4ID: 12478641 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	343.34	NA	NA
PROB:	1	NA	NA
RMSE:	12.51	NA	NA

MAX_MEAN: 12.1 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

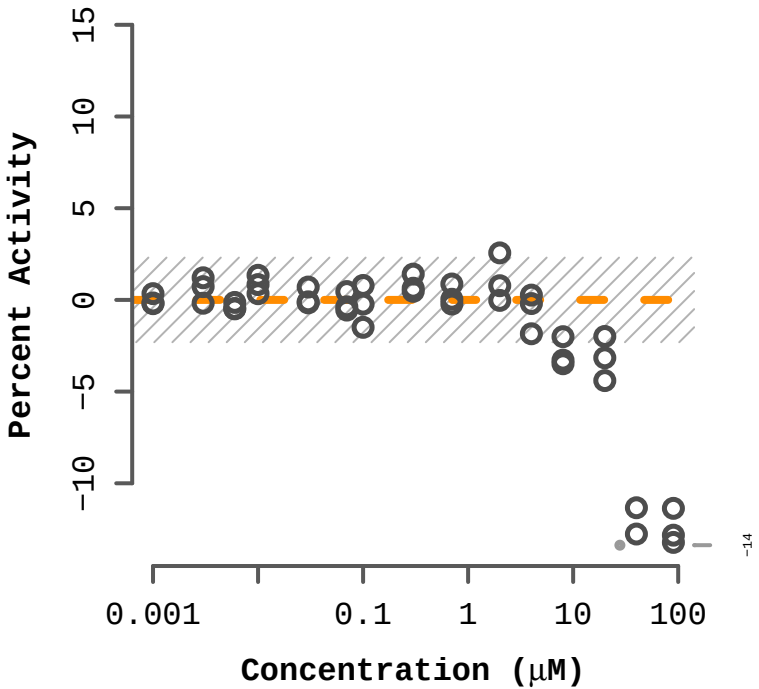
NAME: Mercuric chloride
CHID: 20811 **CASRN:** 7487-94-7
SPID(S): Tox21_202259
M4ID: 12479993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.81	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 0.509 **MAX_MED:** 0.0307 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

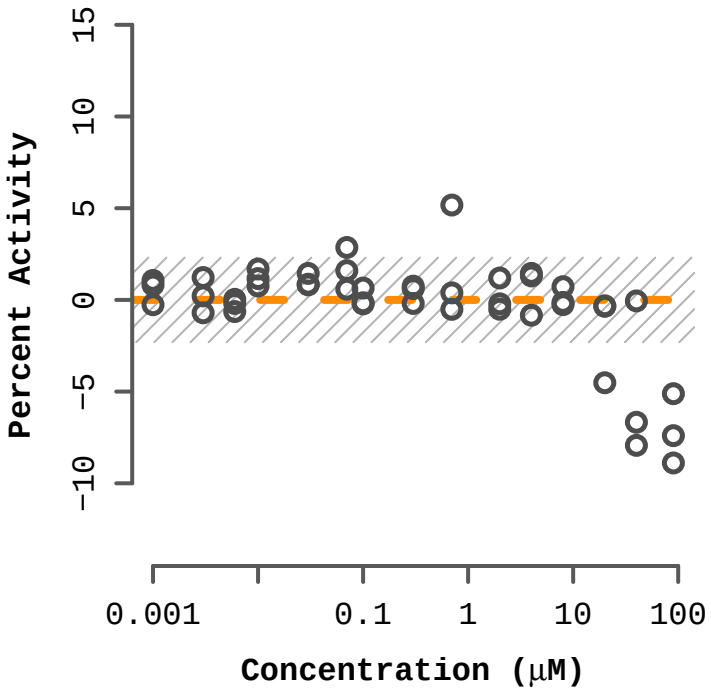
NAME: Methylmercuric(II) chloride
CHID: 20813 **CASRN:** 115-09-3
SPID(S): Tox21_202524
M4ID: 12479728 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	244.84	NA	NA
PROB:	1	NA	NA
RMSE:	4.8	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.838 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

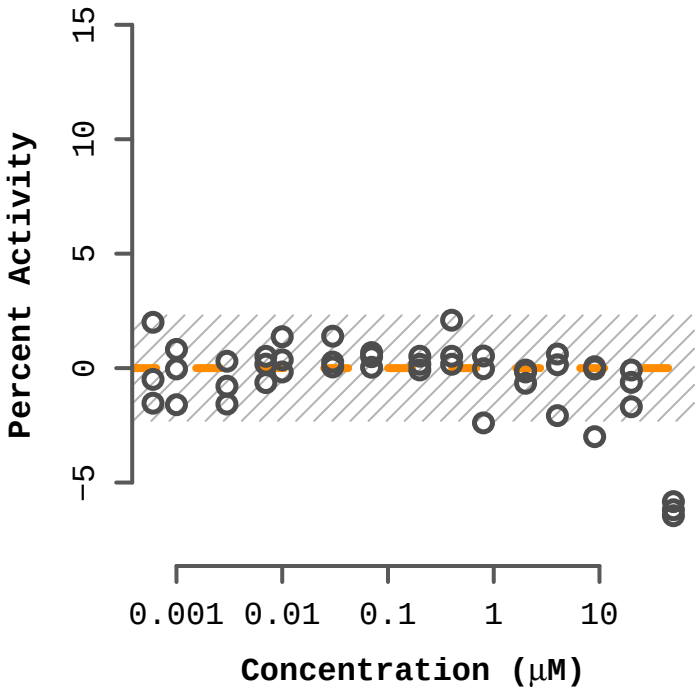
NAME: Mestranol
CHID: 20814 **CASRN:** 72-33-3
SPID(S): Tox21_301837
M4ID: 12477296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.48	NA	NA
PROB:	1	NA	NA
RMSE:	2.78	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

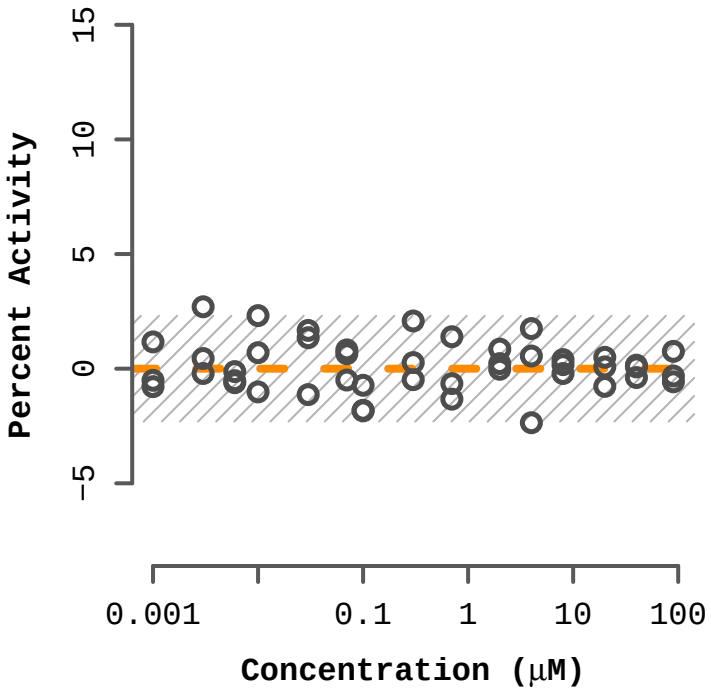
NAME: Mestranol
CHID: 20814 CASRN: 72-33-3
SPID(S): Tox21_111200_1
M4ID: 12483846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.928 **MAX_MED:** 0.519 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

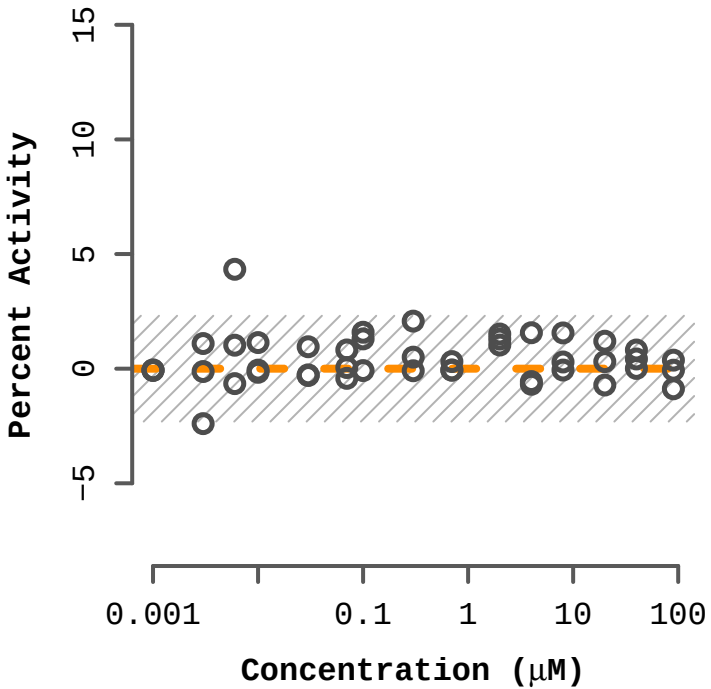
NAME: Metepa
CHID: 20815 CASRN: 57-39-6
SPID(S): Tox21_301807
M4ID: 12477326

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.979 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

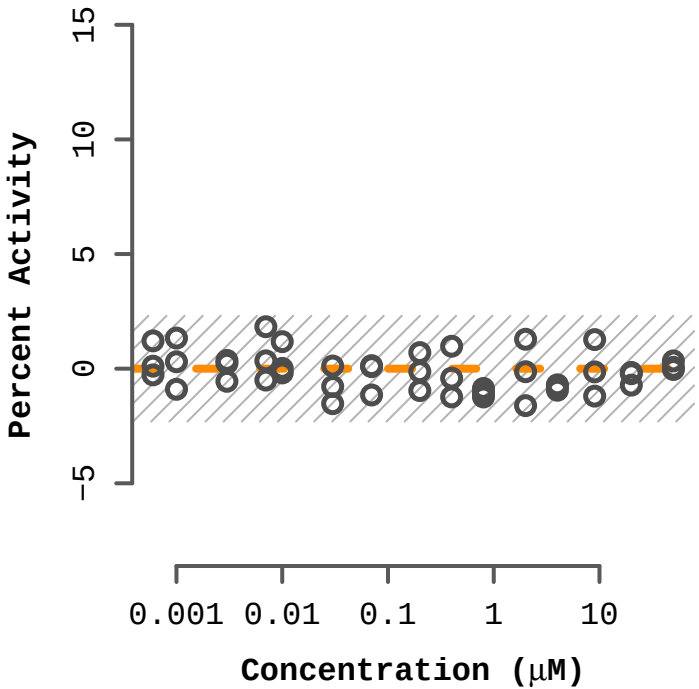
NAME: Methapyrilene hydrochloride
CHID: 20818 **CASRN:** 135-23-9
SPID(S): Tox21_201134
M4ID: 12481118

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

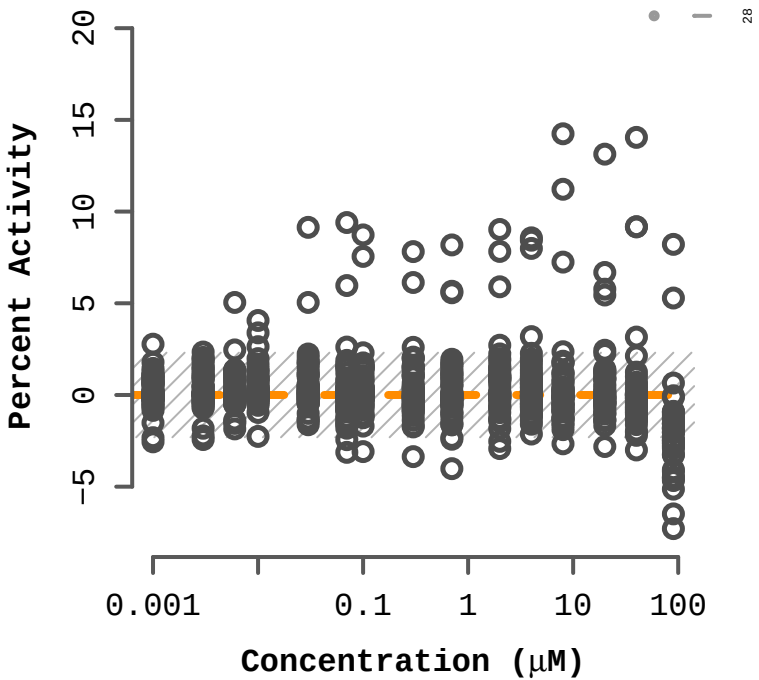
NAME: Methapyrilene hydrochloride
CHID: 20818 CASRN: 135-23-9
SPID(S): Tox21_111256_1
M4ID: 12483812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.56 **MAX_MED:** 0.343 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

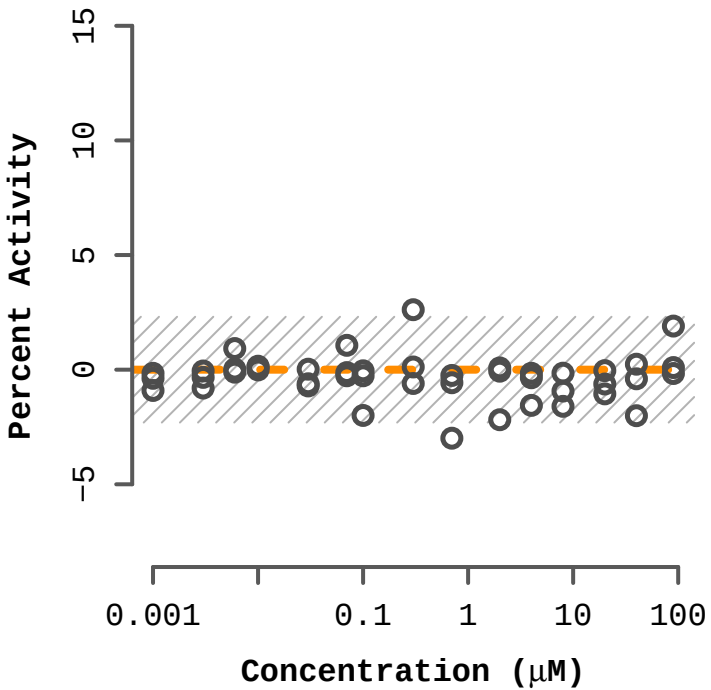
NAME: Methidathion
CHID: 20819 CASRN: 950-37-8
SPID(S): Tox21_400049
M4ID: 12475088 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2693.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.36	NA	NA

MAX_MEAN: 0.688 MAX_MED: 0.172 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

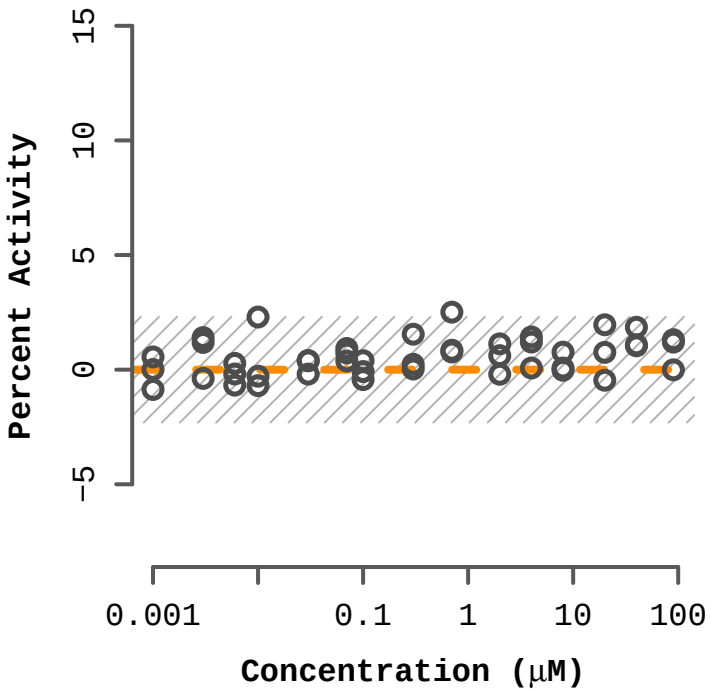
NAME: Methimazole
CHID: 20820 CASRN: 60-56-0
SPID(S): Tox21_300532
M4ID: 12478600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.712 MAX_MED: 0.119 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

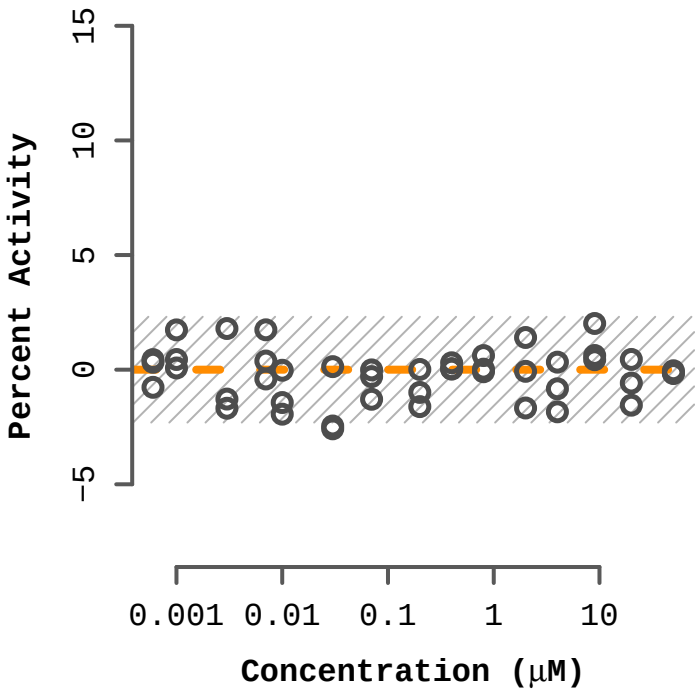
NAME: Methimazole
CHID: 20820 CASRN: 60-56-0
SPID(S): Tox21_201341
M4ID: 12480911

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

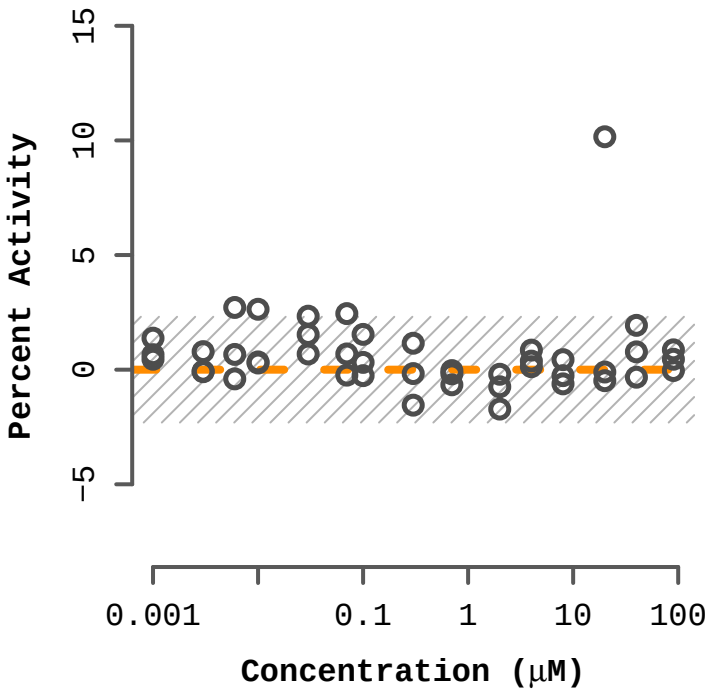
NAME: Methimazole
CHID: 20820 **CASRN:** 60-56-0
SPID(S): Tox21_110341_1
M4ID: 12484441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

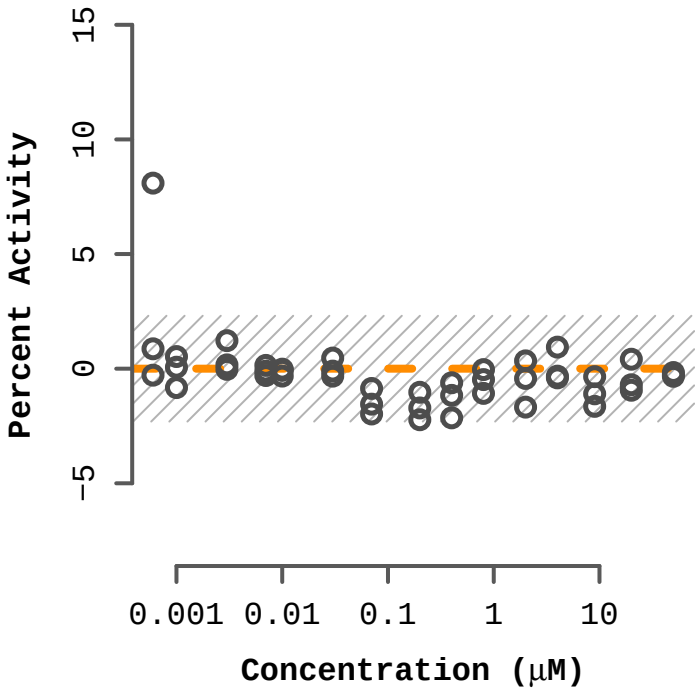
NAME: Methotrexate
CHID: 20822 **CASRN:** 59-05-2
SPID(S): Tox21_300269
M4ID: 12478861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 3.19 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

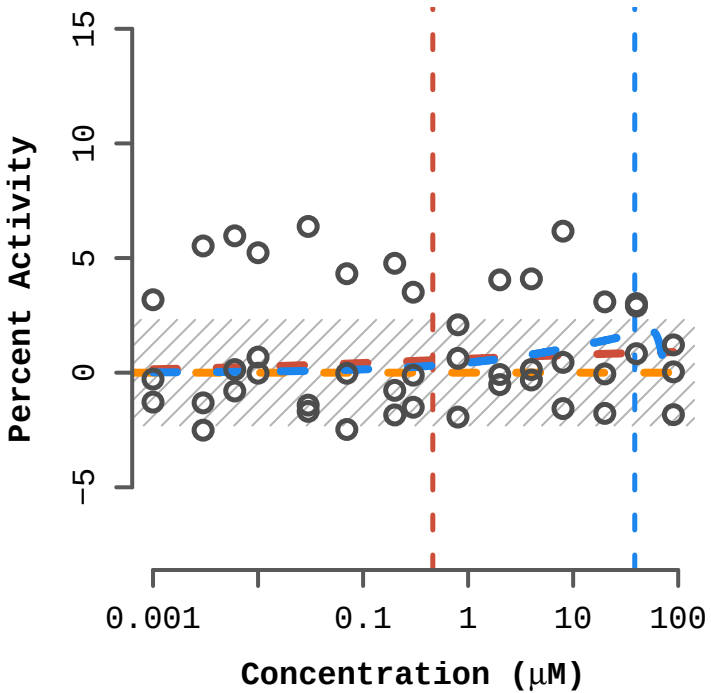
NAME: Methotrexate
CHID: 20822 **CASRN:** 59-05-2
SPID(S): Tox21_110944_1
M4ID: 12483994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.89 **MAX_MED:** 0.868 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methoxy-3-aminodibenzofuran
CHID: 20825 CASRN: 5834-17-3
SPID(S): Tox21_200262
M4ID: 12481990

HILL MODEL (in red):

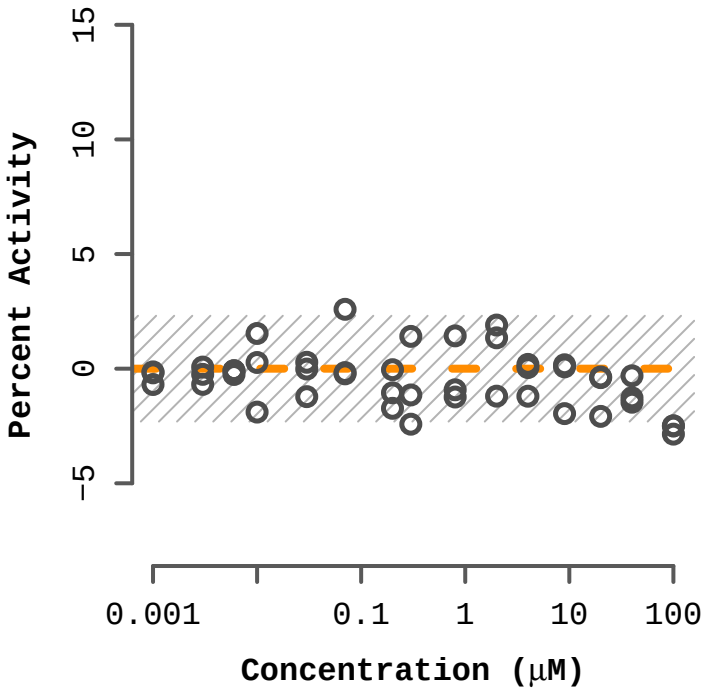
	tp	ga	gw
val:	1.08	-0.336	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.38	1.59	0.522	1.84	18
sd:	11.5	4.92	0.827	0.755	113

	CNST	HILL	GNLS
AIC:	221.92	225.56	228.3
PROB:	0.83	0.13	0.03
RMSE:	2.77	2.64	2.64

MAX_MEAN: 2.25 MAX_MED: 2.91 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

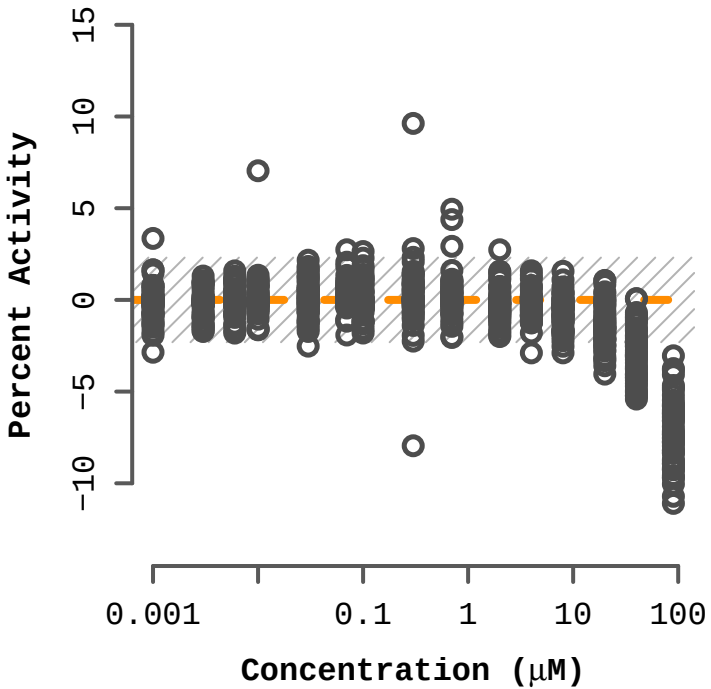
NAME: 3-Methoxycatechol
CHID: 20826 **CASRN:** 934-00-9
SPID(S): Tox21_200504
M4ID: 12481748

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.732 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

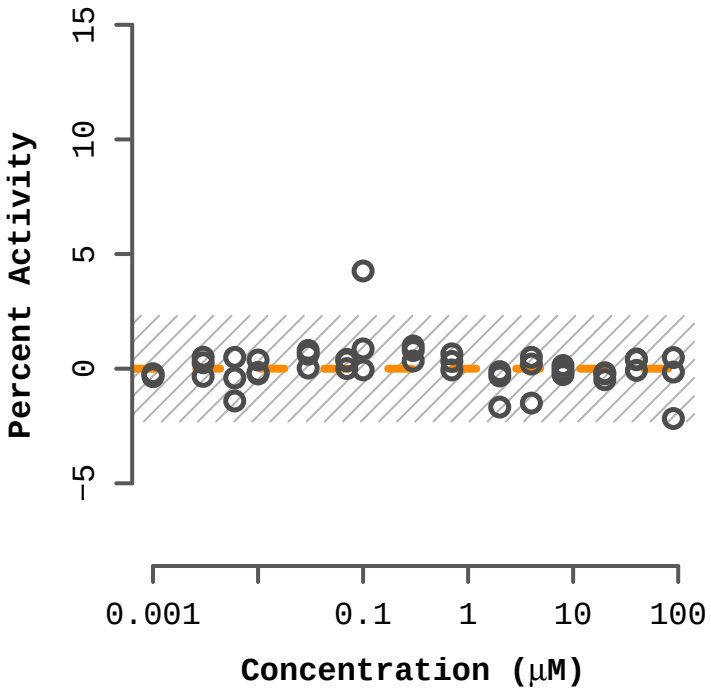
NAME: Methoxychlor
CHID: 20827 **CASRN:** 72-43-5
SPID(S): Tox21_400075
M4ID: 12475062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2904.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 0.273 **MAX_MED:** 0.0805 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

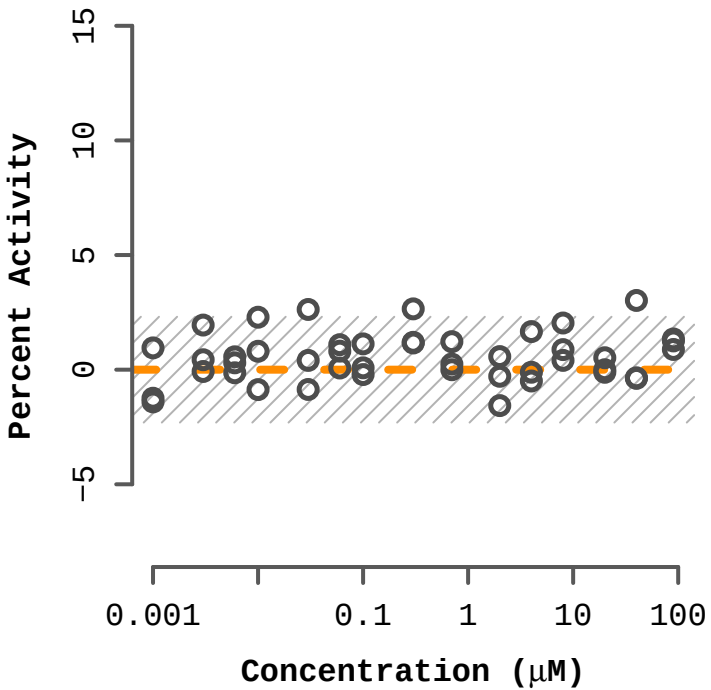
NAME: 4-Methoxyphenol
CHID: 20828 **CASRN:** 150-76-5
SPID(S): Tox21_302876
M4ID: 12476257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 0.862 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

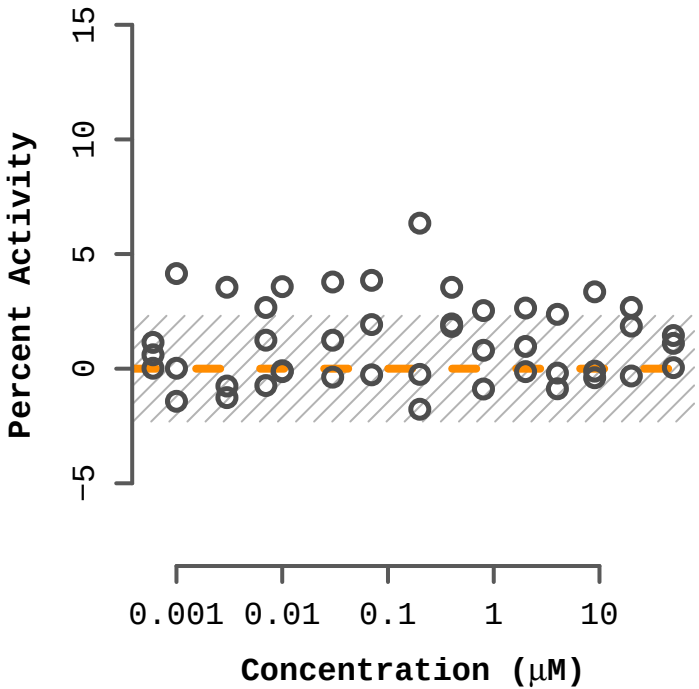
NAME: 4-Methoxyphenol
CHID: 20828 **CASRN:** 150-76-5
SPID(S): Tox21_202367
M4ID: 12479885

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

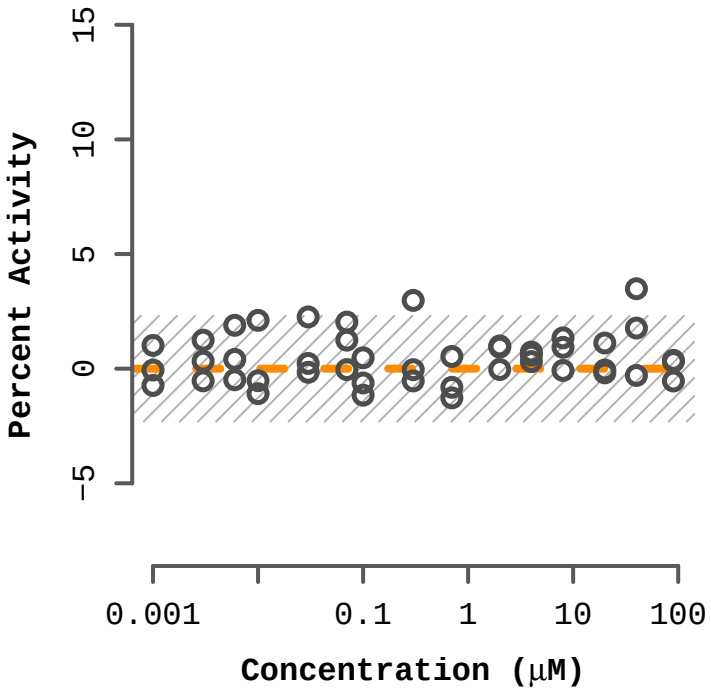
NAME: 4-Methoxyphenol
CHID: 20828 **CASRN:** 150-76-5
SPID(S): Tox21_111125_1
M4ID: 12483893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 2.45 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

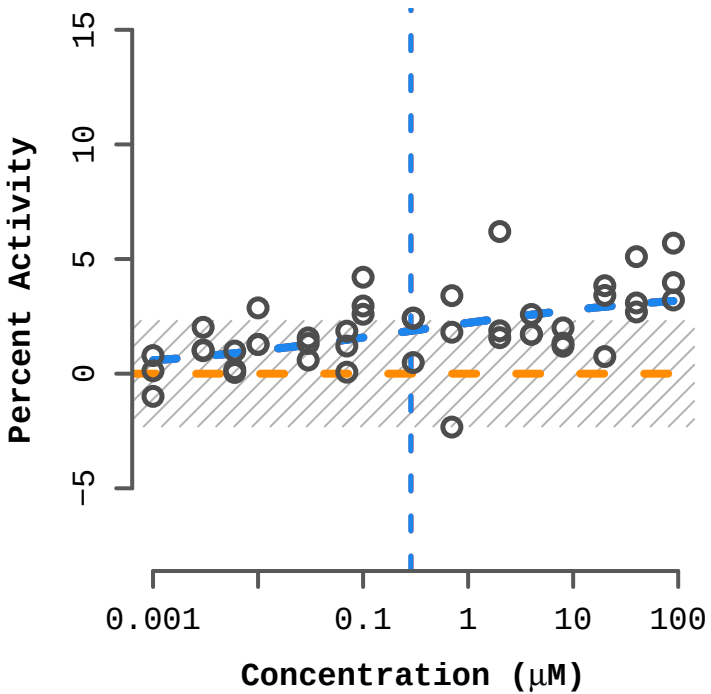
NAME: Methoxyphenylacetic acid
CHID: 20829 **CASRN:** 1701-77-5
SPID(S): Tox21_301985
M4ID: 12477148

HILL MODEL: Not applicable.

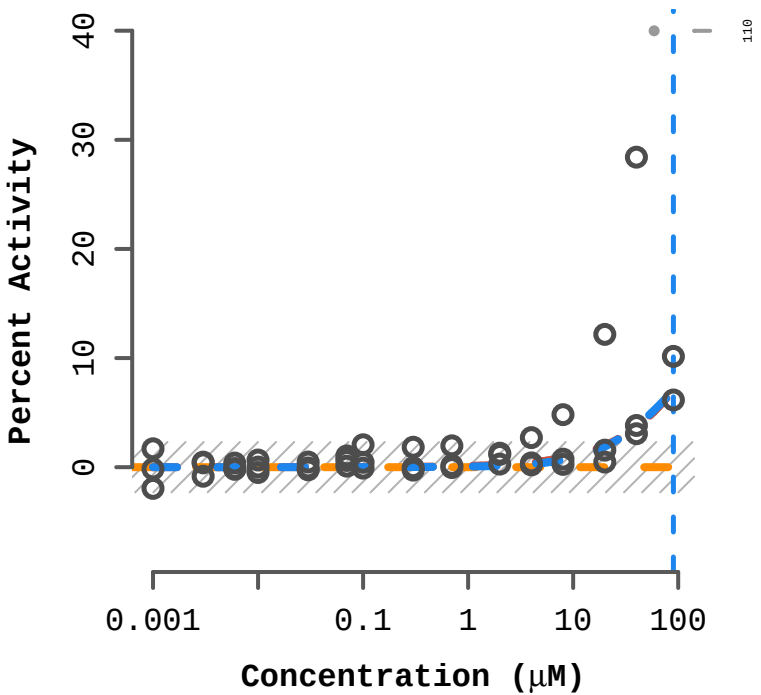
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.77 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    8-Methoxypsoralen
CHID:    20830   CASRN: 298-81-7
SPID(S): Tox21_302816
M4ID:    12476317

HILL MODEL (in red):
      tp       ga       gw
val:  3.74     -0.543   0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.74     -0.546   0.3      3.95     18
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  216.68      159.86      163.86
PROB: 0           0.88        0.12
RMSE: 2.53        1.37        1.37

MAX_MEAN: 4.29      MAX_MED: 3.97      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 8-Methoxypsoralen
CHID: 20830 CASRN: 298-81-7
SPID(S): Tox21_201767
M4ID: 12480485 BRK

HILL MODEL (in red):

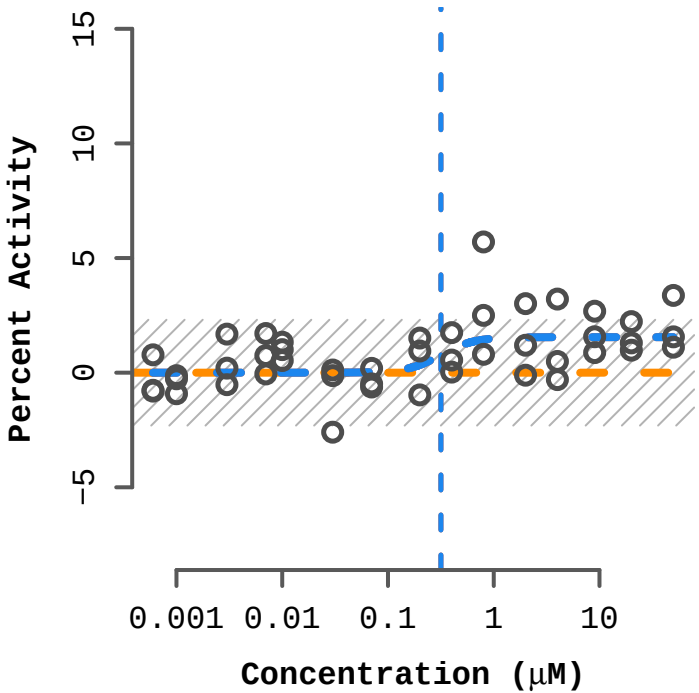
	tp	ga	gw
val:	29	2.45	0.982
sd:	46.4	1.07	0.416

GAIN-LOSS MODEL (in blue):

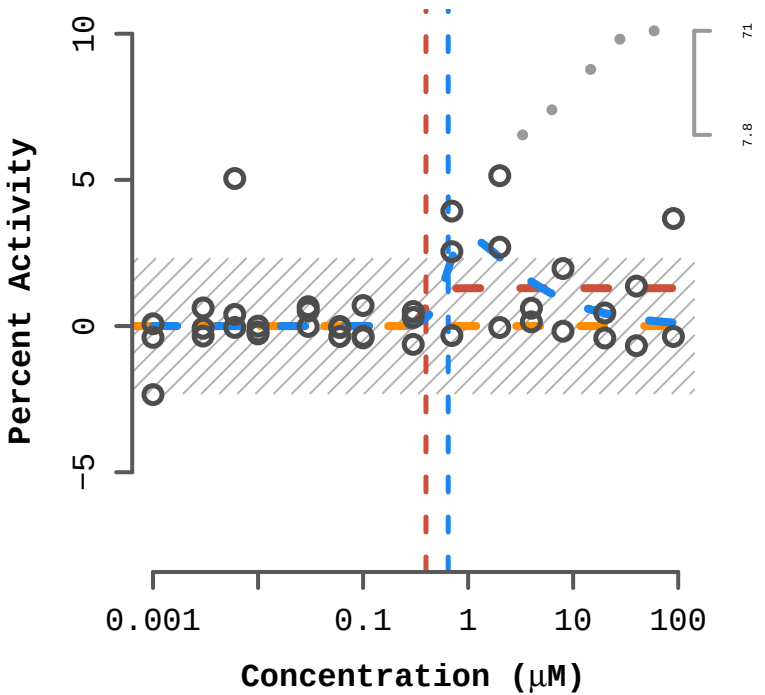
	tp	ga	gw	la	lw
val:	14	1.95	1.24	2.96	6.85
sd:	11.1	0.517	0.624	336	2290

	CNST	HILL	GNLS
AIC:	252.24	222.72	227.62
PROB:	0	0.92	0.08
RMSE:	17.45	16.17	16.17

MAX_MEAN: 42.7 MAX_MED: 10.2 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    8-Methoxypsoralen
CHID:    20830   CASRN: 298-81-7
SPID(S): Tox21_110432_1
M4ID:    12484362

HILL MODEL (in red):
      tp       ga       gw
val:  1.55     -0.499   2.78
sd:   0.289    0.279    2.52

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.55     -0.499   2.78     3.65     3.54
sd:   0.289    0.279    2.52     891      1620

      CNST        HILL        GNLS
AIC:  170.88      148.66      152.66
PROB: 0           0.88        0.12
RMSE: 1.64        1.19        1.19

MAX_MEAN: 3         MAX_MED: 2.5       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl tert-butyl ether
CHID: 20833 CASRN: 1634-04-4
SPID(S): Tox21_201184
M4ID: 12481068 BRK

HILL MODEL (in red):

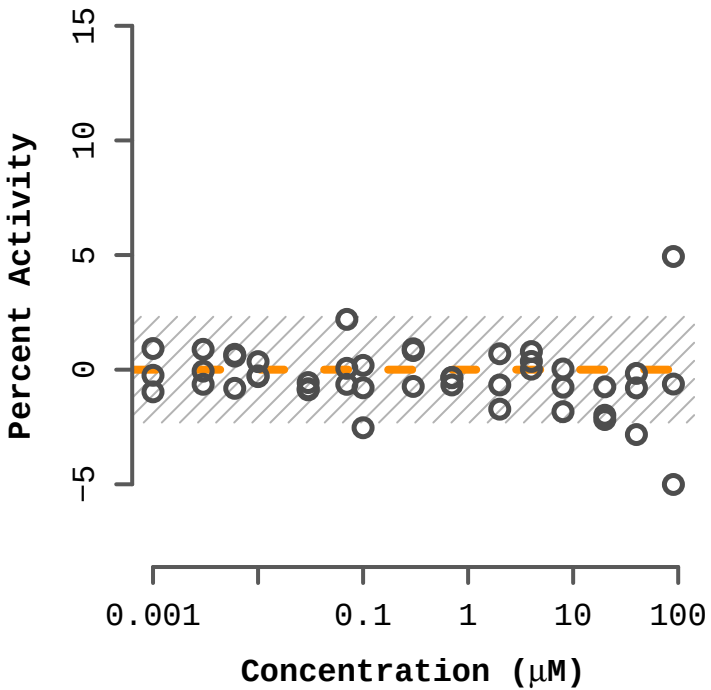
	tp	ga	gw
val:	1.3	−0.402	8
sd:	0.525	0.309	15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.23	−0.19	5.57	0.0605	0.902
sd:	22.8	0.323	13.9	2.86	1.26

	CNST	HILL	GNLS
AIC:	283.82	282.95	284.81
PROB:	0.32	0.49	0.19
RMSE:	16.62	16.23	16.49

MAX_MEAN: 24.8 MAX_MED: 3.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

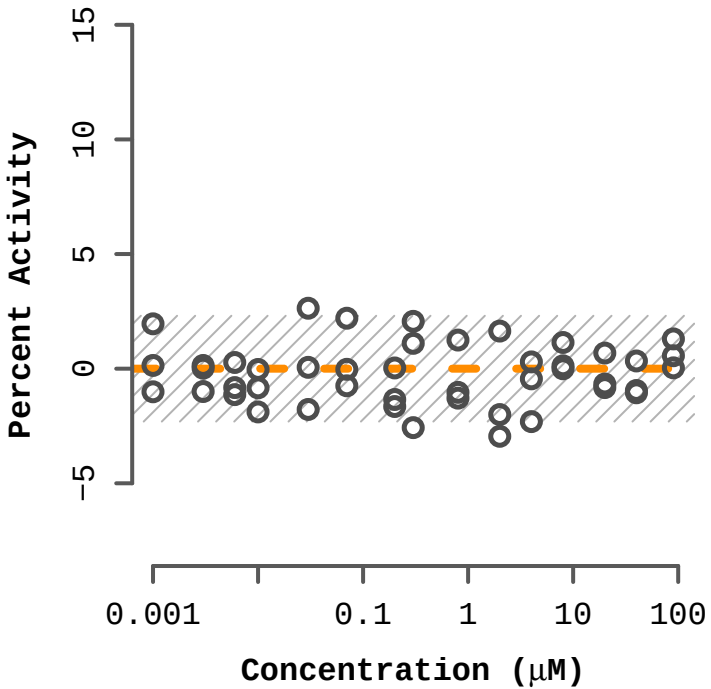
NAME: Methyl carbamate
CHID: 20834 CASRN: 598-55-0
SPID(S): Tox21_301388
M4ID: 12477745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.539 MAX_MED: 0.835 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

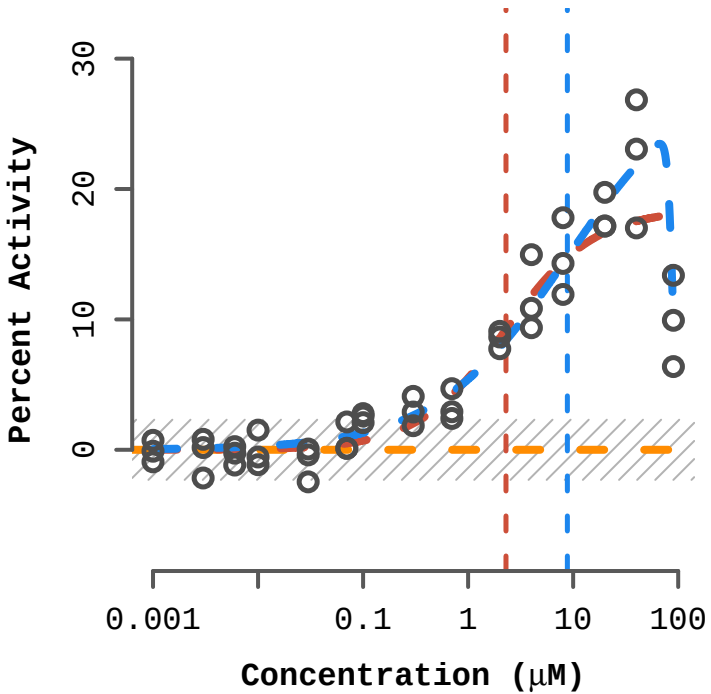
NAME: Methyl carbazate
CHID: 20835 CASRN: 6294-89-9
SPID(S): Tox21_200879
M4ID: 12481373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.634 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3'-Methyl-4-dimethylaminoazobenzene
CHID: 20838 CASRN: 55-80-1
SPID(S): Tox21_303022
M4ID: 12476111

HILL MODEL (in red):

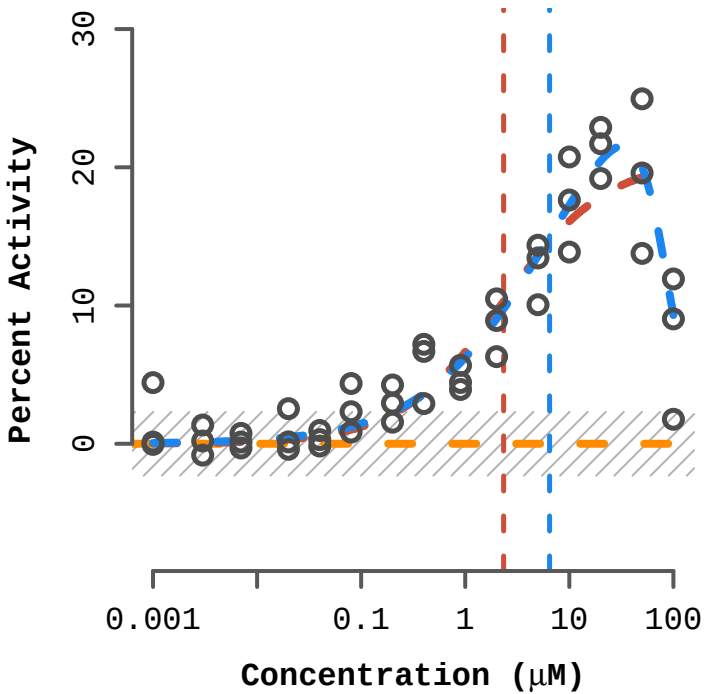
	tp	ga	gw
val:	18.5	0.36	1.03
sd:	1.7	0.114	0.199

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29.5	0.945	0.687	1.94	17.6
sd:	8.22	0.386	0.129	0.00806	14.2

	CNST	HILL	GNLS
AIC:	331.57	219.75	195.43
PROB:	0	0	1
RMSE:	9.73	3.09	1.89

MAX_MEAN: 22.3 MAX_MED: 23.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3'-Methyl-4-dimethylaminoazobenzene
CHID: 20838 CASRN: 55-80-1
SPID(S): Tox21_201755
M4ID: 12480497

HILL MODEL (in red):

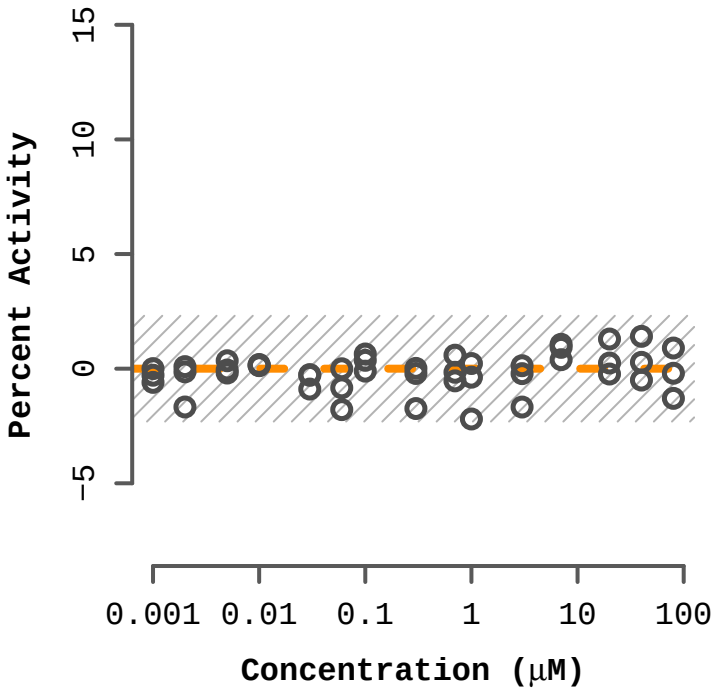
	tp	ga	gw
val:	20.6	0.369	0.875
sd:	2.59	0.163	0.18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29.9	0.81	0.716	1.92	3.09
sd:	5.58	0.243	0.106	0.0502	0.901

	CNST	HILL	GNLS
AIC:	337.37	242.74	213.3
PROB:	0	0	1
RMSE:	10.21	4.07	2.39

MAX_MEAN: 21.3 MAX_MED: 21.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

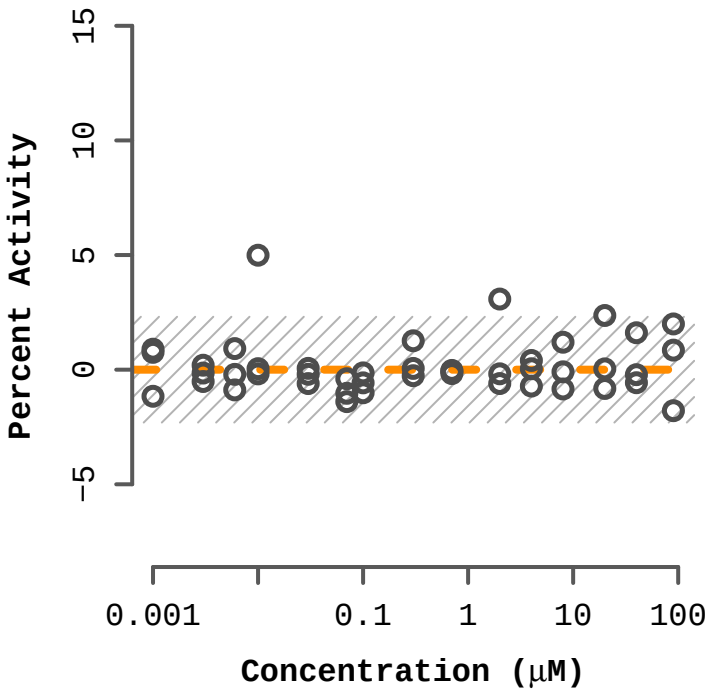
NAME: Methyl hesperidin
CHID: 20841 **CASRN:** 11013-97-1
SPID(S): Tox21_302739
M4ID: 12476394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.796 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

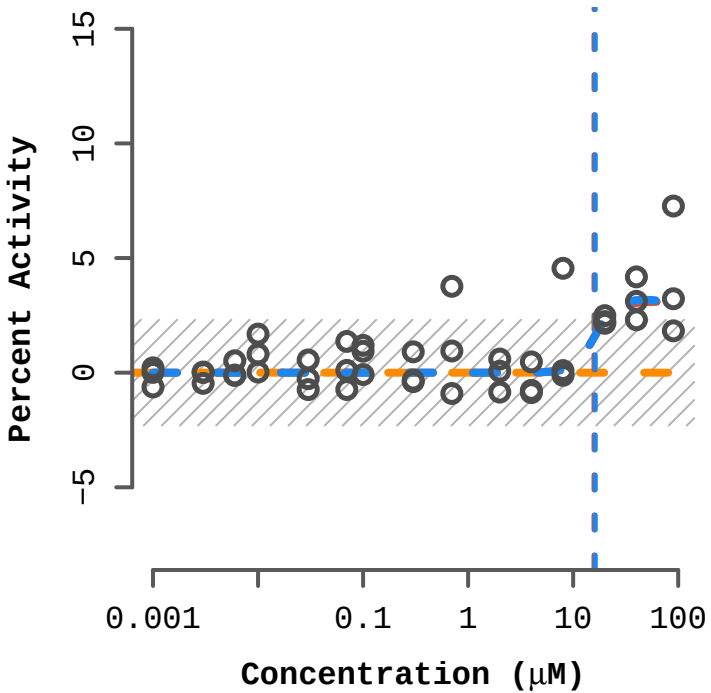
NAME: Methyl hesperidin
CHID: 20841 **CASRN:** 11013-97-1
SPID(S): Tox21_202328
M4ID: 12479924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl linoleate
CHID: 20843 CASRN: 112-63-0
SPID(S): Tox21_302917
M4ID: 12476216

HILL MODEL (in red):

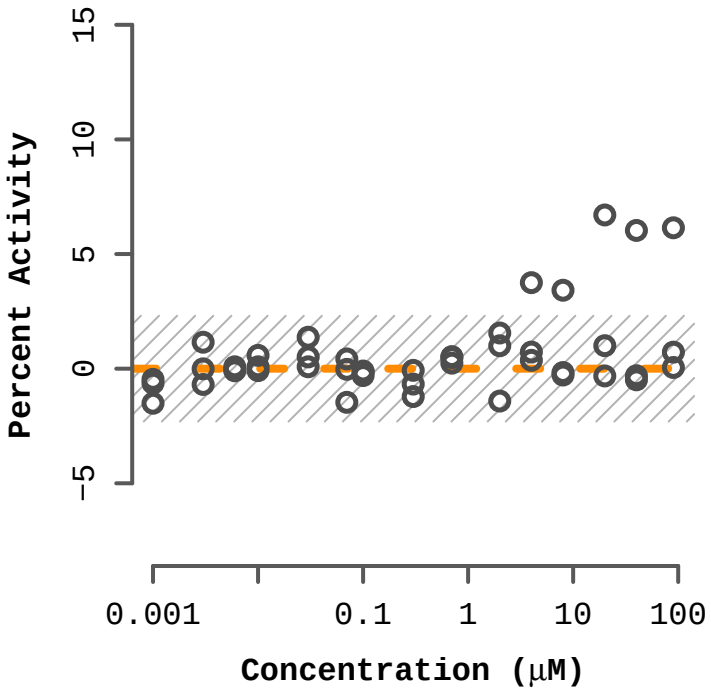
	tp	ga	gw
val:	3.1	1.2	4.5
sd:	0.426	0.0998	3.51

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.24	1.21	4.24	2.22	3.73
sd:	1.14	0.121	3.28	4.19	63.2

	CNST	HILL	GNLS
AIC:	176.75	136.67	140.56
PROB:	0	0.88	0.12
RMSE:	1.92	1.25	1.26

MAX_MEAN: 4.11 MAX_MED: 3.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

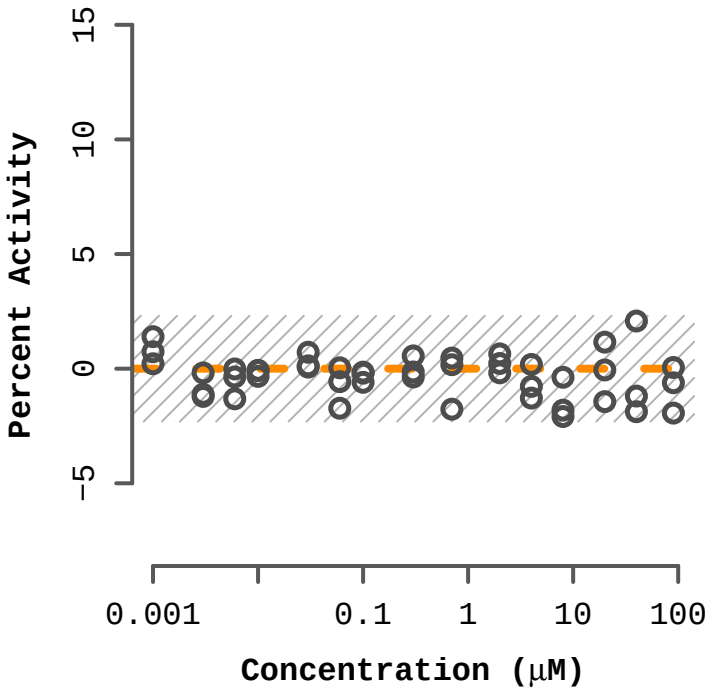
NAME: Methyl linoleate
CHID: 20843 **CASRN:** 112-63-0
SPID(S): Tox21_201403
M4ID: 12480849

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 2.47 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

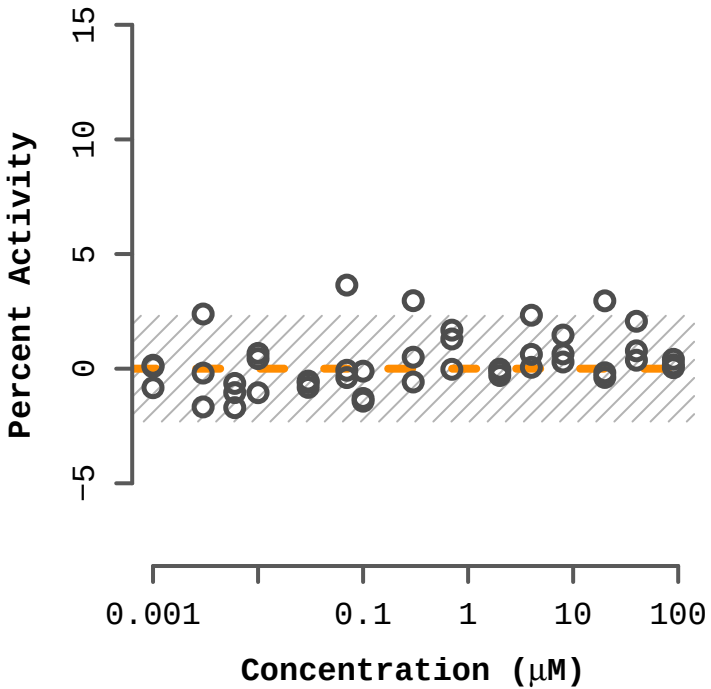
NAME: Methyl methacrylate
CHID: 20844 CASRN: 80-62-6
SPID(S): Tox21_200367
M4ID: 12481885

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.784 MAX_MED: 0.739 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

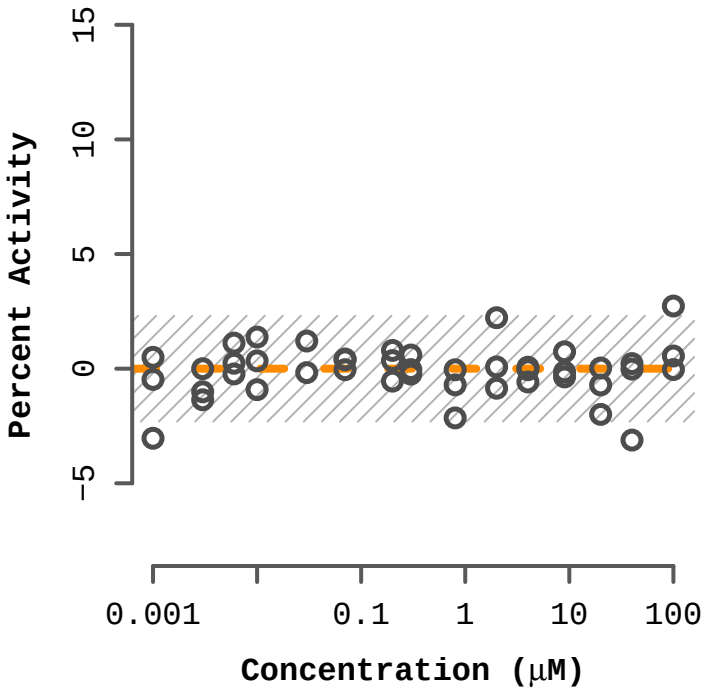
NAME: Methyl methanesulfonate
CHID: 20845 CASRN: 66-27-3
SPID(S): Tox21_300299
M4ID: 12478831

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.07 MAX_MED: 1.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

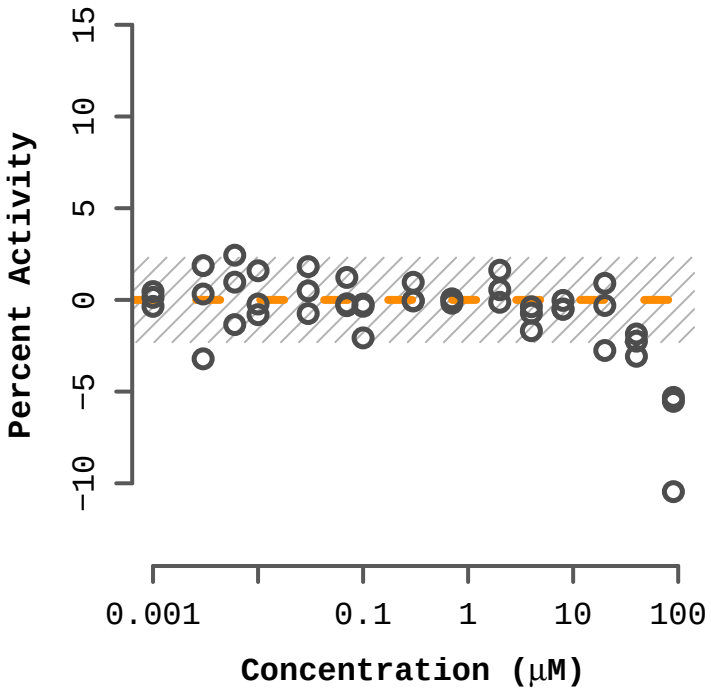
NAME: Methyl methanesulfonate
CHID: 20845 CASRN: 66-27-3
SPID(S): Tox21_202094
M4ID: 12480158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.555 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

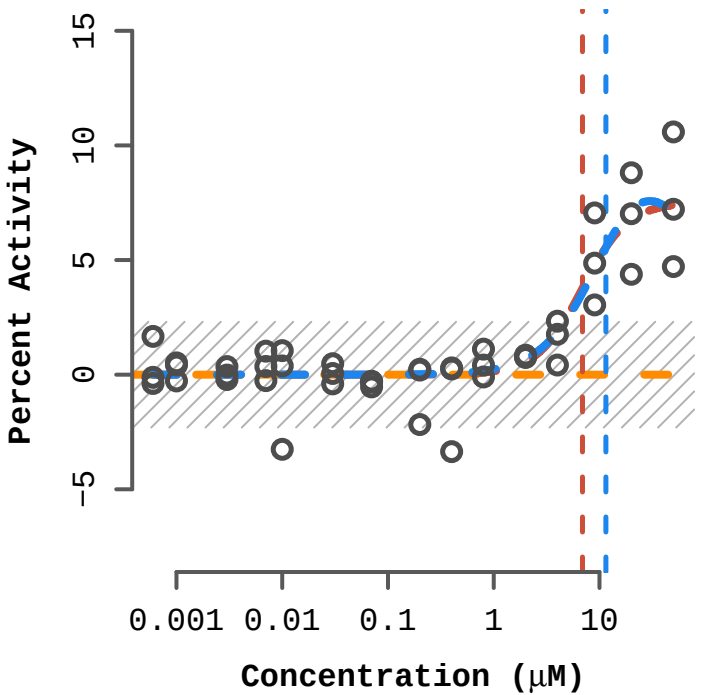
NAME: N-Methyl-N'-nitro-N-nitrosoguanidine
CHID: 20846 **CASRN:** 70-25-7
SPID(S): Tox21_201126
M4ID: 12481126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.3	NA	NA

MAX_MEAN: 0.687 **MAX_MED:** 0.969 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methyl-1-nitroanthraquinone
CHID: 20847 CASRN: 129-15-7
SPID(S): Tox21_202474
M4ID: 12479778

HILL MODEL (in red):

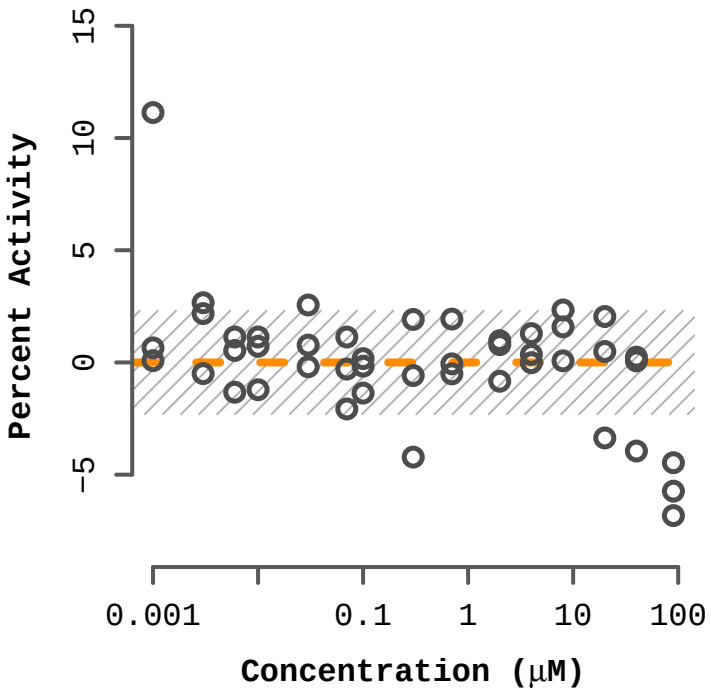
	tp	ga	gw
val:	7.54	0.839	2.02
sd:	0.862	0.092	0.605

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.7	1.06	1.62	1.88	1.02
sd:	28.5	0.573	0.695	1.69	3.83

	CNST	HILL	GNLS
AIC:	219.92	150.34	153.65
PROB:	0	0.84	0.16
RMSE:	3.2	1.28	1.29

MAX_MEAN: 7.51 MAX_MED: 7.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

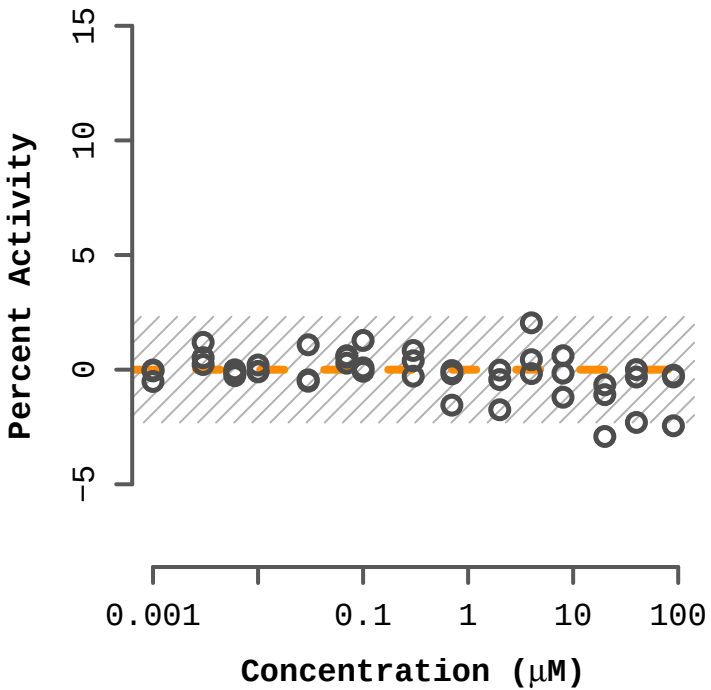
NAME: Methyl parathion
CHID: 20855 CASRN: 298-00-0
SPID(S): Tox21_300998
M4ID: 12478135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.69	NA	NA

MAX_MEAN: 3.96 MAX_MED: 2.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

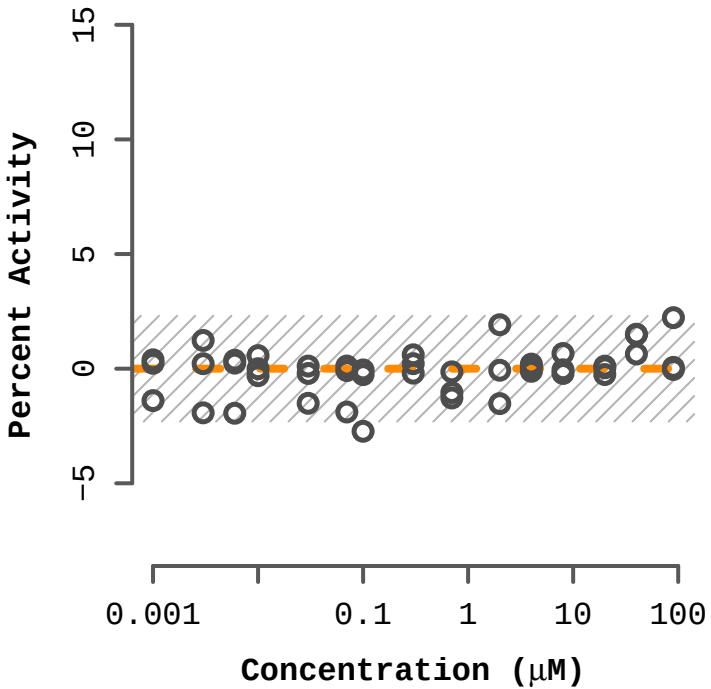
NAME: Methyl parathion
CHID: 20855 CASRN: 298-00-0
SPID(S): Tox21_202303
M4ID: 12479949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.771 MAX_MED: 0.544 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

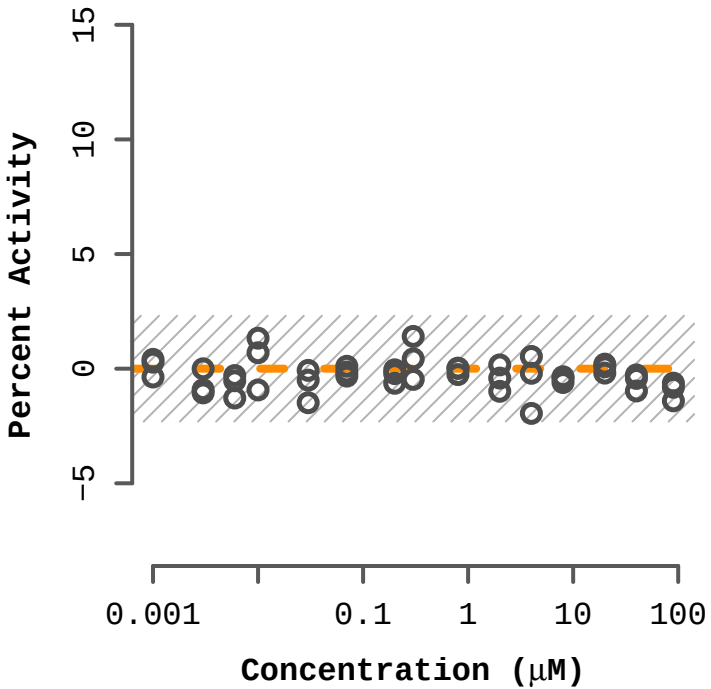
NAME: N-Methyl-2-pyrrolidone
CHID: 20856 **CASRN:** 872-50-4
SPID(S): Tox21_300097
M4ID: 12479033

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.45	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

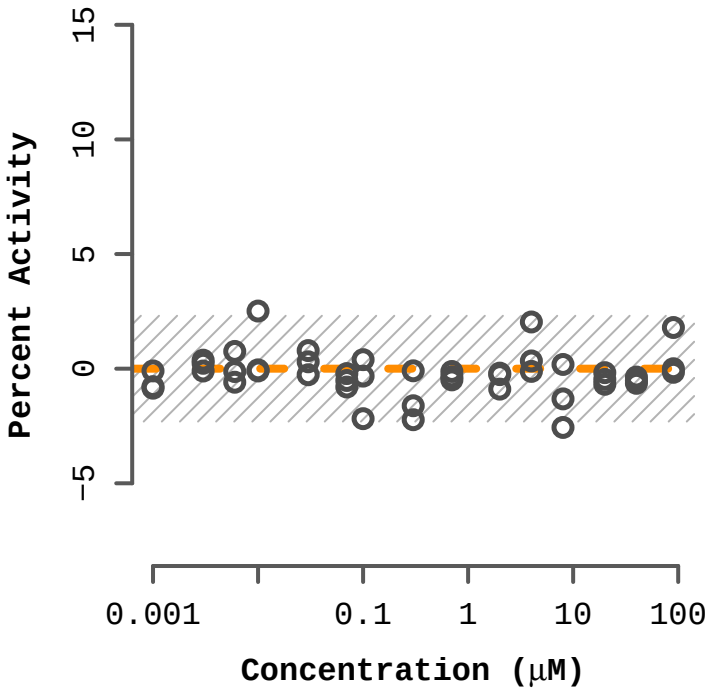
NAME: N-Methyl-2-pyrrolidone
CHID: 20856 **CASRN:** 872-50-4
SPID(S): Tox21_202350
M4ID: 12479902

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.458 **MAX_MED:** 0.697 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

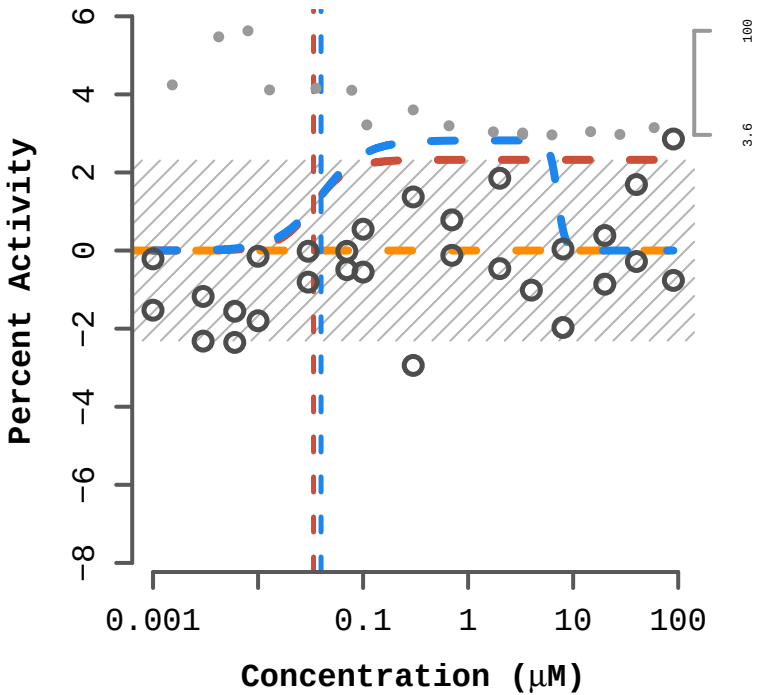
NAME: (N-6)-Methyladenine
CHID: 20857 **CASRN:** 443-72-1
SPID(S): Tox21_200016
M4ID: 12482236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.789 **MAX_MED:** 0.339 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: alpha-Methylbenzyl alcohol
CHID: 20859 CASRN: 98-85-1
SPID(S): Tox21_200505
M4ID: 12481747 BRK

HILL MODEL (in red):

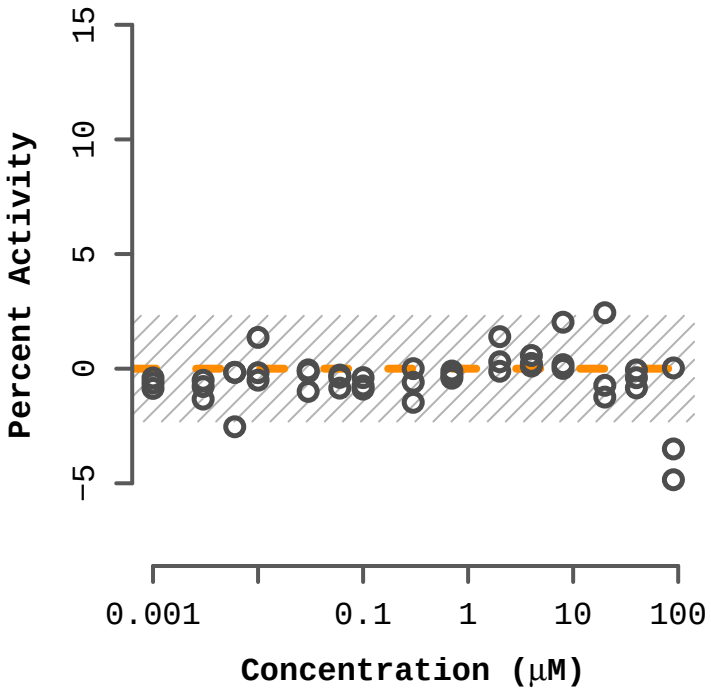
	tp	ga	gw
val:	2.32	-1.47	2.6
sd:	1.24	1.16	9.46

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.82	-1.4	2.1	0.85	11.9
sd:	2.04	1.15	6.45	4.06	905

	CNST	HILL	GNLS
AIC:	375.76	377.78	382.87
PROB:	0.72	0.26	0.02
RMSE:	25.68	25.44	25.44

MAX_MEAN: 32.4 MAX_MED: 3.93 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

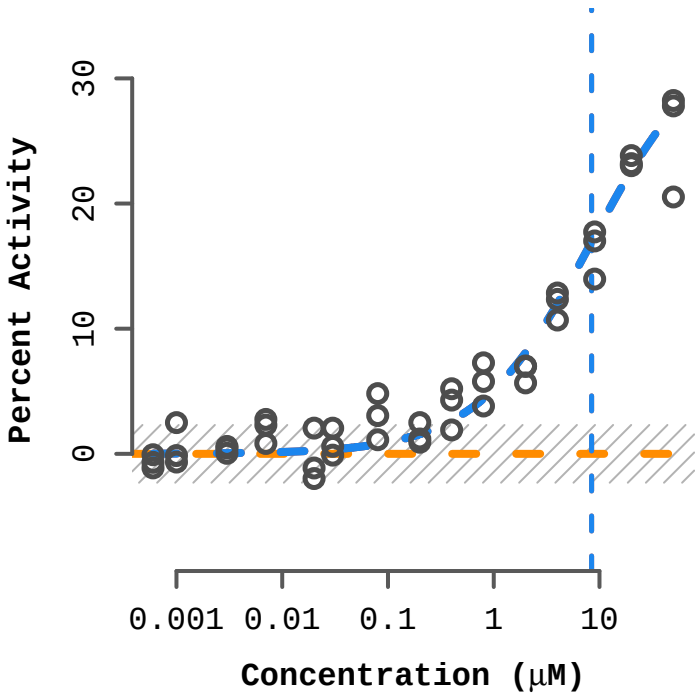
NAME: 4-Methylcatechol
CHID: 20861 **CASRN:** 452-86-8
SPID(S): Tox21_200632
M4ID: 12481620

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.74 **MAX_MED:** 0.304 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methylcholanthrene
CHID: 20862 CASRN: 56-49-5
SPID(S): Tox21_202592
M4ID: 12479660

HILL MODEL (in red):

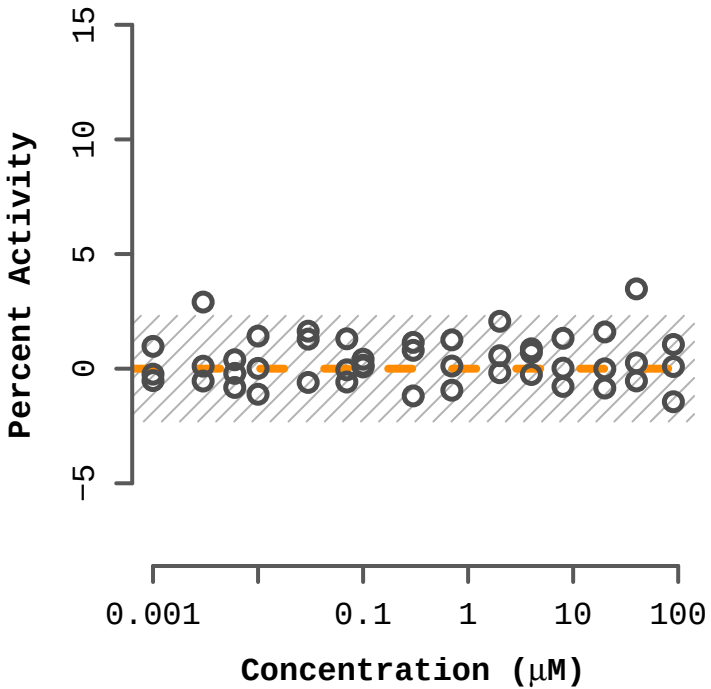
	tp	ga	gw
val:	33.9	0.926	0.807
sd:	2.82	0.108	0.0847

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	33.9	0.926	0.807	3.68	12.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	336.7	184.53	188.53
PROB:	0	0.88	0.12
RMSE:	10.77	1.83	1.83

MAX_MEAN: 25.5 MAX_MED: 27.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

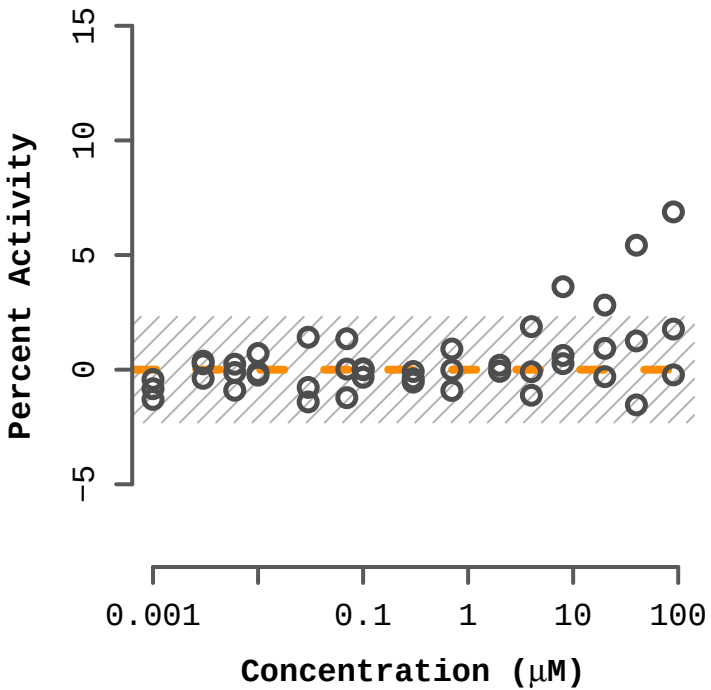
NAME: Methyldopa sesquihydrate
CHID: 20863 **CASRN:** 41372-08-1
SPID(S): Tox21_300482
M4ID: 12478650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

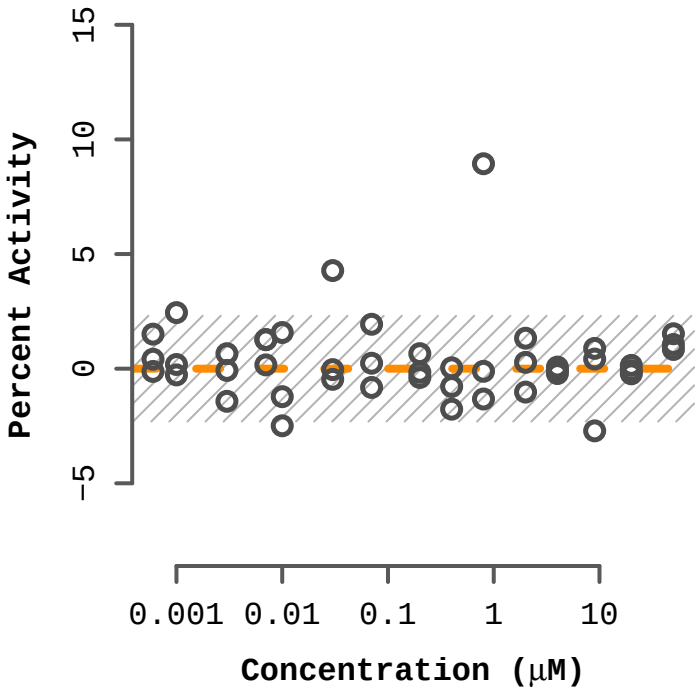
NAME: Methyldopa sesquihydrate
CHID: 20863 **CASRN:** 41372-08-1
SPID(S): Tox21_202031
M4ID: 12480221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 2.81 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

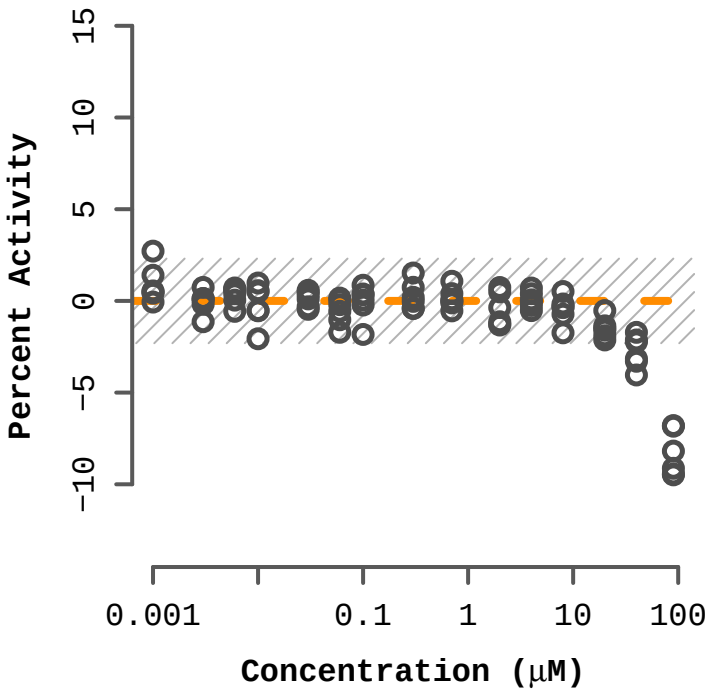
NAME: Methyldopa sesquihydrate
CHID: 20863 **CASRN:** 41372-08-1
SPID(S): Tox21_110917_1
M4ID: 12484016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 2.5 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

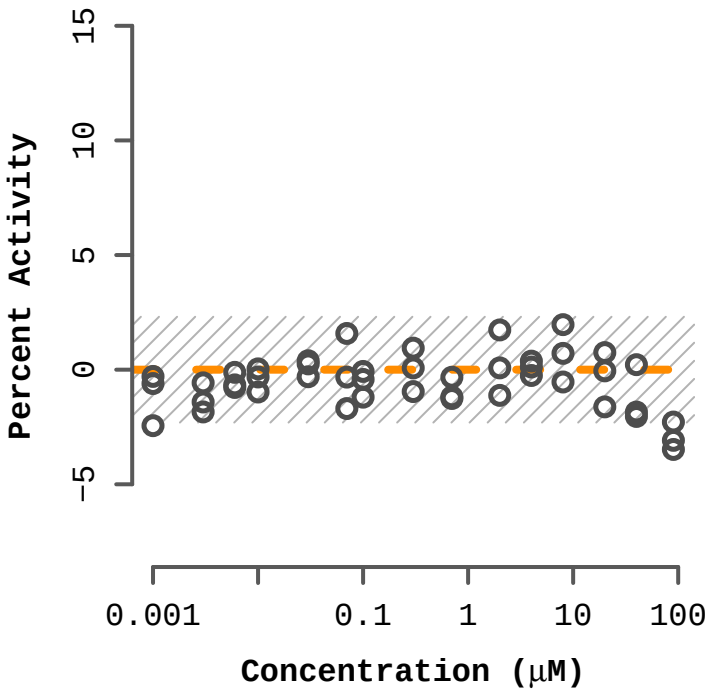
NAME: 4,4'−Methylenebis(2−chloroaniline)
CHID: 20865 **CASRN:** 101−14−4
SPID(S): Tox21_200651
M4ID: 12481601

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	354.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 0.919 **MAX_MED:** 0.519 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

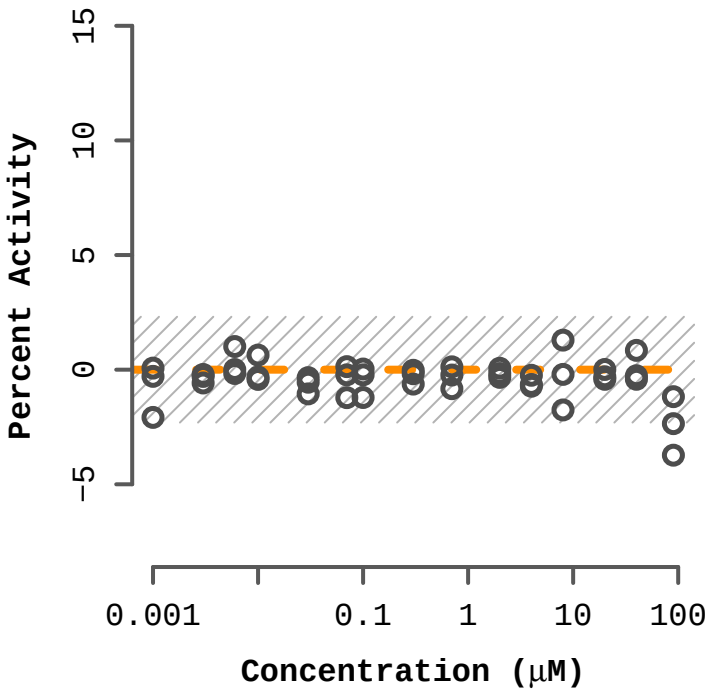
NAME: 4,4'−Methylenebis(2−methylaniline)
CHID: 20867 **CASRN:** 838−88−0
SPID(S): Tox21_300201
M4ID: 12478929

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.714 **MAX_MED:** 0.712 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

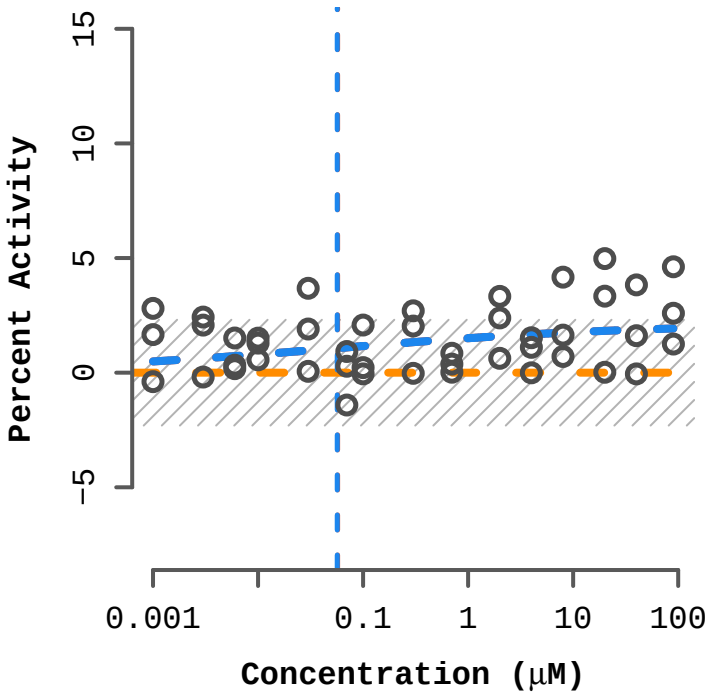
NAME: 4,4'−Methylenebis(2−methylaniline)
CHID: 20867 **CASRN:** 838−88−0
SPID(S): Tox21_202372
M4ID: 12479880

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.285 **MAX_MED:** 0.00865 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dichloromethane
CHID: 20868 CASRN: 75-09-2
SPID(S): Tox21_202526
M4ID: 12479726

HILL MODEL (in red):

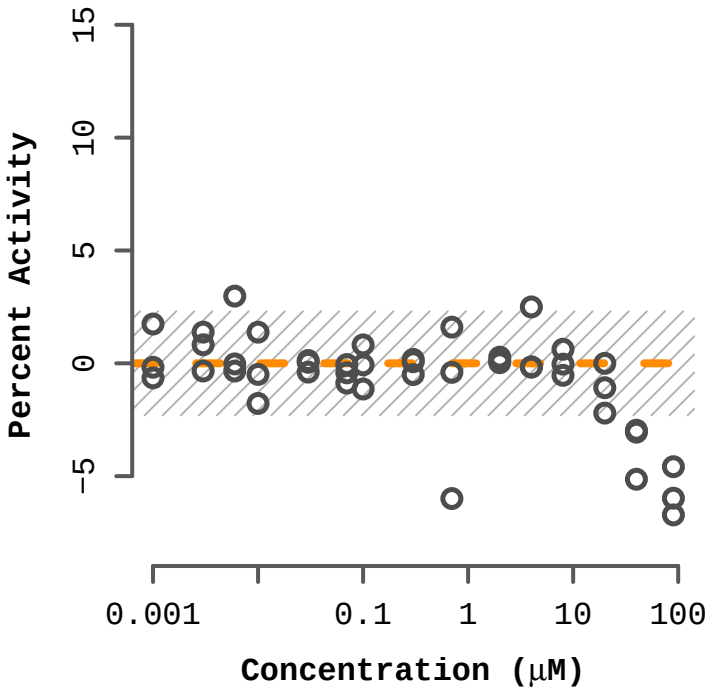
	tp	ga	gw
val:	2.14	−1.24	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.14	−1.25	0.3	3.95	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	195.62	170.73	174.73
PROB:	0	0.88	0.12
RMSE:	2.05	1.4	1.4

MAX_MEAN: 2.82 **MAX_MED:** 3.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

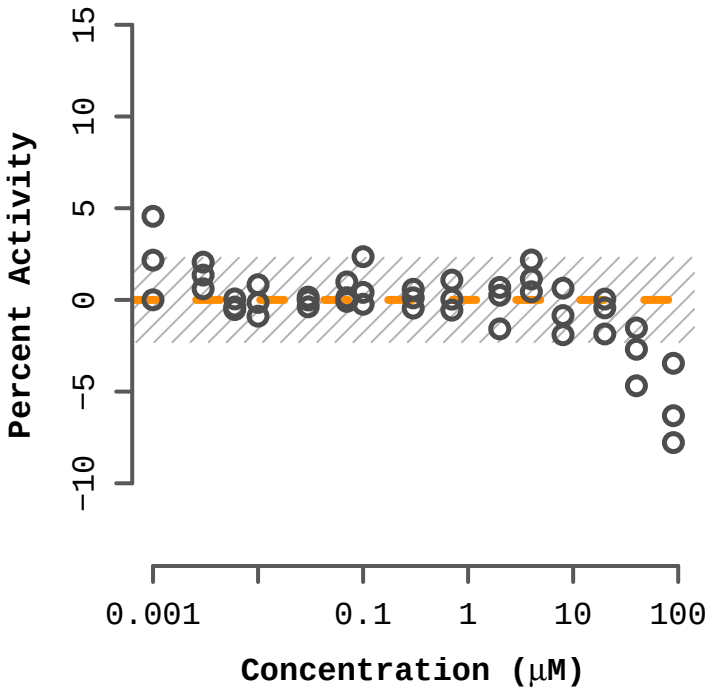
NAME: 4,4'−Methylenebis(N,N−dimethylaniline)
CHID: 20869 CASRN: 101−61−1
SPID(S): Tox21_300130
M4ID: 12479000

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.01	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 0.87 MAX_MED: 0.824 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

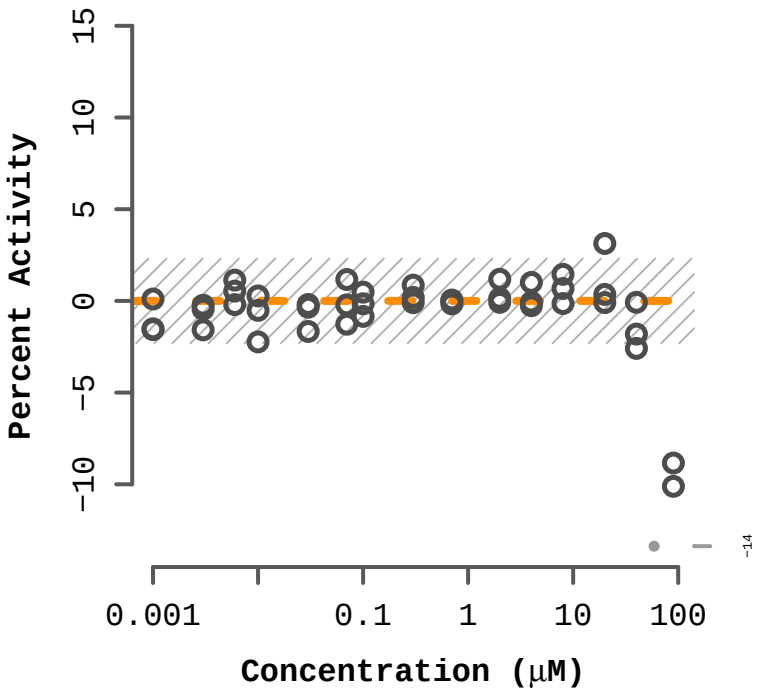
NAME: 4,4'-Methylenebis(N,N-dimethylaniline)
CHID: 20869 **CASRN:** 101-61-1
SPID(S): Tox21_201389
M4ID: 12480863

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

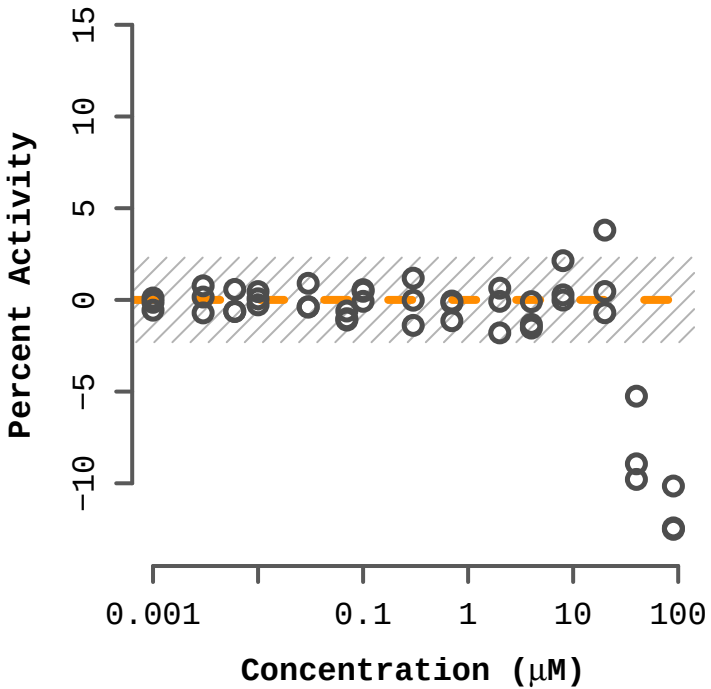
NAME: 2,2'-Methylenebis(4-methyl-6-tert-butylphenol)
CHID: 20870 **CASRN:** 119-47-1
SPID(S): Tox21_302923
M4ID: 12476210 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.59	NA	NA
PROB:	1	NA	NA
RMSE:	3.04	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.678 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

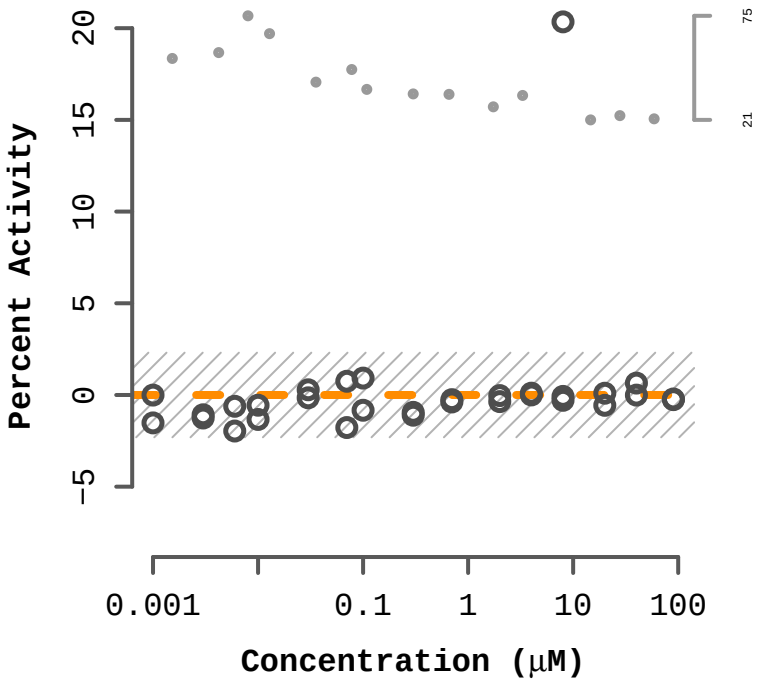
NAME: 2,2'-Methylenebis(4-methyl-6-tert-butylphenol)
CHID: 20870 **CASRN:** 119-47-1
SPID(S): Tox21_201529
M4ID: 12480723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.99	NA	NA
PROB:	1	NA	NA
RMSE:	3.82	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.472 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

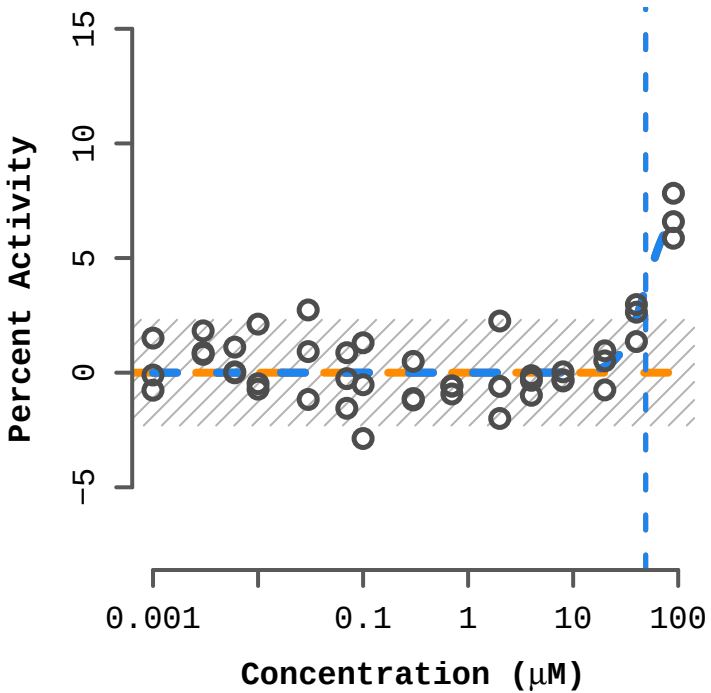
NAME: Methylhydrazine sulfate
CHID: 20875 CASRN: 302-15-8
SPID(S): Tox21_200033
M4ID: 12482219 BRK

HILL MODEL: Not applicable.

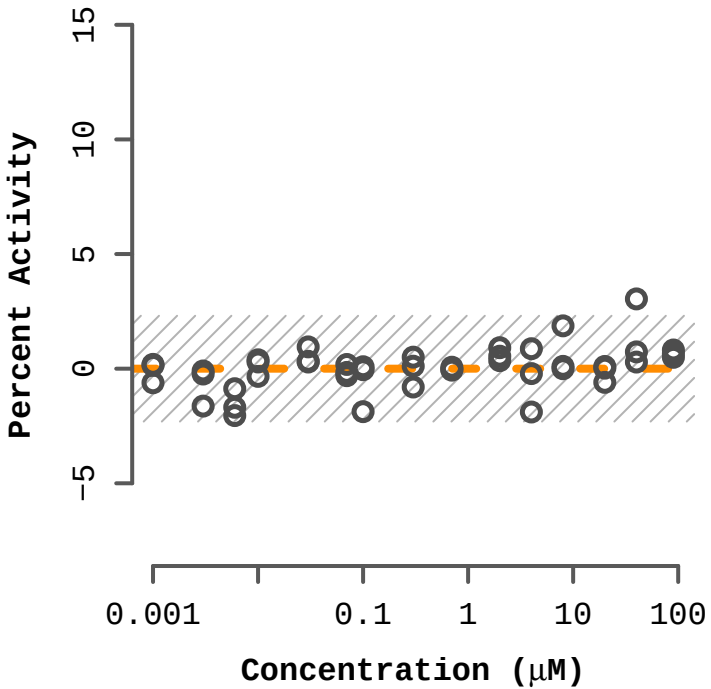
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	410.83	NA	NA
PROB:	1	NA	NA
RMSE:	24.71	NA	NA

MAX_MEAN: 24.3 **MAX_MED:** 0.922 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Methylhydroquinone
CHID:    20876   CASRN: 95-71-6
SPID(S): Tox21_200506
M4ID:    12481746

HILL MODEL (in red):
      tp       ga       gw
val:  7.43     1.69     3.67
sd:   2.37     0.144    3.17

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.43     1.69     3.67     3.27     4.26
sd:   2.38     0.144    3.17     1960     6560

      CNST         HILL         GNLS
AIC:  185.46       148.44       152.44
PROB: 0            0.88         0.12
RMSE: 2.17         1.13         1.13

MAX_MEAN: 6.76      MAX_MED: 6.59      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

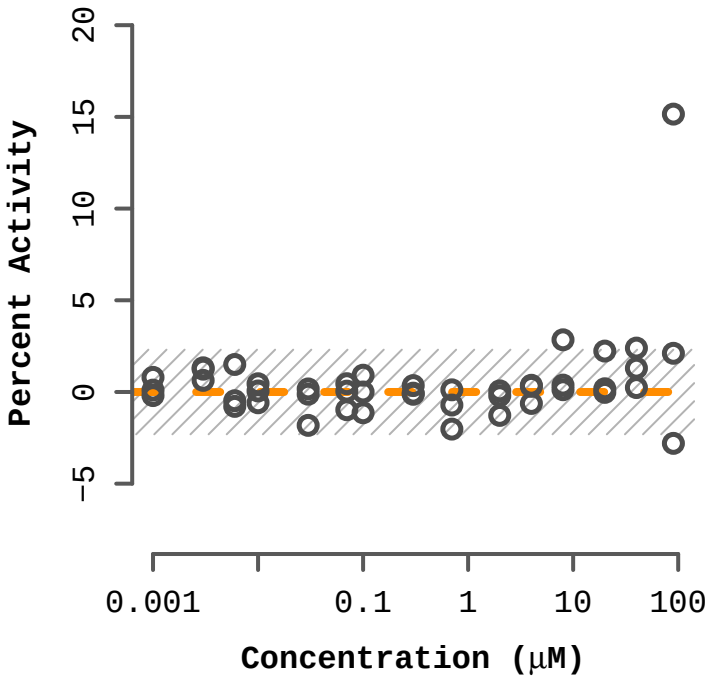
NAME: 1-Methylnaphthalene
CHID: 20877 **CASRN:** 90-12-0
SPID(S): Tox21_300339
M4ID: 12478793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.734 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

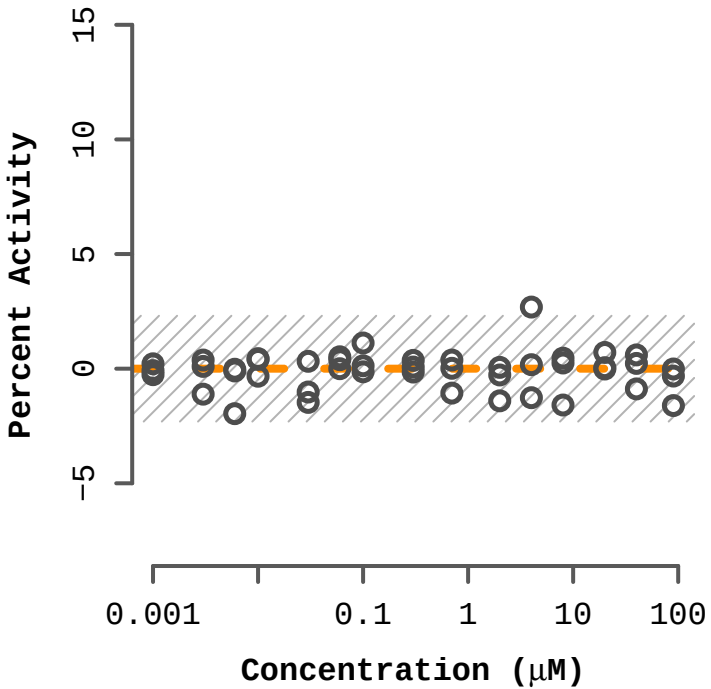
NAME: 1-Methylnaphthalene
CHID: 20877 CASRN: 90-12-0
SPID(S): Tox21_201768
M4ID: 12480484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.5	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 4.82 MAX_MED: 2.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

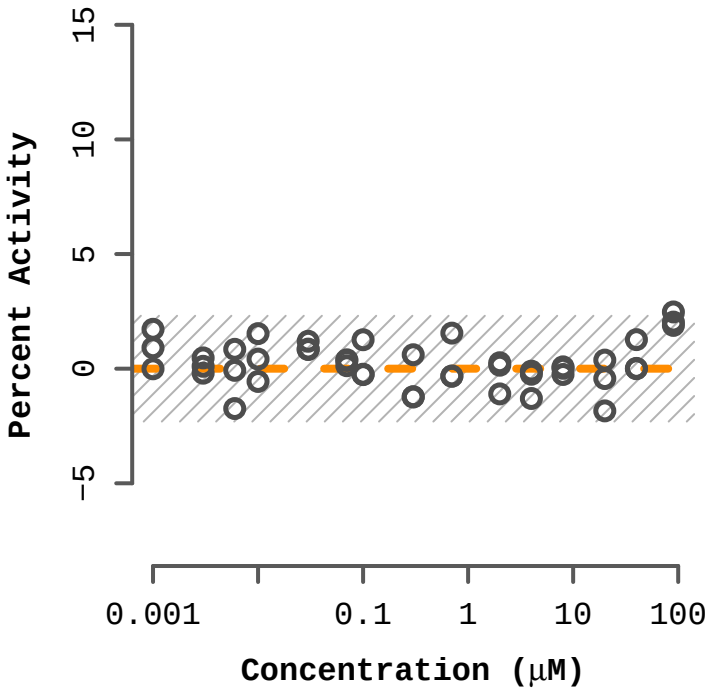
NAME: 2-Methylnaphthalene
CHID: 20878 **CASRN:** 91-57-6
SPID(S): Tox21_200839
M4ID: 12481413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.534 **MAX_MED:** 0.405 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

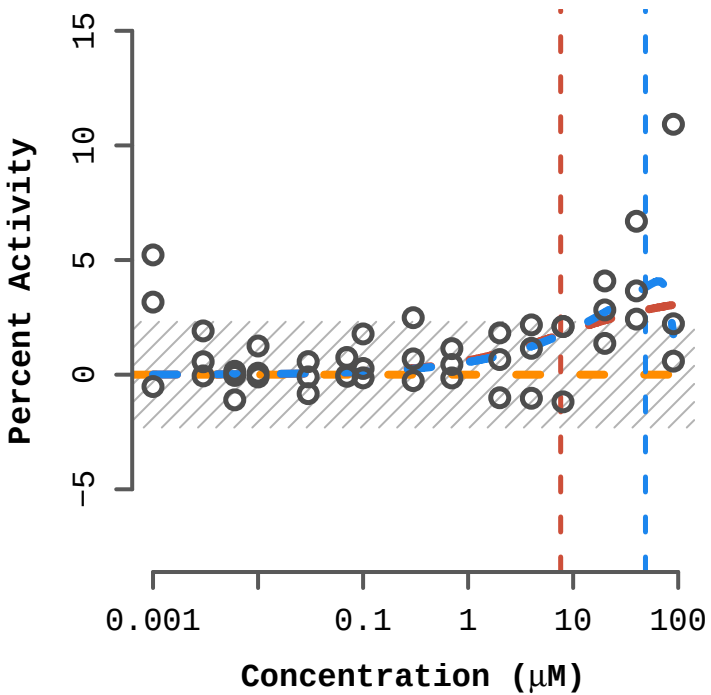
NAME: 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol
CHID: 20880 **CASRN:** 76014-81-8
SPID(S): Tox21_303708
M4ID: 12475480

HILL MODEL: Not applicable.

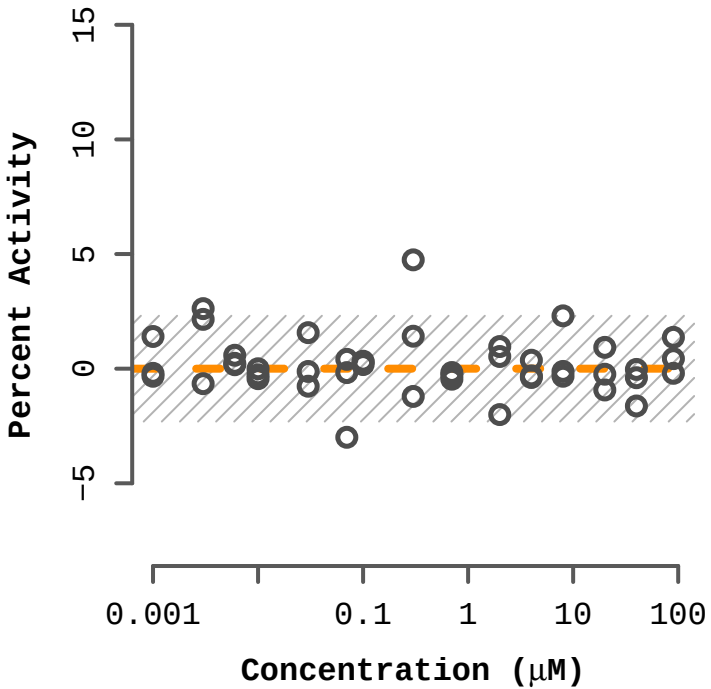
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 2.03 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-(N-Methyl-N-nitrosamino)-1-(3-pyridyl)-1-buta
CHID:    20881   CASRN: 64091-91-4
SPID(S): Tox21_303771
M4ID:    12475417

HILL MODEL (in red):
      tp       ga       gw
val:  3.51     0.881    0.757
sd:   2.01     0.778    0.862

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.62     1.69     0.658    1.94     13
sd:   9.75     1.52     0.38     0.0453   36.7

      CNST        HILL        GNLS
AIC:  198.51      177.56      177.72
PROB: 0           0.52        0.48
RMSE: 2.56        1.91        1.97

MAX_MEAN: 4.58      MAX_MED: 3.66      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

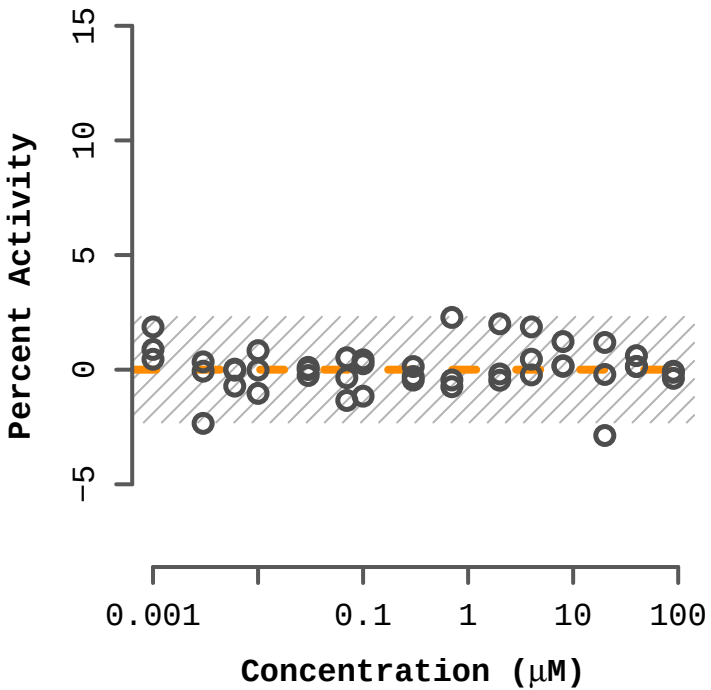
NAME: Methylphenidate hydrochloride
CHID: 20886 CASRN: 298-59-9
SPID(S): Tox21_200309
M4ID: 12481943

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

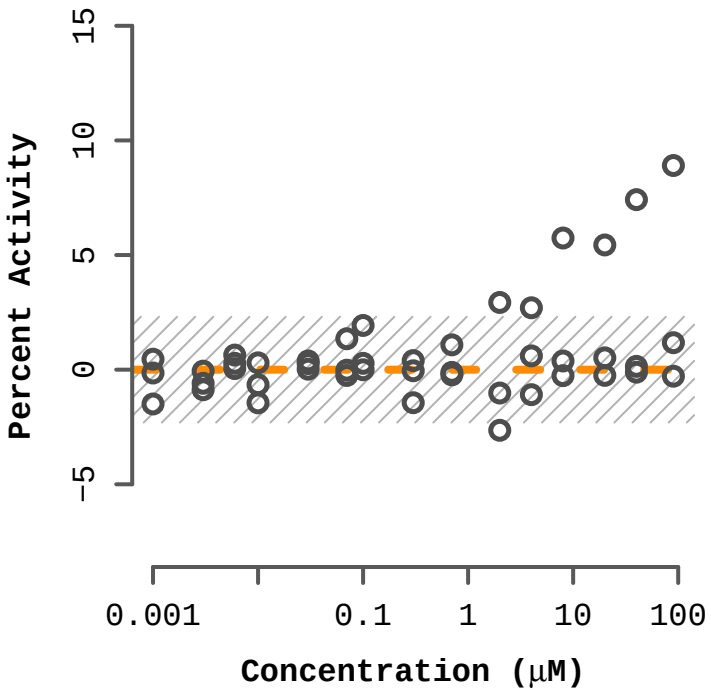
NAME: 6-Methylquinoline
CHID: 20887 **CASRN:** 91-62-3
SPID(S): Tox21_300320
M4ID: 12478811

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.885 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

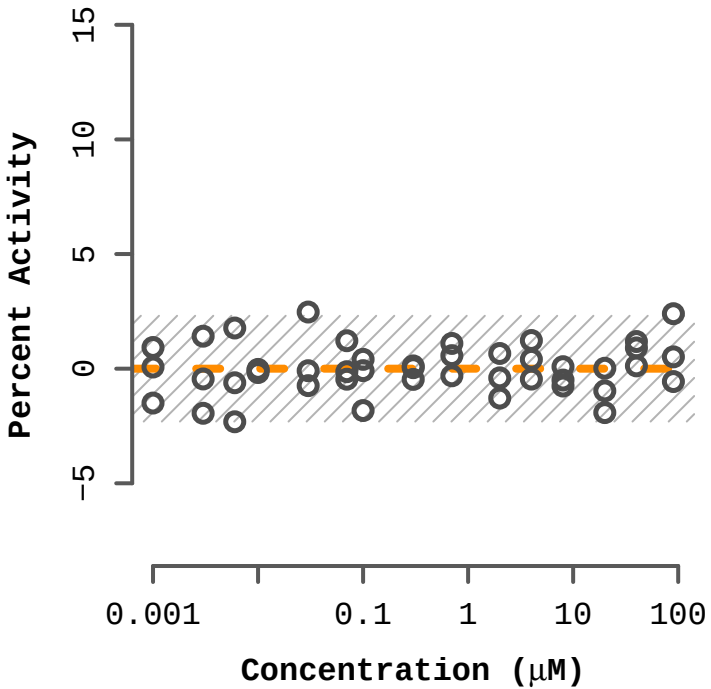
NAME: 6-Methylquinoline
CHID: 20887 **CASRN:** 91-62-3
SPID(S): Tox21_202379
M4ID: 12479873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.31	NA	NA

MAX_MEAN: 3.27 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

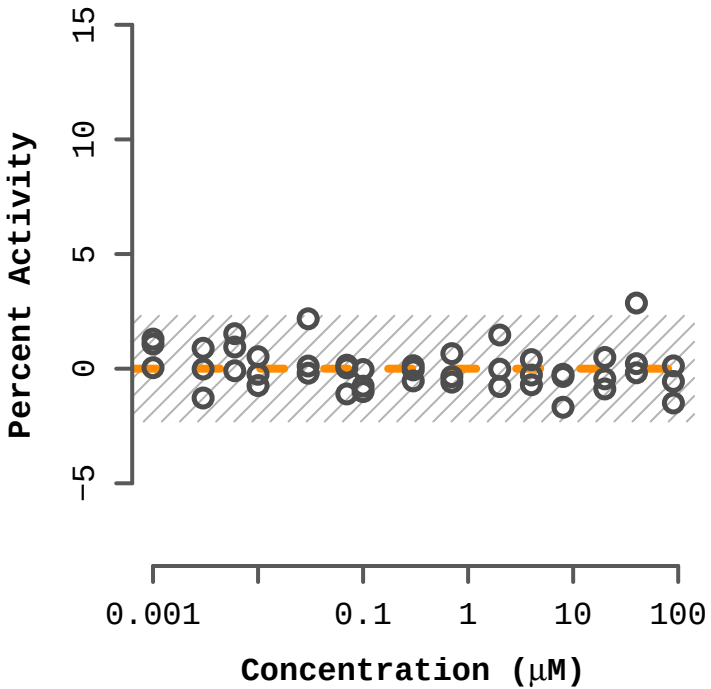
NAME: 8-Methylquinoline
CHID: 20888 **CASRN:** 611-32-5
SPID(S): Tox21_200341
M4ID: 12481911

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.786 **MAX_MED:** 0.908 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

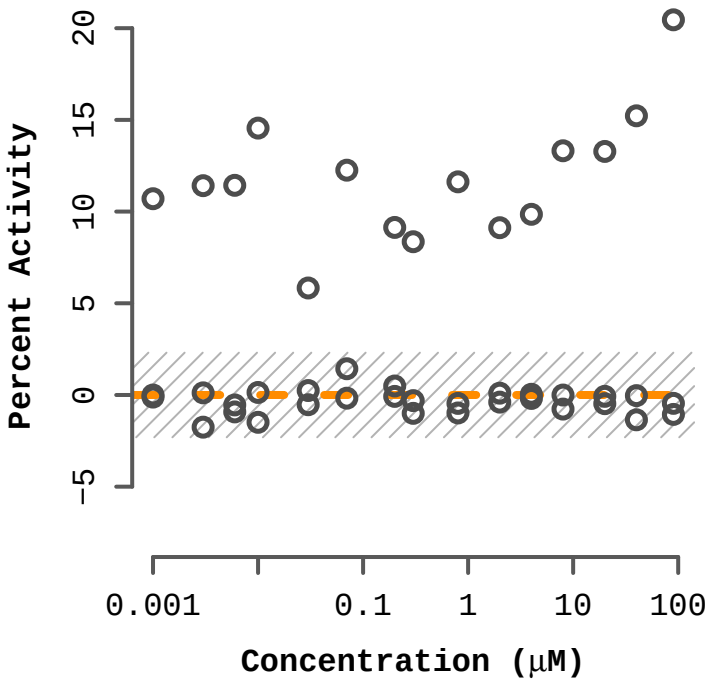
NAME: 4-Methylstyrene
CHID: 20889 **CASRN:** 622-97-9
SPID(S): Tox21_302751
M4ID: 12476382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.969 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

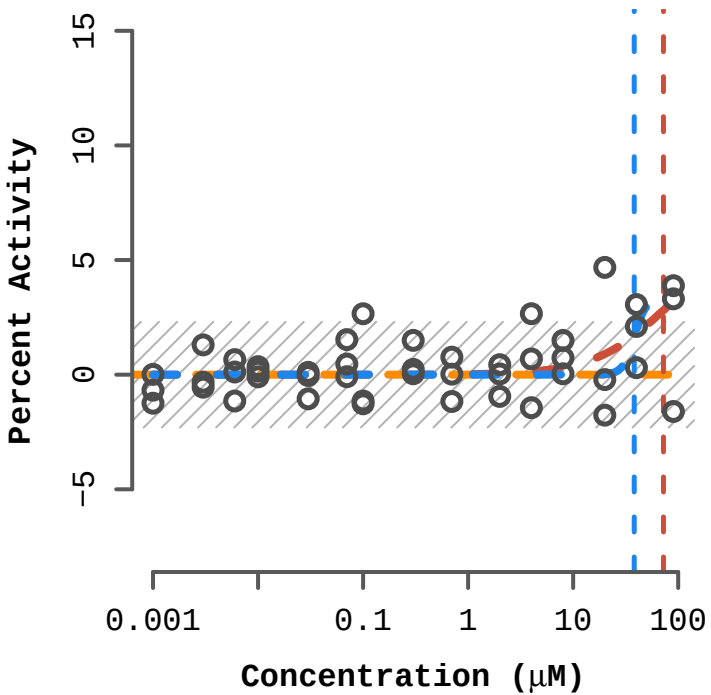
NAME: 4-Methylstyrene
CHID: 20889 CASRN: 622-97-9
SPID(S): Tox21_202394
M4ID: 12479858

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.43	NA	NA
PROB:	1	NA	NA
RMSE:	7.09	NA	NA

MAX_MEAN: 6.32 MAX_MED: 1.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Methyl-2-thiouracil
CHID: 20890 CASRN: 56-04-2
SPID(S): Tox21_300497
M4ID: 12478635

HILL MODEL (in red):

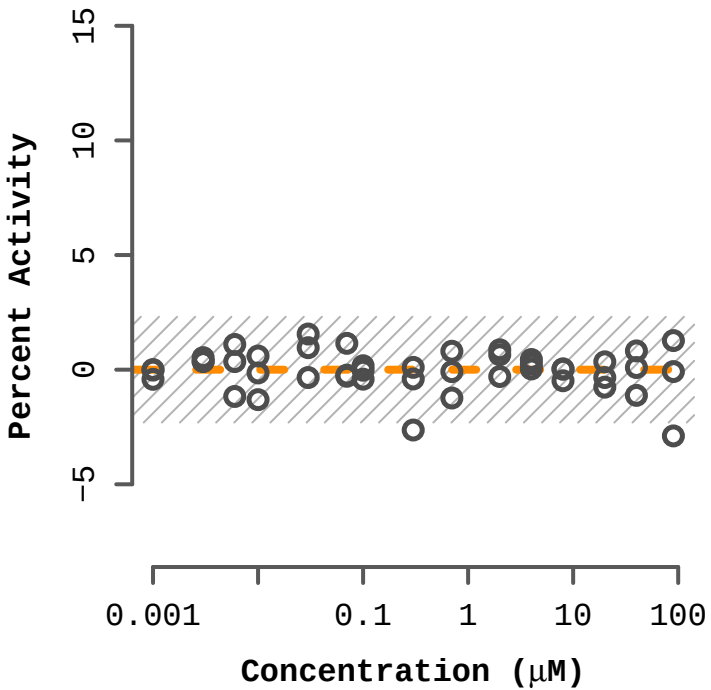
	tp	ga	gw
val:	5.62	1.86	1.29
sd:	7.38	0.929	1.49

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.37	1.58	8	3.32	1.05
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.72	158.1	161.36
PROB:	0.05	0.8	0.16
RMSE:	1.53	1.38	1.42

MAX_MEAN: 1.86 MAX_MED: 3.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

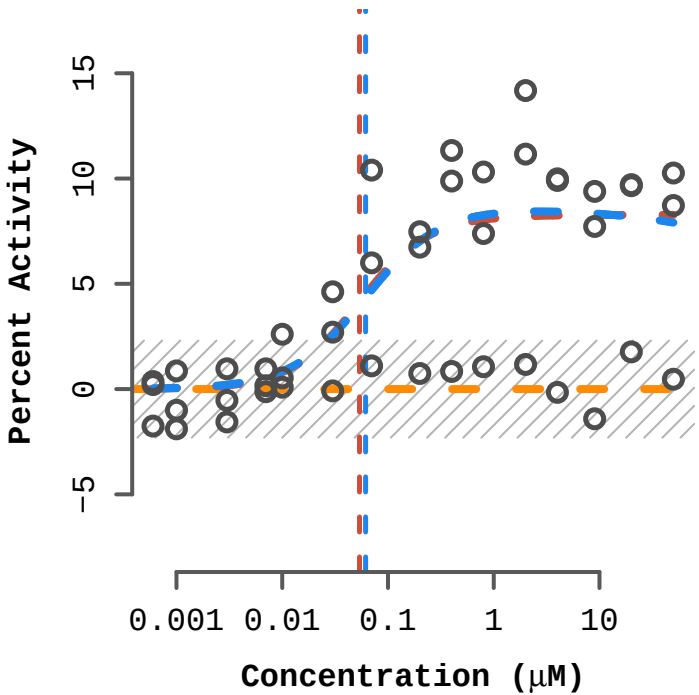
NAME: 6-Methyl-2-thiouracil
CHID: 20890 CASRN: 56-04-2
SPID(S): Tox21_201870
M4ID: 12480382

HILL MODEL: Not applicable.

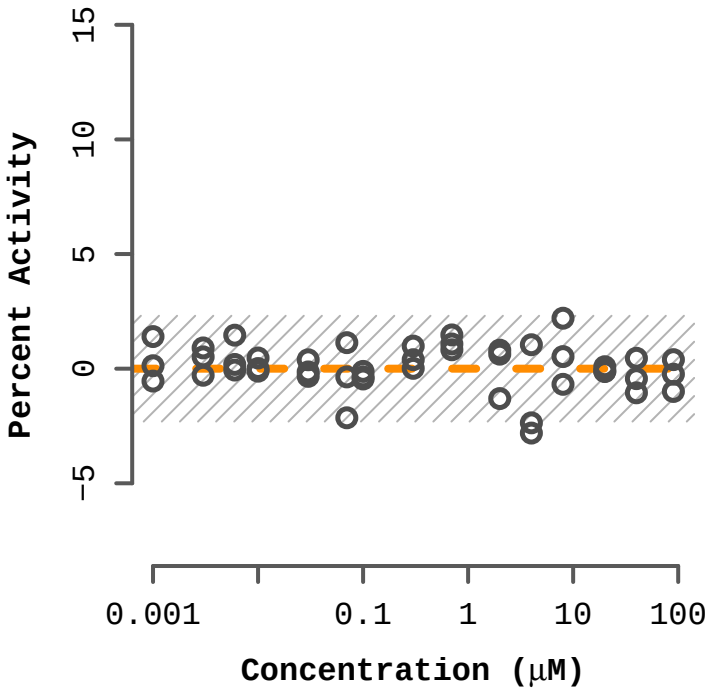
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 0.961 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    6-Methyl-2-thiouracil
CHID:    20890   CASRN: 56-04-2
SPID(S): Tox21_111088_1
M4ID:    12483915

HILL MODEL (in red):
      tp       ga       gw
val:  8.27     -1.27    1.33
sd:   0.941    0.248    0.64

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.73     -1.21    1.23     3.7      0.493
sd:   3.79     0.45     0.744    9.95     3.04

      CNST        HILL        GNLS
AIC:  295.56      249.9       253.85
PROB: 0           0.88        0.12
RMSE: 6.2         3.69        3.69

MAX_MEAN: 8.84      MAX_MED: 11.2      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

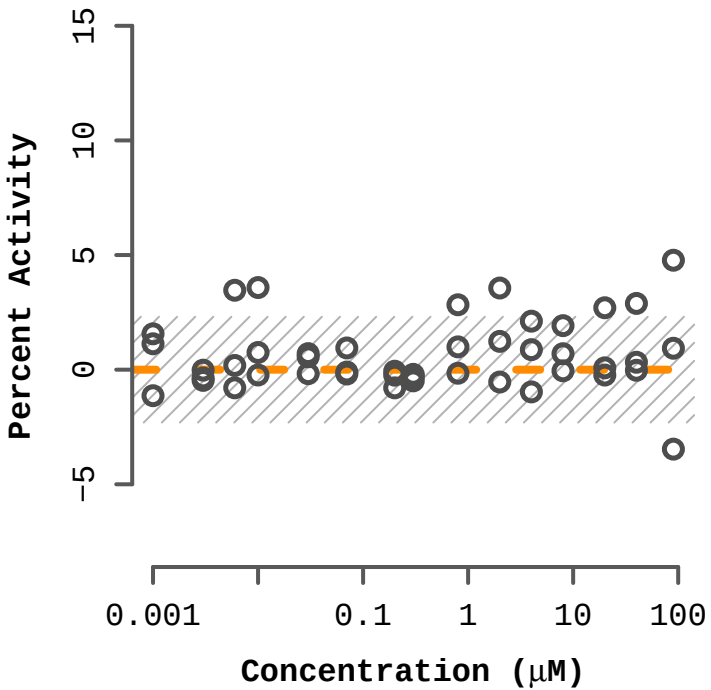
NAME: Metronidazole
CHID: 20892 **CASRN:** 443-48-1
SPID(S): Tox21_302794
M4ID: 12476339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

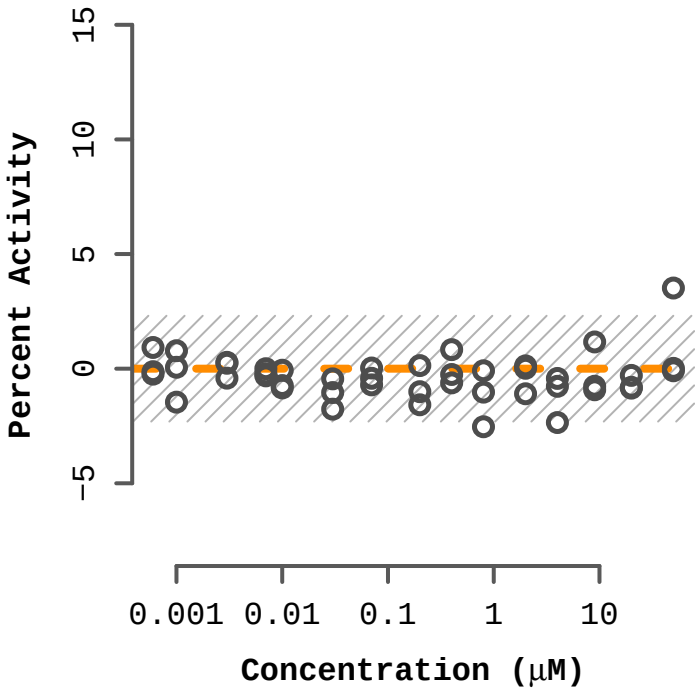
NAME: Metronidazole
CHID: 20892 **CASRN:** 443-48-1
SPID(S): Tox21_202413
M4ID: 12479839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

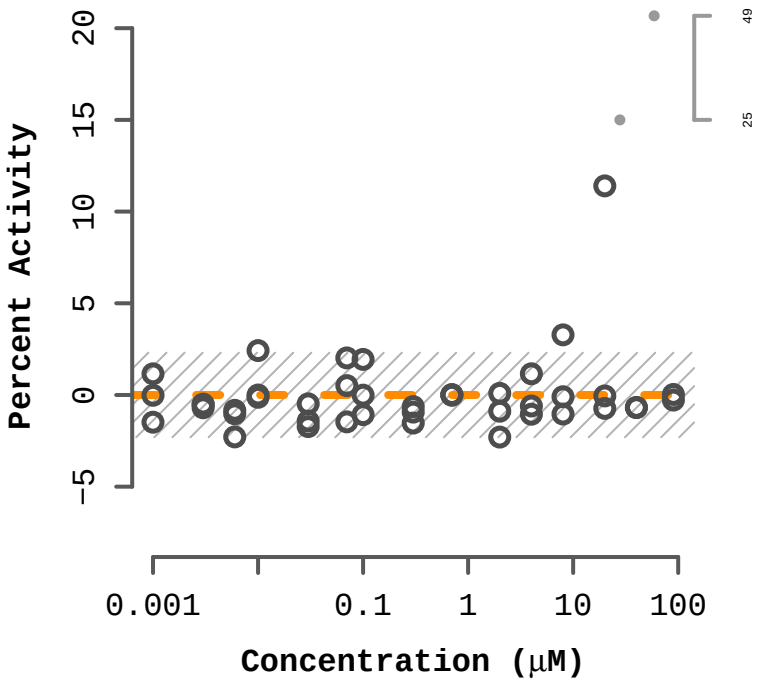
NAME: Metronidazole
CHID: 20892 **CASRN:** 443-48-1
SPID(S): Tox21_110441_1
M4ID: 12484354

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.237 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

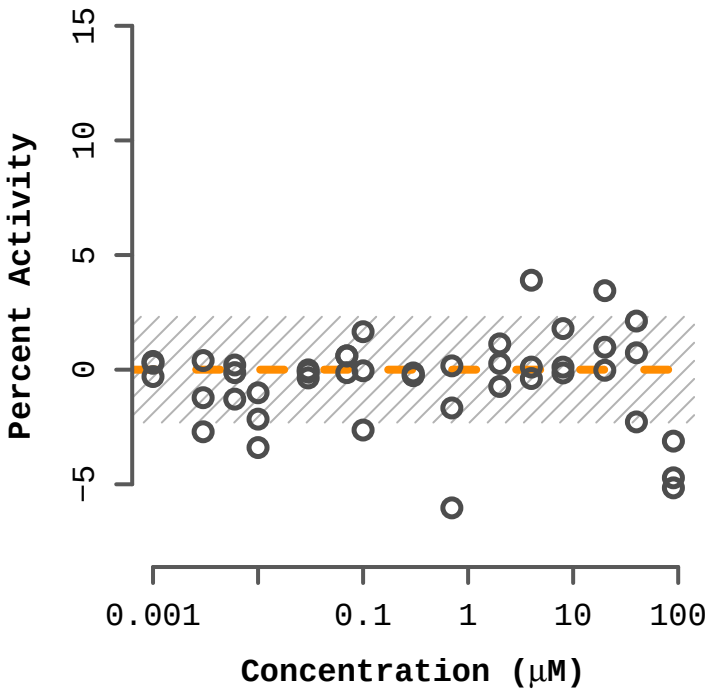
NAME: Mexacarbate
CHID: 20893 CASRN: 315-18-4
SPID(S): Tox21_200649
M4ID: 12481603 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.76	NA	NA
PROB:	1	NA	NA
RMSE:	8.43	NA	NA

MAX_MEAN: 16.1 MAX_MED: 0.513 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

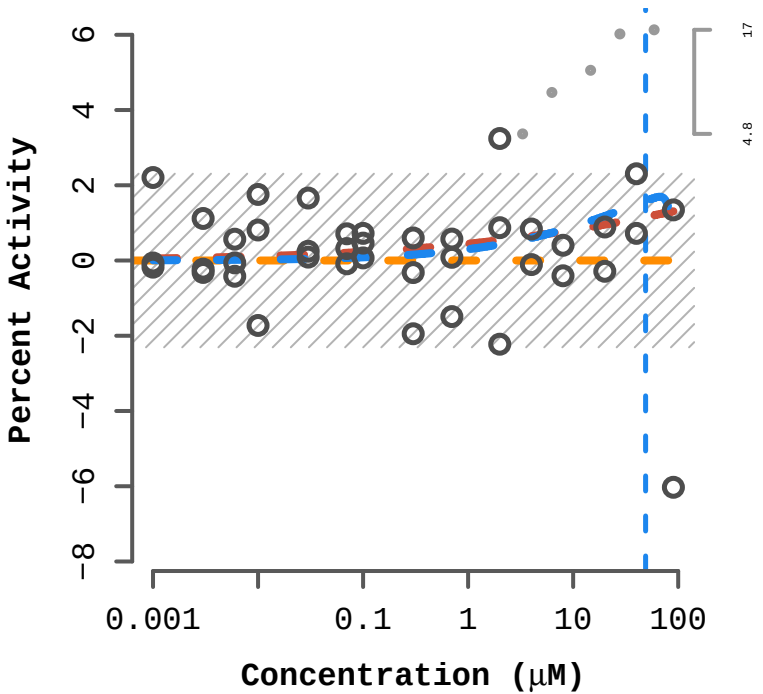
NAME: Michler's ketone
CHID: 20894 CASRN: 90-94-8
SPID(S): Tox21_300279
M4ID: 12478851

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.76	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 1.47 MAX_MED: 0.981 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Michler's ketone
CHID: 20894 **CASRN:** 90-94-8
SPID(S): Tox21_202416
M4ID: 12479836 **BRK**

HILL MODEL (in red):

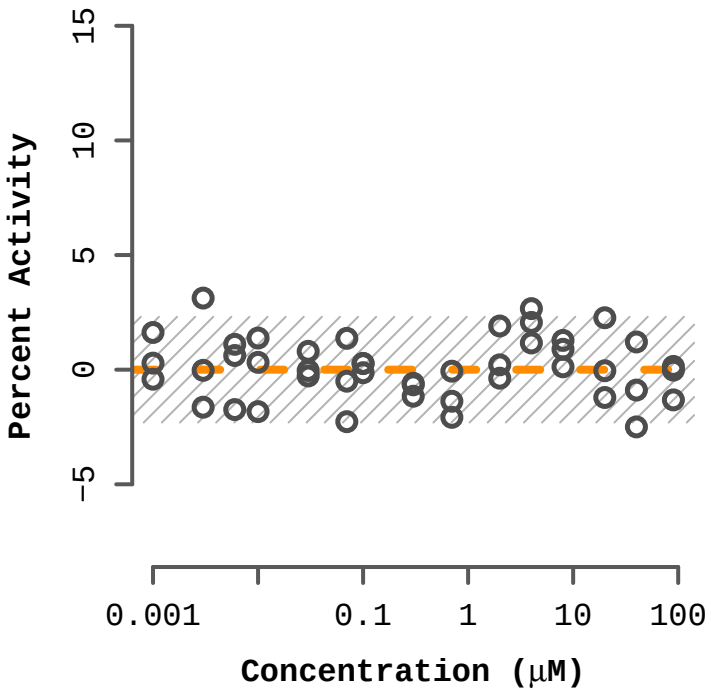
	tp	ga	gw
val:	3.21	2.45	0.323
sd:	13.3	9.57	0.539

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.17	1.69	0.58	1.94	14.7
sd:	11.5	4.87	1.07	0.138	179

	CNST	HILL	GNLS
AIC:	225.74	227.42	231.19
PROB:	0.67	0.29	0.04
RMSE:	4.56	4.28	4.27

MAX_MEAN: 6.59 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

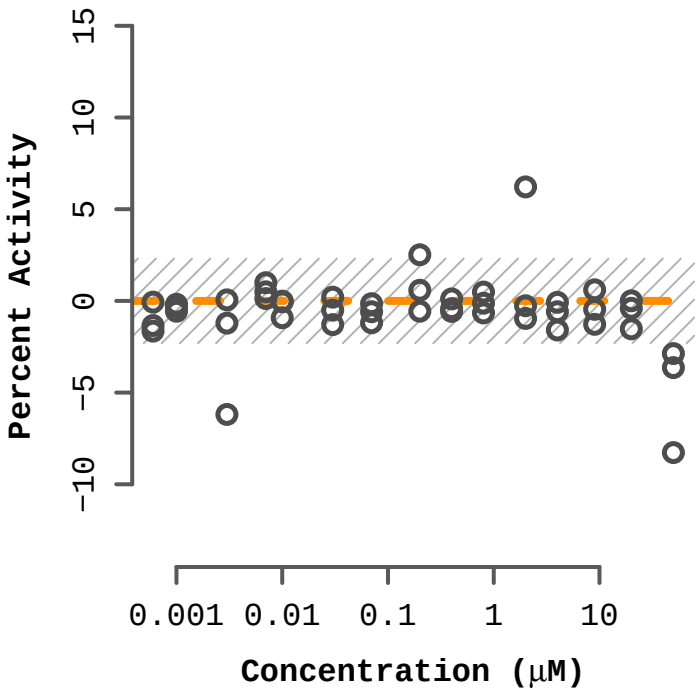
NAME: Mirex
CHID: 20895 CASRN: 2385-85-5
SPID(S): Tox21_300592
M4ID: 12478541

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

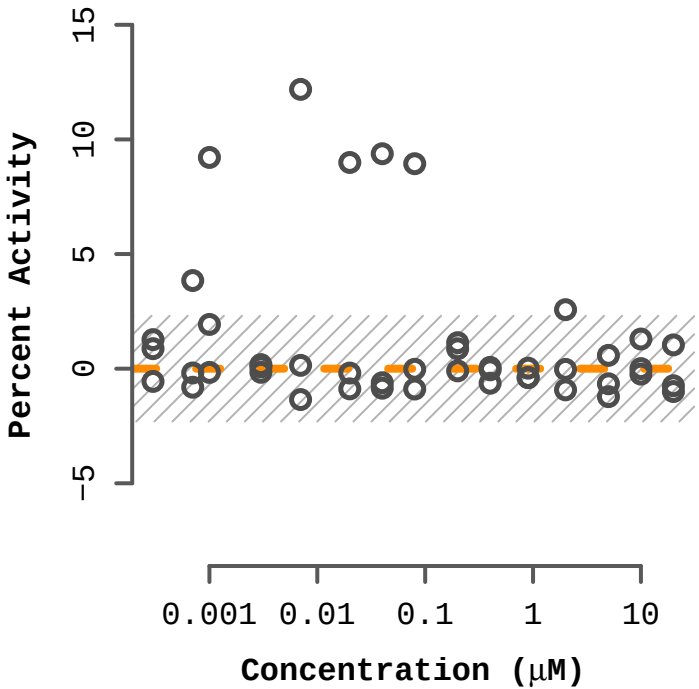
NAME: Mitomycin C
CHID: 20898 **CASRN:** 50-07-7
SPID(S): Tox21_111493_1
M4ID: 12483652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.08	NA	NA
PROB:	1	NA	NA
RMSE:	2.09	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 0.582 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

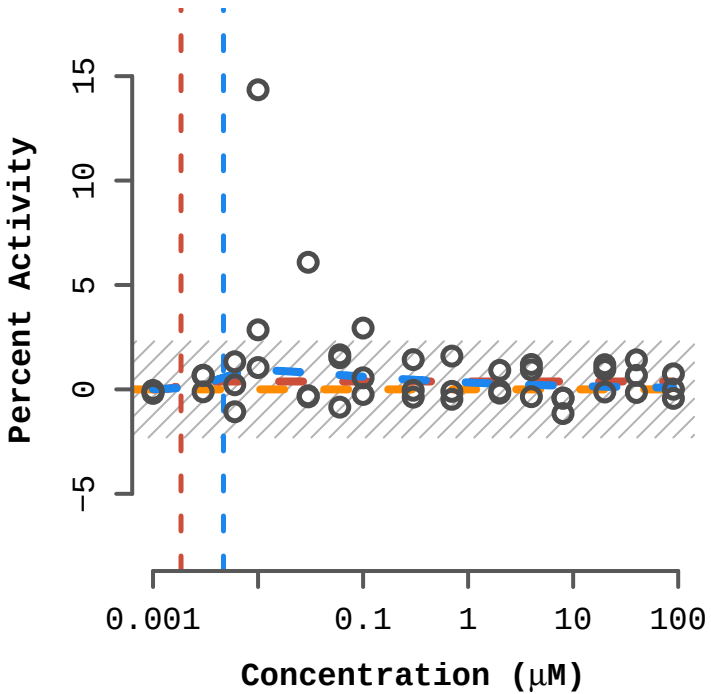
NAME: Molybdenum trioxide
CHID: 20899 CASRN: 1313-27-5
SPID(S): Tox21_202785
M4ID: 12479467

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.09	NA	NA
PROB:	1	NA	NA
RMSE:	3.42	NA	NA

MAX_MEAN: 3.66 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloroacetic acid
CHID: 20901 CASRN: 79-11-8
SPID(S): Tox21_201114
M4ID: 12481138

HILL MODEL (in red):

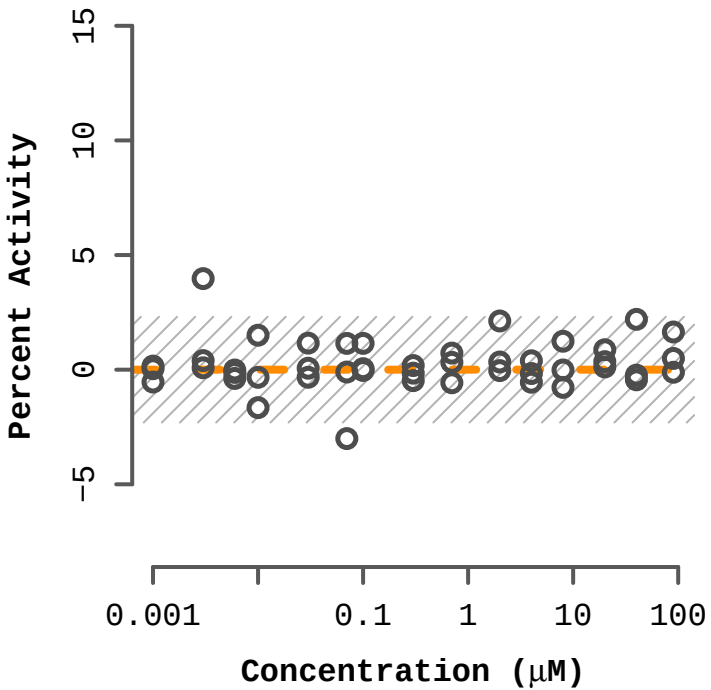
	tp	ga	gw
val:	0.378	−2.73	8
sd:	0.165	0.94	31.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.05	−2.33	2.92	−2.08	0.344
sd:	9.29	1	3.67	7.21	0.507

	CNST	HILL	GNLS
AIC:	161.04	161.65	164.51
PROB:	0.52	0.39	0.09
RMSE:	2.52	2.42	2.33

MAX_MEAN: 6.08 **MAX_MED:** 2.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

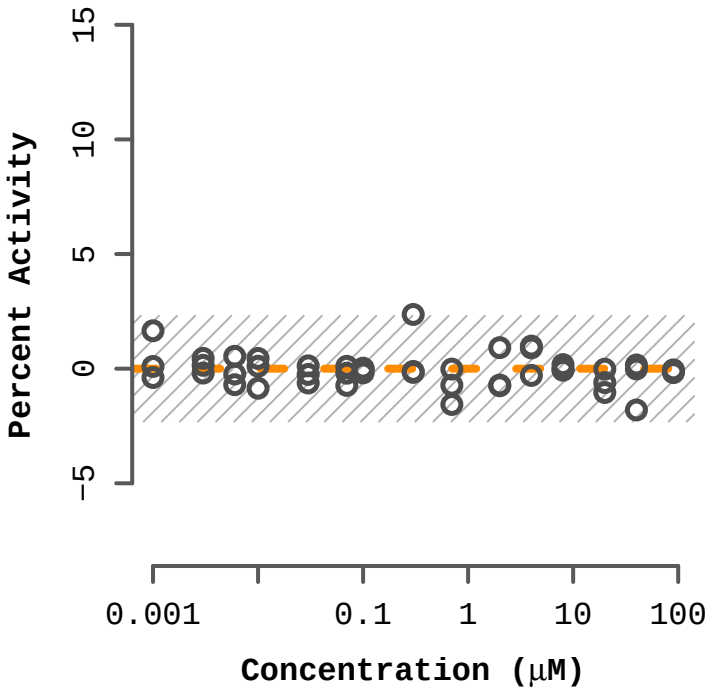
NAME: Monocrotaline
CHID: 20902 CASRN: 315-22-0
SPID(S): Tox21_302874
M4ID: 12476259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.49 MAX_MED: 0.491 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

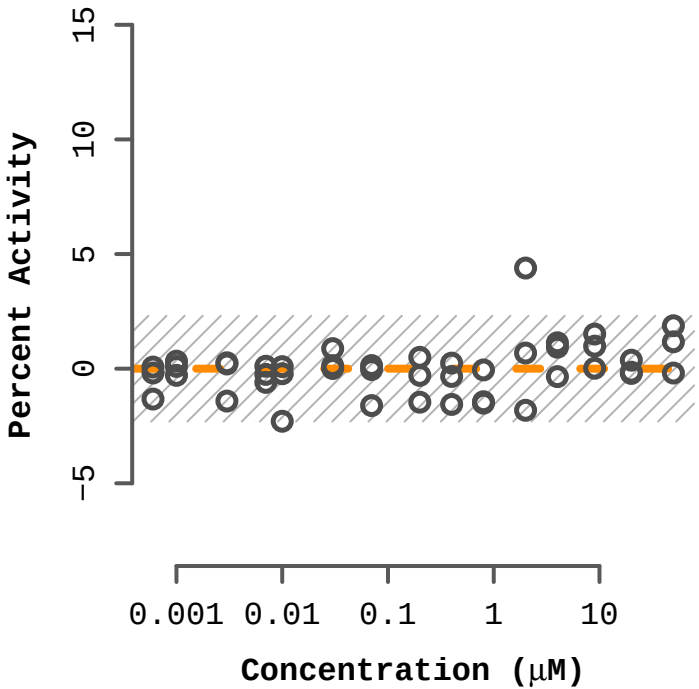
NAME: Monocrotaline
CHID: 20902 CASRN: 315-22-0
SPID(S): Tox21_201509
M4ID: 12480743

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.695 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

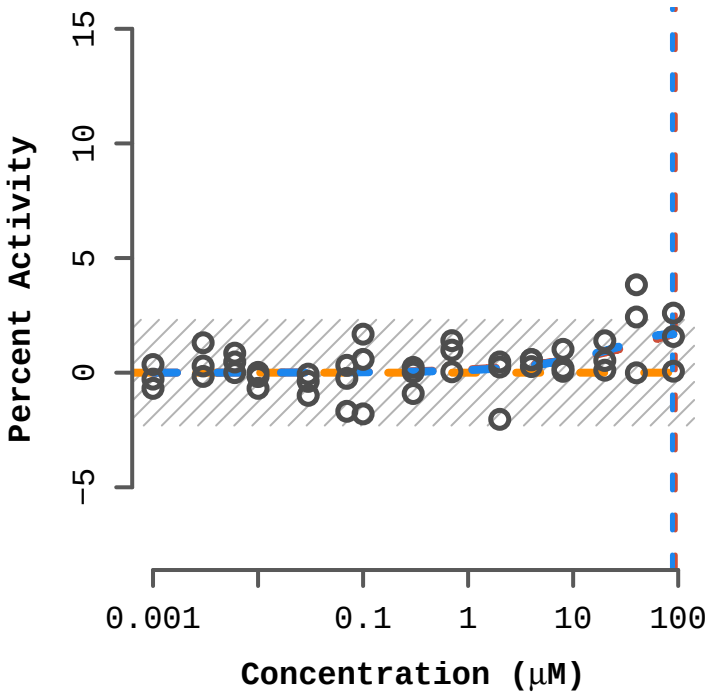
NAME: Monocrotaline
CHID: 20902 **CASRN:** 315-22-0
SPID(S): Tox21_112094_1
M4ID: 12483325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Busulfan
CHID: 20910 CASRN: 55-98-1
SPID(S): Tox21_300318
M4ID: 12478813

HILL MODEL (in red):

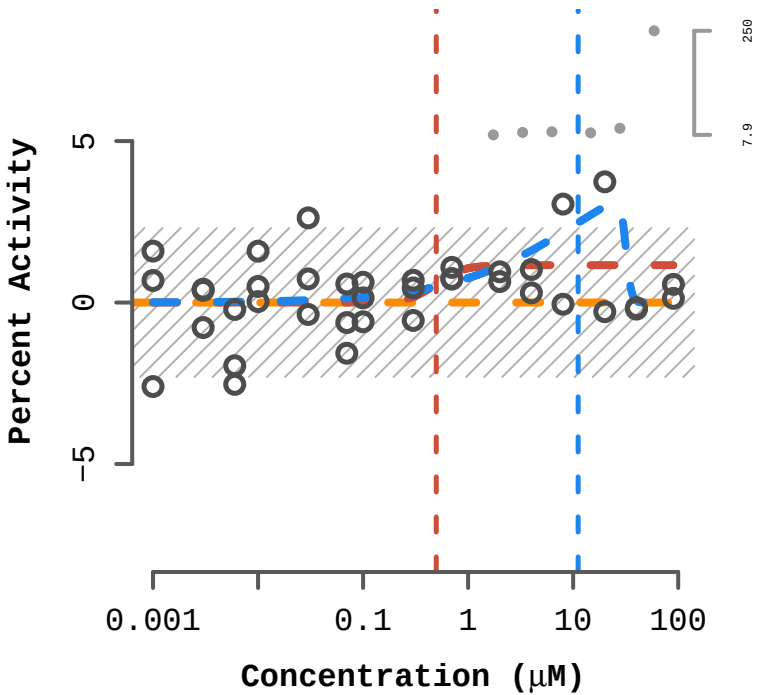
	tp	ga	gw
val:	3.43	1.97	0.691
sd:	8.43	2.95	0.753

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.09	1.95	0.802	2.2	2.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	134.25	126.28	130.1
PROB:	0.02	0.86	0.13
RMSE:	1.12	0.92	0.91

MAX_MEAN: 2.09 MAX_MED: 2.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Busulfan
CHID: 20910 CASRN: 55-98-1
SPID(S): Tox21_201848
M4ID: 12480404 BRK

HILL MODEL (in red):

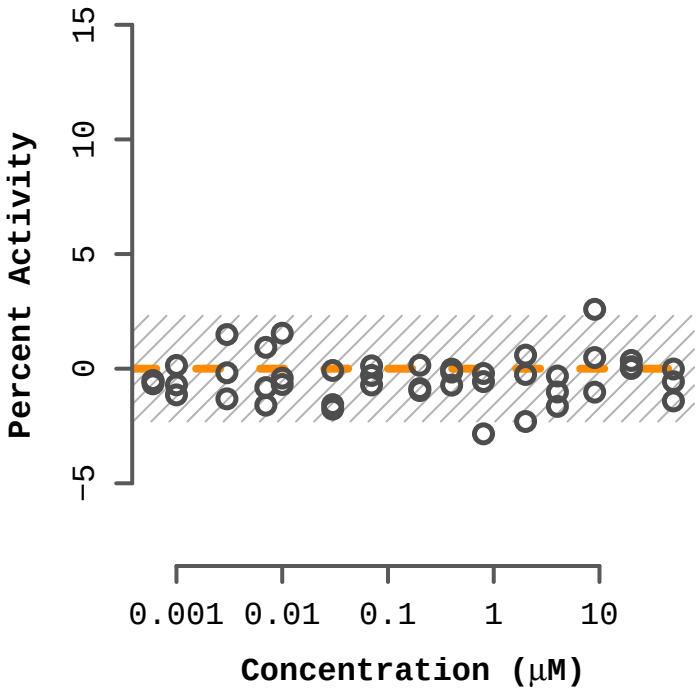
	tp	ga	gw
val:	1.16	−0.303	3.42
sd:	0.582	0.524	7.55

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.94	1.05	0.709	1.5	17.5
sd:	13.9	3.4	0.912	0.858	148

	CNST	HILL	GNLS
AIC:	275.29	275.48	276.87
PROB:	0.42	0.38	0.19
RMSE:	38.35	38.13	38.3

MAX_MEAN: 85.2 MAX_MED: 3.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

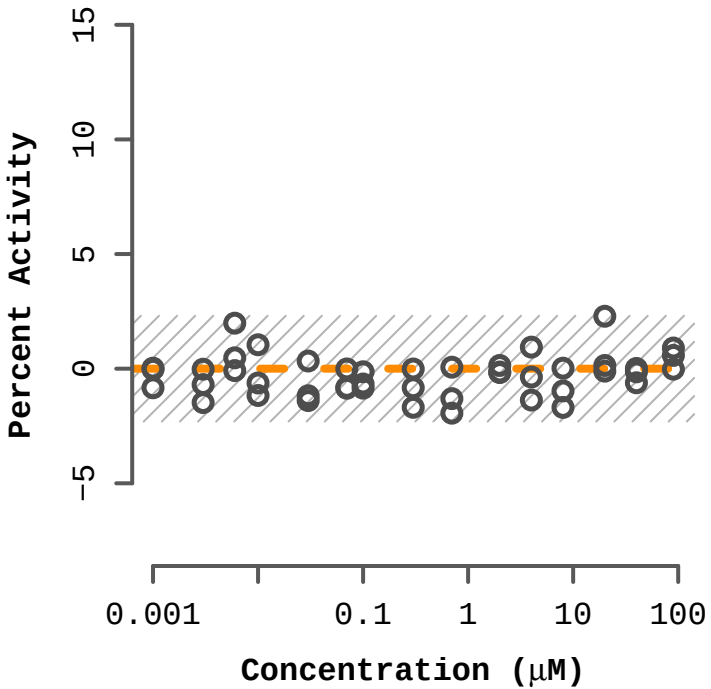
NAME: Busulfan
CHID: 20910 CASRN: 55-98-1
SPID(S): Tox21_111038_1
M4ID: 12483935

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.685 **MAX_MED:** 0.486 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

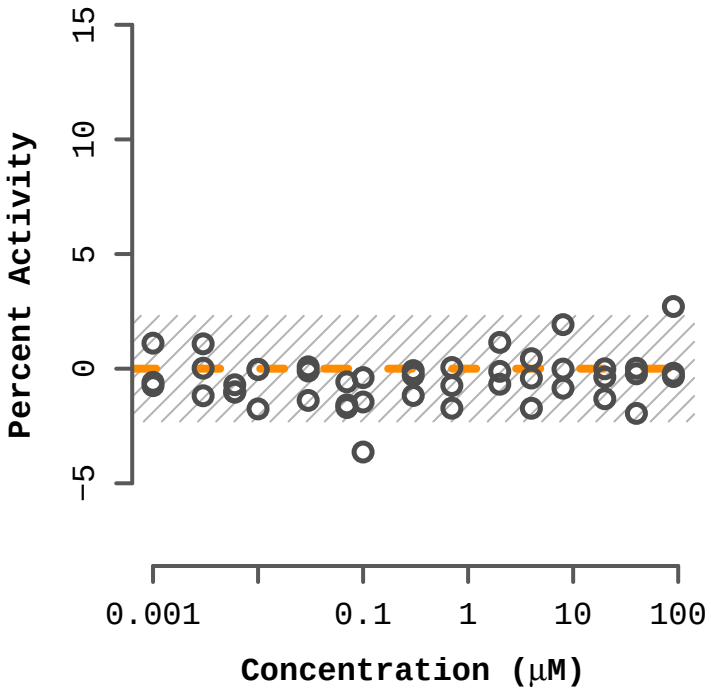
NAME: Nalidixic acid
CHID: 20912 **CASRN:** 389-08-2
SPID(S): Tox21_302754
M4ID: 12476379

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 0.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

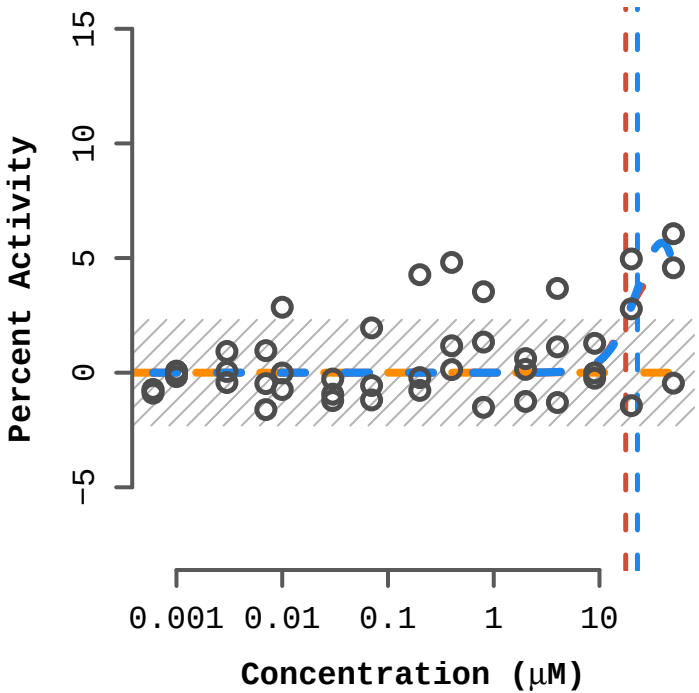
NAME: Nalidixic acid
CHID: 20912 **CASRN:** 389-08-2
SPID(S): Tox21_201477
M4ID: 12480775

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.724 **MAX_MED:** 0.0226 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nalidixic acid
CHID: 20912 **CASRN:** 389-08-2
SPID(S): Tox21_110835_1
M4ID: 12484082

HILL MODEL (in red):

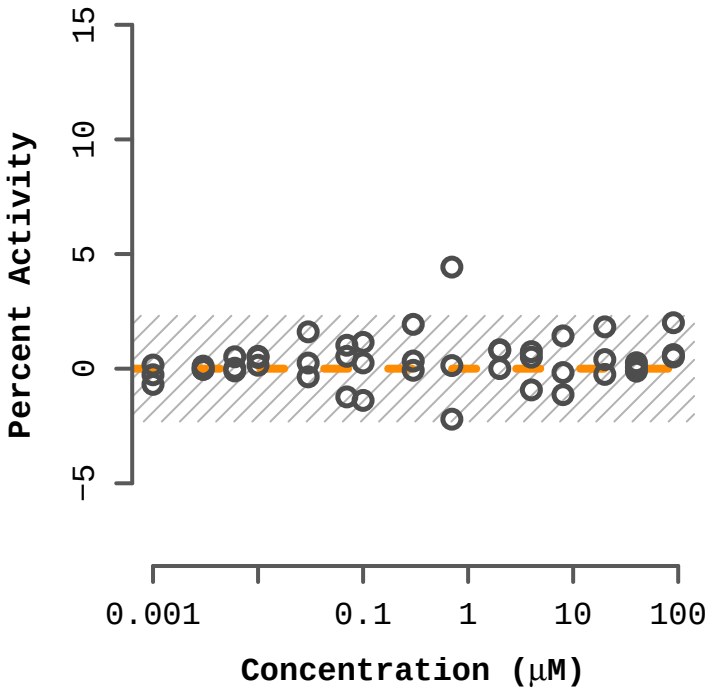
	tp	ga	gw
val:	4.75	1.25	3.67
sd:	1.22	0.134	3.55

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.28	1.36	3.08	1.75	7.03
sd:	385	13.1	46.6	3.28	737

	CNST	HILL	GNLS
AIC:	189.95	185.09	189.07
PROB:	0.07	0.82	0.11
RMSE:	2.09	1.85	1.85

MAX_MEAN: 3.4 **MAX_MED:** 4.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

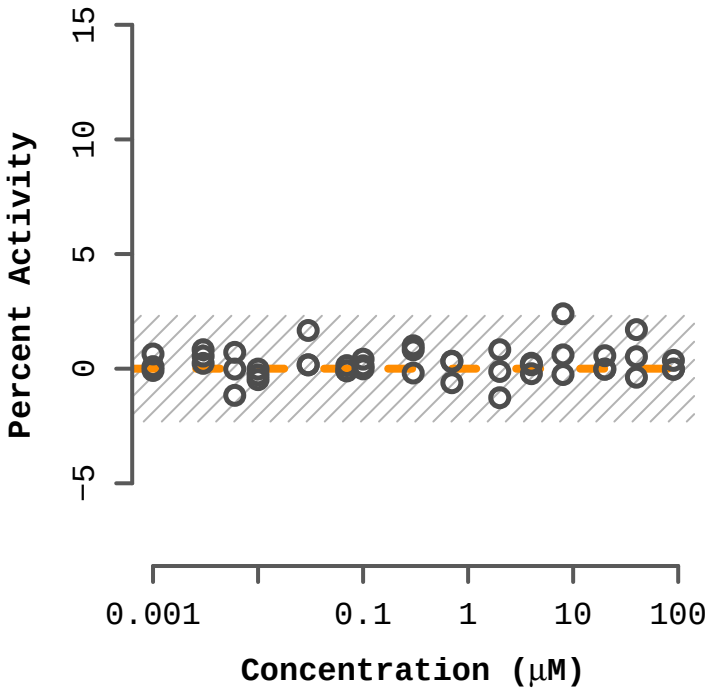
NAME: Naphthalene
CHID: 20913 CASRN: 91-20-3
SPID(S): Tox21_300008
M4ID: 12479122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.04 MAX_MED: 0.801 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

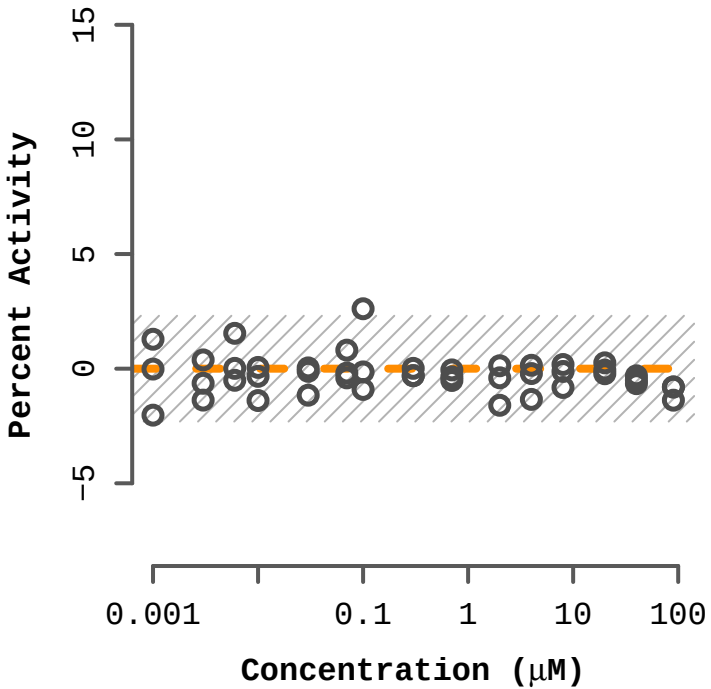
NAME: Naphthalene
CHID: 20913 CASRN: 91-20-3
SPID(S): Tox21_202004
M4ID: 12480248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.915 MAX_MED: 0.823 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

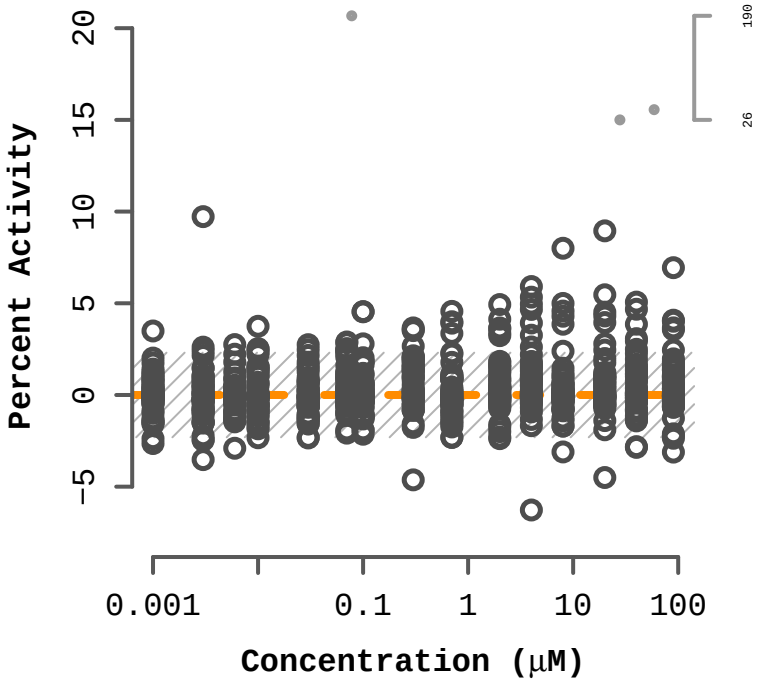
NAME: 1-Naphthaleneacetamide
CHID: 20914 **CASRN:** 86-86-2
SPID(S): Tox21_200049
M4ID: 12482203

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.524 **MAX_MED:** 0.015 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

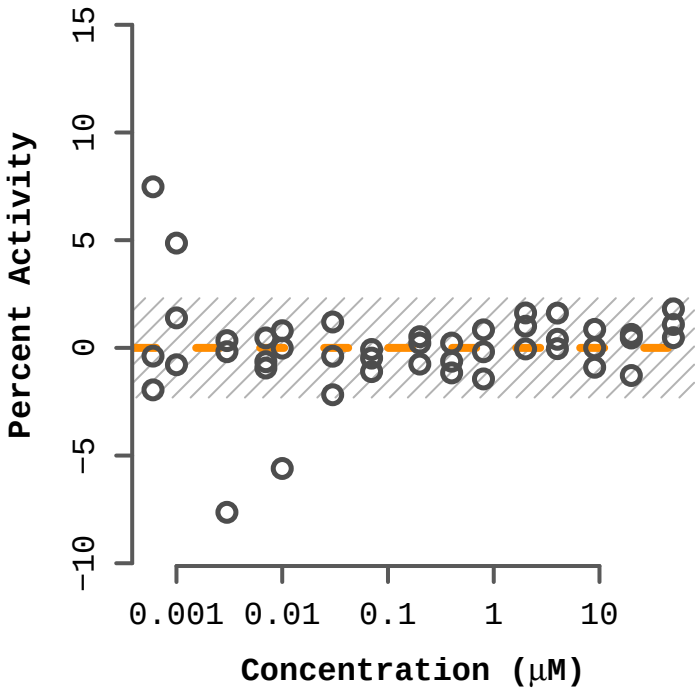
NAME: 1-Naphthaleneacetic acid
CHID: 20915 **CASRN:** 86-87-3
SPID(S): Tox21_400007
M4ID: 12475130 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2649.34	NA	NA
PROB:	1	NA	NA
RMSE:	7.63	NA	NA

MAX_MEAN: 4.39 **MAX_MED:** 0.435 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

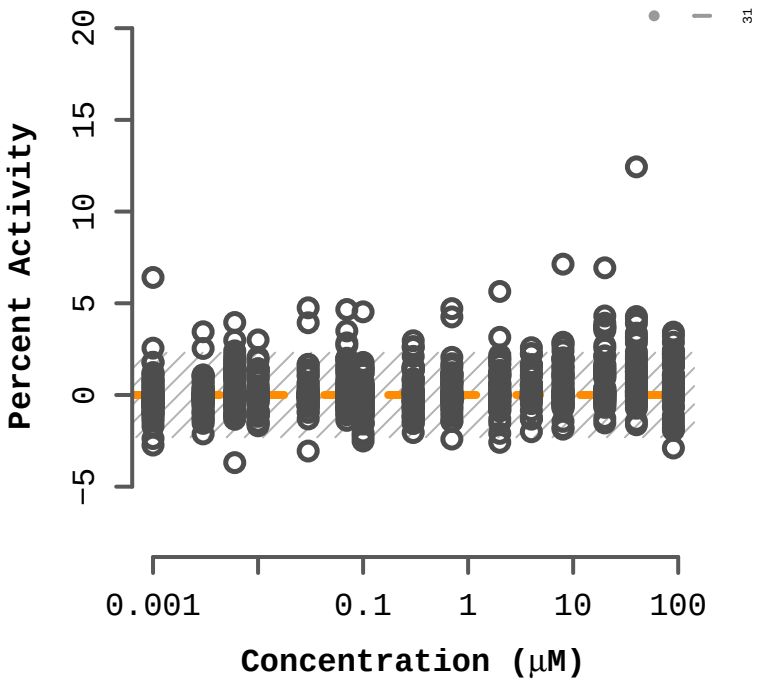
NAME: 1-Naphthaleneacetic acid
CHID: 20915 **CASRN:** 86-87-3
SPID(S): Tox21_111051_1
M4ID: 12483931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.97	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

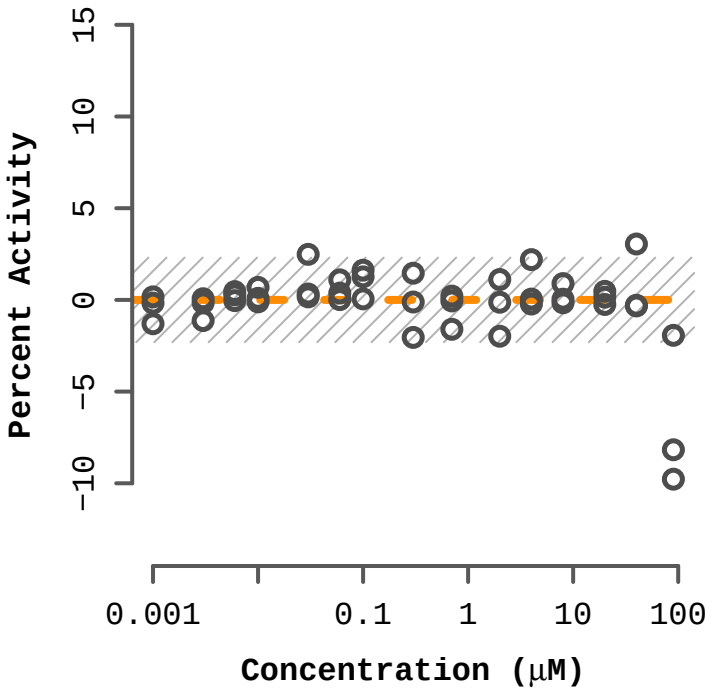
NAME: 1,5-Naphthalenediamine
CHID: 20916 **CASRN:** 2243-62-1
SPID(S): Tox21_400040
M4ID: 12475097 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2486.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.865 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

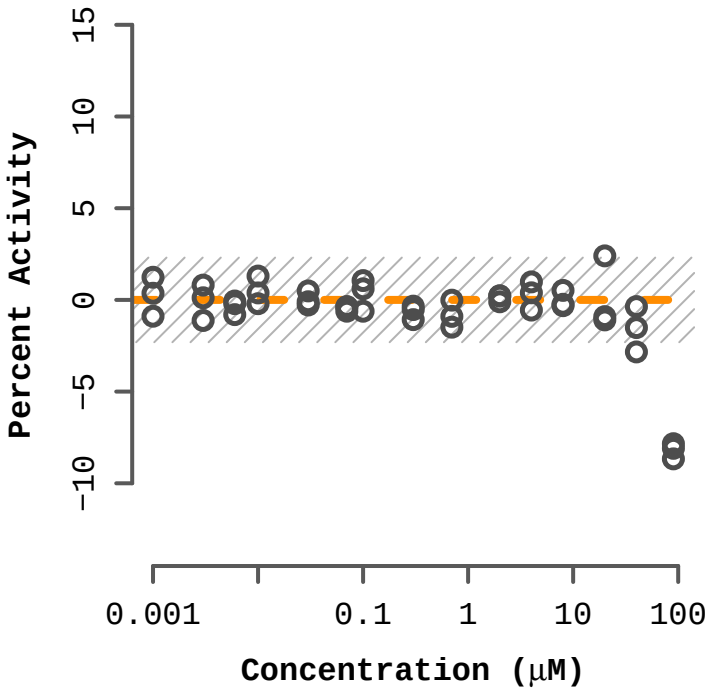
NAME: N-(1-Naphthyl)ethylenediamine dihydrochloride
CHID: 20917 **CASRN:** 1465-25-4
SPID(S): Tox21_302783
M4ID: 12476350

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 0.992 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

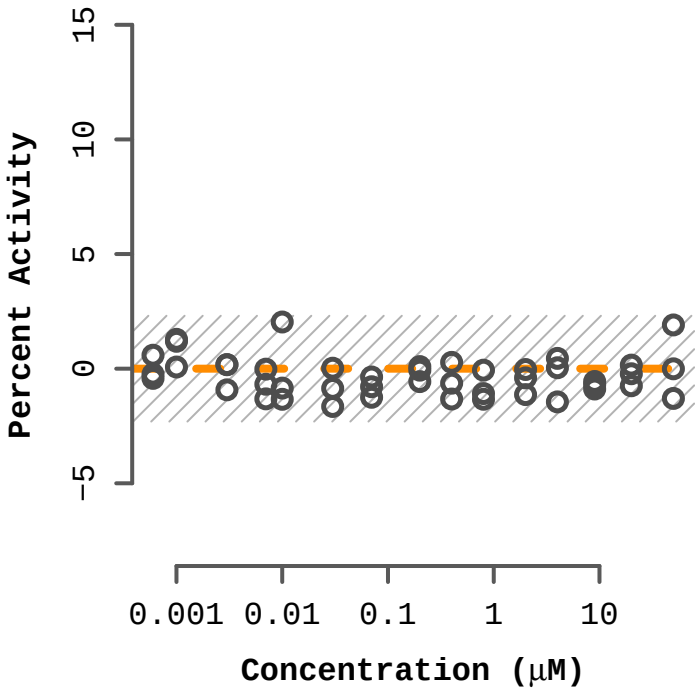
NAME: N-(1-Naphthyl)ethylenediamine dihydrochloride
CHID: 20917 CASRN: 1465-25-4
SPID(S): Tox21_201928
M4ID: 12480324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 0.493 **MAX_MED:** 0.606 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

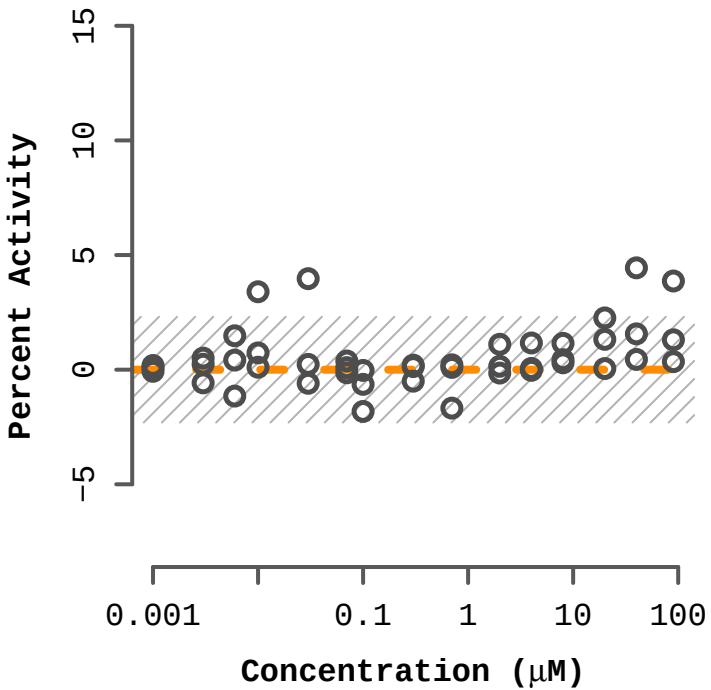
NAME: N−(1−Naphthyl)ethylenediamine dihydrochloride
CHID: 20917 CASRN: 1465−25−4
SPID(S): Tox21_111184_1
M4ID: 12483860

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

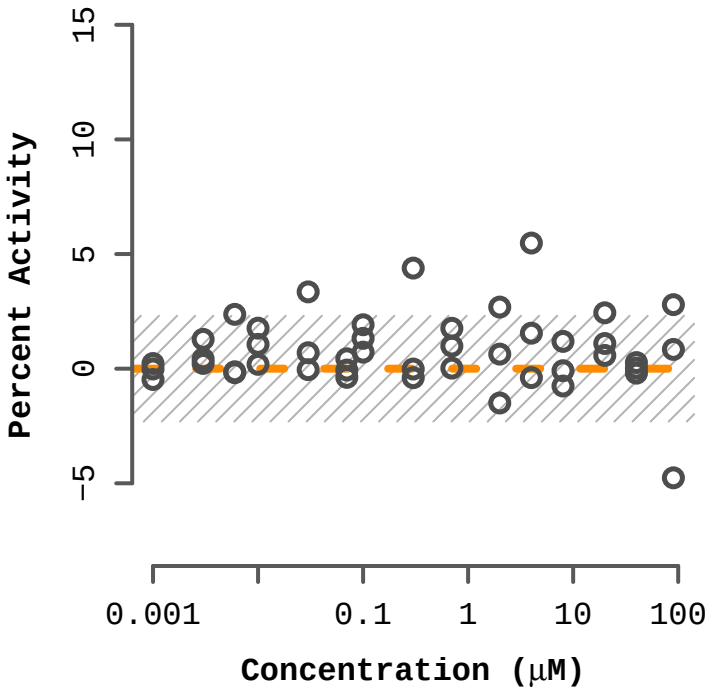
NAME: N,N'−Di−2−naphthyl−p−phenylenediamine
CHID: 20918 CASRN: 93−46−9
SPID(S): Tox21_302849
M4ID: 12476284

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

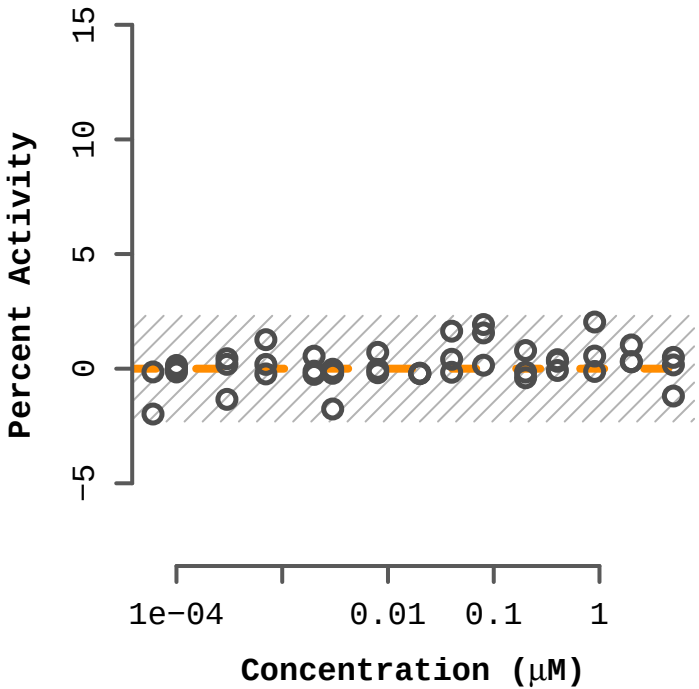
NAME: N,N'−Di−2−naphthyl−p−phenylenediamine
CHID: 20918 CASRN: 93−46−9
SPID(S): Tox21_202063
M4ID: 12480189

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

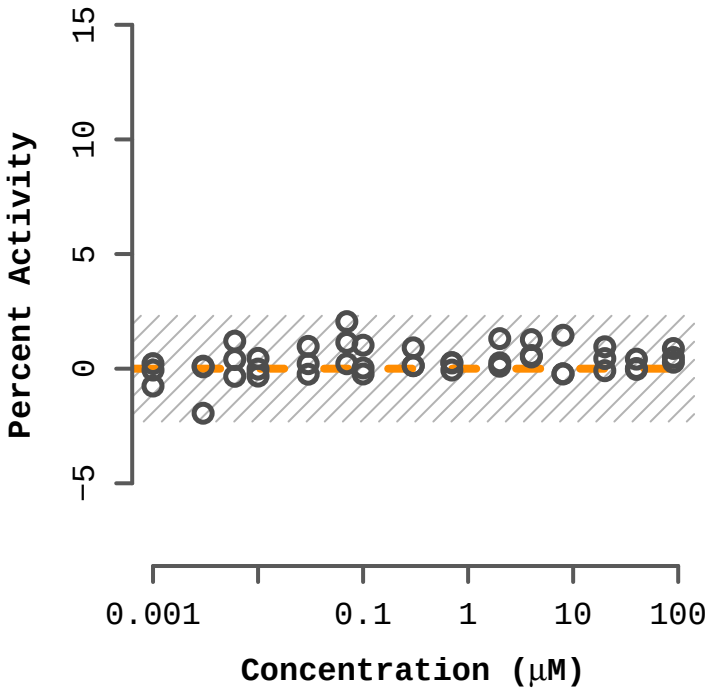
NAME: 1-(1-Naphthyl)-2-thiourea
CHID: 20919 **CASRN:** 86-88-4
SPID(S): Tox21_203002
M4ID: 12479250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

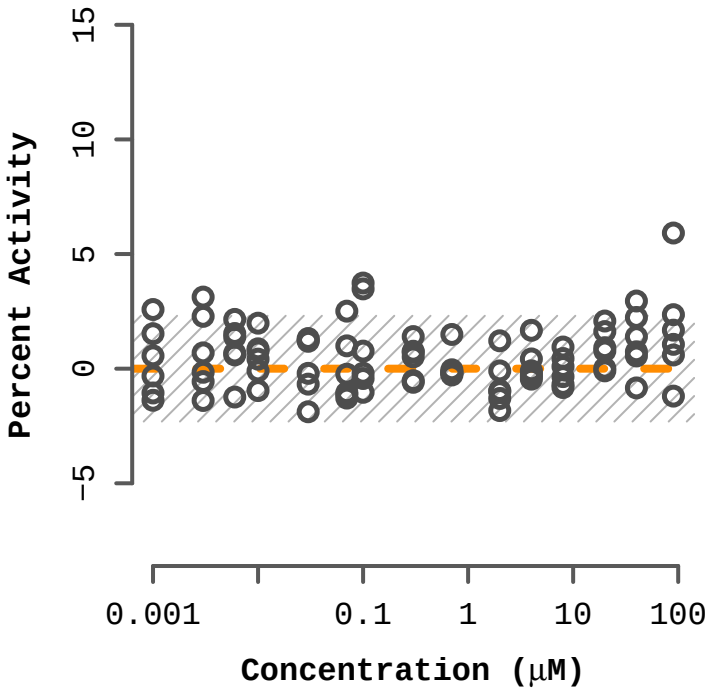
NAME: 1-Naphthylamine
CHID: 20920 **CASRN:** 134-32-7
SPID(S): Tox21_302805
M4ID: 12476328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

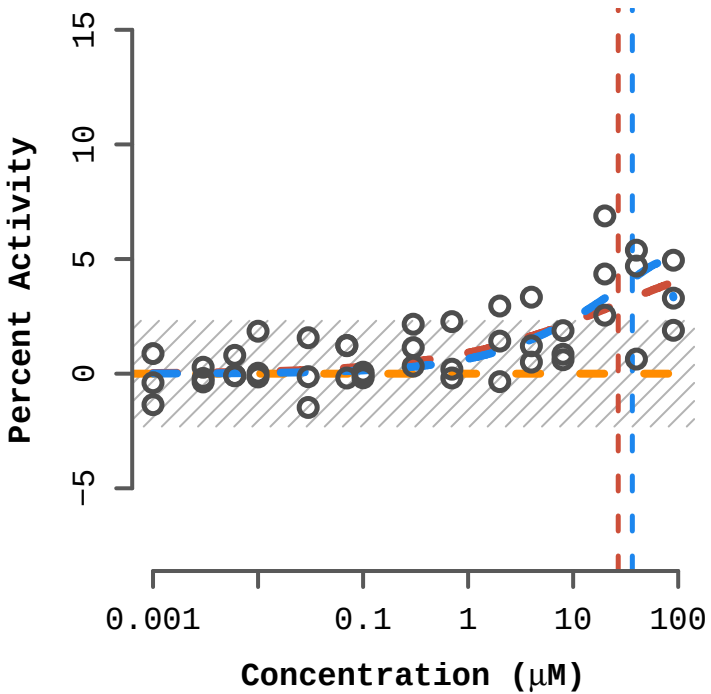
NAME: 1-Naphthylamine
CHID: 20920 **CASRN:** 134-32-7
SPID(S): Tox21_201233
M4ID: 12481019

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	318.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Naphthylamine
CHID: 20921 **CASRN:** 91-59-8
SPID(S): Tox21_300048
M4ID: 12479082

HILL MODEL (in red):

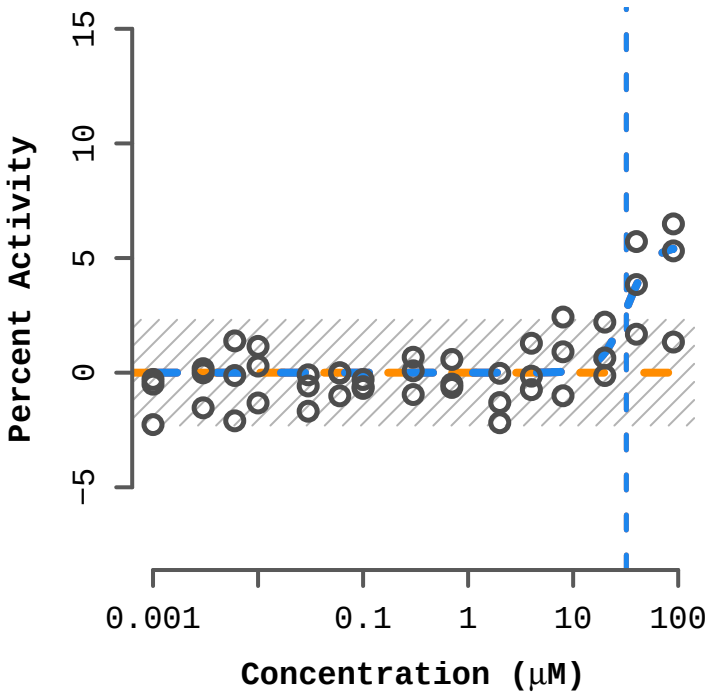
	tp	ga	gw
val:	6.1	1.43	0.528
sd:	4.55	1.33	0.301

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.26	1.56	0.683	1.97	10.3
sd:	4.17	0.647	0.341	0.0598	29.4

	CNST	HILL	GNLS
AIC:	194.34	157.53	158.94
PROB:	0	0.67	0.33
RMSE:	2.2	1.27	1.25

MAX_MEAN: 4.6 **MAX_MED:** 4.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Naphthylamine
CHID: 20921 CASRN: 91-59-8
SPID(S): Tox21_202091
M4ID: 12480161

HILL MODEL (in red):

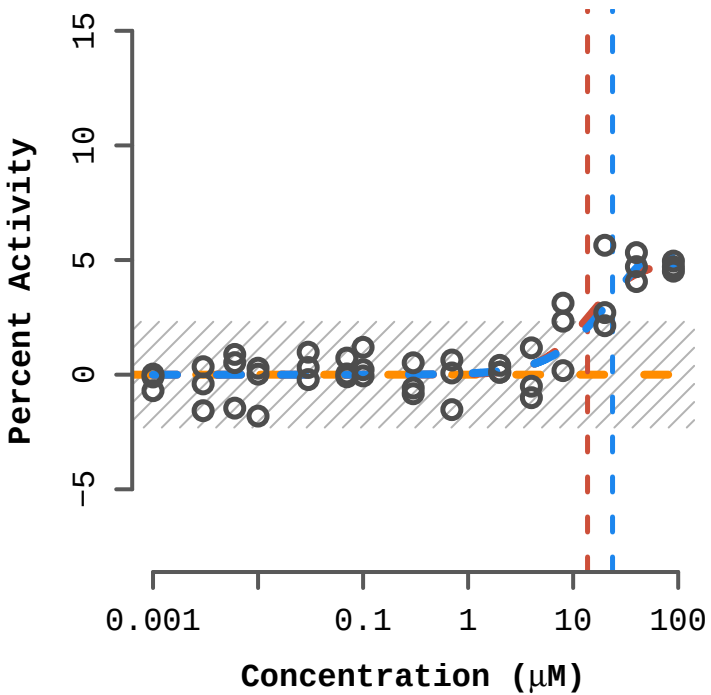
	tp	ga	gw
val:	5.54	1.51	3.56
sd:	0.982	0.0946	2.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.54	1.51	3.56	3.6	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	177.56	154.35	158.35
PROB:	0	0.88	0.12
RMSE:	1.94	1.25	1.25

MAX_MEAN: 4.38 MAX_MED: 5.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-1-naphthalenesulfonic acid
CHID: 20922 **CASRN:** 81-16-3
SPID(S): Tox21_200507
M4ID: 12481745

HILL MODEL (in red):

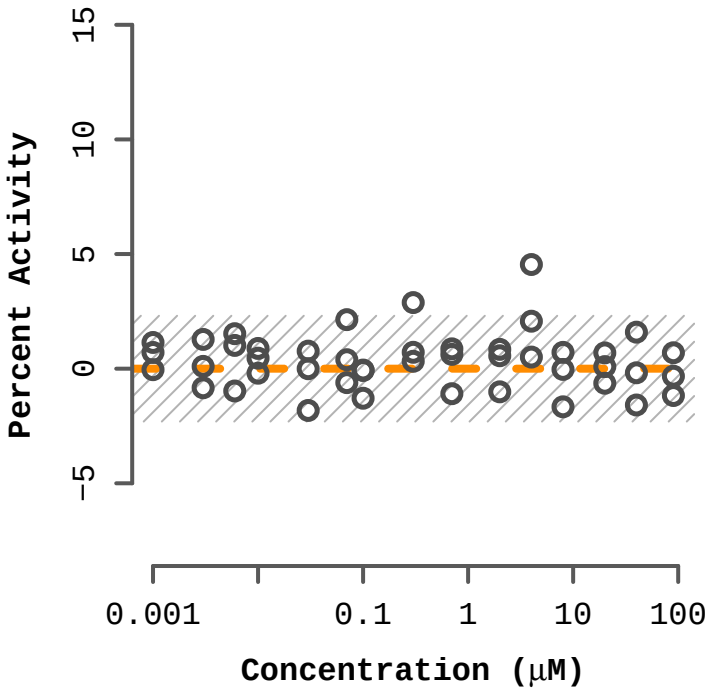
	tp	ga	gw
val:	4.95	1.14	1.93
sd:	0.484	0.164	0.664

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.77	1.37	1.5	2	12.4
sd:	4.06	0.418	0.741	0.0236	14.3

	CNST	HILL	GNLS
AIC:	192.61	124.84	128.05
PROB:	0	0.83	0.17
RMSE:	2.18	0.88	0.89

MAX_MEAN: 4.73 **MAX_MED:** 4.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

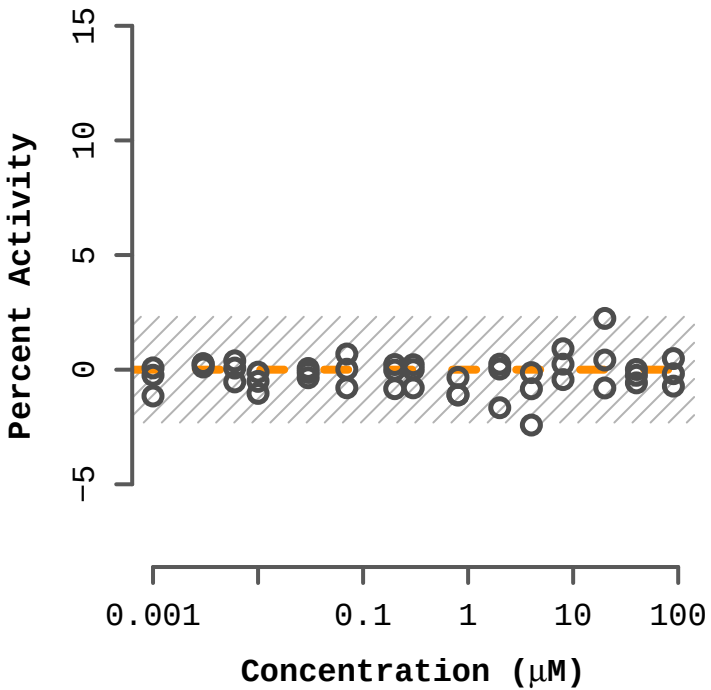
NAME: Nefiracetam
CHID: 20923 CASRN: 77191-36-7
SPID(S): Tox21_303025
M4ID: 12476108

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 2.37 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

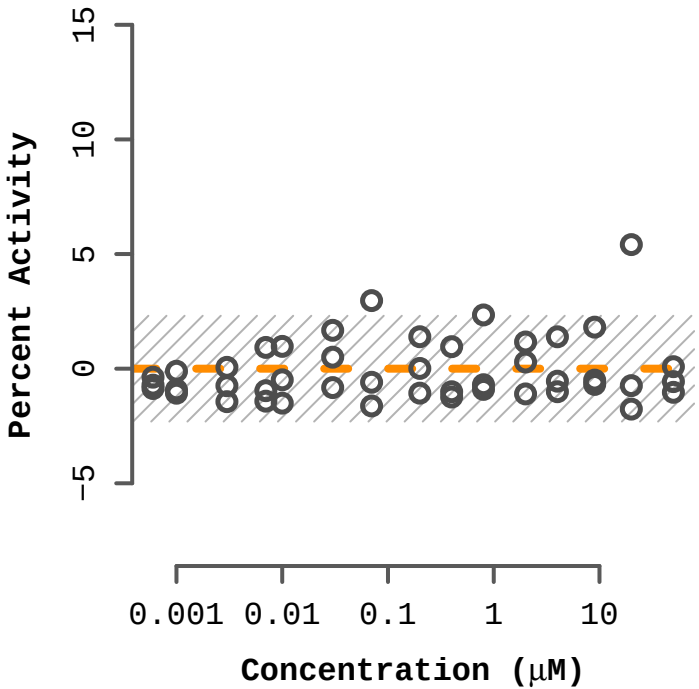
NAME: Nefiracetam
CHID: 20923 **CASRN:** 77191-36-7
SPID(S): Tox21_201916
M4ID: 12480336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.621 **MAX_MED:** 0.422 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

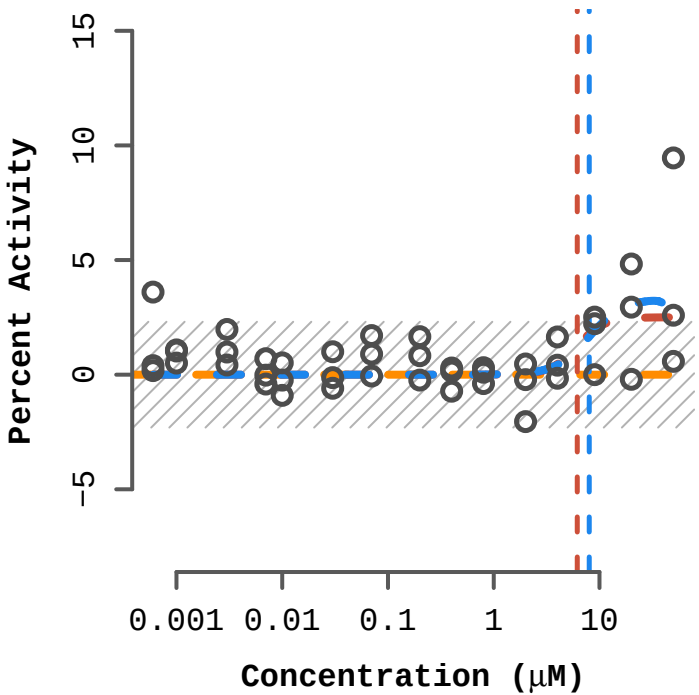
NAME: Nefiracetam
CHID: 20923 **CASRN:** 77191-36-7
SPID(S): Tox21_113521_1
M4ID: 12482622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 0.503 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nickel dibutyldithiocarbamate
CHID: 20927 CASRN: 13927-77-0
SPID(S): Tox21_202593
M4ID: 12479659

HILL MODEL (in red):

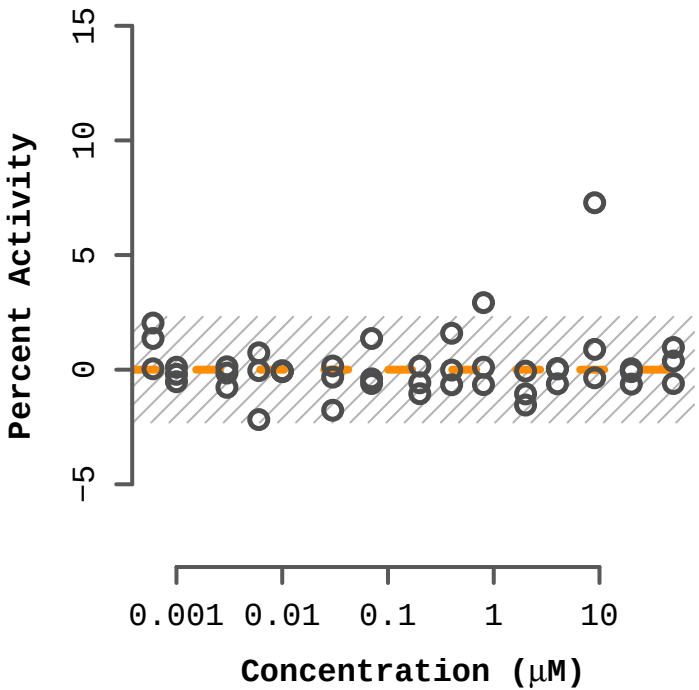
	tp	ga	gw
val:	2.5	0.79	3.45
sd:	0.708	0.188	2.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.31	0.903	2.74	1.72	10.9
sd:	1.42	0.212	1.98	0.291	143

	CNST	HILL	GNLS
AIC:	168.98	158.49	161.84
PROB:	0	0.84	0.16
RMSE:	2	1.55	1.59

MAX_MEAN: 4.21 **MAX_MED:** 2.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

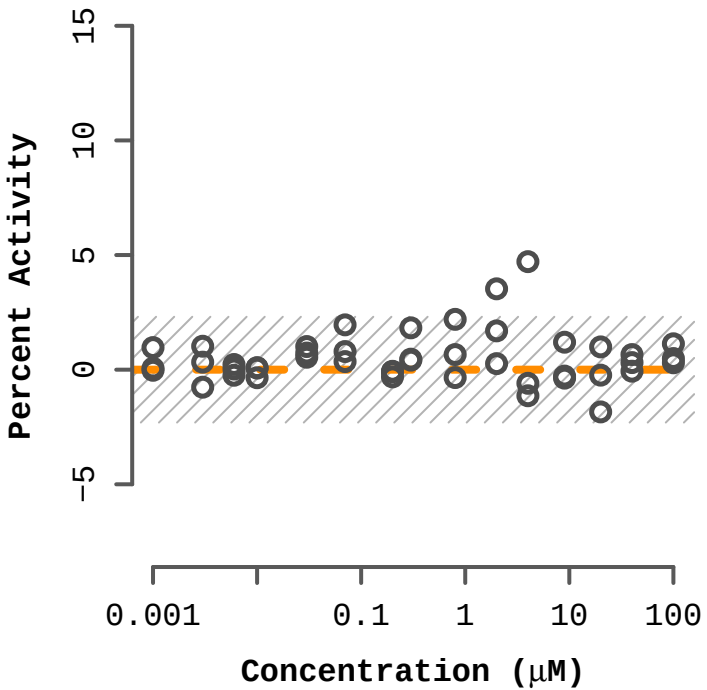
NAME: Nickel(II) sulfate hexahydrate
CHID: 20928 **CASRN:** 10101-97-0
SPID(S): Tox21_202594
M4ID: 12479658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.61 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

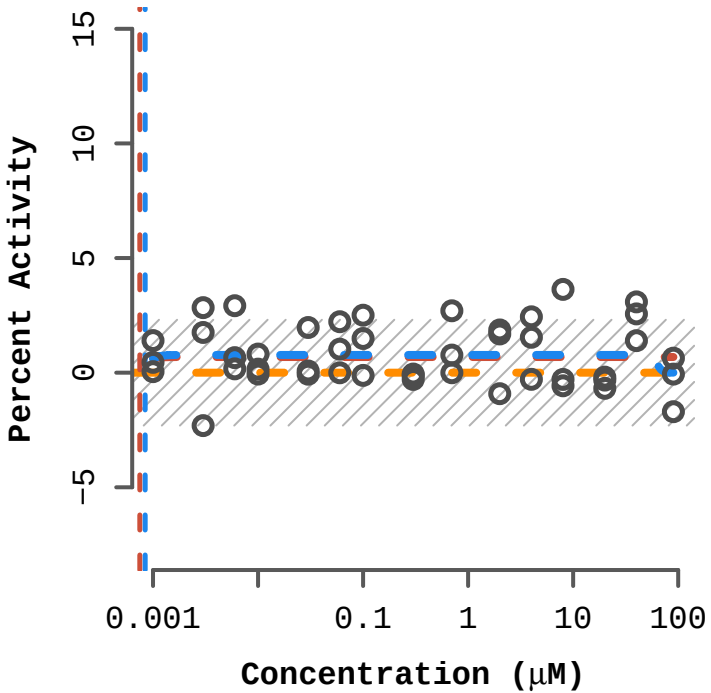
NAME: Niacinamide
CHID: 20929 **CASRN:** 98-92-0
SPID(S): Tox21_302776
M4ID: 12476357

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Niacinamide
CHID: 20929 CASRN: 98-92-0
SPID(S): Tox21_201716
M4ID: 12480536

HILL MODEL (in red):

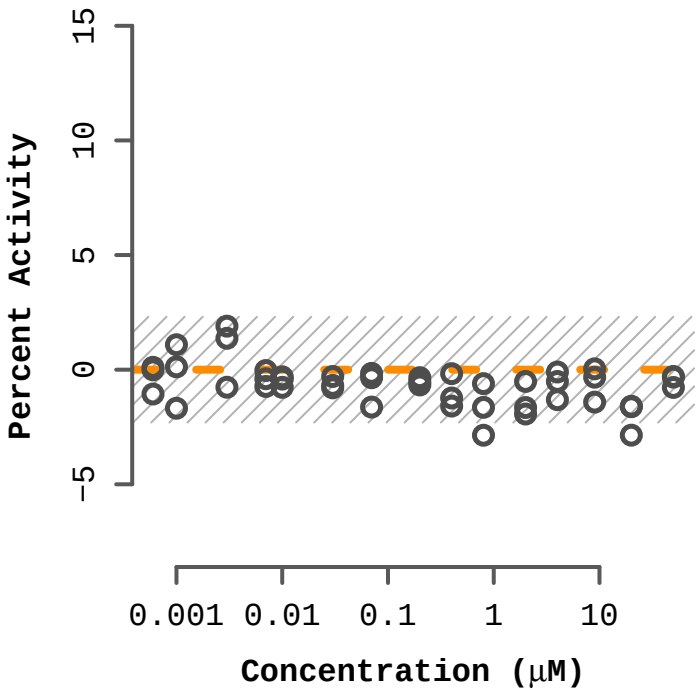
	tp	ga	gw
val:	0.683	−3.13	7.77
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.774	−3.07	7.95	1.8	17.4
sd:	0.231	6.77	707	0.618	60.6

	CNST	HILL	GNLS
AIC:	169.87	165.26	167.49
PROB:	0.07	0.7	0.23
RMSE:	1.53	1.33	1.3

MAX_MEAN: 2.35 MAX_MED: 2.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

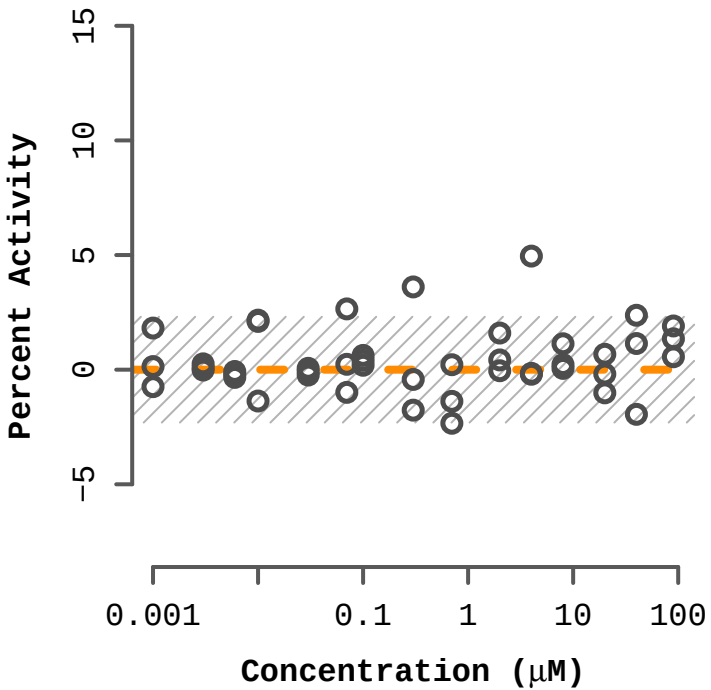
NAME: Niacinamide
CHID: 20929 **CASRN:** 98-92-0
SPID(S): Tox21_111202_1
M4ID: 12483844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.835 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

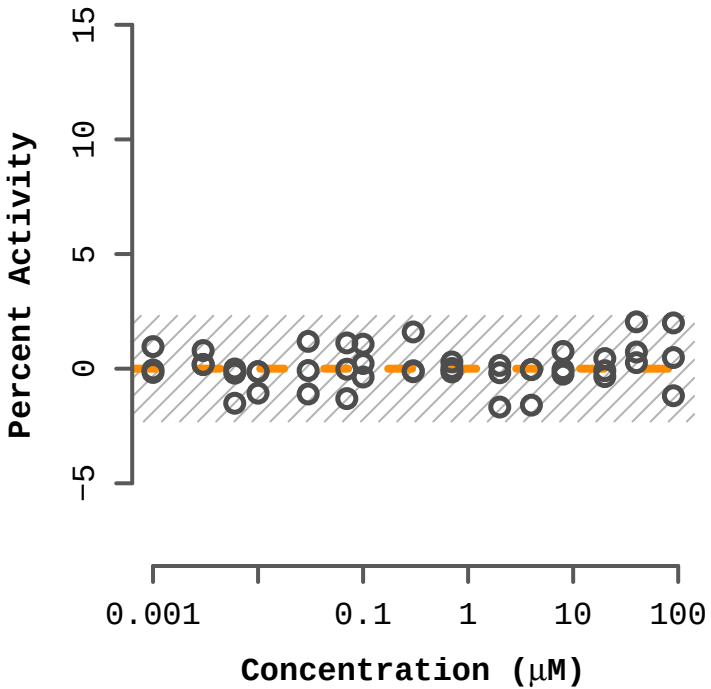
NAME: Nicotine
CHID: 20930 CASRN: 54-11-5
SPID(S): Tox21_300174
M4ID: 12478956

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.53 MAX_MED: 2.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

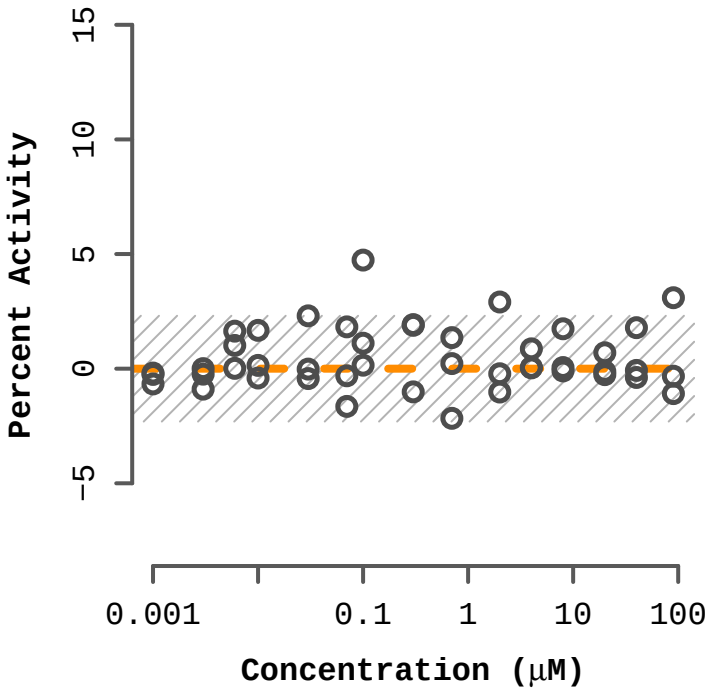
NAME: Nicotine
CHID: 20930 CASRN: 54-11-5
SPID(S): Tox21_201814
M4ID: 12480438

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.01 MAX_MED: 0.729 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

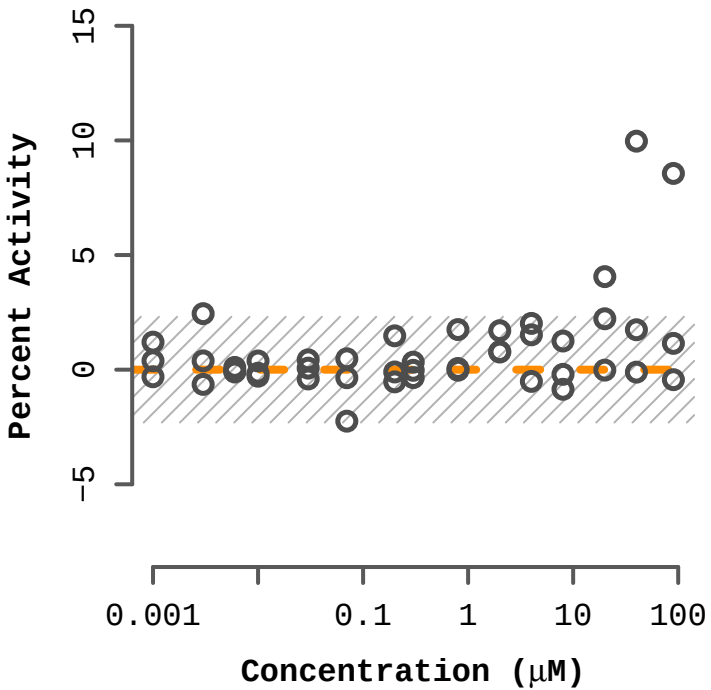
NAME: Nicotinic acid
CHID: 20932 **CASRN:** 59-67-6
SPID(S): Tox21_302904
M4ID: 12476229

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

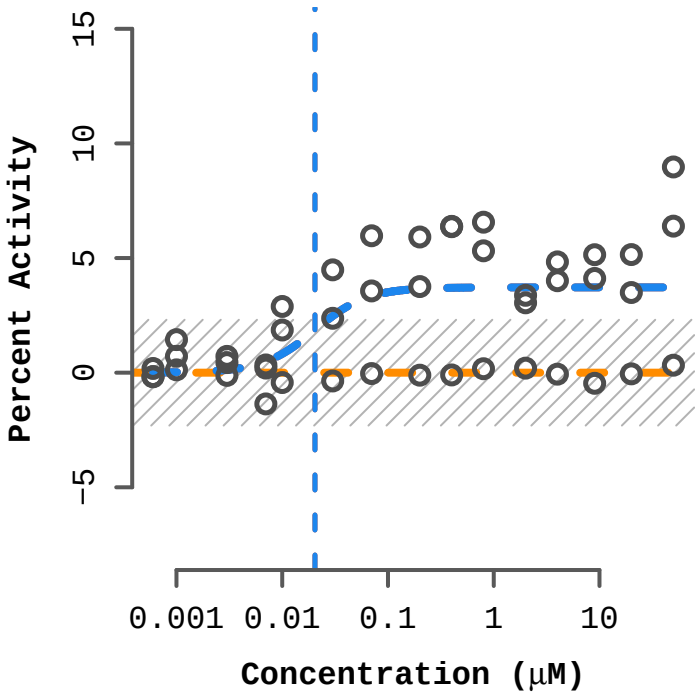
NAME: Nicotinic acid
CHID: 20932 CASRN: 59-67-6
SPID(S): Tox21_201420
M4ID: 12480832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.83	NA	NA
PROB:	1	NA	NA
RMSE:	2.27	NA	NA

MAX_MEAN: 3.87 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nicotinic acid
CHID: 20932 CASRN: 59-67-6
SPID(S): Tox21_110337_1
M4ID: 12484444

HILL MODEL (in red):

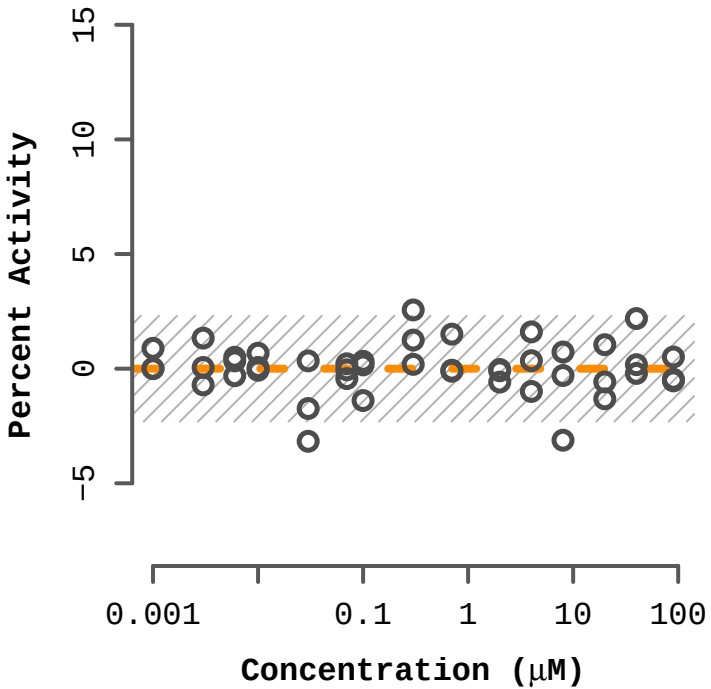
	tp	ga	gw
val:	3.72	−1.69	1.77
sd:	0.551	0.291	1.39

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.72	−1.69	1.77	2.54	12.6
sd:	0.551	0.291	1.39	12700	191000

	CNST	HILL	GNLS
AIC:	244.04	211.54	215.54
PROB:	0	0.88	0.12
RMSE:	3.52	2.24	2.24

MAX_MEAN: 5.23 MAX_MED: 6.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

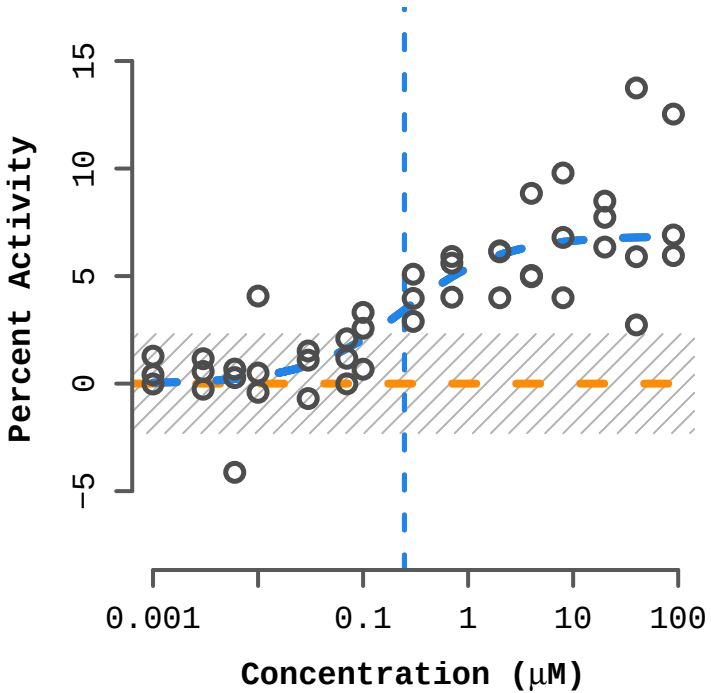
NAME: Nicotinic acid hydrazide
CHID: 20933 **CASRN:** 553-53-7
SPID(S): Tox21_200666
M4ID: 12481586

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium nitrate
CHID: 20937 CASRN: 7631-99-4
SPID(S): Tox21_202595
M4ID: 12479657

HILL MODEL (in red):

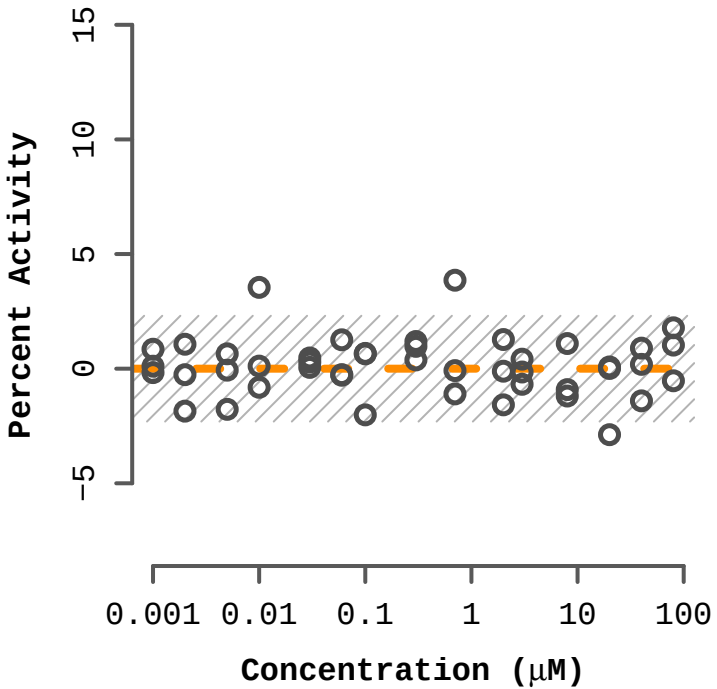
	tp	ga	gw
val:	6.86	−0.606	0.922
sd:	0.632	0.18	0.304

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.86	−0.606	0.922	3.69	4.35
sd:	0.632	0.18	0.304	1590	4090

	CNST	HILL	GNLS
AIC:	280.01	189.8	193.8
PROB:	0	0.88	0.12
RMSE:	5.21	2.03	2.03

MAX_MEAN: 8.47 MAX_MED: 7.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

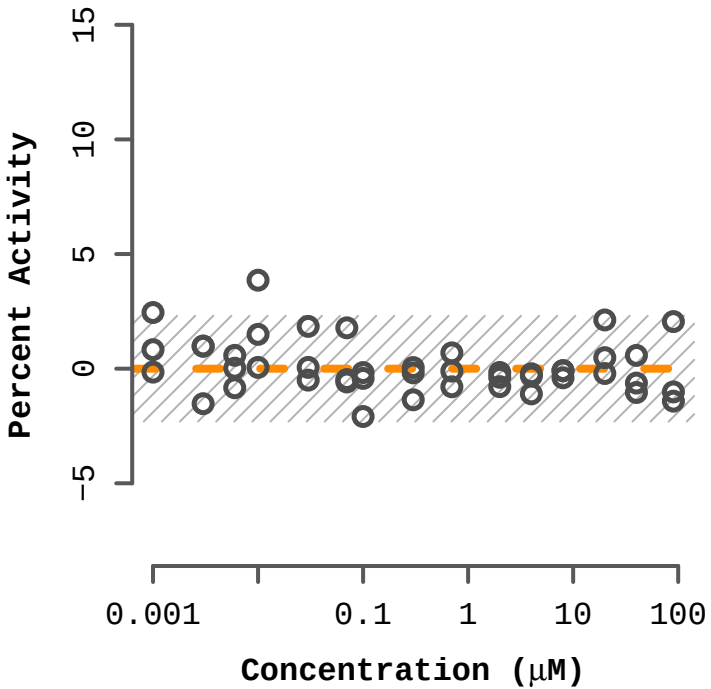
NAME: Nitrilotriacetic acid
CHID: 20939 **CASRN:** 139-13-9
SPID(S): Tox21_300156
M4ID: 12478974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

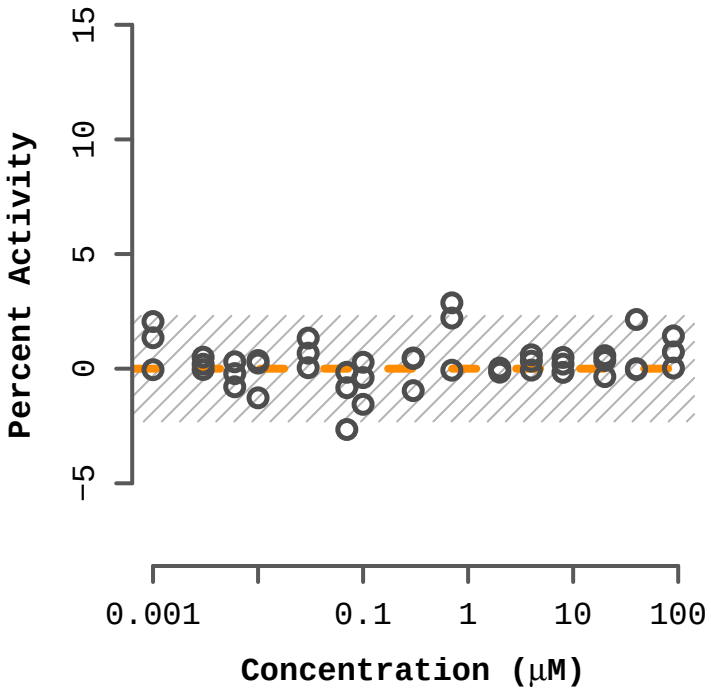
NAME: Nitrilotriacetic acid
CHID: 20939 **CASRN:** 139-13-9
SPID(S): Tox21_202195
M4ID: 12480057

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

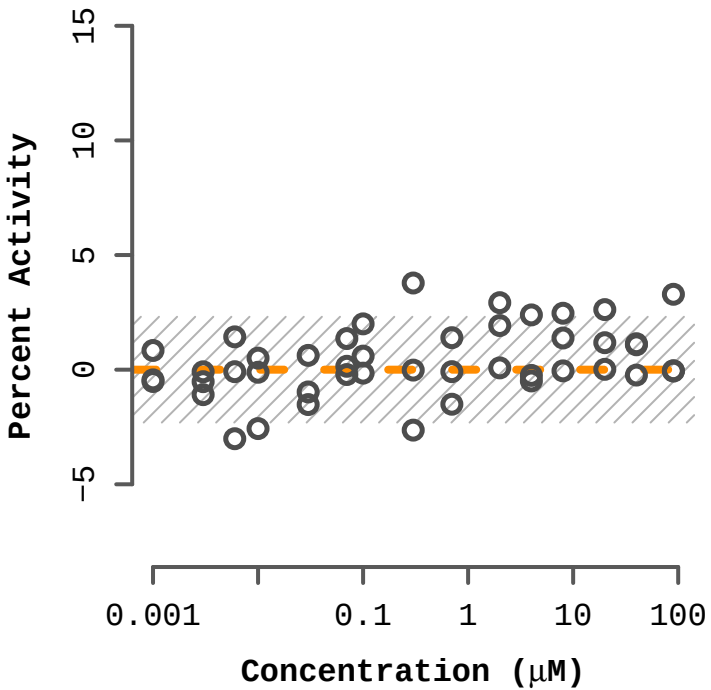
NAME: Sodium nitrite
CHID: 20941 **CASRN:** 7632-00-0
SPID(S): Tox21_300025
M4ID: 12479105

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.72	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

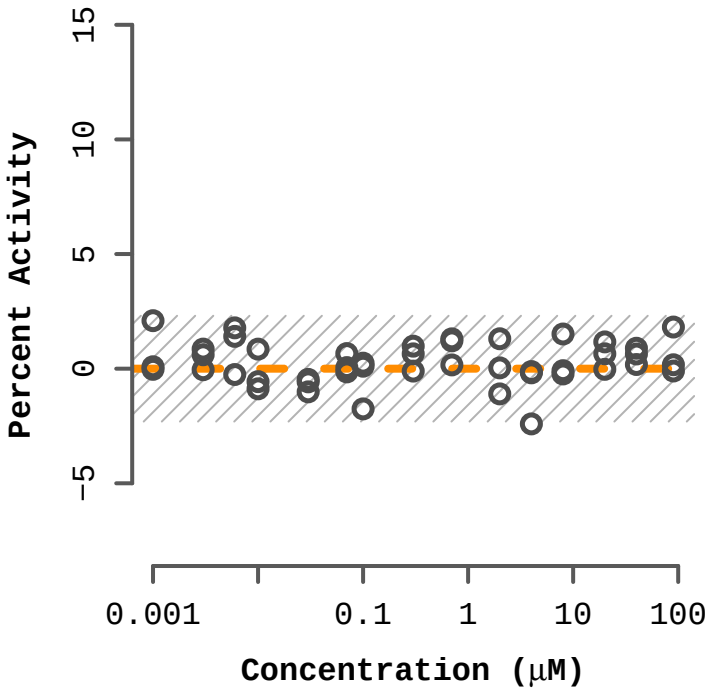
NAME: Sodium nitrite
CHID: 20941 **CASRN:** 7632-00-0
SPID(S): Tox21_202155
M4ID: 12480097

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

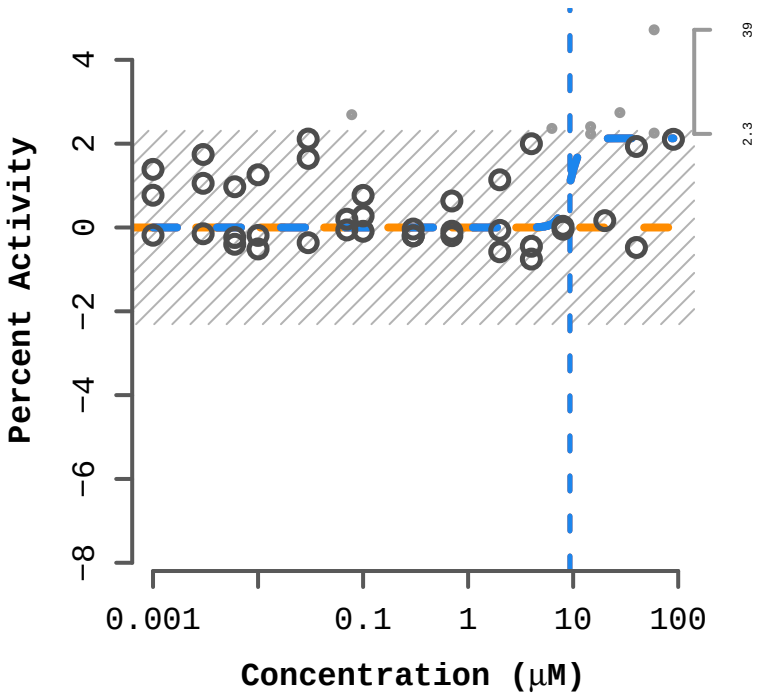
NAME: 2-Methoxy-5-nitroaniline
CHID: 20943 **CASRN:** 99-59-2
SPID(S): Tox21_300122
M4ID: 12479008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.98 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methoxy-5-nitroaniline
CHID: 20943 CASRN: 99-59-2
SPID(S): Tox21_201636
M4ID: 12480616 BRK

HILL MODEL (in red):

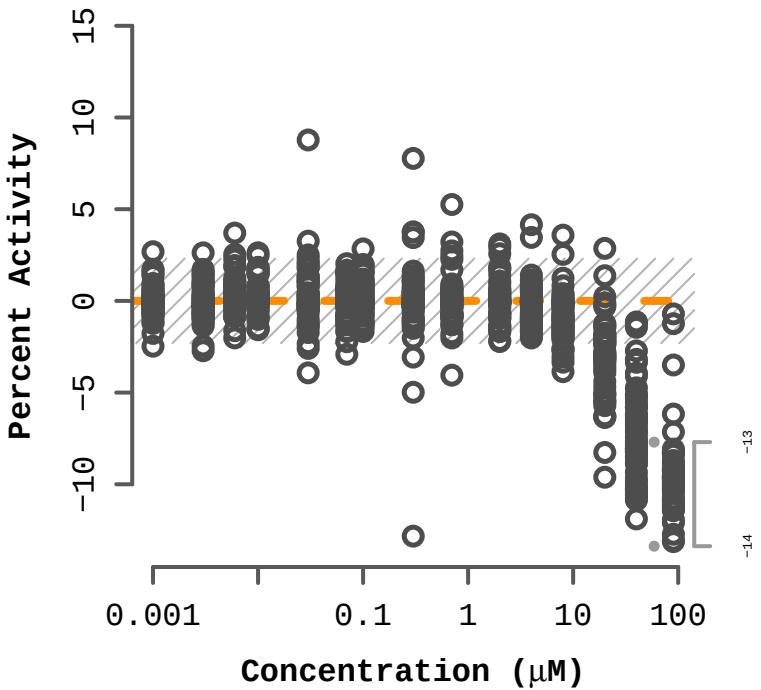
	tp	ga	gw
val:	2.13	0.969	8
sd:	0.507	0.335	38.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.13	0.969	8	3.58	11.3
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	208.23	200.61	204.61
PROB:	0.02	0.86	0.12
RMSE:	6.29	5.88	5.88

MAX_MEAN: 14.6 **MAX_MED:** 2.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

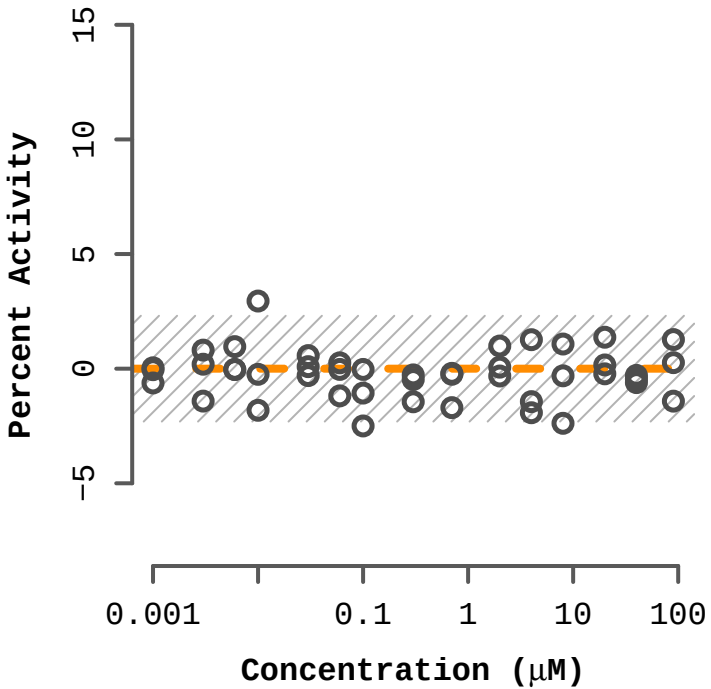
NAME: Nitrofurazone
CHID: 20944 **CASRN:** 59-87-0
SPID(S): Tox21_400035
M4ID: 12475102 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3761.87	NA	NA
PROB:	1	NA	NA
RMSE:	3.59	NA	NA

MAX_MEAN: 0.325 **MAX_MED:** 0.101 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

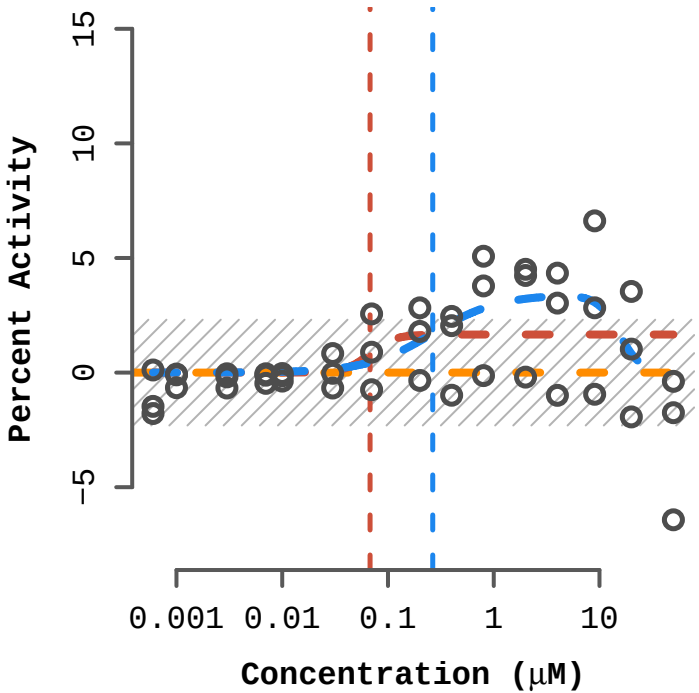
NAME: Nitrofurazone
CHID: 20944 **CASRN:** 59-87-0
SPID(S): Tox21_202988
M4ID: 12479264

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.438 **MAX_MED:** 0.264 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nitrofurazone
CHID: 20944 CASRN: 59-87-0
SPID(S): Tox21_110997_1
M4ID: 12483957

HILL MODEL (in red):

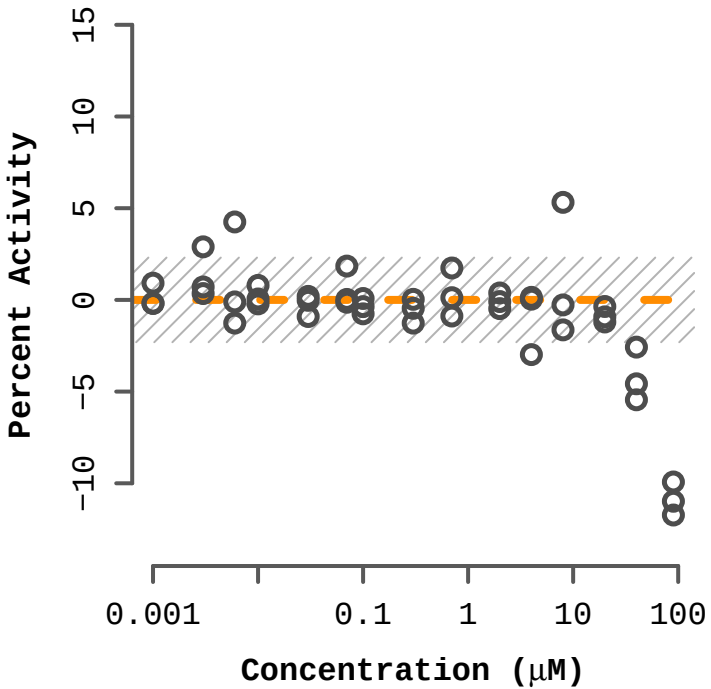
	tp	ga	gw
val:	1.66	−1.17	3.82
sd:	0.541	0.299	15.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.42	−0.577	1.39	1.19	4.23
sd:	1.21	0.363	0.88	0.47	8.65

	CNST	HILL	GNLS
AIC:	204.95	200.2	193.13
PROB:	0	0.03	0.97
RMSE:	2.4	2.16	1.93

MAX_MEAN: 2.91 MAX_MED: 4.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

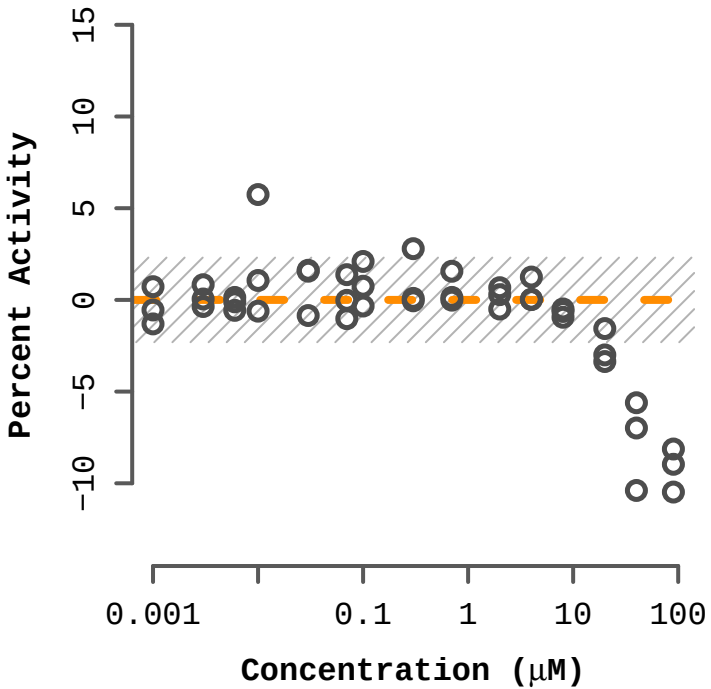
NAME: 5-Nitro-2-furanmethanediol diacetate
CHID: 20946 **CASRN:** 92-55-7
SPID(S): Tox21_200727
M4ID: 12481525

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.93	NA	NA
PROB:	1	NA	NA
RMSE:	3.32	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.706 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

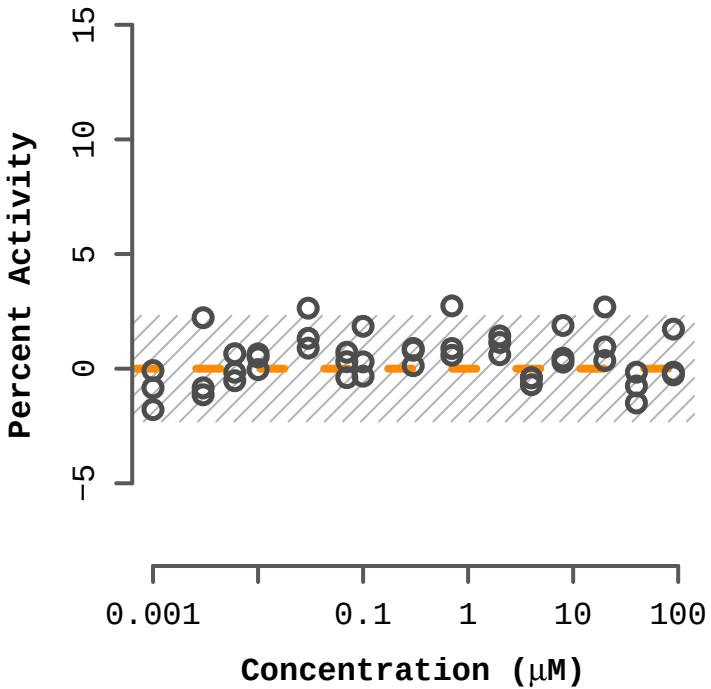
NAME: 5-(5-Nitro-2-furyl)-1,3,4-oxadiazole-2-ol
CHID: 20948 **CASRN:** 2122-86-3
SPID(S): Tox21_301880
M4ID: 12477253

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.83	NA	NA
PROB:	1	NA	NA
RMSE:	3.44	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

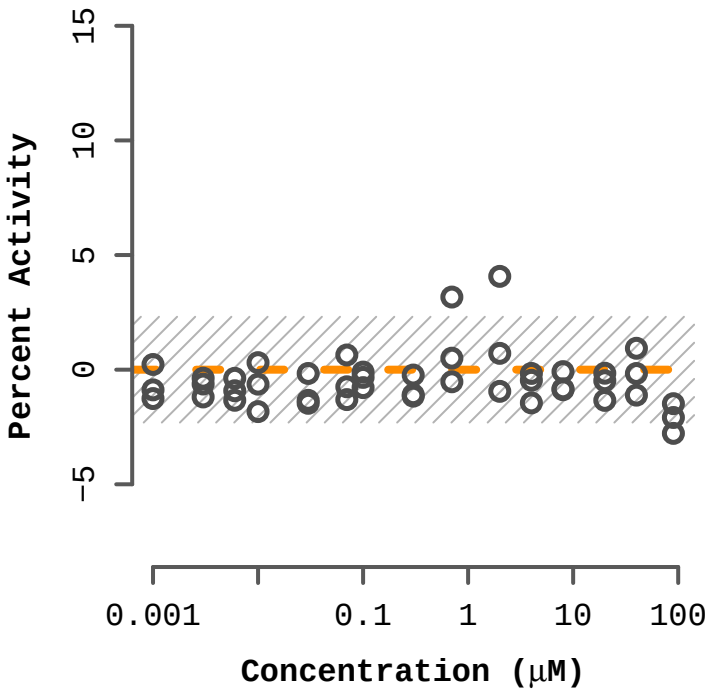
NAME: 4-Hydroxy-3-nitrophenylarsonic acid
CHID: 20956 **CASRN:** 121-19-7
SPID(S): Tox21_302842
M4ID: 12476291

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

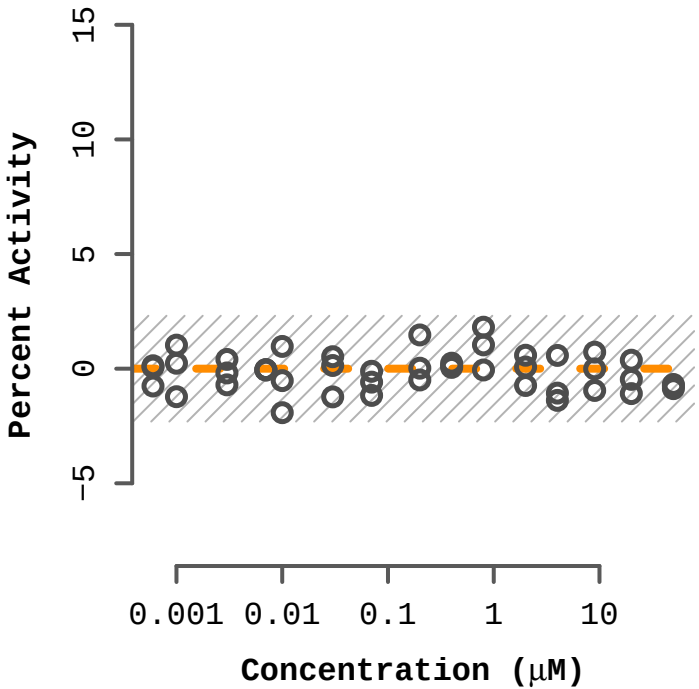
NAME: 4-Hydroxy-3-nitrophenylarsonic acid
CHID: 20956 **CASRN:** 121-19-7
SPID(S): Tox21_201465
M4ID: 12480787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.713 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

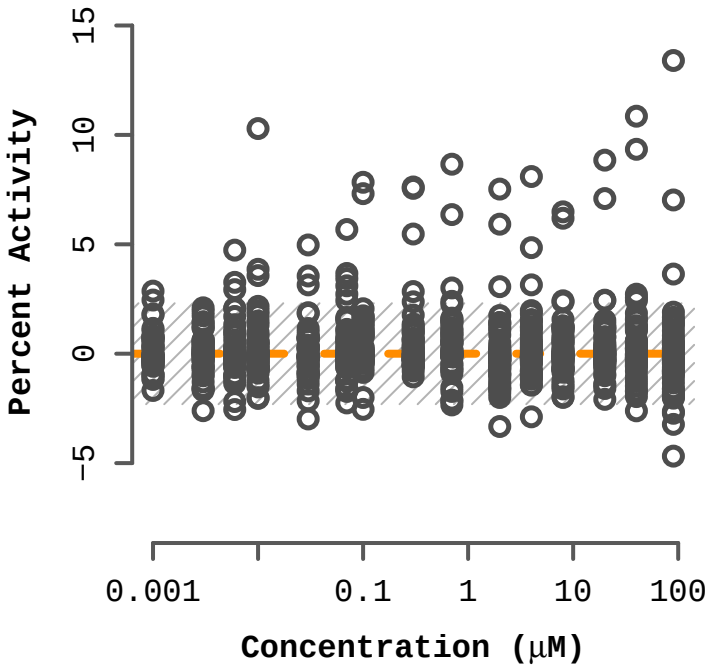
NAME: 4-Hydroxy-3-nitrophenylarsonic acid
CHID: 20956 **CASRN:** 121-19-7
SPID(S): Tox21_110402_1
M4ID: 12484390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.931 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

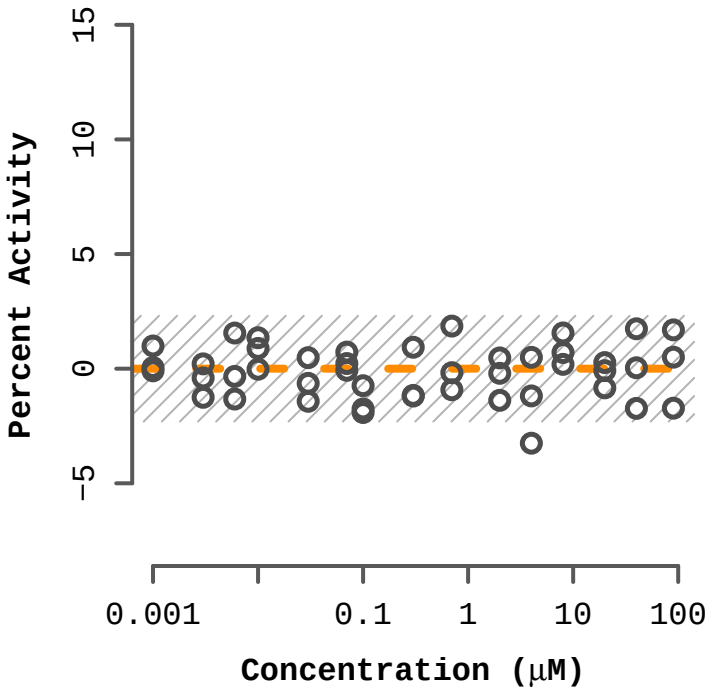
NAME: 2-Nitro-1,4-phenylenediamine
CHID: 20957 **CASRN:** 5307-14-2
SPID(S): Tox21_400026
M4ID: 12475111

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2434.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 0.631 **MAX_MED:** 0.165 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

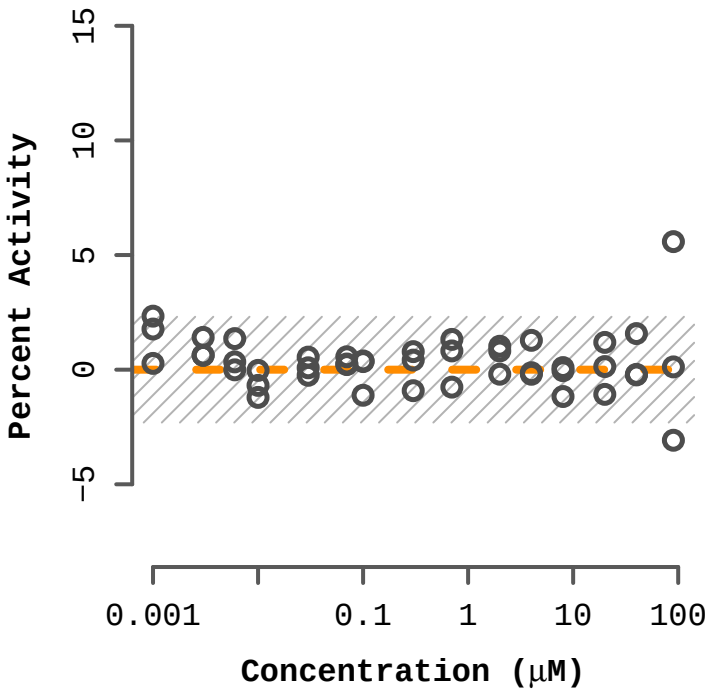
NAME: 4-Nitro-1,2-phenylenediamine
CHID: 20958 **CASRN:** 99-56-9
SPID(S): Tox21_302811
M4ID: 12476322

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.819 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

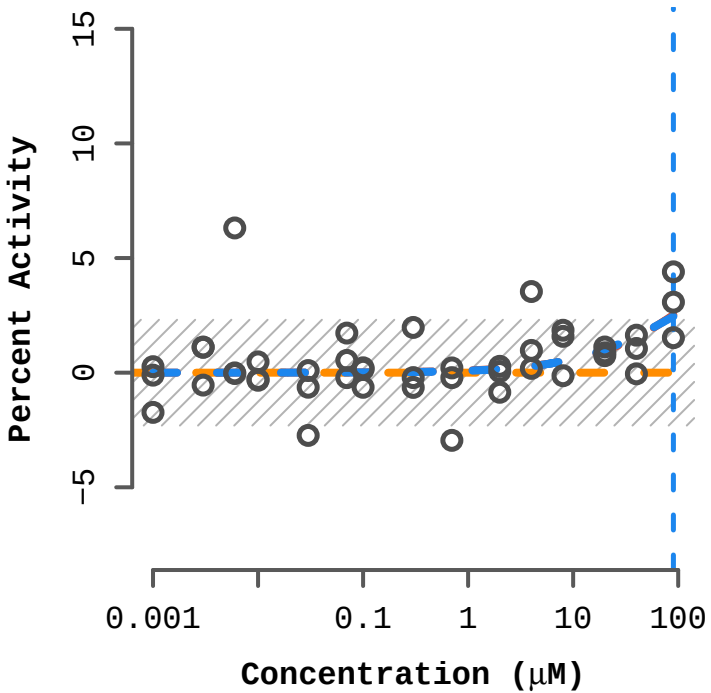
NAME: 4-Nitro-1,2-phenylenediamine
CHID: 20958 **CASRN:** 99-56-9
SPID(S): Tox21_202313
M4ID: 12479939

HILL MODEL: Not applicable.

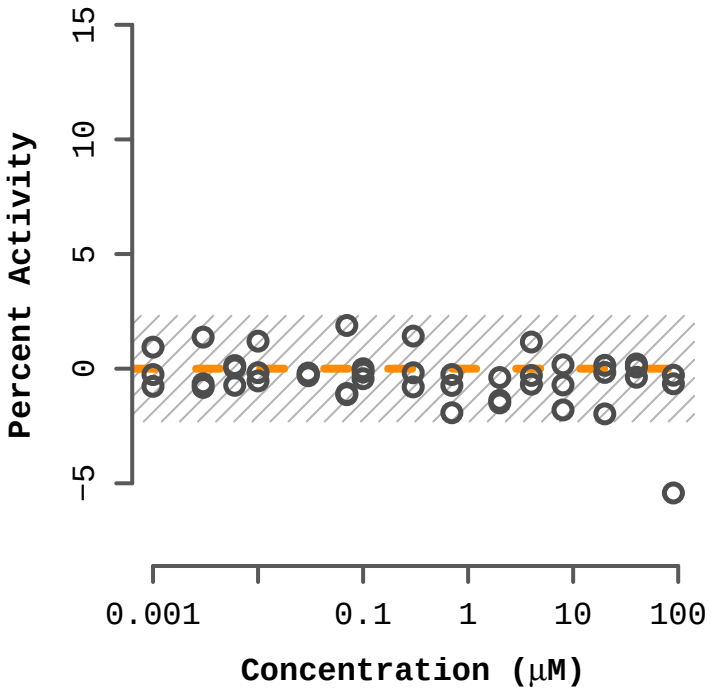
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.77 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Methyl-5-nitroaniline
CHID:    20959   CASRN: 99-55-8
SPID(S): Tox21_300134
M4ID:    12478996

HILL MODEL (in red):
      tp       ga       gw
val:  7.58     2.33     0.812
sd:   9.79     1.05     0.393

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.91     1.95     0.899    3.93     3.43
sd:   6.6      1.03     0.425    536      948

      CNST        HILL        GNLS
AIC:  166.39      152.39      156.71
PROB: 0           0.9         0.1
RMSE: 1.69        1.45        1.45

MAX_MEAN: 3         MAX_MED: 3.08      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

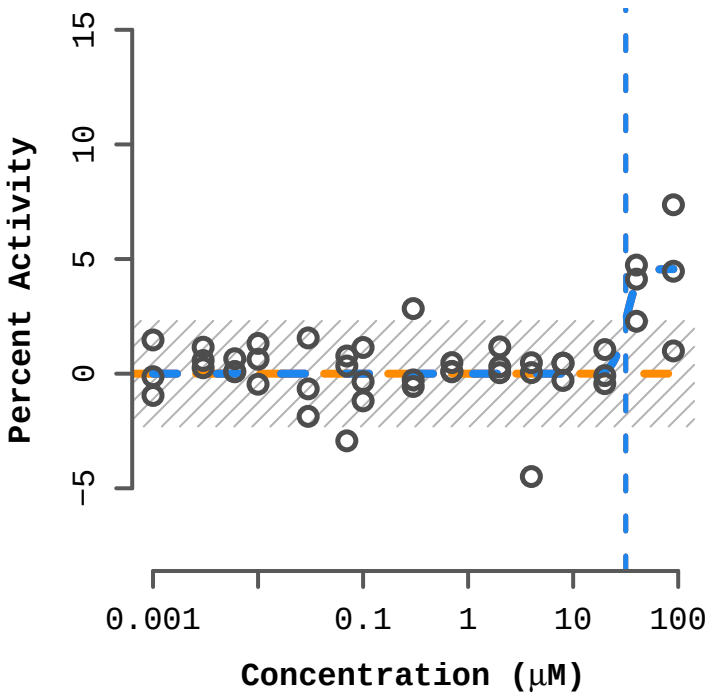
NAME: 2-Methyl-5-nitroaniline
CHID: 20959 **CASRN:** 99-55-8
SPID(S): Tox21_201945
M4ID: 12480307

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.166 **MAX_MED:** 0.0735 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Nitroacenaphthene
CHID: 20960 CASRN: 602-87-9
SPID(S): Tox21_302877
M4ID: 12476256

HILL MODEL (in red):

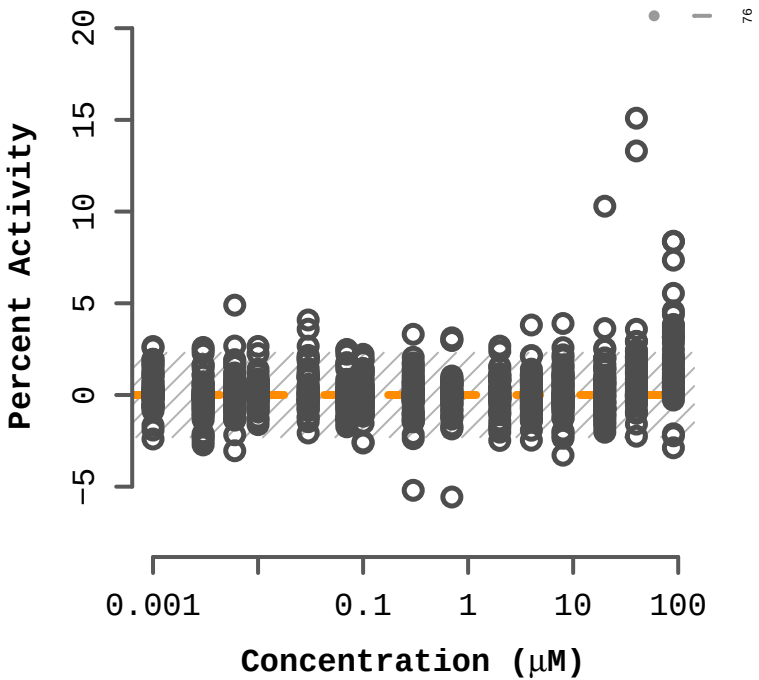
	tp	ga	gw
val:	4.57	1.5	7.62
sd:	0.938	0.109	6.59

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.57	1.5	7.62	3.2	5.38
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	177.74	154.81	158.81
PROB:	0	0.88	0.12
RMSE:	1.99	1.35	1.35

MAX_MEAN: 4.28 MAX_MED: 4.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

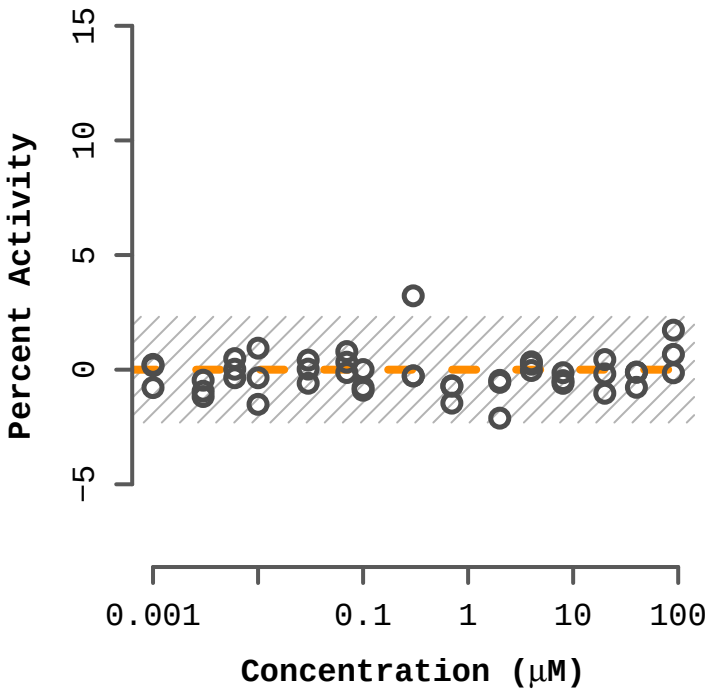
NAME: 4-Nitroaniline
CHID: 20961 **CASRN:** 100-01-6
SPID(S): Tox21_400031
M4ID: 12475106 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2539.7	NA	NA
PROB:	1	NA	NA
RMSE:	3.18	NA	NA

MAX_MEAN: 3.2 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

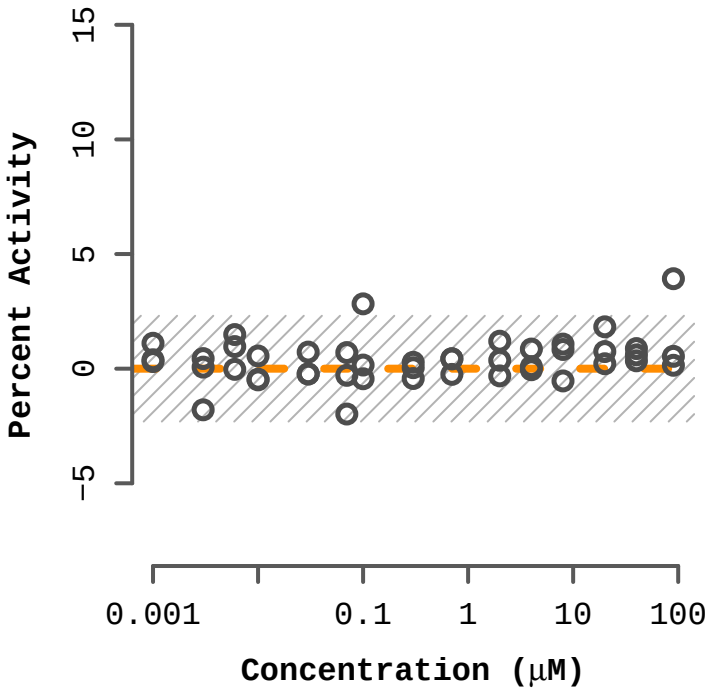
NAME: 1-Methoxy-2-nitrobenzene
CHID: 20962 **CASRN:** 91-23-6
SPID(S): Tox21_302981
M4ID: 12476152

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 0.671 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

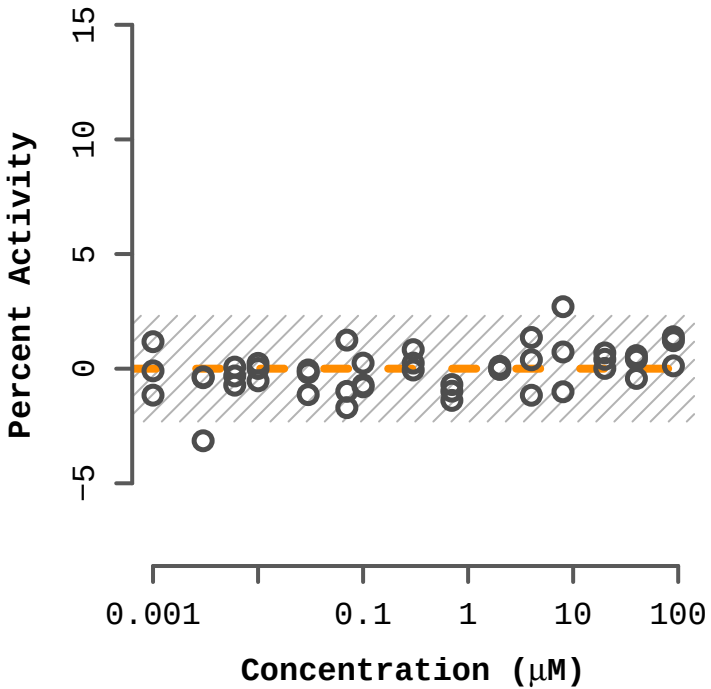
NAME: 1-Methoxy-2-nitrobenzene
CHID: 20962 **CASRN:** 91-23-6
SPID(S): Tox21_201984
M4ID: 12480268

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

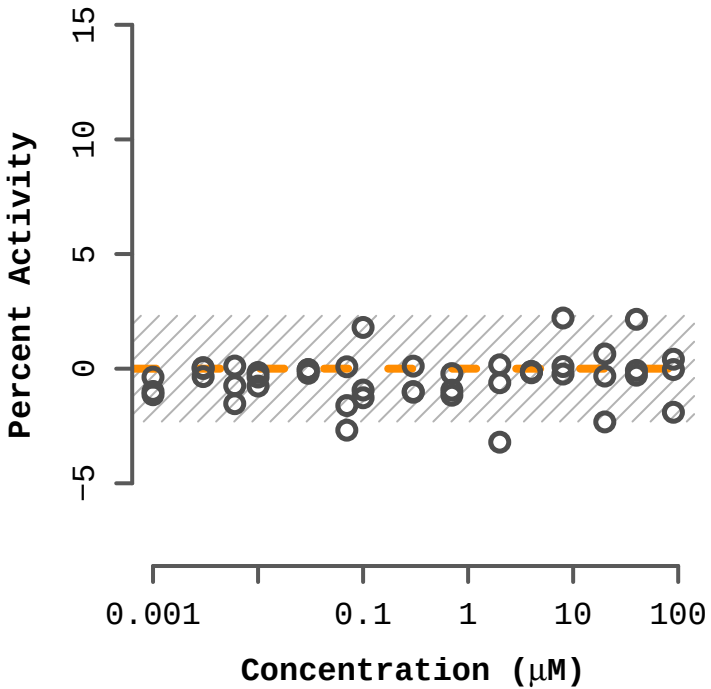
NAME: 4-Nitroanthranilic acid
CHID: 20963 **CASRN:** 619-17-0
SPID(S): Tox21_302942
M4ID: 12476191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

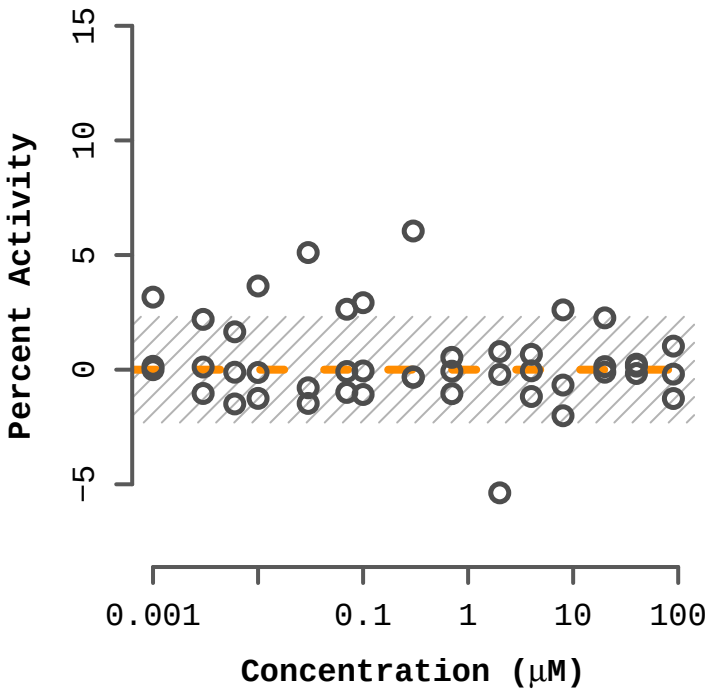
NAME: 4-Nitroanthranilic acid
CHID: 20963 CASRN: 619-17-0
SPID(S): Tox21_201312
M4ID: 12480940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.69 MAX_MED: 0.0942 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

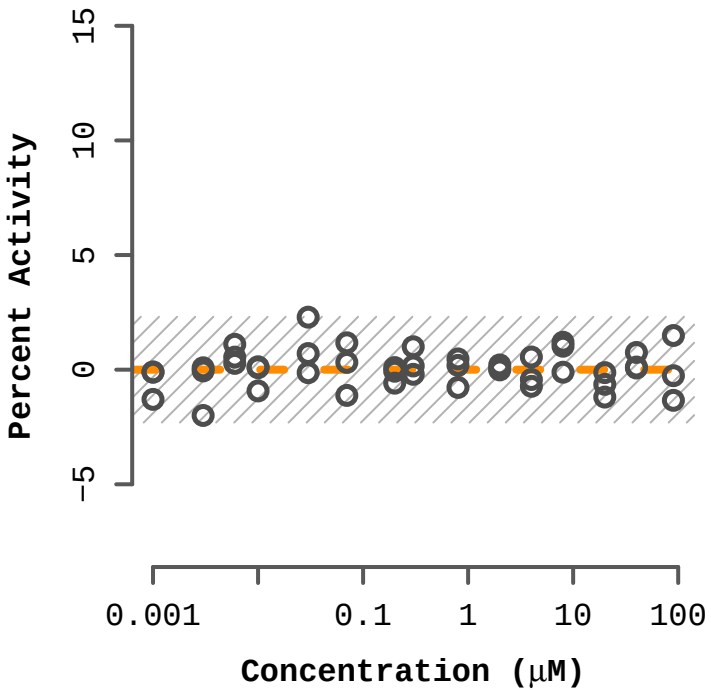
NAME: Nitrobenzene
CHID: 20964 **CASRN:** 98-95-3
SPID(S): Tox21_300508
M4ID: 12478624

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 0.155 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

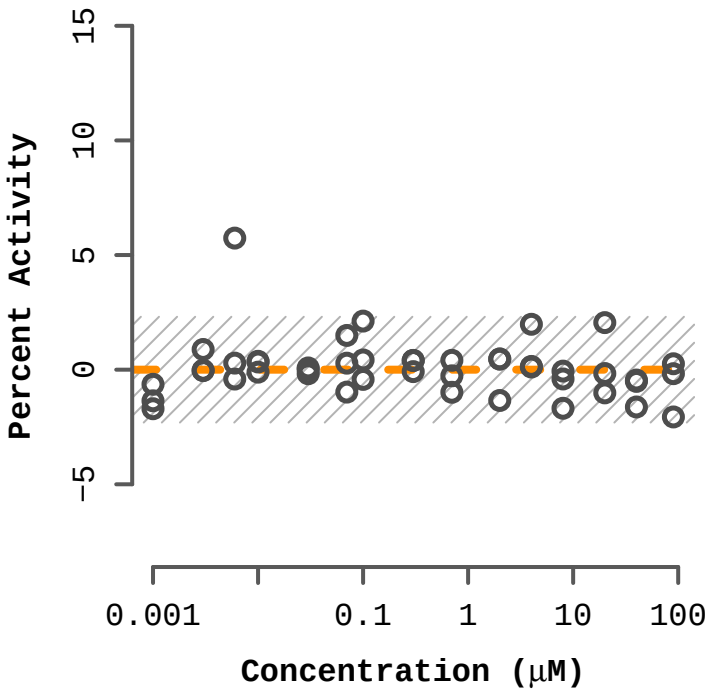
NAME: Nitrobenzene
CHID: 20964 CASRN: 98-95-3
SPID(S): Tox21_201750
M4ID: 12480502

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.956 MAX_MED: 1.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

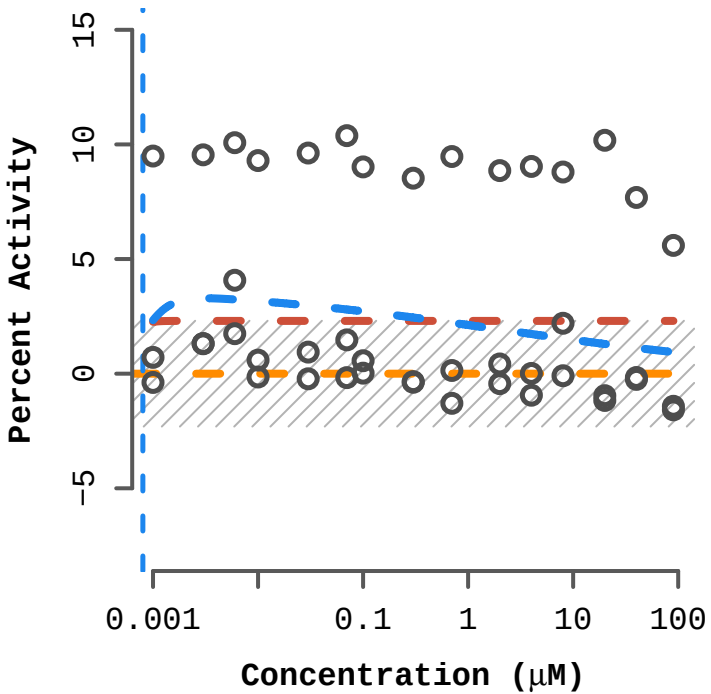
NAME: 6-Nitrobenzimidazole
CHID: 20965 **CASRN:** 94-52-0
SPID(S): Tox21_302828
M4ID: 12476305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 0.463 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Nitrobenzimidazole
CHID: 20965 CASRN: 94-52-0
SPID(S): Tox21_201684
M4ID: 12480568

HILL MODEL (in red):

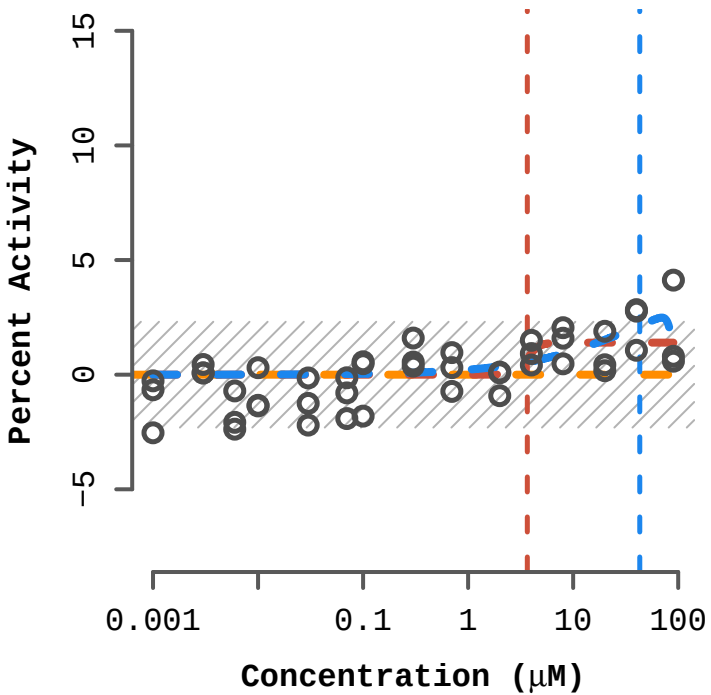
	tp	ga	gw
val:	2.3	-3.24	7.18
sd:	0.752	12.7	361

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.79	-3.1	3.3	0.351	0.3
sd:	24.8	1.66	21.7	24.4	3.12

	CNST	HILL	GNLS
AIC:	279.88	274.35	277.22
PROB:	0.05	0.77	0.18
RMSE:	5.35	4.41	4.37

MAX_MEAN: 5.3 MAX_MED: 4.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitrobenzoic acid
CHID: 20966 CASRN: 62-23-7
SPID(S): Tox21_300131
M4ID: 12478999

HILL MODEL (in red):

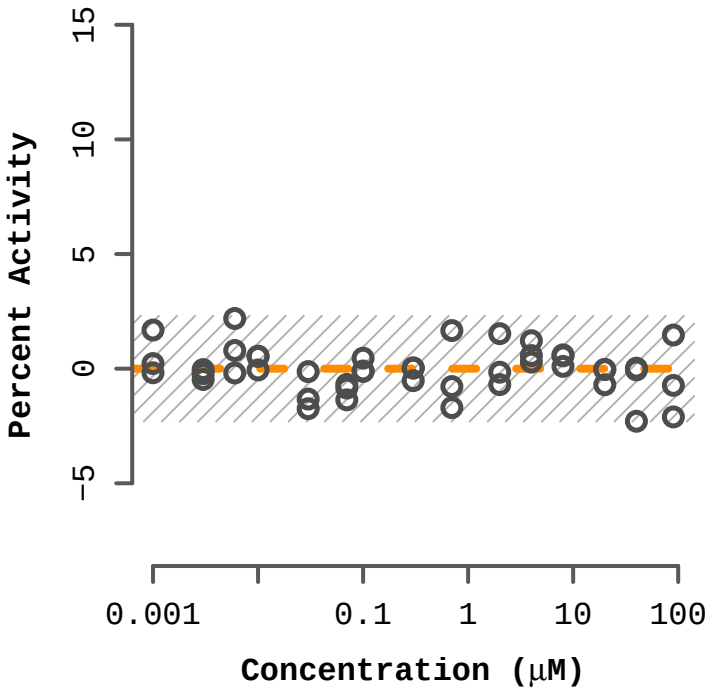
	tp	ga	gw
val:	1.4	0.563	8
sd:	0.336	0.112	15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.28	1.63	0.778	1.95	17
sd:	14.8	3.49	0.773	0.0559	123

	CNST	HILL	GNLS
AIC:	161.5	148.92	153.22
PROB:	0	0.89	0.1
RMSE:	1.42	1.14	1.15

MAX_MEAN: 2.23 MAX_MED: 2.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

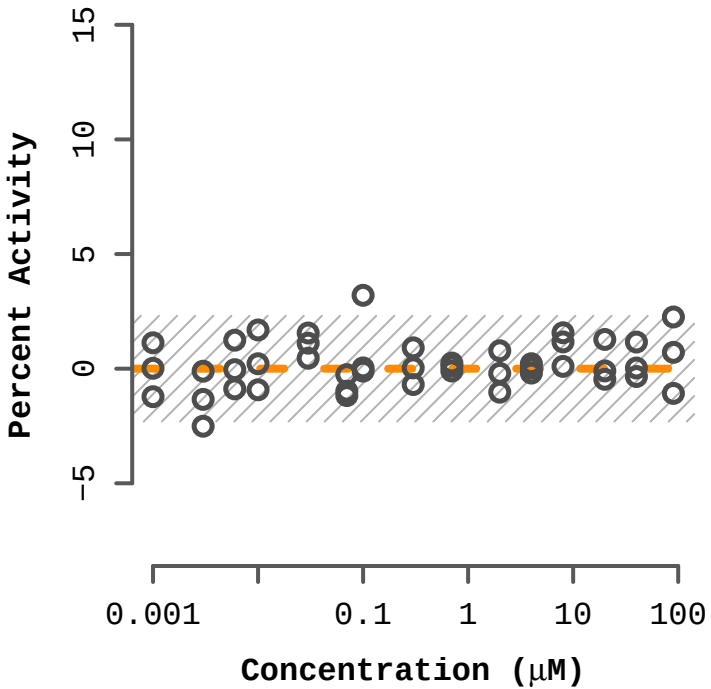
NAME: 4-Nitrobenzoic acid
CHID: 20966 CASRN: 62-23-7
SPID(S): Tox21_201258
M4ID: 12480994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.933 MAX_MED: 0.794 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

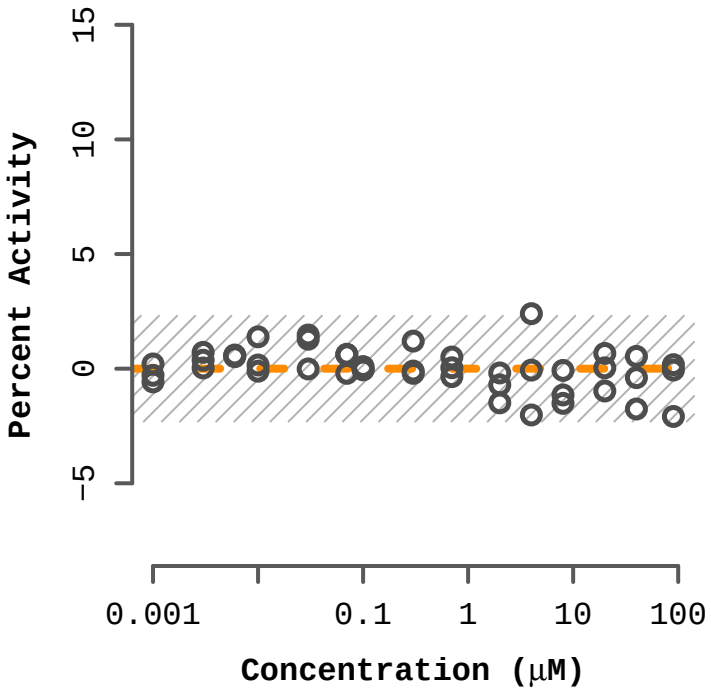
NAME: 1-Nitrobutane
CHID: 20967 **CASRN:** 627-05-4
SPID(S): Tox21_200346
M4ID: 12481906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

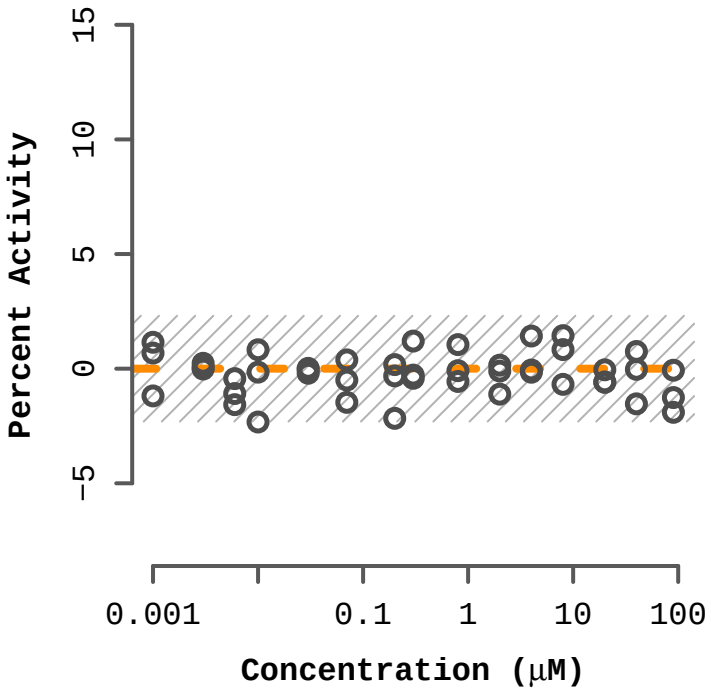
NAME: Nitroethane
CHID: 20969 CASRN: 79-24-3
SPID(S): Tox21_302823
M4ID: 12476310

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.915 MAX_MED: 1.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

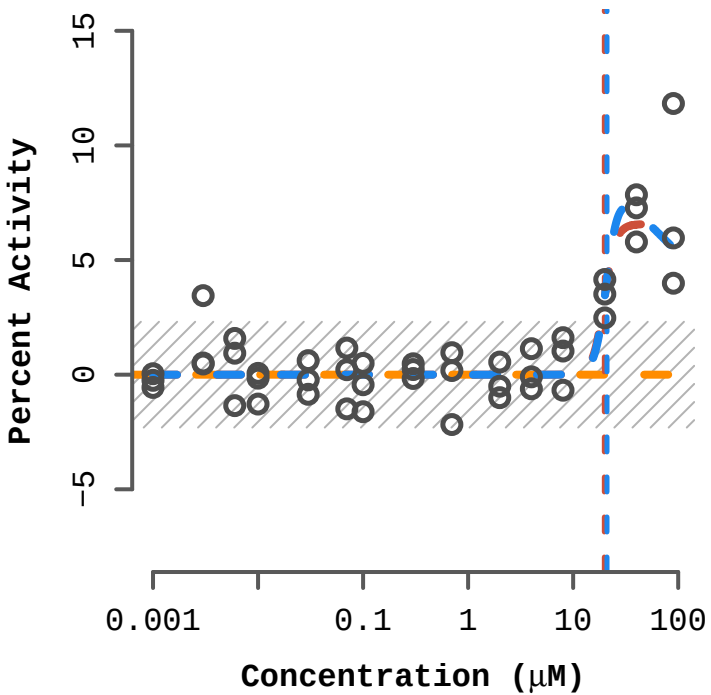
NAME: Nitroethane
CHID: 20969 **CASRN:** 79-24-3
SPID(S): Tox21_202217
M4ID: 12480035

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.532 **MAX_MED:** 0.834 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nitrofen
CHID: 20970 CASRN: 1836-75-5
SPID(S): Tox21_300276
M4ID: 12478854

HILL MODEL (in red):

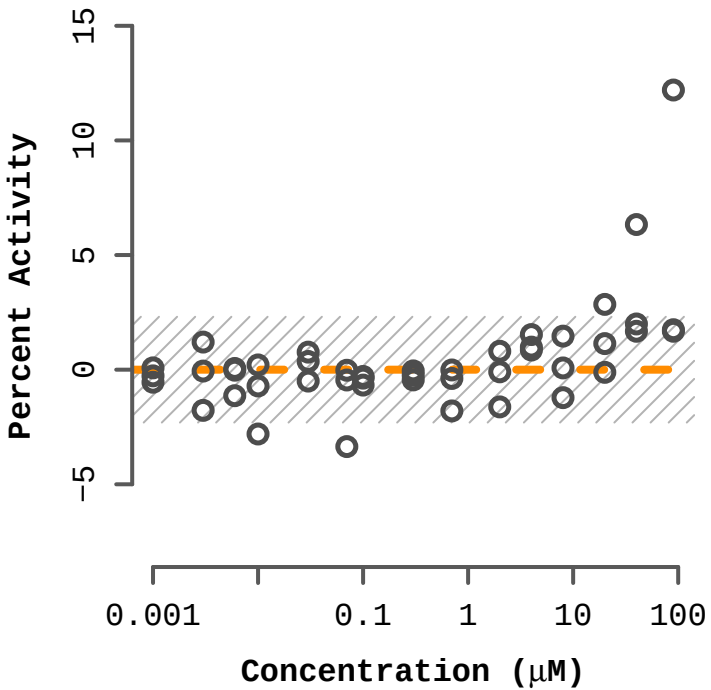
	tp	ga	gw
val:	6.57	1.3	8
sd:	0.594	0.0225	11.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.8	1.32	7.94	1.76	0.619
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	212.22	152.55	154.38
PROB:	0	0.71	0.29
RMSE:	3.04	1.33	1.39

MAX_MEAN: 7.26 MAX_MED: 7.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

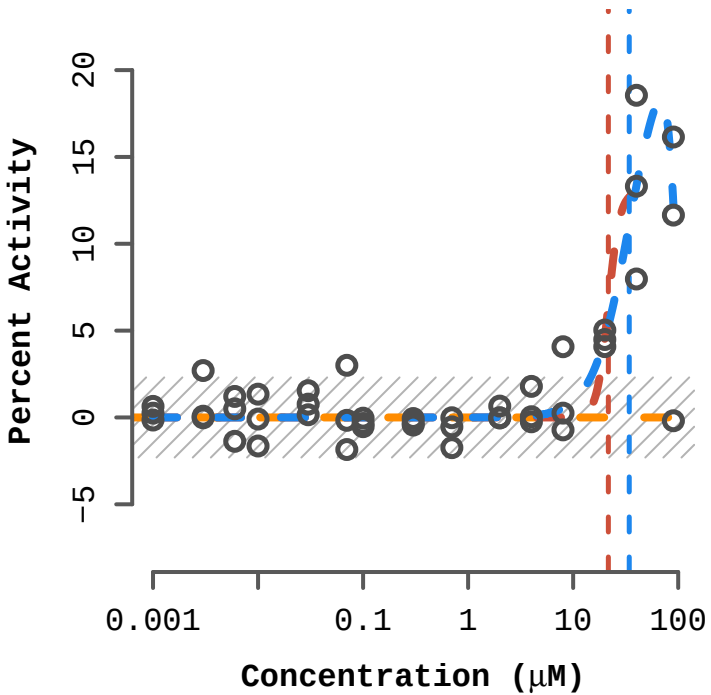
NAME: Nitrofen
CHID: 20970 CASRN: 1836-75-5
SPID(S): Tox21_202438
M4ID: 12479814

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.56	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 5.21 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Nitrofluorene
CHID: 20971 CASRN: 607-57-8
SPID(S): Tox21_302770
M4ID: 12476363

HILL MODEL (in red):

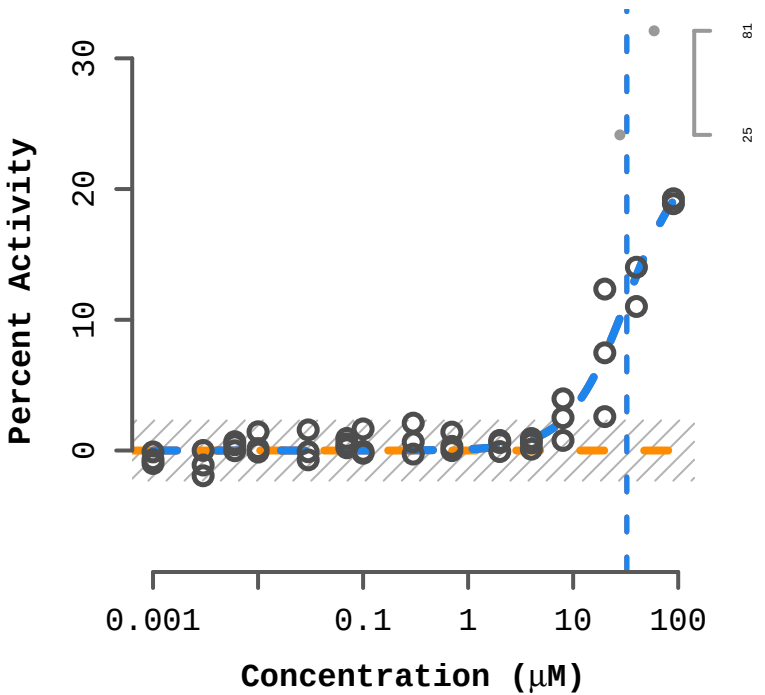
	tp	ga	gw
val:	13	1.33	8
sd:	1.08	0.0284	6.01

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.3	1.53	2.55	1.97	10.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	241	186.94	190.22
PROB:	0	0.84	0.16
RMSE:	4.94	2.58	2.49

MAX_MEAN: 13.3 MAX_MED: 13.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Nitrofluorene
CHID: 20971 CASRN: 607-57-8
SPID(S): Tox21_201765
M4ID: 12480487 BRK

HILL MODEL (in red):

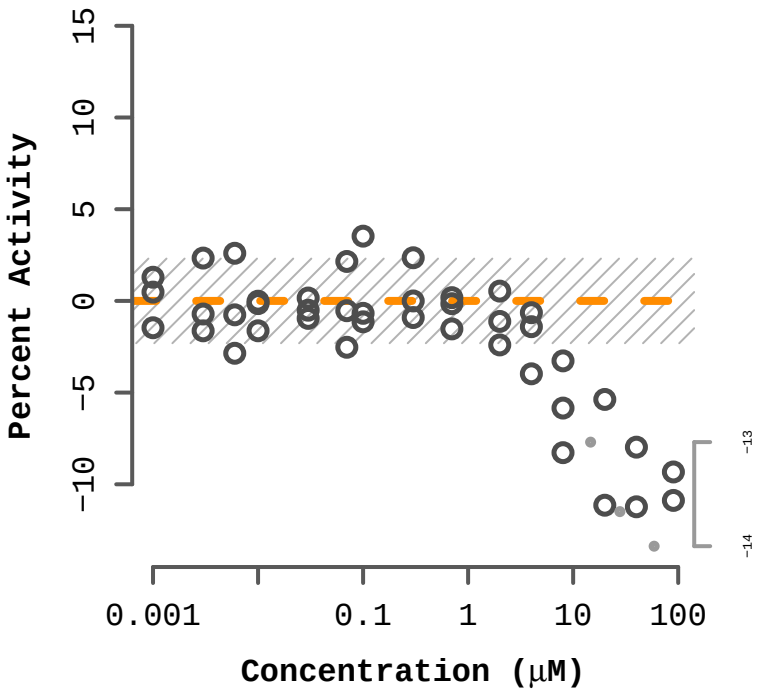
	tp	ga	gw
val:	23	1.51	1.56
sd:	2.77	0.104	0.279

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23	1.51	1.56	3.58	4.21
sd:	2.77	0.104	0.279	1170	3090

	CNST	HILL	GNLS
AIC:	289.56	201.7	205.7
PROB:	0	0.88	0.12
RMSE:	13.72	9.46	9.46

MAX_MEAN: 39.6 MAX_MED: 19.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

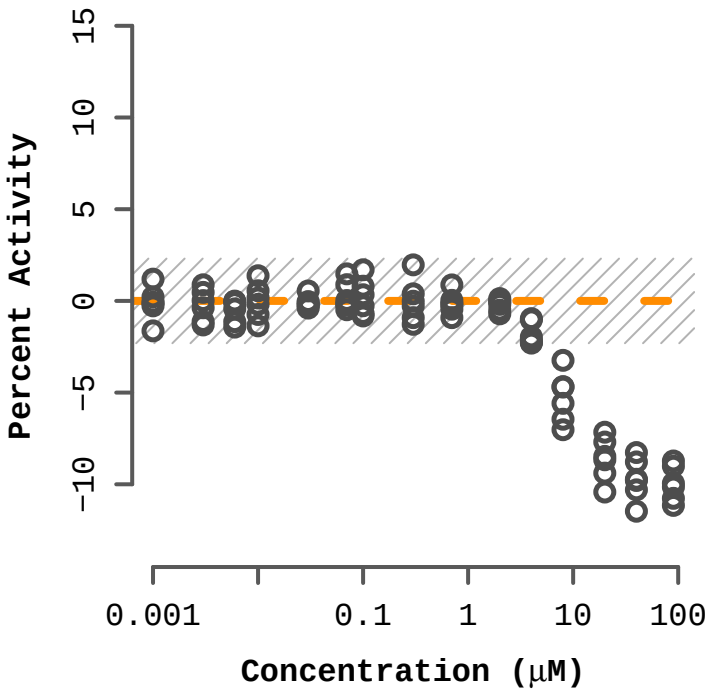
NAME: Nitrofurantoin
CHID: 20972 **CASRN:** 67-20-9
SPID(S): Tox21_300602
M4ID: 12478531 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	274.1	NA	NA
PROB:	1	NA	NA
RMSE:	5.44	NA	NA

MAX_MEAN: 0.573 **MAX_MED:** 0.481 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

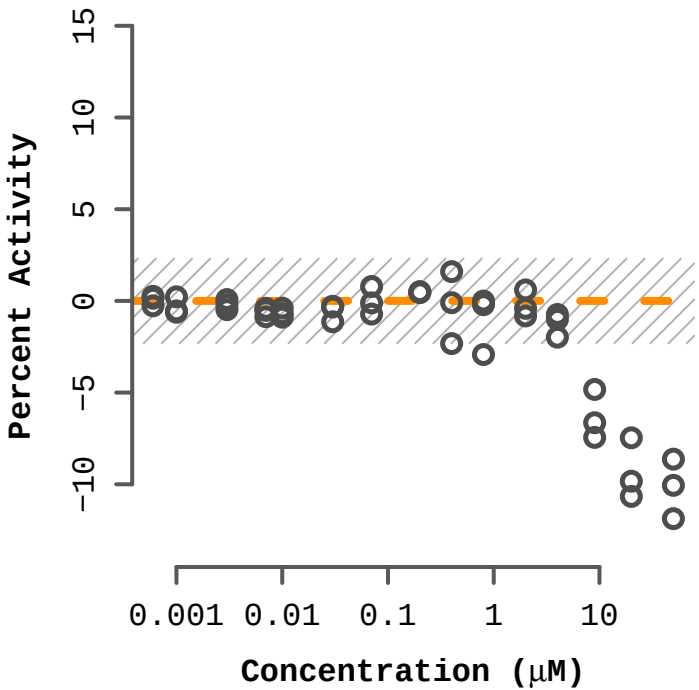
NAME: Nitrofurantoin
CHID: 20972 **CASRN:** 67-20-9
SPID(S): Tox21_201924
M4ID: 12480328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	512.06	NA	NA
PROB:	1	NA	NA
RMSE:	4.54	NA	NA

MAX_MEAN: 0.253 **MAX_MED:** 0.0379 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

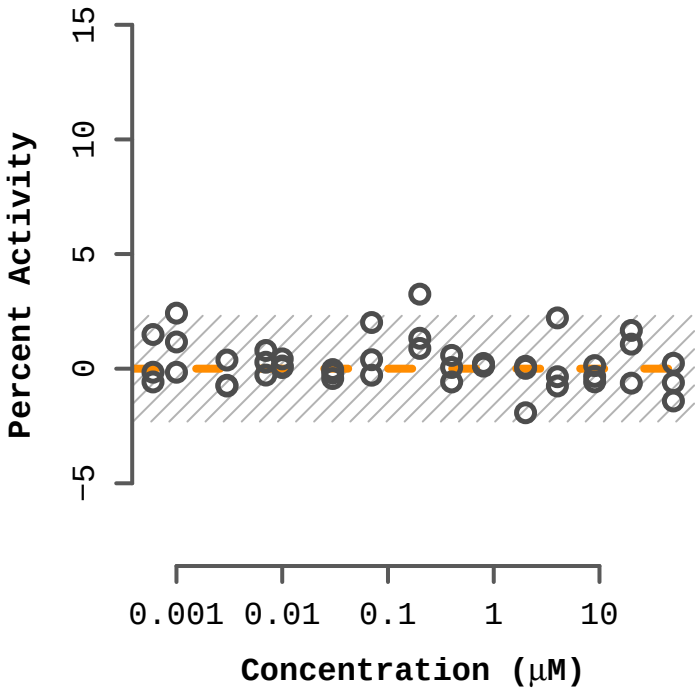
NAME: Nitrofurantoin
CHID: 20972 **CASRN:** 67-20-9
SPID(S): Tox21_111142_1
M4ID: 12483880

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.38	NA	NA
PROB:	1	NA	NA
RMSE:	4.04	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** 0.487 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

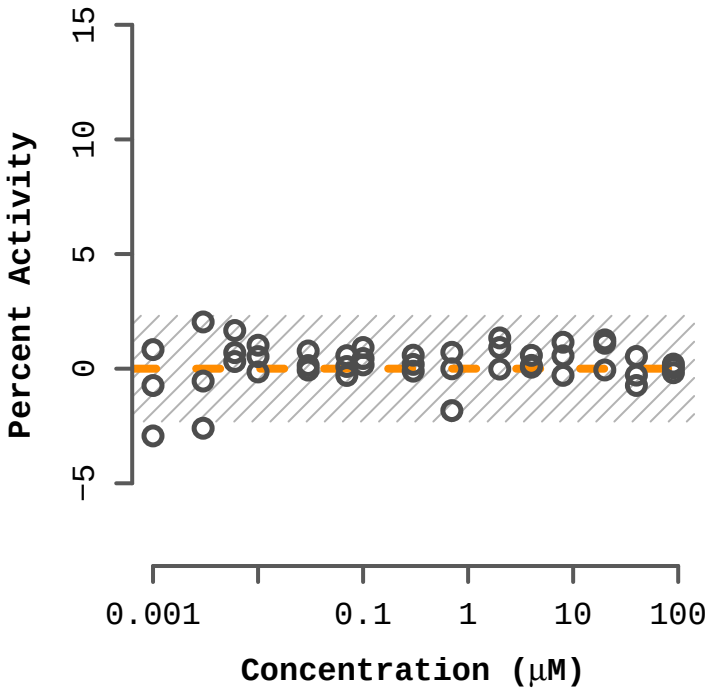
NAME: Nitrogen mustard N-oxide
CHID: 20976 CASRN: 126-85-2
SPID(S): Tox21_113709
M4ID: 12482505

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

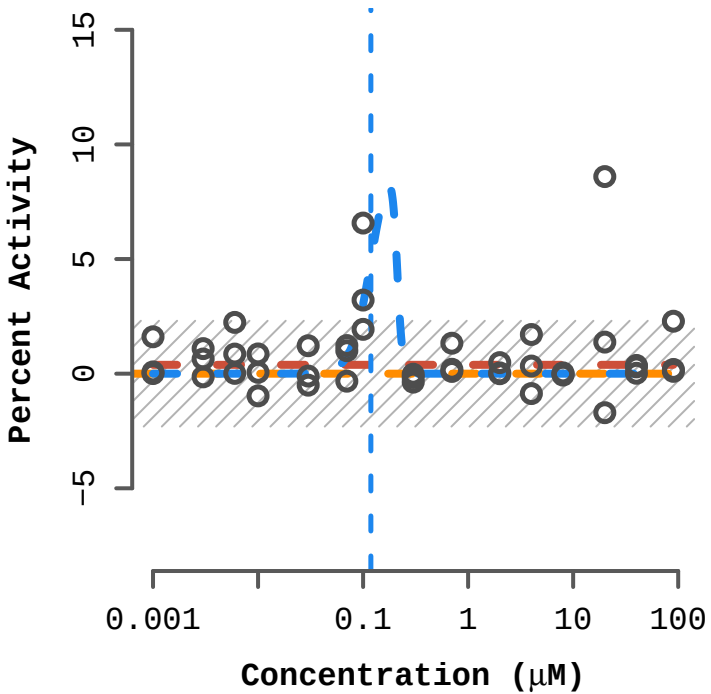
NAME: Nitromethane
CHID: 20977 **CASRN:** 75-52-5
SPID(S): Tox21_200822
M4ID: 12481430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Nitronaphthalene
CHID: 20978 CASRN: 86-57-7
SPID(S): Tox21_302759
M4ID: 12476374

HILL MODEL (in red):

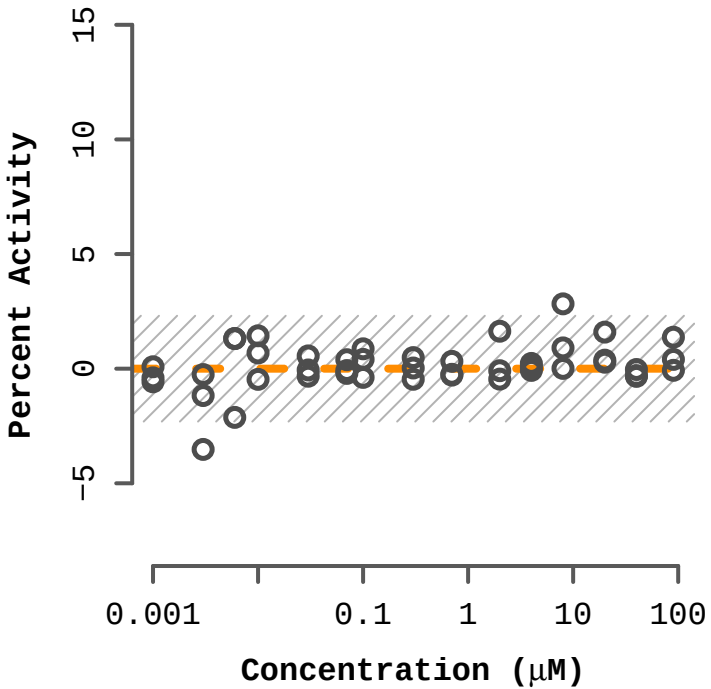
	tp	ga	gw
val:	0.386	-4.99	3.5
sd:	0.147	3300	5720

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.83	-0.926	4.75	-0.676	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.8	156.75	150.25
PROB:	0.02	0.04	0.94
RMSE:	1.91	1.78	1.63

MAX_MEAN: 3.91 MAX_MED: 3.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

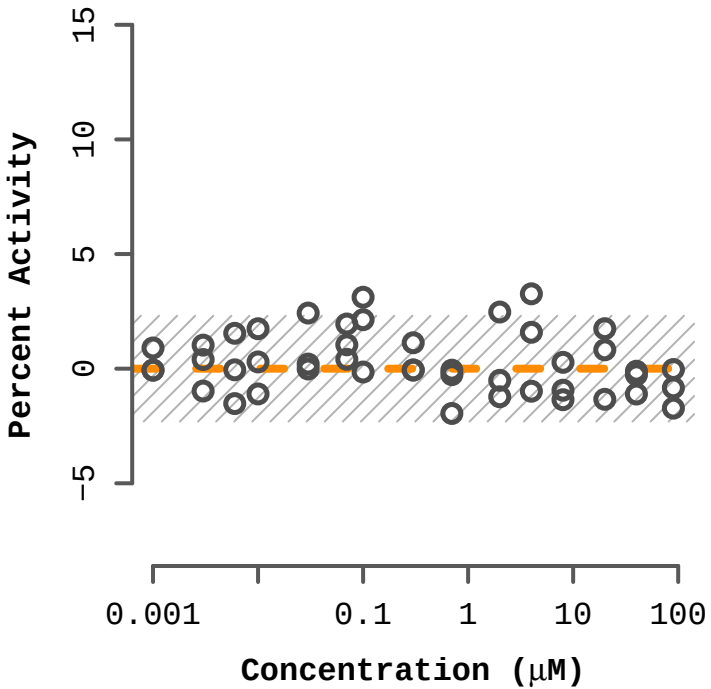
NAME: 1-Nitronaphthalene
CHID: 20978 CASRN: 86-57-7
SPID(S): Tox21_201407
M4ID: 12480845

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.25 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

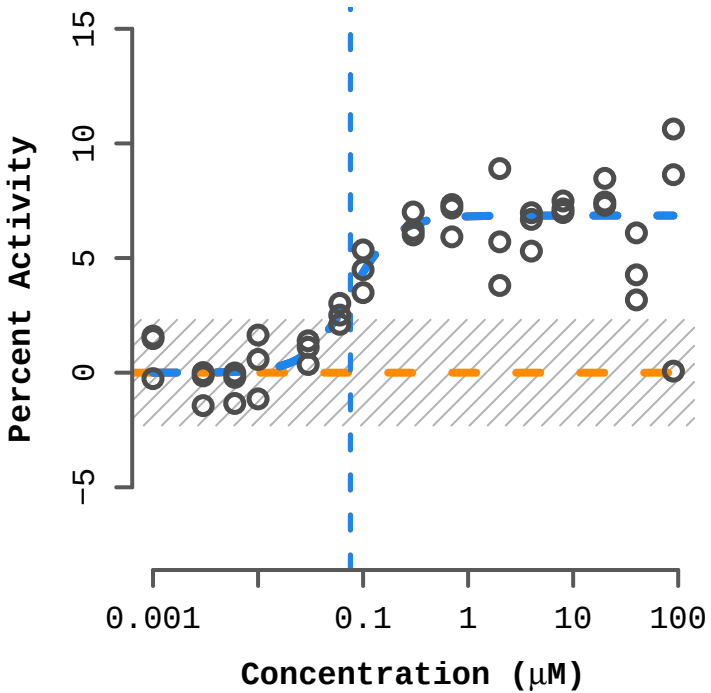
NAME: 1-Nitropropane
CHID: 20980 **CASRN:** 108-03-2
SPID(S): Tox21_303024
M4ID: 12476109

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Nitropropane
CHID: 20980 CASRN: 108-03-2
SPID(S): Tox21_202289
M4ID: 12479963

HILL MODEL (in red):

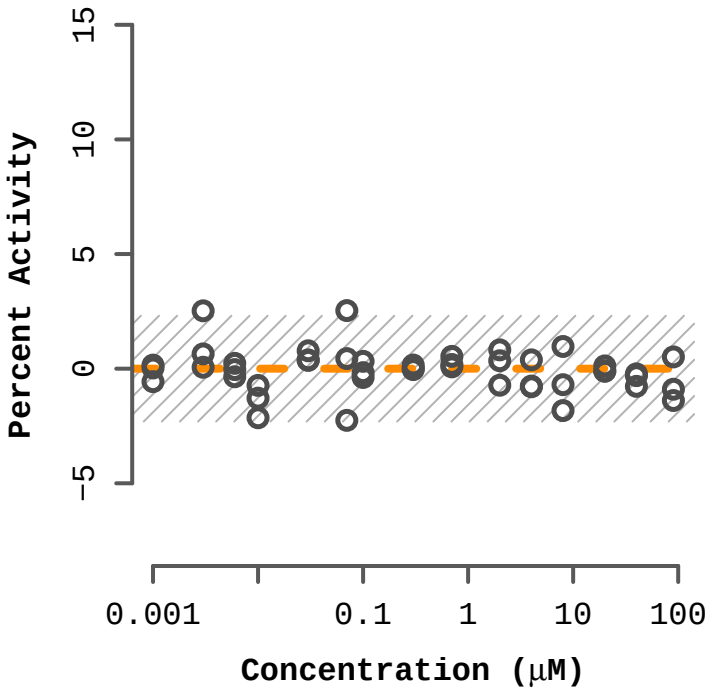
	tp	ga	gw
val:	6.85	-1.12	2.04
sd:	0.296	0.0591	0.587

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.85	-1.12	2.04	3.31	11.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	282.95	167.99	171.99
PROB:	0	0.88	0.12
RMSE:	5.16	1.65	1.65

MAX_MEAN: 7.74 MAX_MED: 8.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

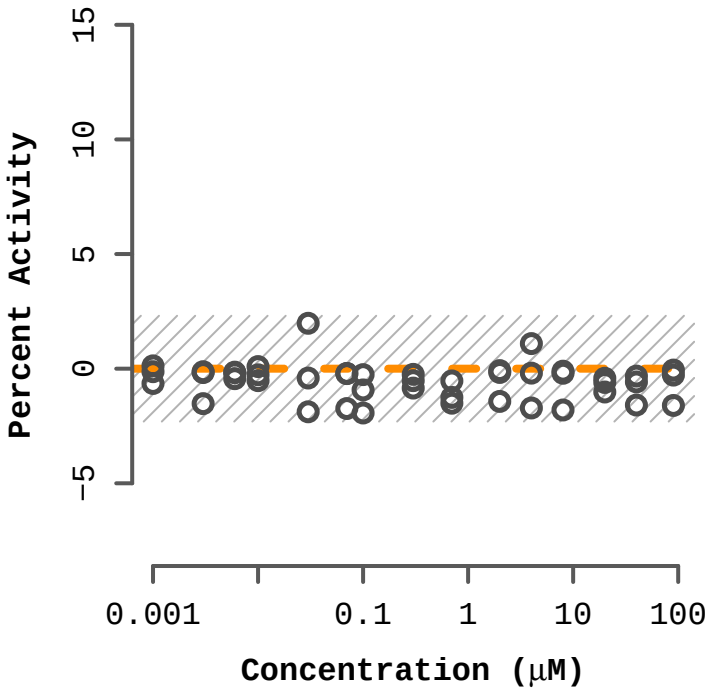
NAME: 2-Nitropropane
CHID: 20981 **CASRN:** 79-46-9
SPID(S): Tox21_200365
M4ID: 12481887

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.646 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

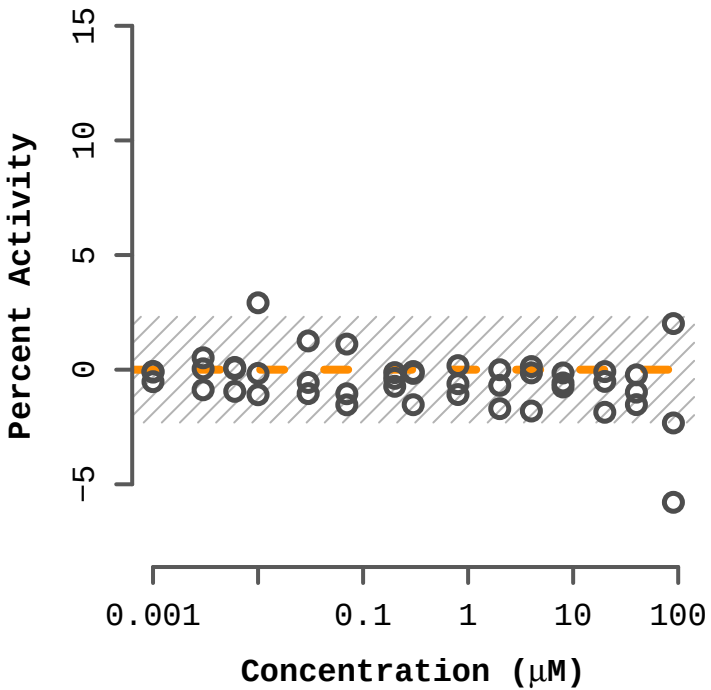
NAME: 3-Nitropropionic acid
CHID: 20982 CASRN: 504-88-1
SPID(S): Tox21_303007
M4ID: 12476126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: −0.102 **MAX_MED:** −0.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

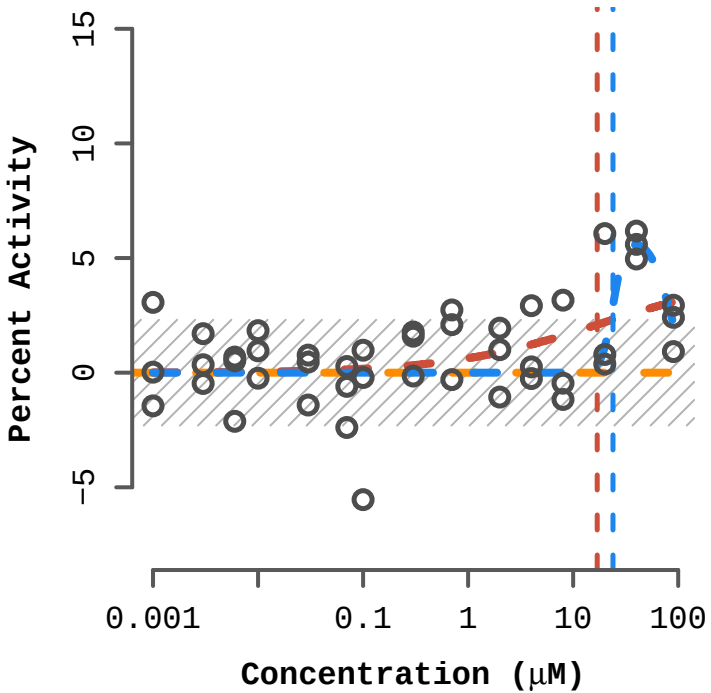
NAME: 3-Nitropropionic acid
CHID: 20982 CASRN: 504-88-1
SPID(S): Tox21_202460
M4ID: 12479792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.555 MAX_MED: 0.0403 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Nitropyrene
CHID: 20983 CASRN: 5522-43-0
SPID(S): Tox21_200066
M4ID: 12482186

HILL MODEL (in red):

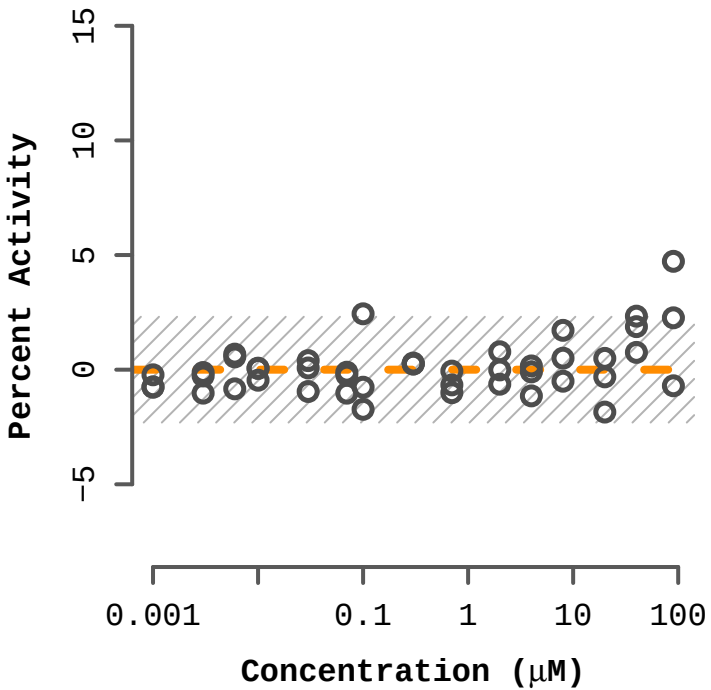
	tp	ga	gw
val:	4.19	1.23	0.612
sd:	3.58	1.46	0.674

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.87	1.38	7.96	1.9	4.81
sd:	15.2	0.895	82.6	1.16	78.8

	CNST	HILL	GNLS
AIC:	204.42	193.14	185.32
PROB:	0	0.02	0.98
RMSE:	2.38	1.87	1.74

MAX_MEAN: 5.58 MAX_MED: 5.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

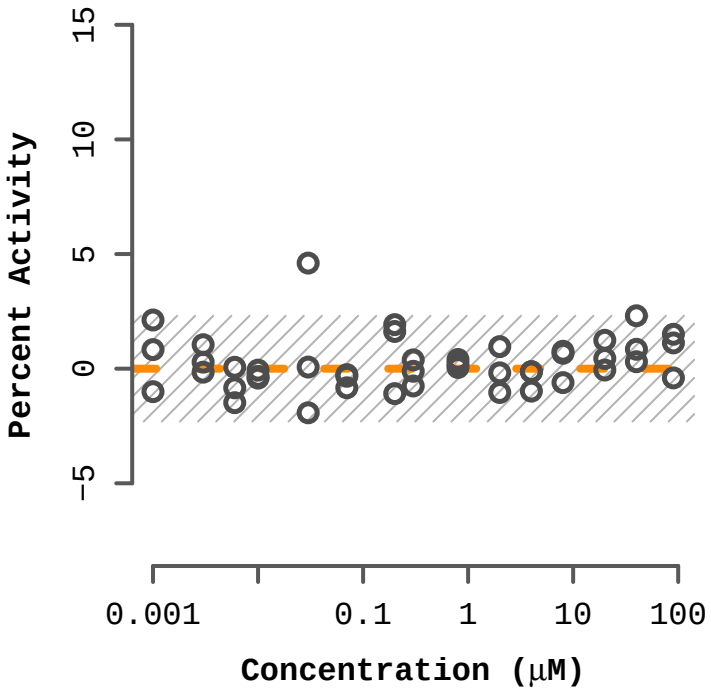
NAME: 6-Nitroquinoline
CHID: 20984 **CASRN:** 613-50-3
SPID(S): Tox21_200508
M4ID: 12481744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

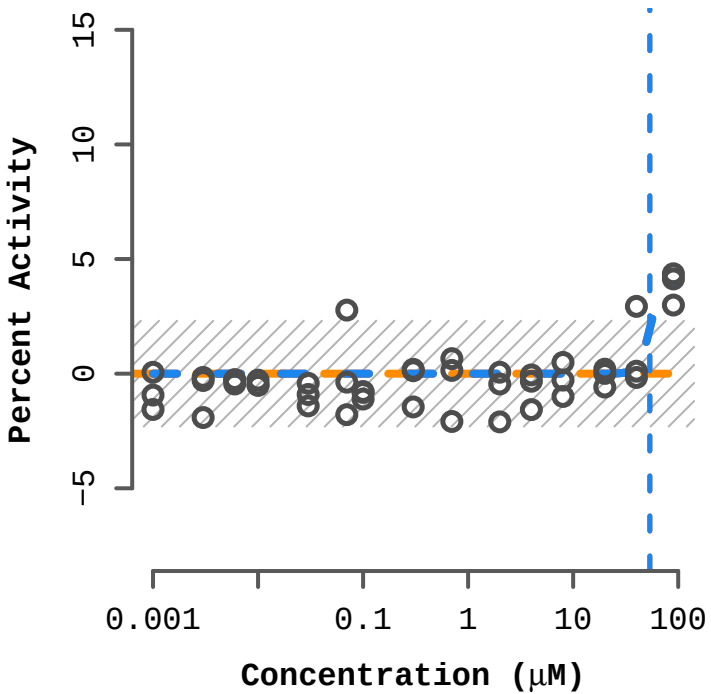
NAME: 8-Nitroquinoline
CHID: 20985 **CASRN:** 607-35-2
SPID(S): Tox21_200683
M4ID: 12481569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Nitroso-N-methyl-4-nitroaniline
CHID: 21002 CASRN: 943-41-9
SPID(S): Tox21_302256
M4ID: 12476877

HILL MODEL (in red):

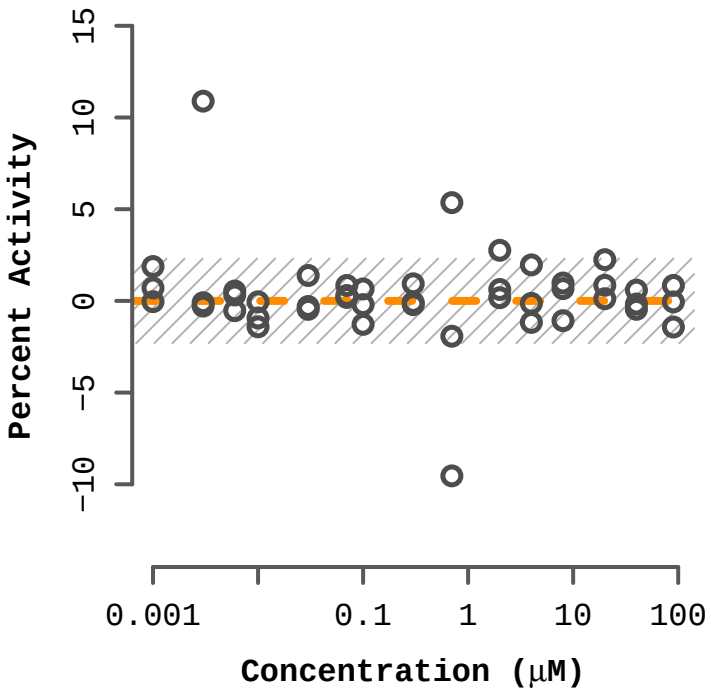
	tp	ga	gw
val:	3.95	1.73	8
sd:	3.5	1.14	67

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.98	1.73	8	3.75	1.19
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	156.14	137.05	141.05
PROB:	0	0.88	0.12
RMSE:	1.45	1.04	1.04

MAX_MEAN: 3.83 MAX_MED: 4.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

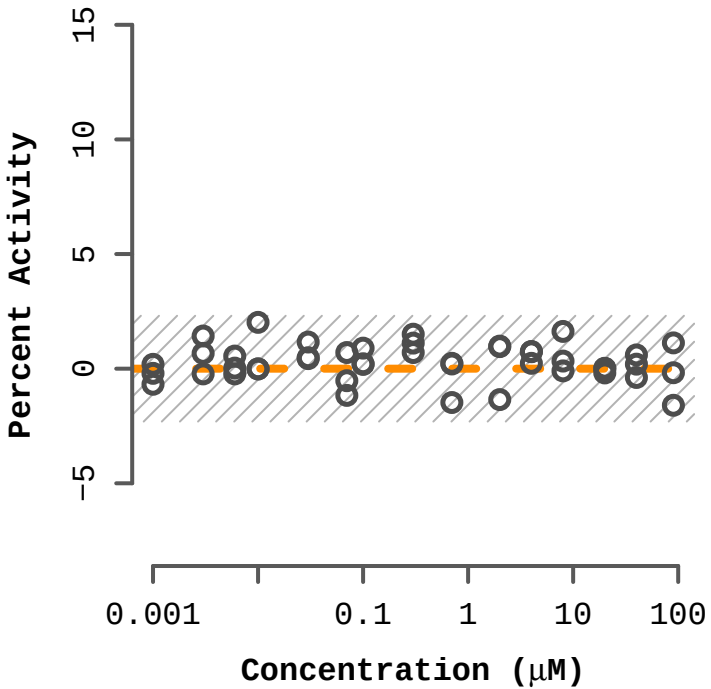
NAME: N-Nitroso-N-methylurea
CHID: 21006 **CASRN:** 684-93-5
SPID(S): Tox21_302850
M4ID: 12476283

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.5	NA	NA

MAX_MEAN: 3.51 **MAX_MED:** 0.853 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

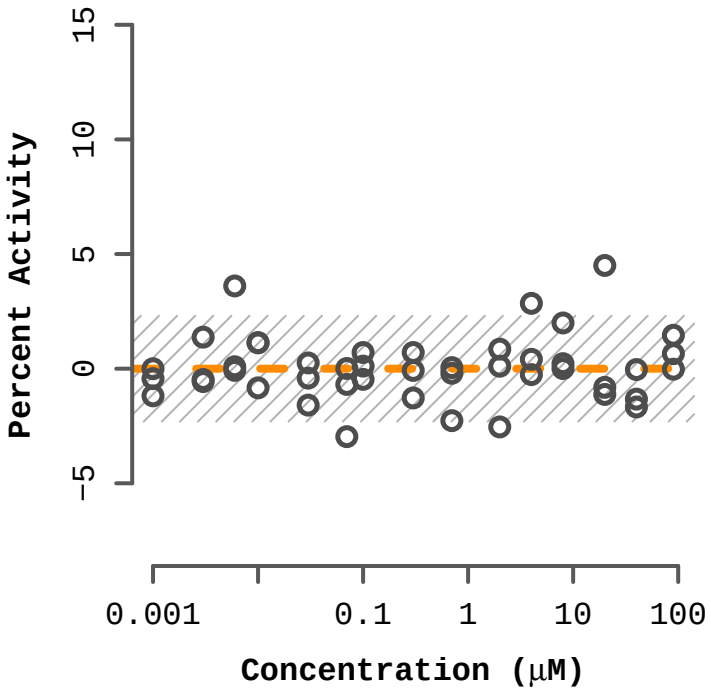
NAME: N-Nitrosobis(2-oxopropyl)amine
CHID: 21022 **CASRN:** 60599-38-4
SPID(S): Tox21_301235
M4ID: 12477898

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

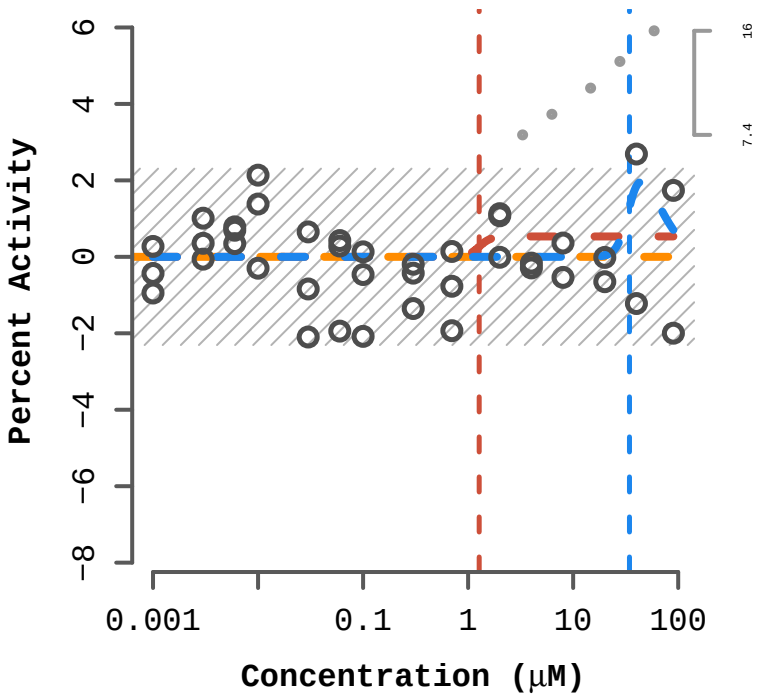
NAME: N-Nitrosodibutylamine
CHID: 21026 **CASRN:** 924-16-3
SPID(S): Tox21_300425
M4ID: 12478707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Nitrosodibutylamine
CHID: 21026 **CASRN:** 924-16-3
SPID(S): Tox21_202334
M4ID: 12479918 **BRK**

HILL MODEL (in red):

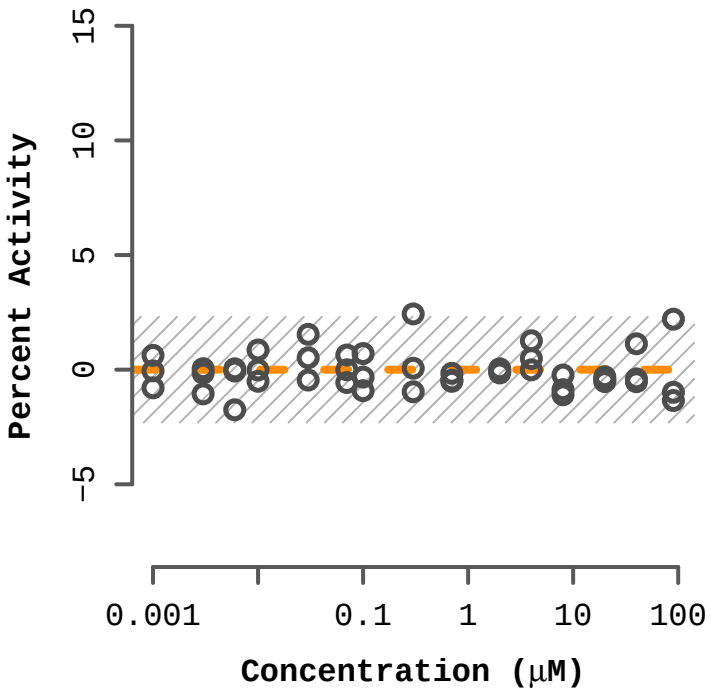
	tp	ga	gw
val:	0.533	0.105	8
sd:	0.471	0.555	19.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.04	1.54	8	1.79	3.1
sd:	30.7	1.59	51.6	2.92	33.8

	CNST	HILL	GNLS
AIC:	217.59	222.18	226.26
PROB:	0.9	0.09	0.01
RMSE:	4.13	3.97	3.94

MAX_MEAN: 5.33 **MAX_MED:** 2.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

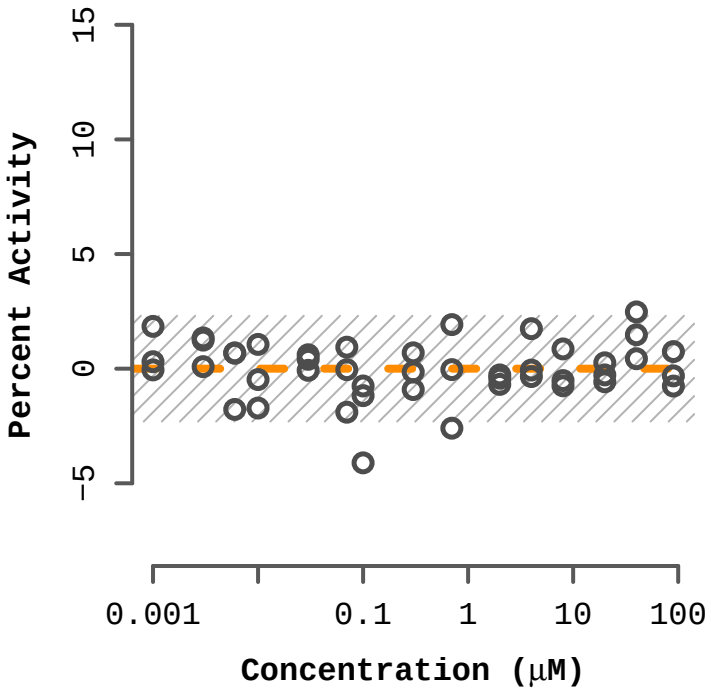
NAME: N-Nitrosodiethanolamine
CHID: 21027 **CASRN:** 1116-54-7
SPID(S): Tox21_200283
M4ID: 12481969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.582 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

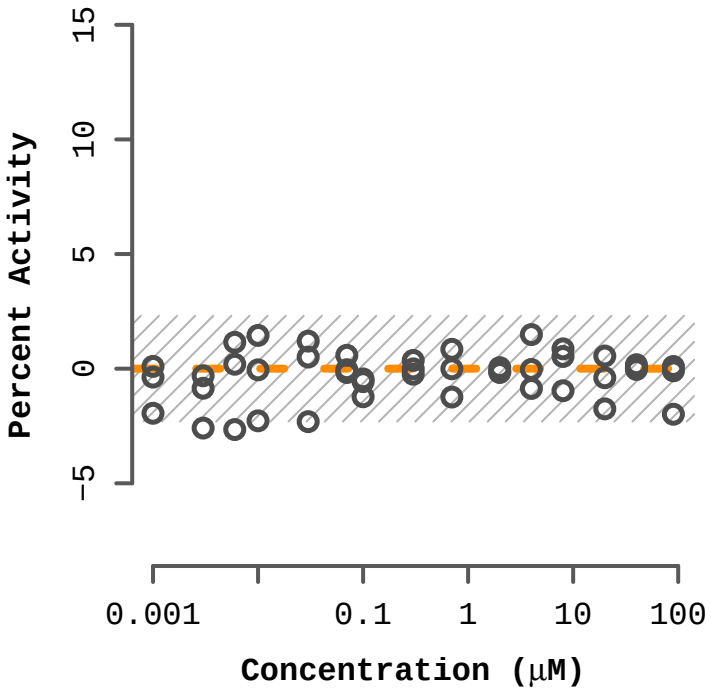
NAME: N-Nitrosodiethylamine
CHID: 21028 **CASRN:** 55-18-5
SPID(S): Tox21_300533
M4ID: 12478599

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

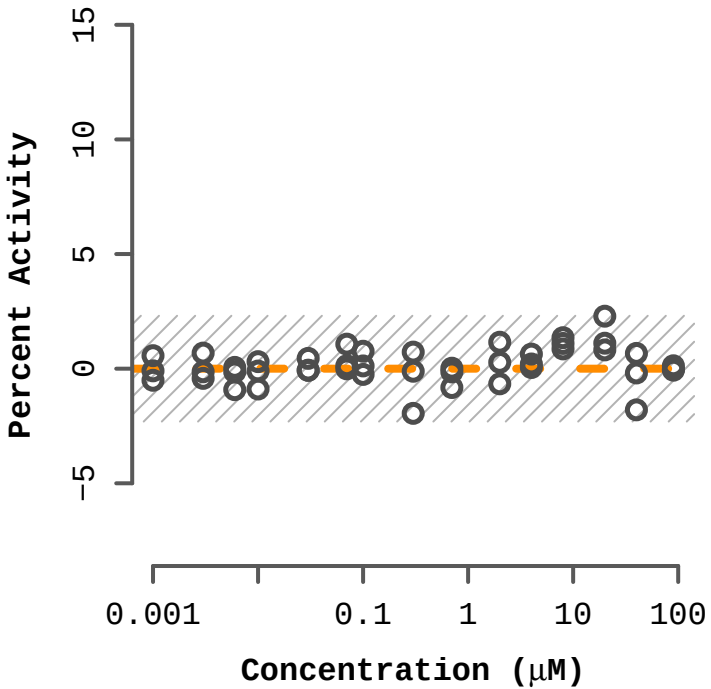
NAME: N-Nitrosodiethylamine
CHID: 21028 **CASRN:** 55-18-5
SPID(S): Tox21_201255
M4ID: 12480997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.198 **MAX_MED:** 0.533 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

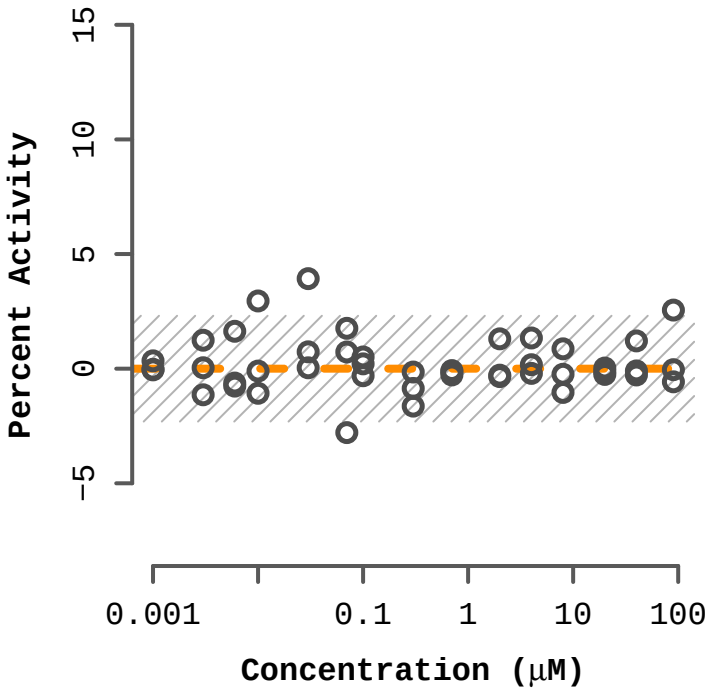
NAME: N-Nitrosodimethylamine
CHID: 21029 **CASRN:** 62-75-9
SPID(S): Tox21_302873
M4ID: 12476260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

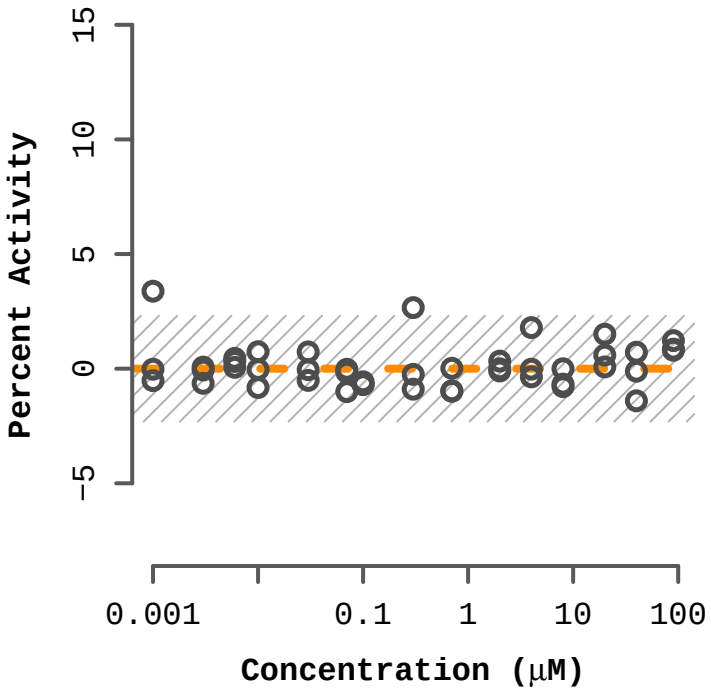
NAME: N-Nitrosodimethylamine
CHID: 21029 **CASRN:** 62-75-9
SPID(S): Tox21_201663
M4ID: 12480589

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 0.737 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

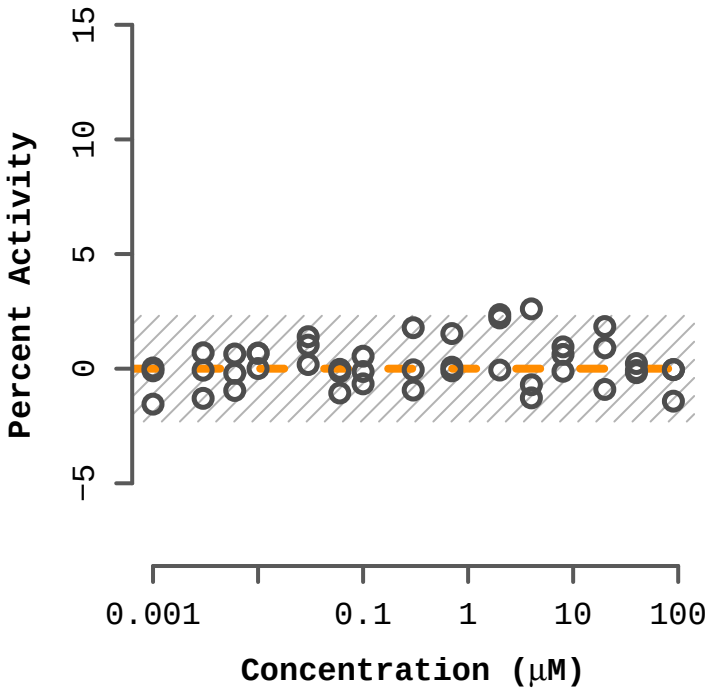
NAME: N-Nitrosodiphenylamine
CHID: 21030 CASRN: 86-30-6
SPID(S): Tox21_300574
M4ID: 12478559

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.961 MAX_MED: 0.853 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

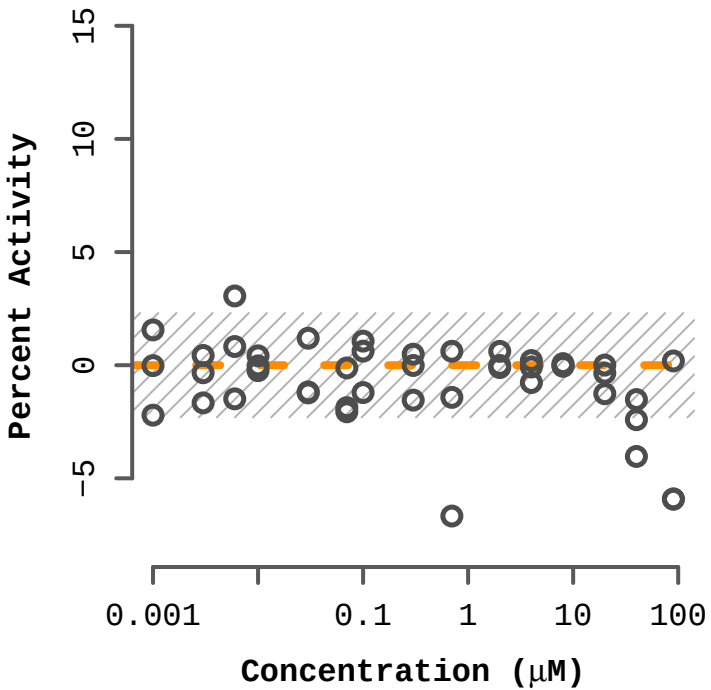
NAME: N-Nitrosodiphenylamine
CHID: 21030 **CASRN:** 86-30-6
SPID(S): Tox21_201457
M4ID: 12480795

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

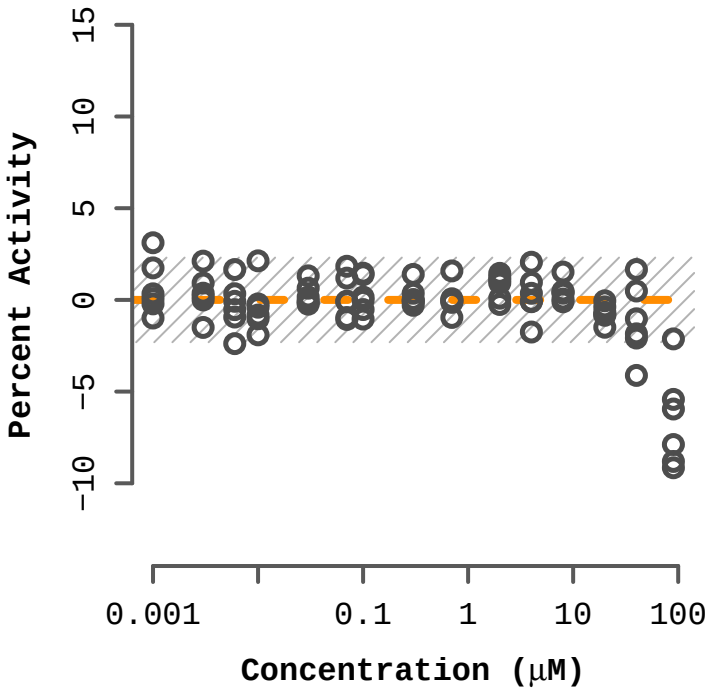
NAME: 4-Nitrosodiphenylamine
CHID: 21031 **CASRN:** 156-10-5
SPID(S): Tox21_302822
M4ID: 12476311

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

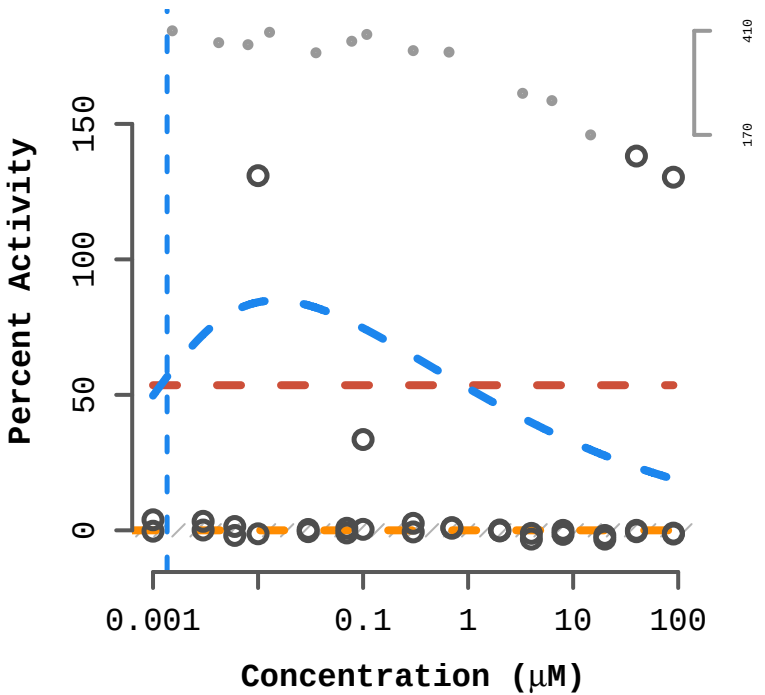
NAME: 4-Nitrosodiphenylamine
CHID: 21031 **CASRN:** 156-10-5
SPID(S): Tox21_201708
M4ID: 12480544

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	344.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.12	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 0.998 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Nitrosodipropylamine
CHID: 21032 CASRN: 621-64-7
SPID(S): Tox21_300388
M4ID: 12478744 BRK

HILL MODEL (in red):

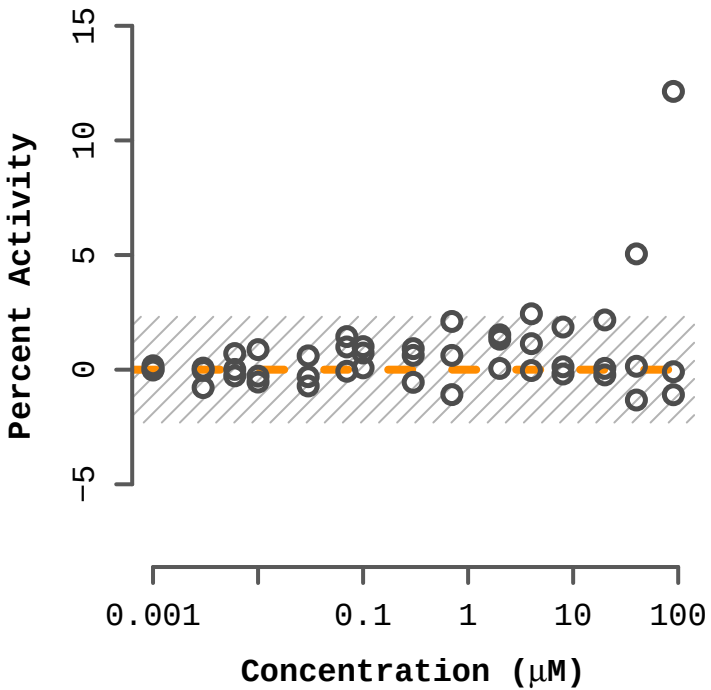
	tp	ga	gw
val:	53.6	-3.74	7.96
sd:	21.4	762	8170

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	139	-2.87	0.892	-0.718	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	643.2	589.51	593.19
PROB:	0	0.86	0.14
RMSE:	184.09	161.07	157.07

MAX_MEAN: 178 MAX_MED: 131 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

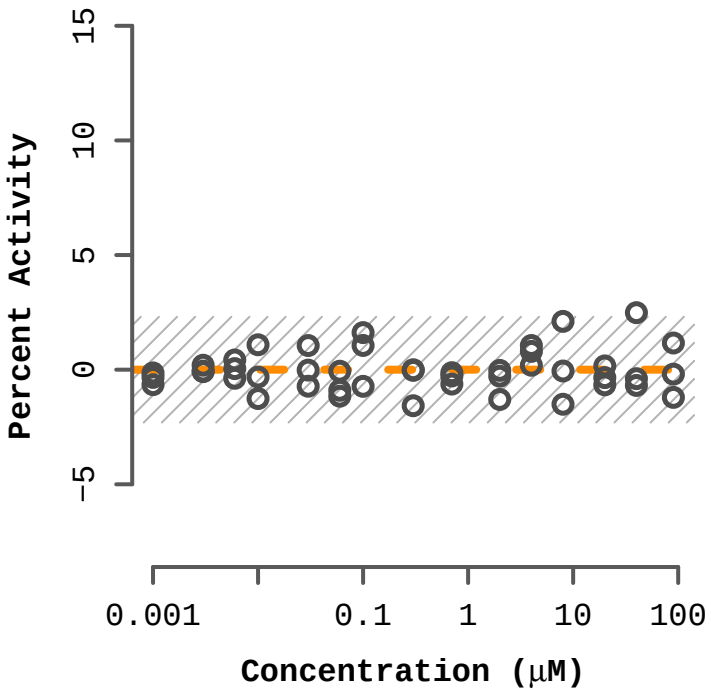
NAME: N-Nitrosodipropylamine
CHID: 21032 **CASRN:** 621-64-7
SPID(S): Tox21_201860
M4ID: 12480392

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 3.65 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

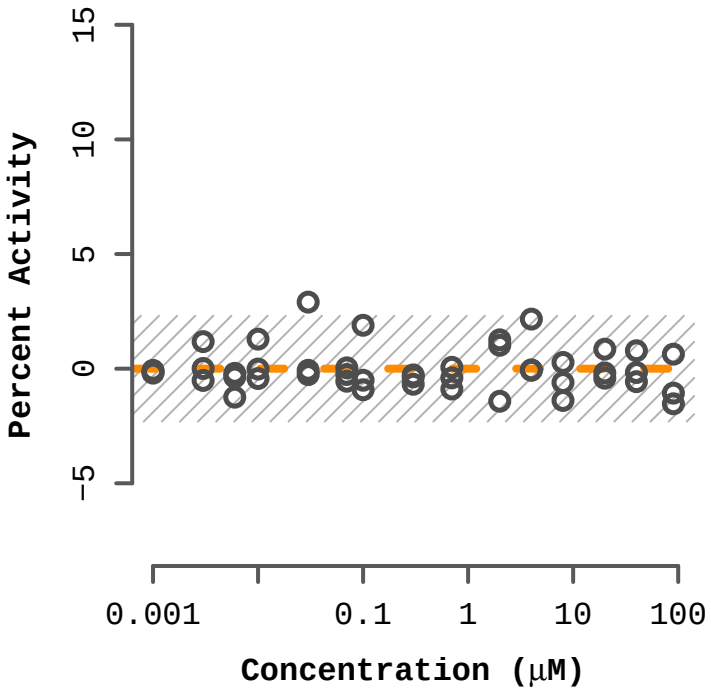
NAME: N-Nitroso-N-methylethylamine
CHID: 21036 **CASRN:** 10595-95-6
SPID(S): Tox21_200744
M4ID: 12481508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.683 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

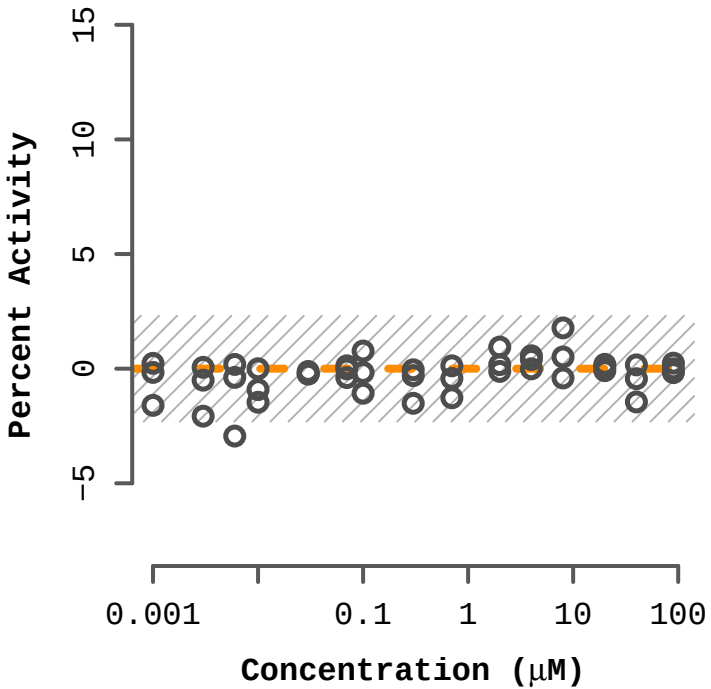
NAME: Nitrosoheptamethyleneimine
CHID: 21039 **CASRN:** 20917-49-1
SPID(S): Tox21_302962
M4ID: 12476171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

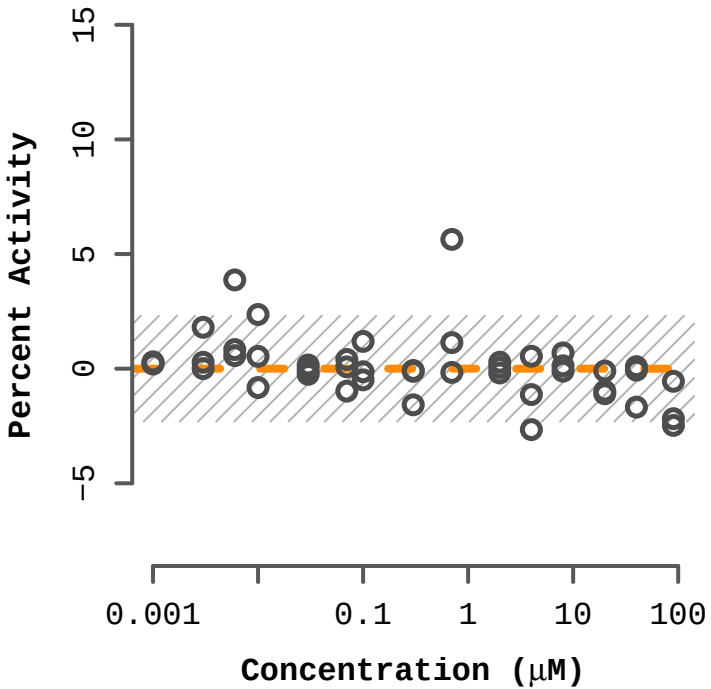
NAME: Nitrosoheptamethyleneimine
CHID: 21039 **CASRN:** 20917-49-1
SPID(S): Tox21_201434
M4ID: 12480818

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.63 **MAX_MED:** 0.512 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

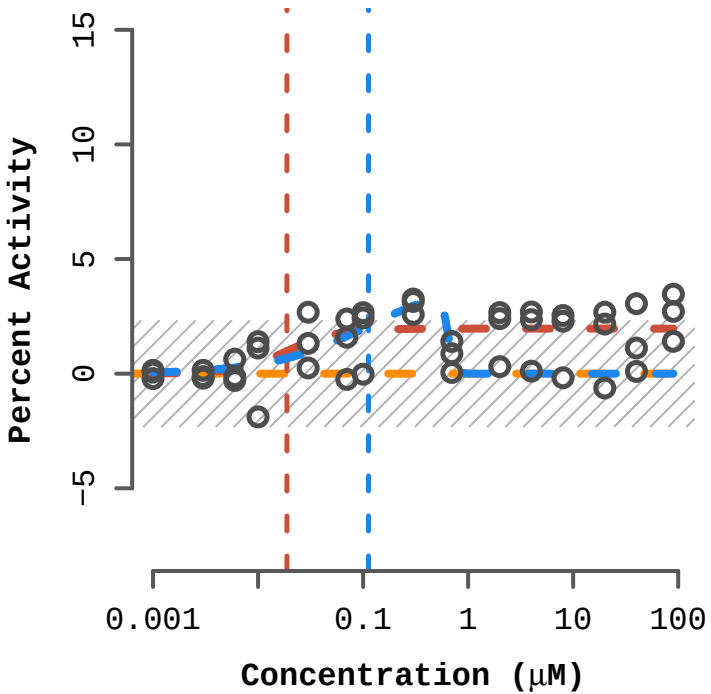
NAME: N-Nitrosohexamethyleneimine
CHID: 21040 **CASRN:** 932-83-2
SPID(S): Tox21_302820
M4ID: 12476313

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nitrosomethylaniline
CHID: 21053 **CASRN:** 614-00-6
SPID(S): Tox21_302747
M4ID: 12476386

HILL MODEL (in red):

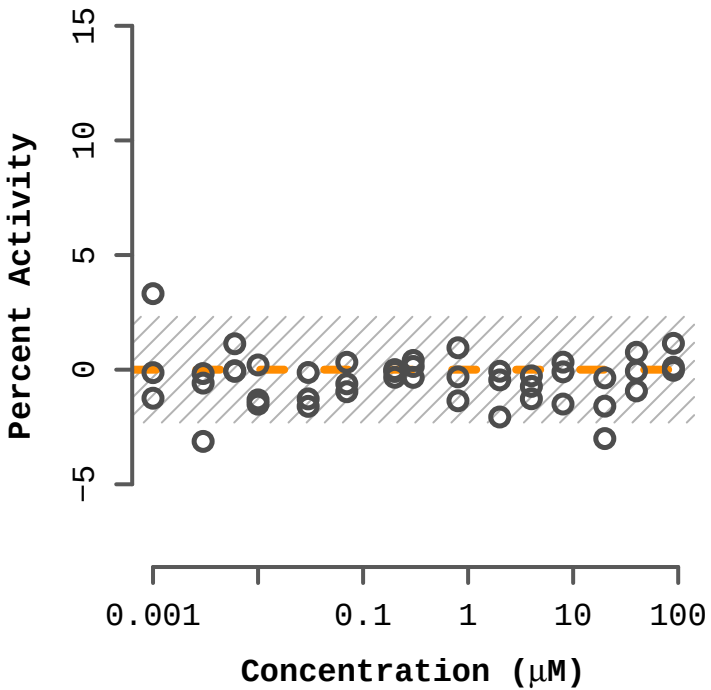
	tp	ga	gw
val:	1.97	−1.73	1.85
sd:	0.251	0.305	1.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.16	−0.948	0.918	−0.192	14.4
sd:	3.88	1.04	0.722	1.18	453

	CNST	HILL	GNLS
AIC:	188.6	148.74	178.06
PROB:	0	1	0
RMSE:	1.82	1.12	1.51

MAX_MEAN: 3 **MAX_MED:** 3.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

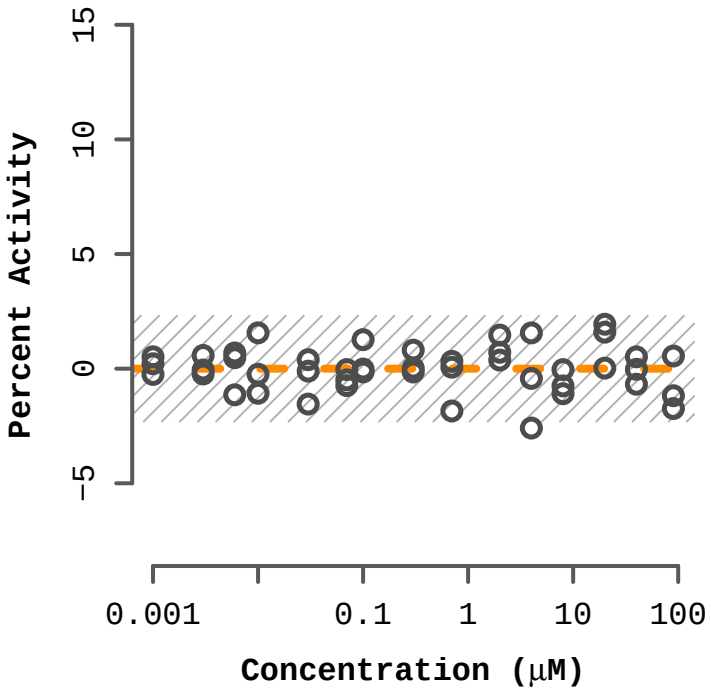
NAME: Nitrosomethylaniline
CHID: 21053 **CASRN:** 614-00-6
SPID(S): Tox21_201508
M4ID: 12480744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.649 **MAX_MED:** 0.141 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

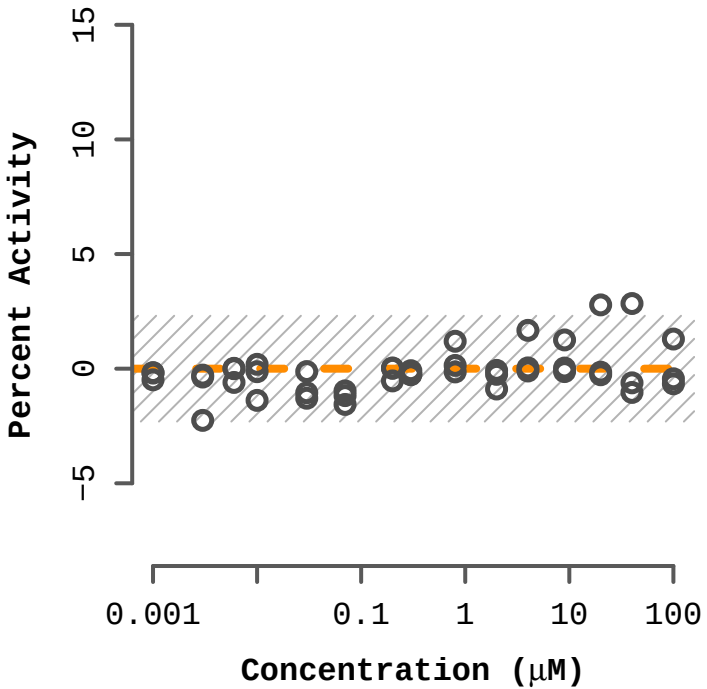
NAME: N-Nitrosomorpholine
CHID: 21056 **CASRN:** 59-89-2
SPID(S): Tox21_302867
M4ID: 12476266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

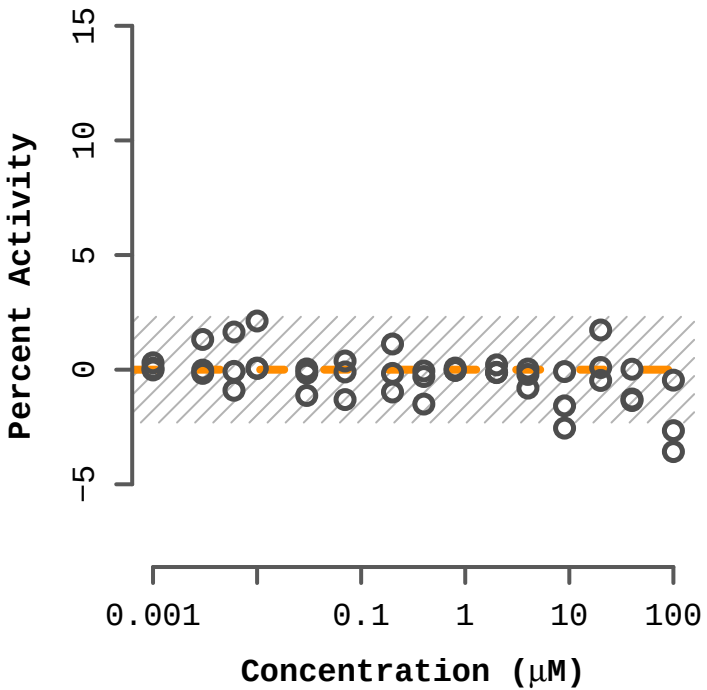
NAME: N-Nitrosomorpholine
CHID: 21056 **CASRN:** 59-89-2
SPID(S): Tox21_202132
M4ID: 12480120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.143 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

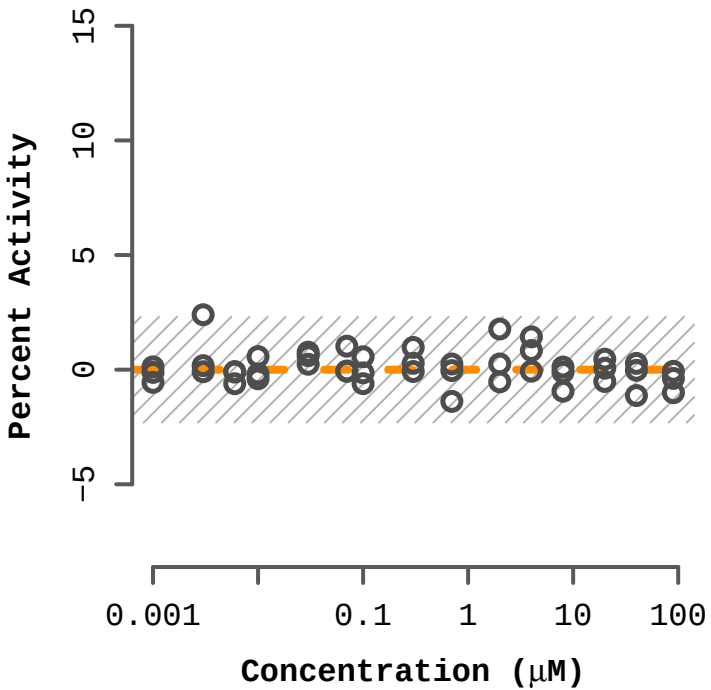
NAME: N-Nitrosopiperazine
CHID: 21059 **CASRN:** 5632-47-3
SPID(S): Tox21_202786
M4ID: 12479466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.75 **MAX_MED:** 0.096 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

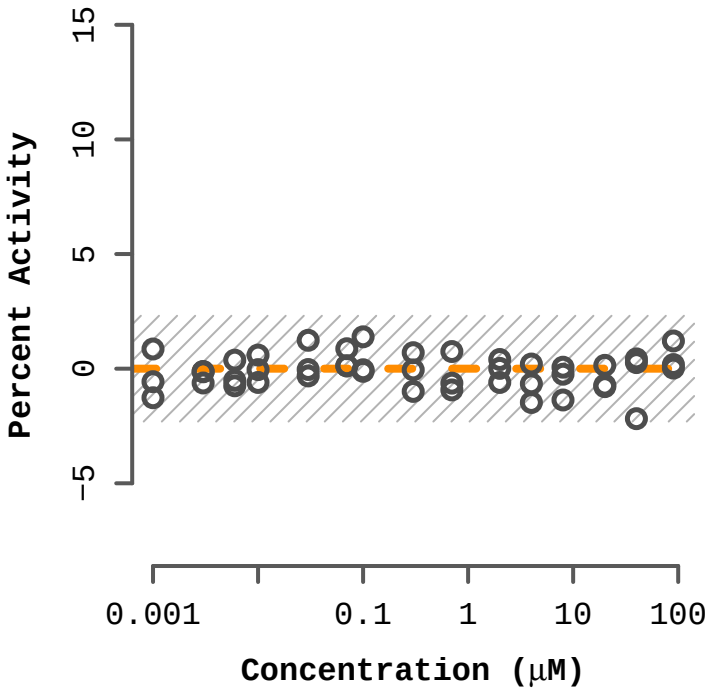
NAME: N-Nitrosopiperidine
CHID: 21060 **CASRN:** 100-75-4
SPID(S): Tox21_200267
M4ID: 12481985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.83 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

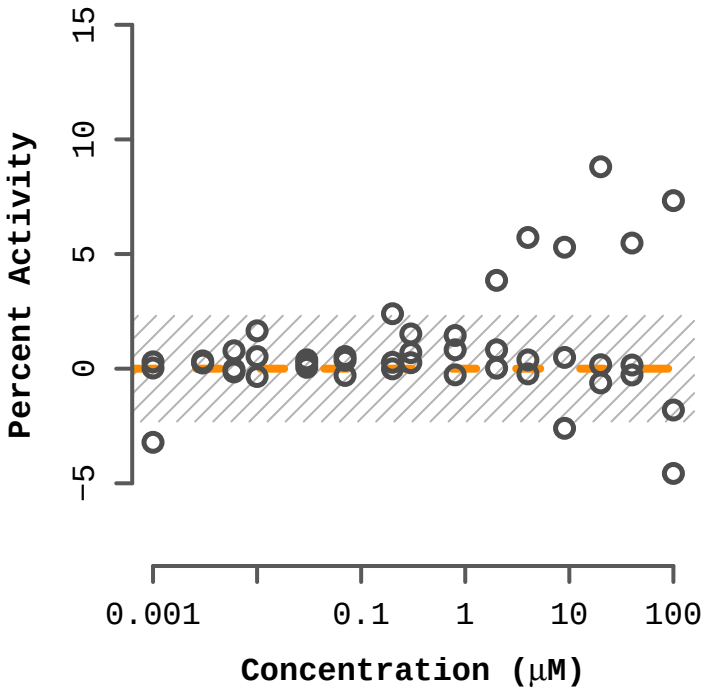
NAME: N-Nitrosopyrrolidine
CHID: 21062 **CASRN:** 930-55-2
SPID(S): Tox21_302913
M4ID: 12476220

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.473 **MAX_MED:** 0.267 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

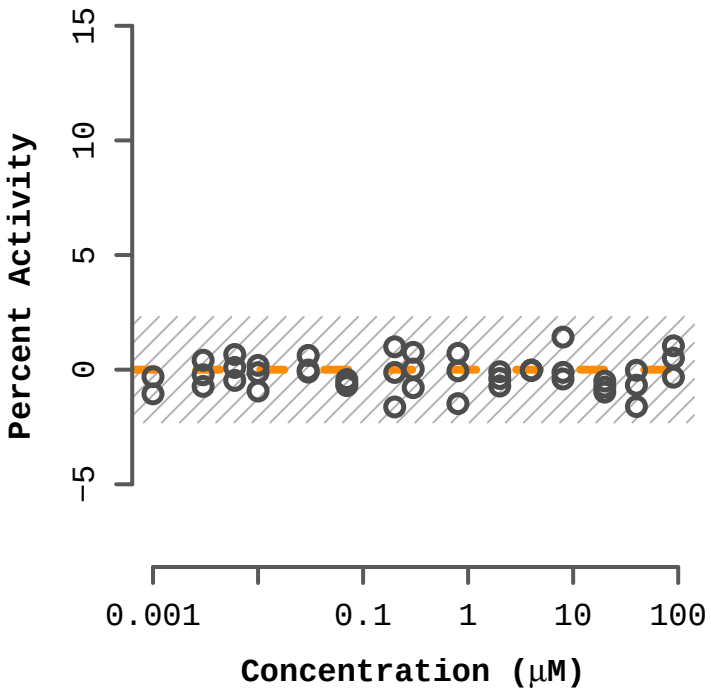
NAME: N-Nitrosopyrrolidine
CHID: 21062 **CASRN:** 930-55-2
SPID(S): Tox21_202356
M4ID: 12479896

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.57	NA	NA

MAX_MEAN: 2.79 **MAX_MED:** 0.826 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

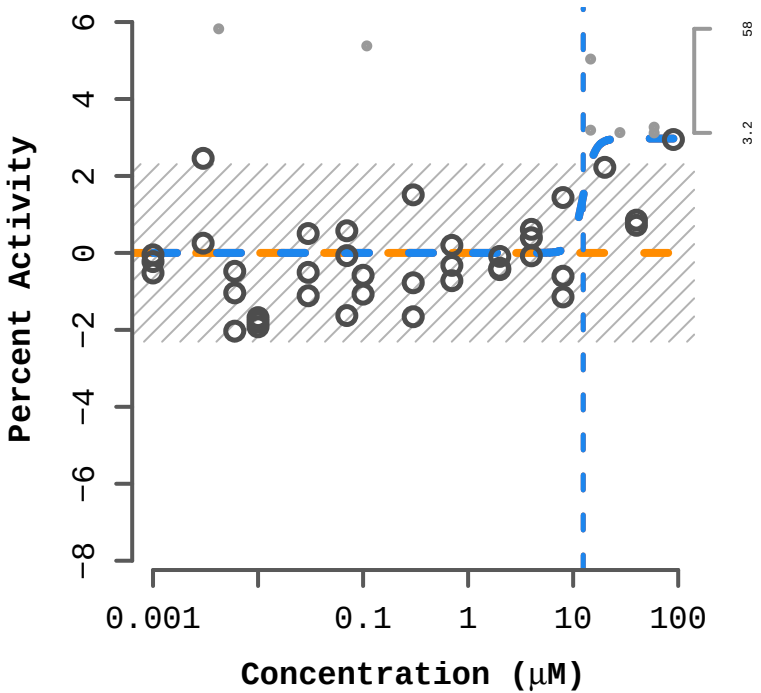
NAME: 2-Nitrosotoluene
CHID: 21065 CASRN: 611-23-4
SPID(S): Tox21_200917
M4ID: 12481335

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.407 MAX_MED: 0.504 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norharman
CHID: 21070 CASRN: 244-63-3
SPID(S): Tox21_200083
M4ID: 12482169 BRK

HILL MODEL (in red):

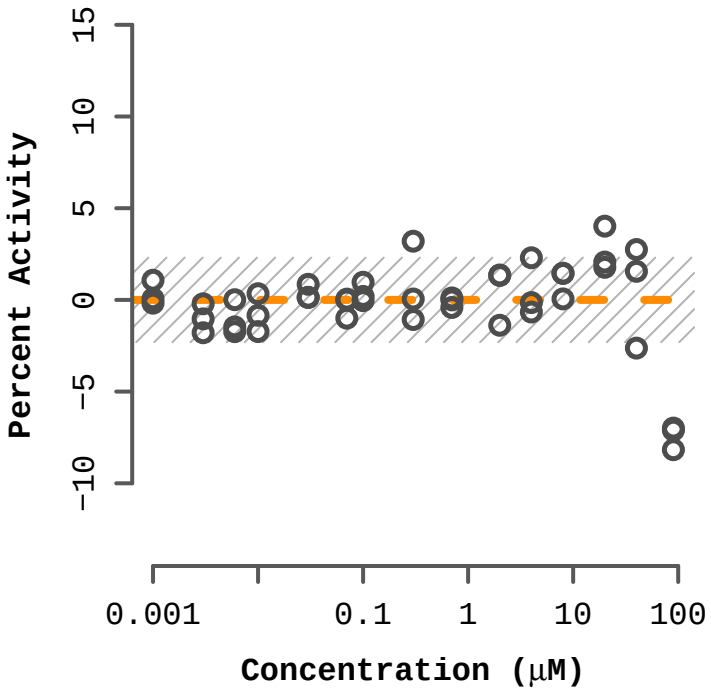
	tp	ga	gw
val:	2.97	1.1	8
sd:	0.579	0.195	8.02

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.97	1.1	8	2.54	17.7
sd:	0.579	0.195	8.01	2810	81700

	CNST	HILL	GNLS
AIC:	257.77	244.09	248.09
PROB:	0	0.88	0.12
RMSE:	13.13	12.86	12.86

MAX_MEAN: 20.3 MAX_MED: 4.65 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

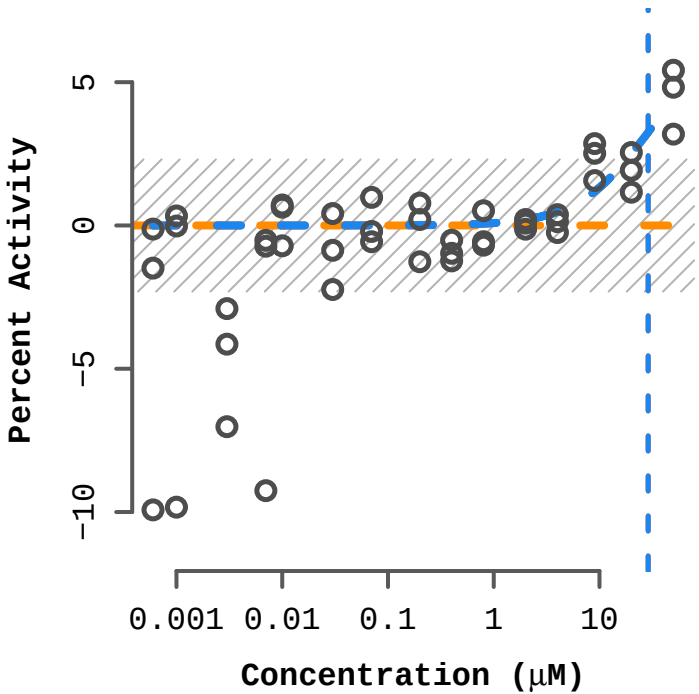
NAME: Omeprazole
CHID: 21080 CASRN: 73590-58-6
SPID(S): Tox21_200509
M4ID: 12481743

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.36	NA	NA

MAX_MEAN: 2.62 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Omeprazole
CHID: 21080 CASRN: 73590-58-6
SPID(S): Tox21_110686_1
M4ID: 12484179

HILL MODEL (in red):

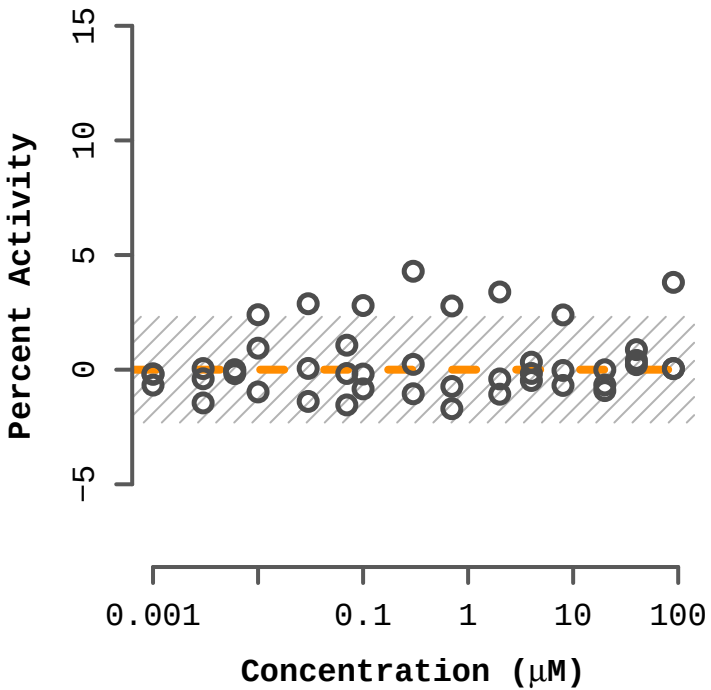
	tp	ga	gw
val:	6.5	1.46	1.29
sd:	4.68	0.55	0.582

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.5	1.46	1.29	3.18	4.05
sd:	4.69	0.551	0.583	234	649

	CNST	HILL	GNLS
AIC:	218.86	199.47	203.47
PROB:	0	0.88	0.12
RMSE:	3.21	2.92	2.92

MAX_MEAN: 4.48 MAX_MED: 4.82 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

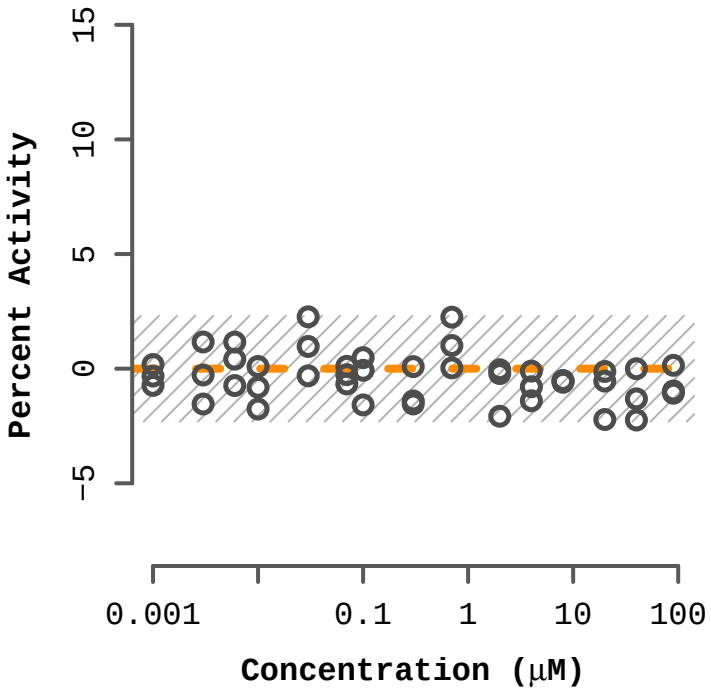
NAME: C.I. Acid Orange 3
CHID: 21081 **CASRN:** 6373-74-6
SPID(S): Tox21_301886
M4ID: 12477247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

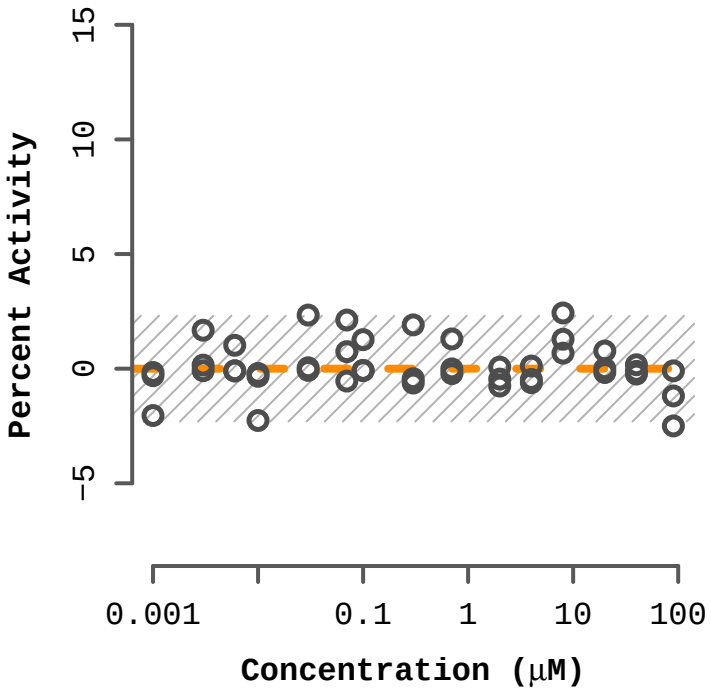
NAME: C.I. Acid Orange 10
CHID: 21082 **CASRN:** 1936-15-8
SPID(S): Tox21_303019
M4ID: 12476114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

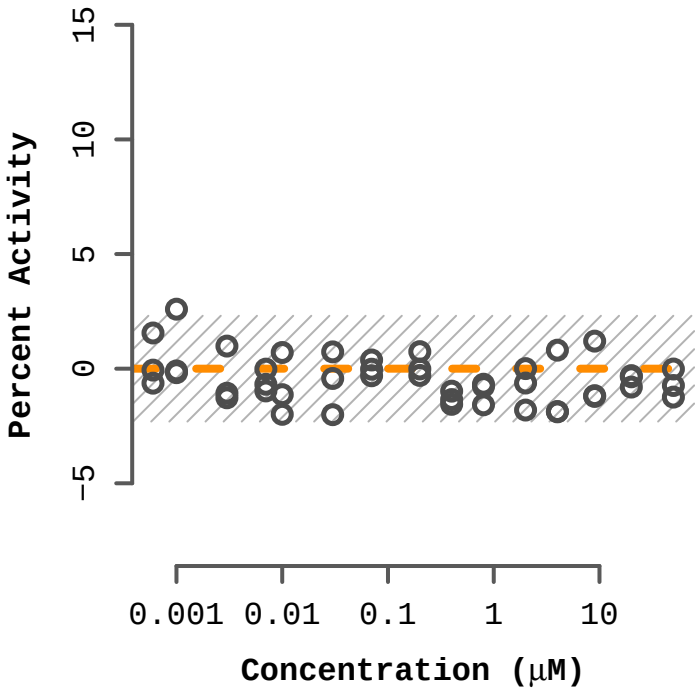
NAME: C.I. Acid Orange 10
CHID: 21082 CASRN: 1936-15-8
SPID(S): Tox21_202154
M4ID: 12480098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.46 MAX_MED: 1.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

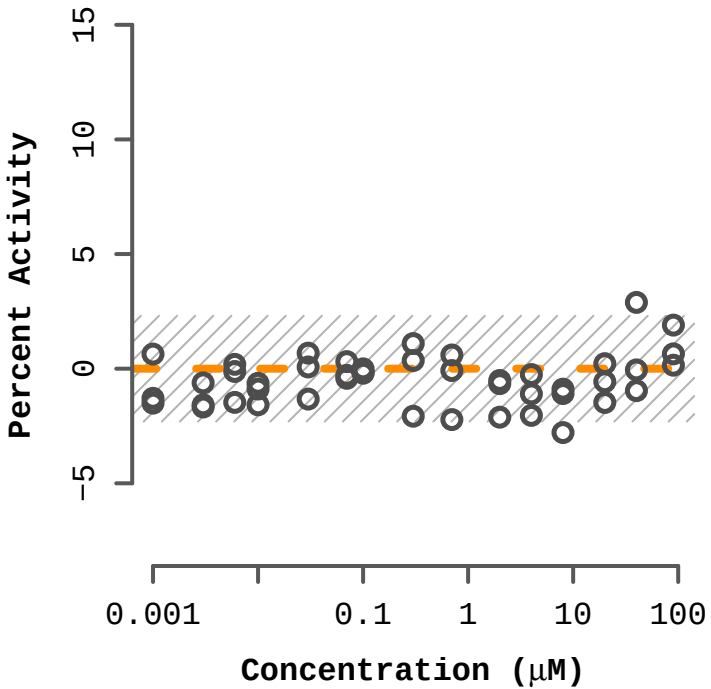
NAME: gamma-Oryzanol
CHID: 21084 **CASRN:** 11042-64-1
SPID(S): Tox21_112482_1
M4ID: 12483075

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.776 **MAX_MED:** −0.0122 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

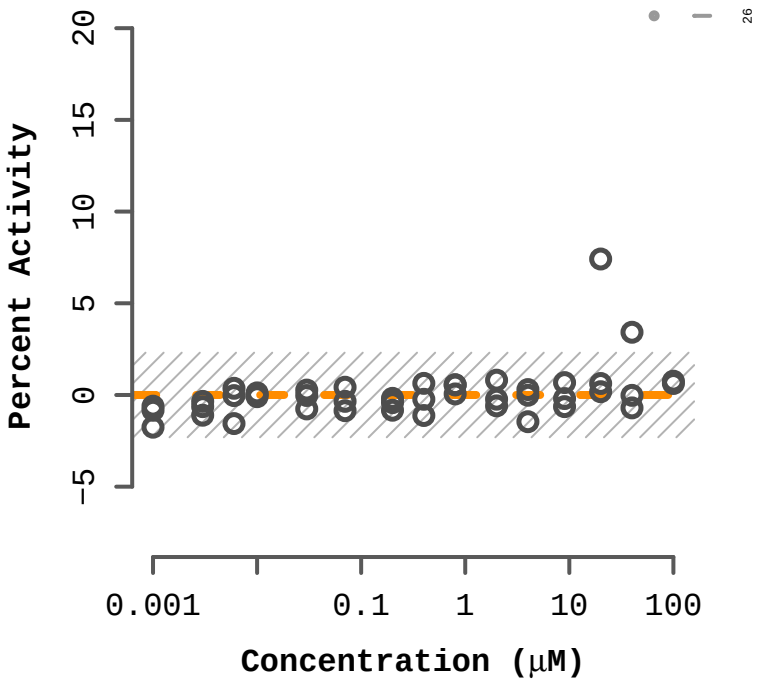
NAME: Oxamyl
CHID: 21086 **CASRN:** 23135-22-0
SPID(S): Tox21_301156
M4ID: 12477977

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.901 **MAX_MED:** 0.647 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

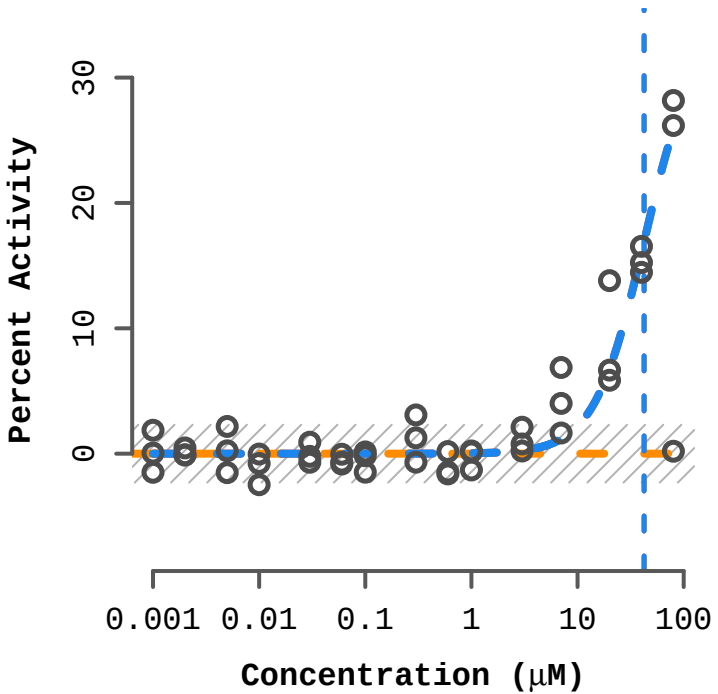
NAME: Oxamyl
CHID: 21086 **CASRN:** 23135-22-0
SPID(S): Tox21_201731
M4ID: 12480521 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.54	NA	NA
PROB:	1	NA	NA
RMSE:	4.1	NA	NA

MAX_MEAN: 9.08 **MAX_MED:** 0.753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxazepam
CHID: 21087 CASRN: 604-75-1
SPID(S): Tox21_303501
M4ID: 12475641

HILL MODEL (in red):

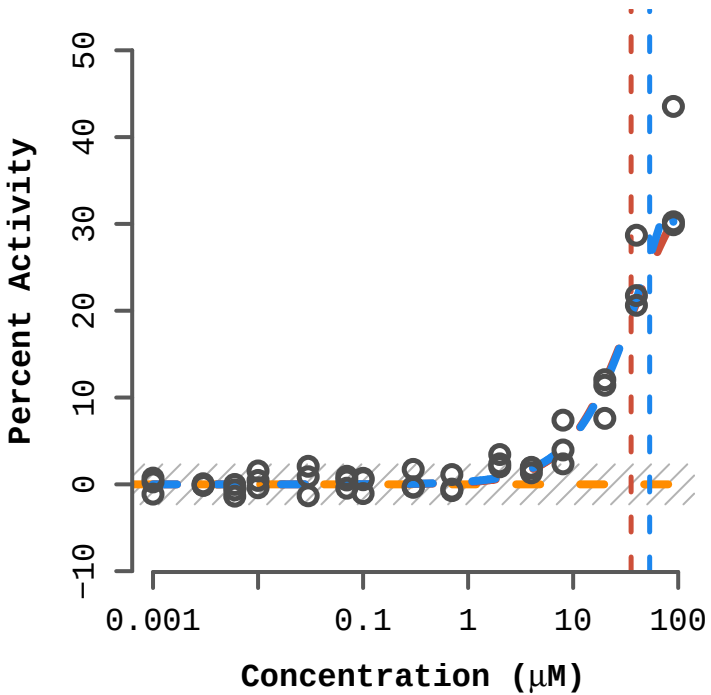
	tp	ga	gw
val:	33.8	1.63	1.85
sd:	4.05	0.0654	0.285

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	33.8	1.63	1.85	3.89	14.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	279.24	198.98	202.98
PROB:	0	0.88	0.12
RMSE:	7.57	4.23	4.23

MAX_MEAN: 18.2 MAX_MED: 26.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxazepam
CHID: 21087 CASRN: 604-75-1
SPID(S): Tox21_200700
M4ID: 12481552

HILL MODEL (in red):

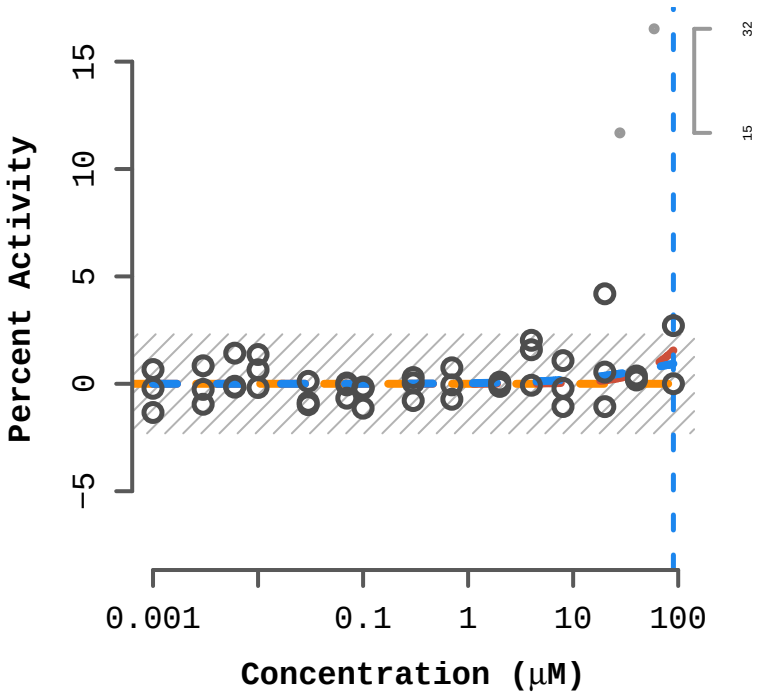
	tp	ga	gw
val:	38.6	1.55	1.41
sd:	3.46	0.0698	0.169

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	52.2	1.73	1.28	2	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	316.55	181.7	183.76
PROB:	0	0.74	0.26
RMSE:	11.44	2.59	2.56

MAX_MEAN: 34.6 MAX_MED: 30.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxolinic acid
CHID: 21089 CASRN: 14698-29-4
SPID(S): Tox21_202787
M4ID: 12479465 BRK

HILL MODEL (in red):

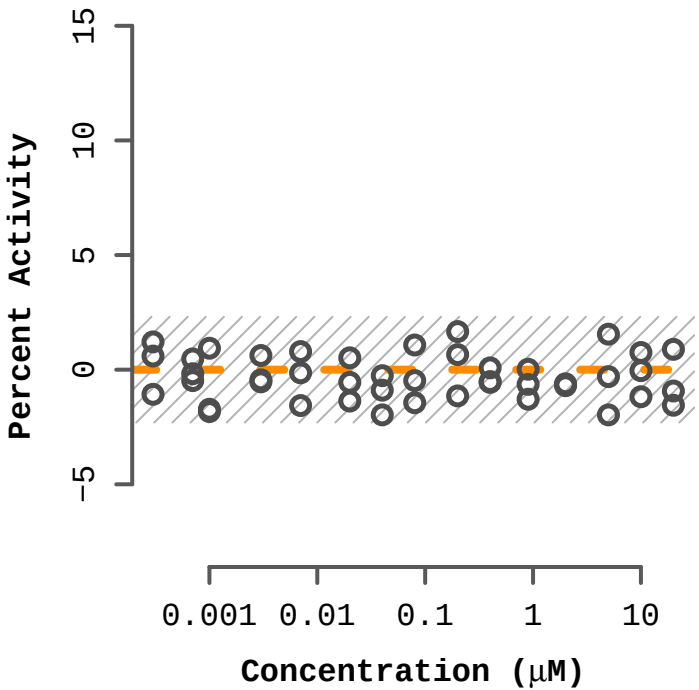
	tp	ga	gw
val:	11.1	2.45	1.58
sd:	116	4.09	3.37

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.87	1.95	0.92	3.6	3.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	175.98	179.46	183.58
PROB:	0.84	0.15	0.02
RMSE:	5.36	5.11	5.18

MAX_MEAN: 11.6 **MAX_MED:** 2.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

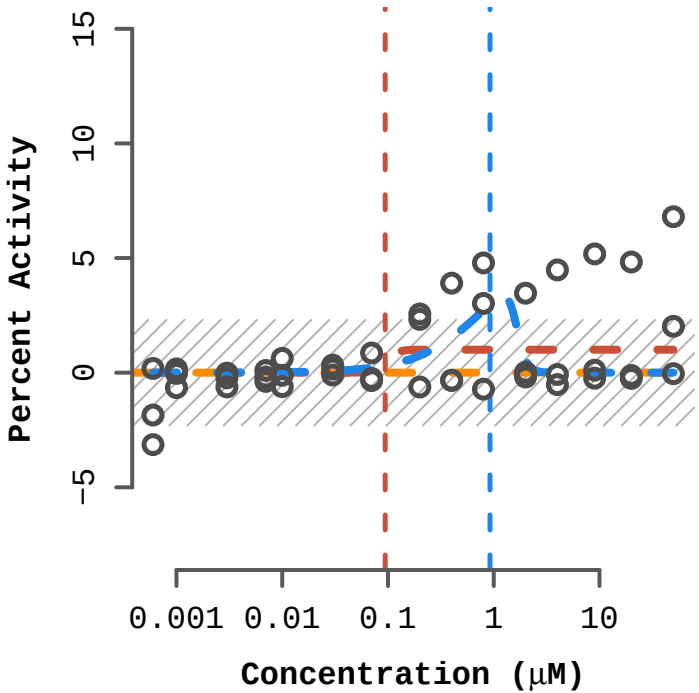
NAME: Oxolinic acid
CHID: 21089 **CASRN:** 14698-29-4
SPID(S): Tox21_110216_1
M4ID: 12484544

HILL MODEL: Not applicable.

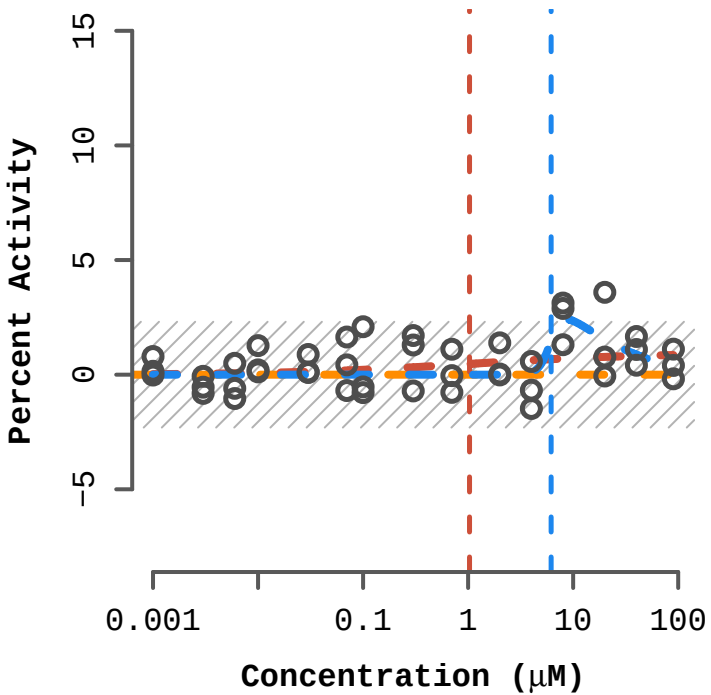
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

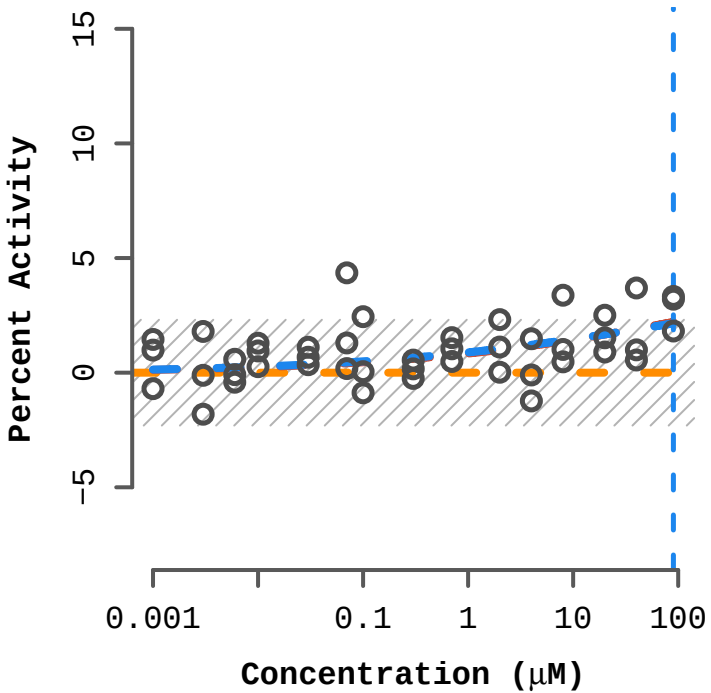
MAX_MEAN: 0.394 **MAX_MED:** 0.659 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Oxprenolol hydrochloride
CHID:    21093   CASRN: 6452-73-9
SPID(S): Tox21_110556_1
M4ID:    12484268

HILL MODEL (in red):
      tp       ga       gw
val:  1        -1.03    8
sd:   0.453    0.508    24.8

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.01     -0.0351  1.28     0.215    9.54
sd:   18.3     1.76     0.995    0.488    52.7

      CNST        HILL        GNLS
AIC:  187.71      187.32      192.04
PROB: 0.43        0.52        0.05
RMSE: 2.16        1.85        2.02

MAX_MEAN: 2.93      MAX_MED: 3.02      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4,4'-Oxydianiline
CHID:    21094   CASRN: 101-80-4
SPID(S): Tox21_300133
M4ID:    12478997

HILL MODEL (in red):
      tp       ga       gw
val:  0.939    0.0134   0.525
sd:   0.571    1.62     0.558

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.31     0.79     8        1.08     1.15
sd:   3.92     0.0947   4.34     0.696    0.704

      CNST        HILL        GNLS
AIC:  143.91      140.36      134.95
PROB: 0.01        0.06        0.93
RMSE: 1.2         1.04        0.91

MAX_MEAN: 2.44      MAX_MED: 2.89      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Oxydianiline
CHID: 21094 CASRN: 101−80−4
SPID(S): Tox21_202035
M4ID: 12480217

HILL MODEL (in red):

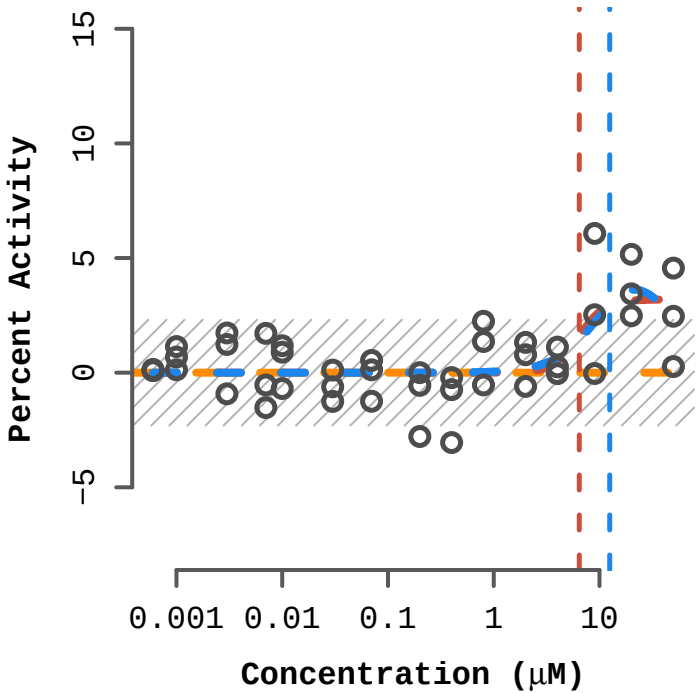
	tp	ga	gw
val:	5.23	2.4	0.3
sd:	5.37	2.52	0.15

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.3	1.95	0.3	3.39	6.05
sd:	4.74	2.65	0.131	2430	10300

	CNST	HILL	GNLS
AIC:	173.05	148.86	153.05
PROB:	0	0.89	0.11
RMSE:	1.62	1.17	1.17

MAX_MEAN: 2.78 MAX_MED: 3.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Oxydiethylenebenzothiazole-2-sulfenamide
CHID: 21096 CASRN: 102-77-2
SPID(S): Tox21_110976_1
M4ID: 12483973

HILL MODEL (in red):

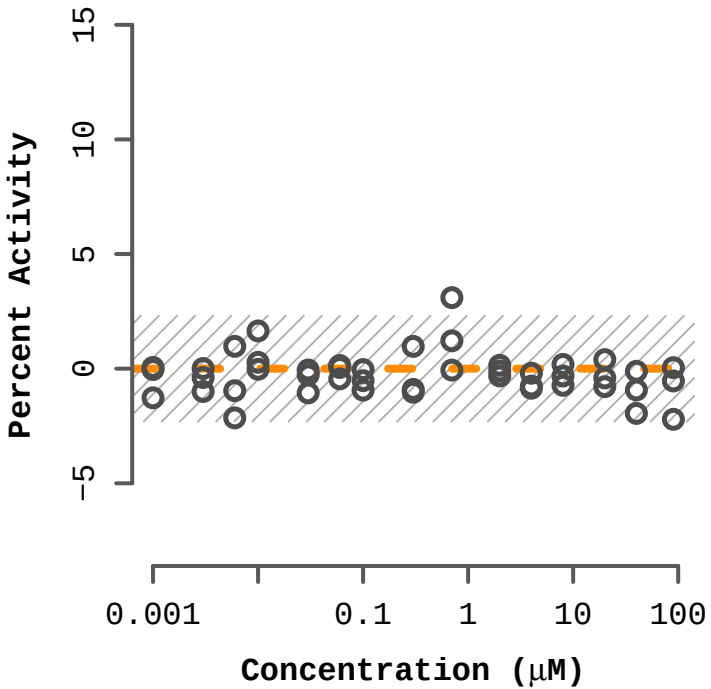
	tp	ga	gw
val:	3.19	0.809	3.62
sd:	0.627	0.155	2.98

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.29	1.1	1.99	1.53	1.51
sd:	31.1	1.18	2.87	2.21	4.91

	CNST	HILL	GNLS
AIC:	181.42	162.8	165.7
PROB:	0	0.81	0.19
RMSE:	1.9	1.35	1.34

MAX_MEAN: 3.7 MAX_MED: 3.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

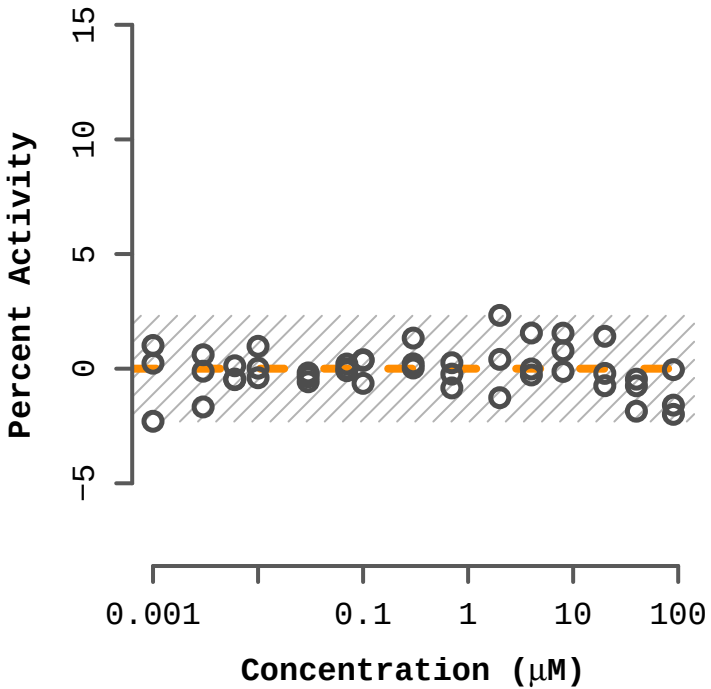
NAME: Oxytetracycline hydrochloride
CHID: 21097 CASRN: 2058-46-0
SPID(S): Tox21_300601
M4ID: 12478532

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

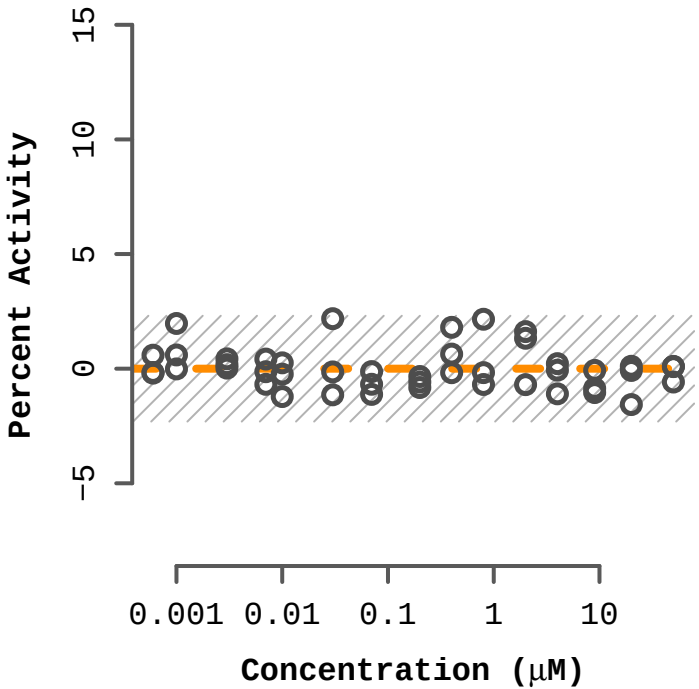
NAME: Oxytetracycline hydrochloride
CHID: 21097 CASRN: 2058-46-0
SPID(S): Tox21_201850
M4ID: 12480402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.738 **MAX_MED:** 0.785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

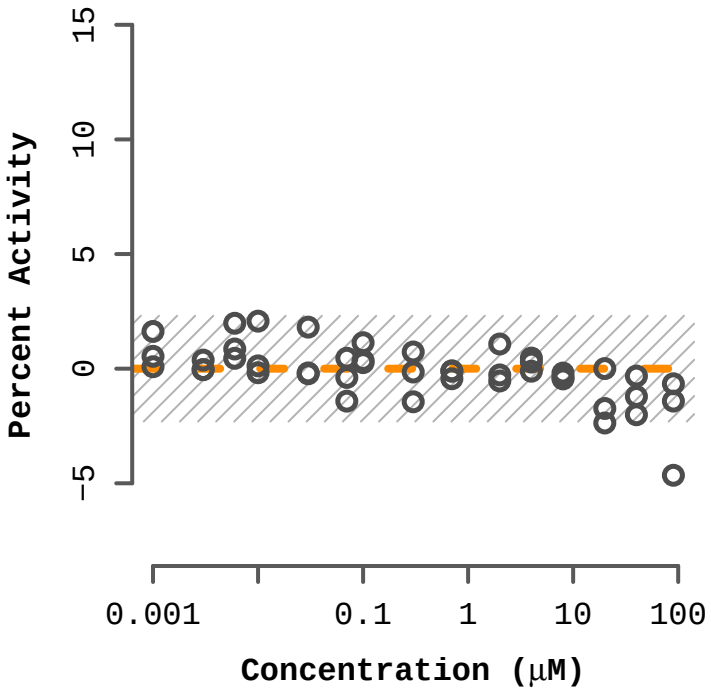
NAME: Parathion
CHID: 21100 **CASRN:** 56-38-2
SPID(S): Tox21_300663
M4ID: 12478470

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

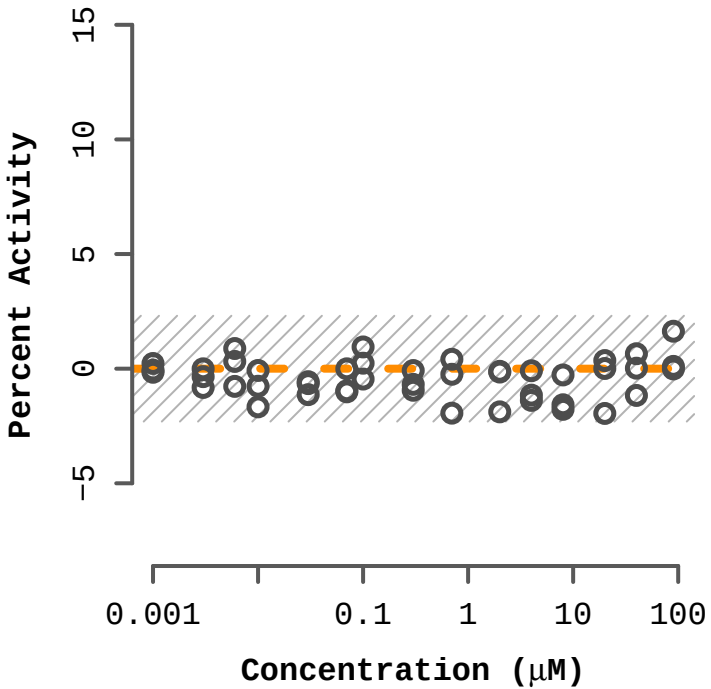
NAME: Parathion
CHID: 21100 **CASRN:** 56-38-2
SPID(S): Tox21_202005
M4ID: 12480247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

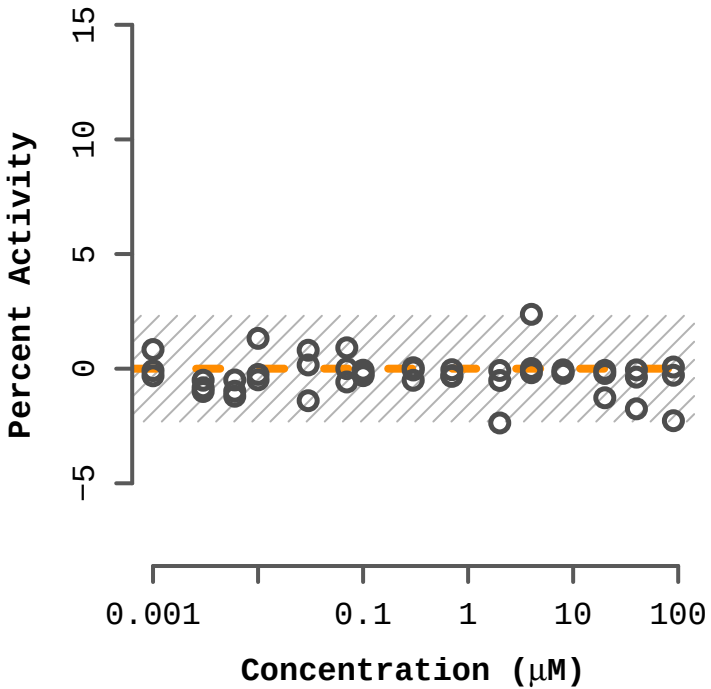
NAME: Penicillin VK
CHID: 21102 **CASRN:** 132-98-9
SPID(S): Tox21_302914
M4ID: 12476219

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.575 **MAX_MED:** 0.316 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

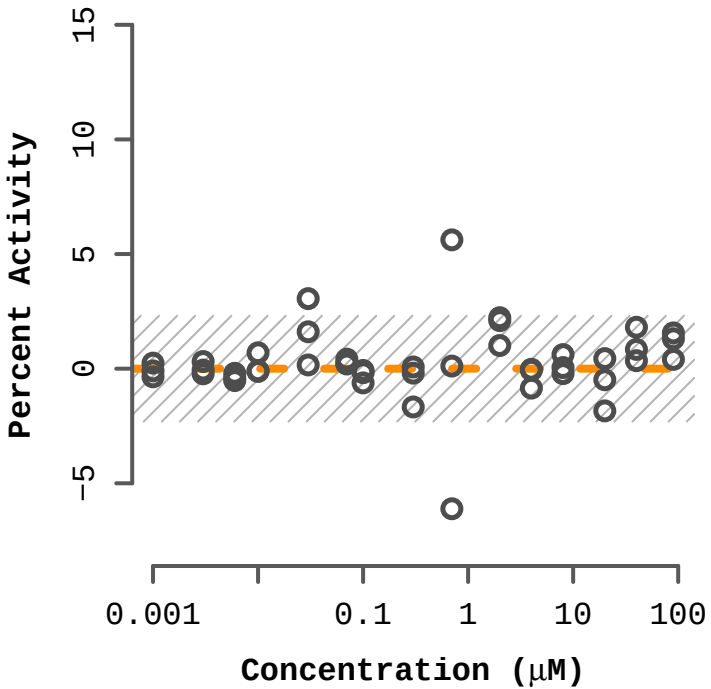
NAME: Penicillin VK
CHID: 21102 **CASRN:** 132-98-9
SPID(S): Tox21_202176
M4ID: 12480076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.736 **MAX_MED:** 0.165 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

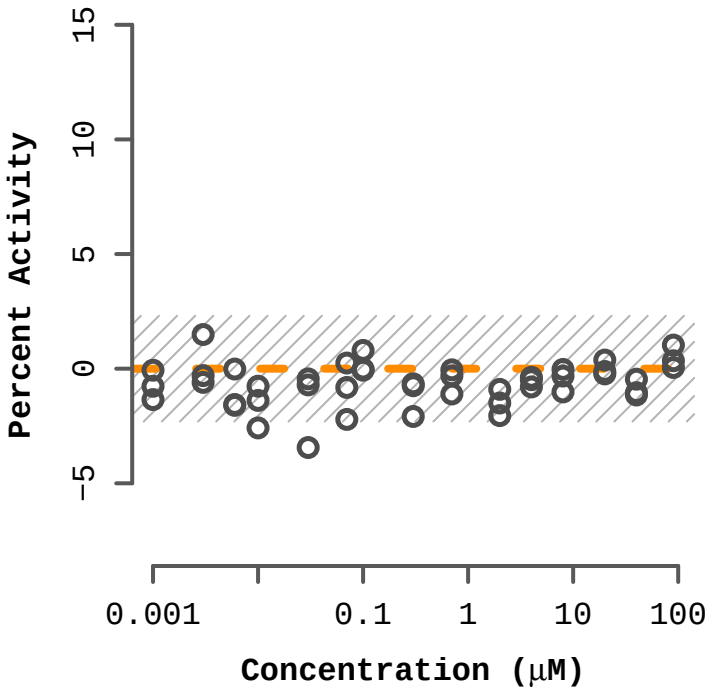
NAME: Pentachloroanisole
CHID: 21103 **CASRN:** 1825-21-4
SPID(S): Tox21_302835
M4ID: 12476298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

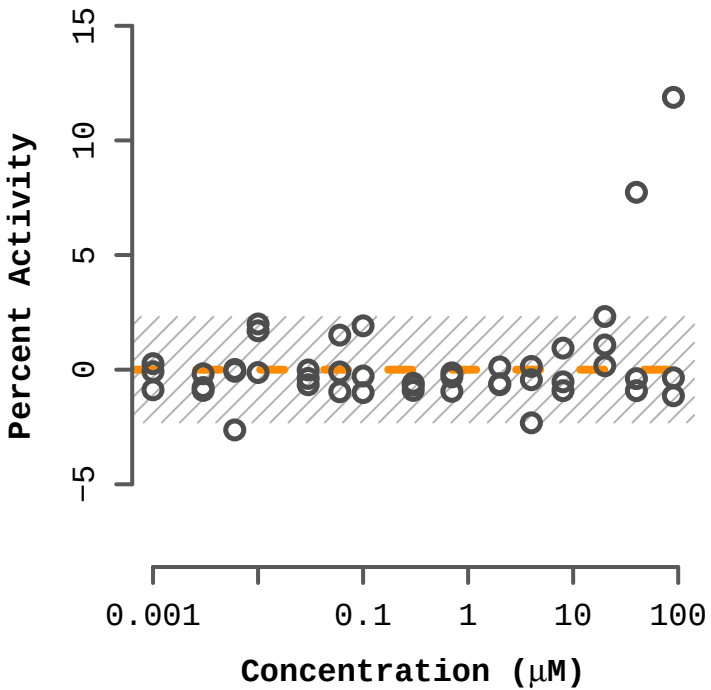
NAME: Pentachloroanisole
CHID: 21103 **CASRN:** 1825-21-4
SPID(S): Tox21_201560
M4ID: 12480692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.477 **MAX_MED:** 0.347 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

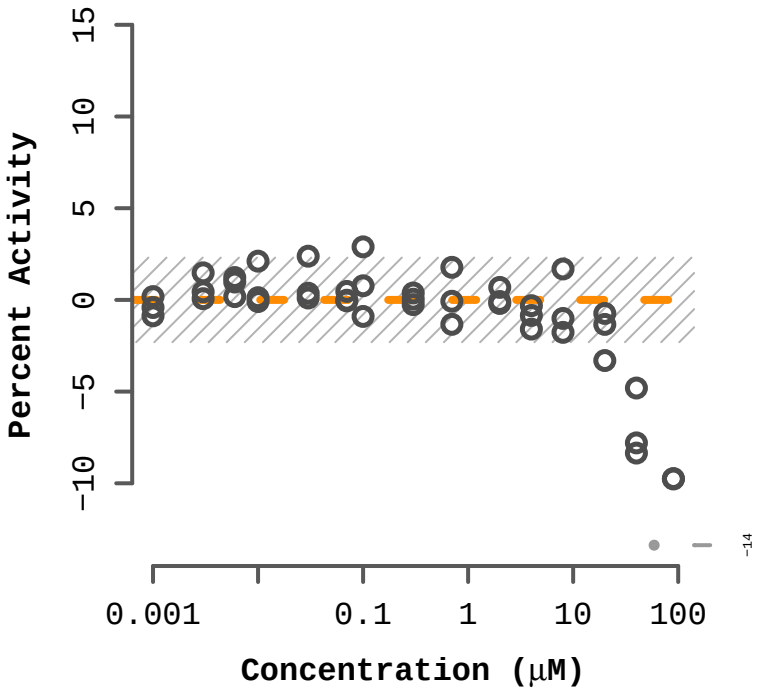
NAME: Pentachloroethane
CHID: 21104 **CASRN:** 76-01-7
SPID(S): Tox21_201141
M4ID: 12481111

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.27	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 3.46 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

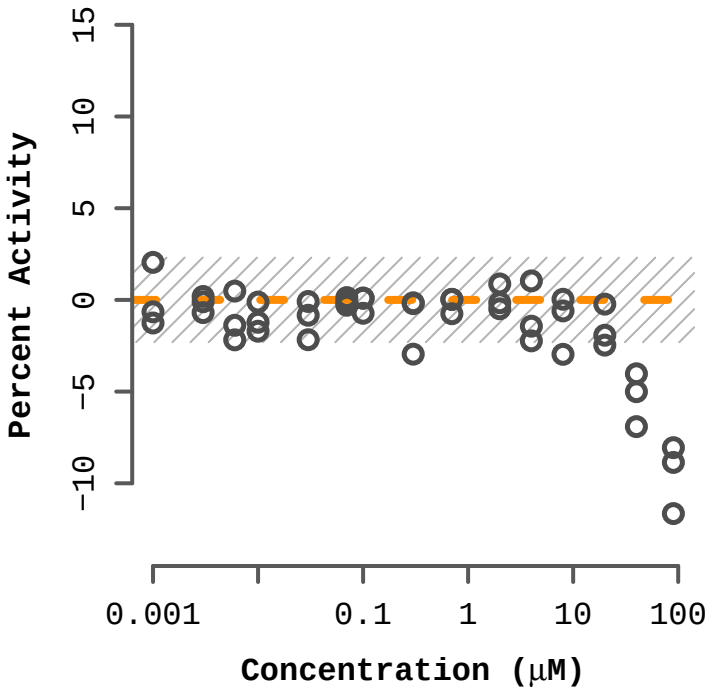
NAME: Pentachloronitrobenzene
CHID: 21105 CASRN: 82-68-8
SPID(S): Tox21_301060
M4ID: 12478073 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.7	NA	NA
PROB:	1	NA	NA
RMSE:	3.6	NA	NA

MAX_MEAN: 0.952 MAX_MED: 0.975 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

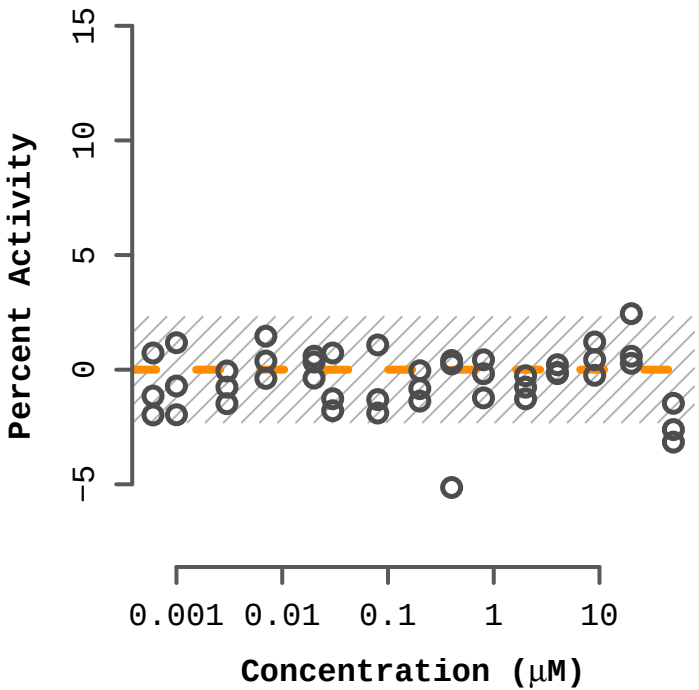
NAME: Pentachloronitrobenzene
CHID: 21105 **CASRN:** 82-68-8
SPID(S): Tox21_201947
M4ID: 12480305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.89	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 0.0778 **MAX_MED:** 0.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

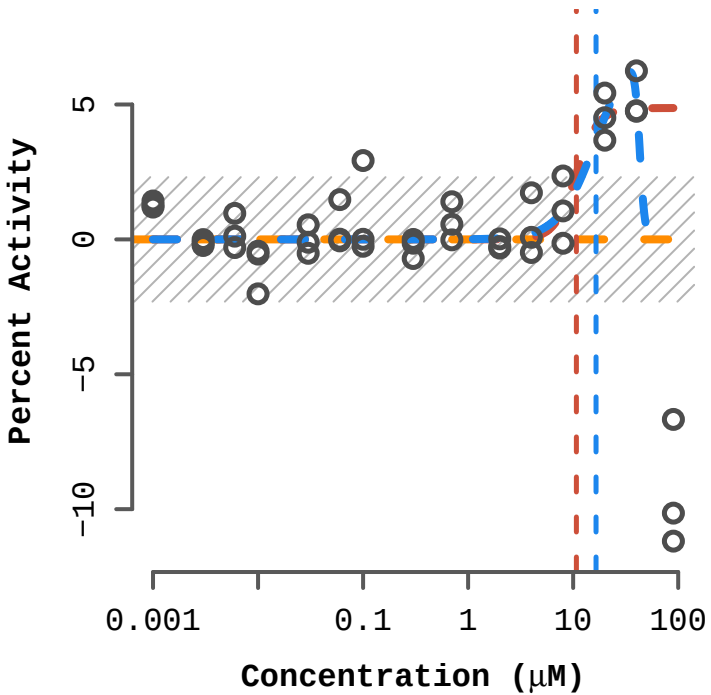
NAME: Pentachlorophenol
CHID: 21106 **CASRN:** 87-86-5
SPID(S): Tox21_300023
M4ID: 12479107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.587 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentachlorophenol
CHID: 21106 CASRN: 87-86-5
SPID(S): Tox21_202131
M4ID: 12480121

HILL MODEL (in red):

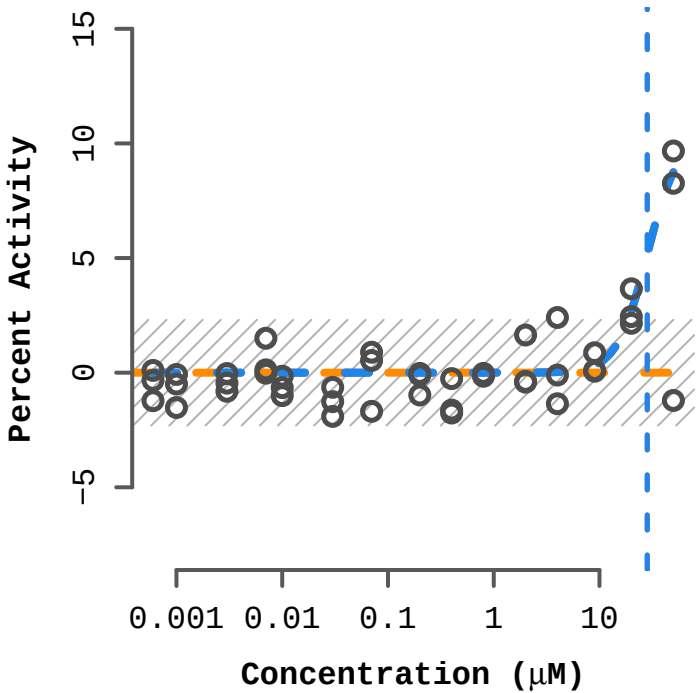
	tp	ga	gw
val:	4.87	1.03	4.2
sd:	0.571	0.102	2.62

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.36	1.22	2.46	1.63	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	216.27	187.09	178.04
PROB:	0	0.01	0.99
RMSE:	3.18	3.8	2.61

MAX_MEAN: 5.26 MAX_MED: 4.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Peppermint oil
CHID: 21113 **CASRN:** 8006-90-4
SPID(S): Tox21_302664
M4ID: 12476469

HILL MODEL (in red):

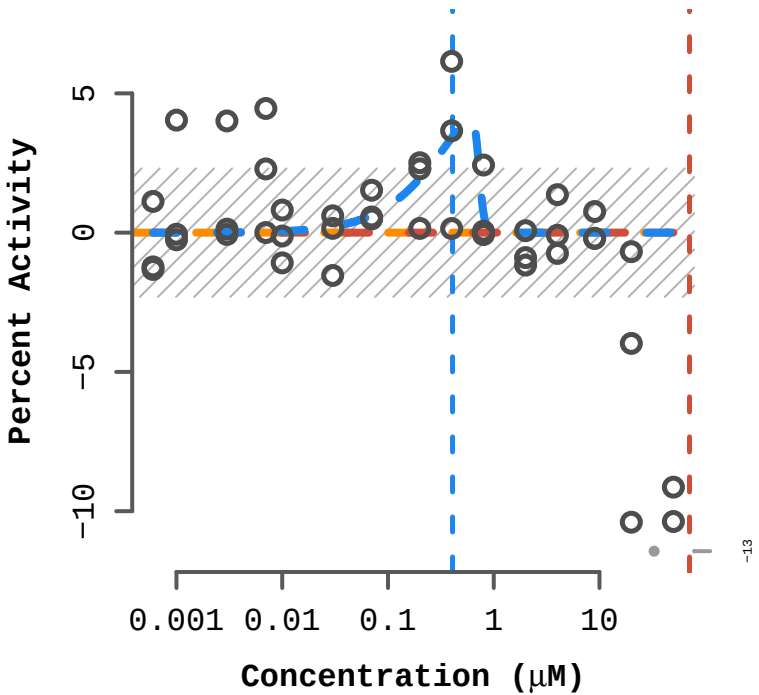
	tp	ga	gw
val:	10.3	1.45	3.01
sd:	3.78	0.178	1.93

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.3	1.45	3.01	3.67	13.5
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	173.15	148.23	152.23
PROB:	0	0.88	0.12
RMSE:	2.23	1.75	1.75

MAX_MEAN: 5.57 **MAX_MED:** 8.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Perhexiline maleate
CHID: 21114 CASRN: 6724-53-4
SPID(S): Tox21_111395_1
M4ID: 12483714 BRK

HILL MODEL (in red):

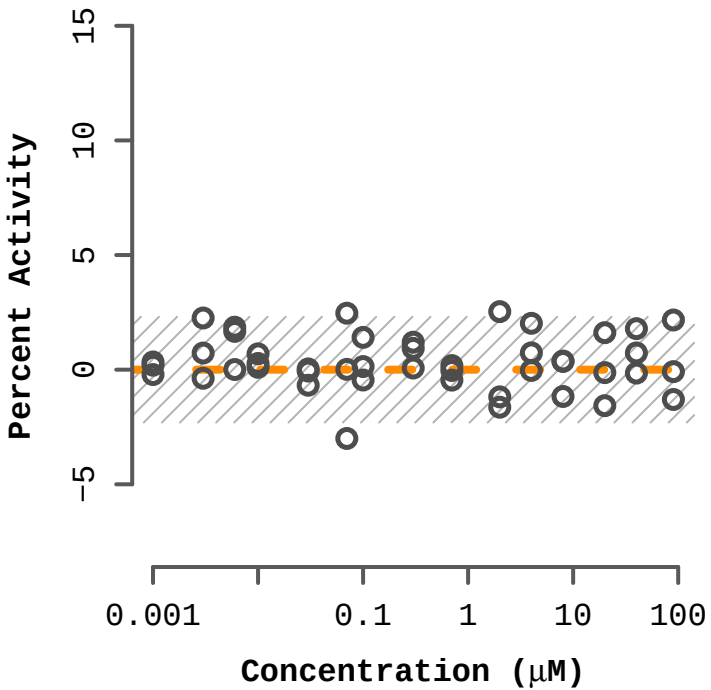
	tp	ga	gw
val:	5.44e-09	1.85	1.83
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.9	-0.39	1.31	-0.14	17.9
sd:	17.5	1.57	1.66	0.329	138

	CNST	HILL	GNLS
AIC:	229.41	235.41	230.85
PROB:	0.65	0.03	0.32
RMSE:	3.73	3.73	3.6

MAX_MEAN: 3.32 MAX_MED: 3.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

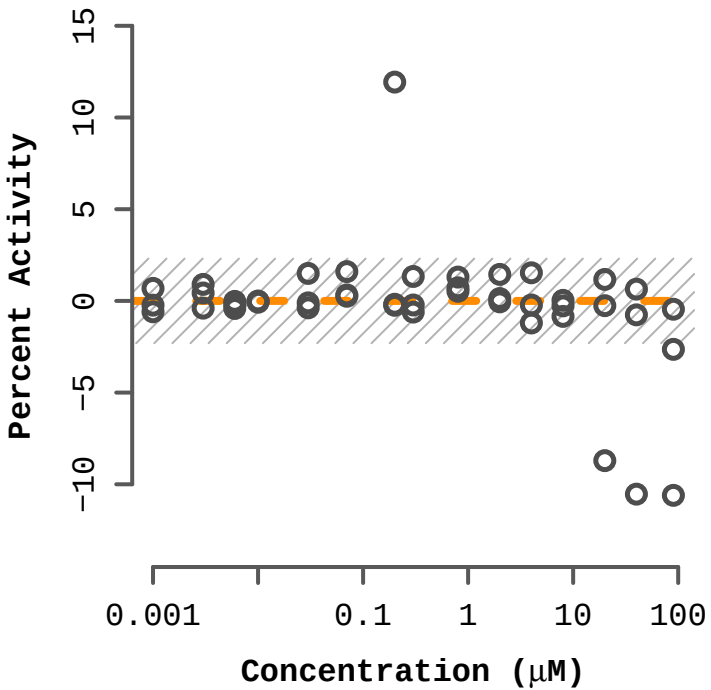
NAME: Phenacetin
CHID: 21116 **CASRN:** 62-44-2
SPID(S): Tox21_302895
M4ID: 12476238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

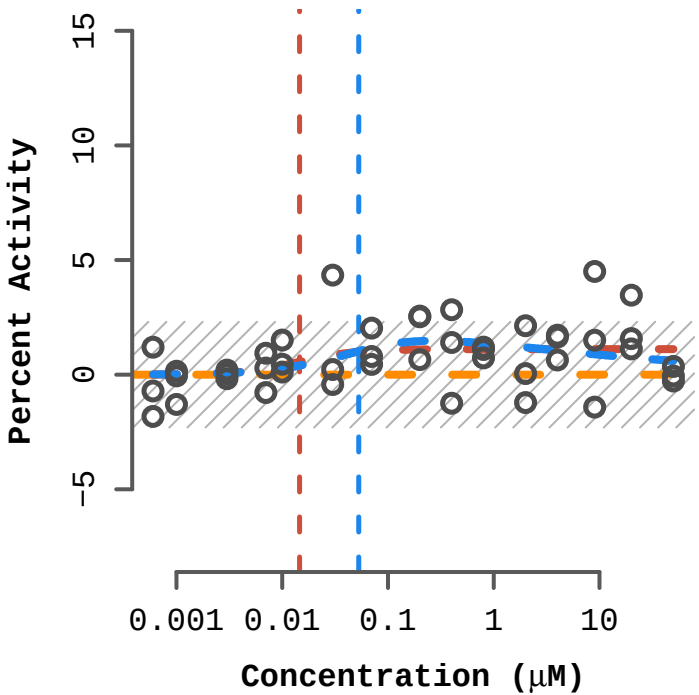
NAME: Phenacetin
CHID: 21116 **CASRN:** 62-44-2
SPID(S): Tox21_201926
M4ID: 12480326

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.52	NA	NA
PROB:	1	NA	NA
RMSE:	3.23	NA	NA

MAX_MEAN: 3.84 **MAX_MED:** 0.716 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenacetin
CHID: 21116 **CASRN:** 62-44-2
SPID(S): Tox21_110347_1
M4ID: 12484436

HILL MODEL (in red):

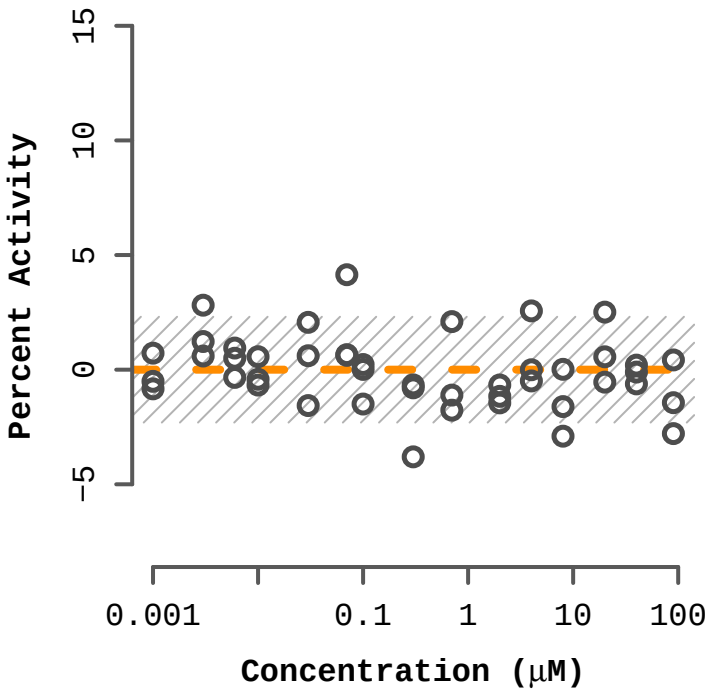
	tp	ga	gw
val:	1.11	−1.84	1.63
sd:	0.254	0.57	1.55

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.18	−1.28	1.23	−0.412	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	170.95	157.34	160.03
PROB:	0	0.79	0.21
RMSE:	1.61	1.29	1.3

MAX_MEAN: 2.06 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

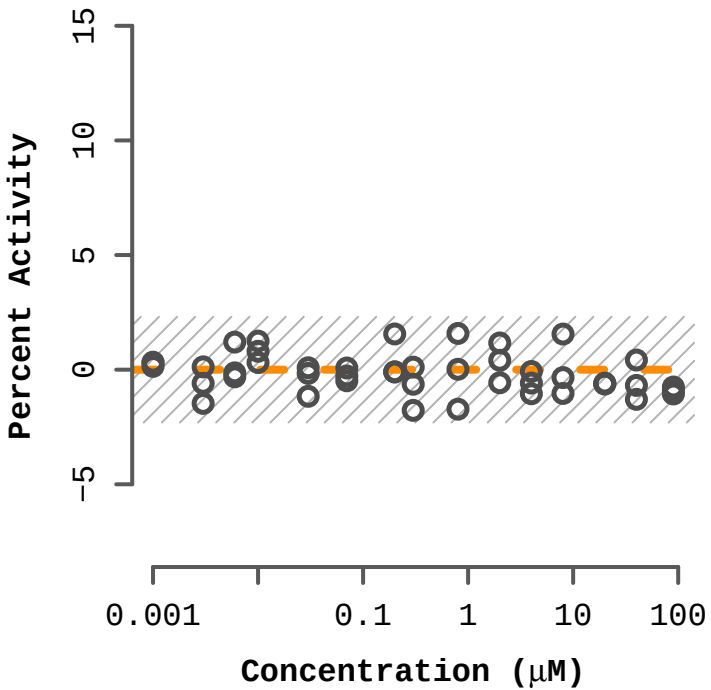
NAME: Phenazone
CHID: 21117 **CASRN:** 60-80-0
SPID(S): Tox21_303026
M4ID: 12476107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

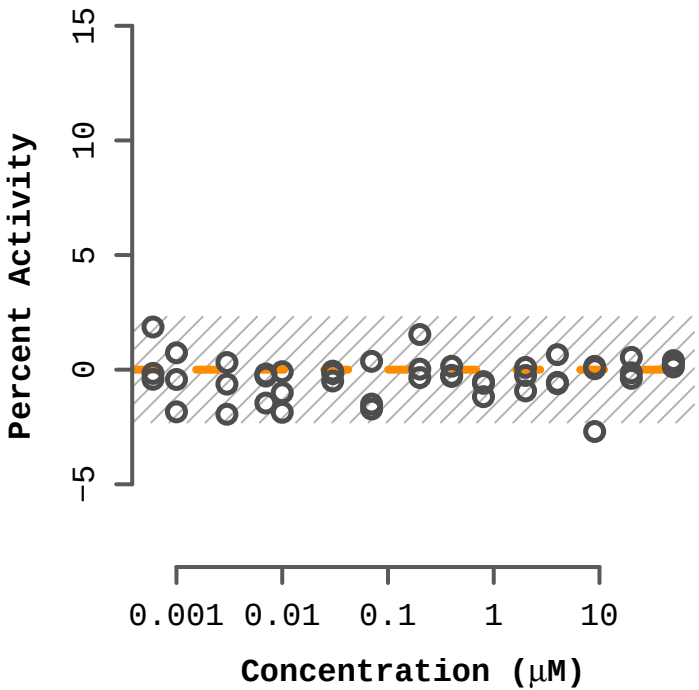
NAME: Phenazone
CHID: 21117 **CASRN:** 60-80-0
SPID(S): Tox21_201600
M4ID: 12480652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.789 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

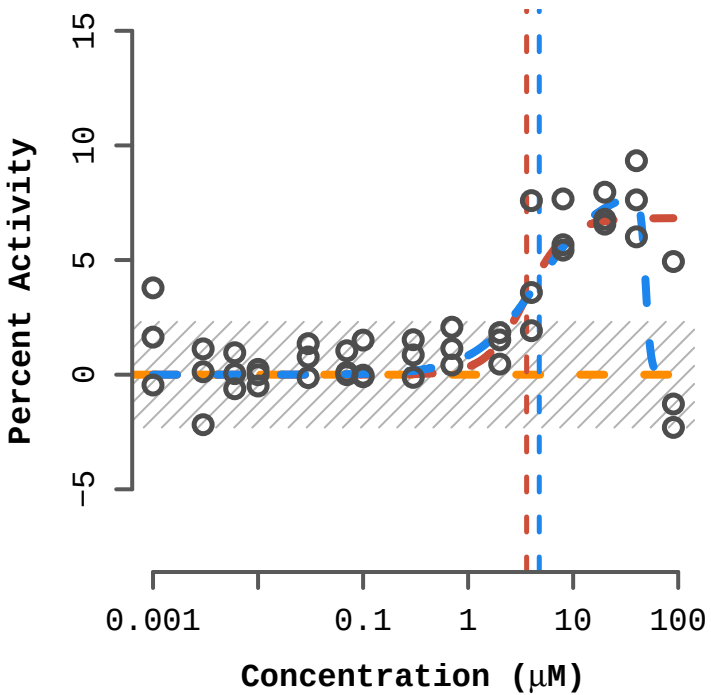
NAME: Phenazone
CHID: 21117 **CASRN:** 60-80-0
SPID(S): Tox21_110342_1
M4ID: 12484440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.428 **MAX_MED:** 0.322 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenazopyridine hydrochloride
CHID: 21118 CASRN: 136-40-3
SPID(S): Tox21_302738
M4ID: 12476395

HILL MODEL (in red):

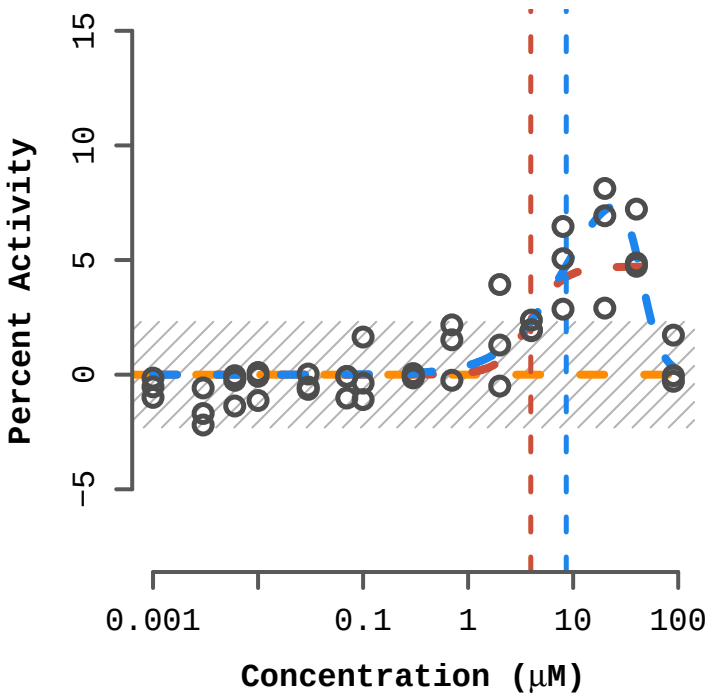
	tp	ga	gw
val:	6.83	0.557	2.3
sd:	0.577	0.0837	0.905

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.24	0.677	1.4	1.69	17.9
sd:	2.96	0.285	1.19	0.22	38.6

	CNST	HILL	GNLS
AIC:	242.91	182.96	168.27
PROB:	0	0	1
RMSE:	3.67	2.22	1.48

MAX_MEAN: 7.66 MAX_MED: 7.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenazopyridine hydrochloride
CHID: 21118 CASRN: 136-40-3
SPID(S): Tox21_202153
M4ID: 12480099

HILL MODEL (in red):

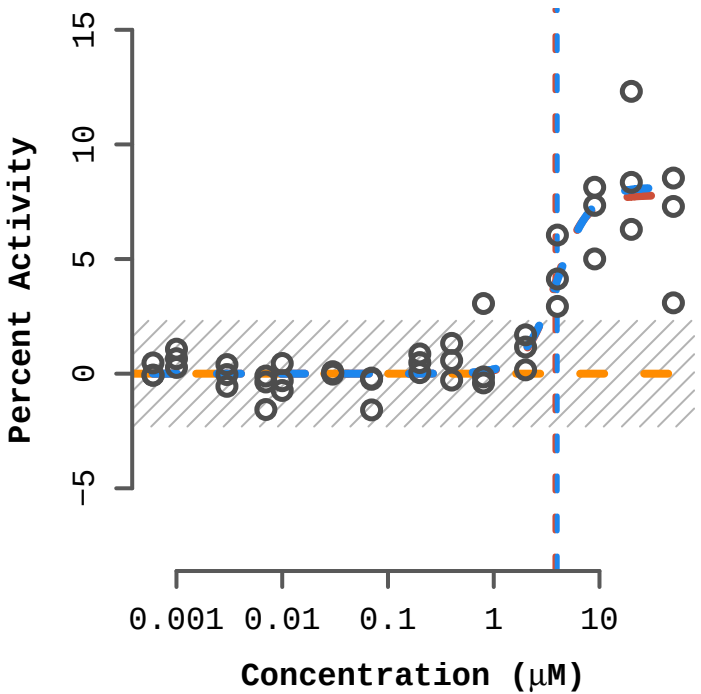
	tp	ga	gw
val:	4.72	0.597	2.86
sd:	0.726	0.117	2.63

GAIN-LOSS MODEL (in blue):

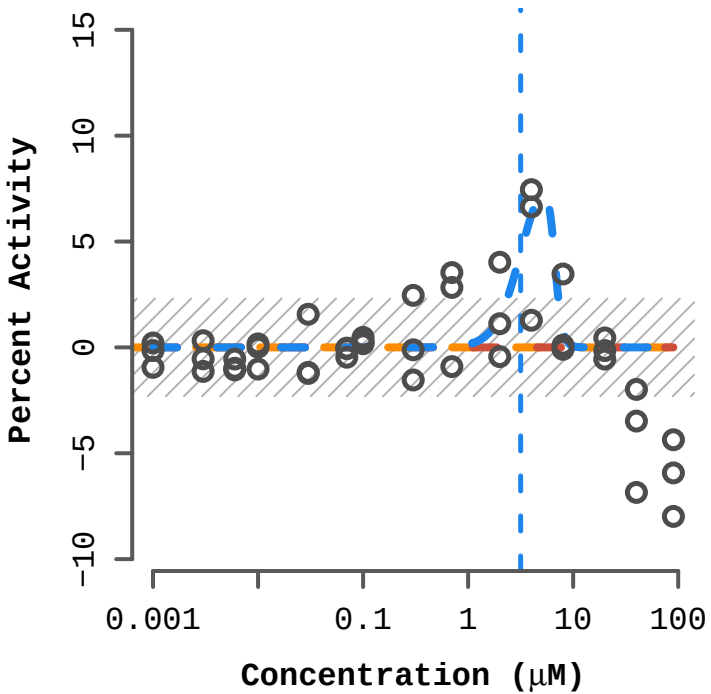
	tp	ga	gw	la	lw
val:	9.53	0.934	1.45	1.65	4.59
sd:	5.39	0.427	0.974	0.0735	2.52

	CNST	HILL	GNLS
AIC:	214.77	178.58	153.99
PROB:	0	0	1
RMSE:	2.81	1.7	1.23

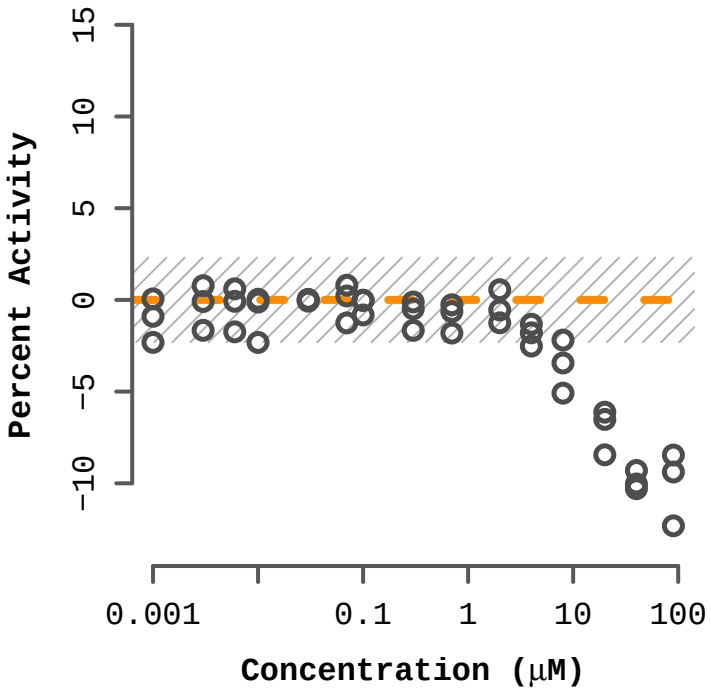
MAX_MEAN: 5.99 MAX_MED: 6.93 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenazopyridine hydrochloride
CHID:    21118   CASRN: 136-40-3
SPID(S): Tox21_110829_1
M4ID:    12484087

HILL MODEL (in red):
      tp       ga       gw
val:  7.78     0.579    2.94
sd:   0.489    0.0513   0.813

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.13     0.6      2.7      1.82     9.48
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  236.17      145.04      148.69
PROB: 0           0.86        0.14
RMSE: 3.74        1.32        1.29

MAX_MEAN: 8.99      MAX_MED: 8.35      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenethyl isothiocyanate
CHID:    21120   CASRN: 2257-09-2
SPID(S): Tox21_200100
M4ID:    12482152

HILL MODEL (in red):
      tp        ga        gw
val:  5.64e-10  2.27      1.23
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  8.94      0.5       3.58      0.824     12.4
sd:   28.3      0.965     11.9      0.544     85.9

      CNST          HILL          GNLS
AIC:  213.02        219.02        209.63
PROB: 0.15          0.01          0.84
RMSE: 2.8           2.8           2.44

MAX_MEAN: 5.12      MAX_MED: 6.64      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

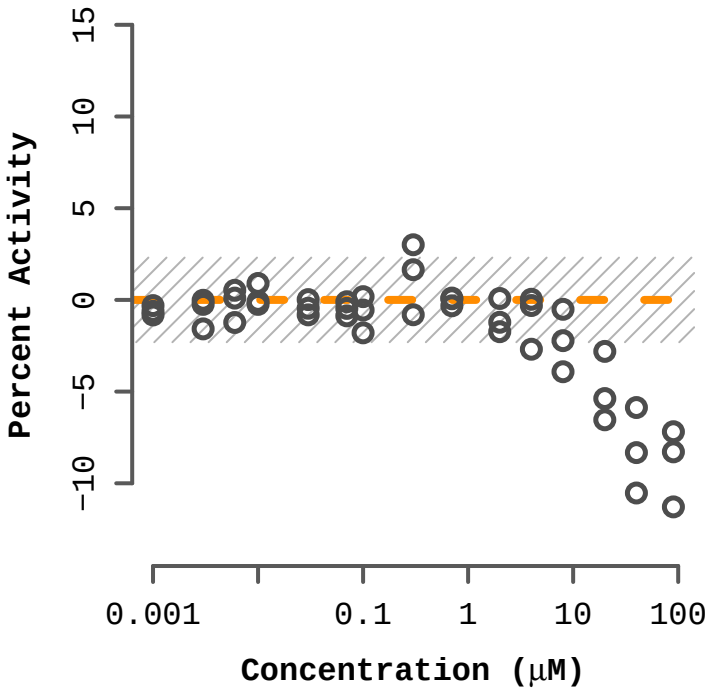
NAME: Phenformin hydrochloride
CHID: 21121 **CASRN:** 834-28-6
SPID(S): Tox21_303004
M4ID: 12476129

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.01	NA	NA
PROB:	1	NA	NA
RMSE:	4.32	NA	NA

MAX_MEAN: −0.00625 **MAX_MED:** 0.216 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

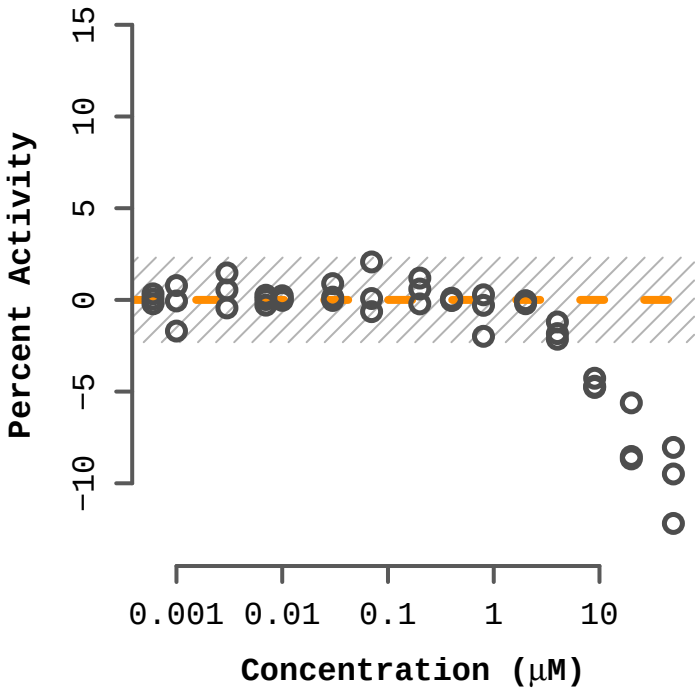
NAME: Phenformin hydrochloride
CHID: 21121 **CASRN:** 834-28-6
SPID(S): Tox21_202197
M4ID: 12480055

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232	NA	NA
PROB:	1	NA	NA
RMSE:	3.65	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

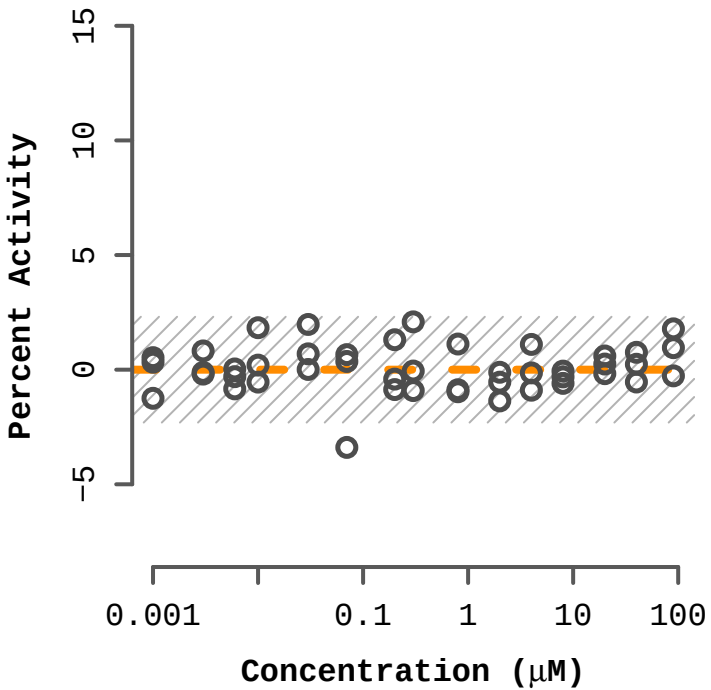
NAME: Phenformin hydrochloride
CHID: 21121 **CASRN:** 834-28-6
SPID(S): Tox21_111185_1
M4ID: 12483859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.14	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** 0.596 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

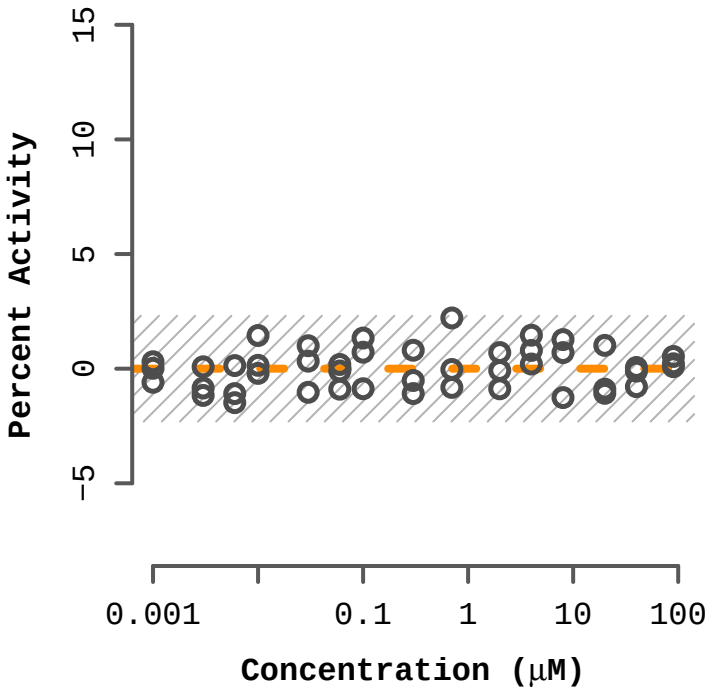
NAME: Phenobarbital
CHID: 21122 **CASRN:** 50-06-6
SPID(S): Tox21_200510
M4ID: 12481742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 0.962 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

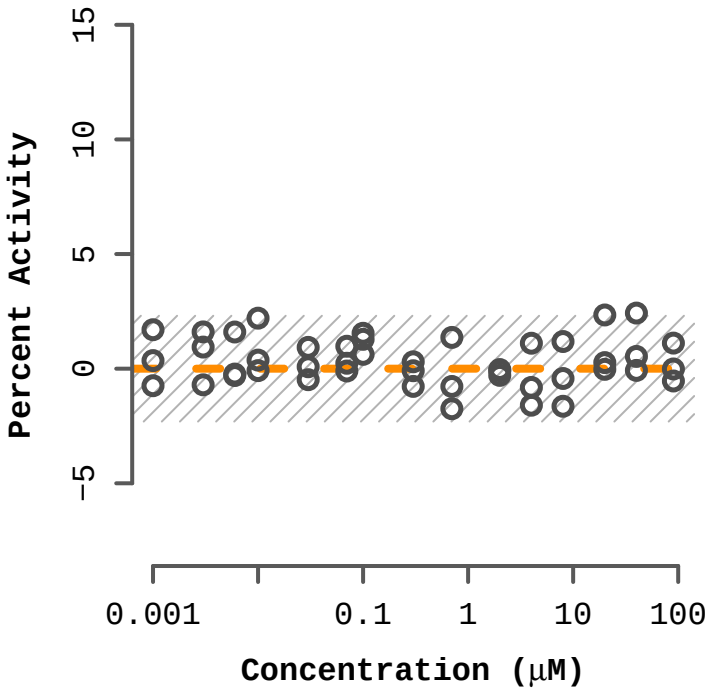
NAME: Phenobarbital sodium
CHID: 21123 CASRN: 57-30-7
SPID(S): Tox21_300271
M4ID: 12478859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.821 **MAX_MED:** 0.797 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

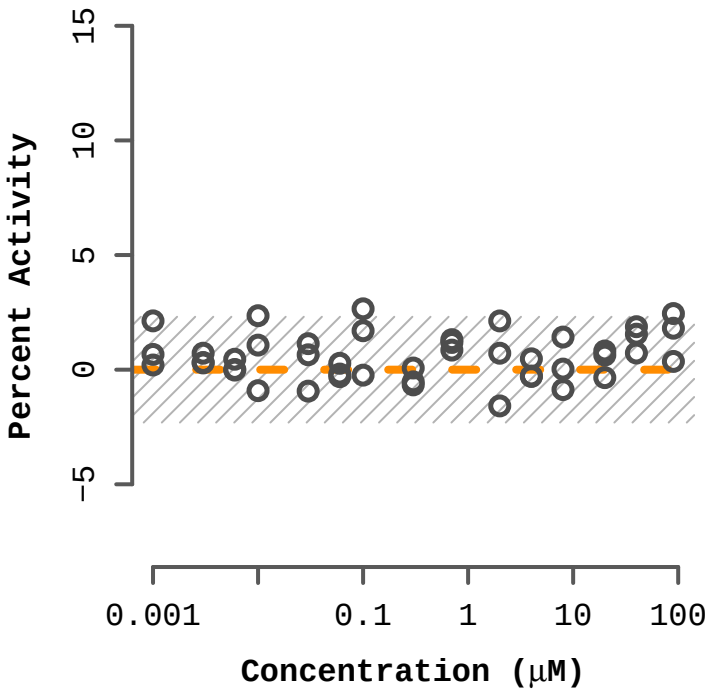
NAME: Phenol
CHID: 21124 **CASRN:** 108-95-2
SPID(S): Tox21_300042
M4ID: 12479088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

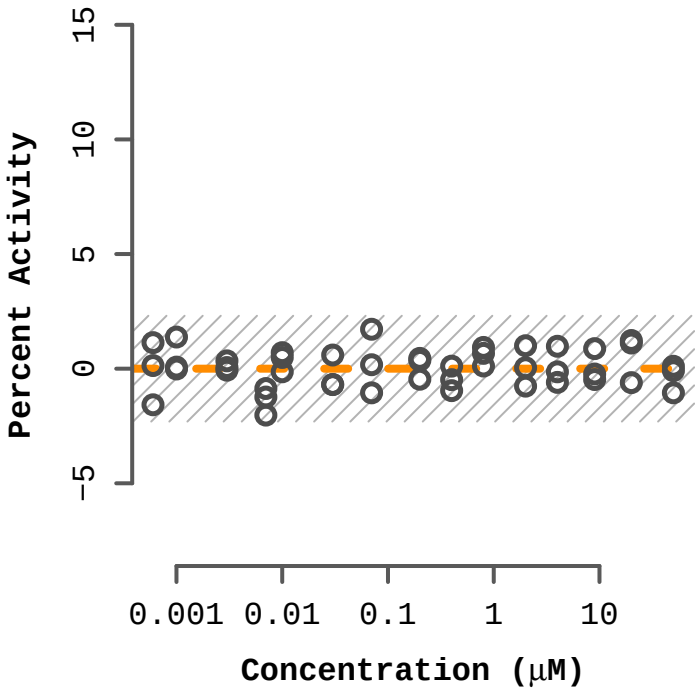
NAME: Phenol
CHID: 21124 **CASRN:** 108-95-2
SPID(S): Tox21_201639
M4ID: 12480613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

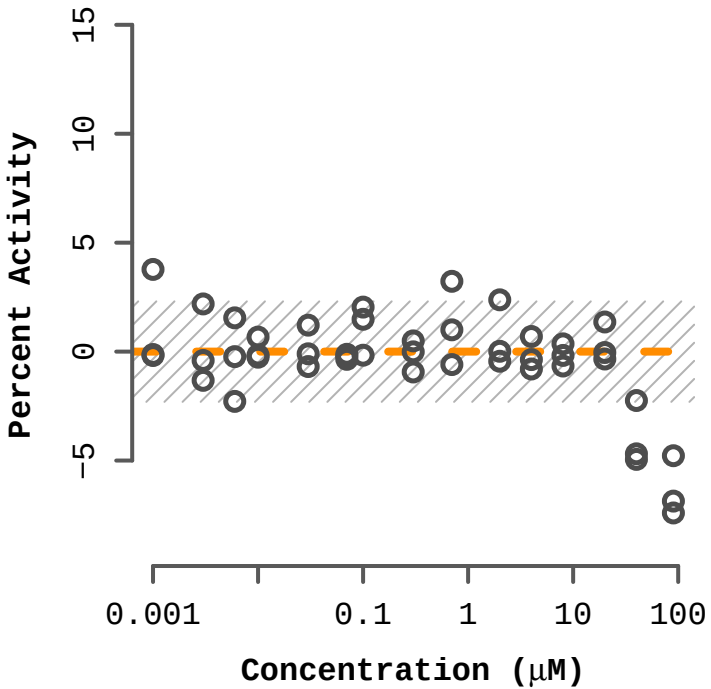
NAME: Phenol
CHID: 21124 **CASRN:** 108-95-2
SPID(S): Tox21_113463_1
M4ID: 12482644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.581 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

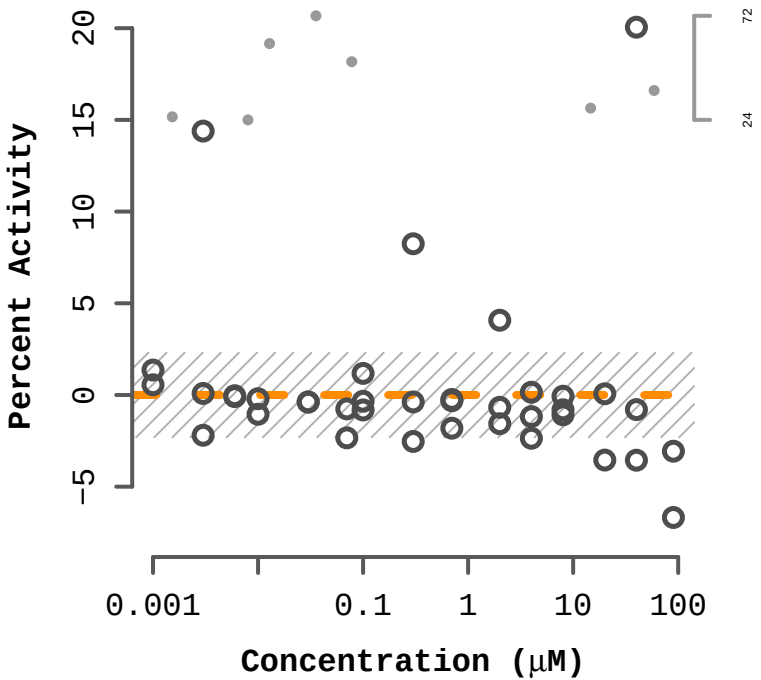
NAME: Phenolphthalein
CHID: 21125 CASRN: 77-09-8
SPID(S): Tox21_300282
M4ID: 12478848

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.19	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

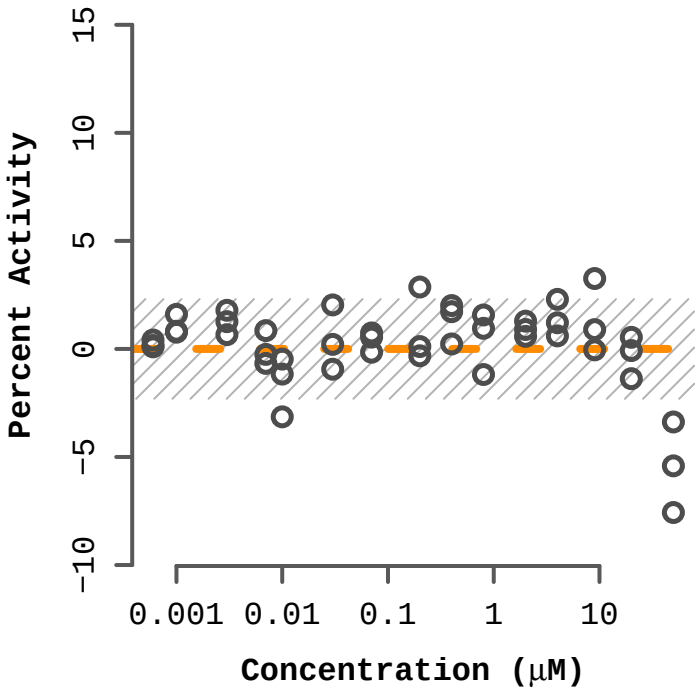
NAME: Phenolphthalein
CHID: 21125 CASRN: 77-09-8
SPID(S): Tox21_202219
M4ID: 12480033 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	355.62	NA	NA
PROB:	1	NA	NA
RMSE:	18.61	NA	NA

MAX_MEAN: 23.9 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

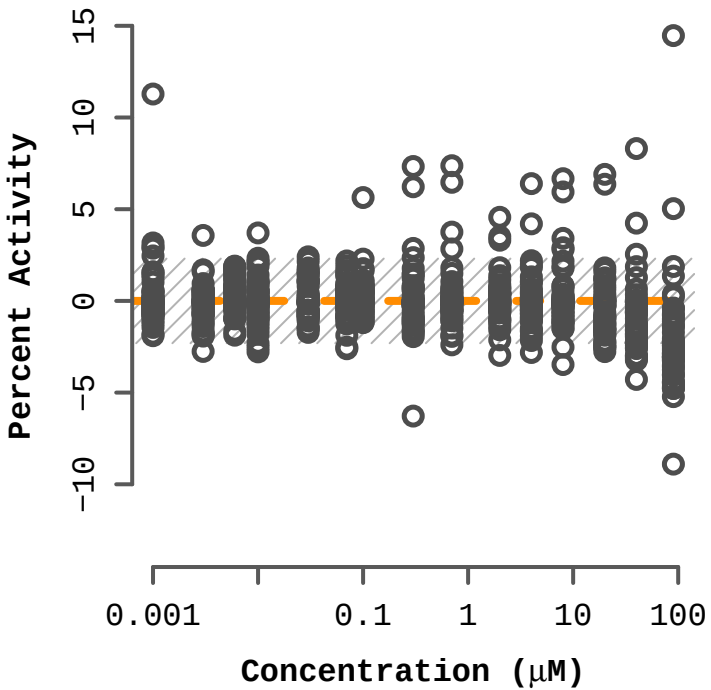
NAME: Phenolphthalein
CHID: 21125 CASRN: 77-09-8
SPID(S): Tox21_110838_1
M4ID: 12484080

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.94	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

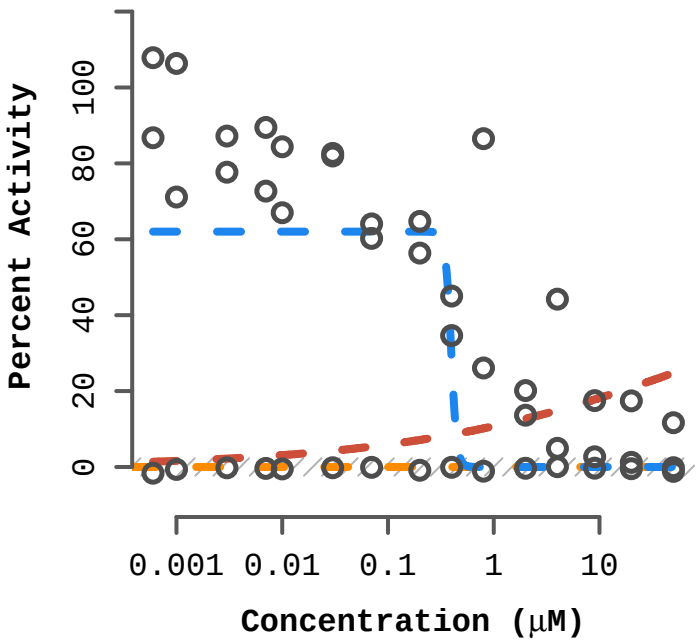
NAME: Phenothiazine
CHID: 21126 **CASRN:** 92-84-2
SPID(S): Tox21_400010
M4ID: 12475127

HILL MODEL: Not applicable.

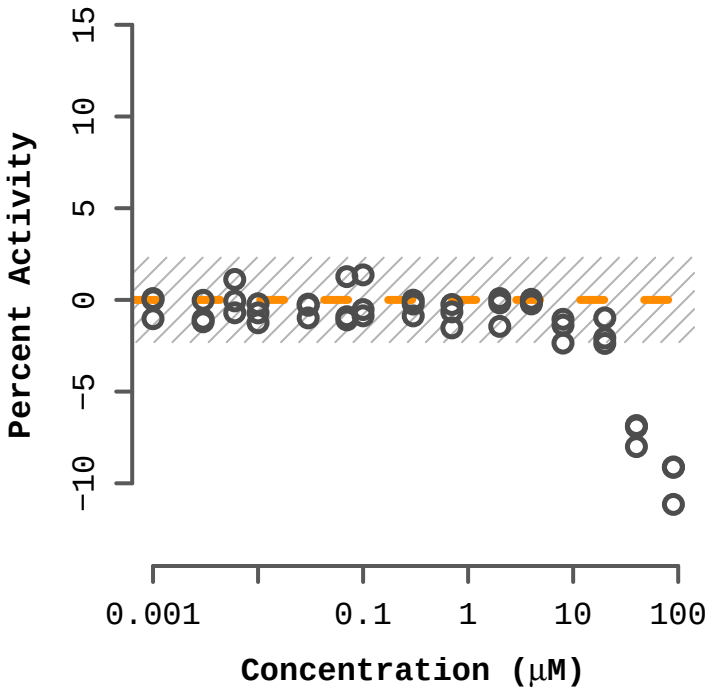
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2603.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.78	NA	NA

MAX_MEAN: 0.335 **MAX_MED:** 0.0867 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenothiazine
CHID:    21126   CASRN: 92-84-2
SPID(S): Tox21_111090_1
M4ID:    12483913

HILL MODEL (in red):
      tp       ga       gw
val:  59.8     2.2      0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  62       -5.13    8        -0.403   16.1
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  485.49      487.71      456.18
PROB: 0           0           1
RMSE: 51.09       48.89       33.95

MAX_MEAN: 64.3      MAX_MED: 86.8      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

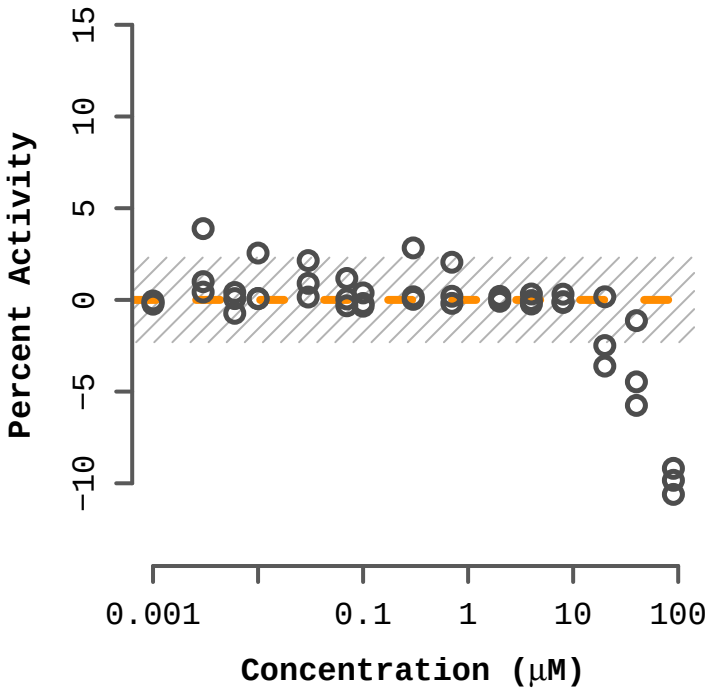
NAME: Phenoxybenzamine hydrochloride
CHID: 21127 CASRN: 63-92-3
SPID(S): Tox21_302978
M4ID: 12476155

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.91	NA	NA
PROB:	1	NA	NA
RMSE:	3.3	NA	NA

MAX_MEAN: 0.122 **MAX_MED:** 0.00417 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

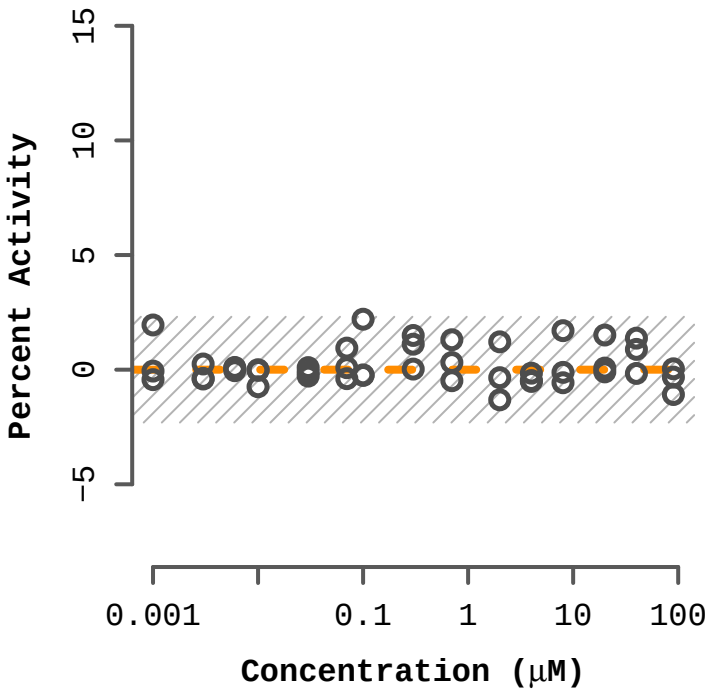
NAME: Phenoxybenzamine hydrochloride
CHID: 21127 **CASRN:** 63-92-3
SPID(S): Tox21_201588
M4ID: 12480664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.82	NA	NA
PROB:	1	NA	NA
RMSE:	3.02	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 0.998 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

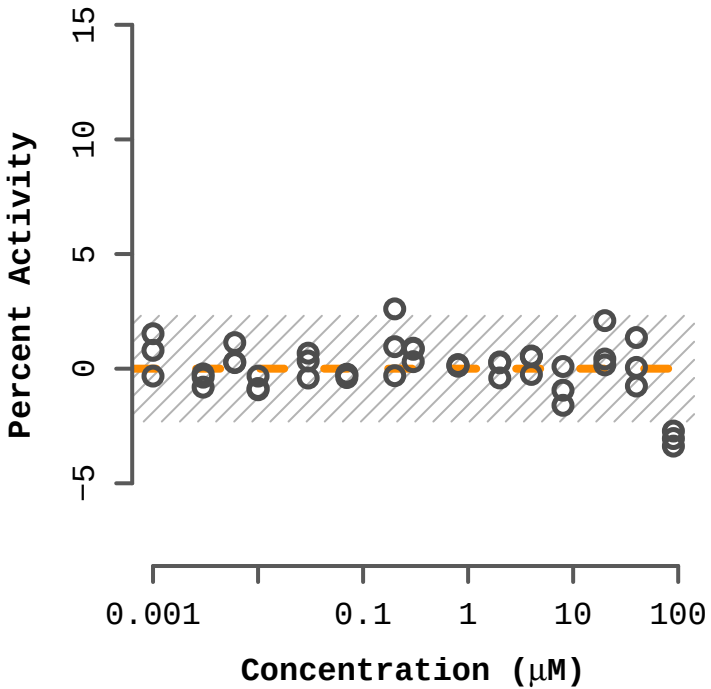
NAME: 1−Phenyl−3,3−dimethyltriazene
CHID: 21128 **CASRN:** 7227−91−0
SPID(S): Tox21_301876
M4ID: 12477257

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

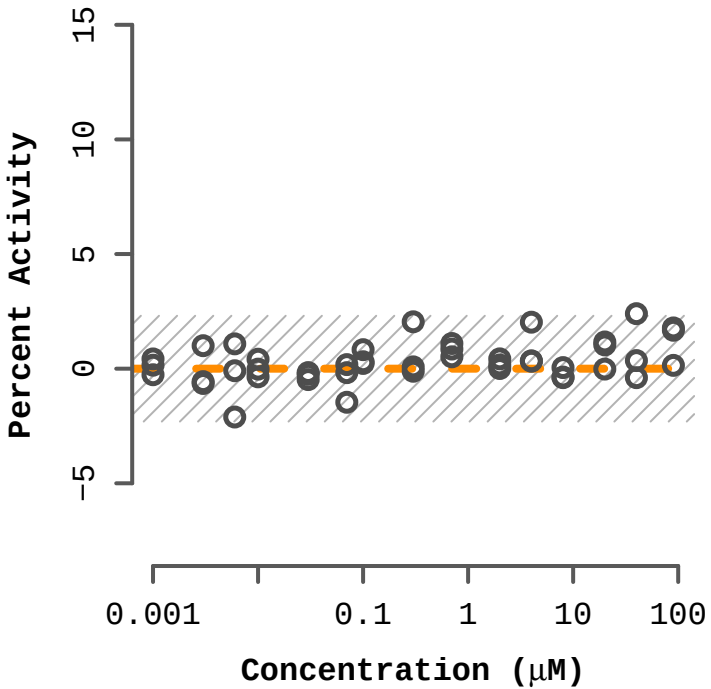
NAME: Phenyl isothiocyanate
CHID: 21129 **CASRN:** 103-72-0
SPID(S): Tox21_201128
M4ID: 12481124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.961 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

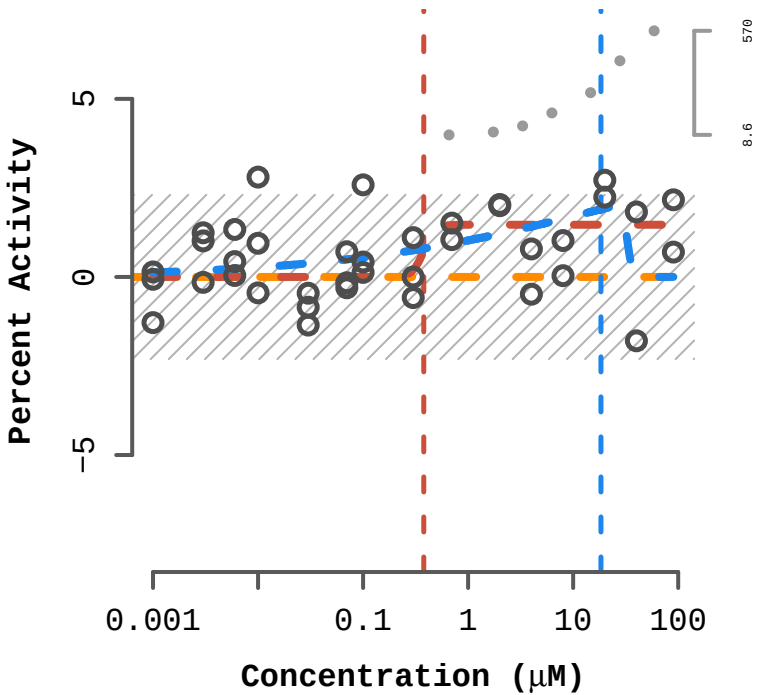
NAME: 1-Phenyl-3-methyl-5-pyrazolone
CHID: 21130 **CASRN:** 89-25-8
SPID(S): Tox21_302819
M4ID: 12476314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Phenyl-3-methyl-5-pyrazolone
CHID: 21130 CASRN: 89-25-8
SPID(S): Tox21_201747
M4ID: 12480505 BRK

HILL MODEL (in red):

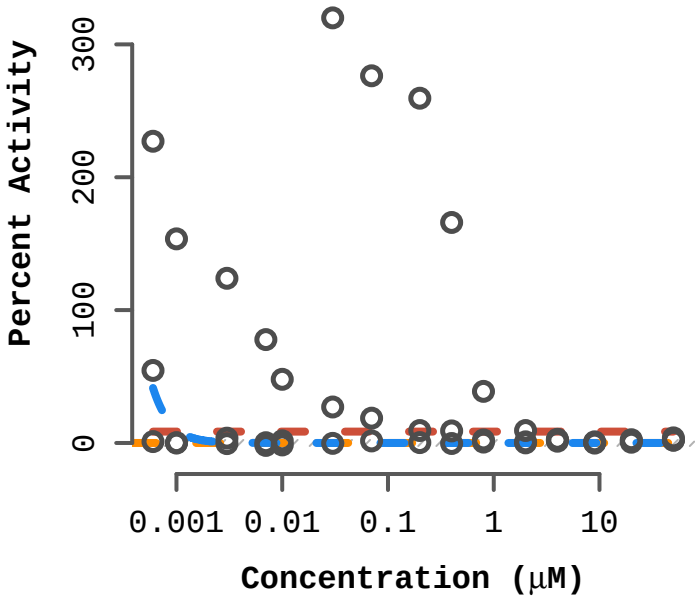
	tp	ga	gw
val:	1.47	−0.422	8
sd:	0.542	0.325	19.2

GAIN-LOSS MODEL (in blue):

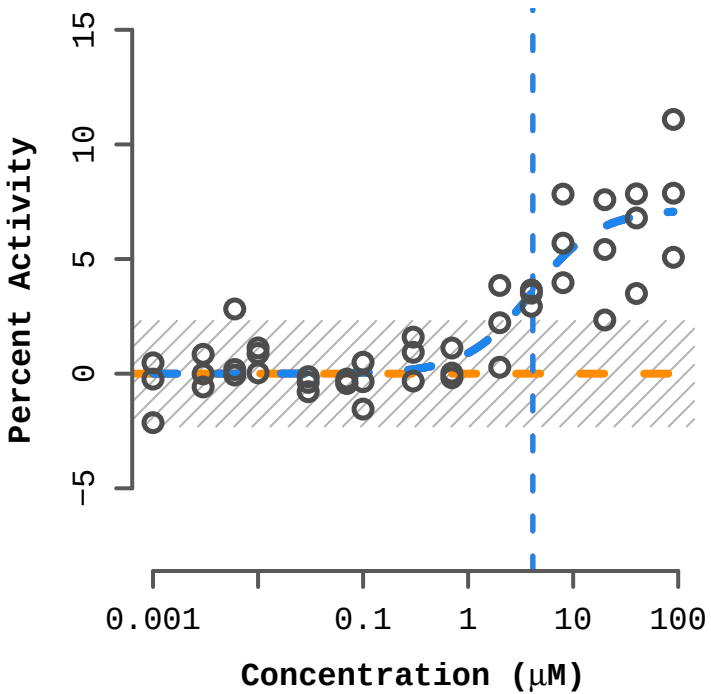
	tp	ga	gw	la	lw
val:	3.8	1.26	0.342	1.51	17.4
sd:	51.6	32.3	1.81	0.775	129

	CNST	HILL	GNLS
AIC:	394.11	393.72	398.6
PROB:	0.43	0.52	0.05
RMSE:	112.41	111.99	112.25

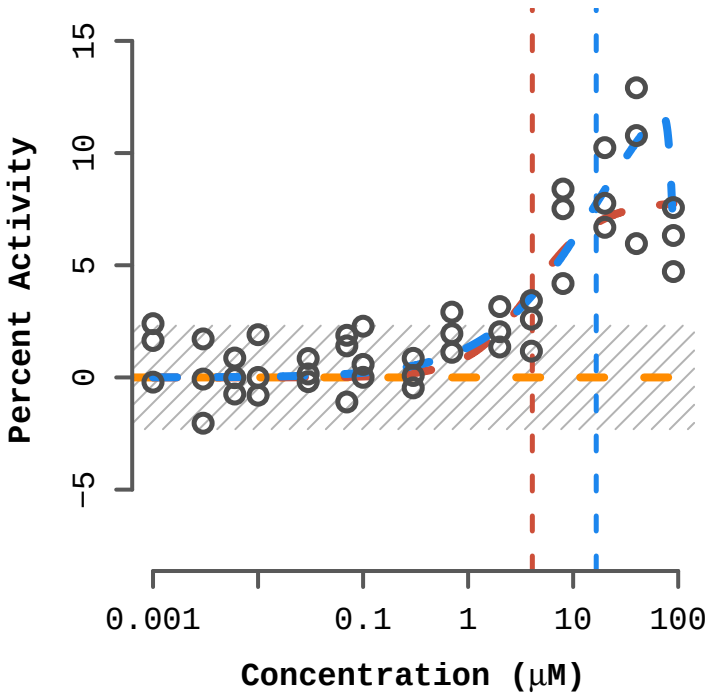
MAX_MEAN: 191 **MAX_MED:** 2.72 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Phenyl-3-methyl-5-pyrazolone
CHID:    21130   CASRN: 89-25-8
SPID(S): Tox21_112077_1
M4ID:    12483334

HILL MODEL (in red):
      tp       ga       gw
val:  8.55     -4.17    8
sd:   4.44     1400     11800

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  361      -3.87    8        -3.53    2.91
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  500.29      501.69      506.99
PROB: 0.65        0.32        0.02
RMSE: 91.71       88.21       89.1

MAX_MEAN: 116       MAX_MED: 54.6      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Phenyl-2-naphthylamine
CHID:    21131   CASRN: 135-88-6
SPID(S): Tox21_302900
M4ID:    12476233

HILL MODEL (in red):
      tp       ga       gw
val:  7.17     0.616    1.37
sd:   0.873    0.128    0.493

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.17     0.616    1.37     3.76     6.18
sd:   0.873    0.128    0.493    43600    149000

      CNST        HILL        GNLS
AIC:  241.95      162.51      166.51
PROB: 0           0.88        0.12
RMSE: 3.69        1.43        1.43

MAX_MEAN: 8.01      MAX_MED: 7.87      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Phenyl-2-naphthylamine
CHID: 21131 CASRN: 135-88-6
SPID(S): Tox21_201891
M4ID: 12480361

HILL MODEL (in red):

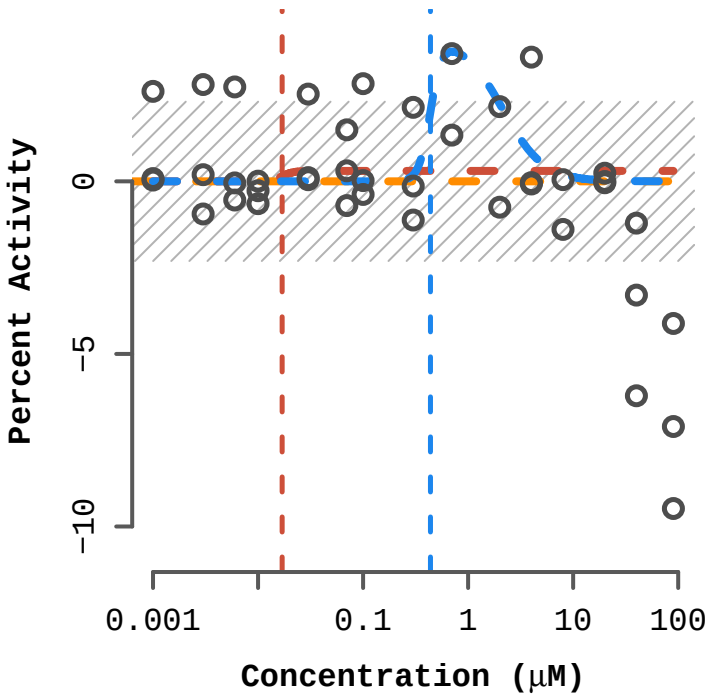
	tp	ga	gw
val:	7.84	0.611	1.4
sd:	0.844	0.121	0.676

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.5	1.22	0.838	1.95	16.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	258.12	183.28	176.24
PROB:	0	0.03	0.97
RMSE:	4.42	1.7	1.48

MAX_MEAN: 9.89 MAX_MED: 10.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Phenyl-1,4-benzenediamine hydrochloride
CHID: 21132 CASRN: 2198-59-6
SPID(S): Tox21_200117
M4ID: 12482135

HILL MODEL (in red):

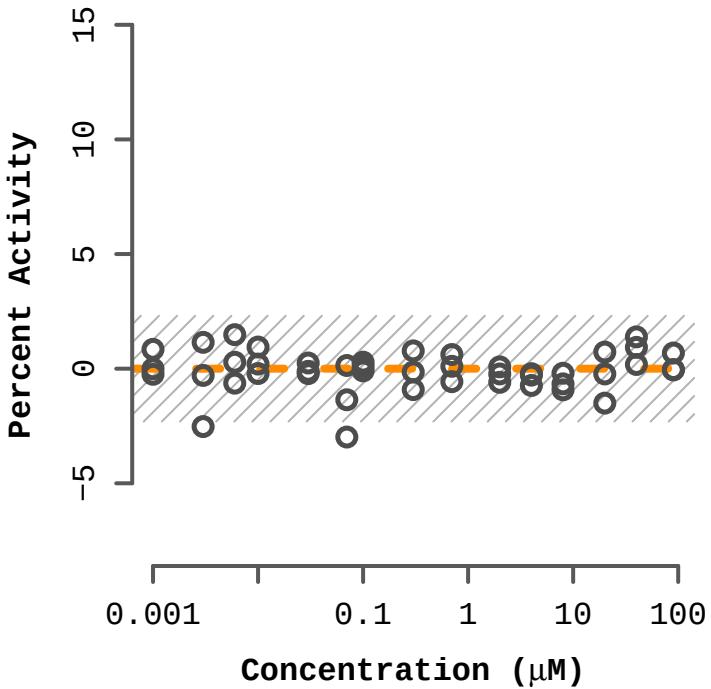
	tp	ga	gw
val:	0.302	−1.77	8
sd:	0.41	1.09	37.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.15	−0.359	8	0.332	2.26
sd:	8.1	1.61	73.7	0.823	3.02

	CNST	HILL	GNLS
AIC:	219.23	224.68	219.35
PROB:	0.5	0.03	0.47
RMSE:	2.93	2.94	2.67

MAX_MEAN: 3.87 **MAX_MED:** 3.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

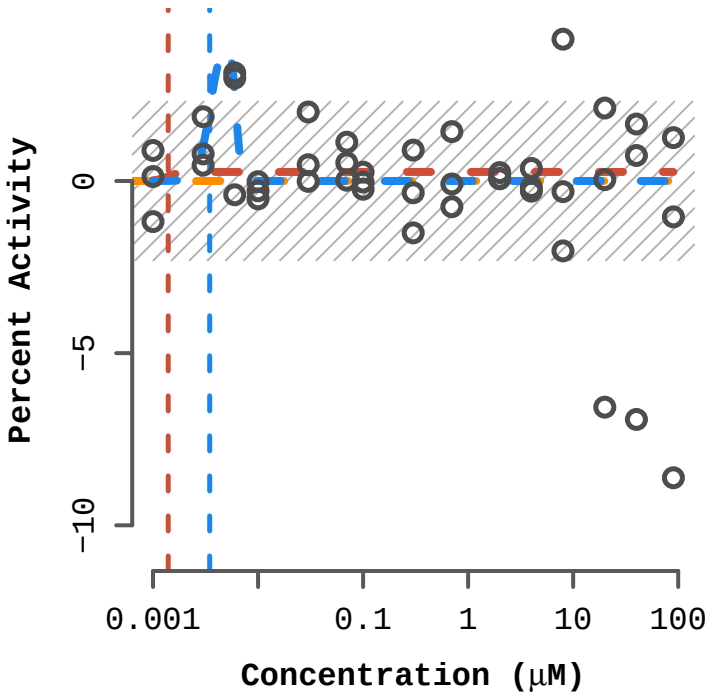
NAME: 1-Phenyl-2-thiourea
CHID: 21134 **CASRN:** 103-85-5
SPID(S): Tox21_302998
M4ID: 12476135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.835 **MAX_MED:** 0.931 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Phenyl-2-thiourea
CHID: 21134 CASRN: 103-85-5
SPID(S): Tox21_201682
M4ID: 12480570

HILL MODEL (in red):

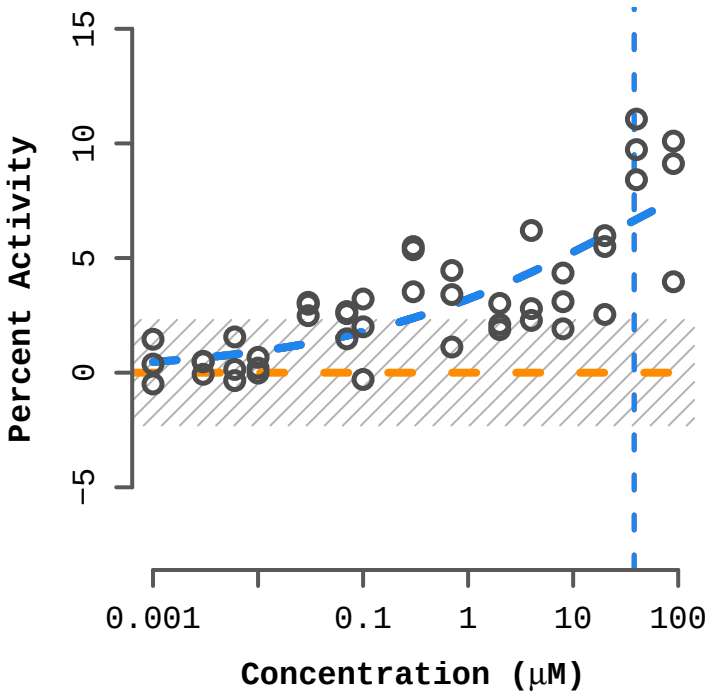
	tp	ga	gw
val:	0.262	−2.86	8
sd:	0.201	1.15	38

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.18	−2.46	7.95	−2.21	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	182.44	186.75	184.7
PROB:	0.69	0.08	0.23
RMSE:	2.28	2.31	2.22

MAX_MEAN: 1.91 MAX_MED: 2.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Solvent Yellow 14
CHID: 21135 CASRN: 842-07-9
SPID(S): Tox21_300297
M4ID: 12478833

HILL MODEL (in red):

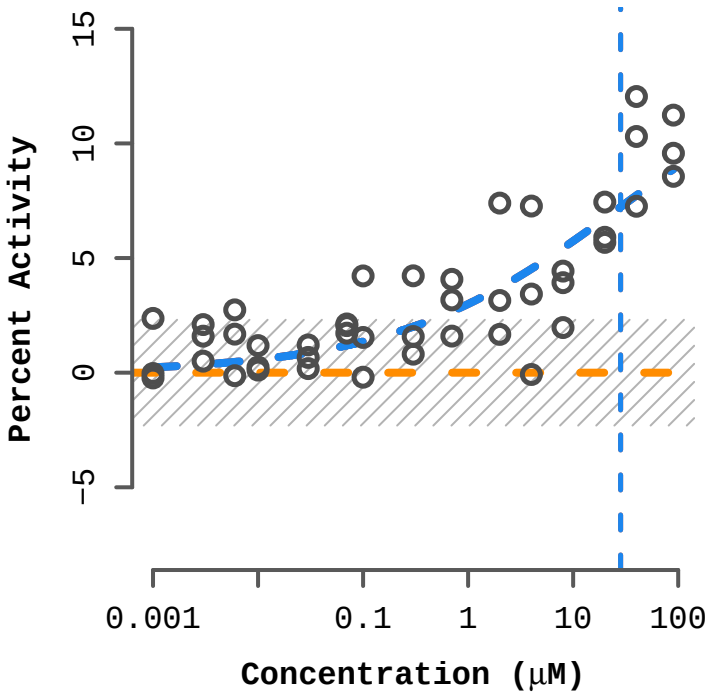
	tp	ga	gw
val:	13.3	1.58	0.314
sd:	5.76	1.03	0.0633

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.3	1.58	0.314	3.04	8.35
sd:	5.76	1.03	0.0633	2530	19400

	CNST	HILL	GNLS
AIC:	259.96	191.68	195.68
PROB:	0	0.88	0.12
RMSE:	4.29	1.79	1.79

MAX_MEAN: 9.74 MAX_MED: 9.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Solvent Yellow 14
CHID: 21135 CASRN: 842-07-9
SPID(S): Tox21_200511
M4ID: 12481741

HILL MODEL (in red):

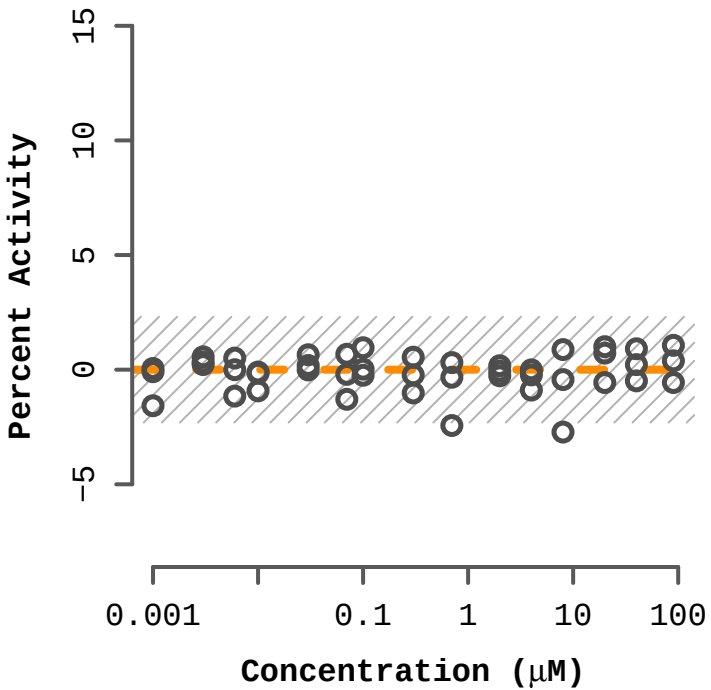
	tp	ga	gw
val:	14.5	1.45	0.401
sd:	3.69	0.558	0.0732

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.5	1.45	0.402	3.55	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	267.7	185.64	189.64
PROB:	0	0.88	0.12
RMSE:	4.71	1.75	1.75

MAX_MEAN: 9.87 MAX_MED: 10.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

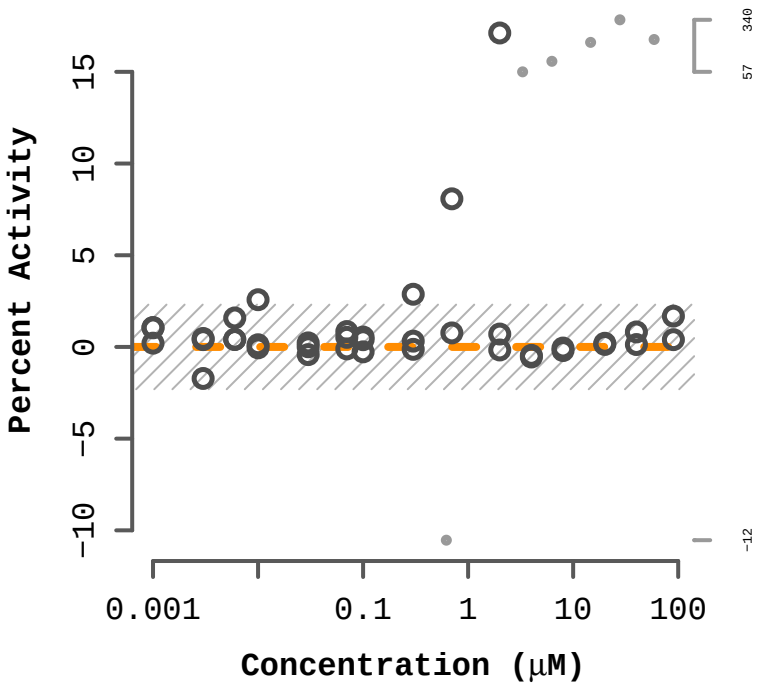
NAME: Phenylbutazone
CHID: 21136 **CASRN:** 50-33-9
SPID(S): Tox21_302763
M4ID: 12476370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.389 **MAX_MED:** 0.723 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

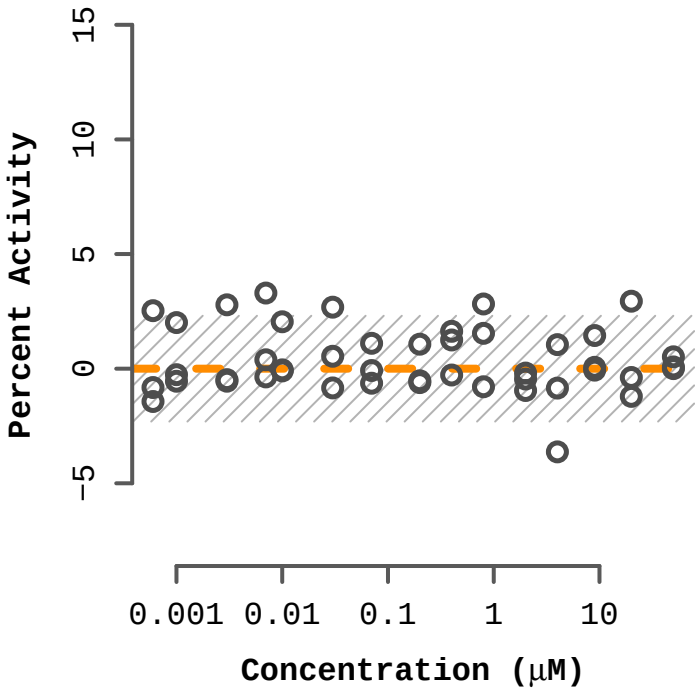
NAME: Phenylbutazone
CHID: 21136 **CASRN:** 50-33-9
SPID(S): Tox21_201809
M4ID: 12480443 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	380.29	NA	NA
PROB:	1	NA	NA
RMSE:	71.87	NA	NA

MAX_MEAN: 113 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

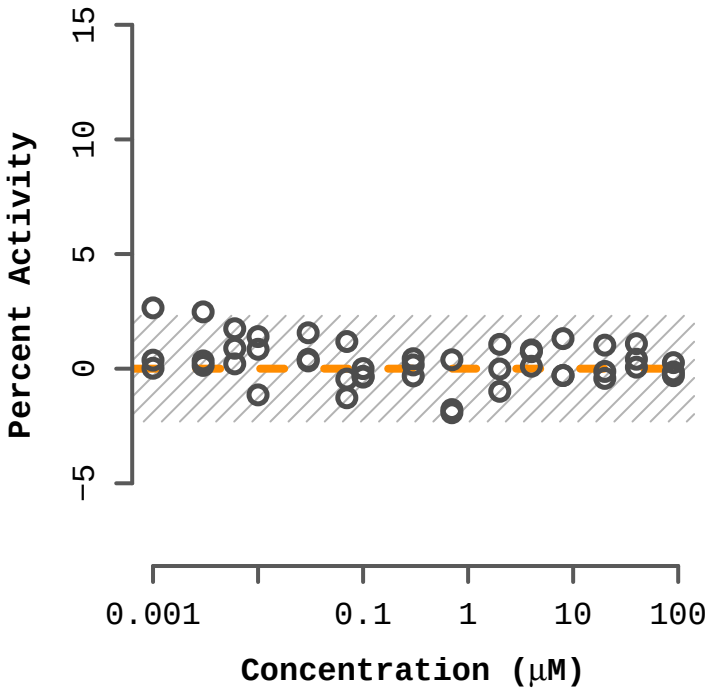
NAME: Phenylbutazone
CHID: 21136 **CASRN:** 50-33-9
SPID(S): Tox21_110242_1
M4ID: 12484521

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

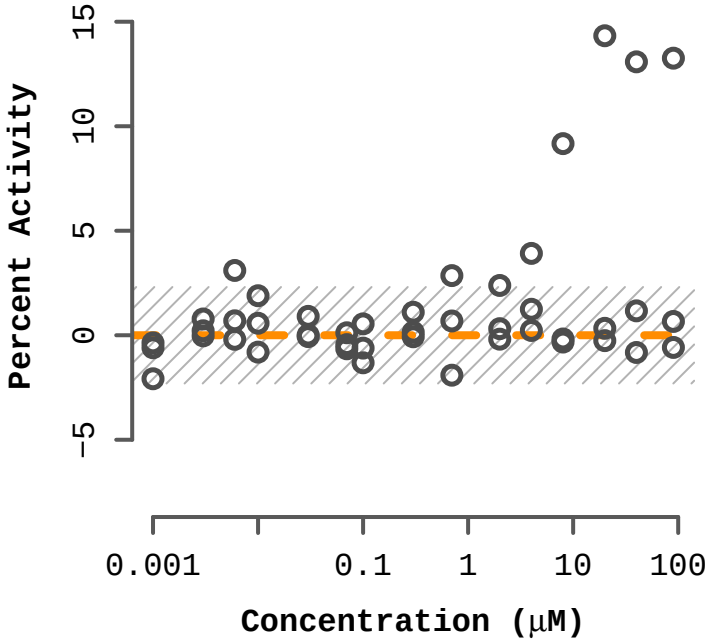
NAME: 1,3−Benzenediamine
CHID: 21137 **CASRN:** 108−45−2
SPID(S): Tox21_300490
M4ID: 12478642

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.892 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

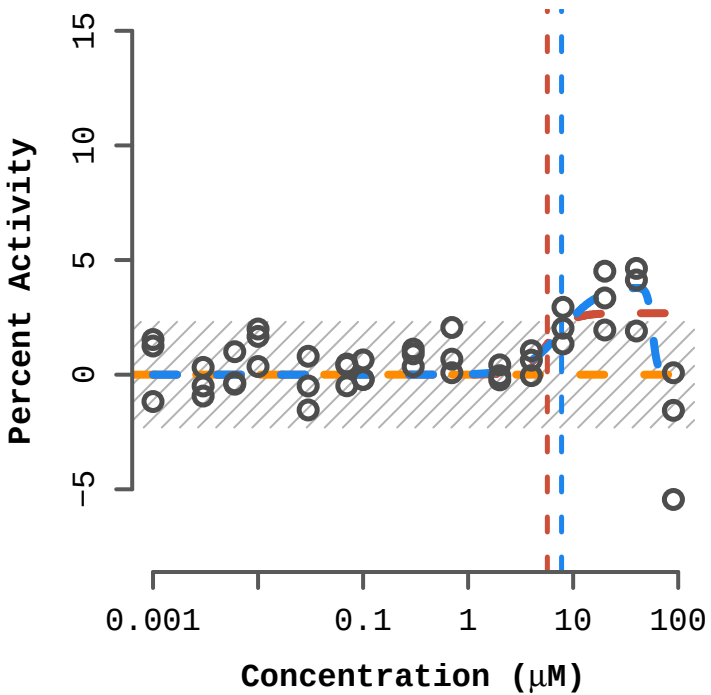
NAME: 1,3-Benzenediamine
CHID: 21137 CASRN: 108-45-2
SPID(S): Tox21_202106
M4ID: 12480146

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.13	NA	NA
PROB:	1	NA	NA
RMSE:	3.94	NA	NA

MAX_MEAN: 4.8 MAX_MED: 1.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Benzenediamine
CHID: 21138 CASRN: 106−50−3
SPID(S): Tox21_302943
M4ID: 12476190

HILL MODEL (in red):

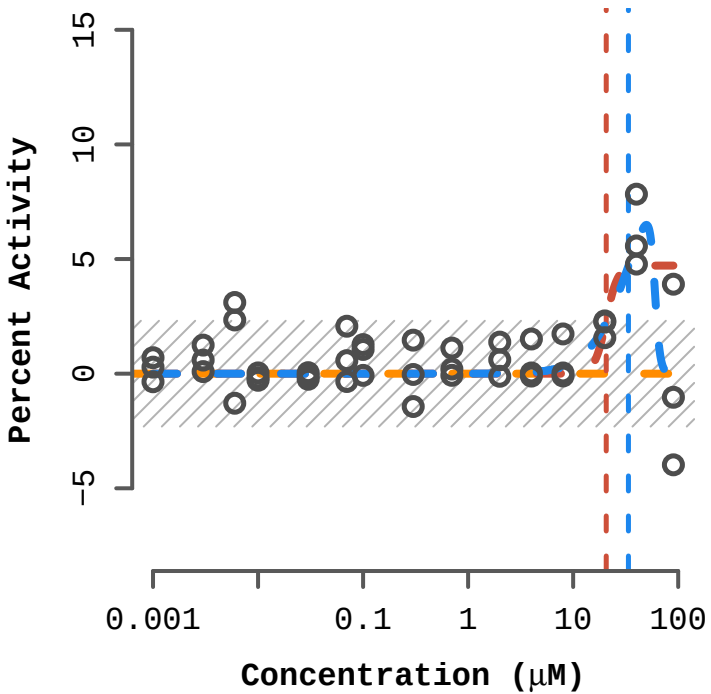
	tp	ga	gw
val:	2.68	0.754	3.96
sd:	0.638	0.13	2.59

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.85	0.89	2.48	1.76	18
sd:	0.777	0.142	1.72	0.366	37.1

	CNST	HILL	GNLS
AIC:	178.98	162.85	147.79
PROB:	0	0	1
RMSE:	1.84	1.7	1.23

MAX_MEAN: 3.56 MAX_MED: 4.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Benzenediamine
CHID: 21138 **CASRN:** 106−50−3
SPID(S): Tox21_201993
M4ID: 12480259

HILL MODEL (in red):

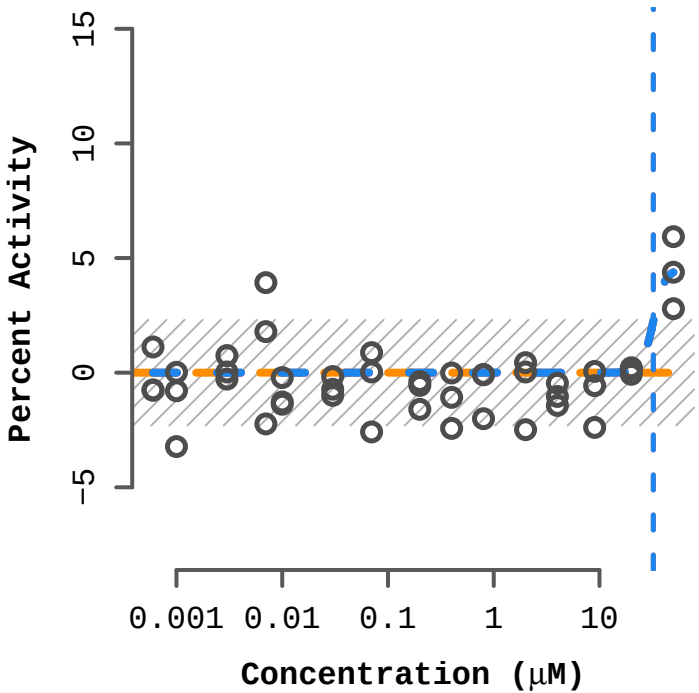
	tp	ga	gw
val:	4.71	1.31	8
sd:	0.618	0.0279	6.47

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.4	1.53	2.36	1.78	17.9
sd:	9.12	0.392	1.79	0.403	40.6

	CNST	HILL	GNLS
AIC:	184.81	165.94	156.84
PROB:	0	0.01	0.99
RMSE:	2.11	1.89	1.31

MAX_MEAN: 6.06 **MAX_MED:** 5.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Benzenediamine
CHID: 21138 CASRN: 106−50−3
SPID(S): Tox21_111615_1
M4ID: 12483585

HILL MODEL (in red):

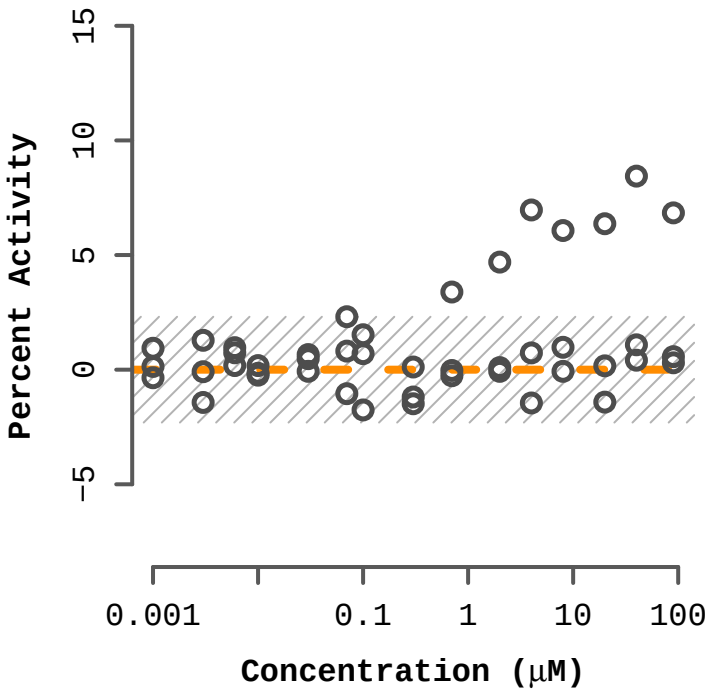
	tp	ga	gw
val:	4.51	1.51	8
sd:	9.46	2.1	74.2

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.51	1.51	8	3.26	5.46
sd:	8.59	1.91	67.4	120000	413000

	CNST	HILL	GNLS
AIC:	175.9	163.26	167.26
PROB:	0	0.88	0.12
RMSE:	1.78	1.37	1.37

MAX_MEAN: 4.37 MAX_MED: 4.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

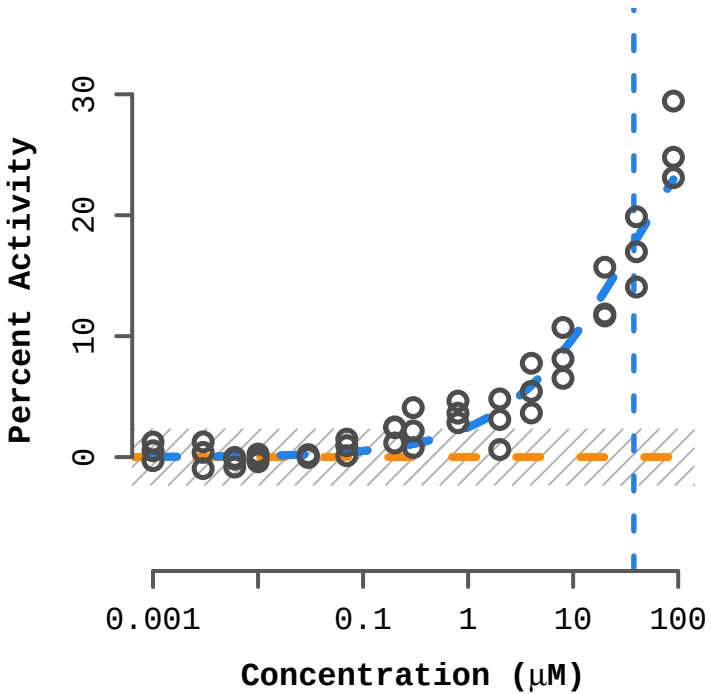
NAME: 1,3−Benzenediamine dihydrochloride
CHID: 21139 CASRN: 541−69−5
SPID(S): Tox21_200734
M4ID: 12481518

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 3.31 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Phenylenediamine dihydrochloride
CHID: 21140 CASRN: 615-28-1
SPID(S): Tox21_200980
M4ID: 12481272

HILL MODEL (in red):

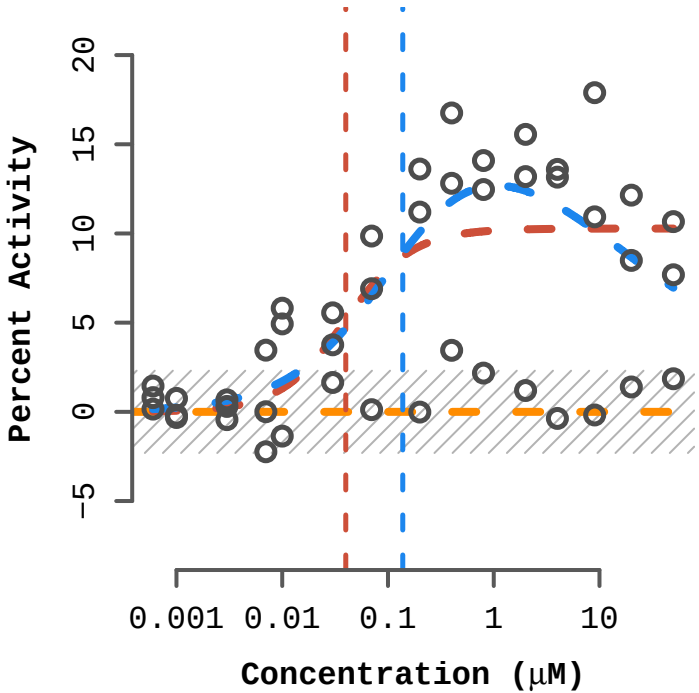
	tp	ga	gw
val:	35.3	1.58	0.713
sd:	5.18	0.193	0.0828

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	35.3	1.58	0.713	3.83	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	318.39	182.15	186.15
PROB:	0	0.88	0.12
RMSE:	9.27	1.76	1.76

MAX_MEAN: 25.8 MAX_MED: 24.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Benzenediamine dihydrochloride
CHID: 21141 CASRN: 624−18−0
SPID(S): Tox21_303880
M4ID: 12475308

HILL MODEL (in red):

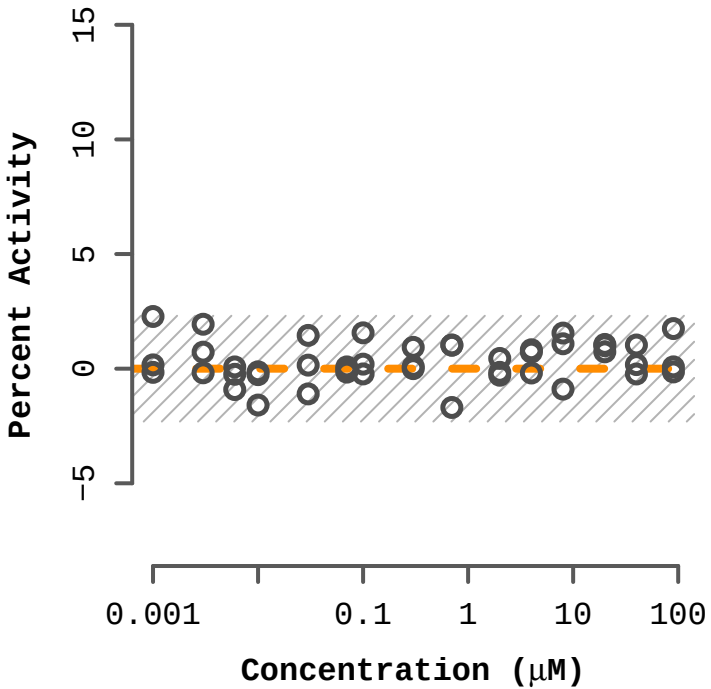
	tp	ga	gw
val:	10.3	−1.4	1.39
sd:	1.22	0.218	0.709

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.5	−0.86	0.902	0.888	0.39
sd:	38.7	0.68	0.394	4.18	0.813

	CNST	HILL	GNLS
AIC:	320.59	275.96	275.63
PROB:	0	0.46	0.54
RMSE:	8.18	4.71	4.71

MAX_MEAN: 11 MAX_MED: 13.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

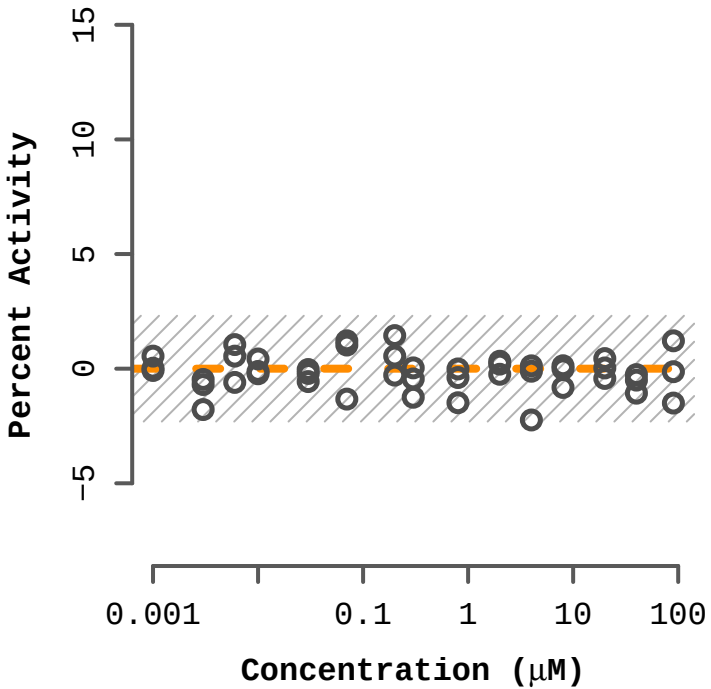
NAME: Phenylephrine hydrochloride
CHID: 21142 CASRN: 61-76-7
SPID(S): Tox21_302846
M4ID: 12476287

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.933 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

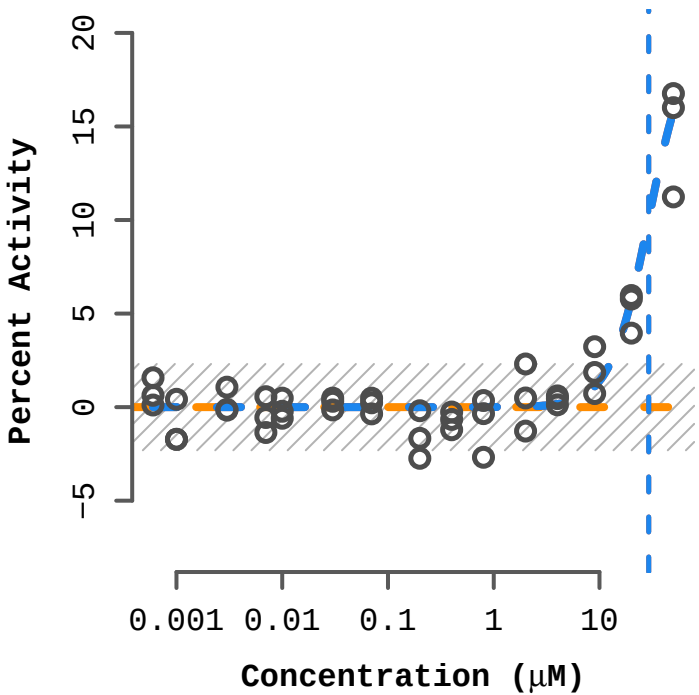
NAME: Phenylephrine hydrochloride
CHID: 21142 CASRN: 61-76-7
SPID(S): Tox21_201261
M4ID: 12480991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.572 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylephrine hydrochloride
CHID: 21142 CASRN: 61-76-7
SPID(S): Tox21_110897_1
M4ID: 12484031

HILL MODEL (in red):

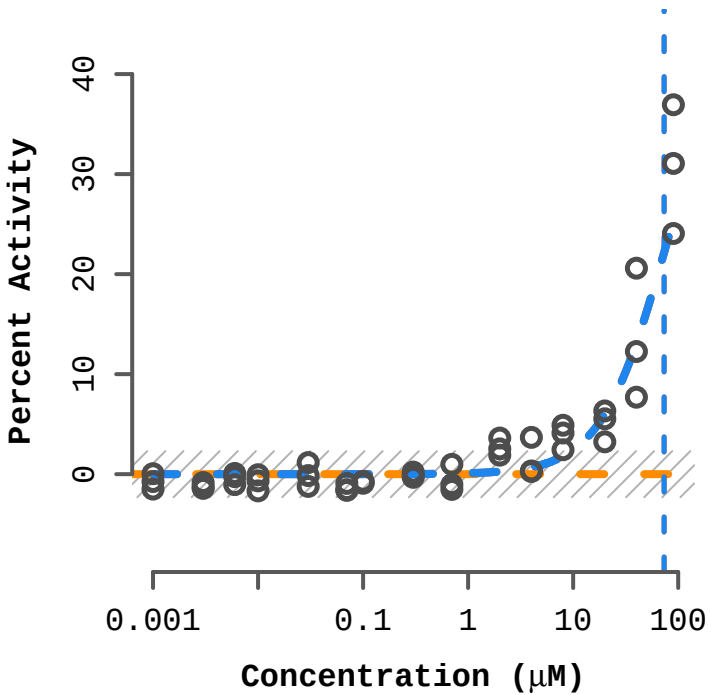
	tp	ga	gw
val:	20.1	1.47	2.42
sd:	3.24	0.0788	0.56

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	20.1	1.47	2.42	3.17	6.15
sd:	3.25	0.0788	0.561	2390	10000

	CNST	HILL	GNLS
AIC:	220.23	149.57	153.57
PROB:	0	0.88	0.12
RMSE:	4.23	1.26	1.26

MAX_MEAN: 14.7 MAX_MED: 16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylethylhydrazine sulfate
CHID: 21144 **CASRN:** 156-51-4
SPID(S): Tox21_200134
M4ID: 12482118

HILL MODEL (in red):

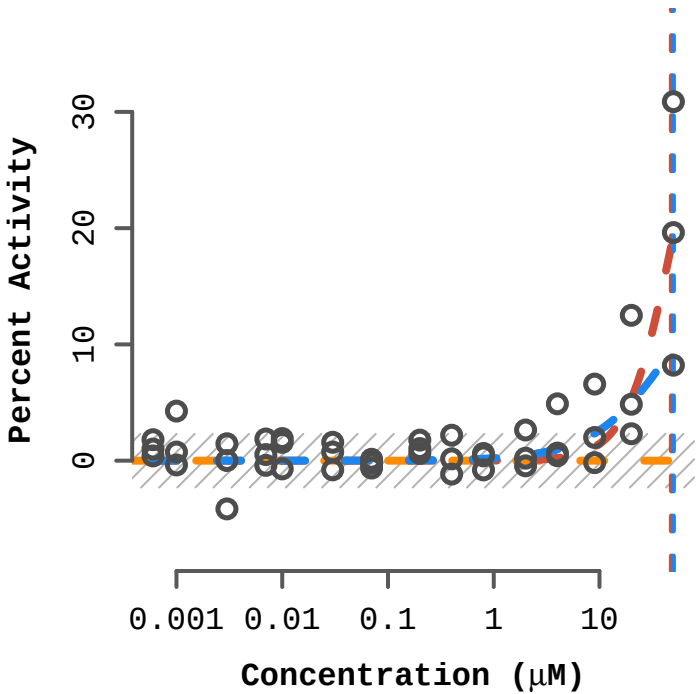
	tp	ga	gw
val:	44.3	1.87	1.43
sd:	11.9	0.17	0.28

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	44.3	1.87	1.43	3.63	11.1
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	285.51	206.96	210.96
PROB:	0	0.88	0.12
RMSE:	9.11	2.72	2.72

MAX_MEAN: 30.7 **MAX_MED:** 31.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylethylhydrazine sulfate
CHID: 21144 CASRN: 156-51-4
SPID(S): Tox21_110236_1
M4ID: 12484527

HILL MODEL (in red):

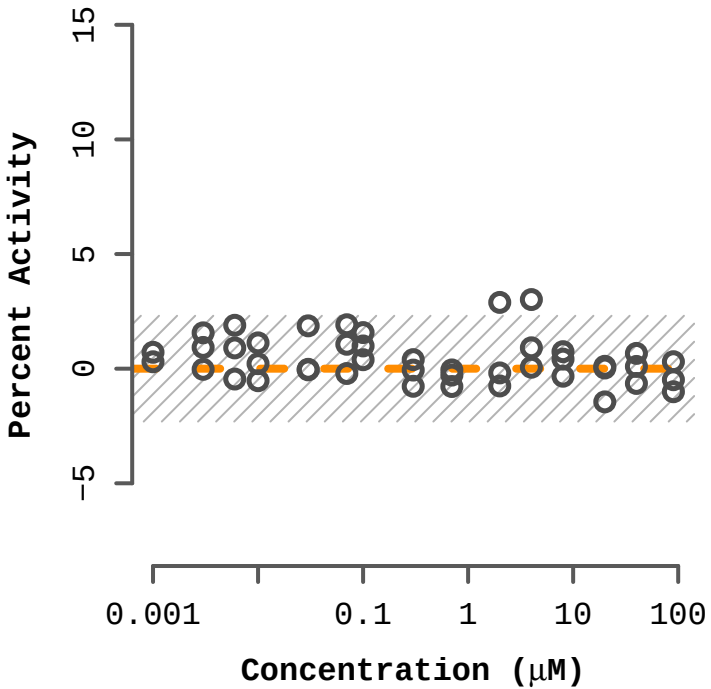
	tp	ga	gw
val:	37.1	1.68	2.05
sd:	21	0.246	0.724

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.4	1.7	1.16	2.52	8.43
sd:	21	0.742	0.559	399	4100

	CNST	HILL	GNLS
AIC:	246.94	218.02	225.61
PROB:	0	0.98	0.02
RMSE:	6.22	3.16	4.02

MAX_MEAN: 19.6 MAX_MED: 19.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

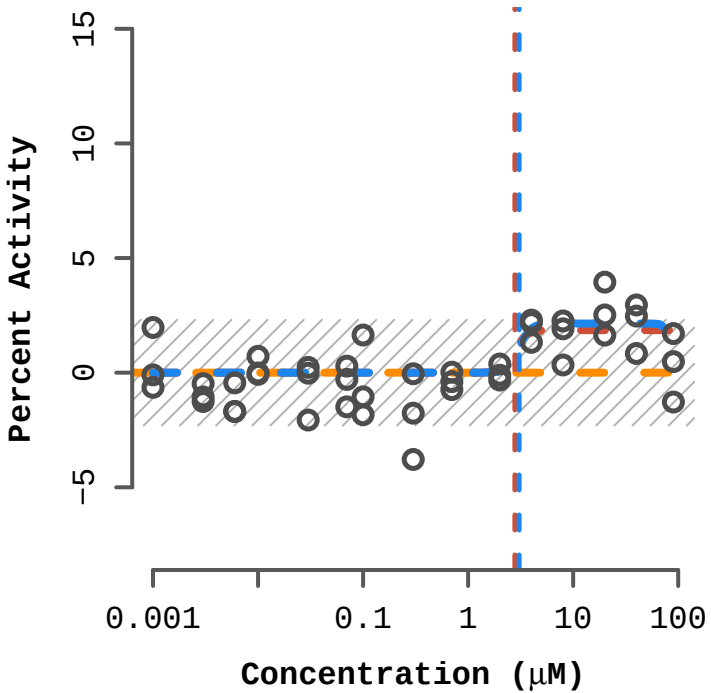
NAME: Phenyl glycidyl ether
CHID: 21145 **CASRN:** 122-60-1
SPID(S): Tox21_200289
M4ID: 12481963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylhydrazine
CHID: 21147 CASRN: 100-63-0
SPID(S): Tox21_303018
M4ID: 12476115

HILL MODEL (in red):

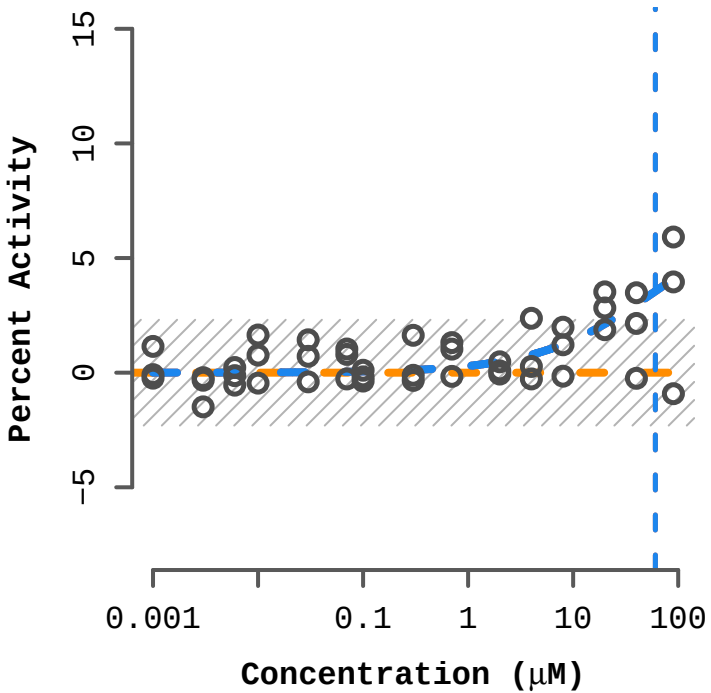
	tp	ga	gw
val:	1.86	0.445	8
sd:	0.301	0.127	6.71

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.14	0.486	8	1.92	17.6
sd:	0.343	0.136	8.17	0.178	95

	CNST	HILL	GNLS
AIC:	172.88	152.68	151.93
PROB:	0	0.41	0.59
RMSE:	1.57	1.23	1.16

MAX_MEAN: 2.7 **MAX_MED:** 2.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylhydrazine
CHID: 21147 CASRN: 100-63-0
SPID(S): Tox21_201977
M4ID: 12480275

HILL MODEL (in red):

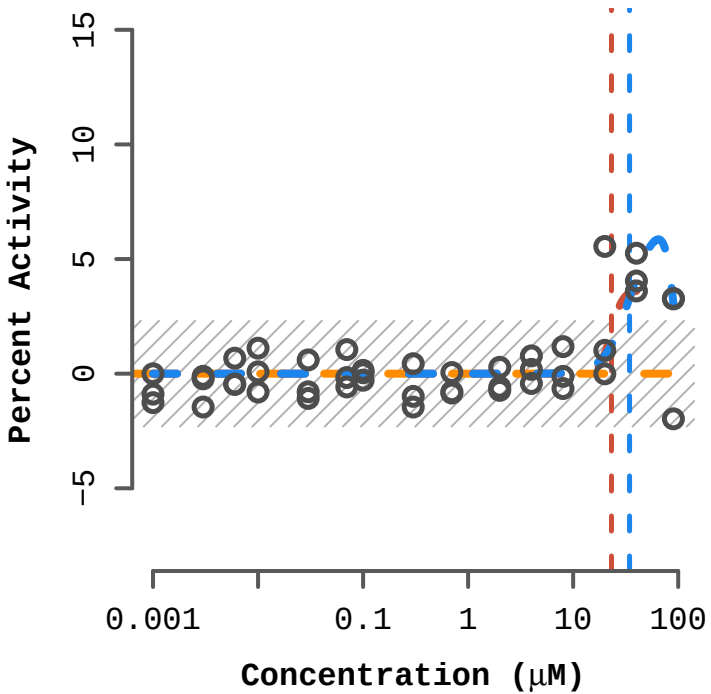
	tp	ga	gw
val:	7.1	1.78	0.769
sd:	10.3	1.65	0.607

GAIN-LOSS MODEL (in blue):

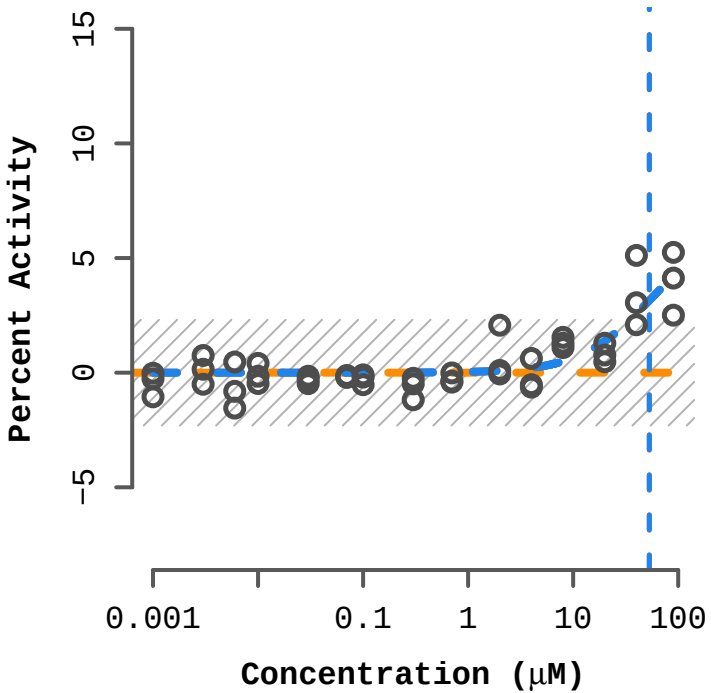
	tp	ga	gw	la	lw
val:	7.1	1.78	0.769	3.5	6.32
sd:	10.3	1.65	0.607	14000	57700

	CNST	HILL	GNLS
AIC:	165.5	142	146
PROB:	0	0.88	0.12
RMSE:	1.64	1.21	1.21

MAX_MEAN: 2.99 **MAX_MED:** 3.96 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenylhydrazine hydrochloride
CHID:    21148   CASRN: 59-88-1
SPID(S): Tox21_302936
M4ID:    12476197

HILL MODEL (in red):
      tp       ga       gw
val:  3.66     1.36     8
sd:   0.366    0.0506   4.35

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.64     1.54     3.67     1.95     10.7
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  165.59      137.24      138.07
PROB: 0           0.6         0.4
RMSE: 1.72        1.31        1.24

MAX_MEAN: 4.3       MAX_MED: 4.05      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylhydrazine hydrochloride
CHID: 21148 CASRN: 59-88-1
SPID(S): Tox21_202198
M4ID: 12480054

HILL MODEL (in red):

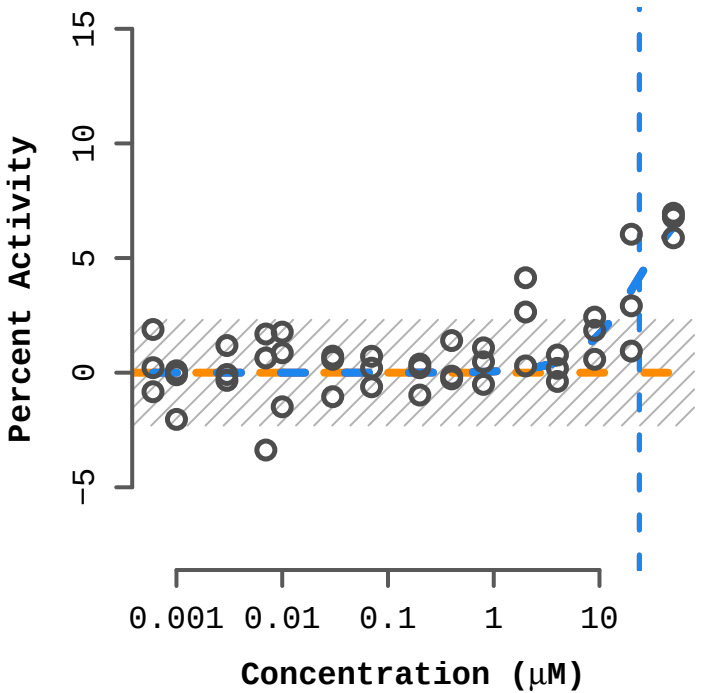
	tp	ga	gw
val:	6.3	1.72	1.31
sd:	3.16	0.371	0.568

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.3	1.72	1.3	2.54	16.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.37	111.05	115.05
PROB:	0	0.88	0.12
RMSE:	1.58	0.79	0.79

MAX_MEAN: 3.96 MAX_MED: 4.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenylhydrazine hydrochloride
CHID: 21148 **CASRN:** 59-88-1
SPID(S): Tox21_111618_1
M4ID: 12483582

HILL MODEL (in red):

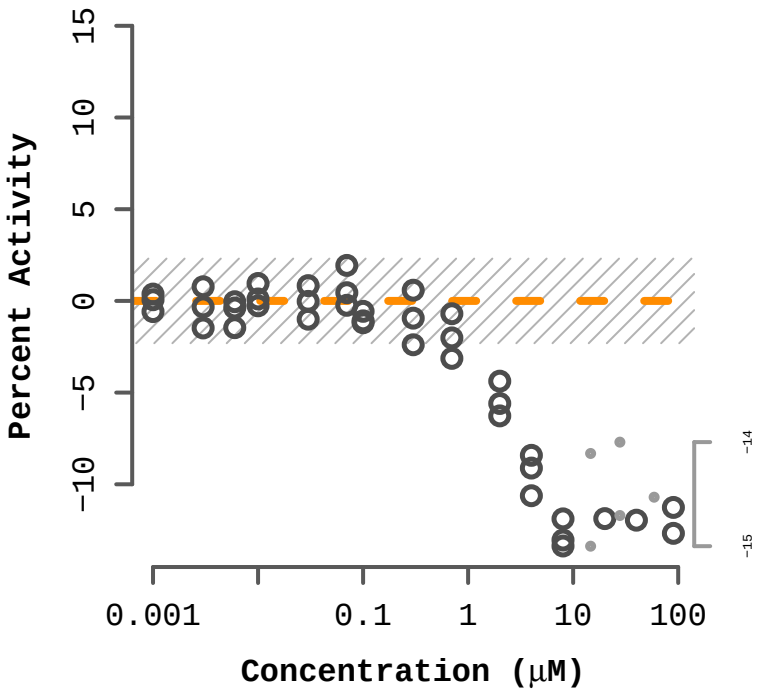
	tp	ga	gw
val:	8.35	1.38	1.58
sd:	2.58	0.236	0.607

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.35	1.38	1.58	3.45	4.29
sd:	2.58	0.236	0.607	869	2130

	CNST	HILL	GNLS
AIC:	195.32	156.82	160.82
PROB:	0	0.88	0.12
RMSE:	2.35	1.31	1.31

MAX_MEAN: 6.54 **MAX_MED:** 6.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

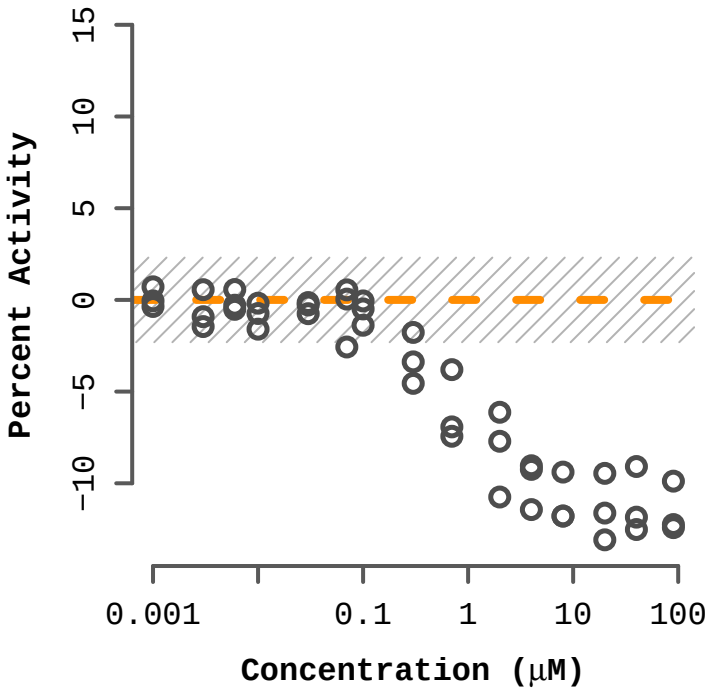
NAME: Phenylmercuric acetate
CHID: 21150 **CASRN:** 62-38-4
SPID(S): Tox21_300589
M4ID: 12478544 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	310.2	NA	NA
PROB:	1	NA	NA
RMSE:	7.47	NA	NA

MAX_MEAN: 0.716 **MAX_MED:** 0.449 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

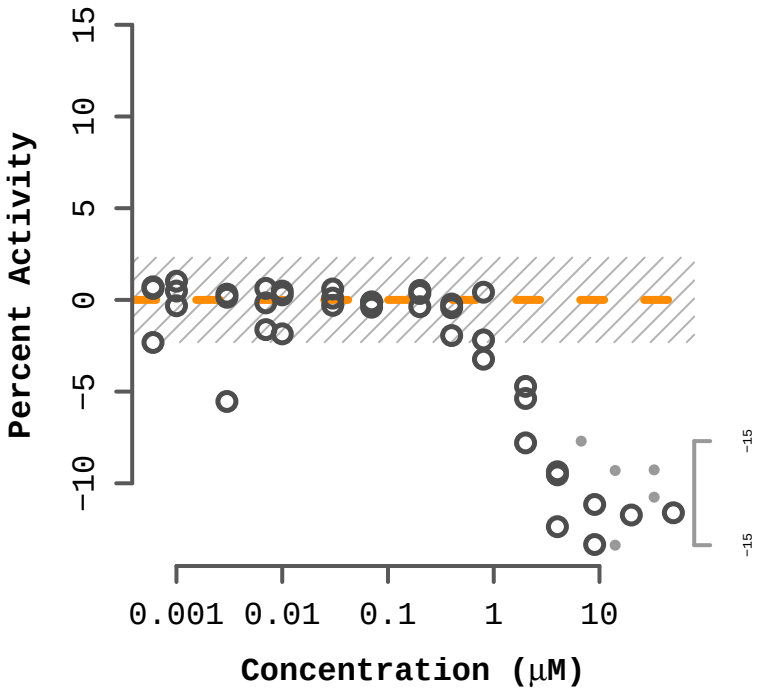
NAME: Phenylmercuric acetate
CHID: 21150 **CASRN:** 62-38-4
SPID(S): Tox21_202241
M4ID: 12480011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	308.34	NA	NA
PROB:	1	NA	NA
RMSE:	7.03	NA	NA

MAX_MEAN: 0.102 **MAX_MED:** 0.0454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

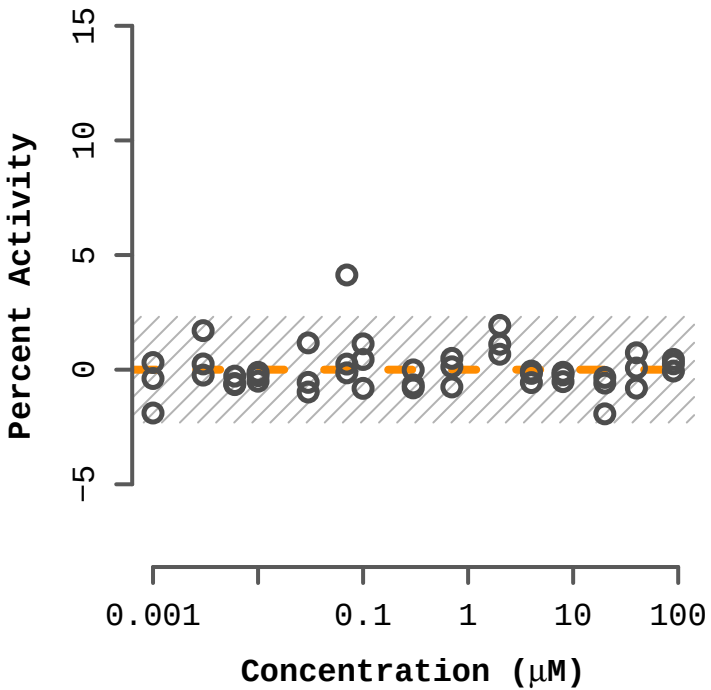
NAME: Phenylmercuric acetate
CHID: 21150 **CASRN:** 62-38-4
SPID(S): Tox21_111068_1
M4ID: 12483925 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.67	NA	NA
PROB:	1	NA	NA
RMSE:	6.97	NA	NA

MAX_MEAN: 0.396 **MAX_MED:** 0.625 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

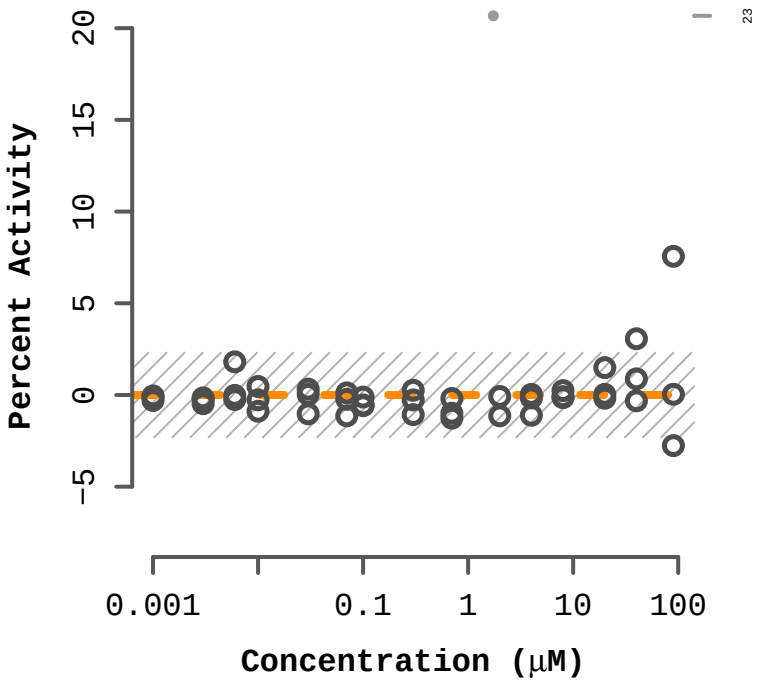
NAME: 2-Phenylphenol
CHID: 21151 **CASRN:** 90-43-7
SPID(S): Tox21_300674
M4ID: 12478459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

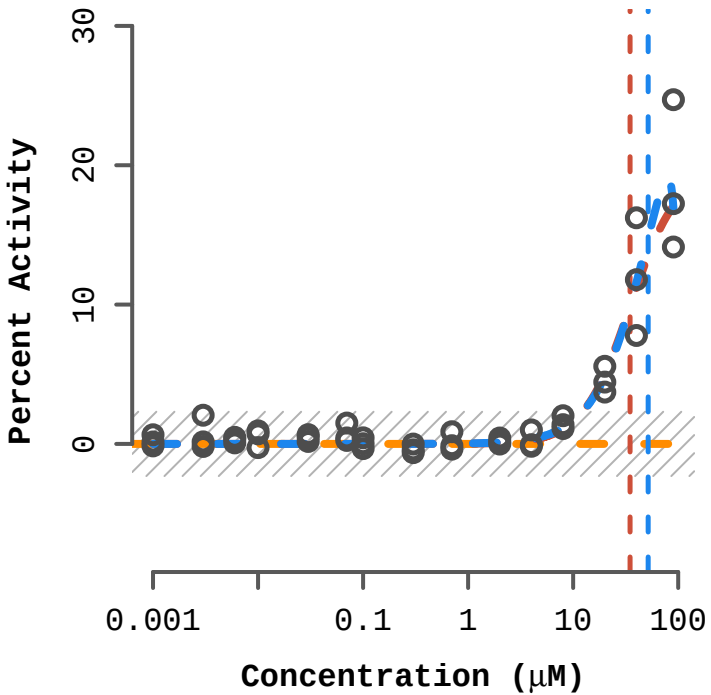
NAME: 2-Phenylphenol
CHID: 21151 CASRN: 90-43-7
SPID(S): Tox21_202415
M4ID: 12479837 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.77	NA	NA

MAX_MEAN: 7.39 MAX_MED: 0.882 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Phenylphenol
CHID: 21152 CASRN: 92-69-3
SPID(S): Tox21_302734
M4ID: 12476399

HILL MODEL (in red):

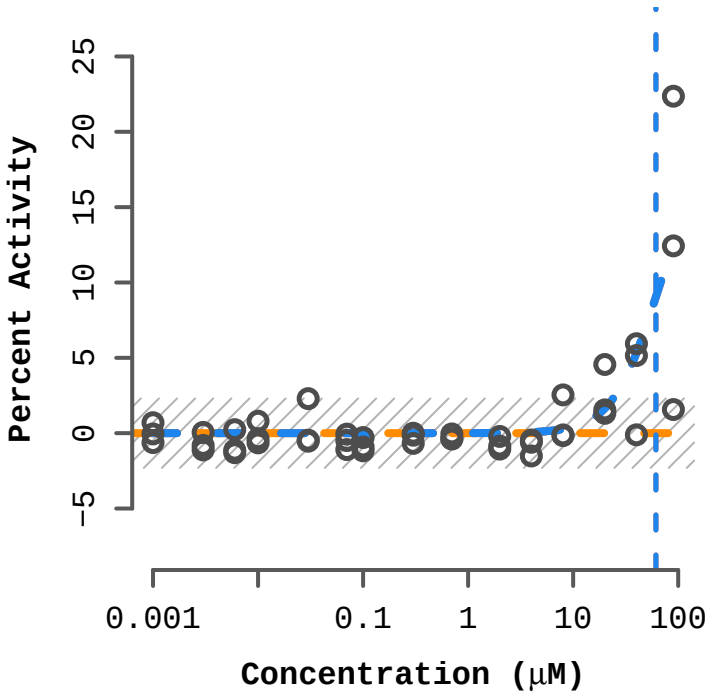
	tp	ga	gw
val:	19.8	1.54	1.95
sd:	2.01	0.0713	0.343

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29.6	1.71	1.72	1.99	14.4
sd:	7.55	0.111	0.2	0.0114	7.46

	CNST	HILL	GNLS
AIC:	250.13	143.83	146.28
PROB:	0	0.77	0.23
RMSE:	6.07	1.63	1.63

MAX_MEAN: 18.7 MAX_MED: 17.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Phenylphenol
CHID: 21152 **CASRN:** 92-69-3
SPID(S): Tox21_202220
M4ID: 12480032

HILL MODEL (in red):

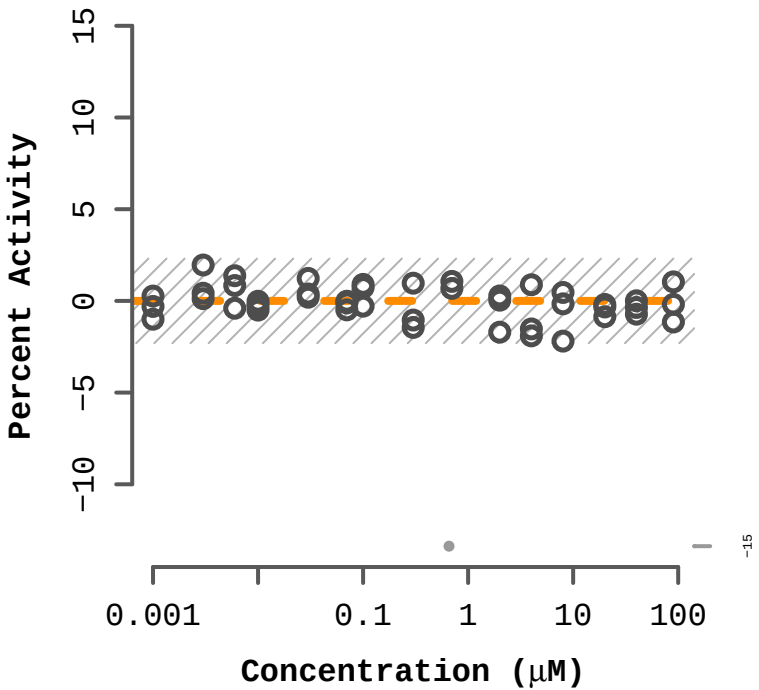
	tp	ga	gw
val:	18.1	1.79	2.05
sd:	6.35	0.177	0.605

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.1	1.79	2.05	3.75	4.54
sd:	6.34	0.177	0.605	6170	15900

	CNST	HILL	GNLS
AIC:	196.84	173.68	177.68
PROB:	0	0.88	0.12
RMSE:	4.14	2.51	2.51

MAX_MEAN: 12.1 **MAX_MED:** 12.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

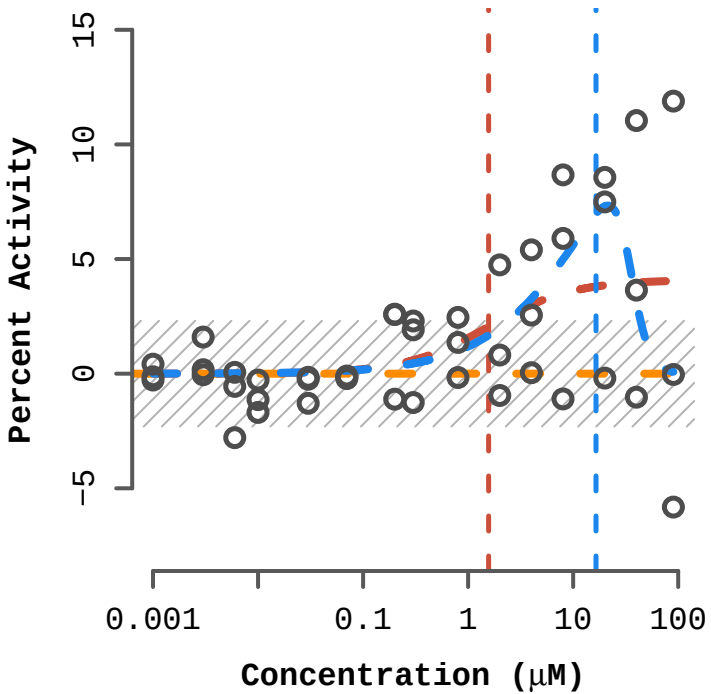
NAME: Phosphamidon
CHID: 21156 **CASRN:** 13171-21-6
SPID(S): Tox21_302848
M4ID: 12476285 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 0.835 **MAX_MED:** 0.841 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phosphamidon
CHID: 21156 CASRN: 13171-21-6
SPID(S): Tox21_202100
M4ID: 12480152

HILL MODEL (in red):

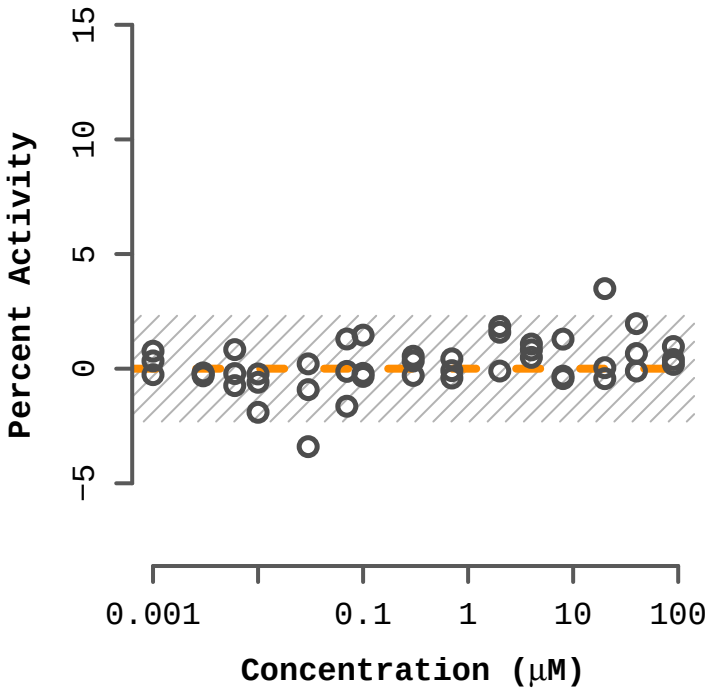
	tp	ga	gw
val:	4.1	0.195	1.08
sd:	2.09	0.593	0.716

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.3	1.22	0.857	1.54	5.17
sd:	28.8	1.57	0.545	0.371	16.6

	CNST	HILL	GNLS
AIC:	239.43	232.8	228.92
PROB:	0	0.13	0.87
RMSE:	3.84	3.09	3.12

MAX_MEAN: 5.29 MAX_MED: 7.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

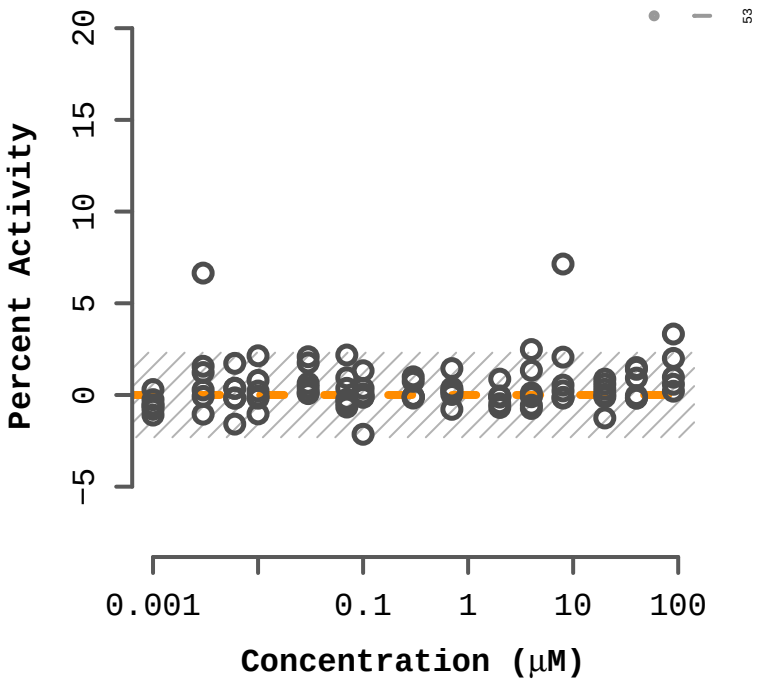
NAME: Phthalamide
CHID: 21158 **CASRN:** 88-96-0
SPID(S): Tox21_200512
M4ID: 12481740

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

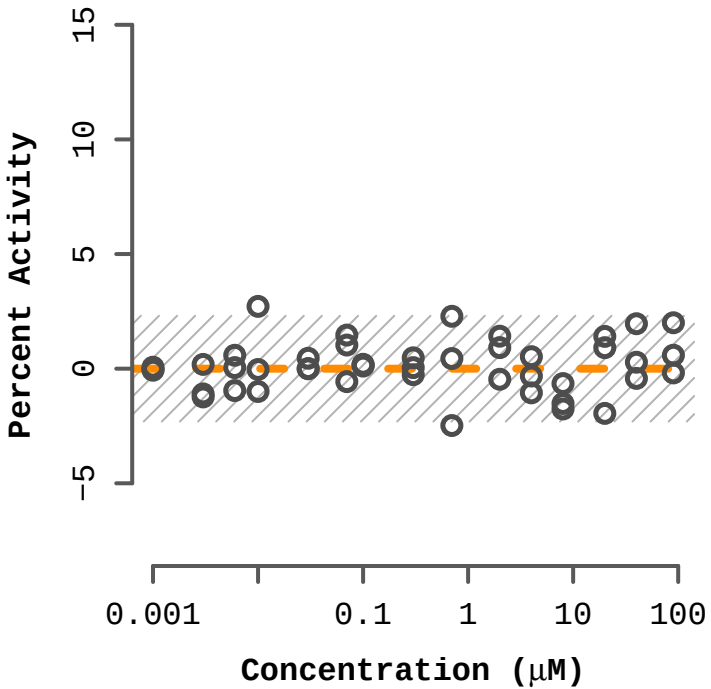
NAME: Phthalic anhydride
CHID: 21159 CASRN: 85-44-9
SPID(S): Tox21_200142
M4ID: 12482110 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	310.43	NA	NA
PROB:	1	NA	NA
RMSE:	5.71	NA	NA

MAX_MEAN: 9.93 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

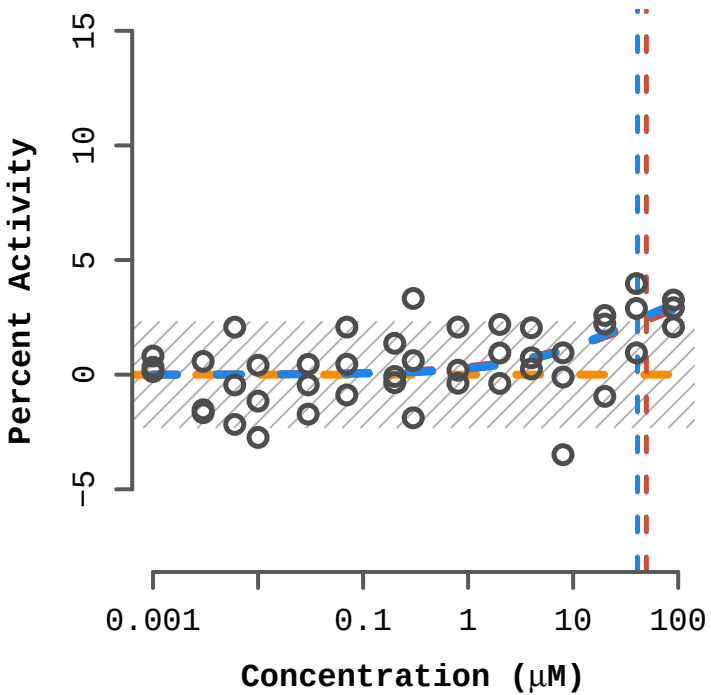
NAME: Picloram
CHID: 21160 CASRN: 1918-02-1
SPID(S): Tox21_301048
M4ID: 12478085

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.803 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Picloram
CHID: 21160 CASRN: 1918-02-1
SPID(S): Tox21_201298
M4ID: 12480954

HILL MODEL (in red):

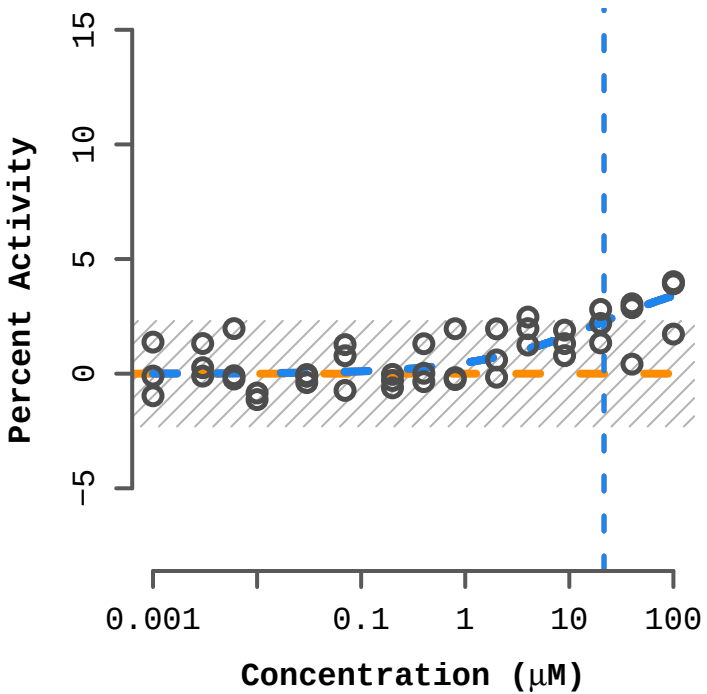
	tp	ga	gw
val:	4.77	1.7	0.671
sd:	4.99	1.42	0.479

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.77	1.61	0.762	2.04	10.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	184.05	168.77	172.7
PROB:	0	0.88	0.12
RMSE:	1.76	1.45	1.45

MAX_MEAN: 2.76 **MAX_MED:** 2.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Picloram
CHID: 21160 CASRN: 1918-02-1
SPID(S): Tox21_200043
M4ID: 12482209

HILL MODEL (in red):

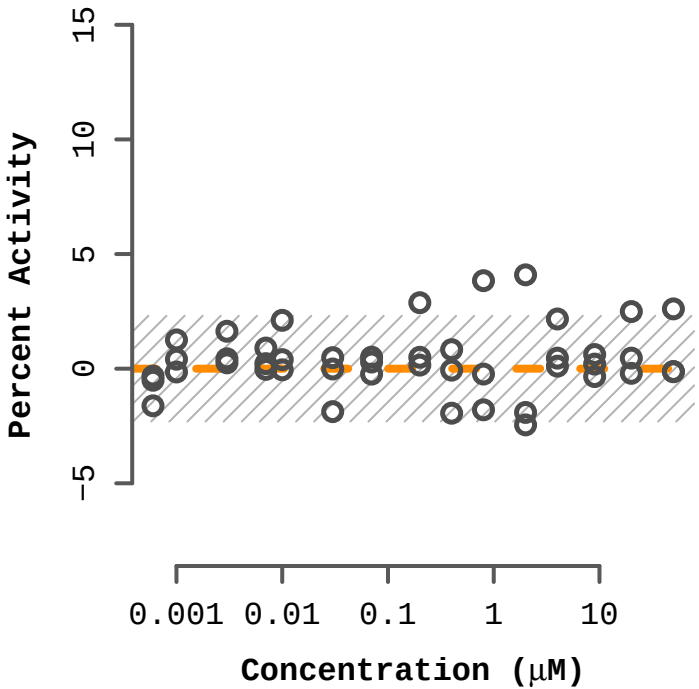
	tp	ga	gw
val:	4.56	1.33	0.699
sd:	2.68	0.828	0.309

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.56	1.33	0.699	3.52	5.1
sd:	2.68	0.828	0.309	1430	4780

	CNST	HILL	GNLS
AIC:	166.72	125.1	129.1
PROB:	0	0.88	0.12
RMSE:	1.57	0.89	0.89

MAX_MEAN: 3.22 MAX_MED: 3.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

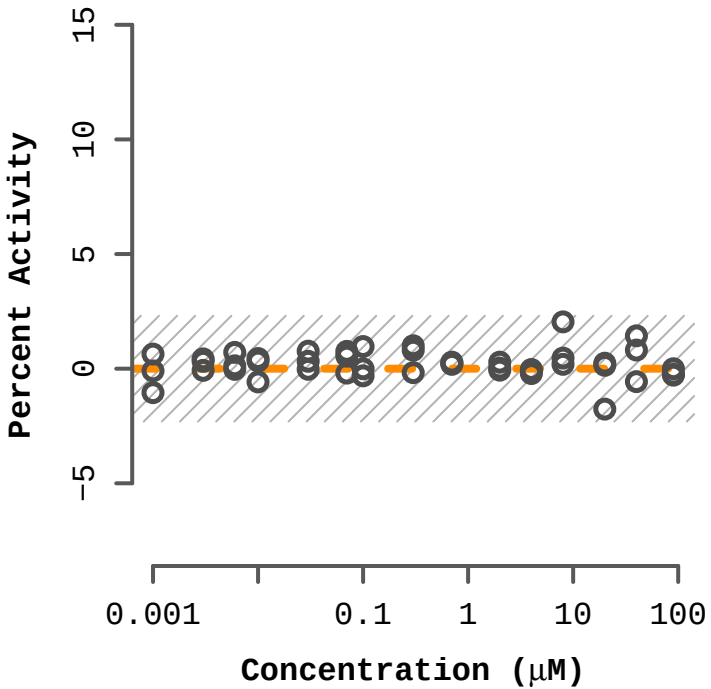
NAME: Pilocarpine
CHID: 21162 **CASRN:** 92-13-7
SPID(S): Tox21_110887_1
M4ID: 12484040

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.498 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

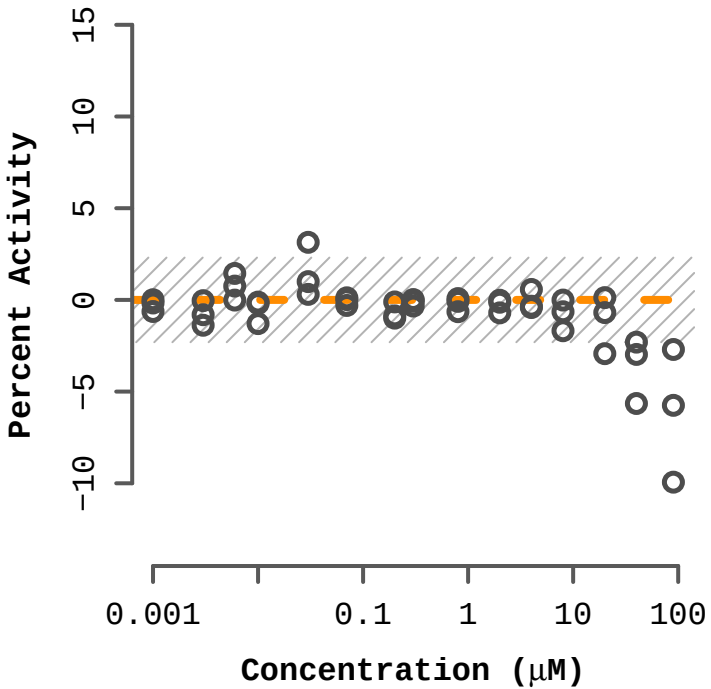
NAME: Piperazine
CHID: 21164 CASRN: 110-85-0
SPID(S): Tox21_300104
M4ID: 12479026

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	84.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.899 MAX_MED: 0.813 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

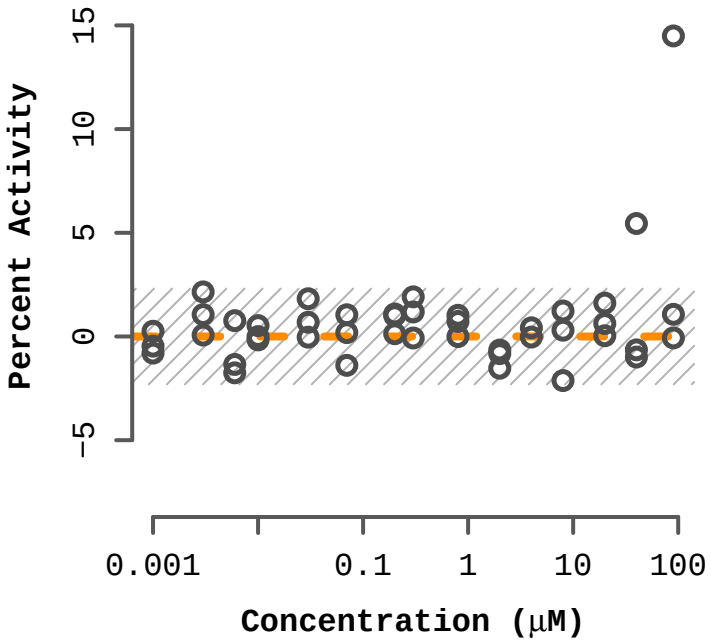
NAME: Piperazine
CHID: 21164 **CASRN:** 110-85-0
SPID(S): Tox21_202242
M4ID: 12480010

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.66	NA	NA
PROB:	1	NA	NA
RMSE:	2.21	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 0.999 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

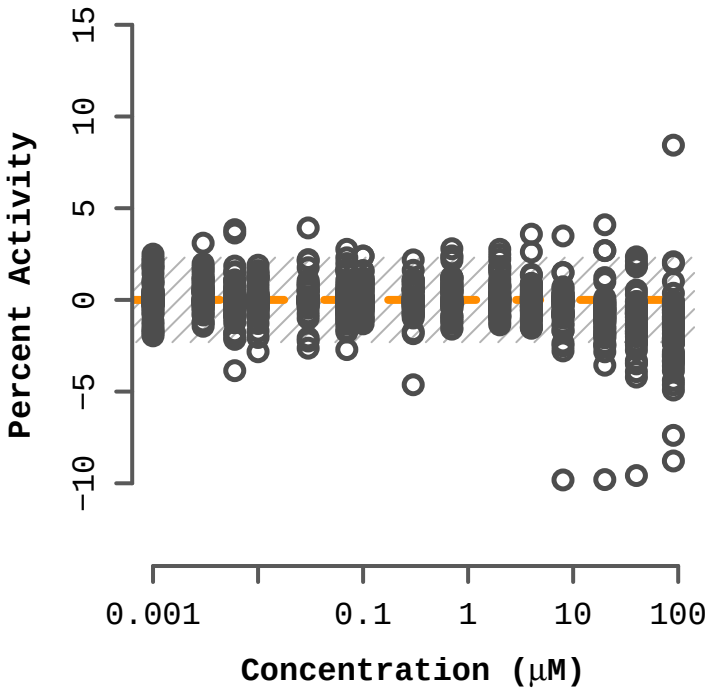
NAME: Piperidine
CHID: 21165 CASRN: 110-89-4
SPID(S): Tox21_201175
M4ID: 12481077

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 5.17 MAX_MED: 1.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

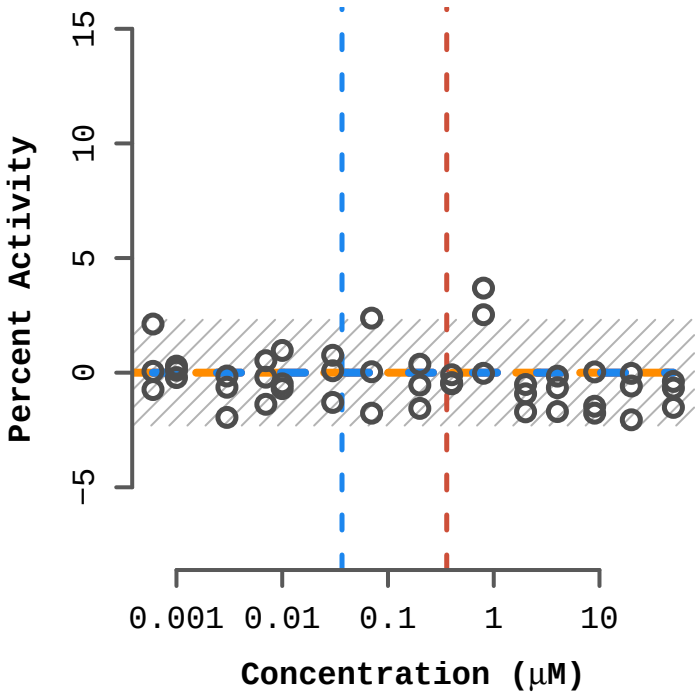
NAME: Piperonyl butoxide
CHID: 21166 **CASRN:** 51-03-6
SPID(S): Tox21_400086
M4ID: 12475051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2353.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.302 **MAX_MED:** 0.213 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piperonyl butoxide
CHID: 21166 **CASRN:** 51-03-6
SPID(S): Tox21_111034_1
M4ID: 12483938

HILL MODEL (in red):

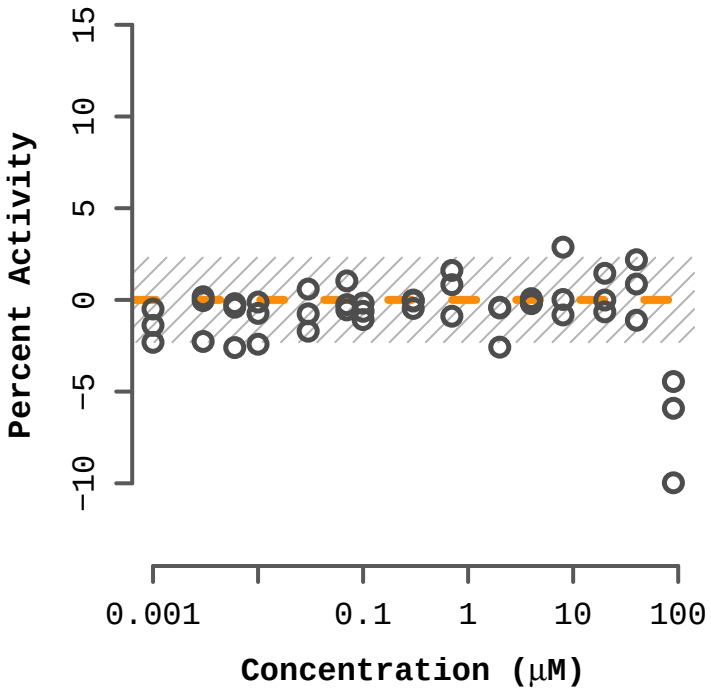
	tp	ga	gw
val:	1.54e-10	-0.444	0.902
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.36e-09	-1.43	1.09	-1.17	8.17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	147.42	153.42	157.42
PROB:	0.95	0.05	0.01
RMSE:	1.23	1.23	1.23

MAX_MEAN: 2.07 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

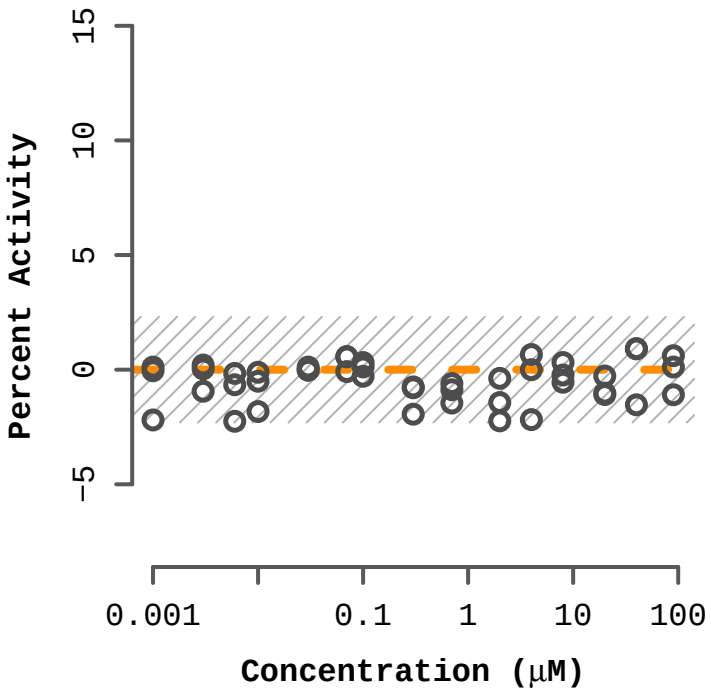
NAME: Piperonyl sulfoxide
CHID: 21168 **CASRN:** 120-62-7
SPID(S): Tox21_200395
M4ID: 12481857

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.19	NA	NA

MAX_MEAN: 0.694 **MAX_MED:** 0.867 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

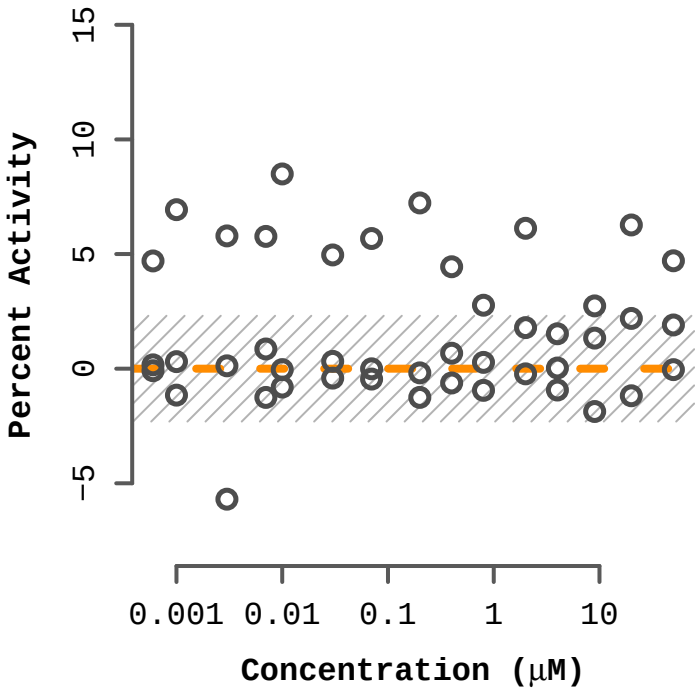
NAME: Piroxicam
CHID: 21170 **CASRN:** 36322-90-4
SPID(S): Tox21_200151
M4ID: 12482101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.07	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.351 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

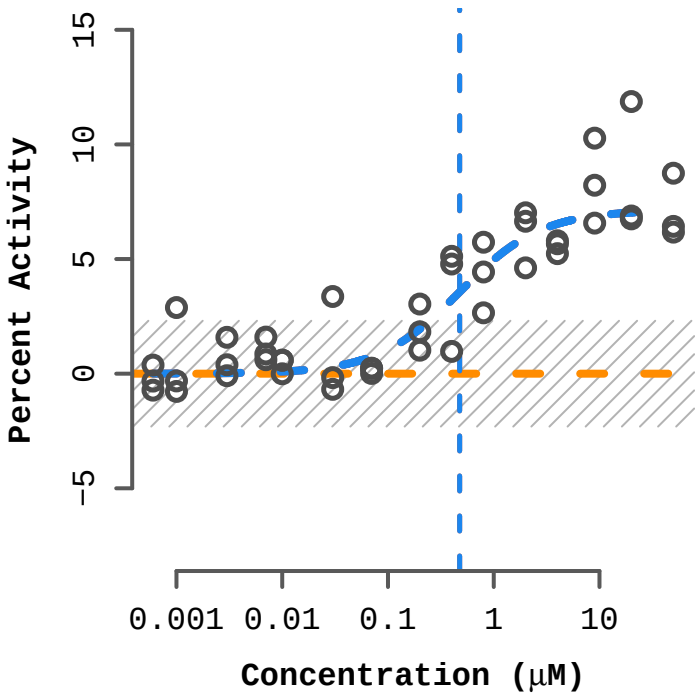
NAME: Piroxicam
CHID: 21170 **CASRN:** 36322-90-4
SPID(S): Tox21_110231_1
M4ID: 12484530

HILL MODEL: Not applicable.

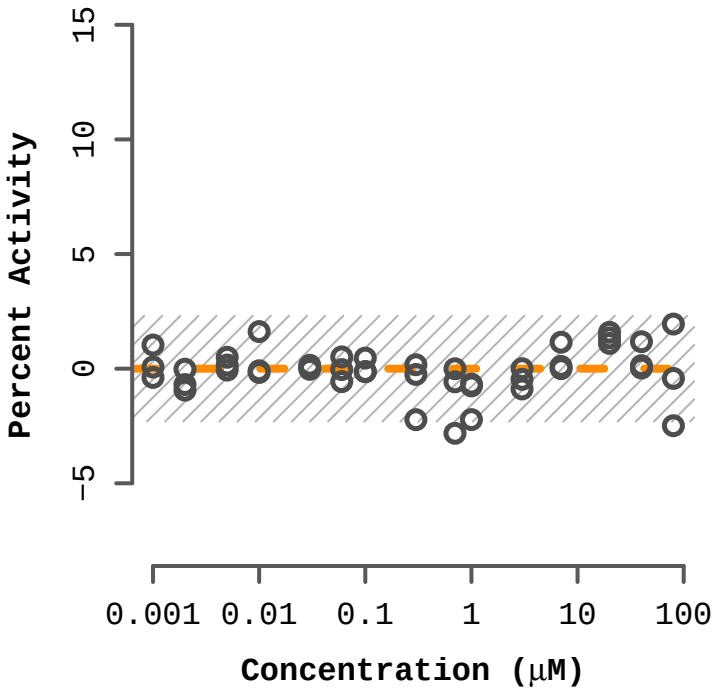
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.65	NA	NA
PROB:	1	NA	NA
RMSE:	3.38	NA	NA

MAX_MEAN: 2.56 **MAX_MED:** 2.19 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Polybrominated biphenyls (PBB)
CHID:    21174   CASRN: 59536-65-1
SPID(S): Tox21_202596
M4ID:    12479656

HILL MODEL (in red):
      tp       ga       gw
val:  7.13     -0.322   1.12
sd:   0.595    0.159    0.361

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.13     -0.322   1.12     3.61     4.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  269.12      164.88      168.88
PROB: 0           0.88        0.12
RMSE: 4.63        1.44        1.44

MAX_MEAN: 8.5       MAX_MED: 8.22      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

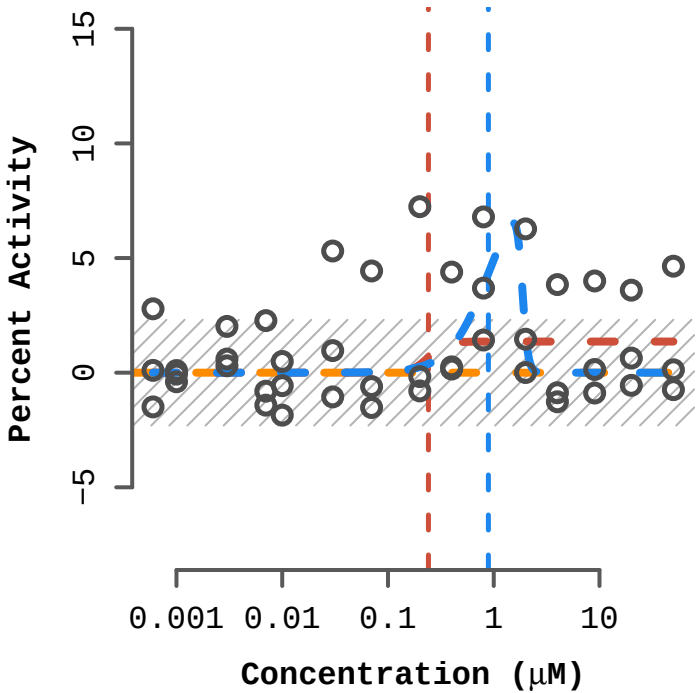
NAME: Polysorbate 80
CHID: 21175 **CASRN:** 9005-65-6
SPID(S): Tox21_303472
M4ID: 12475668

HILL MODEL: Not applicable.

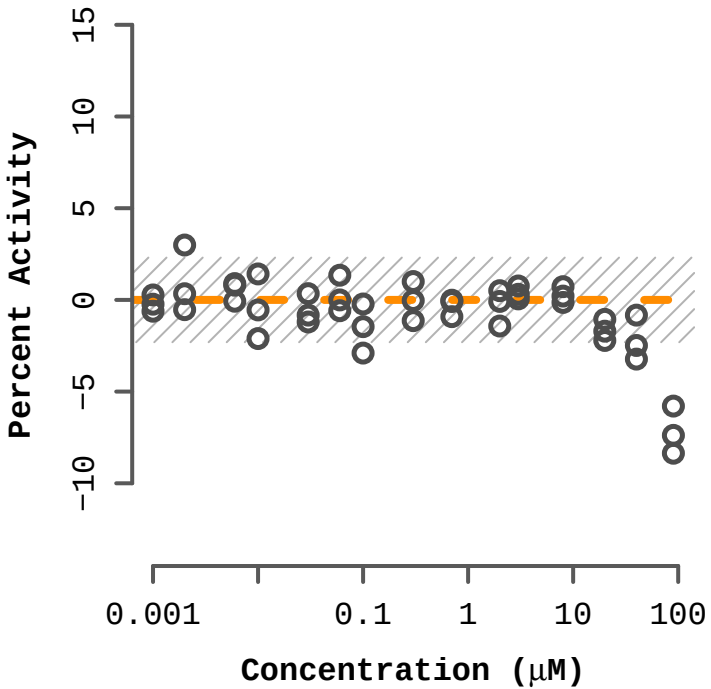
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.01	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.34 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Practolol
CHID:    21179   CASRN: 6673-35-4
SPID(S): Tox21_110928_1
M4ID:    12484007

HILL MODEL (in red):
      tp       ga       gw
val:  1.36     -0.617   5.7
sd:   0.581    0.452    18.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.66     -0.0506  2.36     0.27     16.8
sd:   89       3.52     8.84     1.54     832

      CNST        HILL        GNLS
AIC:  214.38      213.7       214.03
PROB: 0.28        0.39        0.33
RMSE: 2.69        2.4         2.35

MAX_MEAN: 3.97      MAX_MED: 3.69      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

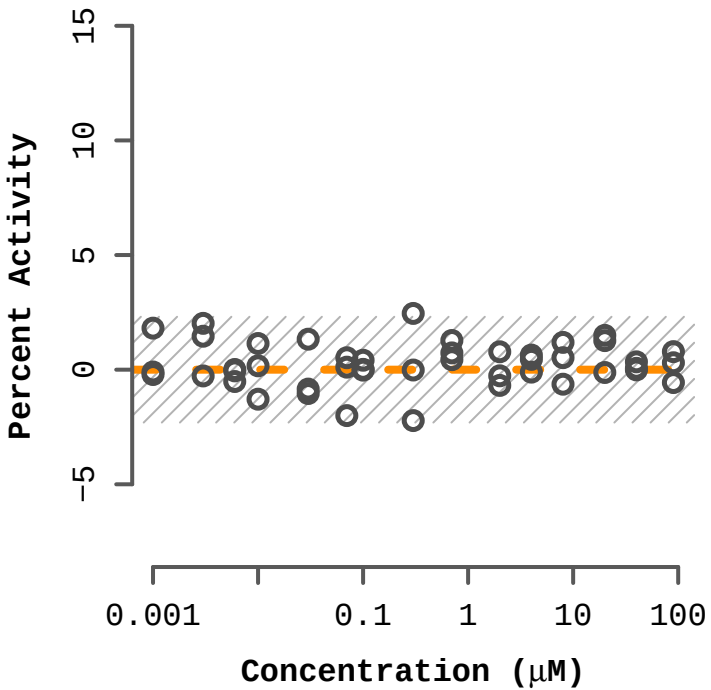
NAME: Prazepam
CHID: 21181 **CASRN:** 2955-38-6
SPID(S): Tox21_200076
M4ID: 12482176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 0.934 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

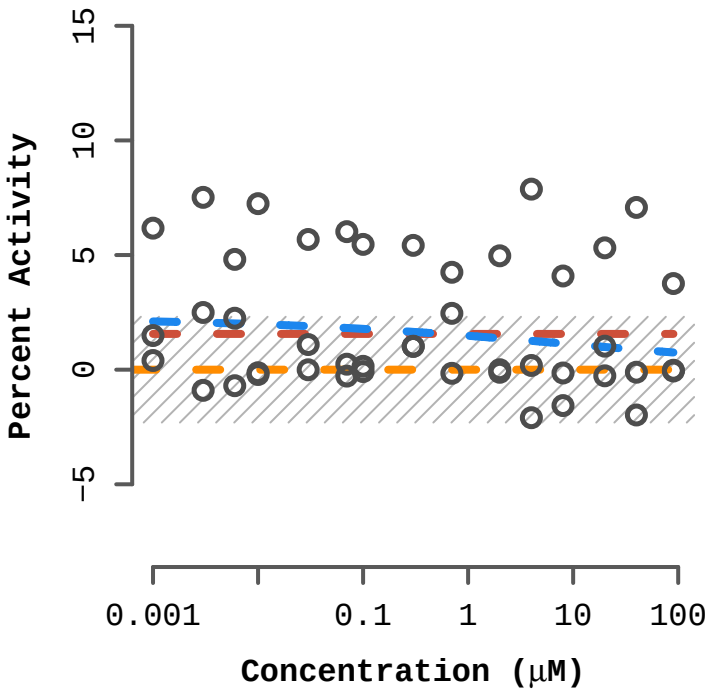
NAME: Praziquantel
CHID: 21182 **CASRN:** 55268-74-1
SPID(S): Tox21_302927
M4ID: 12476206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Praziquantel
CHID: 21182 CASRN: 55268-74-1
SPID(S): Tox21_201950
M4ID: 12480302

HILL MODEL (in red):

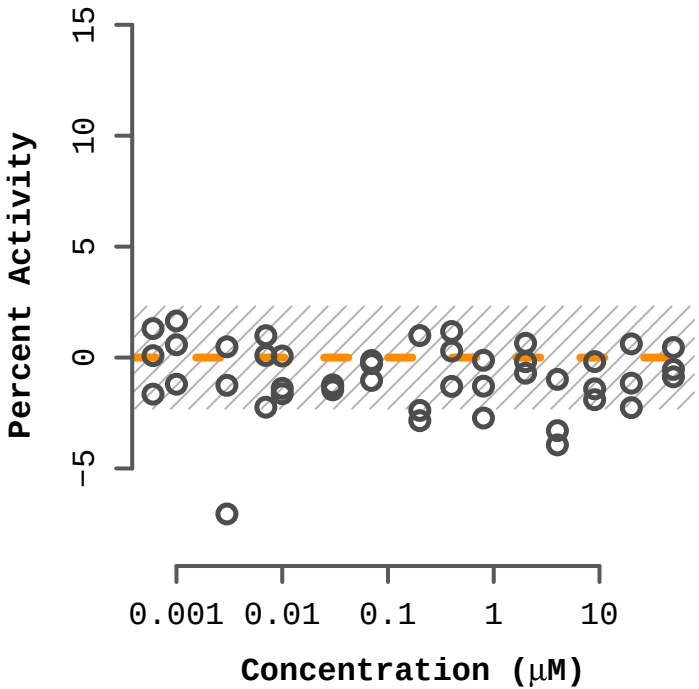
	tp	ga	gw
val:	1.56	−4.74	4.01
sd:	0.463	1460	3350

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.24	−4.79	3.37	0.96	0.3
sd:	3.06	968	1800	4.55	1.14

	CNST	HILL	GNLS
AIC:	241.73	235.37	238.47
PROB:	0.03	0.8	0.17
RMSE:	3.49	2.89	2.86

MAX_MEAN: 3.04 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

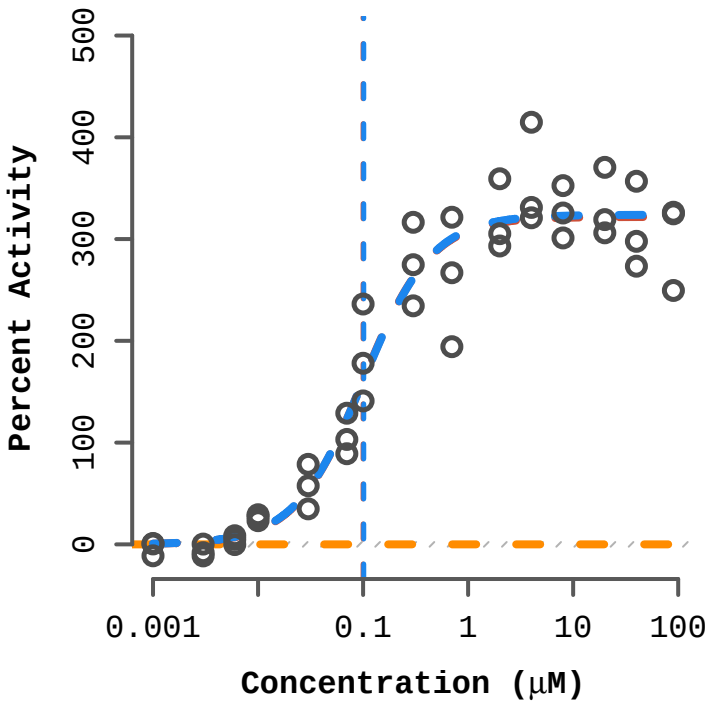
NAME: Praziquantel
CHID: 21182 **CASRN:** 55268-74-1
SPID(S): Tox21_110660_1
M4ID: 12484198

HILL MODEL: Not applicable.

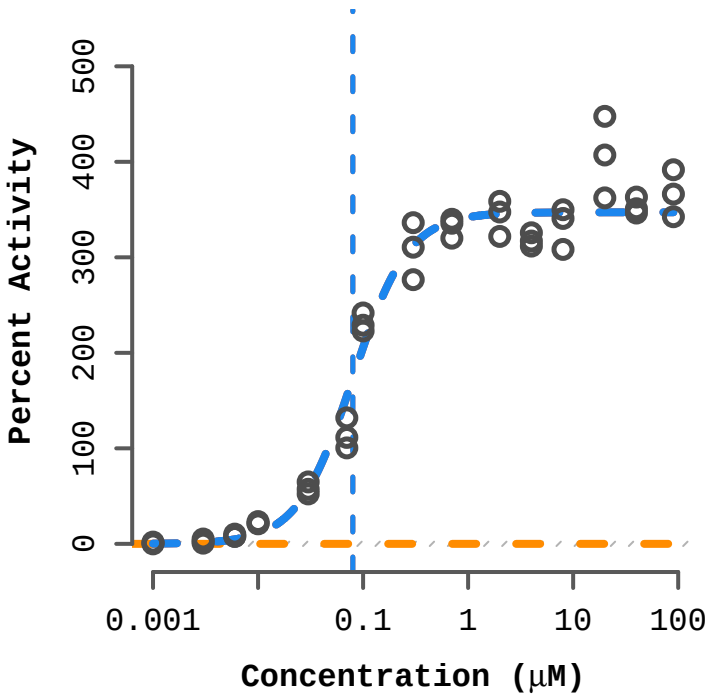
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 0.343 **MAX_MED:** 0.578 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Prednisolone
CHID:    21184   CASRN: 50-24-8
SPID(S): Tox21_302987
M4ID:    12476146

HILL MODEL (in red):
      tp       ga       gw
val:  322      -1       1.34
sd:   7.21     0.05     0.195

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  324      -0.994   1.32     2.05     15.6
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  628.02      446.42      450.11
PROB: 0           0.86        0.14
RMSE: 236.21      33.9        33.56

MAX_MEAN: 356       MAX_MED: 331       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisolone
CHID: 21184 CASRN: 50-24-8
SPID(S): Tox21_201673
M4ID: 12480579

HILL MODEL (in red):

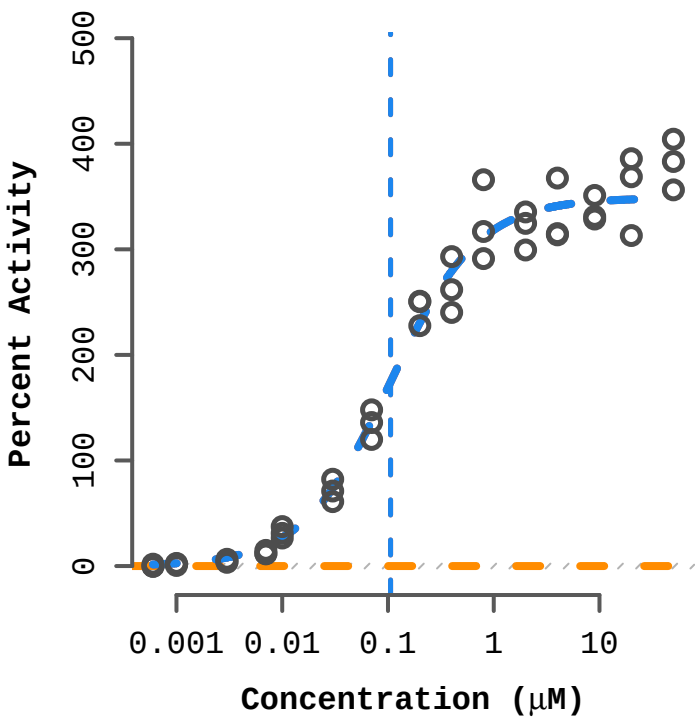
	tp	ga	gw
val:	347	-1.1	1.66
sd:	5.24	0.04	0.202

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	347	-1.1	1.66	3.76	11.3
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	637.84	422.17	426.17
PROB:	0	0.88	0.12
RMSE:	262.34	26.49	26.49

MAX_MEAN: 406 MAX_MED: 407 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisolone
CHID: 21184 CASRN: 50-24-8
SPID(S): Tox21_111327_1
M4ID: 12483765

HILL MODEL (in red):

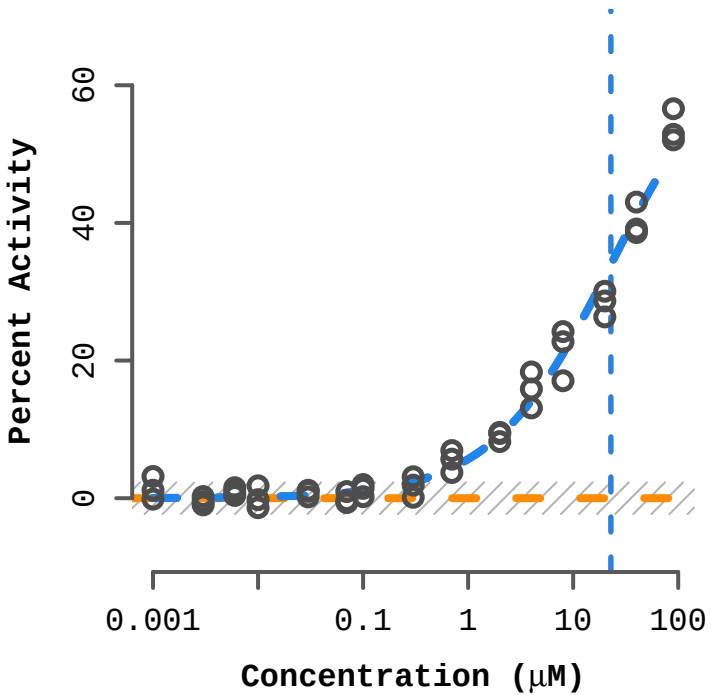
	tp	ga	gw
val:	349	-0.976	1.05
sd:	7.84	0.0425	0.08

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	349	-0.976	1.05	2.26	17.9
sd:	7.84	0.0425	0.08	602	18900

	CNST	HILL	GNLS
AIC:	628.69	404.52	408.52
PROB:	0	0.88	0.12
RMSE:	239.65	20.37	20.37

MAX_MEAN: 381 **MAX_MED:** 383 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisone
CHID: 21185 CASRN: 53-03-2
SPID(S): Tox21_300196
M4ID: 12478934

HILL MODEL (in red):

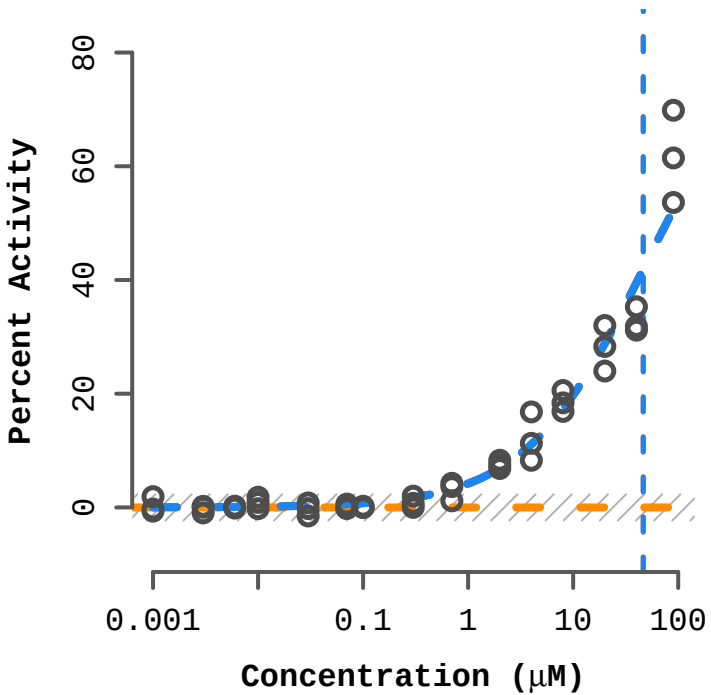
	tp	ga	gw
val:	67.9	1.36	0.765
sd:	6.73	0.129	0.0526

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	67.9	1.36	0.765	3.92	6.65
sd:	6.73	0.129	0.0526	63700	215000

	CNST	HILL	GNLS
AIC:	391.35	202.4	206.4
PROB:	0	0.88	0.12
RMSE:	20.3	2.15	2.15

MAX_MEAN: 53.8 MAX_MED: 52.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisone
CHID: 21185 CASRN: 53-03-2
SPID(S): Tox21_201564
M4ID: 12480688

HILL MODEL (in red):

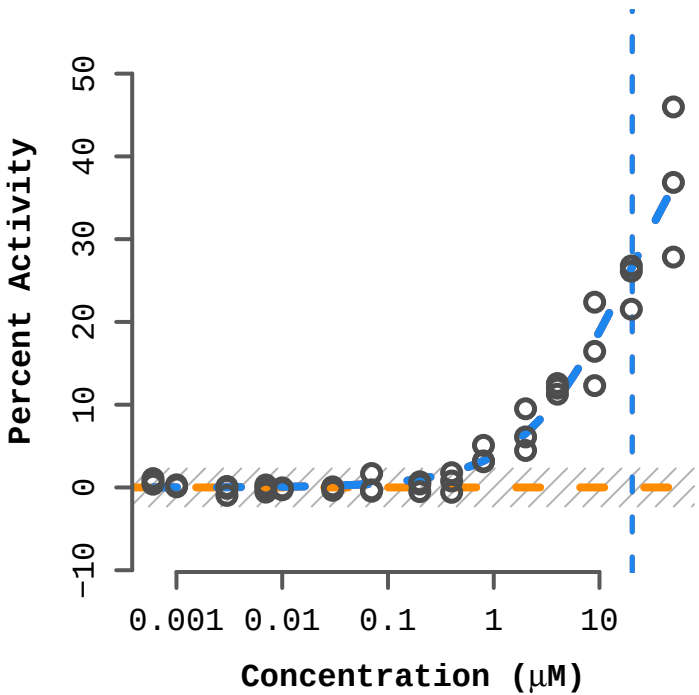
	tp	ga	gw
val:	83.8	1.67	0.767
sd:	11.8	0.164	0.0597

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	83.8	1.67	0.767	3.7	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	385.11	227.79	231.79
PROB:	0	0.88	0.12
RMSE:	20.5	3.81	3.81

MAX_MEAN: 61.7 MAX_MED: 61.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisone
CHID: 21185 **CASRN:** 53-03-2
SPID(S): Tox21_111014_1
M4ID: 12483948

HILL MODEL (in red):

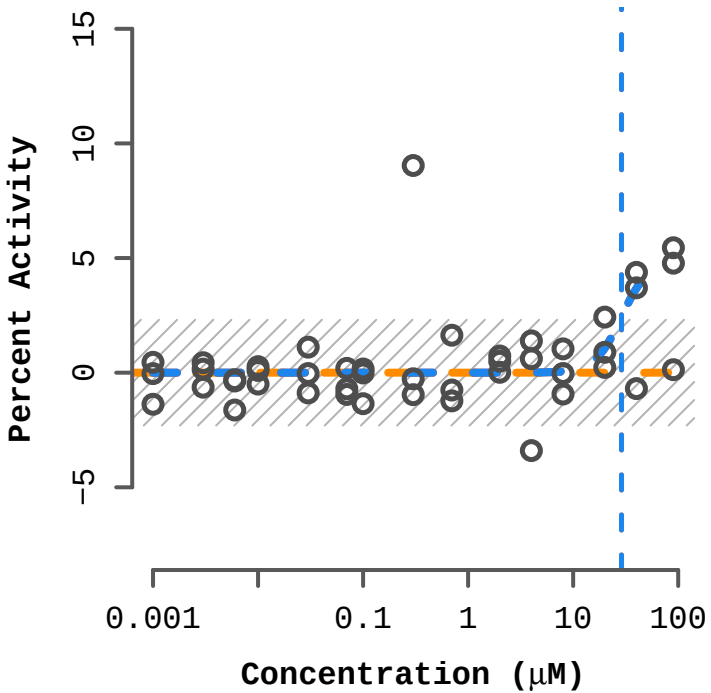
	tp	ga	gw
val:	53.3	1.31	0.847
sd:	7.65	0.161	0.0756

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	53.3	1.31	0.847	3.57	14.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	343.7	192.52	196.52
PROB:	0	0.88	0.12
RMSE:	13.05	2.5	2.5

MAX_MEAN: 36.9 **MAX_MED:** 36.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Probenecid
CHID: 21188 CASRN: 57-66-9
SPID(S): Tox21_302928
M4ID: 12476205

HILL MODEL (in red):

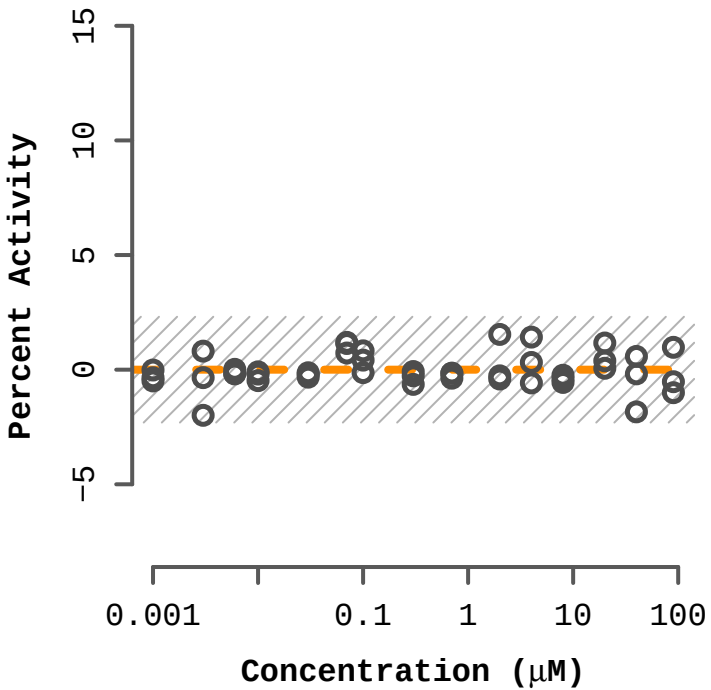
	tp	ga	gw
val:	4.86	1.46	3.45
sd:	0.796	0.0898	1.78

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.86	1.46	3.45	3.83	9.71
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	177.73	163.23	167.23
PROB:	0	0.88	0.12
RMSE:	2.15	1.88	1.88

MAX_MEAN: 3.45 MAX_MED: 4.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

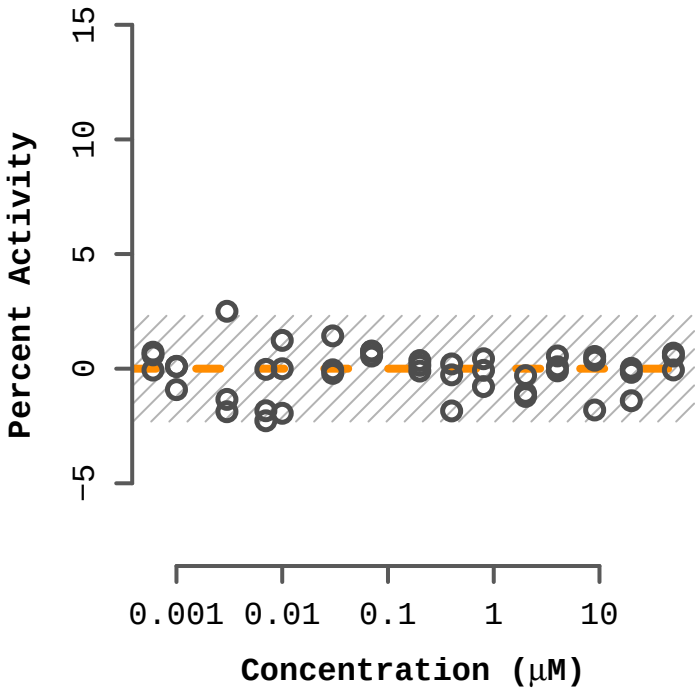
NAME: Probenecid
CHID: 21188 CASRN: 57-66-9
SPID(S): Tox21_202110
M4ID: 12480142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

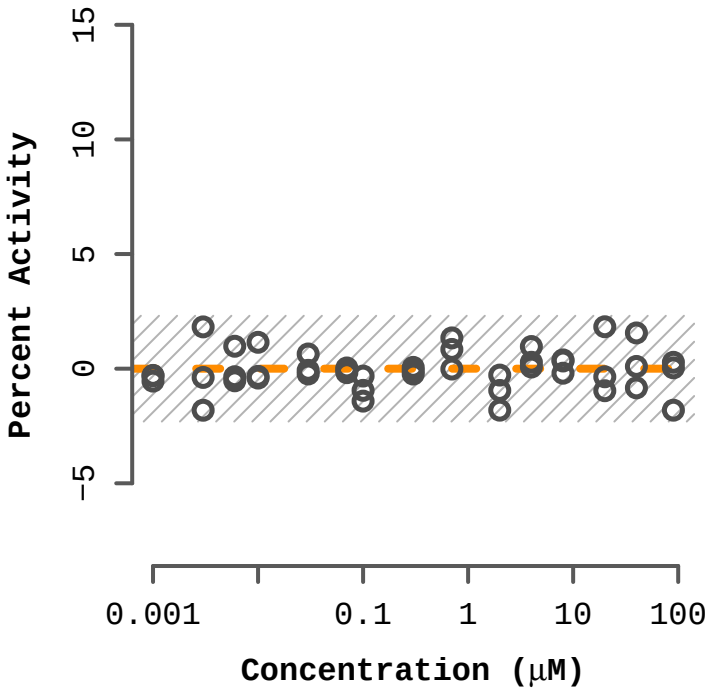
NAME: Probenecid
CHID: 21188 **CASRN:** 57-66-9
SPID(S): Tox21_110328_1
M4ID: 12484452

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.78	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.694 **MAX_MED:** 0.759 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

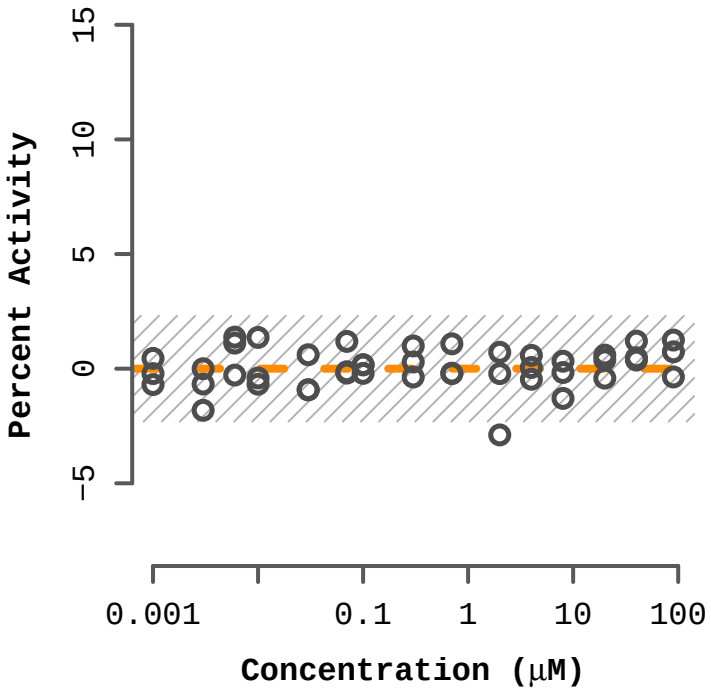
NAME: Procarbazine
CHID: 21189 CASRN: 671-16-9
SPID(S): Tox21_301738
M4ID: 12477395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.723 MAX_MED: 0.842 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

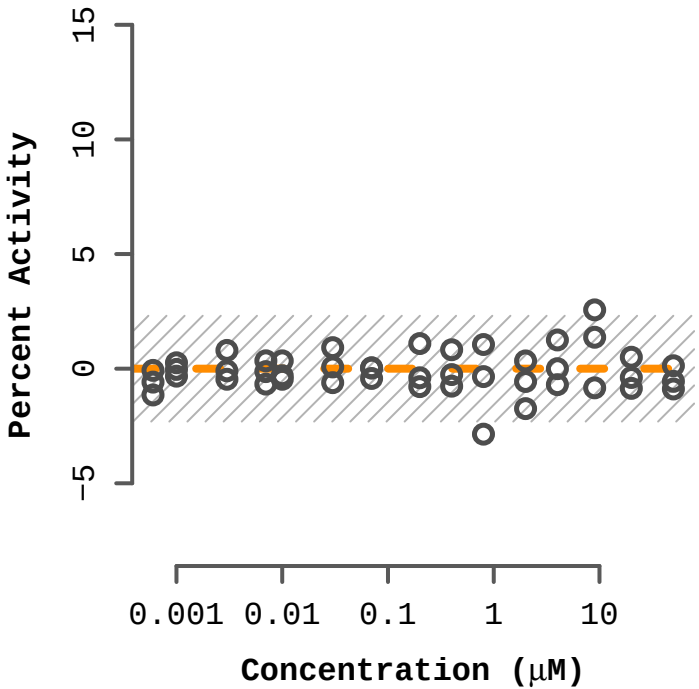
NAME: Procarbazine hydrochloride
CHID: 21190 CASRN: 366-70-1
SPID(S): Tox21_302318
M4ID: 12476815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

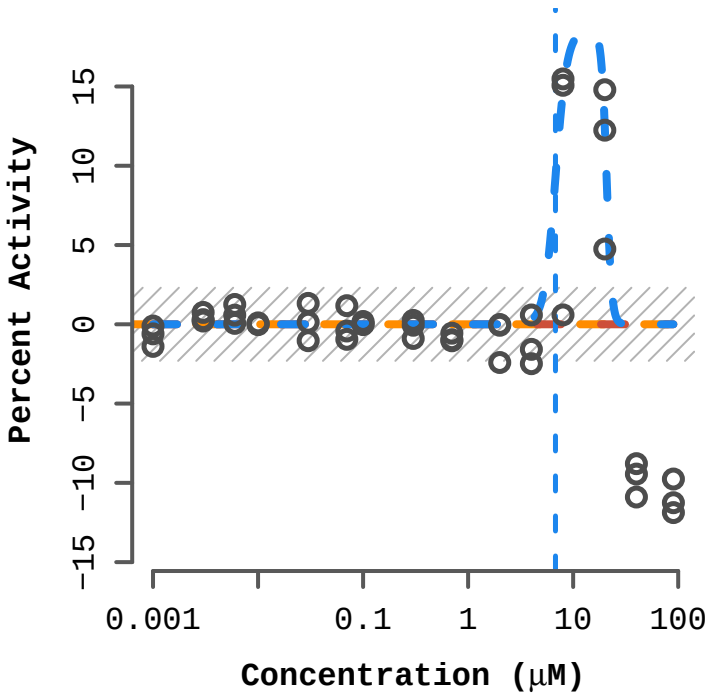
NAME: Procarbazine hydrochloride
CHID: 21190 CASRN: 366-70-1
SPID(S): Tox21_110439_1
M4ID: 12484356

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Proflavin hydrochloride
CHID: 21191 CASRN: 952-23-8
SPID(S): Tox21_200513
M4ID: 12481739

HILL MODEL (in red):

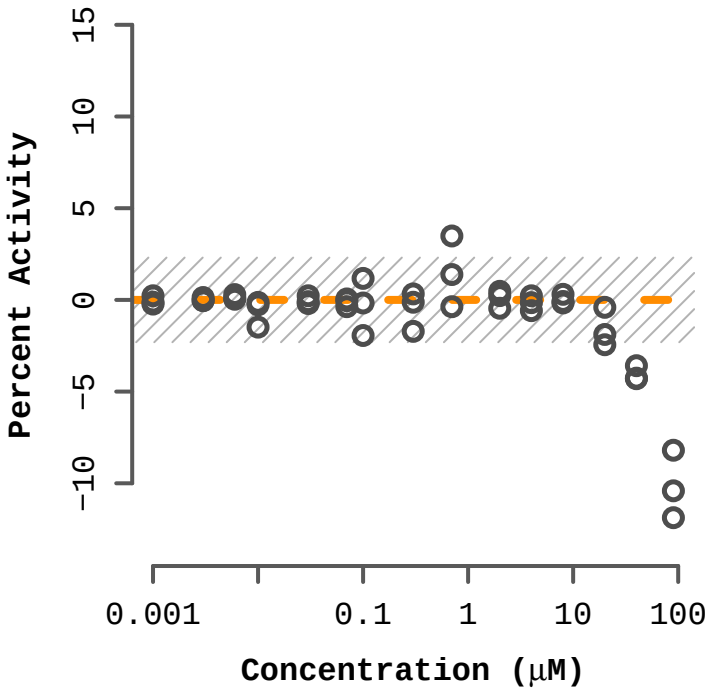
	tp	ga	gw
val:	1.24e-07	2.25	6.05
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.6	0.832	8	1.32	17.7
sd:	7.76	0.0893	3.45	0.0192	32.7

	CNST	HILL	GNLS
AIC:	274.73	280.73	254.52
PROB:	0	0	1
RMSE:	5.84	5.84	4.57

MAX_MEAN: 10.6 **MAX_MED:** 15.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

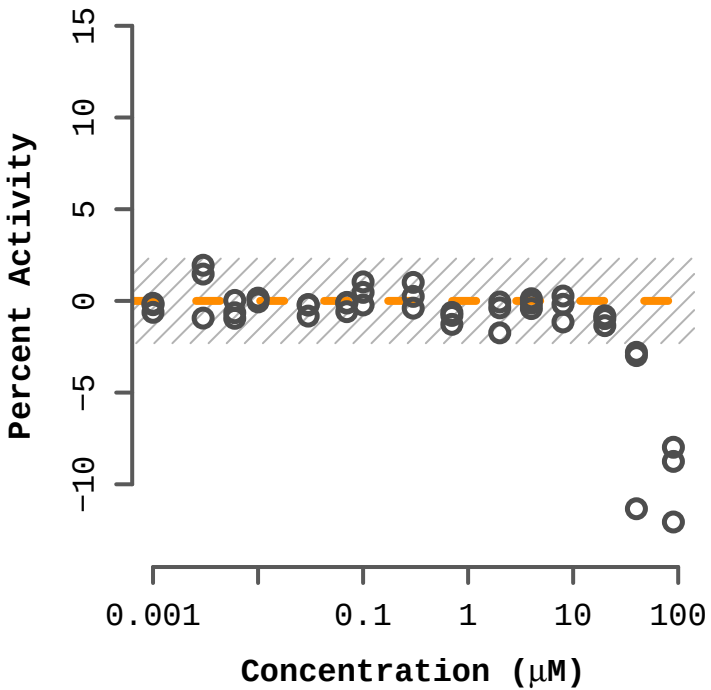
NAME: Promethazine hydrochloride
CHID: 21192 **CASRN:** 58-33-3
SPID(S): Tox21_302878
M4ID: 12476255

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

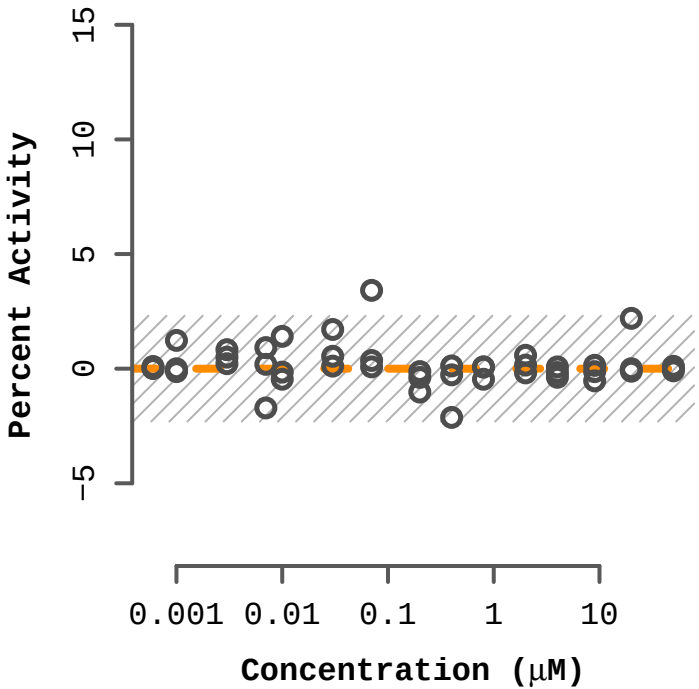
NAME: Promethazine hydrochloride
CHID: 21192 **CASRN:** 58-33-3
SPID(S): Tox21_202264
M4ID: 12479988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.43	NA	NA
PROB:	1	NA	NA
RMSE:	3.18	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

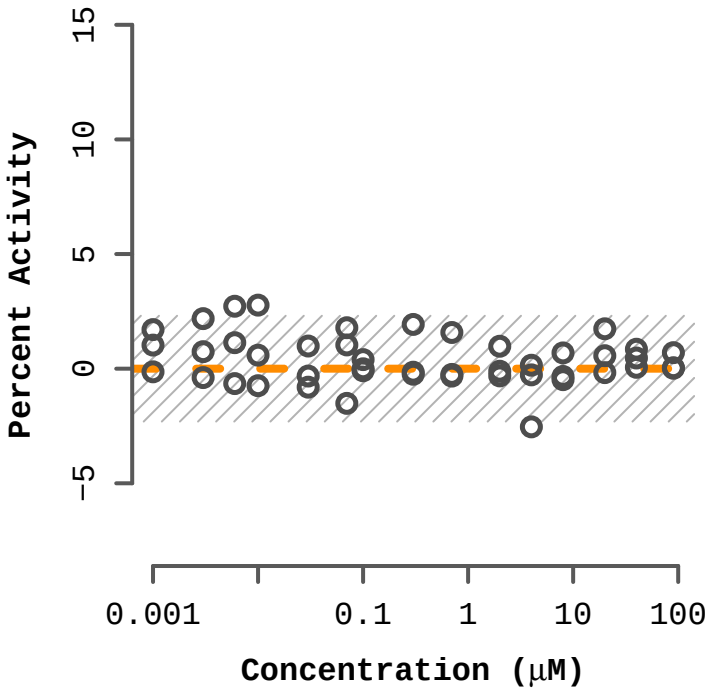
NAME: Pronethalol
CHID: 21193 **CASRN:** 54-80-8
SPID(S): Tox21_110927_1
M4ID: 12484008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.541 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

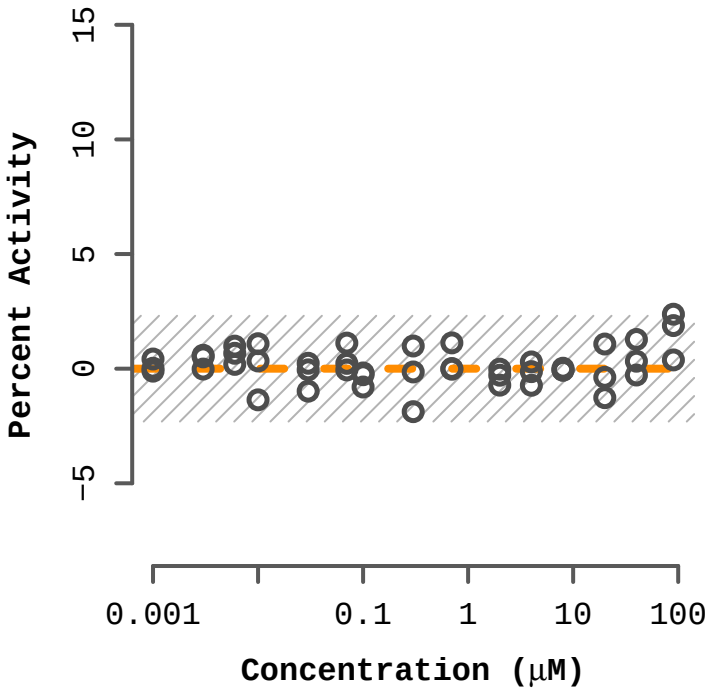
NAME: 1,3-Propane sultone
CHID: 21195 **CASRN:** 1120-71-4
SPID(S): Tox21_300066
M4ID: 12479064

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

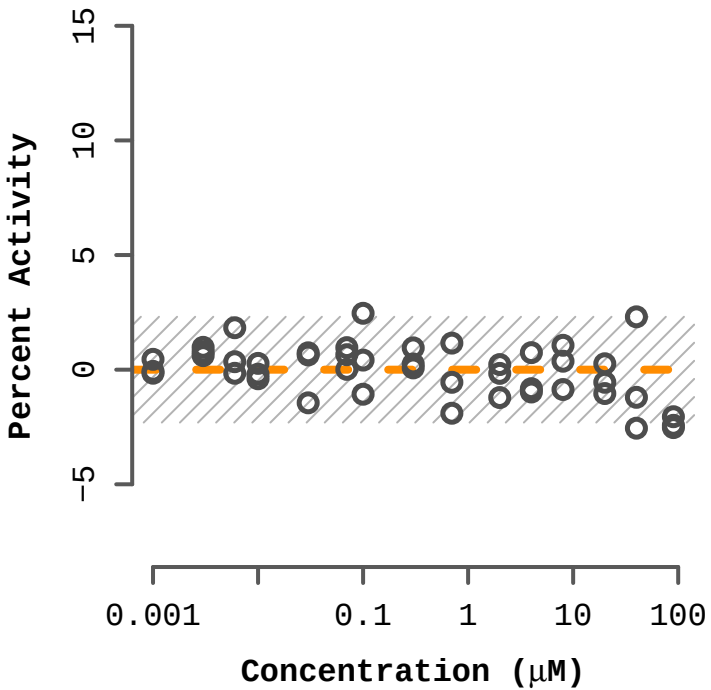
NAME: 1,3-Propane sultone
CHID: 21195 CASRN: 1120-71-4
SPID(S): Tox21_201419
M4ID: 12480833

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.55 MAX_MED: 1.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

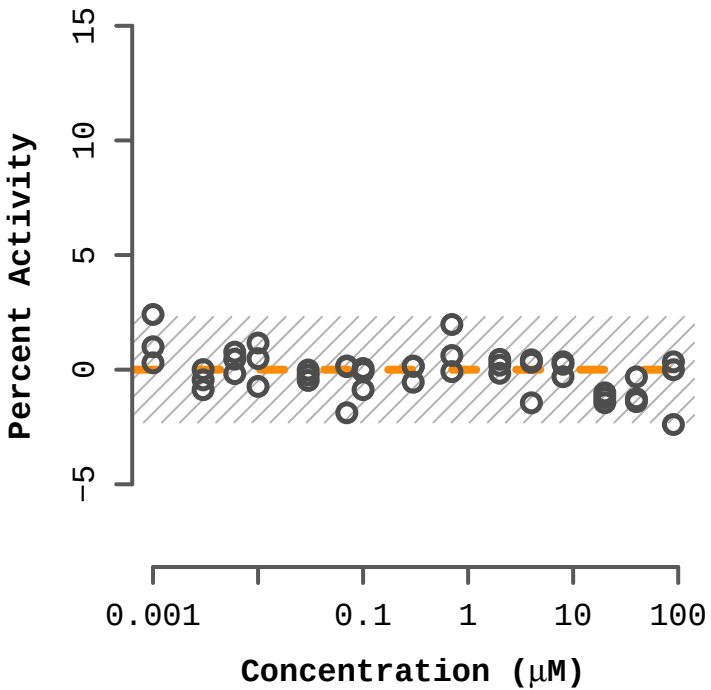
NAME: Propazine
CHID: 21196 **CASRN:** 139-40-2
SPID(S): Tox21_300984
M4ID: 12478149

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.788 **MAX_MED:** 0.775 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

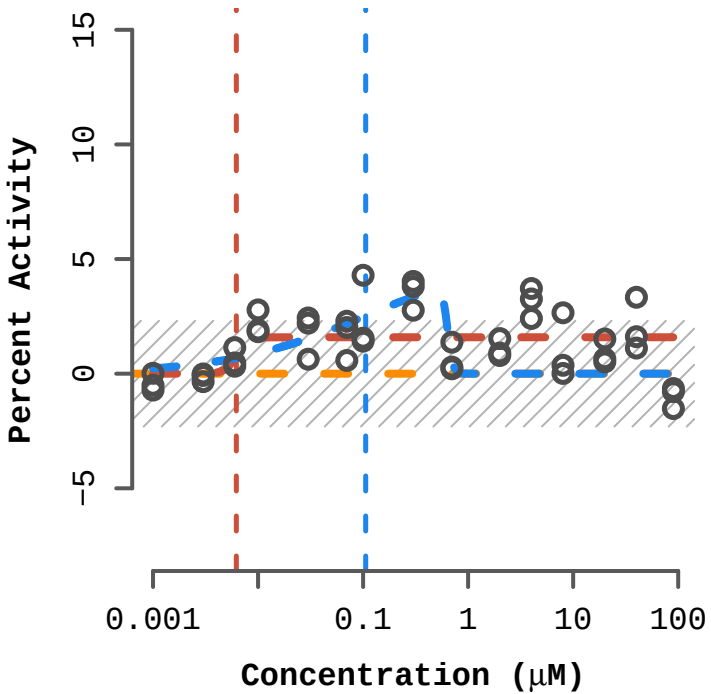
NAME: Propazine
CHID: 21196 **CASRN:** 139-40-2
SPID(S): Tox21_201394
M4ID: 12480858

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propranolol hydrochloride
CHID: 21198 CASRN: 318-98-9
SPID(S): Tox21_302905
M4ID: 12476228

HILL MODEL (in red):

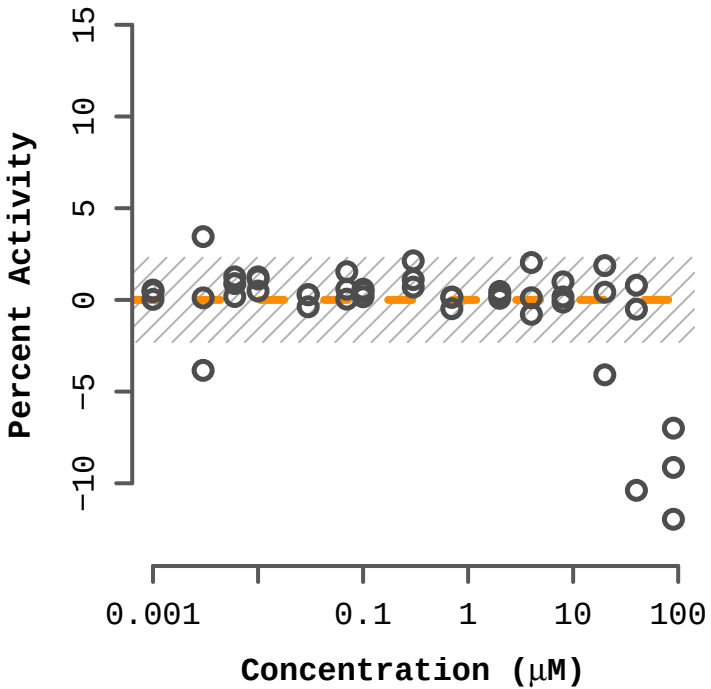
	tp	ga	gw
val:	1.59	−2.21	8
sd:	0.217	0.0724	7.87

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.05	−0.975	0.653	−0.196	17.8
sd:	5.67	1.64	0.438	1.36	583

	CNST	HILL	GNLS
AIC:	190.48	156.65	166.04
PROB:	0	0.99	0.01
RMSE:	1.91	1.24	1.36

MAX_MEAN: 3.53 MAX_MED: 3.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

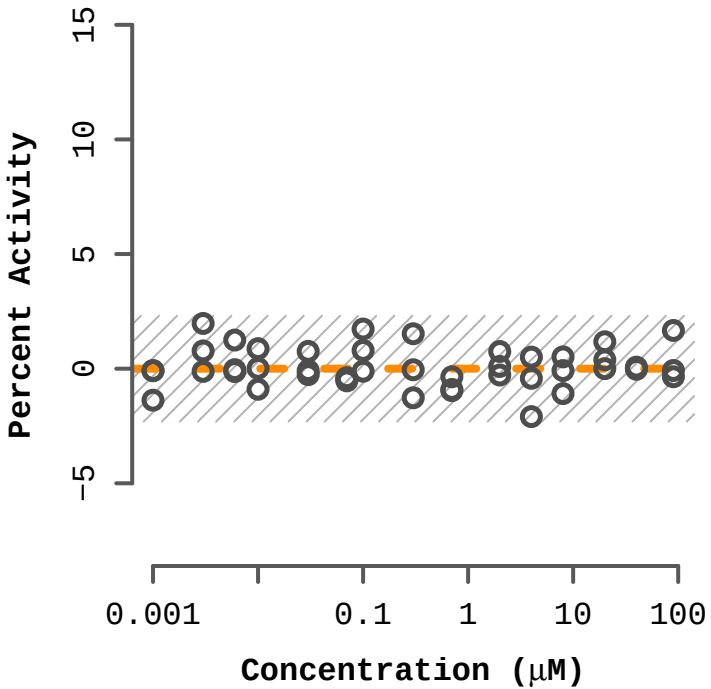
NAME: Propranolol hydrochloride
CHID: 21198 **CASRN:** 318-98-9
SPID(S): Tox21_201886
M4ID: 12480366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.11	NA	NA
PROB:	1	NA	NA
RMSE:	3.17	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

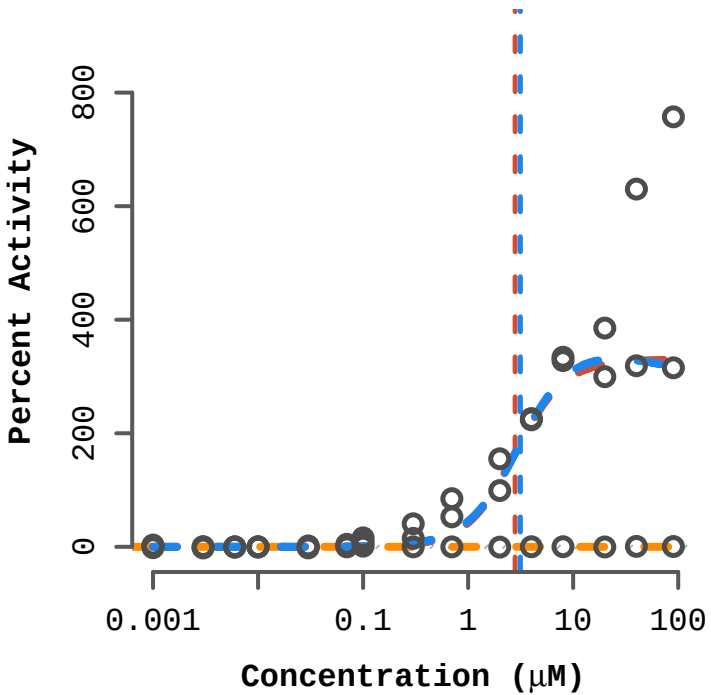
NAME: Pebulate
CHID: 21199 CASRN: 1114-71-2
SPID(S): Tox21_302868
M4ID: 12476265

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.878 MAX_MED: 0.797 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pebulate
CHID: 21199 CASRN: 1114-71-2
SPID(S): Tox21_201796
M4ID: 12480456

HILL MODEL (in red):

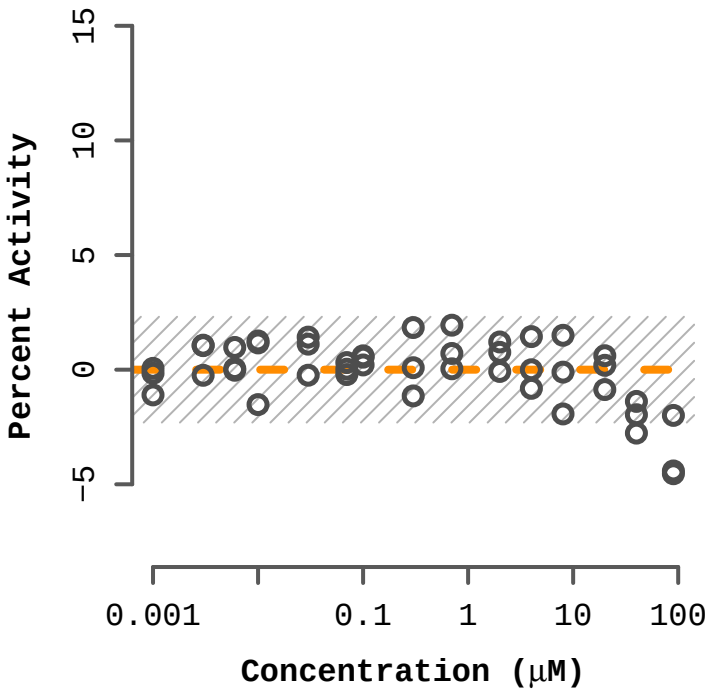
	tp	ga	gw
val:	330	0.447	1.86
sd:	24.1	0.0781	0.711

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	399	0.497	1.73	3.94	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	617.94	542.78	545.96
PROB:	0	0.83	0.17
RMSE:	198.71	129.49	130.39

MAX_MEAN: 358 MAX_MED: 328 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

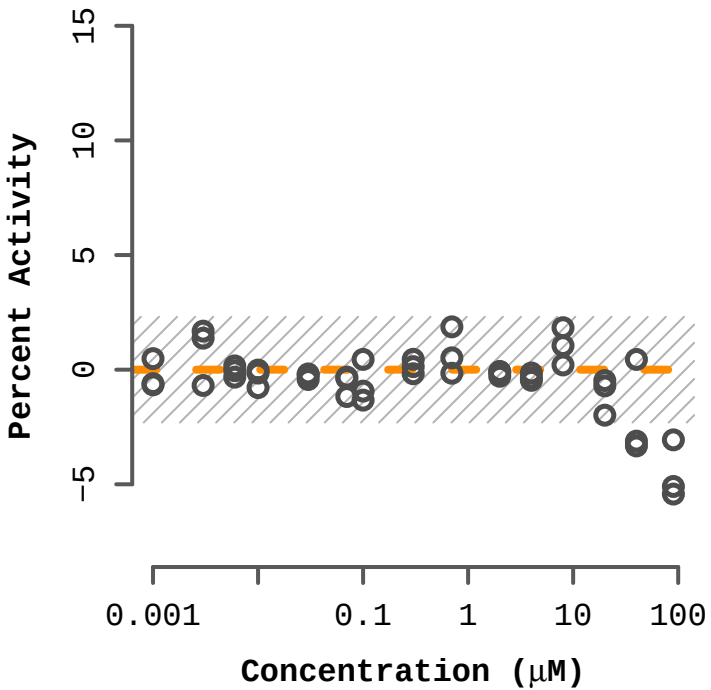
NAME: Propyl gallate
CHID: 21201 CASRN: 121-79-9
SPID(S): Tox21_300060
M4ID: 12479070

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 0.897 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

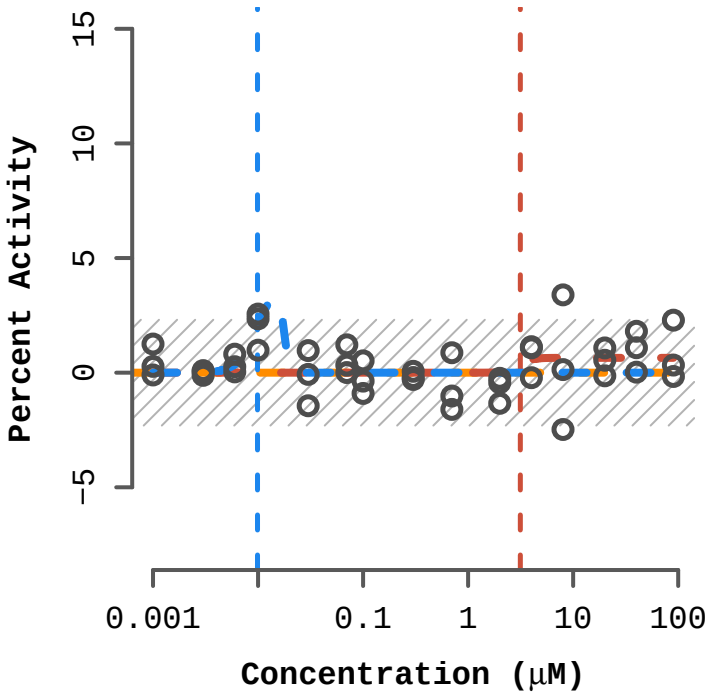
NAME: Propyl gallate
CHID: 21201 **CASRN:** 121-79-9
SPID(S): Tox21_202286
M4ID: 12479966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Propylene glycol
CHID: 21206 CASRN: 57-55-6
SPID(S): Tox21_300006
M4ID: 12479124

HILL MODEL (in red):

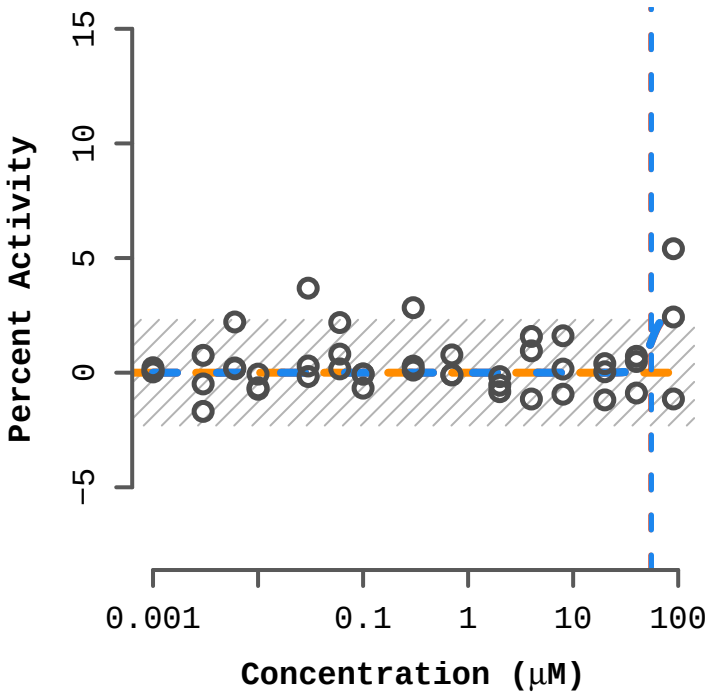
	tp	ga	gw
val:	0.646	0.497	8
sd:	0.273	0.18	9.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.03	−2.01	4.65	−1.76	17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	139.57	139.81	137.63
PROB:	0.22	0.2	0.58
RMSE:	1.15	1.08	1.03

MAX_MEAN: 1.96 MAX_MED: 2.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Propylene glycol
CHID: 21206 CASRN: 57-55-6
SPID(S): Tox21_201812
M4ID: 12480440

HILL MODEL (in red):

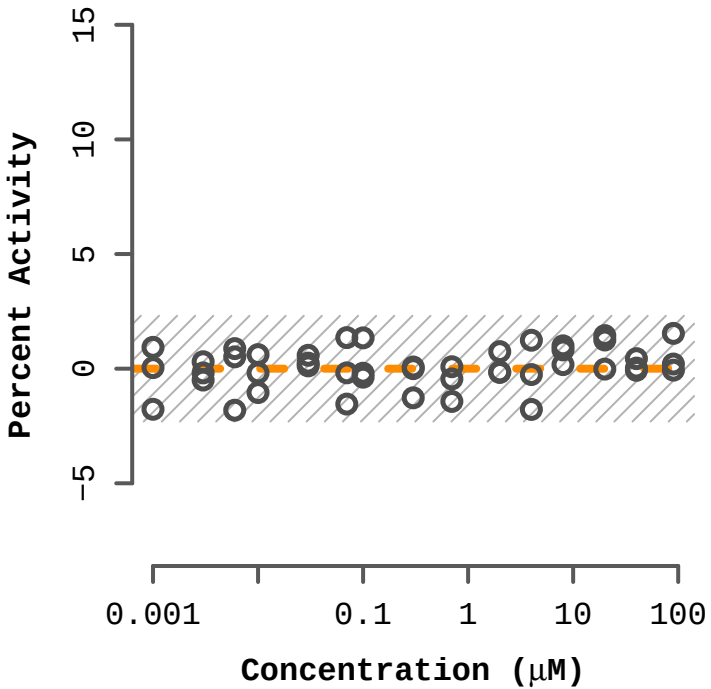
	tp	ga	gw
val:	2.57	1.74	8
sd:	2.48	1.08	58.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5	1.75	7.98	2.05	0.305
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	147.16	149.03	153.03
PROB:	0.69	0.27	0.04
RMSE:	1.39	1.27	1.27

MAX_MEAN: 2.23 MAX_MED: 2.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

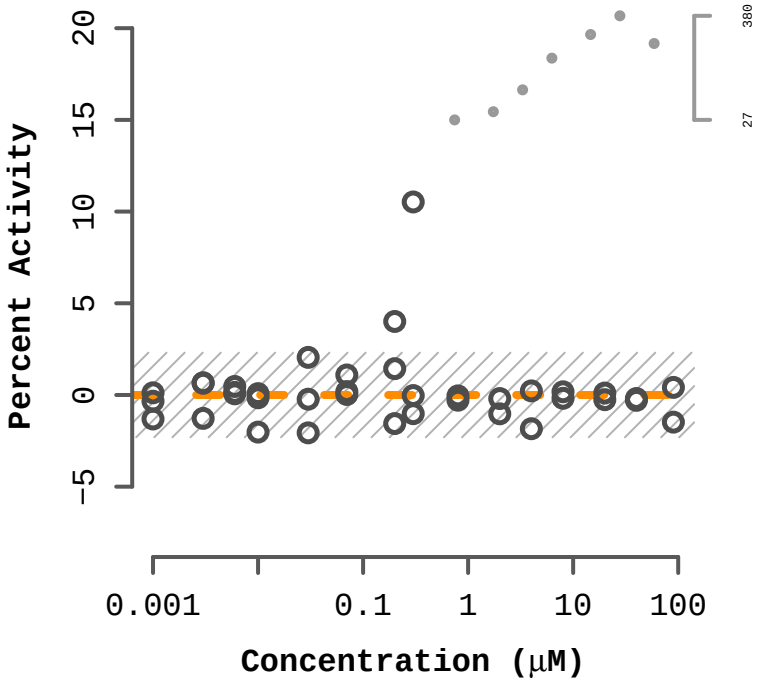
NAME: 6-Propyl-2-thiouracil
CHID: 21209 CASRN: 51-52-5
SPID(S): Tox21_300280
M4ID: 12478850

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.893 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

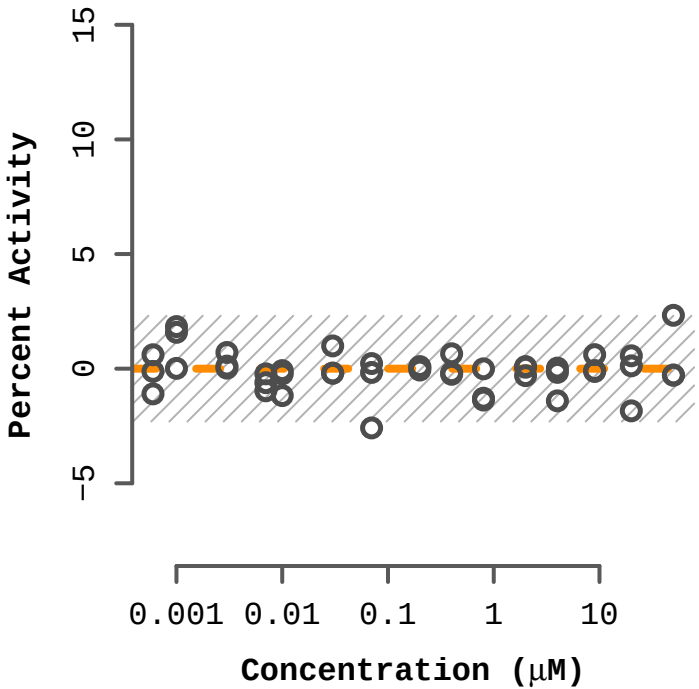
NAME: 6-Propyl-2-thiouracil
CHID: 21209 **CASRN:** 51-52-5
SPID(S): Tox21_201741
M4ID: 12480511 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	427.11	NA	NA
PROB:	1	NA	NA
RMSE:	95.18	NA	NA

MAX_MEAN: 127 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

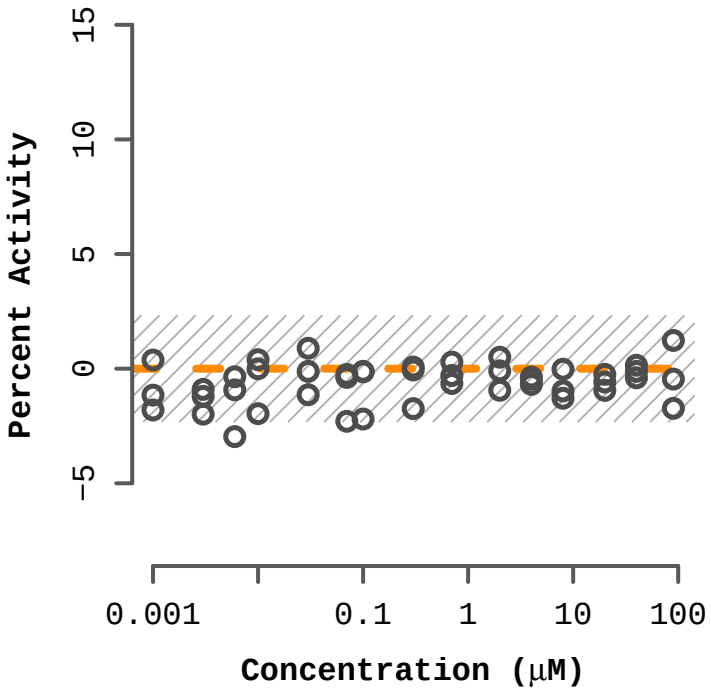
NAME: 6-Propyl-2-thiouracil
CHID: 21209 **CASRN:** 51-52-5
SPID(S): Tox21_110882_1
M4ID: 12484045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

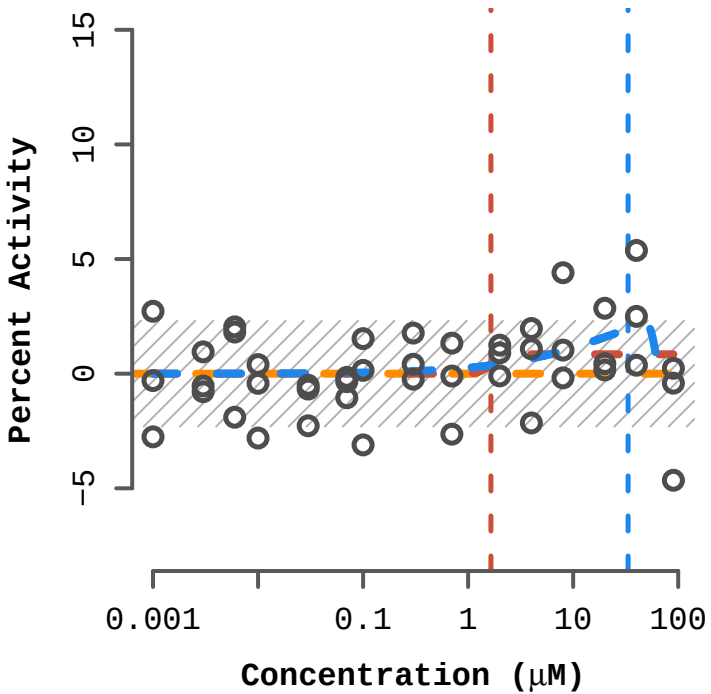
NAME: 3,4−Dihydroxybenzoic acid
CHID: 21212 CASRN: 99−50−3
SPID(S): Tox21_200167
M4ID: 12482085

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: −0.12 **MAX_MED:** −0.00155 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Purpurin
CHID: 21214 **CASRN:** 81-54-9
SPID(S): Tox21_301526
M4ID: 12477607

HILL MODEL (in red):

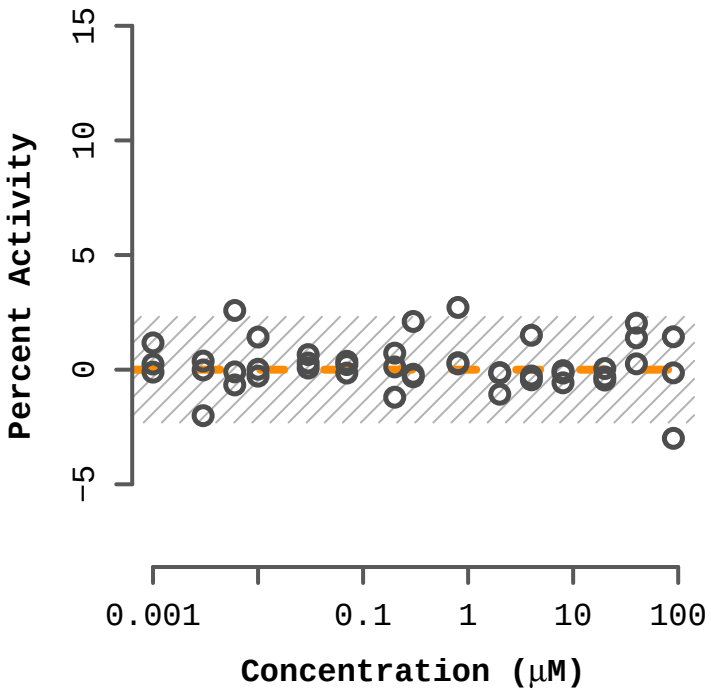
	tp	ga	gw
val:	0.845	0.217	8
sd:	0.458	0.763	68.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.93	1.52	0.756	1.77	18
sd:	15.1	4.06	0.878	0.592	59.6

	CNST	HILL	GNLS
AIC:	187.36	189.24	189.43
PROB:	0.57	0.22	0.2
RMSE:	1.92	1.84	1.72

MAX_MEAN: 2.75 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

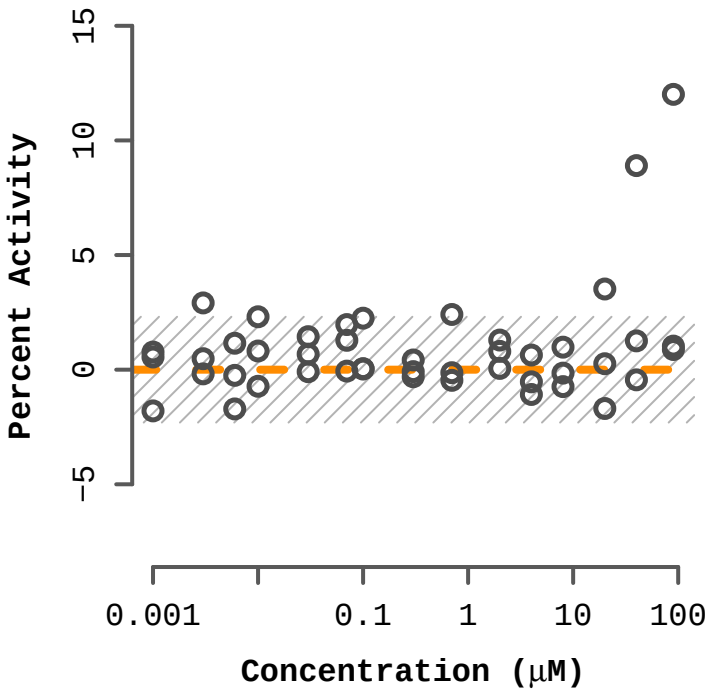
NAME: Pyrazinamide
CHID: 21215 **CASRN:** 98-96-4
SPID(S): Tox21_302771
M4ID: 12476362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

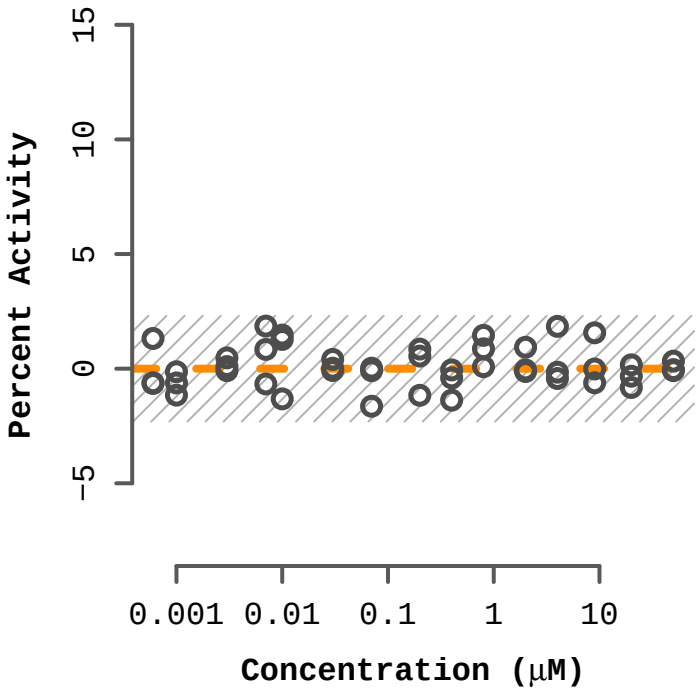
NAME: Pyrazinamide
CHID: 21215 **CASRN:** 98-96-4
SPID(S): Tox21_202059
M4ID: 12480193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 4.64 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

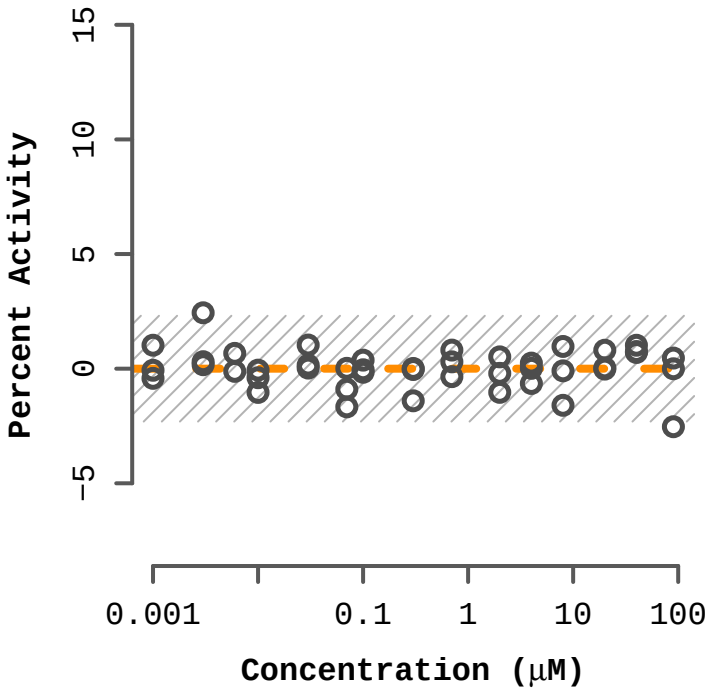
NAME: Pyrazinamide
CHID: 21215 **CASRN:** 98-96-4
SPID(S): Tox21_110237_1
M4ID: 12484526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.804 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

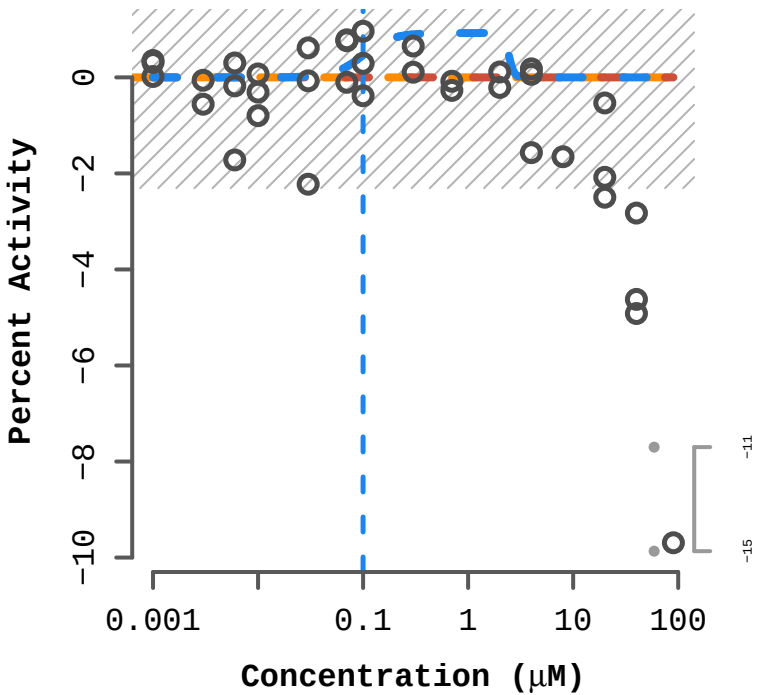
NAME: Pyrilamine maleate
CHID: 21216 **CASRN:** 59-33-6
SPID(S): Tox21_200514
M4ID: 12481738

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.973 **MAX_MED:** 0.749 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pyrimethamine
CHID: 21217 **CASRN:** 58-14-0
SPID(S): Tox21_300129
M4ID: 12479001 **BRK**

HILL MODEL (in red):

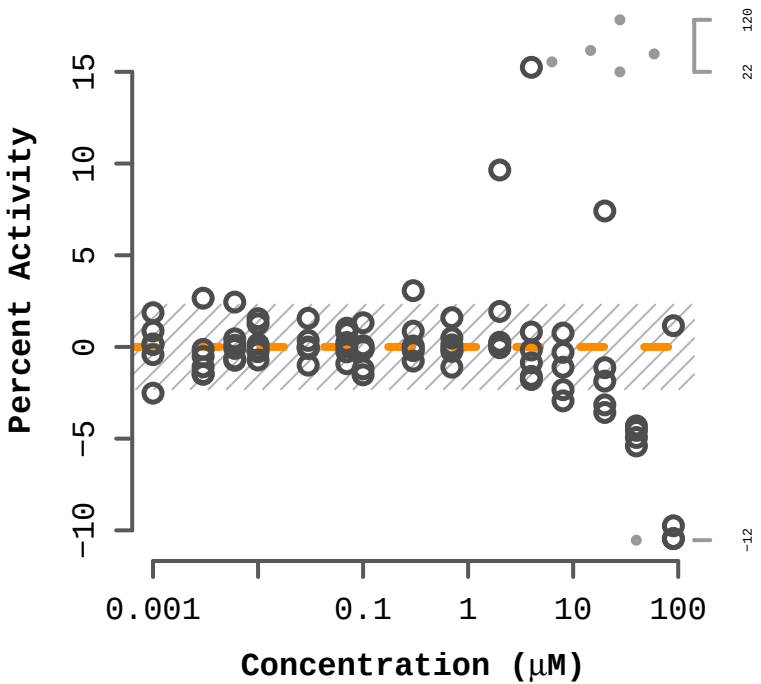
	tp	ga	gw
val:	5.79e-09	2.24	2.9
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.924	−1	3.14	0.387	17.6
sd:	1.17	0.737	8.56	1.57	234

	CNST	HILL	GNLS
AIC:	244.99	250.99	253.68
PROB:	0.94	0.05	0.01
RMSE:	4.45	4.45	4.32

MAX_MEAN: 4.4 **MAX_MED:** 3.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

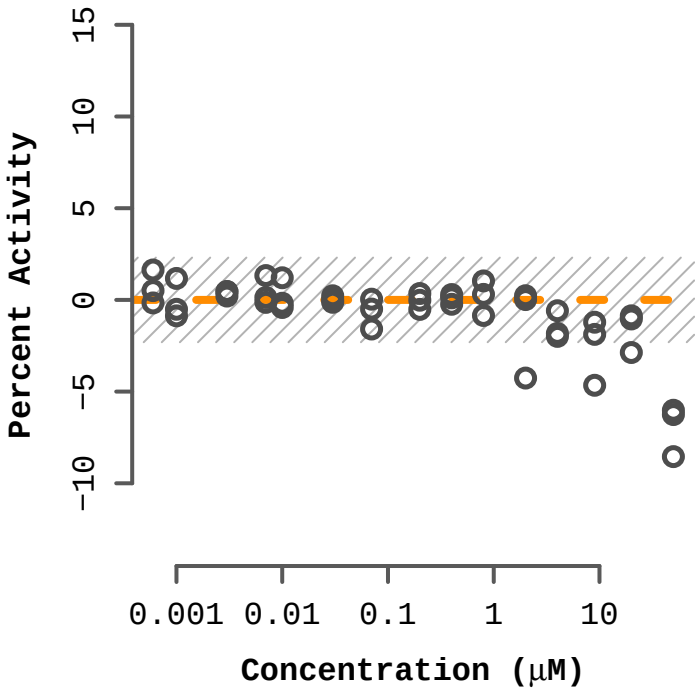
NAME: Pyrimethamine
CHID: 21217 **CASRN:** 58-14-0
SPID(S): Tox21_201834
M4ID: 12480418 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	553.72	NA	NA
PROB:	1	NA	NA
RMSE:	16.74	NA	NA

MAX_MEAN: 20.7 **MAX_MED:** 0.227 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

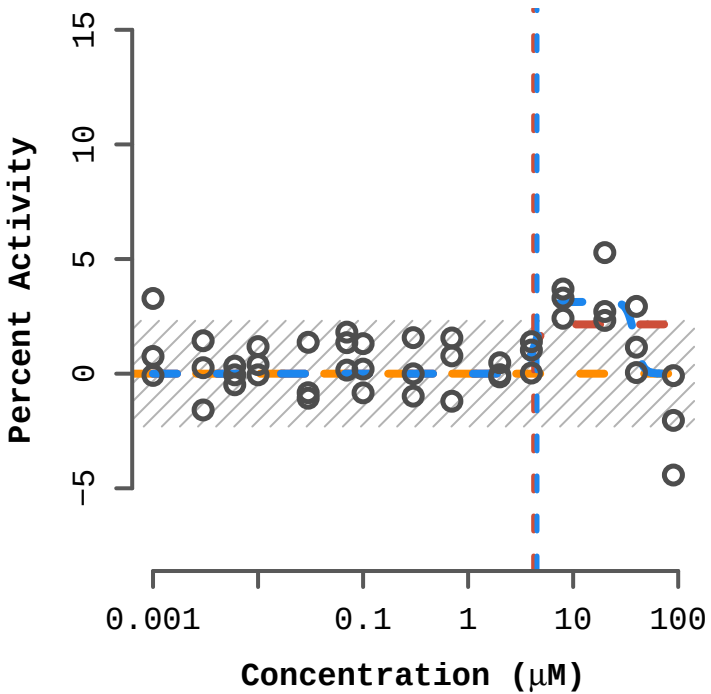
NAME: Pyrimethamine
CHID: 21217 **CASRN:** 58-14-0
SPID(S): Tox21_110332_1
M4ID: 12484448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 0.66 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Quercetin
CHID: 21218 **CASRN:** 117-39-5
SPID(S): Tox21_300285
M4ID: 12478845

HILL MODEL (in red):

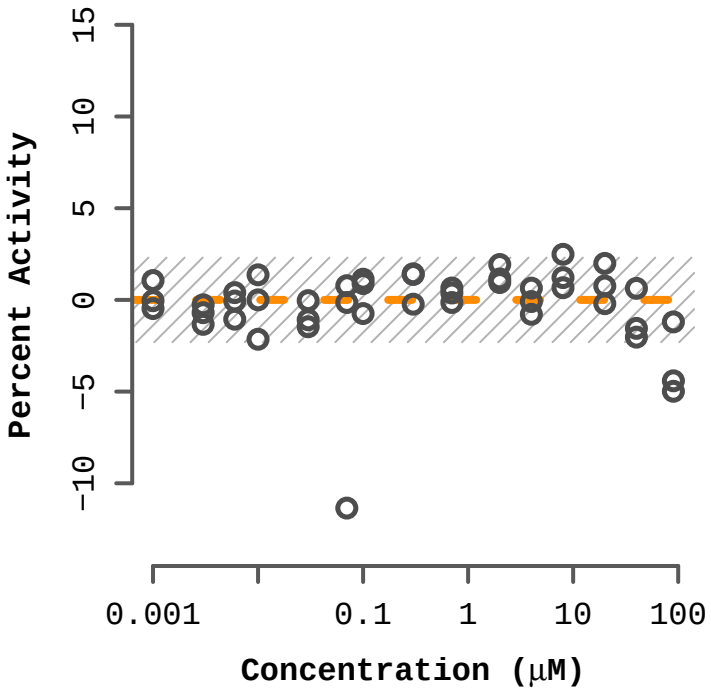
	tp	ga	gw
val:	2.15	0.624	8
sd:	0.483	0.0686	9.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.13	0.656	8	1.59	11.6
sd:	0.513	0.137	19	0.0985	68

	CNST	HILL	GNLS
AIC:	180.35	171.59	157.66
PROB:	0	0	1
RMSE:	1.8	1.66	1.27

MAX_MEAN: 3.44 **MAX_MED:** 3.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

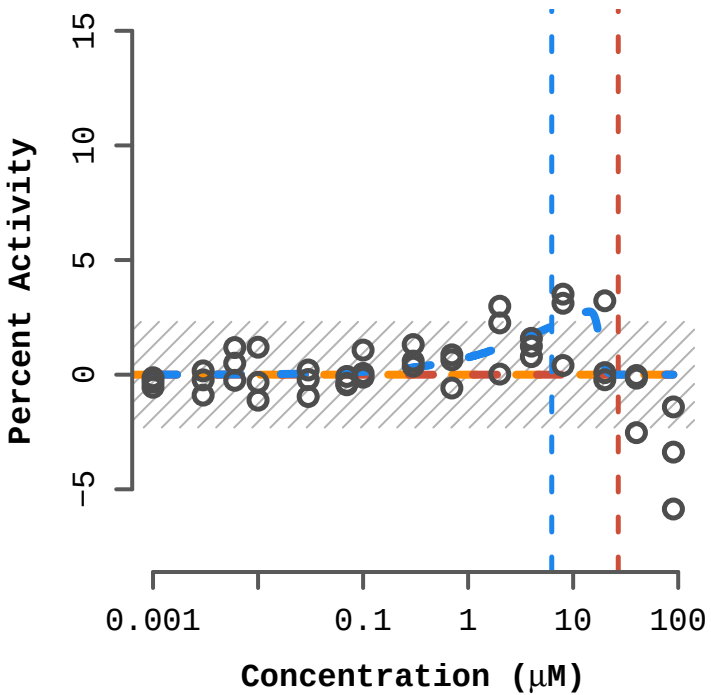
NAME: Quercetin
CHID: 21218 **CASRN:** 117-39-5
SPID(S): Tox21_202308
M4ID: 12479944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Quercetin dihydrate
CHID: 21219 CASRN: 6151-25-3
SPID(S): Tox21_201150
M4ID: 12481102

HILL MODEL (in red):

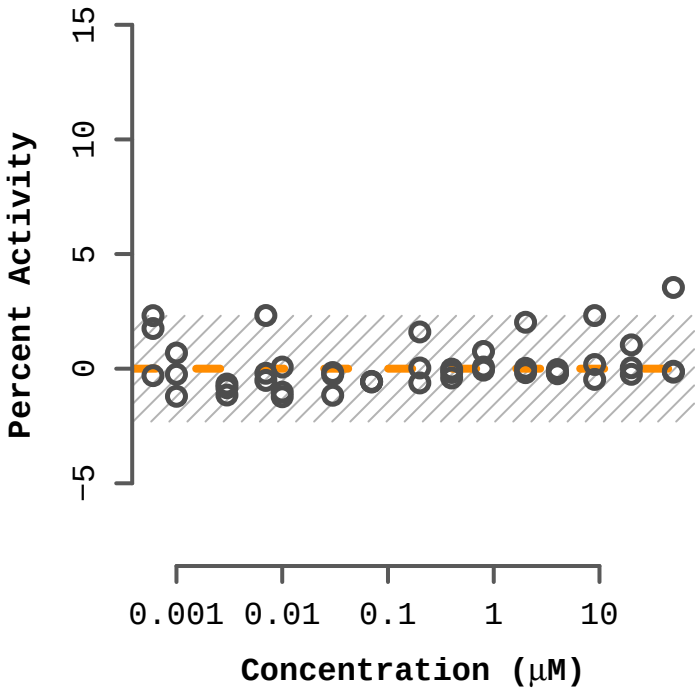
	tp	ga	gw
val:	5.46e-10	1.43	1.79
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.22	0.796	0.832	1.25	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.12	169.12	154.74
PROB:	0.01	0	0.98
RMSE:	1.62	1.62	1.39

MAX_MEAN: 2.34 MAX_MED: 3.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

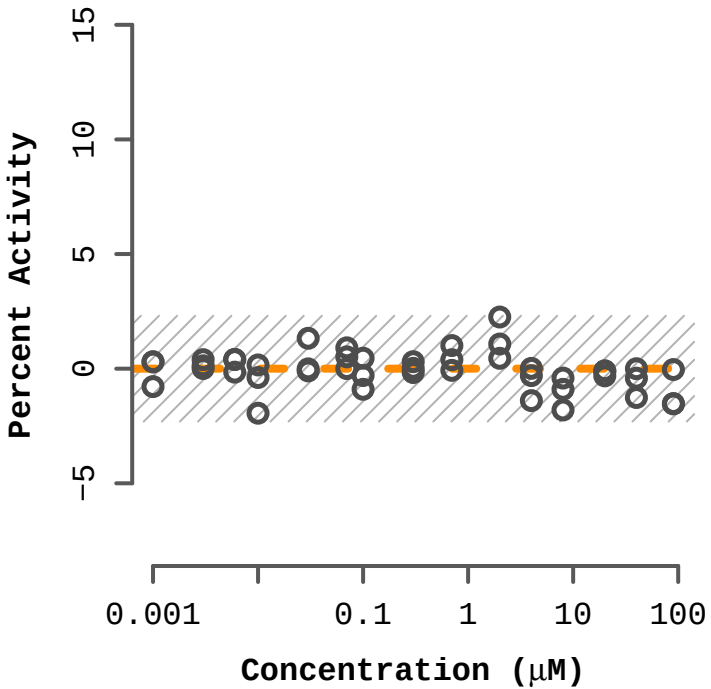
NAME: Quercetin dihydrate
CHID: 21219 **CASRN:** 6151-25-3
SPID(S): Tox21_110761_1
M4ID: 12484129

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

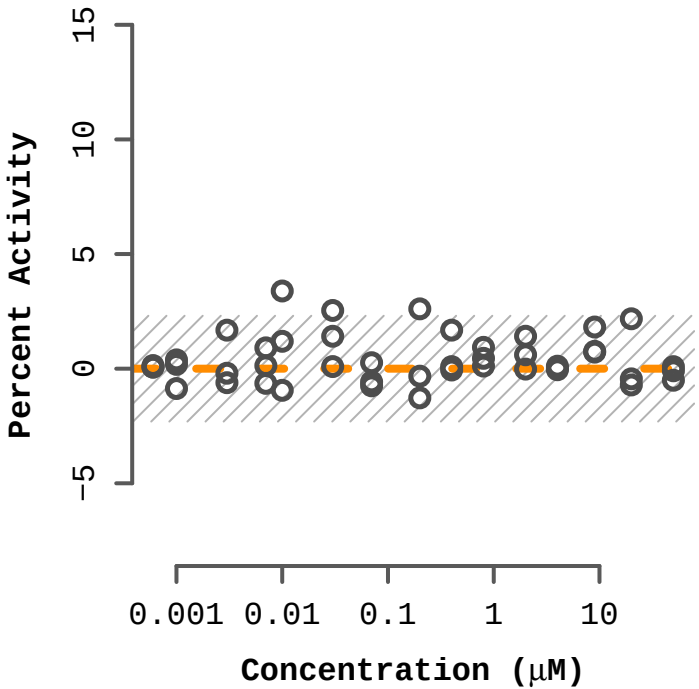
NAME: Quinapril hydrochloride
CHID: 21221 CASRN: 82586-55-8
SPID(S): Tox21_200390
M4ID: 12481862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

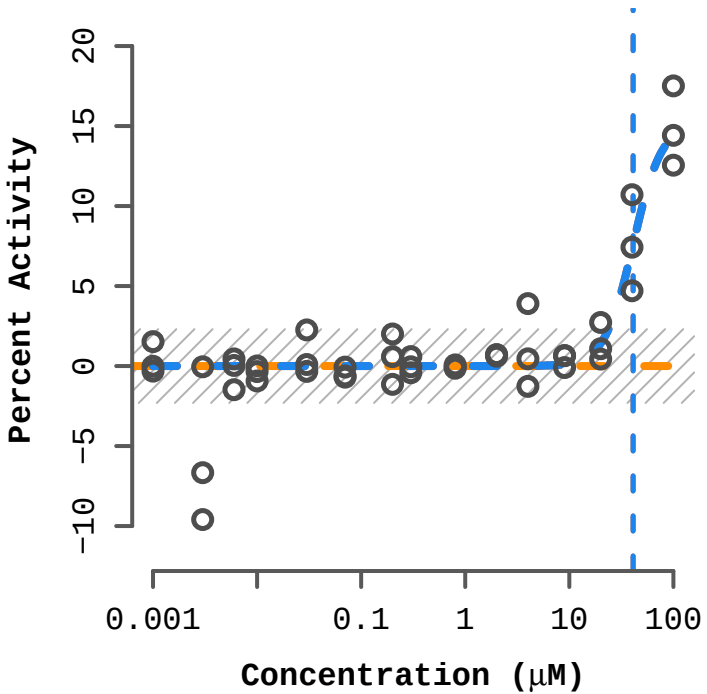
NAME: Quinapril hydrochloride
CHID: 21221 CASRN: 82586-55-8
SPID(S): Tox21_111381_1
M4ID: 12483724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: p-Benzoquinone dioxime
CHID: 21222 CASRN: 105-11-3
SPID(S): Tox21_200273
M4ID: 12481979

HILL MODEL (in red):

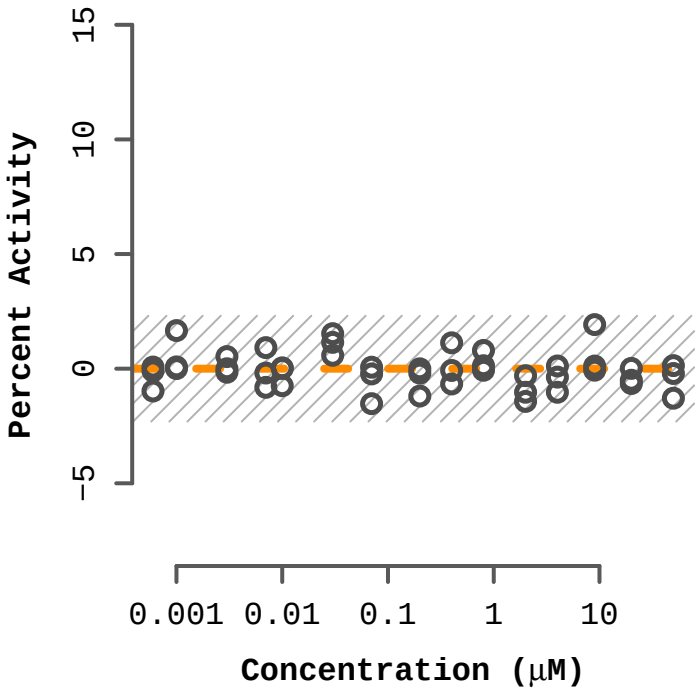
	tp	ga	gw
val:	15.2	1.61	3.17
sd:	1.58	0.0578	0.998

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.2	1.61	3.17	3.98	6.54
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	243.31	177.98	181.98
PROB:	0	0.88	0.12
RMSE:	4.82	2.15	2.15

MAX_MEAN: 14.8 MAX_MED: 14.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

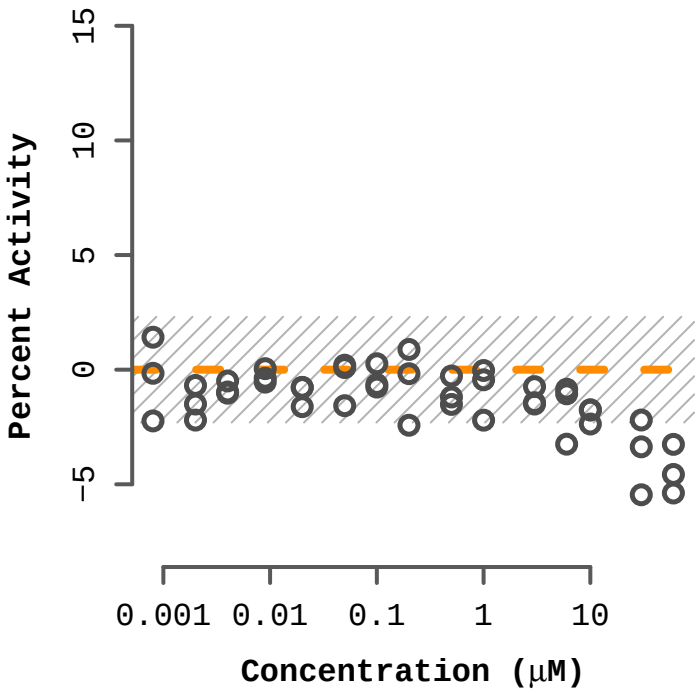
NAME: Ramosetron hydrochloride
CHID: 21223 **CASRN:** 132907-72-3
SPID(S): Tox21_112441_1
M4ID: 12483101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

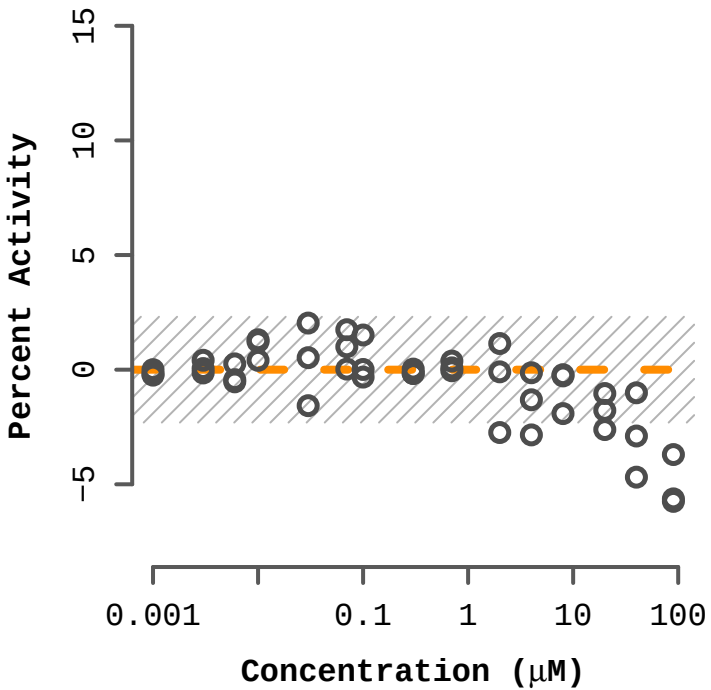
NAME: C.I. Acid Red 114
CHID: 21224 **CASRN:** 6459-94-5
SPID(S): Tox21_302977
M4ID: 12476156

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: −0.29 **MAX_MED:** 0.0929 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

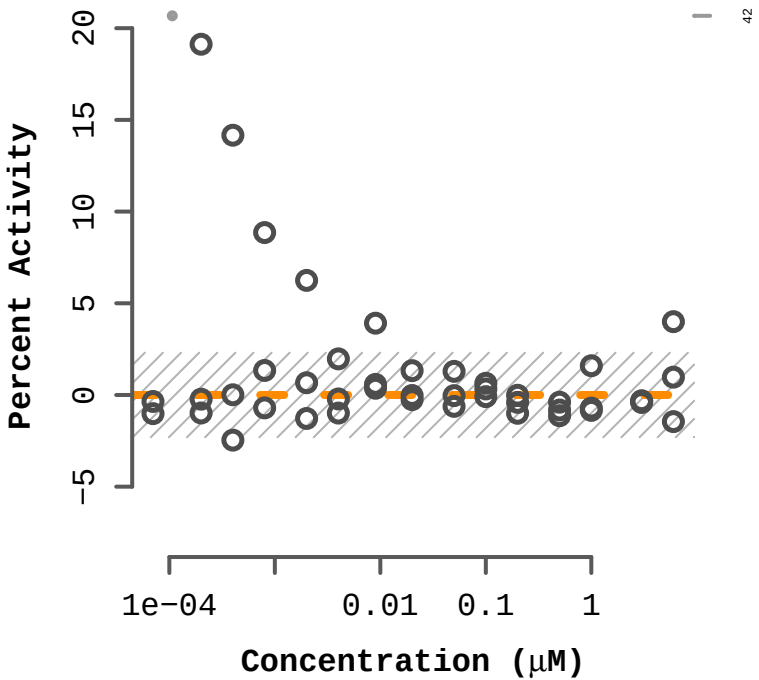
NAME: C.I. Acid Red 114
CHID: 21224 **CASRN:** 6459-94-5
SPID(S): Tox21_202139
M4ID: 12480113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.98 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

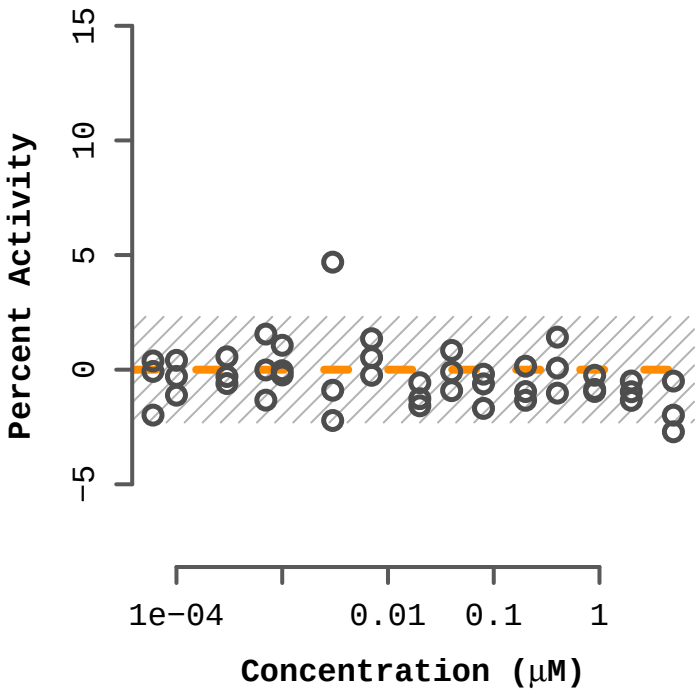
NAME: Ponceau 3R
CHID: 21231 **CASRN:** 3564-09-8
SPID(S): Tox21_202788
M4ID: 12479464 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233.56	NA	NA
PROB:	1	NA	NA
RMSE:	7.46	NA	NA

MAX_MEAN: 13.5 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

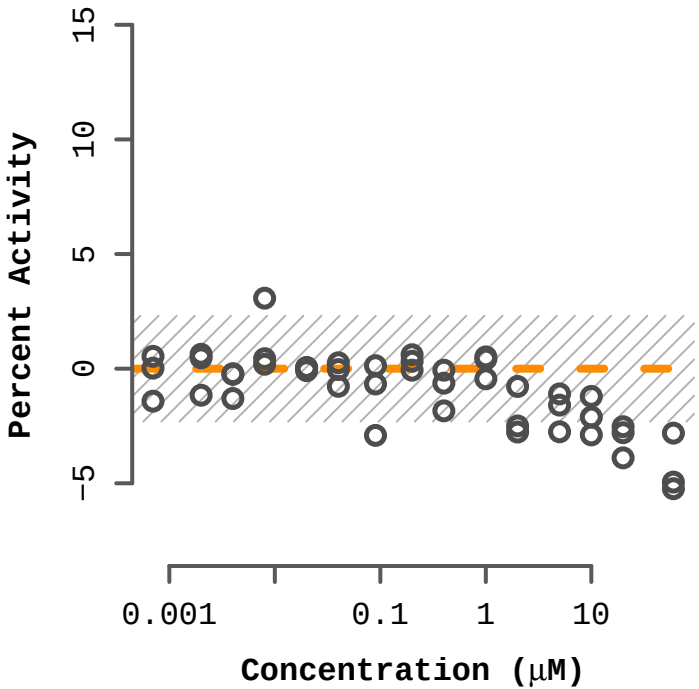
NAME: Amaranth
CHID: 21232 **CASRN:** 915-67-3
SPID(S): Tox21_202789
M4ID: 12479463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.545 **MAX_MED:** 0.527 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

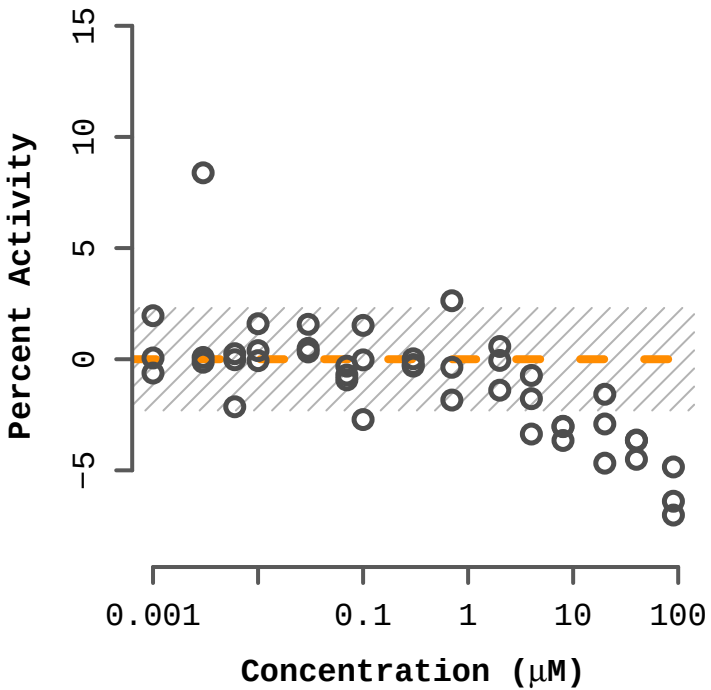
NAME: FD&C Red 3
CHID: 21233 **CASRN:** 16423-68-0
SPID(S): Tox21_302085
M4ID: 12477048

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

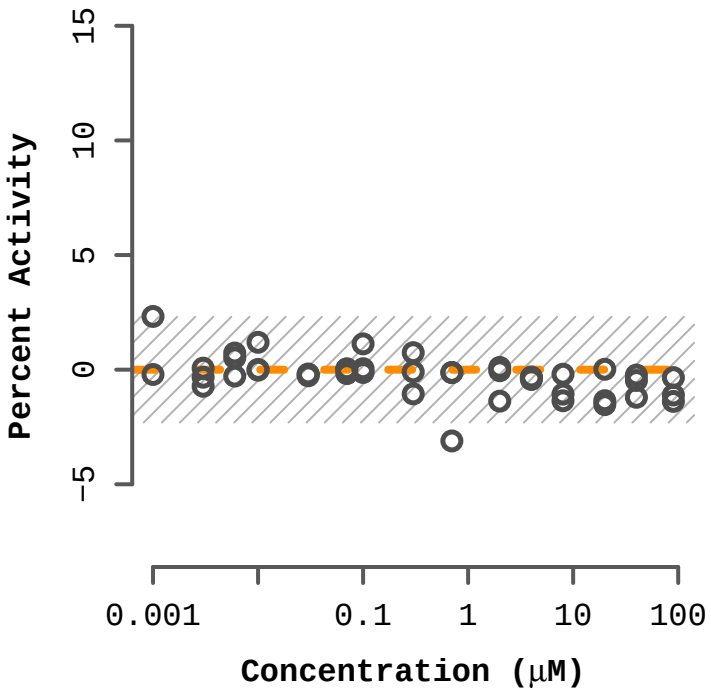
NAME: FD&C Red 3
CHID: 21233 CASRN: 16423-68-0
SPID(S): Tox21_202932
M4ID: 12479320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.78	NA	NA

MAX_MEAN: 2.78 **MAX_MED:** 0.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

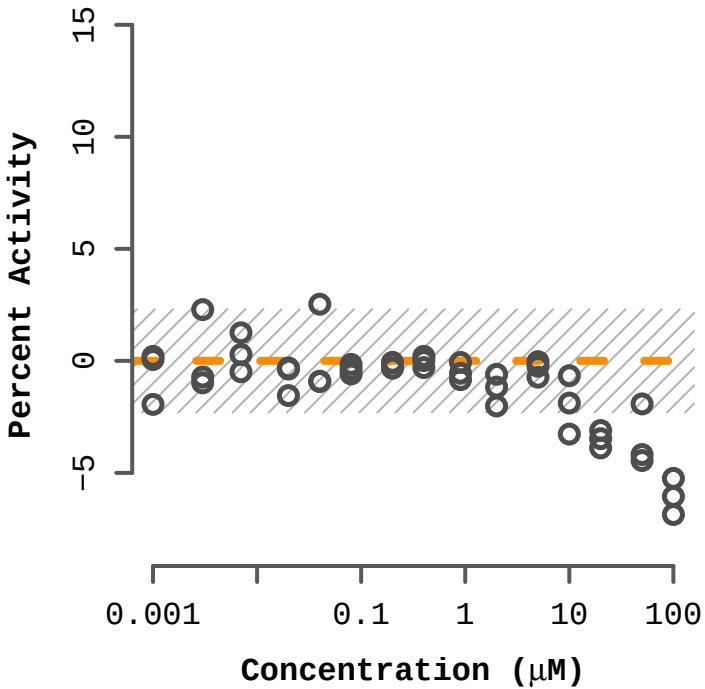
NAME: FD&C Red 4
CHID: 21234 **CASRN:** 4548-53-2
SPID(S): Tox21_302855
M4ID: 12476278

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

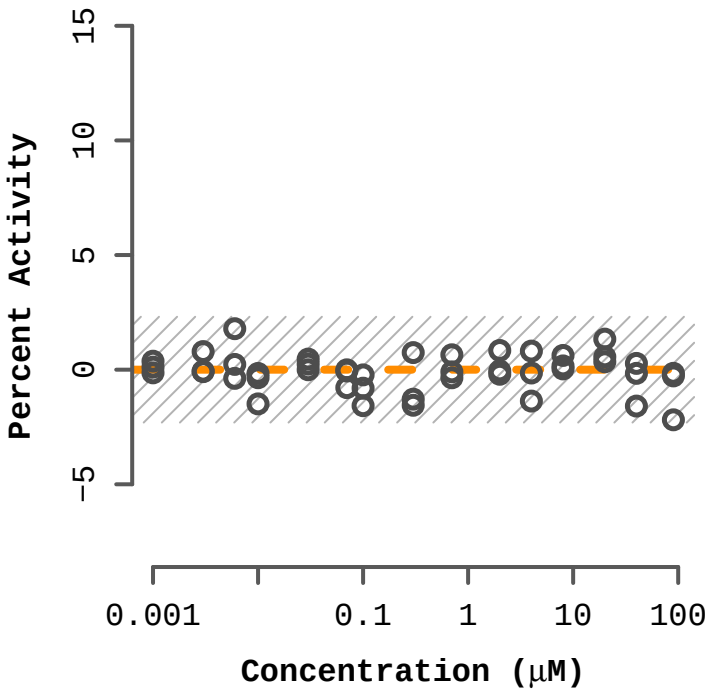
NAME: C.I. Acid Red 52
CHID: 21235 **CASRN:** 3520-42-1
SPID(S): Tox21_200080
M4ID: 12482172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.28	NA	NA

MAX_MEAN: 0.351 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

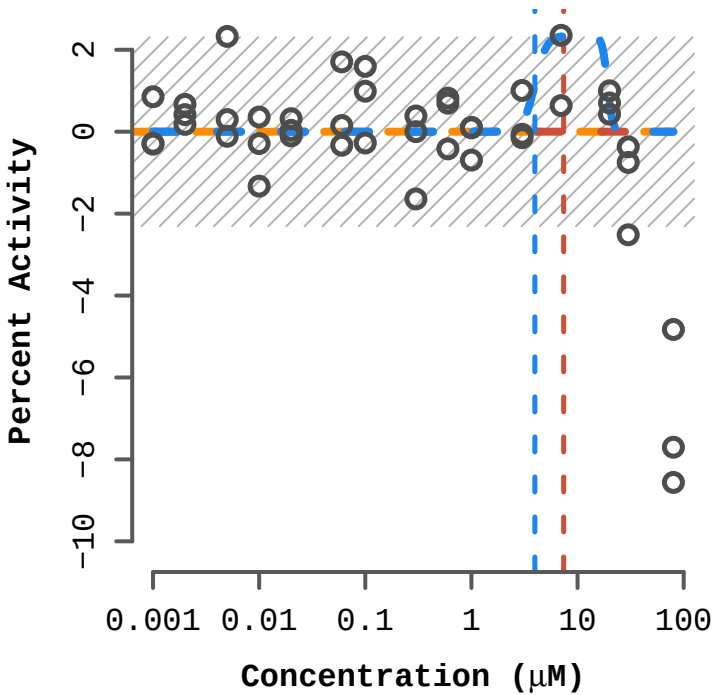
NAME: HC Red 3
CHID: 21236 CASRN: 2871-01-4
SPID(S): Tox21_302416
M4ID: 12476717

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.747 MAX_MED: 0.563 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Reserpine
CHID: 21237 CASRN: 50-55-5
SPID(S): Tox21_300537
M4ID: 12478595

HILL MODEL (in red):

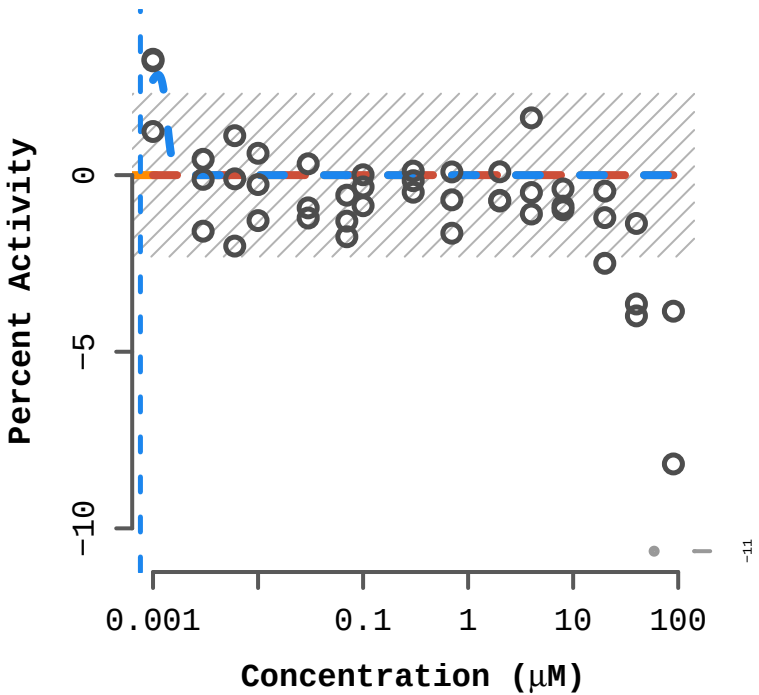
	tp	ga	gw
val:	8.48e-10	0.869	1.74
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.35	0.598	7.99	1.28	18
sd:	6.35	4.63	295	0.0901	38.7

	CNST	HILL	GNLS
AIC:	169.02	175.02	168.26
PROB:	0.4	0.02	0.58
RMSE:	2.13	2.13	2.05

MAX_MEAN: 2.19 MAX_MED: 2.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Reserpine
CHID: 21237 CASRN: 50-55-5
SPID(S): Tox21_202395
M4ID: 12479857 BRK

HILL MODEL (in red):

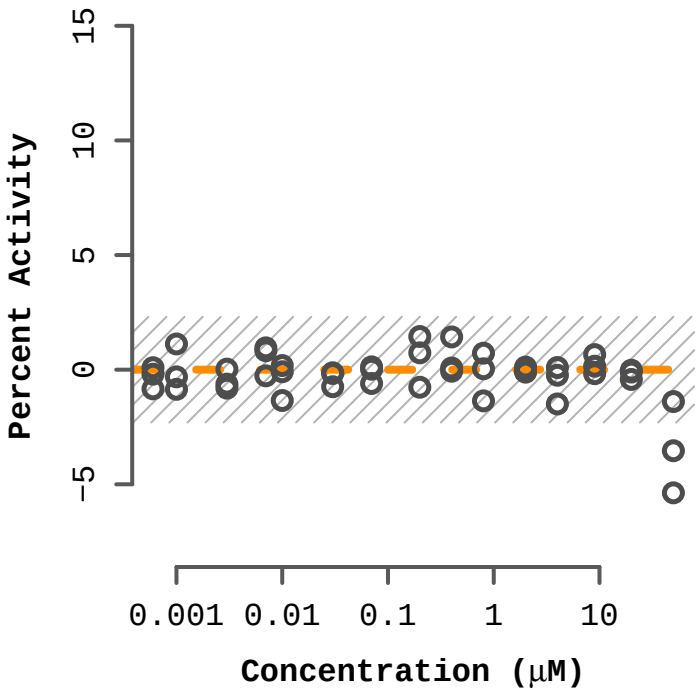
	tp	ga	gw
val:	2.6e-11	-4.54	1.46
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.89	-3.12	3.02	-2.87	16.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	192.35	198.35	193.71
PROB:	0.64	0.03	0.33
RMSE:	2.54	2.54	2.45

MAX_MEAN: 2.58 **MAX_MED:** 3.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

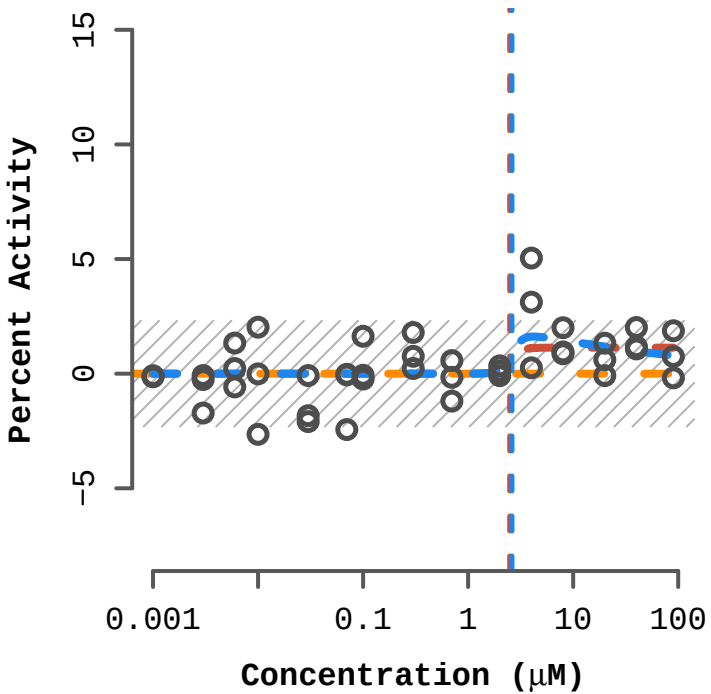
NAME: Reserpine
CHID: 21237 CASRN: 50-55-5
SPID(S): Tox21_111107_1
M4ID: 12483903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.504 **MAX_MED:** 0.826 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Resorcinol
CHID: 21238 **CASRN:** 108-46-3
SPID(S): Tox21_300140
M4ID: 12478990

HILL MODEL (in red):

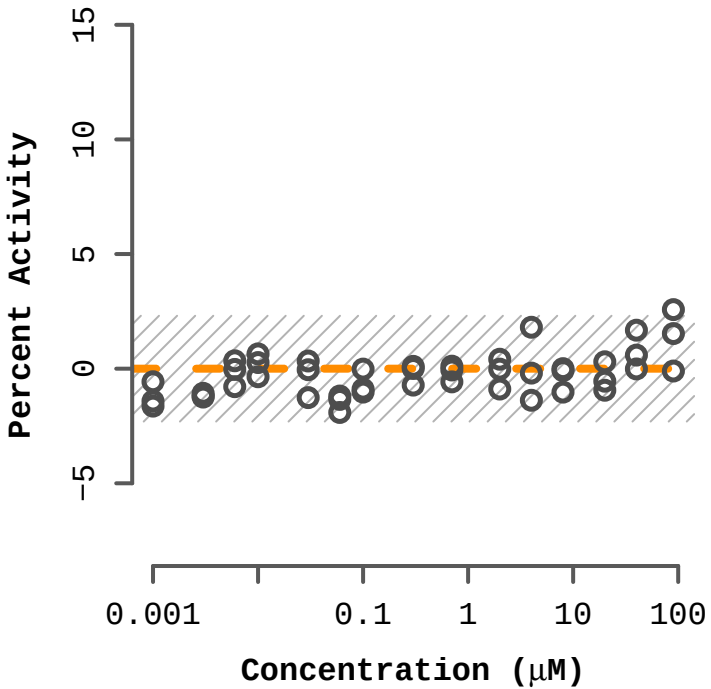
	tp	ga	gw
val:	1.14	0.396	8
sd:	0.259	0.142	9.07

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.26	0.417	7.78	0.667	0.388
sd:	10.5	0.114	6.96	6	0.443

	CNST	HILL	GNLS
AIC:	157.76	147.25	150.42
PROB:	0	0.83	0.17
RMSE:	1.43	1.2	1.16

MAX_MEAN: 2.81 **MAX_MED:** 3.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

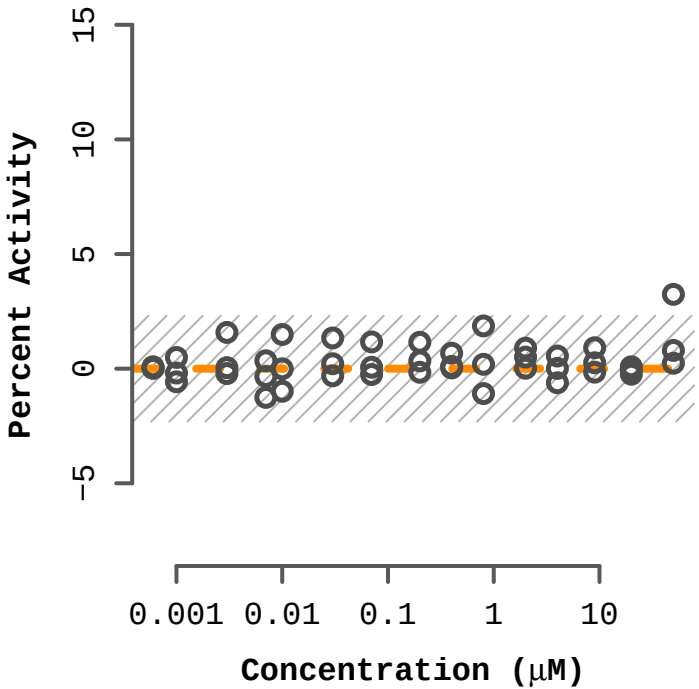
NAME: Resorcinol
CHID: 21238 **CASRN:** 108-46-3
SPID(S): Tox21_202417
M4ID: 12479835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

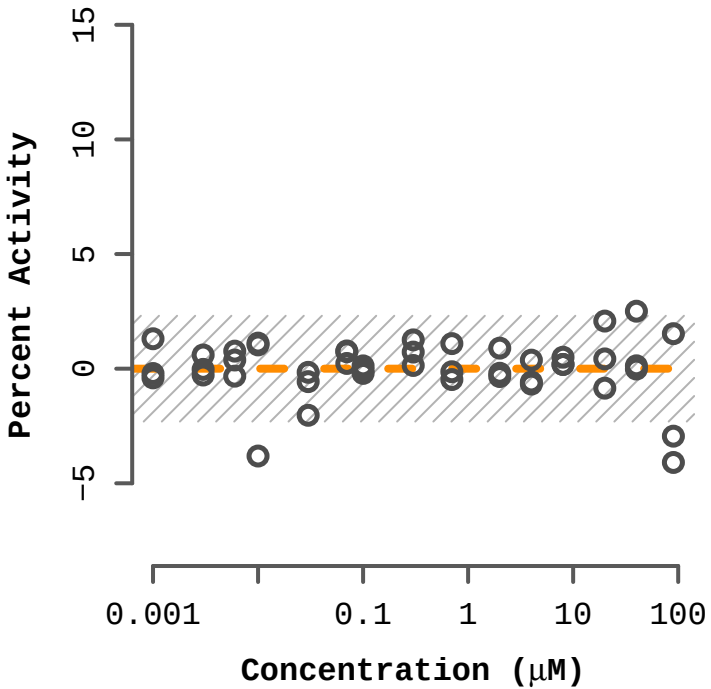
NAME: Resorcinol
CHID: 21238 **CASRN:** 108-46-3
SPID(S): Tox21_111140_1
M4ID: 12483882

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.797 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

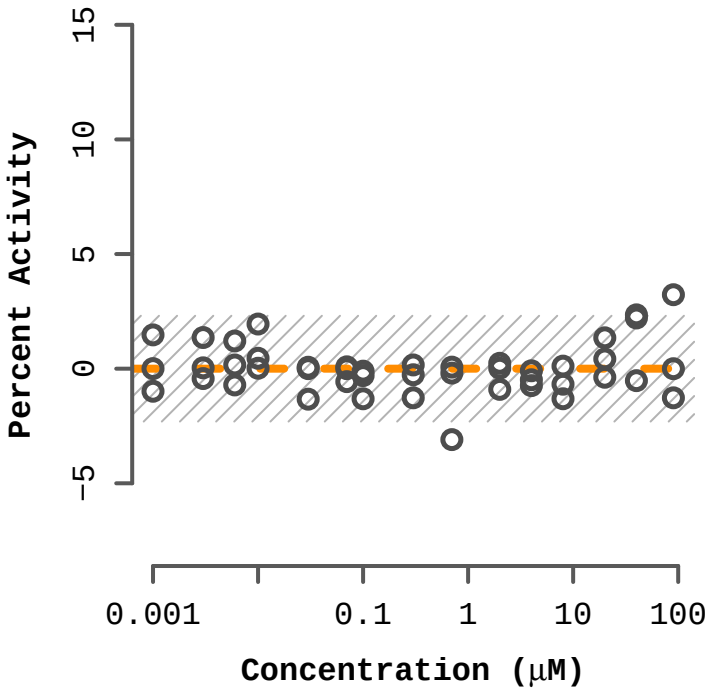
NAME: all-trans-Retinoic acid
CHID: 21239 **CASRN:** 302-79-4
SPID(S): Tox21_300305
M4ID: 12478825

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.873 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

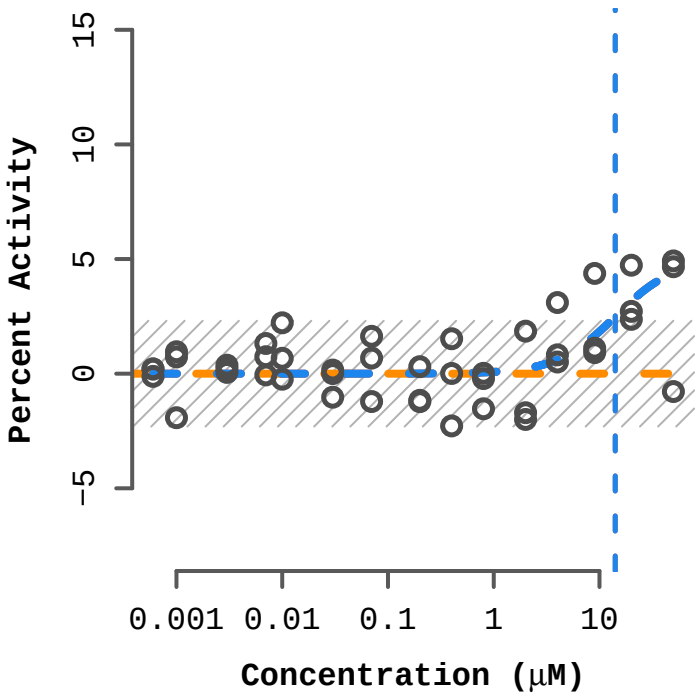
NAME: all-trans-Retinoic acid
CHID: 21239 **CASRN:** 302-79-4
SPID(S): Tox21_202330
M4ID: 12479922

HILL MODEL: Not applicable.

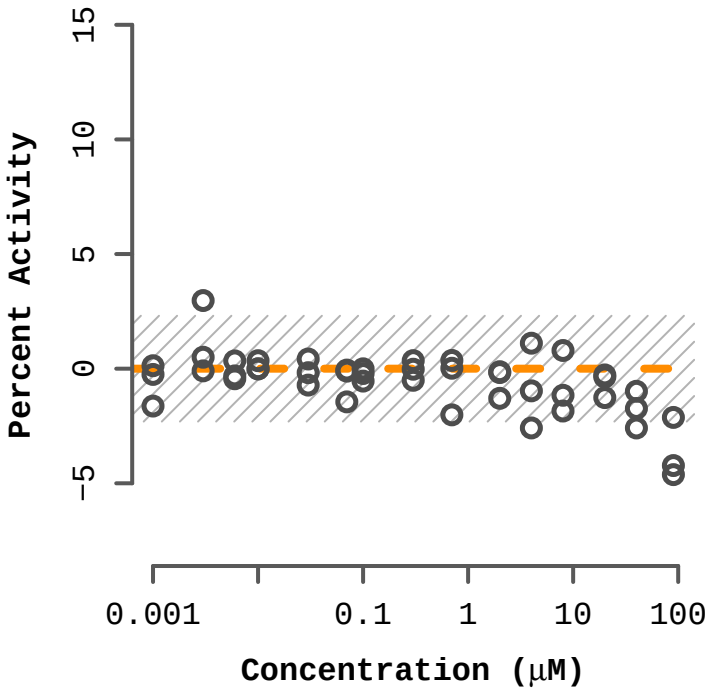
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 2.21 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    all-trans-Retinoic acid
CHID:    21239   CASRN: 302-79-4
SPID(S): Tox21_110812_1
M4ID:    12484100

HILL MODEL (in red):
      tp       ga       gw
val:  4.99     1.15     1.57
sd:   1.67     0.284    0.784

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.99     1.15     1.57     2.72     7.65
sd:   1.67     0.284    0.784    2180     16400

      CNST        HILL        GNLS
AIC:  182.04      161.43      165.43
PROB: 0           0.88        0.12
RMSE: 1.86        1.4         1.4

MAX_MEAN: 3.27      MAX_MED: 4.67      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

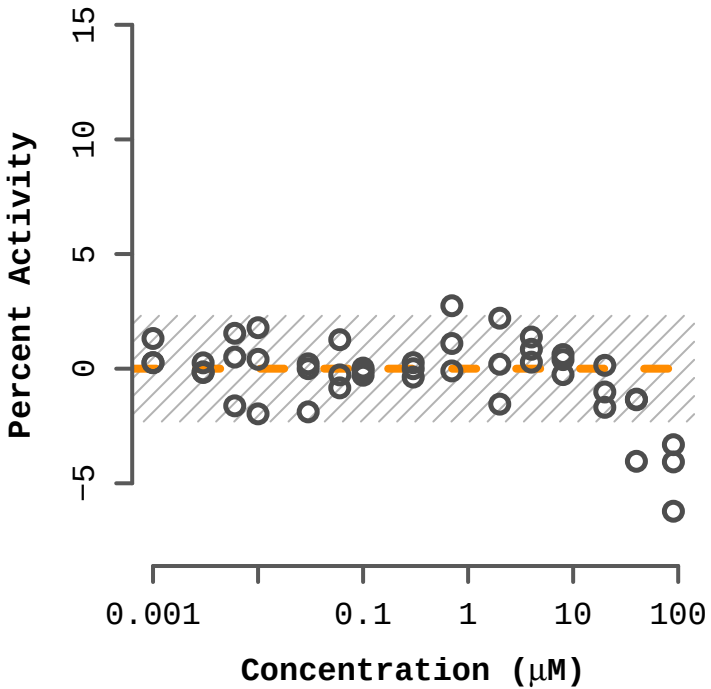
NAME: Retinol acetate
CHID: 21240 **CASRN:** 127-47-9
SPID(S): Tox21_302737
M4ID: 12476396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

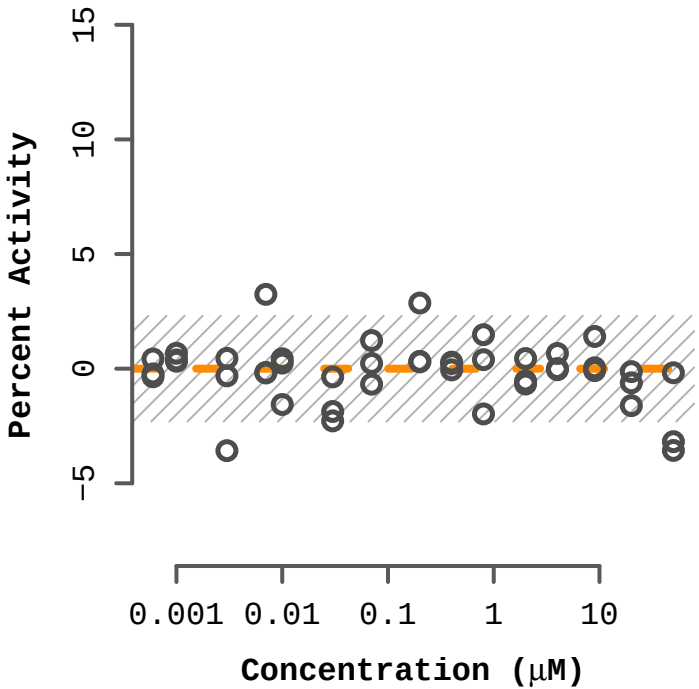
NAME: Retinol acetate
CHID: 21240 **CASRN:** 127-47-9
SPID(S): Tox21_201423
M4ID: 12480829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

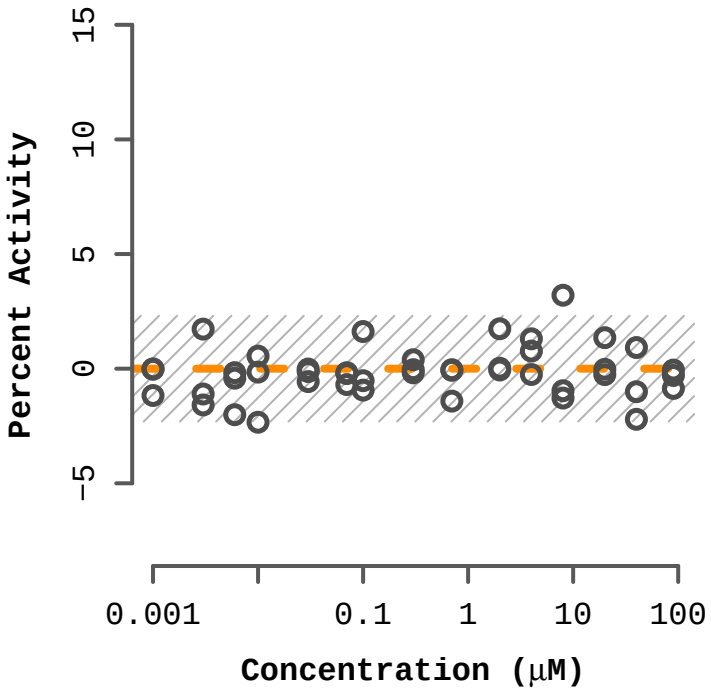
NAME: Retinol acetate
CHID: 21240 **CASRN:** 127-47-9
SPID(S): Tox21_113549_1
M4ID: 12482612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.394 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

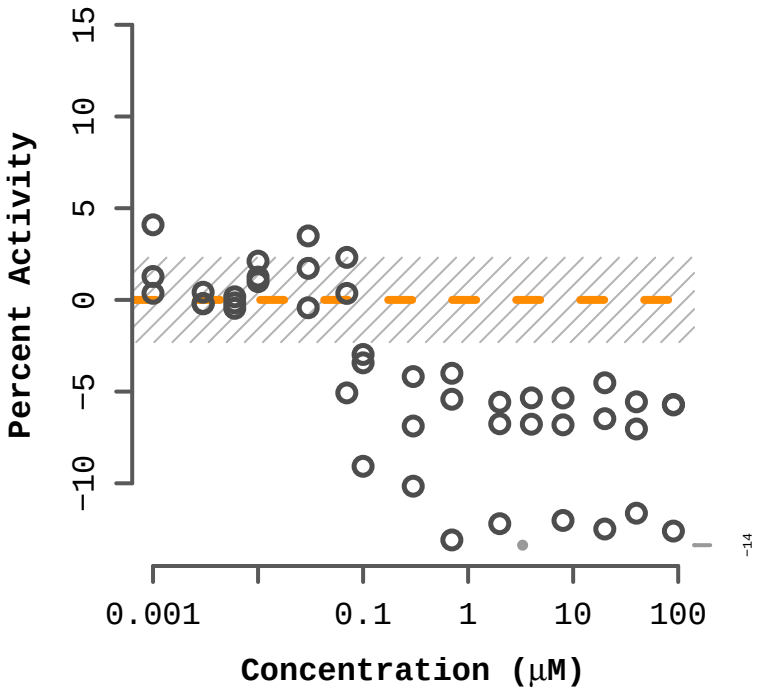
NAME: Retinol palmitate
CHID: 21241 **CASRN:** 79-81-2
SPID(S): Tox21_303008
M4ID: 12476125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.607 **MAX_MED:** 0.769 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

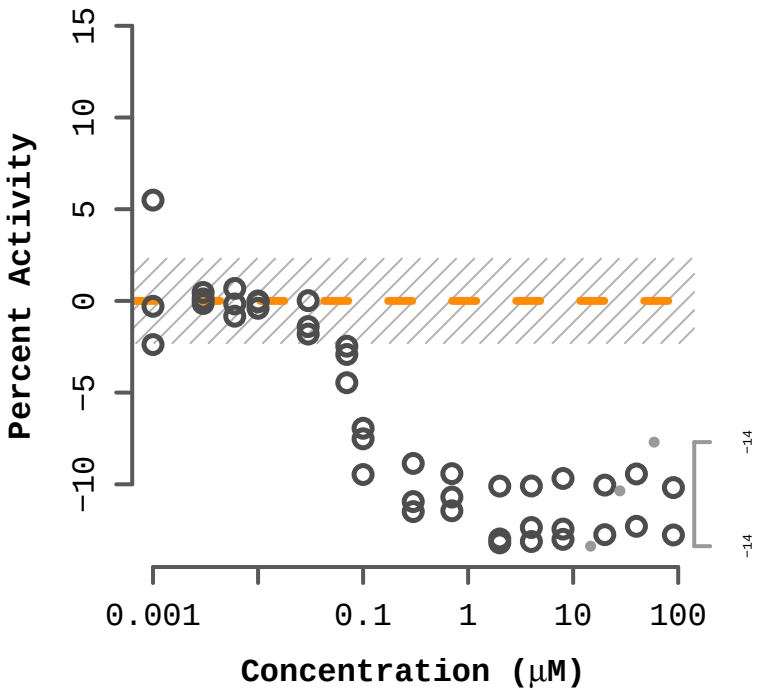
NAME: Rhodamine 6G
CHID: 21243 **CASRN:** 989-38-8
SPID(S): Tox21_302898
M4ID: 12476235 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	301.79	NA	NA
PROB:	1	NA	NA
RMSE:	6.54	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

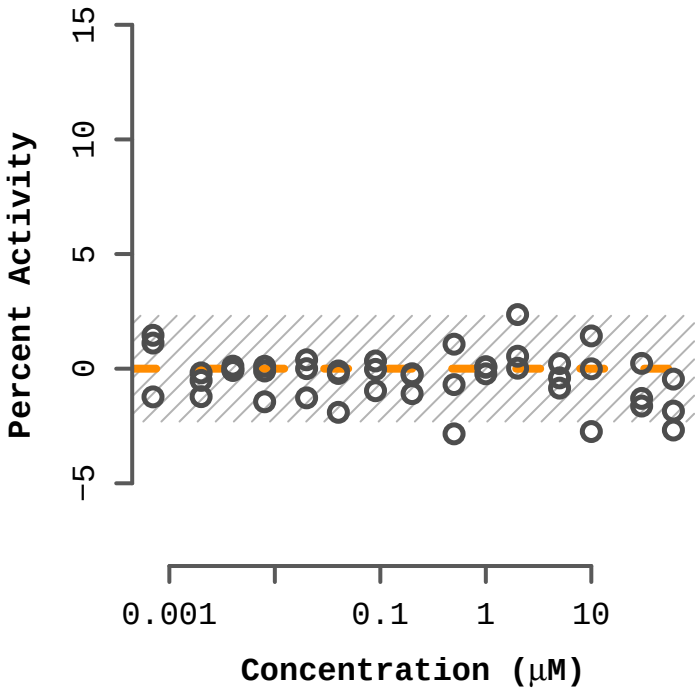
NAME: Rhodamine 6G
CHID: 21243 **CASRN:** 989-38-8
SPID(S): Tox21_201597
M4ID: 12480655 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	333.11	NA	NA
PROB:	1	NA	NA
RMSE:	8.89	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 0.111 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

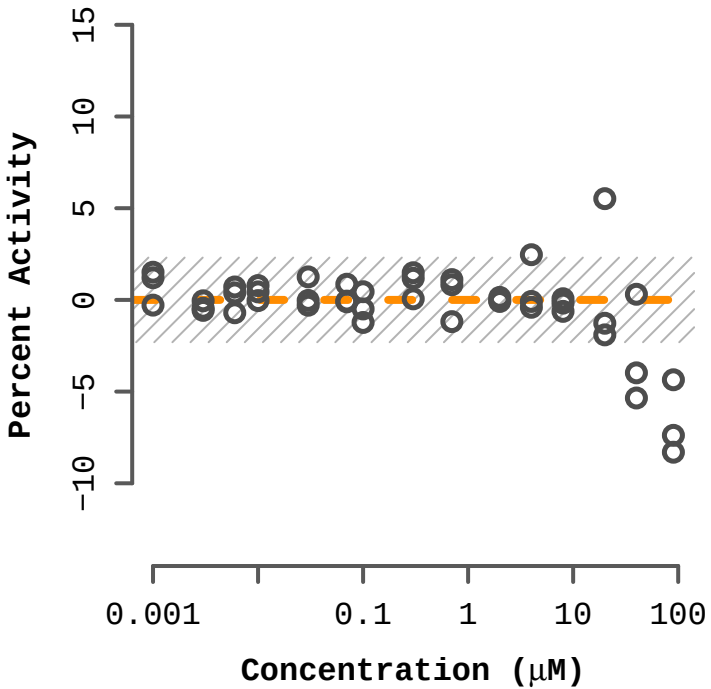
NAME: Rifampicin
CHID: 21244 CASRN: 13292-46-1
SPID(S): Tox21_300550
M4ID: 12478582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

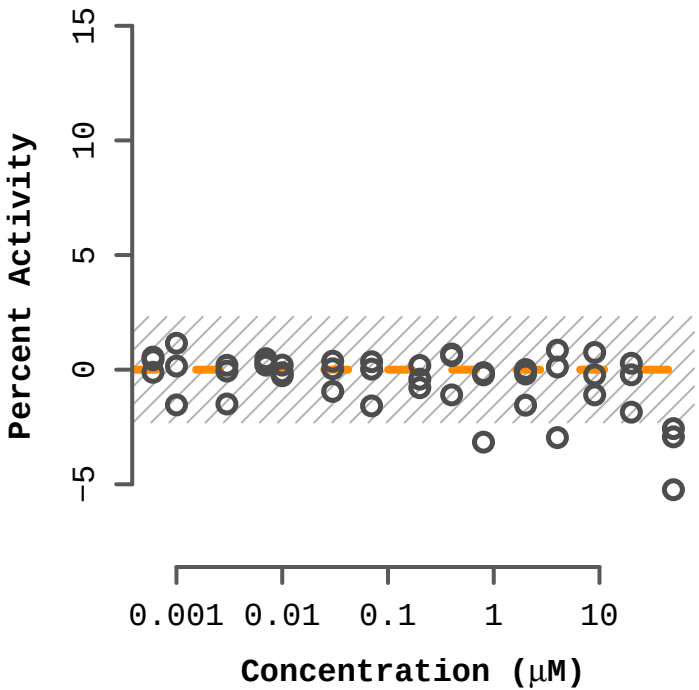
NAME: Rifampicin
CHID: 21244 **CASRN:** 13292-46-1
SPID(S): Tox21_201385
M4ID: 12480867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.79	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 0.907 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

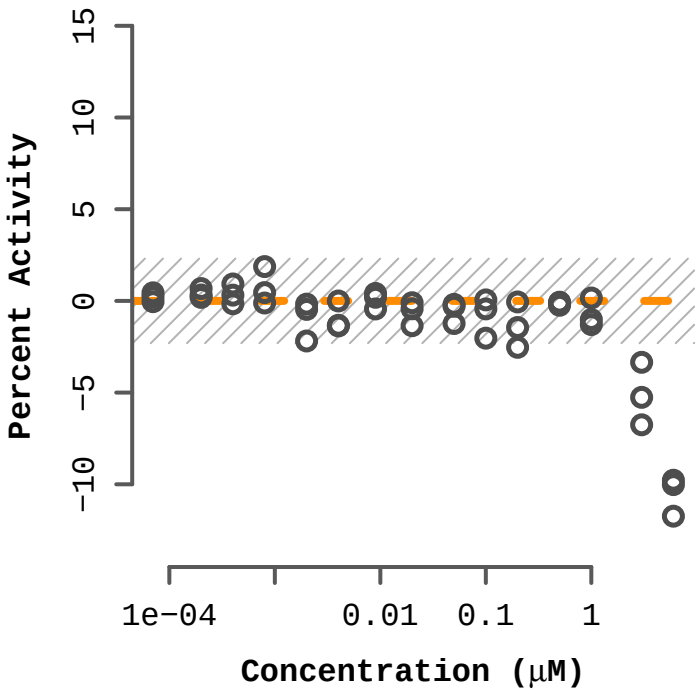
NAME: Rifampicin
CHID: 21244 CASRN: 13292-46-1
SPID(S): Tox21_111329_1
M4ID: 12483763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.333 **MAX_MED:** 0.615 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

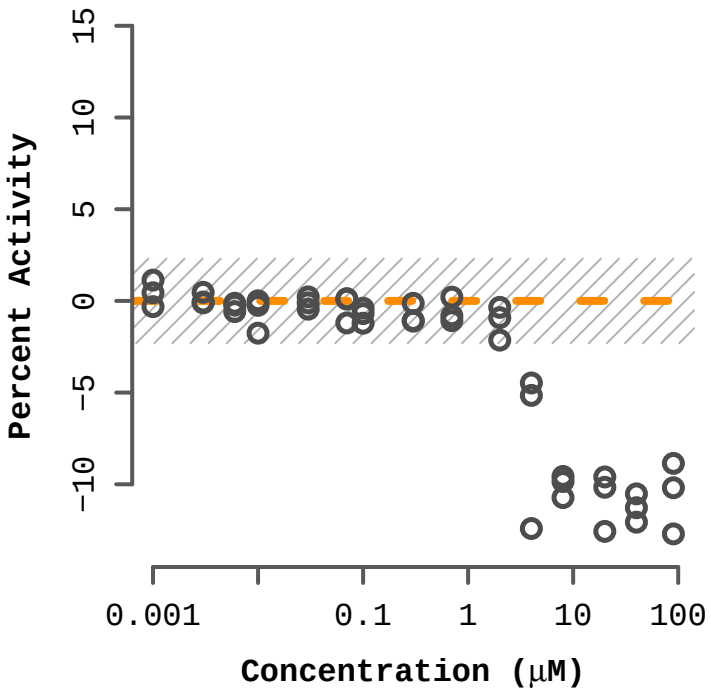
NAME: C.I. Basic Violet 14
CHID: 21246 **CASRN:** 632-99-5
SPID(S): Tox21_202790
M4ID: 12479462

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.3	NA	NA
PROB:	1	NA	NA
RMSE:	3.17	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** 0.456 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

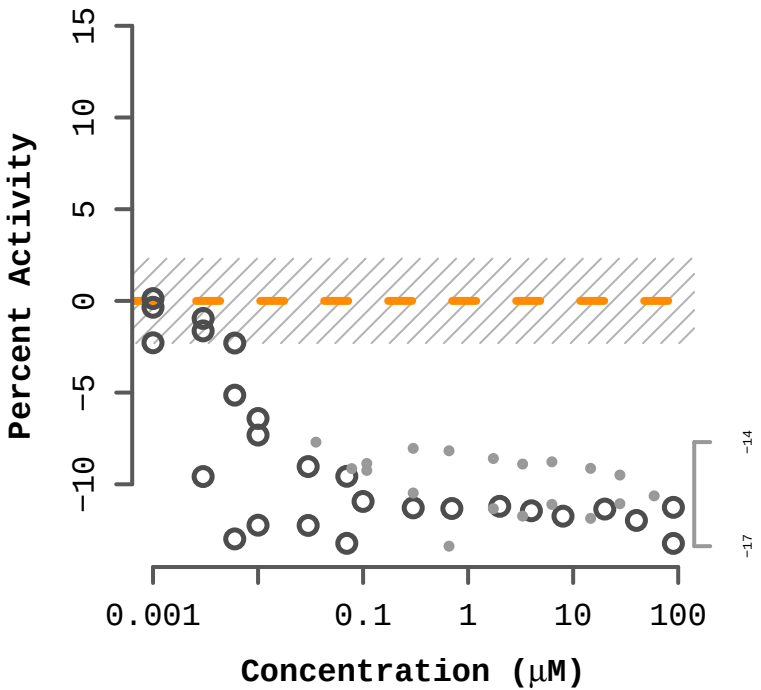
NAME: C.I. Basic Red 9 monohydrochloride
CHID: 21247 **CASRN:** 569-61-9
SPID(S): Tox21_303581
M4ID: 12475564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.91	NA	NA
PROB:	1	NA	NA
RMSE:	5.97	NA	NA

MAX_MEAN: 0.423 **MAX_MED:** 0.446 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

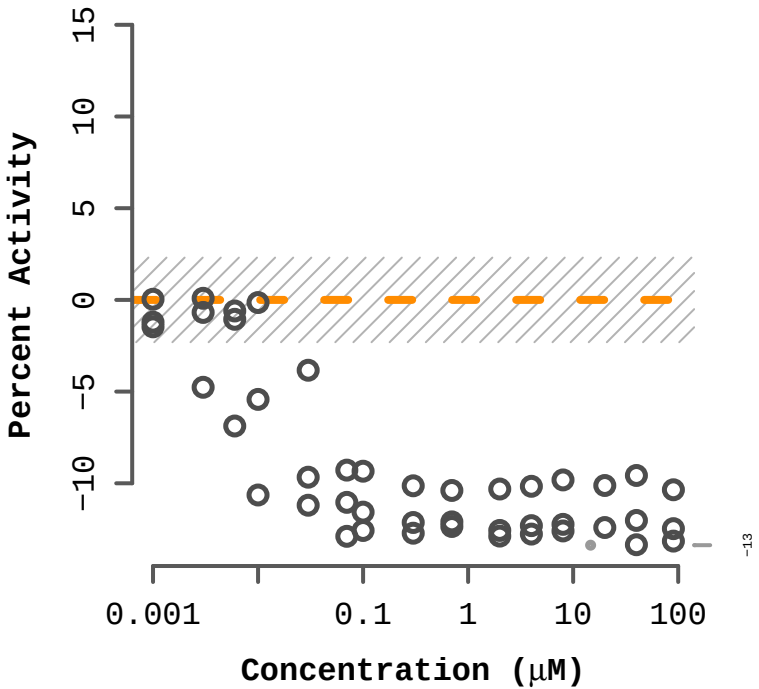
NAME: Rotenone
CHID: 21248 **CASRN:** 83-79-4
SPID(S): Tox21_300695
M4ID: 12478438 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	363.02	NA	NA
PROB:	1	NA	NA
RMSE:	12.05	NA	NA

MAX_MEAN: −0.833 **MAX_MED:** −0.346 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

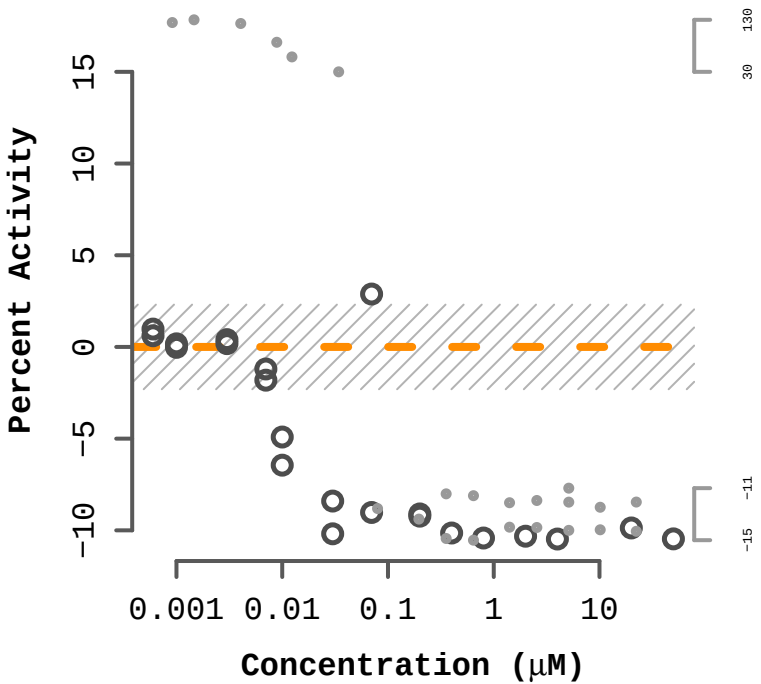
NAME: Rotenone
CHID: 21248 **CASRN:** 83-79-4
SPID(S): Tox21_201904
M4ID: 12480348 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	346.46	NA	NA
PROB:	1	NA	NA
RMSE:	10.07	NA	NA

MAX_MEAN: −0.881 **MAX_MED:** −0.681 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

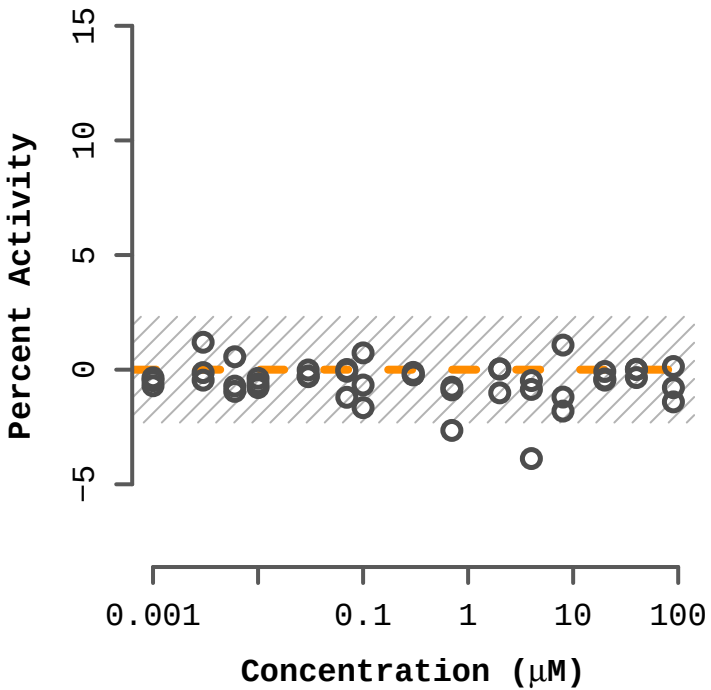
NAME: Rotenone
CHID: 21248 **CASRN:** 83-79-4
SPID(S): Tox21_110819_1
M4ID: 12484097 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	420.01	NA	NA
PROB:	1	NA	NA
RMSE:	36.75	NA	NA

MAX_MEAN: 42.3 **MAX_MED:** 0.976 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

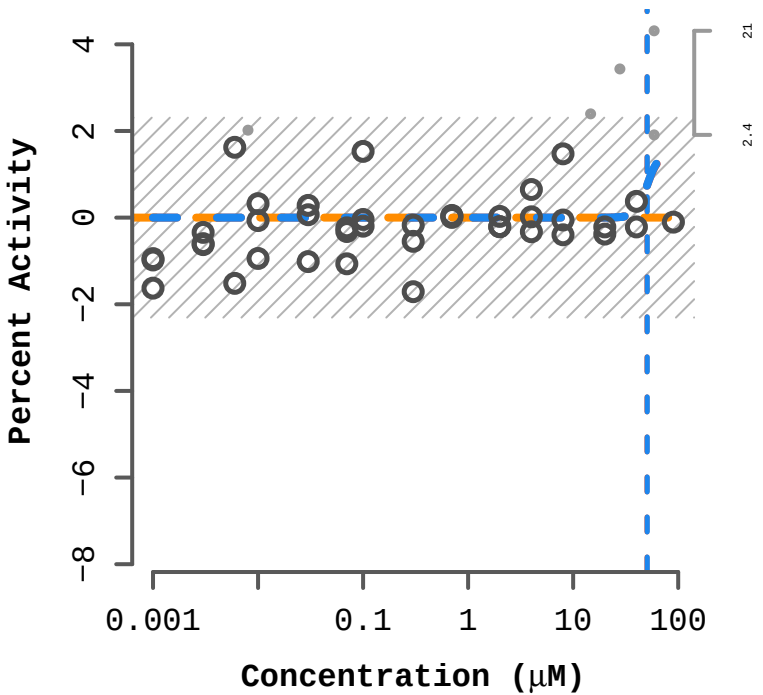
NAME: Saccharin
CHID: 21251 **CASRN:** 81-07-2
SPID(S): Tox21_302950
M4ID: 12476183

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.5	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.205 **MAX_MED:** 0.0257 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Saccharin
CHID: 21251 CASRN: 81-07-2
SPID(S): Tox21_201880
M4ID: 12480372 BRK

HILL MODEL (in red):

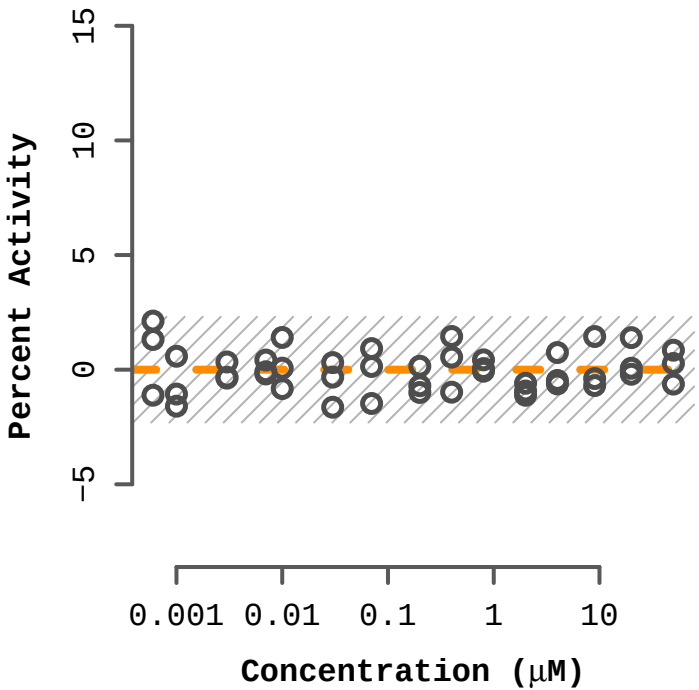
	tp	ga	gw
val:	1.46	1.7	8
sd:	2.02	1.93	146

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.82	1.71	7.99	3.76	0.34
sd:	24.7	1.67	122	73.2	14

	CNST	HILL	GNLS
AIC:	178.75	182.82	186.82
PROB:	0.87	0.11	0.02
RMSE:	4	3.81	3.81

MAX_MEAN: 7.76 MAX_MED: 2.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

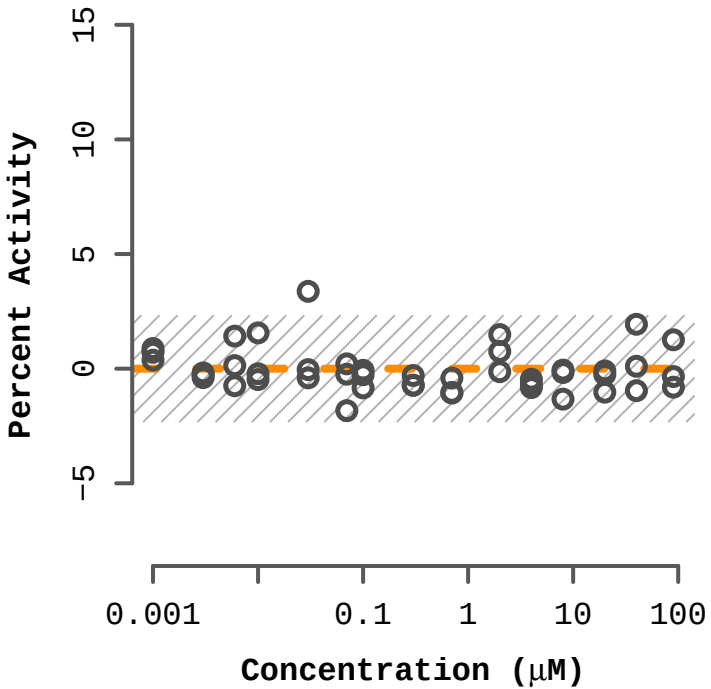
NAME: Saccharin
CHID: 21251 **CASRN:** 81-07-2
SPID(S): Tox21_111358_1
M4ID: 12483741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.776 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

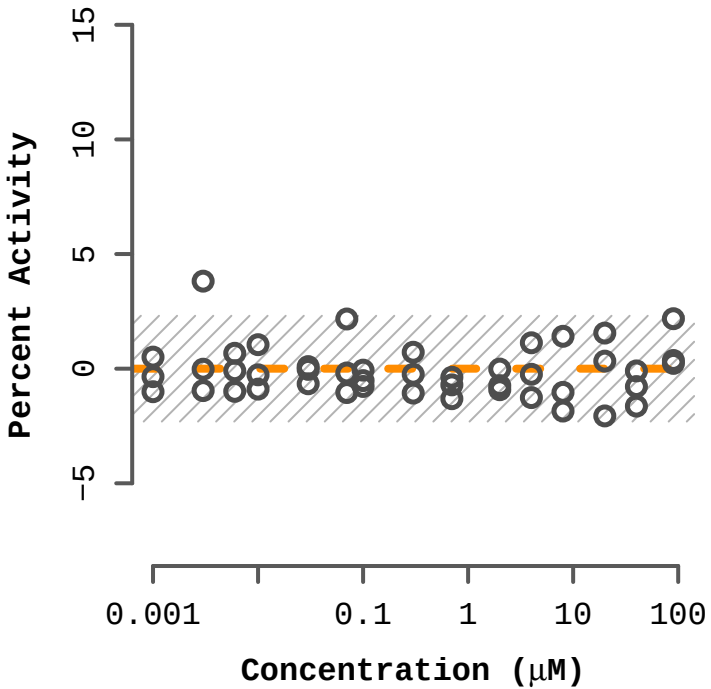
NAME: Sodium saccharin
CHID: 21253 CASRN: 128-44-9
SPID(S): Tox21_200515
M4ID: 12481737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 0.753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

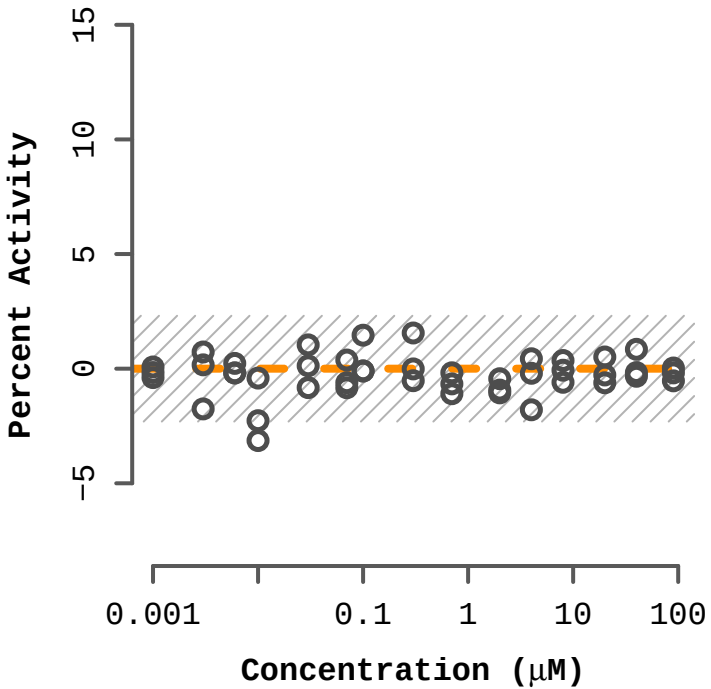
NAME: Safrole
CHID: 21254 **CASRN:** 94-59-7
SPID(S): Tox21_300520
M4ID: 12478612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.947 **MAX_MED:** 0.359 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

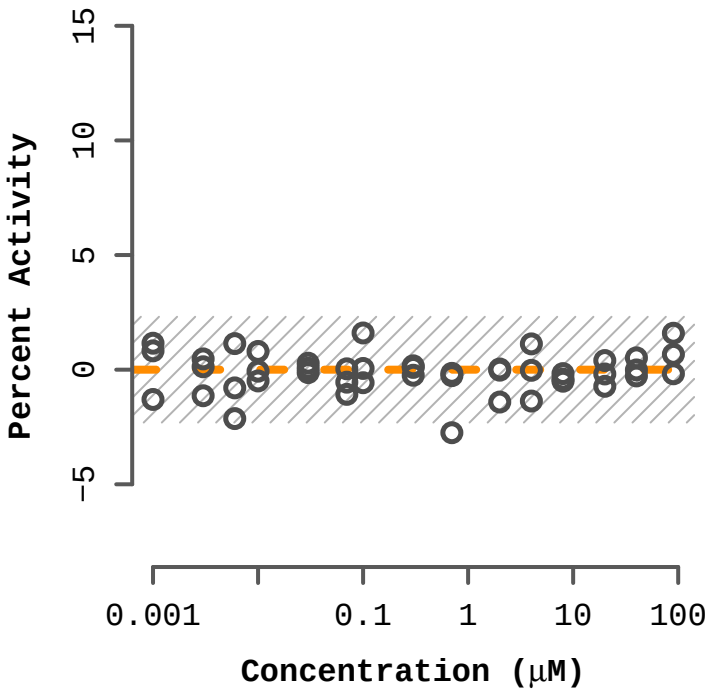
NAME: Safrole
CHID: 21254 **CASRN:** 94-59-7
SPID(S): Tox21_202439
M4ID: 12479813

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.421 **MAX_MED:** 0.169 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

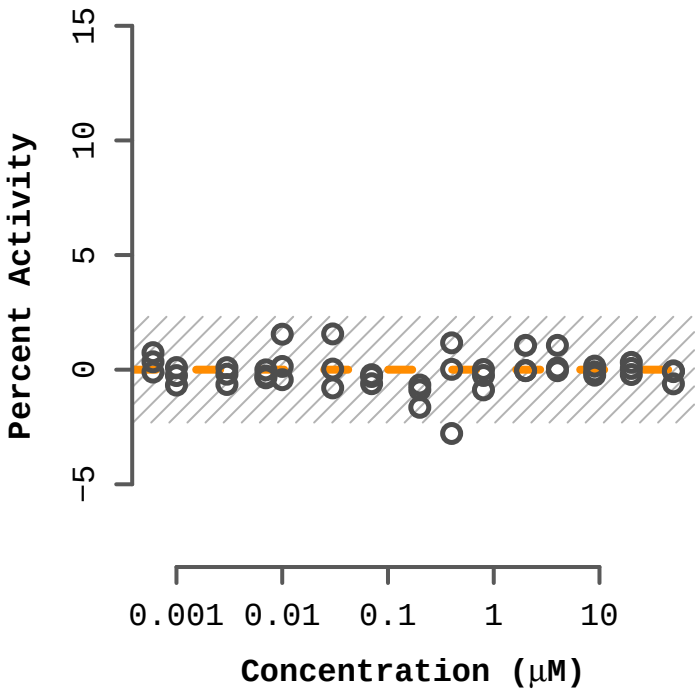
NAME: Albuterol
CHID: 21255 CASRN: 18559-94-9
SPID(S): Tox21_200800
M4ID: 12481452

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.694 **MAX_MED:** 0.823 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

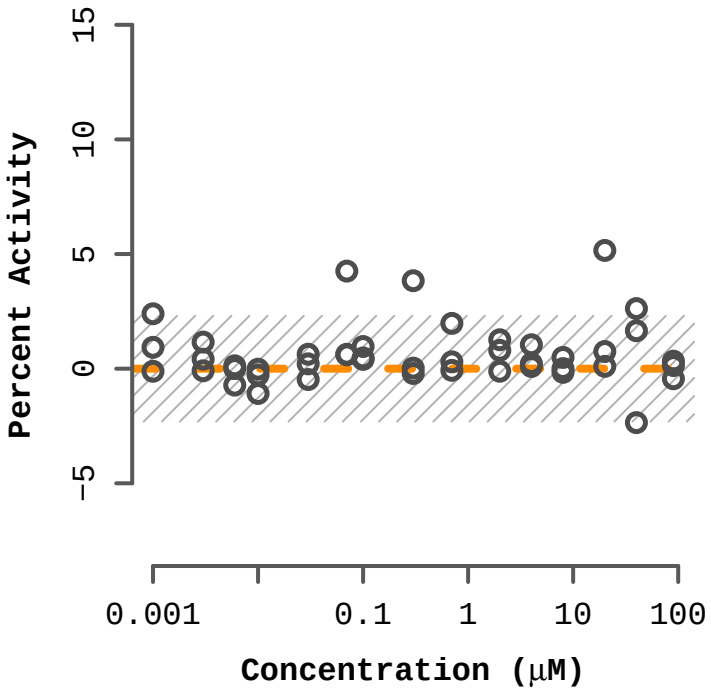
NAME: Albuterol
CHID: 21255 CASRN: 18559-94-9
SPID(S): Tox21_110266_1
M4ID: 12484500

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.419 **MAX_MED:** 0.345 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

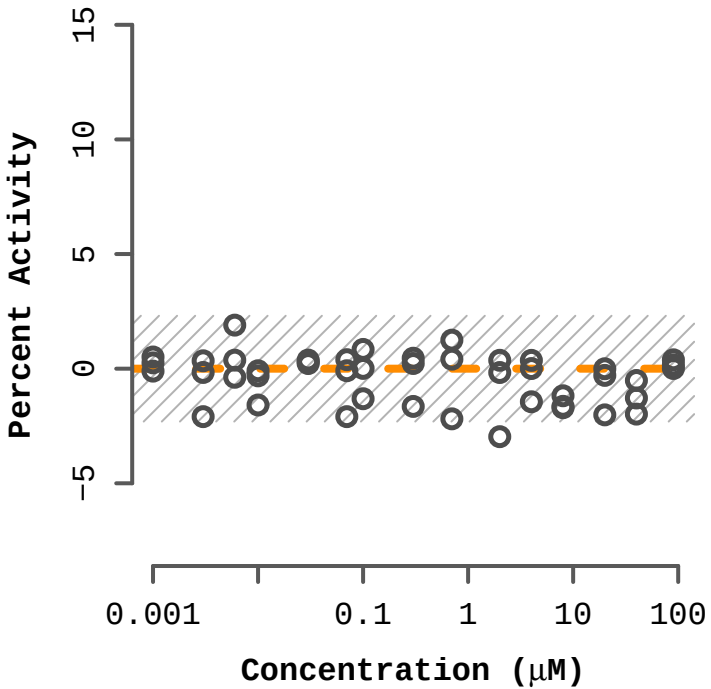
NAME: Sulfasalazine
CHID: 21256 **CASRN:** 599-79-1
SPID(S): Tox21_300541
M4ID: 12478591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

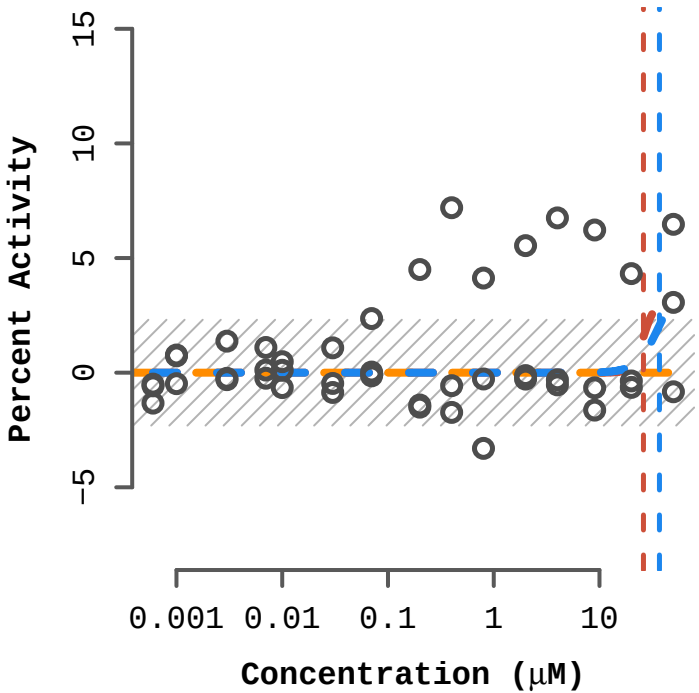
NAME: Sulfasalazine
CHID: 21256 **CASRN:** 599-79-1
SPID(S): Tox21_201239
M4ID: 12481013

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.633 **MAX_MED:** 0.414 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfasalazine
CHID: 21256 CASRN: 599-79-1
SPID(S): Tox21_111037_1
M4ID: 12483936

HILL MODEL (in red):

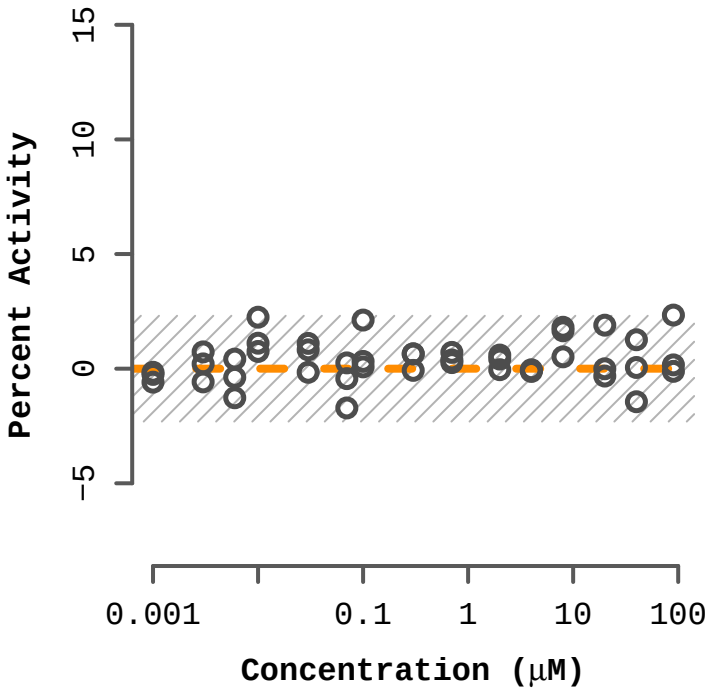
	tp	ga	gw
val:	3.11	1.42	8
sd:	2.09	1.37	91.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.6	1.57	4.31	1.82	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	207.65	210.19	214.19
PROB:	0.76	0.21	0.03
RMSE:	2.64	2.52	2.52

MAX_MEAN: 2.9 MAX_MED: 3.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

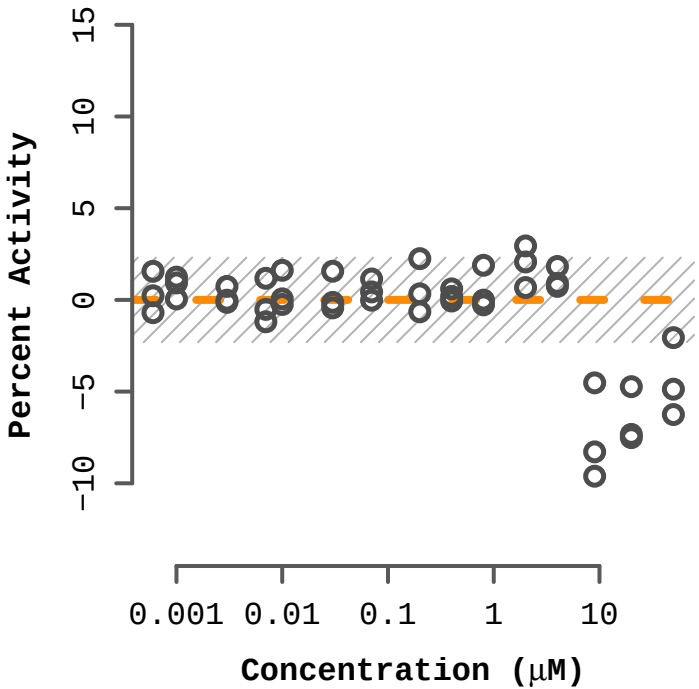
NAME: Scopolamine hydrobromide trihydrate
CHID: 21258 CASRN: 6533-68-2
SPID(S): Tox21_200867
M4ID: 12481385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

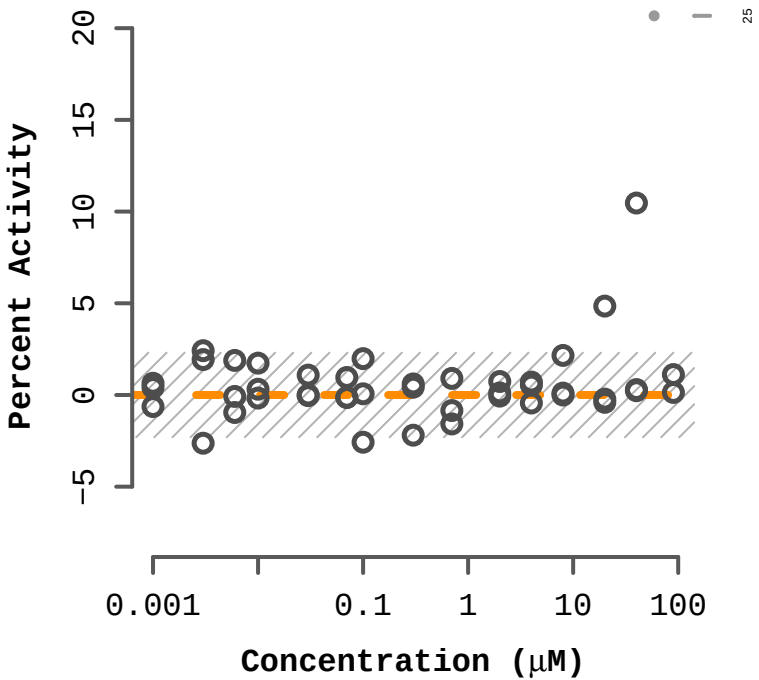
NAME: Selenium dioxide
CHID: 21264 **CASRN:** 7446-08-4
SPID(S): Tox21_202597
M4ID: 12479655

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.52	NA	NA
PROB:	1	NA	NA
RMSE:	3.07	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

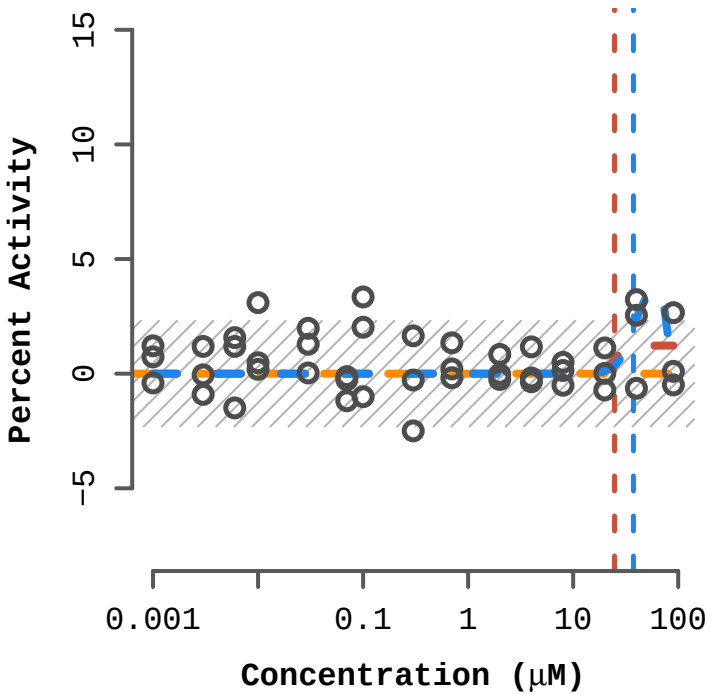
NAME: Sesamol
CHID: 21267 CASRN: 533-31-3
SPID(S): Tox21_201211
M4ID: 12481041 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.32	NA	NA
PROB:	1	NA	NA
RMSE:	4.2	NA	NA

MAX_MEAN: 8.61 MAX_MED: 1.93 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Simazine
CHID: 21268 CASRN: 122-34-9
SPID(S): Tox21_300748
M4ID: 12478385

HILL MODEL (in red):

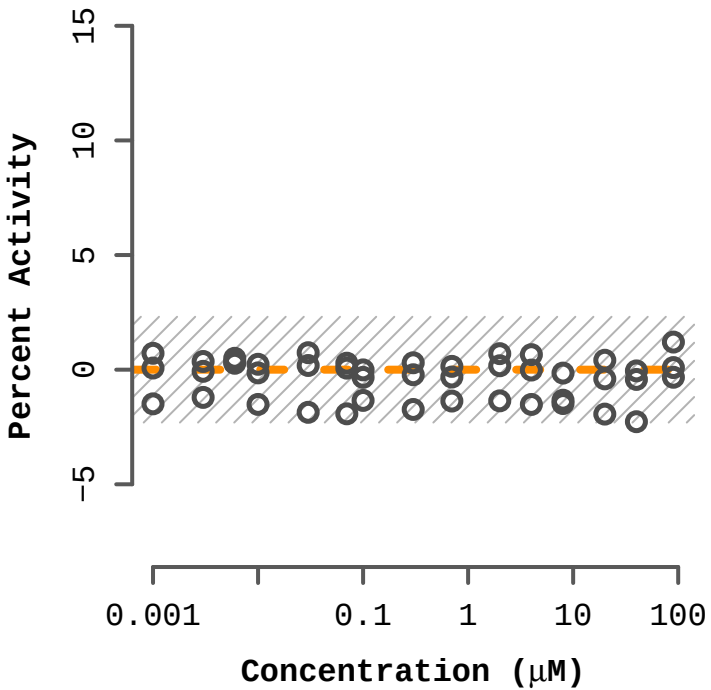
	tp	ga	gw
val:	1.22	1.39	8
sd:	0.869	0.172	10.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4	1.57	5.59	1.89	16.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.26	160.72	162.19
PROB:	0.79	0.14	0.07
RMSE:	1.37	1.29	1.29

MAX_MEAN: 1.72 MAX_MED: 2.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

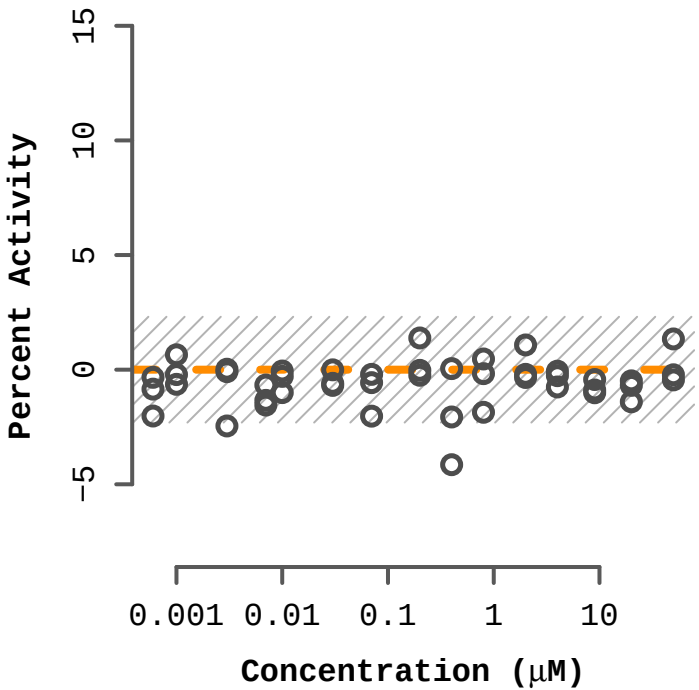
NAME: Simazine
CHID: 21268 CASRN: 122-34-9
SPID(S): Tox21_202378
M4ID: 12479874

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.374 **MAX_MED:** 0.343 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

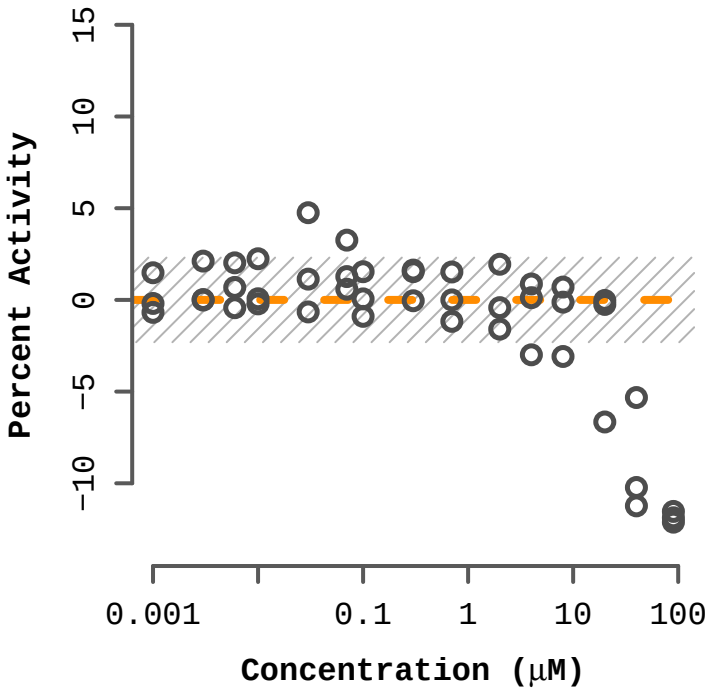
NAME: Simazine
CHID: 21268 CASRN: 122-34-9
SPID(S): Tox21_111291_1
M4ID: 12483787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.371 MAX_MED: −0.028 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

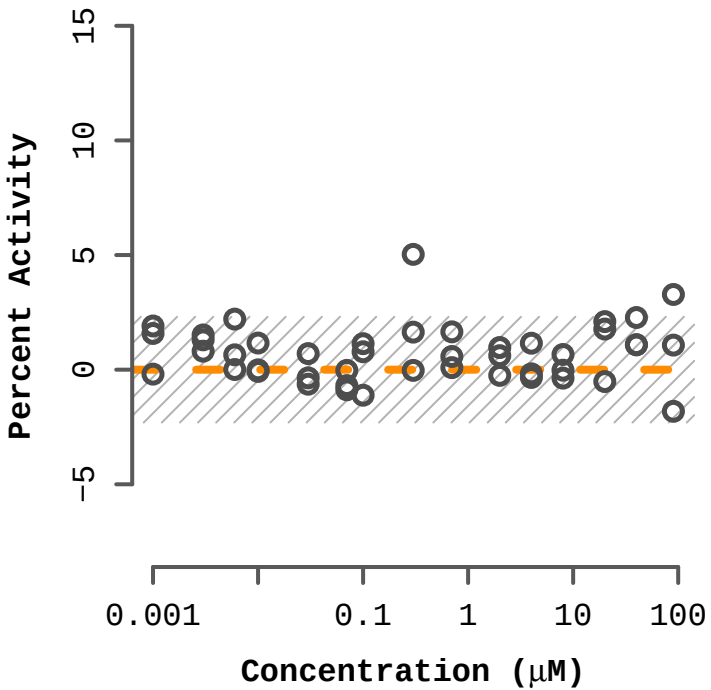
NAME: Sodium bithionolate
CHID: 21270 CASRN: 6385-58-6
SPID(S): Tox21_202791
M4ID: 12479461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	242.38	NA	NA
PROB:	1	NA	NA
RMSE:	4.26	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

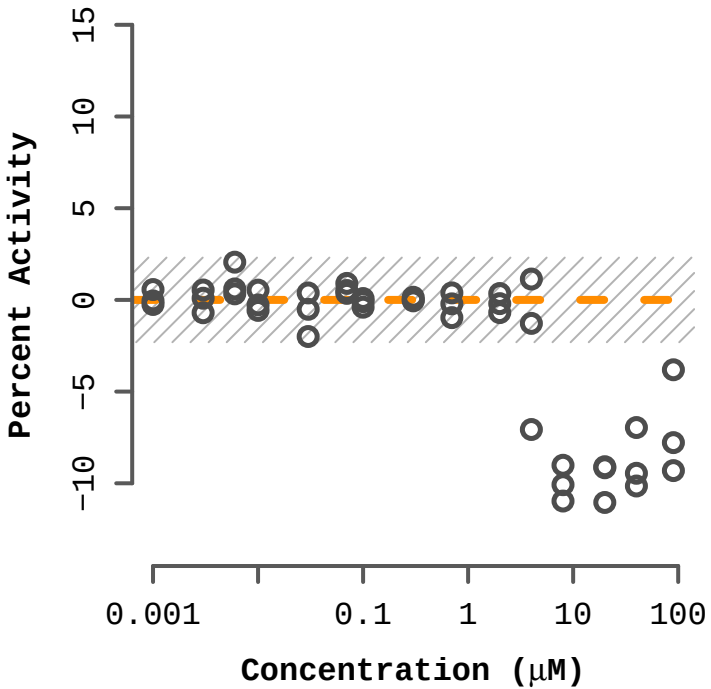
NAME: Sodium chlorite
CHID: 21272 CASRN: 7758-19-2
SPID(S): Tox21_302800
M4ID: 12476333

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.21 MAX_MED: 1.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

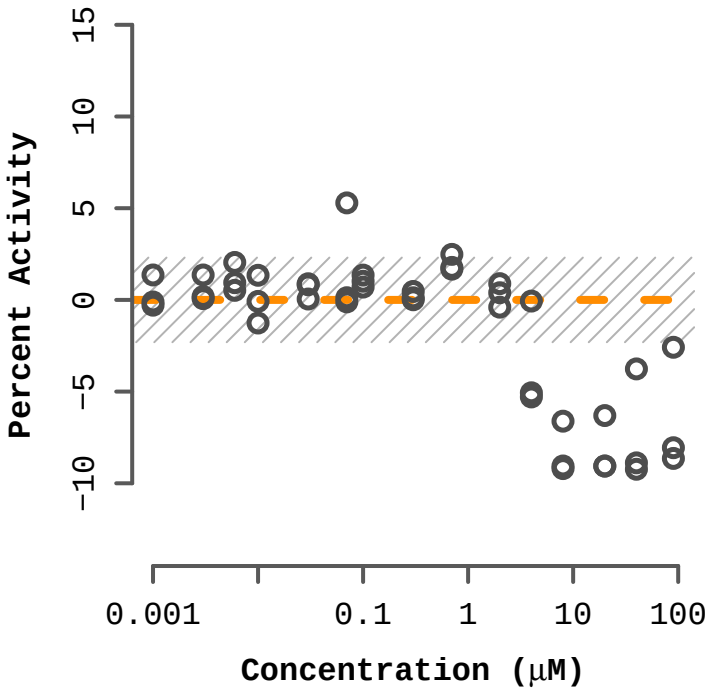
NAME: Sodium diethyldithiocarbamate trihydrate
CHID: 21275 **CASRN:** 20624-25-3
SPID(S): Tox21_302812
M4ID: 12476321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.11	NA	NA
PROB:	1	NA	NA
RMSE:	4.85	NA	NA

MAX_MEAN: 0.996 **MAX_MED:** 0.599 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

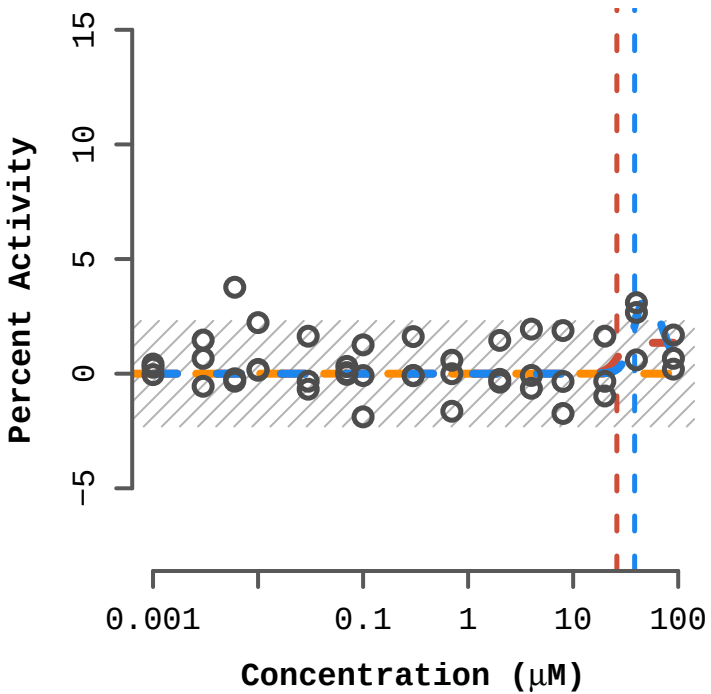
NAME: Sodium diethyldithiocarbamate trihydrate
CHID: 21275 CASRN: 20624-25-3
SPID(S): Tox21_201267
M4ID: 12480985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.41	NA	NA
PROB:	1	NA	NA
RMSE:	4.35	NA	NA

MAX_MEAN: 1.98 MAX_MED: 1.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sorbic acid
CHID: 21277 CASRN: 110-44-1
SPID(S): Tox21_300182
M4ID: 12478948

HILL MODEL (in red):

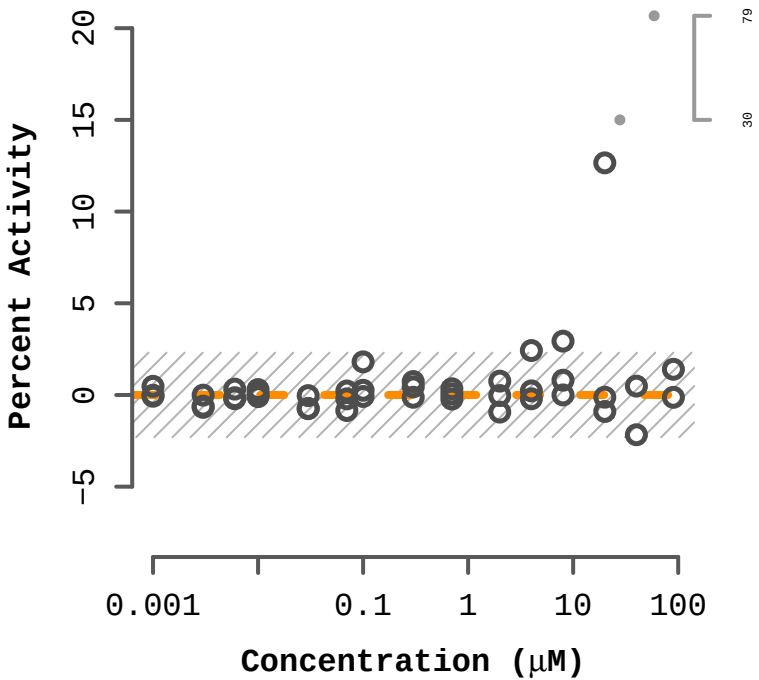
	tp	ga	gw
val:	1.35	1.42	8
sd:	0.502	0.137	7.32

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.4	1.59	8	1.84	5.4
sd:	31.6	0.845	22.9	4.89	201

	CNST	HILL	GNLS
AIC:	150.19	148.41	149.09
PROB:	0.19	0.47	0.33
RMSE:	1.28	1.16	1.14

MAX_MEAN: 2.12 **MAX_MED:** 2.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

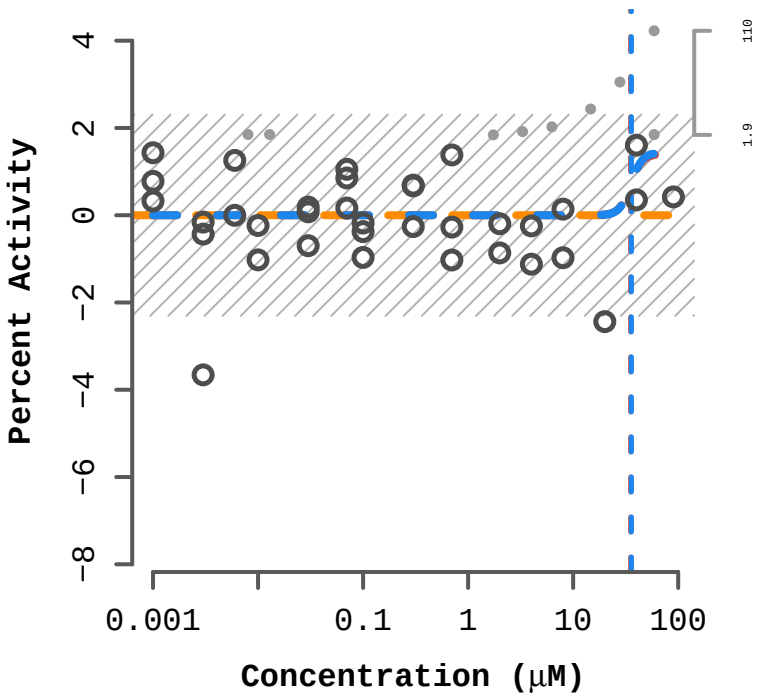
NAME: Sorbic acid
CHID: 21277 CASRN: 110-44-1
SPID(S): Tox21_201719
M4ID: 12480533 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.04	NA	NA
PROB:	1	NA	NA
RMSE:	12.85	NA	NA

MAX_MEAN: 26.9 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sotalol hydrochloride
CHID: 21278 CASRN: 959-24-0
SPID(S): Tox21_200127
M4ID: 12482125 BRK

HILL MODEL (in red):

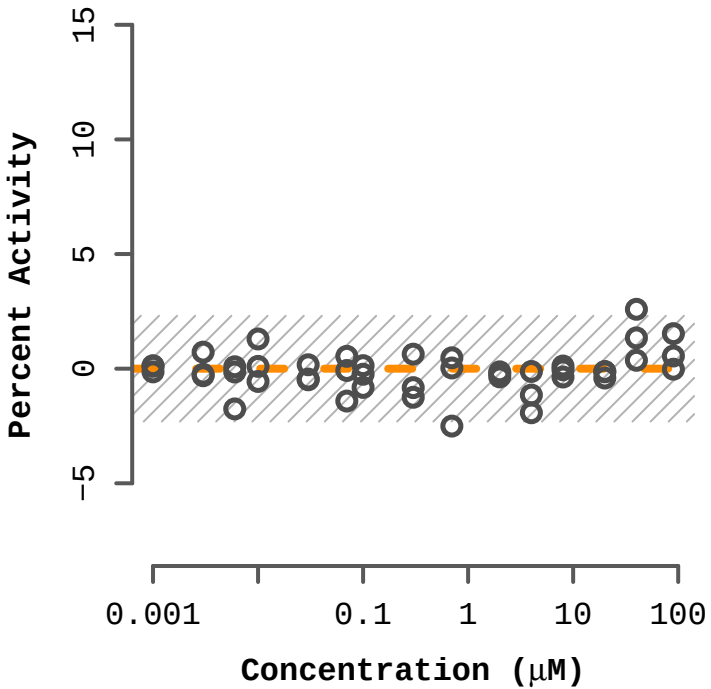
	tp	ga	gw
val:	1.4	1.55	8
sd:	1.03	0.217	15.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.75	1.55	8	3.95	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	257.77	261.1	265.1
PROB:	0.82	0.16	0.02
RMSE:	19.52	19.26	19.26

MAX_MEAN: 38 MAX_MED: 13.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

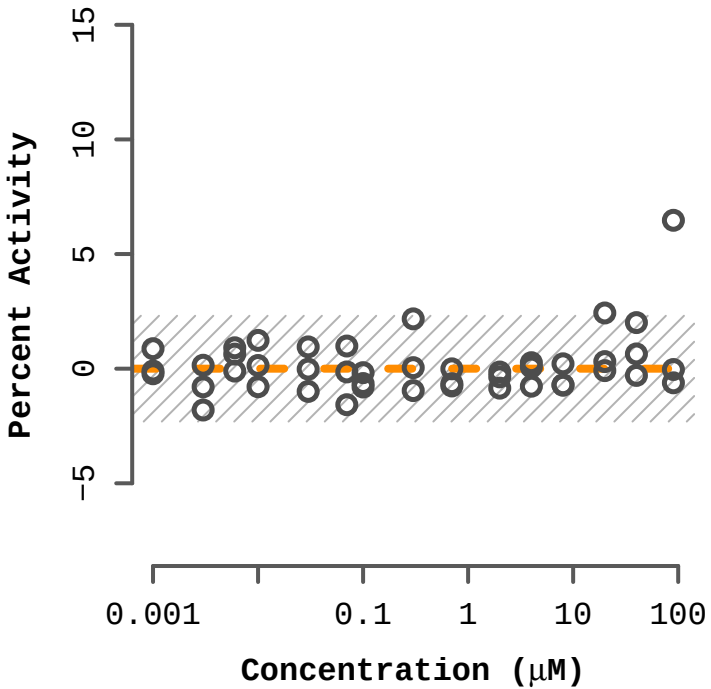
NAME: Streptozotocin
CHID: 21282 **CASRN:** 18883-66-4
SPID(S): Tox21_302974
M4ID: 12476159

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

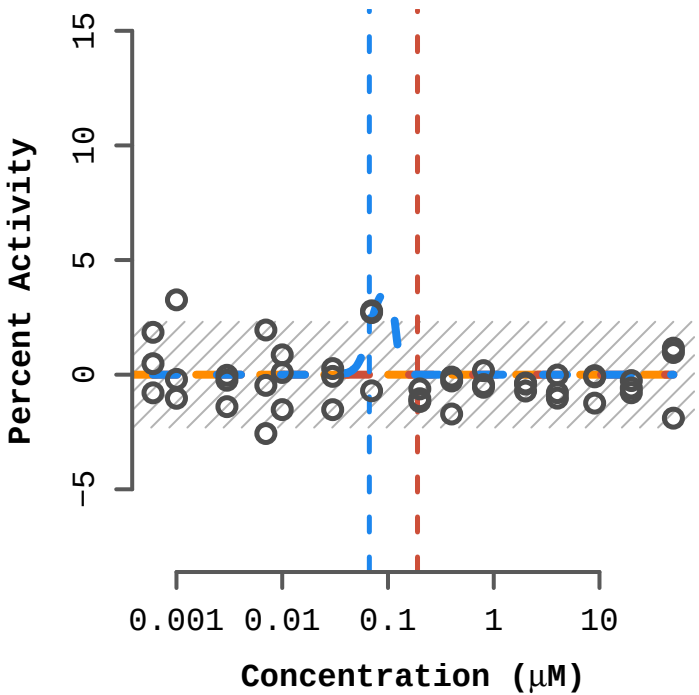
NAME: Streptozotocin
CHID: 21282 **CASRN:** 18883-66-4
SPID(S): Tox21_201859
M4ID: 12480393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 0.644 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Streptozotocin
CHID: 21282 **CASRN:** 18883-66-4
SPID(S): Tox21_110585_1
M4ID: 12484249

HILL MODEL (in red):

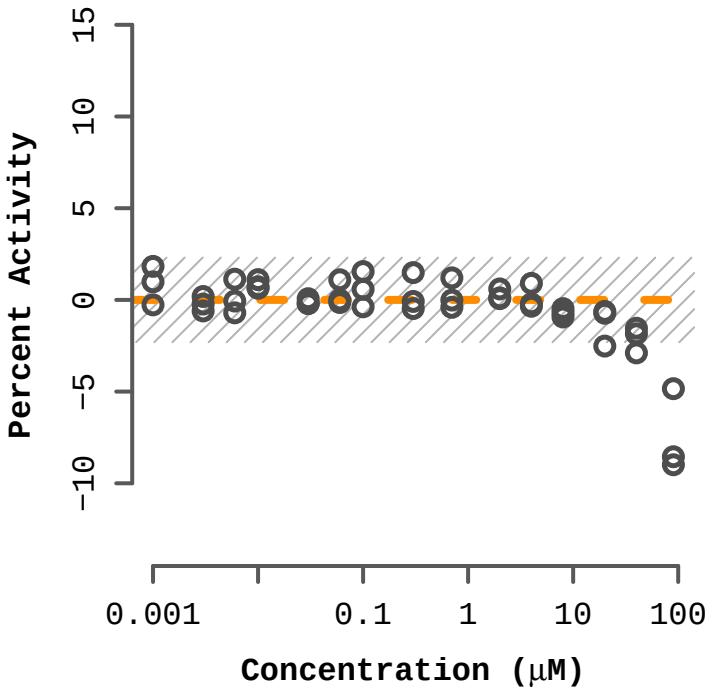
	tp	ga	gw
val:	2.69e-13	-0.721	1.72
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.91	-1.18	8	-0.926	18
sd:	26.1	0.872	17.4	1.64	130

	CNST	HILL	GNLS
AIC:	147.23	153.23	151.92
PROB:	0.87	0.04	0.08
RMSE:	1.22	1.22	1.16

MAX_MEAN: 1.6 **MAX_MED:** 2.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

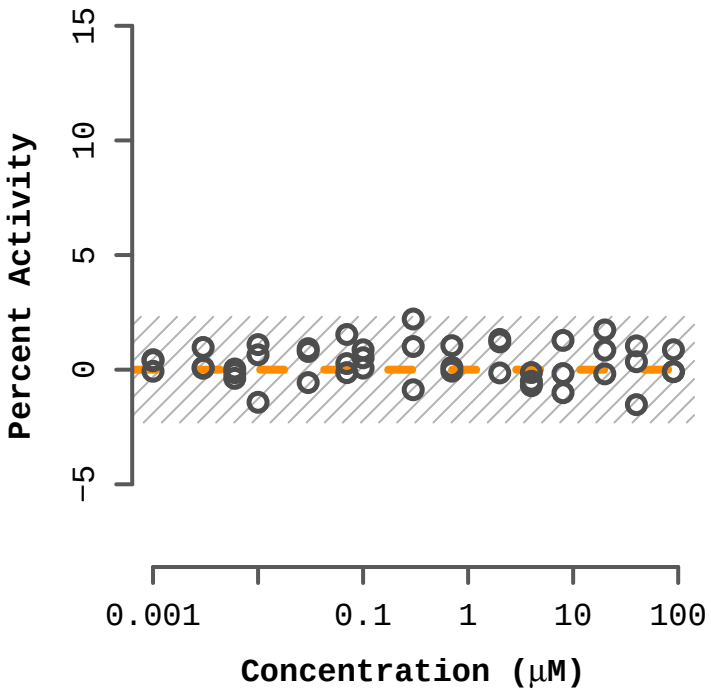
NAME: Strobane
CHID: 21283 **CASRN:** 8001-50-1
SPID(S): Tox21_200659
M4ID: 12481593

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 0.986 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

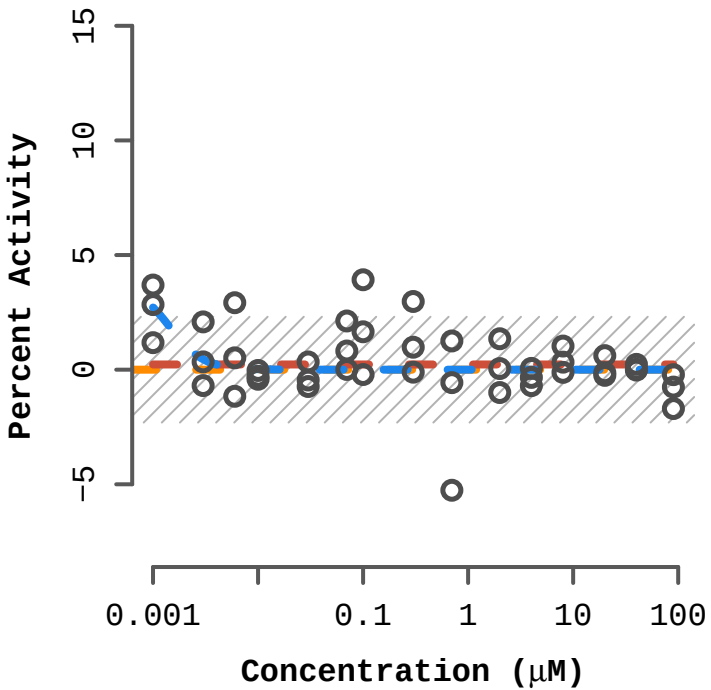
NAME: Styrene
CHID: 21284 **CASRN:** 100-42-5
SPID(S): Tox21_200808
M4ID: 12481444

HILL MODEL: Not applicable.

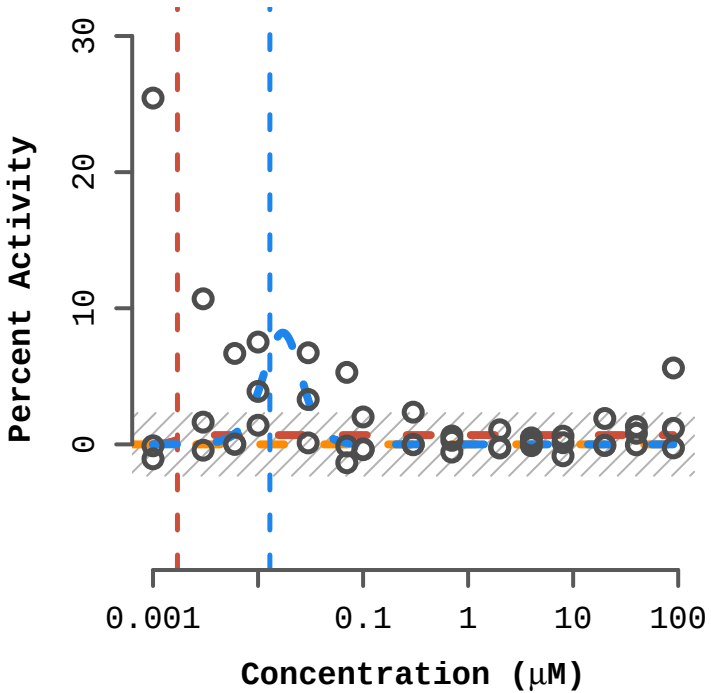
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 1.21 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Styrene oxide
CHID:    21286   CASRN: 96-09-3
SPID(S): Tox21_300110
M4ID:    12479020

HILL MODEL (in red):
      tp       ga       gw
val:  0.226    -5       3.34
sd:   0.18     939      1570

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.62     -3.96    0.763    -2.87    2.69
sd:   104      73.5     34.9     2.49     7.53

      CNST        HILL        GNLS
AIC:  161.4       165.76      159.39
PROB: 0.26        0.03        0.71
RMSE: 1.57        1.53        1.41

MAX_MEAN: 2.57      MAX_MED: 2.84      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Styrene oxide
CHID: 21286 CASRN: 96-09-3
SPID(S): Tox21_202112
M4ID: 12480140

HILL MODEL (in red):

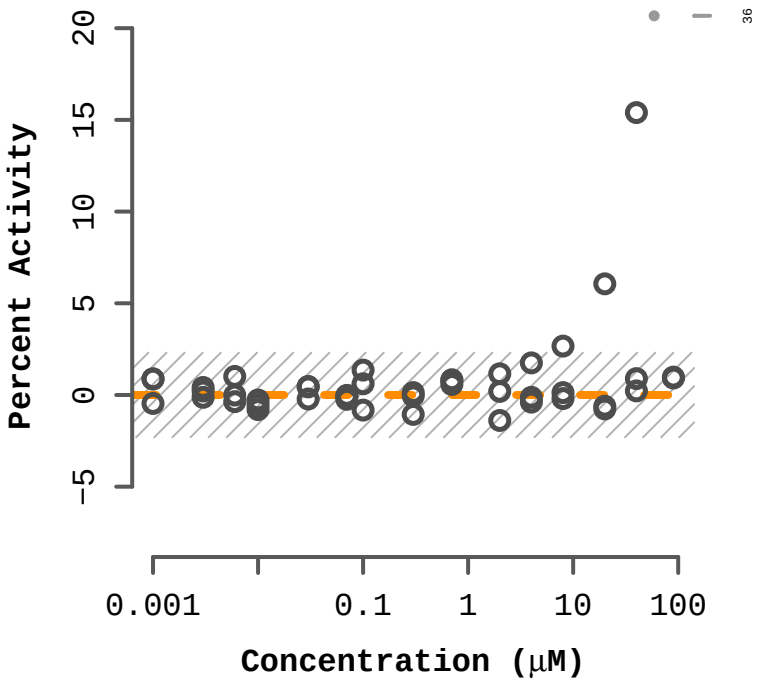
	tp	ga	gw
val:	0.682	-2.77	8
sd:	0.289	0.706	23.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.2	-1.89	3.7	-1.64	4.33
sd:	215	2.63	9.68	1.96	15.7

	CNST	HILL	GNLS
AIC:	226.23	226.03	222.21
PROB:	0.1	0.12	0.78
RMSE:	4.77	4.62	4.53

MAX_MEAN: 8.09 MAX_MED: 3.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

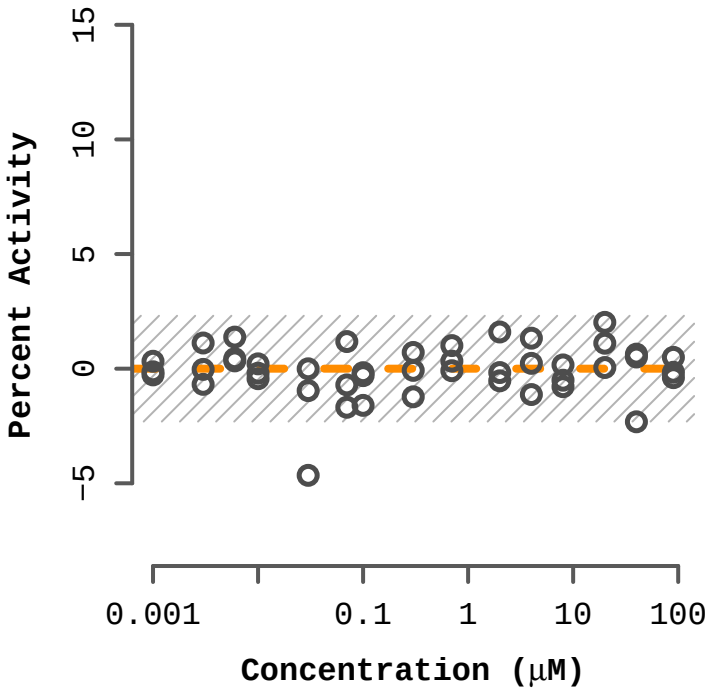
NAME: Succinic anhydride
CHID: 21287 CASRN: 108-30-5
SPID(S): Tox21_201179
M4ID: 12481073 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.4	NA	NA
PROB:	1	NA	NA
RMSE:	6.01	NA	NA

MAX_MEAN: 12.8 **MAX_MED:** 0.976 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

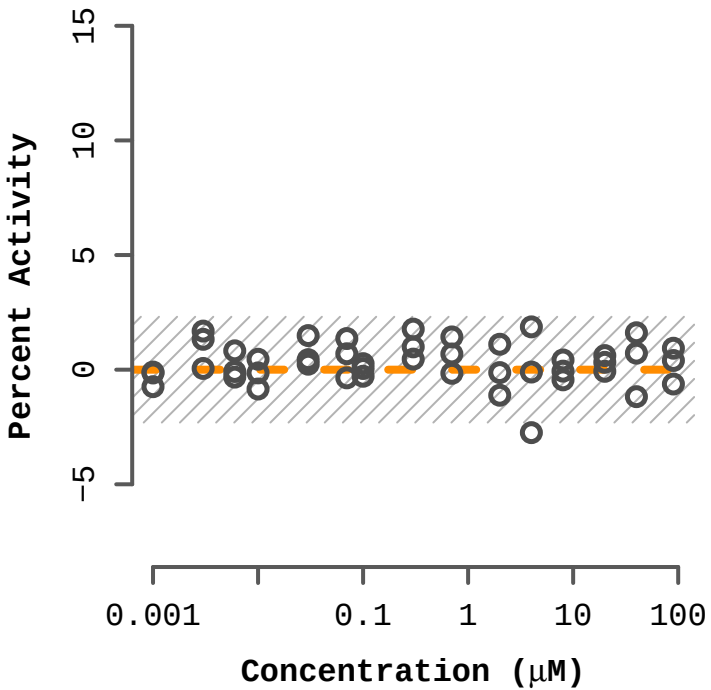
NAME: Sucrose
CHID: 21288 CASRN: 57-50-1
SPID(S): Tox21_300410
M4ID: 12478722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.06 MAX_MED: 1.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

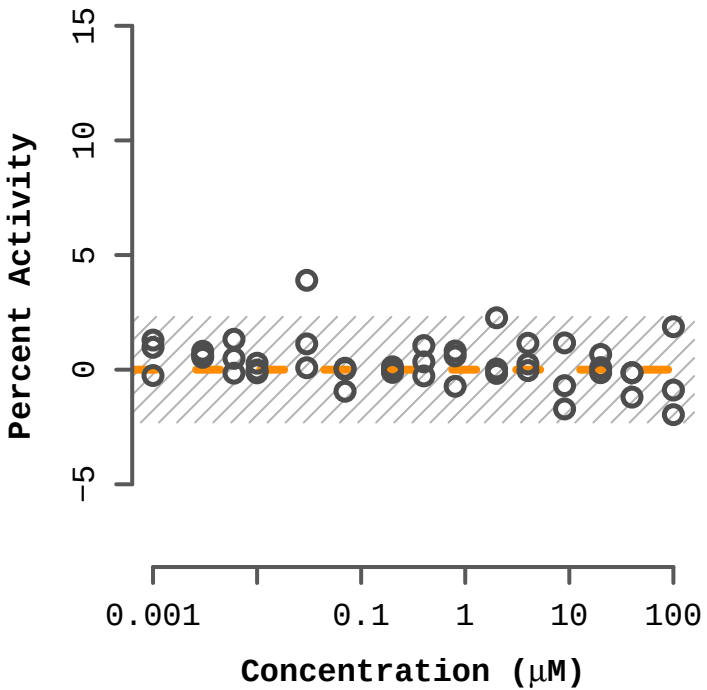
NAME: Sucrose
CHID: 21288 CASRN: 57-50-1
SPID(S): Tox21_201397
M4ID: 12480855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.08 MAX_MED: 1.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

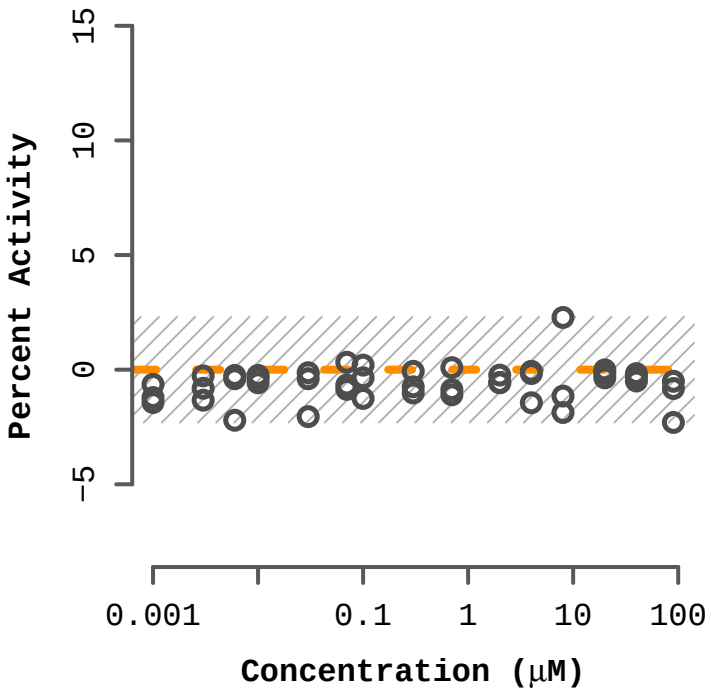
NAME: Sulfallate
CHID: 21289 **CASRN:** 95-06-7
SPID(S): Tox21_200042
M4ID: 12482210

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

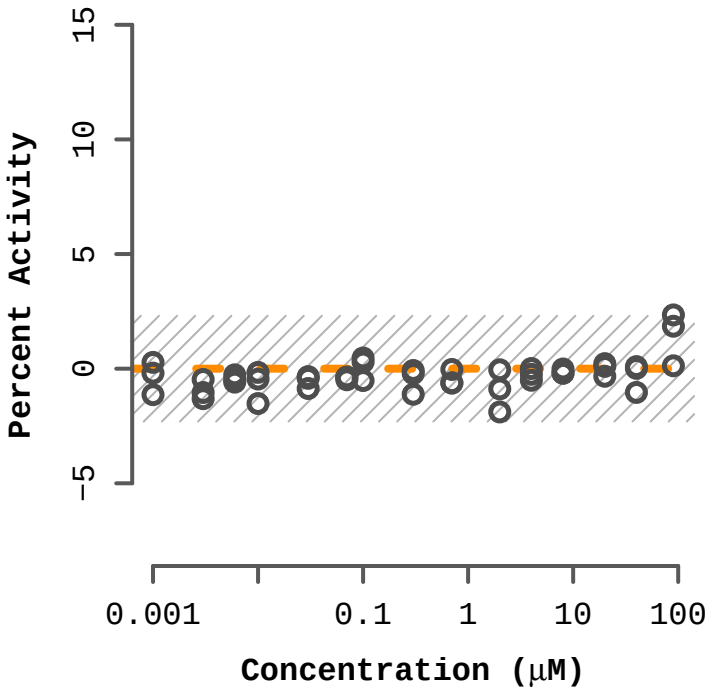
NAME: Sulfamethazine
CHID: 21290 **CASRN:** 57-68-1
SPID(S): Tox21_303006
M4ID: 12476127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: −0.173 **MAX_MED:** −0.156 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

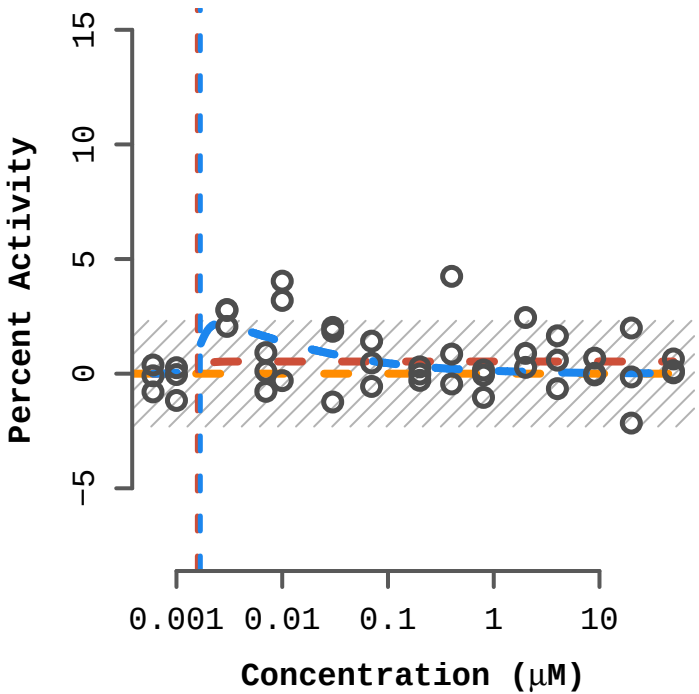
NAME: Sulfamethazine
CHID: 21290 **CASRN:** 57-68-1
SPID(S): Tox21_202221
M4ID: 12480031

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfamethazine
CHID: 21290 CASRN: 57-68-1
SPID(S): Tox21_110847_1
M4ID: 12484072

HILL MODEL (in red):

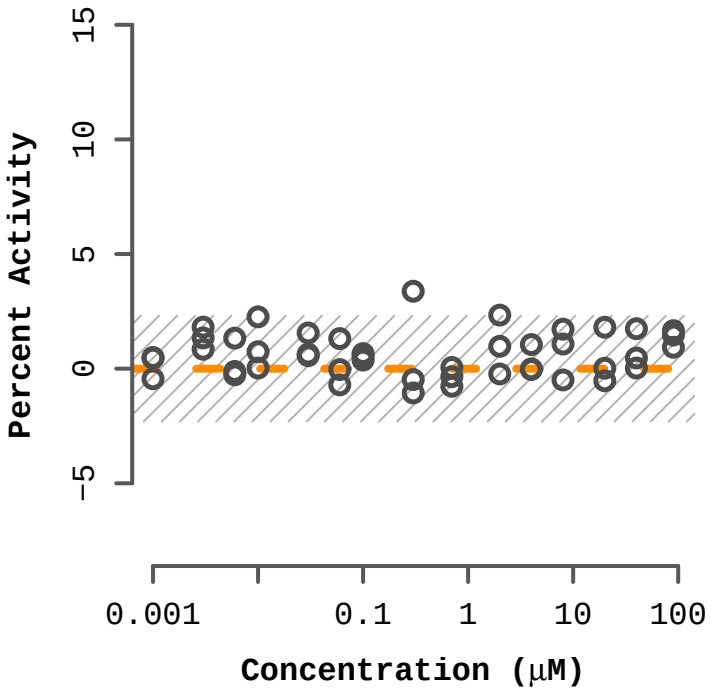
	tp	ga	gw
val:	0.53	−2.8	8
sd:	0.207	0.377	12.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.32	−2.77	8	−2.52	0.607
sd:	6.24	0.197	6.53	1.89	0.388

	CNST	HILL	GNLS
AIC:	162.54	161.69	158.25
PROB:	0.09	0.14	0.77
RMSE:	1.5	1.35	1.26

MAX_MEAN: 2.54 **MAX_MED:** 3.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

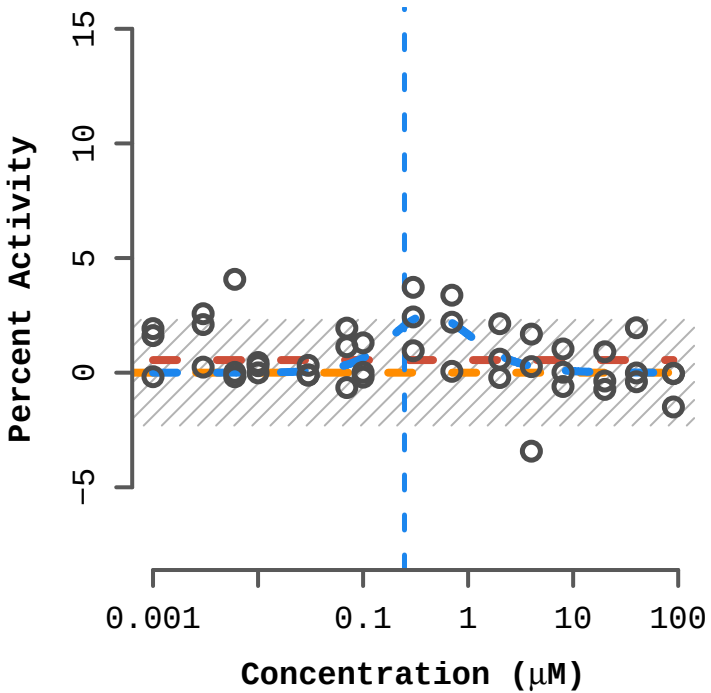
NAME: Sodium sulfate anyhdrous
CHID: 21291 **CASRN:** 7757-82-6
SPID(S): Tox21_201045
M4ID: 12481207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfisoxazole
CHID: 21292 **CASRN:** 127-69-5
SPID(S): Tox21_302851
M4ID: 12476282

HILL MODEL (in red):

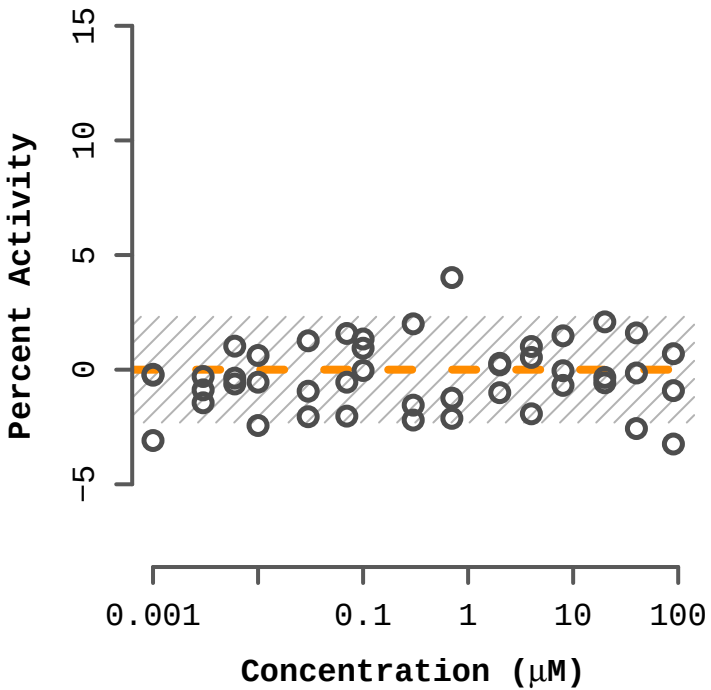
	tp	ga	gw
val:	0.55	−5	3.29
sd:	0.194	822	1340

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.89	−0.606	2.02	−0.155	1.6
sd:	10.5	0.702	1.97	0.956	1.42

	CNST	HILL	GNLS
AIC:	166.55	164.24	160.31
PROB:	0.04	0.12	0.84
RMSE:	1.55	1.39	1.31

MAX_MEAN: 2.37 **MAX_MED:** 2.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

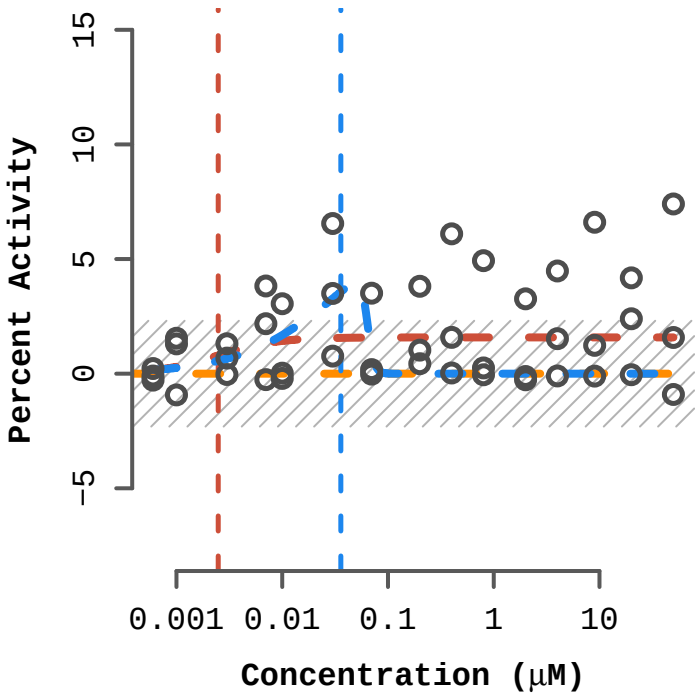
NAME: Sulfisoxazole
CHID: 21292 **CASRN:** 127-69-5
SPID(S): Tox21_202265
M4ID: 12479987

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 0.747 **MAX_MED:** 0.937 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfisoxazole
CHID: 21292 CASRN: 127-69-5
SPID(S): Tox21_110409_1
M4ID: 12484384

HILL MODEL (in red):

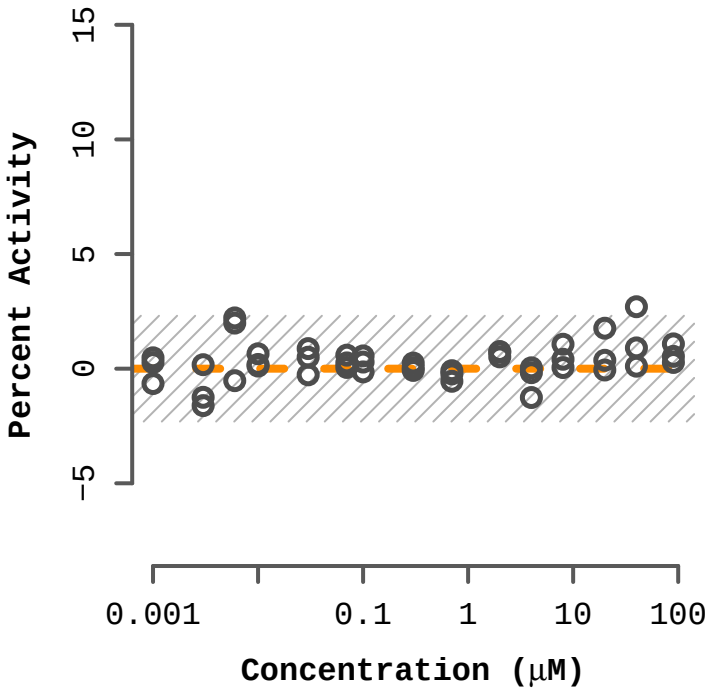
	tp	ga	gw
val:	1.58	−2.61	1.6
sd:	0.406	0.56	2.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.14	−1.45	0.923	−1.2	14.1
sd:	17.5	2.03	0.862	1.8	618

	CNST	HILL	GNLS
AIC:	217.07	203.67	218.01
PROB:	0	1	0
RMSE:	2.76	2.13	2.53

MAX_MEAN: 3.61 MAX_MED: 3.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

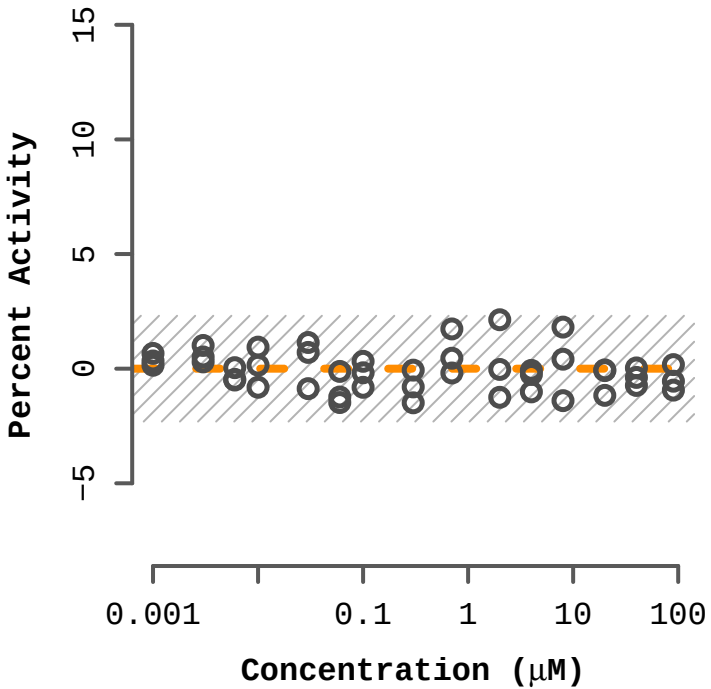
NAME: 3-Sulfolene
CHID: 21294 **CASRN:** 77-79-2
SPID(S): Tox21_302817
M4ID: 12476316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

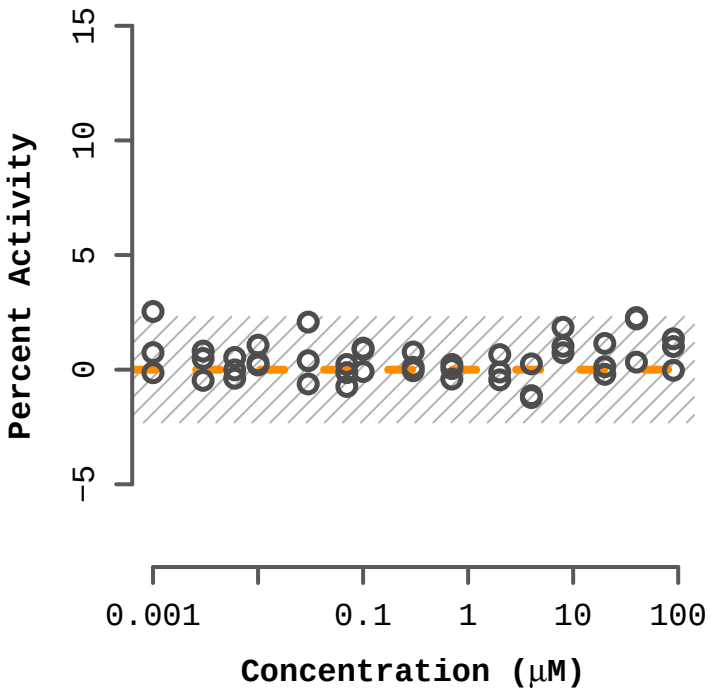
NAME: 3-Sulfolene
CHID: 21294 CASRN: 77-79-2
SPID(S): Tox21_201532
M4ID: 12480720

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.668 MAX_MED: 0.711 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

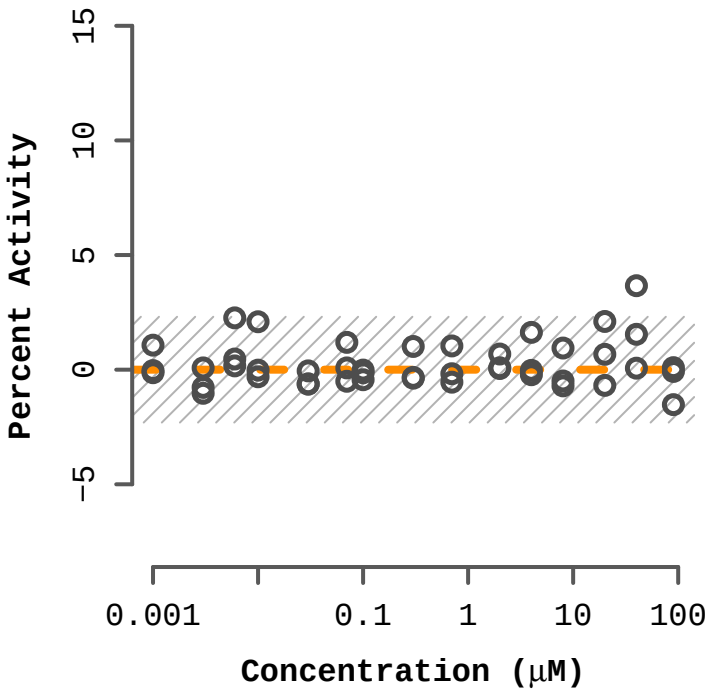
NAME: Suxibuzone
CHID: 21296 **CASRN:** 27470-51-5
SPID(S): Tox21_302778
M4ID: 12476355

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

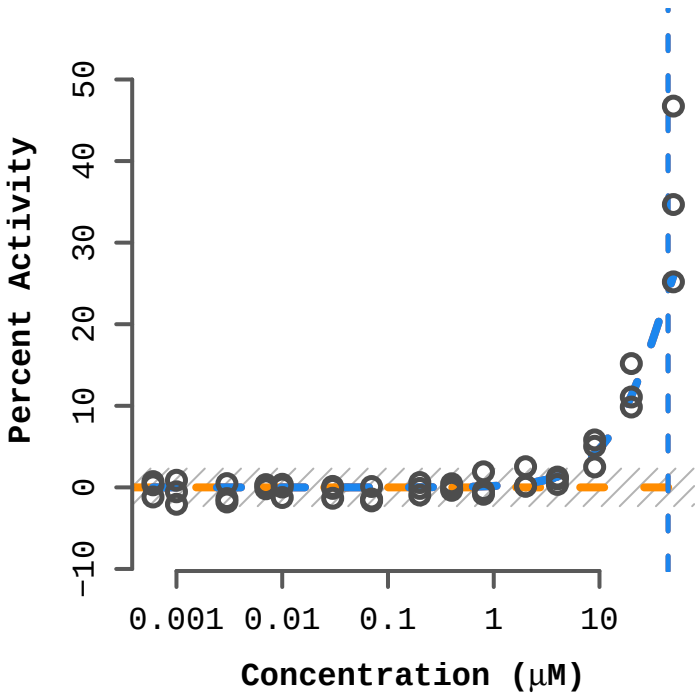
NAME: Suxibuzone
CHID: 21296 **CASRN:** 27470-51-5
SPID(S): Tox21_202352
M4ID: 12479900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Suxibuzone
CHID: 21296 **CASRN:** 27470-51-5
SPID(S): Tox21_110615_1
M4ID: 12484230

HILL MODEL (in red):

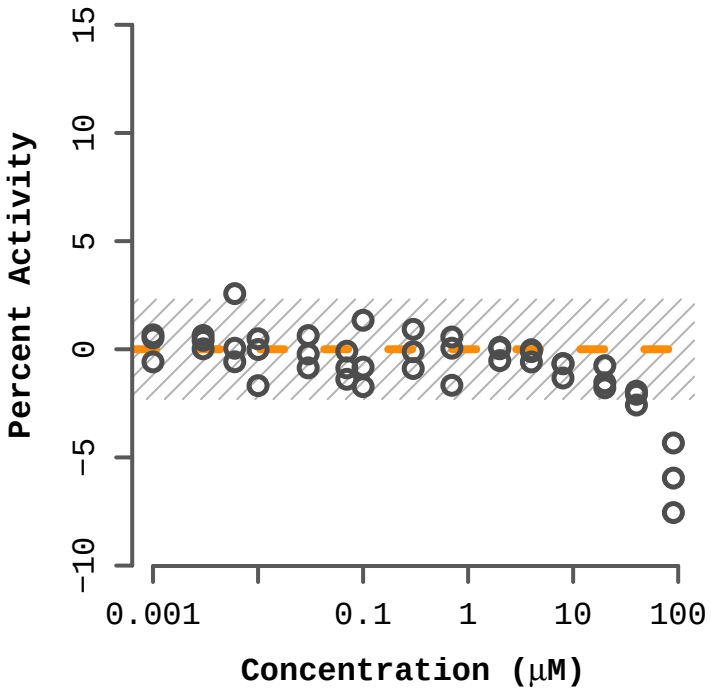
	tp	ga	gw
val:	47.8	1.65	1.48
sd:	24	0.296	0.348

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	47.8	1.65	1.48	3.4	4.17
sd:	24	0.296	0.348	1290	3240

	CNST	HILL	GNLS
AIC:	274.28	183.35	187.35
PROB:	0	0.88	0.12
RMSE:	10.08	3.55	3.55

MAX_MEAN: 35.5 **MAX_MED:** 34.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

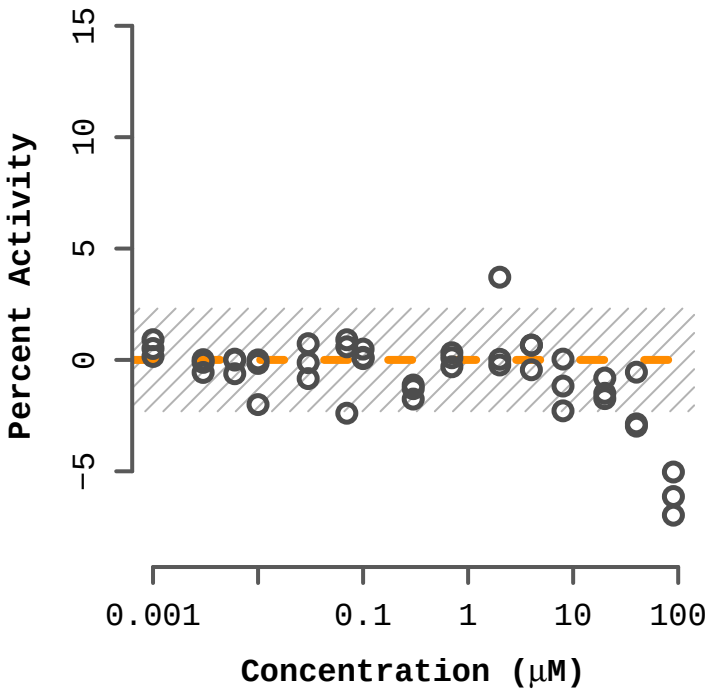
NAME: Chlorotrianisene
CHID: 21299 **CASRN:** 569-57-3
SPID(S): Tox21_302897
M4ID: 12476236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.683 **MAX_MED:** 0.527 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

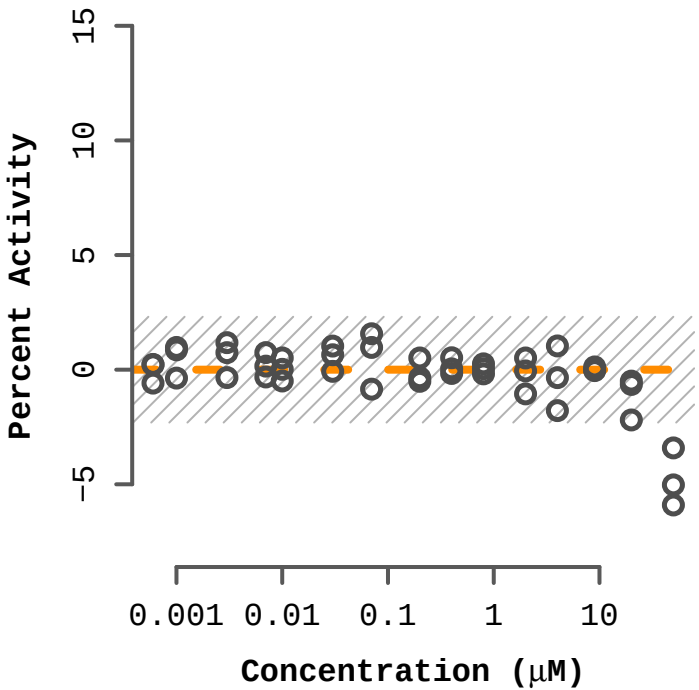
NAME: Chlorotrianisene
CHID: 21299 **CASRN:** 569-57-3
SPID(S): Tox21_202361
M4ID: 12479891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.661 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

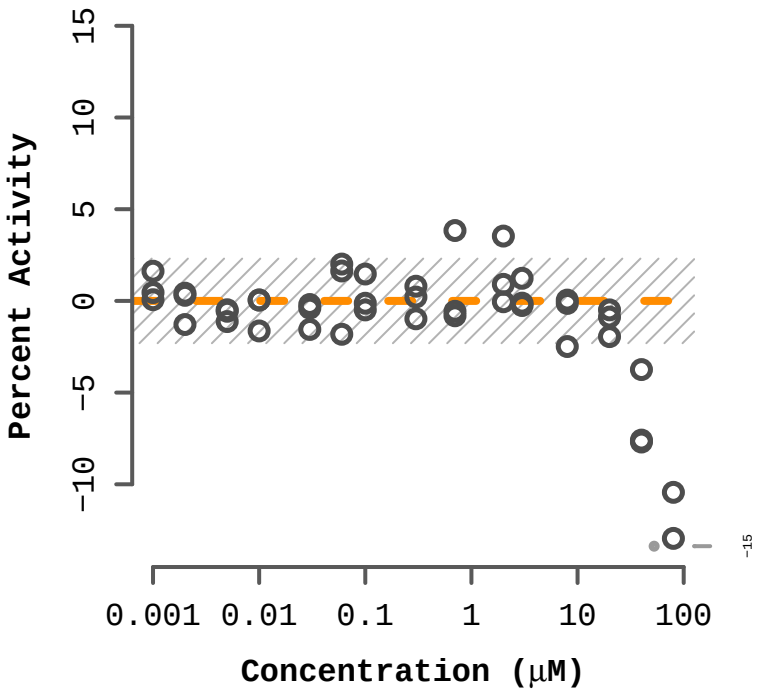
NAME: Chlorotrianisene
CHID: 21299 **CASRN:** 569-57-3
SPID(S): Tox21_110466_1
M4ID: 12484334

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 0.563 **MAX_MED:** 0.971 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

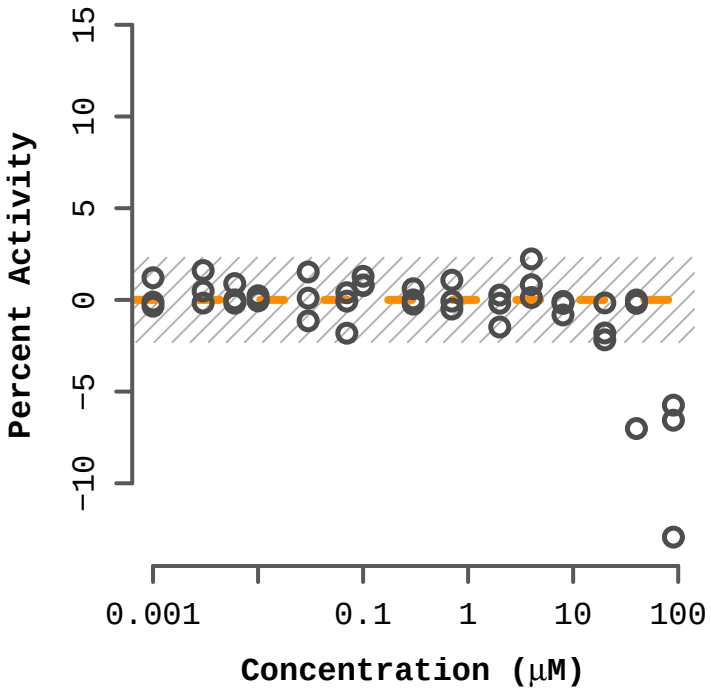
NAME: Tamoxifen citrate
CHID: 21301 CASRN: 54965-24-1
SPID(S): Tox21_300274
M4ID: 12478856 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	223.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.92	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

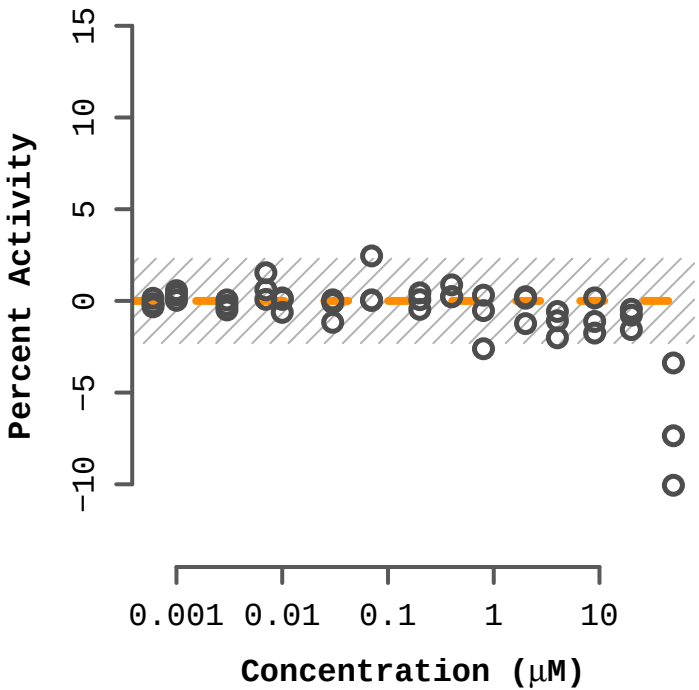
NAME: Tamoxifen citrate
CHID: 21301 **CASRN:** 54965-24-1
SPID(S): Tox21_202070
M4ID: 12480182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.18	NA	NA
PROB:	1	NA	NA
RMSE:	2.69	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.831 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

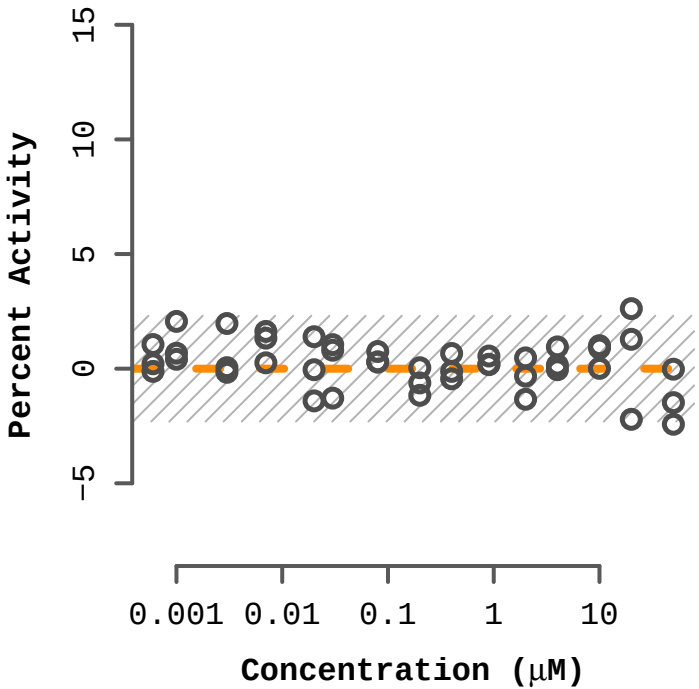
NAME: Tamoxifen citrate
CHID: 21301 CASRN: 54965-24-1
SPID(S): Tox21_110938_1
M4ID: 12484000

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.11	NA	NA

MAX_MEAN: 0.847 **MAX_MED:** 0.609 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

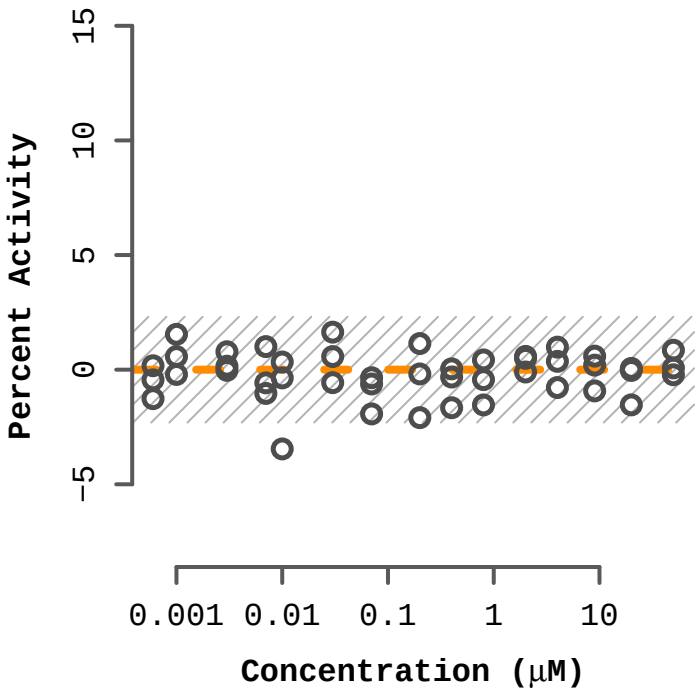
NAME: l−Taurine
CHID: 21304 **CASRN:** 107−35−7
SPID(S): Tox21_202520
M4ID: 12479732

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

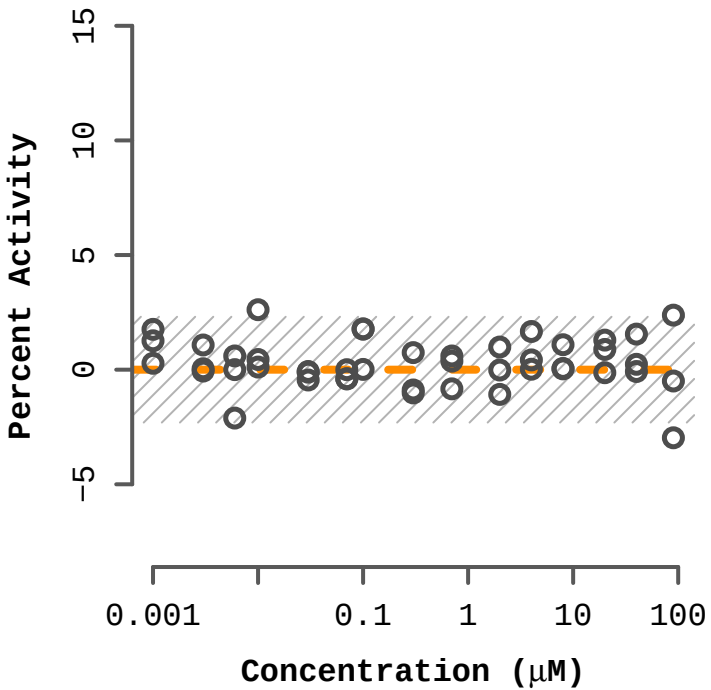
NAME: l-Taurine
CHID: 21304 **CASRN:** 107-35-7
SPID(S): Tox21_110277_1
M4ID: 12484490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.01	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.637 **MAX_MED:** 0.574 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

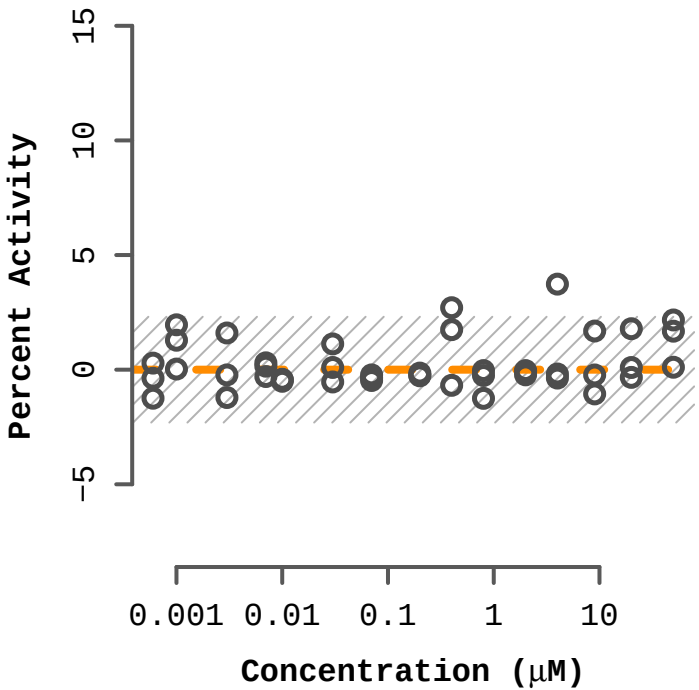
NAME: Tegafur
CHID: 21305 CASRN: 37076-68-9
SPID(S): Tox21_301812
M4ID: 12477321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.19 MAX_MED: 1.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

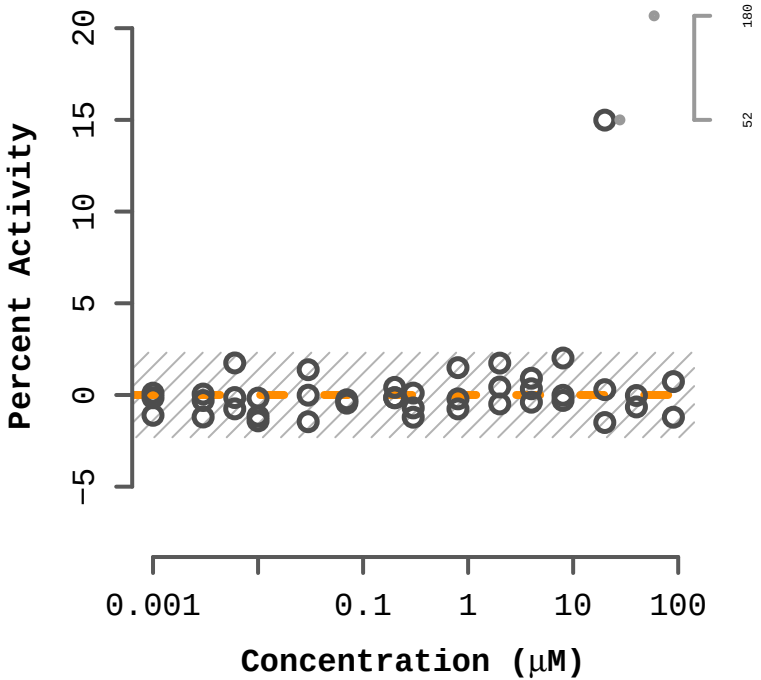
NAME: Tegafur
CHID: 21305 CASRN: 37076-68-9
SPID(S): Tox21_111649_1
M4ID: 12483559

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.32 MAX_MED: 1.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

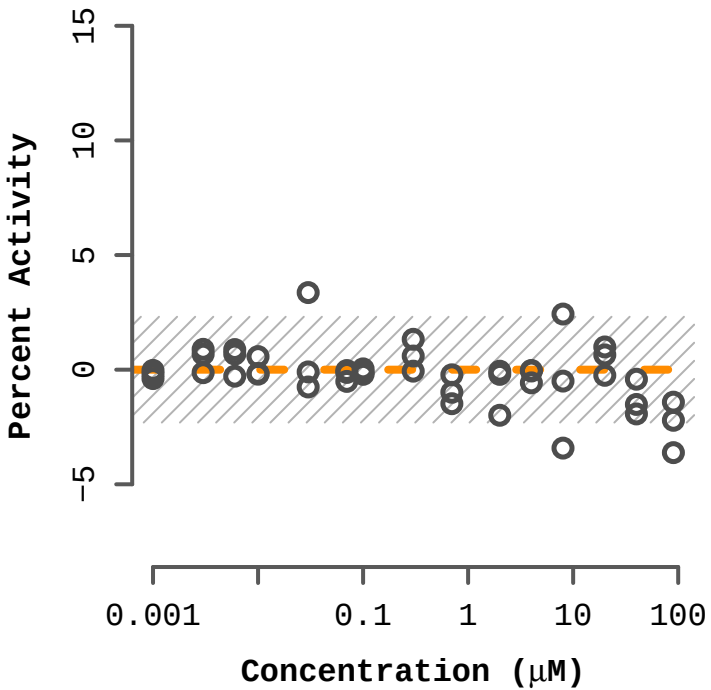
NAME: Temazepam
CHID: 21309 **CASRN:** 846-50-4
SPID(S): Tox21_200044
M4ID: 12482208 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.22	NA	NA
PROB:	1	NA	NA
RMSE:	28.39	NA	NA

MAX_MEAN: 60.7 **MAX_MED:** 0.732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

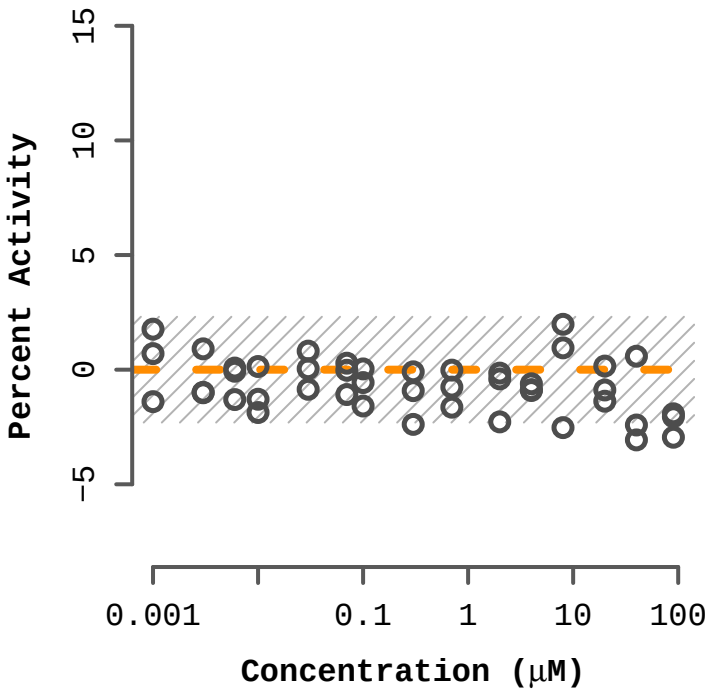
NAME: 2,4,6-Tris(tert-butyl)phenol
CHID: 21311 **CASRN:** 732-26-3
SPID(S): Tox21_300121
M4ID: 12479009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.838 **MAX_MED:** 0.683 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

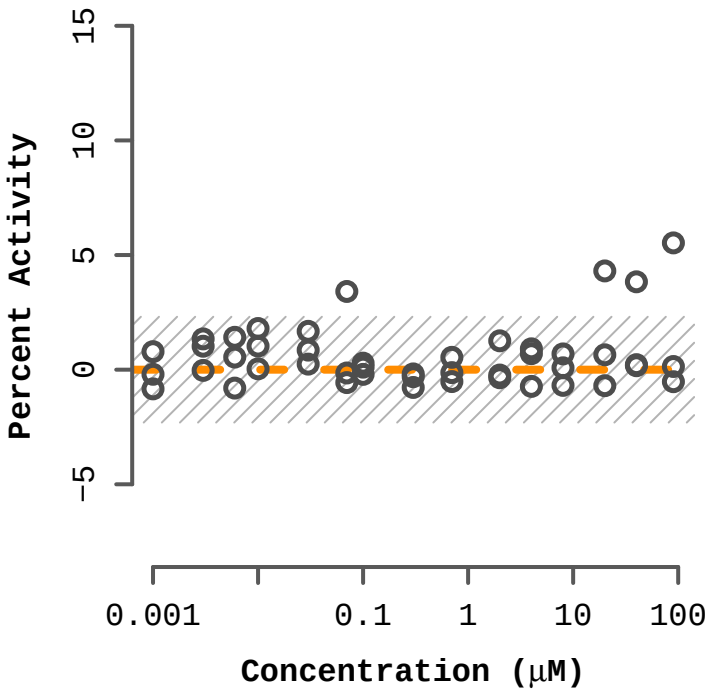
NAME: 2,4,6-Tris(tert-butyl)phenol
CHID: 21311 **CASRN:** 732-26-3
SPID(S): Tox21_202374
M4ID: 12479878

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.359 **MAX_MED:** 0.953 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3',4,4'−Tetraaminobiphenyl tetrahydrochlorid

CHID: 21312 **CASRN:** 7411−49−6

SPID(S): Tox21_202598

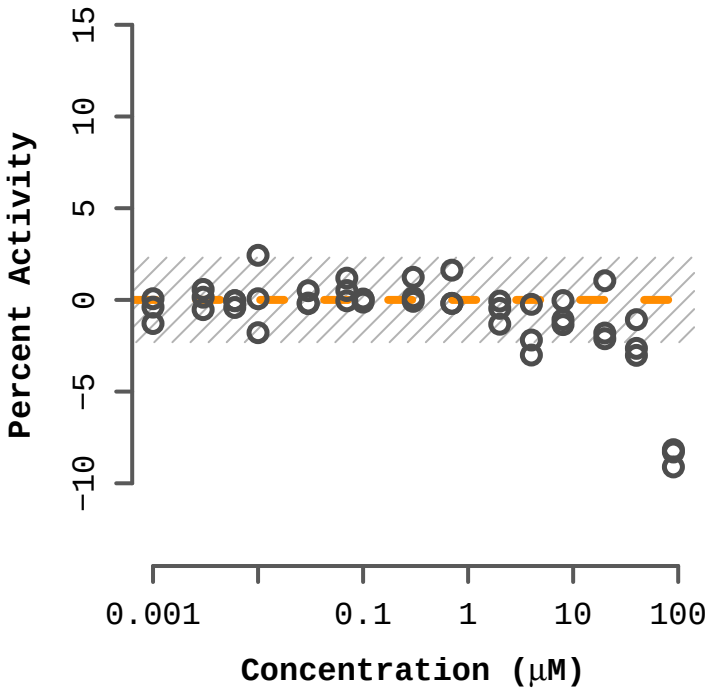
M4ID: 12479654

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

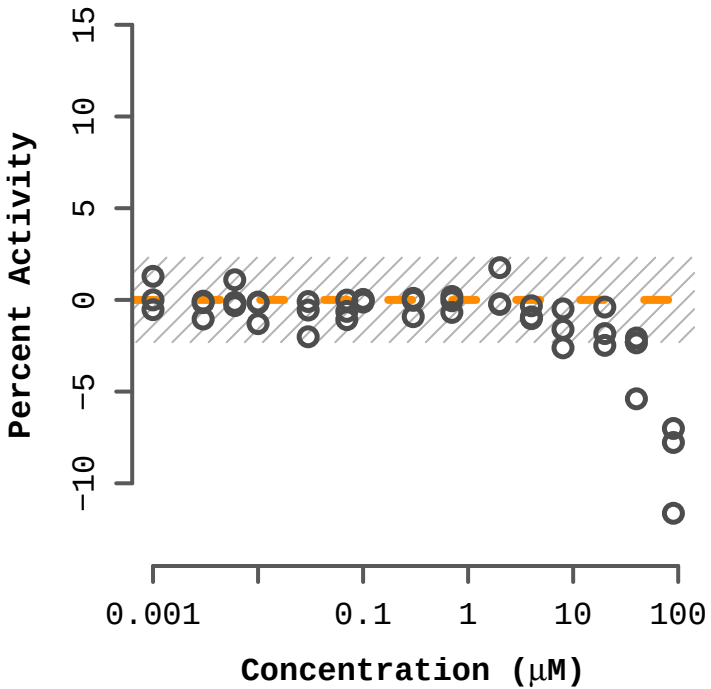
NAME: 2,2',5,5'-Tetrachlorobenzidine
CHID: 21314 **CASRN:** 15721-02-5
SPID(S): Tox21_302911
M4ID: 12476222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.57	NA	NA
PROB:	1	NA	NA
RMSE:	2.5	NA	NA

MAX_MEAN: 0.551 **MAX_MED:** 0.512 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

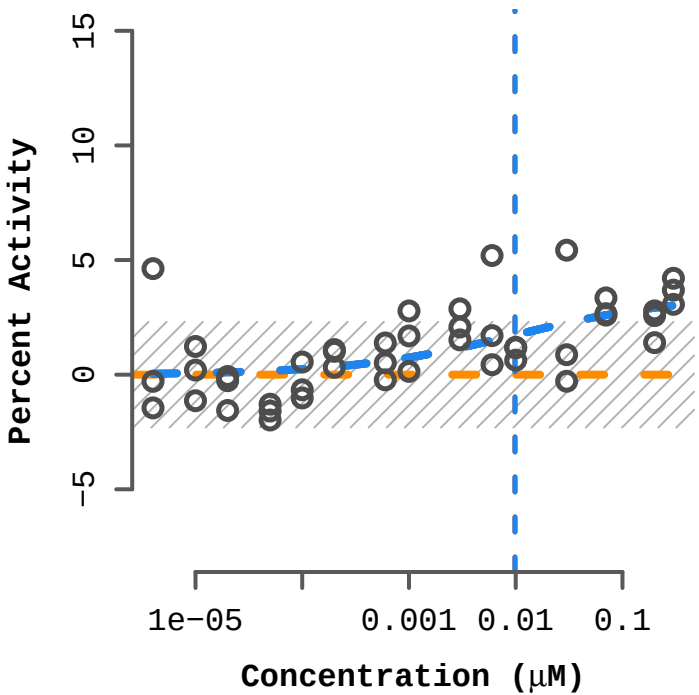
NAME: 2,2',5,5'-Tetrachlorobenzidine
CHID: 21314 **CASRN:** 15721-02-5
SPID(S): Tox21_202027
M4ID: 12480225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 0.437 **MAX_MED:** 0.00147 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,7,8−Tetrachlorodibenzo−p−dioxin
CHID: 21315 CASRN: 1746−01−6
SPID(S): Tox21_202792
M4ID: 12479460

HILL MODEL (in red):

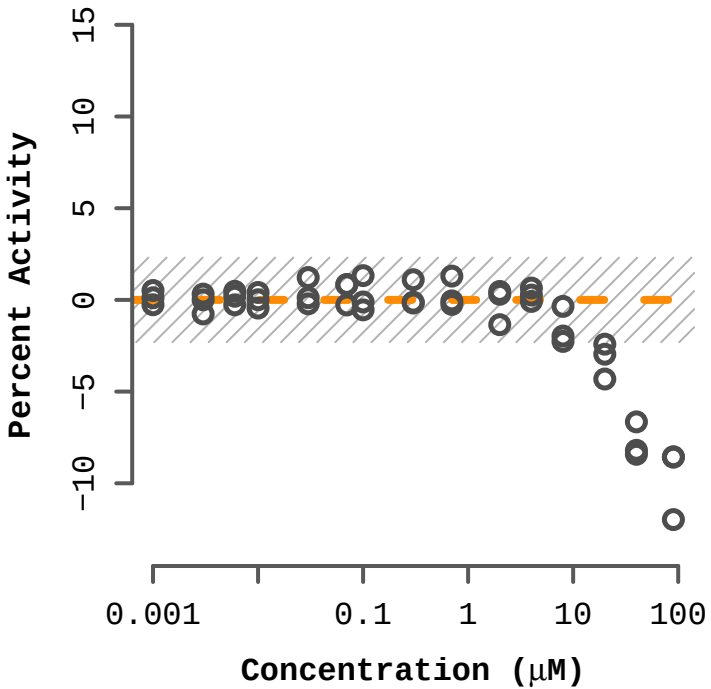
	tp	ga	gw
val:	3.46	−2.01	0.562
sd:	1.58	1.12	0.298

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.46	−2.01	0.562	0.923	6
sd:	1.58	1.12	0.298	2330	9780

	CNST	HILL	GNLS
AIC:	201.26	165.36	169.36
PROB:	0	0.88	0.12
RMSE:	2.18	1.44	1.44

MAX_MEAN: 3.65 **MAX_MED:** 3.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

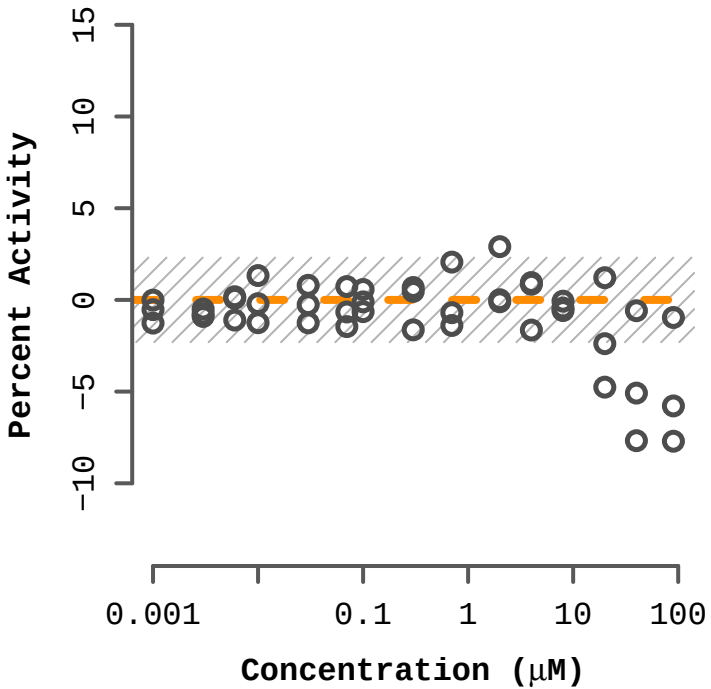
NAME: Tetradifon
CHID: 21316 **CASRN:** 116-29-0
SPID(S): Tox21_302766
M4ID: 12476367

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.6	NA	NA
PROB:	1	NA	NA
RMSE:	3.42	NA	NA

MAX_MEAN: 0.466 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

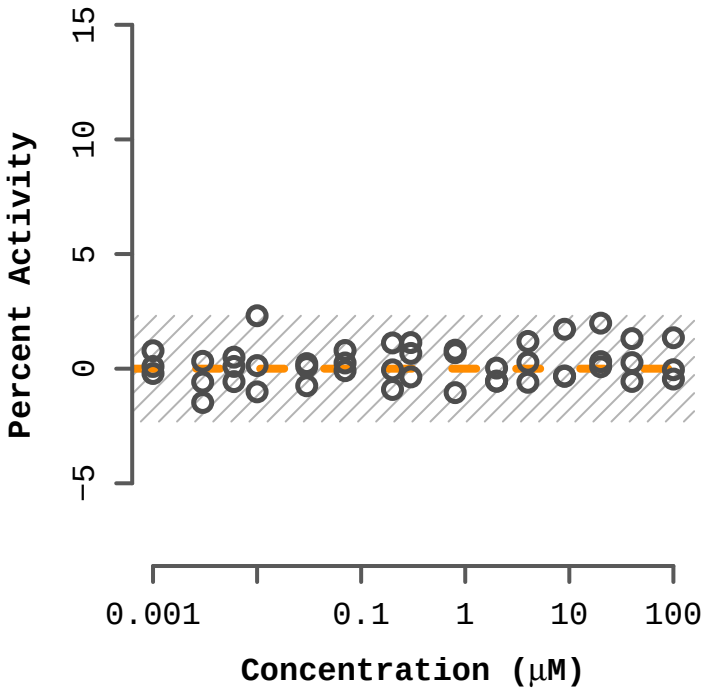
NAME: Tetradifon
CHID: 21316 **CASRN:** 116-29-0
SPID(S): Tox21_202396
M4ID: 12479856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.76	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

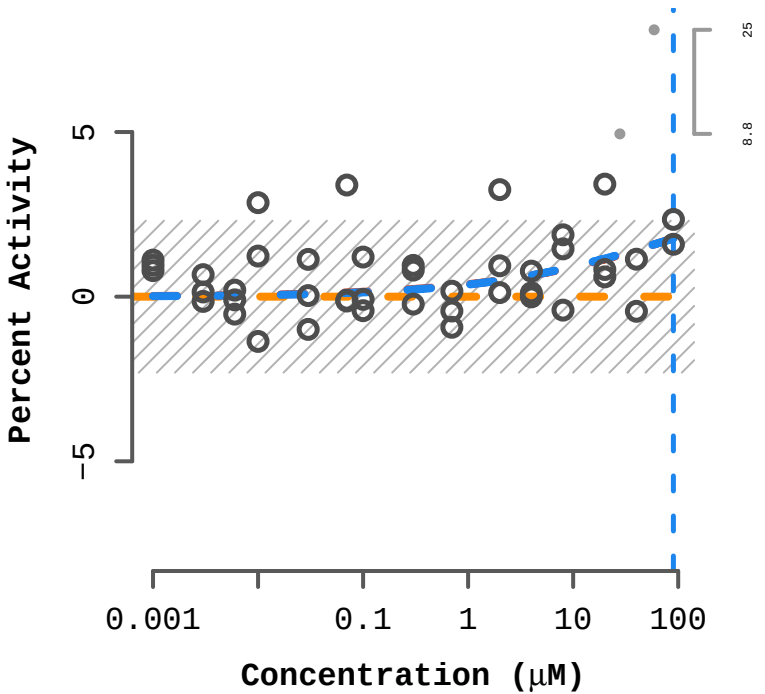
NAME: 1,1,1,2−Tetrachloroethane
CHID: 21317 CASRN: 630−20−6
SPID(S): Tox21_201109
M4ID: 12481143

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.794 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1,2,2−Tetrachloroethane
CHID: 21318 CASRN: 79−34−5
SPID(S): Tox21_200074
M4ID: 12482178 BRK

HILL MODEL (in red):

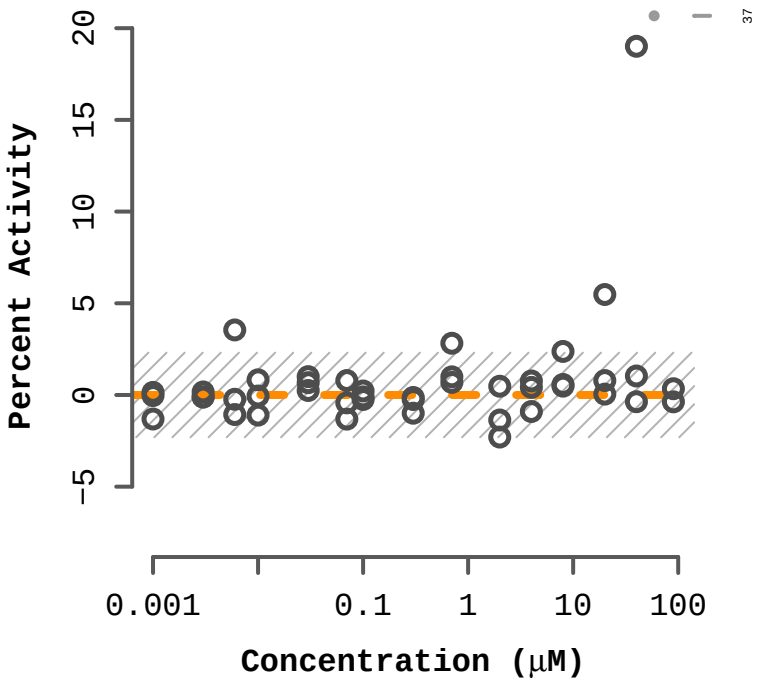
	tp	ga	gw
val:	4.71	2.45	0.432
sd:	10.6	3.83	0.371

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.53	1.95	0.479	2.53	13.2
sd:	6.41	3.05	0.448	529	12000

	CNST	HILL	GNLS
AIC:	187.52	179.9	183.99
PROB:	0.02	0.87	0.11
RMSE:	4.21	3.85	3.85

MAX_MEAN: 9.78 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

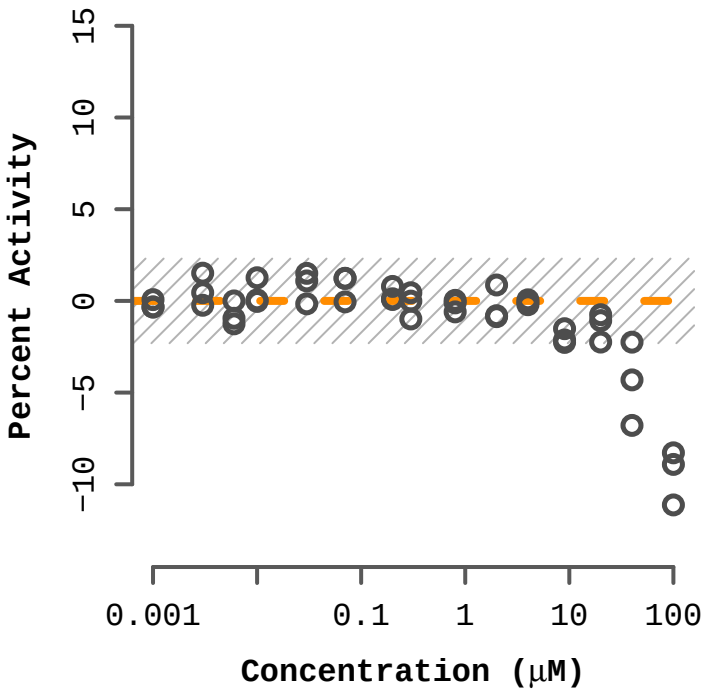
NAME: Tetrachloroethylene
CHID: 21319 CASRN: 127-18-4
SPID(S): Tox21_201196
M4ID: 12481056 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.86	NA	NA
PROB:	1	NA	NA
RMSE:	6.38	NA	NA

MAX_MEAN: 12.4 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

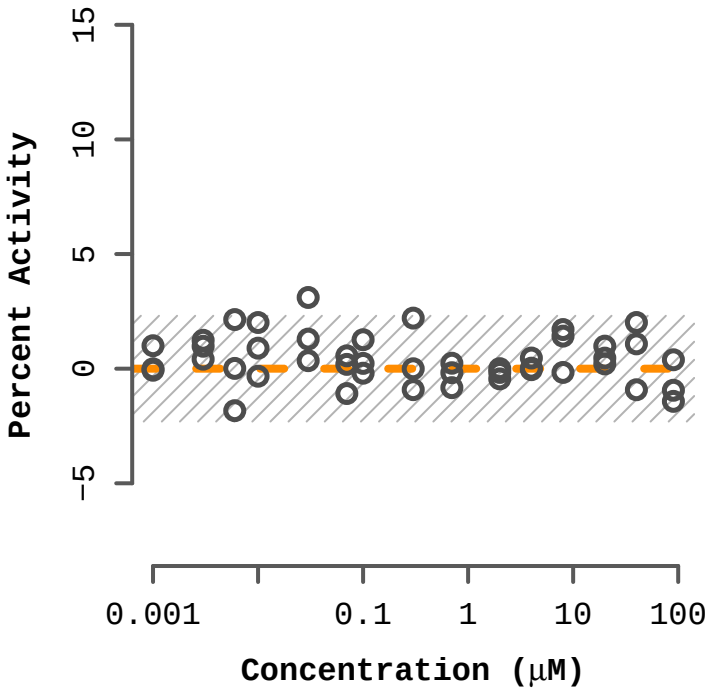
NAME: Tetrachlorovinphos
CHID: 21320 **CASRN:** 961-11-5
SPID(S): Tox21_200092
M4ID: 12482160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.9	NA	NA

MAX_MEAN: 0.812 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

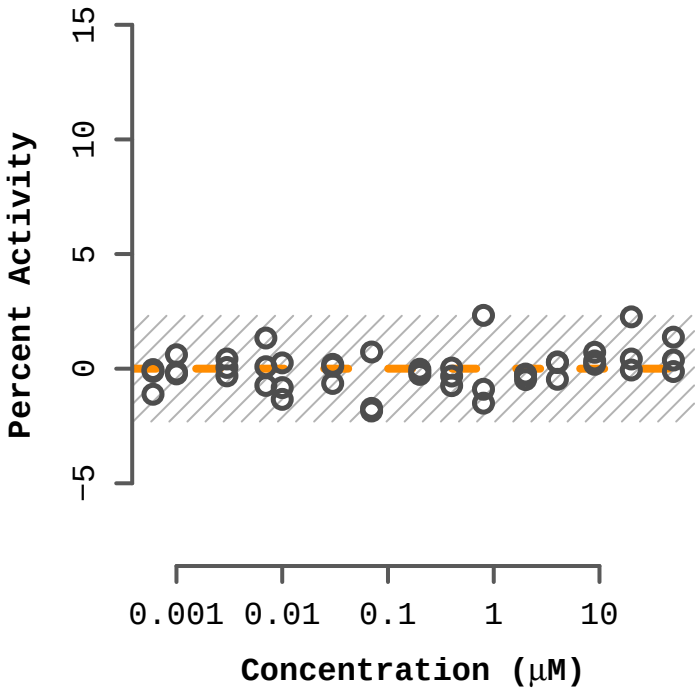
NAME: Tetracycline hydrochloride
CHID: 21321 CASRN: 64-75-5
SPID(S): Tox21_200516
M4ID: 12481736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

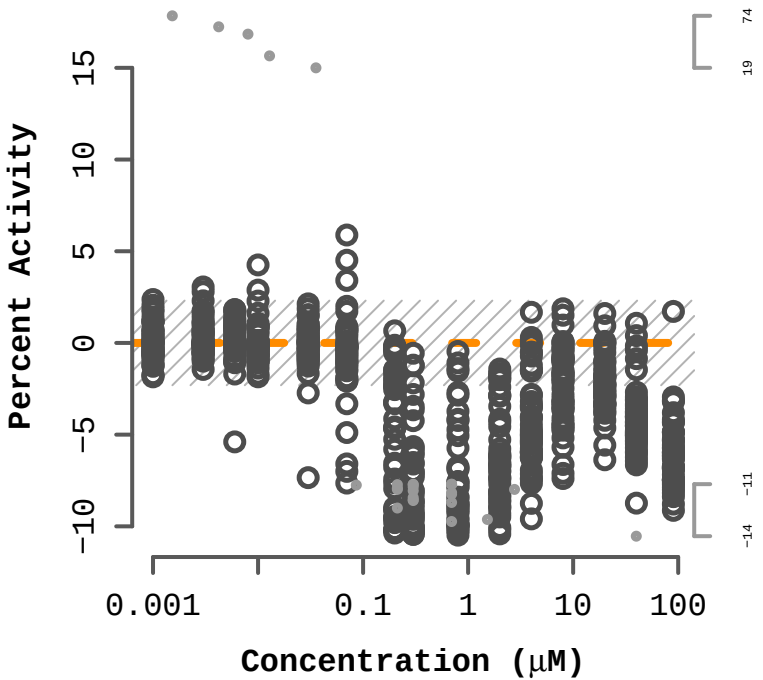
NAME: Tetracycline hydrochloride
CHID: 21321 CASRN: 64-75-5
SPID(S): Tox21_110355_1
M4ID: 12484430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 0.423 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

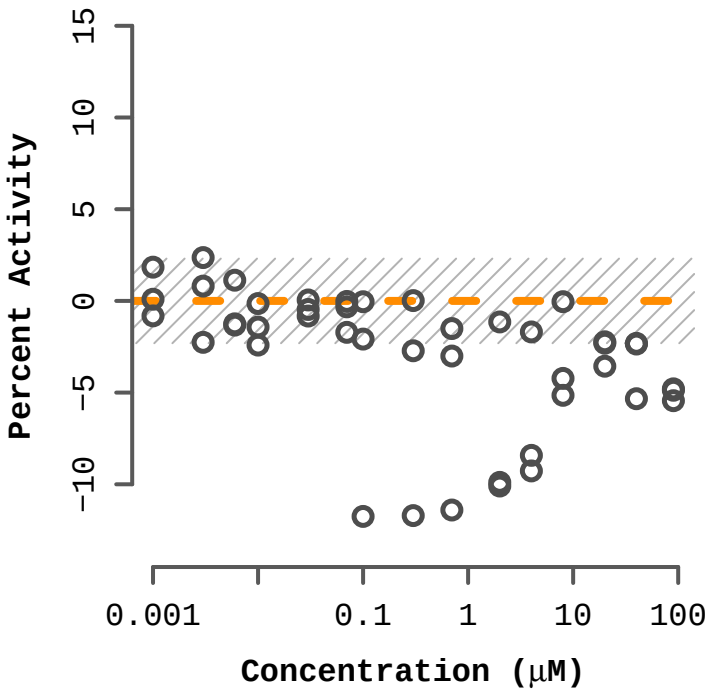
NAME: Disulfiram
CHID: 21322 **CASRN:** 97-77-8
SPID(S): Tox21_400072
M4ID: 12475065 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	4411.15	NA	NA
PROB:	1	NA	NA
RMSE:	6.52	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 0.0471 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

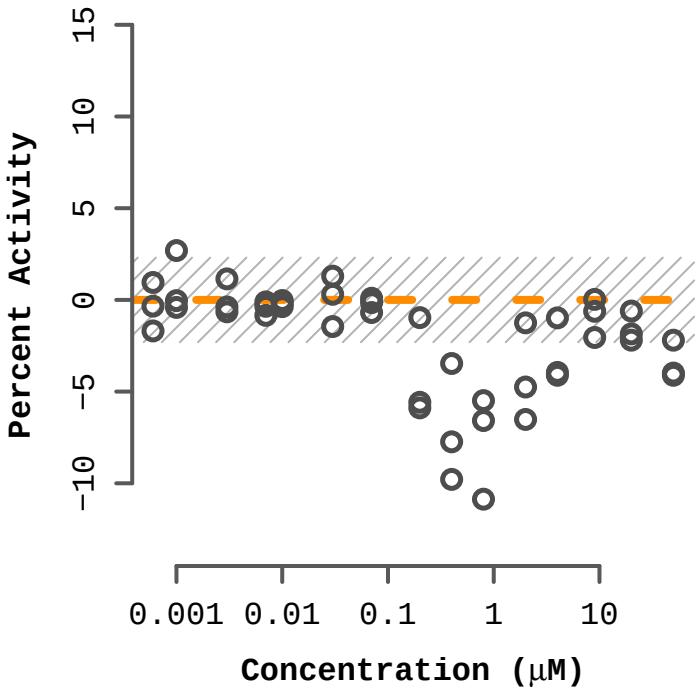
NAME: Disulfiram
CHID: 21322 **CASRN:** 97-77-8
SPID(S): Tox21_300403
M4ID: 12478729

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.55	NA	NA
PROB:	1	NA	NA
RMSE:	4.72	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

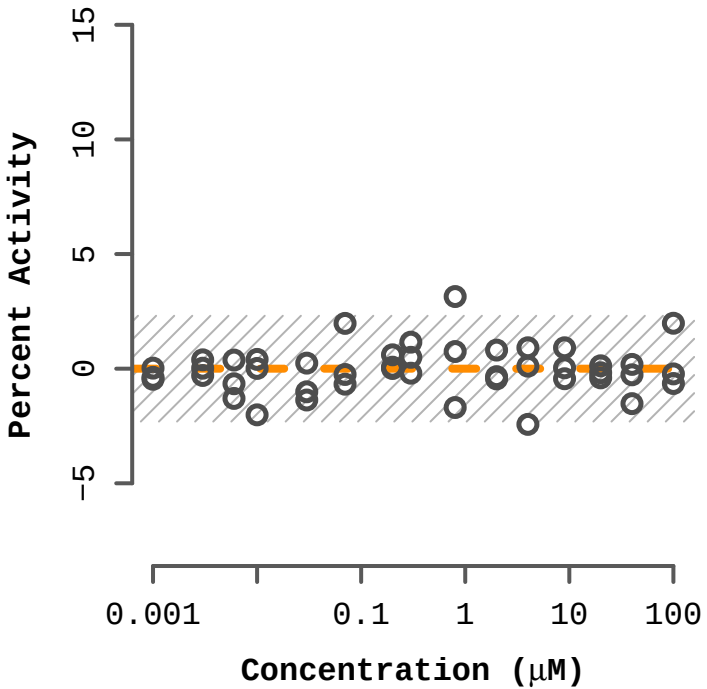
NAME: Disulfiram
CHID: 21322 **CASRN:** 97-77-8
SPID(S): Tox21_110280_1
M4ID: 12484488

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	240.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 0.749 **MAX_MED:** 0.307 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

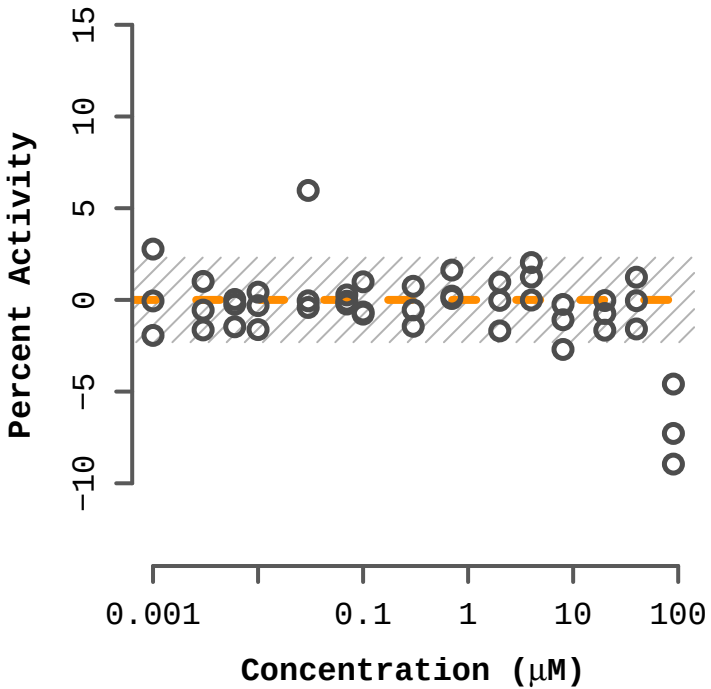
NAME: Tetrahydrofuran
CHID: 21328 **CASRN:** 109-99-9
SPID(S): Tox21_201026
M4ID: 12481226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.735 **MAX_MED:** 0.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

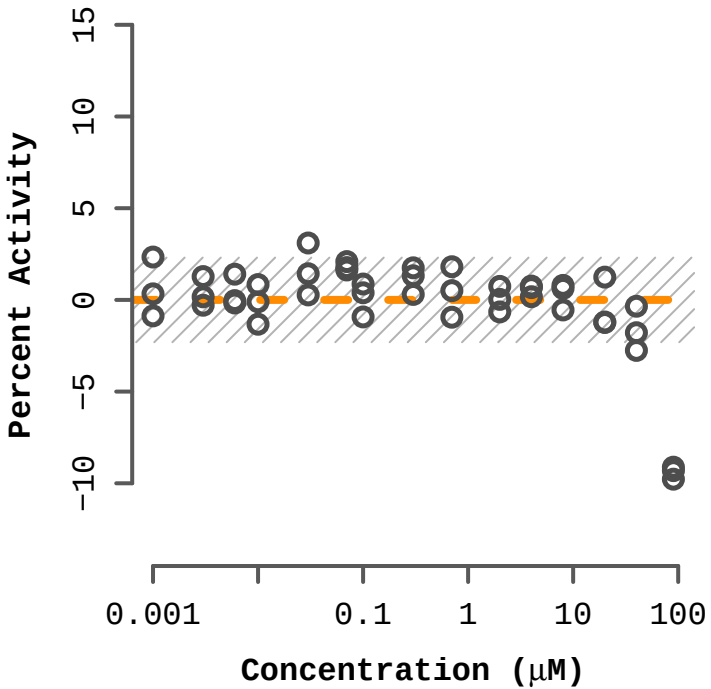
NAME: Tetrakis(hydroxymethyl)phosphonium chloride
CHID: 21330 **CASRN:** 124-64-1
SPID(S): Tox21_302070
M4ID: 12477063

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.33	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

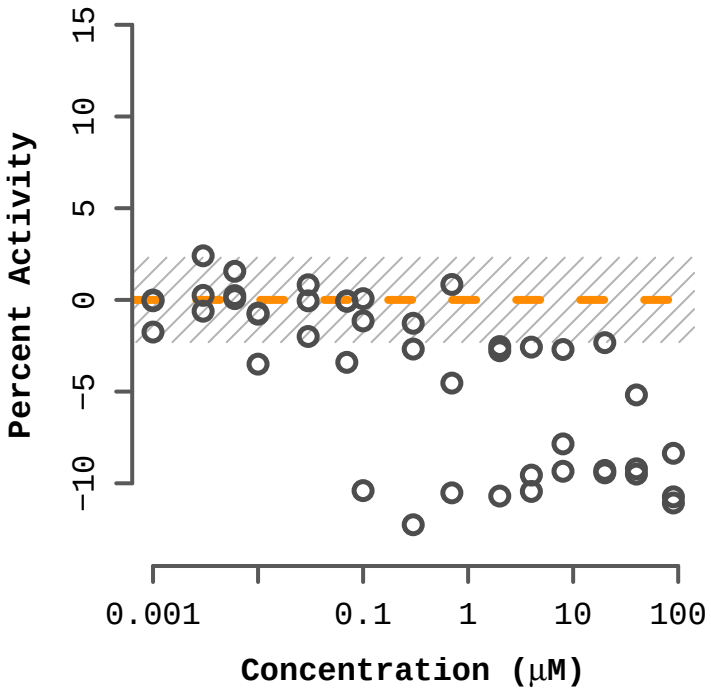
NAME: Tetrakis(hydroxymethyl)phosphonium sulfate
CHID: 21331 **CASRN:** 55566-30-8
SPID(S): Tox21_200928
M4ID: 12481324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

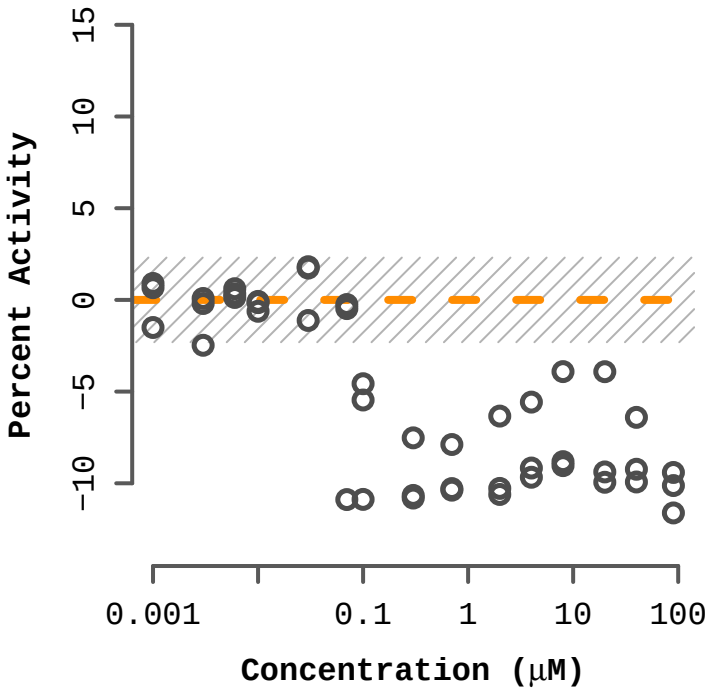
NAME: Thiram
CHID: 21332 **CASRN:** 137-26-8
SPID(S): Tox21_301102
M4ID: 12478031

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.61	NA	NA
PROB:	1	NA	NA
RMSE:	6.01	NA	NA

MAX_MEAN: 0.681 **MAX_MED:** 0.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

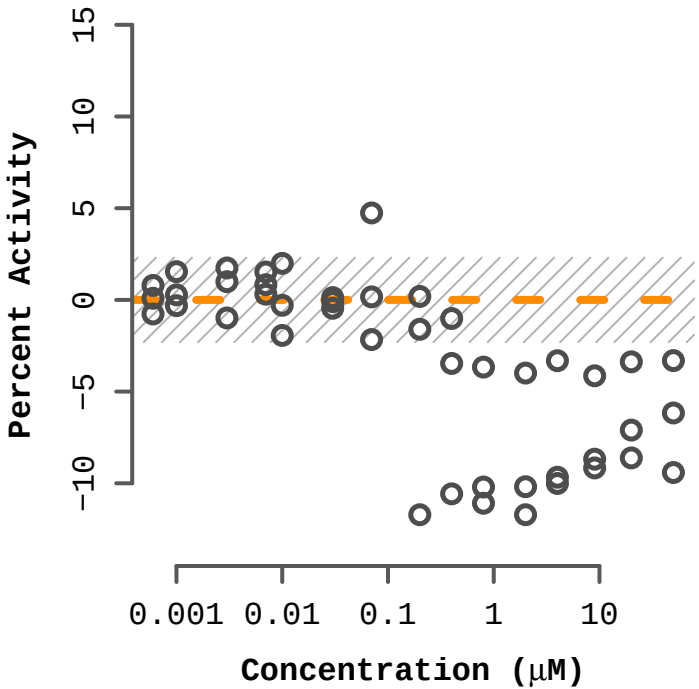
NAME: Thiram
CHID: 21332 CASRN: 137-26-8
SPID(S): Tox21_201569
M4ID: 12480683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	312.1	NA	NA
PROB:	1	NA	NA
RMSE:	7.09	NA	NA

MAX_MEAN: 0.809 MAX_MED: 1.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

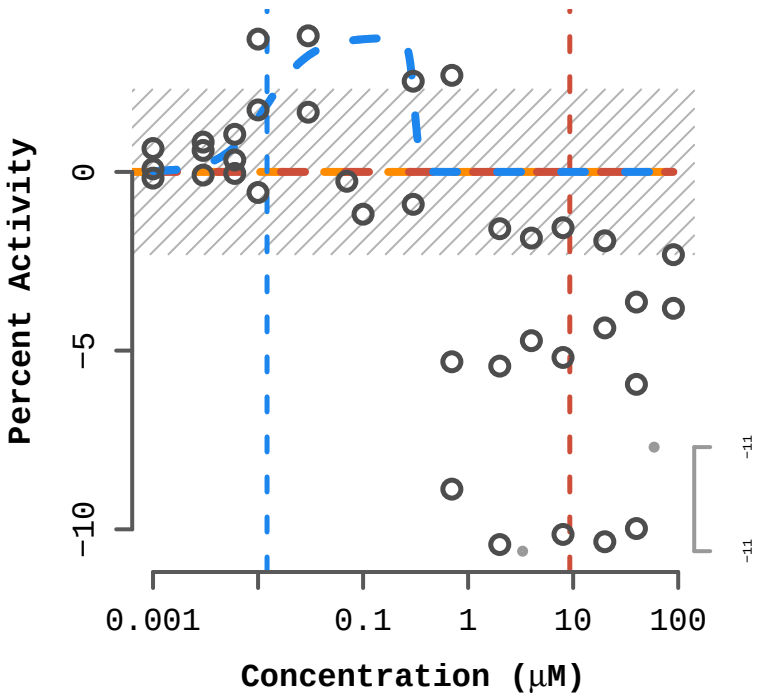
NAME: Thiram
CHID: 21332 **CASRN:** 137-26-8
SPID(S): Tox21_111150_1
M4ID: 12483877

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.91	NA	NA
PROB:	1	NA	NA
RMSE:	5.7	NA	NA

MAX_MEAN: 0.917 **MAX_MED:** 0.995 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetramethylthiuram monosulfide
CHID: 21333 CASRN: 97-74-5
SPID(S): Tox21_302880
M4ID: 12476253 BRK

HILL MODEL (in red):

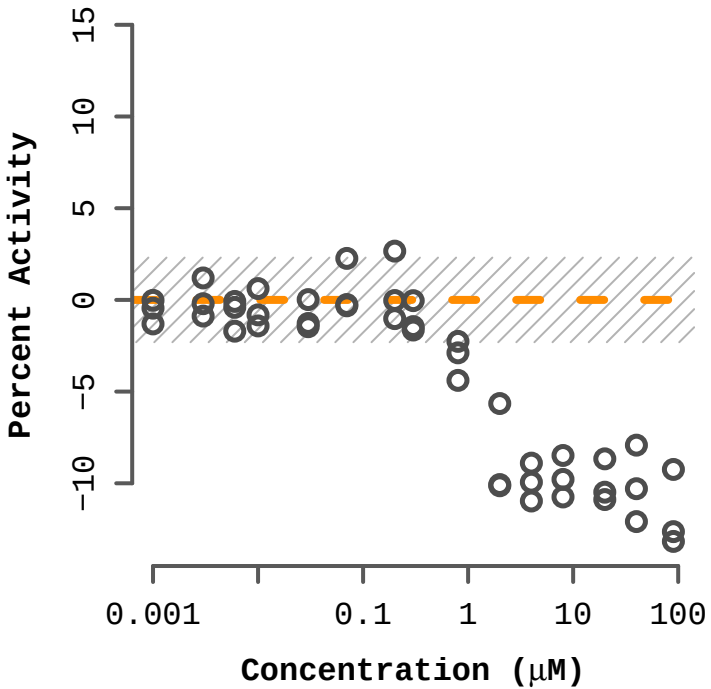
	tp	ga	gw
val:	1.16e-09	0.968	2.35
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.76	-1.91	2.06	-0.512	16.3
sd:	2.26	0.612	5.04	0.476	719

	CNST	HILL	GNLS
AIC:	276.96	282.96	278.72
PROB:	0.68	0.03	0.28
RMSE:	5.07	5.07	4.8

MAX_MEAN: 3.53 MAX_MED: 5.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

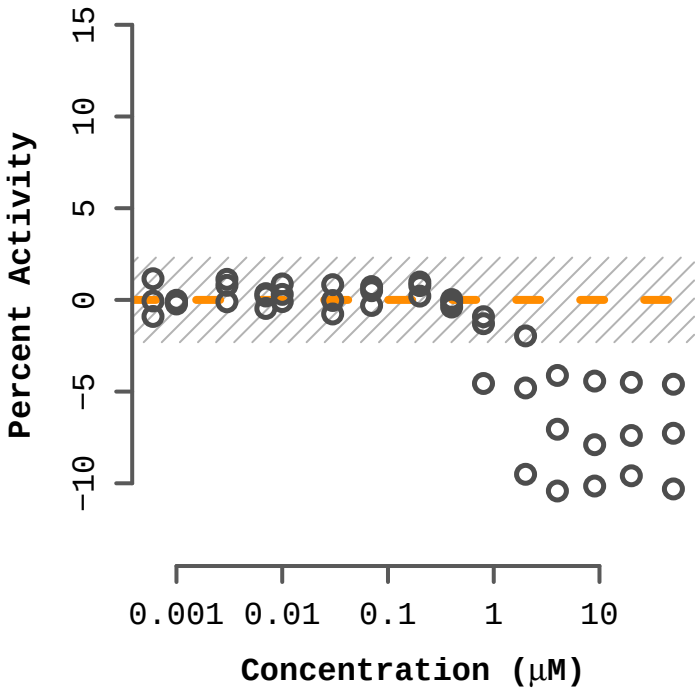
NAME: Tetramethylthiuram monosulfide
CHID: 21333 **CASRN:** 97-74-5
SPID(S): Tox21_201554
M4ID: 12480698

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.59	NA	NA
PROB:	1	NA	NA
RMSE:	6.53	NA	NA

MAX_MEAN: 0.565 **MAX_MED:** −0.0316 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

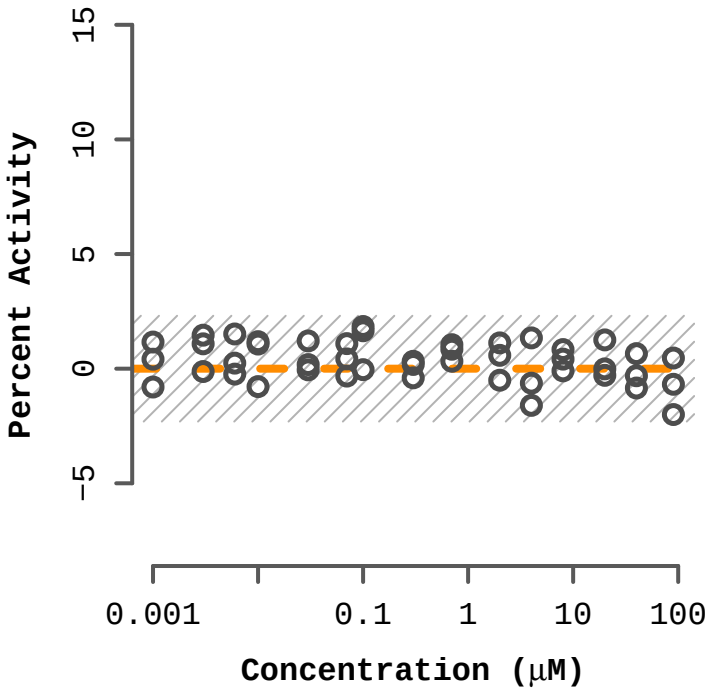
NAME: Tetramethylthiuram monosulfide
CHID: 21333 **CASRN:** 97-74-5
SPID(S): Tox21_111656_1
M4ID: 12483553

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	256.27	NA	NA
PROB:	1	NA	NA
RMSE:	4.36	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 0.796 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

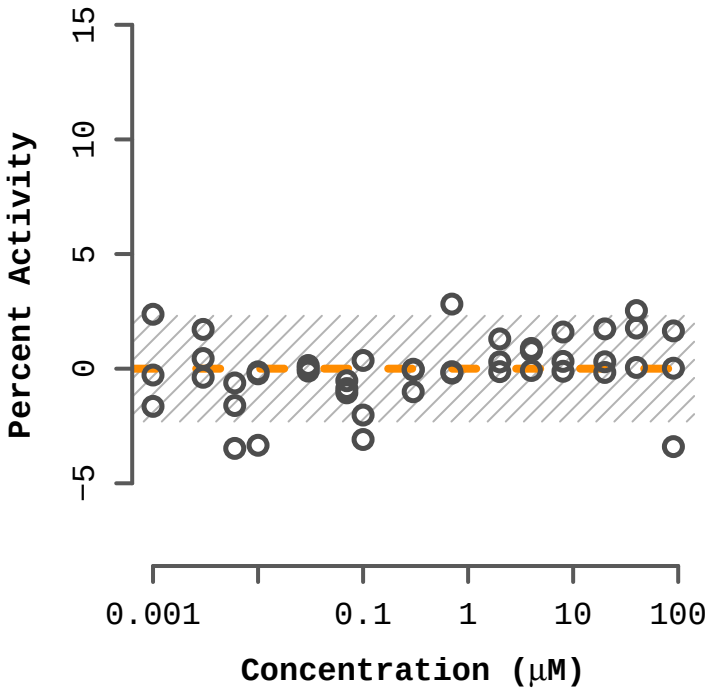
NAME: Tetranitromethane
CHID: 21334 **CASRN:** 509-14-8
SPID(S): Tox21_302834
M4ID: 12476299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

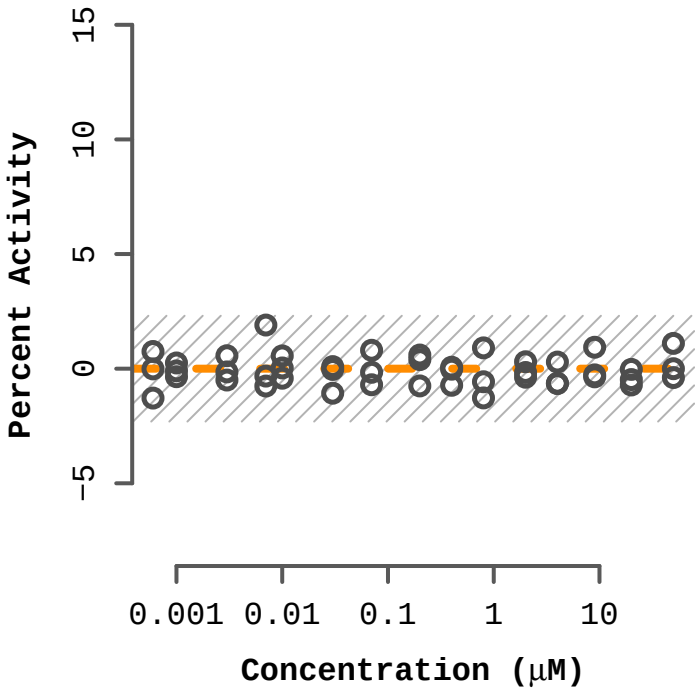
NAME: Tetranitromethane
CHID: 21334 **CASRN:** 509-14-8
SPID(S): Tox21_202353
M4ID: 12479899

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

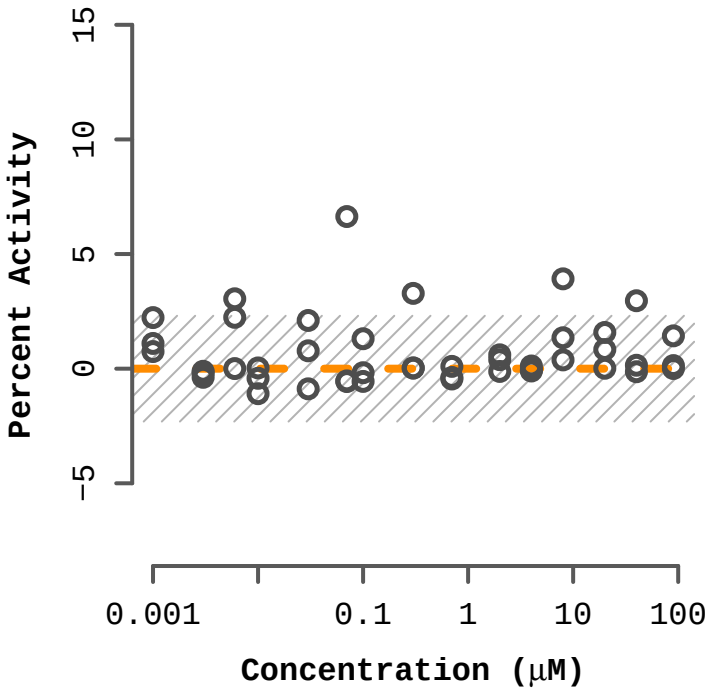
NAME: Thenyldiamine
CHID: 21335 **CASRN:** 91-79-2
SPID(S): Tox21_113737
M4ID: 12482477

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.275 **MAX_MED:** 0.397 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

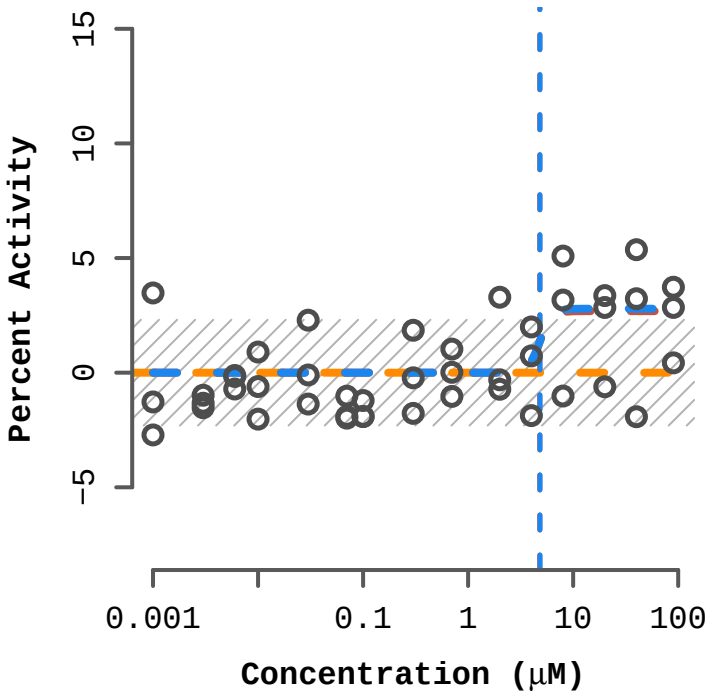
NAME: Theophylline
CHID: 21336 **CASRN:** 58-55-9
SPID(S): Tox21_300028
M4ID: 12479102

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Theophylline
CHID: 21336 CASRN: 58-55-9
SPID(S): Tox21_202375
M4ID: 12479877

HILL MODEL (in red):

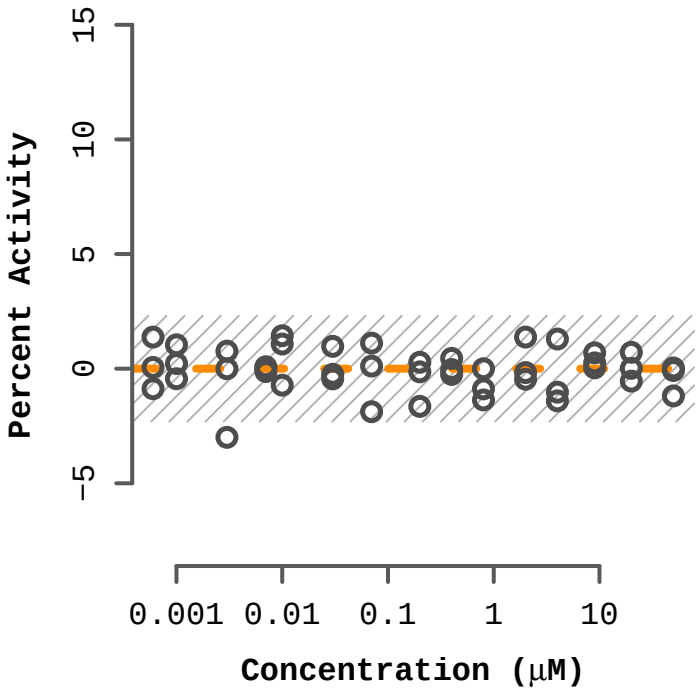
	tp	ga	gw
val:	2.69	0.681	8
sd:	0.595	0.169	14.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.79	0.684	7.99	2.02	14.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	201.25	193.22	197.16
PROB:	0.02	0.86	0.12
RMSE:	2.14	1.83	1.83

MAX_MEAN: 2.41 MAX_MED: 3.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

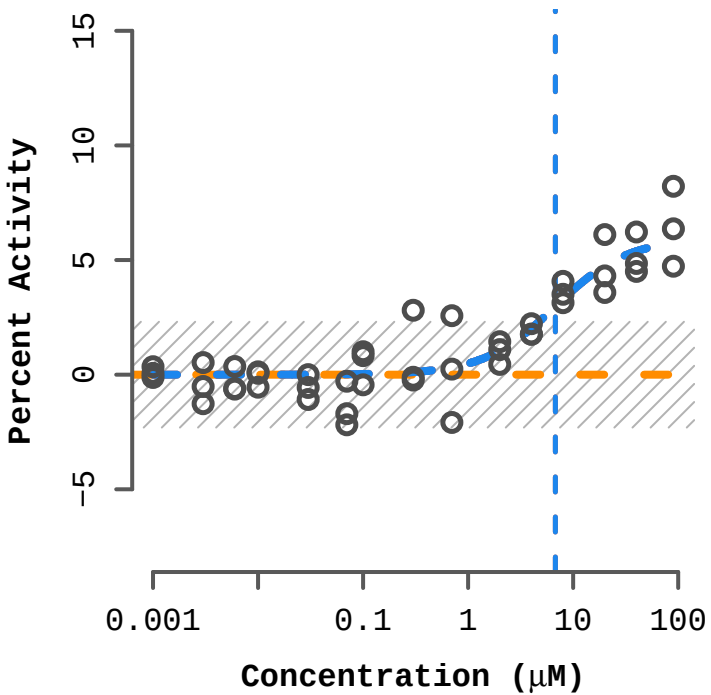
NAME: Theophylline
CHID: 21336 **CASRN:** 58-55-9
SPID(S): Tox21_110827_1
M4ID: 12484089

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.598 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiabendazole
CHID: 21337 **CASRN:** 148-79-8
SPID(S): Tox21_300970
M4ID: 12478163

HILL MODEL (in red):

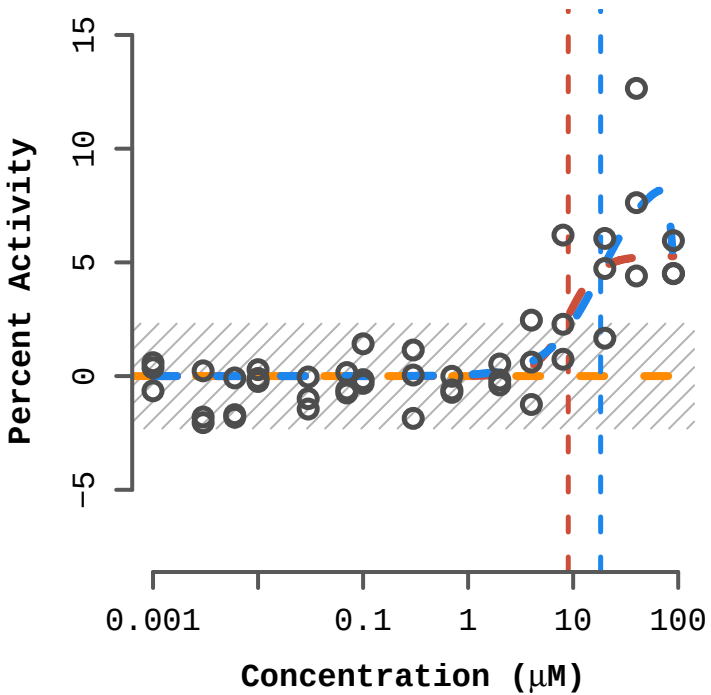
	tp	ga	gw
val:	5.95	0.831	1.27
sd:	0.903	0.161	0.435

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.95	0.831	1.27	3.64	5.82
sd:	0.903	0.161	0.435	7770	26900

	CNST	HILL	GNLS
AIC:	221.33	134.55	138.55
PROB:	0	0.88	0.12
RMSE:	2.86	1.02	1.02

MAX_MEAN: 6.44 **MAX_MED:** 6.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiabendazole
CHID: 21337 **CASRN:** 148-79-8
SPID(S): Tox21_202397
M4ID: 12479855

HILL MODEL (in red):

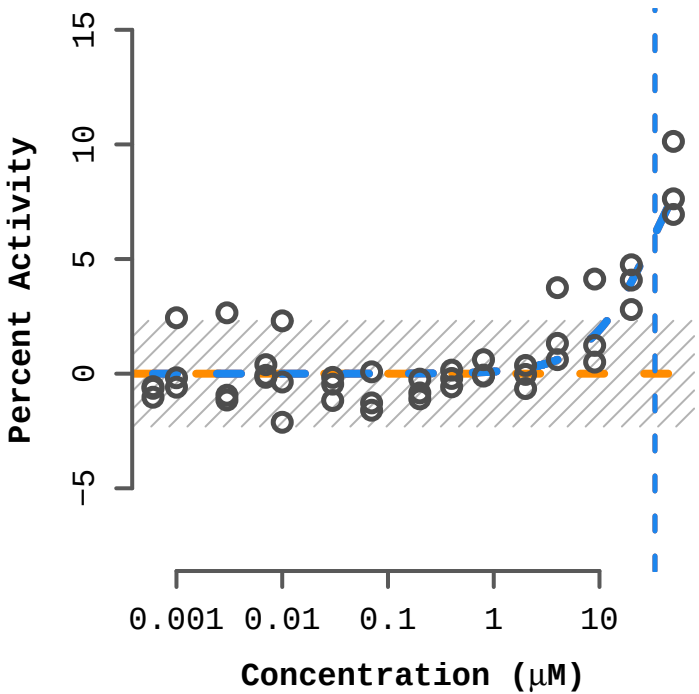
	tp	ga	gw
val:	5.28	0.953	2.95
sd:	0.565	0.106	1.64

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.13	1.26	1.71	1.96	14.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	218.84	167.44	169.13
PROB:	0	0.7	0.3
RMSE:	3.18	1.68	1.53

MAX_MEAN: 8.23 **MAX_MED:** 7.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiabendazole
CHID: 21337 **CASRN:** 148-79-8
SPID(S): Tox21_110427_1
M4ID: 12484367

HILL MODEL (in red):

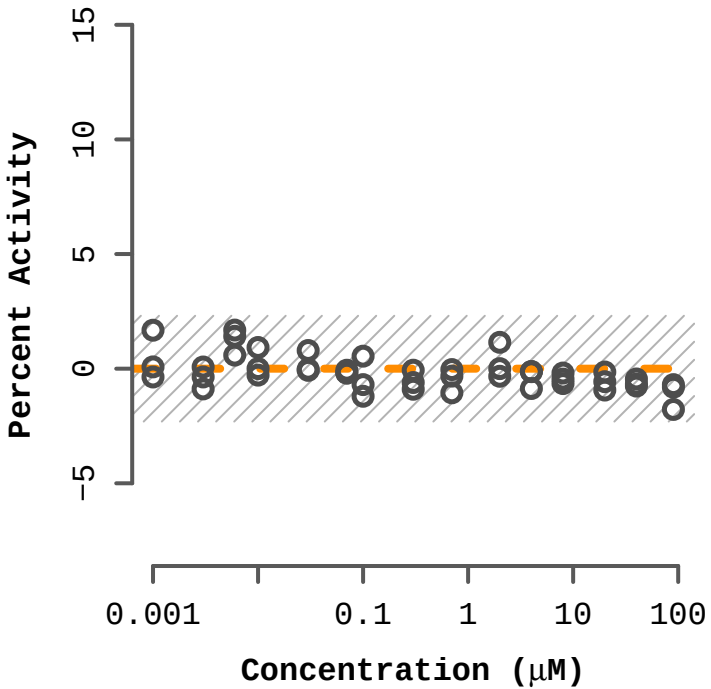
	tp	ga	gw
val:	12.2	1.52	1.39
sd:	5.48	0.311	0.477

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.2	1.52	1.39	3.44	4.17
sd:	5.48	0.311	0.477	1230	2960

	CNST	HILL	GNLS
AIC:	202.28	149.24	153.24
PROB:	0	0.88	0.12
RMSE:	2.7	1.19	1.19

MAX_MEAN: 8.24 **MAX_MED:** 7.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

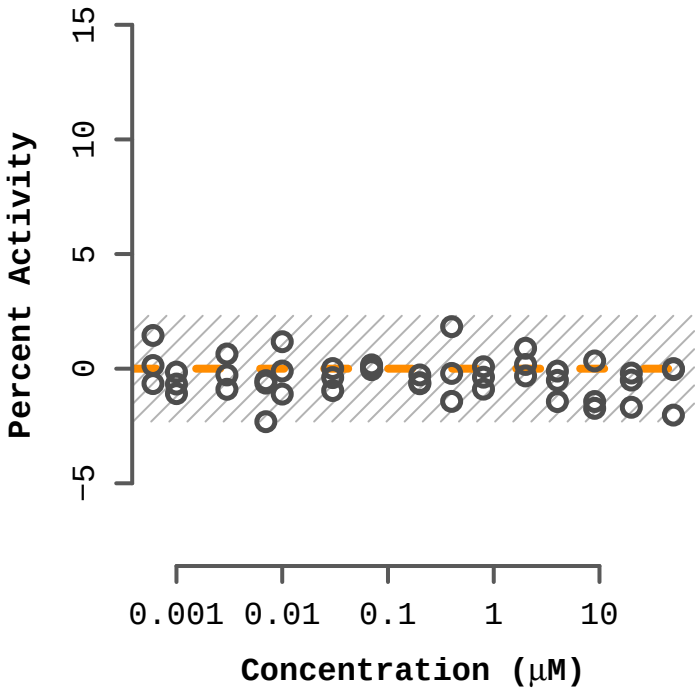
NAME: Thiamphenicol
CHID: 21338 **CASRN:** 15318-45-3
SPID(S): Tox21_200816
M4ID: 12481436

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

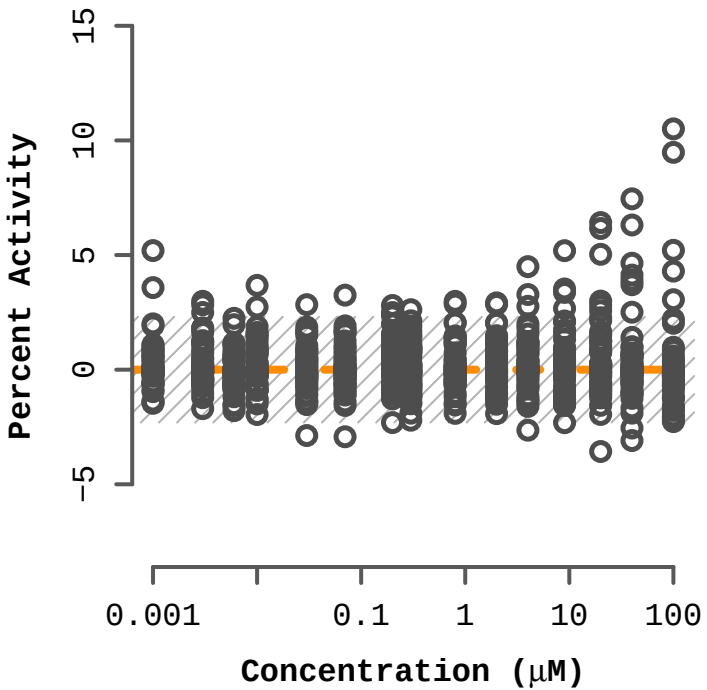
NAME: Thiamphenicol
CHID: 21338 **CASRN:** 15318-45-3
SPID(S): Tox21_110577_1
M4ID: 12484255

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.314 **MAX_MED:** 0.186 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

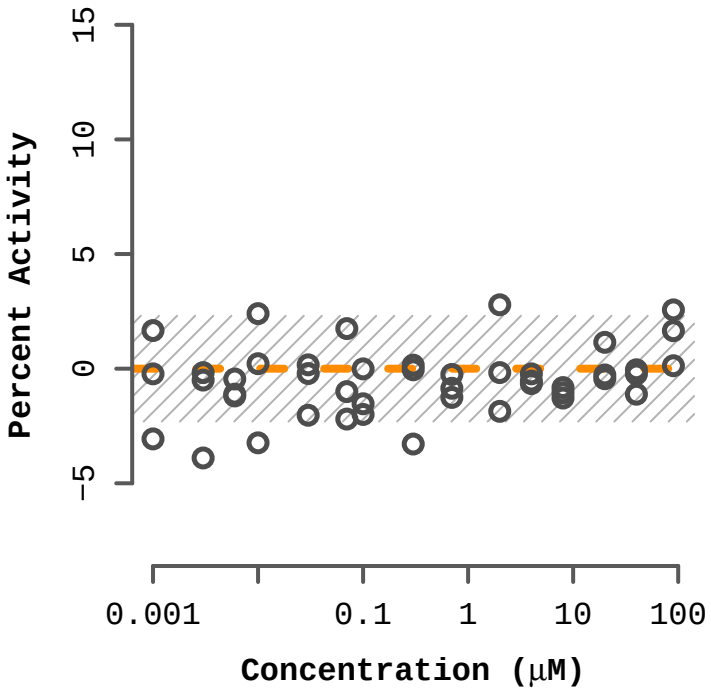
NAME: Thiotepa
CHID: 21339 **CASRN:** 52-24-4
SPID(S): Tox21_400065
M4ID: 12475072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2258.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.552 **MAX_MED:** 0.182 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

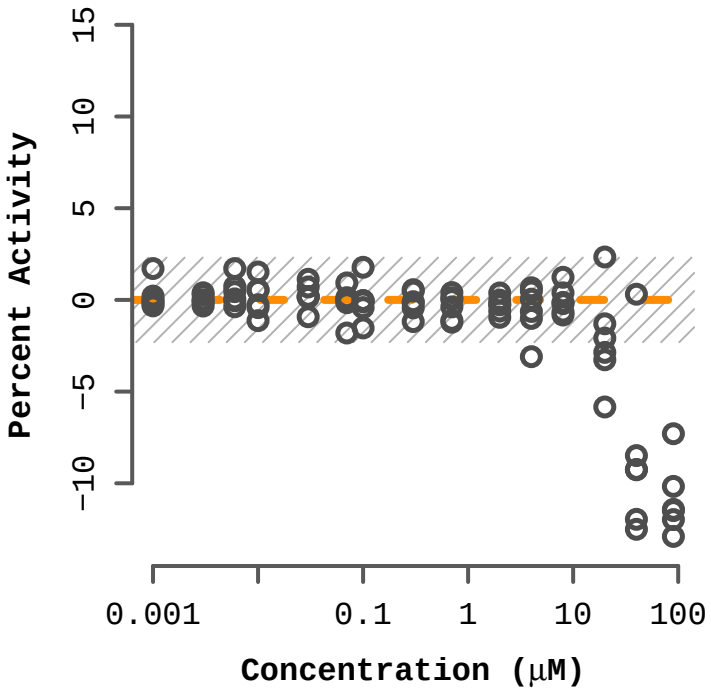
NAME: Thioacetamide
CHID: 21340 **CASRN:** 62-55-5
SPID(S): Tox21_301295
M4ID: 12477838

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

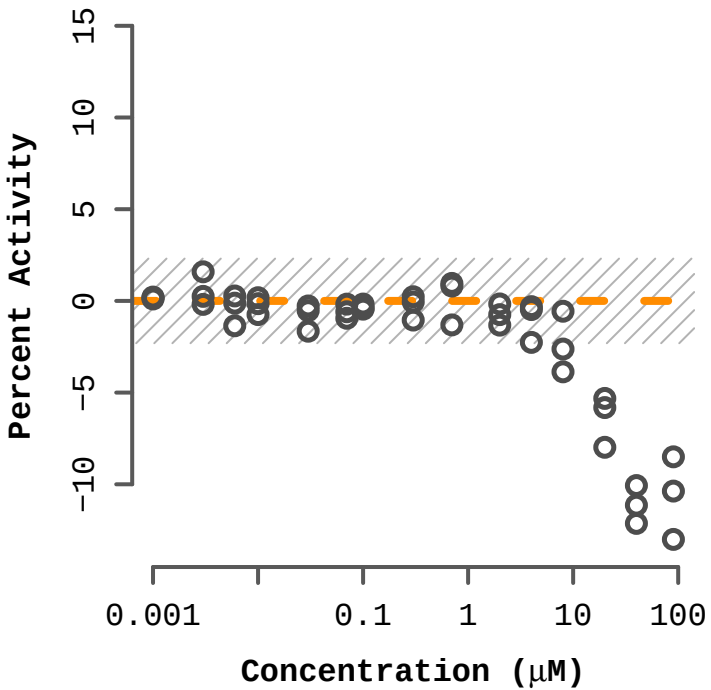
NAME: 4,4'-Thiobis(6-tert-butyl-m-cresol)
CHID: 21341 **CASRN:** 96-69-5
SPID(S): Tox21_201022
M4ID: 12481230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	434.76	NA	NA
PROB:	1	NA	NA
RMSE:	3.92	NA	NA

MAX_MEAN: 0.423 **MAX_MED:** 0.254 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

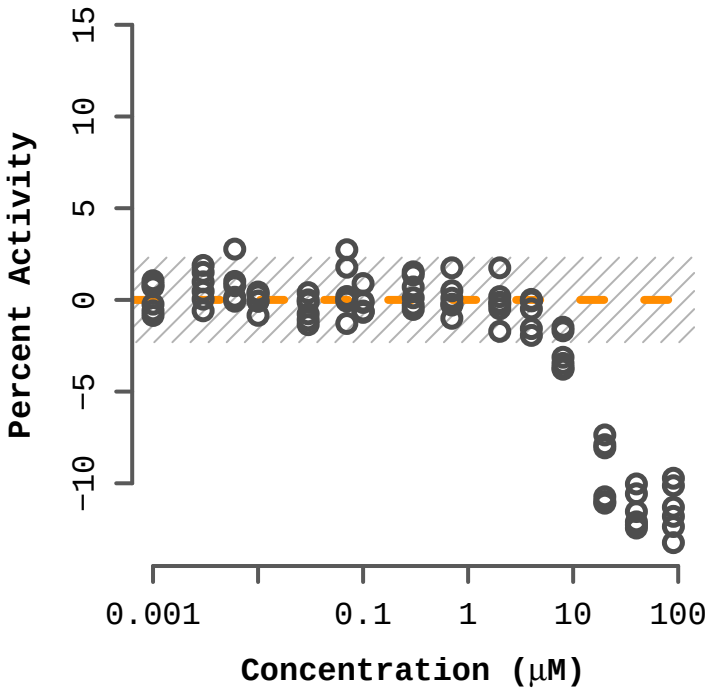
NAME: Bithionol
CHID: 21342 CASRN: 97-18-7
SPID(S): Tox21_302919
M4ID: 12476214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.39	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: 0.549 **MAX_MED:** 0.811 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

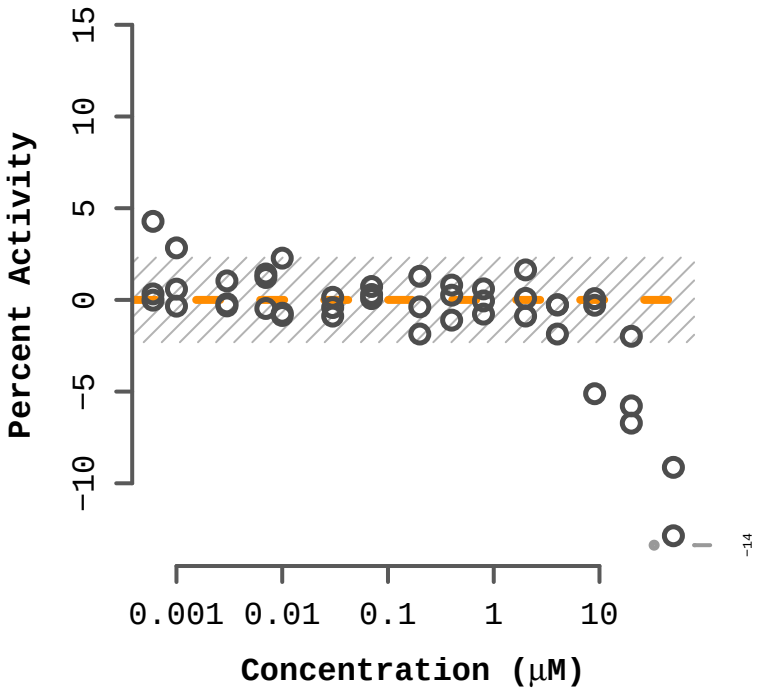
NAME: Bithionol
CHID: 21342 **CASRN:** 97-18-7
SPID(S): Tox21_200384
M4ID: 12481868

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	518.43	NA	NA
PROB:	1	NA	NA
RMSE:	5	NA	NA

MAX_MEAN: 0.776 **MAX_MED:** 0.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

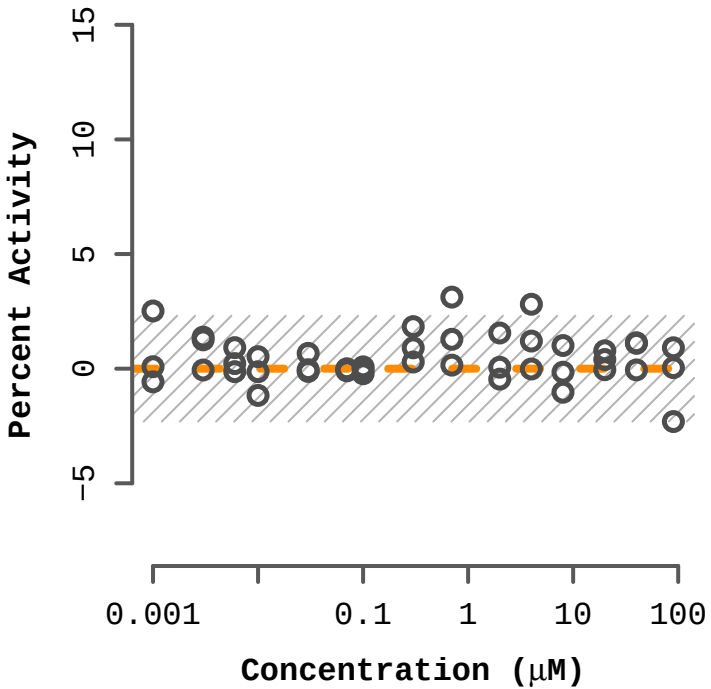
NAME: Bithionol
CHID: 21342 CASRN: 97-18-7
SPID(S): Tox21_110832_1
M4ID: 12484084 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

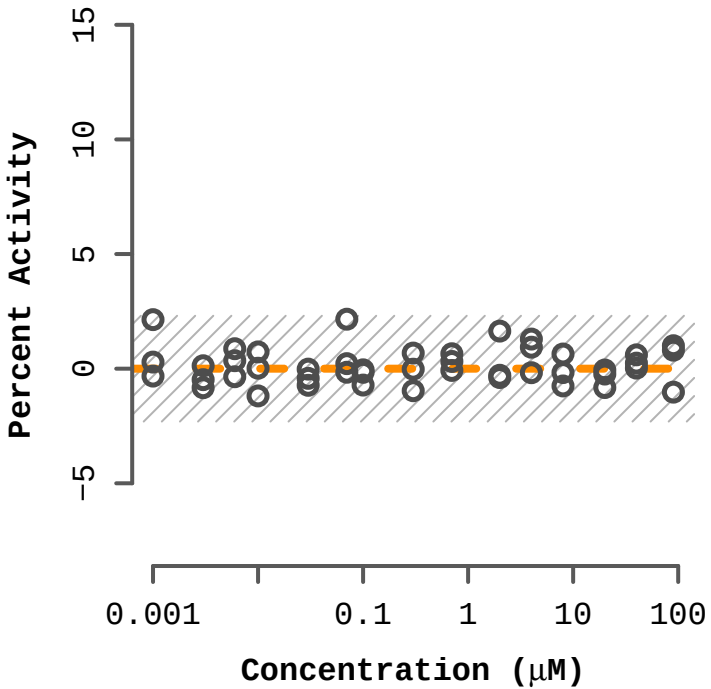
NAME: Sodium thiocyanate
CHID: 21343 **CASRN:** 540-72-7
SPID(S): Tox21_302975
M4ID: 12476158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

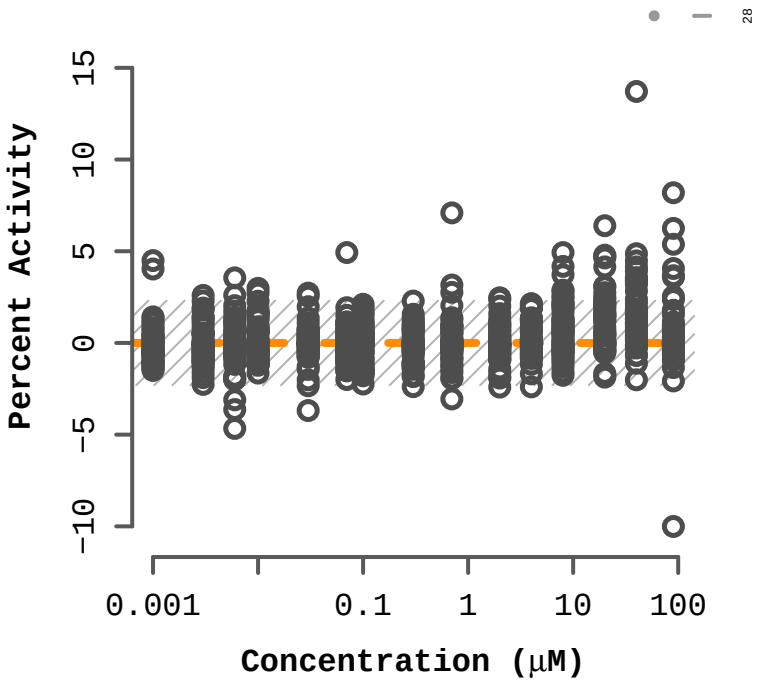
NAME: Sodium thiocyanate
CHID: 21343 **CASRN:** 540-72-7
SPID(S): Tox21_201621
M4ID: 12480631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.938 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

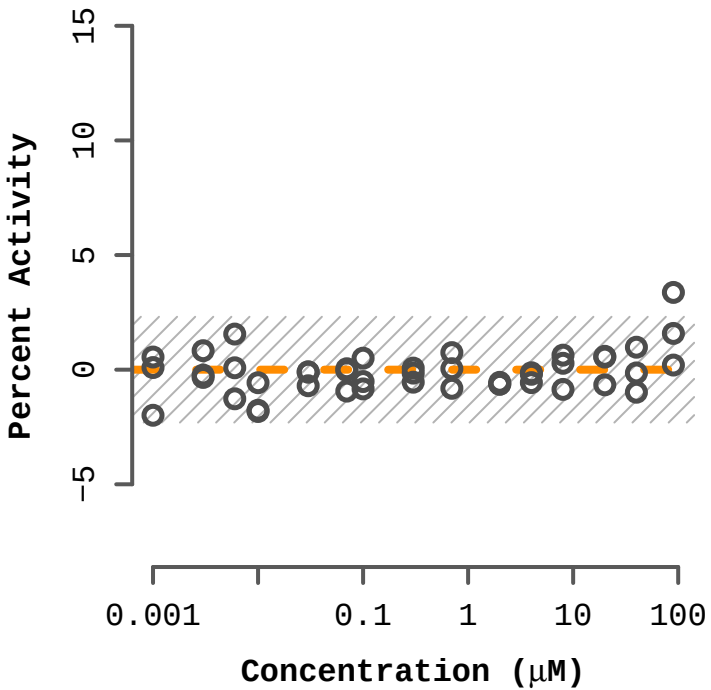
NAME: 4,4'−Thiodianiline
CHID: 21344 **CASRN:** 139−65−1
SPID(S): Tox21_400005
M4ID: 12475132 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2473.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.87	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

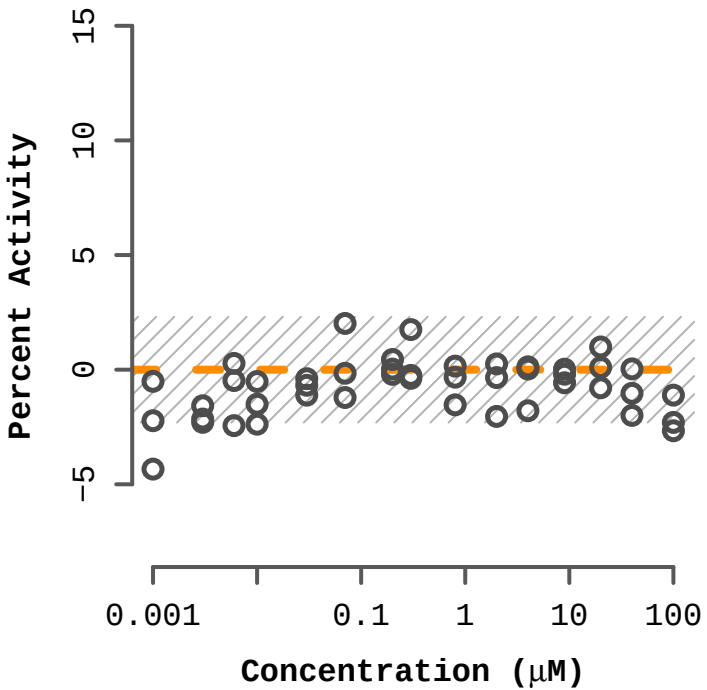
NAME: Thiosemicarbazide
CHID: 21346 **CASRN:** 79-19-6
SPID(S): Tox21_302983
M4ID: 12476150

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

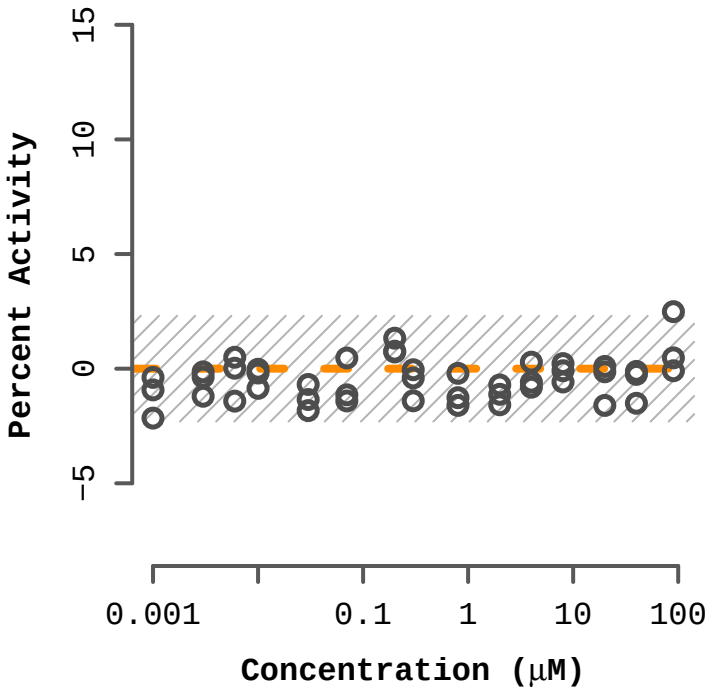
NAME: Thiosemicarbazide
CHID: 21346 **CASRN:** 79-19-6
SPID(S): Tox21_201348
M4ID: 12480904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 0.375 **MAX_MED:** 0.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

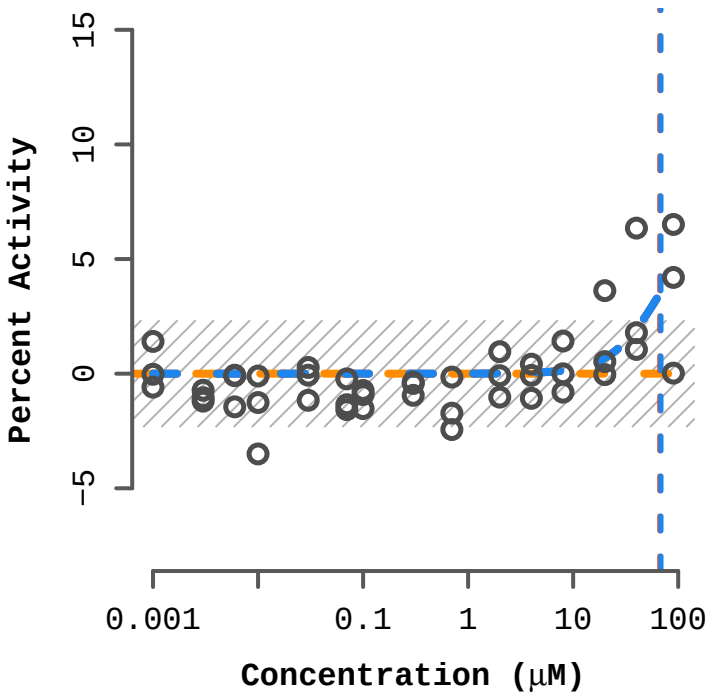
NAME: Thiouracil
CHID: 21347 **CASRN:** 141-90-2
SPID(S): Tox21_302955
M4ID: 12476178

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.958 **MAX_MED:** 0.764 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiouracil
CHID: 21347 CASRN: 141-90-2
SPID(S): Tox21_202418
M4ID: 12479834

HILL MODEL (in red):

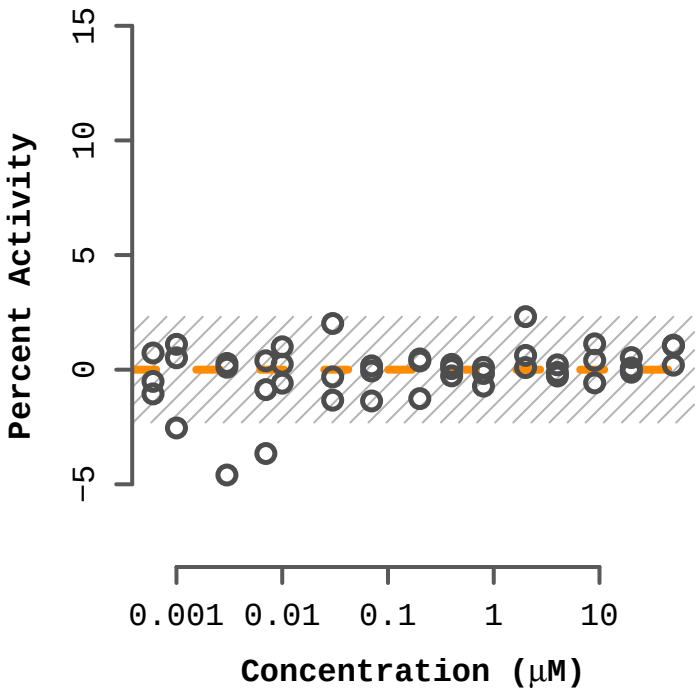
	tp	ga	gw
val:	6.96	1.82	1.84
sd:	9.18	0.691	1.63

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.37	1.84	1.84	3.95	0.713
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	175.07	166.39	170.39
PROB:	0.01	0.87	0.12
RMSE:	1.91	1.49	1.49

MAX_MEAN: 3.58 MAX_MED: 4.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

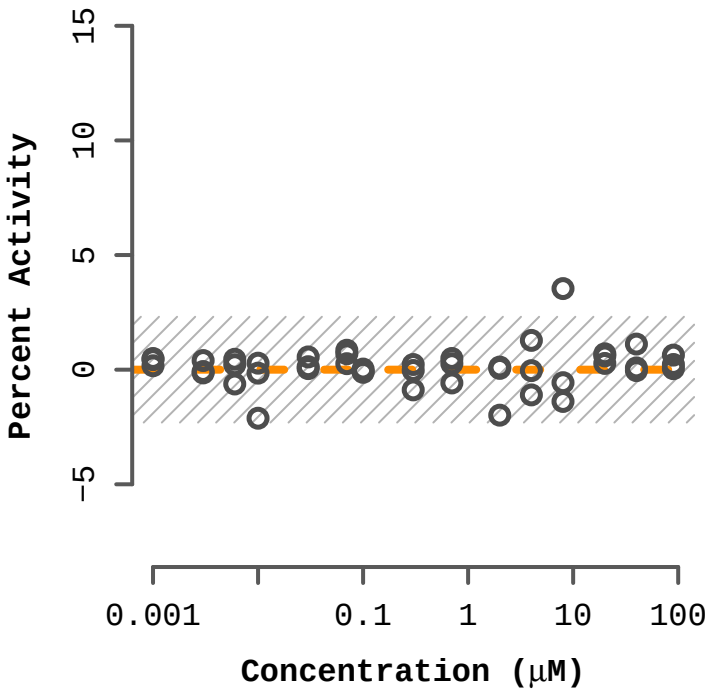
NAME: Thiouracil
CHID: 21347 **CASRN:** 141-90-2
SPID(S): Tox21_111418_1
M4ID: 12483701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

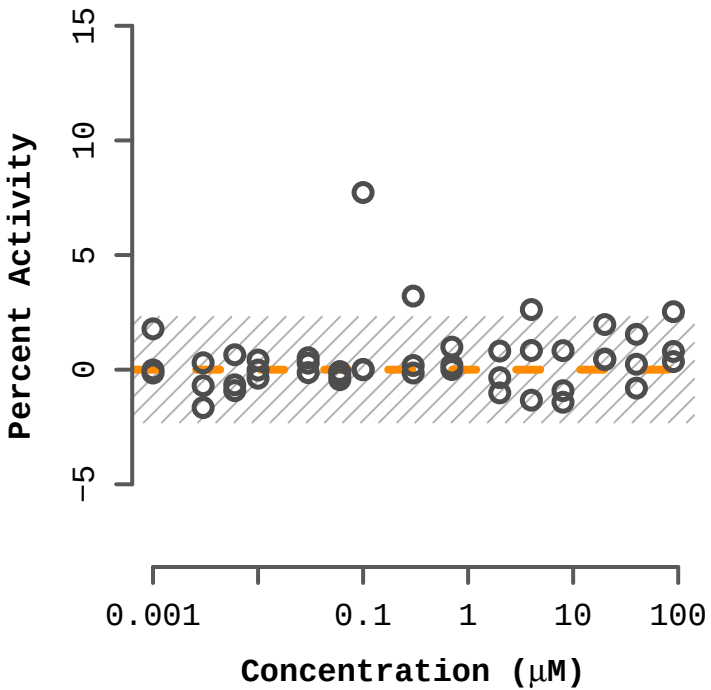
NAME: Thiourea
CHID: 21348 CASRN: 62-56-6
SPID(S): Tox21_302767
M4ID: 12476366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.603 MAX_MED: 0.696 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

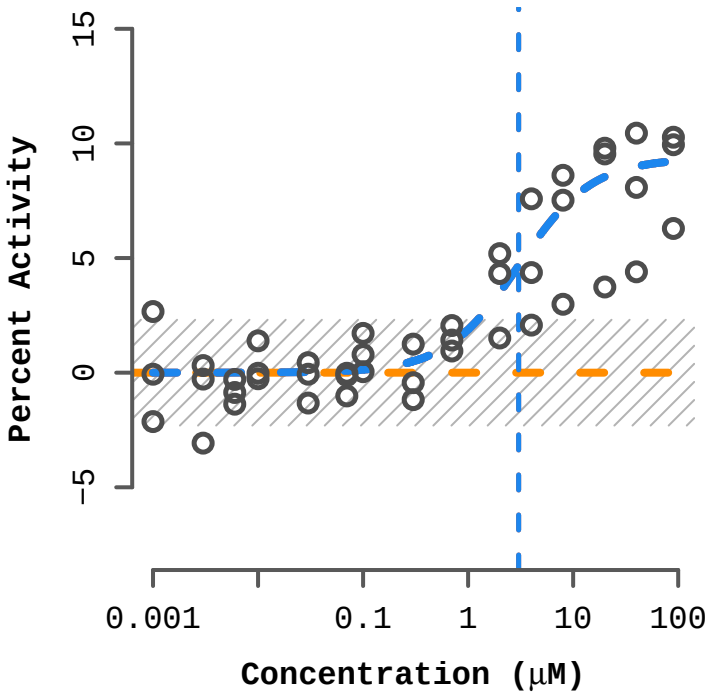
NAME: Thiourea
CHID: 21348 **CASRN:** 62-56-6
SPID(S): Tox21_201873
M4ID: 12480379

HILL MODEL: Not applicable.

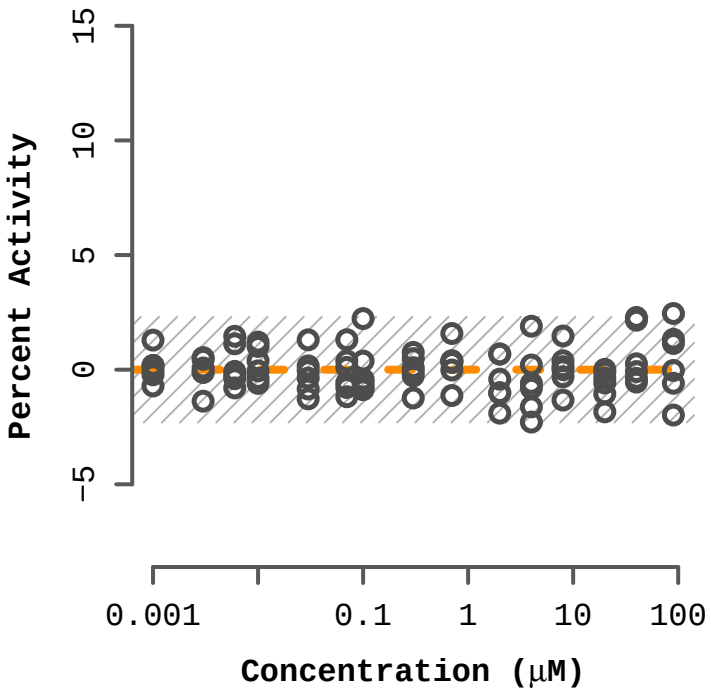
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.58 **MAX_MED:** 0.839 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tin(II) chloride
CHID:    21351   CASRN: 7772-99-8
SPID(S): Tox21_202599
M4ID:    12479653

HILL MODEL (in red):
      tp       ga       gw
val:  9.35     0.481    1.25
sd:   0.894    0.146    0.332

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.35     0.481    1.25     2.84     9.28
sd:   0.894    0.146    0.332    1450     15100

      CNST        HILL        GNLS
AIC:  264.26      185.11      189.11
PROB: 0           0.88        0.12
RMSE: 4.6         1.77        1.77

MAX_MEAN: 8.84      MAX_MED: 9.95      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

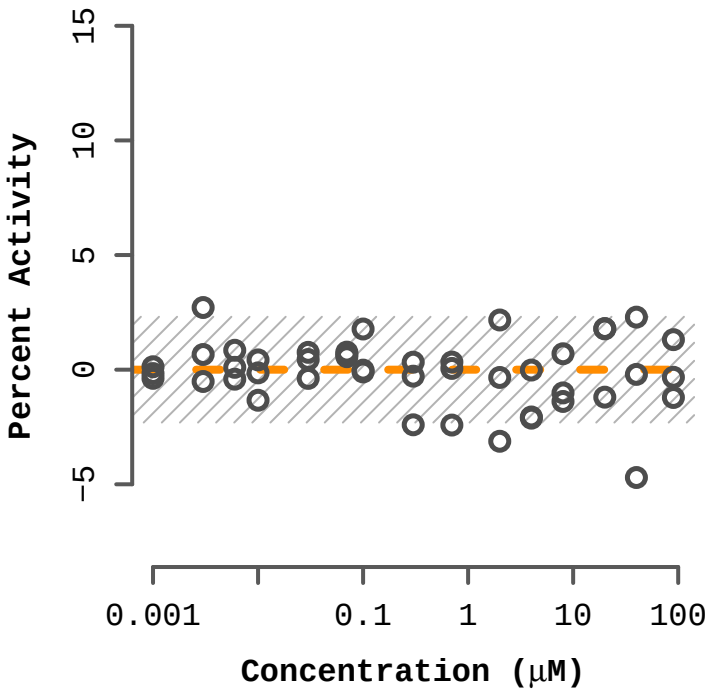
NAME: Titanocene dichloride
CHID: 21354 **CASRN:** 1271-19-8
SPID(S): Tox21_202542
M4ID: 12479710

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	255.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.615 **MAX_MED:** 0.556 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

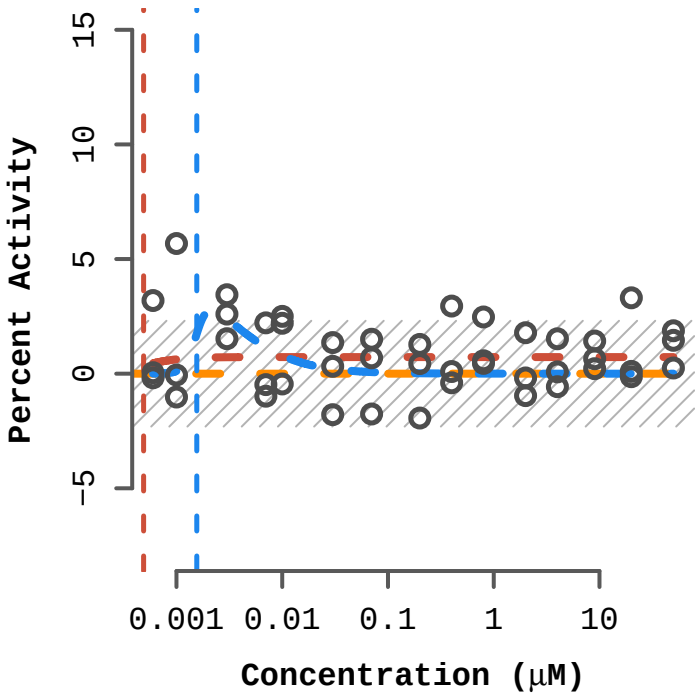
NAME: dl-alpha-Tocopheryl acetate
CHID: 21356 CASRN: 52225-20-4
SPID(S): Tox21_303444
M4ID: 12475696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.954 MAX_MED: 1.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: dl-alpha-Tocopheryl acetate
CHID: 21356 **CASRN:** 52225-20-4
SPID(S): Tox21_113467_1
M4ID: 12482640

HILL MODEL (in red):

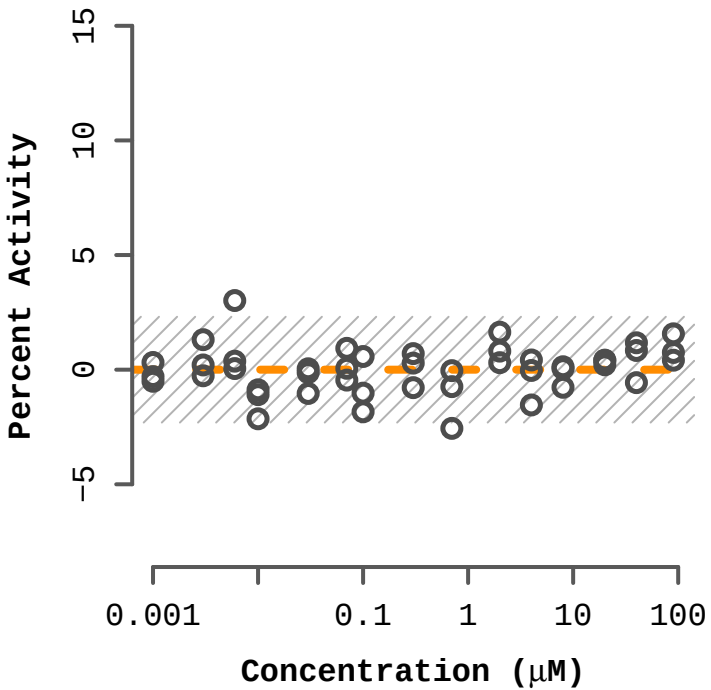
	tp	ga	gw
val:	0.724	−3.31	2.56
sd:	0.242	1.13	5.75

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.11	−2.81	8	−2.56	1.33
sd:	10.4	0.392	16.8	1.25	1.86

	CNST	HILL	GNLS
AIC:	180	176.74	180.71
PROB:	0.15	0.75	0.1
RMSE:	1.76	1.57	1.61

MAX_MEAN: 2.52 **MAX_MED:** 2.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

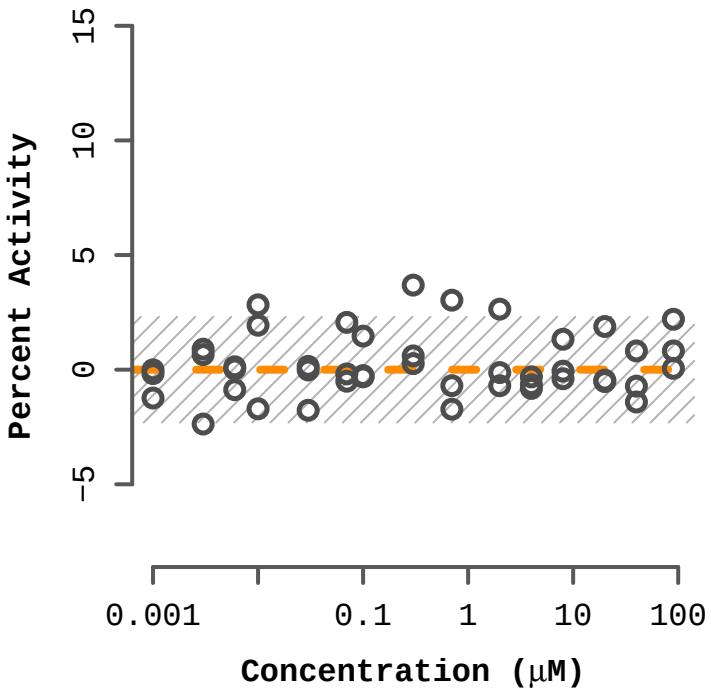
NAME: Tolazamide
CHID: 21358 **CASRN:** 1156-19-0
SPID(S): Tox21_300416
M4ID: 12478716

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.839 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

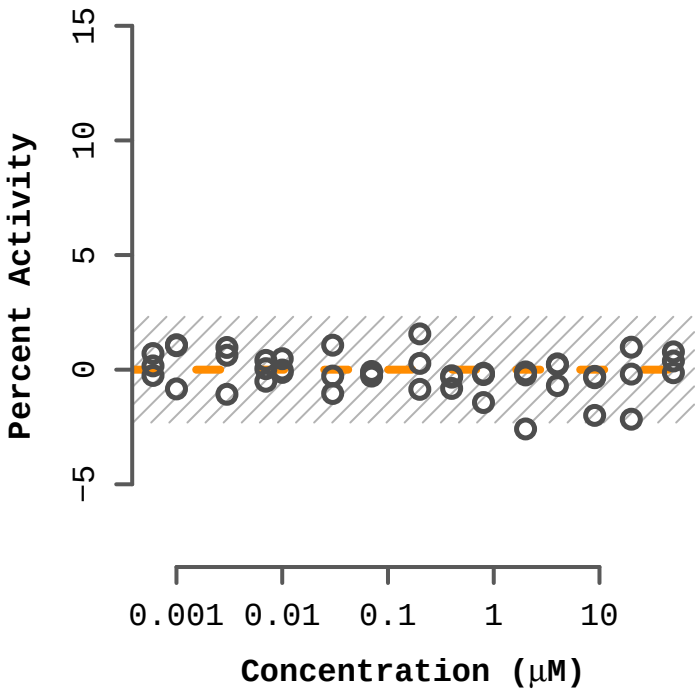
NAME: Tolazamide
CHID: 21358 **CASRN:** 1156-19-0
SPID(S): Tox21_201507
M4ID: 12480745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

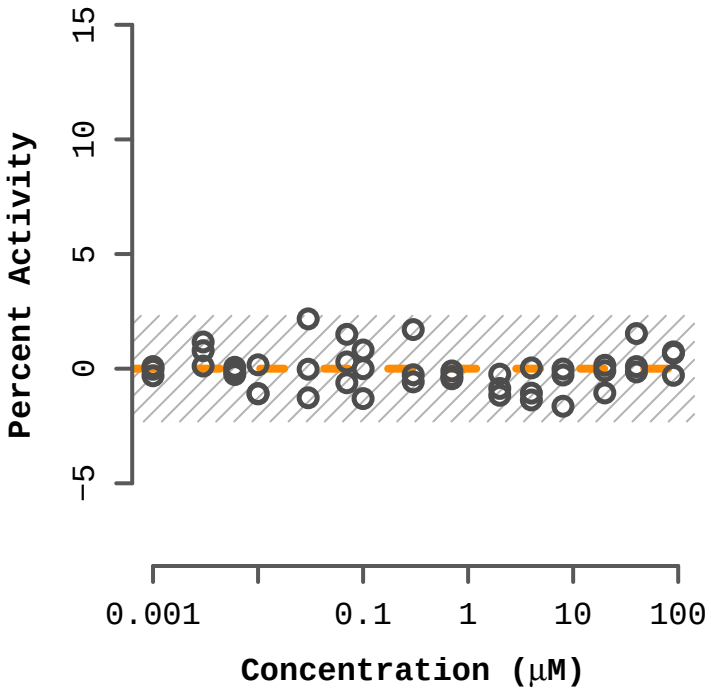
NAME: Tolazamide
CHID: 21358 **CASRN:** 1156-19-0
SPID(S): Tox21_110281_1
M4ID: 12484487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.433 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

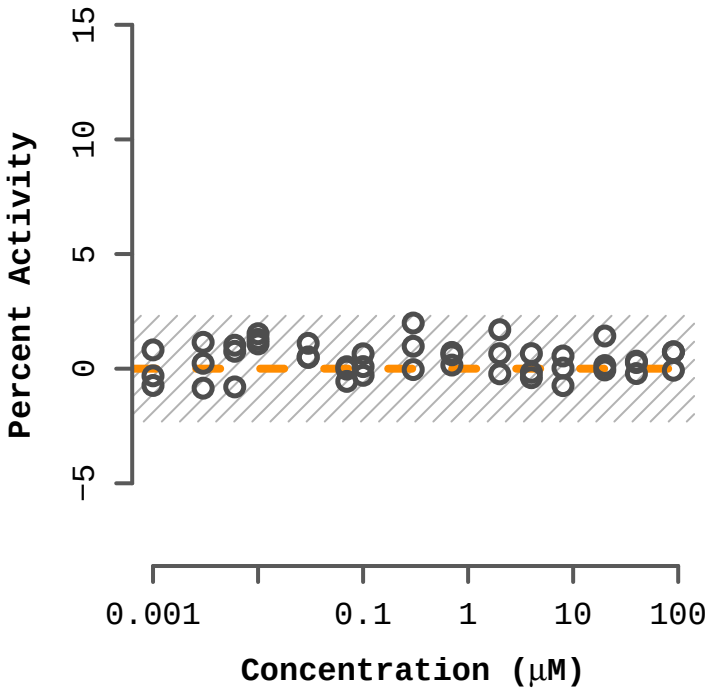
NAME: Tolbutamide
CHID: 21359 **CASRN:** 64-77-7
SPID(S): Tox21_302795
M4ID: 12476338

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.69 **MAX_MED:** 0.788 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

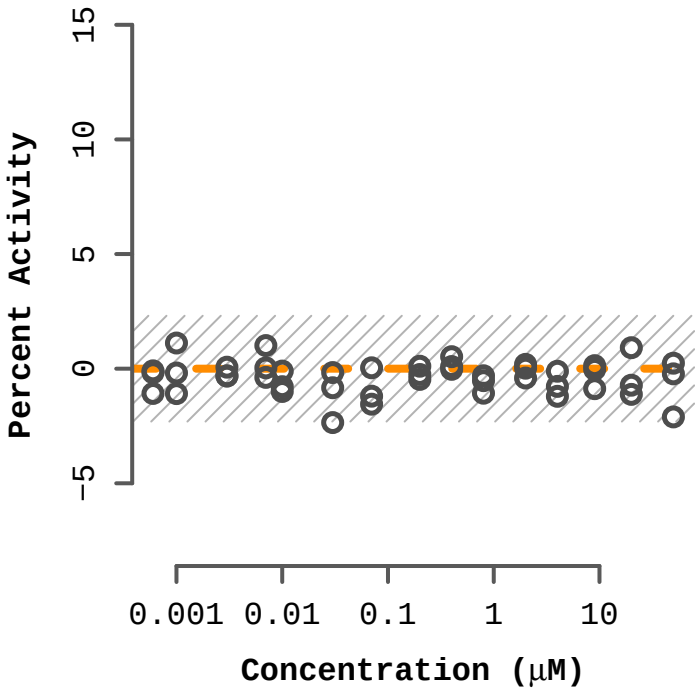
NAME: Tolbutamide
CHID: 21359 **CASRN:** 64-77-7
SPID(S): Tox21_201612
M4ID: 12480640

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

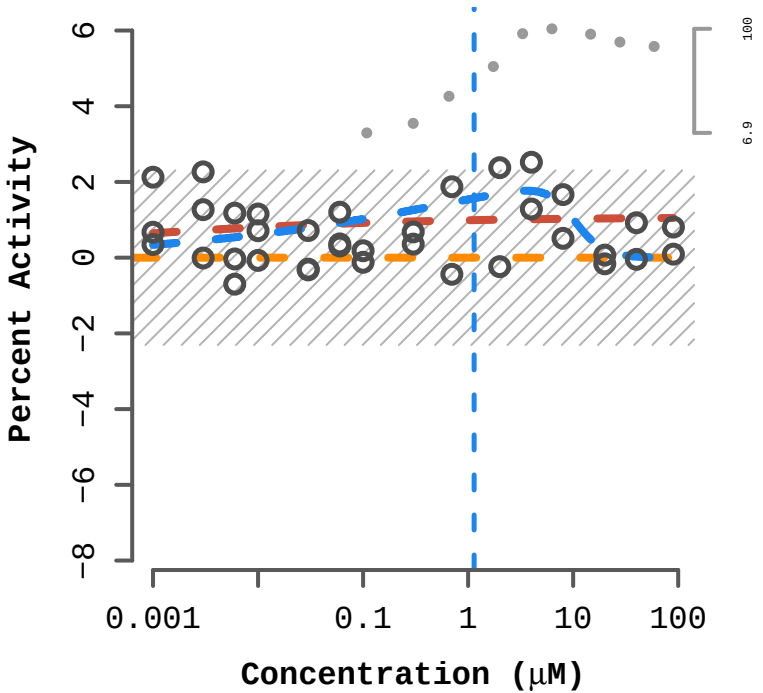
NAME: Tolbutamide
CHID: 21359 **CASRN:** 64-77-7
SPID(S): Tox21_110279_1
M4ID: 12484489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.222 **MAX_MED:** 0.0942 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Toluene
CHID: 21360 **CASRN:** 108-88-3
SPID(S): Tox21_201224
M4ID: 12481028 BRK

HILL MODEL (in red):

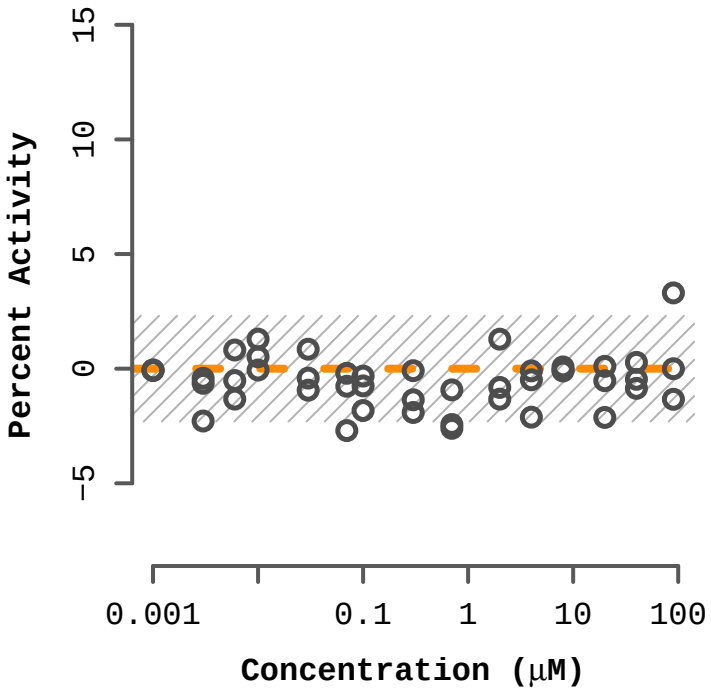
	tp	ga	gw
val:	1.07	−3.6	0.3
sd:	1.08	9.39	1.36

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.14	0.057	0.3	0.998	3.18
sd:	38.5	35.8	2.28	1.2	34.9

	CNST	HILL	GNLS
AIC:	389.8	392.41	396.02
PROB:	0.76	0.21	0.03
RMSE:	33.74	33.33	33.39

MAX_MEAN: 34.7 **MAX_MED:** 2.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

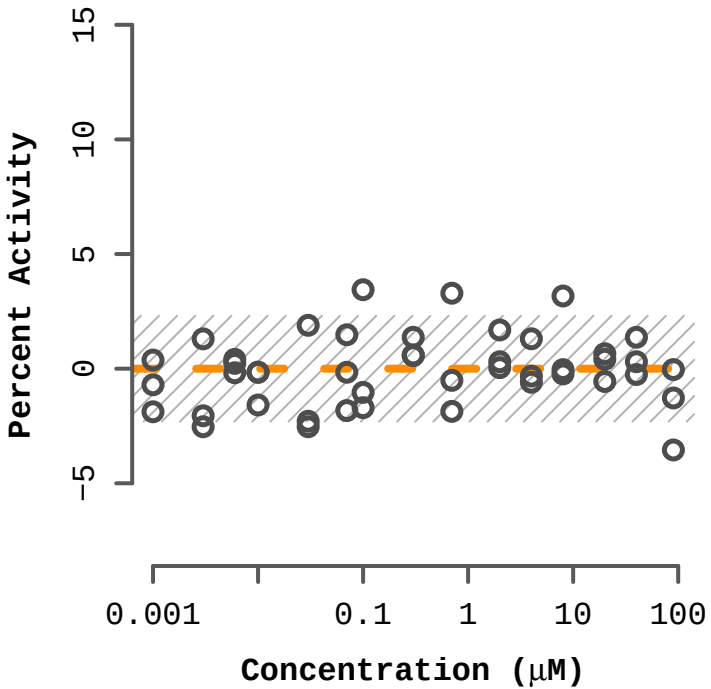
NAME: o-Toluenesulfonamide
CHID: 21362 **CASRN:** 88-19-7
SPID(S): Tox21_301641
M4ID: 12477492

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.658 **MAX_MED:** 0.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

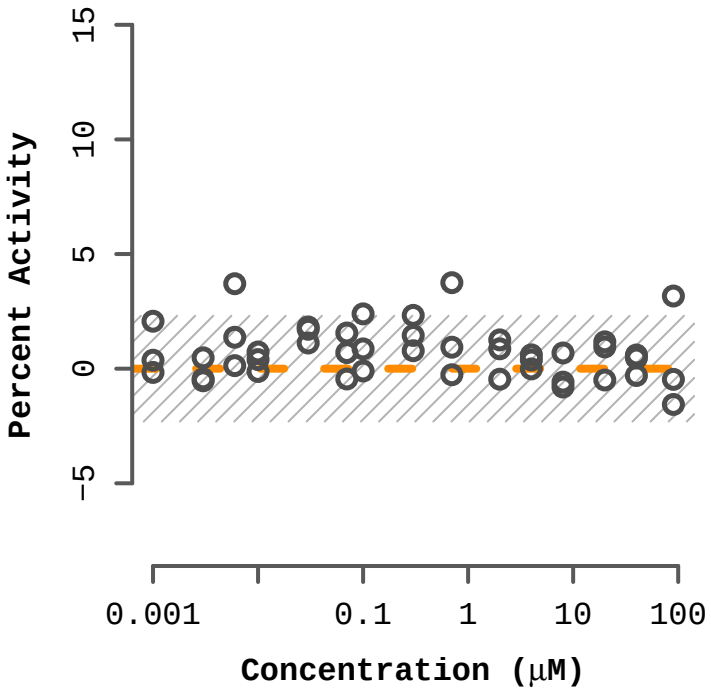
NAME: 3-Methylaniline hydrochloride
CHID: 21363 **CASRN:** 638-03-9
SPID(S): Tox21_200215
M4ID: 12482037

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 0.968 **MAX_MED:** 0.598 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

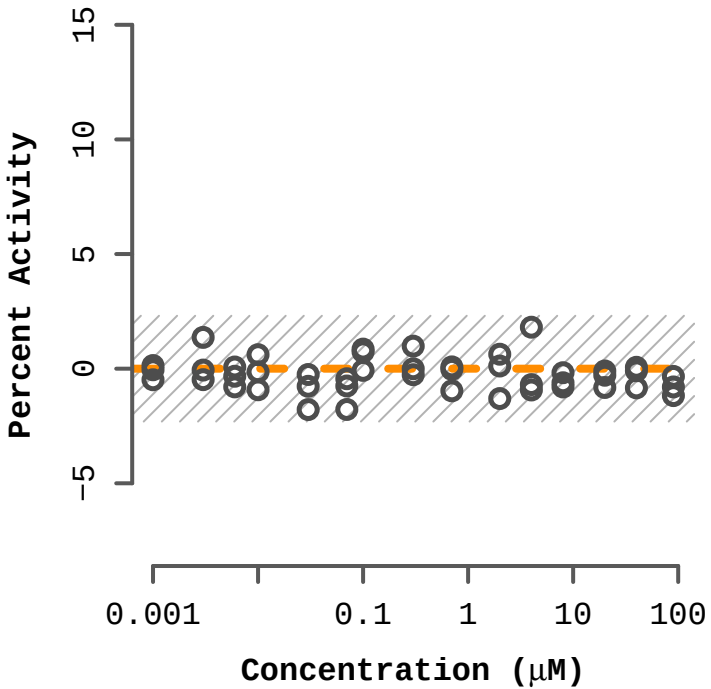
NAME: 2-Methylaniline hydrochloride
CHID: 21364 **CASRN:** 636-21-5
SPID(S): Tox21_302772
M4ID: 12476361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

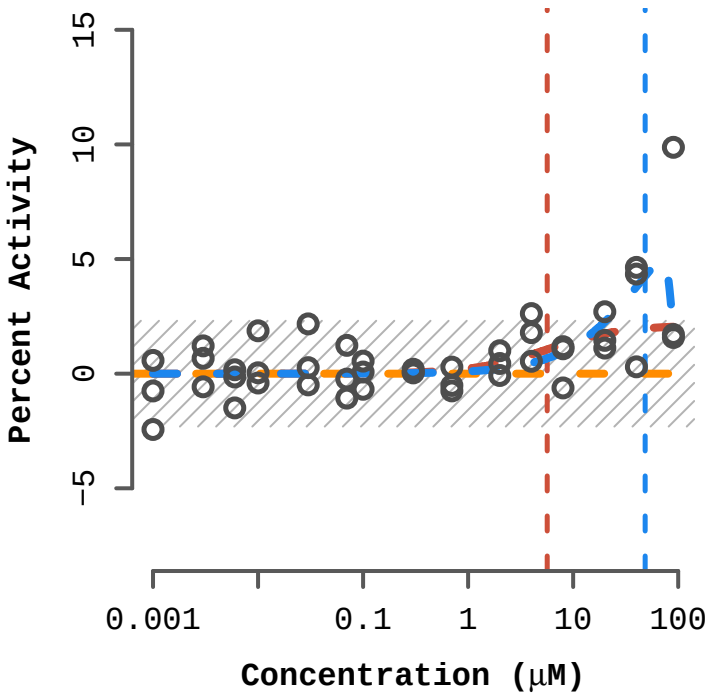
NAME: 2-Methylaniline hydrochloride
CHID: 21364 CASRN: 636-21-5
SPID(S): Tox21_201277
M4ID: 12480975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.506 MAX_MED: 0.736 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylaniline hydrochloride
CHID: 21365 CASRN: 540-23-8
SPID(S): Tox21_200517
M4ID: 12481735

HILL MODEL (in red):

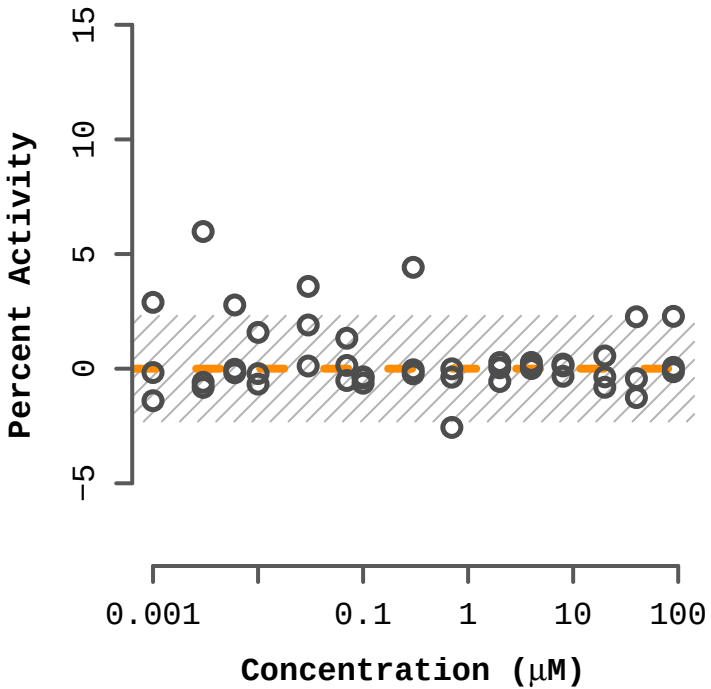
	tp	ga	gw
val:	2.11	0.753	1.24
sd:	0.813	0.47	0.822

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.49	1.69	1.15	1.94	16.9
sd:	9.78	0.691	0.472	0.0177	19.8

	CNST	HILL	GNLS
AIC:	173.44	155.23	156.02
PROB:	0	0.6	0.4
RMSE:	2.07	1.58	1.59

MAX_MEAN: 4.39 MAX_MED: 4.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

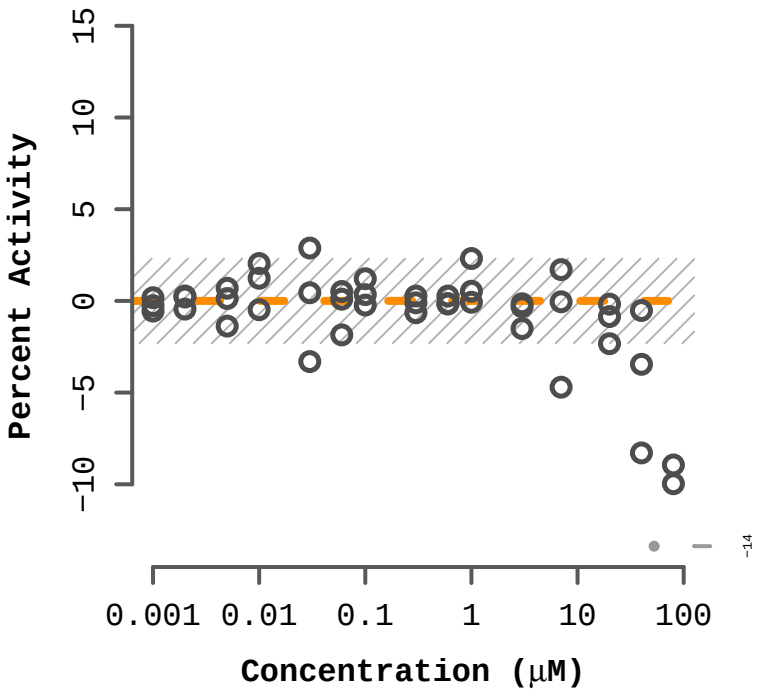
NAME: p-Tolylurea
CHID: 21366 **CASRN:** 622-51-5
SPID(S): Tox21_200832
M4ID: 12481420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

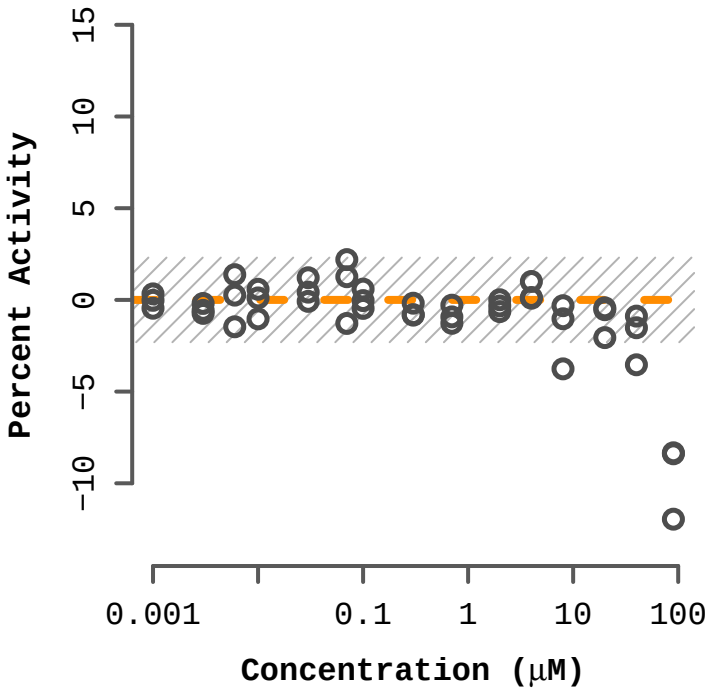
NAME: Toremifene citrate
CHID: 21367 CASRN: 89778-27-8
SPID(S): Tox21_301740
M4ID: 12477393 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.4	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

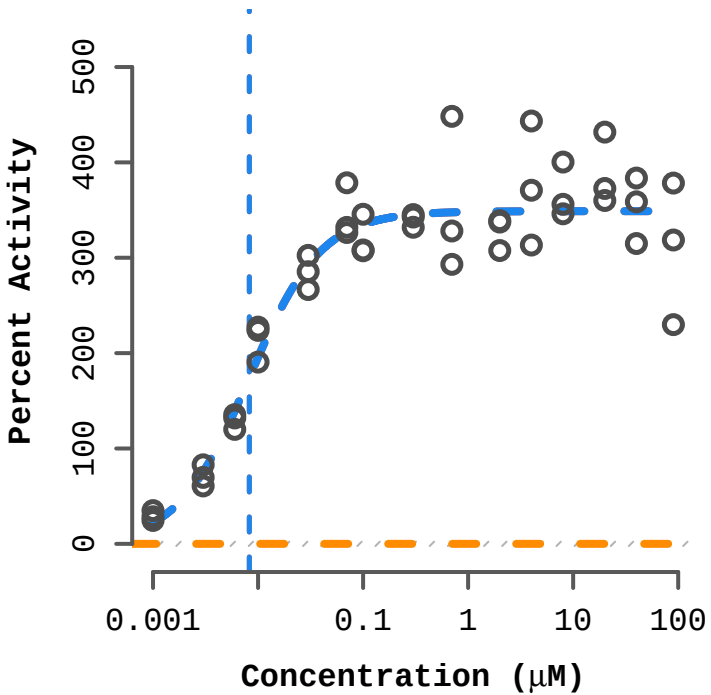
NAME: Toxaphene
CHID: 21368 **CASRN:** 8001-35-2
SPID(S): Tox21_200912
M4ID: 12481340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamcinolone acetonide
CHID: 21371 CASRN: 76-25-5
SPID(S): Tox21_303014
M4ID: 12476119

HILL MODEL (in red):

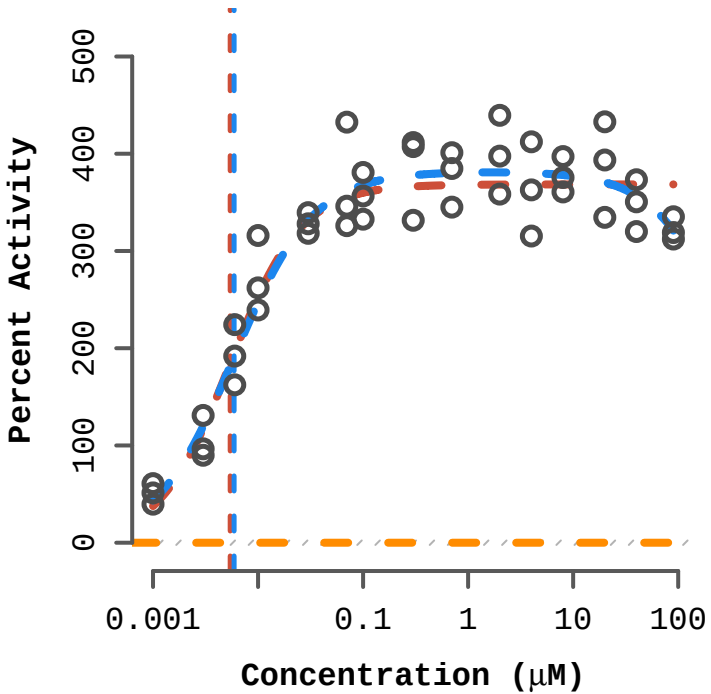
	tp	ga	gw
val:	349	-2.08	1.27
sd:	6.79	0.0416	0.154

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	349	-2.08	1.27	3.79	5.28
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	653.24	453.64	457.64
PROB:	0	0.88	0.12
RMSE:	303.73	37.35	37.35

MAX_MEAN: 388 MAX_MED: 373 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamcinolone acetonide
CHID: 21371 CASRN: 76-25-5
SPID(S): Tox21_201795
M4ID: 12480457

HILL MODEL (in red):

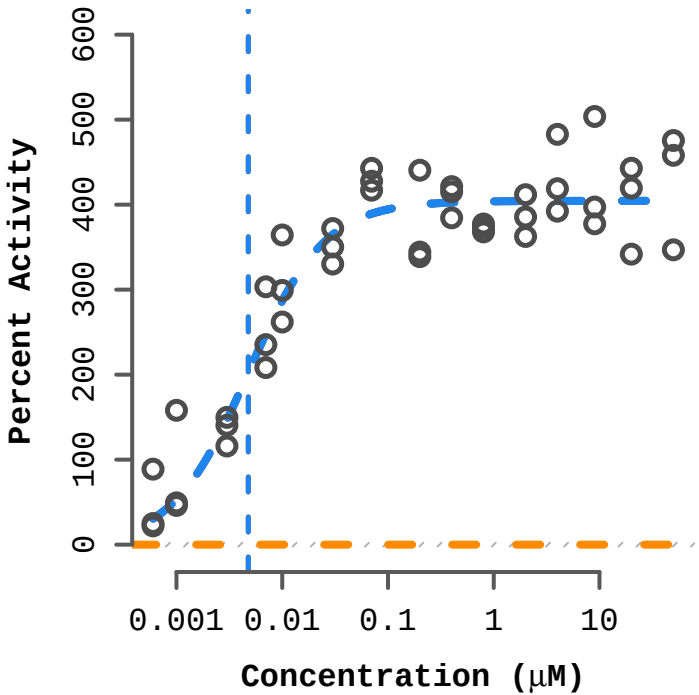
	tp	ga	gw
val:	368	-2.27	1.28
sd:	7.26	0.0442	0.171

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	382	-2.23	1.16	2.55	1.22
sd:	9.5	0.0461	0.141	0.393	0.785

	CNST	HILL	GNLS
AIC:	660.37	455.27	448.17
PROB:	0	0.03	0.97
RMSE:	327.14	33.51	30.22

MAX_MEAN: 399 MAX_MED: 407 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamcinolone acetonide
CHID: 21371 **CASRN:** 76-25-5
SPID(S): Tox21_110885_1
M4ID: 12484042

HILL MODEL (in red):

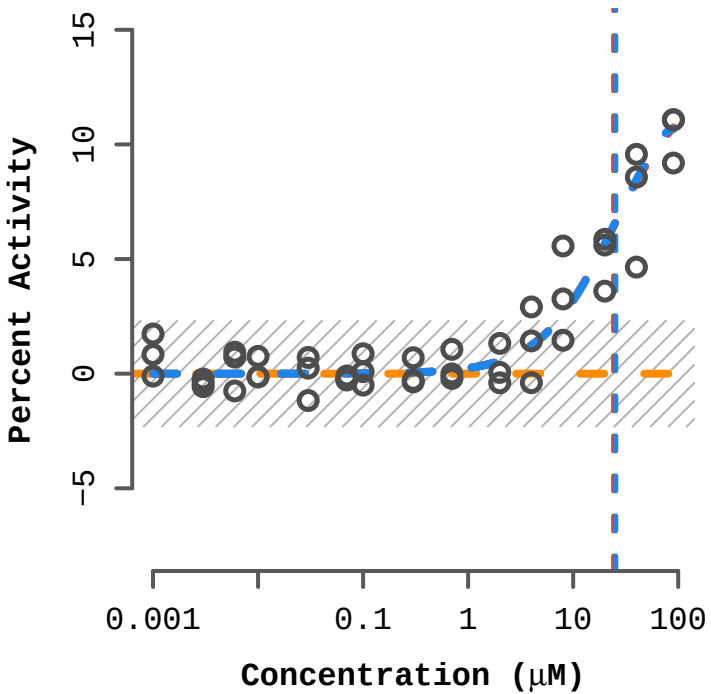
	tp	ga	gw
val:	404	-2.32	1.21
sd:	8.98	0.0531	0.168

GAIN-LOSS MODEL (in blue):

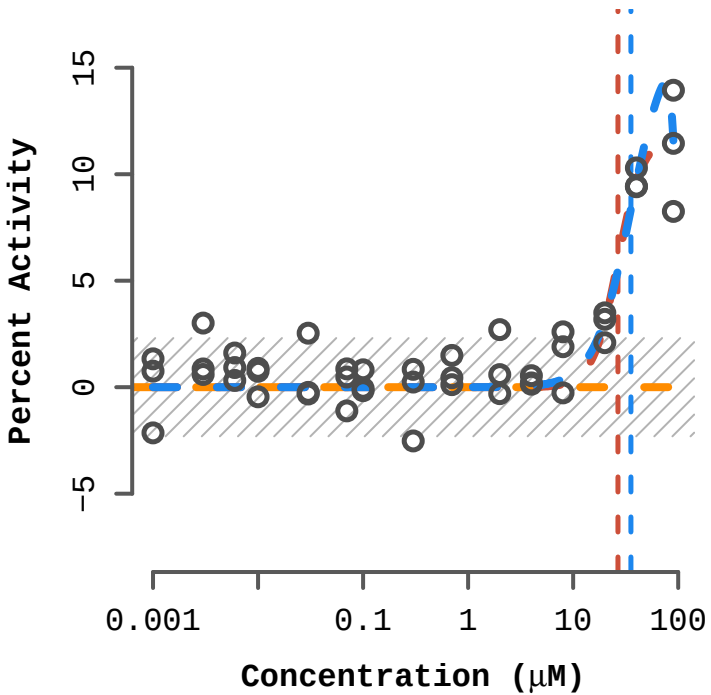
	tp	ga	gw	la	lw
val:	404	-2.32	1.21	2.19	16.7
sd:	8.98	0.0531	0.168	245	8250

	CNST	HILL	GNLS
AIC:	665.55	476.06	480.06
PROB:	0	0.88	0.12
RMSE:	348.09	42.71	42.71

MAX_MEAN: 431 **MAX_MED:** 458 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3,4,4'-Triaminodiphenyl ether
CHID:    21372   CASRN: 6264-66-0
SPID(S): Tox21_301531
M4ID:    12477602

HILL MODEL (in red):
      tp       ga       gw
val:  12.9     1.38     1.24
sd:   1.72     0.125    0.261

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.3     1.41     1.24     2.13     8.83
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  235.45      135.89      139.77
PROB: 0           0.87        0.13
RMSE: 3.84        1.07        1.08

MAX_MEAN: 10.4      MAX_MED: 11.1      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamterene
CHID: 21373 CASRN: 396-01-0
SPID(S): Tox21_302833
M4ID: 12476300

HILL MODEL (in red):

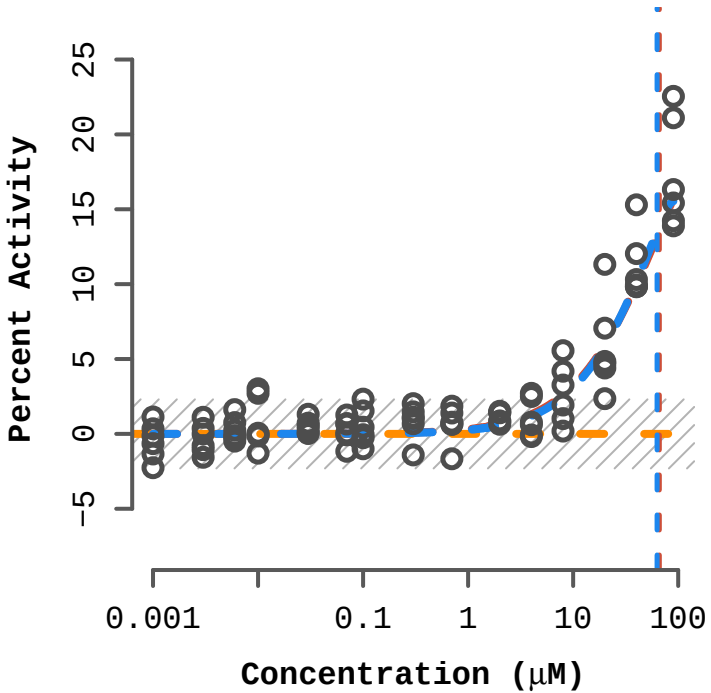
	tp	ga	gw
val:	11.8	1.43	3.64
sd:	1.16	0.0414	0.902

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.7	1.55	2.53	1.99	15.8
sd:	23.8	0.524	2.47	0.0353	46.9

	CNST	HILL	GNLS
AIC:	236.64	158.37	161.45
PROB:	0	0.82	0.18
RMSE:	4.12	1.31	1.29

MAX_MEAN: 11.2 MAX_MED: 11.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamterene
CHID: 21373 CASRN: 396-01-0
SPID(S): Tox21_202021
M4ID: 12480231

HILL MODEL (in red):

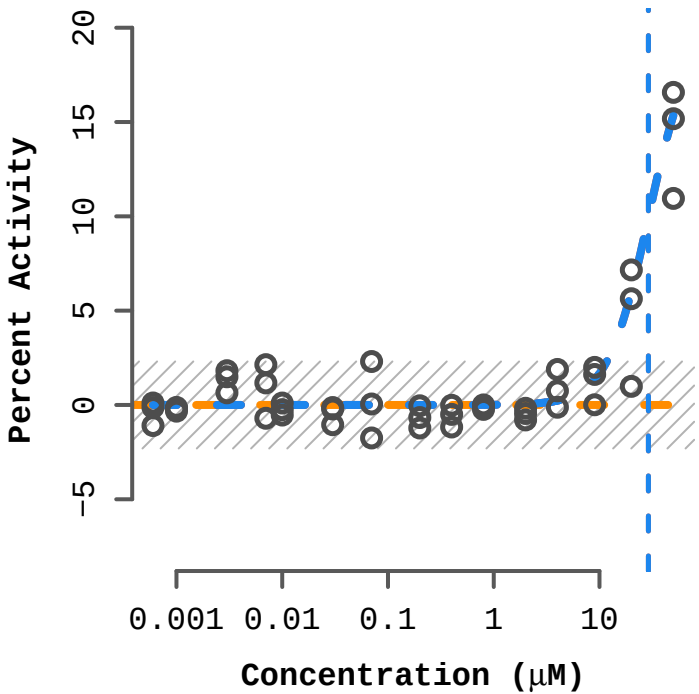
	tp	ga	gw
val:	27.1	1.82	1.06
sd:	8.73	0.271	0.222

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27.1	1.8	1.12	2.08	10.8
sd:	261	6.13	2.12	4.58	110

	CNST	HILL	GNLS
AIC:	524.64	340.76	344.53
PROB:	0	0.87	0.13
RMSE:	5.81	1.71	1.72

MAX_MEAN: 17.3 MAX_MED: 15.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamterene
CHID: 21373 CASRN: 396-01-0
SPID(S): Tox21_110283_1
M4ID: 12484485

HILL MODEL (in red):

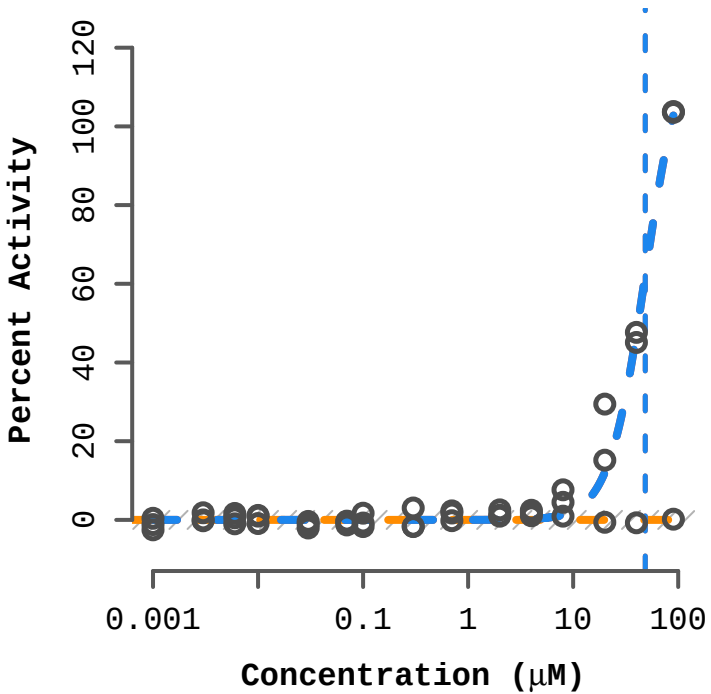
	tp	ga	gw
val:	19.9	1.46	2.24
sd:	4.39	0.119	0.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.9	1.46	2.24	3.68	3.62
sd:	4.39	0.119	0.601	1020	1880

	CNST	HILL	GNLS
AIC:	208.96	149.54	153.54
PROB:	0	0.88	0.12
RMSE:	4.08	1.34	1.34

MAX_MEAN: 14.2 MAX_MED: 15.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bromoform
CHID: 21374 CASRN: 75-25-2
SPID(S): Tox21_200189
M4ID: 12482063

HILL MODEL (in red):

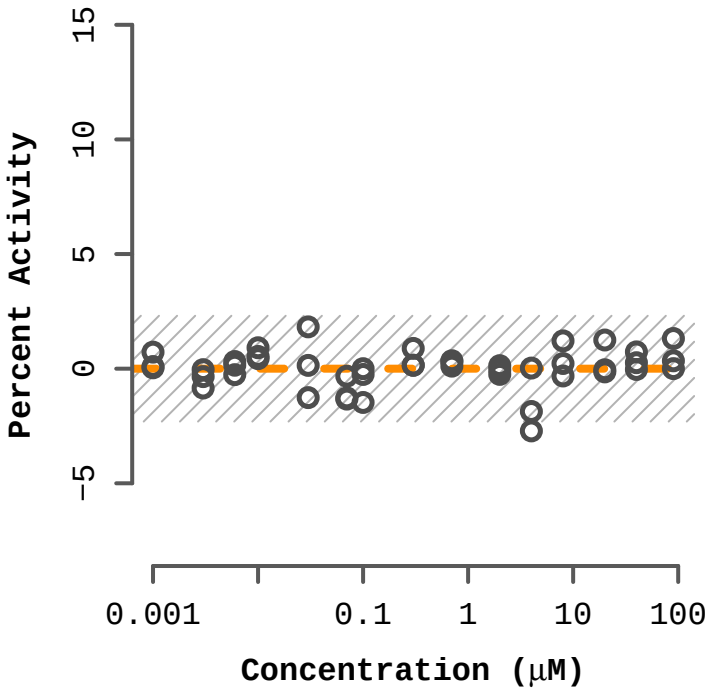
	tp	ga	gw
val:	125	1.69	2.52
sd:	5.88	0.0213	0.265

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	125	1.69	2.52	3.93	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	330.33	275.92	279.92
PROB:	0	0.88	0.12
RMSE:	24.52	17.28	17.28

MAX_MEAN: 69.2 MAX_MED: 104 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

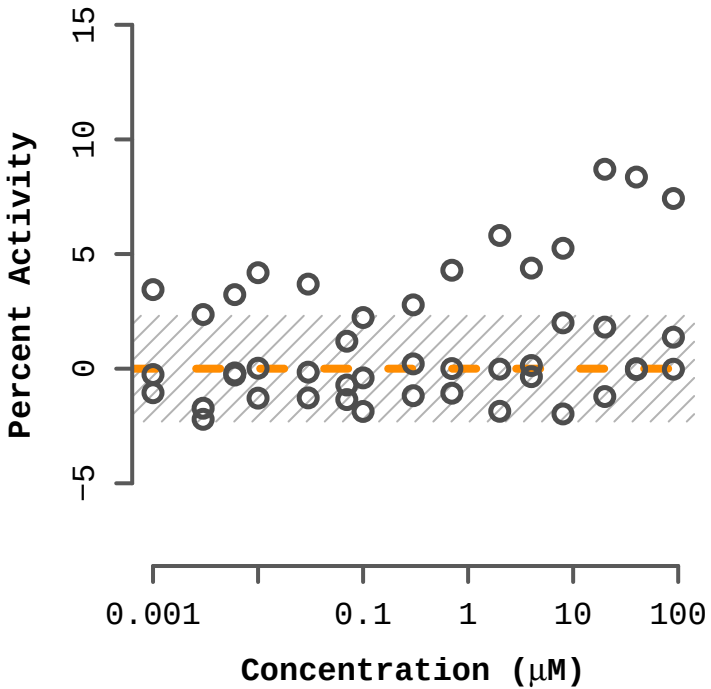
NAME: Tricaprylin
CHID: 21375 **CASRN:** 538-23-8
SPID(S): Tox21_302762
M4ID: 12476371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.629 **MAX_MED:** 0.535 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

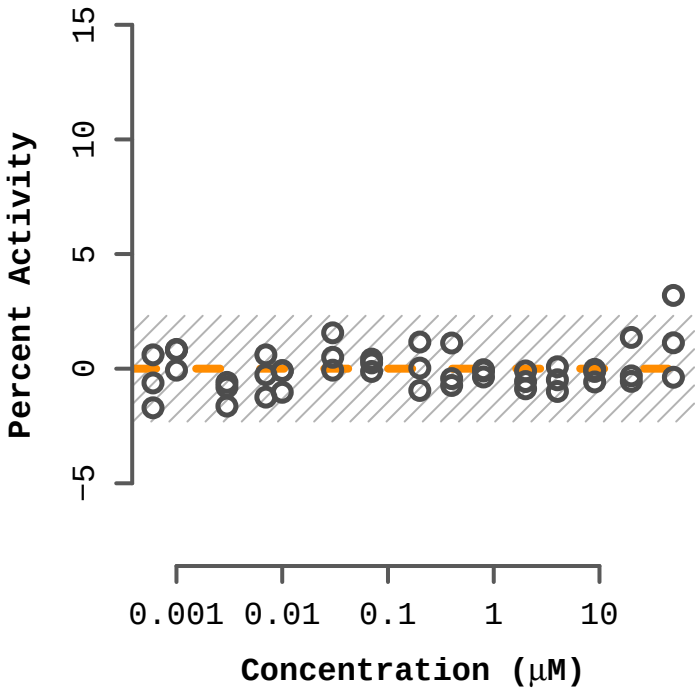
NAME: Tricaprylin
CHID: 21375 CASRN: 538-23-8
SPID(S): Tox21_201480
M4ID: 12480772

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.08	NA	NA
PROB:	1	NA	NA
RMSE:	3.03	NA	NA

MAX_MEAN: 3.1 MAX_MED: 2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

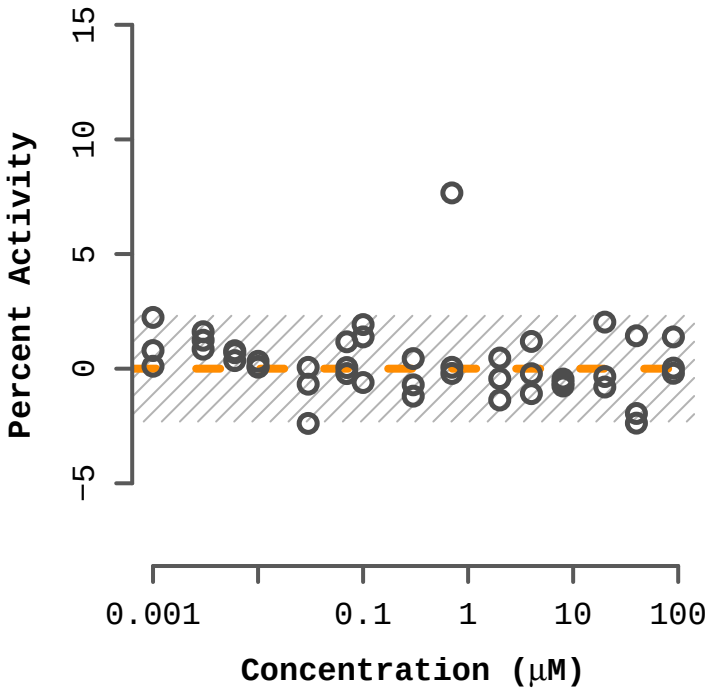
NAME: Tricaprylin
CHID: 21375 CASRN: 538-23-8
SPID(S): Tox21_111110_1
M4ID: 12483902

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

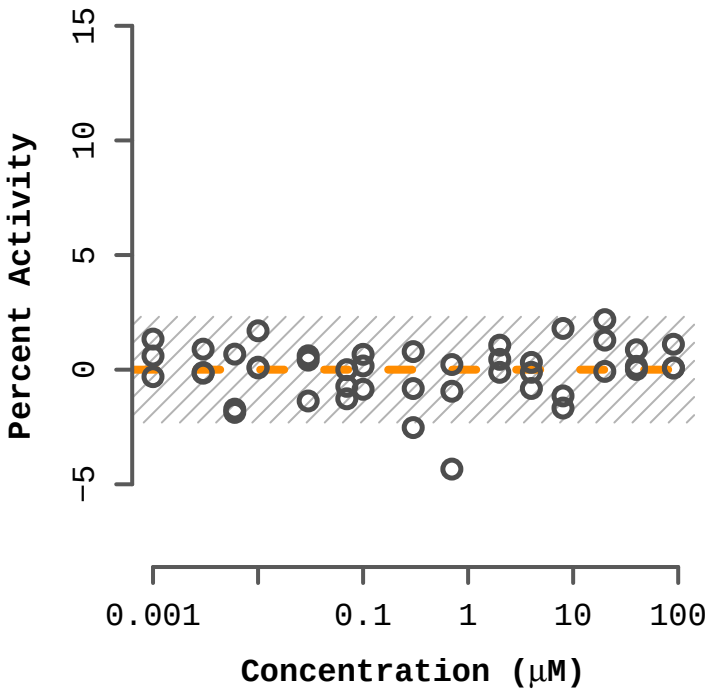
NAME: 1,1,2−Trichloro−1,2,2−trifluoroethane
CHID: 21377 CASRN: 76−13−1
SPID(S): Tox21_200401
M4ID: 12481851

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 2.51 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

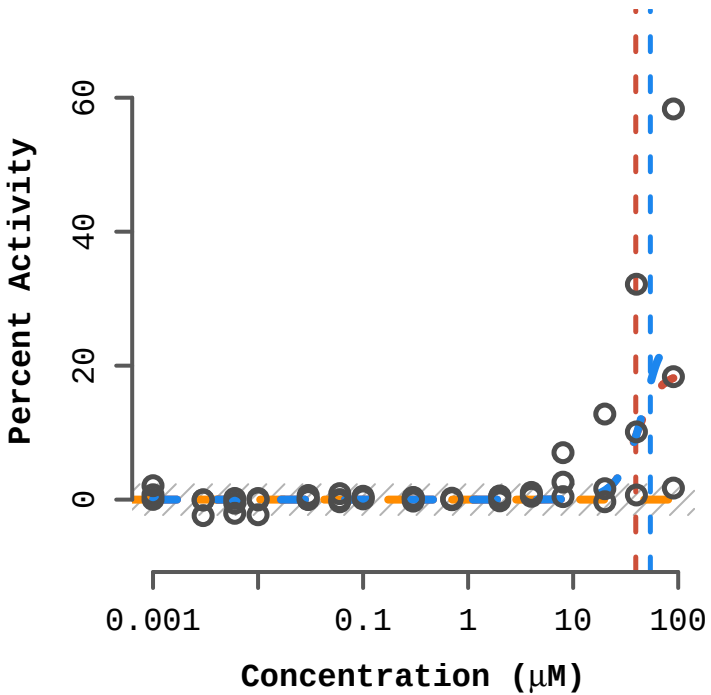
NAME: Trichloroacetic acid
CHID: 21378 **CASRN:** 76-03-9
SPID(S): Tox21_300187
M4ID: 12478943

HILL MODEL: Not applicable.

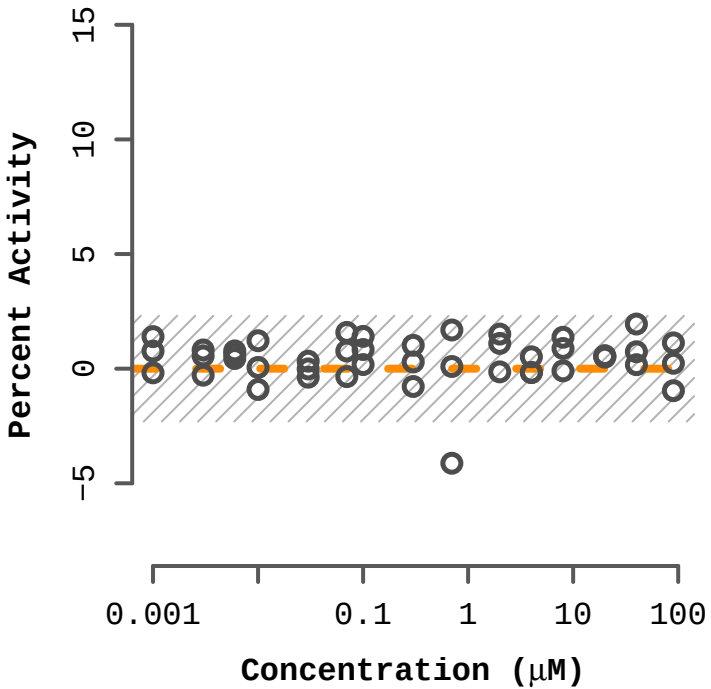
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.29 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Trichloroacetic acid
CHID:    21378   CASRN: 76-03-9
SPID(S): Tox21_201632
M4ID:    12480620

HILL MODEL (in red):
      tp       ga       gw
val:  18.9     1.6      3.91
sd:   1.79     0.0404   1.64

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  35.8     1.73     3.23     1.98     6.05
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  252.36      245.79      249.68
PROB: 0.03        0.85        0.12
RMSE: 10.67       7.73        7.72

MAX_MEAN: 26.1      MAX_MED: 18.4      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

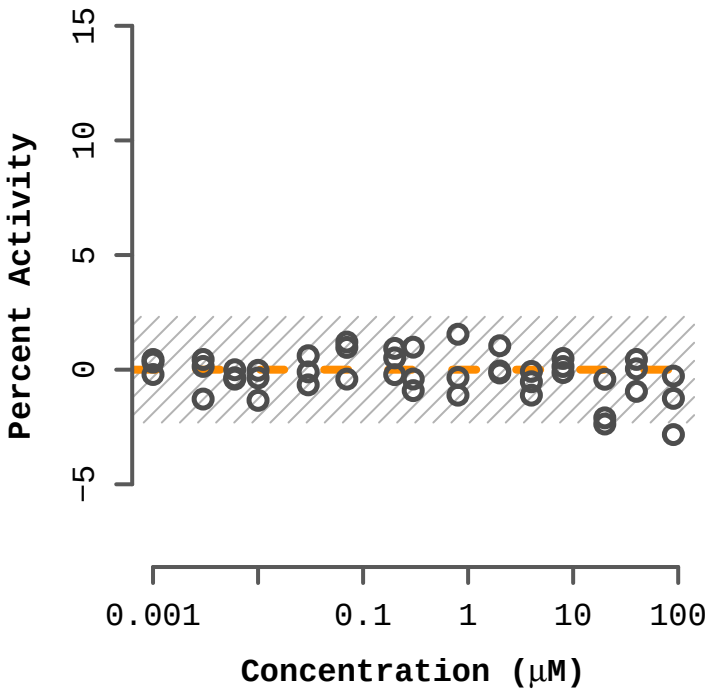
NAME: 2,4,6-Trichloroaniline
CHID: 21379 **CASRN:** 634-93-5
SPID(S): Tox21_201063
M4ID: 12481189

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.955 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

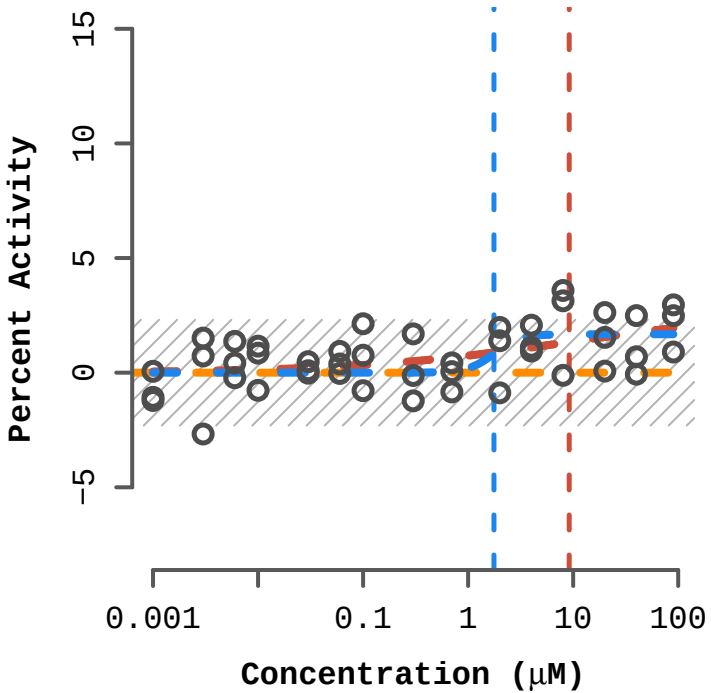
NAME: 1,1,2−Trichloroethane
CHID: 21380 **CASRN:** 79−00−5
SPID(S): Tox21_202465
M4ID: 12479787

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.589 **MAX_MED:** 0.972 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1,1−Trichloroethane
CHID: 21381 **CASRN:** 71−55−6
SPID(S): Tox21_203122
M4ID: 12479130

HILL MODEL (in red):

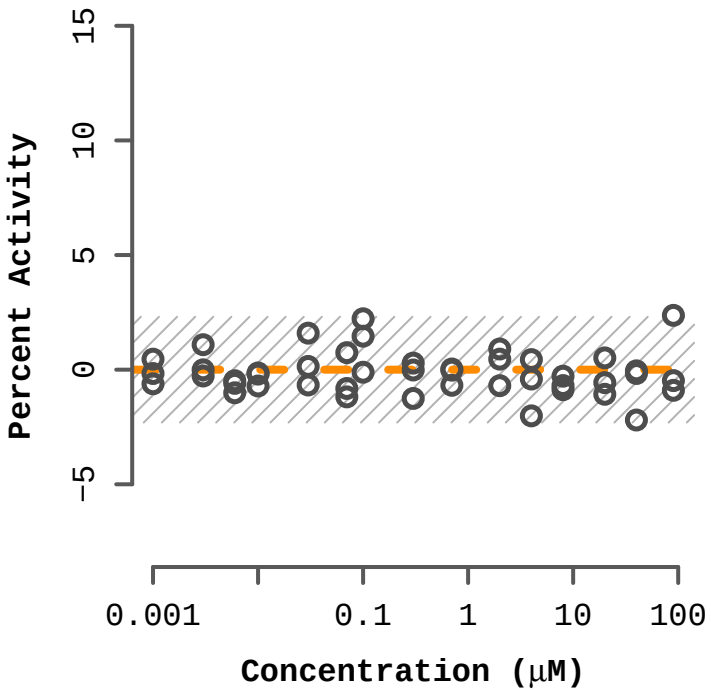
	tp	ga	gw
val:	2.67	0.962	0.43
sd:	3.7	3.25	0.549

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.68	0.246	3.6	3.72	5.66
sd:	0.425	0.248	6.71	18600	59900

	CNST	HILL	GNLS
AIC:	166.13	150.54	153.44
PROB:	0	0.81	0.19
RMSE:	1.47	1.12	1.11

MAX_MEAN: 2.2 **MAX_MED:** 3.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

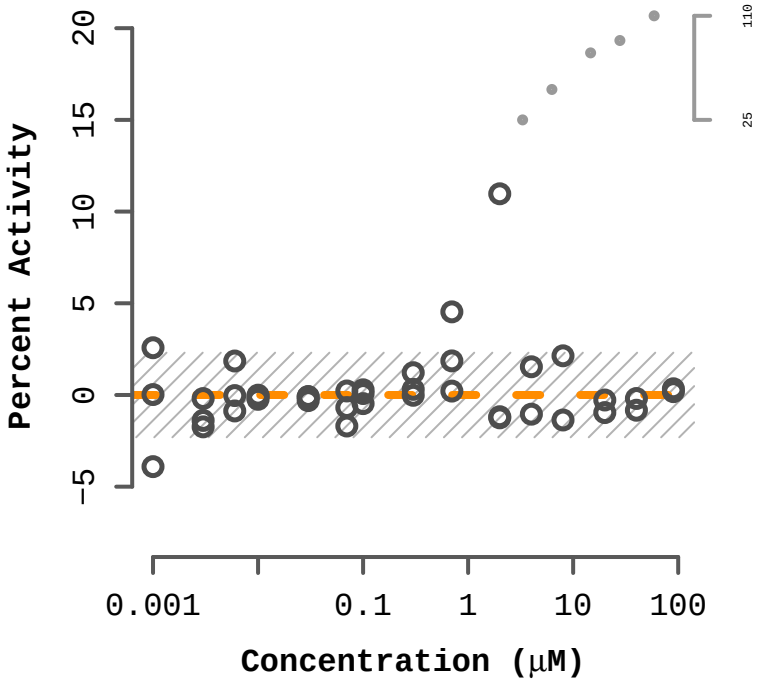
NAME: Trichloroethylene
CHID: 21383 **CASRN:** 79-01-6
SPID(S): Tox21_202543
M4ID: 12479709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

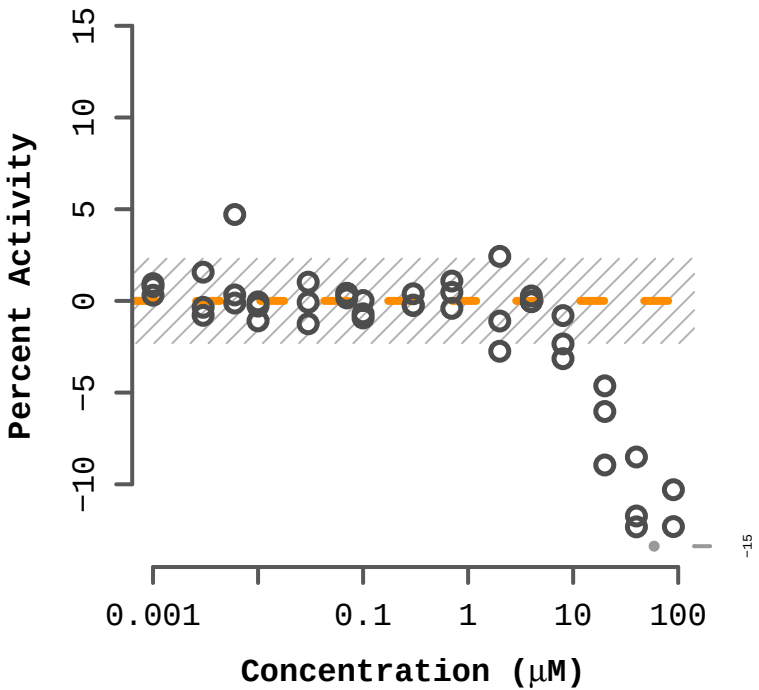
NAME: Trichlorofluoromethane
CHID: 21384 **CASRN:** 75-69-4
SPID(S): Tox21_201190
M4ID: 12481062 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	321.36	NA	NA
PROB:	1	NA	NA
RMSE:	26.7	NA	NA

MAX_MEAN: 38.4 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

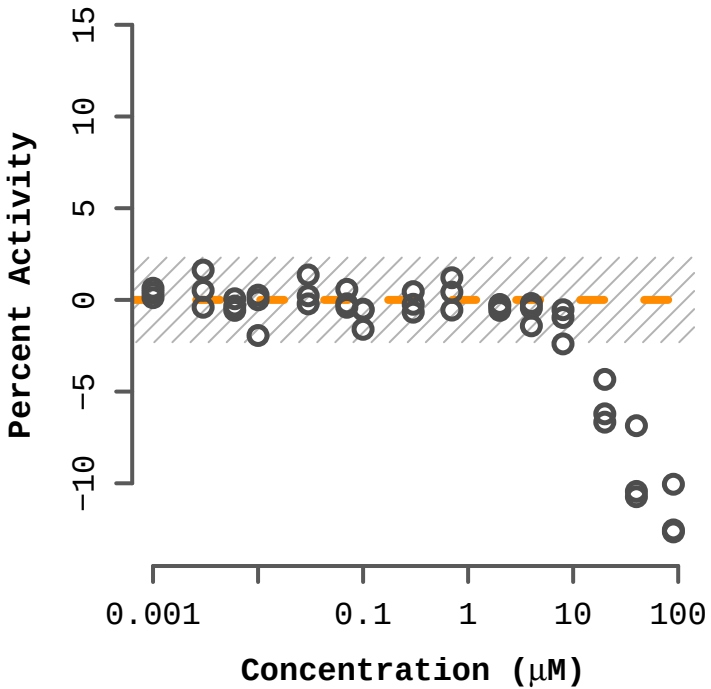
NAME: Folpet
CHID: 21385 **CASRN:** 133-07-3
SPID(S): Tox21_301077
M4ID: 12478056 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253.85	NA	NA
PROB:	1	NA	NA
RMSE:	4.81	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 0.781 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

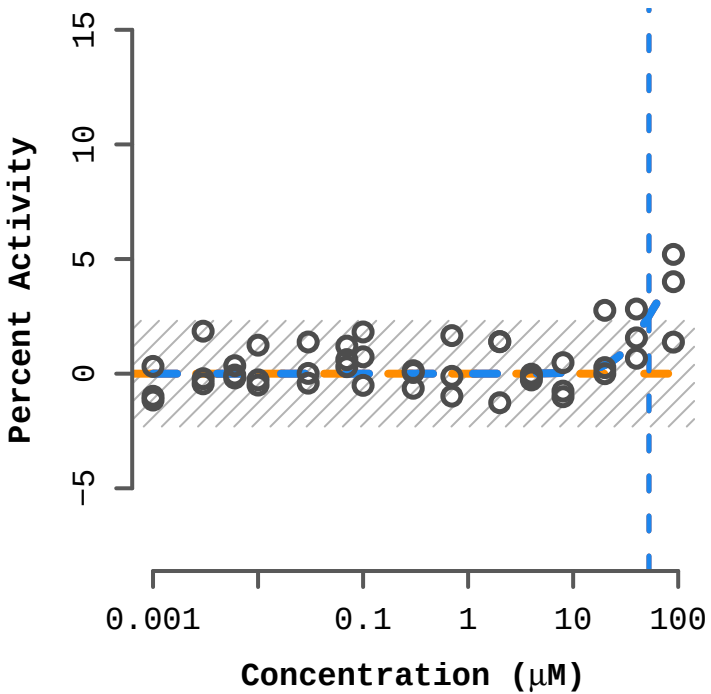
NAME: Folpet
CHID: 21385 **CASRN:** 133-07-3
SPID(S): Tox21_201987
M4ID: 12480265

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	238.1	NA	NA
PROB:	1	NA	NA
RMSE:	4.26	NA	NA

MAX_MEAN: 0.583 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,6-Trichlorophenol
CHID: 21386 CASRN: 88-06-2
SPID(S): Tox21_300189
M4ID: 12478941

HILL MODEL (in red):

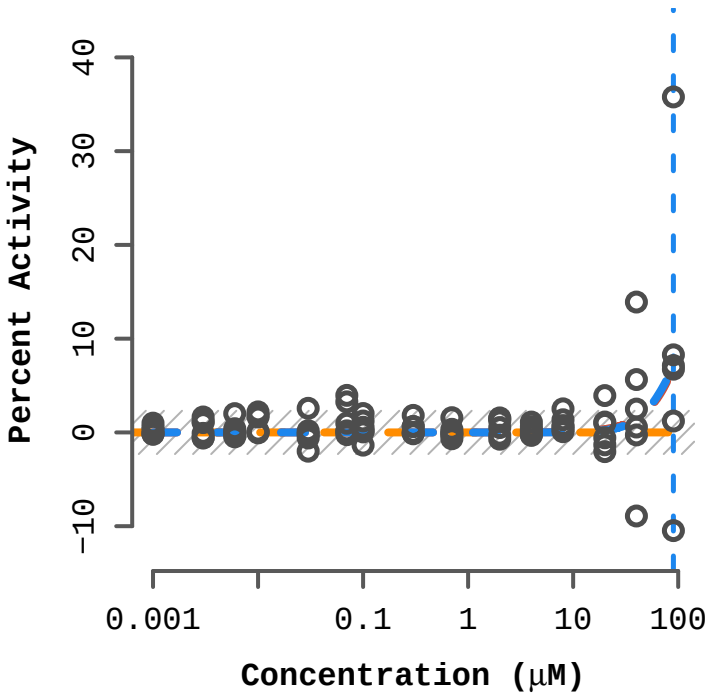
	tp	ga	gw
val:	5.07	1.72	2.6
sd:	2.95	0.277	2.01

GAIN-LOSS MODEL (in blue):

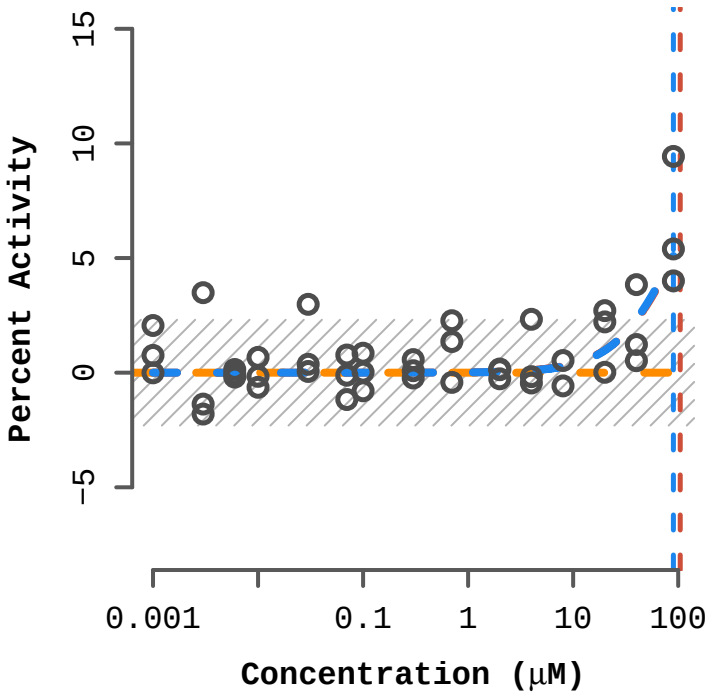
	tp	ga	gw	la	lw
val:	5.07	1.72	2.6	3.61	3.3
sd:	2.96	0.277	2.01	858	1800

	CNST	HILL	GNLS
AIC:	152.87	136.11	140.11
PROB:	0	0.88	0.12
RMSE:	1.43	1	1

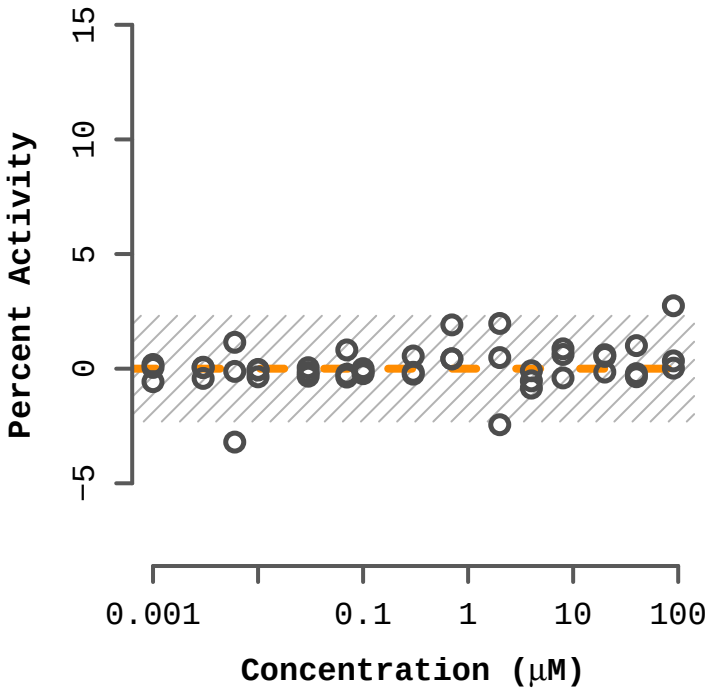
MAX_MEAN: 3.53 MAX_MED: 4.01 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,4,6-Trichlorophenol
CHID:    21386   CASRN: 88-06-2
SPID(S): Tox21_202037
M4ID:    12480215

HILL MODEL (in red):
      tp       ga       gw
val:  42.9     2.29     2.11
sd:   53.4     0.272    0.723

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  14       1.95     2.72     3.25     11.2
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  405.38      386.35      390.46
PROB: 0           0.89        0.11
RMSE: 4.7         4.18        4.18

MAX_MEAN: 8.12      MAX_MED: 6.94      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-(2,4,5-Trichlorophenoxy)propionic acid
CHID:    21387   CASRN: 93-72-1
SPID(S): Tox21_200761
M4ID:    12481491

HILL MODEL (in red):
      tp       ga       gw
val:  11.3     2.02     1.42
sd:   11.3     0.563    0.731

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.2     1.95     1.5      3.77     6.75
sd:   10.9     0.596    0.786    225000   832000

      CNST        HILL        GNLS
AIC:  178.94      155.67      159.75
PROB: 0           0.88        0.12
RMSE: 2.2         1.36        1.36

MAX_MEAN: 6.28      MAX_MED: 5.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

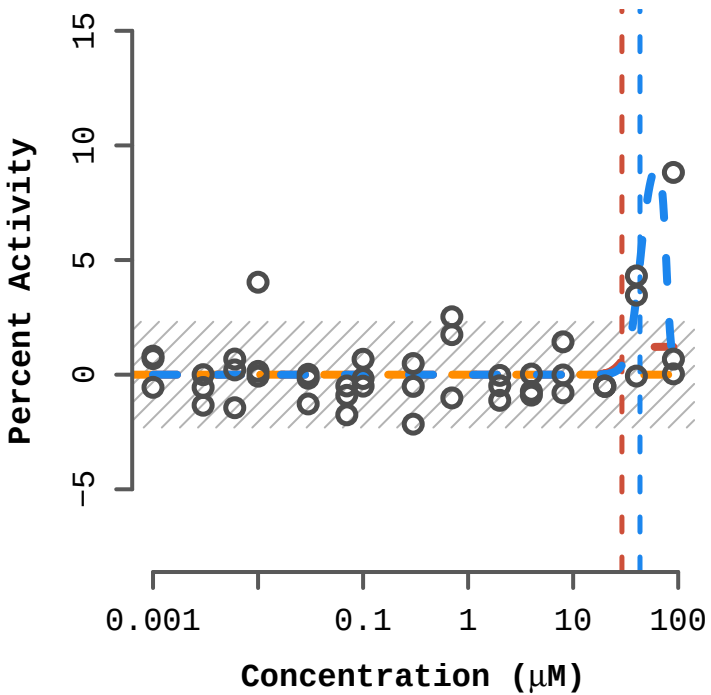
NAME: 2,4,5−Trichlorophenoxyacetic acid
CHID: 21388 **CASRN:** 93−76−5
SPID(S): Tox21_302882
M4ID: 12476251

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.622 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,5−Trichlorophenoxyacetic acid
CHID: 21388 CASRN: 93−76−5
SPID(S): Tox21_201605
M4ID: 12480647

HILL MODEL (in red):

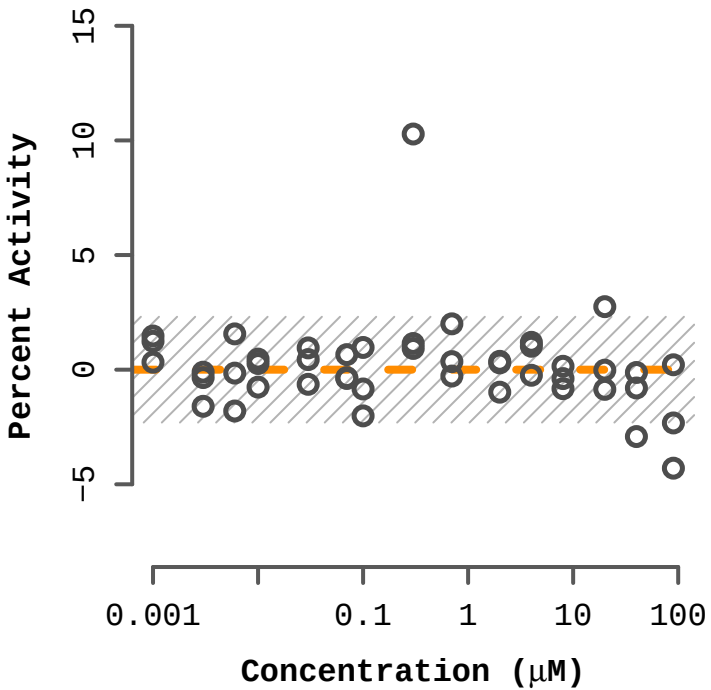
	tp	ga	gw
val:	1.22	1.46	8
sd:	0.88	0.125	6.91

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.78	1.64	7.92	1.89	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.01	165.66	164.16
PROB:	0.55	0.15	0.31
RMSE:	1.88	1.68	1.71

MAX_MEAN: 3.18 MAX_MED: 3.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

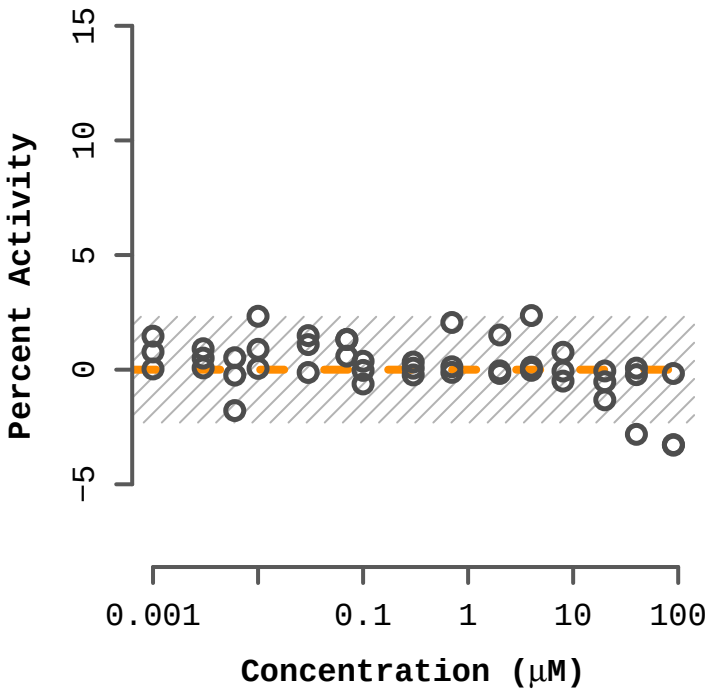
NAME: Trichlorfon
CHID: 21389 **CASRN:** 52-68-6
SPID(S): Tox21_300860
M4ID: 12478273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 4.12 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

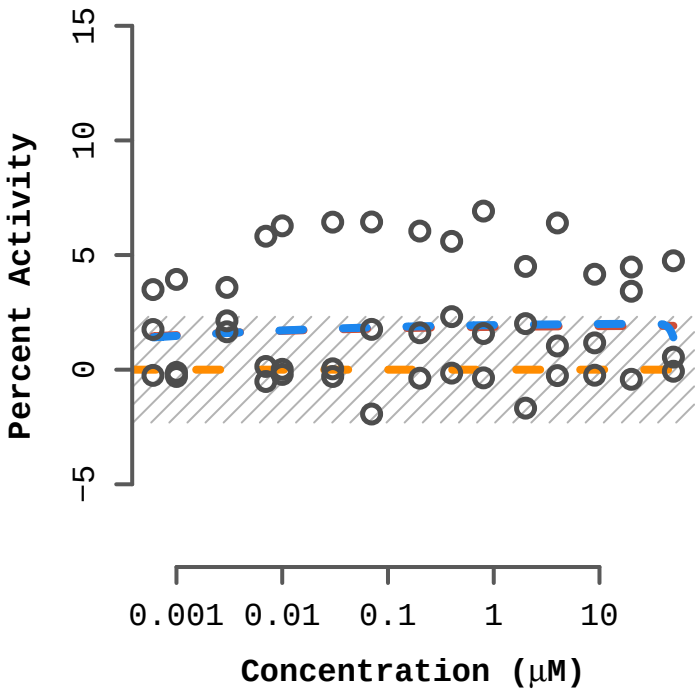
NAME: Trichlorfon
CHID: 21389 **CASRN:** 52-68-6
SPID(S): Tox21_201607
M4ID: 12480645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trichlorfon
CHID: 21389 CASRN: 52-68-6
SPID(S): Tox21_110843_1
M4ID: 12484076

HILL MODEL (in red):

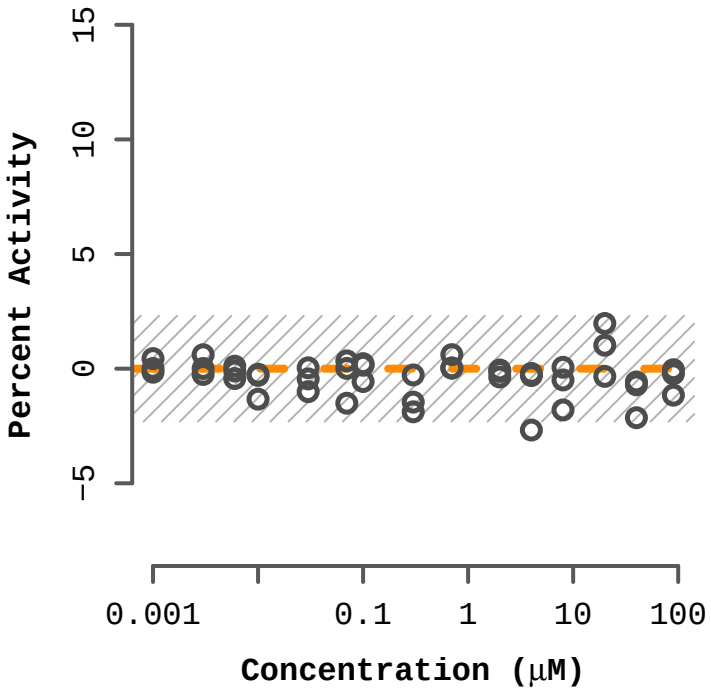
	tp	ga	gw
val:	1.93	−4.83	0.3
sd:	1.25	10.3	2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.04	−4.38	0.3	1.73	13.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	237.62	225.72	229.59
PROB:	0	0.87	0.13
RMSE:	3.28	2.56	2.55

MAX_MEAN: 2.71 **MAX_MED:** 3.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

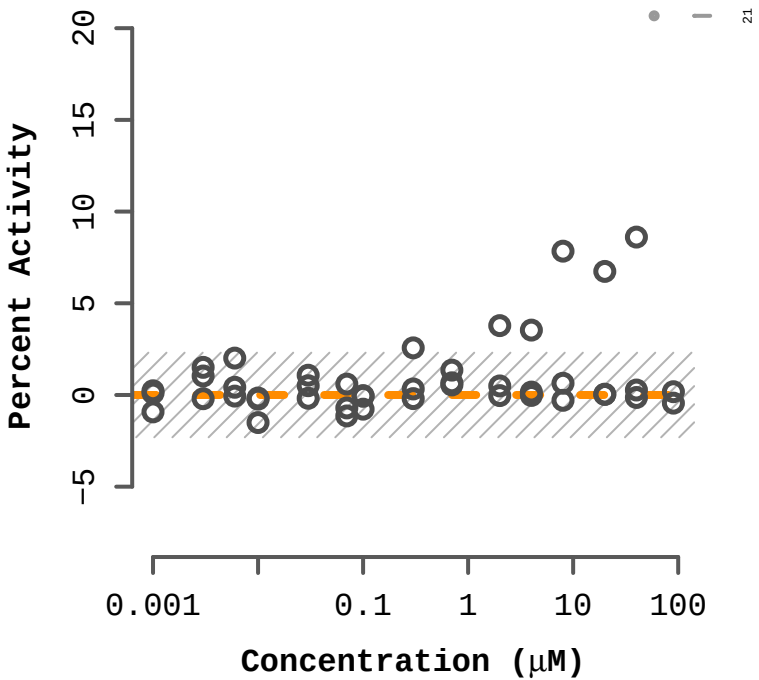
NAME: 1,2,3-Trichloropropane
CHID: 21390 **CASRN:** 96-18-4
SPID(S): Tox21_302963
M4ID: 12476170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.887 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

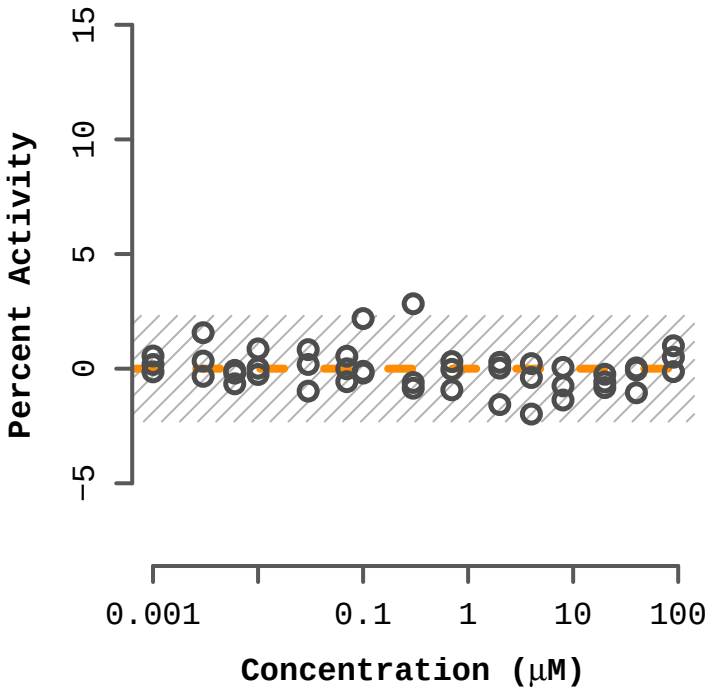
NAME: 1,2,3-Trichloropropane
CHID: 21390 CASRN: 96-18-4
SPID(S): Tox21_202023
M4ID: 12480229 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.25	NA	NA
PROB:	1	NA	NA
RMSE:	3.84	NA	NA

MAX_MEAN: 6.83 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

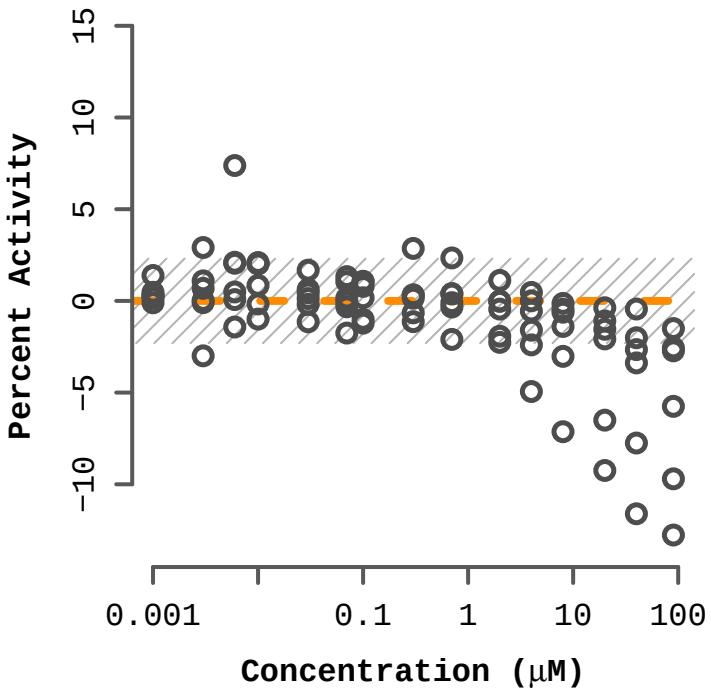
NAME: Tricresyl phosphate
CHID: 21391 **CASRN:** 1330-78-5
SPID(S): Tox21_302886
M4ID: 12476247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.627 **MAX_MED:** 0.501 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

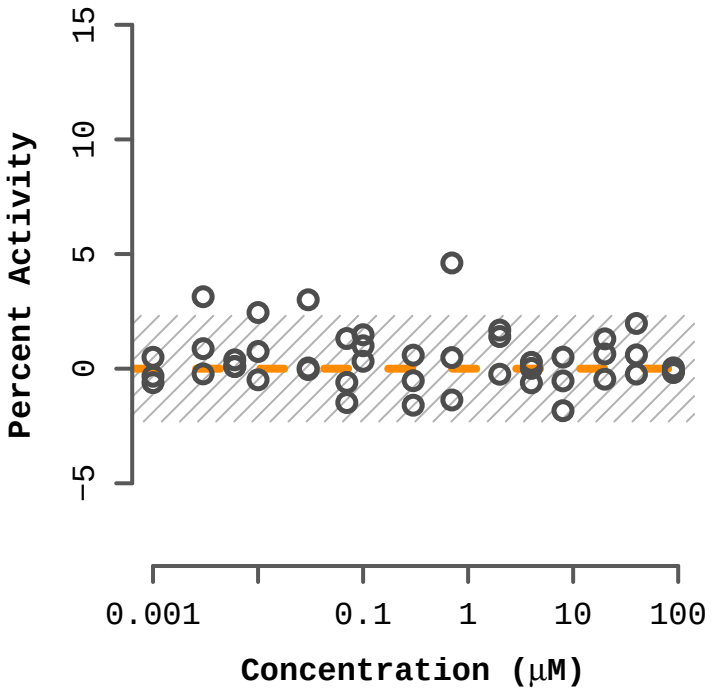
NAME: Tricresyl phosphate
CHID: 21391 **CASRN:** 1330-78-5
SPID(S): Tox21_201546
M4ID: 12480706

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	425.95	NA	NA
PROB:	1	NA	NA
RMSE:	3.17	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

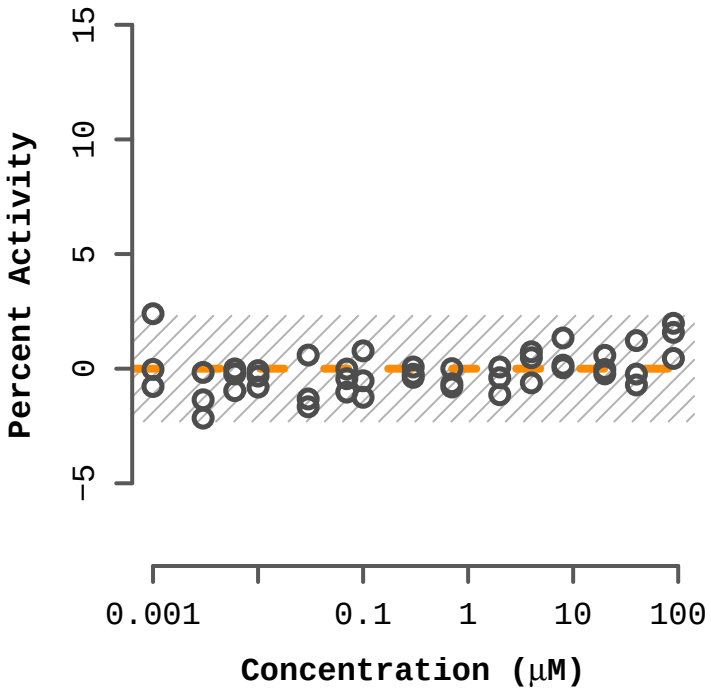
NAME: Triethanolamine
CHID: 21392 **CASRN:** 102-71-6
SPID(S): Tox21_300527
M4ID: 12478605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

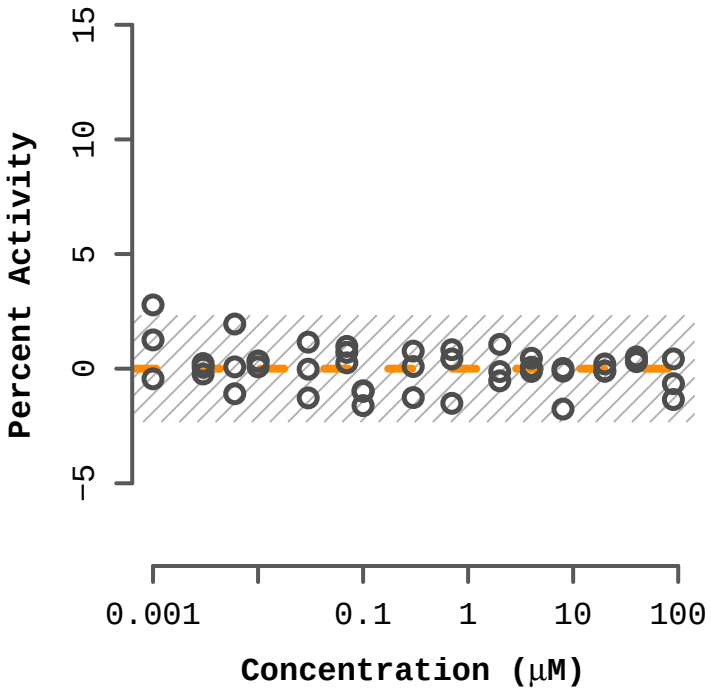
NAME: Triethanolamine
CHID: 21392 **CASRN:** 102-71-6
SPID(S): Tox21_202062
M4ID: 12480190

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

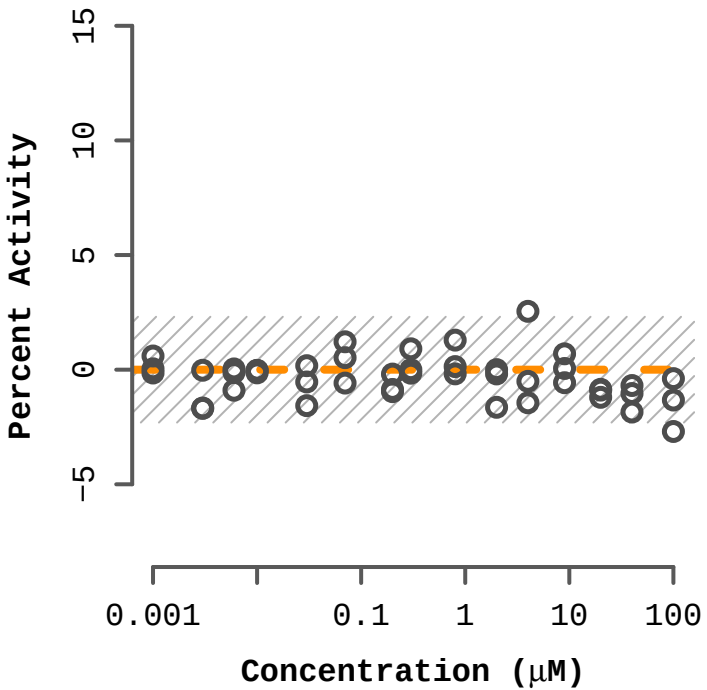
NAME: Triethylene glycol
CHID: 21393 CASRN: 112-27-6
SPID(S): Tox21_300306
M4ID: 12478824

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.2 MAX_MED: 1.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

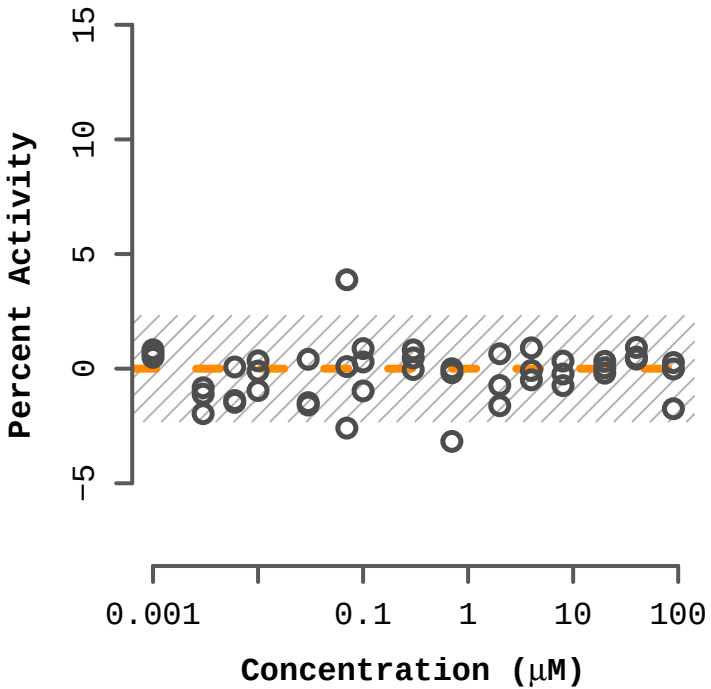
NAME: Triethylene glycol
CHID: 21393 CASRN: 112-27-6
SPID(S): Tox21_202440
M4ID: 12479812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.415 **MAX_MED:** 0.526 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

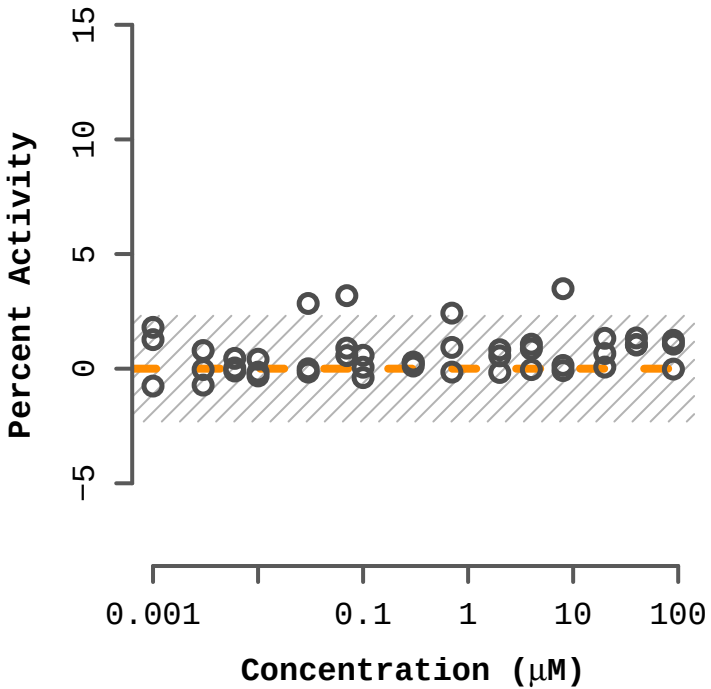
NAME: Trifluralin
CHID: 21395 **CASRN:** 1582-09-8
SPID(S): Tox21_300918
M4ID: 12478215

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.661 **MAX_MED:** 0.662 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

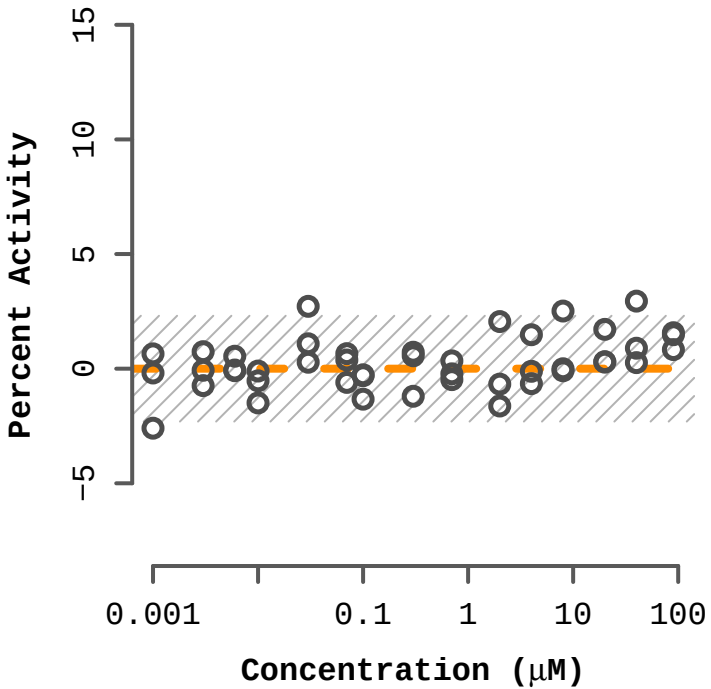
NAME: Trifluralin
CHID: 21395 CASRN: 1582-09-8
SPID(S): Tox21_201352
M4ID: 12480900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.55 MAX_MED: 1.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

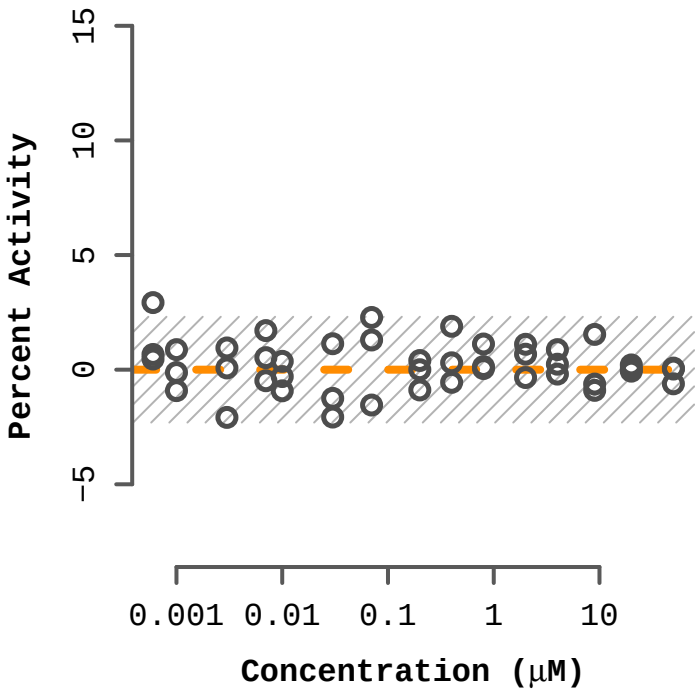
NAME: Trimethadione
CHID: 21396 **CASRN:** 127-48-0
SPID(S): Tox21_200231
M4ID: 12482021

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (+−)−7−(3,5,6−trimethyl−1,4−benzoquinon−2−yl)−

CHID: 21397 **CASRN:** 112665−43−7

SPID(S): Tox21_112774_1

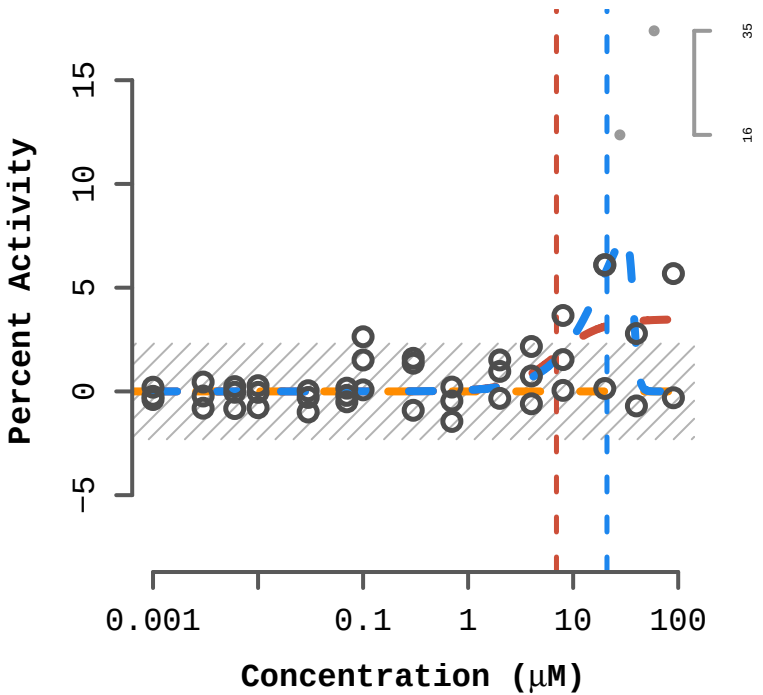
M4ID: 12482959

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,5-Trimethylaniline
CHID: 21398 CASRN: 137-17-7
SPID(S): Tox21_201118
M4ID: 12481134 BRK

HILL MODEL (in red):

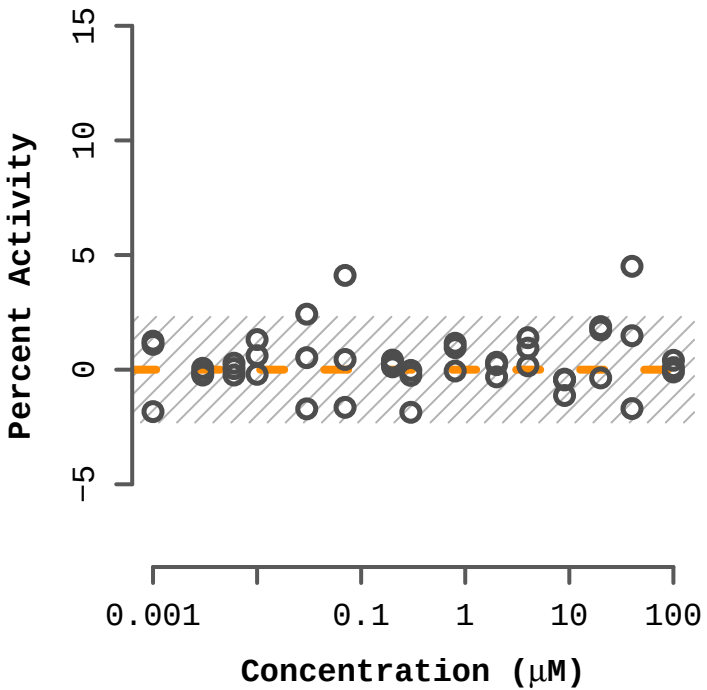
	tp	ga	gw
val:	3.48	0.841	2.04
sd:	1.6	0.255	2.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.8	1.32	1.69	1.57	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	214.86	208.99	208.54
PROB:	0.02	0.43	0.54
RMSE:	6.01	5.25	5.8

MAX_MEAN: 13.5 MAX_MED: 6.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

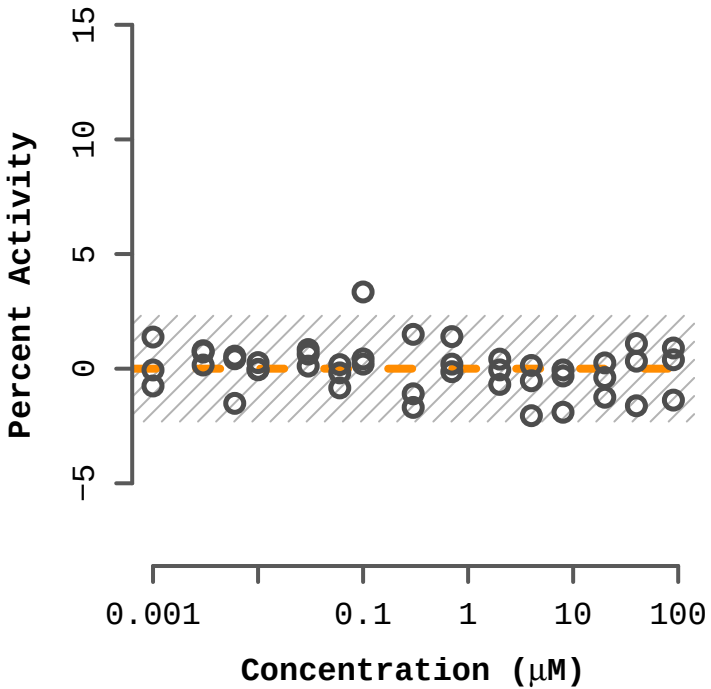
NAME: 1,2,4−Trimethylbenzene
CHID: 21402 **CASRN:** 95−63−6
SPID(S): Tox21_300049
M4ID: 12479081

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

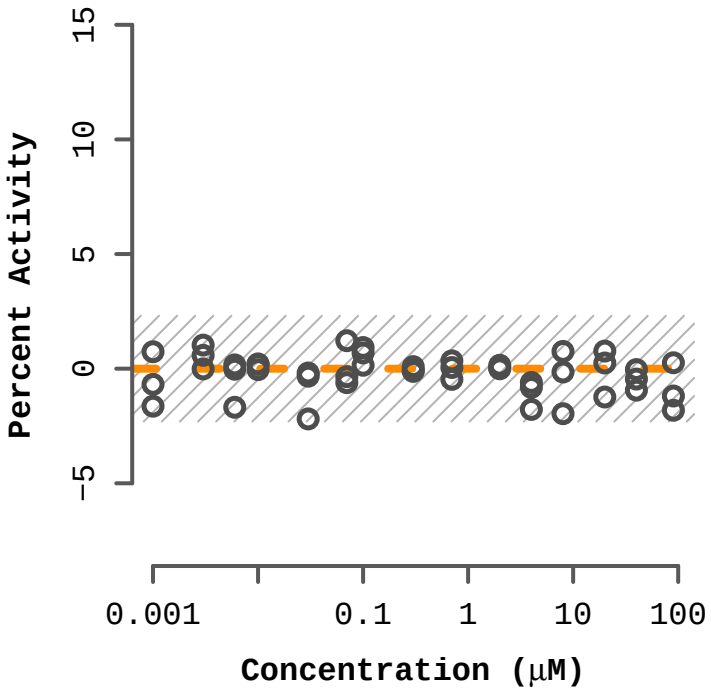
NAME: 1,2,4−Trimethylbenzene
CHID: 21402 **CASRN:** 95−63−6
SPID(S): Tox21_200518
M4ID: 12481734

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.728 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

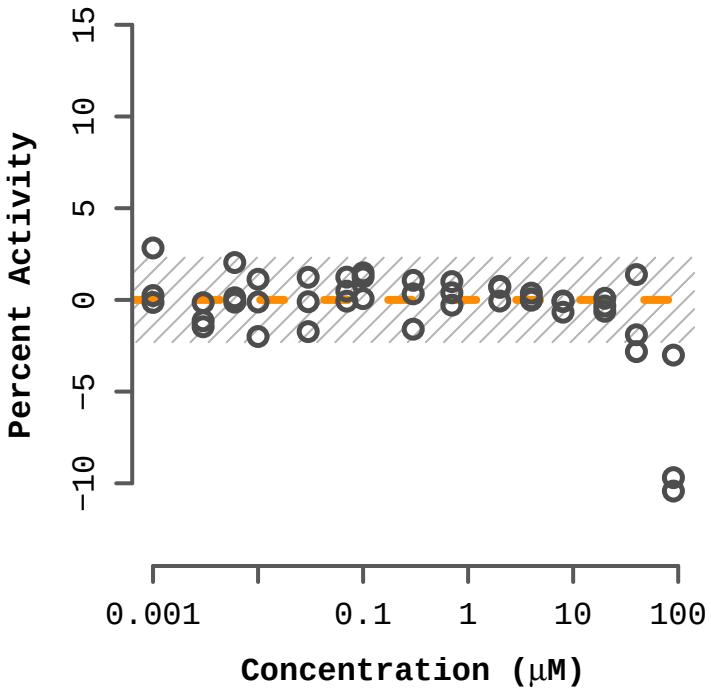
NAME: Trimethyl phosphate
CHID: 21403 CASRN: 512-56-1
SPID(S): Tox21_302740
M4ID: 12476393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.587 **MAX_MED:** 0.688 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

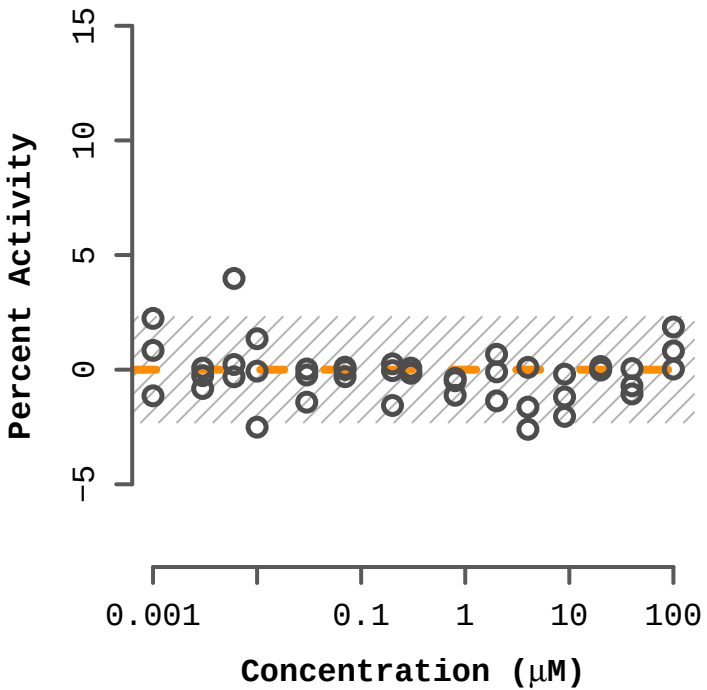
NAME: Trimethyl phosphate
CHID: 21403 **CASRN:** 512-56-1
SPID(S): Tox21_201576
M4ID: 12480676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.42	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

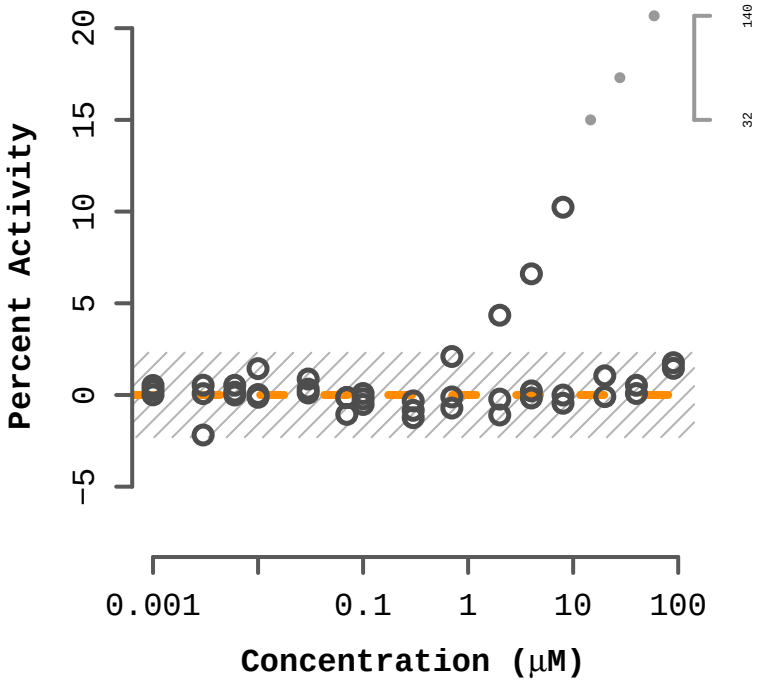
NAME: 1,1,3-Trimethyl-2-thiourea
CHID: 21404 **CASRN:** 2489-77-2
SPID(S): Tox21_302853
M4ID: 12476280

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.842 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

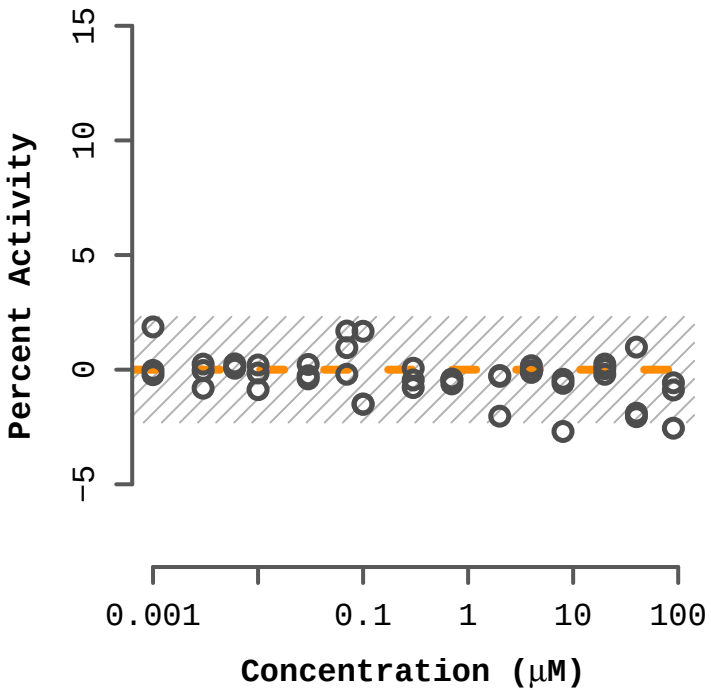
NAME: 1,1,3-Trimethyl-2-thiourea
CHID: 21404 **CASRN:** 2489-77-2
SPID(S): Tox21_201733
M4ID: 12480519 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	259.14	NA	NA
PROB:	1	NA	NA
RMSE:	24.7	NA	NA

MAX_MEAN: 48.7 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

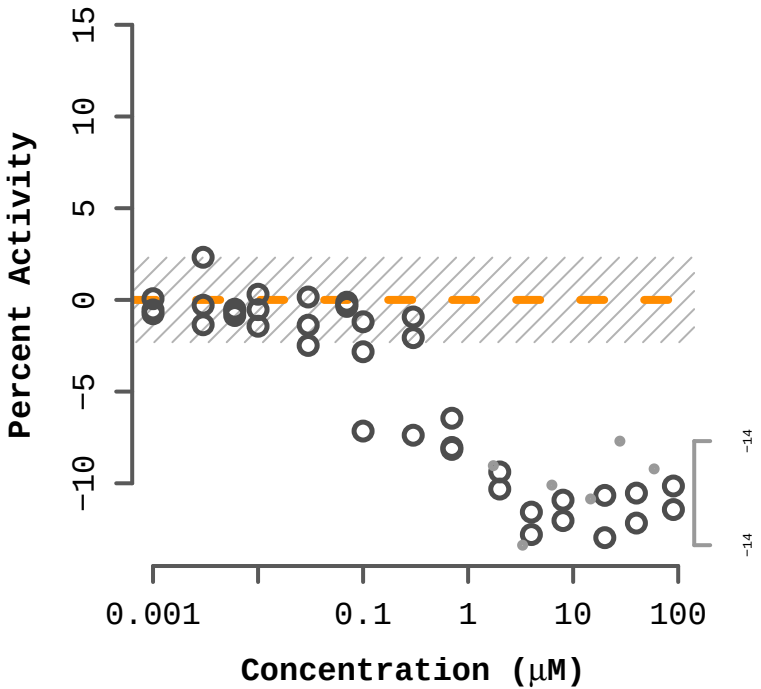
NAME: 2,4,6-Trinitro-1,3-dimethyl-5-tert-butylbenzen
CHID: 21405 **CASRN:** 81-15-2
SPID(S): Tox21_302248
M4ID: 12476885

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.817 **MAX_MED:** 0.961 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

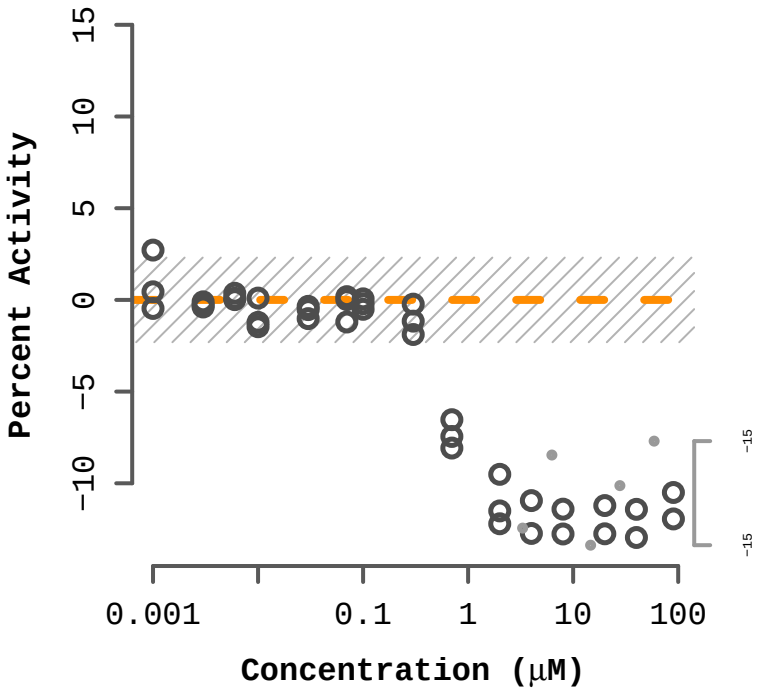
NAME: Triphenyltin acetate
CHID: 21408 **CASRN:** 900-95-8
SPID(S): Tox21_202600
M4ID: 12479652 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	322.69	NA	NA
PROB:	1	NA	NA
RMSE:	8.14	NA	NA

MAX_MEAN: 0.228 **MAX_MED:** −0.267 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

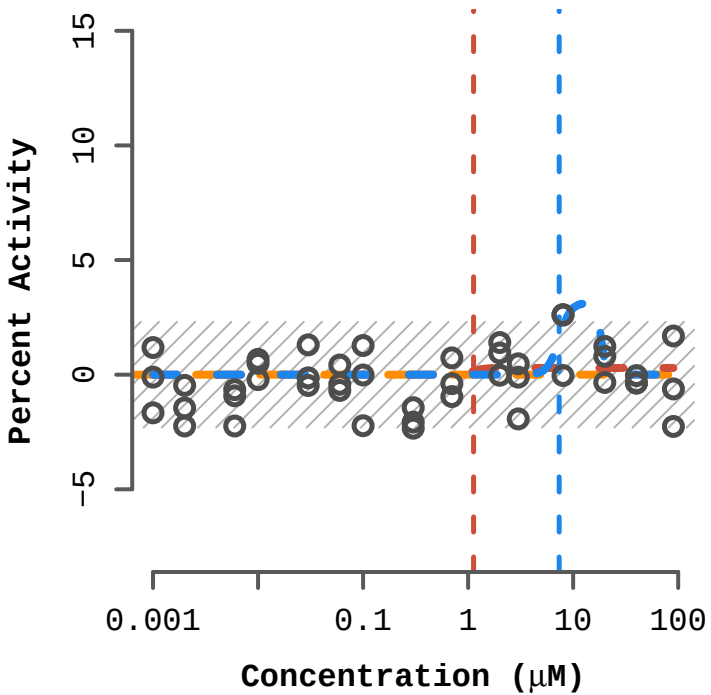
NAME: Triphenyltin hydroxide
CHID: 21409 CASRN: 76-87-9
SPID(S): Tox21_300754
M4ID: 12478379 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	322.95	NA	NA
PROB:	1	NA	NA
RMSE:	8.28	NA	NA

MAX_MEAN: 0.898 MAX_MED: 0.444 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triprolidine hydrochloride monohydrate
CHID: 21410 CASRN: 6138-79-0
SPID(S): Tox21_200848
M4ID: 12481404

HILL MODEL (in red):

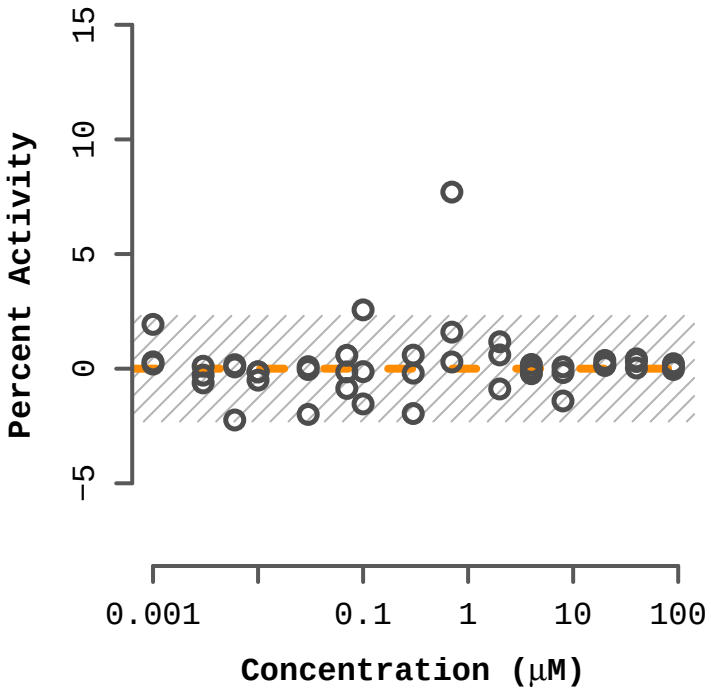
	tp	ga	gw
val:	0.292	0.0518	8
sd:	0.297	0.64	22.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.15	0.867	8	1.27	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	154.33	159.36	158.04
PROB:	0.81	0.07	0.13
RMSE:	1.27	1.25	1.18

MAX_MEAN: 1.73 **MAX_MED:** 2.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

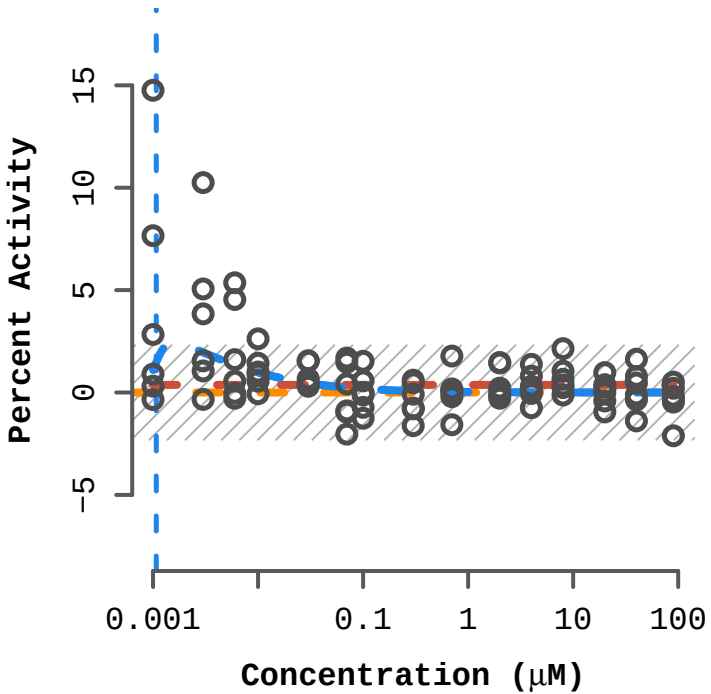
NAME: Tris(2-chloroethyl) phosphate
CHID: 21411 **CASRN:** 115-96-8
SPID(S): Tox21_300074
M4ID: 12479056

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 3.2 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tris(2-chloroethyl) phosphate
CHID: 21411 CASRN: 115-96-8
SPID(S): Tox21_201254
M4ID: 12480998

HILL MODEL (in red):

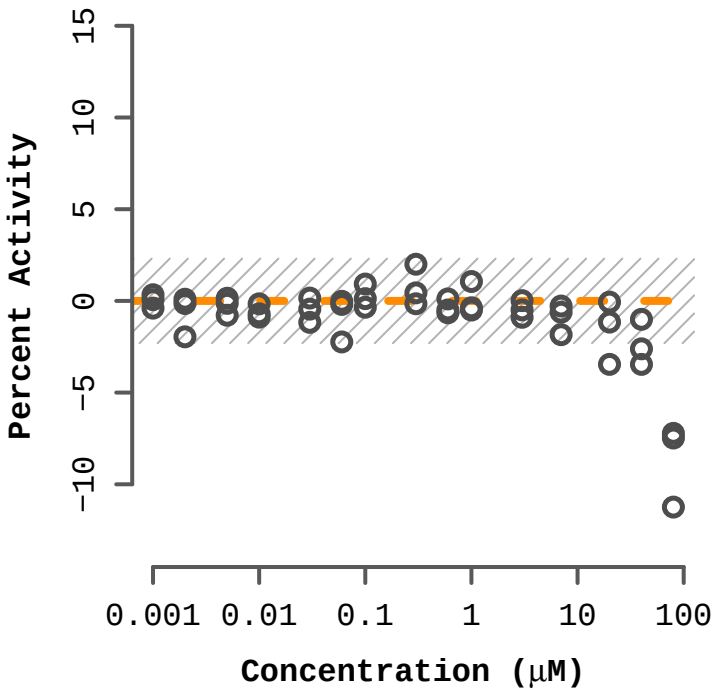
	tp	ga	gw
val:	0.372	-5	3.31
sd:	0.124	853	1390

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.79	-2.97	7.78	-2.72	0.817
sd:	36.7	0.192	41.6	6.84	1.66

	CNST	HILL	GNLS
AIC:	346.65	343.72	334.42
PROB:	0	0.01	0.99
RMSE:	2.49	2.39	2.15

MAX_MEAN: 4.35 MAX_MED: 2.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

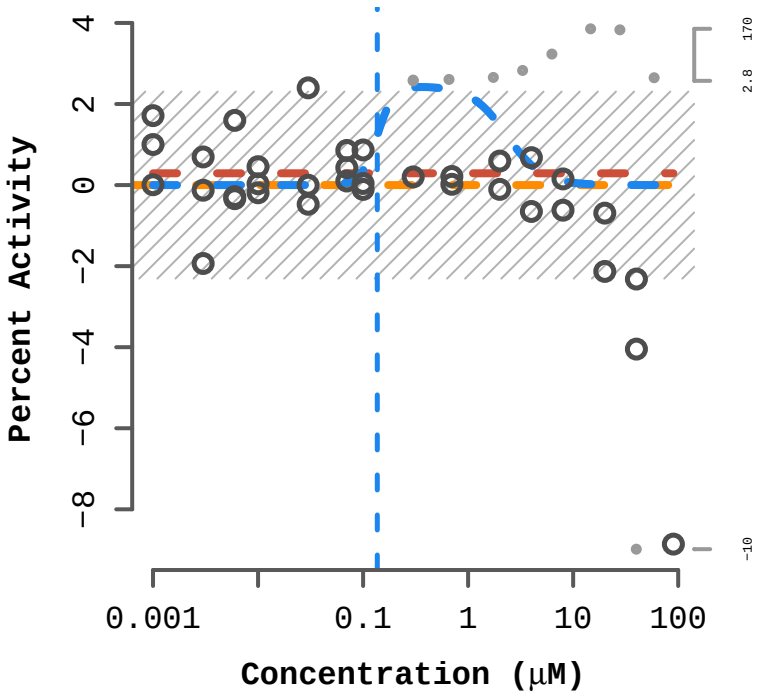
NAME: Tris(2,3-dibromopropyl) phosphate
CHID: 21413 **CASRN:** 126-72-7
SPID(S): Tox21_302967
M4ID: 12476166

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.55	NA	NA

MAX_MEAN: 0.762 **MAX_MED:** 0.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tris(2,3-dibromopropyl) phosphate
CHID: 21413 **CASRN:** 126-72-7
SPID(S): Tox21_201798
M4ID: 12480454 **BRK**

HILL MODEL (in red):

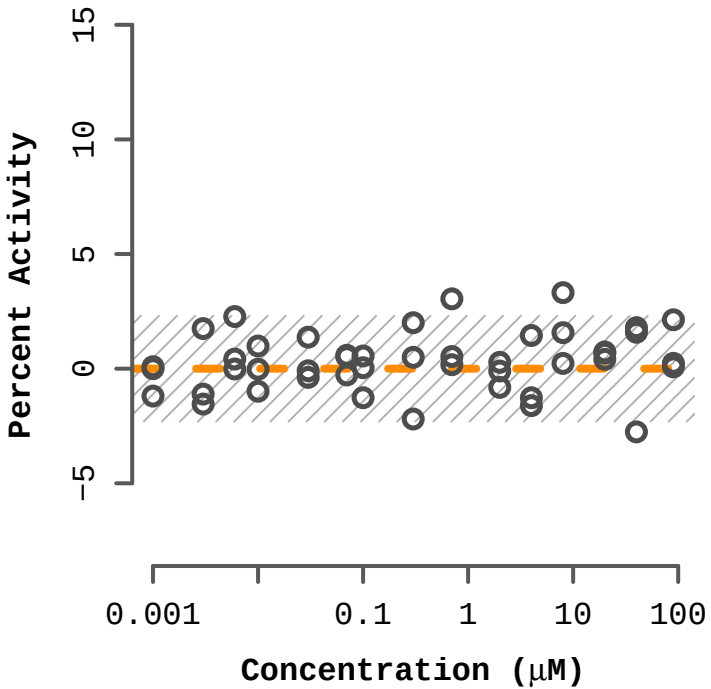
	tp	ga	gw
val:	0.291	−4.99	2.83
sd:	0.522	1080	1570

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.45	−0.865	5.62	0.368	2.57
sd:	1.98	0.517	24.7	0.829	7.71

	CNST	HILL	GNLS
AIC:	346.69	352.38	353.37
PROB:	0.91	0.05	0.03
RMSE:	39.25	39.17	39.21

MAX_MEAN: 56.9 **MAX_MED:** 2.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

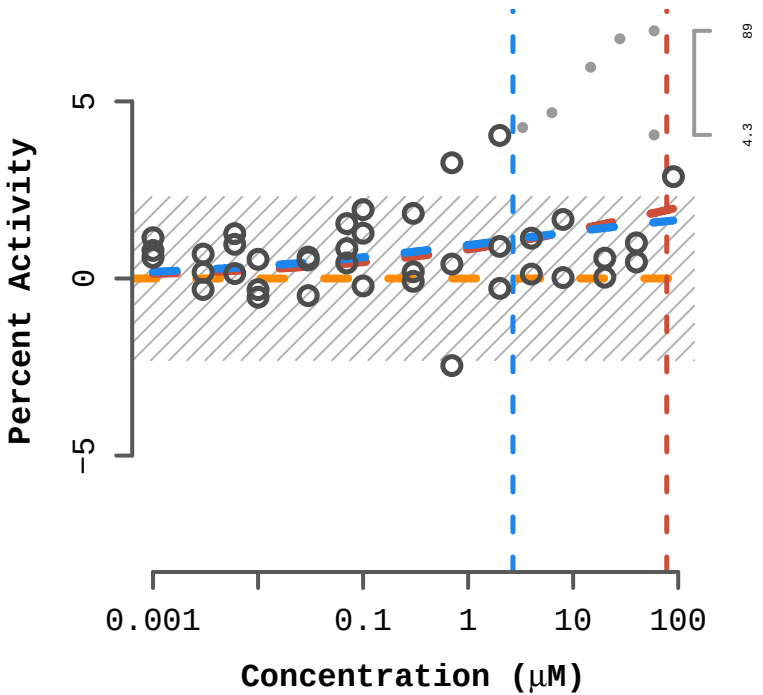
NAME: Tris(2-ethylhexyl) phosphate
CHID: 21414 **CASRN:** 78-42-2
SPID(S): Tox21_300321
M4ID: 12478810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tris(2-ethylhexyl) phosphate
CHID: 21414 CASRN: 78-42-2
SPID(S): Tox21_201369
M4ID: 12480883 BRK

HILL MODEL (in red):

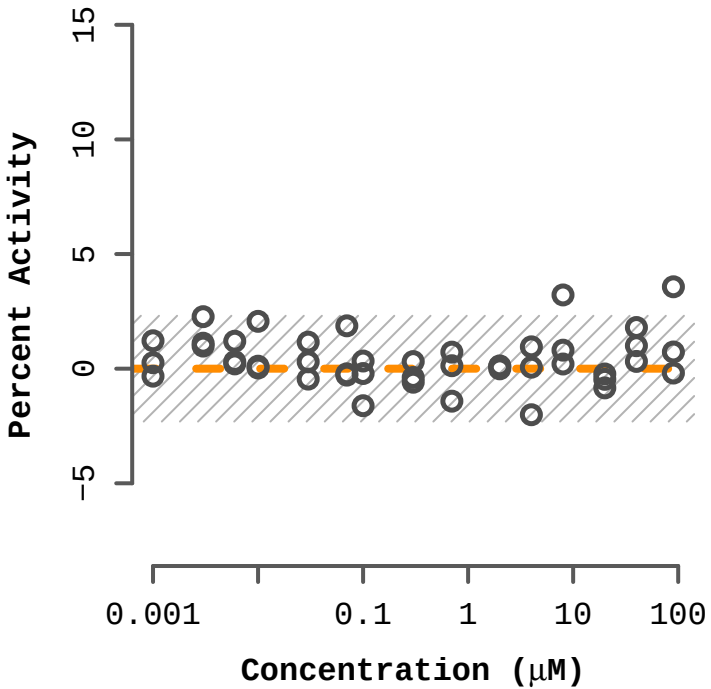
	tp	ga	gw
val:	3.86	1.89	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.21	0.427	0.3	3.56	8.38
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	289.47	284.92	288.88
PROB:	0.08	0.81	0.11
RMSE:	20.6	20.09	20.15

MAX_MEAN: 32.2 MAX_MED: 4.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

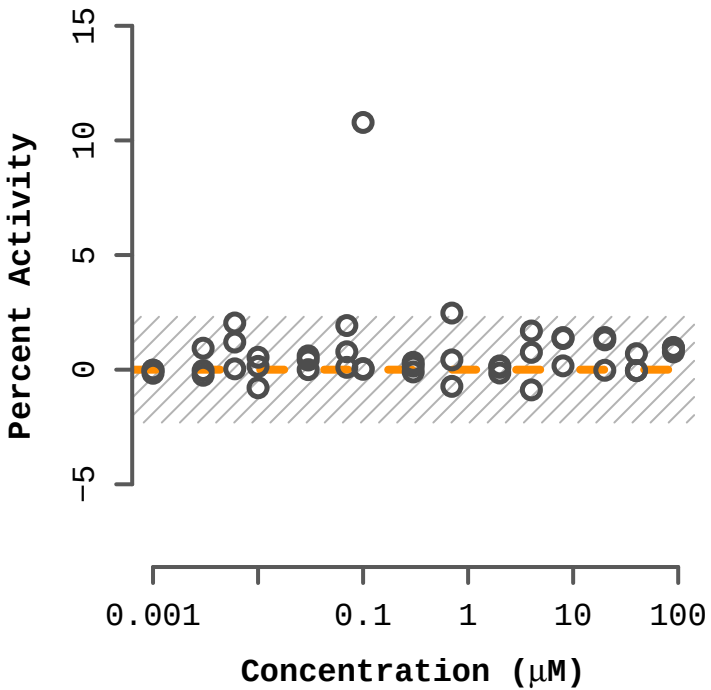
NAME: Triisopropanolamine
CHID: 21415 **CASRN:** 122-20-3
SPID(S): Tox21_302748
M4ID: 12476385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

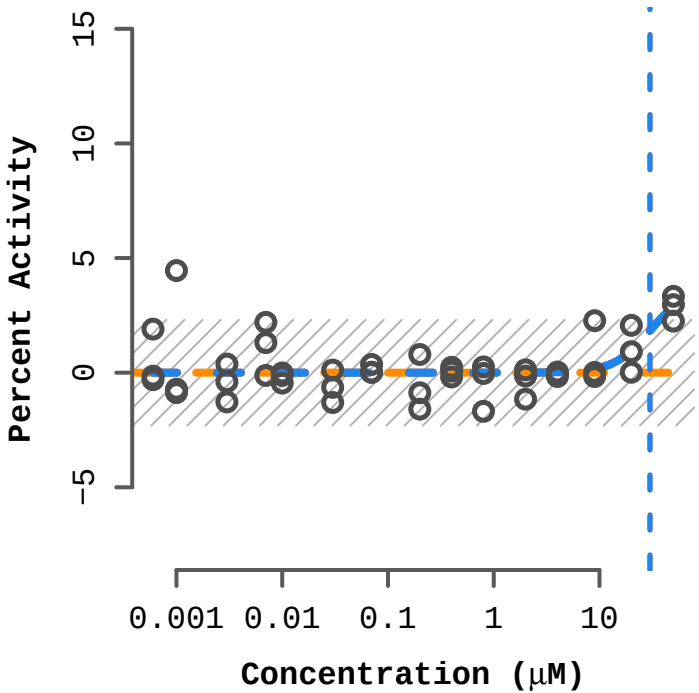
NAME: Triisopropanolamine
CHID: 21415 **CASRN:** 122-20-3
SPID(S): Tox21_201952
M4ID: 12480300

HILL MODEL: Not applicable.

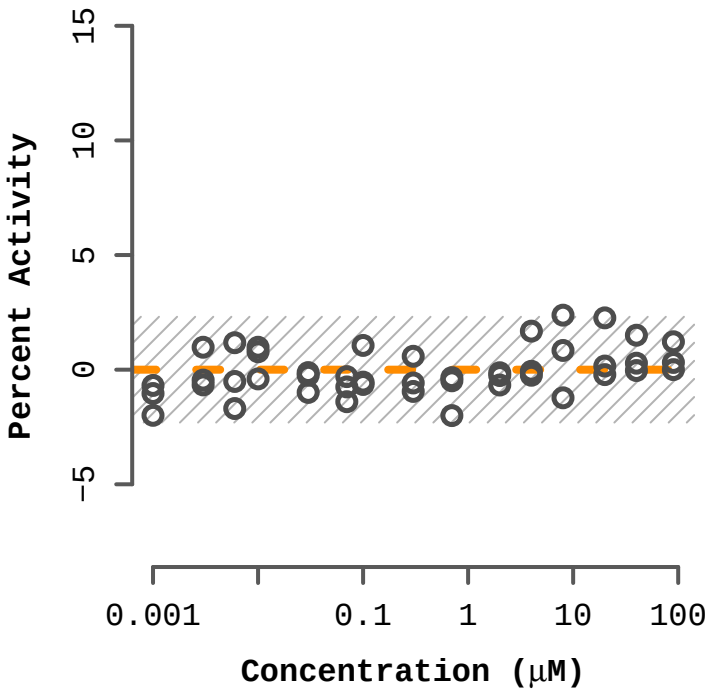
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 3.62 **MAX_MED:** 1.36 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    dl-Tryptophan
CHID:    21418   CASRN: 54-12-6
SPID(S): Tox21_202793
M4ID:    12479459

HILL MODEL (in red):
      tp       ga       gw
val:  3.66     1.48     2.53
sd:   3.36     0.469    2.94

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.66     1.48     2.53     3.34     3.42
sd:   3.36     0.468    2.94     1840     4030

      CNST        HILL        GNLS
AIC:  147.66      129.4       133.4
PROB: 0           0.88        0.12
RMSE: 1.33        1.07        1.07

MAX_MEAN: 2.85      MAX_MED: 2.97      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

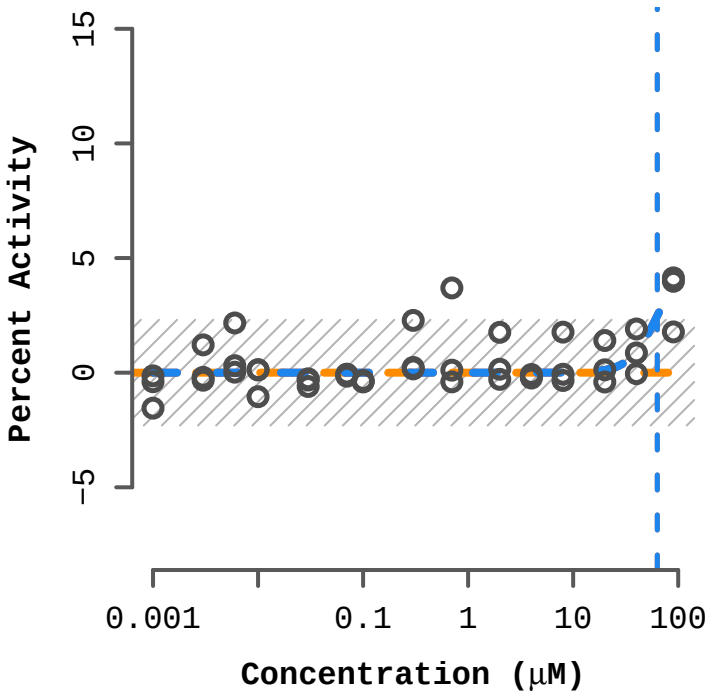
NAME: l-Tryptophan
CHID: 21419 **CASRN:** 73-22-3
SPID(S): Tox21_300359
M4ID: 12478773

HILL MODEL: Not applicable.

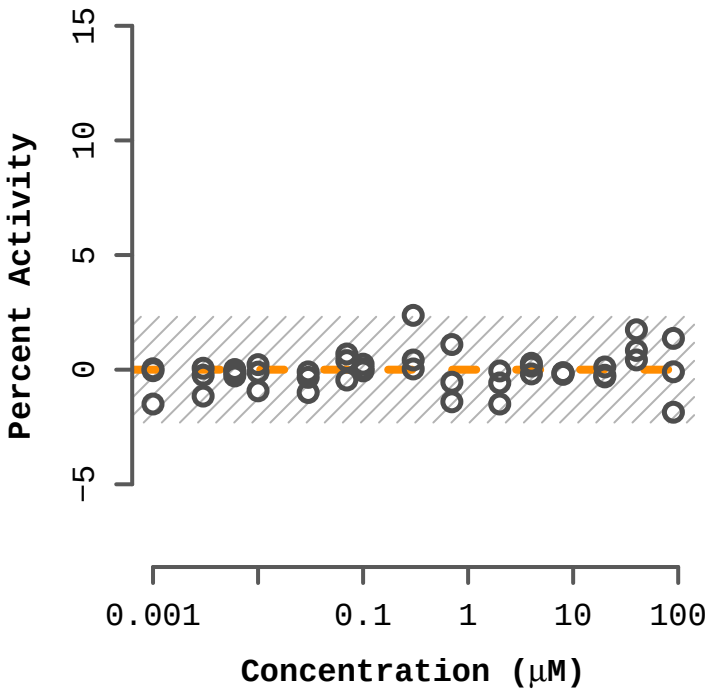
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.14	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.736 **MAX_MED:** 0.84 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    l-Tryptophan
CHID:    21419   CASRN: 73-22-3
SPID(S): Tox21_201246
M4ID:    12481006

HILL MODEL (in red):
      tp       ga       gw
val:  4.96     1.8      3.24
sd:   5.23     0.406    3.86

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.96     1.8      3.24     3.93     2.91
sd:   5.28     0.41     3.89     609      907

      CNST        HILL        GNLS
AIC:  142.28      123.35      127.35
PROB: 0           0.88        0.12
RMSE: 1.33        1           1

MAX_MEAN: 3.3       MAX_MED: 3.99      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

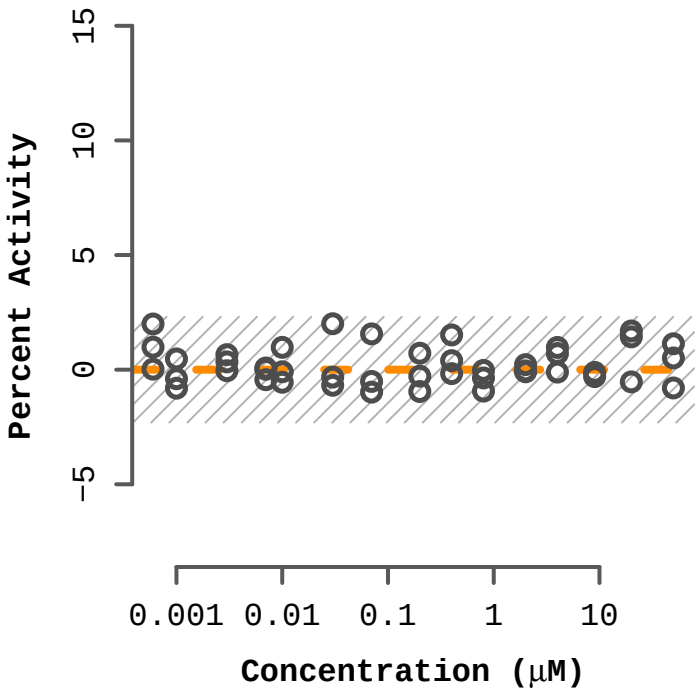
NAME: Uracil
CHID: 21424 **CASRN:** 66-22-8
SPID(S): Tox21_201023
M4ID: 12481229

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.842 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

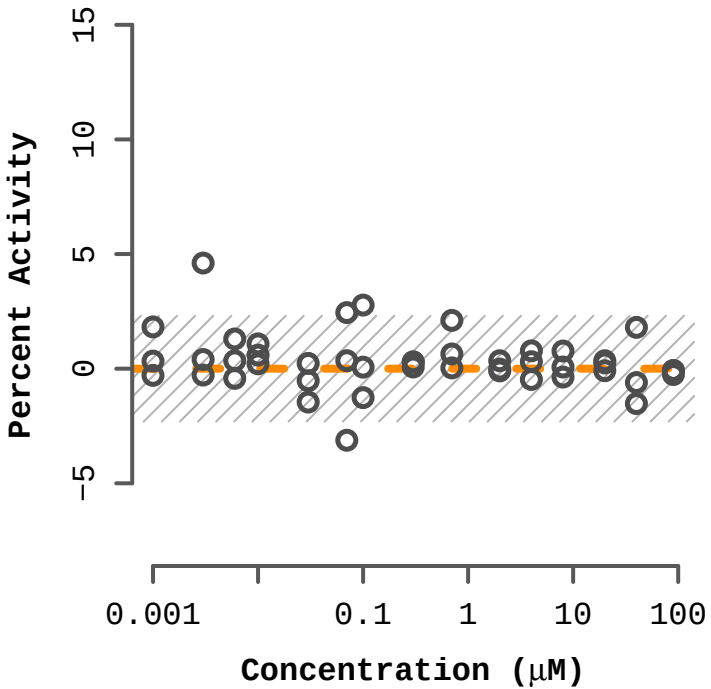
NAME: Uracil
CHID: 21424 **CASRN:** 66-22-8
SPID(S): Tox21_112680_1
M4ID: 12482984

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

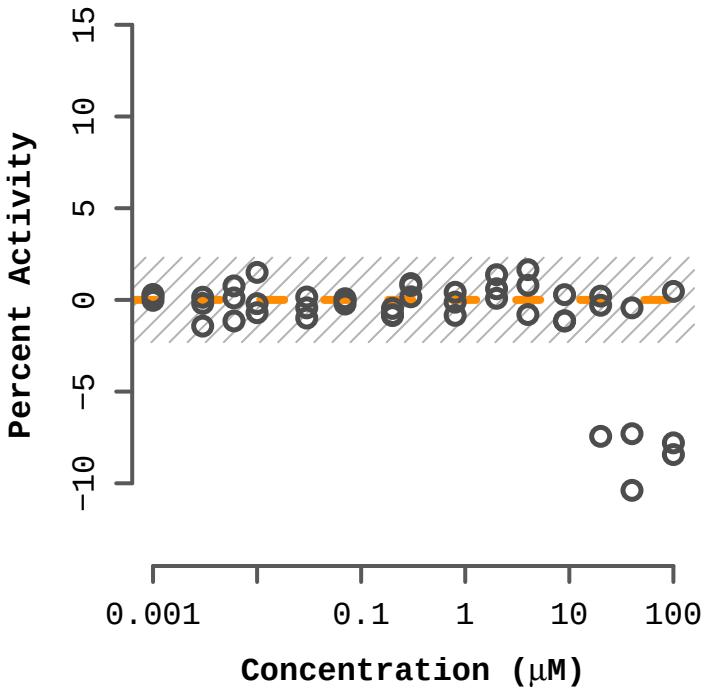
NAME: Urea
CHID: 21426 **CASRN:** 57-13-6
SPID(S): Tox21_300035
M4ID: 12479095

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

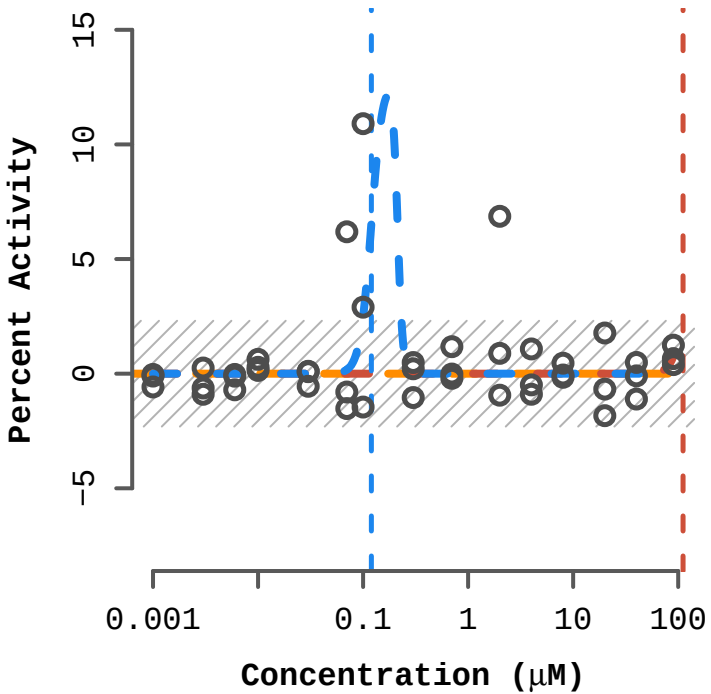
NAME: Urea
CHID: 21426 **CASRN:** 57-13-6
SPID(S): Tox21_202158
M4ID: 12480094

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.87	NA	NA

MAX_MEAN: 0.691 **MAX_MED:** 0.797 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Urethane
CHID: 21427 CASRN: 51-79-6
SPID(S): Tox21_300494
M4ID: 12478638

HILL MODEL (in red):

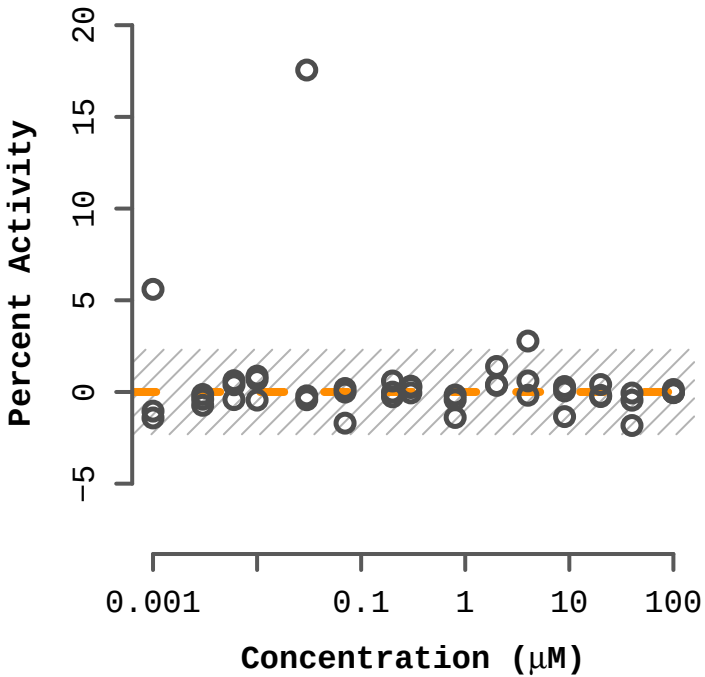
	tp	ga	gw
val:	4.9	2.05	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.1	−0.921	7.99	−0.671	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.89	167.51	172.11
PROB:	0.85	0.14	0.01
RMSE:	2.3	2.29	2.08

MAX_MEAN: 4.12 MAX_MED: 2.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

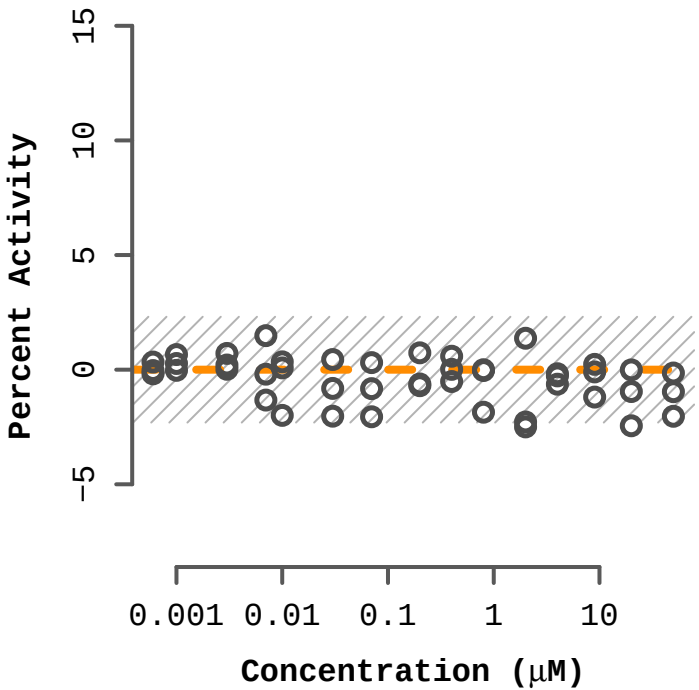
NAME: Urethane
CHID: 21427 CASRN: 51-79-6
SPID(S): Tox21_201761
M4ID: 12480491

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.86	NA	NA

MAX_MEAN: 5.64 MAX_MED: 0.679 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

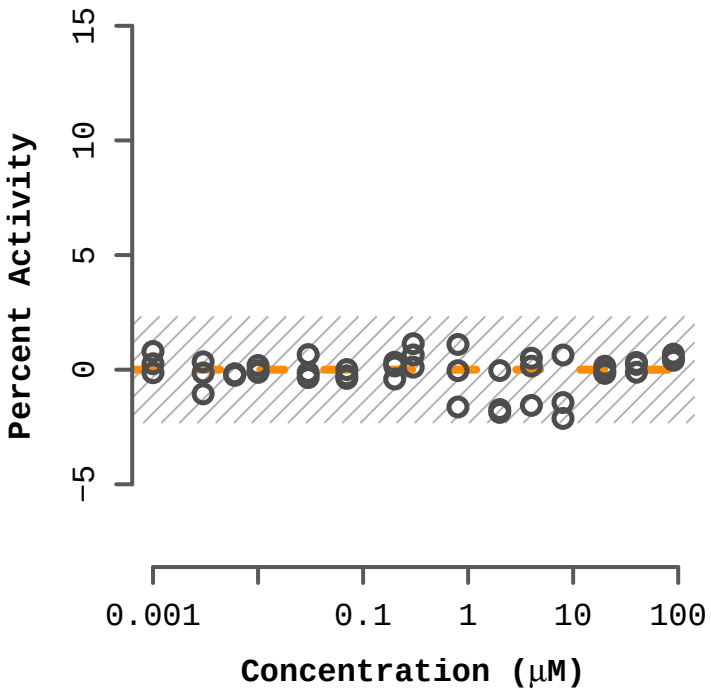
NAME: Urethane
CHID: 21427 **CASRN:** 51-79-6
SPID(S): Tox21_111398_1
M4ID: 12483712

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.311 **MAX_MED:** 0.271 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

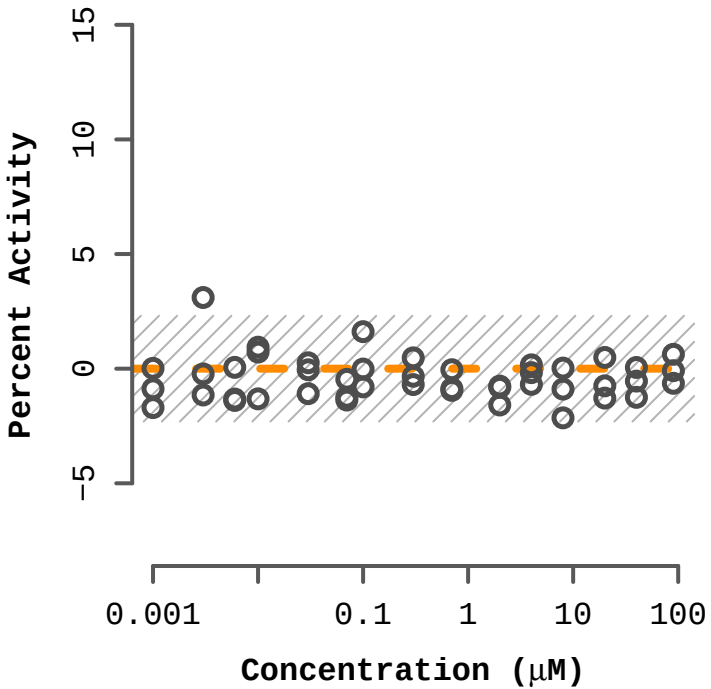
NAME: Vinyl acetate
CHID: 21431 CASRN: 108-05-4
SPID(S): Tox21_200817
M4ID: 12481435

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.63 MAX_MED: 0.645 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

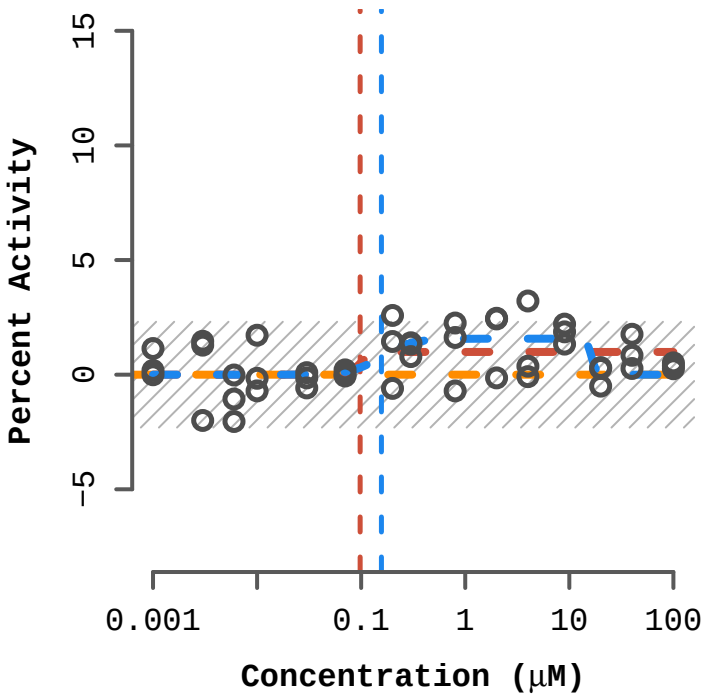
NAME: 4-Vinylcyclohexene
CHID: 21437 **CASRN:** 100-40-3
SPID(S): Tox21_200388
M4ID: 12481864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** 0.725 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1−Dichloroethylene
CHID: 21438 CASRN: 75−35−4
SPID(S): Tox21_200357
M4ID: 12481895

HILL MODEL (in red):

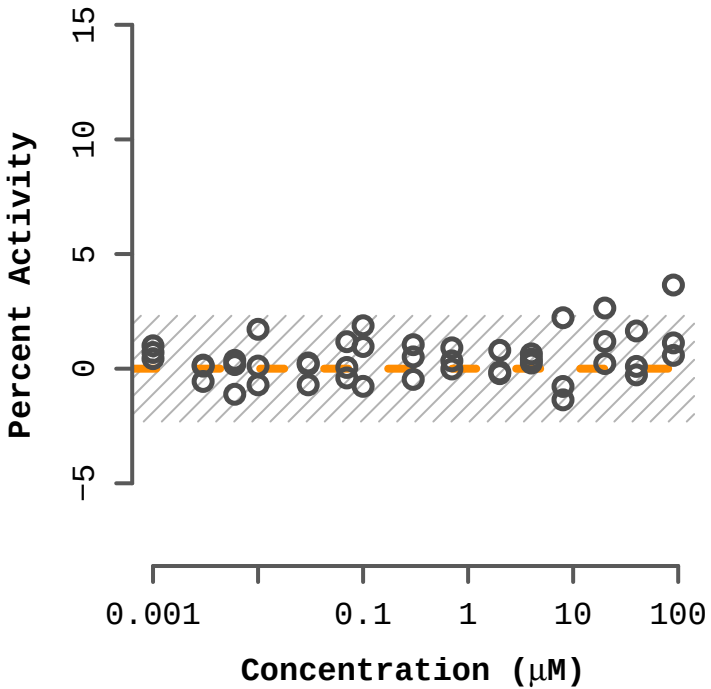
	tp	ga	gw
val:	0.991	−1.01	8
sd:	0.218	0.45	20.5

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.57	−0.805	3	1.21	17.7
sd:	0.396	0.299	3.54	0.727	143

	CNST	HILL	GNLS
AIC:	156.29	143.5	142.86
PROB:	0	0.42	0.58
RMSE:	1.31	1.04	1.01

MAX_MEAN: 1.8 MAX_MED: 2.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

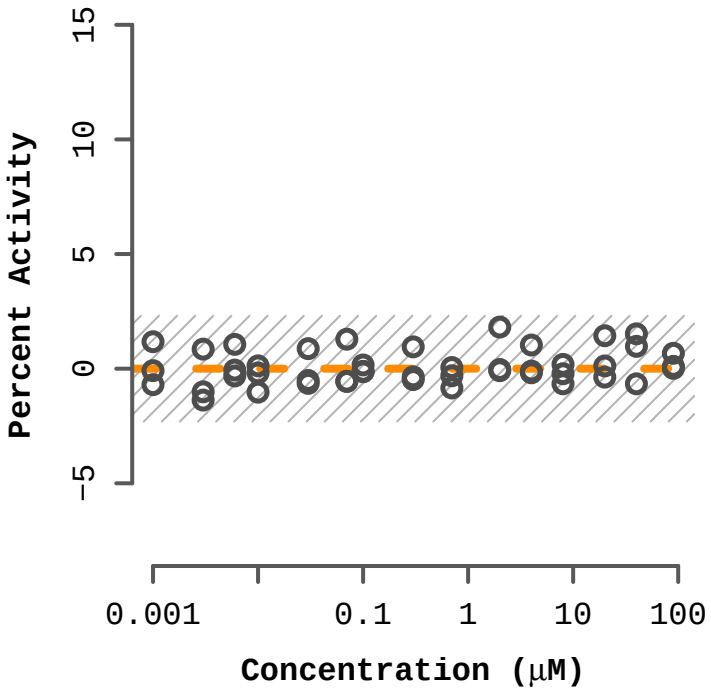
NAME: N-Vinyl-2-pyrrolidone
CHID: 21440 **CASRN:** 88-12-0
SPID(S): Tox21_300073
M4ID: 12479057

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

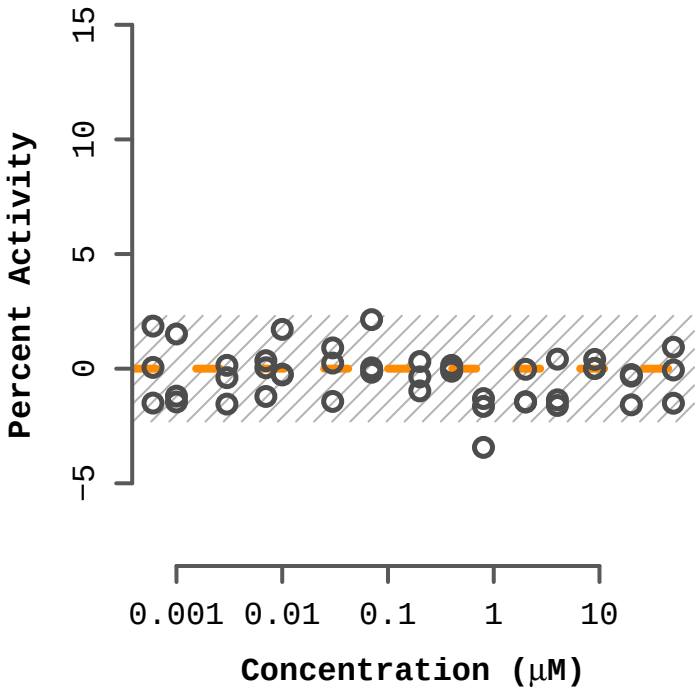
NAME: N-Vinyl-2-pyrrolidone
CHID: 21440 **CASRN:** 88-12-0
SPID(S): Tox21_202462
M4ID: 12479790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.612 **MAX_MED:** 0.975 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

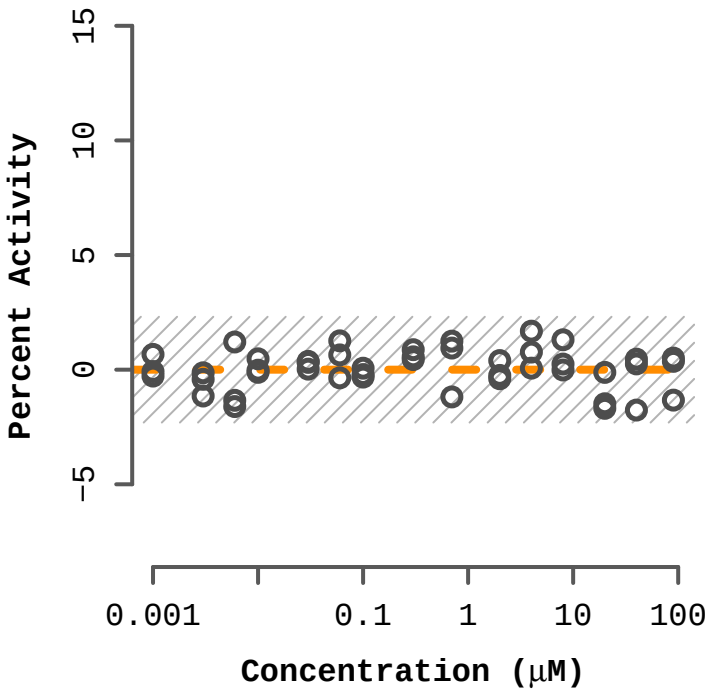
NAME: Voglibose
CHID: 21442 **CASRN:** 83480-29-9
SPID(S): Tox21_112220_1
M4ID: 12483225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.675 **MAX_MED:** 0.246 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

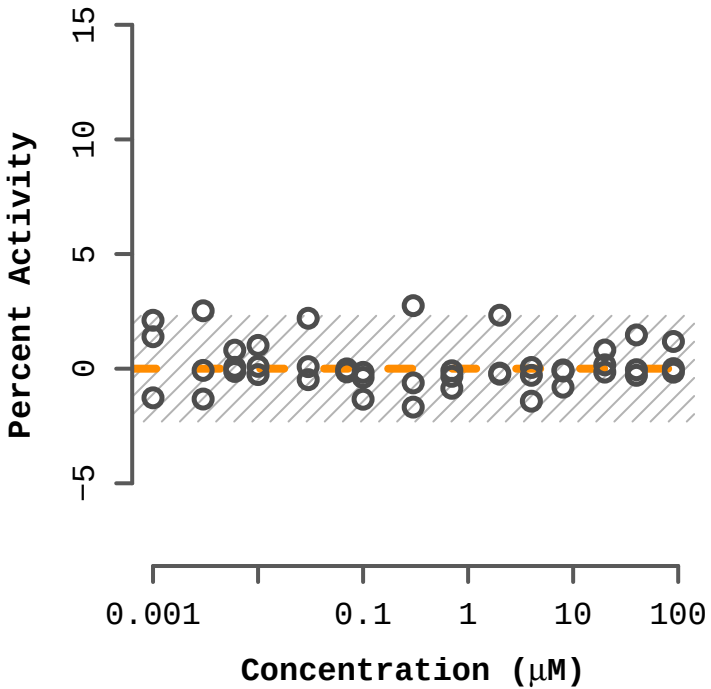
NAME: Xylenes
CHID: 21446 **CASRN:** 1330-20-7
SPID(S): Tox21_200292
M4ID: 12481960

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.839 **MAX_MED:** 0.944 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

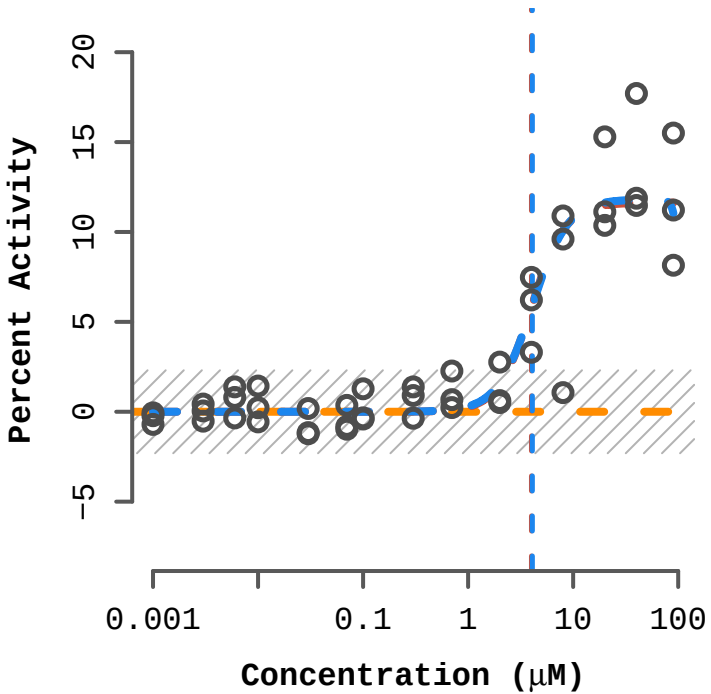
NAME: 2,4-Dimethylaniline hydrochloride
CHID: 21448 CASRN: 21436-96-4
SPID(S): Tox21_200519
M4ID: 12481733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.746 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Disperse Yellow 3
CHID: 21450 CASRN: 2832-40-8
SPID(S): Tox21_304042
M4ID: 12475146

HILL MODEL (in red):

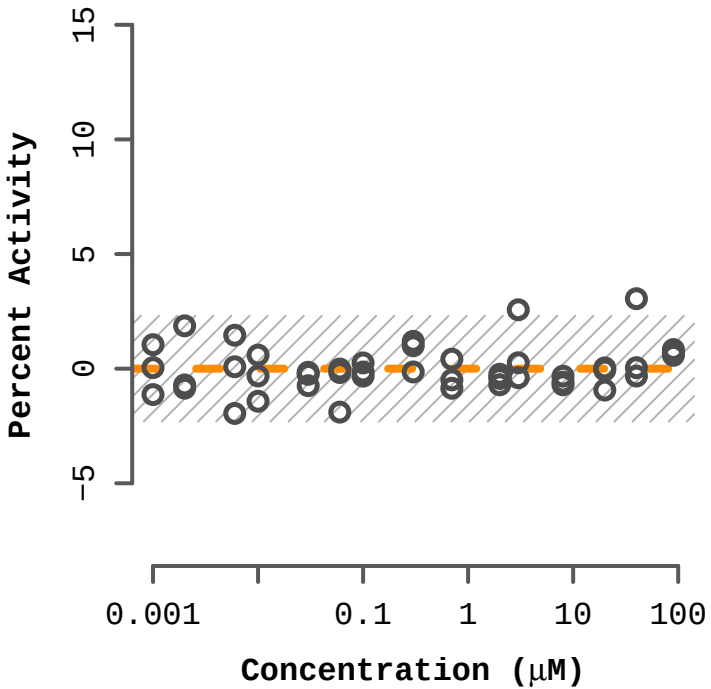
	tp	ga	gw
val:	11.6	0.603	2.72
sd:	0.567	0.0496	0.761

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.8	0.611	2.6	2.03	15.1
sd:	0.73	0.0547	0.77	0.368	74.8

	CNST	HILL	GNLS
AIC:	288.44	180.24	183.89
PROB:	0	0.86	0.14
RMSE:	6.38	2.09	2.07

MAX_MEAN: 13.7 **MAX_MED:** 11.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

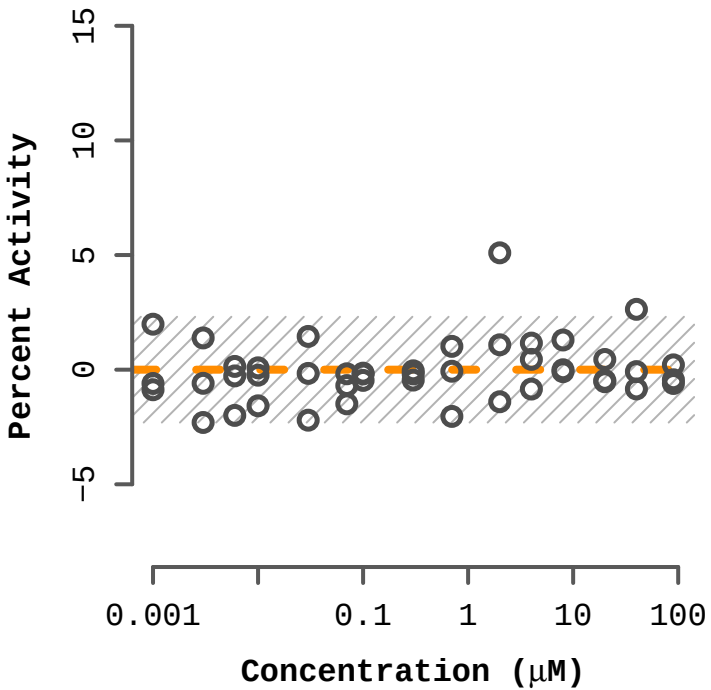
NAME: FD&C Yellow 5
CHID: 21455 **CASRN:** 1934-21-0
SPID(S): Tox21_300554
M4ID: 12478579

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.927 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

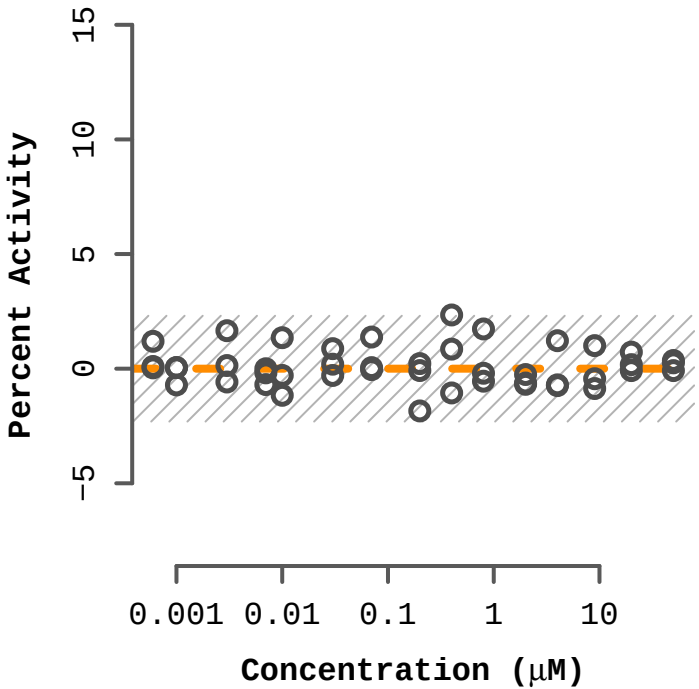
NAME: FD&C Yellow 5
CHID: 21455 CASRN: 1934-21-0
SPID(S): Tox21_201539
M4ID: 12480713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

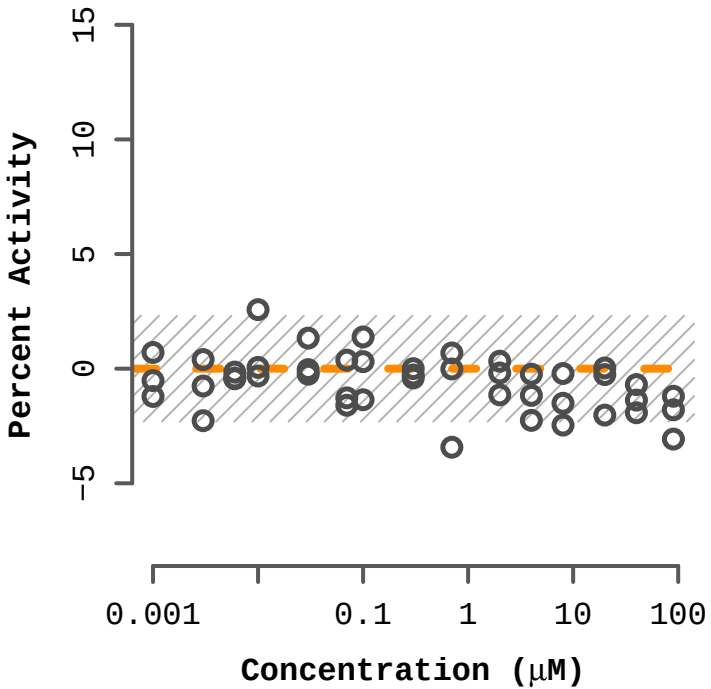
NAME: FD&C Yellow 5
CHID: 21455 **CASRN:** 1934-21-0
SPID(S): Tox21_113411
M4ID: 12482658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.714 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

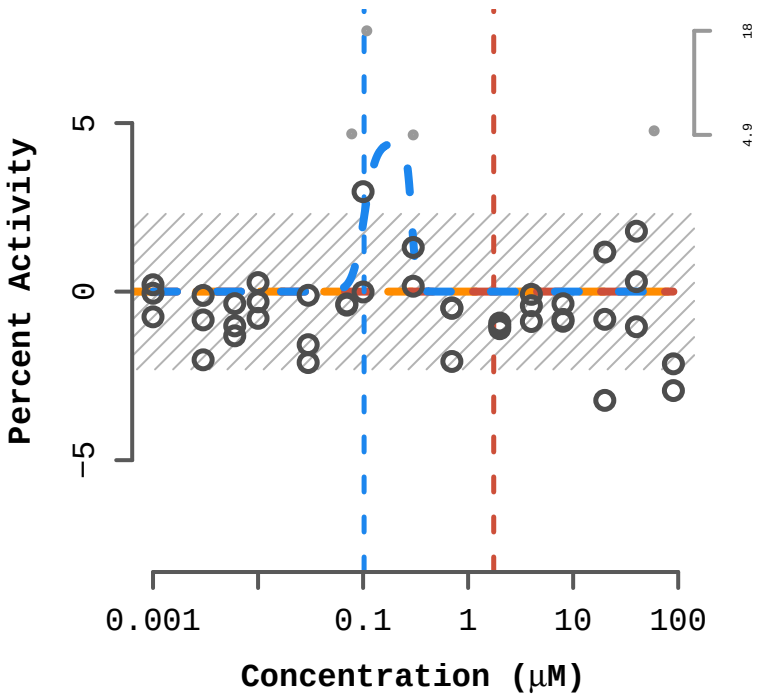
NAME: FD&C Yellow 6
CHID: 21456 CASRN: 2783-94-0
SPID(S): Tox21_300407
M4ID: 12478725

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.772 **MAX_MED:** 0.307 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: FD&C Yellow 6
CHID: 21456 CASRN: 2783-94-0
SPID(S): Tox21_201897
M4ID: 12480355 BRK

HILL MODEL (in red):

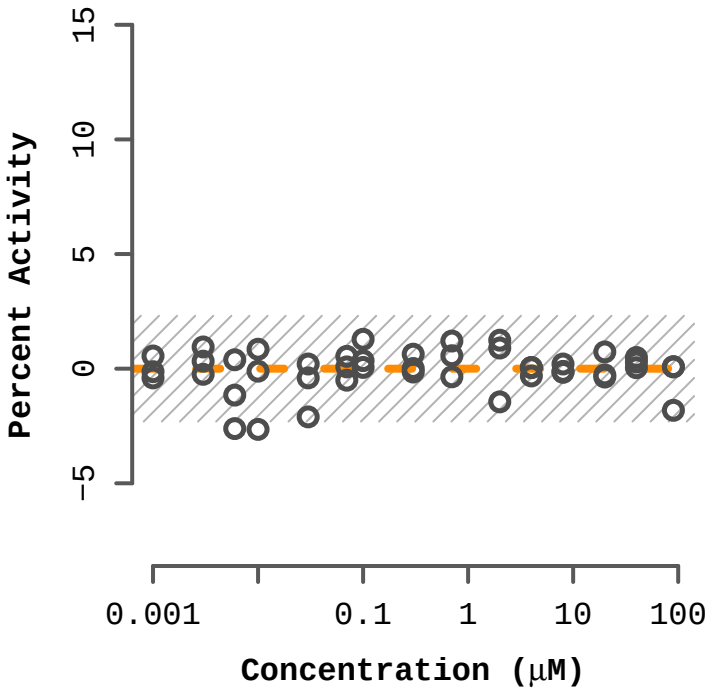
	tp	ga	gw
val:	2.45e-10	0.244	3.67
sd:	2.56e-05	6050	479000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.43	-0.99	8	-0.538	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	194.33	200.33	199.44
PROB:	0.89	0.04	0.07
RMSE:	3.17	3.17	2.86

MAX_MEAN: 6.83 MAX_MED: 2.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

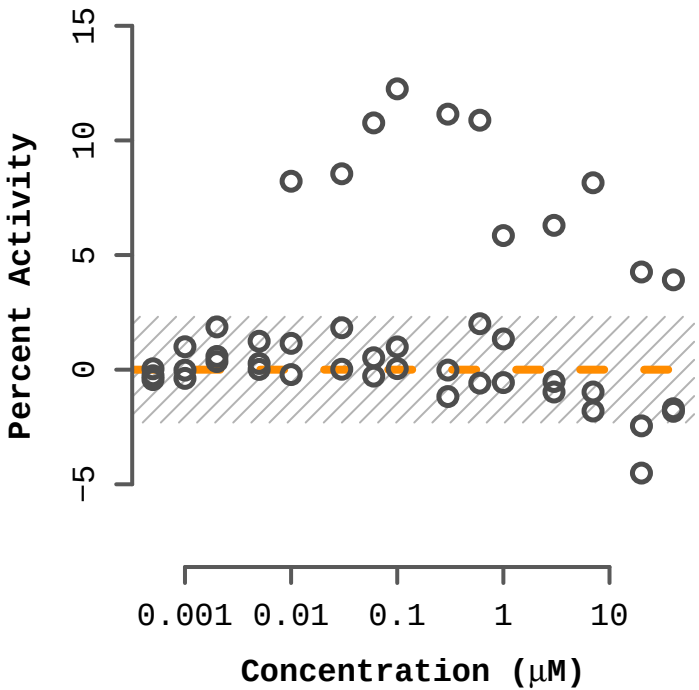
NAME: HC Yellow 4
CHID: 21458 **CASRN:** 59820-43-8
SPID(S): Tox21_201014
M4ID: 12481238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.563 **MAX_MED:** 0.901 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

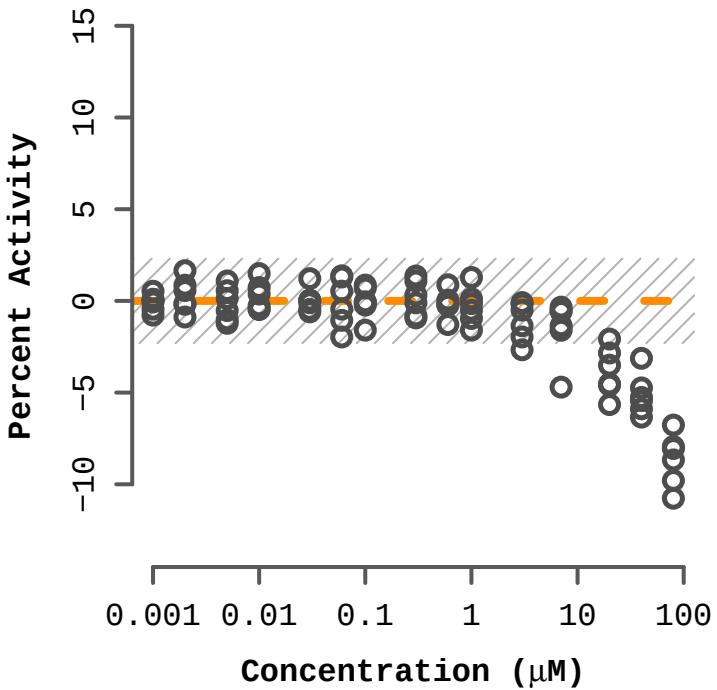
NAME: Zearalenone
CHID: 21460 **CASRN:** 17924-92-4
SPID(S): Tox21_303510
M4ID: 12475632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253	NA	NA
PROB:	1	NA	NA
RMSE:	4.43	NA	NA

MAX_MEAN: 4.43 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

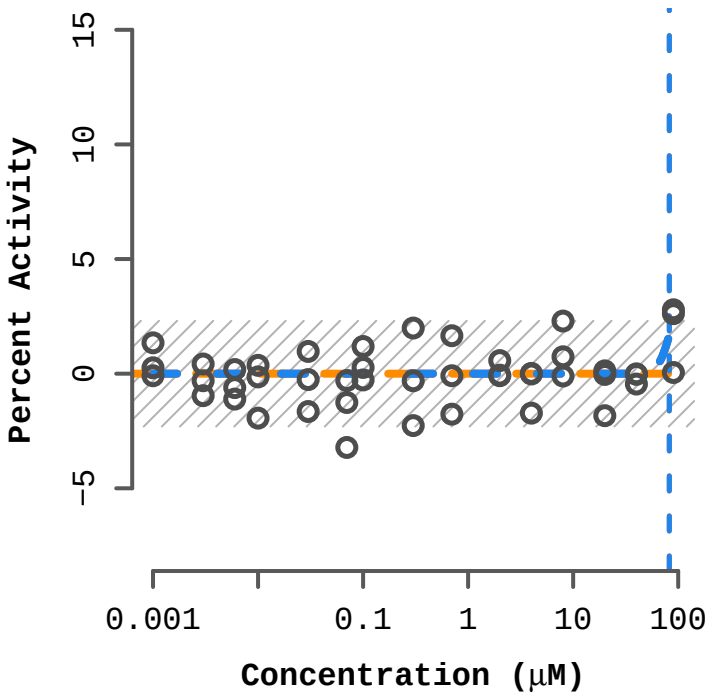
NAME: Zearalenone
CHID: 21460 **CASRN:** 17924-92-4
SPID(S): Tox21_201153
M4ID: 12481099

HILL MODEL: Not applicable.

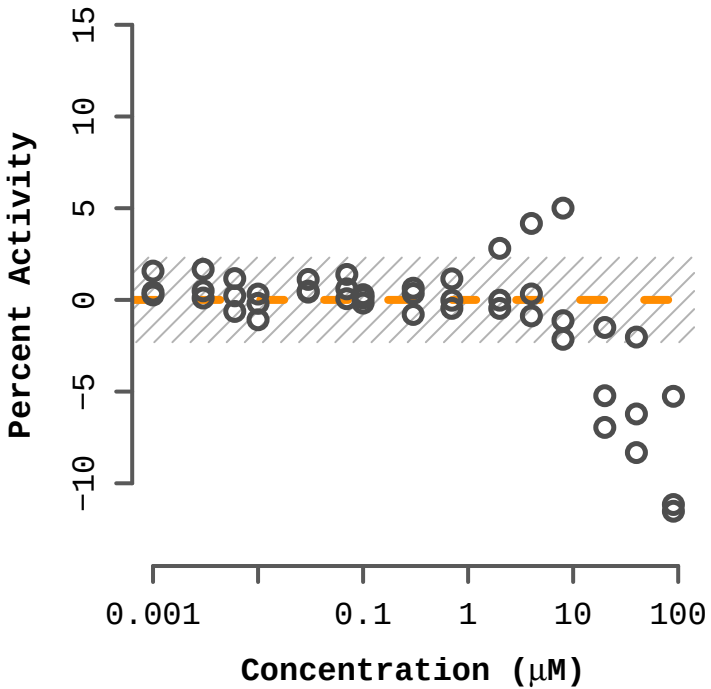
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	422.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 0.312 **MAX_MED:** 0.213 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Zinc(II) acetate dihydrate
CHID:    21461   CASRN: 5970-45-6
SPID(S): Tox21_200864
M4ID:    12481388

HILL MODEL (in red):
      tp       ga       gw
val:  3.35     1.92     8
sd:   9.55     0.428    16.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.35     1.92     8        3.91     12.7
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  147.17      146.52      150.52
PROB: 0.39        0.54        0.07
RMSE: 1.23        1.14        1.14

MAX_MEAN: 1.82      MAX_MED: 2.62      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

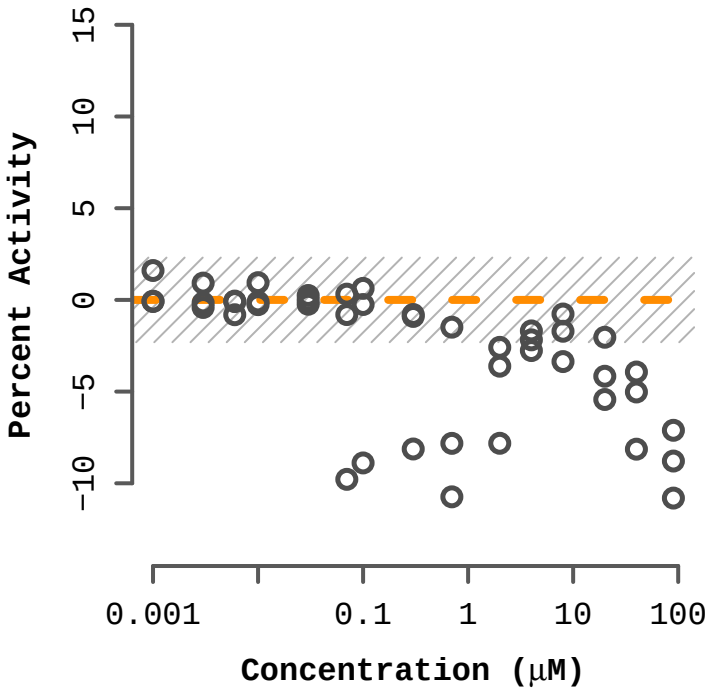
NAME: Zinc dibutyldithiocarbamate
CHID: 21462 **CASRN:** 136-23-2
SPID(S): Tox21_202601
M4ID: 12479651

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.66	NA	NA
PROB:	1	NA	NA
RMSE:	3.49	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.605 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

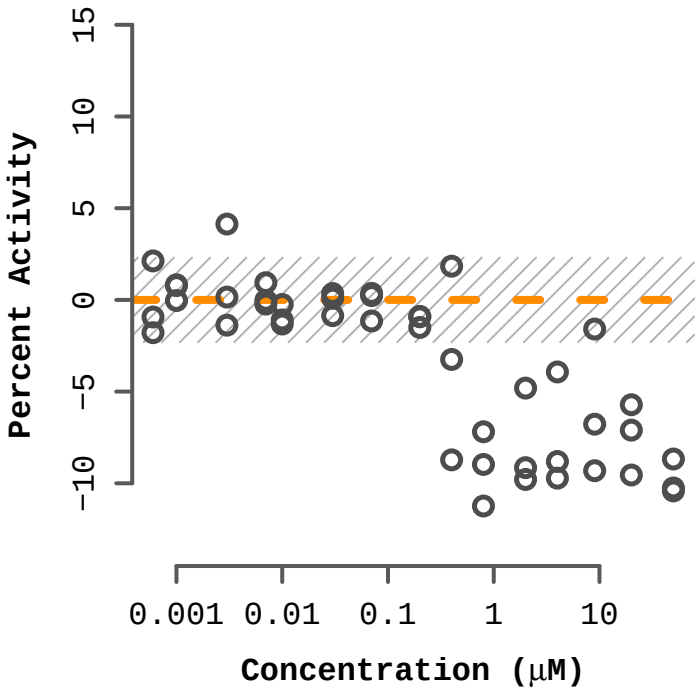
NAME: Zinc diethyldithiocarbamate
CHID: 21463 CASRN: 14324-55-1
SPID(S): Tox21_200263
M4ID: 12481989

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	263.52	NA	NA
PROB:	1	NA	NA
RMSE:	4.57	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** −0.00868 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

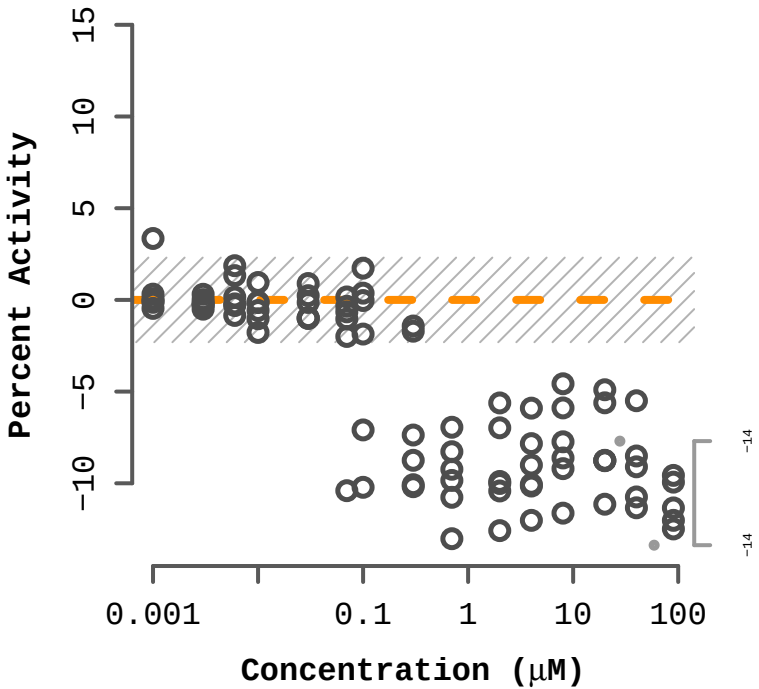
NAME: Ziram
CHID: 21464 **CASRN:** 137-30-4
SPID(S): Tox21_300503
M4ID: 12478629

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	285.06	NA	NA
PROB:	1	NA	NA
RMSE:	5.53	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 0.783 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

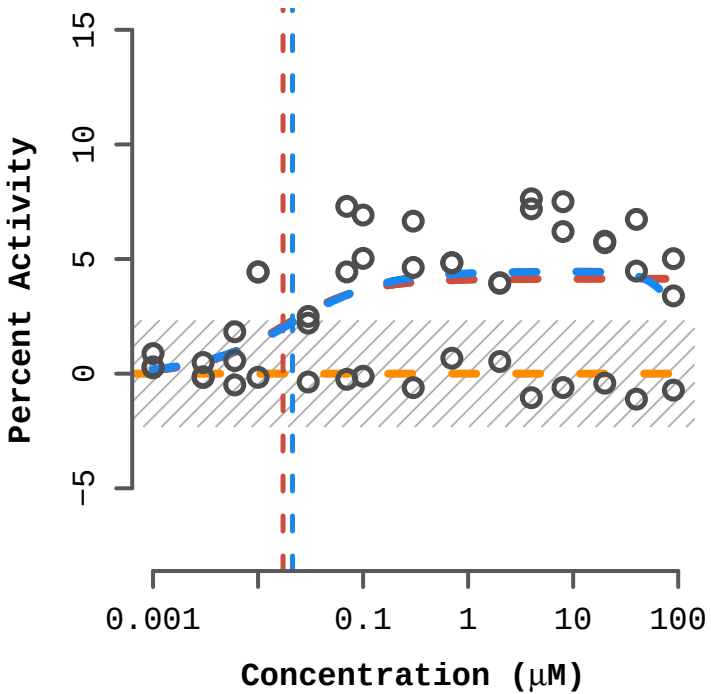
NAME: Ziram
CHID: 21464 **CASRN:** 137-30-4
SPID(S): Tox21_201910
M4ID: 12480342 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	619.87	NA	NA
PROB:	1	NA	NA
RMSE:	7.12	NA	NA

MAX_MEAN: 0.512 **MAX_MED:** −0.00139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Nitroso-N-methylurethane
CHID: 21472 CASRN: 615-53-2
SPID(S): Tox21_302872
M4ID: 12476261

HILL MODEL (in red):

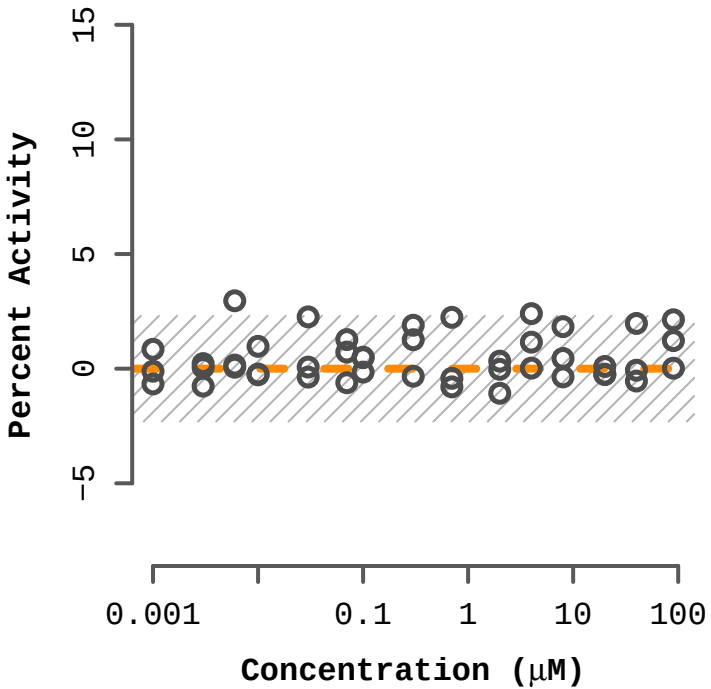
	tp	ga	gw
val:	4.14	−1.76	1.14
sd:	0.649	0.377	0.756

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.46	−1.67	1.02	2.05	3.01
sd:	0.845	0.408	0.751	0.38	9.83

	CNST	HILL	GNLS
AIC:	258.5	227.58	230.79
PROB:	0	0.83	0.17
RMSE:	4.01	2.65	2.64

MAX_MEAN: 4.59 MAX_MED: 7.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

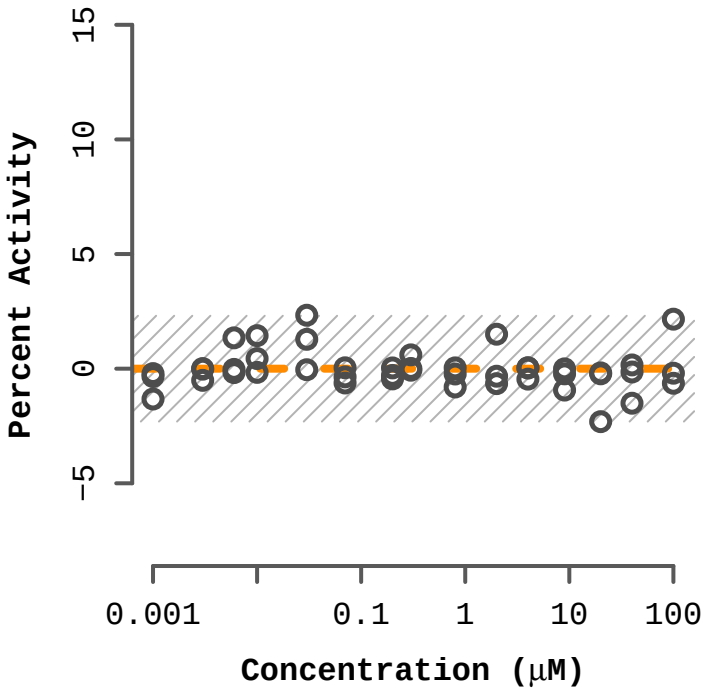
NAME: Sodium tetrafluoroborate
CHID: 21477 **CASRN:** 13755-29-8
SPID(S): Tox21_303450
M4ID: 12475690

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

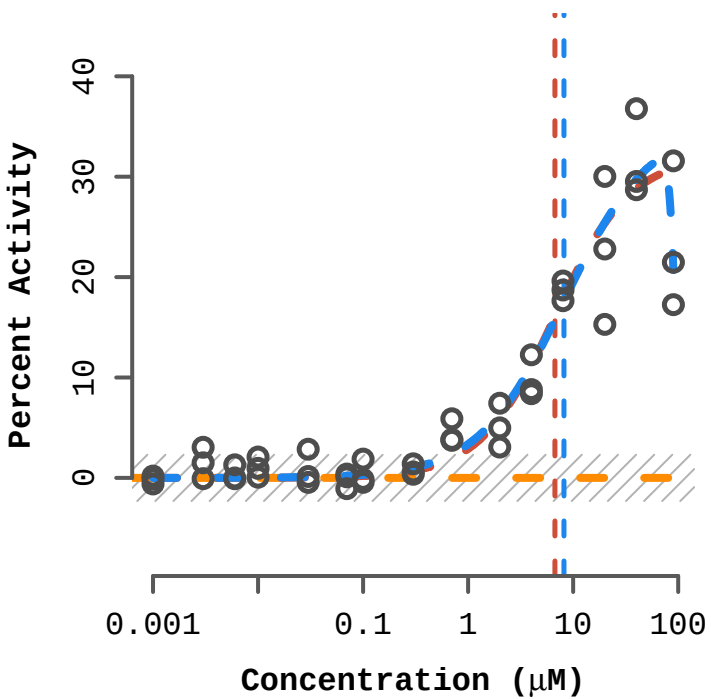
NAME: Sodium tetrafluoroborate
CHID: 21477 **CASRN:** 13755-29-8
SPID(S): Tox21_200520
M4ID: 12481732

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lynestrenol
CHID: 21478 CASRN: 52-76-6
SPID(S): Tox21_301969
M4ID: 12477164

HILL MODEL (in red):

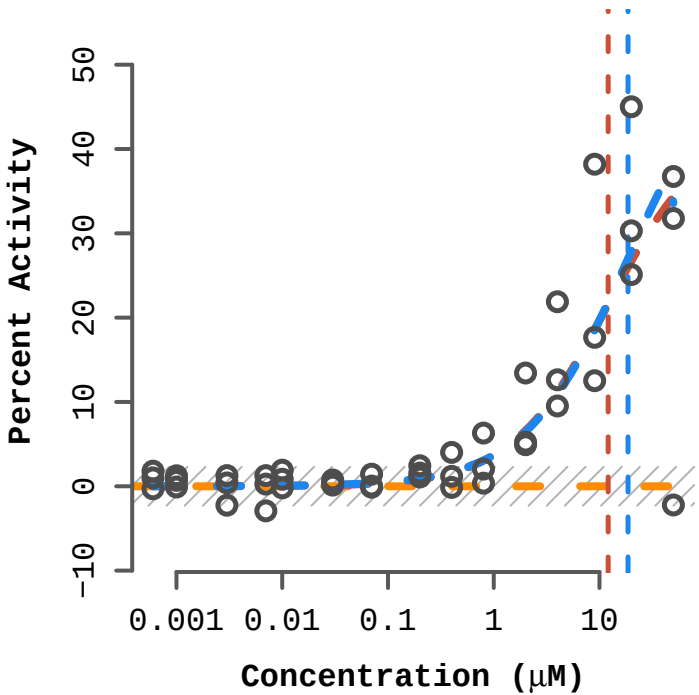
	tp	ga	gw
val:	32.1	0.826	1.21
sd:	2.08	0.0701	0.222

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	35.2	0.912	1.07	1.97	15.2
sd:	4.32	0.135	0.216	0.00764	8.19

	CNST	HILL	GNLS
AIC:	355.56	226.69	220.65
PROB:	0	0.05	0.95
RMSE:	13.33	3.5	2.97

MAX_MEAN: 31.7 MAX_MED: 29.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lynestrenol
CHID: 21478 **CASRN:** 52-76-6
SPID(S): Tox21_110319_1
M4ID: 12484459

HILL MODEL (in red):

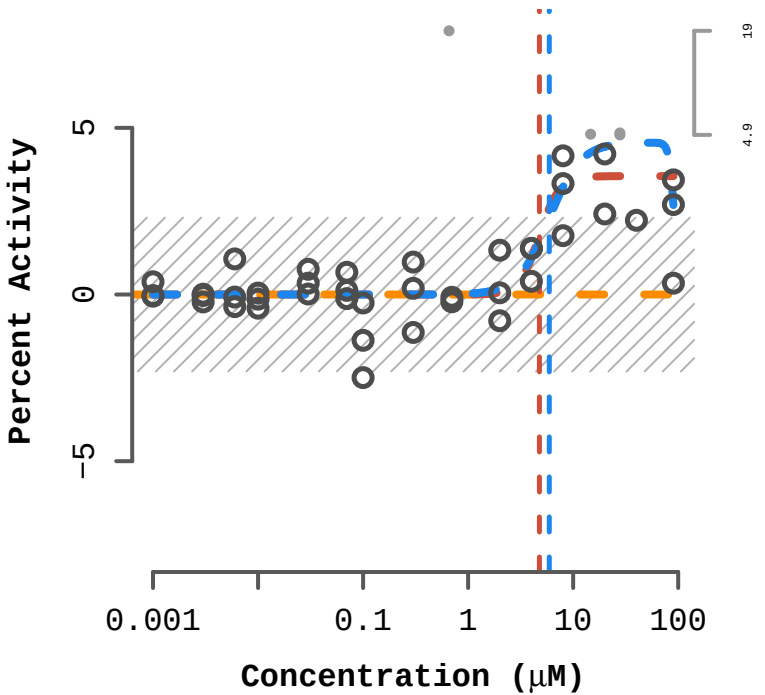
	tp	ga	gw
val:	43.2	1.08	0.952
sd:	7.96	0.214	0.186

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	54	1.27	0.893	1.75	18
sd:	26.9	0.46	0.194	0.0345	23.5

	CNST	HILL	GNLS
AIC:	349.37	261.61	264.69
PROB:	0	0.82	0.18
RMSE:	14.09	7.23	7.09

MAX_MEAN: 33.5 **MAX_MED:** 31.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,7-Acetylaminofluorene
CHID: 21479 CASRN: 304-28-9
SPID(S): Tox21_302864
M4ID: 12476269 BRK

HILL MODEL (in red):

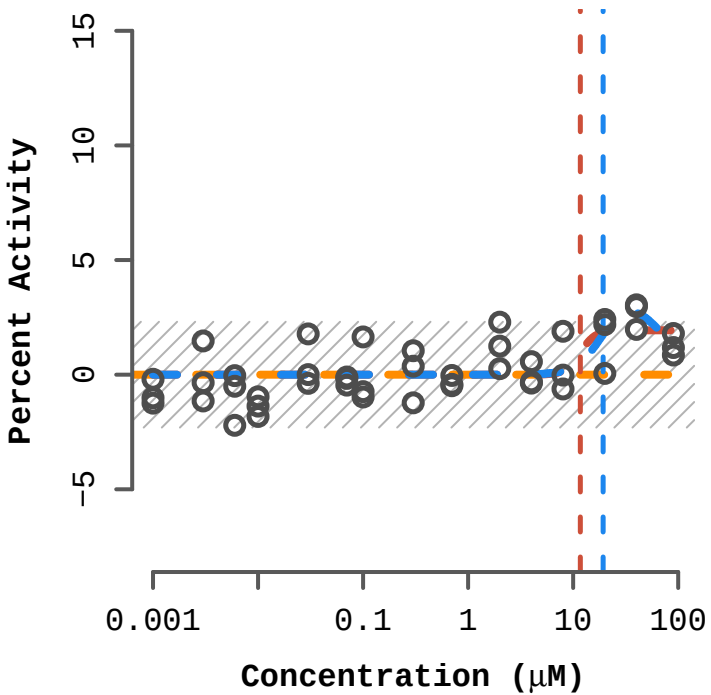
	tp	ga	gw
val:	3.55	0.679	4.59
sd:	0.457	0.0788	3.36

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.56	0.773	2.93	1.96	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	203.34	152.32	150.09
PROB:	0	0.25	0.75
RMSE:	3.45	2.98	2.96

MAX_MEAN: 6.22 MAX_MED: 4.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,7-Acetylaminofluorene
CHID: 21479 CASRN: 304-28-9
SPID(S): Tox21_201518
M4ID: 12480734

HILL MODEL (in red):

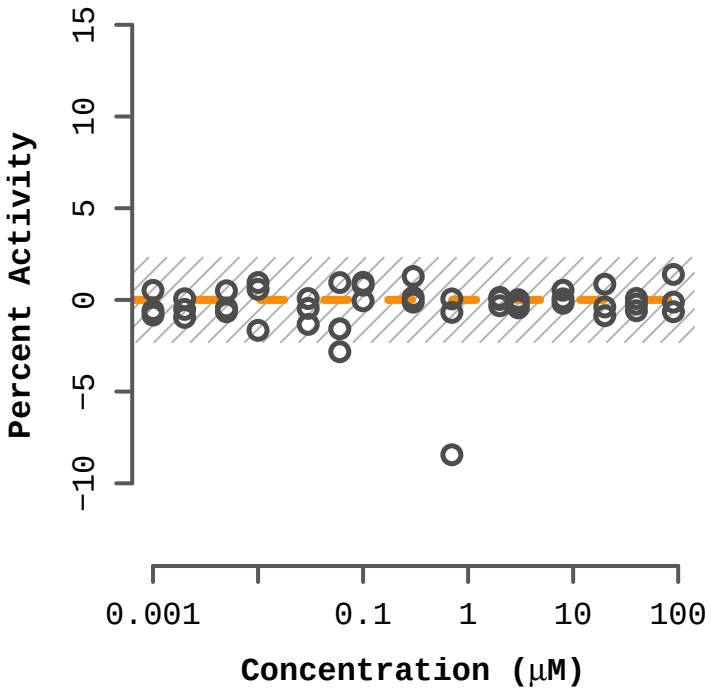
	tp	ga	gw
val:	1.94	1.07	6.01
sd:	0.4	0.333	9.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.66	1.29	3.47	1.84	2.45
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.05	141.25	141.11
PROB:	0	0.48	0.52
RMSE:	1.31	1.02	0.99

MAX_MEAN: 2.67 MAX_MED: 2.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

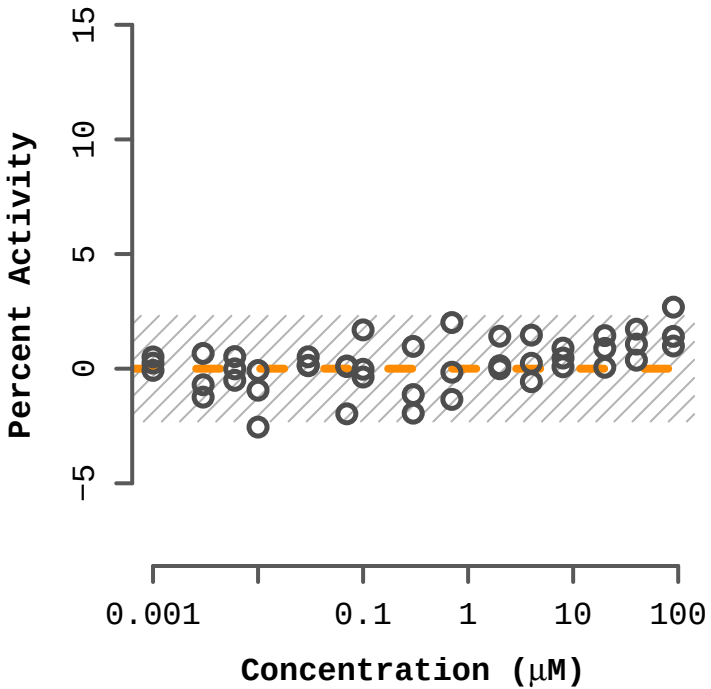
NAME: Acetone
CHID: 21482 **CASRN:** 67-64-1
SPID(S): Tox21_202480
M4ID: 12479772

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.571 **MAX_MED:** 0.803 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

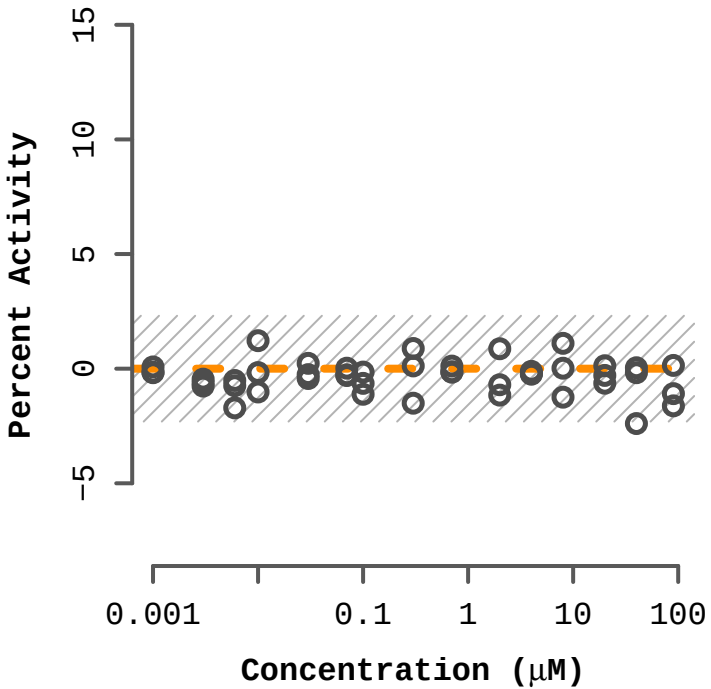
NAME: Phenylacetaldehyde
CHID: 21483 **CASRN:** 122-78-1
SPID(S): Tox21_302945
M4ID: 12476188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

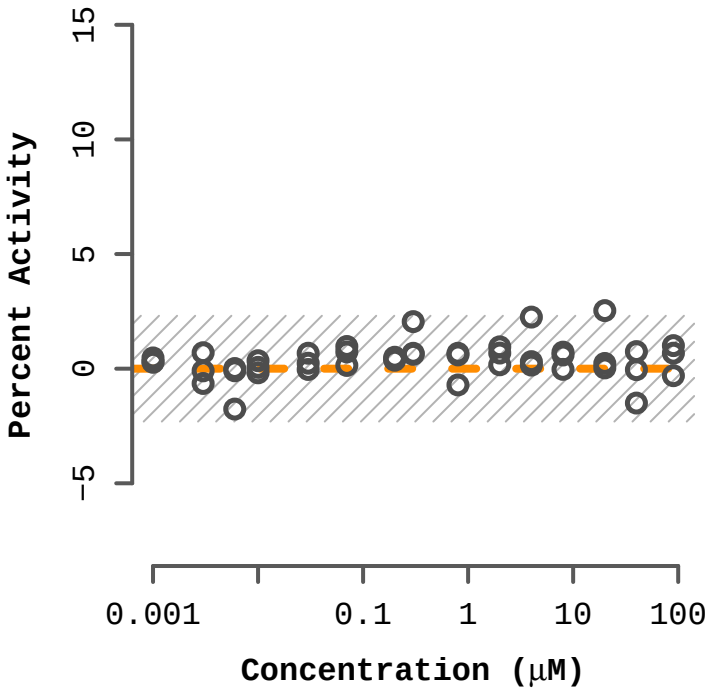
NAME: Phenylacetaldehyde
CHID: 21483 **CASRN:** 122-78-1
SPID(S): Tox21_201582
M4ID: 12480670

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.0134 **MAX_MED:** 0.121 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

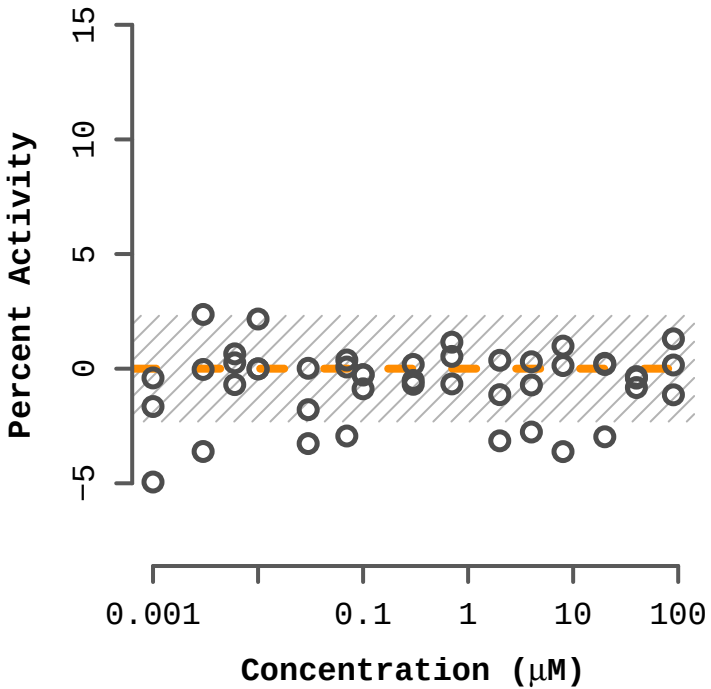
NAME: Phthalic acid
CHID: 21484 CASRN: 88-99-3
SPID(S): Tox21_200915
M4ID: 12481337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.12 MAX_MED: 0.733 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

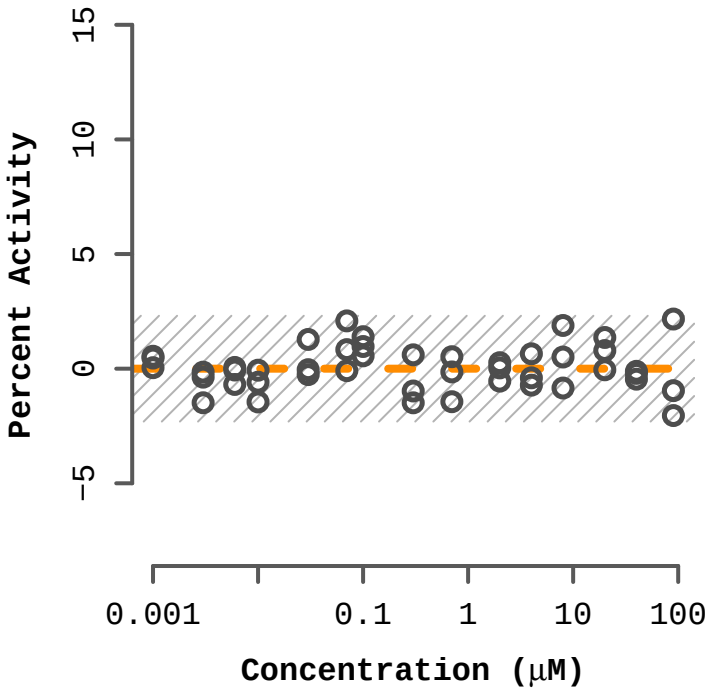
NAME: 1,3-Benzenedicarboxylic acid
CHID: 21485 **CASRN:** 121-91-5
SPID(S): Tox21_300106
M4ID: 12479024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 0.717 **MAX_MED:** 0.537 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

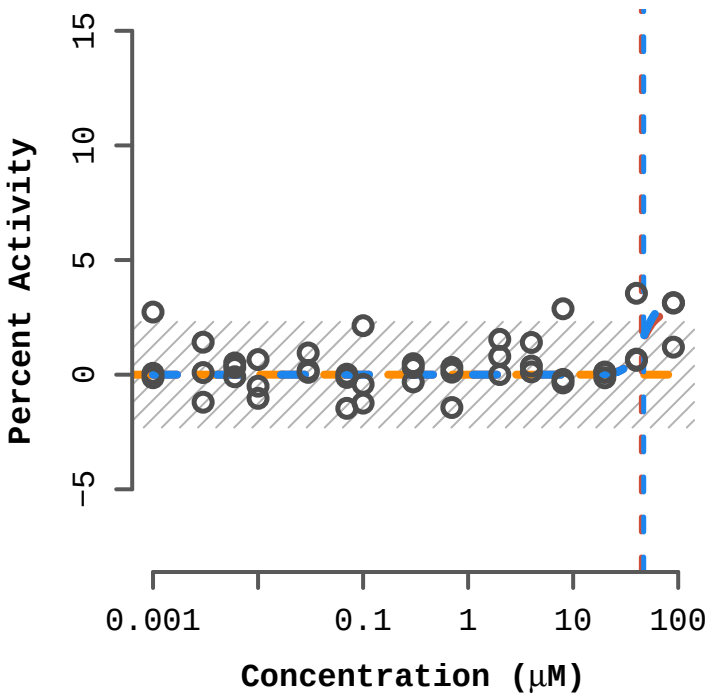
NAME: 1,3-Benzenedicarboxylic acid
CHID: 21485 **CASRN:** 121-91-5
SPID(S): Tox21_200409
M4ID: 12481843

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.975 **MAX_MED:** 0.968 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2,3−Benzenetricarboxylic acid
CHID: 21486 CASRN: 36362−97−7
SPID(S): Tox21_200979
M4ID: 12481273

HILL MODEL (in red):

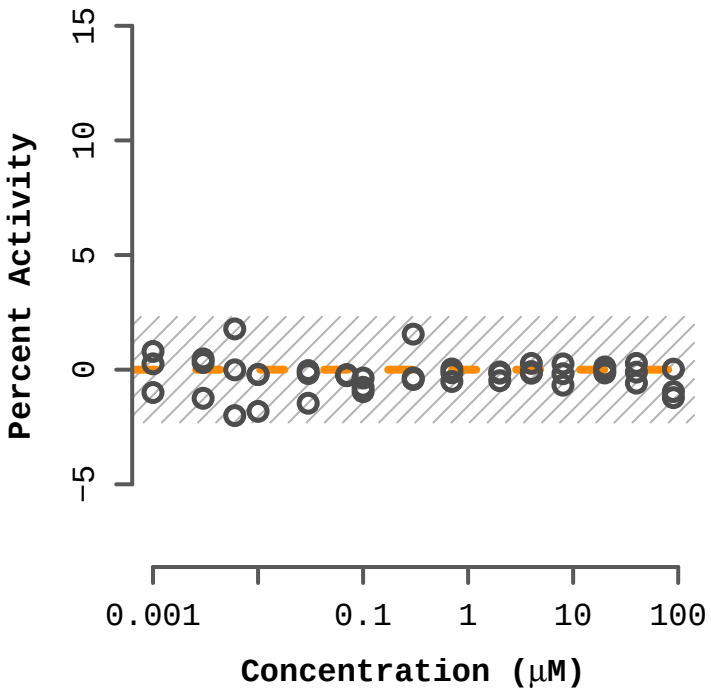
	tp	ga	gw
val:	2.8	1.65	5.75
sd:	0.978	0.213	20.1

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.38	1.67	5.63	2.08	5.82
sd:	112	3.54	20.2	2.96	788

	CNST	HILL	GNLS
AIC:	145.64	133.71	137.71
PROB:	0	0.88	0.12
RMSE:	1.28	1.04	1.04

MAX_MEAN: 2.49 MAX_MED: 3.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

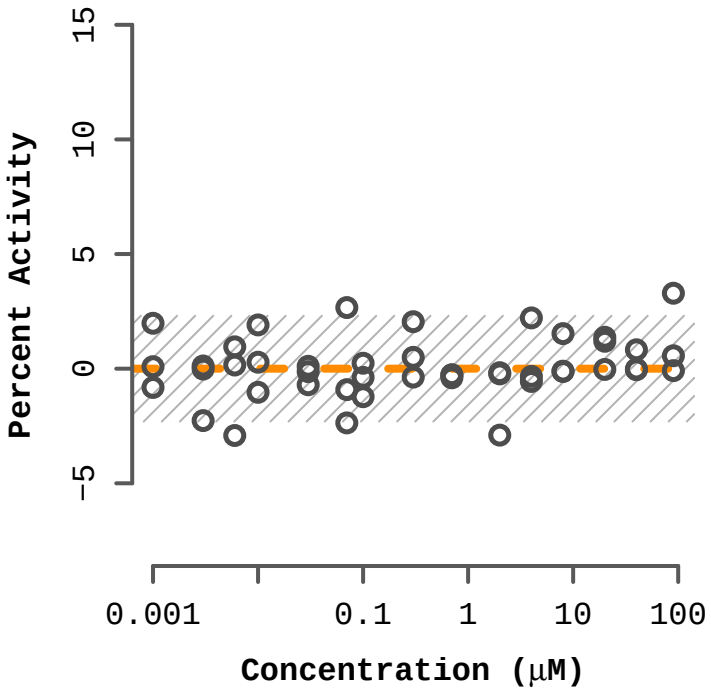
NAME: 1,2,4−Benzenetricarboxylic acid
CHID: 21487 **CASRN:** 528−44−9
SPID(S): Tox21_302990
M4ID: 12476143

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.256 **MAX_MED:** 0.315 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

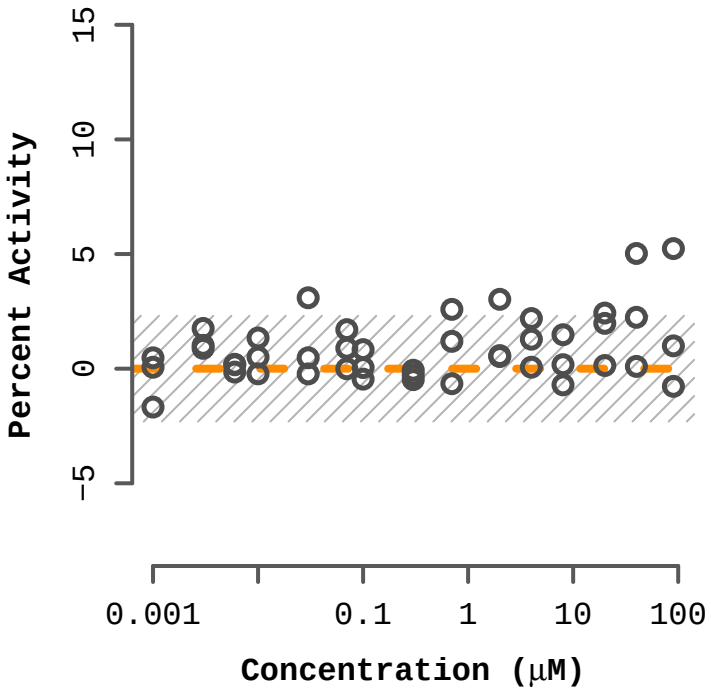
NAME: 1,2,4−Benzenetricarboxylic acid
CHID: 21487 **CASRN:** 528−44−9
SPID(S): Tox21_201939
M4ID: 12480313

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

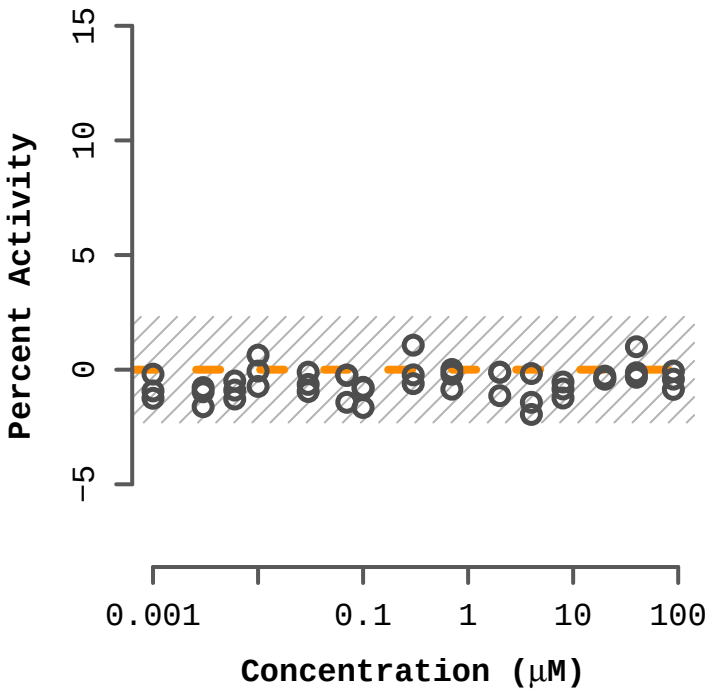
NAME: 1,3,5−Benzenetricarboxylic acid
CHID: 21488 CASRN: 554−95−0
SPID(S): Tox21_200017
M4ID: 12482235

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 2.46 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

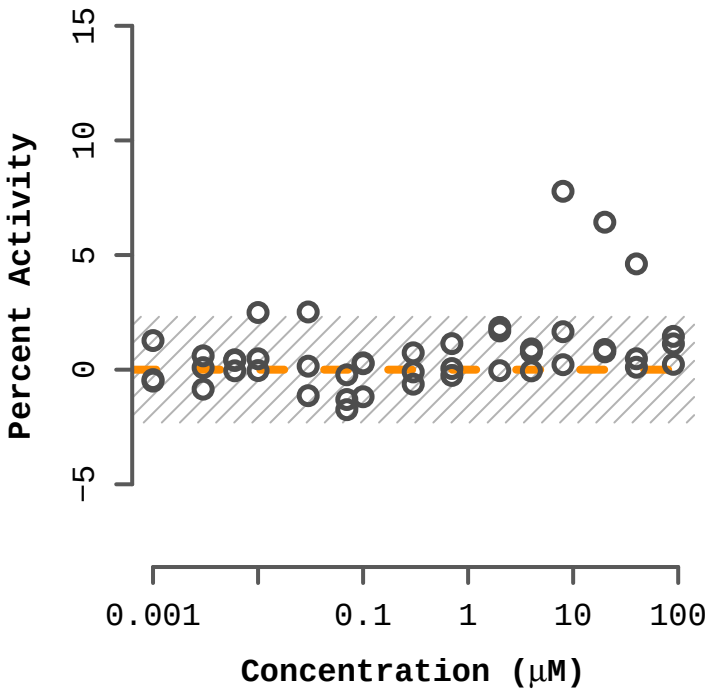
NAME: Benzonitrile
CHID: 21491 **CASRN:** 100-47-0
SPID(S): Tox21_302979
M4ID: 12476154

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.18 **MAX_MED:** −0.059 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

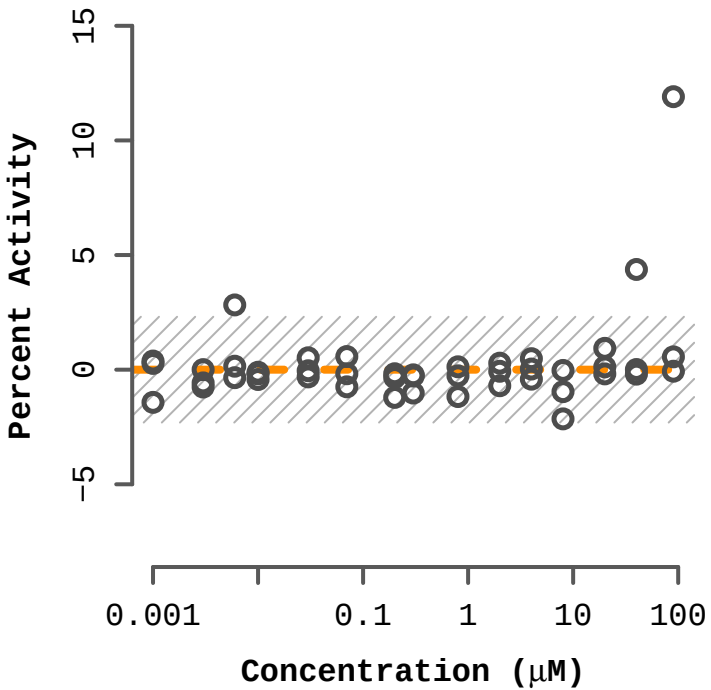
NAME: Benzonitrile
CHID: 21491 **CASRN:** 100-47-0
SPID(S): Tox21_201982
M4ID: 12480270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 3.22 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

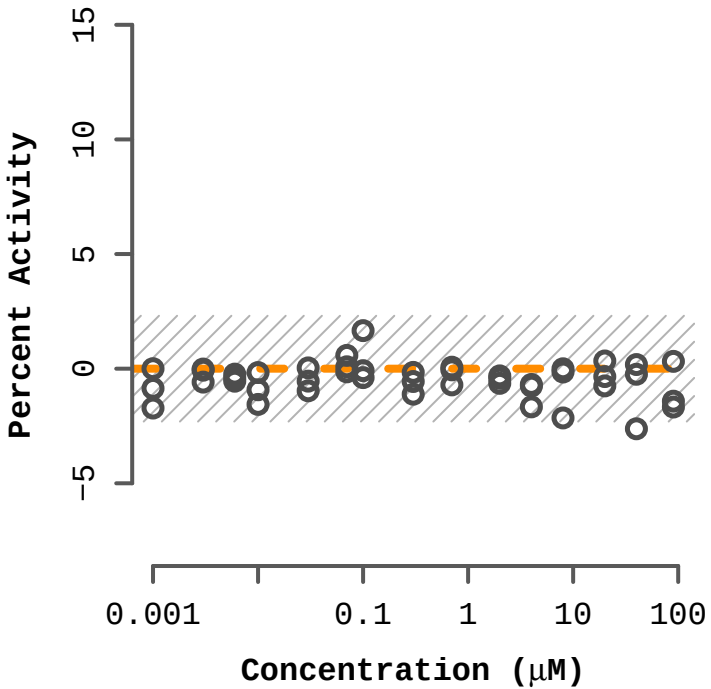
NAME: Benzyl cyanide
CHID: 21492 **CASRN:** 140-29-4
SPID(S): Tox21_200217
M4ID: 12482035

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 4.13 **MAX_MED:** 0.561 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

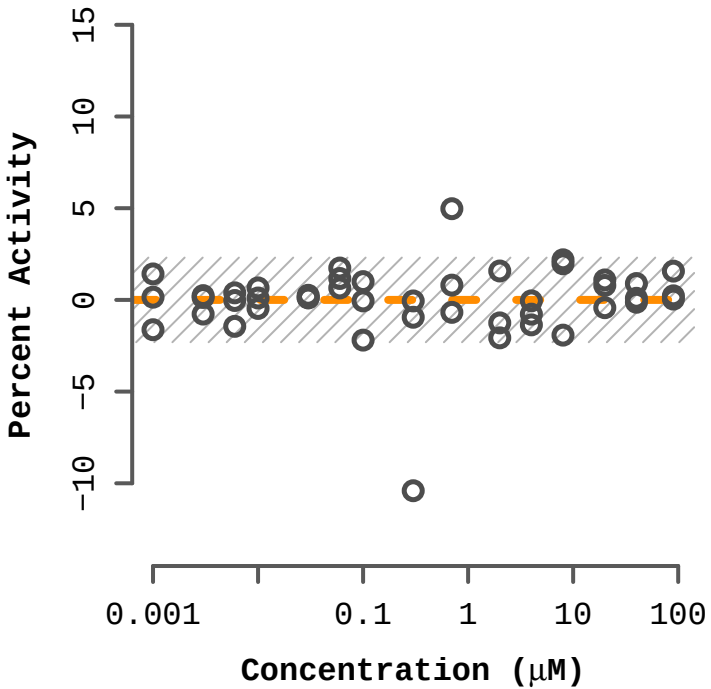
NAME: 2,6-Bis-(1,1-dimethylethyl)-2,5-cyclohexadiene-
CHID: 21493 **CASRN:** 719-22-2
SPID(S): Tox21_200521
M4ID: 12481731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.396 **MAX_MED:** 0.0837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

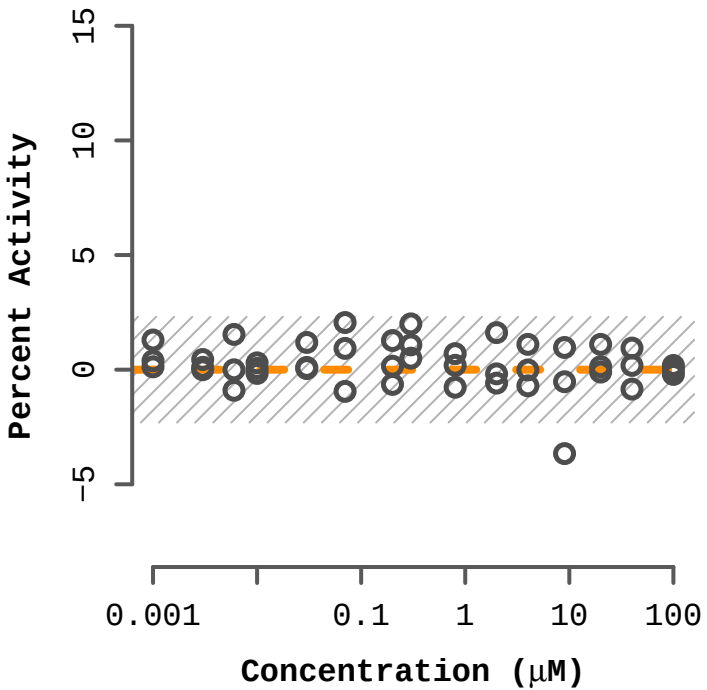
NAME: Bromoacetic acid
CHID: 21495 **CASRN:** 79-08-3
SPID(S): Tox21_200657
M4ID: 12481595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

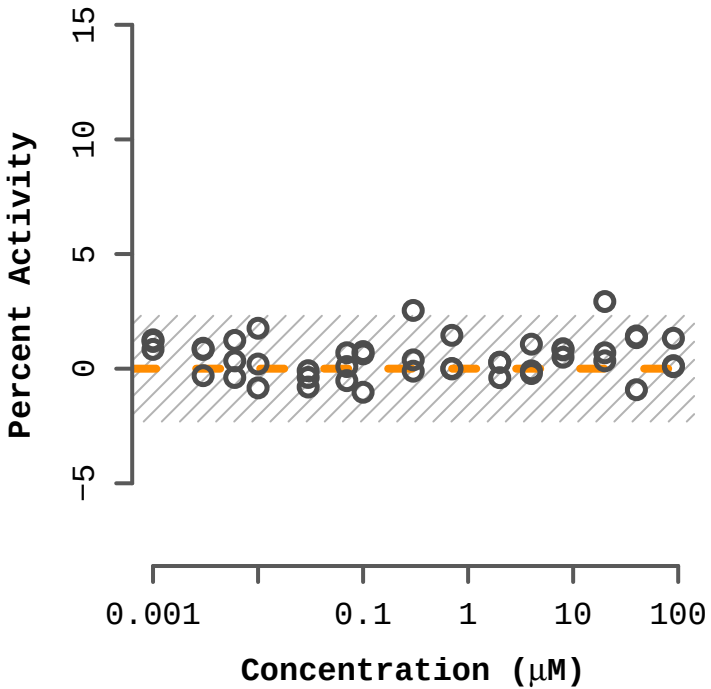
NAME: Bromoacetonitrile
CHID: 21496 **CASRN:** 590-17-0
SPID(S): Tox21_202207
M4ID: 12480045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

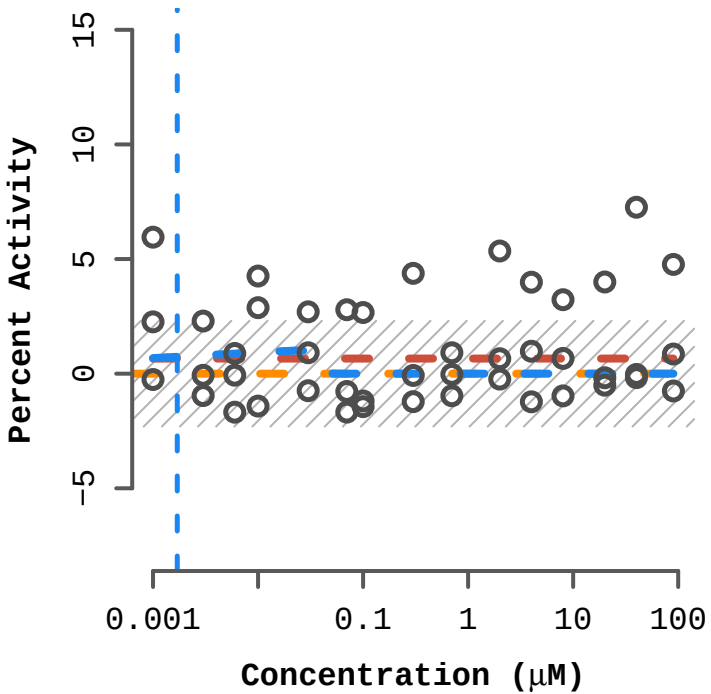
NAME: 2-Bromobenzothiazole
CHID: 21498 **CASRN:** 2516-40-7
SPID(S): Tox21_302813
M4ID: 12476320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Bromobenzothiazole
CHID: 21498 CASRN: 2516-40-7
SPID(S): Tox21_202134
M4ID: 12480118

HILL MODEL (in red):

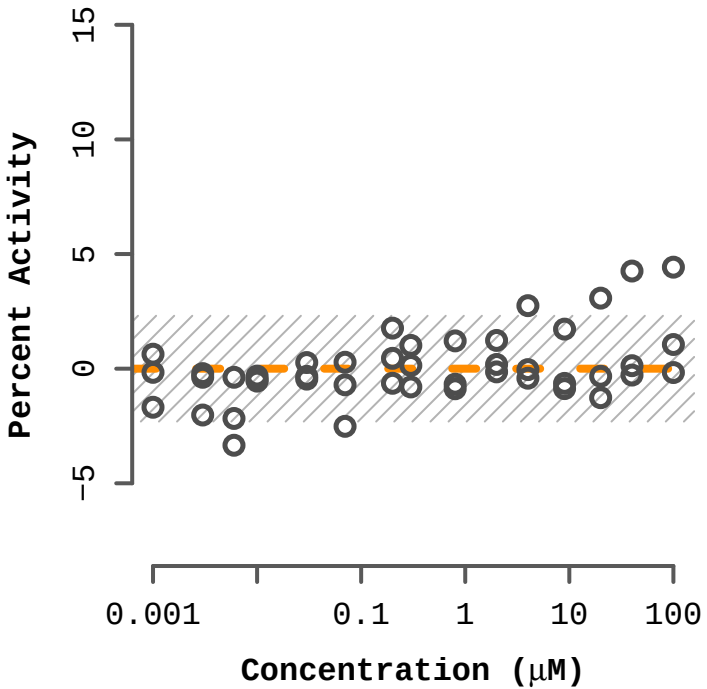
	tp	ga	gw
val:	0.659	-4.68	4.29
sd:	0.343	1650	4210

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.47	-2.77	0.3	-1.45	13.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	210	212.04	217.77
PROB:	0.72	0.26	0.01
RMSE:	2.51	2.31	2.44

MAX_MEAN: 2.65 MAX_MED: 2.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

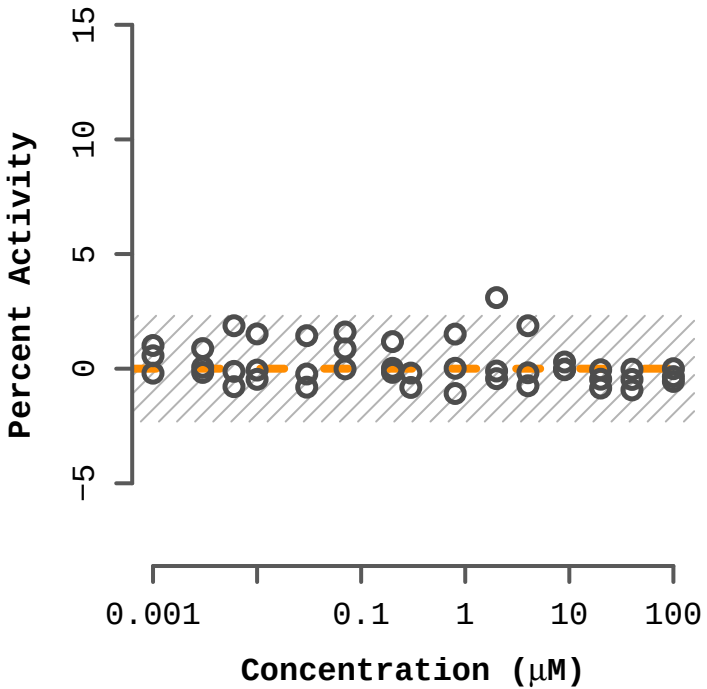
NAME: 2-Bromobutane
CHID: 21499 CASRN: 78-76-2
SPID(S): Tox21_200633
M4ID: 12481619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.77 MAX_MED: 1.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

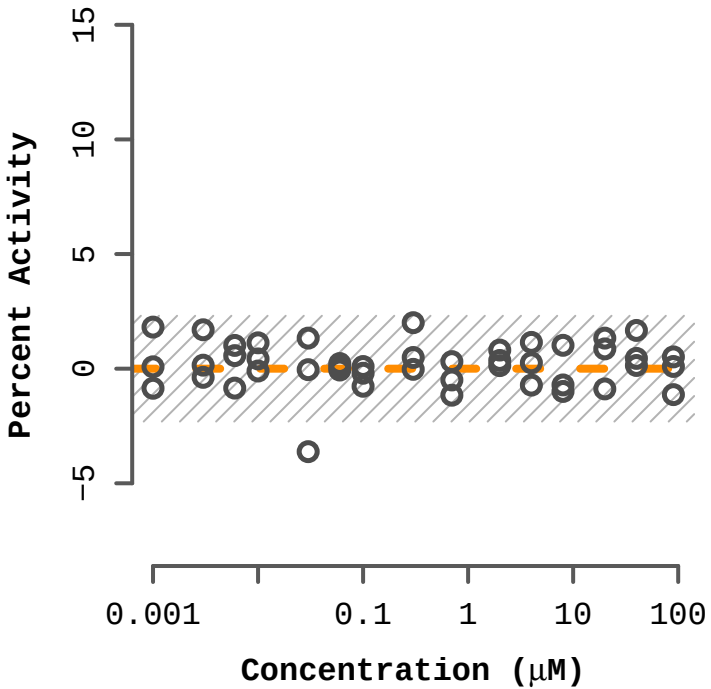
NAME: Bromochloromethane
CHID: 21503 **CASRN:** 74-97-5
SPID(S): Tox21_200790
M4ID: 12481462

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.856 **MAX_MED:** 0.863 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

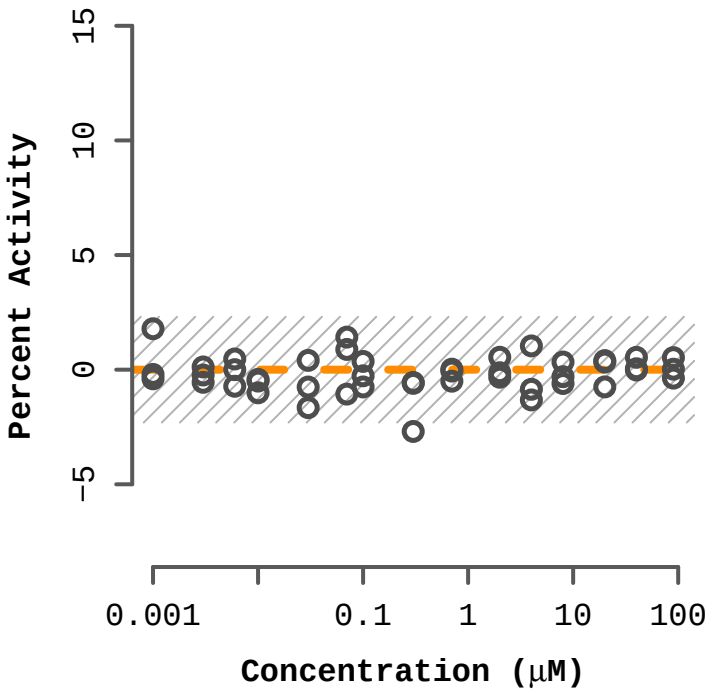
NAME: Butyraldehyde
CHID: 21513 **CASRN:** 123-72-8
SPID(S): Tox21_202491
M4ID: 12479761

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.97	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.824 **MAX_MED:** 0.865 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

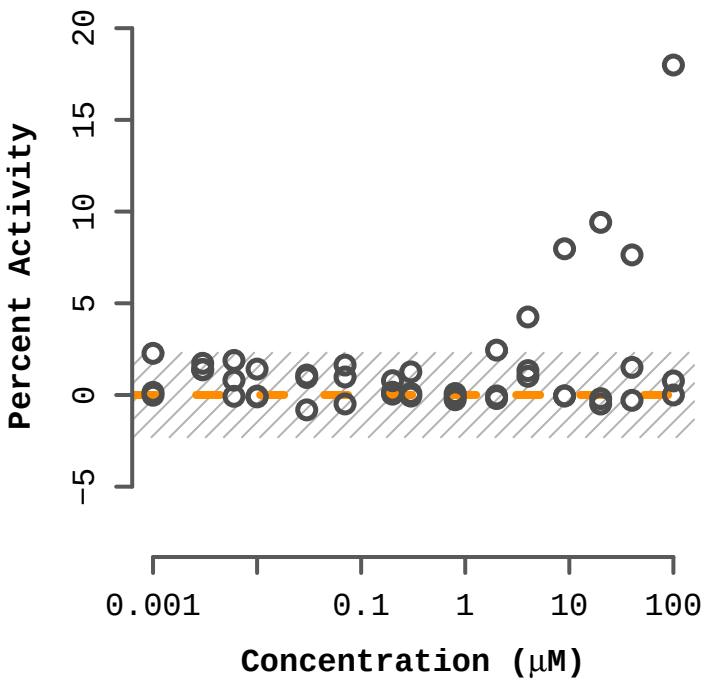
NAME: Butanoic acid
CHID: 21515 **CASRN:** 107-92-6
SPID(S): Tox21_300164
M4ID: 12478966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.414 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

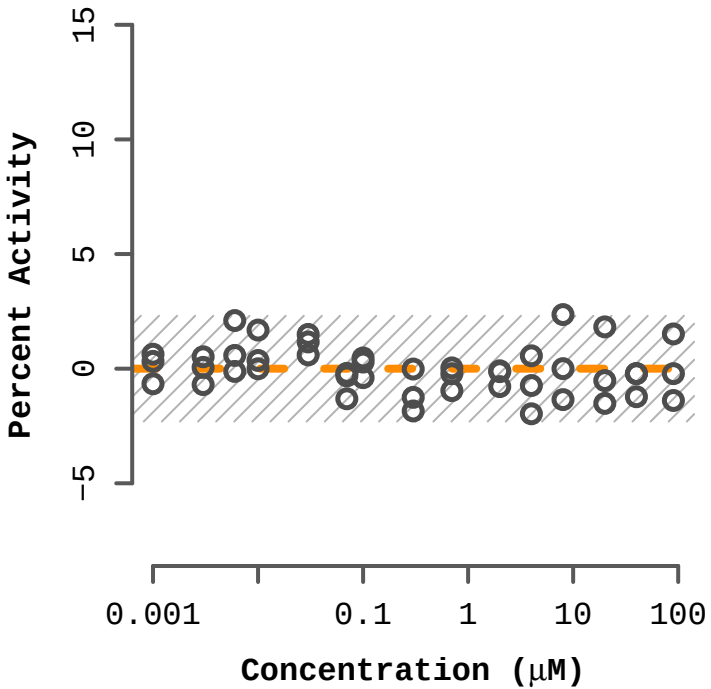
NAME: Butanoic acid
CHID: 21515 CASRN: 107-92-6
SPID(S): Tox21_202382
M4ID: 12479870

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.25	NA	NA
PROB:	1	NA	NA
RMSE:	3.63	NA	NA

MAX_MEAN: 6.25 MAX_MED: 1.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

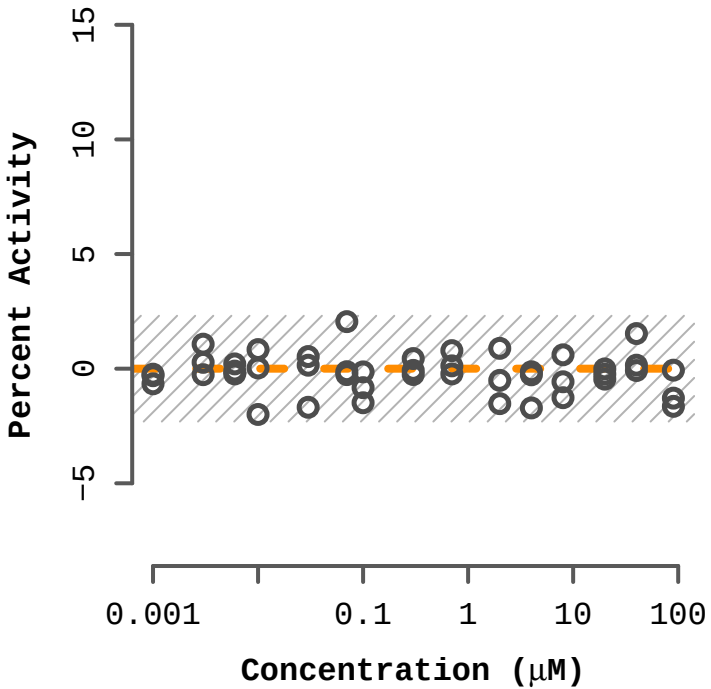
NAME: Methyl ethyl ketone
CHID: 21516 CASRN: 78-93-3
SPID(S): Tox21_200041
M4ID: 12482211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.09 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

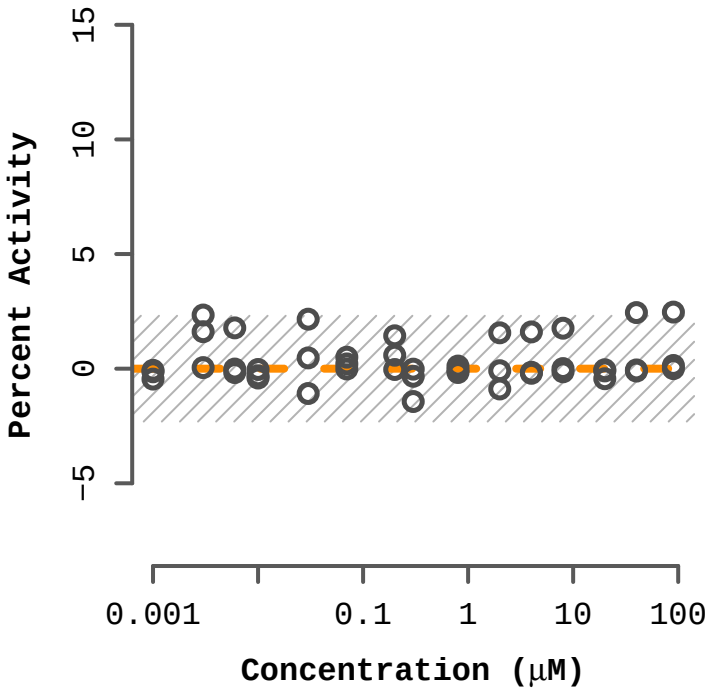
NAME: Maleic acid
CHID: 21517 **CASRN:** 110-16-7
SPID(S): Tox21_303045
M4ID: 12476088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.555 **MAX_MED:** 0.277 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

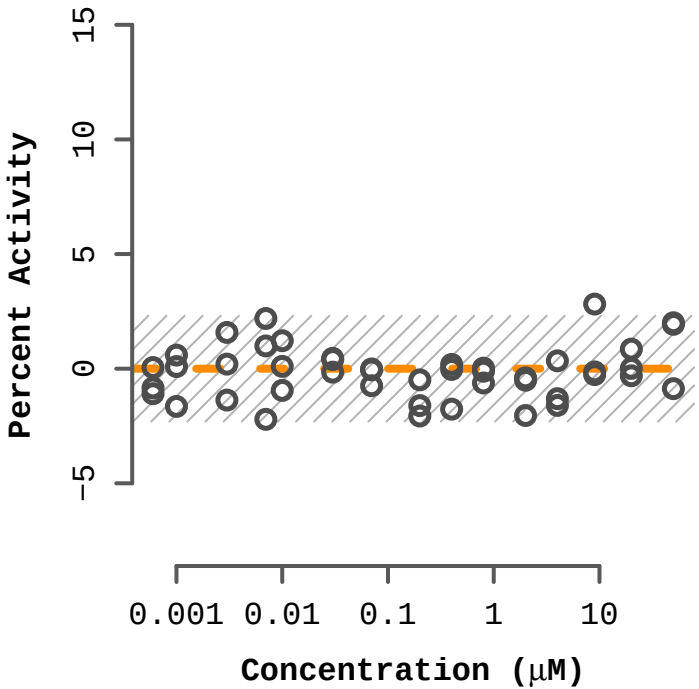
NAME: Maleic acid
CHID: 21517 **CASRN:** 110-16-7
SPID(S): Tox21_202193
M4ID: 12480059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

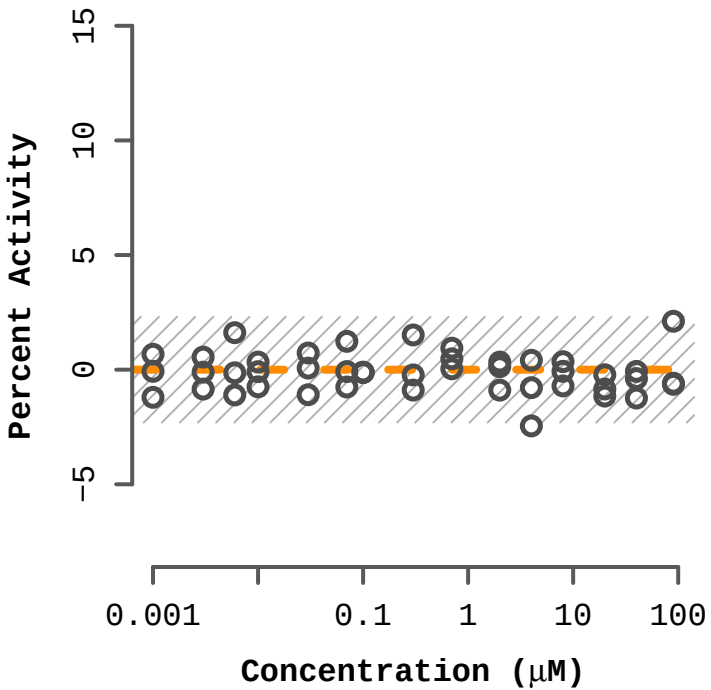
NAME: Maleic acid
CHID: 21517 **CASRN:** 110-16-7
SPID(S): Tox21_113105_1
M4ID: 12482805

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

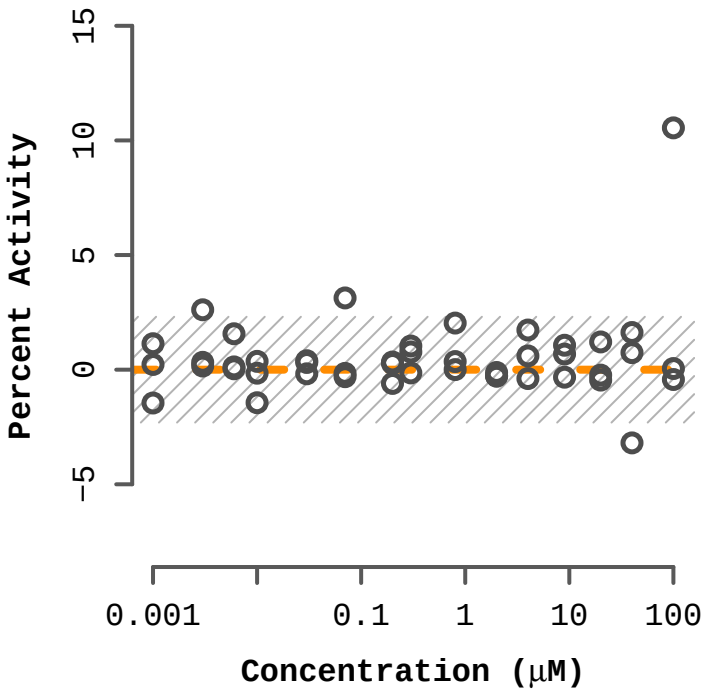
NAME: Fumaric acid
CHID: 21518 **CASRN:** 110-17-8
SPID(S): Tox21_302826
M4ID: 12476307

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 0.472 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

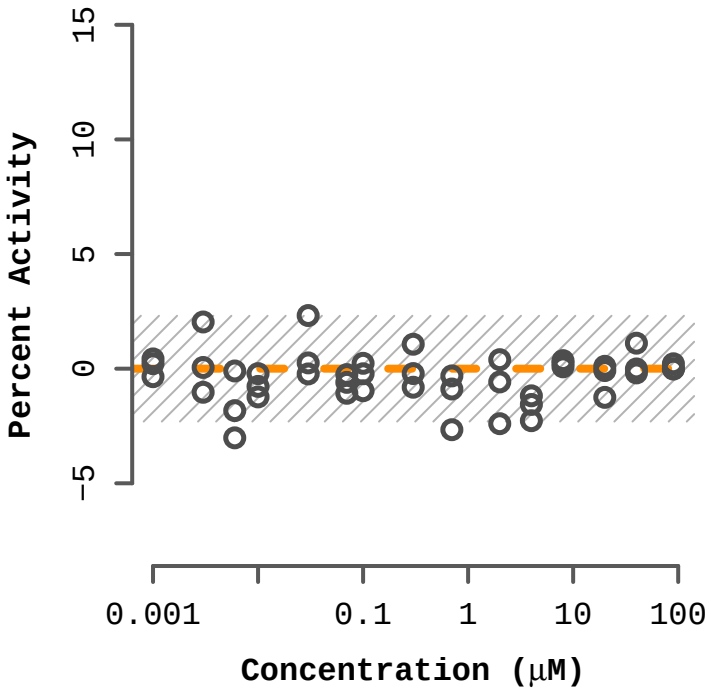
NAME: Fumaric acid
CHID: 21518 **CASRN:** 110-17-8
SPID(S): Tox21_201769
M4ID: 12480483

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.91	NA	NA

MAX_MEAN: 3.39 **MAX_MED:** 0.777 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

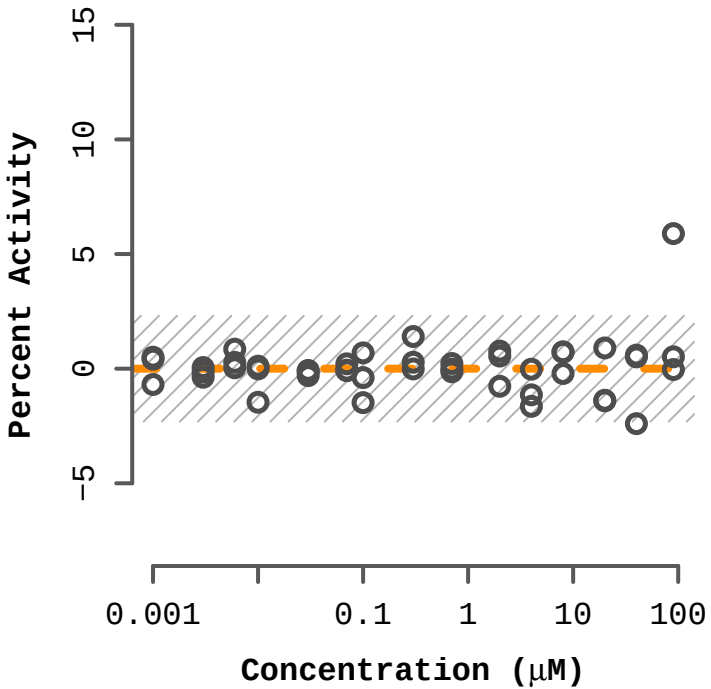
NAME: 2-(2-Butoxyethoxy)ethanol
CHID: 21519 **CASRN:** 112-34-5
SPID(S): Tox21_300084
M4ID: 12479046

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.782 **MAX_MED:** 0.254 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

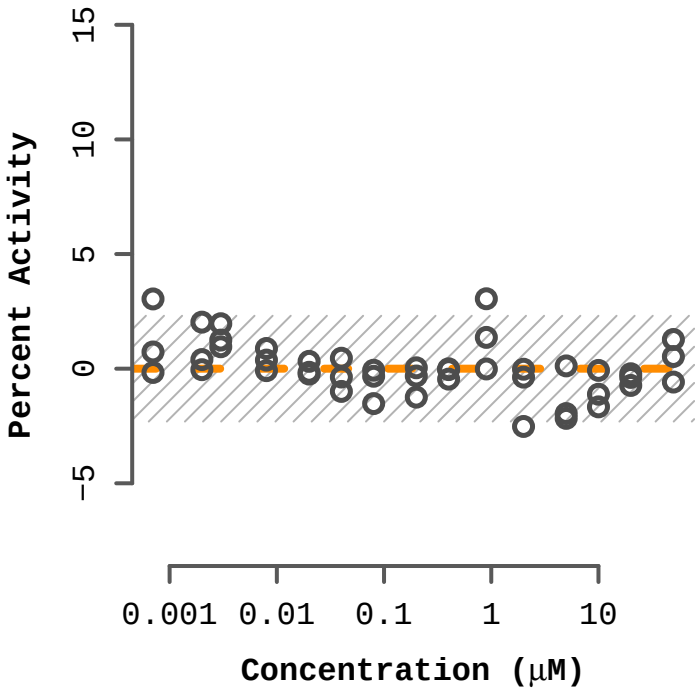
NAME: 2-(2-Butoxyethoxy)ethanol
CHID: 21519 **CASRN:** 112-34-5
SPID(S): Tox21_202404
M4ID: 12479848

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 0.718 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

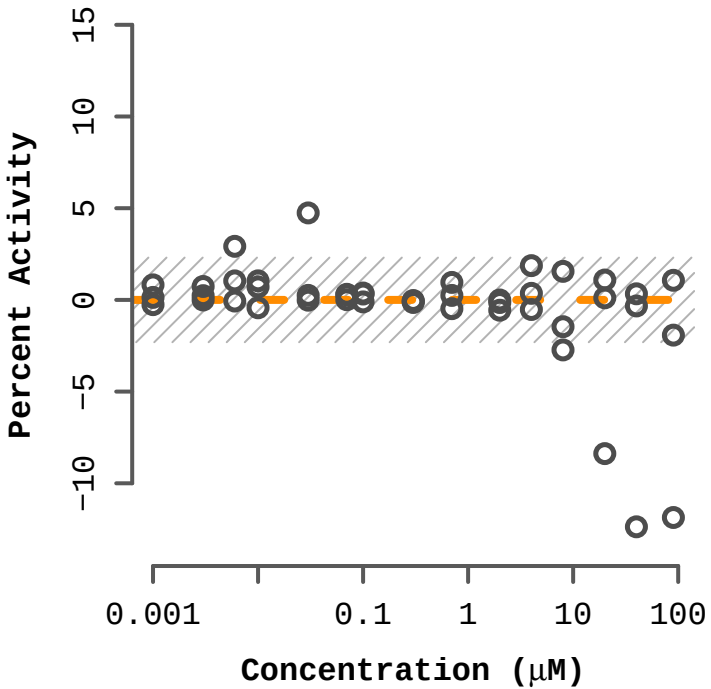
NAME: 2-[2-(2-Butoxyethoxy)ethoxy]ethanol
CHID: 21520 **CASRN:** 143-22-6
SPID(S): Tox21_302836
M4ID: 12476297

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

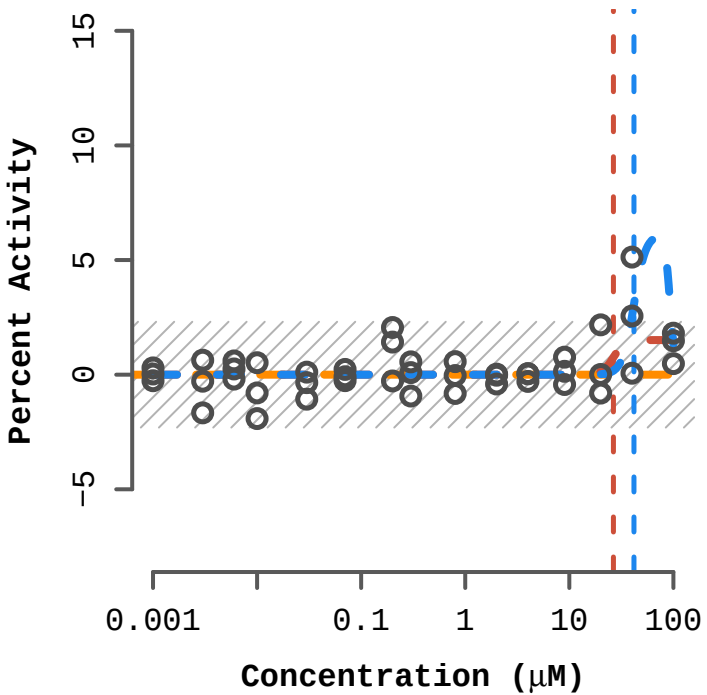
NAME: 2-[2-(2-Butoxyethoxy)ethoxy]ethanol
CHID: 21520 **CASRN:** 143-22-6
SPID(S): Tox21_201885
M4ID: 12480367

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.07	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloroacetonitrile
CHID: 21524 **CASRN:** 107-14-2
SPID(S): Tox21_200957
M4ID: 12481295

HILL MODEL (in red):

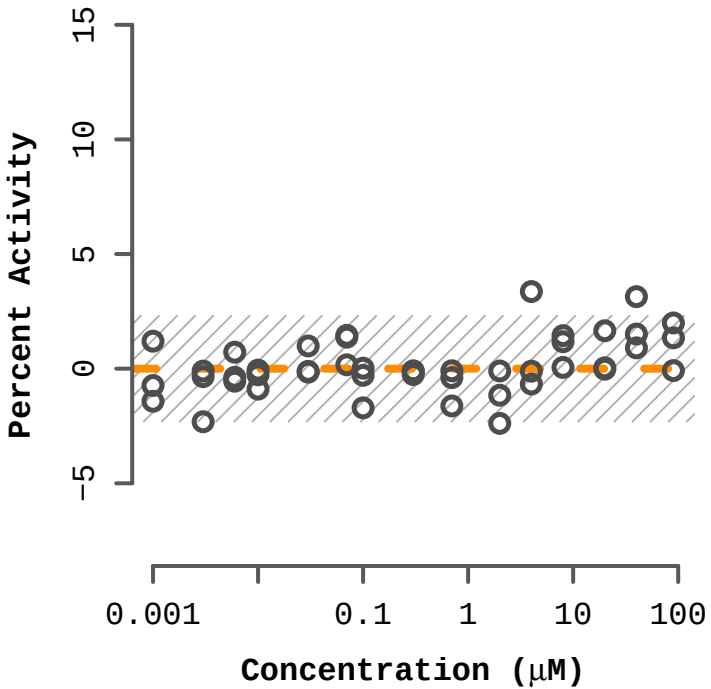
	tp	ga	gw
val:	1.51	1.42	8
sd:	0.415	0.136	7.66

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.14	1.62	7.78	1.97	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	129.75	124.08	125.88
PROB:	0.04	0.68	0.28
RMSE:	1.19	0.97	0.93

MAX_MEAN: 2.59 **MAX_MED:** 2.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

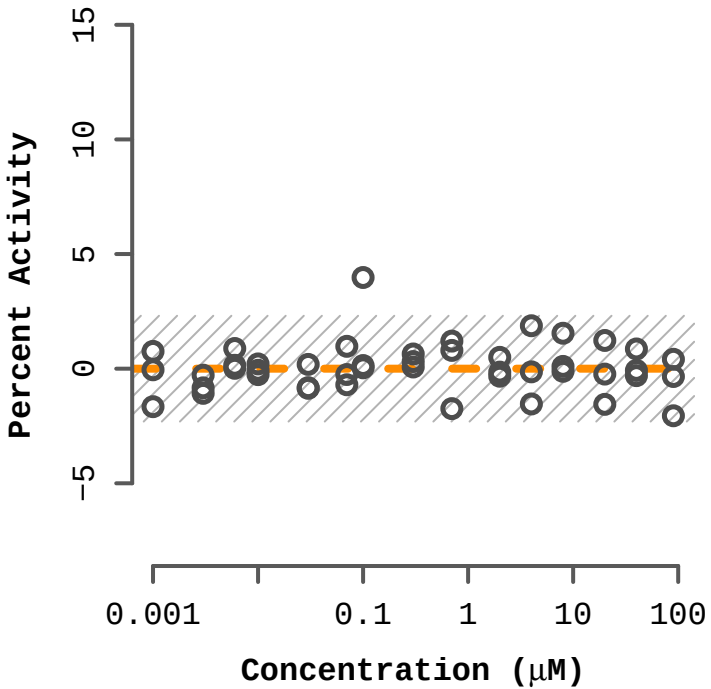
NAME: Chlorobutanedioic acid
CHID: 21526 **CASRN:** 16045-92-4
SPID(S): Tox21_200034
M4ID: 12482218

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

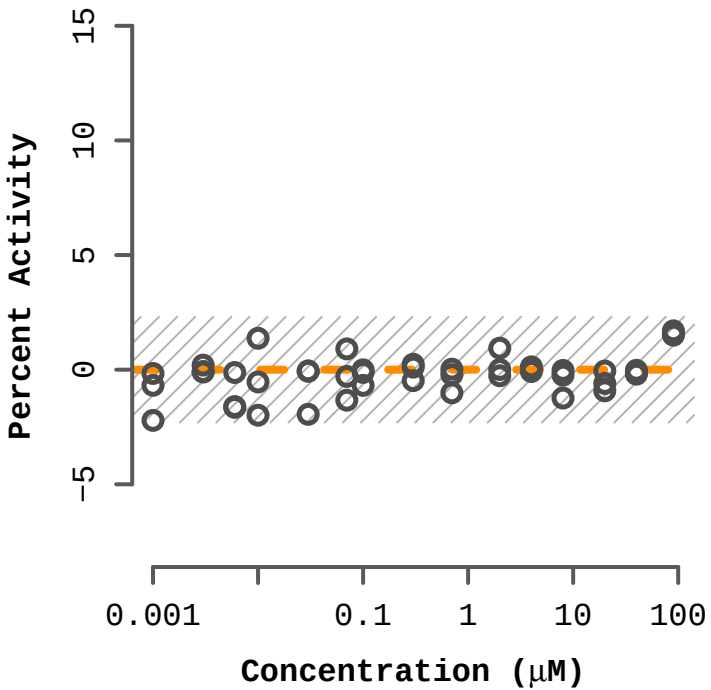
NAME: 2-Chlorocyclohexanone
CHID: 21530 CASRN: 822-87-7
SPID(S): Tox21_200522
M4ID: 12481730

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.38 MAX_MED: 0.798 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

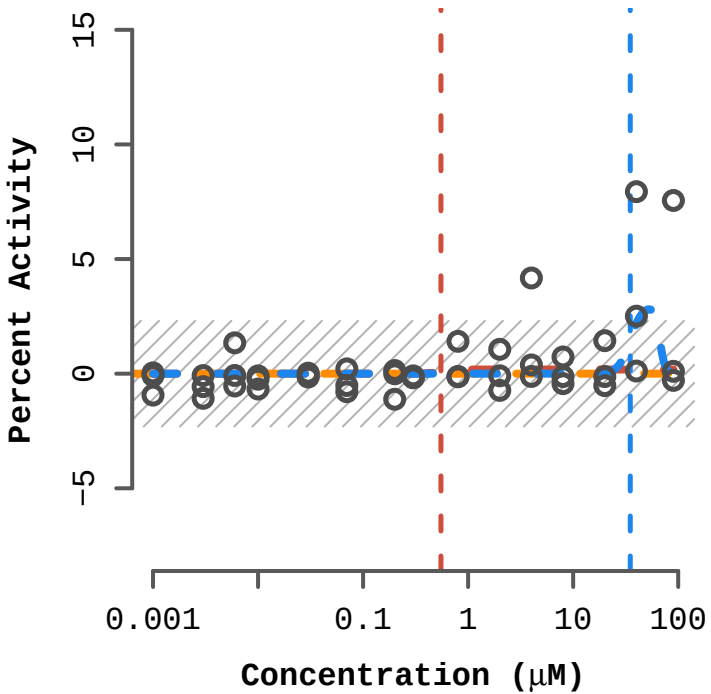
NAME: 1-Chlorooctane
CHID: 21543 **CASRN:** 111-85-3
SPID(S): Tox21_302948
M4ID: 12476185

HILL MODEL: Not applicable.

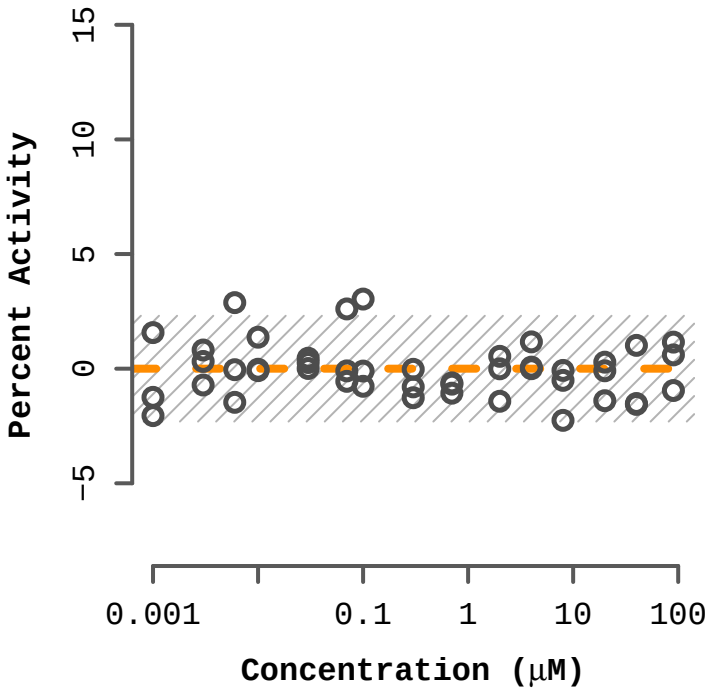
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.58 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Chlorooctane
CHID:    21543   CASRN: 111-85-3
SPID(S): Tox21_201715
M4ID:    12480537

HILL MODEL (in red):
      tp       ga       gw
val:  0.182    -0.259   8
sd:   0.188    0.89     31.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.98     1.54     7.73     1.82     17.2
sd:   35.2     2.12     58.3     1.42     171

      CNST        HILL        GNLS
AIC:  139.71      144.68      145.4
PROB: 0.88        0.07        0.05
RMSE: 1.88        1.83        1.67

MAX_MEAN: 3.52      MAX_MED: 2.51      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

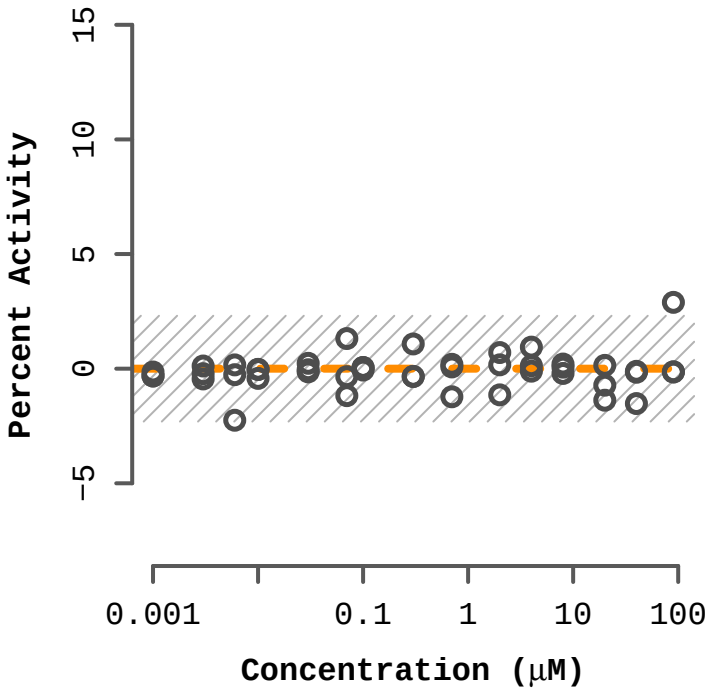
NAME: 2-Chlorophenol
CHID: 21544 **CASRN:** 95-57-8
SPID(S): Tox21_300340
M4ID: 12478792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.722 **MAX_MED:** 0.602 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

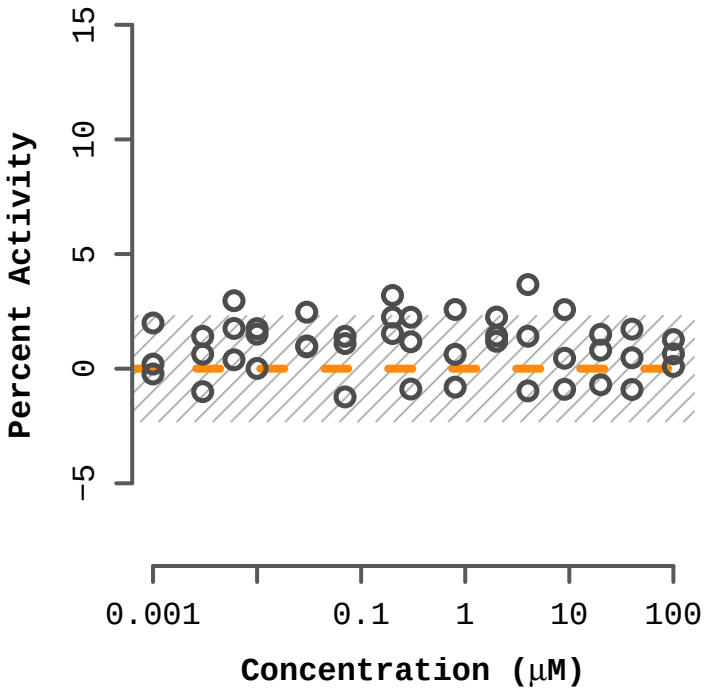
NAME: 2-Chlorophenol
CHID: 21544 **CASRN:** 95-57-8
SPID(S): Tox21_201410
M4ID: 12480842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.872 **MAX_MED:** 0.169 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

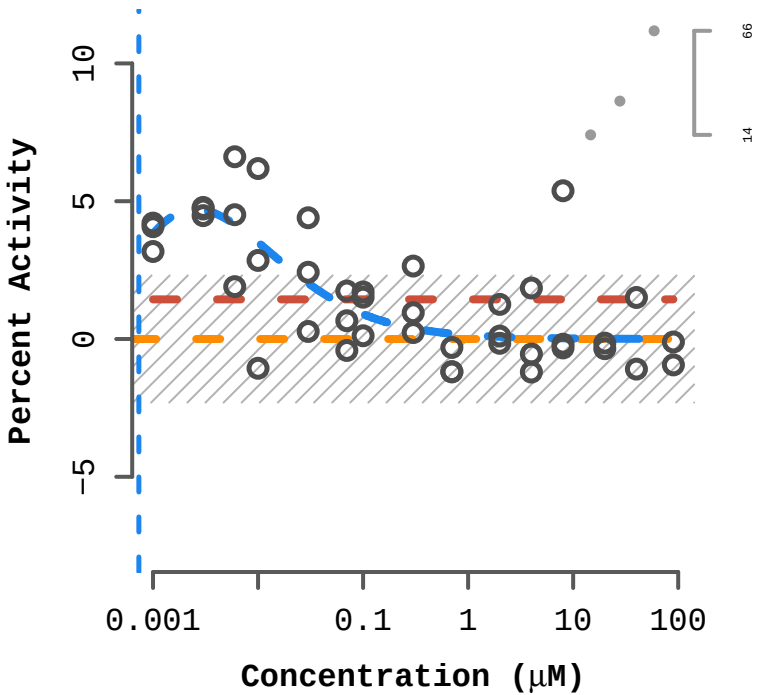
NAME: 2-Chloropropanoic acid
CHID: 21545 **CASRN:** 598-78-7
SPID(S): Tox21_200650
M4ID: 12481602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Chloropropanoic acid
CHID: 21546 CASRN: 107-94-8
SPID(S): Tox21_201185
M4ID: 12481067 BRK

HILL MODEL (in red):

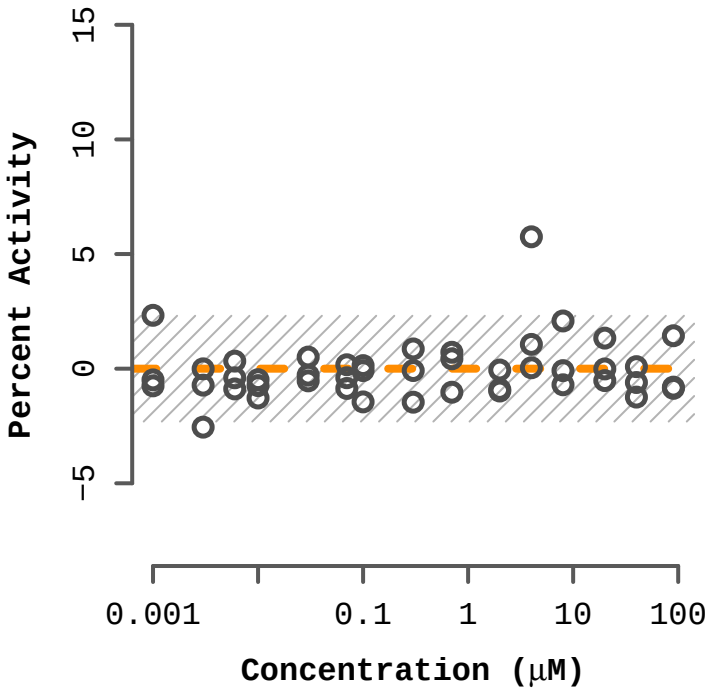
	tp	ga	gw
val:	1.44	-4.96	3.98
sd:	0.431	1960	3970

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.05	-3.13	1.55	-1.99	0.845
sd:	22.7	1.02	8.38	2.92	0.964

	CNST	HILL	GNLS
AIC:	272.65	267.49	245.01
PROB:	0	0	1
RMSE:	11.36	10.95	11.16

MAX_MEAN: 21.6 MAX_MED: 4.72 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

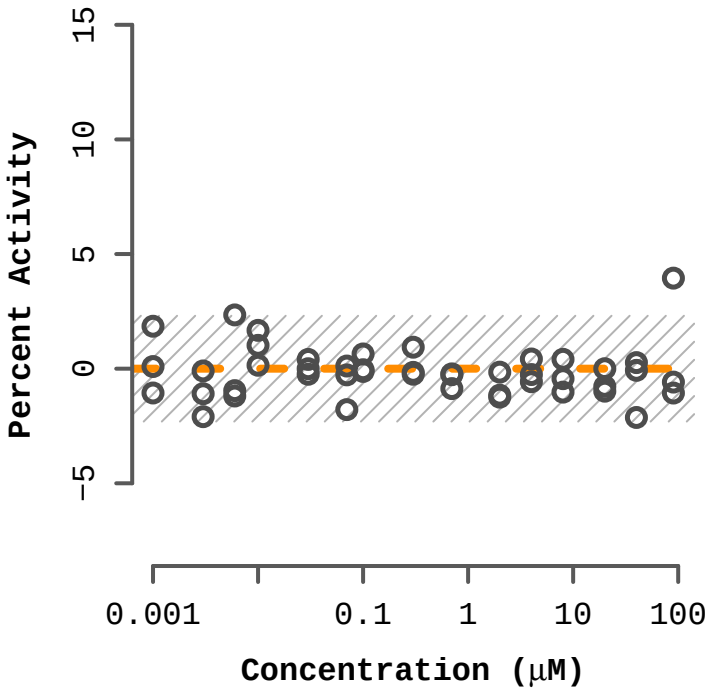
NAME: 1-Chloropropan-2-one
CHID: 21547 **CASRN:** 78-95-5
SPID(S): Tox21_200027
M4ID: 12482225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.29 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

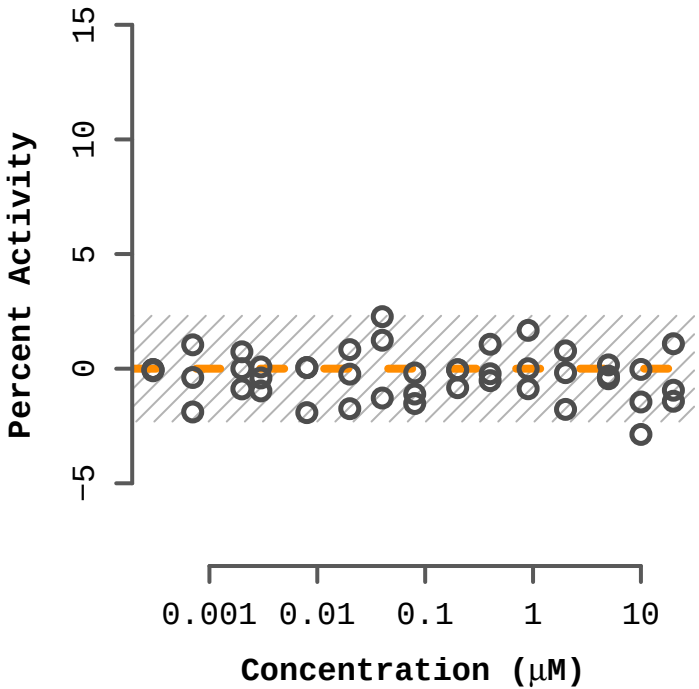
NAME: Cyanogen bromide
CHID: 21550 **CASRN:** 506-68-3
SPID(S): Tox21_303779
M4ID: 12475409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.947 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

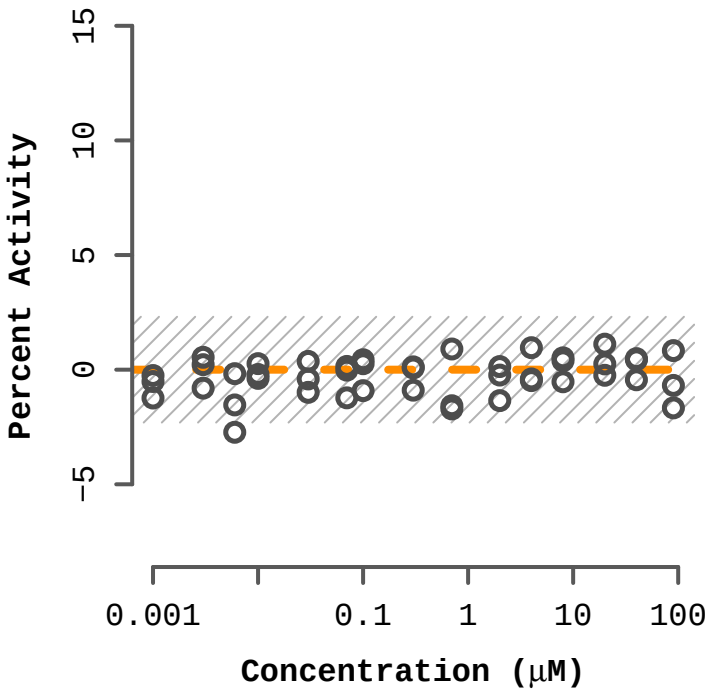
NAME: Cyclododecane
CHID: 21552 **CASRN:** 294-62-2
SPID(S): Tox21_202734
M4ID: 12479518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.745 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

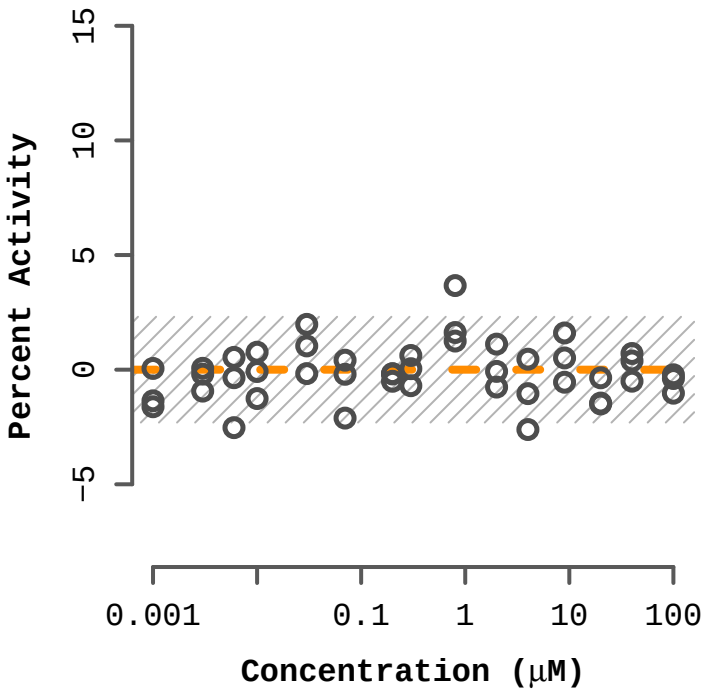
NAME: Decanal
CHID: 21553 **CASRN:** 112-31-2
SPID(S): Tox21_302656
M4ID: 12476477

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.374 **MAX_MED:** 0.432 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

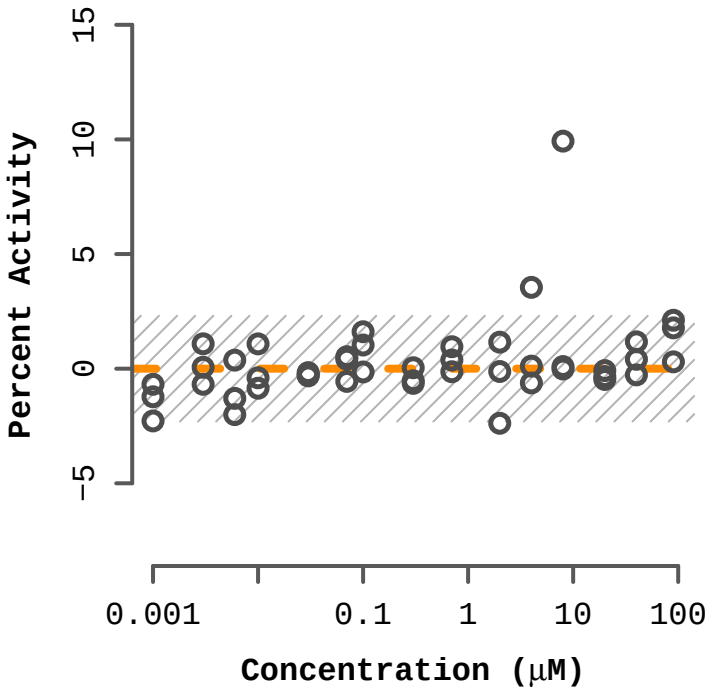
NAME: Decanoic acid
CHID: 21554 CASRN: 334-48-5
SPID(S): Tox21_300366
M4ID: 12478766

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 2.18 MAX_MED: 1.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

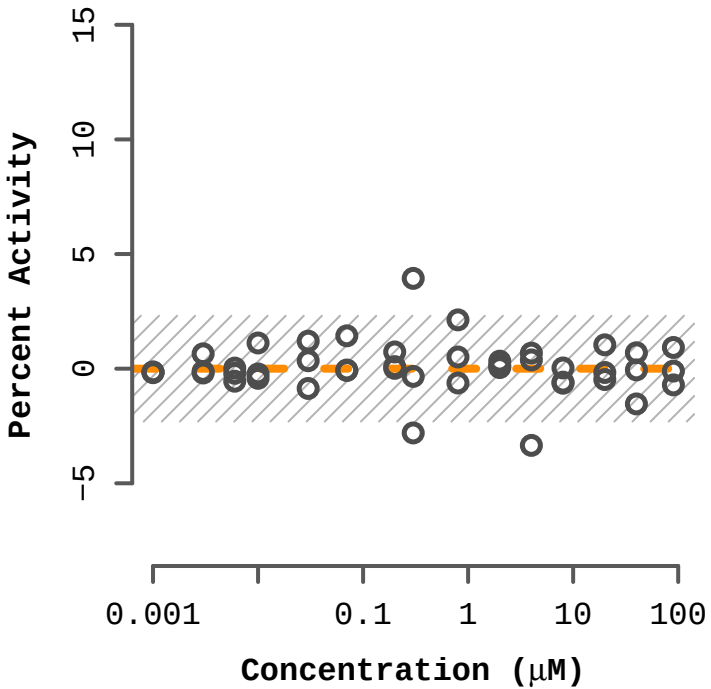
NAME: Decanoic acid
CHID: 21554 CASRN: 334-48-5
SPID(S): Tox21_202209
M4ID: 12480043

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 3.34 MAX_MED: 1.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

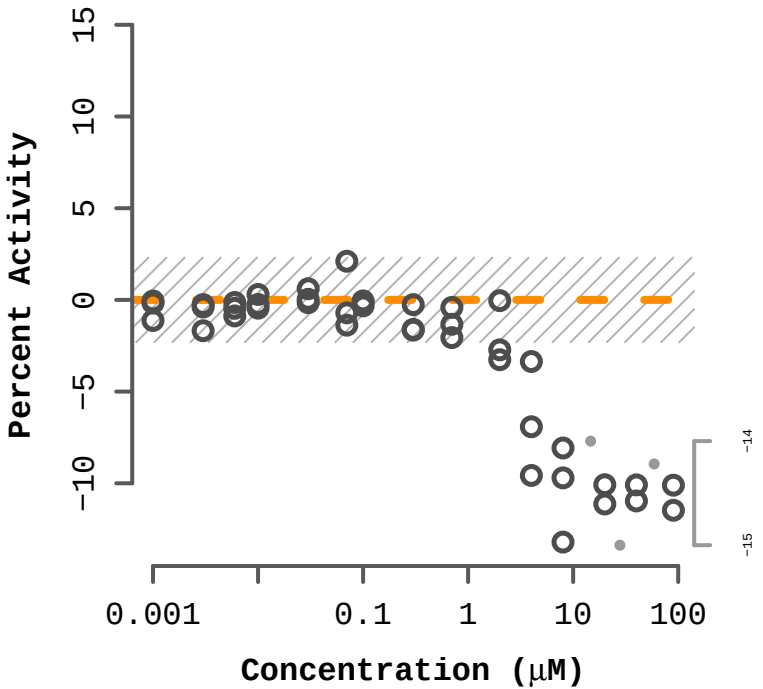
NAME: Dibromomethane
CHID: 21557 CASRN: 74-95-3
SPID(S): Tox21_200410
M4ID: 12481842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.672 MAX_MED: 0.511 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

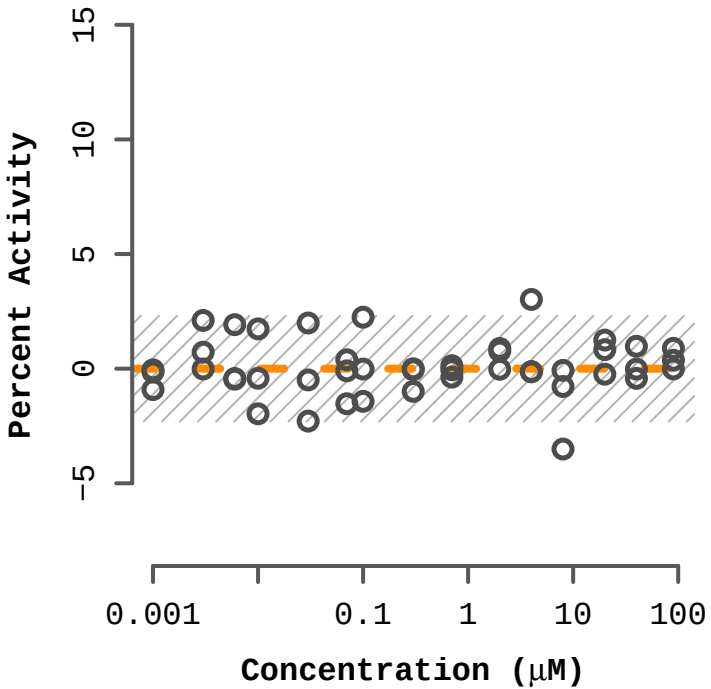
NAME: 2,6-Di-tert-butyl-4-nitrophenol
CHID: 21559 **CASRN:** 728-40-5
SPID(S): Tox21_301750
M4ID: 12477383 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	293.17	NA	NA
PROB:	1	NA	NA
RMSE:	6.42	NA	NA

MAX_MEAN: 0.166 **MAX_MED:** 0.0344 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

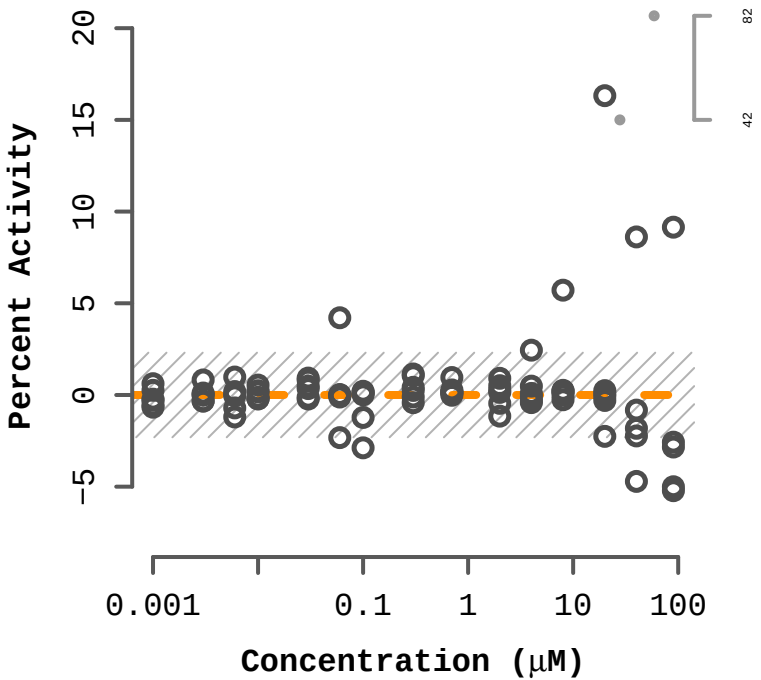
NAME: 2,2-Dichloroacetamide
CHID: 21561 **CASRN:** 683-72-7
SPID(S): Tox21_200050
M4ID: 12482202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 0.832 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

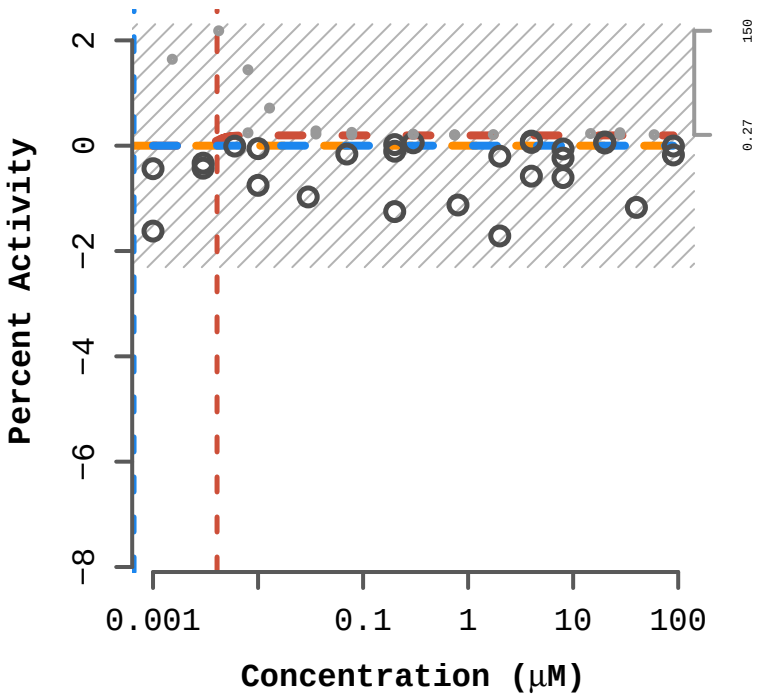
NAME: Dichloroacetonitrile
CHID: 21562 **CASRN:** 3018-12-0
SPID(S): Tox21_200218
M4ID: 12482034 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	402.09	NA	NA
PROB:	1	NA	NA
RMSE:	10	NA	NA

MAX_MEAN: 12.5 **MAX_MED:** 0.418 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,6-Dichloro-1,3-benzenediol
CHID: 21563 CASRN: 137-19-9
SPID(S): Tox21_200523
M4ID: 12481729 BRK

HILL MODEL (in red):

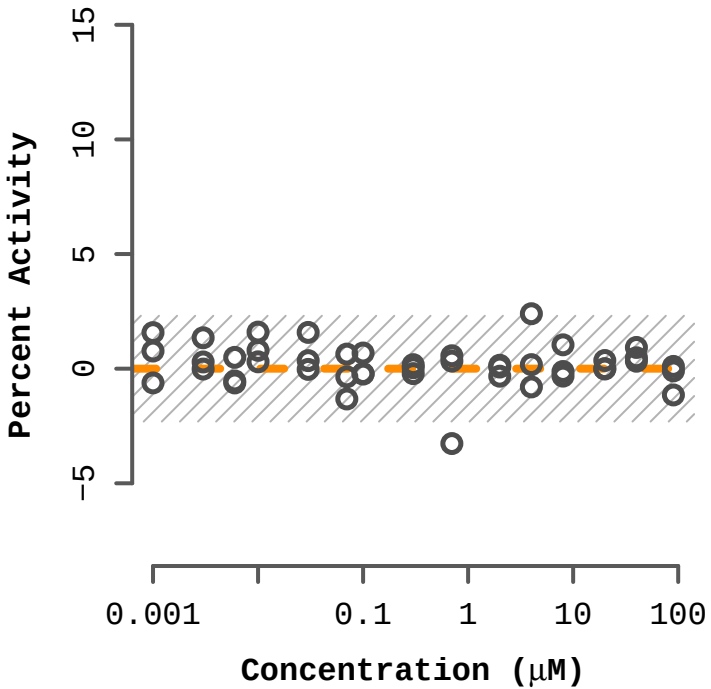
	tp	ga	gw
val:	0.196	-2.39	8
sd:	0.249	0.507	27.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.85e-09	-3.18	6.93	-2.73	7.45
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	292.89	298.25	302.89
PROB:	0.93	0.06	0.01
RMSE:	30.67	30.64	30.67

MAX_MEAN: 48.3 MAX_MED: 3.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

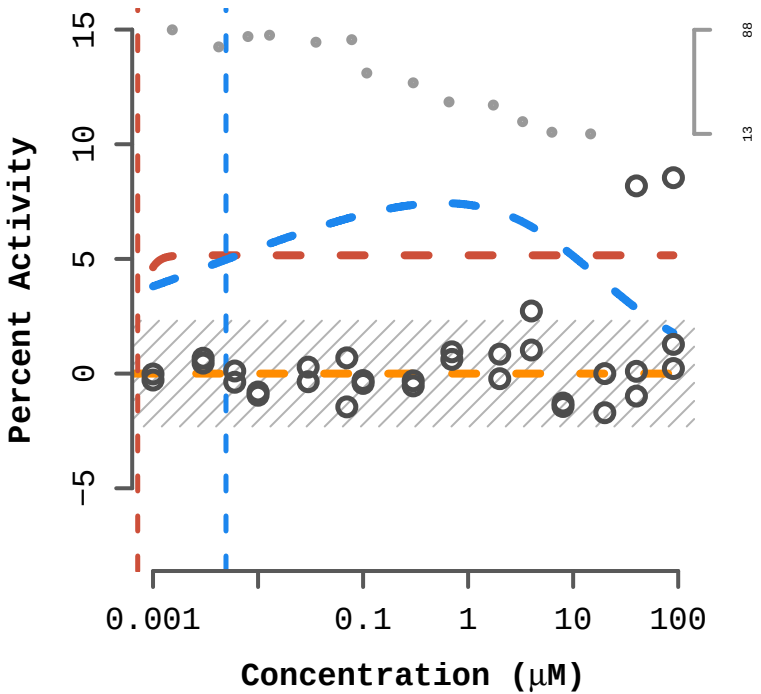
NAME: 2,3-Dichlorobutane
CHID: 21565 **CASRN:** 7581-97-7
SPID(S): Tox21_200667
M4ID: 12481585

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.9 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dalapon
CHID: 21575 CASRN: 75-99-0
SPID(S): Tox21_300364
M4ID: 12478768 BRK

HILL MODEL (in red):

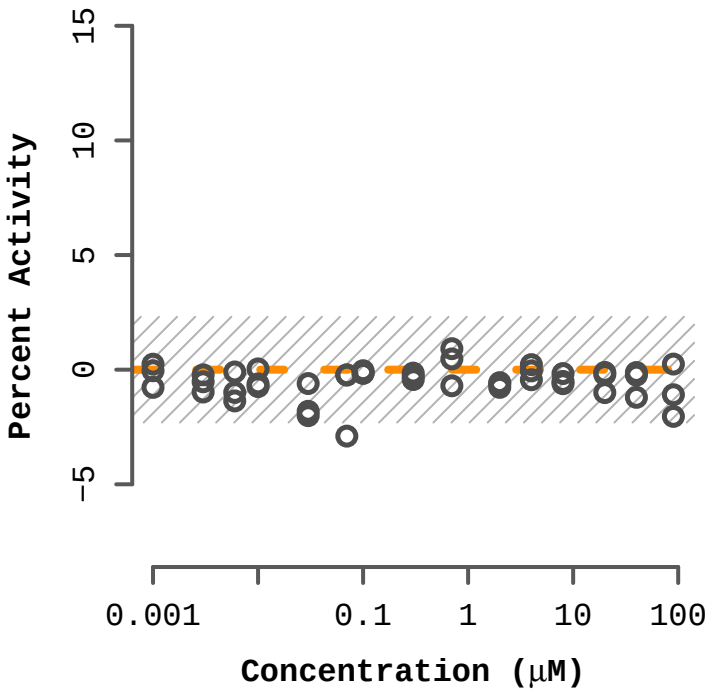
	tp	ga	gw
val:	5.16	−3.15	6.51
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.95	−2.31	0.3	1.15	0.791
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	425.75	427.08	430.69
PROB:	0.63	0.32	0.05
RMSE:	33.23	31.05	30.82

MAX_MEAN: 29.3 MAX_MED: 2.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

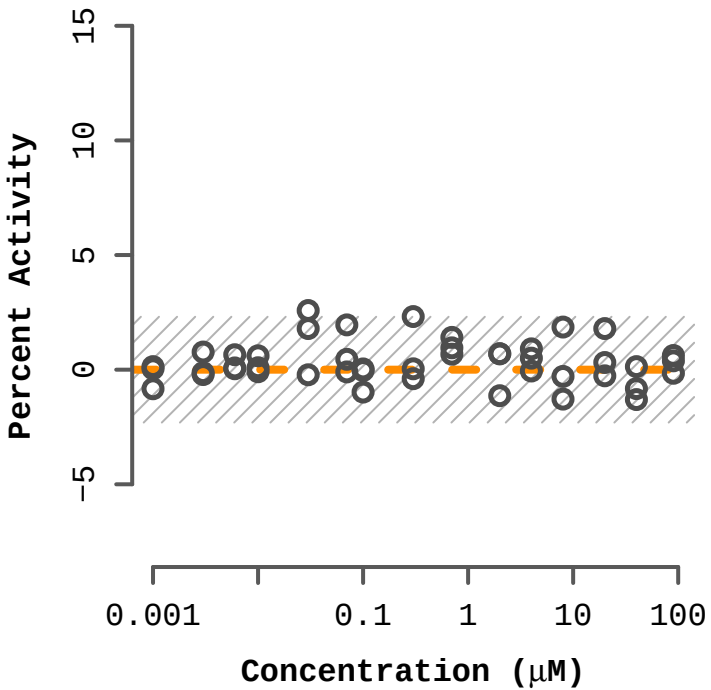
NAME: Dalapon
CHID: 21575 CASRN: 75-99-0
SPID(S): Tox21_201510
M4ID: 12480742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.228 MAX_MED: 0.469 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

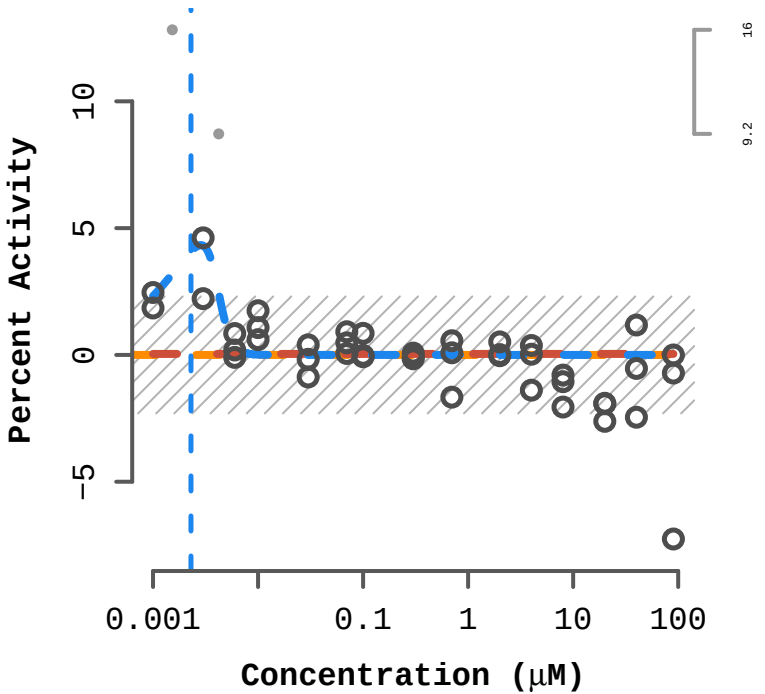
NAME: 1,1−Dichloropropanone
CHID: 21576 **CASRN:** 513−88−2
SPID(S): Tox21_201090
M4ID: 12481162

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3−Dichloropropanone
CHID: 21577 CASRN: 534−07−6
SPID(S): Tox21_302809
M4ID: 12476324 BRK

HILL MODEL (in red):

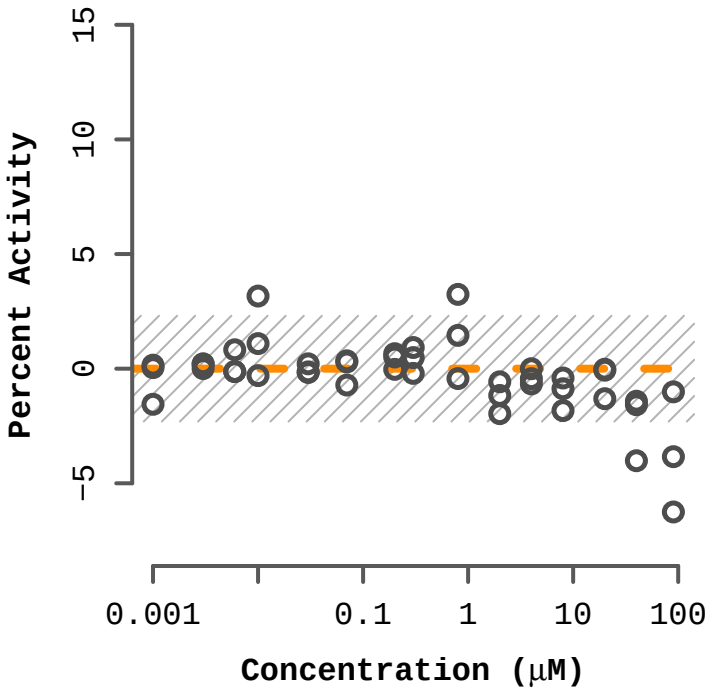
	tp	ga	gw
val:	0.0396	−4.9	7.6
sd:	0.219	20600	4620000

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.3	−2.64	1.14	−2.39	7.17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	196.49	202.46	184.74
PROB:	0	0	1
RMSE:	3.28	3.27	2.67

MAX_MEAN: 6.9 MAX_MED: 4.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

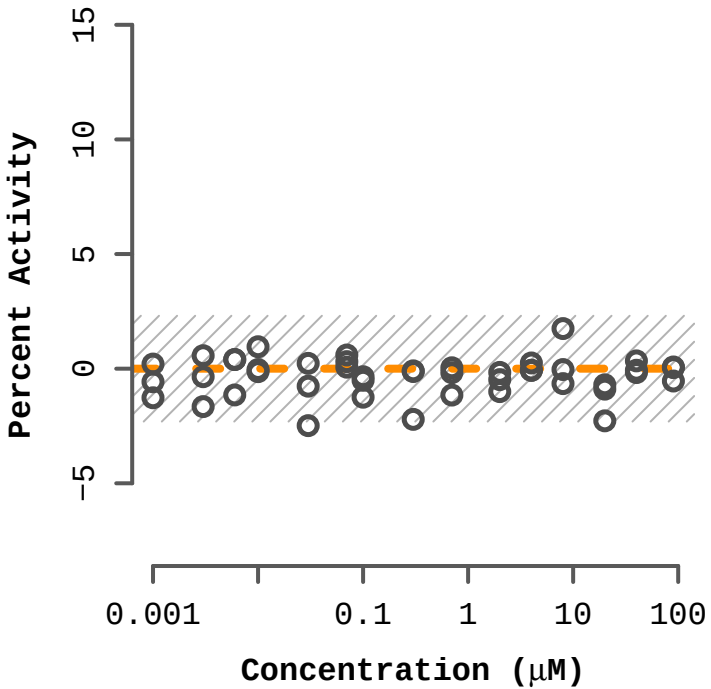
NAME: 1,3-Dichloropropanone
CHID: 21577 CASRN: 534-07-6
SPID(S): Tox21_201433
M4ID: 12480819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.42 MAX_MED: 1.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

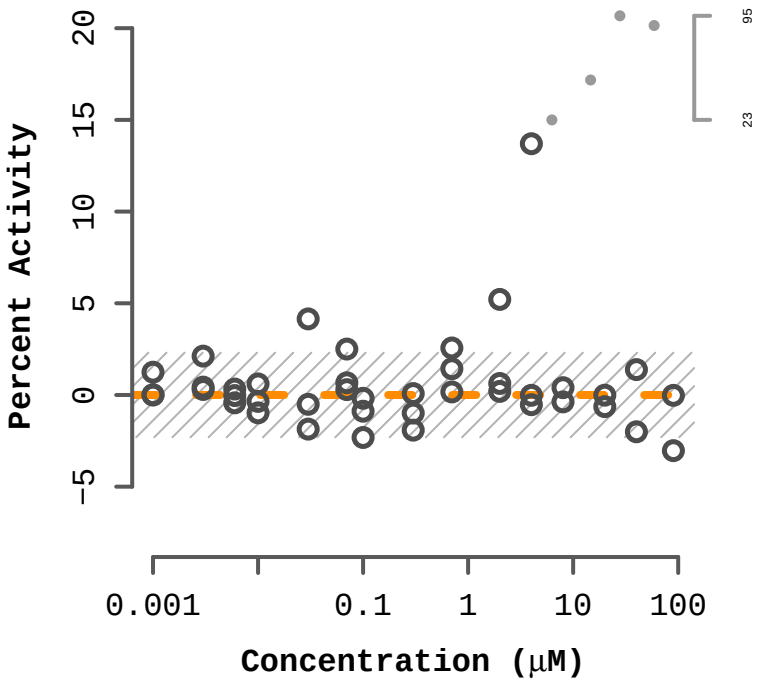
NAME: 2,2−Dimethylbutanedioic acid
CHID: 21581 **CASRN:** 597−43−3
SPID(S): Tox21_200524
M4ID: 12481728

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.355 **MAX_MED:** 0.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

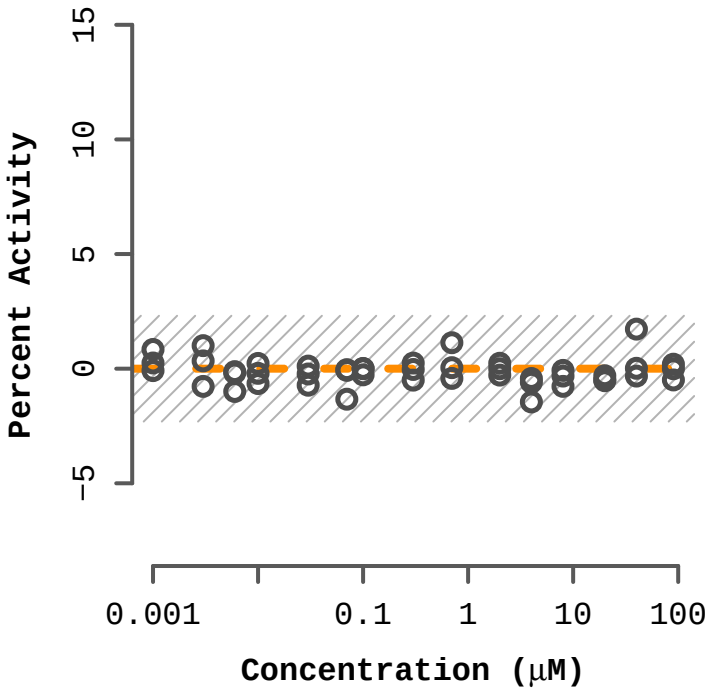
NAME: 2,3-Butanedione
CHID: 21583 **CASRN:** 431-03-8
SPID(S): Tox21_201218
M4ID: 12481034 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	294.58	NA	NA
PROB:	1	NA	NA
RMSE:	21.17	NA	NA

MAX_MEAN: 31.4 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

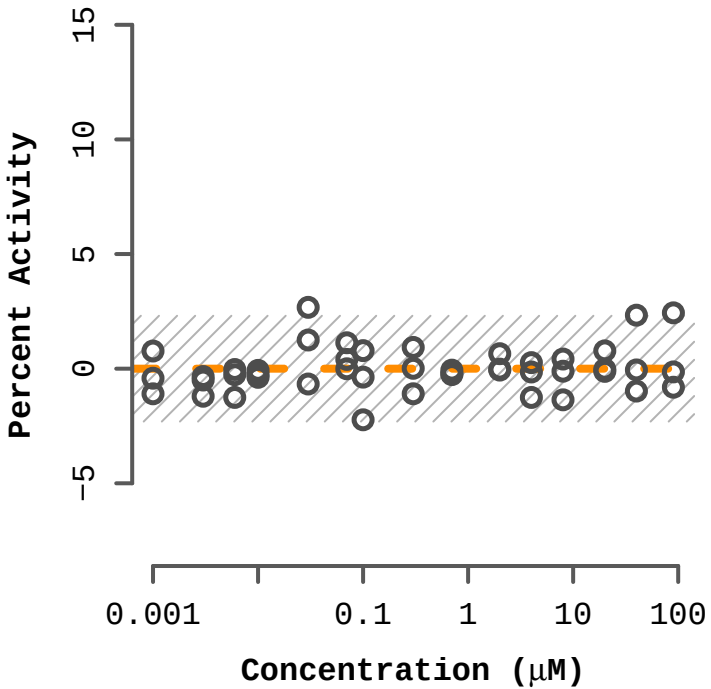
NAME: Phorone
CHID: 21584 CASRN: 504-20-1
SPID(S): Tox21_201097
M4ID: 12481155

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	79.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.59	NA	NA

MAX_MEAN: 0.474 MAX_MED: 0.341 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

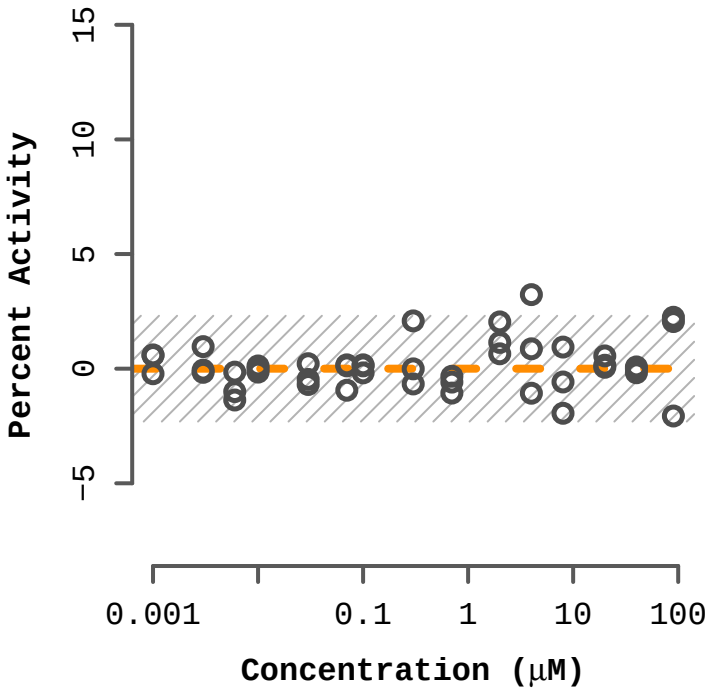
NAME: 2,2−Dimethylpentanedioic acid
CHID: 21585 **CASRN:** 681−57−2
SPID(S): Tox21_200525
M4ID: 12481727

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

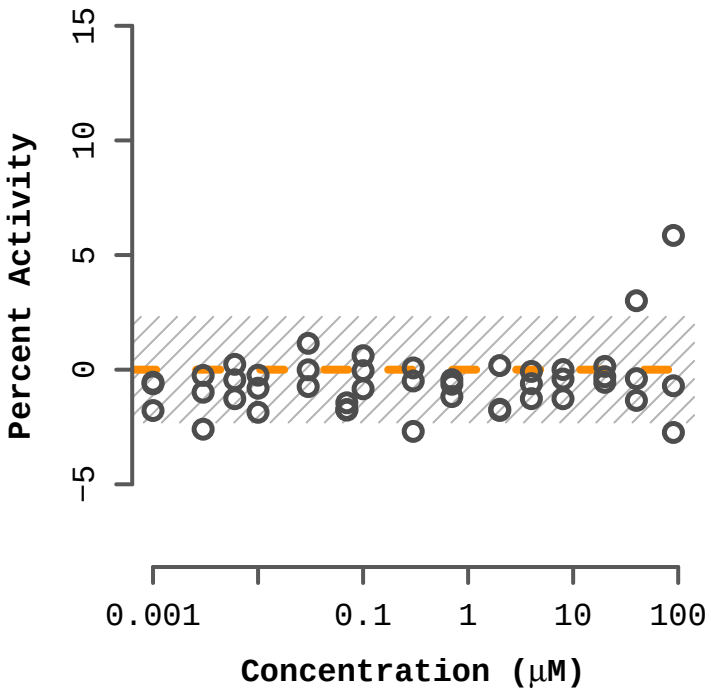
NAME: 6,10-Dimethyl-5,9-undecadiene-2-one
CHID: 21586 **CASRN:** 689-67-8
SPID(S): Tox21_302933
M4ID: 12476200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

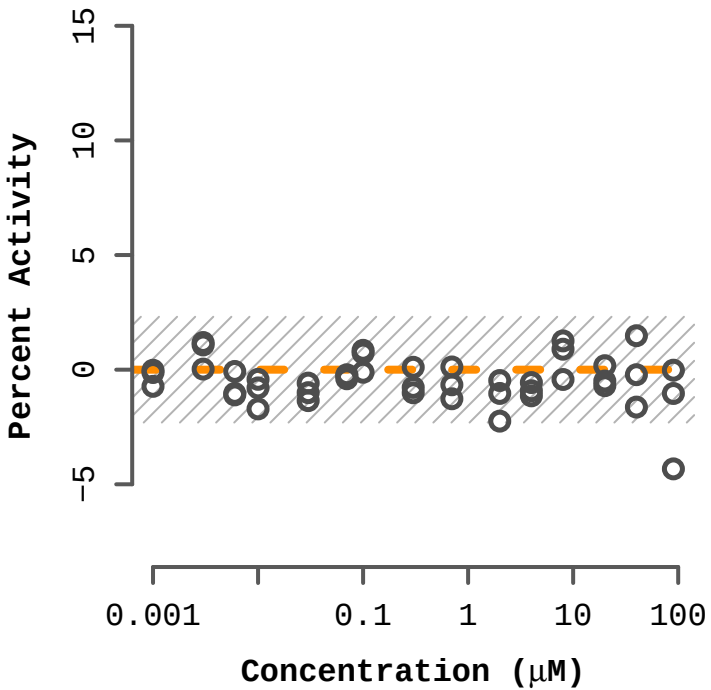
NAME: 6,10-Dimethyl-5,9-undecadiene-2-one
CHID: 21586 **CASRN:** 689-67-8
SPID(S): Tox21_202156
M4ID: 12480096

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.806 **MAX_MED:** −0.0029 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

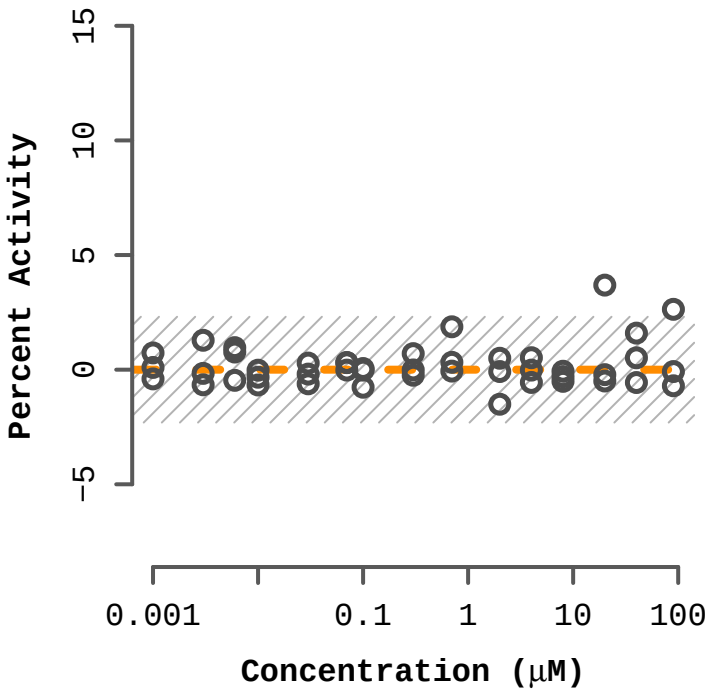
NAME: Dodecanoic acid
CHID: 21590 **CASRN:** 143-07-7
SPID(S): Tox21_303010
M4ID: 12476123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.765 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

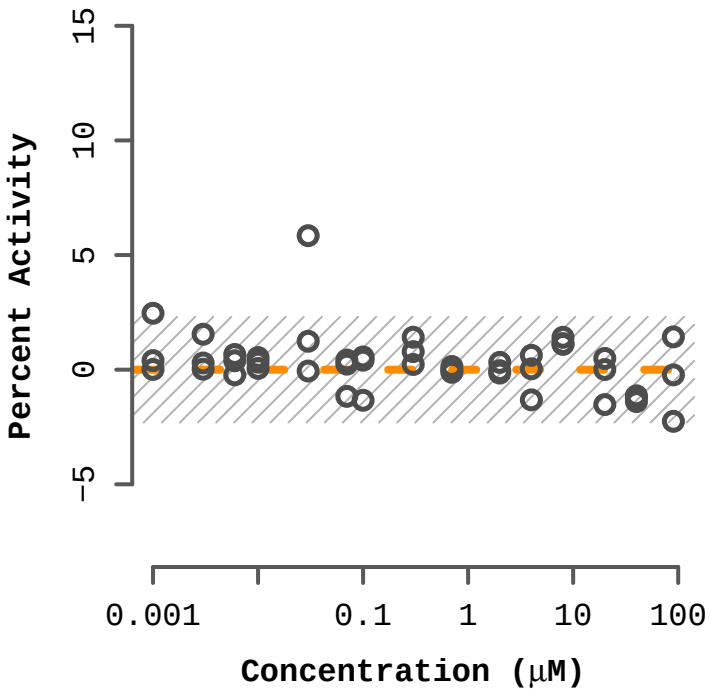
NAME: Dodecanoic acid
CHID: 21590 **CASRN:** 143-07-7
SPID(S): Tox21_202149
M4ID: 12480103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.994 **MAX_MED:** 0.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

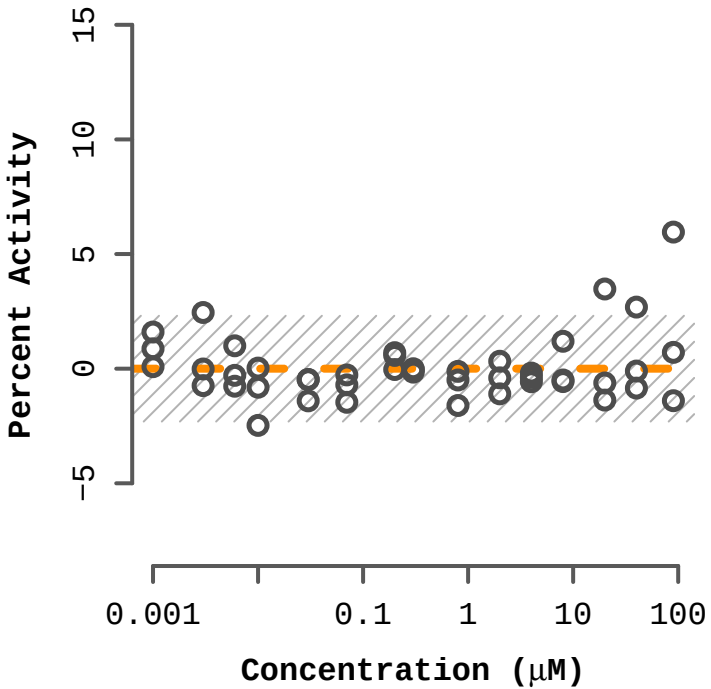
NAME: Heptanal
CHID: 21597 **CASRN:** 111-71-7
SPID(S): Tox21_302779
M4ID: 12476354

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

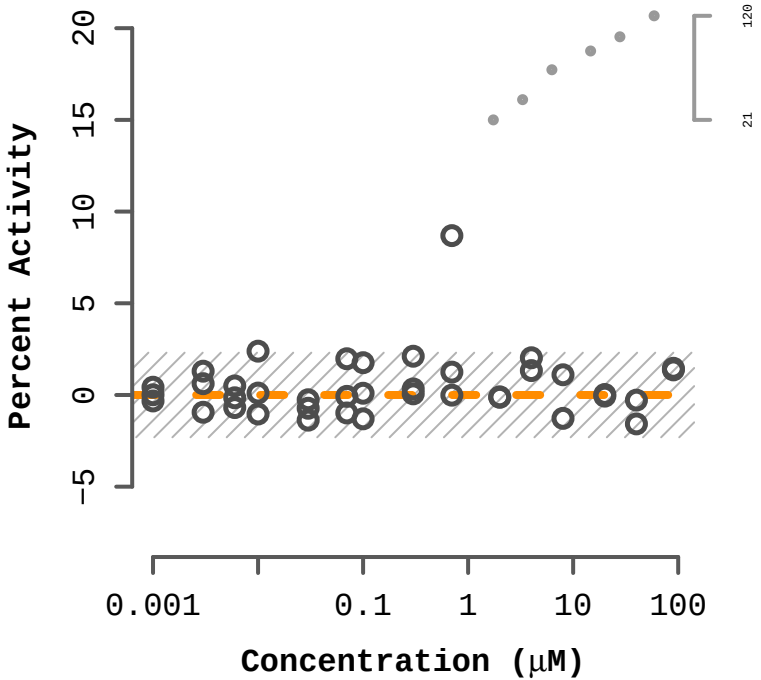
NAME: Heptanal
CHID: 21597 CASRN: 111-71-7
SPID(S): Tox21_202173
M4ID: 12480079

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.76 MAX_MED: 0.869 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

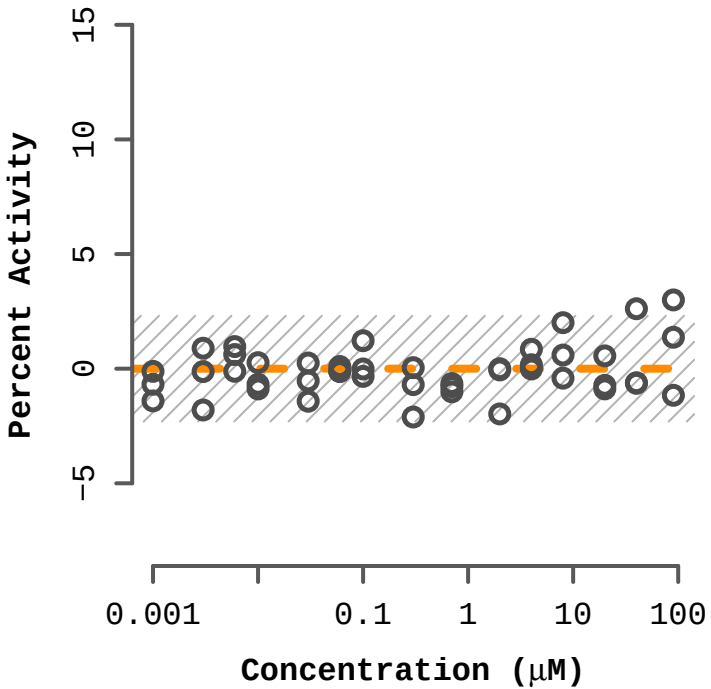
NAME: Heptanedioic acid
CHID: 21598 **CASRN:** 111-16-0
SPID(S): Tox21_201171
M4ID: 12481081 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	339.52	NA	NA
PROB:	1	NA	NA
RMSE:	29.23	NA	NA

MAX_MEAN: 40.7 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

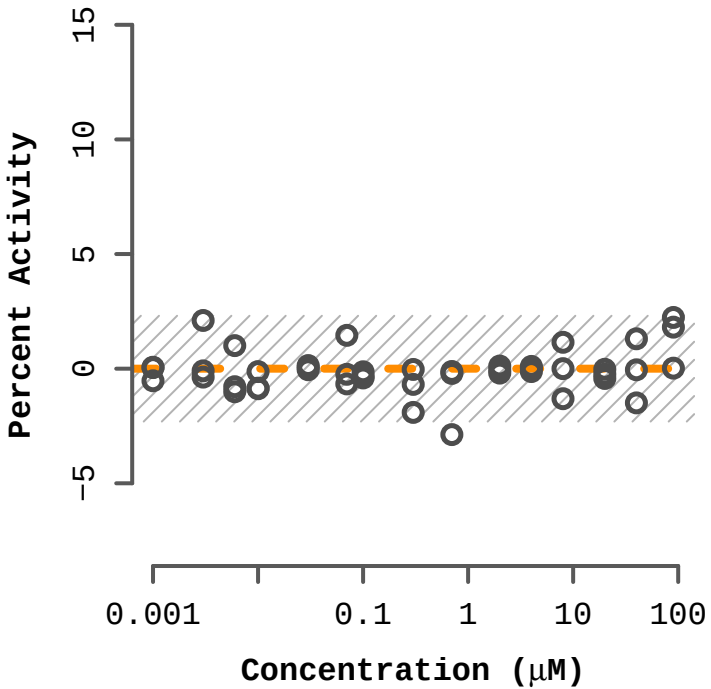
NAME: Heptanenitrile
CHID: 21599 **CASRN:** 629-08-3
SPID(S): Tox21_200526
M4ID: 12481726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

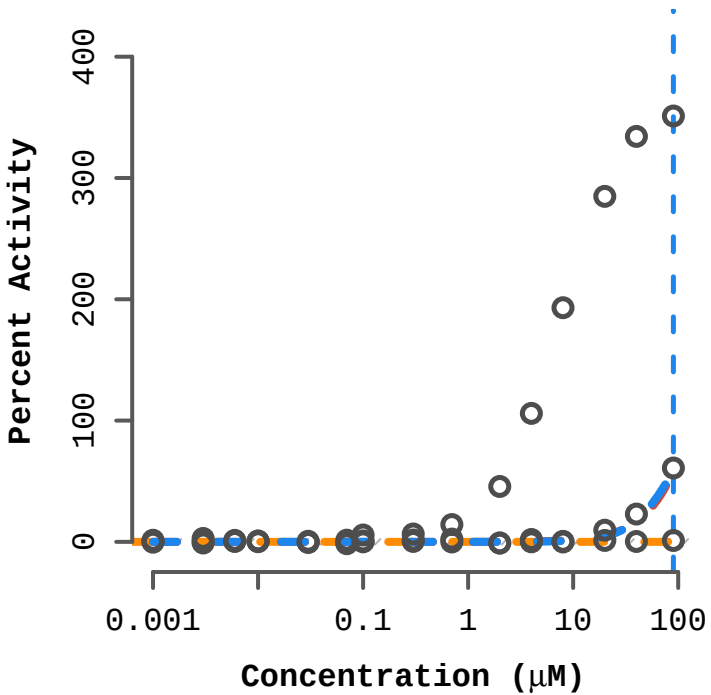
NAME: Heptanoic acid
CHID: 21600 **CASRN:** 111-14-8
SPID(S): Tox21_300342
M4ID: 12478790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Heptanoic acid
CHID: 21600 CASRN: 111-14-8
SPID(S): Tox21_201830
M4ID: 12480422

HILL MODEL (in red):

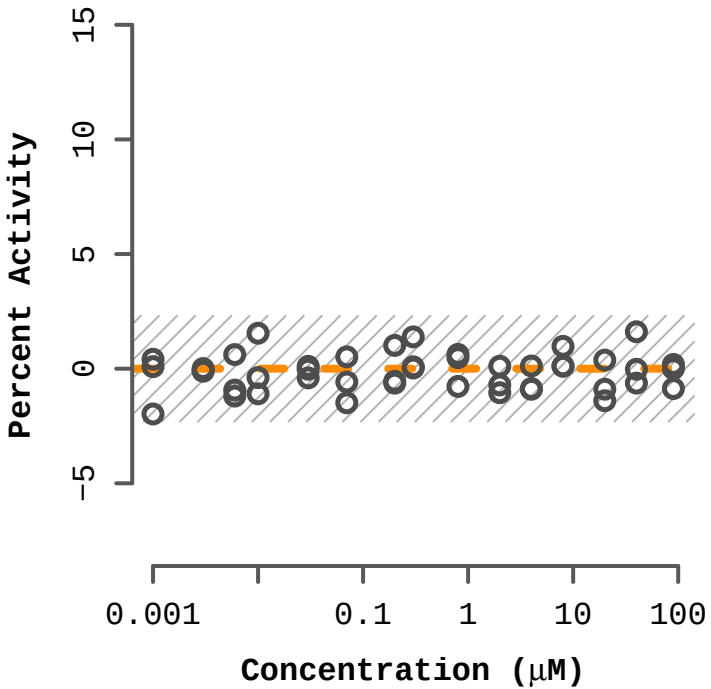
	tp	ga	gw
val:	421	2.42	1.69
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	117	1.95	2.13	3.68	3.72
sd:	146	0.508	1.16	937	2070

	CNST	HILL	GNLS
AIC:	448.04	448.47	452.62
PROB:	0.52	0.42	0.05
RMSE:	90.85	84.17	84.16

MAX_MEAN: 138 MAX_MED: 60.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

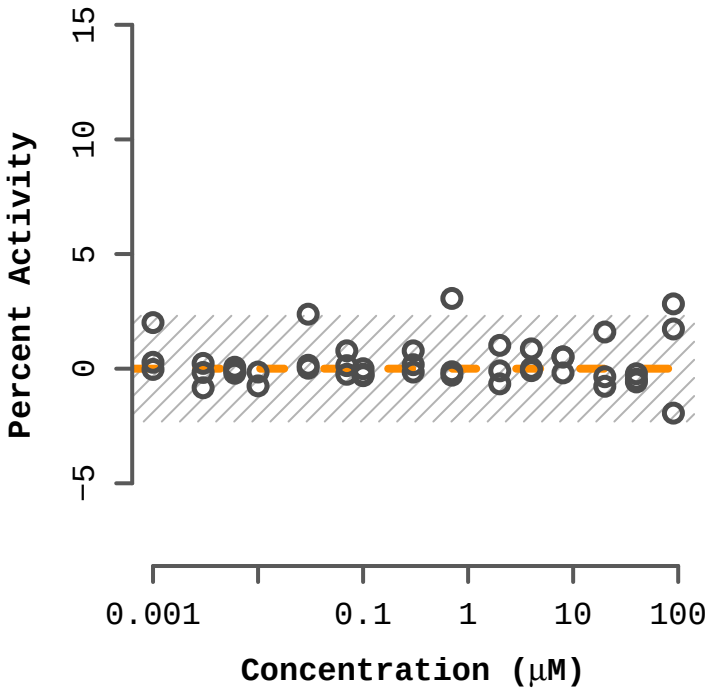
NAME: Hexachloroacetone
CHID: 21601 **CASRN:** 116-16-5
SPID(S): Tox21_201773
M4ID: 12480479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.501 **MAX_MED:** 0.482 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

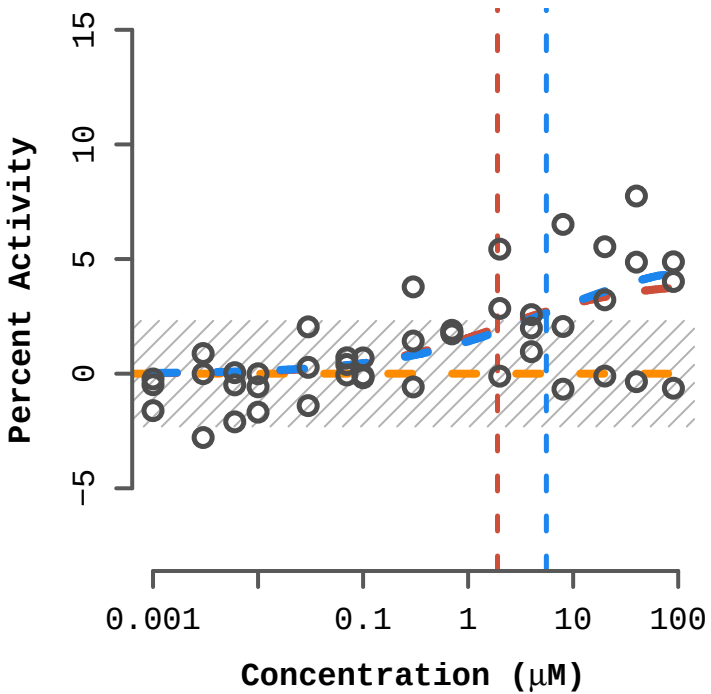
NAME: Hexadecanoic acid
CHID: 21602 **CASRN:** 57-10-3
SPID(S): Tox21_302966
M4ID: 12476167

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.91	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.883 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexadecanoic acid
CHID: 21602 CASRN: 57-10-3
SPID(S): Tox21_201671
M4ID: 12480581

HILL MODEL (in red):

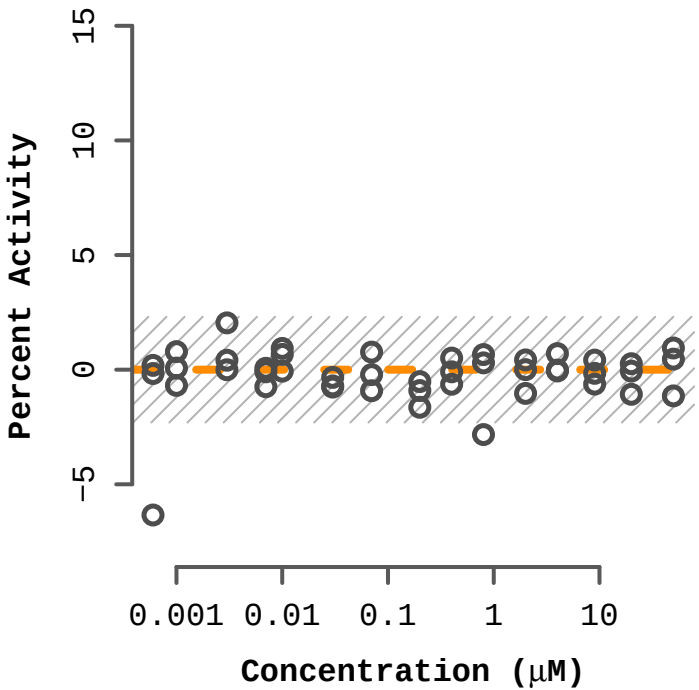
	tp	ga	gw
val:	4	0.28	0.698
sd:	1.71	0.854	0.37

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.29	0.745	0.591	2	15.1
sd:	8.42	2.65	0.49	0.154	62.9

	CNST	HILL	GNLS
AIC:	213.2	191.21	195.18
PROB:	0	0.88	0.12
RMSE:	2.64	1.87	1.87

MAX_MEAN: 4.09 **MAX_MED:** 4.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

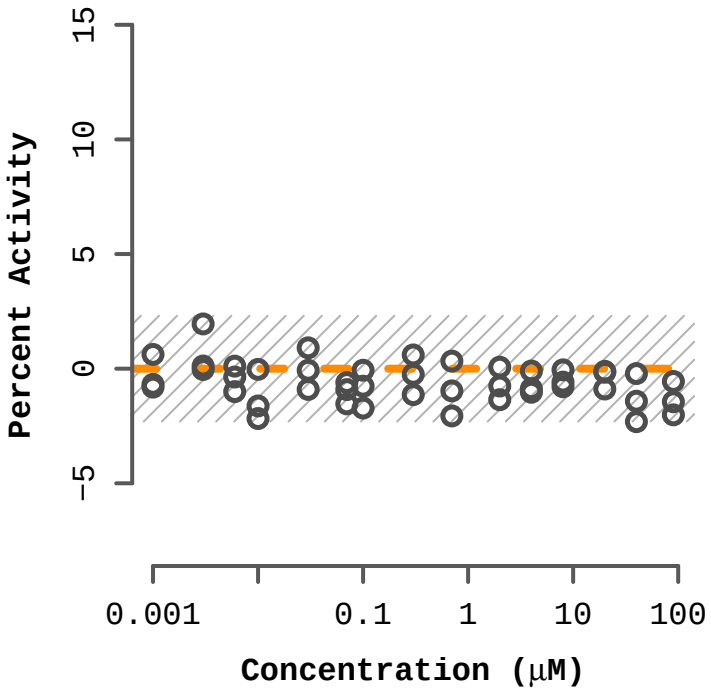
NAME: Hexadecanoic acid
CHID: 21602 **CASRN:** 57-10-3
SPID(S): Tox21_112105_1
M4ID: 12483316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 0.667 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

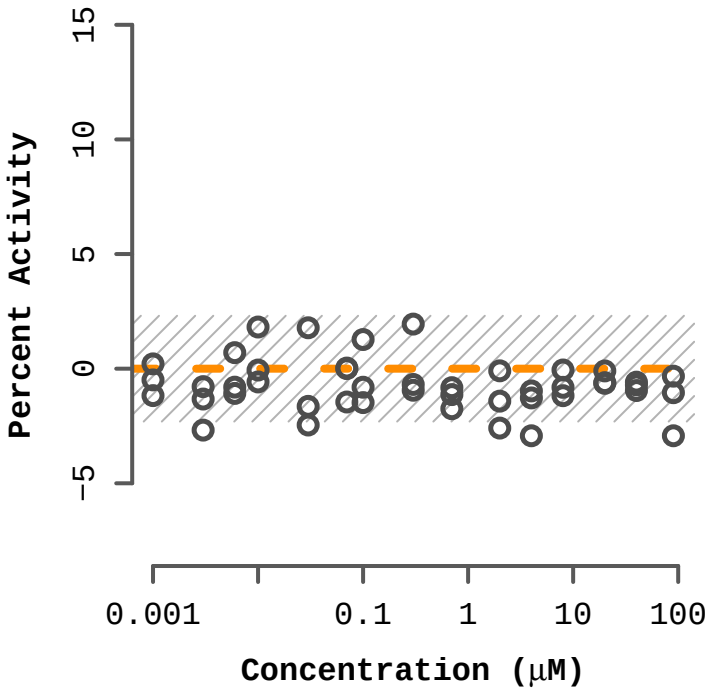
NAME: (E)−Hexadec−9−enoic acid
CHID: 21603 **CASRN:** 10030−73−6
SPID(S): Tox21_302976
M4ID: 12476157

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.679 **MAX_MED:** 0.118 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

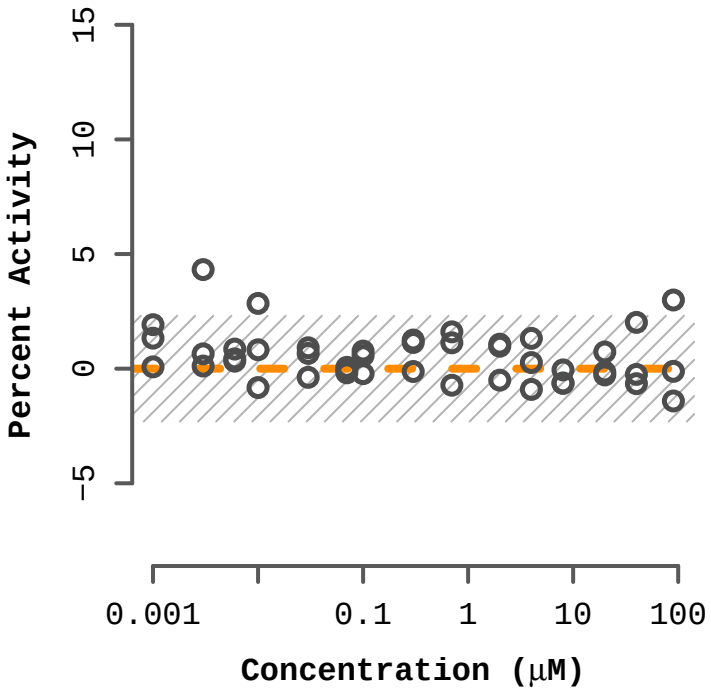
NAME: (E)-Hexadec-9-enoic acid
CHID: 21603 **CASRN:** 10030-73-6
SPID(S): Tox21_202178
M4ID: 12480074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.394 **MAX_MED:** 0.0044 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

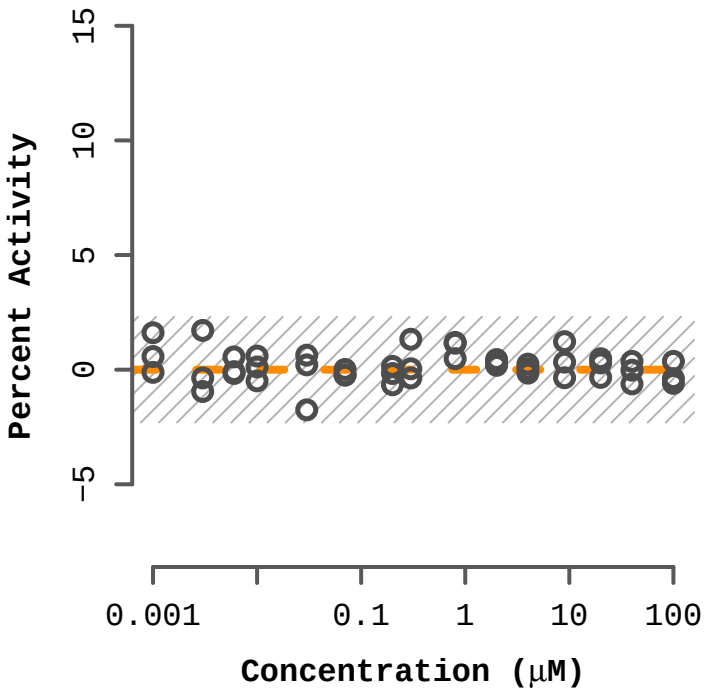
NAME: Hexanal
CHID: 21604 **CASRN:** 66-25-1
SPID(S): Tox21_303342
M4ID: 12475791

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

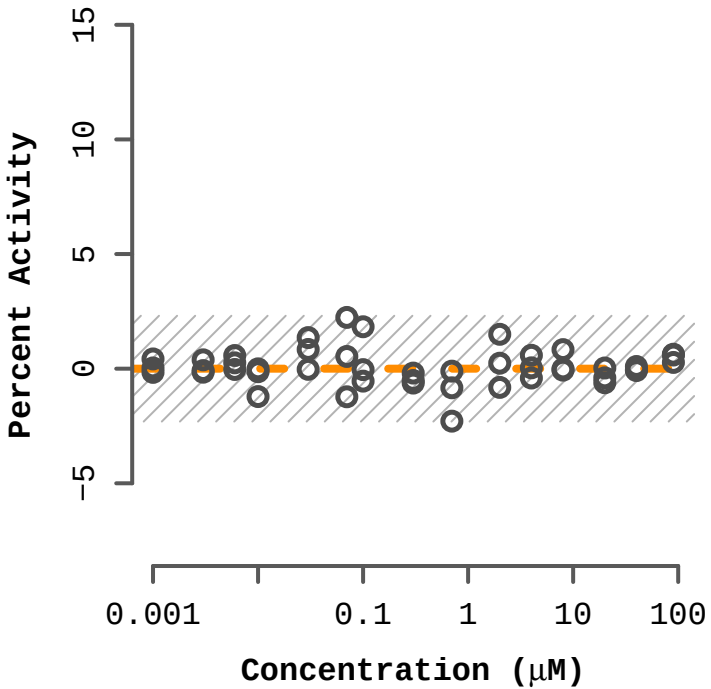
NAME: Hexanal
CHID: 21604 **CASRN:** 66-25-1
SPID(S): Tox21_201933
M4ID: 12480319

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

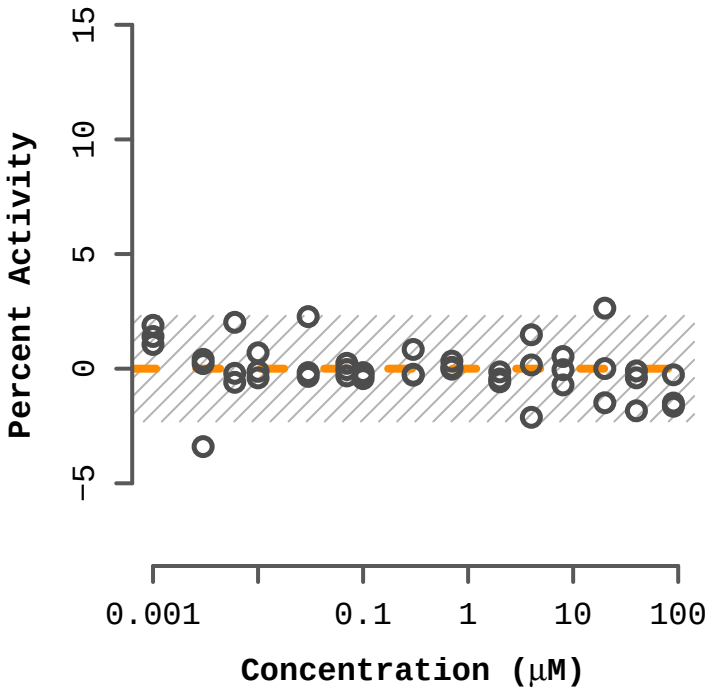
NAME: Hexanedioic acid
CHID: 21605 **CASRN:** 124-04-9
SPID(S): Tox21_300344
M4ID: 12478788

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.723 **MAX_MED:** 0.841 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

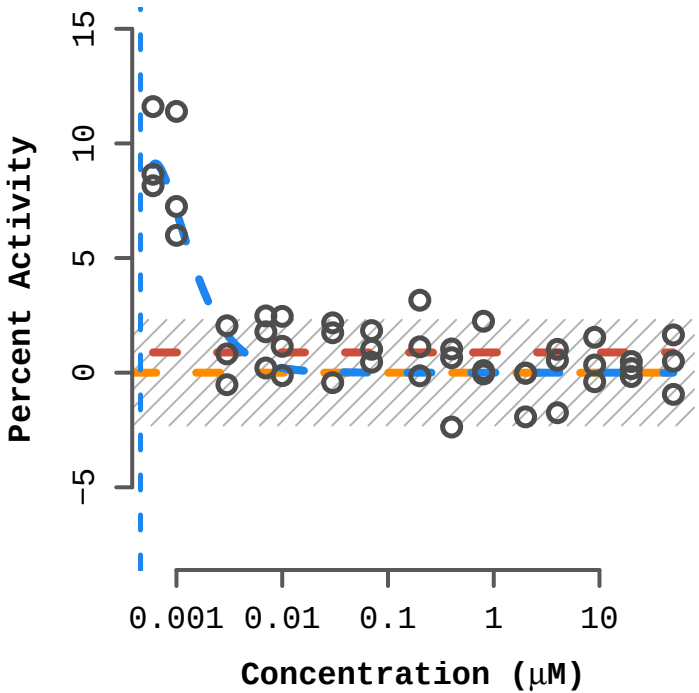
NAME: Hexanedioic acid
CHID: 21605 **CASRN:** 124-04-9
SPID(S): Tox21_202161
M4ID: 12480091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexanedioic acid
CHID: 21605 CASRN: 124-04-9
SPID(S): Tox21_111118_1
M4ID: 12483896

HILL MODEL (in red):

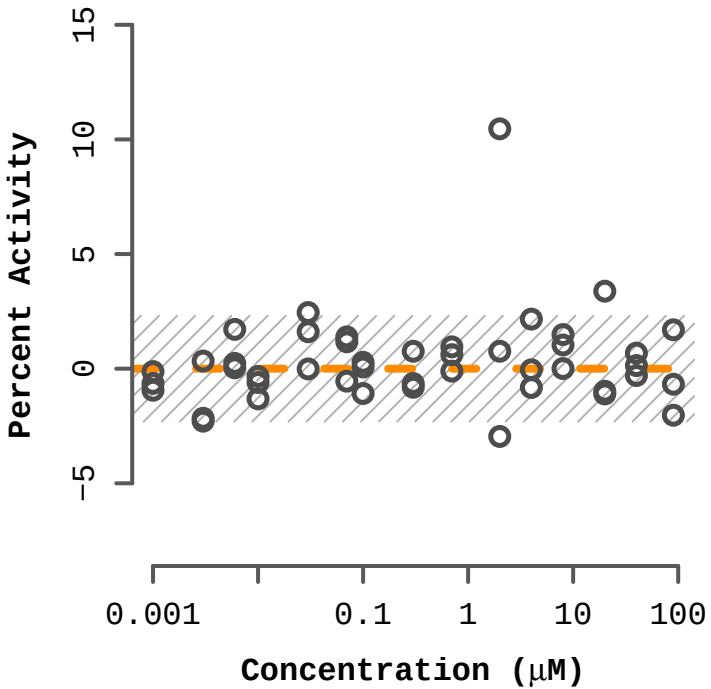
	tp	ga	gw
val:	0.882	−4.49	6
sd:	0.284	1130	5290

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.9	−3.34	7.99	−2.99	1.84
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	224.81	221.33	174.52
PROB:	0	0	1
RMSE:	3.55	3.22	1.46

MAX_MEAN: 9.47 MAX_MED: 8.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

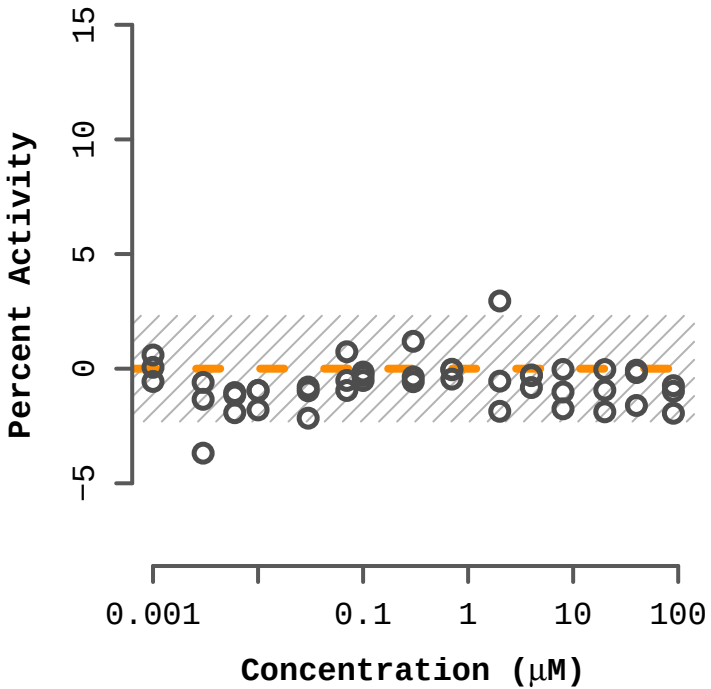
NAME: Hexanoic acid
CHID: 21607 **CASRN:** 142-62-1
SPID(S): Tox21_300406
M4ID: 12478726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.11	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 2.76 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

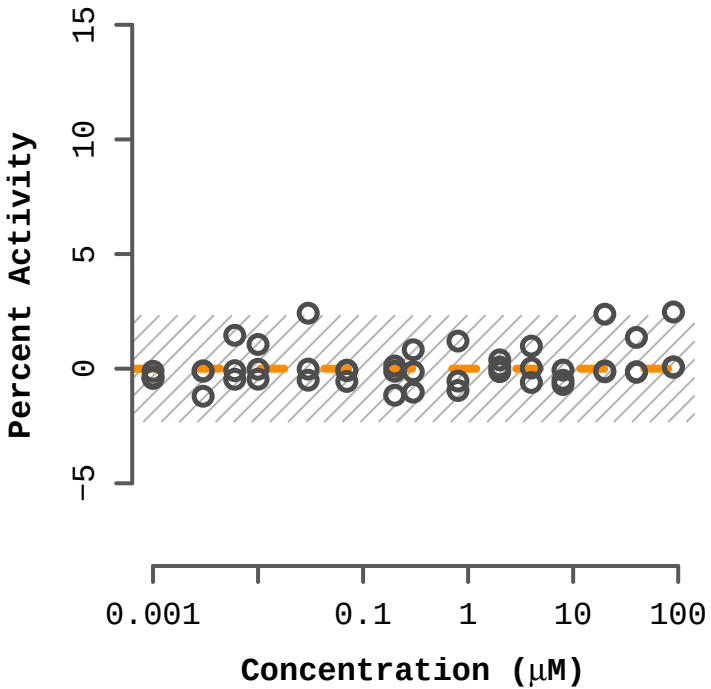
NAME: Hexanoic acid
CHID: 21607 **CASRN:** 142-62-1
SPID(S): Tox21_201517
M4ID: 12480735

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.184 **MAX_MED:** 0.0595 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

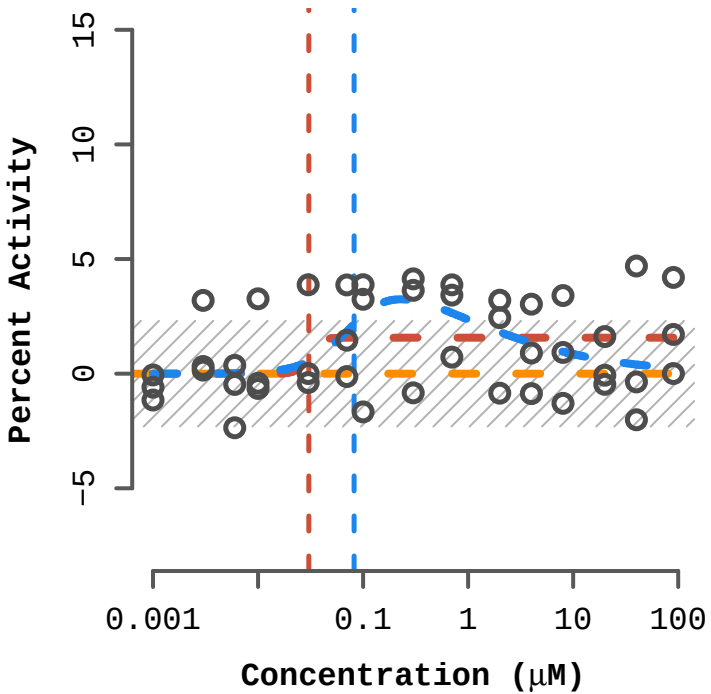
NAME: 3-Hexanone
CHID: 21608 **CASRN:** 589-38-8
SPID(S): Tox21_201119
M4ID: 12481133

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.873 **MAX_MED:** 0.082 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Hydroxybenzoic acid
CHID: 21610 CASRN: 99-06-9
SPID(S): Tox21_200527
M4ID: 12481725

HILL MODEL (in red):

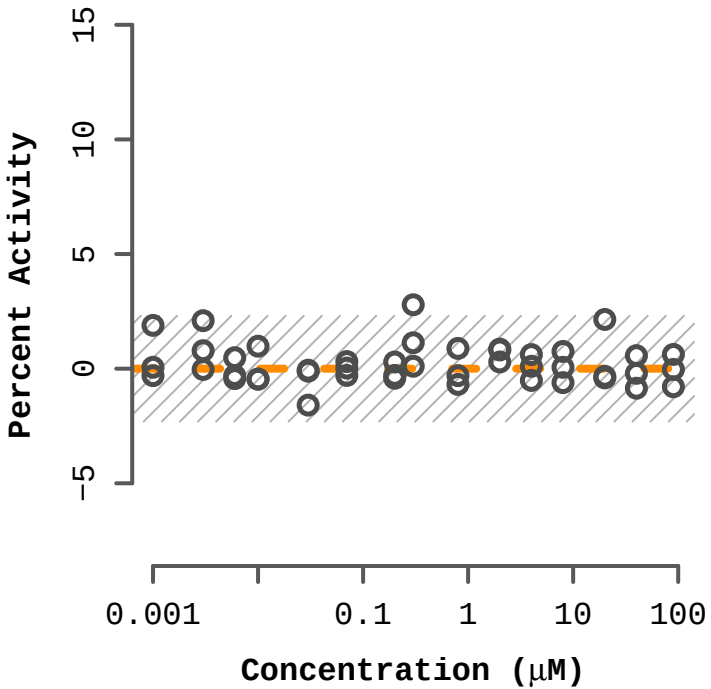
	tp	ga	gw
val:	1.57	−1.52	8
sd:	0.419	0.183	104

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.64	−1.09	2.11	−0.226	0.611
sd:	10.2	0.371	2.36	2.61	0.765

	CNST	HILL	GNLS
AIC:	208.4	200.7	200.24
PROB:	0.01	0.44	0.55
RMSE:	2.31	1.92	1.92

MAX_MEAN: 2.68 **MAX_MED:** 3.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

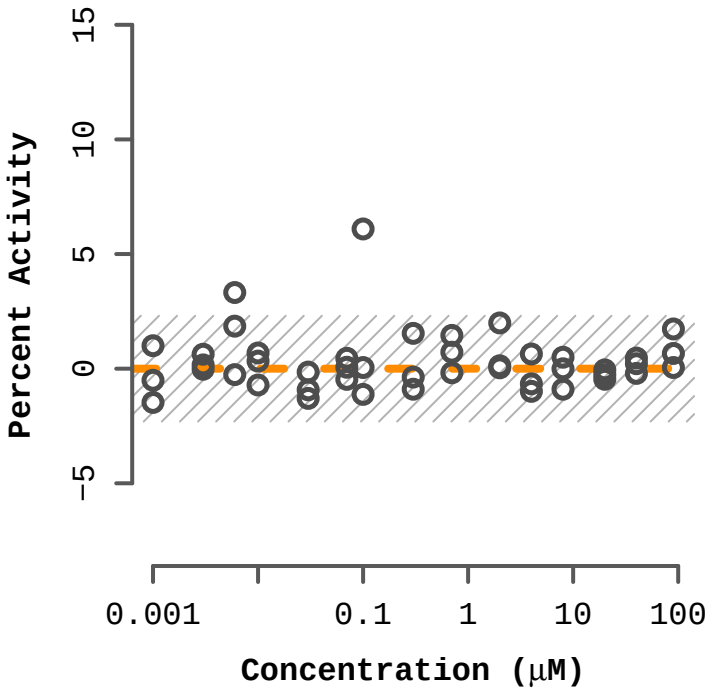
NAME: Methanesulfonyl chloride
CHID: 21615 **CASRN:** 124-63-0
SPID(S): Tox21_200643
M4ID: 12481609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

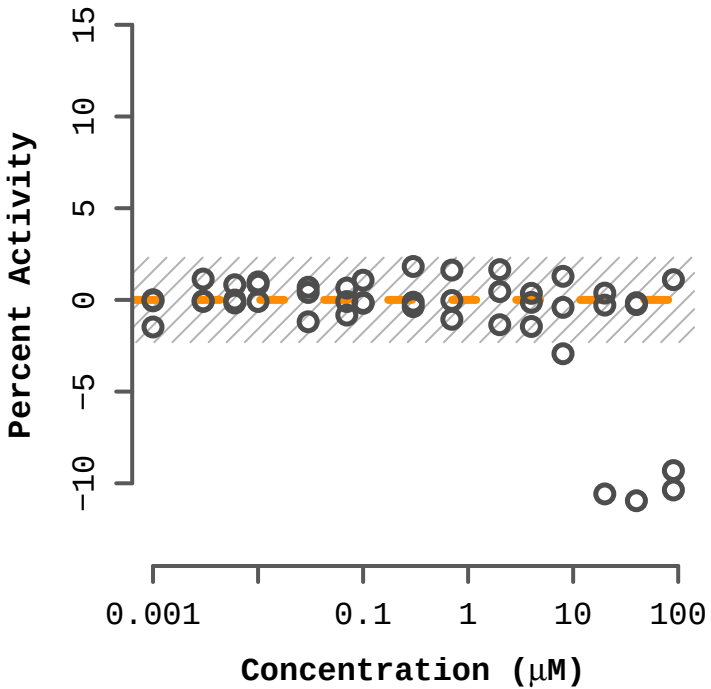
NAME: 3-Methylbenzoic acid
CHID: 21617 **CASRN:** 99-04-7
SPID(S): Tox21_302796
M4ID: 12476337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

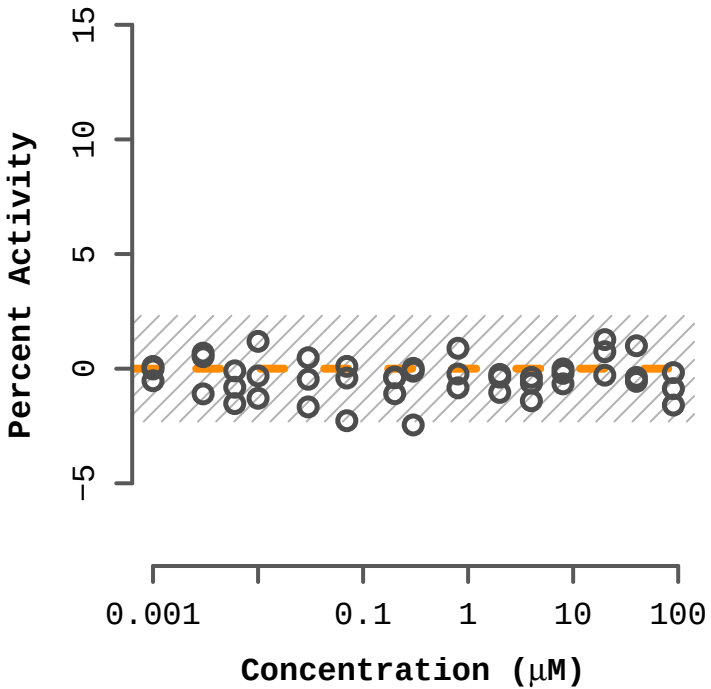
NAME: 3-Methylbenzoic acid
CHID: 21617 **CASRN:** 99-04-7
SPID(S): Tox21_201591
M4ID: 12480661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.05	NA	NA
PROB:	1	NA	NA
RMSE:	3.2	NA	NA

MAX_MEAN: 0.584 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

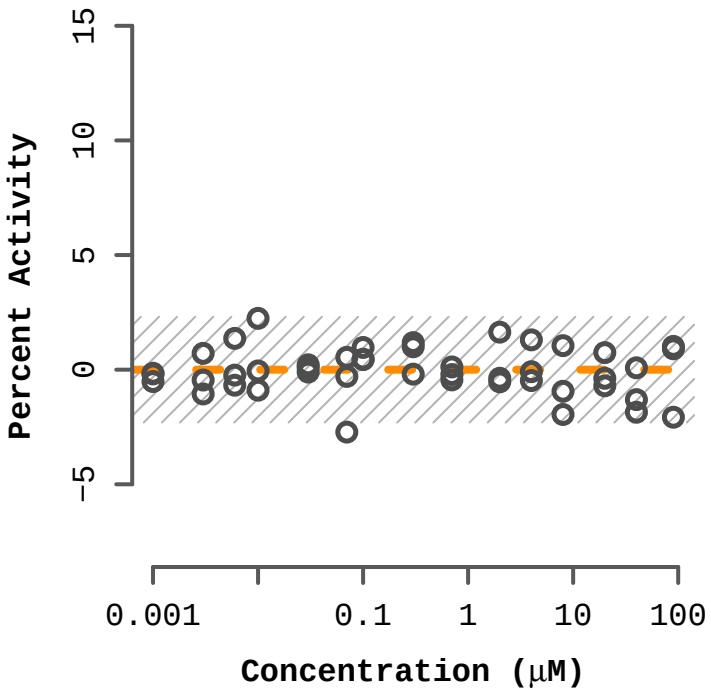
NAME: 4-Methylbenzoic acid
CHID: 21618 **CASRN:** 99-94-5
SPID(S): Tox21_201091
M4ID: 12481161

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.576 **MAX_MED:** 0.741 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

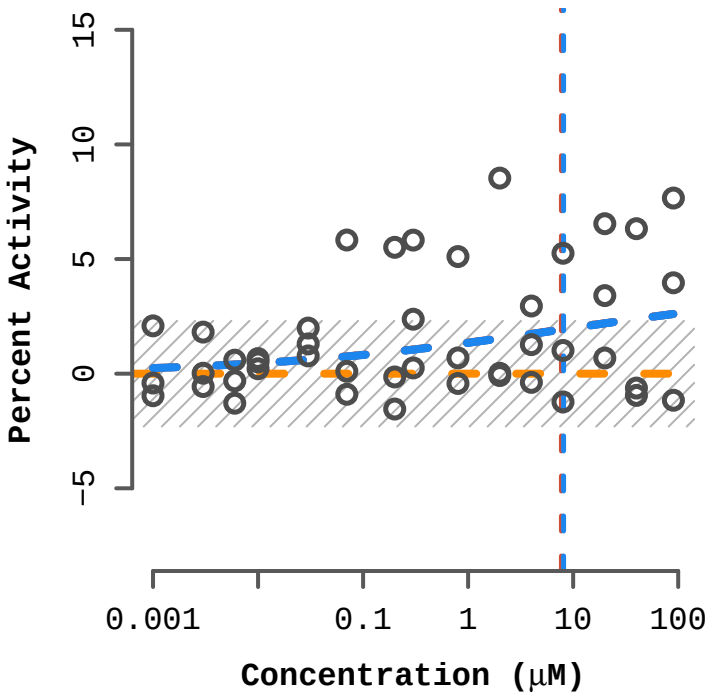
NAME: 3-Methylbutanal
CHID: 21619 CASRN: 590-86-3
SPID(S): Tox21_200891
M4ID: 12481361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.663 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isovaleronitrile
CHID: 21620 CASRN: 625-28-5
SPID(S): Tox21_200528
M4ID: 12481724

HILL MODEL (in red):

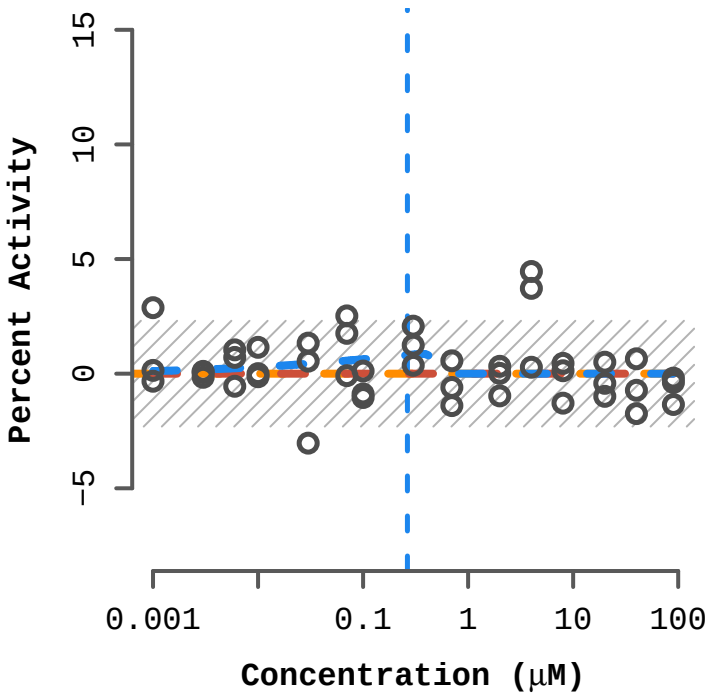
	tp	ga	gw
val:	3.85	0.888	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

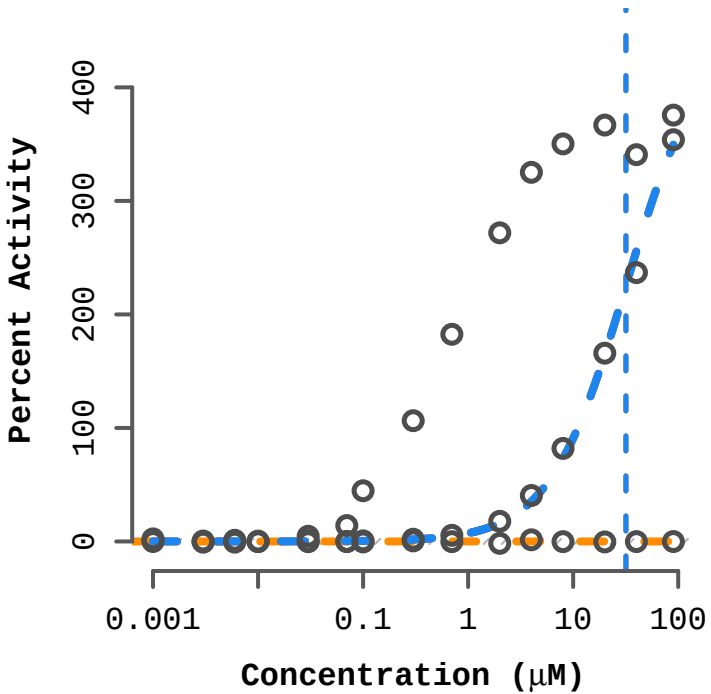
	tp	ga	gw	la	lw
val:	3.87	0.909	0.3	3.34	5.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	226.6	221.3	225.3
PROB:	0.06	0.83	0.11
RMSE:	3.12	2.57	2.57

MAX_MEAN: 3.55 MAX_MED: 3.97 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Methylbutanoic acid
CHID:    21621   CASRN: 116-53-0
SPID(S): Tox21_303584
M4ID:    12475561

HILL MODEL (in red):
      tp       ga       gw
val:  4.2e-09  2.31     1.96
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.62     -0.578   0.466    -0.328   18
sd:   5.2      5.07     0.543    0.728    73.4

      CNST        HILL        GNLS
AIC:  153.1       159.1       159.29
PROB: 0.91        0.05        0.04
RMSE: 1.39        1.39        1.36

MAX_MEAN: 2.82      MAX_MED: 3.72      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylbutanoic acid
CHID: 21621 CASRN: 116-53-0
SPID(S): Tox21_201807
M4ID: 12480445

HILL MODEL (in red):

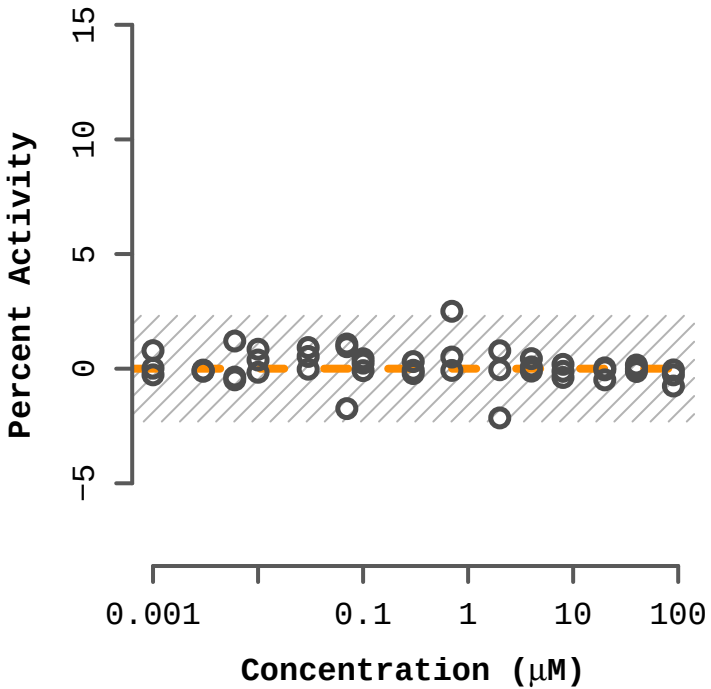
	tp	ga	gw
val:	451	1.5	1.19
sd:	141	0.299	0.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	451	1.5	1.19	3.7	3.75
sd:	141	0.299	0.47	461	990

	CNST	HILL	GNLS
AIC:	603.19	535.82	539.82
PROB:	0	0.88	0.12
RMSE:	145.96	109.76	109.76

MAX_MEAN: 243 MAX_MED: 354 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

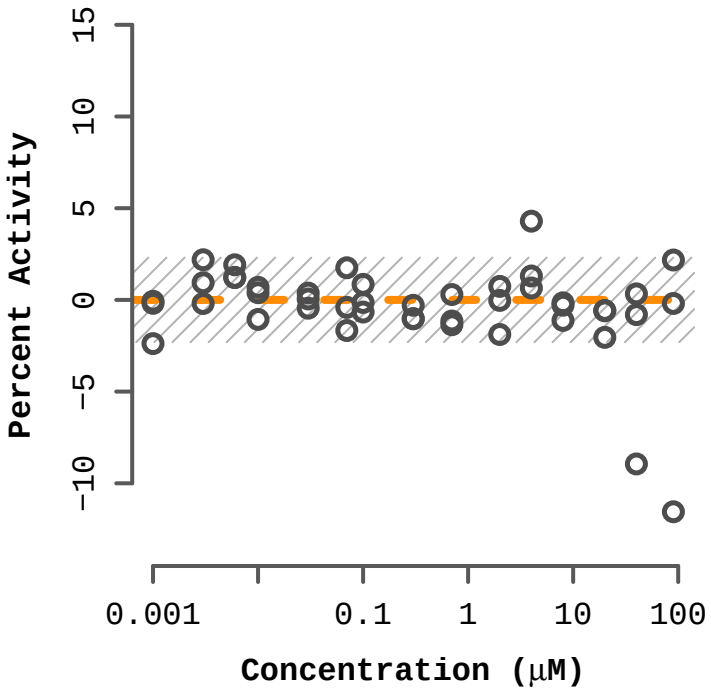
NAME: 4-Isopropylbenzyl alcohol
CHID: 21626 **CASRN:** 536-60-7
SPID(S): Tox21_302797
M4ID: 12476336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 0.958 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

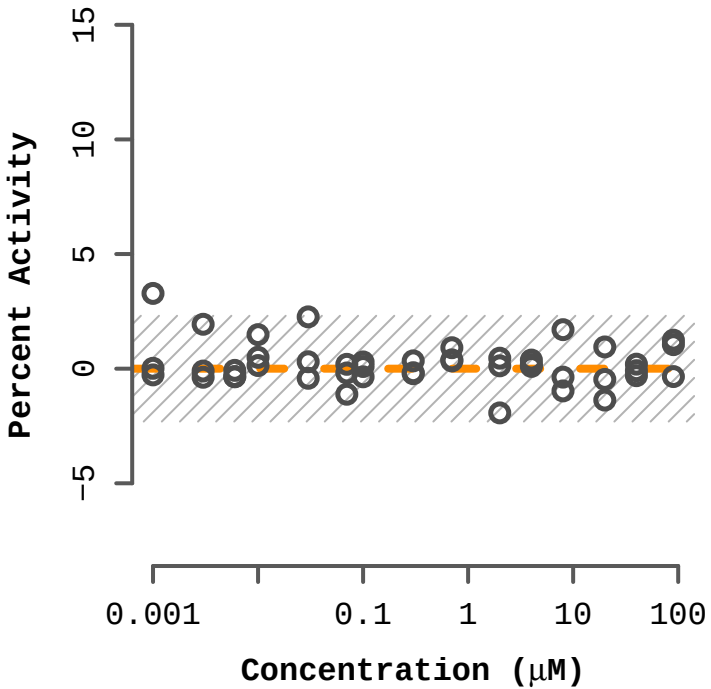
NAME: 4-Isopropylbenzyl alcohol
CHID: 21626 **CASRN:** 536-60-7
SPID(S): Tox21_202025
M4ID: 12480227

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

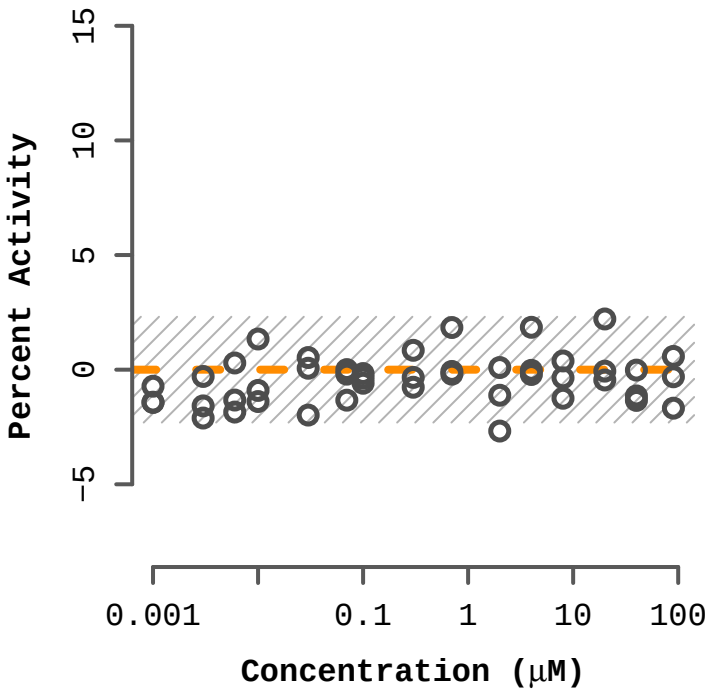
NAME: 5-Methyl-2-furancarboxylic acid
CHID: 21627 **CASRN:** 1917-15-3
SPID(S): Tox21_302827
M4ID: 12476306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

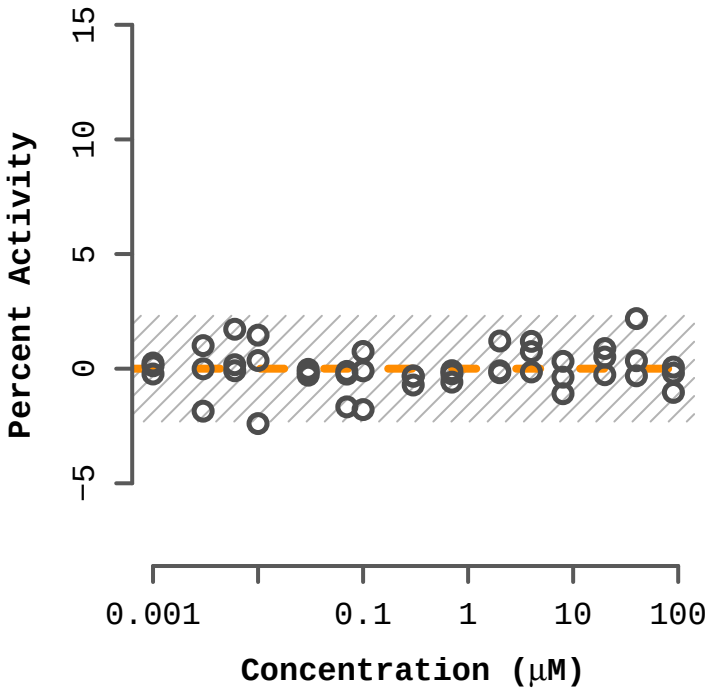
NAME: 5-Methyl-2-furancarboxylic acid
CHID: 21627 **CASRN:** 1917-15-3
SPID(S): Tox21_202200
M4ID: 12480052

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.567 **MAX_MED:** 0.0628 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

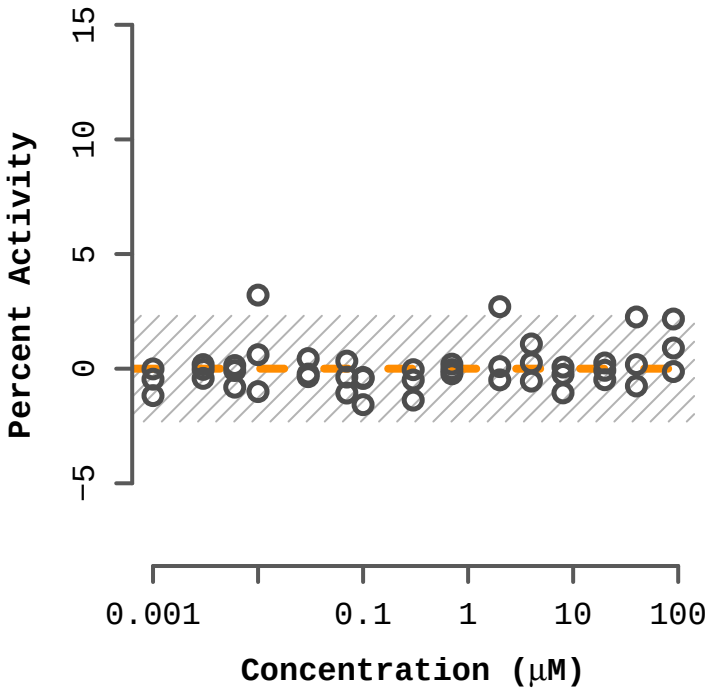
NAME: Methyl glyoxal
CHID: 21628 **CASRN:** 78-98-8
SPID(S): Tox21_303931
M4ID: 12475257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.747 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

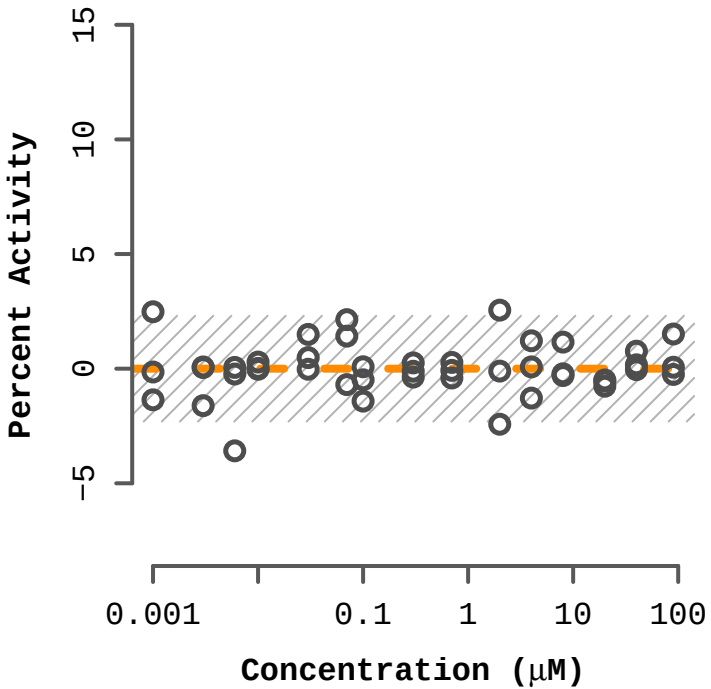
NAME: 6-Methyl-5-hepten-2-one
CHID: 21629 **CASRN:** 110-93-0
SPID(S): Tox21_302899
M4ID: 12476234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.903 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

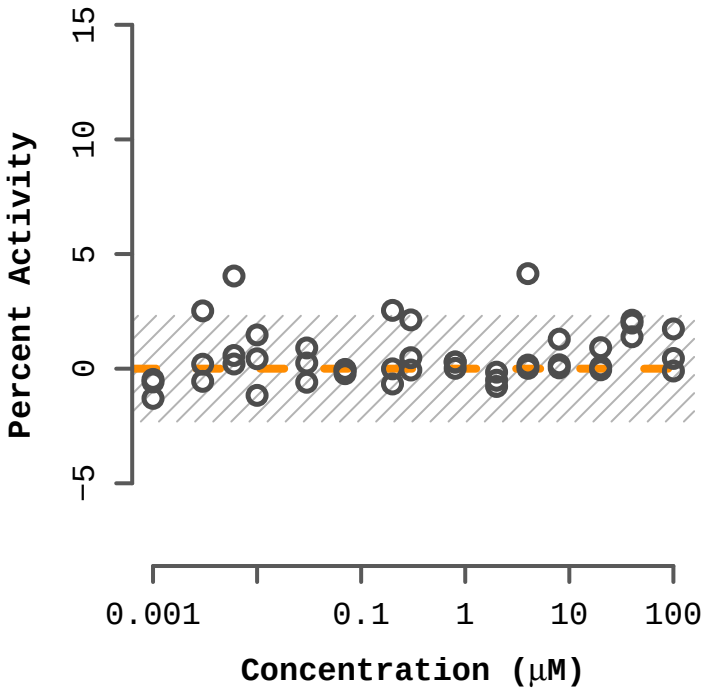
NAME: 6-Methyl-5-hepten-2-one
CHID: 21629 **CASRN:** 110-93-0
SPID(S): Tox21_201381
M4ID: 12480871

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

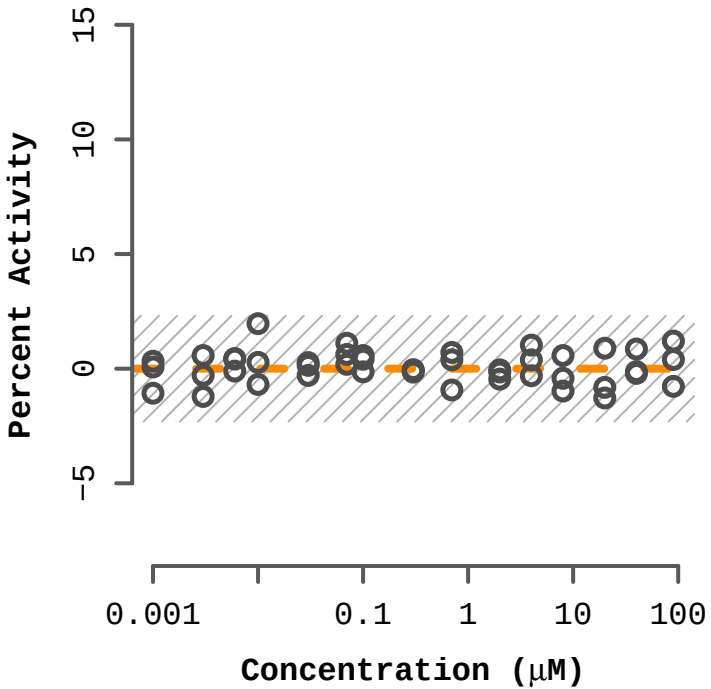
NAME: 5-Methyl-3-isoxazolamine
CHID: 21631 **CASRN:** 1072-67-9
SPID(S): Tox21_201149
M4ID: 12481103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

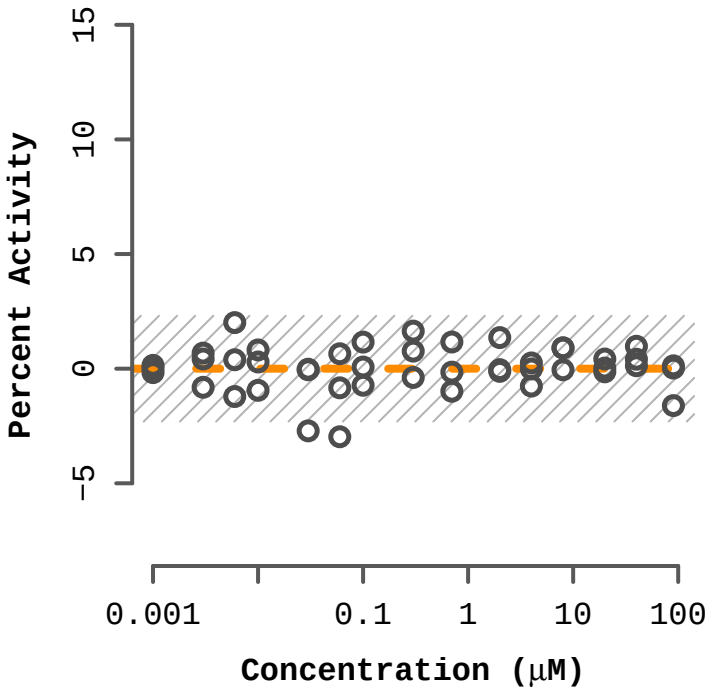
NAME: 2-Methylpentanedioic acid
CHID: 21632 **CASRN:** 18069-17-5
SPID(S): Tox21_200529
M4ID: 12481723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.642 **MAX_MED:** 0.622 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

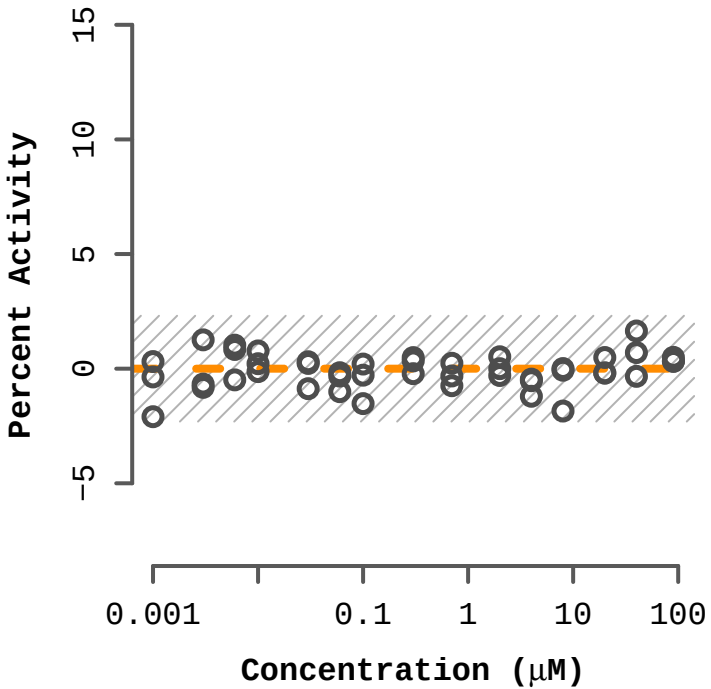
NAME: 2-Methylpentanoic acid
CHID: 21633 **CASRN:** 97-61-0
SPID(S): Tox21_200935
M4ID: 12481317

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.675 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

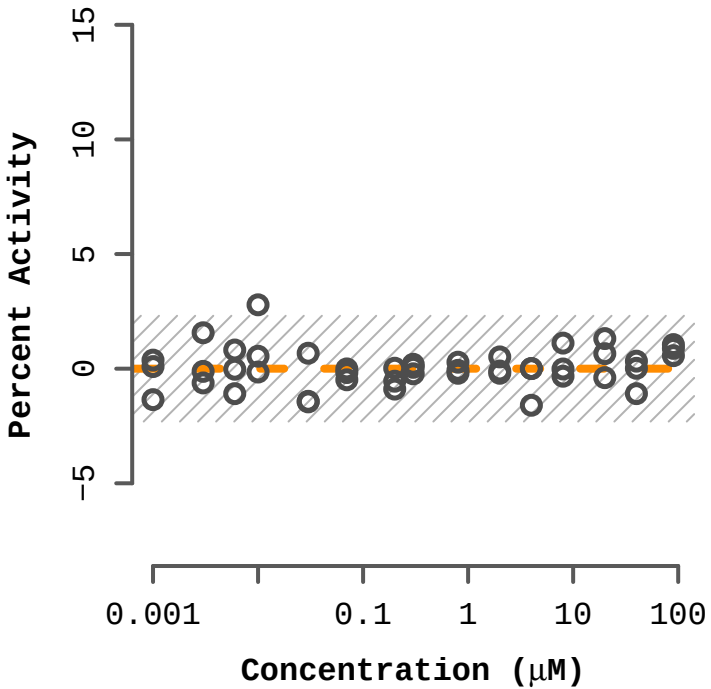
NAME: 3-Methyl-2-pentanone
CHID: 21634 **CASRN:** 565-61-7
SPID(S): Tox21_200530
M4ID: 12481722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 0.839 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

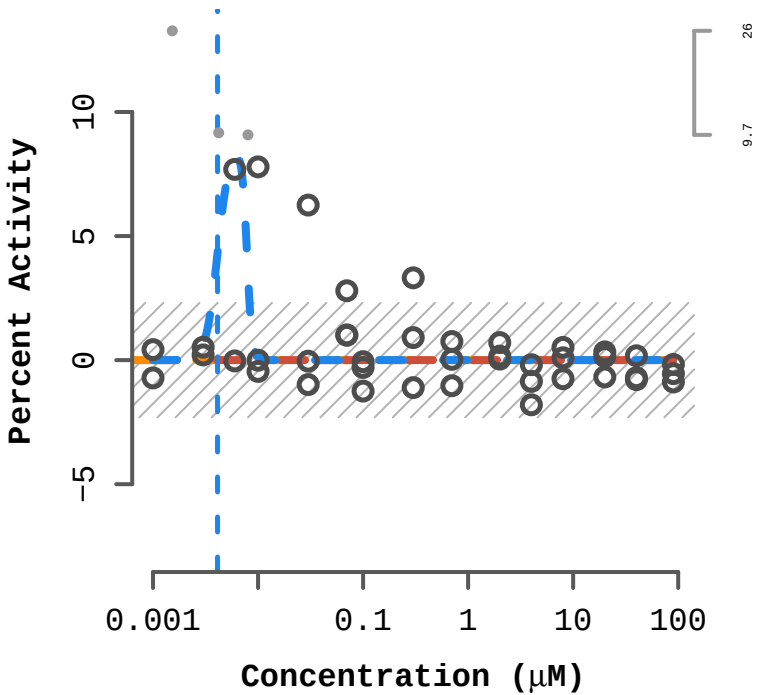
NAME: 2-Methylpropanal
CHID: 21635 **CASRN:** 78-84-2
SPID(S): Tox21_200024
M4ID: 12482228

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.886 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylpropanoic acid
CHID: 21636 CASRN: 79-31-2
SPID(S): Tox21_201207
M4ID: 12481045 BRK

HILL MODEL (in red):

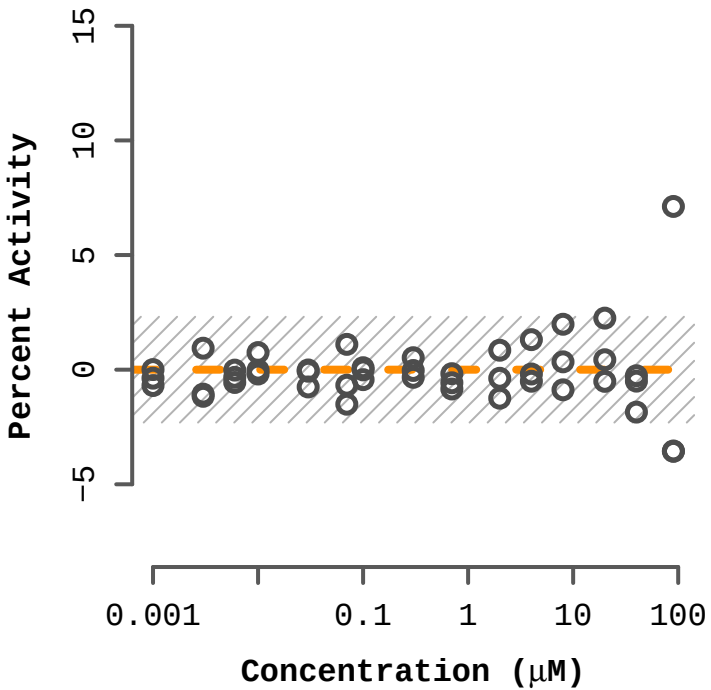
	tp	ga	gw
val:	1.54e-09	2.28	0.545
sd:	5.7e-05	21100	22600

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.65	-2.39	7.99	-2.11	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	217.53	223.53	215.12
PROB:	0.23	0.01	0.76
RMSE:	4.86	4.86	4.63

MAX_MEAN: 8.54 MAX_MED: 7.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

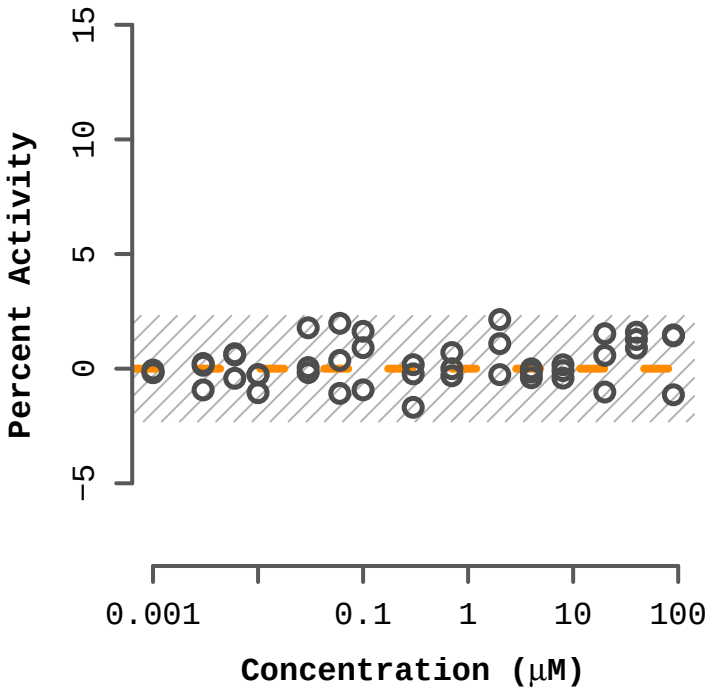
NAME: Dibromonitromethane
CHID: 21637 **CASRN:** 598-91-4
SPID(S): Tox21_200899
M4ID: 12481353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 0.726 **MAX_MED:** 0.435 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

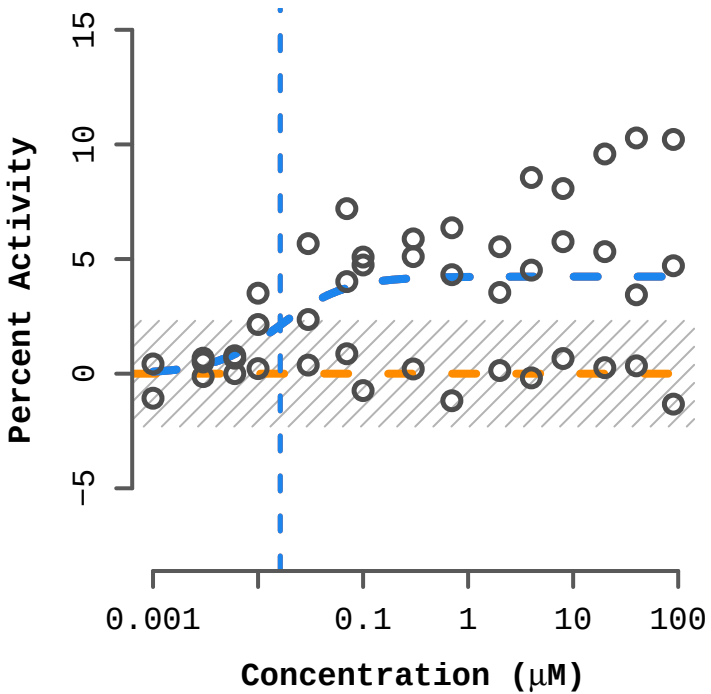
NAME: 1,1-Dichloro-1-nitroethane
CHID: 21638 **CASRN:** 594-72-9
SPID(S): Tox21_201178
M4ID: 12481074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nonanal
CHID: 21639 CASRN: 124-19-6
SPID(S): Tox21_303603
M4ID: 12475542

HILL MODEL (in red):

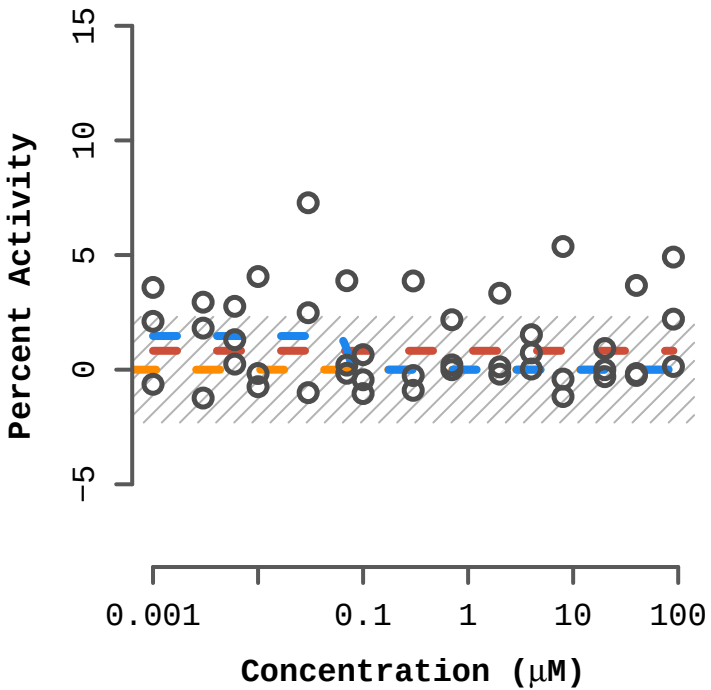
	tp	ga	gw
val:	4.23	-1.79	1.38
sd:	0.718	0.369	1.16

GAIN-LOSS MODEL (in blue):

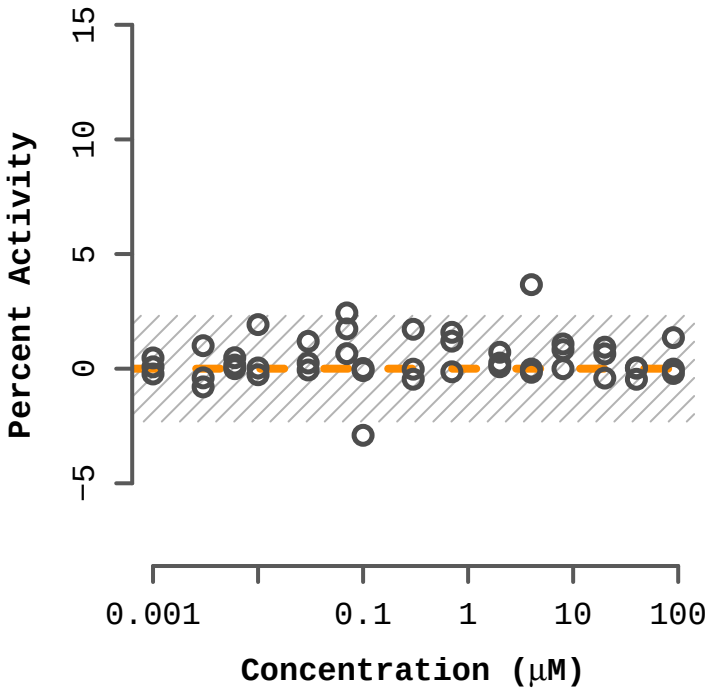
	tp	ga	gw	la	lw
val:	4.23	-1.79	1.38	3.24	5.52
sd:	0.718	0.369	1.16	1250	5440

	CNST	HILL	GNLS
AIC:	261.11	229.4	233.4
PROB:	0	0.88	0.12
RMSE:	4.52	2.91	2.91

MAX_MEAN: 5.06 MAX_MED: 5.76 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Nonanedioic acid
CHID:    21640   CASRN: 123-99-9
SPID(S): Tox21_303011
M4ID:    12476122

HILL MODEL (in red):
      tp       ga       gw
val:  0.823    -4.89    3.62
sd:   0.298    1180     2250

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.47     -4.13    5.46     -1.15    18
sd:   0.539    396      1900     0.0812   76.8

      CNST        HILL        GNLS
AIC:  201.64      199.38      203.91
PROB: 0.23        0.7         0.07
RMSE: 2.33        2.03        2.1

MAX_MEAN: 2.92      MAX_MED: 2.49      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

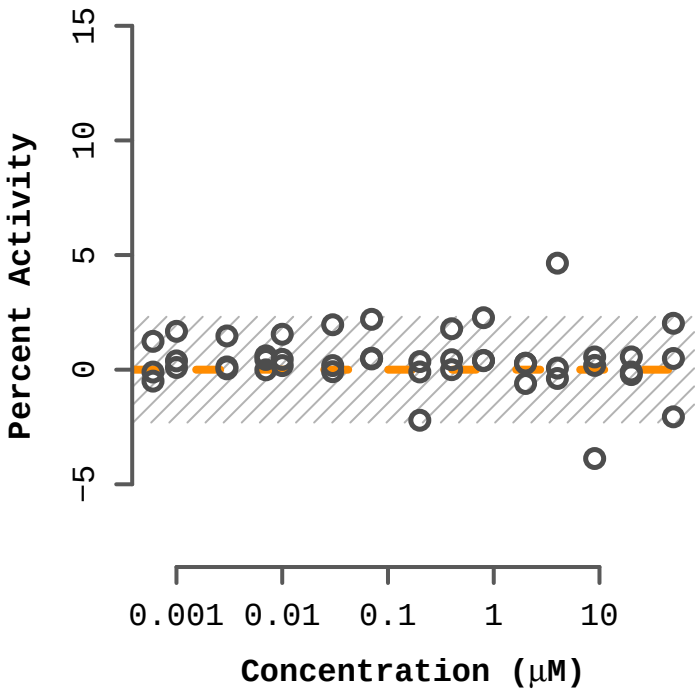
NAME: Nonanedioic acid
CHID: 21640 **CASRN:** 123-99-9
SPID(S): Tox21_201989
M4ID: 12480263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

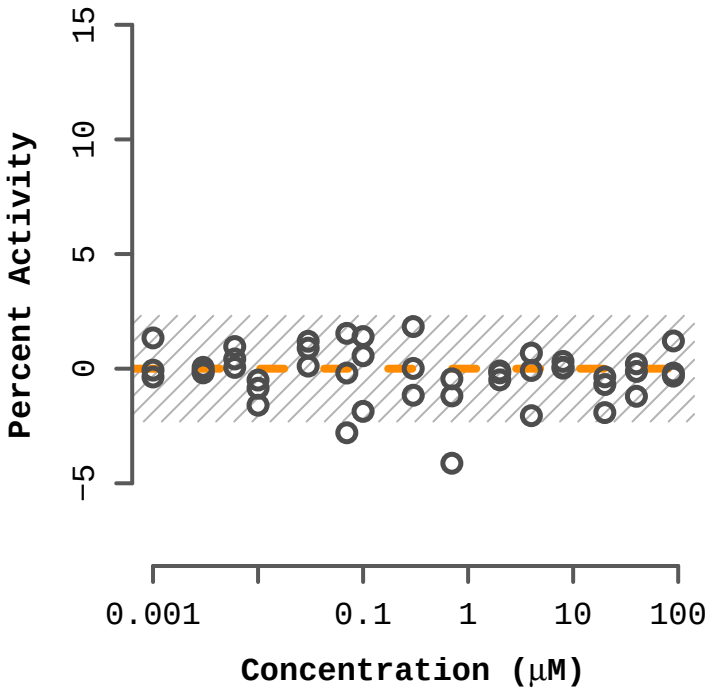
NAME: Nonanedioic acid
CHID: 21640 **CASRN:** 123-99-9
SPID(S): Tox21_110063_1
M4ID: 12484687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 0.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

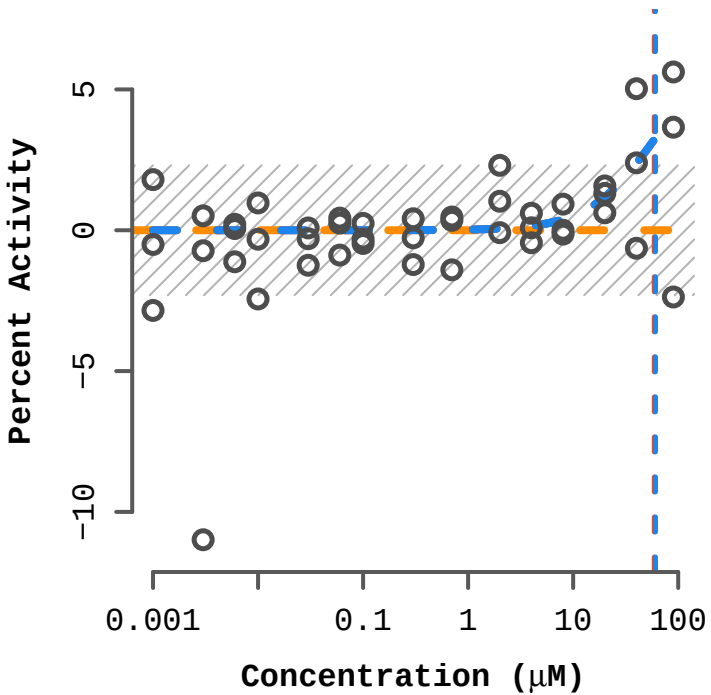
NAME: Nonanoic acid
CHID: 21641 **CASRN:** 112-05-0
SPID(S): Tox21_300022
M4ID: 12479108

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.736 **MAX_MED:** 0.897 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nonanoic acid
CHID: 21641 CASRN: 112-05-0
SPID(S): Tox21_202426
M4ID: 12479826

HILL MODEL (in red):

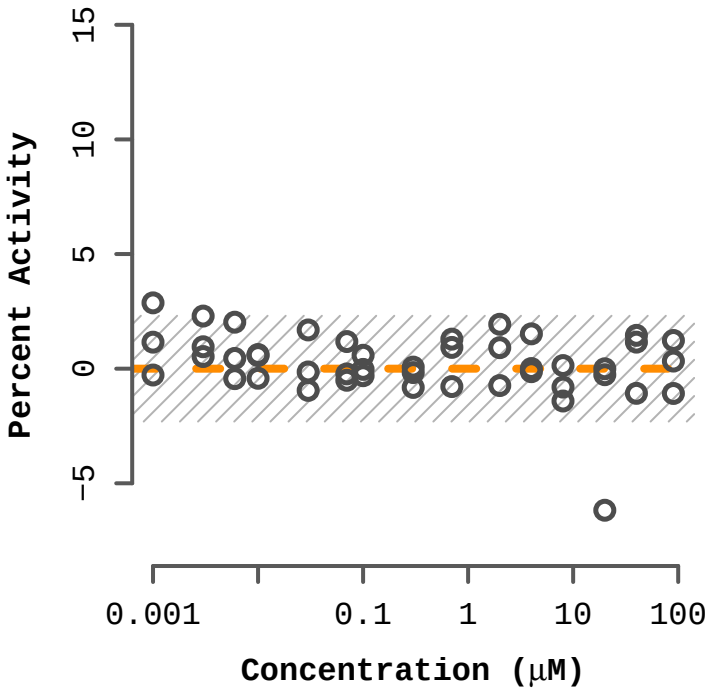
	tp	ga	gw
val:	6.43	1.77	1.38
sd:	9.88	1.09	1.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.74	1.78	1.38	3.69	0.822
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	180.28	170.99	174.98
PROB:	0.01	0.87	0.12
RMSE:	2.32	2.2	2.2

MAX_MEAN: 2.3 MAX_MED: 3.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

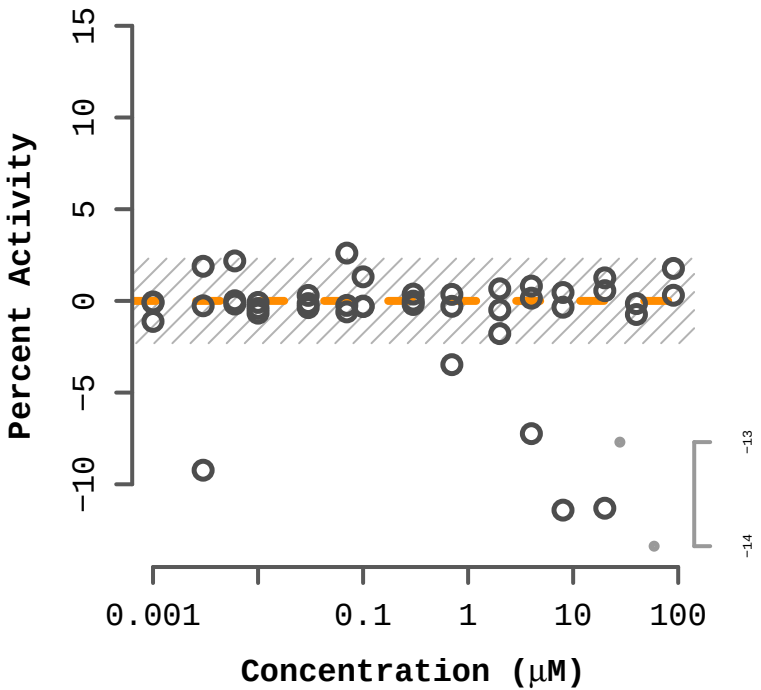
NAME: Octadecanoic acid
CHID: 21642 **CASRN:** 57-11-4
SPID(S): Tox21_300562
M4ID: 12478571

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

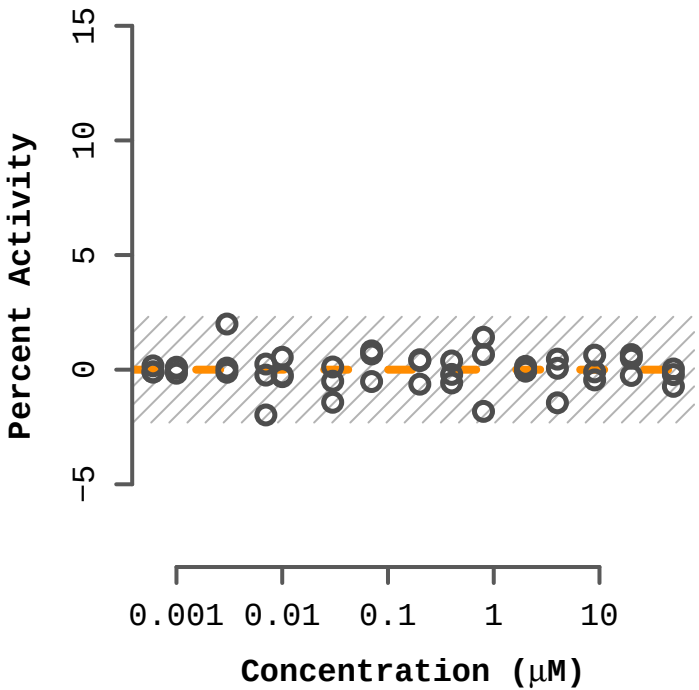
NAME: Octadecanoic acid
CHID: 21642 **CASRN:** 57-11-4
SPID(S): Tox21_201887
M4ID: 12480365 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.63	NA	NA
PROB:	1	NA	NA
RMSE:	4.23	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

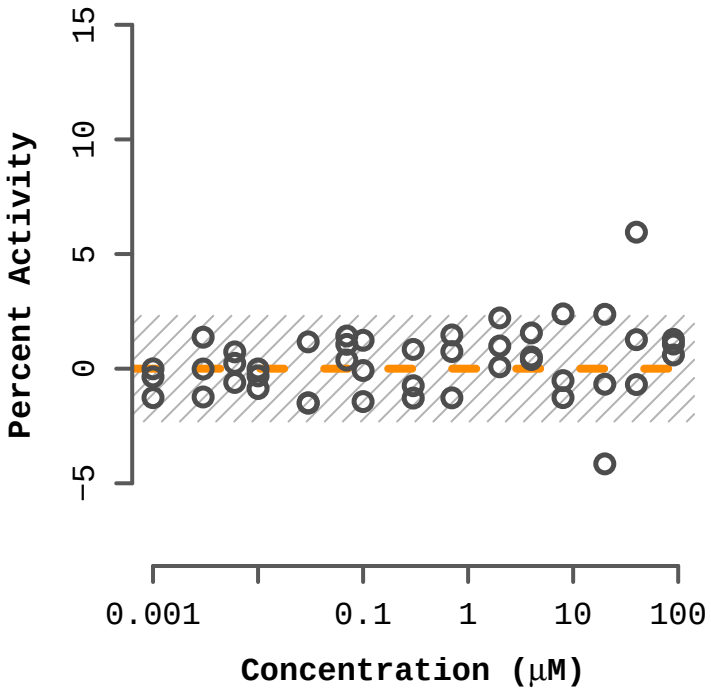
NAME: Octadecanoic acid
CHID: 21642 **CASRN:** 57-11-4
SPID(S): Tox21_111154_1
M4ID: 12483874

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.651 **MAX_MED:** 0.686 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

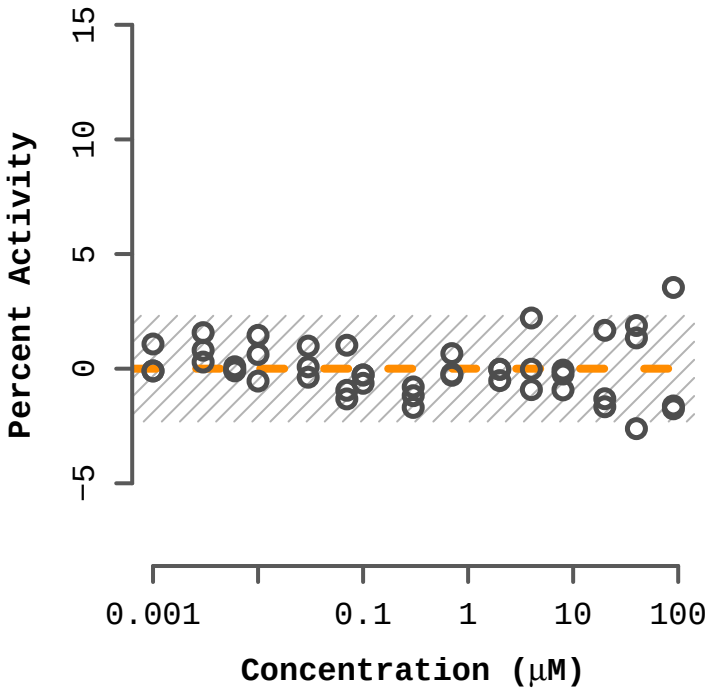
NAME: Octanal
CHID: 21643 **CASRN:** 124-13-0
SPID(S): Tox21_300337
M4ID: 12478795

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 2.18 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

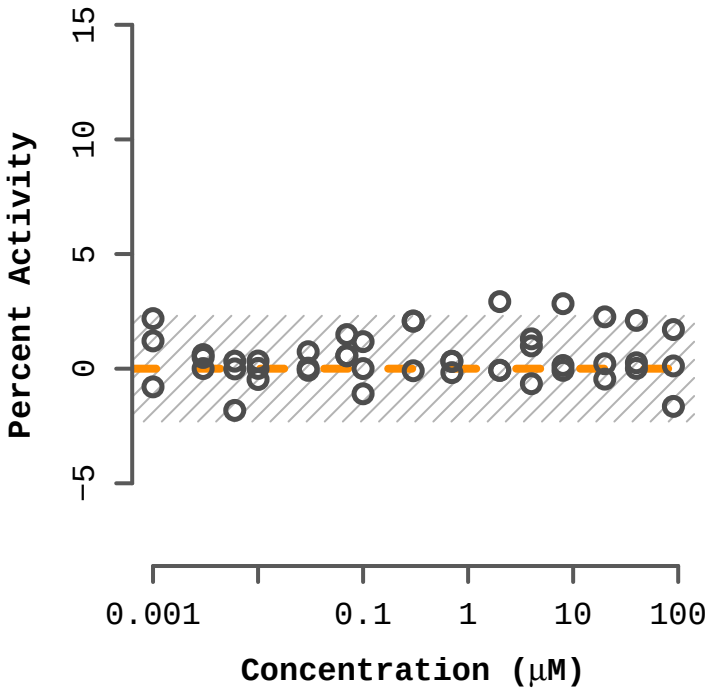
NAME: Octanal
CHID: 21643 CASRN: 124-13-0
SPID(S): Tox21_201415
M4ID: 12480837

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.89 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

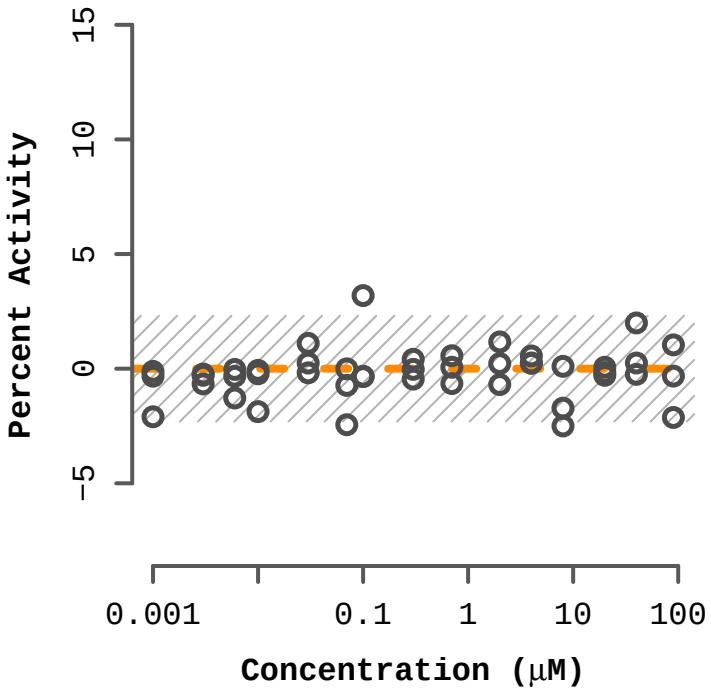
NAME: Octanedioic acid
CHID: 21644 CASRN: 505-48-6
SPID(S): Tox21_200531
M4ID: 12481721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.36 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

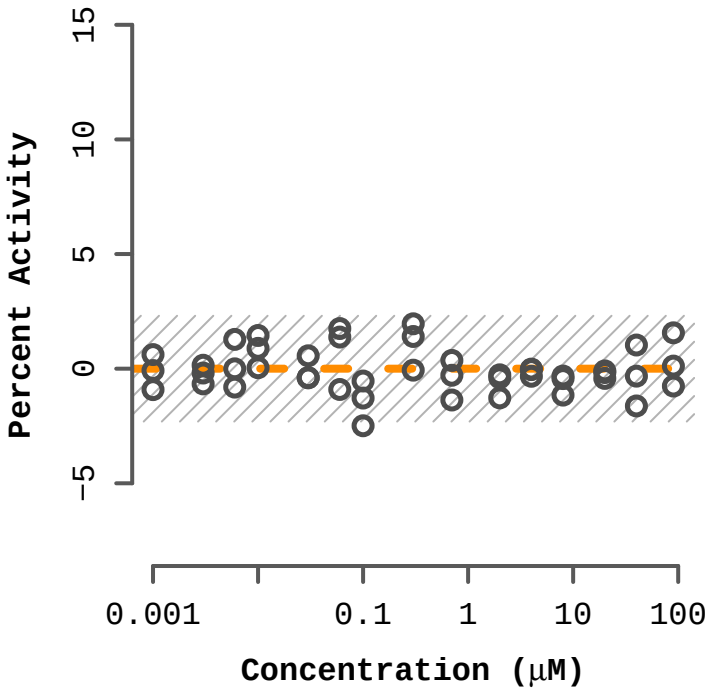
NAME: Octanoic acid
CHID: 21645 **CASRN:** 124-07-2
SPID(S): Tox21_300345
M4ID: 12478787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.839 **MAX_MED:** 0.248 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

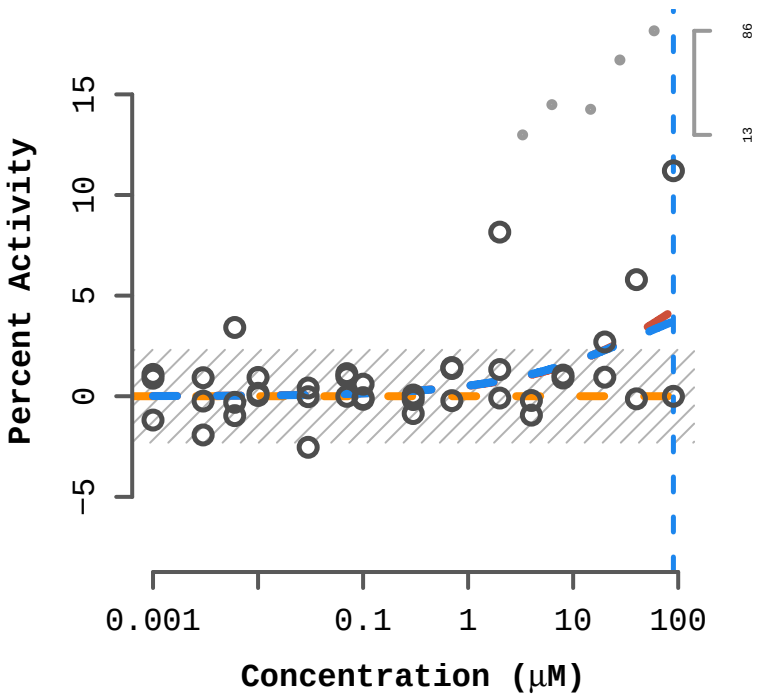
NAME: Octanoic acid
CHID: 21645 CASRN: 124-07-2
SPID(S): Tox21_201279
M4ID: 12480973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Oxobutanedioic acid
CHID: 21646 CASRN: 328-42-7
SPID(S): Tox21_201215
M4ID: 12481037 BRK

HILL MODEL (in red):

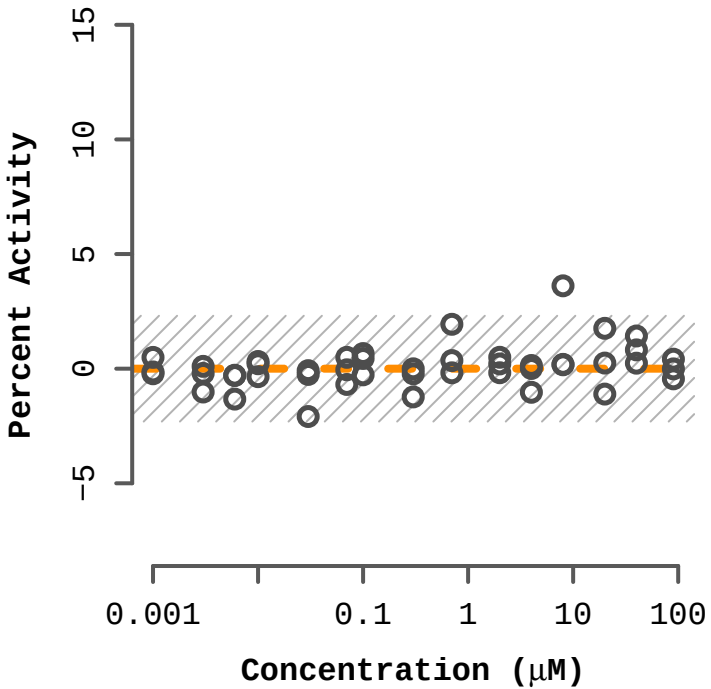
	tp	ga	gw
val:	12.4	2.45	0.554
sd:	111	8.78	0.551

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.05	1.95	0.609	3.95	0.332
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	303.25	302.72	306.77
PROB:	0.4	0.53	0.07
RMSE:	17.8	16.86	16.93

MAX_MEAN: 32.4 MAX_MED: 11.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

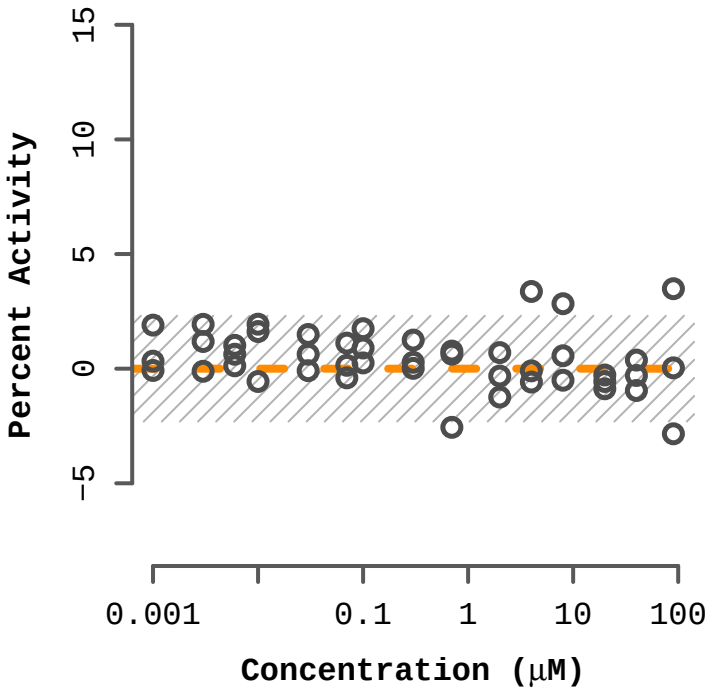
NAME: 2-Oxopentanoic acid
CHID: 21647 **CASRN:** 1821-02-9
SPID(S): Tox21_200532
M4ID: 12481720

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

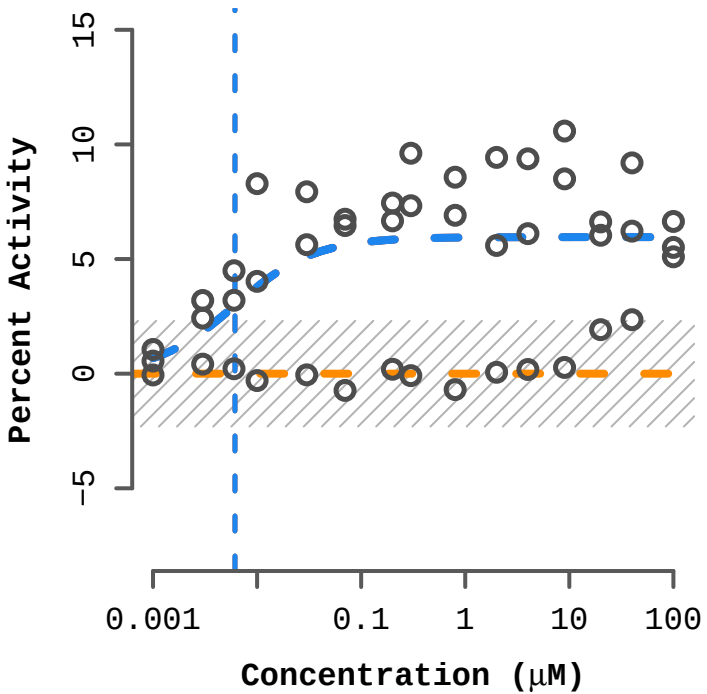
NAME: 4-Oxopentanoic acid
CHID: 21648 **CASRN:** 123-76-2
SPID(S): Tox21_302729
M4ID: 12476404

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Oxopentanoic acid
CHID: 21648 CASRN: 123-76-2
SPID(S): Tox21_201483
M4ID: 12480769

HILL MODEL (in red):

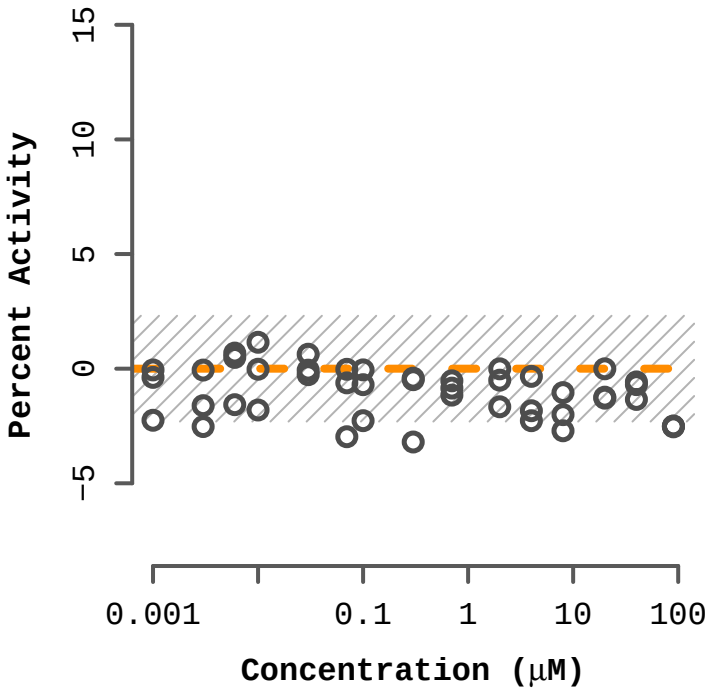
	tp	ga	gw
val:	5.96	-2.21	1.13
sd:	0.665	0.282	0.817

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.96	-2.21	1.13	3.59	5.32
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	291.02	243.01	247.01
PROB:	0	0.88	0.12
RMSE:	5.63	3.2	3.2

MAX_MEAN: 6.45 MAX_MED: 8.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

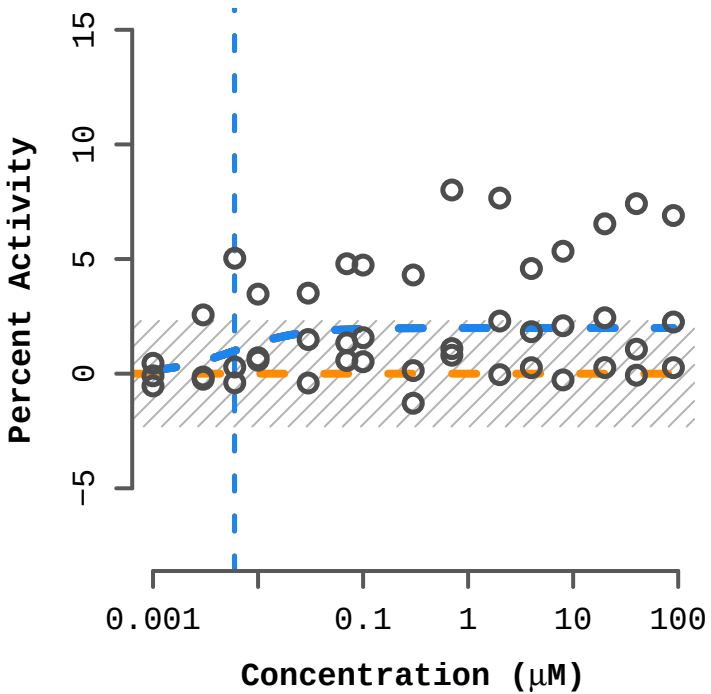
NAME: 2-Oxopropanoic acid
CHID: 21650 **CASRN:** 127-17-3
SPID(S): Tox21_303284
M4ID: 12475849

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.103 **MAX_MED:** 0.492 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Oxopropanoic acid
CHID: 21650 **CASRN:** 127-17-3
SPID(S): Tox21_202096
M4ID: 12480156

HILL MODEL (in red):

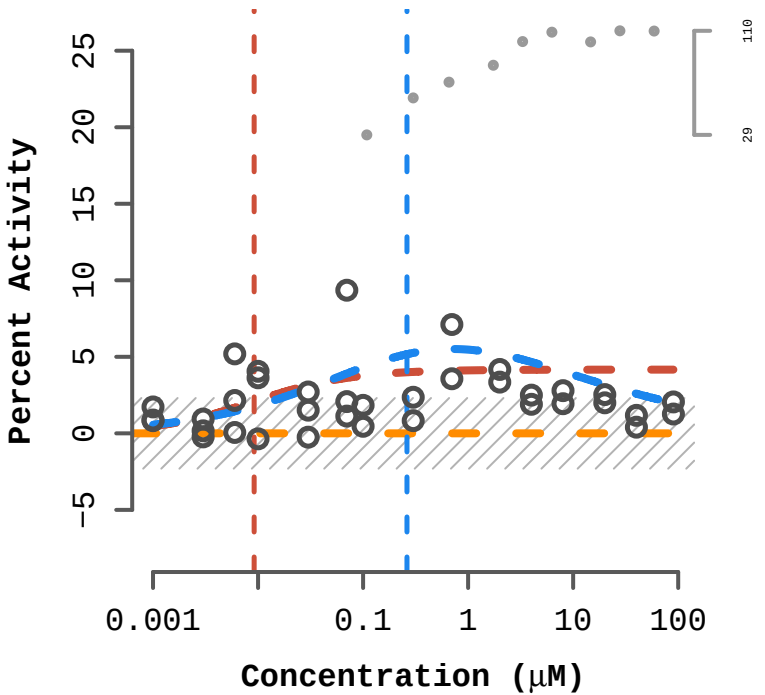
	tp	ga	gw
val:	1.99	−2.22	1.4
sd:	0.528	0.577	2.78

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.99	−2.22	1.4	3.72	5.29
sd:	0.528	0.577	2.78	18900	57000

	CNST	HILL	GNLS
AIC:	232.94	215.68	219.68
PROB:	0	0.88	0.12
RMSE:	3.25	2.42	2.42

MAX_MEAN: 3.31 **MAX_MED:** 2.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentadecanoic acid
CHID: 21652 **CASRN:** 1002-84-2
SPID(S): Tox21_201197
M4ID: 12481055 **BRK**

HILL MODEL (in red):

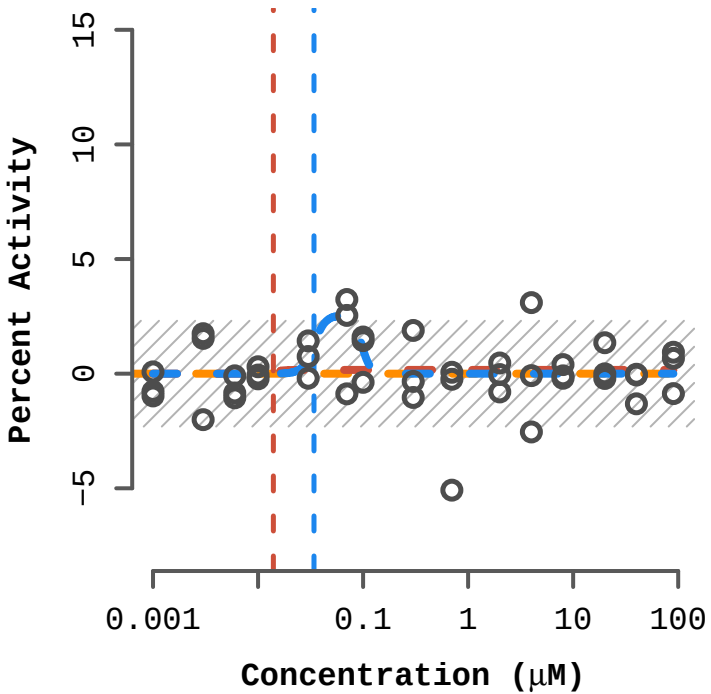
	tp	ga	gw
val:	4.16	−2.04	0.938
sd:	2.26	1.28	1.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.6	−0.582	0.609	−0.332	0.397
sd:	232	5.71	1.51	22.1	1.64

	CNST	HILL	GNLS
AIC:	432.63	432.49	436.03
PROB:	0.44	0.48	0.08
RMSE:	41.7	39.91	40.02

MAX_MEAN: 39.2 **MAX_MED:** 7.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentanal
CHID: 21653 **CASRN:** 110-62-3
SPID(S): Tox21_300061
M4ID: 12479069

HILL MODEL (in red):

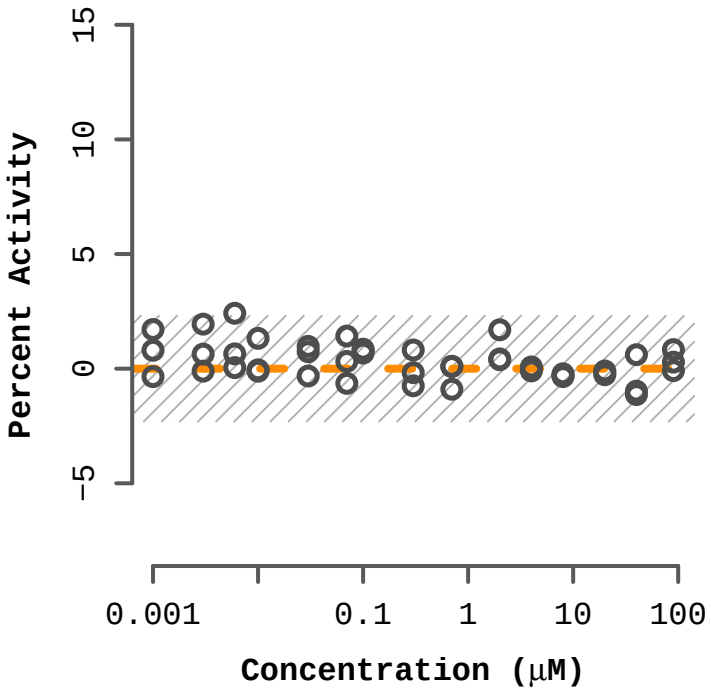
	tp	ga	gw
val:	0.164	−1.85	8
sd:	0.207	1.49	40.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.56	−1.47	7.96	−1.01	10.3
sd:	7.31	2.44	338	0.483	202

	CNST	HILL	GNLS
AIC:	155.49	160.86	156.63
PROB:	0.61	0.04	0.35
RMSE:	1.43	1.42	1.35

MAX_MEAN: 1.63 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

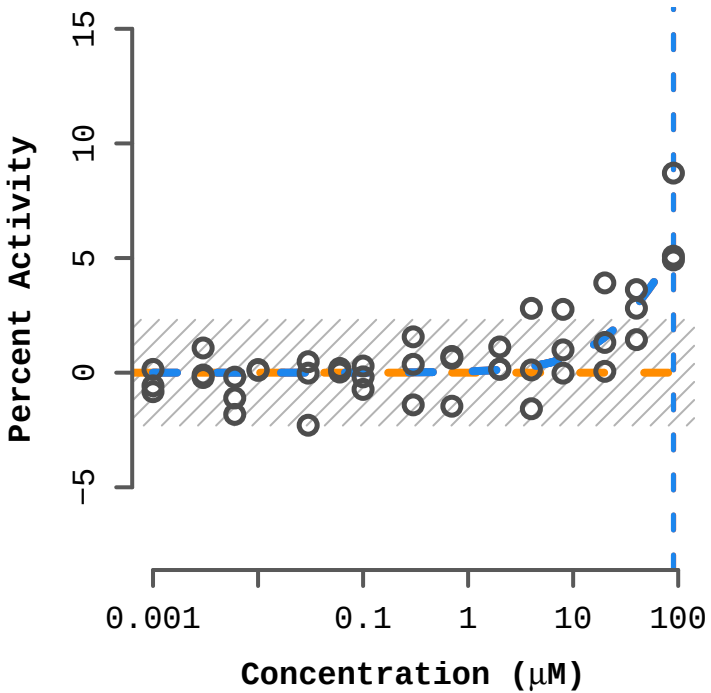
NAME: Pentanedioic acid
CHID: 21654 **CASRN:** 110-94-1
SPID(S): Tox21_302871
M4ID: 12476262

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentanedioic acid
CHID: 21654 CASRN: 110-94-1
SPID(S): Tox21_202448
M4ID: 12479804

HILL MODEL (in red):

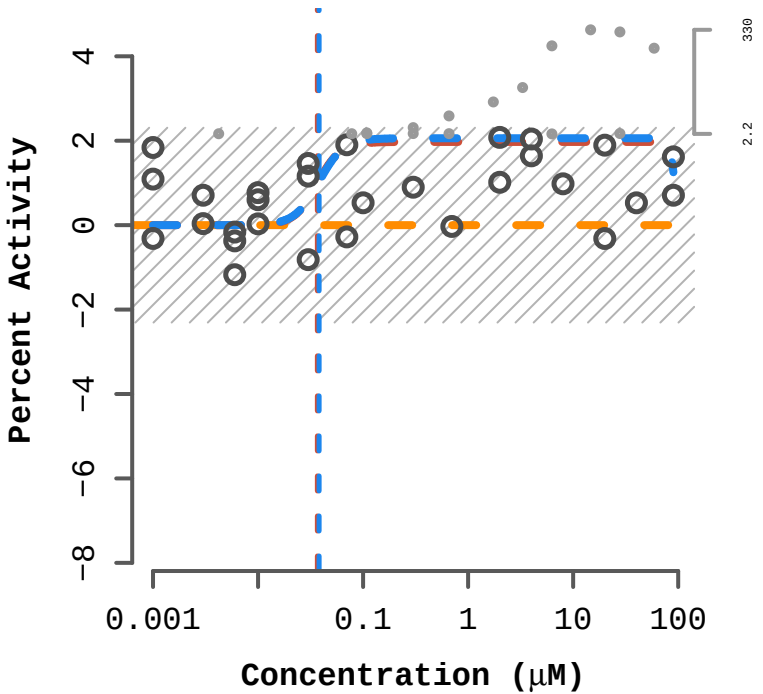
	tp	ga	gw
val:	10.4	1.96	1.15
sd:	7.15	0.503	0.486

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.4	1.95	1.16	3.79	4.2
sd:	7.67	0.534	0.499	1530	3530

	CNST	HILL	GNLS
AIC:	180.78	143.25	147.25
PROB:	0	0.88	0.12
RMSE:	2.17	1.16	1.16

MAX_MEAN: 6.24 MAX_MED: 5.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentanoic acid
CHID: 21655 CASRN: 109-52-4
SPID(S): Tox21_303030
M4ID: 12476103 BRK

HILL MODEL (in red):

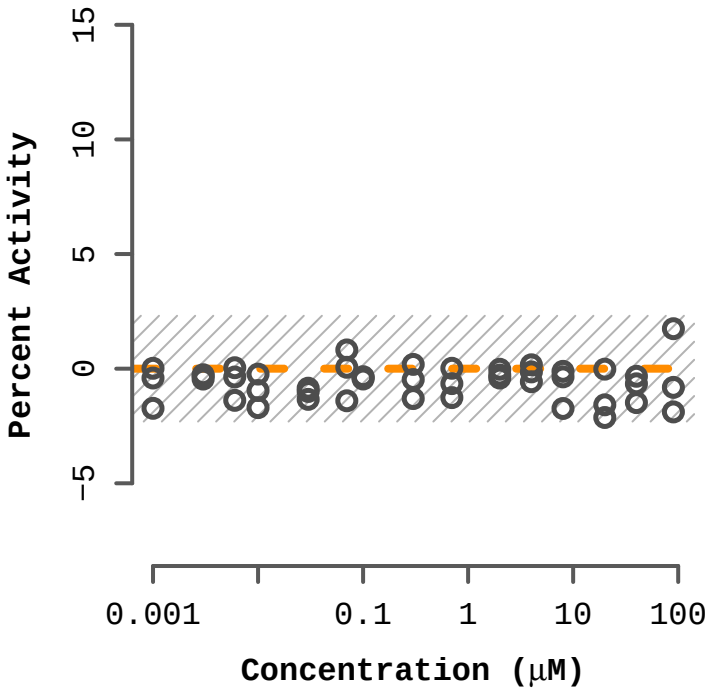
	tp	ga	gw
val:	1.97	−1.44	4.02
sd:	0.757	0.493	11.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.06	−1.42	3.74	1.97	17.7
sd:	0.814	0.506	9.45	0.135	221

	CNST	HILL	GNLS
AIC:	454.65	454.56	458.44
PROB:	0.45	0.48	0.07
RMSE:	95.07	94.35	94.37

MAX_MEAN: 111 MAX_MED: 3.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

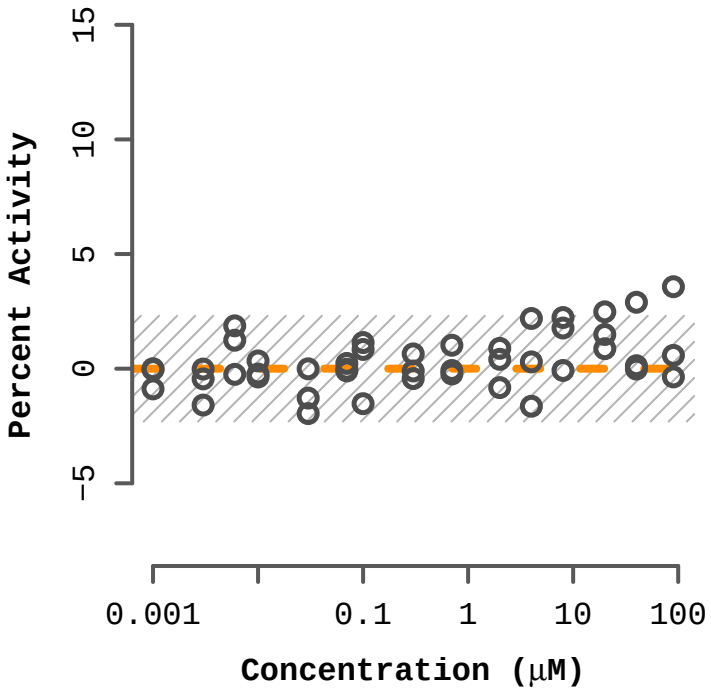
NAME: Pentanoic acid
CHID: 21655 **CASRN:** 109-52-4
SPID(S): Tox21_201561
M4ID: 12480691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: −0.173 **MAX_MED:** 0.0618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

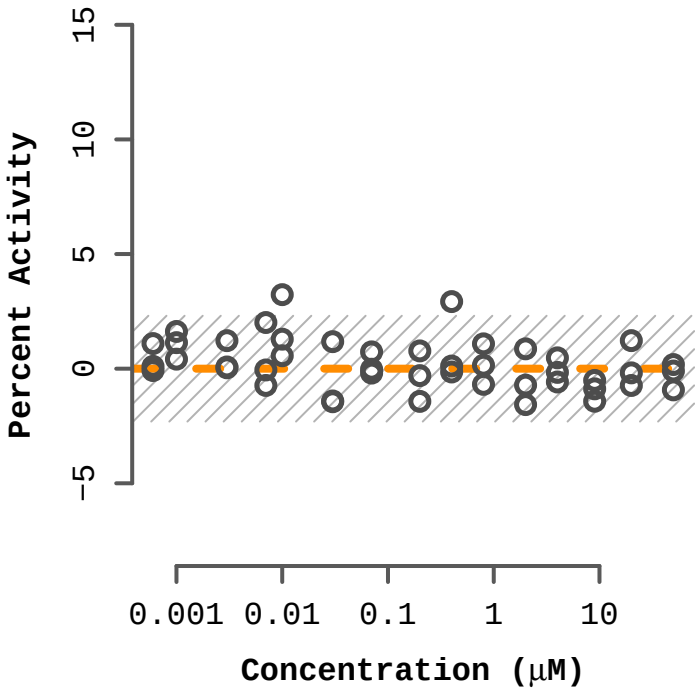
NAME: Phenylacetic acid
CHID: 21656 **CASRN:** 103-82-2
SPID(S): Tox21_200533
M4ID: 12481719

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

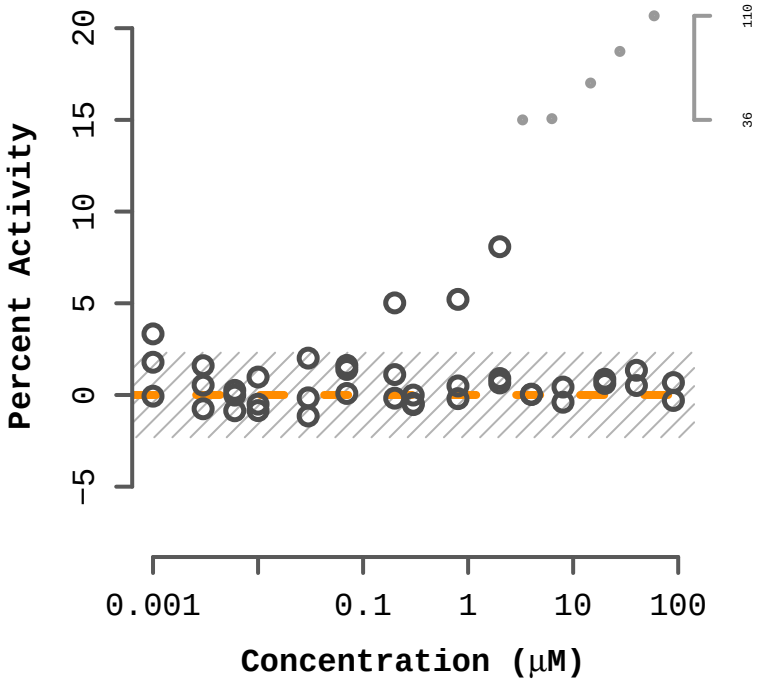
NAME: Phenylacetic acid
CHID: 21656 **CASRN:** 103-82-2
SPID(S): Tox21_113042_1
M4ID: 12482833

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

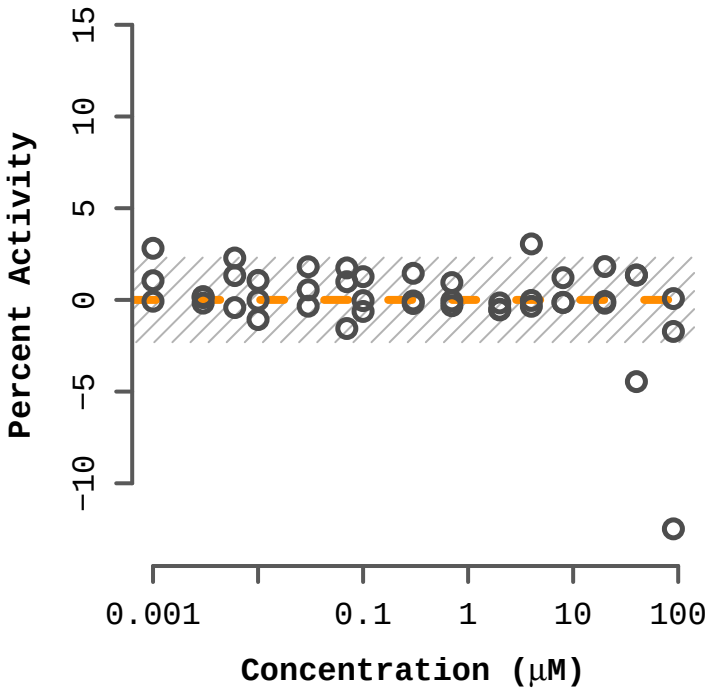
NAME: 1,1−(1,4−Phenylene)bis−ethanone
CHID: 21657 **CASRN:** 1009−61−6
SPID(S): Tox21_201219
M4ID: 12481033 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	315.28	NA	NA
PROB:	1	NA	NA
RMSE:	23.26	NA	NA

MAX_MEAN: 35.4 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

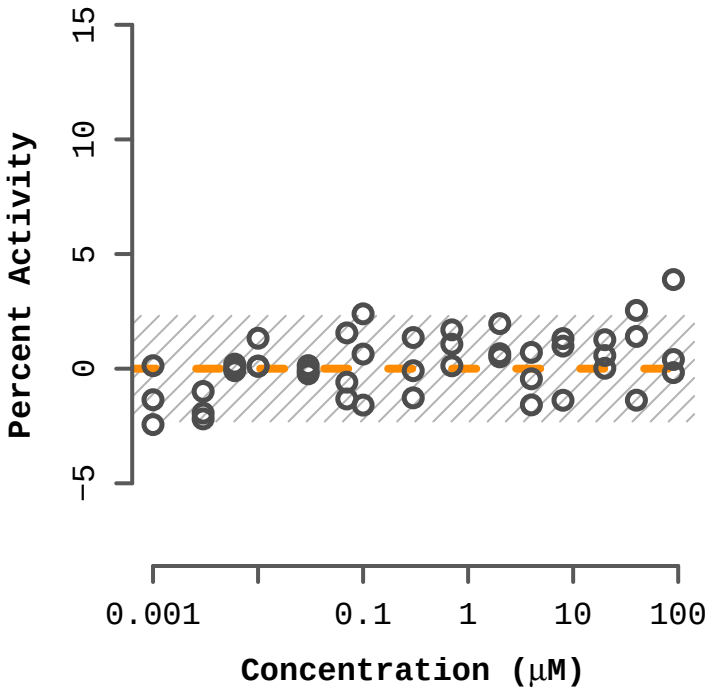
NAME: Propanal
CHID: 21658 **CASRN:** 123-38-6
SPID(S): Tox21_201071
M4ID: 12481181

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.27	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

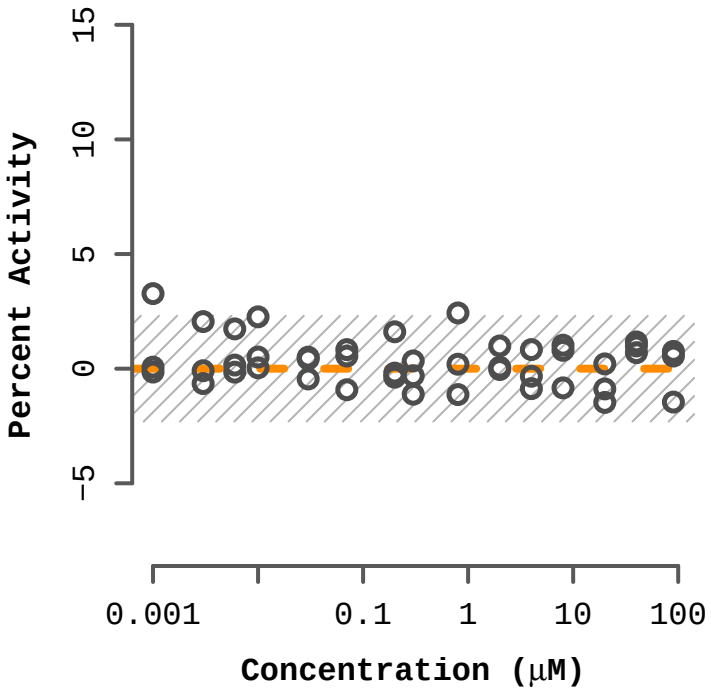
NAME: Propanedioic acid
CHID: 21659 **CASRN:** 141-82-2
SPID(S): Tox21_200534
M4ID: 12481718

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

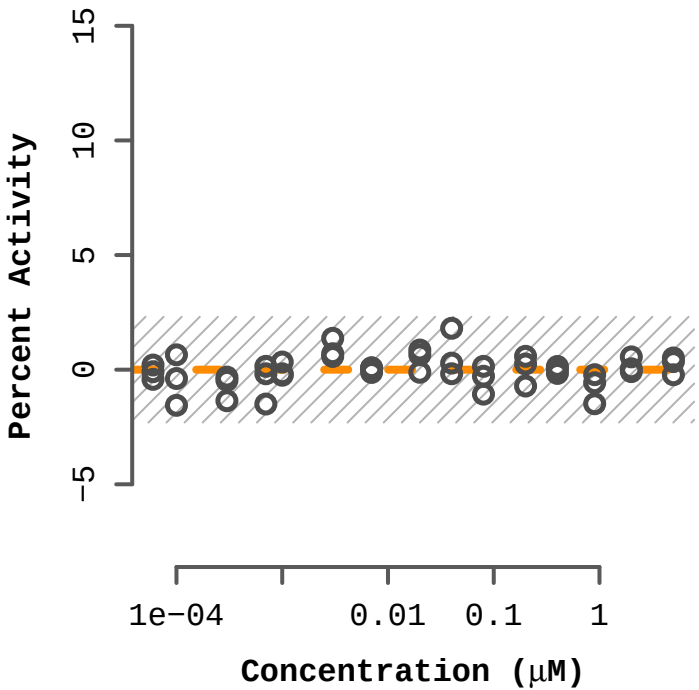
NAME: Tetrachlorocyclopropene
CHID: 21660 CASRN: 6262-42-6
SPID(S): Tox21_201046
M4ID: 12481206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.07 MAX_MED: 0.991 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

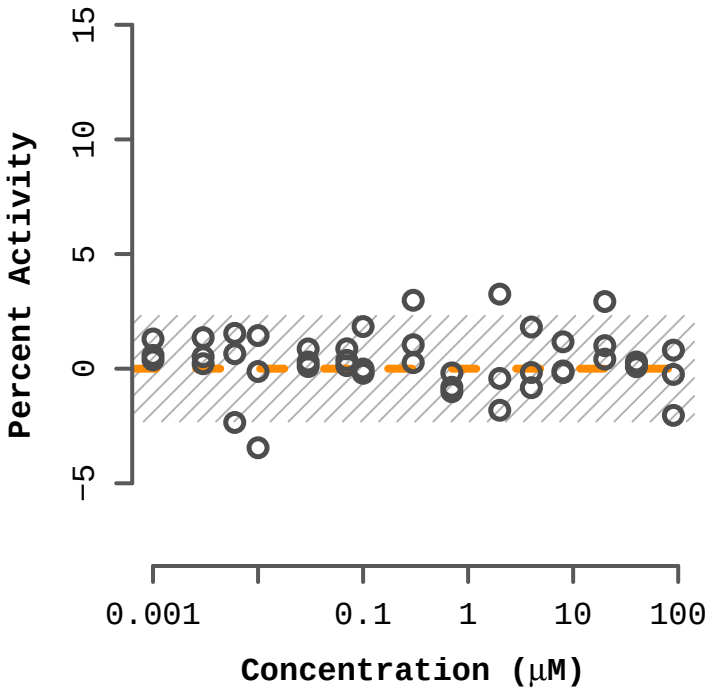
NAME: Tetradecanal
CHID: 21665 **CASRN:** 124-25-4
SPID(S): Tox21_202794
M4ID: 12479458

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.882 **MAX_MED:** 0.699 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

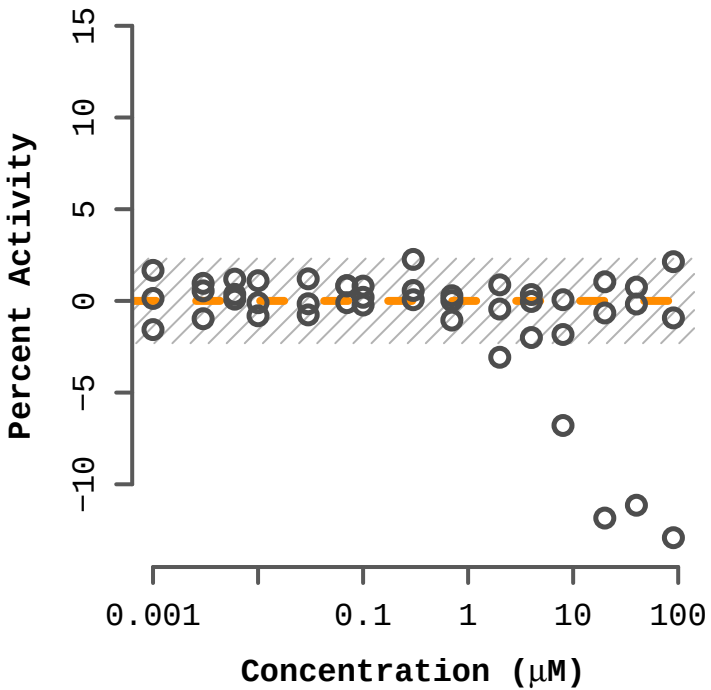
NAME: Tetradecanoic acid
CHID: 21666 **CASRN:** 544-63-8
SPID(S): Tox21_302781
M4ID: 12476352

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

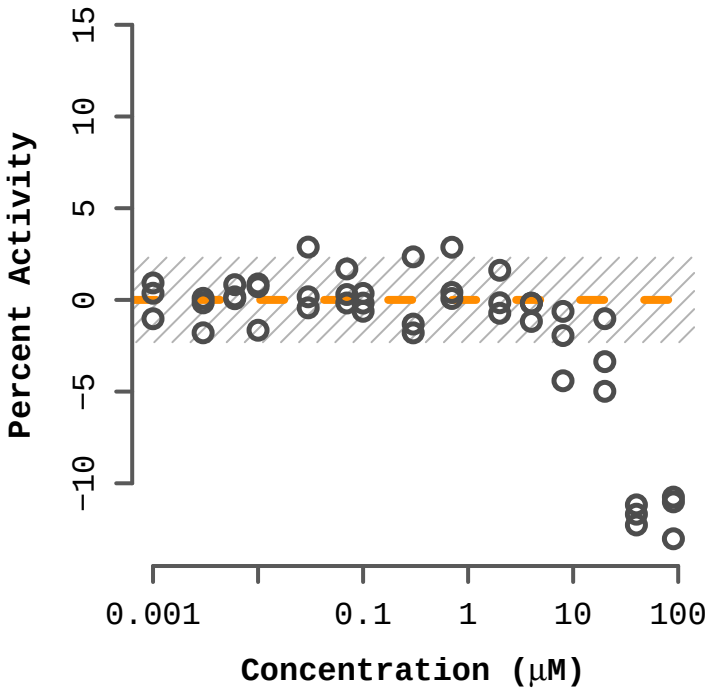
NAME: Tetradecanoic acid
CHID: 21666 **CASRN:** 544-63-8
SPID(S): Tox21_201852
M4ID: 12480400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.41	NA	NA
PROB:	1	NA	NA
RMSE:	3.41	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.814 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

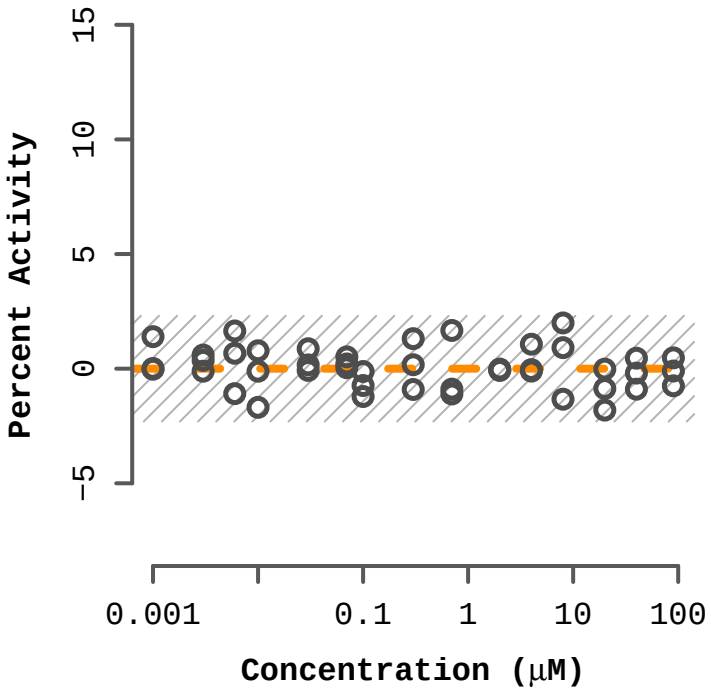
NAME: Tribromoacetaldehyde
CHID: 21667 **CASRN:** 115-17-3
SPID(S): Tox21_200535
M4ID: 12481717

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.27	NA	NA
PROB:	1	NA	NA
RMSE:	4.53	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.719 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

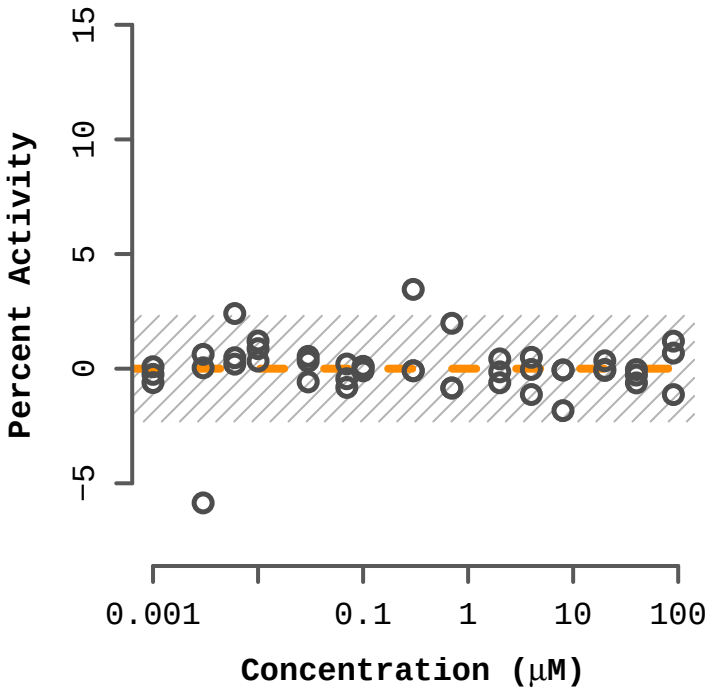
NAME: Tribromoacetic acid
CHID: 21668 **CASRN:** 75-96-7
SPID(S): Tox21_200913
M4ID: 12481339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

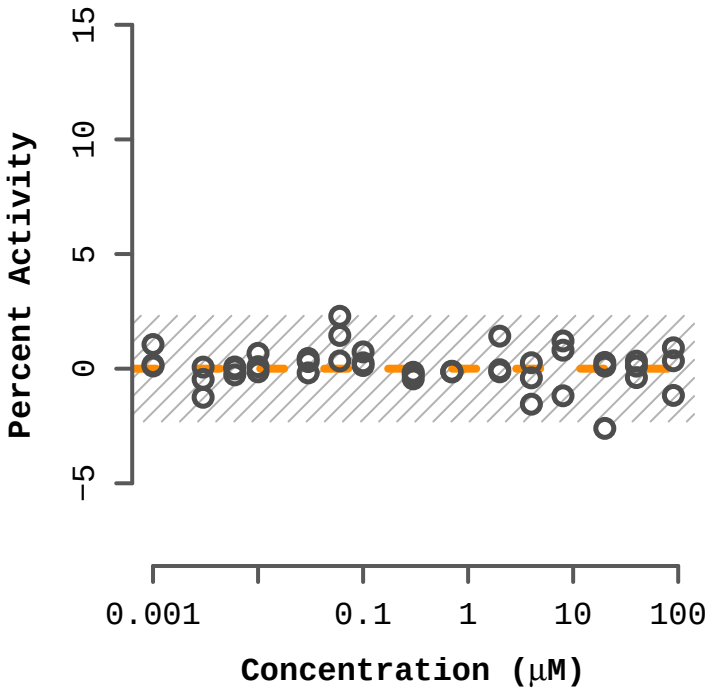
NAME: 2,2,2-Trichloroacetamide
CHID: 21671 **CASRN:** 594-65-0
SPID(S): Tox21_200536
M4ID: 12481716

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.875 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

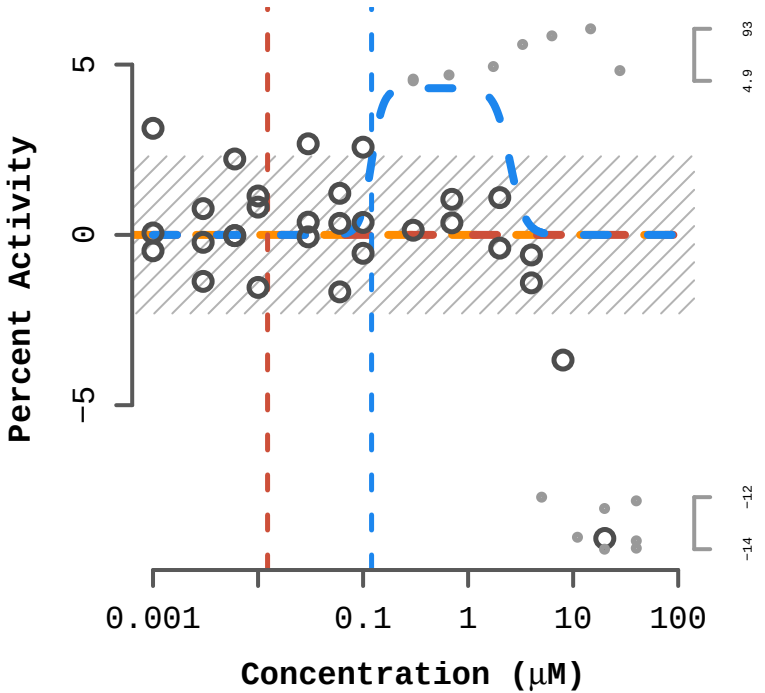
NAME: Trichloroacetonitrile
CHID: 21672 **CASRN:** 545-06-2
SPID(S): Tox21_201058
M4ID: 12481194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1,1−Trichloropropanone
CHID: 21679 **CASRN:** 918−00−3
SPID(S): Tox21_201222
M4ID: 12481030 **BRK**

HILL MODEL (in red):

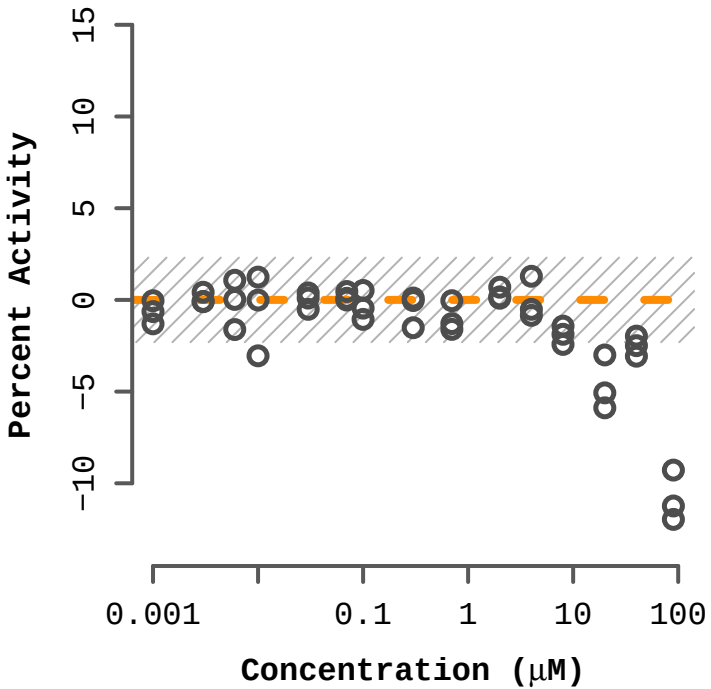
	tp	ga	gw
val:	5.67e−09	−1.91	6.03
sd:	0.00111	16100	1130000

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.31	−0.919	7.99	0.398	5.98
sd:	2.99	2.07	201	0.576	22.4

	CNST	HILL	GNLS
AIC:	363.22	369.22	370.53
PROB:	0.93	0.05	0.02
RMSE:	22.47	22.47	22.3

MAX_MEAN: 23.6 **MAX_MED:** 4.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

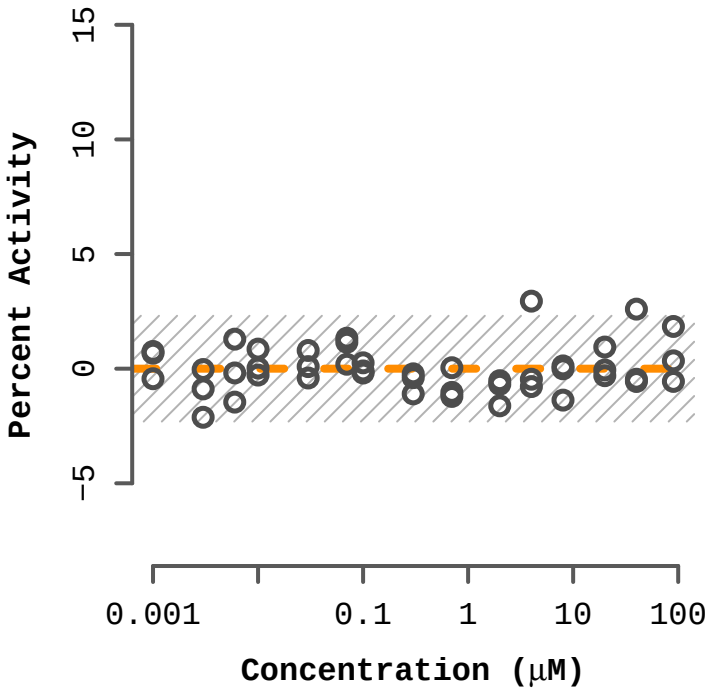
NAME: 1,1,3-Trichloropropanone
CHID: 21680 **CASRN:** 921-03-9
SPID(S): Tox21_202795
M4ID: 12479457

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.99	NA	NA
PROB:	1	NA	NA
RMSE:	3.28	NA	NA

MAX_MEAN: 0.317 **MAX_MED:** 0.165 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

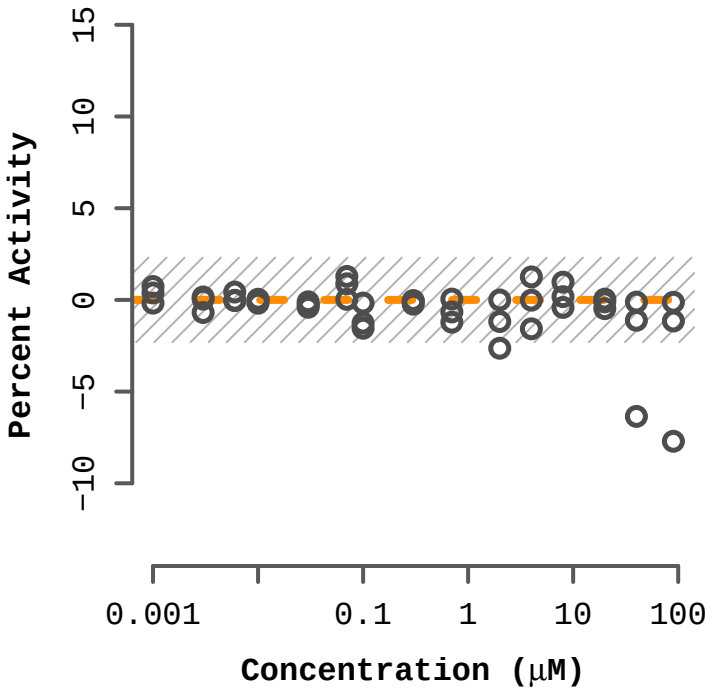
NAME: Tridecanedioic acid
CHID: 21683 **CASRN:** 505-52-2
SPID(S): Tox21_302982
M4ID: 12476151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.893 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

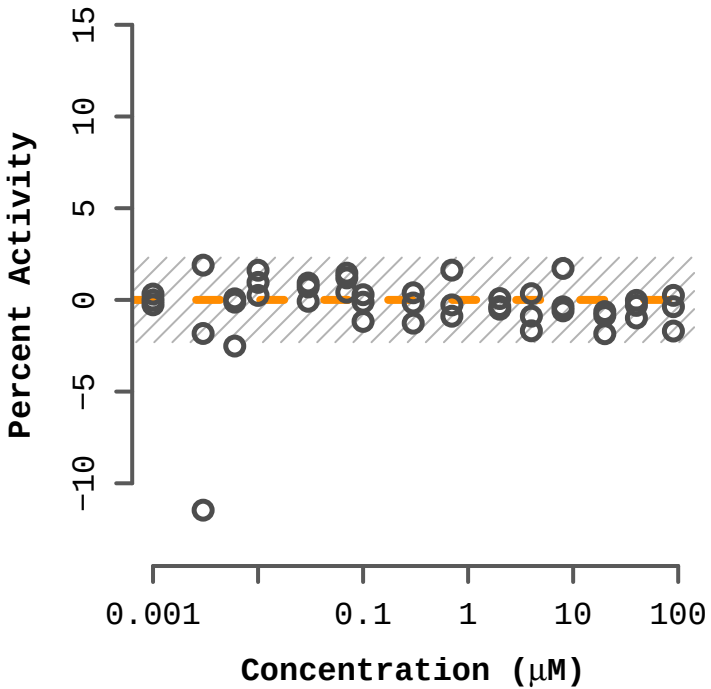
NAME: Tridecanedioic acid
CHID: 21683 **CASRN:** 505-52-2
SPID(S): Tox21_201301
M4ID: 12480951

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.73 **MAX_MED:** 0.879 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

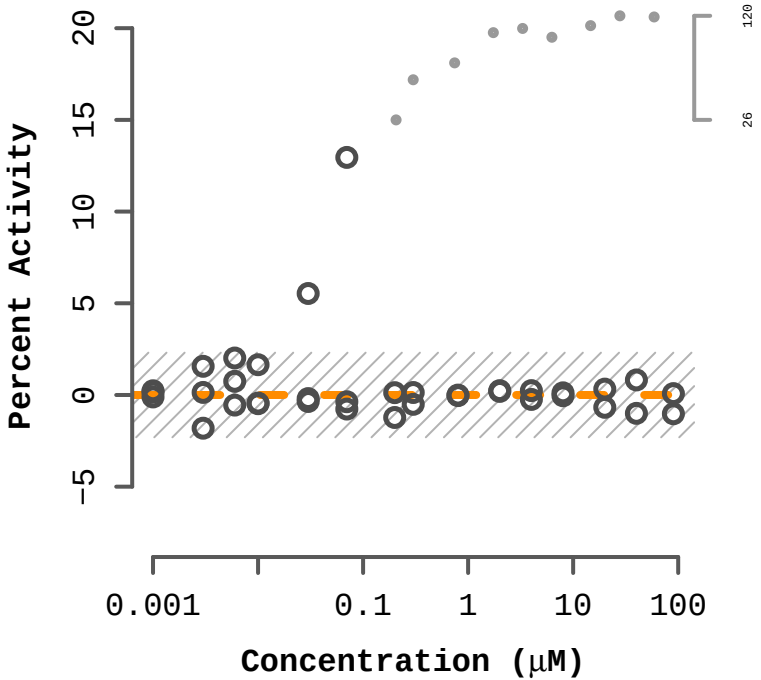
NAME: Tridecanoic acid
CHID: 21684 **CASRN:** 638-53-9
SPID(S): Tox21_200537
M4ID: 12481715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

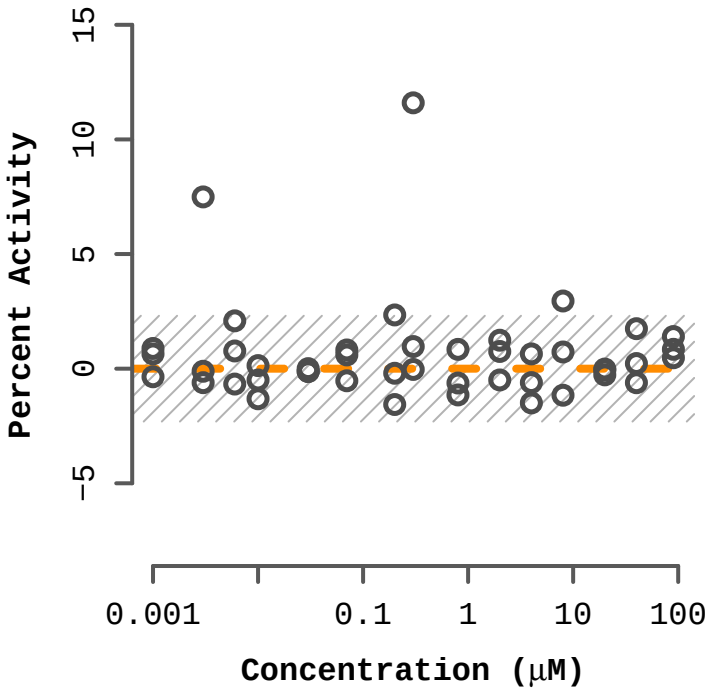
NAME: 2,6,6-Trimethyl-2-cyclohexene-1,4-dione
CHID: 21685 **CASRN:** 1125-21-9
SPID(S): Tox21_201193
M4ID: 12481059 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	435.25	NA	NA
PROB:	1	NA	NA
RMSE:	44.16	NA	NA

MAX_MEAN: 40.8 **MAX_MED:** 0.821 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

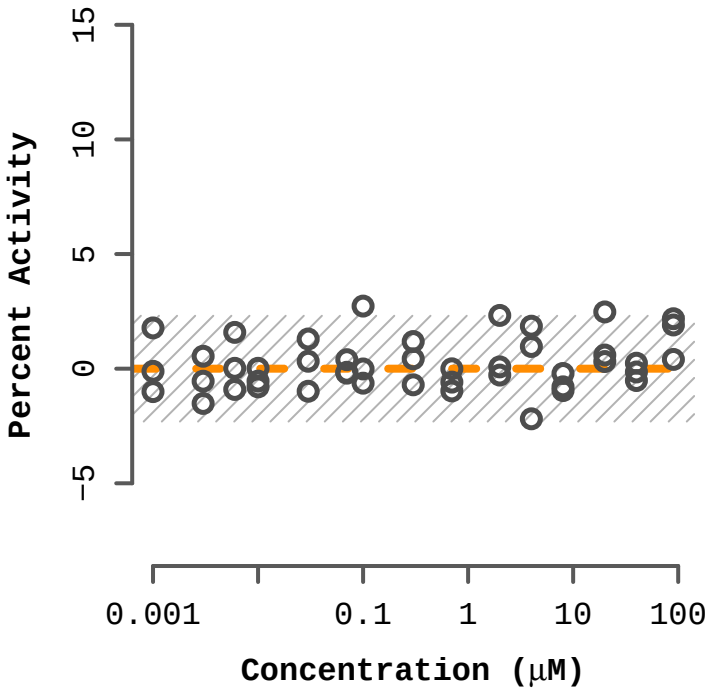
NAME: Undecanal
CHID: 21688 **CASRN:** 112-44-7
SPID(S): Tox21_200538
M4ID: 12481714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.63	NA	NA
PROB:	1	NA	NA
RMSE:	2.28	NA	NA

MAX_MEAN: 4.18 **MAX_MED:** 0.967 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

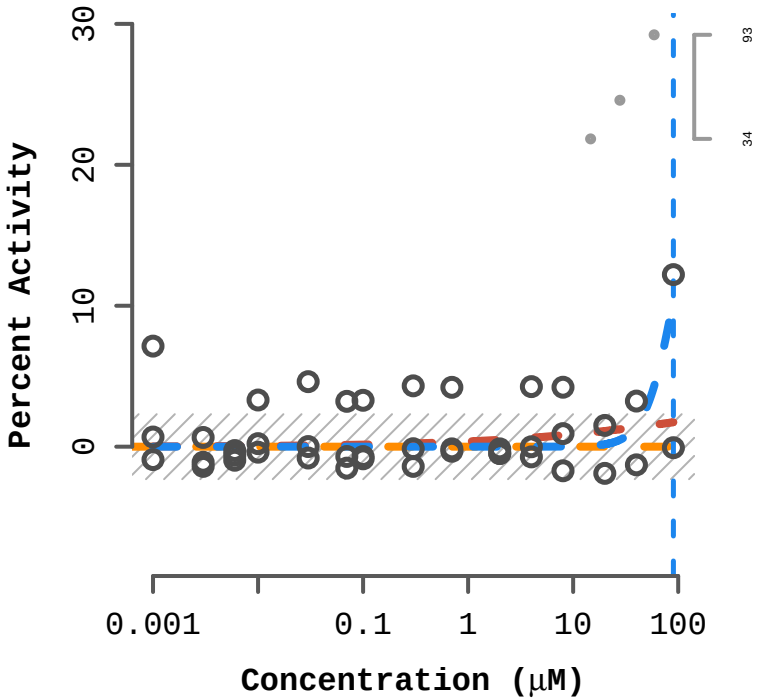
NAME: Undecane
CHID: 21689 **CASRN:** 1120-21-4
SPID(S): Tox21_300076
M4ID: 12479054

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Undecanoic acid
CHID: 21690 CASRN: 112-37-8
SPID(S): Tox21_201031
M4ID: 12481221 BRK

HILL MODEL (in red):

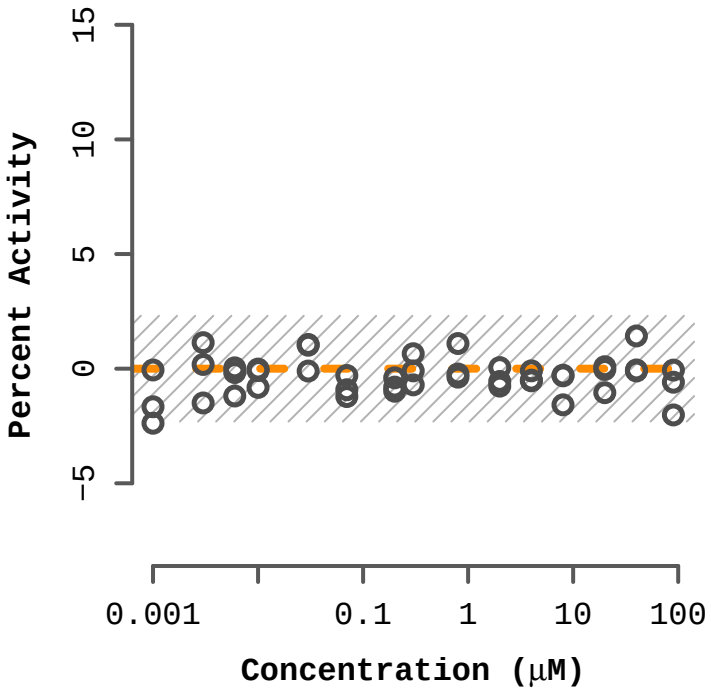
	tp	ga	gw
val:	4.58	2.45	0.429
sd:	28.5	7.98	0.956

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	20.8	1.95	3.19	2.94	5.29
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	286.87	291.07	294.59
PROB:	0.87	0.11	0.02
RMSE:	17.28	16.89	15.91

MAX_MEAN: 35.2 MAX_MED: 12.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

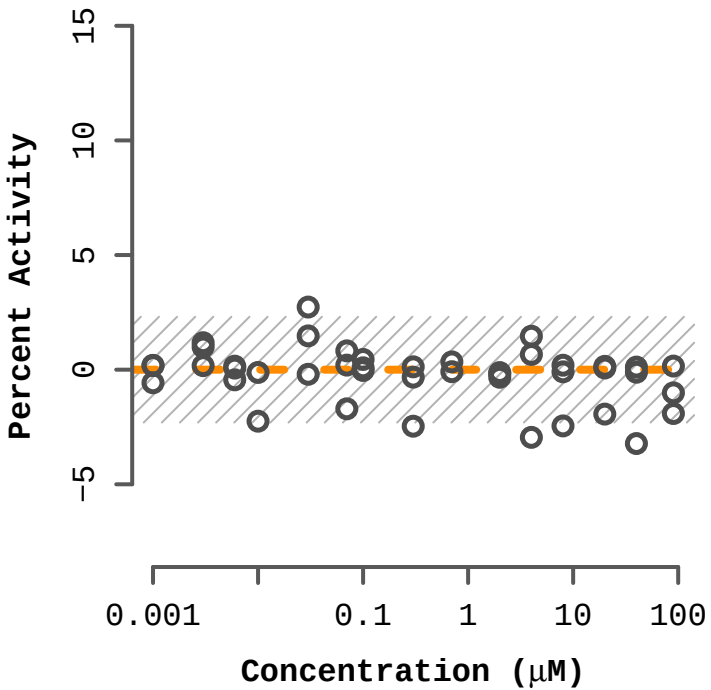
NAME: Sodium salicylate
CHID: 21708 CASRN: 54-21-7
SPID(S): Tox21_200411
M4ID: 12481841

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.66 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

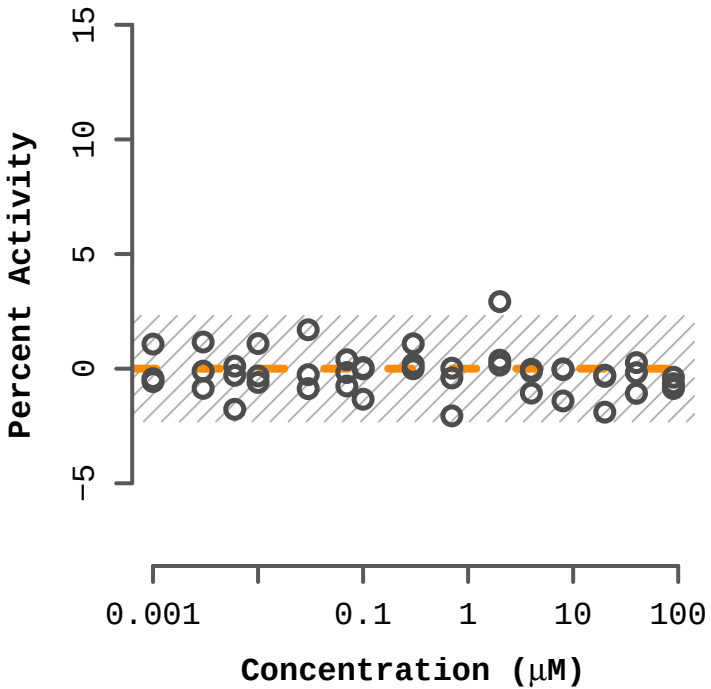
NAME: Benzamide
CHID: 21709 **CASRN:** 55-21-0
SPID(S): Tox21_200621
M4ID: 12481631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

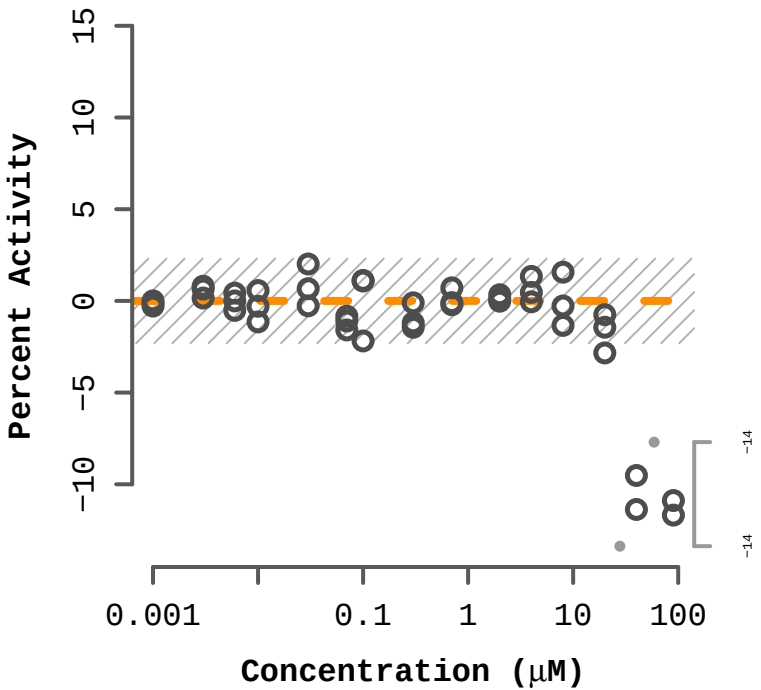
NAME: Benzyltriethylammonium chloride
CHID: 21710 CASRN: 56-37-1
SPID(S): Tox21_303914
M4ID: 12475274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

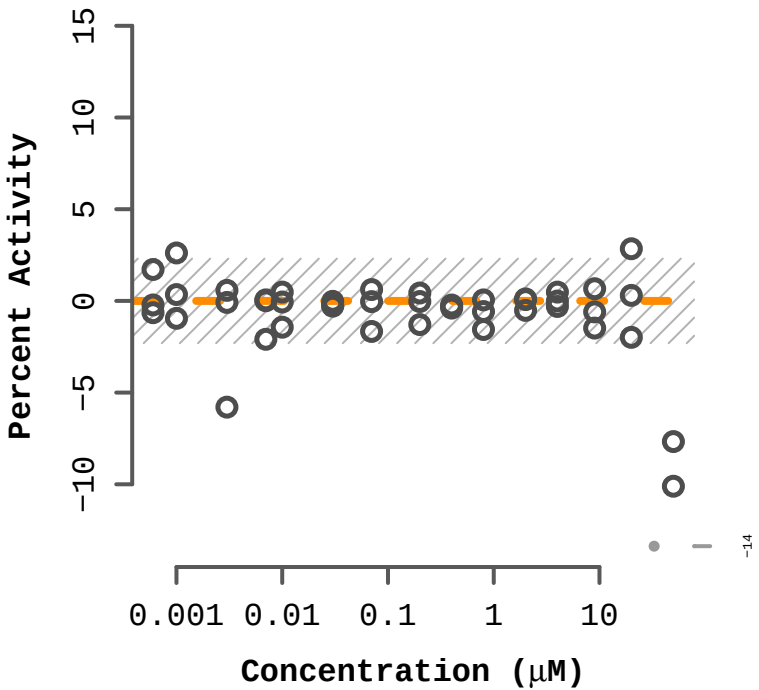
NAME: Menadione
CHID: 21715 **CASRN:** 58-27-5
SPID(S): Tox21_301367
M4ID: 12477766 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.25	NA	NA
PROB:	1	NA	NA
RMSE:	4.49	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

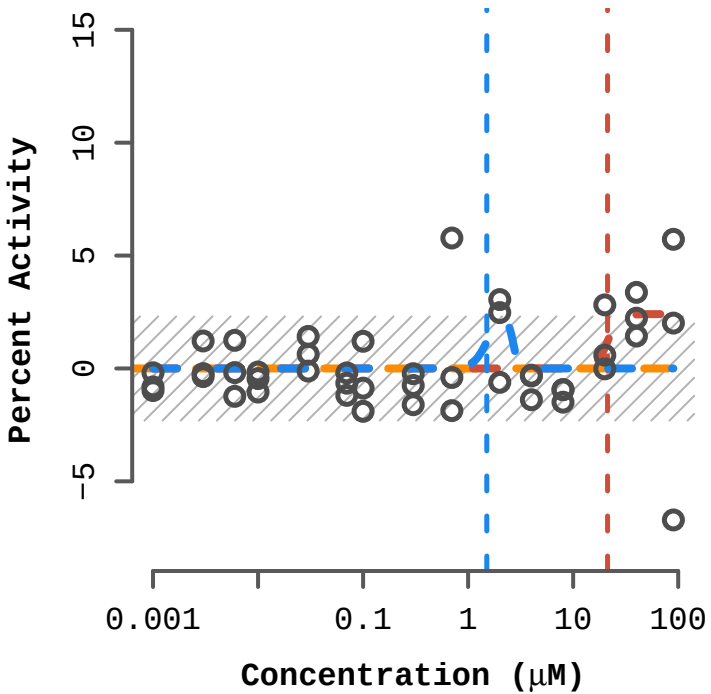
NAME: Menadione
CHID: 21715 **CASRN:** 58-27-5
SPID(S): Tox21_110334_1
M4ID: 12484446 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.23	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 0.671 **MAX_MED:** 0.347 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,4,6-Tetrachlorophenol
CHID: 21716 **CASRN:** 58-90-2
SPID(S): Tox21_302932
M4ID: 12476201

HILL MODEL (in red):

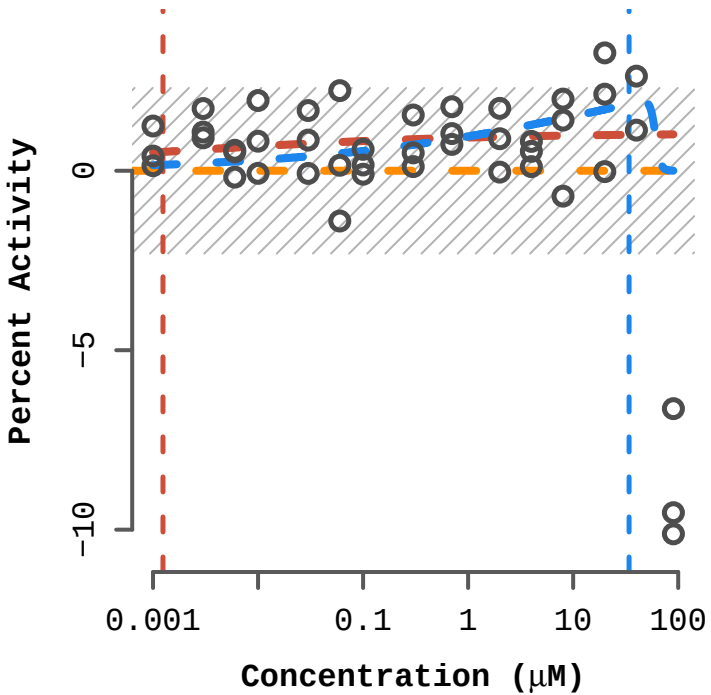
	tp	ga	gw
val:	2.41	1.33	8
sd:	0.663	0.146	30.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.36	0.178	6.68	0.428	16.9
sd:	6.18	1.02	18.9	0.767	73.9

	CNST	HILL	GNLS
AIC:	185.11	177.95	191.82
PROB:	0.03	0.97	0
RMSE:	2.05	2	2

MAX_MEAN: 2.35 **MAX_MED:** 2.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,4,6-Tetrachlorophenol
CHID: 21716 CASRN: 58-90-2
SPID(S): Tox21_201931
M4ID: 12480321

HILL MODEL (in red):

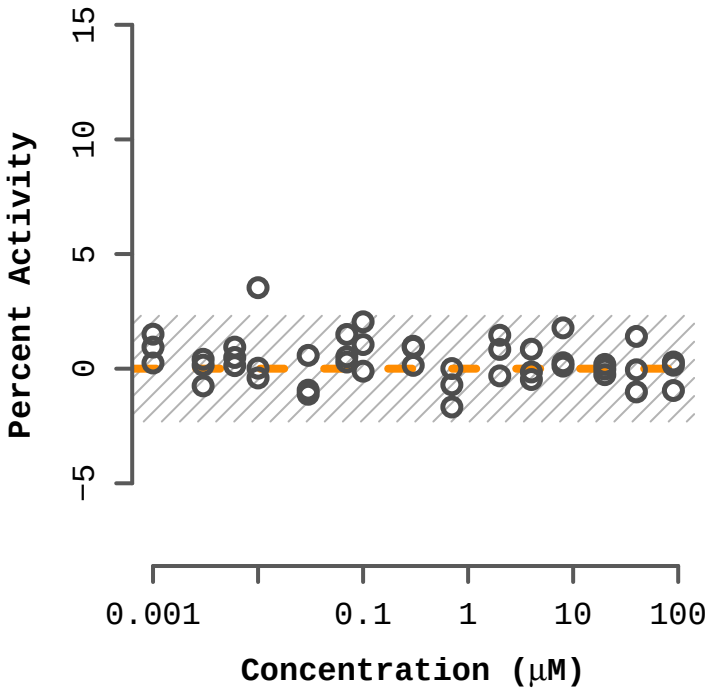
	tp	ga	gw
val:	1.05	−2.91	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.71	1.53	0.3	1.78	18
sd:	9.7	6.49	0.326	0.394	40.6

	CNST	HILL	GNLS
AIC:	195.14	184.63	184.34
PROB:	0	0.46	0.54
RMSE:	2.66	2.74	2.48

MAX_MEAN: 2.64 MAX_MED: 2.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

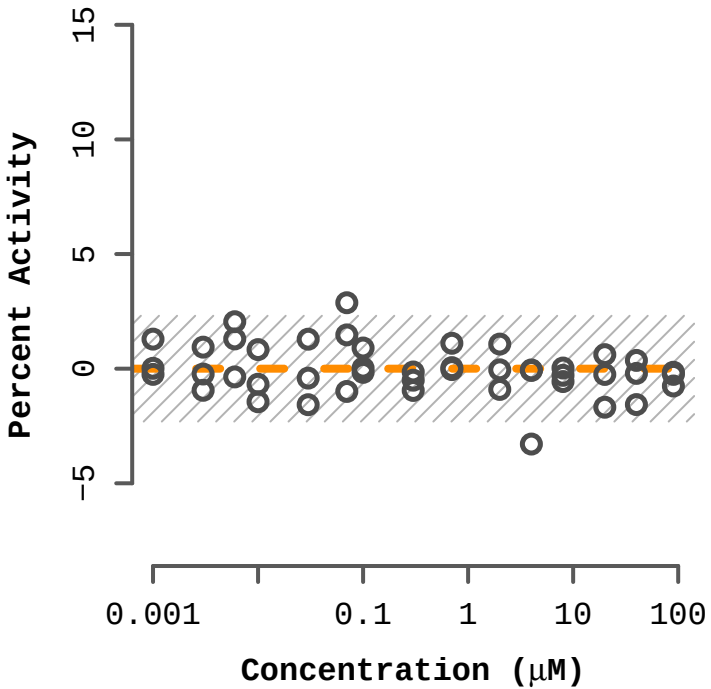
NAME: 4-Chloro-3-methylphenol
CHID: 21717 **CASRN:** 59-50-7
SPID(S): Tox21_300054
M4ID: 12479076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

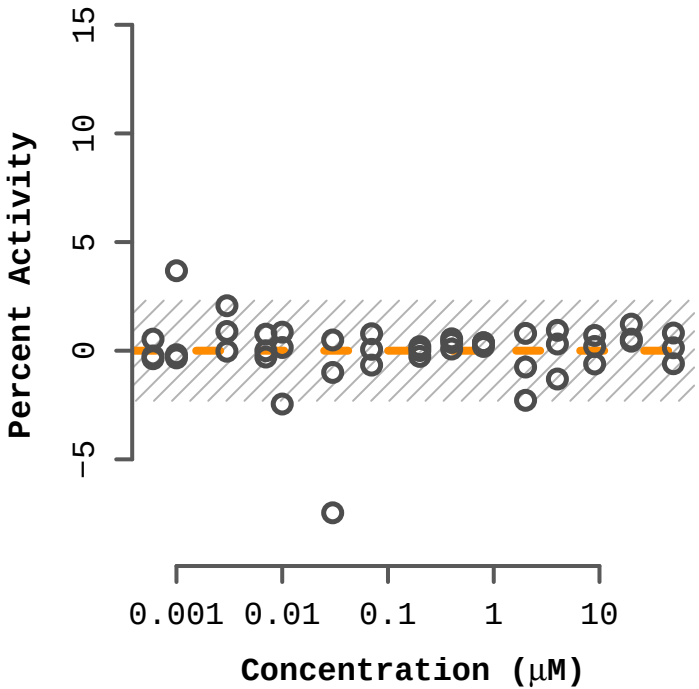
NAME: 4-Chloro-3-methylphenol
CHID: 21717 CASRN: 59-50-7
SPID(S): Tox21_201293
M4ID: 12480959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.12 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

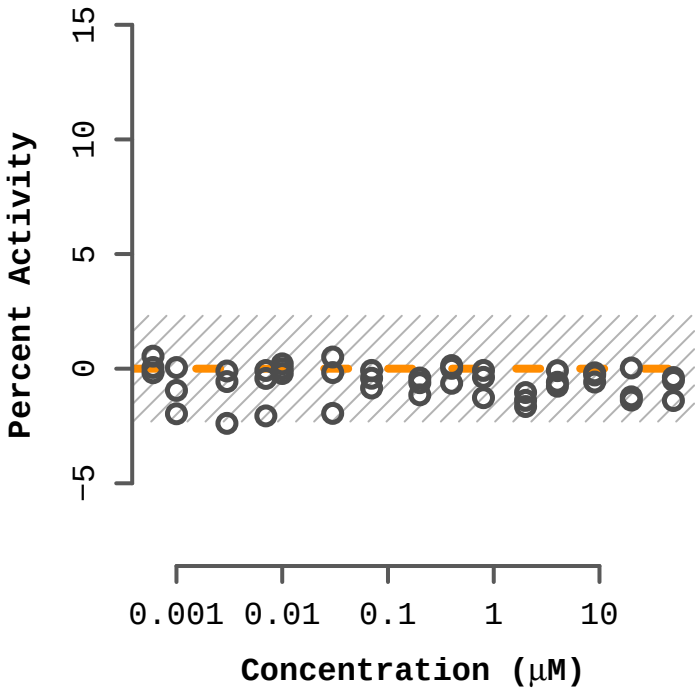
NAME: 4-Chloro-3-methylphenol
CHID: 21717 **CASRN:** 59-50-7
SPID(S): Tox21_111116_1
M4ID: 12483897

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.887 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

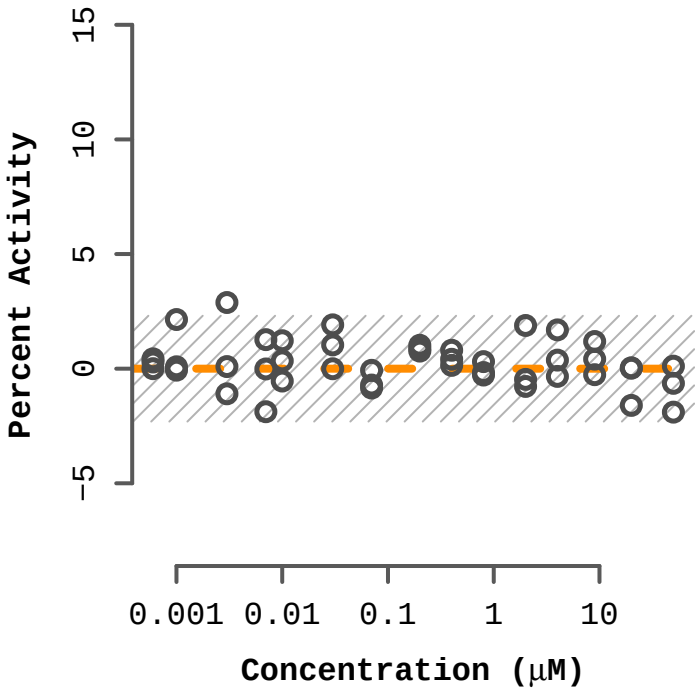
NAME: Tolazoline hydrochloride
CHID: 21718 **CASRN:** 59-97-2
SPID(S): Tox21_110339_1
M4ID: 12484443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.142 **MAX_MED:** 0.0545 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

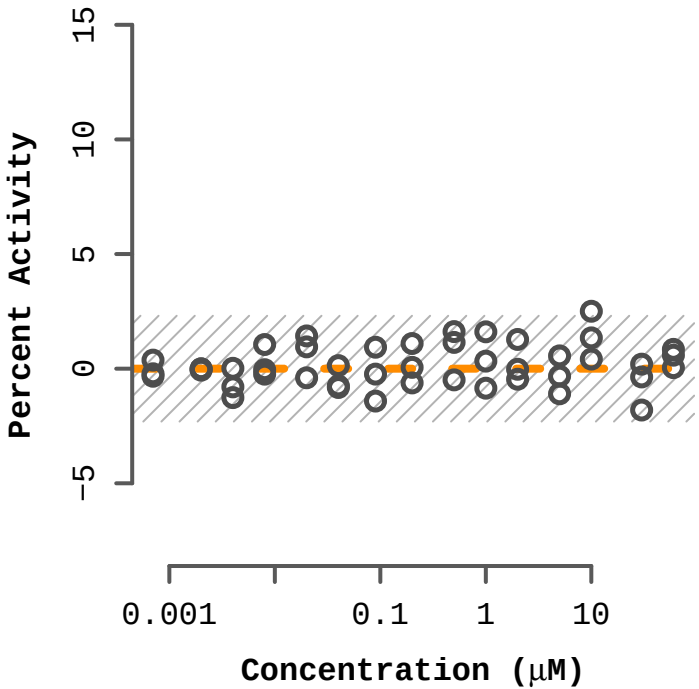
NAME: Strychnine hemisulphate salt
CHID: 21721 **CASRN:** 60-41-3
SPID(S): Tox21_302017
M4ID: 12477116

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

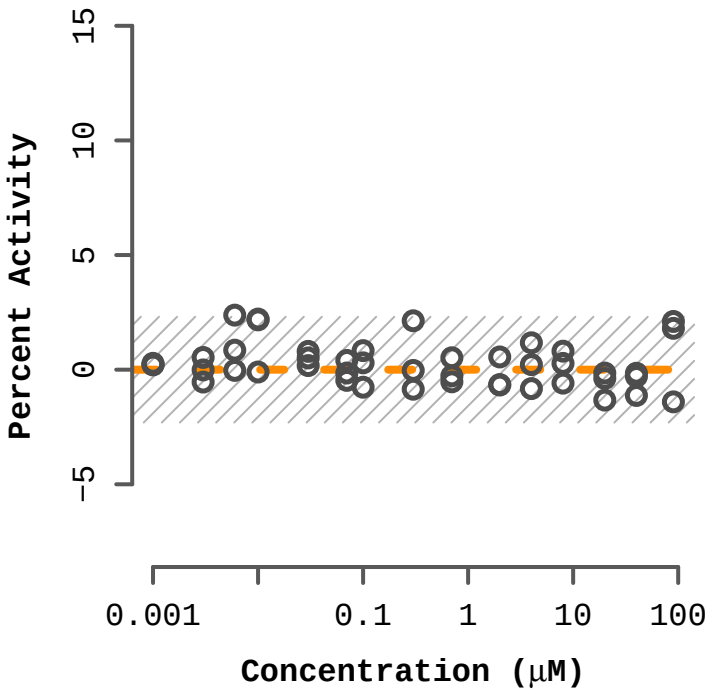
NAME: Nicotine sulfate
CHID: 21725 **CASRN:** 65-30-5
SPID(S): Tox21_302354
M4ID: 12476779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

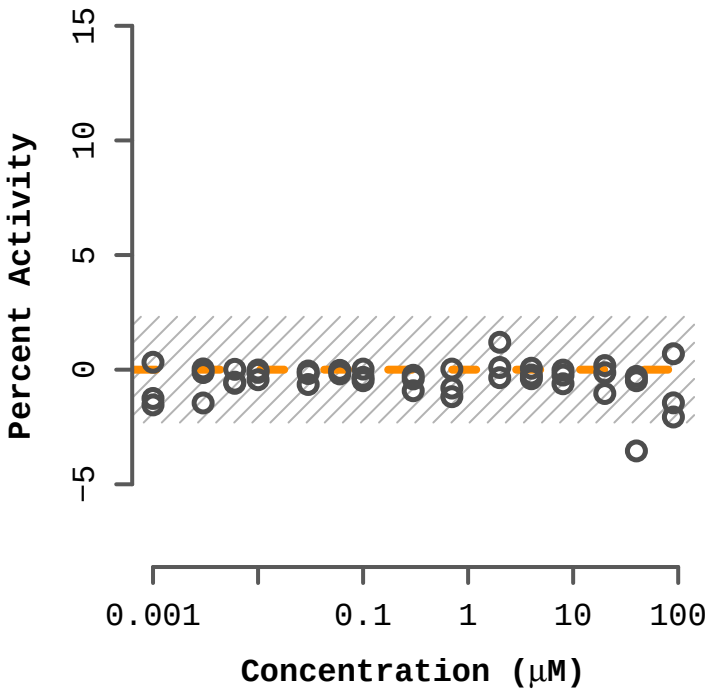
NAME: Salicylamide
CHID: 21726 **CASRN:** 65-45-2
SPID(S): Tox21_302801
M4ID: 12476332

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

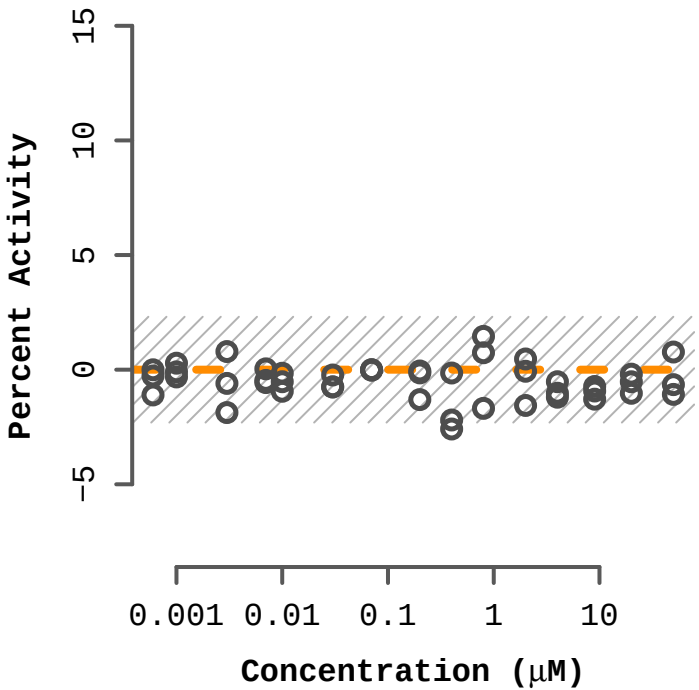
NAME: Salicylamide
CHID: 21726 CASRN: 65-45-2
SPID(S): Tox21_201944
M4ID: 12480308

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.315 MAX_MED: 0.0969 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

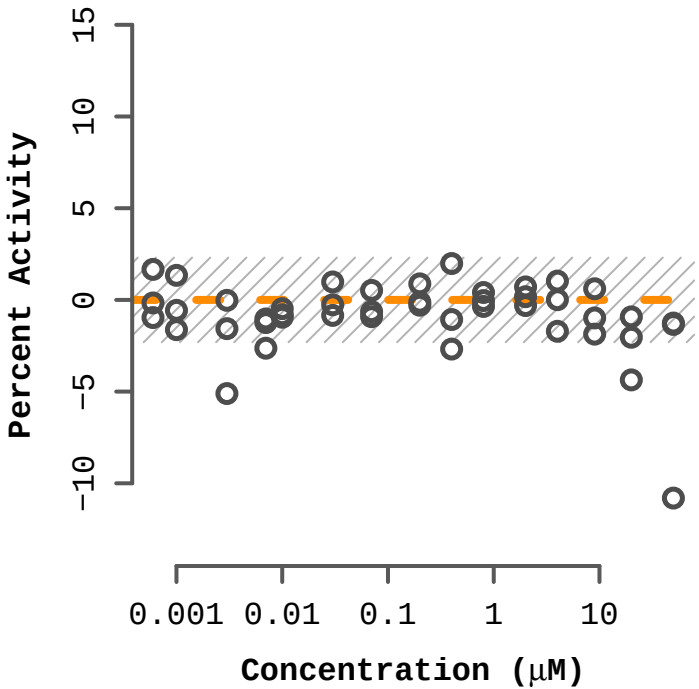
NAME: Salicylamide
CHID: 21726 **CASRN:** 65-45-2
SPID(S): Tox21_111129_1
M4ID: 12483890

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.169 **MAX_MED:** 0.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

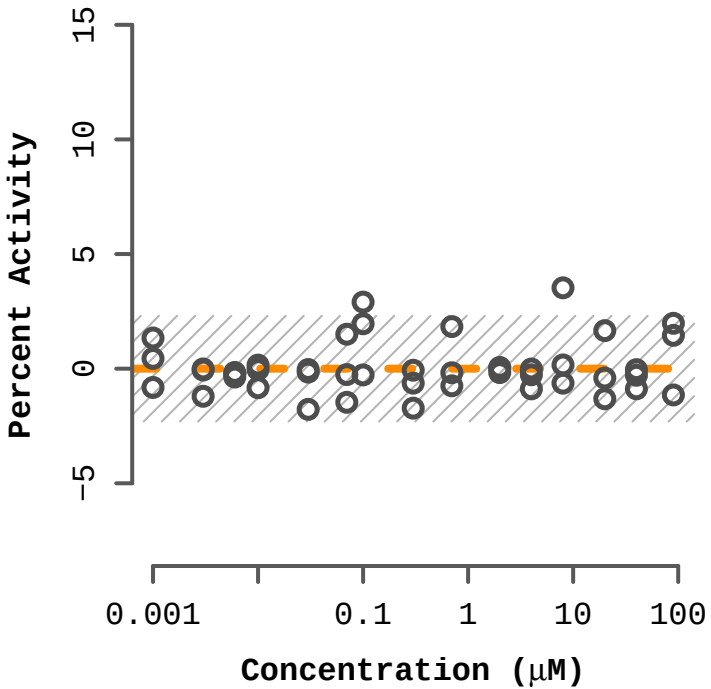
NAME: Dicumarol
CHID: 21729 **CASRN:** 66-76-2
SPID(S): Tox21_110357_1
M4ID: 12484428

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.27	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 0.193 **MAX_MED:** 0.176 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

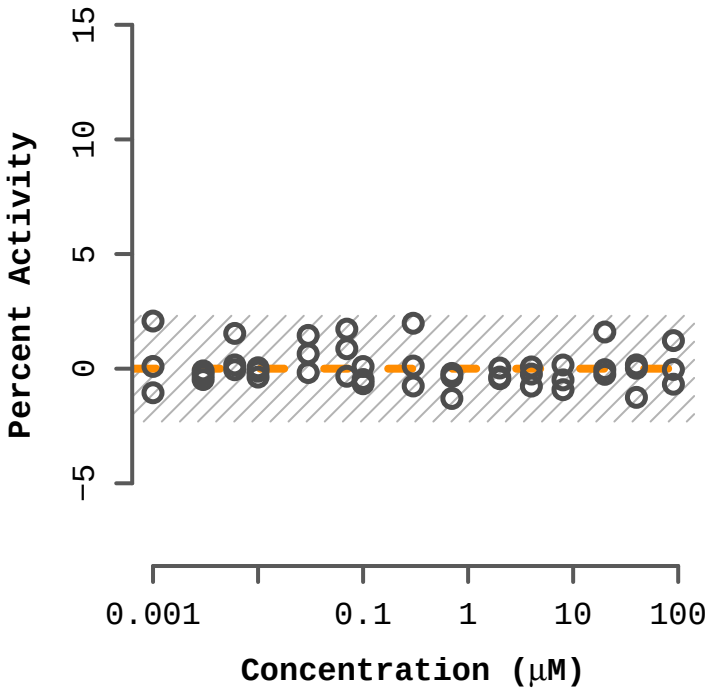
NAME: Methanol
CHID: 21731 **CASRN:** 67-56-1
SPID(S): Tox21_202523
M4ID: 12479729

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

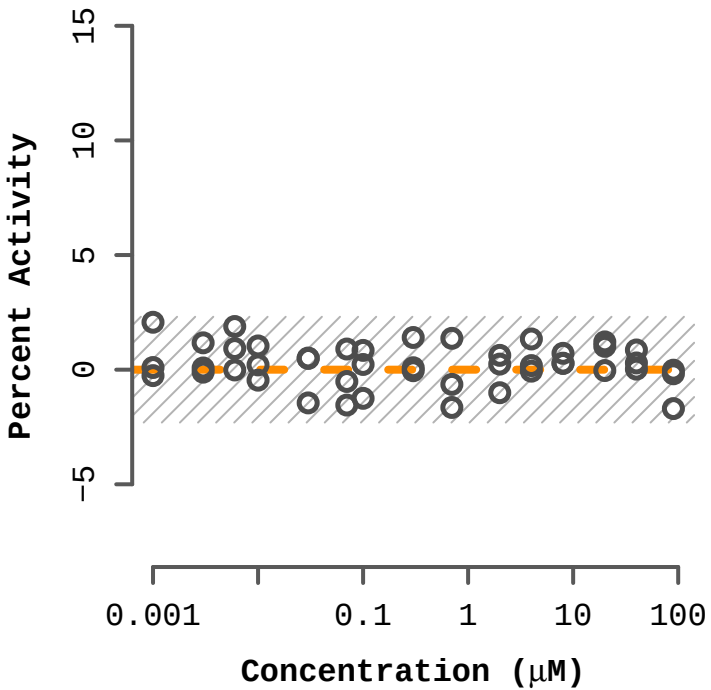
NAME: Dimethyl sulfoxide
CHID: 21735 CASRN: 67-68-5
SPID(S): Tox21_300957
M4ID: 12478176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.756 MAX_MED: 0.871 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

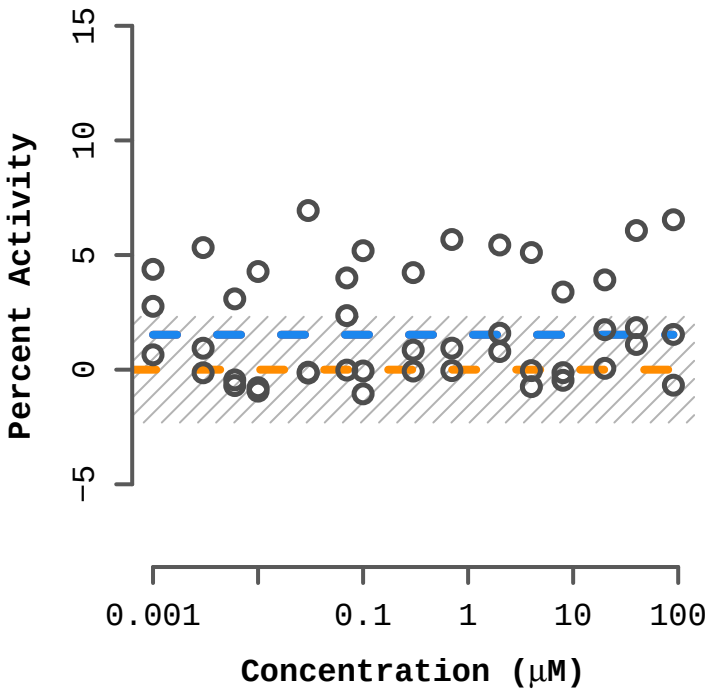
NAME: 1-Propanol
CHID: 21739 **CASRN:** 71-23-8
SPID(S): Tox21_302440
M4ID: 12476693

HILL MODEL: Not applicable.

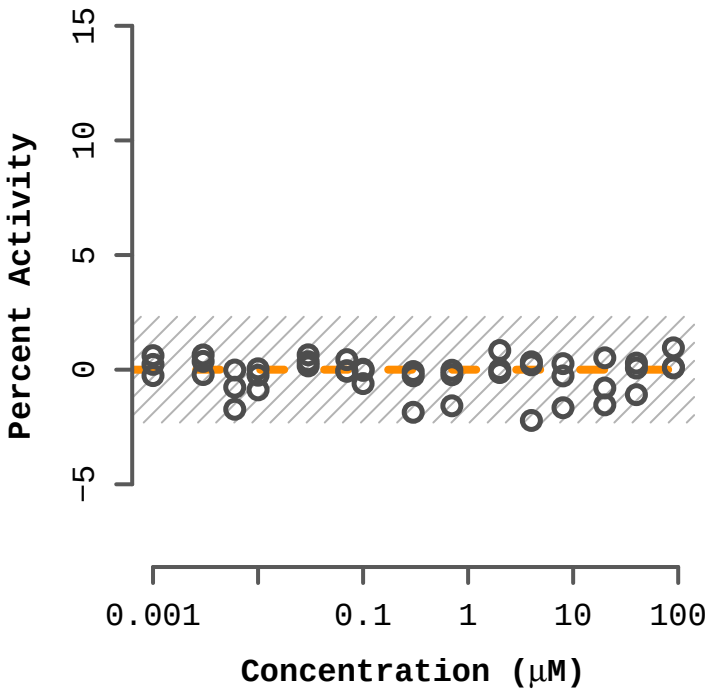
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 1.02 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butanol
CHID:    21740   CASRN: 71-36-3
SPID(S): Tox21_200741
M4ID:    12481511

HILL MODEL (in red):
      tp       ga       gw
val:  1.52     -4.84    3.99
sd:   0.39     1560     3370

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.52     -3.92    7.79     3.36     4.45
sd:   0.39     641      5410     868      2640

      CNST        HILL        GNLS
AIC:  229.49      219.46      223.46
PROB: 0.01        0.88        0.12
RMSE: 3.03        2.41        2.41

MAX_MEAN: 3         MAX_MED: 2.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

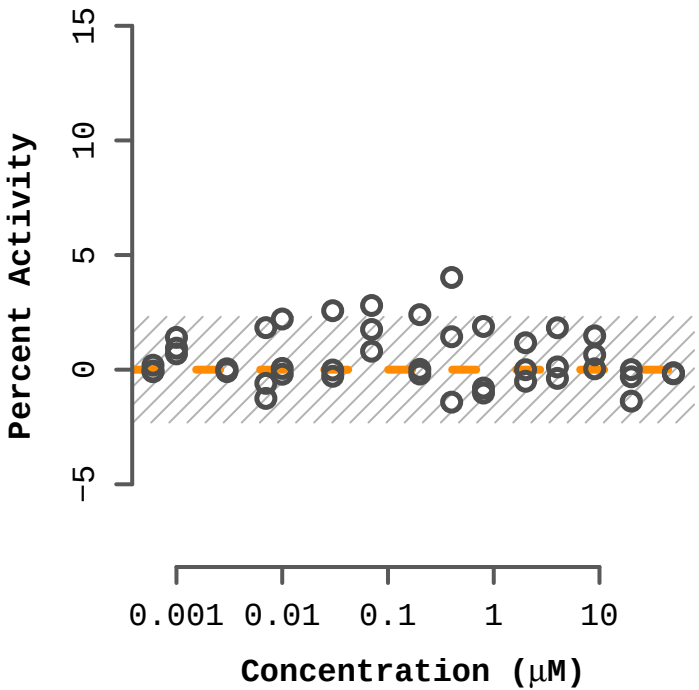
NAME: 1-Pentanol
CHID: 21741 **CASRN:** 71-41-0
SPID(S): Tox21_201107
M4ID: 12481145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.389 **MAX_MED:** 0.363 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

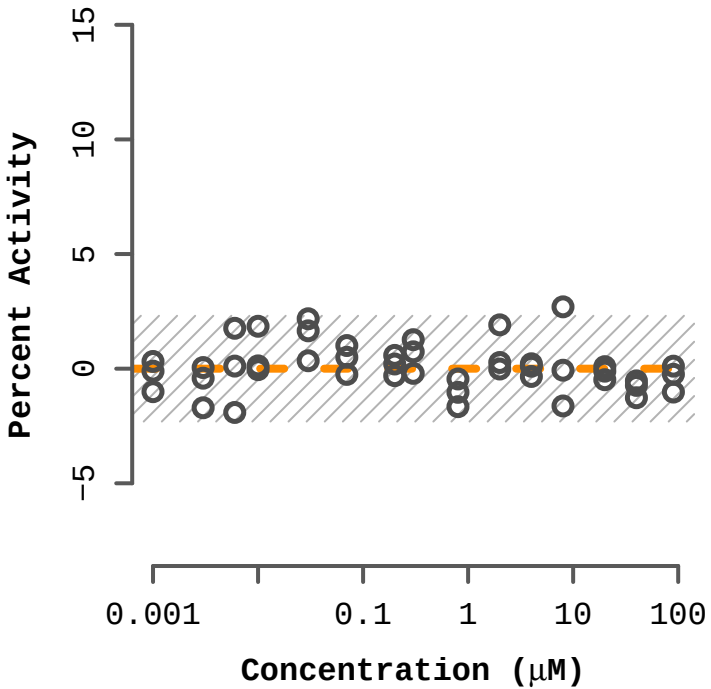
NAME: Thiopental sodium
CHID: 21744 **CASRN:** 71-73-8
SPID(S): Tox21_111741_1
M4ID: 12483508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

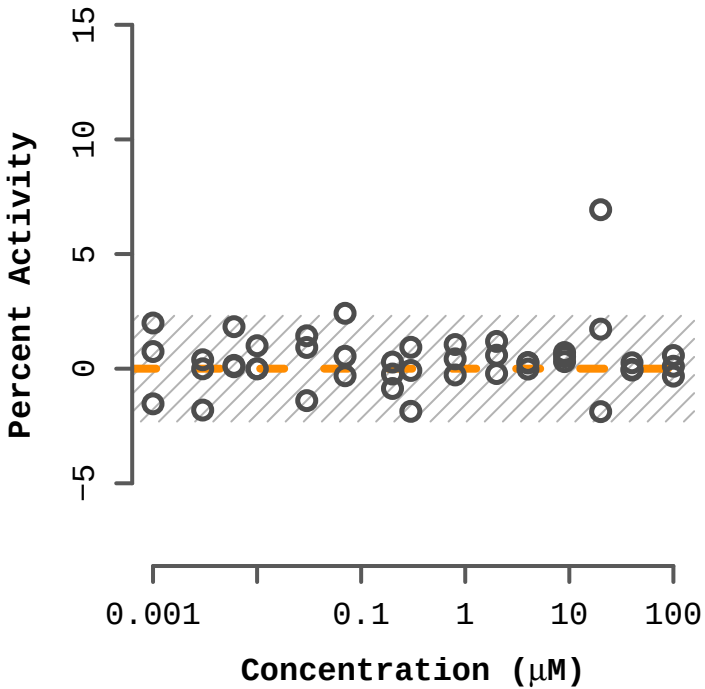
NAME: Tetramethylammonium chloride
CHID: 21749 **CASRN:** 75-57-0
SPID(S): Tox21_200660
M4ID: 12481592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

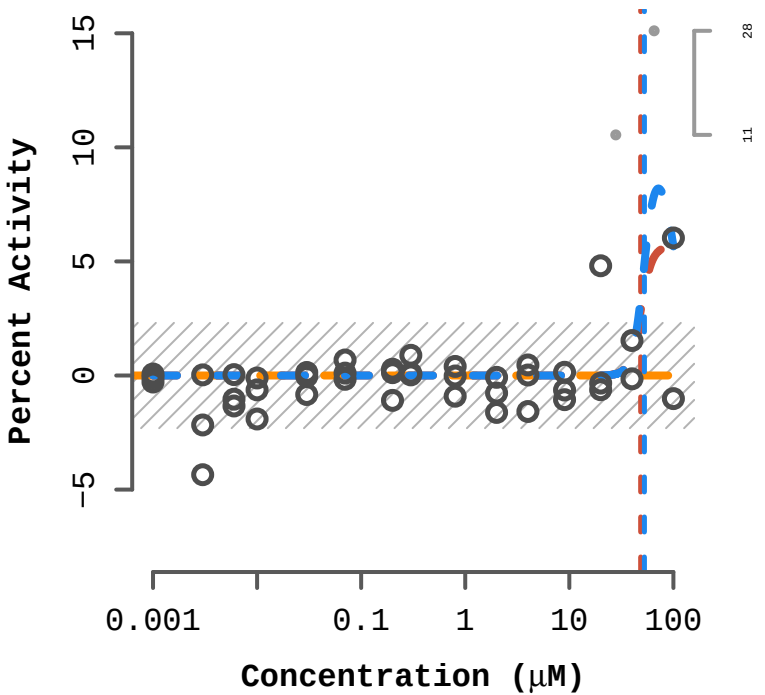
NAME: 2,2,2-Trifluoroethanol
CHID: 21751 **CASRN:** 75-89-8
SPID(S): Tox21_200905
M4ID: 12481347

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.26 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3-Dimethyl-2-butanone
CHID: 21752 CASRN: 75-97-8
SPID(S): Tox21_200060
M4ID: 12482192 BRK

HILL MODEL (in red):

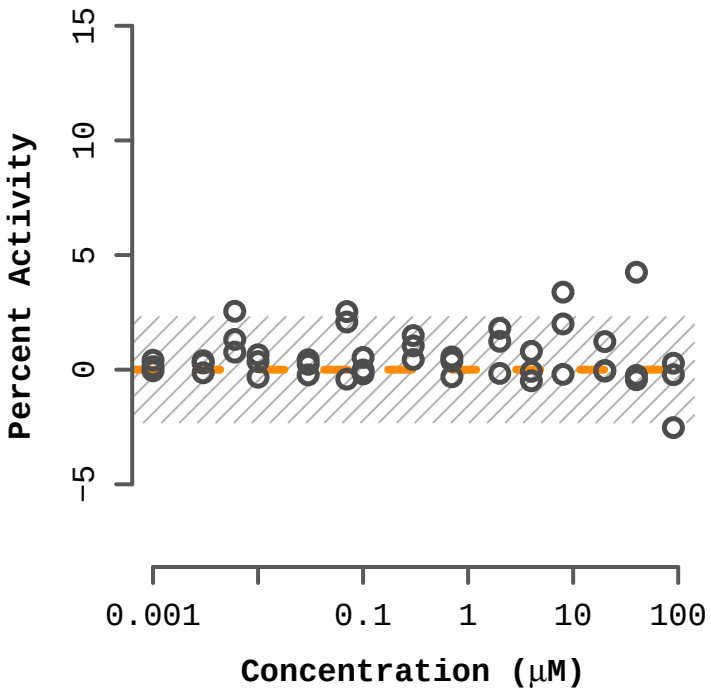
	tp	ga	gw
val:	5.68	1.69	8
sd:	1.82	1.02	95

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10	1.72	7.98	2.02	5.34
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	191.47	193.71	197.71
PROB:	0.73	0.24	0.03
RMSE:	4.79	4.03	4.03

MAX_MEAN: 11.1 MAX_MED: 6.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

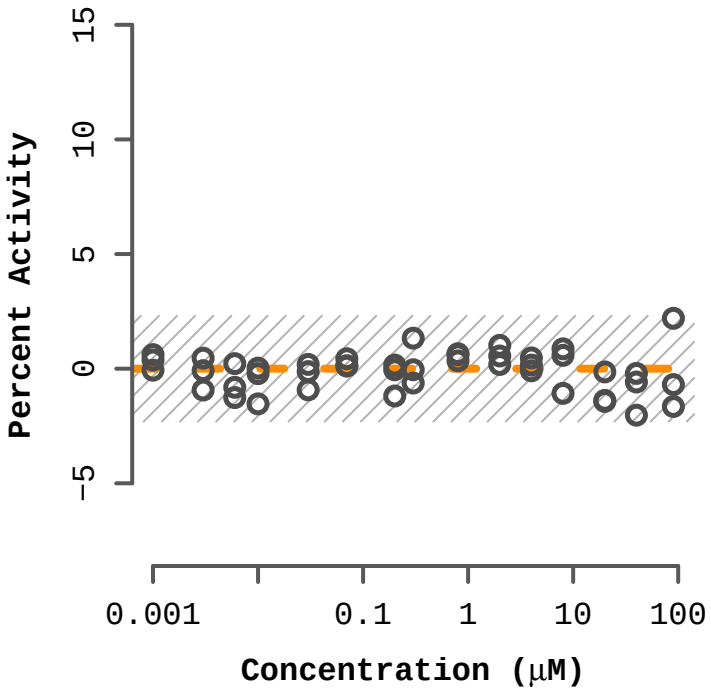
NAME: 5,5-Dimethylhydantoin
CHID: 21754 **CASRN:** 77-71-4
SPID(S): Tox21_300361
M4ID: 12478771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

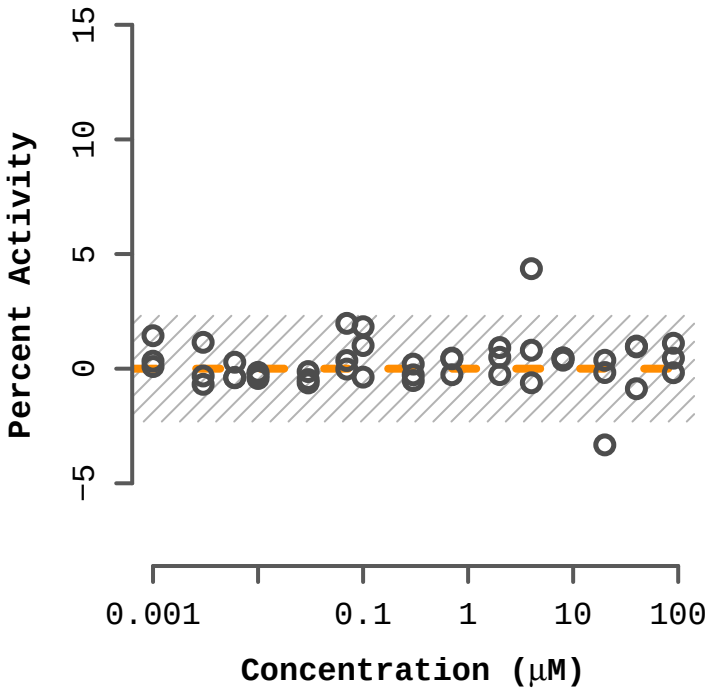
NAME: 5,5-Dimethylhydantoin
CHID: 21754 **CASRN:** 77-71-4
SPID(S): Tox21_202049
M4ID: 12480203

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.606 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

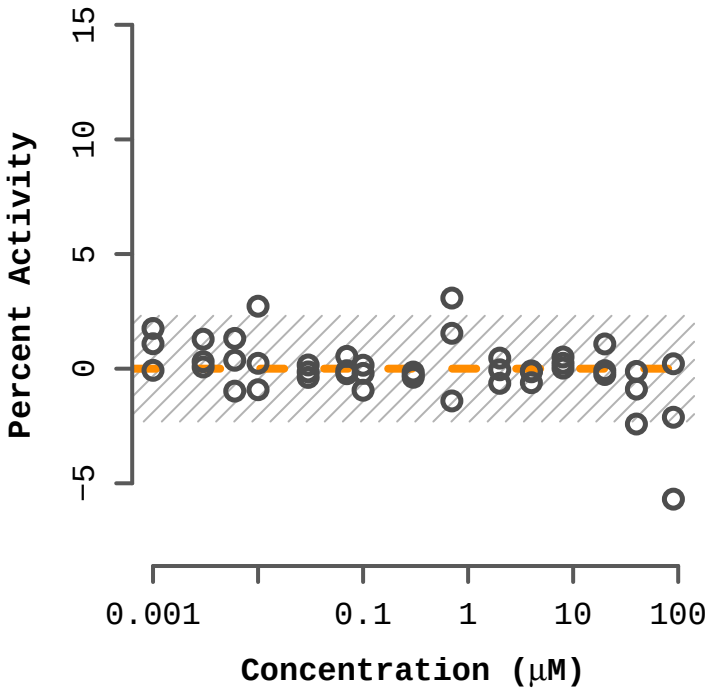
NAME: 1-Ethynylcyclohexanol
CHID: 21757 **CASRN:** 78-27-3
SPID(S): Tox21_302106
M4ID: 12477027

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

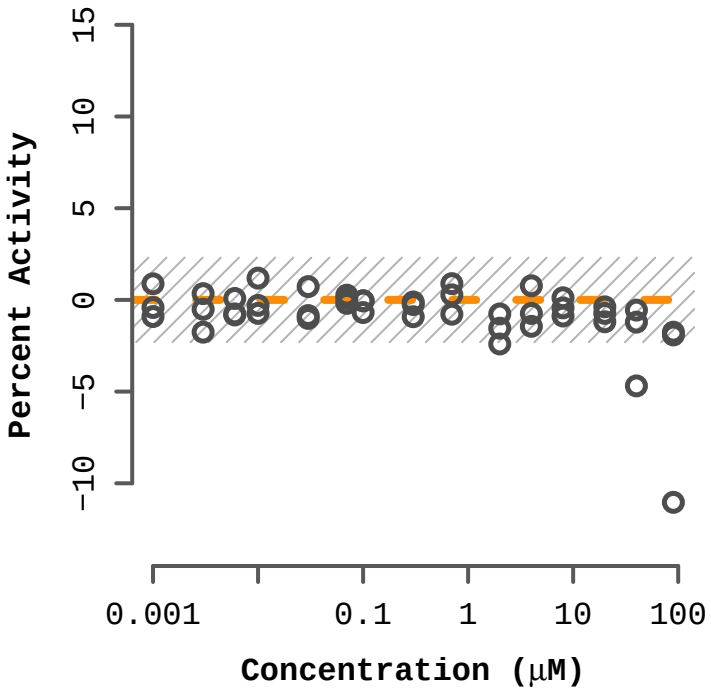
NAME: Tris(2-butoxyethyl) phosphate
CHID: 21758 **CASRN:** 78-51-3
SPID(S): Tox21_302891
M4ID: 12476242

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

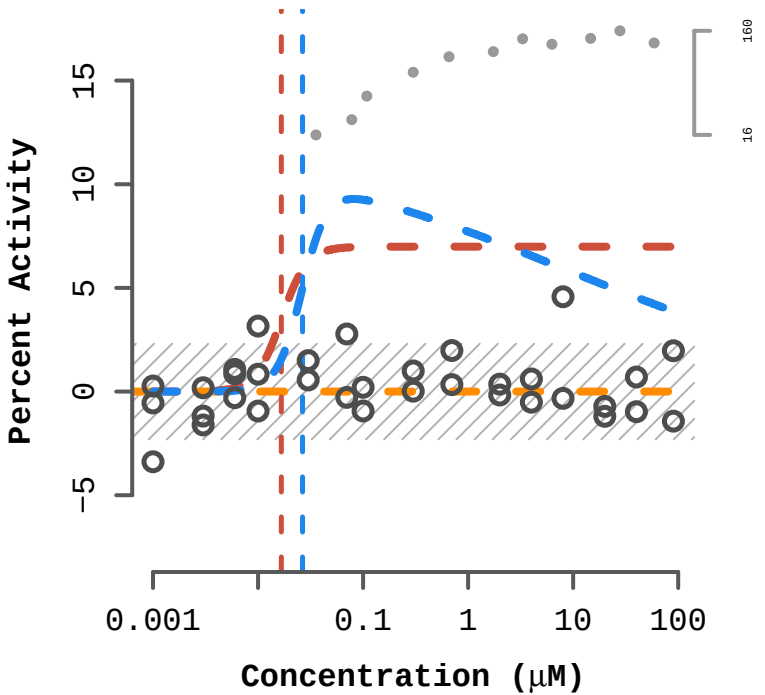
NAME: Tris(2-butoxyethyl) phosphate
CHID: 21758 **CASRN:** 78-51-3
SPID(S): Tox21_201593
M4ID: 12480659

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.88	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 0.129 **MAX_MED:** 0.277 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methyl-1-propanol
CHID: 21759 CASRN: 78-83-1
SPID(S): Tox21_201214
M4ID: 12481038 BRK

HILL MODEL (in red):

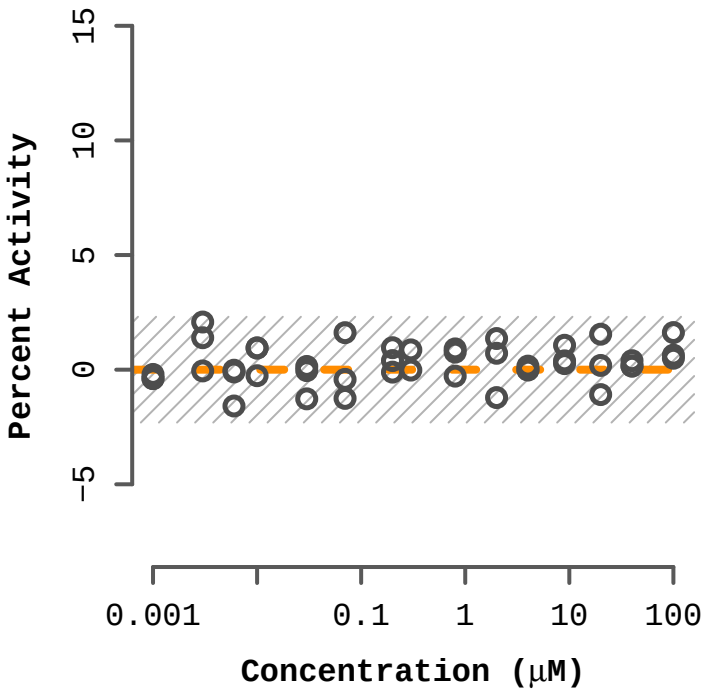
	tp	ga	gw
val:	6.99	-1.78	3.57
sd:	5.38	1.32	14.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.8	-1.58	3.66	0.924	0.3
sd:	87.1	1.69	63.5	24.2	3.25

	CNST	HILL	GNLS
AIC:	472.97	475.62	479.47
PROB:	0.77	0.2	0.03
RMSE:	59.84	56.85	57.16

MAX_MEAN: 53.4 MAX_MED: 4.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

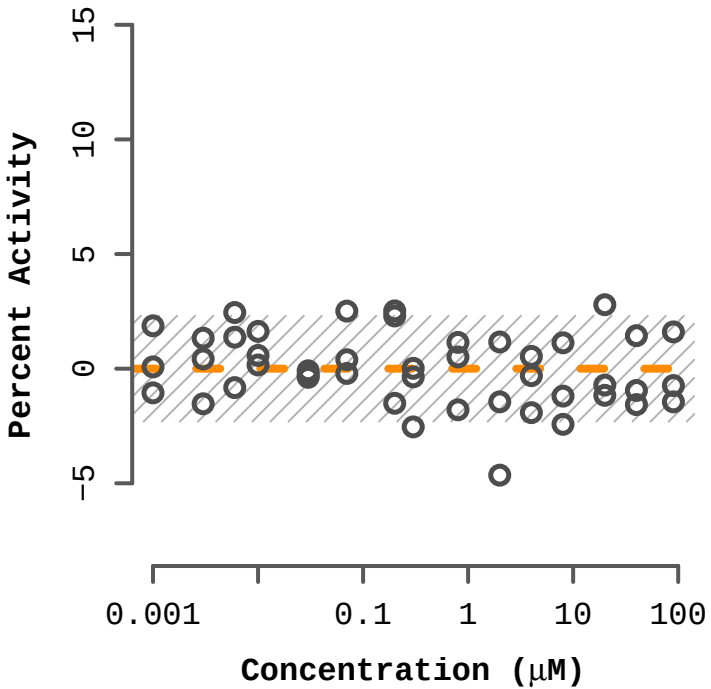
NAME: 1,2−Diaminopropane
CHID: 21761 **CASRN:** 78−90−0
SPID(S): Tox21_202135
M4ID: 12480117

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

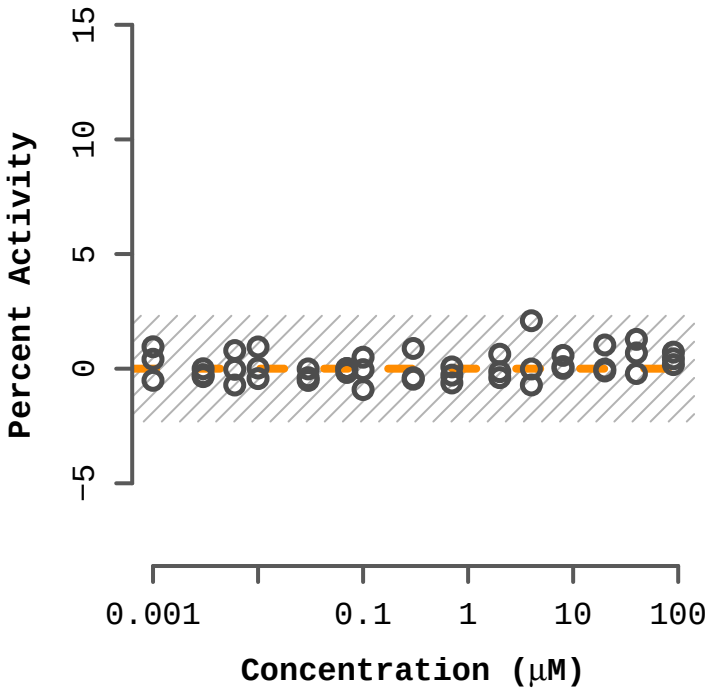
NAME: 2-Butanol
CHID: 21762 **CASRN:** 78-92-2
SPID(S): Tox21_201092
M4ID: 12481160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

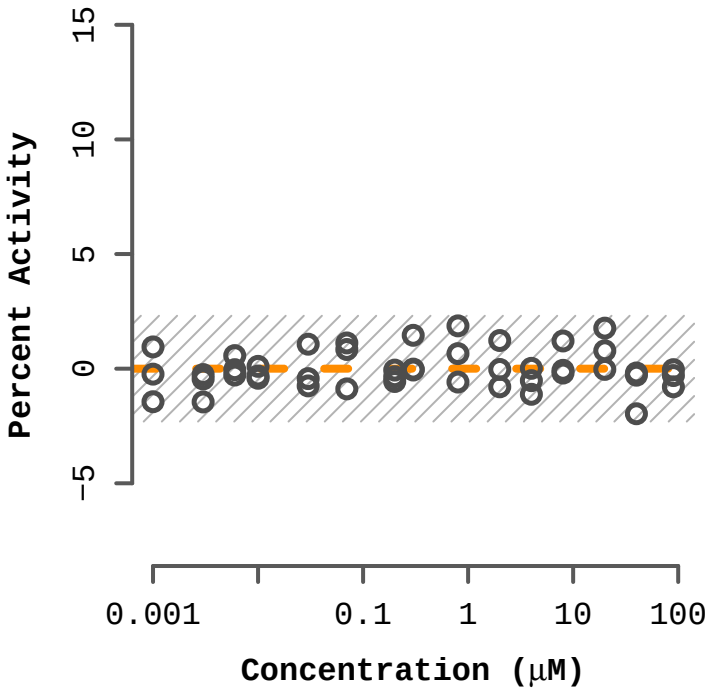
NAME: 1-Amino-2-propanol
CHID: 21764 **CASRN:** 78-96-6
SPID(S): Tox21_301704
M4ID: 12477429

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	83.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.689 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

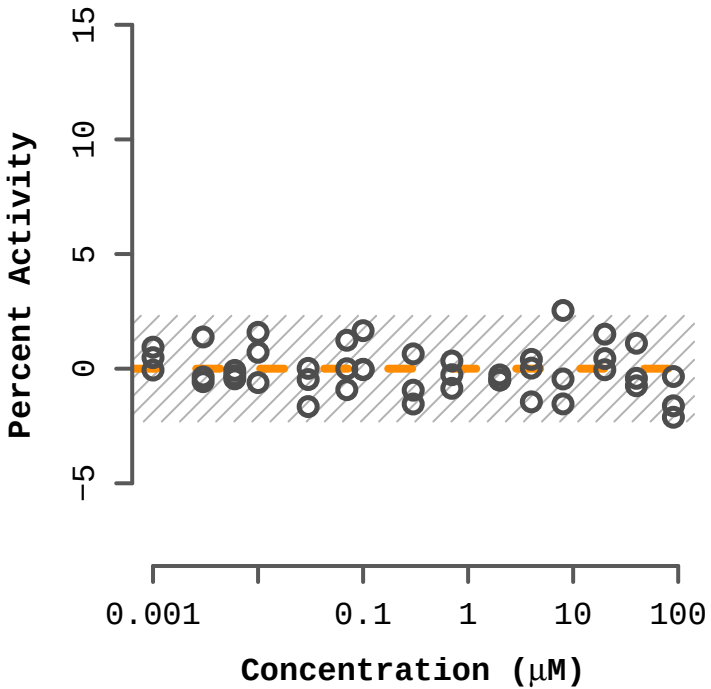
NAME: Methyl acetate
CHID: 21767 CASRN: 79-20-9
SPID(S): Tox21_200057
M4ID: 12482195

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.841 MAX_MED: 0.839 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

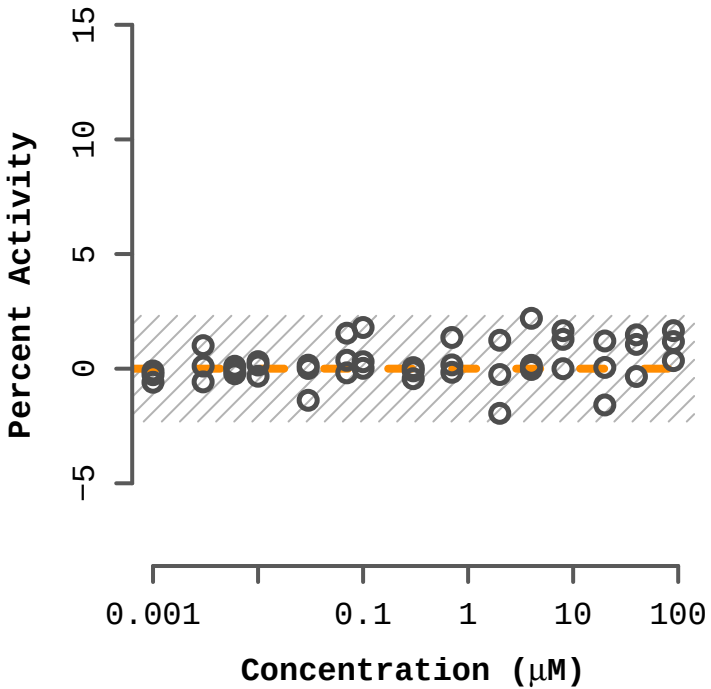
NAME: beta−Ionone
CHID: 21769 **CASRN:** 79−77−6
SPID(S): Tox21_302862
M4ID: 12476271

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.634 **MAX_MED:** 0.715 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

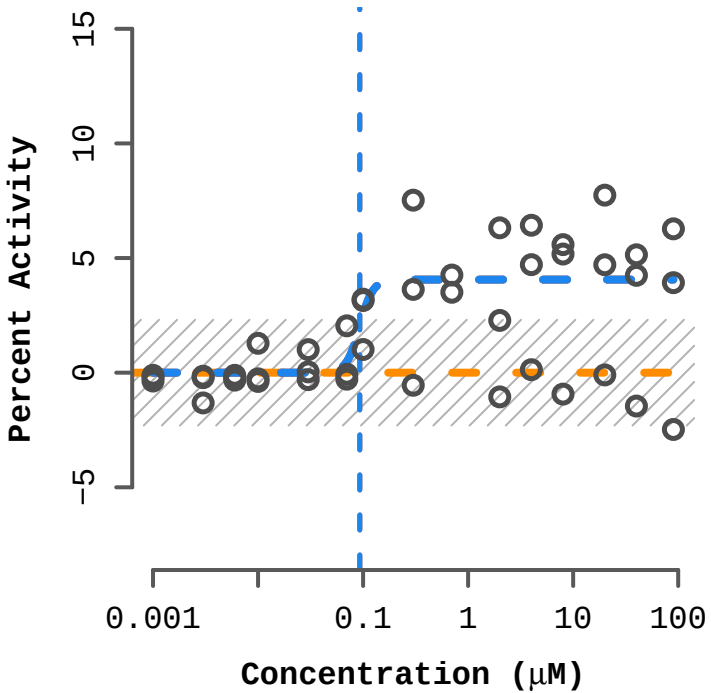
NAME: beta-Ionone
CHID: 21769 **CASRN:** 79-77-6
SPID(S): Tox21_201454
M4ID: 12480798

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2',6,6'−Tetrachlorobisphenol A
CHID: 21770 CASRN: 79−95−8
SPID(S): Tox21_303582
M4ID: 12475563

HILL MODEL (in red):

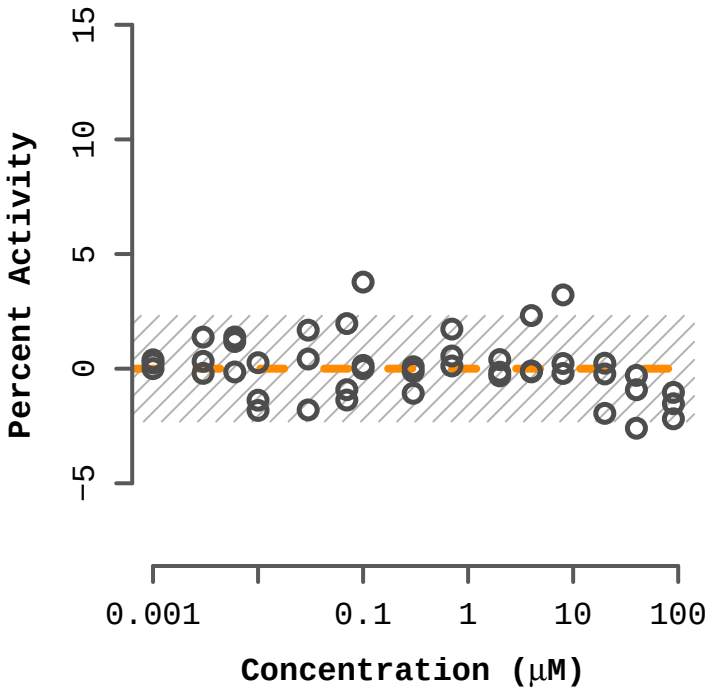
	tp	ga	gw
val:	4.06	−1.03	7
sd:	0.502	0.059	6.93

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.06	−1.03	7	2.97	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	233.21	202.16	206.16
PROB:	0	0.88	0.12
RMSE:	3.34	2.34	2.34

MAX_MEAN: 4.12 MAX_MED: 5.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

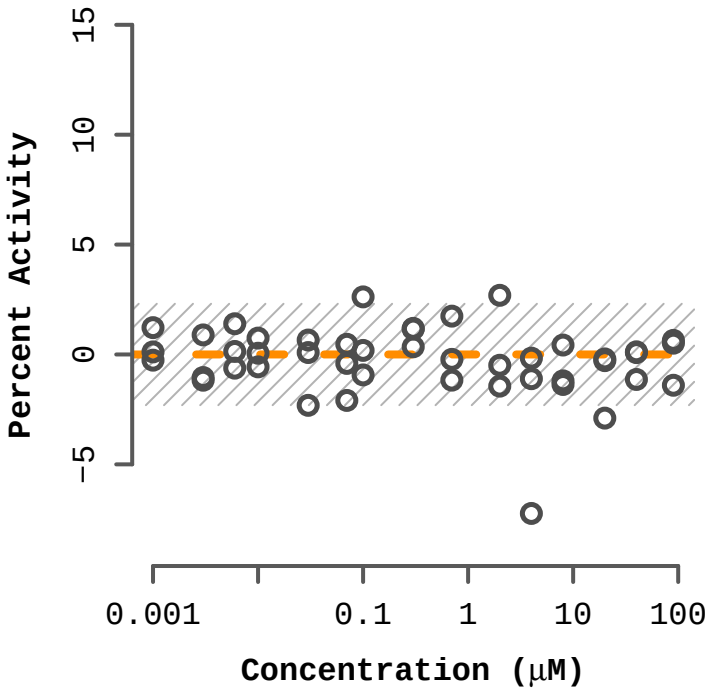
NAME: 2,2',6,6'−Tetrachlorobisphenol A
CHID: 21770 **CASRN:** 79−95−8
SPID(S): Tox21_200557
M4ID: 12481695

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

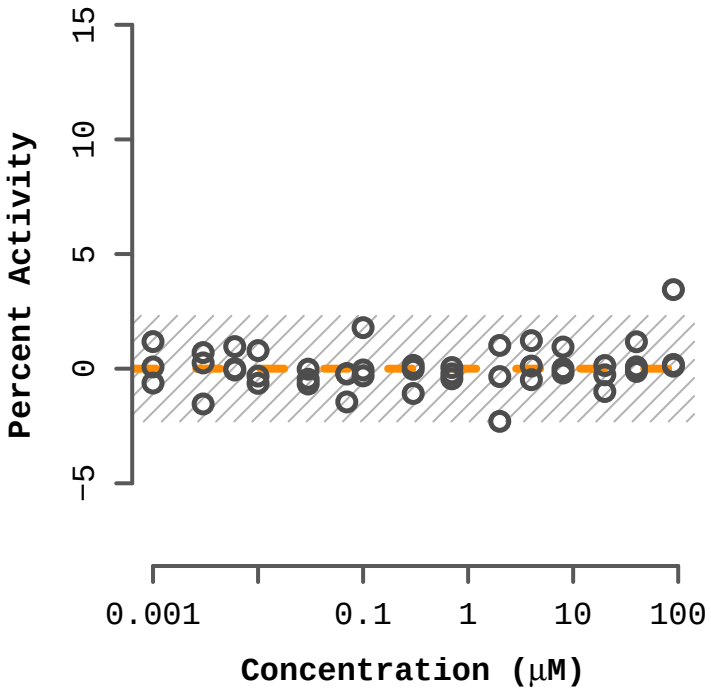
NAME: 4-(2-Methylbutan-2-yl)phenol
CHID: 21771 **CASRN:** 80-46-6
SPID(S): Tox21_300088
M4ID: 12479042

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 0.9 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

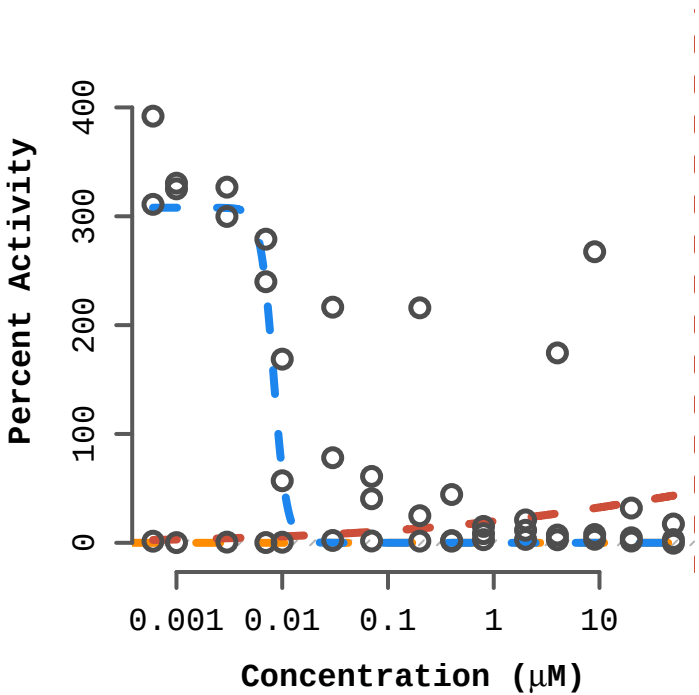
NAME: 4-(2-Methylbutan-2-yl)phenol
CHID: 21771 **CASRN:** 80-46-6
SPID(S): Tox21_202351
M4ID: 12479901

HILL MODEL: Not applicable.

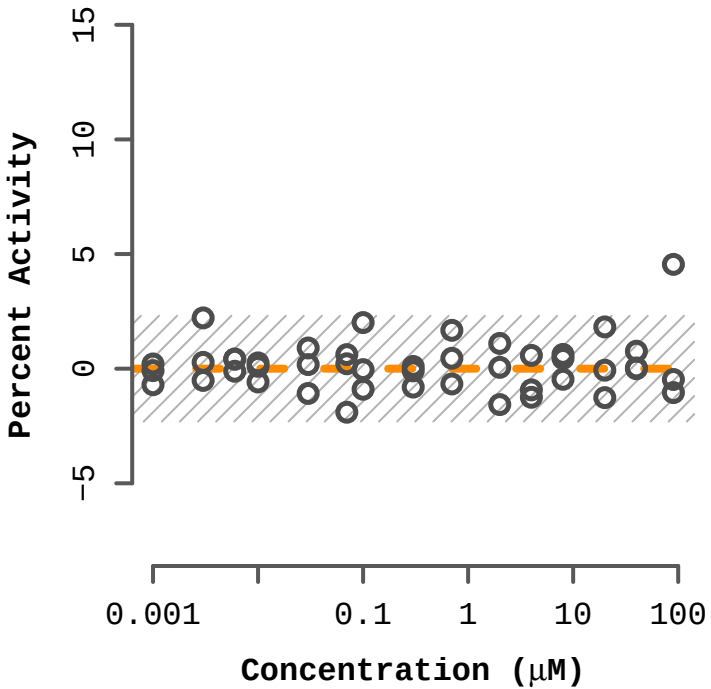
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.253 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-(2-Methylbutan-2-yl)phenol
CHID:    21771   CASRN: 80-46-6
SPID(S): Tox21_111159_1
M4ID:    12483869

HILL MODEL (in red):
      tp       ga       gw
val:  93.8     1.92     0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  308      -5.09    5.92     -2.08    6.97
sd:   24       55400    177000   0.0364   3.25

      CNST       HILL       GNLS
AIC:  574.72     578.22     548.11
PROB: 0          0          1
RMSE: 152.1      148.33     113.03

MAX_MEAN: 235       MAX_MED: 325       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

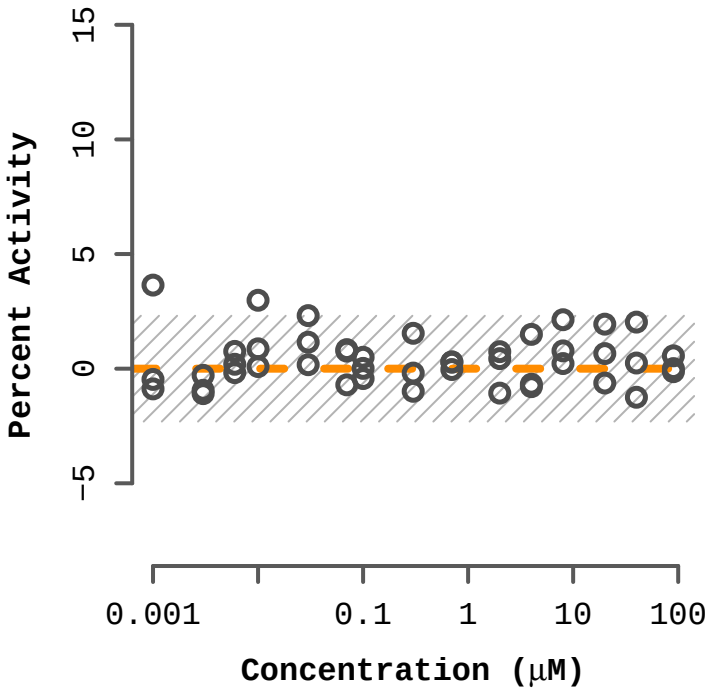
NAME: 1,8-Diamino-p-menthane
CHID: 21772 **CASRN:** 80-52-4
SPID(S): Tox21_201132
M4ID: 12481120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

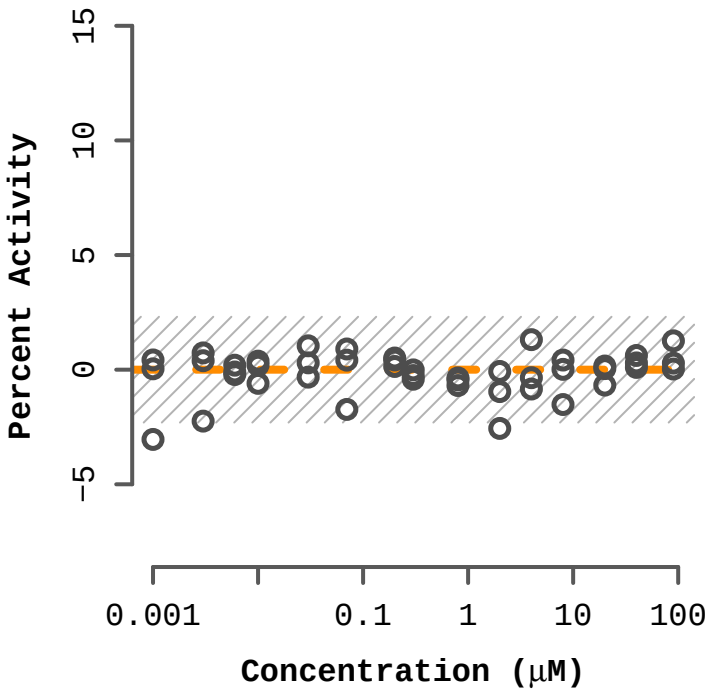
NAME: Acenaphthene
CHID: 21774 **CASRN:** 83-32-9
SPID(S): Tox21_300013
M4ID: 12479117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

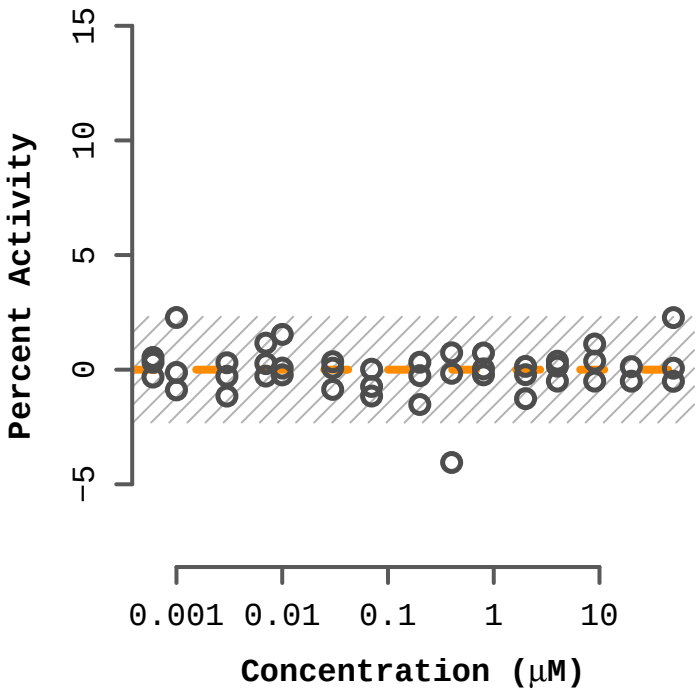
NAME: Acenaphthene
CHID: 21774 **CASRN:** 83-32-9
SPID(S): Tox21_202400
M4ID: 12479852

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.525 **MAX_MED:** 0.423 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

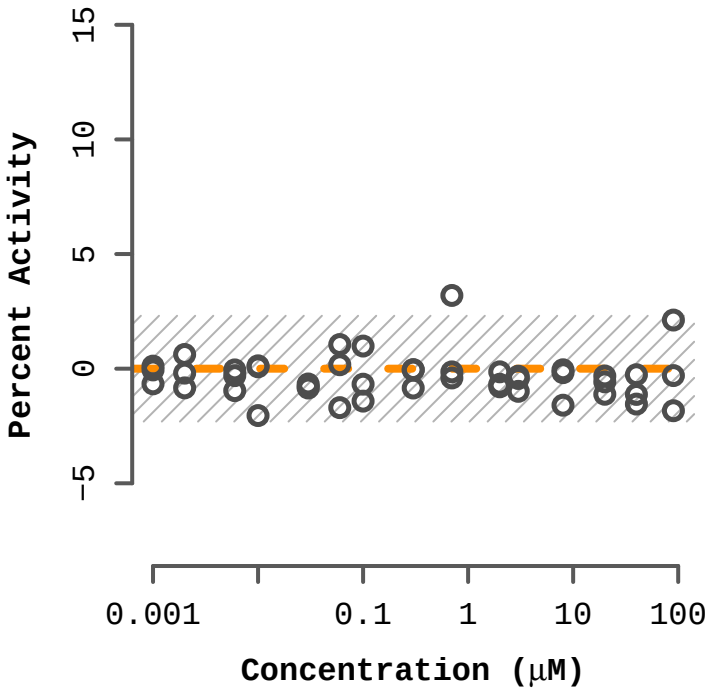
NAME: 3-Methylindole
CHID: 21775 **CASRN:** 83-34-1
SPID(S): Tox21_112537_1
M4ID: 12483038

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.06	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.611 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

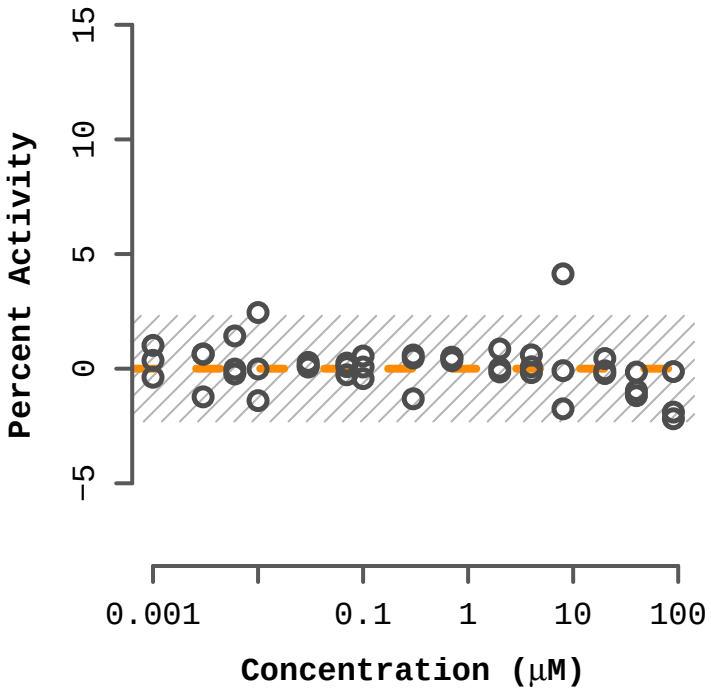
NAME: Riboflavin
CHID: 21777 CASRN: 83-88-5
SPID(S): Tox21_302980
M4ID: 12476153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.43	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.885 **MAX_MED:** 0.173 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

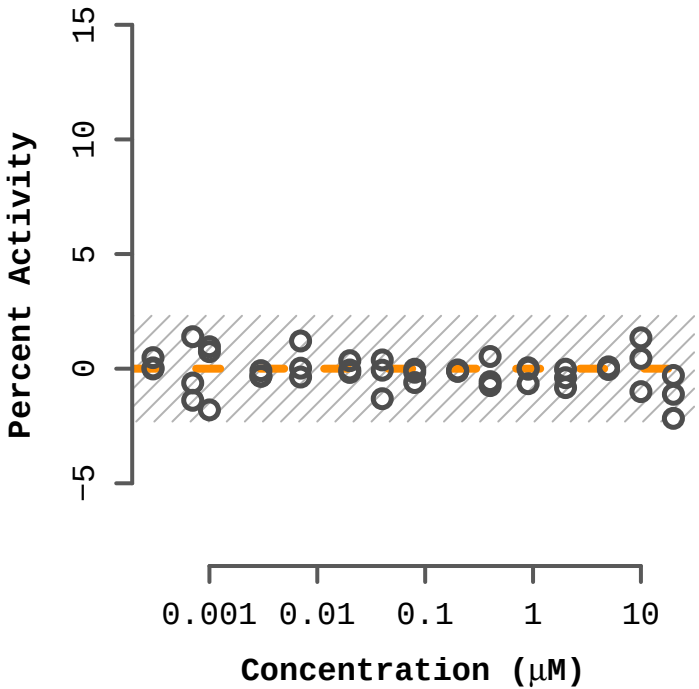
NAME: Riboflavin
CHID: 21777 CASRN: 83-88-5
SPID(S): Tox21_201633
M4ID: 12480619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.768 MAX_MED: 0.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

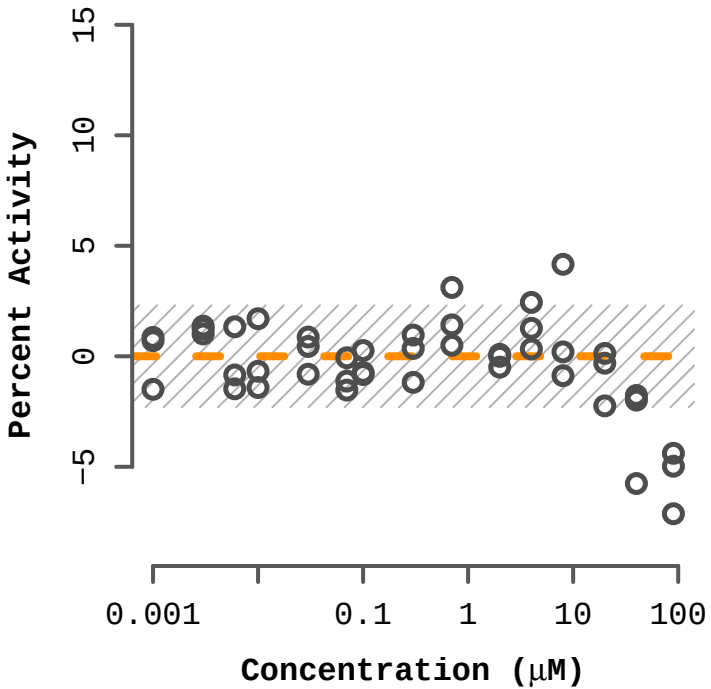
NAME: Riboflavin
CHID: 21777 **CASRN:** 83-88-5
SPID(S): Tox21_111714_1
M4ID: 12483522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.29 **MAX_MED:** 0.745 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

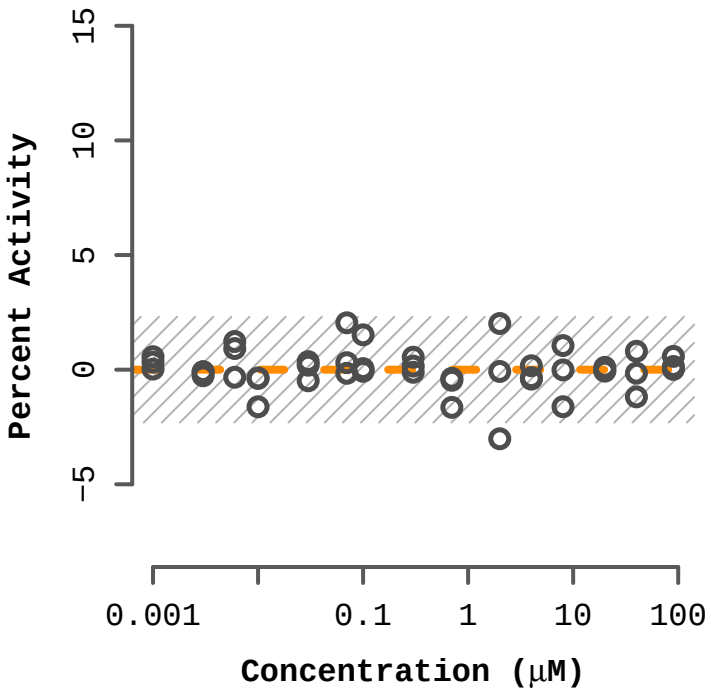
NAME: Diphenyl phthalate
CHID: 21778 **CASRN:** 84-62-8
SPID(S): Tox21_300937
M4ID: 12478196

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

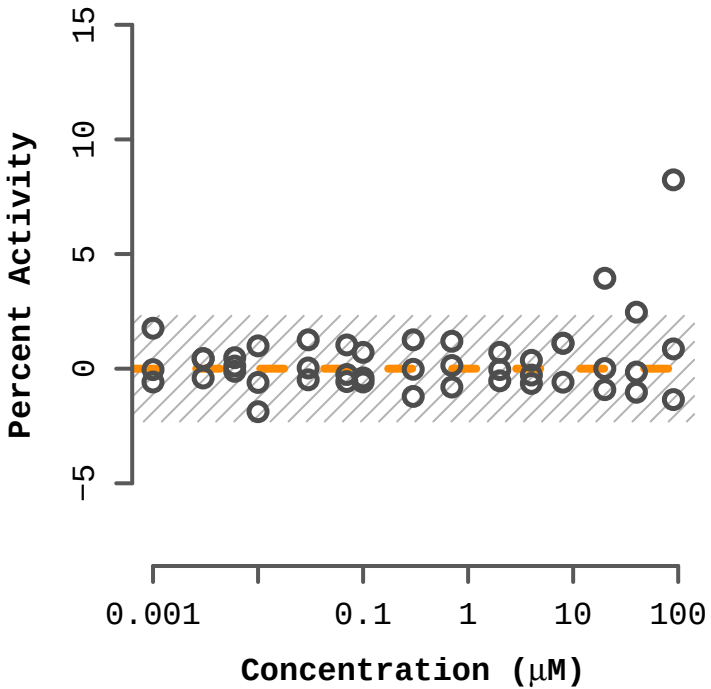
NAME: Diethyl phthalate
CHID: 21780 **CASRN:** 84-66-2
SPID(S): Tox21_300183
M4ID: 12478947

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.732 **MAX_MED:** 0.922 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

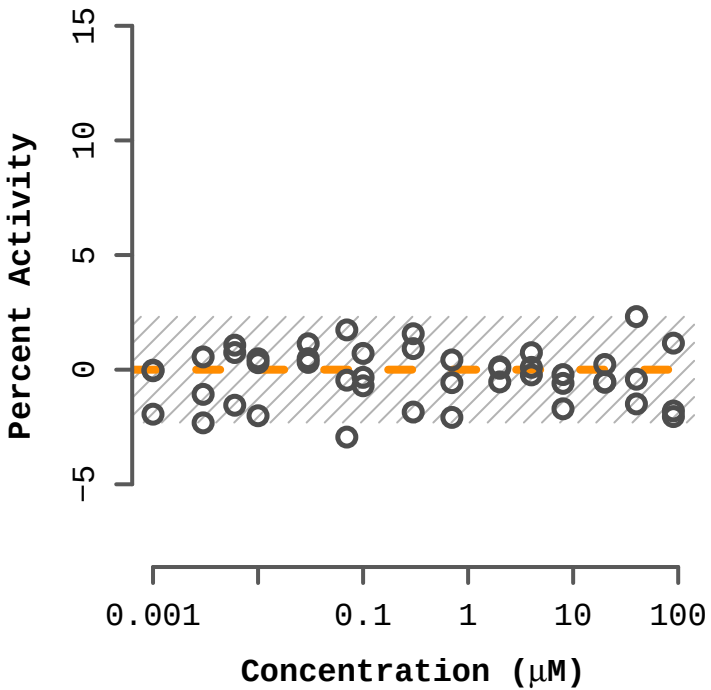
NAME: Diethyl phthalate
CHID: 21780 **CASRN:** 84-66-2
SPID(S): Tox21_201874
M4ID: 12480378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.59 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

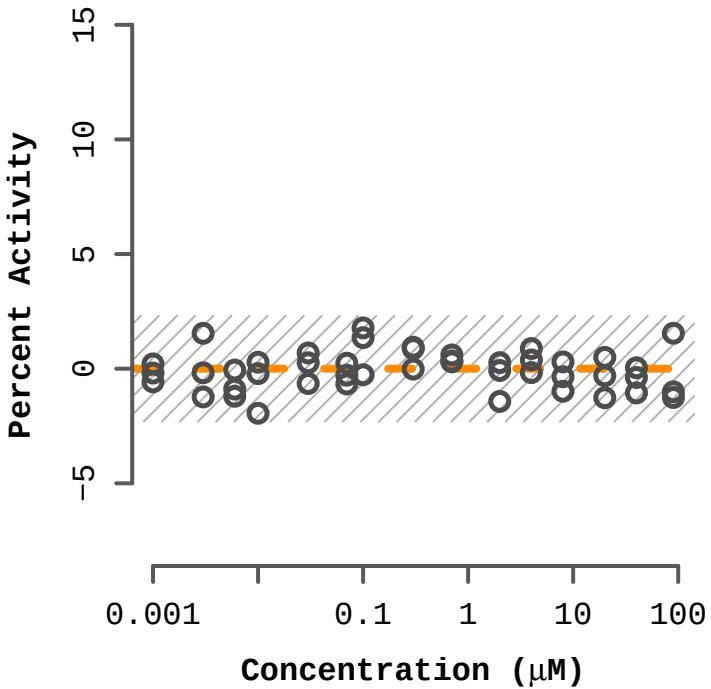
NAME: Dibutyl phthalate
CHID: 21781 **CASRN:** 84-74-2
SPID(S): Tox21_300980
M4ID: 12478153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.645 **MAX_MED:** 0.921 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

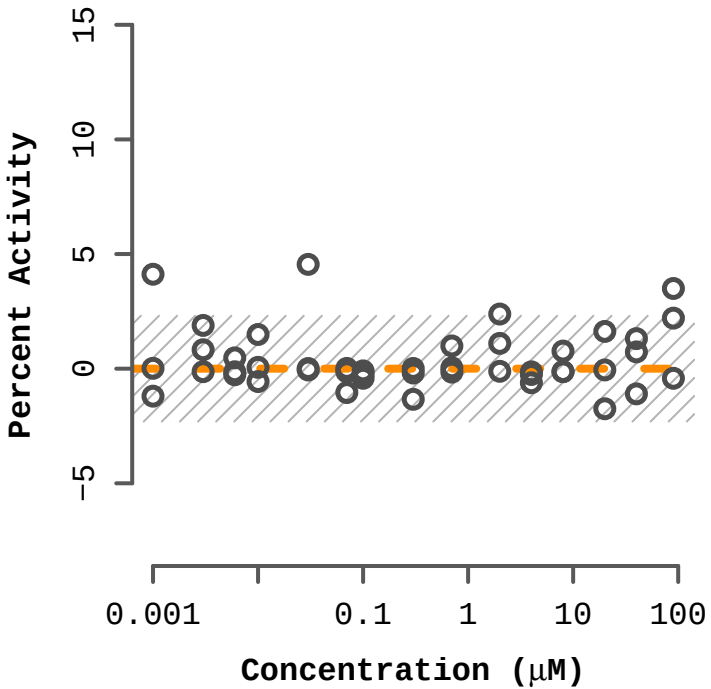
NAME: Dibutyl phthalate
CHID: 21781 **CASRN:** 84-74-2
SPID(S): Tox21_201729
M4ID: 12480523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

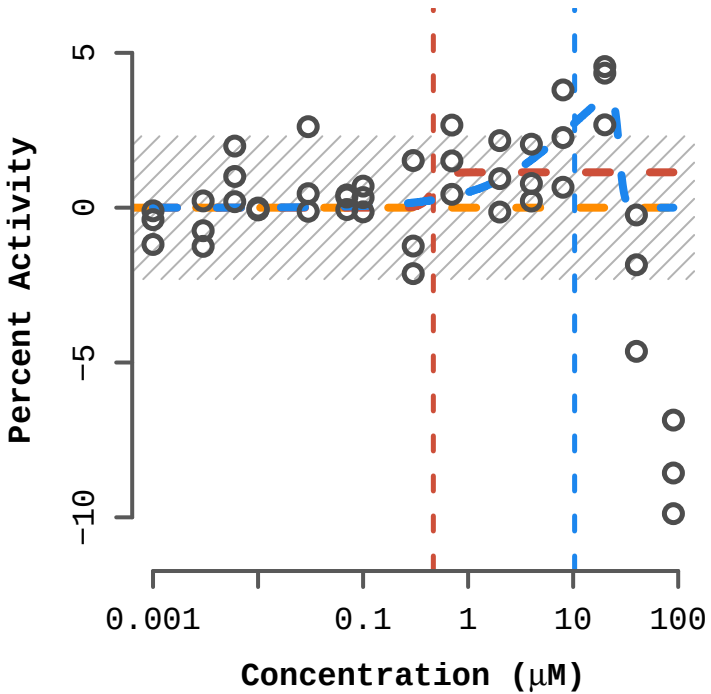
NAME: 2,3,4,5,6-Pentabromoethylbenzene
CHID: 21782 **CASRN:** 85-22-3
SPID(S): Tox21_303981
M4ID: 12475207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Salicylanilide
CHID: 21784 **CASRN:** 87-17-2
SPID(S): Tox21_301301
M4ID: 12477832

HILL MODEL (in red):

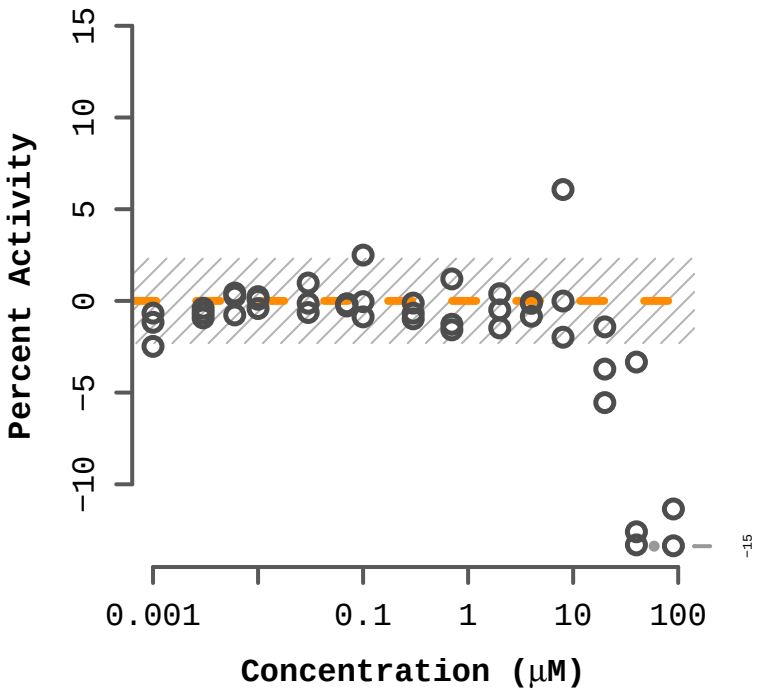
	tp	ga	gw
val:	1.14	−0.331	8
sd:	0.444	0.252	10.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.47	1.01	0.984	1.44	17.9
sd:	3.12	0.54	0.681	0.183	21.5

	CNST	HILL	GNLS
AIC:	209.12	209.46	196.6
PROB:	0	0	1
RMSE:	2.81	2.94	2.53

MAX_MEAN: 3.86 **MAX_MED:** 4.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

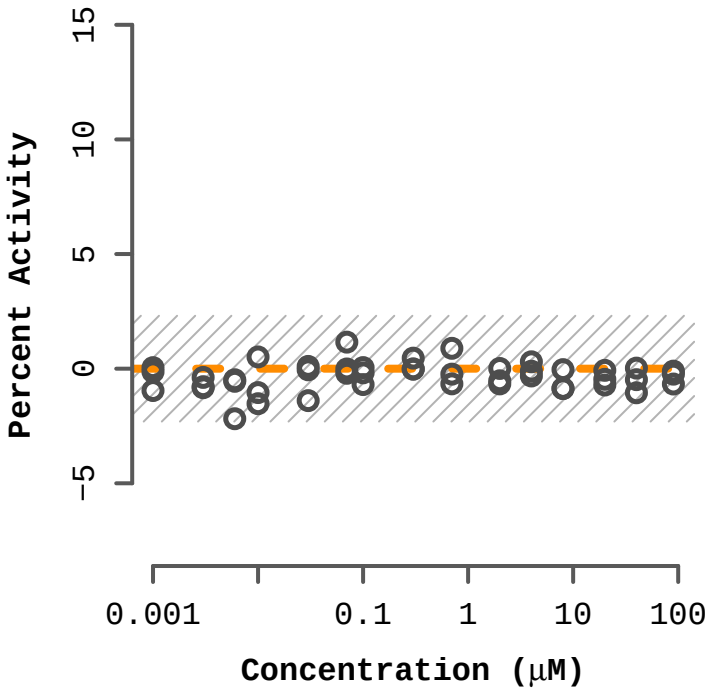
NAME: 3-Trifluoromethyl-4-nitrophenol
CHID: 21788 **CASRN:** 88-30-2
SPID(S): Tox21_300905
M4ID: 12478228 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	240.99	NA	NA
PROB:	1	NA	NA
RMSE:	4.69	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.262 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

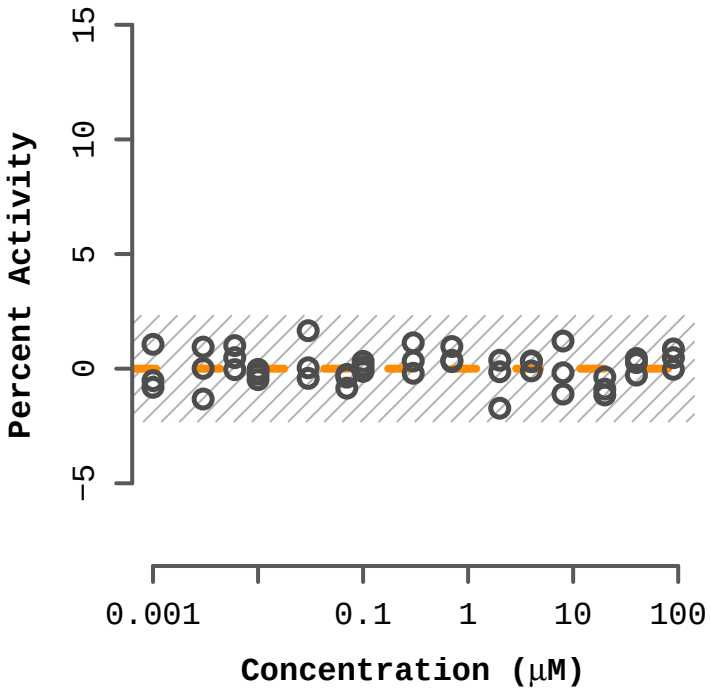
NAME: 2-Aminobenzamide
CHID: 21789 **CASRN:** 88-68-6
SPID(S): Tox21_200412
M4ID: 12481840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.316 **MAX_MED:** −0.00672 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

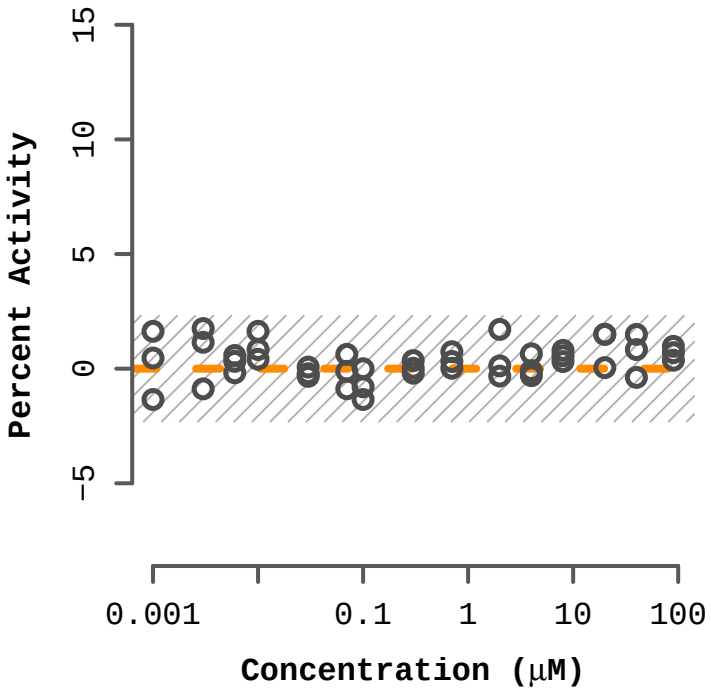
NAME: 2-Nitrophenol
CHID: 21790 **CASRN:** 88-75-5
SPID(S): Tox21_302758
M4ID: 12476375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.482 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

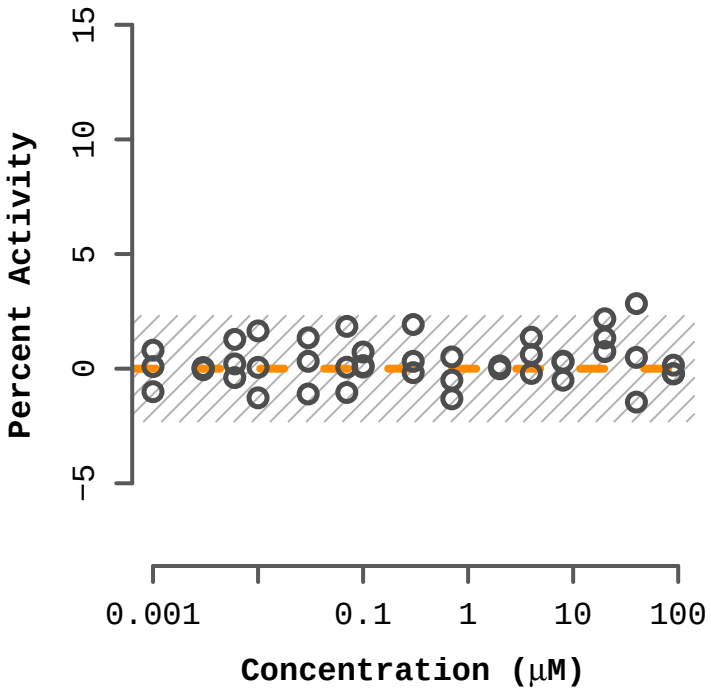
NAME: 2-Nitrophenol
CHID: 21790 **CASRN:** 88-75-5
SPID(S): Tox21_201442
M4ID: 12480810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

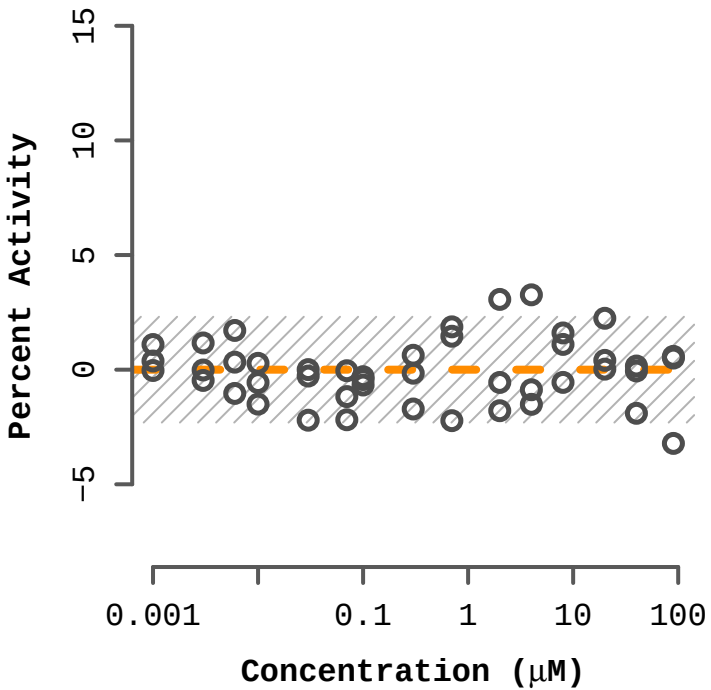
NAME: Salicylaldehyde
CHID: 21792 **CASRN:** 90-02-8
SPID(S): Tox21_302929
M4ID: 12476204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

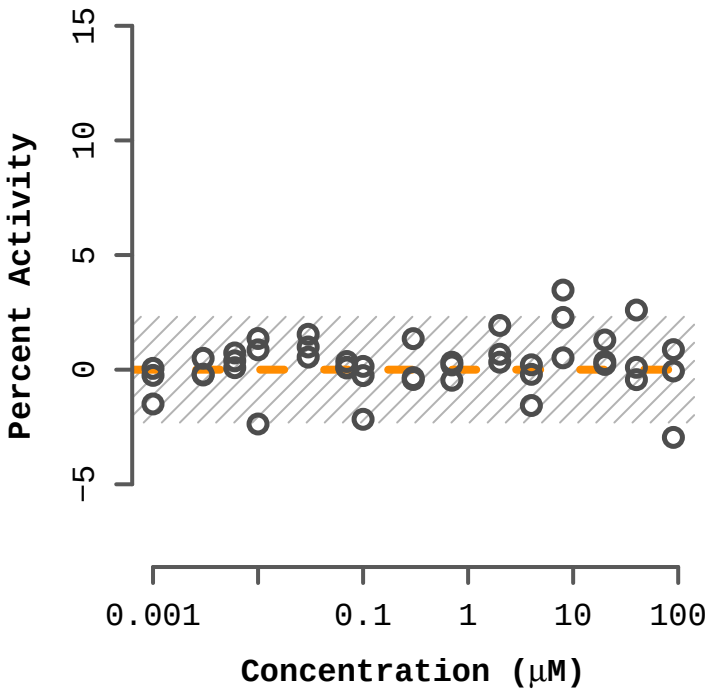
NAME: Salicylaldehyde
CHID: 21792 **CASRN:** 90-02-8
SPID(S): Tox21_201737
M4ID: 12480515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

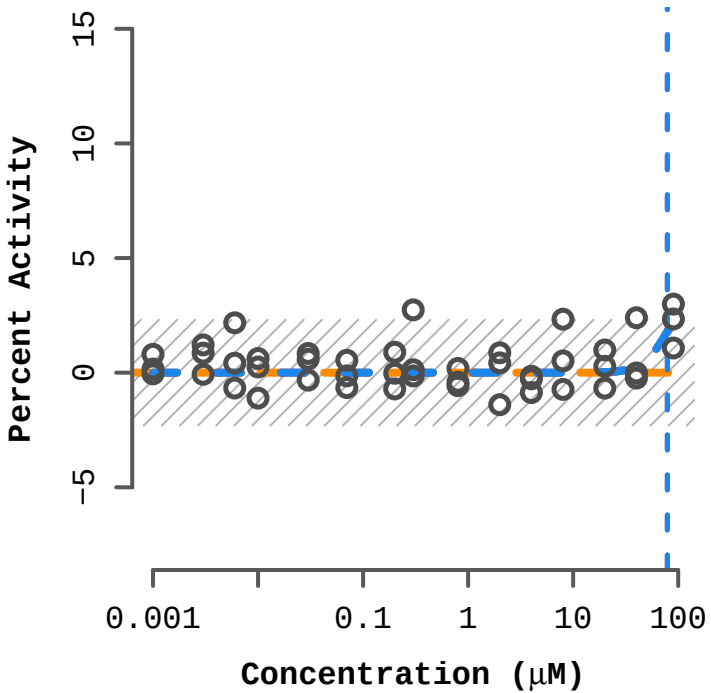
NAME: 1-Naphthol
CHID: 21793 **CASRN:** 90-15-3
SPID(S): Tox21_302768
M4ID: 12476365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Naphthol
CHID: 21793 **CASRN:** 90-15-3
SPID(S): Tox21_202120
M4ID: 12480132

HILL MODEL (in red):

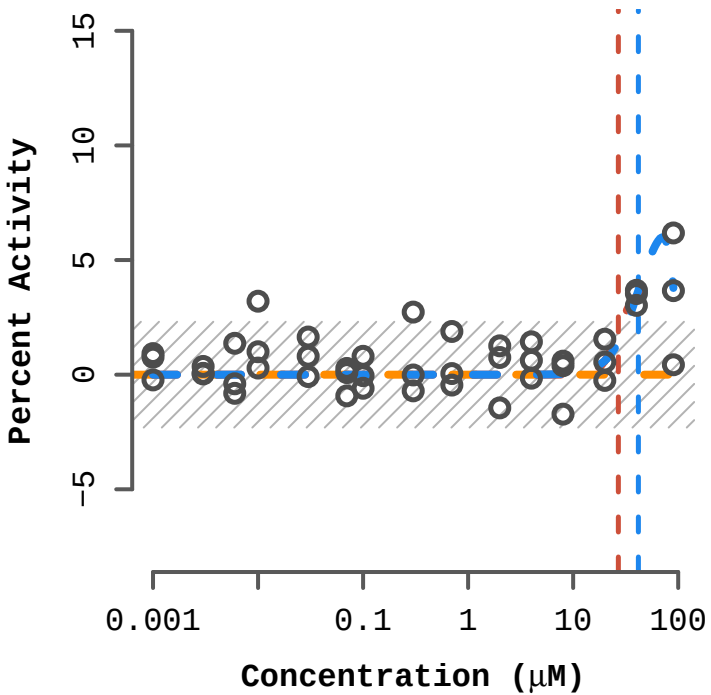
	tp	ga	gw
val:	3.59	1.9	3.72
sd:	14.9	1.14	9.65

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.59	1.9	3.72	3.31	4.41
sd:	14.9	1.14	9.66	1240	4060

	CNST	HILL	GNLS
AIC:	134.39	127.37	131.37
PROB:	0.03	0.86	0.12
RMSE:	1.1	0.94	0.94

MAX_MEAN: 2.14 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Xanthone
CHID: 21795 **CASRN:** 90-47-1
SPID(S): Tox21_301151
M4ID: 12477982

HILL MODEL (in red):

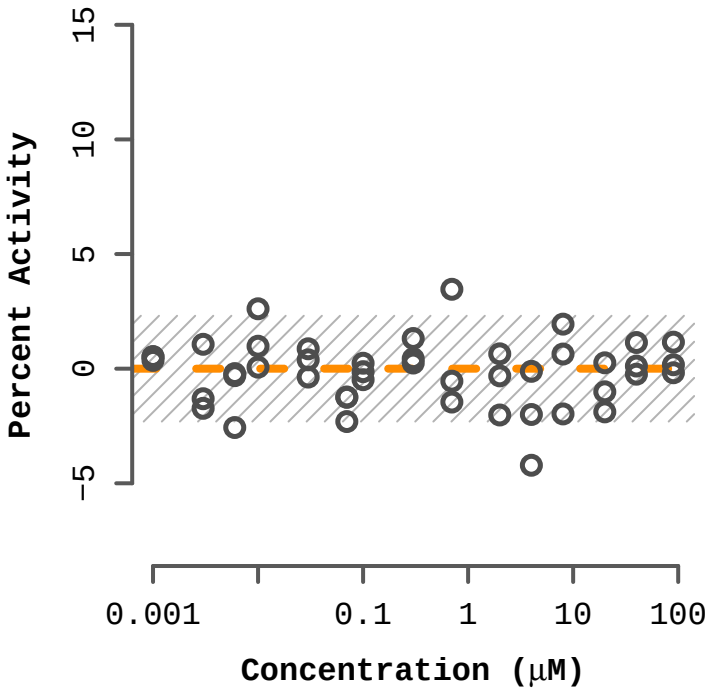
	tp	ga	gw
val:	3.79	1.43	5.62
sd:	0.897	0.114	4.05

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.36	1.62	3.25	1.96	12.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	169.74	145.88	149.87
PROB:	0	0.88	0.12
RMSE:	1.72	1.17	1.17

MAX_MEAN: 3.43 **MAX_MED:** 3.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

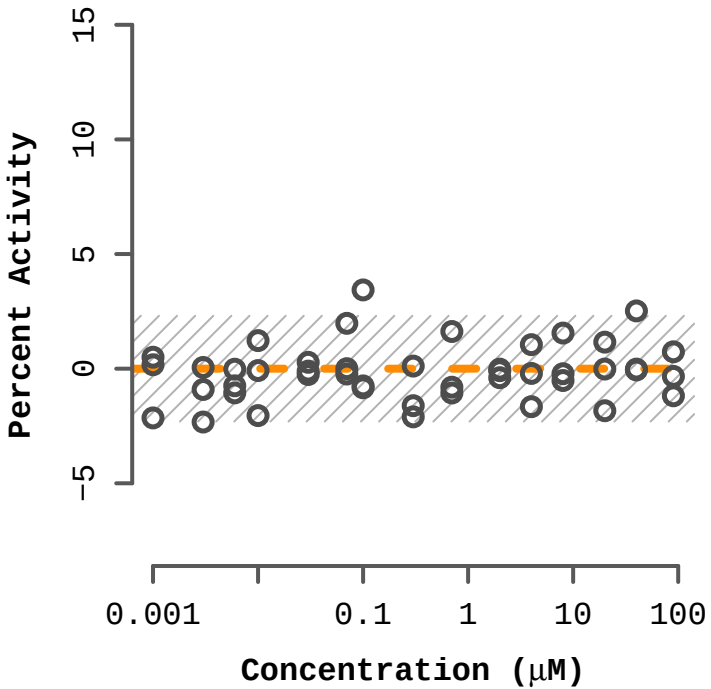
NAME: Quinoline
CHID: 21798 CASRN: 91-22-5
SPID(S): Tox21_300068
M4ID: 12479062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

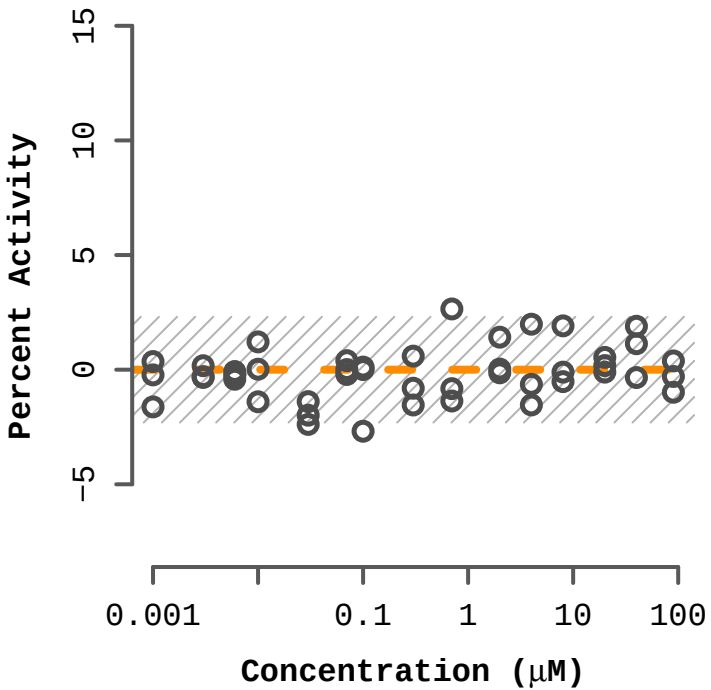
NAME: Quinoline
CHID: 21798 **CASRN:** 91-22-5
SPID(S): Tox21_201478
M4ID: 12480774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.816 **MAX_MED:** 0.172 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

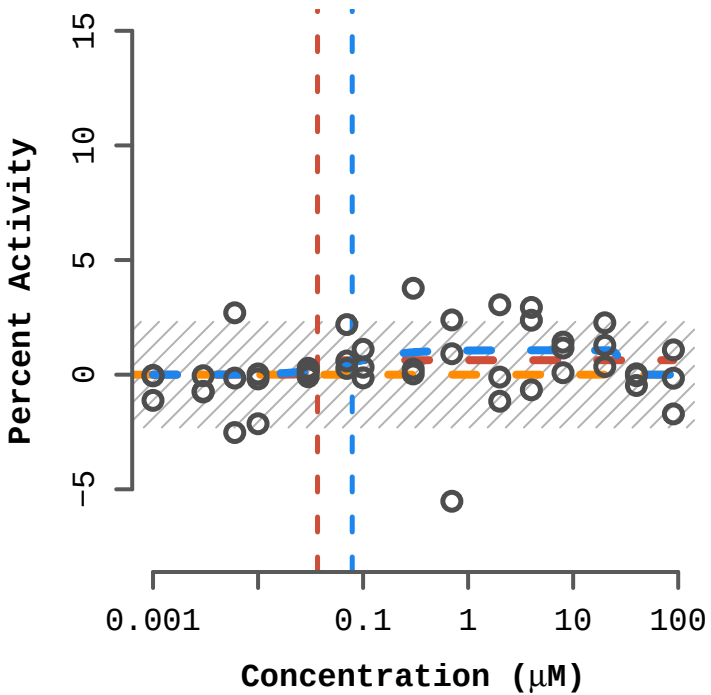
NAME: N,N−Diethylcyclohexylamine
CHID: 21799 **CASRN:** 91−65−6
SPID(S): Tox21_301799
M4ID: 12477334

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N,N−Diethylaniline
CHID: 21800 CASRN: 91−66−7
SPID(S): Tox21_300569
M4ID: 12478564

HILL MODEL (in red):

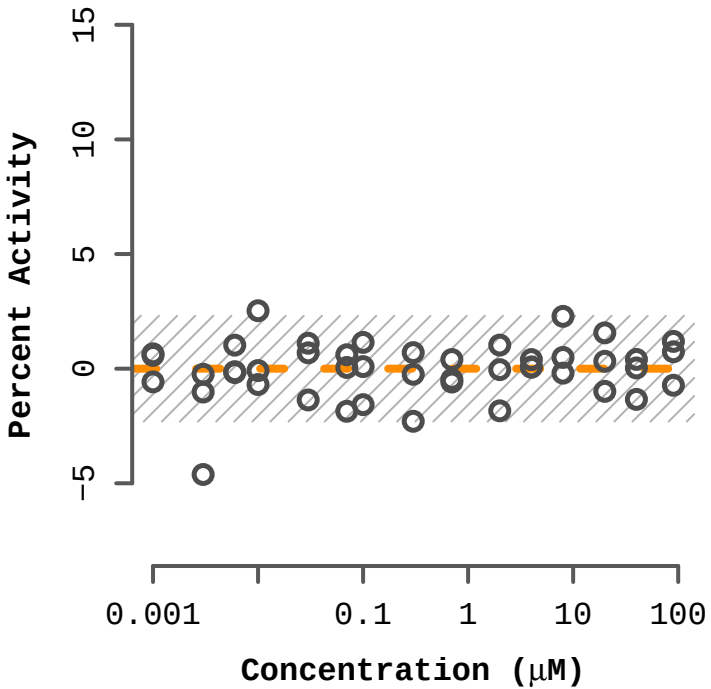
	tp	ga	gw
val:	0.632	−1.43	8
sd:	0.238	0.371	25.2

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.06	−1.1	1.79	1.45	18
sd:	0.415	0.629	2.76	0.491	58.7

	CNST	HILL	GNLS
AIC:	167.87	166.85	166.51
PROB:	0.22	0.36	0.42
RMSE:	1.62	1.55	1.53

MAX_MEAN: 1.55 **MAX_MED:** 2.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

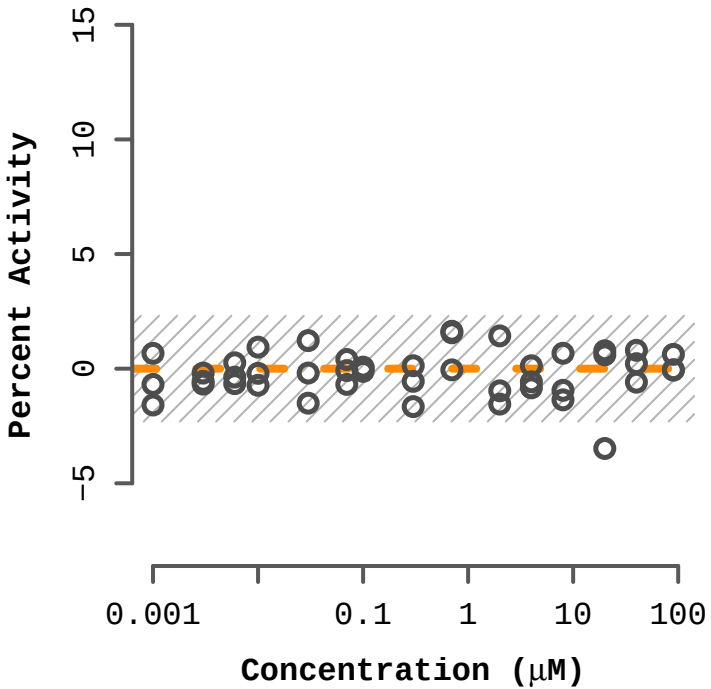
NAME: N,N−Diethylaniline
CHID: 21800 **CASRN:** 91−66−7
SPID(S): Tox21_201496
M4ID: 12480756

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 0.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

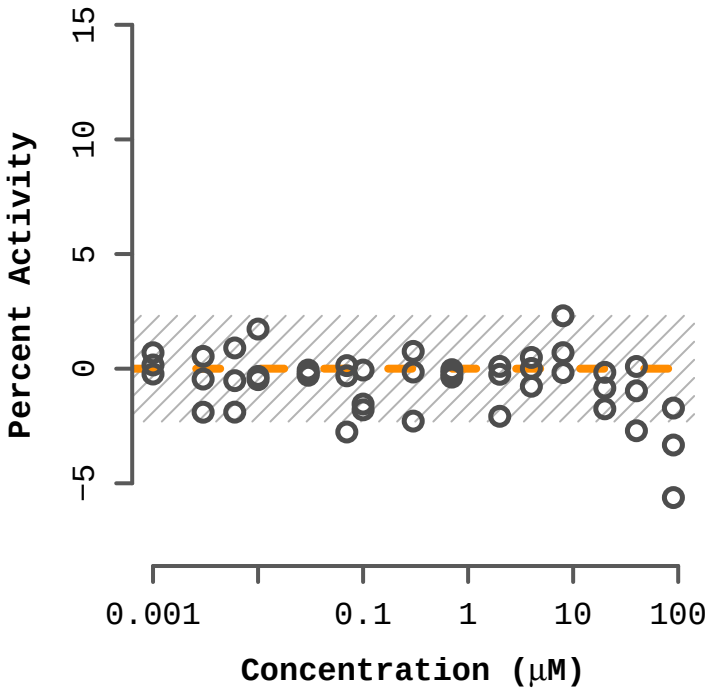
NAME: 2-(N-Ethyl-m-toluidino)ethanol
CHID: 21801 **CASRN:** 91-88-3
SPID(S): Tox21_301735
M4ID: 12477398

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

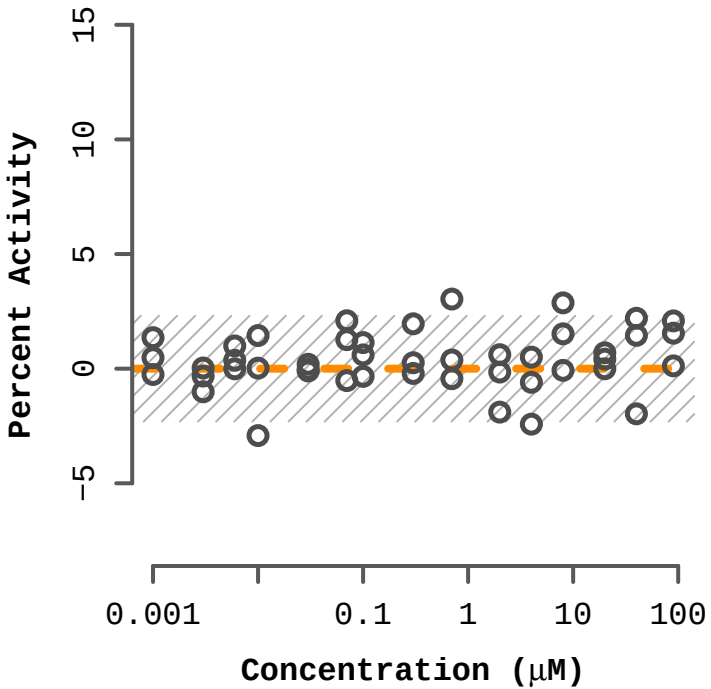
NAME: Dicyclohexyl
CHID: 21802 **CASRN:** 92-51-3
SPID(S): Tox21_302104
M4ID: 12477029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.948 **MAX_MED:** 0.701 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

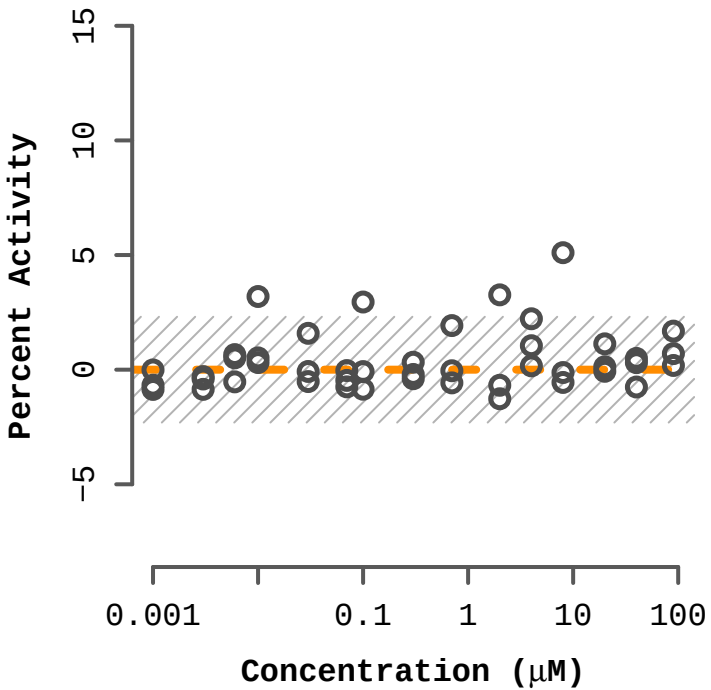
NAME: 1-Benzoylacetone
CHID: 21803 **CASRN:** 93-91-4
SPID(S): Tox21_202879
M4ID: 12479373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

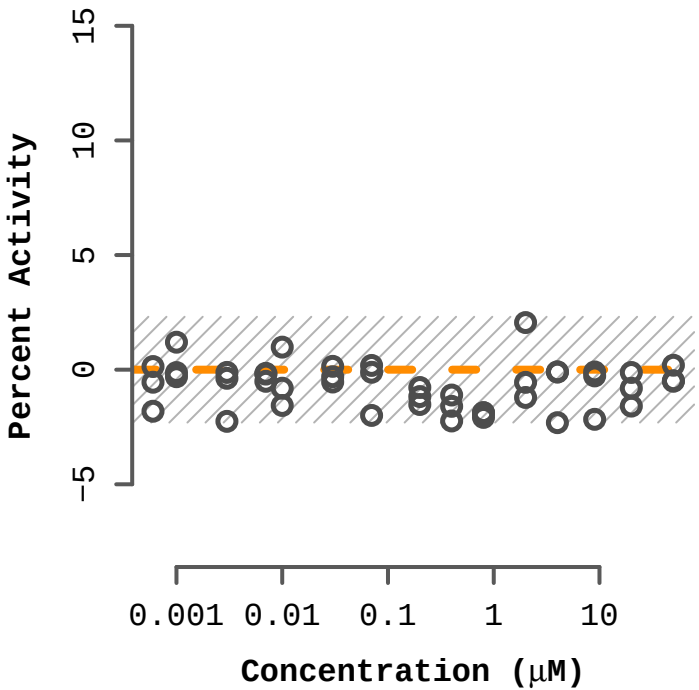
NAME: Benzocaine
CHID: 21804 **CASRN:** 94-09-7
SPID(S): Tox21_301149
M4ID: 12477984

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

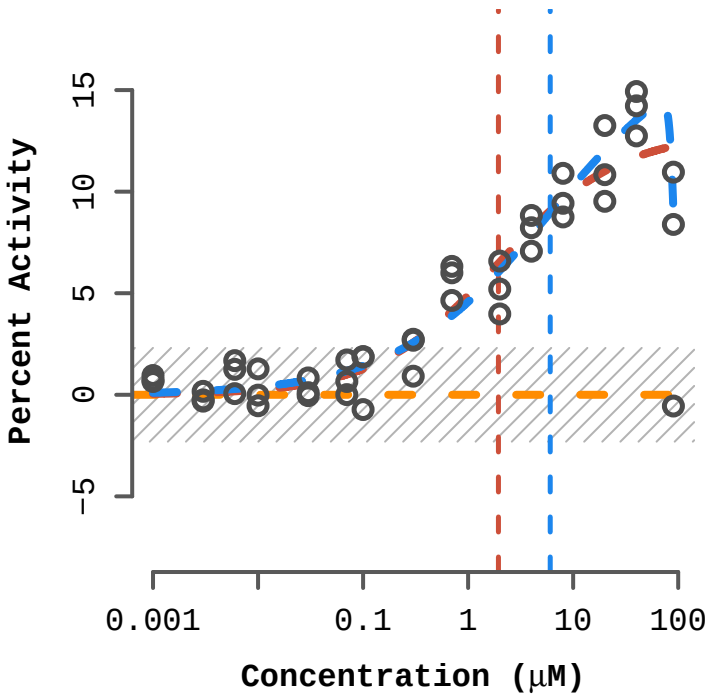
NAME: Benzocaine
CHID: 21804 **CASRN:** 94-09-7
SPID(S): Tox21_110391_1
M4ID: 12484400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.256 **MAX_MED:** −0.102 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piperine
CHID: 21805 CASRN: 94-62-2
SPID(S): Tox21_302746
M4ID: 12476387

HILL MODEL (in red):

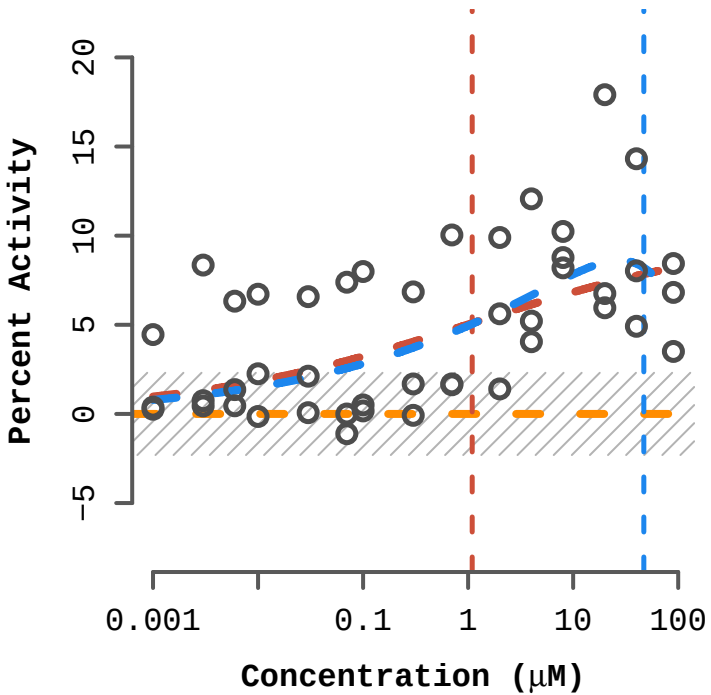
	tp	ga	gw
val:	12.9	0.289	0.747
sd:	1.47	0.184	0.117

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.9	0.781	0.596	1.96	17.9
sd:	2.9	0.276	0.0861	0.0127	21.6

	CNST	HILL	GNLS
AIC:	297.26	178.32	167.3
PROB:	0	0	1
RMSE:	6.43	2.32	1.81

MAX_MEAN: 14 MAX_MED: 14.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piperine
CHID: 21805 CASRN: 94-62-2
SPID(S): Tox21_201990
M4ID: 12480262

HILL MODEL (in red):

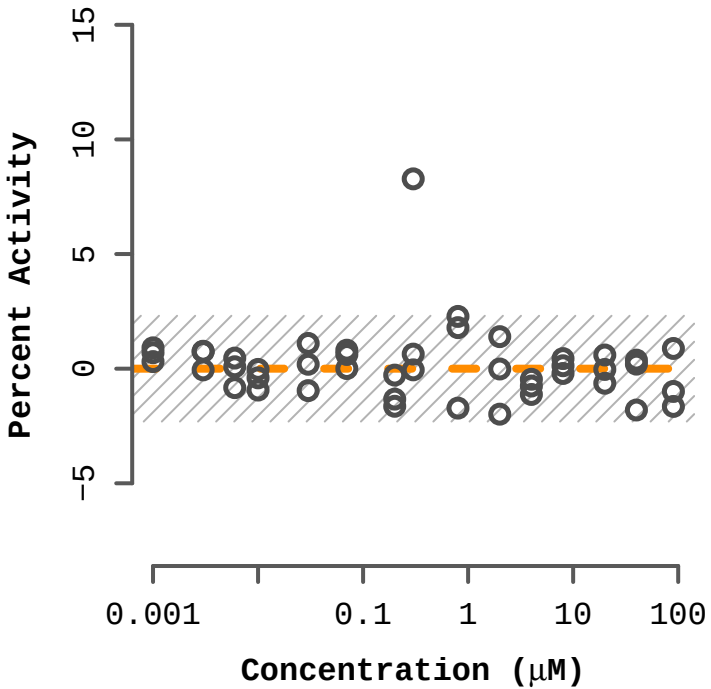
	tp	ga	gw
val:	10.2	0.0388	0.321
sd:	4.77	1.53	0.201

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	20.7	1.67	0.3	2.02	1.71
sd:	21.9	2.72	0.158	0.243	2

	CNST	HILL	GNLS
AIC:	300.18	253.64	255.26
PROB:	0	0.69	0.31
RMSE:	6.5	3.61	3.49

MAX_MEAN: 10.2 MAX_MED: 8.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

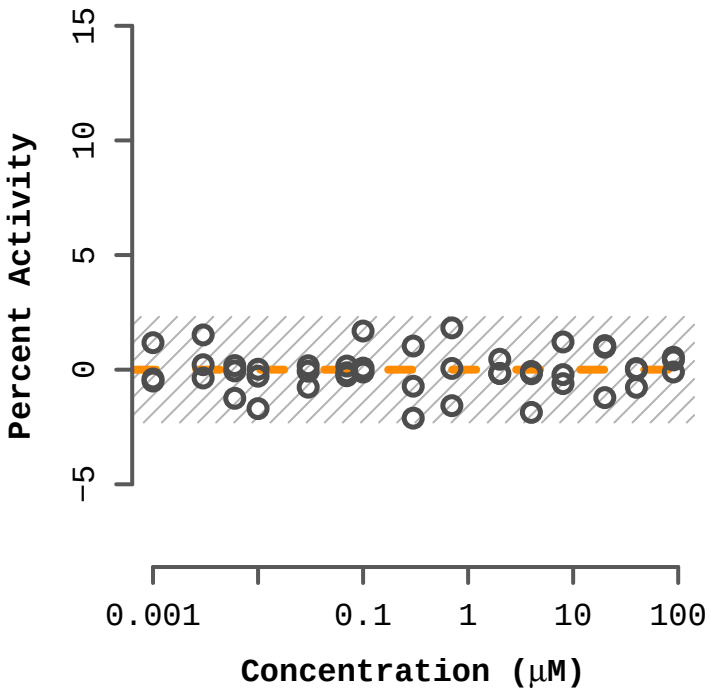
NAME: o-Xylene
CHID: 21807 CASRN: 95-47-6
SPID(S): Tox21_200658
M4ID: 12481594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.96 MAX_MED: 1.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

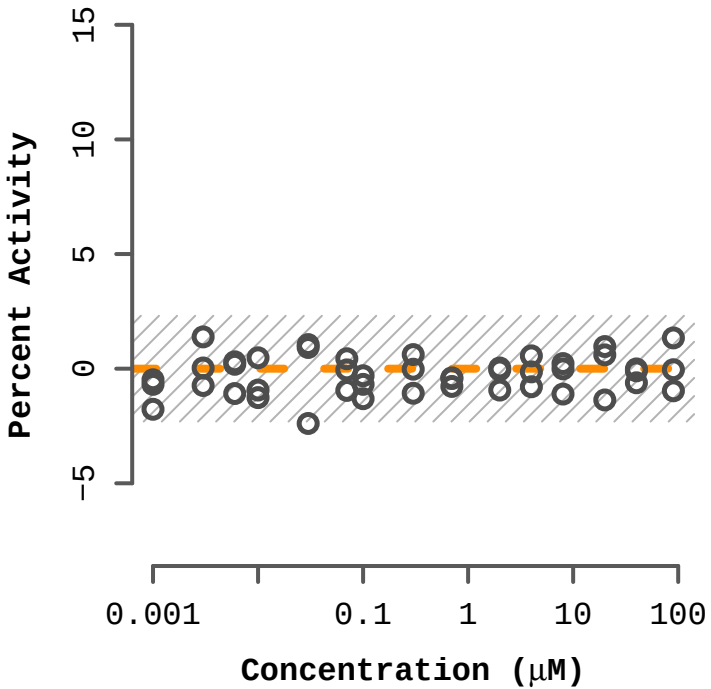
NAME: o-Cresol
CHID: 21808 **CASRN:** 95-48-7
SPID(S): Tox21_300021
M4ID: 12479109

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.552 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

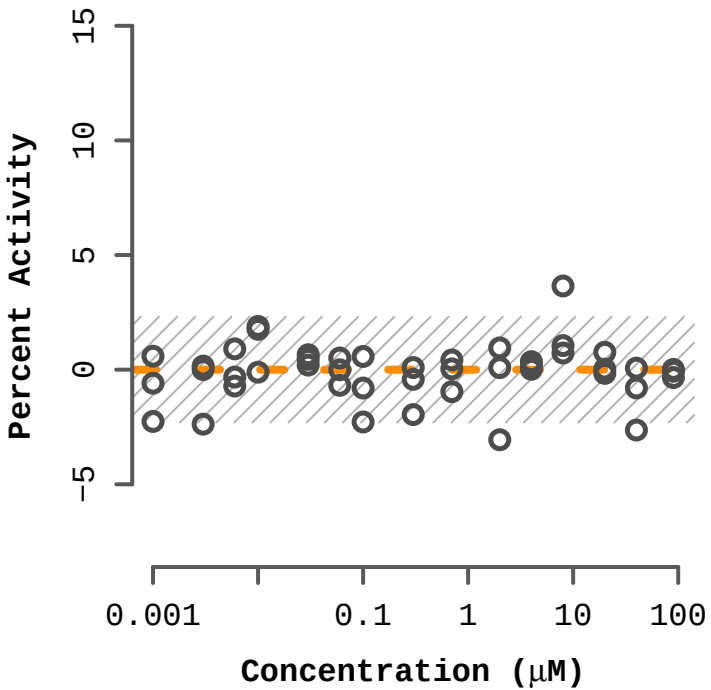
NAME: o-Cresol
CHID: 21808 CASRN: 95-48-7
SPID(S): Tox21_202305
M4ID: 12479947

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.229 MAX_MED: 0.926 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

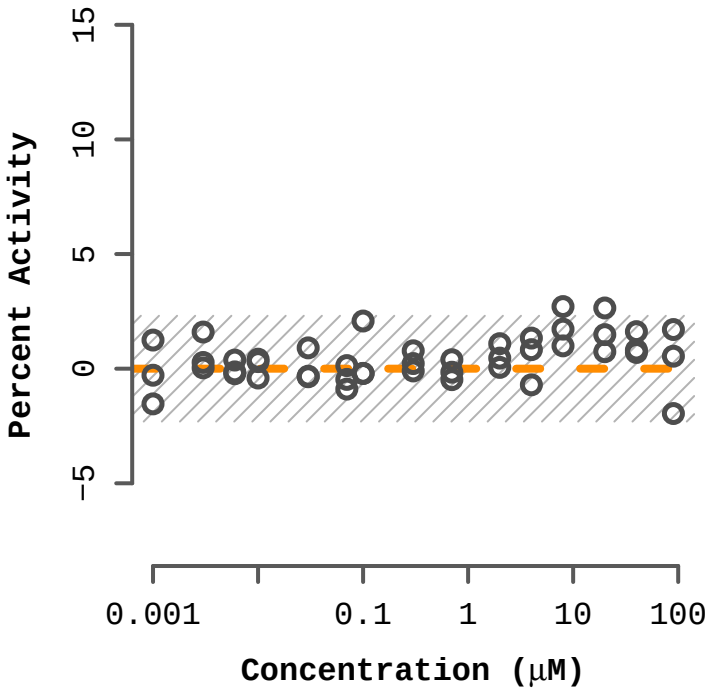
NAME: 2-Chloroaniline
CHID: 21810 **CASRN:** 95-51-2
SPID(S): Tox21_200802
M4ID: 12481450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

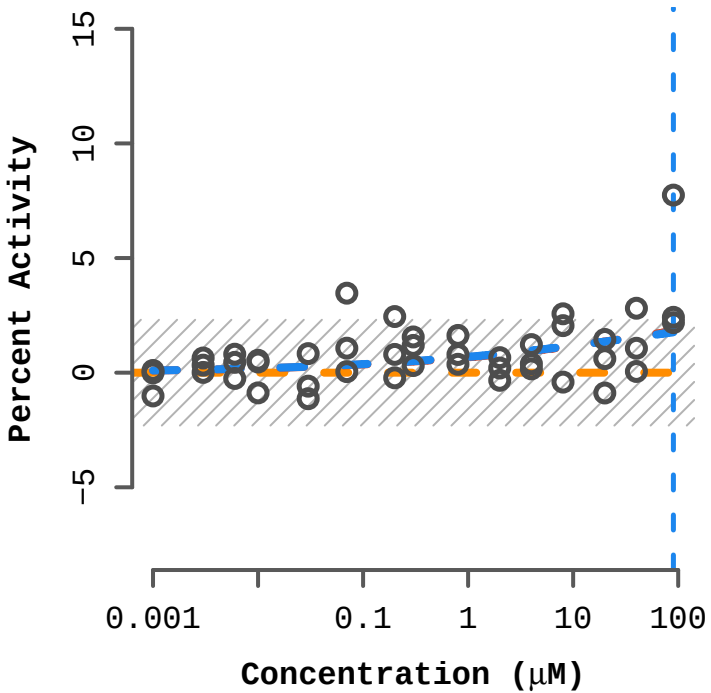
NAME: 3,4−Dichloroaniline
CHID: 21815 **CASRN:** 95−76−1
SPID(S): Tox21_302839
M4ID: 12476294

HILL MODEL: Not applicable.

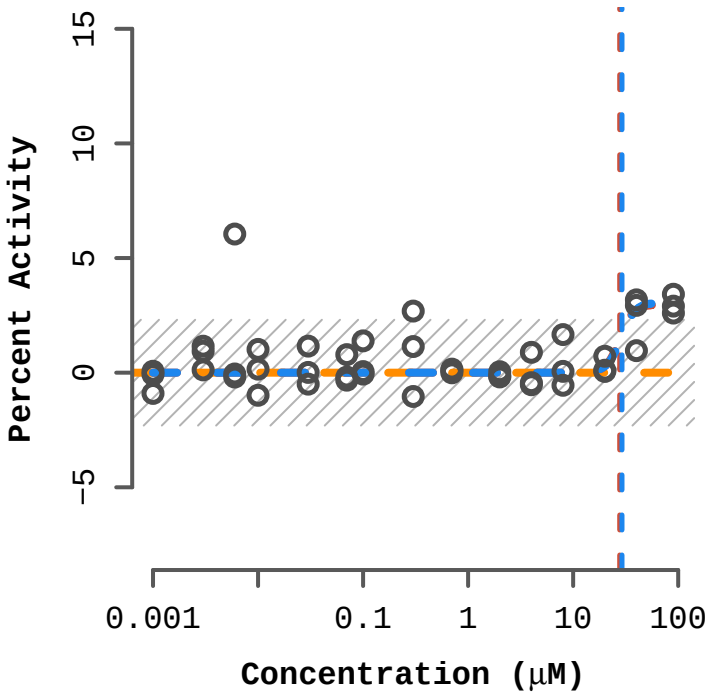
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.73 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3,4-Dichloroaniline
CHID:    21815   CASRN: 95-76-1
SPID(S): Tox21_202115
M4ID:    12480137

HILL MODEL (in red):
      tp       ga       gw
val:  4.41     2.45     0.305
sd:   7.02     3.42     0.128

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.53     1.95     0.314    3.27     5.97
sd:   4.97     3.15     0.134    876      3990

      CNST        HILL        GNLS
AIC:  161.85      145.3       149.49
PROB: 0           0.89        0.11
RMSE: 1.7         1.31        1.32

MAX_MEAN: 4.12      MAX_MED: 2.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Allyl methacrylate
CHID: 21816 CASRN: 96-05-9
SPID(S): Tox21_302944
M4ID: 12476189

HILL MODEL (in red):

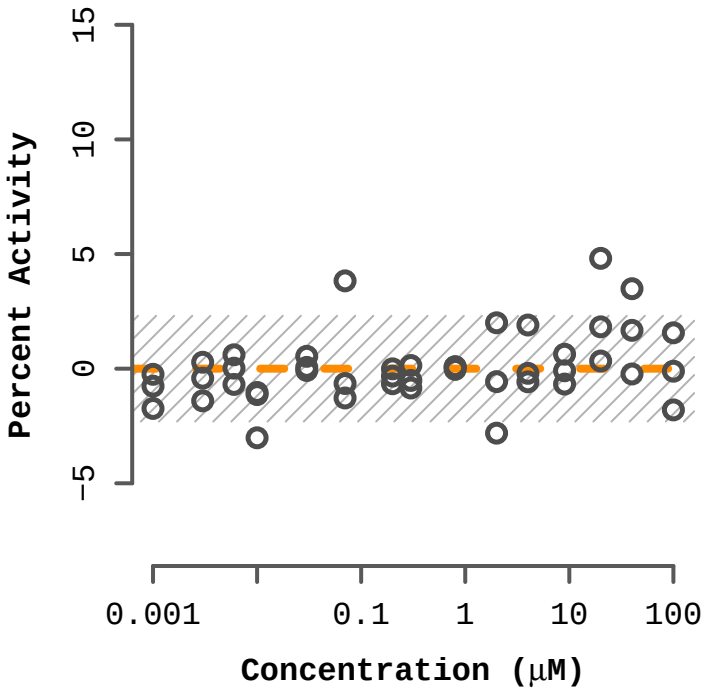
	tp	ga	gw
val:	2.97	1.44	6.89
sd:	0.354	0.0951	4.32

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.88	1.46	6.24	3.67	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.46	124.7	128.7
PROB:	0	0.88	0.12
RMSE:	1.54	1.19	1.19

MAX_MEAN: 2.98 MAX_MED: 2.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

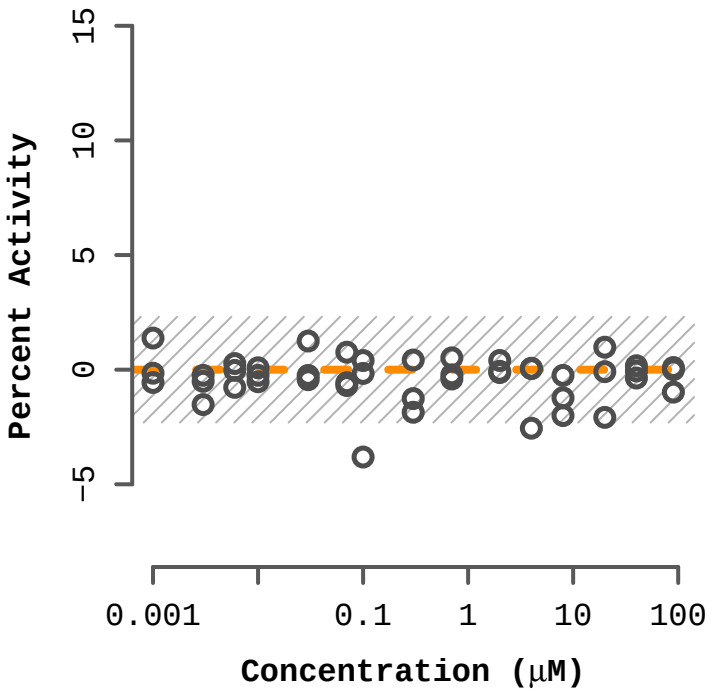
NAME: Allyl methacrylate
CHID: 21816 **CASRN:** 96-05-9
SPID(S): Tox21_201759
M4ID: 12480493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

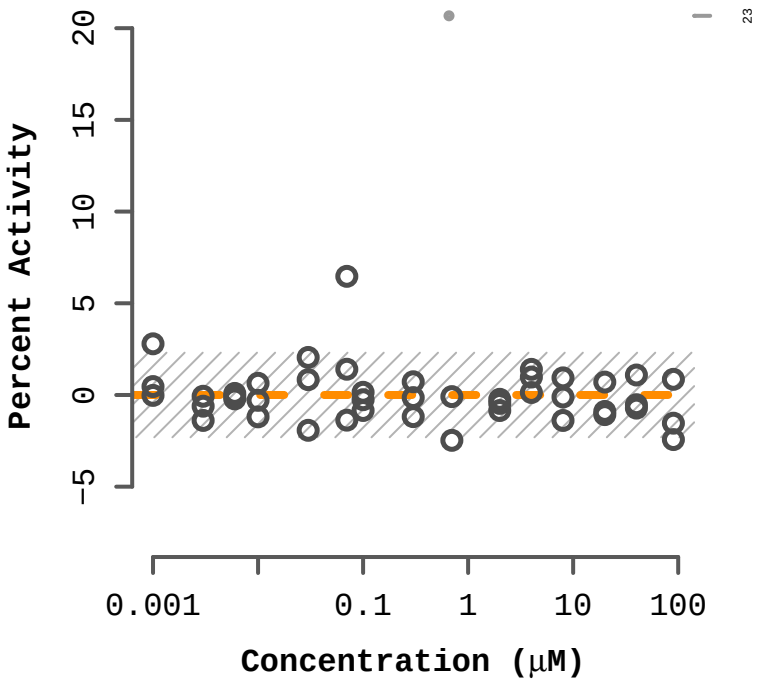
NAME: 2,3-Dibromopropanol
CHID: 21817 CASRN: 96-13-9
SPID(S): Tox21_200709
M4ID: 12481543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.223 MAX_MED: 0.0468 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

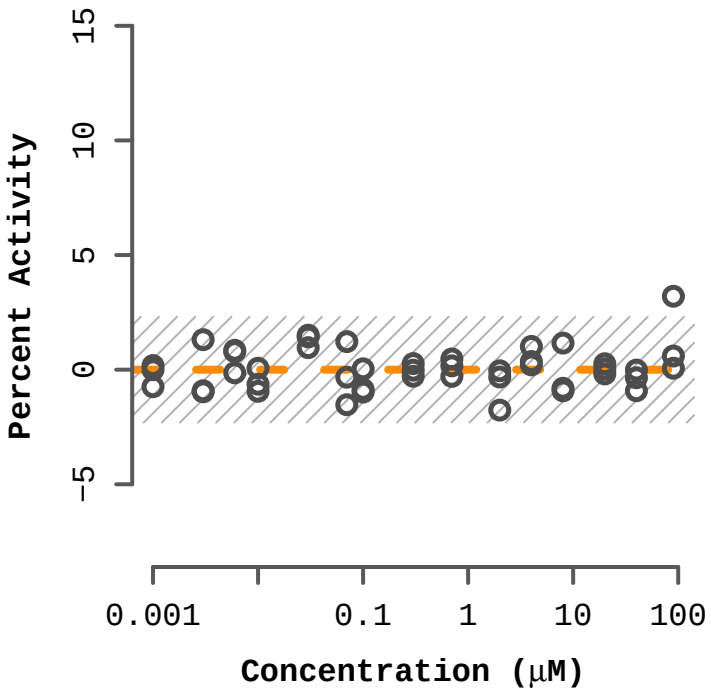
NAME: 2-Methylbutanal
CHID: 21818 CASRN: 96-17-3
SPID(S): Tox21_302866
M4ID: 12476267 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.11	NA	NA
PROB:	1	NA	NA
RMSE:	3.7	NA	NA

MAX_MEAN: 6.75 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

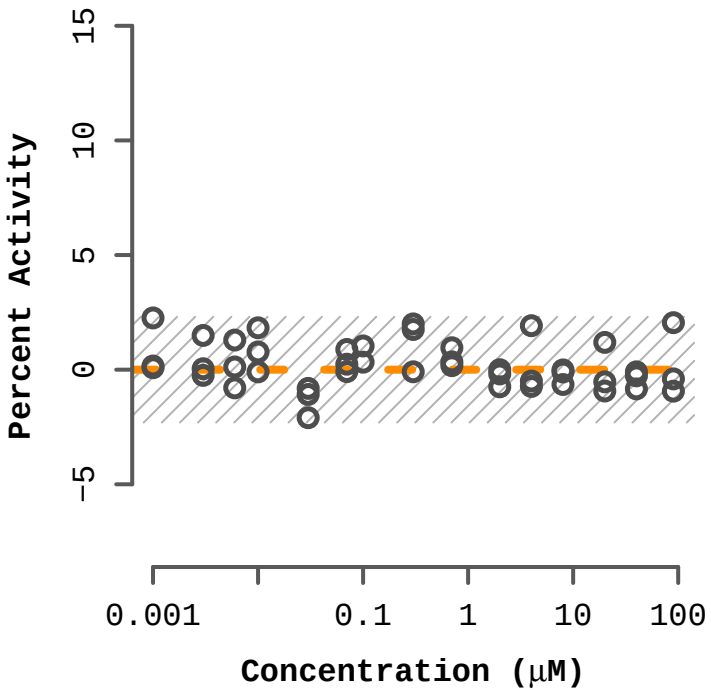
NAME: 2-Methylbutanal
CHID: 21818 **CASRN:** 96-17-3
SPID(S): Tox21_201242
M4ID: 12481010

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

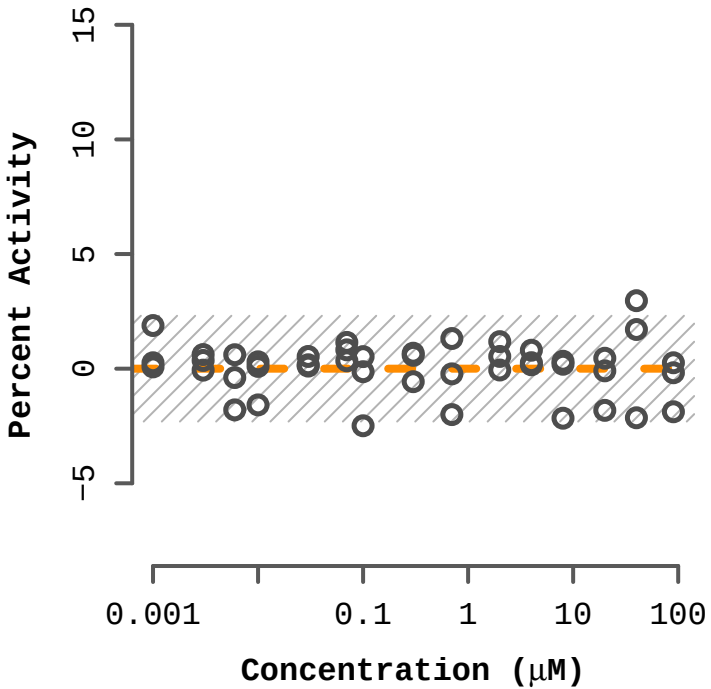
NAME: 3-Pentanone
CHID: 21820 CASRN: 96-22-0
SPID(S): Tox21_200677
M4ID: 12481575

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.13	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

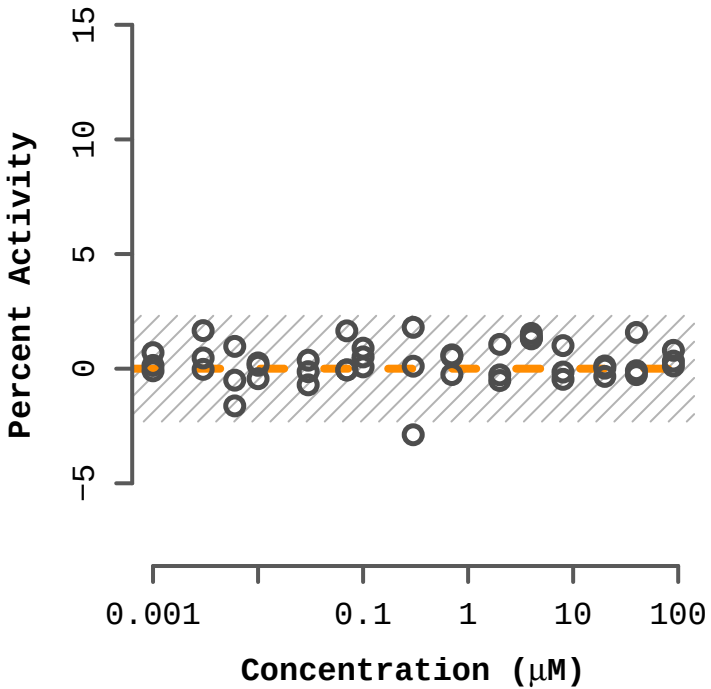
NAME: 2-Butanone oxime
CHID: 21821 **CASRN:** 96-29-7
SPID(S): Tox21_300162
M4ID: 12478968

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.846 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

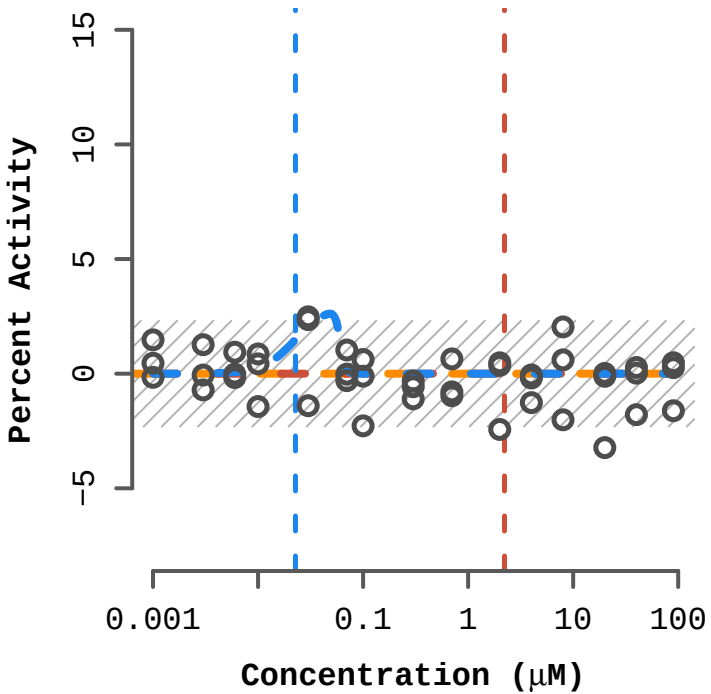
NAME: 2-Butanone oxime
CHID: 21821 **CASRN:** 96-29-7
SPID(S): Tox21_201706
M4ID: 12480546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Diisopropylamino)ethanol
CHID: 21822 CASRN: 96-80-0
SPID(S): Tox21_301869
M4ID: 12477264

HILL MODEL (in red):

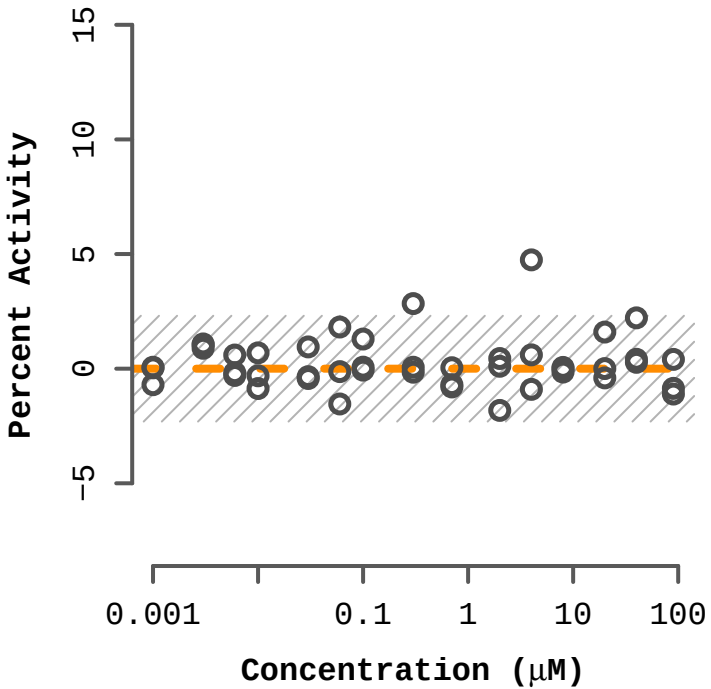
	tp	ga	gw
val:	1.94e-10	0.346	1.64
sd:	1.31e-05	18400	276000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.98	-1.64	2.82	-1.22	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	146.55	152.55	151.75
PROB:	0.89	0.04	0.07
RMSE:	1.21	1.21	1.19

MAX_MEAN: 1.15 MAX_MED: 2.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

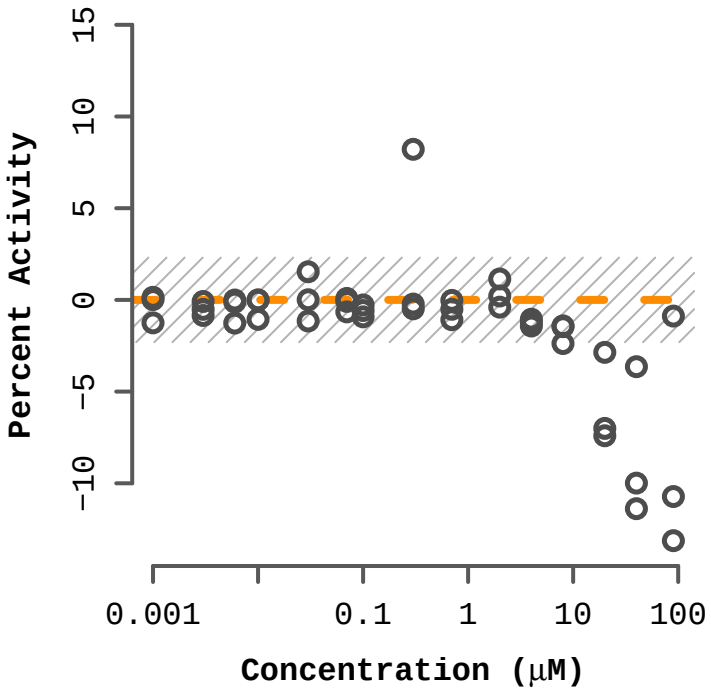
NAME: 2,4−Dinitroaniline
CHID: 21823 **CASRN:** 97−02−9
SPID(S): Tox21_200126
M4ID: 12482126

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

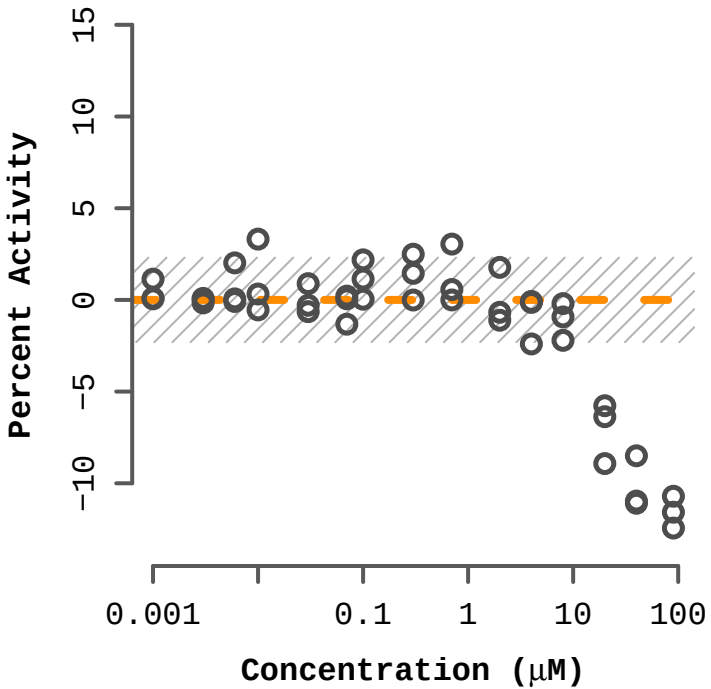
NAME: Dichlorophen
CHID: 21824 **CASRN:** 97-23-4
SPID(S): Tox21_303013
M4ID: 12476120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.27	NA	NA
PROB:	1	NA	NA
RMSE:	4.05	NA	NA

MAX_MEAN: 2.5 **MAX_MED:** 0.215 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

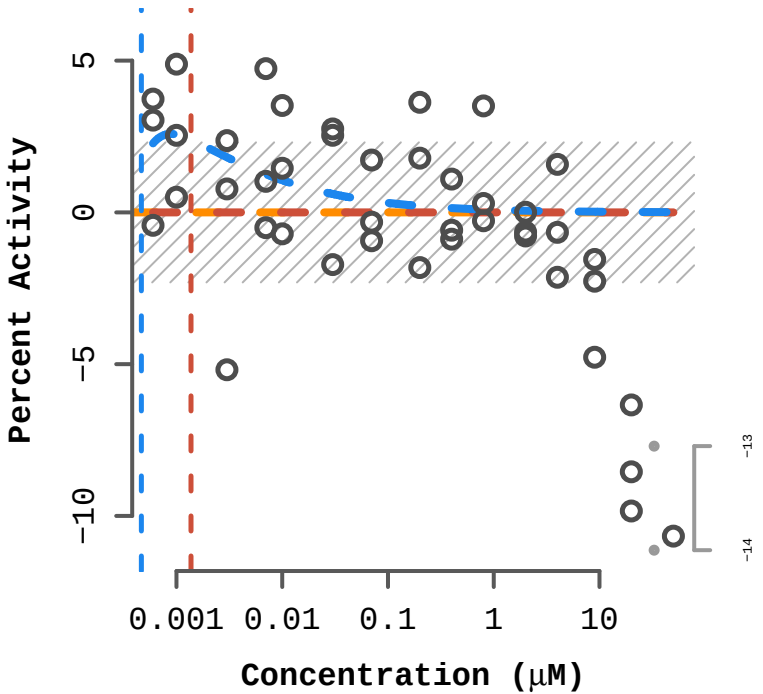
NAME: Dichlorophen
CHID: 21824 **CASRN:** 97-23-4
SPID(S): Tox21_201429
M4ID: 12480823

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.95	NA	NA
PROB:	1	NA	NA
RMSE:	4.55	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dichlorophen
CHID: 21824 CASRN: 97-23-4
SPID(S): Tox21_111112_1
M4ID: 12483900 BRK

HILL MODEL (in red):

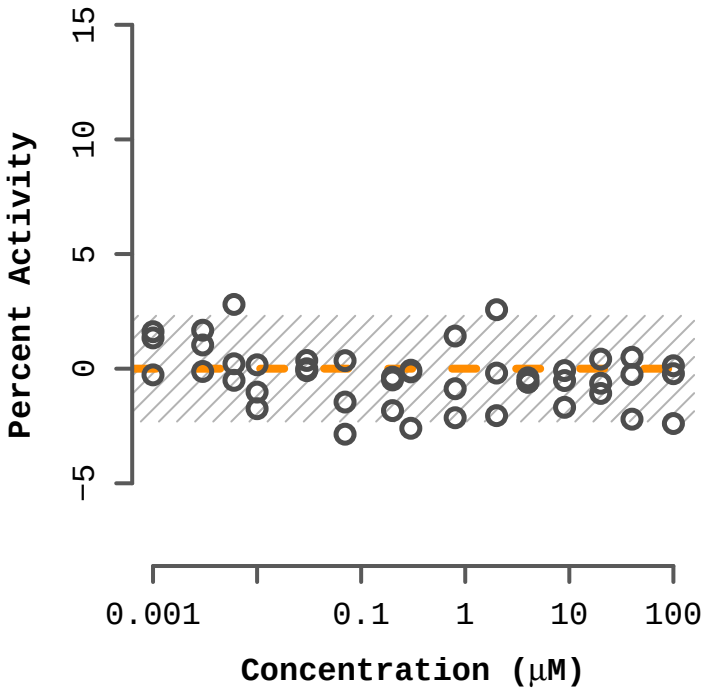
	tp	ga	gw
val:	1.34e-09	-2.86	2.36
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.73	-3.33	3.81	-3.08	0.594
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	256.07	262.07	260.92
PROB:	0.88	0.04	0.08
RMSE:	4.52	4.52	4.43

MAX_MEAN: 2.64 MAX_MED: 3.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

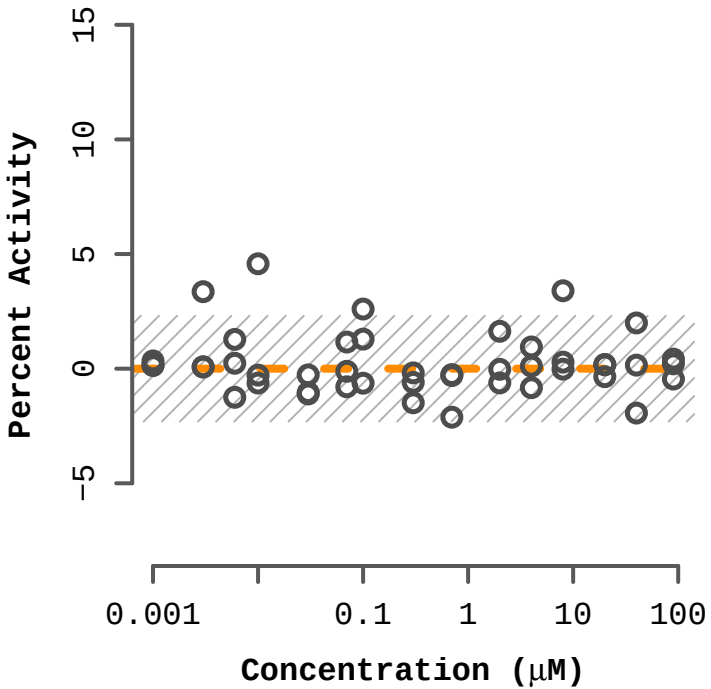
NAME: Cumene
CHID: 21827 **CASRN:** 98-82-8
SPID(S): Tox21_202503
M4ID: 12479749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.897 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

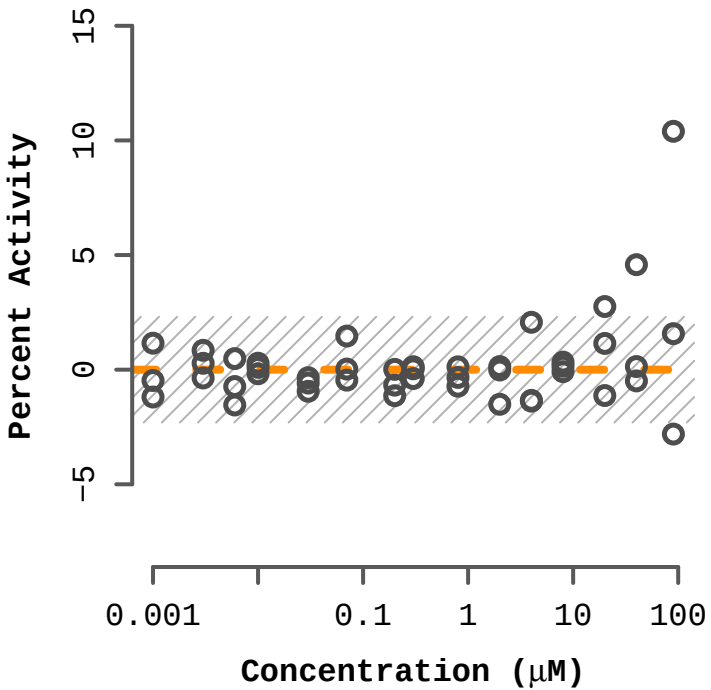
NAME: Acetophenone
CHID: 21828 CASRN: 98-86-2
SPID(S): Tox21_300343
M4ID: 12478789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

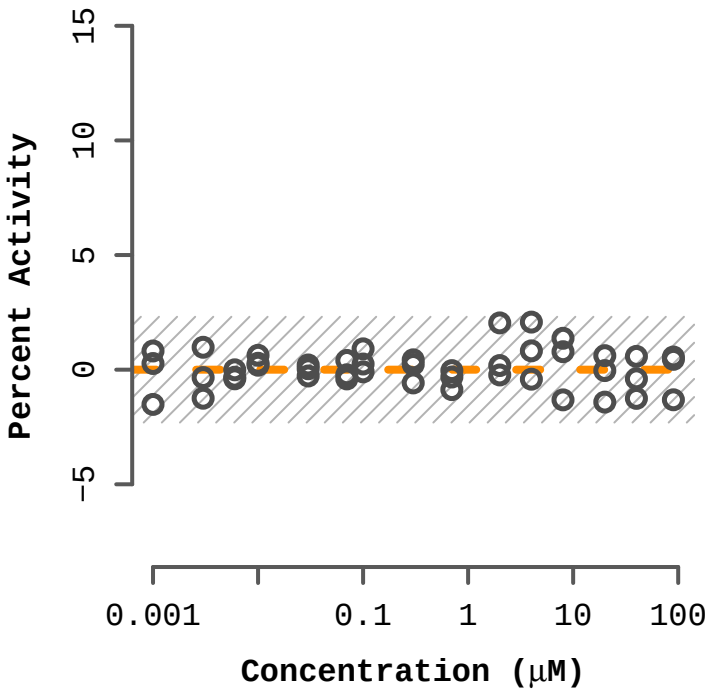
NAME: Acetophenone
CHID: 21828 **CASRN:** 98-86-2
SPID(S): Tox21_202422
M4ID: 12479830

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 3.05 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

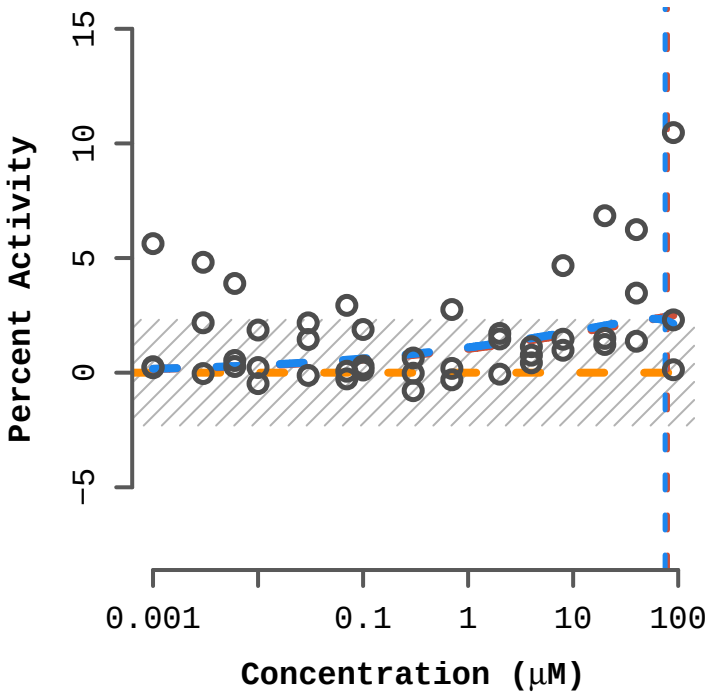
NAME: 3-Nitrotoluene
CHID: 21831 **CASRN:** 99-08-1
SPID(S): Tox21_300007
M4ID: 12479123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.828 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Nitrotoluene
CHID: 21831 CASRN: 99-08-1
SPID(S): Tox21_202435
M4ID: 12479817

HILL MODEL (in red):

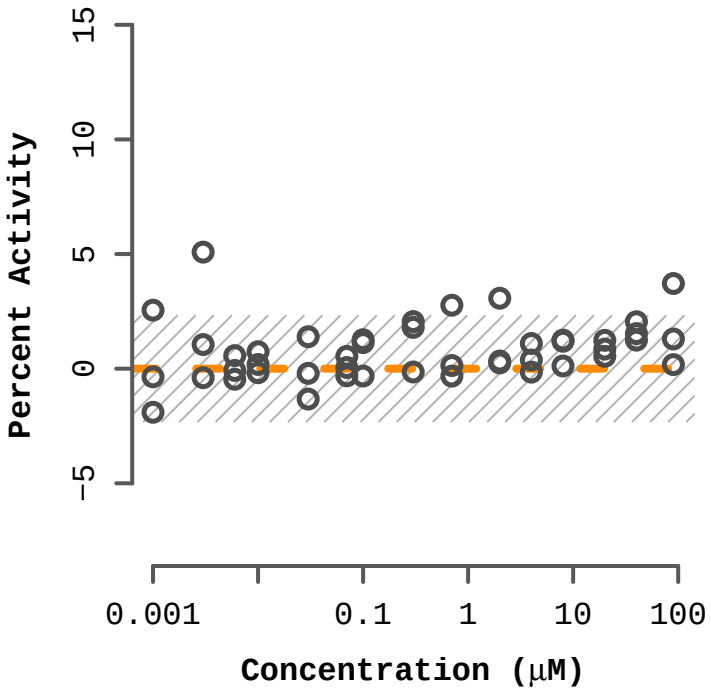
	tp	ga	gw
val:	4.9	1.9	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.12	1.88	0.3	2.13	3.67
sd:	9.09	4.25	0.233	0.225	10.6

	CNST	HILL	GNLS
AIC:	211.74	195.81	199.56
PROB:	0	0.87	0.13
RMSE:	2.82	2.2	2.22

MAX_MEAN: 4.3 MAX_MED: 3.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

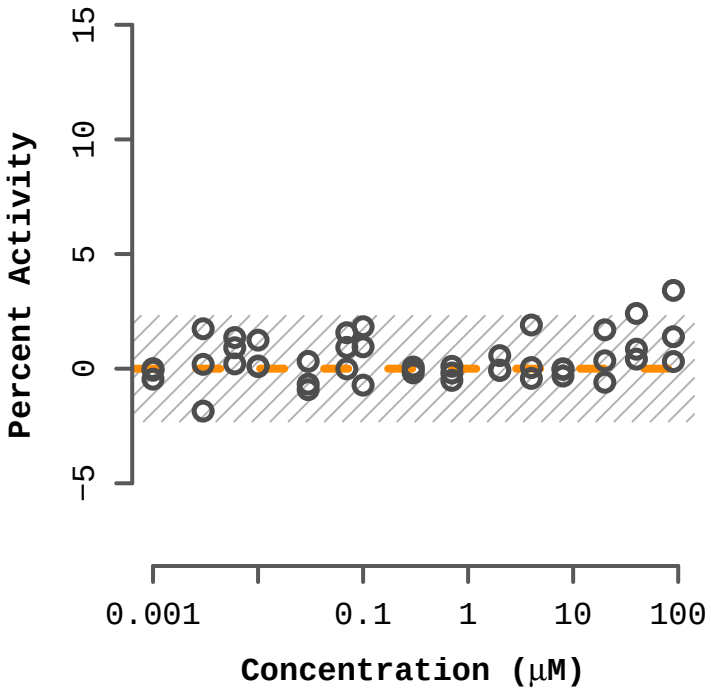
NAME: N,N,4−Trimethylaniline
CHID: 21832 **CASRN:** 99−97−8
SPID(S): Tox21_300062
M4ID: 12479068

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

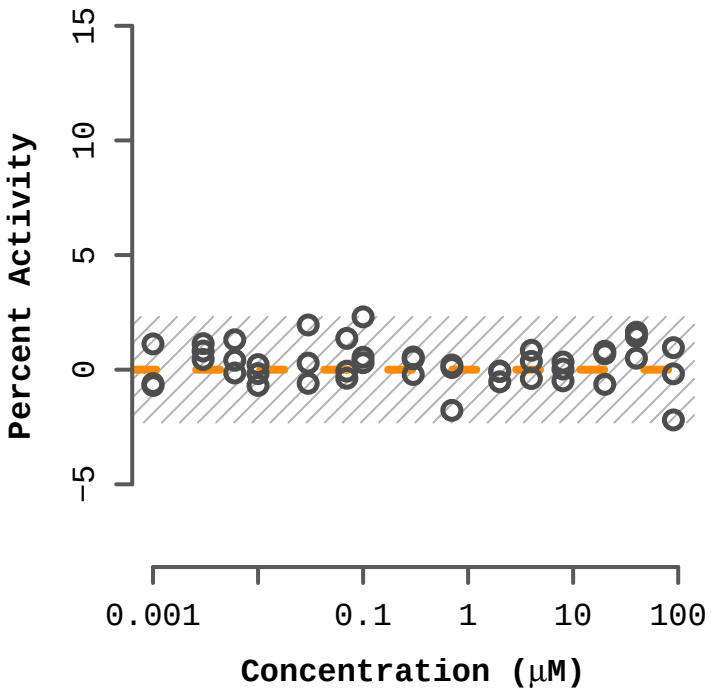
NAME: N,N,4−Trimethylaniline
CHID: 21832 **CASRN:** 99−97−8
SPID(S): Tox21_201370
M4ID: 12480882

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

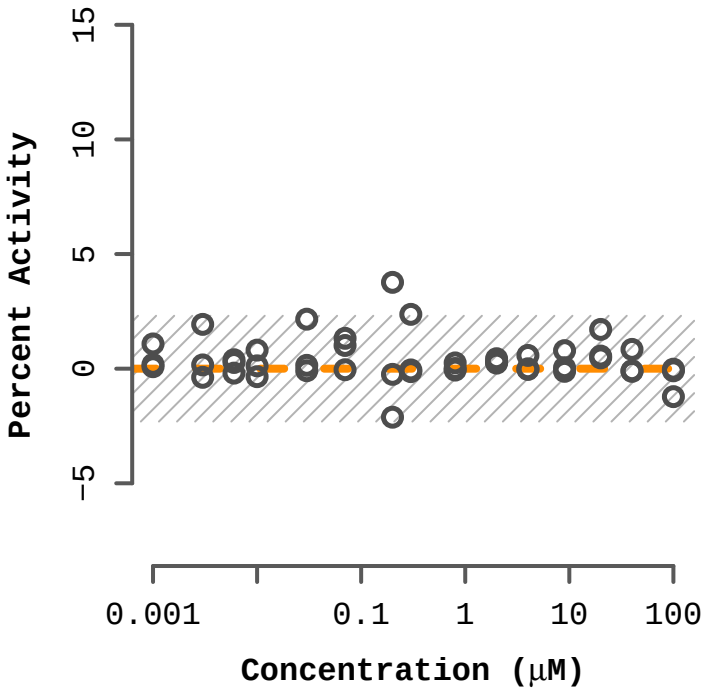
NAME: 4-Nitrophenol
CHID: 21834 **CASRN:** 100-02-7
SPID(S): Tox21_300117
M4ID: 12479013

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

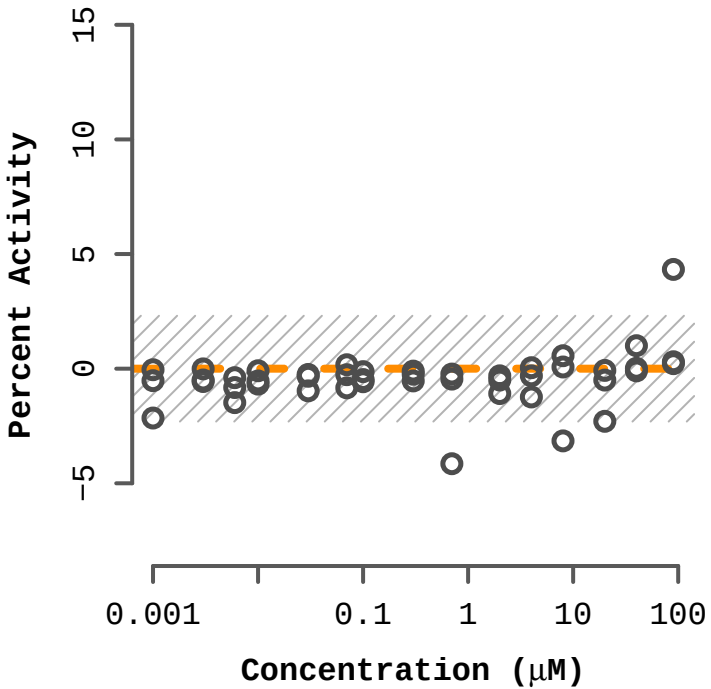
NAME: 4-Nitrophenol
CHID: 21834 **CASRN:** 100-02-7
SPID(S): Tox21_202444
M4ID: 12479808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.9	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

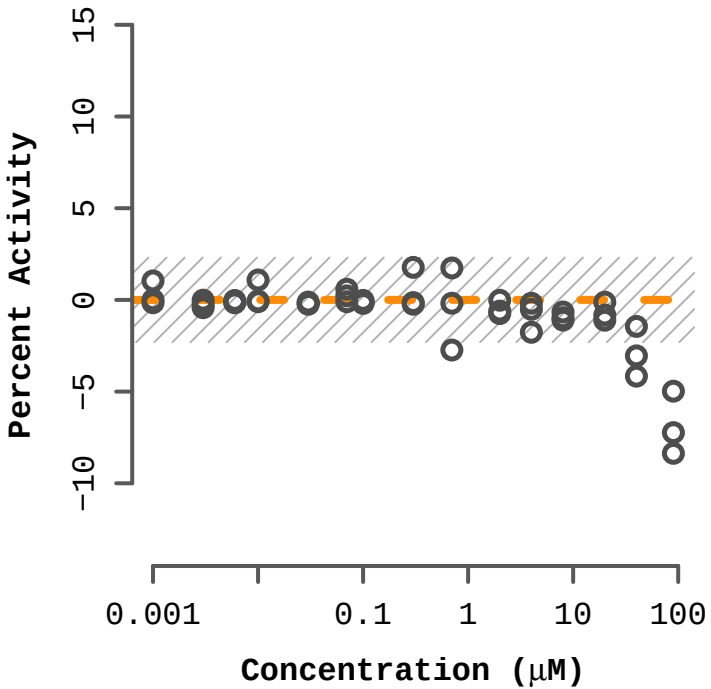
NAME: 4-Dimethylaminobenzaldehyde
CHID: 21835 **CASRN:** 100-10-7
SPID(S): Tox21_300707
M4ID: 12478426

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 0.304 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

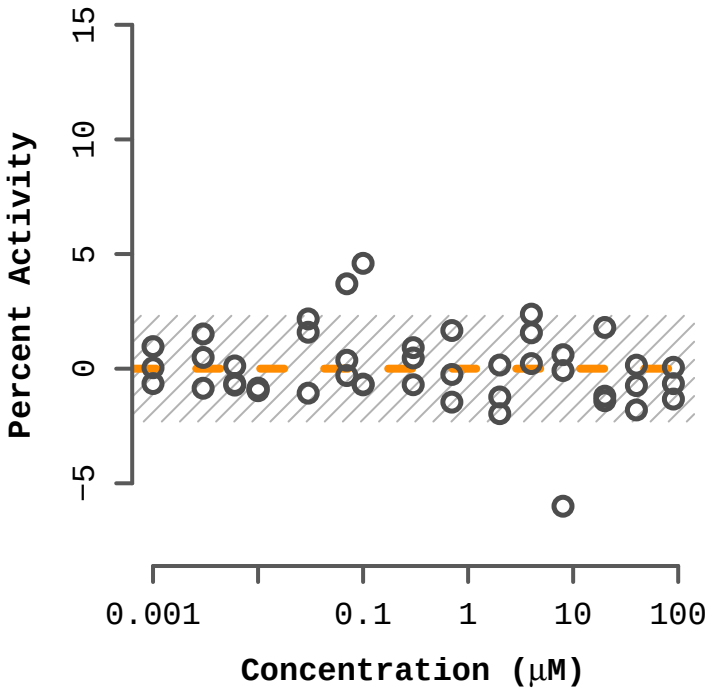
NAME: 1,4-Dinitrobenzene
CHID: 21836 **CASRN:** 100-25-4
SPID(S): Tox21_303785
M4ID: 12475403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.18	NA	NA
PROB:	1	NA	NA
RMSE:	2.12	NA	NA

MAX_MEAN: 0.466 **MAX_MED:** 0.221 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

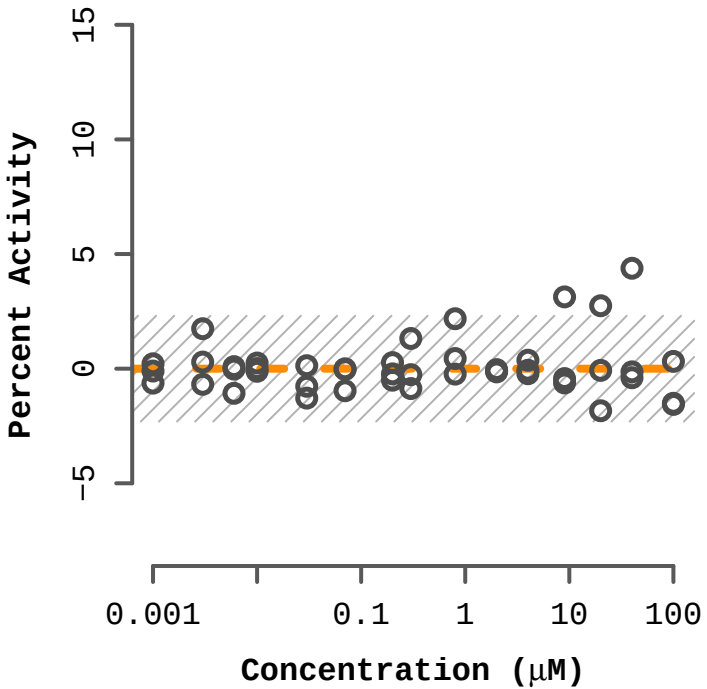
NAME: N,N−Diethylethanolamine
CHID: 21837 **CASRN:** 100−37−8
SPID(S): Tox21_300037
M4ID: 12479093

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

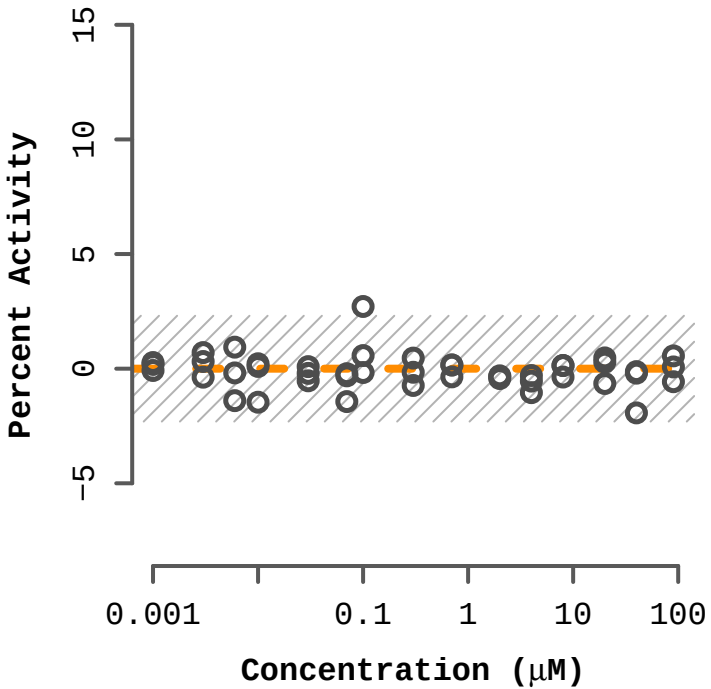
NAME: N,N−Diethylethanolamine
CHID: 21837 **CASRN:** 100−37−8
SPID(S): Tox21_201463
M4ID: 12480789

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.445 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

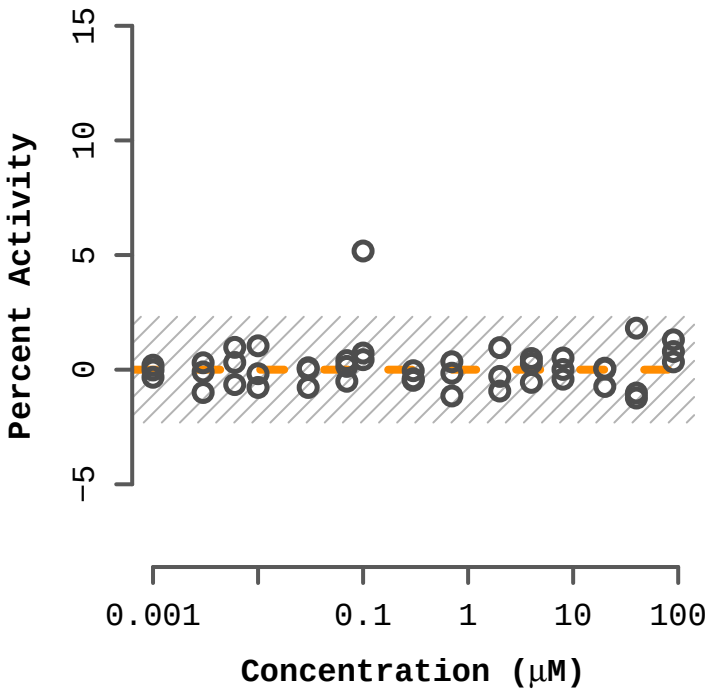
NAME: Benzylamine
CHID: 21839 **CASRN:** 100-46-9
SPID(S): Tox21_300933
M4ID: 12478200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.574 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

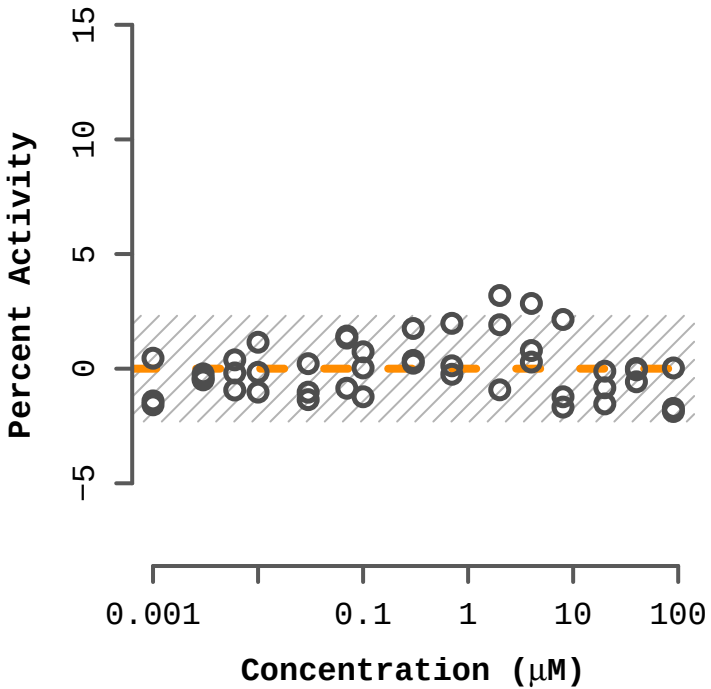
NAME: N-Methylaniline
CHID: 21841 **CASRN:** 100-61-8
SPID(S): Tox21_200298
M4ID: 12481954

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 0.793 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

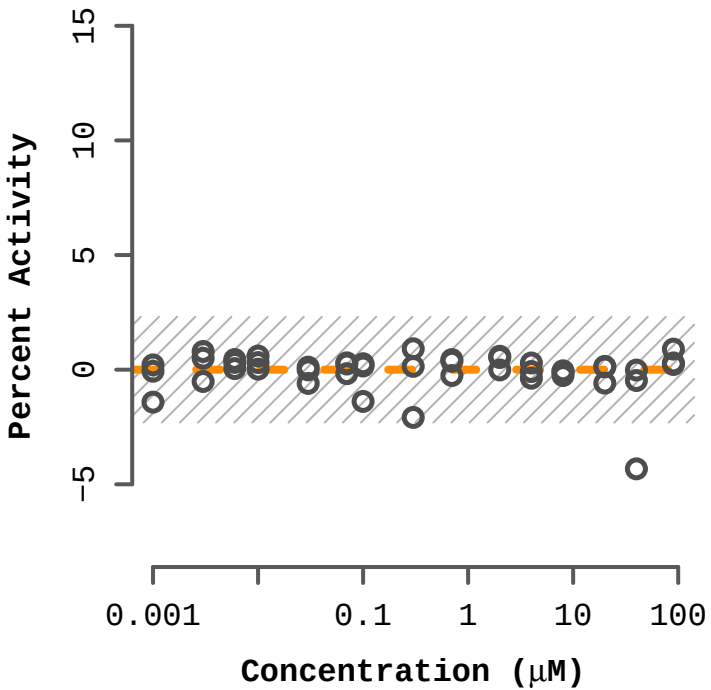
NAME: Cyclohexanone oxime
CHID: 21842 **CASRN:** 100-64-1
SPID(S): Tox21_303015
M4ID: 12476118

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

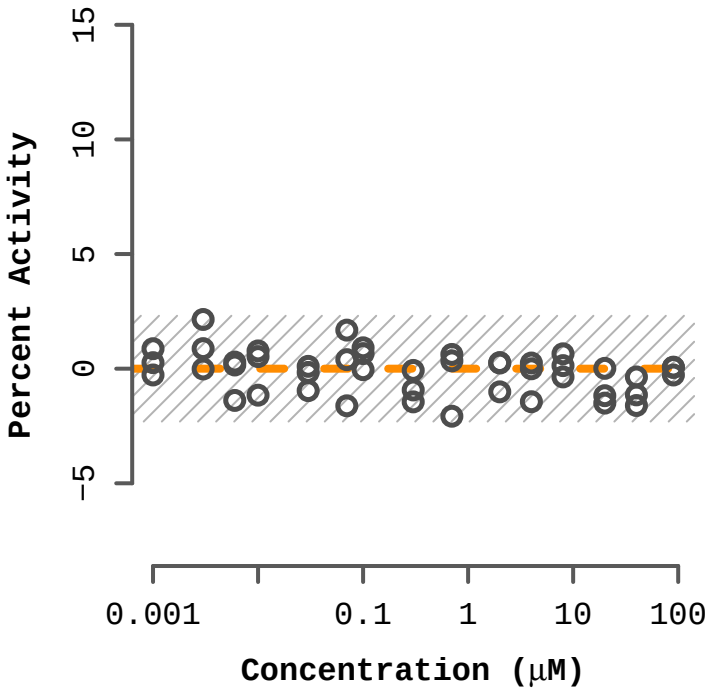
NAME: Cyclohexanone oxime
CHID: 21842 **CASRN:** 100-64-1
SPID(S): Tox21_202143
M4ID: 12480109

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.474 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

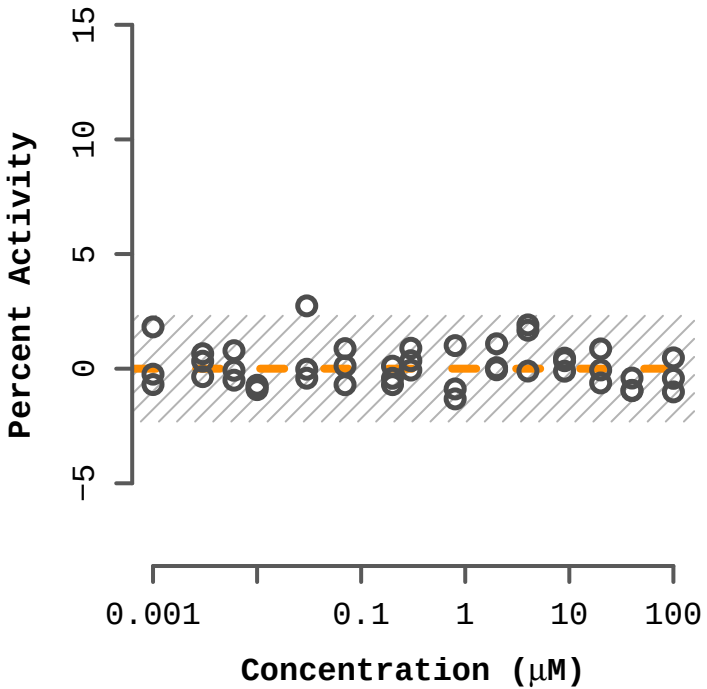
NAME: 2-Pyridinecarbonitrile
CHID: 21843 **CASRN:** 100-70-9
SPID(S): Tox21_302832
M4ID: 12476301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.876 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

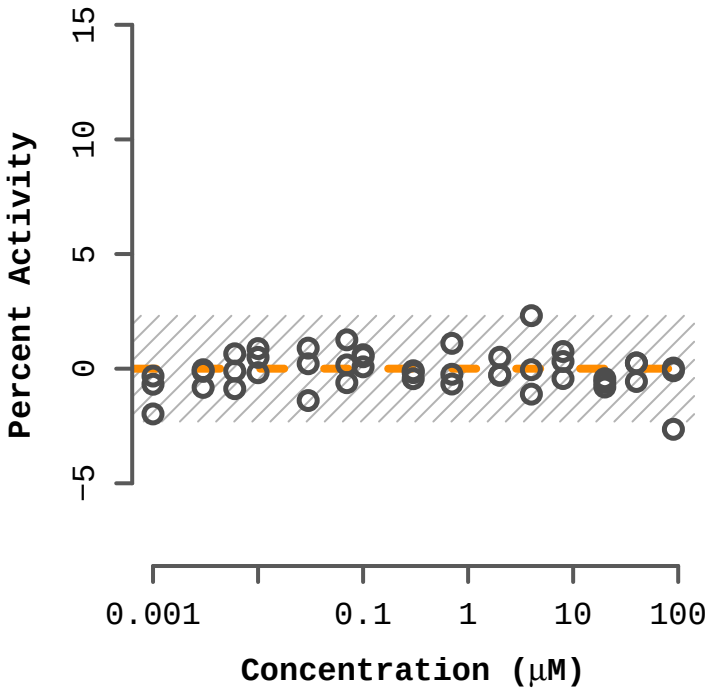
NAME: 2-Pyridinecarbonitrile
CHID: 21843 **CASRN:** 100-70-9
SPID(S): Tox21_201343
M4ID: 12480909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

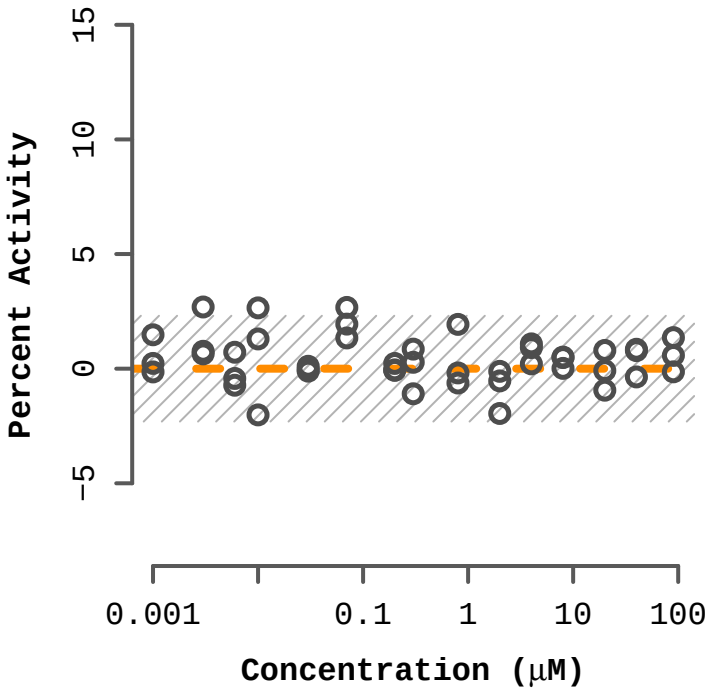
NAME: Diphenyl oxide
CHID: 21847 CASRN: 101-84-8
SPID(S): Tox21_302777
M4ID: 12476356

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.405 MAX_MED: 0.522 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

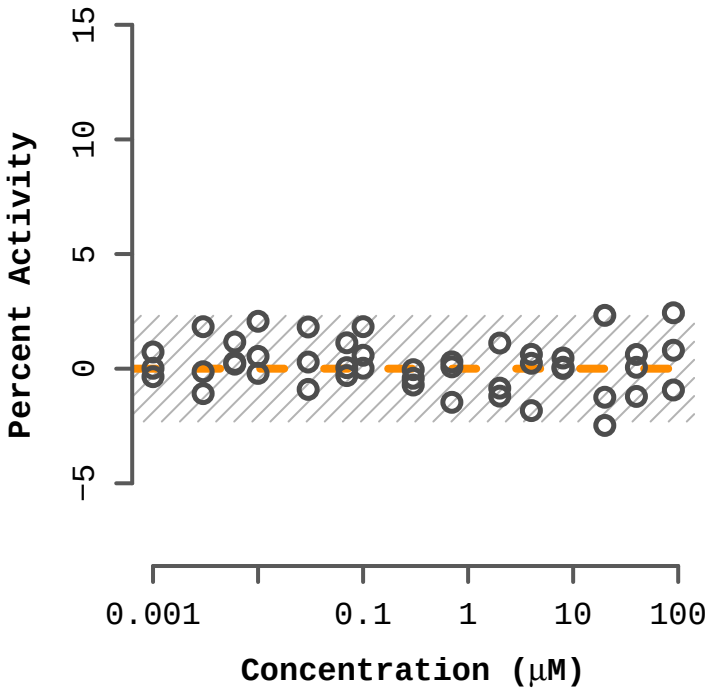
NAME: Diphenyl oxide
CHID: 21847 **CASRN:** 101-84-8
SPID(S): Tox21_202277
M4ID: 12479975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

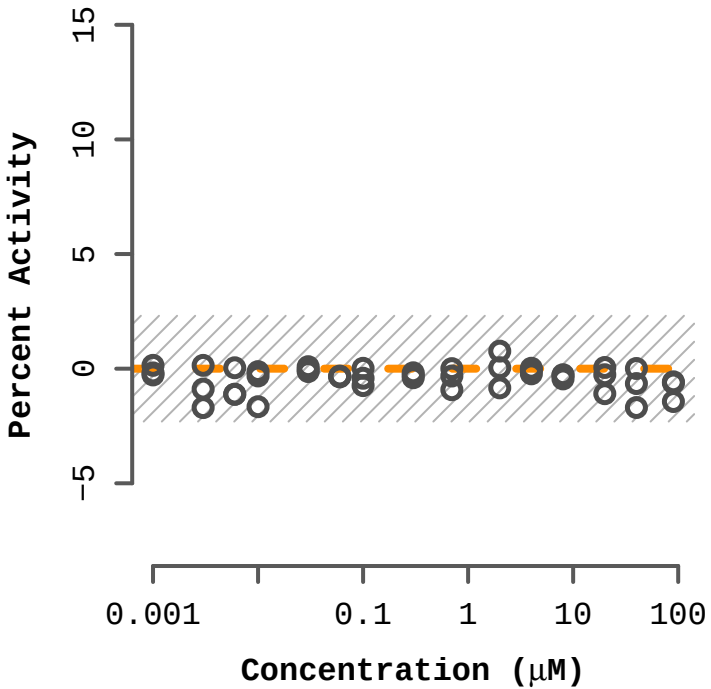
NAME: N-Ethyl-3-methylaniline
CHID: 21848 **CASRN:** 102-27-2
SPID(S): Tox21_300513
M4ID: 12478619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.814 **MAX_MED:** 0.805 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

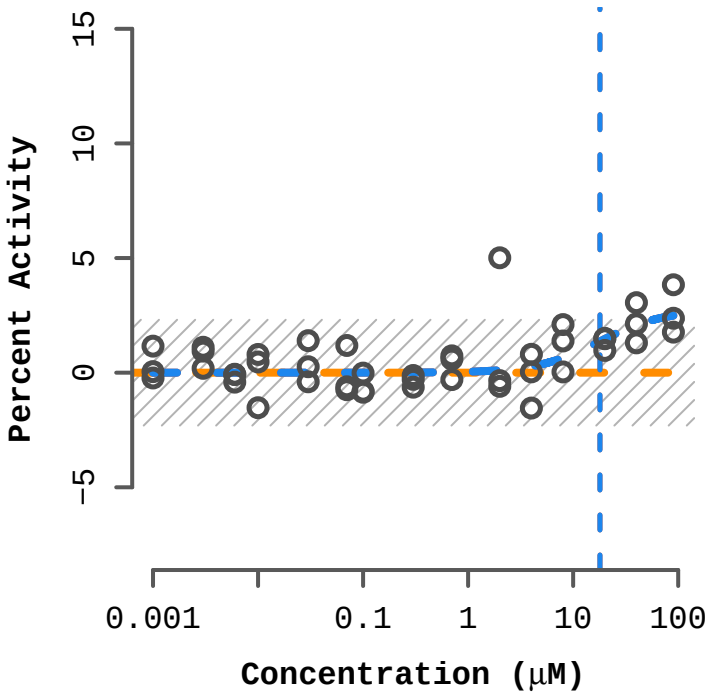
NAME: N-Ethyl-3-methylaniline
CHID: 21848 CASRN: 102-27-2
SPID(S): Tox21_201647
M4ID: 12480605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: −0.00858 MAX_MED: 0.0444 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methyl-4-phenylbutan-2-ol
CHID: 21851 **CASRN:** 103-05-9
SPID(S): Tox21_302631
M4ID: 12476502

HILL MODEL (in red):

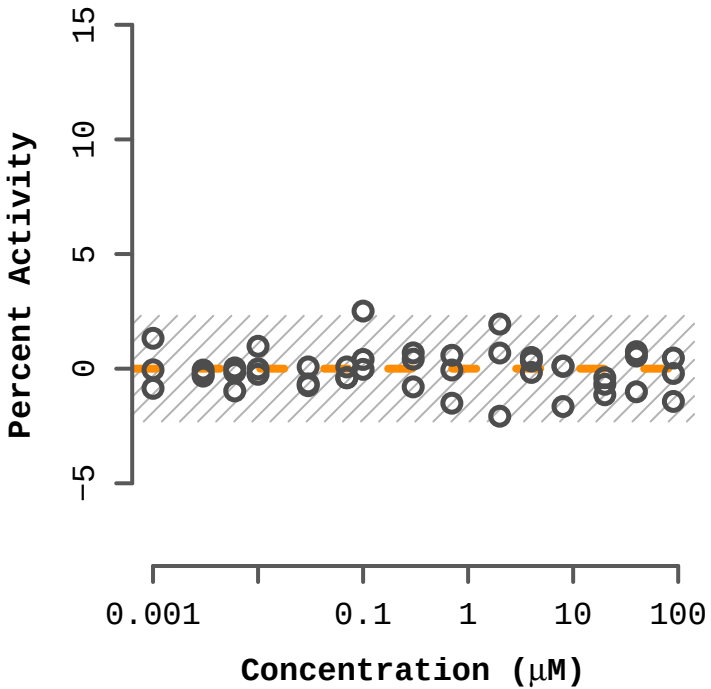
	tp	ga	gw
val:	2.73	1.26	1.45
sd:	0.921	0.299	0.798

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.73	1.26	1.45	3.32	4.74
sd:	0.921	0.299	0.798	1390	4660

	CNST	HILL	GNLS
AIC:	157.19	127.35	131.35
PROB:	0	0.88	0.12
RMSE:	1.44	1.05	1.05

MAX_MEAN: 2.66 **MAX_MED:** 2.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

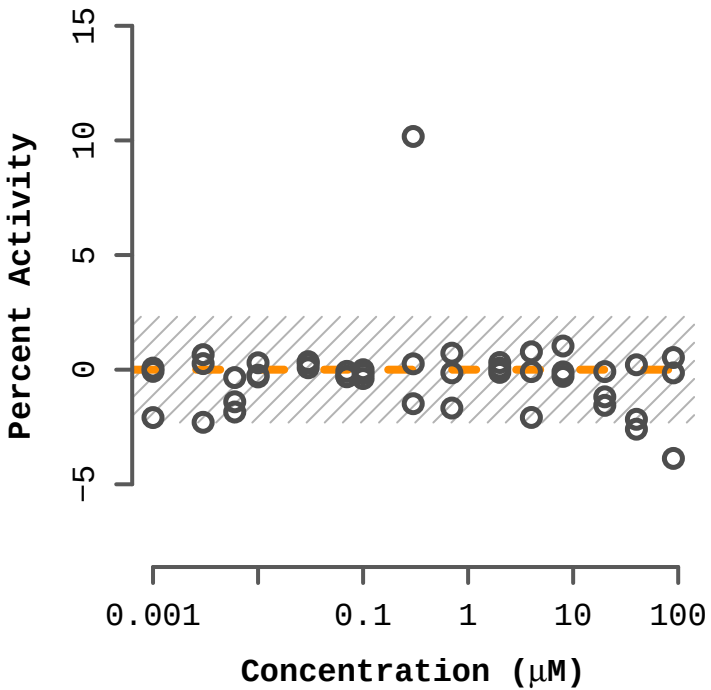
NAME: 1-Piperazineethanol
CHID: 21853 **CASRN:** 103-76-4
SPID(S): Tox21_302881
M4ID: 12476252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

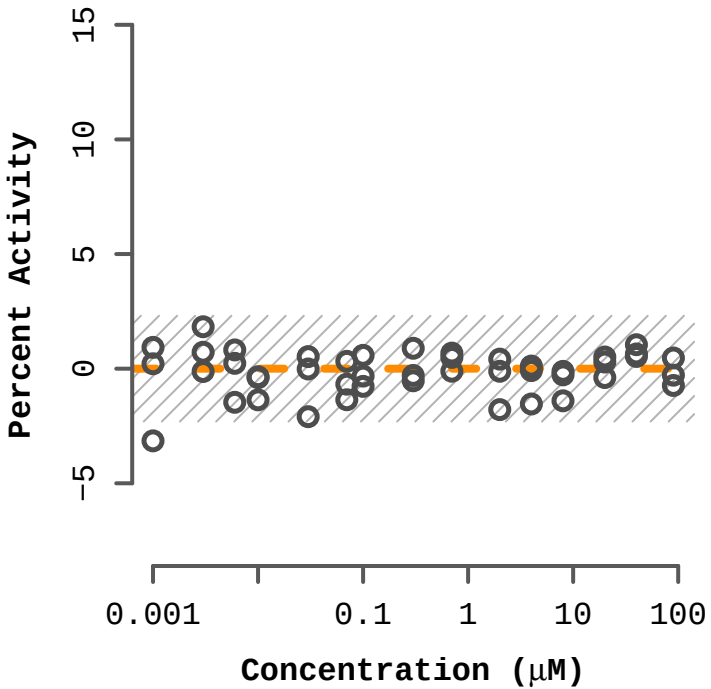
NAME: 1-Piperazineethanol
CHID: 21853 **CASRN:** 103-76-4
SPID(S): Tox21_201974
M4ID: 12480278

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 2.98 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

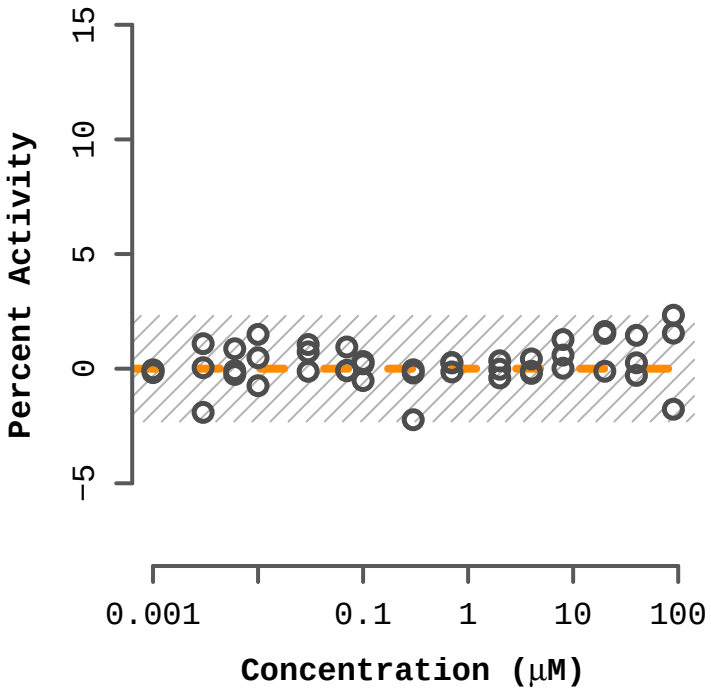
NAME: N,N−Dimethylbenzylamine
CHID: 21854 CASRN: 103−83−3
SPID(S): Tox21_200719
M4ID: 12481533

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.809 MAX_MED: 0.719 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

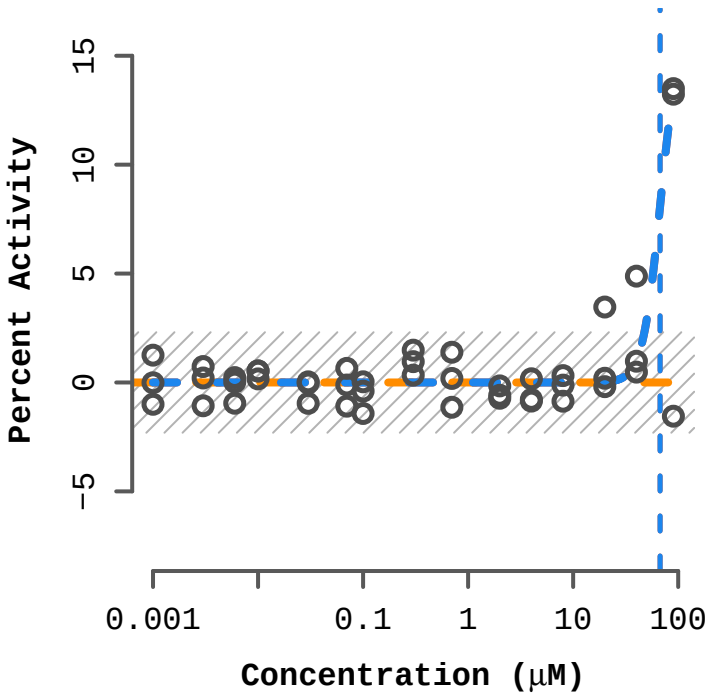
NAME: 4-Butylaniline
CHID: 21856 **CASRN:** 104-13-2
SPID(S): Tox21_303446
M4ID: 12475694

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chlorobenzaldehyde
CHID: 21860 CASRN: 104-88-1
SPID(S): Tox21_200136
M4ID: 12482116

HILL MODEL (in red):

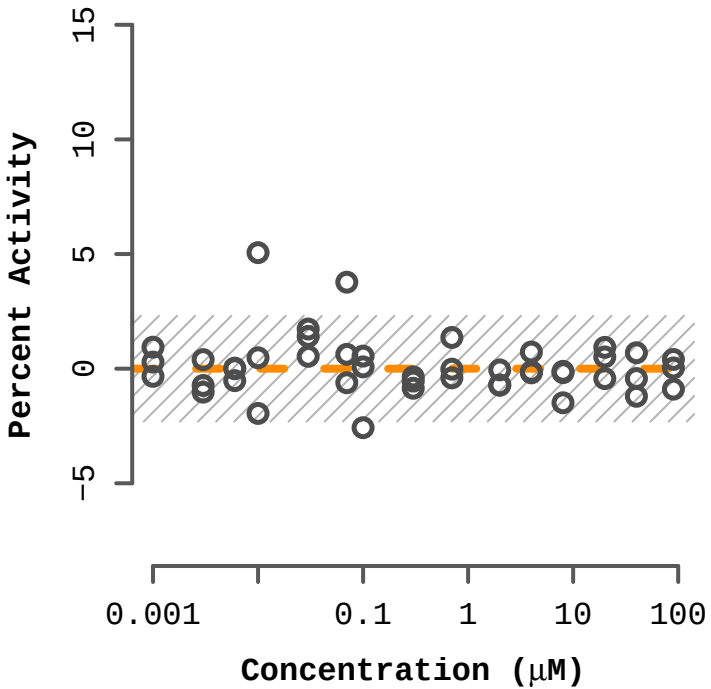
	tp	ga	gw
val:	16.2	1.83	5.21
sd:	4.94	0.0972	2.09

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.2	1.83	5.21	3.18	7
sd:	4.95	0.0974	2.1	10100	57800

	CNST	HILL	GNLS
AIC:	170.37	149.49	153.49
PROB:	0	0.88	0.12
RMSE:	3.04	2.44	2.44

MAX_MEAN: 8.39 MAX_MED: 13.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

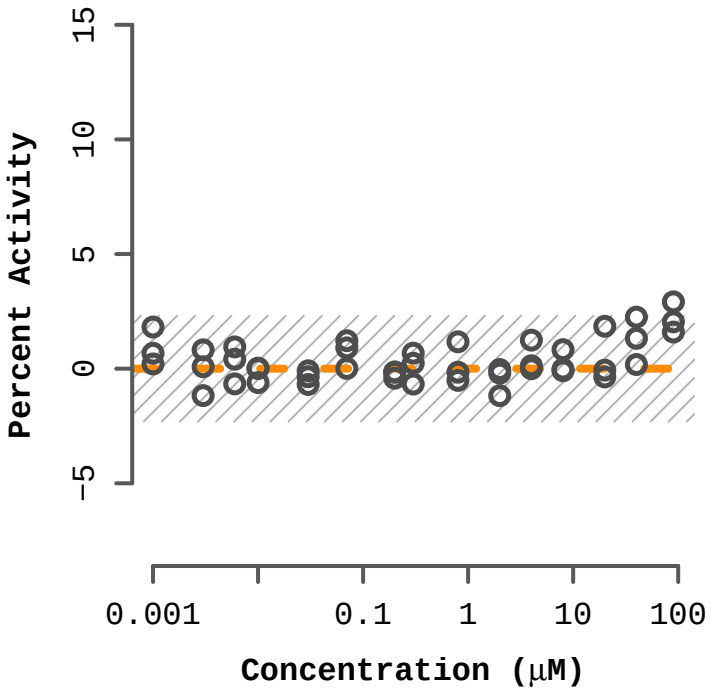
NAME: 5-Ethyl-2-methylpyridine
CHID: 21861 **CASRN:** 104-90-5
SPID(S): Tox21_303710
M4ID: 12475478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

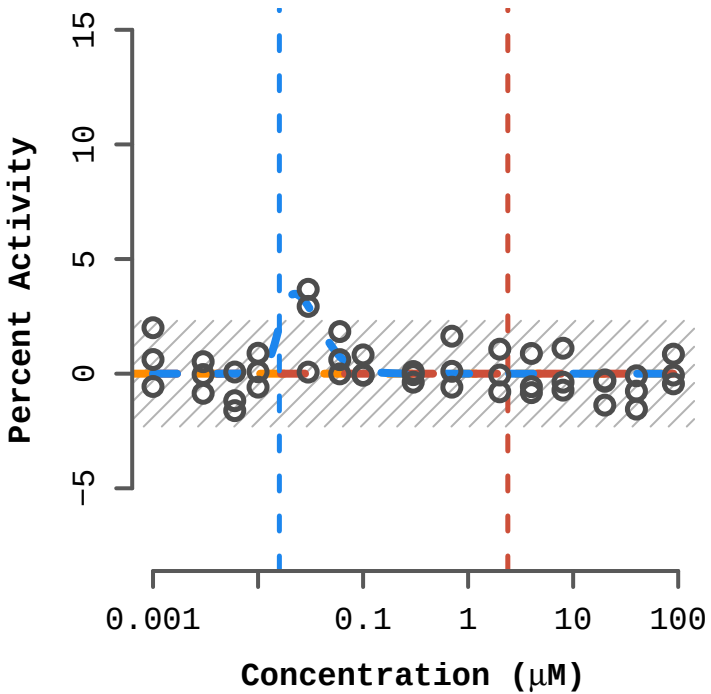
NAME: Diethyl propanedioate
CHID: 21863 CASRN: 105-53-3
SPID(S): Tox21_302931
M4ID: 12476202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 2.19 MAX_MED: 2.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethyl propanedioate
CHID: 21863 CASRN: 105-53-3
SPID(S): Tox21_201362
M4ID: 12480890

HILL MODEL (in red):

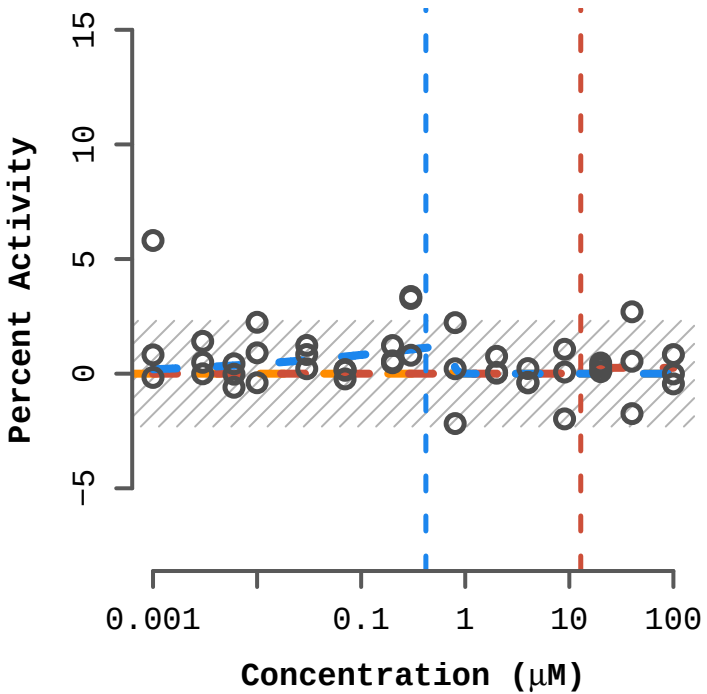
	tp	ga	gw
val:	2.66e-11	0.378	2.09
sd:	3.12e-06	123000	404000

GAIN-LOSS MODEL (in blue):

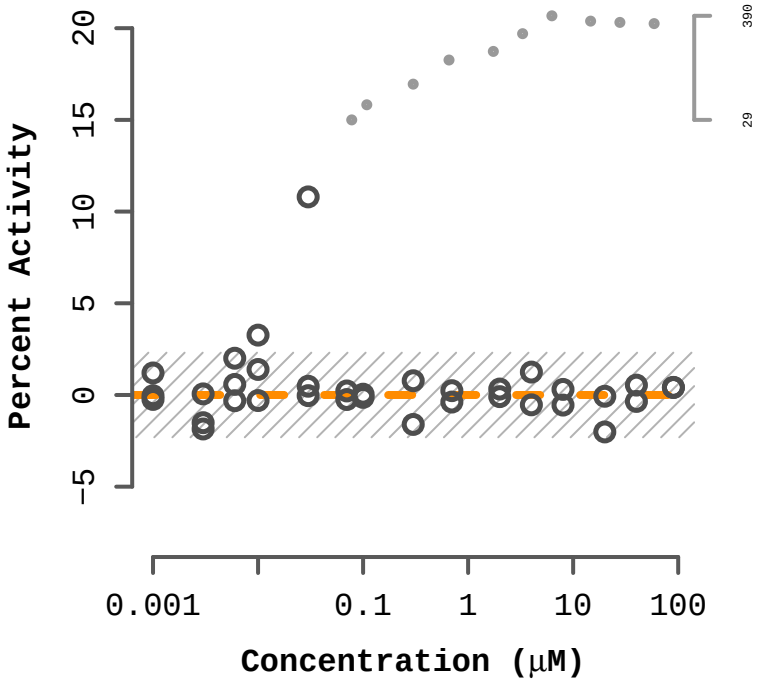
	tp	ga	gw	la	lw
val:	4.42	-1.8	7.89	-1.43	3.3
sd:	7.47	0.638	20.3	0.548	4.15

	CNST	HILL	GNLS
AIC:	130.97	136.97	129.65
PROB:	0.34	0.02	0.65
RMSE:	1.08	1.08	0.9

MAX_MEAN: 2.23 MAX_MED: 2.94 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,4-Dimethylphenol
CHID:    21864   CASRN: 105-67-9
SPID(S): Tox21_300051
M4ID:    12479079

HILL MODEL (in red):
      tp       ga       gw
val:  0.255    1.11     8
sd:   0.345    1.09     47.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.26     -0.378   0.392    -0.128   18
sd:   8.64     6.03     0.447    0.348    200

      CNST        HILL        GNLS
AIC:  152.58      158         152
PROB: 0.42        0.03        0.56
RMSE: 1.48        1.47        1.33

MAX_MEAN: 2.49      MAX_MED: 3.28      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

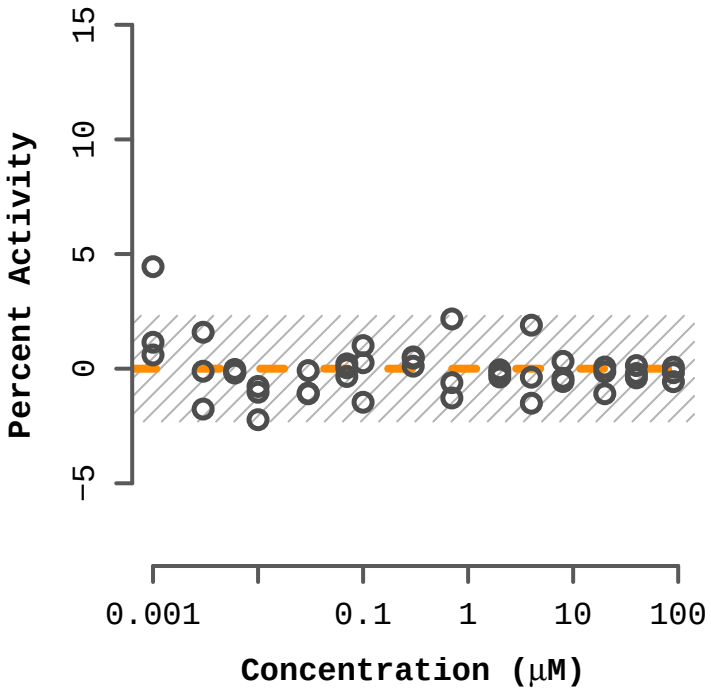
NAME: 2,4-Dimethylphenol
CHID: 21864 **CASRN:** 105-67-9
SPID(S): Tox21_201787
M4ID: 12480465 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	538.54	NA	NA
PROB:	1	NA	NA
RMSE:	136.05	NA	NA

MAX_MEAN: 131 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

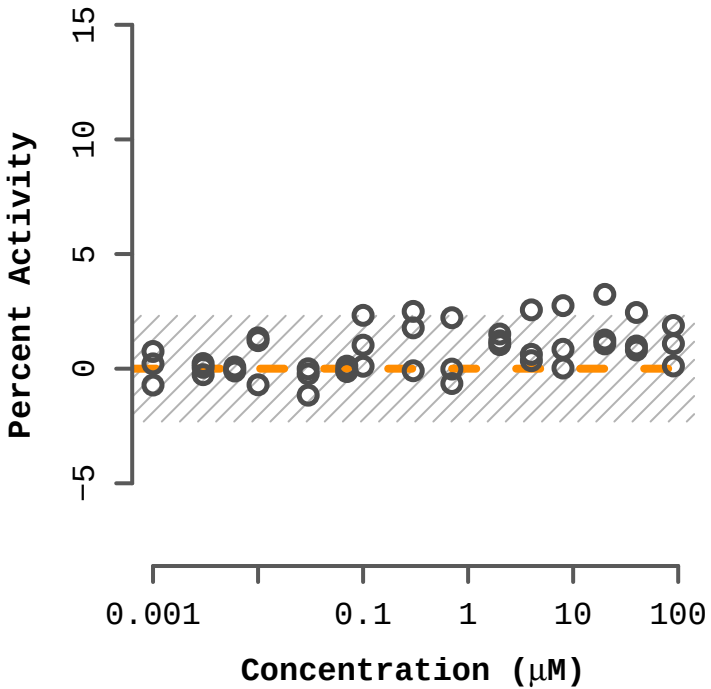
NAME: Dibutyl hexanedioate
CHID: 21866 **CASRN:** 105-99-7
SPID(S): Tox21_300166
M4ID: 12478964

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

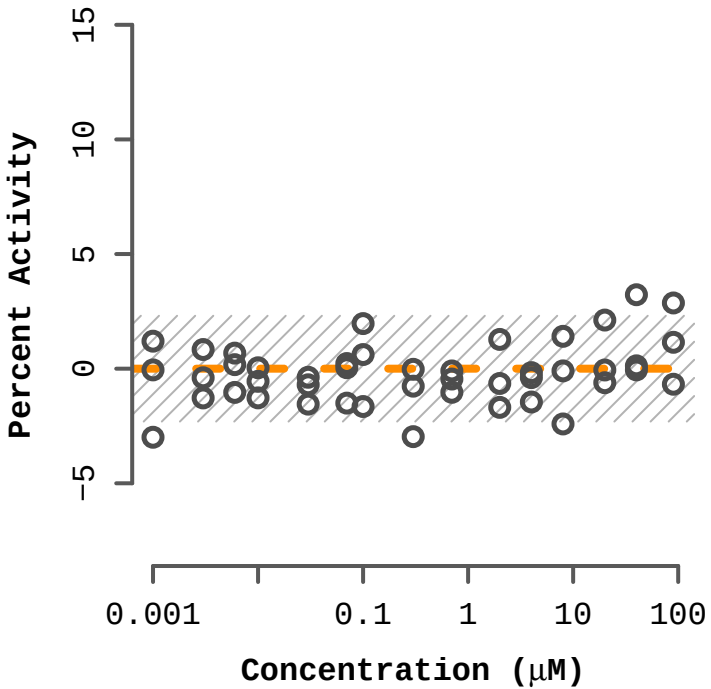
NAME: 4-Bromoaniline
CHID: 21867 **CASRN:** 106-40-1
SPID(S): Tox21_302910
M4ID: 12476223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

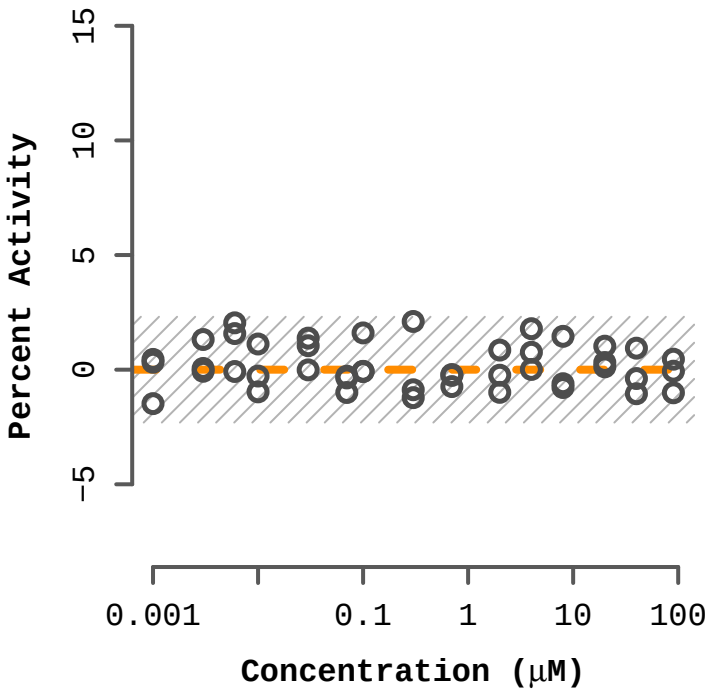
NAME: 4-Bromoaniline
CHID: 21867 **CASRN:** 106-40-1
SPID(S): Tox21_202459
M4ID: 12479793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

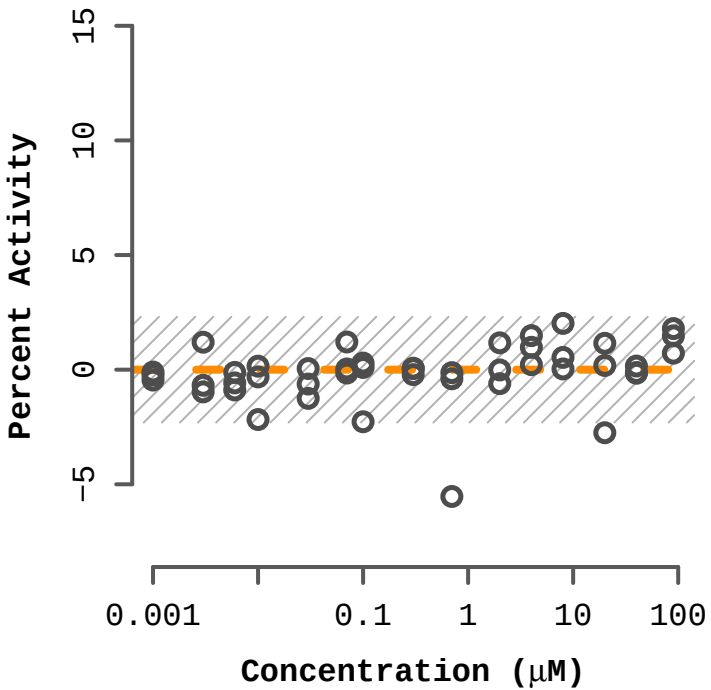
NAME: p-Xylene
CHID: 21868 **CASRN:** 106-42-3
SPID(S): Tox21_201113
M4ID: 12481139

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

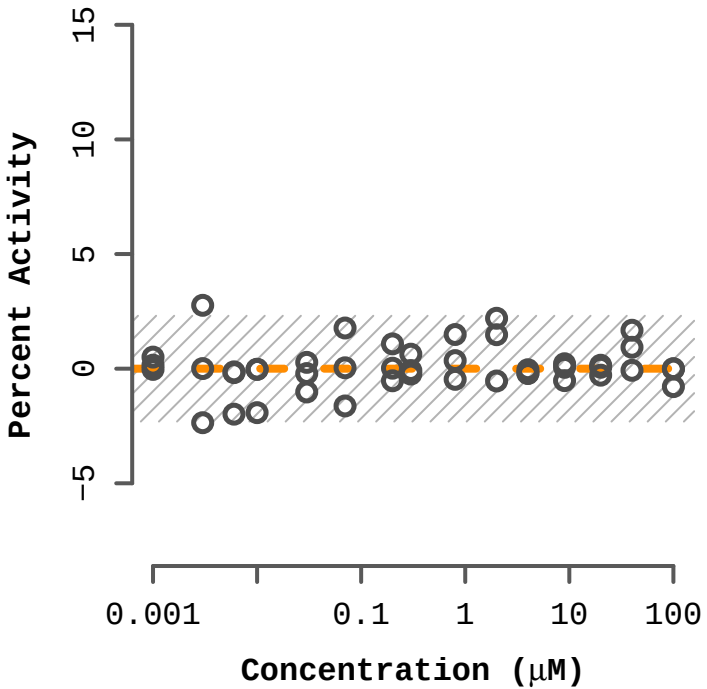
NAME: p-Cresol
CHID: 21869 **CASRN:** 106-44-5
SPID(S): Tox21_300029
M4ID: 12479101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

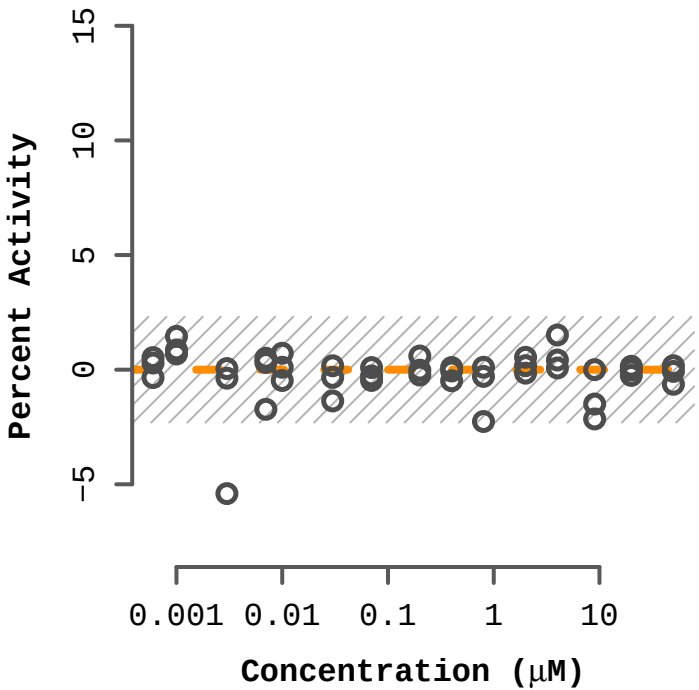
NAME: p-Cresol
CHID: 21869 **CASRN:** 106-44-5
SPID(S): Tox21_200402
M4ID: 12481850

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.15	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

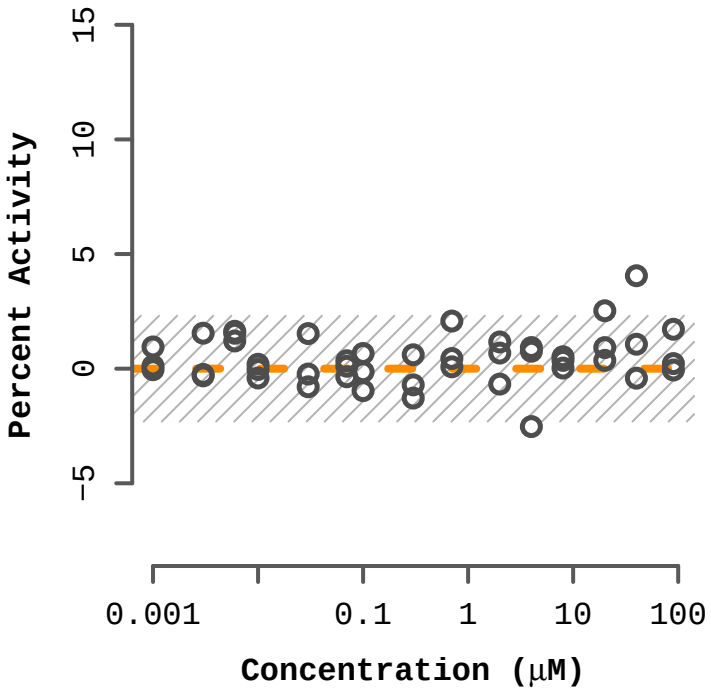
NAME: p-Cresol
CHID: 21869 CASRN: 106-44-5
SPID(S): Tox21_113445_1
M4ID: 12482650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.864 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

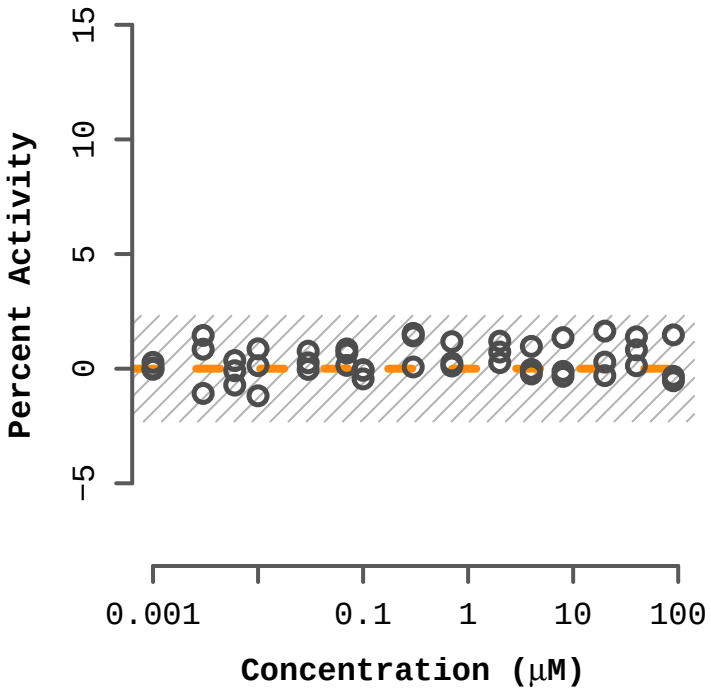
NAME: 4-Chlorophenol
CHID: 21871 CASRN: 106-48-9
SPID(S): Tox21_302860
M4ID: 12476273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.57 MAX_MED: 1.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

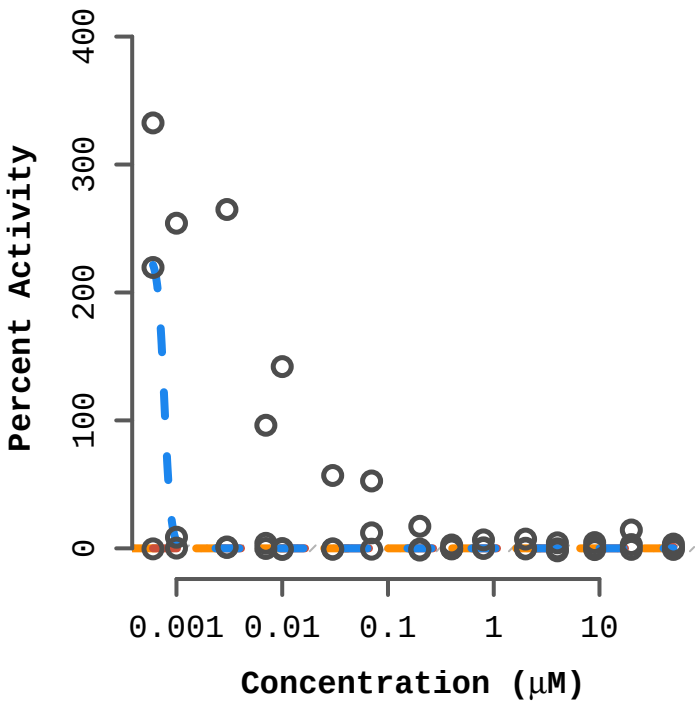
NAME: 4-Chlorophenol
CHID: 21871 **CASRN:** 106-48-9
SPID(S): Tox21_201704
M4ID: 12480548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chlorophenol
CHID: 21871 CASRN: 106-48-9
SPID(S): Tox21_111028_1
M4ID: 12483942

HILL MODEL (in red):

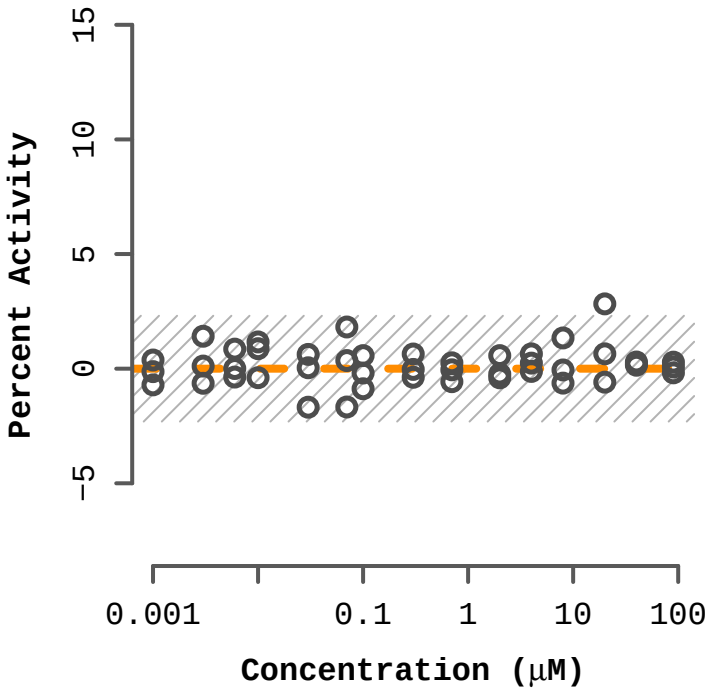
	tp	ga	gw
val:	214	2.2	4.53
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	230	-4.18	2.23	-3.11	14
sd:	888	101	14.6	0.011	12.1

	CNST	HILL	GNLS
AIC:	467.43	473.39	466.21
PROB:	0.35	0.02	0.64
RMSE:	85.63	85.63	71.48

MAX_MEAN: 184 MAX_MED: 220 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

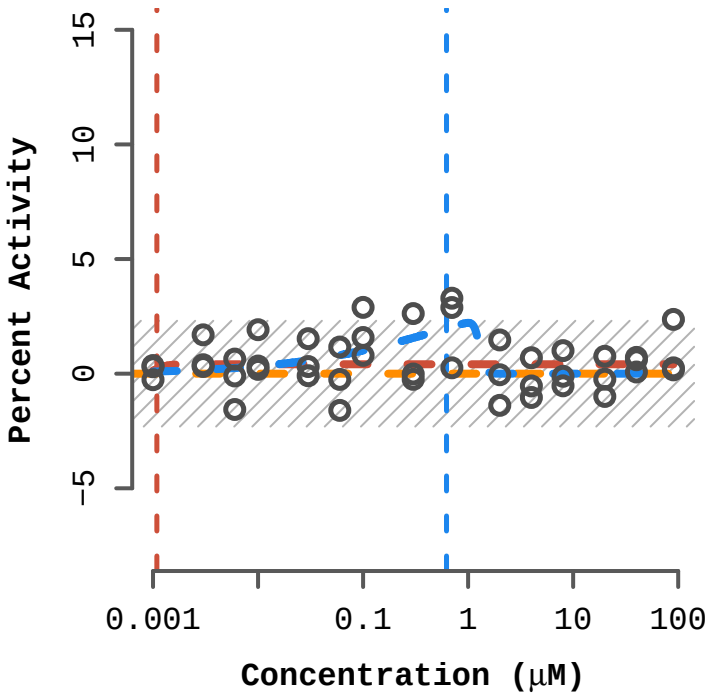
NAME: 4-Methylaniline
CHID: 21872 CASRN: 106-49-0
SPID(S): Tox21_300168
M4ID: 12478962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.963 MAX_MED: 0.874 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylaniline
CHID: 21872 **CASRN:** 106-49-0
SPID(S): Tox21_202142
M4ID: 12480110

HILL MODEL (in red):

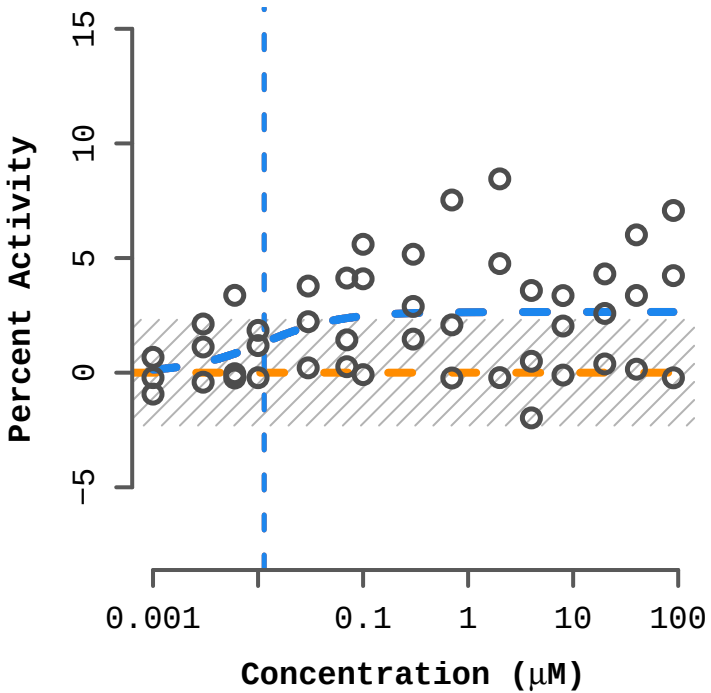
	tp	ga	gw
val:	0.411	−2.96	8
sd:	0.165	0.392	69.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.95	−0.206	0.583	0.105	17.7
sd:	4.42	1.45	0.376	2.36	182

	CNST	HILL	GNLS
AIC:	147.44	147.16	145.81
PROB:	0.23	0.26	0.51
RMSE:	1.24	1.14	1.04

MAX_MEAN: 2.15 **MAX_MED:** 2.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isobutyl acrylate
CHID: 21873 CASRN: 106-63-8
SPID(S): Tox21_200184
M4ID: 12482068

HILL MODEL (in red):

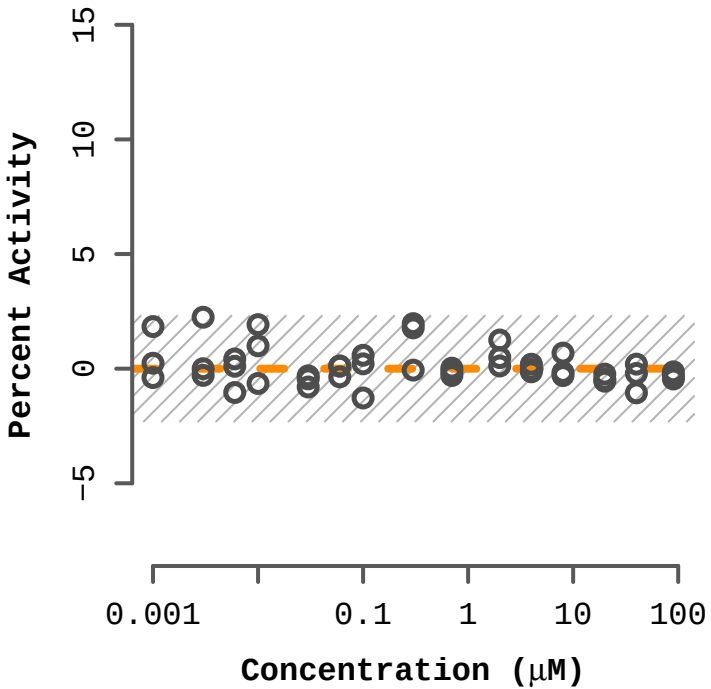
	tp	ga	gw
val:	2.65	−1.94	1.21
sd:	0.509	0.418	1.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.65	−1.94	1.21	3.54	17.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	235.97	211.52	215.52
PROB:	0	0.88	0.12
RMSE:	3.25	2.25	2.25

MAX_MEAN: 4.33 MAX_MED: 4.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

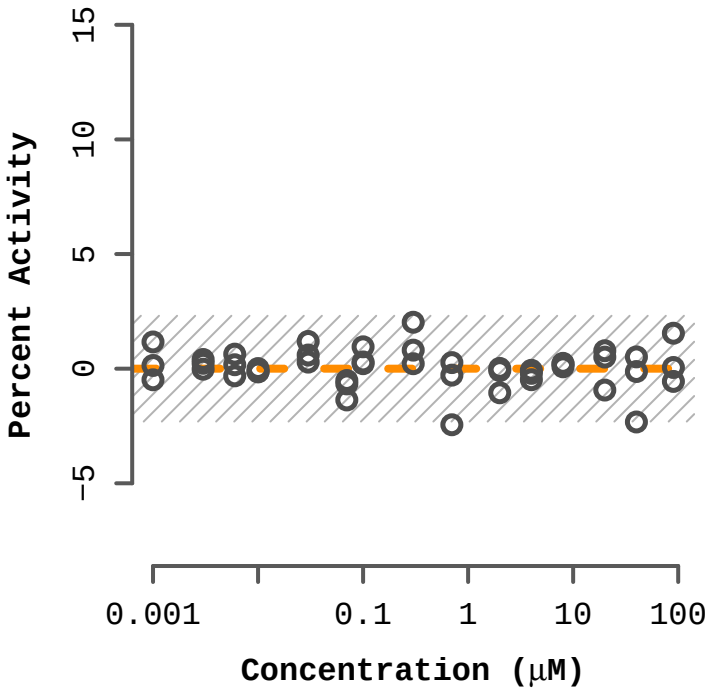
NAME: 1-Bromopropane
CHID: 21874 CASRN: 106-94-5
SPID(S): Tox21_200619
M4ID: 12481633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.23 MAX_MED: 1.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

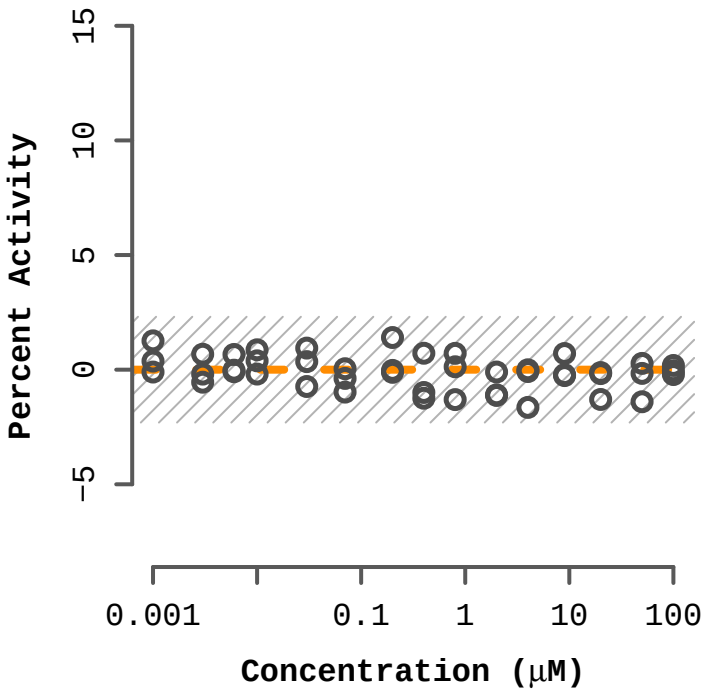
NAME: 2-Chloroethanol
CHID: 21877 CASRN: 107-07-3
SPID(S): Tox21_300043
M4ID: 12479087

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.02 MAX_MED: 0.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

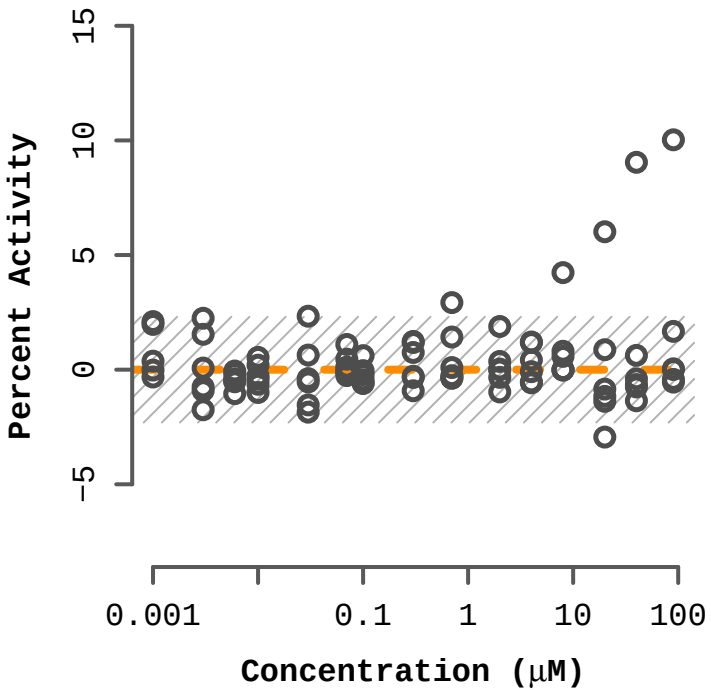
NAME: Propionitrile
CHID: 21879 **CASRN:** 107-12-0
SPID(S): Tox21_201135
M4ID: 12481117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.511 **MAX_MED:** 0.388 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

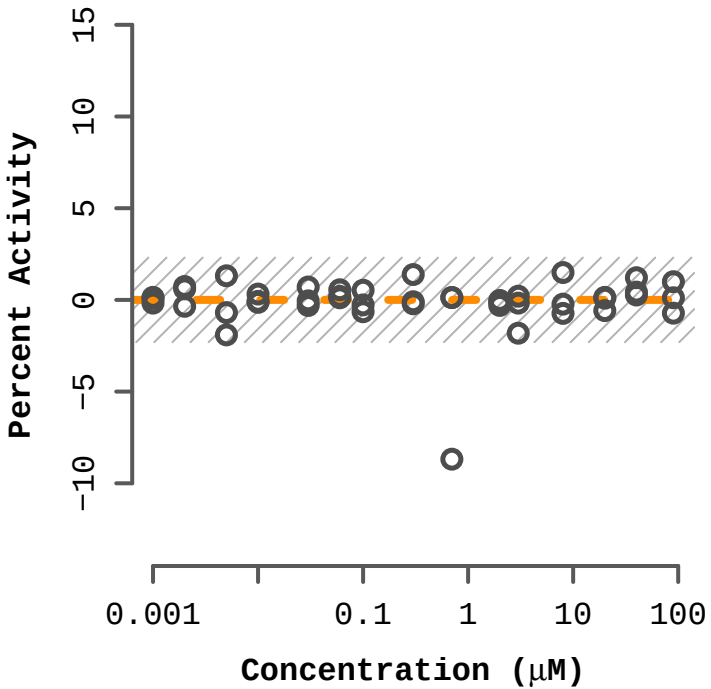
NAME: Ethylenediamine
CHID: 21881 **CASRN:** 107-15-3
SPID(S): Tox21_201202
M4ID: 12481050

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	304.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 0.373 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

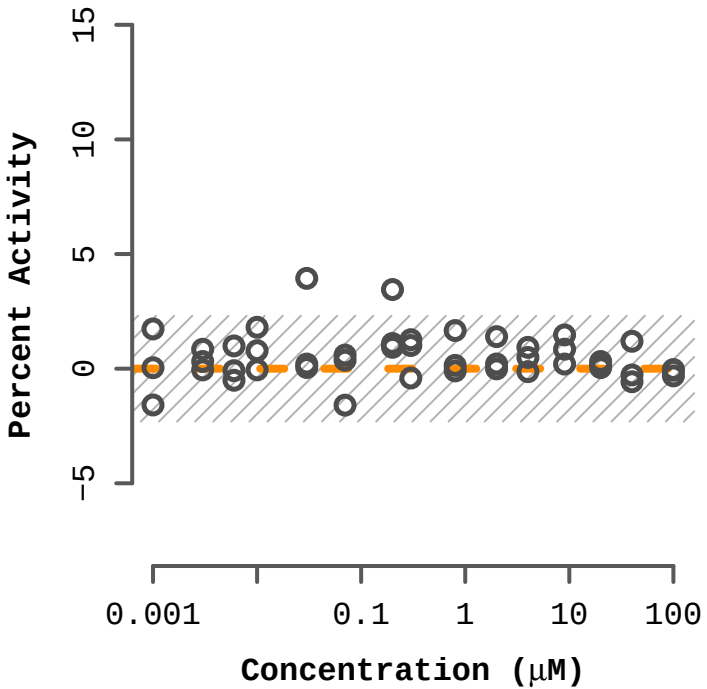
NAME: Propargyl alcohol
CHID: 21883 **CASRN:** 107-19-7
SPID(S): Tox21_200976
M4ID: 12481276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 0.603 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

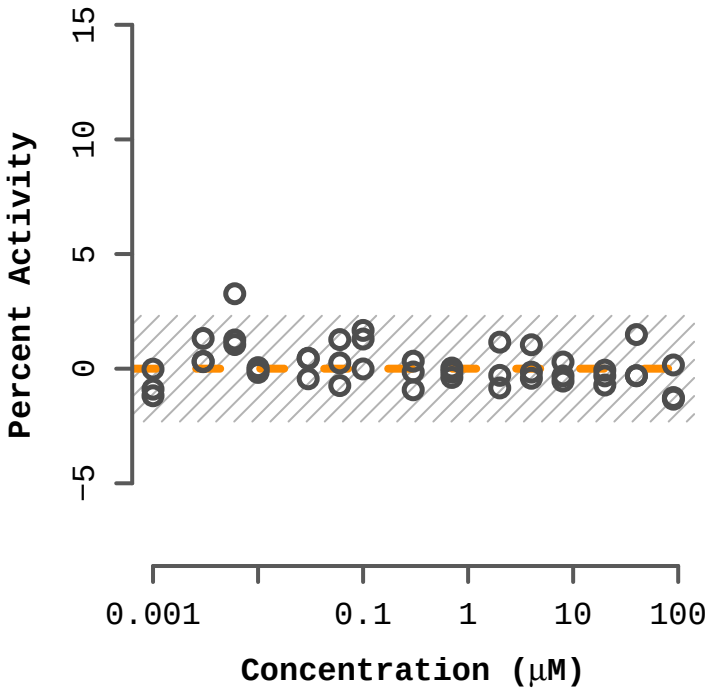
NAME: 2-Methyl-2,4-pentanediol
CHID: 21885 **CASRN:** 107-41-5
SPID(S): Tox21_302818
M4ID: 12476315

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

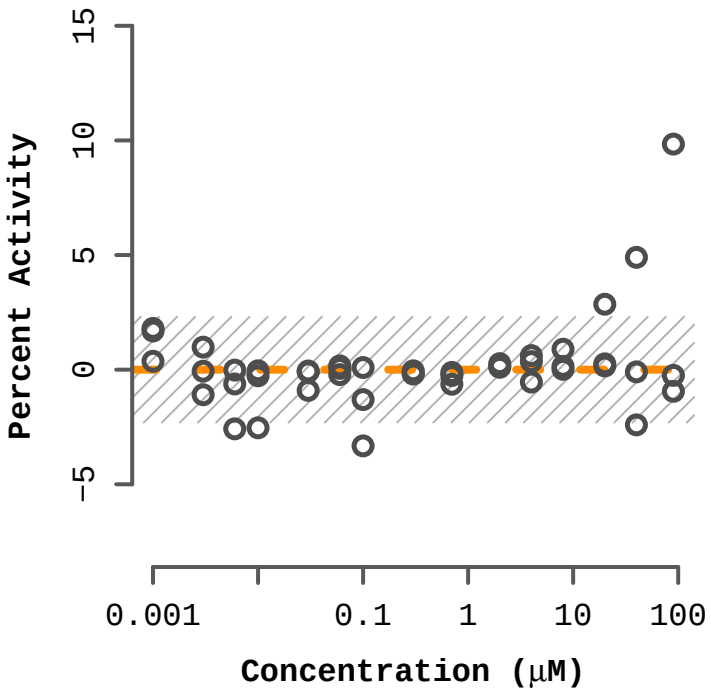
NAME: 2-Methyl-2,4-pentanediol
CHID: 21885 **CASRN:** 107-41-5
SPID(S): Tox21_201975
M4ID: 12480277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

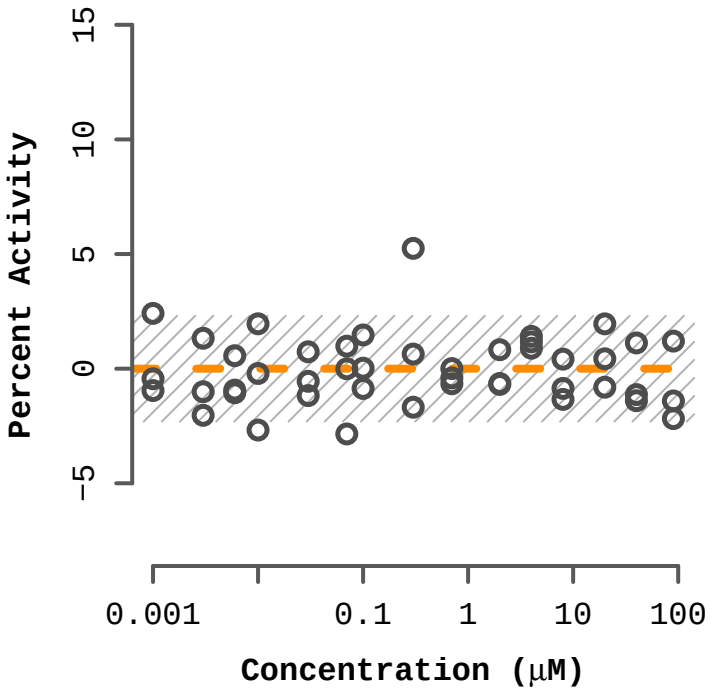
NAME: 2,4,4−Trimethyl−2−pentanamine
CHID: 21886 **CASRN:** 107−45−9
SPID(S): Tox21_200077
M4ID: 12482175

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 2.88 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

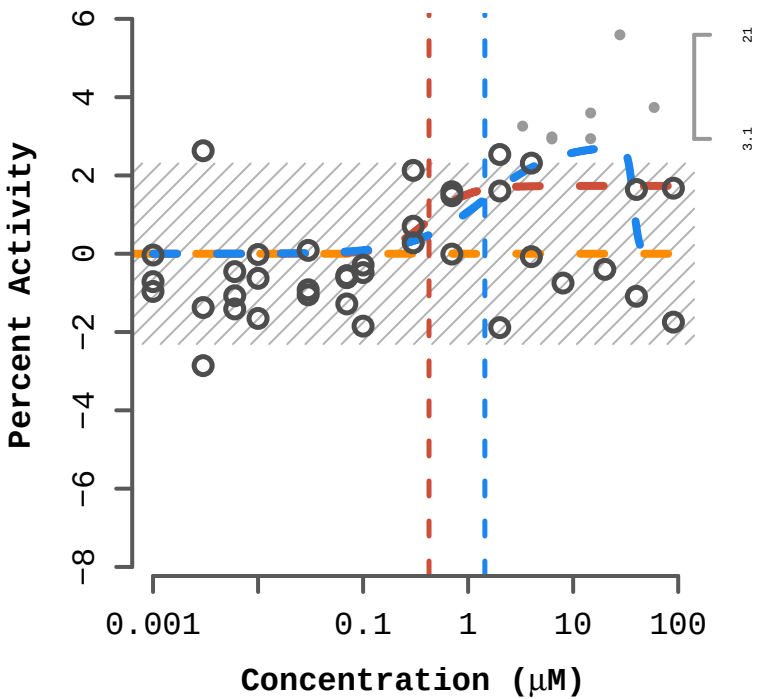
NAME: 2-Pentanone
CHID: 21888 **CASRN:** 107-87-9
SPID(S): Tox21_303016
M4ID: 12476117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Pentanone
CHID: 21888 CASRN: 107-87-9
SPID(S): Tox21_201670
M4ID: 12480582 BRK

HILL MODEL (in red):

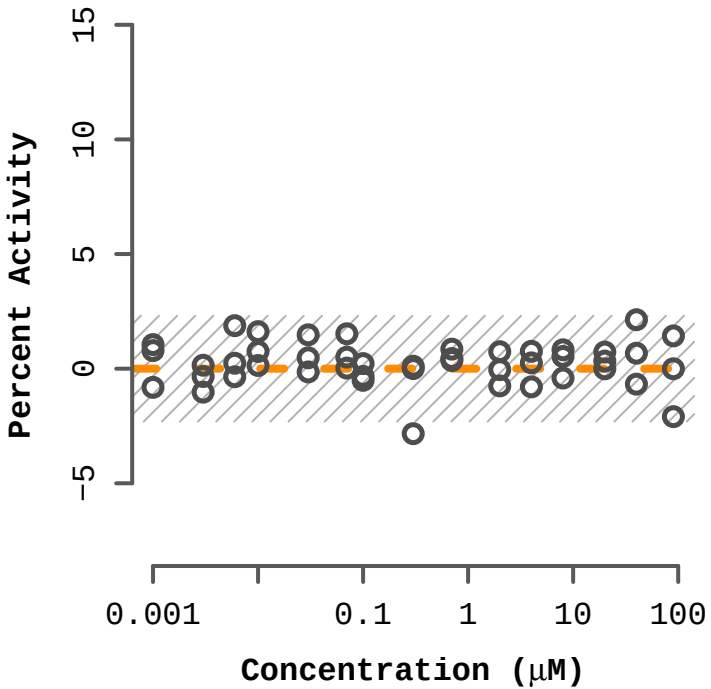
	tp	ga	gw
val:	1.73	-0.372	2.34
sd:	0.854	0.875	3.89

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.79	0.159	1.29	1.57	16.4
sd:	1.58	0.735	0.953	0.249	138

	CNST	HILL	GNLS
AIC:	217.59	212.38	215.54
PROB:	0.06	0.78	0.16
RMSE:	3.99	3.56	3.72

MAX_MEAN: 7.29 MAX_MED: 3.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

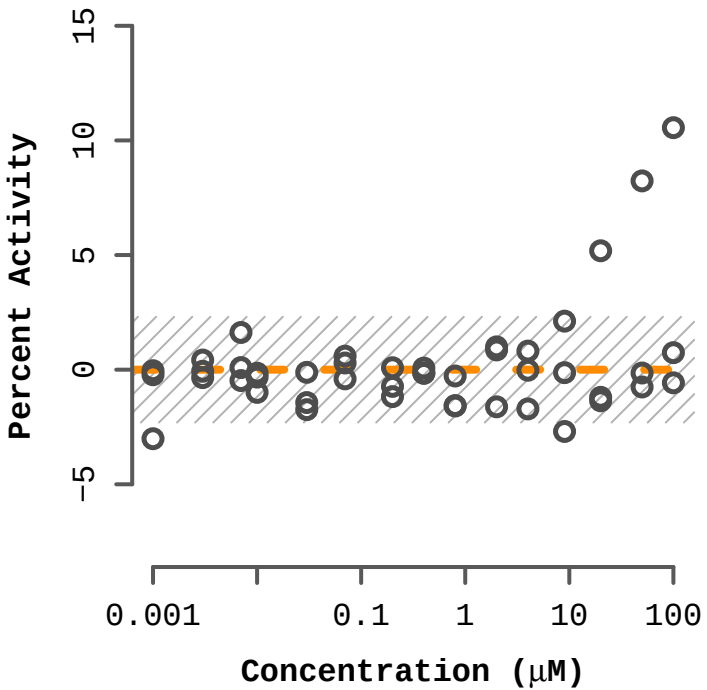
NAME: 4-Methyl-2-pentanone
CHID: 21889 **CASRN:** 108-10-1
SPID(S): Tox21_201108
M4ID: 12481144

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.837 **MAX_MED:** 0.789 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

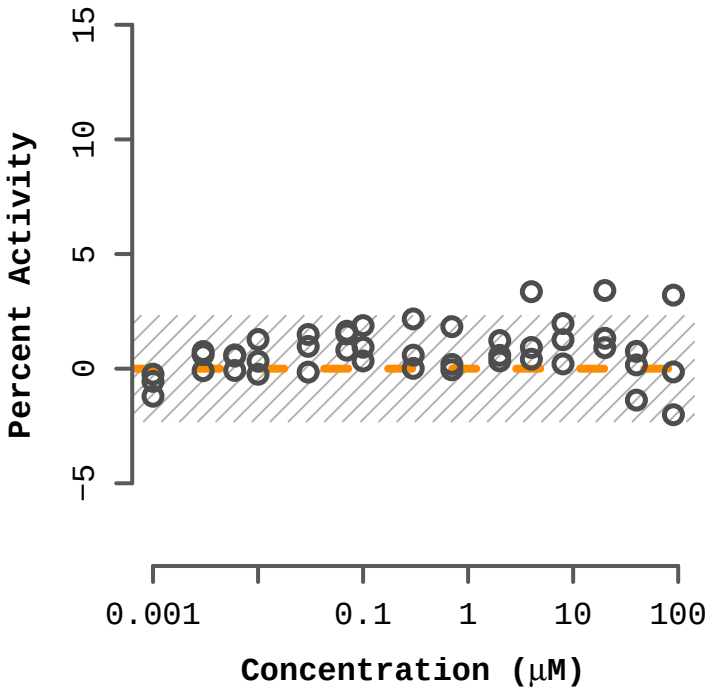
NAME: Isopropyl ether
CHID: 21890 **CASRN:** 108-20-3
SPID(S): Tox21_202551
M4ID: 12479701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.69	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 3.58 **MAX_MED:** 0.863 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

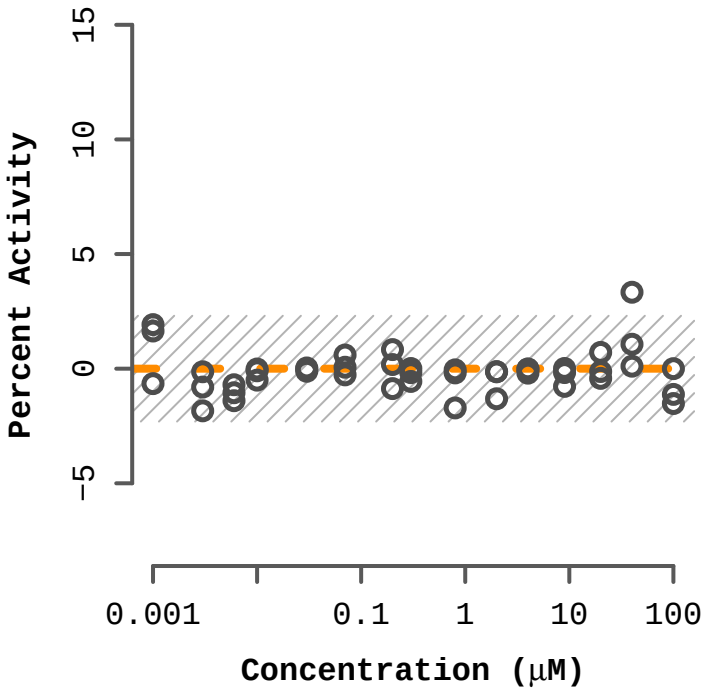
NAME: 4-Methylpyridine
CHID: 21892 **CASRN:** 108-89-4
SPID(S): Tox21_302961
M4ID: 12476172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

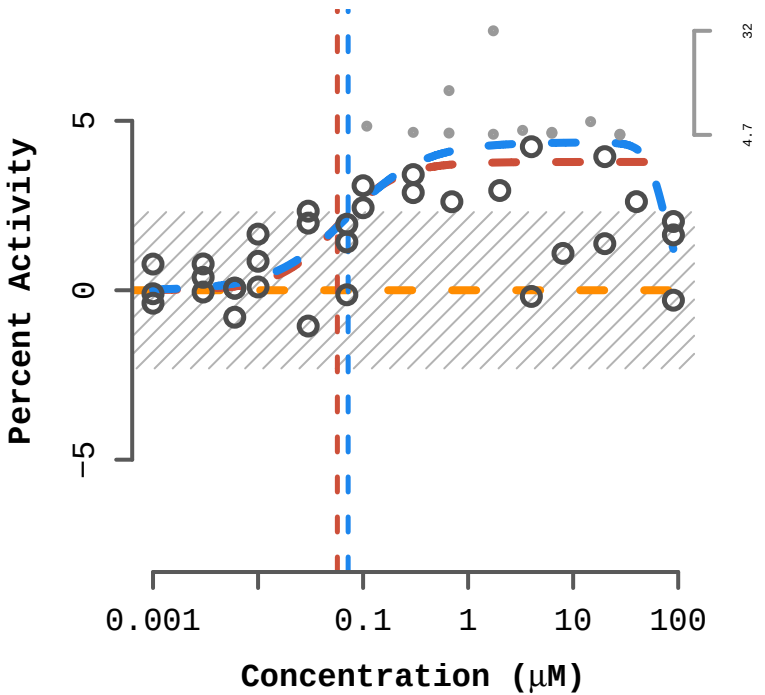
NAME: 4-Methylpyridine
CHID: 21892 CASRN: 108-89-4
SPID(S): Tox21_201400
M4ID: 12480852

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.5 MAX_MED: 1.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclohexanol
CHID: 21894 CASRN: 108-93-0
SPID(S): Tox21_302803
M4ID: 12476330 BRK

HILL MODEL (in red):

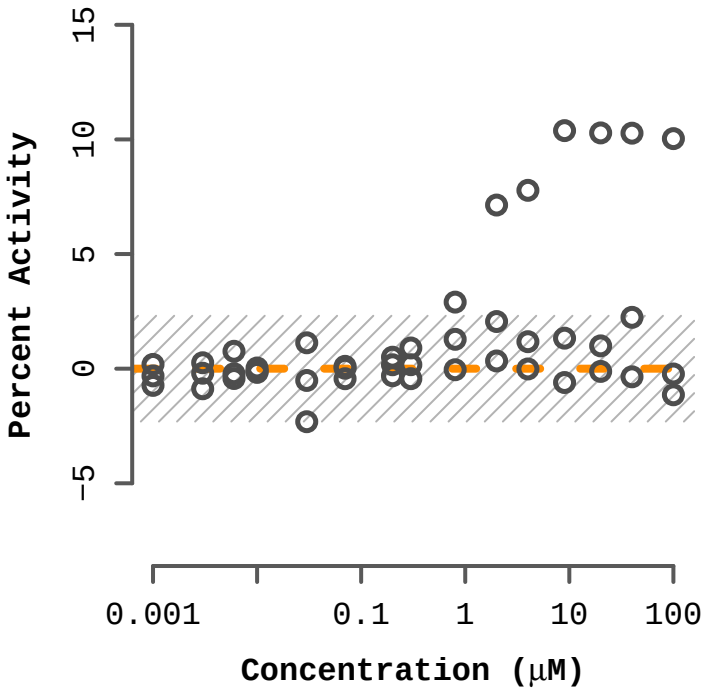
	tp	ga	gw
val:	3.79	−1.24	1.55
sd:	0.454	0.251	1.18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.37	−1.14	1.22	1.87	4.96
sd:	0.566	0.207	0.691	0.14	7.09

	CNST	HILL	GNLS
AIC:	263.93	219.89	215.29
PROB:	0	0.09	0.91
RMSE:	6.23	4.92	4.78

MAX_MEAN: 13.3 MAX_MED: 5.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

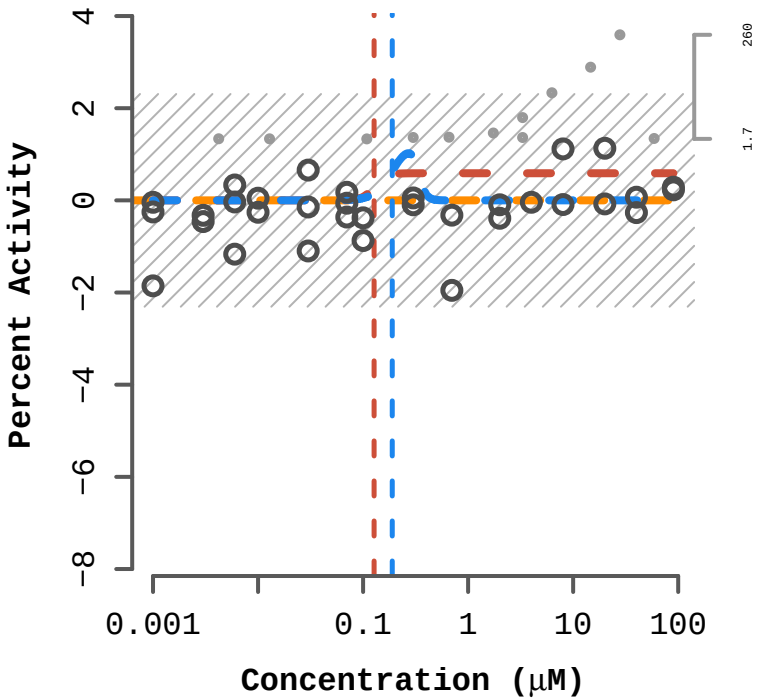
NAME: Cyclohexanol
CHID: 21894 **CASRN:** 108-93-0
SPID(S): Tox21_201481
M4ID: 12480771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.52	NA	NA
PROB:	1	NA	NA
RMSE:	3.55	NA	NA

MAX_MEAN: 4.05 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methylpyridine
CHID: 21897 CASRN: 108-99-6
SPID(S): Tox21_303001
M4ID: 12476132 BRK

HILL MODEL (in red):

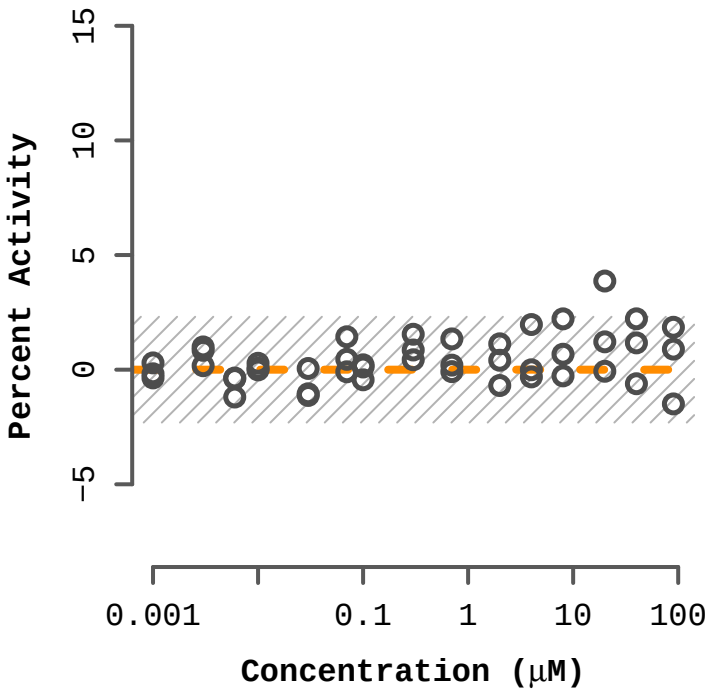
	tp	ga	gw
val:	0.588	−0.895	8
sd:	0.472	1.23	66.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.27	−0.722	5.02	−0.472	12.5
sd:	25.8	11.6	143	2.7	351

	CNST	HILL	GNLS
AIC:	330.95	335.22	340.38
PROB:	0.89	0.1	0.01
RMSE:	50.81	50.64	50.81

MAX_MEAN: 86.4 MAX_MED: 5.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

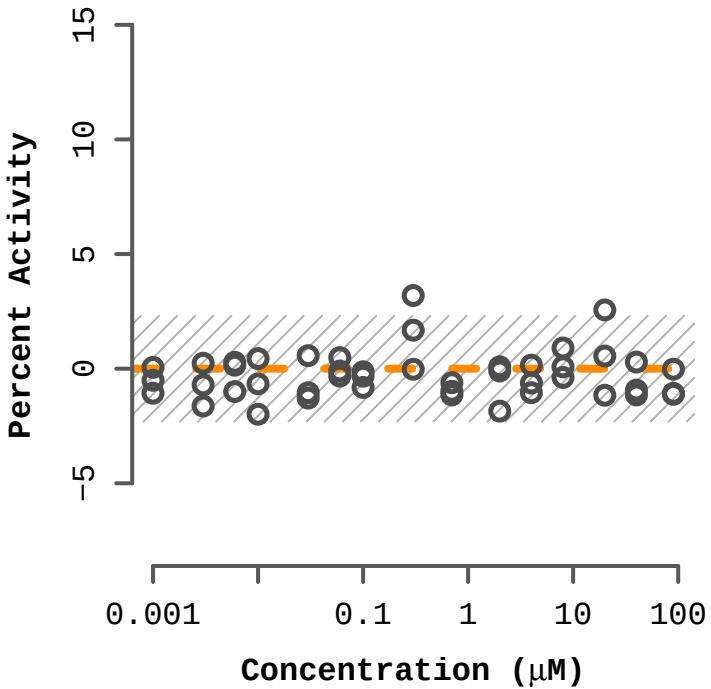
NAME: 3-Methylpyridine
CHID: 21897 **CASRN:** 108-99-6
SPID(S): Tox21_201966
M4ID: 12480286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

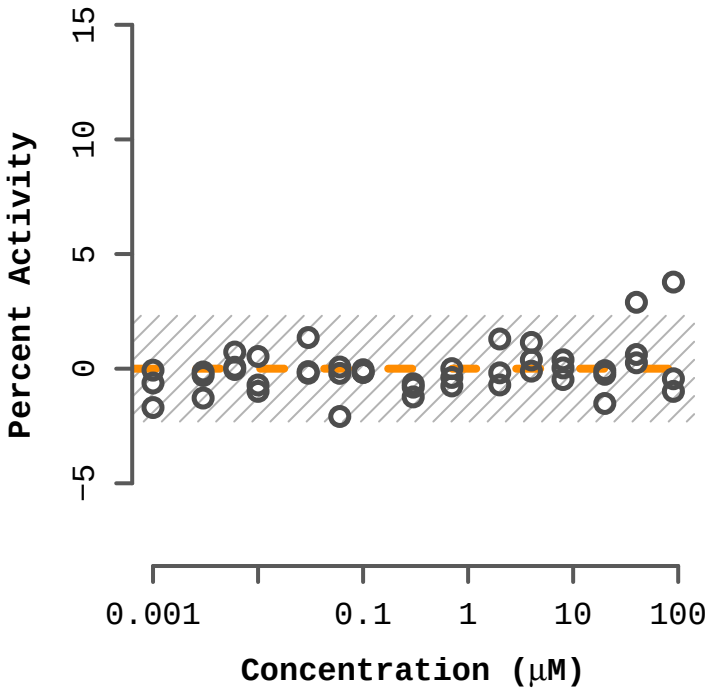
NAME: 2-Methylpyridine
CHID: 21899 CASRN: 109-06-8
SPID(S): Tox21_201693
M4ID: 12480559

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.62 MAX_MED: 1.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

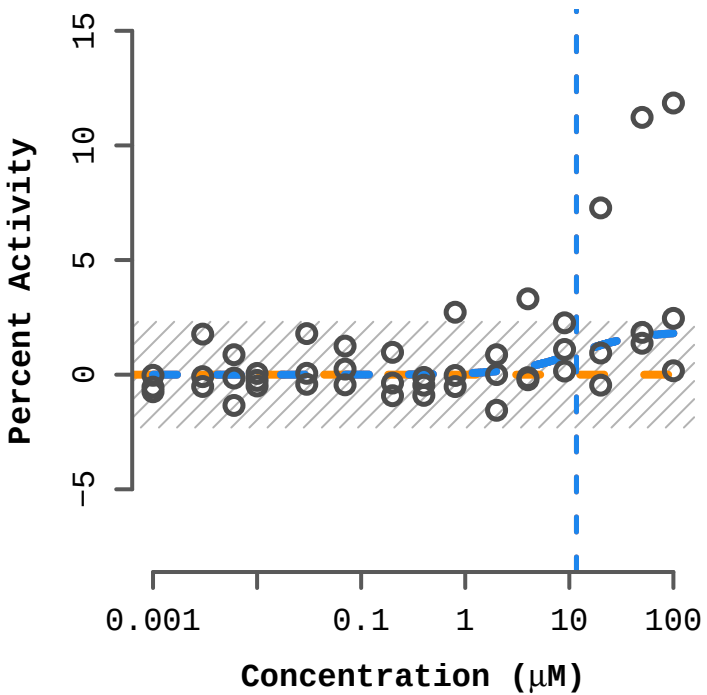
NAME: Propyl acetate
CHID: 21901 CASRN: 109-60-4
SPID(S): Tox21_202012
M4ID: 12480240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.26 MAX_MED: 0.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3-Dibromopropane
CHID: 21902 CASRN: 109-64-8
SPID(S): Tox21_202716
M4ID: 12479536

HILL MODEL (in red):

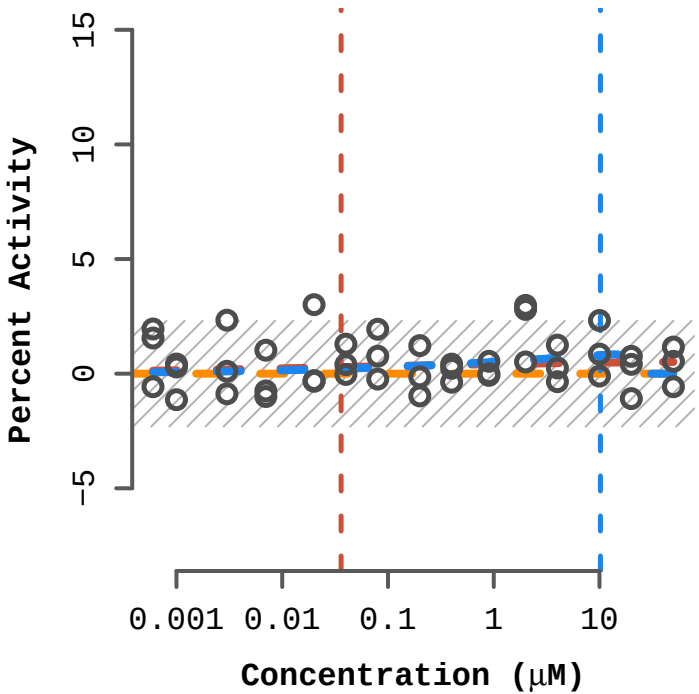
	tp	ga	gw
val:	1.89	1.07	1.4
sd:	1.35	0.841	1.72

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.89	1.07	1.4	3.37	3.97
sd:	1.35	0.841	1.72	1260	2800

	CNST	HILL	GNLS
AIC:	186.04	180.2	184.2
PROB:	0.05	0.84	0.11
RMSE:	2.89	2.46	2.46

MAX_MEAN: 4.83 MAX_MED: 2.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butylamine
CHID: 21904 **CASRN:** 109-73-9
SPID(S): Tox21_301131
M4ID: 12478002

HILL MODEL (in red):

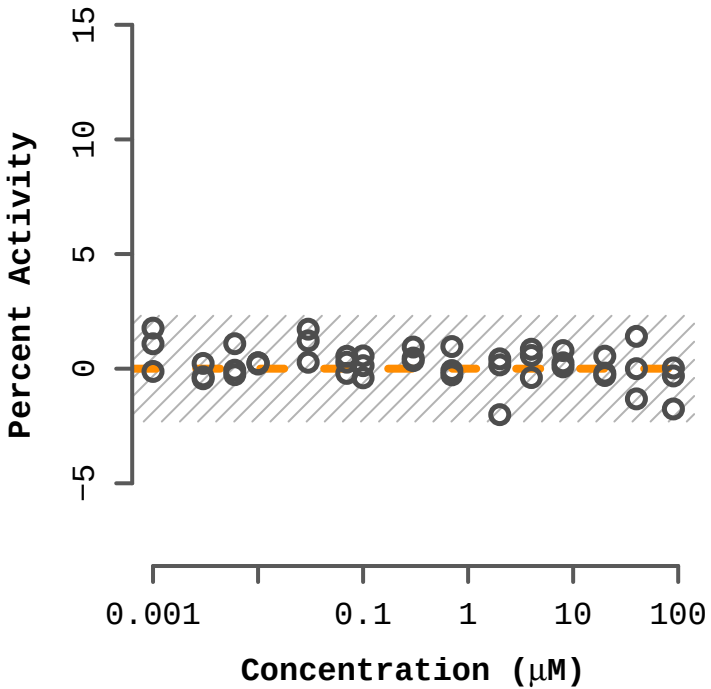
	tp	ga	gw
val:	0.57	-1.44	0.3
sd:	0.805	4.69	1.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.62	1.01	0.333	1.26	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	144.41	144.69	148.25
PROB:	0.5	0.43	0.07
RMSE:	1.2	1.1	1.08

MAX_MEAN: 2.1 **MAX_MED:** 2.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

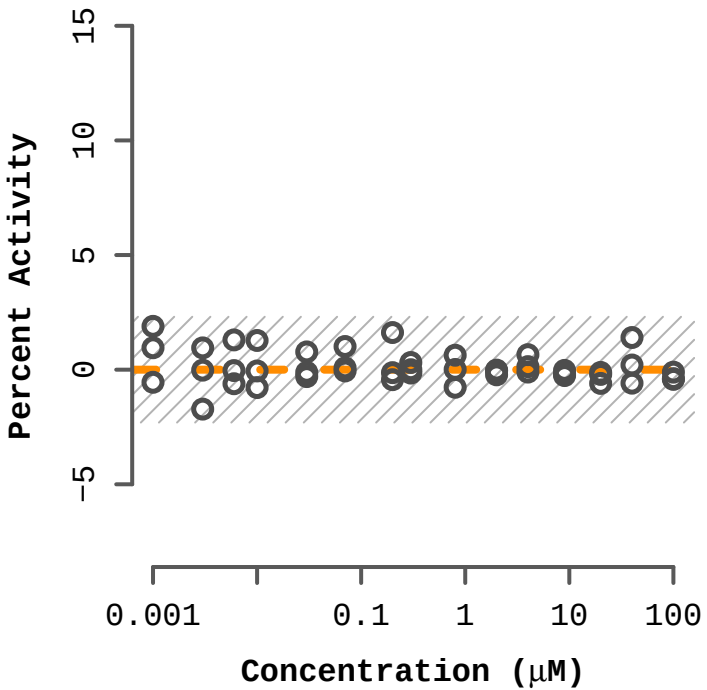
NAME: Propanedinitrile
CHID: 21907 CASRN: 109-77-3
SPID(S): Tox21_301196
M4ID: 12477937

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

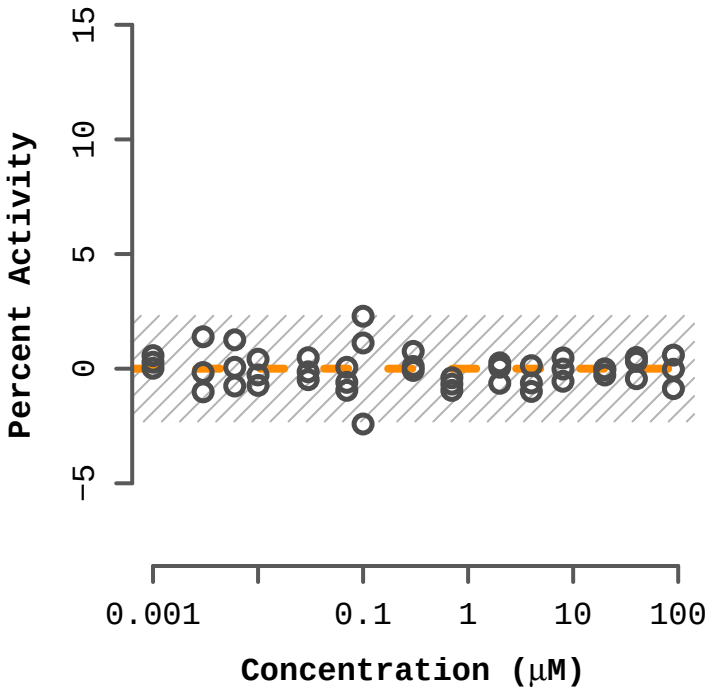
NAME: Diethylamine
CHID: 21909 **CASRN:** 109-89-7
SPID(S): Tox21_202506
M4ID: 12479746

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.767 **MAX_MED:** 0.958 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

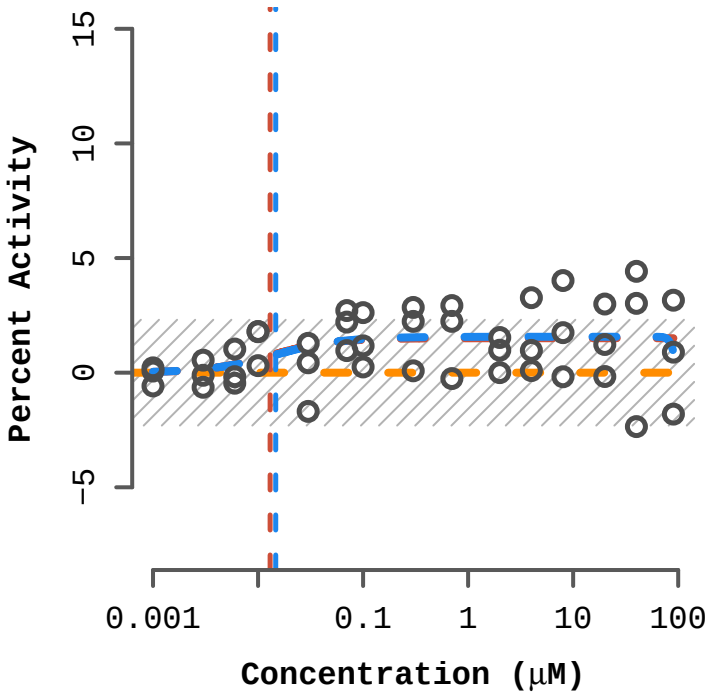
NAME: Pyrrole
CHID: 21910 CASRN: 109-97-7
SPID(S): Tox21_303910
M4ID: 12475278

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.333 MAX_MED: 1.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Methyl-2-hexanone
CHID: 21914 **CASRN:** 110-12-3
SPID(S): Tox21_302906
M4ID: 12476227

HILL MODEL (in red):

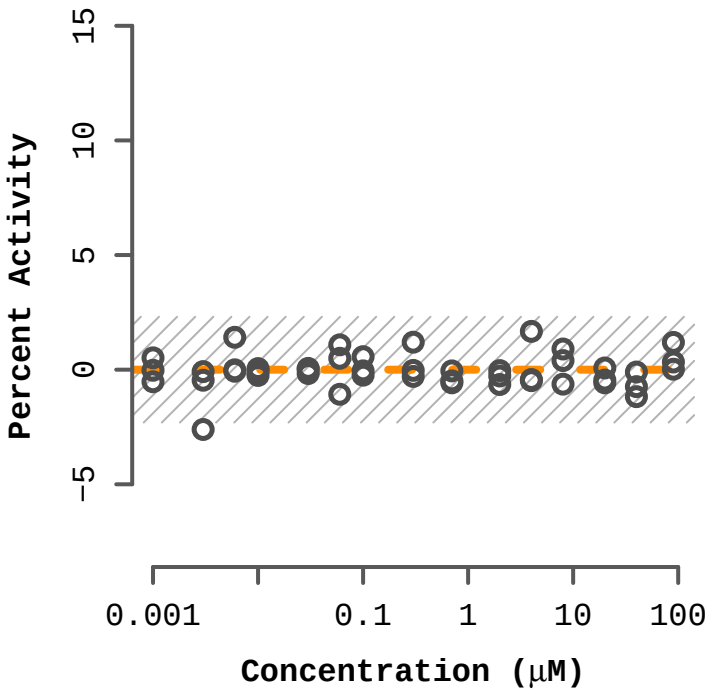
	tp	ga	gw
val:	1.5	−1.89	1.47
sd:	0.332	0.545	1.35

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.57	−1.83	1.38	1.96	17.6
sd:	0.35	0.517	1.1	0.0868	186

	CNST	HILL	GNLS
AIC:	188.04	169.08	172.73
PROB:	0	0.86	0.14
RMSE:	1.86	1.43	1.42

MAX_MEAN: 1.96 **MAX_MED:** 3.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

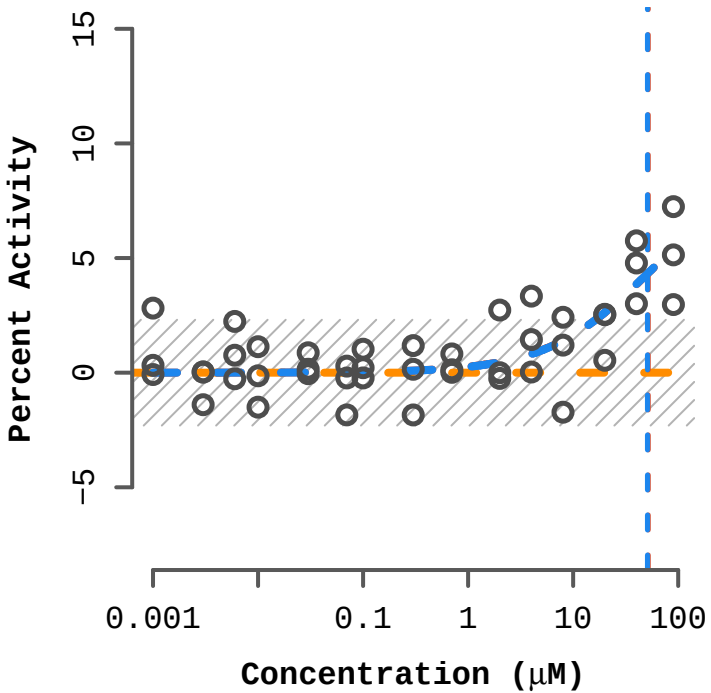
NAME: 5-Methyl-2-hexanone
CHID: 21914 **CASRN:** 110-12-3
SPID(S): Tox21_201346
M4ID: 12480906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.516 **MAX_MED:** 0.498 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethyl decanedioate
CHID: 21915 **CASRN:** 110-40-7
SPID(S): Tox21_301167
M4ID: 12477966

HILL MODEL (in red):

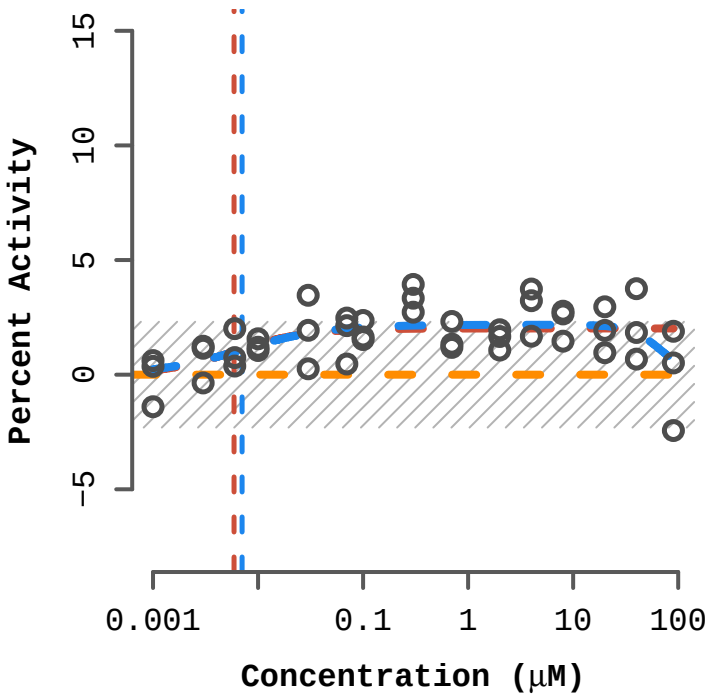
	tp	ga	gw
val:	8.69	1.71	0.883
sd:	6.47	0.765	0.465

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.69	1.71	0.894	3.57	1.22
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	196.44	157.54	161.53
PROB:	0	0.88	0.12
RMSE:	2.25	1.27	1.27

MAX_MEAN: 5.12 **MAX_MED:** 5.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Heptanone
CHID: 21916 CASRN: 110-43-0
SPID(S): Tox21_302935
M4ID: 12476198

HILL MODEL (in red):

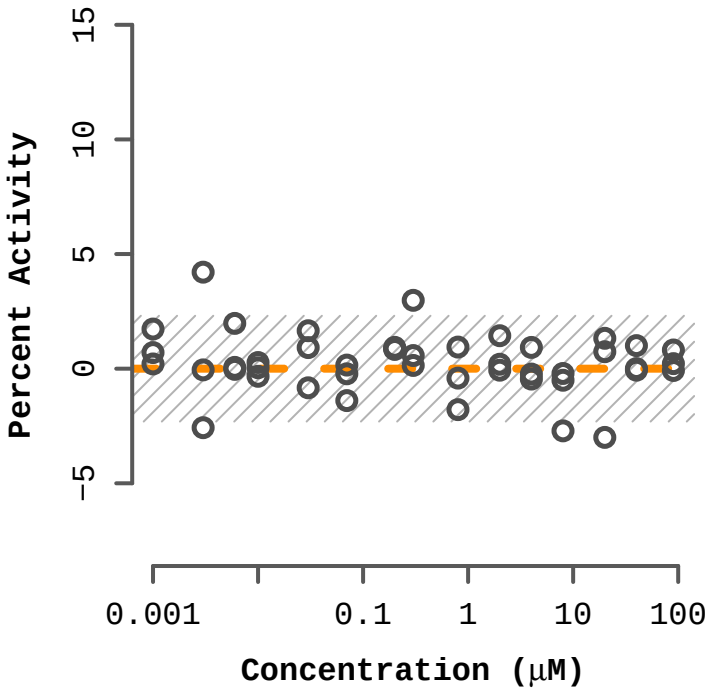
	tp	ga	gw
val:	2.02	−2.23	1.28
sd:	0.198	0.228	0.796

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.18	−2.15	1.08	1.83	3
sd:	0.254	0.25	0.665	0.192	3.65

	CNST	HILL	GNLS
AIC:	200.4	141.64	141.32
PROB:	0	0.46	0.54
RMSE:	2.05	1.13	1.01

MAX_MEAN: 3.33 MAX_MED: 3.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

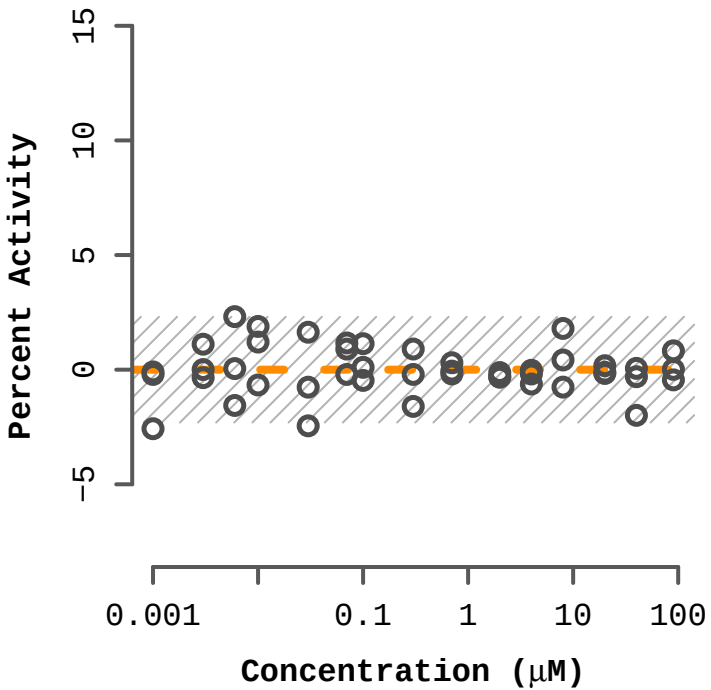
NAME: 2-Heptanone
CHID: 21916 **CASRN:** 110-43-0
SPID(S): Tox21_202164
M4ID: 12480088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.921 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

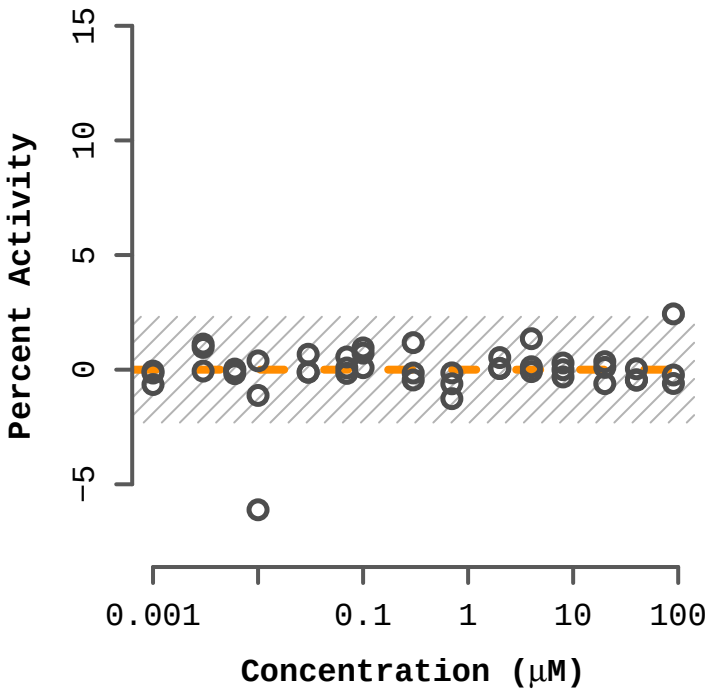
NAME: n-Hexane
CHID: 21917 **CASRN:** 110-54-3
SPID(S): Tox21_200777
M4ID: 12481475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.809 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

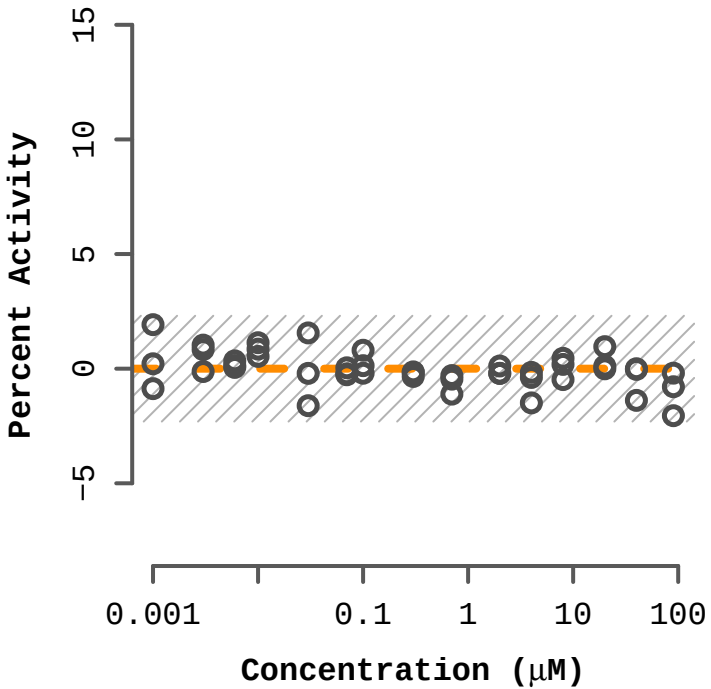
NAME: 2-Butyne-1,4-diol
CHID: 21921 **CASRN:** 110-65-6
SPID(S): Tox21_302875
M4ID: 12476258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.677 **MAX_MED:** 0.972 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

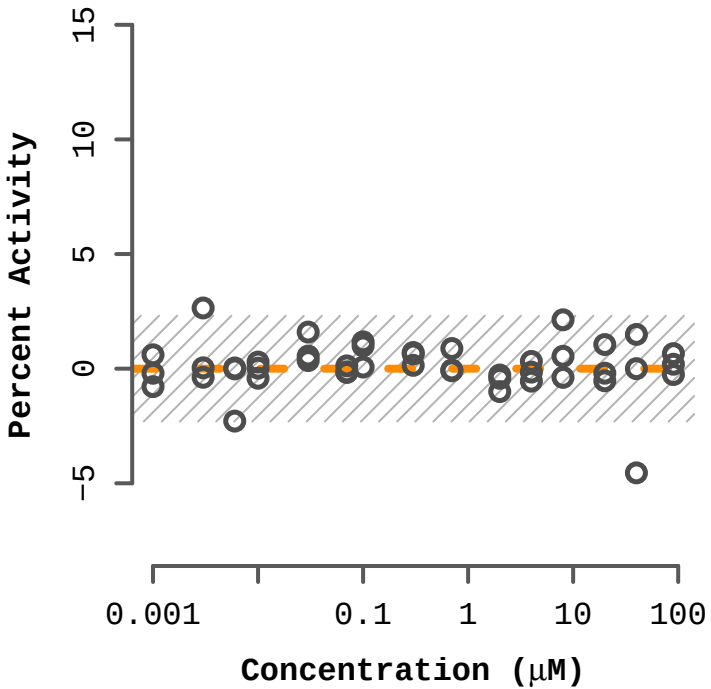
NAME: 2-Butyne-1,4-diol
CHID: 21921 **CASRN:** 110-65-6
SPID(S): Tox21_201284
M4ID: 12480968

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

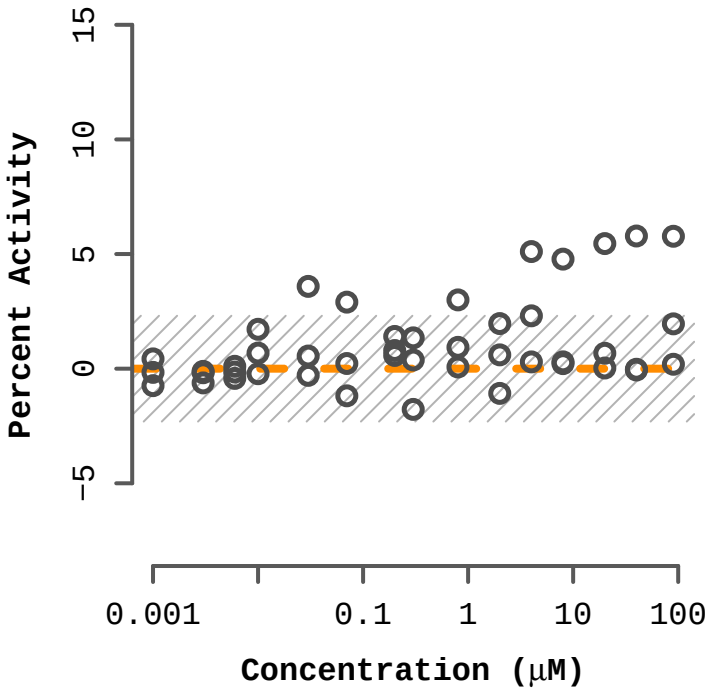
NAME: 2-(Ethylamino)ethanol
CHID: 21922 **CASRN:** 110-73-6
SPID(S): Tox21_301171
M4ID: 12477962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.835 **MAX_MED:** 0.995 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

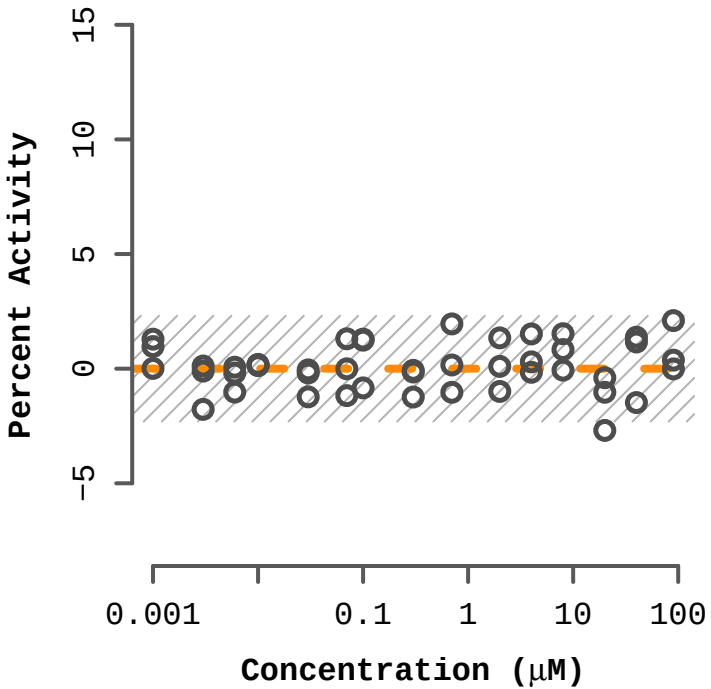
NAME: Cyclohexane
CHID: 21923 **CASRN:** 110-82-7
SPID(S): Tox21_201087
M4ID: 12481165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.28	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 2.64 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

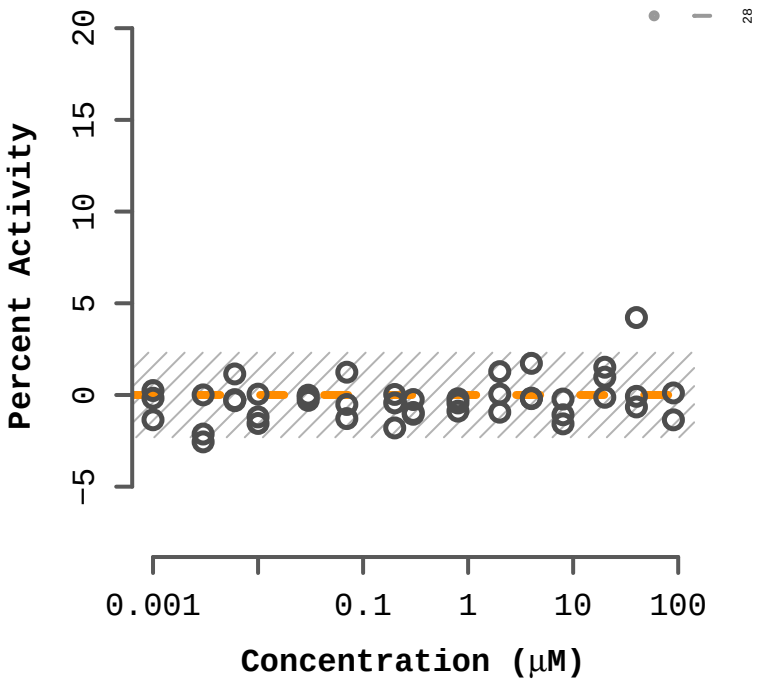
NAME: Pyridine
CHID: 21924 **CASRN:** 110-86-1
SPID(S): Tox21_200960
M4ID: 12481292

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.821 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

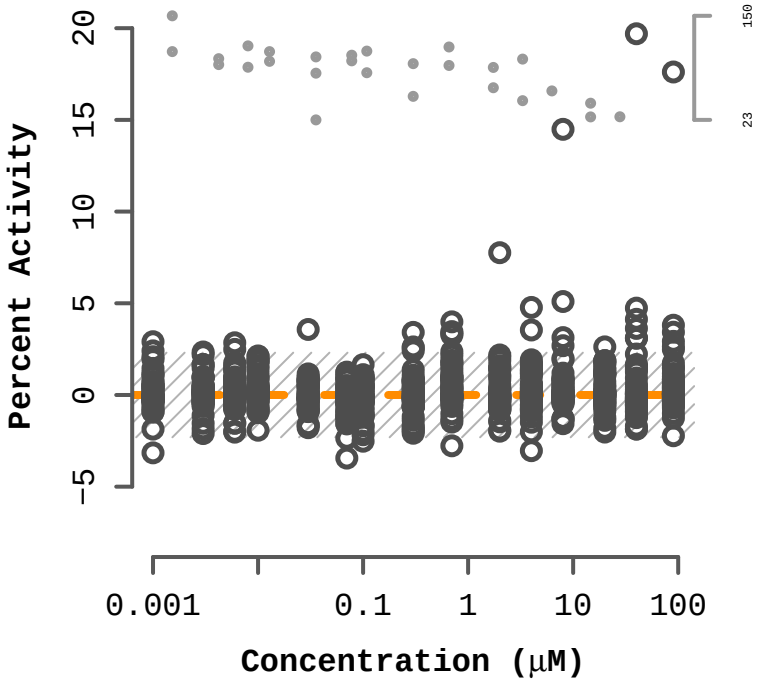
NAME: 1,3,5-Trioxane
CHID: 21925 CASRN: 110-88-3
SPID(S): Tox21_200942
M4ID: 12481310 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.77	NA	NA
PROB:	1	NA	NA
RMSE:	4.36	NA	NA

MAX_MEAN: 8.98 MAX_MED: 0.972 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

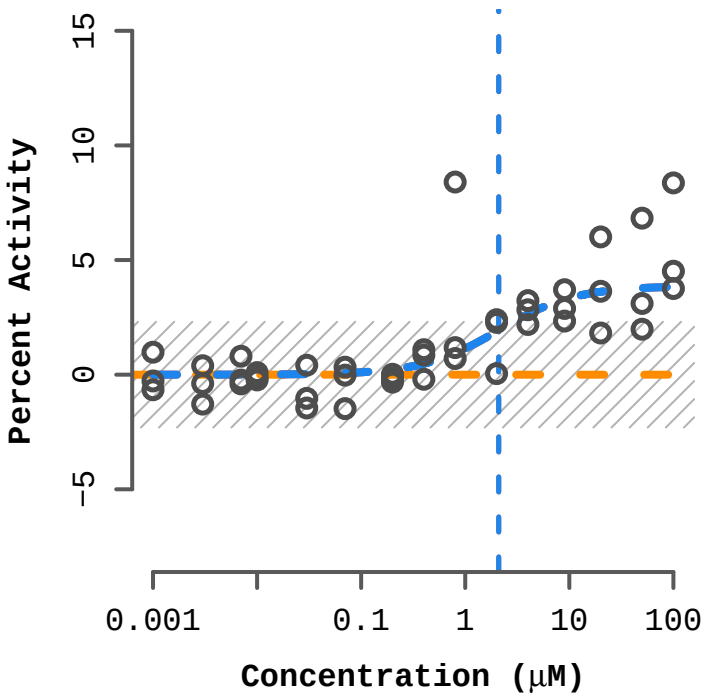
NAME: 2-Ethoxyethyl acetate
CHID: 21928 **CASRN:** 111-15-9
SPID(S): Tox21_400028
M4ID: 12475109 **BRK**

HILL MODEL: Not applicable.

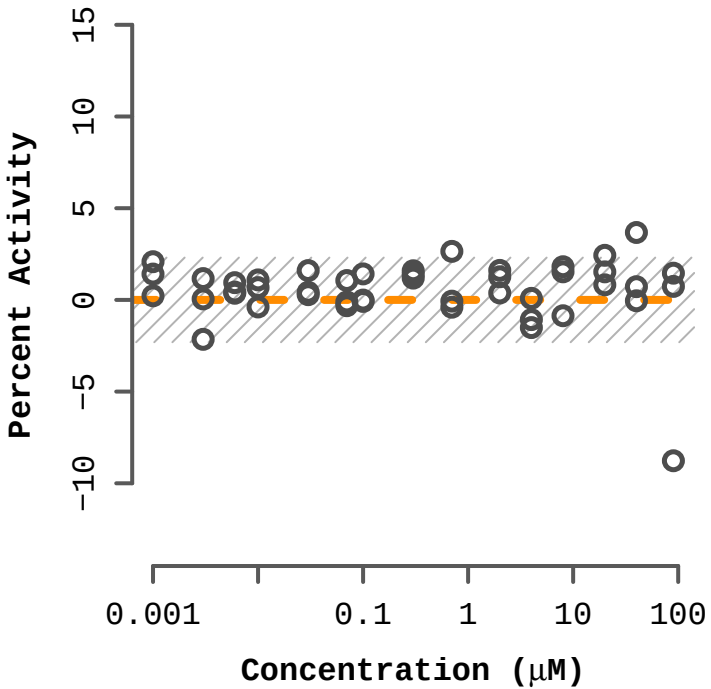
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3159.27	NA	NA
PROB:	1	NA	NA
RMSE:	17.4	NA	NA

MAX_MEAN: 5.61 **MAX_MED:** 0.399 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Bromohexane
CHID:    21929   CASRN: 111-25-1
SPID(S): Tox21_202719
M4ID:    12479533

HILL MODEL (in red):
      tp       ga       gw
val:  3.87     0.322    1.18
sd:   0.582    0.213    0.405

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.87     0.322    1.18     3.65     4.95
sd:   0.582    0.213    0.405    1230     3710

      CNST        HILL        GNLS
AIC:  216.53      153.23      157.23
PROB: 0           0.88        0.12
RMSE: 2.84        1.61        1.61

MAX_MEAN: 5.55      MAX_MED: 4.51      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

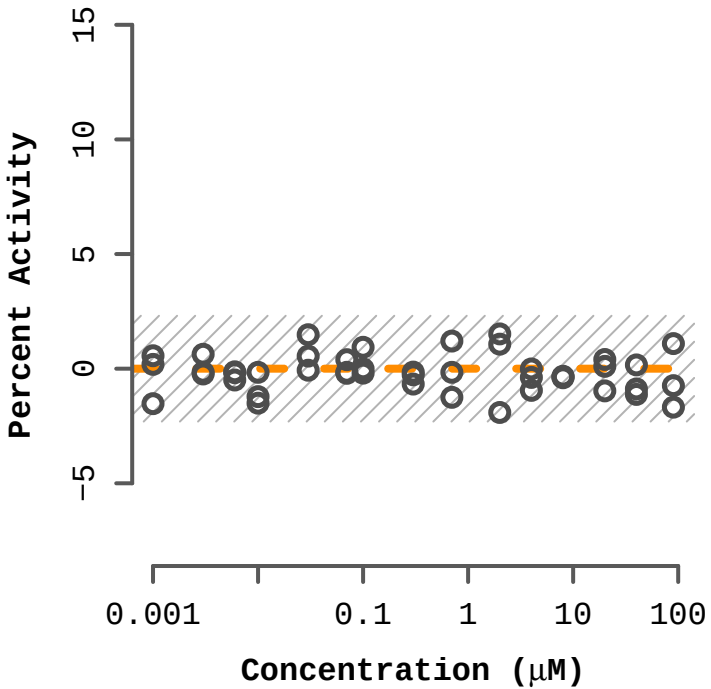
NAME: Hexylamine
CHID: 21930 **CASRN:** 111-26-2
SPID(S): Tox21_200036
M4ID: 12482216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

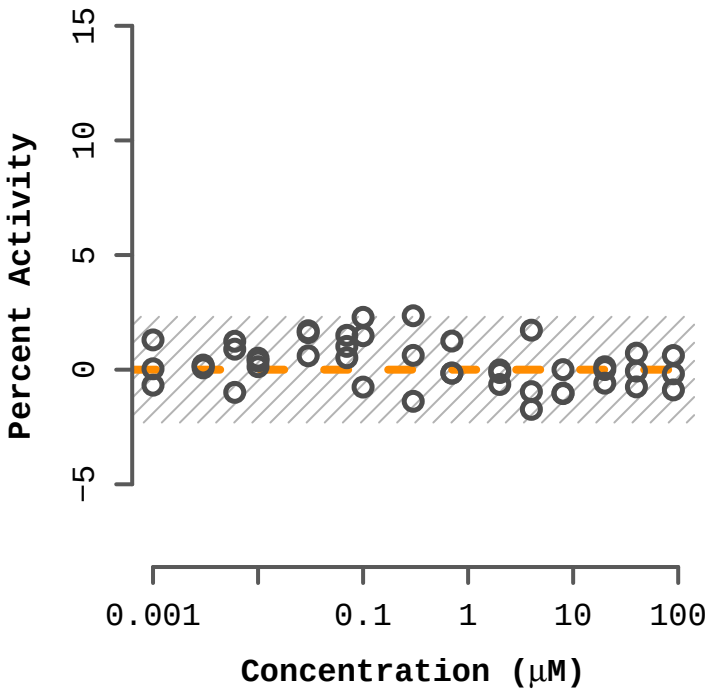
NAME: 1-Hexanol
CHID: 21931 **CASRN:** 111-27-3
SPID(S): Tox21_302953
M4ID: 12476180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

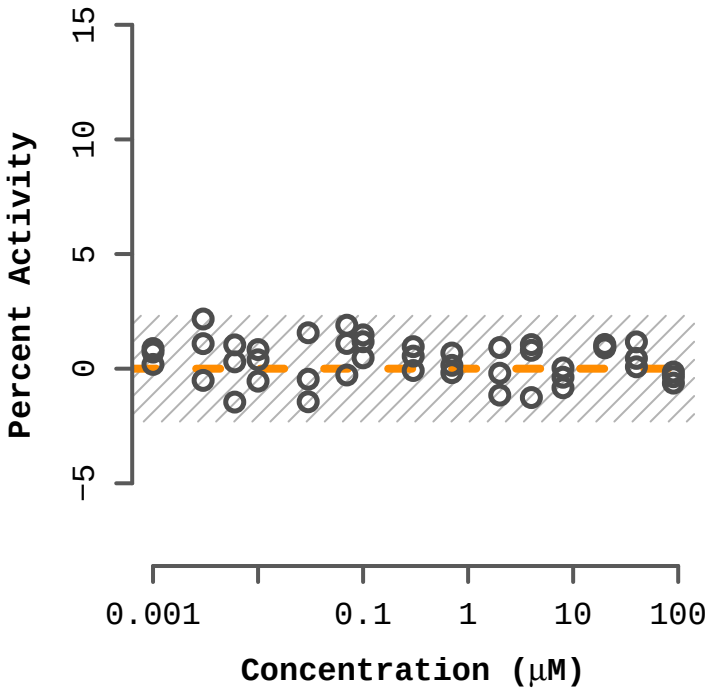
NAME: 1-Hexanol
CHID: 21931 **CASRN:** 111-27-3
SPID(S): Tox21_201335
M4ID: 12480917

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.6	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

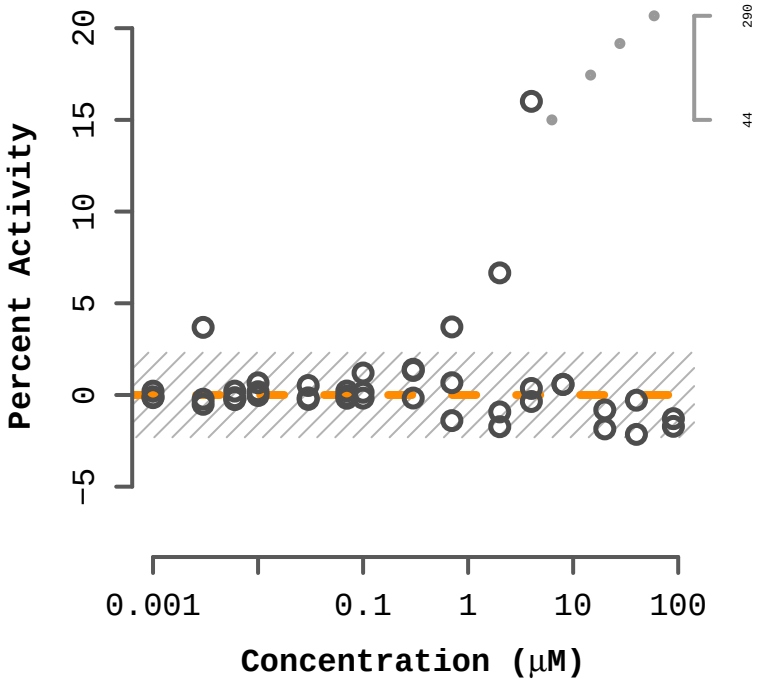
NAME: Diethanolamine
CHID: 21932 **CASRN:** 111-42-2
SPID(S): Tox21_300034
M4ID: 12479096

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

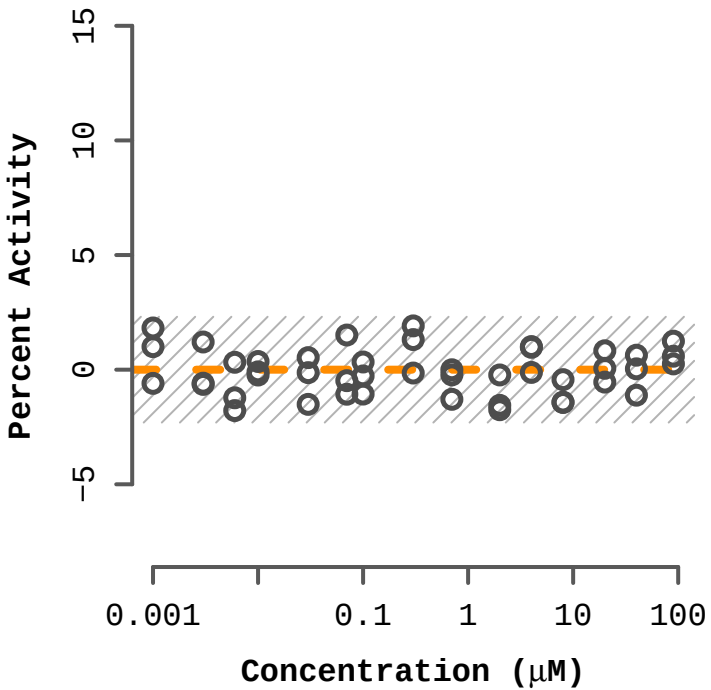
NAME: Diethanolamine
CHID: 21932 **CASRN:** 111-42-2
SPID(S): Tox21_201701
M4ID: 12480551 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	329.43	NA	NA
PROB:	1	NA	NA
RMSE:	58.6	NA	NA

MAX_MEAN: 94.2 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

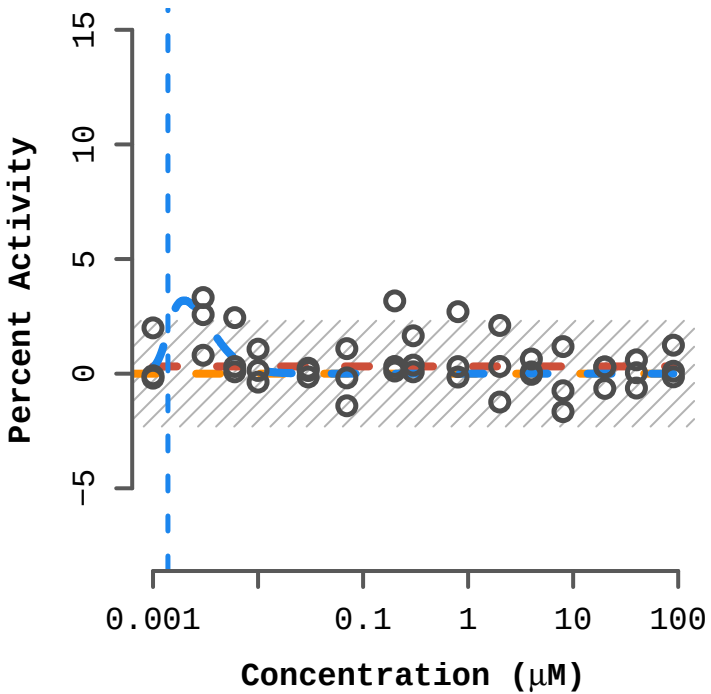
NAME: Hexanedinitrile
CHID: 21936 CASRN: 111-69-3
SPID(S): Tox21_300026
M4ID: 12479104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.03 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexanedinitrile
CHID: 21936 CASRN: 111-69-3
SPID(S): Tox21_202183
M4ID: 12480069

HILL MODEL (in red):

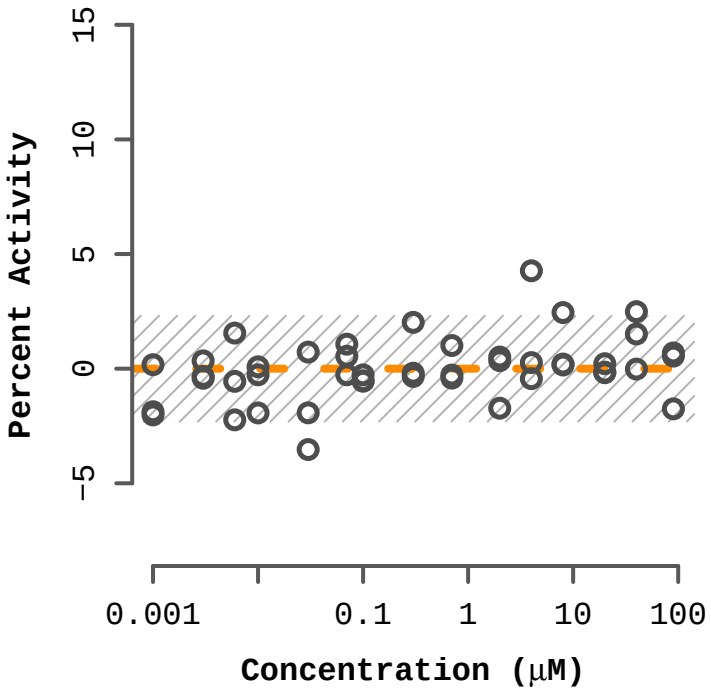
	tp	ga	gw
val:	0.316	−4.79	2.76
sd:	0.145	660	758

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.99	−2.86	8	−2.45	2.99
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	143.15	144.21	140.43
PROB:	0.18	0.11	0.71
RMSE:	1.23	1.14	1.05

MAX_MEAN: 2.23 MAX_MED: 2.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

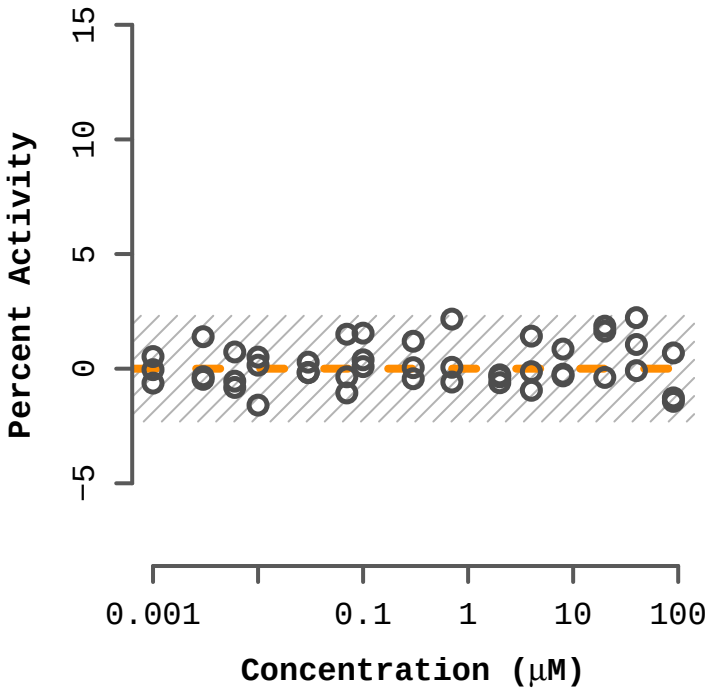
NAME: 1-Heptanol
CHID: 21937 **CASRN:** 111-70-6
SPID(S): Tox21_303470
M4ID: 12475670

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

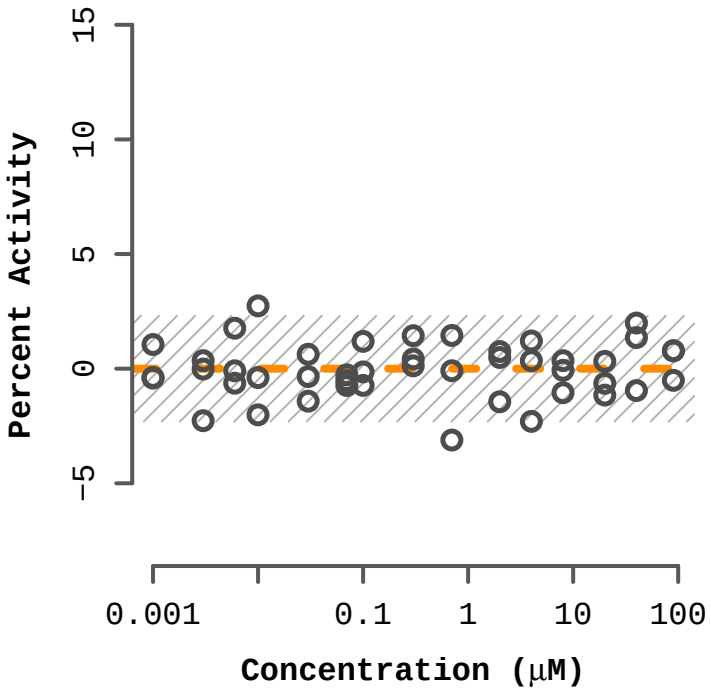
NAME: 1-Heptanol
CHID: 21937 **CASRN:** 111-70-6
SPID(S): Tox21_201247
M4ID: 12481005

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

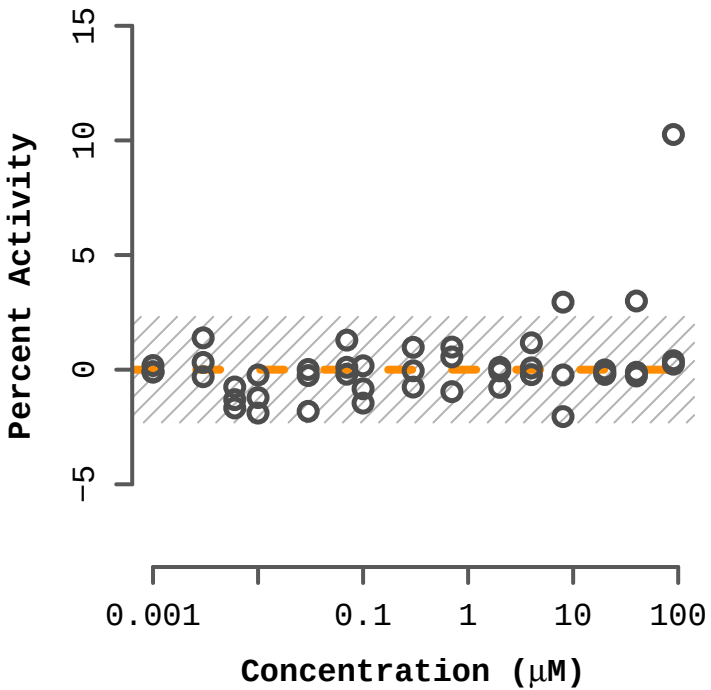
NAME: 1-Bromooctane
CHID: 21938 **CASRN:** 111-83-1
SPID(S): Tox21_302112
M4ID: 12477021

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.799 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

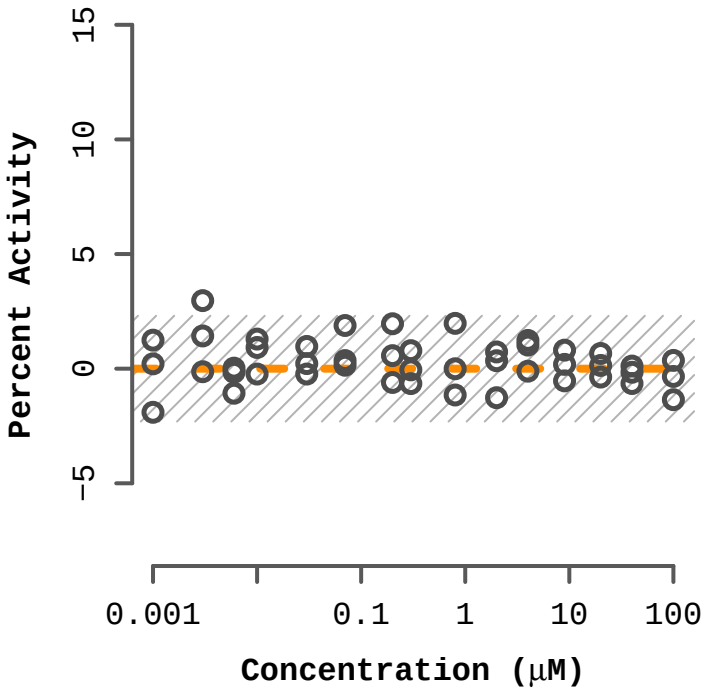
NAME: 1-Octanamine
CHID: 21939 **CASRN:** 111-86-4
SPID(S): Tox21_200052
M4ID: 12482200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 3.63 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

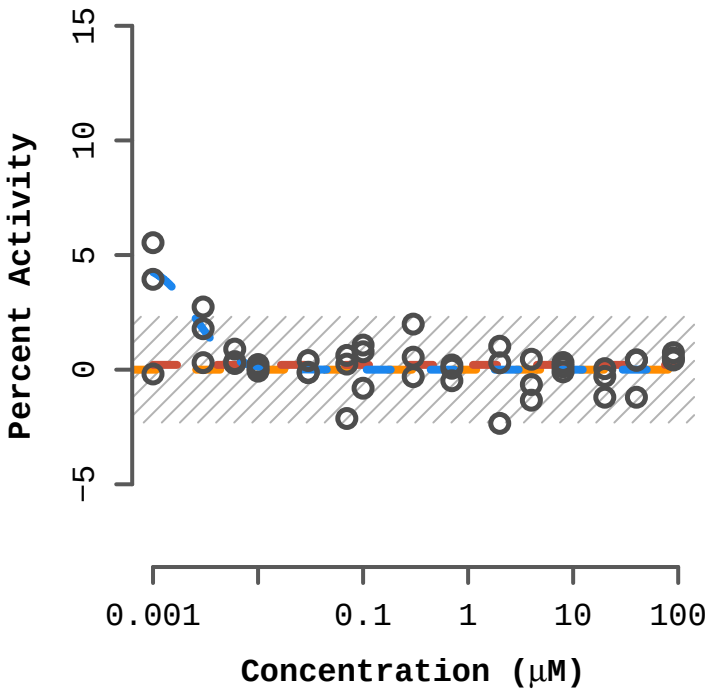
NAME: 1-Octanol
CHID: 21940 **CASRN:** 111-87-5
SPID(S): Tox21_300096
M4ID: 12479034

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Octanol
CHID: 21940 **CASRN:** 111-87-5
SPID(S): Tox21_201373
M4ID: 12480879

HILL MODEL (in red):

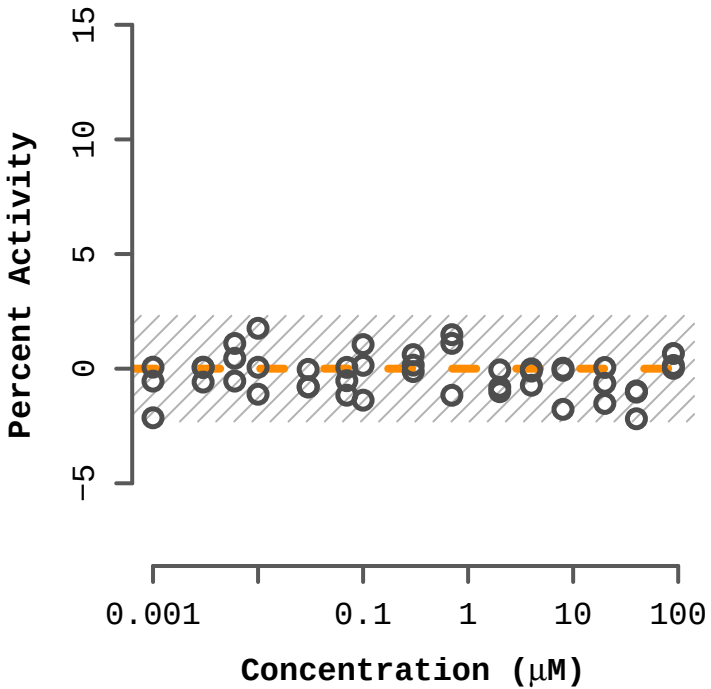
	tp	ga	gw
val:	0.209	-3.92	7.55
sd:	0.126	990	8110

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	-4.35	3.66	-2.61	2.46
sd:	1.43	621	1730	0.191	1.38

	CNST	HILL	GNLS
AIC:	140.8	144.15	132.5
PROB:	0.02	0	0.98
RMSE:	1.36	1.33	1.06

MAX_MEAN: 3.1 **MAX_MED:** 3.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

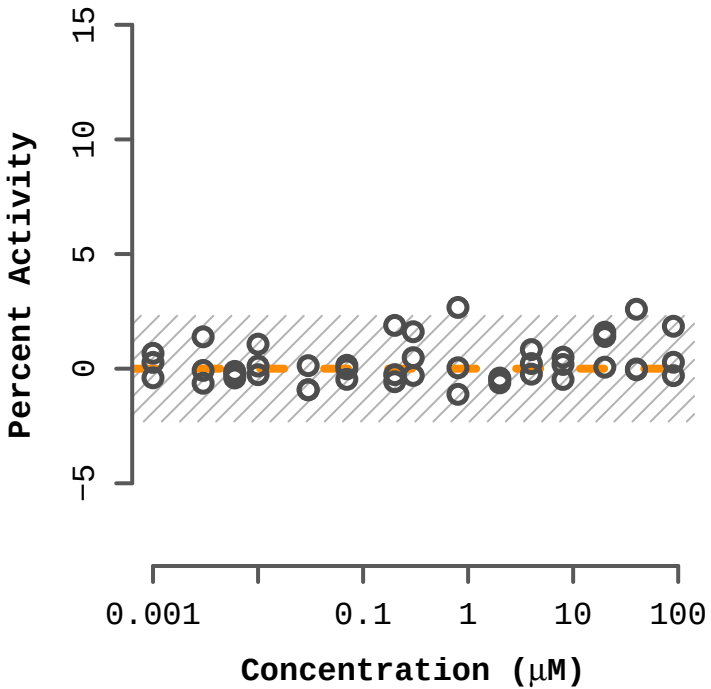
NAME: 2-(2-Ethoxyethoxy)ethanol
CHID: 21941 **CASRN:** 111-90-0
SPID(S): Tox21_300080
M4ID: 12479050

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.477 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

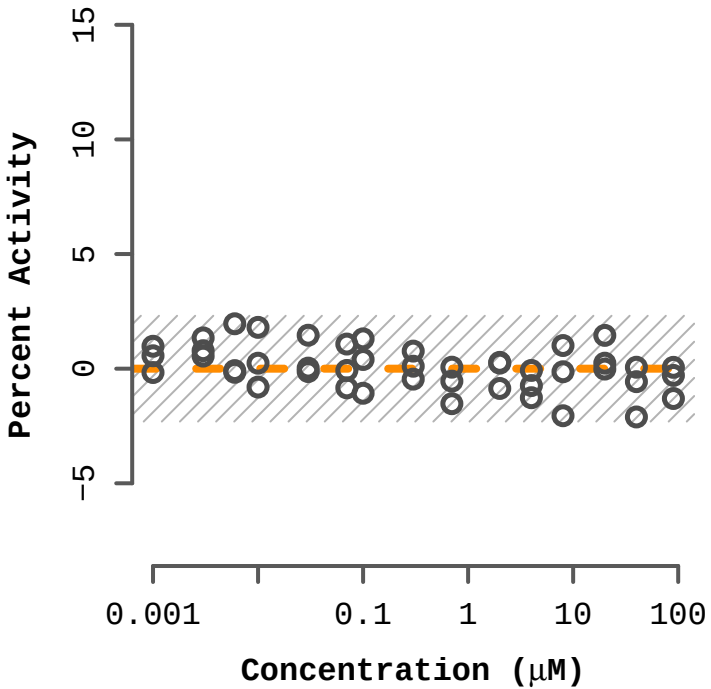
NAME: 2-(2-Ethoxyethoxy)ethanol
CHID: 21941 **CASRN:** 111-90-0
SPID(S): Tox21_200413
M4ID: 12481839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

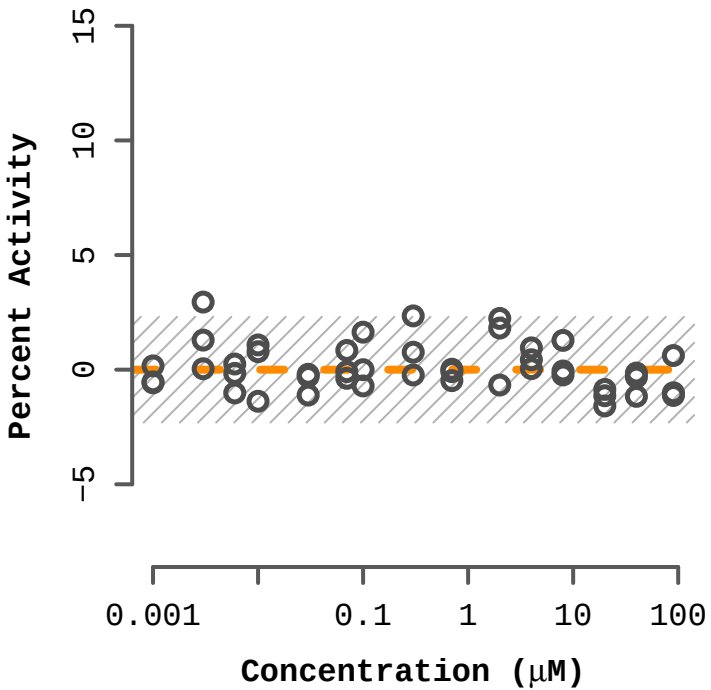
NAME: 2-Undecanone
CHID: 21943 **CASRN:** 112-12-9
SPID(S): Tox21_301385
M4ID: 12477748

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 0.787 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

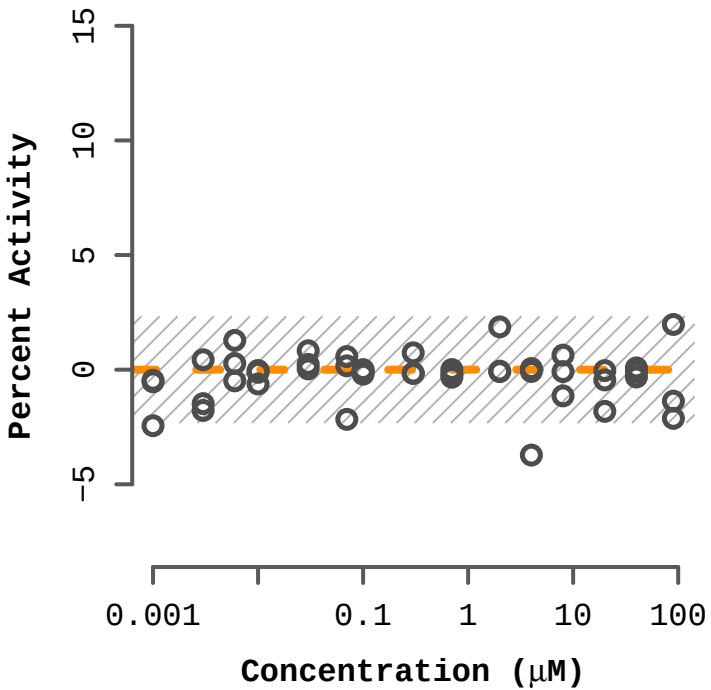
NAME: 1-Decanol
CHID: 21946 **CASRN:** 112-30-1
SPID(S): Tox21_300078
M4ID: 12479052

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

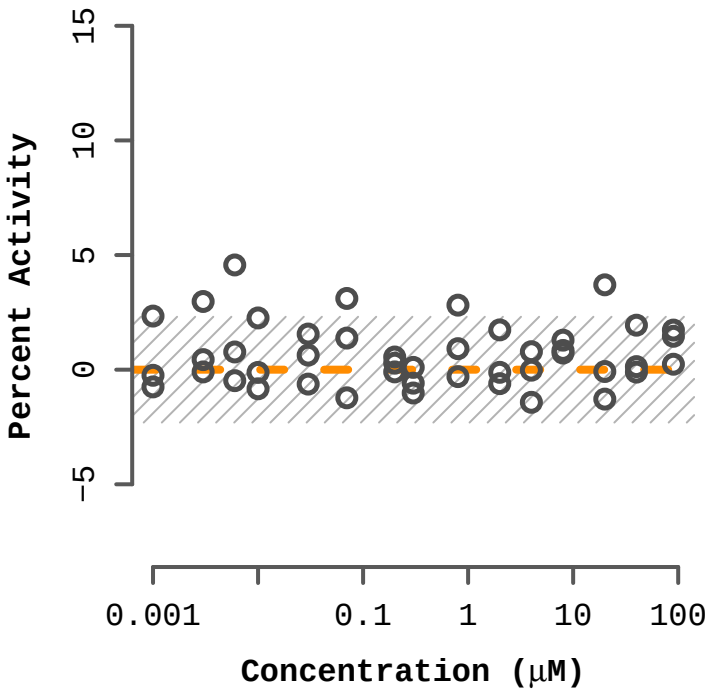
NAME: 1-Decanol
CHID: 21946 **CASRN:** 112-30-1
SPID(S): Tox21_202186
M4ID: 12480066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 0.271 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

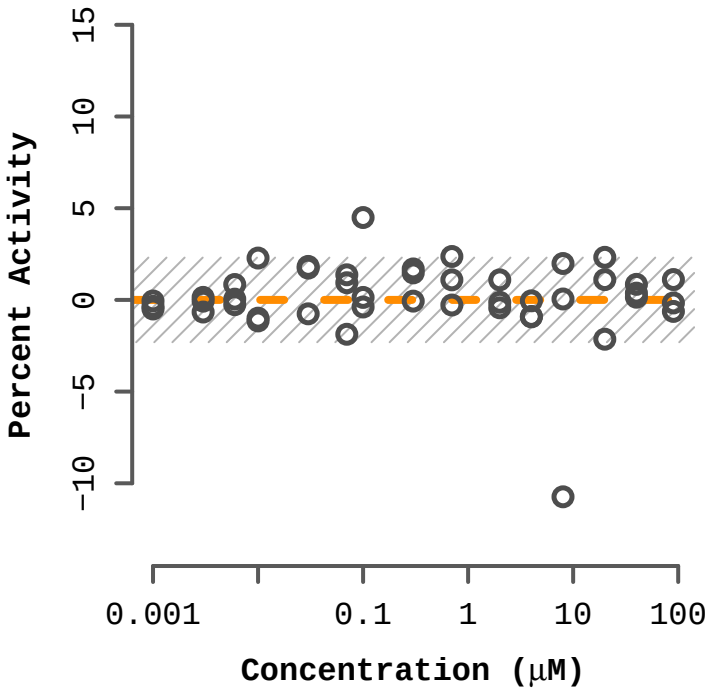
NAME: 1-Tridecanol
CHID: 21947 **CASRN:** 112-70-9
SPID(S): Tox21_300138
M4ID: 12478992

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

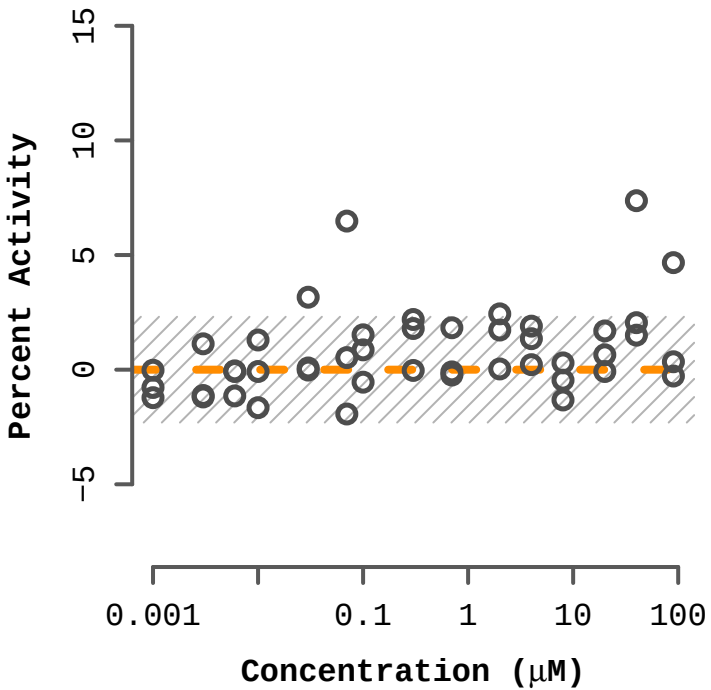
NAME: 1-Tridecanol
CHID: 21947 **CASRN:** 112-70-9
SPID(S): Tox21_202208
M4ID: 12480044

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

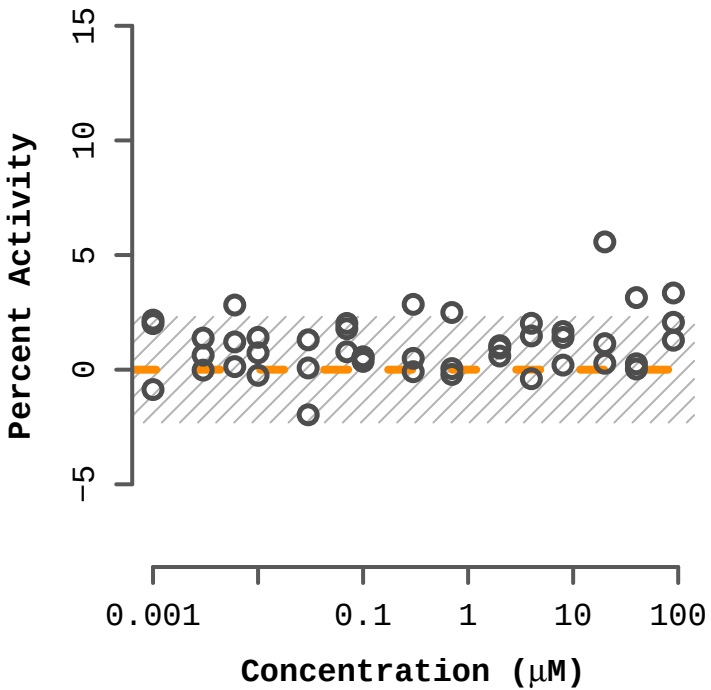
NAME: Propoxur
CHID: 21948 **CASRN:** 114-26-1
SPID(S): Tox21_301207
M4ID: 12477926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.44	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 3.64 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

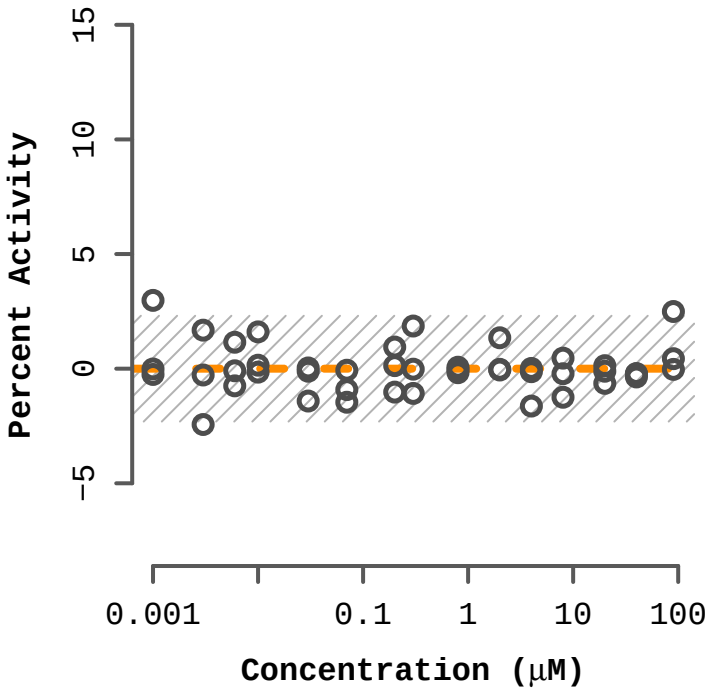
NAME: Propoxur
CHID: 21948 **CASRN:** 114-26-1
SPID(S): Tox21_201968
M4ID: 12480284

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

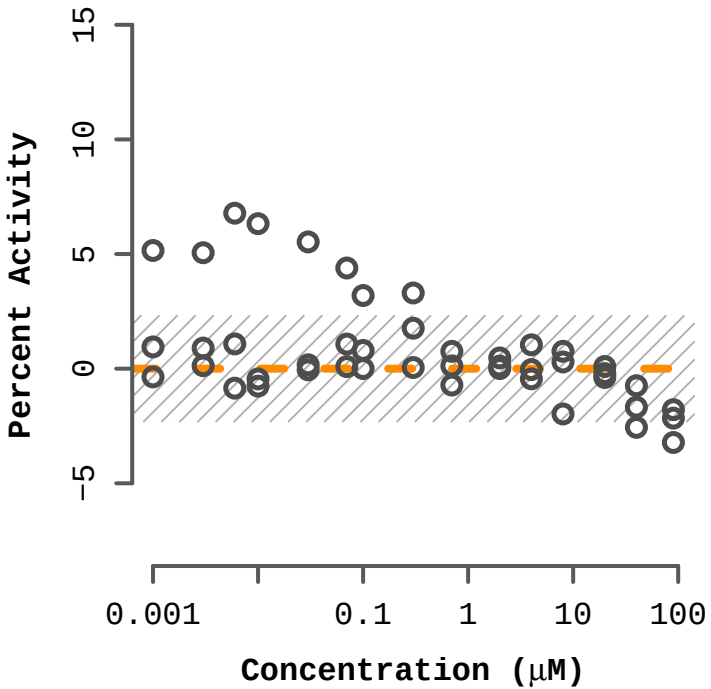
NAME: 2-Methyl-3-butyn-2-ol
CHID: 21949 **CASRN:** 115-19-5
SPID(S): Tox21_200094
M4ID: 12482158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.967 **MAX_MED:** 0.437 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

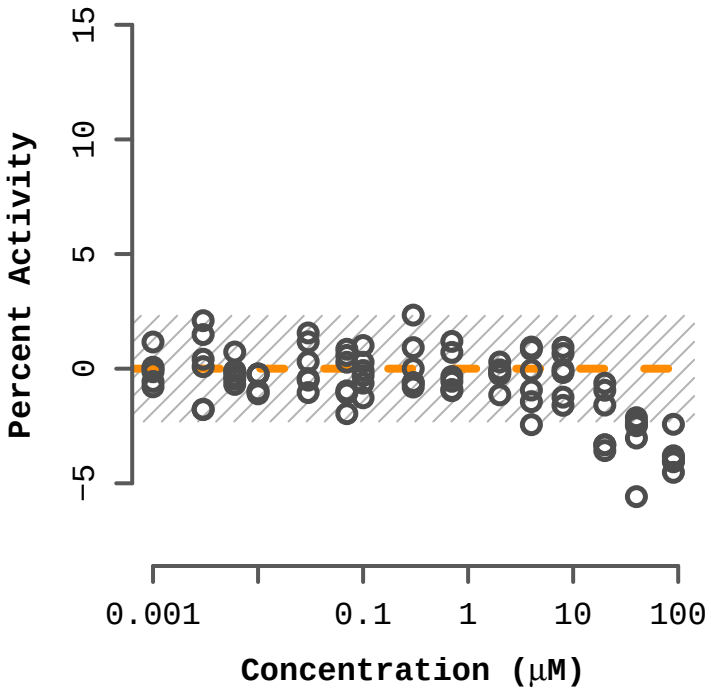
NAME: Triphenyl phosphate
CHID: 21952 **CASRN:** 115-86-6
SPID(S): Tox21_300504
M4ID: 12478628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.38	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

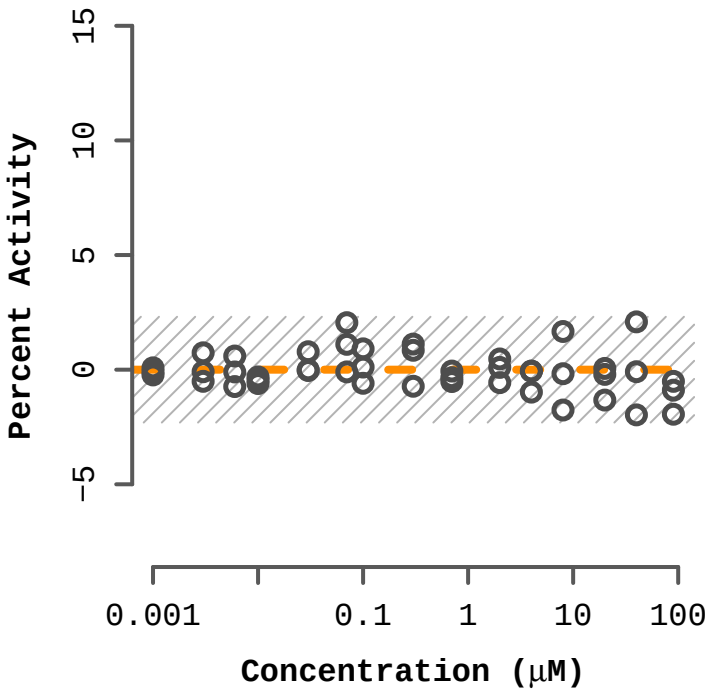
NAME: Triphenyl phosphate
CHID: 21952 **CASRN:** 115-86-6
SPID(S): Tox21_201511
M4ID: 12480741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	342.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 0.207 **MAX_MED:** 0.252 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

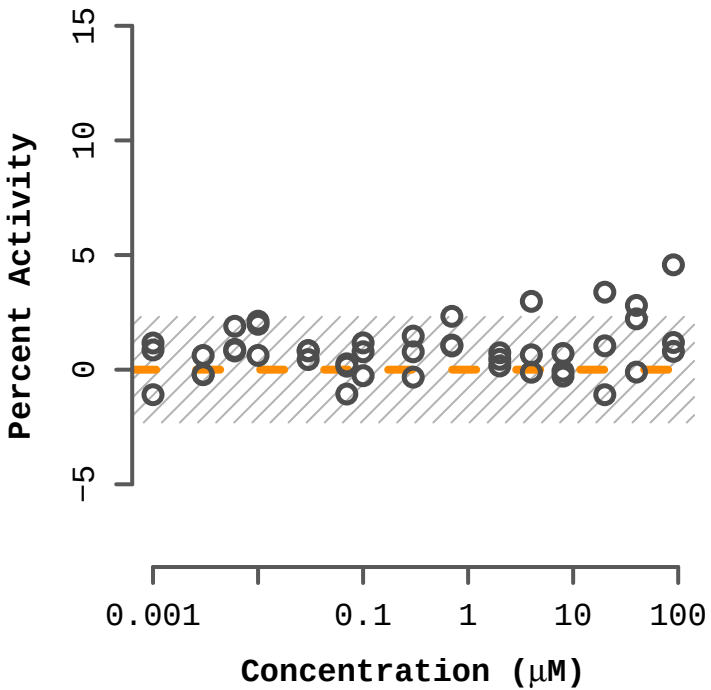
NAME: Fensulfothion
CHID: 21953 **CASRN:** 115-90-2
SPID(S): Tox21_301858
M4ID: 12477275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

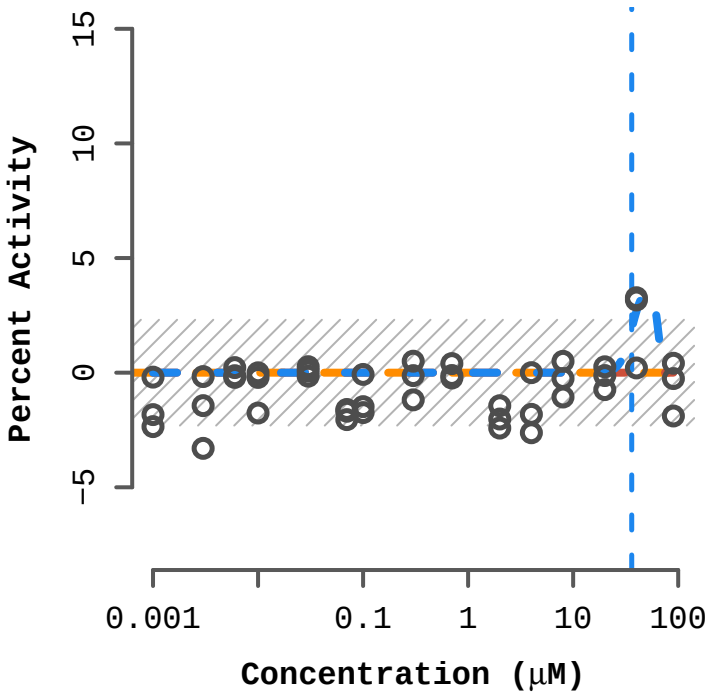
NAME: Dioctyl phthalate
CHID: 21956 **CASRN:** 117-84-0
SPID(S): Tox21_300549
M4ID: 12478583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dioctyl phthalate
CHID: 21956 CASRN: 117-84-0
SPID(S): Tox21_202233
M4ID: 12480019

HILL MODEL (in red):

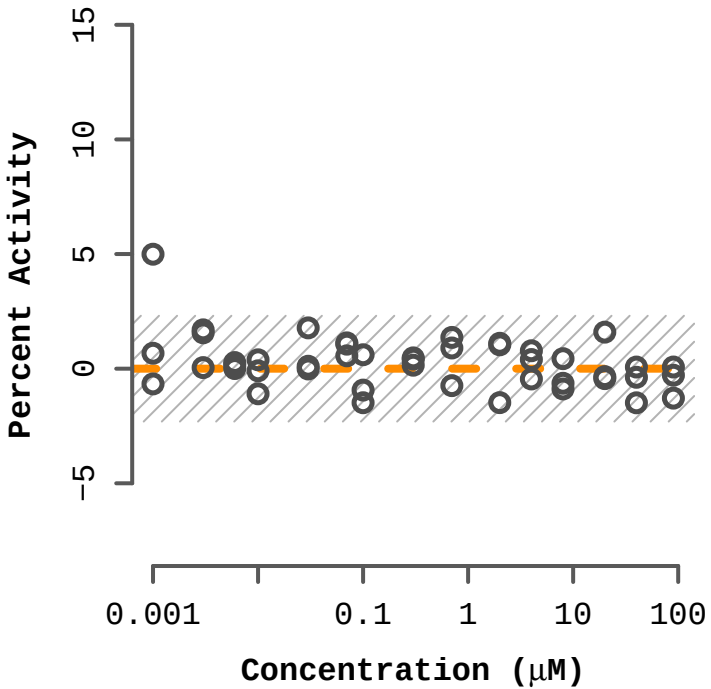
	tp	ga	gw
val:	3.28e-08	2.34	1.75
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.84	1.56	8	1.81	18
sd:	10.9	0.457	12.4	0.462	56.7

	CNST	HILL	GNLS
AIC:	161.64	167.64	164.7
PROB:	0.79	0.04	0.17
RMSE:	1.42	1.42	1.31

MAX_MEAN: 2.22 MAX_MED: 3.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

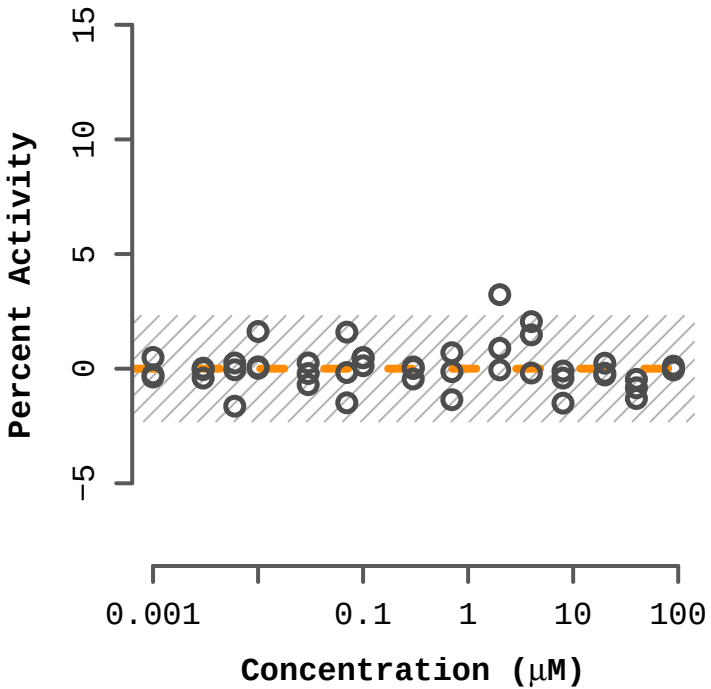
NAME: Phenyl salicylate
CHID: 21957 **CASRN:** 118-55-8
SPID(S): Tox21_302949
M4ID: 12476184

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

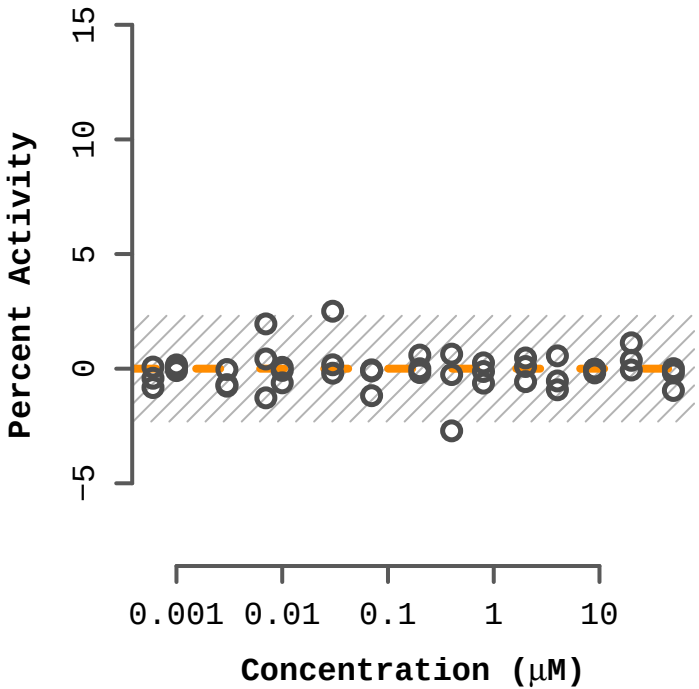
NAME: Phenyl salicylate
CHID: 21957 CASRN: 118-55-8
SPID(S): Tox21_201811
M4ID: 12480441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

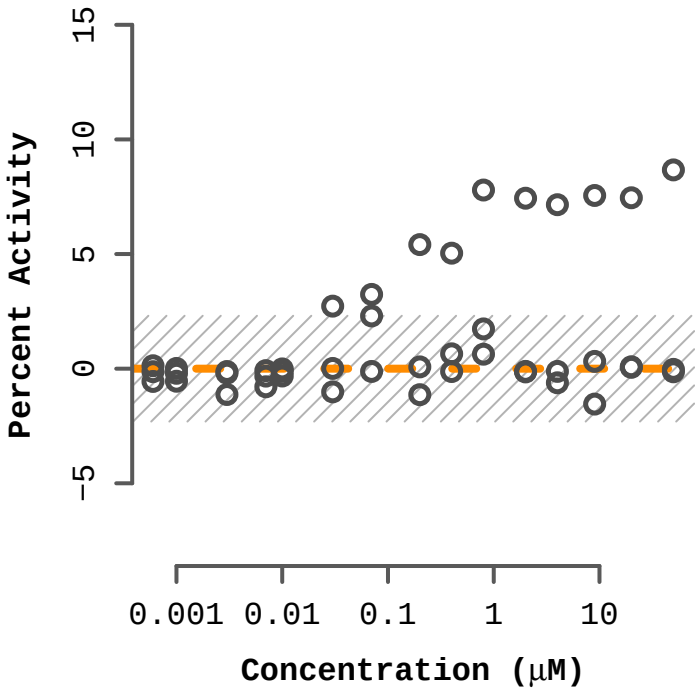
NAME: Phenyl salicylate
CHID: 21957 **CASRN:** 118-55-8
SPID(S): Tox21_113459_1
M4ID: 12482646

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.827 **MAX_MED:** 0.425 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

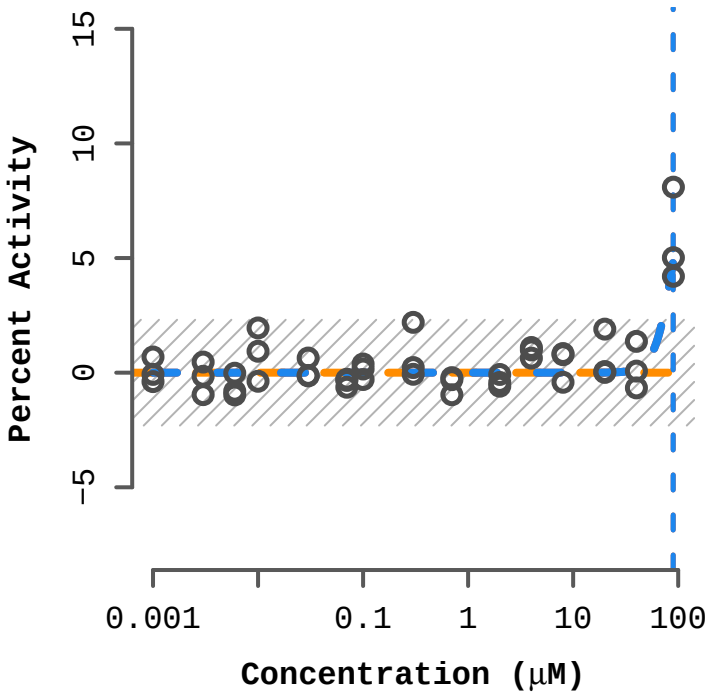
NAME: Ethyl salicylate
CHID: 21958 **CASRN:** 118-61-6
SPID(S): Tox21_112764_1
M4ID: 12482966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.56	NA	NA
PROB:	1	NA	NA
RMSE:	3.14	NA	NA

MAX_MEAN: 3.39 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,6-Tribromophenol
CHID: 21959 **CASRN:** 118-79-6
SPID(S): Tox21_302972
M4ID: 12476161

HILL MODEL (in red):

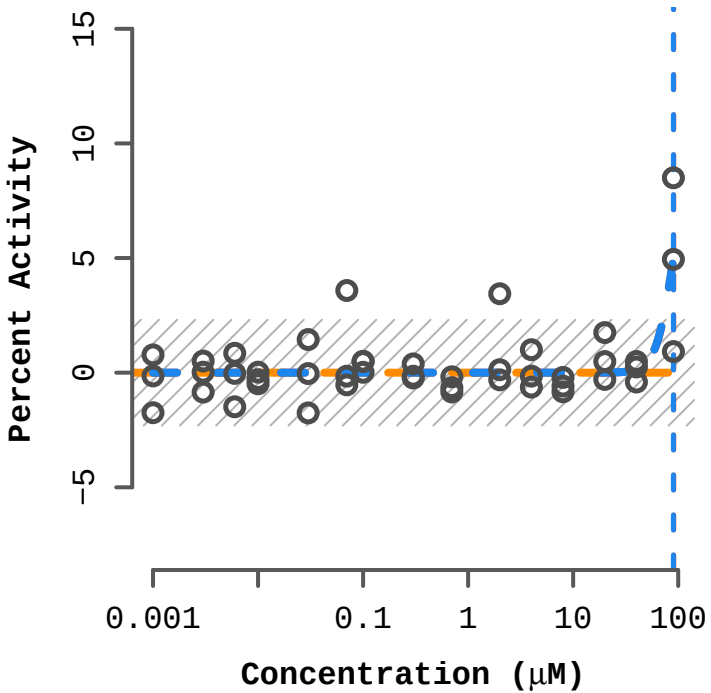
	tp	ga	gw
val:	9.71	1.95	5.04
sd:	5.61	0.101	4.95

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.71	1.95	5.04	3.83	16
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	146.37	120.15	124.15
PROB:	0	0.88	0.12
RMSE:	1.73	0.9	0.9

MAX_MEAN: 5.77 **MAX_MED:** 5.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,6-Tribromophenol
CHID: 21959 CASRN: 118-79-6
SPID(S): Tox21_201273
M4ID: 12480979

HILL MODEL (in red):

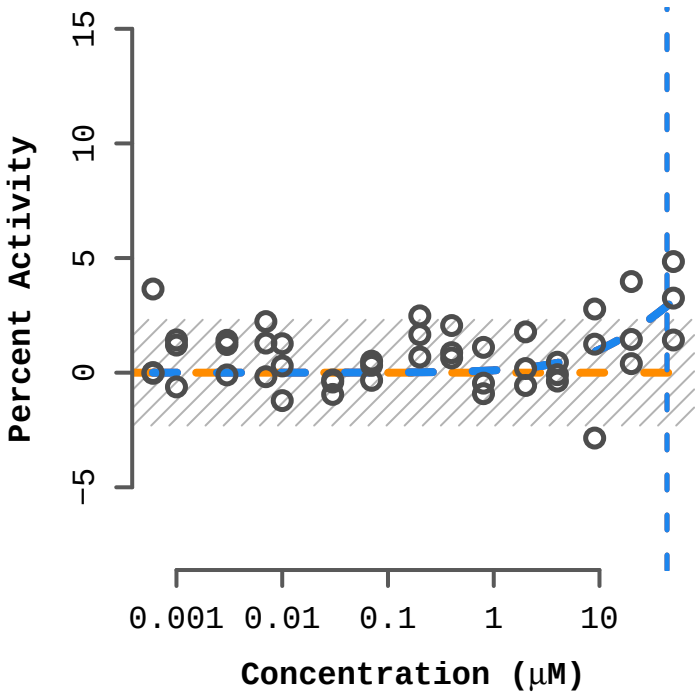
	tp	ga	gw
val:	10.2	1.96	5.22
sd:	4.34	0.0714	4.09

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10	1.95	5.24	3.5	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	150.46	145.02	149.02
PROB:	0.05	0.83	0.11
RMSE:	1.79	1.29	1.29

MAX_MEAN: 4.79 MAX_MED: 4.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,6-Tribromophenol
CHID: 21959 **CASRN:** 118-79-6
SPID(S): Tox21_111098_1
M4ID: 12483909

HILL MODEL (in red):

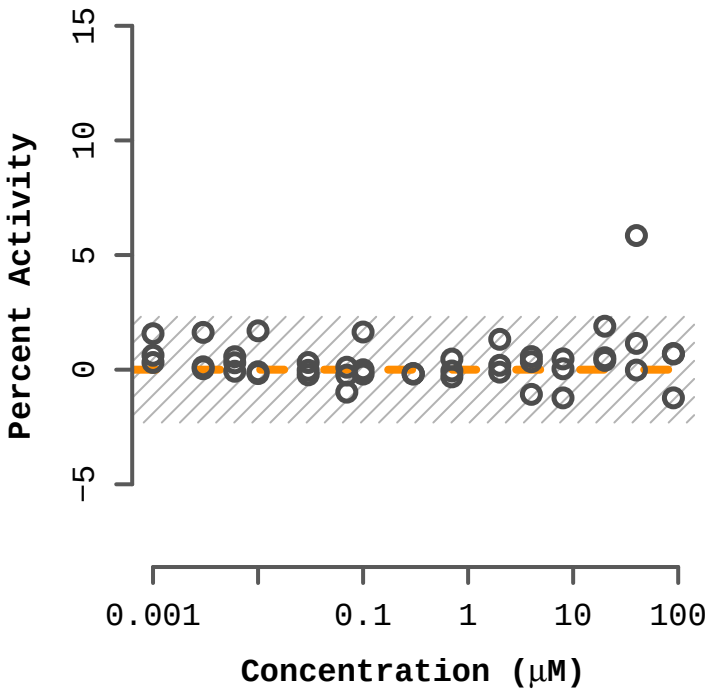
	tp	ga	gw
val:	5.82	1.64	1.06
sd:	11.6	1.69	1.51

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.82	1.64	1.06	3.7	5.91
sd:	11.6	1.7	1.51	196000	564000

	CNST	HILL	GNLS
AIC:	173.67	163.64	167.64
PROB:	0.01	0.88	0.12
RMSE:	1.66	1.36	1.36

MAX_MEAN: 3.18 **MAX_MED:** 3.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

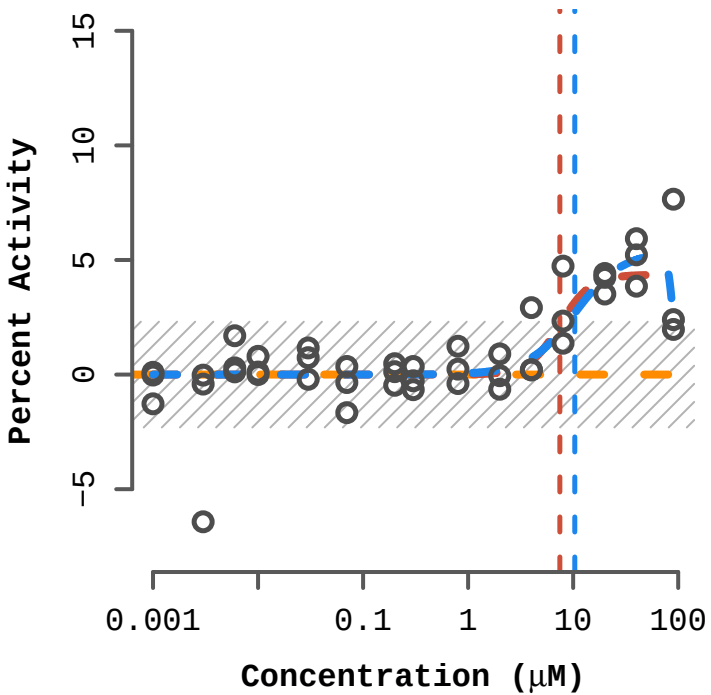
NAME: Benzophenone
CHID: 21961 **CASRN:** 119-61-9
SPID(S): Tox21_300058
M4ID: 12479072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzophenone
CHID: 21961 CASRN: 119-61-9
SPID(S): Tox21_202425
M4ID: 12479827

HILL MODEL (in red):

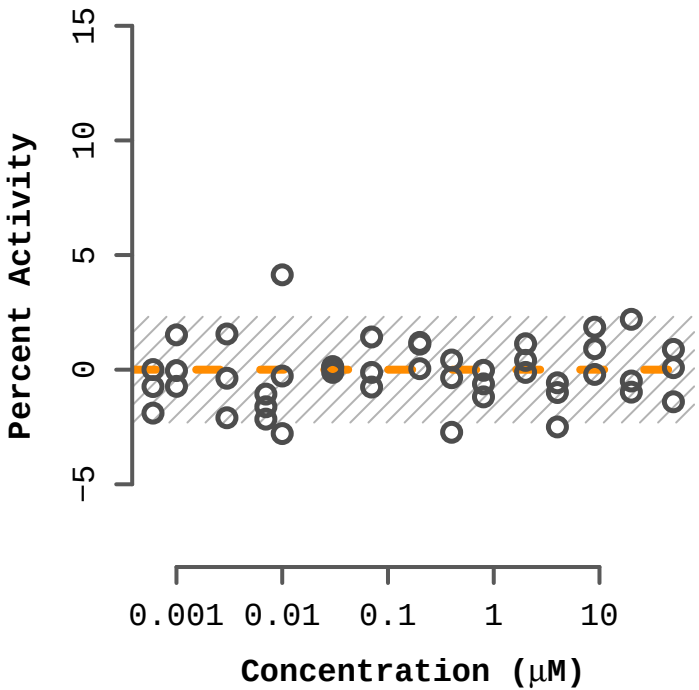
	tp	ga	gw
val:	4.36	0.873	2.94
sd:	0.578	0.102	1.58

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.37	1.02	1.95	1.95	16.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	205.19	150.91	147.22
PROB:	0	0.14	0.86
RMSE:	2.54	1.43	1.49

MAX_MEAN: 5 MAX_MED: 5.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

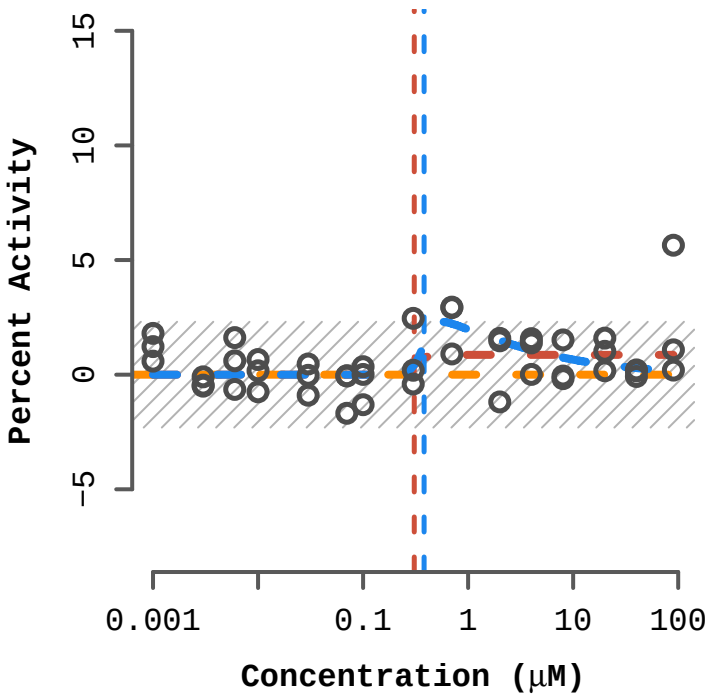
NAME: Benzophenone
CHID: 21961 **CASRN:** 119-61-9
SPID(S): Tox21_113465_1
M4ID: 12482642

HILL MODEL: Not applicable.

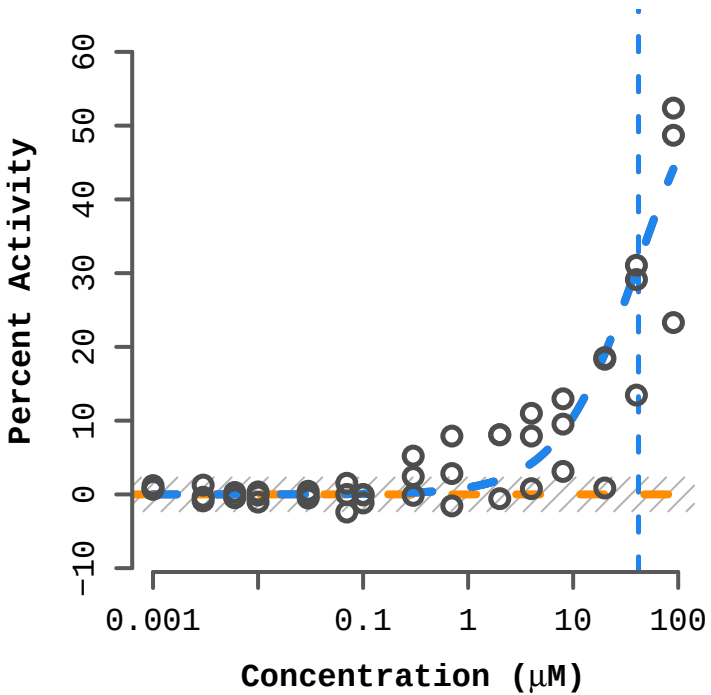
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 1.11 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Phenyldiethanolamine
CHID:    21962   CASRN: 120-07-0
SPID(S): Tox21_301523
M4ID:    12477610

HILL MODEL (in red):
      tp       ga       gw
val:  0.864    -0.513   8
sd:   0.235    0.164    19.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.53     -0.419   7.99     -0.169   0.66
sd:   5.49     0.144    9.47     1.36     0.356

      CNST        HILL        GNLS
AIC:  152.38      145.31      143.66
PROB: 0.01        0.3         0.69
RMSE: 1.41        1.2         1.22

MAX_MEAN: 2.31      MAX_MED: 2.93      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(Diethylamino)benzaldehyde
CHID: 21963 **CASRN:** 120-21-8
SPID(S): Tox21_303895
M4ID: 12475293

HILL MODEL (in red):

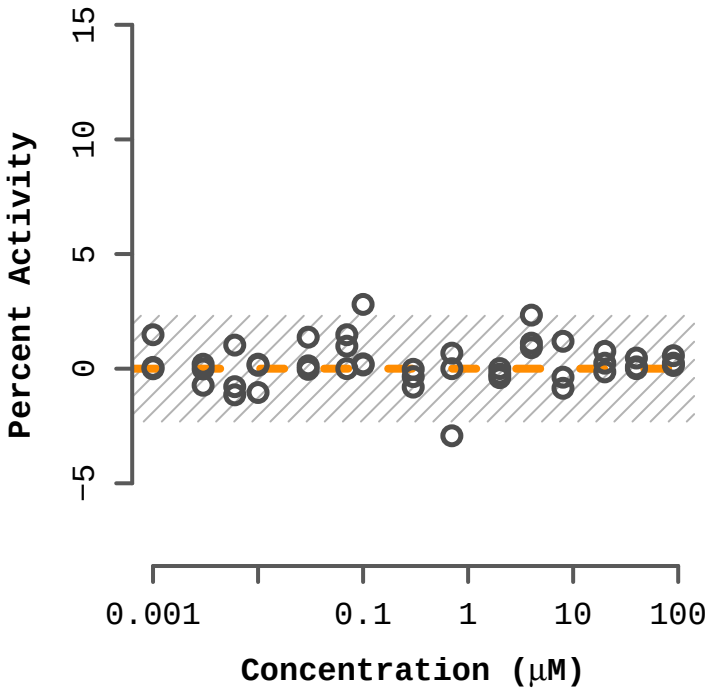
	tp	ga	gw
val:	62.9	1.62	1.12
sd:	21.8	0.216	0.231

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	62.9	1.62	1.12	3.78	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	343.64	270.28	274.28
PROB:	0	0.88	0.12
RMSE:	14.17	5.7	5.7

MAX_MEAN: 41.5 **MAX_MED:** 48.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

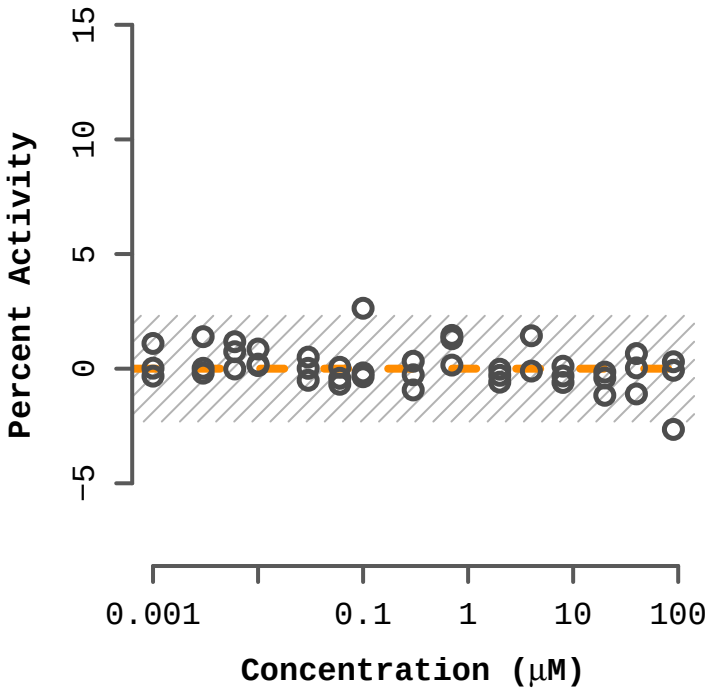
NAME: 1,2,4−Trichlorobenzene
CHID: 21965 CASRN: 120−82−1
SPID(S): Tox21_300563
M4ID: 12478570

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

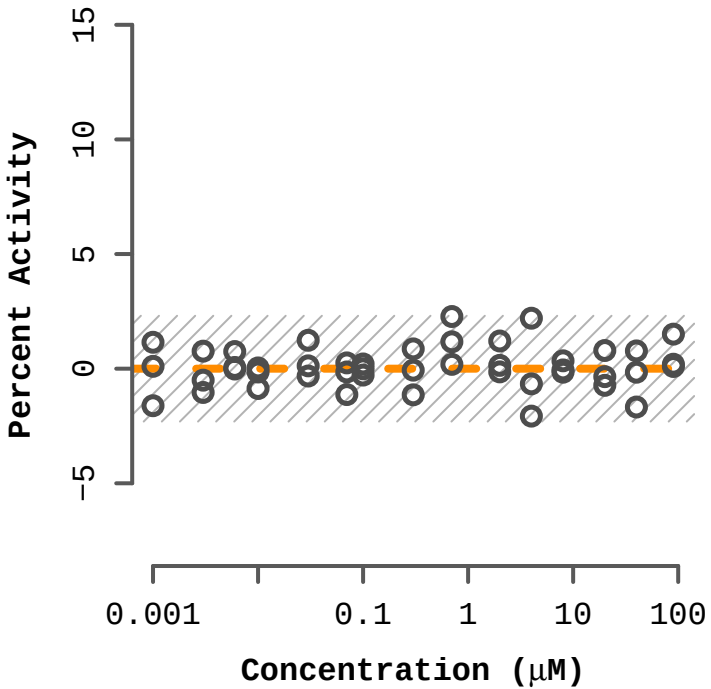
NAME: 1,2,4−Trichlorobenzene
CHID: 21965 **CASRN:** 120−82−1
SPID(S): Tox21_201311
M4ID: 12480941

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.973 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

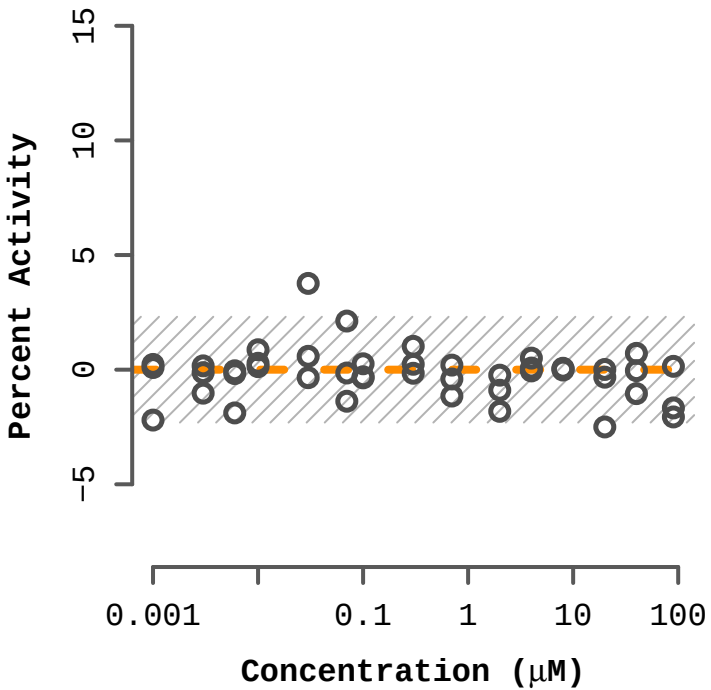
NAME: 3-Ethoxy-4-hydroxybenzaldehyde
CHID: 21968 **CASRN:** 121-32-4
SPID(S): Tox21_302903
M4ID: 12476230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

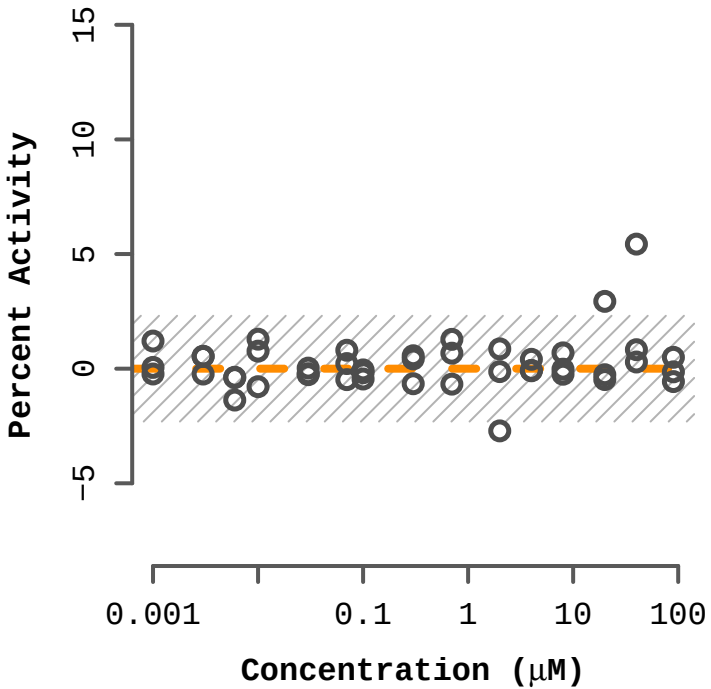
NAME: 3-Ethoxy-4-hydroxybenzaldehyde
CHID: 21968 **CASRN:** 121-32-4
SPID(S): Tox21_202125
M4ID: 12480127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

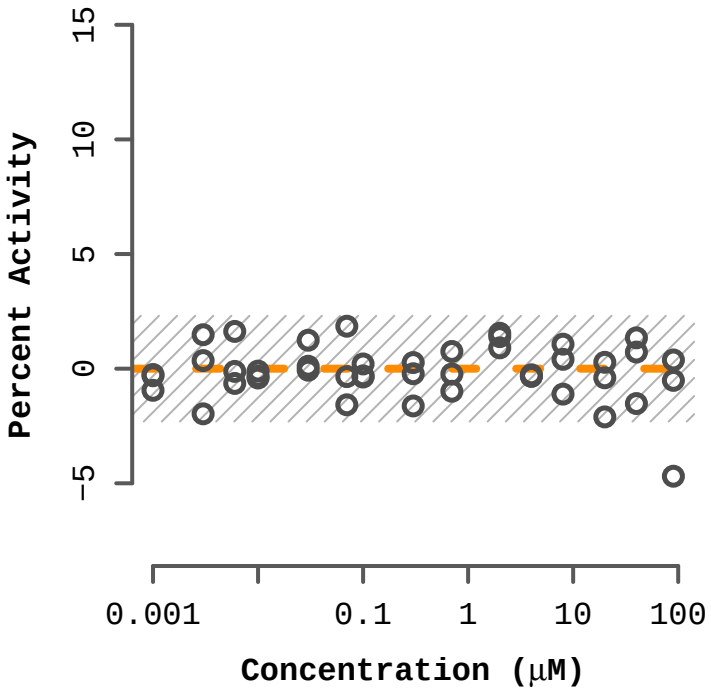
NAME: 4-Hydroxy-3-methoxybenzaldehyde
CHID: 21969 **CASRN:** 121-33-5
SPID(S): Tox21_300352
M4ID: 12478780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

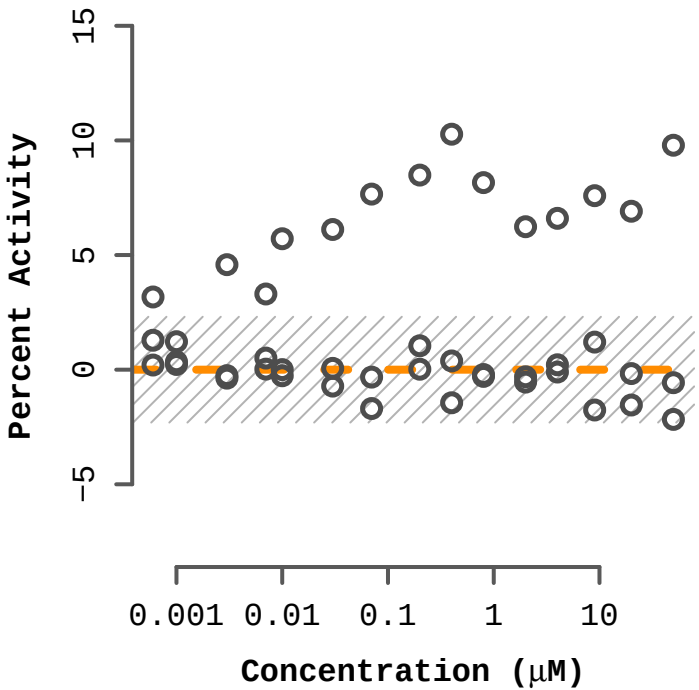
NAME: 4-Hydroxy-3-methoxybenzaldehyde
CHID: 21969 **CASRN:** 121-33-5
SPID(S): Tox21_201925
M4ID: 12480327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

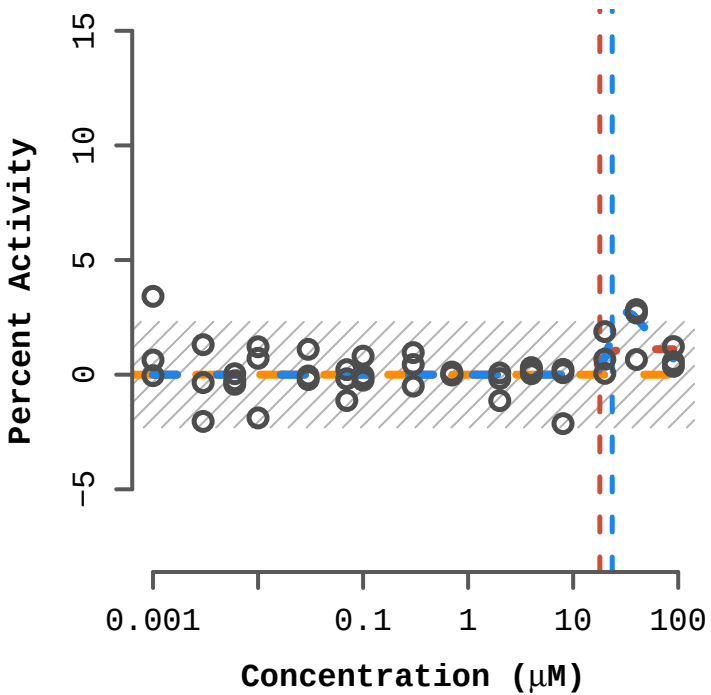
NAME: 4-Hydroxy-3-methoxybenzaldehyde
CHID: 21969 **CASRN:** 121-33-5
SPID(S): Tox21_113534_1
M4ID: 12482618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.87	NA	NA
PROB:	1	NA	NA
RMSE:	4.01	NA	NA

MAX_MEAN: 3.18 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Chloro-3-nitrobenzene
CHID: 21971 CASRN: 121-73-3
SPID(S): Tox21_302825
M4ID: 12476308

HILL MODEL (in red):

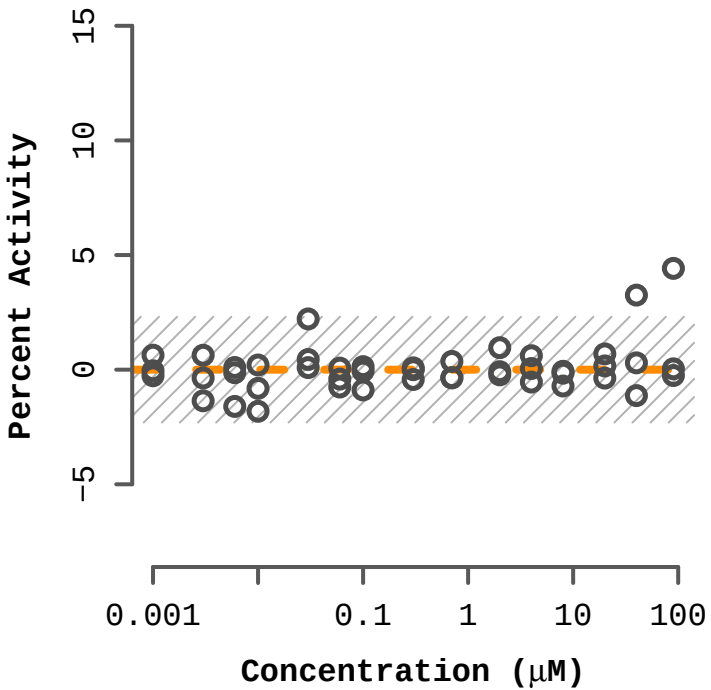
	tp	ga	gw
val:	1.11	1.25	8
sd:	0.382	0.171	17.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.92	1.37	8	1.7	2.56
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	133.47	127.5	126.09
PROB:	0.02	0.32	0.66
RMSE:	1.12	0.98	0.95

MAX_MEAN: 2.06 MAX_MED: 2.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

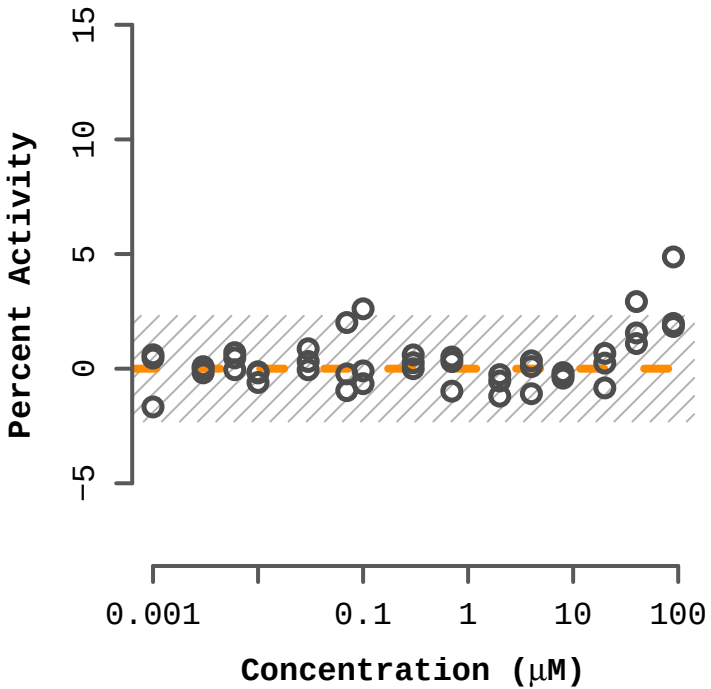
NAME: 1-Chloro-3-nitrobenzene
CHID: 21971 **CASRN:** 121-73-3
SPID(S): Tox21_201330
M4ID: 12480922

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.446 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

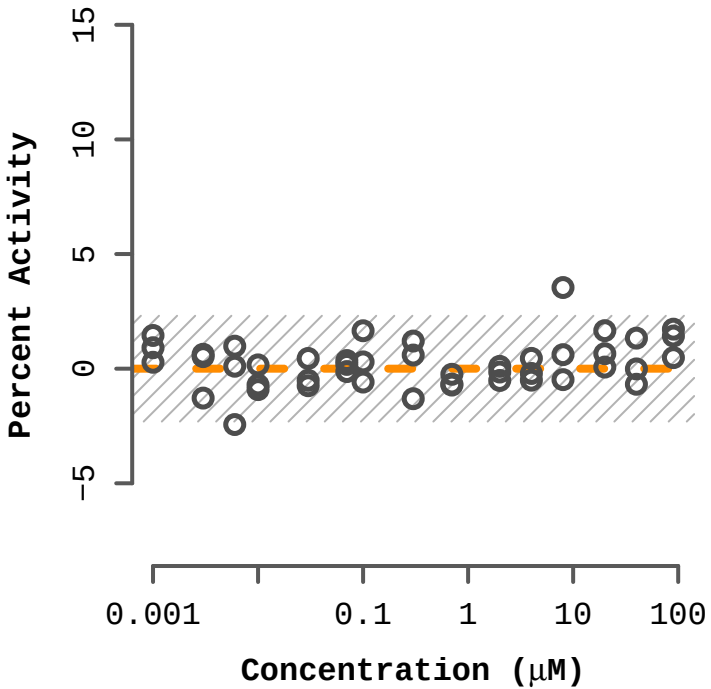
NAME: 2-Chloro-4-nitroaniline
CHID: 21973 **CASRN:** 121-87-9
SPID(S): Tox21_303921
M4ID: 12475267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 2.9 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

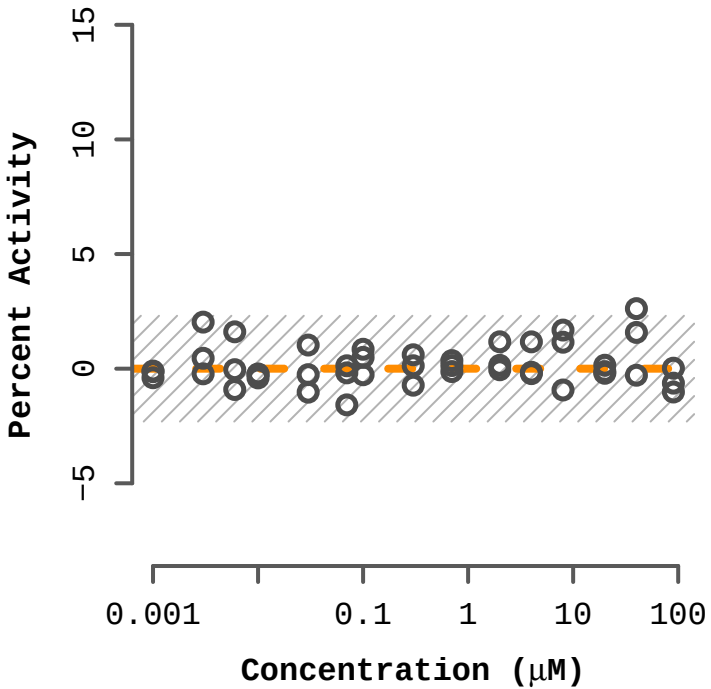
NAME: 4-Isopropylbenzaldehyde
CHID: 21974 **CASRN:** 122-03-2
SPID(S): Tox21_300712
M4ID: 12478421

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

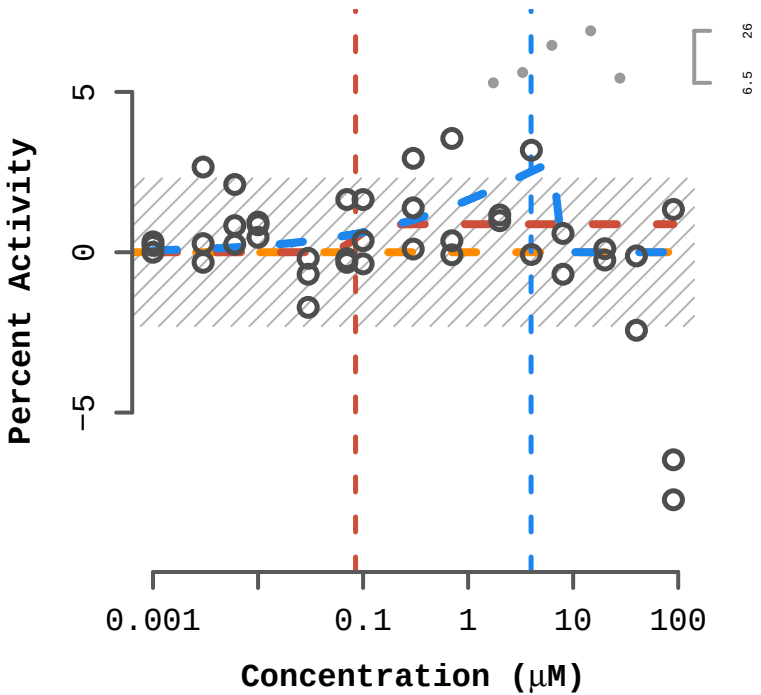
NAME: Diphenylamine
CHID: 21975 **CASRN:** 122-39-4
SPID(S): Tox21_301026
M4ID: 12478107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diphenylamine
CHID: 21975 **CASRN:** 122-39-4
SPID(S): Tox21_201611
M4ID: 12480641 **BRK**

HILL MODEL (in red):

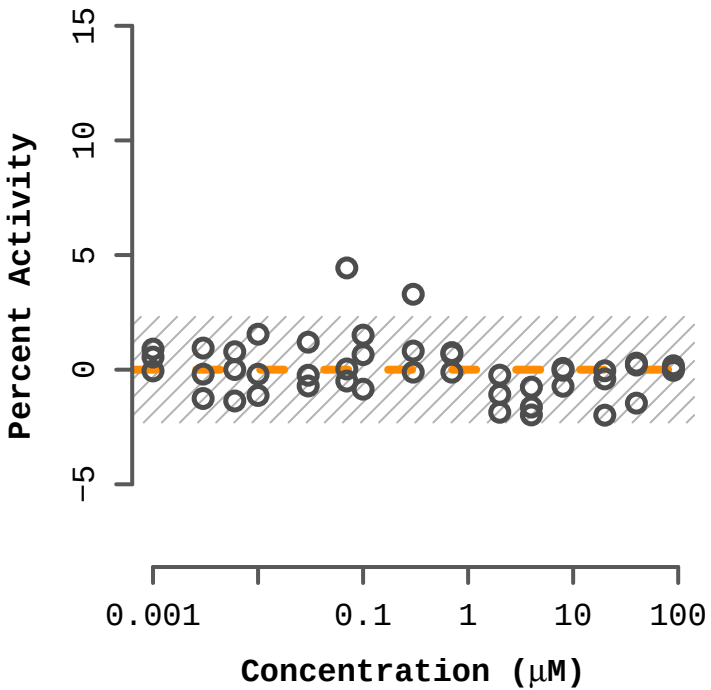
	tp	ga	gw
val:	0.875	−1.07	4.98
sd:	0.5	0.411	12.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.03	0.599	0.533	0.849	17.5
sd:	12.9	3.84	0.666	0.429	139

	CNST	HILL	GNLS
AIC:	245.5	247.95	247.22
PROB:	0.58	0.17	0.25
RMSE:	5.82	5.62	5.63

MAX_MEAN: 8.77 **MAX_MED:** 3.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

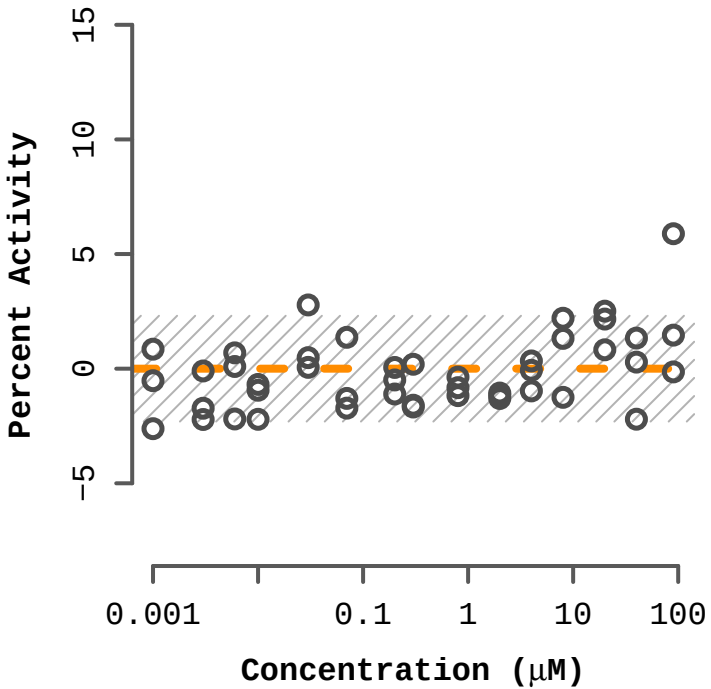
NAME: 2-Phenoxyethanol
CHID: 21976 **CASRN:** 122-99-6
SPID(S): Tox21_300842
M4ID: 12478291

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.814 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

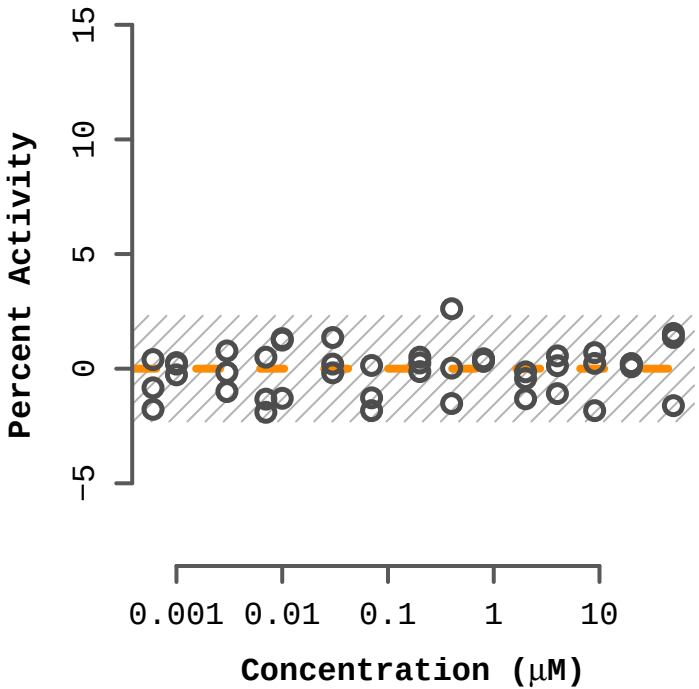
NAME: 2-Phenoxyethanol
CHID: 21976 **CASRN:** 122-99-6
SPID(S): Tox21_202111
M4ID: 12480141

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.4 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

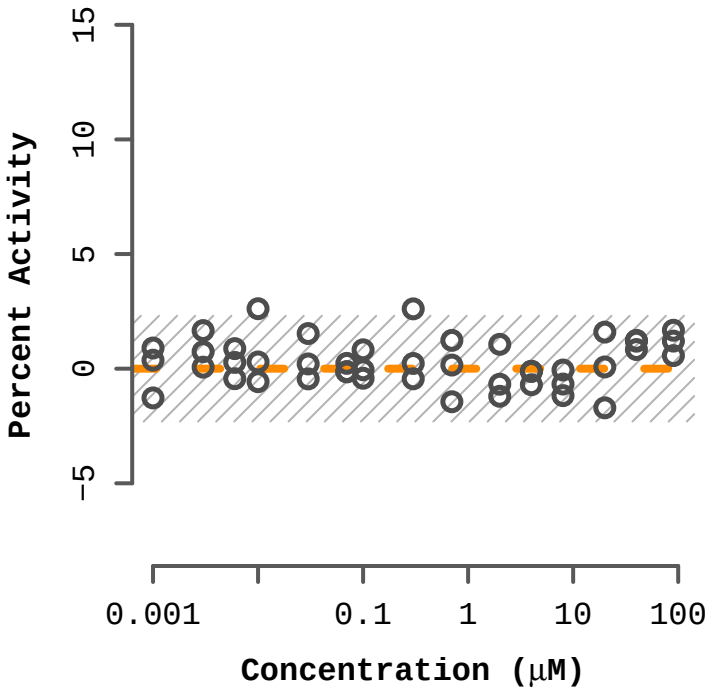
NAME: 2-Phenoxyethanol
CHID: 21976 **CASRN:** 122-99-6
SPID(S): Tox21_111002_1
M4ID: 12483955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.461 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

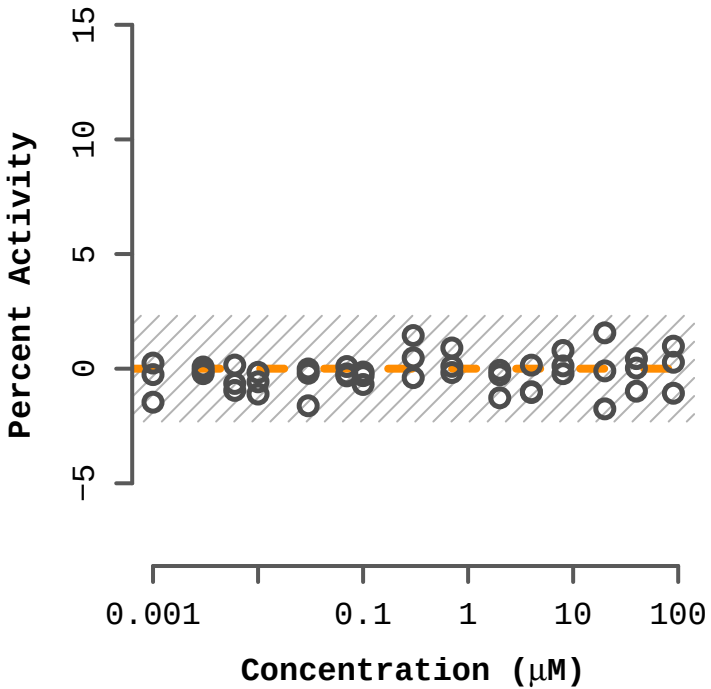
NAME: 4-Ethylphenol
CHID: 21977 **CASRN:** 123-07-9
SPID(S): Tox21_302986
M4ID: 12476147

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

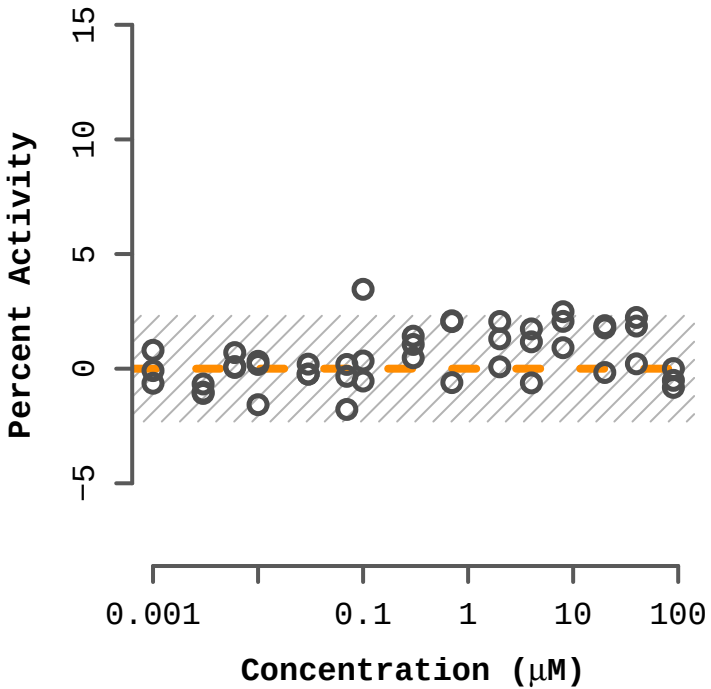
NAME: 4-Ethylphenol
CHID: 21977 **CASRN:** 123-07-9
SPID(S): Tox21_201533
M4ID: 12480719

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.509 **MAX_MED:** 0.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

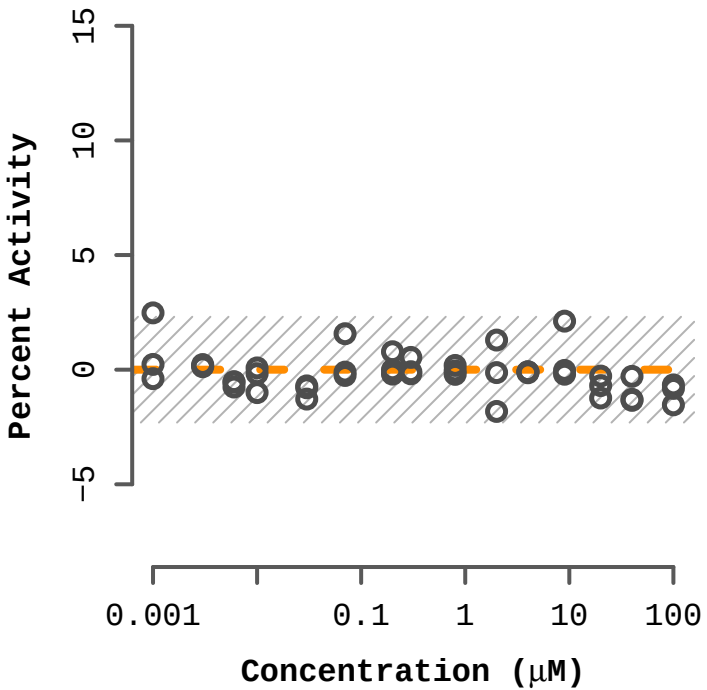
NAME: 2-Methylpentanal
CHID: 21978 **CASRN:** 123-15-9
SPID(S): Tox21_303754
M4ID: 12475434

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

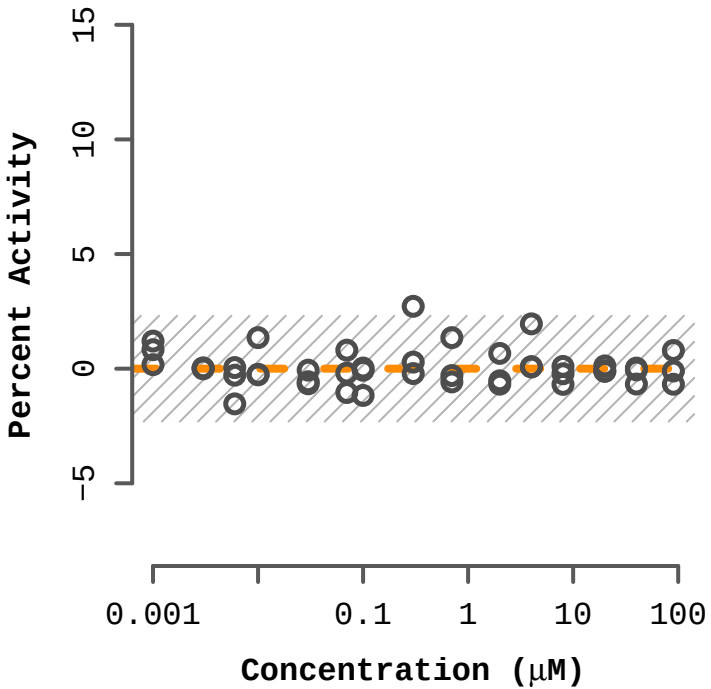
NAME: 2,4−Pentanedione
CHID: 21979 **CASRN:** 123−54−6
SPID(S): Tox21_200414
M4ID: 12481838

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.773 **MAX_MED:** 0.231 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

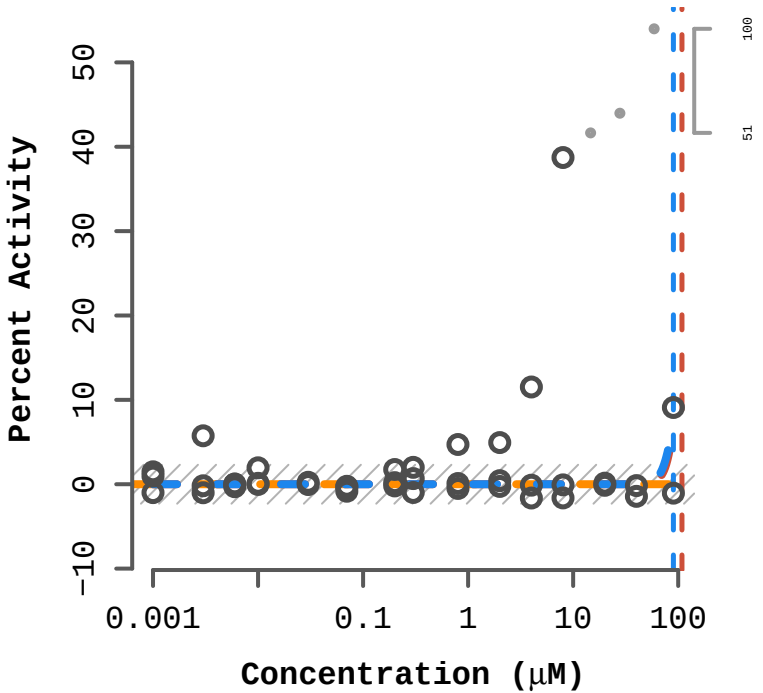
NAME: Ethyl hexanoate
CHID: 21980 **CASRN:** 123-66-0
SPID(S): Tox21_301217
M4ID: 12477916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl acetate
CHID: 21982 CASRN: 123-86-4
SPID(S): Tox21_201052
M4ID: 12481200 BRK

HILL MODEL (in red):

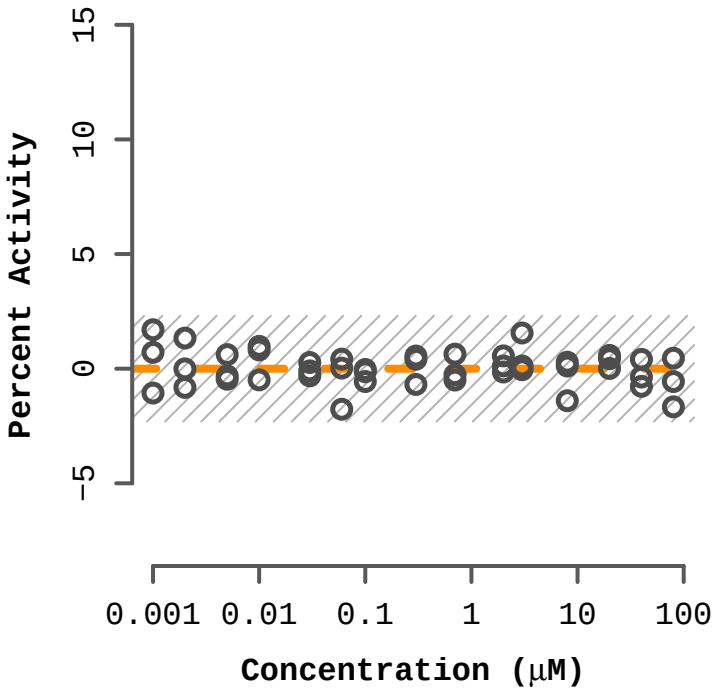
	tp	ga	gw
val:	39.7	2.04	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.5	1.95	8	3.58	4.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	299.62	304.7	308.71
PROB:	0.92	0.07	0.01
RMSE:	20.22	19.42	19.42

MAX_MEAN: 35.9 **MAX_MED:** 9.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

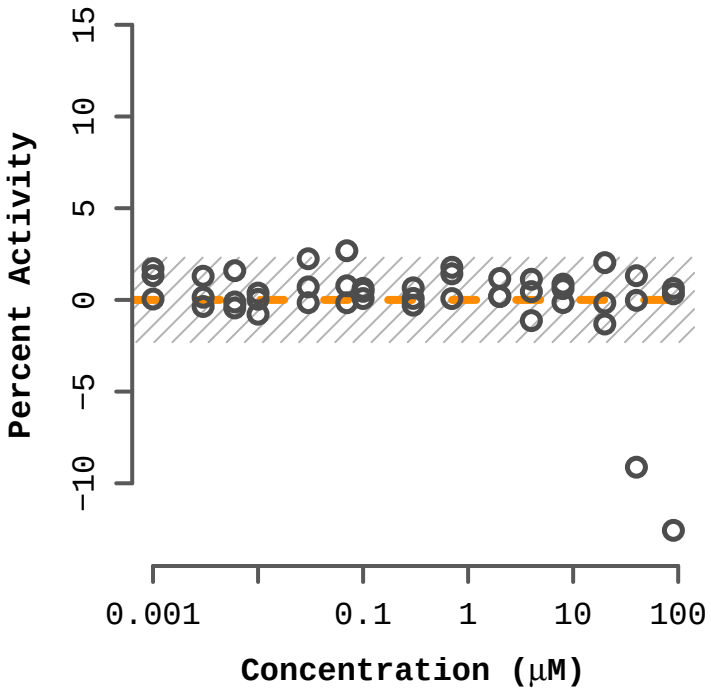
NAME: 1-Dodecanamine
CHID: 21984 **CASRN:** 124-22-1
SPID(S): Tox21_302940
M4ID: 12476193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.543 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

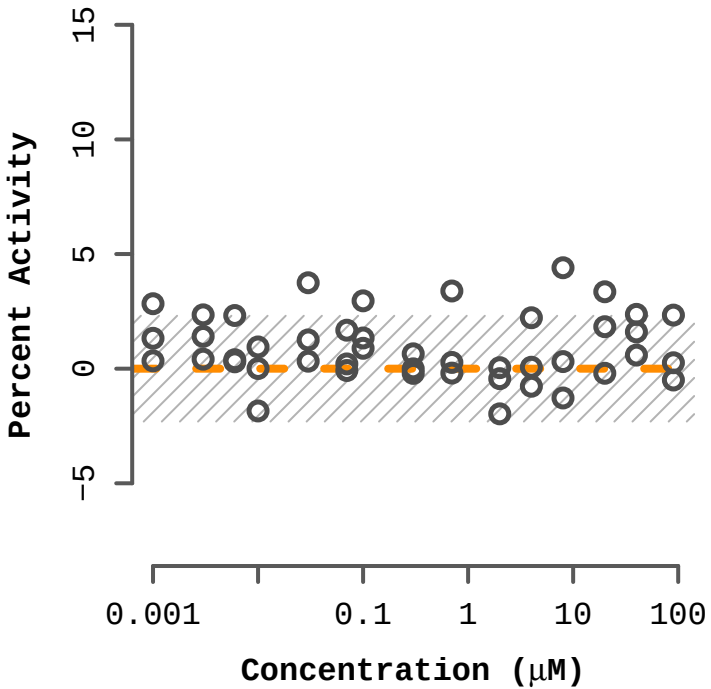
NAME: 1-Dodecanamine
CHID: 21984 **CASRN:** 124-22-1
SPID(S): Tox21_201900
M4ID: 12480352

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

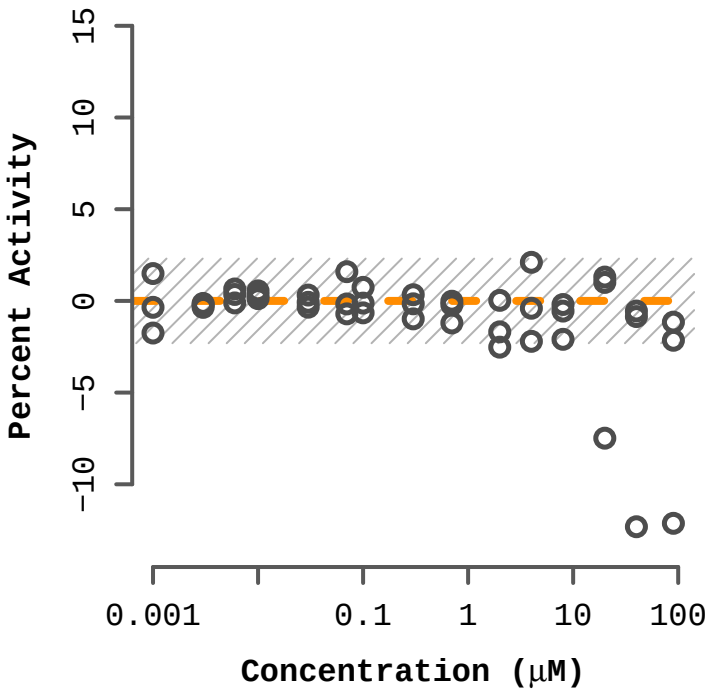
NAME: Tributyl phosphate
CHID: 21986 CASRN: 126-73-8
SPID(S): Tox21_300107
M4ID: 12479023

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

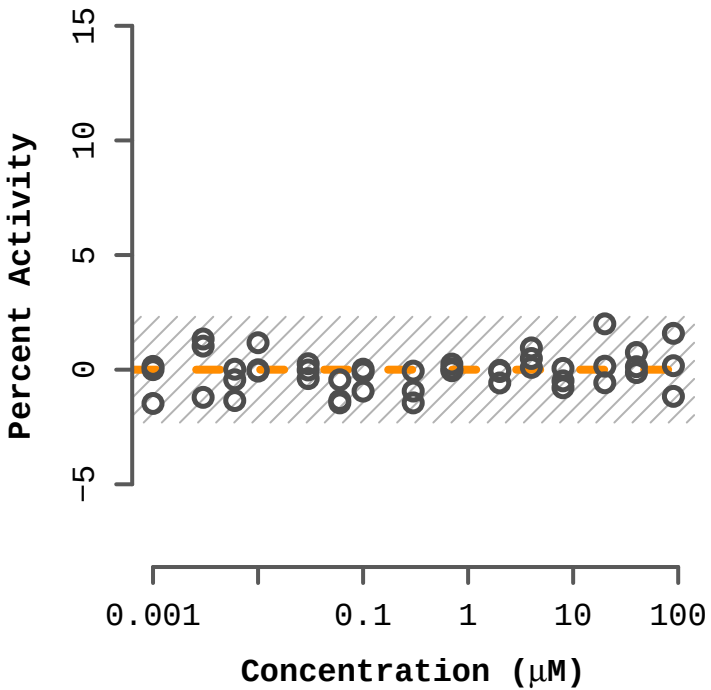
NAME: Tributyl phosphate
CHID: 21986 **CASRN:** 126-73-8
SPID(S): Tox21_201872
M4ID: 12480380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 0.329 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

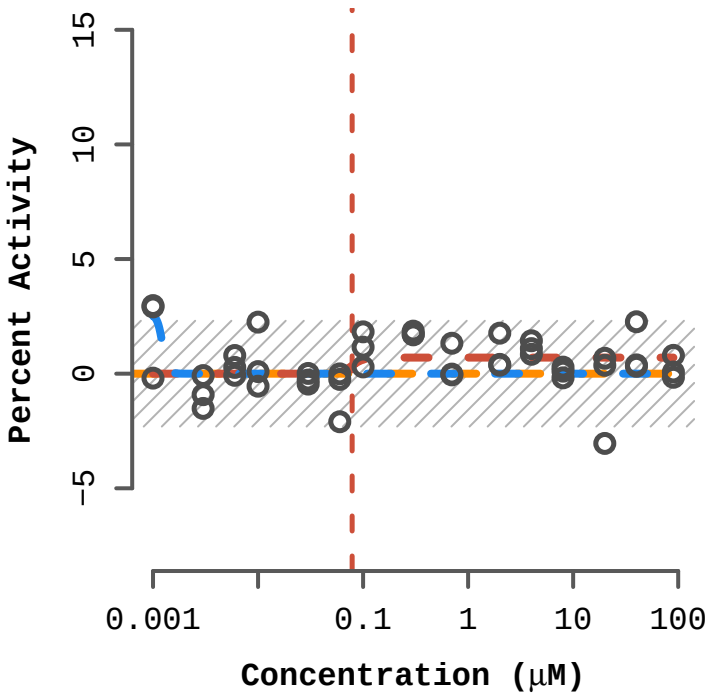
NAME: 1-Chloro-2-propanol, technical grade (~75% 1-cl
CHID: 21988 **CASRN:** NOCAS_21988
SPID(S): Tox21_200998
M4ID: 12481254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium saccharin hydrate
CHID: 21992 CASRN: 82385-42-0
SPID(S): Tox21_300604
M4ID: 12478529

HILL MODEL (in red):

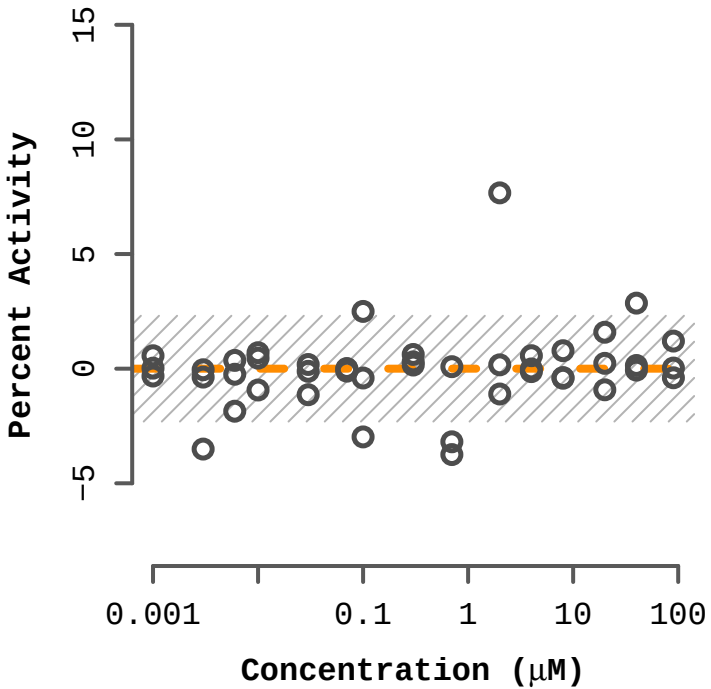
	tp	ga	gw
val:	0.702	−1.1	8
sd:	0.18	0.106	7.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.33	−4.05	0.521	−2.91	17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	148.91	141.14	152.44
PROB:	0.02	0.98	0
RMSE:	1.25	1.15	1.16

MAX_MEAN: 1.9 **MAX_MED:** 2.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

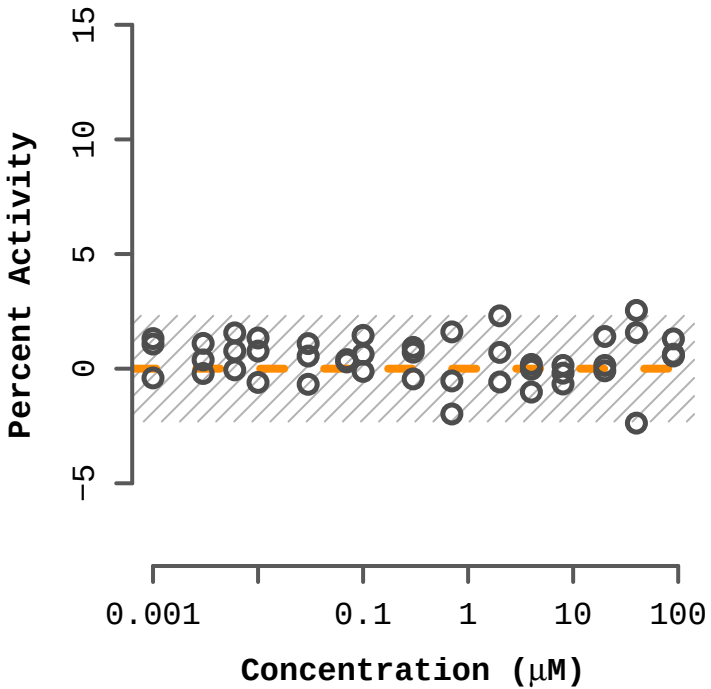
NAME: Dibenzofuran
CHID: 21993 **CASRN:** 132-64-9
SPID(S): Tox21_300052
M4ID: 12479078

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 0.461 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

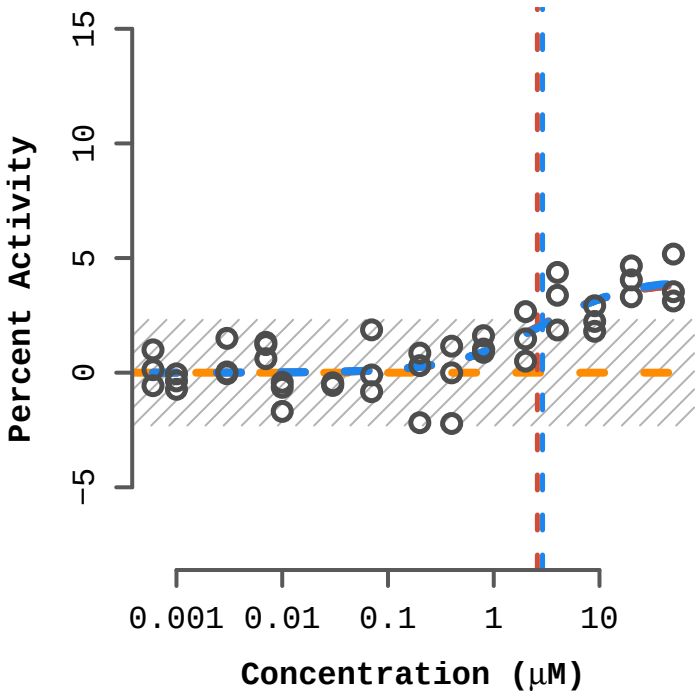
NAME: Dibenzofuran
CHID: 21993 **CASRN:** 132-64-9
SPID(S): Tox21_202116
M4ID: 12480136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.829 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenyl 4-aminosalicylate
CHID: 21994 **CASRN:** 133-11-9
SPID(S): Tox21_111538_1
M4ID: 12483629

HILL MODEL (in red):

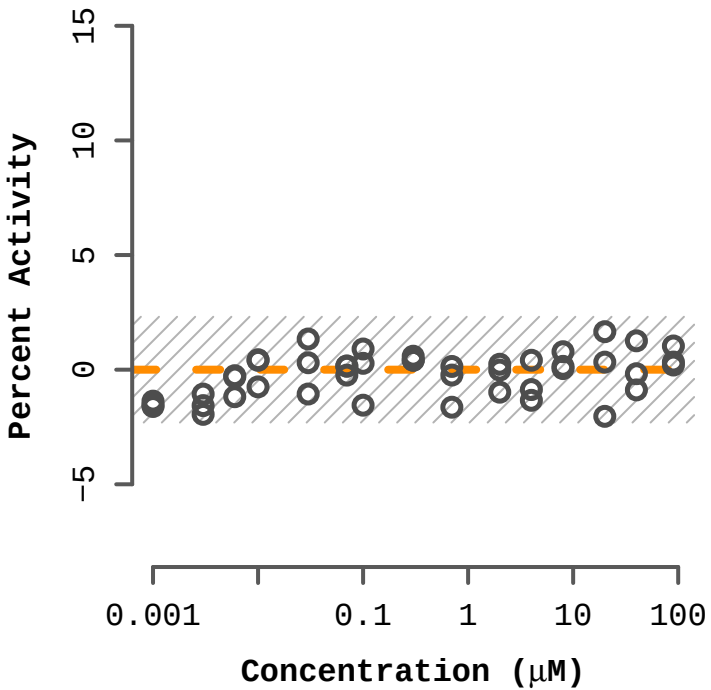
	tp	ga	gw
val:	3.98	0.413	1.05
sd:	0.767	0.297	0.436

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.14	0.461	1	1.83	11.4
sd:	1.81	0.582	0.615	0.597	54.1

	CNST	HILL	GNLS
AIC:	195.16	136.7	140.68
PROB:	0	0.88	0.12
RMSE:	2.06	1	1

MAX_MEAN: 4.01 **MAX_MED:** 4.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

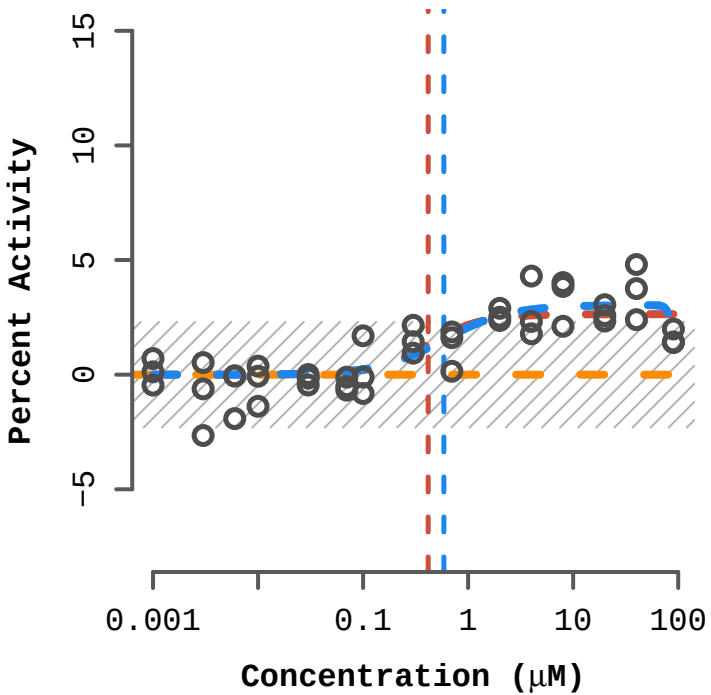
NAME: DEET
CHID: 21995 CASRN: 134-62-3
SPID(S): Tox21_300917
M4ID: 12478216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.524 **MAX_MED:** 0.416 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: DEET
CHID: 21995 CASRN: 134-62-3
SPID(S): Tox21_201980
M4ID: 12480272

HILL MODEL (in red):

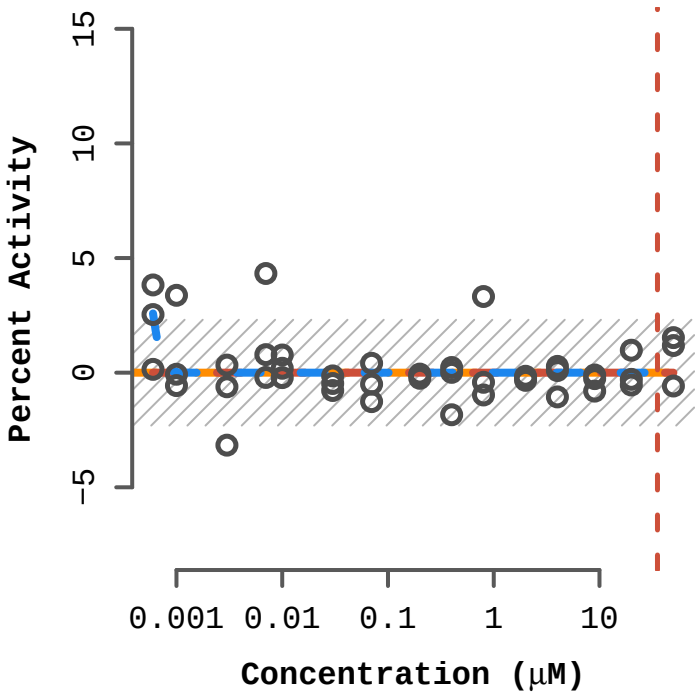
	tp	ga	gw
val:	2.64	−0.38	1.73
sd:	0.263	0.187	0.629

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.04	−0.231	1.4	1.96	16.4
sd:	0.345	0.183	0.454	0.0158	84.4

	CNST	HILL	GNLS
AIC:	196.9	130.85	127.14
PROB:	0	0.14	0.86
RMSE:	2.04	0.95	0.88

MAX_MEAN: 3.65 MAX_MED: 3.85 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: DEET
CHID: 21995 **CASRN:** 134-62-3
SPID(S): Tox21_111103_1
M4ID: 12483906

HILL MODEL (in red):

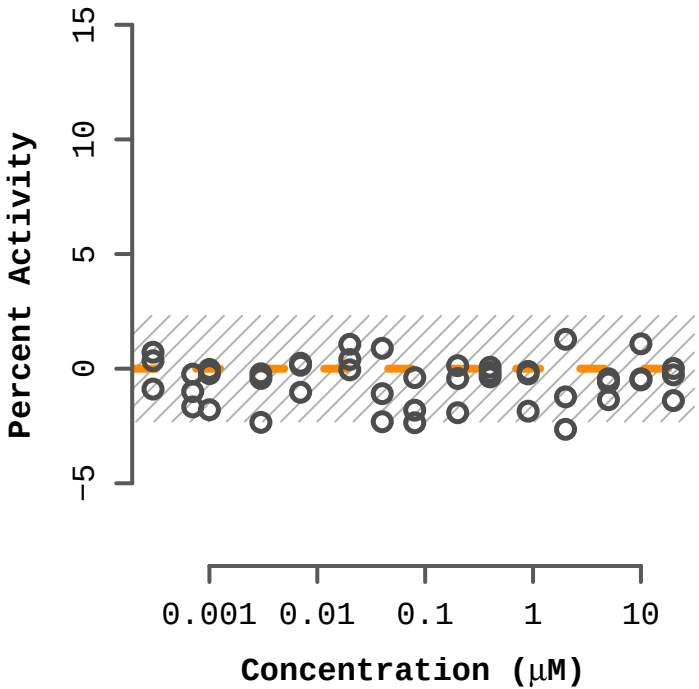
	tp	ga	gw
val:	2.73e-09	1.55	0.458
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.14	−3.59	6.68	−3.22	10.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	148.21	154.21	150.79
PROB:	0.75	0.04	0.21
RMSE:	1.41	1.41	1.3

MAX_MEAN: 2.17 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

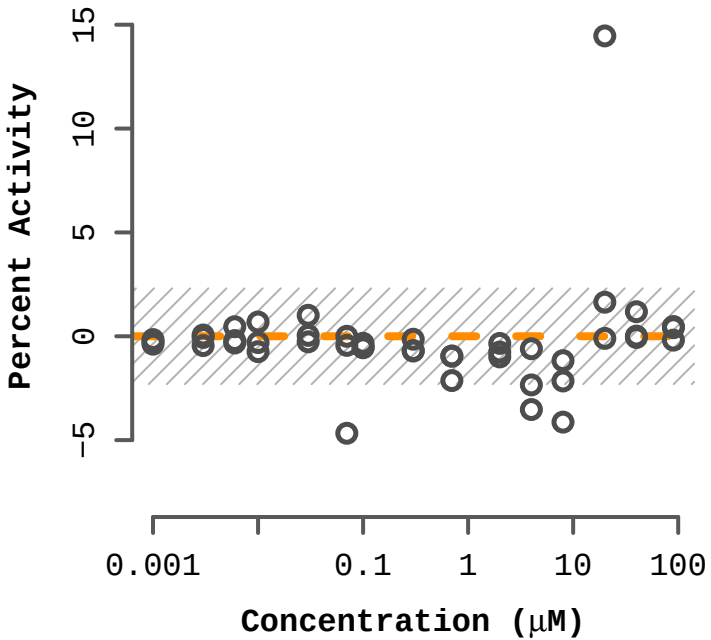
NAME: Sodium propionate
CHID: 21996 CASRN: 137-40-6
SPID(S): Tox21_202735
M4ID: 12479517

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.473 **MAX_MED:** 0.403 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

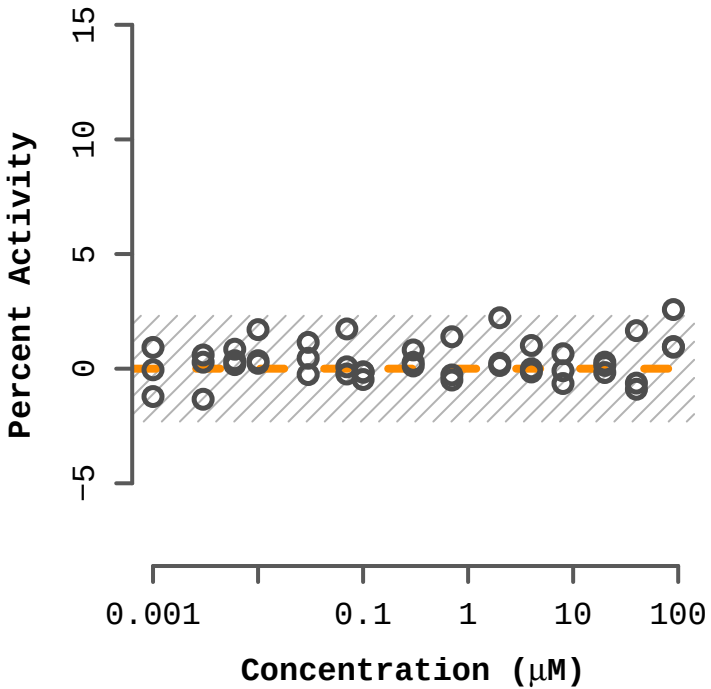
NAME: 1-(2-Aminoethyl)piperazine
CHID: 21997 **CASRN:** 140-31-8
SPID(S): Tox21_302922
M4ID: 12476211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.36	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 5.33 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

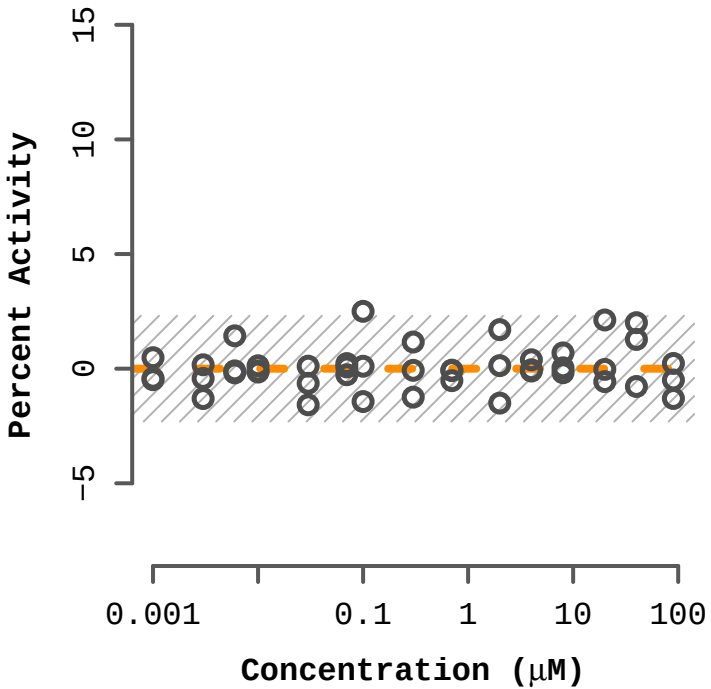
NAME: 1-(2-Aminoethyl)piperazine
CHID: 21997 **CASRN:** 140-31-8
SPID(S): Tox21_202230
M4ID: 12480022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 0.968 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

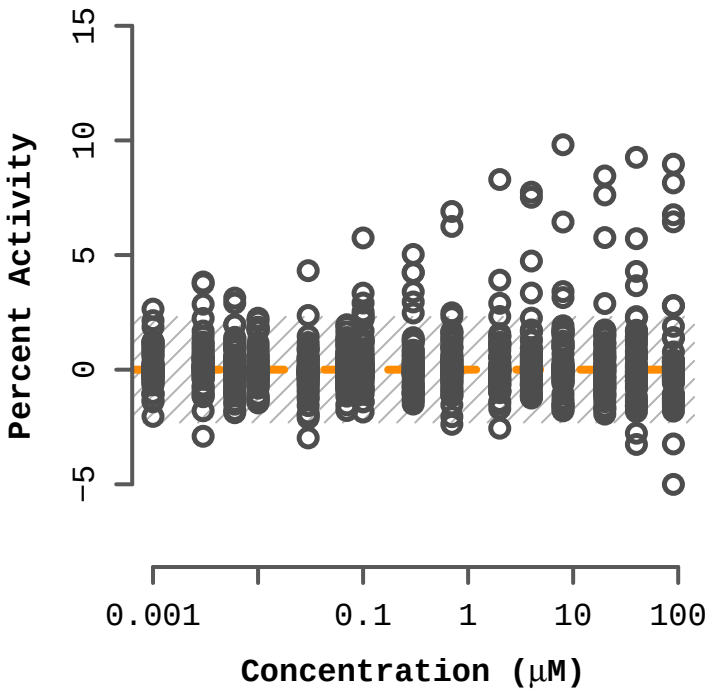
NAME: Dibutyl butanedioate
CHID: 21998 **CASRN:** 141-03-7
SPID(S): Tox21_301514
M4ID: 12477619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.836 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

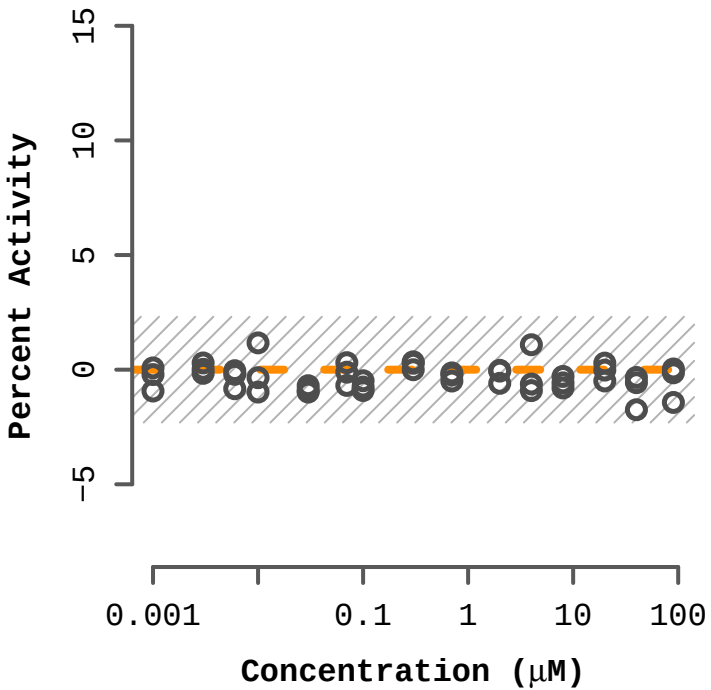
NAME: Ethanolamine
CHID: 22000 **CASRN:** 141-43-5
SPID(S): Tox21_400020
M4ID: 12475117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2510.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 0.542 **MAX_MED:** 0.139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

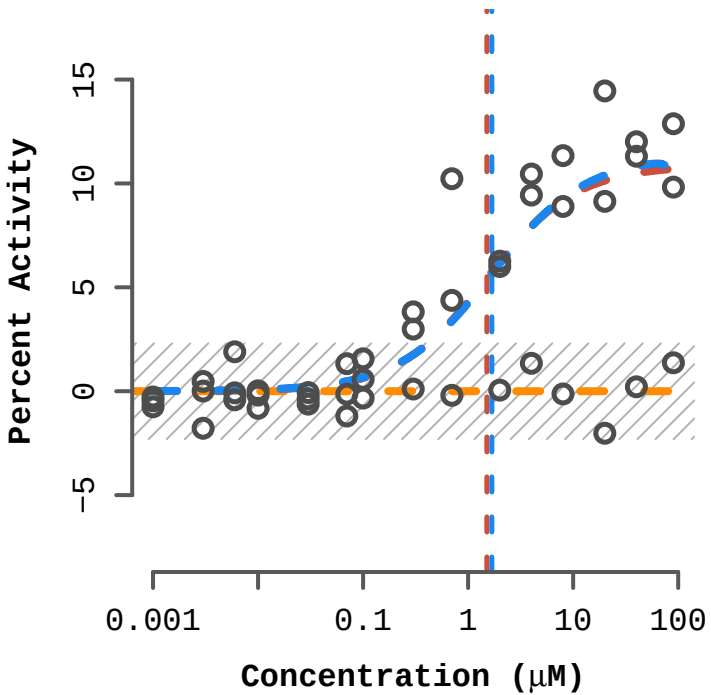
NAME: Ethyl acetate
CHID: 22001 **CASRN:** 141-78-6
SPID(S): Tox21_202512
M4ID: 12479740

HILL MODEL: Not applicable.

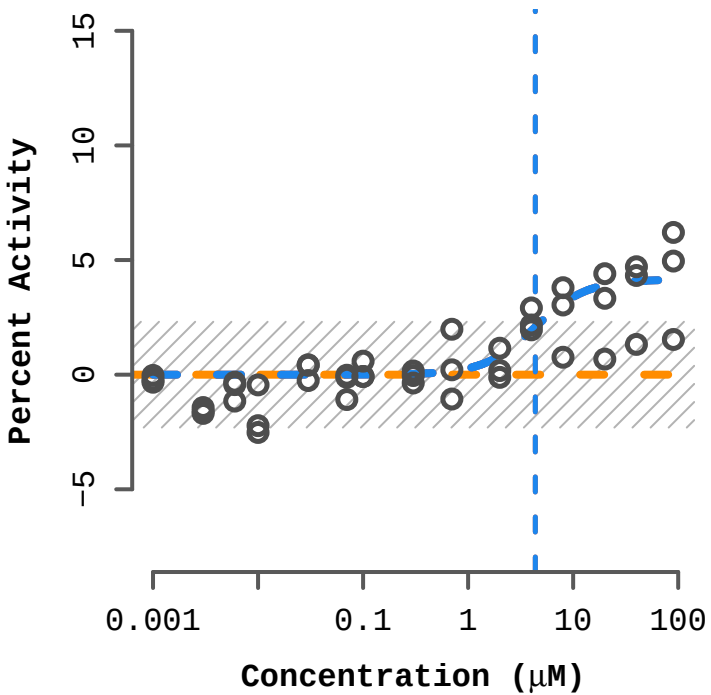
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.208 **MAX_MED:** 0.28 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,6-Dimethyl morpholine
CHID:    22002   CASRN: 141-91-3
SPID(S): Tox21_303829
M4ID:    12475359

HILL MODEL (in red):
      tp       ga       gw
val:  10.9     0.178    1.02
sd:   1.24     0.201    0.299

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  11.3     0.226    0.981    2.06     9.63
sd:   NaN      NaN      NaN      NaN      NaN

      CNST       HILL       GNLS
AIC:  281.89     238.93     242.76
PROB: 0          0.87       0.13
RMSE: 5.73       3.76       3.77

MAX_MEAN: 8.02      MAX_MED: 11.3      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3-Diethylbenzene
CHID: 22003 **CASRN:** 141-93-5
SPID(S): Tox21_303896
M4ID: 12475292

HILL MODEL (in red):

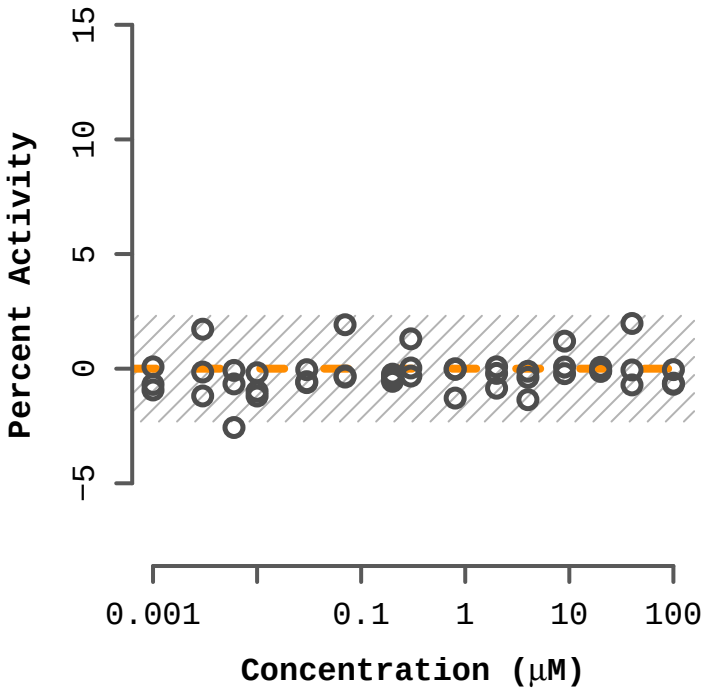
	tp	ga	gw
val:	4.15	0.64	1.79
sd:	0.971	0.229	1.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.15	0.64	1.79	3.24	6.75
sd:	0.971	0.229	1.6	2110	11000

	CNST	HILL	GNLS
AIC:	195.2	151.08	155.08
PROB:	0	0.88	0.12
RMSE:	2.16	1.22	1.22

MAX_MEAN: 4.23 **MAX_MED:** 4.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

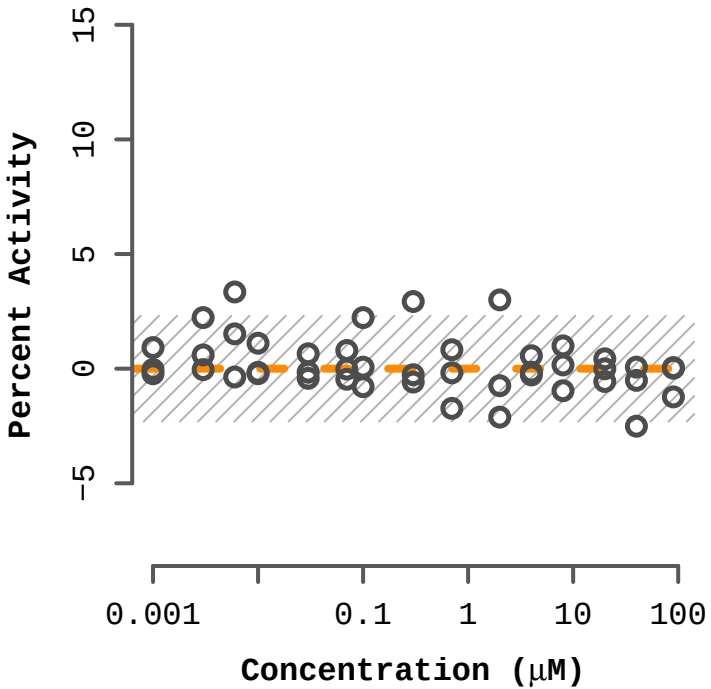
NAME: 1,3-Dichloropropane
CHID: 22004 CASRN: 142-28-9
SPID(S): Tox21_201140
M4ID: 12481112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.413 MAX_MED: 0.0736 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

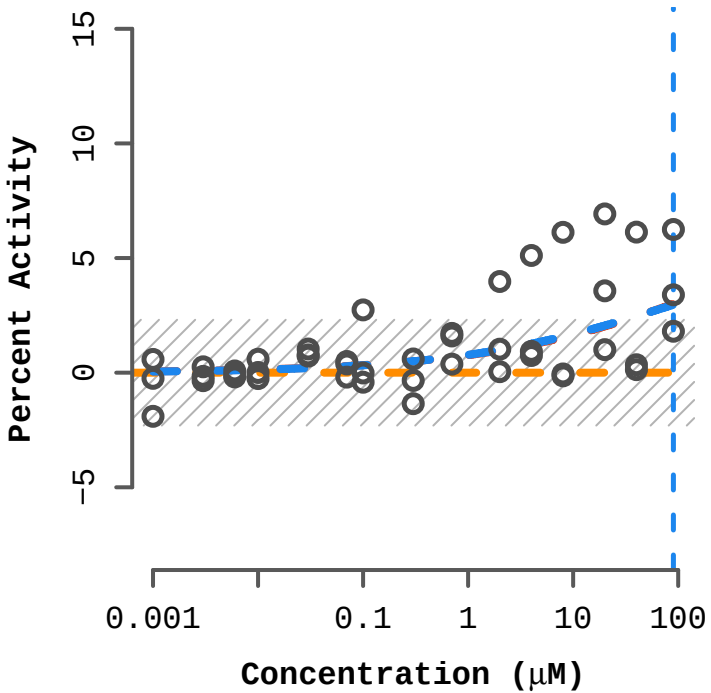
NAME: Hexyl acetate
CHID: 22006 **CASRN:** 142-92-7
SPID(S): Tox21_301393
M4ID: 12477740

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl ether
CHID: 22007 CASRN: 142-96-1
SPID(S): Tox21_201037
M4ID: 12481215

HILL MODEL (in red):

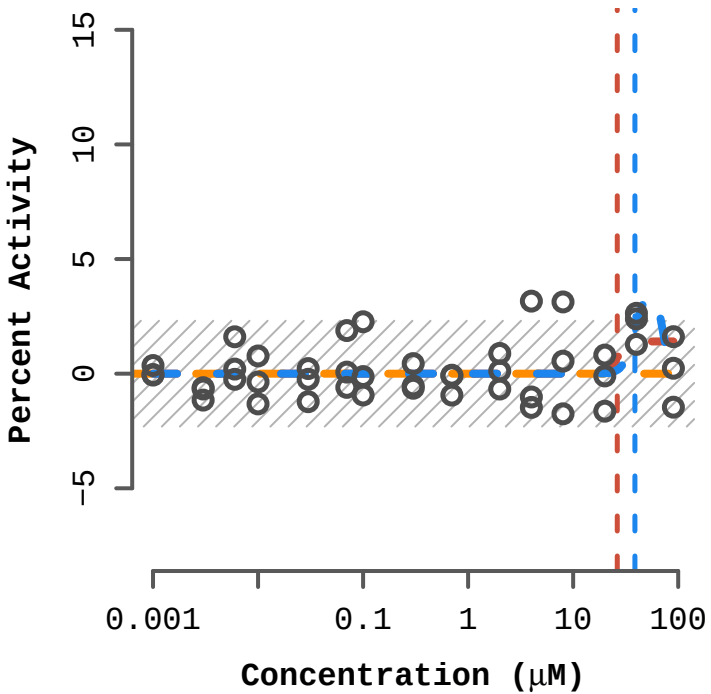
	tp	ga	gw
val:	7.72	2.45	0.391
sd:	21.8	5.18	0.271

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.92	1.95	0.42	3.83	3.33
sd:	11.1	3.55	0.279	404	734

	CNST	HILL	GNLS
AIC:	195.08	179.13	183.17
PROB:	0	0.88	0.12
RMSE:	2.4	1.72	1.72

MAX_MEAN: 3.83 MAX_MED: 3.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Nonanol
CHID: 22008 CASRN: 143-08-8
SPID(S): Tox21_300869
M4ID: 12478264

HILL MODEL (in red):

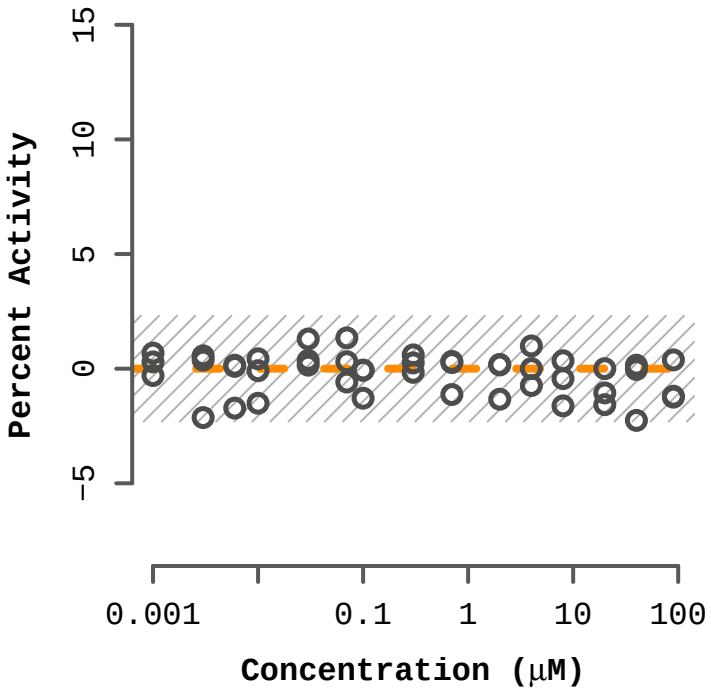
	tp	ga	gw
val:	1.41	1.42	8
sd:	0.508	0.115	6.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.8	1.59	8	1.85	11.9
sd:	16.8	0.539	16.4	0.816	97.2

	CNST	HILL	GNLS
AIC:	150.3	150.15	149.28
PROB:	0.27	0.29	0.44
RMSE:	1.25	1.2	1.13

MAX_MEAN: 2.1 MAX_MED: 2.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

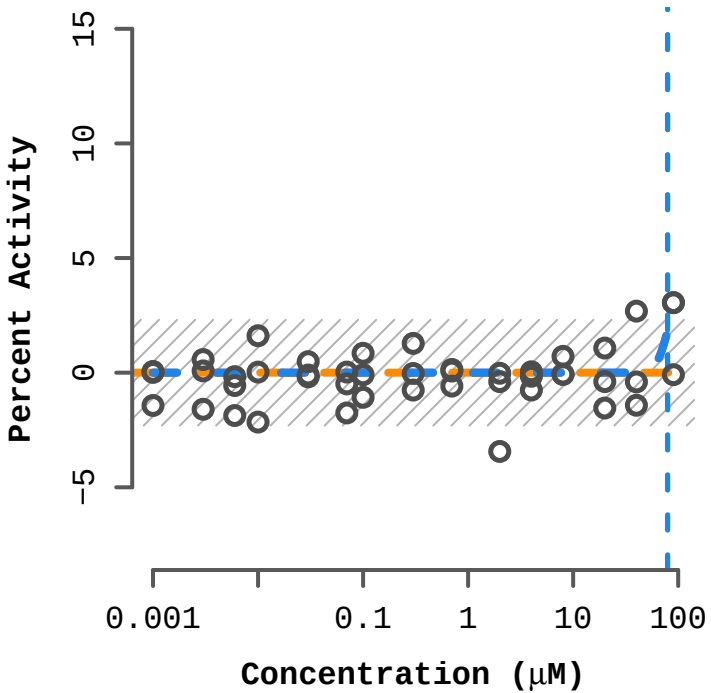
NAME: Dihexylamine
CHID: 22009 **CASRN:** 143-16-8
SPID(S): Tox21_302127
M4ID: 12477006

HILL MODEL: Not applicable.

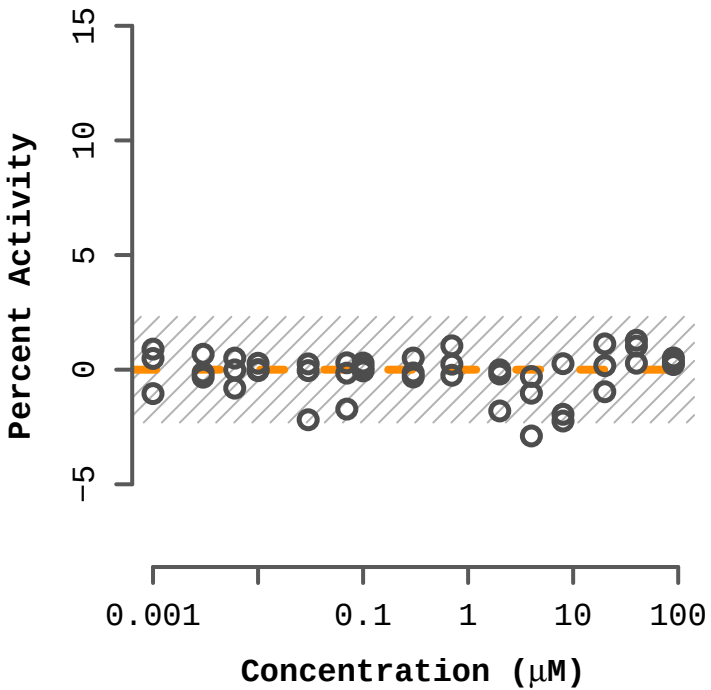
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.604 **MAX_MED:** 0.376 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (9Z)-Octadec-9-en-1-ol
CHID:    22010   CASRN: 143-28-2
SPID(S): Tox21_200111
M4ID:    12482141

HILL MODEL (in red):
      tp       ga       gw
val:  3.64     1.9      8
sd:   6.66     0.325    13.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.67     1.9      8        2.67     10.2
sd:   6.88     0.326    13.3     2410     34300

      CNST        HILL        GNLS
AIC:  144.27      142.69      146.69
PROB: 0.29        0.63        0.09
RMSE: 1.24        1.14        1.14

MAX_MEAN: 2.01      MAX_MED: 3.05      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

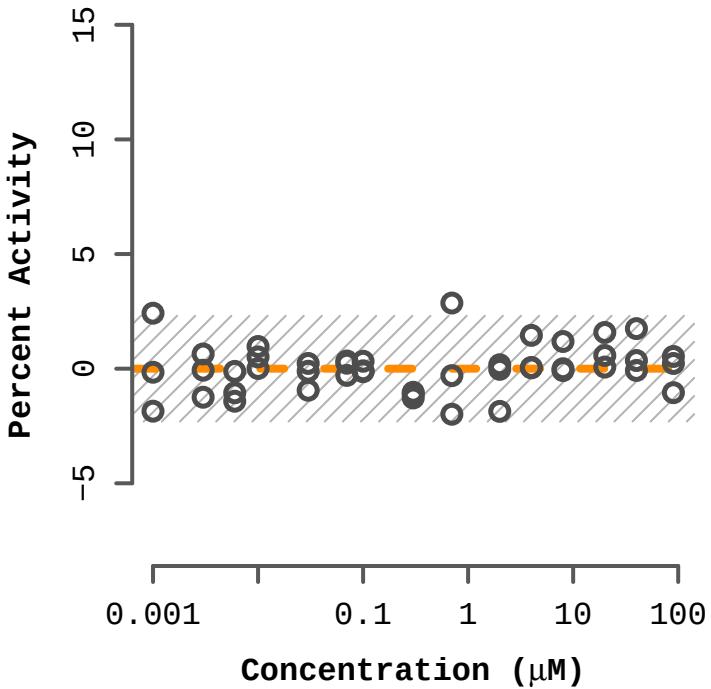
NAME: 3-Methoxyphenol
CHID: 22012 **CASRN:** 150-19-6
SPID(S): Tox21_303820
M4ID: 12475368

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.866 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

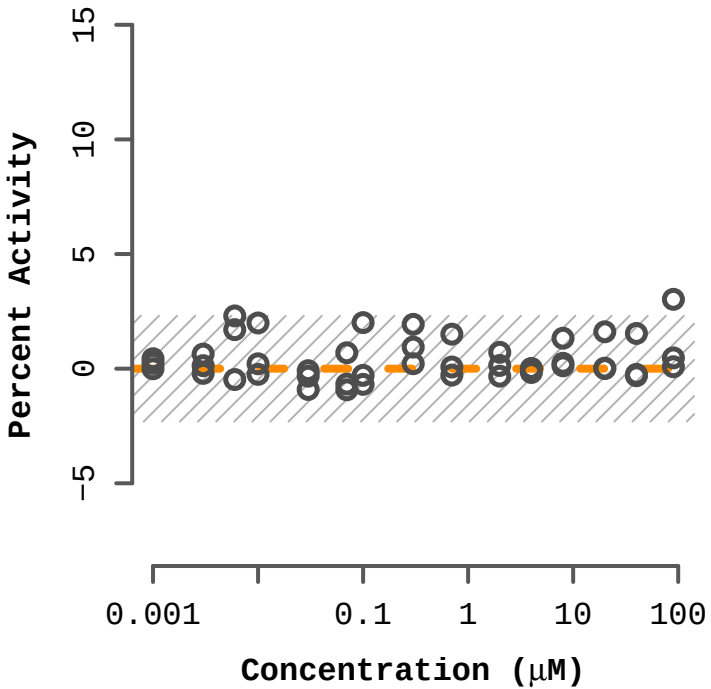
NAME: Hydroquinone dimethyl ether
CHID: 22014 **CASRN:** 150-78-7
SPID(S): Tox21_302782
M4ID: 12476351

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.743 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

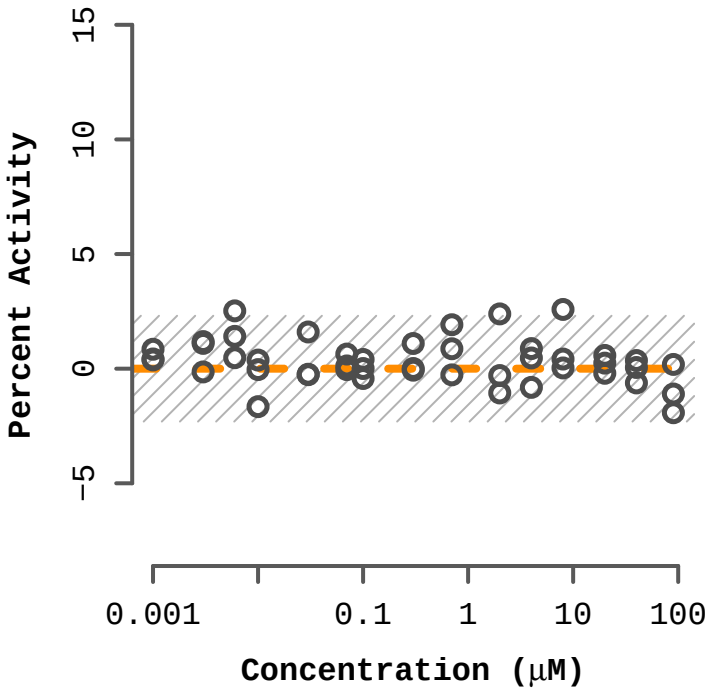
NAME: Hydroquinone dimethyl ether
CHID: 22014 **CASRN:** 150-78-7
SPID(S): Tox21_201333
M4ID: 12480919

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.26	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

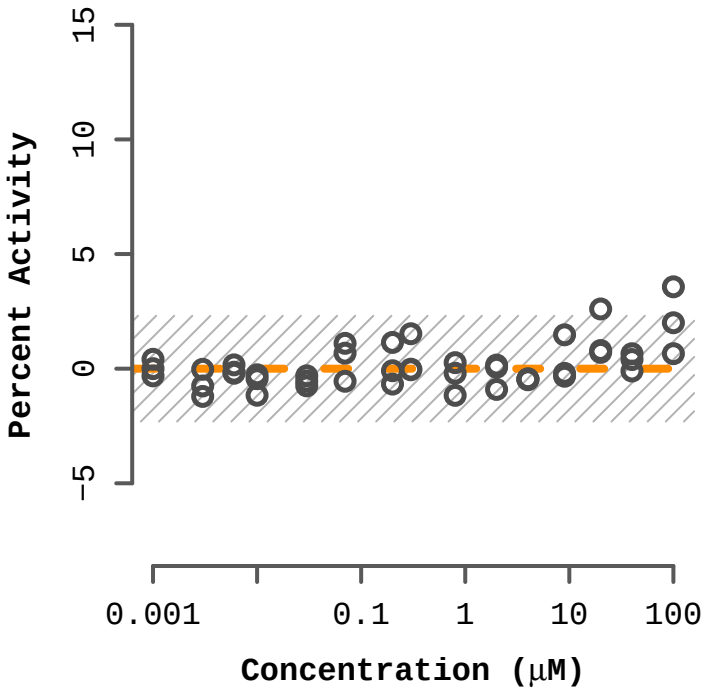
NAME: 1,4−Diazabicyclo[2.2.2]octane
CHID: 22016 **CASRN:** 280−57−9
SPID(S): Tox21_302908
M4ID: 12476225

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

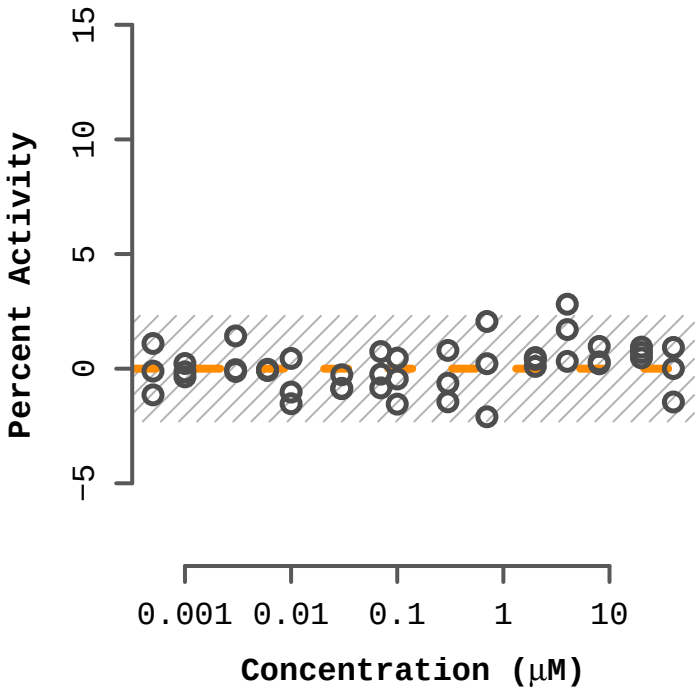
NAME: 1,4−Diazabicyclo[2.2.2]octane
CHID: 22016 **CASRN:** 280−57−9
SPID(S): Tox21_201323
M4ID: 12480929

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

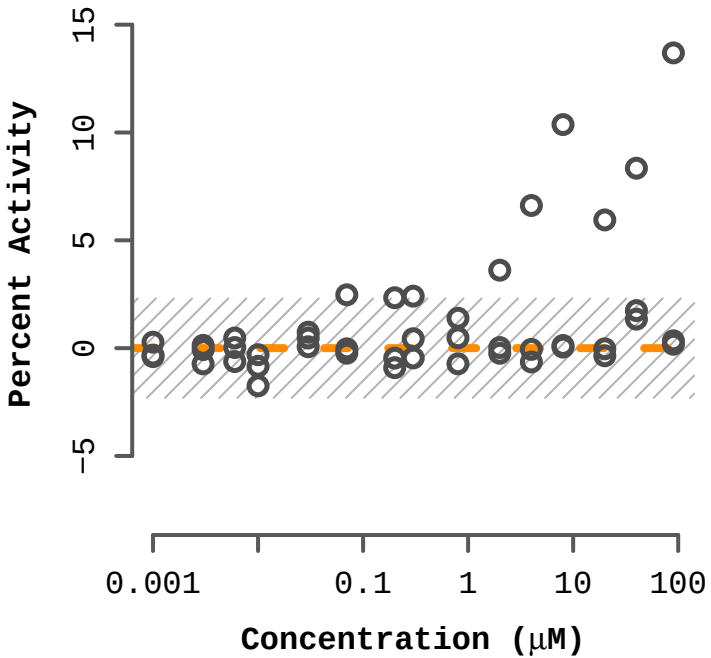
NAME: Disulfoton
CHID: 22018 **CASRN:** 298-04-4
SPID(S): Tox21_300861
M4ID: 12478272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

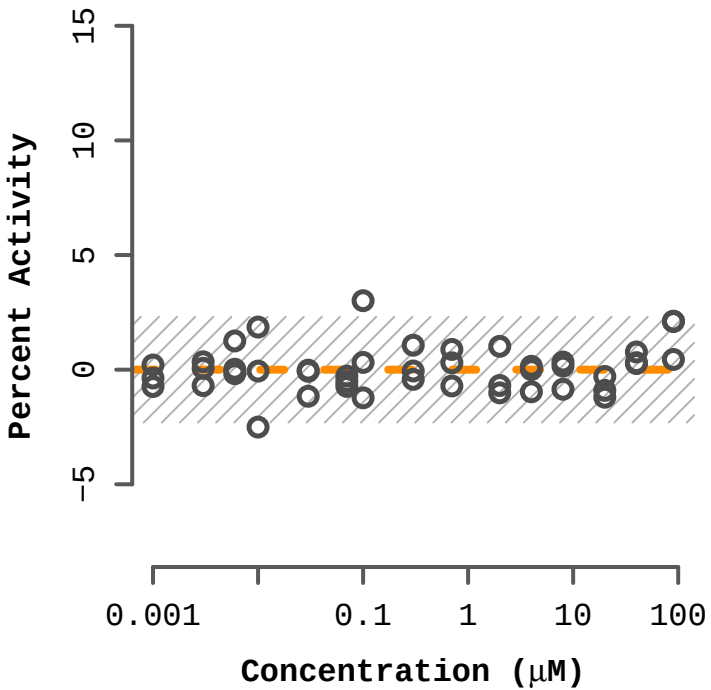
NAME: Disulfoton
CHID: 22018 CASRN: 298-04-4
SPID(S): Tox21_202343
M4ID: 12479909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.11	NA	NA
PROB:	1	NA	NA
RMSE:	3.3	NA	NA

MAX_MEAN: 4.74 MAX_MED: 1.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

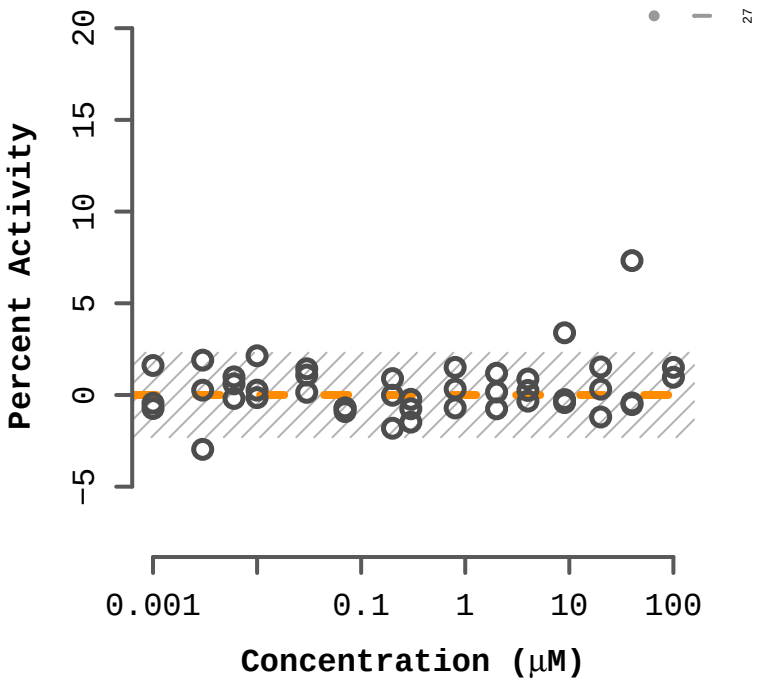
NAME: Bromacil
CHID: 22020 CASRN: 314-40-9
SPID(S): Tox21_301111
M4ID: 12478022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.51	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

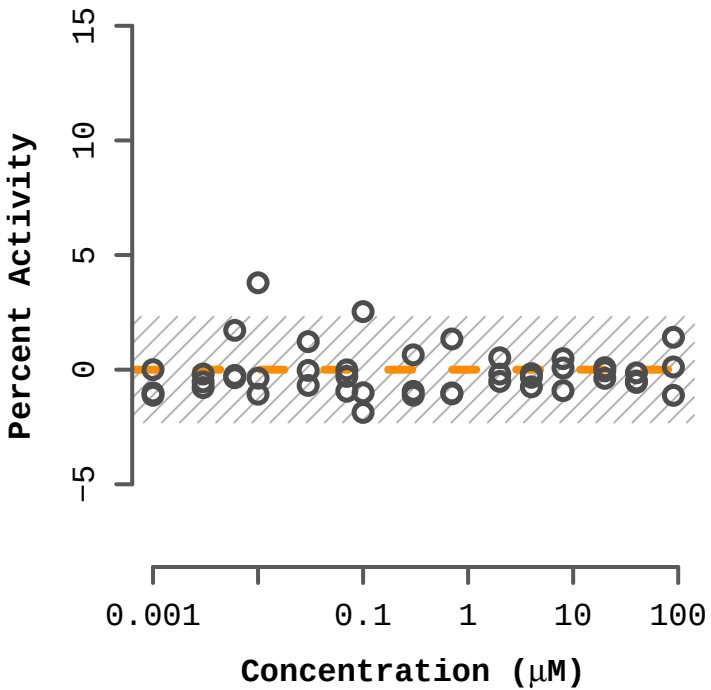
NAME: 4-Fluoroaniline
CHID: 22027 **CASRN:** 371-40-4
SPID(S): Tox21_202828
M4ID: 12479424 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.78	NA	NA
PROB:	1	NA	NA
RMSE:	4.31	NA	NA

MAX_MEAN: 9.79 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

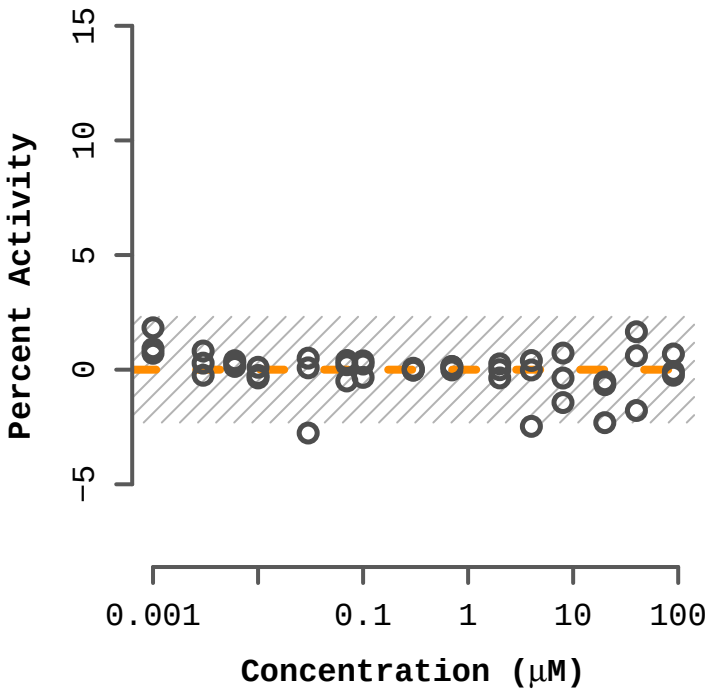
NAME: [(1S)-endo]-(-)-Borneol
CHID: 22035 **CASRN:** 464-45-9
SPID(S): Tox21_302285
M4ID: 12476848

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.785 **MAX_MED:** 0.119 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

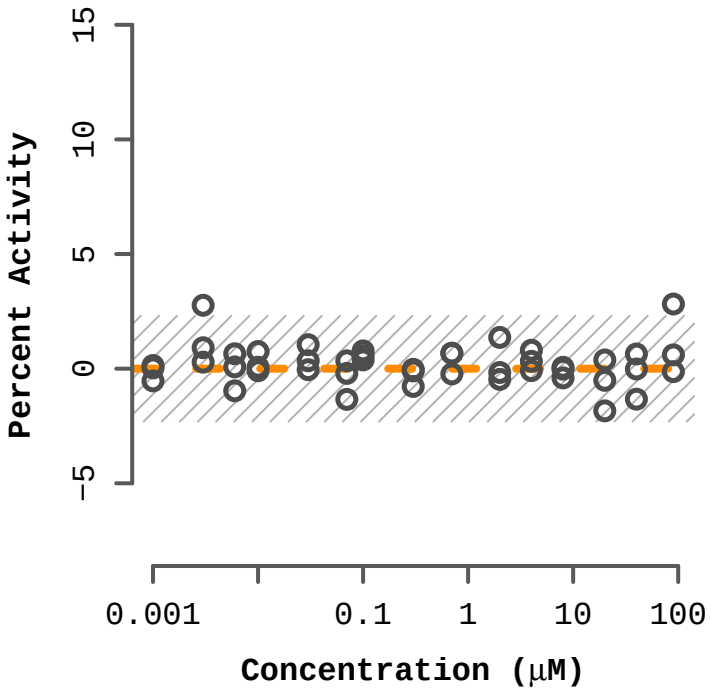
NAME: (1S)−(−)−Camphor
CHID: 22036 **CASRN:** 464−48−2
SPID(S): Tox21_303988
M4ID: 12475200

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.916 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

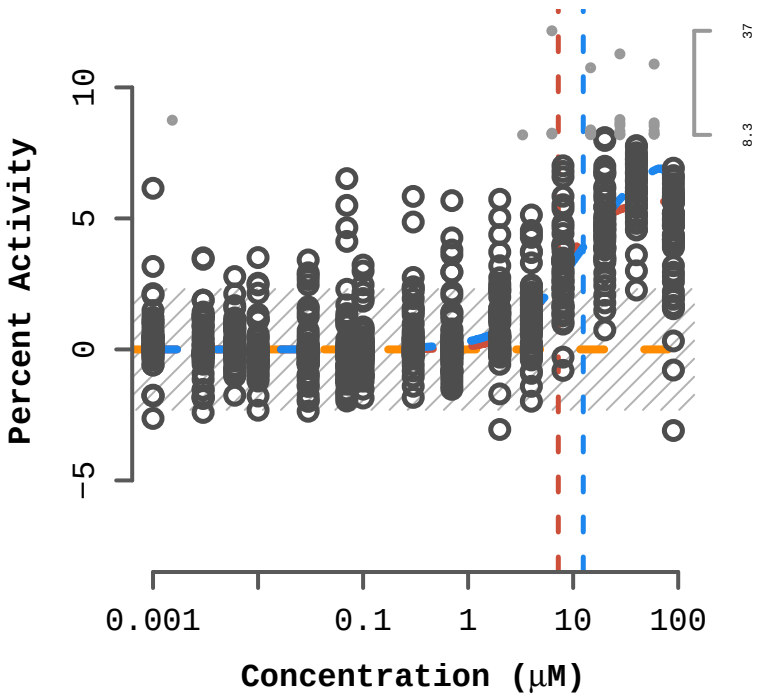
NAME: 2,6-Pyridinedicarboxylic acid
CHID: 22043 **CASRN:** 499-83-2
SPID(S): Tox21_301129
M4ID: 12478004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.916 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flavone
CHID: 22048 CASRN: 525-82-6
SPID(S): Tox21_400059
M4ID: 12475078 BRK

HILL MODEL (in red):

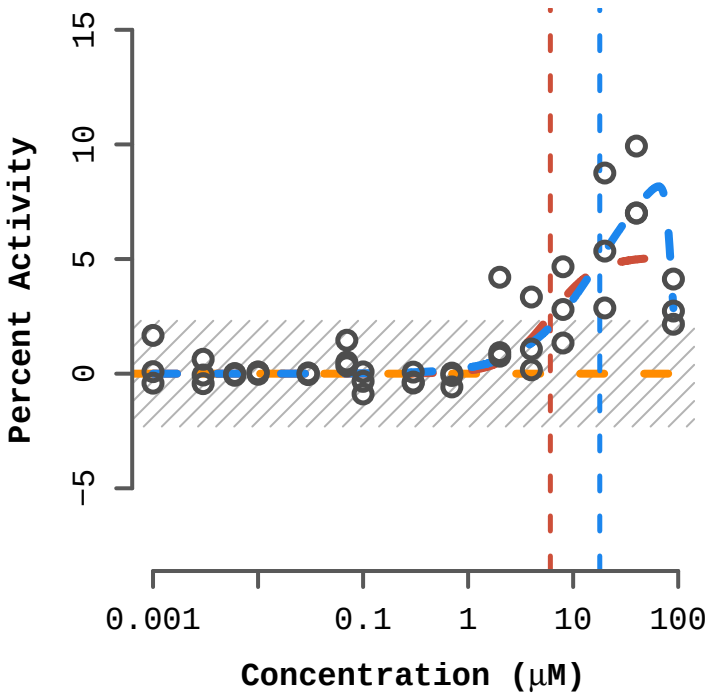
	tp	ga	gw
val:	5.7	0.858	1.98
sd:	0.186	0.0317	0.253

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.8	1.1	1.27	1.97	13.8
sd:	0.945	0.113	0.199	0.00832	6.32

	CNST	HILL	GNLS
AIC:	3644.72	2794.83	2762.93
PROB:	0	0	1
RMSE:	3.89	2.64	2.62

MAX_MEAN: 7.04 MAX_MED: 6.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flavone
CHID: 22048 CASRN: 525-82-6
SPID(S): Tox21_202987
M4ID: 12479265

HILL MODEL (in red):

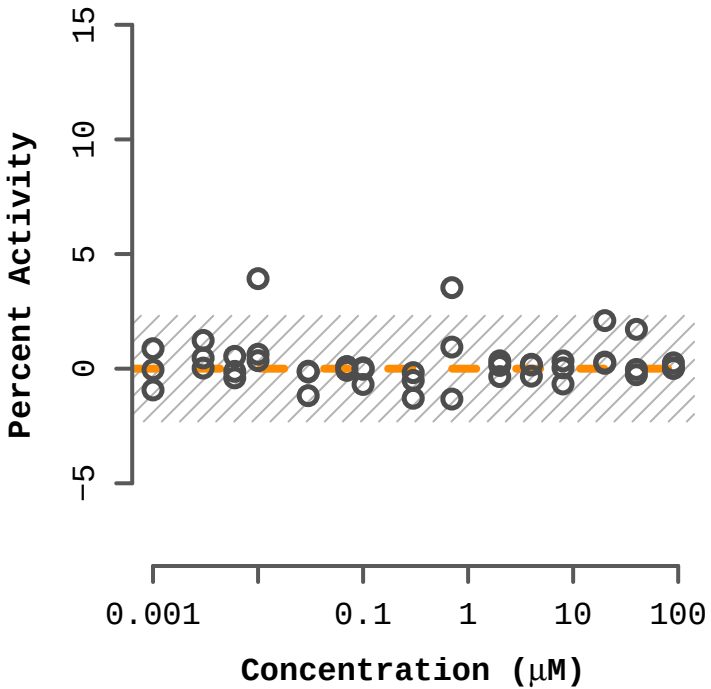
	tp	ga	gw
val:	5.1	0.783	2
sd:	1.19	0.161	0.756

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.95	1.25	1.25	1.93	15.3
sd:	3.51	0.311	0.394	0.0112	8.19

	CNST	HILL	GNLS
AIC:	214.45	162.37	139.98
PROB:	0	0	1
RMSE:	3.02	1.5	1.15

MAX_MEAN: 7.98 MAX_MED: 7.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

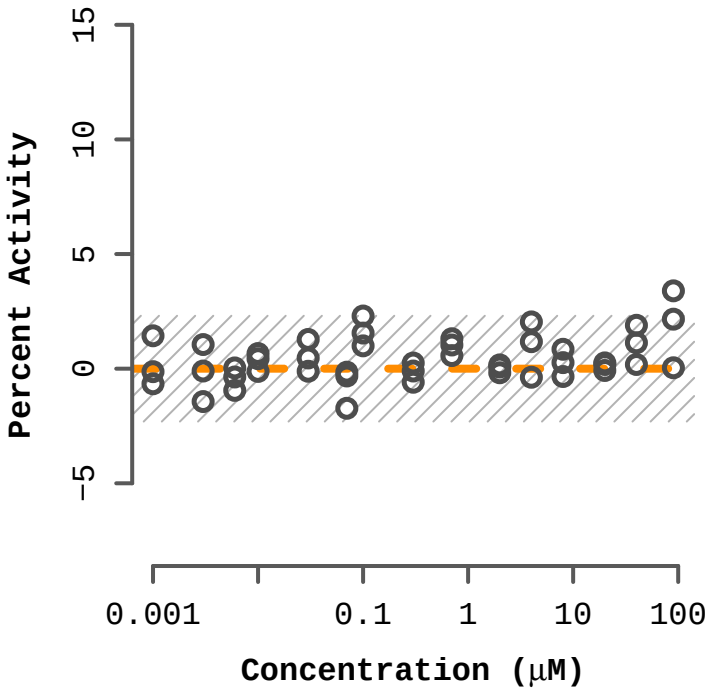
NAME: 2,4,6-Trimethylphenol
CHID: 22049 **CASRN:** 527-60-6
SPID(S): Tox21_300348
M4ID: 12478784

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 0.944 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

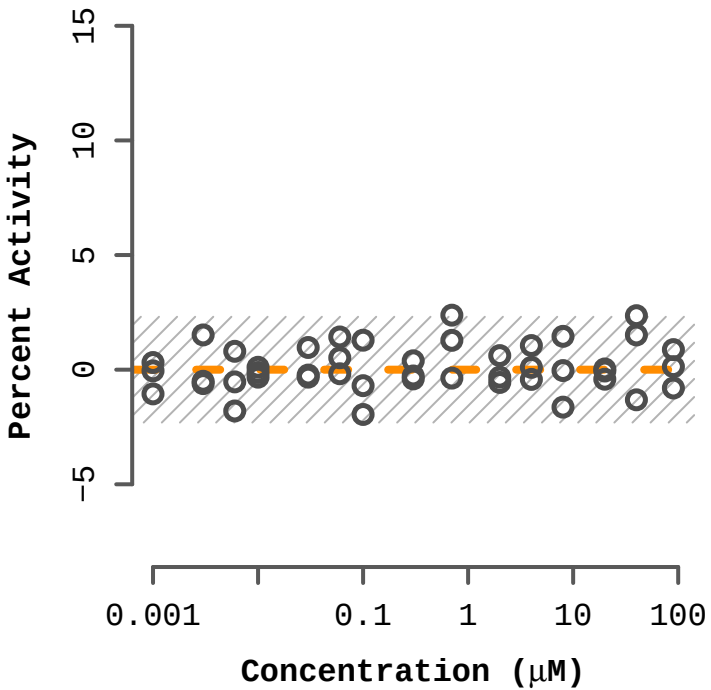
NAME: 2,4,6-Trimethylphenol
CHID: 22049 **CASRN:** 527-60-6
SPID(S): Tox21_202252
M4ID: 12480000

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

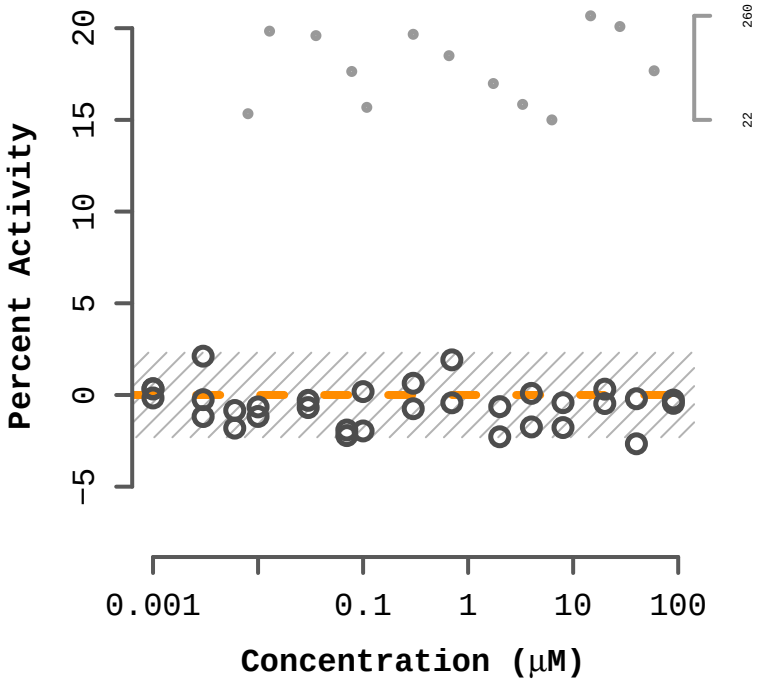
NAME: 2-Tolunitrile
CHID: 22050 CASRN: 529-19-1
SPID(S): Tox21_200324
M4ID: 12481928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

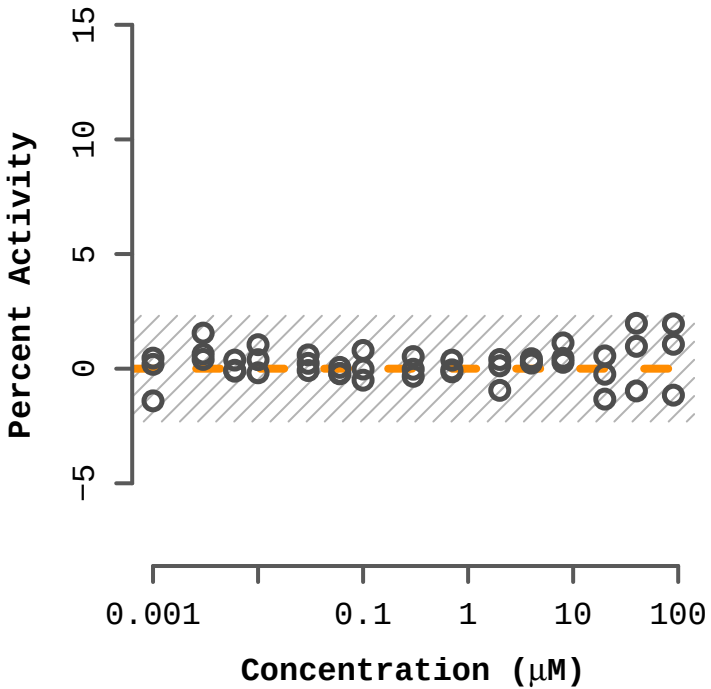
NAME: 2-Tolualdehyde
CHID: 22051 **CASRN:** 529-20-4
SPID(S): Tox21_303012
M4ID: 12476121 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	517.55	NA	NA
PROB:	1	NA	NA
RMSE:	89.69	NA	NA

MAX_MEAN: 88.1 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

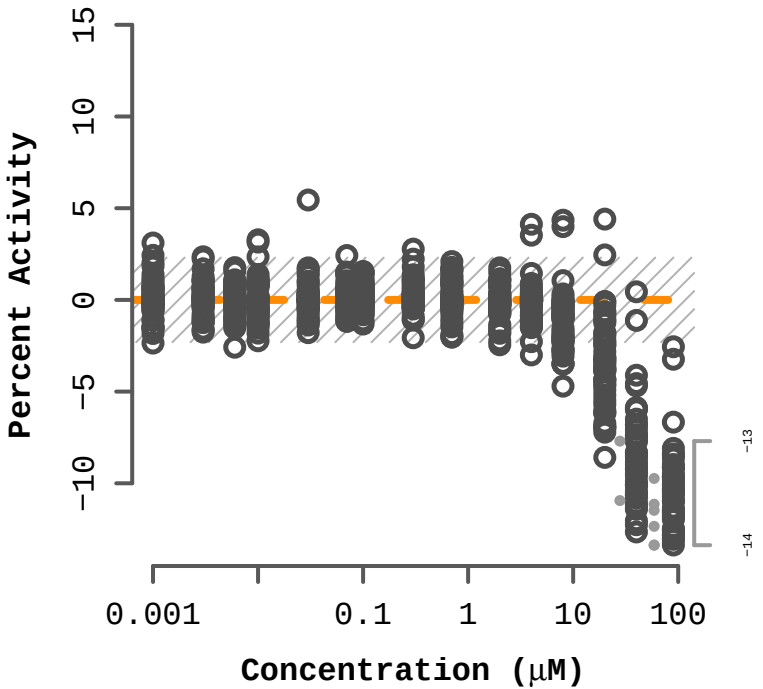
NAME: 2-Tolualdehyde
CHID: 22051 **CASRN:** 529-20-4
SPID(S): Tox21_201764
M4ID: 12480488

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.867 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

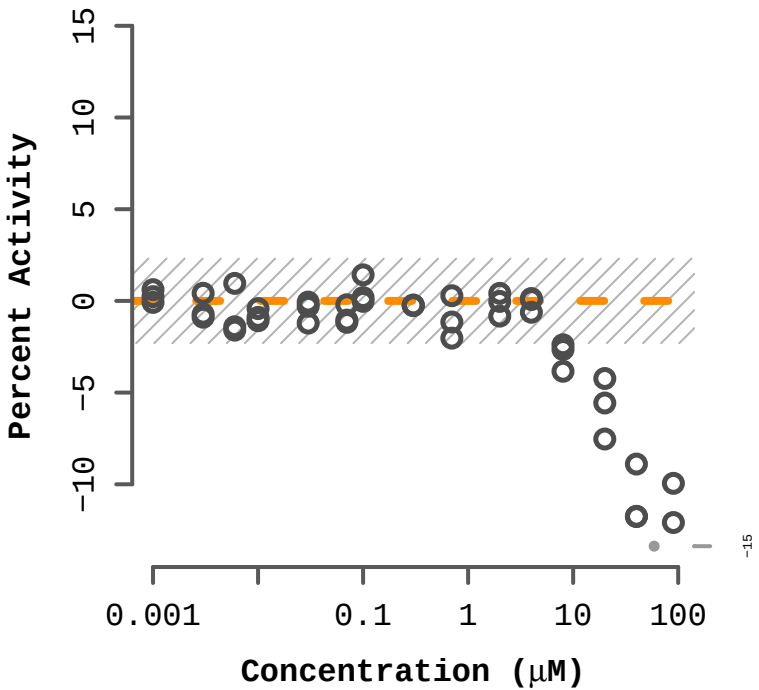
NAME: 2-Methyl-4,6-dinitrophenol
CHID: 22053 **CASRN:** 534-52-1
SPID(S): Tox21_400068
M4ID: 12475069 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3625.16	NA	NA
PROB:	1	NA	NA
RMSE:	3.94	NA	NA

MAX_MEAN: 0.189 **MAX_MED:** 0.182 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

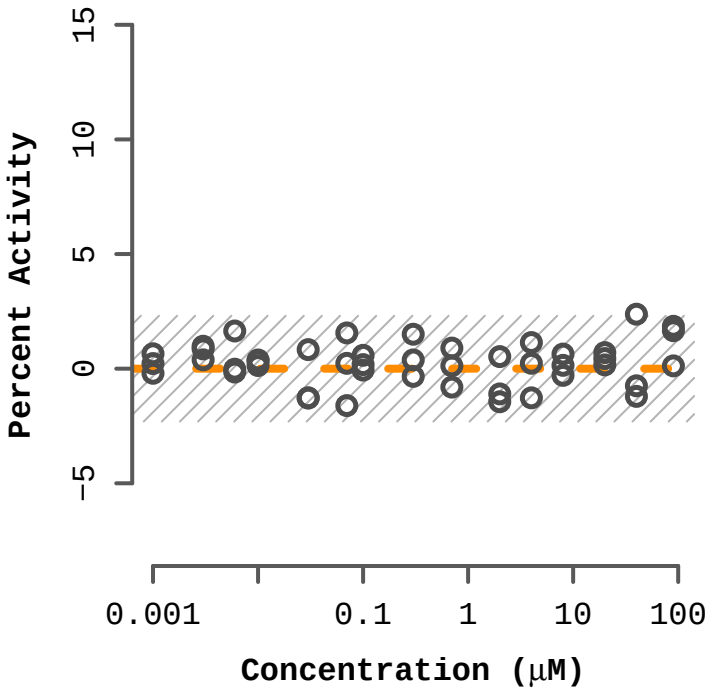
NAME: 2-Methyl-4,6-dinitrophenol
CHID: 22053 **CASRN:** 534-52-1
SPID(S): Tox21_300327
M4ID: 12478805 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.86	NA	NA
PROB:	1	NA	NA
RMSE:	4.66	NA	NA

MAX_MEAN: 0.527 **MAX_MED:** 0.234 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

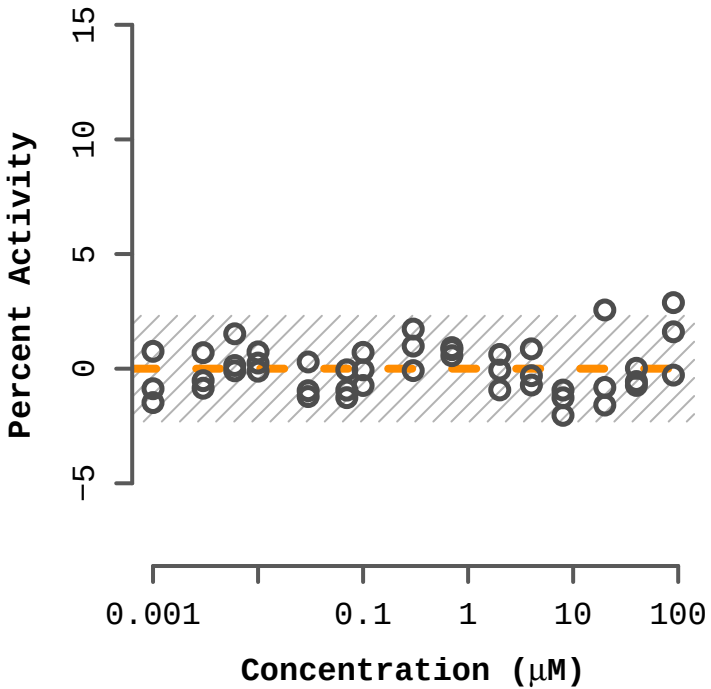
NAME: tert-Butyl acetate
CHID: 22055 **CASRN:** 540-88-5
SPID(S): Tox21_301308
M4ID: 12477825

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

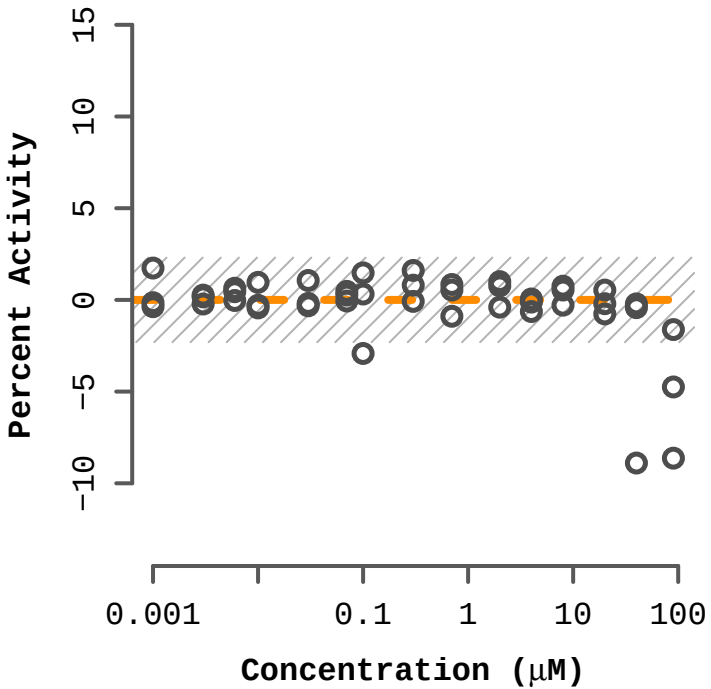
NAME: 1,3-Dichlorobenzene
CHID: 22056 **CASRN:** 541-73-1
SPID(S): Tox21_300005
M4ID: 12479125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

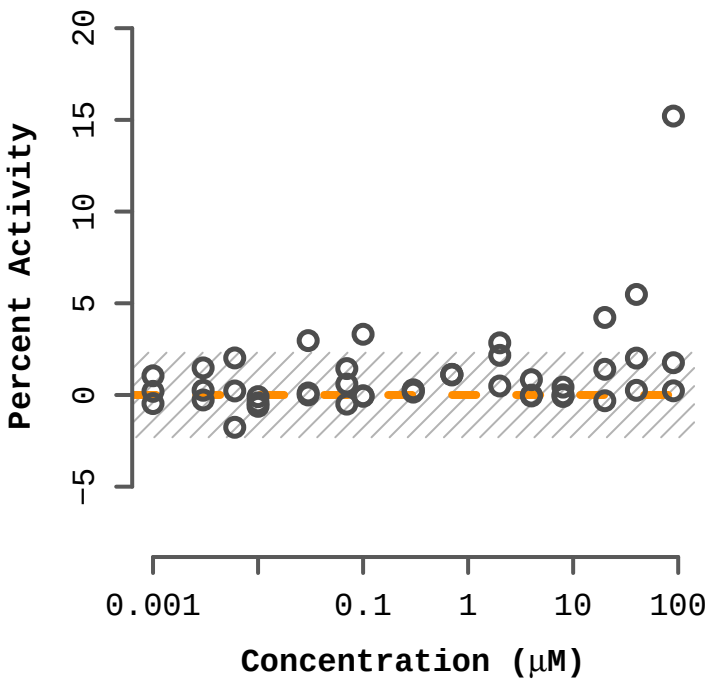
NAME: 1,3-Dichlorobenzene
CHID: 22056 **CASRN:** 541-73-1
SPID(S): Tox21_202179
M4ID: 12480073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 0.778 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

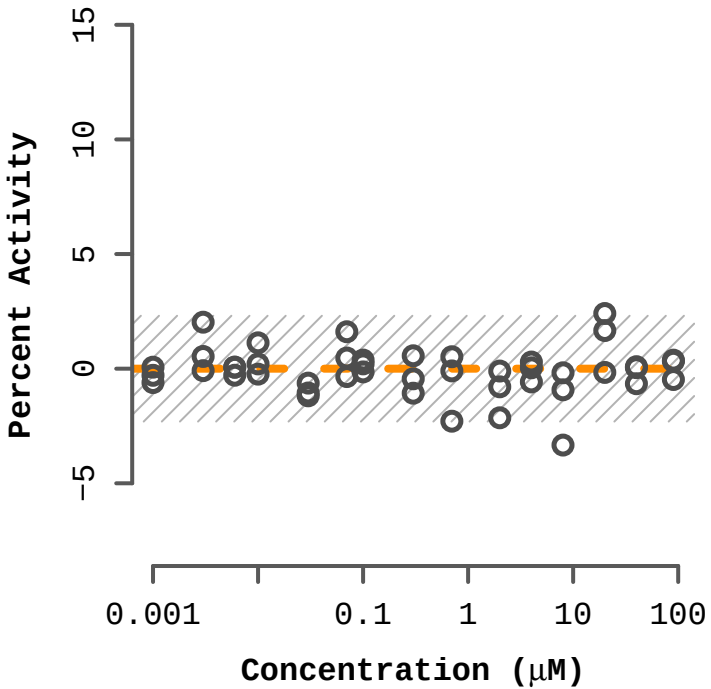
NAME: 1,3-Dichloropropene
CHID: 22057 CASRN: 542-75-6
SPID(S): Tox21_200235
M4ID: 12482017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 5.73 MAX_MED: 2.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

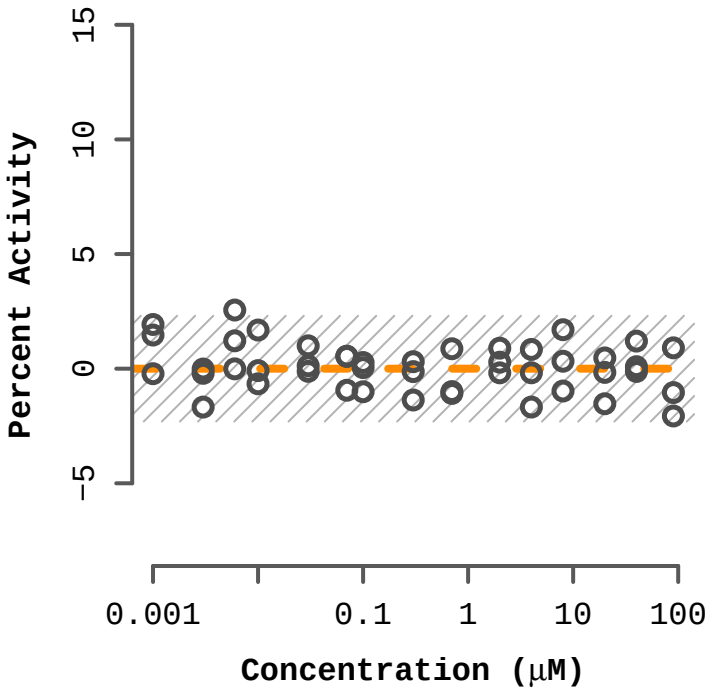
NAME: Dibutyl sulfide
CHID: 22058 **CASRN:** 544-40-1
SPID(S): Tox21_300985
M4ID: 12478148

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

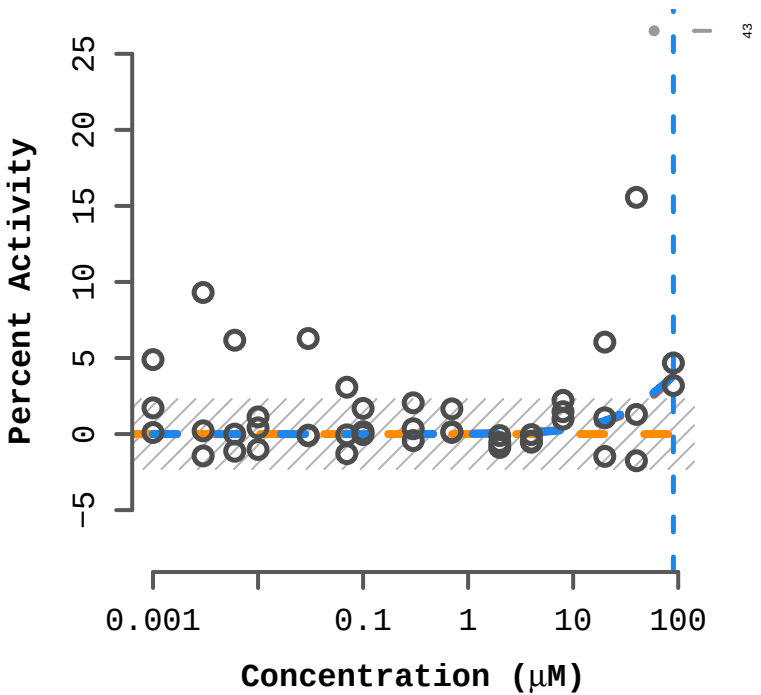
NAME: 2-Nitrobenzaldehyde
CHID: 22060 **CASRN:** 552-89-6
SPID(S): Tox21_202929
M4ID: 12479323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitrobenzaldehyde
CHID: 22061 CASRN: 555-16-8
SPID(S): Tox21_202930
M4ID: 12479322 BRK

HILL MODEL (in red):

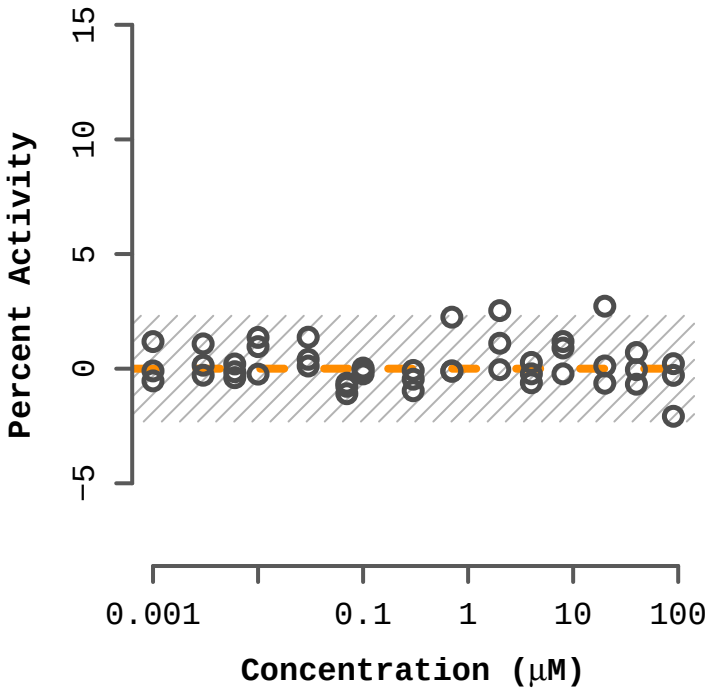
	tp	ga	gw
val:	18.7	2.45	1.16
sd:	64.8	1.82	1.21

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.64	1.95	1.36	3.11	5.81
sd:	12.5	0.93	1.68	536	2710

	CNST	HILL	GNLS
AIC:	242.78	240.13	244.36
PROB:	0.19	0.72	0.09
RMSE:	7.34	6.7	6.7

MAX_MEAN: 17.1 MAX_MED: 4.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

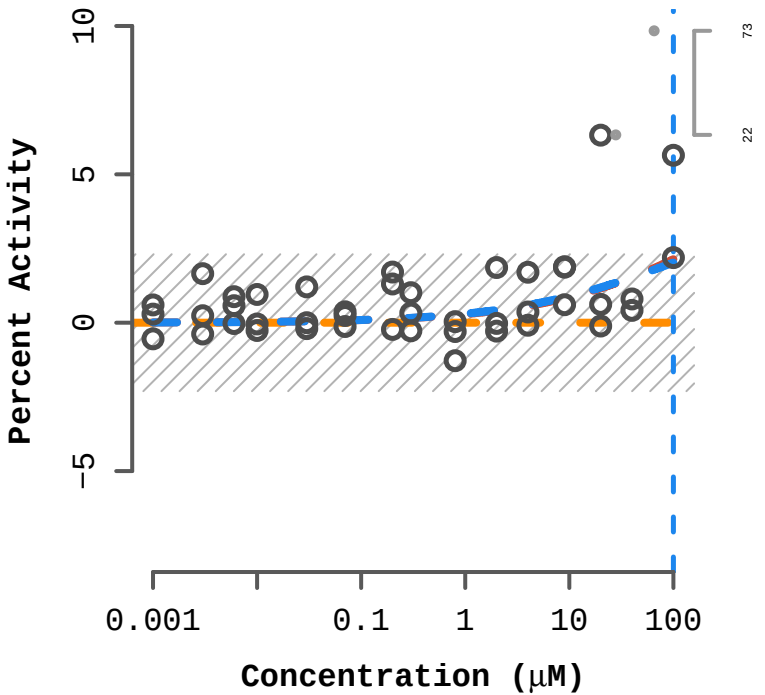
NAME: 3-Methyl-2-butanone
CHID: 22062 **CASRN:** 563-80-4
SPID(S): Tox21_302856
M4ID: 12476277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methyl-2-butanone
CHID: 22062 **CASRN:** 563-80-4
SPID(S): Tox21_201720
M4ID: 12480532 **BRK**

HILL MODEL (in red):

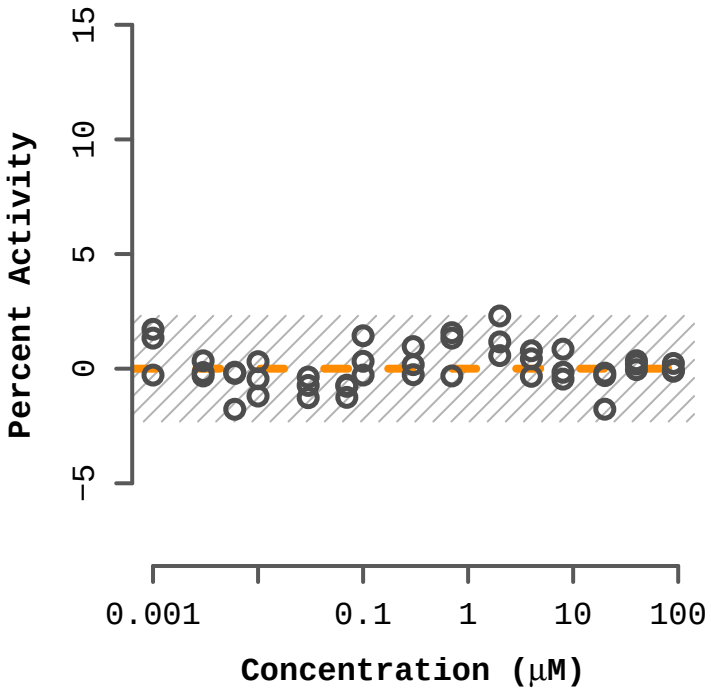
	tp	ga	gw
val:	6.03	2.5	0.52
sd:	12.4	2.4	0.354

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.05	2	0.546	4	5.23
sd:	6.71	2.05	0.383	28100	73700

	CNST	HILL	GNLS
AIC:	207.13	199.16	203.41
PROB:	0.02	0.88	0.1
RMSE:	11.45	11.04	11.05

MAX_MEAN: 26.9 **MAX_MED:** 5.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

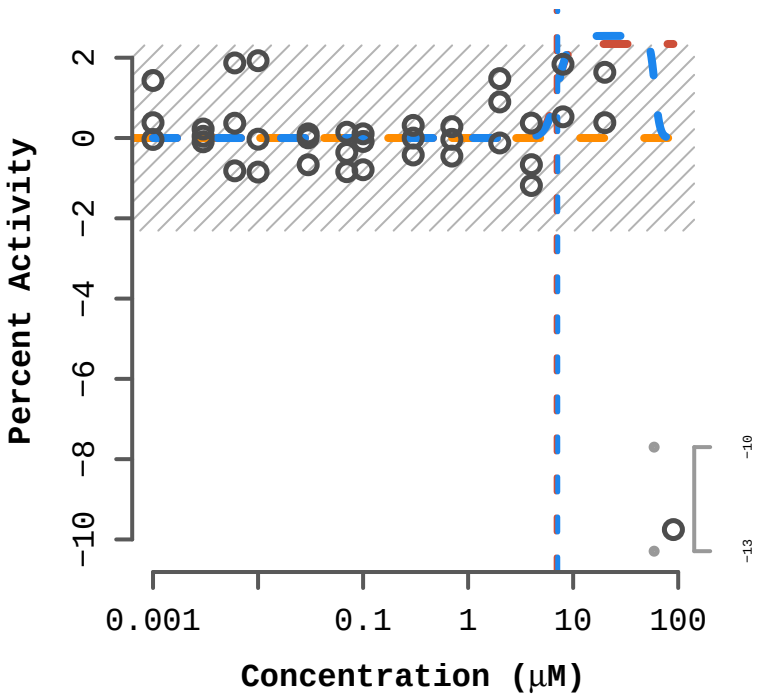
NAME: 2-Tridecanone
CHID: 22070 **CASRN:** 593-08-8
SPID(S): Tox21_301838
M4ID: 12477295

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentabromophenol
CHID: 22079 CASRN: 608-71-9
SPID(S): Tox21_200339
M4ID: 12481913 BRK

HILL MODEL (in red):

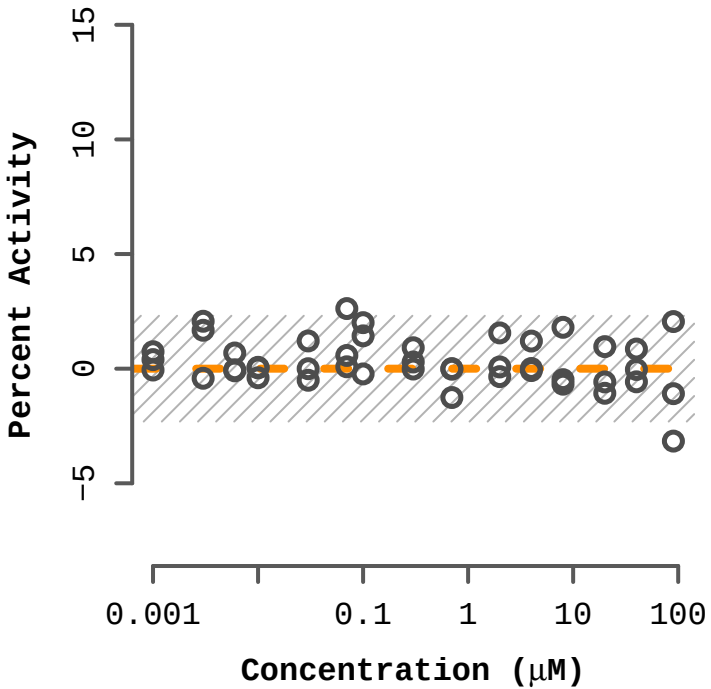
	tp	ga	gw
val:	2.34	0.838	8
sd:	0.439	0.0918	6.77

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.54	0.853	8	1.78	18
sd:	0.414	0.0781	7.25	0.362	37

	CNST	HILL	GNLS
AIC:	195.62	182.32	180.33
PROB:	0	0.27	0.73
RMSE:	3.11	3.53	2.95

MAX_MEAN: 2.79 MAX_MED: 2.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

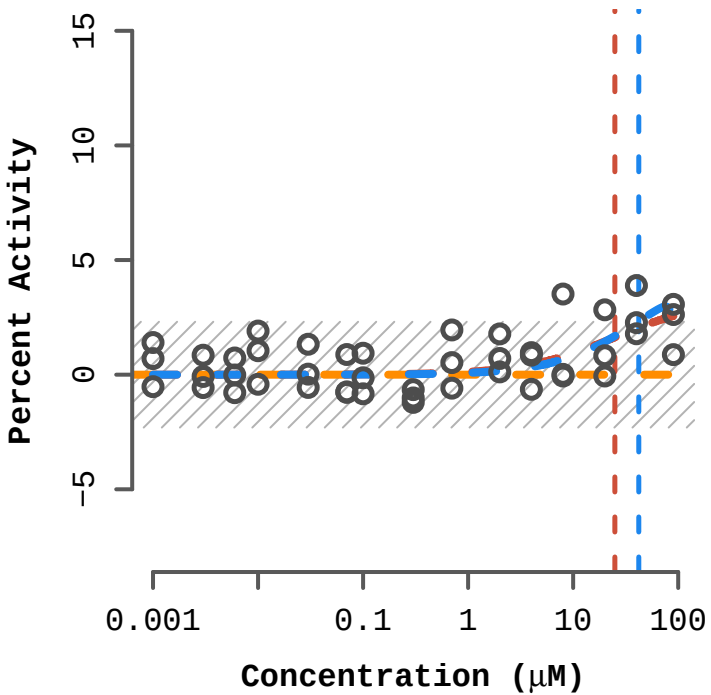
NAME: 2,4,6-Triiodophenol
CHID: 22080 **CASRN:** 609-23-4
SPID(S): Tox21_303909
M4ID: 12475279

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Acetamidophenol
CHID: 22082 **CASRN:** 614-80-2
SPID(S): Tox21_302185
M4ID: 12476948

HILL MODEL (in red):

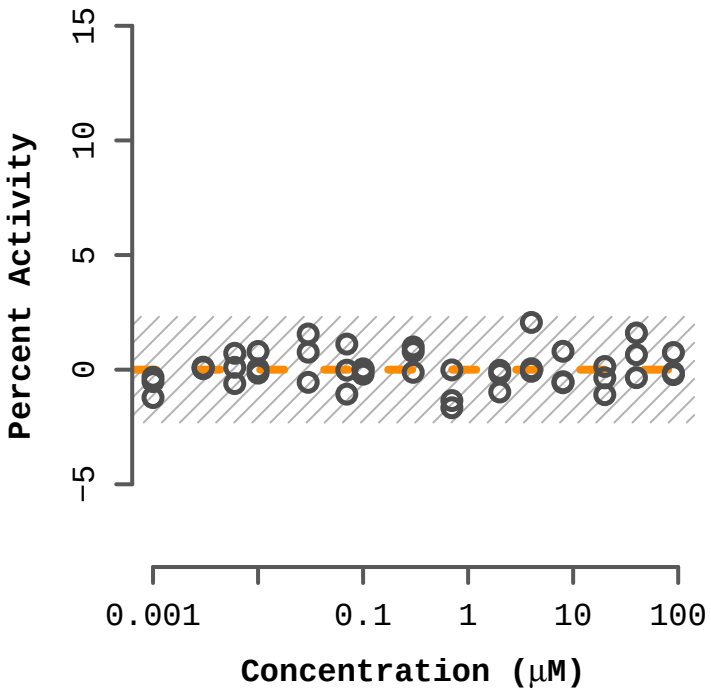
	tp	ga	gw
val:	3.26	1.4	1.01
sd:	2.01	0.668	0.768

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.67	1.62	1.08	1.98	15.3
sd:	5.03	0.781	0.78	0.0538	33

	CNST	HILL	GNLS
AIC:	159.65	141.09	144.53
PROB:	0	0.85	0.15
RMSE:	1.42	1.02	1.02

MAX_MEAN: 2.65 **MAX_MED:** 2.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

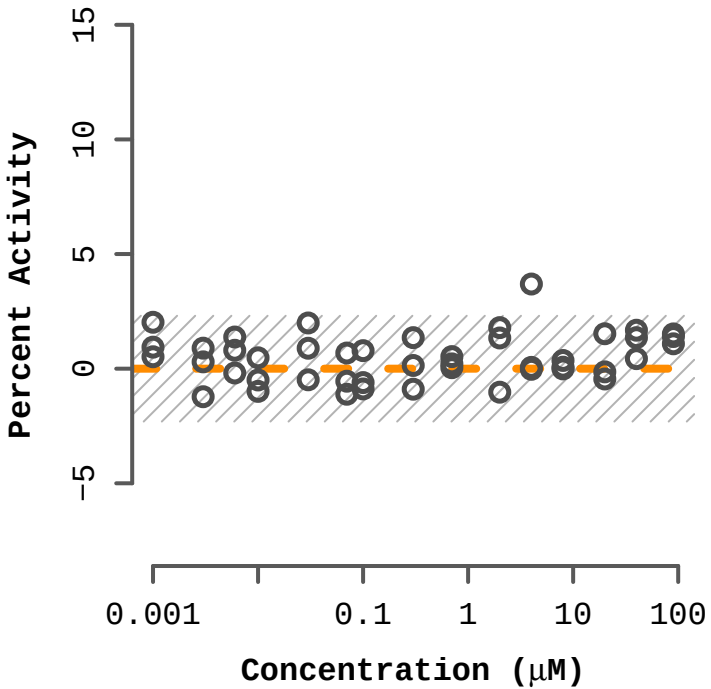
NAME: 4-Ethoxy-2-nitroaniline
CHID: 22084 **CASRN:** 616-86-4
SPID(S): Tox21_301608
M4ID: 12477525

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.679 **MAX_MED:** 0.793 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

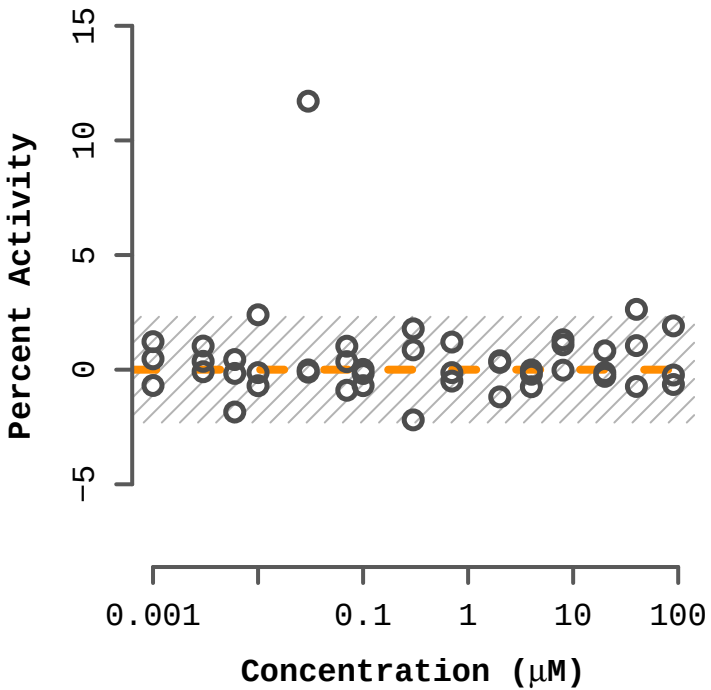
NAME: Methyl p-nitrobenzoate
CHID: 22085 **CASRN:** 619-50-1
SPID(S): Tox21_303702
M4ID: 12475486

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

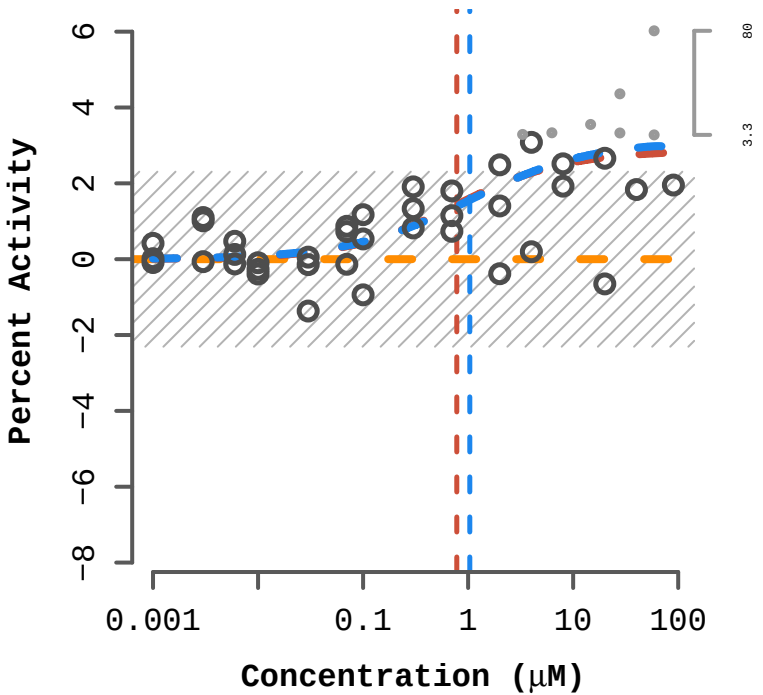
NAME: 4-Nitrobenzamide
CHID: 22086 **CASRN:** 619-80-7
SPID(S): Tox21_200343
M4ID: 12481909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.74	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 3.86 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Acetamidophenol
CHID: 22089 CASRN: 621-42-1
SPID(S): Tox21_200252
M4ID: 12482000 BRK

HILL MODEL (in red):

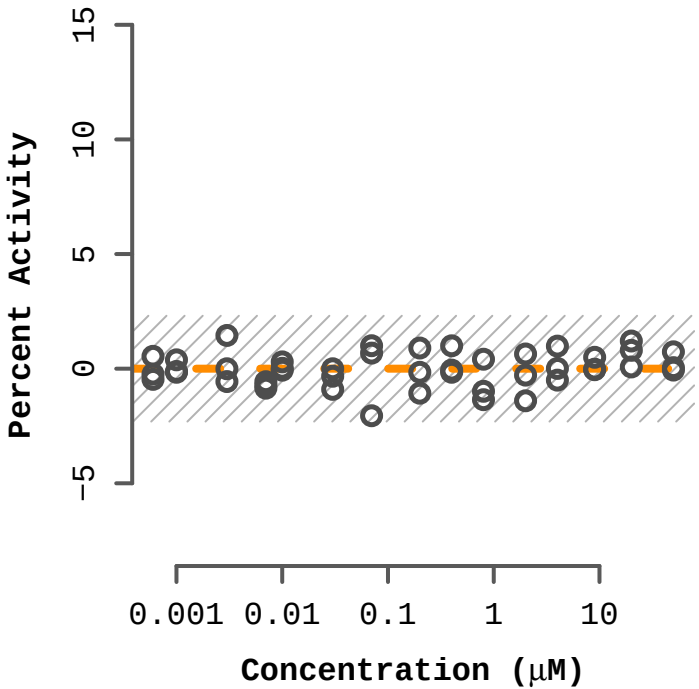
	tp	ga	gw
val:	2.87	-0.108	0.828
sd:	0.638	0.418	0.401

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.12	0.016	0.757	2.03	11.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	245.67	214.21	218.11
PROB:	0	0.88	0.12
RMSE:	13.22	12.57	12.58

MAX_MEAN: 28.6 MAX_MED: 4.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

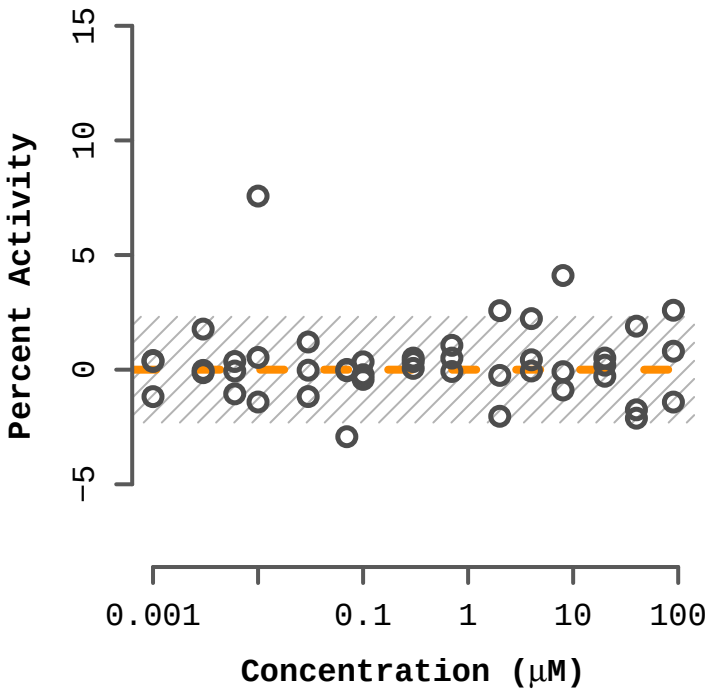
NAME: 3-Acetamidophenol
CHID: 22089 **CASRN:** 621-42-1
SPID(S): Tox21_111130_1
M4ID: 12483889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.696 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

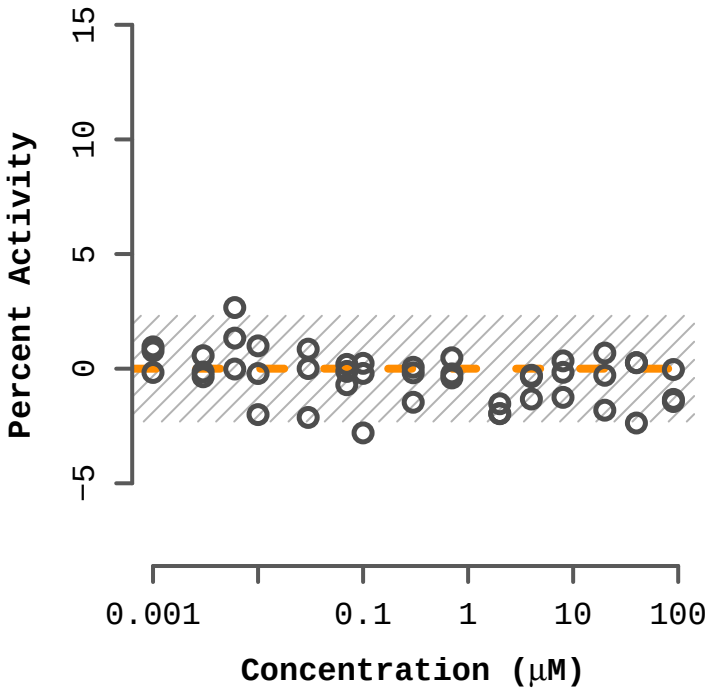
NAME: 4-(2-Hydroxyethyl)morpholine
CHID: 22090 **CASRN:** 622-40-2
SPID(S): Tox21_302022
M4ID: 12477111

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 0.806 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

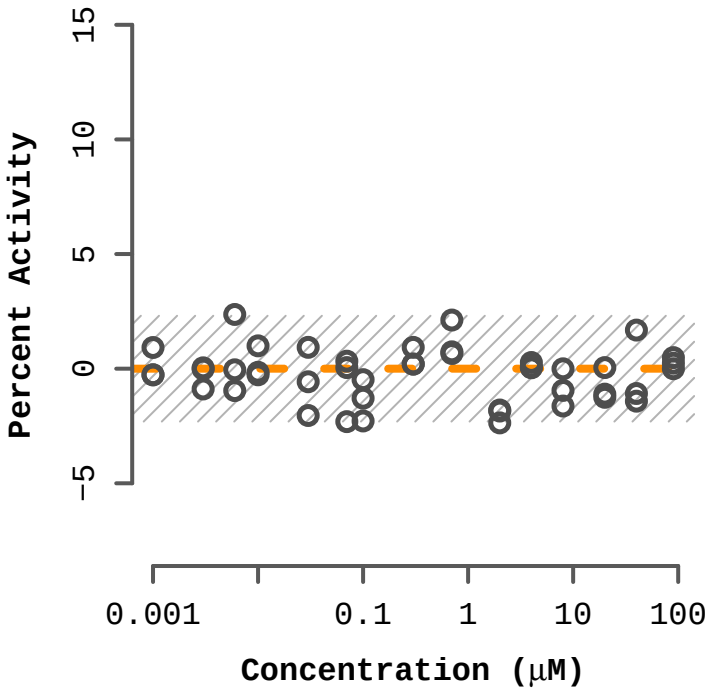
NAME: 2,5-Dimethylfuran
CHID: 22093 **CASRN:** 625-86-5
SPID(S): Tox21_202472
M4ID: 12479780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

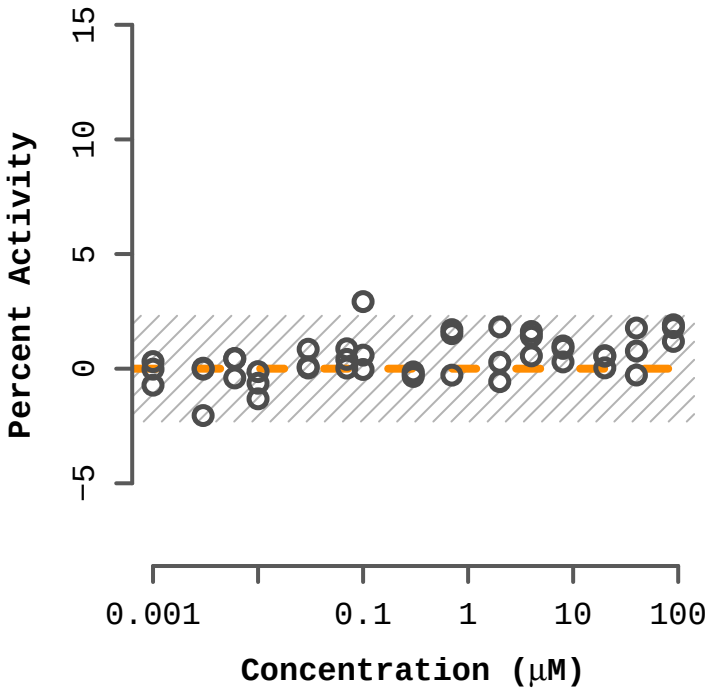
NAME: Dipropyl disulfide
CHID: 22096 **CASRN:** 629-19-6
SPID(S): Tox21_301499
M4ID: 12477634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.737 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

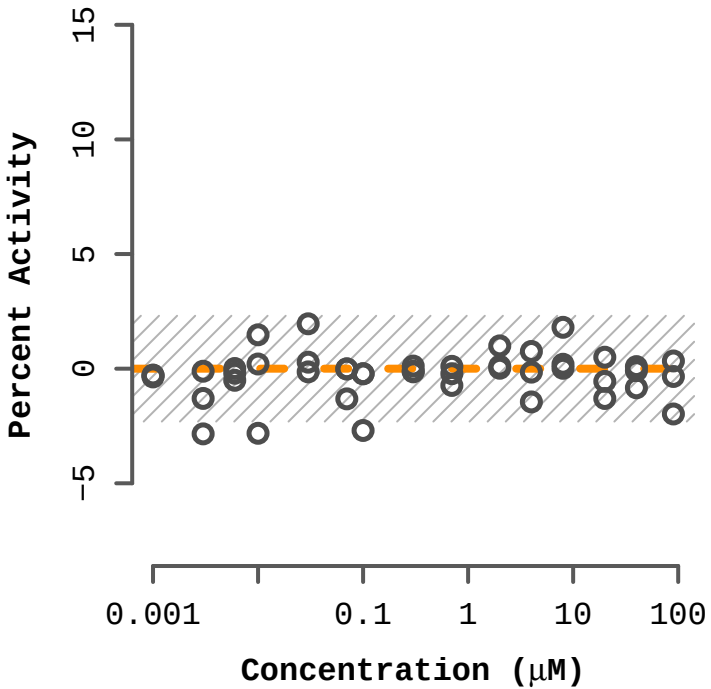
NAME: 4-Propylphenol
CHID: 22100 **CASRN:** 645-56-7
SPID(S): Tox21_302642
M4ID: 12476491

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

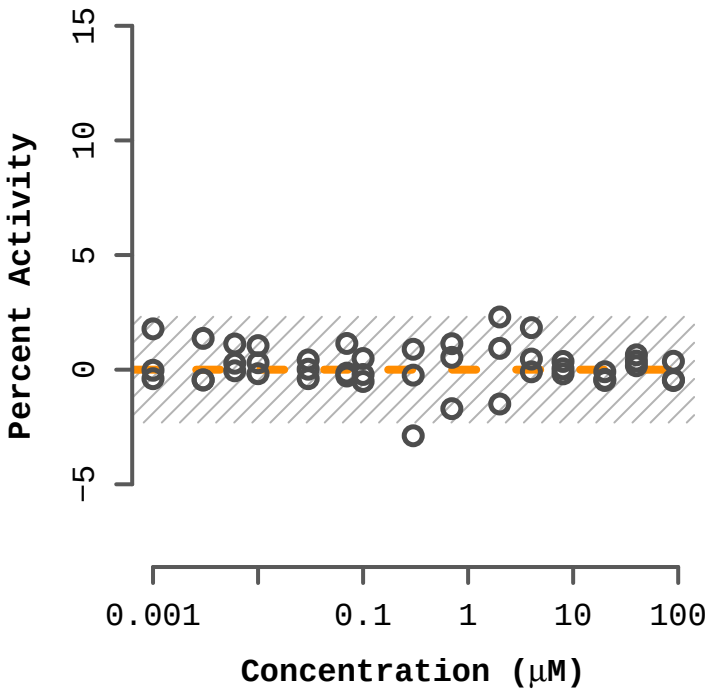
NAME: 2-Decanone
CHID: 22104 **CASRN:** 693-54-9
SPID(S): Tox21_303799
M4ID: 12475389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.702 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

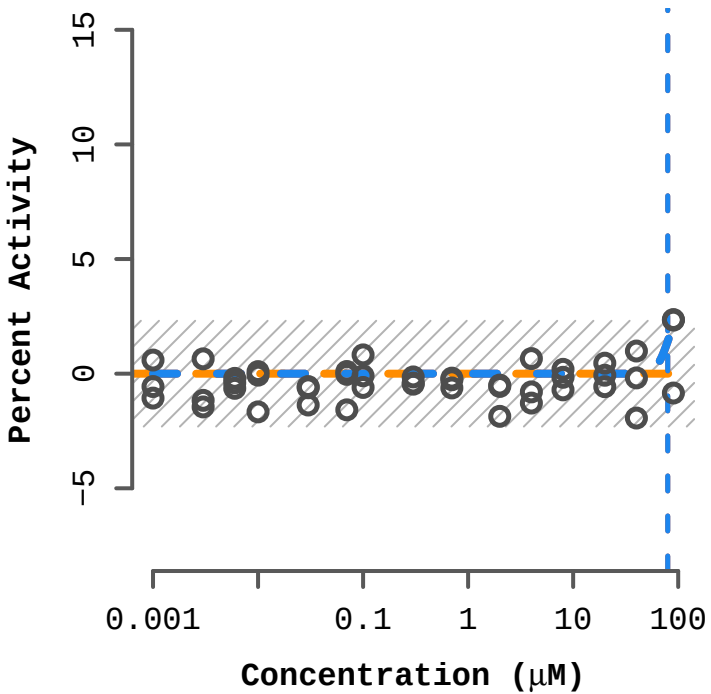
NAME: 2-Methylimidazole
CHID: 22107 **CASRN:** 693-98-1
SPID(S): Tox21_302808
M4ID: 12476325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.736 **MAX_MED:** 0.931 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylimidazole
CHID: 22107 CASRN: 693-98-1
SPID(S): Tox21_201316
M4ID: 12480936

HILL MODEL (in red):

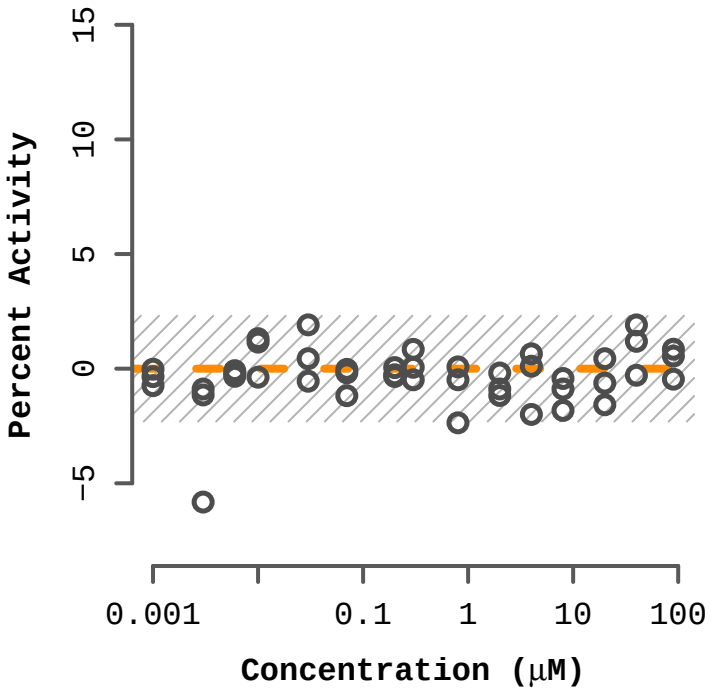
	tp	ga	gw
val:	2.83	1.9	8
sd:	7.69	0.455	20.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.83	1.9	8	2.45	11.3
sd:	8	0.474	21.1	390	8890

	CNST	HILL	GNLS
AIC:	125.22	125.32	129.32
PROB:	0.48	0.46	0.06
RMSE:	0.95	0.91	0.91

MAX_MEAN: 1.29 MAX_MED: 2.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

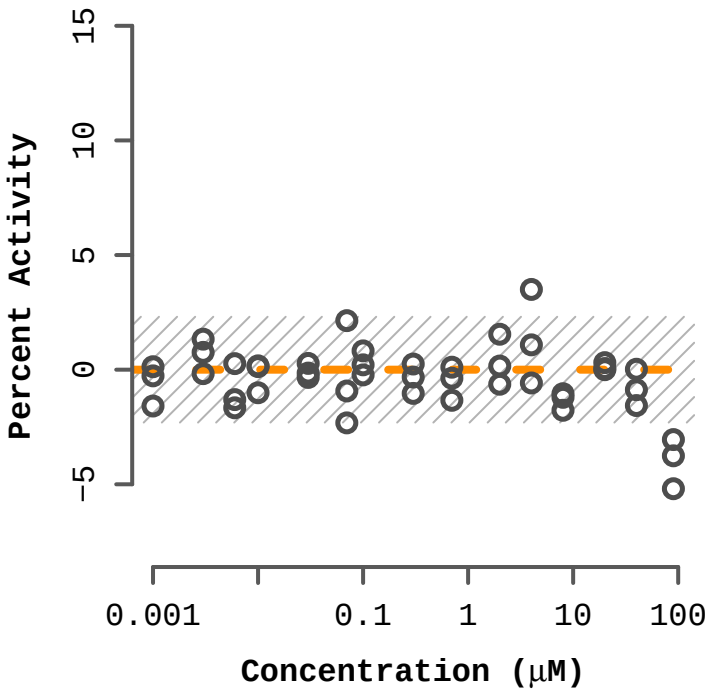
NAME: gamma-Decanolactone
CHID: 22109 **CASRN:** 706-14-9
SPID(S): Tox21_301095
M4ID: 12478038

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.94 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

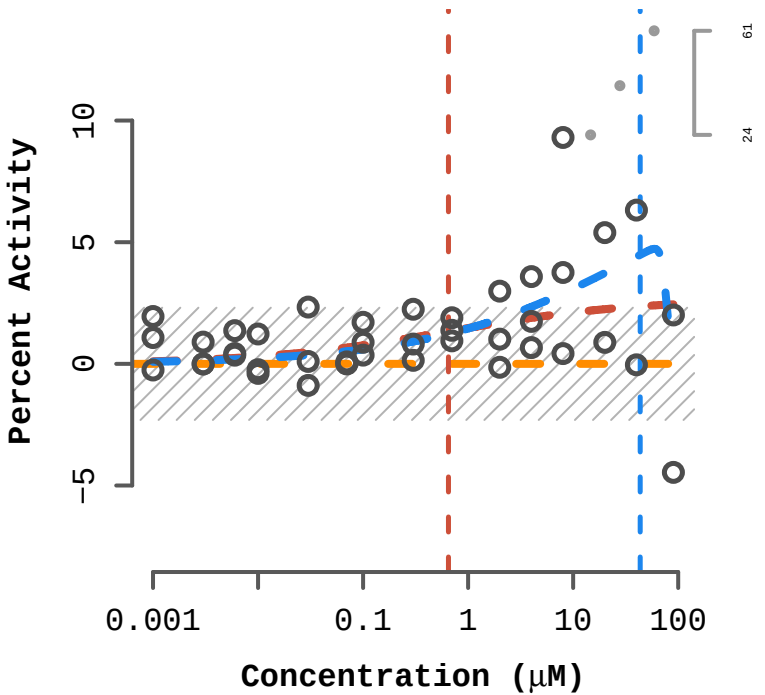
NAME: Propanil
CHID: 22111 **CASRN:** 709-98-8
SPID(S): Tox21_300848
M4ID: 12478285

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propanil
CHID: 22111 CASRN: 709-98-8
SPID(S): Tox21_201774
M4ID: 12480478 BRK

HILL MODEL (in red):

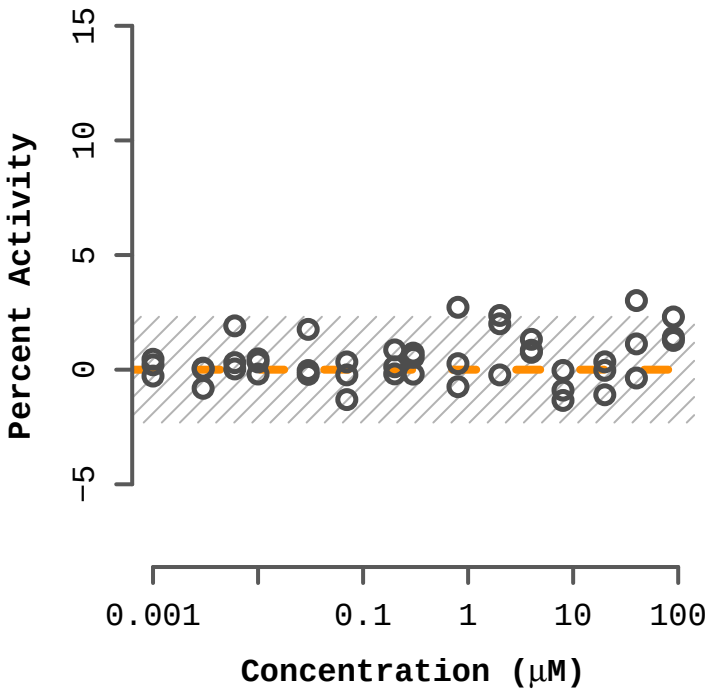
	tp	ga	gw
val:	2.66	-0.187	0.491
sd:	1.62	1.31	0.533

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.96	1.64	0.436	1.89	16.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	266.62	256.26	257.32
PROB:	0	0.63	0.37
RMSE:	11.87	11.22	11.22

MAX_MEAN: 19.6 MAX_MED: 6.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

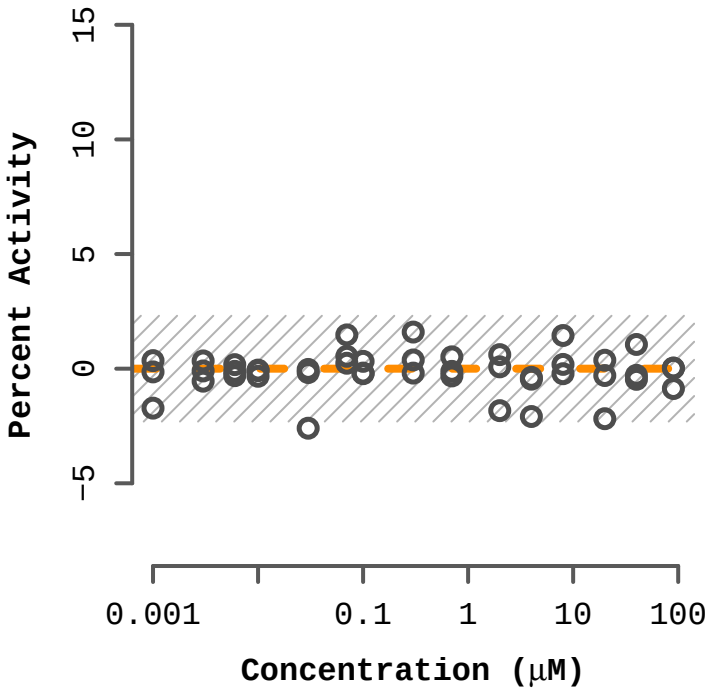
NAME: 3,4-Dichloro-1-butene
CHID: 22113 **CASRN:** 760-23-6
SPID(S): Tox21_302814
M4ID: 12476319

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

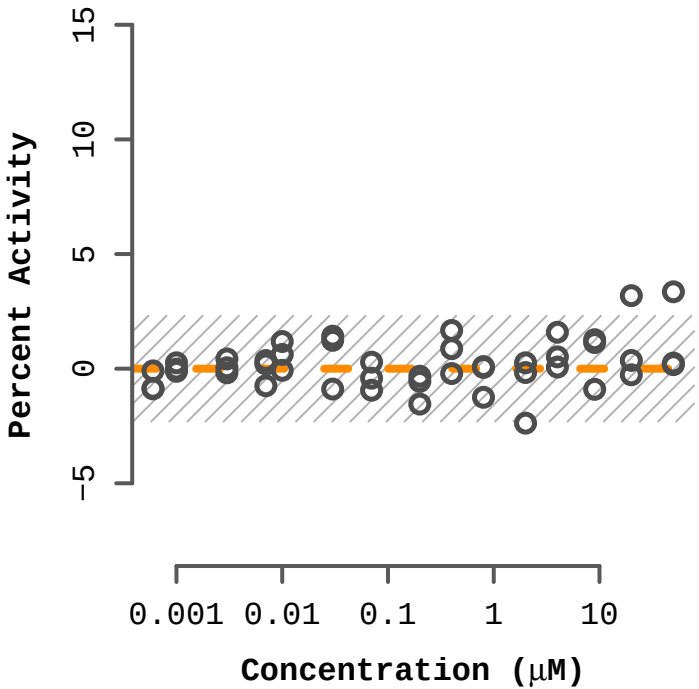
NAME: 3,4-Dichloro-1-butene
CHID: 22113 CASRN: 760-23-6
SPID(S): Tox21_201361
M4ID: 12480891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.752 MAX_MED: 0.541 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

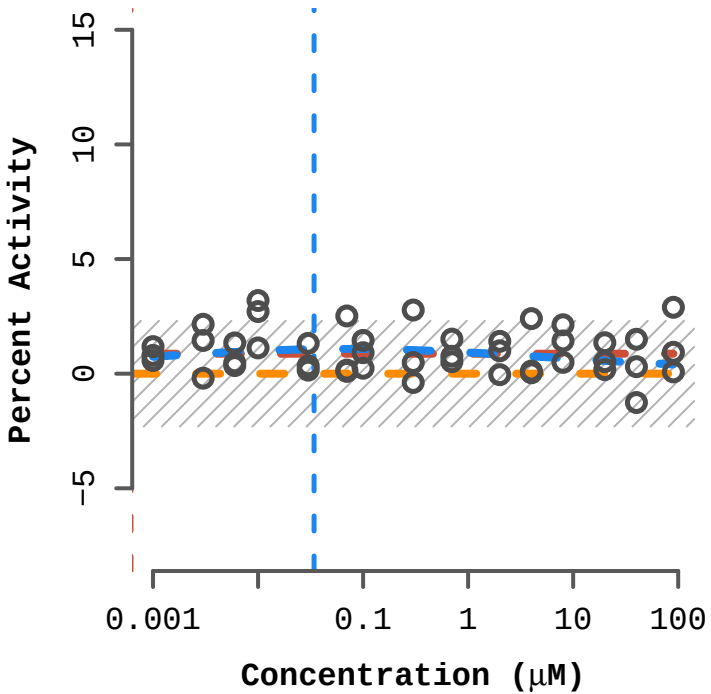
NAME: Amantadine
CHID: 22117 **CASRN:** 768-94-5
SPID(S): Tox21_110068_1
M4ID: 12484682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carbophenothion
CHID: 22120 CASRN: 786-19-6
SPID(S): Tox21_301426
M4ID: 12477707

HILL MODEL (in red):

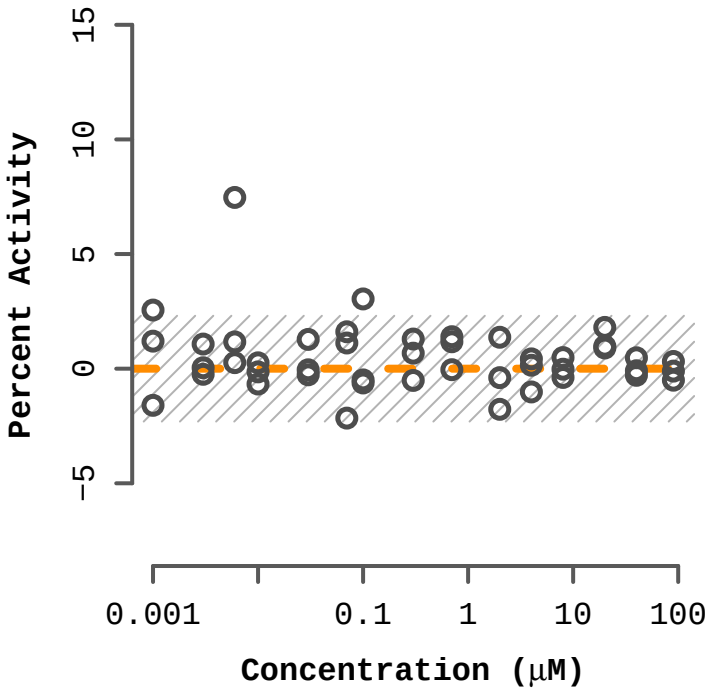
	tp	ga	gw
val:	0.869	−3.21	7.87
sd:	0.15	3.1	116

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.54	−1.47	0.3	−0.86	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	159.31	134.01	139.64
PROB:	0	0.94	0.06
RMSE:	1.36	0.96	0.98

MAX_MEAN: 2.34 **MAX_MED:** 2.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

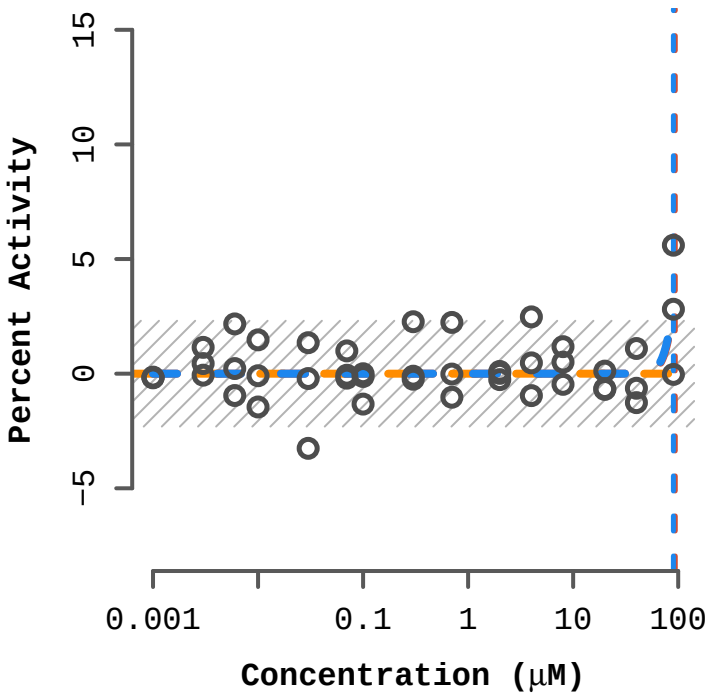
NAME: Triphenylphosphine oxide
CHID: 22121 **CASRN:** 791-28-6
SPID(S): Tox21_302054
M4ID: 12477079

HILL MODEL: Not applicable.

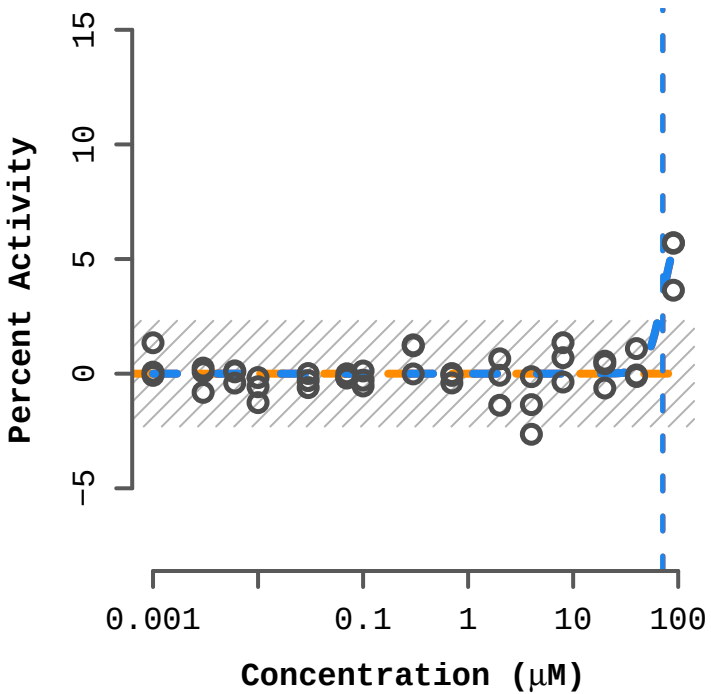
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 2.97 **MAX_MED:** 1.2 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Hydroxyethyl acrylate
CHID:    22123   CASRN: 818-61-1
SPID(S): Tox21_302968
M4ID:    12476165

HILL MODEL (in red):
      tp       ga       gw
val:  6.72     1.97     8
sd:   8.71     0.111    14.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.64     1.95     8        3.73     5.4
sd:   7.69     0.15     13.5     223000   678000

      CNST        HILL        GNLS
AIC:  150.89      151.29      155.29
PROB: 0.52        0.43        0.06
RMSE: 1.42        1.22        1.22

MAX_MEAN: 2.8       MAX_MED: 2.81      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxyethyl acrylate
CHID: 22123 CASRN: 818-61-1
SPID(S): Tox21_201430
M4ID: 12480822

HILL MODEL (in red):

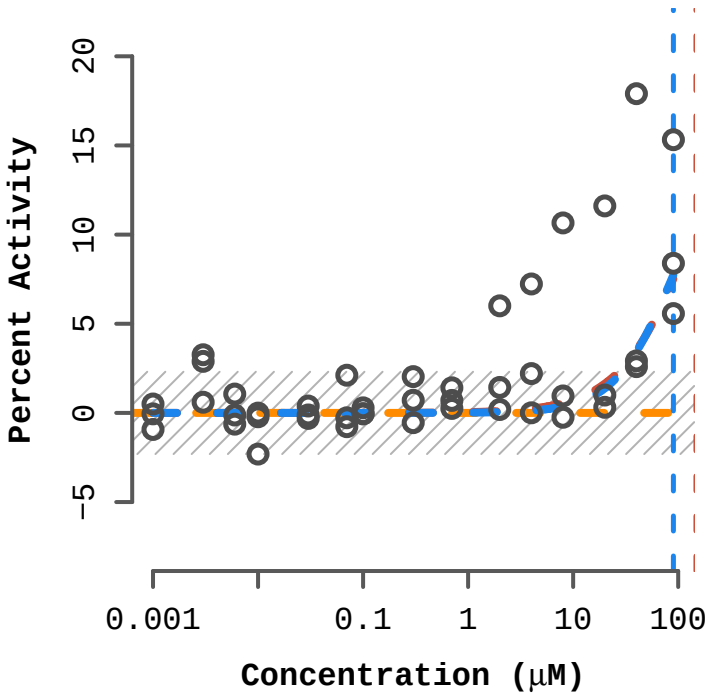
	tp	ga	gw
val:	6.86	1.86	5.93
sd:	5.43	0.208	5.16

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.86	1.85	6.01	3.95	0.905
sd:	10.1	0.251	5.86	39.2	18.6

	CNST	HILL	GNLS
AIC:	139.2	108.79	112.79
PROB:	0	0.88	0.12
RMSE:	1.51	0.78	0.78

MAX_MEAN: 5.02 MAX_MED: 5.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Octyn-3-ol
CHID: 22124 CASRN: 818-72-4
SPID(S): Tox21_202873
M4ID: 12479379

HILL MODEL (in red):

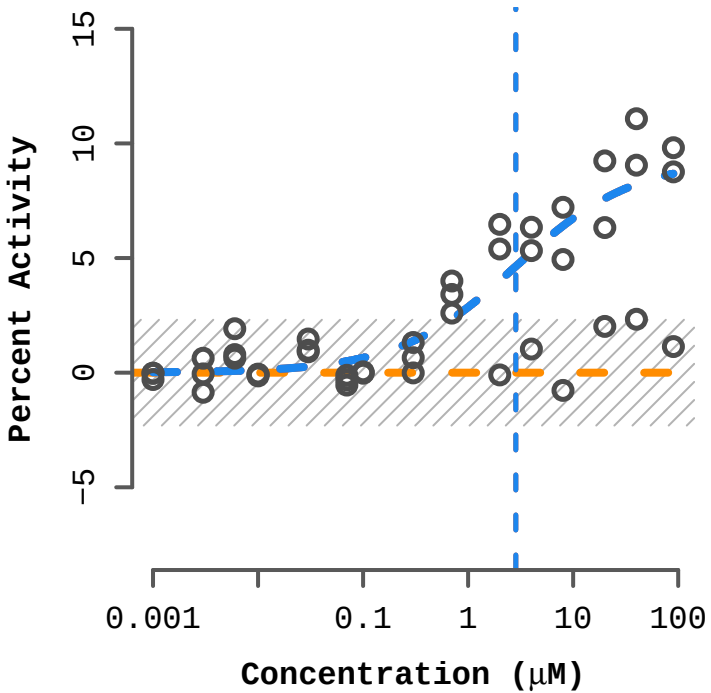
	tp	ga	gw
val:	21.5	2.17	1.25
sd:	25.1	0.783	0.94

GAIN-LOSS MODEL (in blue):

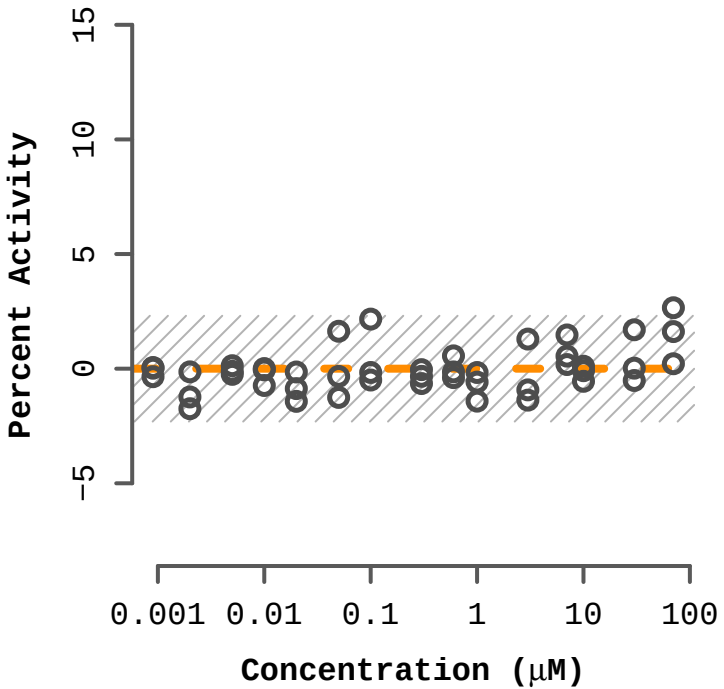
	tp	ga	gw	la	lw
val:	15.5	1.95	1.55	3.67	6.36
sd:	19.7	0.714	1.3	63700	237000

	CNST	HILL	GNLS
AIC:	247.26	225.41	229.7
PROB:	0	0.9	0.1
RMSE:	4.85	3.67	3.71

MAX_MEAN: 9.76 MAX_MED: 8.39 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Nonanone
CHID:    22125   CASRN: 821-55-6
SPID(S): Tox21_303845
M4ID:    12475343

HILL MODEL (in red):
      tp       ga       gw
val:  9.28     0.454    0.774
sd:   1.67     0.345    0.235

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.28     0.454    0.774    3.38     5.15
sd:   1.67     0.345    0.236    1130     3980

      CNST        HILL        GNLS
AIC:  252.28      199.1       203.1
PROB: 0           0.88        0.12
RMSE: 4.16        2.37        2.37

MAX_MEAN: 7.49      MAX_MED: 9.05      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

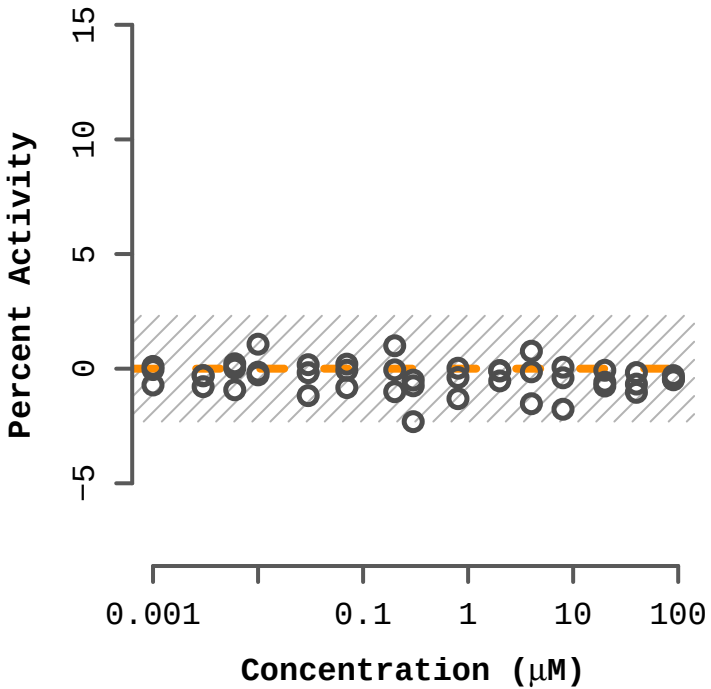
NAME: 4-Phenoxyphenol
CHID: 22127 **CASRN:** 831-82-3
SPID(S): Tox21_302190
M4ID: 12476943

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

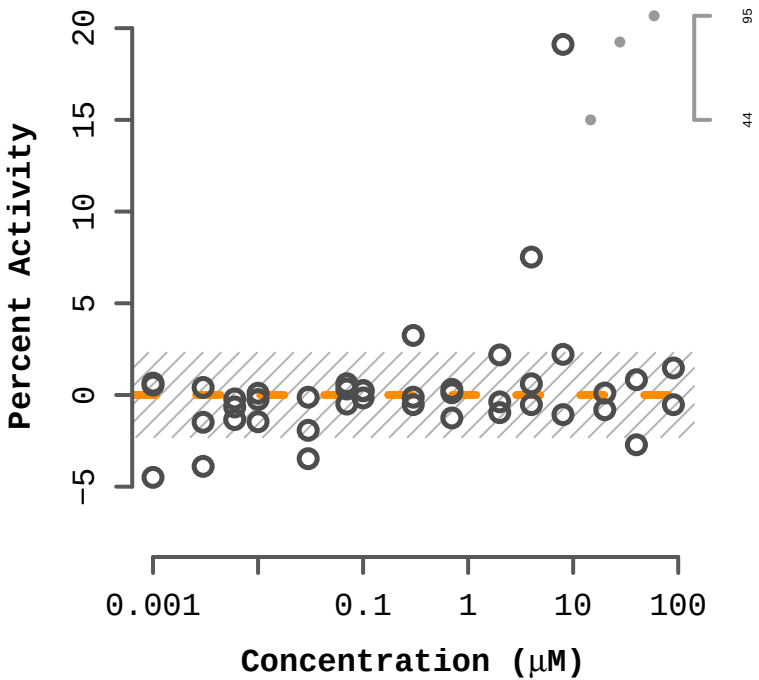
NAME: 2-Hydroxyethyl methacrylate
CHID: 22128 CASRN: 868-77-9
SPID(S): Tox21_200415
M4ID: 12481837

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.217 MAX_MED: 0.0224 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

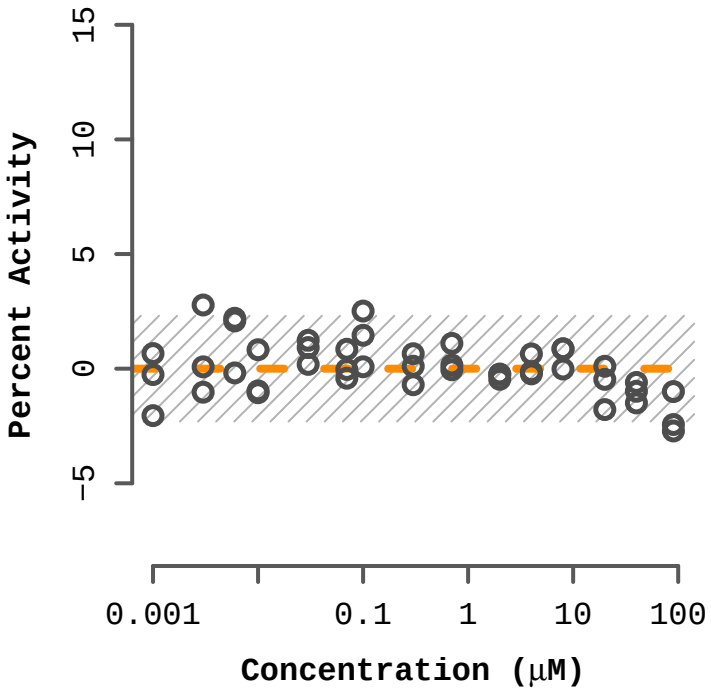
NAME: 2,4-Dichlorobenzaldehyde
CHID: 22130 **CASRN:** 874-42-0
SPID(S): Tox21_201217
M4ID: 12481035 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	285.33	NA	NA
PROB:	1	NA	NA
RMSE:	20.13	NA	NA

MAX_MEAN: 32 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

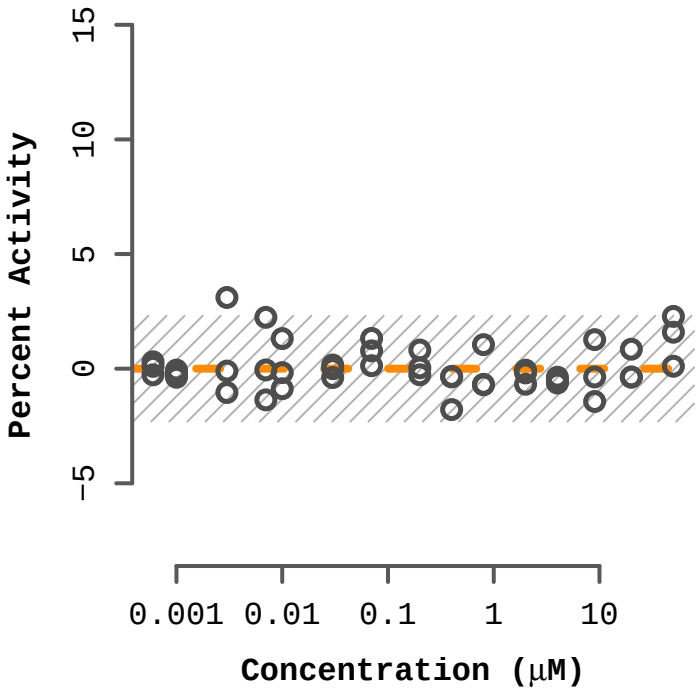
NAME: Diphenyl disulfide
CHID: 22131 **CASRN:** 882-33-7
SPID(S): Tox21_200728
M4ID: 12481524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

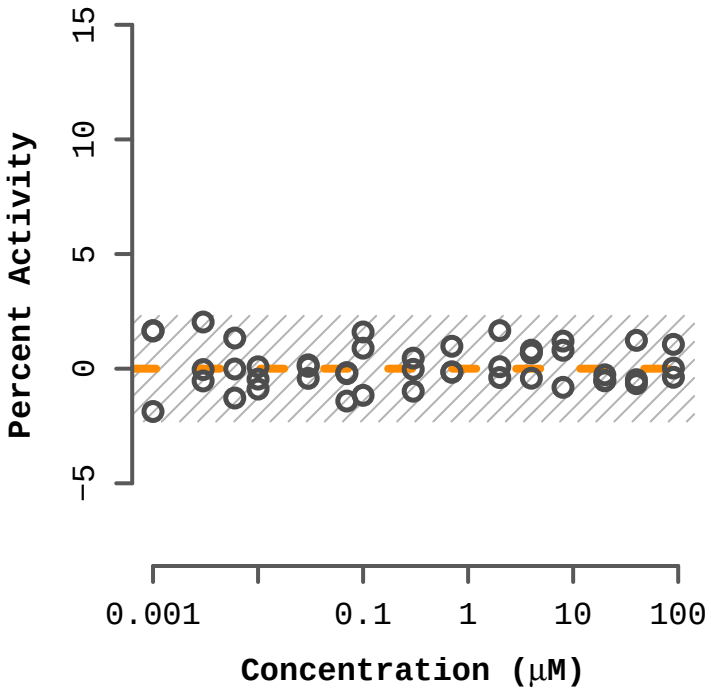
NAME: Ethyl 3-aminobenzoate methanesulfonic acid sal
CHID: 22133 CASRN: 886-86-2
SPID(S): Tox21_112290_1
M4ID: 12483180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

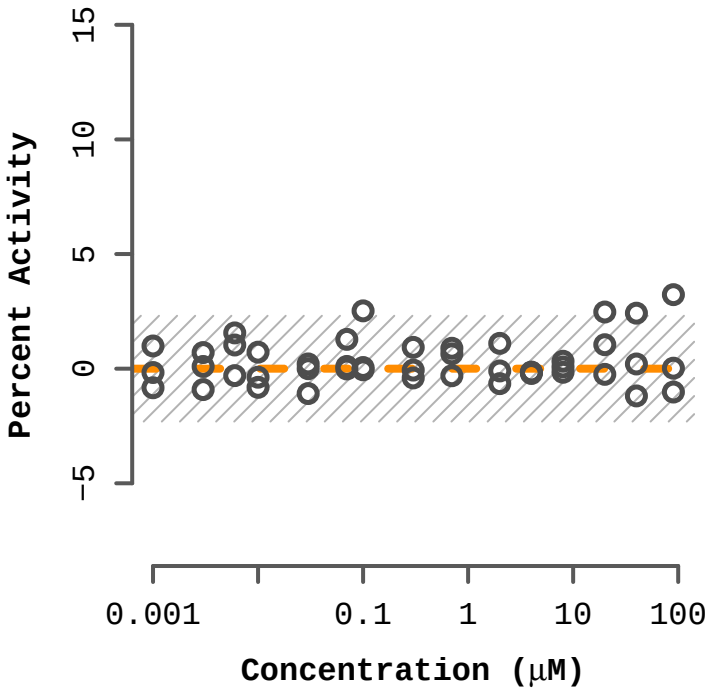
NAME: (Z)−3−Hexen−1−ol
CHID: 22137 **CASRN:** 928−96−1
SPID(S): Tox21_301011
M4ID: 12478122

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.488 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

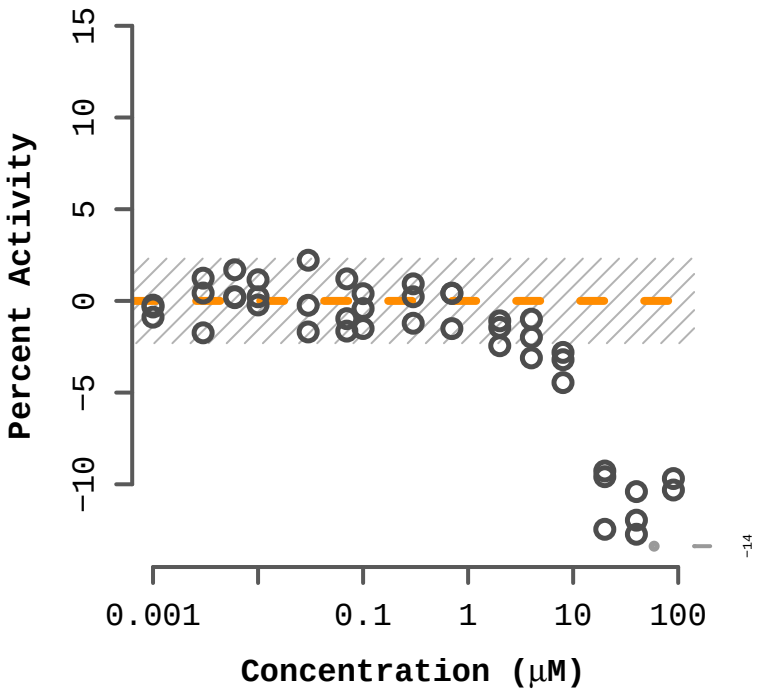
NAME: (E)−3−Hexen−1−ol
CHID: 22138 **CASRN:** 928−97−2
SPID(S): Tox21_301972
M4ID: 12477161

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

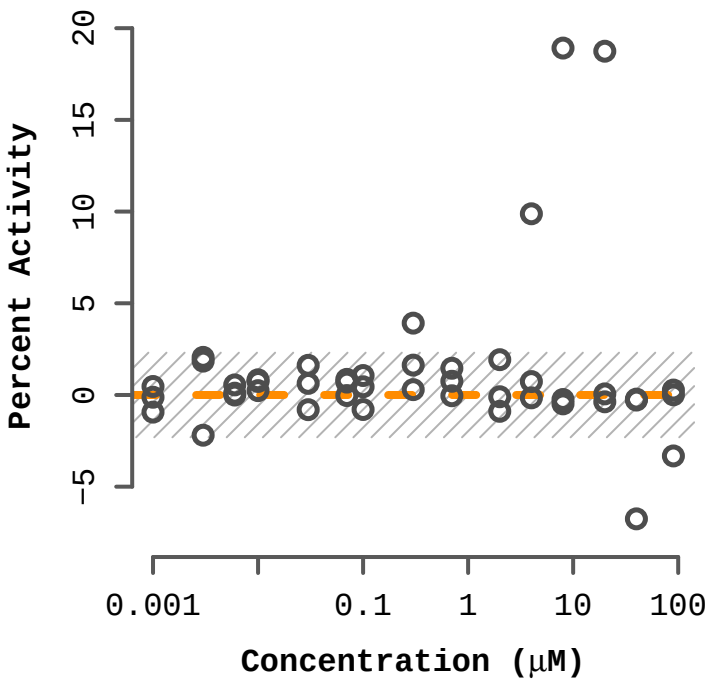
NAME: Tetrabutyltin
CHID: 22153 **CASRN:** 1461-25-2
SPID(S): Tox21_302893
M4ID: 12476240 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.33	NA	NA
PROB:	1	NA	NA
RMSE:	5.21	NA	NA

MAX_MEAN: 0.704 **MAX_MED:** 0.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

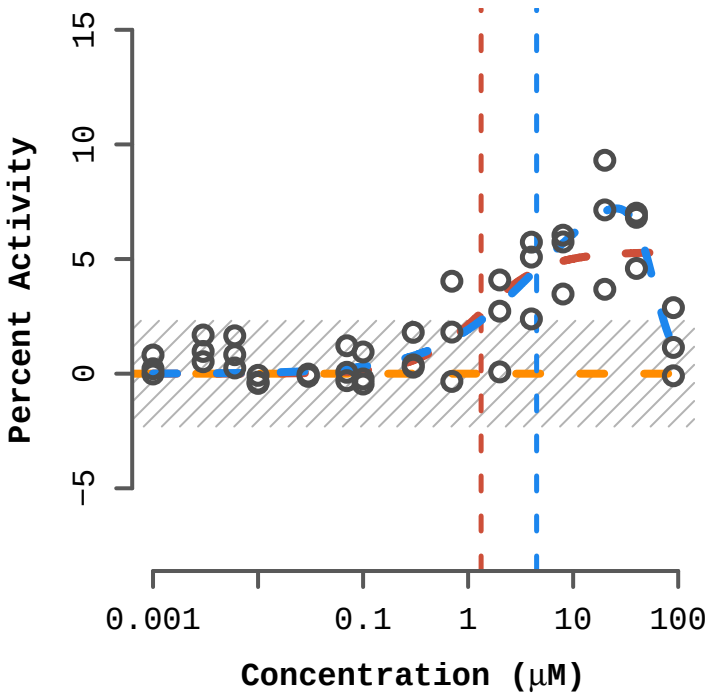
NAME: 1,9-Decadiene
CHID: 22159 CASRN: 1647-16-1
SPID(S): Tox21_200037
M4ID: 12482215

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.06	NA	NA
PROB:	1	NA	NA
RMSE:	4.5	NA	NA

MAX_MEAN: 6.15 MAX_MED: 1.85 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: p-Phenylazophenol
CHID: 22160 CASRN: 1689-82-3
SPID(S): Tox21_202968
M4ID: 12479284

HILL MODEL (in red):

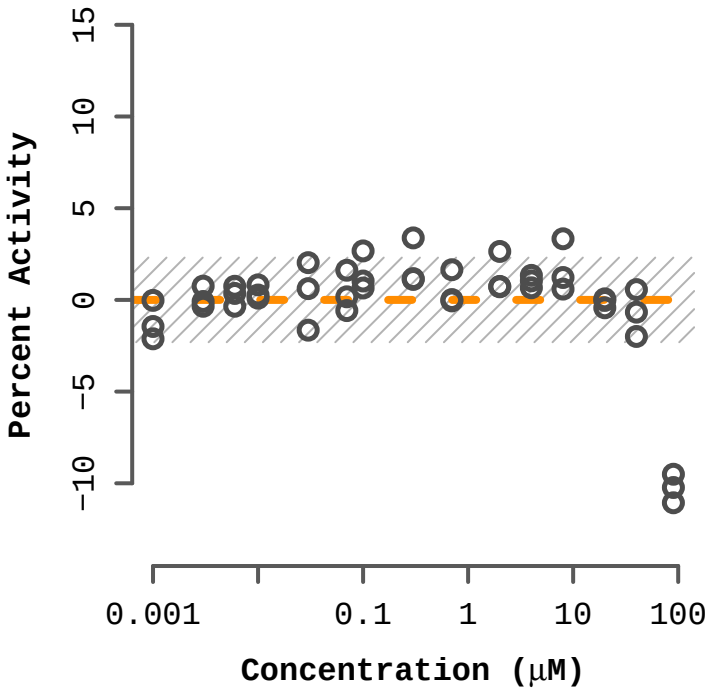
	tp	ga	gw
val:	5.31	0.123	1.41
sd:	0.749	0.198	0.513

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.12	0.652	0.878	1.76	4
sd:	4.07	0.522	0.341	0.104	1.57

	CNST	HILL	GNLS
AIC:	232.43	176.93	157.66
PROB:	0	0	1
RMSE:	3.27	1.67	1.23

MAX_MEAN: 6.71 MAX_MED: 7.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

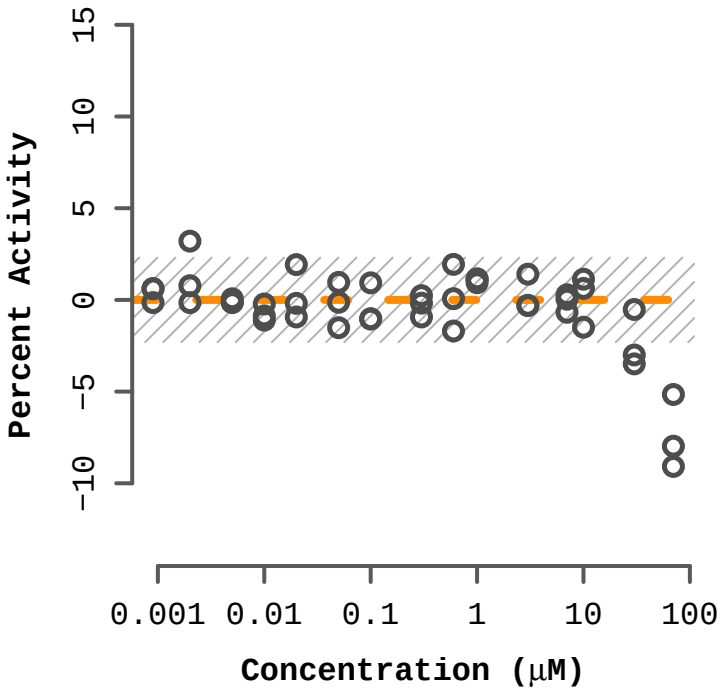
NAME: Ioxynil
CHID: 22161 **CASRN:** 1689-83-4
SPID(S): Tox21_301330
M4ID: 12477803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.4	NA	NA
PROB:	1	NA	NA
RMSE:	2.95	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

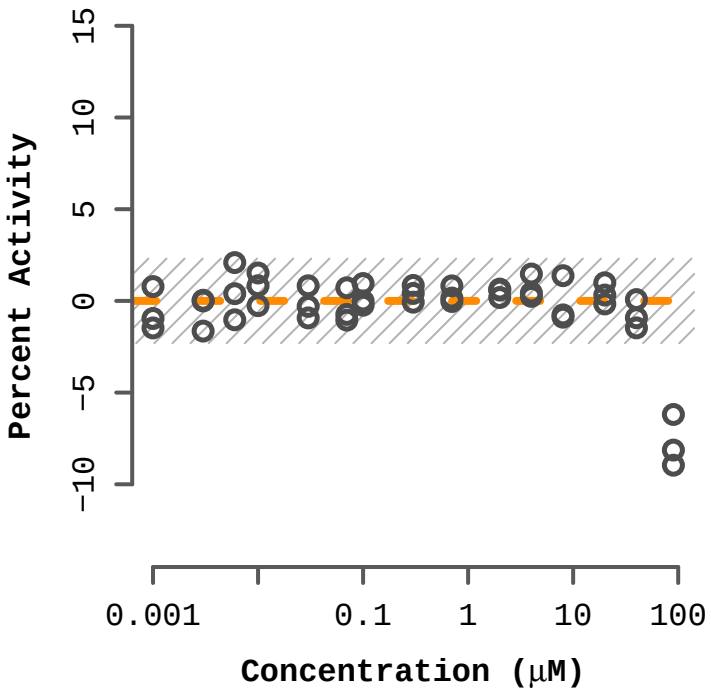
NAME: Bromoxynil
CHID: 22162 **CASRN:** 1689-84-5
SPID(S): Tox21_301202
M4ID: 12477931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.04	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

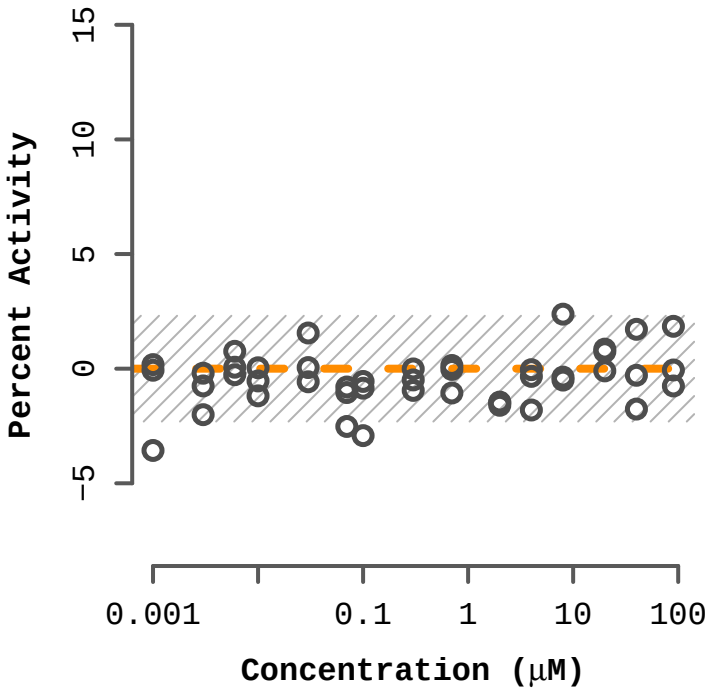
NAME: Bromoxynil
CHID: 22162 **CASRN:** 1689-84-5
SPID(S): Tox21_201421
M4ID: 12480831

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.19	NA	NA

MAX_MEAN: 0.717 **MAX_MED:** 0.828 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

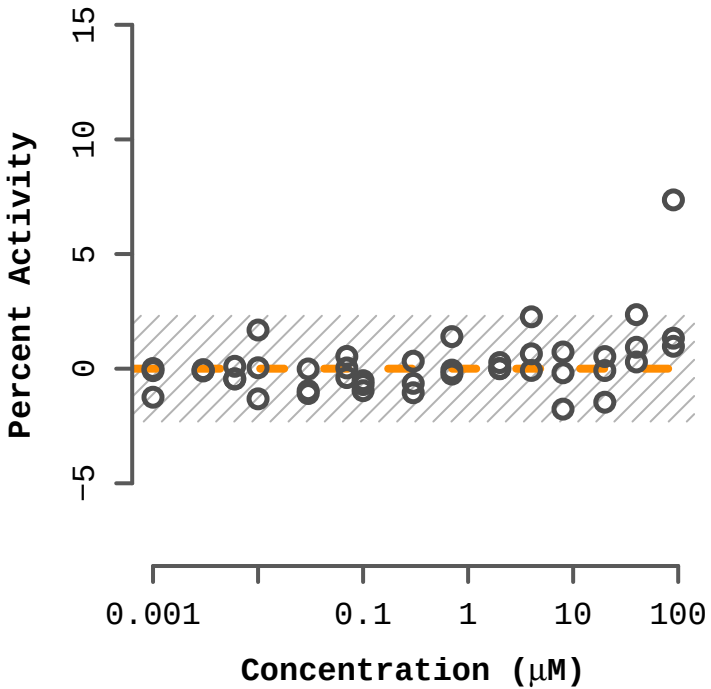
NAME: 2-Allylphenol
CHID: 22164 **CASRN:** 1745-81-9
SPID(S): Tox21_302056
M4ID: 12477077

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.505 **MAX_MED:** 0.742 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

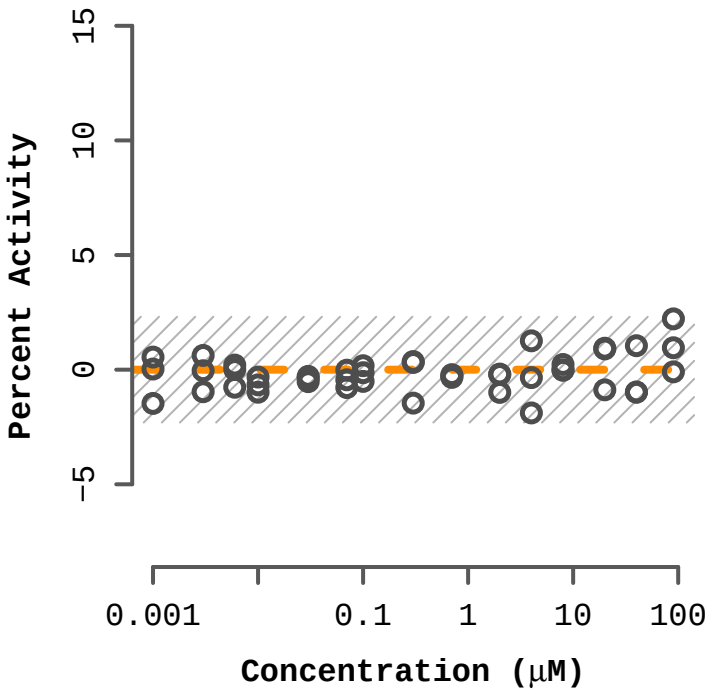
NAME: 2,6-Dichlorobenzamide
CHID: 22170 **CASRN:** 2008-58-4
SPID(S): Tox21_301922
M4ID: 12477211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 3.22 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

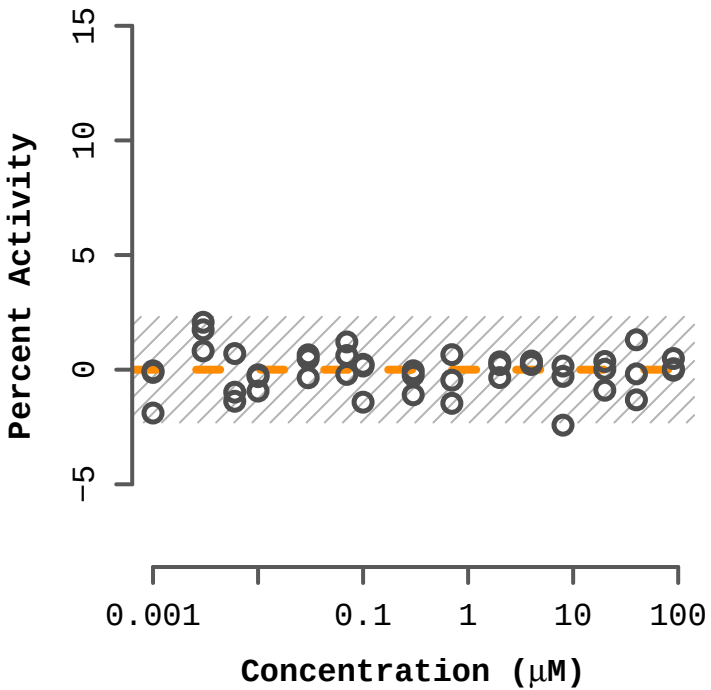
NAME: 1-Decanamine
CHID: 22171 **CASRN:** 2016-57-1
SPID(S): Tox21_302938
M4ID: 12476195

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.958 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

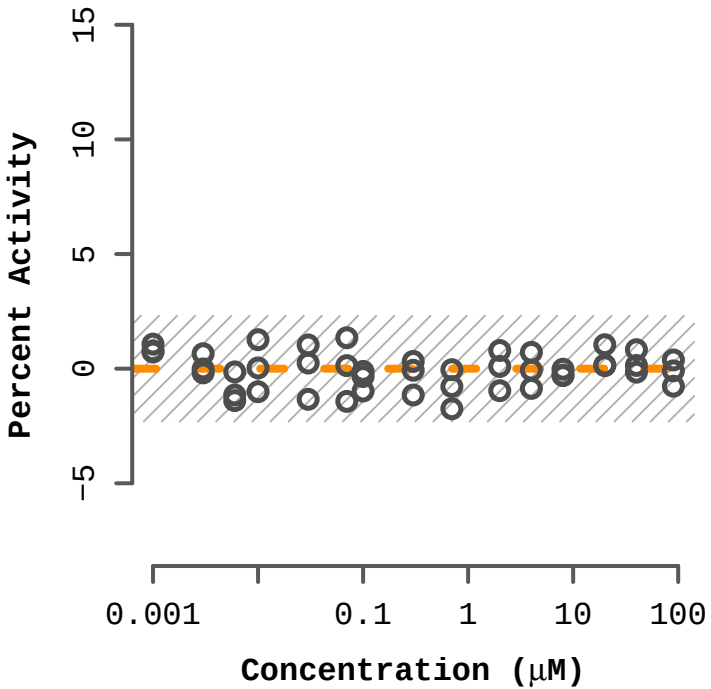
NAME: 1-Decanamine
CHID: 22171 **CASRN:** 2016-57-1
SPID(S): Tox21_201303
M4ID: 12480949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

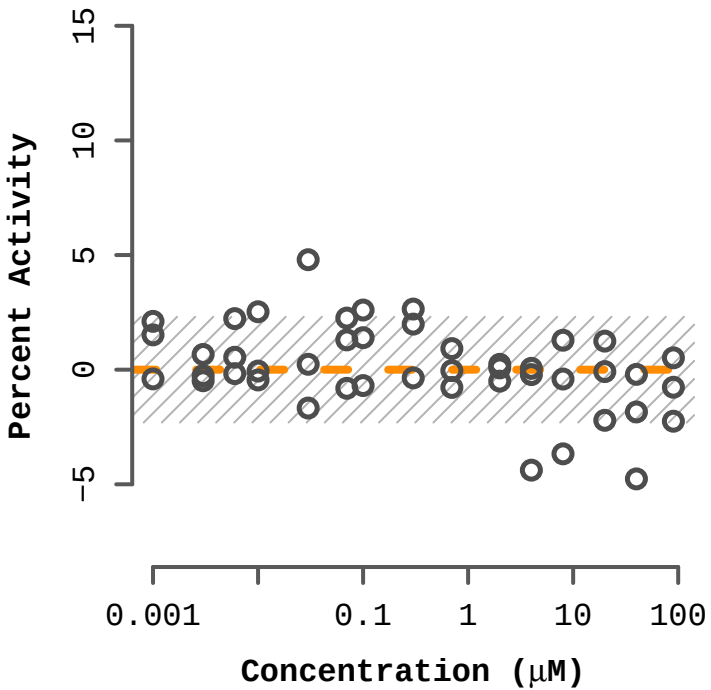
NAME: Aminocarb
CHID: 22172 **CASRN:** 2032-59-9
SPID(S): Tox21_301423
M4ID: 12477710

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 0.778 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

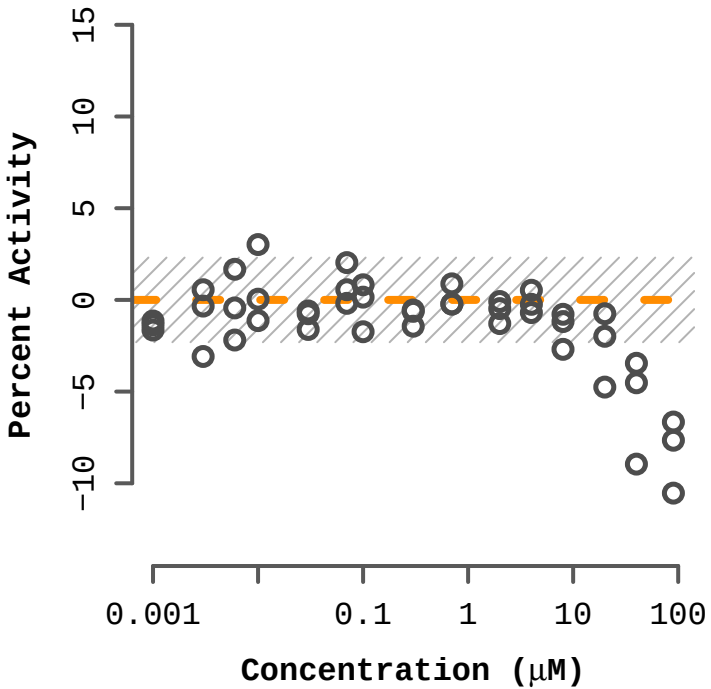
NAME: EPN
CHID: 22174 **CASRN:** 2104-64-5
SPID(S): Tox21_300424
M4ID: 12478708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

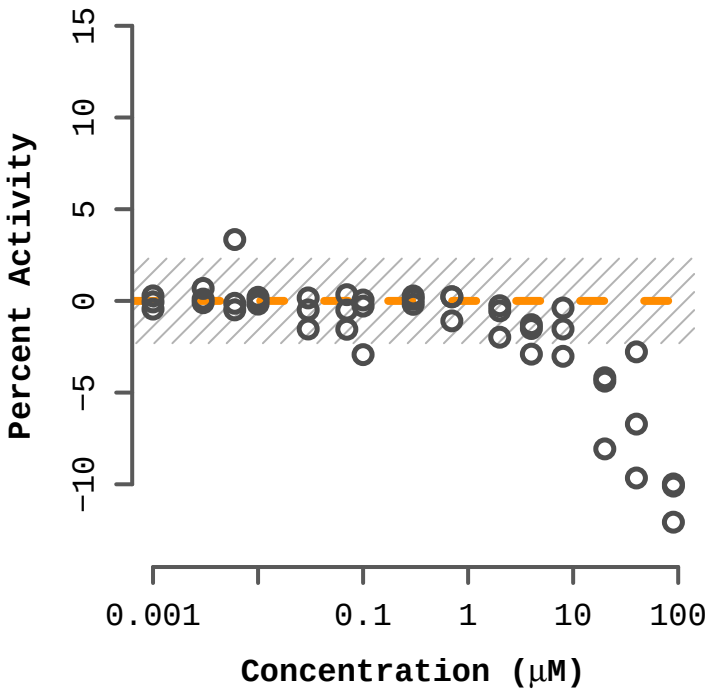
NAME: Pentachloropyridine
CHID: 22179 **CASRN:** 2176-62-7
SPID(S): Tox21_300371
M4ID: 12478761

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.01	NA	NA
PROB:	1	NA	NA
RMSE:	3.04	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 0.558 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

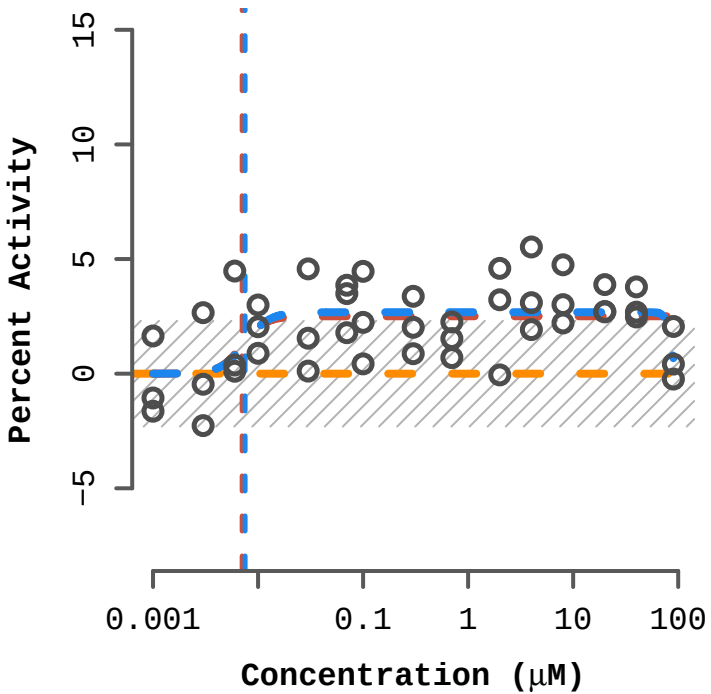
NAME: Pentachloropyridine
CHID: 22179 **CASRN:** 2176-62-7
SPID(S): Tox21_201578
M4ID: 12480674

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.73	NA	NA
PROB:	1	NA	NA
RMSE:	3.8	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 0.223 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (1R,2S,5R)-(-)-Menthol
CHID: 22180 CASRN: 2216-51-5
SPID(S): Tox21_303028
M4ID: 12476105

HILL MODEL (in red):

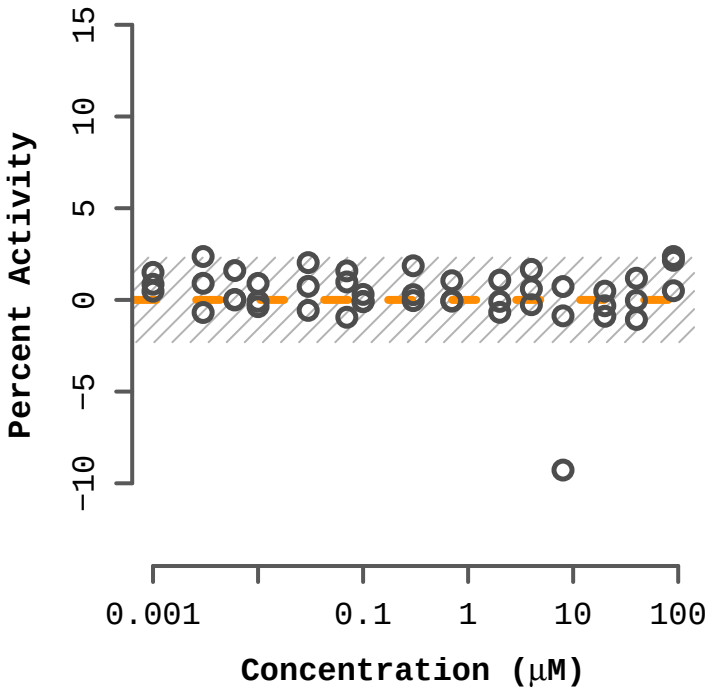
	tp	ga	gw
val:	2.5	-2.15	4.16
sd:	0.277	0.142	4.57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.68	-2.12	3.84	1.93	16.7
sd:	0.274	0.128	3.9	0.0717	42.9

	CNST	HILL	GNLS
AIC:	225.33	179.1	178.16
PROB:	0	0.39	0.61
RMSE:	2.71	1.55	1.48

MAX_MEAN: 3.52 MAX_MED: 3.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

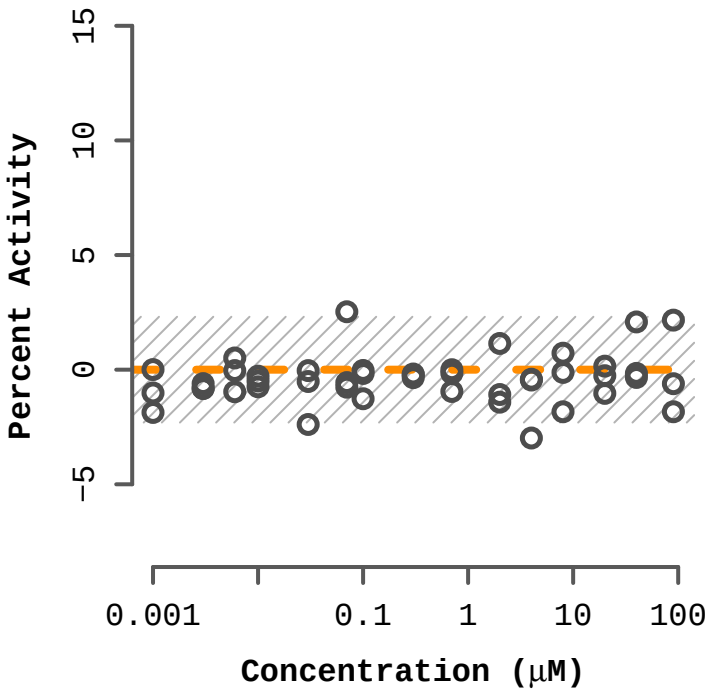
NAME: (1R,2S,5R)-(-)-Menthol
CHID: 22180 CASRN: 2216-51-5
SPID(S): Tox21_201919
M4ID: 12480333

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 1.68 MAX_MED: 2.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

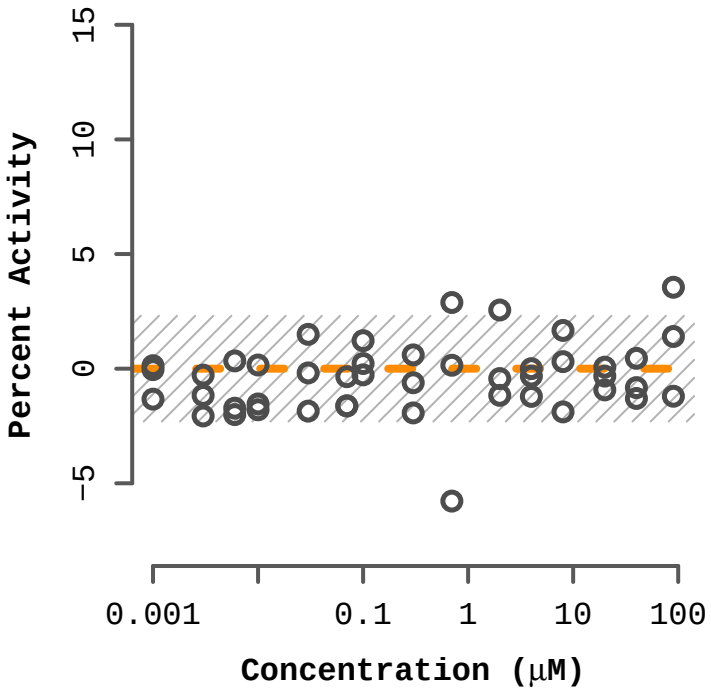
NAME: 2-Ethoxyethyl methacrylate
CHID: 22186 **CASRN:** 2370-63-0
SPID(S): Tox21_202814
M4ID: 12479438

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** −0.0373 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

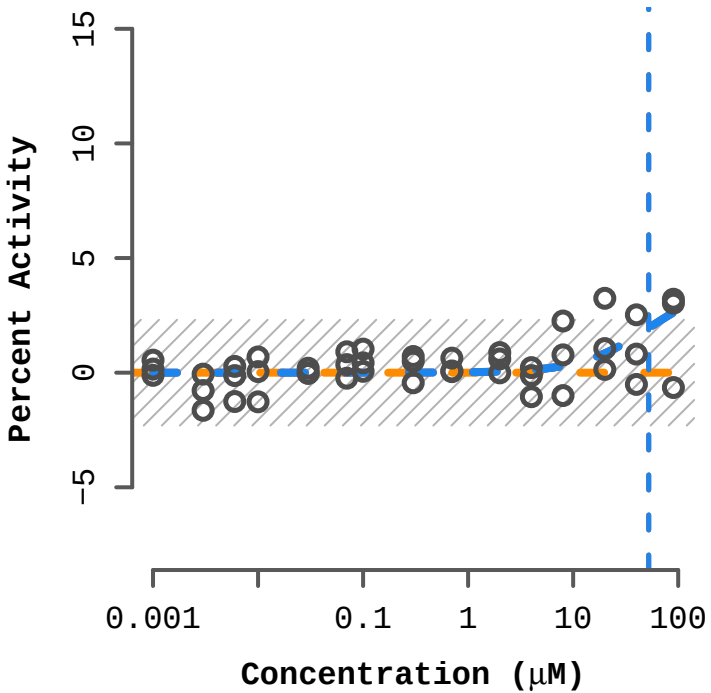
NAME: 2,3,6-Trimethylphenol
CHID: 22187 **CASRN:** 2416-94-6
SPID(S): Tox21_300059
M4ID: 12479071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,6-Trimethylphenol
CHID: 22187 CASRN: 2416-94-6
SPID(S): Tox21_202274
M4ID: 12479978

HILL MODEL (in red):

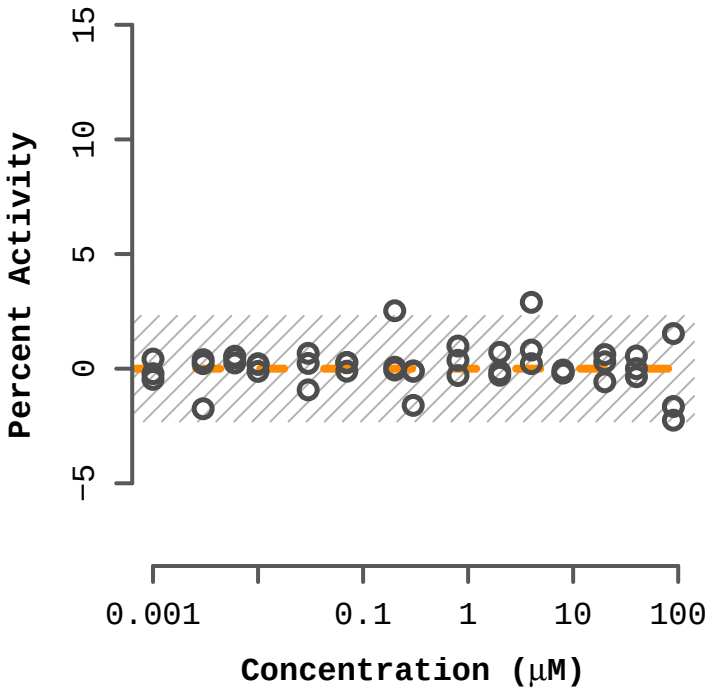
	tp	ga	gw
val:	3.89	1.72	1.33
sd:	2.29	0.43	0.904

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.89	1.72	1.33	3.25	5.8
sd:	2.28	0.428	0.901	783	3520

	CNST	HILL	GNLS
AIC:	134.06	127.87	131.87
PROB:	0.04	0.85	0.11
RMSE:	1.14	0.97	0.97

MAX_MEAN: 1.86 MAX_MED: 3.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

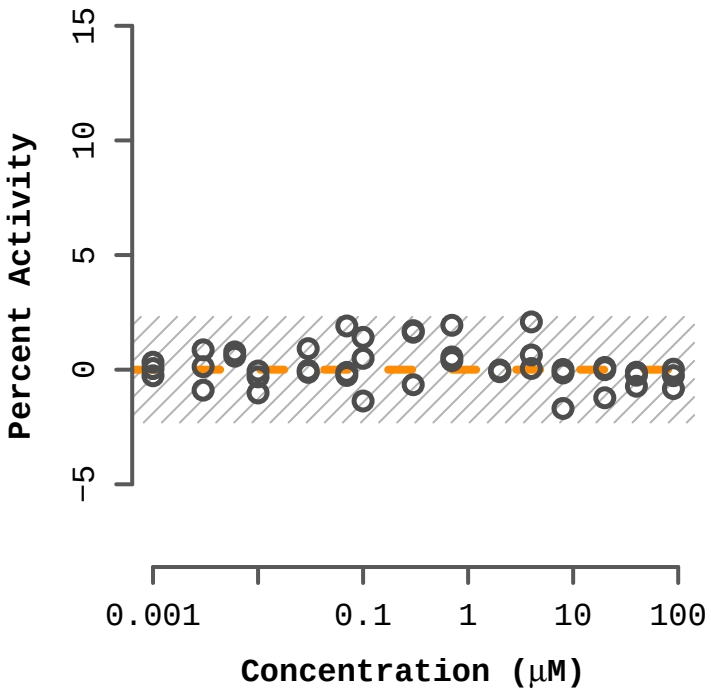
NAME: Dodecanenitrile
CHID: 22188 CASRN: 2437-25-4
SPID(S): Tox21_302921
M4ID: 12476212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.31 MAX_MED: 0.814 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

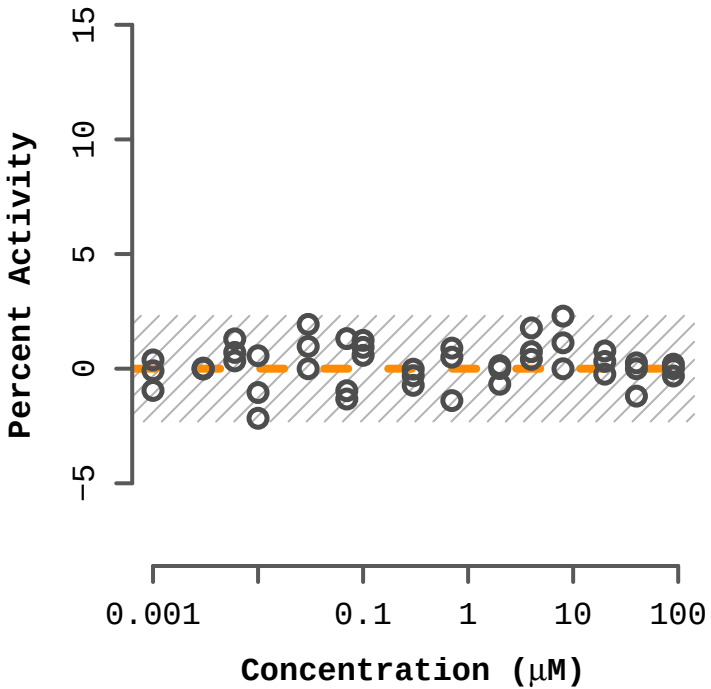
NAME: Dodecanenitrile
CHID: 22188 **CASRN:** 2437-25-4
SPID(S): Tox21_201304
M4ID: 12480948

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.964 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

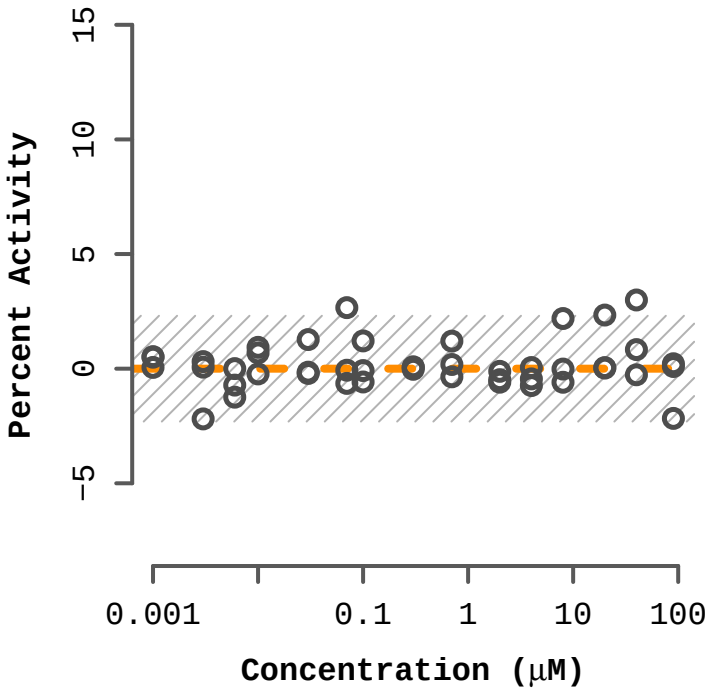
NAME: Tetrahydrofurfuryl methacrylate
CHID: 22191 CASRN: 2455-24-5
SPID(S): Tox21_301715
M4ID: 12477418

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

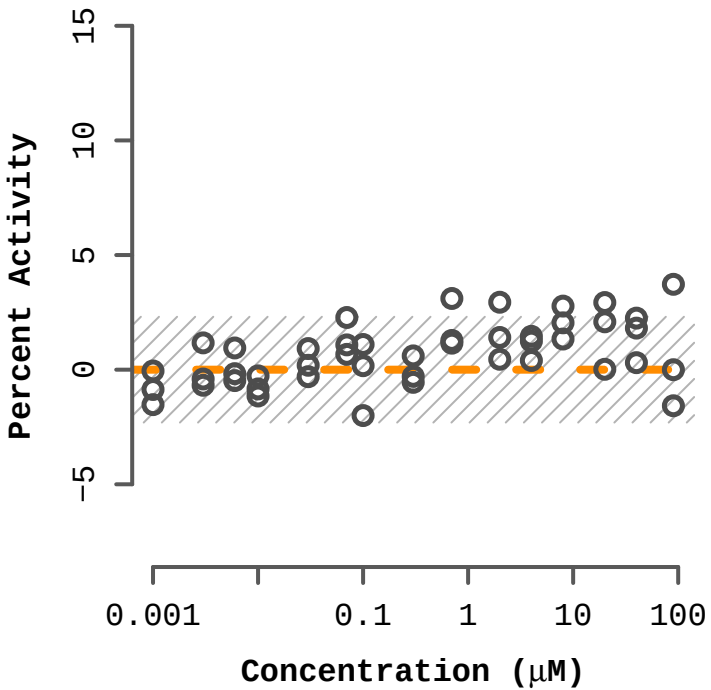
NAME: Benzyl methacrylate
CHID: 22193 **CASRN:** 2495-37-6
SPID(S): Tox21_301712
M4ID: 12477421

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.834 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

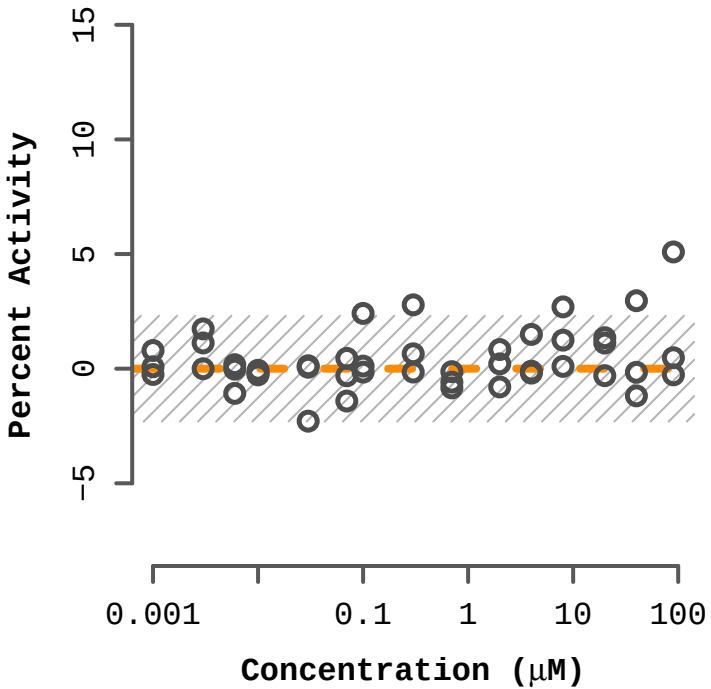
NAME: Hexyl acrylate
CHID: 22194 CASRN: 2499-95-8
SPID(S): Tox21_301720
M4ID: 12477413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

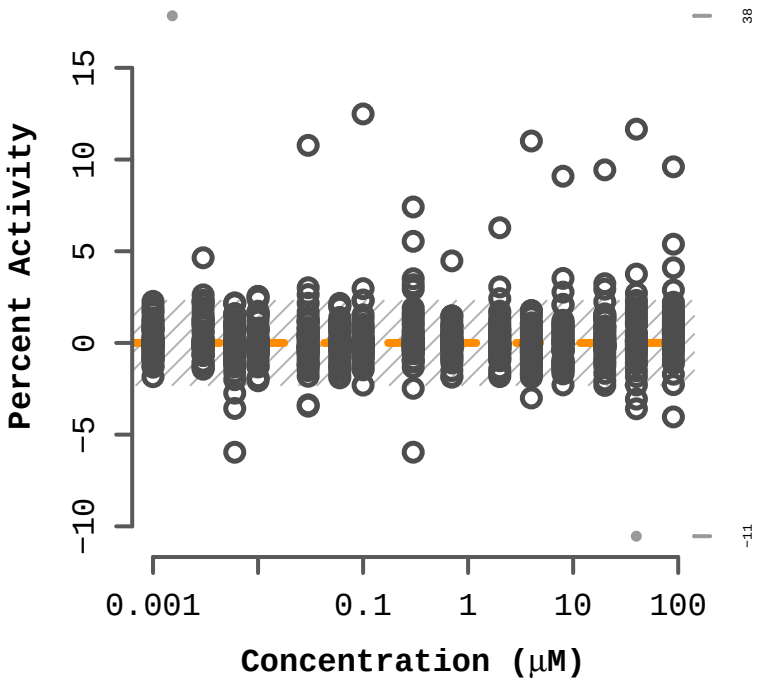
NAME: 3-(3-Pyridyl)-1-propanol
CHID: 22198 CASRN: 2859-67-8
SPID(S): Tox21_303737
M4ID: 12475451

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

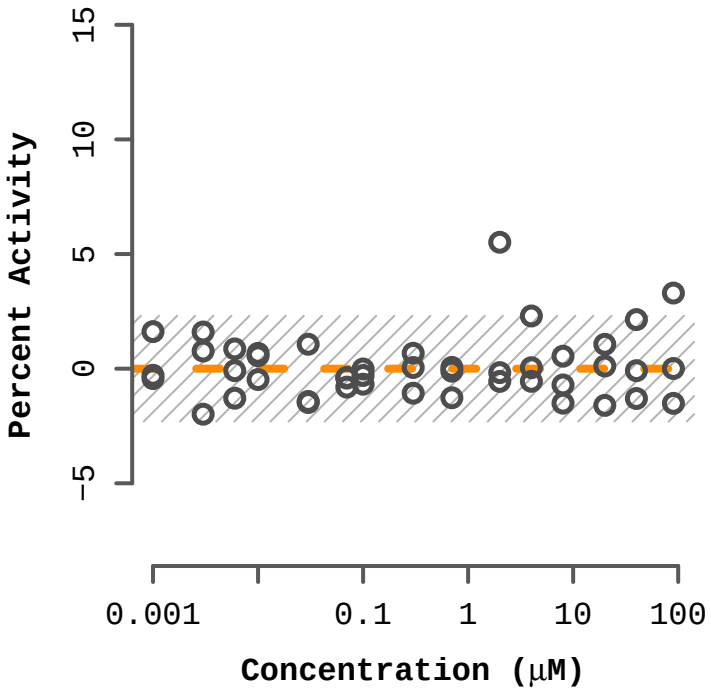
NAME: 2,4,5−Trimethoxybenzaldehyde
CHID: 22217 **CASRN:** 4460−86−0
SPID(S): Tox21_400070
M4ID: 12475067 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2390.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 0.901 **MAX_MED:** 0.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

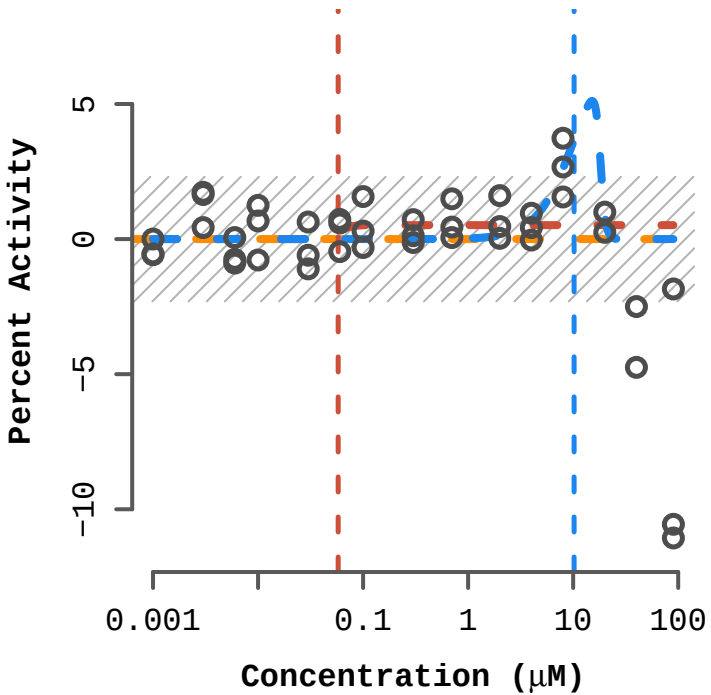
NAME: Isopropyl methacrylate
CHID: 22218 **CASRN:** 4655-34-9
SPID(S): Tox21_202609
M4ID: 12479643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 0.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,4,5-Tetrachlorophenol
CHID: 22220 CASRN: 4901-51-3
SPID(S): Tox21_200105
M4ID: 12482147

HILL MODEL (in red):

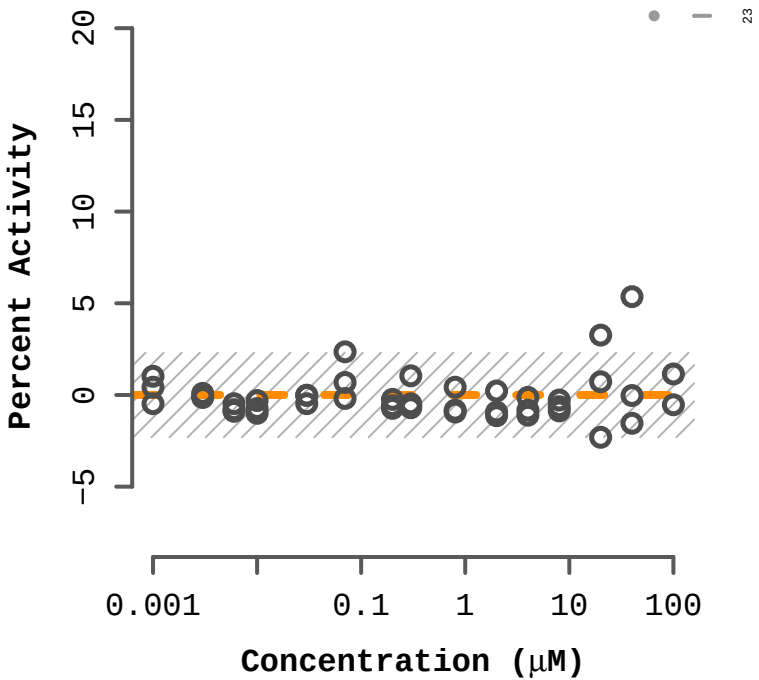
	tp	ga	gw
val:	0.517	−1.24	8
sd:	0.306	0.31	36.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.34	1.01	2.44	1.26	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	208.96	212.13	207.93
PROB:	0.35	0.07	0.58
RMSE:	3.36	3.36	3.21

MAX_MEAN: 4.11 MAX_MED: 2.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

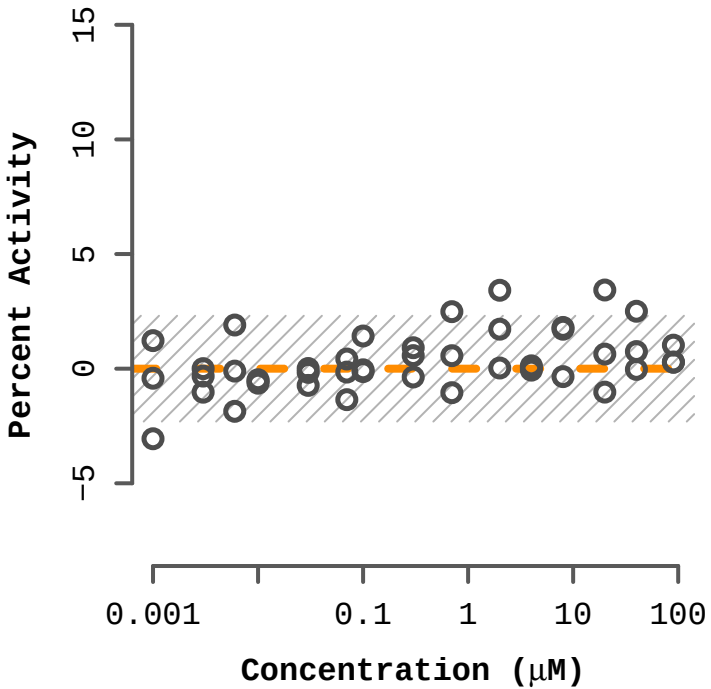
NAME: Dimethylaminopropyl chloride hydrochloride
CHID: 22227 CASRN: 5407-04-5
SPID(S): Tox21_201208
M4ID: 12481044 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.54	NA	NA
PROB:	1	NA	NA
RMSE:	3.63	NA	NA

MAX_MEAN: 7.82 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

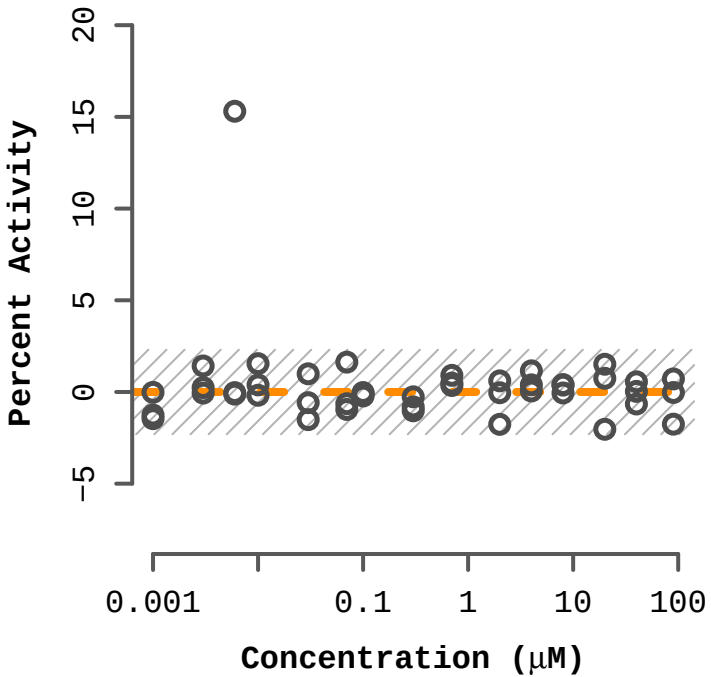
NAME: 1,4-bis(3-Aminopropyl)piperazine
CHID: 22246 **CASRN:** 7209-38-3
SPID(S): Tox21_301407
M4ID: 12477726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

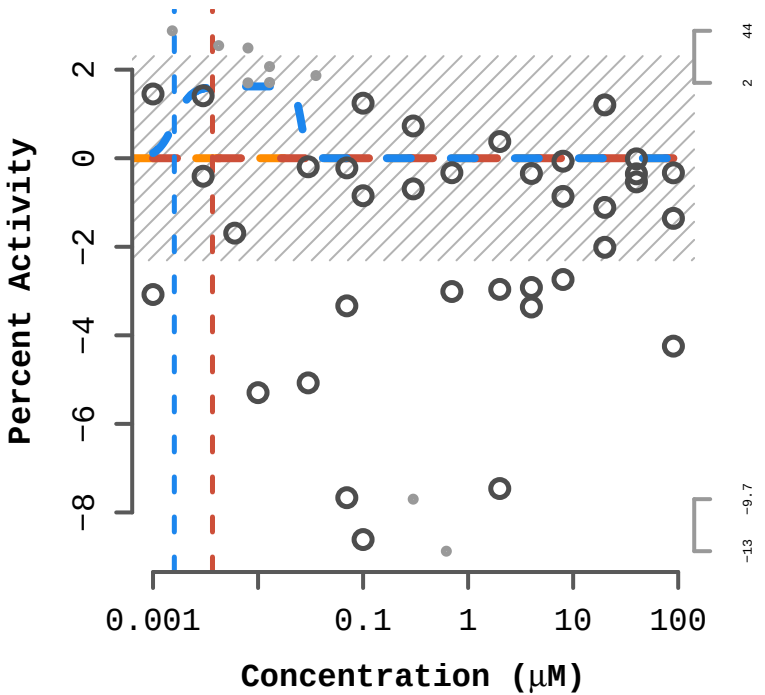
NAME: Nerolidol
CHID: 22247 CASRN: 7212-44-4
SPID(S): Tox21_301382
M4ID: 12477751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.45	NA	NA

MAX_MEAN: 5.05 MAX_MED: 0.746 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Resmethrin
CHID: 22253 **CASRN:** 10453-86-8
SPID(S): Tox21_300920
M4ID: 12478213 **BRK**

HILL MODEL (in red):

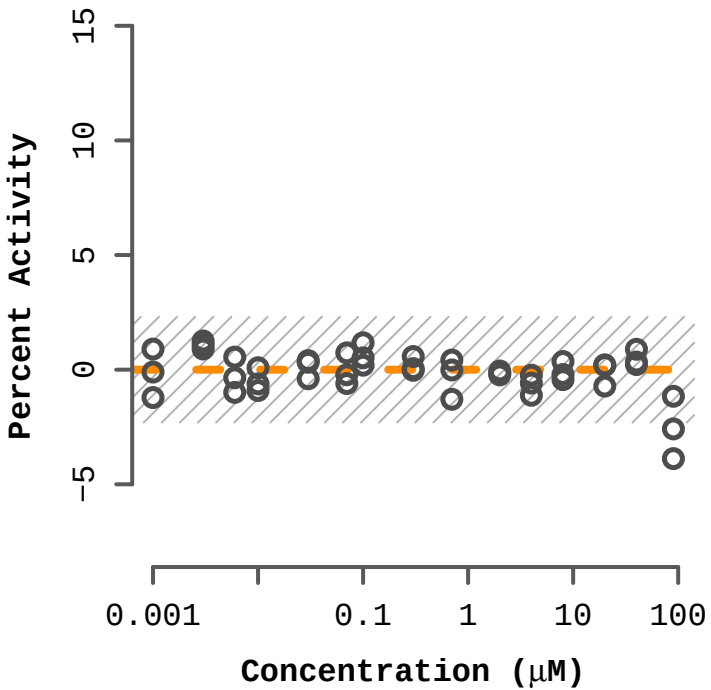
	tp	ga	gw
val:	3.47e-10	-2.43	3.19
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.62	-2.8	5.5	-1.59	14
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	304.03	310.03	313.18
PROB:	0.94	0.05	0.01
RMSE:	10.31	10.31	10.06

MAX_MEAN: 14.1 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

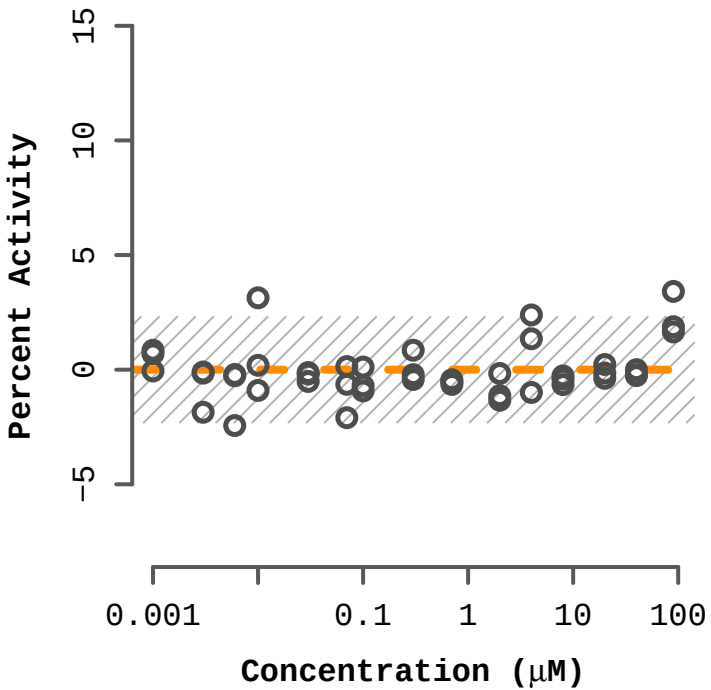
NAME: Resmethrin
CHID: 22253 **CASRN:** 10453-86-8
SPID(S): Tox21_202138
M4ID: 12480114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

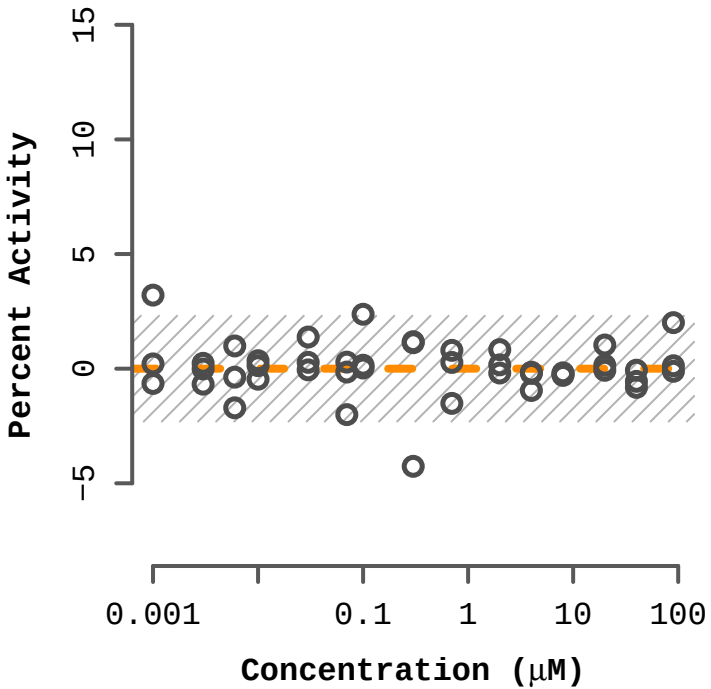
NAME: Terbufos
CHID: 22254 CASRN: 13071-79-9
SPID(S): Tox21_302994
M4ID: 12476139

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.31 MAX_MED: 1.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

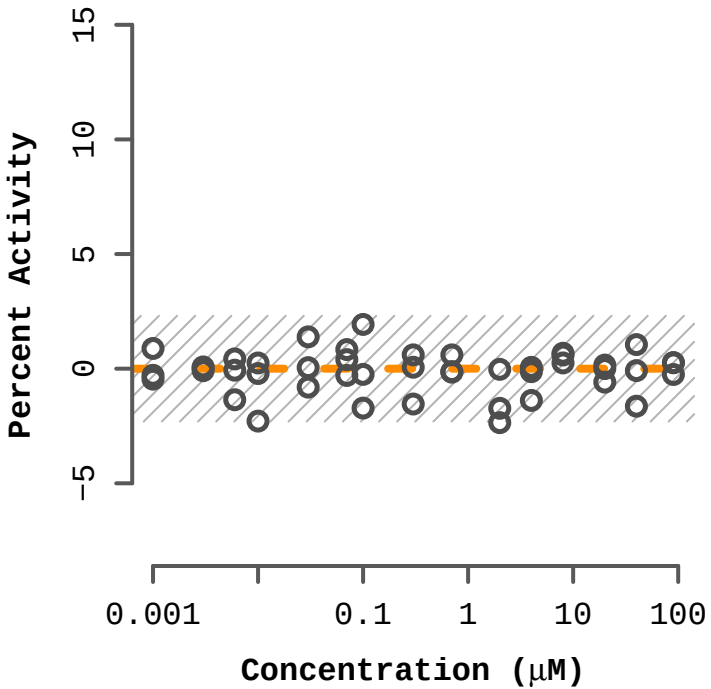
NAME: Terbufos
CHID: 22254 **CASRN:** 13071-79-9
SPID(S): Tox21_201634
M4ID: 12480618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.925 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

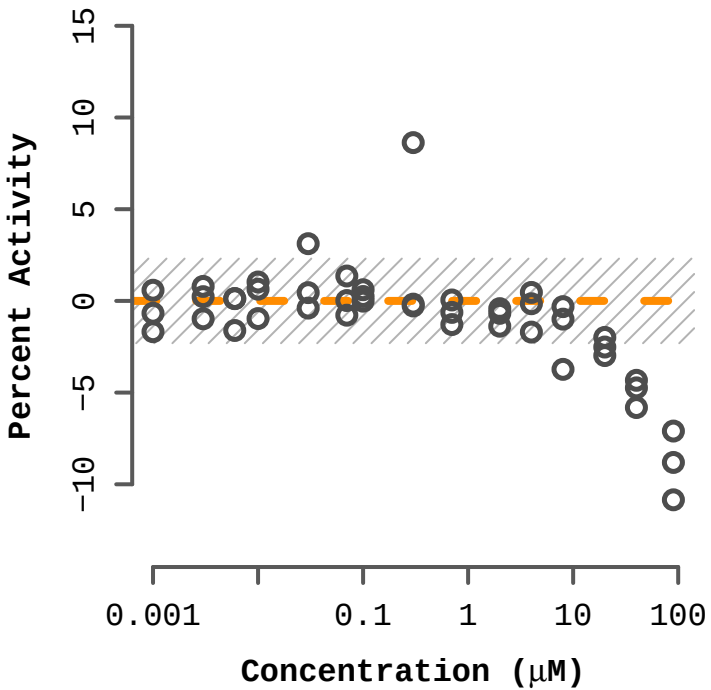
NAME: 2',3',4'−Trichloroacetophenone
CHID: 22256 CASRN: 13608−87−2
SPID(S): Tox21_200293
M4ID: 12481959

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.507 MAX_MED: 0.597 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

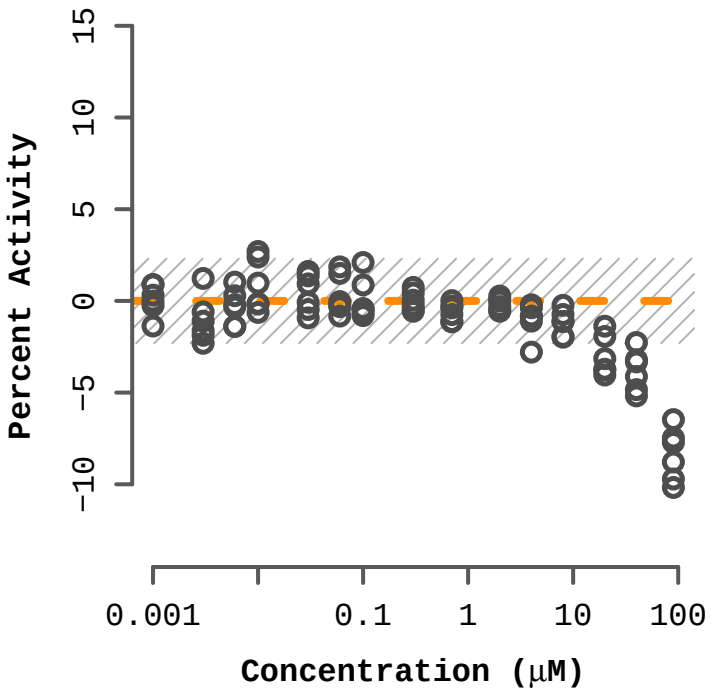
NAME: Alachlor
CHID: 22265 **CASRN:** 15972-60-8
SPID(S): Tox21_300713
M4ID: 12478420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.31	NA	NA
PROB:	1	NA	NA
RMSE:	3.2	NA	NA

MAX_MEAN: 2.73 **MAX_MED:** 0.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

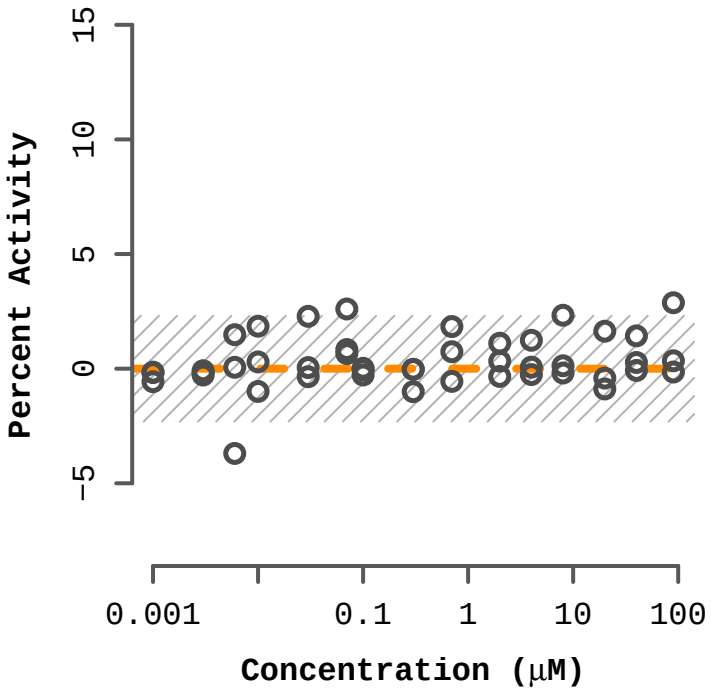
NAME: Alachlor
CHID: 22265 **CASRN:** 15972-60-8
SPID(S): Tox21_202205
M4ID: 12480047

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	405.63	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 0.428 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

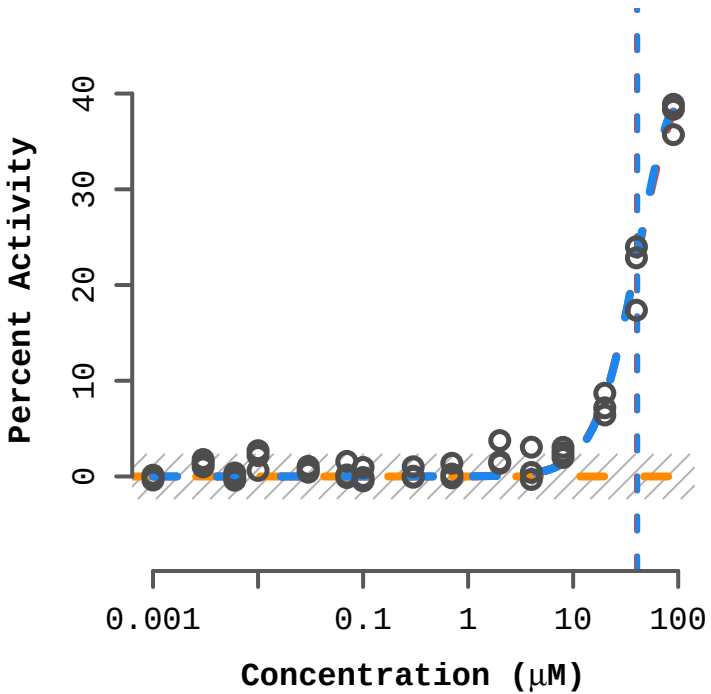
NAME: Methomyl
CHID: 22267 **CASRN:** 16752-77-5
SPID(S): Tox21_301118
M4ID: 12478015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(Diethylamino)salicylaldehyde
CHID: 22271 CASRN: 17754-90-4
SPID(S): Tox21_303946
M4ID: 12475242

HILL MODEL (in red):

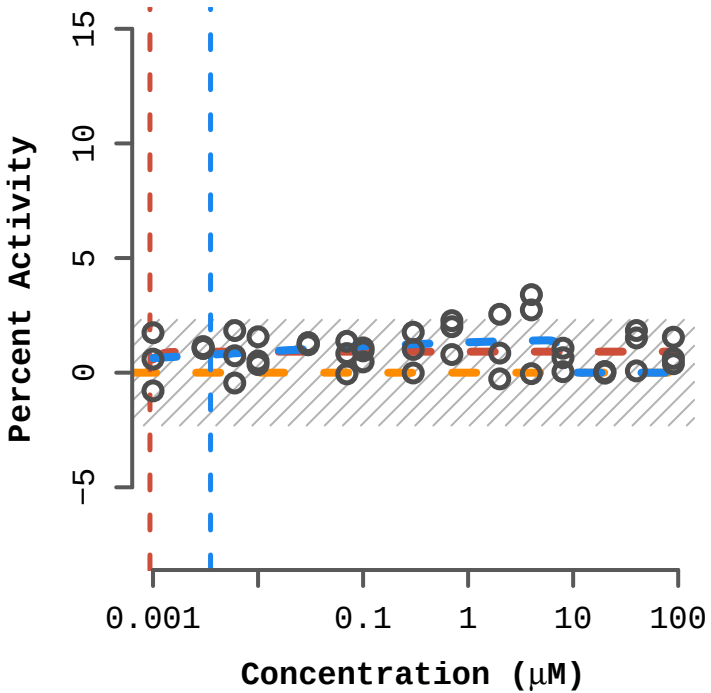
	tp	ga	gw
val:	44.9	1.6	2.14
sd:	3.32	0.0447	0.297

GAIN-LOSS MODEL (in blue):

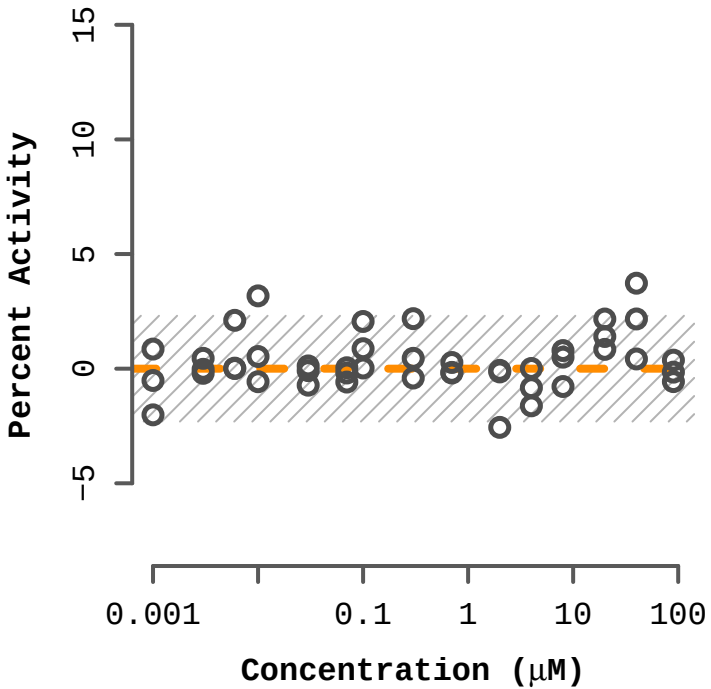
	tp	ga	gw	la	lw
val:	46.7	1.61	2.15	2.07	12.3
sd:	12.2	0.103	0.34	0.0561	18

	CNST	HILL	GNLS
AIC:	307.09	165.47	169.09
PROB:	0	0.86	0.14
RMSE:	11.45	1.47	1.47

MAX_MEAN: 37.7 MAX_MED: 38.4 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,6-Diisopropylaniline
CHID:    22279   CASRN: 24544-04-5
SPID(S): Tox21_302145
M4ID:    12476988

HILL MODEL (in red):
      tp       ga       gw
val:  0.917    -3.03    8
sd:   0.132    0.26     64.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.57     -2.45    0.3      0.895    17.5
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  155.34      124.82      129.78
PROB: 0           0.92        0.08
RMSE: 1.29        0.87        0.87

MAX_MEAN: 2.03      MAX_MED: 2.74      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

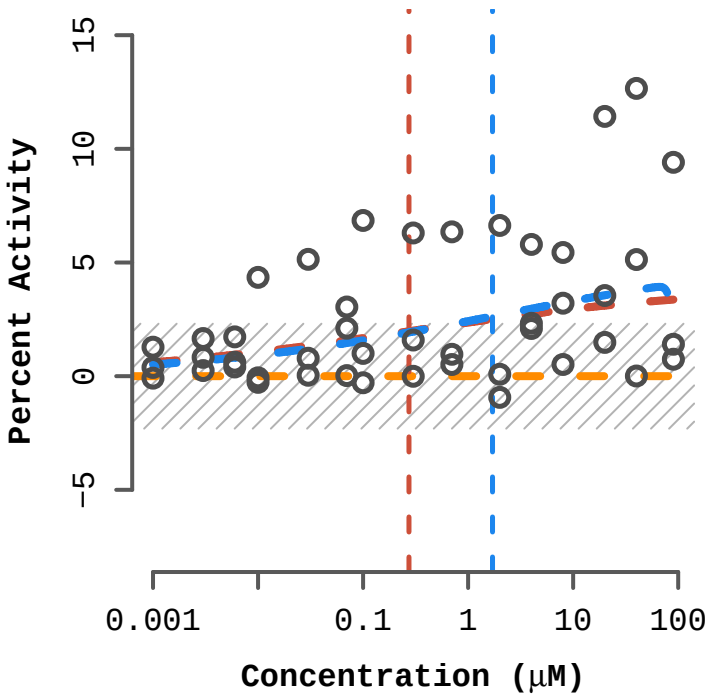
NAME: 2-Butanamine
CHID: 22284 **CASRN:** 13952-84-6
SPID(S): Tox21_301321
M4ID: 12477812

HILL MODEL: Not applicable.

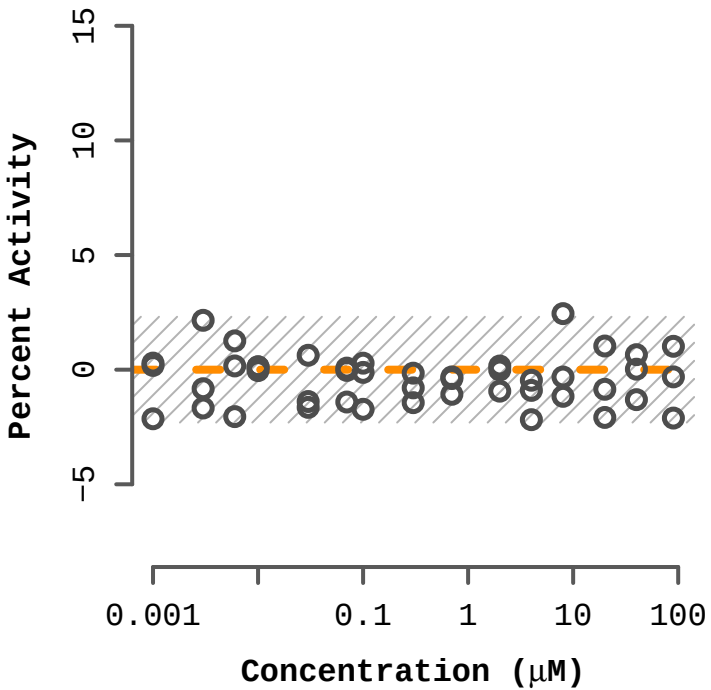
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 2.17 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Hexyloxyaniline
CHID:    22288   CASRN: 39905-57-2
SPID(S): Tox21_303490
M4ID:    12475651

HILL MODEL (in red):
      tp       ga       gw
val:  3.95     -0.563   0.304
sd:   3.54     3.17     0.345

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.26     0.232    0.3      1.95     17.7
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  249.13      228.8       231.92
PROB: 0           0.83        0.17
RMSE: 4.09        2.95        2.94

MAX_MEAN: 5.93      MAX_MED: 5.13      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

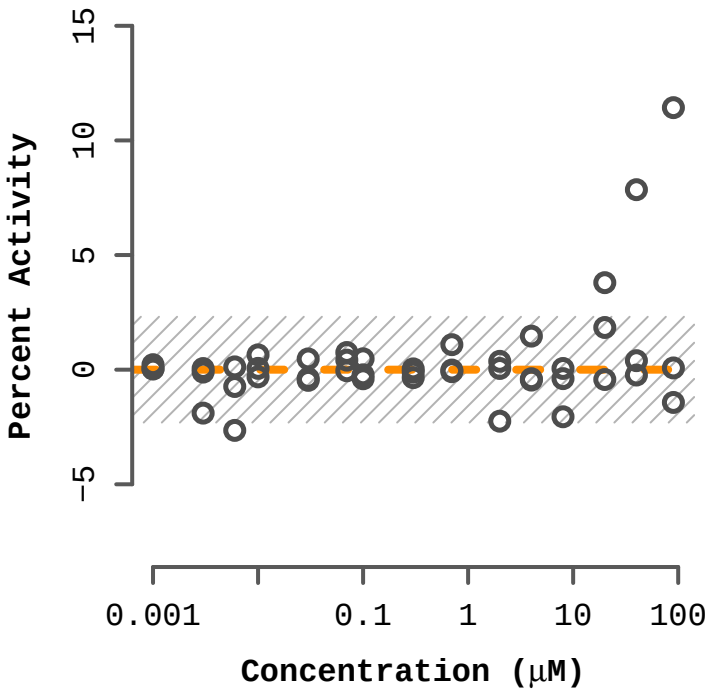
NAME: Permethrin
CHID: 22292 **CASRN:** 52645-53-1
SPID(S): Tox21_300691
M4ID: 12478442

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.322 **MAX_MED:** 0.187 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

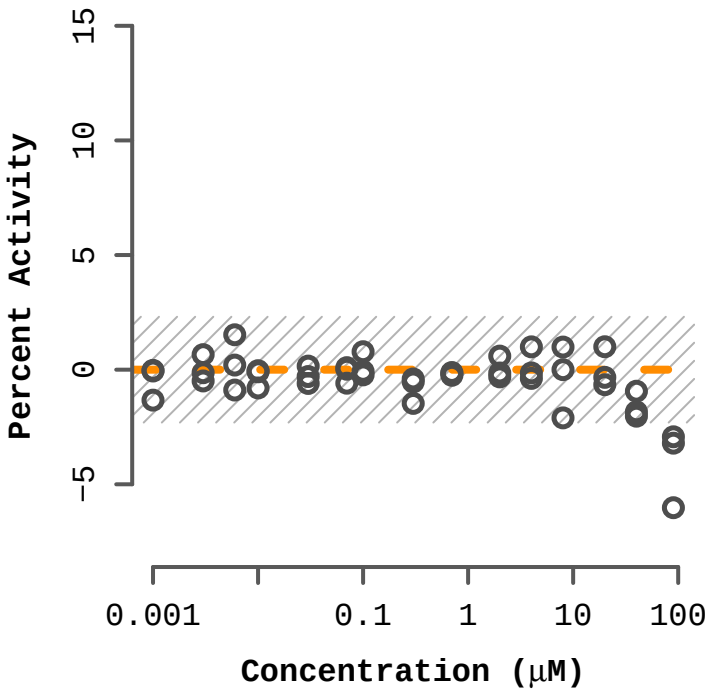
NAME: Permethrin
CHID: 22292 **CASRN:** 52645-53-1
SPID(S): Tox21_201586
M4ID: 12480666

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.36	NA	NA
PROB:	1	NA	NA
RMSE:	2.31	NA	NA

MAX_MEAN: 3.36 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

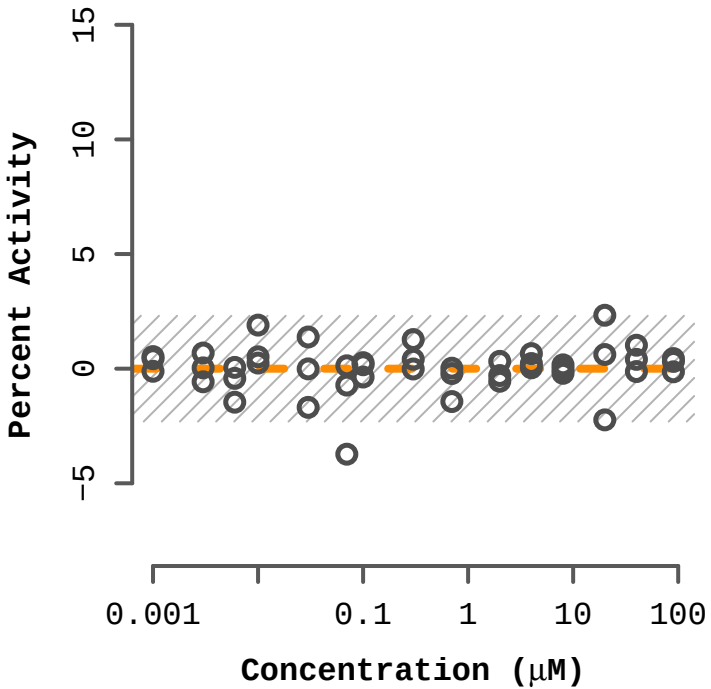
NAME: Flucythrinate
CHID: 22301 **CASRN:** 70124-77-5
SPID(S): Tox21_302254
M4ID: 12476879

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.28 **MAX_MED:** 0.203 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

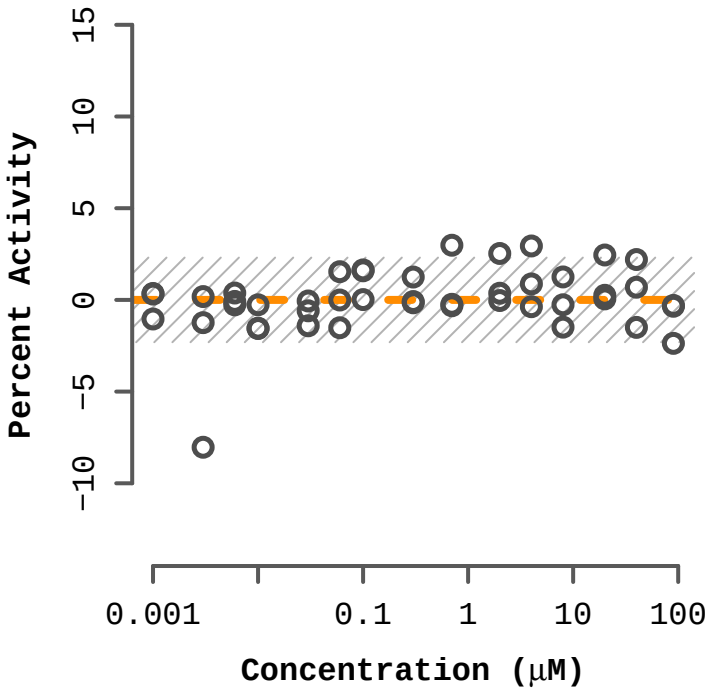
NAME: 4-tert-Butylstyrene
CHID: 22305 **CASRN:** 1746-23-2
SPID(S): Tox21_301673
M4ID: 12477460

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 0.619 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

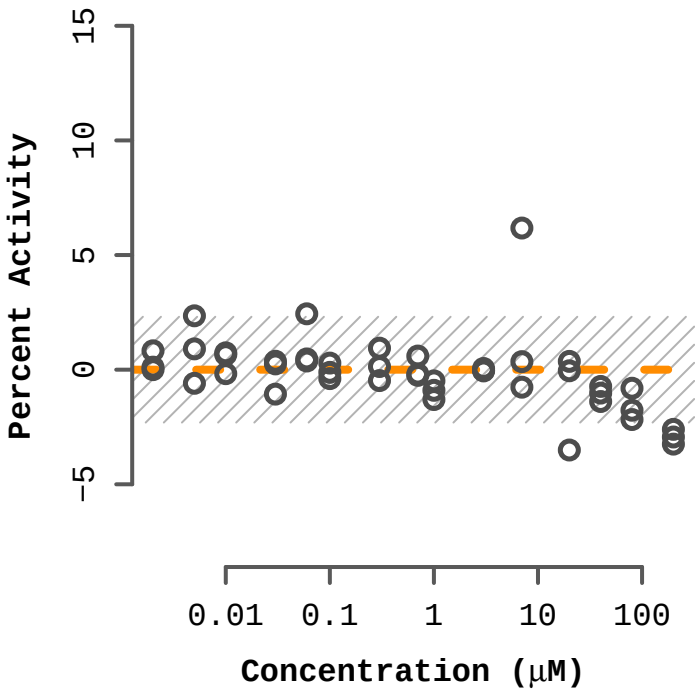
NAME: Demeton
CHID: 22306 **CASRN:** 8065-48-3
SPID(S): Tox21_200239
M4ID: 12482013

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

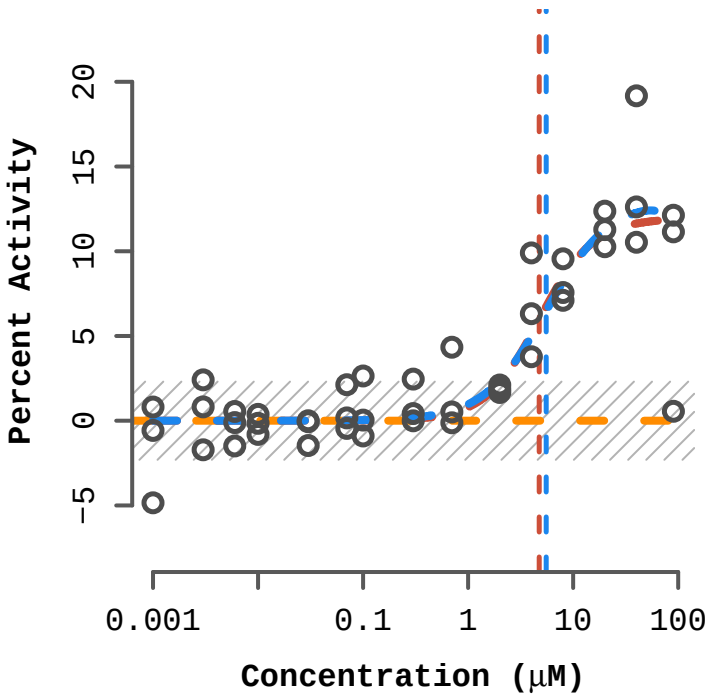
NAME: Chloromethyl styrene
CHID: 22307 **CASRN:** 30030-25-2
SPID(S): Tox21_301268
M4ID: 12477865

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Genistein
CHID: 22308 **CASRN:** 446-72-0
SPID(S): Tox21_300585
M4ID: 12478548

HILL MODEL (in red):

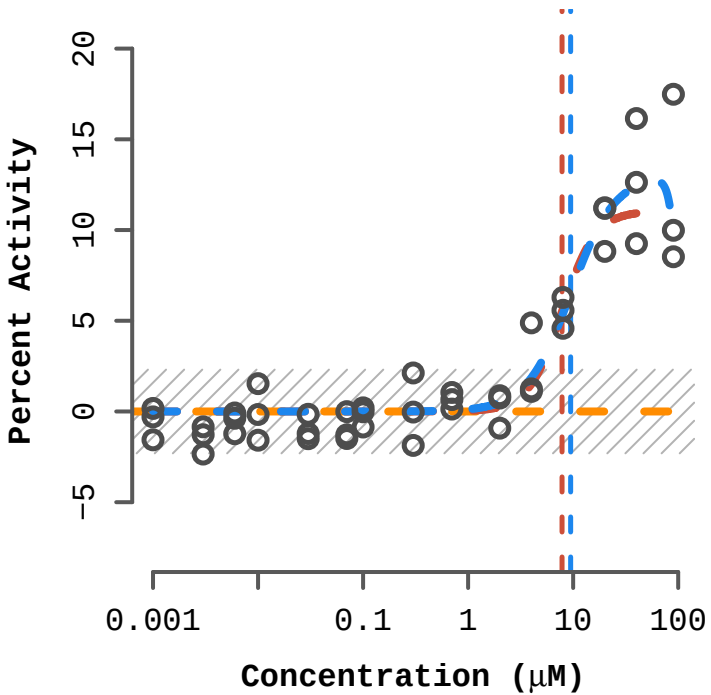
	tp	ga	gw
val:	11.9	0.677	1.69
sd:	0.714	0.0728	0.366

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13	0.743	1.47	2.13	5.13
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	288.51	195.27	198.29
PROB:	0	0.82	0.18
RMSE:	6.21	2.55	2.46

MAX_MEAN: 14.1 **MAX_MED:** 12.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Genistein
CHID: 22308 **CASRN:** 446-72-0
SPID(S): Tox21_201428
M4ID: 12480824

HILL MODEL (in red):

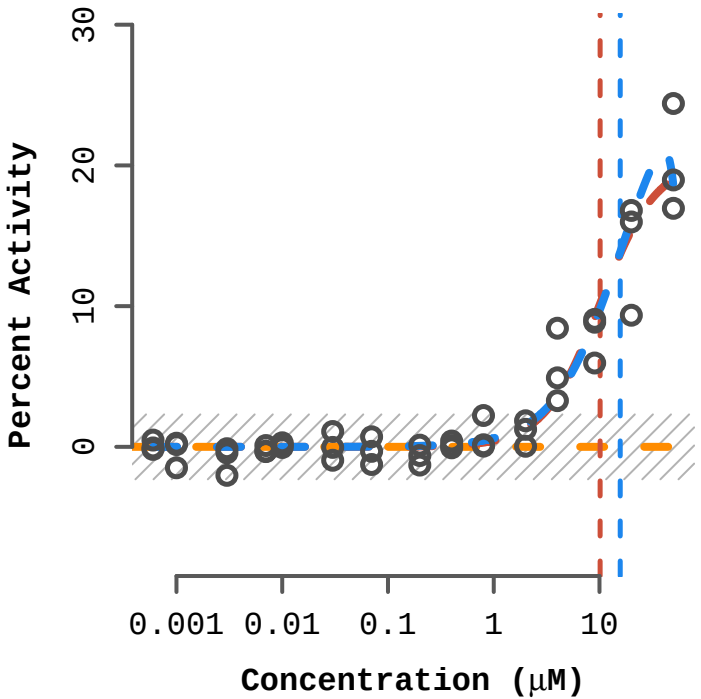
	tp	ga	gw
val:	11	0.894	2.75
sd:	0.918	0.0483	0.769

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13	0.976	2.08	2	11.1
sd:	1.75	0.0887	0.607	0.0237	7.13

	CNST	HILL	GNLS
AIC:	275.07	176.71	176.85
PROB:	0	0.52	0.48
RMSE:	5.71	1.74	1.76

MAX_MEAN: 12.7 **MAX_MED:** 12.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Genistein
CHID: 22308 CASRN: 446-72-0
SPID(S): Tox21_110161_1
M4ID: 12484596

HILL MODEL (in red):

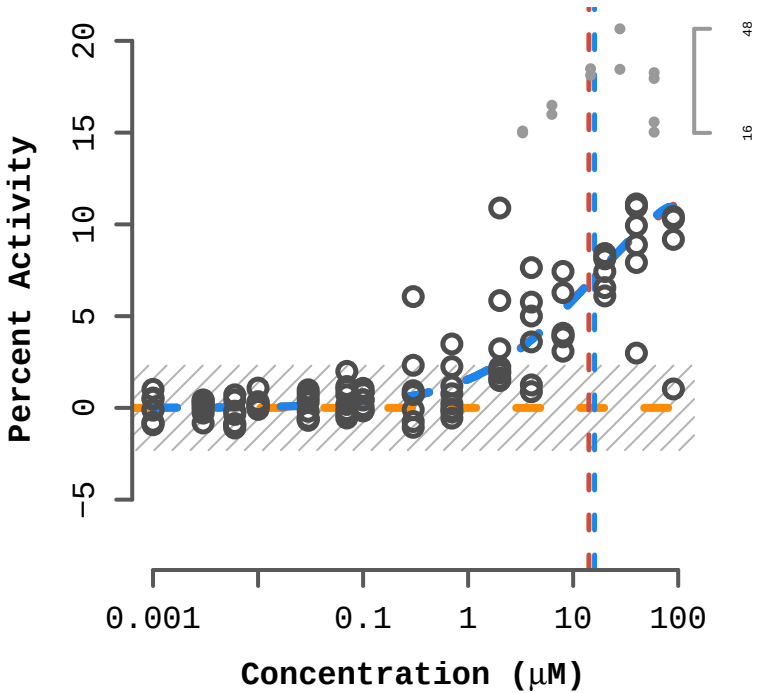
	tp	ga	gw
val:	20.4	1.01	1.65
sd:	1.25	0.0485	0.215

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27.7	1.2	1.38	1.76	9.51
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	281.61	161.11	162.52
PROB:	0	0.67	0.33
RMSE:	6.98	1.68	1.74

MAX_MEAN: 20.1 MAX_MED: 19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Daidzein
CHID: 22310 CASRN: 486-66-8
SPID(S): Tox21_303650
M4ID: 12475498 BRK

HILL MODEL (in red):

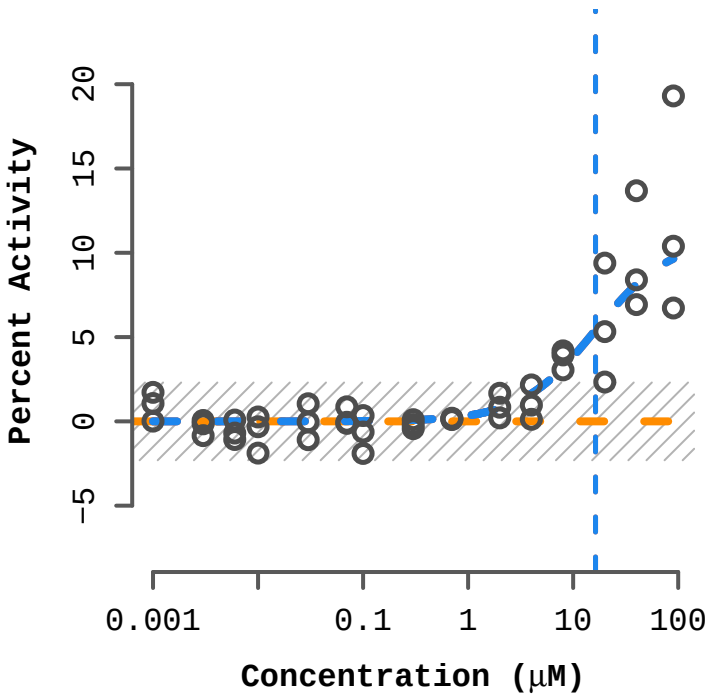
	tp	ga	gw
val:	13.6	1.15	0.775
sd:	2.98	0.296	0.161

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.3	1.2	0.758	2.08	11.7
sd:	6.4	0.562	0.216	0.271	23.5

	CNST	HILL	GNLS
AIC:	807.37	650.02	653.98
PROB:	0	0.88	0.12
RMSE:	9.98	7.01	7.02

MAX_MEAN: 16.8 **MAX_MED:** 13.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Daidzein
CHID: 22310 CASRN: 486-66-8
SPID(S): Tox21_201444
M4ID: 12480808

HILL MODEL (in red):

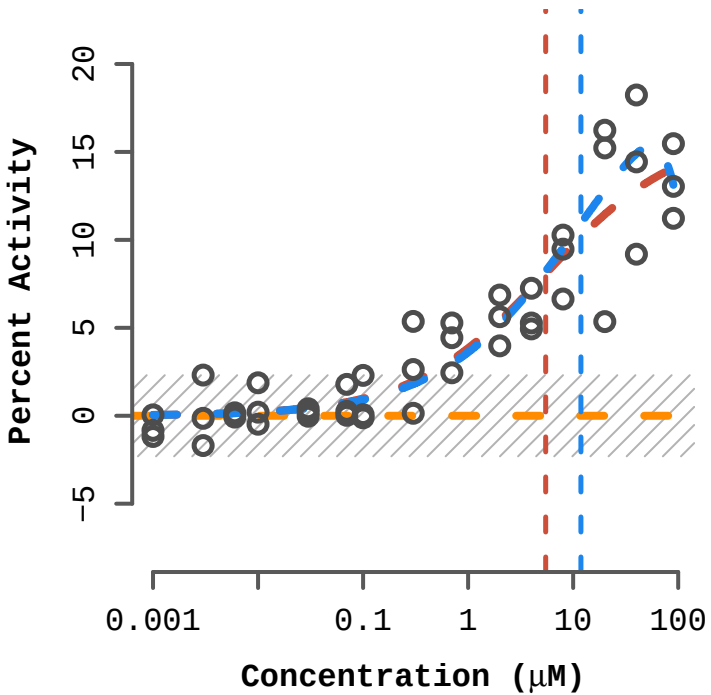
	tp	ga	gw
val:	10.8	1.21	1.22
sd:	2.53	0.239	0.348

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.8	1.21	1.22	3.35	5.4
sd:	2.53	0.239	0.348	1060	4110

	CNST	HILL	GNLS
AIC:	246.43	169.76	173.76
PROB:	0	0.88	0.12
RMSE:	4.77	2.02	2.02

MAX_MEAN: 12.1 **MAX_MED:** 10.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Formononetin
CHID: 22311 CASRN: 485-72-3
SPID(S): Tox21_301848
M4ID: 12477285

HILL MODEL (in red):

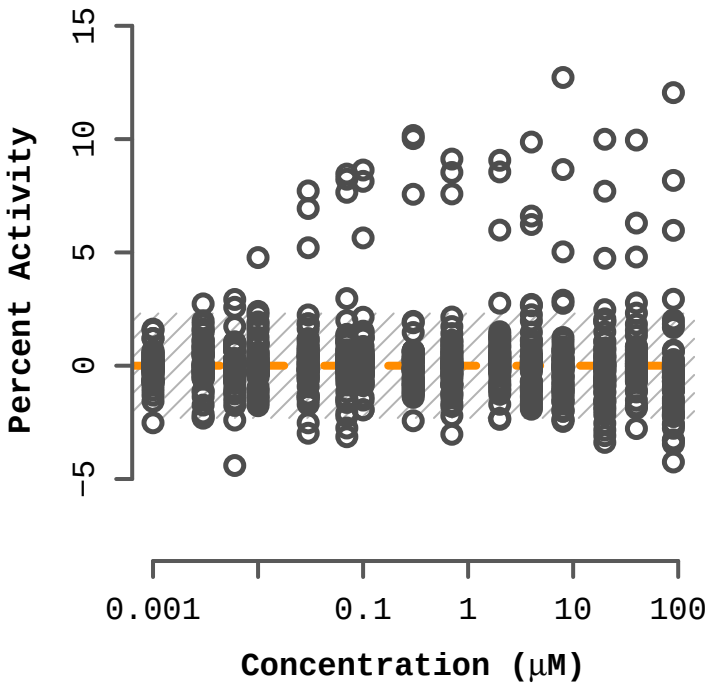
	tp	ga	gw
val:	16.2	0.738	0.686
sd:	2.29	0.233	0.137

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.9	1.07	0.656	2.08	3.96
sd:	6.58	0.378	0.117	0.225	8.21

	CNST	HILL	GNLS
AIC:	302.24	197.96	198.19
PROB:	0	0.53	0.47
RMSE:	7.05	2.07	2.07

MAX_MEAN: 14 MAX_MED: 15.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

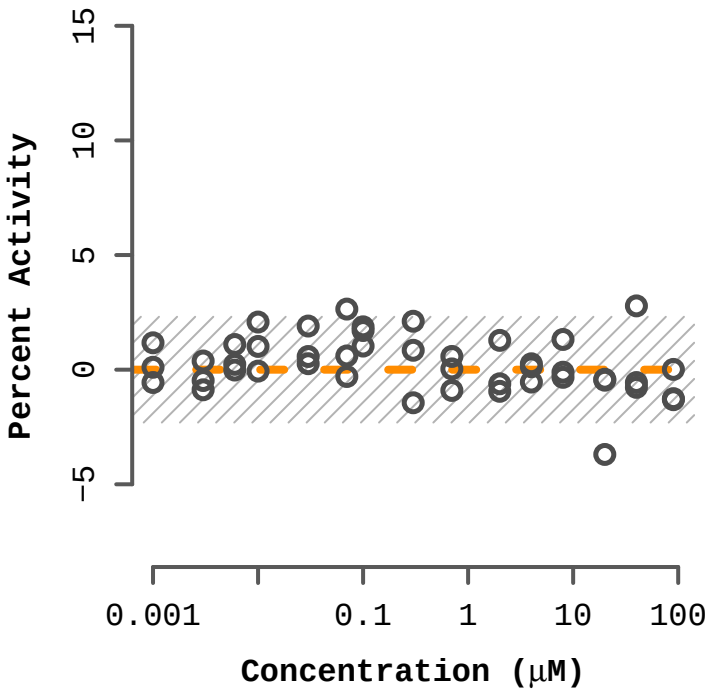
NAME: 4-Octylphenol
CHID: 22312 **CASRN:** 1806-26-4
SPID(S): Tox21_400015
M4ID: 12475122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2710.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.155 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

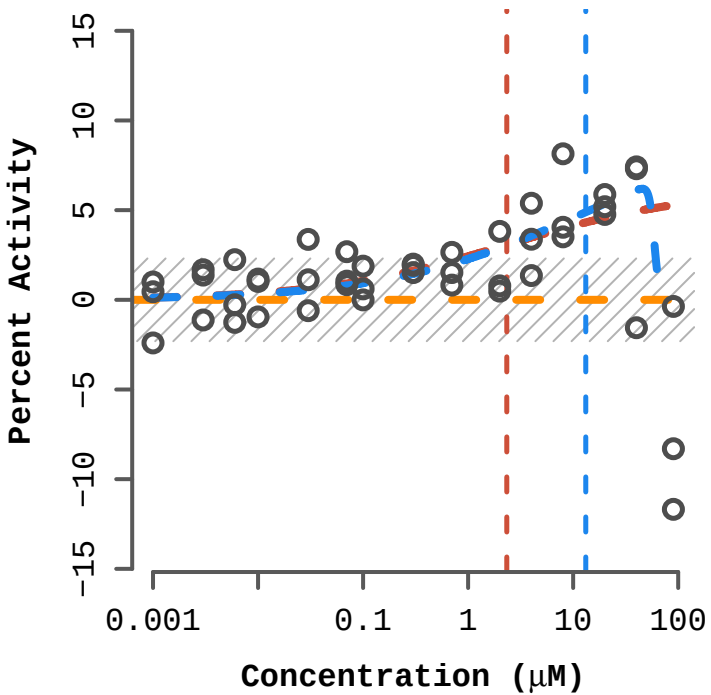
NAME: o,p'−DDE
CHID: 22313 CASRN: 3424−82−6
SPID(S): Tox21_304022
M4ID: 12475166

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.54 MAX_MED: 1.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zearalanol
CHID: 22315 CASRN: 26538-44-3
SPID(S): Tox21_201203
M4ID: 12481049

HILL MODEL (in red):

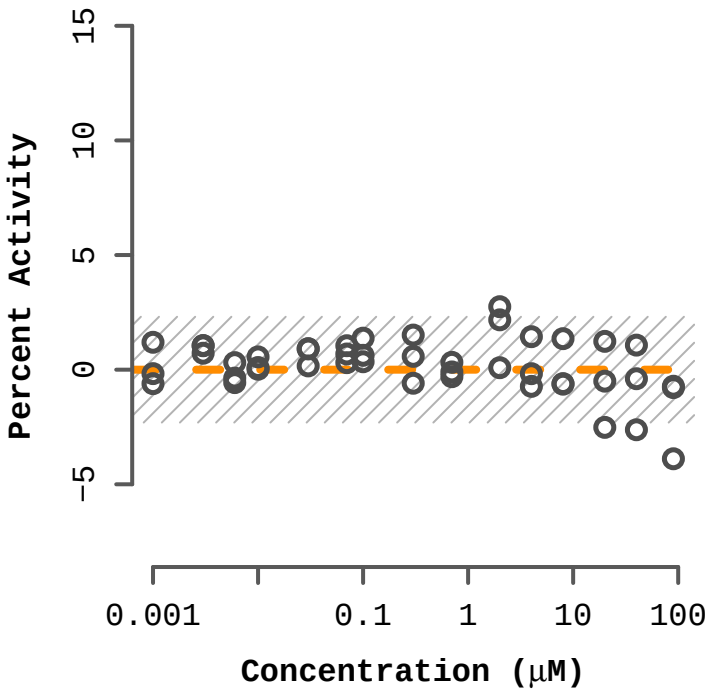
	tp	ga	gw
val:	6.14	0.368	0.499
sd:	2.91	0.941	0.237

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.77	1.12	0.462	1.77	18
sd:	4.21	0.813	0.132	0.265	27

	CNST	HILL	GNLS
AIC:	243.78	220.24	205.8
PROB:	0	0	1
RMSE:	3.72	3.76	2.76

MAX_MEAN: 5.28 MAX_MED: 7.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

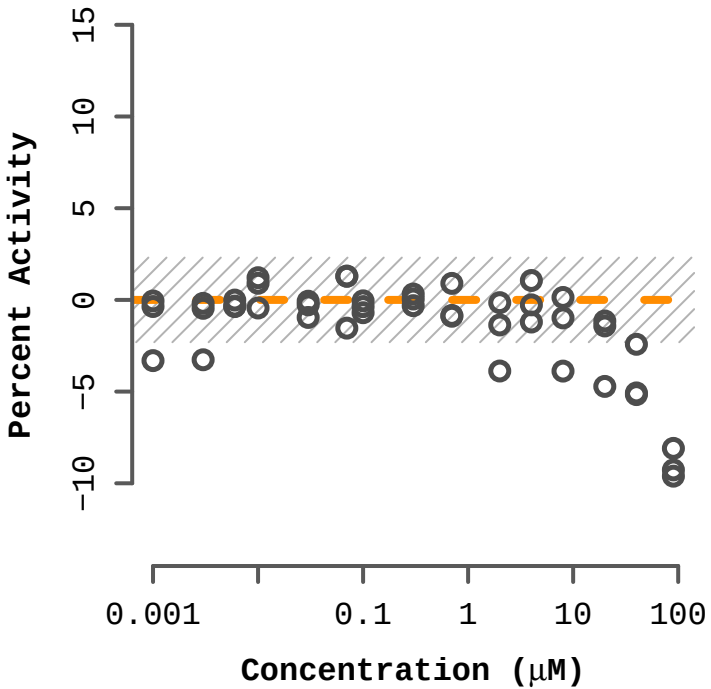
NAME: Triphenylethylene
CHID: 22320 **CASRN:** 58-72-0
SPID(S): Tox21_302425
M4ID: 12476708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

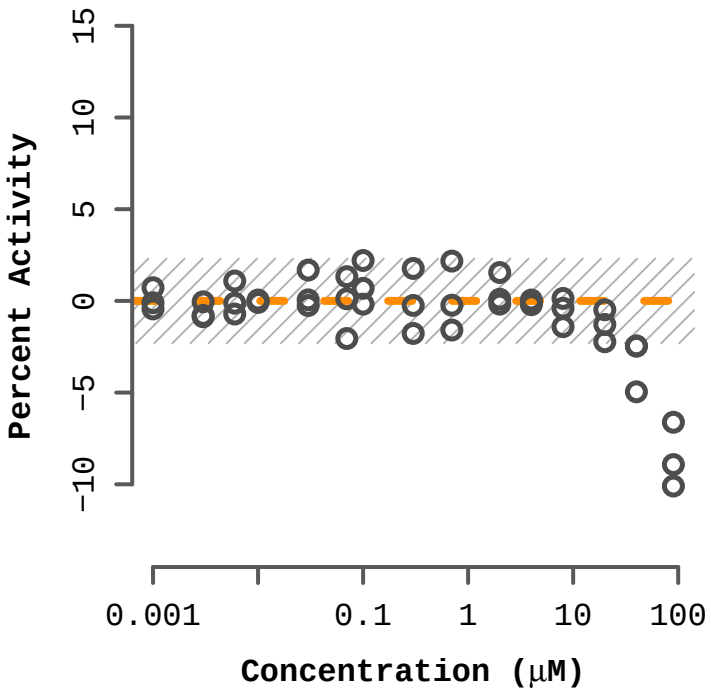
NAME: 2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane
CHID: 22325 **CASRN:** 2971-36-0
SPID(S): Tox21_300656
M4ID: 12478477

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.97	NA	NA

MAX_MEAN: 0.561 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

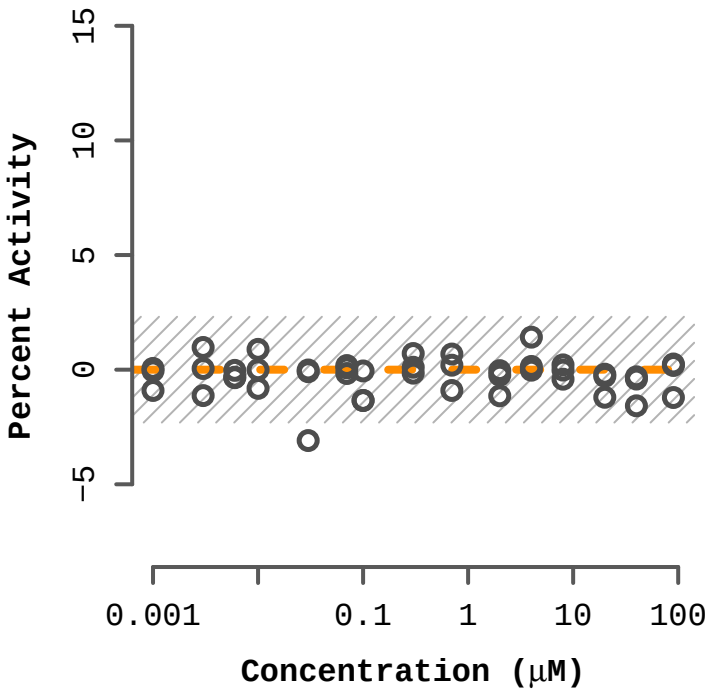
NAME: 2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane
CHID: 22325 **CASRN:** 2971-36-0
SPID(S): Tox21_201736
M4ID: 12480516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.86	NA	NA
PROB:	1	NA	NA
RMSE:	2.6	NA	NA

MAX_MEAN: 0.905 **MAX_MED:** 0.687 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

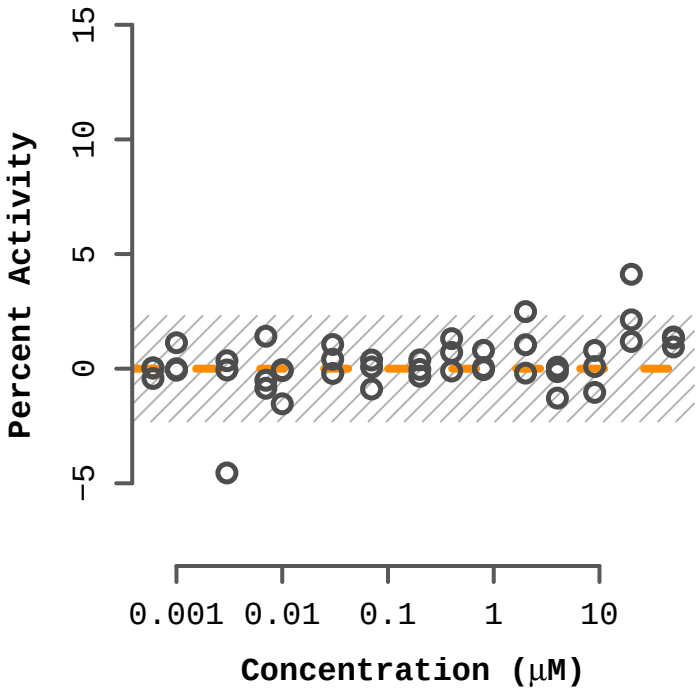
NAME: Rutin trihydrate
CHID: 22326 CASRN: 153-18-4
SPID(S): Tox21_202602
M4ID: 12479650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.514 **MAX_MED:** 0.197 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

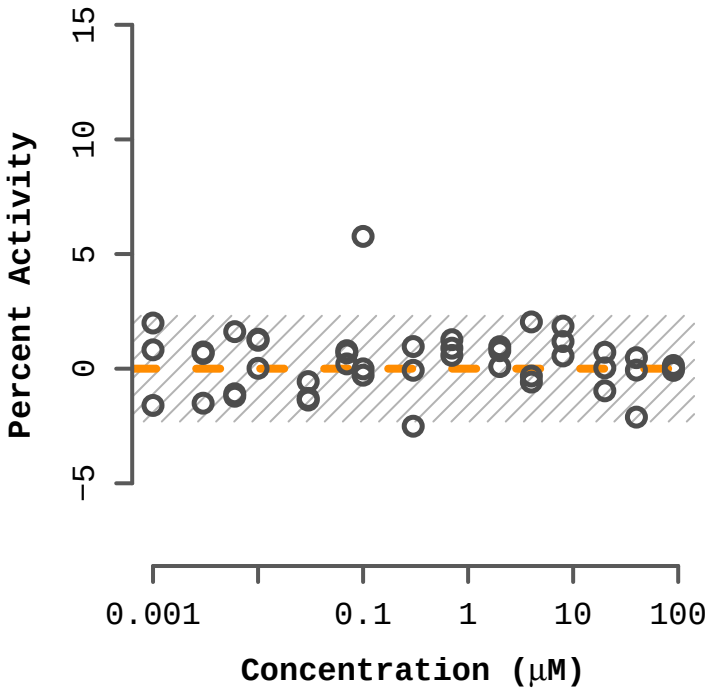
NAME: Rutin trihydrate
CHID: 22326 CASRN: 153-18-4
SPID(S): Tox21_111945_1
M4ID: 12483417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 2.48 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

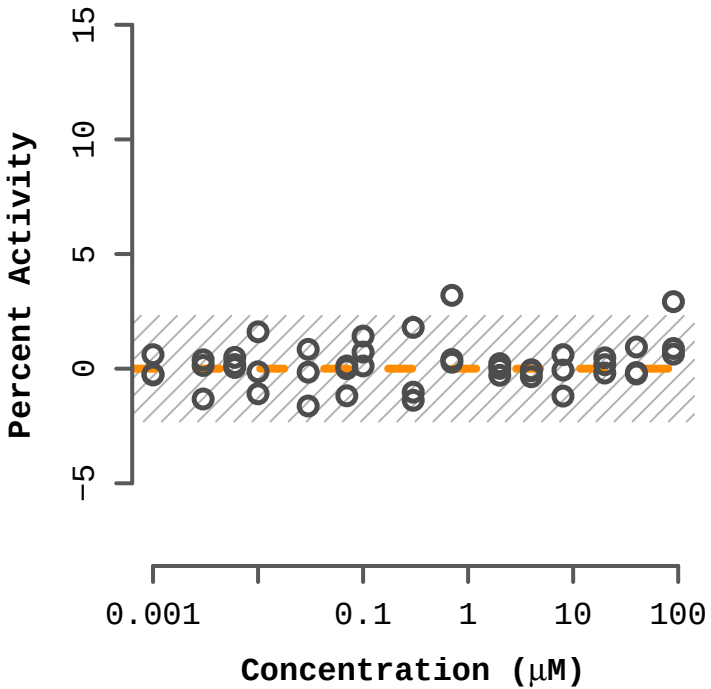
NAME: 2-(Butan-2-yl)phenol
CHID: 22331 CASRN: 89-72-5
SPID(S): Tox21_300047
M4ID: 12479083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.83 MAX_MED: 1.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

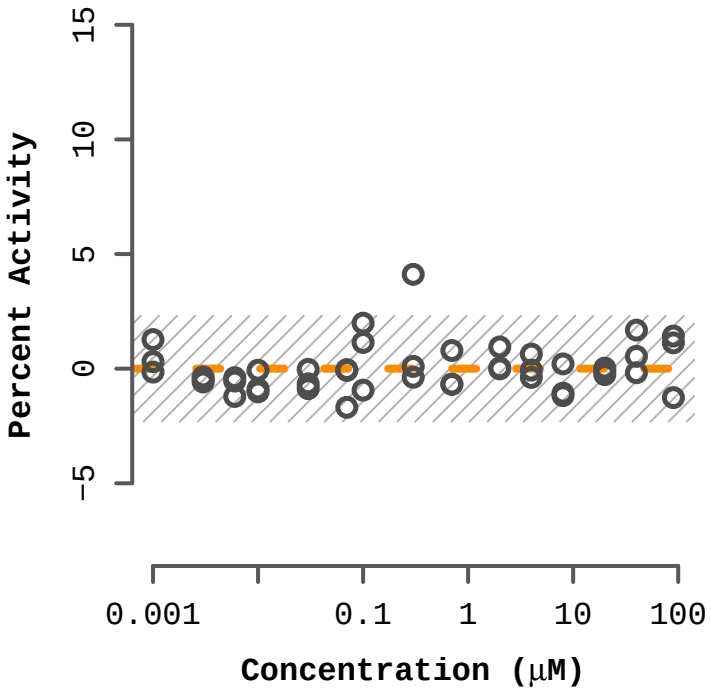
NAME: 2-(Butan-2-yl)phenol
CHID: 22331 CASRN: 89-72-5
SPID(S): Tox21_201372
M4ID: 12480880

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.48 MAX_MED: 0.883 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

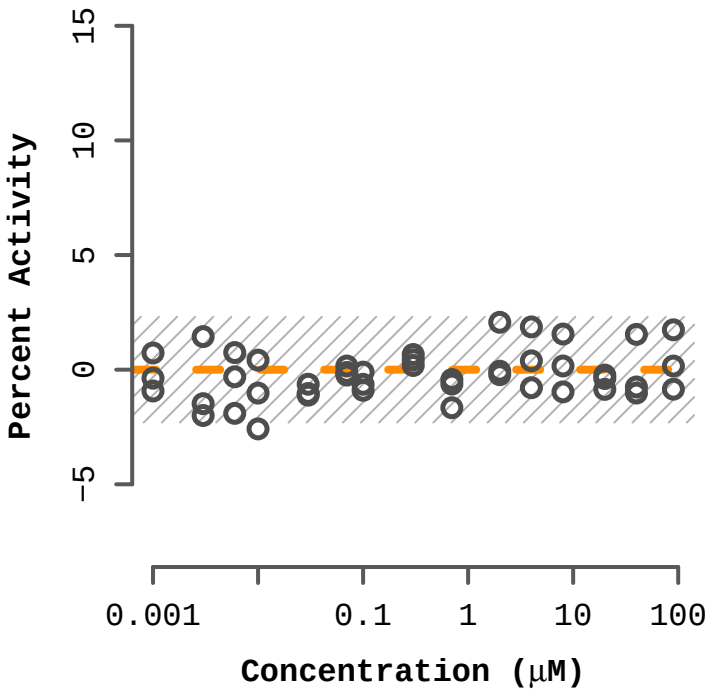
NAME: 4-(Butan-2-yl)phenol
CHID: 22332 **CASRN:** 99-71-8
SPID(S): Tox21_300086
M4ID: 12479044

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

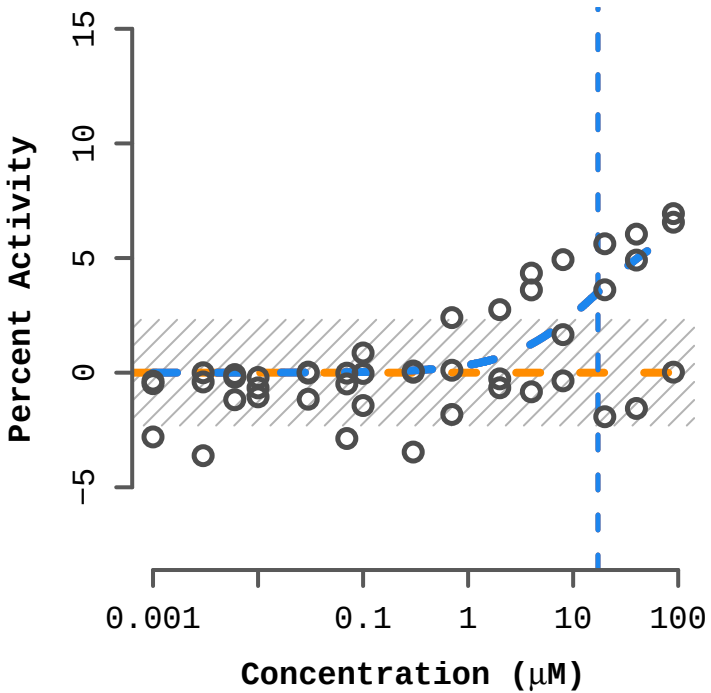
NAME: 4-(Butan-2-yl)phenol
CHID: 22332 **CASRN:** 99-71-8
SPID(S): Tox21_200416
M4ID: 12481836

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.436 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: sec-Butylbenzene
CHID: 22333 CASRN: 135-98-8
SPID(S): Tox21_303828
M4ID: 12475360

HILL MODEL (in red):

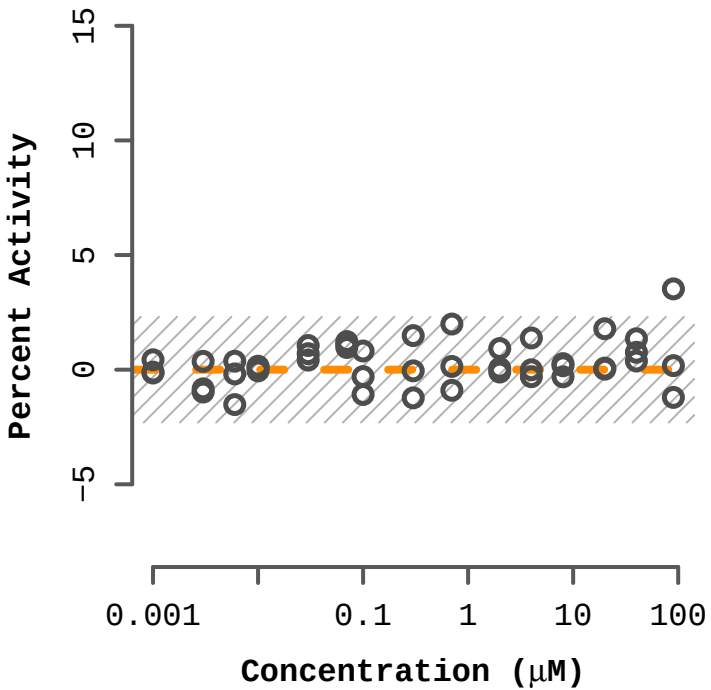
	tp	ga	gw
val:	7.01	1.24	1.05
sd:	3	0.511	0.533

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.01	1.24	1.05	3.3	5.46
sd:	3	0.511	0.533	1300	5290

	CNST	HILL	GNLS
AIC:	216.22	200.75	204.75
PROB:	0	0.88	0.12
RMSE:	2.7	2.19	2.19

MAX_MEAN: 4.51 MAX_MED: 6.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

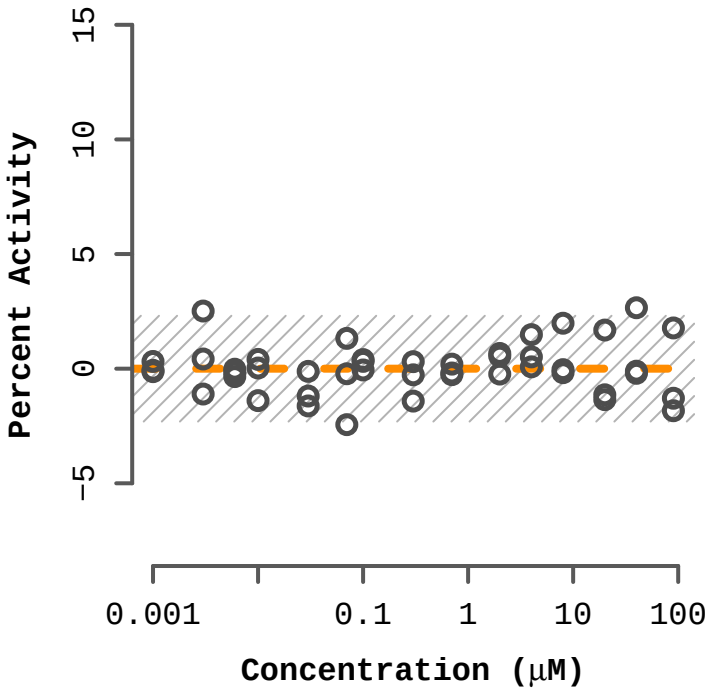
NAME: Prometon
CHID: 22341 **CASRN:** 1610-18-0
SPID(S): Tox21_300893
M4ID: 12478240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

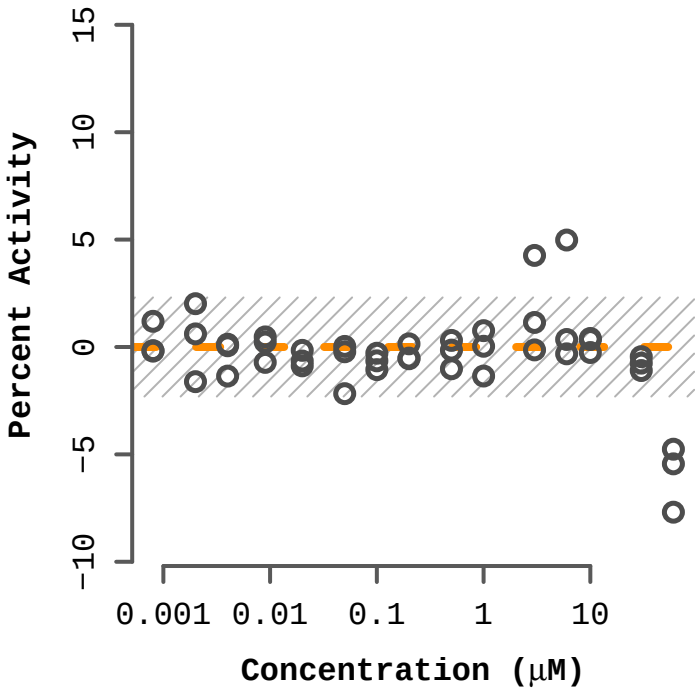
NAME: Prometon
CHID: 22341 **CASRN:** 1610-18-0
SPID(S): Tox21_202098
M4ID: 12480154

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.783 **MAX_MED:** 0.548 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

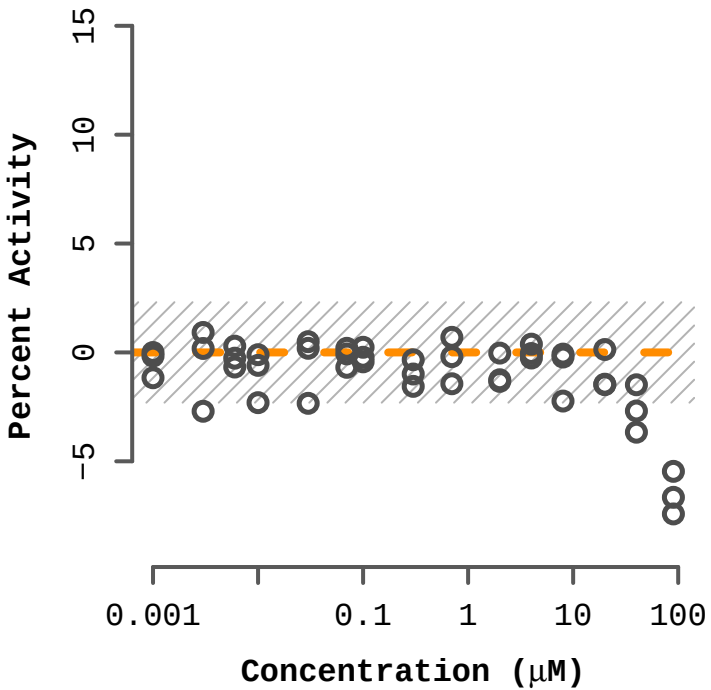
NAME: o,p'−DDT
CHID: 22345 **CASRN:** 789−02−6
SPID(S): Tox21_300622
M4ID: 12478511

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

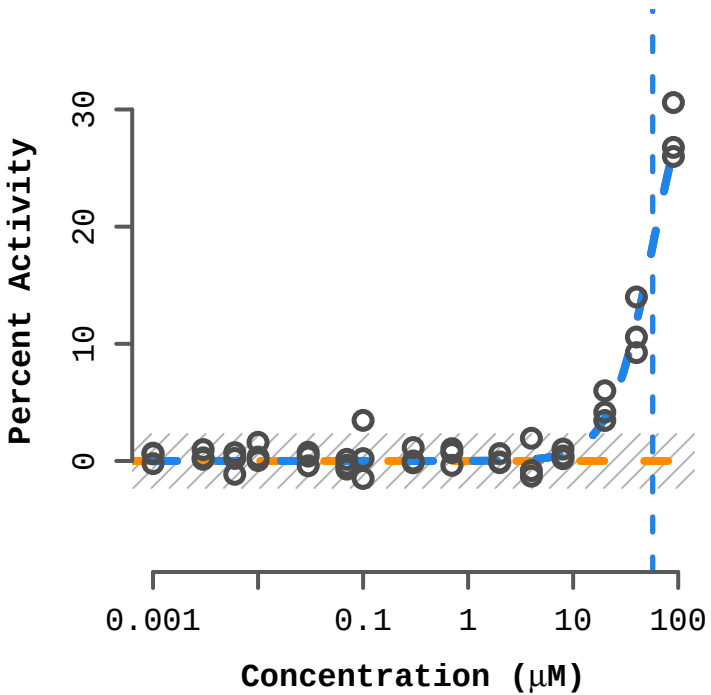
NAME: o,p'−DDT
CHID: 22345 CASRN: 789−02−6
SPID(S): Tox21_202239
M4ID: 12480013

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.88	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 0.026 MAX_MED: 0.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-4-phenylphenol
CHID: 22353 **CASRN:** 92-04-6
SPID(S): Tox21_301478
M4ID: 12477655

HILL MODEL (in red):

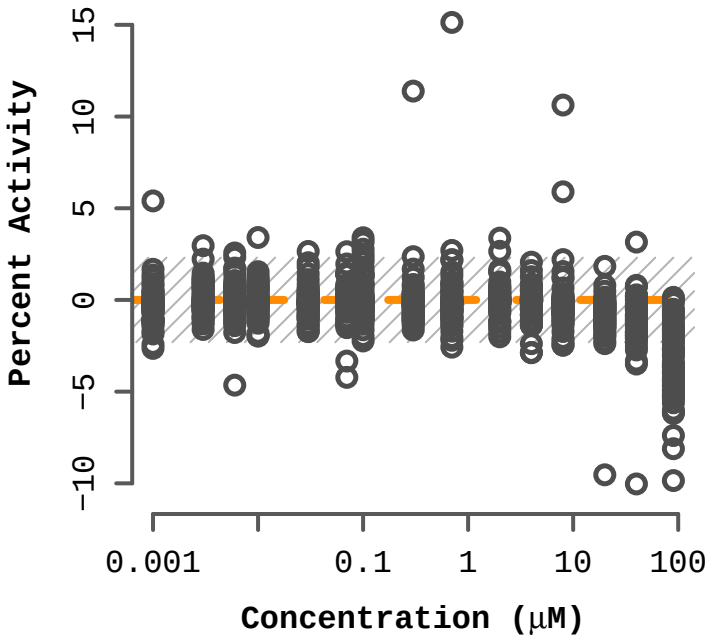
	tp	ga	gw
val:	36.7	1.76	2.1
sd:	6.86	0.111	0.324

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	36.7	1.76	2.1	3.73	9.82
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	264.99	146.83	150.83
PROB:	0	0.88	0.12
RMSE:	7.92	1.23	1.23

MAX_MEAN: 27.8 **MAX_MED:** 26.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

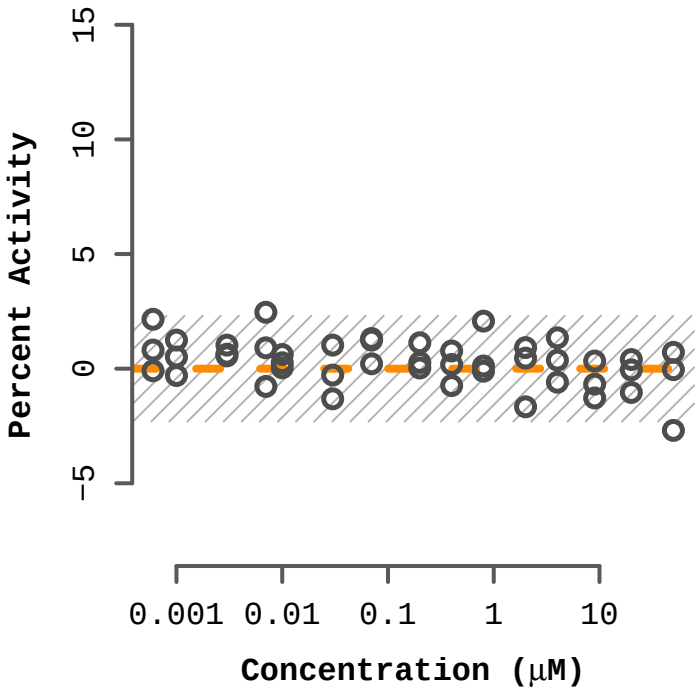
NAME: 4-(1,1,3,3-Tetramethylbutyl)phenol
CHID: 22360 **CASRN:** 140-66-9
SPID(S): Tox21_400011
M4ID: 12475126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2629.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 0.188 **MAX_MED:** −0.0251 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

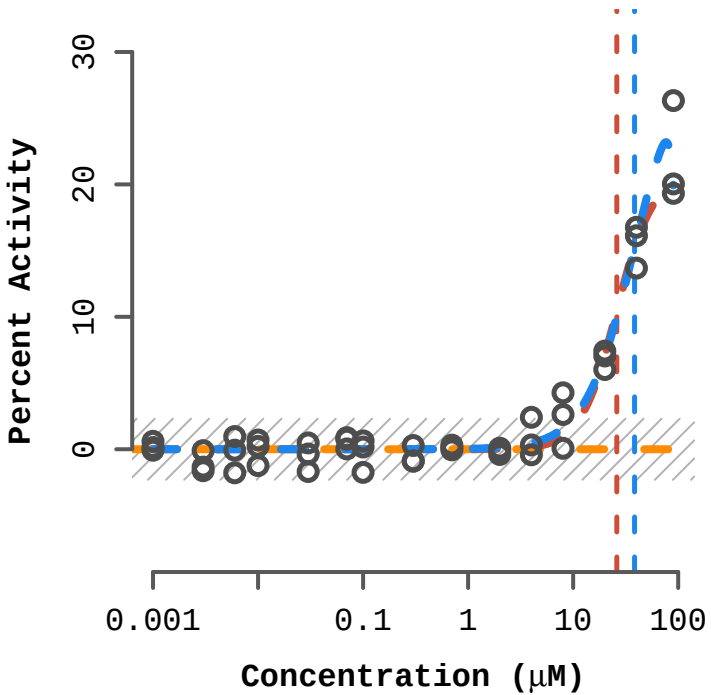
NAME: 4-(1,1,3,3-Tetramethylbutyl)phenol
CHID: 22360 **CASRN:** 140-66-9
SPID(S): Tox21_112084_1
M4ID: 12483331

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.96 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vinclozolin
CHID: 22361 CASRN: 50471-44-8
SPID(S): Tox21_301101
M4ID: 12478032

HILL MODEL (in red):

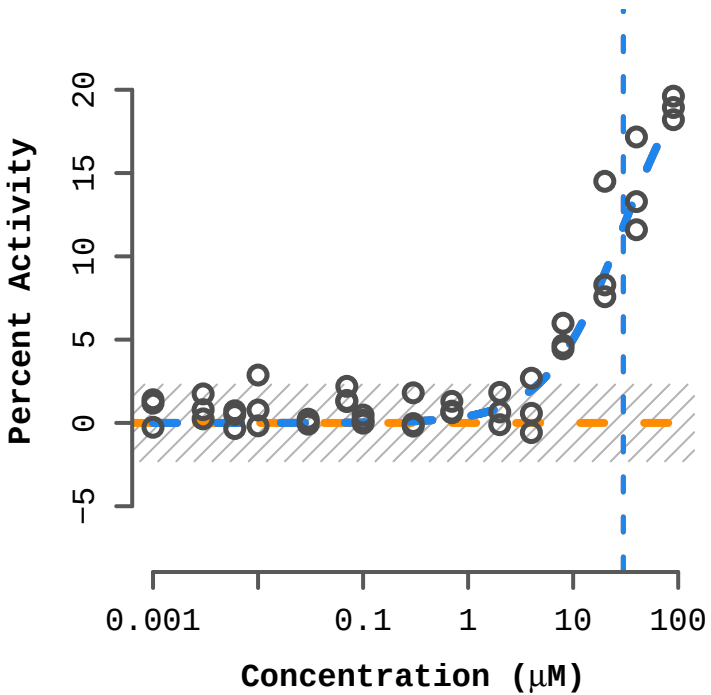
	tp	ga	gw
val:	20.9	1.42	2.54
sd:	1.05	0.03	0.464

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	30.6	1.58	1.85	2	13.4
sd:	11.9	0.183	0.426	0.00679	10.1

	CNST	HILL	GNLS
AIC:	277.78	149.96	152.09
PROB:	0	0.74	0.26
RMSE:	7.29	1.39	1.37

MAX_MEAN: 21.9 MAX_MED: 20 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vinclozolin
CHID: 22361 CASRN: 50471-44-8
SPID(S): Tox21_202160
M4ID: 12480092

HILL MODEL (in red):

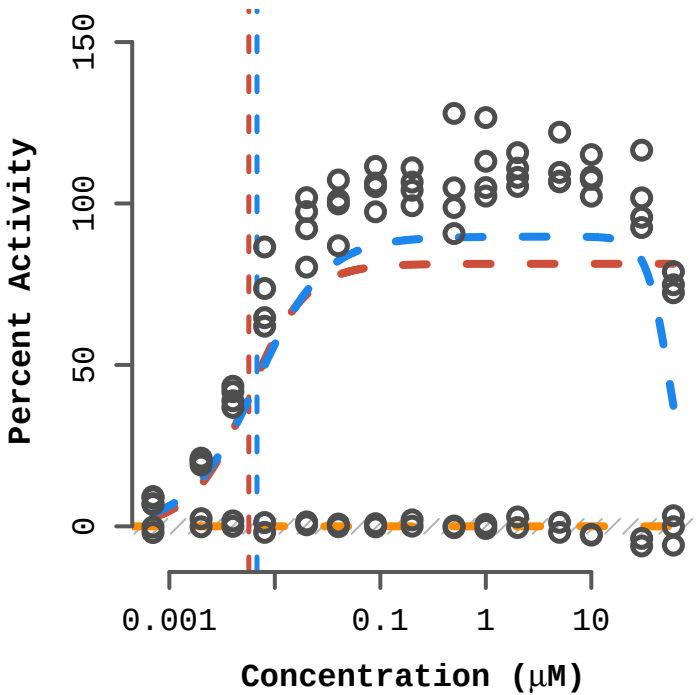
	tp	ga	gw
val:	23.5	1.48	1.18
sd:	2.73	0.118	0.17

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.5	1.48	1.18	3.85	4.65
sd:	2.73	0.118	0.17	1640	4020

	CNST	HILL	GNLS
AIC:	285.8	162.61	166.61
PROB:	0	0.88	0.12
RMSE:	6.89	1.46	1.46

MAX_MEAN: 18.9 MAX_MED: 18.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5alpha-Dihydrotestosterone
CHID: 22364 CASRN: 521-18-6
SPID(S): Tox21_303655
M4ID: 12475493

HILL MODEL (in red):

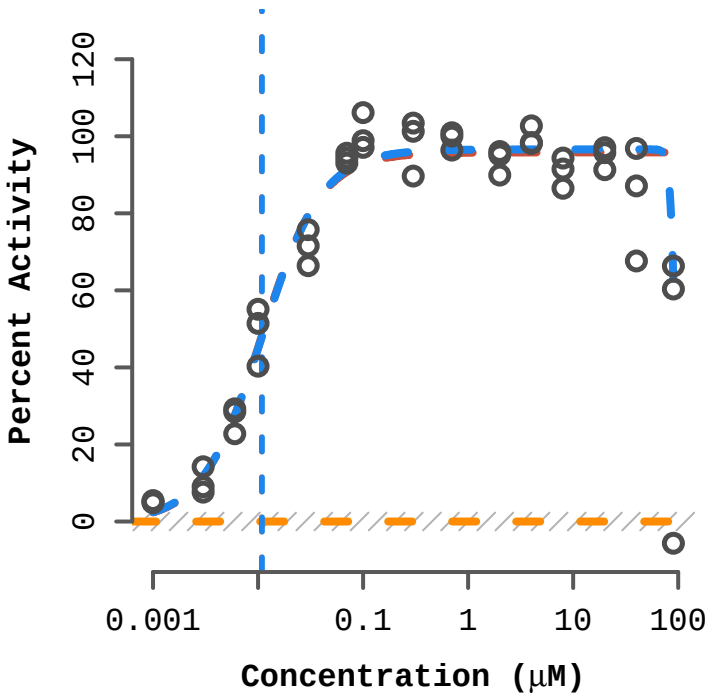
	tp	ga	gw
val:	81.3	-2.25	1.6
sd:	7.11	0.158	0.84

GAIN-LOSS MODEL (in blue):

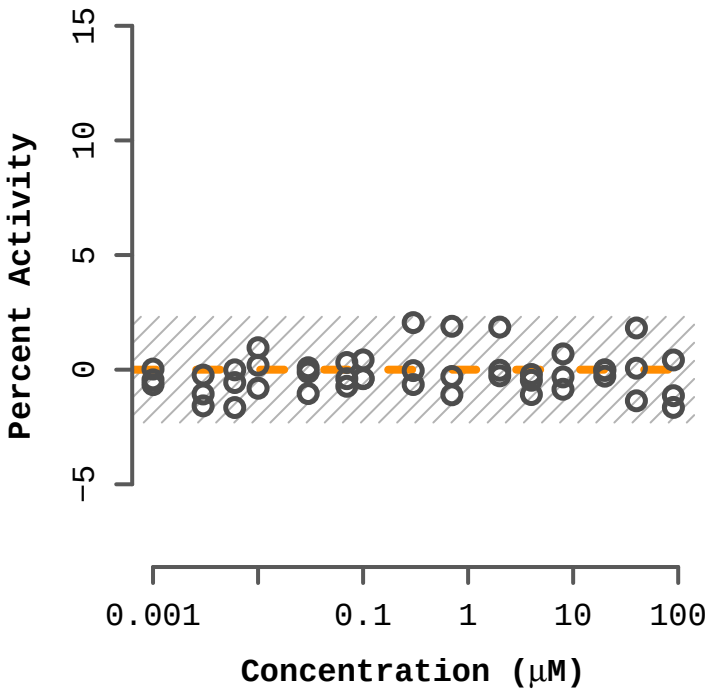
	tp	ga	gw	la	lw
val:	89.7	-2.17	1.35	1.74	3.98
sd:	7.84	0.168	0.631	0.0979	4.29

	CNST	HILL	GNLS
AIC:	1042.76	956.34	954.16
PROB:	0	0.25	0.75
RMSE:	73.92	45.72	45.49

MAX_MEAN: 74.5 MAX_MED: 107 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    5alpha-Dihydrotestosterone
CHID:    22364   CASRN: 521-18-6
SPID(S): Tox21_200987
M4ID:    12481265

HILL MODEL (in red):
      tp       ga       gw
val:  95.8     -1.97    1.54
sd:   1.47     0.0389   0.162

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  96.6     -1.96    1.52     1.97     18
sd:   1.27     0.0357   0.14     0.00614  5.54

      CNST        HILL        GNLS
AIC:  531.31      344.18      322.67
PROB: 0           0           1
RMSE: 78.65       17.92       12.21

MAX_MEAN: 101       MAX_MED: 101       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

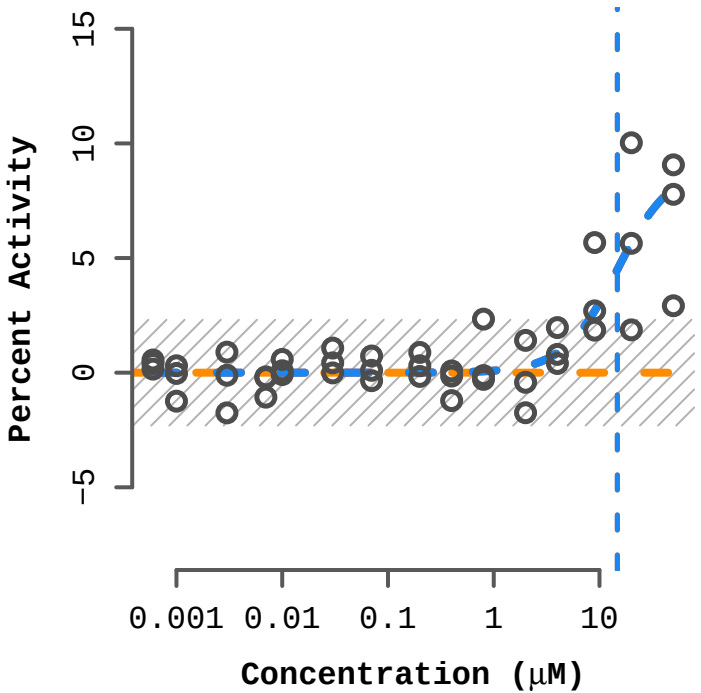
NAME: Estriol
CHID: 22366 **CASRN:** 50-27-1
SPID(S): Tox21_301604
M4ID: 12477529

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.522 **MAX_MED:** 0.194 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estriol
CHID: 22366 **CASRN:** 50-27-1
SPID(S): Tox21_112320_1
M4ID: 12483165

HILL MODEL (in red):

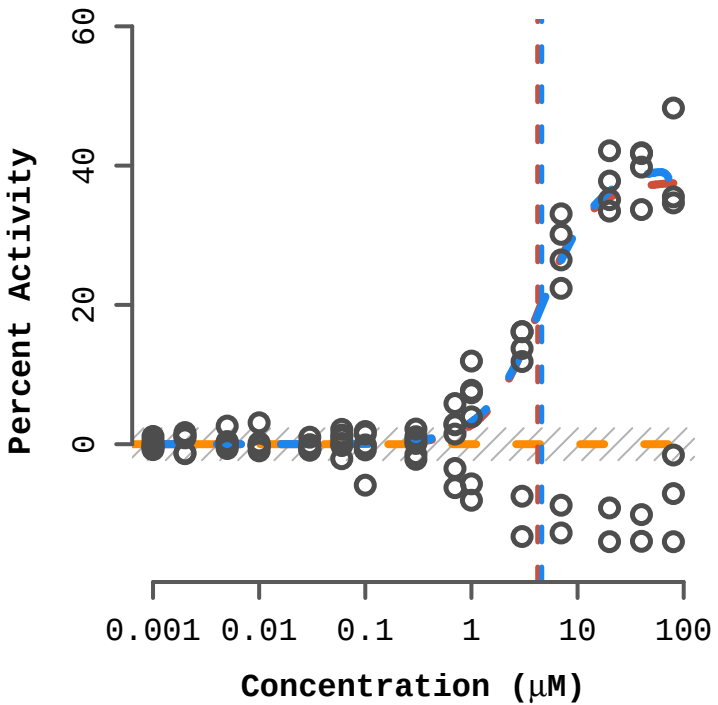
	tp	ga	gw
val:	9	1.17	1.72
sd:	1.62	0.147	0.545

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9	1.17	1.72	2.91	5.65
sd:	1.62	0.147	0.545	899	4220

	CNST	HILL	GNLS
AIC:	198.6	153.57	157.57
PROB:	0	0.88	0.12
RMSE:	2.82	1.45	1.45

MAX_MEAN: 6.59 **MAX_MED:** 7.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estrone
CHID: 22367 CASRN: 53-16-7
SPID(S): Tox21_303651
M4ID: 12475497

HILL MODEL (in red):

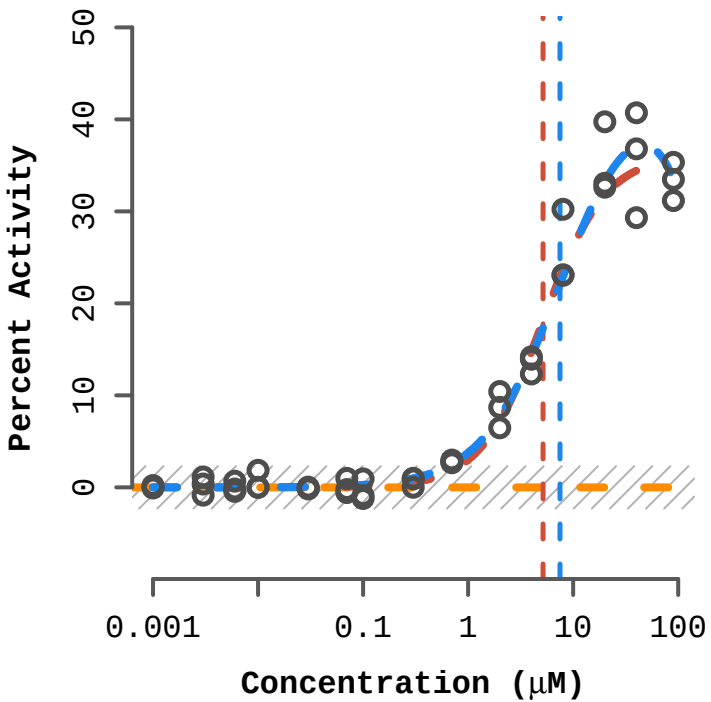
	tp	ga	gw
val:	37.7	0.625	1.77
sd:	1.97	0.0588	0.362

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	39.8	0.663	1.6	1.96	15
sd:	2.68	0.0721	0.329	0.0354	10.3

	CNST	HILL	GNLS
AIC:	727.23	662.07	664.29
PROB:	0	0.75	0.25
RMSE:	15.81	14.99	14.88

MAX_MEAN: 22.2 MAX_MED: 36.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estrone
CHID: 22367 CASRN: 53-16-7
SPID(S): Tox21_201375
M4ID: 12480877

HILL MODEL (in red):

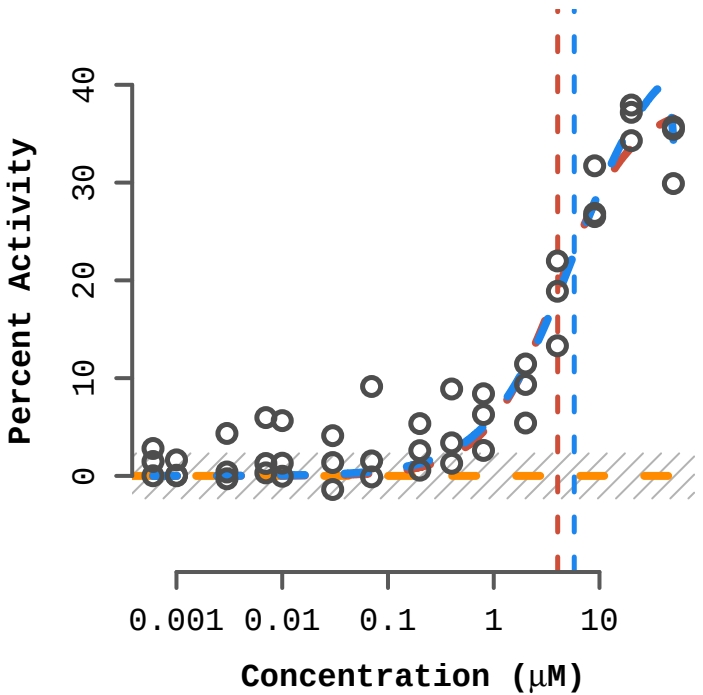
	tp	ga	gw
val:	36.2	0.713	1.46
sd:	1.16	0.0304	0.124

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	44.2	0.874	1.18	2.24	2.09
sd:	4.42	0.0799	0.0989	0.0773	1.03

	CNST	HILL	GNLS
AIC:	382.1	193.6	179.96
PROB:	0	0	1
RMSE:	17.47	2.31	2.14

MAX_MEAN: 35.6 MAX_MED: 36.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estrone
CHID: 22367 CASRN: 53-16-7
SPID(S): Tox21_113567_1
M4ID: 12482607

HILL MODEL (in red):

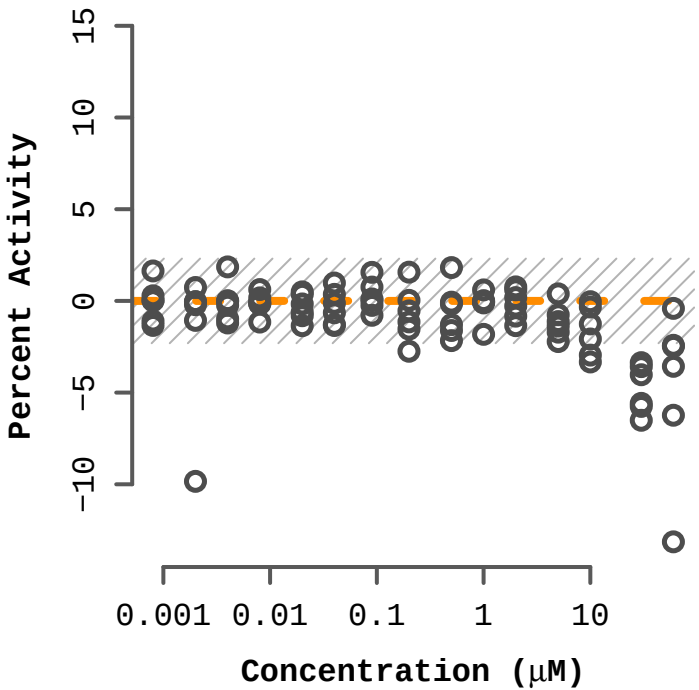
	tp	ga	gw
val:	38.2	0.605	1.24
sd:	2.21	0.0647	0.211

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	45.5	0.761	1.05	1.75	12.8
sd:	5.66	0.129	0.172	0.0237	5.86

	CNST	HILL	GNLS
AIC:	373.13	240.72	237.01
PROB:	0	0.13	0.87
RMSE:	16.04	3.24	2.99

MAX_MEAN: 36.5 MAX_MED: 37.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

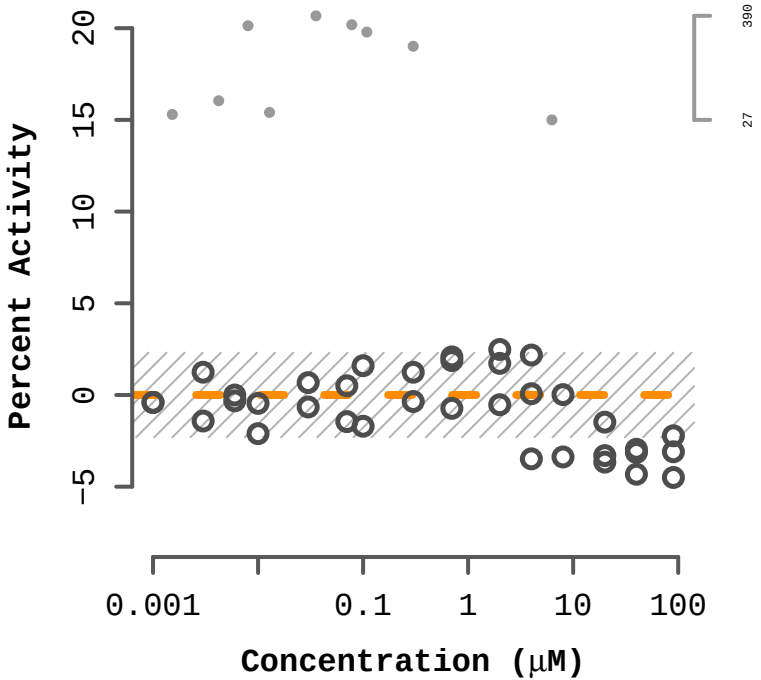
NAME: Fulvestrant
CHID: 22369 **CASRN:** 129453-61-8
SPID(S): Tox21_303656
M4ID: 12475492

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	378.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.53	NA	NA

MAX_MEAN: 0.236 **MAX_MED:** 0.0629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

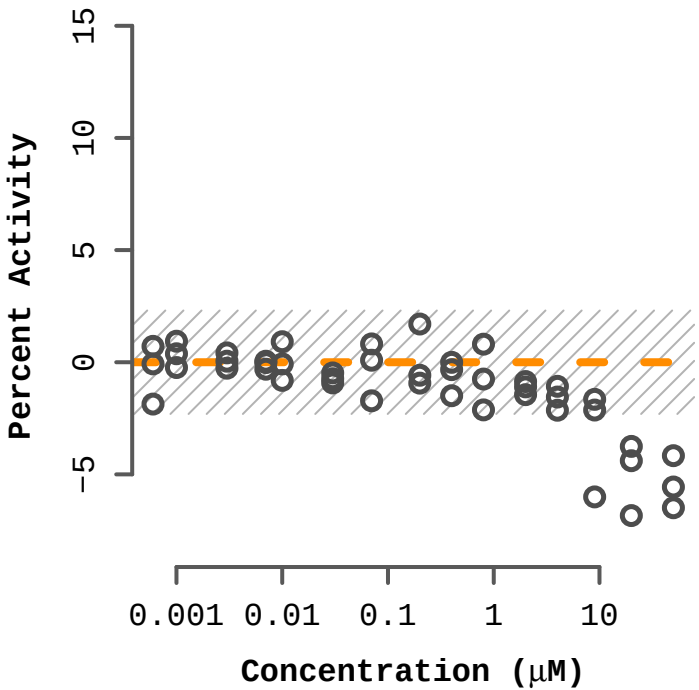
NAME: Fulvestrant
CHID: 22369 **CASRN:** 129453-61-8
SPID(S): Tox21_202604
M4ID: 12479648 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	482.4	NA	NA
PROB:	1	NA	NA
RMSE:	117.83	NA	NA

MAX_MEAN: 131 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

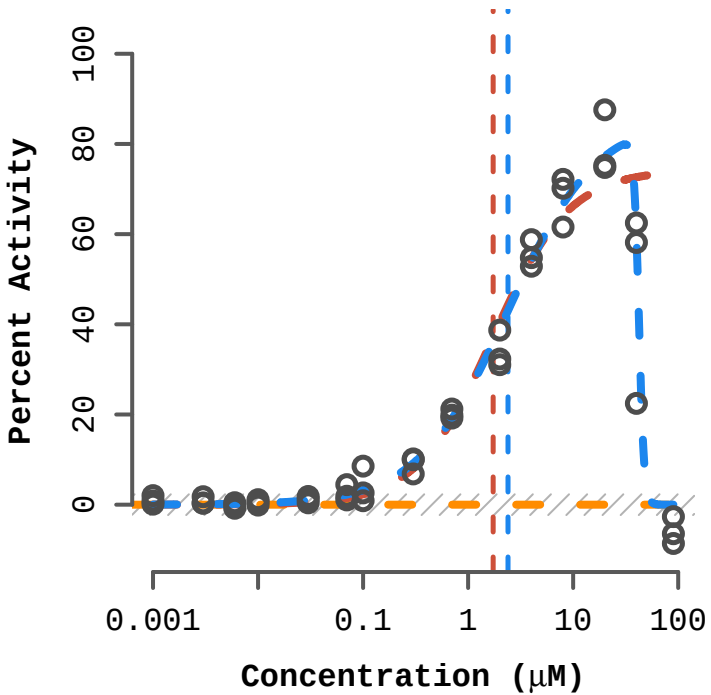
NAME: Fulvestrant
CHID: 22369 **CASRN:** 129453-61-8
SPID(S): Tox21_110939_1
M4ID: 12483999

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.36	NA	NA

MAX_MEAN: 0.361 **MAX_MED:** 0.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Progesterone
CHID: 22370 CASRN: 57-83-0
SPID(S): Tox21_300307
M4ID: 12478823

HILL MODEL (in red):

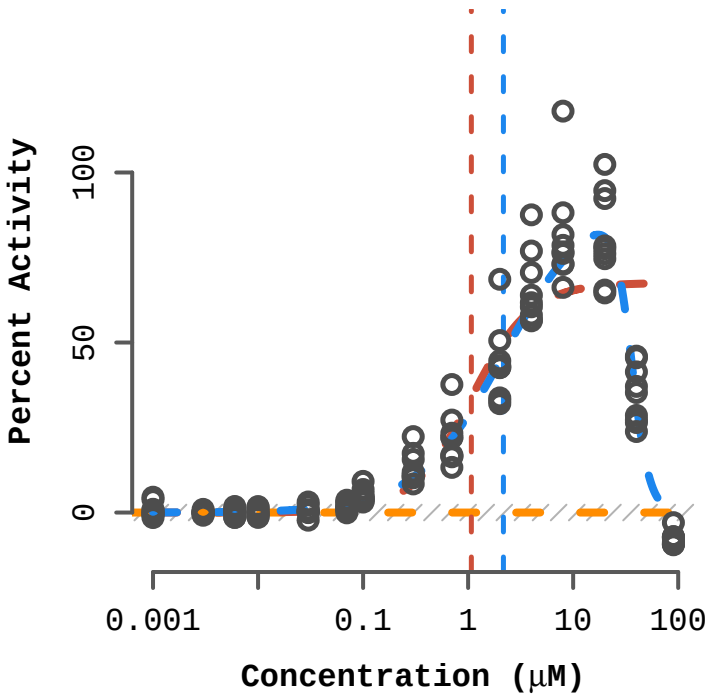
	tp	ga	gw
val:	74.3	0.238	1.2
sd:	5.9	0.0828	0.148

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	86	0.38	1.02	1.63	18
sd:	4.28	0.0589	0.0723	0.00458	3.44

	CNST	HILL	GNLS
AIC:	445.27	352.3	262.9
PROB:	0	0	1
RMSE:	35	22.37	6.51

MAX_MEAN: 79.2 MAX_MED: 75.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Progesterone
CHID: 22370 CASRN: 57-83-0
SPID(S): Tox21_201792
M4ID: 12480460

HILL MODEL (in red):

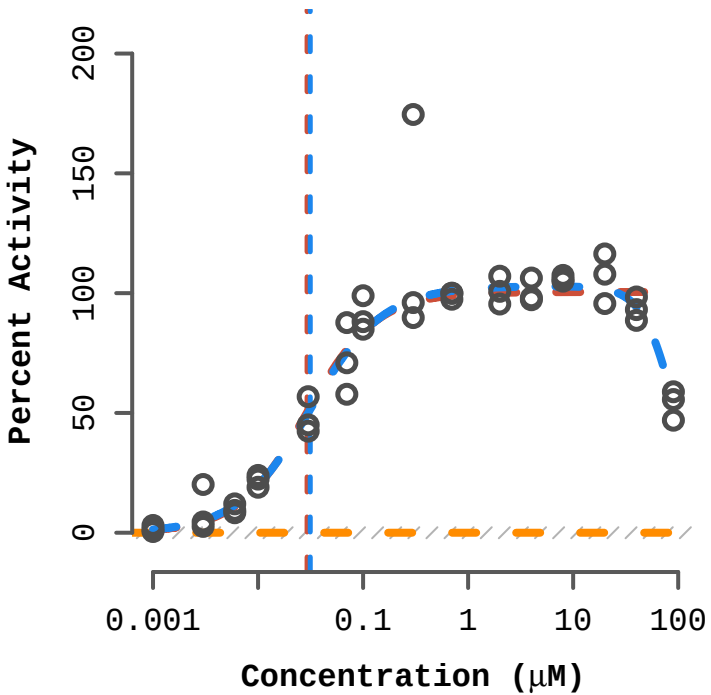
	tp	ga	gw
val:	67.5	0.0306	1.52
sd:	4.13	0.0653	0.203

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	92.9	0.336	1.05	1.56	5.26
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	1352.62	1154.21	890.56
PROB:	0	0	1
RMSE:	38.28	23.09	7.65

MAX_MEAN: 81.3 MAX_MED: 77.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Testosterone
CHID: 22371 CASRN: 58-22-0
SPID(S): Tox21_200689
M4ID: 12481563

HILL MODEL (in red):

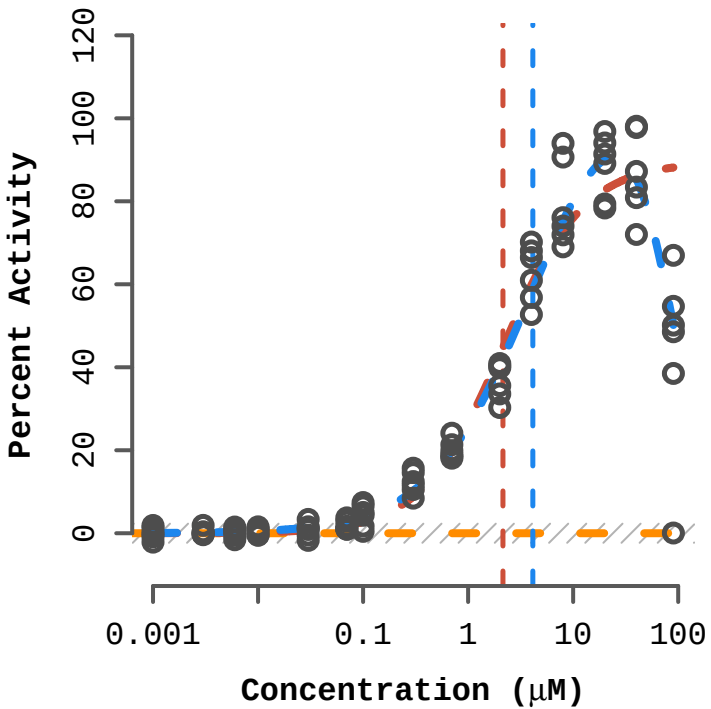
	tp	ga	gw
val:	100	-1.53	1.32
sd:	1.94	0.0476	0.14

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	103	-1.5	1.25	1.97	2.81
sd:	1.69	0.0417	0.106	0.0229	0.537

	CNST	HILL	GNLS
AIC:	531.8	362.99	323.79
PROB:	0	0	1
RMSE:	80.49	18.1	13.16

MAX_MEAN: 120 MAX_MED: 108 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Estradiol
CHID: 22377 **CASRN:** 57-91-0
SPID(S): Tox21_303644
M4ID: 12475502

HILL MODEL (in red):

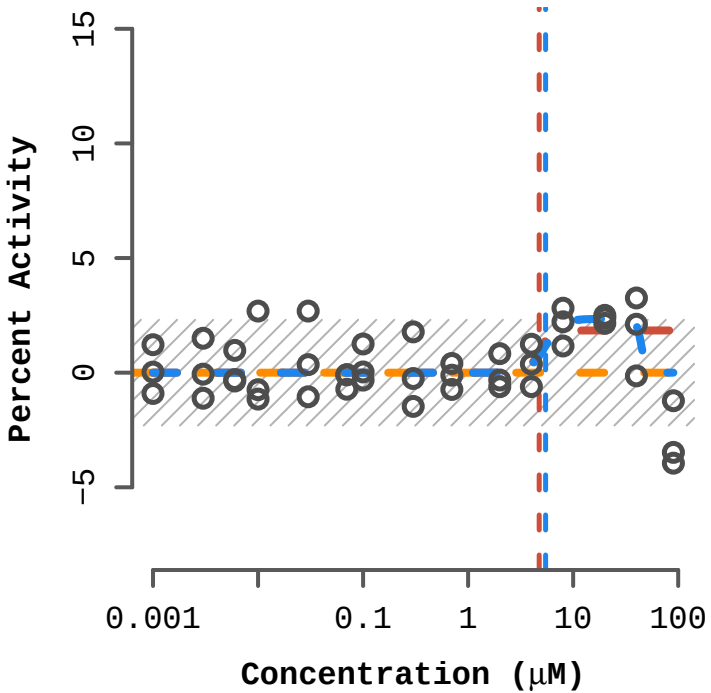
	tp	ga	gw
val:	89.5	0.331	1.12
sd:	3.23	0.0448	0.0832

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	118	0.616	0.898	1.92	2.1
sd:	10.8	0.0974	0.0601	0.0344	0.362

	CNST	HILL	GNLS
AIC:	938.79	640.96	564.9
PROB:	0	0	1
RMSE:	44.73	13.91	7.56

MAX_MEAN: 88.2 **MAX_MED:** 90.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Estradiol
CHID: 22377 CASRN: 57-91-0
SPID(S): Tox21_201262
M4ID: 12480990

HILL MODEL (in red):

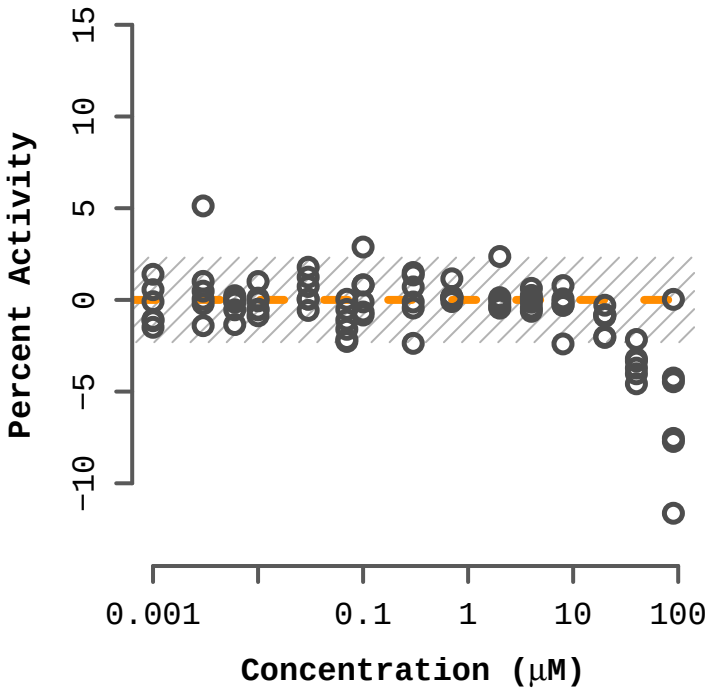
	tp	ga	gw
val:	1.84	0.676	8
sd:	0.404	0.125	10.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.35	0.738	5.66	1.65	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	171.35	165.23	156.48
PROB:	0	0.01	0.99
RMSE:	1.57	1.6	1.27

MAX_MEAN: 2.35 MAX_MED: 2.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

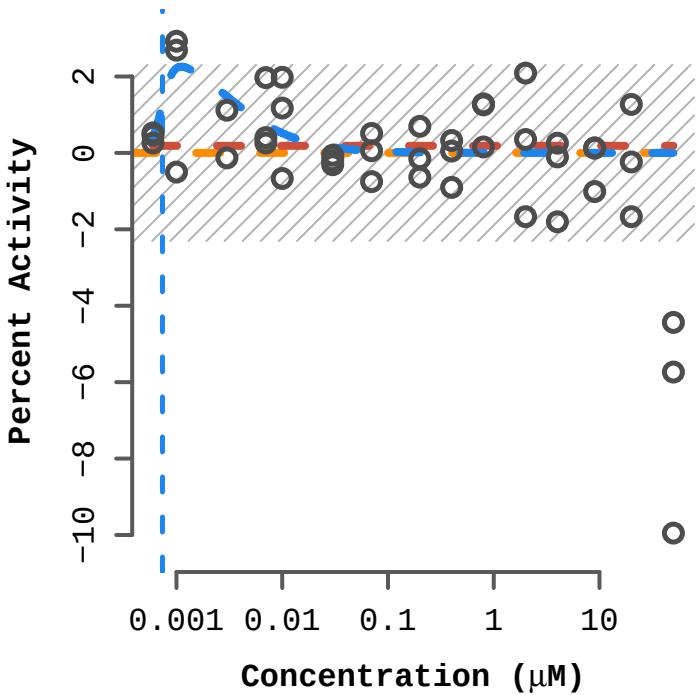
NAME: meso-Hexestrol
CHID: 22381 **CASRN:** 84-16-2
SPID(S): Tox21_301456
M4ID: 12477677

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	363.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 0.841 **MAX_MED:** 0.389 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: meso-Hexestrol
CHID: 22381 **CASRN:** 84-16-2
SPID(S): Tox21_110377_1
M4ID: 12484411

HILL MODEL (in red):

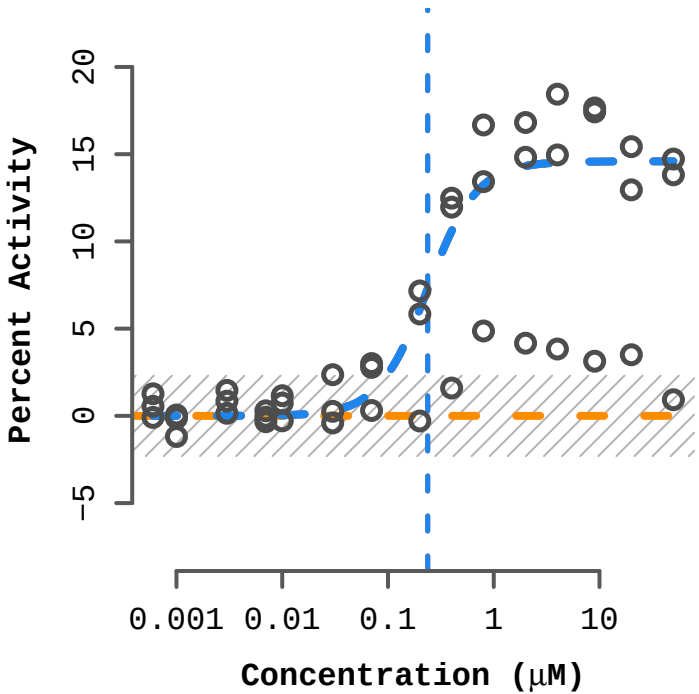
	tp	ga	gw
val:	0.185	−4.4	5.82
sd:	0.192	1520	7330

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.04	−3.13	8	−2.54	1.27
sd:	6.21	0.251	15.8	1.55	1.63

	CNST	HILL	GNLS
AIC:	177.29	182.37	177.56
PROB:	0.51	0.04	0.45
RMSE:	2.19	2.2	2.08

MAX_MEAN: 1.7 **MAX_MED:** 2.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dienestrol
CHID: 22382 CASRN: 84-17-3
SPID(S): Tox21_110378_1
M4ID: 12484410

HILL MODEL (in red):

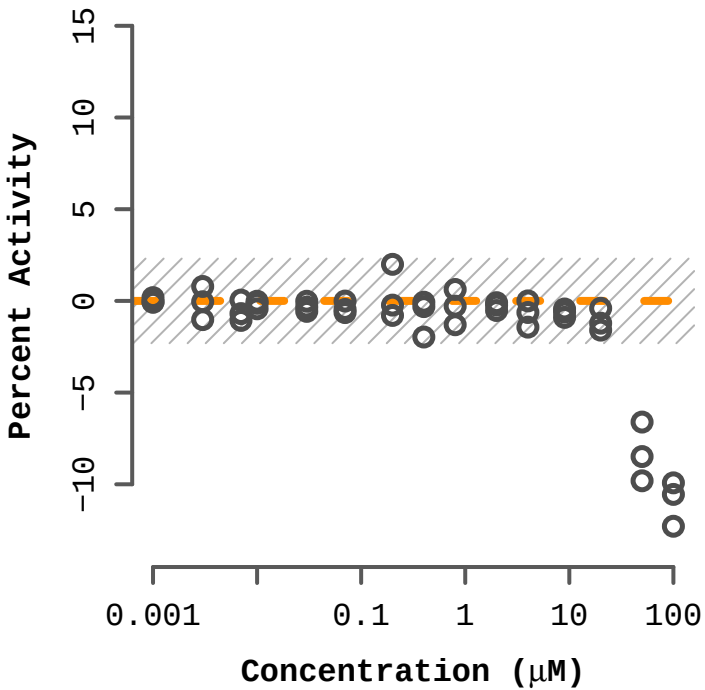
	tp	ga	gw
val:	14.6	−0.624	1.87
sd:	0.925	0.0889	0.71

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.6	−0.624	1.87	3.36	6.58
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	323.95	257.15	261.15
PROB:	0	0.88	0.12
RMSE:	8.76	4.55	4.55

MAX_MEAN: 12.7 MAX_MED: 17.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

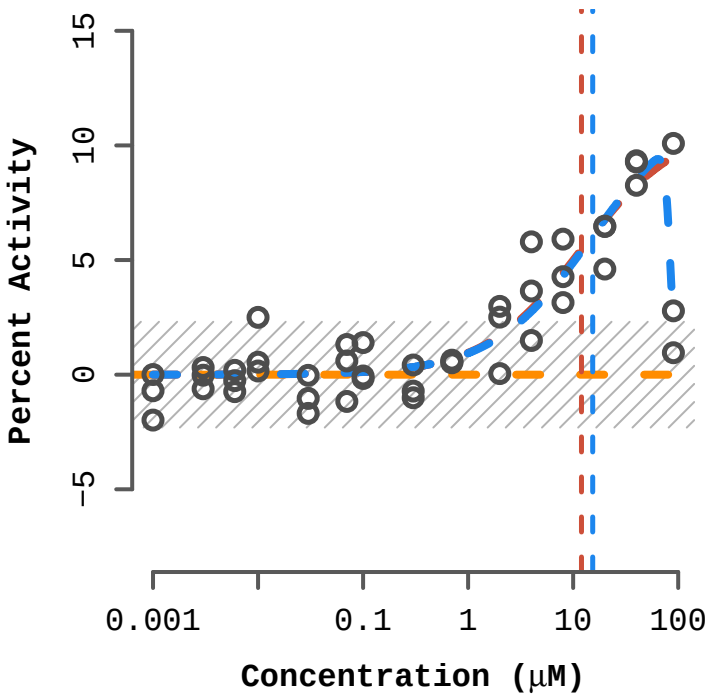
NAME: (Z)−4−Hydroxytamoxifen
CHID: 22384 **CASRN:** 68047−06−3
SPID(S): Tox21_200943
M4ID: 12481309

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.41	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 0.326 **MAX_MED:** −0.0413 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Apigenin
CHID: 22391 CASRN: 520-36-5
SPID(S): Tox21_302884
M4ID: 12476249

HILL MODEL (in red):

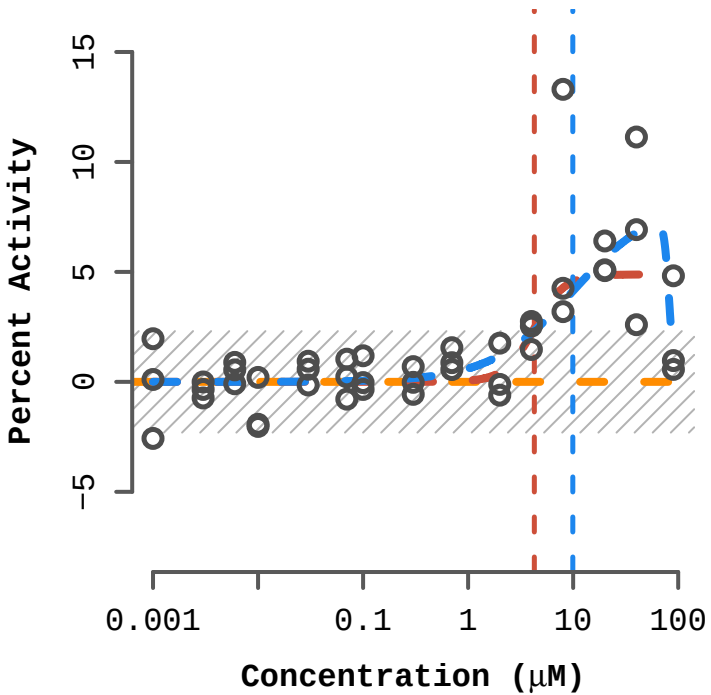
	tp	ga	gw
val:	10.9	1.08	0.945
sd:	2.11	0.235	0.213

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.1	1.19	0.908	1.92	16.9
sd:	3.43	0.32	0.203	0.0158	8.55

	CNST	HILL	GNLS
AIC:	239.61	170.8	162.5
PROB:	0	0.02	0.98
RMSE:	3.68	1.94	1.59

MAX_MEAN: 8.96 MAX_MED: 9.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Apigenin
CHID: 22391 **CASRN:** 520-36-5
SPID(S): Tox21_201542
M4ID: 12480710

HILL MODEL (in red):

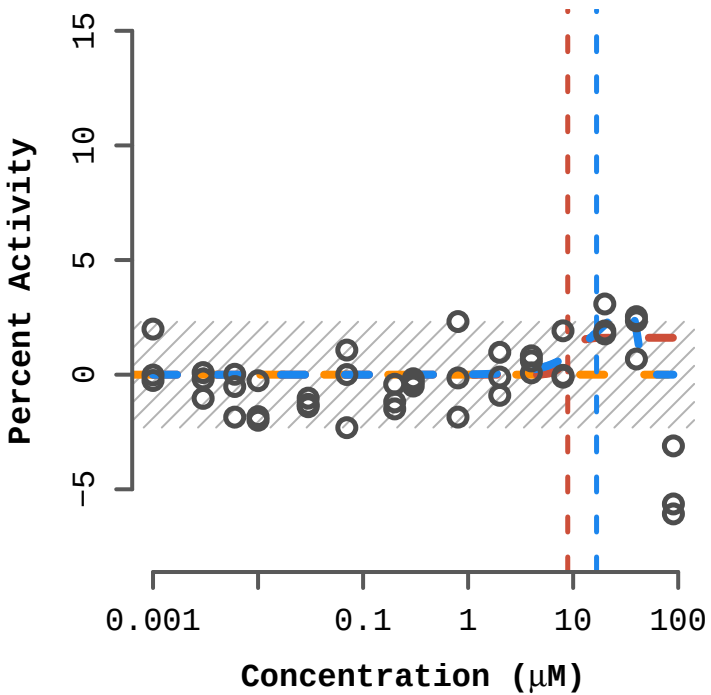
	tp	ga	gw
val:	4.88	0.63	3.1
sd:	0.628	0.0855	1.91

GAIN-LOSS MODEL (in blue):

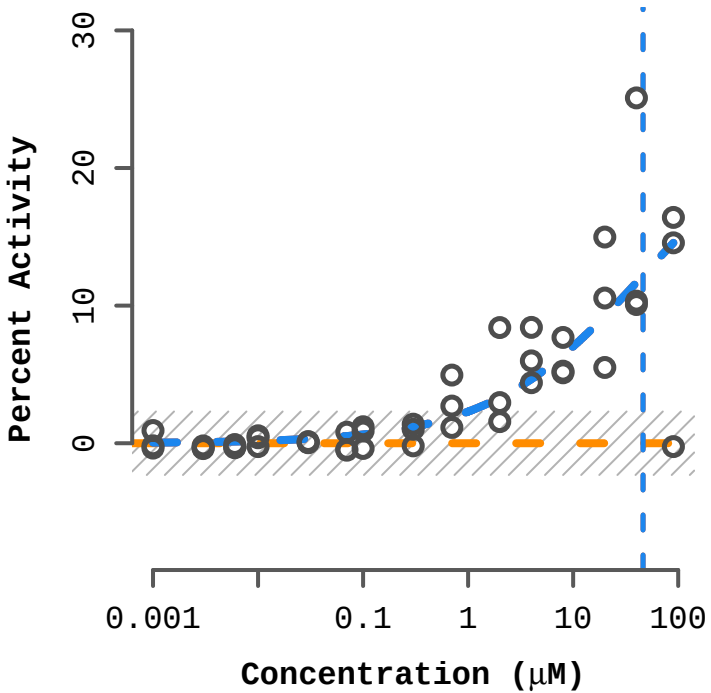
	tp	ga	gw	la	lw
val:	8.24	0.997	1.1	1.91	17.5
sd:	3.72	0.441	0.602	0.0259	11

	CNST	HILL	GNLS
AIC:	225.16	181.99	174.41
PROB:	0	0.02	0.98
RMSE:	3.49	2.11	1.99

MAX_MEAN: 6.92 **MAX_MED:** 6.92 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phloretin
CHID:    22393   CASRN: 60-82-2
SPID(S): Tox21_202854
M4ID:    12479398

HILL MODEL (in red):
      tp       ga       gw
val:  1.61     0.948    8
sd:   0.529    0.174    29.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.7      1.22     1.99     1.61     16.8
sd:   7.11     0.9      2.38     0.0568   79.6

      CNST        HILL        GNLS
AIC:  179.86      179.7       174.72
PROB: 0.07        0.07        0.86
RMSE: 1.85        2.02        1.68

MAX_MEAN: 2.26      MAX_MED: 2.35      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Biochanin A
CHID: 22394 CASRN: 491-80-5
SPID(S): Tox21_302901
M4ID: 12476232

HILL MODEL (in red):

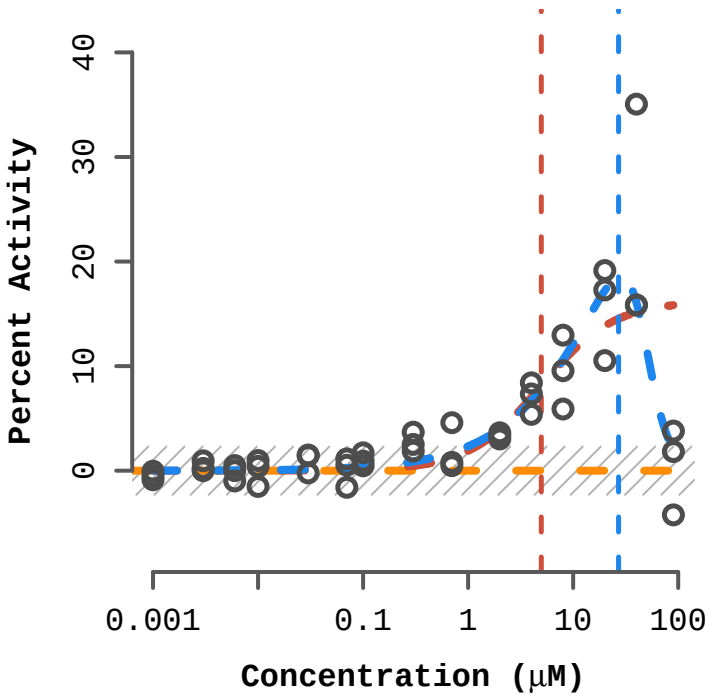
	tp	ga	gw
val:	24.4	1.67	0.59
sd:	10.8	0.678	0.132

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.4	1.67	0.59	3.4	5.8
sd:	10.8	0.678	0.132	1250	5030

	CNST	HILL	GNLS
AIC:	288.2	204.81	208.81
PROB:	0	0.88	0.12
RMSE:	6.75	3.41	3.41

MAX_MEAN: 15.2 MAX_MED: 14.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Biochanin A
CHID: 22394 CASRN: 491-80-5
SPID(S): Tox21_202097
M4ID: 12480155

HILL MODEL (in red):

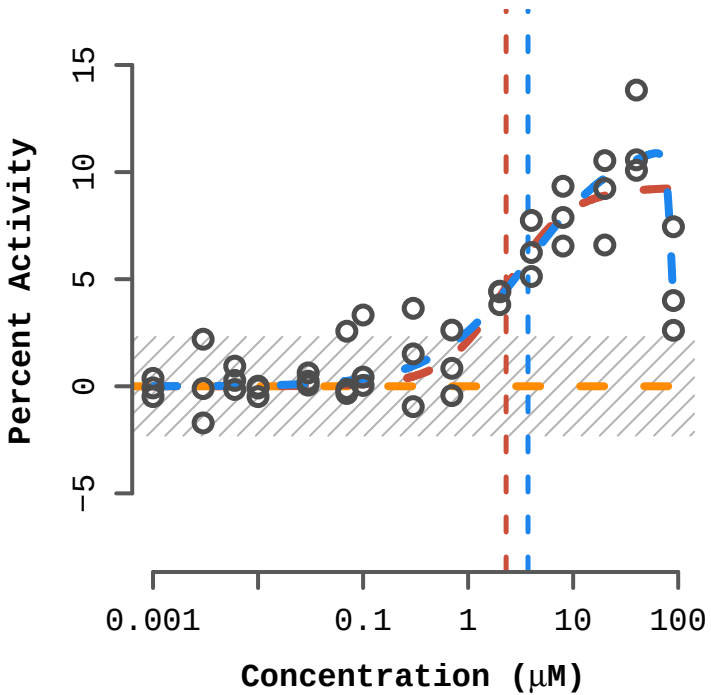
	tp	ga	gw
val:	16.2	0.697	1.26
sd:	2.17	0.133	0.453

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	40.5	1.43	0.848	1.68	4.15
sd:	19.2	0.454	0.179	0.0347	0.828

	CNST	HILL	GNLS
AIC:	300.29	246.7	205.92
PROB:	0	0	1
RMSE:	8.28	5.32	3.42

MAX_MEAN: 22.3 MAX_MED: 17.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chrysin
CHID: 22396 CASRN: 480-40-0
SPID(S): Tox21_302335
M4ID: 12476798

HILL MODEL (in red):

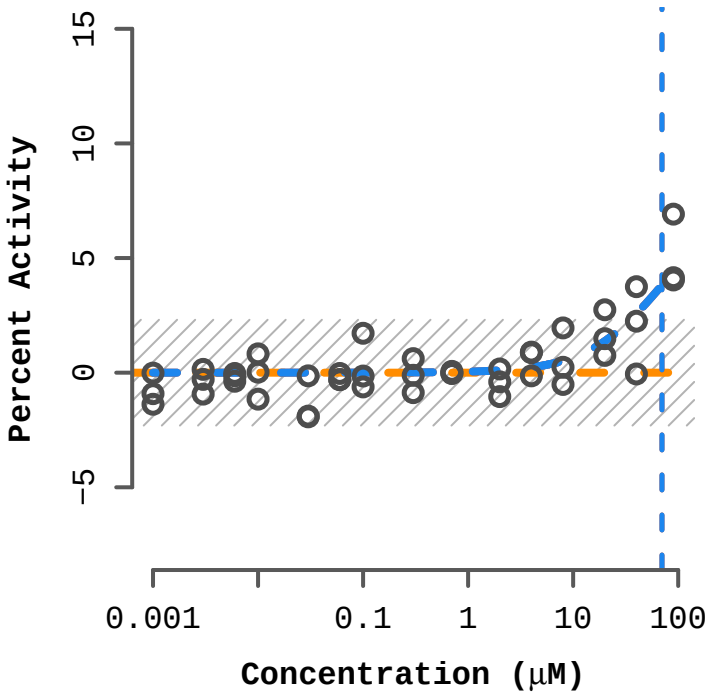
	tp	ga	gw
val:	9.29	0.362	1.45
sd:	0.924	0.0948	0.464

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.7	0.57	0.961	1.94	16.5
sd:	1.72	0.181	0.283	0.039	37.1

	CNST	HILL	GNLS
AIC:	273.34	182.65	166.02
PROB:	0	0	1
RMSE:	5.05	1.89	1.39

MAX_MEAN: 11.5 MAX_MED: 10.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Coumestrol
CHID: 22399 CASRN: 479-13-0
SPID(S): Tox21_200032
M4ID: 12482220

HILL MODEL (in red):

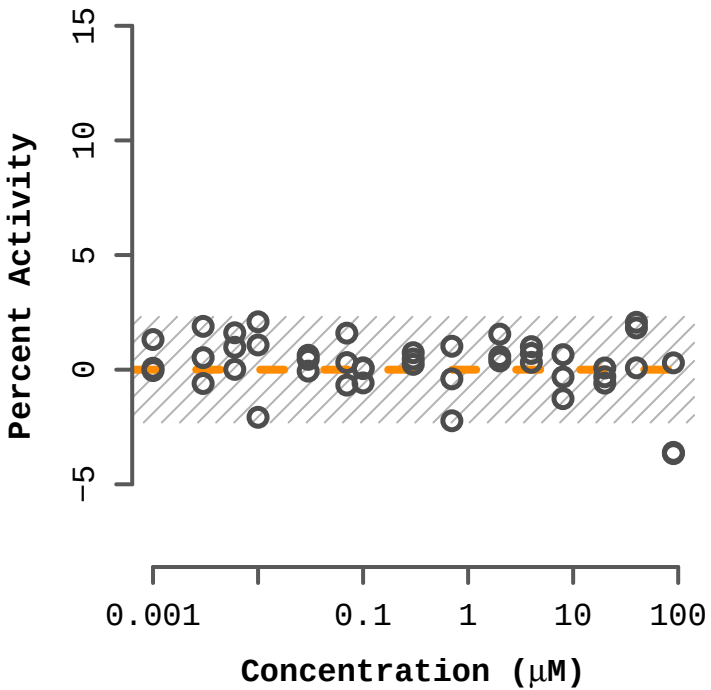
	tp	ga	gw
val:	7.63	1.85	1.21
sd:	7.47	0.74	0.648

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.63	1.85	1.21	3.19	5.68
sd:	7.47	0.74	0.648	1090	5020

	CNST	HILL	GNLS
AIC:	164.05	128.93	132.93
PROB:	0	0.88	0.12
RMSE:	1.74	0.95	0.95

MAX_MEAN: 5.04 MAX_MED: 4.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

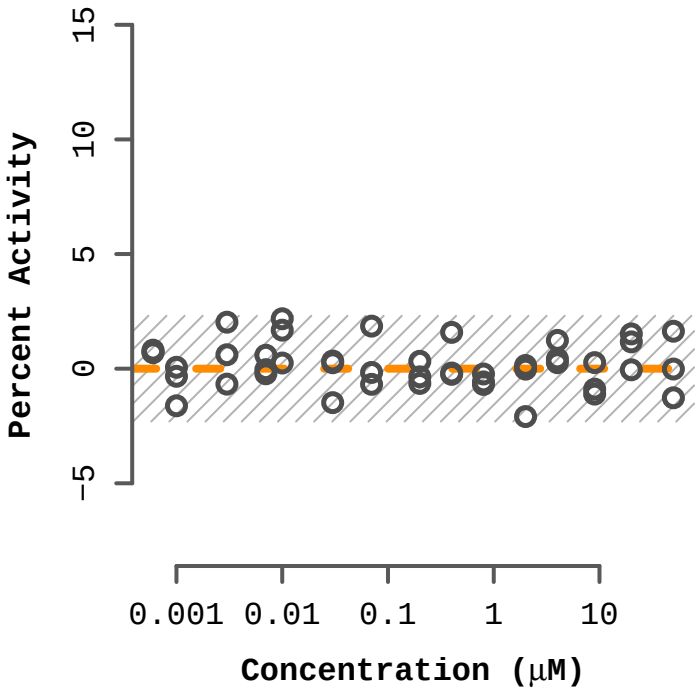
NAME: 2,2'−Dihydroxy−4−methoxybenzophenone
CHID: 22403 **CASRN:** 131−53−3
SPID(S): Tox21_200993
M4ID: 12481259

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

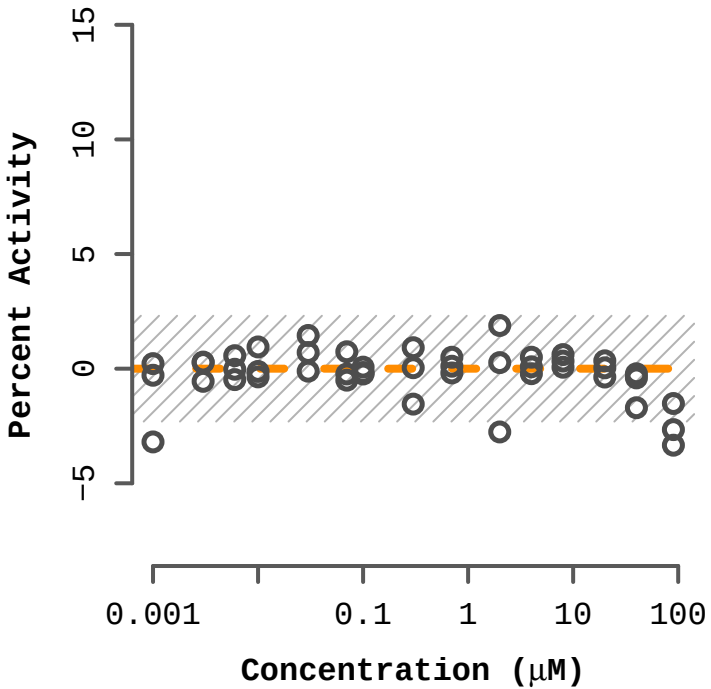
NAME: 2,2'−Dihydroxy−4−methoxybenzophenone
CHID: 22403 **CASRN:** 131−53−3
SPID(S): Tox21_110417_1
M4ID: 12484377

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

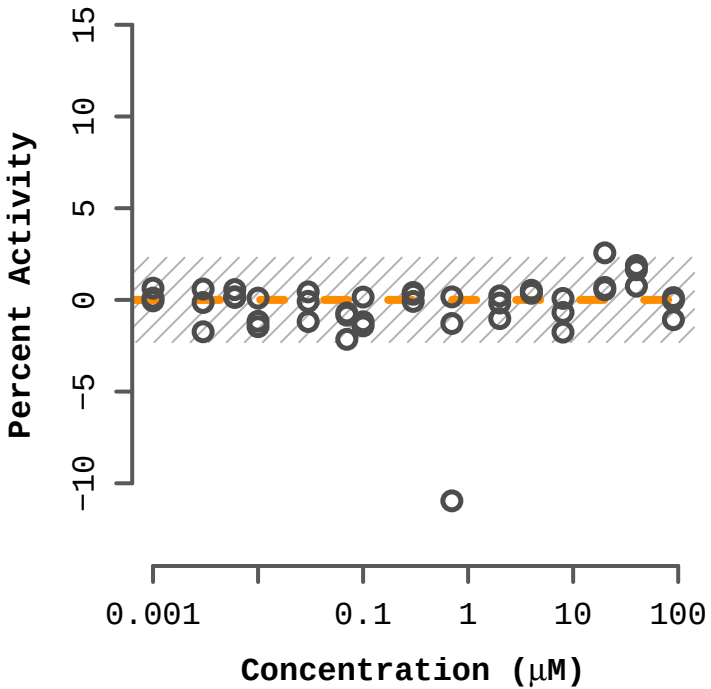
NAME: 2,2'−Dihydroxybenzophenone
CHID: 22404 **CASRN:** 835−11−0
SPID(S): Tox21_201169
M4ID: 12481083

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.683 **MAX_MED:** 0.706 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

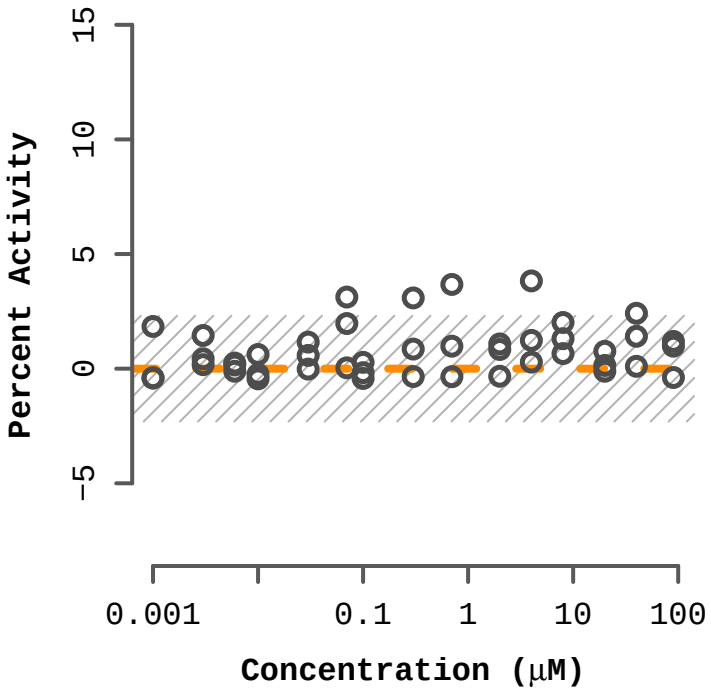
NAME: 2-Hydroxy-4-methoxybenzophenone
CHID: 22405 **CASRN:** 131-57-7
SPID(S): Tox21_302852
M4ID: 12476281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

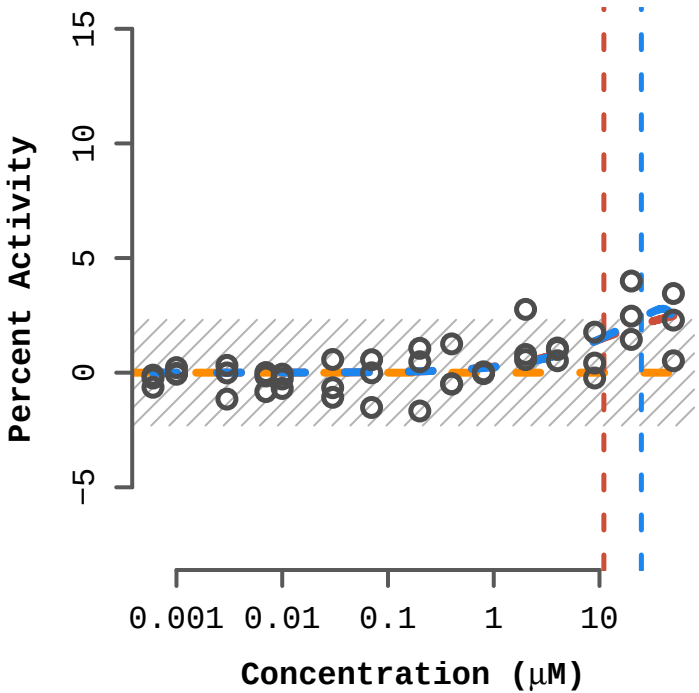
NAME: 2-Hydroxy-4-methoxybenzophenone
CHID: 22405 **CASRN:** 131-57-7
SPID(S): Tox21_201985
M4ID: 12480267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxy-4-methoxybenzophenone
CHID: 22405 **CASRN:** 131-57-7
SPID(S): Tox21_110418_1
M4ID: 12484376

HILL MODEL (in red):

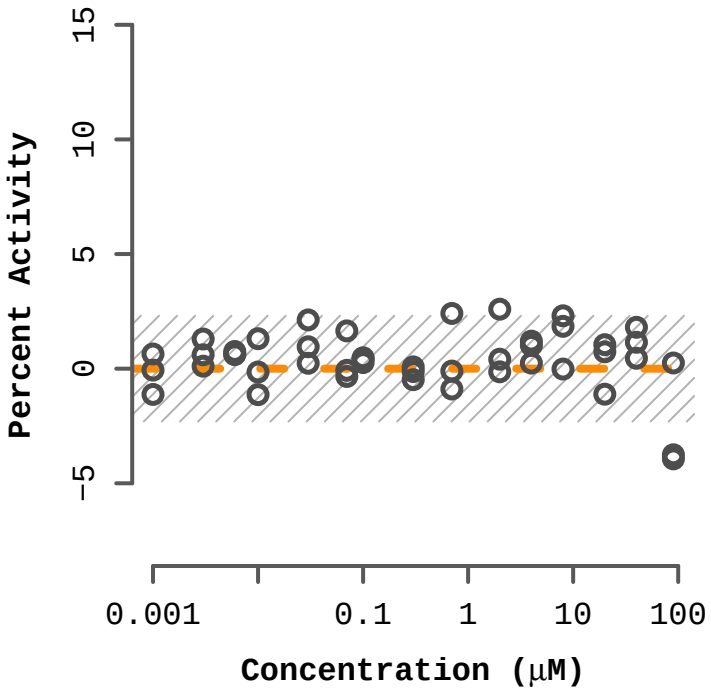
	tp	ga	gw
val:	3.03	1.04	0.981
sd:	1.49	0.549	0.483

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.8	1.4	0.906	1.75	9.28
sd:	5.97	1.03	0.392	0.198	37.8

	CNST	HILL	GNLS
AIC:	142.61	119.38	122.95
PROB:	0	0.86	0.14
RMSE:	1.25	0.85	0.84

MAX_MEAN: 2.64 **MAX_MED:** 2.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

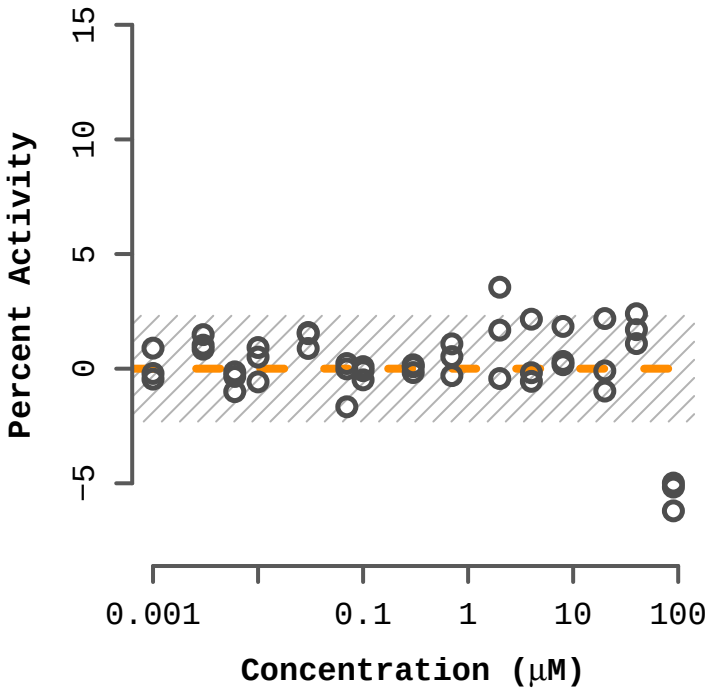
NAME: 2,4−Dihydroxybenzophenone
CHID: 22406 **CASRN:** 131−56−6
SPID(S): Tox21_302865
M4ID: 12476268

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

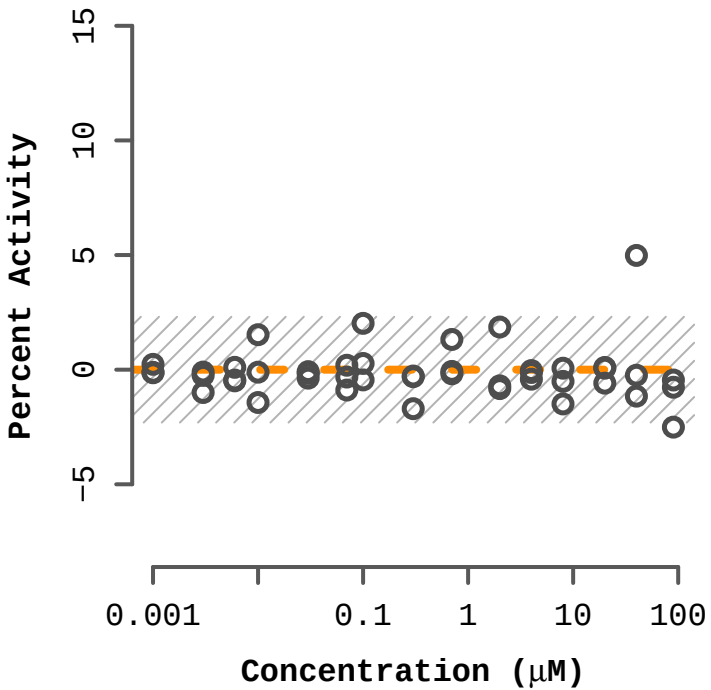
NAME: 2,4−Dihydroxybenzophenone
CHID: 22406 **CASRN:** 131−56−6
SPID(S): Tox21_201285
M4ID: 12480967

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

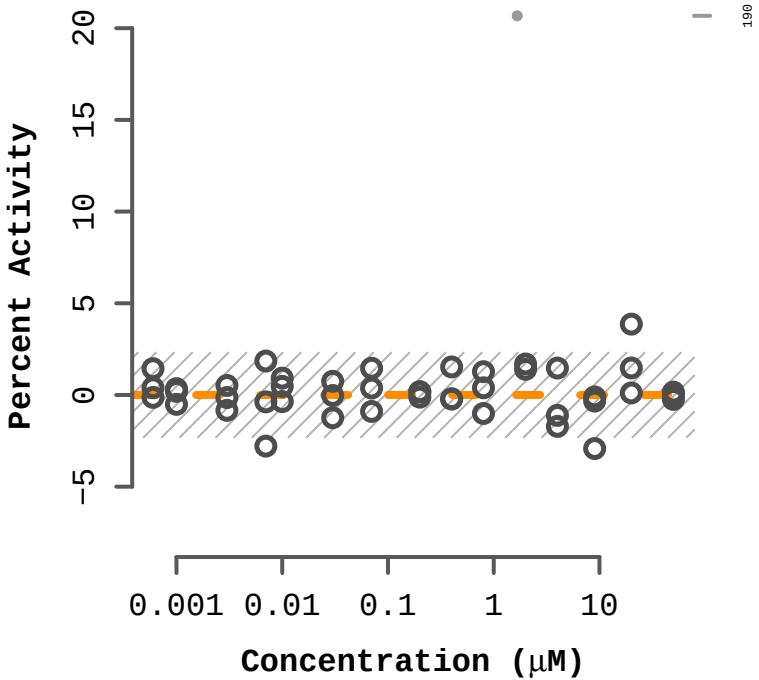
NAME: Phenol red
CHID: 22408 **CASRN:** 143-74-8
SPID(S): Tox21_303570
M4ID: 12475575

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.273 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

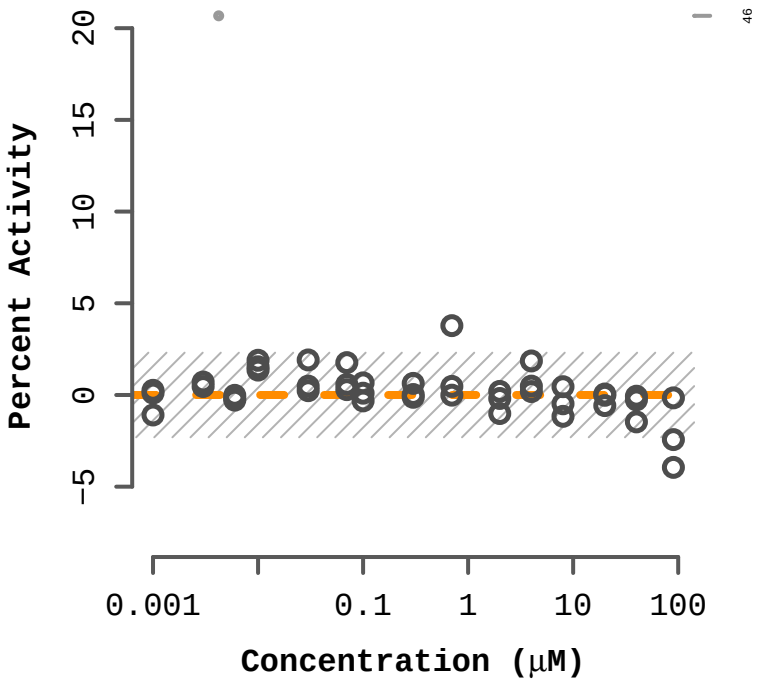
NAME: Phenol red
CHID: 22408 **CASRN:** 143-74-8
SPID(S): Tox21_110012_1
M4ID: 12484712 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.69	NA	NA
PROB:	1	NA	NA
RMSE:	28.53	NA	NA

MAX_MEAN: 64.8 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

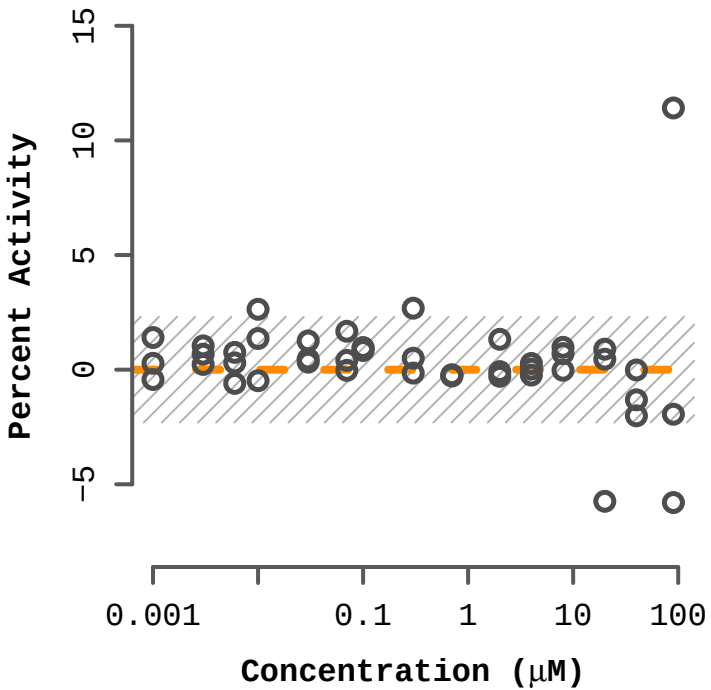
NAME: 4,4'−Sulfonyldiphenol
CHID: 22409 CASRN: 80−09−1
SPID(S): Tox21_302843
M4ID: 12476290 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.05	NA	NA
PROB:	1	NA	NA
RMSE:	6.91	NA	NA

MAX_MEAN: 15.6 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

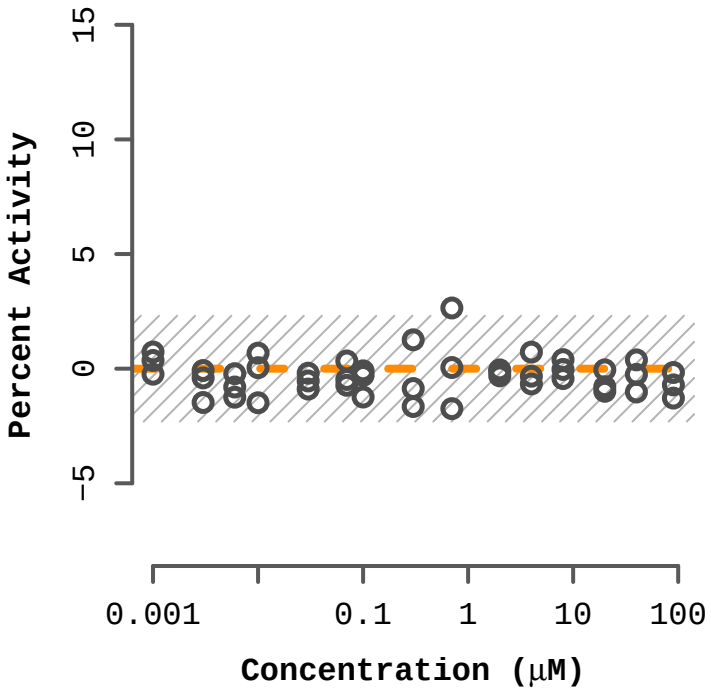
NAME: 4,4'−Sulfonyldiphenol
CHID: 22409 **CASRN:** 80−09−1
SPID(S): Tox21_201743
M4ID: 12480509

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.31	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

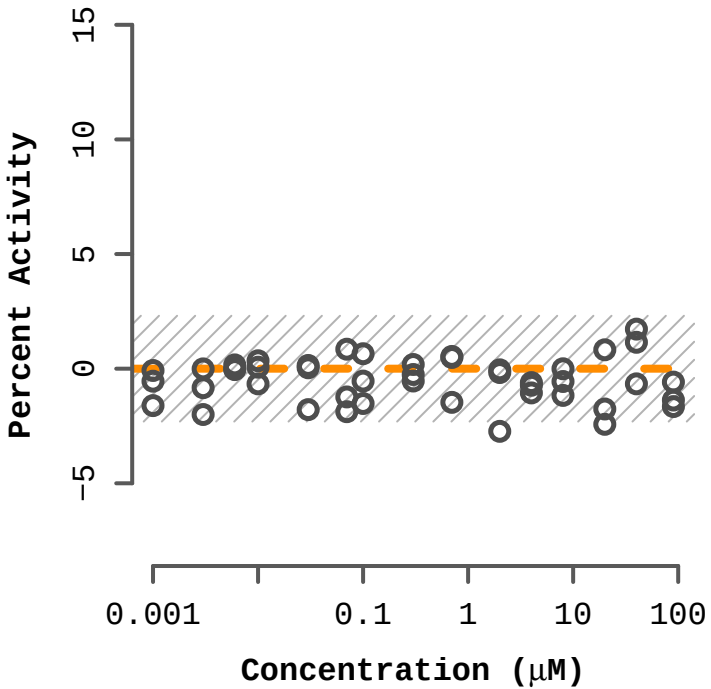
NAME: 4,4'−Methylenebis(2,6−di−t−butylphenol)
CHID: 22411 **CASRN:** 118−82−1
SPID(S): Tox21_303566
M4ID: 12475579

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.319 **MAX_MED:** 0.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

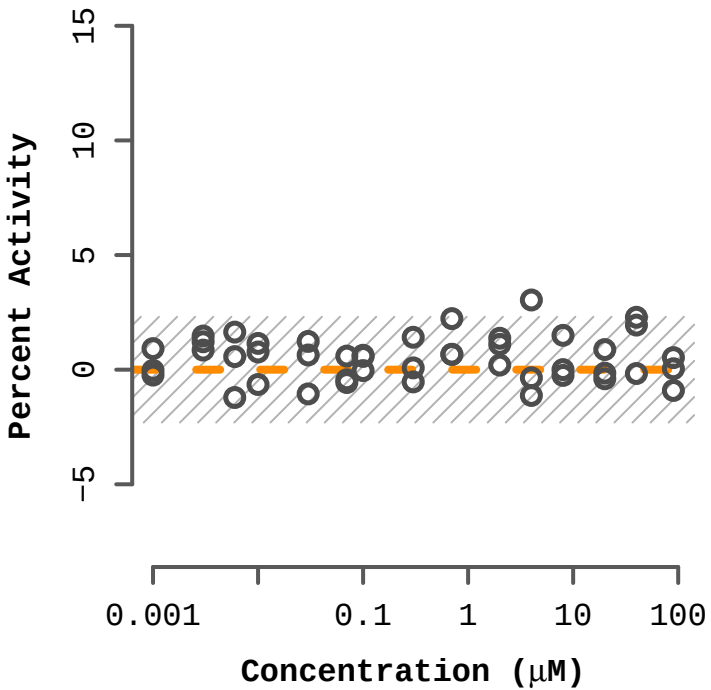
NAME: 4,4'-Methylenebis(2,6-di-t-butylphenol)
CHID: 22411 **CASRN:** 118-82-1
SPID(S): Tox21_201863
M4ID: 12480389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.74 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

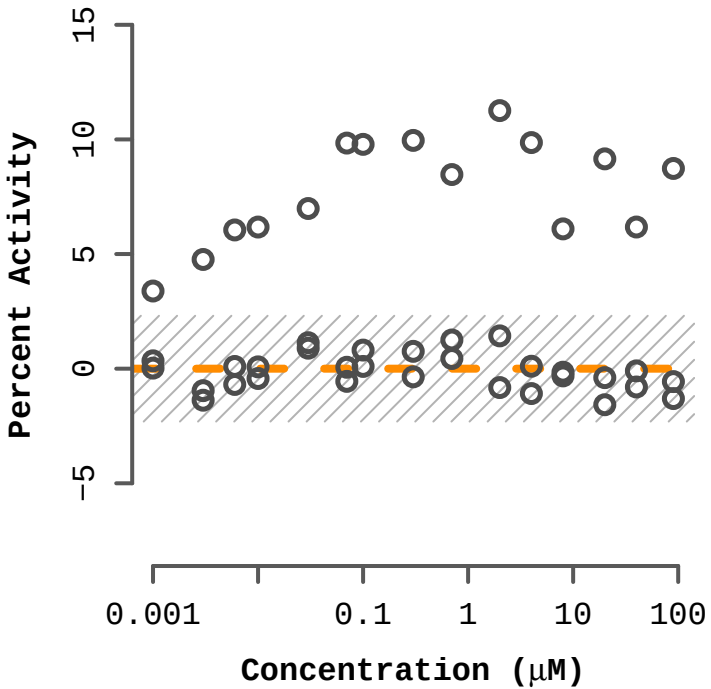
NAME: Isoeugenol
CHID: 22413 **CASRN:** 97-54-1
SPID(S): Tox21_300303
M4ID: 12478827

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

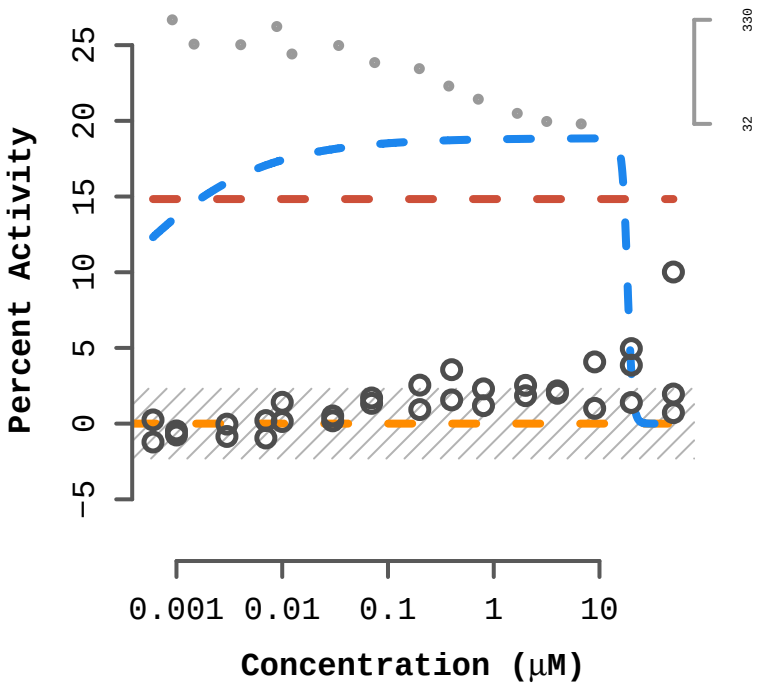
NAME: Isoeugenol
CHID: 22413 **CASRN:** 97-54-1
SPID(S): Tox21_202433
M4ID: 12479819

HILL MODEL: Not applicable.

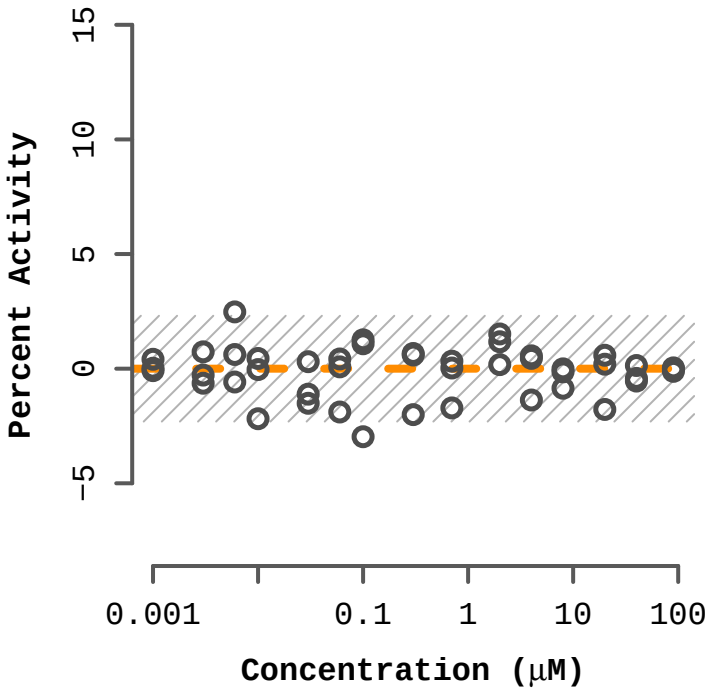
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.81	NA	NA
PROB:	1	NA	NA
RMSE:	4.71	NA	NA

MAX_MEAN: 3.96 **MAX_MED:** 1.43 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Isoeugenol
CHID:    22413   CASRN: 97-54-1
SPID(S): Tox21_111138_1
M4ID:    12483884  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  14.8     -4.24    7.81
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  18.9     -3.64    0.659    1.26     18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  543.91      536.55      540
PROB: 0.02        0.83        0.15
RMSE: 113.93      107.52      106.89

MAX_MEAN: 111       MAX_MED: 4.08      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

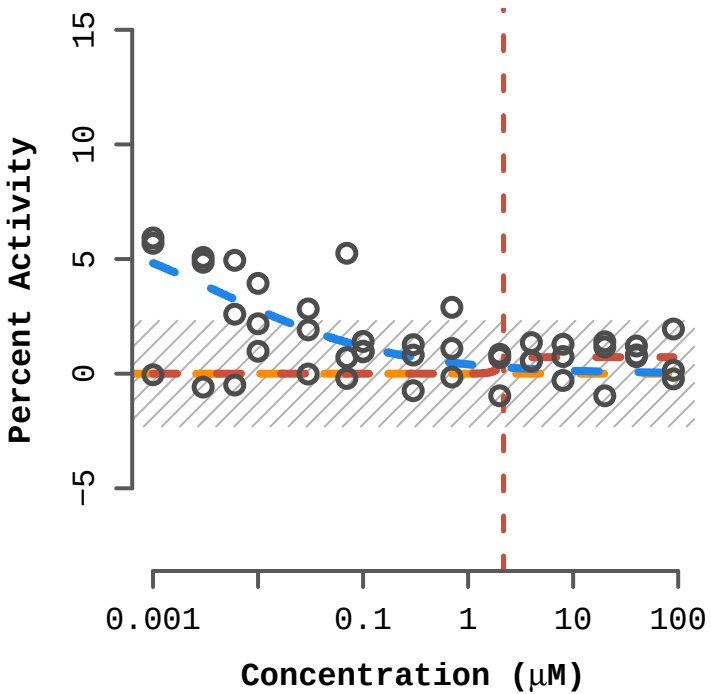
NAME: 1,6-Dimethylnaphthalene
CHID: 22415 **CASRN:** 575-43-9
SPID(S): Tox21_200672
M4ID: 12481580

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl 4-aminobenzoate
CHID: 22417 CASRN: 94-25-7
SPID(S): Tox21_200378
M4ID: 12481874

HILL MODEL (in red):

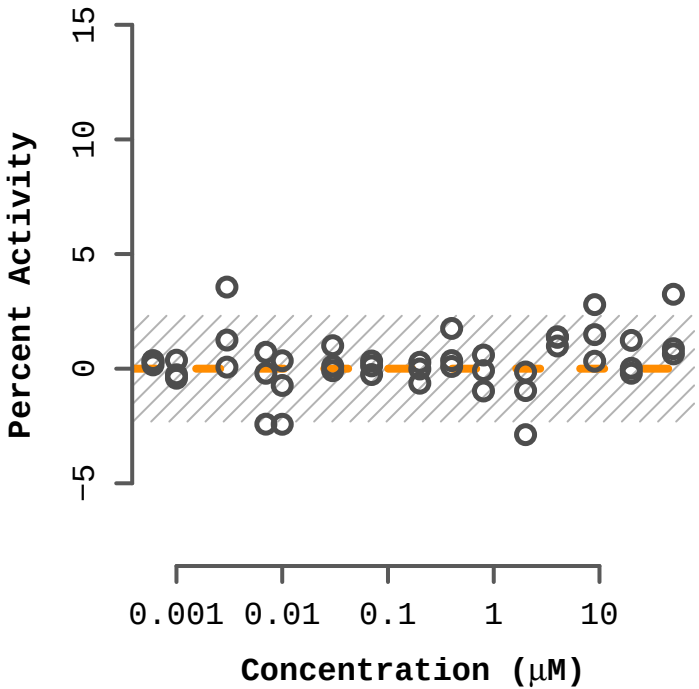
	tp	ga	gw
val:	0.72	0.337	8
sd:	0.383	0.351	57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.11	−4.91	6.1	−2.37	0.514
sd:	2.84	85000	268000	0.692	0.211

	CNST	HILL	GNLS
AIC:	201.06	203.73	177.54
PROB:	0	0	1
RMSE:	2.33	2.29	1.62

MAX_MEAN: 3.85 MAX_MED: 5.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

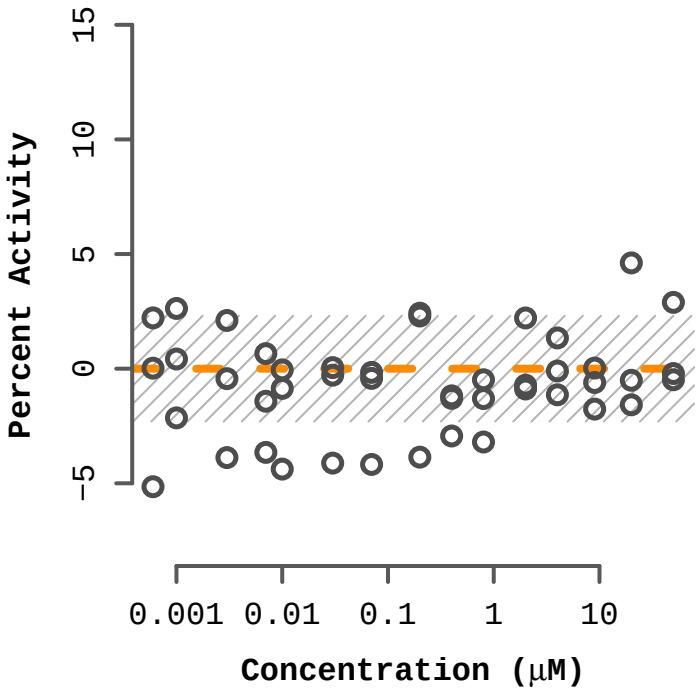
NAME: Butyl 4-aminobenzoate
CHID: 22417 **CASRN:** 94-25-7
SPID(S): Tox21_110392_1
M4ID: 12484399

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

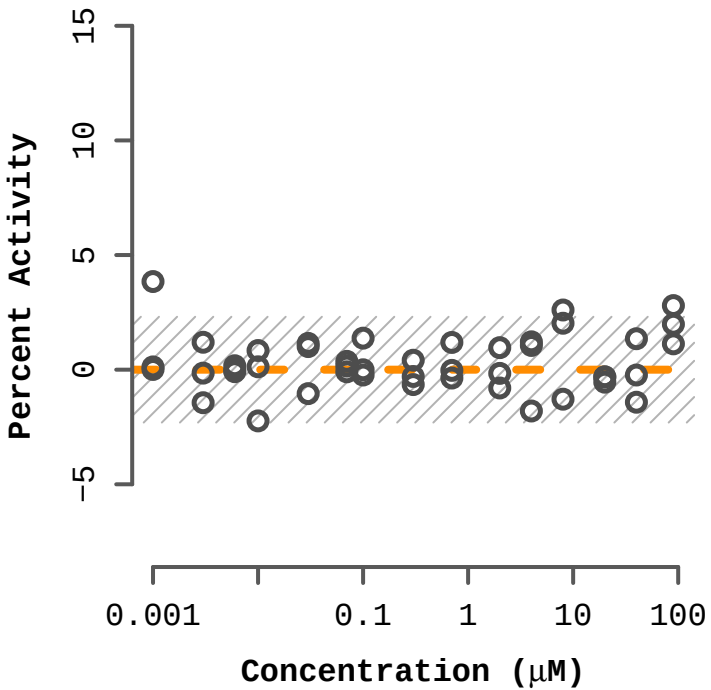
NAME: Dopamine
CHID: 22420 **CASRN:** 51-61-6
SPID(S): Tox21_110167_1
M4ID: 12484590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.25	NA	NA

MAX_MEAN: 0.845 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

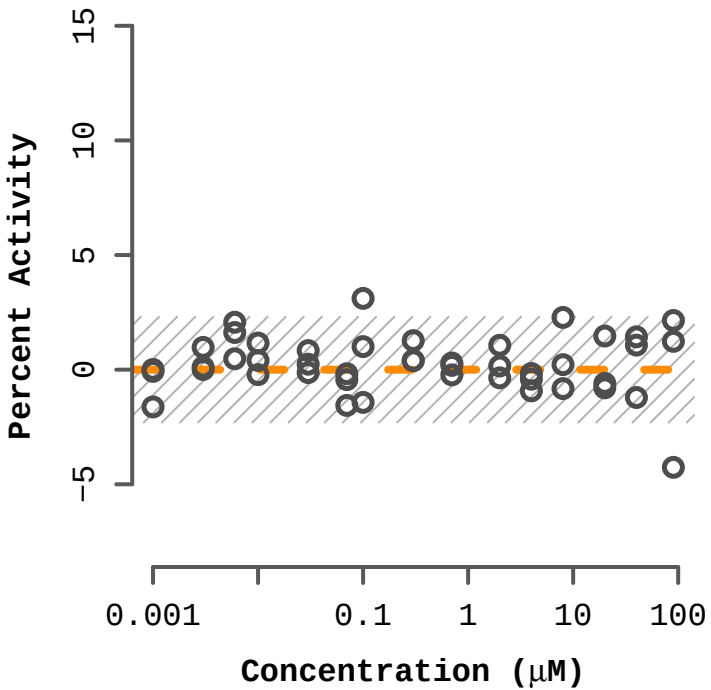
NAME: Melatonin
CHID: 22421 CASRN: 73-31-4
SPID(S): Tox21_302926
M4ID: 12476207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.97 MAX_MED: 2.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

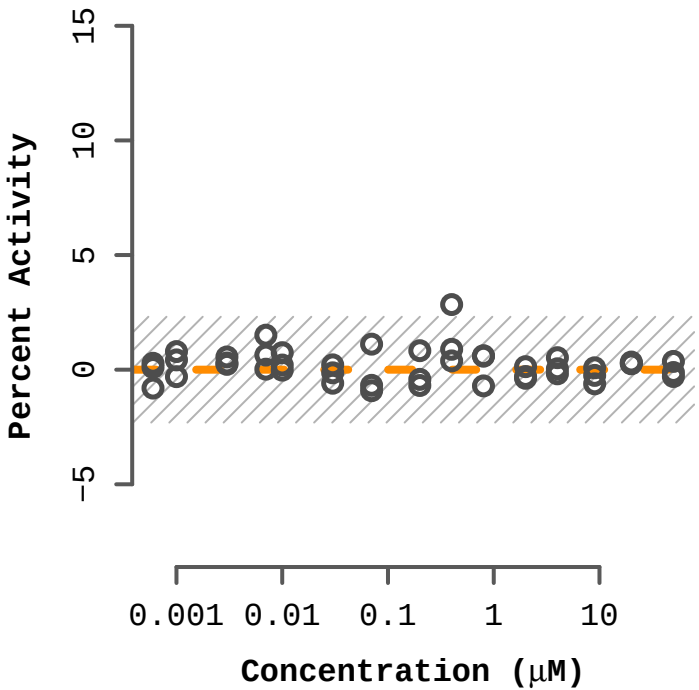
NAME: Melatonin
CHID: 22421 **CASRN:** 73-31-4
SPID(S): Tox21_201527
M4ID: 12480725

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

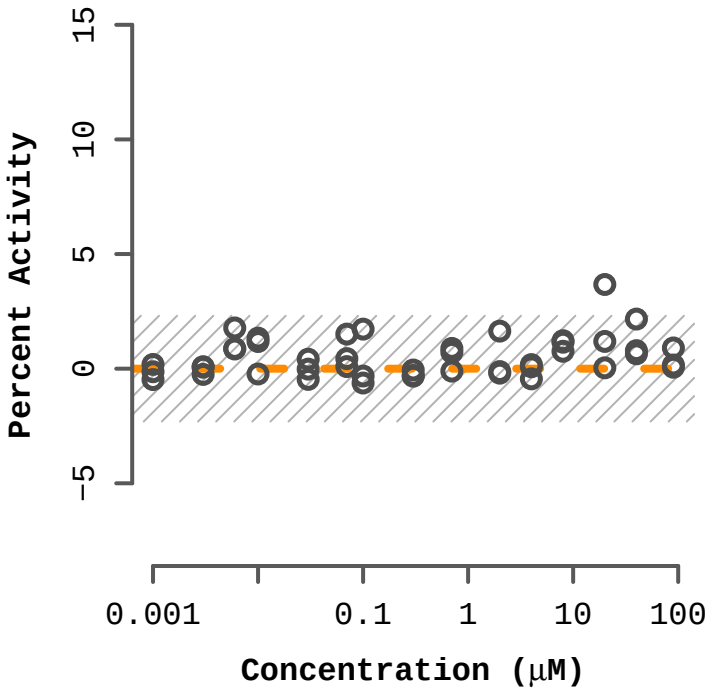
NAME: Melatonin
CHID: 22421 **CASRN:** 73-31-4
SPID(S): Tox21_110195_1
M4ID: 12484564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

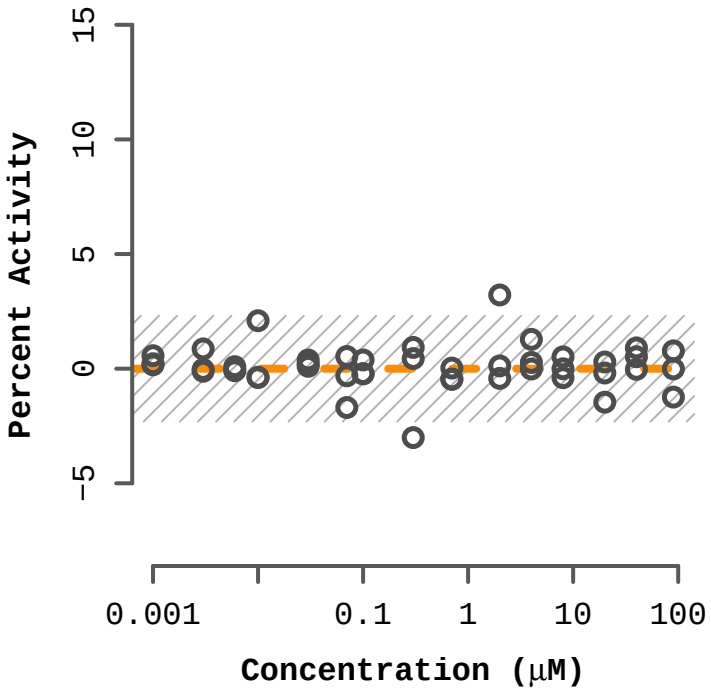
NAME: 4,4'−Methylenedianiline
CHID: 22422 **CASRN:** 101−77−9
SPID(S): Tox21_300141
M4ID: 12478989

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

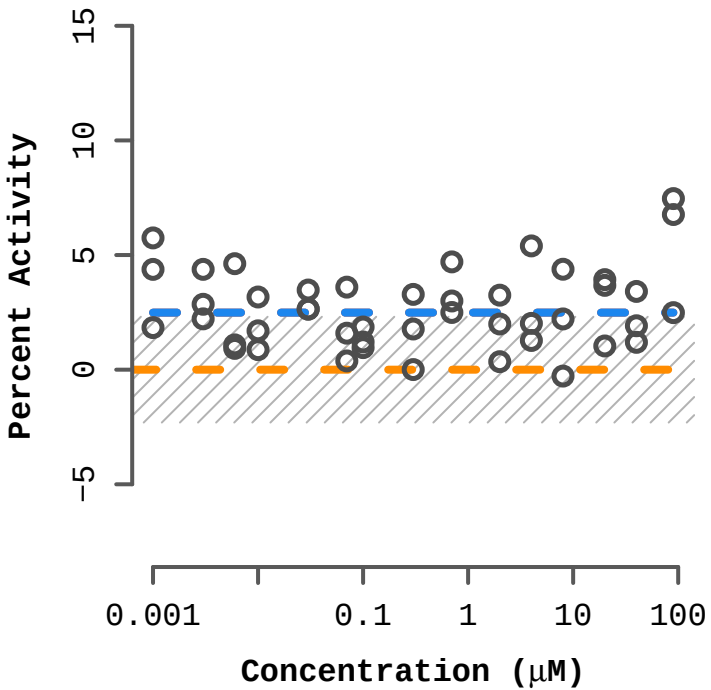
NAME: 4,4'−Methylenedianiline
CHID: 22422 **CASRN:** 101−77−9
SPID(S): Tox21_201723
M4ID: 12480529

HILL MODEL: Not applicable.

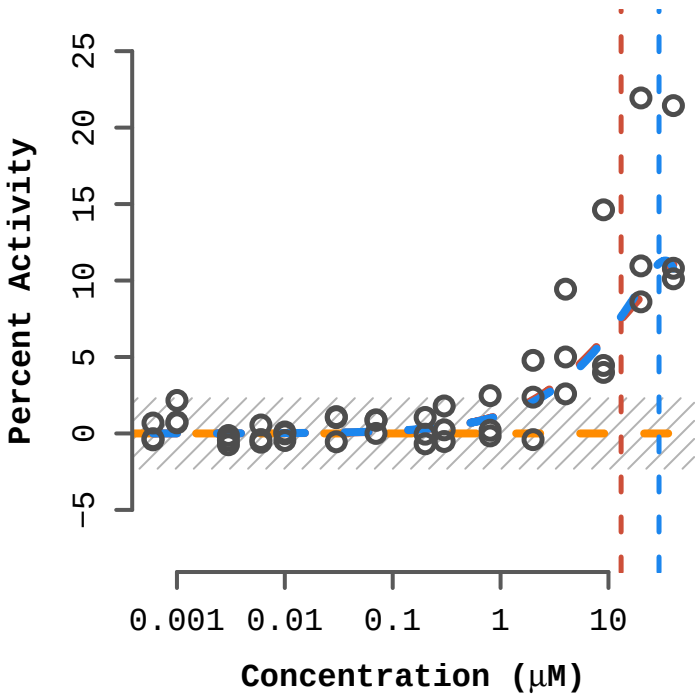
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 0.521 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4,4'-Dihydoxybenzophenone
CHID:    22425   CASRN: 611-99-4
SPID(S): Tox21_200550
M4ID:    12481702

HILL MODEL (in red):
      tp       ga       gw
val:  2.49     -4.5     5.34
sd:   0.251    1420     5040

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.49     -4.38    5.2      3.65     4.53
sd:   0.251    514      1940     1020     2730

      CNST        HILL        GNLS
AIC:  238.22      185.48      189.48
PROB: 0           0.88        0.12
RMSE: 3.17        1.72        1.72

MAX_MEAN: 5.57      MAX_MED: 6.77      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chrysene
CHID: 22432 **CASRN:** 218-01-9
SPID(S): Tox21_202548
M4ID: 12479704

HILL MODEL (in red):

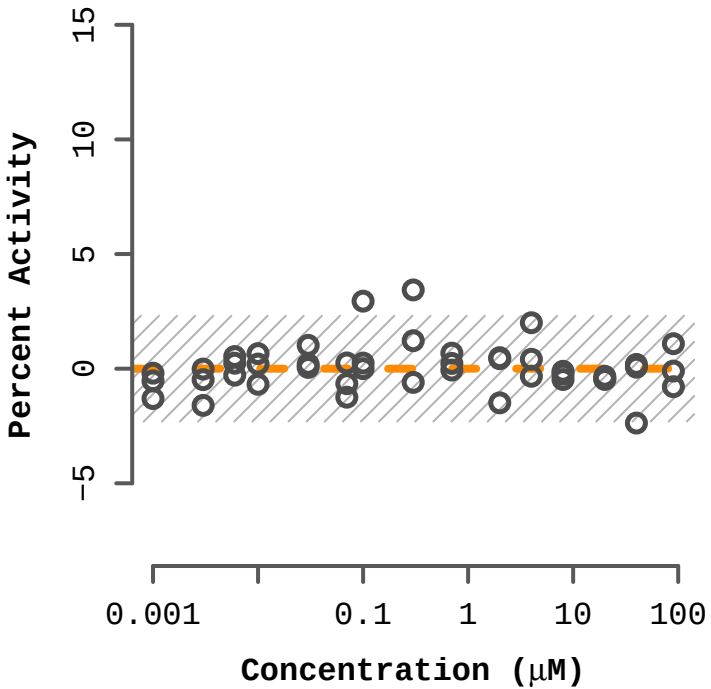
	tp	ga	gw
val:	14.9	1.12	0.936
sd:	5.36	0.426	0.319

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23	1.47	0.862	1.72	5.84
sd:	26	0.977	0.266	0.588	25.2

	CNST	HILL	GNLS
AIC:	272.21	201.35	204.3
PROB:	0	0.81	0.19
RMSE:	6.28	3.1	3.07

MAX_MEAN: 14.1 **MAX_MED:** 11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

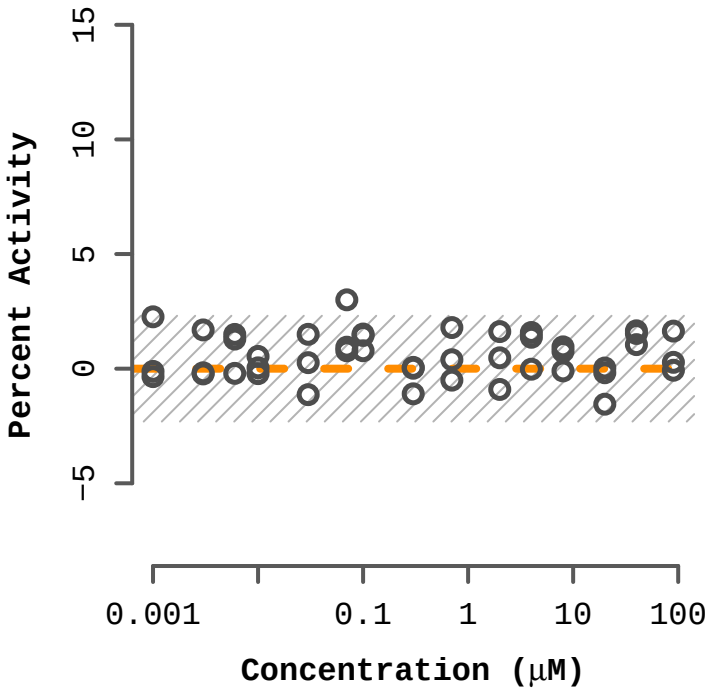
NAME: Diphenolic acid
CHID: 22436 **CASRN:** 126-00-1
SPID(S): Tox21_302993
M4ID: 12476140

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

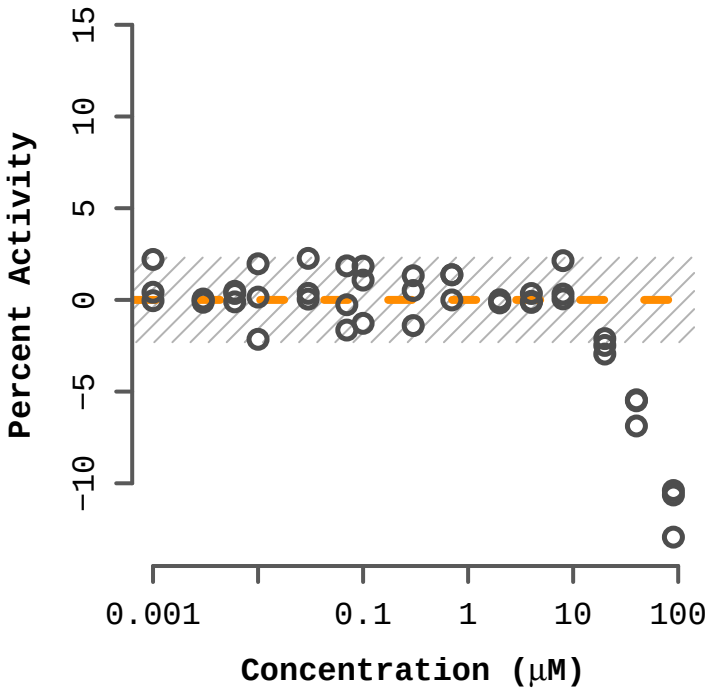
NAME: Diphenolic acid
CHID: 22436 **CASRN:** 126-00-1
SPID(S): Tox21_202255
M4ID: 12479997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

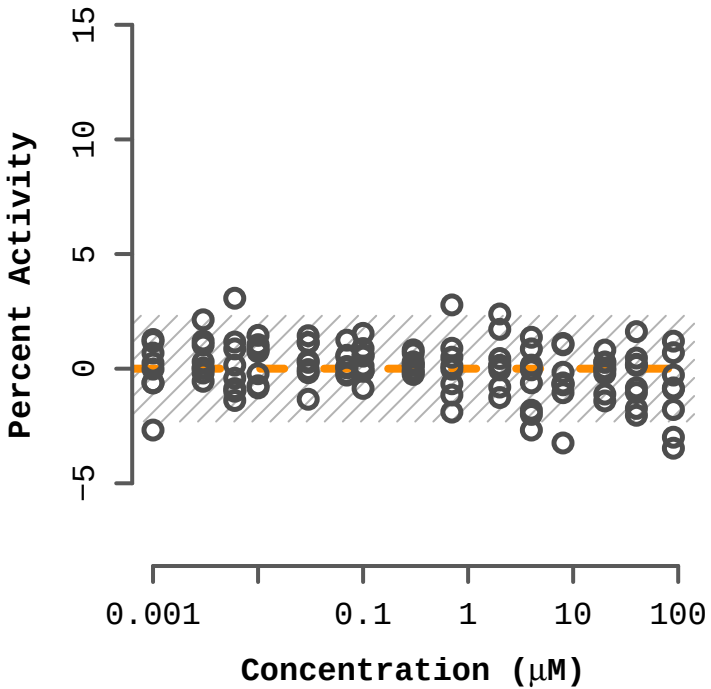
NAME: Nordihydroguaiaretic acid
CHID: 22437 **CASRN:** 500-38-9
SPID(S): Tox21_302171
M4ID: 12476962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.53	NA	NA
PROB:	1	NA	NA
RMSE:	3.52	NA	NA

MAX_MEAN: 0.915 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

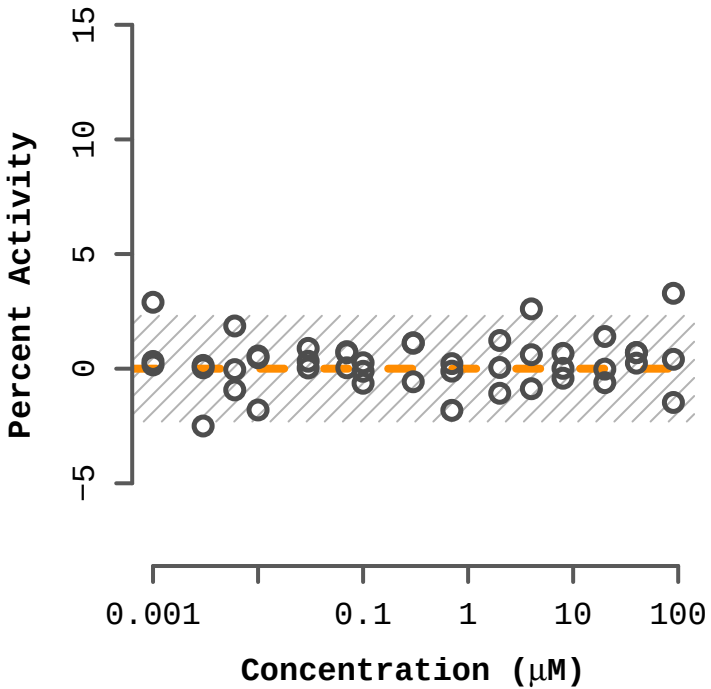
NAME: Phenolphthalin
CHID: 22439 **CASRN:** 81-90-3
SPID(S): Tox21_303646
M4ID: 12475501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	371.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.498 **MAX_MED:** 0.777 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

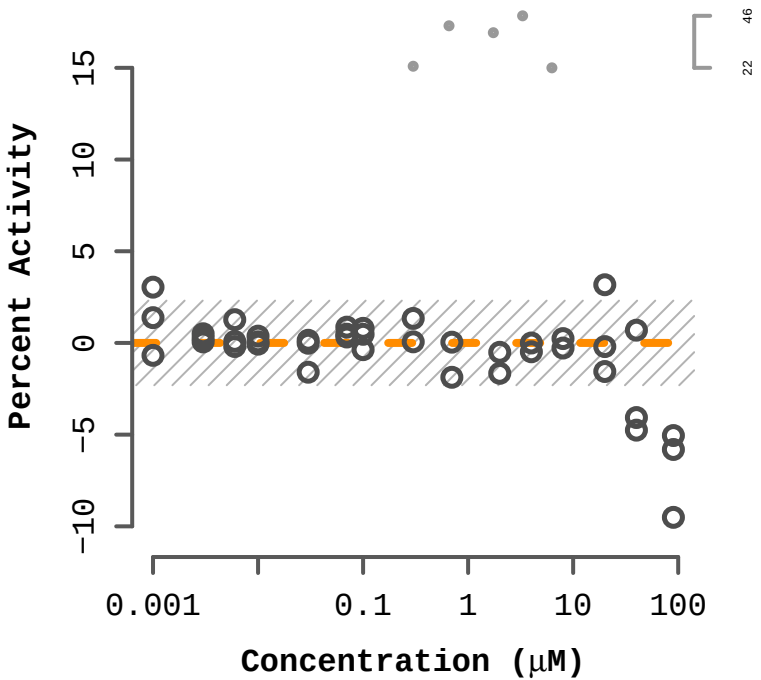
NAME: Phenolphthalin
CHID: 22439 CASRN: 81-90-3
SPID(S): Tox21_201700
M4ID: 12480552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

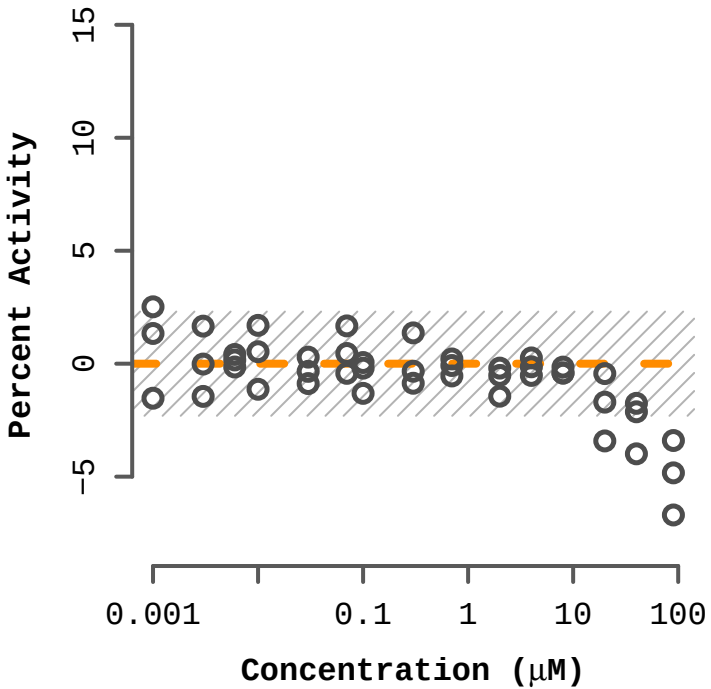
NAME: Bisphenol B
CHID: 22442 **CASRN:** 77-40-7
SPID(S): Tox21_300198
M4ID: 12478932 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	295.38	NA	NA
PROB:	1	NA	NA
RMSE:	11.98	NA	NA

MAX_MEAN: 15.1 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

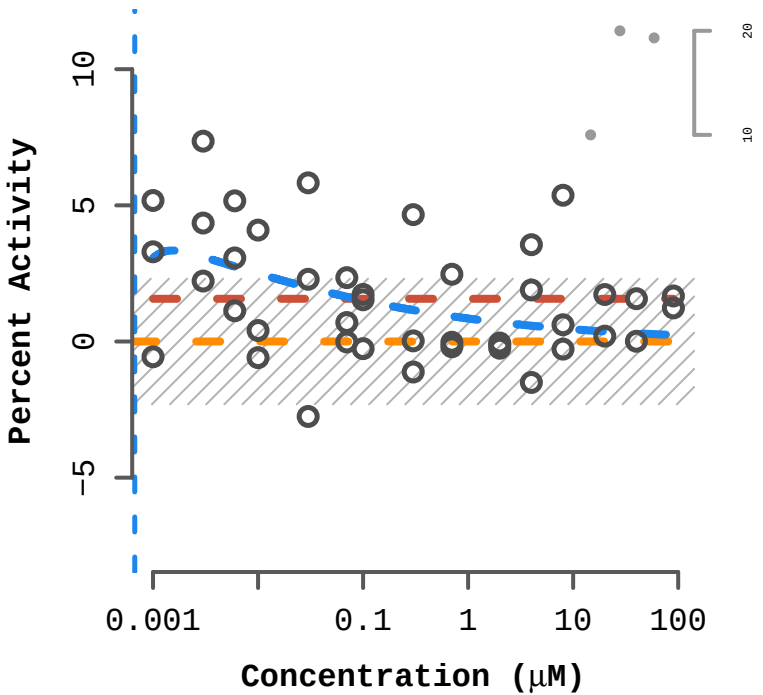
NAME: Bisphenol B
CHID: 22442 CASRN: 77-40-7
SPID(S): Tox21_202222
M4ID: 12480030

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 0.777 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(4−hydroxyphenyl)methane
CHID: 22445 CASRN: 620−92−8
SPID(S): Tox21_201163
M4ID: 12481089 BRK

HILL MODEL (in red):

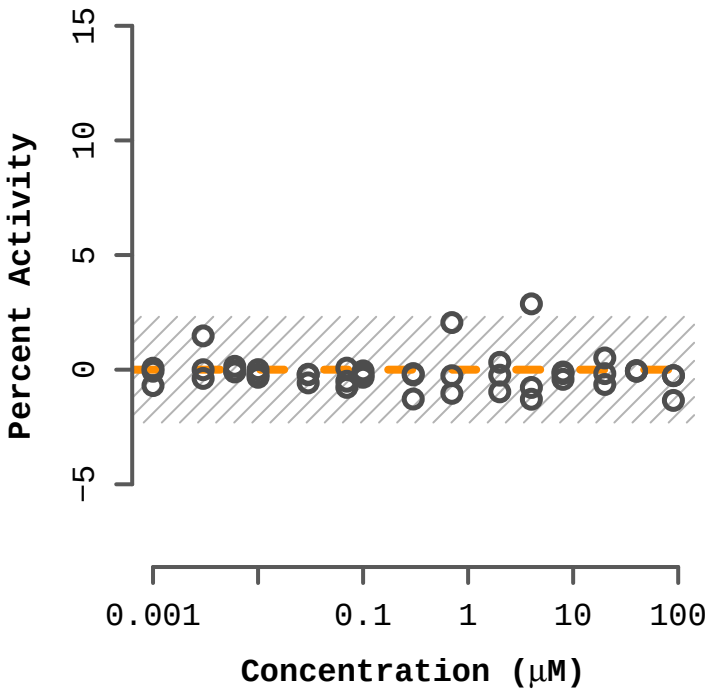
	tp	ga	gw
val:	1.57	−4.54	4.75
sd:	0.405	1440	4410

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.23	−3.17	3.87	−2.92	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	254.67	246.06	247.38
PROB:	0.01	0.65	0.34
RMSE:	5.24	4.65	4.88

MAX_MEAN: 7.57 **MAX_MED:** 4.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

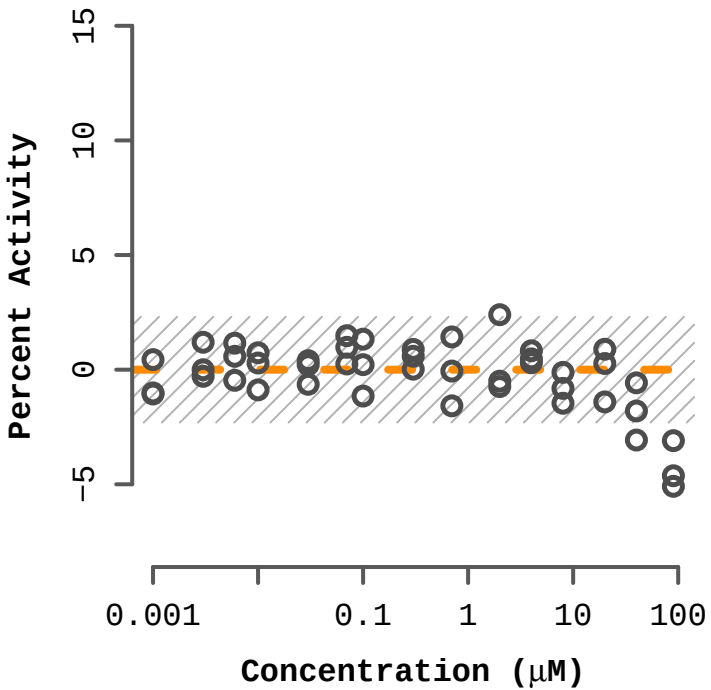
NAME: Bisphenol F
CHID: 22446 CASRN: 2467-02-9
SPID(S): Tox21_303599
M4ID: 12475546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.365 MAX_MED: 0 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

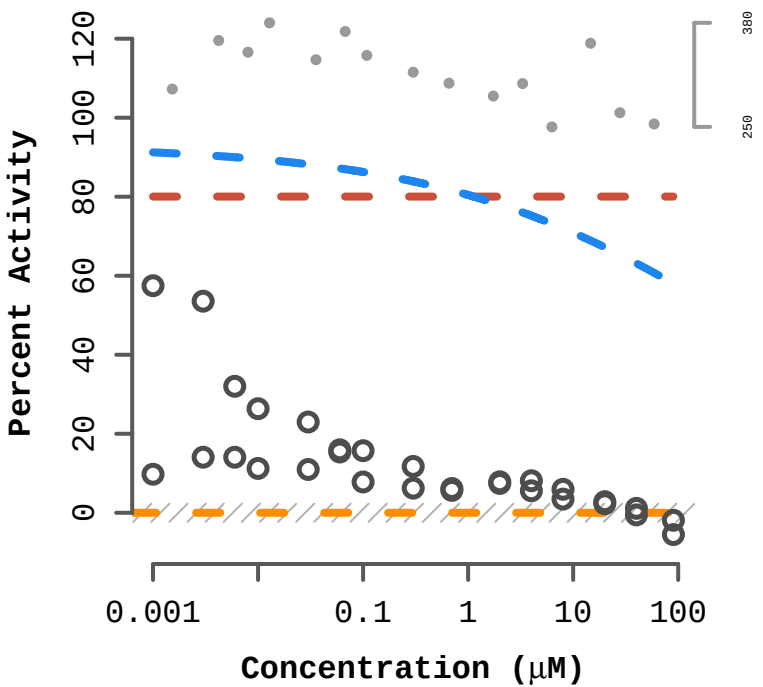
NAME: Metolachlor
CHID: 22448 **CASRN:** 51218-45-2
SPID(S): Tox21_300982
M4ID: 12478151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 0.904 **MAX_MED:** 0.977 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Metolachlor
CHID: 22448 CASRN: 51218-45-2
SPID(S): Tox21_201376
M4ID: 12480876 BRK

HILL MODEL (in red):

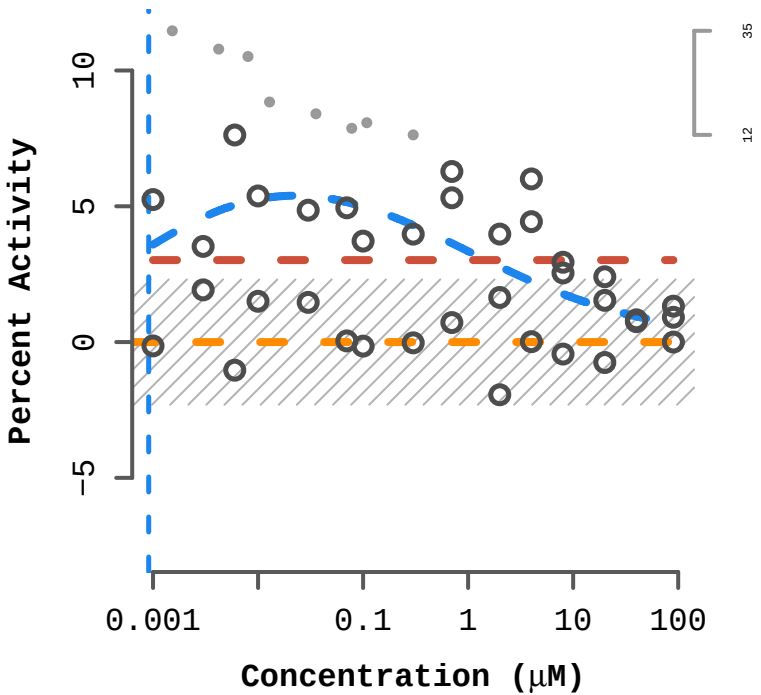
	tp	ga	gw
val:	80	-4.84	3.38
sd:	24.4	927	1690

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	93	-5	8	2.68	0.3
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	598.33	591.01	594.81
PROB:	0.02	0.85	0.13
RMSE:	187.22	151.71	151.01

MAX_MEAN: 143 MAX_MED: 57.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethyl phthalate
CHID: 22455 CASRN: 131-11-3
SPID(S): Tox21_301045
M4ID: 12478088 BRK

HILL MODEL (in red):

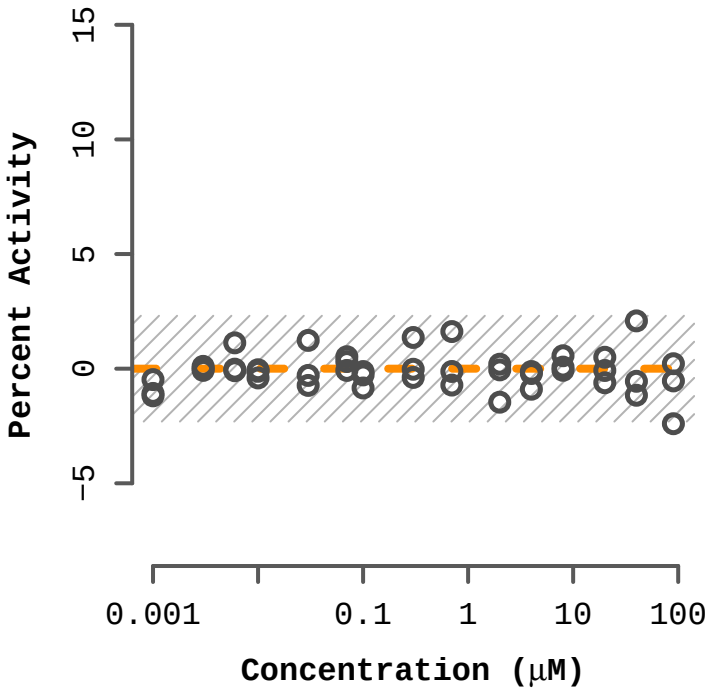
	tp	ga	gw
val:	3.02	-4.98	3.28
sd:	0.713	1150	1880

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.27	-3.04	0.621	-0.122	0.478
sd:	20.7	3.32	2.81	4.98	0.808

	CNST	HILL	GNLS
AIC:	317.07	305.52	303.02
PROB:	0	0.22	0.78
RMSE:	10.01	8.7	8.14

MAX_MEAN: 13.3 MAX_MED: 7.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

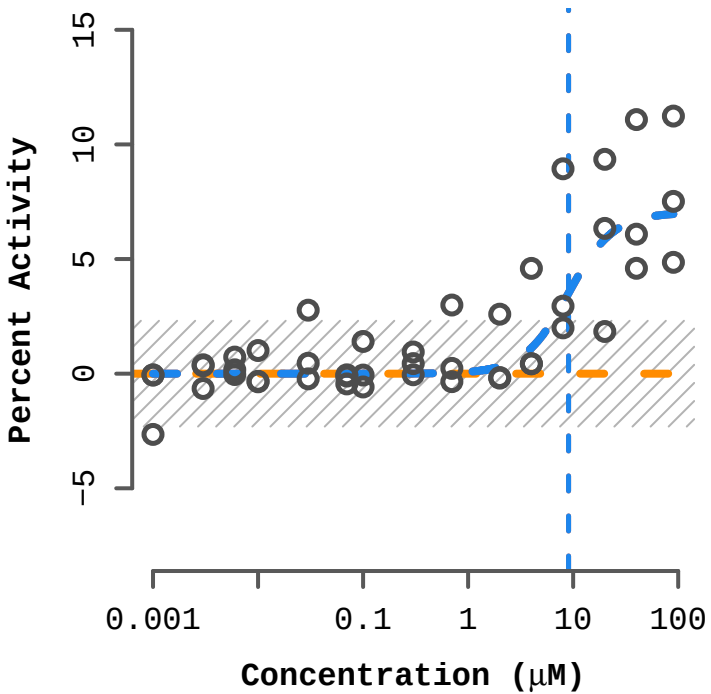
NAME: Dimethyl phthalate
CHID: 22455 **CASRN:** 131-11-3
SPID(S): Tox21_202145
M4ID: 12480107

HILL MODEL: Not applicable.

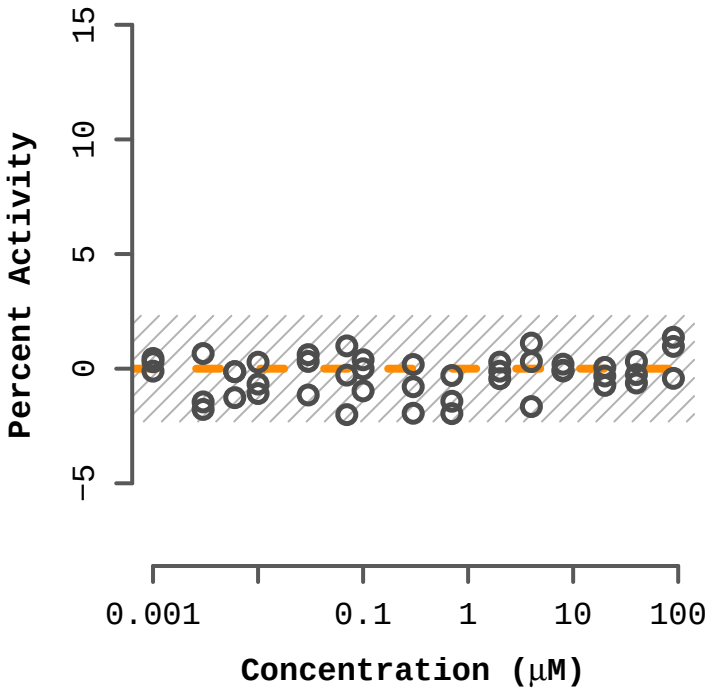
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.341 **MAX_MED:** 0.313 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-Phenylphenol
CHID:    22462   CASRN: 580-51-8
SPID(S): Tox21_303813
M4ID:    12475375

HILL MODEL (in red):
      tp       ga       gw
val:  7.03     0.956    2.04
sd:   1.17     0.145    1.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.03     0.956    2.04     3.27     5.78
sd:   1.17     0.145    1.4      992      4370

      CNST        HILL        GNLS
AIC:  239.13      184.81      188.81
PROB: 0           0.88        0.12
RMSE: 3.86        1.88        1.88

MAX_MEAN: 7.87      MAX_MED: 7.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

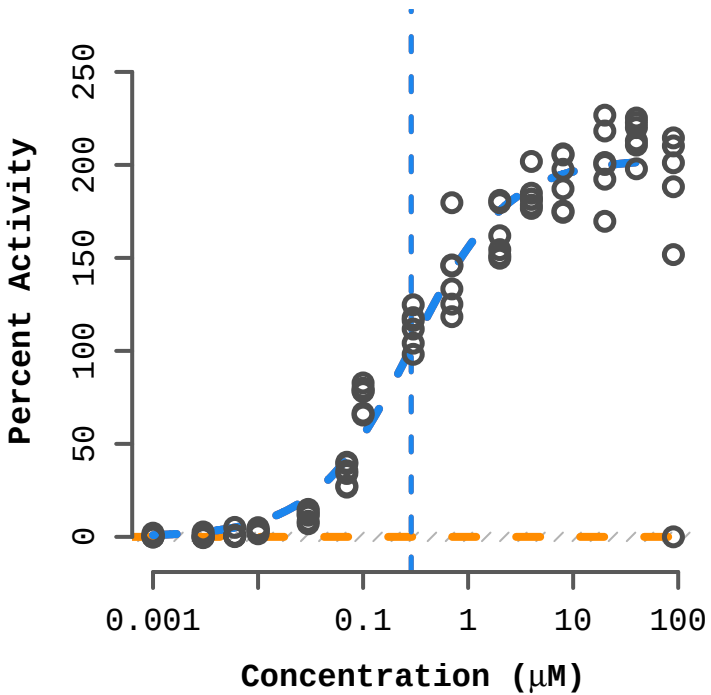
NAME: Butylbenzene
CHID: 22472 **CASRN:** 104-51-8
SPID(S): Tox21_300511
M4ID: 12478621

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.641 **MAX_MED:** 0.973 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Corticosterone
CHID: 22474 CASRN: 50-22-6
SPID(S): Tox21_303642
M4ID: 12475503

HILL MODEL (in red):

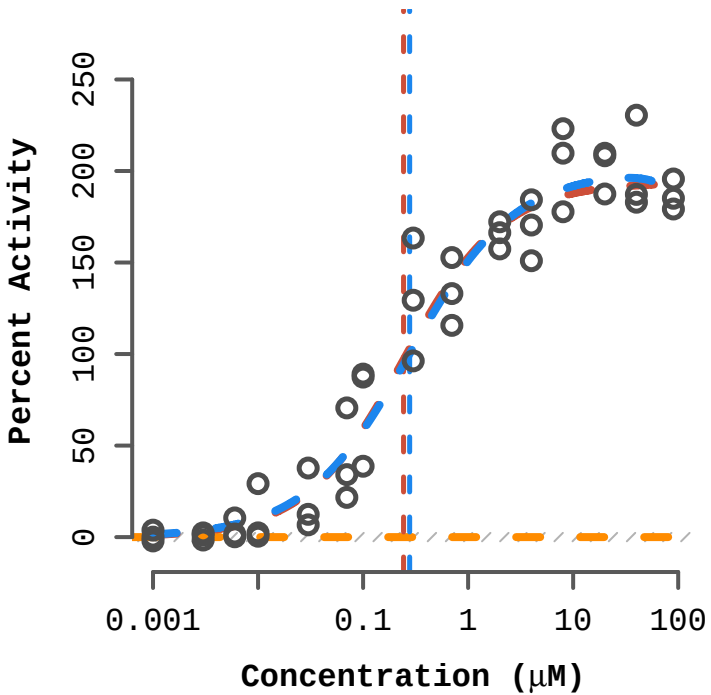
	tp	ga	gw
val:	203	-0.542	0.949
sd:	3.89	0.0457	0.0647

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	203	-0.542	0.949	3.93	14.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	1144.71	757.73	761.73
PROB:	0	0.88	0.12
RMSE:	130.69	25.53	25.53

MAX_MEAN: 215 MAX_MED: 217 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Corticosterone
CHID: 22474 CASRN: 50-22-6
SPID(S): Tox21_201366
M4ID: 12480886

HILL MODEL (in red):

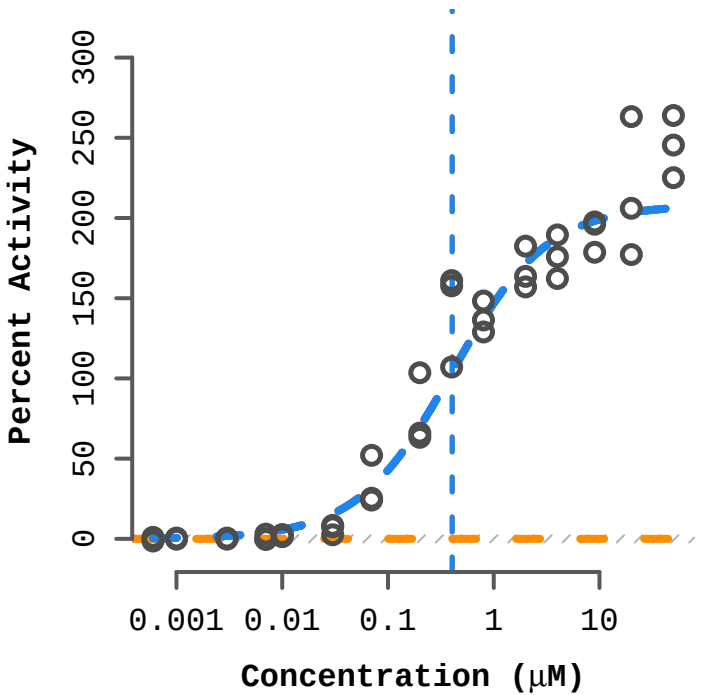
	tp	ga	gw
val:	194	-0.615	0.927
sd:	5.85	0.0887	0.11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	200	-0.557	0.871	2.4	2.65
sd:	9.9	0.11	0.115	0.873	5.4

	CNST	HILL	GNLS
AIC:	574.33	397.02	399.86
PROB:	0	0.81	0.19
RMSE:	131.29	18.31	18.16

MAX_MEAN: 204 MAX_MED: 210 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Corticosterone
CHID: 22474 CASRN: 50-22-6
SPID(S): Tox21_110879_1
M4ID: 12484048

HILL MODEL (in red):

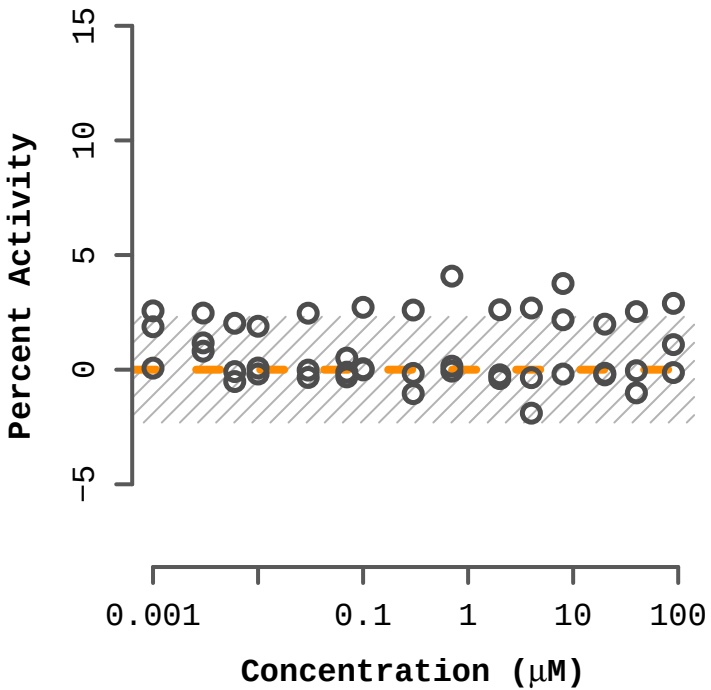
	tp	ga	gw
val:	208	-0.393	0.967
sd:	10.3	0.0804	0.122

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	208	-0.393	0.967	3.66	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	570.69	395.5	399.5
PROB:	0	0.88	0.12
RMSE:	129.43	20.88	20.88

MAX_MEAN: 245 MAX_MED: 245 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

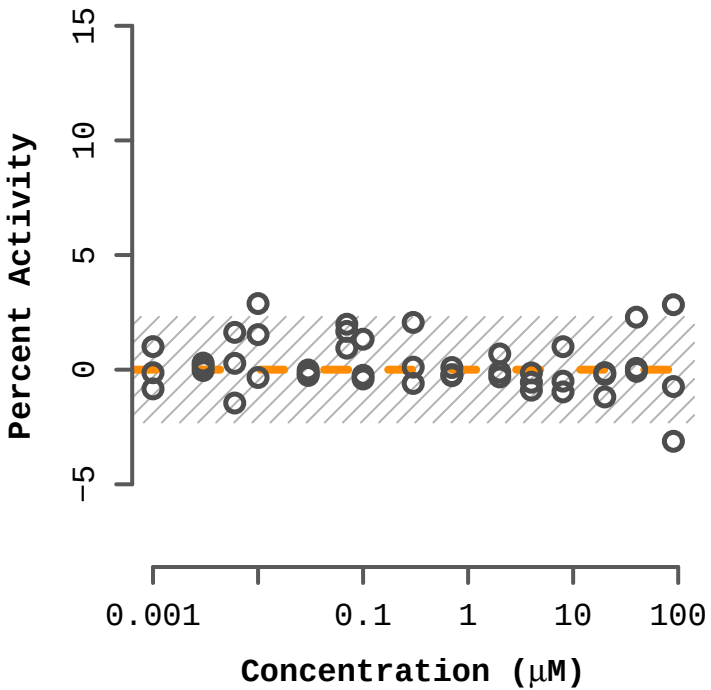
NAME: 2-Ethylphenol
CHID: 22479 **CASRN:** 90-00-6
SPID(S): Tox21_302885
M4ID: 12476248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

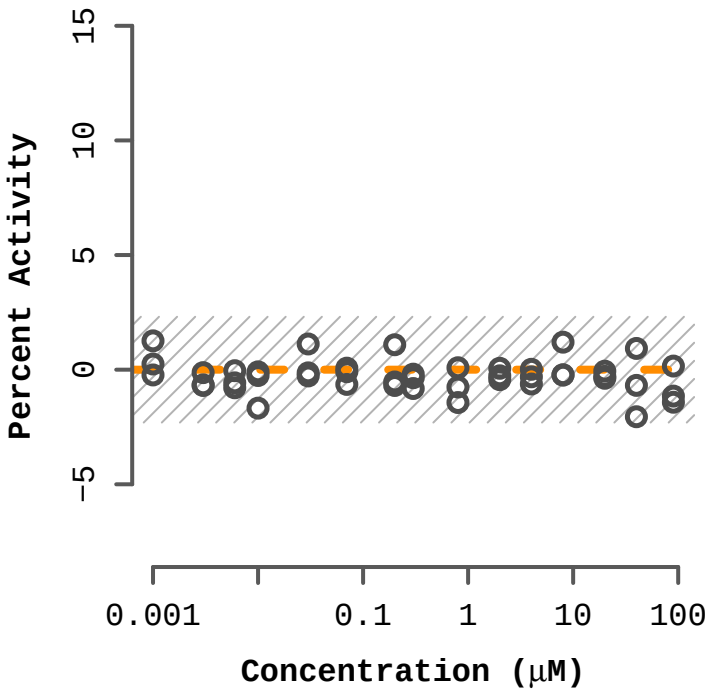
NAME: 2-Ethylphenol
CHID: 22479 **CASRN:** 90-00-6
SPID(S): Tox21_202327
M4ID: 12479925

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

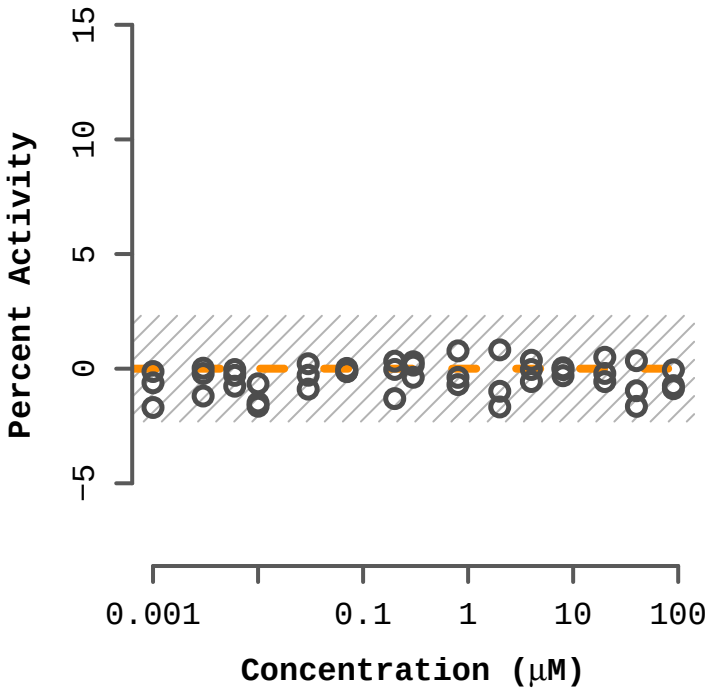
NAME: 3-Ethylphenol
CHID: 22480 **CASRN:** 620-17-7
SPID(S): Tox21_302992
M4ID: 12476141

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.426 **MAX_MED:** 0.248 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

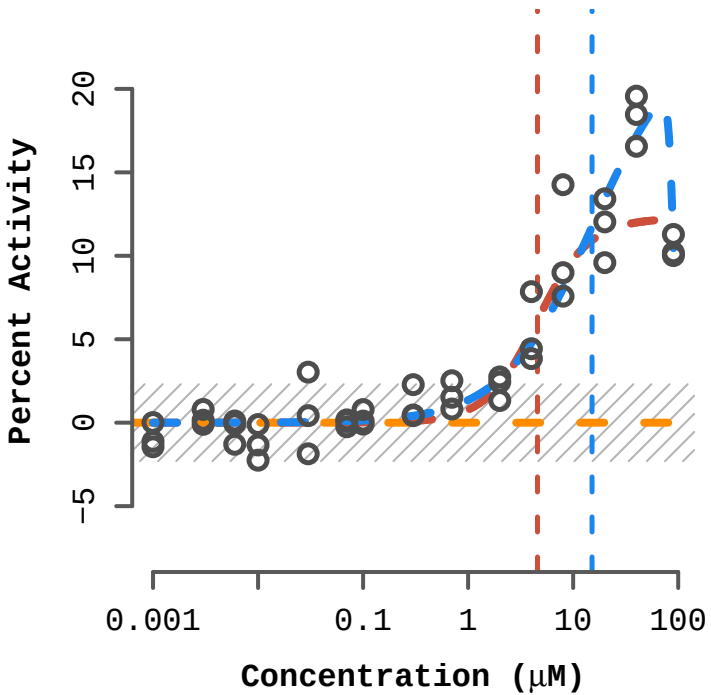
NAME: 3-Ethylphenol
CHID: 22480 CASRN: 620-17-7
SPID(S): Tox21_201623
M4ID: 12480629

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.028 MAX_MED: 0.155 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dihydroxymethoxychlor olefin
CHID: 22485 CASRN: 14868-03-2
SPID(S): Tox21_200558
M4ID: 12481694

HILL MODEL (in red):

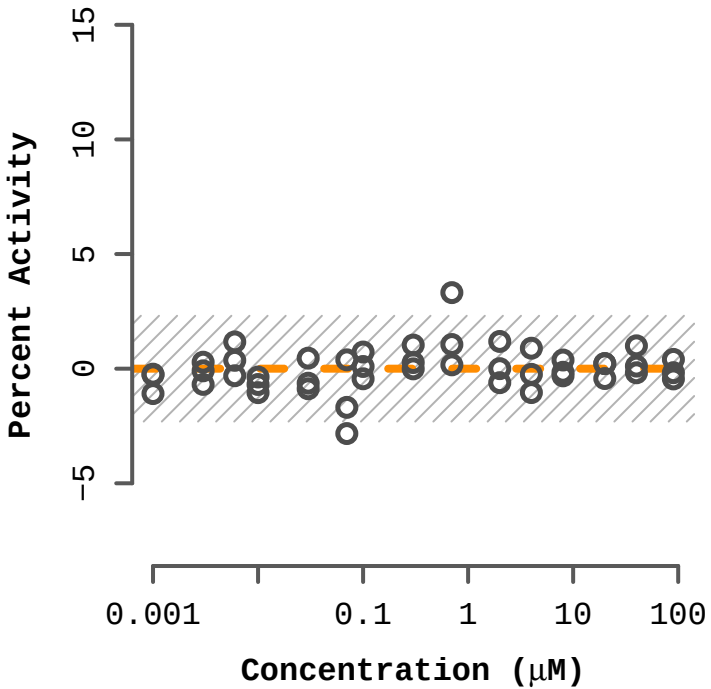
	tp	ga	gw
val:	12.3	0.66	1.77
sd:	1.06	0.0756	0.447

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.5	1.18	1.03	1.96	17.8
sd:	3.7	0.156	0.139	0.00429	54.5

	CNST	HILL	GNLS
AIC:	298.19	194.67	167.73
PROB:	0	0	1
RMSE:	7.06	2.19	1.56

MAX_MEAN: 18.2 MAX_MED: 18.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

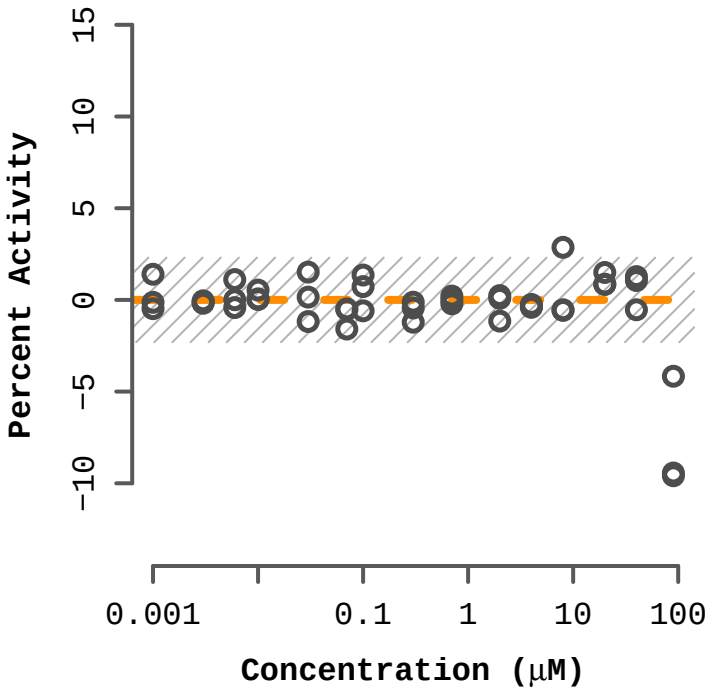
NAME: E−Cinnamic acid
CHID: 22489 CASRN: 140−10−3
SPID(S): Tox21_302137
M4ID: 12476996

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.51 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

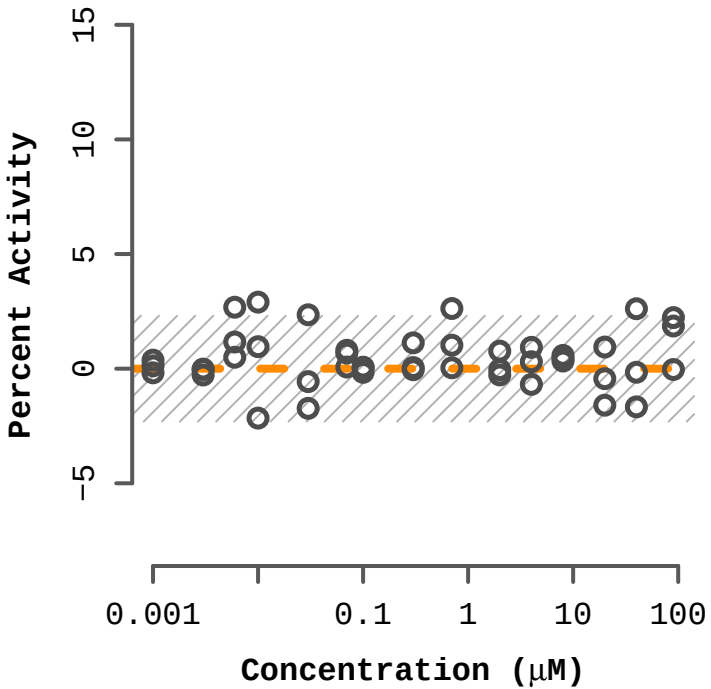
NAME: 4-Dodecylphenol
CHID: 22508 **CASRN:** 104-43-8
SPID(S): Tox21_301020
M4ID: 12478113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.89	NA	NA
PROB:	1	NA	NA
RMSE:	2.26	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

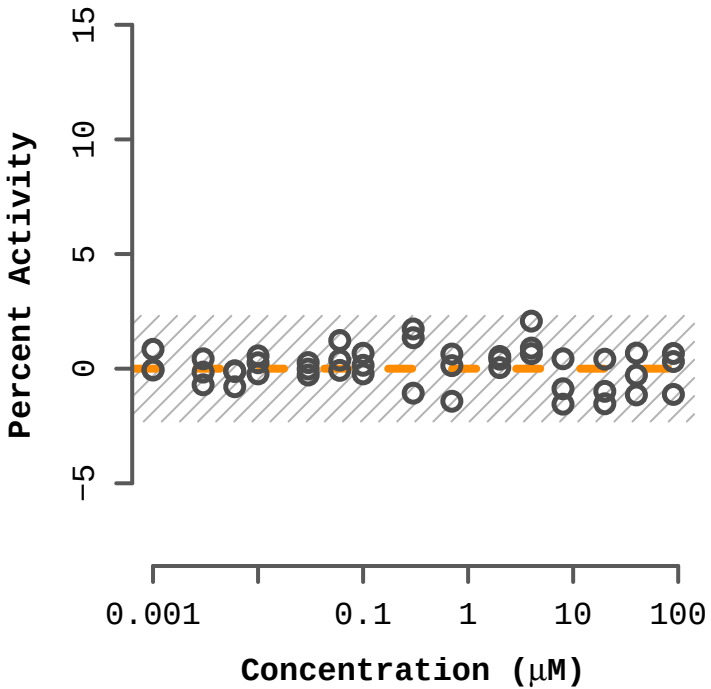
NAME: 4-Chloro-2-methylphenol
CHID: 22510 **CASRN:** 1570-64-5
SPID(S): Tox21_302888
M4ID: 12476245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

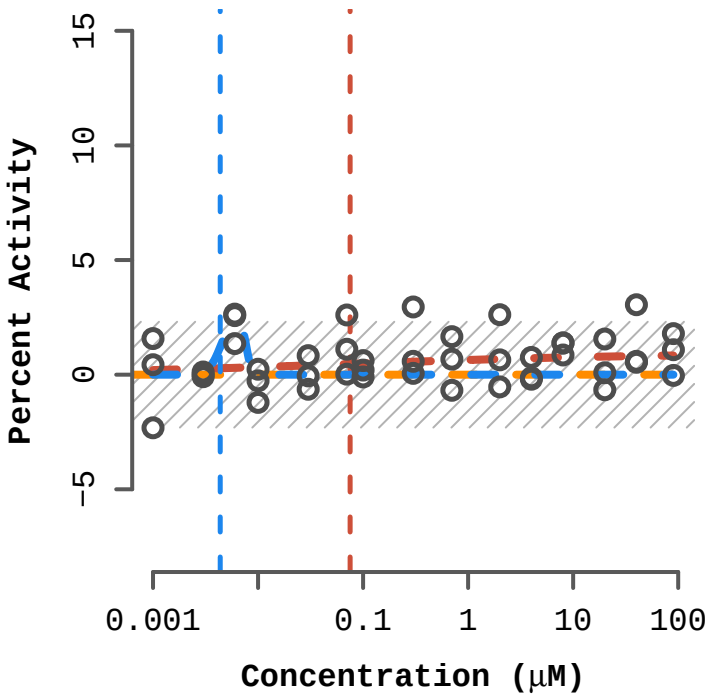
NAME: 4-Chloro-2-methylphenol
CHID: 22510 **CASRN:** 1570-64-5
SPID(S): Tox21_202018
M4ID: 12480234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Folic acid
CHID: 22519 CASRN: 59-30-3
SPID(S): Tox21_300127
M4ID: 12479003

HILL MODEL (in red):

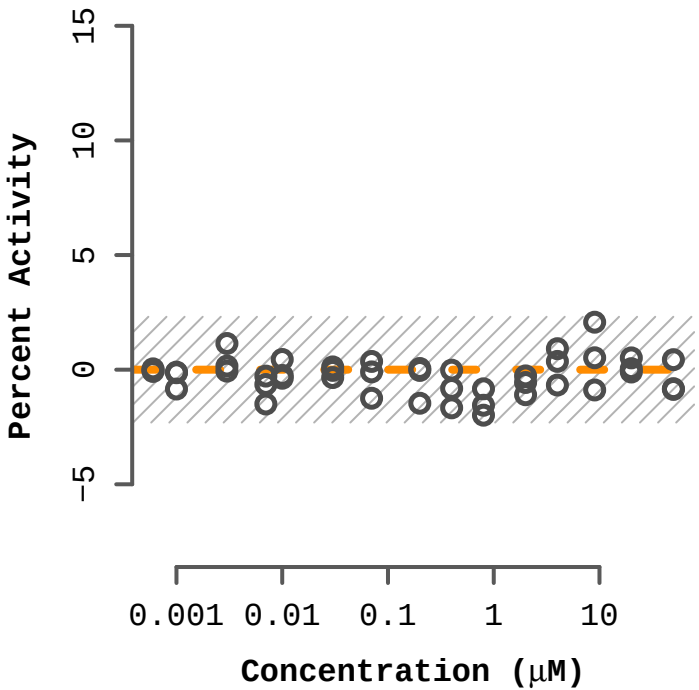
	tp	ga	gw
val:	0.936	−1.12	0.3
sd:	1.94	7.46	1.16

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.43	−2.36	8	−2.11	18
sd:	1.58	0.27	11.7	0.185	29.8

	CNST	HILL	GNLS
AIC:	154	146.76	152.83
PROB:	0.02	0.93	0.04
RMSE:	1.31	1.12	1.18

MAX_MEAN: 2.19 MAX_MED: 2.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

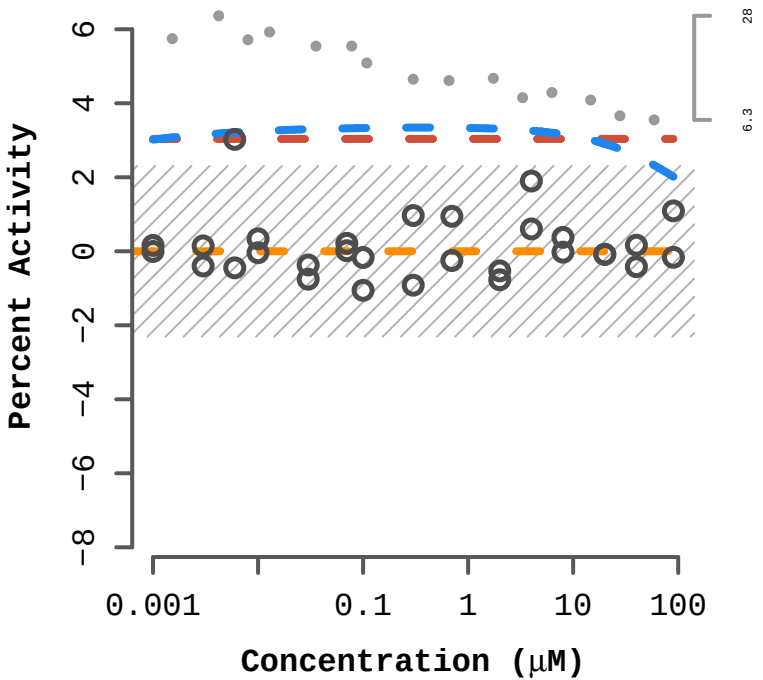
NAME: Folic acid
CHID: 22519 **CASRN:** 59-30-3
SPID(S): Tox21_111559_1
M4ID: 12483618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.569 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl cinnamate
CHID: 22520 CASRN: 103-36-6
SPID(S): Tox21_302638
M4ID: 12476495 BRK

HILL MODEL (in red):

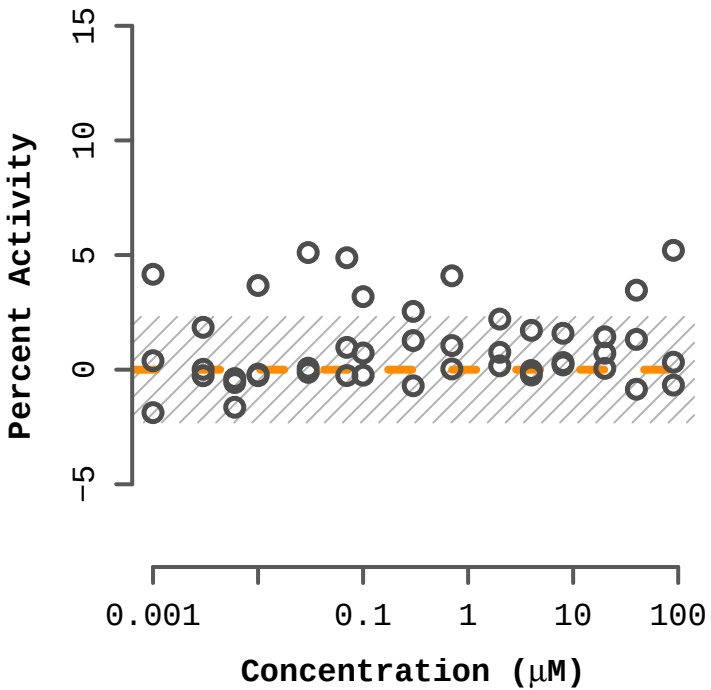
	tp	ga	gw
val:	3.04	−4.7	2.18
sd:	1.17	878	911

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.38	−5	0.459	2.13	0.952
sd:	12.1	158	43.9	3.47	8.19

	CNST	HILL	GNLS
AIC:	331.19	328.83	332.71
PROB:	0.21	0.69	0.1
RMSE:	10.35	9.06	9

MAX_MEAN: 9.2 **MAX_MED:** 3.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

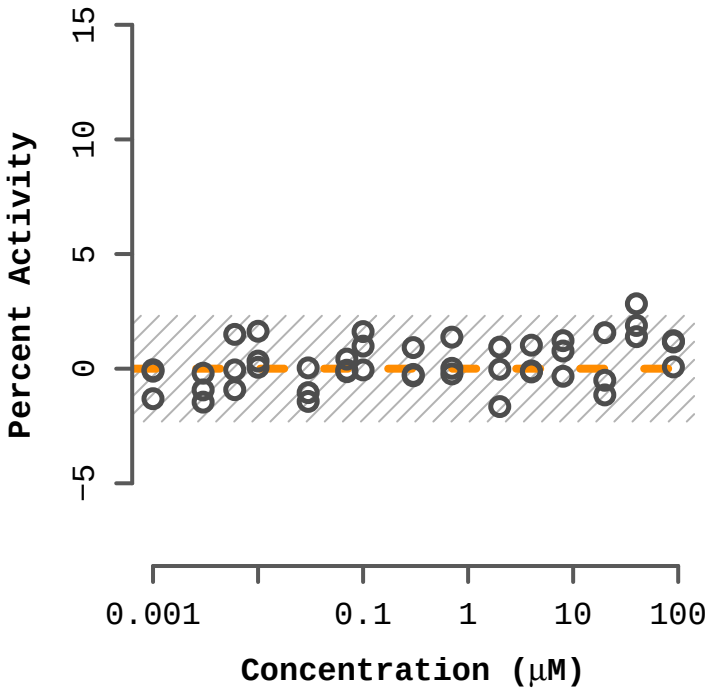
NAME: DINP
CHID: 22521 CASRN: 28553-12-0
SPID(S): Tox21_200745
M4ID: 12481507

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 1.87 MAX_MED: 1.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

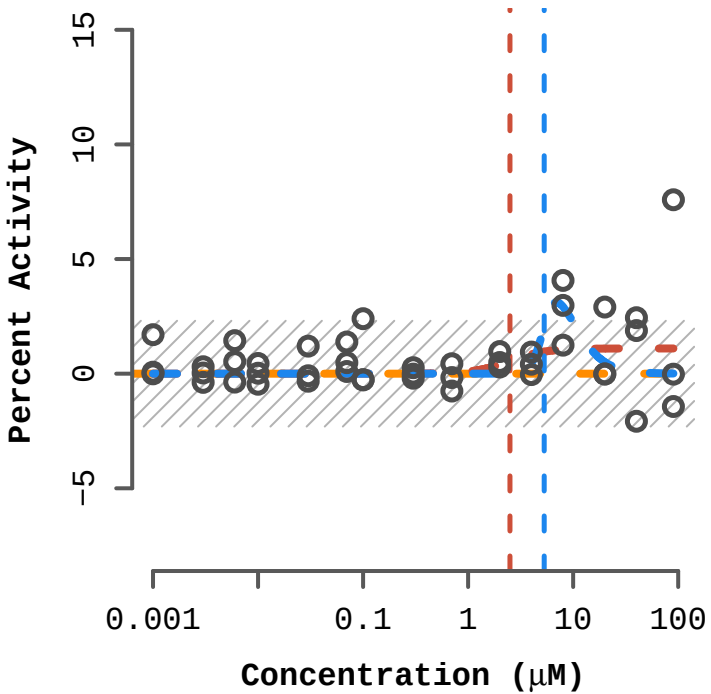
NAME: Diisobutyl phthalate
CHID: 22522 **CASRN:** 84-69-5
SPID(S): Tox21_300612
M4ID: 12478521

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diisobutyl phthalate
CHID: 22522 CASRN: 84-69-5
SPID(S): Tox21_202429
M4ID: 12479823

HILL MODEL (in red):

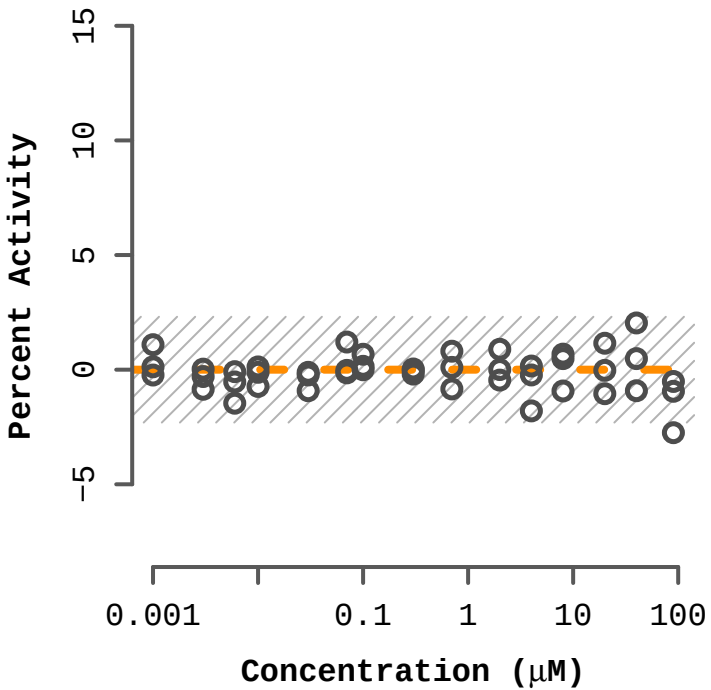
	tp	ga	gw
val:	1.1	0.398	2.58
sd:	0.577	0.396	2.19

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.93	0.724	7.86	0.974	2.88
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	156.88	155.03	152
PROB:	0.07	0.17	0.77
RMSE:	1.69	1.48	1.5

MAX_MEAN: 2.77 **MAX_MED:** 2.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

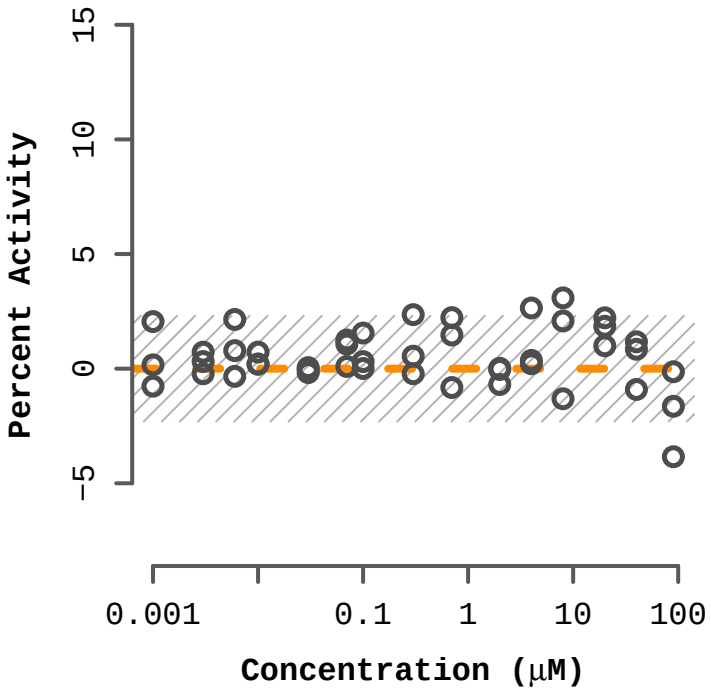
NAME: Heptylparaben
CHID: 22523 **CASRN:** 1085-12-7
SPID(S): Tox21_303458
M4ID: 12475682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.536 **MAX_MED:** 0.484 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

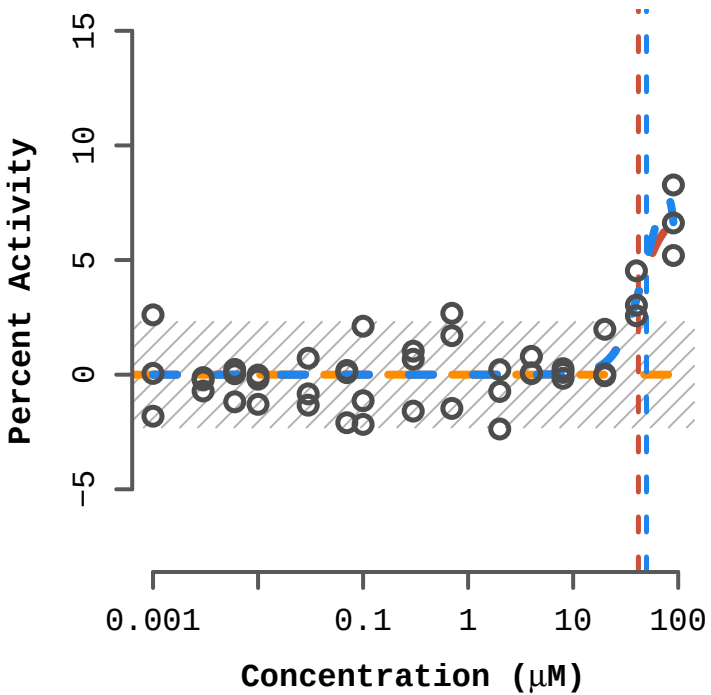
NAME: Heptylparaben
CHID: 22523 **CASRN:** 1085-12-7
SPID(S): Tox21_200540
M4ID: 12481712

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thalidomide
CHID: 22524 CASRN: 50-35-1
SPID(S): Tox21_300580
M4ID: 12478553

HILL MODEL (in red):

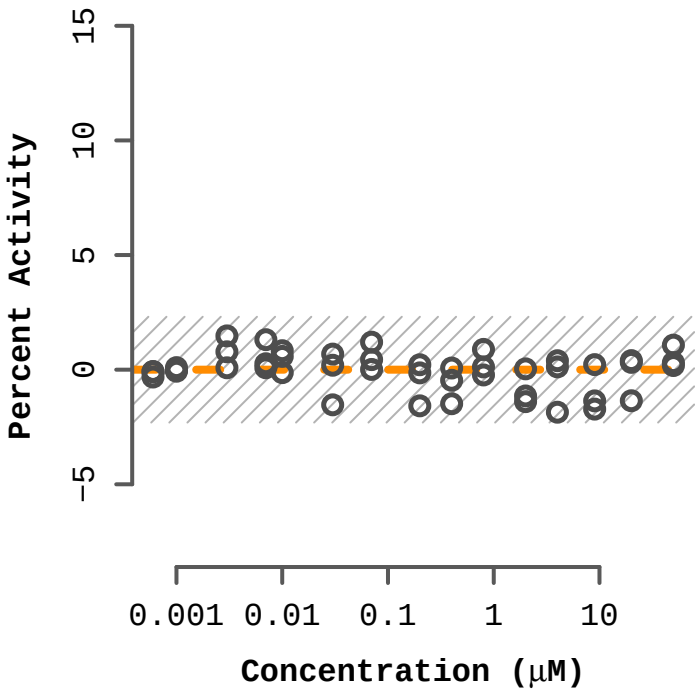
	tp	ga	gw
val:	7.11	1.62	3.47
sd:	1.45	0.0831	2.26

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.93	1.7	3.18	1.99	14.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	192.51	154.19	158.18
PROB:	0	0.88	0.12
RMSE:	2.28	1.2	1.2

MAX_MEAN: 6.7 MAX_MED: 6.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

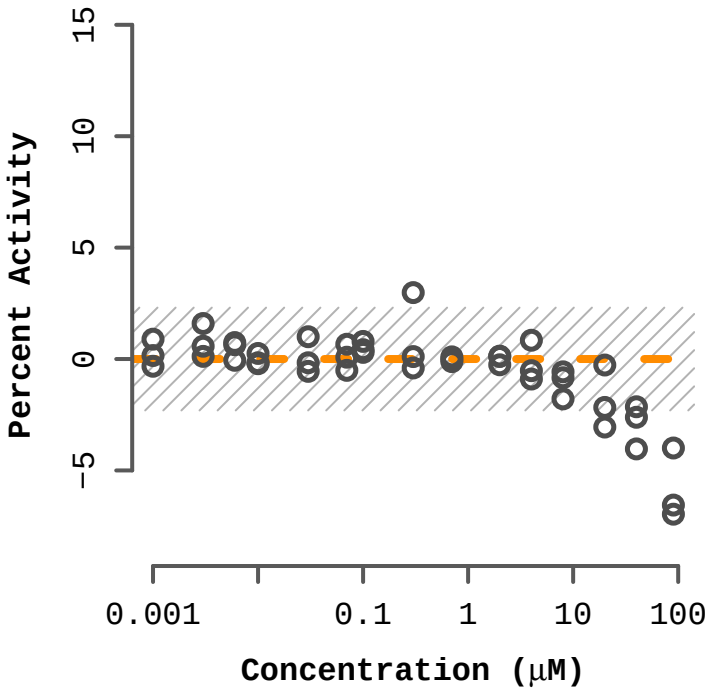
NAME: Thalidomide
CHID: 22524 **CASRN:** 50-35-1
SPID(S): Tox21_110275_1
M4ID: 12484492

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.782 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

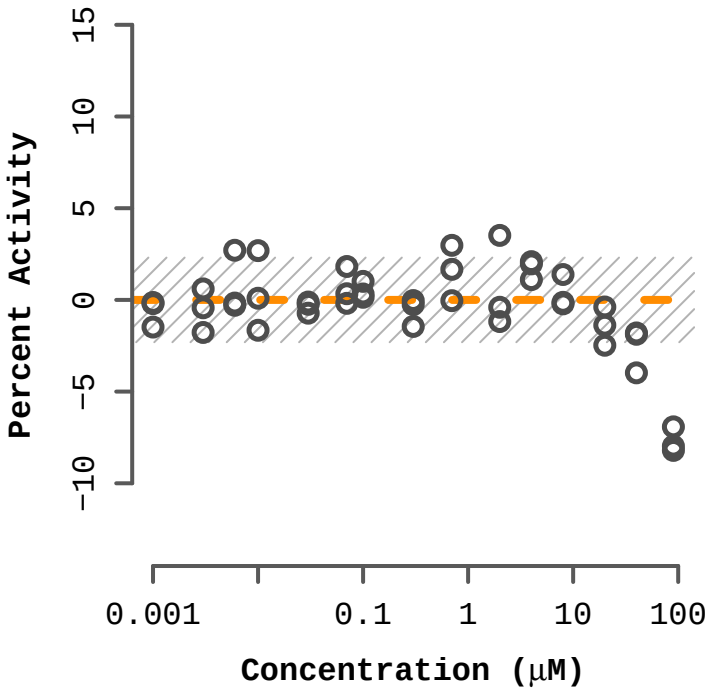
NAME: 2-Ethylhexylparaben
CHID: 22525 **CASRN:** 5153-25-3
SPID(S): Tox21_302793
M4ID: 12476340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 0.899 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

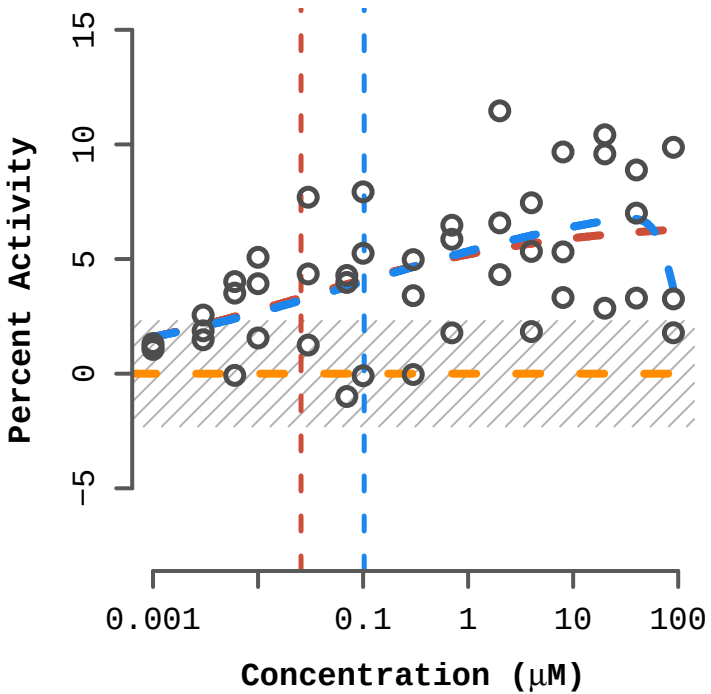
NAME: 2-Ethylhexylparaben
CHID: 22525 CASRN: 5153-25-3
SPID(S): Tox21_202354
M4ID: 12479898

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.48	NA	NA

MAX_MEAN: 1.72 MAX_MED: 1.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzylparaben
CHID: 22526 CASRN: 94-18-8
SPID(S): Tox21_302330
M4ID: 12476803

HILL MODEL (in red):

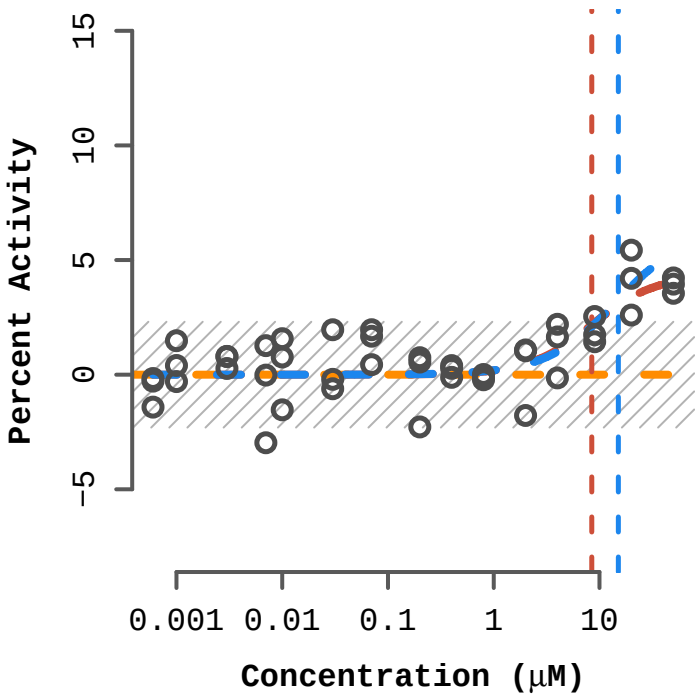
	tp	ga	gw
val:	6.63	−1.59	0.353
sd:	2.04	1.04	0.231

GAIN-LOSS MODEL (in blue):

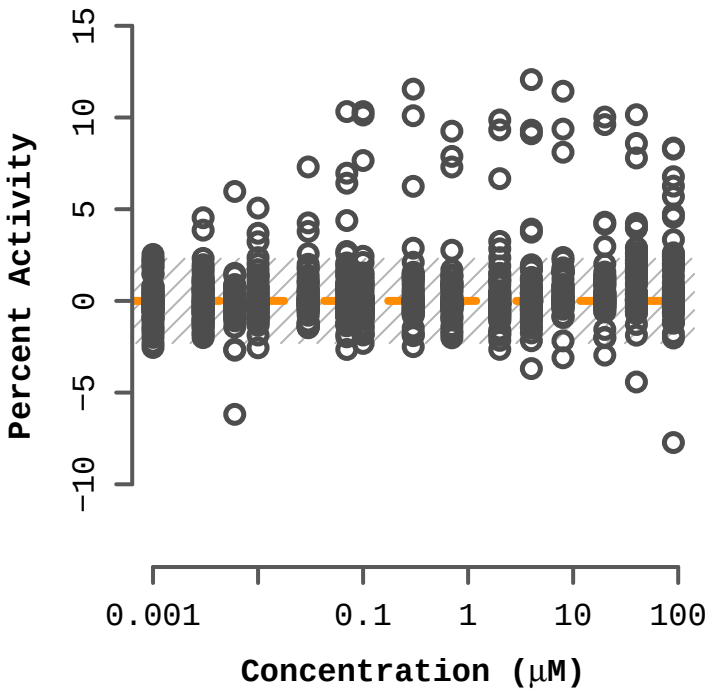
	tp	ga	gw	la	lw
val:	8.03	−0.989	0.3	1.96	4.69
sd:	5.73	2.5	0.26	0.103	15

	CNST	HILL	GNLS
AIC:	284.86	227.4	229.26
PROB:	0	0.72	0.28
RMSE:	5.34	2.65	2.63

MAX_MEAN: 7.62 MAX_MED: 9.59 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzylparaben
CHID:    22526   CASRN: 94-18-8
SPID(S): Tox21_112088_1
M4ID:    12483328

HILL MODEL (in red):
      tp       ga       gw
val:  4.34     0.927    1.46
sd:   0.801    0.18     0.751

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.52     1.18     1.29     1.75     8.49
sd:   4.34     0.451    0.63     0.0994   18.3

      CNST        HILL        GNLS
AIC:  186.57      145.22      148.17
PROB: 0           0.81        0.19
RMSE: 1.91        1.1         1.09

MAX_MEAN: 4.08      MAX_MED: 4.2       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

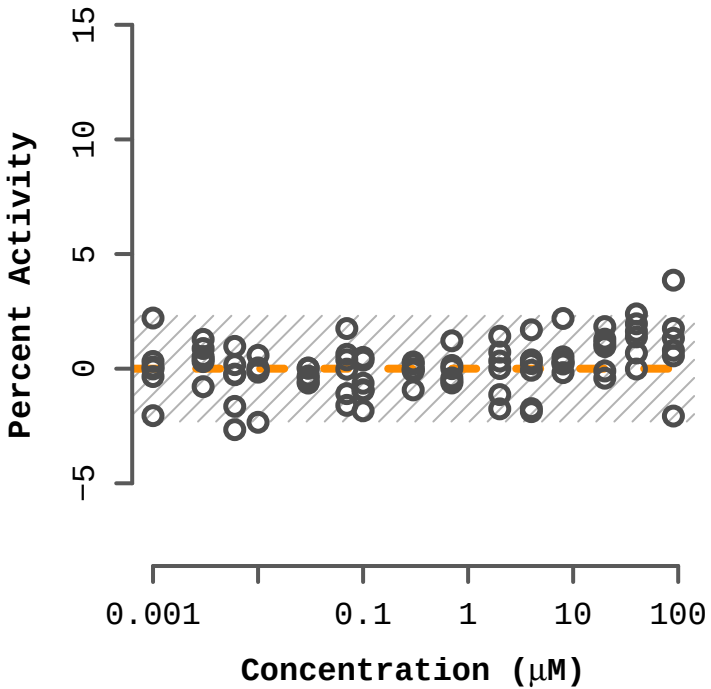
NAME: Propylparaben
CHID: 22527 **CASRN:** 94-13-3
SPID(S): Tox21_400012
M4ID: 12475125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2888.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.483 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

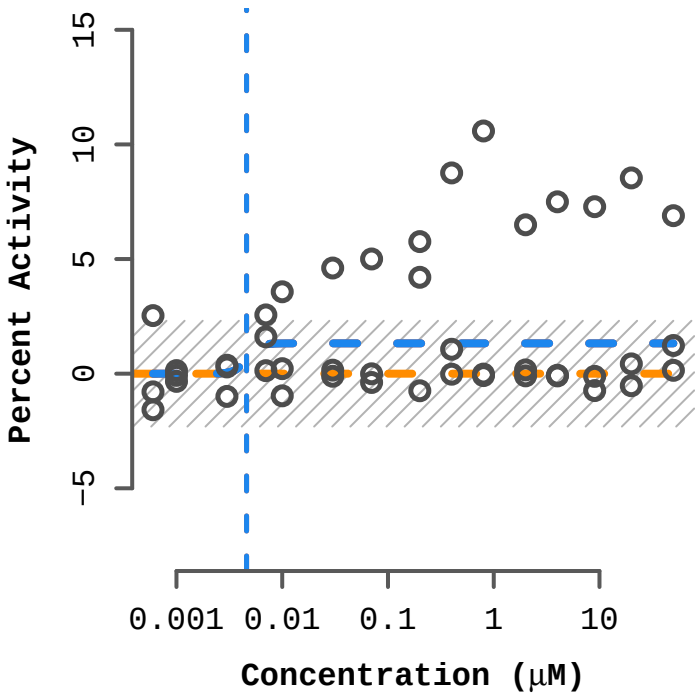
NAME: Ethylparaben
CHID: 22528 **CASRN:** 120-47-8
SPID(S): Tox21_300335
M4ID: 12478797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	278.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethylparaben
CHID: 22528 **CASRN:** 120-47-8
SPID(S): Tox21_111961_1
M4ID: 12483405

HILL MODEL (in red):

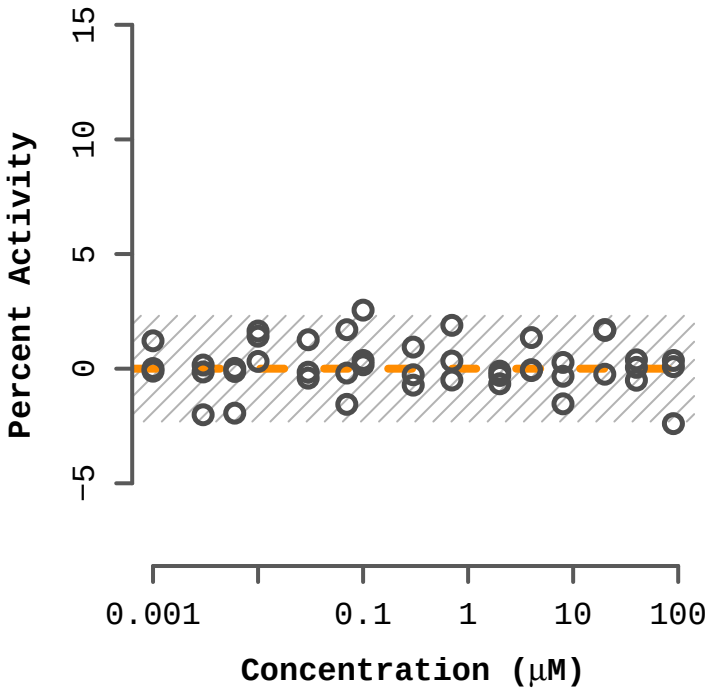
	tp	ga	gw
val:	1.32	−2.34	8
sd:	0.509	0.554	26.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.32	−2.34	8	3.49	3.97
sd:	0.509	0.554	26.3	2010	4480

	CNST	HILL	GNLS
AIC:	236.65	233.91	237.91
PROB:	0.18	0.72	0.1
RMSE:	3.64	3.13	3.13

MAX_MEAN: 3.5 **MAX_MED:** 4.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

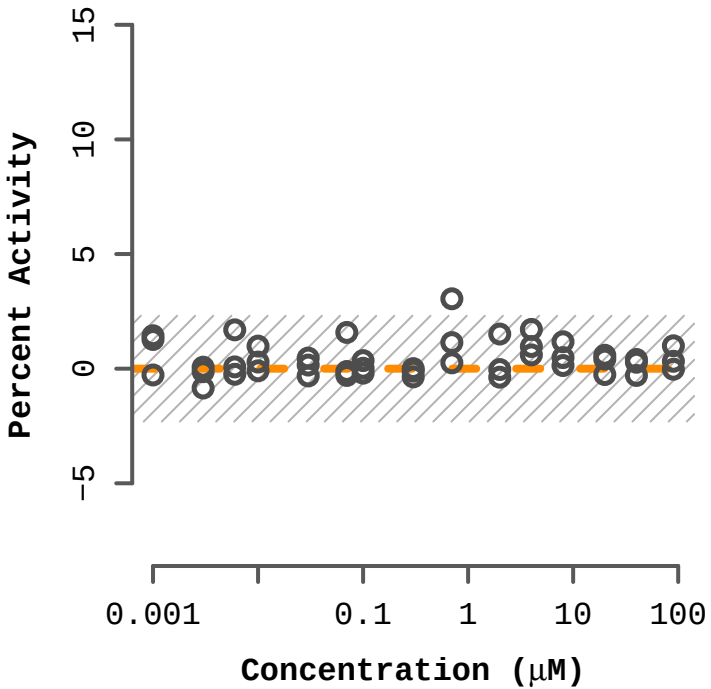
NAME: Methylparaben
CHID: 22529 CASRN: 99-76-3
SPID(S): Tox21_300009
M4ID: 12479121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.13 MAX_MED: 1.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

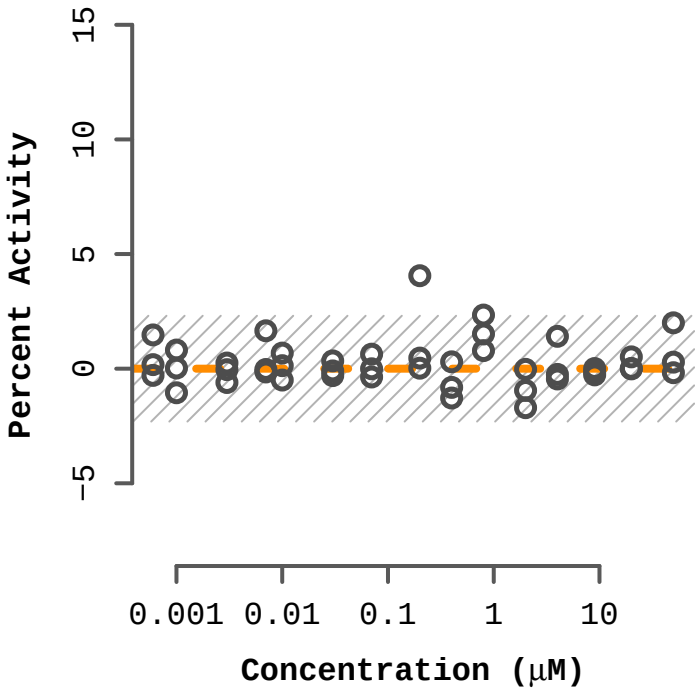
NAME: Methylparaben
CHID: 22529 **CASRN:** 99-76-3
SPID(S): Tox21_202318
M4ID: 12479934

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

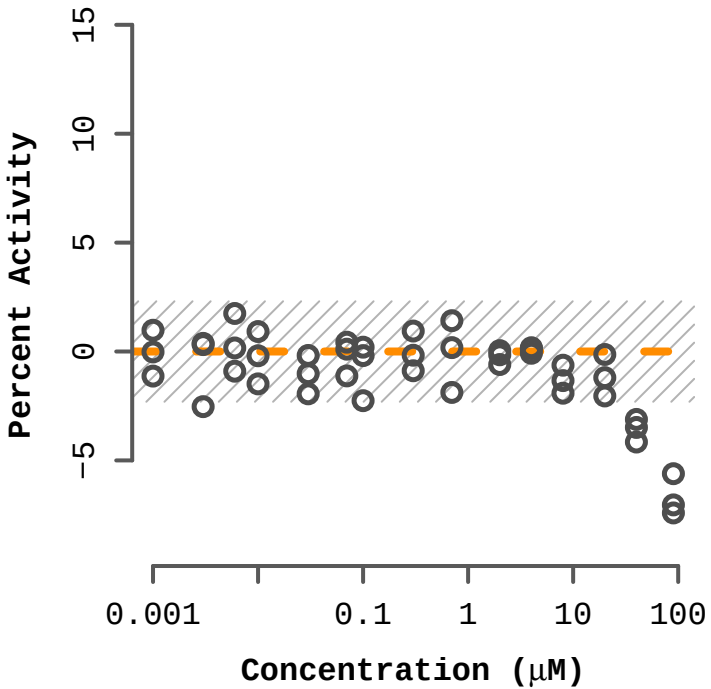
NAME: Methylparaben
CHID: 22529 **CASRN:** 99-76-3
SPID(S): Tox21_111616_1
M4ID: 12483584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

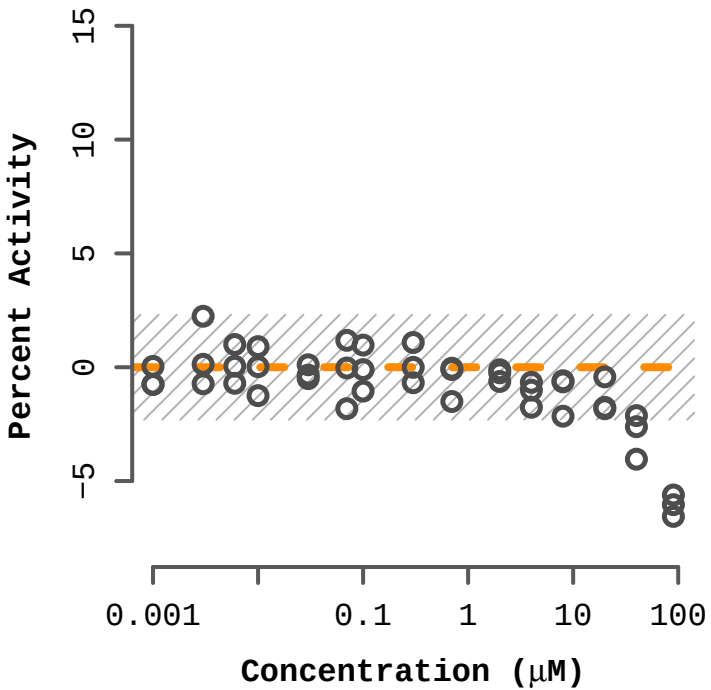
NAME: 4-Cumylphenol
CHID: 22536 **CASRN:** 599-64-4
SPID(S): Tox21_300056
M4ID: 12479074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 0.337 **MAX_MED:** 0.319 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

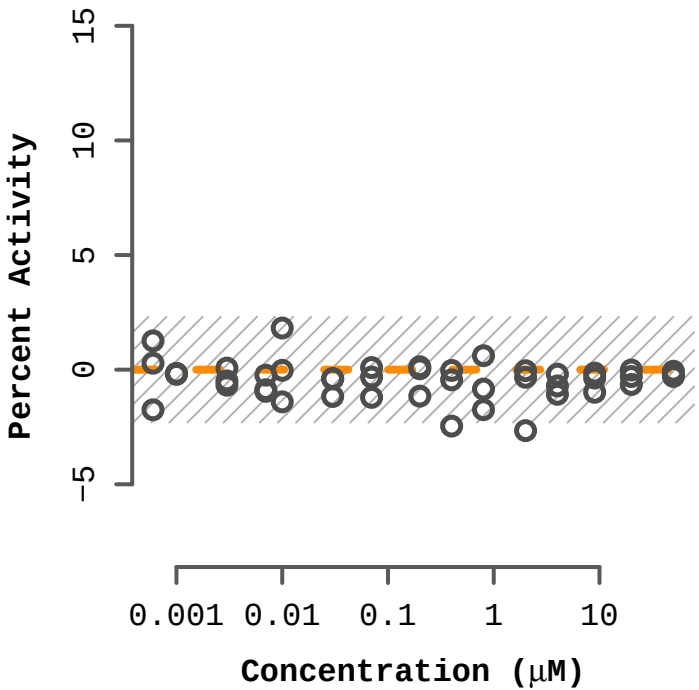
NAME: 4-Cumylphenol
CHID: 22536 **CASRN:** 599-64-4
SPID(S): Tox21_201297
M4ID: 12480955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

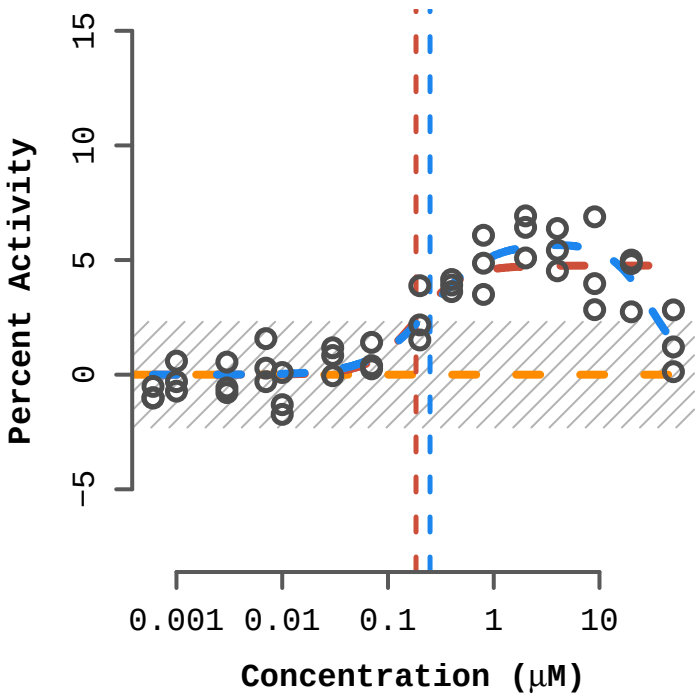
NAME: Acemetacin
CHID: 22540 **CASRN:** 53164-05-9
SPID(S): Tox21_113473_1
M4ID: 12482639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.129 **MAX_MED:** 0.283 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acenocoumarol
CHID: 22541 **CASRN:** 152-72-7
SPID(S): Tox21_110430_1
M4ID: 12484364

HILL MODEL (in red):

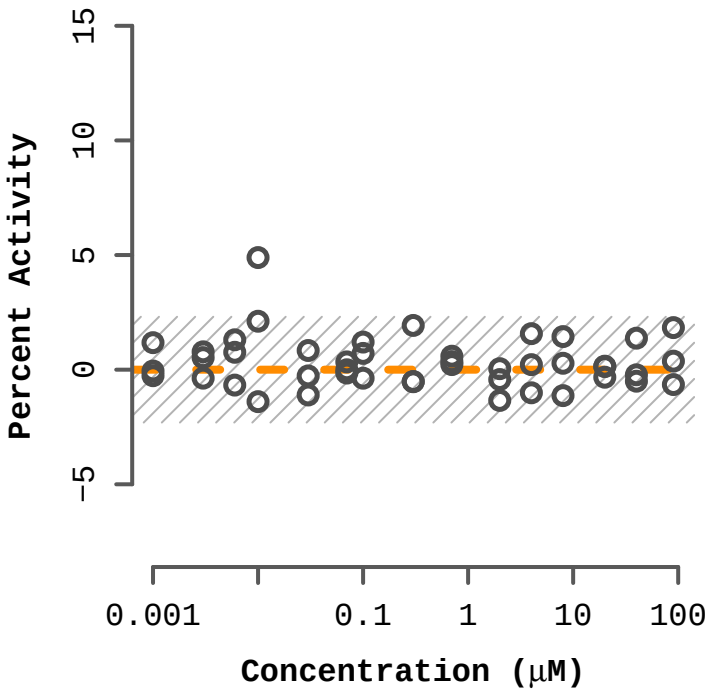
	tp	ga	gw
val:	4.76	−0.735	2.02
sd:	0.365	0.114	0.711

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.79	−0.602	1.56	1.48	2.23
sd:	0.62	0.104	0.455	0.11	1.56

	CNST	HILL	GNLS
AIC:	240.53	159.67	142.17
PROB:	0	0	1
RMSE:	3.33	1.36	0.98

MAX_MEAN: 6.15 **MAX_MED:** 6.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

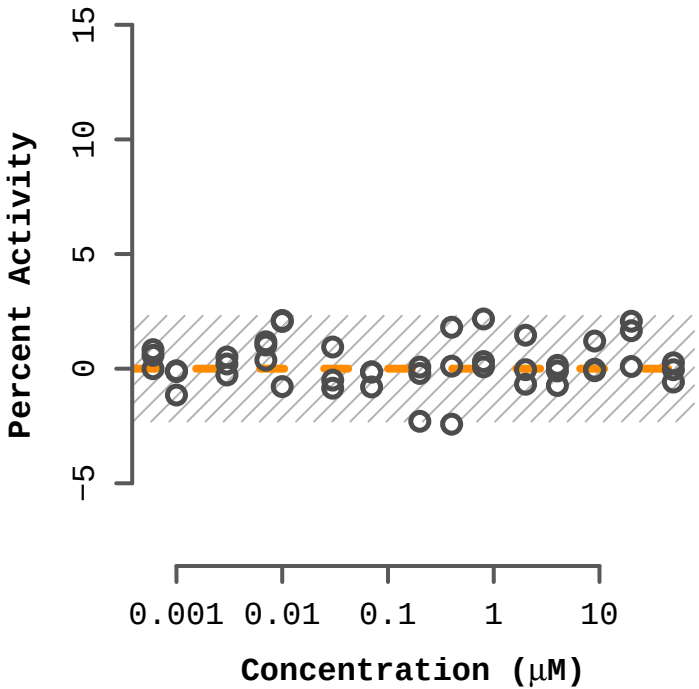
NAME: Acetanilide
CHID: 22543 CASRN: 103-84-4
SPID(S): Tox21_200925
M4ID: 12481327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.87 MAX_MED: 2.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

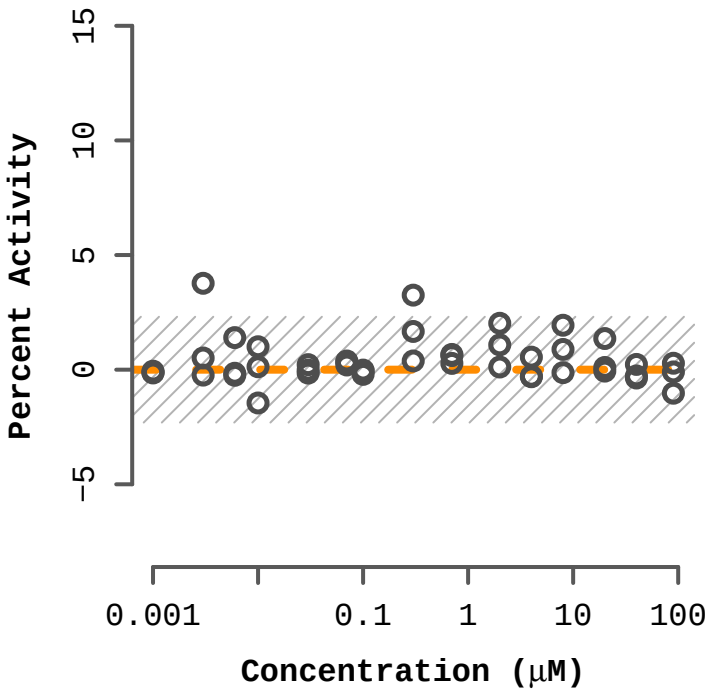
NAME: Acetanilide
CHID: 22543 **CASRN:** 103-84-4
SPID(S): Tox21_111113_1
M4ID: 12483899

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

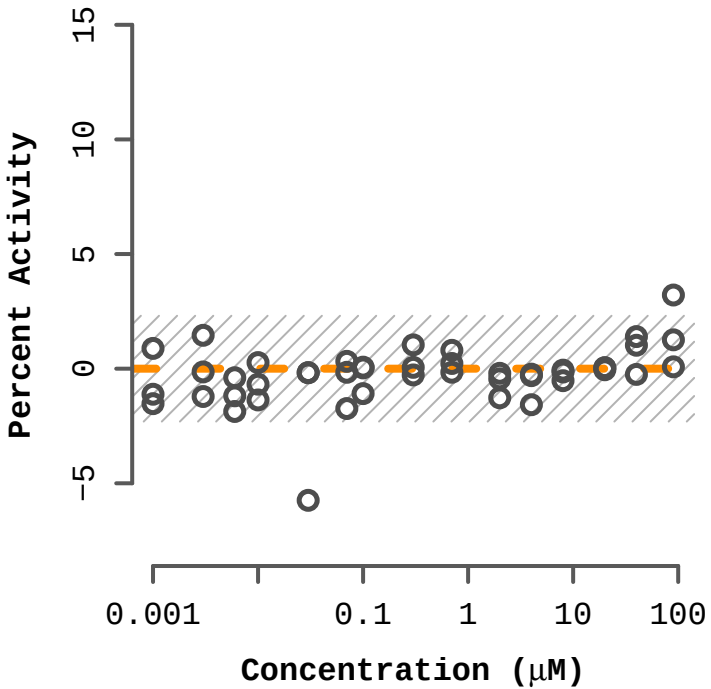
NAME: Acetazolamide
CHID: 22544 **CASRN:** 59-66-5
SPID(S): Tox21_302773
M4ID: 12476360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

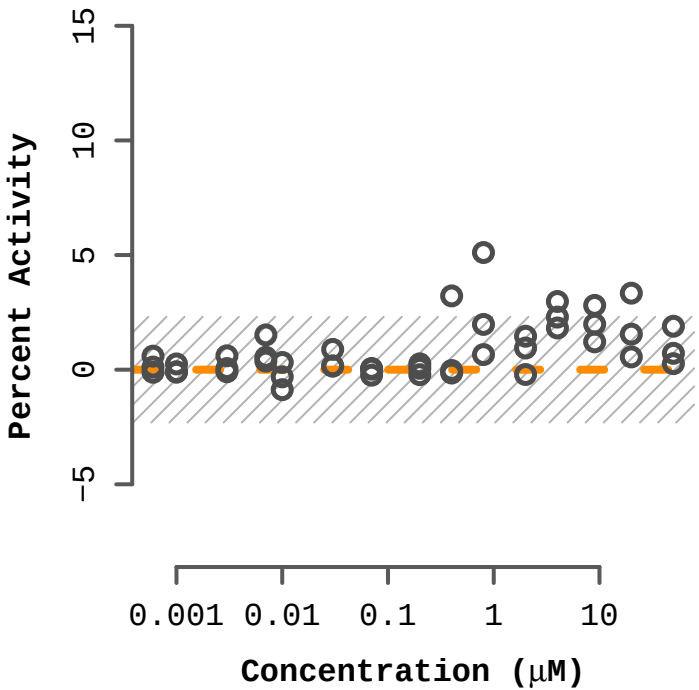
NAME: Acetazolamide
CHID: 22544 CASRN: 59-66-5
SPID(S): Tox21_201559
M4ID: 12480693

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.52 MAX_MED: 1.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

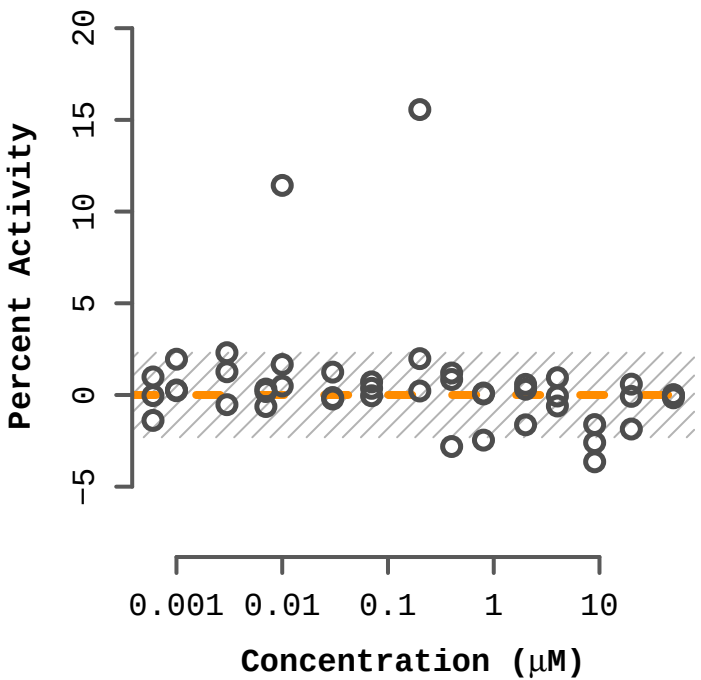
NAME: Acetazolamide
CHID: 22544 **CASRN:** 59-66-5
SPID(S): Tox21_110078_1
M4ID: 12484674

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.58 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

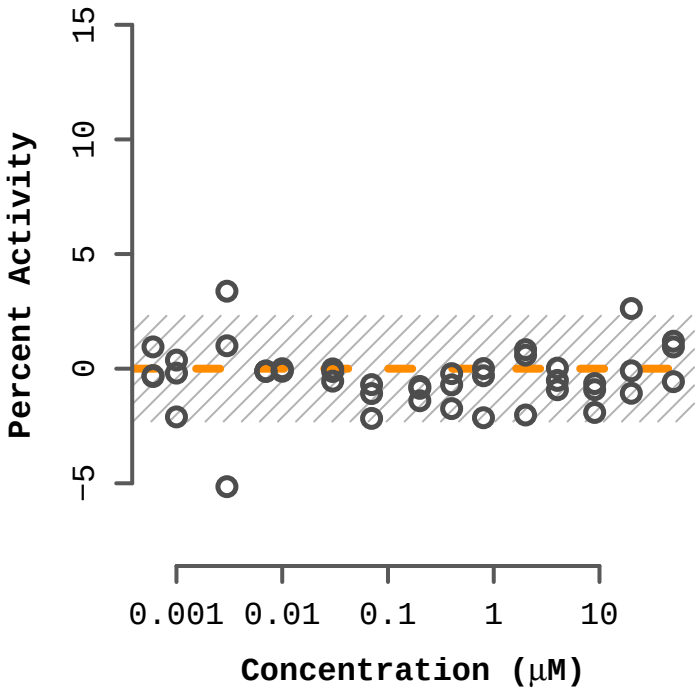
NAME: Acetohydroxamic acid
CHID: 22546 **CASRN:** 546-88-3
SPID(S): Tox21_111301_1
M4ID: 12483780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.17	NA	NA
PROB:	1	NA	NA
RMSE:	3.14	NA	NA

MAX_MEAN: 5.92 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

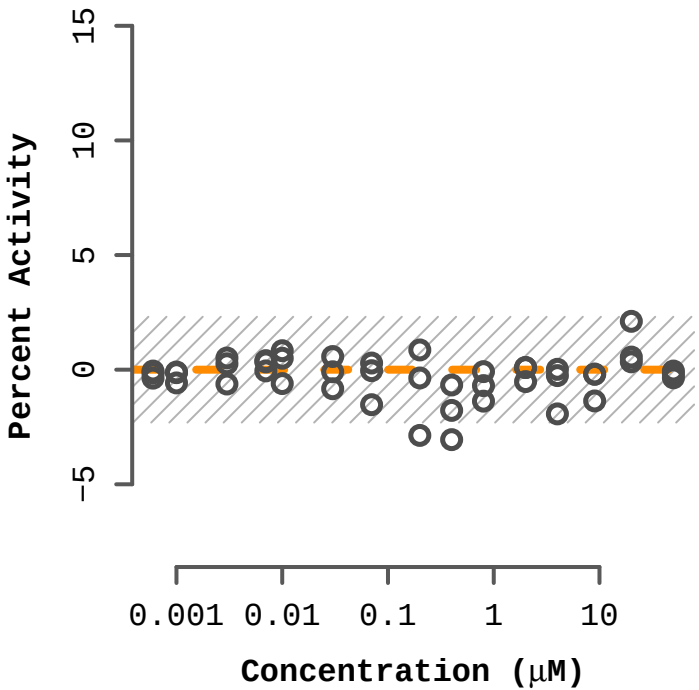
NAME: Acetrizoic acid
CHID: 22549 **CASRN:** 85-36-9
SPID(S): Tox21_111423_1
M4ID: 12483699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

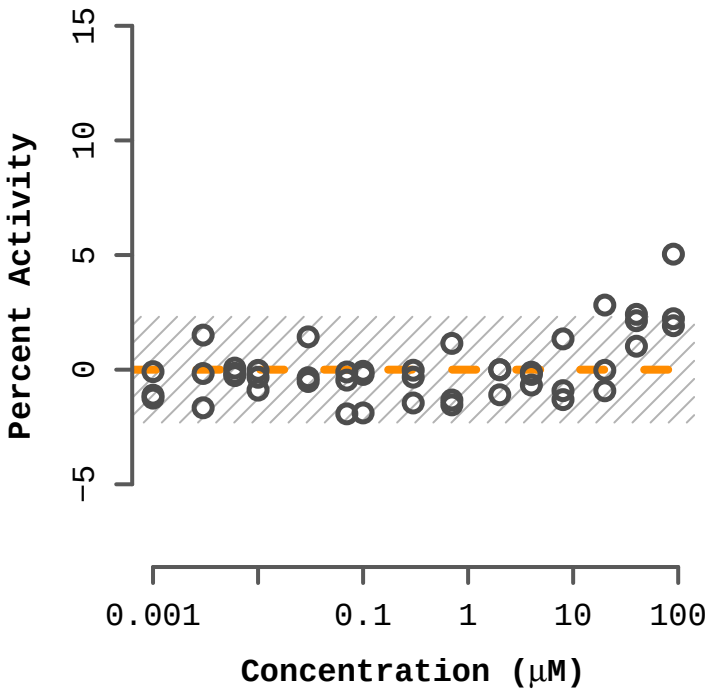
NAME: Acyclovir
CHID: 22556 **CASRN:** 59277-89-3
SPID(S): Tox21_110075_1
M4ID: 12484677

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.552 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

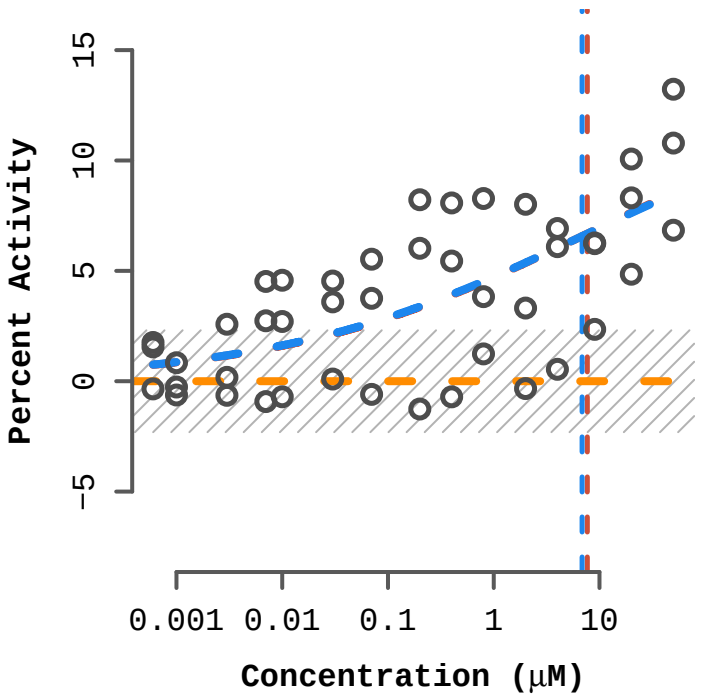
NAME: Adenine
CHID: 22557 **CASRN:** 73-24-5
SPID(S): Tox21_302108
M4ID: 12477025

HILL MODEL: Not applicable.

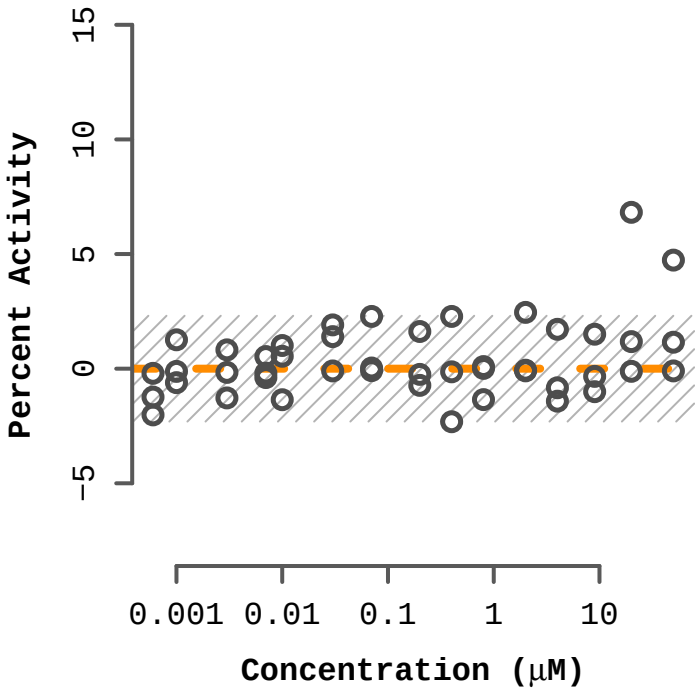
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 3.06 **MAX_MED:** 2.22 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Adenine
CHID:    22557   CASRN: 73-24-5
SPID(S): Tox21_111348_1
M4ID:    12483748

HILL MODEL (in red):
      tp       ga       gw
val:  13.4     0.885    0.3
sd:   48.4     10.7     0.505

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.1     0.835    0.3      3.7      3.97
sd:   27.6     6.28     0.302    1370     2720

      CNST        HILL        GNLS
AIC:  280.38      230.82      234.82
PROB: 0           0.88        0.12
RMSE: 5.19        2.73        2.73

MAX_MEAN: 10.3      MAX_MED: 10.8      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

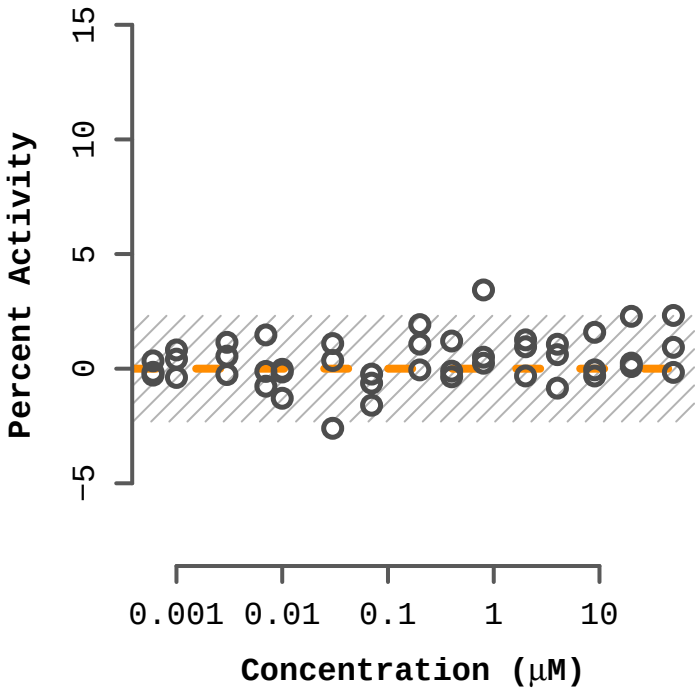
NAME: Adenosine
CHID: 22558 **CASRN:** 58-61-7
SPID(S): Tox21_110891_1
M4ID: 12484036

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2.63 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

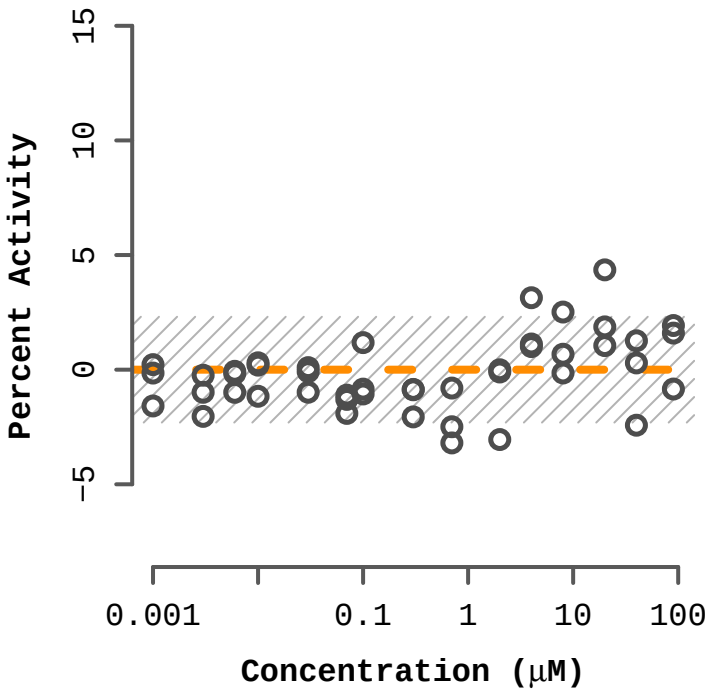
NAME: Adenosine−5−phosphate
CHID: 22560 **CASRN:** 61−19−8
SPID(S): Tox21_112046_1
M4ID: 12483350

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

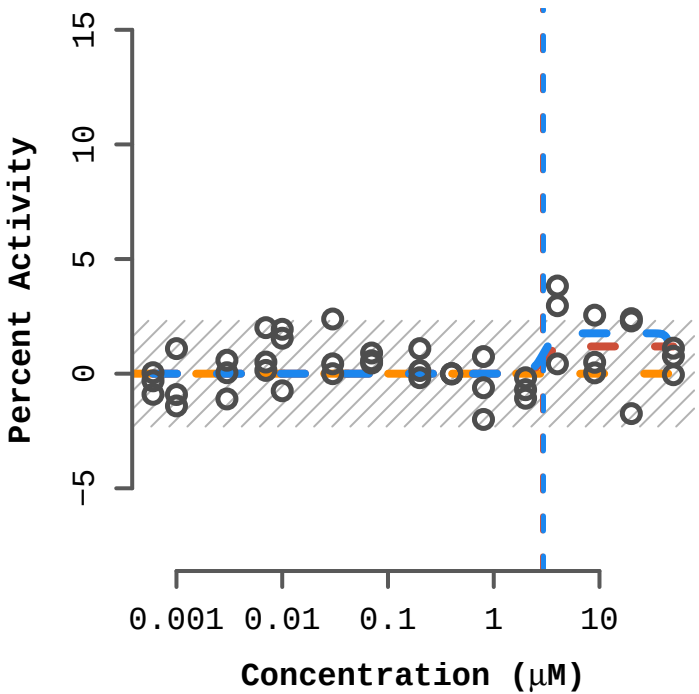
NAME: Albendazole
CHID: 22563 **CASRN:** 54965-21-8
SPID(S): Tox21_302300
M4ID: 12476833

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.43 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Albendazole
CHID: 22563 **CASRN:** 54965-21-8
SPID(S): Tox21_110659_1
M4ID: 12484199

HILL MODEL (in red):

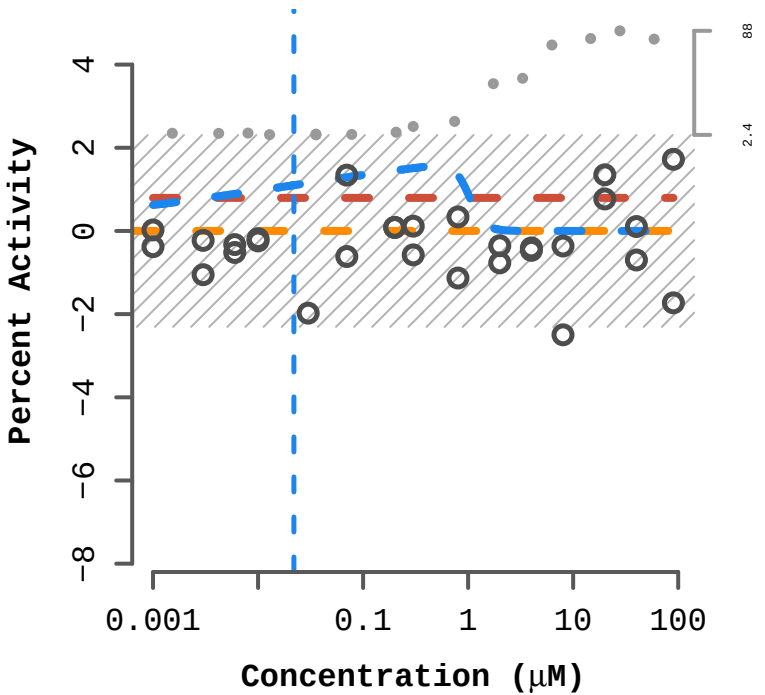
	tp	ga	gw
val:	1.19	0.462	8
sd:	0.409	0.11	5.88

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.76	0.47	8	1.68	18
sd:	0.531	0.094	5.01	0.0457	56.9

	CNST	HILL	GNLS
AIC:	153.86	150.85	152.64
PROB:	0.14	0.61	0.25
RMSE:	1.32	1.16	1.15

MAX_MEAN: 2.41 **MAX_MED:** 2.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Allopurinol
CHID: 22573 CASRN: 315-30-0
SPID(S): Tox21_200922
M4ID: 12481330 BRK

HILL MODEL (in red):

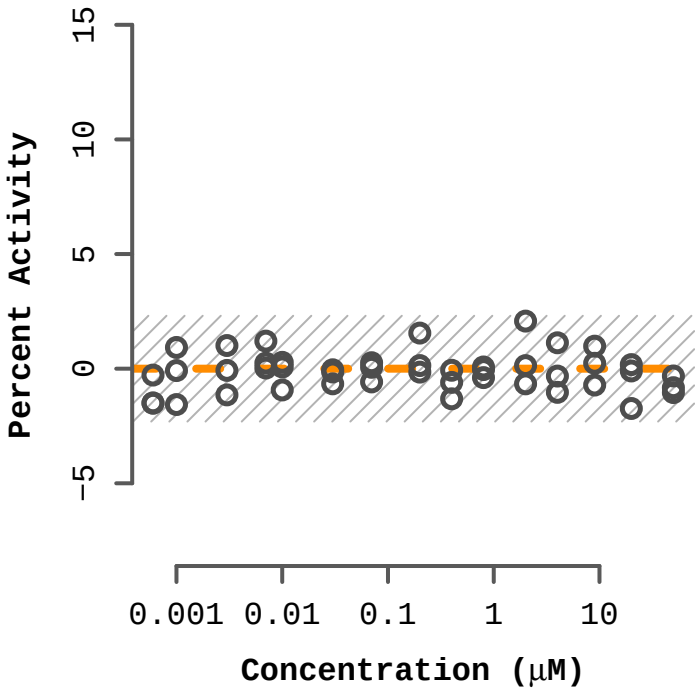
	tp	ga	gw
val:	0.795	−4.97	2.81
sd:	0.611	1110	1590

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.2	−1.66	0.3	0.00934	6.07
sd:	88.5	124	12	3.03	79.3

	CNST	HILL	GNLS
AIC:	363.08	367.28	370.59
PROB:	0.87	0.11	0.02
RMSE:	26.5	26.2	26.47

MAX_MEAN: 29.1 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

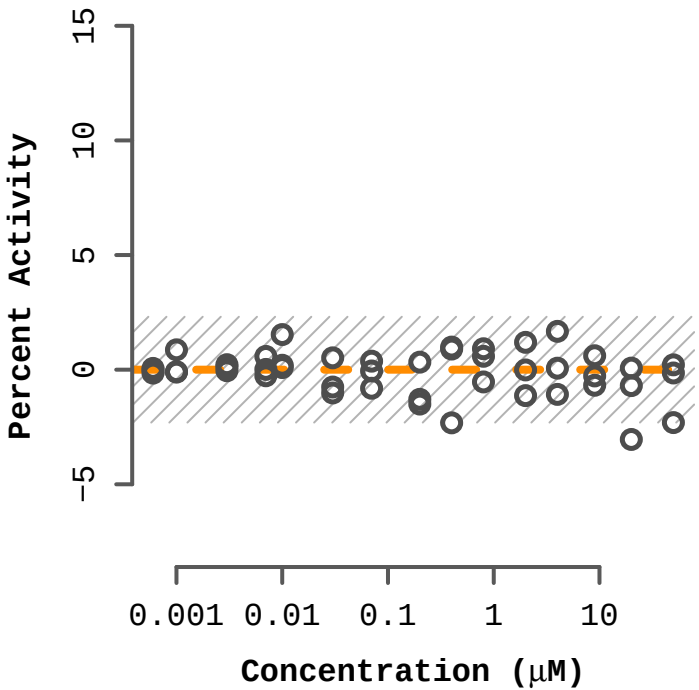
NAME: Allopurinol
CHID: 22573 **CASRN:** 315-30-0
SPID(S): Tox21_110082_1
M4ID: 12484670

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.517 **MAX_MED:** 0.244 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

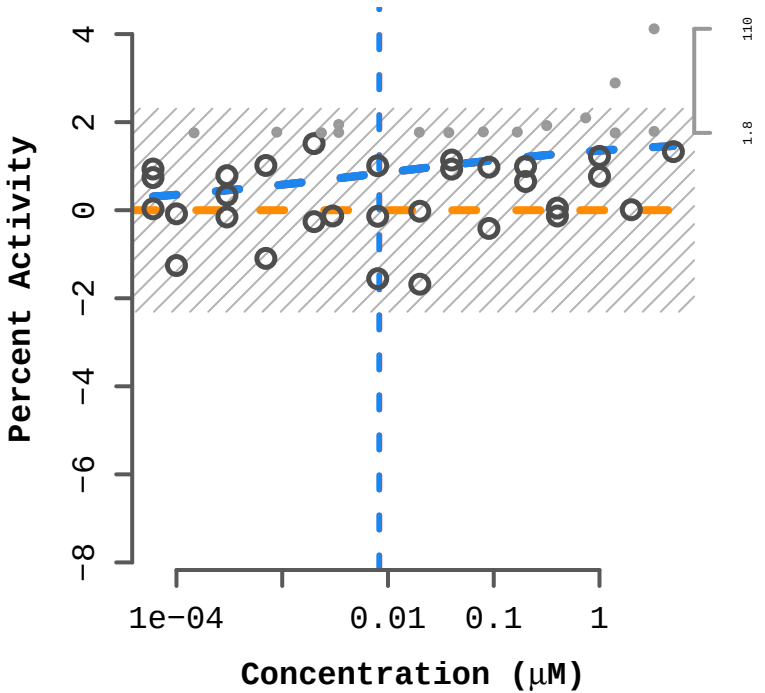
NAME: Alphaxalone
CHID: 22576 **CASRN:** 23930-19-0
SPID(S): Tox21_110884_1
M4ID: 12484043

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.607 **MAX_MED:** 0.901 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexamethylmelamine
CHID: 22579 **CASRN:** 645-05-6
SPID(S): Tox21_202784
M4ID: 12479468 **BRK**

HILL MODEL (in red):

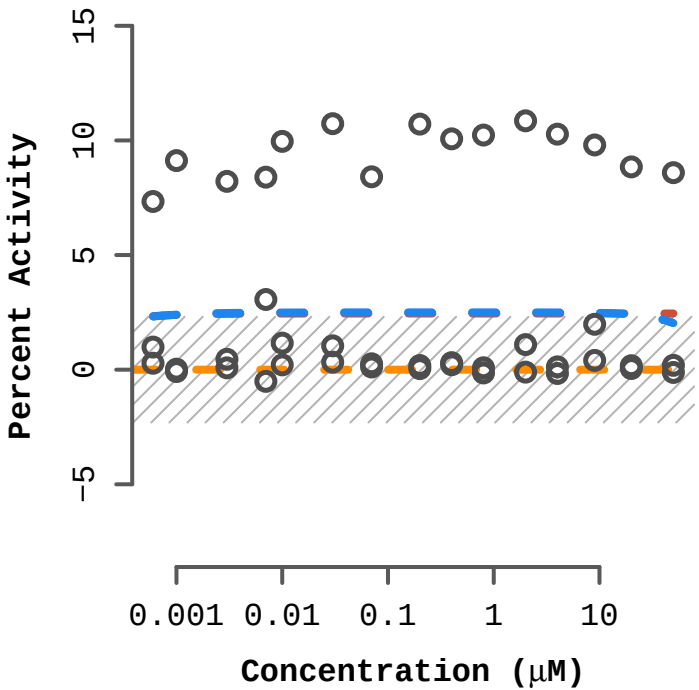
	tp	ga	gw
val:	1.67	−2.08	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.67	−2.09	0.3	2.7	11.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	269.93	264.55	268.55
PROB:	0.06	0.83	0.11
RMSE:	19.05	18.7	18.7

MAX_MEAN: 39.1 **MAX_MED:** 3.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexamethylmelamine
CHID: 22579 **CASRN:** 645-05-6
SPID(S): Tox21_110085_1
M4ID: 12484667

HILL MODEL (in red):

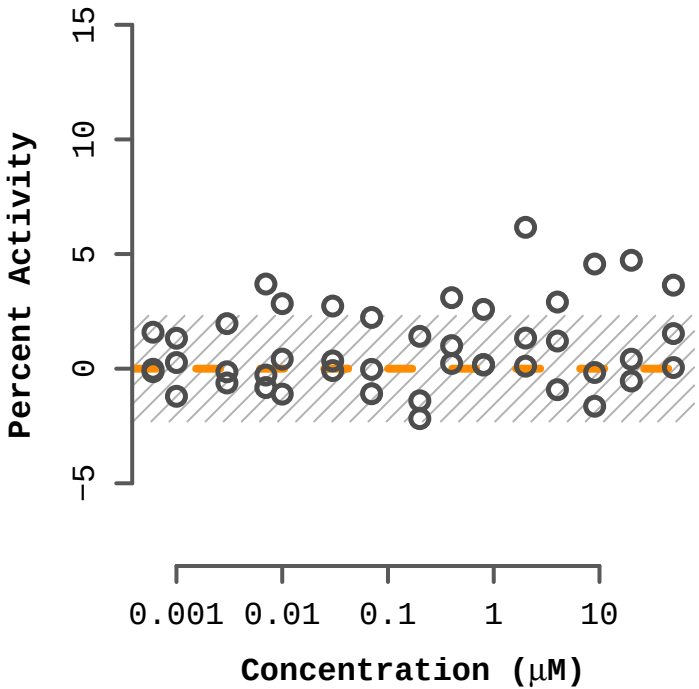
	tp	ga	gw
val:	2.45	−4.22	1.29
sd:	0.8	14.6	15.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.5	−4.14	1.21	2.01	2.04
sd:	0.879	10.9	12	3.35	18.9

	CNST	HILL	GNLS
AIC:	281.81	274.18	278.15
PROB:	0.02	0.86	0.12
RMSE:	5.52	4.45	4.45

MAX_MEAN: 4.06 **MAX_MED:** 3.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

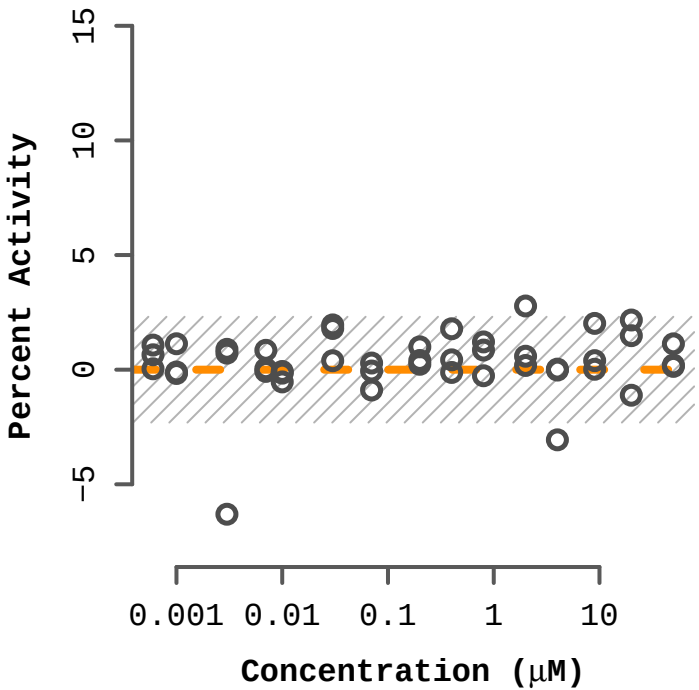
NAME: Ambenonium chloride
CHID: 22582 **CASRN:** 115-79-7
SPID(S): Tox21_112030_1
M4ID: 12483361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.86	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 2.54 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

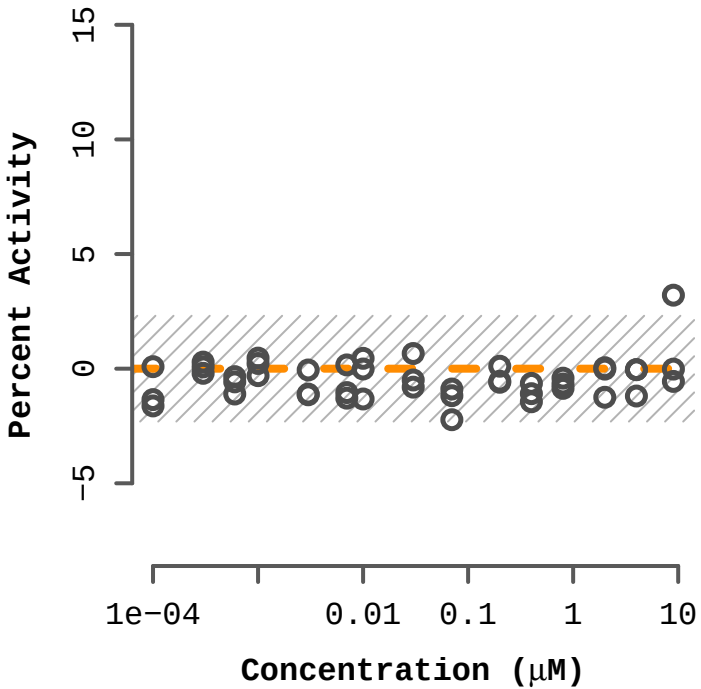
NAME: Amdinocillin
CHID: 22584 **CASRN:** 32887-01-7
SPID(S): Tox21_112209_1
M4ID: 12483234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

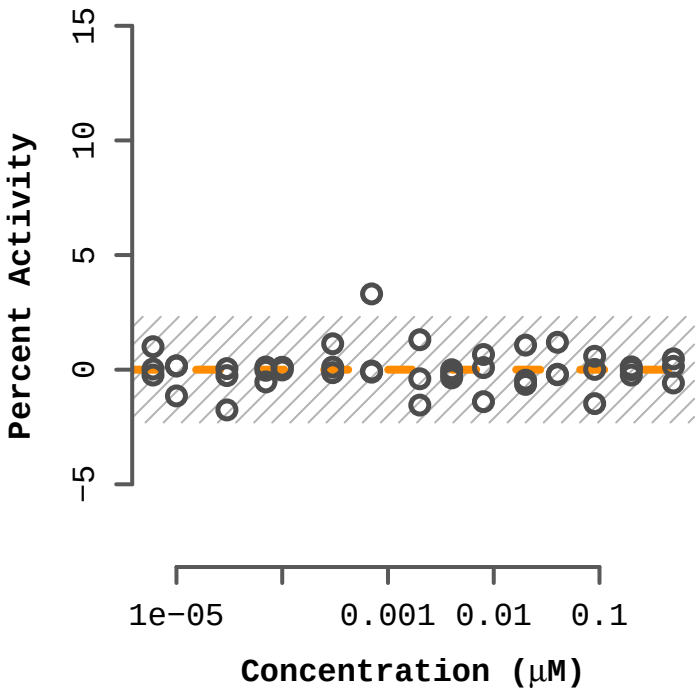
NAME: Amifostine
CHID: 22585 **CASRN:** 20537-88-6
SPID(S): Tox21_110077_1
M4ID: 12484675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 0.228 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

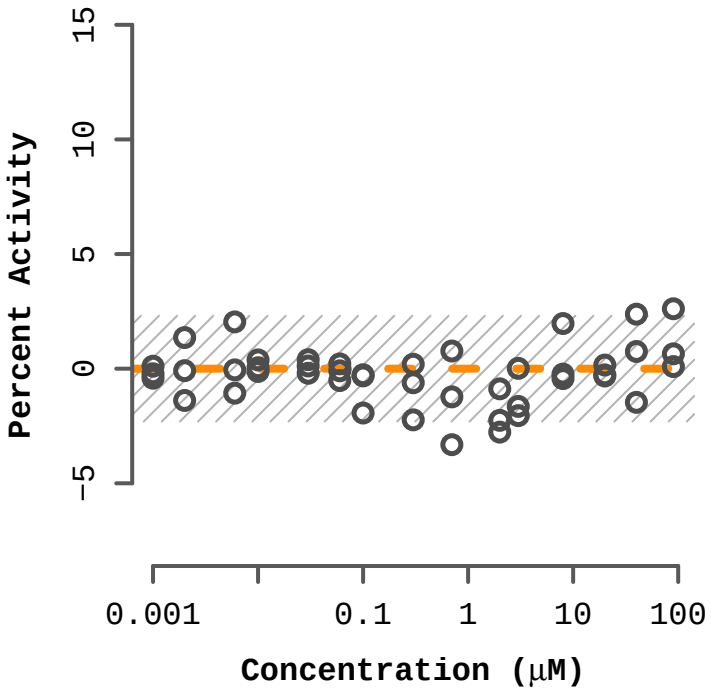
NAME: Amikacin
CHID: 22586 **CASRN:** 37517-28-5
SPID(S): Tox21_111201_1
M4ID: 12483845

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.165 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

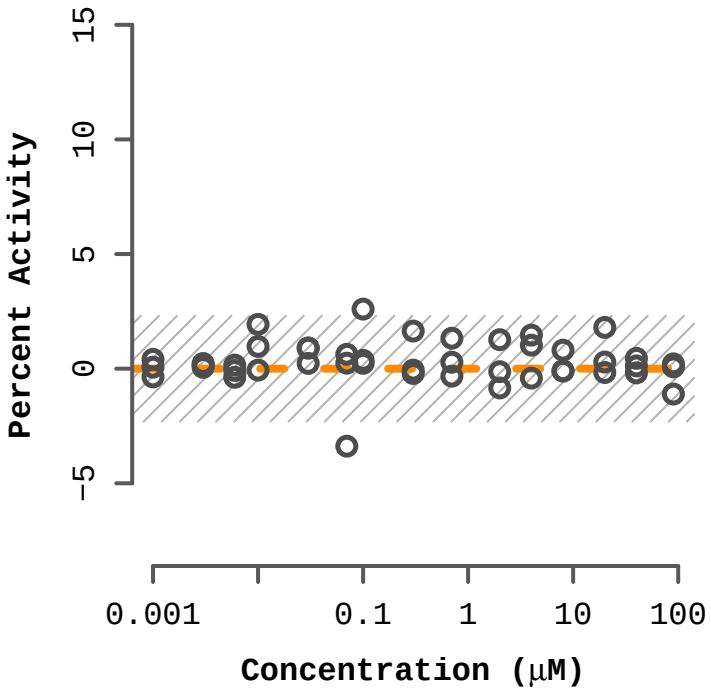
NAME: 4-Aminofolic acid
CHID: 22588 **CASRN:** 54-62-6
SPID(S): Tox21_300627
M4ID: 12478506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.752 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

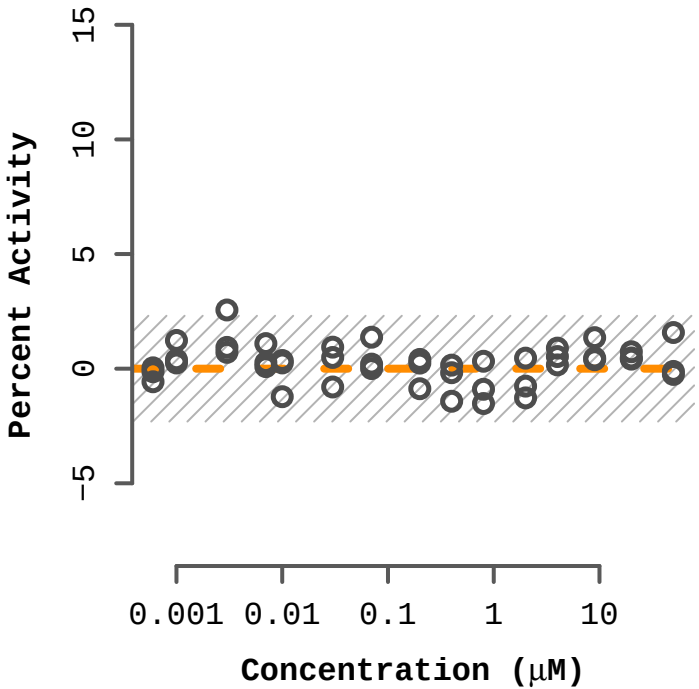
NAME: Aminoglutethimide
CHID: 22589 **CASRN:** 125-84-8
SPID(S): Tox21_303497
M4ID: 12475645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

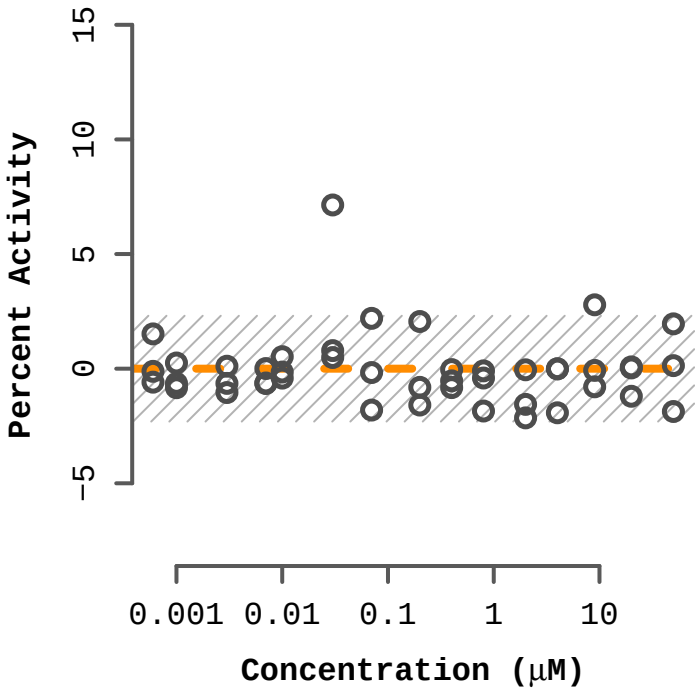
NAME: Aminoglutethimide
CHID: 22589 **CASRN:** 125-84-8
SPID(S): Tox21_110406_1
M4ID: 12484386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

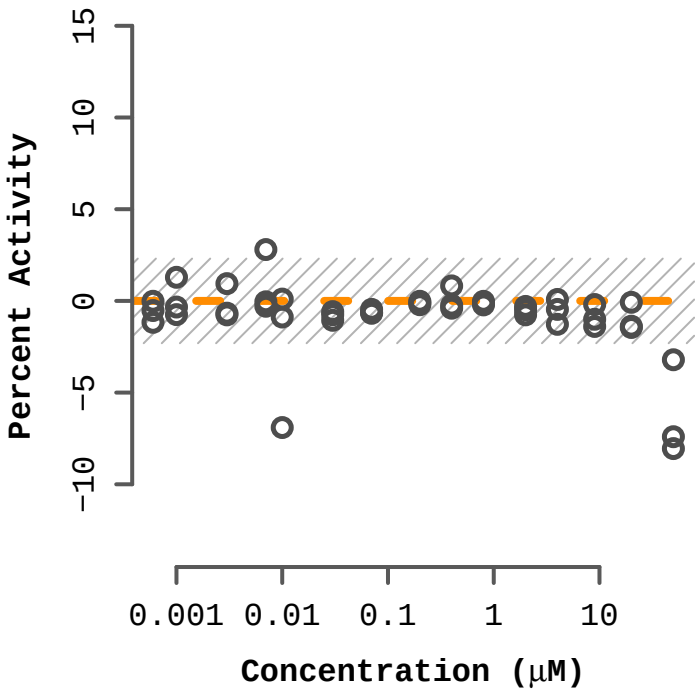
NAME: Aminohippuric acid
CHID: 22590 **CASRN:** 61-78-9
SPID(S): Tox21_110345_1
M4ID: 12484438

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 2.81 **MAX_MED:** 0.791 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

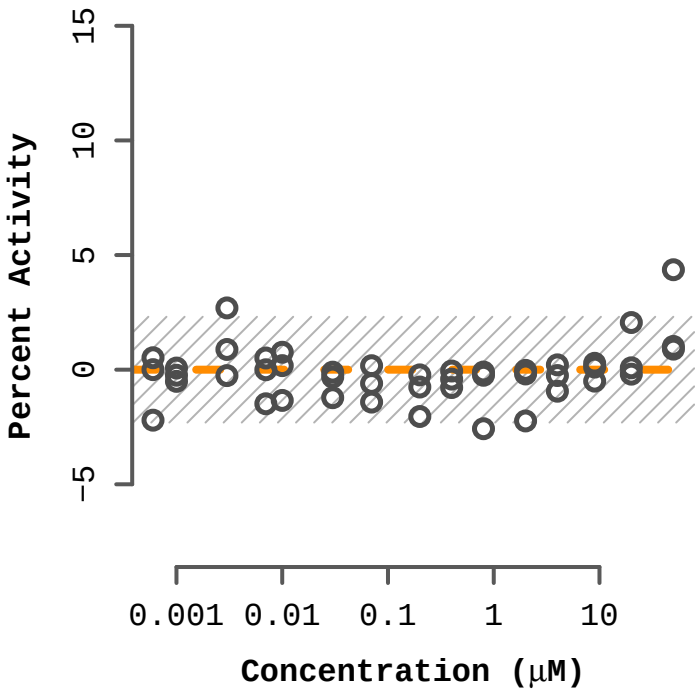
NAME: Amiodarone
CHID: 22592 **CASRN:** 1951-25-3
SPID(S): Tox21_110083_1
M4ID: 12484669

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 0.821 **MAX_MED:** −0.0459 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

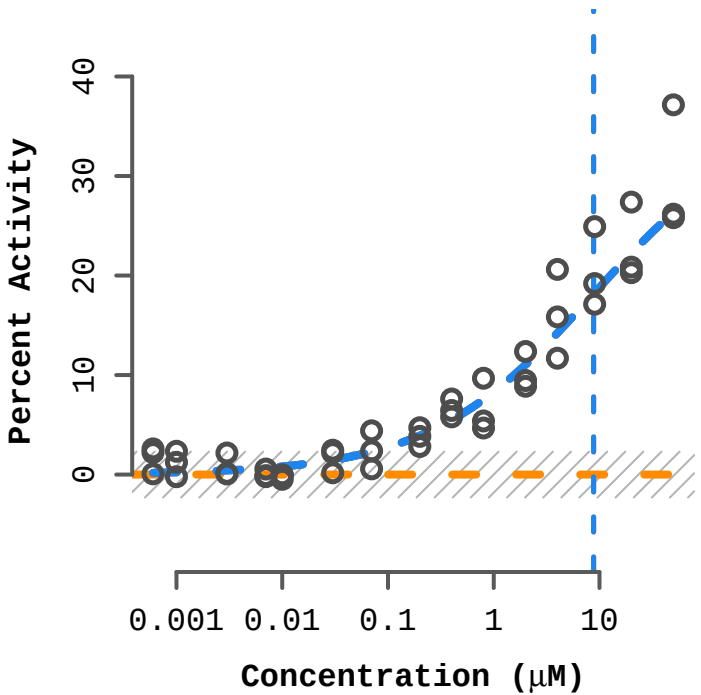
NAME: Amithiozone
CHID: 22593 **CASRN:** 104-06-3
SPID(S): Tox21_111625_1
M4ID: 12483577

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amlenanox
CHID: 22595 CASRN: 68302-57-8
SPID(S): Tox21_112476_1
M4ID: 12483079

HILL MODEL (in red):

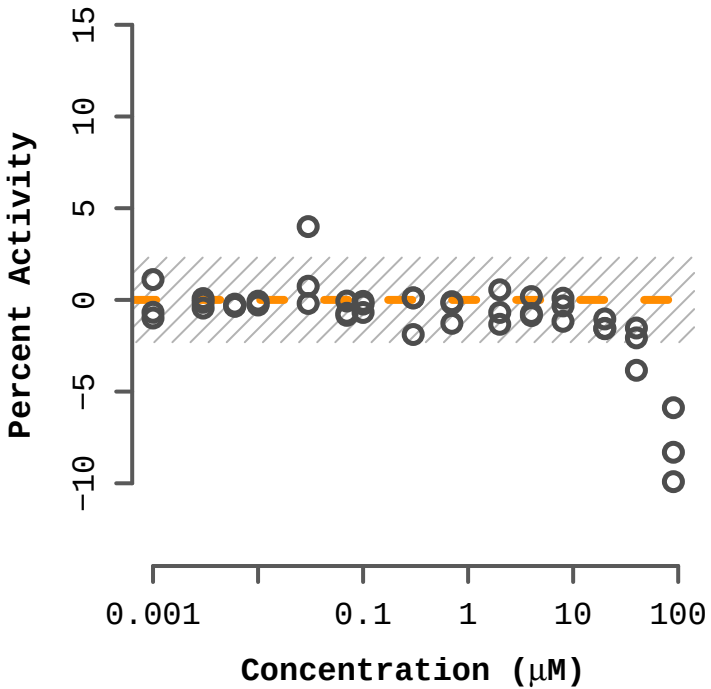
	tp	ga	gw
val:	36.3	0.945	0.558
sd:	6.01	0.307	0.0771

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	36.3	0.945	0.558	3.46	4.52
sd:	6.01	0.307	0.0771	1670	4340

	CNST	HILL	GNLS
AIC:	352.86	209.04	213.04
PROB:	0	0.88	0.12
RMSE:	12.59	2.64	2.64

MAX_MEAN: 29.7 MAX_MED: 26.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

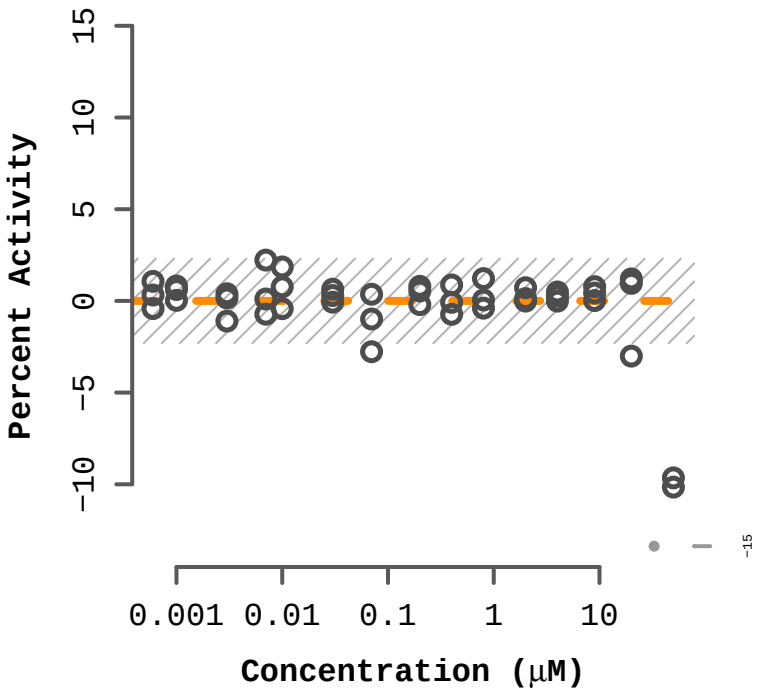
NAME: Amoxapine
CHID: 22598 **CASRN:** 14028-44-5
SPID(S): Tox21_302352
M4ID: 12476781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.28	NA	NA
PROB:	1	NA	NA
RMSE:	2.41	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 0.747 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

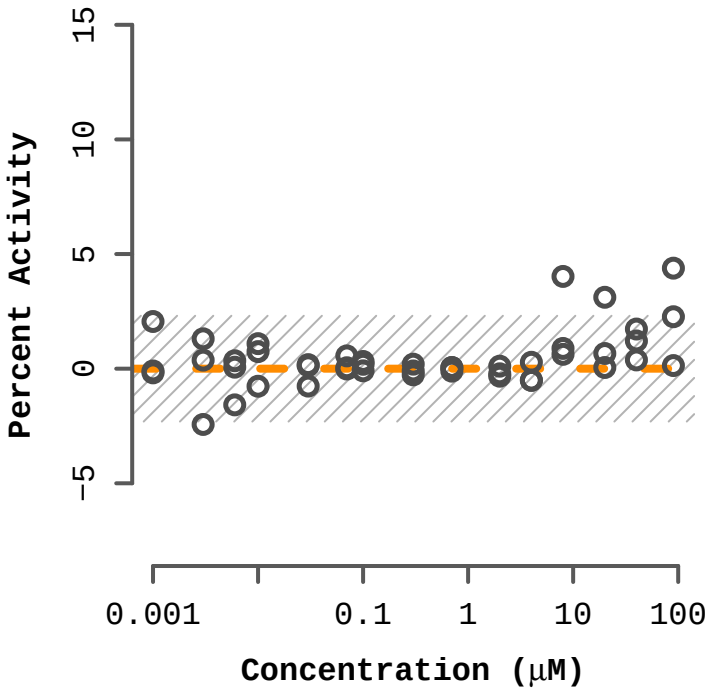
NAME: Amoxapine
CHID: 22598 **CASRN:** 14028-44-5
SPID(S): Tox21_110064_1
M4ID: 12484686 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.41	NA	NA
PROB:	1	NA	NA
RMSE:	3.16	NA	NA

MAX_MEAN: 0.733 **MAX_MED:** 0.959 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

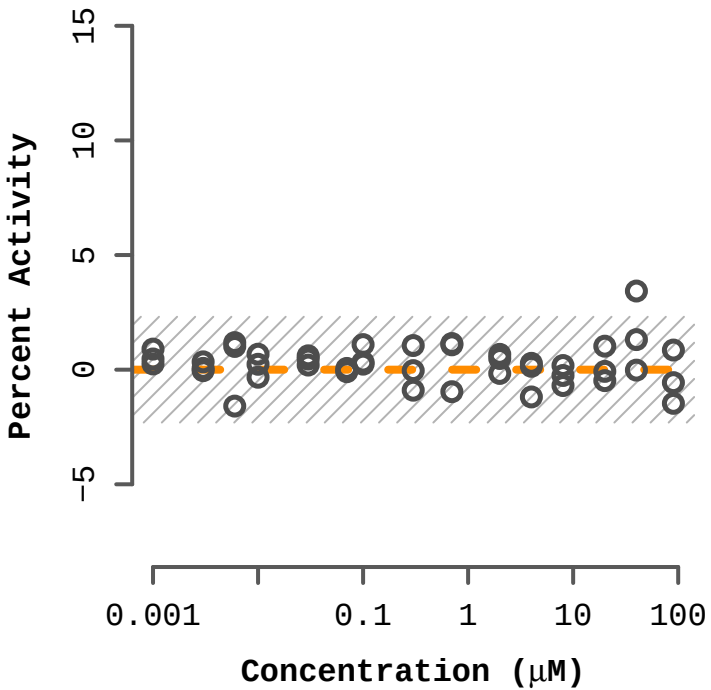
NAME: Amphotericin B
CHID: 22601 **CASRN:** 1397-89-3
SPID(S): Tox21_202484
M4ID: 12479768

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.26 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

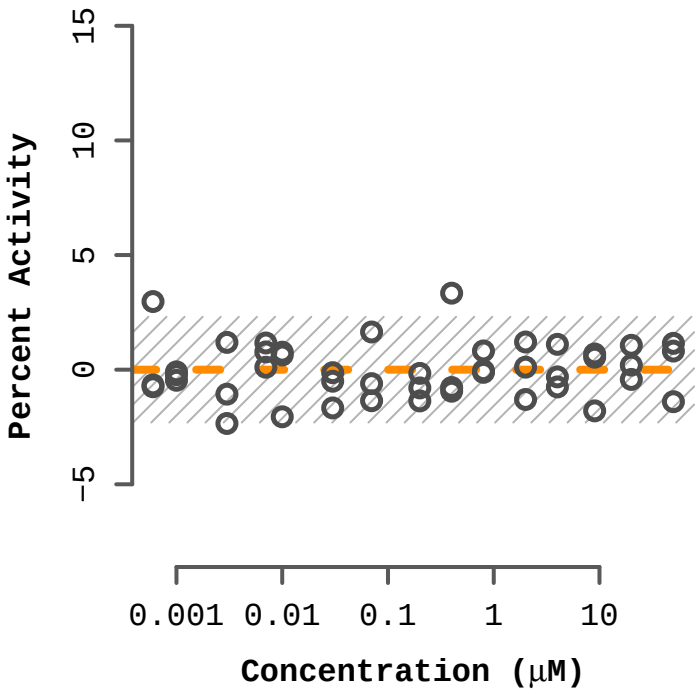
NAME: Ampicillin
CHID: 22602 **CASRN:** 69-53-4
SPID(S): Tox21_301416
M4ID: 12477717

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

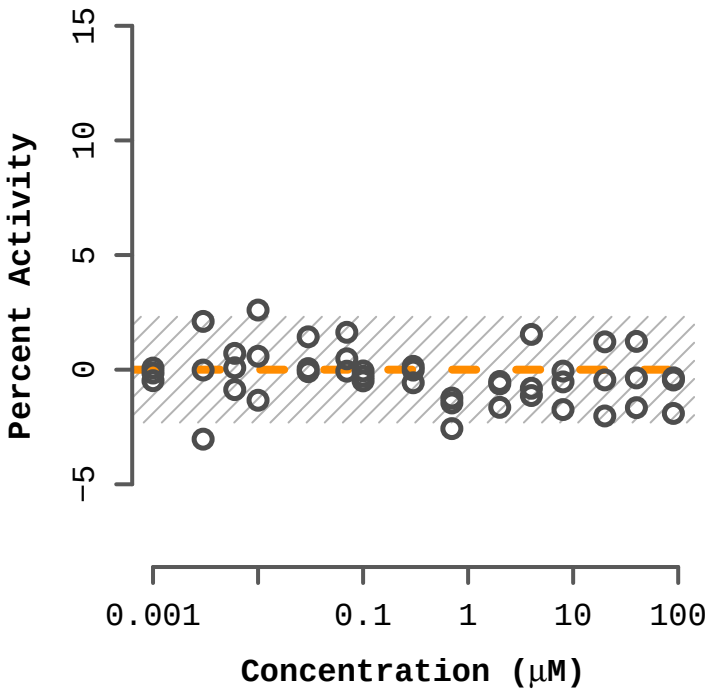
NAME: Ampicillin
CHID: 22602 **CASRN:** 69-53-4
SPID(S): Tox21_113049_1
M4ID: 12482828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.683 **MAX_MED:** 0.813 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

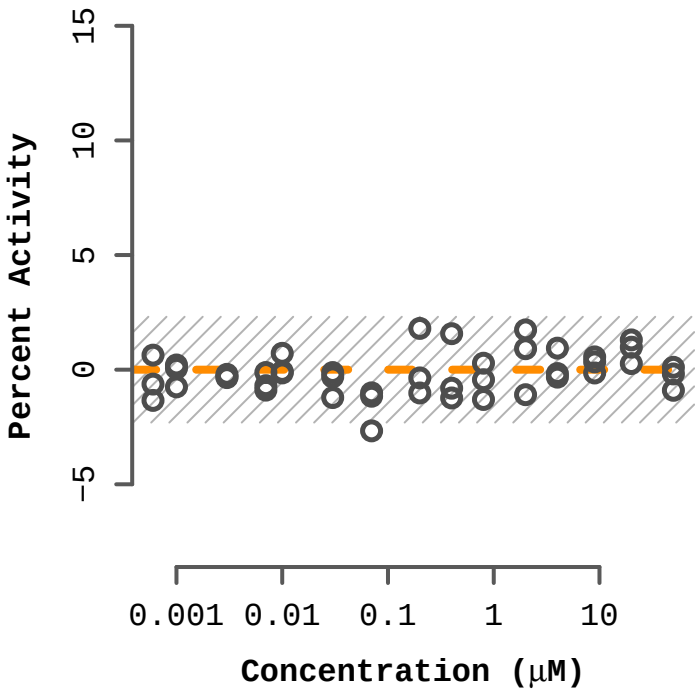
NAME: Amrinone
CHID: 22603 **CASRN:** 60719-84-8
SPID(S): Tox21_301847
M4ID: 12477286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.681 **MAX_MED:** 0.587 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

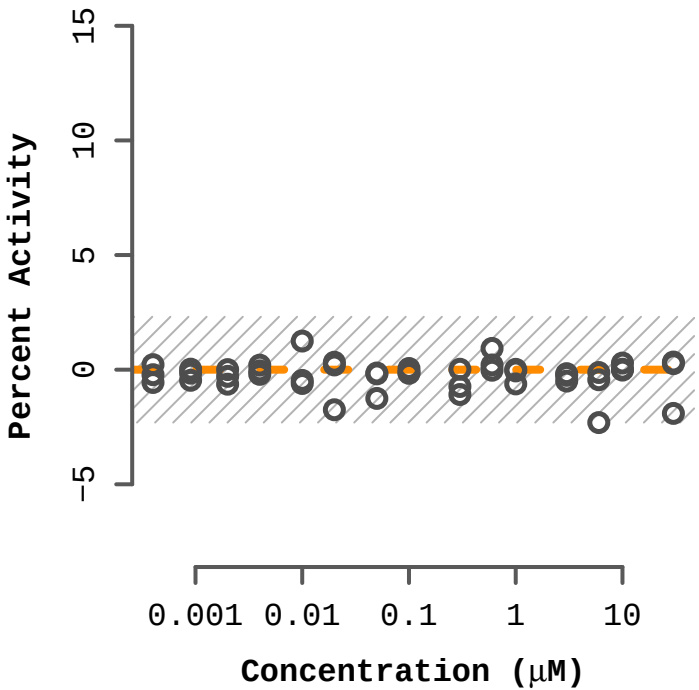
NAME: Amrinone
CHID: 22603 **CASRN:** 60719-84-8
SPID(S): Tox21_112110_1
M4ID: 12483314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

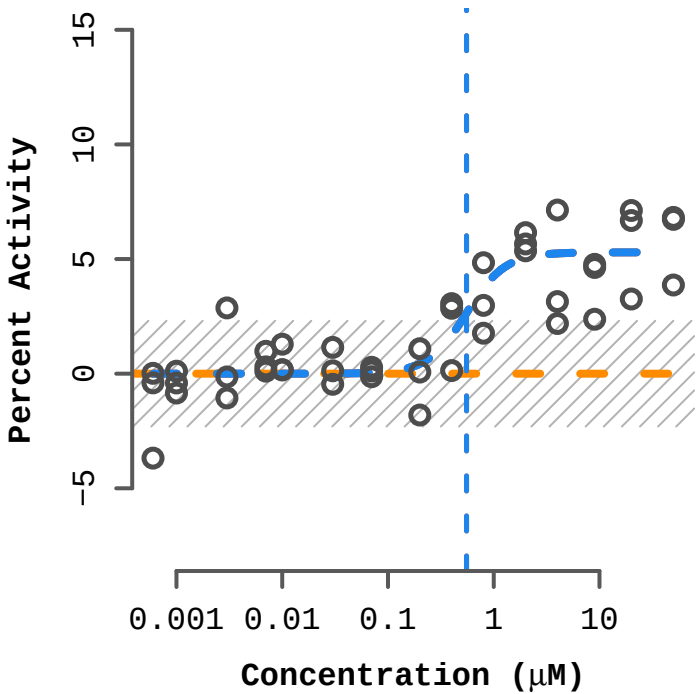
NAME: Anastrozole
CHID: 22607 **CASRN:** 120511-73-1
SPID(S): Tox21_303568
M4ID: 12475577

HILL MODEL: Not applicable.

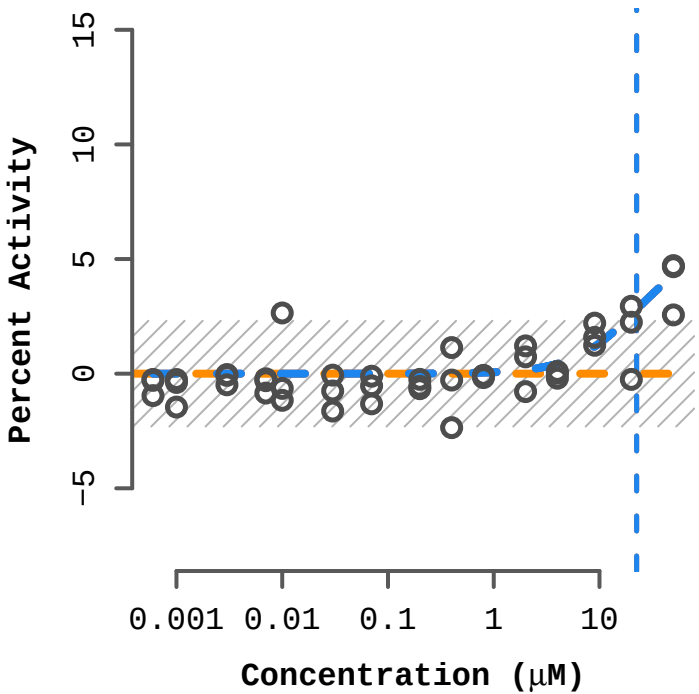
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	83.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

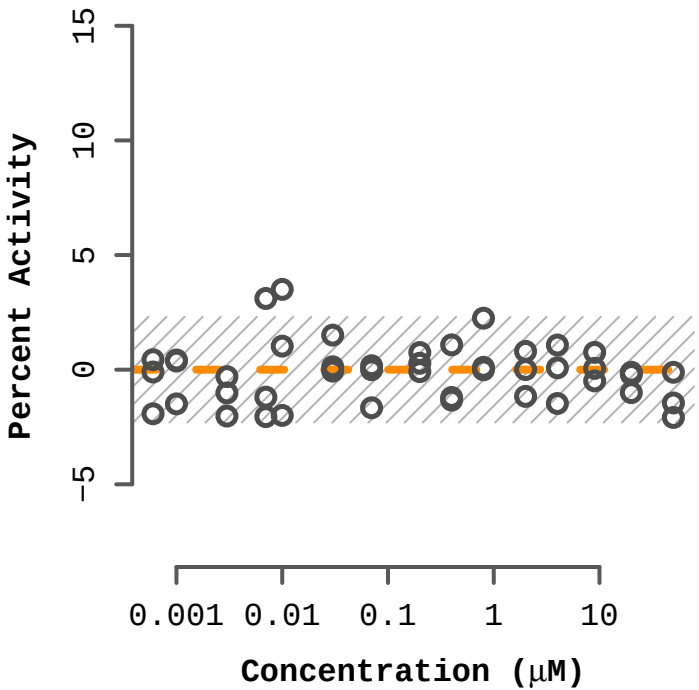
MAX_MEAN: 0.371 **MAX_MED:** 0.264 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Anastrozole
CHID:    22607   CASRN: 120511-73-1
SPID(S): Tox21_112238_1
M4ID:    12483213

HILL MODEL (in red):
      tp       ga       gw
val:  5.29     -0.257   2.38
sd:   0.507    0.12     0.957

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.29     -0.257   2.38     2.62     9.81
sd:   0.507    0.12     0.957    1920     20500

      CNST        HILL        GNLS
AIC:  239.93      167.82      171.82
PROB: 0           0.88        0.12
RMSE: 3.38        1.41        1.41

MAX_MEAN: 5.81      MAX_MED: 6.73      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Androstenediol
CHID:    22609   CASRN: 521-17-5
SPID(S): Tox21_112495_1
M4ID:    12483068

HILL MODEL (in red):
      tp       ga       gw
val:  5.59     1.35     1.44
sd:   2.53     0.346    0.606

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.59     1.35     1.44     3.39     4.29
sd:   2.53     0.346    0.606    1160     2980

      CNST        HILL        GNLS
AIC:  158.88      128.42      132.42
PROB: 0           0.88        0.12
RMSE: 1.51        0.97        0.97

MAX_MEAN: 3.98      MAX_MED: 4.67      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

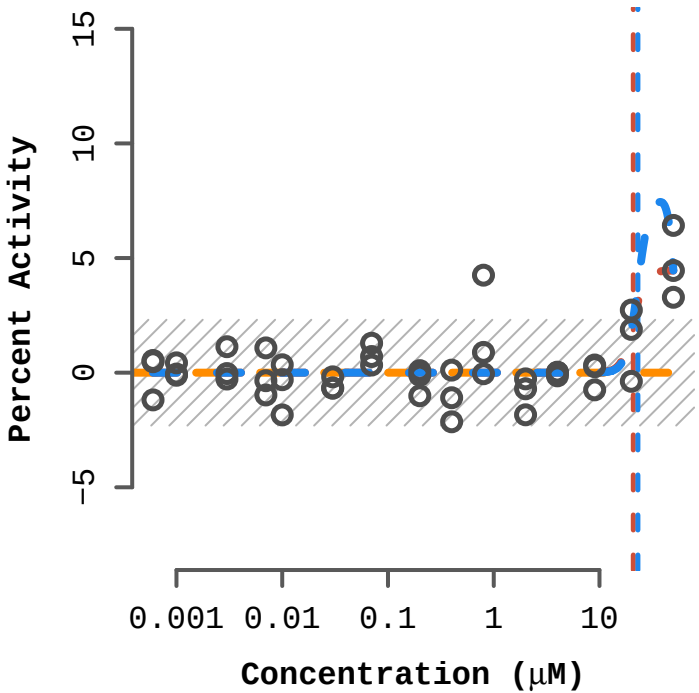
NAME: Anileridine
CHID: 22610 **CASRN:** 144-14-9
SPID(S): Tox21_113744
M4ID: 12482470

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.846 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Anisindione
CHID: 22611 **CASRN:** 117-37-3
SPID(S): Tox21_111370_1
M4ID: 12483734

HILL MODEL (in red):

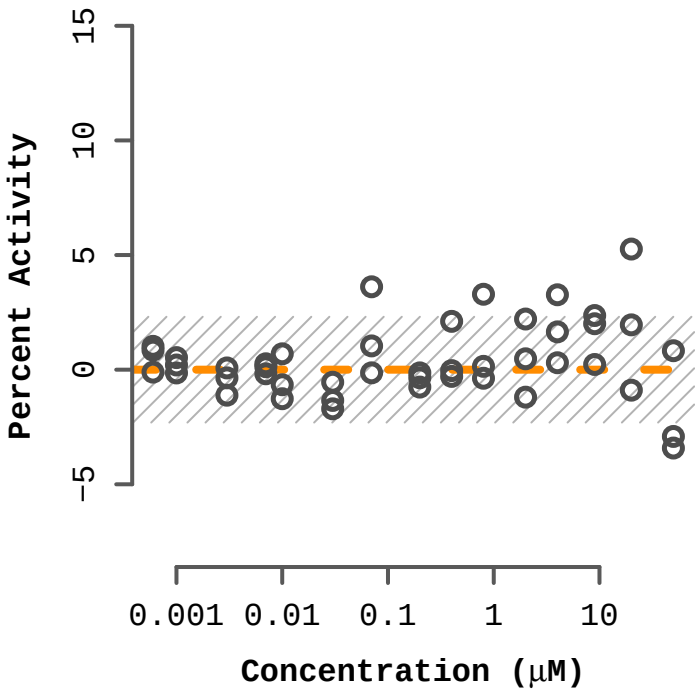
	tp	ga	gw
val:	4.46	1.32	8
sd:	0.674	0.11	44.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.68	1.36	8	1.71	14.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	160.05	135.9	139.9
PROB:	0	0.88	0.12
RMSE:	1.67	1.09	1.09

MAX_MEAN: 4.72 **MAX_MED:** 4.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

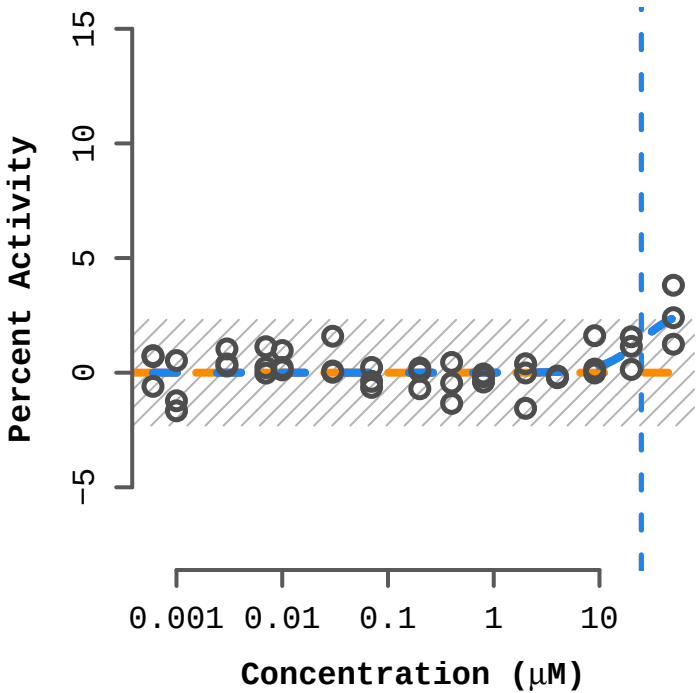
NAME: Apomorphine
CHID: 22614 **CASRN:** 58-00-4
SPID(S): Tox21_110967_1
M4ID: 12483978

HILL MODEL: Not applicable.

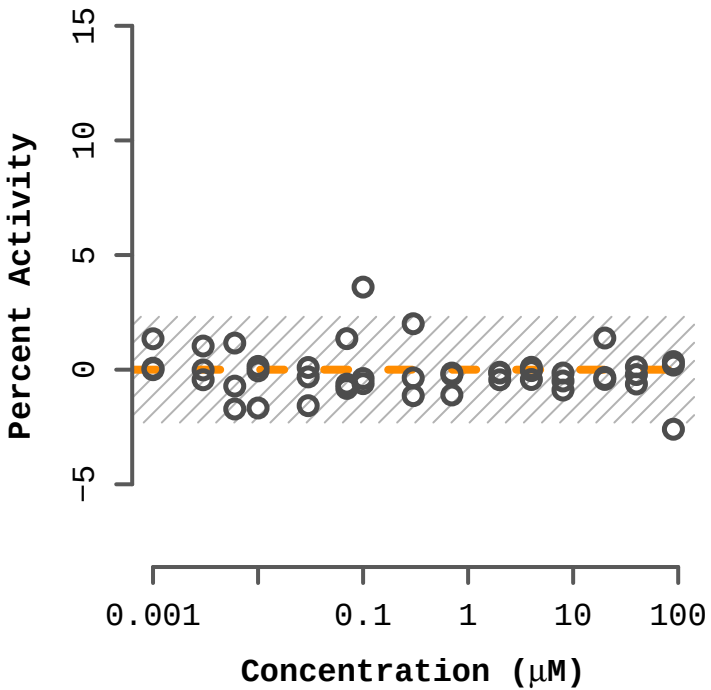
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 2.01 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Arecoline
CHID:    22617   CASRN: 63-75-2
SPID(S): Tox21_110079_1
M4ID:    12484673

HILL MODEL (in red):
      tp       ga       gw
val:  2.84     1.4      2.37
sd:   1.52     0.282    1.82

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.84     1.4      2.37     3.16     4.25
sd:   1.52     0.282    1.82     1400     4140

      CNST        HILL        GNLS
AIC:  124.42      109.81      113.81
PROB: 0           0.88        0.12
RMSE: 1.02        0.74        0.74

MAX_MEAN: 2.49      MAX_MED: 2.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

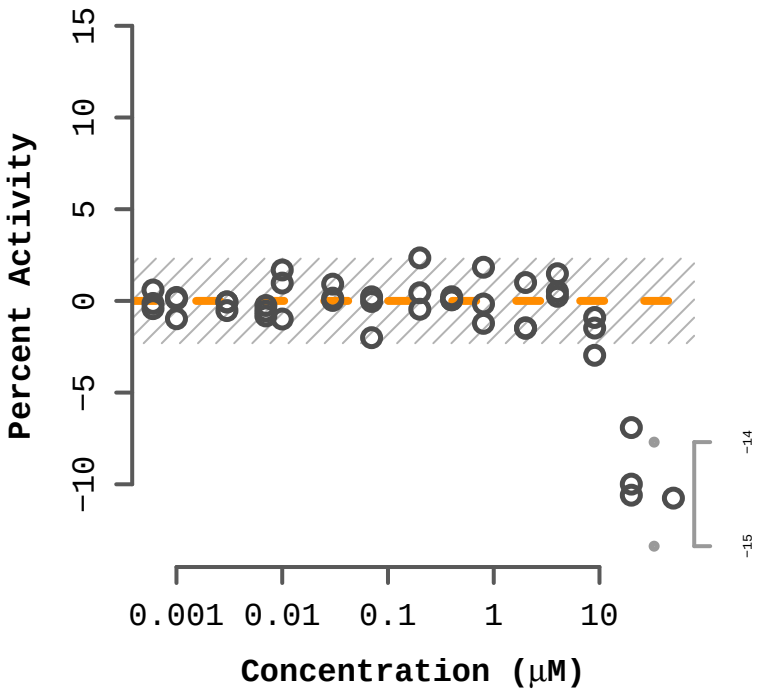
NAME: Atenolol
CHID: 22628 **CASRN:** 29122-68-7
SPID(S): Tox21_302426
M4ID: 12476707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.869 **MAX_MED:** 0.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

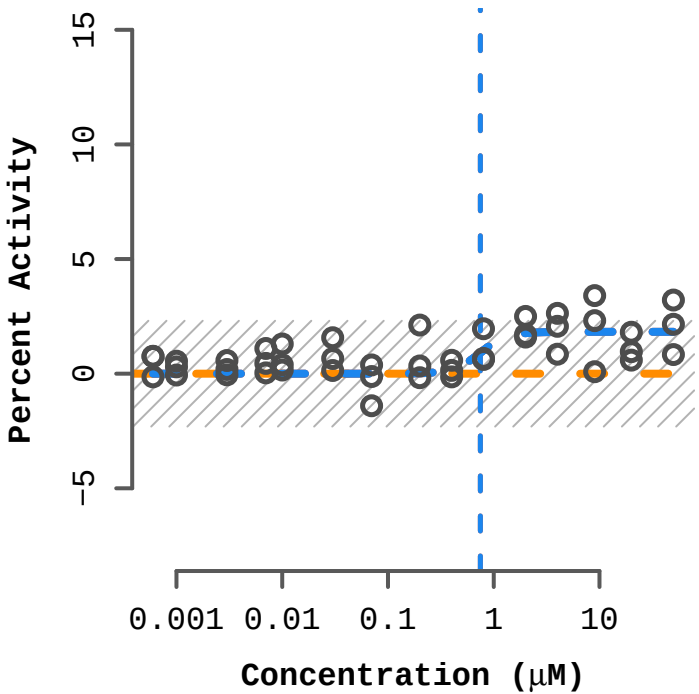
NAME: Atovaquone
CHID: 22629 **CASRN:** 95233-18-4
SPID(S): Tox21_110714_1
M4ID: 12484154 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227	NA	NA
PROB:	1	NA	NA
RMSE:	4.36	NA	NA

MAX_MEAN: 0.78 **MAX_MED:** 0.973 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Azaribine
CHID: 22635 **CASRN:** 2169-64-4
SPID(S): Tox21_110878_1
M4ID: 12484049

HILL MODEL (in red):

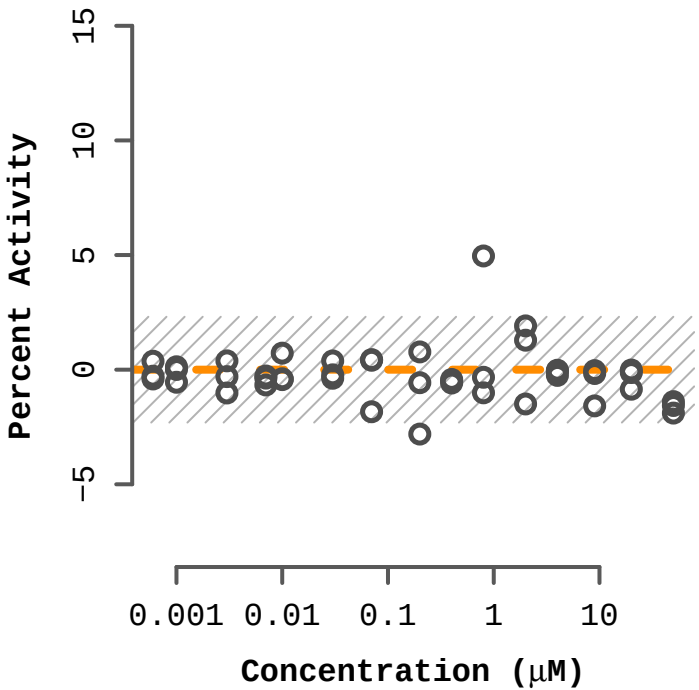
	tp	ga	gw
val:	1.83	−0.127	3.47
sd:	0.244	0.118	3.12

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.83	−0.127	3.46	2.81	7.33
sd:	0.244	0.118	3.12	1650	10900

	CNST	HILL	GNLS
AIC:	155.87	117.59	121.59
PROB:	0	0.88	0.12
RMSE:	1.34	0.81	0.81

MAX_MEAN: 2.07 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

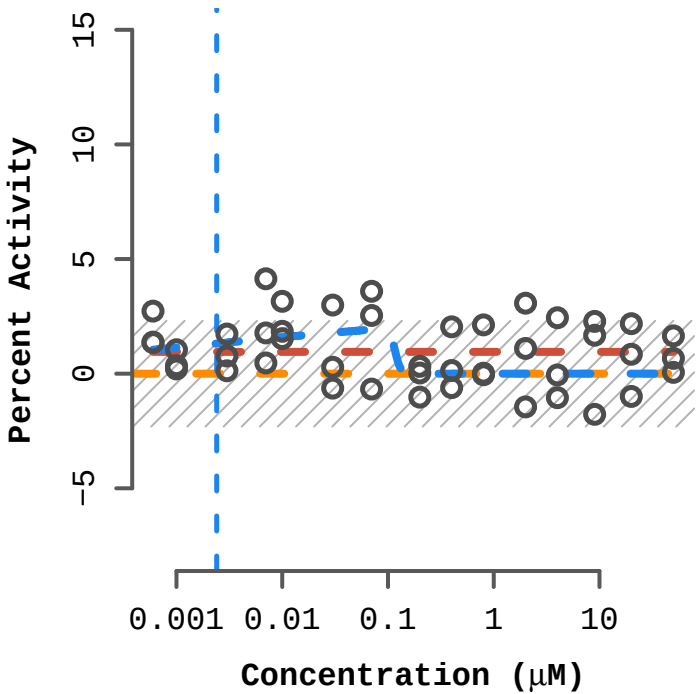
NAME: Azatadine
CHID: 22636 **CASRN:** 3964-81-6
SPID(S): Tox21_112982_1
M4ID: 12482856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Aztreonam
CHID: 22640 **CASRN:** 78110-38-0
SPID(S): Tox21_110692_1
M4ID: 12484174

HILL MODEL (in red):

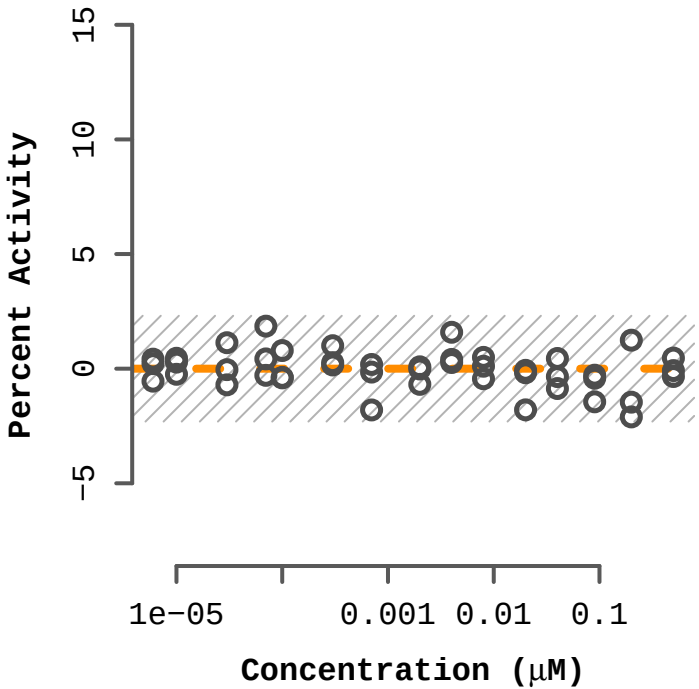
	tp	ga	gw
val:	0.951	−4.98	4.42
sd:	0.223	1880	4780

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.62	−2.62	0.3	−0.933	16.8
sd:	11.1	12.8	1.62	1.59	118

	CNST	HILL	GNLS
AIC:	181.49	171.03	173.59
PROB:	0	0.78	0.22
RMSE:	1.72	1.4	1.39

MAX_MEAN: 2.18 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

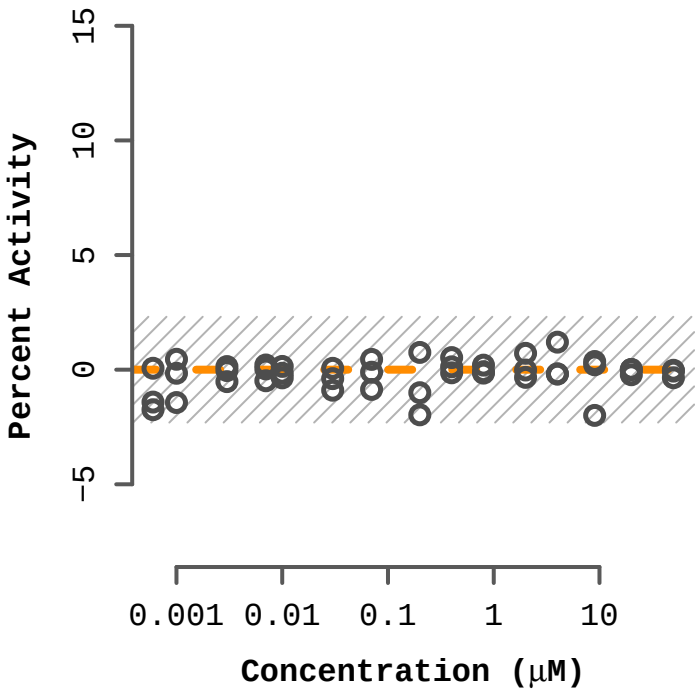
NAME: Baclofen
CHID: 22641 **CASRN:** 1134-47-0
SPID(S): Tox21_110090_1
M4ID: 12484662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.755 **MAX_MED:** 0.427 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

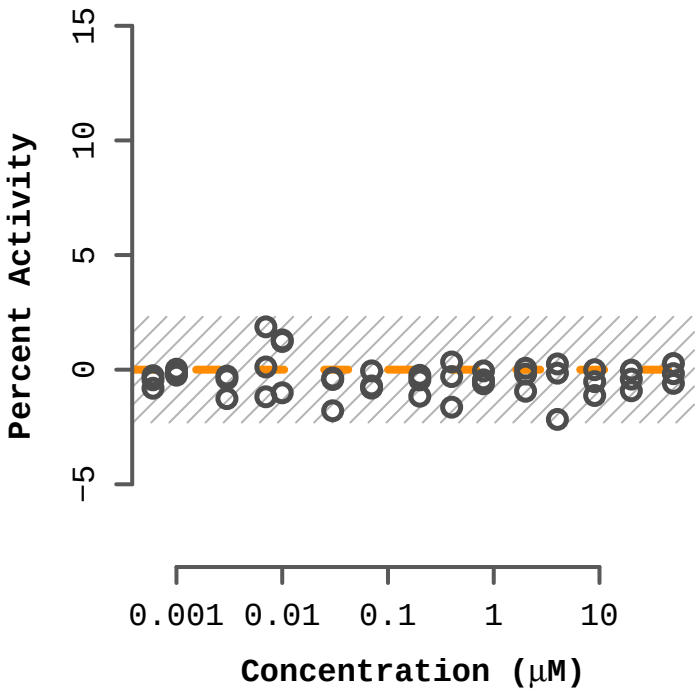
NAME: Barbital
CHID: 22643 CASRN: 57-44-3
SPID(S): Tox21_111650_1
M4ID: 12483558

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.277 **MAX_MED:** 0.215 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

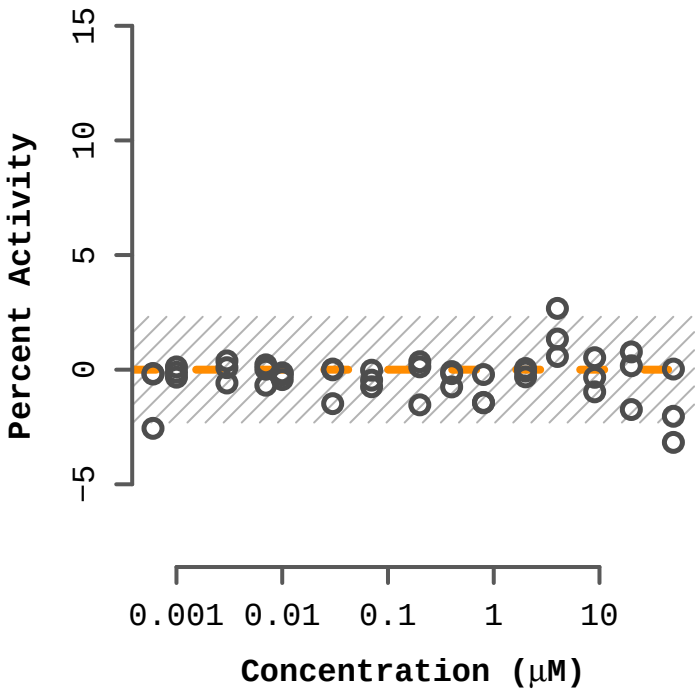
NAME: Benactyzine
CHID: 22644 **CASRN:** 302-40-9
SPID(S): Tox21_111665_1
M4ID: 12483547

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.508 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

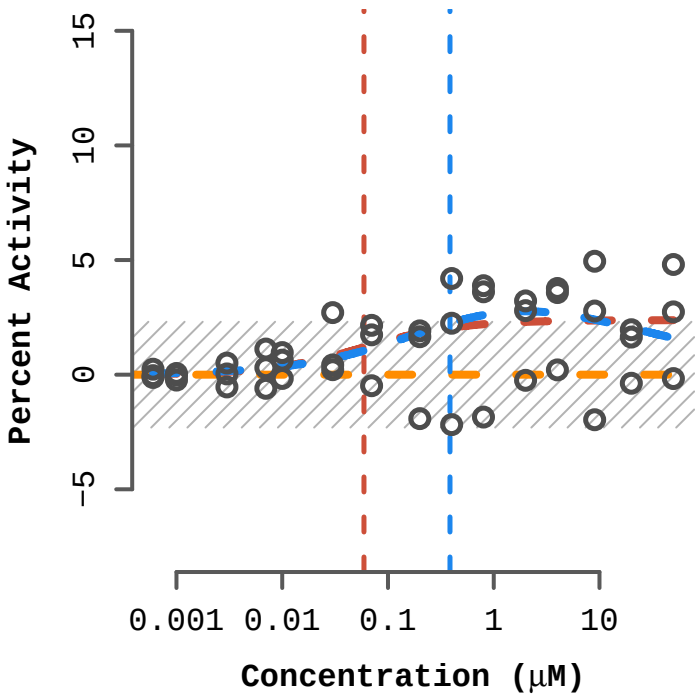
NAME: Bencyclane
CHID: 22646 CASRN: 2179-37-5
SPID(S): Tox21_113690
M4ID: 12482524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bendroflumethiazide
CHID: 22647 **CASRN:** 73-48-3
SPID(S): Tox21_110365_1
M4ID: 12484423

HILL MODEL (in red):

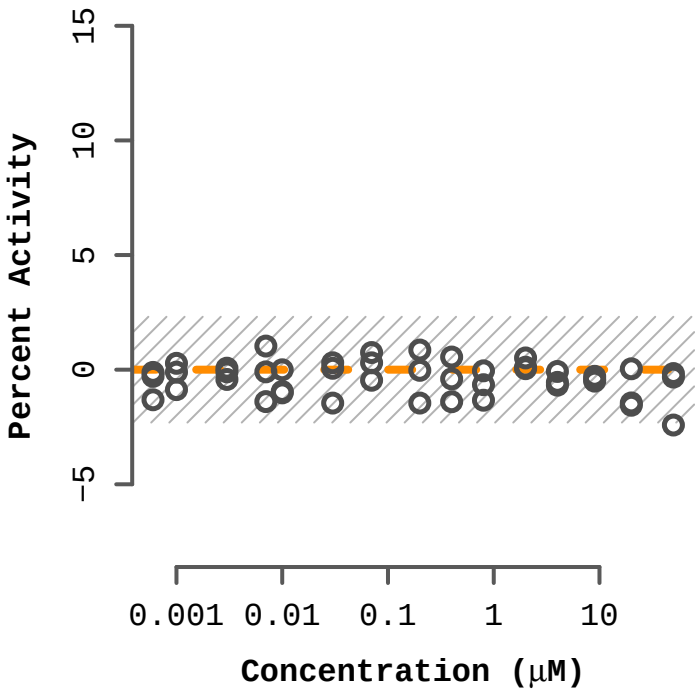
	tp	ga	gw
val:	2.38	−1.23	0.966
sd:	0.481	0.438	0.553

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.94	−0.414	0.736	0.727	0.43
sd:	14.5	1.55	0.435	4.35	0.694

	CNST	HILL	GNLS
AIC:	200.1	180.97	183.97
PROB:	0	0.82	0.18
RMSE:	2.14	1.71	1.73

MAX_MEAN: 2.52 **MAX_MED:** 3.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

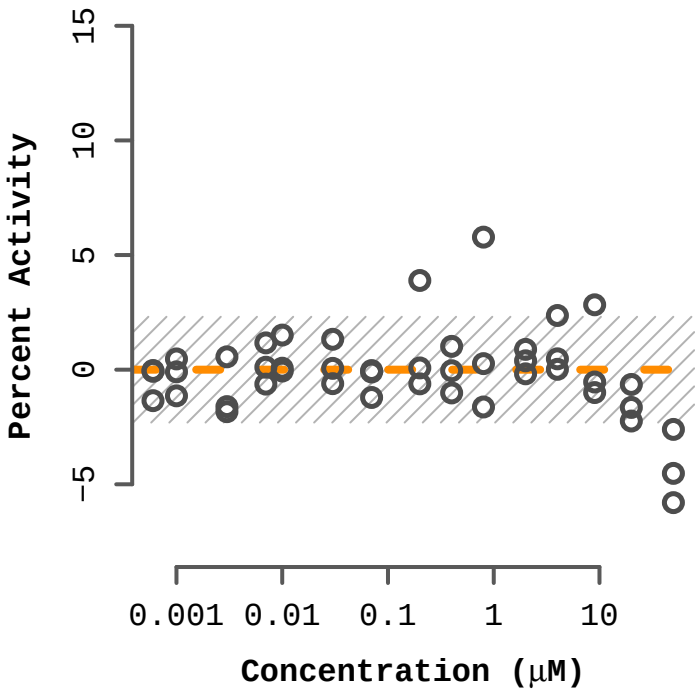
NAME: Benorylate
CHID: 22649 **CASRN:** 5003-48-5
SPID(S): Tox21_112472_1
M4ID: 12483081

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.222 **MAX_MED:** 0.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

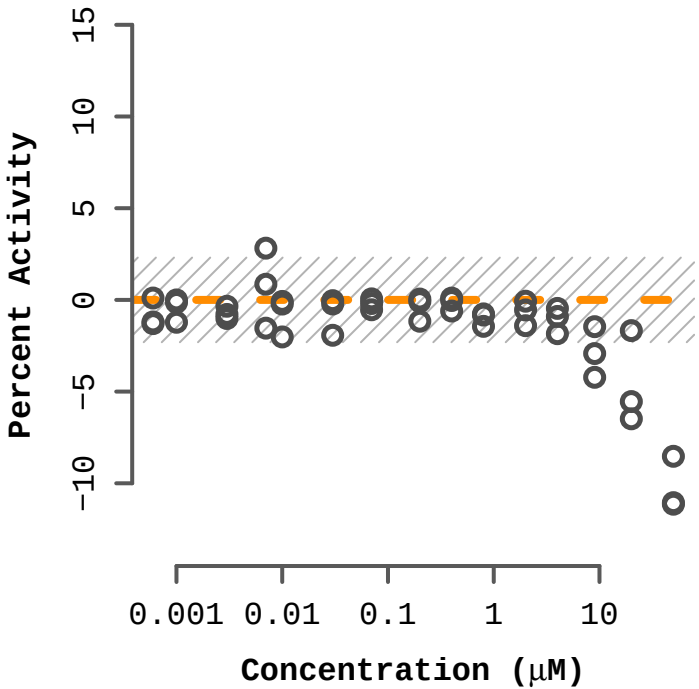
NAME: Benzbromarone
CHID: 22652 **CASRN:** 3562-84-3
SPID(S): Tox21_110041_1
M4ID: 12484697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 0.474 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

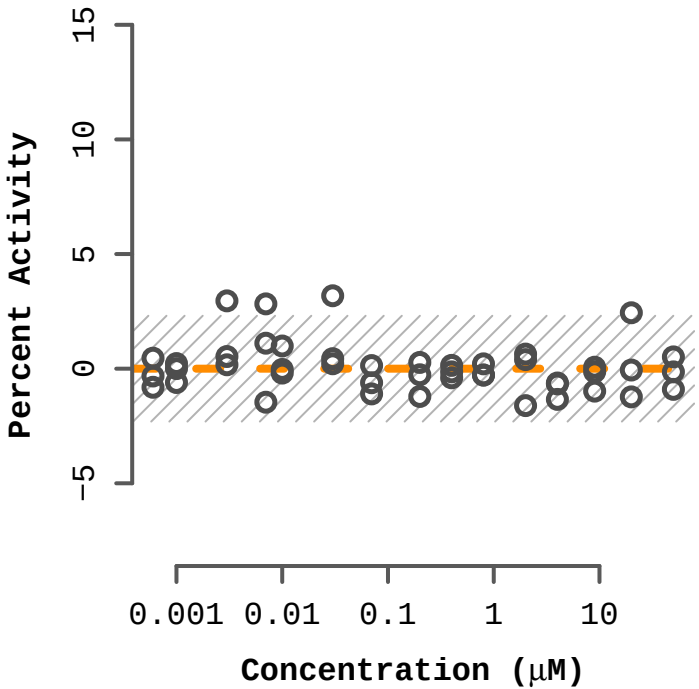
NAME: Benzonatate
CHID: 22655 **CASRN:** 104-31-4
SPID(S): Tox21_110398_1
M4ID: 12484393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.76	NA	NA
PROB:	1	NA	NA
RMSE:	3.2	NA	NA

MAX_MEAN: 0.713 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

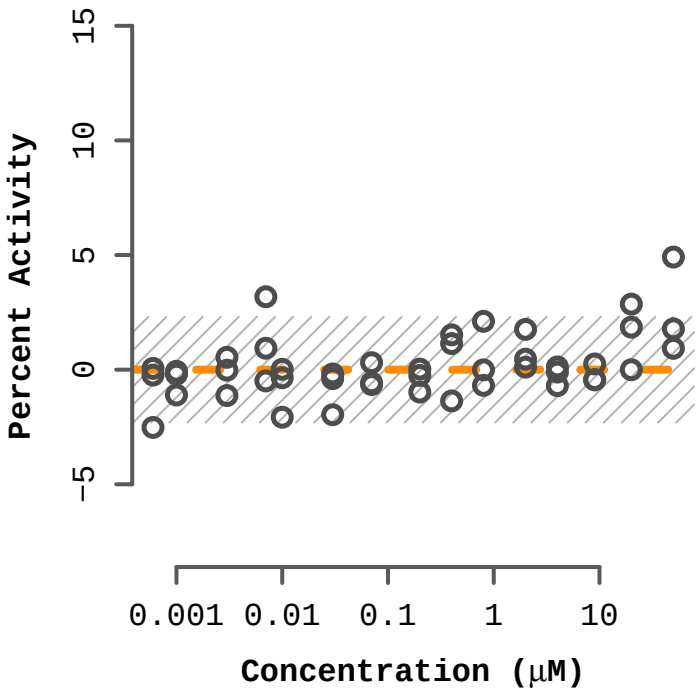
NAME: Benzquinamide
CHID: 22657 **CASRN:** 63-12-7
SPID(S): Tox21_113977
M4ID: 12482263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

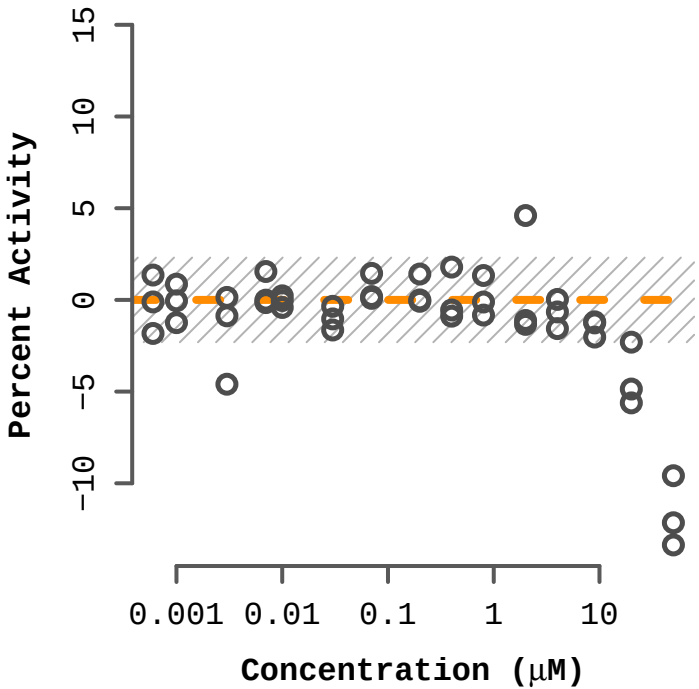
NAME: Benzthiazide
CHID: 22658 **CASRN:** 91-33-8
SPID(S): Tox21_110387_1
M4ID: 12484403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 2.54 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

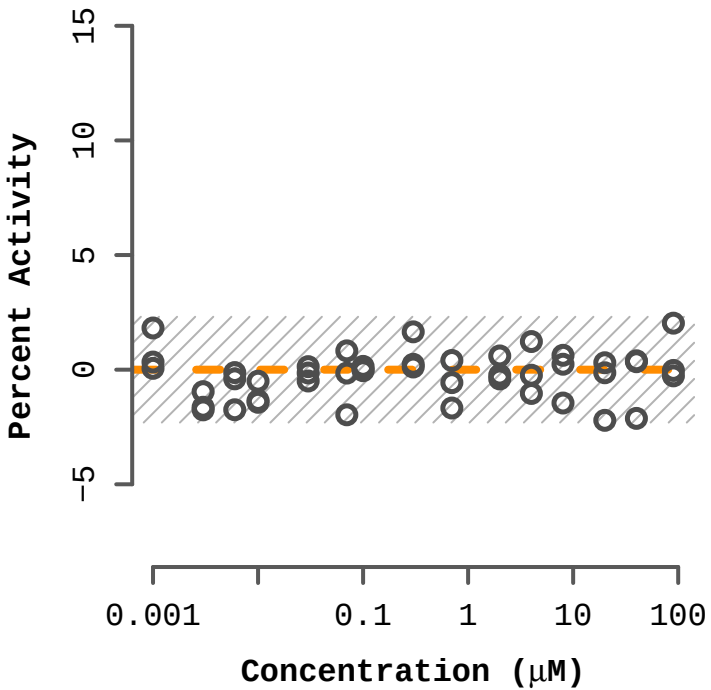
NAME: Bepridil
CHID: 22663 **CASRN:** 64706-54-3
SPID(S): Tox21_110089_1
M4ID: 12484663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.71	NA	NA
PROB:	1	NA	NA
RMSE:	3.53	NA	NA

MAX_MEAN: 0.716 **MAX_MED:** 0.184 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

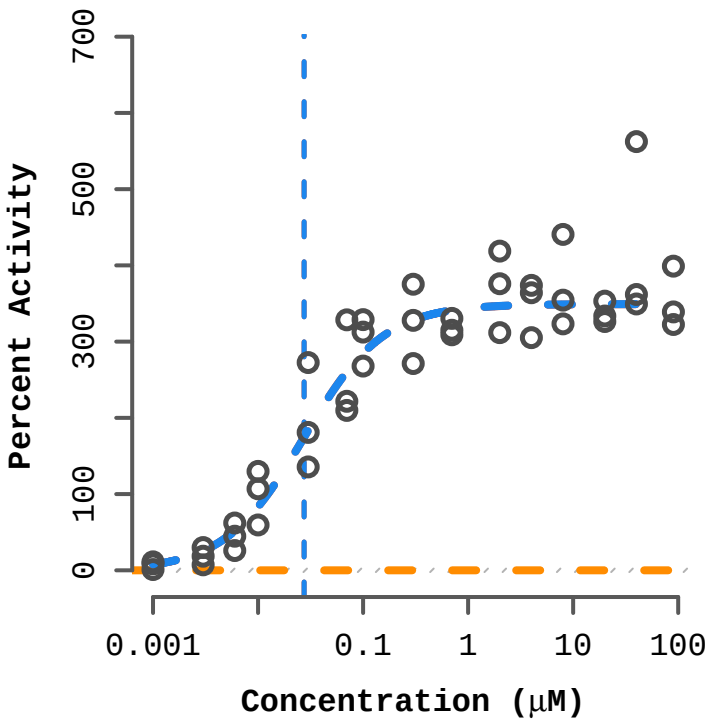
NAME: Betaine
CHID: 22666 **CASRN:** 107-43-7
SPID(S): Tox21_301159
M4ID: 12477974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.738 **MAX_MED:** 0.348 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Betamethasone
CHID: 22667 **CASRN:** 378-44-9
SPID(S): Tox21_301455
M4ID: 12477678

HILL MODEL (in red):

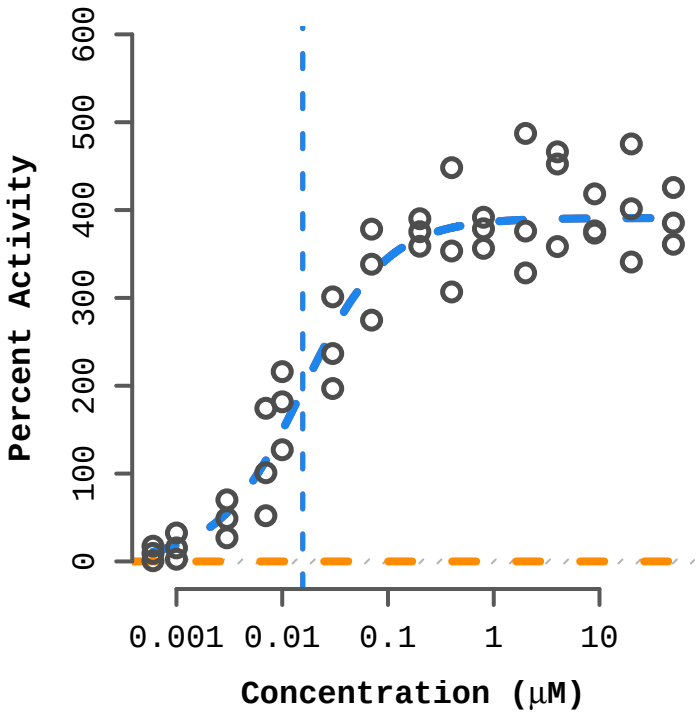
	tp	ga	gw
val:	349	-1.56	1.15
sd:	8.44	0.0744	0.156

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	349	-1.56	1.15	2.18	10.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	647.56	471.15	475.14
PROB:	0	0.88	0.12
RMSE:	289.23	47.77	47.76

MAX_MEAN: 425 **MAX_MED:** 376 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Betamethasone
CHID: 22667 **CASRN:** 378-44-9
SPID(S): Tox21_112115_1
M4ID: 12483310

HILL MODEL (in red):

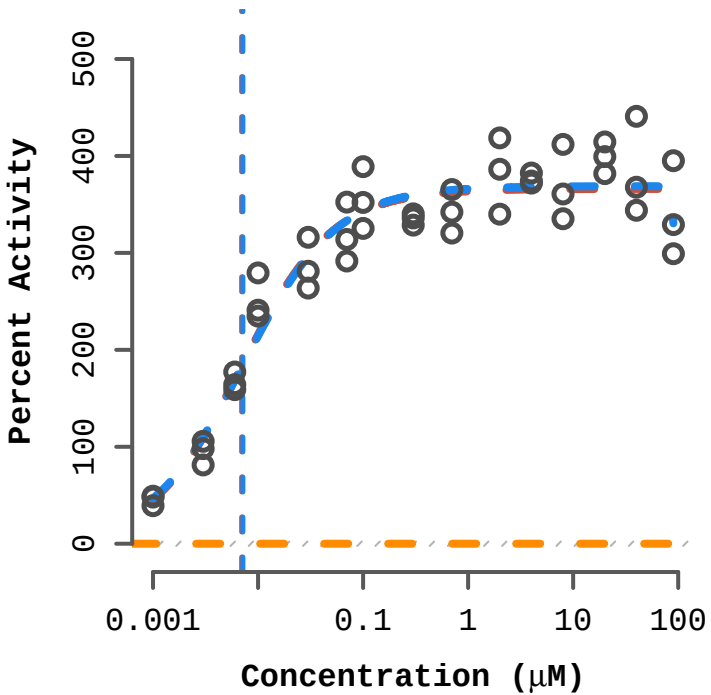
	tp	ga	gw
val:	391	-1.81	1.09
sd:	10.1	0.0755	0.152

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	391	-1.81	1.09	2.78	7.97
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	654.61	473.29	477.29
PROB:	0	0.88	0.12
RMSE:	312.37	41.37	41.37

MAX_MEAN: 426 **MAX_MED:** 452 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Betamethasone valerate
CHID: 22673 CASRN: 2152-44-5
SPID(S): Tox21_302288
M4ID: 12476845

HILL MODEL (in red):

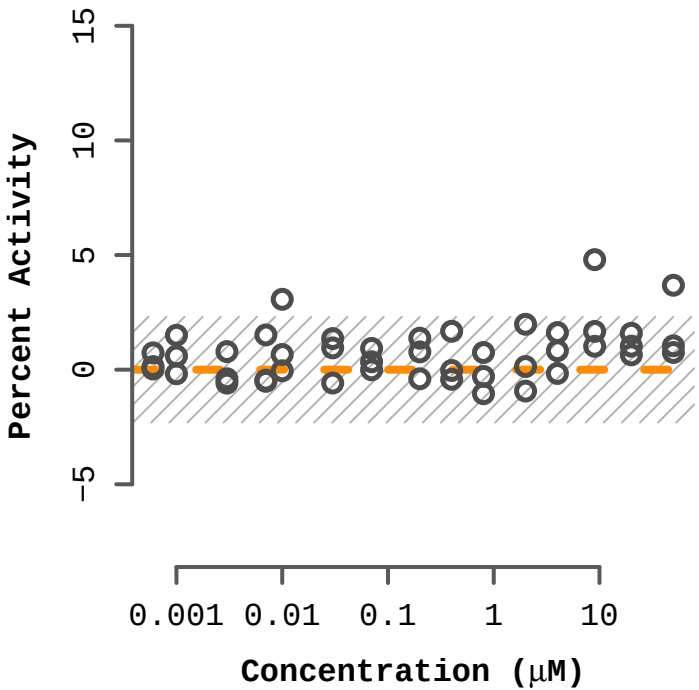
	tp	ga	gw
val:	366	-2.16	1.01
sd:	7.29	0.0504	0.127

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	369	-2.14	0.981	2.01	16
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	657.1	444.54	446.17
PROB:	0	0.69	0.31
RMSE:	315.95	30.12	29.39

MAX_MEAN: 399 MAX_MED: 399 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

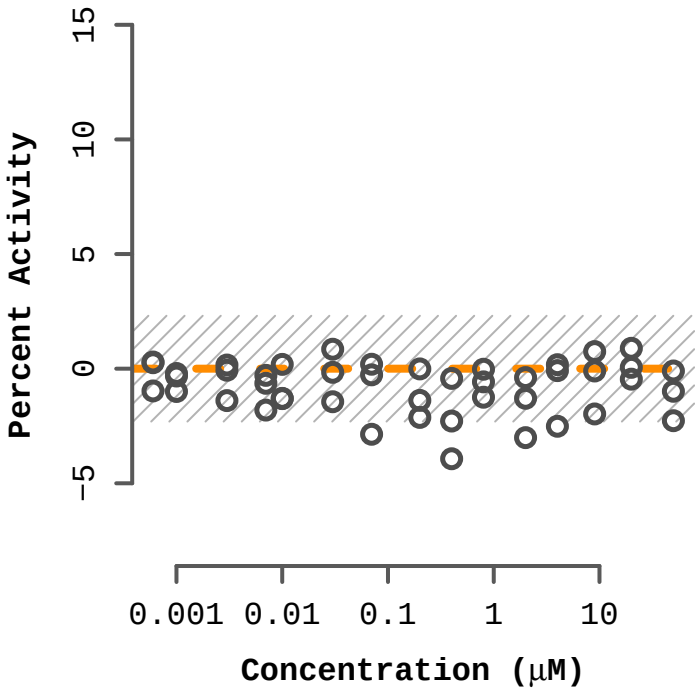
NAME: Betaxolol
CHID: 22674 **CASRN:** 63659-18-7
SPID(S): Tox21_110091_1
M4ID: 12484661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 2.5 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

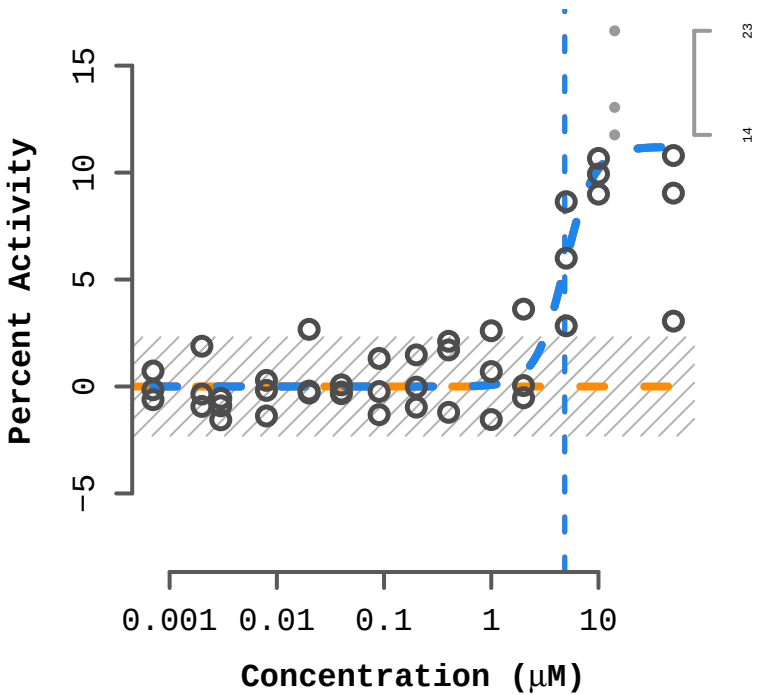
NAME: Bethanechol
CHID: 22676 **CASRN:** 590-63-6
SPID(S): Tox21_112028_1
M4ID: 12483363

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.164 **MAX_MED:** 0.261 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bicalutamide
CHID: 22678 CASRN: 90357-06-5
SPID(S): Tox21_303560
M4ID: 12475585 BRK

HILL MODEL (in red):

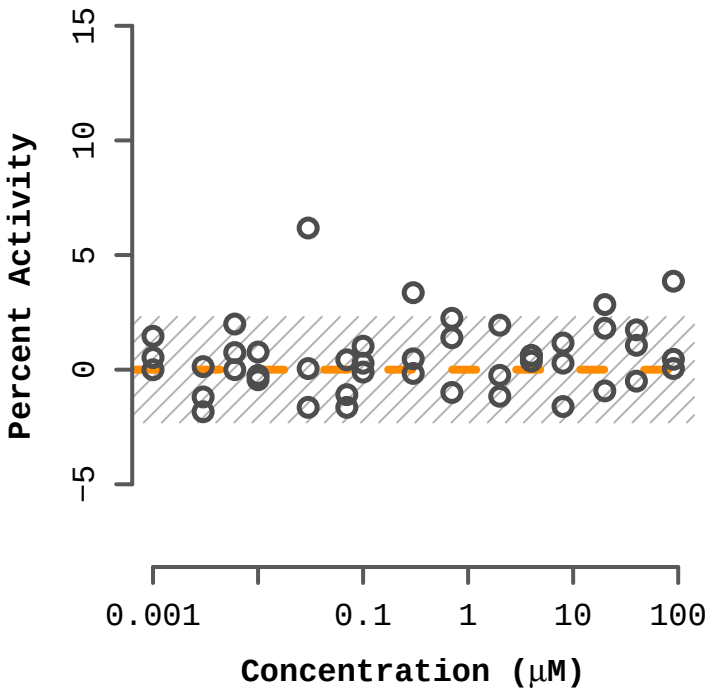
	tp	ga	gw
val:	11.2	0.685	3.16
sd:	1.13	0.0714	1.21

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.2	0.685	3.16	3.66	5.61
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	273.94	201.47	205.47
PROB:	0	0.88	0.12
RMSE:	6.05	2.64	2.64

MAX_MEAN: 17.6 MAX_MED: 16.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

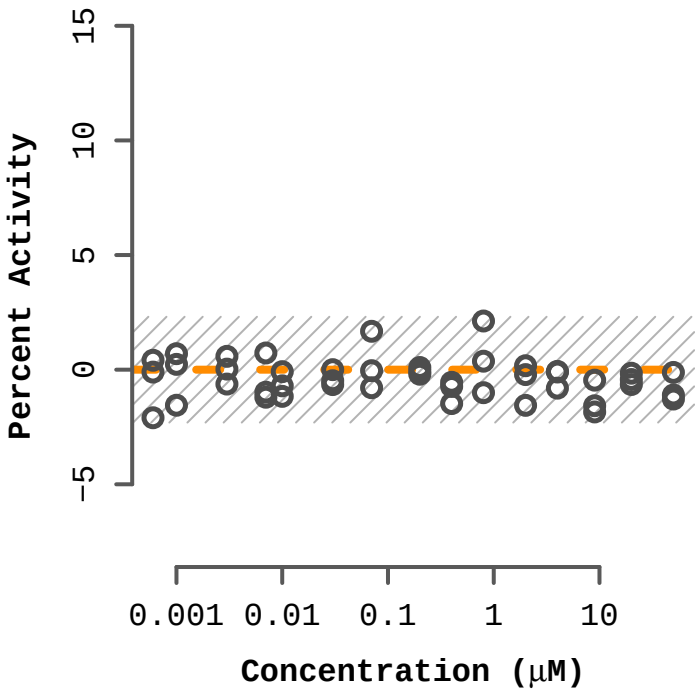
NAME: Biotin
CHID: 22679 **CASRN:** 58-85-5
SPID(S): Tox21_302161
M4ID: 12476972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

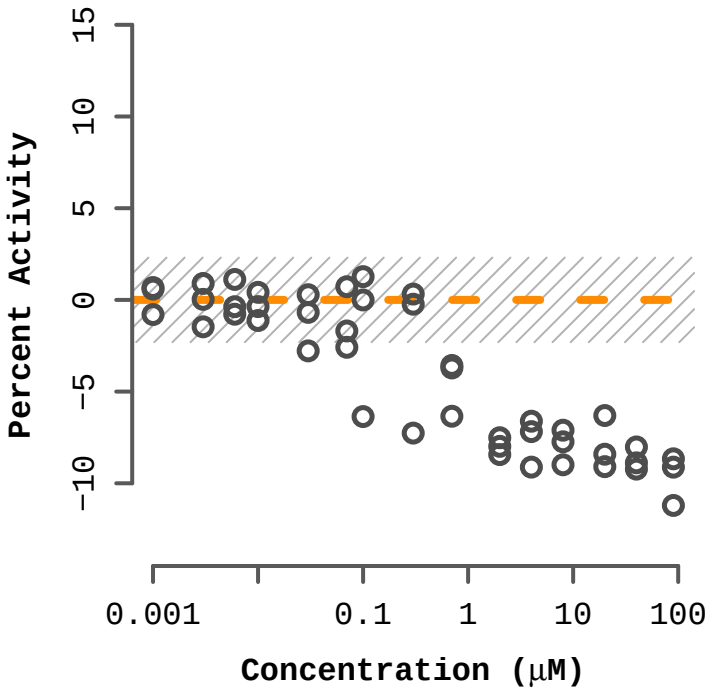
NAME: Biotin
CHID: 22679 **CASRN:** 58-85-5
SPID(S): Tox21_113050_1
M4ID: 12482827

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.498 **MAX_MED:** 0.371 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

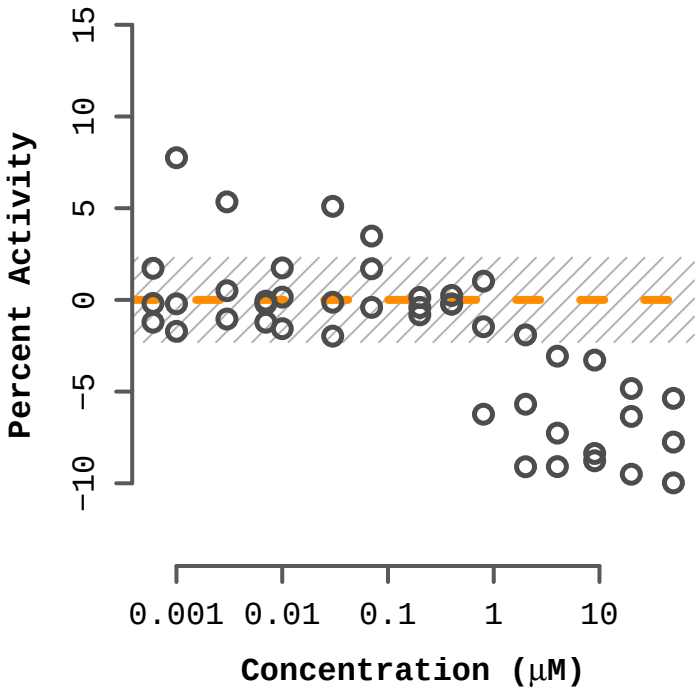
NAME: Bisacodyl
CHID: 22681 CASRN: 603-50-9
SPID(S): Tox21_200338
M4ID: 12481914

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.59	NA	NA
PROB:	1	NA	NA
RMSE:	5.68	NA	NA

MAX_MEAN: 0.157 **MAX_MED:** 0.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

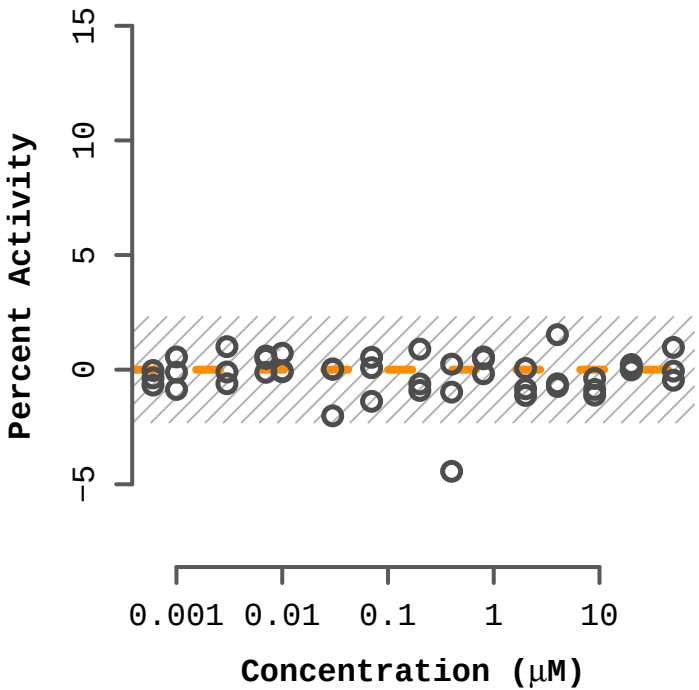
NAME: Bisacodyl
CHID: 22681 **CASRN:** 603-50-9
SPID(S): Tox21_110472_1
M4ID: 12484329

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.63	NA	NA
PROB:	1	NA	NA
RMSE:	4.61	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

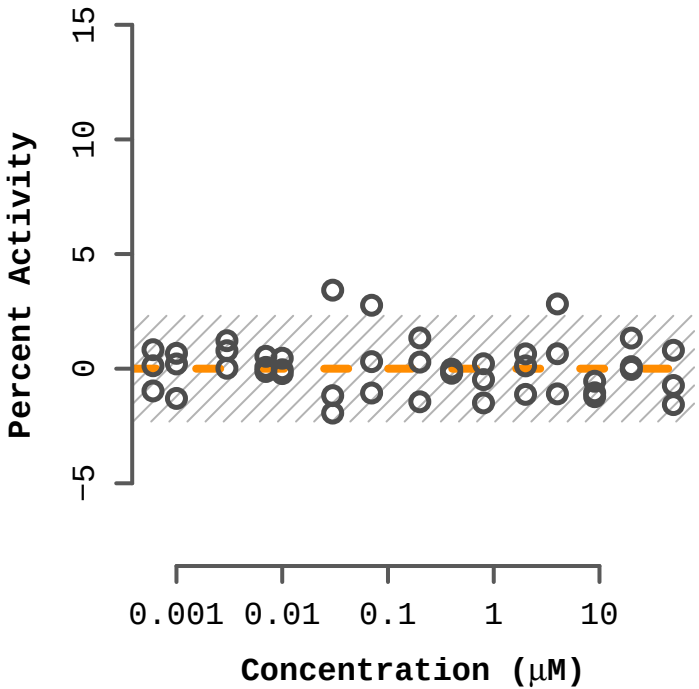
NAME: Bitolterol
CHID: 22683 CASRN: 30392-40-6
SPID(S): Tox21_113730
M4ID: 12482484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.325 MAX_MED: 0.492 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

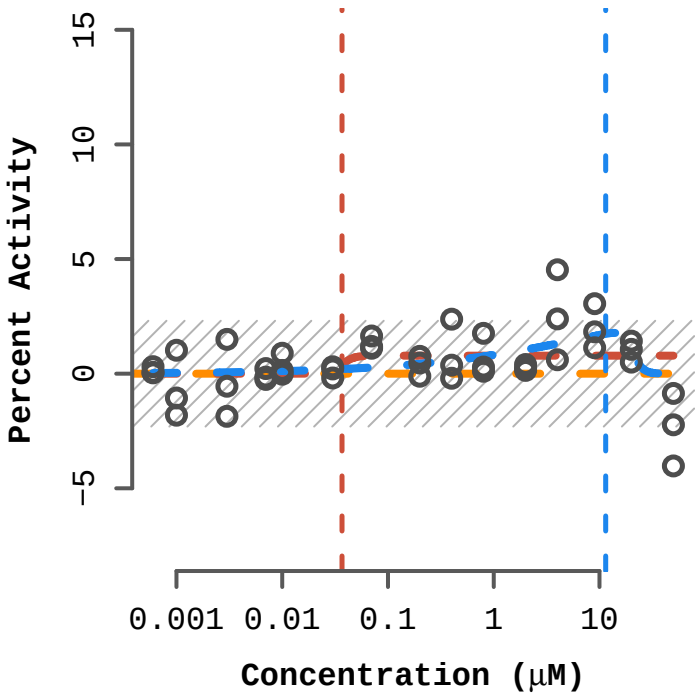
NAME: Bopindolol
CHID: 22684 **CASRN:** 62658-63-3
SPID(S): Tox21_112017_1
M4ID: 12483369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.794 **MAX_MED:** 0.785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bromodiphenhydramine
CHID: 22688 CASRN: 118-23-0
SPID(S): Tox21_113667
M4ID: 12482547

HILL MODEL (in red):

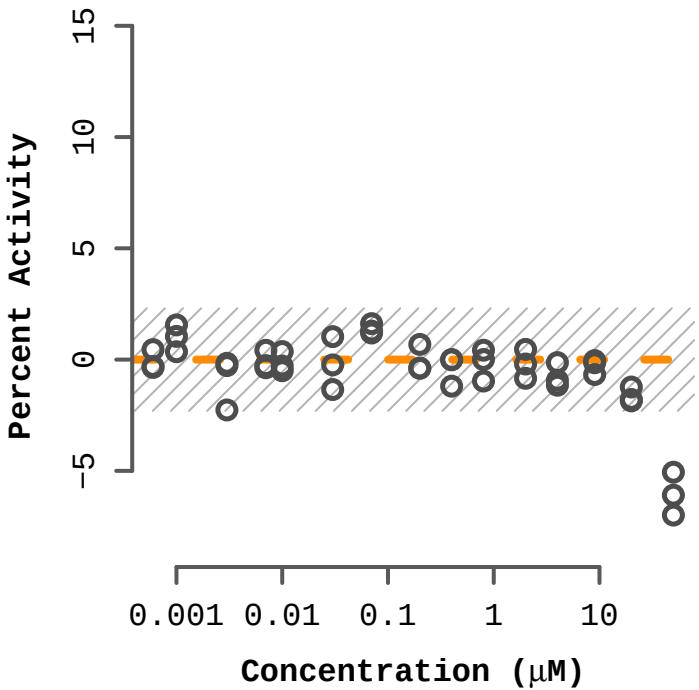
	tp	ga	gw
val:	0.785	−1.43	8
sd:	0.205	0.208	12.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.5	1.06	0.486	1.31	9.13
sd:	6.18	2.46	0.264	0.113	28.5

	CNST	HILL	GNLS
AIC:	158.02	151.01	147.18
PROB:	0	0.13	0.87
RMSE:	1.45	1.33	1.16

MAX_MEAN: 2.51 **MAX_MED:** 2.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

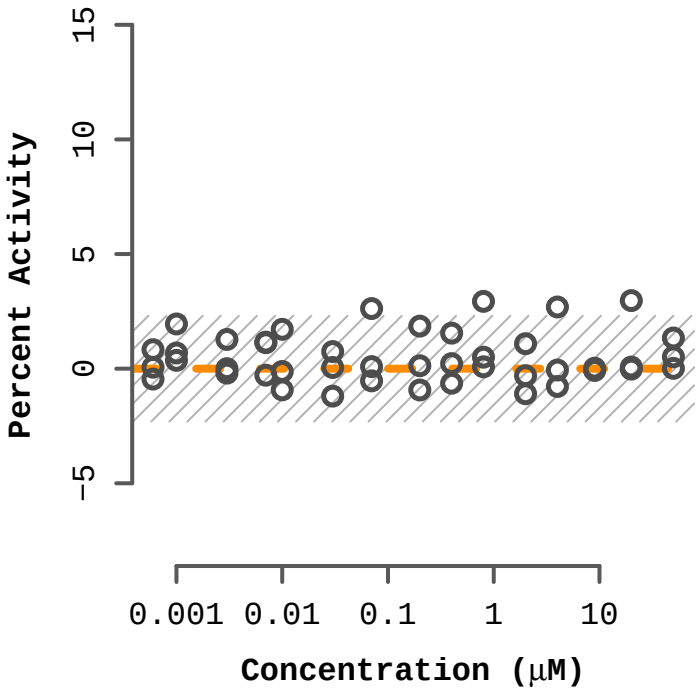
NAME: Bromperidol
CHID: 22690 **CASRN:** 10457-90-6
SPID(S): Tox21_110565_1
M4ID: 12484264

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

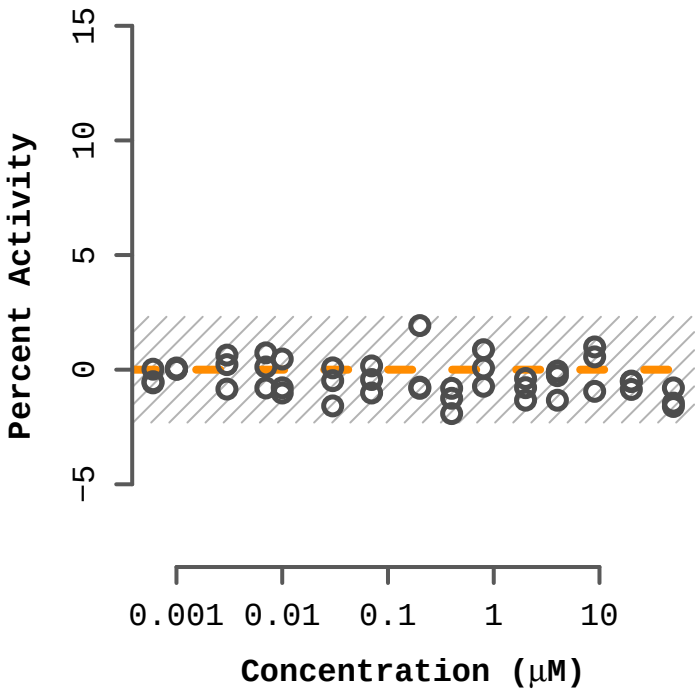
NAME: Bumetanide
CHID: 22699 CASRN: 28395-03-1
SPID(S): Tox21_110088_1
M4ID: 12484664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.17 MAX_MED: 1.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

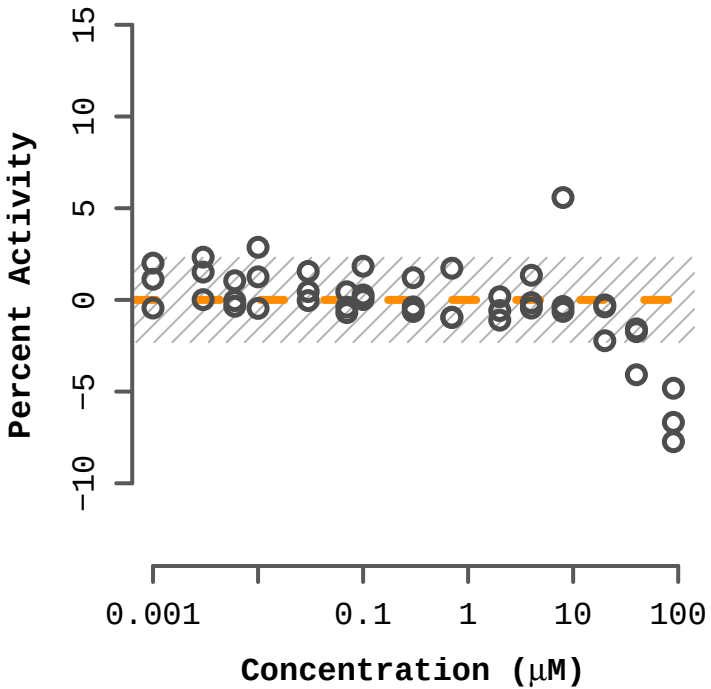
NAME: Bupranolol
CHID: 22704 **CASRN:** 14556-46-8
SPID(S): Tox21_113691
M4ID: 12482523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.203 **MAX_MED:** 0.559 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

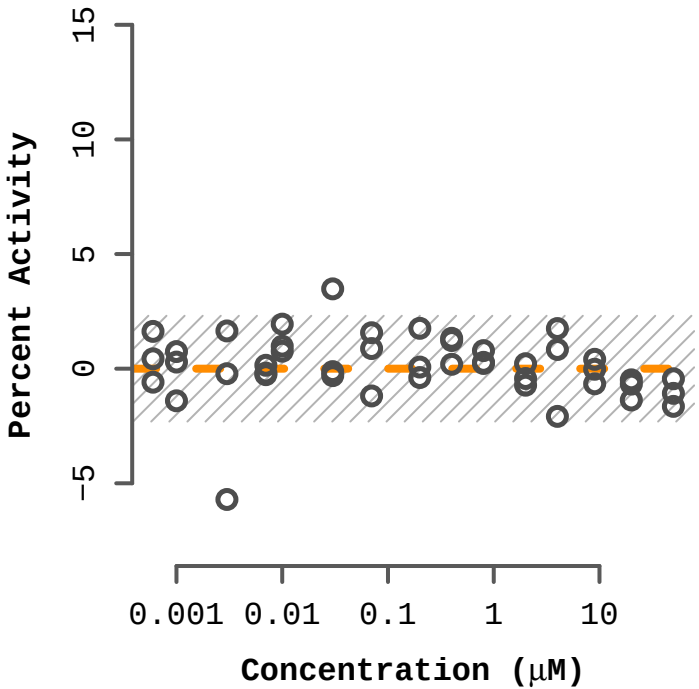
NAME: Buspirone
CHID: 22707 **CASRN:** 36505-84-7
SPID(S): Tox21_302371
M4ID: 12476762

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.25	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

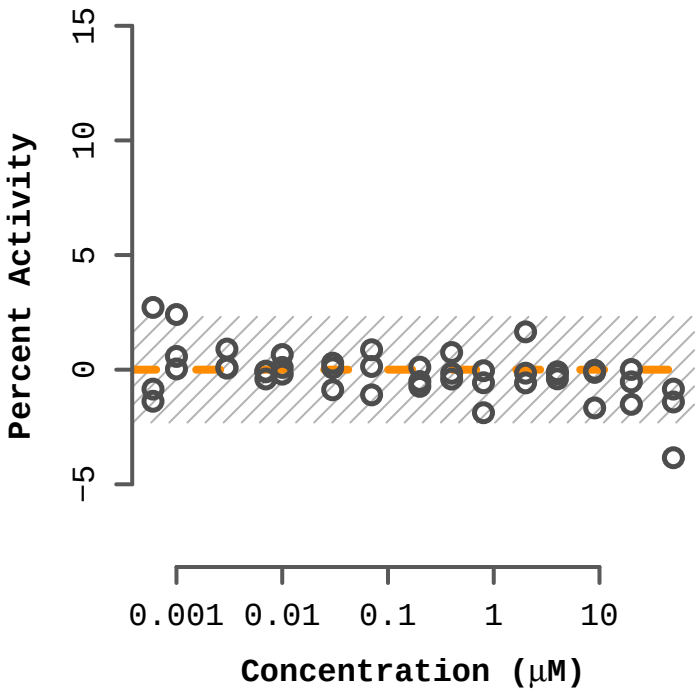
NAME: Buspirone
CHID: 22707 **CASRN:** 36505-84-7
SPID(S): Tox21_110092_1
M4ID: 12484660

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

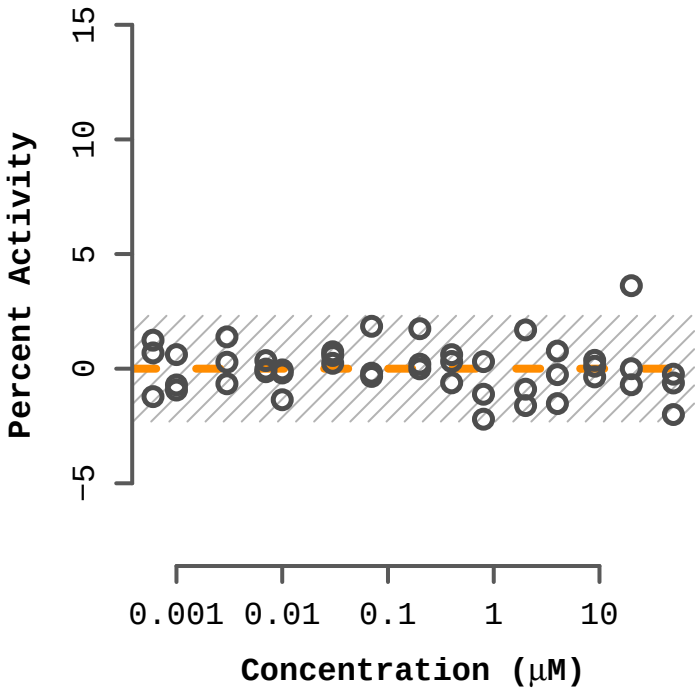
NAME: Butriptyline
CHID: 22715 CASRN: 35941-65-2
SPID(S): Tox21_113980
M4ID: 12482261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

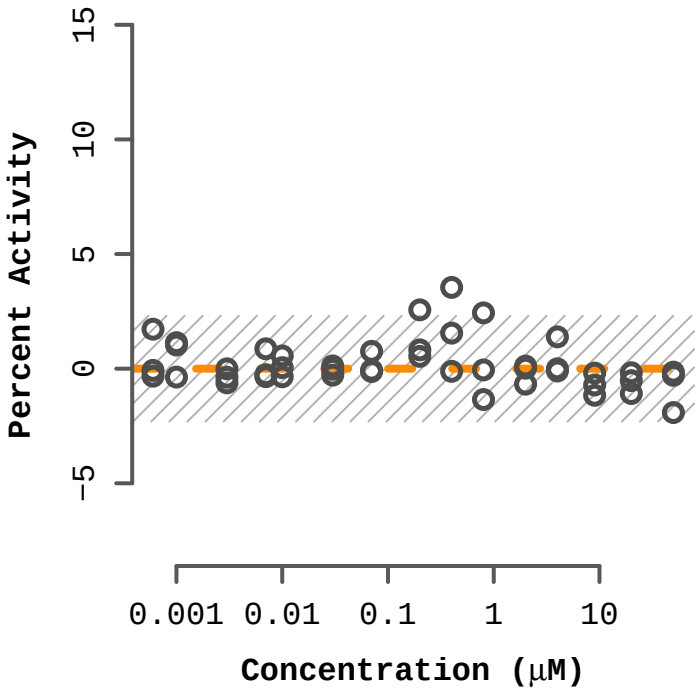
NAME: Butylscopolammonium bromide
CHID: 22718 CASRN: 149-64-4
SPID(S): Tox21_112031_1
M4ID: 12483360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.974 **MAX_MED:** 0.689 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

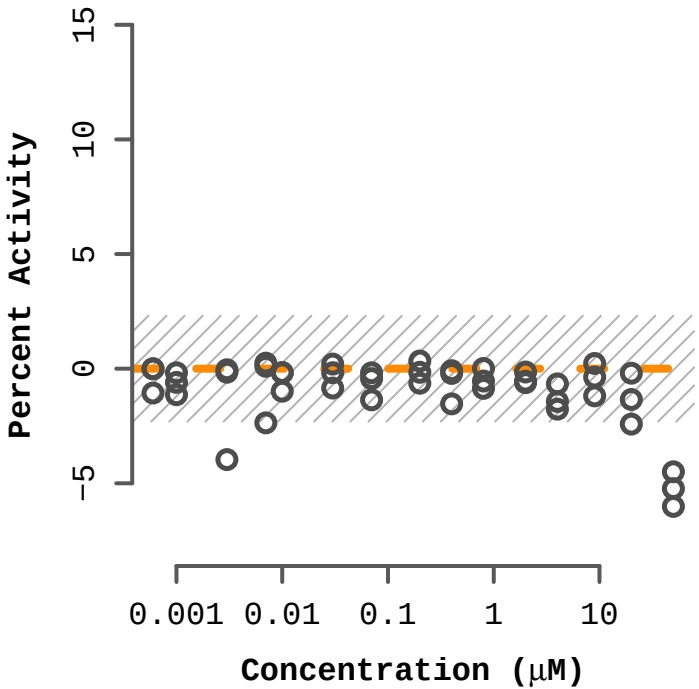
NAME: Cabergoline
CHID: 22719 **CASRN:** 81409-90-7
SPID(S): Tox21_112589_1
M4ID: 12483017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

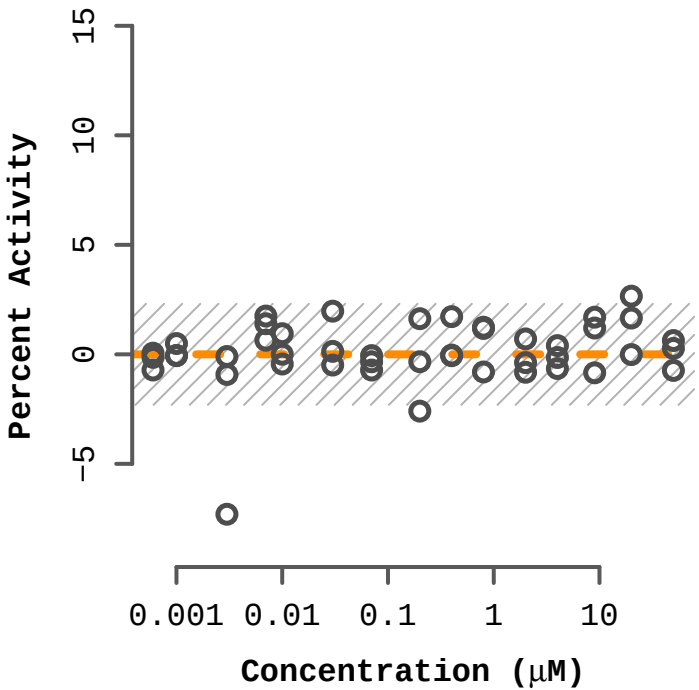
NAME: Canadine
CHID: 22724 **CASRN:** 522-97-4
SPID(S): Tox21_110451_1
M4ID: 12484345

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: −0.151 **MAX_MED:** 0.106 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

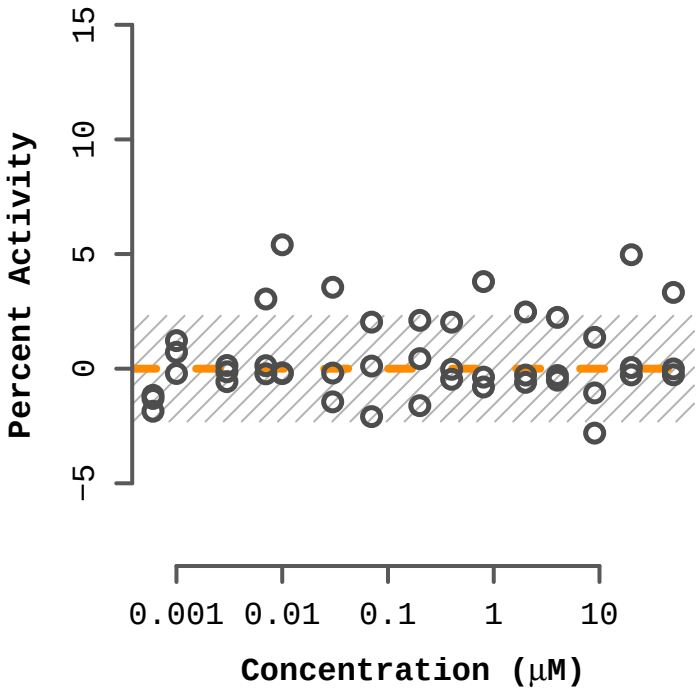
NAME: Candesartan
CHID: 22725 **CASRN:** 139481-59-7
SPID(S): Tox21_112478_1
M4ID: 12483077

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

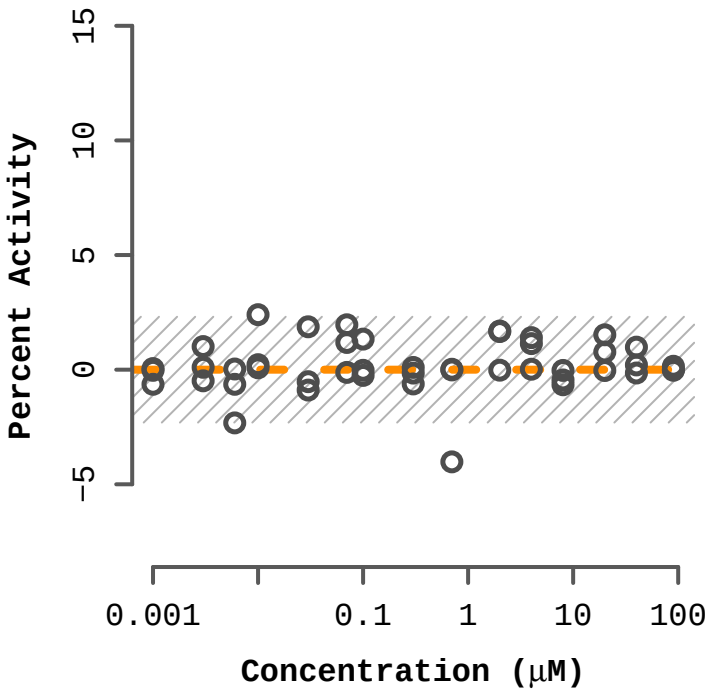
NAME: Carbachol
CHID: 22730 **CASRN:** 51-83-2
SPID(S): Tox21_112029_1
M4ID: 12483362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 0.716 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

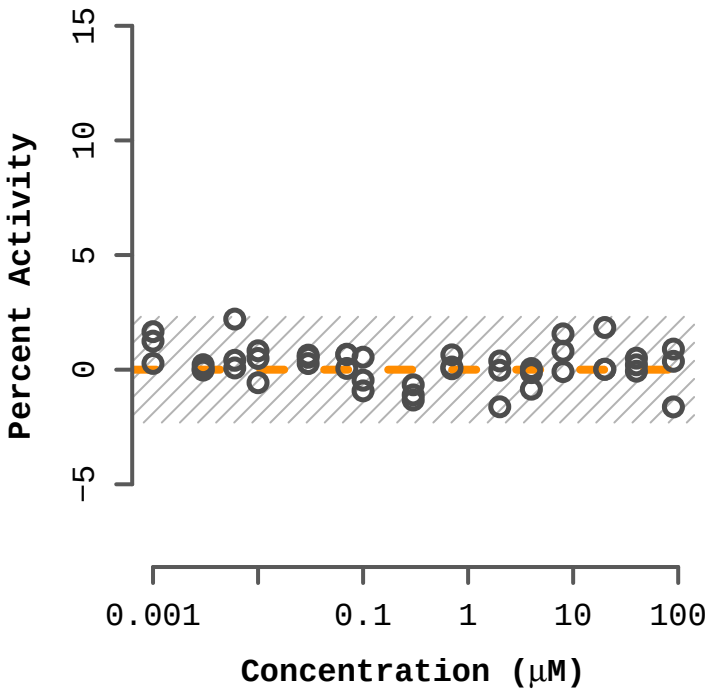
NAME: Carbamazepine
CHID: 22731 **CASRN:** 298-46-4
SPID(S): Tox21_300195
M4ID: 12478935

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

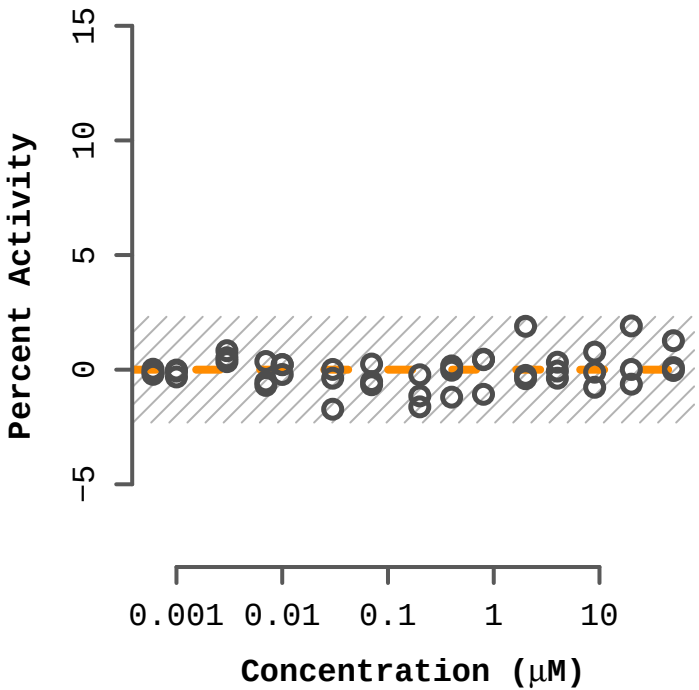
NAME: Carbamazepine
CHID: 22731 **CASRN:** 298-46-4
SPID(S): Tox21_202273
M4ID: 12479979

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

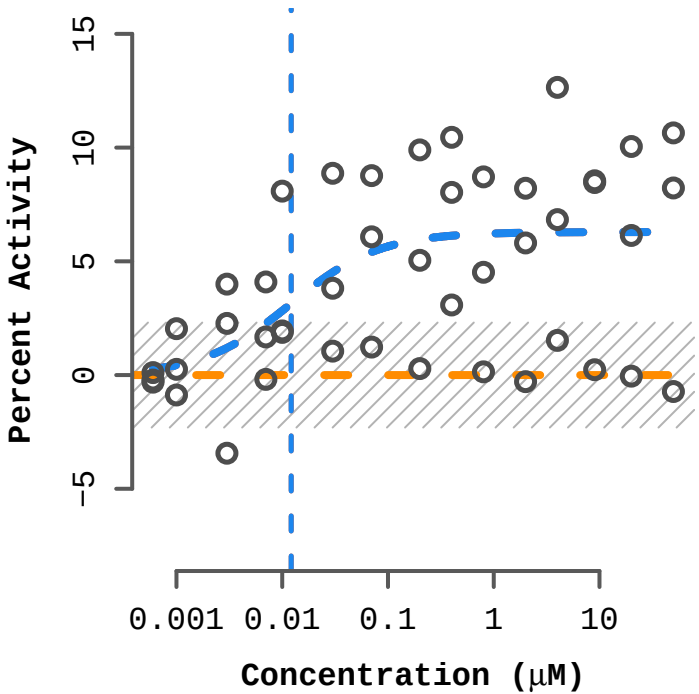
NAME: Carbamazepine
CHID: 22731 **CASRN:** 298-46-4
SPID(S): Tox21_110104_1
M4ID: 12484649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.568 **MAX_MED:** 0.522 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carbetapentane
CHID: 22734 **CASRN:** 77-23-6
SPID(S): Tox21_110909_1
M4ID: 12484023

HILL MODEL (in red):

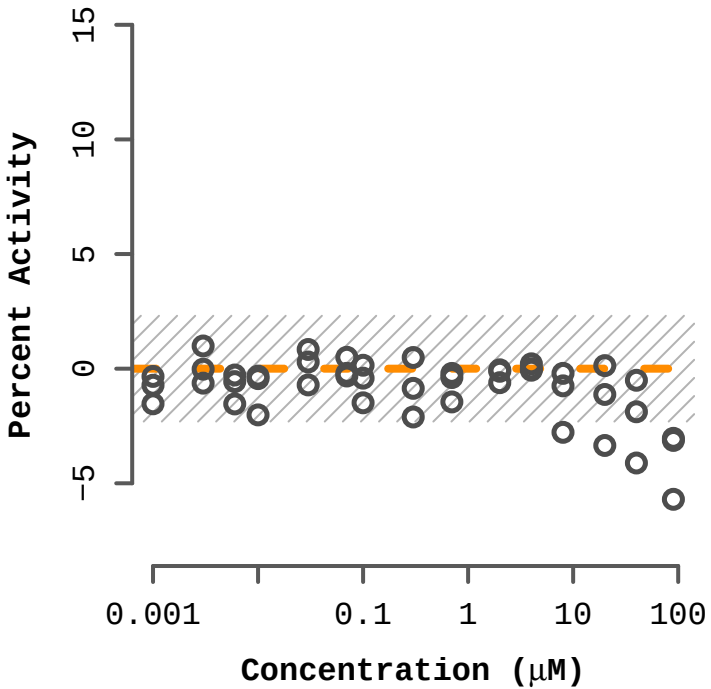
	tp	ga	gw
val:	6.29	−1.92	1.04
sd:	0.966	0.364	0.805

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.29	−1.92	1.04	3.45	7.83
sd:	0.966	0.364	0.805	430000	791000

	CNST	HILL	GNLS
AIC:	291.55	252.02	256.02
PROB:	0	0.88	0.12
RMSE:	5.81	3.48	3.48

MAX_MEAN: 7.19 **MAX_MED:** 8.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

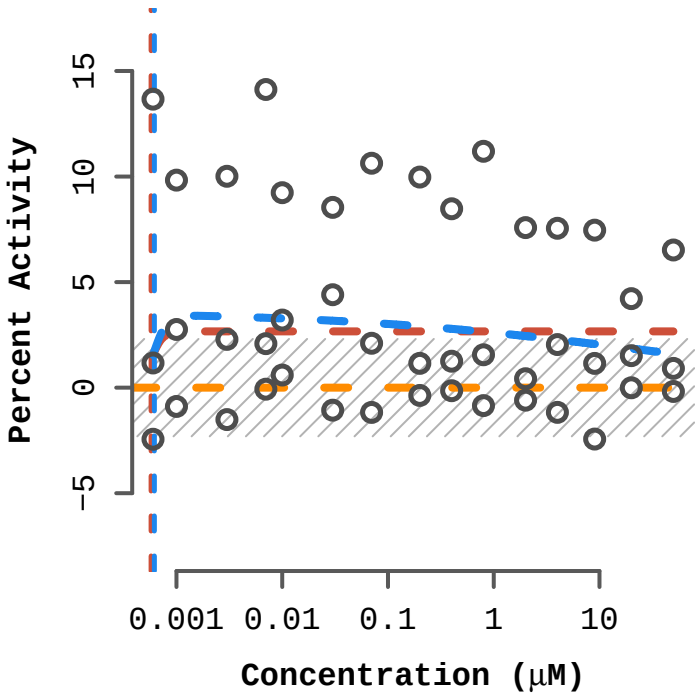
NAME: Carbimazole
CHID: 22736 **CASRN:** 22232-54-8
SPID(S): Tox21_302320
M4ID: 12476813

HILL MODEL: Not applicable.

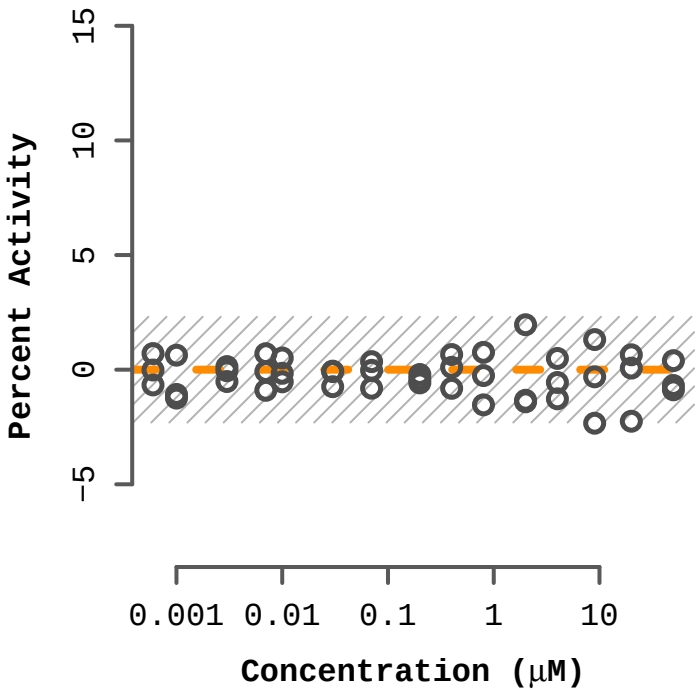
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 0.141 **MAX_MED:** 0.292 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Carbimazole
CHID:    22736   CASRN: 22232-54-8
SPID(S): Tox21_110596_1
M4ID:    12484242

HILL MODEL (in red):
      tp       ga       gw
val:  2.66     -3.24    8
sd:   0.725    0.278    36.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.6      -3.21    7.26     1.39     0.3
sd:   3.7      0.249    70.8     3.46     0.939

      CNST        HILL        GNLS
AIC:  284.85      276.14      279.49
PROB: 0.01        0.83        0.16
RMSE: 5.71        4.66        4.59

MAX_MEAN: 5.38      MAX_MED: 4.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

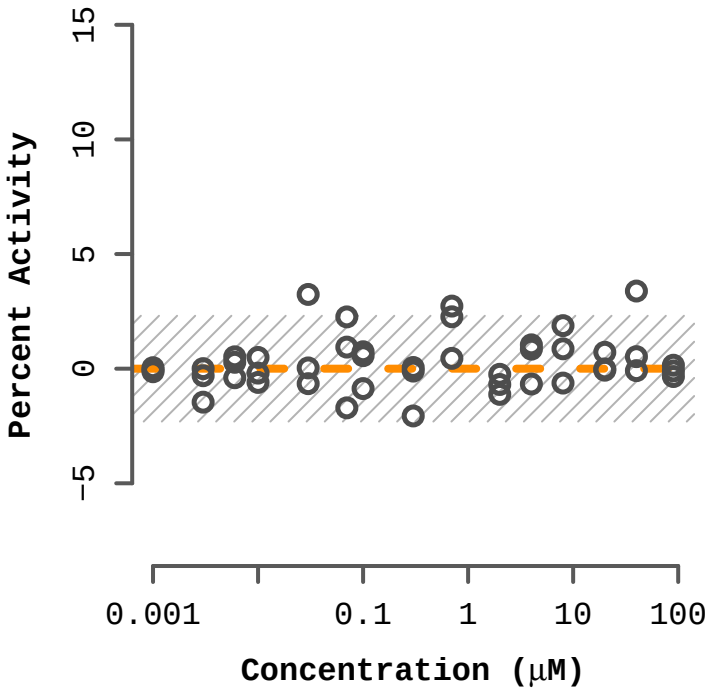
NAME: Carbocysteine
CHID: 22738 **CASRN:** 2387-59-9
SPID(S): Tox21_111658_1
M4ID: 12483551

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.00908 **MAX_MED:** 0.103 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

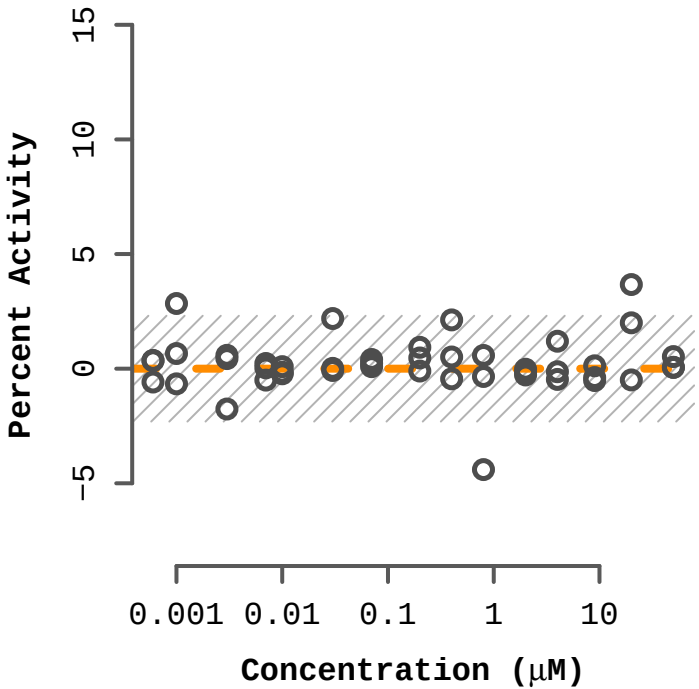
NAME: Carbutamide
CHID: 22741 **CASRN:** 339-43-5
SPID(S): Tox21_301817
M4ID: 12477316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

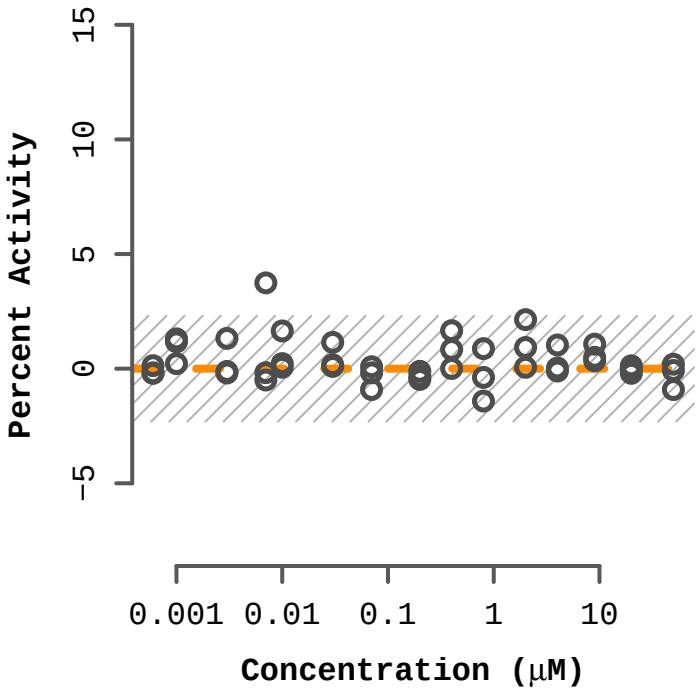
NAME: Carbutamide
CHID: 22741 **CASRN:** 339-43-5
SPID(S): Tox21_111673_1
M4ID: 12483544

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

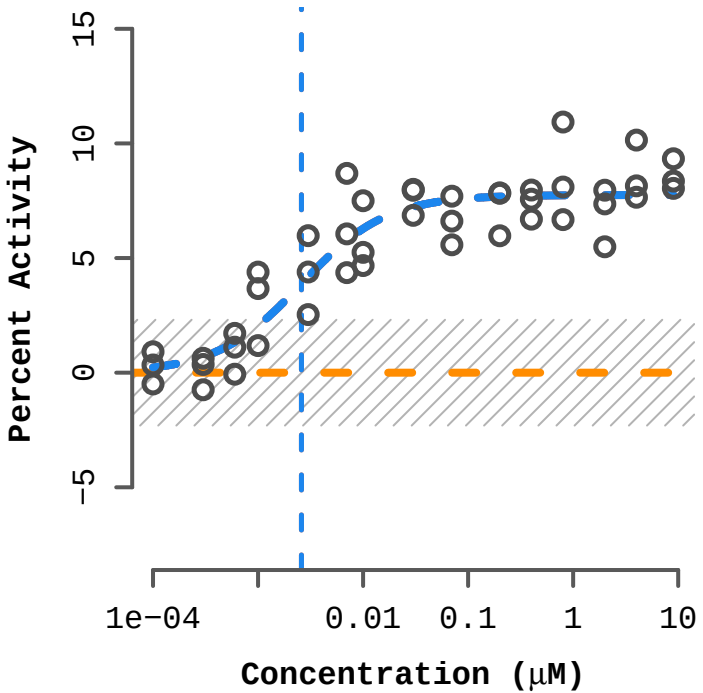
NAME: Carmustine
CHID: 22743 **CASRN:** 154-93-8
SPID(S): Tox21_110097_1
M4ID: 12484656

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cefaclor
CHID: 22748 CASRN: 53994-73-3
SPID(S): Tox21_110880_1
M4ID: 12484047

HILL MODEL (in red):

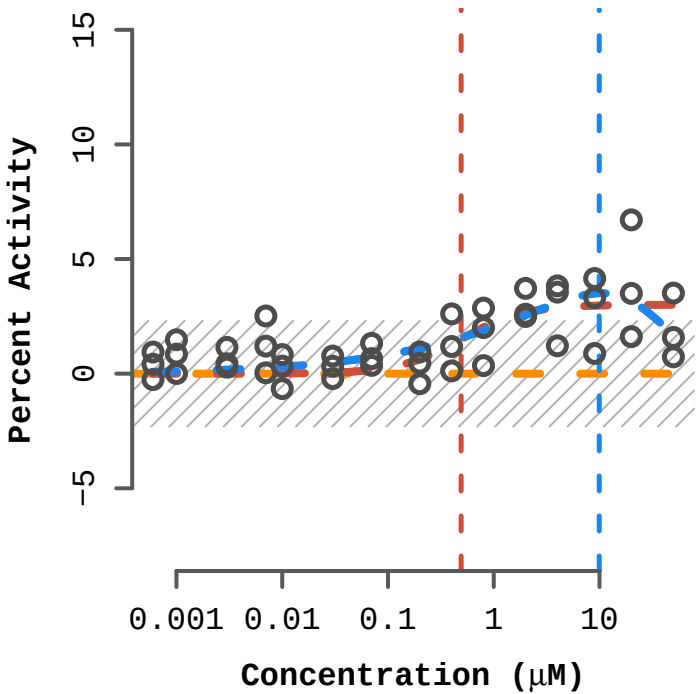
	tp	ga	gw
val:	7.75	−2.59	1.07
sd:	0.276	0.117	0.227

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.75	−2.59	1.07	2.88	4.3
sd:	0.276	0.117	0.227	1020	2280

	CNST	HILL	GNLS
AIC:	303.66	157.85	161.85
PROB:	0	0.88	0.12
RMSE:	6.32	1.26	1.26

MAX_MEAN: 8.65 MAX_MED: 8.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cefadroxil
CHID: 22749 **CASRN:** 50370-12-2
SPID(S): Tox21_110651_1
M4ID: 12484204

HILL MODEL (in red):

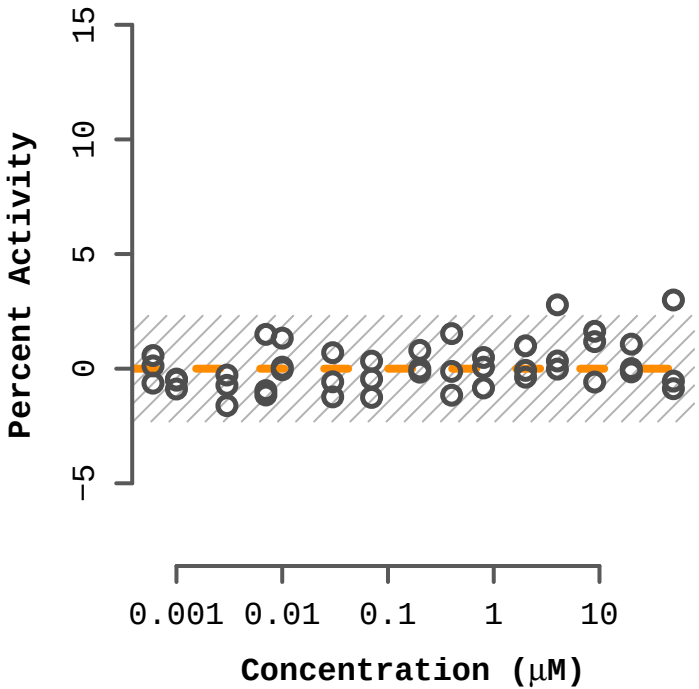
	tp	ga	gw
val:	3.01	−0.308	1.48
sd:	0.431	0.185	1.19

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.05	0.998	0.47	1.49	1.67
sd:	7.72	1.57	0.226	0.278	1.2

	CNST	HILL	GNLS
AIC:	194.81	147.21	145.63
PROB:	0	0.31	0.69
RMSE:	2.11	1.15	1.1

MAX_MEAN: 3.94 **MAX_MED:** 3.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

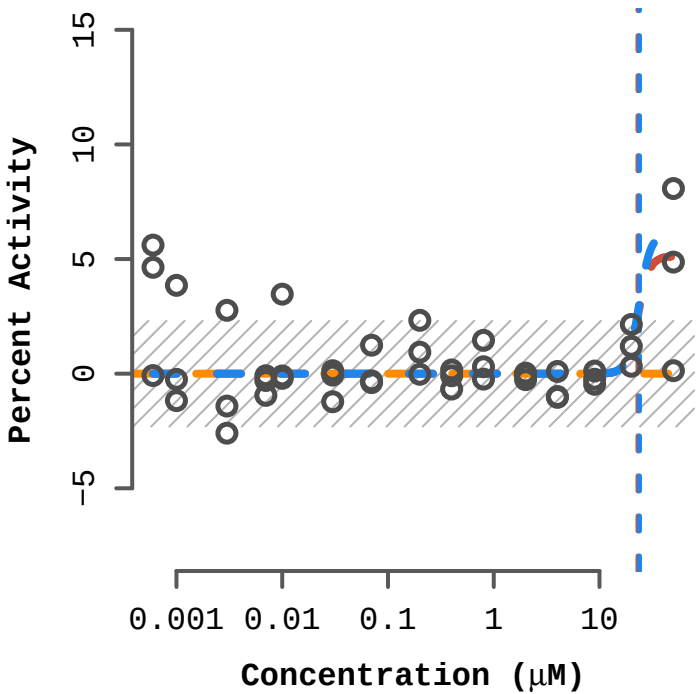
NAME: Cefazolin
CHID: 22753 **CASRN:** 25953-19-9
SPID(S): Tox21_111691_1
M4ID: 12483533

HILL MODEL: Not applicable.

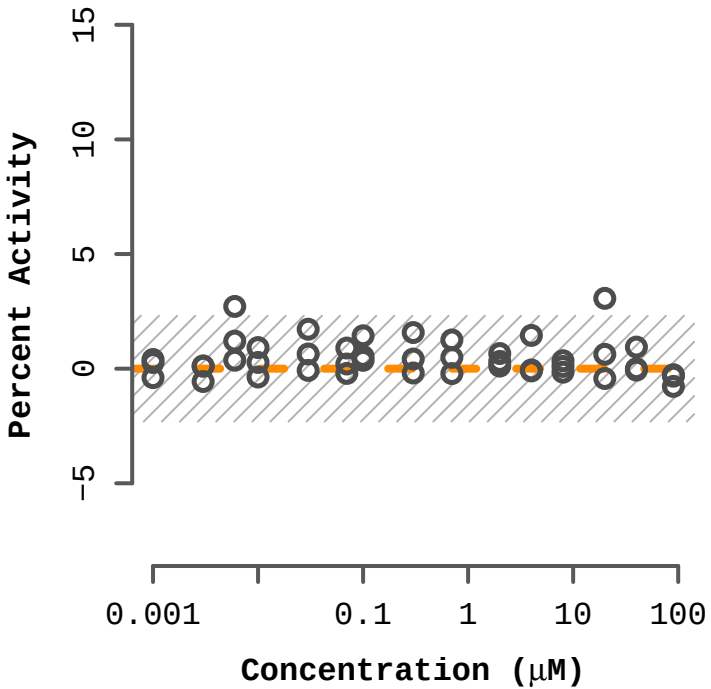
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.18 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cefoxitin
CHID:    22764   CASRN: 35607-66-0
SPID(S): Tox21_113009_1
M4ID:    12482846

HILL MODEL (in red):
      tp       ga       gw
val:  5.12     1.36     8
sd:   1.17     0.249    30.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.25     1.38     7.99     1.8      6.27
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  182.91      178.05      182.05
PROB: 0.07        0.82        0.11
RMSE: 2.15        1.82        1.82

MAX_MEAN: 4.36      MAX_MED: 4.87      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

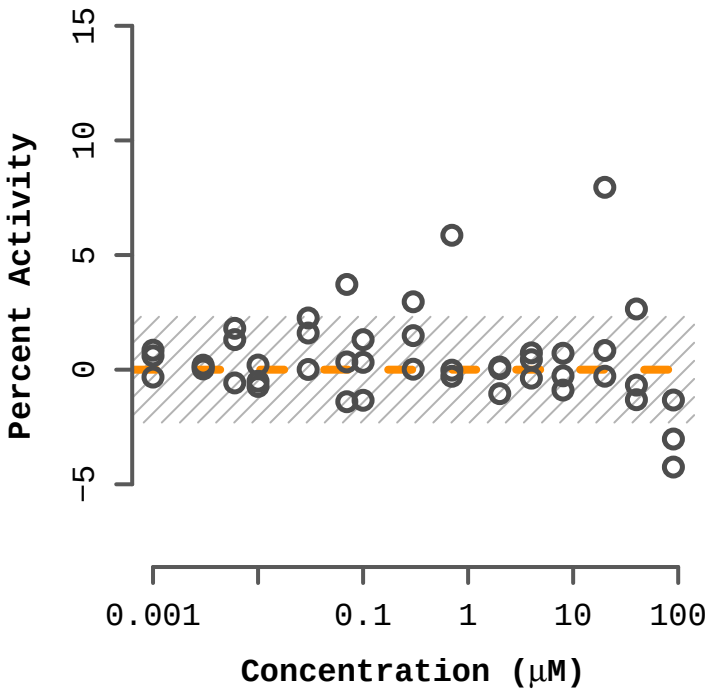
NAME: Cefuroxime
CHID: 22774 **CASRN:** 55268-75-2
SPID(S): Tox21_200884
M4ID: 12481368

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

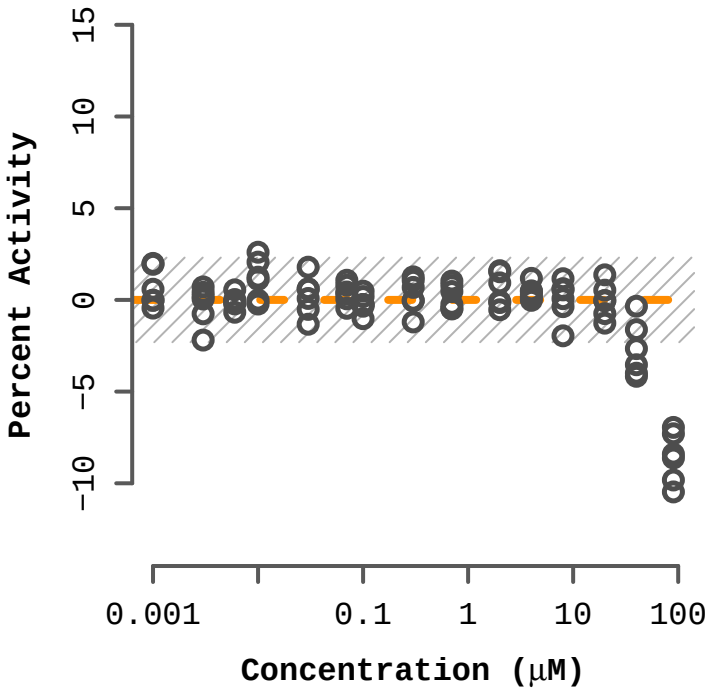
NAME: Celecoxib
CHID: 22777 **CASRN:** 169590-42-5
SPID(S): Tox21_300599
M4ID: 12478534

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 2.84 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

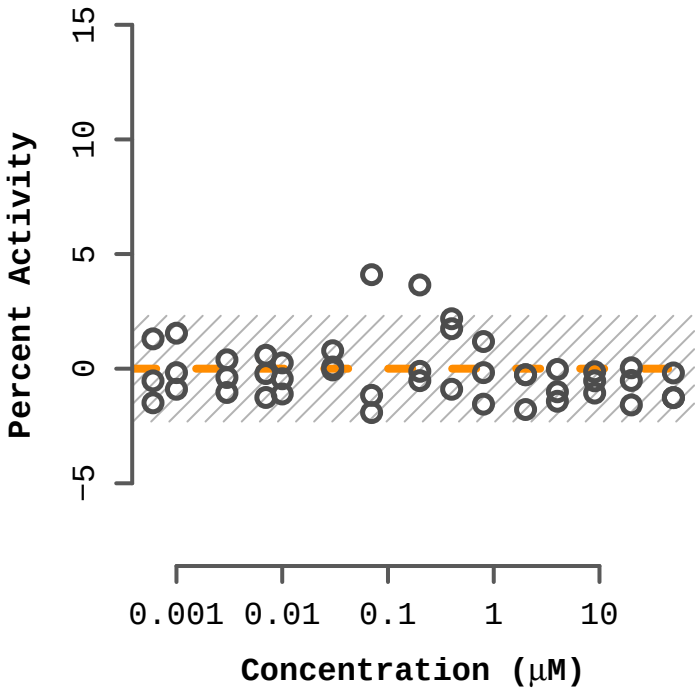
NAME: Celecoxib
CHID: 22777 **CASRN:** 169590-42-5
SPID(S): Tox21_201964
M4ID: 12480288

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	360.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.52	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

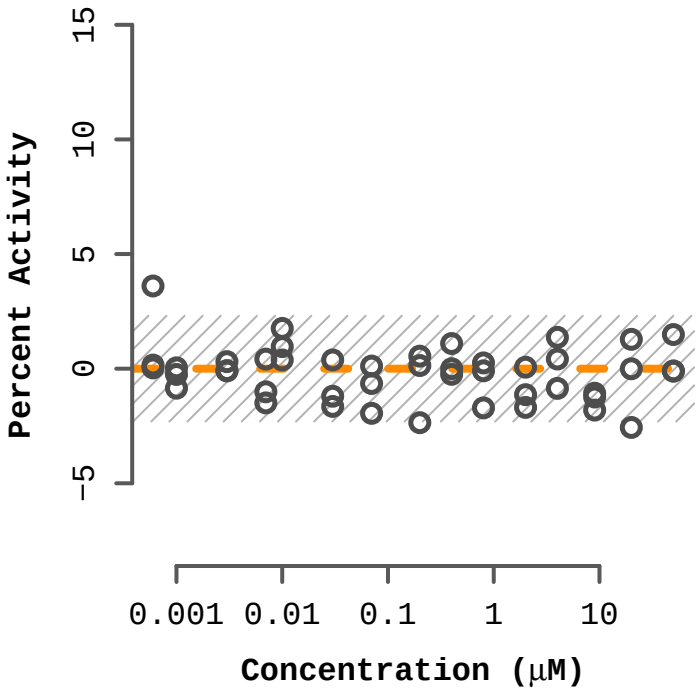
NAME: Celecoxib
CHID: 22777 CASRN: 169590-42-5
SPID(S): Tox21_111135_1
M4ID: 12483885

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

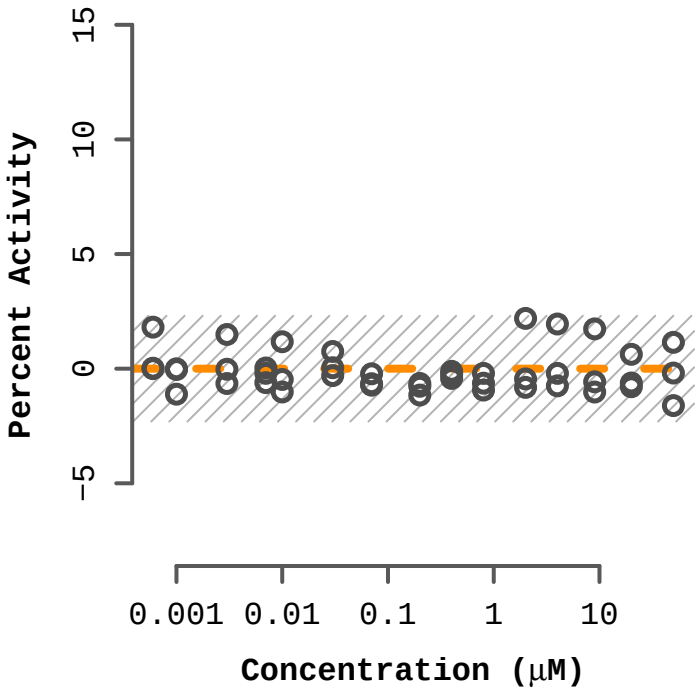
NAME: Cephalexin
CHID: 22780 CASRN: 15686-71-2
SPID(S): Tox21_111740_1
M4ID: 12483509

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.964 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

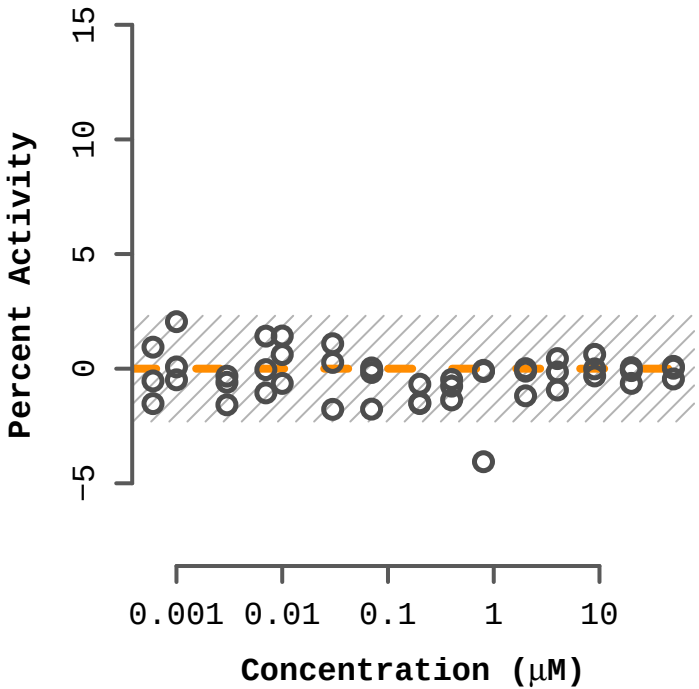
NAME: Cephalothin
CHID: 22783 **CASRN:** 153-61-7
SPID(S): Tox21_111579_1
M4ID: 12483607

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.613 **MAX_MED:** 0.043 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

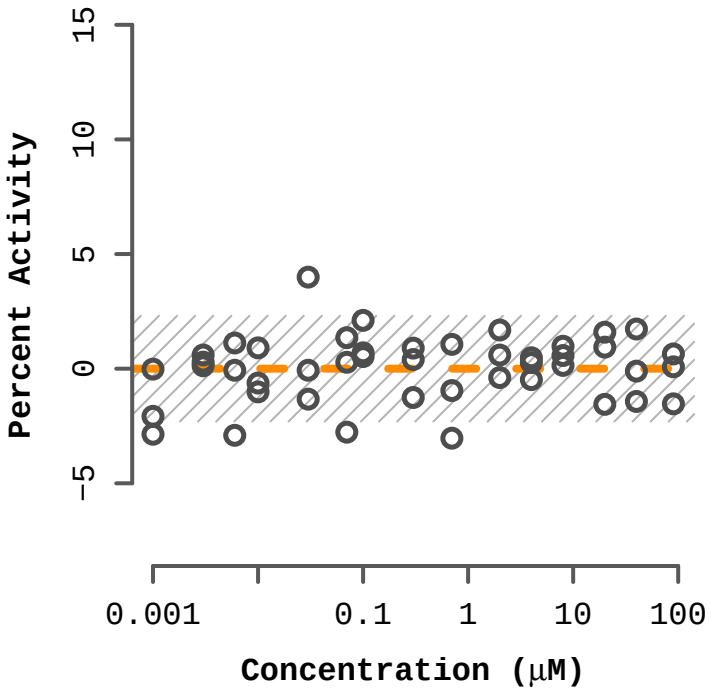
NAME: Cephradine
CHID: 22785 **CASRN:** 38821-53-3
SPID(S): Tox21_113488_1
M4ID: 12482634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.617 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

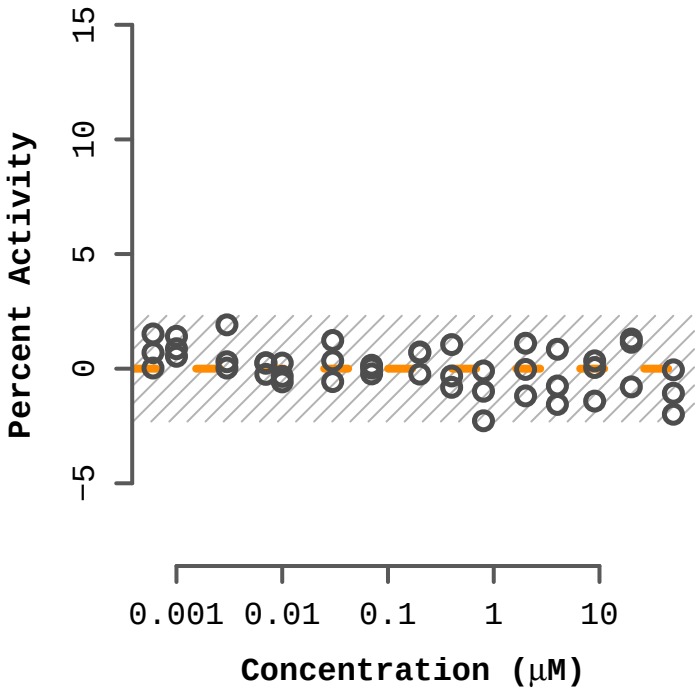
NAME: Chlormezanone
CHID: 22798 **CASRN:** 80-77-3
SPID(S): Tox21_302197
M4ID: 12476936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

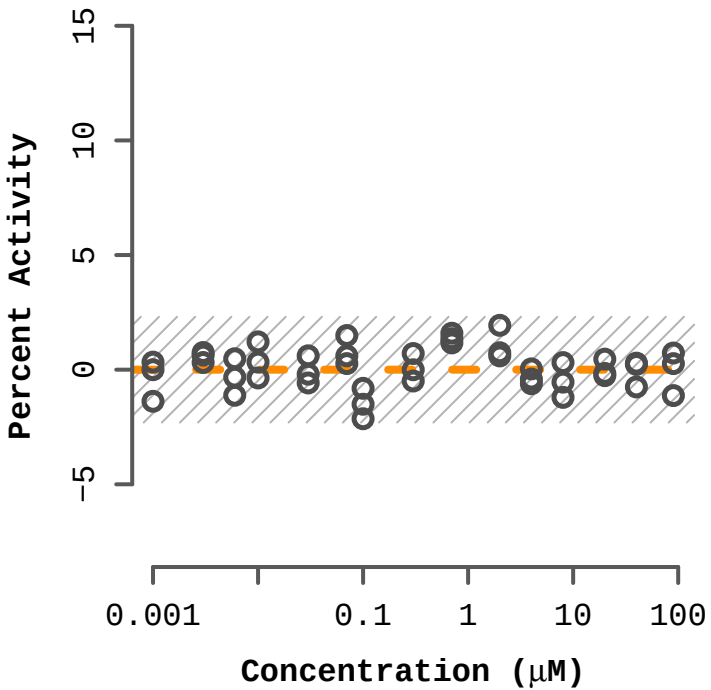
NAME: Chlormezanone
CHID: 22798 **CASRN:** 80-77-3
SPID(S): Tox21_110093_1
M4ID: 12484659

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

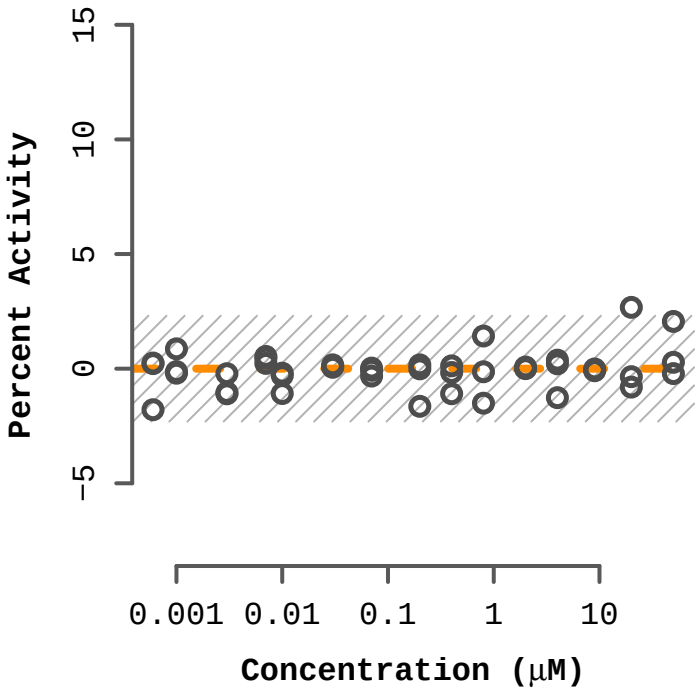
NAME: Chlorothiazide
CHID: 22800 **CASRN:** 58-94-6
SPID(S): Tox21_200972
M4ID: 12481280

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

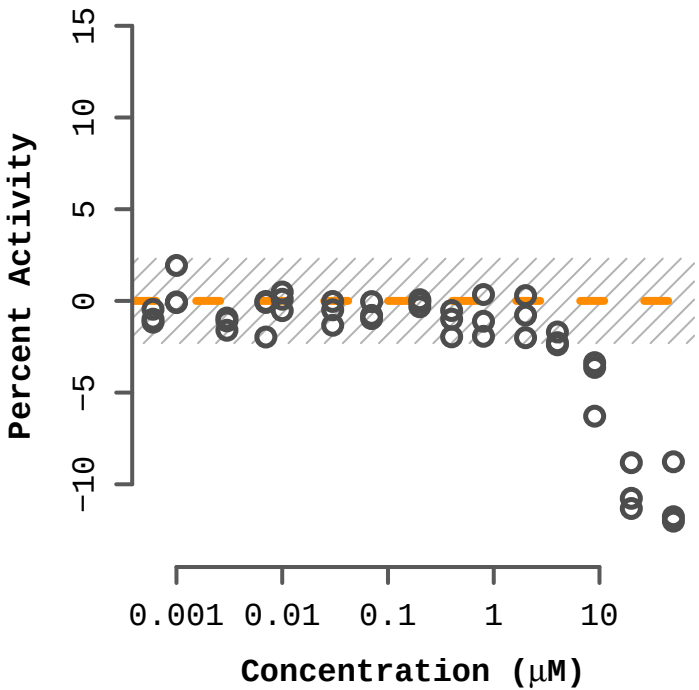
NAME: Chlorothiazide
CHID: 22800 **CASRN:** 58-94-6
SPID(S): Tox21_110107_1
M4ID: 12484646

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.71 **MAX_MED:** 0.454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

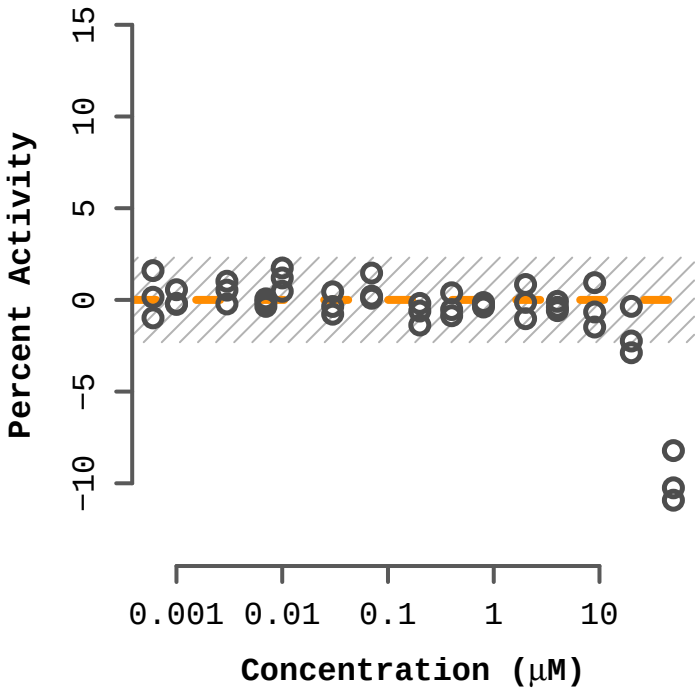
NAME: Chloroxine
CHID: 22801 **CASRN:** 773-76-2
SPID(S): Tox21_111494_1
M4ID: 12483651

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	240.06	NA	NA
PROB:	1	NA	NA
RMSE:	4.2	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.0916 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

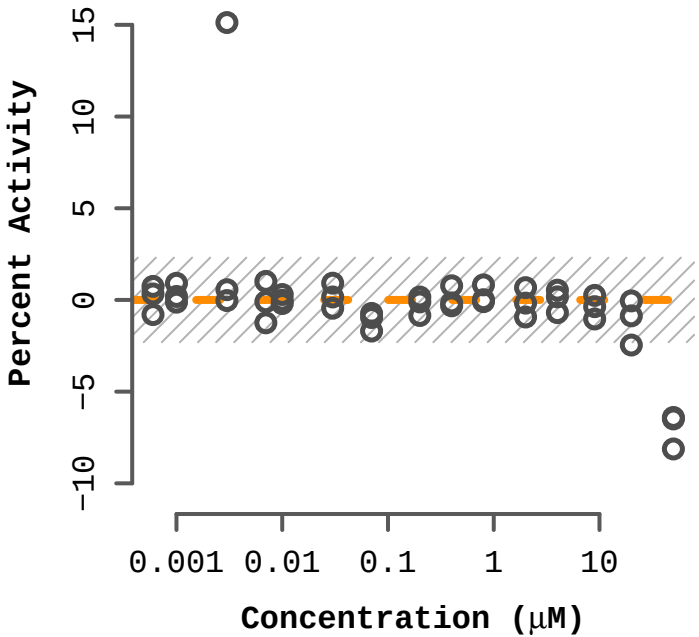
NAME: Chlorpromazine
CHID: 22808 **CASRN:** 50-53-3
SPID(S): Tox21_110120_1
M4ID: 12484633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.7	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

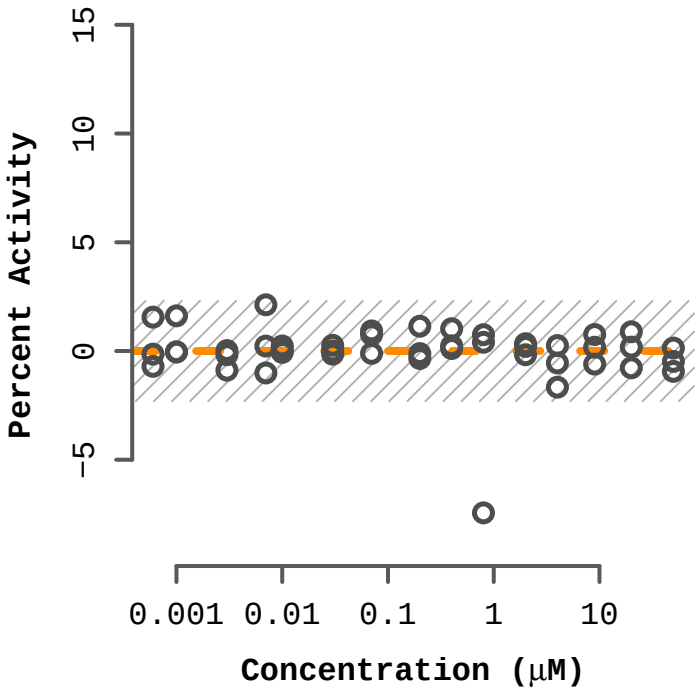
NAME: Chlorprothixene
CHID: 22810 **CASRN:** 113-59-7
SPID(S): Tox21_110032_1
M4ID: 12484701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.98	NA	NA

MAX_MEAN: 5.22 **MAX_MED:** 0.561 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

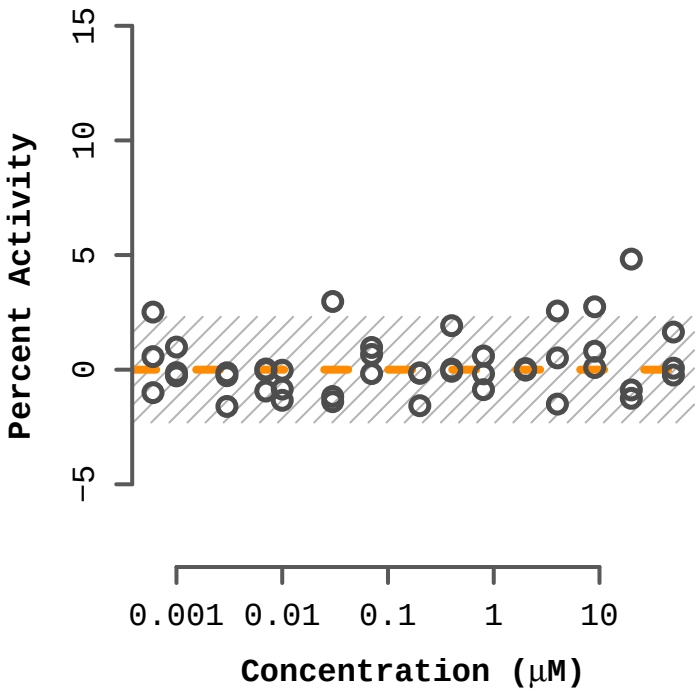
NAME: Chlorthalidone
CHID: 22812 **CASRN:** 77-36-1
SPID(S): Tox21_110369_1
M4ID: 12484419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.525 **MAX_MED:** 0.758 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

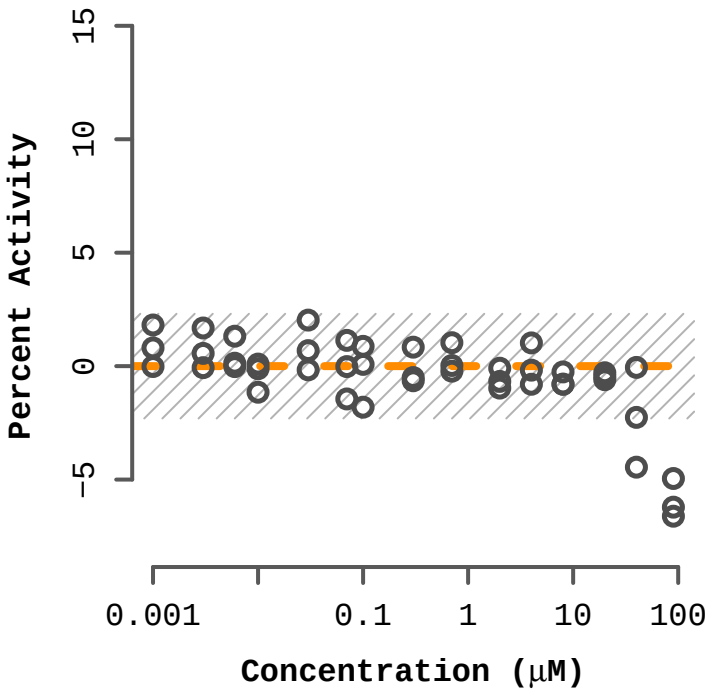
NAME: Chlorzoxazone
CHID: 22813 **CASRN:** 95-25-0
SPID(S): Tox21_110105_1
M4ID: 12484648

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.805 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

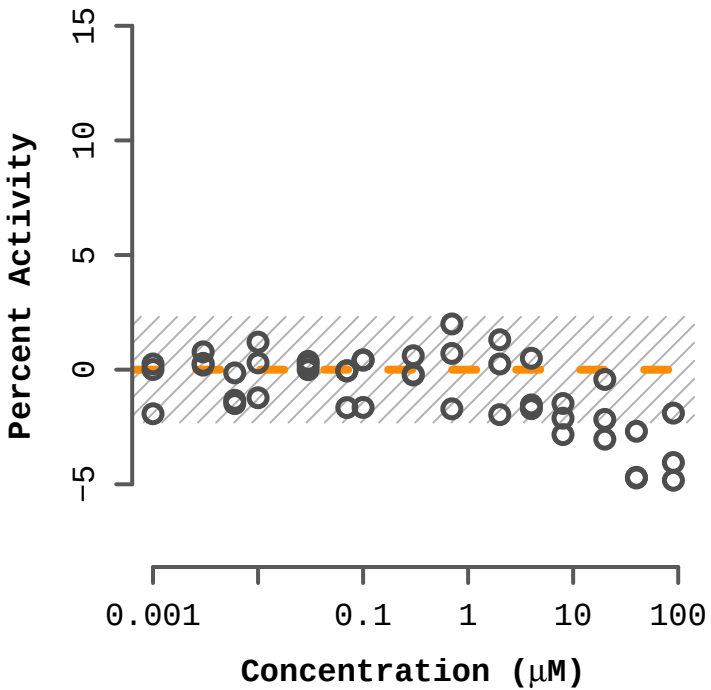
NAME: C.I. Direct Red 28
CHID: 22816 **CASRN:** 573-58-0
SPID(S): Tox21_202934
M4ID: 12479318

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 0.867 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

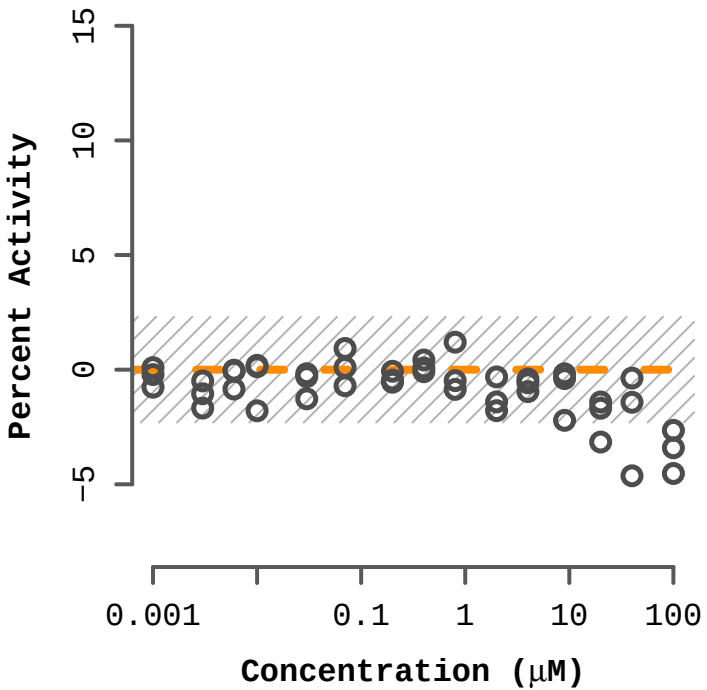
NAME: Carminic acid
CHID: 22817 **CASRN:** 1260-17-9
SPID(S): Tox21_300294
M4ID: 12478836

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.419 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

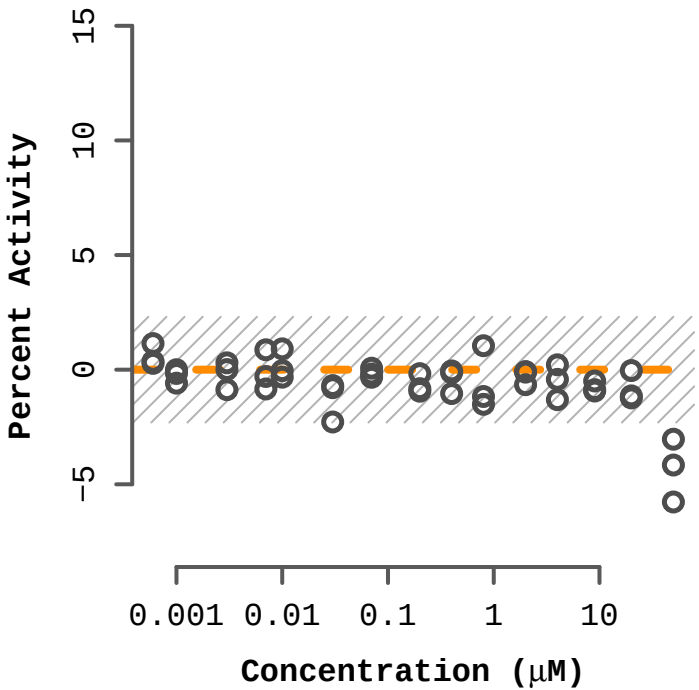
NAME: Carminic acid
CHID: 22817 **CASRN:** 1260-17-9
SPID(S): Tox21_201979
M4ID: 12480273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.139 **MAX_MED:** 0.132 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

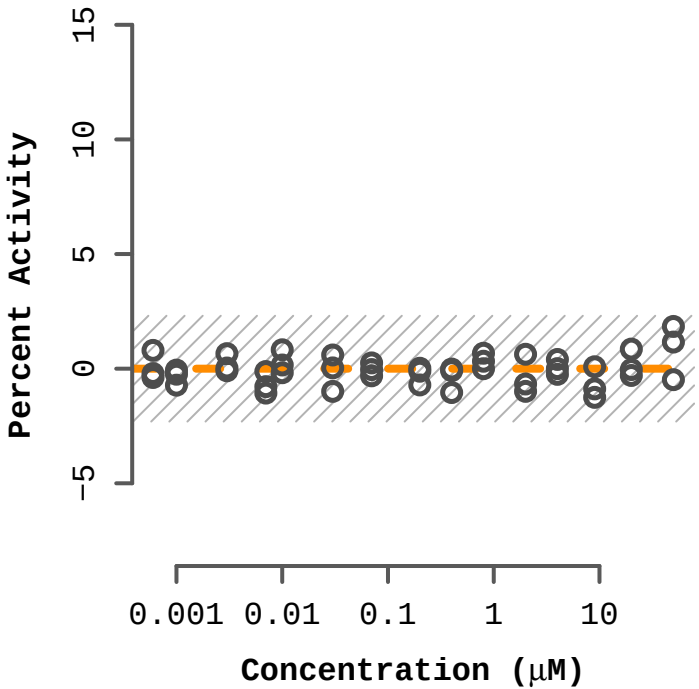
NAME: Cinnarizine
CHID: 22821 **CASRN:** 298-57-7
SPID(S): Tox21_110109_1
M4ID: 12484644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.595 **MAX_MED:** 0.367 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

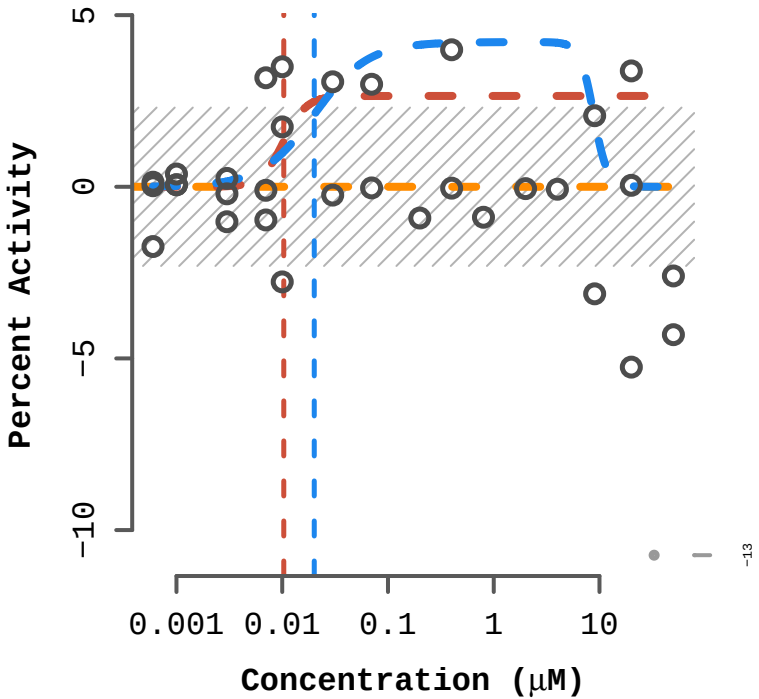
NAME: Cinoxacin
CHID: 22822 **CASRN:** 28657-80-9
SPID(S): Tox21_110121_1
M4ID: 12484632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cisapride
CHID: 22825 CASRN: 81098-60-4
SPID(S): Tox21_110699_1
M4ID: 12484169 BRK

HILL MODEL (in red):

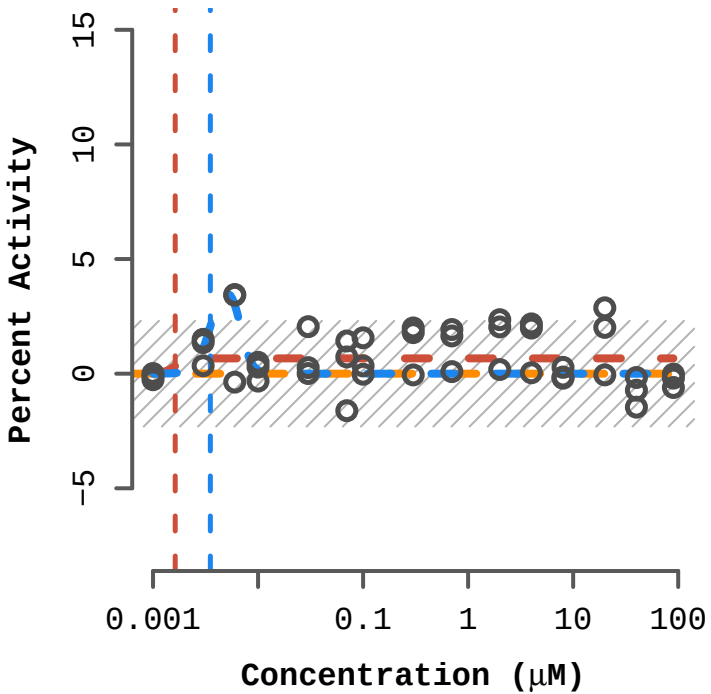
	tp	ga	gw
val:	2.65	−1.99	4.09
sd:	0.722	0.284	8.92

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.22	−1.7	1.72	0.945	6.71
sd:	0.961	0.425	1.86	0.177	67

	CNST	HILL	GNLS
AIC:	257.62	251.26	243.73
PROB:	0	0.02	0.98
RMSE:	4.14	3.87	3.33

MAX_MEAN: 4.3 MAX_MED: 5.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cladribine
CHID: 22828 CASRN: 4291-63-8
SPID(S): Tox21_300596
M4ID: 12478537

HILL MODEL (in red):

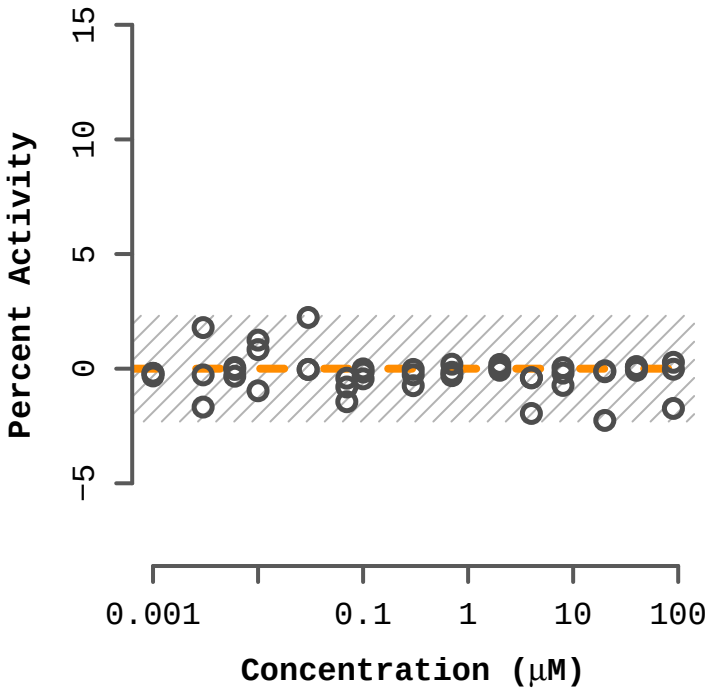
	tp	ga	gw
val:	0.667	−2.79	8
sd:	0.198	0.484	16.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.15	−2.45	6.5	−2.17	8.44
sd:	12.8	0.5	30.9	0.453	19.7

	CNST	HILL	GNLS
AIC:	160.26	154.54	160.44
PROB:	0.05	0.9	0.05
RMSE:	1.4	1.19	1.27

MAX_MEAN: 2.17 **MAX_MED:** 3.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

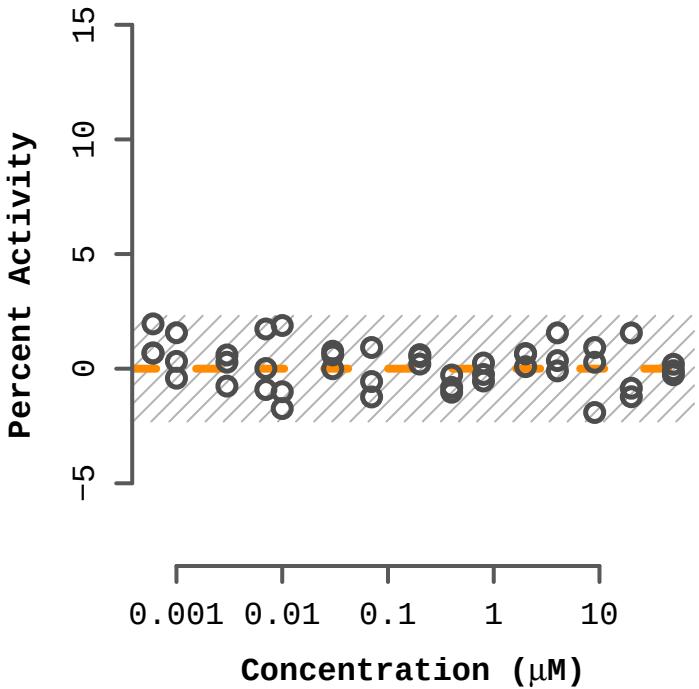
NAME: Clarithromycin
CHID: 22829 CASRN: 81103-11-9
SPID(S): Tox21_202903
M4ID: 12479349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 0.834 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

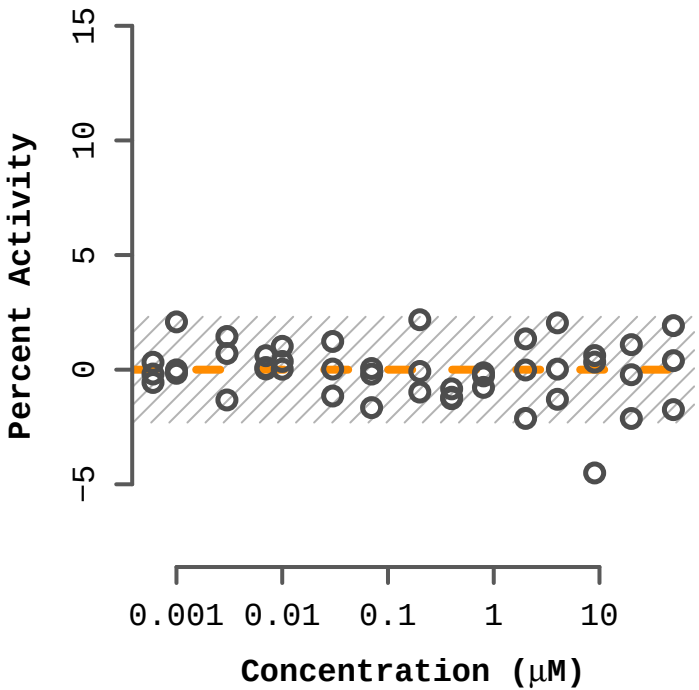
NAME: Clenbuterol
CHID: 22833 **CASRN:** 37148-27-9
SPID(S): Tox21_112016_1
M4ID: 12483370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

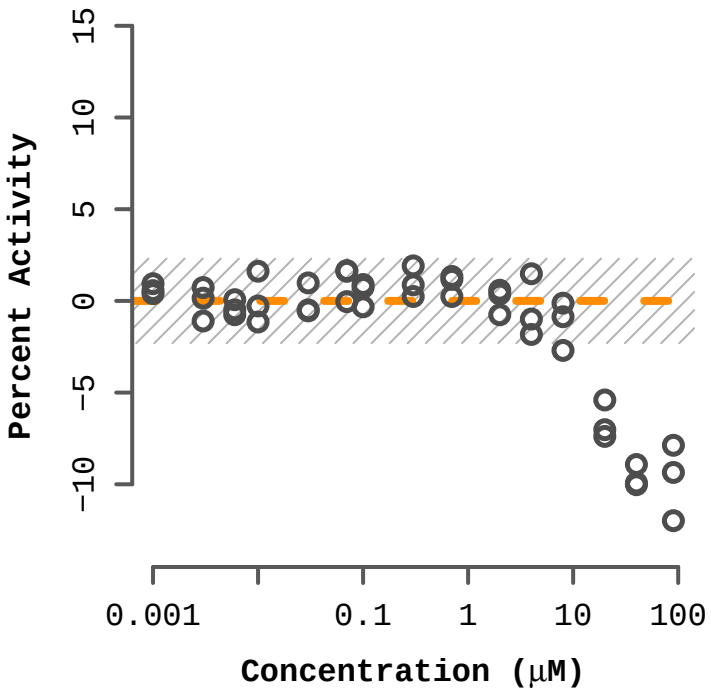
NAME: Clidinium bromide
CHID: 22835 **CASRN:** 3485-62-9
SPID(S): Tox21_110535_1
M4ID: 12484285

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.641 **MAX_MED:** 0.708 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

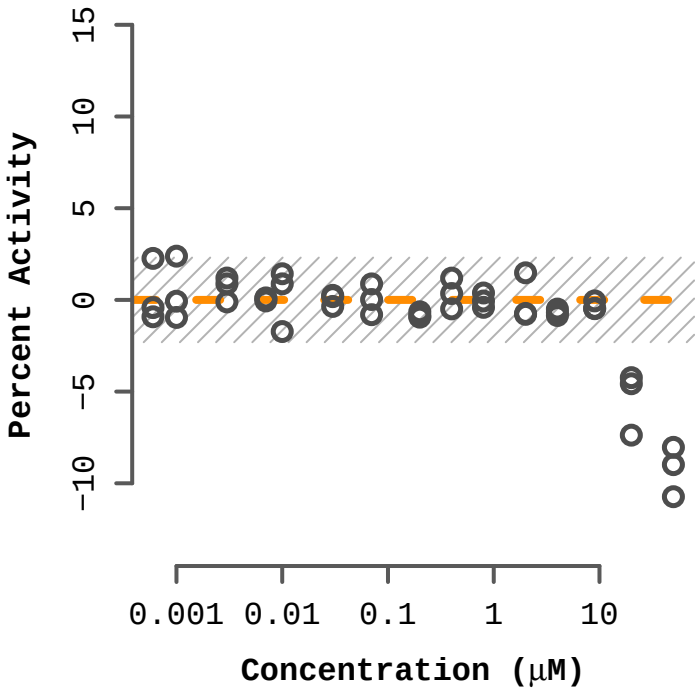
NAME: Clioquinol
CHID: 22837 **CASRN:** 130-26-7
SPID(S): Tox21_200291
M4ID: 12481961

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.02	NA	NA
PROB:	1	NA	NA
RMSE:	4.07	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

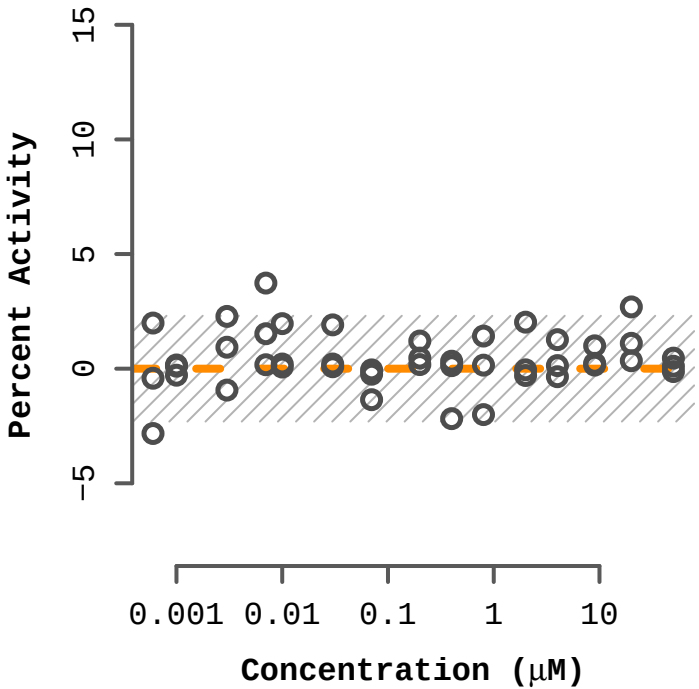
NAME: Clioquinol
CHID: 22837 **CASRN:** 130-26-7
SPID(S): Tox21_110416_1
M4ID: 12484378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.41	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 0.655 **MAX_MED:** 0.879 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

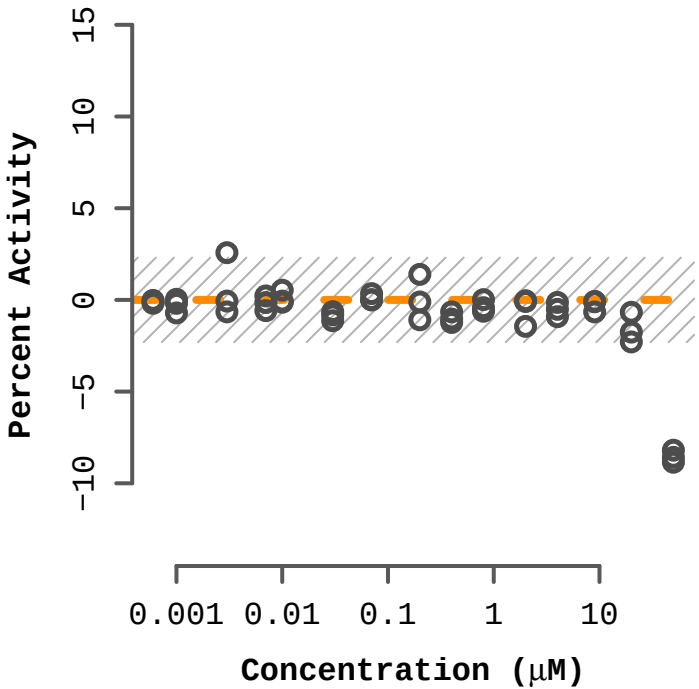
NAME: Clomethiazole
CHID: 22842 **CASRN:** 533-45-9
SPID(S): Tox21_110931_1
M4ID: 12484006

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

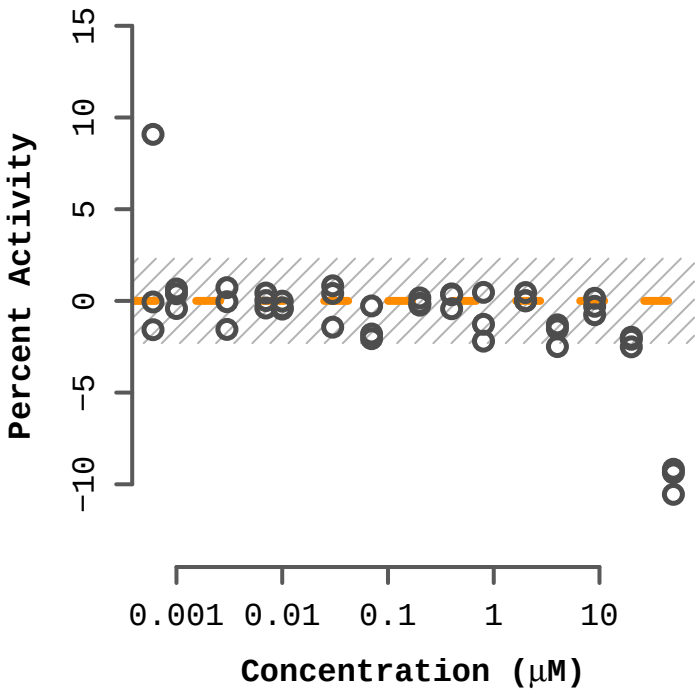
NAME: Clomiphene
CHID: 22843 **CASRN:** 911-45-5
SPID(S): Tox21_113110_1
M4ID: 12482803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.35	NA	NA

MAX_MEAN: 0.621 **MAX_MED:** 0.0156 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

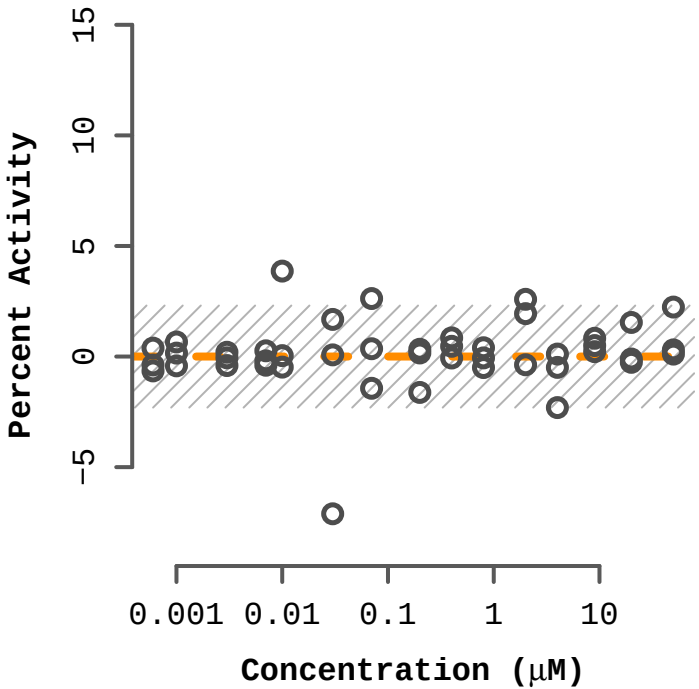
NAME: Clomipramine
CHID: 22844 **CASRN:** 303-49-1
SPID(S): Tox21_110117_1
M4ID: 12484636

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.04	NA	NA

MAX_MEAN: 2.49 **MAX_MED:** 0.406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

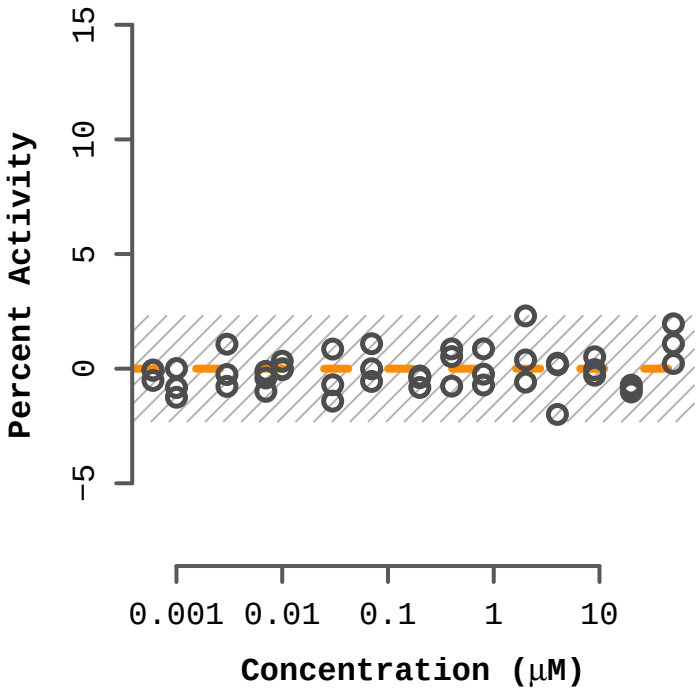
NAME: Clonidine
CHID: 22846 **CASRN:** 4205-90-7
SPID(S): Tox21_110118_1
M4ID: 12484635

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

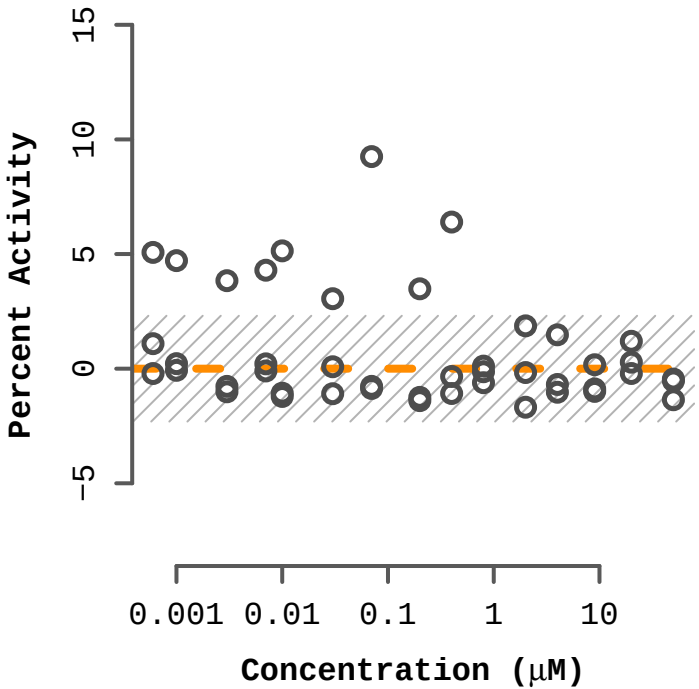
NAME: Clortermine
CHID: 22850 **CASRN:** 10389-73-8
SPID(S): Tox21_113863
M4ID: 12482362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

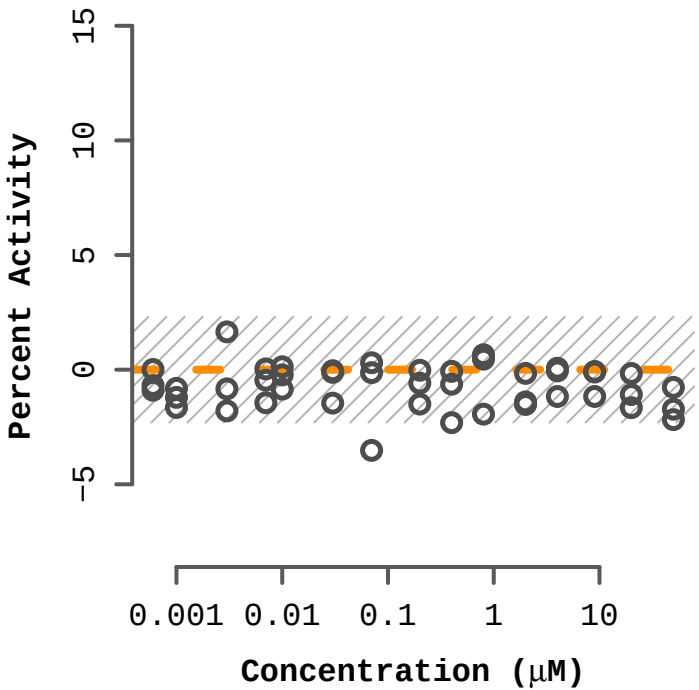
NAME: Clothiapine
CHID: 22851 **CASRN:** 2058-52-8
SPID(S): Tox21_111779_1
M4ID: 12483487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.96	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 2.54 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

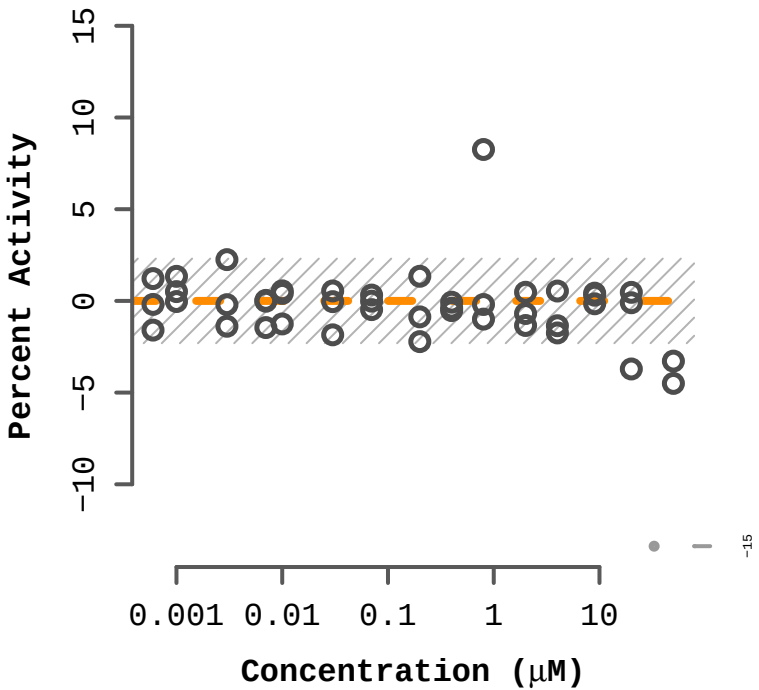
NAME: Cloxazolam
CHID: 22854 **CASRN:** 24166-13-0
SPID(S): Tox21_113693
M4ID: 12482521

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: −0.275 **MAX_MED:** 0.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

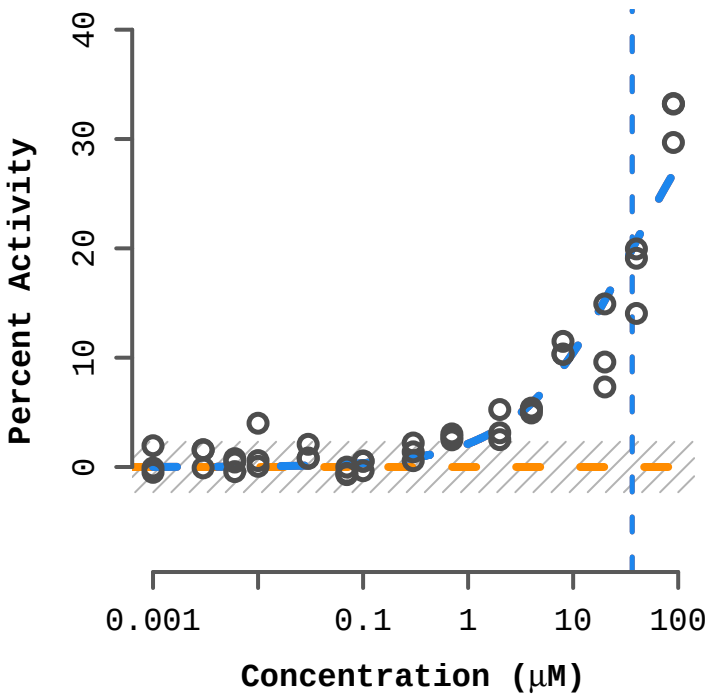
NAME: Clozapine
CHID: 22855 **CASRN:** 5786-21-0
SPID(S): Tox21_110113_1
M4ID: 12484640 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.87	NA	NA

MAX_MEAN: 2.36 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cortisone
CHID: 22857 CASRN: 53-06-5
SPID(S): Tox21_301440
M4ID: 12477693

HILL MODEL (in red):

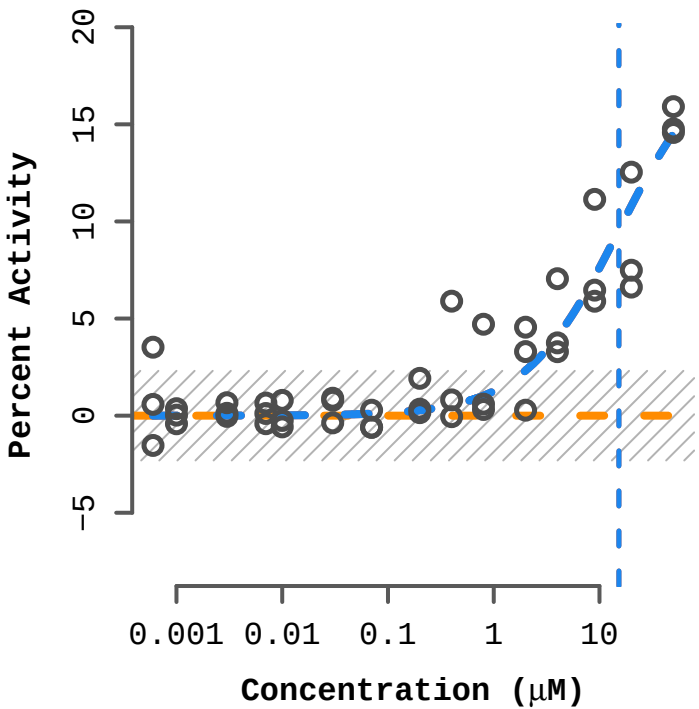
	tp	ga	gw
val:	39.9	1.56	0.799
sd:	12	0.266	0.0774

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	39.9	1.56	0.799	3.03	9.2
sd:	12	0.266	0.0774	1690	14500

	CNST	HILL	GNLS
AIC:	323.62	204.57	208.57
PROB:	0	0.88	0.12
RMSE:	10.49	2.51	2.51

MAX_MEAN: 32 MAX_MED: 33.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cortisone
CHID: 22857 CASRN: 53-06-5
SPID(S): Tox21_111539_1
M4ID: 12483628

HILL MODEL (in red):

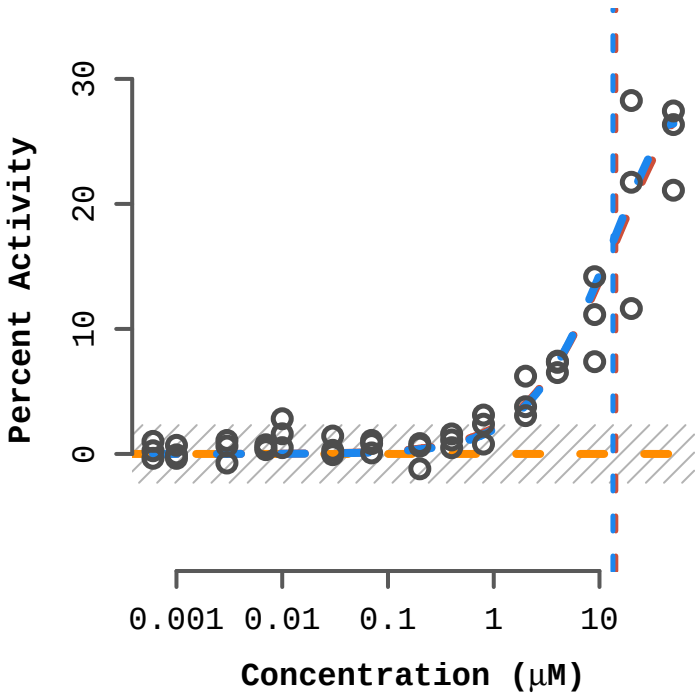
	tp	ga	gw
val:	19.1	1.18	0.972
sd:	2.93	0.185	0.175

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.1	1.18	0.972	3.69	4.2
sd:	2.92	0.184	0.175	1170	2470

	CNST	HILL	GNLS
AIC:	270.45	178.26	182.26
PROB:	0	0.88	0.12
RMSE:	5.44	1.75	1.75

MAX_MEAN: 15.1 MAX_MED: 14.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cortisone acetate
CHID: 22858 CASRN: 50-04-4
SPID(S): Tox21_113482_1
M4ID: 12482636

HILL MODEL (in red):

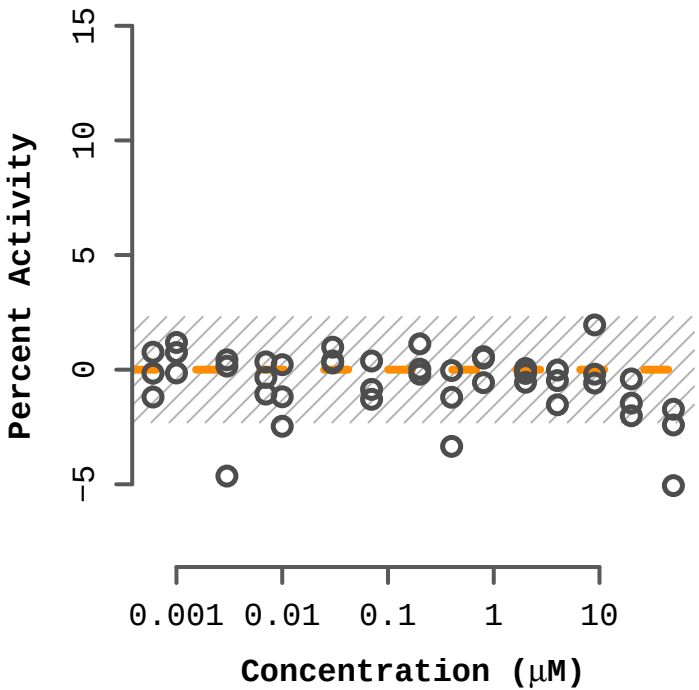
	tp	ga	gw
val:	33.9	1.15	1.02
sd:	4.47	0.163	0.163

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	33.9	1.13	1.08	1.87	8.53
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	310.95	185.43	189.18
PROB:	0	0.87	0.13
RMSE:	9.35	2.32	2.33

MAX_MEAN: 25 MAX_MED: 26.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

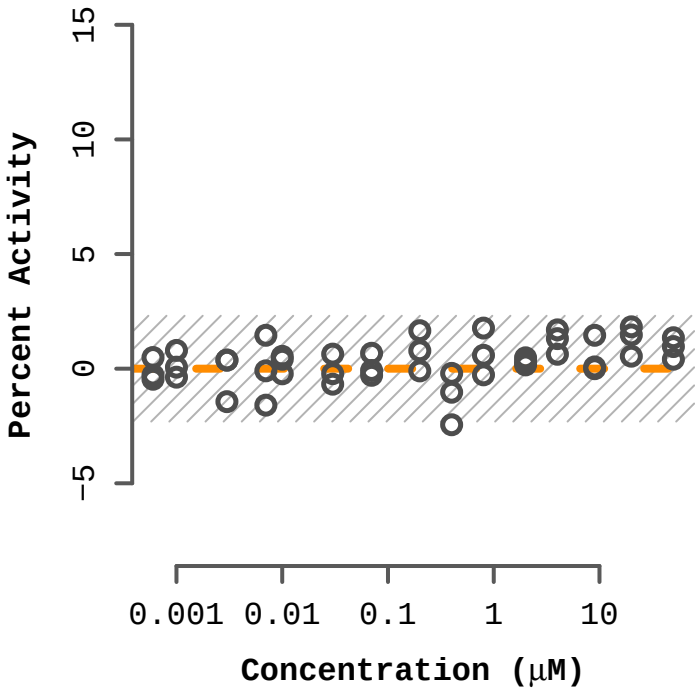
NAME: Cyclofenil
CHID: 22866 **CASRN:** 2624-43-3
SPID(S): Tox21_112259_1
M4ID: 12483197

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.599 **MAX_MED:** 0.749 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

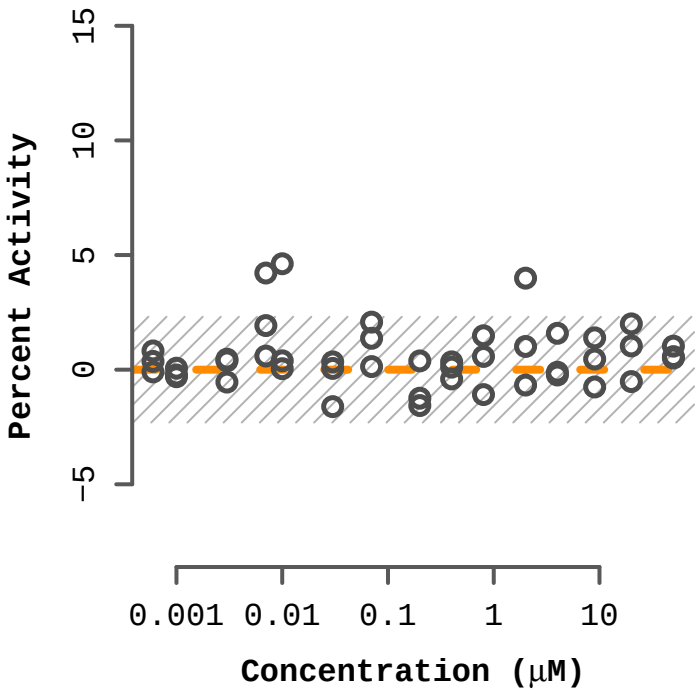
NAME: Cyclopenthiazide
CHID: 22868 **CASRN:** 742-20-1
SPID(S): Tox21_110481_1
M4ID: 12484322

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

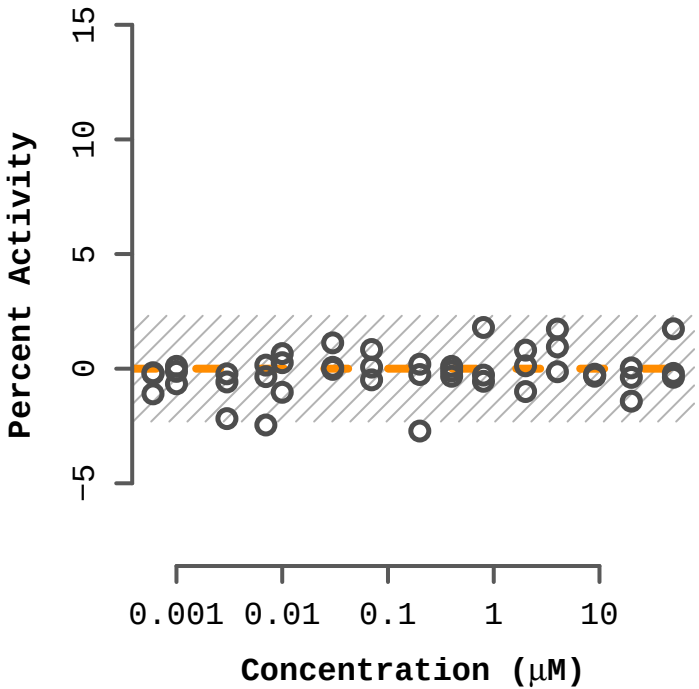
NAME: Cycloserine
CHID: 22870 **CASRN:** 68-41-7
SPID(S): Tox21_110361_1
M4ID: 12484427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

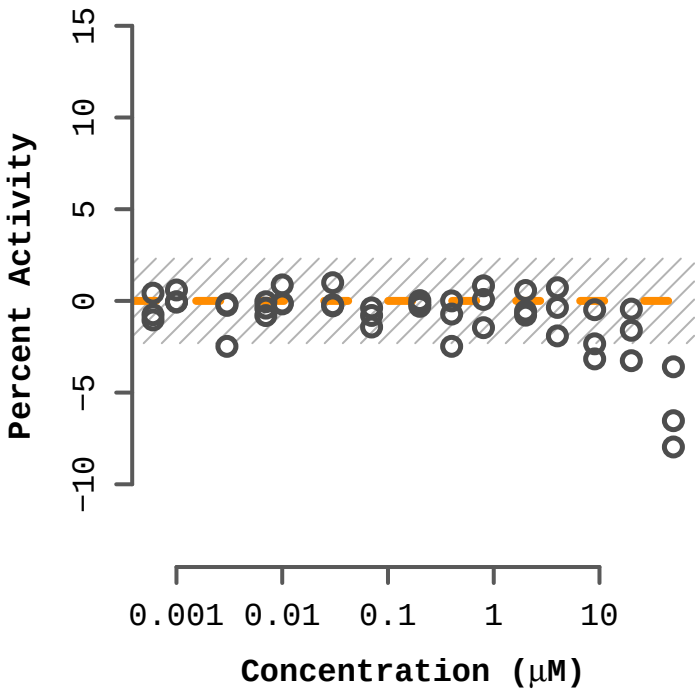
NAME: Cyclothiazide
CHID: 22871 **CASRN:** 2259-96-3
SPID(S): Tox21_110124_1
M4ID: 12484629

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 0.951 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

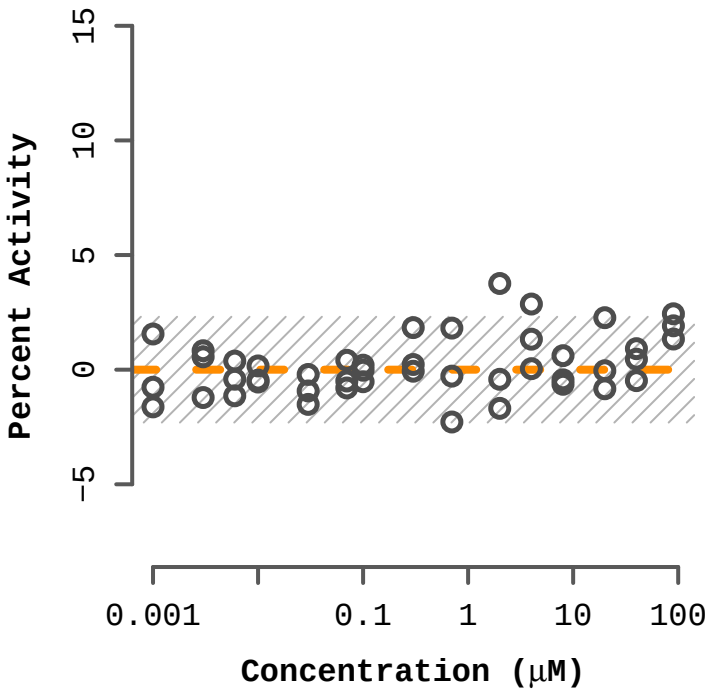
NAME: Cyproheptadine
CHID: 22872 **CASRN:** 129-03-3
SPID(S): Tox21_110112_1
M4ID: 12484641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 0.201 **MAX_MED:** 0.0812 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

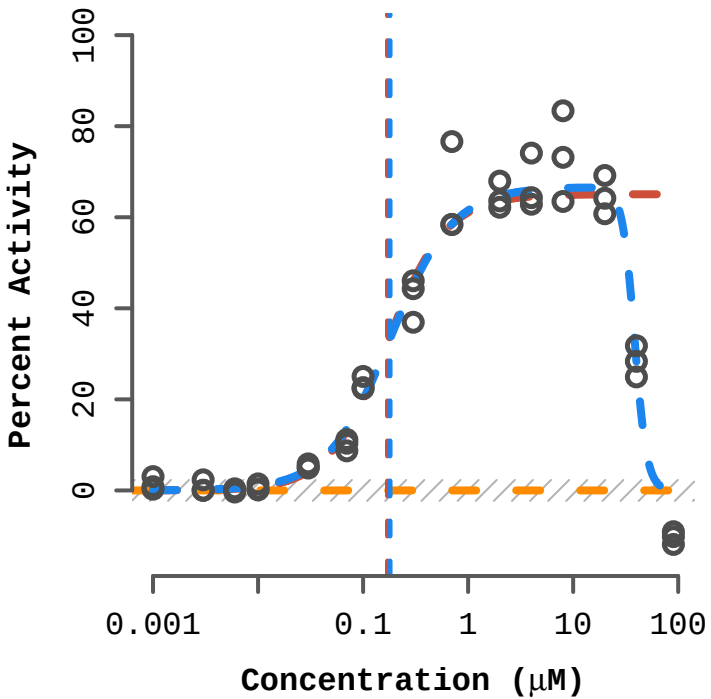
NAME: Cytarabine
CHID: 22877 **CASRN:** 147-94-4
SPID(S): Tox21_301971
M4ID: 12477162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Danazol
CHID: 22880 CASRN: 17230-88-5
SPID(S): Tox21_301940
M4ID: 12477193

HILL MODEL (in red):

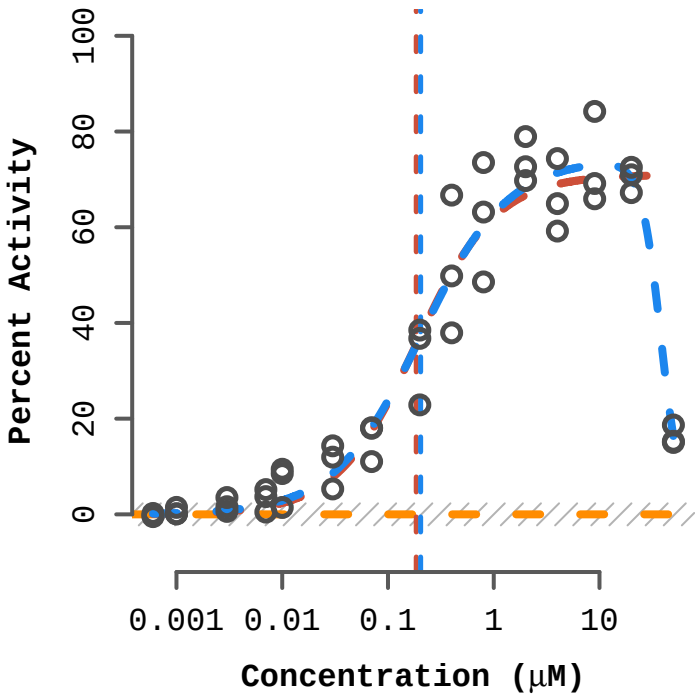
	tp	ga	gw
val:	65.1	-0.768	1.54
sd:	2.11	0.0538	0.209

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	66.7	-0.744	1.45	1.58	7.41
sd:	1.59	0.0369	0.125	0.0138	4.46

	CNST	HILL	GNLS
AIC:	468.18	371.85	280.29
PROB:	0	0	1
RMSE:	41.63	22.2	5.44

MAX_MEAN: 73.3 MAX_MED: 73.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Danazol
CHID: 22880 CASRN: 17230-88-5
SPID(S): Tox21_112114_1
M4ID: 12483311

HILL MODEL (in red):

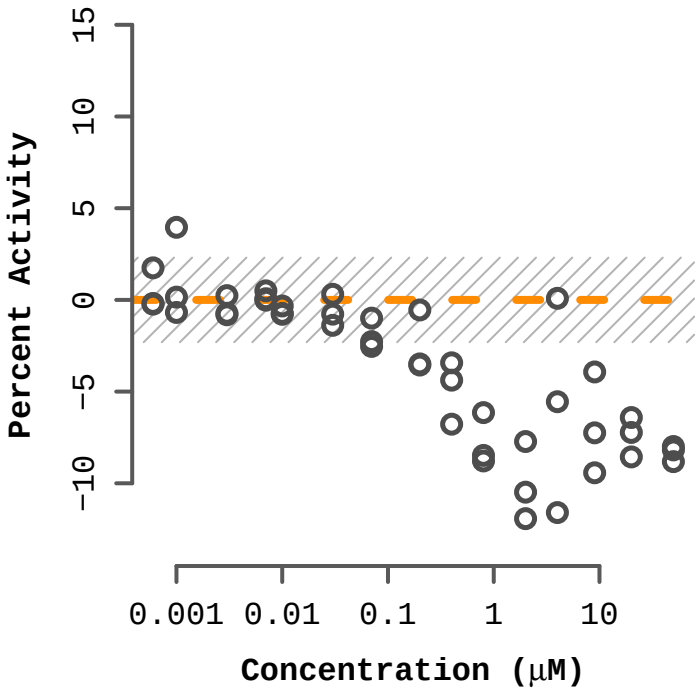
	tp	ga	gw
val:	71	−0.733	1.15
sd:	2.4	0.0646	0.177

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	74.4	−0.691	1.06	1.58	4.63
sd:	3.44	0.0657	0.139	0.0369	1.22

	CNST	HILL	GNLS
AIC:	472.94	346.16	299.01
PROB:	0	0	1
RMSE:	43.8	15.4	6.14

MAX_MEAN: 73.8 **MAX_MED:** 72.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

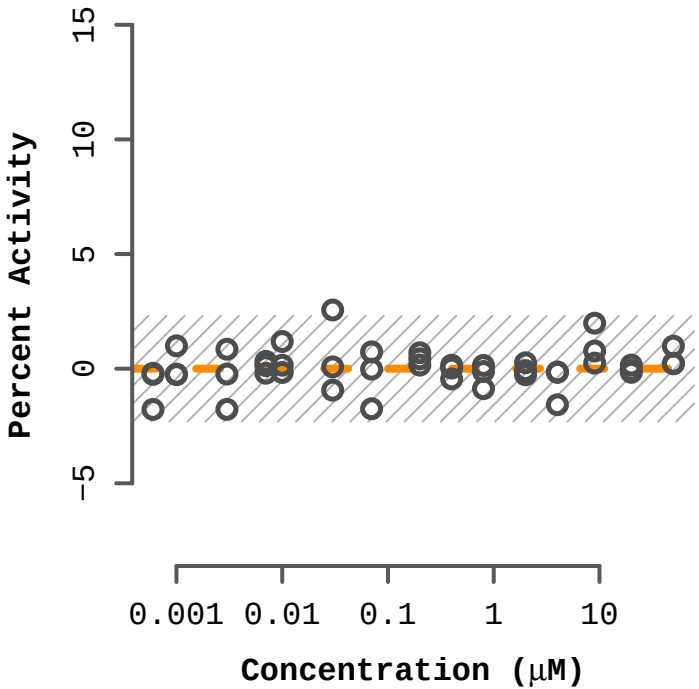
NAME: Daunorubicin
CHID: 22883 **CASRN:** 20830-81-3
SPID(S): Tox21_110896_1
M4ID: 12484032

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	284.4	NA	NA
PROB:	1	NA	NA
RMSE:	5.45	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.153 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

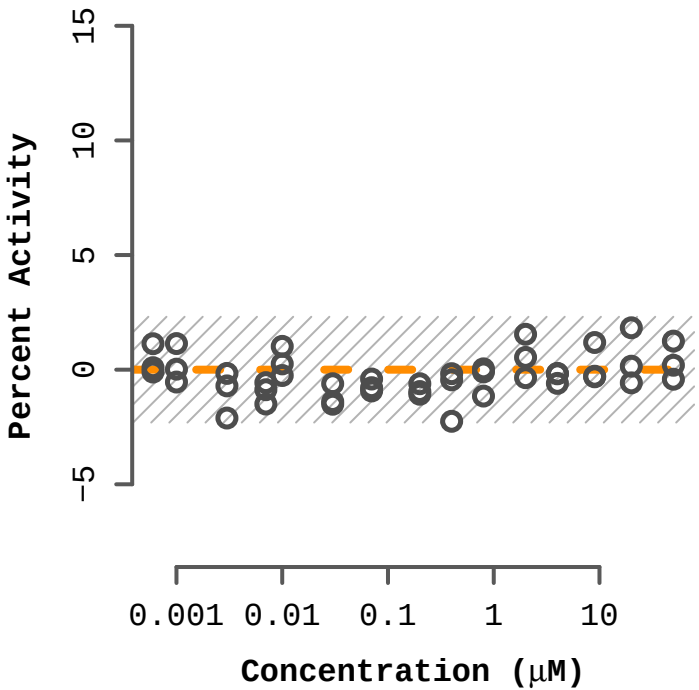
NAME: Decamethonium bromide
CHID: 22886 **CASRN:** 541-22-0
SPID(S): Tox21_112035_1
M4ID: 12483358

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.773 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

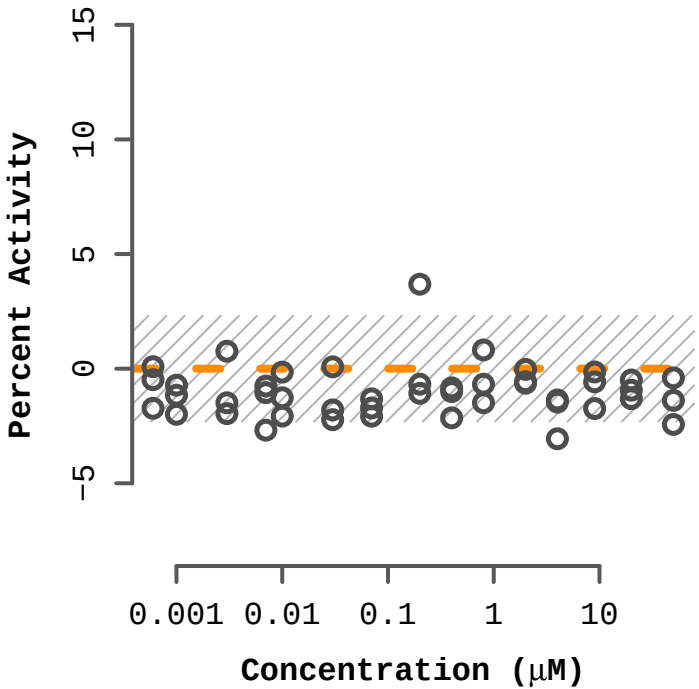
NAME: Dehydrocholic acid
CHID: 22888 **CASRN:** 81-23-2
SPID(S): Tox21_111519_1
M4ID: 12483638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.578 **MAX_MED:** 0.536 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

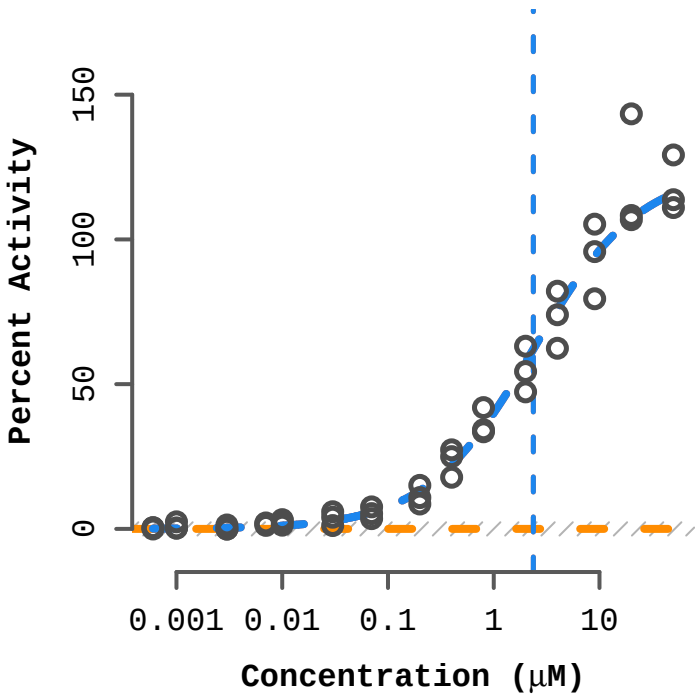
NAME: Delavirdine
CHID: 22892 CASRN: 136817-59-9
SPID(S): Tox21_112637_1
M4ID: 12482999

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.645 **MAX_MED:** −0.479 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Deoxycorticosterone acetate
CHID: 22894 CASRN: 56-47-3
SPID(S): Tox21_110876_1
M4ID: 12484051

HILL MODEL (in red):

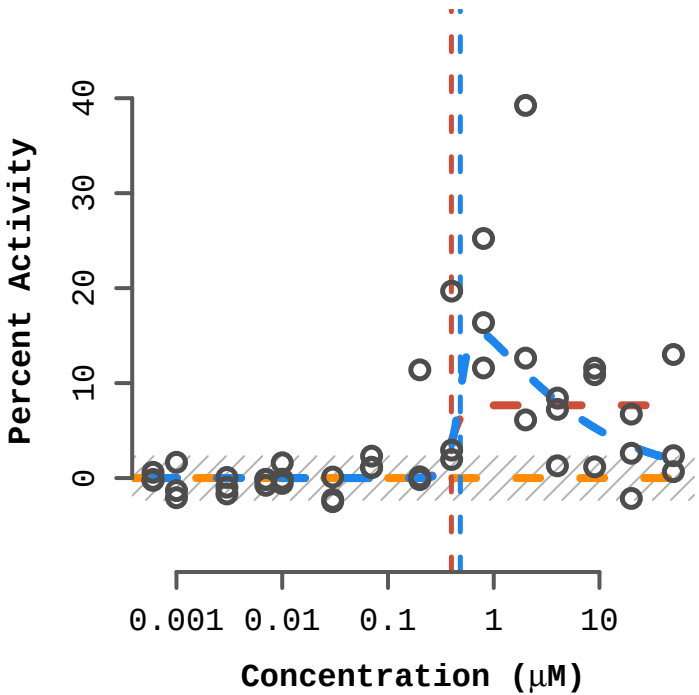
	tp	ga	gw
val:	124	0.375	0.861
sd:	4.47	0.0608	0.0581

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	124	0.375	0.861	3.65	6.33
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	489.49	285.57	289.57
PROB:	0	0.88	0.12
RMSE:	56.54	7.32	7.32

MAX_MEAN: 119 MAX_MED: 114 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Deslanoside
CHID: 22897 CASRN: 17598-65-1
SPID(S): Tox21_111671_1
M4ID: 12483545

HILL MODEL (in red):

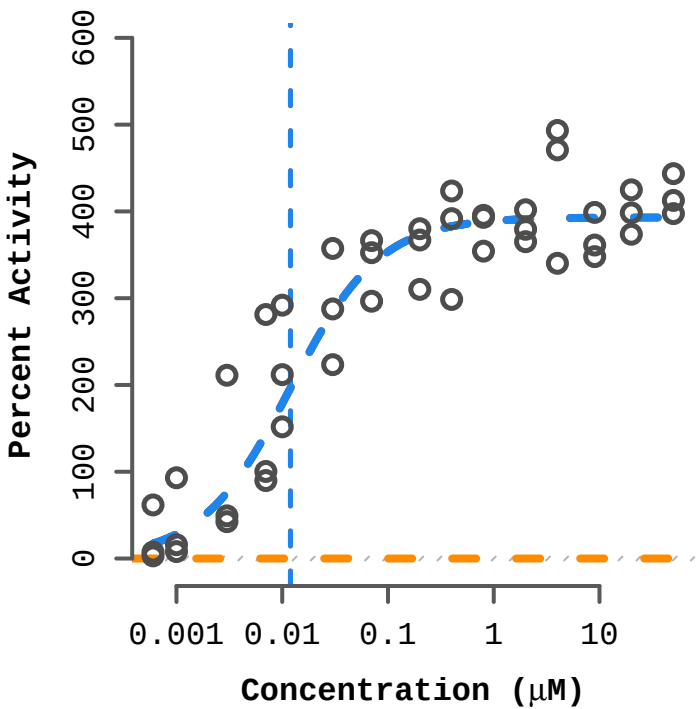
	tp	ga	gw
val:	7.66	-0.4	8
sd:	1.33	0.0788	12.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	30.3	-0.316	7.95	-0.0659	0.66
sd:	28.1	0.0884	7.51	1.12	0.282

	CNST	HILL	GNLS
AIC:	311.43	286.22	274.34
PROB:	0	0	1
RMSE:	9.37	6.96	6.09

MAX_MEAN: 19.3 MAX_MED: 16.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexamethasone acetate
CHID: 22901 CASRN: 1177-87-3
SPID(S): Tox21_112928_1
M4ID: 12482873

HILL MODEL (in red):

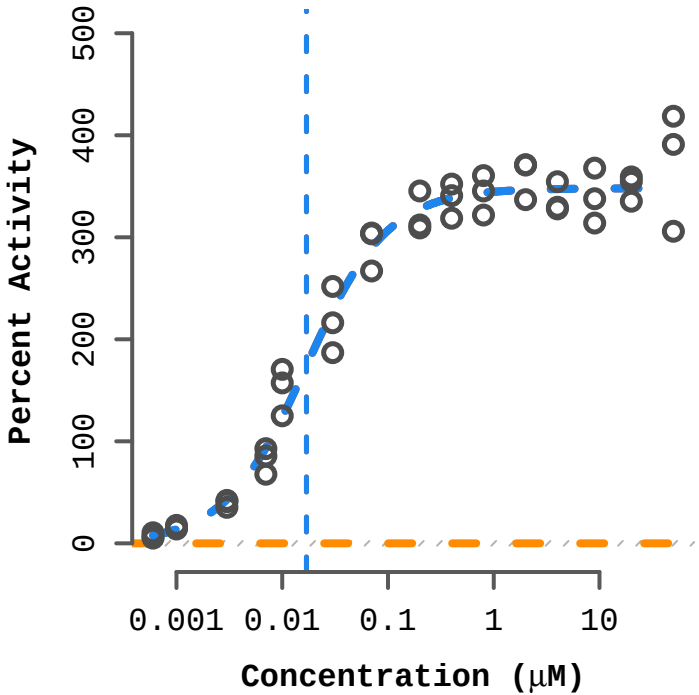
	tp	ga	gw
val:	393	-1.92	1.03
sd:	10.5	0.0887	0.192

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	393	-1.92	1.03	3.17	8.12
sd:	10.5	0.0887	0.192	38800	215000

	CNST	HILL	GNLS
AIC:	657.19	489.08	493.08
PROB:	0	0.88	0.12
RMSE:	319.28	51.42	51.42

MAX_MEAN: 435 **MAX_MED:** 471 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexamethasone valerate
CHID: 22904 CASRN: 33755-46-3
SPID(S): Tox21_111565_1
M4ID: 12483614

HILL MODEL (in red):

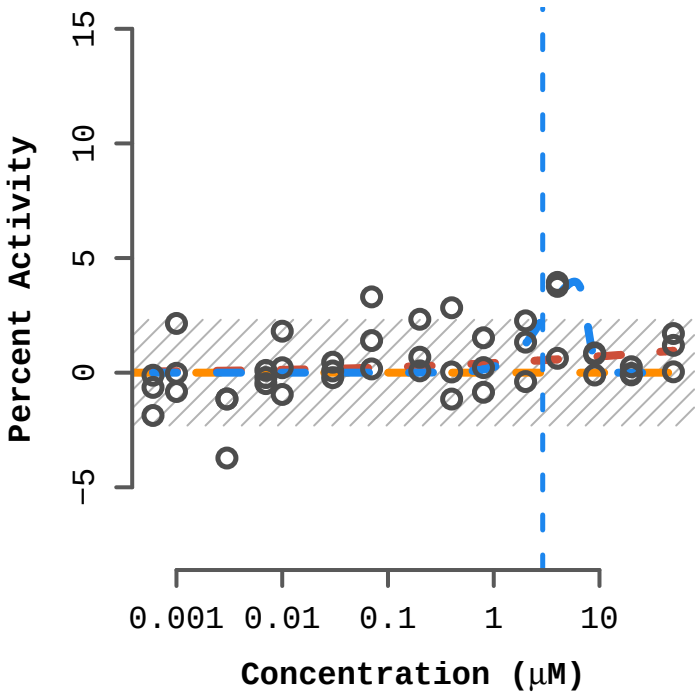
	tp	ga	gw
val:	348	−1.77	1.13
sd:	5.32	0.043	0.0909

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	348	−1.77	1.13	3.7	15.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	642.87	413.97	417.97
PROB:	0	0.88	0.12
RMSE:	273.72	22.31	22.31

MAX_MEAN: 372 **MAX_MED:** 391 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexpanthenol
CHID: 22906 **CASRN:** 81-13-0
SPID(S): Tox21_111563_1
M4ID: 12483615

HILL MODEL (in red):

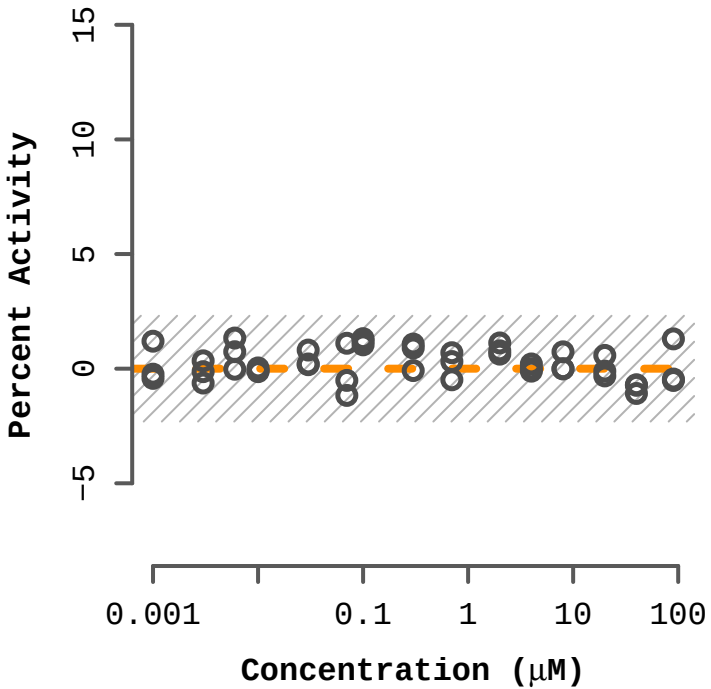
	tp	ga	gw
val:	2.21	2.09	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	0.463	2.69	0.885	12.5
sd:	7.47	0.617	5.03	0.713	129

	CNST	HILL	GNLS
AIC:	164.65	163.99	161.61
PROB:	0.14	0.2	0.66
RMSE:	1.53	1.4	1.32

MAX_MEAN: 2.78 **MAX_MED:** 3.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

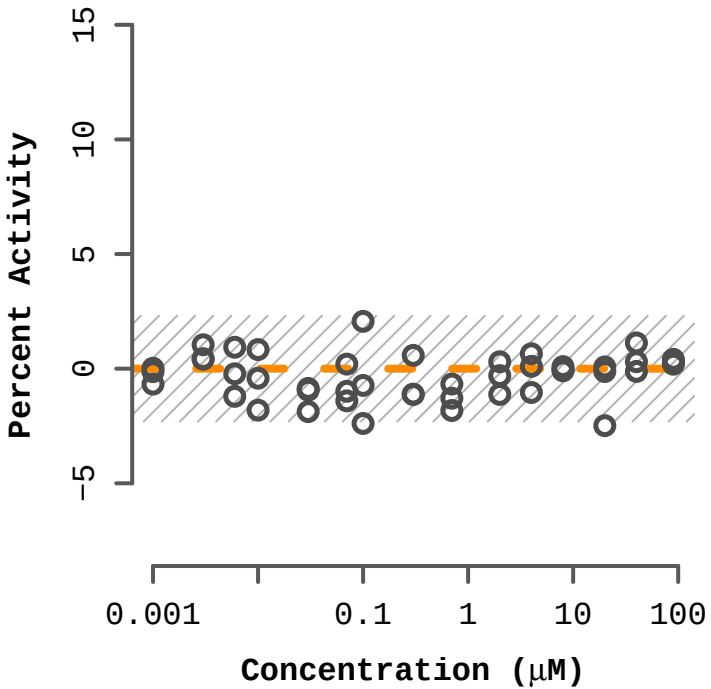
NAME: D-Glucose
CHID: 22910 **CASRN:** 50-99-7
SPID(S): Tox21_200145
M4ID: 12482107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

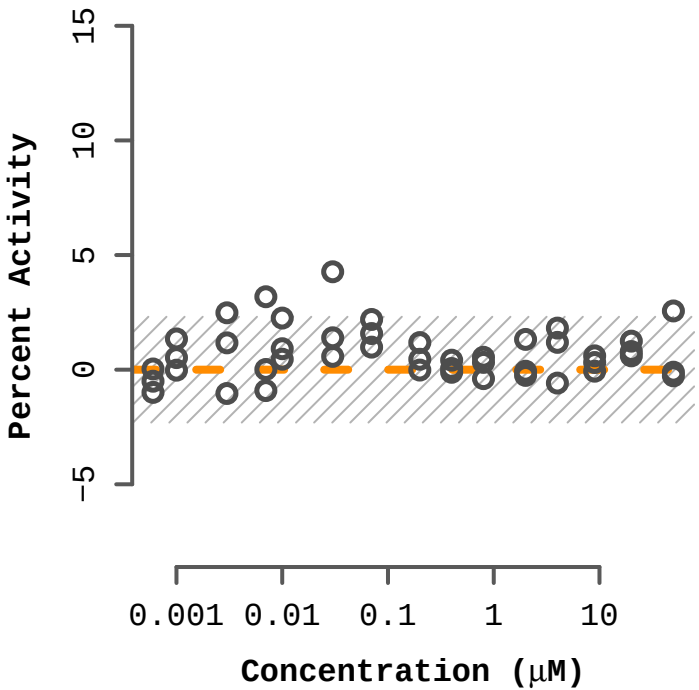
NAME: Diatrizoate sodium
CHID: 22912 **CASRN:** 737-31-5
SPID(S): Tox21_301439
M4ID: 12477694

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.632 **MAX_MED:** 0.437 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

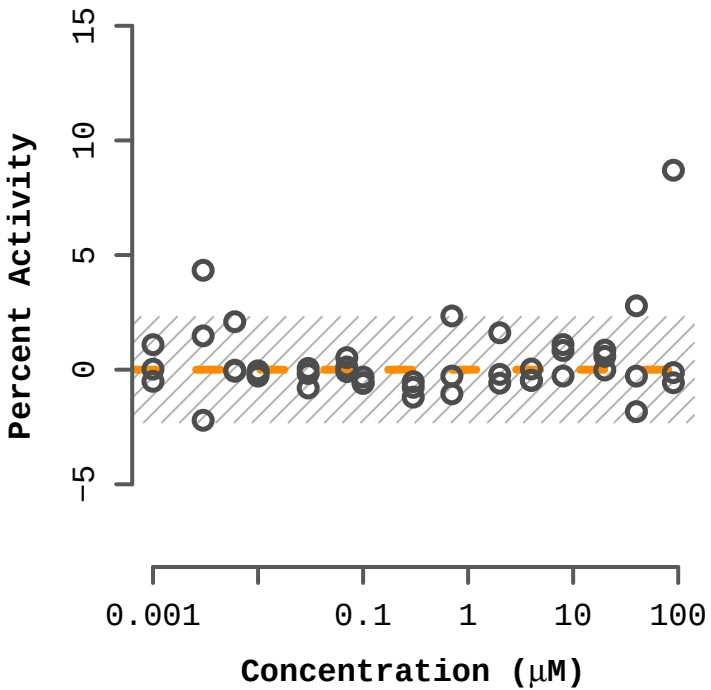
NAME: Diazoxide
CHID: 22914 **CASRN:** 364-98-7
SPID(S): Tox21_110132_1
M4ID: 12484622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

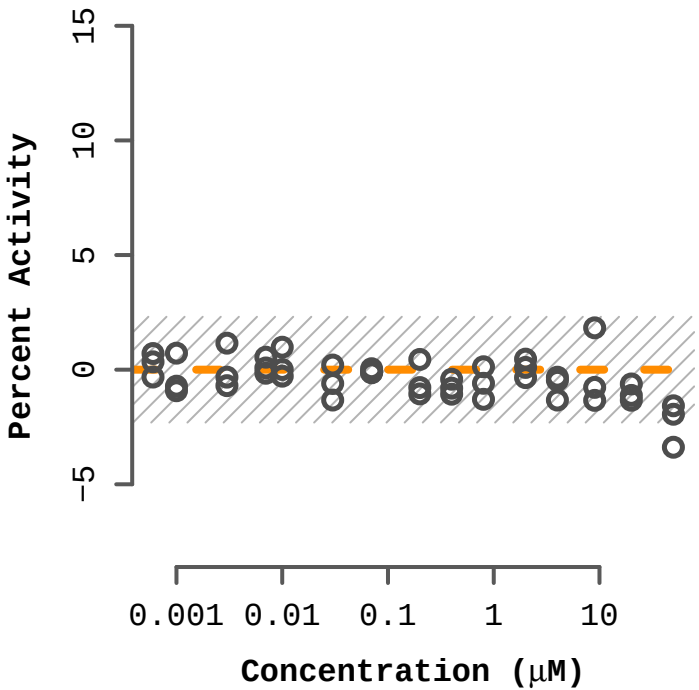
NAME: Dibromomannitol
CHID: 22918 **CASRN:** 488-41-5
SPID(S): Tox21_201164
M4ID: 12481088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 2.67 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

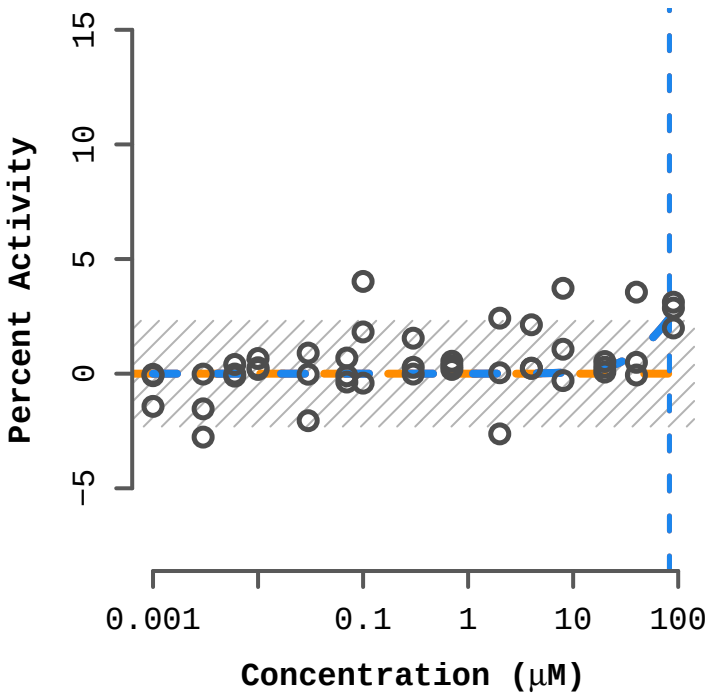
NAME: Dicyclomine
CHID: 22926 **CASRN:** 77-19-0
SPID(S): Tox21_113571_1
M4ID: 12482604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.243 **MAX_MED:** 0.344 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2',3'−Dideoxyinosine
CHID: 22927 CASRN: 69655−05−6
SPID(S): Tox21_300575
M4ID: 12478558

HILL MODEL (in red):

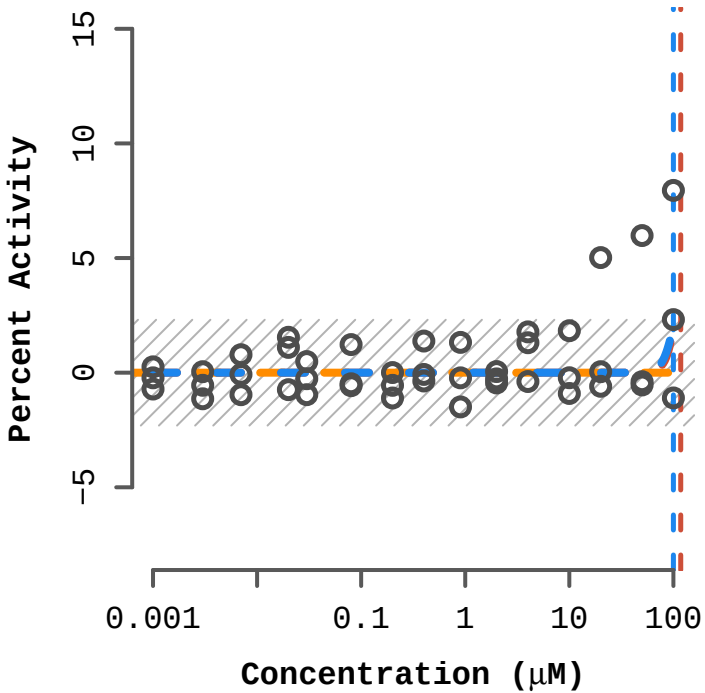
	tp	ga	gw
val:	4.83	1.92	2
sd:	7.01	0.658	2.48

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.83	1.92	2	3.35	6.51
sd:	7.01	0.658	2.48	10300	48200

	CNST	HILL	GNLS
AIC:	165.48	155.2	159.2
PROB:	0.01	0.88	0.12
RMSE:	1.55	1.35	1.35

MAX_MEAN: 2.66 **MAX_MED:** 2.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2',3'−Dideoxyinosine
CHID: 22927 CASRN: 69655−05−6
SPID(S): Tox21_202333
M4ID: 12479919

HILL MODEL (in red):

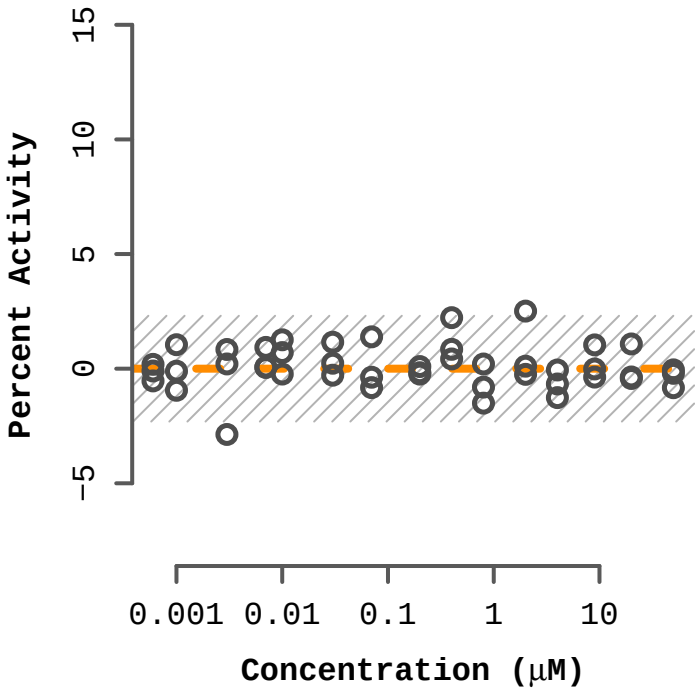
	tp	ga	gw
val:	9.38	2.07	8
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.02	2	8	3.97	4.09
sd:	29.7	0.801	16.4	33700	70500

	CNST	HILL	GNLS
AIC:	161.7	165.66	169.66
PROB:	0.86	0.12	0.02
RMSE:	1.89	1.73	1.73

MAX_MEAN: 3.06 **MAX_MED:** 2.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

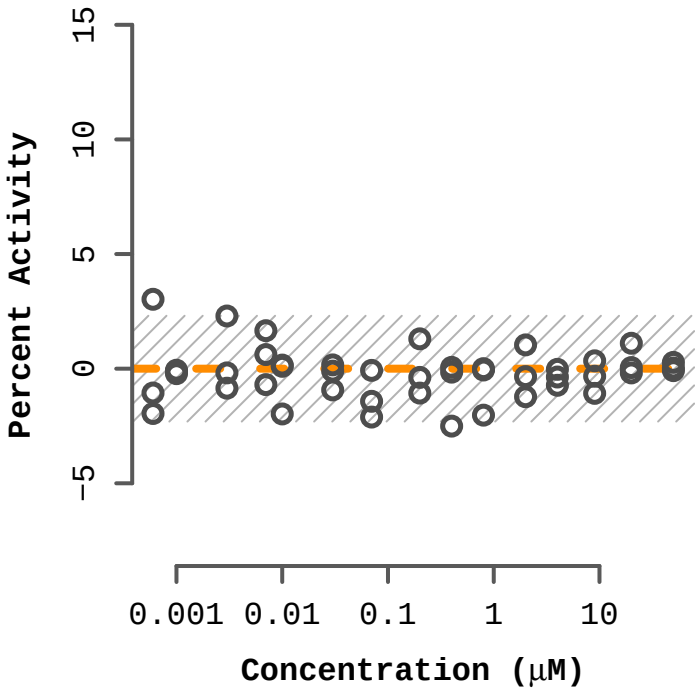
NAME: 2',3'−Dideoxyinosine
CHID: 22927 **CASRN:** 69655−05−6
SPID(S): Tox21_111732_1
M4ID: 12483516

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.845 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

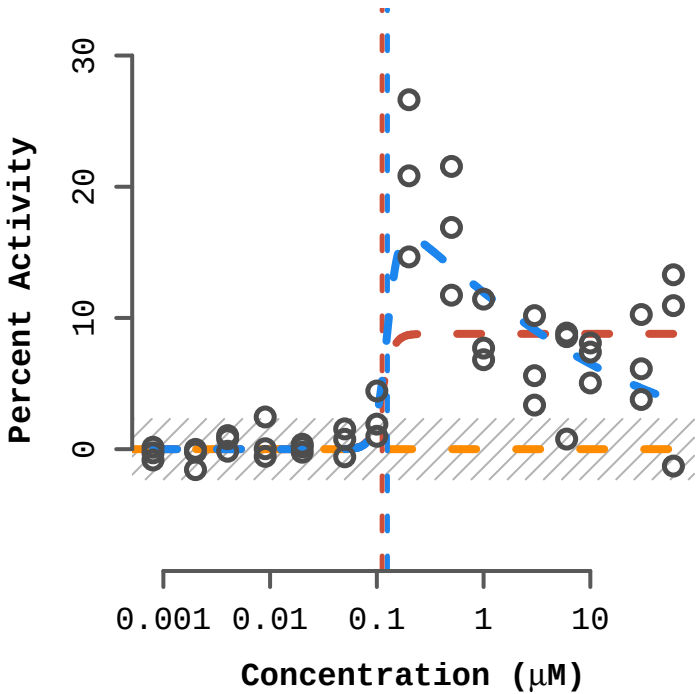
NAME: Diflunisal
CHID: 22932 CASRN: 22494-42-4
SPID(S): Tox21_110598_1
M4ID: 12484240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.527 **MAX_MED:** 0.617 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Digitoxin
CHID: 22933 CASRN: 71-63-6
SPID(S): Tox21_302269
M4ID: 12476864

HILL MODEL (in red):

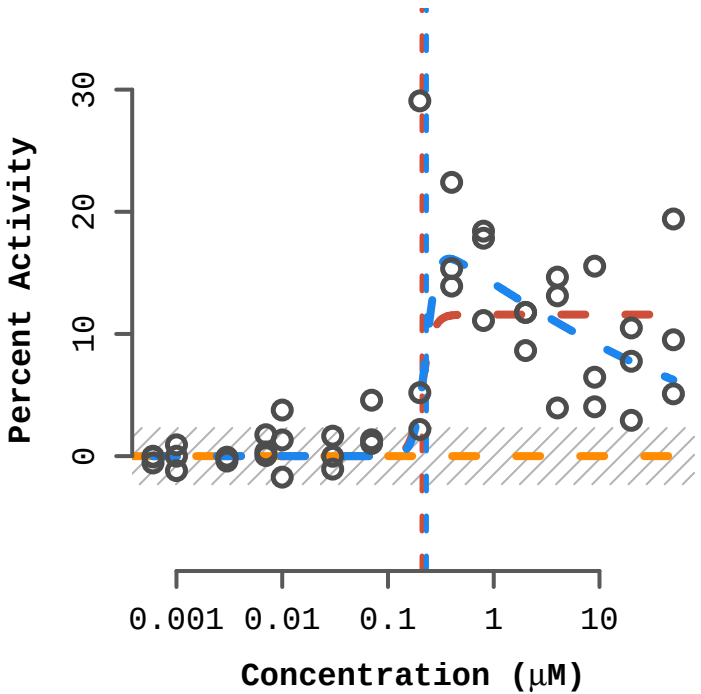
	tp	ga	gw
val:	8.79	-0.95	8
sd:	0.81	0.0494	5.18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	32	-0.901	8	-0.606	0.369
sd:	13.8	0.0447	3.1	0.914	0.102

	CNST	HILL	GNLS
AIC:	319.71	261.97	248.07
PROB:	0	0	1
RMSE:	8.72	4.85	3.57

MAX_MEAN: 20.7 MAX_MED: 20.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Digitoxin
CHID: 22933 CASRN: 71-63-6
SPID(S): Tox21_111659_1
M4ID: 12483550

HILL MODEL (in red):

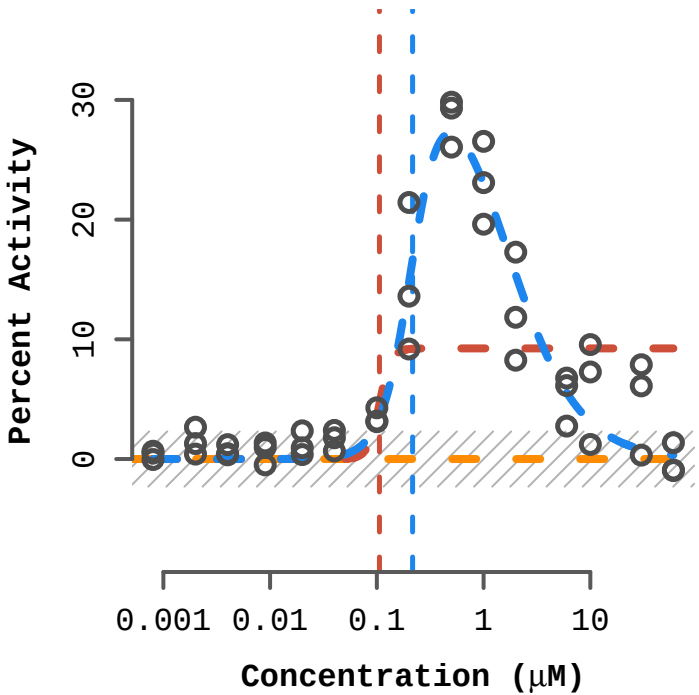
	tp	ga	gw
val:	11.6	-0.678	8
sd:	1	0.0433	5.88

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	32.5	-0.637	7.99	-0.383	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	333.05	267.76	258.06
PROB:	0	0.01	0.99
RMSE:	9.85	5.28	5

MAX_MEAN: 17.2 **MAX_MED:** 17.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Digoxin
CHID: 22934 CASRN: 20830-75-5
SPID(S): Tox21_303050
M4ID: 12476083

HILL MODEL (in red):

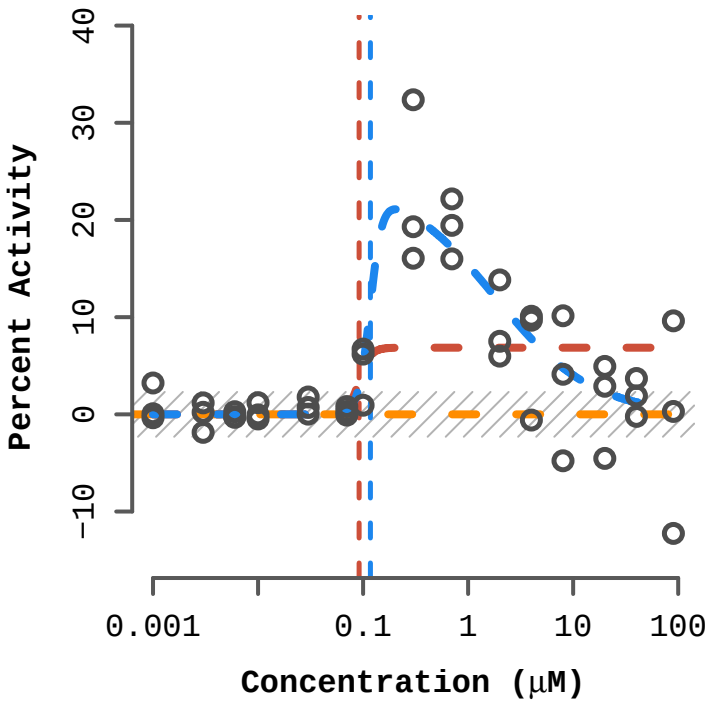
	tp	ga	gw
val:	9.24	-0.976	8
sd:	1.55	0.064	9.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	35.8	-0.665	3.08	0.207	1.29
sd:	5.26	0.0506	0.592	0.124	0.227

	CNST	HILL	GNLS
AIC:	338.78	308.1	230.64
PROB:	0	0	1
RMSE:	11.25	7.41	2.85

MAX_MEAN: 28.4 MAX_MED: 29.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Digoxin
CHID: 22934 **CASRN:** 20830-75-5
SPID(S): Tox21_201678
M4ID: 12480574

HILL MODEL (in red):

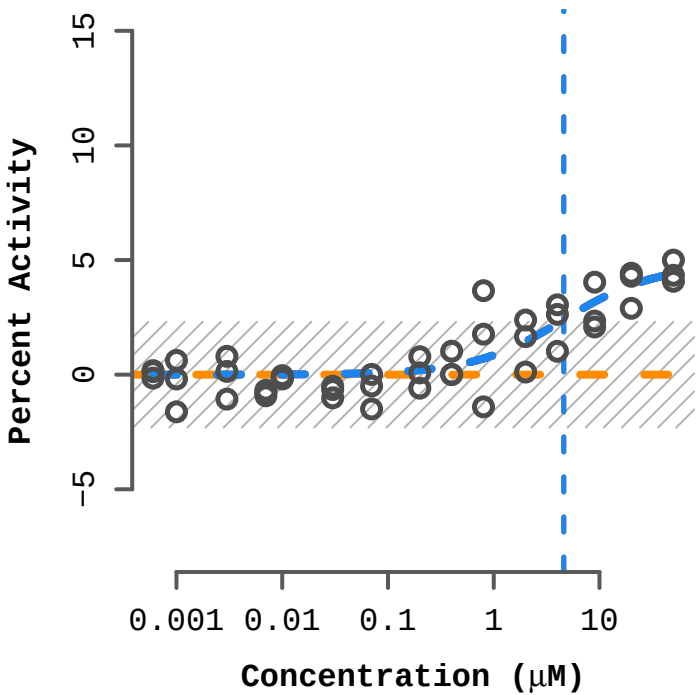
	tp	ga	gw
val:	6.86	−1.04	8
sd:	1.43	0.0848	9.68

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.1	−0.93	7.78	0.259	0.942
sd:	6.27	0.124	12.7	0.321	0.335

	CNST	HILL	GNLS
AIC:	320.45	303.22	259.89
PROB:	0	0	1
RMSE:	9.25	7.21	4.21

MAX_MEAN: 22.6 **MAX_MED:** 19.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dihydralazine
CHID: 22935 **CASRN:** 484-23-1
SPID(S): Tox21_111653_1
M4ID: 12483556

HILL MODEL (in red):

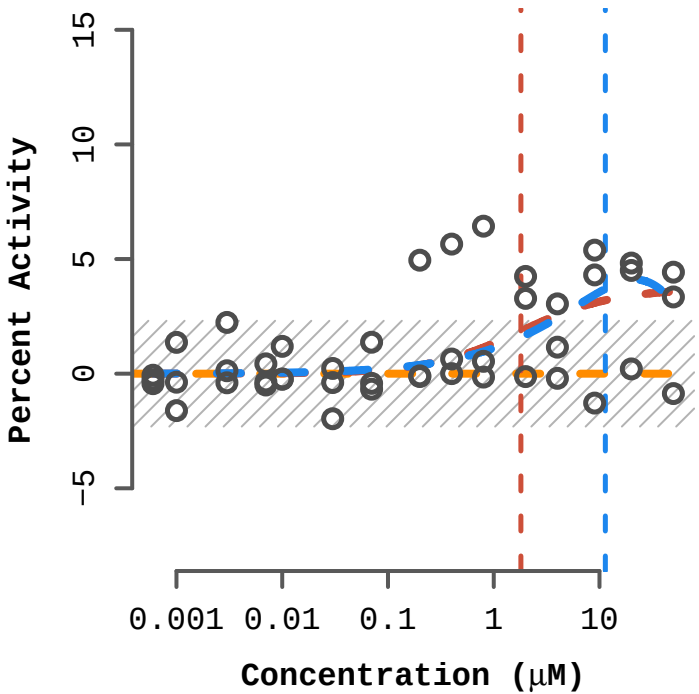
	tp	ga	gw
val:	4.8	0.662	1
sd:	0.775	0.251	0.29

GAIN-LOSS MODEL (in blue):

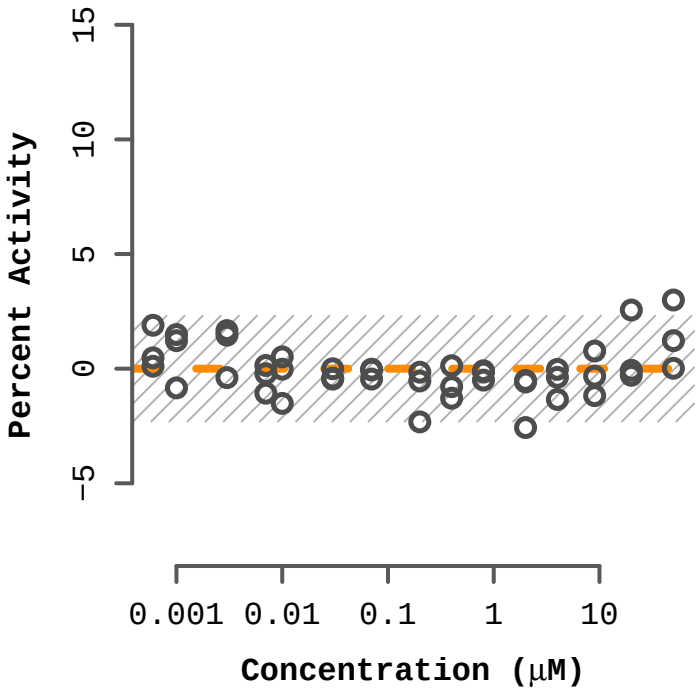
	tp	ga	gw	la	lw
val:	4.8	0.662	1	3.4	4.19
sd:	0.775	0.251	0.29	890	2190

	CNST	HILL	GNLS
AIC:	192.96	126.58	130.58
PROB:	0	0.88	0.12
RMSE:	2.06	0.91	0.91

MAX_MEAN: 4.47 **MAX_MED:** 4.34 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diltiazem
CHID:    22940   CASRN: 42399-41-7
SPID(S): Tox21_110898_1
M4ID:    12484030

HILL MODEL (in red):
      tp       ga       gw
val:  3.71     0.257    0.998
sd:   1.07     0.478    0.609

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.72     1.06     0.733    1.73     2.01
sd:   21.8     2.77     0.564    0.679    5.05

      CNST        HILL        GNLS
AIC:  208.01      192.73      195.98
PROB: 0           0.84        0.16
RMSE: 2.5         1.98        2

MAX_MEAN: 3.18      MAX_MED: 4.5       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

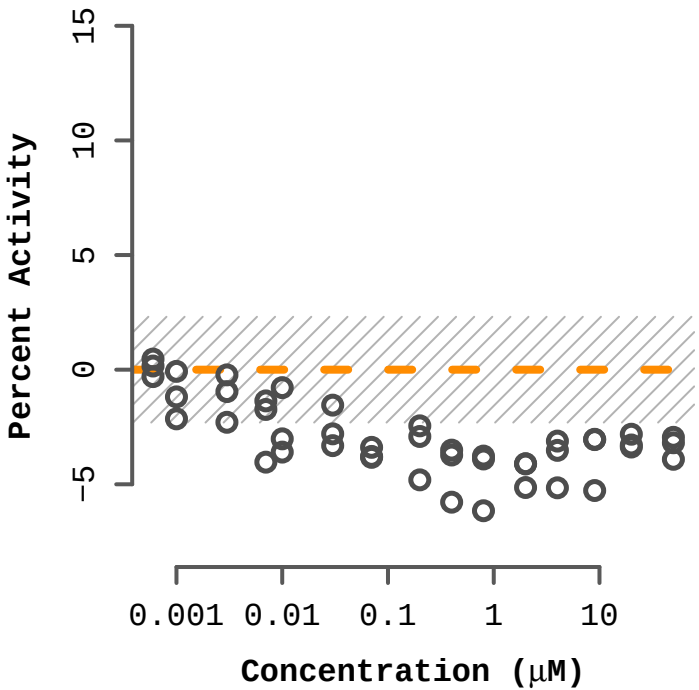
NAME: Metocurine iodide
CHID: 22944 **CASRN:** 7601-55-0
SPID(S): Tox21_112755_1
M4ID: 12482968

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

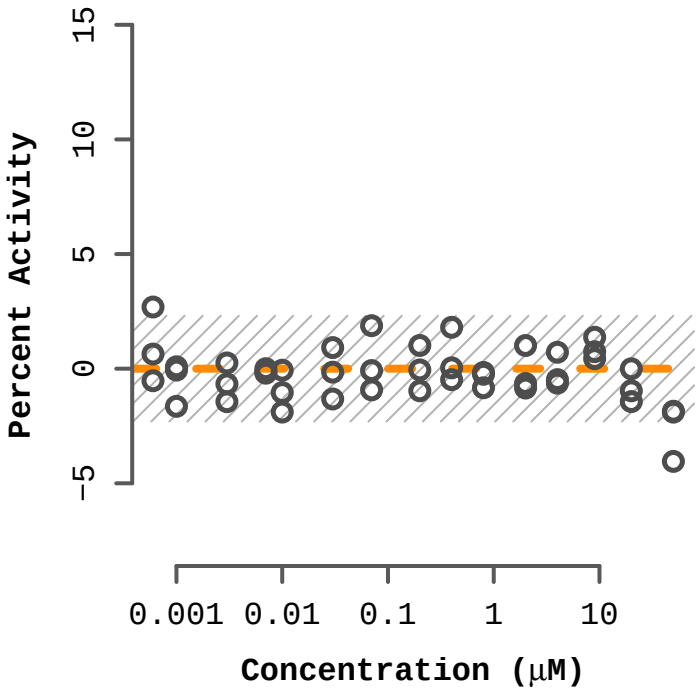
NAME: Dinoprostone
CHID: 22947 CASRN: 363-24-6
SPID(S): Tox21_111196_1
M4ID: 12483850

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.99	NA	NA
PROB:	1	NA	NA
RMSE:	3.34	NA	NA

MAX_MEAN: 0.107 MAX_MED: 0.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

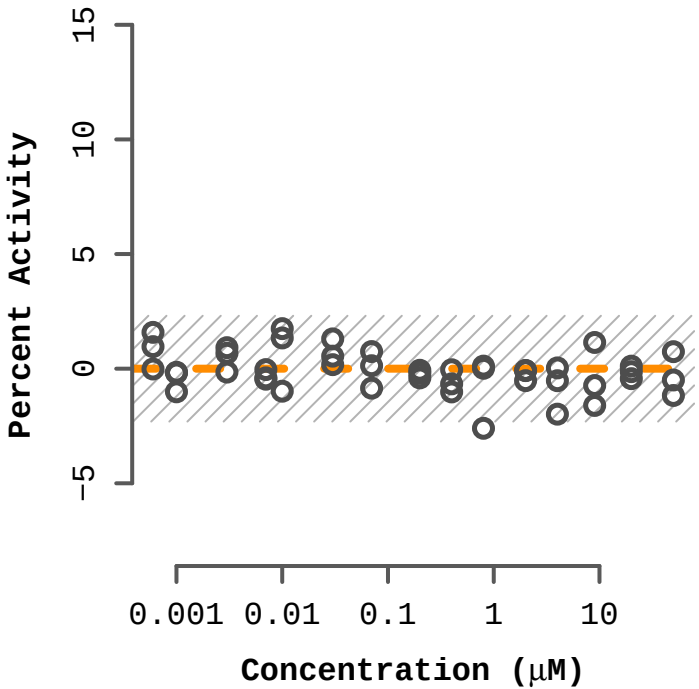
NAME: Diphemanil methylsulfate
CHID: 22948 **CASRN:** 62-97-5
SPID(S): Tox21_110349_1
M4ID: 12484434

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.742 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

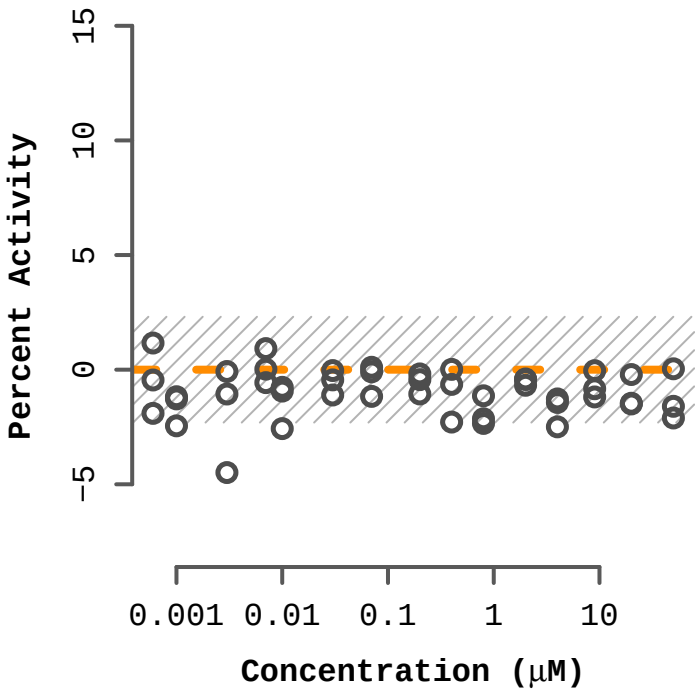
NAME: Diphenhydramine
CHID: 22949 **CASRN:** 58-73-1
SPID(S): Tox21_110127_1
M4ID: 12484626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.845 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

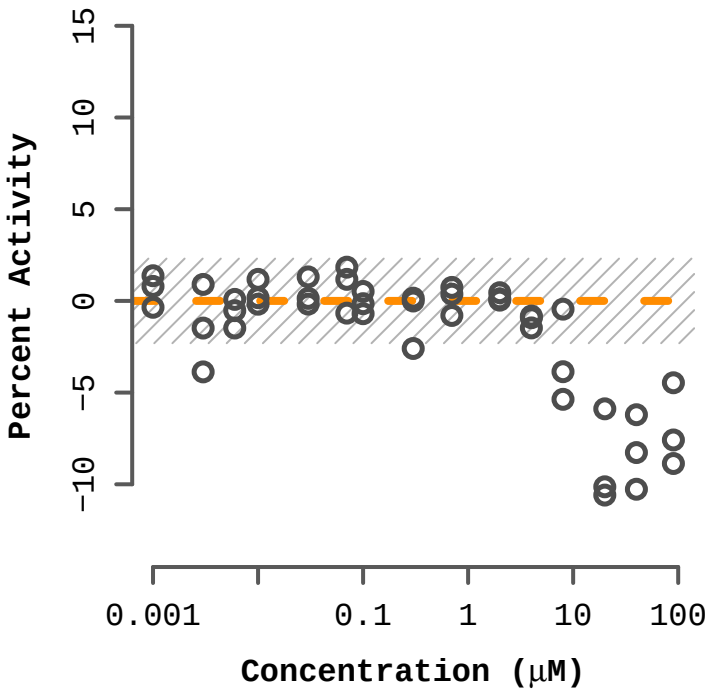
NAME: Diphenidol
CHID: 22950 CASRN: 972-02-1
SPID(S): Tox21_113073_1
M4ID: 12482819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 0.127 **MAX_MED:** 0.0228 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

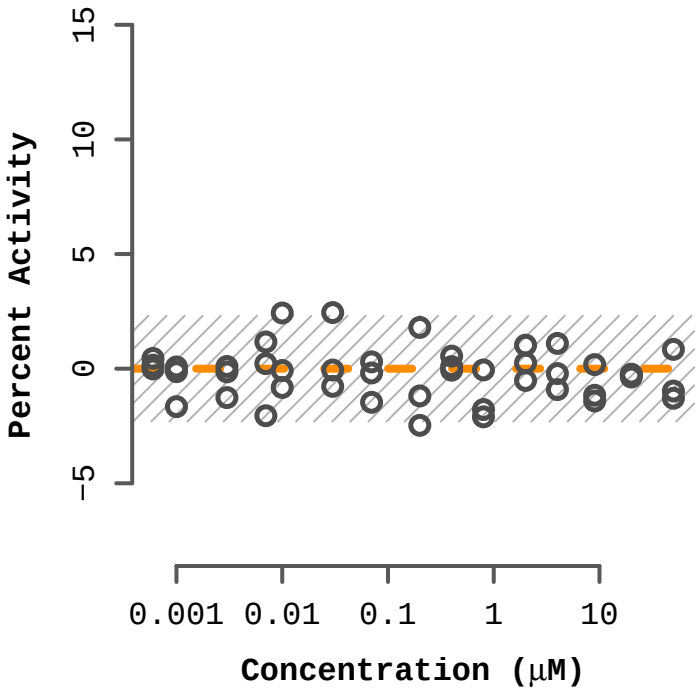
NAME: Sodium diethyldithiocarbamate
CHID: 22956 CASRN: 148-18-5
SPID(S): Tox21_200403
M4ID: 12481849

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	243.25	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 0.784 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

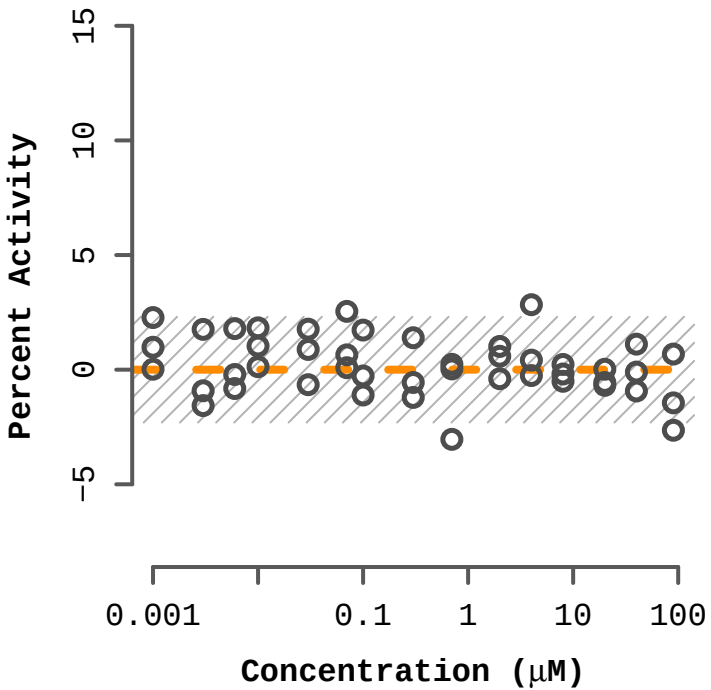
NAME: Dobutamine
CHID: 22958 **CASRN:** 34368-04-2
SPID(S): Tox21_110126_1
M4ID: 12484627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.54 **MAX_MED:** 0.253 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

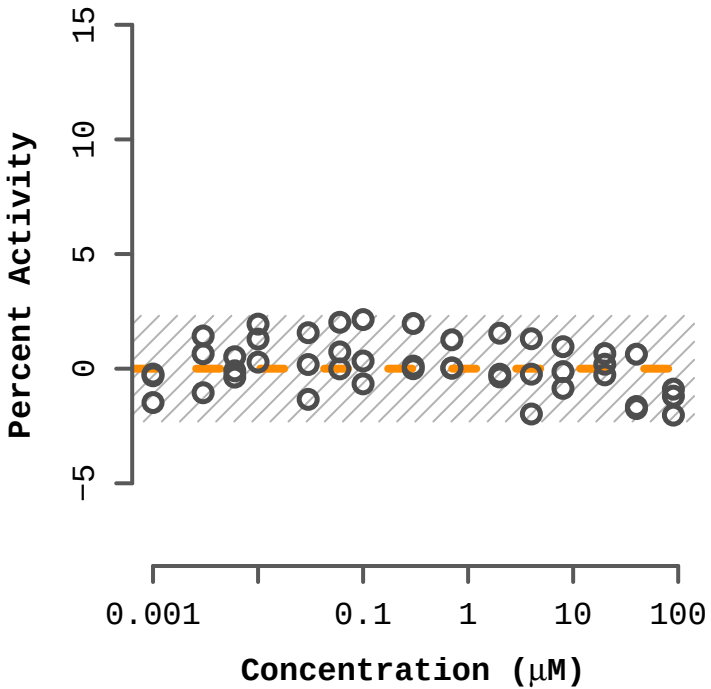
NAME: Docusate sodium
CHID: 22959 **CASRN:** 577-11-7
SPID(S): Tox21_300496
M4ID: 12478636

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

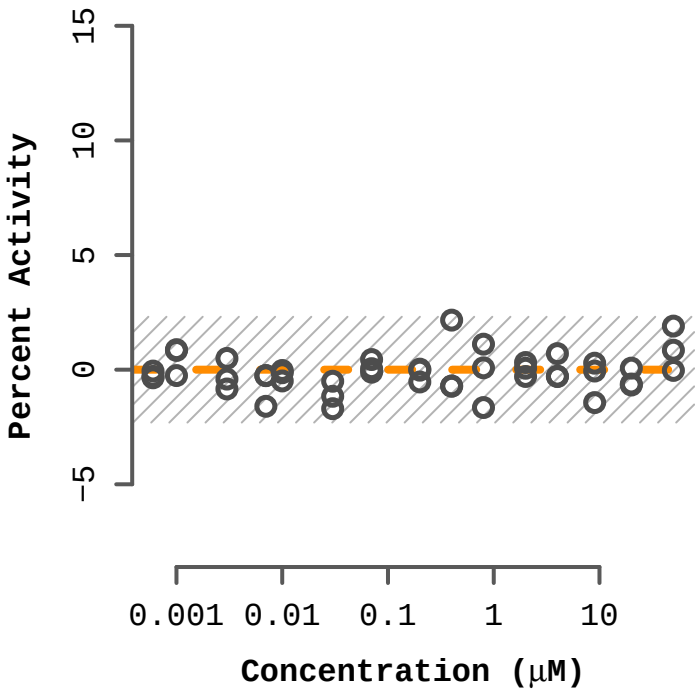
NAME: Docusate sodium
CHID: 22959 **CASRN:** 577-11-7
SPID(S): Tox21_201342
M4ID: 12480910

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

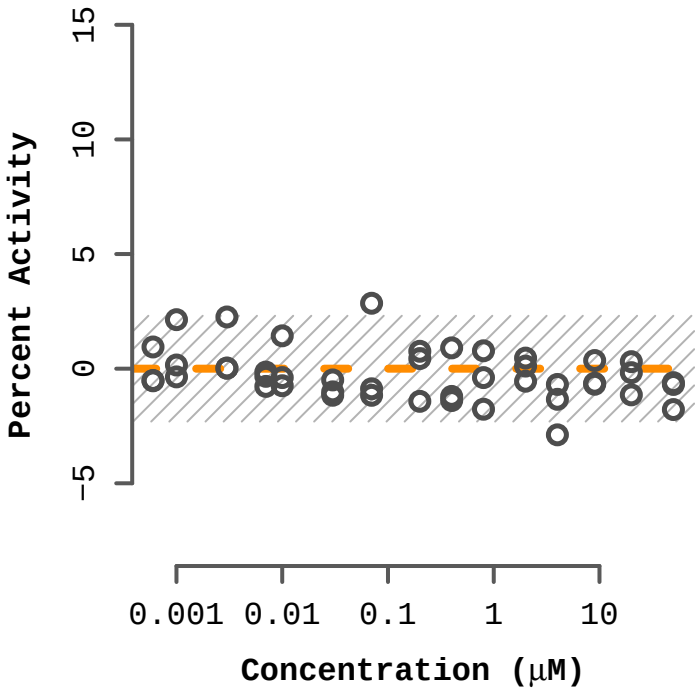
NAME: Doxifluridine
CHID: 22967 **CASRN:** 3094-09-5
SPID(S): Tox21_111231_1
M4ID: 12483826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.908 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

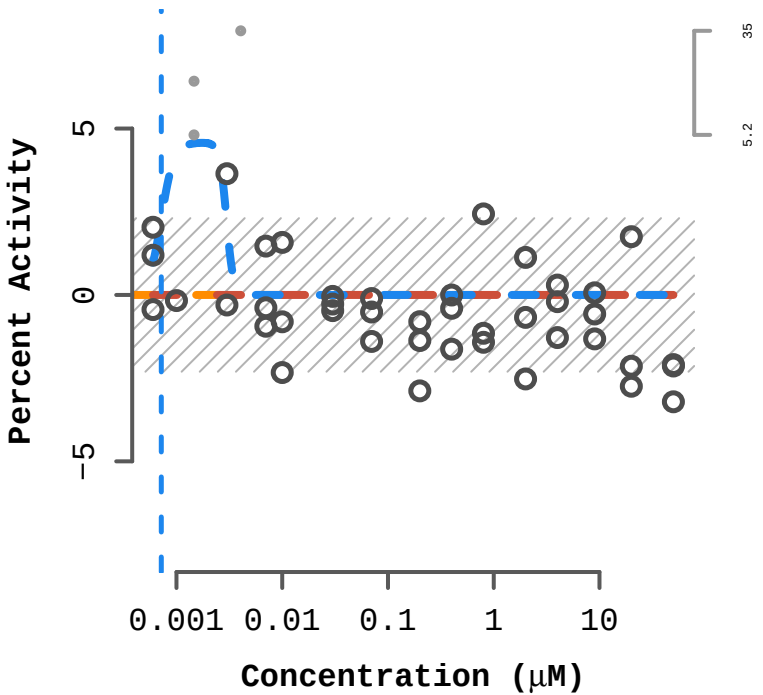
NAME: Doxofylline
CHID: 22968 **CASRN:** 69975-86-6
SPID(S): Tox21_111577_1
M4ID: 12483608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.769 **MAX_MED:** 0.444 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Droperidol
CHID: 22973 CASRN: 548-73-2
SPID(S): Tox21_110461_1
M4ID: 12484337 BRK

HILL MODEL (in red):

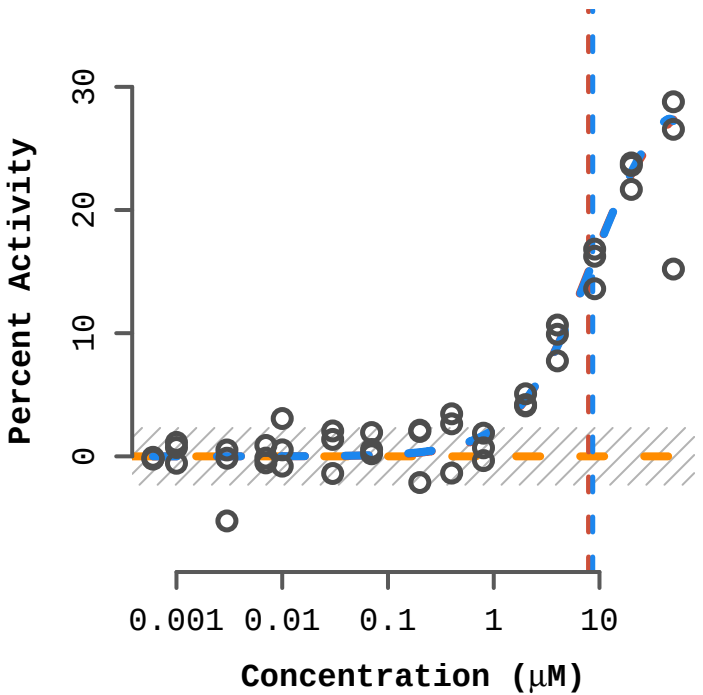
	tp	ga	gw
val:	8.51e-10	-4.78	7.16
sd:	NA	NA	NA

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.58	-3.14	7.3	-2.53	13.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	221.75	227.75	226.28
PROB:	0.87	0.04	0.09
RMSE:	6.32	6.32	5.74

MAX_MEAN: 12.8 MAX_MED: 5.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dydrogesterone
CHID: 22974 CASRN: 152-62-5
SPID(S): Tox21_110429_1
M4ID: 12484365

HILL MODEL (in red):

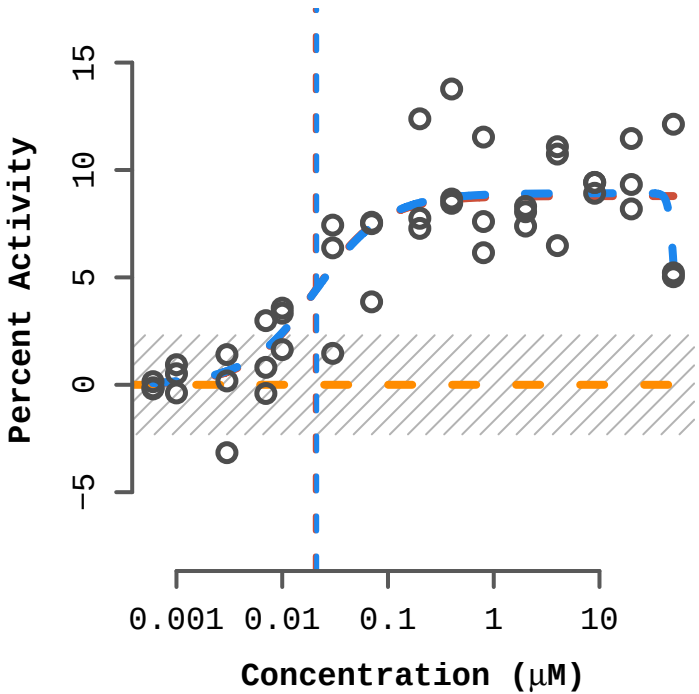
	tp	ga	gw
val:	30	0.897	1.25
sd:	2.03	0.067	0.138

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	31.5	0.936	1.2	1.84	10.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	324.85	187.89	191.8
PROB:	0	0.88	0.12
RMSE:	10.02	2.37	2.35

MAX_MEAN: 23.5 MAX_MED: 26.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dyphylline
CHID: 22975 CASRN: 479-18-5
SPID(S): Tox21_110444_1
M4ID: 12484351

HILL MODEL (in red):

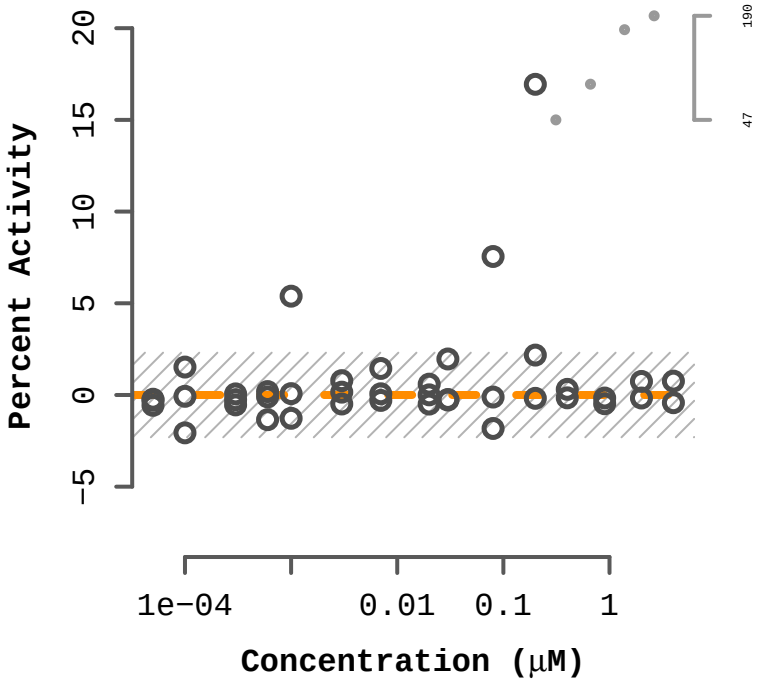
	tp	ga	gw
val:	8.79	−1.69	1.37
sd:	0.461	0.134	0.415

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.92	−1.67	1.31	1.71	16
sd:	0.451	0.132	0.383	0.015	15.8

	CNST	HILL	GNLS
AIC:	313.43	198.88	198.64
PROB:	0	0.47	0.53
RMSE:	7.18	2.01	2.03

MAX_MEAN: 10.3 MAX_MED: 10.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

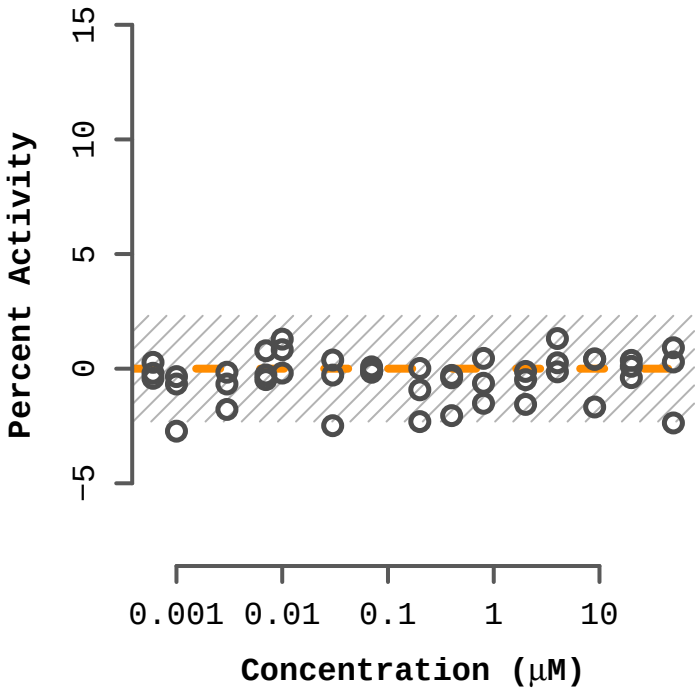
NAME: Ethylenediaminetetraacetic acid
CHID: 22977 **CASRN:** 60-00-4
SPID(S): Tox21_202736
M4ID: 12479516 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	318.58	NA	NA
PROB:	1	NA	NA
RMSE:	40.61	NA	NA

MAX_MEAN: 62.1 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

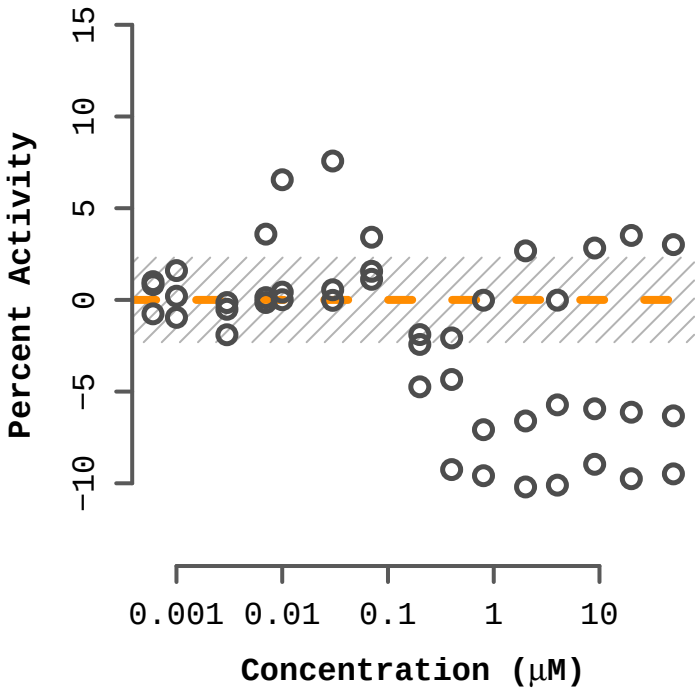
NAME: Edrophonium chloride
CHID: 22978 **CASRN:** 116-38-1
SPID(S): Tox21_110138_1
M4ID: 12484617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.643 **MAX_MED:** 0.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

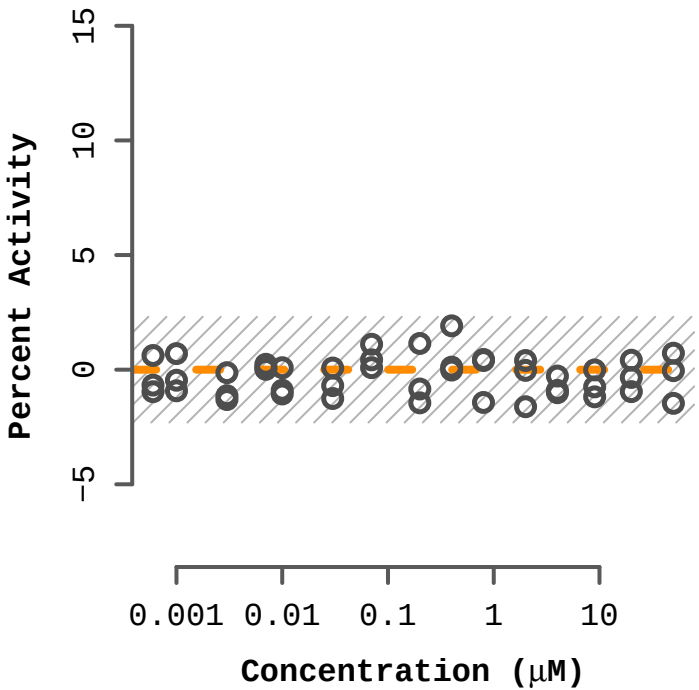
NAME: Emetine
CHID: 22980 **CASRN:** 483-18-1
SPID(S): Tox21_110901_1
M4ID: 12484029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	275.89	NA	NA
PROB:	1	NA	NA
RMSE:	4.98	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

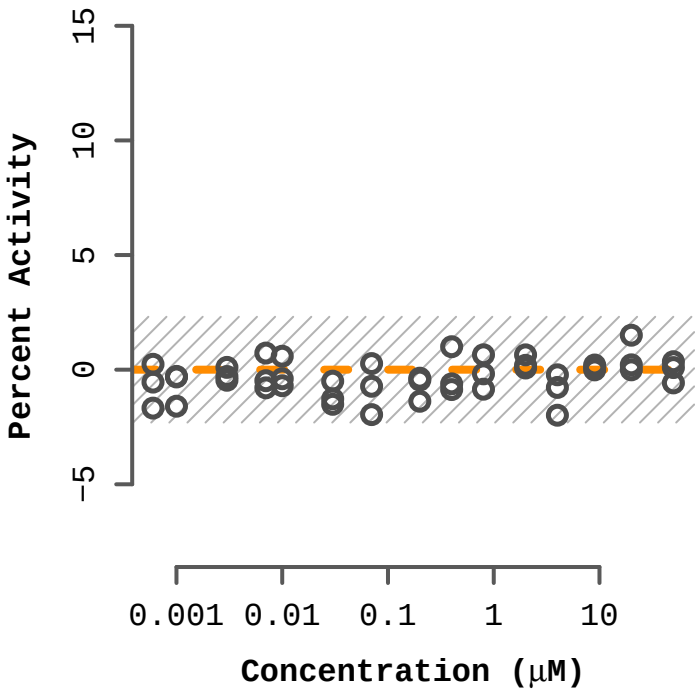
NAME: Emorfazone
CHID: 22981 CASRN: 38957-41-4
SPID(S): Tox21_113708
M4ID: 12482506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.67 MAX_MED: 0.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

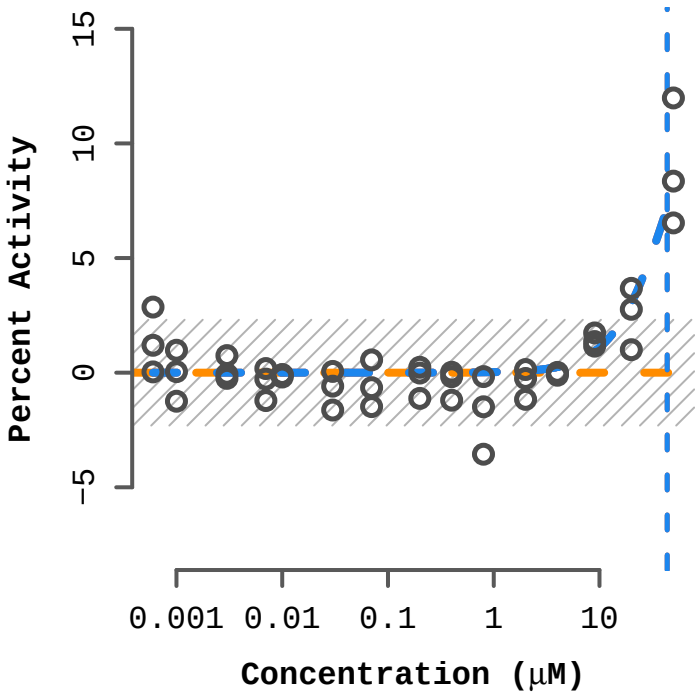
NAME: Enalapril
CHID: 22982 **CASRN:** 75847-73-3
SPID(S): Tox21_110872_1
M4ID: 12484055

HILL MODEL: Not applicable.

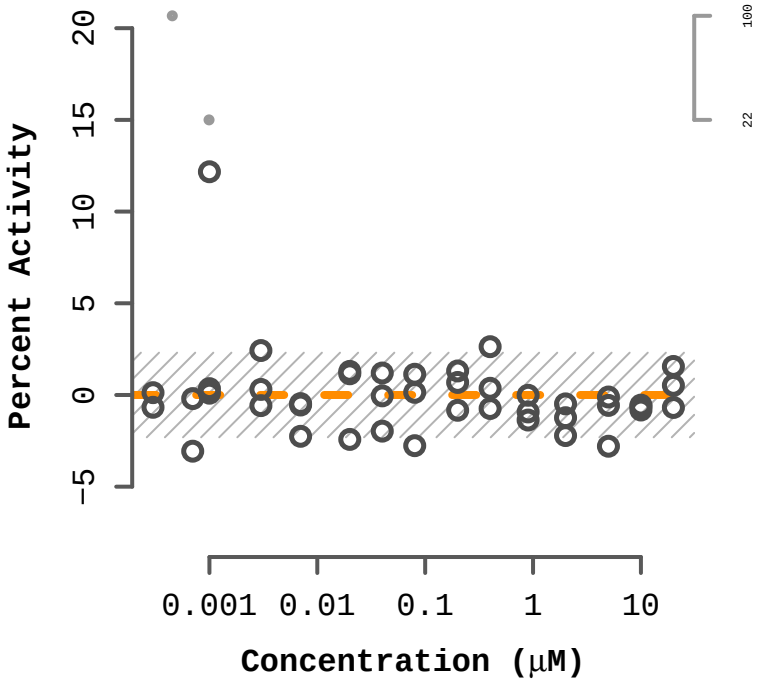
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.571 **MAX_MED:** 0.213 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Enoxacin
CHID:    22984   CASRN: 74011-58-8
SPID(S): Tox21_110688_1
M4ID:    12484178

HILL MODEL (in red):
      tp       ga       gw
val:  14.4     1.64     1.69
sd:   8.34     0.305    0.486

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  14.4     1.64     1.69     3.62     18
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  186.54      141.91      145.91
PROB: 0           0.88        0.12
RMSE: 2.68        1.19        1.19

MAX_MEAN: 8.96      MAX_MED: 8.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

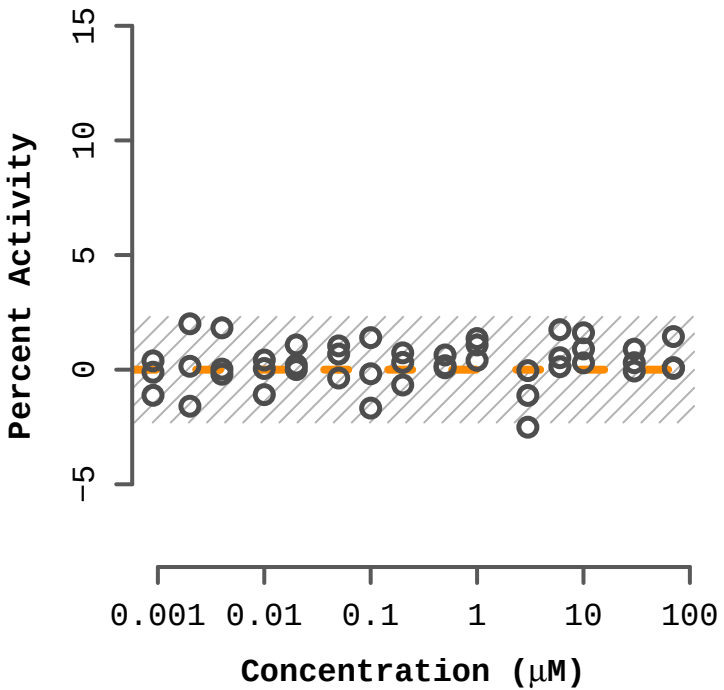
NAME: Epinephrine
CHID: 22986 **CASRN:** 51-43-4
SPID(S): Tox21_111562_1
M4ID: 12483616 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.99	NA	NA
PROB:	1	NA	NA
RMSE:	16.01	NA	NA

MAX_MEAN: 34.5 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

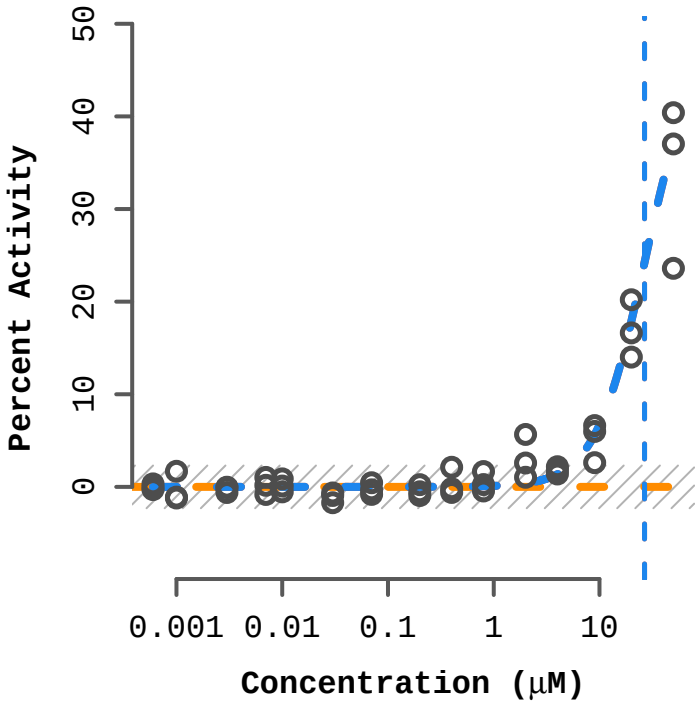
NAME: Erythromycin
CHID: 22991 **CASRN:** 114-07-8
SPID(S): Tox21_300515
M4ID: 12478617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Erythromycin propionate
CHID: 22994 **CASRN:** 134-36-1
SPID(S): Tox21_113189_1
M4ID: 12482776

HILL MODEL (in red):

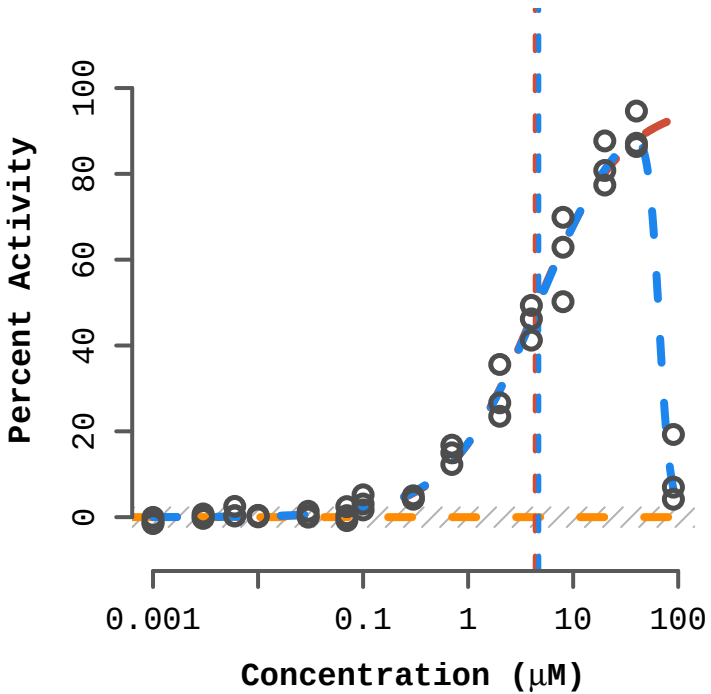
	tp	ga	gw
val:	48.5	1.43	1.87
sd:	5.62	0.0772	0.238

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	48.5	1.43	1.87	3.7	11.1
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	289.71	181.72	185.72
PROB:	0	0.88	0.12
RMSE:	10.11	2.5	2.5

MAX_MEAN: 33.7 **MAX_MED:** 37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estradiol cypionate
CHID: 22999 CASRN: 313-06-4
SPID(S): Tox21_301818
M4ID: 12477315

HILL MODEL (in red):

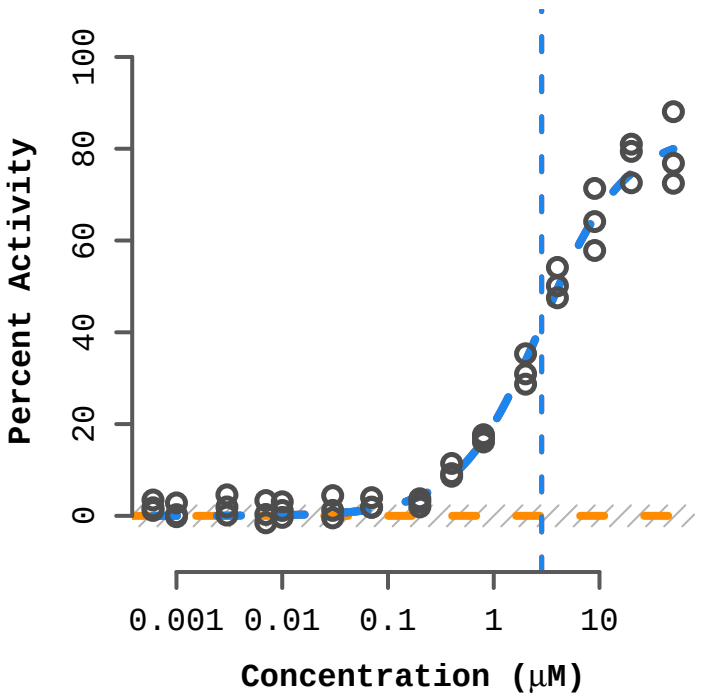
	tp	ga	gw
val:	96.7	0.639	1.04
sd:	3.79	0.0521	0.0801

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	99.8	0.673	1.01	1.82	8.18
sd:	5.81	0.0679	0.0737	0.042	2.35

	CNST	HILL	GNLS
AIC:	450.35	315.98	247.49
PROB:	0	0	1
RMSE:	38.18	21.65	3.82

MAX_MEAN: 89.4 MAX_MED: 87.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estradiol cypionate
CHID: 22999 **CASRN:** 313-06-4
SPID(S): Tox21_112331_1
M4ID: 12483156

HILL MODEL (in red):

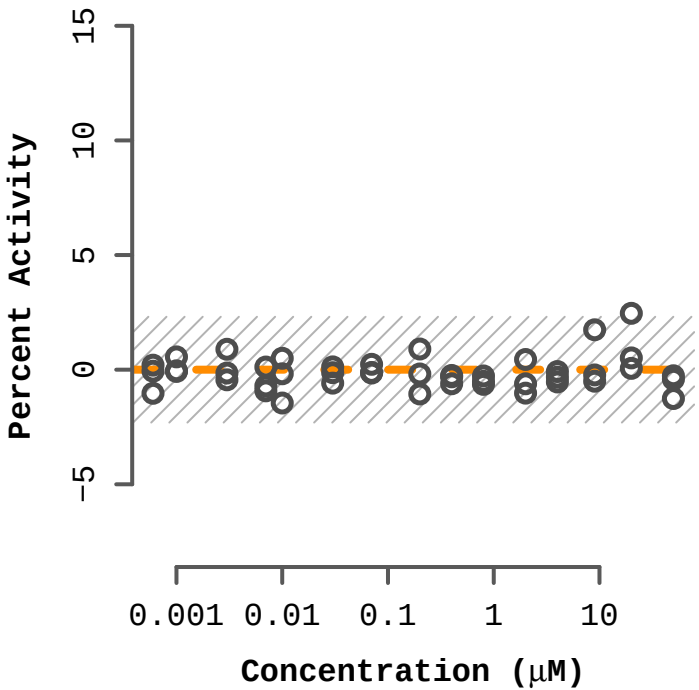
	tp	ga	gw
val:	83.3	0.453	1.1
sd:	4.54	0.0573	0.0774

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	83.3	0.453	1.1	2.86	15
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	449.97	240.24	244.24
PROB:	0	0.88	0.12
RMSE:	37.01	3.22	3.22

MAX_MEAN: 79.1 **MAX_MED:** 79.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

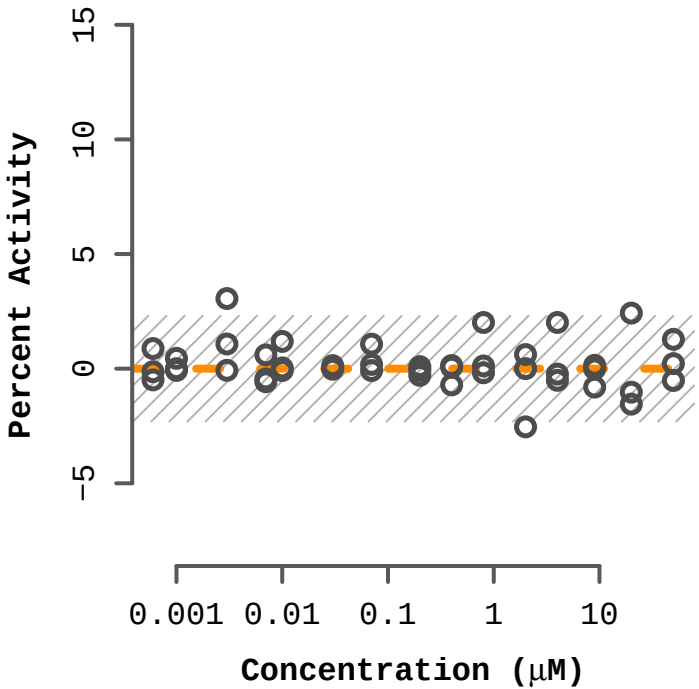
NAME: Ethamivan
CHID: 23007 **CASRN:** 304-84-7
SPID(S): Tox21_110135_1
M4ID: 12484619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.515 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

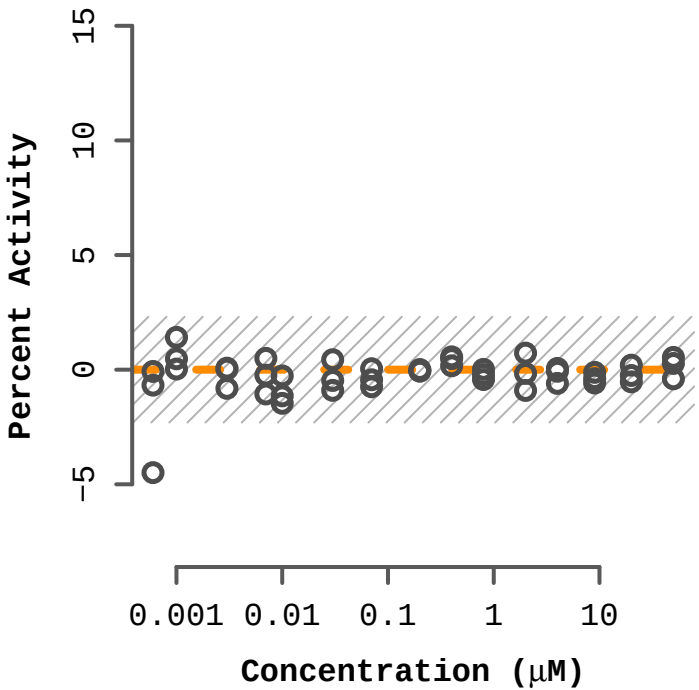
NAME: Ethchlorvynol
CHID: 23010 **CASRN:** 113-18-8
SPID(S): Tox21_113732
M4ID: 12482482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

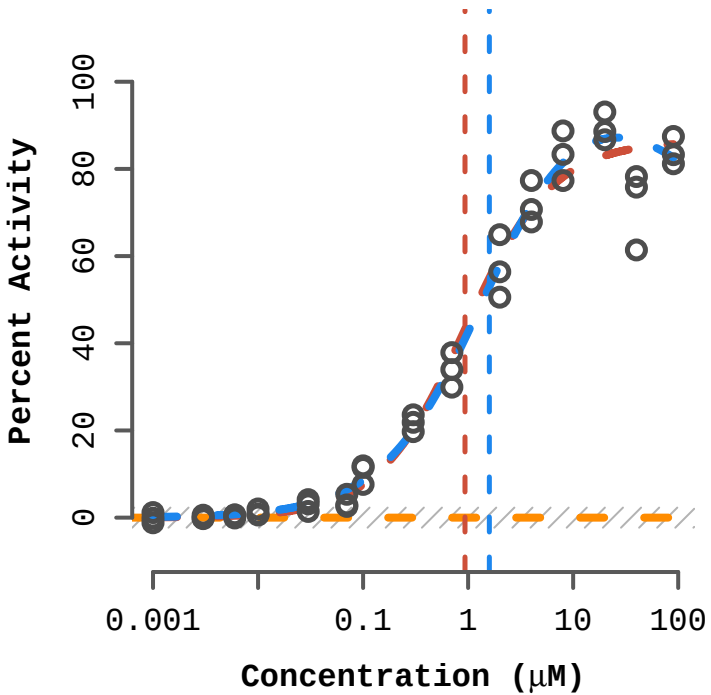
NAME: Ethebenecid
CHID: 23011 **CASRN:** 1213-06-5
SPID(S): Tox21_111810_1
M4ID: 12483466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.639 **MAX_MED:** 0.485 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethisterone
CHID: 23016 **CASRN:** 434-03-7
SPID(S): Tox21_302324
M4ID: 12476809

HILL MODEL (in red):

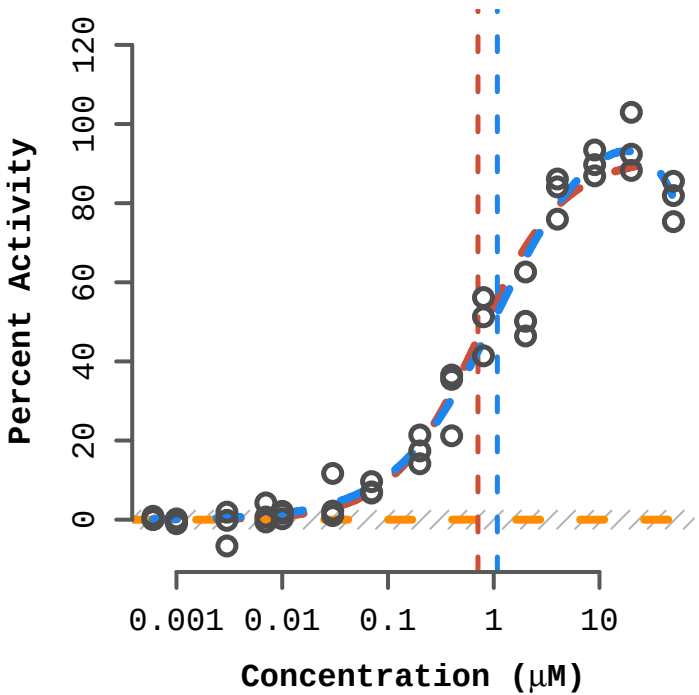
	tp	ga	gw
val:	86.4	-0.0299	1.05
sd:	2.08	0.041	0.0679

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	112	0.202	0.892	3.09	0.44
sd:	23.5	0.119	0.0633	0.452	0.359

	CNST	HILL	GNLS
AIC:	484.44	272.12	267.16
PROB:	0	0.08	0.92
RMSE:	50	5.33	5.2

MAX_MEAN: 89.5 **MAX_MED:** 88.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethisterone
CHID: 23016 **CASRN:** 434-03-7
SPID(S): Tox21_111604_1
M4ID: 12483593

HILL MODEL (in red):

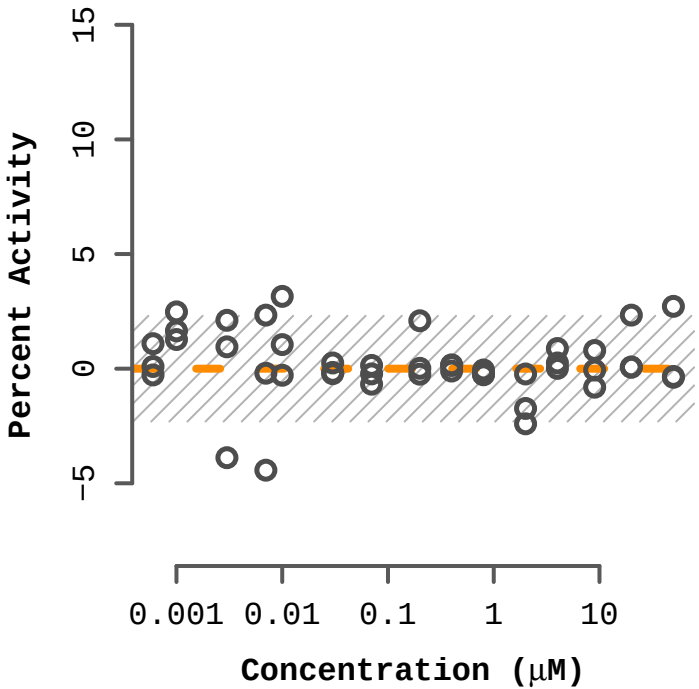
	tp	ga	gw
val:	91.6	-0.149	1.07
sd:	2.97	0.0608	0.105

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	104	0.0341	0.892	2.03	1.84
sd:	11.6	0.155	0.11	0.22	1.63

	CNST	HILL	GNLS
AIC:	482.64	298.92	287.89
PROB:	0	0	1
RMSE:	49.83	6.74	5.64

MAX_MEAN: 94.5 **MAX_MED:** 92.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

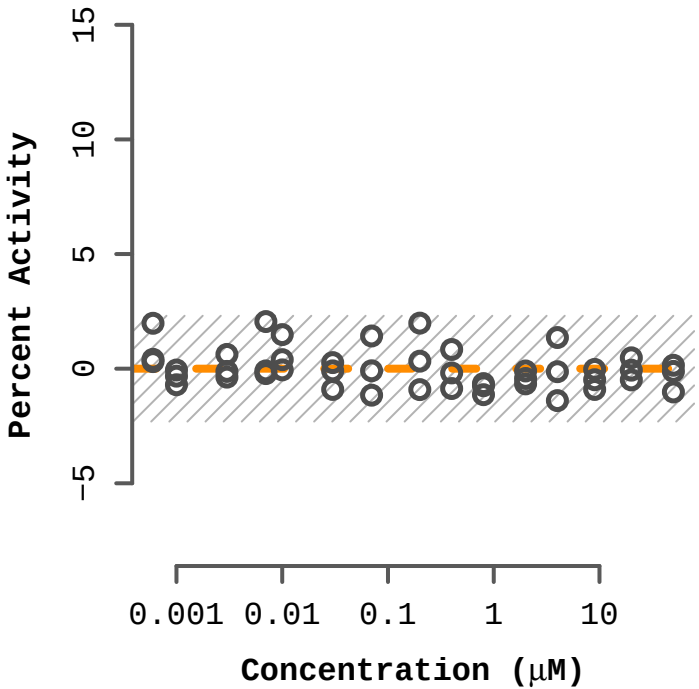
NAME: Ethosuximide
CHID: 23019 **CASRN:** 77-67-8
SPID(S): Tox21_110370_1
M4ID: 12484418

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

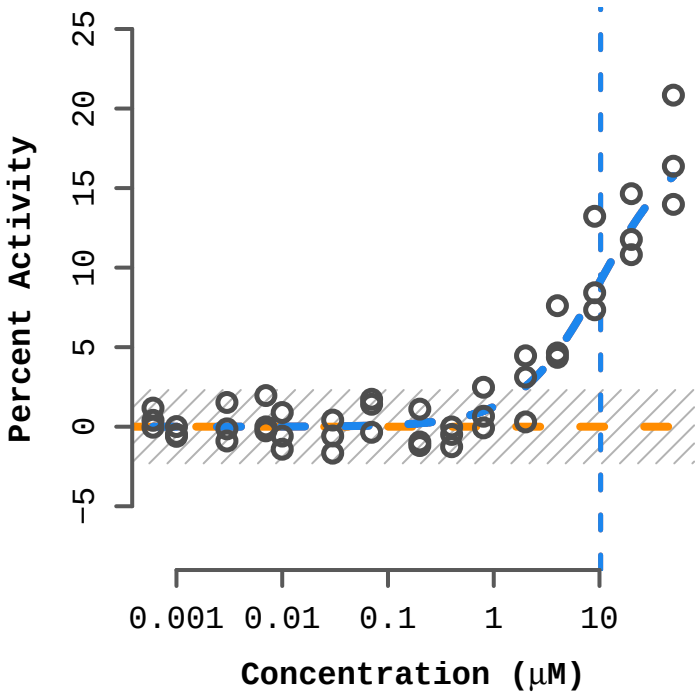
NAME: Ethoxzolamide
CHID: 23021 **CASRN:** 452-35-7
SPID(S): Tox21_110848_1
M4ID: 12484071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.9 **MAX_MED:** 0.408 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethylestrenol
CHID: 23024 **CASRN:** 965-90-2
SPID(S): Tox21_112512_1
M4ID: 12483057

HILL MODEL (in red):

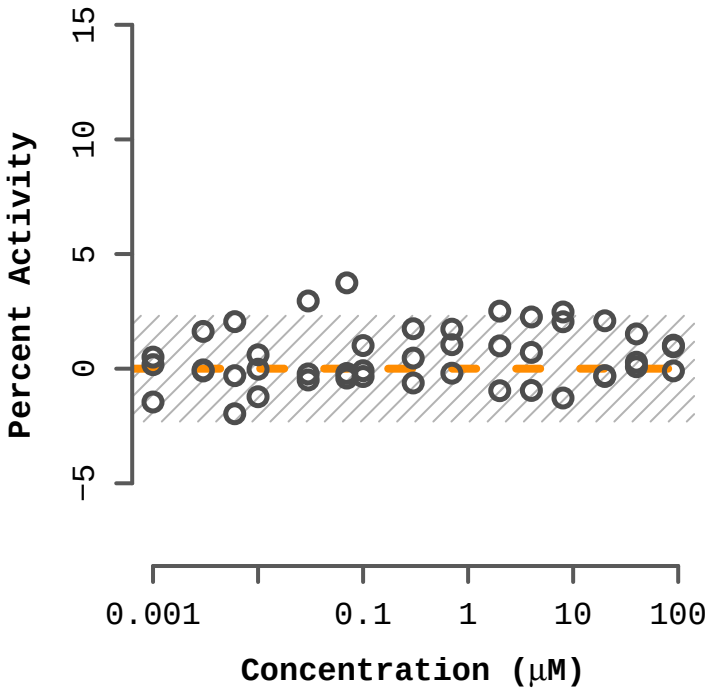
	tp	ga	gw
val:	18.4	1.01	1.13
sd:	2.85	0.16	0.214

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.4	1.01	1.13	3.08	5.69
sd:	2.85	0.16	0.214	910	3750

	CNST	HILL	GNLS
AIC:	282.07	172.36	176.36
PROB:	0	0.88	0.12
RMSE:	6.38	1.57	1.57

MAX_MEAN: 17.1 **MAX_MED:** 16.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

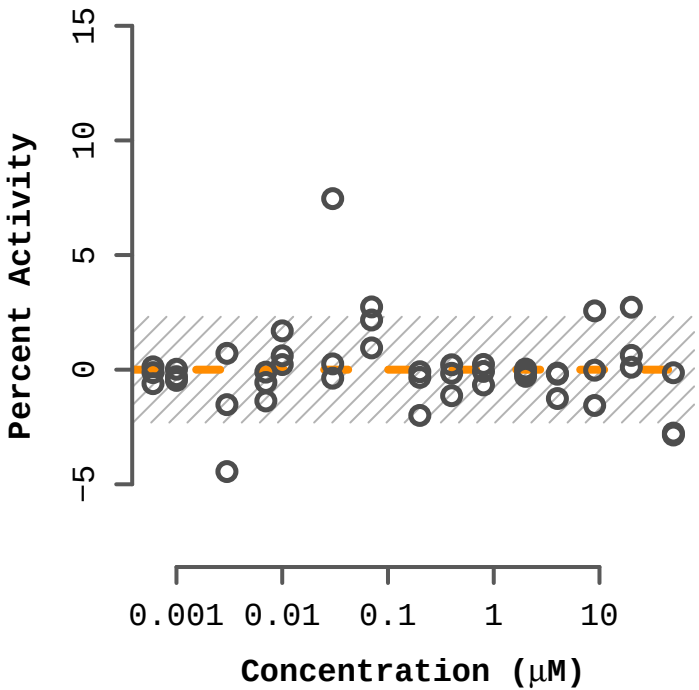
NAME: Etidronic acid
CHID: 23028 **CASRN:** 2809-21-4
SPID(S): Tox21_200417
M4ID: 12481835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

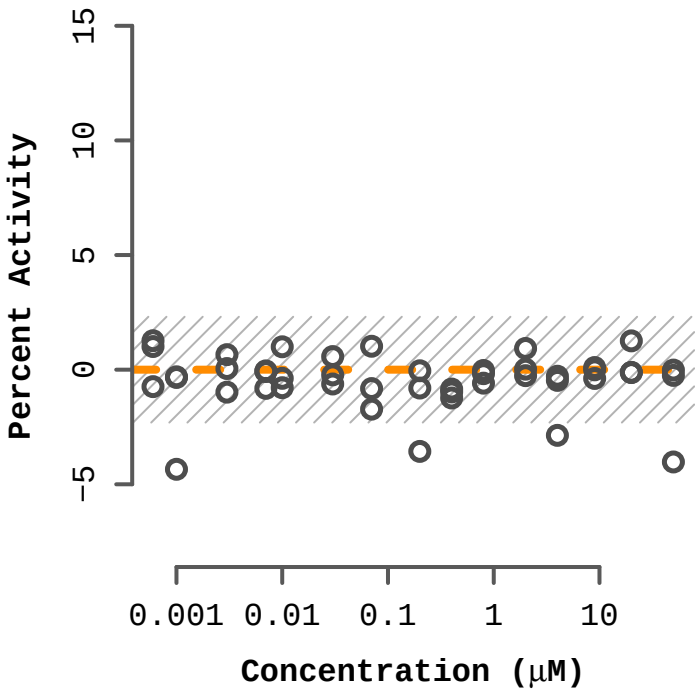
NAME: Etizolam
CHID: 23030 CASRN: 40054-69-1
SPID(S): Tox21_112931
M4ID: 12482871

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 2.45 MAX_MED: 2.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

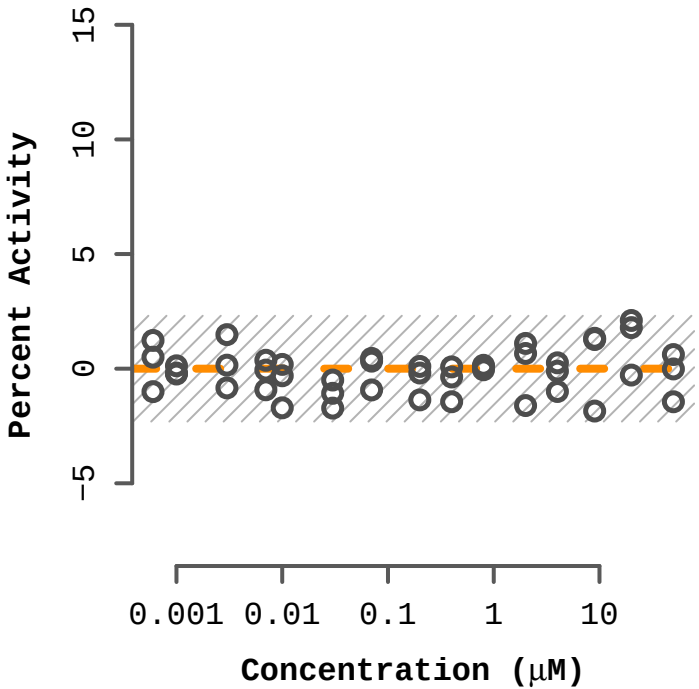
NAME: Etofylline
CHID: 23031 **CASRN:** 519-37-9
SPID(S): Tox21_110447_1
M4ID: 12484348

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.513 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

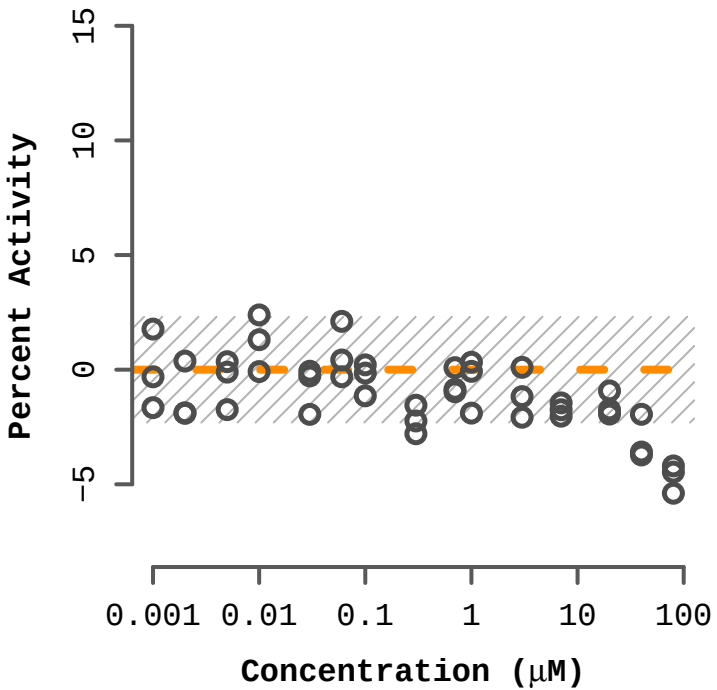
NAME: Etomidate
CHID: 23033 **CASRN:** 33125-97-2
SPID(S): Tox21_110628_1
M4ID: 12484221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

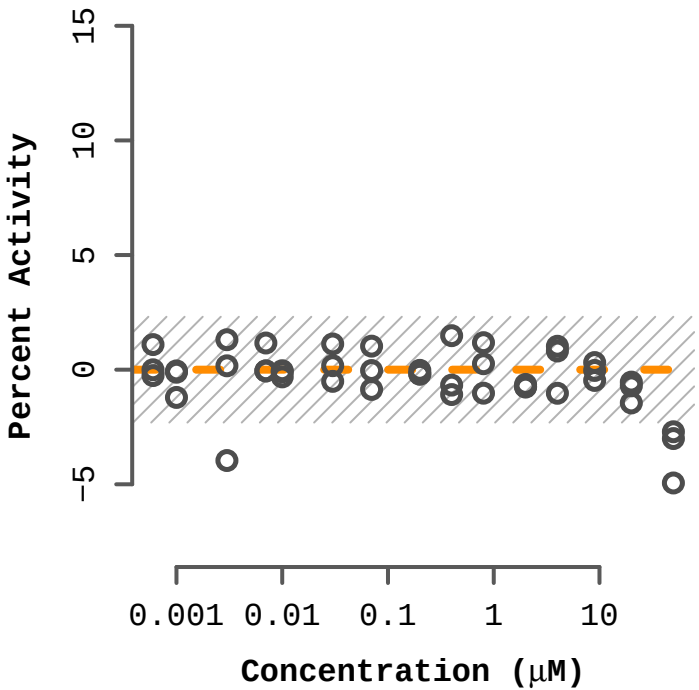
NAME: Etoposide
CHID: 23035 **CASRN:** 33419-42-0
SPID(S): Tox21_302201
M4ID: 12476932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

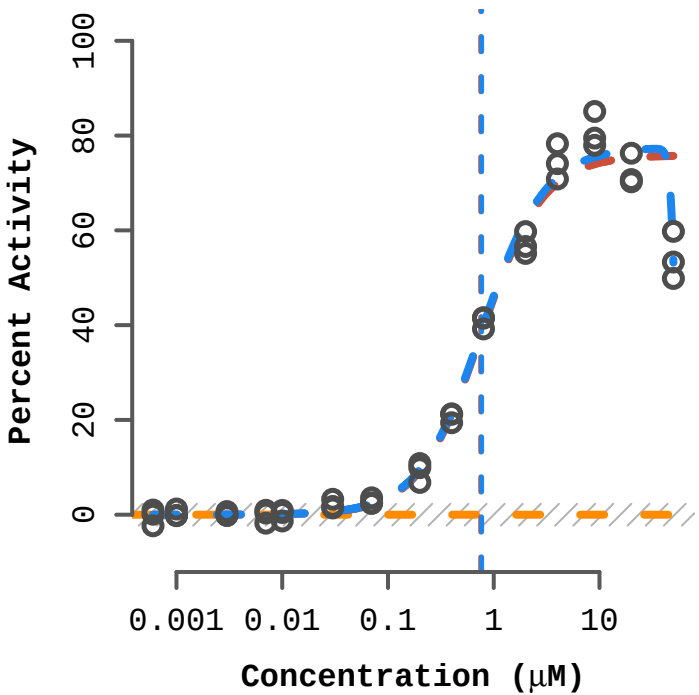
NAME: Etretinate
CHID: 23036 **CASRN:** 54350-48-0
SPID(S): Tox21_112501_1
M4ID: 12483065

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.353 **MAX_MED:** 0.816 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Exemestane
CHID: 23037 CASRN: 107868-30-4
SPID(S): Tox21_111499_1
M4ID: 12483649

HILL MODEL (in red):

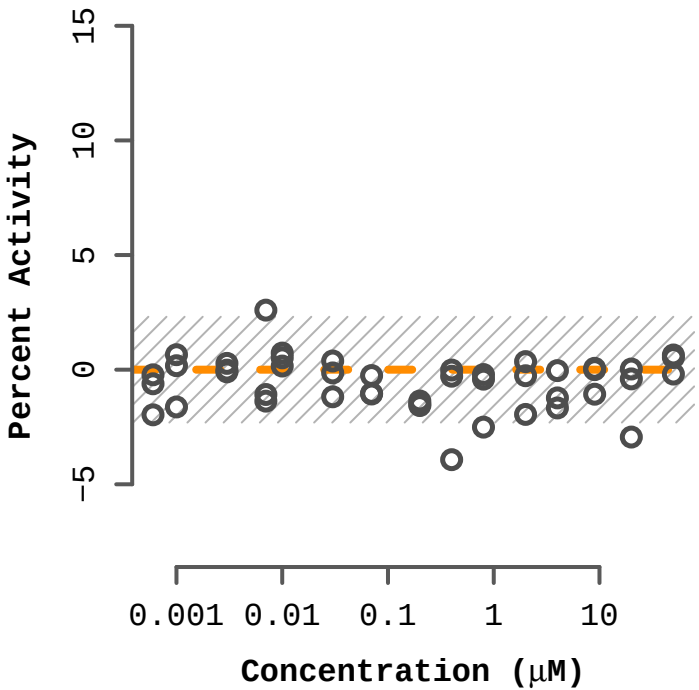
	tp	ga	gw
val:	75.9	-0.123	1.49
sd:	2.24	0.0287	0.108

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	77.6	-0.115	1.46	1.72	18
sd:	1.77	0.0237	0.0898	0.00385	3.16

	CNST	HILL	GNLS
AIC:	465.6	270.94	235.28
PROB:	0	0	1
RMSE:	41.45	6.39	3.14

MAX_MEAN: 80.8 **MAX_MED:** 79.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

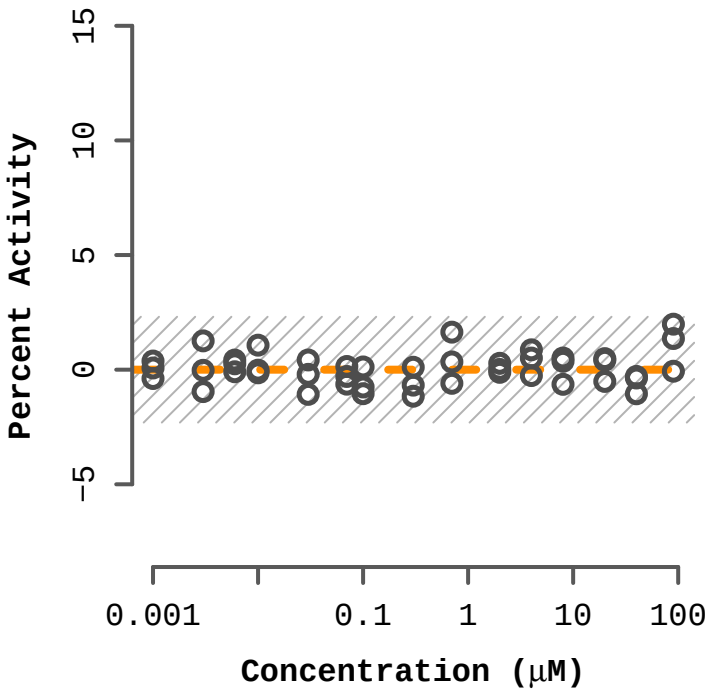
NAME: Famciclovir
CHID: 23038 **CASRN:** 104227-87-4
SPID(S): Tox21_111442_1
M4ID: 12483683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.468 **MAX_MED:** 0.531 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

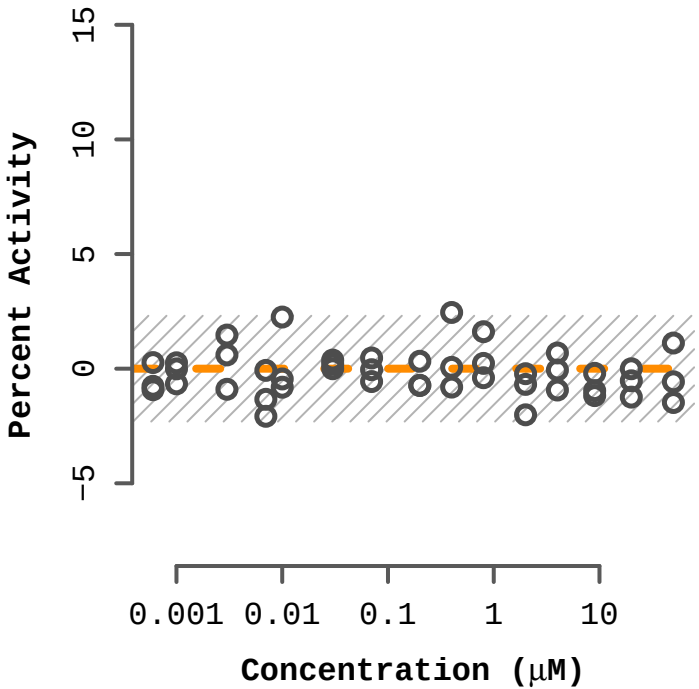
NAME: Famotidine
CHID: 23039 **CASRN:** 76824-35-6
SPID(S): Tox21_301827
M4ID: 12477306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

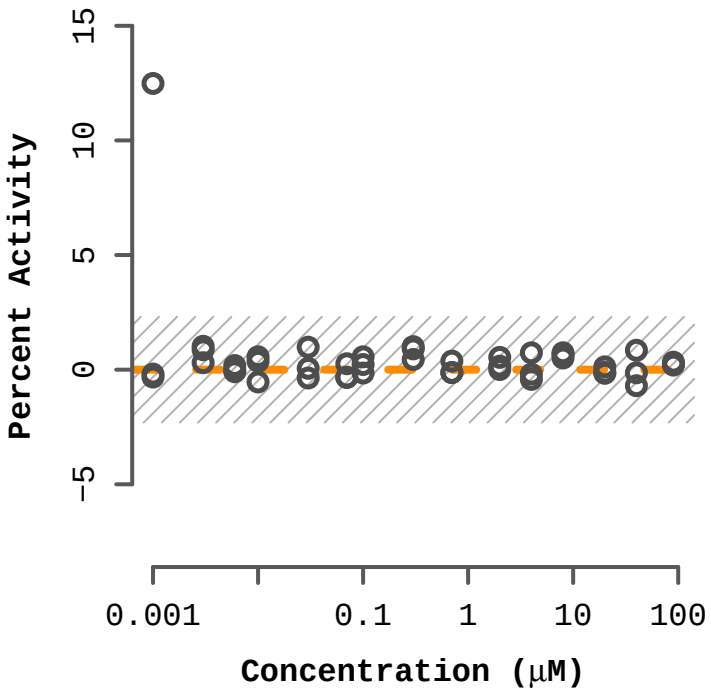
NAME: Famotidine
CHID: 23039 **CASRN:** 76824-35-6
SPID(S): Tox21_110153_1
M4ID: 12484604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.57 **MAX_MED:** 0.601 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

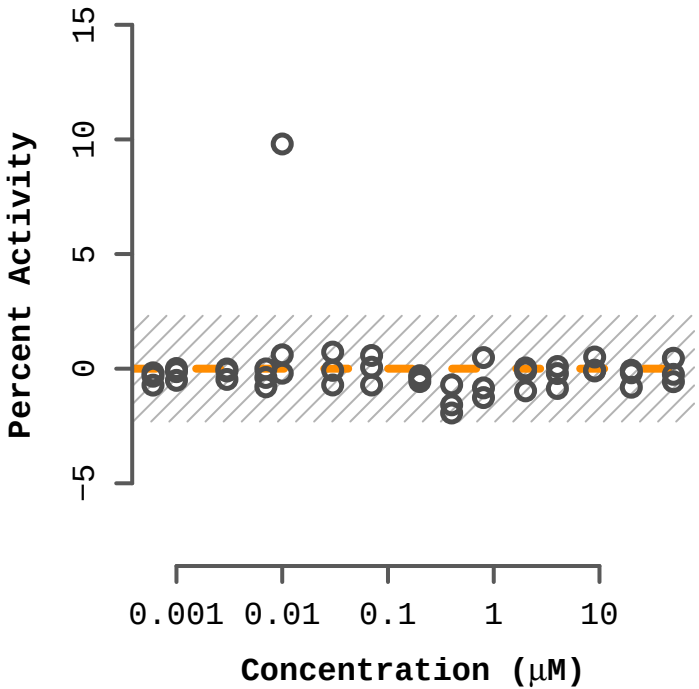
NAME: Felbamate
CHID: 23041 **CASRN:** 25451-15-4
SPID(S): Tox21_302368
M4ID: 12476765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 3.99 **MAX_MED:** 0.908 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

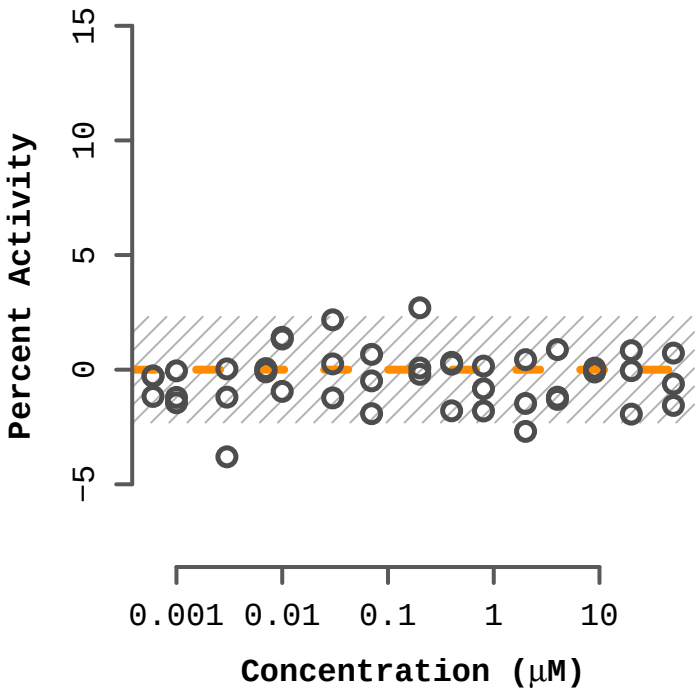
NAME: Felbamate
CHID: 23041 **CASRN:** 25451-15-4
SPID(S): Tox21_110145_1
M4ID: 12484611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 3.4 **MAX_MED:** 0.606 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

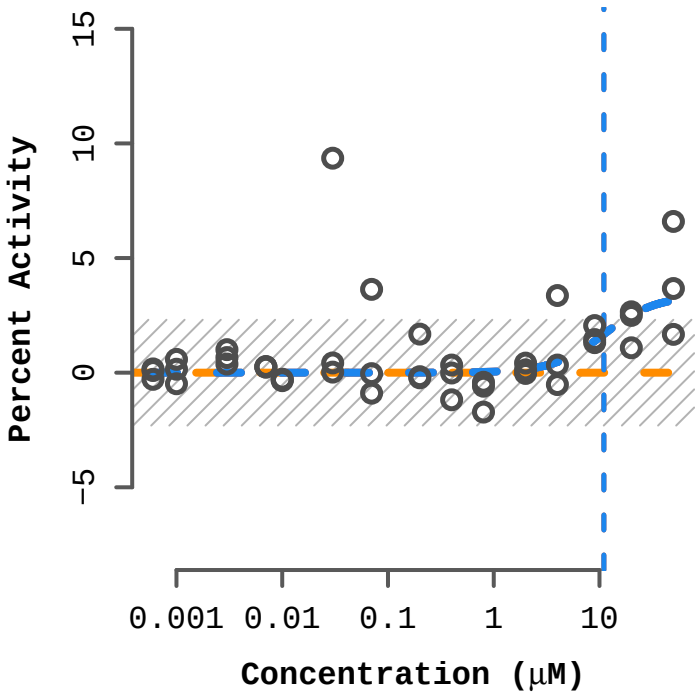
NAME: Felodipine
CHID: 23042 **CASRN:** 72509-76-3
SPID(S): Tox21_110155_1
M4ID: 12484602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenbufen
CHID: 23043 CASRN: 36330-85-5
SPID(S): Tox21_110638_1
M4ID: 12484214

HILL MODEL (in red):

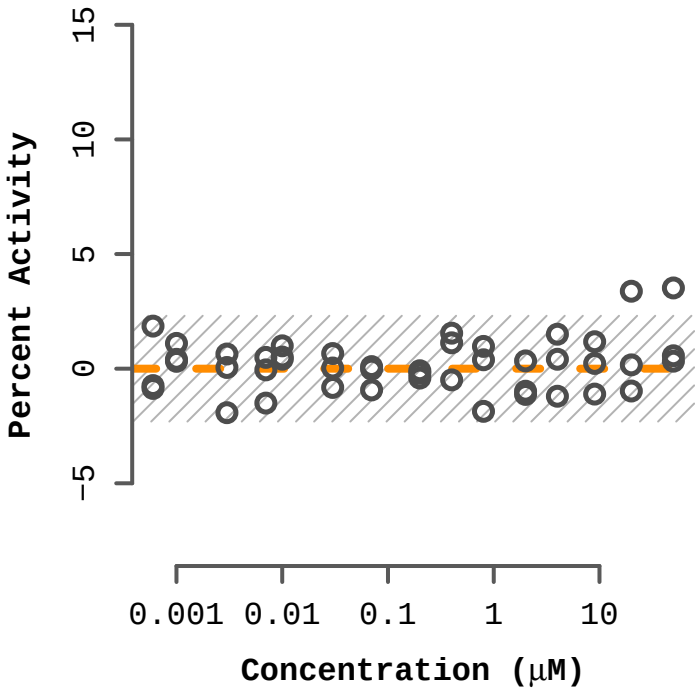
	tp	ga	gw
val:	3.36	1.04	1.8
sd:	1.57	0.322	1.09

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.36	1.04	1.8	2.61	8.97
sd:	1.57	0.322	1.09	1330	13000

	CNST	HILL	GNLS
AIC:	173.73	145.23	149.23
PROB:	0	0.88	0.12
RMSE:	2.14	1.76	1.76

MAX_MEAN: 3.98 MAX_MED: 3.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

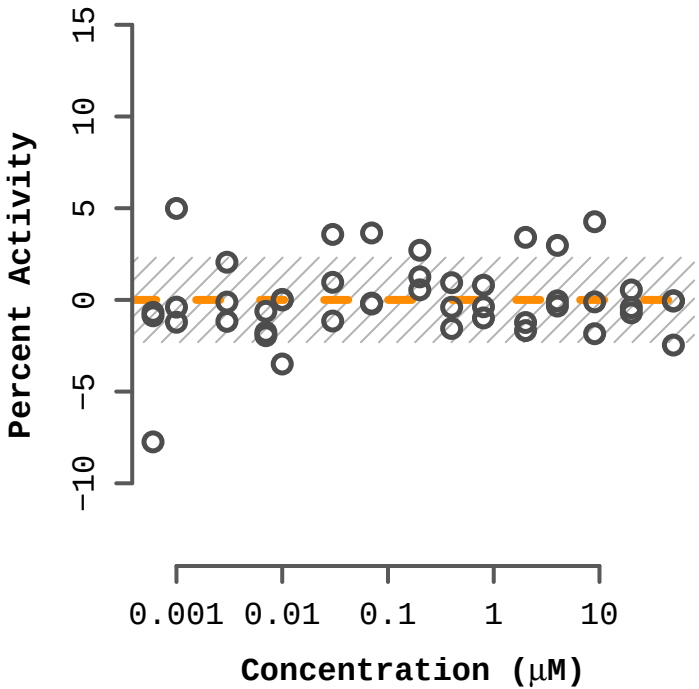
NAME: Fentiazac
CHID: 23050 CASRN: 18046-21-4
SPID(S): Tox21_111788_1
M4ID: 12483480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.47 MAX_MED: 1.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

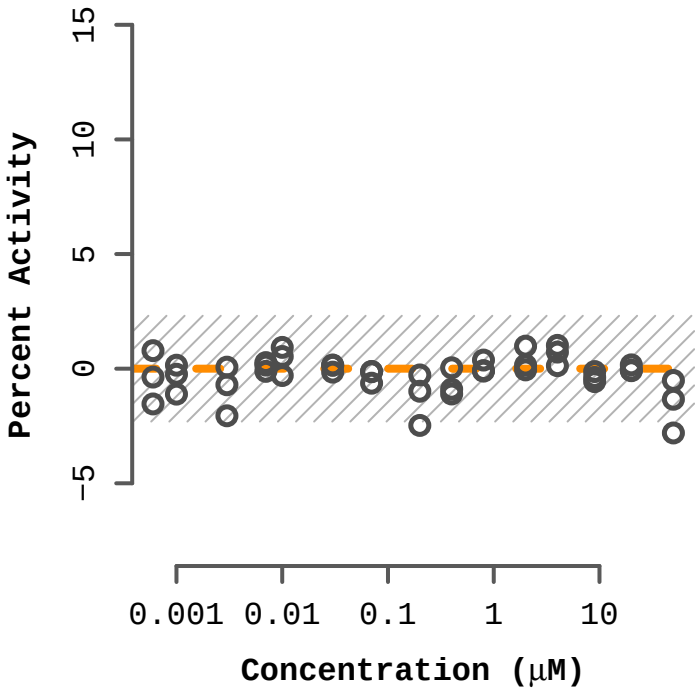
NAME: Feprazone
CHID: 23051 **CASRN:** 30748-29-9
SPID(S): Tox21_112208_1
M4ID: 12483235

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.27	NA	NA
PROB:	1	NA	NA
RMSE:	2.16	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

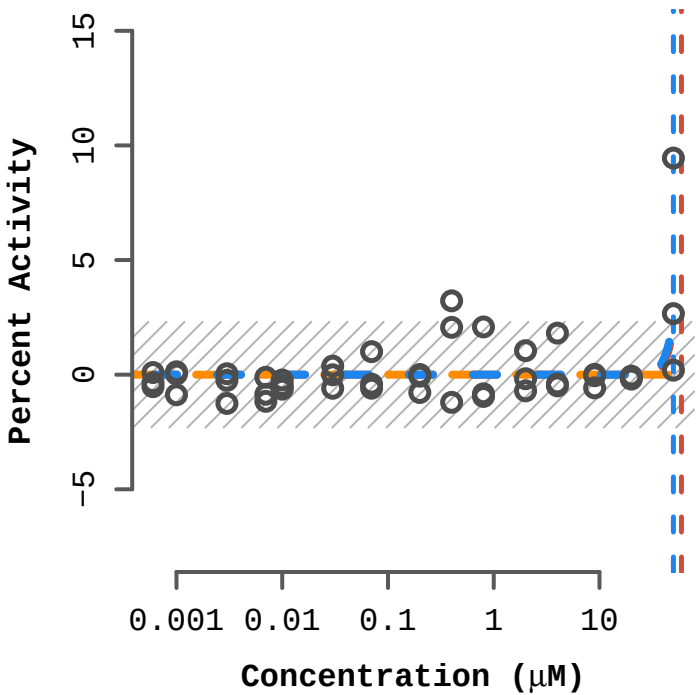
NAME: Flecainide
CHID: 23054 **CASRN:** 54143-55-4
SPID(S): Tox21_110151_1
M4ID: 12484606

HILL MODEL: Not applicable.

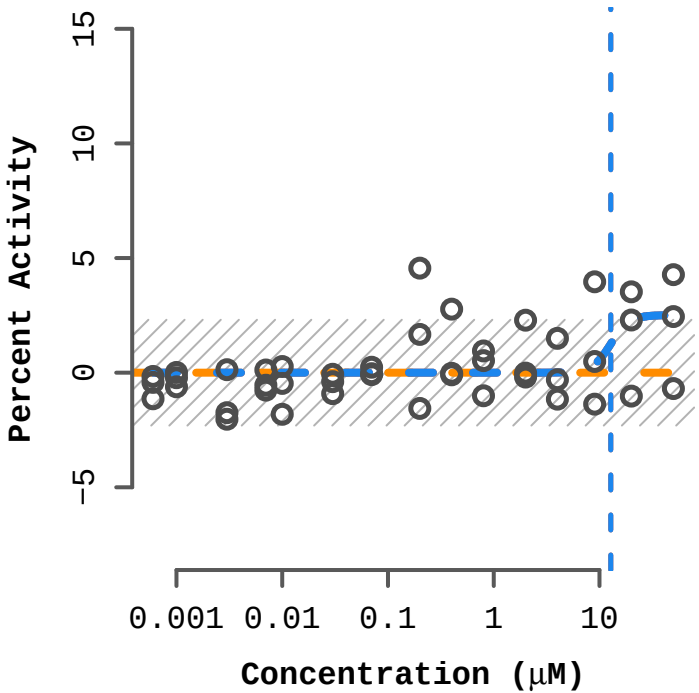
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

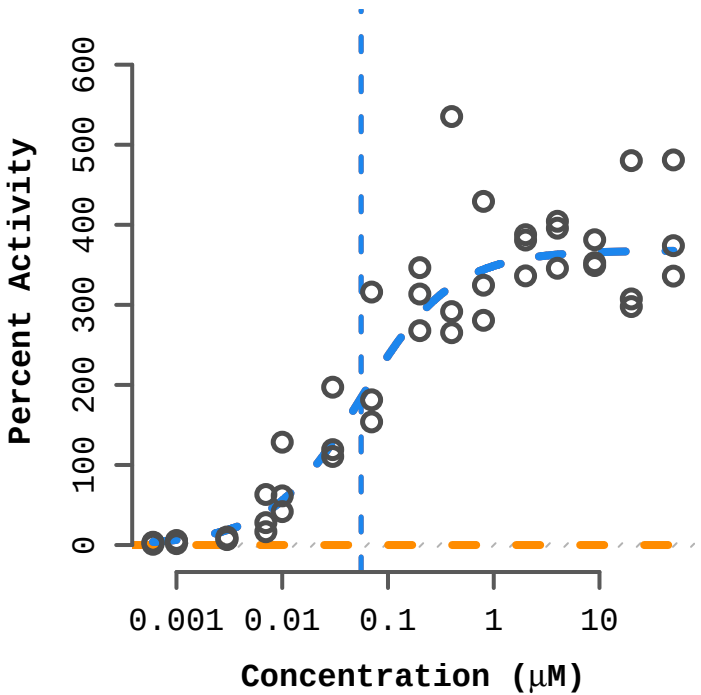
MAX_MEAN: 0.625 **MAX_MED:** 0.725 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Floxuridine
CHID:    23057   CASRN: 50-91-9
SPID(S): Tox21_110892_1
M4ID:    12484035

HILL MODEL (in red):
      tp       ga       gw
val:  11.2     1.78     8
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.44     1.7      8        3.67     1.23
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  139.66      141.45      145.45
PROB: 0.68        0.28        0.04
RMSE: 1.72        1.43        1.43

MAX_MEAN: 4.1       MAX_MED: 2.67      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Flucytosine
CHID:    23059   CASRN: 2022-85-7
SPID(S): Tox21_110515_1
M4ID:    12484302

HILL MODEL (in red):
      tp       ga       gw
val:  2.51     1.11     4.97
sd:   0.991    0.28     7.57

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.51     1.11     4.97     3.68     11.1
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  169.73      167.79      171.79
PROB: 0.25        0.66        0.09
RMSE: 1.64        1.5         1.5

MAX_MEAN: 2.01      MAX_MED: 2.45      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fludrocortisone
CHID: 23061 CASRN: 127-31-1
SPID(S): Tox21_113344_1
M4ID: 12482684

HILL MODEL (in red):

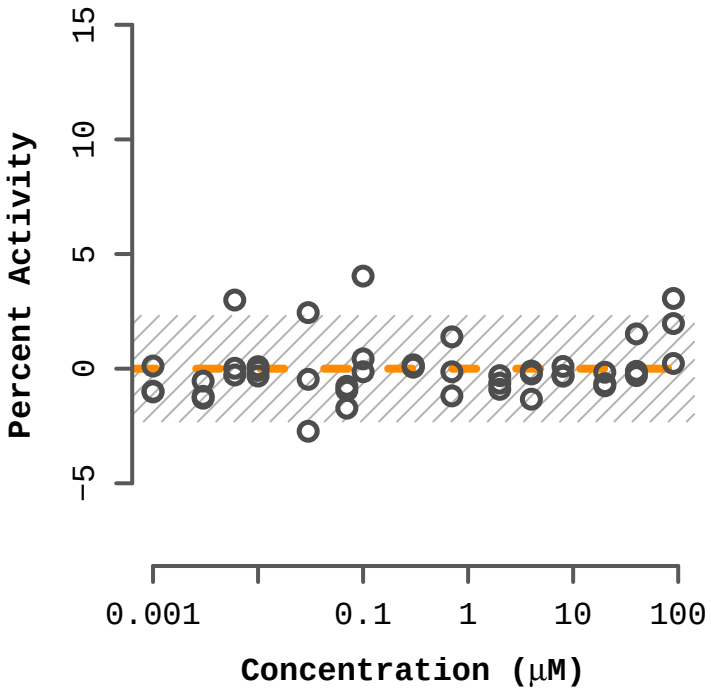
	tp	ga	gw
val:	368	-1.25	1
sd:	12.7	0.094	0.148

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	368	-1.25	1	2.17	15.9
sd:	12.7	0.094	0.148	207	6950

	CNST	HILL	GNLS
AIC:	642.49	486.37	490.37
PROB:	0	0.88	0.12
RMSE:	278.42	54.58	54.58

MAX_MEAN: 397 MAX_MED: 396 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

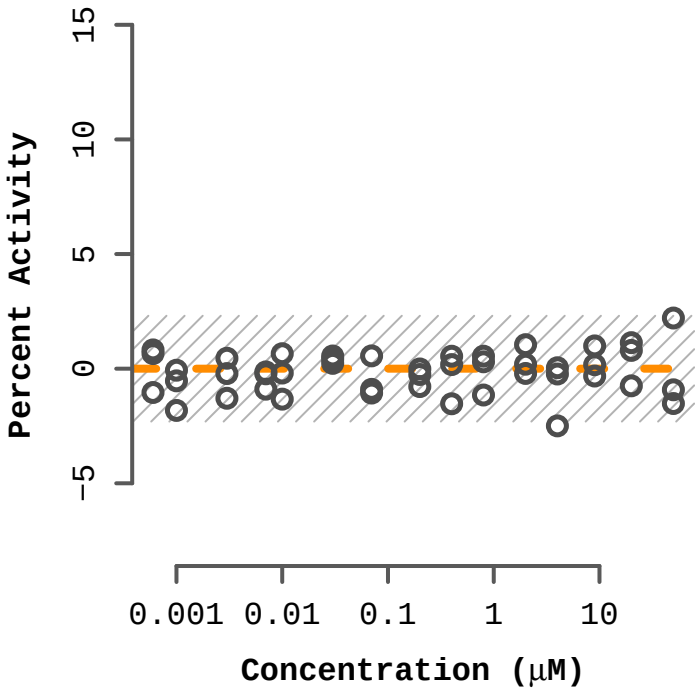
NAME: Flufenamic acid
CHID: 23063 CASRN: 530-78-9
SPID(S): Tox21_302111
M4ID: 12477022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.75 MAX_MED: 1.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

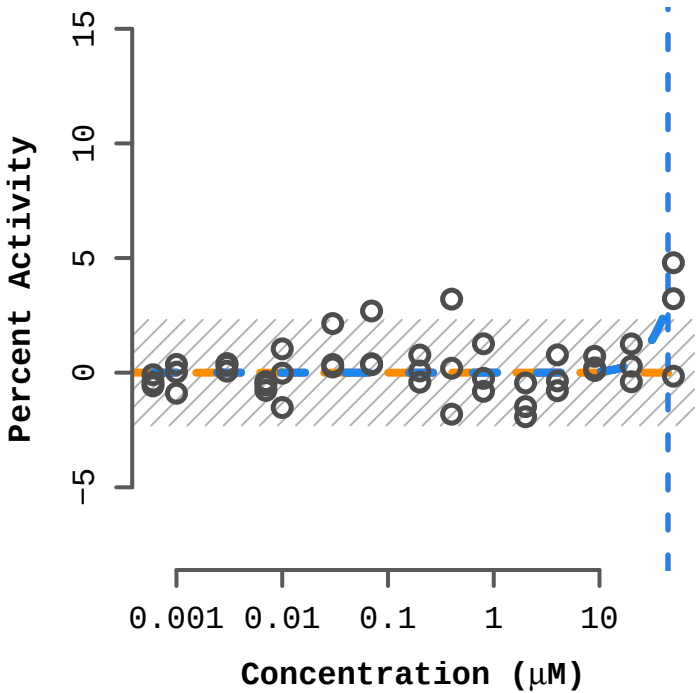
NAME: Flufenamic acid
CHID: 23063 **CASRN:** 530-78-9
SPID(S): Tox21_110452_1
M4ID: 12484344

HILL MODEL: Not applicable.

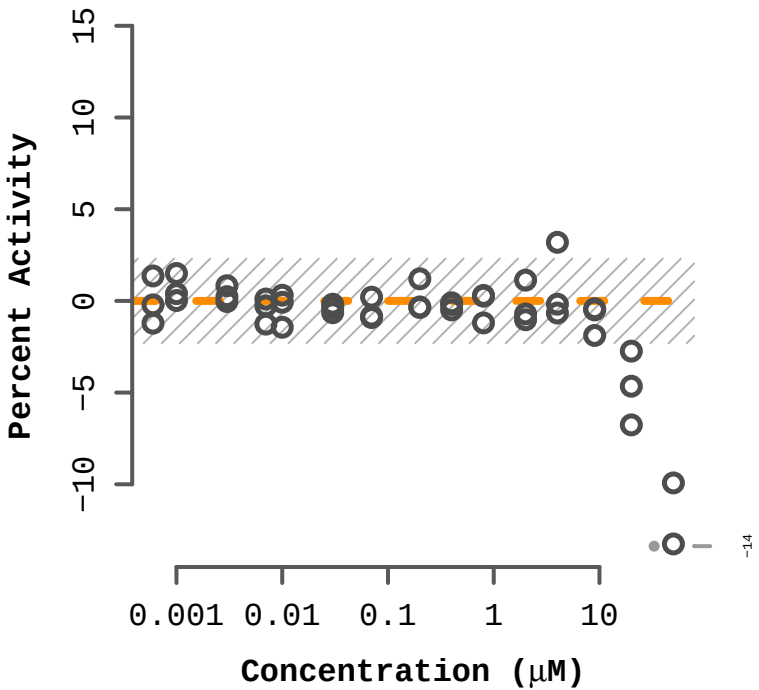
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.403 **MAX_MED:** 0.799 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Flumazenil
CHID:    23064   CASRN: 78755-81-4
SPID(S): Tox21_110148_1
M4ID:    12484608

HILL MODEL (in red):
      tp       ga       gw
val:  5.76     1.65     3.18
sd:   14.7     0.789    4.53

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.76     1.65     3.18     3.68     3.36
sd:   14.8     0.794    4.55     2450     4200

      CNST        HILL        GNLS
AIC:  143.93      141.56      145.56
PROB: 0.21        0.69        0.09
RMSE: 1.32        1.15        1.15

MAX_MEAN: 2.62      MAX_MED: 3.23      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

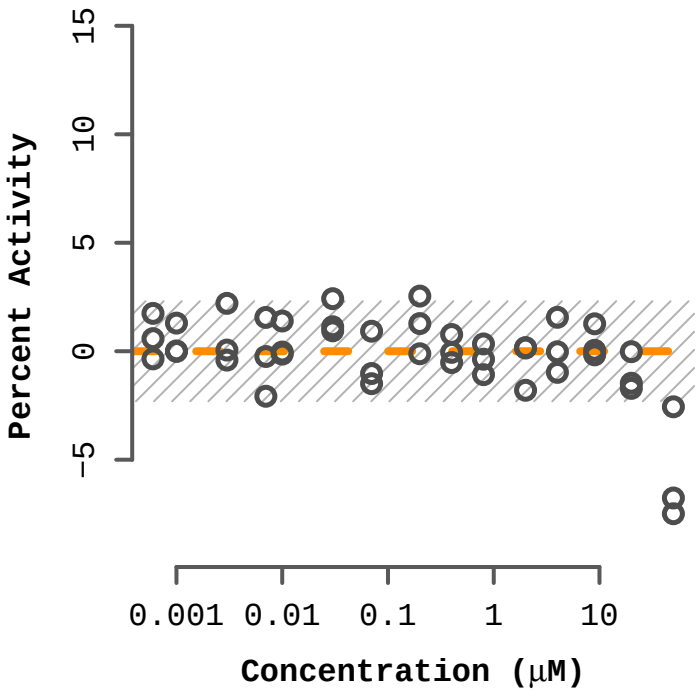
NAME: (+/−) −Fluoxetine
CHID: 23067 CASRN: 54910−89−3
SPID(S): Tox21_110144_1
M4ID: 12484612 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.58	NA	NA

MAX_MEAN: 0.787 **MAX_MED:** 0.398 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

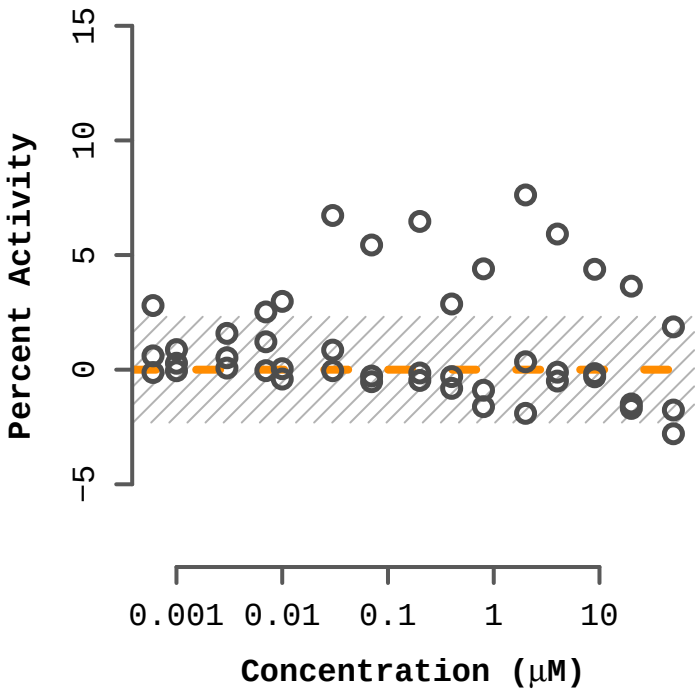
NAME: Fluphenazine
CHID: 23068 **CASRN:** 69-23-8
SPID(S): Tox21_110146_1
M4ID: 12484610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.91	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

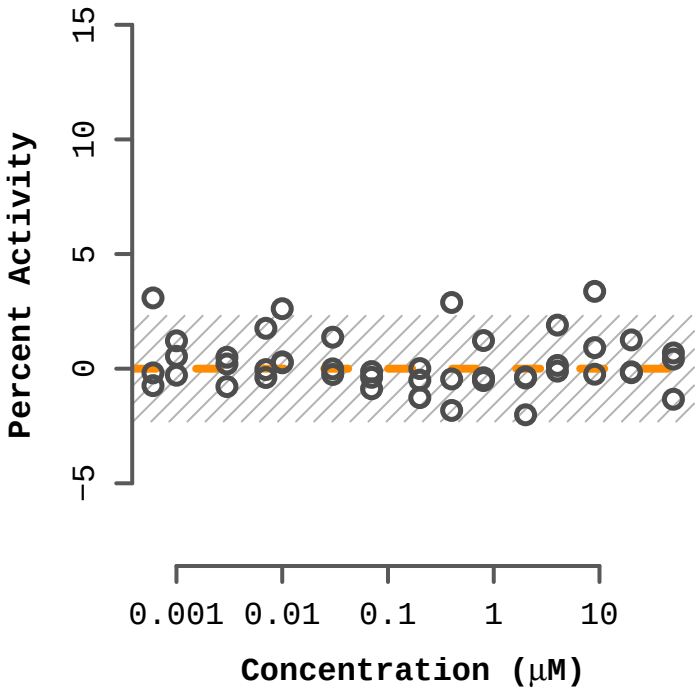
NAME: Flurazepam
CHID: 23071 **CASRN:** 17617-23-1
SPID(S): Tox21_112201_1
M4ID: 12483241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.85	NA	NA
PROB:	1	NA	NA
RMSE:	2.7	NA	NA

MAX_MEAN: 2.51 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

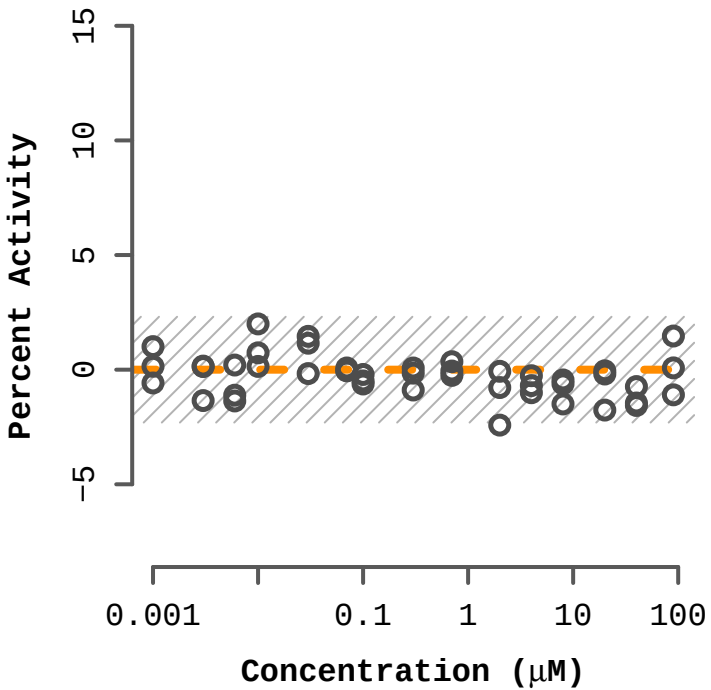
NAME: Foscarnet trisodium
CHID: 23078 **CASRN:** 63585-09-1
SPID(S): Tox21_111364_1
M4ID: 12483737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

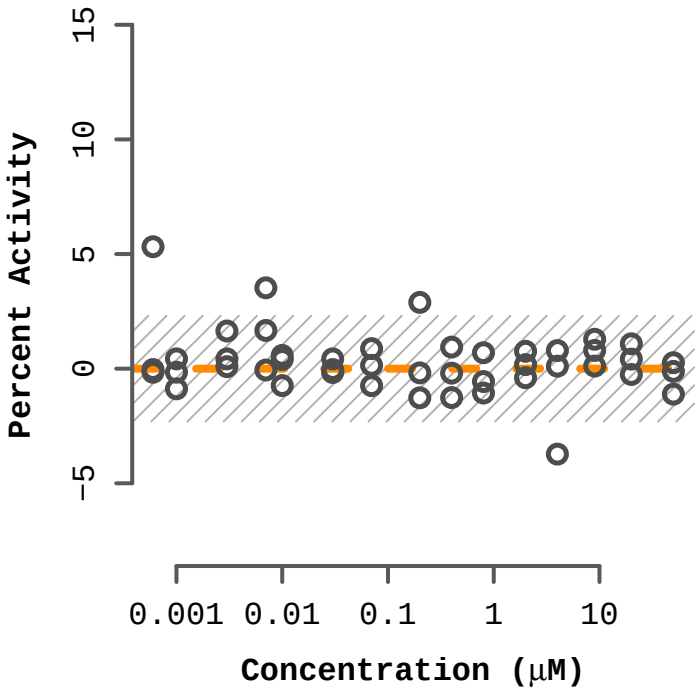
NAME: D-Fructose
CHID: 23081 CASRN: 57-48-7
SPID(S): Tox21_200762
M4ID: 12481490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.959 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

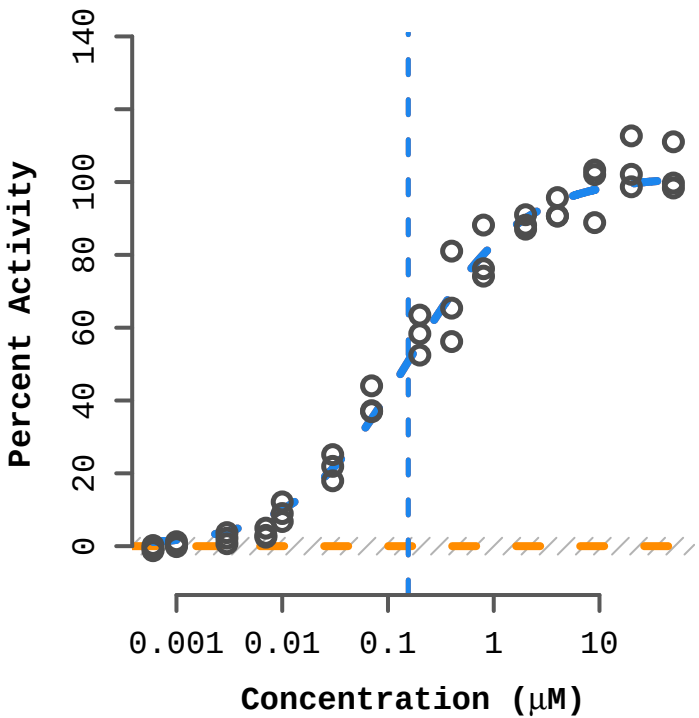
NAME: Gallamine triethiodide
CHID: 23089 **CASRN:** 65-29-2
SPID(S): Tox21_112040_1
M4ID: 12483354

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Gestrinone
CHID: 23094 CASRN: 16320-04-0
SPID(S): Tox21_112461_1
M4ID: 12483087

HILL MODEL (in red):

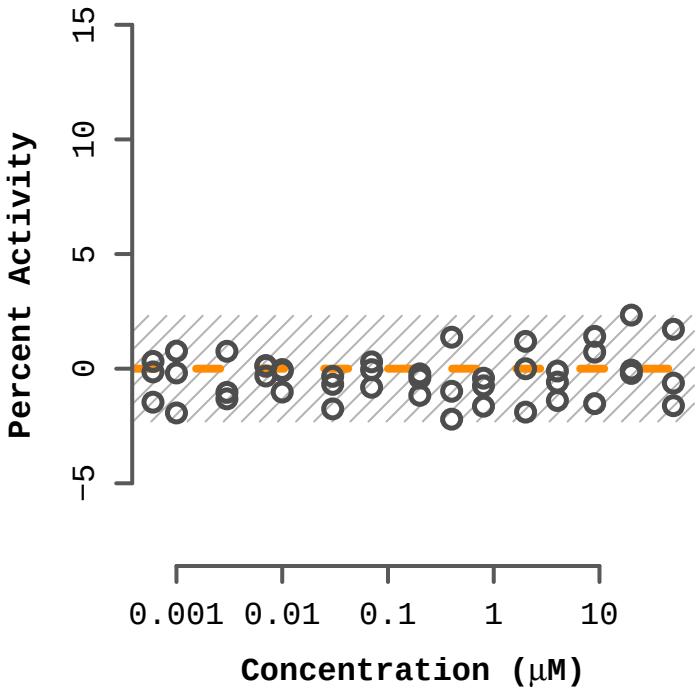
	tp	ga	gw
val:	102	-0.808	0.806
sd:	2.06	0.054	0.0519

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	102	-0.808	0.806	3.1	17.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	511.61	282.48	286.48
PROB:	0	0.88	0.12
RMSE:	65.46	5.17	5.17

MAX_MEAN: 105 MAX_MED: 102 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

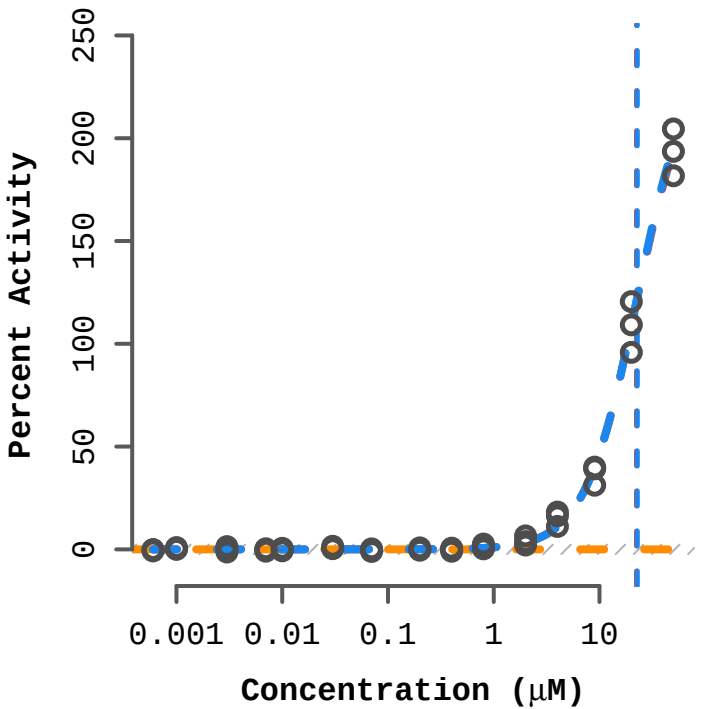
NAME: Gliclazide
CHID: 23095 CASRN: 21187-98-4
SPID(S): Tox21_110590_1
M4ID: 12484245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.691 **MAX_MED:** 0.722 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Gliquidone
CHID: 23096 CASRN: 33342-05-1
SPID(S): Tox21_110629_1
M4ID: 12484220

HILL MODEL (in red):

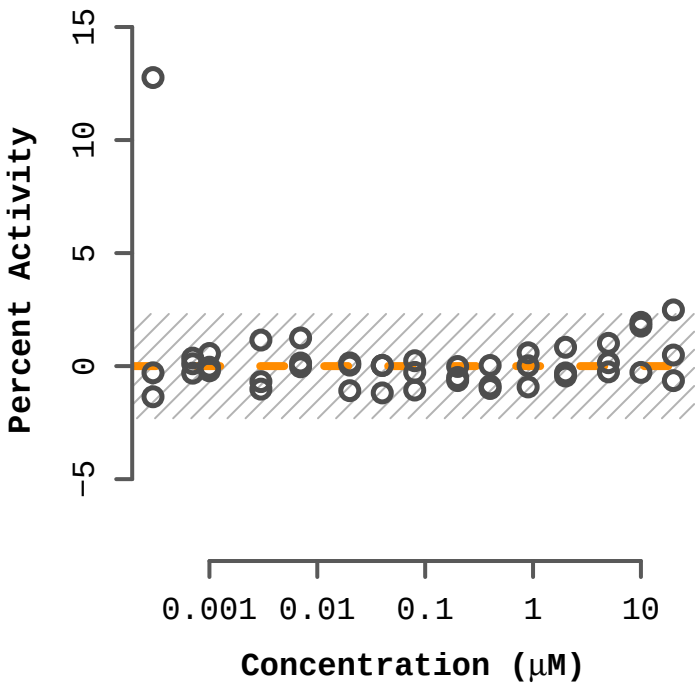
	tp	ga	gw
val:	241	1.35	1.76
sd:	2.53	0.00765	0.0261

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	245	1.36	1.76	1.8	17.9
sd:	9.98	0.0244	0.0342	0.0506	9.12

	CNST	HILL	GNLS
AIC:	446.59	230.97	234.55
PROB:	0	0.86	0.14
RMSE:	58.3	4.1	4.09

MAX_MEAN: 193 **MAX_MED:** 194 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

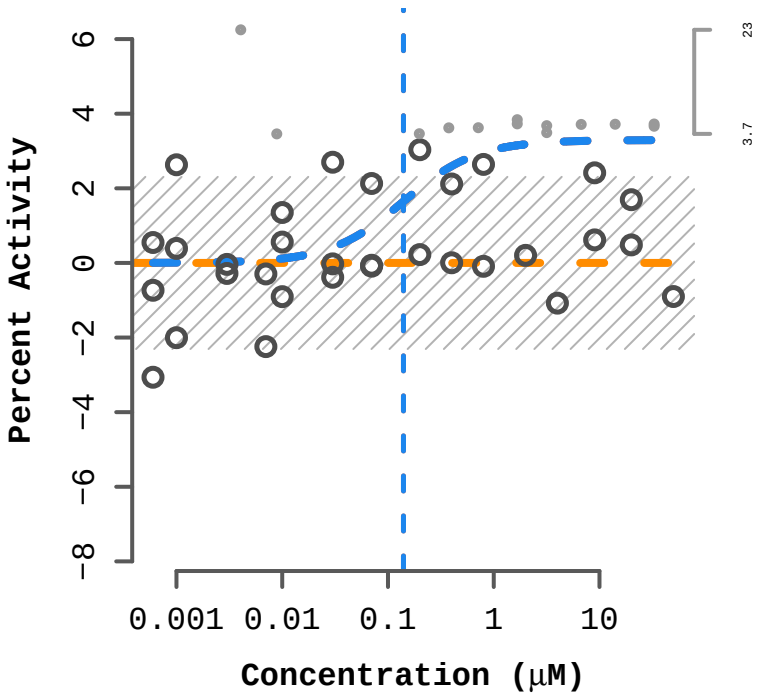
NAME: Glutathione
CHID: 23101 **CASRN:** 70-18-8
SPID(S): Tox21_111371_1
M4ID: 12483733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 3.71 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glutethimide
CHID: 23102 **CASRN:** 77-21-4
SPID(S): Tox21_111641_1
M4ID: 12483566 **BRK**

HILL MODEL (in red):

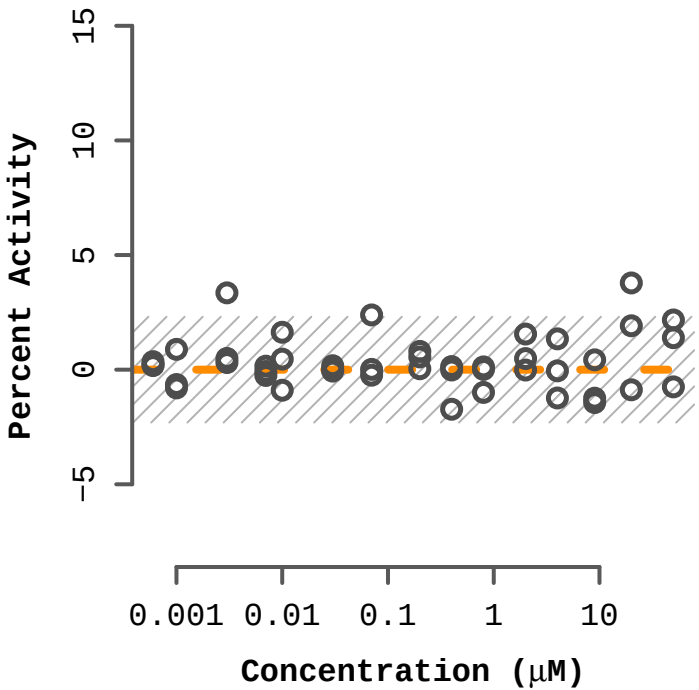
	tp	ga	gw
val:	3.29	−0.853	1.25
sd:	0.78	0.403	1.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.29	−0.853	1.25	3.23	5.04
sd:	0.78	0.403	1.23	1610	5350

	CNST	HILL	GNLS
AIC:	242.77	223.15	227.15
PROB:	0	0.88	0.12
RMSE:	4.52	4.01	4.01

MAX_MEAN: 7.64 **MAX_MED:** 5.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

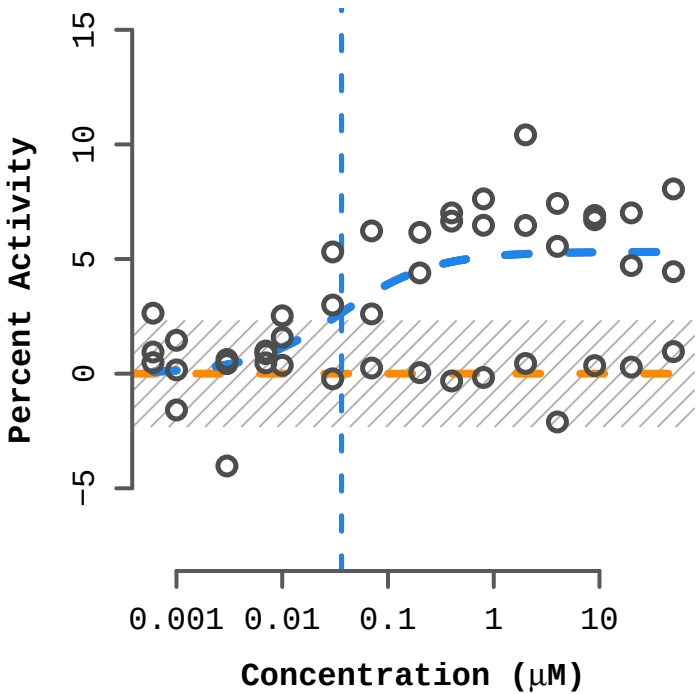
NAME: Glybuzole
CHID: 23103 **CASRN:** 1492-02-0
SPID(S): Tox21_113322
M4ID: 12482705

HILL MODEL: Not applicable.

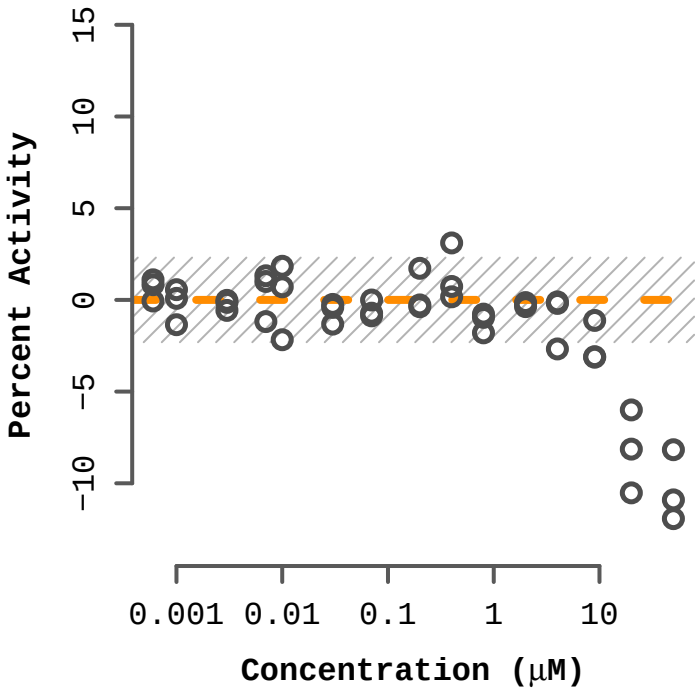
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.92 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Glycopyrrolate bromide
CHID:    23109   CASRN: 596-51-0
SPID(S): Tox21_113144_1
M4ID:    12482791

HILL MODEL (in red):
      tp       ga       gw
val:  5.32     -1.44    1.01
sd:   0.793    0.347    0.527

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.32     -1.44    1.01     3.42     5.02
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  265.36      230.23      234.23
PROB: 0           0.88        0.12
RMSE: 4.39        2.82        2.82

MAX_MEAN: 5.78      MAX_MED: 6.72      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

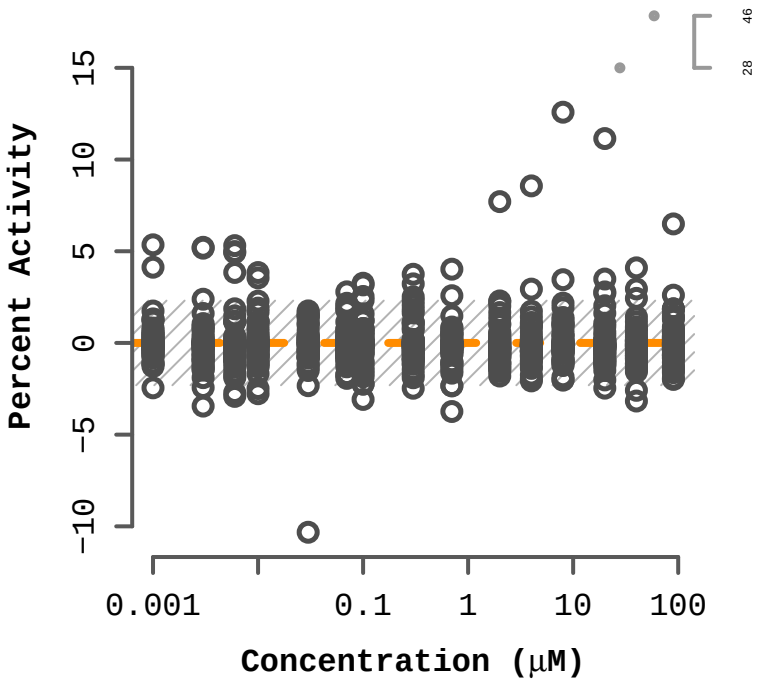
NAME: Gossypol
CHID: 23110 **CASRN:** 303-45-7
SPID(S): Tox21_110434_1
M4ID: 12484360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.52	NA	NA
PROB:	1	NA	NA
RMSE:	3.67	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

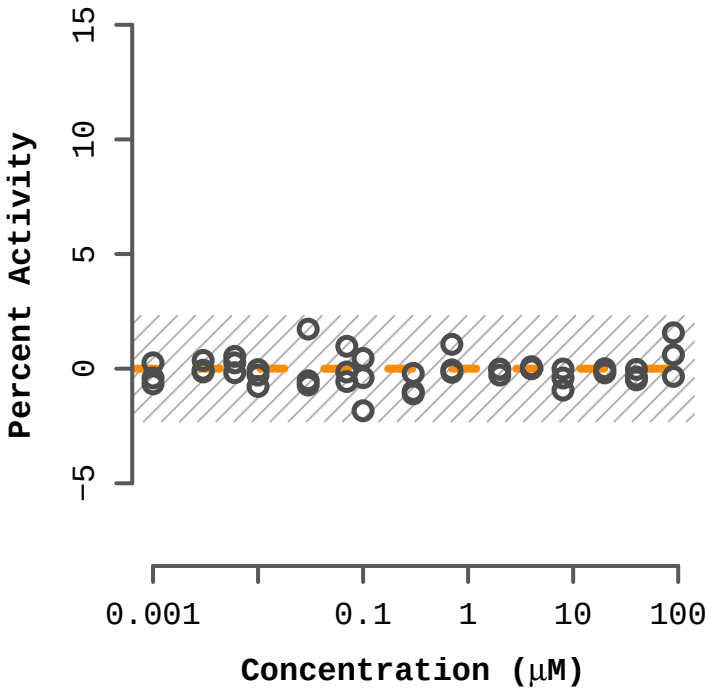
NAME: 2-Methoxyphenol
CHID: 23113 **CASRN:** 90-05-1
SPID(S): Tox21_400004
M4ID: 12475133 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2287.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.00905 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

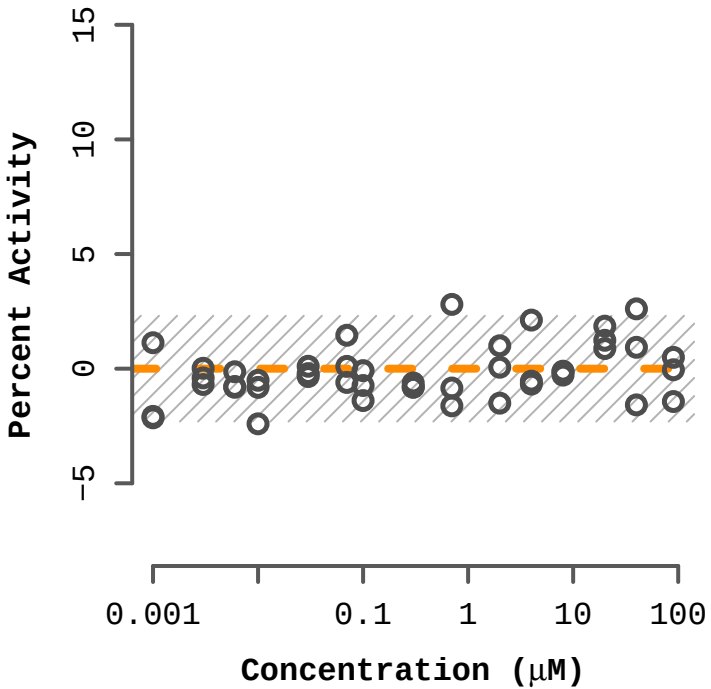
NAME: 2-Methoxyphenol
CHID: 23113 CASRN: 90-05-1
SPID(S): Tox21_202990
M4ID: 12479262

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	85.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.612 MAX_MED: 0.606 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

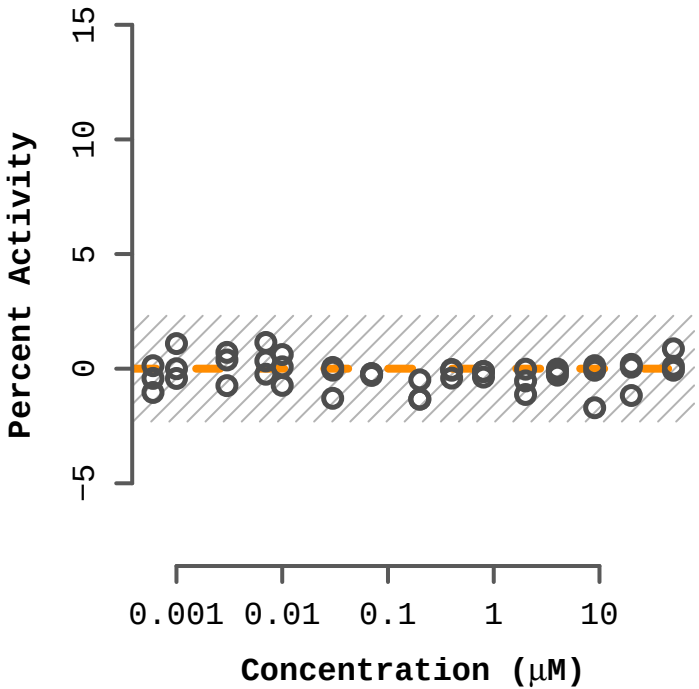
NAME: Guaifenesin
CHID: 23114 **CASRN:** 93-14-1
SPID(S): Tox21_302094
M4ID: 12477039

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

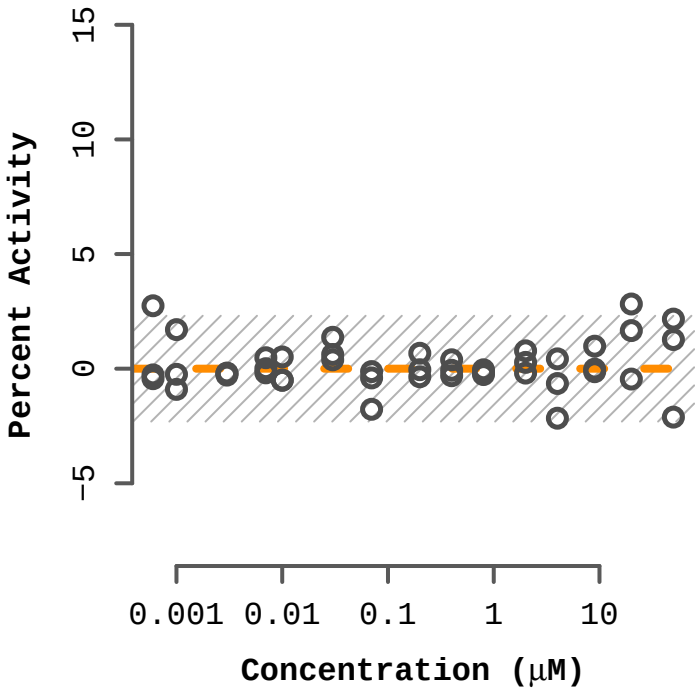
NAME: Guaifenesin
CHID: 23114 **CASRN:** 93-14-1
SPID(S): Tox21_110389_1
M4ID: 12484402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.415 **MAX_MED:** 0.381 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

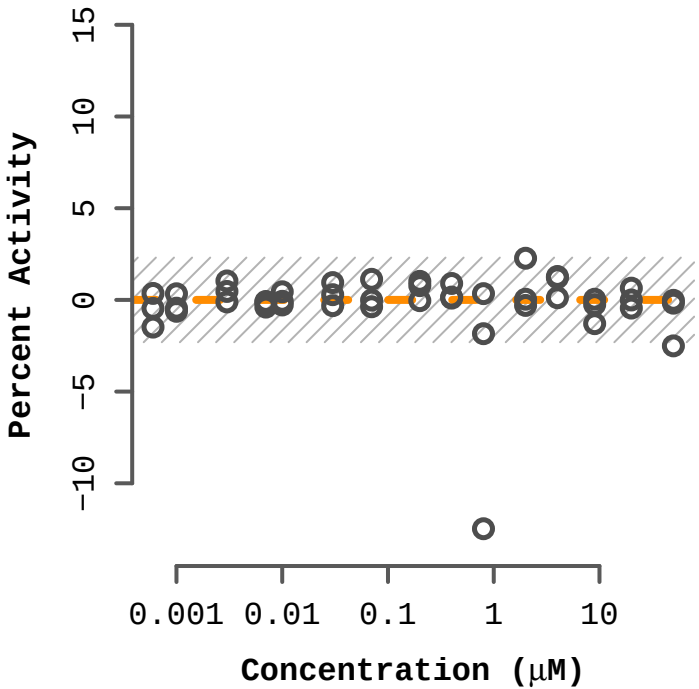
NAME: Hexobarbital
CHID: 23122 **CASRN:** 56-29-1
SPID(S): Tox21_111661_1
M4ID: 12483549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

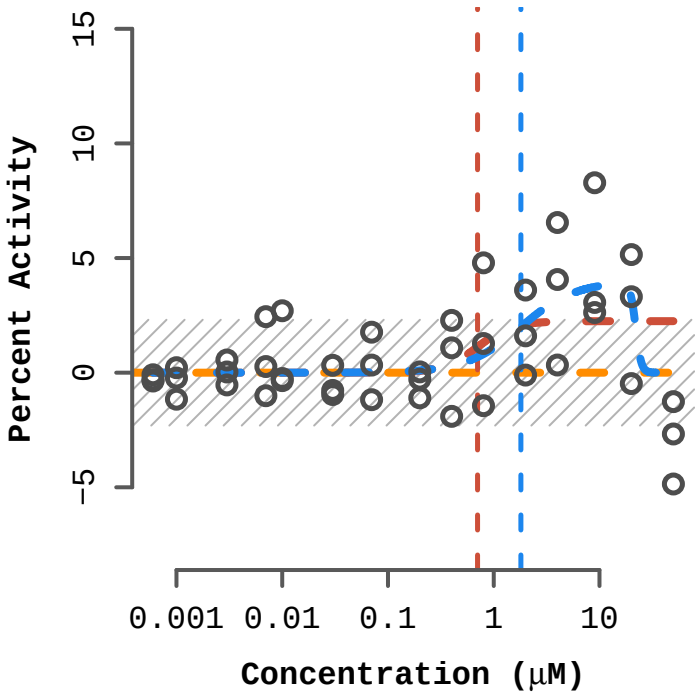
NAME: Histamine
CHID: 23125 **CASRN:** 51-45-6
SPID(S): Tox21_110166_1
M4ID: 12484591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.18	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 0.87 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hycanthone
CHID: 23128 **CASRN:** 3105-97-3
SPID(S): Tox21_110531_1
M4ID: 12484288

HILL MODEL (in red):

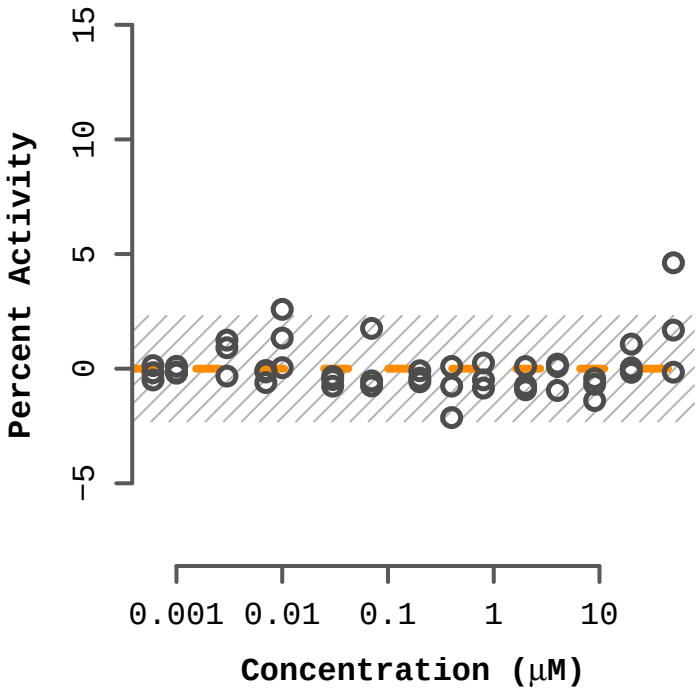
	tp	ga	gw
val:	2.25	−0.153	2.66
sd:	0.802	0.441	3.22

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.99	0.257	1.68	1.34	16.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	207.69	203.49	194.24
PROB:	0	0.01	0.99
RMSE:	2.54	2.25	1.86

MAX_MEAN: 4.66 **MAX_MED:** 4.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

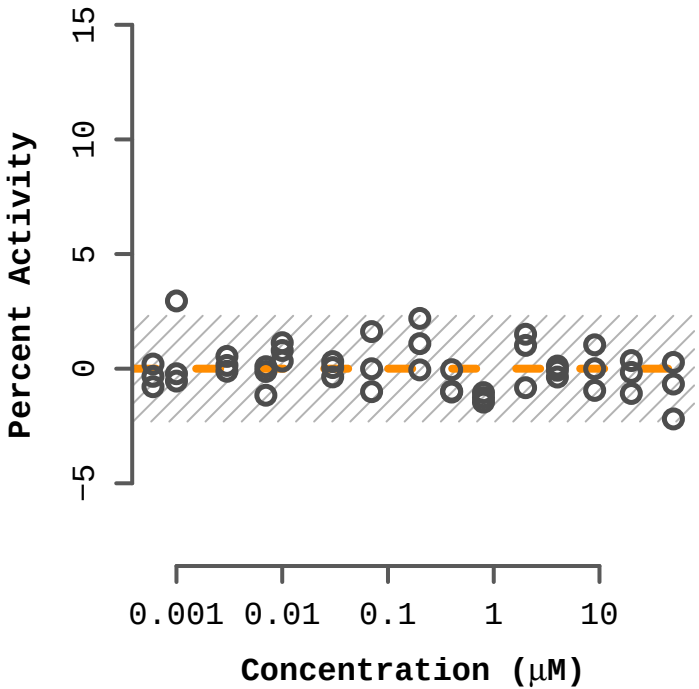
NAME: Hydroflumethiazide
CHID: 23132 **CASRN:** 135-09-1
SPID(S): Tox21_110422_1
M4ID: 12484372

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

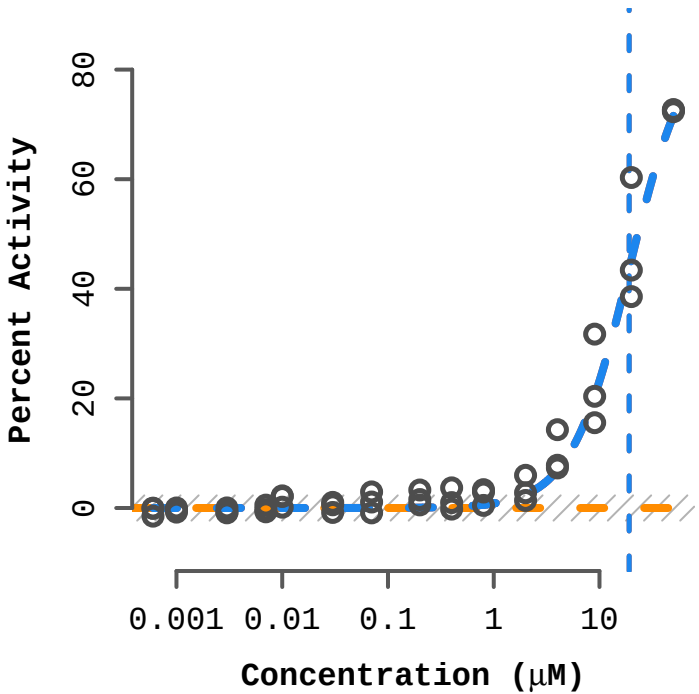
NAME: Hydroxyzine
CHID: 23137 **CASRN:** 68-88-2
SPID(S): Tox21_113569_1
M4ID: 12482606

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ibuprofen piconol
CHID: 23140 CASRN: 64622-45-3
SPID(S): Tox21_113700
M4ID: 12482514

HILL MODEL (in red):

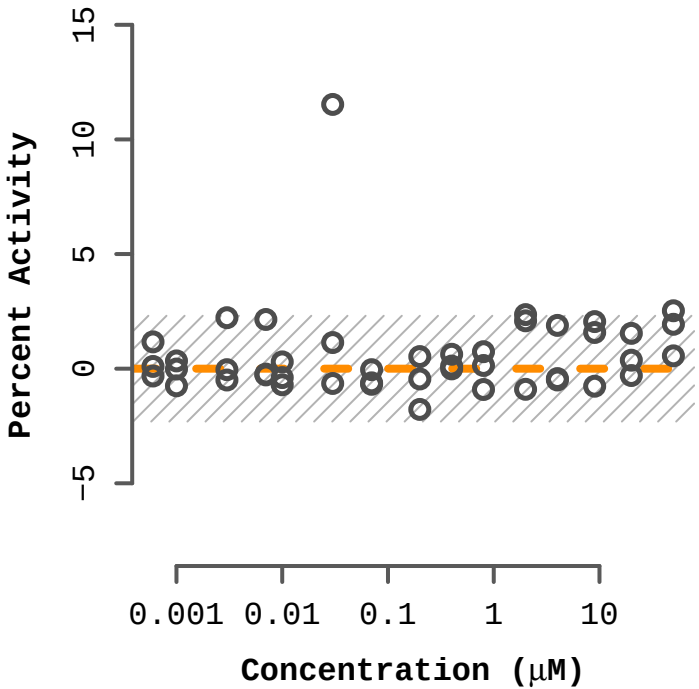
	tp	ga	gw
val:	87.3	1.28	1.57
sd:	4.94	0.05	0.127

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	87.3	1.28	1.57	2.74	11.3
sd:	4.94	0.05	0.127	8990	97300

	CNST	HILL	GNLS
AIC:	380.56	223.5	227.5
PROB:	0	0.88	0.12
RMSE:	23.52	3.54	3.54

MAX_MEAN: 72.5 **MAX_MED:** 72.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

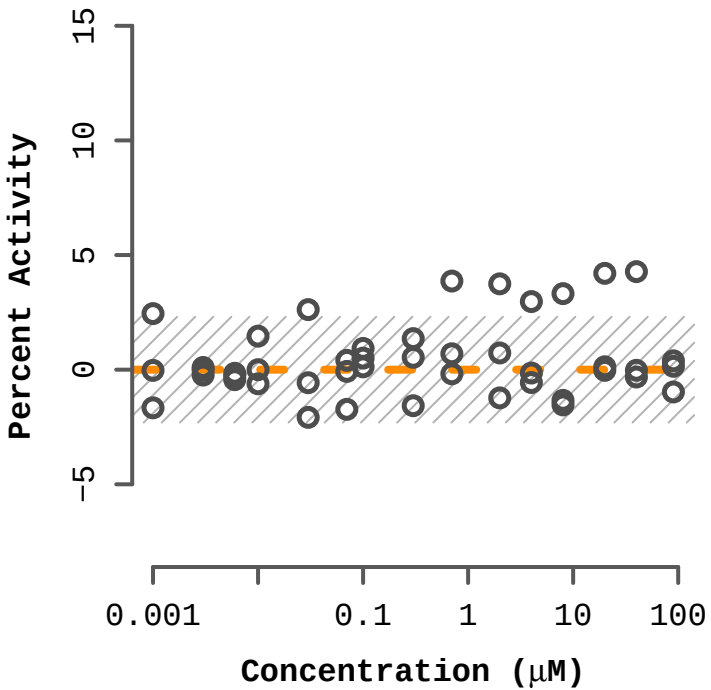
NAME: Imipenem
CHID: 23143 CASRN: 64221-86-9
SPID(S): Tox21_110689_1
M4ID: 12484177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 4.01 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

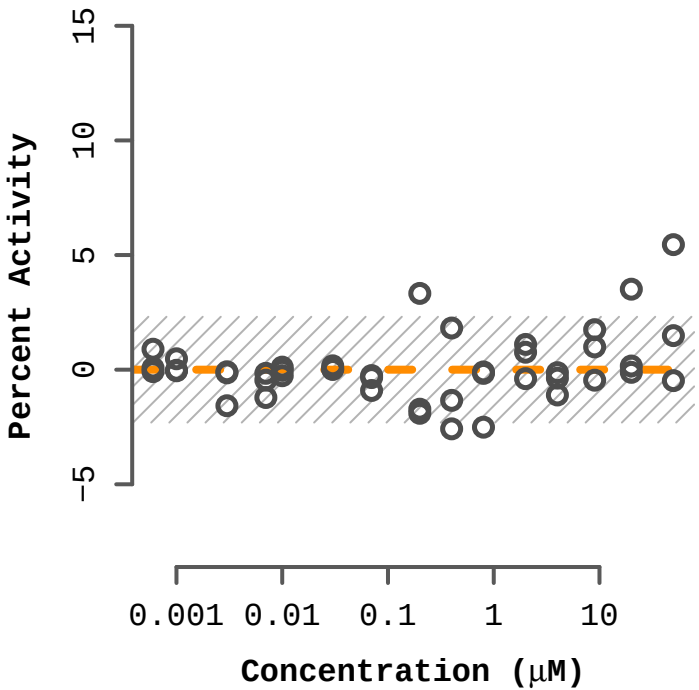
NAME: myo-Inositol
CHID: 23146 **CASRN:** 87-89-8
SPID(S): Tox21_302035
M4ID: 12477098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 0.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

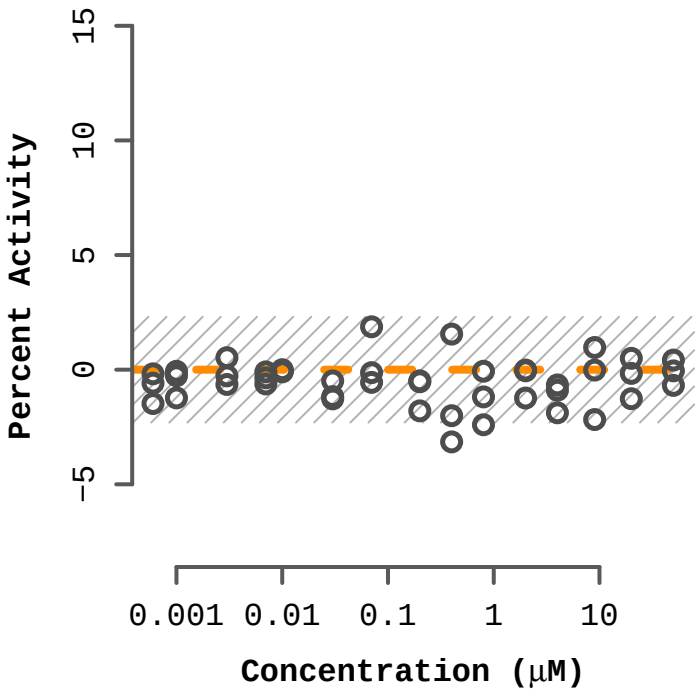
NAME: myo-Inositol
CHID: 23146 **CASRN:** 87-89-8
SPID(S): Tox21_111642_1
M4ID: 12483565

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

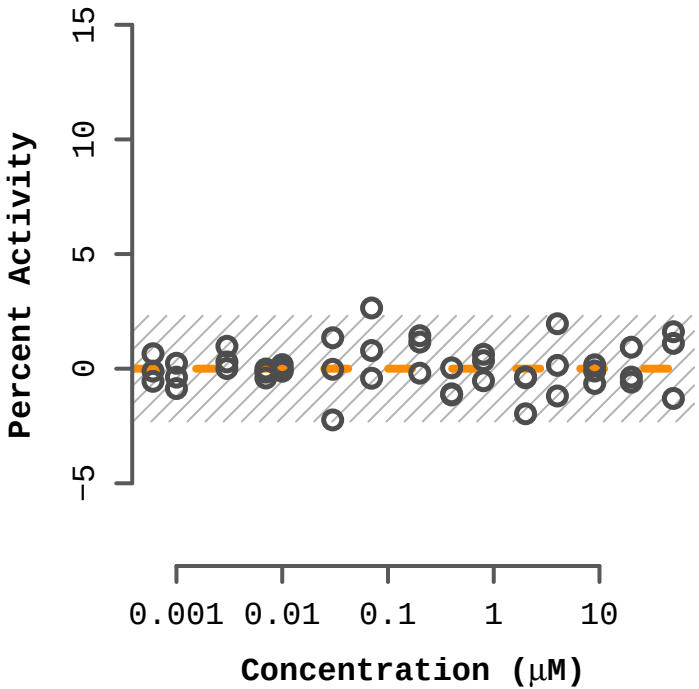
NAME: Iocarmic acid
CHID: 23148 **CASRN:** 10397-75-8
SPID(S): Tox21_113712
M4ID: 12482502

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.397 **MAX_MED:** −0.0172 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

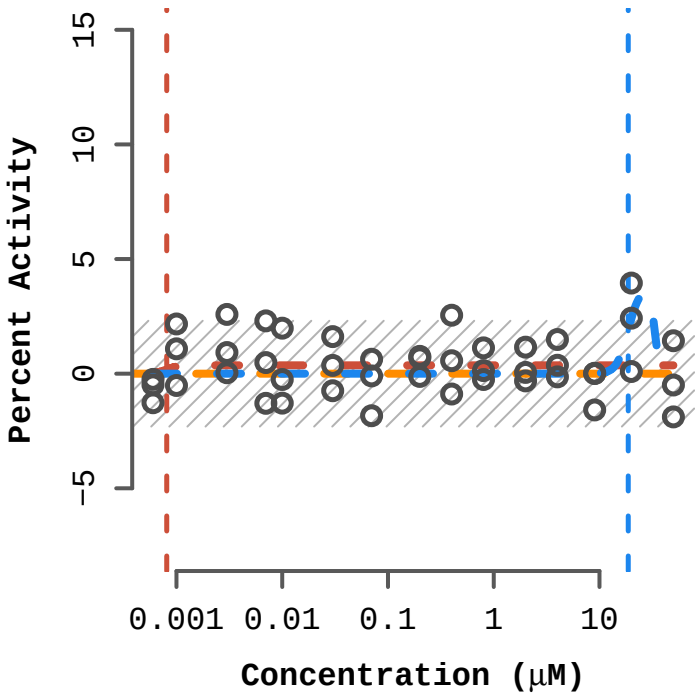
NAME: Iodamide
CHID: 23150 CASRN: 440-58-4
SPID(S): Tox21_111346_1
M4ID: 12483750

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.01 MAX_MED: 1.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iodipamide
CHID: 23153 **CASRN:** 606-17-7
SPID(S): Tox21_113504_1
M4ID: 12482625

HILL MODEL (in red):

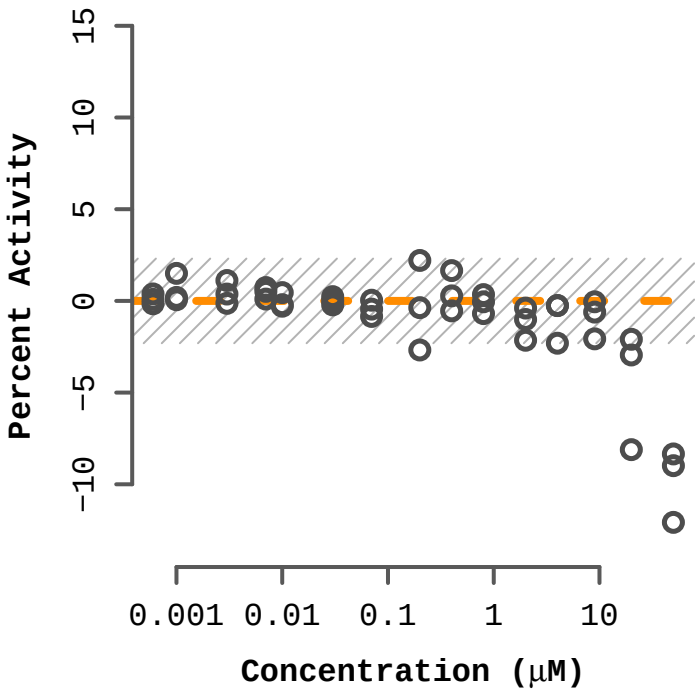
	tp	ga	gw
val:	0.363	−3.09	8
sd:	0.194	0.184	13.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.79	1.27	8	1.52	17.9
sd:	16.4	0.602	14	1.17	118

	CNST	HILL	GNLS
AIC:	155.23	157.61	159.47
PROB:	0.7	0.21	0.08
RMSE:	1.33	1.26	1.21

MAX_MEAN: 2.16 **MAX_MED:** 2.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

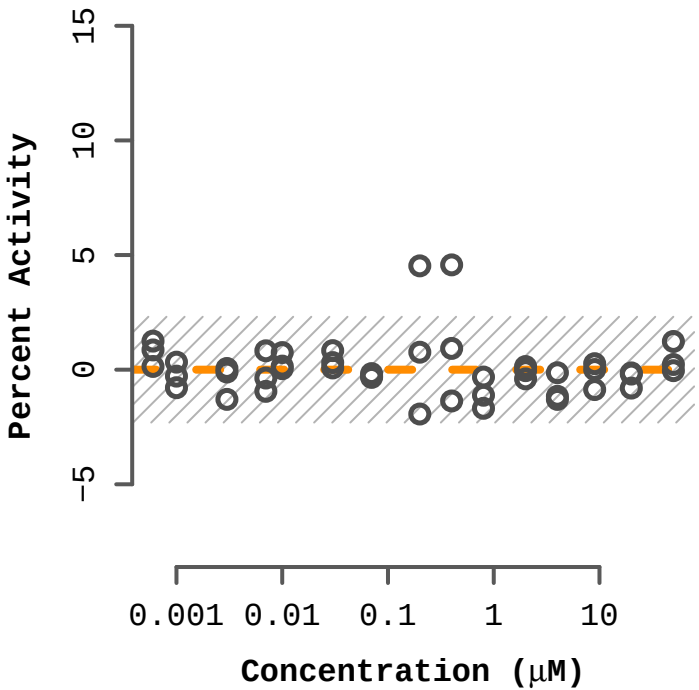
NAME: Iodoquinol
CHID: 23155 **CASRN:** 83-73-8
SPID(S): Tox21_110823_1
M4ID: 12484093

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.03	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.522 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

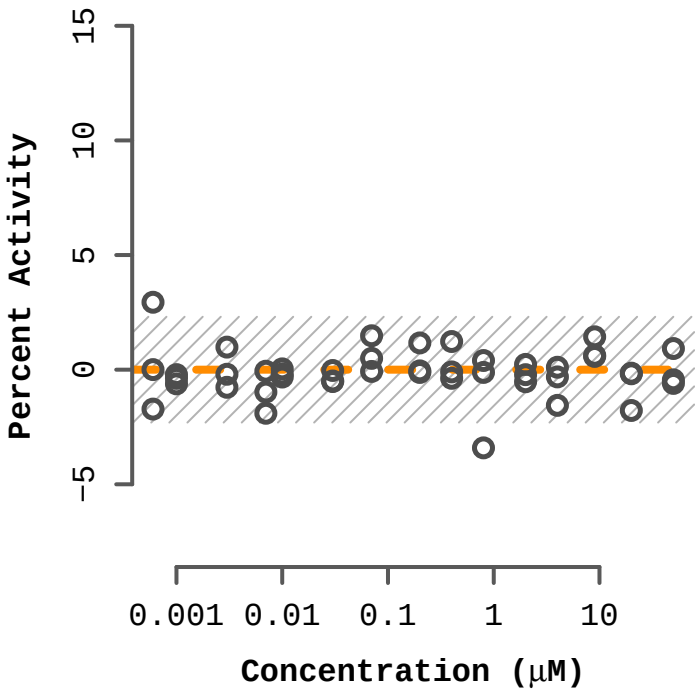
NAME: Iohexol
CHID: 23157 **CASRN:** 66108-95-0
SPID(S): Tox21_112286_1
M4ID: 12483181

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 0.929 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

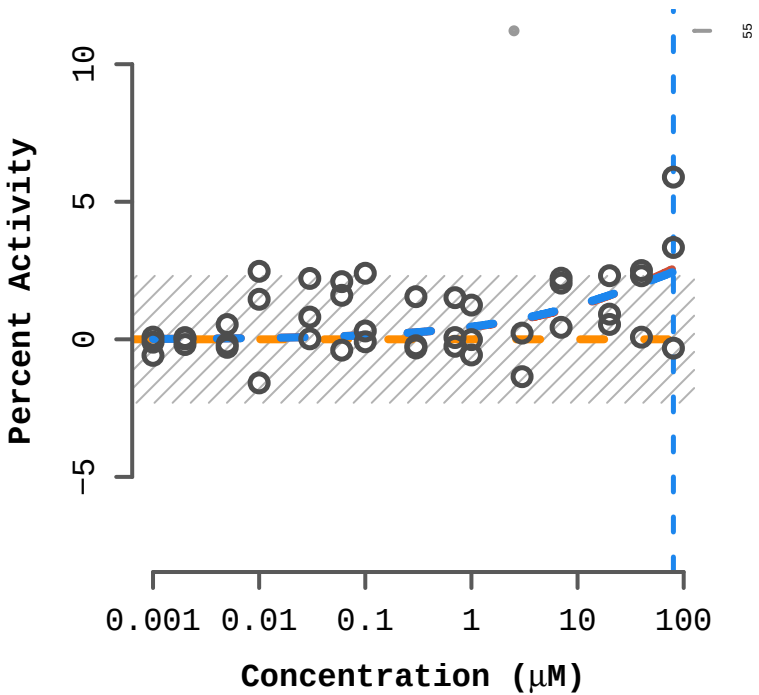
NAME: Iopamidol
CHID: 23158 **CASRN:** 60166-93-0
SPID(S): Tox21_110668_1
M4ID: 12484191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 0.628 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iopanoic acid
CHID: 23159 **CASRN:** 96-83-3
SPID(S): Tox21_303477
M4ID: 12475663 **BRK**

HILL MODEL (in red):

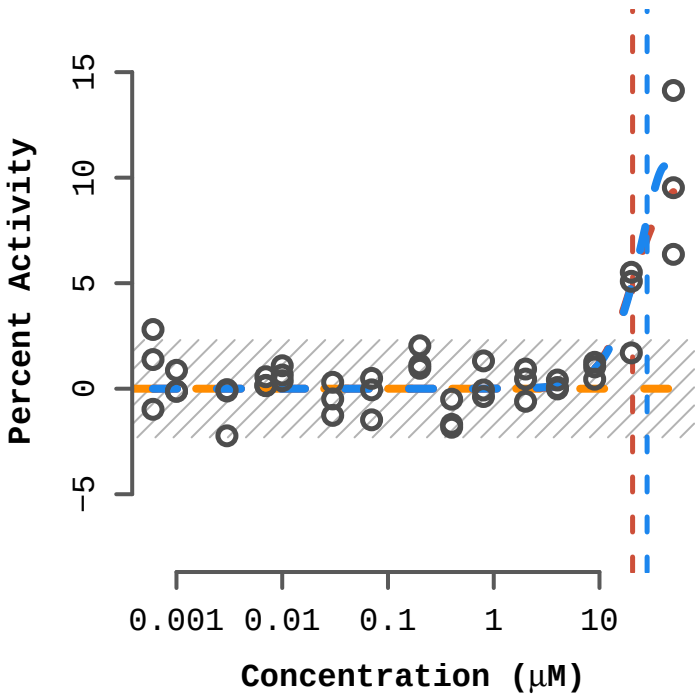
	tp	ga	gw
val:	7.08	2.4	0.488
sd:	13.7	2.47	0.383

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.9	1.9	0.518	3.53	6.9
sd:	7.46	1.97	0.453	73100	312000

	CNST	HILL	GNLS
AIC:	196.57	186.45	190.69
PROB:	0.01	0.89	0.11
RMSE:	8.39	8.23	8.22

MAX_MEAN: 18.1 **MAX_MED:** 3.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iopanoic acid
CHID: 23159 CASRN: 96-83-3
SPID(S): Tox21_110394_1
M4ID: 12484397

HILL MODEL (in red):

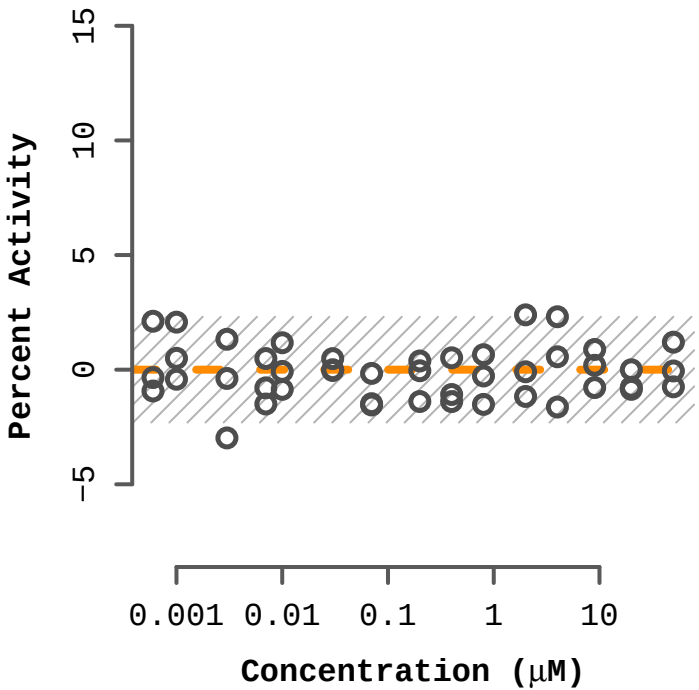
	tp	ga	gw
val:	10.1	1.31	2.75
sd:	1.6	0.0769	0.883

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.1	1.45	2.43	1.76	7.34
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	197.85	154.67	158.64
PROB:	0	0.88	0.12
RMSE:	3.1	1.35	1.35

MAX_MEAN: 10 MAX_MED: 9.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

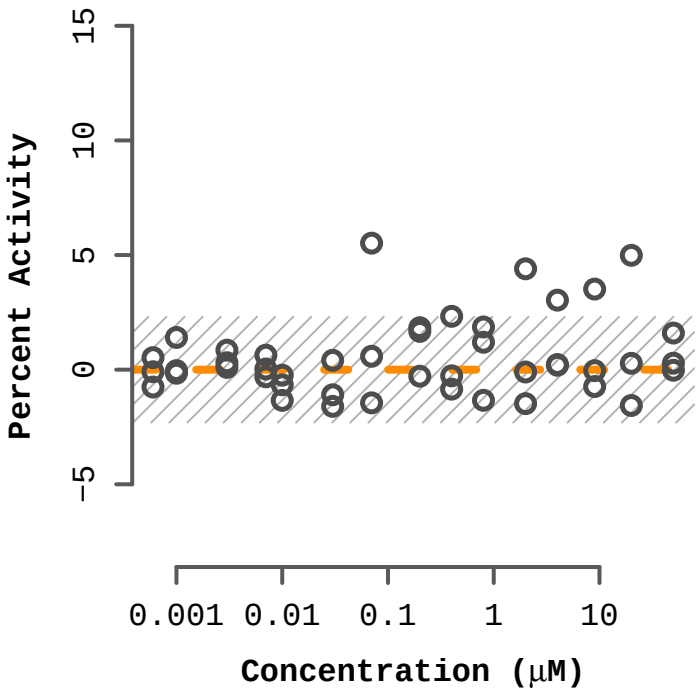
NAME: Iopromide
CHID: 23163 **CASRN:** 73334-07-3
SPID(S): Tox21_110684_1
M4ID: 12484180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.564 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

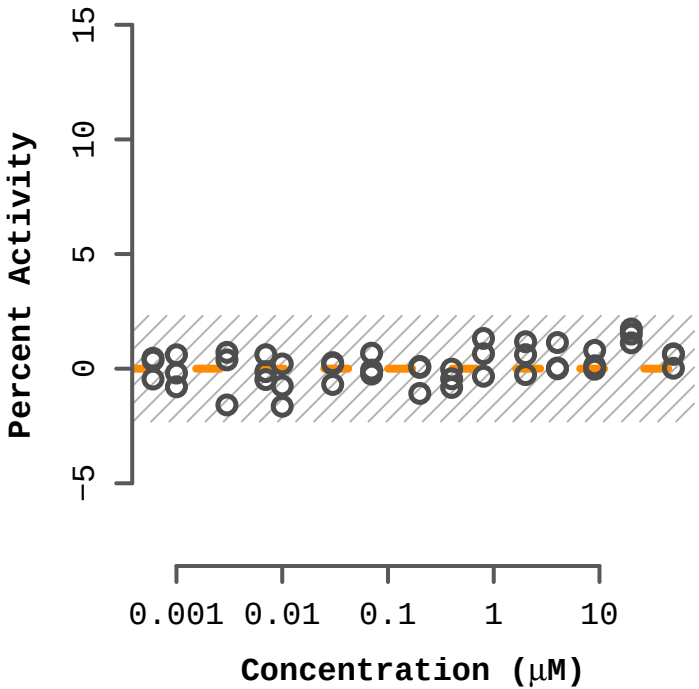
NAME: Irbesartan
CHID: 23169 **CASRN:** 138402-11-6
SPID(S): Tox21_111433_1
M4ID: 12483692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

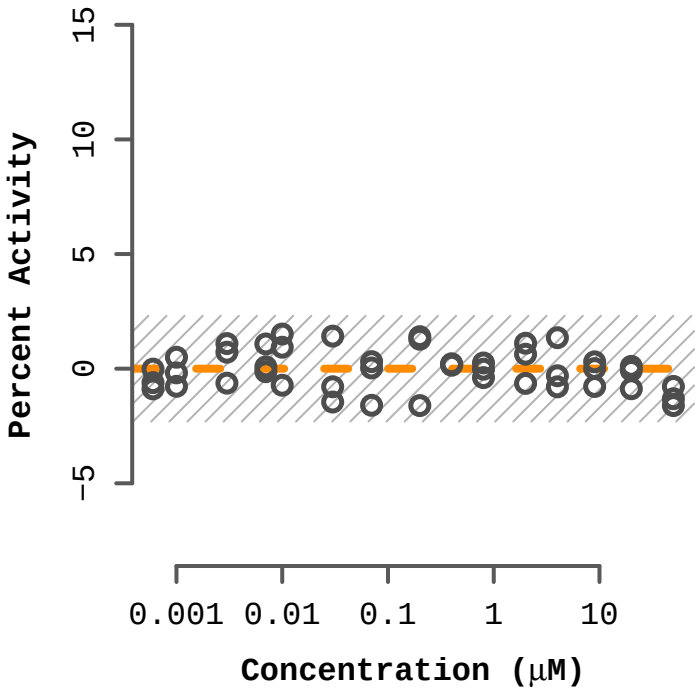
NAME: Isocaine
CHID: 23170 **CASRN:** 94-14-4
SPID(S): Tox21_111985_1
M4ID: 12483387

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

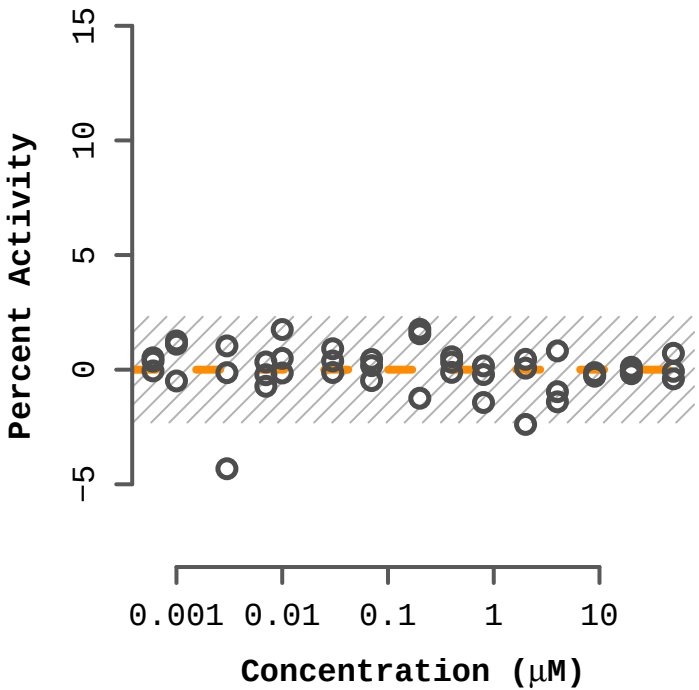
NAME: Isopropamide
CHID: 23174 **CASRN:** 7492-32-2
SPID(S): Tox21_110362_1
M4ID: 12484426

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.575 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

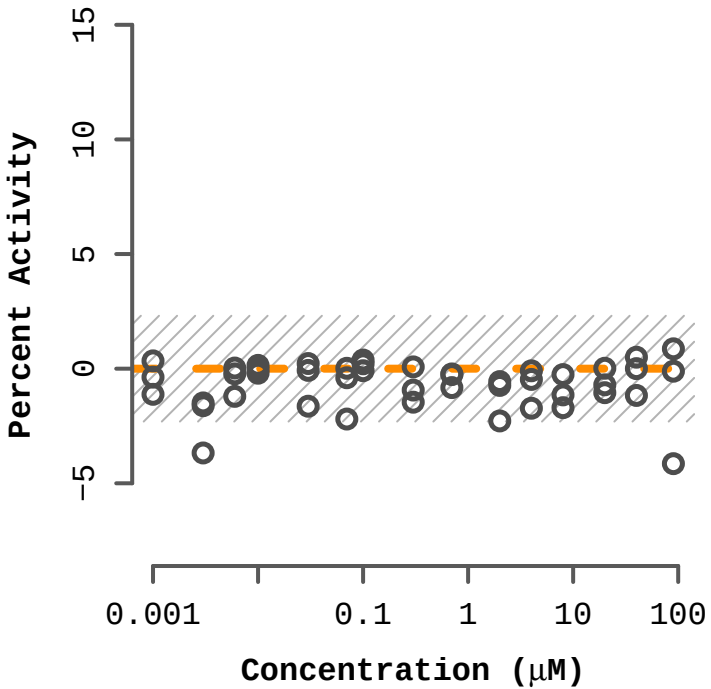
NAME: Isoproterenol
CHID: 23175 **CASRN:** 7683-59-2
SPID(S): Tox21_110172_1
M4ID: 12484586

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.701 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

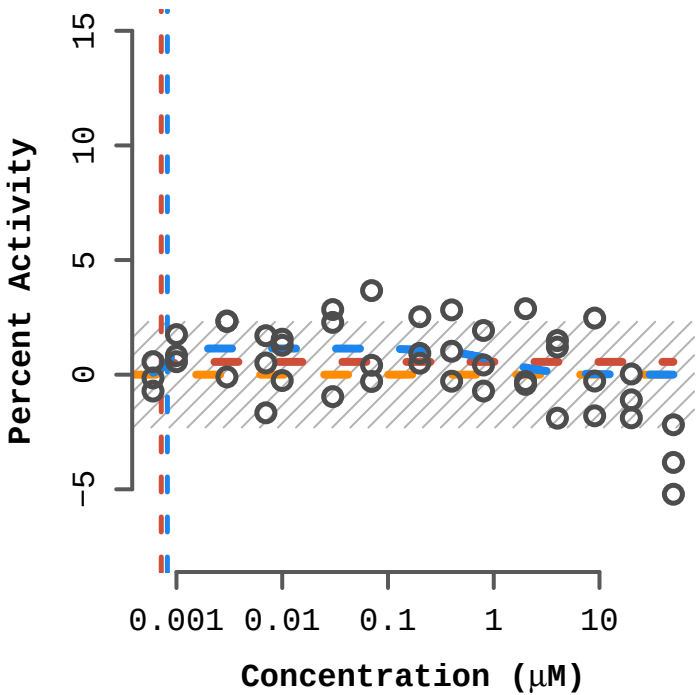
NAME: 13-cis Retinoic acid
CHID: 23177 **CASRN:** 4759-48-2
SPID(S): Tox21_200093
M4ID: 12482159

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.168 **MAX_MED:** 0.214 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isradipine
CHID: 23179 **CASRN:** 75695-93-1
SPID(S): Tox21_110690_1
M4ID: 12484176

HILL MODEL (in red):

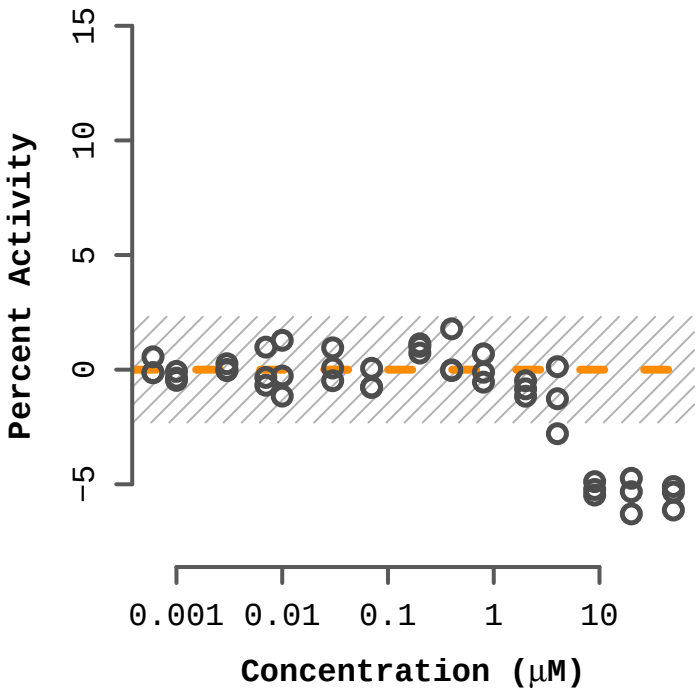
	tp	ga	gw
val:	0.559	−3.14	8
sd:	0.273	0.233	16.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.14	−3.09	8	0.0529	1.76
sd:	0.369	0.174	12.7	0.684	2.21

	CNST	HILL	GNLS
AIC:	186.05	188.01	184.24
PROB:	0.26	0.1	0.64
RMSE:	1.83	1.8	1.64

MAX_MEAN: 1.52 **MAX_MED:** 2.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

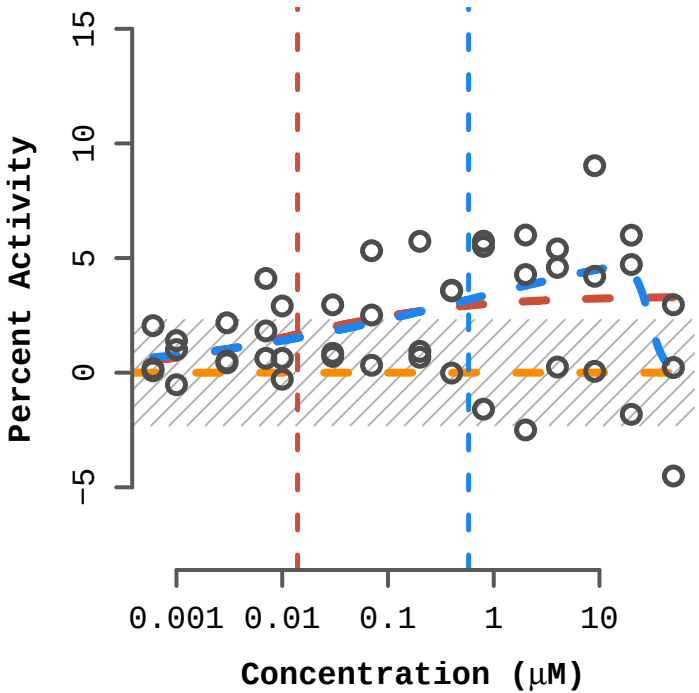
NAME: Itraconazole
CHID: 23180 CASRN: 84625-61-6
SPID(S): Tox21_110854_1
M4ID: 12484066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.09	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 0.958 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ketanserin
CHID: 23188 **CASRN:** 74050-98-9
SPID(S): Tox21_110865_1
M4ID: 12484058

HILL MODEL (in red):

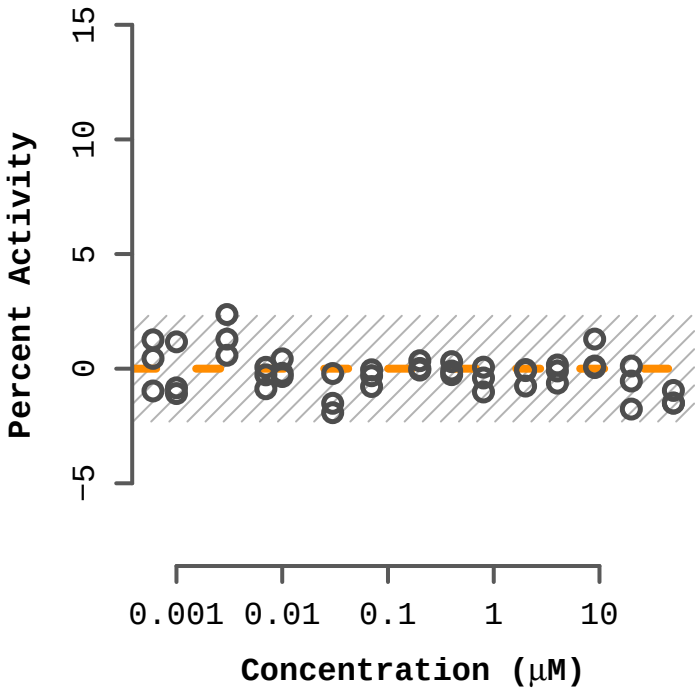
	tp	ga	gw
val:	3.33	−1.86	0.532
sd:	0.916	0.764	0.36

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.37	−0.238	0.313	1.47	6.19
sd:	7.61	3.63	0.287	0.359	11.7

	CNST	HILL	GNLS
AIC:	241.29	221.49	219.92
PROB:	0	0.31	0.69
RMSE:	3.38	2.61	2.46

MAX_MEAN: 4.43 **MAX_MED:** 5.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

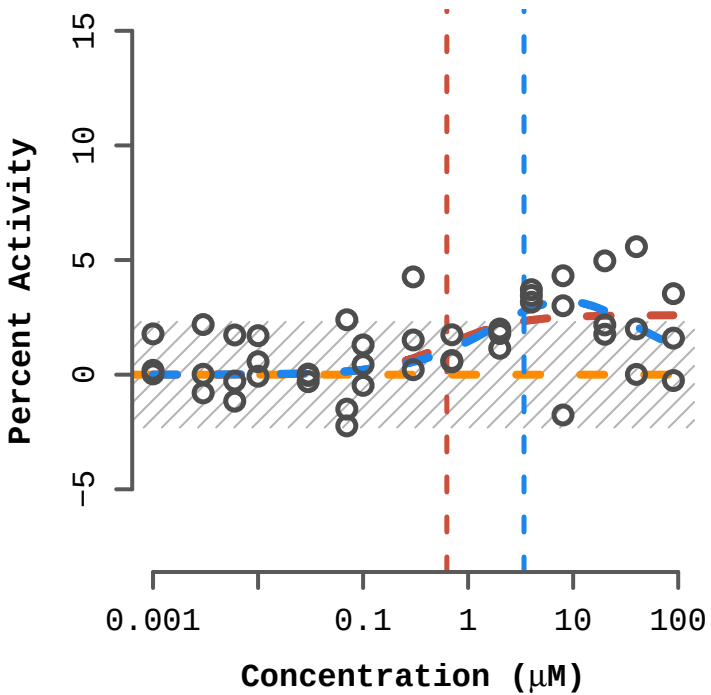
NAME: Ketotifen
CHID: 23190 CASRN: 34580-13-7
SPID(S): Tox21_110176_1
M4ID: 12484582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lactic acid
CHID: 23192 CASRN: 50-21-5
SPID(S): Tox21_303616
M4ID: 12475529

HILL MODEL (in red):

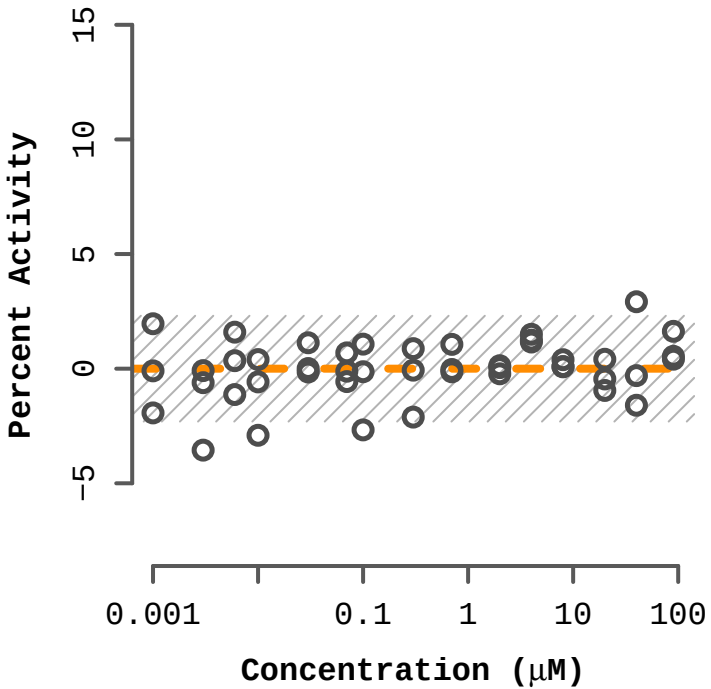
	tp	ga	gw
val:	2.6	−0.203	1.3
sd:	0.477	0.343	0.733

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.7	0.532	0.977	1.28	0.893
sd:	8.59	0.826	0.649	1.04	0.777

	CNST	HILL	GNLS
AIC:	200.95	173.68	174.28
PROB:	0	0.58	0.42
RMSE:	2.18	1.53	1.53

MAX_MEAN: 3.44 MAX_MED: 3.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

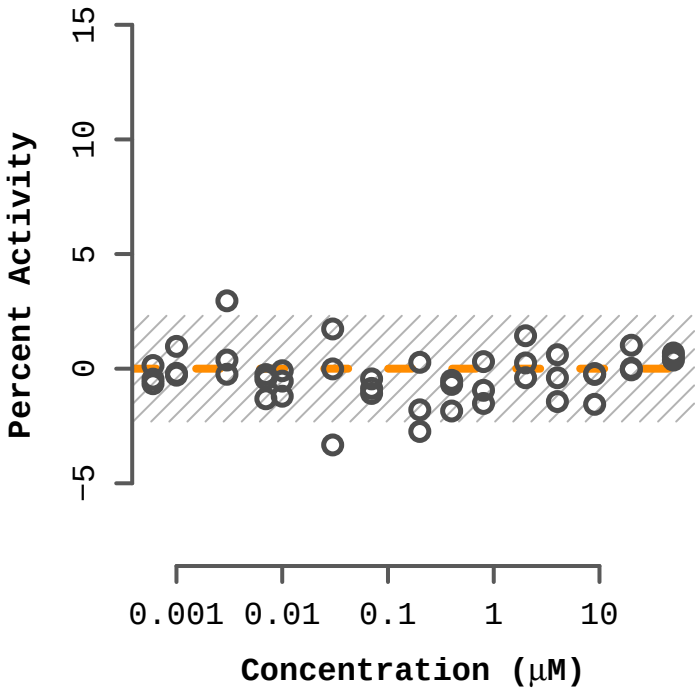
NAME: Lactic acid
CHID: 23192 CASRN: 50-21-5
SPID(S): Tox21_202455
M4ID: 12479797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.3 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

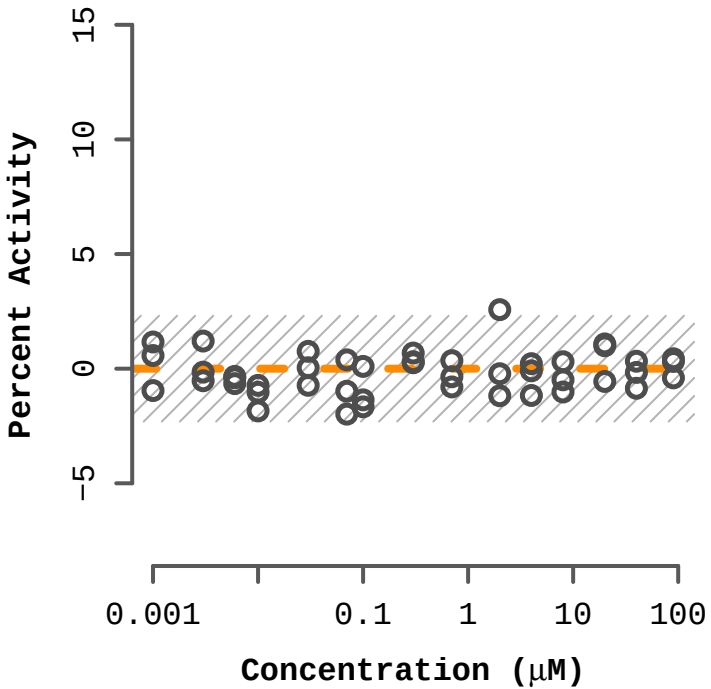
NAME: Lactic acid
CHID: 23192 **CASRN:** 50-21-5
SPID(S): Tox21_111049_1
M4ID: 12483932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.537 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

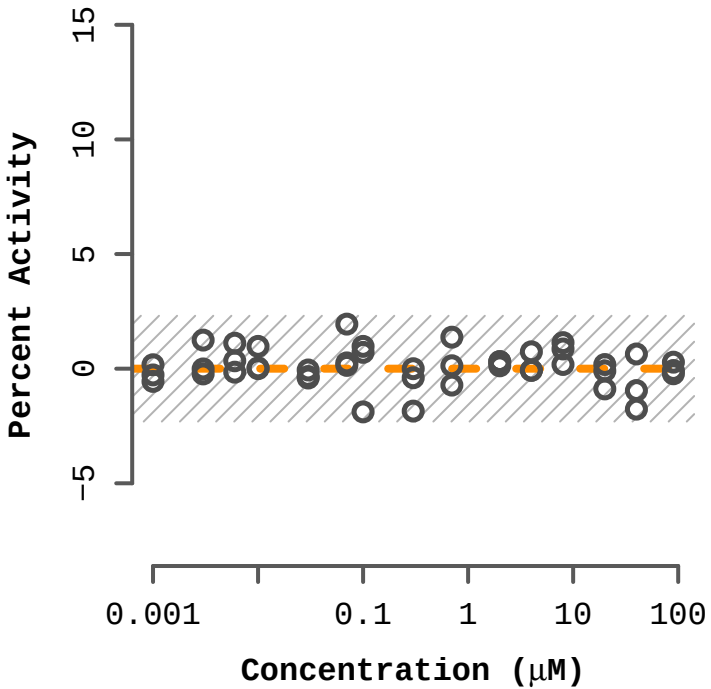
NAME: Lactose
CHID: 23193 CASRN: 63-42-3
SPID(S): Tox21_301866
M4ID: 12477267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.509 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

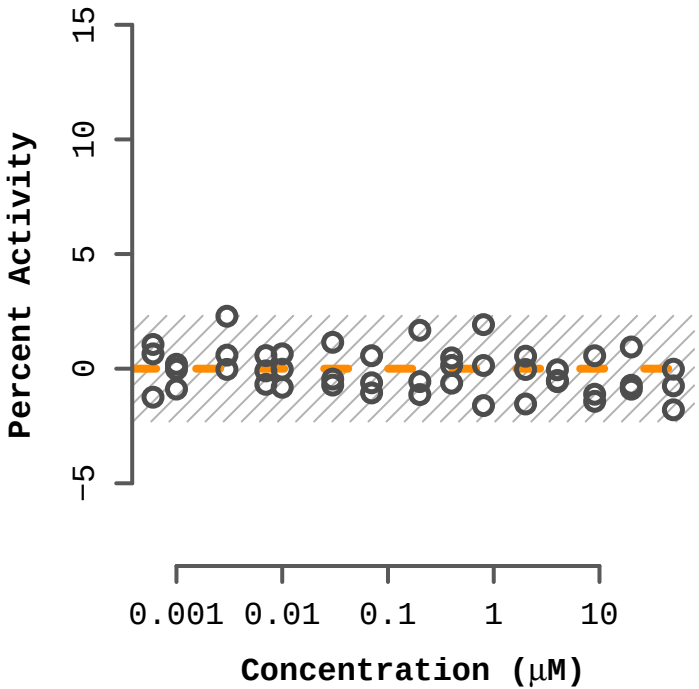
NAME: Lamivudine
CHID: 23194 **CASRN:** 134678-17-4
SPID(S): Tox21_303147
M4ID: 12475986

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

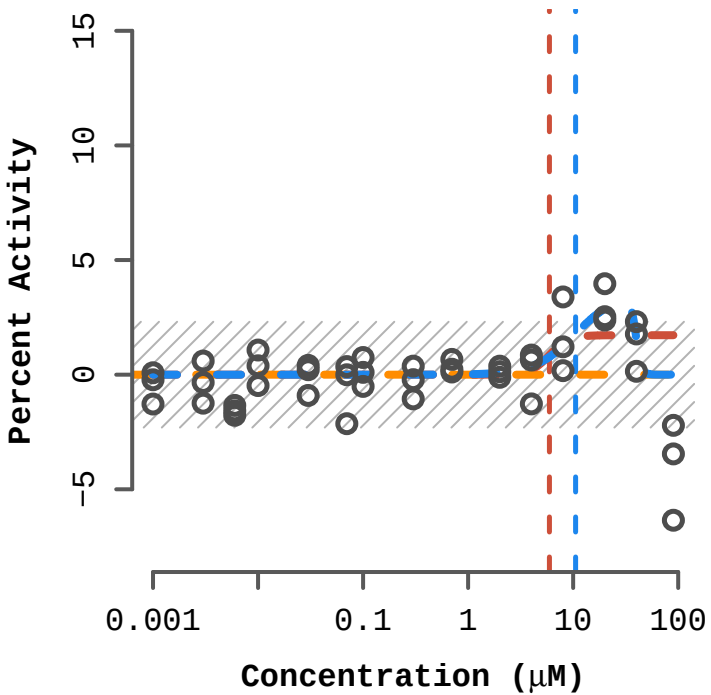
NAME: Lamotrigine
CHID: 23195 **CASRN:** 84057-84-1
SPID(S): Tox21_110179_1
M4ID: 12484579

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 0.647 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lansoprazole
CHID: 23200 CASRN: 103577-45-3
SPID(S): Tox21_301023
M4ID: 12478110

HILL MODEL (in red):

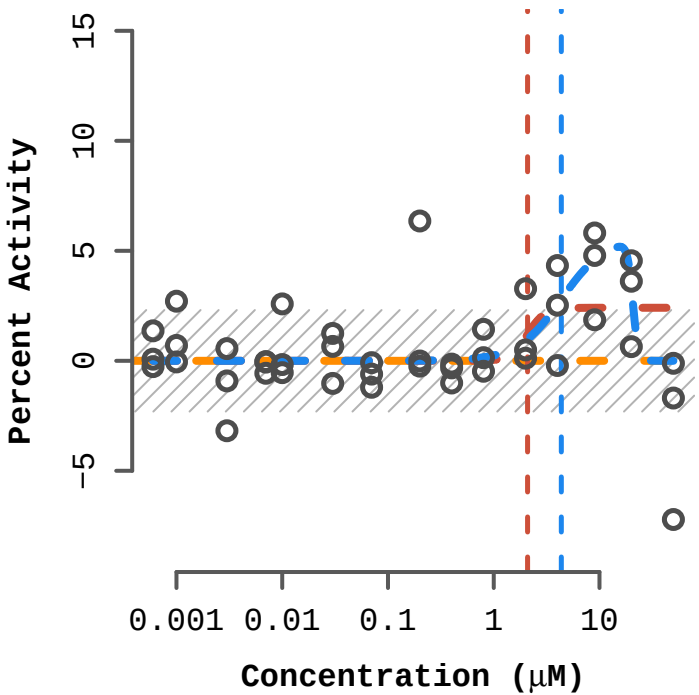
	tp	ga	gw
val:	1.72	0.774	4.84
sd:	0.519	0.232	5.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.57	1.02	2.23	1.6	16.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	169.4	166.08	156.08
PROB:	0	0.01	0.99
RMSE:	1.7	1.8	1.42

MAX_MEAN: 2.96 MAX_MED: 2.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lansoprazole
CHID: 23200 CASRN: 103577-45-3
SPID(S): Tox21_110184_1
M4ID: 12484574

HILL MODEL (in red):

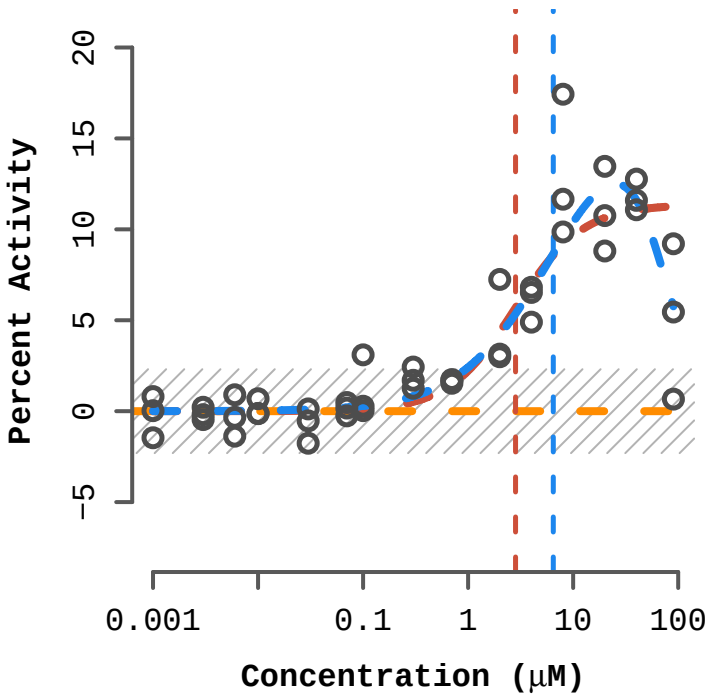
	tp	ga	gw
val:	2.41	0.32	5.32
sd:	0.808	0.145	22.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.59	0.639	2.1	1.31	17
sd:	3.4	0.364	1.78	0.0649	81.7

	CNST	HILL	GNLS
AIC:	201.09	195.58	184.52
PROB:	0	0	1
RMSE:	2.42	2.29	1.93

MAX_MEAN: 4.16 MAX_MED: 4.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Leflunomide
CHID: 23201 CASRN: 75706-12-6
SPID(S): Tox21_301873
M4ID: 12477260

HILL MODEL (in red):

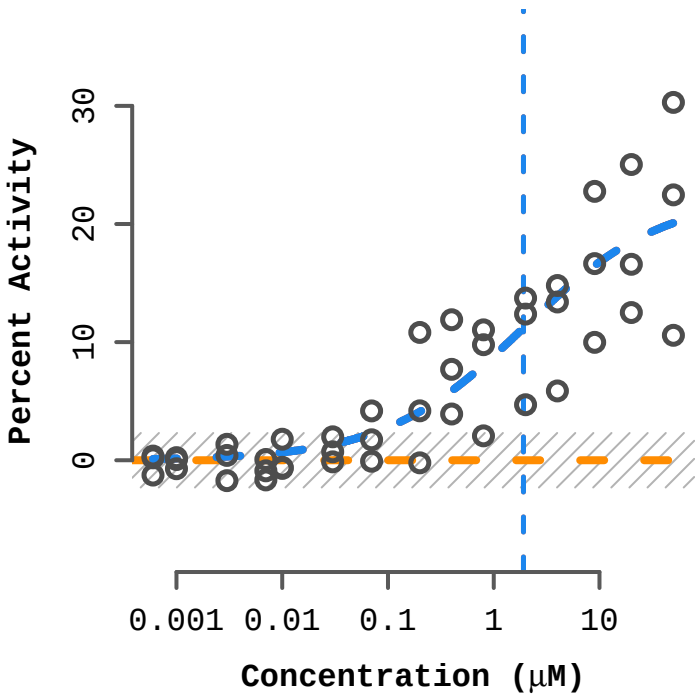
	tp	ga	gw
val:	11.4	0.451	1.36
sd:	0.774	0.0855	0.333

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.4	0.811	0.978	1.84	2.28
sd:	9.6	0.47	0.284	0.18	1.45

	CNST	HILL	GNLS
AIC:	287.53	192.57	179.55
PROB:	0	0	1
RMSE:	6.09	2.5	1.89

MAX_MEAN: 13 MAX_MED: 11.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Leflunomide
CHID: 23201 CASRN: 75706-12-6
SPID(S): Tox21_110182_1
M4ID: 12484576

HILL MODEL (in red):

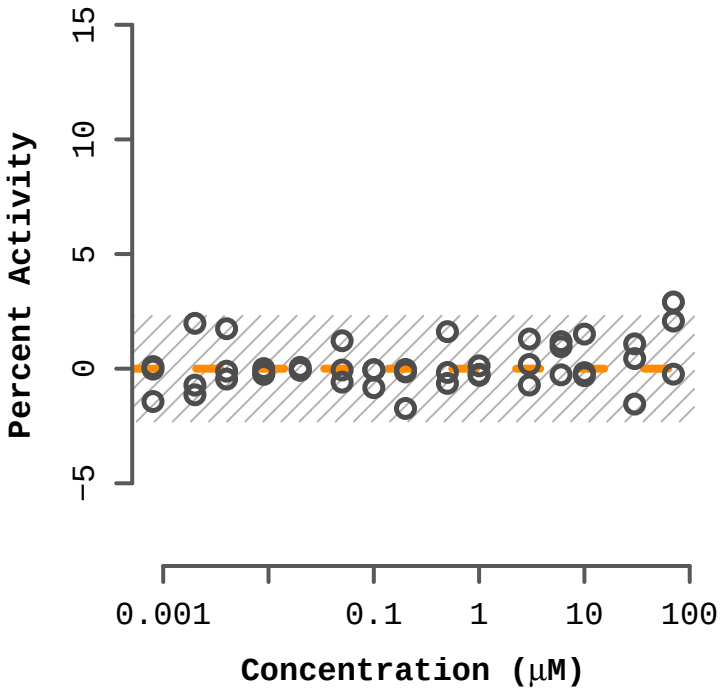
	tp	ga	gw
val:	22.4	0.281	0.662
sd:	6.72	0.509	0.193

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.4	0.281	0.662	3.29	5.09
sd:	6.72	0.509	0.193	1170	3760

	CNST	HILL	GNLS
AIC:	337.22	254.13	258.13
PROB:	0	0.88	0.12
RMSE:	10.43	3.85	3.85

MAX_MEAN: 21.1 MAX_MED: 22.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

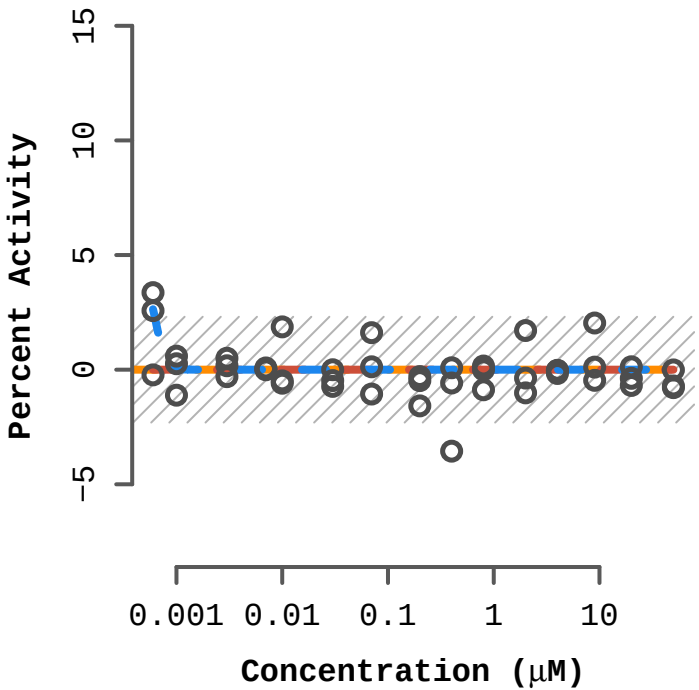
NAME: Letrozole
CHID: 23202 **CASRN:** 112809-51-5
SPID(S): Tox21_303572
M4ID: 12475573

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Levallorphan
CHID: 23205 **CASRN:** 152-02-3
SPID(S): Tox21_112005_1
M4ID: 12483377

HILL MODEL (in red):

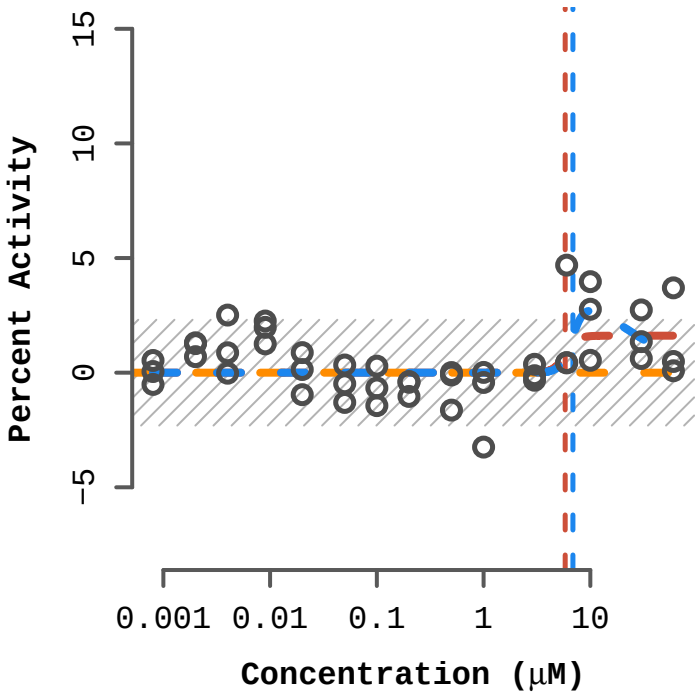
	tp	ga	gw
val:	1.08e-10	-3.55	0.87
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.01	-4.92	1.3	-3.19	9.48
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	129.11	135.11	131.28
PROB:	0.72	0.04	0.24
RMSE:	1.11	1.11	1.01

MAX_MEAN: 1.9 **MAX_MED:** 2.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Levothyroxine
CHID: 23214 **CASRN:** 51-48-9
SPID(S): Tox21_302156
M4ID: 12476977

HILL MODEL (in red):

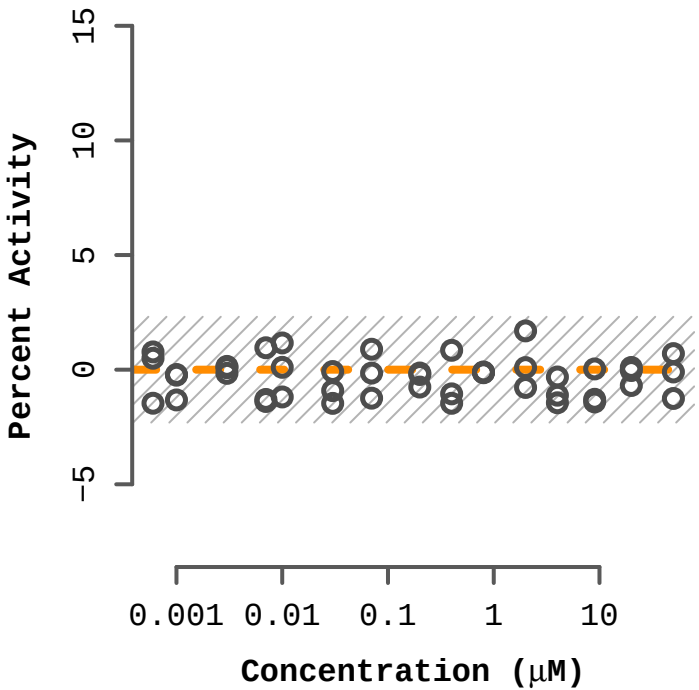
	tp	ga	gw
val:	1.61	0.764	8
sd:	0.516	0.115	12.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.8	0.837	7.91	1.34	1.37
sd:	13.6	0.504	47.4	2.25	3.38

	CNST	HILL	GNLS
AIC:	166.09	158.9	160.28
PROB:	0.02	0.65	0.33
RMSE:	1.59	1.3	1.3

MAX_MEAN: 2.43 **MAX_MED:** 2.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

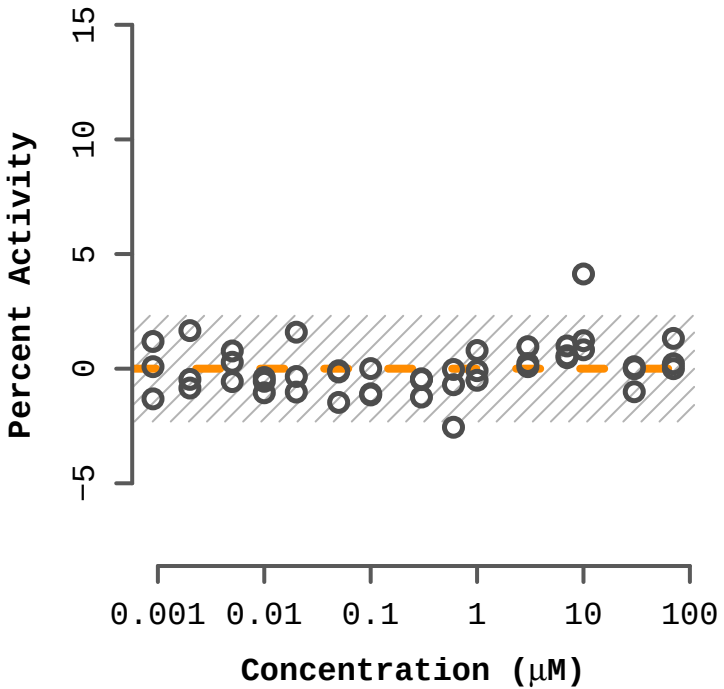
NAME: Levothyroxine
CHID: 23214 **CASRN:** 51-48-9
SPID(S): Tox21_112101_1
M4ID: 12483320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.337 **MAX_MED:** 0.499 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

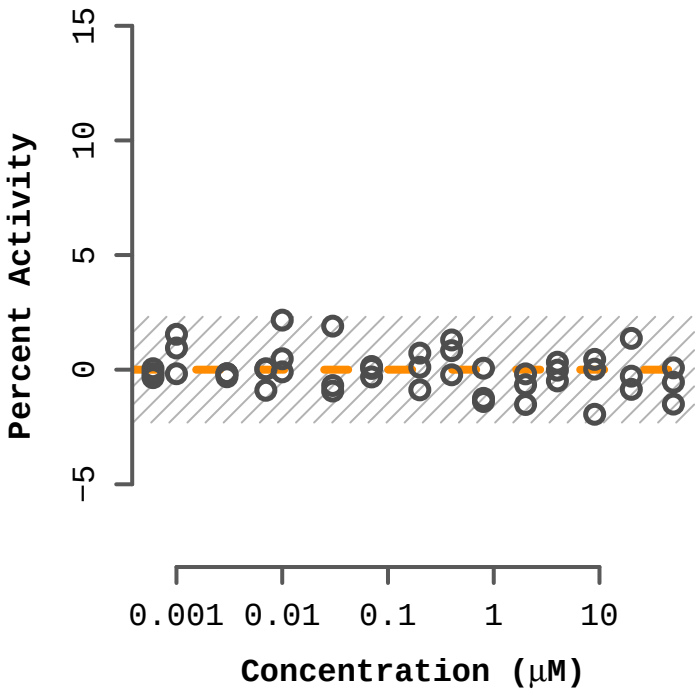
NAME: 3,5,3'−Triiodothyronine
CHID: 23216 **CASRN:** 6893−02−3
SPID(S): Tox21_301943
M4ID: 12477190

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

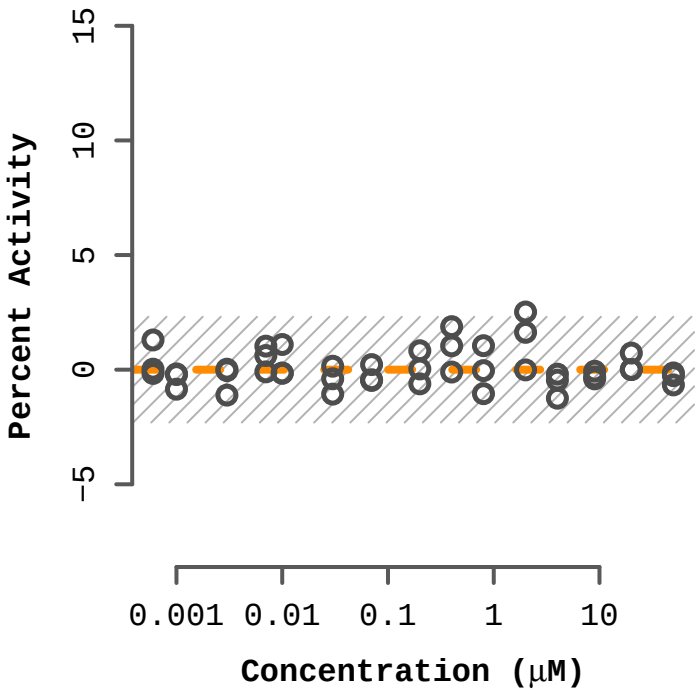
NAME: Lofexidine
CHID: 23221 CASRN: 31036-80-3
SPID(S): Tox21_113963
M4ID: 12482270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 0.947 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

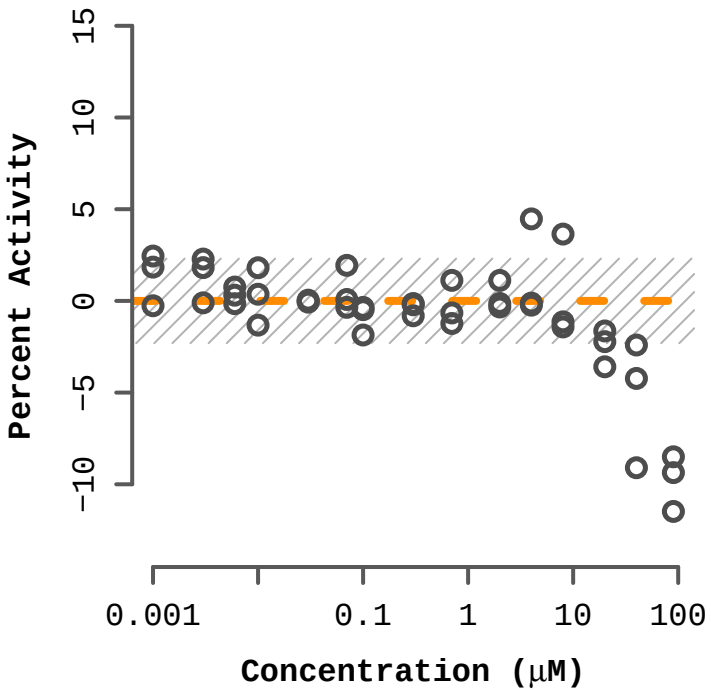
NAME: Lomustine
CHID: 23222 CASRN: 13010-47-4
SPID(S): Tox21_112470_1
M4ID: 12483083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

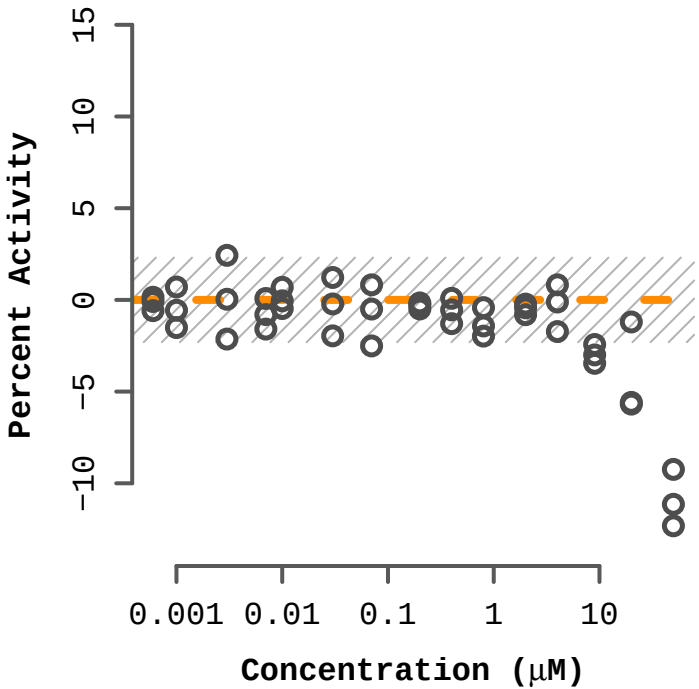
NAME: Loratadine
CHID: 23224 **CASRN:** 79794-75-5
SPID(S): Tox21_301532
M4ID: 12477601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.08	NA	NA
PROB:	1	NA	NA
RMSE:	3.31	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

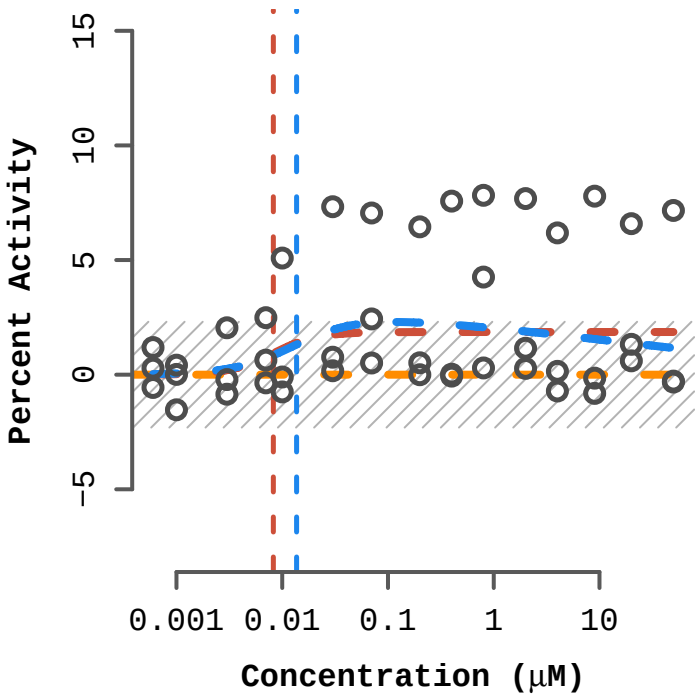
NAME: Loratadine
CHID: 23224 **CASRN:** 79794-75-5
SPID(S): Tox21_110185_1
M4ID: 12484573

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.74	NA	NA
PROB:	1	NA	NA
RMSE:	3.32	NA	NA

MAX_MEAN: 0.112 **MAX_MED:** 0.0369 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Losartan
CHID: 23227 CASRN: 114798-26-4
SPID(S): Tox21_111435_1
M4ID: 12483690

HILL MODEL (in red):

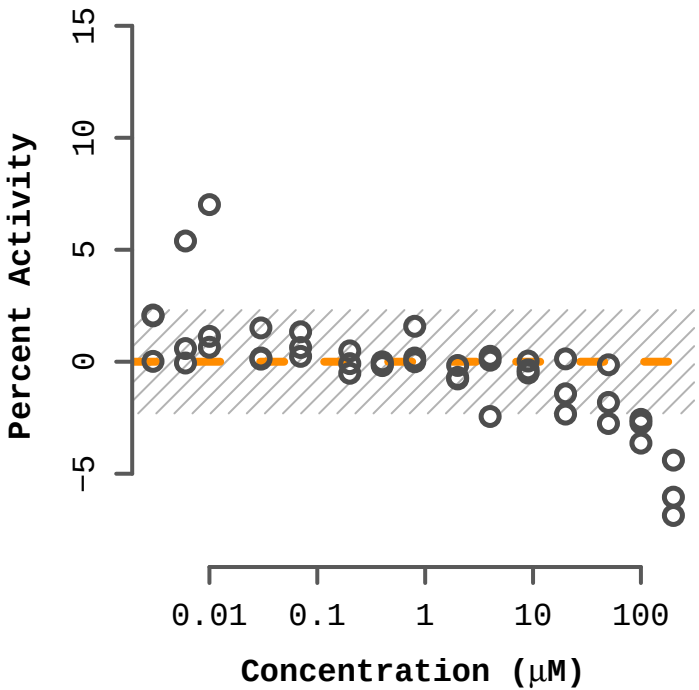
	tp	ga	gw
val:	1.86	−2.08	2.11
sd:	0.639	0.494	3.87

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.93	−1.86	1.51	1.12	0.314
sd:	9.88	1.14	2.66	9.74	1.86

	CNST	HILL	GNLS
AIC:	240.02	233.6	237.16
PROB:	0.03	0.83	0.14
RMSE:	3.62	2.91	2.91

MAX_MEAN: 4.13 **MAX_MED:** 4.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

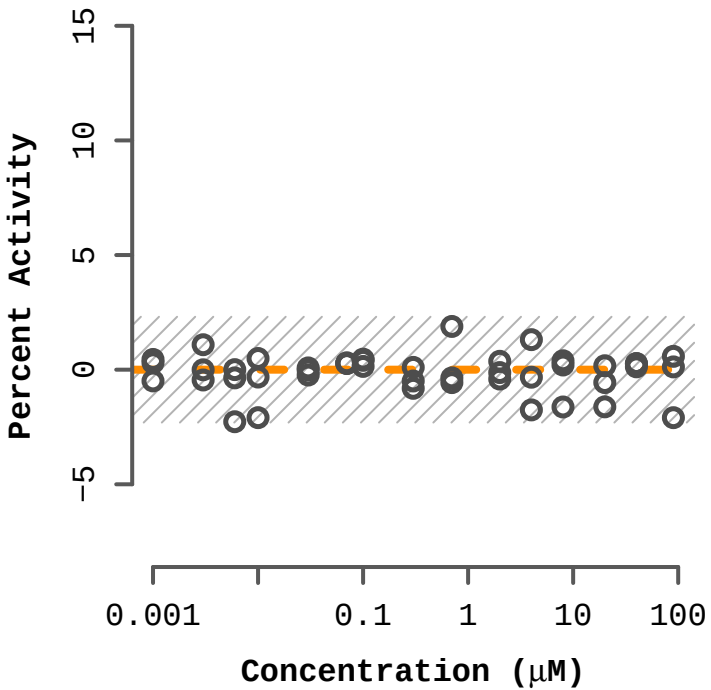
NAME: Lysergide
CHID: 23231 **CASRN:** 50-37-3
SPID(S): Tox21_112872
M4ID: 12482909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.83	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 2.93 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

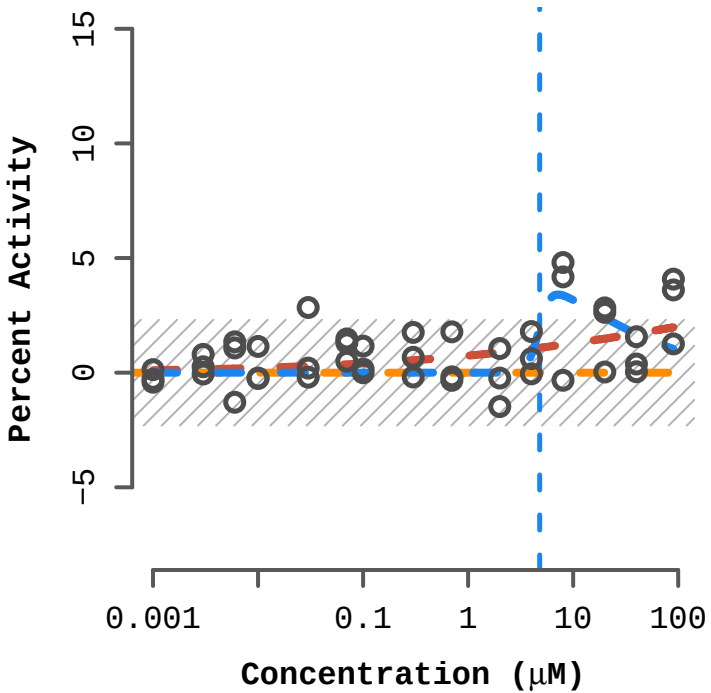
NAME: D−Mannitol
CHID: 23235 **CASRN:** 69−65−8
SPID(S): Tox21_300483
M4ID: 12478649

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.337 **MAX_MED:** 0.407 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D-Mannitol
CHID: 23235 CASRN: 69-65-8
SPID(S): Tox21_201487
M4ID: 12480765

HILL MODEL (in red):

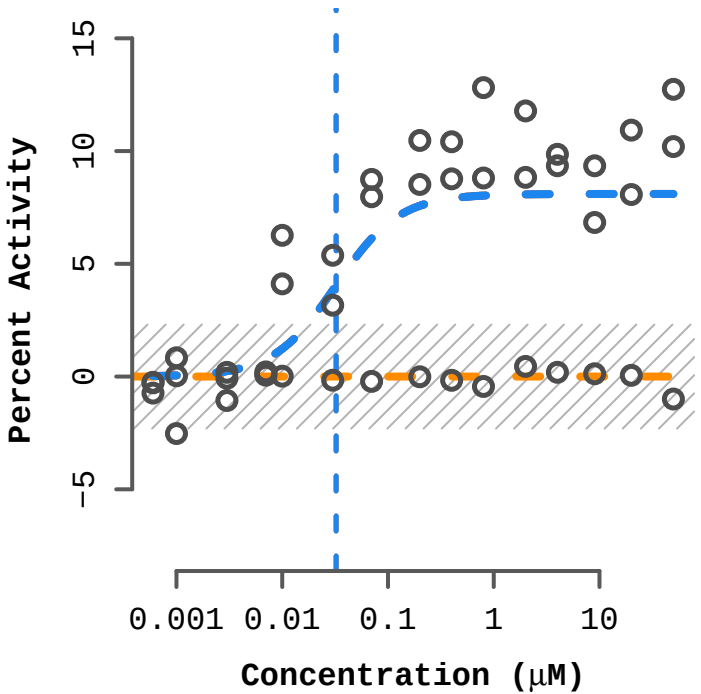
	tp	ga	gw
val:	4.77	2.45	0.3
sd:	8.92	4.07	0.159

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.77	0.681	8	1.11	0.785
sd:	4.99	0.0856	6.05	0.757	0.933

	CNST	HILL	GNLS
AIC:	169.97	157.39	161.51
PROB:	0	0.89	0.11
RMSE:	1.66	1.26	1.29

MAX_MEAN: 2.98 MAX_MED: 4.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D−Mannitol
CHID: 23235 CASRN: 69−65−8
SPID(S): Tox21_112092_1
M4ID: 12483326

HILL MODEL (in red):

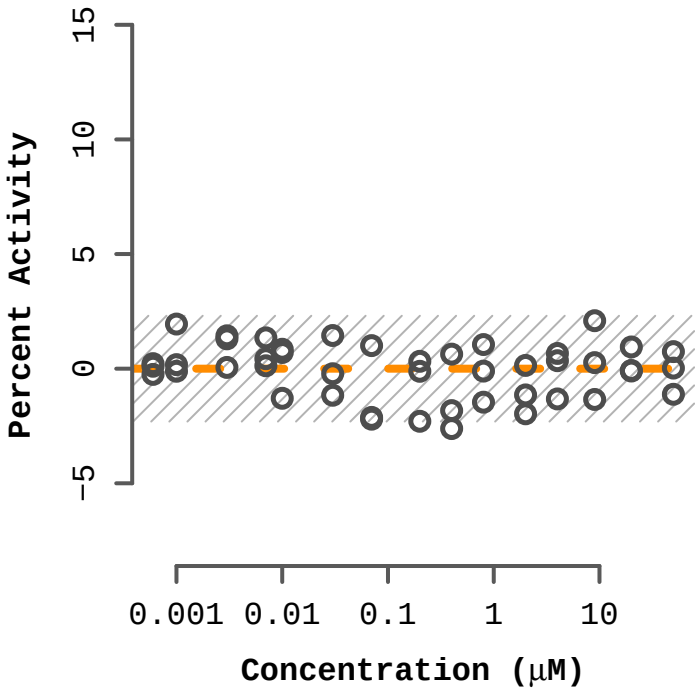
	tp	ga	gw
val:	8.1	−1.49	1.46
sd:	0.954	0.232	0.782

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.1	−1.49	1.46	3.66	8.13
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	299.36	260.53	264.53
PROB:	0	0.88	0.12
RMSE:	6.4	4.05	4.05

MAX_MEAN: 7.31 MAX_MED: 10.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

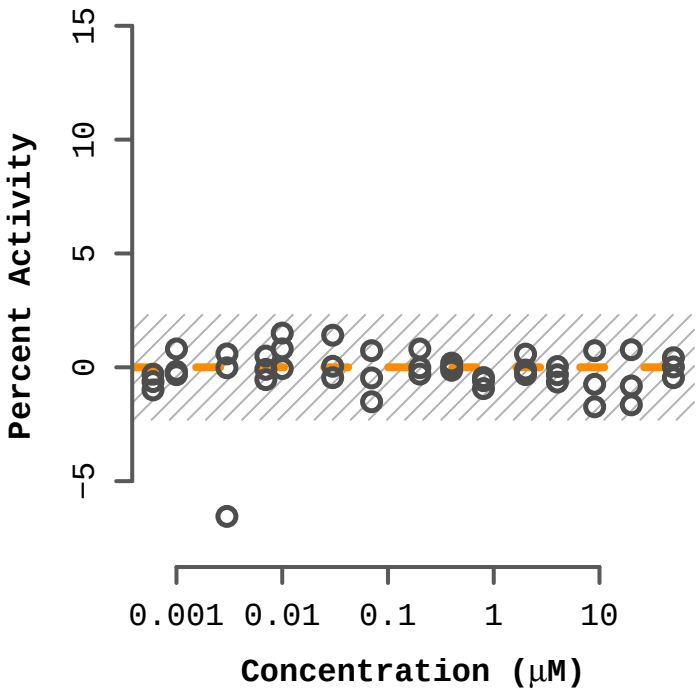
NAME: Mebutamate
CHID: 23239 **CASRN:** 64-55-1
SPID(S): Tox21_113666
M4ID: 12482548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

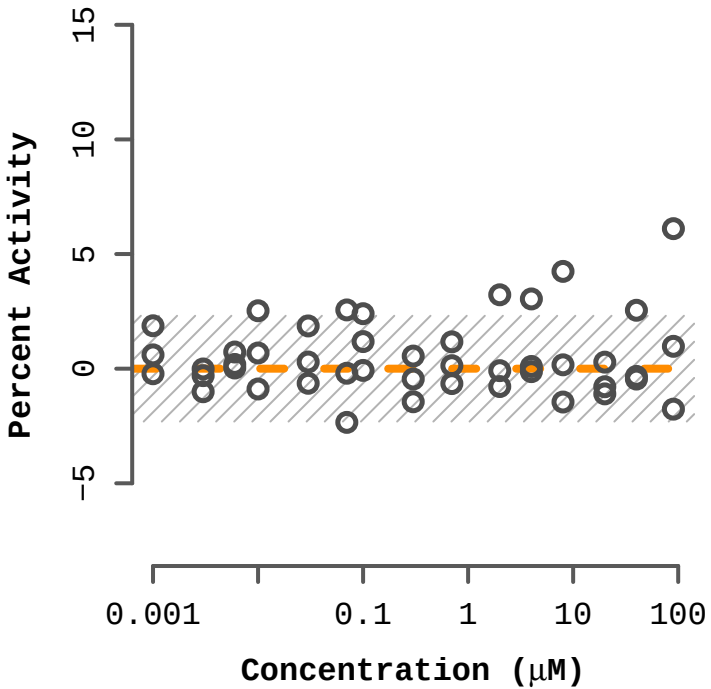
NAME: Mecamylamine
CHID: 23240 **CASRN:** 60-40-2
SPID(S): Tox21_110198_1
M4ID: 12484561

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 0.811 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

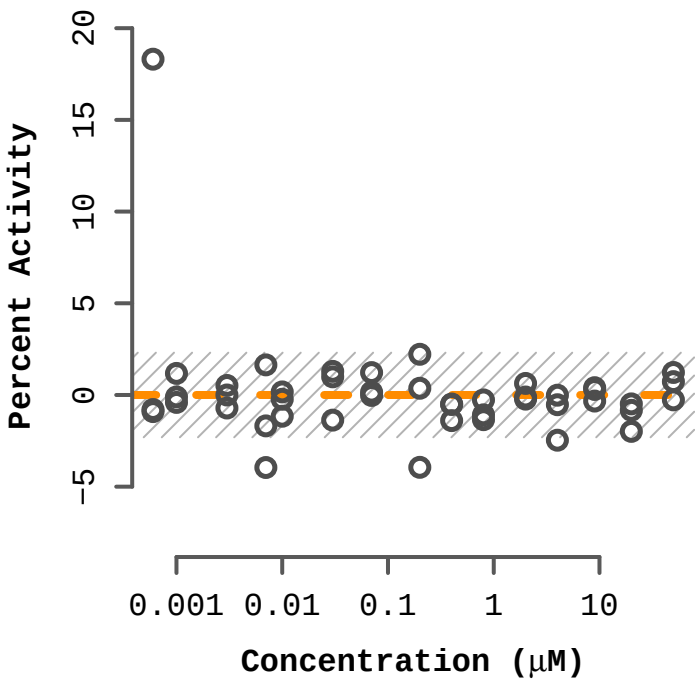
NAME: Mefenamic acid
CHID: 23243 **CASRN:** 61-68-7
SPID(S): Tox21_301983
M4ID: 12477150

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

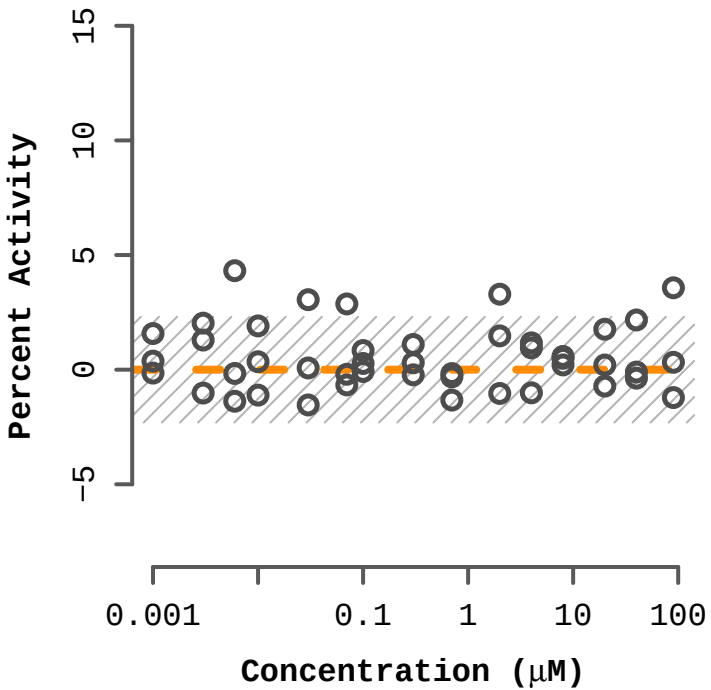
NAME: Mefenamic acid
CHID: 23243 **CASRN:** 61-68-7
SPID(S): Tox21_110344_1
M4ID: 12484439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.61	NA	NA
PROB:	1	NA	NA
RMSE:	3.01	NA	NA

MAX_MEAN: 5.54 **MAX_MED:** 0.992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

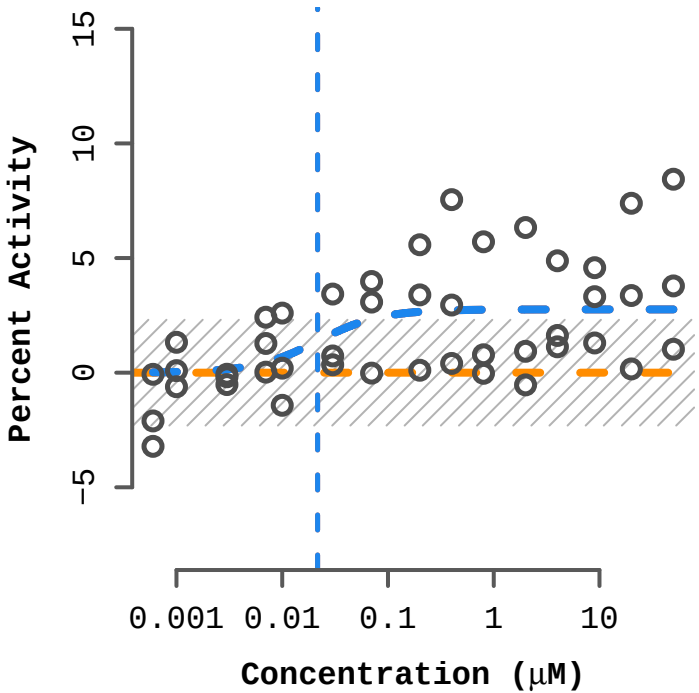
NAME: Meglumine
CHID: 23244 **CASRN:** 6284-40-8
SPID(S): Tox21_302037
M4ID: 12477096

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Meglumine
CHID: 23244 CASRN: 6284-40-8
SPID(S): Tox21_112330_1
M4ID: 12483157

HILL MODEL (in red):

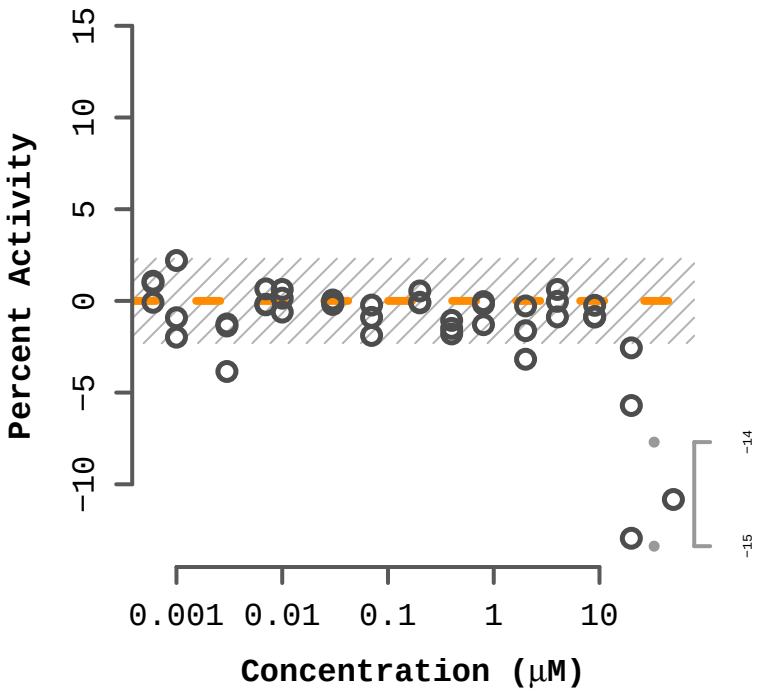
	tp	ga	gw
val:	2.76	−1.67	1.46
sd:	0.543	0.403	1.16

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.76	−1.67	1.46	3.04	5.86
sd:	0.543	0.403	1.16	1700	7440

	CNST	HILL	GNLS
AIC:	233.7	209.21	213.21
PROB:	0	0.88	0.12
RMSE:	3.23	2.19	2.19

MAX_MEAN: 4.42 MAX_MED: 3.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

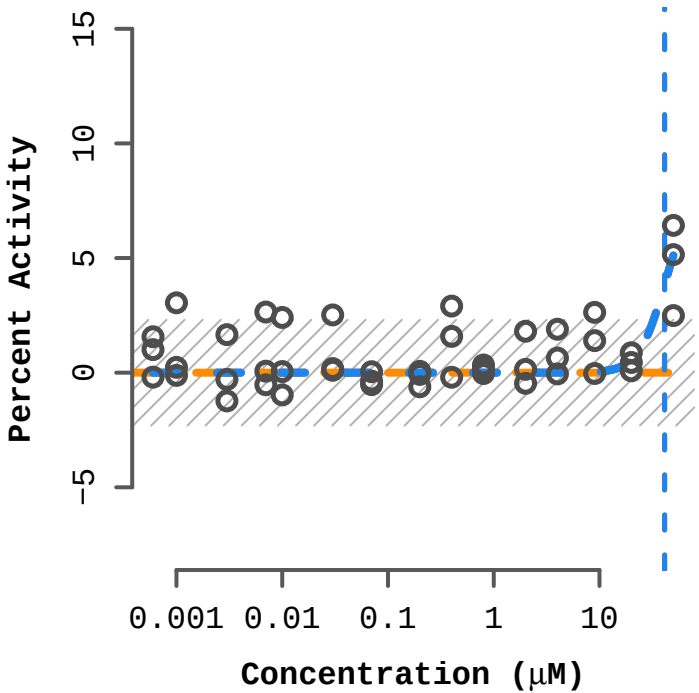
NAME: Menadiol
CHID: 23247 **CASRN:** 481-85-6
SPID(S): Tox21_113729
M4ID: 12482485 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.84	NA	NA
PROB:	1	NA	NA
RMSE:	4.22	NA	NA

MAX_MEAN: 0.66 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mepenzolate bromide
CHID: 23252 CASRN: 76-90-4
SPID(S): Tox21_110367_1
M4ID: 12484421

HILL MODEL (in red):

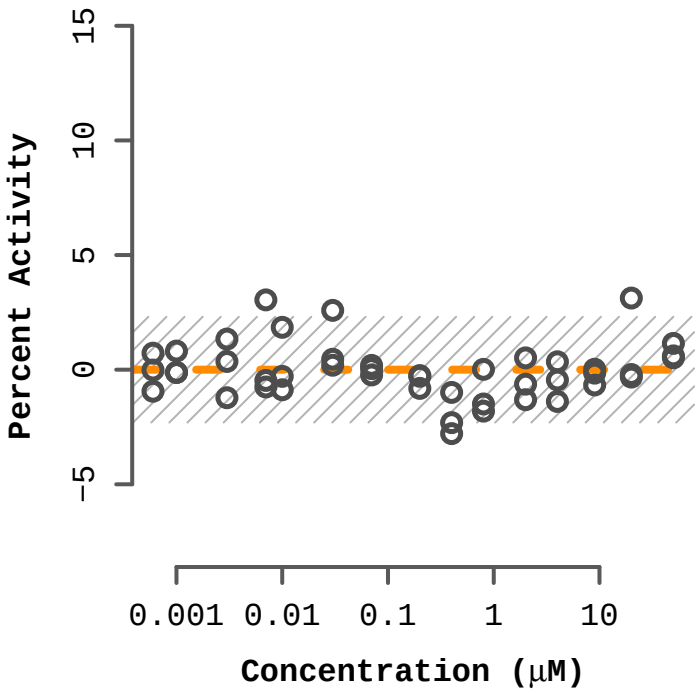
	tp	ga	gw
val:	7.71	1.62	3.54
sd:	14.7	0.59	4.81

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.71	1.62	3.54	3.7	2.73
sd:	14.7	0.589	4.8	456	631

	CNST	HILL	GNLS
AIC:	170.78	156.16	160.16
PROB:	0	0.88	0.12
RMSE:	1.77	1.29	1.29

MAX_MEAN: 4.69 **MAX_MED:** 5.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

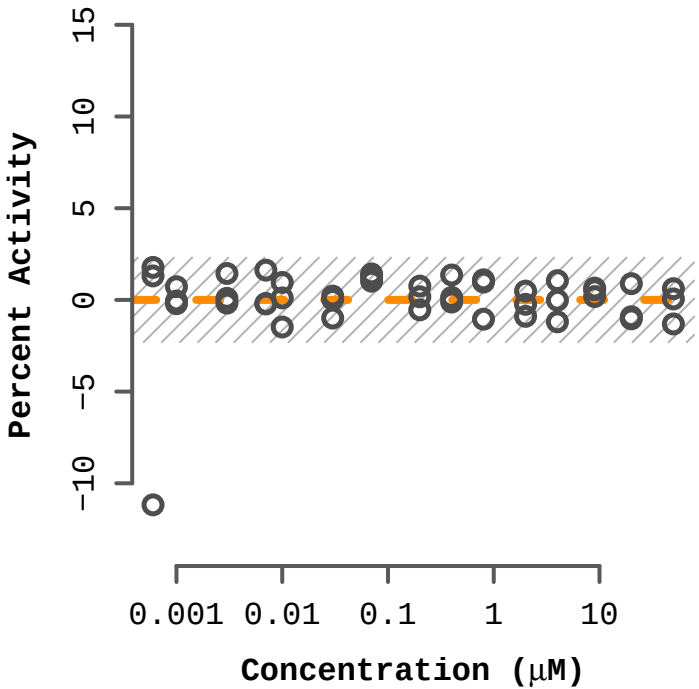
NAME: Mephenesin
CHID: 23254 **CASRN:** 59-47-2
SPID(S): Tox21_111356_1
M4ID: 12483742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.603 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

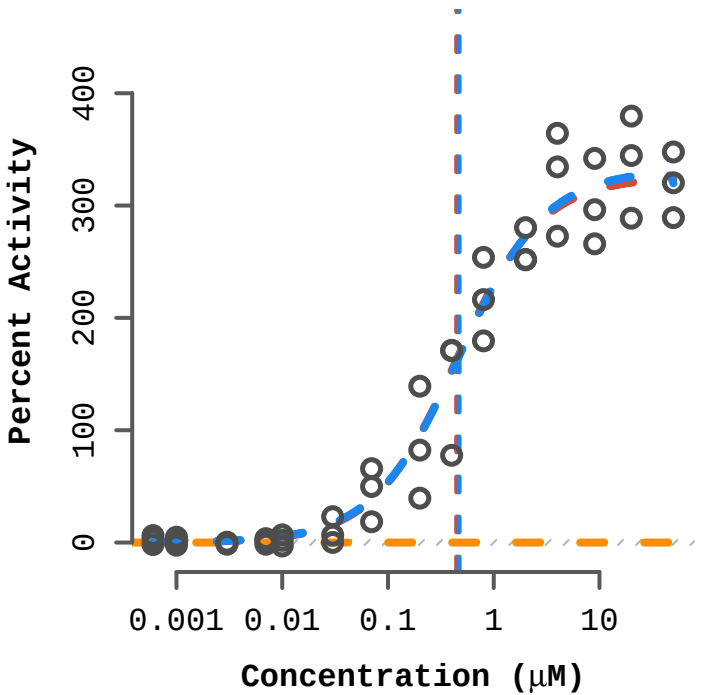
NAME: Mephenoxalone
CHID: 23255 **CASRN:** 70-07-5
SPID(S): Tox21_113149_1
M4ID: 12482788

HILL MODEL: Not applicable.

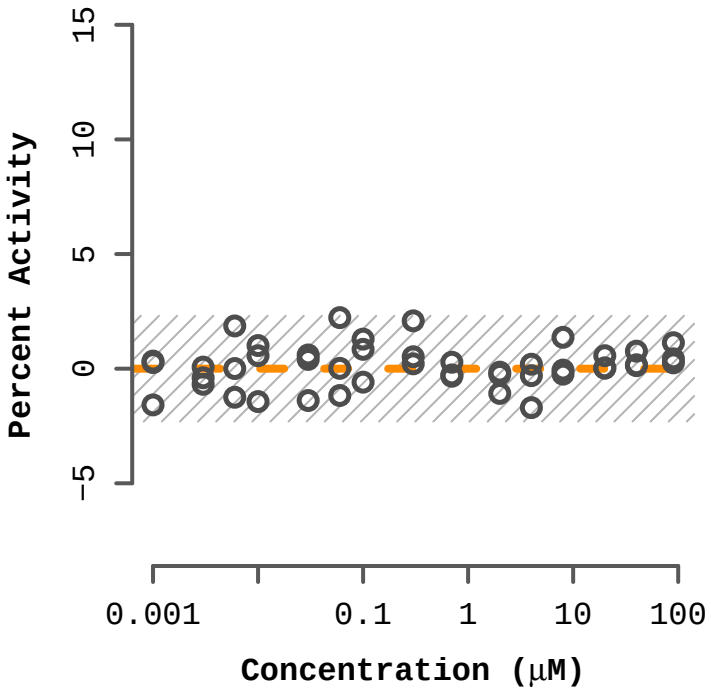
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.31 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Meprednisone
CHID:    23260   CASRN: 1247-42-3
SPID(S): Tox21_113612_1
M4ID:    12482580

HILL MODEL (in red):
      tp       ga       gw
val:  326      -0.35    1.09
sd:   12.7     0.0681   0.131

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  332      -0.327   1.06     1.79     15.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  606.53      431.87      435.71
PROB: 0           0.87        0.13
RMSE: 194.2       27.37       27.15

MAX_MEAN: 338       MAX_MED: 345       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

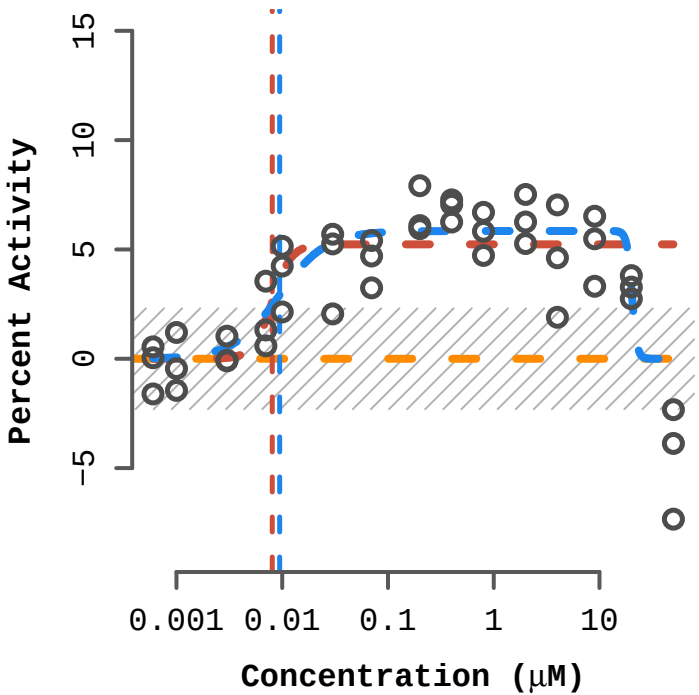
NAME: Meprobamate
CHID: 23261 **CASRN:** 57-53-4
SPID(S): Tox21_200332
M4ID: 12481920

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.941 **MAX_MED:** 0.845 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mequitazine
CHID: 23262 **CASRN:** 29216-28-2
SPID(S): Tox21_113648_1
M4ID: 12482563

HILL MODEL (in red):

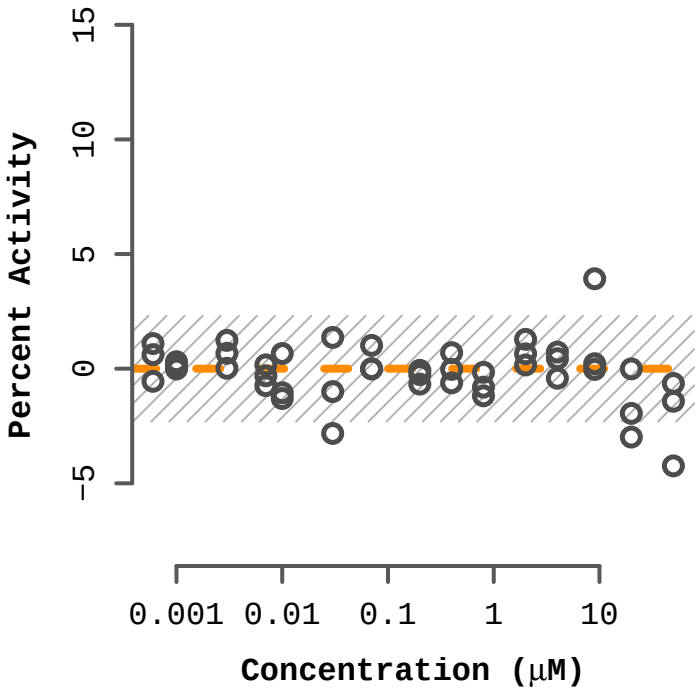
	tp	ga	gw
val:	5.23	−2.09	4.9
sd:	0.361	0.0588	4.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.84	−2.02	1.99	1.31	18
sd:	0.438	0.199	2.03	0.0188	56.9

	CNST	HILL	GNLS
AIC:	274.62	208.94	185.26
PROB:	0	0	1
RMSE:	4.63	2.94	1.83

MAX_MEAN: 6.86 **MAX_MED:** 7.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

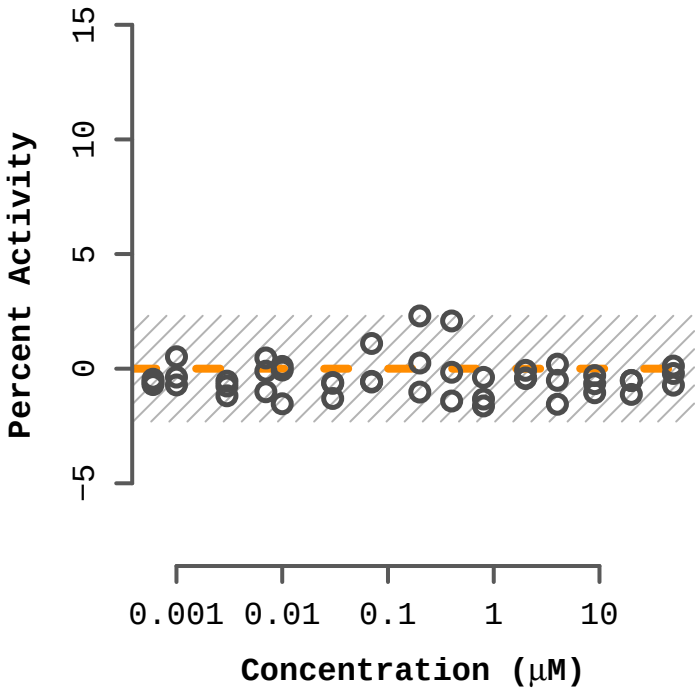
NAME: Mesoridazine
CHID: 23265 **CASRN:** 5588-33-0
SPID(S): Tox21_110052_1
M4ID: 12484694

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.672 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

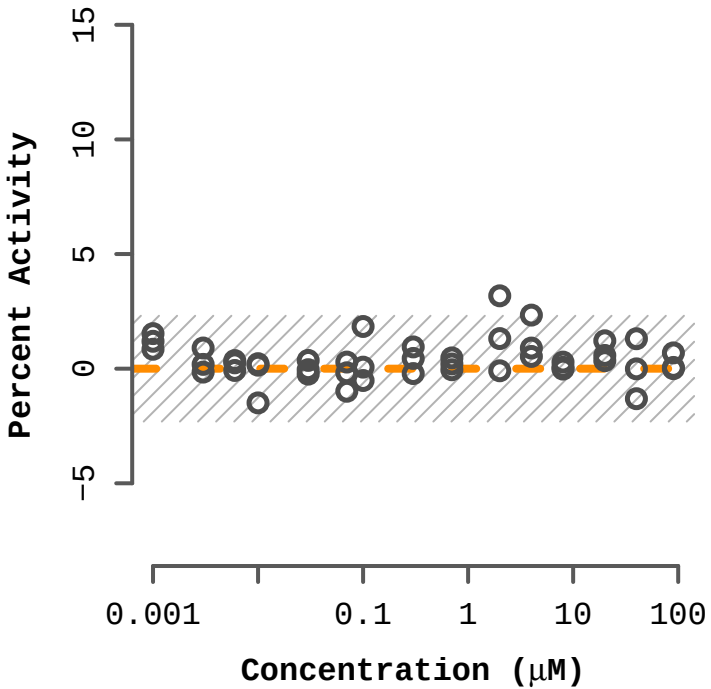
NAME: Metaxalone
CHID: 23269 **CASRN:** 1665-48-1
SPID(S): Tox21_111428_1
M4ID: 12483695

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.51 **MAX_MED:** 0.248 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

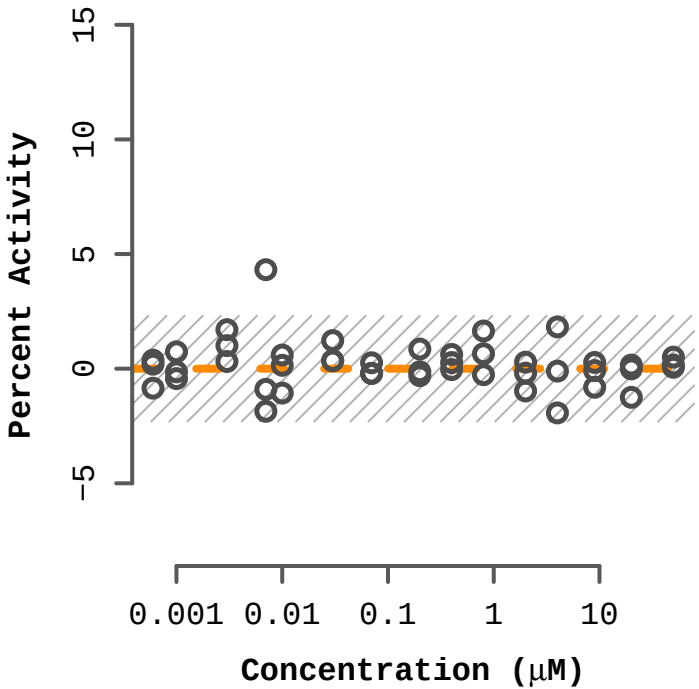
NAME: Metformin
CHID: 23270 **CASRN:** 657-24-9
SPID(S): Tox21_302370
M4ID: 12476763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

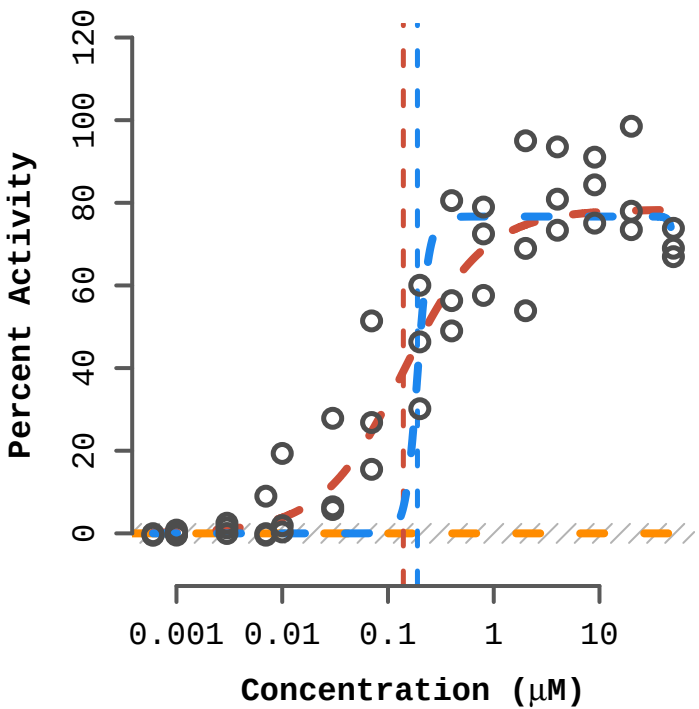
NAME: Methacholine chloride
CHID: 23271 **CASRN:** 62-51-1
SPID(S): Tox21_110348_1
M4ID: 12484435

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methandrostenolone
CHID: 23276 CASRN: 72-63-9
SPID(S): Tox21_111647_1
M4ID: 12483561

HILL MODEL (in red):

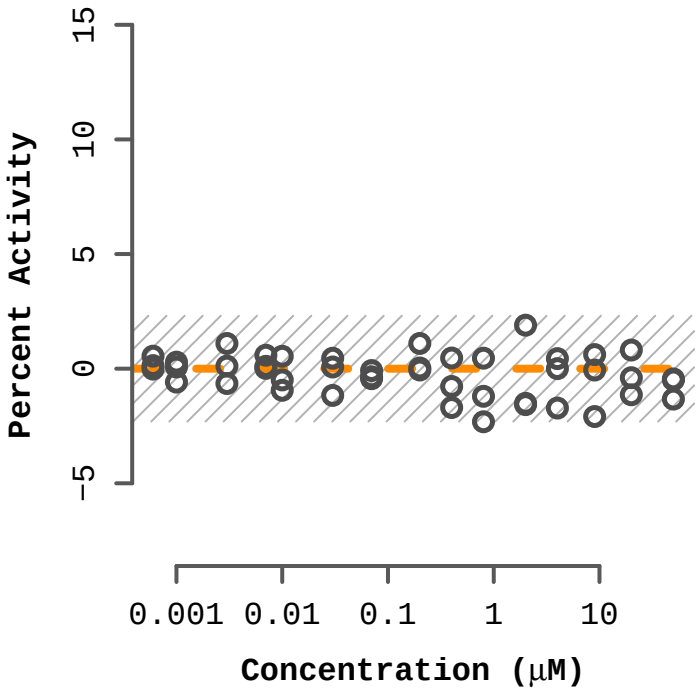
	tp	ga	gw
val:	78.4	-0.855	1.13
sd:	3	0.0916	0.194

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	76.7	-0.721	7.84	1.76	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	494.45	345.66	370.78
PROB:	0	1	0
RMSE:	54.32	10.32	14.09

MAX_MEAN: 83.5 MAX_MED: 84.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

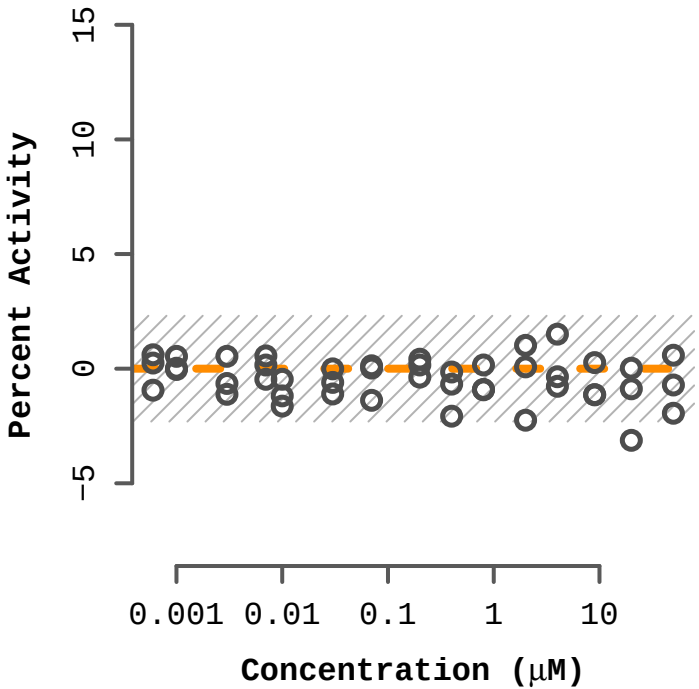
NAME: Methantheline bromide
CHID: 23277 CASRN: 53-46-3
SPID(S): Tox21_110320_1
M4ID: 12484458

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.359 **MAX_MED:** 0.135 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

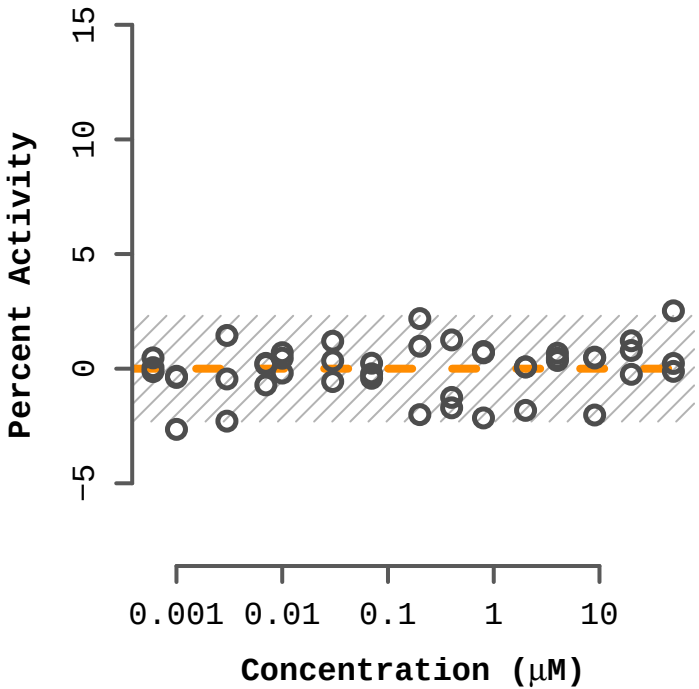
NAME: Methergine
CHID: 23283 CASRN: 113-42-8
SPID(S): Tox21_110809_1
M4ID: 12484102

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.175 **MAX_MED:** 0.247 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

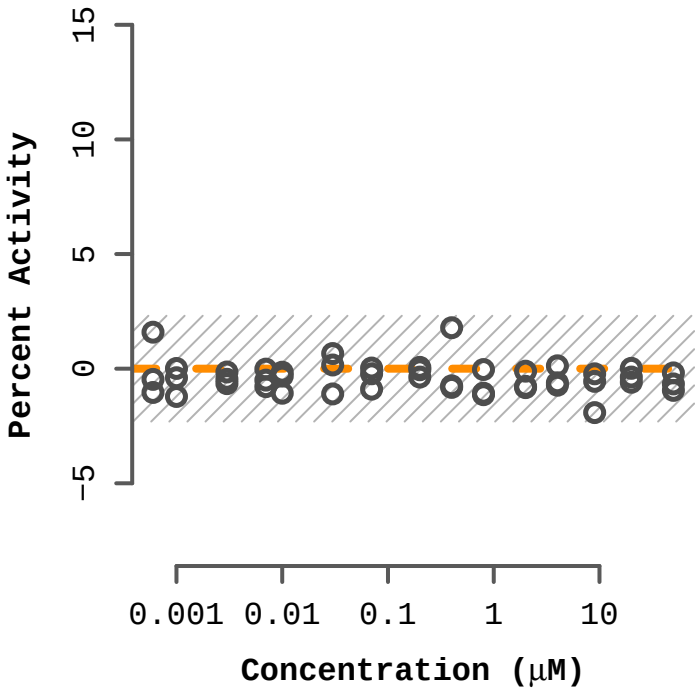
NAME: Methocarbamol
CHID: 23286 **CASRN:** 532-03-6
SPID(S): Tox21_110454_1
M4ID: 12484343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.879 **MAX_MED:** 0.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

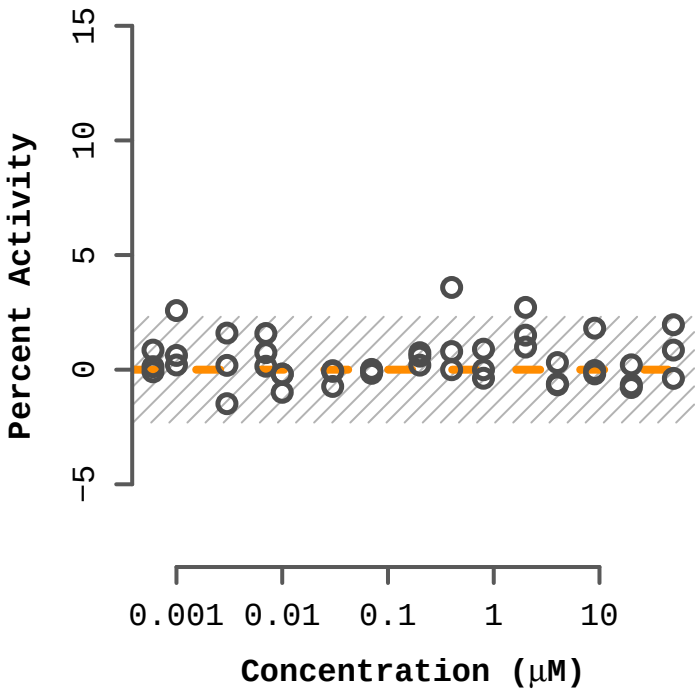
NAME: Methoxyphenamine
CHID: 23292 **CASRN:** 93-30-1
SPID(S): Tox21_113045_1
M4ID: 12482831

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.0755 **MAX_MED:** 0.162 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

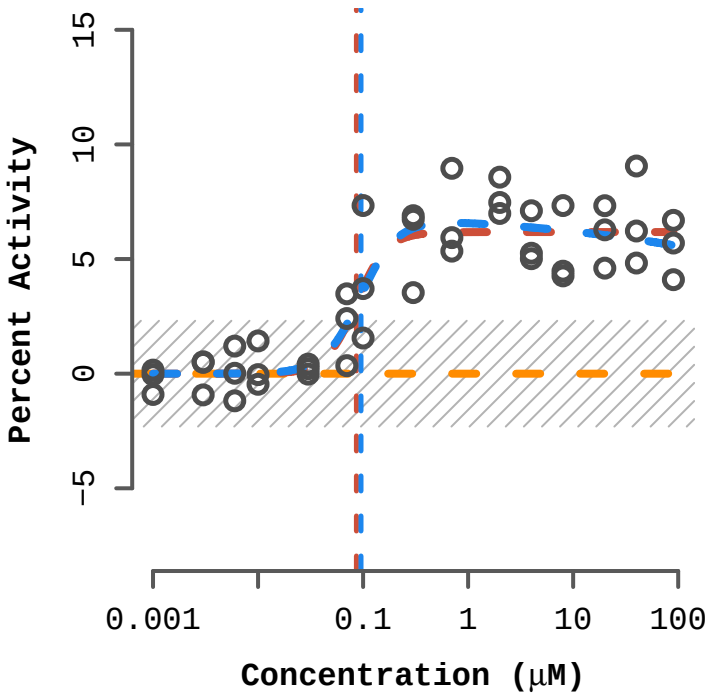
NAME: Methsuximide
CHID: 23293 **CASRN:** 77-41-8
SPID(S): Tox21_113613
M4ID: 12482579

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyldopa
CHID: 23295 CASRN: 555-30-6
SPID(S): Tox21_202610
M4ID: 12479642

HILL MODEL (in red):

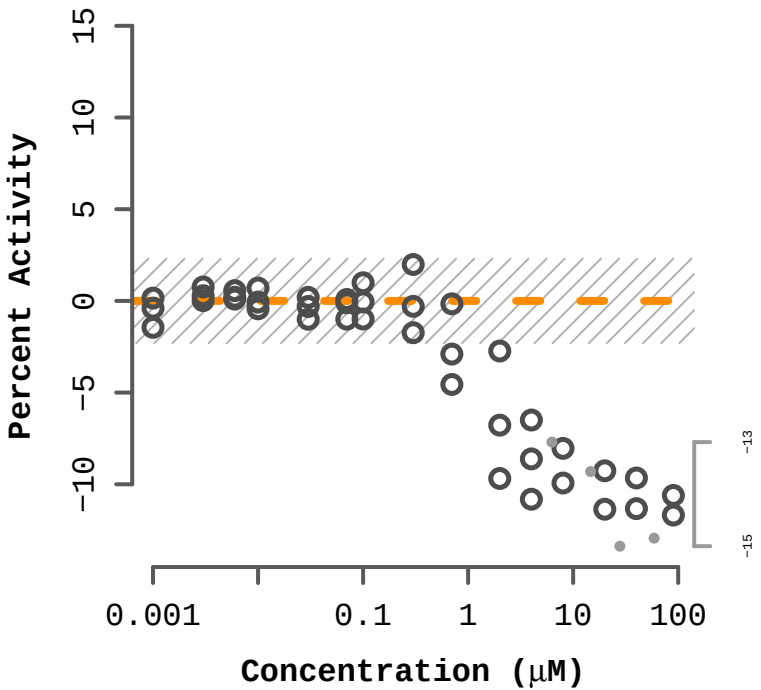
	tp	ga	gw
val:	6.18	−1.06	2.99
sd:	0.308	0.0706	1.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.01	−1.02	2.49	3.95	0.3
sd:	4.13	0.149	1.55	4.95	1.29

	CNST	HILL	GNLS
AIC:	277.89	165.44	168.12
PROB:	0	0.79	0.21
RMSE:	4.88	1.37	1.36

MAX_MEAN: 7.68 MAX_MED: 7.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

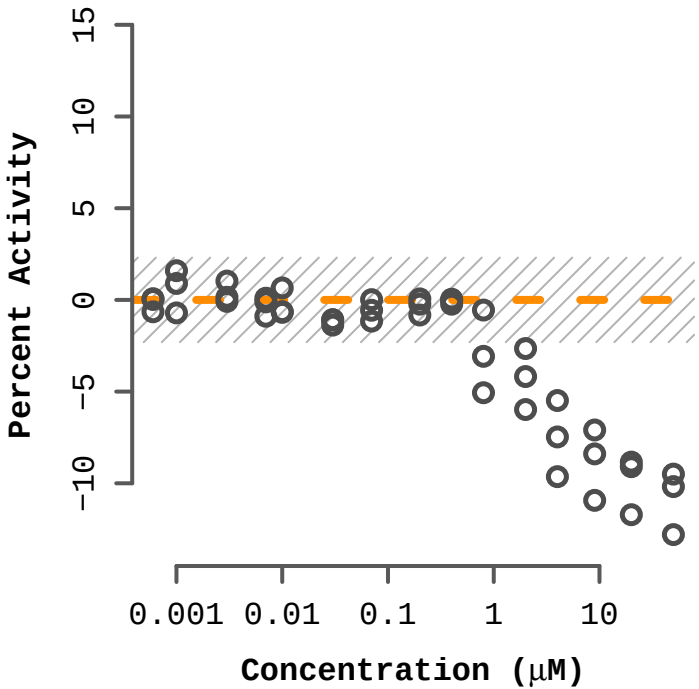
NAME: Methylene blue
CHID: 23296 **CASRN:** 61-73-4
SPID(S): Tox21_302087
M4ID: 12477046 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	302.29	NA	NA
PROB:	1	NA	NA
RMSE:	6.85	NA	NA

MAX_MEAN: 0.355 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

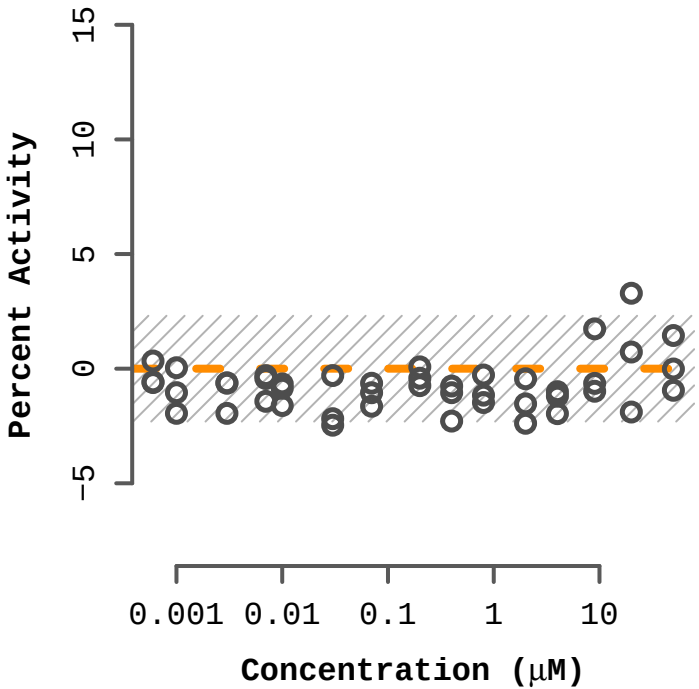
NAME: Methylene blue
CHID: 23296 **CASRN:** 61-73-4
SPID(S): Tox21_112497_1
M4ID: 12483067

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	272.68	NA	NA
PROB:	1	NA	NA
RMSE:	5.13	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

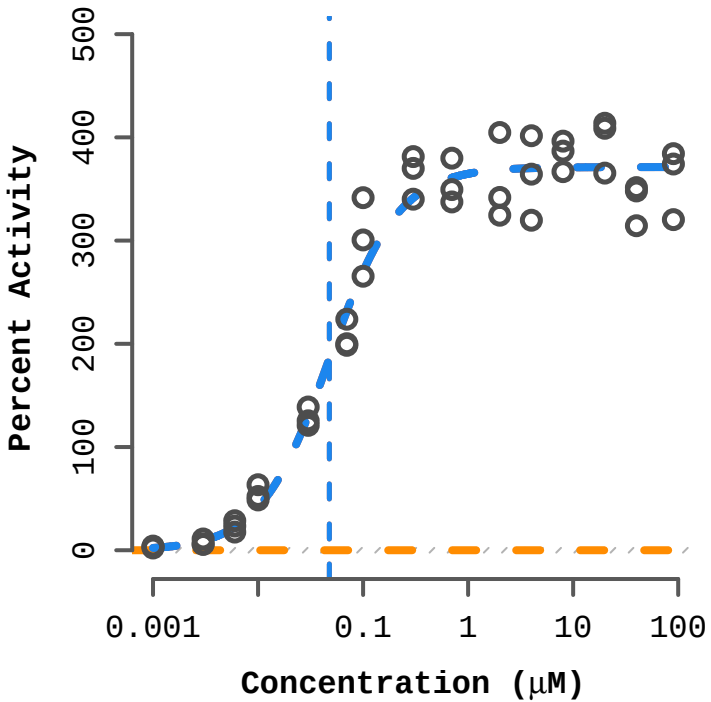
NAME: Methylperone
CHID: 23298 **CASRN:** 3575-80-2
SPID(S): Tox21_112583_1
M4ID: 12483022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.709 **MAX_MED:** 0.727 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methylprednisolone
CHID: 23300 CASRN: 83-43-2
SPID(S): Tox21_302018
M4ID: 12477115

HILL MODEL (in red):

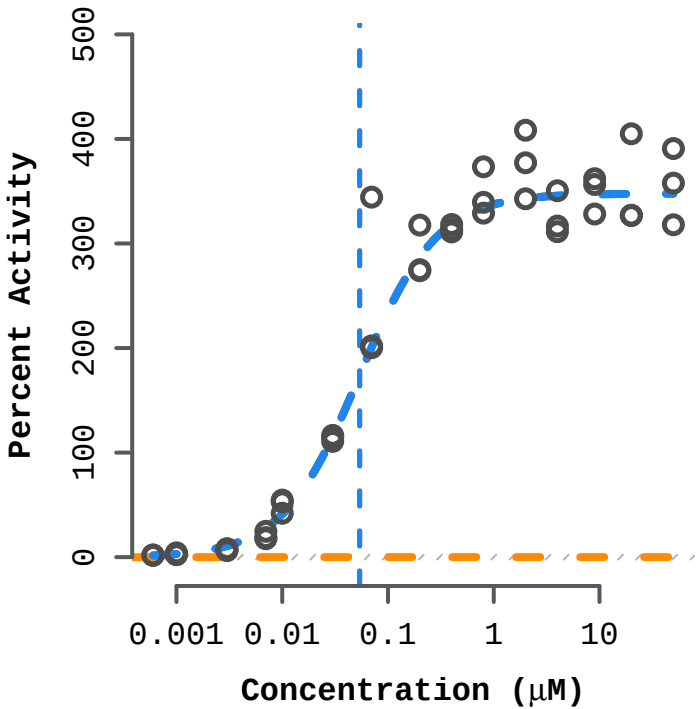
	tp	ga	gw
val:	371	-1.32	1.32
sd:	6.49	0.0347	0.118

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	371	-1.32	1.32	2.73	17.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	646.44	430.71	434.71
PROB:	0	0.88	0.12
RMSE:	285.79	26.37	26.37

MAX_MEAN: 396 MAX_MED: 409 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methylprednisolone
CHID: 23300 CASRN: 83-43-2
SPID(S): Tox21_110376_1
M4ID: 12484412

HILL MODEL (in red):

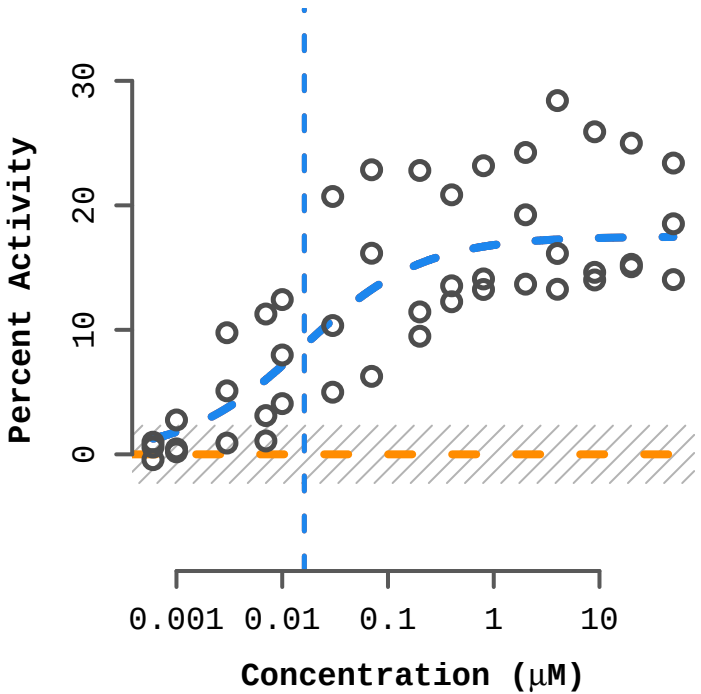
	tp	ga	gw
val:	348	-1.27	1.19
sd:	5.9	0.0313	0.0792

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	348	-1.27	1.19	2.93	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	636.86	414.76	418.76
PROB:	0	0.88	0.12
RMSE:	259.49	29.56	29.56

MAX_MEAN: 376 **MAX_MED:** 377 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methysergide
CHID: 23307 CASRN: 361-37-5
SPID(S): Tox21_110895_1
M4ID: 12484033

HILL MODEL (in red):

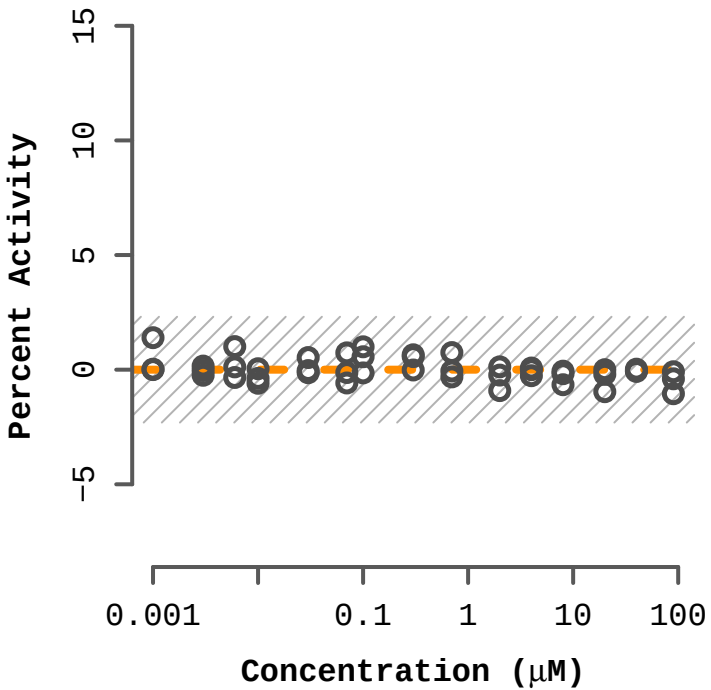
	tp	ga	gw
val:	17.5	-1.79	0.777
sd:	1.51	0.281	0.312

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.5	-1.79	0.777	2.85	15.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	378.94	282.13	286.13
PROB:	0	0.88	0.12
RMSE:	14.87	4.86	4.86

MAX_MEAN: 19.3 MAX_MED: 19.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

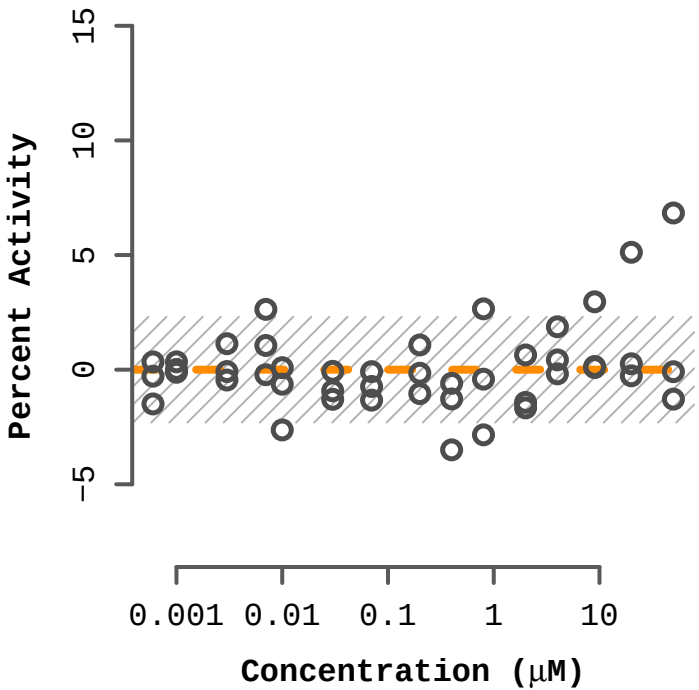
NAME: Metoprolol
CHID: 23309 **CASRN:** 51384-51-1
SPID(S): Tox21_303972
M4ID: 12475216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	65.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.5	NA	NA

MAX_MEAN: 0.475 **MAX_MED:** 0.572 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

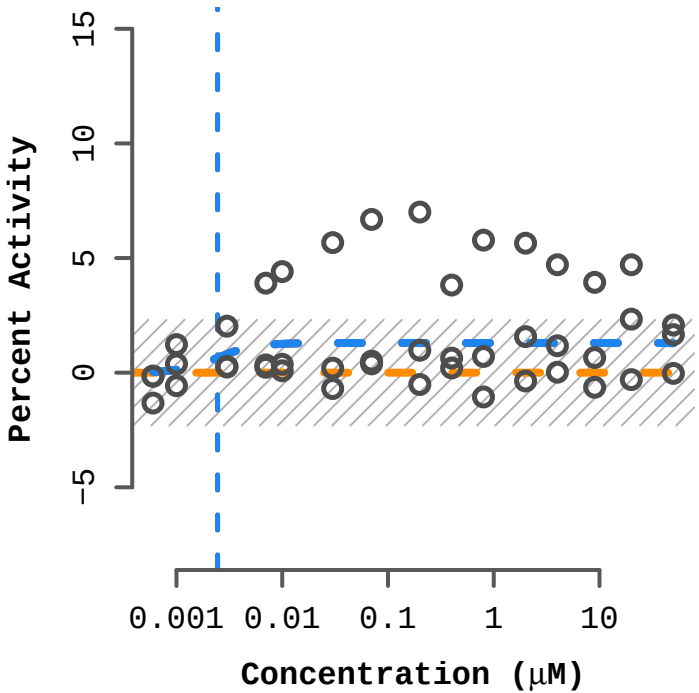
NAME: Methyclothiazide
CHID: 23313 CASRN: 135-07-9
SPID(S): Tox21_112450_1
M4ID: 12483095

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Metyrapone
CHID: 23314 **CASRN:** 54-36-4
SPID(S): Tox21_110323_1
M4ID: 12484456

HILL MODEL (in red):

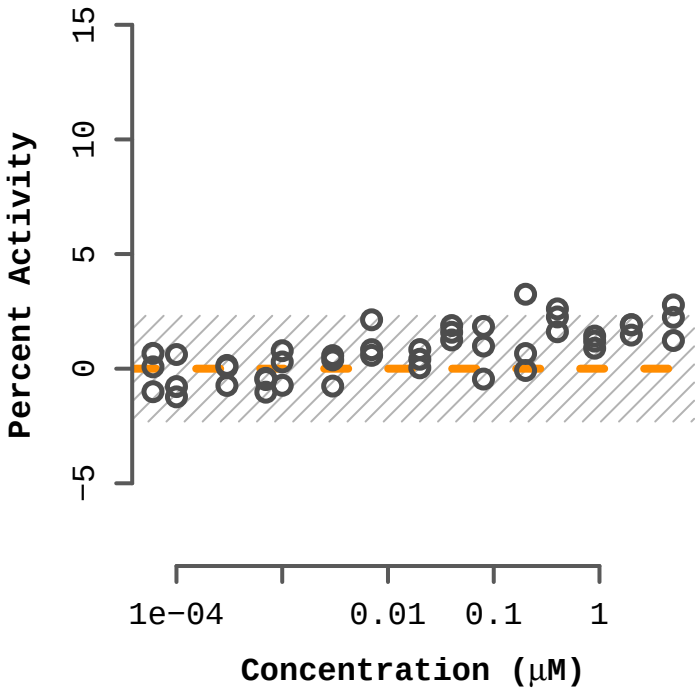
	tp	ga	gw
val:	1.29	−2.61	2.5
sd:	0.397	0.543	5.26

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.3	−2.61	2.49	1.87	10.6
sd:	0.437	0.55	5.29	18.6	1120

	CNST	HILL	GNLS
AIC:	213.92	205.29	209.29
PROB:	0.01	0.87	0.12
RMSE:	2.71	2.19	2.19

MAX_MEAN: 2.52 **MAX_MED:** 2.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

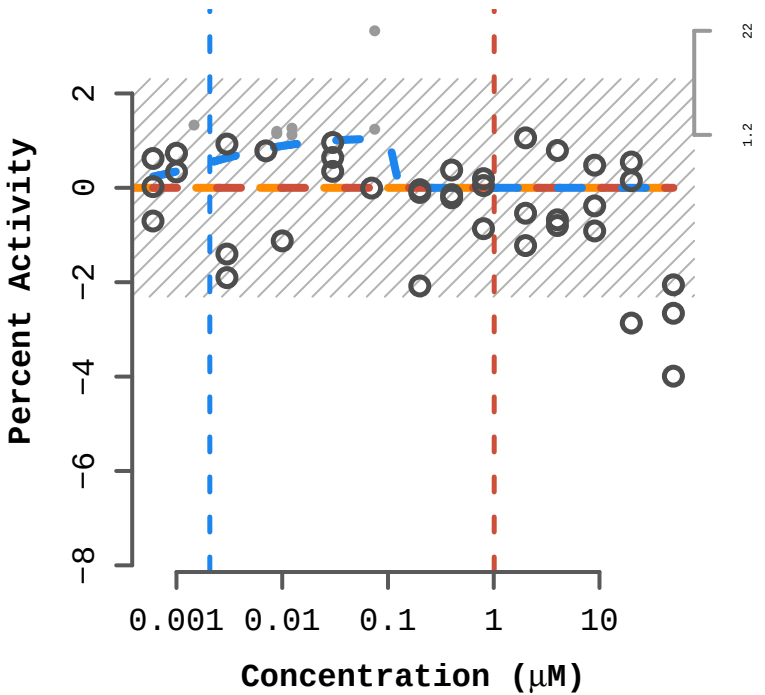
NAME: Metyrosine
CHID: 23315 **CASRN:** 672-87-7
SPID(S): Tox21_111253_1
M4ID: 12483814

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mianserin
CHID: 23317 **CASRN:** 24219-97-4
SPID(S): Tox21_110191_1
M4ID: 12484568 **BRK**

HILL MODEL (in red):

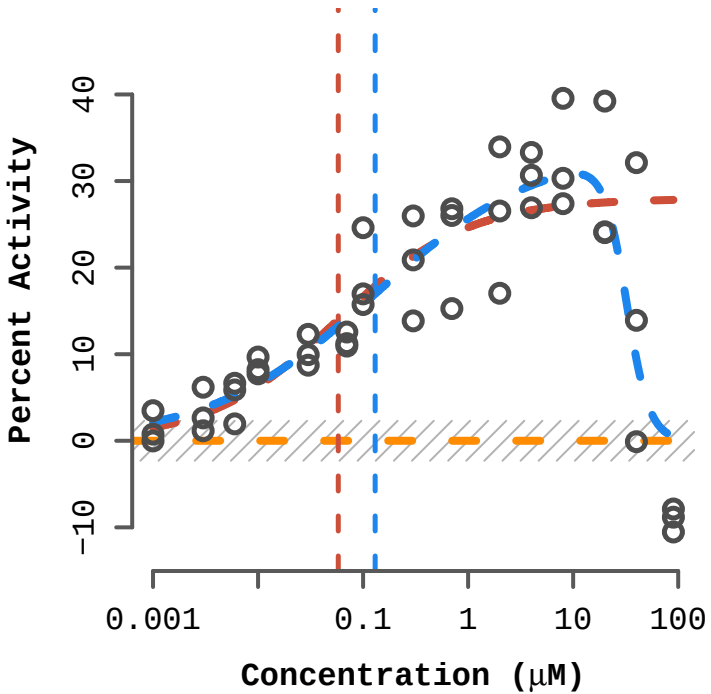
	tp	ga	gw
val:	1.91e-10	0.00434	1.41
sd:	4.19e-05	7910	41800

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.07	-2.68	1.01	-0.943	17.9
sd:	0.683	1.03	1.7	2.21	173

	CNST	HILL	GNLS
AIC:	181.58	187.58	185.06
PROB:	0.82	0.04	0.14
RMSE:	3.57	3.57	3.4

MAX_MEAN: 8.13 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mifepristone
CHID: 23322 CASRN: 84371-65-3
SPID(S): Tox21_301841
M4ID: 12477292

HILL MODEL (in red):

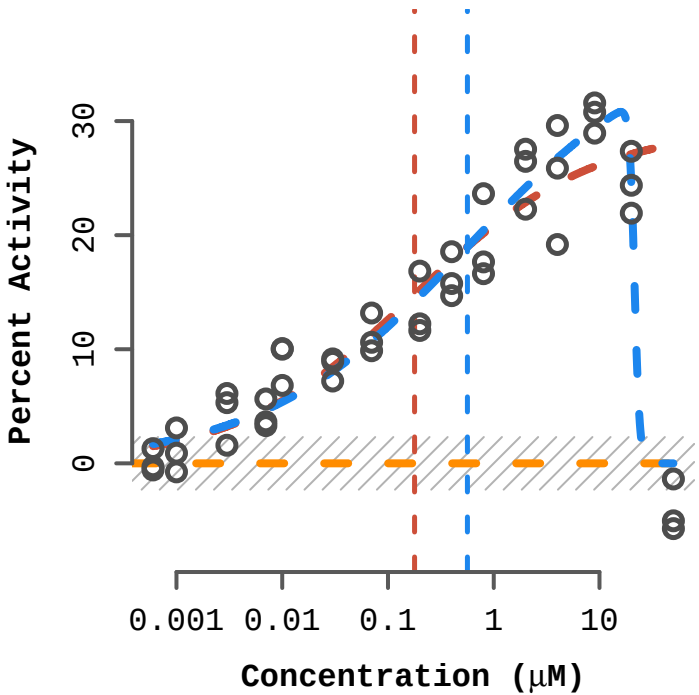
	tp	ga	gw
val:	28	−1.24	0.703
sd:	2.4	0.191	0.157

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	33.9	−0.885	0.553	1.5	4.02
sd:	5.1	0.332	0.131	0.122	1.6

	CNST	HILL	GNLS
AIC:	403.03	330.3	295.64
PROB:	0	0	1
RMSE:	19.72	11.47	6.06

MAX_MEAN: 32.4 MAX_MED: 30.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mifepristone
CHID: 23322 CASRN: 84371-65-3
SPID(S): Tox21_110952_1
M4ID: 12483989

HILL MODEL (in red):

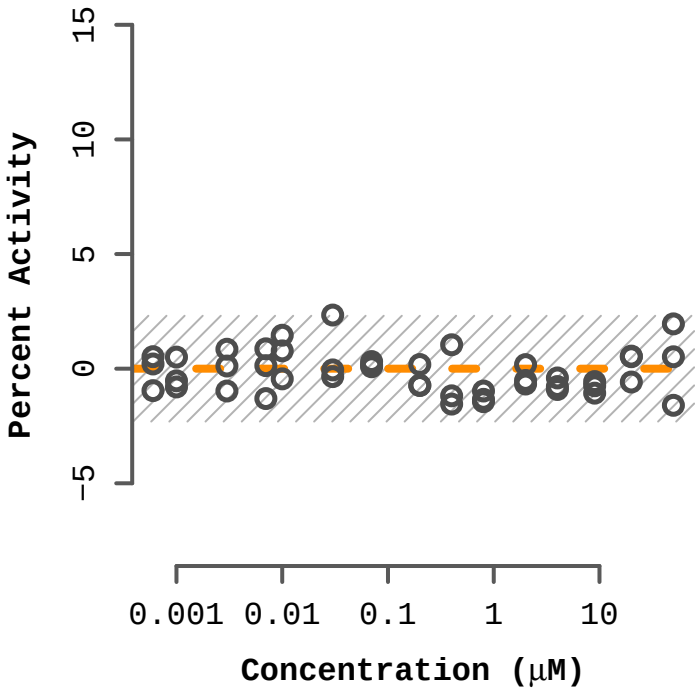
	tp	ga	gw
val:	29.5	-0.749	0.513
sd:	2.85	0.227	0.078

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	37.9	-0.249	0.446	1.33	18
sd:	4.44	0.277	0.0525	0.0116	7.55

	CNST	HILL	GNLS
AIC:	385.66	284.99	231.62
PROB:	0	0	1
RMSE:	16.36	8.73	2.69

MAX_MEAN: 30.4 MAX_MED: 30.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

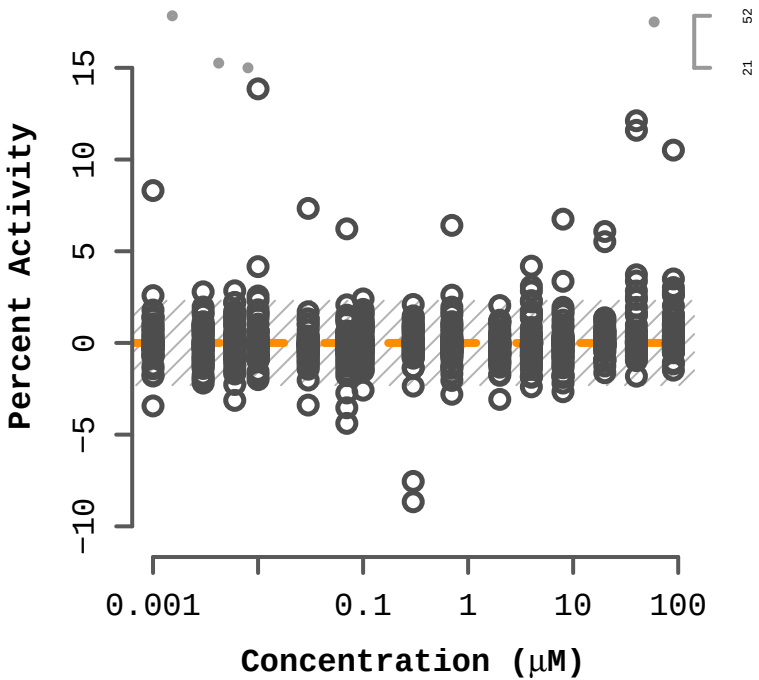
NAME: Miglitol
CHID: 23323 CASRN: 72432-03-2
SPID(S): Tox21_111436_1
M4ID: 12483689

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.648 **MAX_MED:** 0.778 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

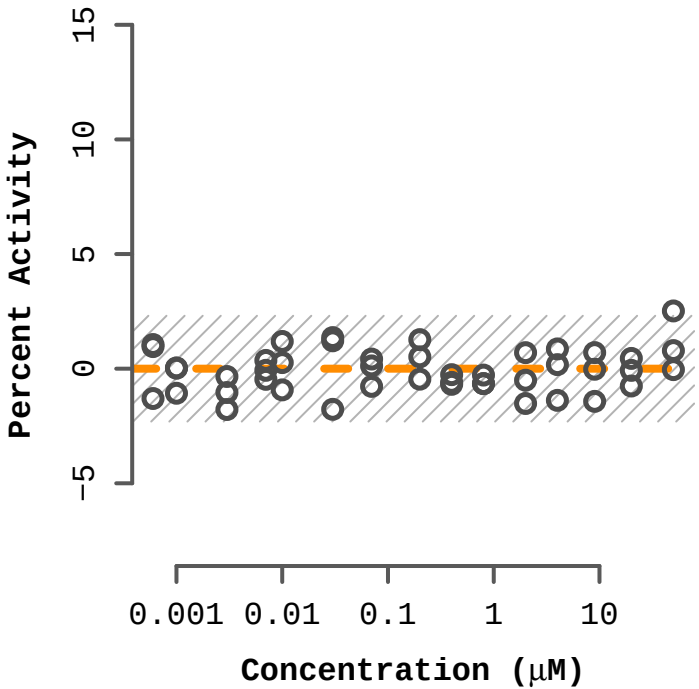
NAME: Milrinone
CHID: 23324 **CASRN:** 78415-72-2
SPID(S): Tox21_400069
M4ID: 12475068 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2354.61	NA	NA
PROB:	1	NA	NA
RMSE:	3.32	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 0.208 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

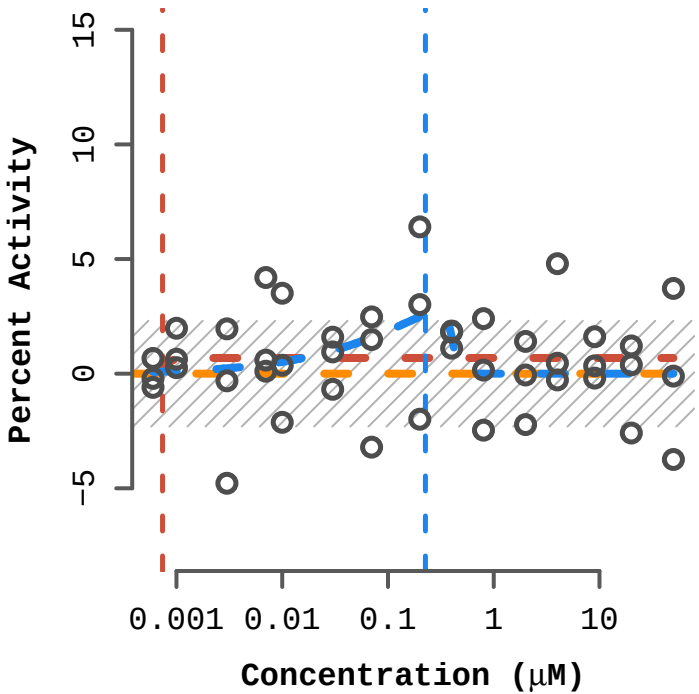
NAME: Milrinone
CHID: 23324 **CASRN:** 78415-72-2
SPID(S): Tox21_112113_1
M4ID: 12483312

HILL MODEL: Not applicable.

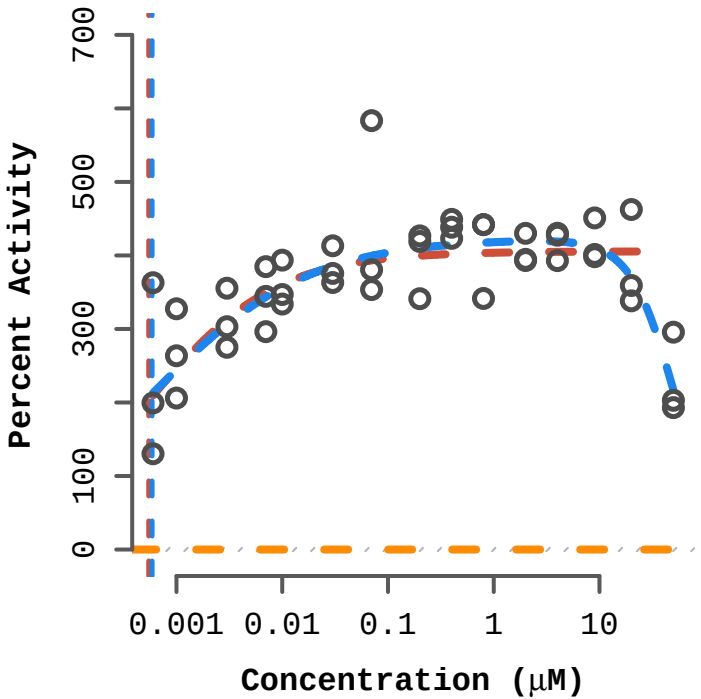
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.22 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Modafinil
CHID:    23329   CASRN: 68693-11-8
SPID(S): Tox21_111470_1
M4ID:    12483665

HILL MODEL (in red):
      tp       ga       gw
val:  0.684    -3.13    8
sd:   0.315    0.27     19.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.2      -0.646   0.708    -0.396   12.9
sd:   15.2     2.47     0.895    0.141    265

      CNST        HILL        GNLS
AIC:  203.93      205.48      206.86
PROB: 0.59        0.27        0.14
RMSE: 2.27        2.19        2.15

MAX_MEAN: 2.48      MAX_MED: 3.02      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mometasone furoate
CHID: 23333 CASRN: 83919-23-7
SPID(S): Tox21_110705_1
M4ID: 12484163

HILL MODEL (in red):

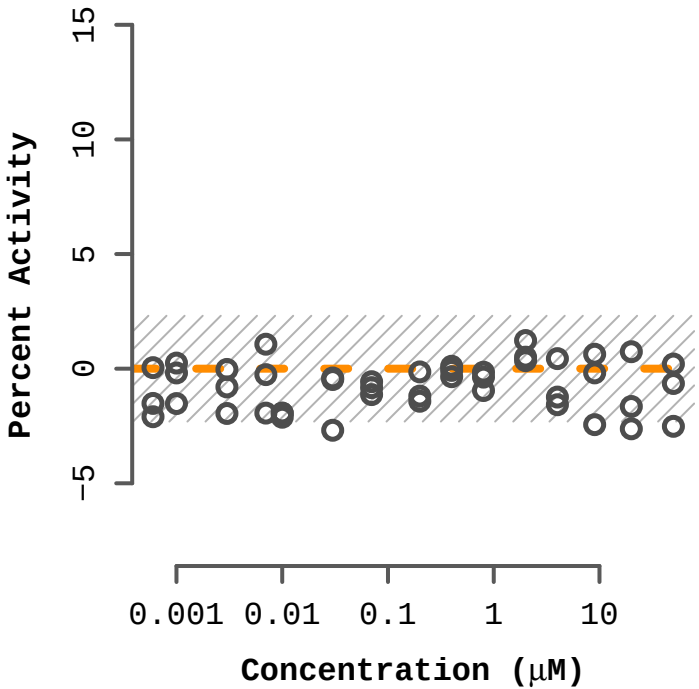
	tp	ga	gw
val:	406	-3.26	0.715
sd:	11.7	0.174	0.191

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	423	-3.23	0.589	1.71	2.07
sd:	13.7	0.165	0.152	0.0525	0.691

	CNST	HILL	GNLS
AIC:	672.29	507.08	486.7
PROB:	0	0	1
RMSE:	371.67	69.1	51.64

MAX_MEAN: 439 MAX_MED: 442 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

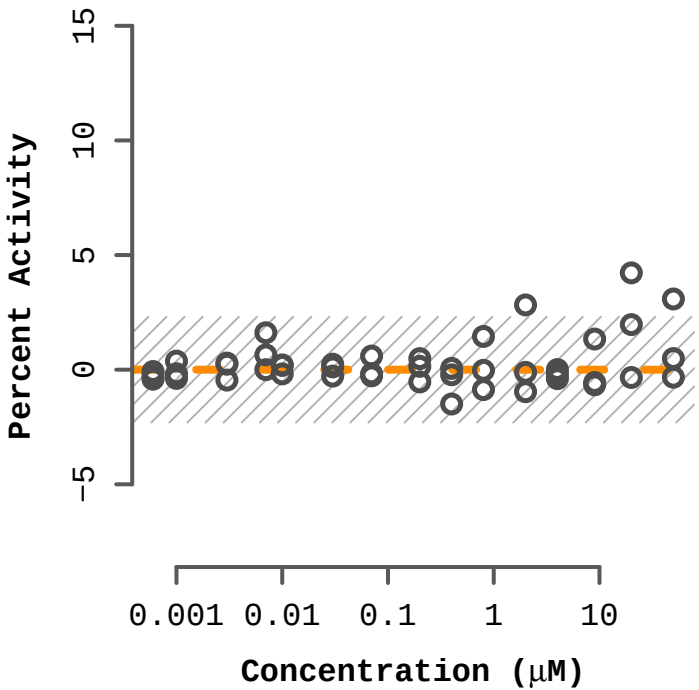
NAME: Mycophenolate mofetil
CHID: 23340 CASRN: 128794-94-5
SPID(S): Tox21_111686_1
M4ID: 12483535

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.695 **MAX_MED:** 0.504 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

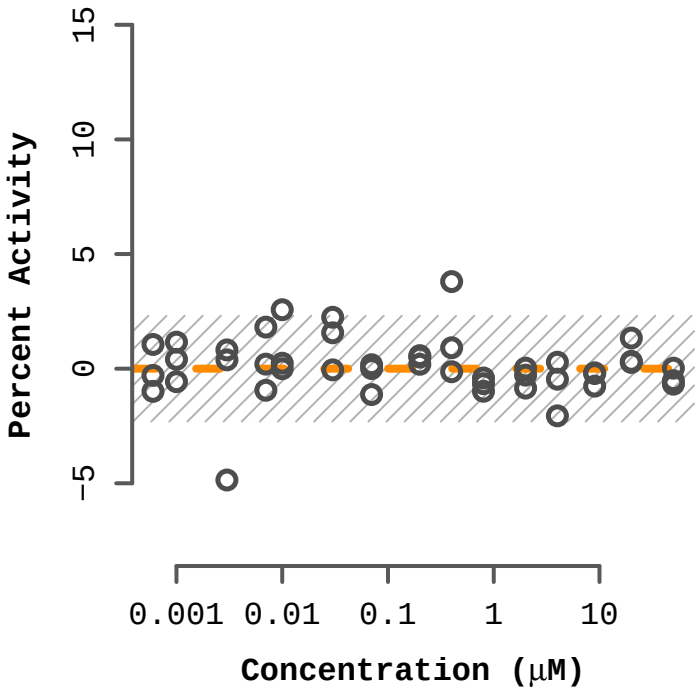
NAME: Nadolol
CHID: 23342 CASRN: 42200-33-9
SPID(S): Tox21_110646_1
M4ID: 12484209

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.95 MAX_MED: 1.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

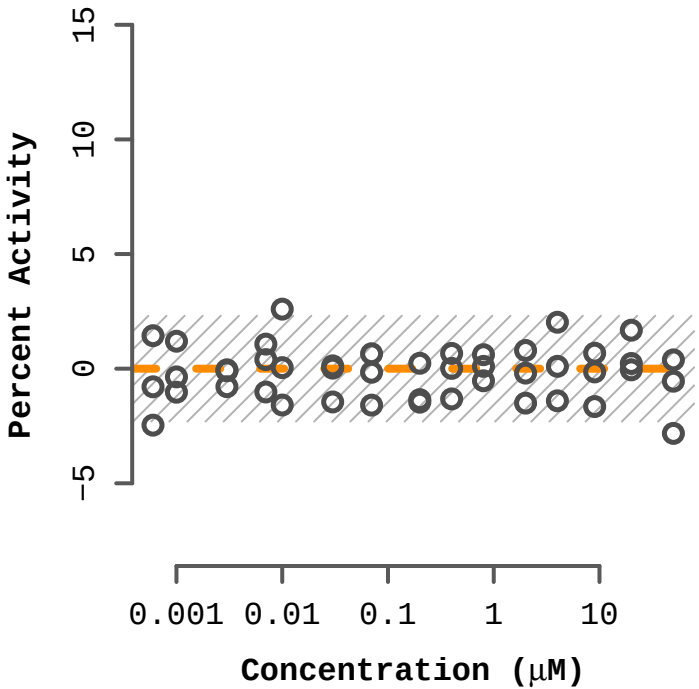
NAME: Nalmefene
CHID: 23347 **CASRN:** 55096-26-9
SPID(S): Tox21_110873_1
M4ID: 12484054

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

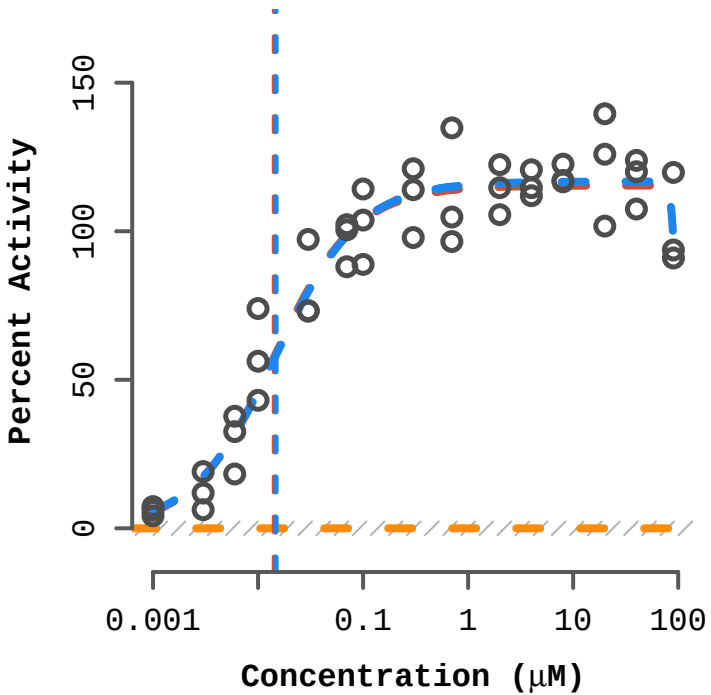
NAME: Naloxone
CHID: 23349 CASRN: 465-65-6
SPID(S): Tox21_112006_1
M4ID: 12483376

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.619 **MAX_MED:** 0.398 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nandrolone
CHID: 23350 CASRN: 434-22-0
SPID(S): Tox21_201212
M4ID: 12481040

HILL MODEL (in red):

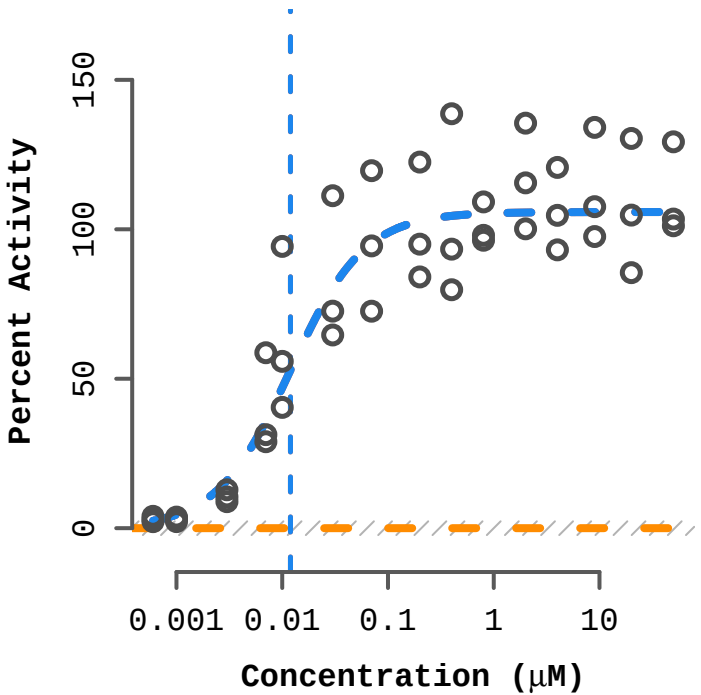
	tp	ga	gw
val:	115	-1.85	1.12
sd:	2.46	0.059	0.127

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	117	-1.83	1.09	1.99	17.8
sd:	2.43	0.0568	0.117	0.0101	5.18

	CNST	HILL	GNLS
AIC:	548.86	353.7	352.73
PROB:	0	0.38	0.62
RMSE:	95.47	11.12	10.58

MAX_MEAN: 122 MAX_MED: 126 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nandrolone
CHID: 23350 CASRN: 434-22-0
SPID(S): Tox21_113167_1
M4ID: 12482784

HILL MODEL (in red):

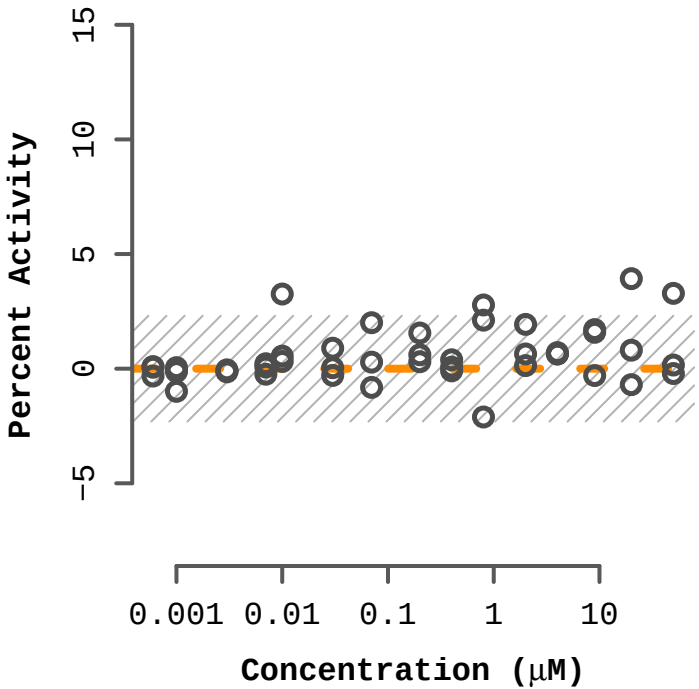
	tp	ga	gw
val:	106	-1.92	1.25
sd:	3.56	0.0977	0.299

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	106	-1.92	1.25	3.69	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	541.36	387.38	391.38
PROB:	0	0.88	0.12
RMSE:	88.67	16.43	16.43

MAX_MEAN: 117 MAX_MED: 116 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

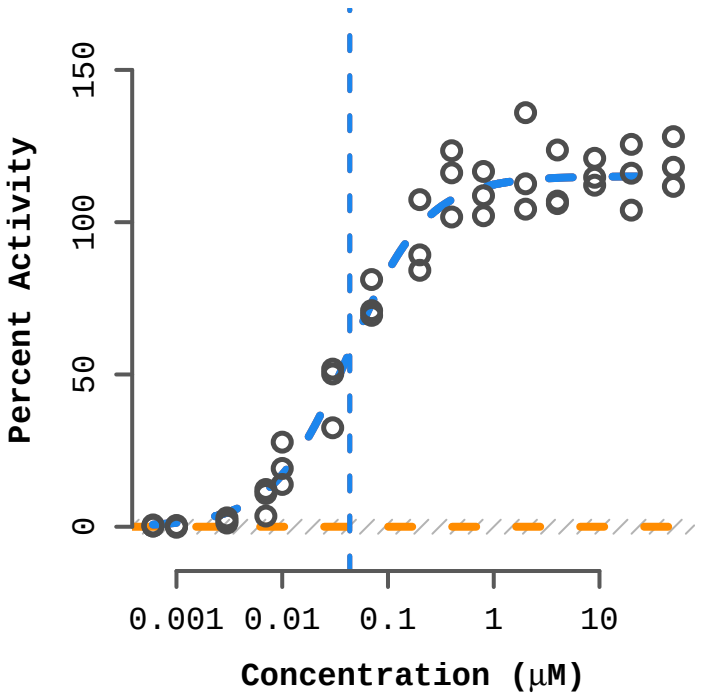
NAME: Nandrolone decanoate
CHID: 23352 CASRN: 360-70-3
SPID(S): Tox21_111638_1
M4ID: 12483569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nandrolone phenpropionate
CHID: 23353 CASRN: 62-90-8
SPID(S): Tox21_113342_1
M4ID: 12482685

HILL MODEL (in red):

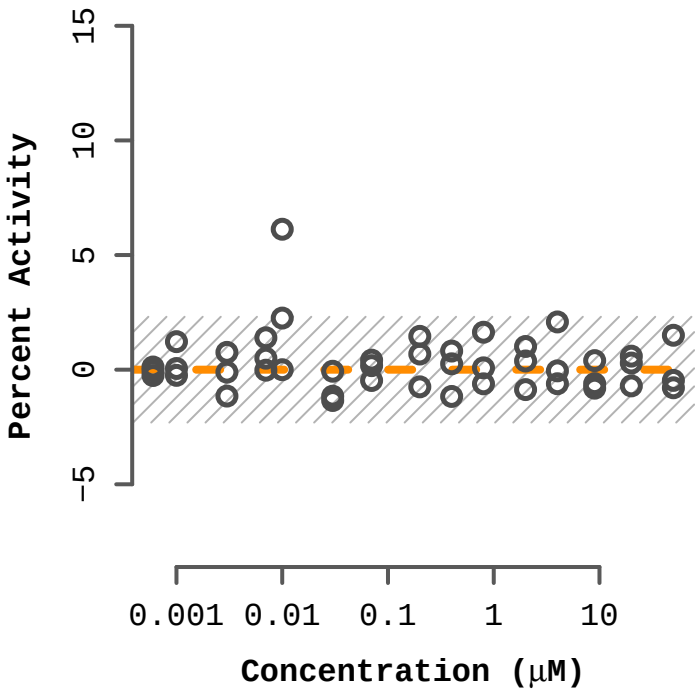
	tp	ga	gw
val:	115	-1.36	1.19
sd:	2.03	0.0439	0.107

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	115	-1.36	1.19	3.17	5.52
sd:	2.03	0.0439	0.107	596	2230

	CNST	HILL	GNLS
AIC:	537.1	320.87	324.87
PROB:	0	0.88	0.12
RMSE:	85.53	7.71	7.71

MAX_MEAN: 119 **MAX_MED:** 118 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

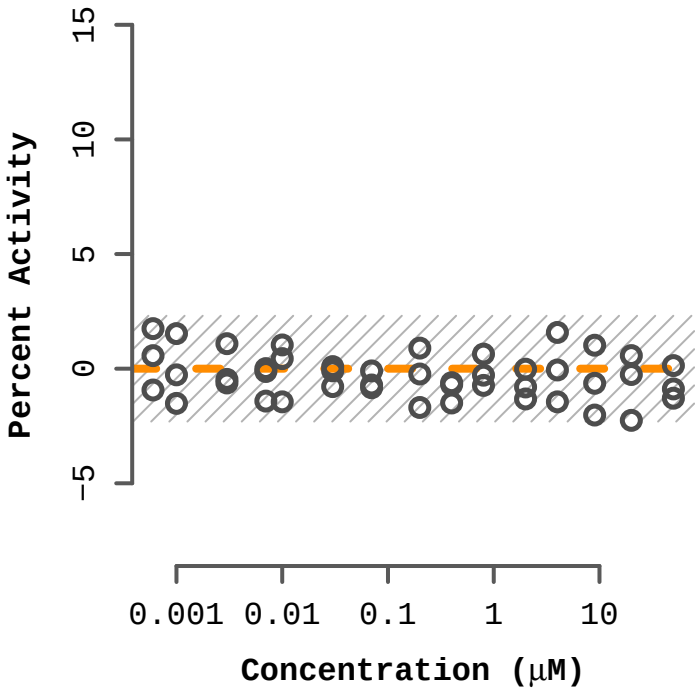
NAME: Nedocromil
CHID: 23356 **CASRN:** 69049-73-6
SPID(S): Tox21_113148_1
M4ID: 12482789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 2.79 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

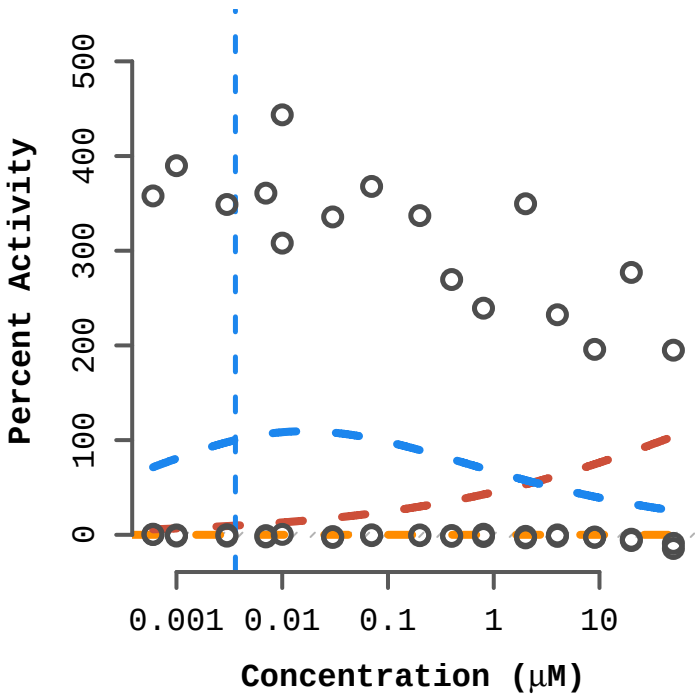
NAME: Nialamide
CHID: 23362 **CASRN:** 51-12-7
SPID(S): Tox21_110208_1
M4ID: 12484551

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.463 **MAX_MED:** 0.571 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nicardipine
CHID: 23363 **CASRN:** 55985-32-5
SPID(S): Tox21_110211_1
M4ID: 12484549

HILL MODEL (in red):

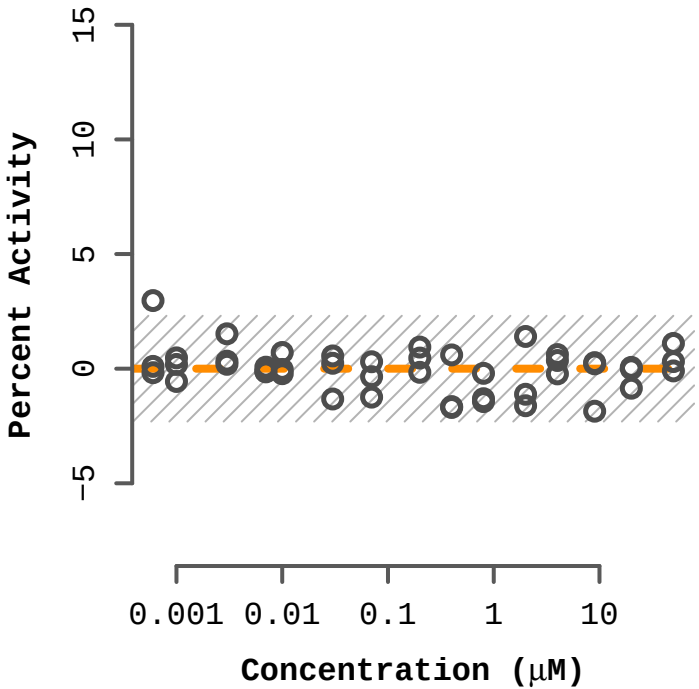
	tp	ga	gw
val:	251	2.2	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	339	-2.44	0.483	-1.91	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	664.77	600.79	599.41
PROB:	0	0.33	0.67
RMSE:	191.21	179.21	157.87

MAX_MEAN: 251 **MAX_MED:** 308 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

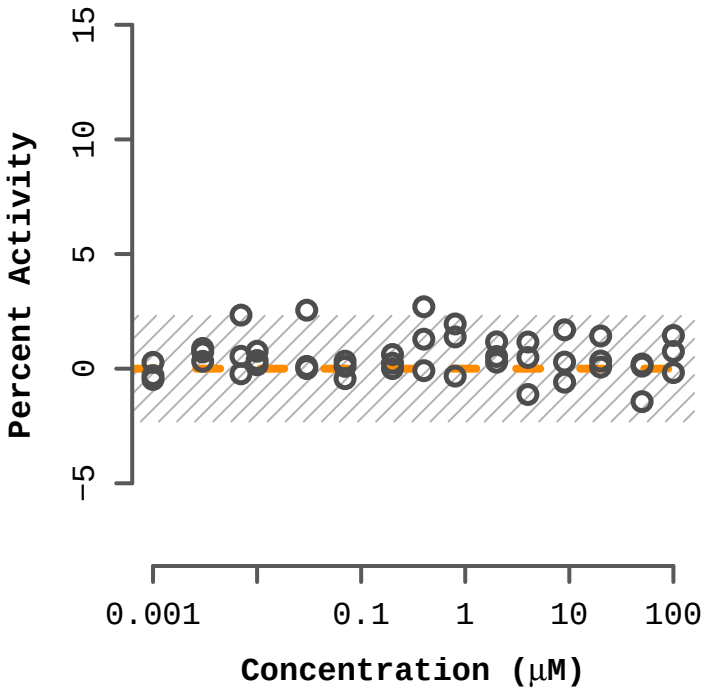
NAME: Niceritrol
CHID: 23364 **CASRN:** 5868-05-3
SPID(S): Tox21_113126_1
M4ID: 12482797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.967 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

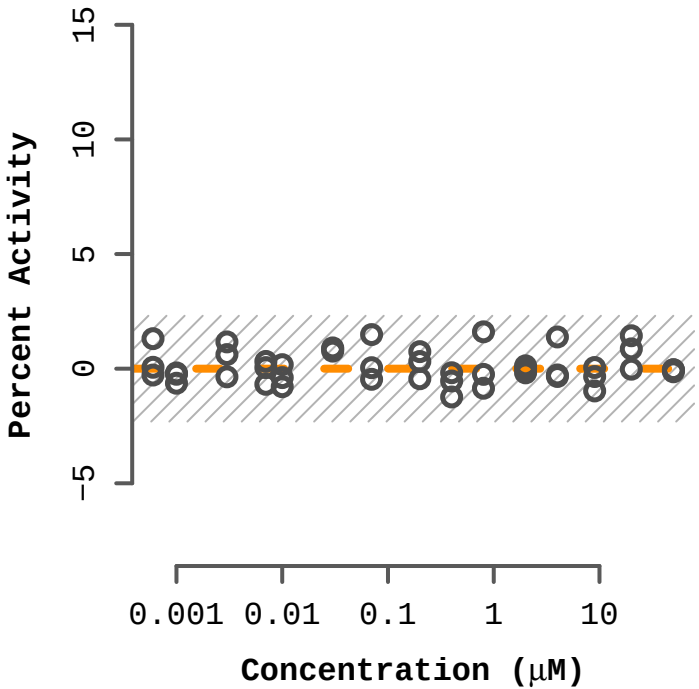
NAME: Nicotinyl alcohol
CHID: 23367 **CASRN:** 100-55-0
SPID(S): Tox21_300839
M4ID: 12478294

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.66	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

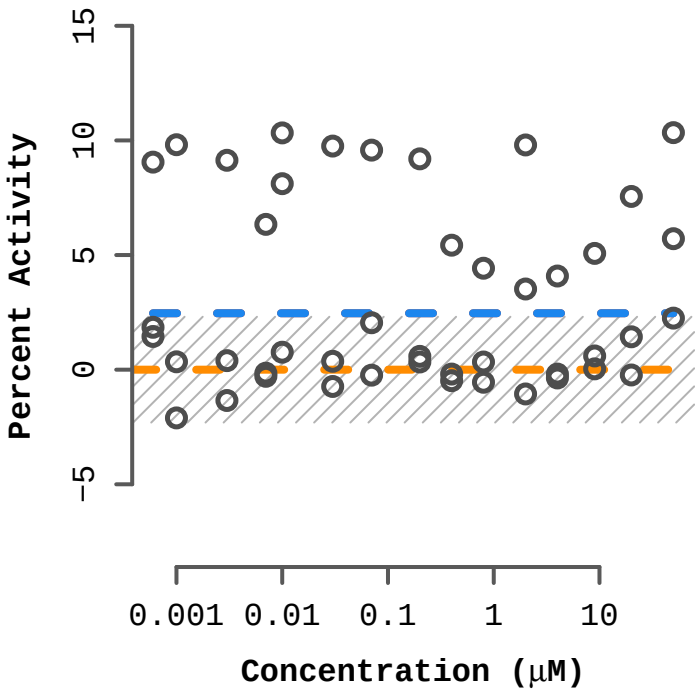
NAME: Nicotinyl alcohol
CHID: 23367 **CASRN:** 100-55-0
SPID(S): Tox21_113448_1
M4ID: 12482649

HILL MODEL: Not applicable.

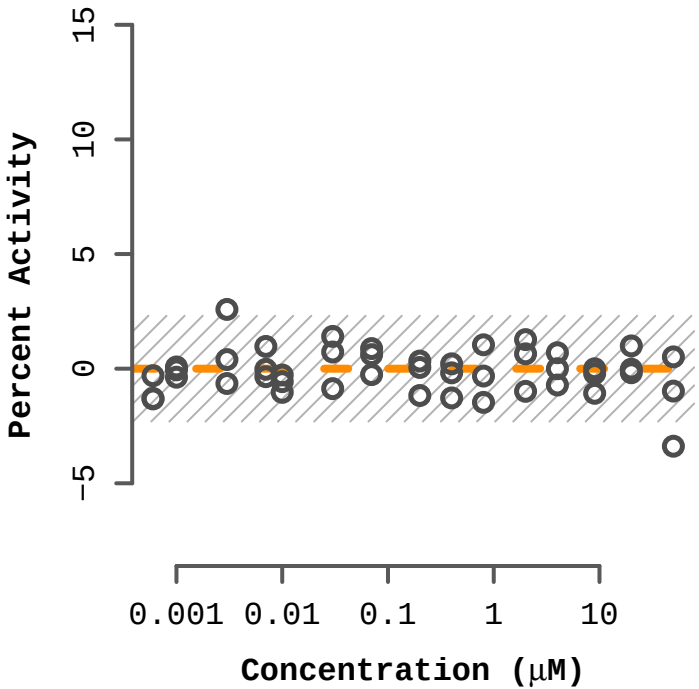
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 0.865 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Niflumic acid
CHID:    23368   CASRN: 4394-00-7
SPID(S): Tox21_110206_1
M4ID:    12484553

HILL MODEL (in red):
      tp       ga       gw
val:  2.46     -4.92    4.02
sd:   0.656    1210     2930

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.46     -4.45    5.49     3.64     3.58
sd:   0.656    811      3650     858      1580

      CNST        HILL        GNLS
AIC:  275.77      266.35      270.35
PROB: 0.01        0.87        0.12
RMSE: 5.1         4.06        4.06

MAX_MEAN: 6.4       MAX_MED: 8.12      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

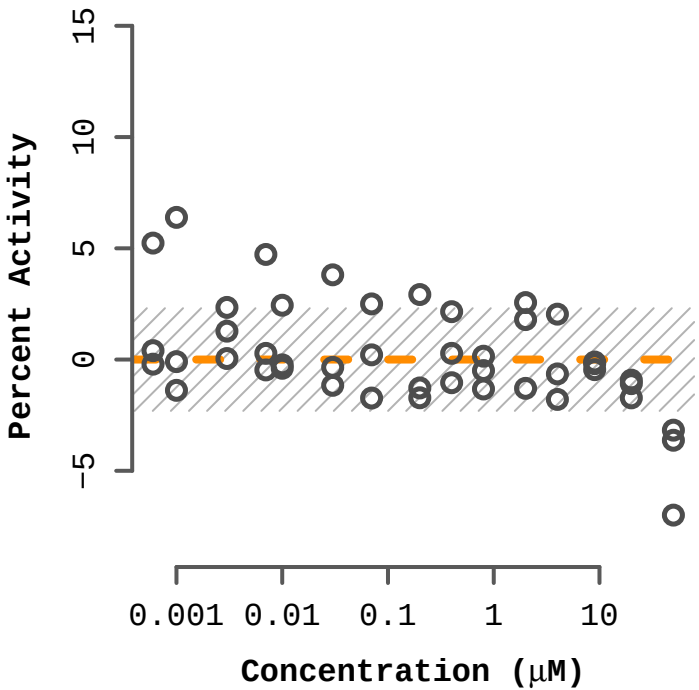
NAME: Nimetazepam
CHID: 23369 **CASRN:** 2011-67-8
SPID(S): Tox21_112205_1
M4ID: 12483238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.78 **MAX_MED:** 0.729 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

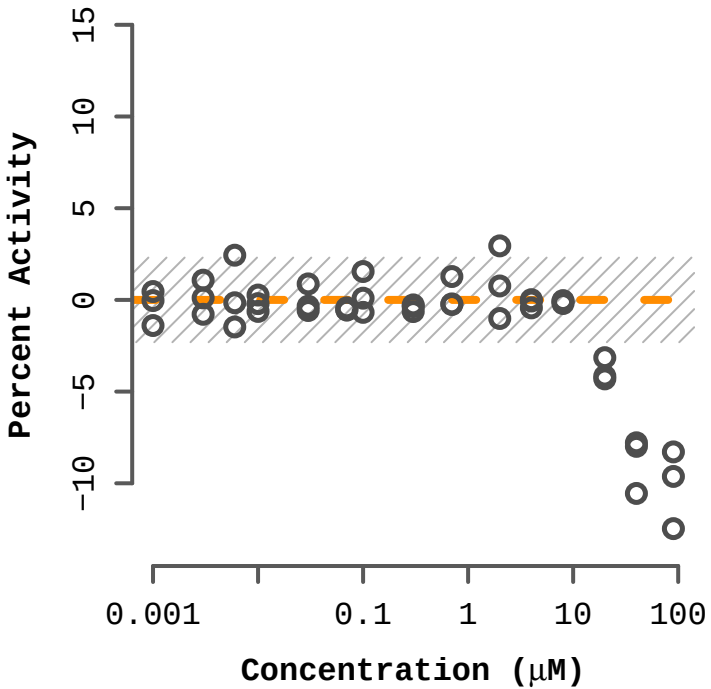
NAME: Nimodipine
CHID: 23370 CASRN: 66085-59-4
SPID(S): Tox21_110202_1
M4ID: 12484557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.35	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

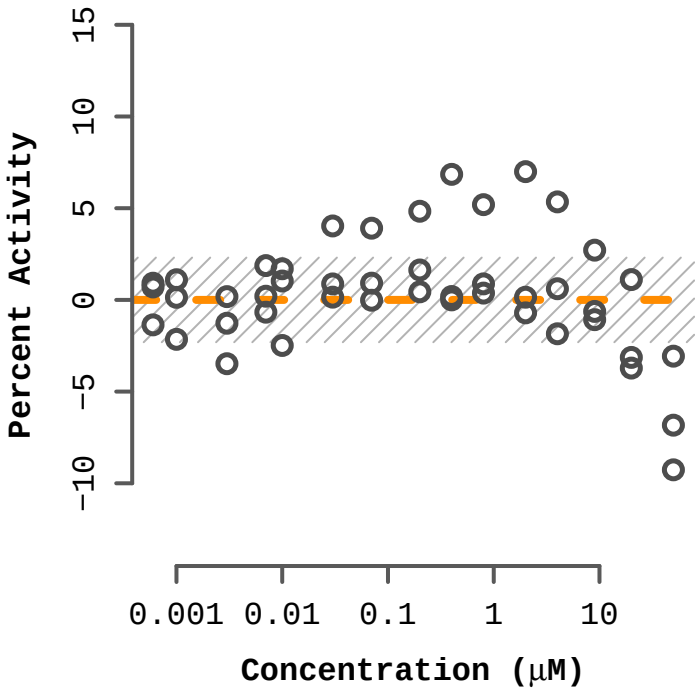
NAME: Nisoldipine
CHID: 23371 **CASRN:** 63675-72-9
SPID(S): Tox21_302365
M4ID: 12476768

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.74	NA	NA

MAX_MEAN: 0.899 **MAX_MED:** 0.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

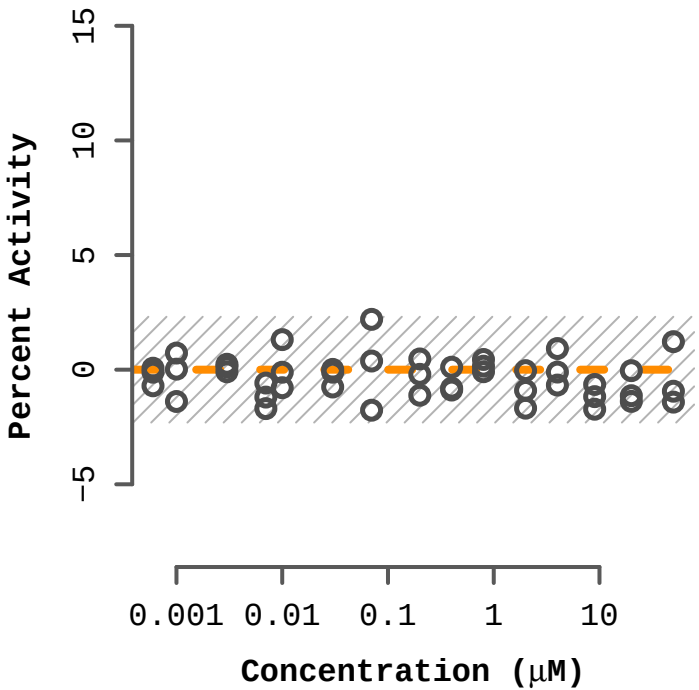
NAME: Nisoldipine
CHID: 23371 **CASRN:** 63675-72-9
SPID(S): Tox21_112251_1
M4ID: 12483201

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.83	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 2.35 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

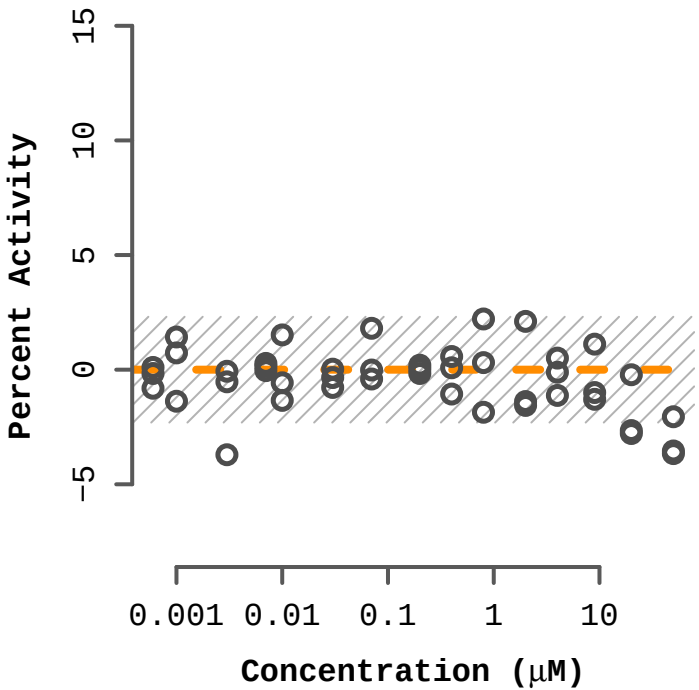
NAME: Nitrazepam
CHID: 23372 **CASRN:** 146-22-5
SPID(S): Tox21_111601_1
M4ID: 12483595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.269 **MAX_MED:** 0.378 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

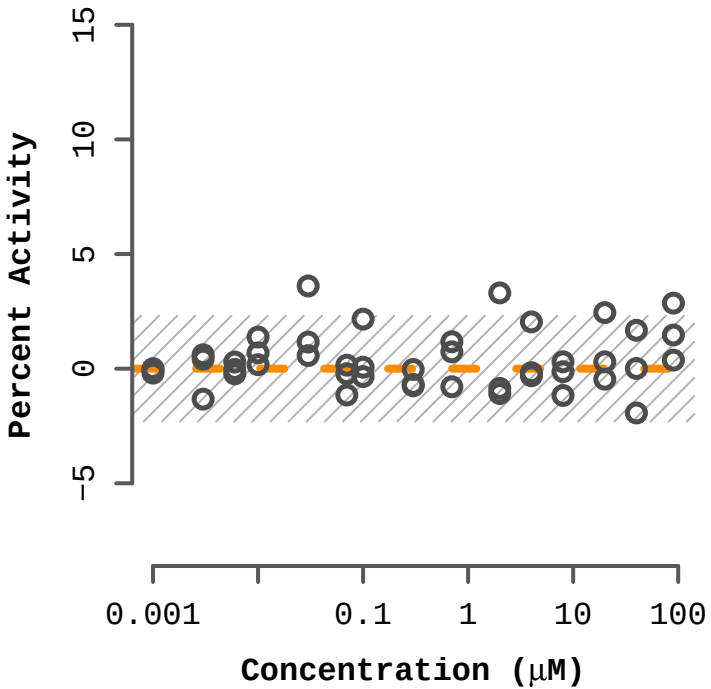
NAME: Nitrendipine
CHID: 23373 **CASRN:** 39562-70-4
SPID(S): Tox21_110201_1
M4ID: 12484558

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.462 **MAX_MED:** 0.733 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

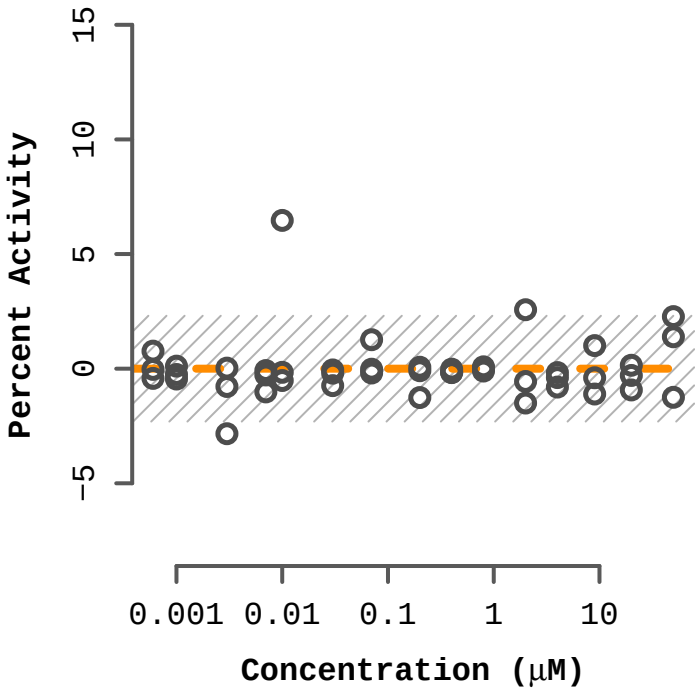
NAME: Nizatidine
CHID: 23376 **CASRN:** 76963-41-2
SPID(S): Tox21_301594
M4ID: 12477539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

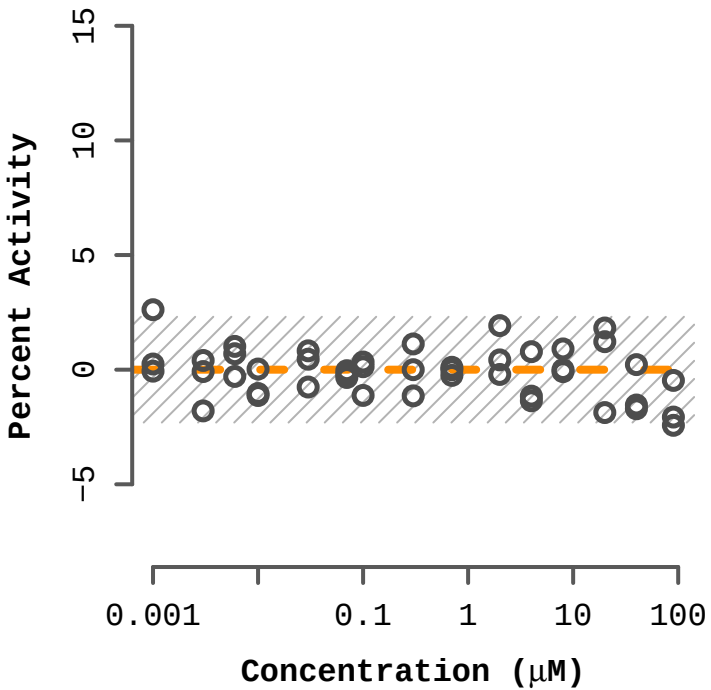
NAME: Nizatidine
CHID: 23376 **CASRN:** 76963-41-2
SPID(S): Tox21_110691_1
M4ID: 12484175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

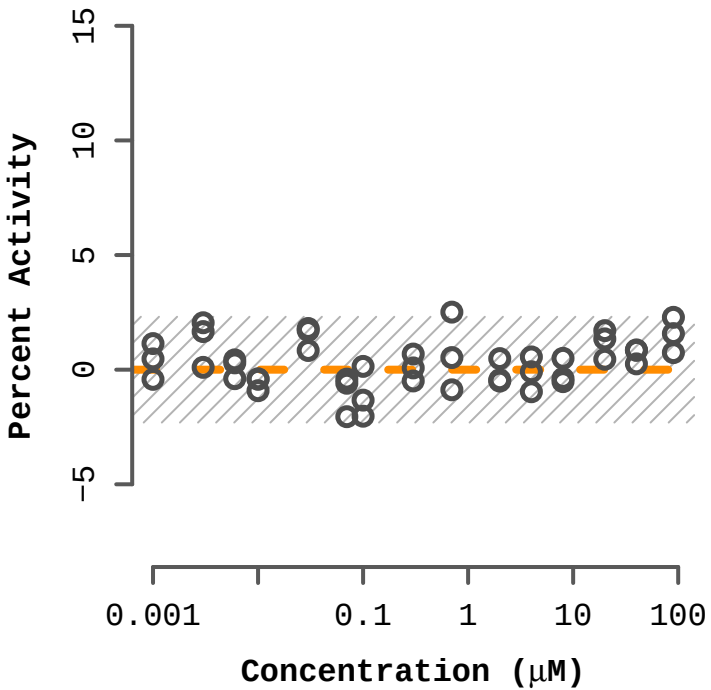
NAME: Nomifensine
CHID: 23377 **CASRN:** 24526-64-5
SPID(S): Tox21_301755
M4ID: 12477378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.934 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

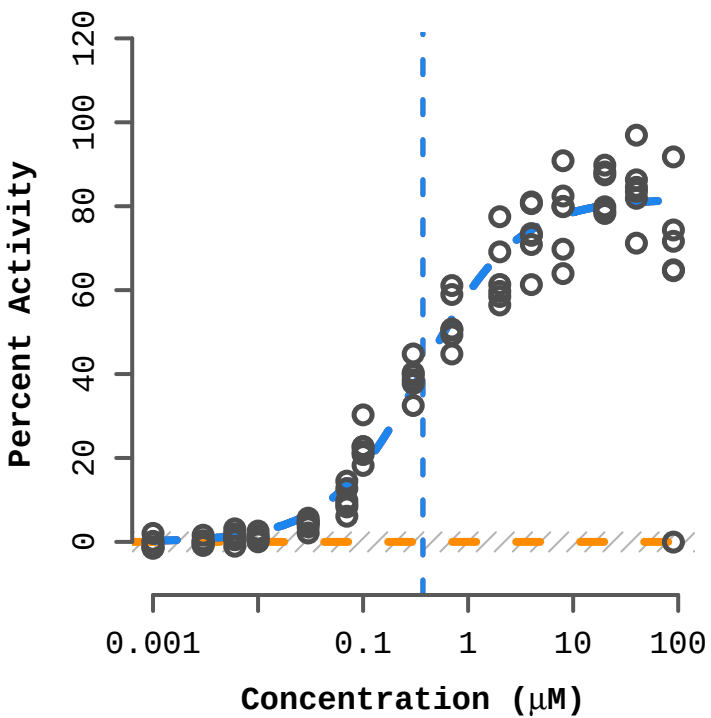
NAME: Norepinephrine
CHID: 23378 **CASRN:** 51-41-2
SPID(S): Tox21_301944
M4ID: 12477189

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norethindrone
CHID: 23380 CASRN: 68-22-4
SPID(S): Tox21_302427
M4ID: 12476706

HILL MODEL (in red):

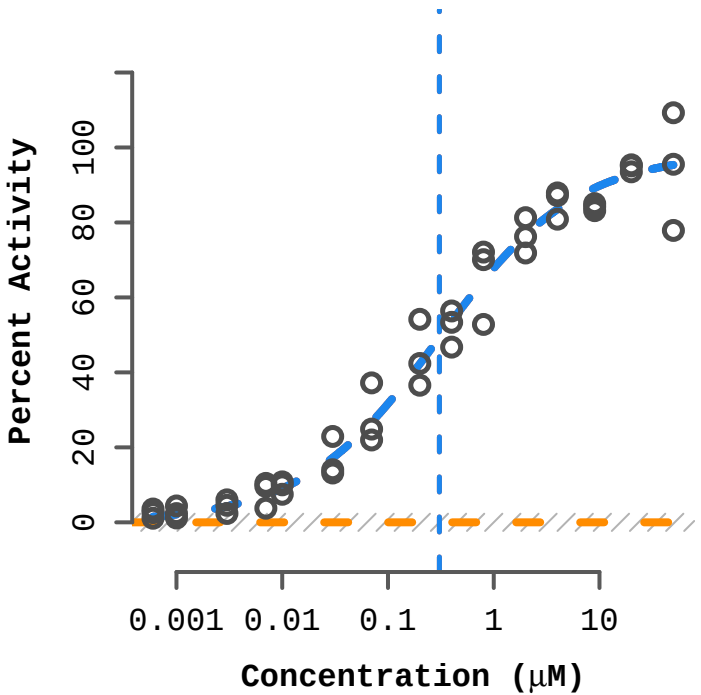
	tp	ga	gw
val:	81.8	-0.43	0.971
sd:	1.85	0.0457	0.0669

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	81.8	-0.43	0.971	3.04	12.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	974.77	605.94	609.94
PROB:	0	0.88	0.12
RMSE:	51.26	10.52	10.52

MAX_MEAN: 84.1 MAX_MED: 84 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norethindrone
CHID: 23380 CASRN: 68-22-4
SPID(S): Tox21_111322_1
M4ID: 12483769

HILL MODEL (in red):

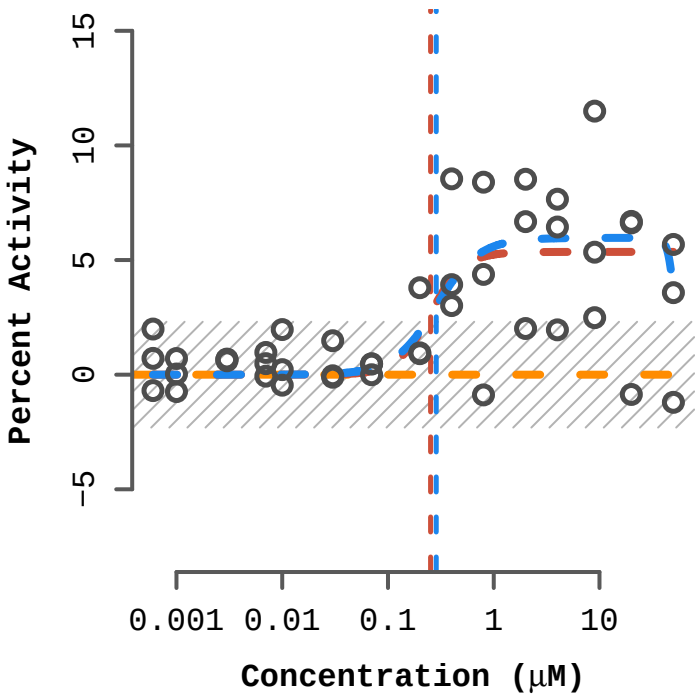
	tp	ga	gw
val:	98.5	-0.514	0.669
sd:	2.88	0.0695	0.0473

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	98.5	-0.514	0.669	3.52	6.96
sd:	2.88	0.0695	0.0473	74200	267000

	CNST	HILL	GNLS
AIC:	498.23	285.23	289.23
PROB:	0	0.88	0.12
RMSE:	56.93	5.53	5.53

MAX_MEAN: 94.7 MAX_MED: 95.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Noscapine
CHID: 23385 **CASRN:** 128-62-1
SPID(S): Tox21_110413_1
M4ID: 12484381

HILL MODEL (in red):

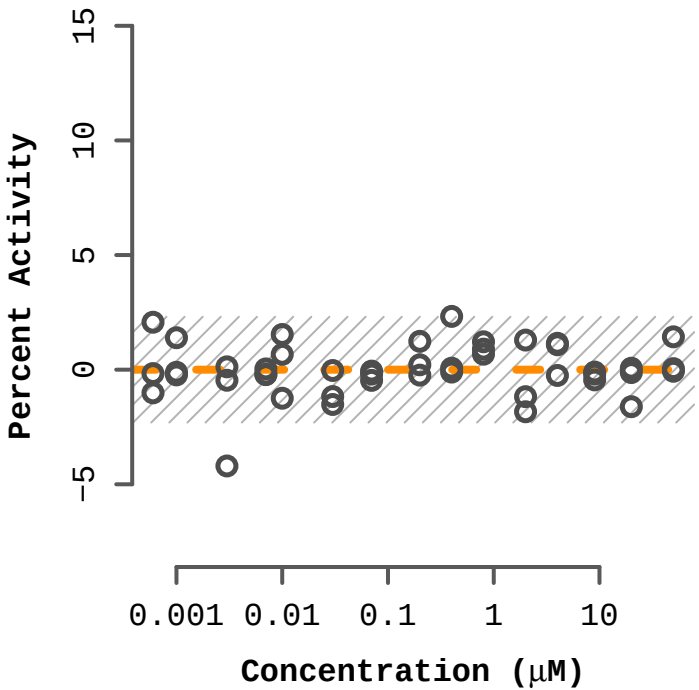
	tp	ga	gw
val:	5.36	−0.597	2.77
sd:	0.66	0.123	2.45

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.97	−0.544	2.16	1.71	13.9
sd:	0.705	0.13	1.53	0.071	76.2

	CNST	HILL	GNLS
AIC:	252.93	208.76	210.08
PROB:	0	0.66	0.34
RMSE:	4.08	2.42	2.36

MAX_MEAN: 6.44 **MAX_MED:** 6.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

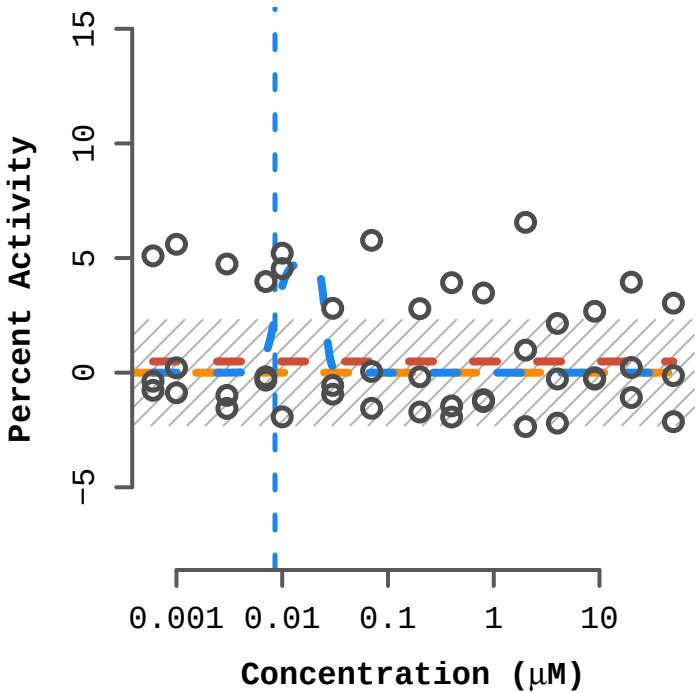
NAME: Novobiocin sodium
CHID: 23386 CASRN: 1476-53-5
SPID(S): Tox21_110747_1
M4ID: 12484137

HILL MODEL: Not applicable.

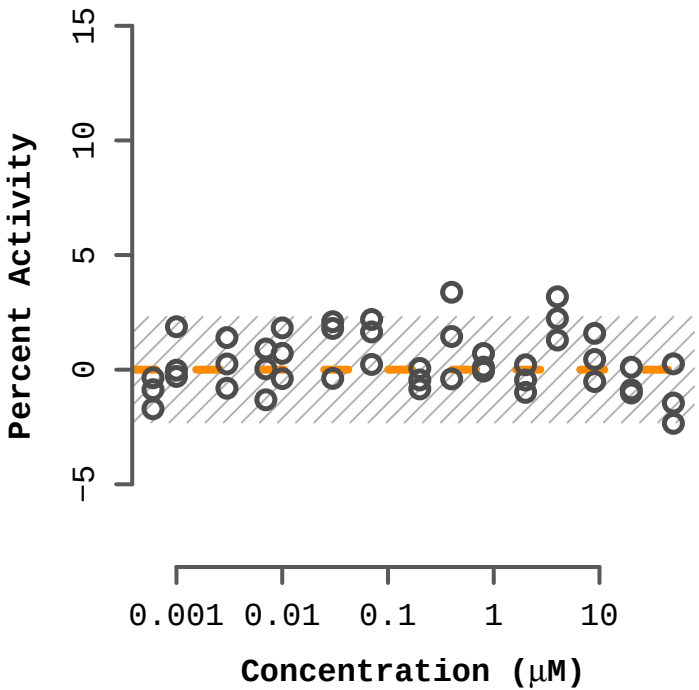
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 1.09 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Nylidrin
CHID:    23387   CASRN: 447-41-6
SPID(S): Tox21_110204_1
M4ID:    12484555

HILL MODEL (in red):
      tp       ga       gw
val:  0.488    -5.19    3.12
sd:   0.42     2060     3150

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.86     -2.07    7.97     -1.59    17.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  222.24      226.82      228.45
PROB: 0.87        0.09        0.04
RMSE: 2.75        2.63        2.67

MAX_MEAN: 2.61      MAX_MED: 4.54      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

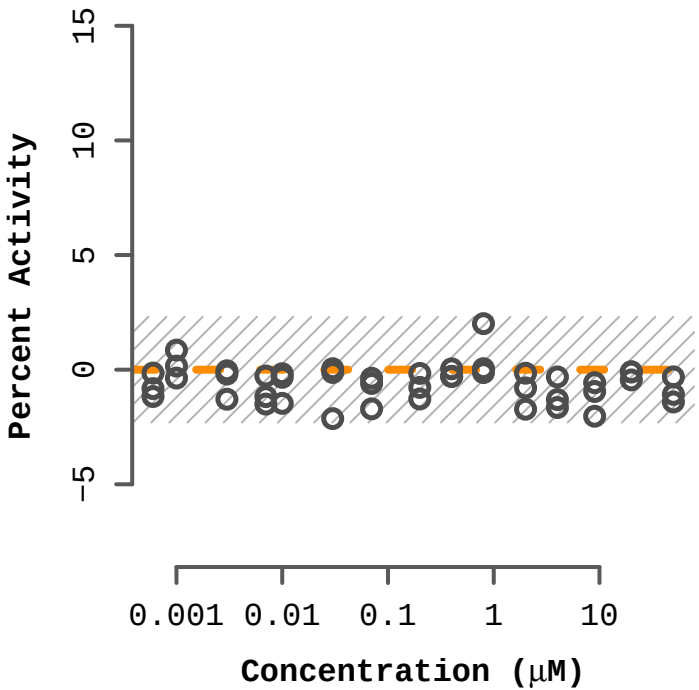
NAME: Olanzapine
CHID: 23388 **CASRN:** 132539-06-1
SPID(S): Tox21_111556_1
M4ID: 12483620

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

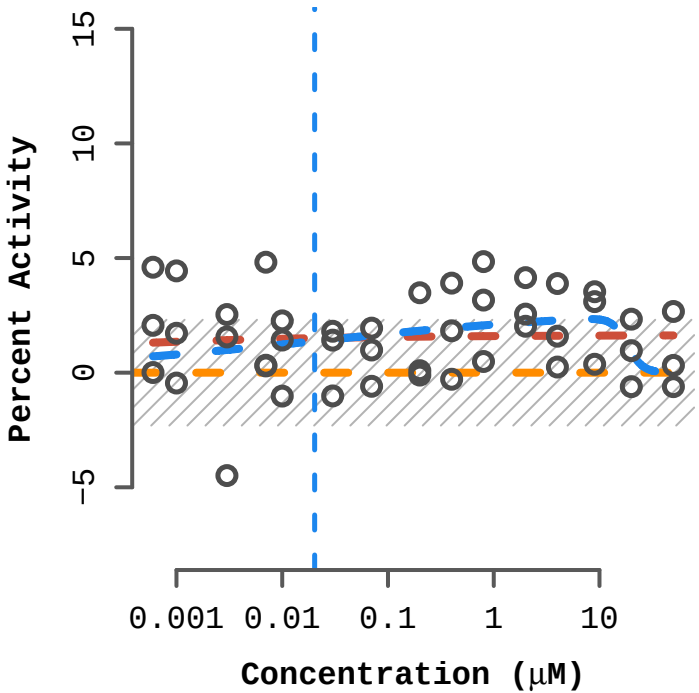
NAME: Ondansetron
CHID: 23393 **CASRN:** 99614-02-5
SPID(S): Tox21_113048_1
M4ID: 12482829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.643 **MAX_MED:** 0.159 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Orlistat
CHID: 23395 CASRN: 96829-58-2
SPID(S): Tox21_111437_1
M4ID: 12483688

HILL MODEL (in red):

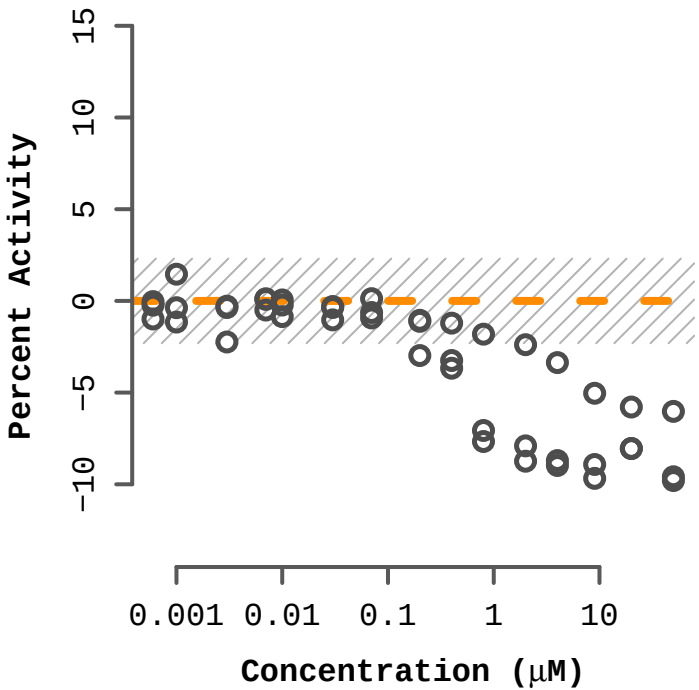
	tp	ga	gw
val:	1.64	−5.22	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.75	−1.69	0.3	1.26	6.03
sd:	13.7	17.6	1.71	1.24	194

	CNST	HILL	GNLS
AIC:	213.45	195.39	197.5
PROB:	0	0.74	0.26
RMSE:	2.44	1.9	1.87

MAX_MEAN: 2.91 **MAX_MED:** 3.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

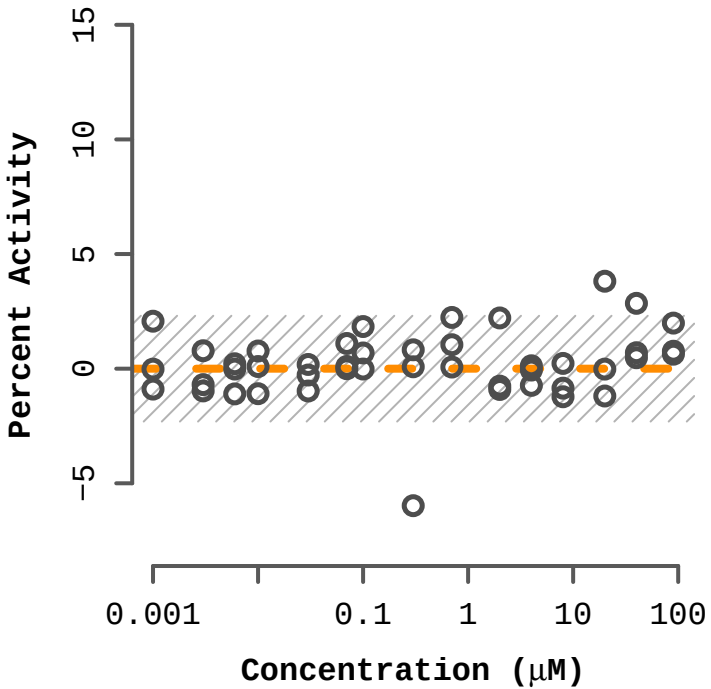
NAME: Oxyphenisatin acetate
CHID: 23411 **CASRN:** 115-33-3
SPID(S): Tox21_111651_1
M4ID: 12483557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	272.03	NA	NA
PROB:	1	NA	NA
RMSE:	4.85	NA	NA

MAX_MEAN: −0.0218 **MAX_MED:** 0.0845 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

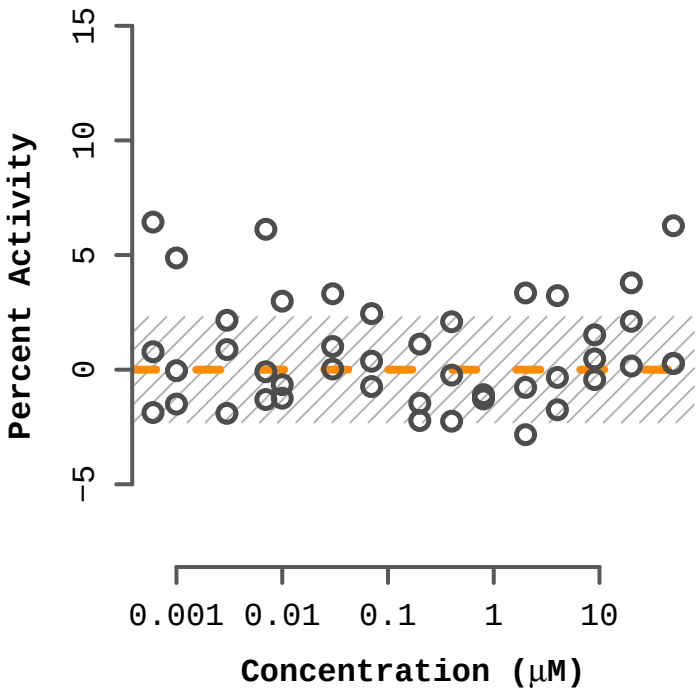
NAME: Oxytetracycline dihydrate
CHID: 23412 **CASRN:** 6153-64-6
SPID(S): Tox21_300679
M4ID: 12478454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

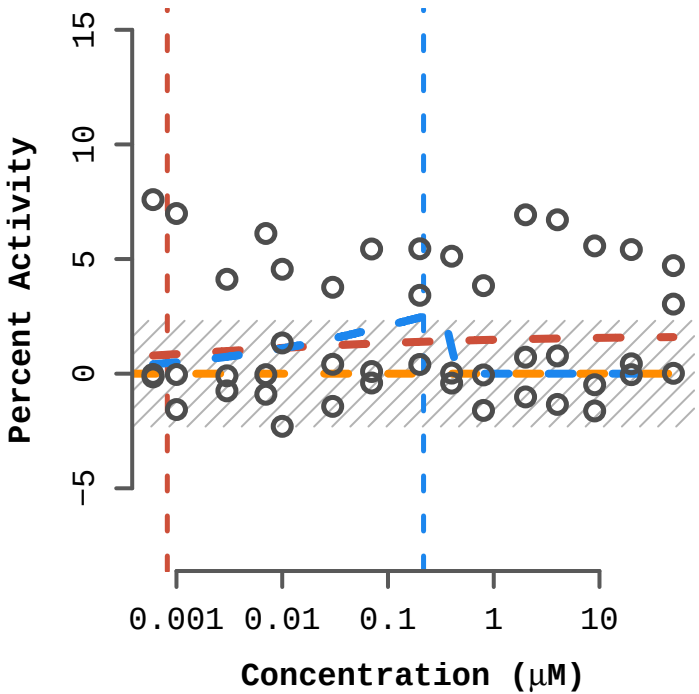
NAME: Pamidronic acid
CHID: 23414 **CASRN:** 40391-99-9
SPID(S): Tox21_111664_1
M4ID: 12483548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.72	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 2.27 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pantoprazole
CHID: 23416 CASRN: 102625-70-7
SPID(S): Tox21_111477_1
M4ID: 12483661

HILL MODEL (in red):

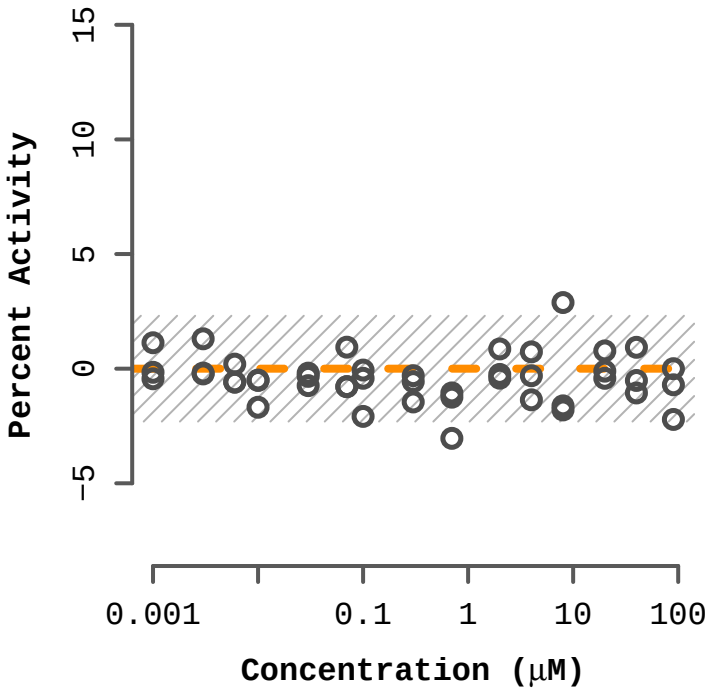
	tp	ga	gw
val:	1.65	−3.09	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.98	−0.664	0.409	−0.411	13
sd:	15.4	5.33	0.516	0.225	190

	CNST	HILL	GNLS
AIC:	239.71	237.41	244.26
PROB:	0.23	0.74	0.02
RMSE:	3.39	2.94	3.15

MAX_MEAN: 3.09 MAX_MED: 3.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

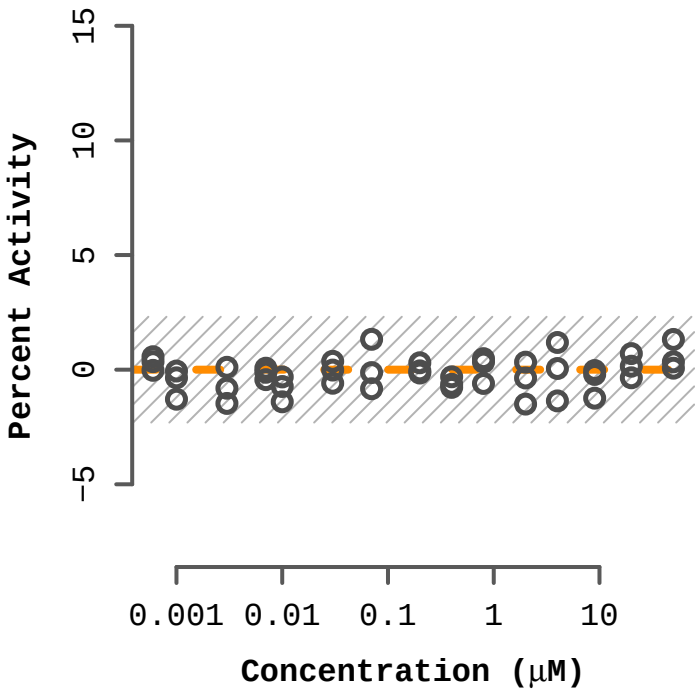
NAME: Paraldehyde
CHID: 23419 **CASRN:** 123-63-7
SPID(S): Tox21_301299
M4ID: 12477834

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.296 **MAX_MED:** −0.107 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

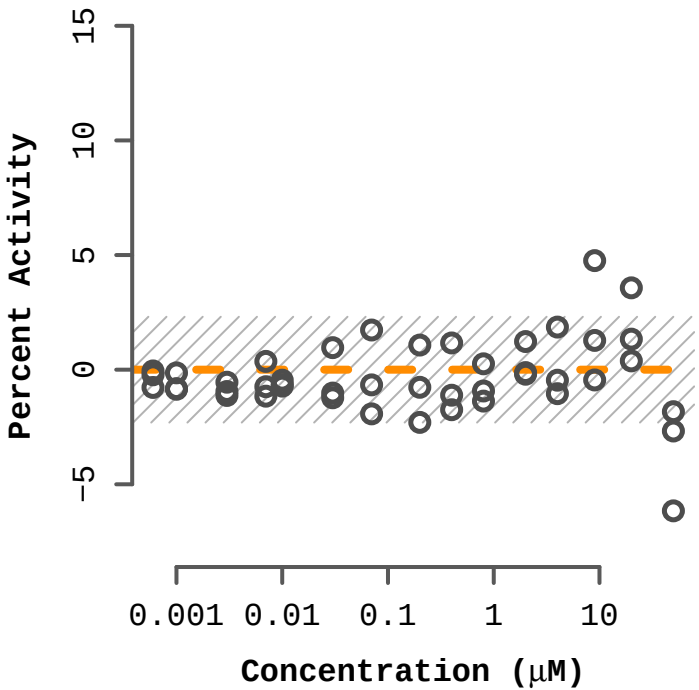
NAME: Paraldehyde
CHID: 23419 **CASRN:** 123-63-7
SPID(S): Tox21_111607_1
M4ID: 12483591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** 0.351 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

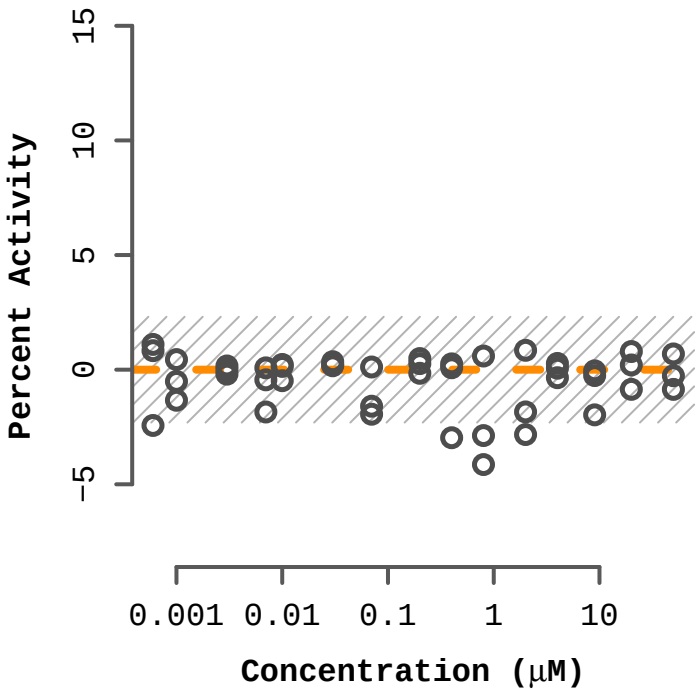
NAME: Paroxetine
CHID: 23425 **CASRN:** 61869-08-7
SPID(S): Tox21_113123_1
M4ID: 12482799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

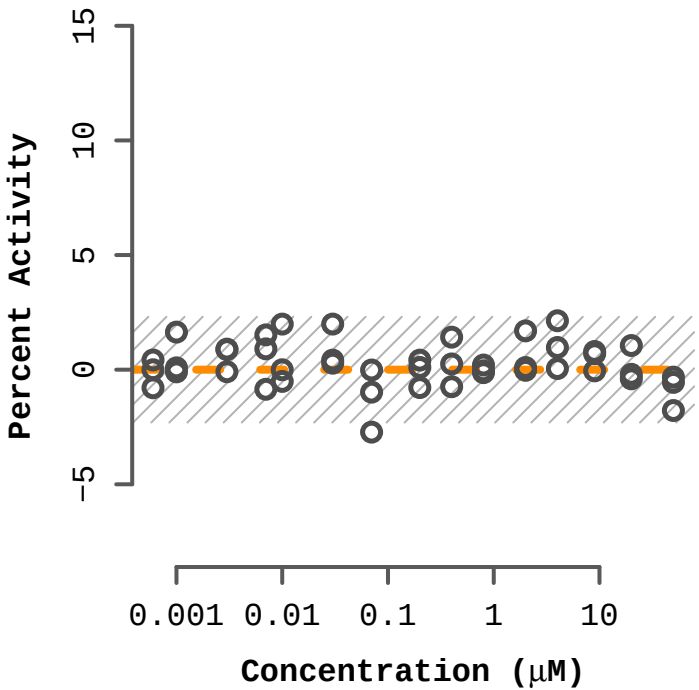
NAME: Paroxypropione
CHID: 23426 **CASRN:** 70-70-2
SPID(S): Tox21_110822_1
M4ID: 12484094

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.249 **MAX_MED:** 0.831 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

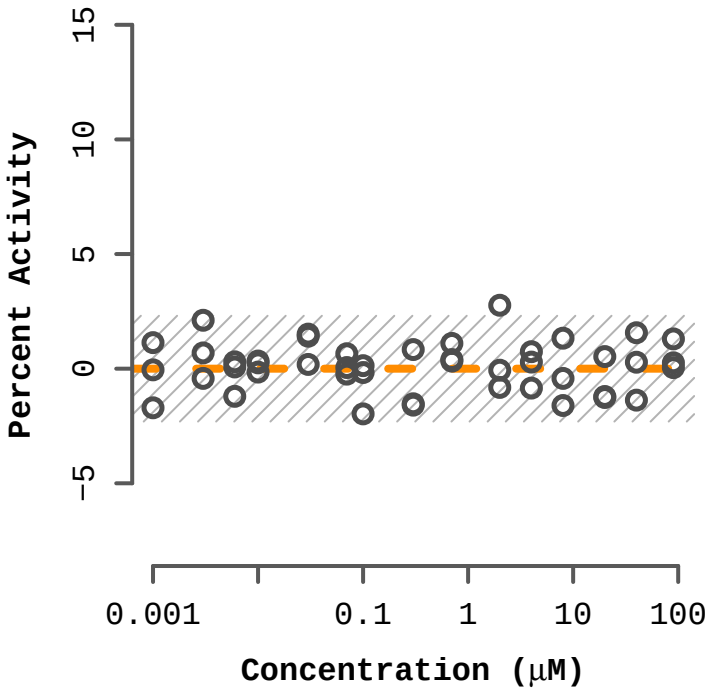
NAME: Pemoline
CHID: 23427 CASRN: 2152-34-3
SPID(S): Tox21_112509_1
M4ID: 12483059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.969 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

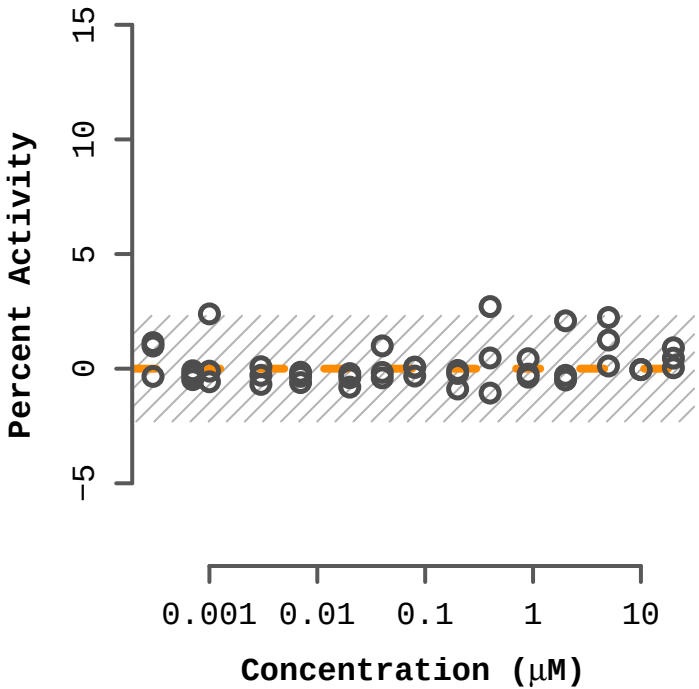
NAME: Pentaerythritol tetranitrate
CHID: 23430 **CASRN:** 78-11-5
SPID(S): Tox21_301747
M4ID: 12477386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

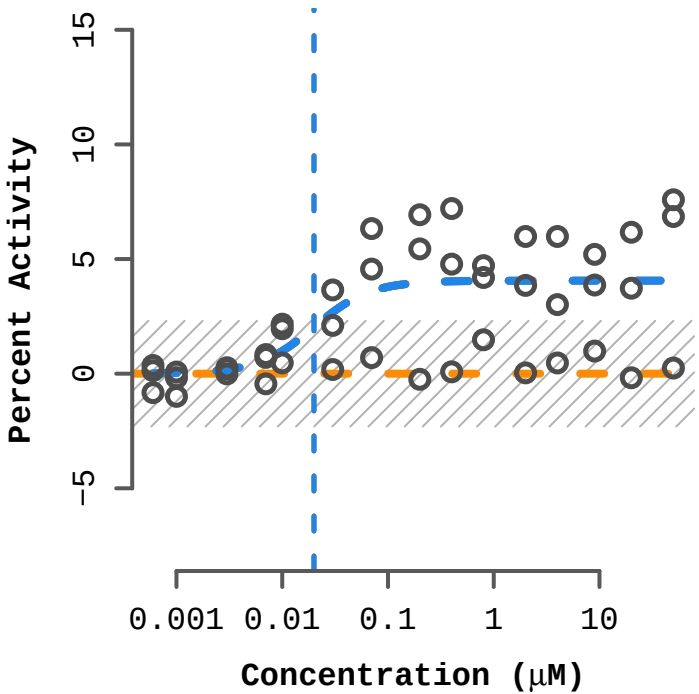
NAME: Pentetic acid
CHID: 23434 **CASRN:** 67-43-6
SPID(S): Tox21_110131_1
M4ID: 12484623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentoxifylline
CHID: 23437 **CASRN:** 6493-05-6
SPID(S): Tox21_110223_1
M4ID: 12484538

HILL MODEL (in red):

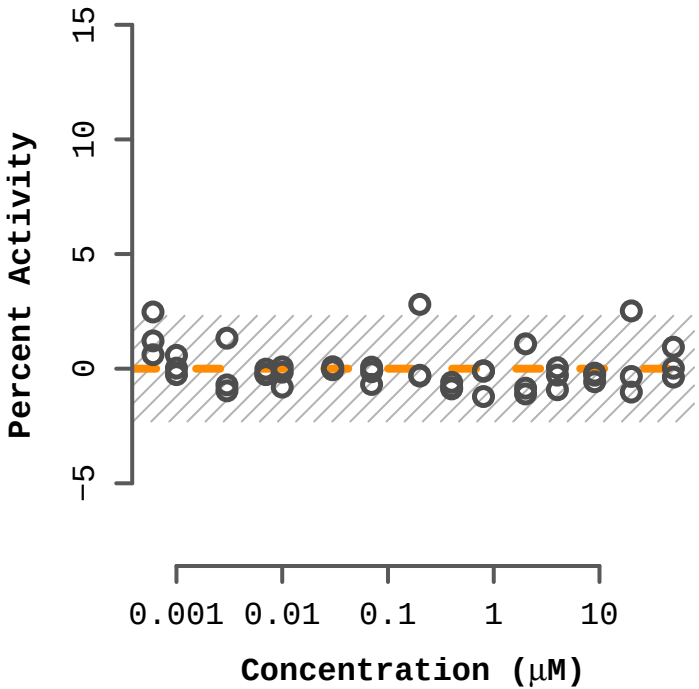
	tp	ga	gw
val:	4.06	−1.7	1.64
sd:	0.515	0.232	0.818

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.06	−1.7	1.64	2.53	10.4
sd:	0.515	0.232	0.818	1630	20500

	CNST	HILL	GNLS
AIC:	246.47	204.74	208.74
PROB:	0	0.88	0.12
RMSE:	3.59	2.1	2.1

MAX_MEAN: 4.9 **MAX_MED:** 6.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

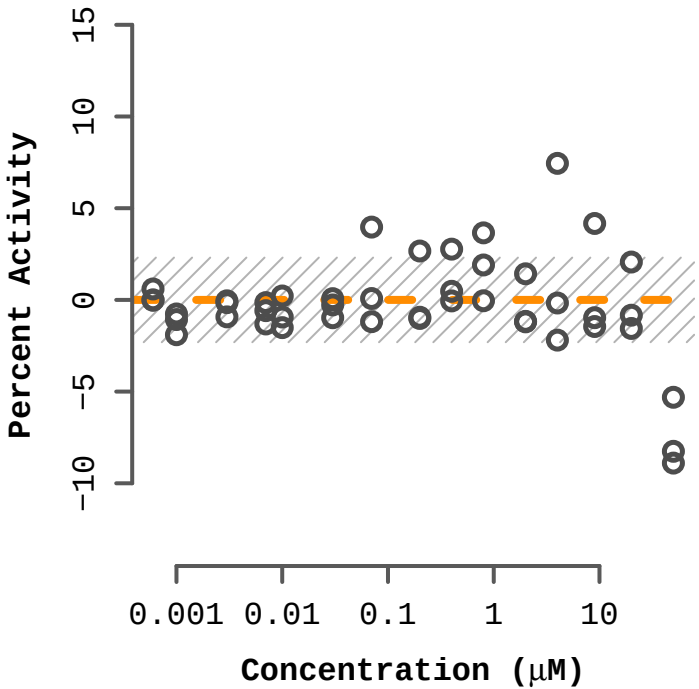
NAME: Perindopril
CHID: 23440 **CASRN:** 82834-16-0
SPID(S): Tox21_113087_1
M4ID: 12482810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

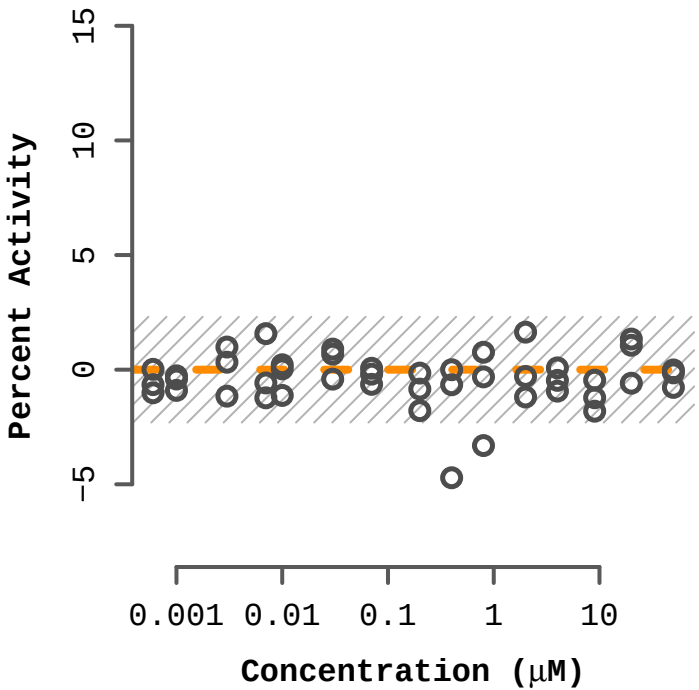
NAME: Perphenazine
CHID: 23441 **CASRN:** 58-39-9
SPID(S): Tox21_110233_1
M4ID: 12484529

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.72	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

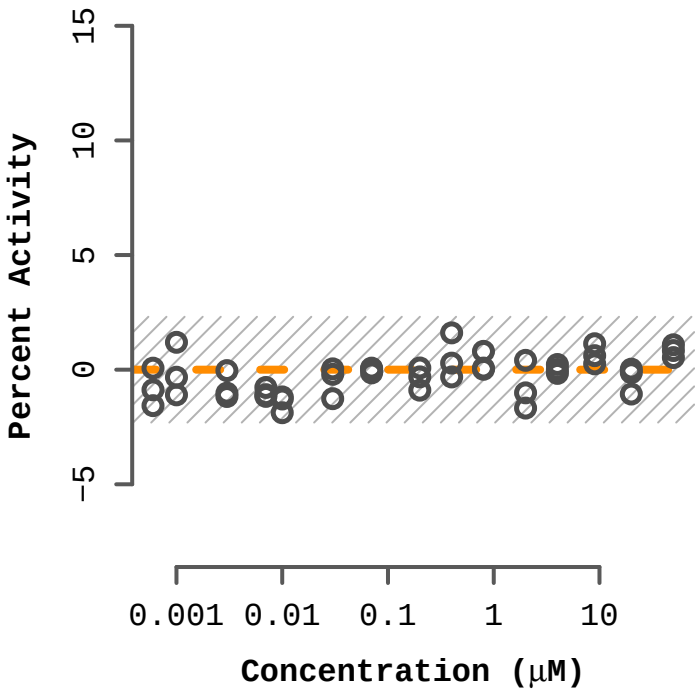
NAME: Phenacemide
CHID: 23442 **CASRN:** 63-98-9
SPID(S): Tox21_111325_1
M4ID: 12483766

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.604 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

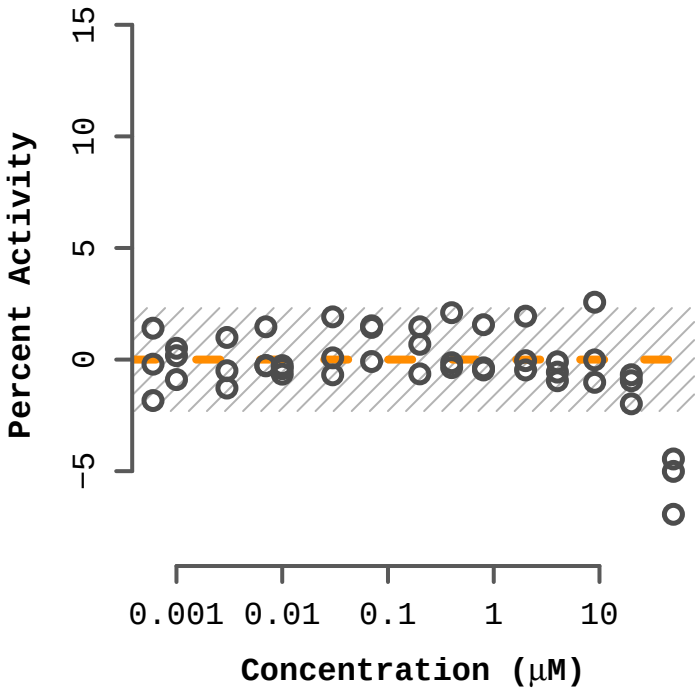
NAME: Phenindione
CHID: 23453 **CASRN:** 83-12-5
SPID(S): Tox21_110375_1
M4ID: 12484413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

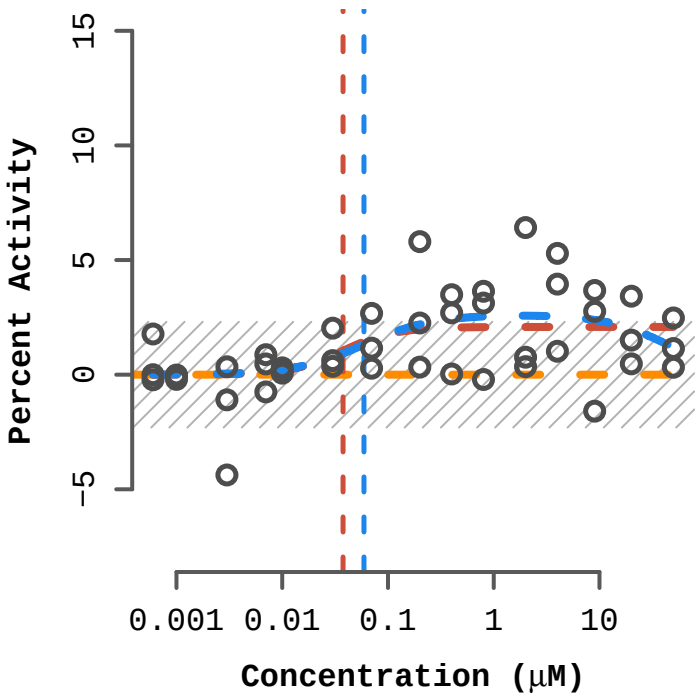
NAME: Phenoxybenzamine
CHID: 23458 **CASRN:** 59-96-1
SPID(S): Tox21_110087_1
M4ID: 12484665

HILL MODEL: Not applicable.

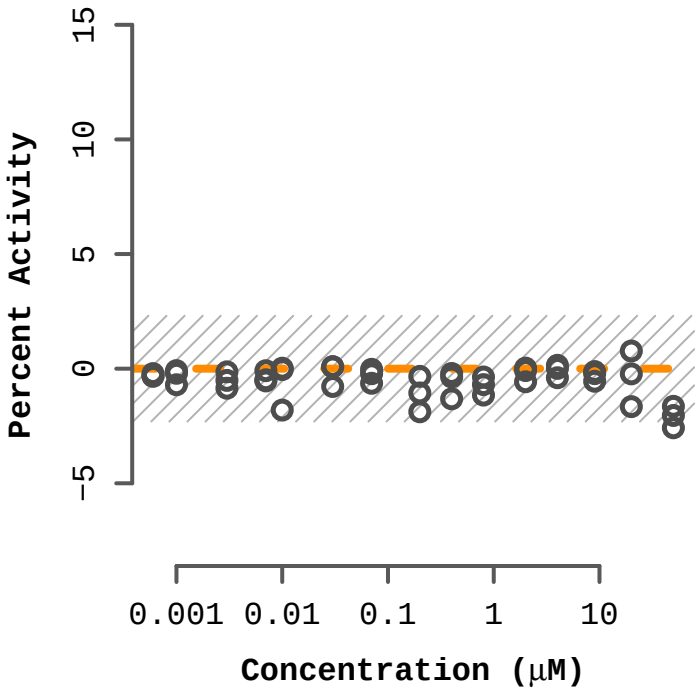
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.78	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 1.44 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phensuximide
CHID:    23460   CASRN: 86-34-0
SPID(S): Tox21_110382_1
M4ID:    12484407

HILL MODEL (in red):
      tp       ga       gw
val:  2.08     -1.42    1.78
sd:   0.394    0.319    1.39

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.63     -1.23    1.33     1.64     1.45
sd:   0.79     0.426    1.06     0.381    1.69

      CNST        HILL        GNLS
AIC:  205.07      180.63      182.76
PROB: 0           0.74        0.26
RMSE: 2.37        1.68        1.65

MAX_MEAN: 3.42      MAX_MED: 3.95      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

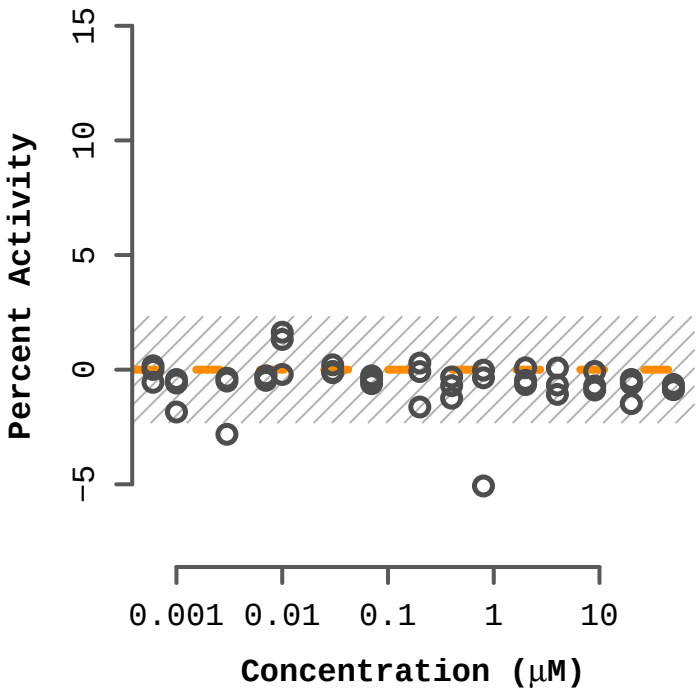
NAME: Phentolamine
CHID: 23462 **CASRN:** 50-60-2
SPID(S): Tox21_110364_1
M4ID: 12484424

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: −0.0774 **MAX_MED:** 0.0852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

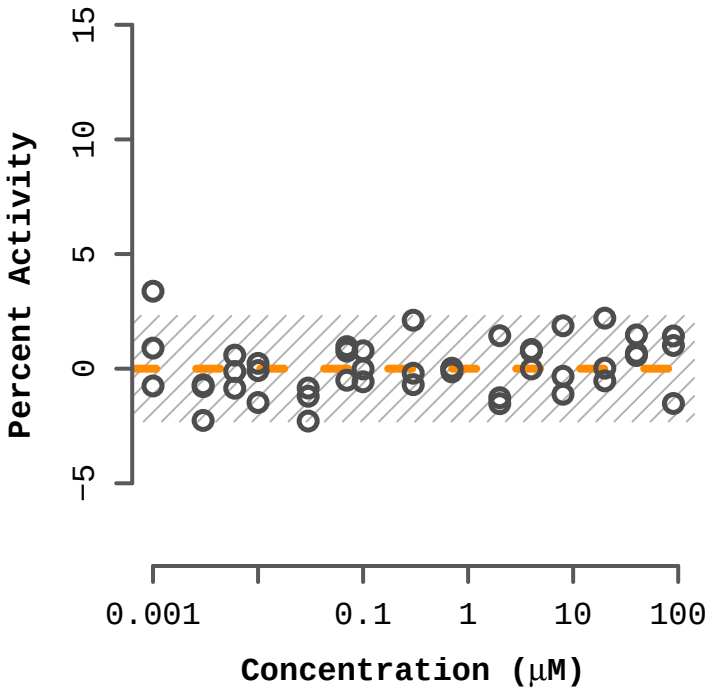
NAME: Phthalylsulfathiazole
CHID: 23470 CASRN: 85-73-4
SPID(S): Tox21_110380_1
M4ID: 12484409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.917 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

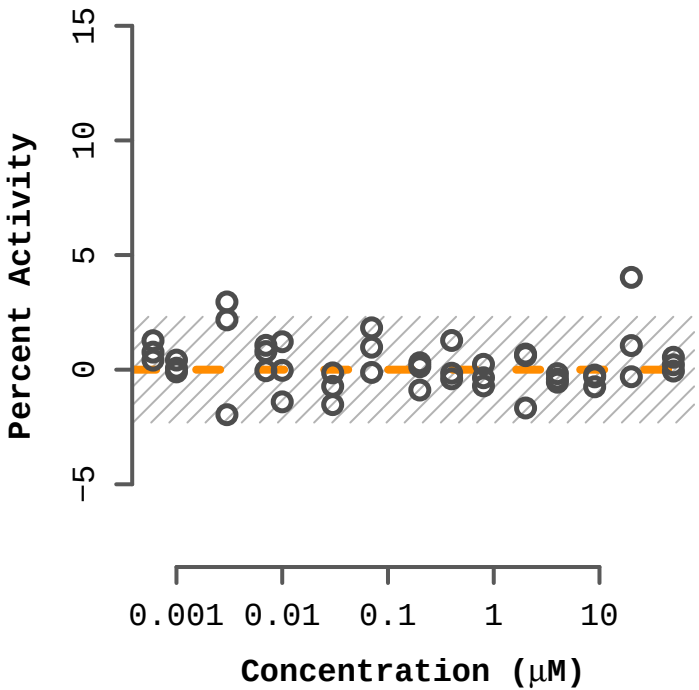
NAME: Physostigmine
CHID: 23471 **CASRN:** 57-47-6
SPID(S): Tox21_301591
M4ID: 12477542

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

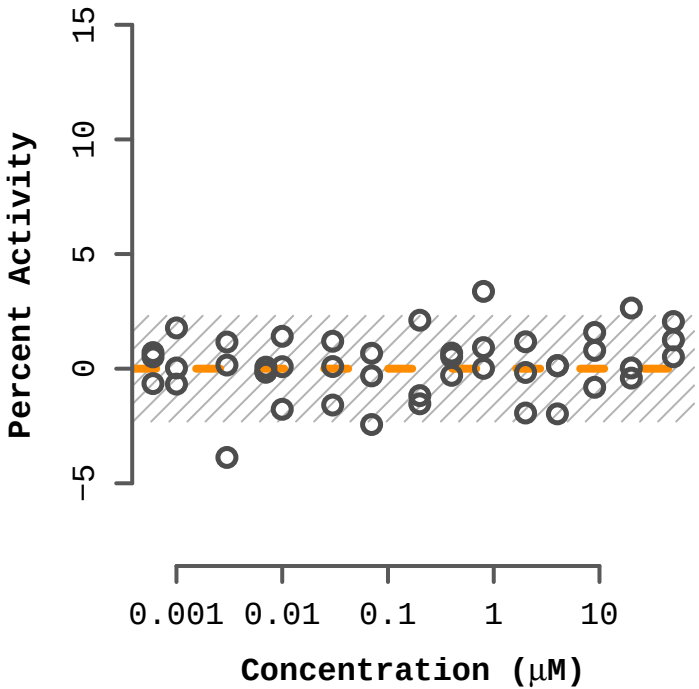
NAME: Physostigmine
CHID: 23471 **CASRN:** 57-47-6
SPID(S): Tox21_111228_1
M4ID: 12483829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

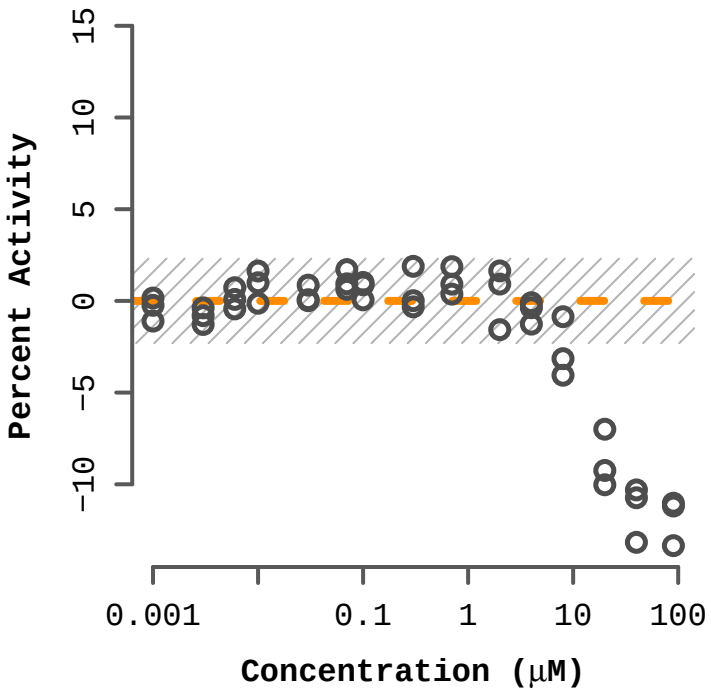
NAME: Phytonadione
CHID: 23472 **CASRN:** 84-80-0
SPID(S): Tox21_111655_1
M4ID: 12483554

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

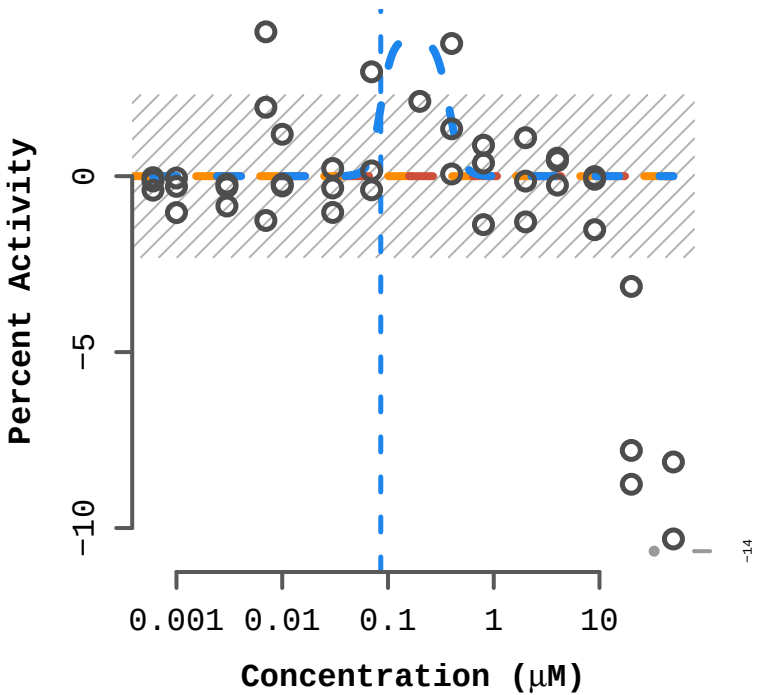
NAME: Pimozide
CHID: 23474 CASRN: 2062-78-4
SPID(S): Tox21_301586
M4ID: 12477547

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	259.42	NA	NA
PROB:	1	NA	NA
RMSE:	4.97	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pimozide
CHID: 23474 CASRN: 2062-78-4
SPID(S): Tox21_110224_1
M4ID: 12484537 BRK

HILL MODEL (in red):

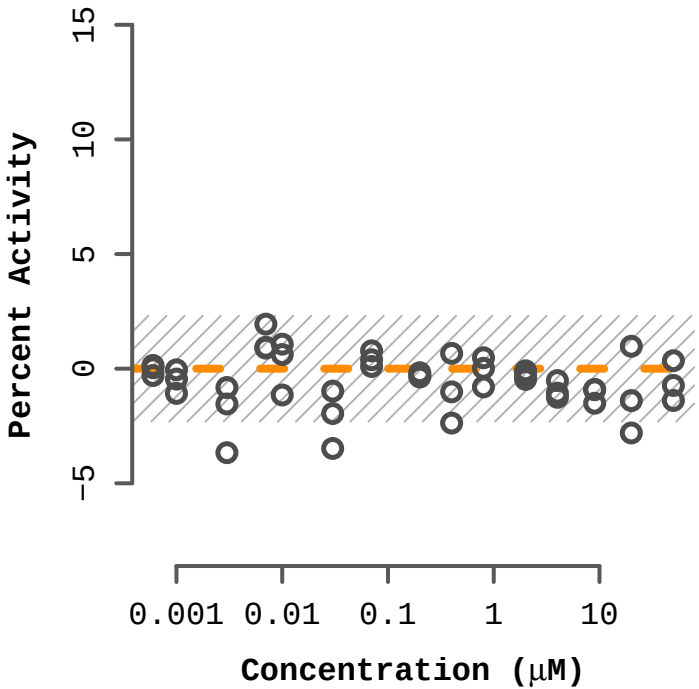
	tp	ga	gw
val:	1.55e-08	2.07	3.24
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.93	-1.07	8	-0.424	7
sd:	2.29	0.569	50.8	0.298	63.4

	CNST	HILL	GNLS
AIC:	227.17	233.17	223.83
PROB:	0.16	0.01	0.84
RMSE:	3.68	3.68	3.52

MAX_MEAN: 3.76 MAX_MED: 4.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

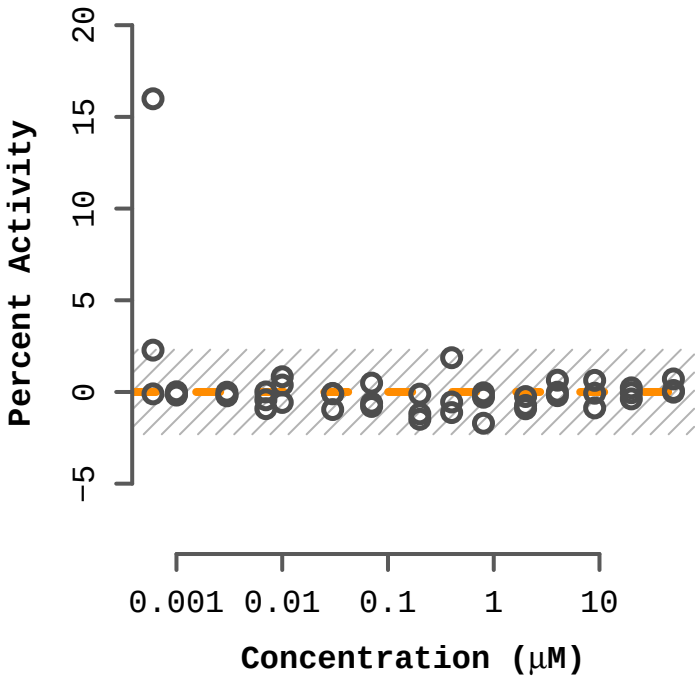
NAME: Pindolol
CHID: 23476 **CASRN:** 13523-86-9
SPID(S): Tox21_110221_1
M4ID: 12484540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

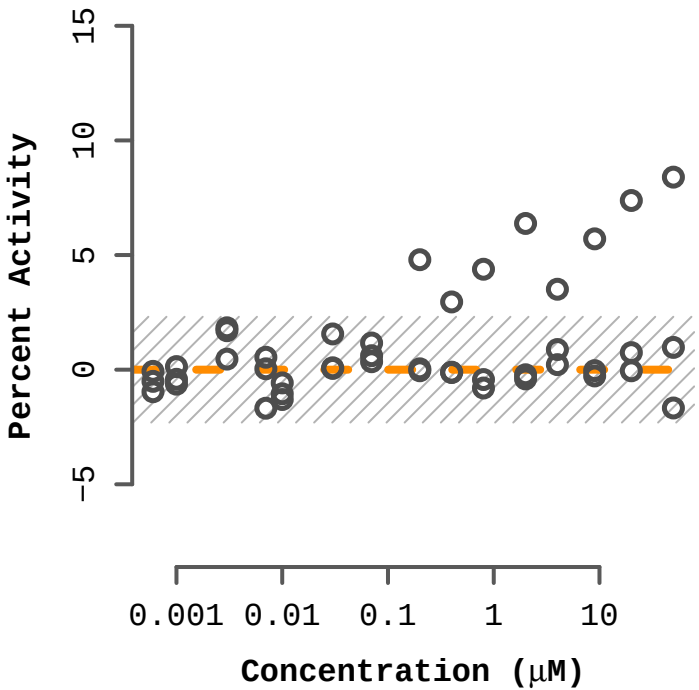
NAME: Pipemidic acid
CHID: 23479 CASRN: 51940-44-4
SPID(S): Tox21_110655_1
M4ID: 12484202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.97	NA	NA
PROB:	1	NA	NA
RMSE:	2.5	NA	NA

MAX_MEAN: 6.06 MAX_MED: 2.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

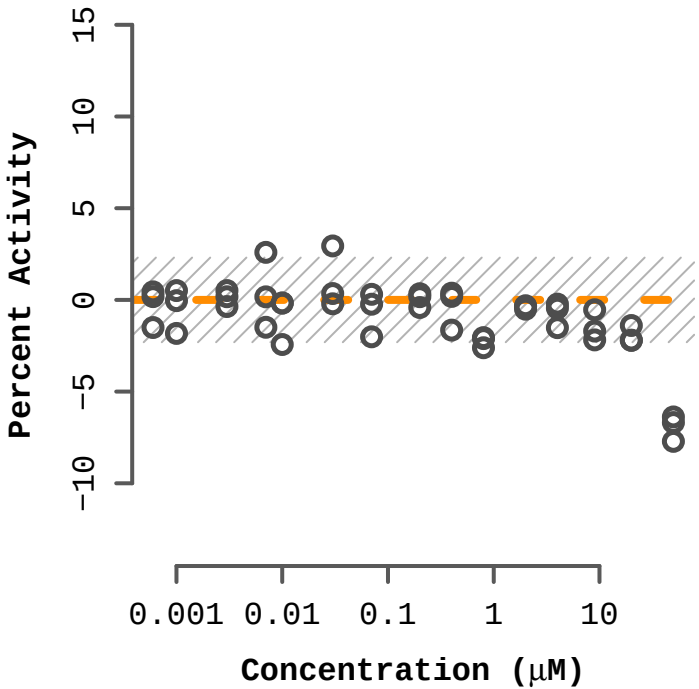
NAME: Pipenzolate bromide
CHID: 23480 **CASRN:** 125-51-9
SPID(S): Tox21_111378_1
M4ID: 12483727

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.38	NA	NA
PROB:	1	NA	NA
RMSE:	2.52	NA	NA

MAX_MEAN: 2.69 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

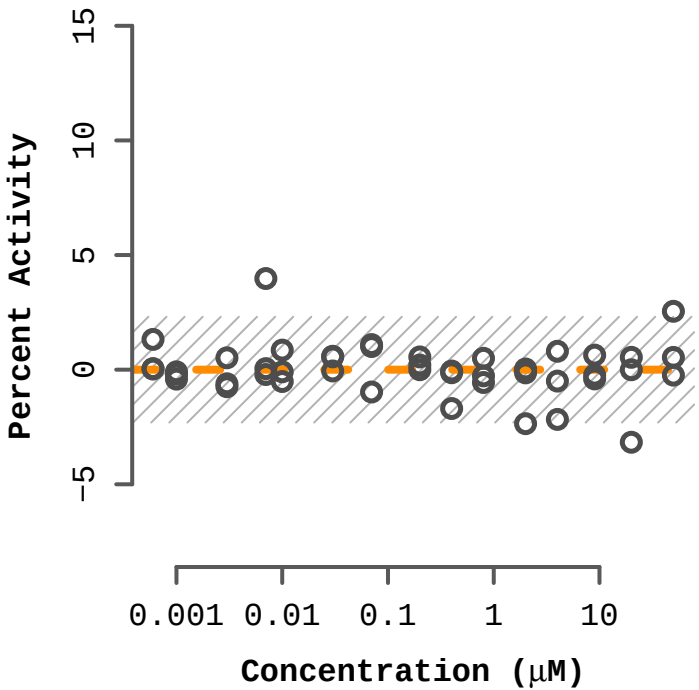
NAME: Piperacetazine
CHID: 23481 **CASRN:** 3819-00-9
SPID(S): Tox21_110540_1
M4ID: 12484280

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.21	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

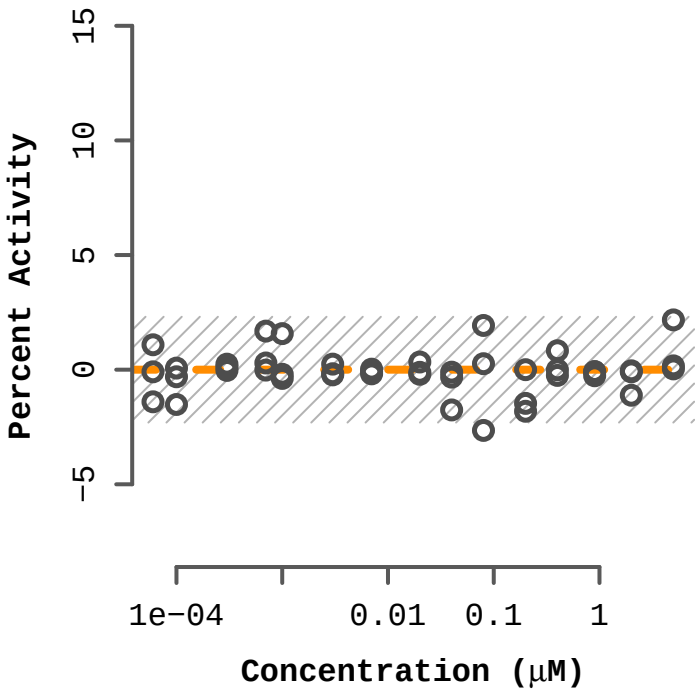
NAME: Pipobroman
CHID: 23485 **CASRN:** 54-91-1
SPID(S): Tox21_111402_1
M4ID: 12483709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

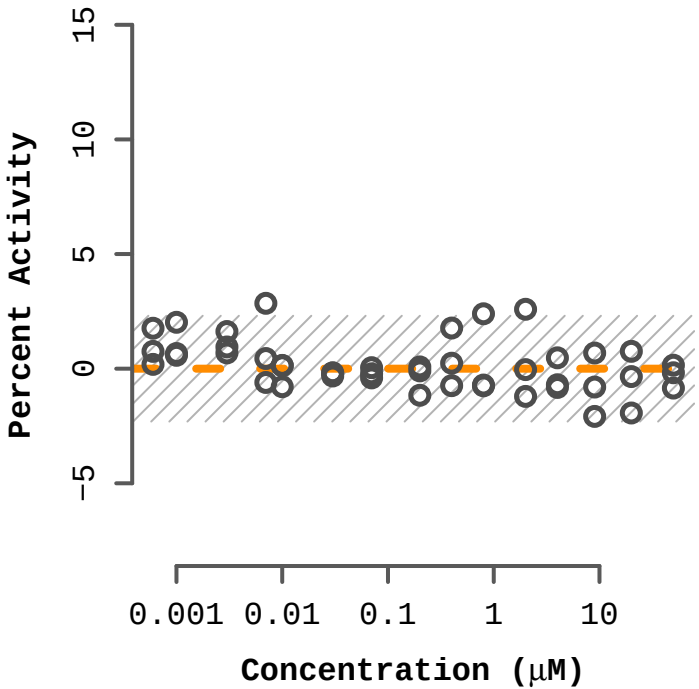
NAME: Pirenzepine
CHID: 23487 **CASRN:** 28797-61-7
SPID(S): Tox21_110239_1
M4ID: 12484524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 0.293 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

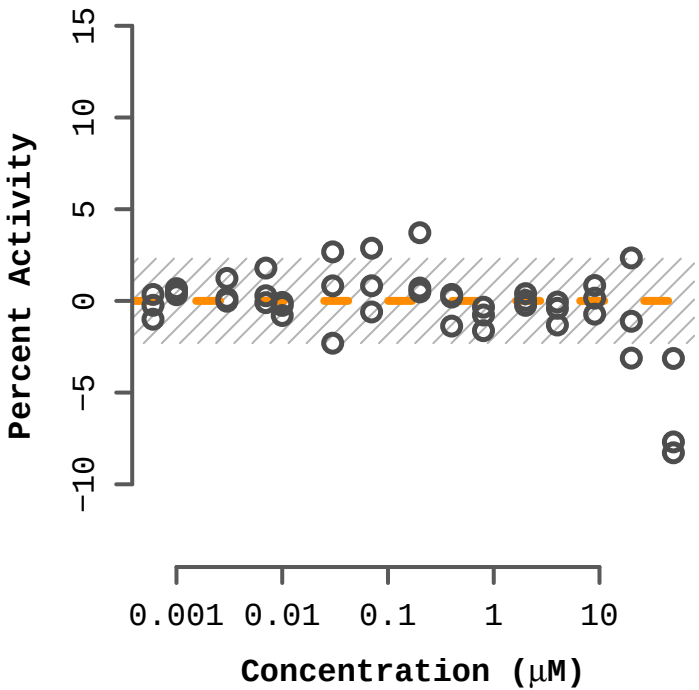
NAME: Piretanide
CHID: 23488 **CASRN:** 55837-27-9
SPID(S): Tox21_110661_1
M4ID: 12484197

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

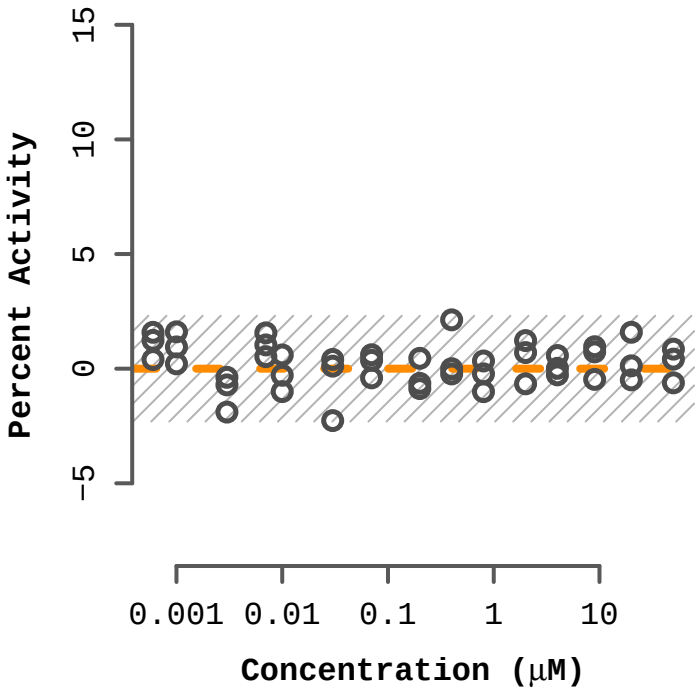
NAME: Pizotyline
CHID: 23490 **CASRN:** 15574-96-6
SPID(S): Tox21_112024_1
M4ID: 12483365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.15	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

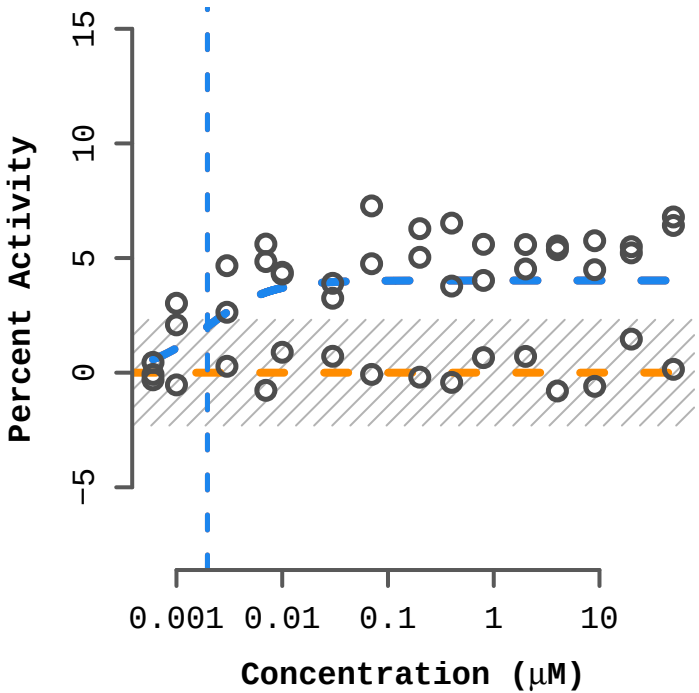
NAME: Pralidoxime chloride
CHID: 23495 **CASRN:** 51-15-0
SPID(S): Tox21_110316_1
M4ID: 12484461

HILL MODEL: Not applicable.

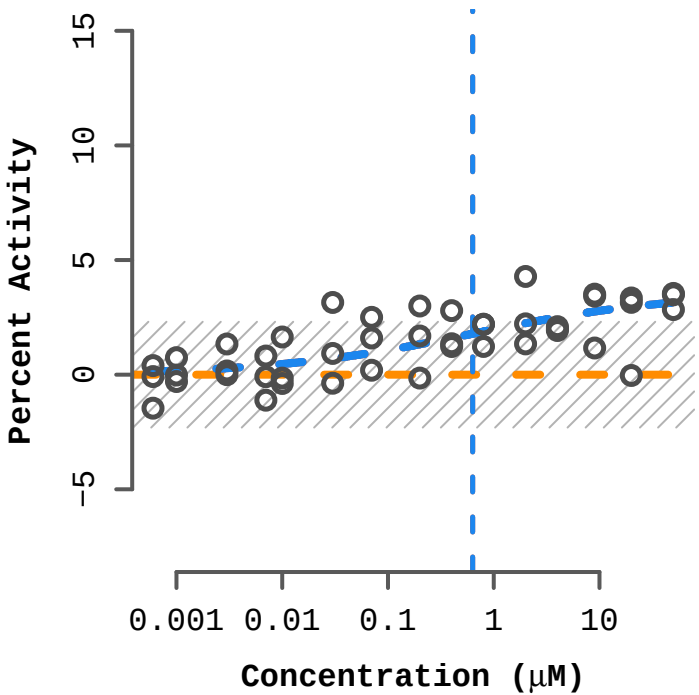
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.24 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pramipexole
CHID:    23496   CASRN: 104632-26-0
SPID(S): Tox21_112445_1
M4ID:    12483098

HILL MODEL (in red):
      tp       ga       gw
val:  4.02     -2.71    1.5
sd:   0.545    0.339    1.53

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.02     -2.71    1.5      2.5      18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  260.65      218.9       222.9
PROB: 0           0.88        0.12
RMSE: 4           2.4         2.4

MAX_MEAN: 4.45      MAX_MED: 6.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pranoprofen
CHID: 23497 **CASRN:** 52549-17-4
SPID(S): Tox21_112601_1
M4ID: 12483012

HILL MODEL (in red):

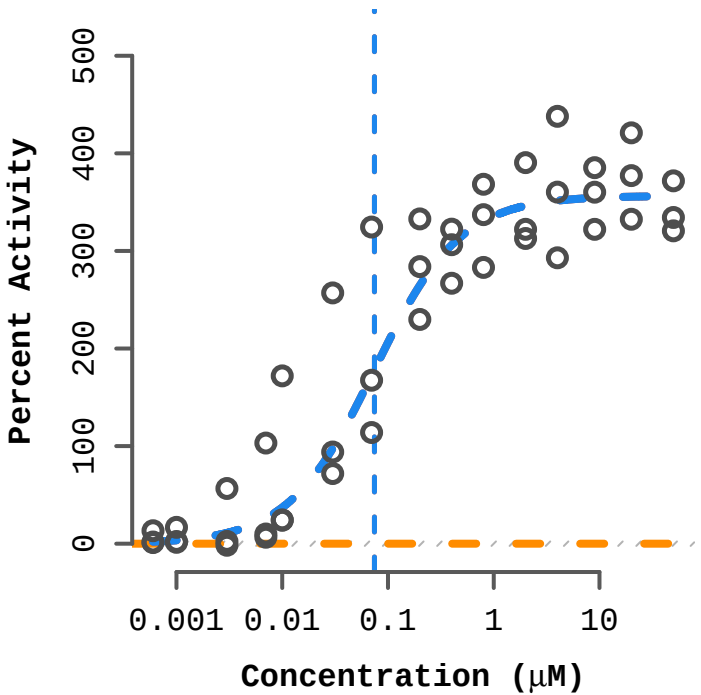
	tp	ga	gw
val:	3.57	−0.199	0.458
sd:	1	0.75	0.181

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.57	−0.199	0.458	3.01	6.15
sd:	1	0.75	0.181	1460	6840

	CNST	HILL	GNLS
AIC:	196.45	136.24	140.24
PROB:	0	0.88	0.12
RMSE:	2	1.02	1.02

MAX_MEAN: 3.29 **MAX_MED:** 3.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisolone acetate
CHID: 23502 CASRN: 52-21-1
SPID(S): Tox21_111328_1
M4ID: 12483764

HILL MODEL (in red):

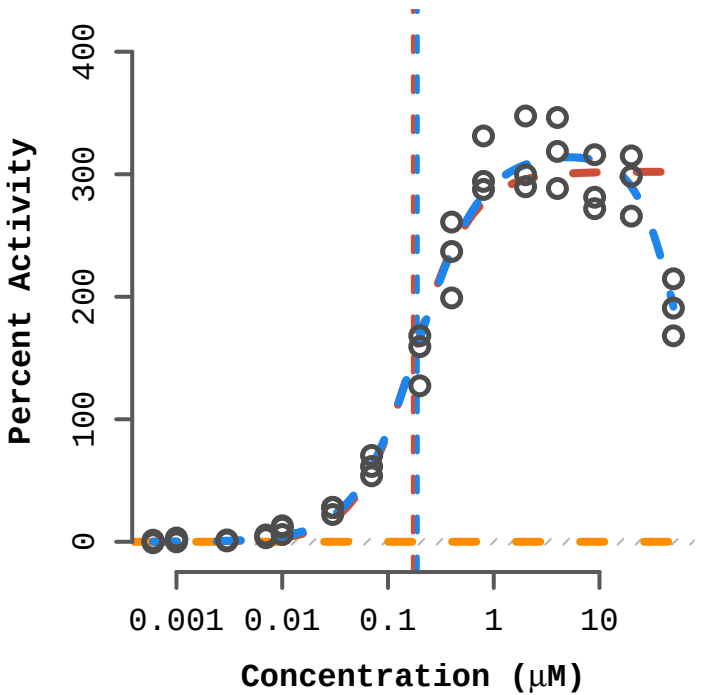
	tp	ga	gw
val:	356	-1.13	1.07
sd:	11.6	0.0841	0.168

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	356	-1.13	1.07	3.58	8
sd:	11.6	0.0841	0.168	496000	1150000

	CNST	HILL	GNLS
AIC:	636.96	480.48	484.48
PROB:	0	0.88	0.12
RMSE:	259.97	50.8	50.8

MAX_MEAN: 377 MAX_MED: 377 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisolone tebutate
CHID: 23505 CASRN: 7681-14-3
SPID(S): Tox21_113662
M4ID: 12482551

HILL MODEL (in red):

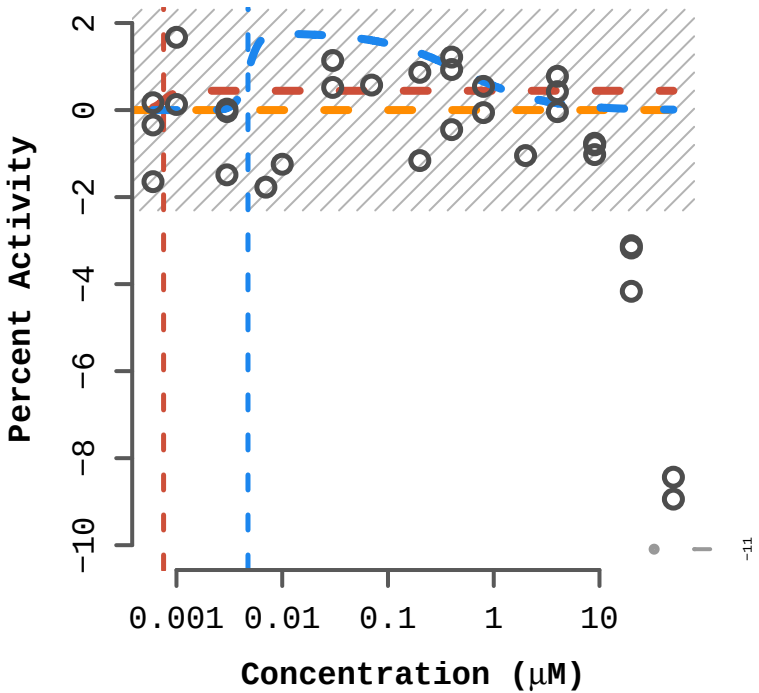
	tp	ga	gw
val:	302	-0.76	1.57
sd:	6.84	0.0341	0.149

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	318	-0.723	1.44	1.79	2.09
sd:	11.2	0.037	0.121	0.0488	0.979

	CNST	HILL	GNLS
AIC:	609.72	432.02	397.21
PROB:	0	0	1
RMSE:	197.14	34.65	18.25

MAX_MEAN: 318 **MAX_MED:** 319 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prifinium bromide
CHID: 23508 CASRN: 4630-95-9
SPID(S): Tox21_113295
M4ID: 12482730 BRK

HILL MODEL (in red):

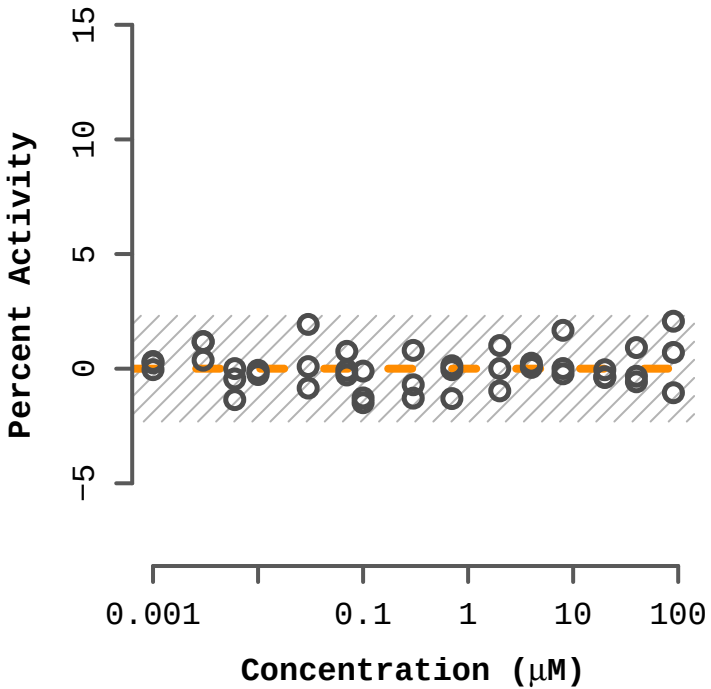
	tp	ga	gw
val:	0.443	−3.12	8
sd:	0.363	0.245	17.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.78	−2.32	8	−0.303	1.13
sd:	0.861	0.246	10.5	0.964	0.992

	CNST	HILL	GNLS
AIC:	220.2	224.72	220.63
PROB:	0.52	0.05	0.42
RMSE:	3.11	3.17	2.98

MAX_MEAN: 2 MAX_MED: 2.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

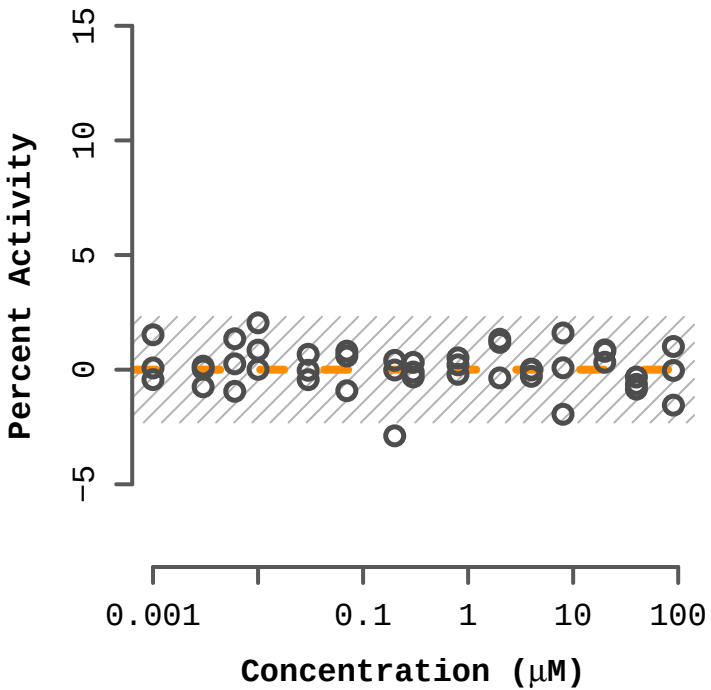
NAME: Primidone
CHID: 23510 **CASRN:** 125-33-7
SPID(S): Tox21_303194
M4ID: 12475939

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.909 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

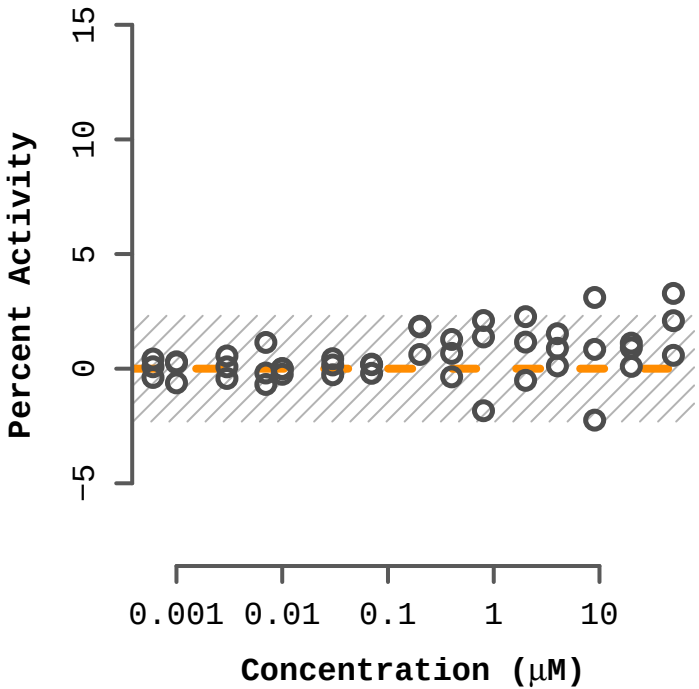
NAME: Primidone
CHID: 23510 **CASRN:** 125-33-7
SPID(S): Tox21_201948
M4ID: 12480304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

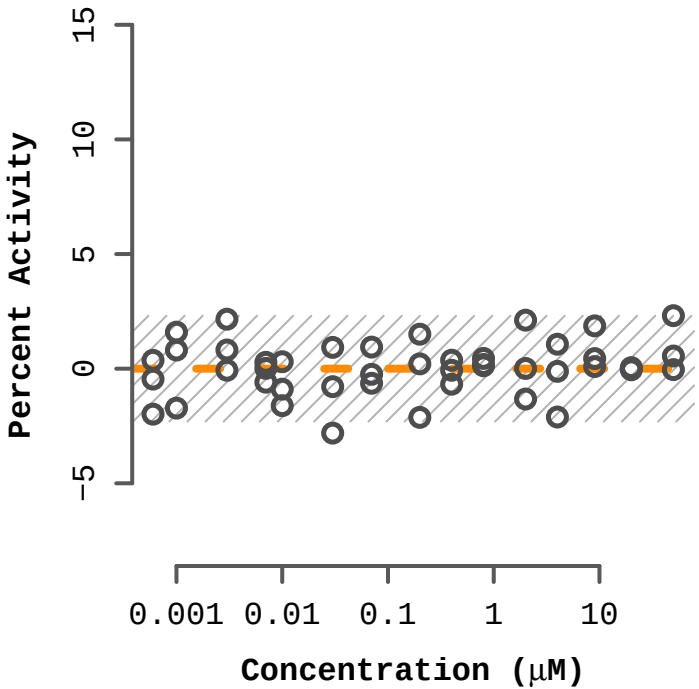
NAME: Primidone
CHID: 23510 **CASRN:** 125-33-7
SPID(S): Tox21_110238_1
M4ID: 12484525

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

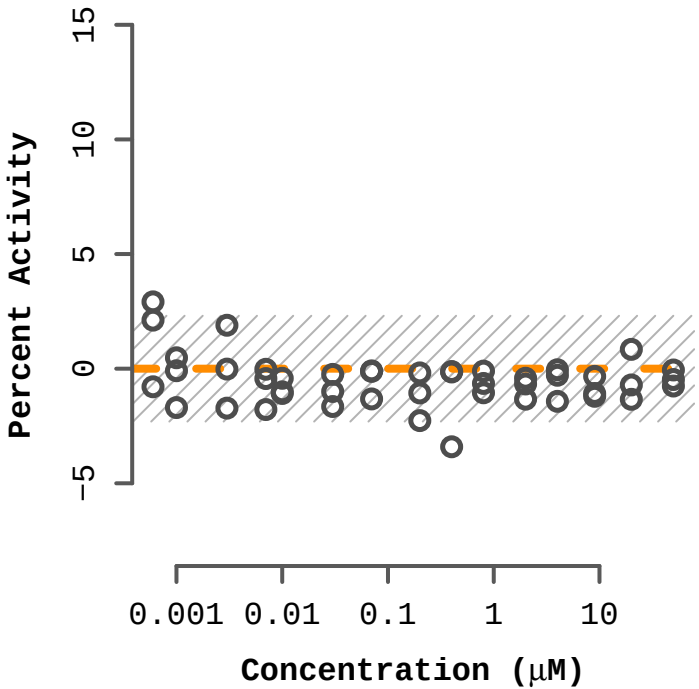
NAME: Procainamide
CHID: 23512 **CASRN:** 51-06-9
SPID(S): Tox21_110246_1
M4ID: 12484518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.97 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

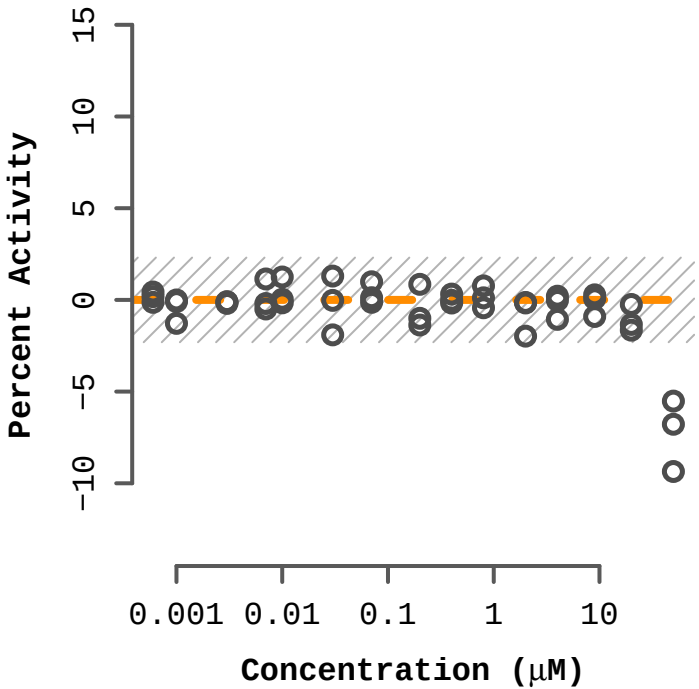
NAME: Proglumide
CHID: 23516 **CASRN:** 6620-60-6
SPID(S): Tox21_110557_1
M4ID: 12484267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

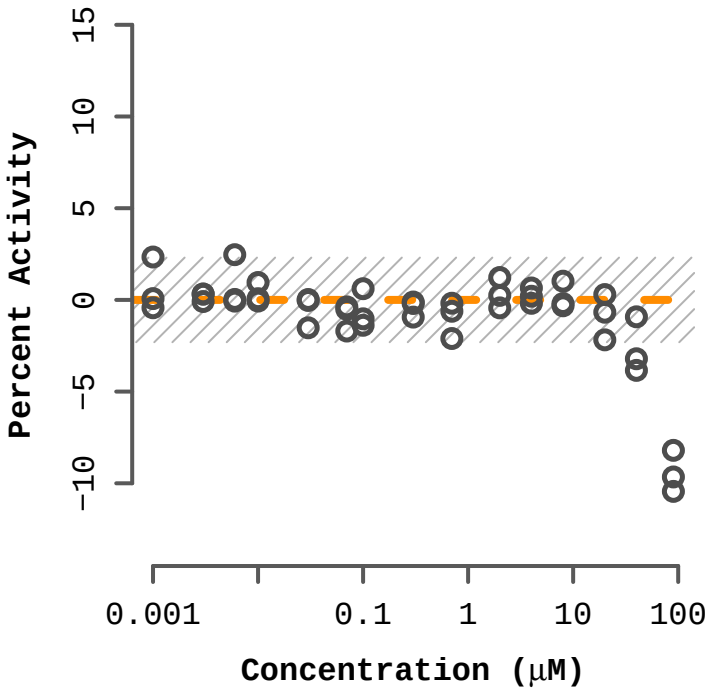
NAME: Promethazine
CHID: 23518 **CASRN:** 60-87-7
SPID(S): Tox21_110227_1
M4ID: 12484534

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.01	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 0.376 **MAX_MED:** 0.182 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

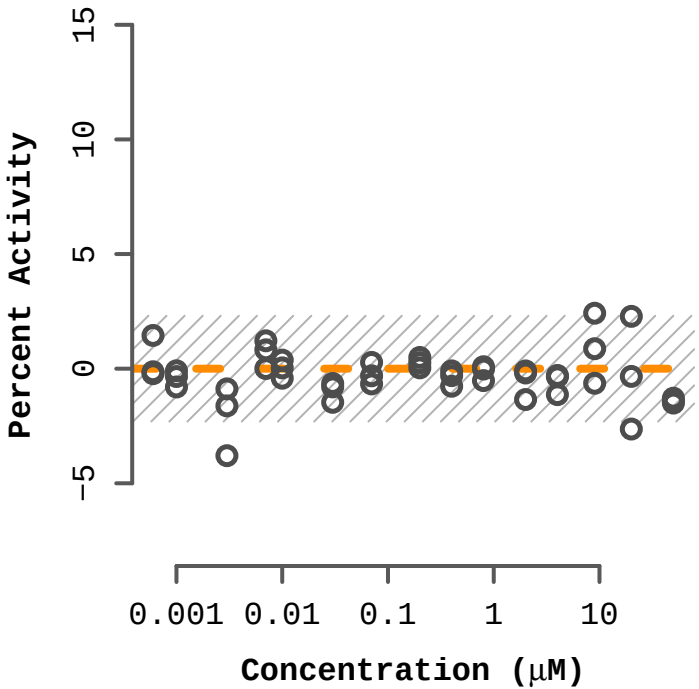
NAME: Propantheline bromide
CHID: 23519 **CASRN:** 50-34-0
SPID(S): Tox21_302331
M4ID: 12476802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 0.81 **MAX_MED:** 0.316 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

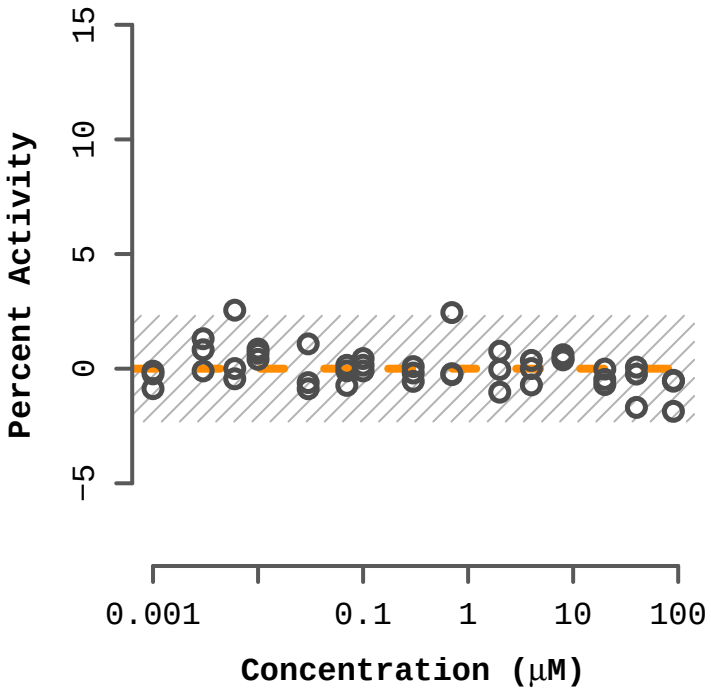
NAME: Propantheline bromide
CHID: 23519 **CASRN:** 50-34-0
SPID(S): Tox21_111265_1
M4ID: 12483807

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.885 **MAX_MED:** 0.873 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

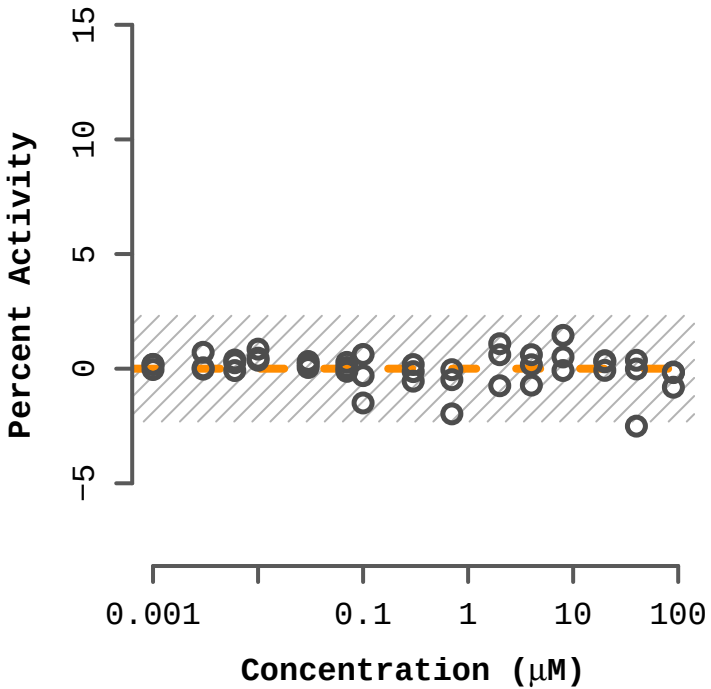
NAME: Propofol
CHID: 23523 CASRN: 2078-54-8
SPID(S): Tox21_303225
M4ID: 12475908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.706 MAX_MED: 0.827 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

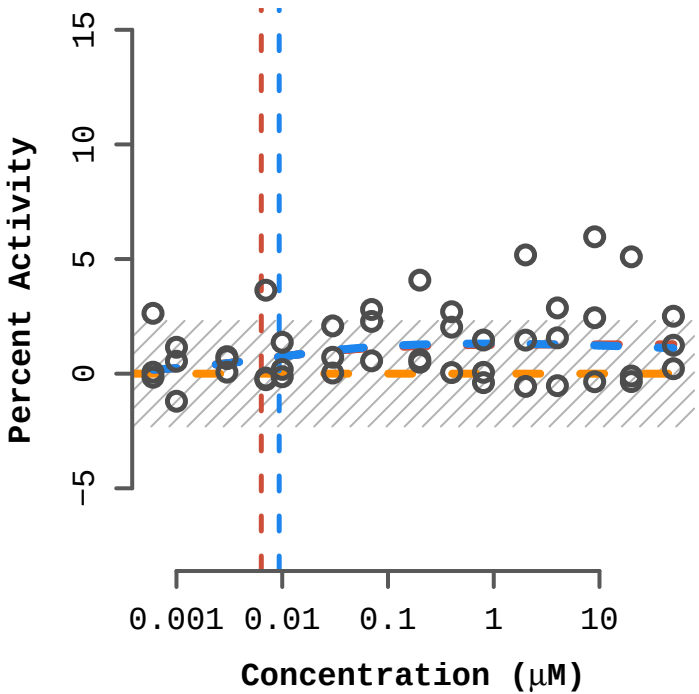
NAME: Propofol
CHID: 23523 CASRN: 2078-54-8
SPID(S): Tox21_201371
M4ID: 12480881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.629 MAX_MED: 0.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propofol
CHID: 23523 **CASRN:** 2078-54-8
SPID(S): Tox21_110134_1
M4ID: 12484620

HILL MODEL (in red):

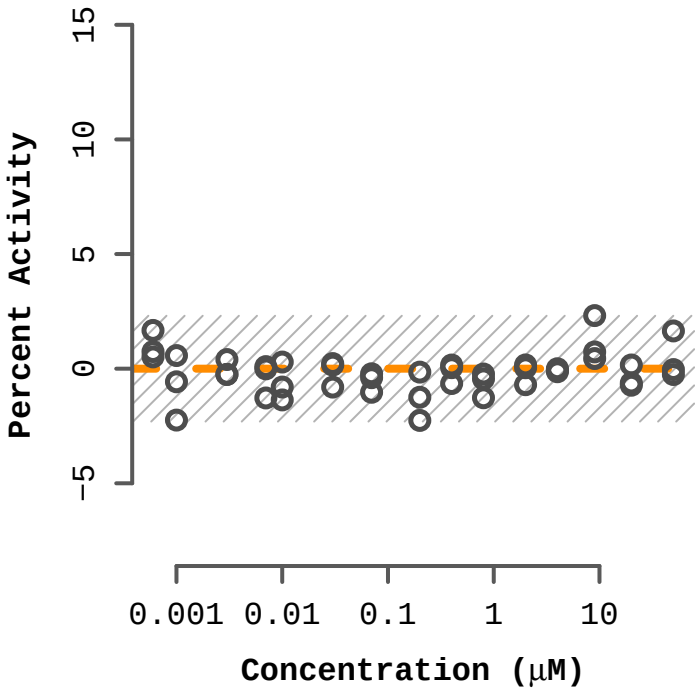
	tp	ga	gw
val:	1.28	−2.2	0.794
sd:	0.359	0.815	1.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.5	−2.03	0.728	3.19	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	190.43	177.89	181.82
PROB:	0	0.88	0.12
RMSE:	2.06	1.62	1.62

MAX_MEAN: 2.69 **MAX_MED:** 2.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

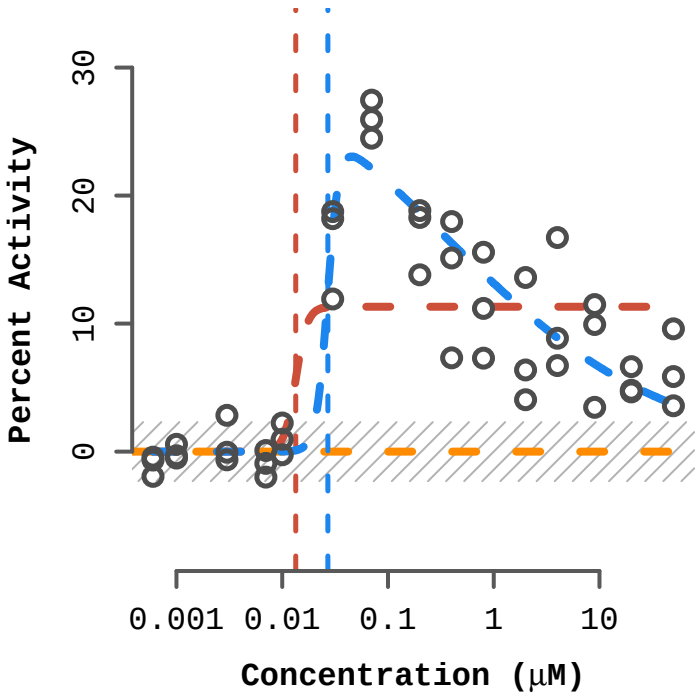
NAME: Propyphenazone
CHID: 23529 **CASRN:** 479-92-5
SPID(S): Tox21_112233_1
M4ID: 12483217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.749 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Proscillaridin
CHID: 23532 CASRN: 466-06-8
SPID(S): Tox21_110442_1
M4ID: 12484353

HILL MODEL (in red):

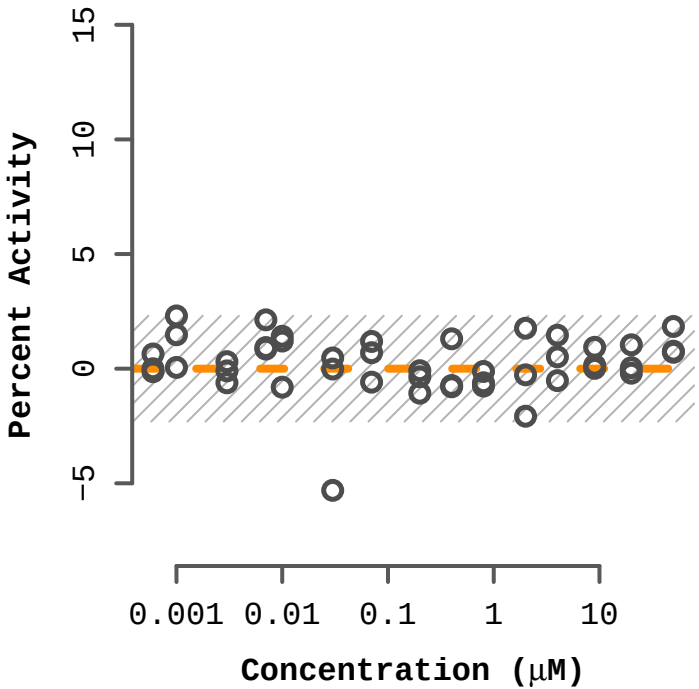
	tp	ga	gw
val:	11.3	-1.87	8
sd:	1.12	0.169	8.18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	32.9	-1.57	8	-0.421	0.423
sd:	7.45	0.0731	11.9	0.469	0.0698

	CNST	HILL	GNLS
AIC:	350.33	288.41	245.84
PROB:	0	0	1
RMSE:	11.45	5.57	3.3

MAX_MEAN: 26 MAX_MED: 25.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

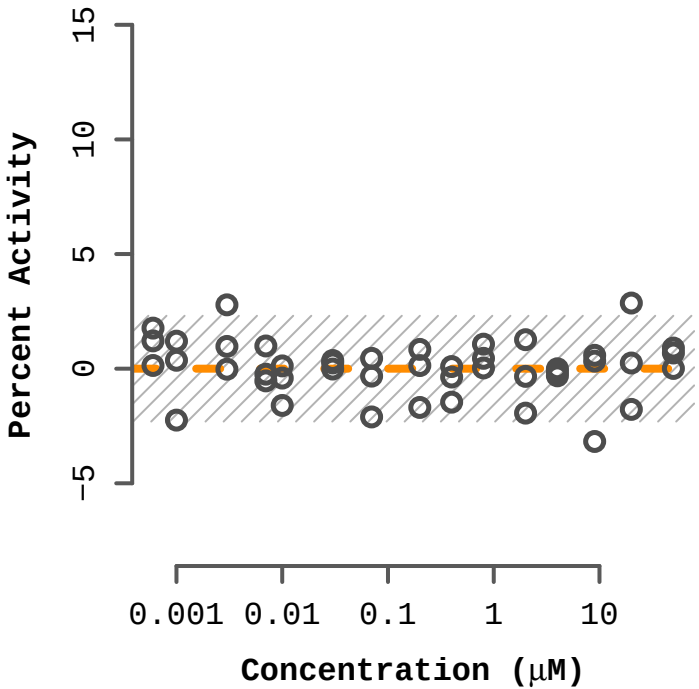
NAME: Proxyphylline
CHID: 23536 **CASRN:** 603-00-9
SPID(S): Tox21_110471_1
M4ID: 12484330

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

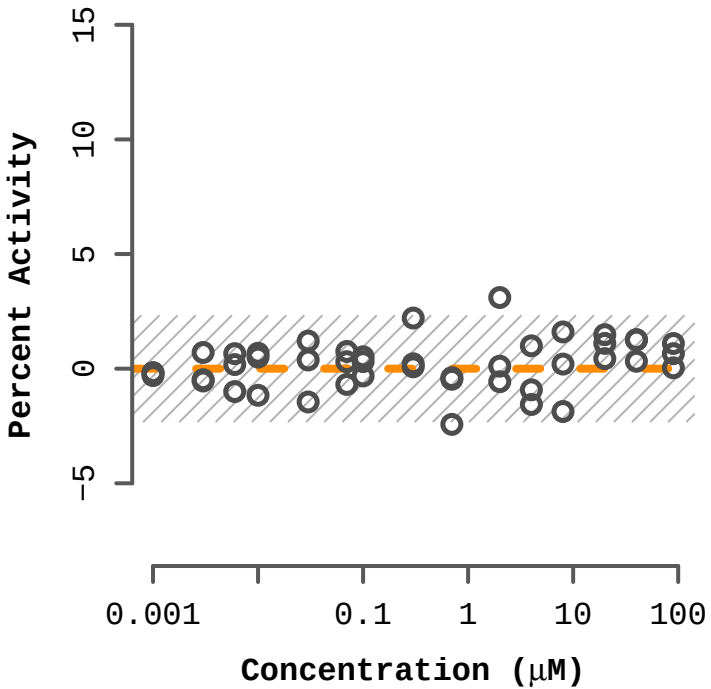
NAME: Pyridostigmine bromide
CHID: 23540 **CASRN:** 101-26-8
SPID(S): Tox21_111266_1
M4ID: 12483806

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

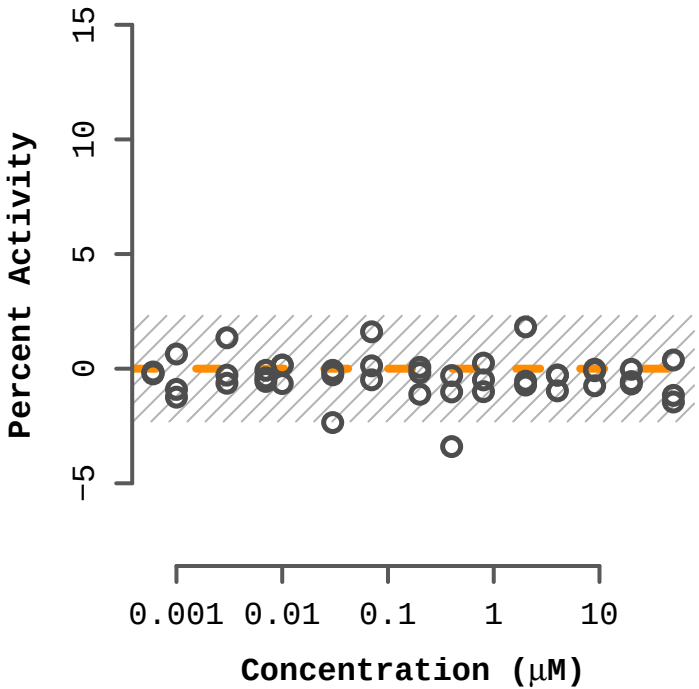
NAME: Pyridoxine
CHID: 23541 **CASRN:** 65-23-6
SPID(S): Tox21_300365
M4ID: 12478767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

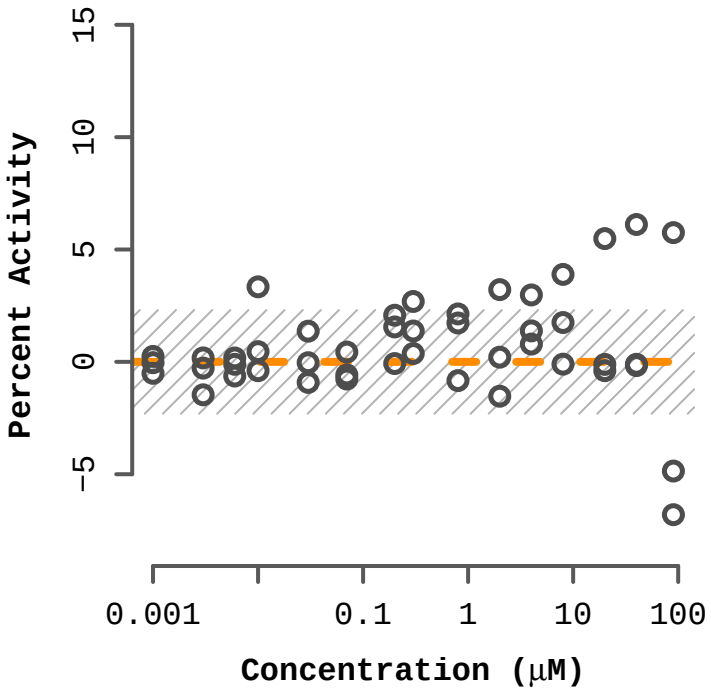
NAME: Pyridoxine
CHID: 23541 **CASRN:** 65-23-6
SPID(S): Tox21_113644_1
M4ID: 12482566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.157 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

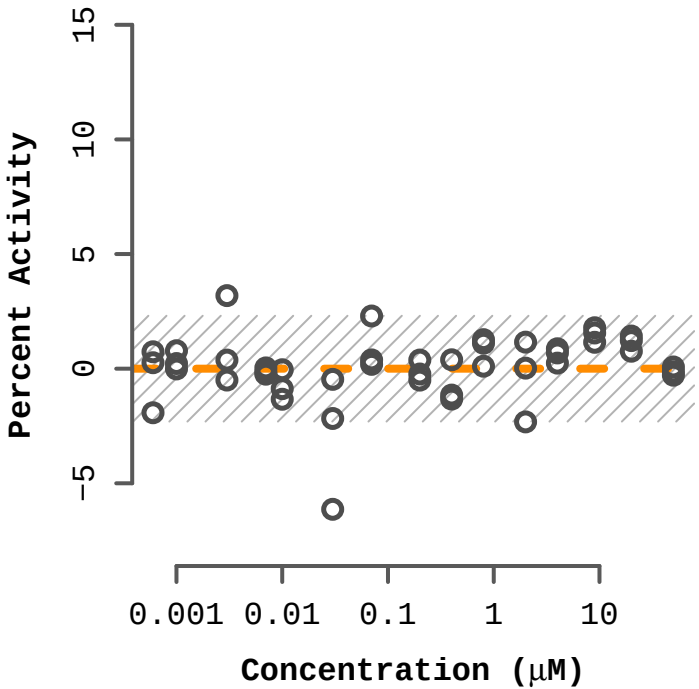
NAME: Pyrilamine
CHID: 23542 **CASRN:** 91-84-9
SPID(S): Tox21_200978
M4ID: 12481274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.38	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

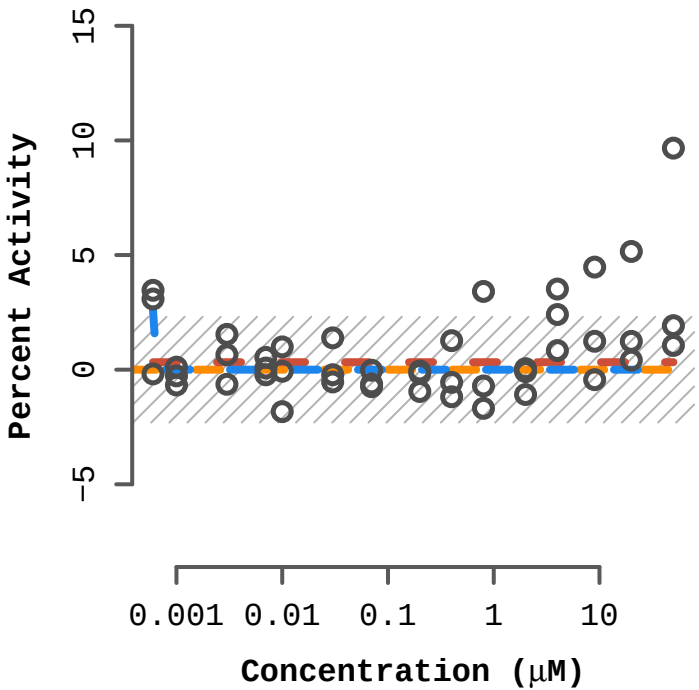
NAME: Pyrilamine
CHID: 23542 **CASRN:** 91-84-9
SPID(S): Tox21_110230_1
M4ID: 12484531

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Quetiapine
CHID: 23546 CASRN: 111974-69-7
SPID(S): Tox21_111537_1
M4ID: 12483630

HILL MODEL (in red):

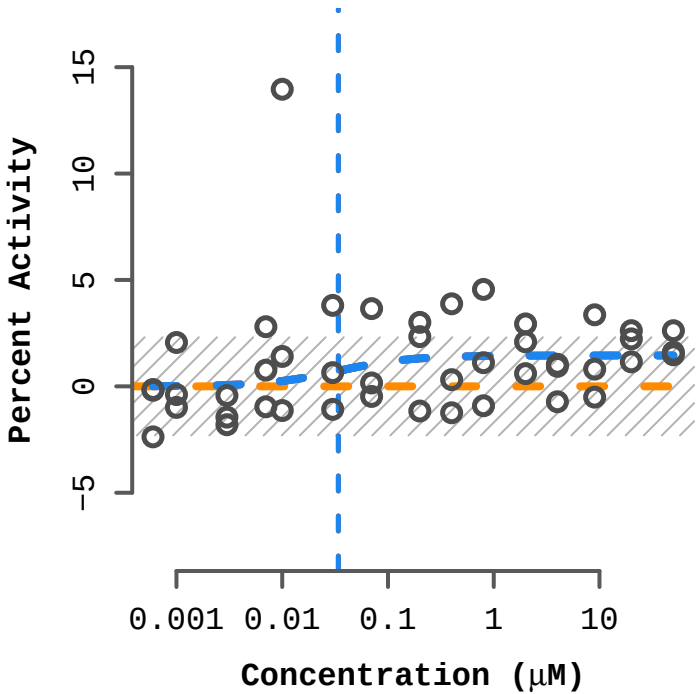
	tp	ga	gw
val:	0.326	−5	3.91
sd:	0.229	1460	3240

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.6	−4.2	1.97	−3.25	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	184.18	188.05	188.9
PROB:	0.81	0.12	0.08
RMSE:	2.21	2.12	2.15

MAX_MEAN: 4.22 **MAX_MED:** 3.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Quinethazone
CHID: 23548 **CASRN:** 73-49-4
SPID(S): Tox21_110366_1
M4ID: 12484422

HILL MODEL (in red):

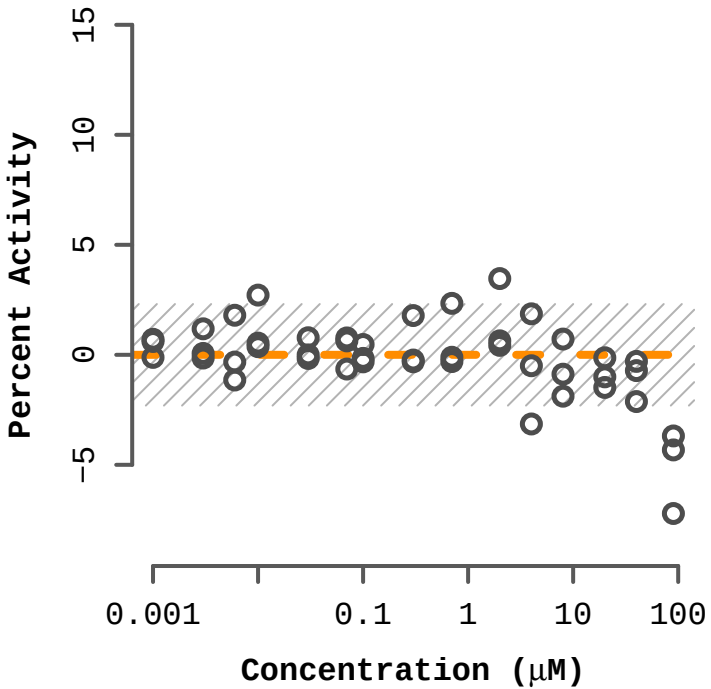
	tp	ga	gw
val:	1.45	−1.47	1.28
sd:	0.418	1.06	1.75

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.45	−1.47	1.28	3.69	3.55
sd:	0.418	1.06	1.75	1210	2130

	CNST	HILL	GNLS
AIC:	206.24	197.26	201.26
PROB:	0.01	0.87	0.12
RMSE:	2.84	2.58	2.58

MAX_MEAN: 4.74 **MAX_MED:** 2.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

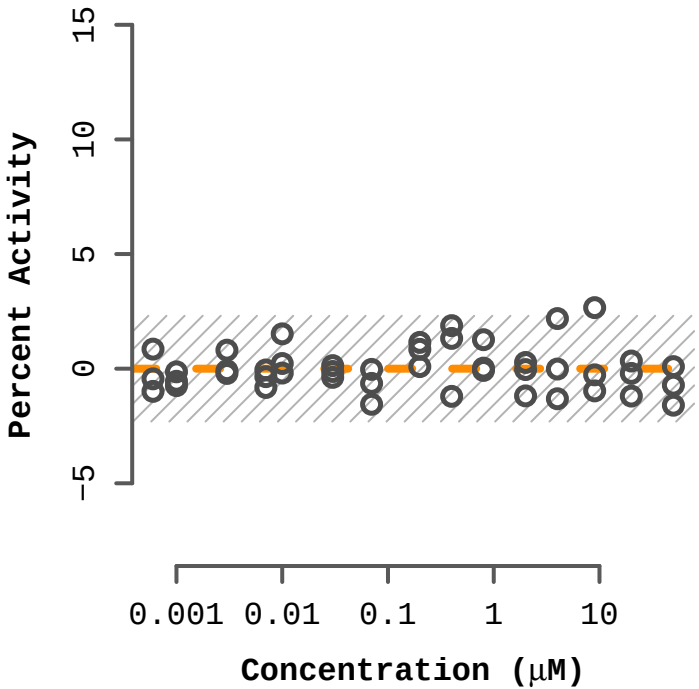
NAME: Quinidine
CHID: 23549 **CASRN:** 56-54-2
SPID(S): Tox21_201110
M4ID: 12481142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 0.637 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

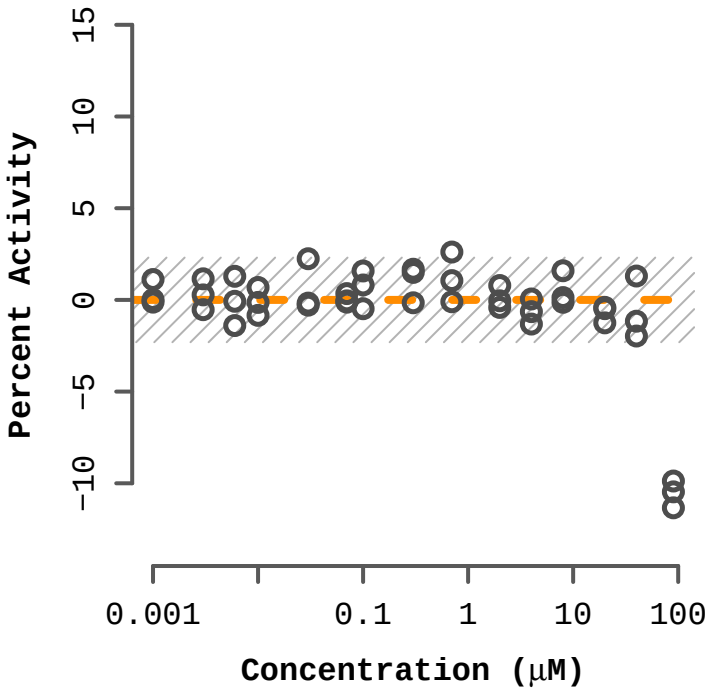
NAME: Quinidine
CHID: 23549 **CASRN:** 56-54-2
SPID(S): Tox21_111720_1
M4ID: 12483520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.695 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

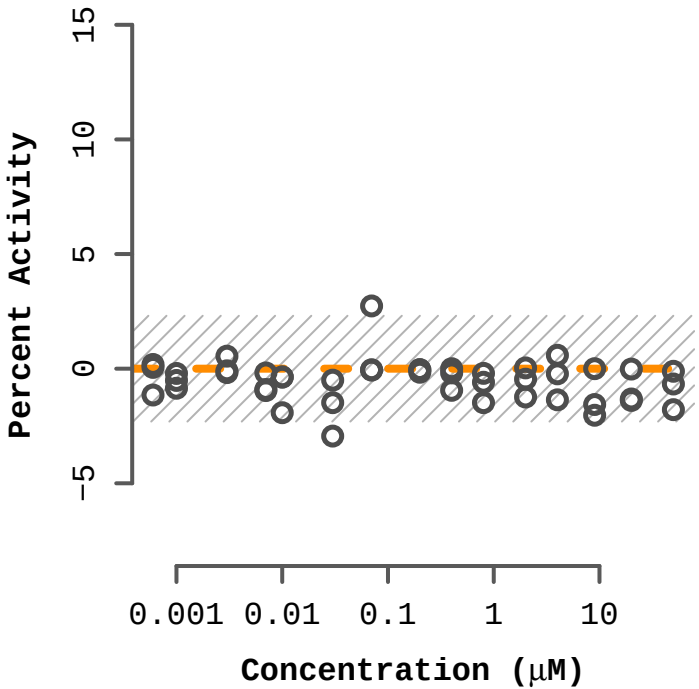
NAME: Raloxifene
CHID: 23550 **CASRN:** 84449-90-1
SPID(S): Tox21_202603
M4ID: 12479649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.27	NA	NA
PROB:	1	NA	NA
RMSE:	2.9	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

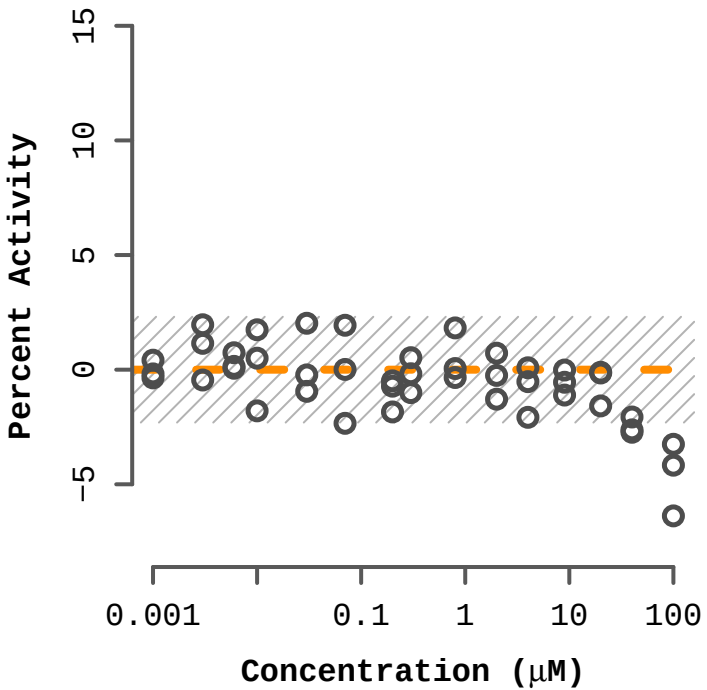
NAME: Ramipril
CHID: 23551 CASRN: 87333-19-5
SPID(S): Tox21_110708_1
M4ID: 12484160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.877 MAX_MED: 0.0571 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

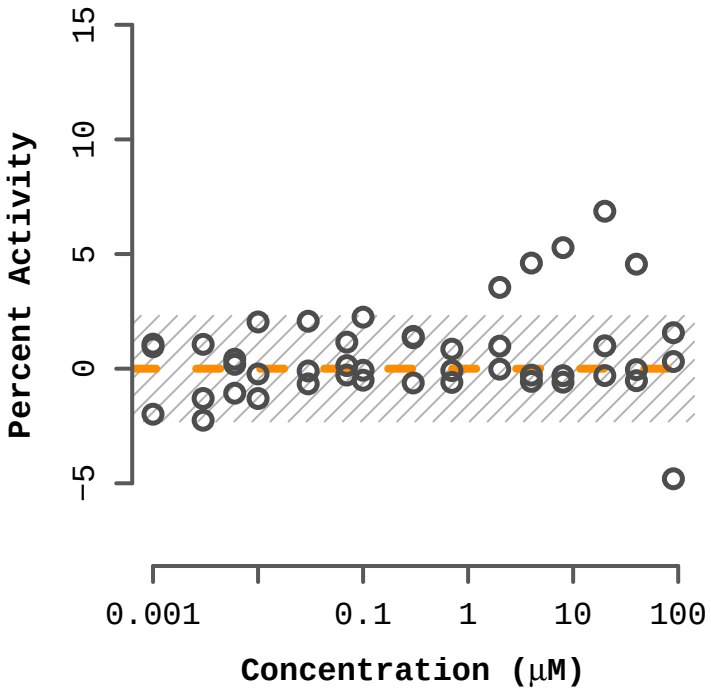
NAME: Retinol
CHID: 23556 **CASRN:** 68-26-8
SPID(S): Tox21_300287
M4ID: 12478843

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 0.887 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

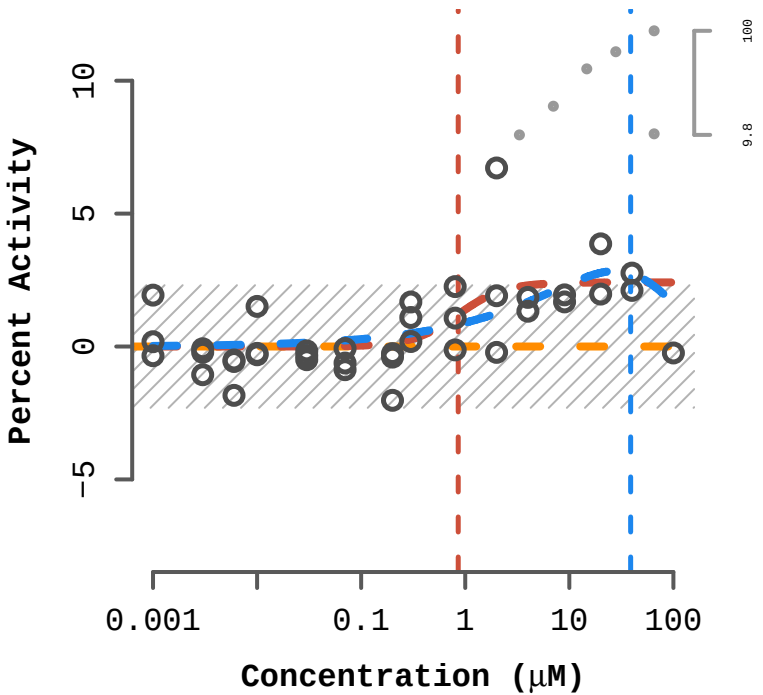
NAME: Retinol
CHID: 23556 **CASRN:** 68-26-8
SPID(S): Tox21_202441
M4ID: 12479811

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.21	NA	NA
PROB:	1	NA	NA
RMSE:	2.09	NA	NA

MAX_MEAN: 2.52 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ribavirin
CHID: 23557 **CASRN:** 36791-04-5
SPID(S): Tox21_200967
M4ID: 12481285 **BRK**

HILL MODEL (in red):

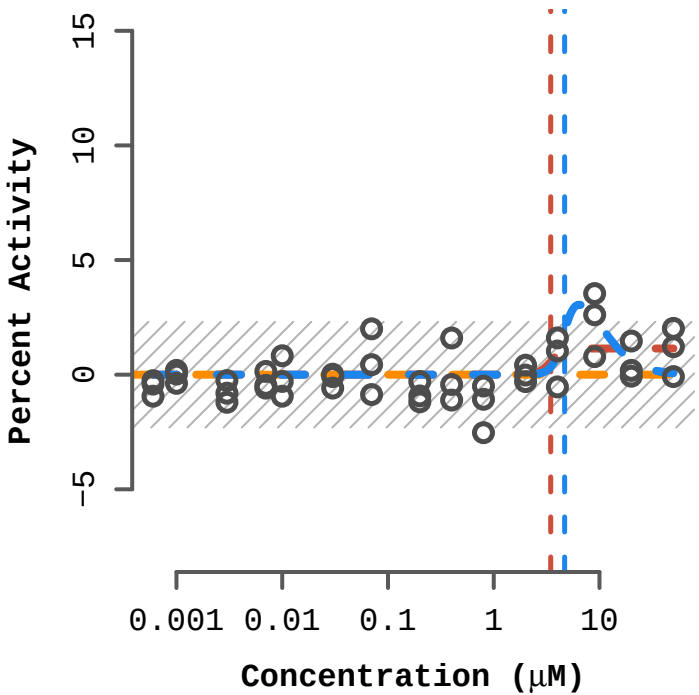
	tp	ga	gw
val:	2.41	−0.0676	1.96
sd:	0.661	0.4	2.09

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.58	1.59	0.548	1.84	1.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	311.43	300.65	305.74
PROB:	0	0.92	0.07
RMSE:	22.75	22	22.04

MAX_MEAN: 37.2 **MAX_MED:** 10.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ribavirin
CHID: 23557 **CASRN:** 36791-04-5
SPID(S): Tox21_110259_1
M4ID: 12484505

HILL MODEL (in red):

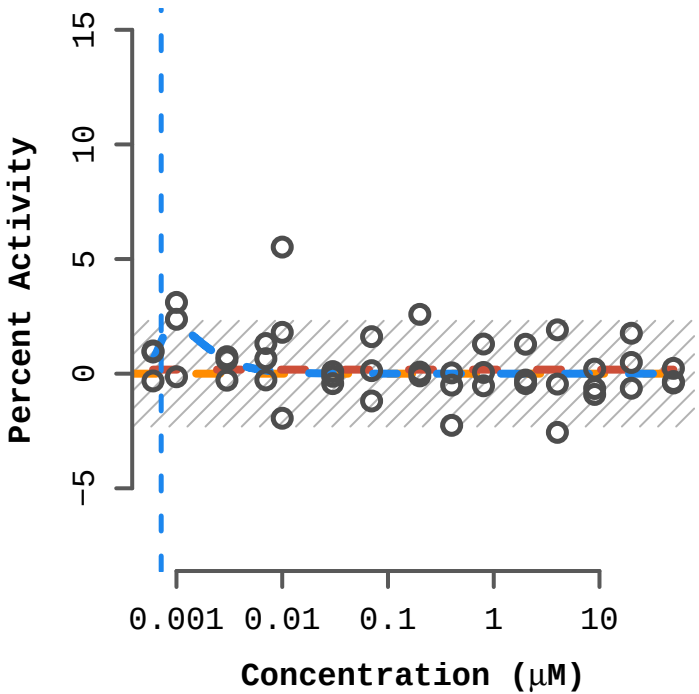
	tp	ga	gw
val:	1.14	0.539	8
sd:	0.363	0.331	34

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.25	0.67	7.92	1.01	2.64
sd:	8	0.227	25.9	0.688	5.67

	CNST	HILL	GNLS
AIC:	137.75	132.05	133.89
PROB:	0.04	0.69	0.27
RMSE:	1.13	0.95	0.92

MAX_MEAN: 2.31 **MAX_MED:** 2.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Rolitetracycline
CHID: 23568 **CASRN:** 751-97-3
SPID(S): Tox21_110483_1
M4ID: 12484321

HILL MODEL (in red):

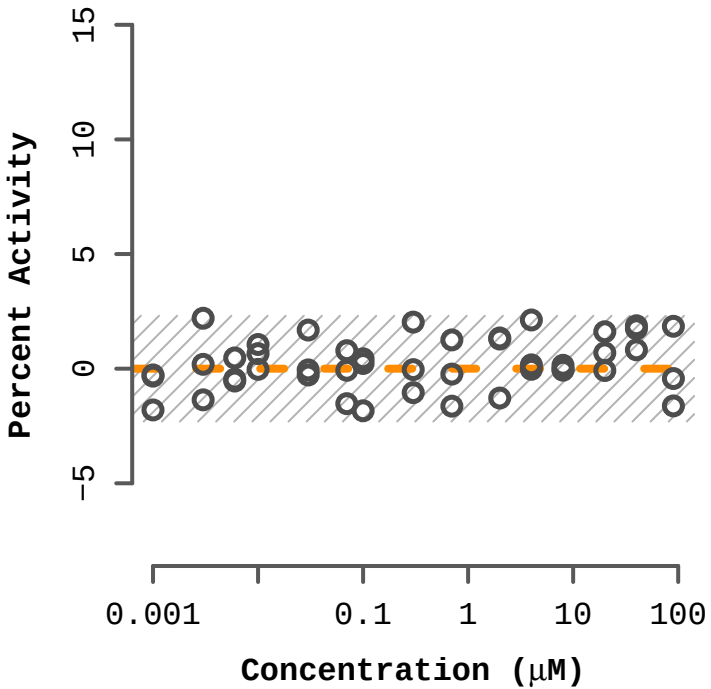
	tp	ga	gw
val:	0.176	−5.09	3.55
sd:	0.175	1400	2590

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.74	−3.14	7.57	−2.89	1.91
sd:	6.09	0.162	11.1	0.779	2.8

	CNST	HILL	GNLS
AIC:	155.41	160.37	158.01
PROB:	0.74	0.06	0.2
RMSE:	1.45	1.41	1.36

MAX_MEAN: 1.79 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

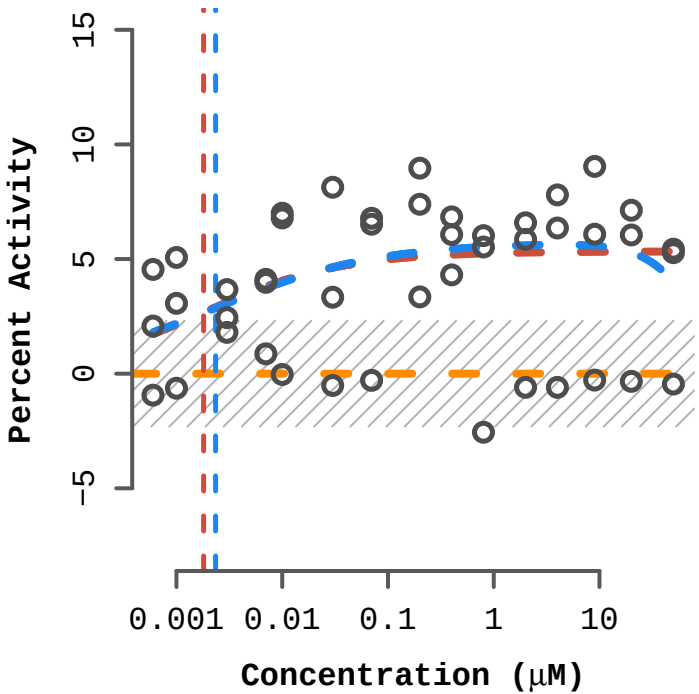
NAME: Rosiglitazone maleate
CHID: 23569 **CASRN:** 155141-29-0
SPID(S): Tox21_302367
M4ID: 12476766

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Salsalate
CHID: 23572 CASRN: 552-94-3
SPID(S): Tox21_111548_1
M4ID: 12483625

HILL MODEL (in red):

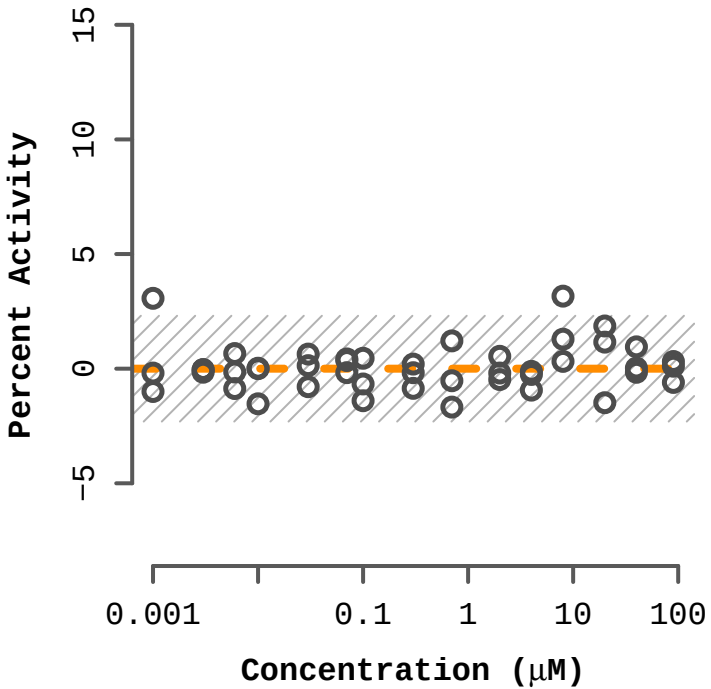
	tp	ga	gw
val:	5.33	−2.74	0.666
sd:	0.688	0.469	0.459

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.73	−2.63	0.568	1.9	1.85
sd:	1.13	0.533	0.471	0.775	5.99

	CNST	HILL	GNLS
AIC:	282.07	239.35	242.56
PROB:	0	0.83	0.17
RMSE:	5.04	3.1	3.09

MAX_MEAN: 6.57 MAX_MED: 7.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

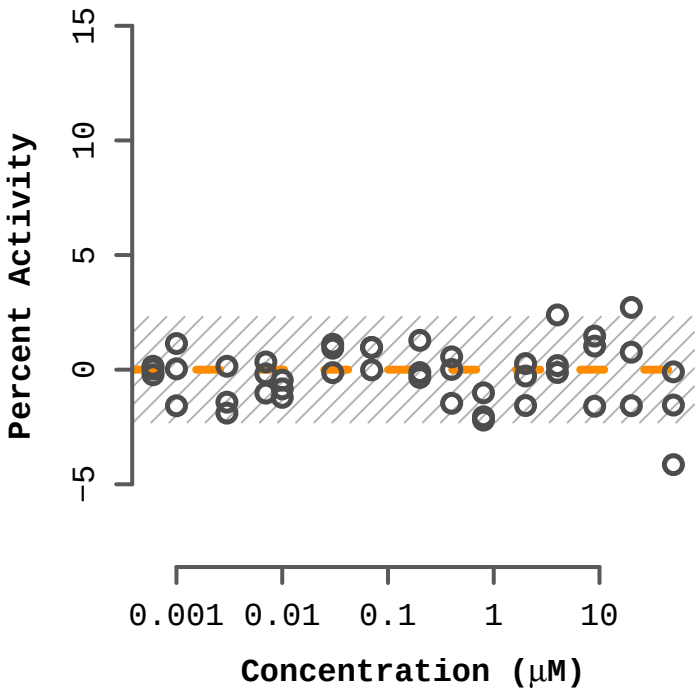
NAME: Simvastatin
CHID: 23581 CASRN: 79902-63-9
SPID(S): Tox21_300400
M4ID: 12478732

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.91	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.59 MAX_MED: 1.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

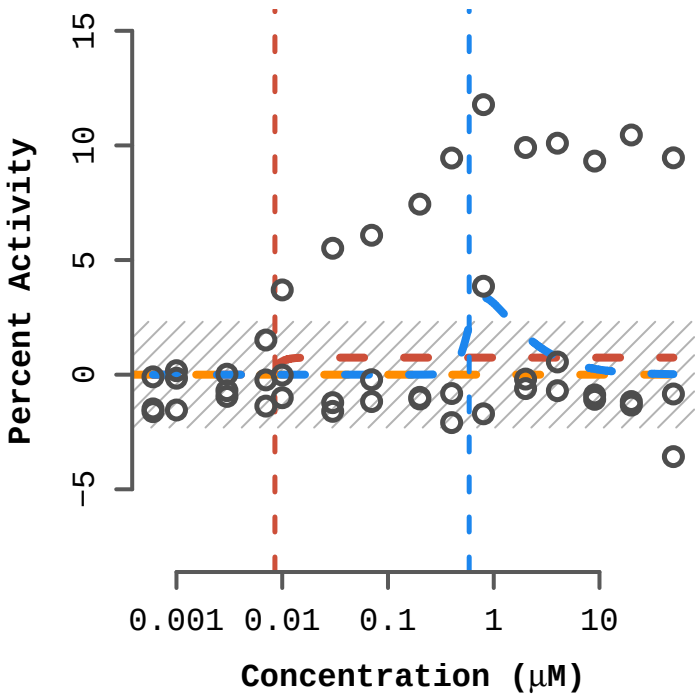
NAME: Simvastatin
CHID: 23581 **CASRN:** 79902-63-9
SPID(S): Tox21_110696_1
M4ID: 12484171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.816 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sofalcone
CHID: 23586 CASRN: 64506-49-6
SPID(S): Tox21_111705_1
M4ID: 12483527

HILL MODEL (in red):

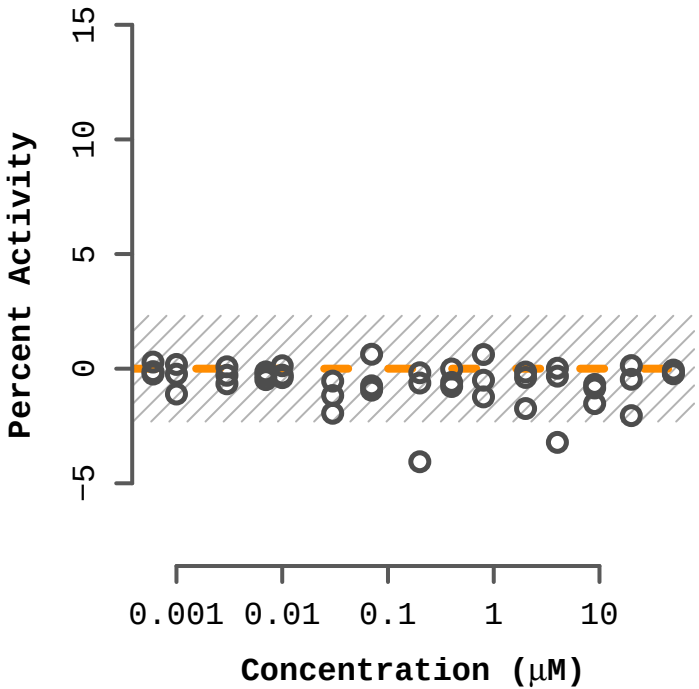
	tp	ga	gw
val:	0.744	−2.07	7.99
sd:	0.769	0.423	41.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.12	−0.232	8	0.0182	1.46
sd:	19.6	0.362	15.8	1.75	2.39

	CNST	HILL	GNLS
AIC:	256.79	261.67	264.4
PROB:	0.9	0.08	0.02
RMSE:	4.51	4.27	4.25

MAX_MEAN: 4.64 MAX_MED: 3.86 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

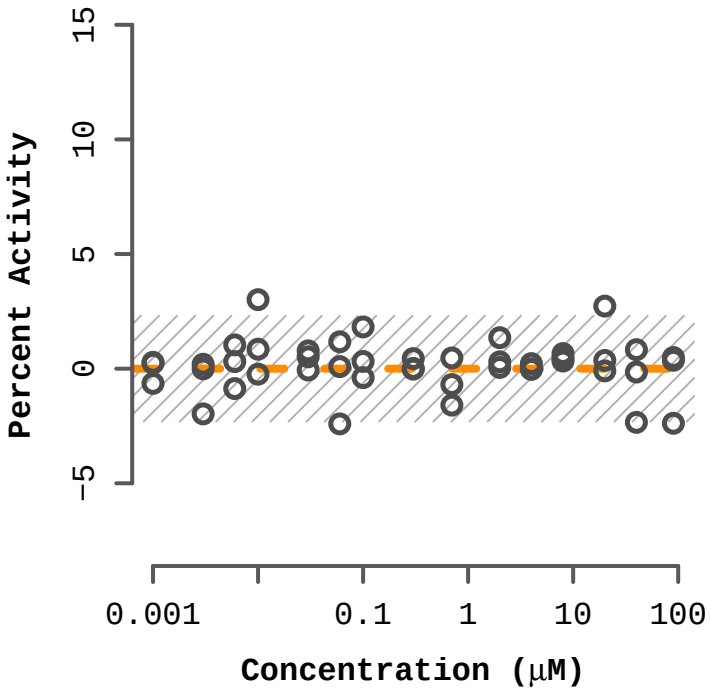
NAME: Sorbinil
CHID: 23587 CASRN: 68367-52-2
SPID(S): Tox21_111679_1
M4ID: 12483540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: −0.0239 **MAX_MED:** −0.128 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

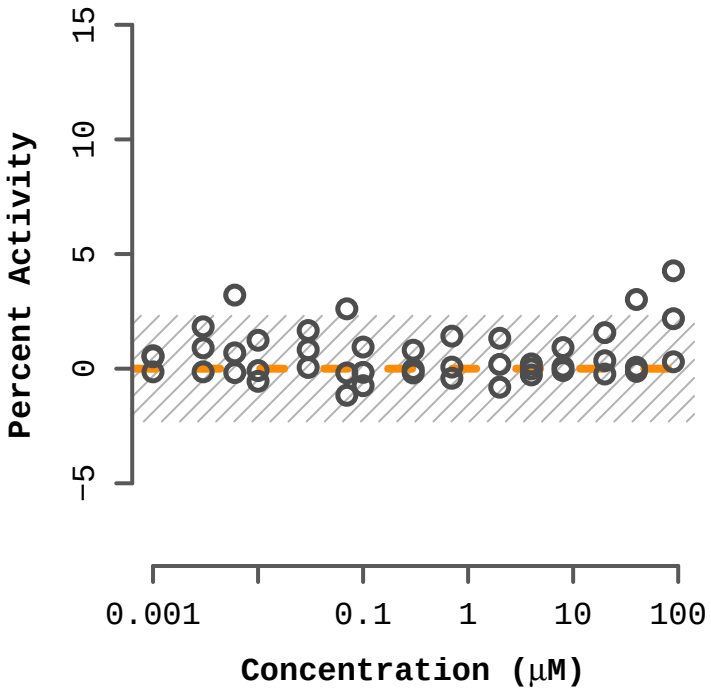
NAME: D-Glucitol
CHID: 23588 **CASRN:** 50-70-4
SPID(S): Tox21_303388
M4ID: 12475750

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

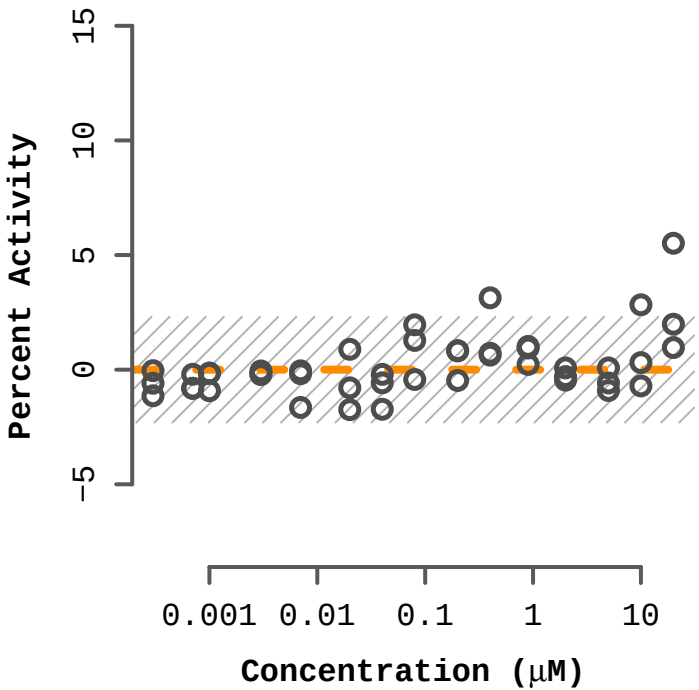
NAME: D-Glucitol
CHID: 23588 **CASRN:** 50-70-4
SPID(S): Tox21_201937
M4ID: 12480315

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

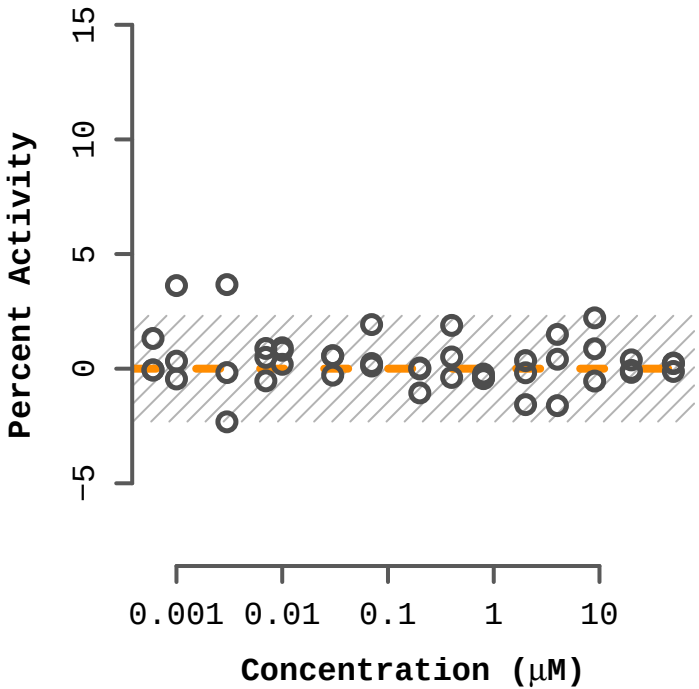
NAME: Sparfloxacin
CHID: 23590 **CASRN:** 110871-86-8
SPID(S): Tox21_111580_1
M4ID: 12483606

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.82 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

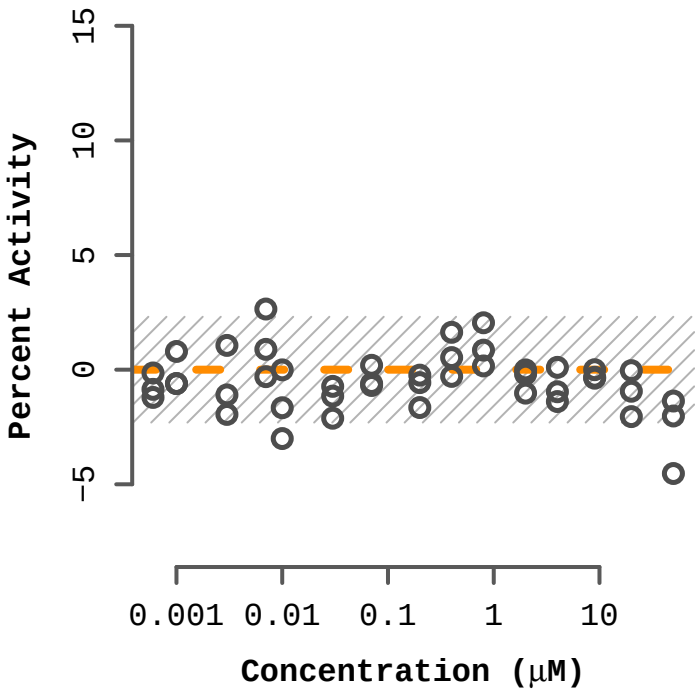
NAME: Sparteine
CHID: 23591 **CASRN:** 90-39-1
SPID(S): Tox21_110386_1
M4ID: 12484404

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.869 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

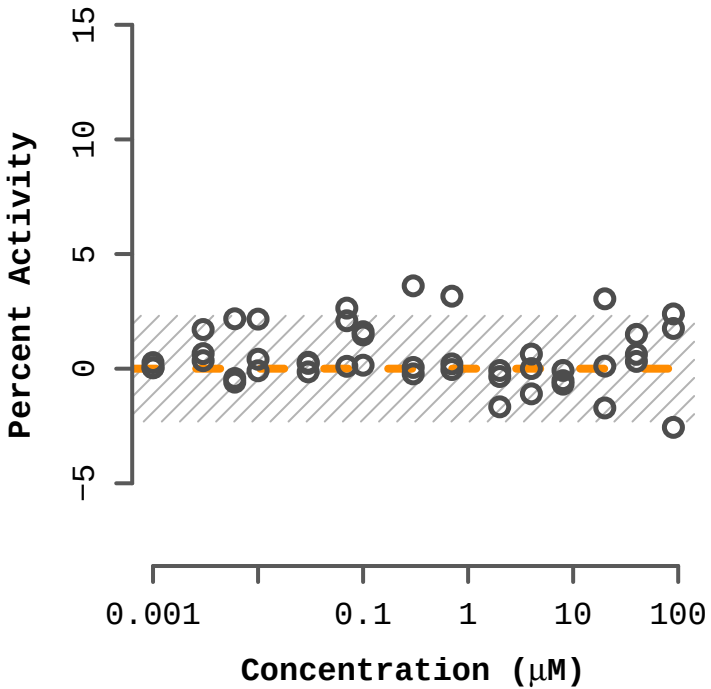
NAME: Spiramycin II
CHID: 23595 CASRN: 24916-51-6
SPID(S): Tox21_113590
M4ID: 12482594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.888 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

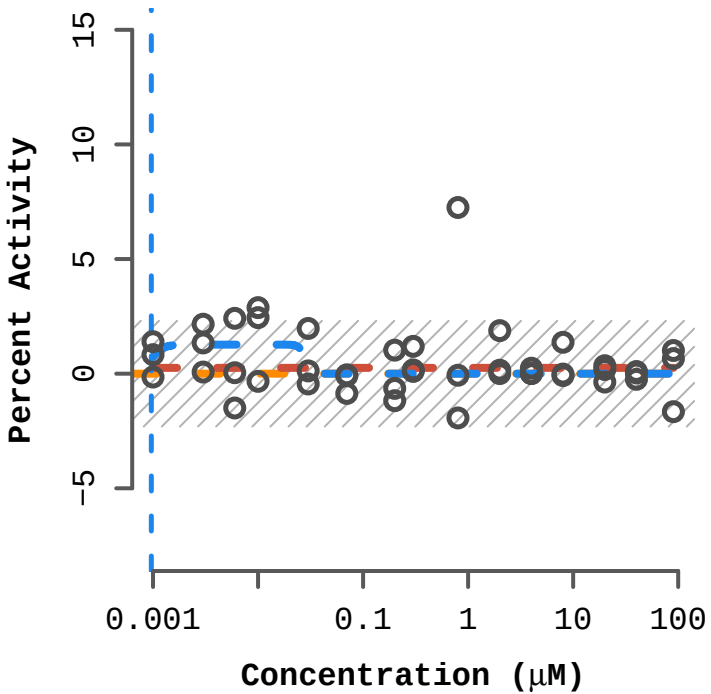
NAME: Butanedioic acid
CHID: 23602 **CASRN:** 110-15-6
SPID(S): Tox21_303247
M4ID: 12475886

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butanedioic acid
CHID: 23602 CASRN: 110-15-6
SPID(S): Tox21_201918
M4ID: 12480334

HILL MODEL (in red):

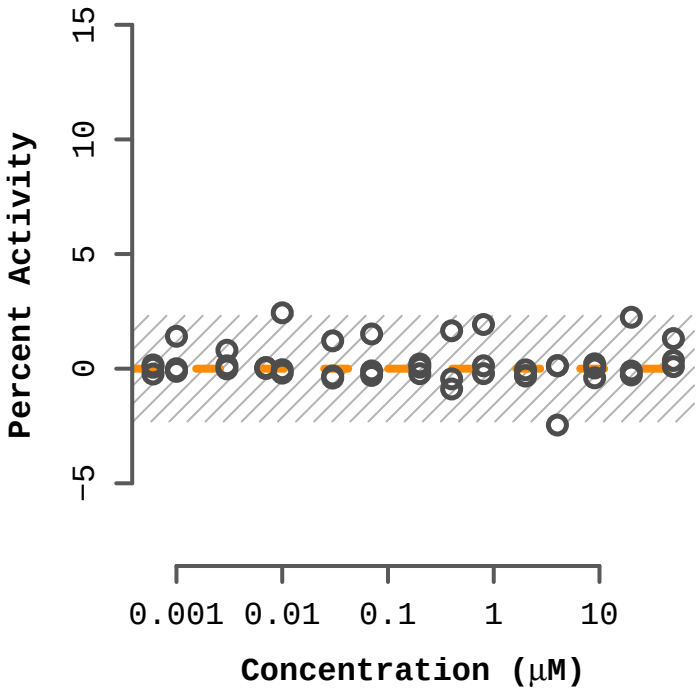
	tp	ga	gw
val:	0.253	-4.99	3.57
sd:	0.157	1970	3510

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.27	-3.02	7.76	-1.55	15.9
sd:	0.513	0.212	105	0.212	119

	CNST	HILL	GNLS
AIC:	151.13	154.44	153.04
PROB:	0.63	0.12	0.24
RMSE:	1.54	1.48	1.45

MAX_MEAN: 1.75 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

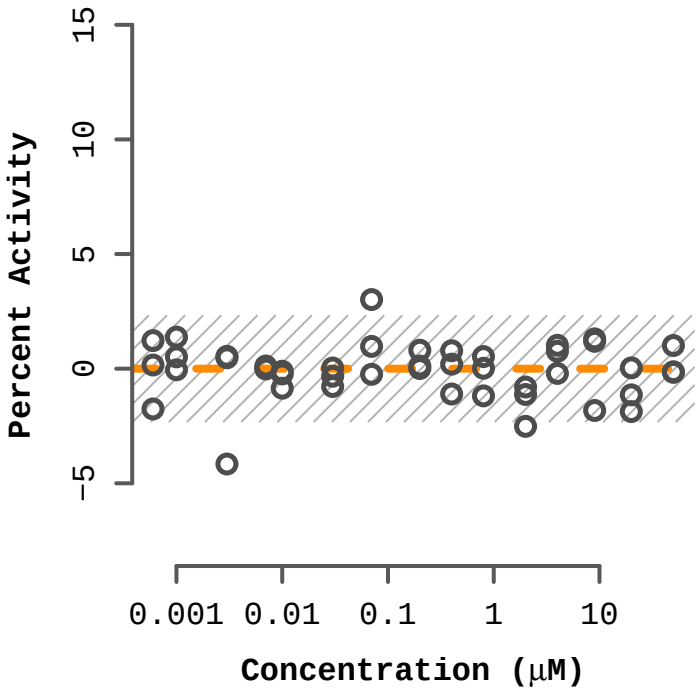
NAME: Butanedioic acid
CHID: 23602 **CASRN:** 110-15-6
SPID(S): Tox21_111612_1
M4ID: 12483588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.734 **MAX_MED:** 0.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

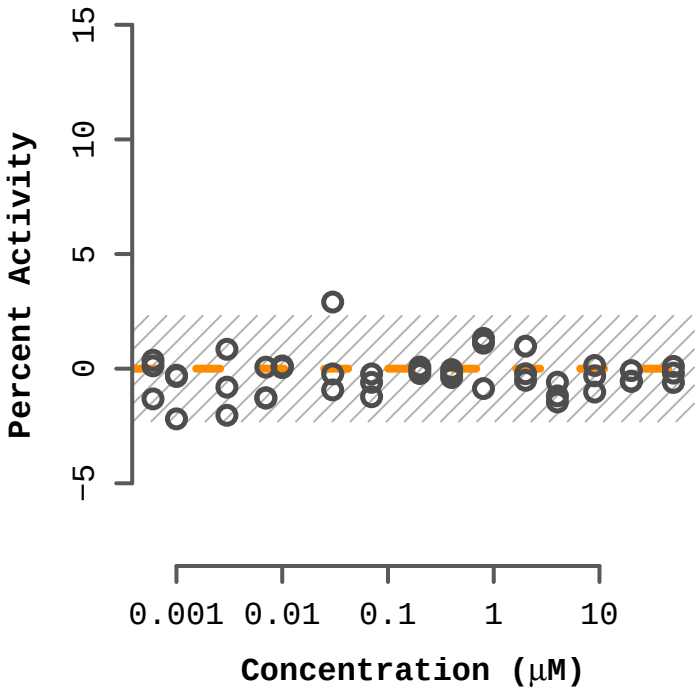
NAME: Succinylcholine chloride
CHID: 23603 **CASRN:** 71-27-2
SPID(S): Tox21_111268_1
M4ID: 12483805

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

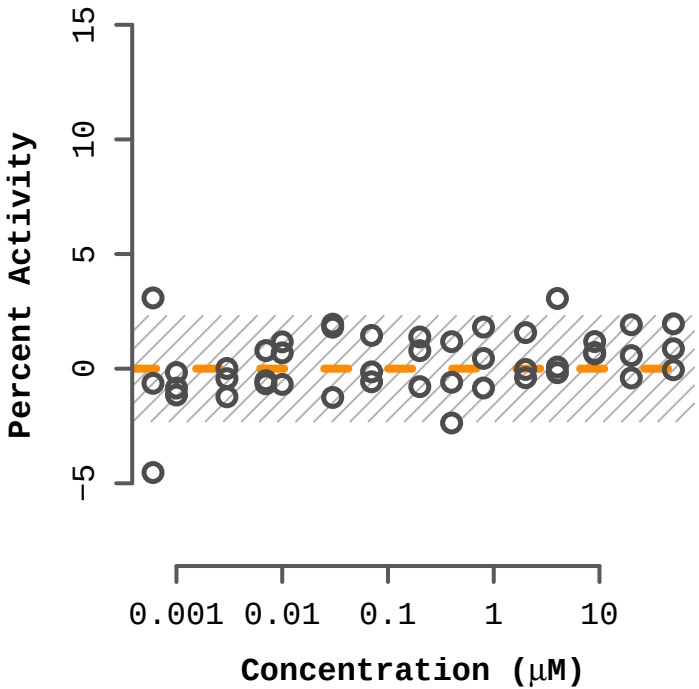
NAME: Sulbactam
CHID: 23605 **CASRN:** 68373-14-8
SPID(S): Tox21_113642_1
M4ID: 12482567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.585 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

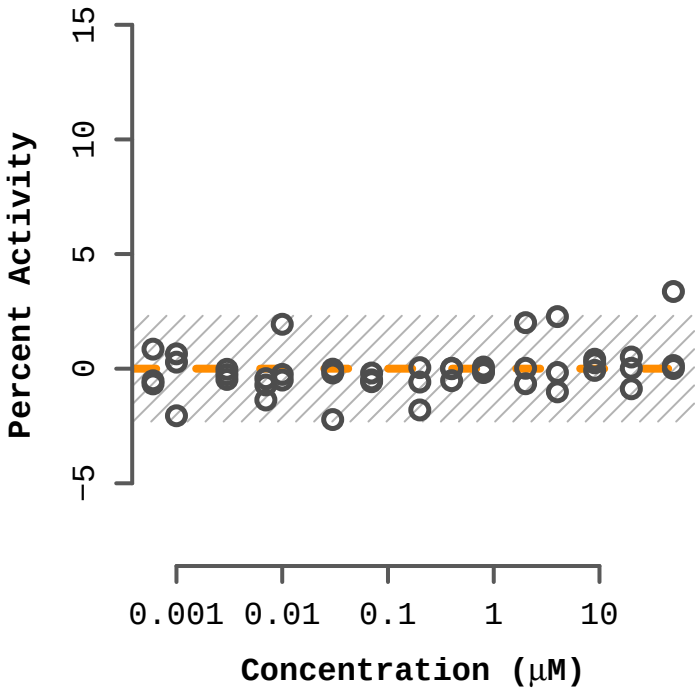
NAME: Sulfacytine
CHID: 23606 **CASRN:** 17784-12-2
SPID(S): Tox21_113734
M4ID: 12482480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.987 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

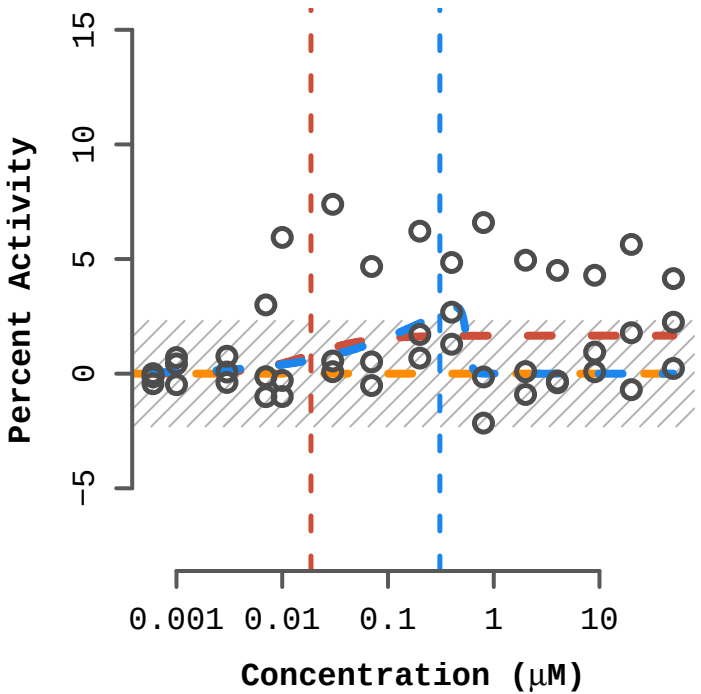
NAME: Sulfadimethoxine
CHID: 23607 **CASRN:** 122-11-2
SPID(S): Tox21_110405_1
M4ID: 12484387

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfadoxine
CHID: 23608 **CASRN:** 2447-57-6
SPID(S): Tox21_110523_1
M4ID: 12484296

HILL MODEL (in red):

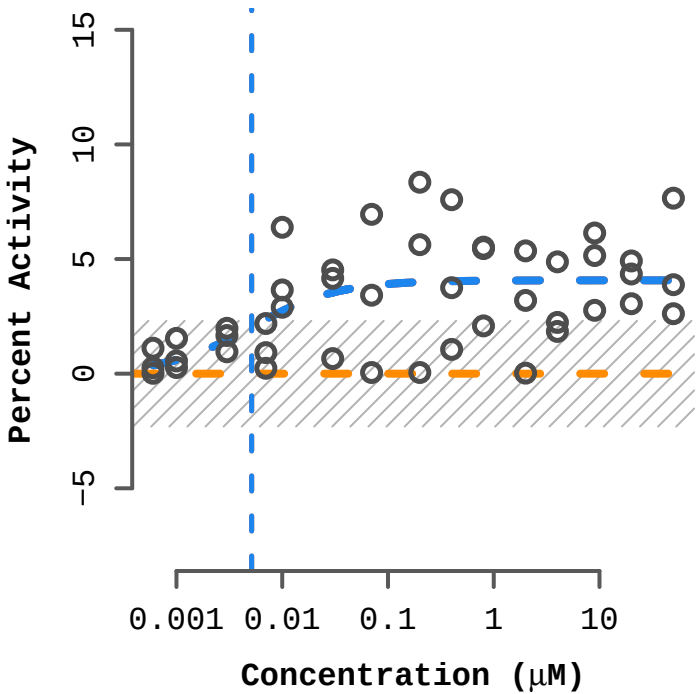
	tp	ga	gw
val:	1.66	−1.73	1.59
sd:	0.518	0.697	2.43

GAIN-LOSS MODEL (in blue):

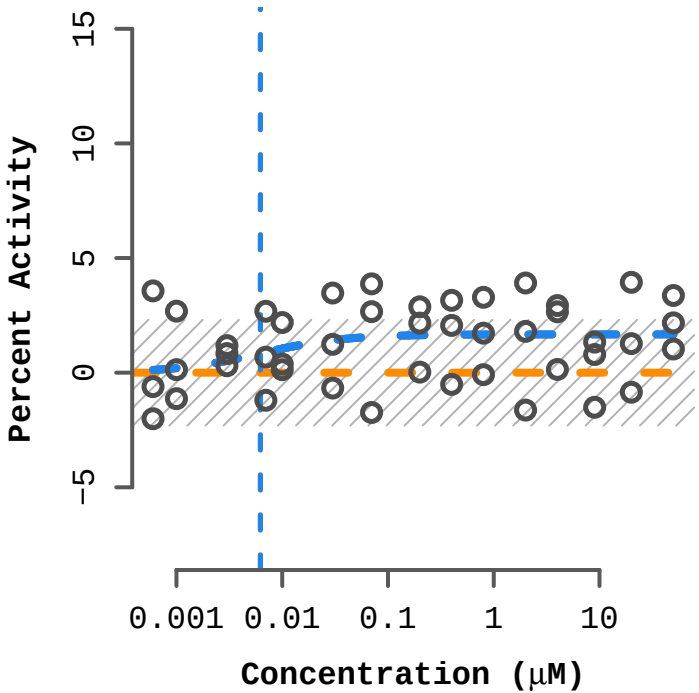
	tp	ga	gw	la	lw
val:	5.22	−0.509	0.728	−0.258	17.9
sd:	15.4	3.46	1	1.05	121

	CNST	HILL	GNLS
AIC:	220.51	213.37	220.45
PROB:	0.03	0.95	0.03
RMSE:	2.87	2.36	2.58

MAX_MEAN: 2.94 **MAX_MED:** 2.68 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Sulfaguanidine
CHID:    23609   CASRN: 57-67-0
SPID(S): Tox21_110329_1
M4ID:    12484451

HILL MODEL (in red):
      tp       ga       gw
val:  4.07     -2.29    1.07
sd:   0.42     0.24     0.589

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.07     -2.29    1.07     3.18     4.89
sd:   0.42     0.24     0.589    1760     5780

      CNST        HILL        GNLS
AIC:  257.15      198.56      202.56
PROB: 0           0.88        0.12
RMSE: 3.92        1.97        1.97

MAX_MEAN: 4.72      MAX_MED: 5.63      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfamethoxypyridazine
CHID: 23611 CASRN: 80-35-3
SPID(S): Tox21_110373_1
M4ID: 12484415

HILL MODEL (in red):

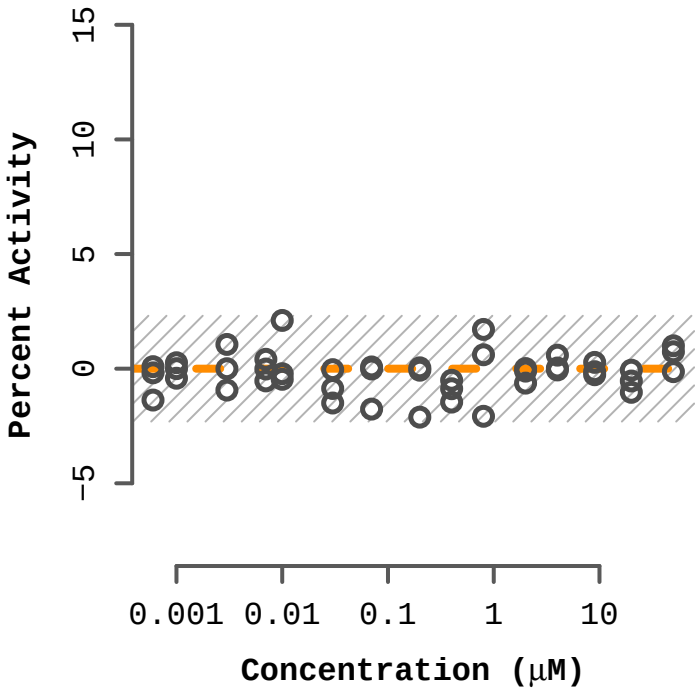
	tp	ga	gw
val:	1.67	−2.21	1.1
sd:	0.362	0.555	1.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.67	−2.21	1.1	2.73	7.86
sd:	0.362	0.555	1.1	1890	14300

	CNST	HILL	GNLS
AIC:	201.89	186.78	190.78
PROB:	0	0.88	0.12
RMSE:	2.1	1.67	1.67

MAX_MEAN: 2.19 **MAX_MED:** 2.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

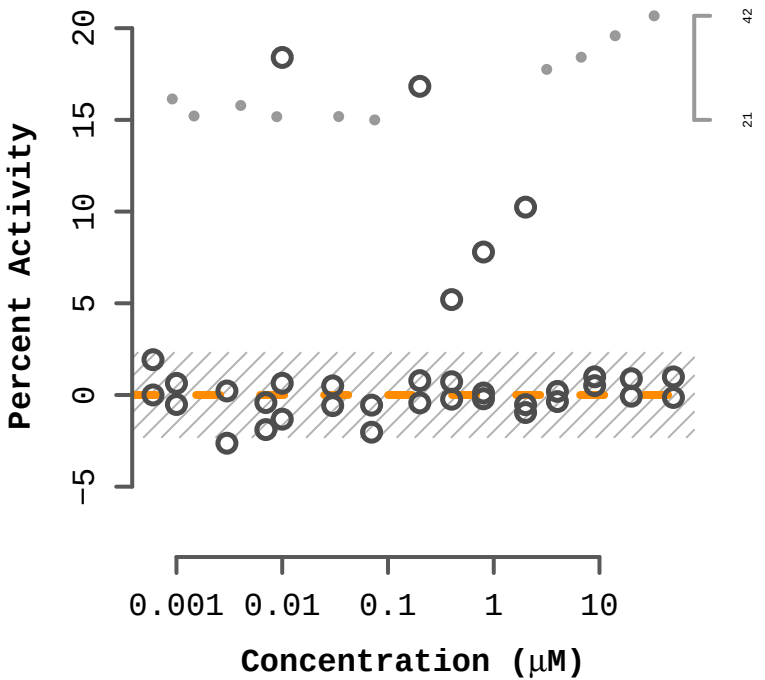
NAME: Sulfamerazine
CHID: 23612 **CASRN:** 127-79-7
SPID(S): Tox21_110411_1
M4ID: 12484382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.537 **MAX_MED:** 0.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

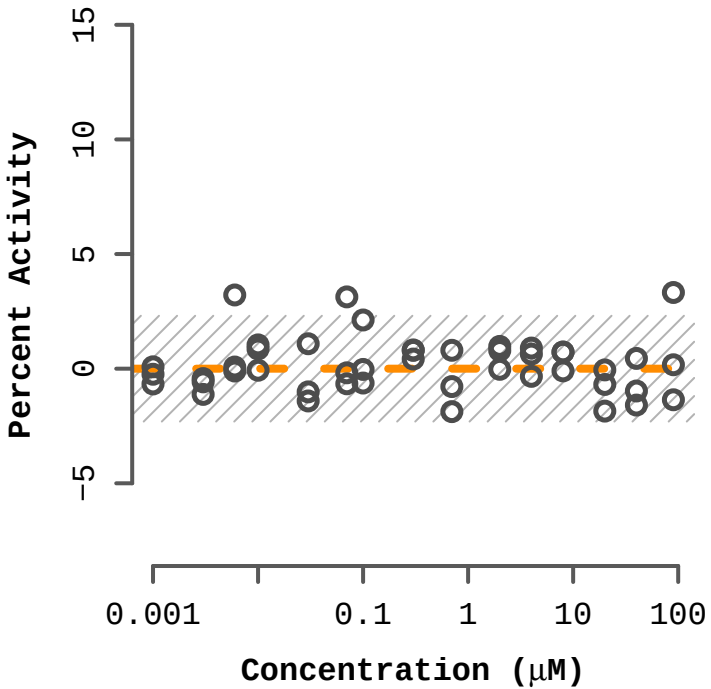
NAME: Sulfameter
CHID: 23613 **CASRN:** 651-06-9
SPID(S): Tox21_110478_1
M4ID: 12484325 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	358.42	NA	NA
PROB:	1	NA	NA
RMSE:	14.37	NA	NA

MAX_MEAN: 14.3 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

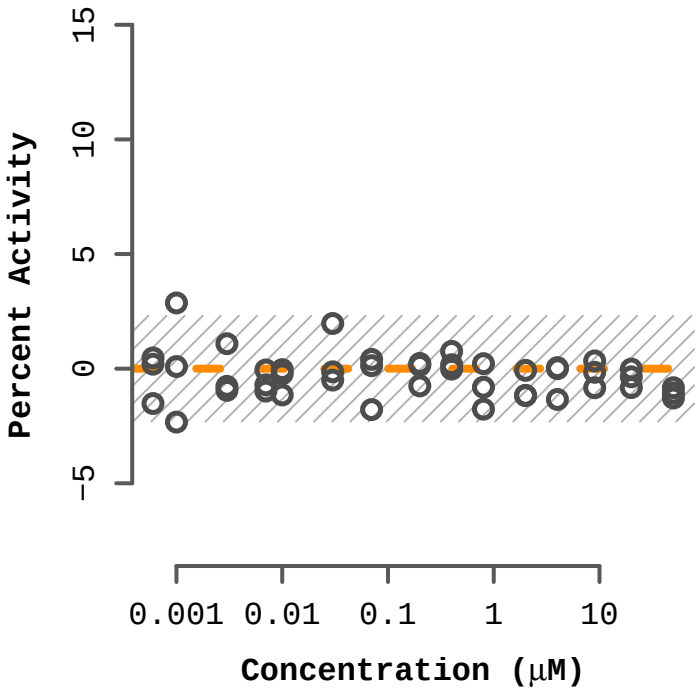
NAME: Sulfamethizole
CHID: 23615 **CASRN:** 144-82-1
SPID(S): Tox21_201035
M4ID: 12481217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

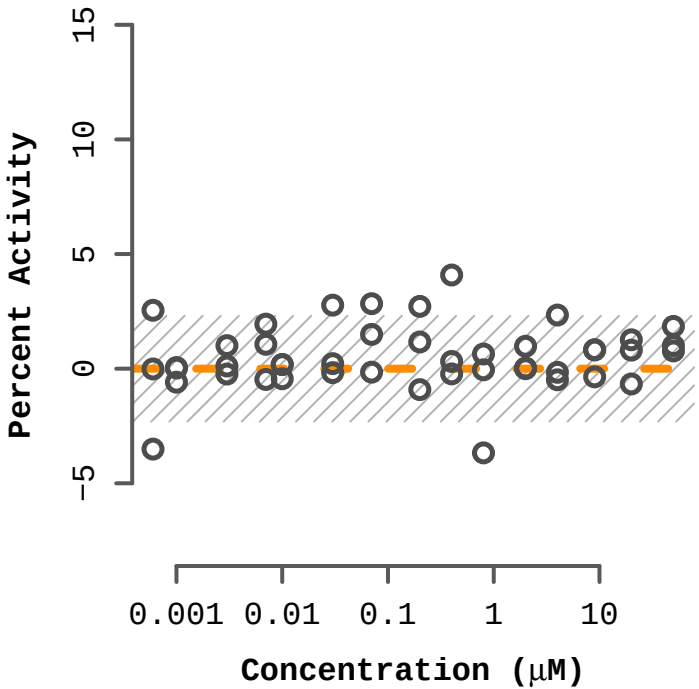
NAME: Sulfamethizole
CHID: 23615 **CASRN:** 144-82-1
SPID(S): Tox21_110425_1
M4ID: 12484369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.447 **MAX_MED:** 0.198 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

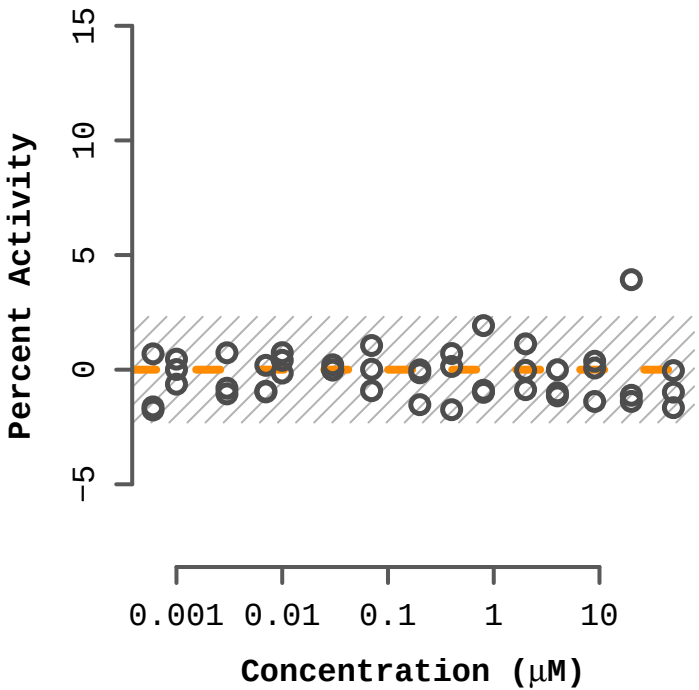
NAME: Sulfamethomidine
CHID: 23616 **CASRN:** 3772-76-7
SPID(S): Tox21_113296
M4ID: 12482729

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

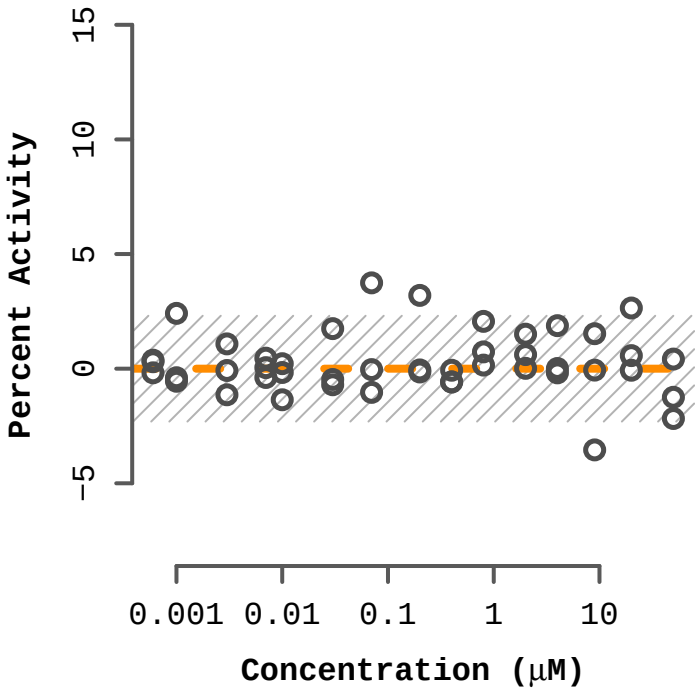
NAME: Sulfinpyrazone
CHID: 23618 **CASRN:** 57-96-5
SPID(S): Tox21_110331_1
M4ID: 12484449

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.476 **MAX_MED:** 0.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

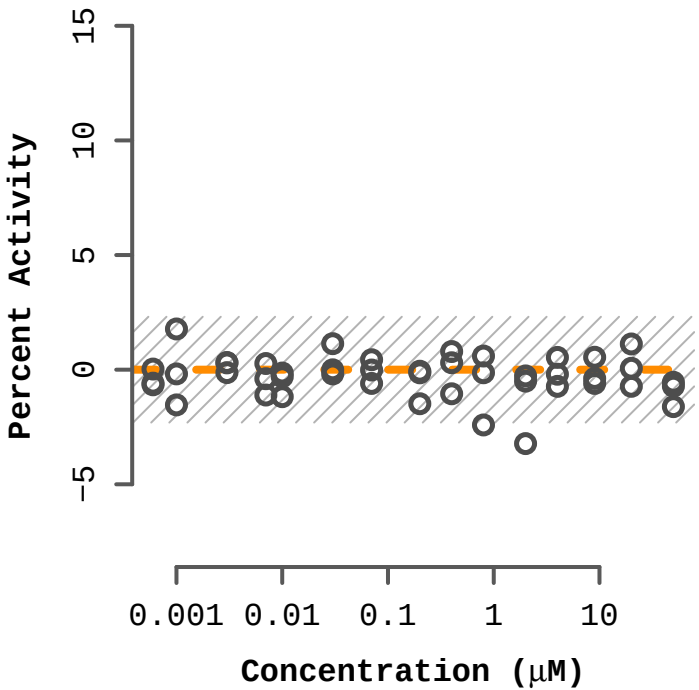
NAME: Sulfisoxazole acetal
CHID: 23620 **CASRN:** 80-74-0
SPID(S): Tox21_113660
M4ID: 12482553

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.734 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

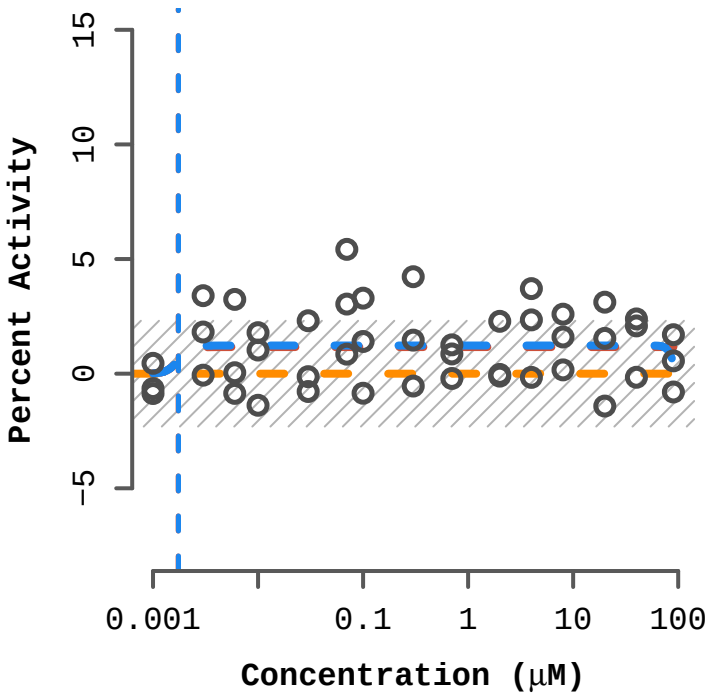
NAME: Sulfobromophthalein
CHID: 23621 **CASRN:** 71-67-0
SPID(S): Tox21_111628_1
M4ID: 12483576

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.316 **MAX_MED:** 0.304 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfanilamide
CHID: 23622 CASRN: 63-74-1
SPID(S): Tox21_303336
M4ID: 12475797

HILL MODEL (in red):

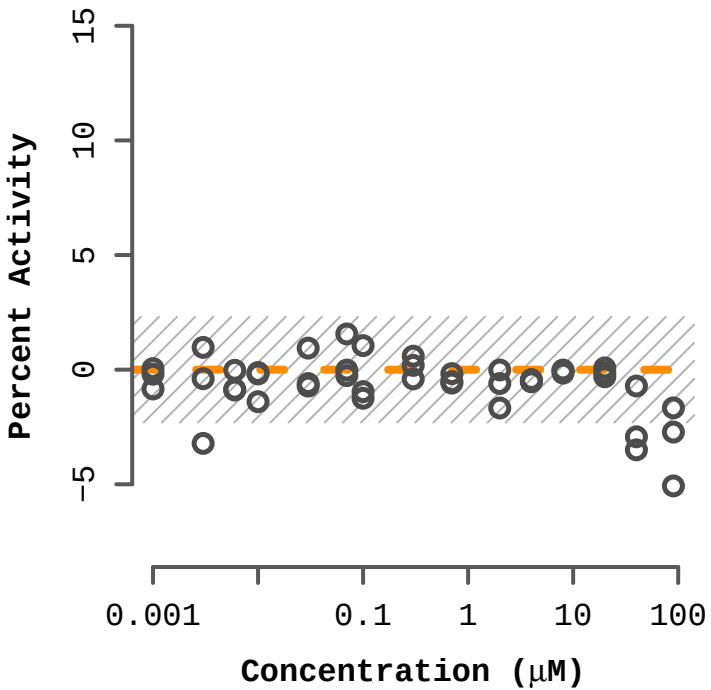
	tp	ga	gw
val:	1.16	−2.76	8
sd:	0.264	0.402	13.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.23	−2.76	8	1.94	15.5
sd:	0.277	0.399	13.5	0.11	168

	CNST	HILL	GNLS
AIC:	192.91	181.24	184.59
PROB:	0	0.84	0.16
RMSE:	1.98	1.58	1.57

MAX_MEAN: 3.1 **MAX_MED:** 3.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

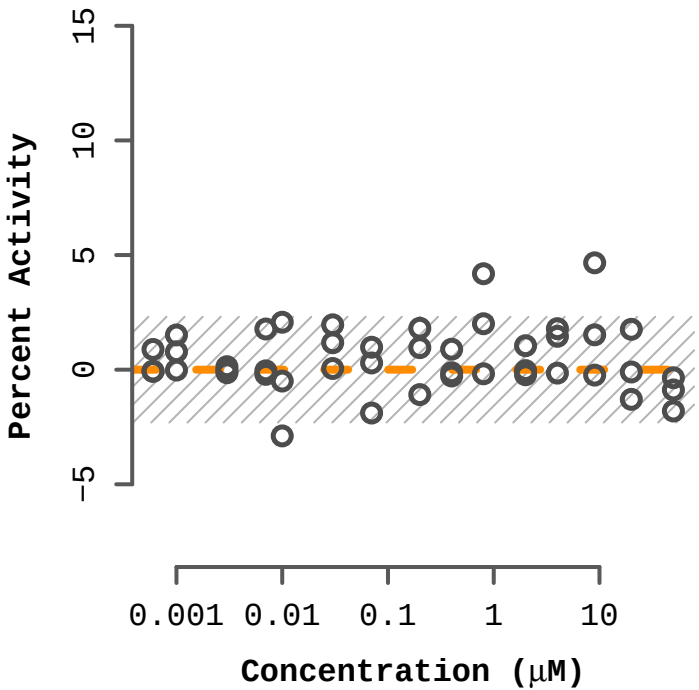
NAME: Sulfanilamide
CHID: 23622 **CASRN:** 63-74-1
SPID(S): Tox21_201331
M4ID: 12480921

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.428 **MAX_MED:** 0.188 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

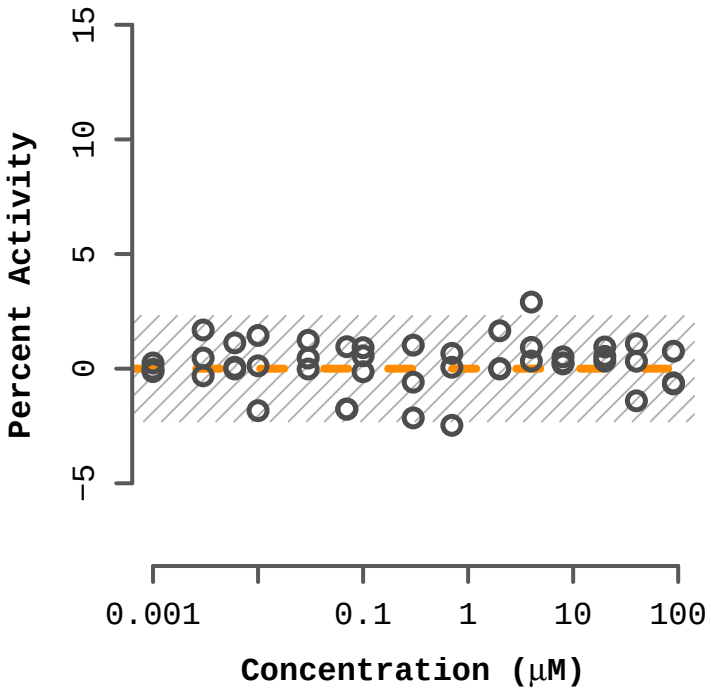
NAME: Sulfanilamide
CHID: 23622 **CASRN:** 63-74-1
SPID(S): Tox21_110351_1
M4ID: 12484432

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

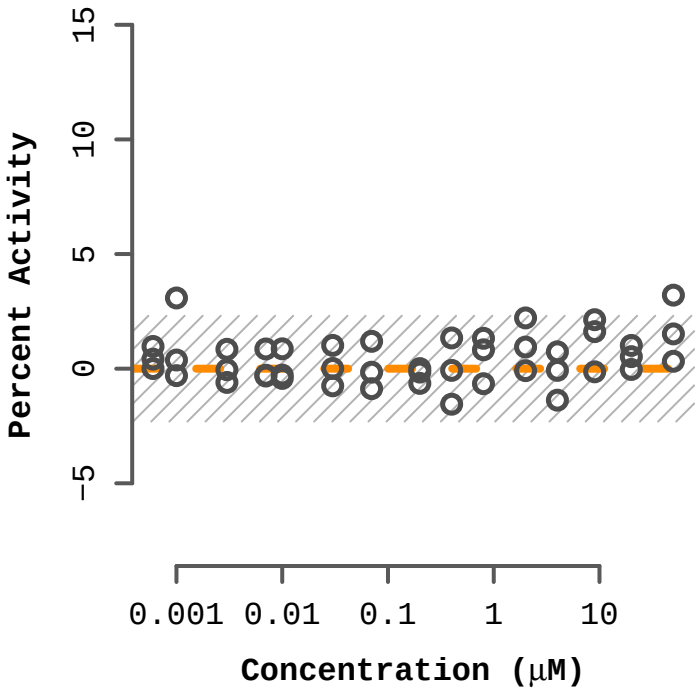
NAME: Sulindac
CHID: 23624 **CASRN:** 38194-50-2
SPID(S): Tox21_301418
M4ID: 12477715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

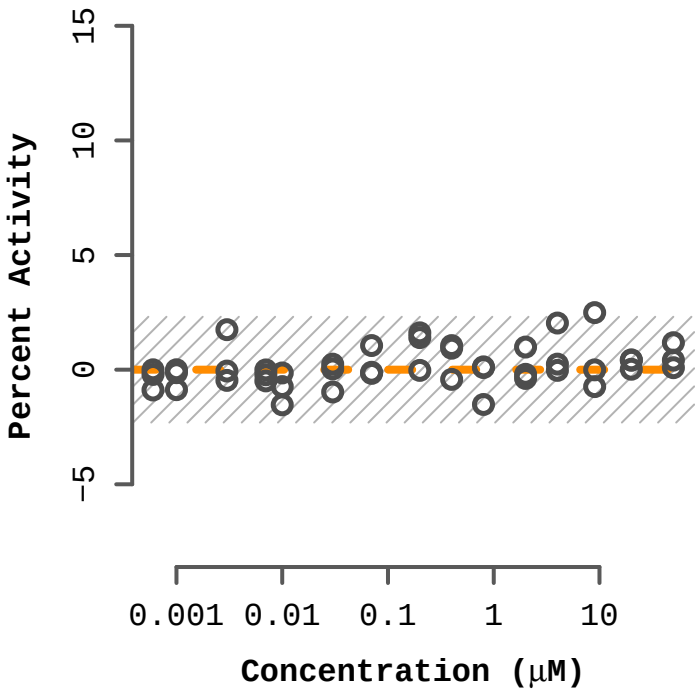
NAME: Sulindac
CHID: 23624 **CASRN:** 38194-50-2
SPID(S): Tox21_110270_1
M4ID: 12484497

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

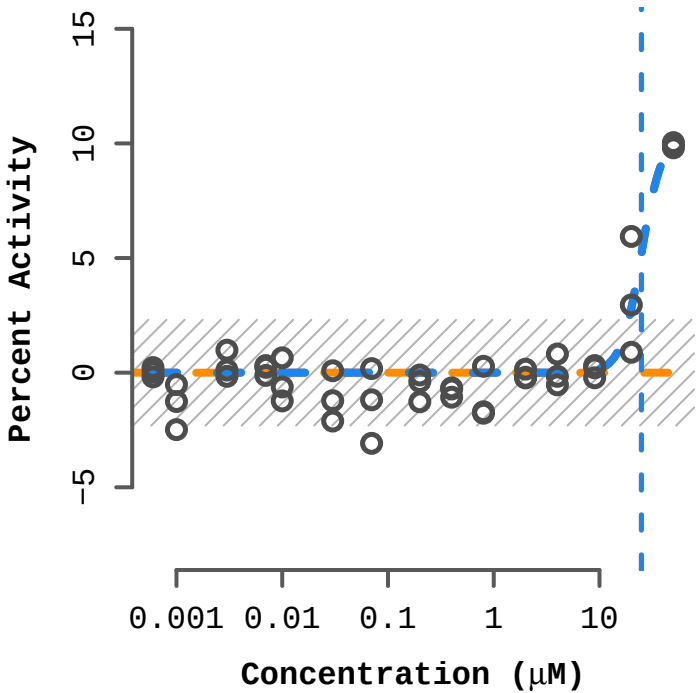
NAME: Sulthiame
CHID: 23626 **CASRN:** 61-56-3
SPID(S): Tox21_113683
M4ID: 12482531

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sumatriptan
CHID: 23628 **CASRN:** 103628-46-2
SPID(S): Tox21_111528_1
M4ID: 12483634

HILL MODEL (in red):

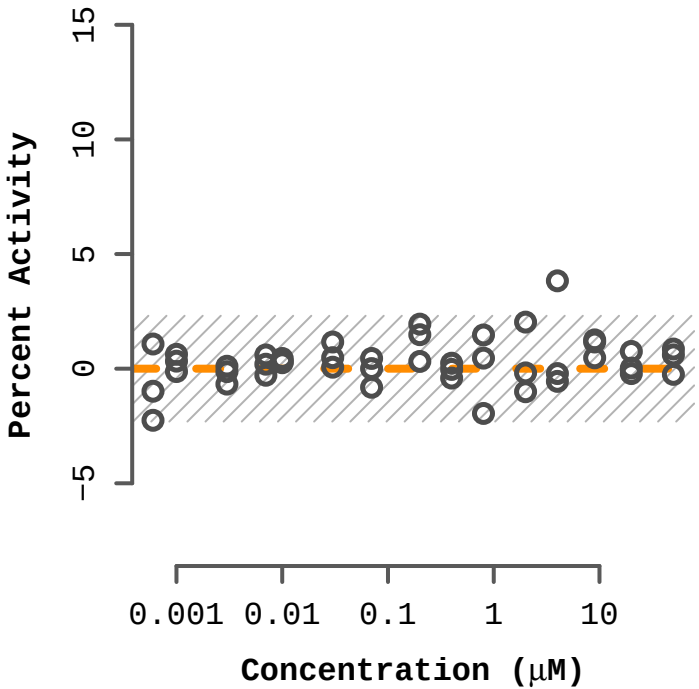
	tp	ga	gw
val:	10.4	1.4	4.51
sd:	1.95	0.128	4.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.4	1.4	4.51	3.21	4.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	191.5	137.16	141.16
PROB:	0	0.88	0.12
RMSE:	2.91	1.09	1.09

MAX_MEAN: 9.93 **MAX_MED:** 9.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

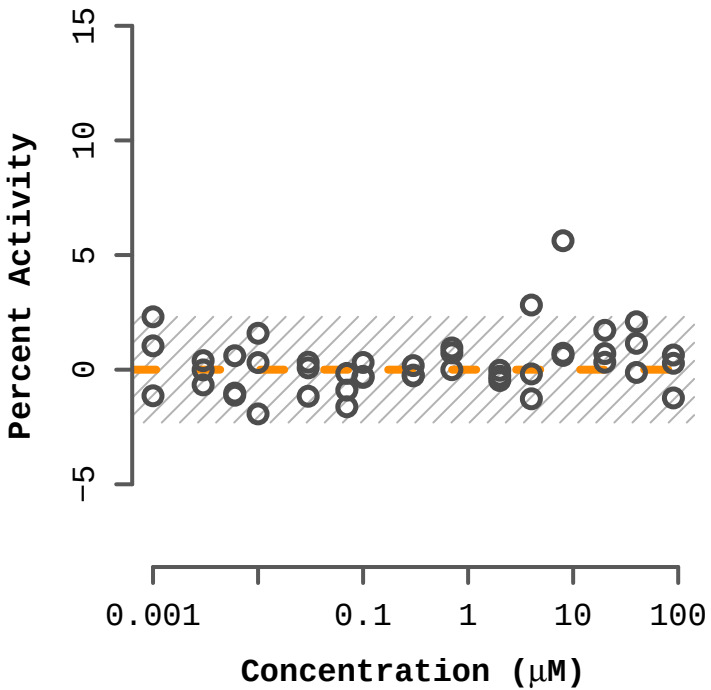
NAME: Talbutal
CHID: 23630 CASRN: 115-44-6
SPID(S): Tox21_113715
M4ID: 12482499

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

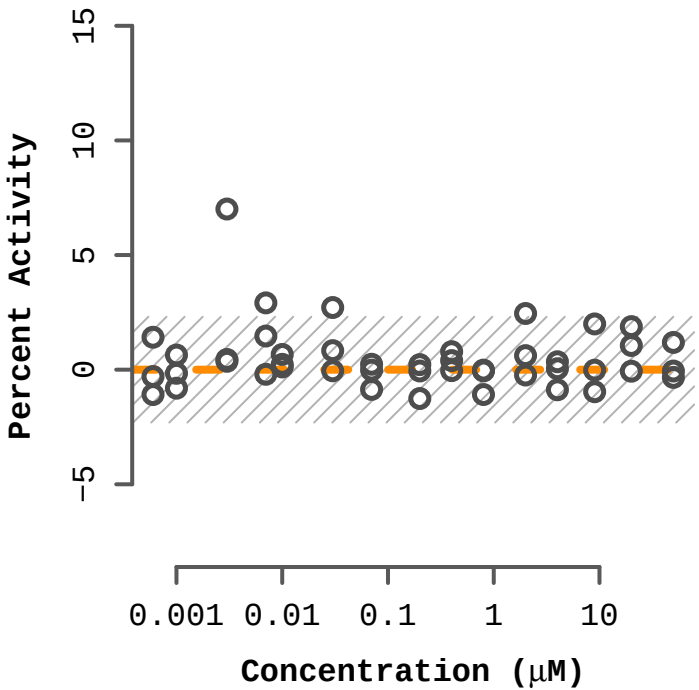
NAME: L−Tartaric acid
CHID: 23632 **CASRN:** 87−69−4
SPID(S): Tox21_300155
M4ID: 12478975

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

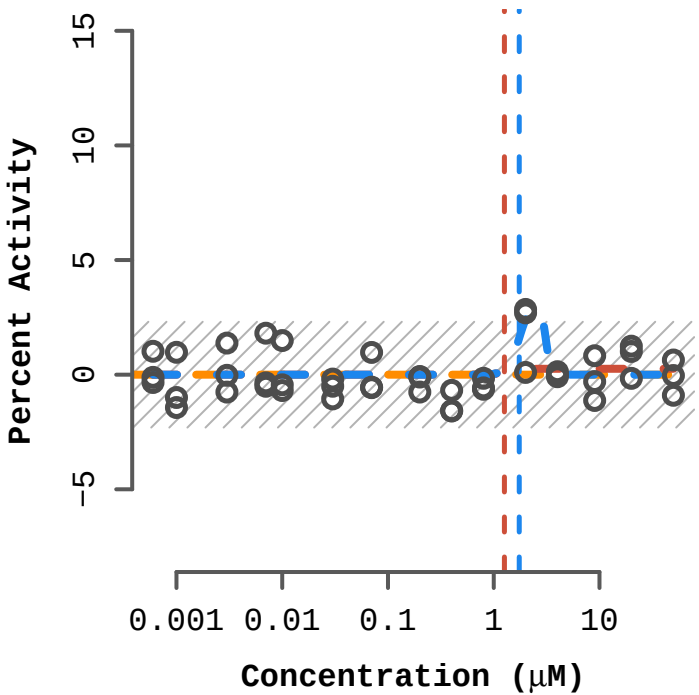
NAME: Telmisartan
CHID: 23636 **CASRN:** 144701-48-4
SPID(S): Tox21_111452_1
M4ID: 12483678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 2.61 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Terbinafine
CHID: 23640 **CASRN:** 91161-71-6
SPID(S): Tox21_111591_1
M4ID: 12483601

HILL MODEL (in red):

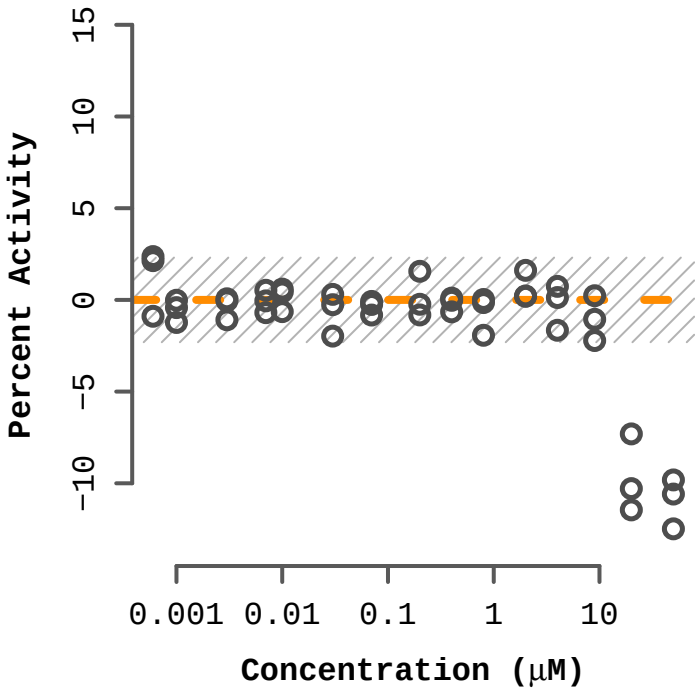
	tp	ga	gw
val:	0.257	0.101	8
sd:	0.248	0.314	12.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.21	0.241	8	0.491	18
sd:	10.4	0.633	12.6	0.591	95.8

	CNST	HILL	GNLS
AIC:	129.89	134.76	131.92
PROB:	0.69	0.06	0.25
RMSE:	1	0.97	0.89

MAX_MEAN: 1.88 **MAX_MED:** 2.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

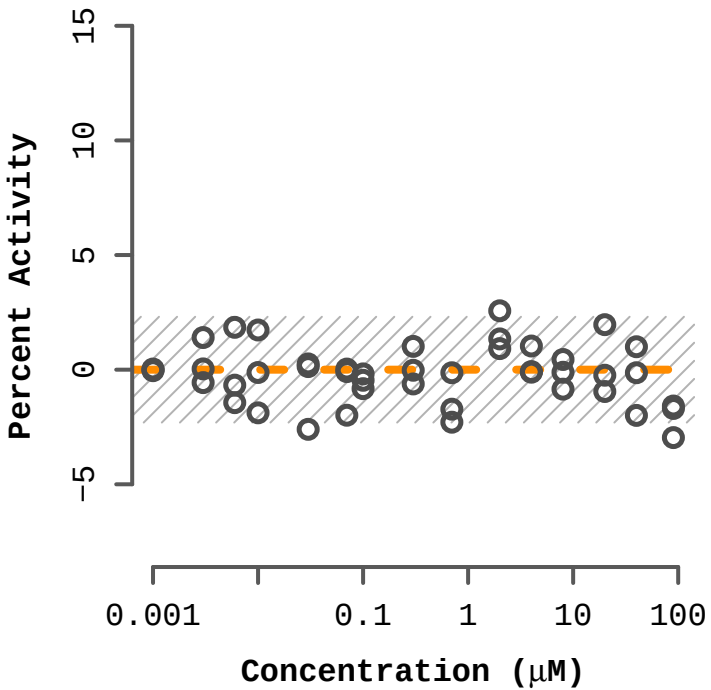
NAME: Terfenadine
CHID: 23642 **CASRN:** 50679-08-8
SPID(S): Tox21_110295_1
M4ID: 12484474

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.59	NA	NA
PROB:	1	NA	NA
RMSE:	3.93	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

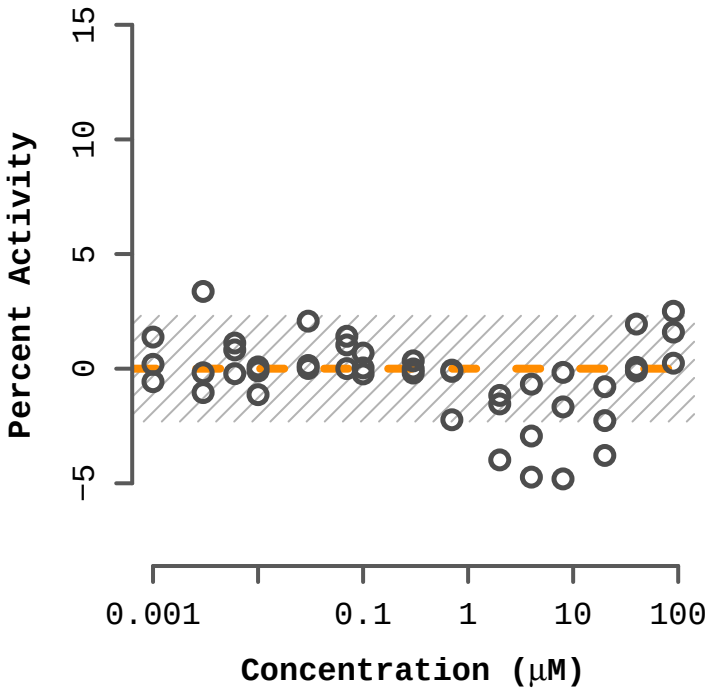
NAME: Tetracycline
CHID: 23645 **CASRN:** 60-54-8
SPID(S): Tox21_300150
M4ID: 12478980

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

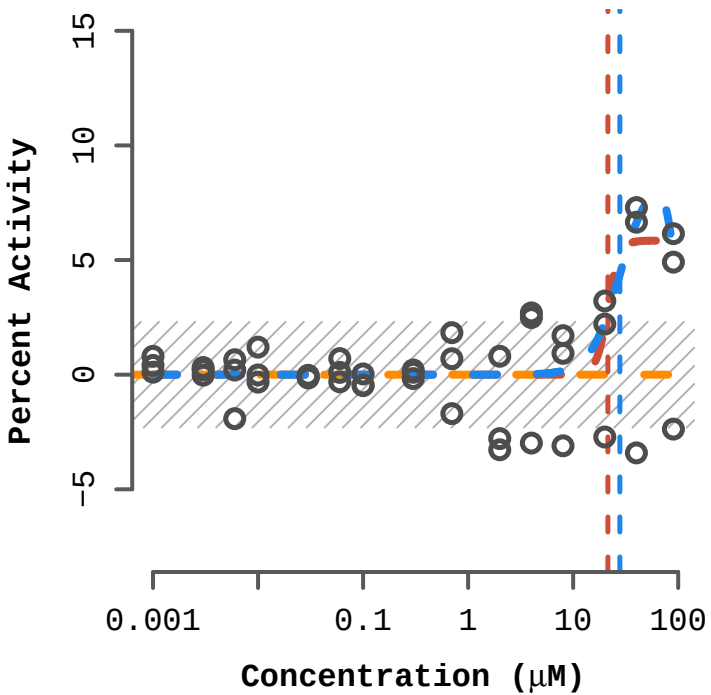
NAME: 6-Thioguanine
CHID: 23652 **CASRN:** 154-42-7
SPID(S): Tox21_300275
M4ID: 12478855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Thioguanine
CHID: 23652 **CASRN:** 154-42-7
SPID(S): Tox21_202401
M4ID: 12479851

HILL MODEL (in red):

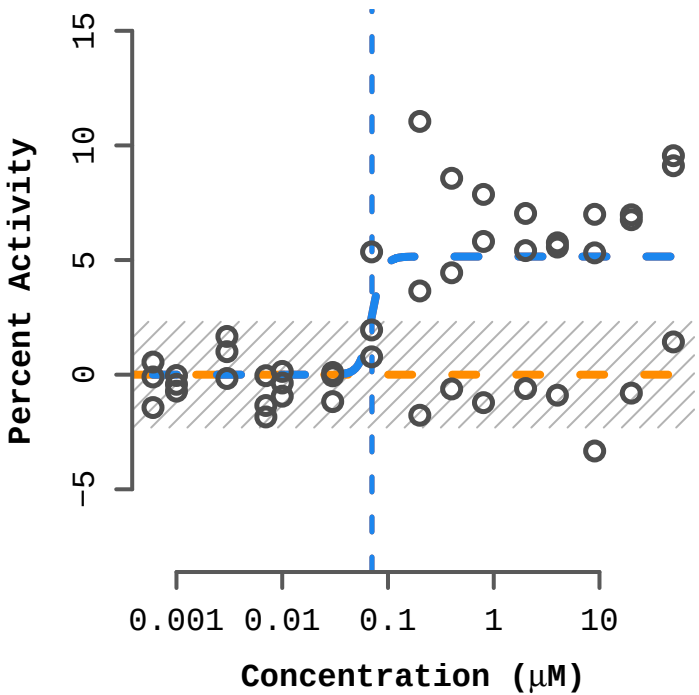
	tp	ga	gw
val:	5.85	1.33	8
sd:	0.711	0.0447	7.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.75	1.44	3.14	1.97	8.85
sd:	8.55	0.345	4.33	0.0741	38.7

	CNST	HILL	GNLS
AIC:	204.07	191.87	193.91
PROB:	0	0.73	0.26
RMSE:	2.44	2.36	2.37

MAX_MEAN: 3.51 **MAX_MED:** 6.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Thioguanine
CHID: 23652 **CASRN:** 154-42-7
SPID(S): Tox21_111035_1
M4ID: 12483937

HILL MODEL (in red):

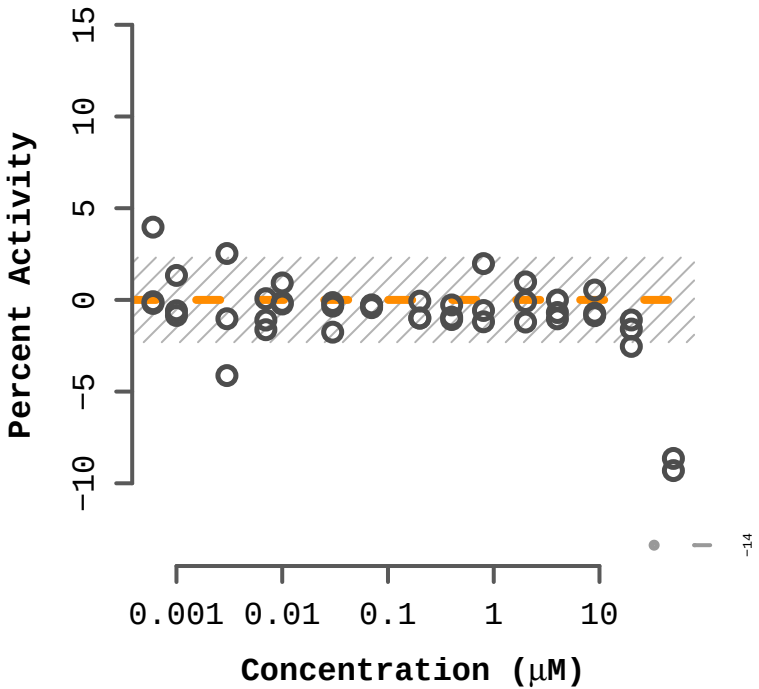
	tp	ga	gw
val:	5.15	−1.15	8
sd:	0.703	0.0671	40.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.15	−1.15	8	2.92	6.79
sd:	0.703	0.067	40	1630	9050

	CNST	HILL	GNLS
AIC:	263.06	235.7	239.7
PROB:	0	0.88	0.12
RMSE:	4.42	3.14	3.14

MAX_MEAN: 6.7 **MAX_MED:** 9.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

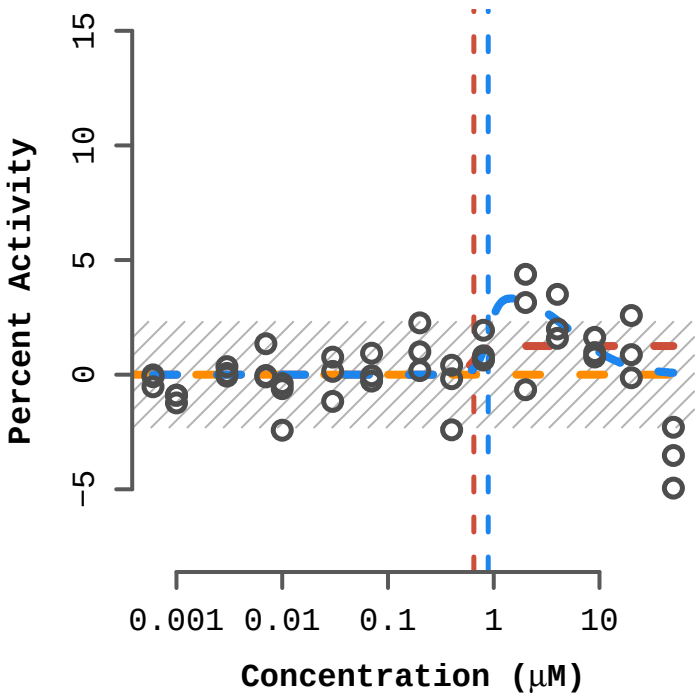
NAME: Thioridazine
CHID: 23656 **CASRN:** 50-52-2
SPID(S): Tox21_110294_1
M4ID: 12484475 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.93	NA	NA
PROB:	1	NA	NA
RMSE:	3.1	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** −0.089 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiphenamil
CHID: 23660 **CASRN:** 82-99-5
SPID(S): Tox21_111675_1
M4ID: 12483543

HILL MODEL (in red):

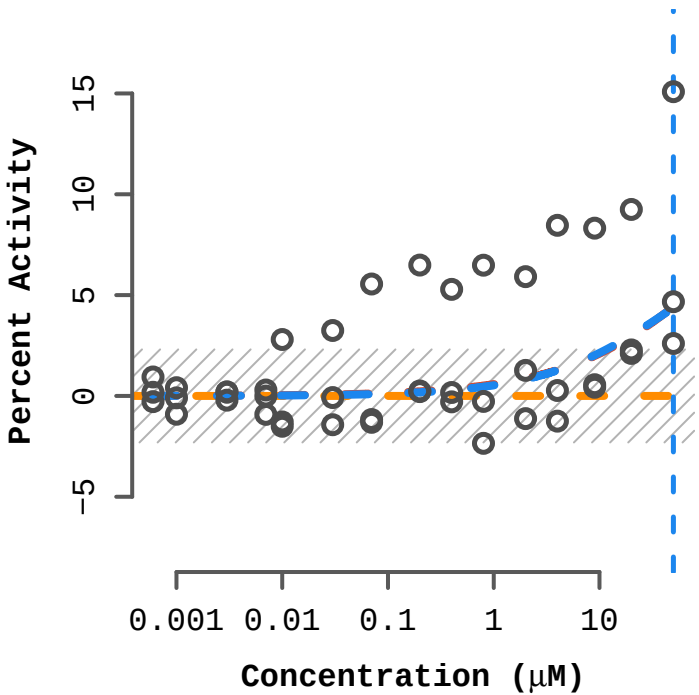
	tp	ga	gw
val:	1.25	−0.188	8
sd:	0.392	0.177	10.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.73	−0.052	8	0.74	1.72
sd:	2.07	0.113	17	0.377	1.13

	CNST	HILL	GNLS
AIC:	175.83	171.96	163.69
PROB:	0	0.02	0.98
RMSE:	1.72	1.69	1.46

MAX_MEAN: 2.36 **MAX_MED:** 3.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tiaprofenic acid
CHID: 23665 CASRN: 33005-95-7
SPID(S): Tox21_110627_1
M4ID: 12484222

HILL MODEL (in red):

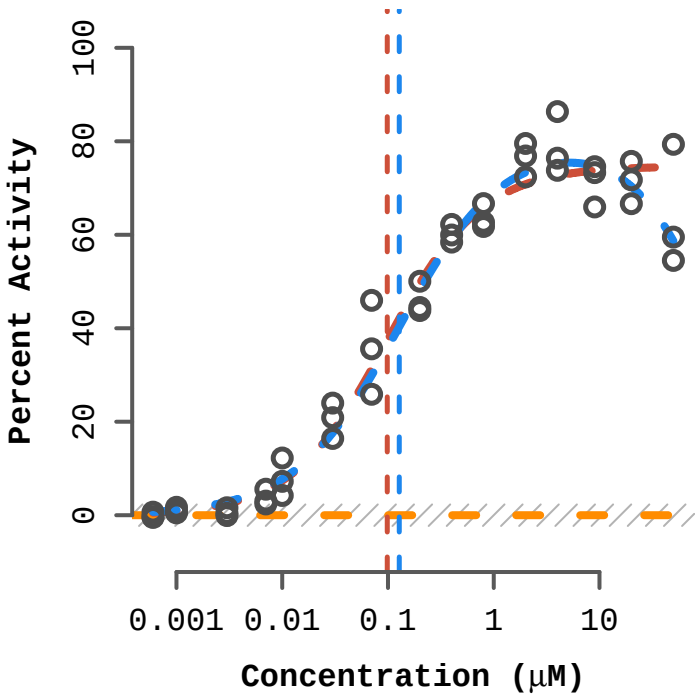
	tp	ga	gw
val:	13.4	2.2	0.61
sd:	42.1	3.61	0.576

GAIN-LOSS MODEL (in blue):

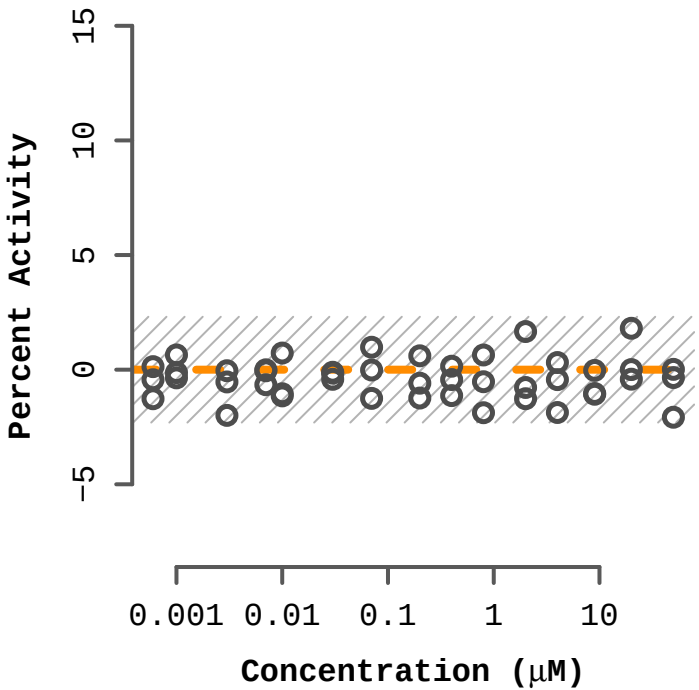
	tp	ga	gw	la	lw
val:	8.75	1.7	0.703	3.43	3.62
sd:	15.7	2.08	0.721	917	1900

	CNST	HILL	GNLS
AIC:	240.54	231.94	236.02
PROB:	0.01	0.87	0.11
RMSE:	3.98	3.2	3.21

MAX_MEAN: 7.45 **MAX_MED:** 4.67 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tibolone
CHID:    23667   CASRN: 5630-53-5
SPID(S): Tox21_112250_1
M4ID:    12483202

HILL MODEL (in red):
      tp       ga       gw
val:  74.7     -1.01    0.966
sd:   1.65     0.0521   0.067

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  80.7     -0.893   0.881    2.09     1.1
sd:   4.91     0.0887   0.0739   0.162    0.519

      CNST        HILL        GNLS
AIC:  488.79      286.18      277.38
PROB: 0           0.01        0.99
RMSE: 50.49       5.9         5.32

MAX_MEAN: 78.9      MAX_MED: 76.9      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

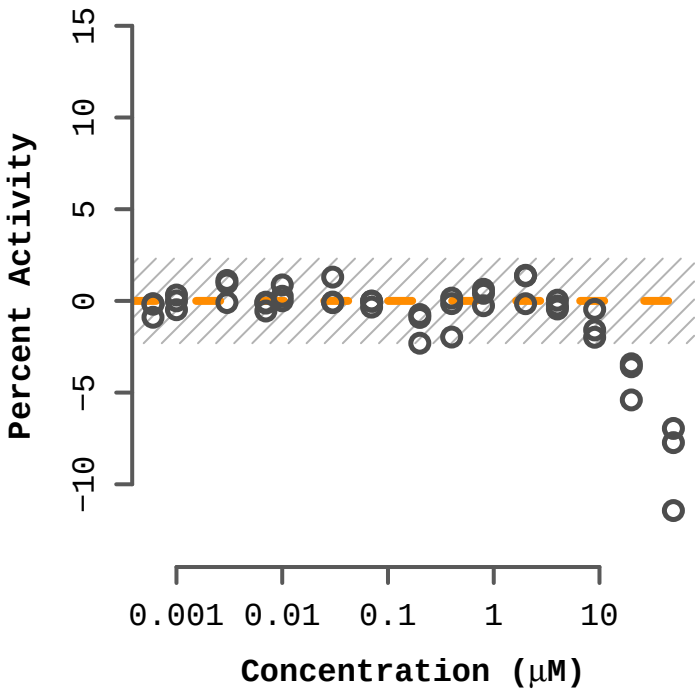
NAME: Ticlopidine
CHID: 23669 **CASRN:** 55142-85-3
SPID(S): Tox21_110658_1
M4ID: 12484200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.466 **MAX_MED:** 0.00558 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

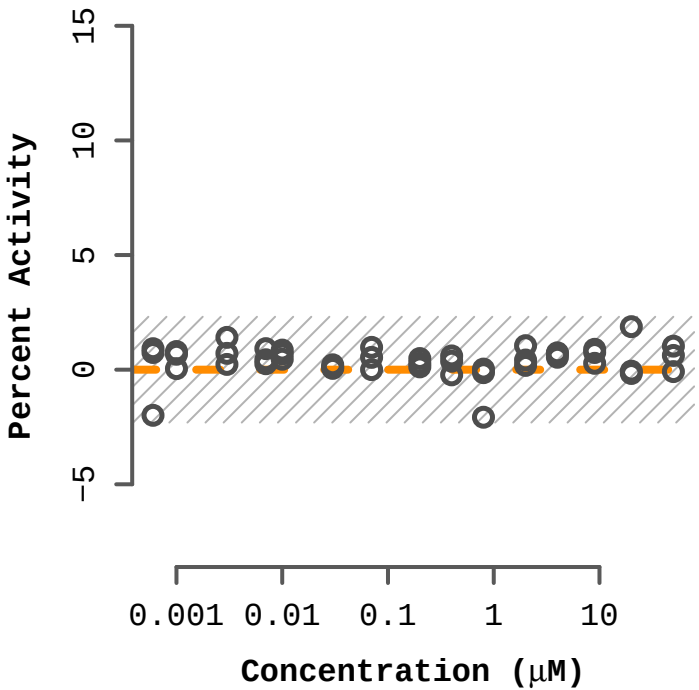
NAME: Timepidium bromide
CHID: 23672 **CASRN:** 35035-05-3
SPID(S): Tox21_112659_1
M4ID: 12482994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 0.87 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

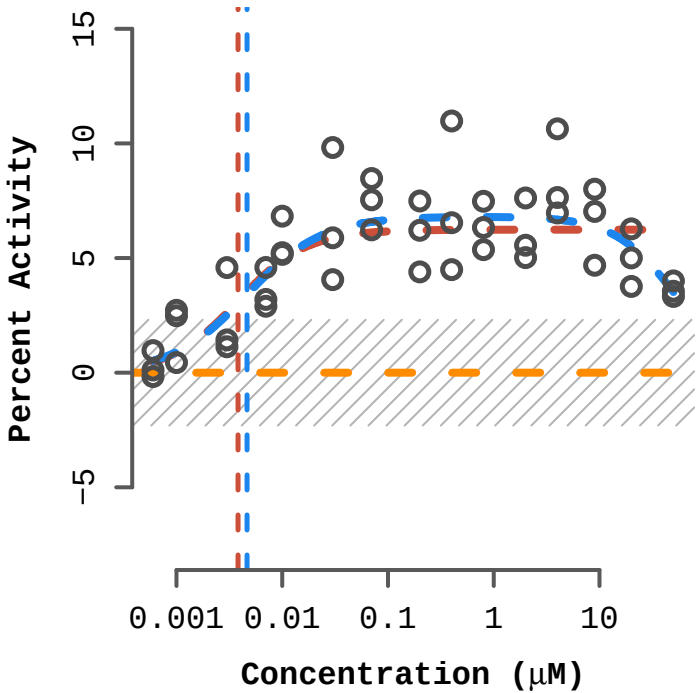
NAME: (S)-Timolol
CHID: 23674 **CASRN:** 26839-75-8
SPID(S): Tox21_110614_1
M4ID: 12484231

HILL MODEL: Not applicable.

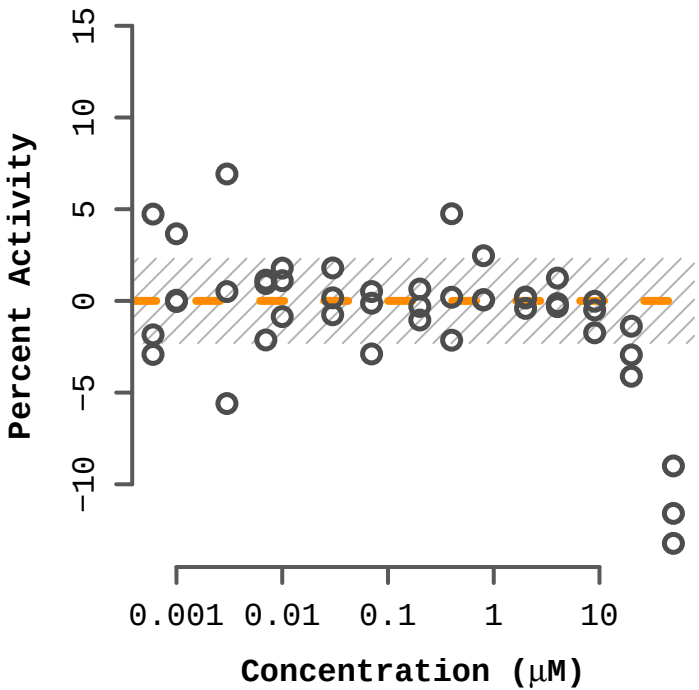
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.785 **MAX_MED:** 0.751 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tinidazole
CHID:    23676   CASRN: 19387-91-8
SPID(S): Tox21_110586_1
M4ID:    12484248

HILL MODEL (in red):
      tp       ga       gw
val:  6.24     -2.42    1.35
sd:   0.345    0.151    0.46

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.82     -2.33    1.22     1.72     1.51
sd:   0.39     0.124    0.398    0.116    0.684

      CNST        HILL        GNLS
AIC:  295.17      188.48      178.98
PROB: 0           0.01        0.99
RMSE: 5.78        1.77        1.55

MAX_MEAN: 8.42      MAX_MED: 7.64      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

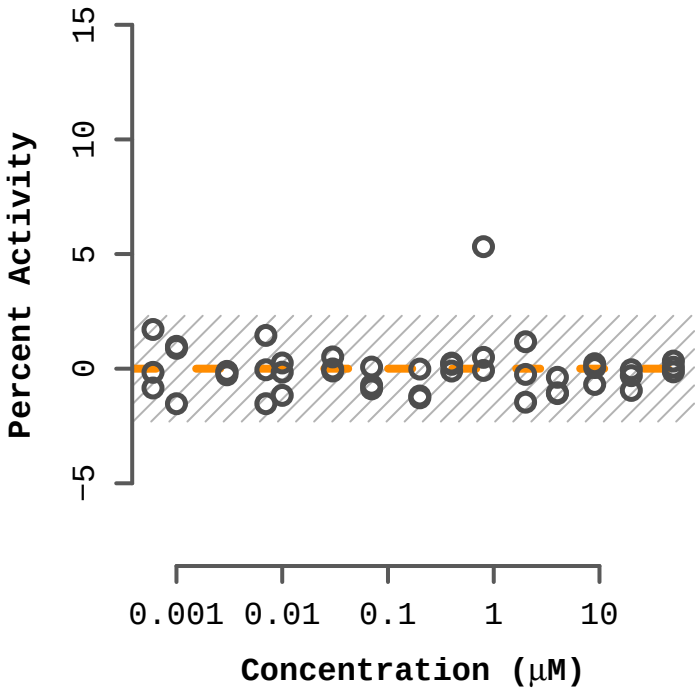
NAME: Tinoridine
CHID: 23677 **CASRN:** 24237-54-5
SPID(S): Tox21_111678_1
M4ID: 12483541

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.48	NA	NA
PROB:	1	NA	NA
RMSE:	3.68	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

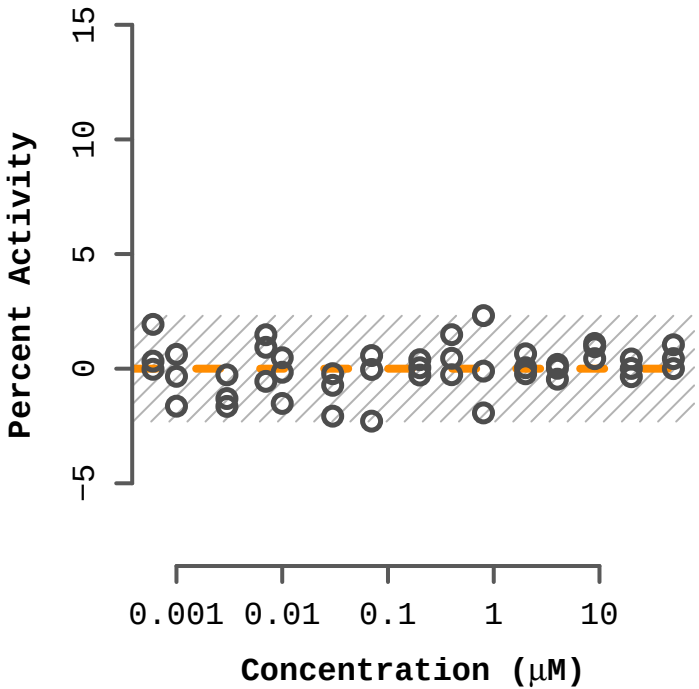
NAME: Tiopronin
CHID: 23678 CASRN: 1953-02-2
SPID(S): Tox21_111654_1
M4ID: 12483555

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 0.889 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

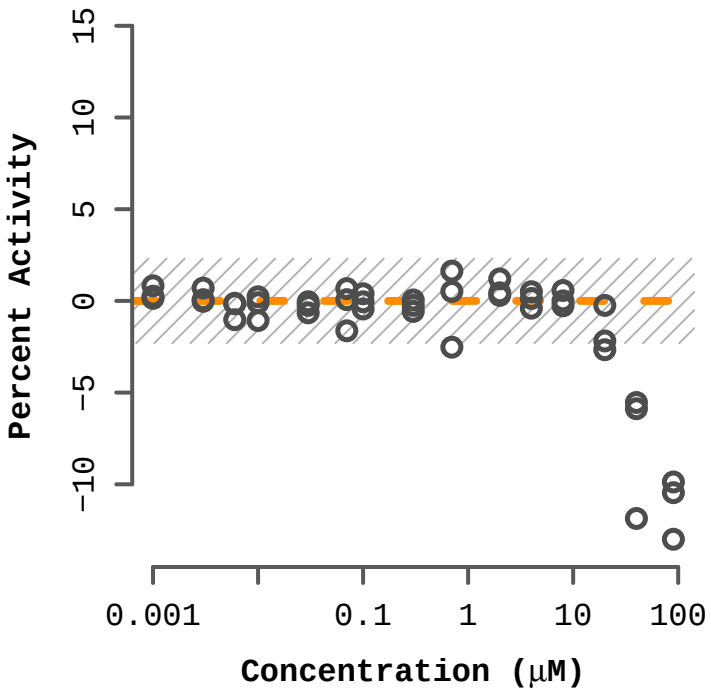
NAME: Tizanidine
CHID: 23679 **CASRN:** 51322-75-9
SPID(S): Tox21_111876_1
M4ID: 12483437

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.834 **MAX_MED:** 0.961 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

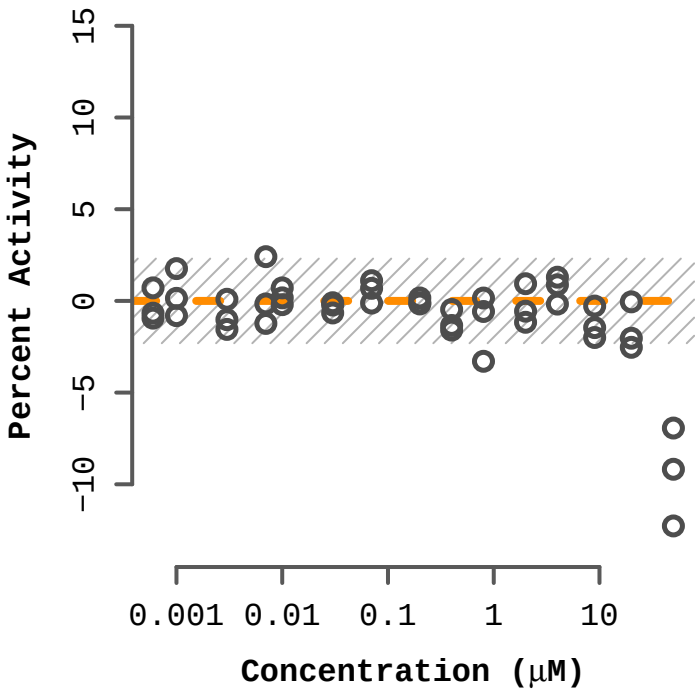
NAME: Tolcapone
CHID: 23685 **CASRN:** 134308-13-7
SPID(S): Tox21_302414
M4ID: 12476719

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.43	NA	NA
PROB:	1	NA	NA
RMSE:	3.69	NA	NA

MAX_MEAN: 0.65 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

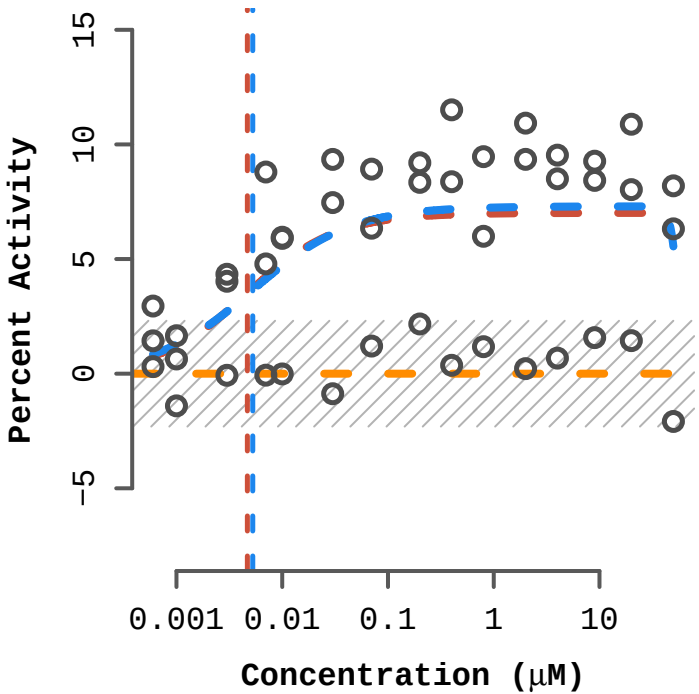
NAME: Tolcapone
CHID: 23685 **CASRN:** 134308-13-7
SPID(S): Tox21_112963_1
M4ID: 12482863

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 0.668 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tolterodine
CHID: 23687 **CASRN:** 124937-51-5
SPID(S): Tox21_111737_1
M4ID: 12483511

HILL MODEL (in red):

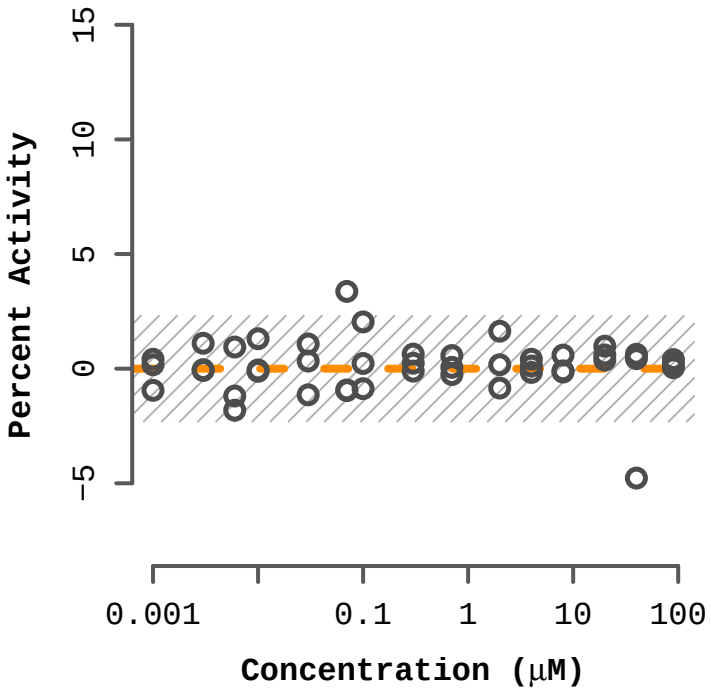
	tp	ga	gw
val:	7.01	−2.33	1.02
sd:	0.864	0.303	0.674

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.3	−2.28	0.935	1.74	12
sd:	0.982	0.328	0.633	0.256	73.6

	CNST	HILL	GNLS
AIC:	301.34	255.77	259.23
PROB:	0	0.85	0.15
RMSE:	6.33	3.67	3.64

MAX_MEAN: 6.83 **MAX_MED:** 9.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

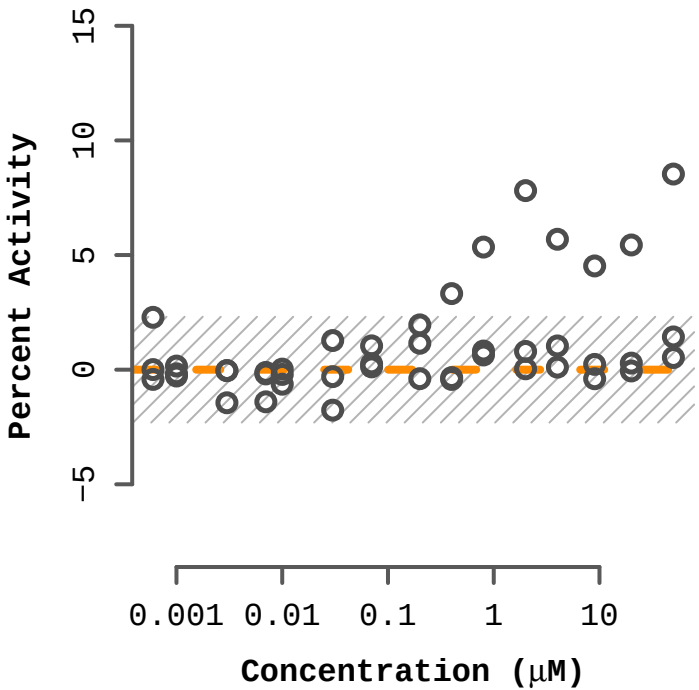
NAME: Topiramate
CHID: 23688 **CASRN:** 97240-79-4
SPID(S): Tox21_302401
M4ID: 12476732

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.653 **MAX_MED:** 0.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

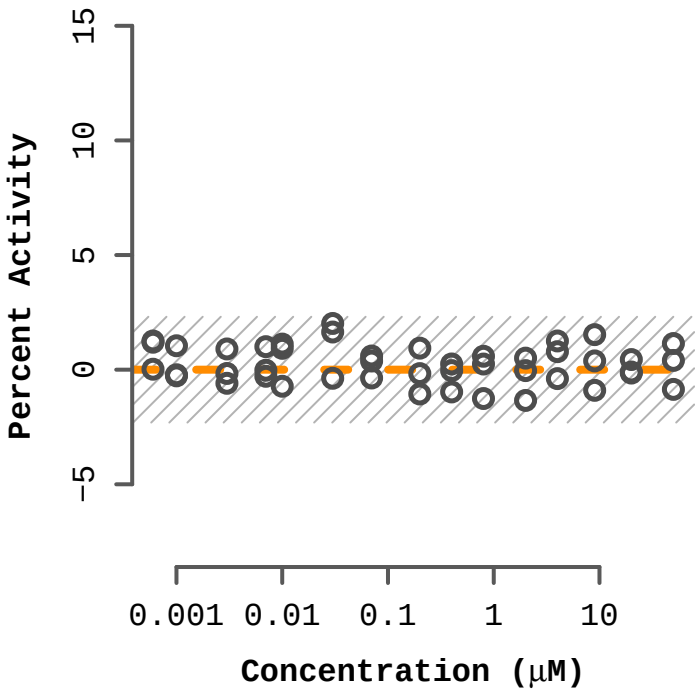
NAME: Topiramate
CHID: 23688 **CASRN:** 97240-79-4
SPID(S): Tox21_111472_1
M4ID: 12483663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.97	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 3.5 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

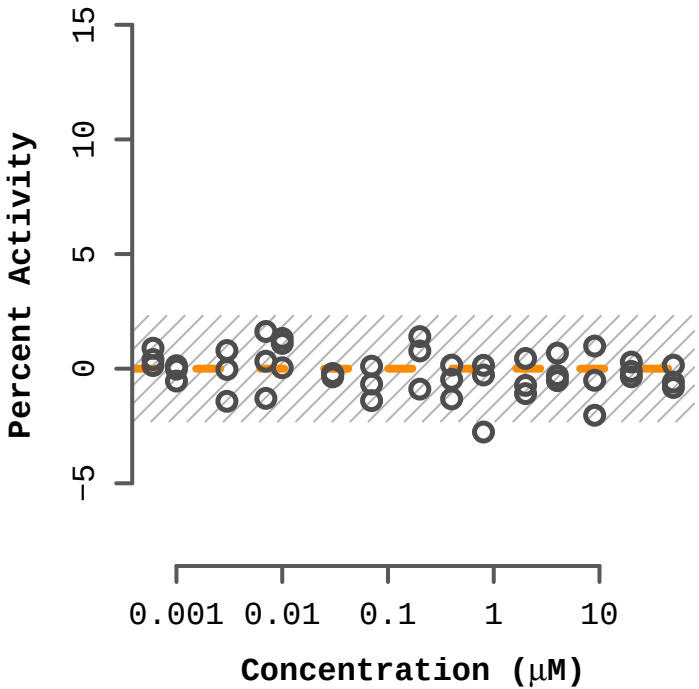
NAME: Torsemide
CHID: 23690 **CASRN:** 56211-40-6
SPID(S): Tox21_110662_1
M4ID: 12484196

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

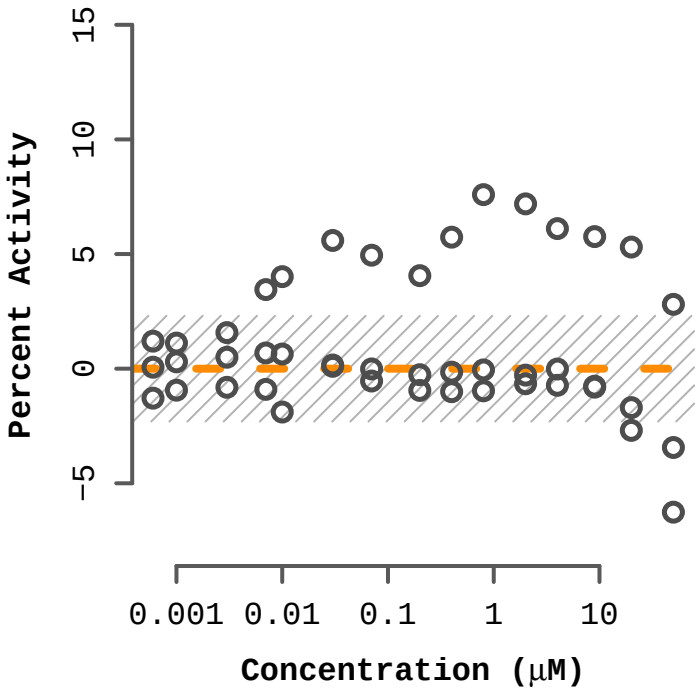
NAME: Tramadol hydrochloride
CHID: 23691 **CASRN:** 36282-47-0
SPID(S): Tox21_111588_1
M4ID: 12483602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.822 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

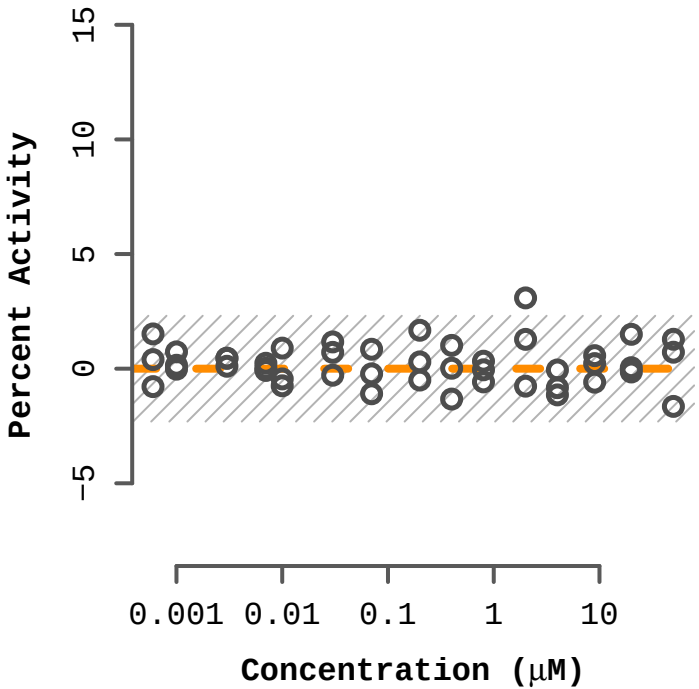
NAME: Tribenoside
CHID: 23697 **CASRN:** 10310-32-4
SPID(S): Tox21_110564_1
M4ID: 12484265

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.6	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 0.687 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

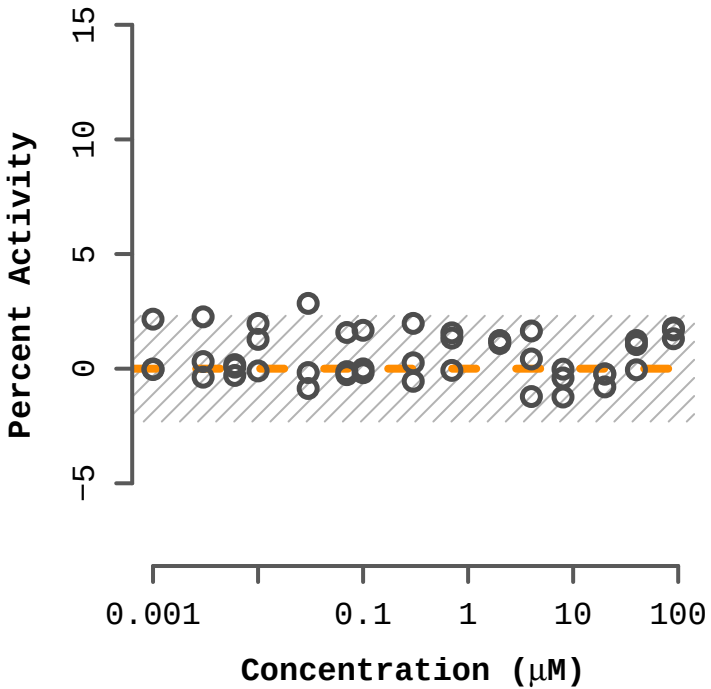
NAME: Trichlormethiazide
CHID: 23699 **CASRN:** 133-67-5
SPID(S): Tox21_110421_1
M4ID: 12484373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

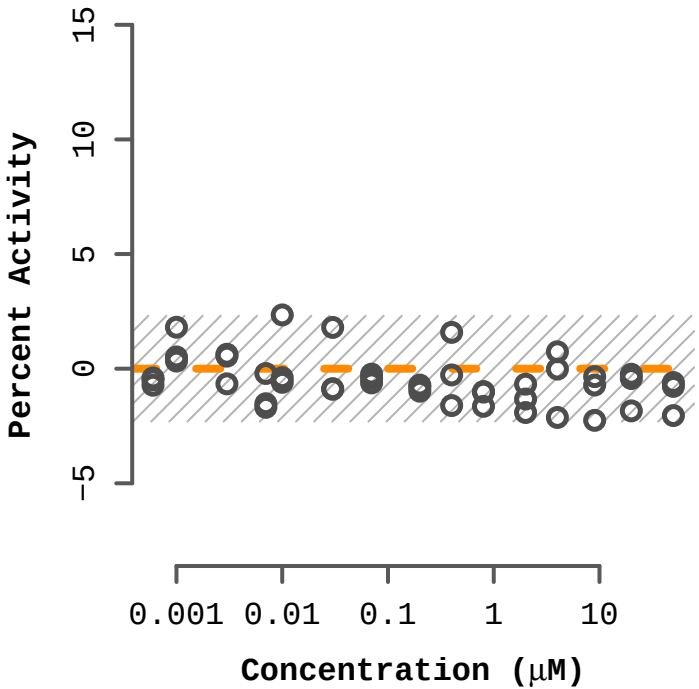
NAME: Triethylenetetramine
CHID: 23702 **CASRN:** 112-24-3
SPID(S): Tox21_201066
M4ID: 12481186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

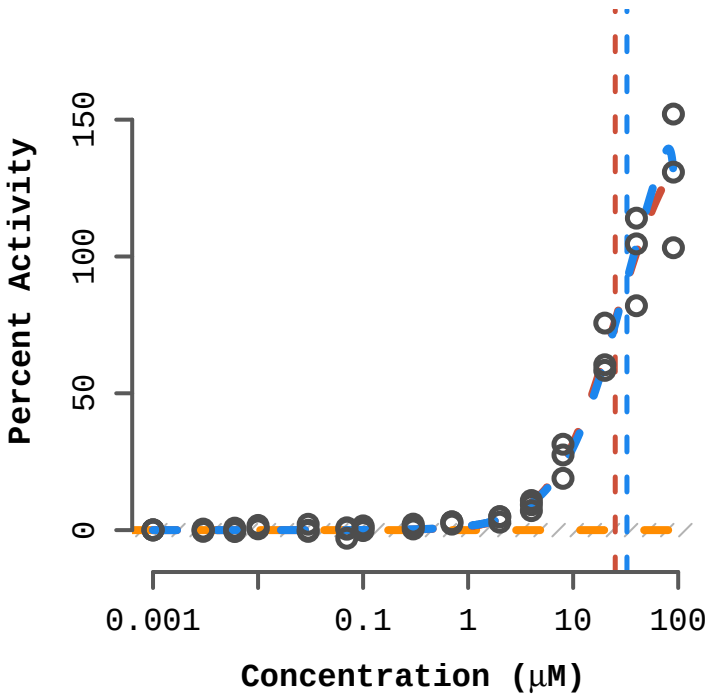
NAME: Triethylenetetramine
CHID: 23702 **CASRN:** 112-24-3
SPID(S): Tox21_111162_1
M4ID: 12483867

HILL MODEL: Not applicable.

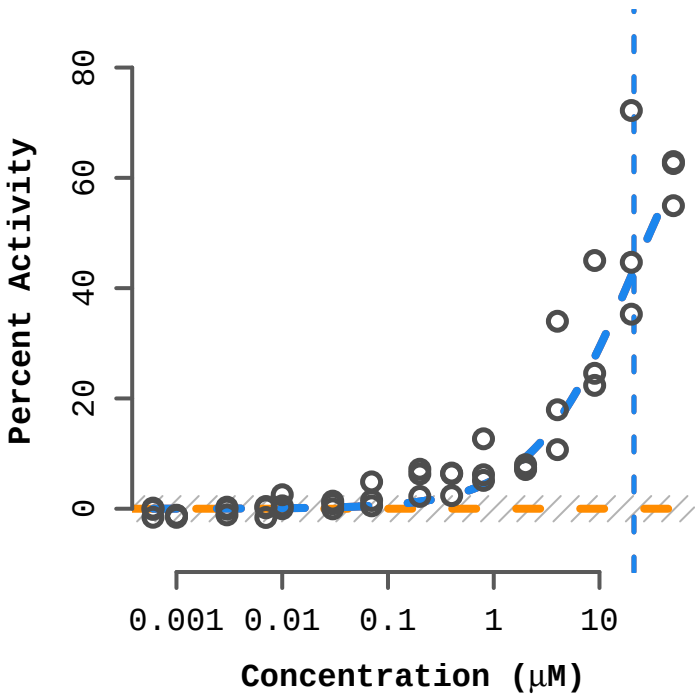
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.885 **MAX_MED:** 0.548 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Trilostane
CHID:    23706   CASRN: 13647-35-3
SPID(S): Tox21_302406
M4ID:    12476727

HILL MODEL (in red):
      tp       ga       gw
val:  153      1.4      1.45
sd:   8.87     0.0675   0.122

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  182      1.51     1.37     2.01     18
sd:   16.8     0.066    0.0965   0.0126   3.08

      CNST        HILL        GNLS
AIC:  451.12      272.33      271.45
PROB: 0           0.39        0.61
RMSE: 46.38       6.84        6.92

MAX_MEAN: 129       MAX_MED: 131       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trilostane
CHID: 23706 **CASRN:** 13647-35-3
SPID(S): Tox21_112454_1
M4ID: 12483092

HILL MODEL (in red):

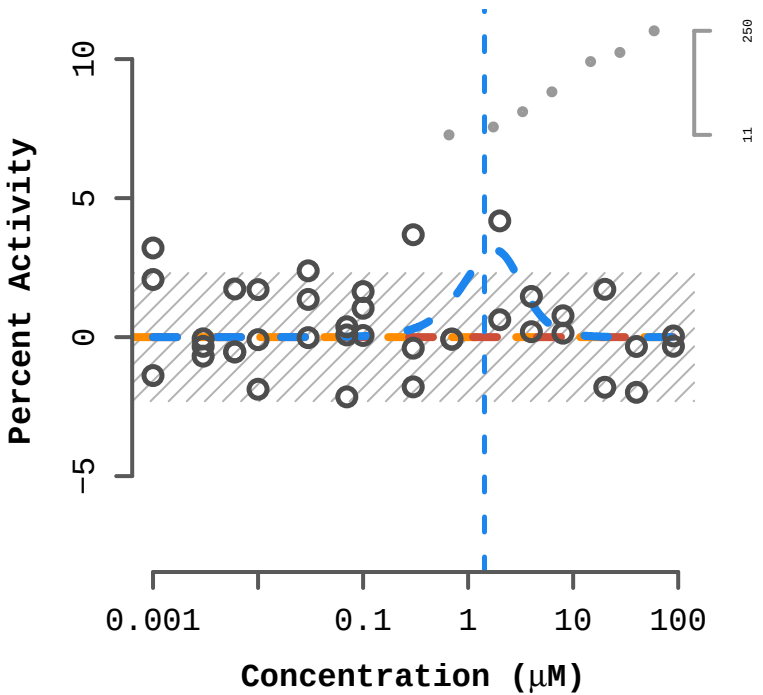
	tp	ga	gw
val:	86.7	1.33	0.897
sd:	13.4	0.172	0.114

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	86.7	1.33	0.897	2.28	16.1
sd:	13.4	0.172	0.114	696	19300

	CNST	HILL	GNLS
AIC:	396.45	273.42	277.42
PROB:	0	0.88	0.12
RMSE:	23.43	6.53	6.53

MAX_MEAN: 60.2 **MAX_MED:** 62.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trimethoprim
CHID: 23712 CASRN: 738-70-5
SPID(S): Tox21_200157
M4ID: 12482095 BRK

HILL MODEL (in red):

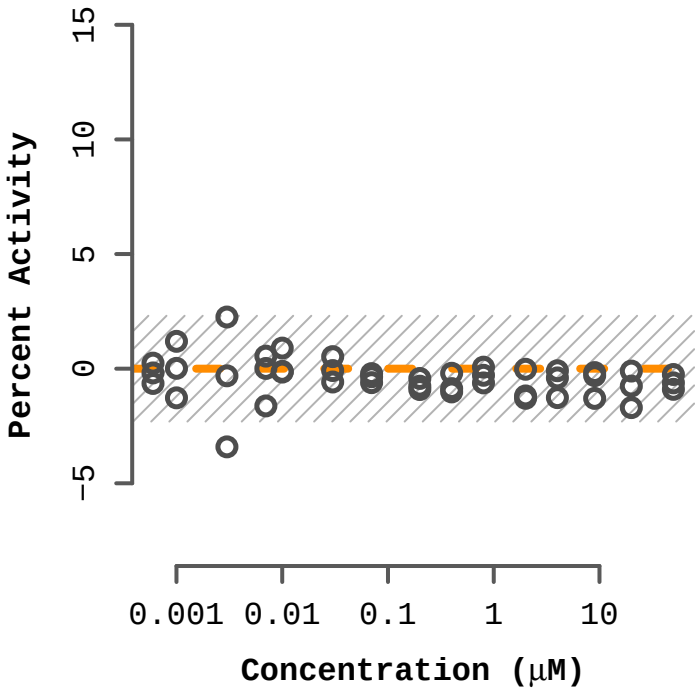
	tp	ga	gw
val:	5.68e-08	2.41	1.16
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.93	0.156	1.98	0.406	3.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	381.9	387.9	388.72
PROB:	0.92	0.05	0.03
RMSE:	57.34	57.34	57.26

MAX_MEAN: 82.1 MAX_MED: 4.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

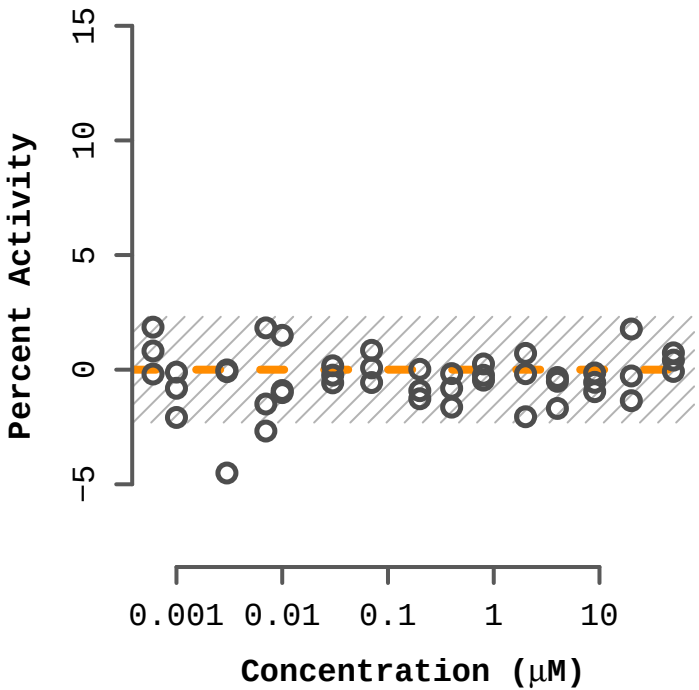
NAME: Trimethoprim
CHID: 23712 **CASRN:** 738-70-5
SPID(S): Tox21_110291_1
M4ID: 12484478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.212 **MAX_MED:** 0.015 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

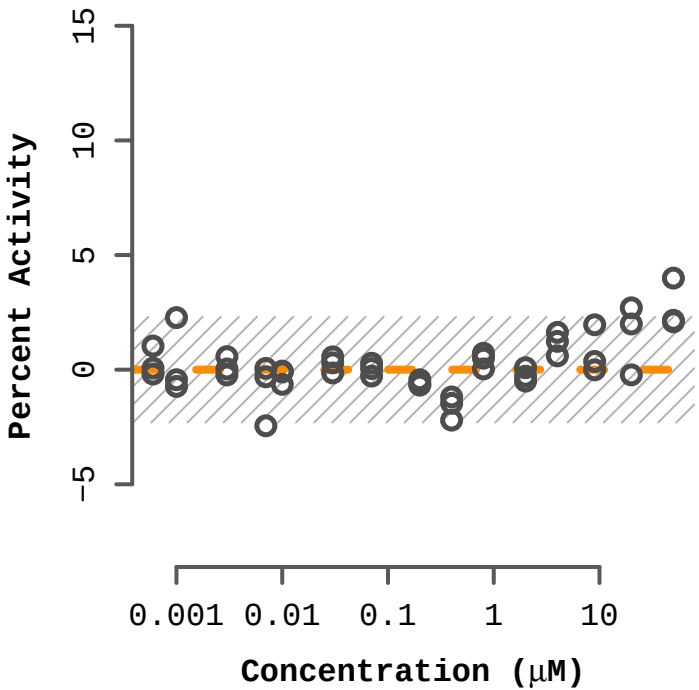
NAME: Trimetozine
CHID: 23713 **CASRN:** 635-41-6
SPID(S): Tox21_111634_1
M4ID: 12483572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.828 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

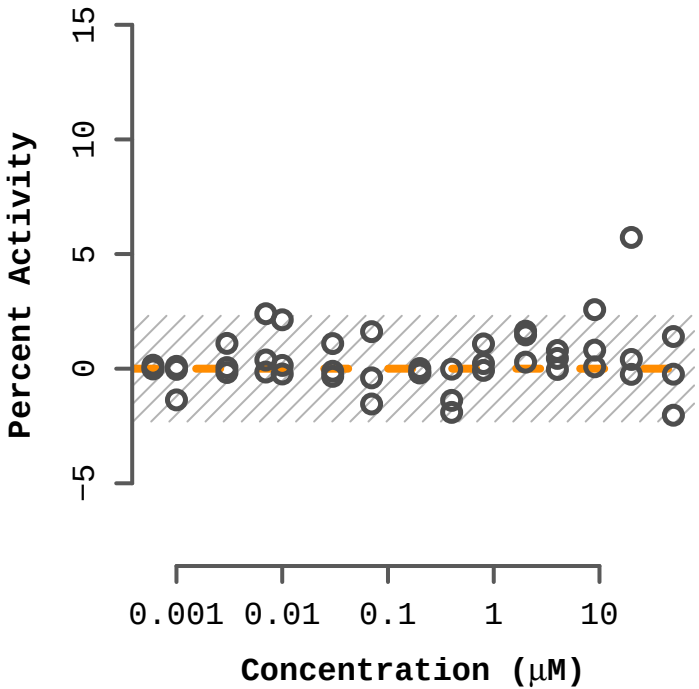
NAME: Trioxsalen
CHID: 23716 CASRN: 3902-71-4
SPID(S): Tox21_110541_1
M4ID: 12484279

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 2.75 MAX_MED: 2.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

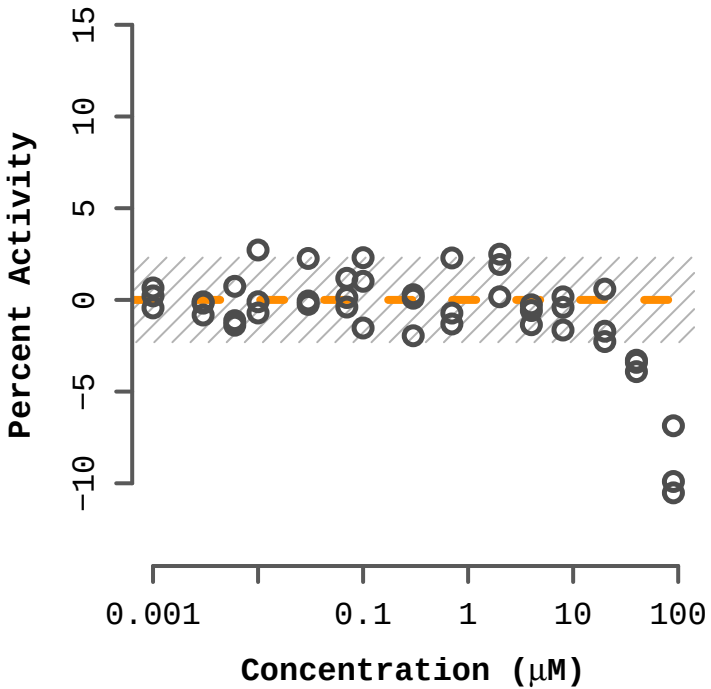
NAME: Triprolidine
CHID: 23718 **CASRN:** 486-12-4
SPID(S): Tox21_110919_1
M4ID: 12484015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

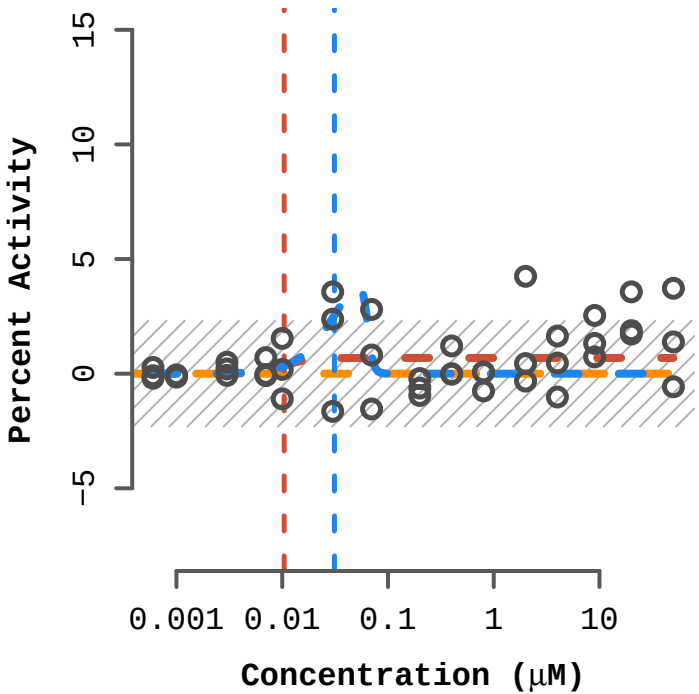
NAME: Troglitazone
CHID: 23719 **CASRN:** 97322-87-7
SPID(S): Tox21_300470
M4ID: 12478662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.33	NA	NA
PROB:	1	NA	NA
RMSE:	2.82	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Troglitazone
CHID: 23719 **CASRN:** 97322-87-7
SPID(S): Tox21_112119_1
M4ID: 12483307

HILL MODEL (in red):

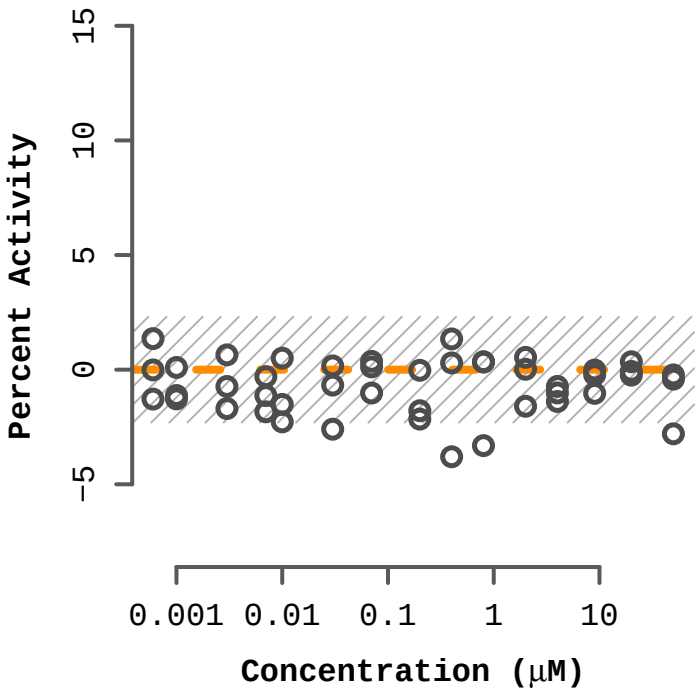
	tp	ga	gw
val:	0.686	−1.98	4.05
sd:	0.27	0.412	11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.1	−1.51	2.43	−1.19	16.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	164.27	163.27	169.18
PROB:	0.37	0.6	0.03
RMSE:	1.54	1.36	1.5

MAX_MEAN: 2.39 **MAX_MED:** 2.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

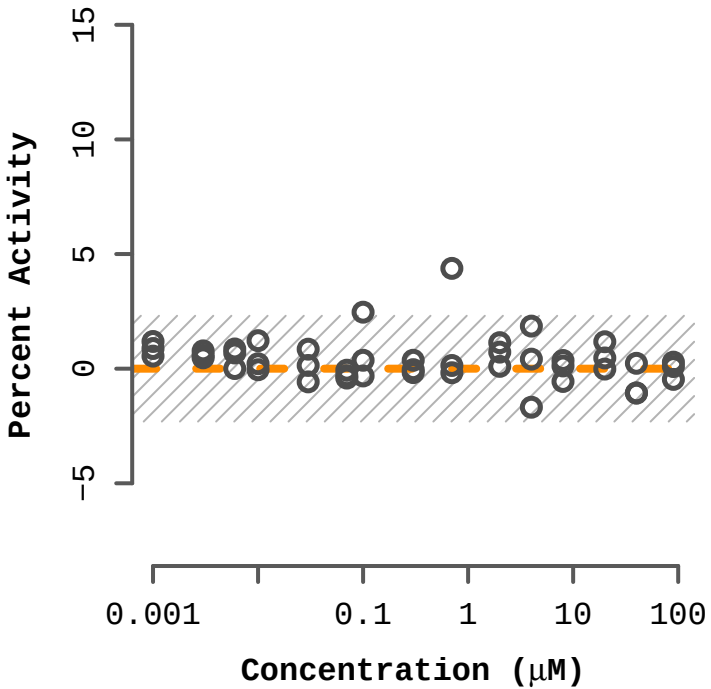
NAME: Trolnitrate
CHID: 23722 **CASRN:** 7077-34-1
SPID(S): Tox21_113331
M4ID: 12482696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.0219 **MAX_MED:** 0.331 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

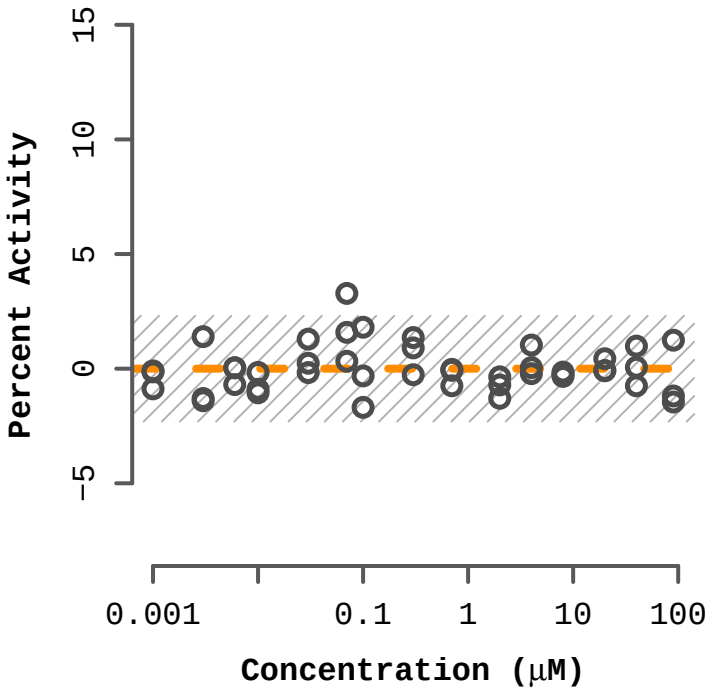
NAME: Tromethamine
CHID: 23723 **CASRN:** 77-86-1
SPID(S): Tox21_303167
M4ID: 12475966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 0.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

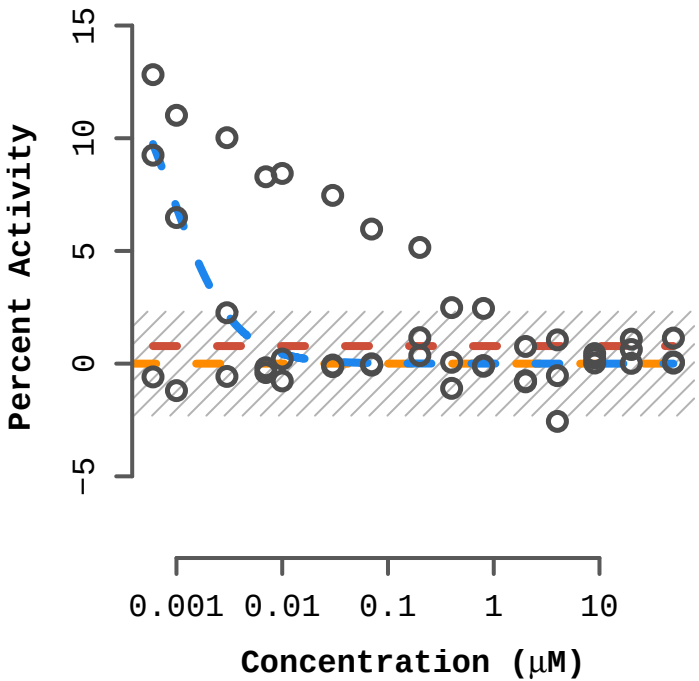
NAME: Tromethamine
CHID: 23723 **CASRN:** 77-86-1
SPID(S): Tox21_201646
M4ID: 12480606

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tromethamine
CHID: 23723 CASRN: 77-86-1
SPID(S): Tox21_111645_1
M4ID: 12483562

HILL MODEL (in red):

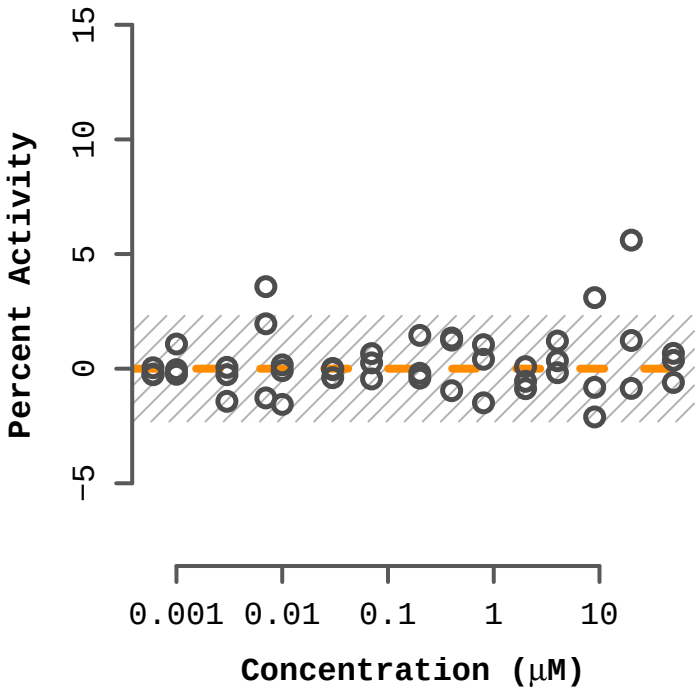
	tp	ga	gw
val:	0.779	−4.44	6.84
sd:	0.416	4460	24800

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.4	−4.75	7.68	−3.06	1.45
sd:	16.9	139000	624000	0.73	1.22

	CNST	HILL	GNLS
AIC:	245.72	247.59	239.44
PROB:	0.04	0.02	0.94
RMSE:	4.24	3.93	3.46

MAX_MEAN: 7.16 **MAX_MED:** 9.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

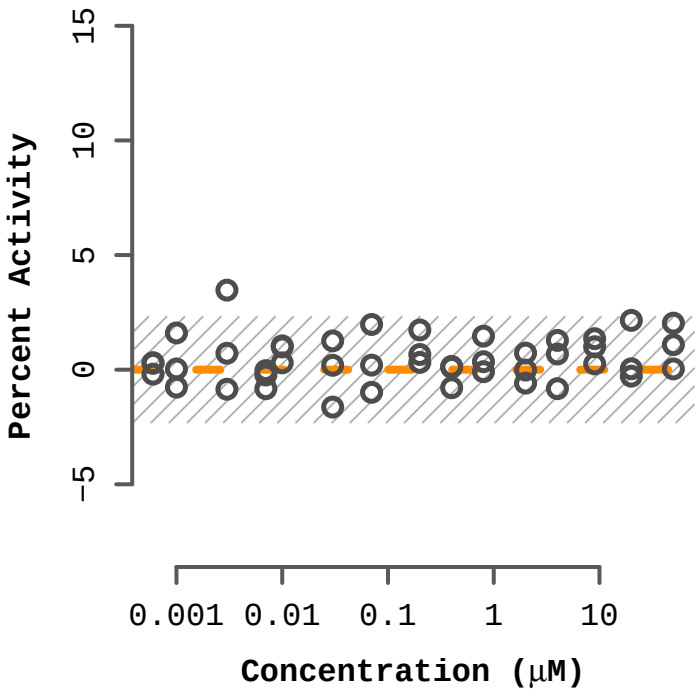
NAME: Trospium chloride
CHID: 23724 CASRN: 10405-02-4
SPID(S): Tox21_112442_1
M4ID: 12483100

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

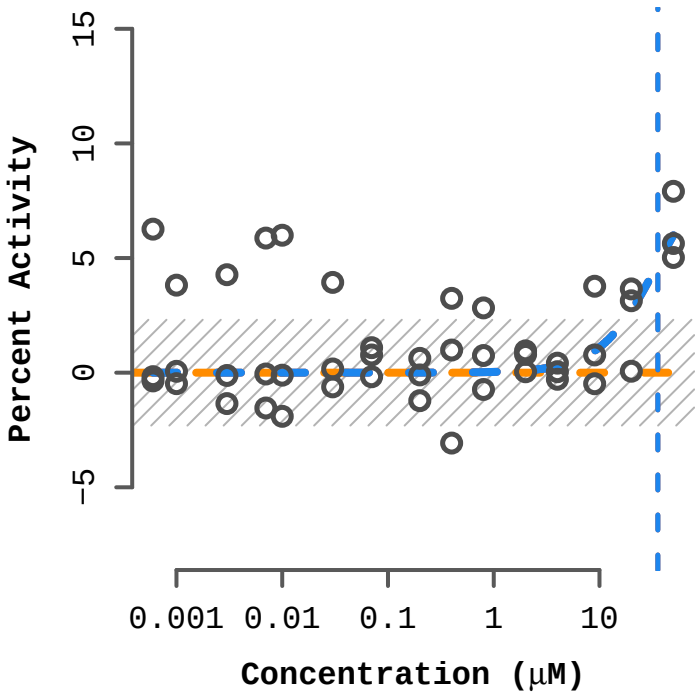
NAME: Troxipide
CHID: 23725 CASRN: 30751-05-4
SPID(S): Tox21_113383_1
M4ID: 12482667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.11 MAX_MED: 1.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (+)−Tubocurarine chloride hydrochloride
CHID: 23727 **CASRN:** 57−94−3
SPID(S): Tox21_112039_1
M4ID: 12483355

HILL MODEL (in red):

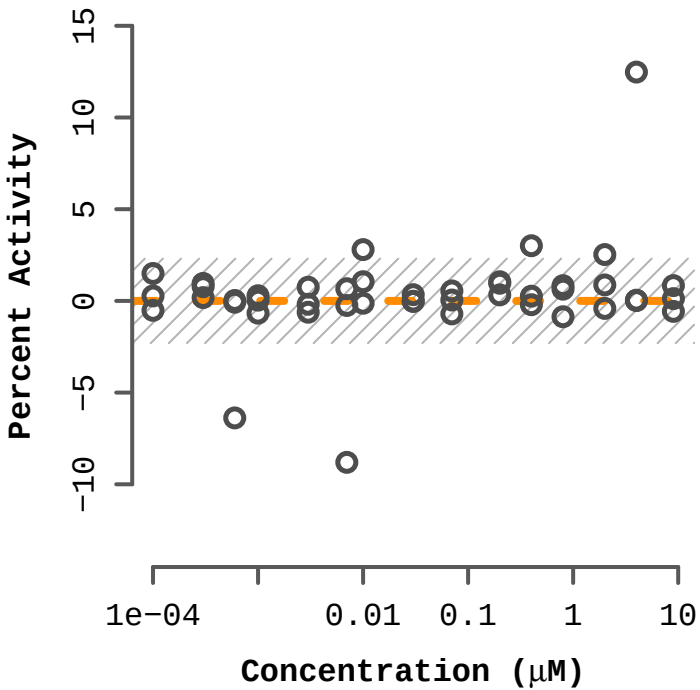
	tp	ga	gw
val:	9.49	1.55	1.59
sd:	10.4	0.672	1.4

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.49	1.55	1.59	3.35	4.25
sd:	10.4	0.673	1.4	1540	3960

	CNST	HILL	GNLS
AIC:	219.64	201.14	205.14
PROB:	0	0.88	0.12
RMSE:	2.83	2.23	2.23

MAX_MEAN: 6.19 **MAX_MED:** 5.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

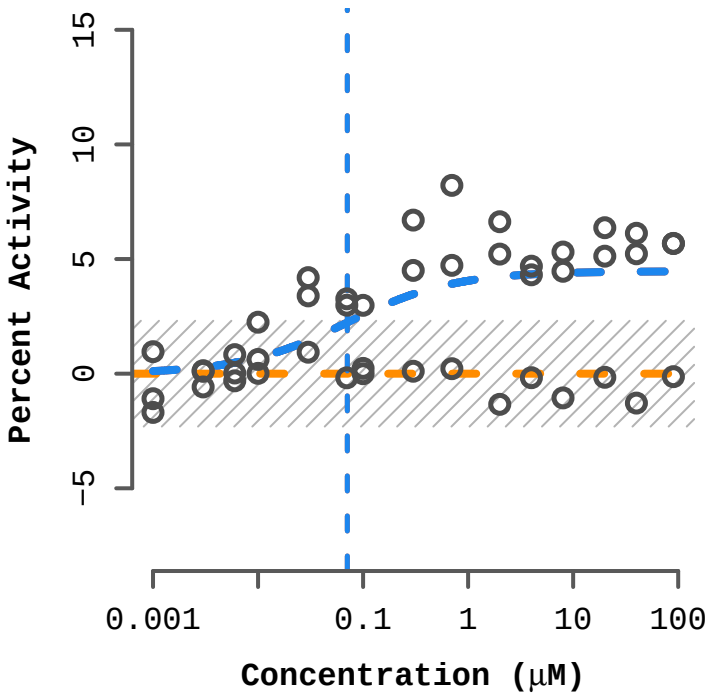
NAME: L-Tyrosine
CHID: 23730 **CASRN:** 60-18-4
SPID(S): Tox21_111594_1
M4ID: 12483598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.63	NA	NA

MAX_MEAN: 4.18 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Valproic acid
CHID: 23733 CASRN: 99-66-1
SPID(S): Tox21_300603
M4ID: 12478530

HILL MODEL (in red):

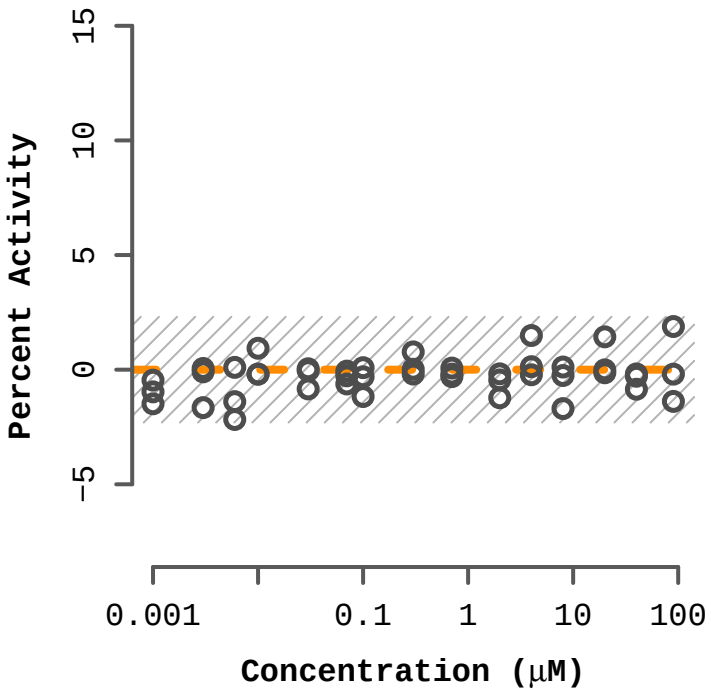
	tp	ga	gw
val:	4.47	−1.15	0.859
sd:	0.68	0.387	0.426

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.47	−1.15	0.859	3.67	3.72
sd:	0.68	0.387	0.426	672	1440

	CNST	HILL	GNLS
AIC:	248	216.43	220.43
PROB:	0	0.88	0.12
RMSE:	3.61	2.45	2.45

MAX_MEAN: 4.39 MAX_MED: 5.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

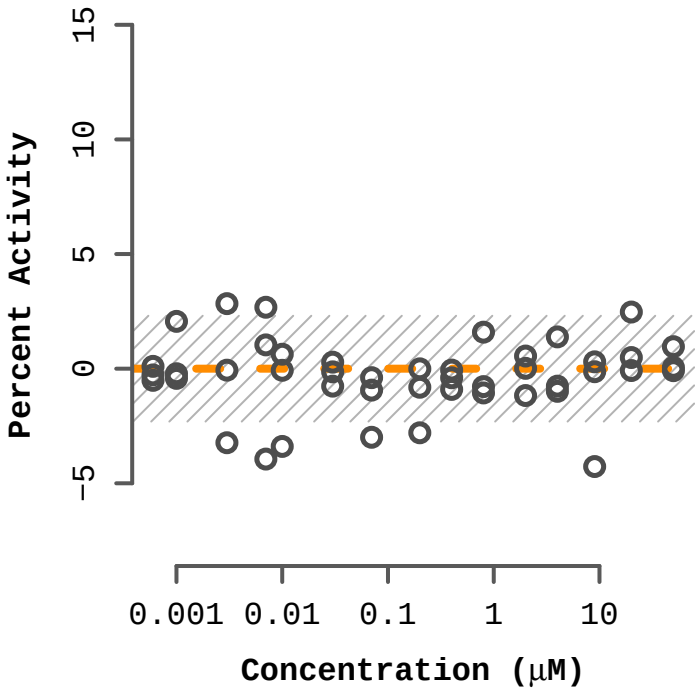
NAME: Valproic acid
CHID: 23733 **CASRN:** 99-66-1
SPID(S): Tox21_201963
M4ID: 12480289

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.468 **MAX_MED:** 0.132 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

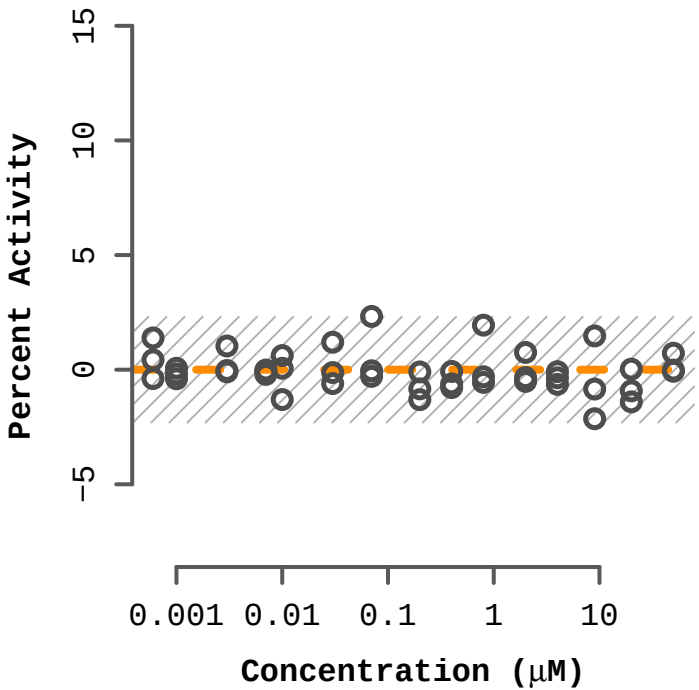
NAME: Valproic acid
CHID: 23733 **CASRN:** 99-66-1
SPID(S): Tox21_111091_1
M4ID: 12483912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 0.96 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

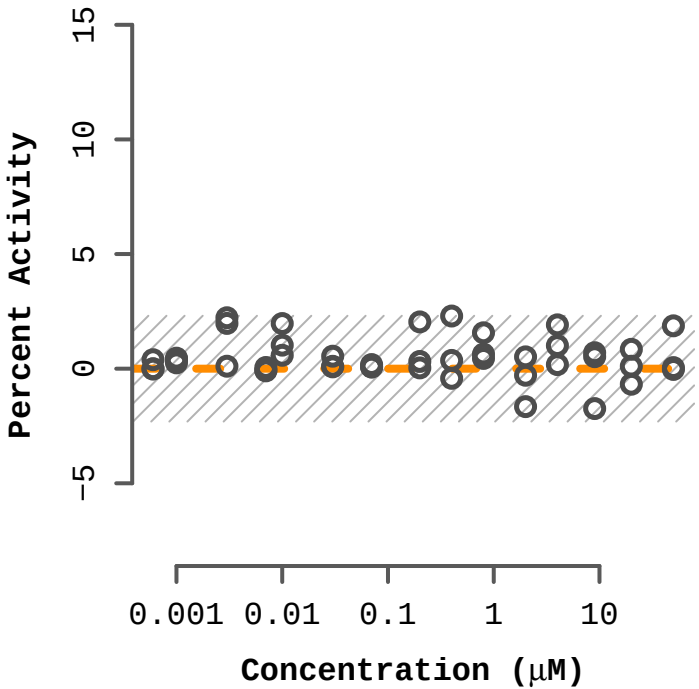
NAME: Vecuronium bromide
CHID: 23736 CASRN: 50700-72-6
SPID(S): Tox21_112471_1
M4ID: 12483082

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.662 **MAX_MED:** 0.429 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

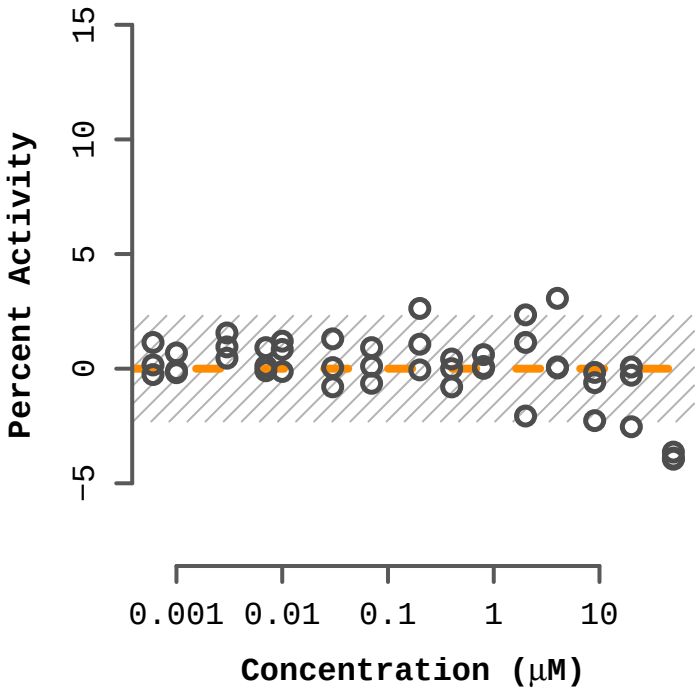
NAME: Venlafaxine
CHID: 23737 **CASRN:** 93413-69-5
SPID(S): Tox21_111425_1
M4ID: 12483698

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

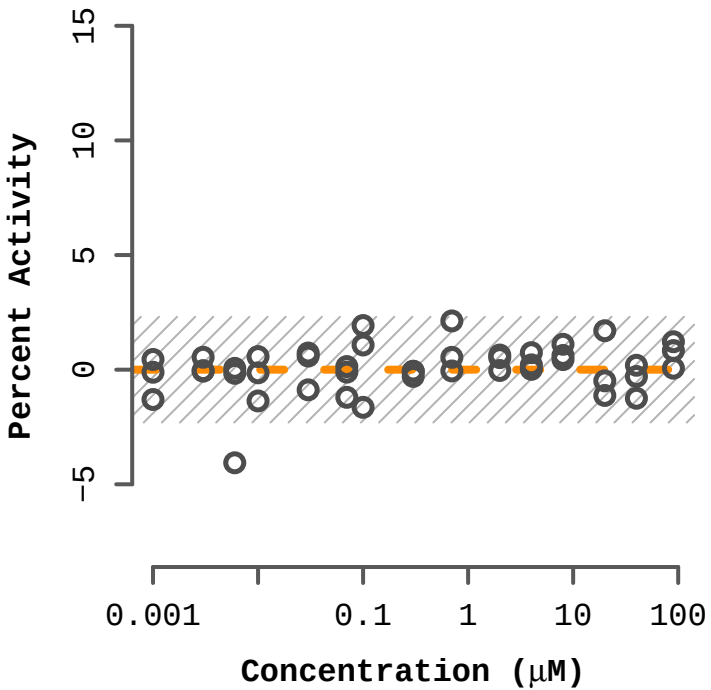
NAME: Vinpocetine
CHID: 23740 CASRN: 42971-09-5
SPID(S): Tox21_110648_1
M4ID: 12484207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.21 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

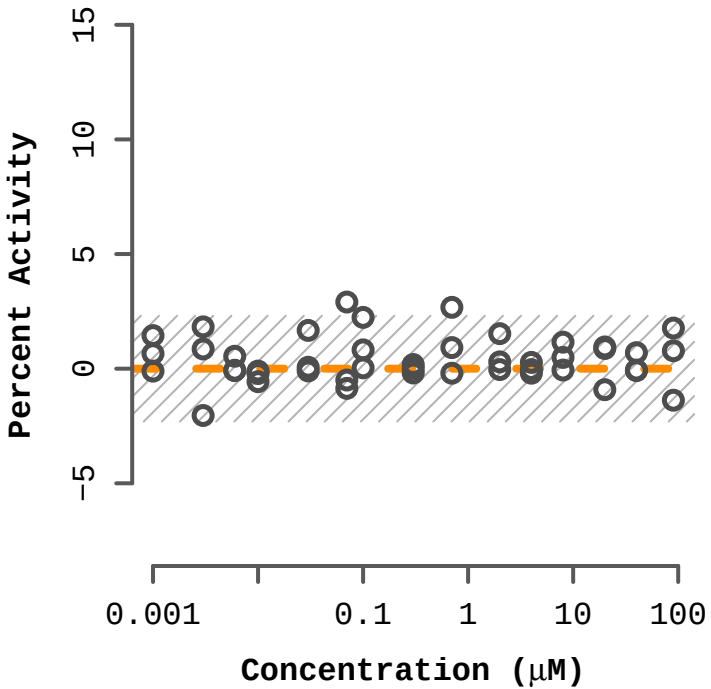
NAME: Warfarin
CHID: 23742 CASRN: 81-81-2
SPID(S): Tox21_300531
M4ID: 12478601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.871 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

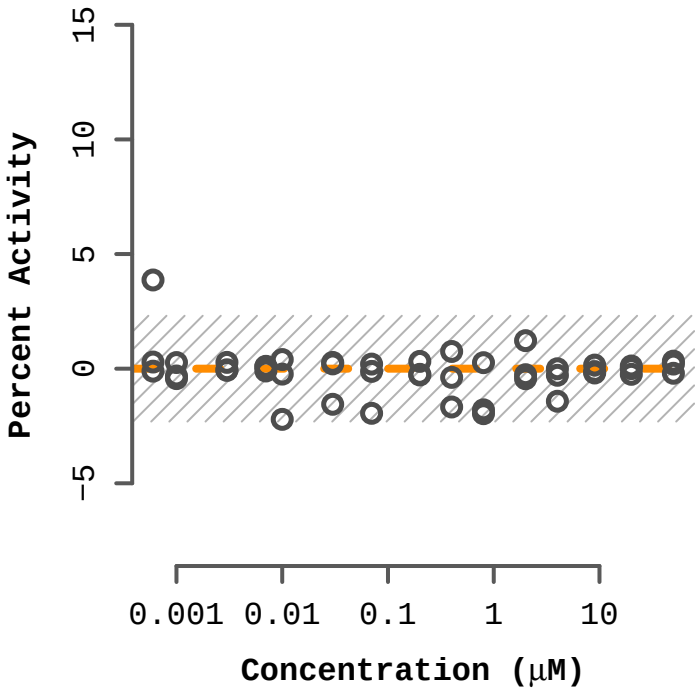
NAME: Warfarin
CHID: 23742 **CASRN:** 81-81-2
SPID(S): Tox21_202182
M4ID: 12480070

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.922 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

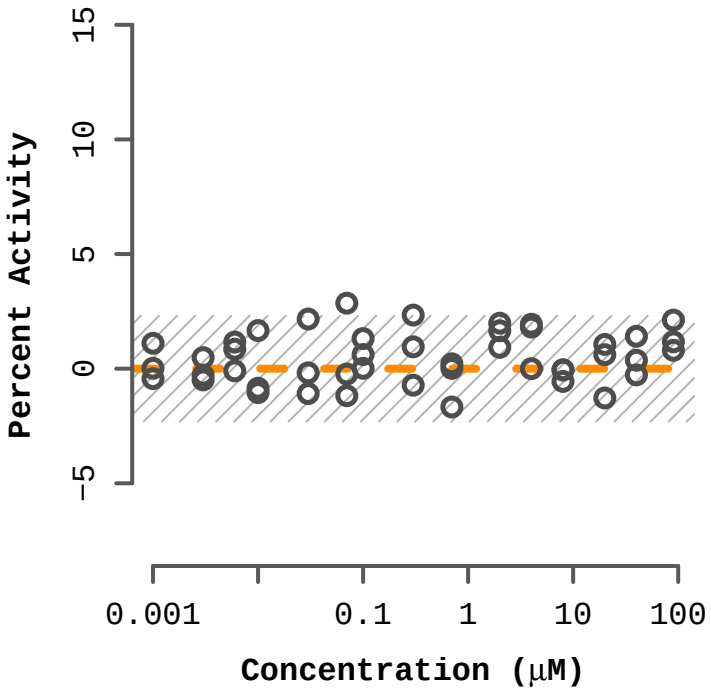
NAME: Xipamide
CHID: 23744 **CASRN:** 14293-44-8
SPID(S): Tox21_112975_1
M4ID: 12482859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.291 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

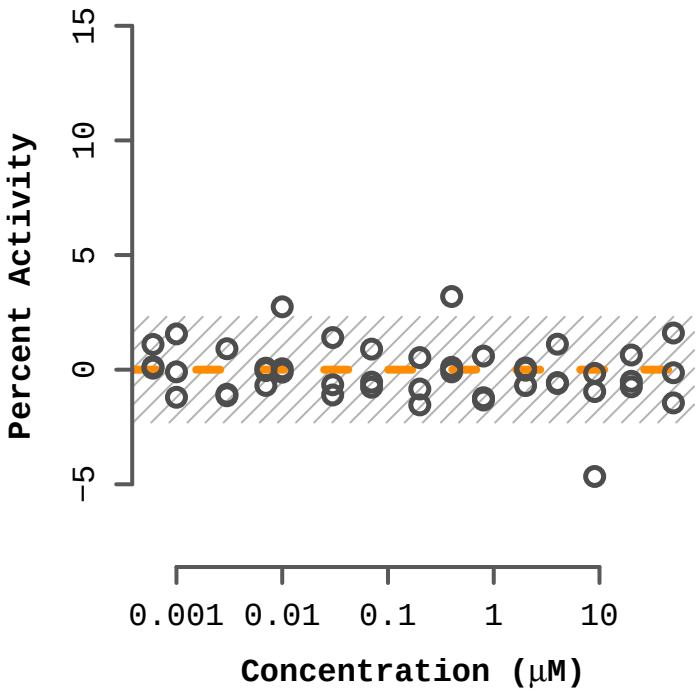
NAME: D-Xylose
CHID: 23745 **CASRN:** 58-86-6
SPID(S): Tox21_302055
M4ID: 12477078

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

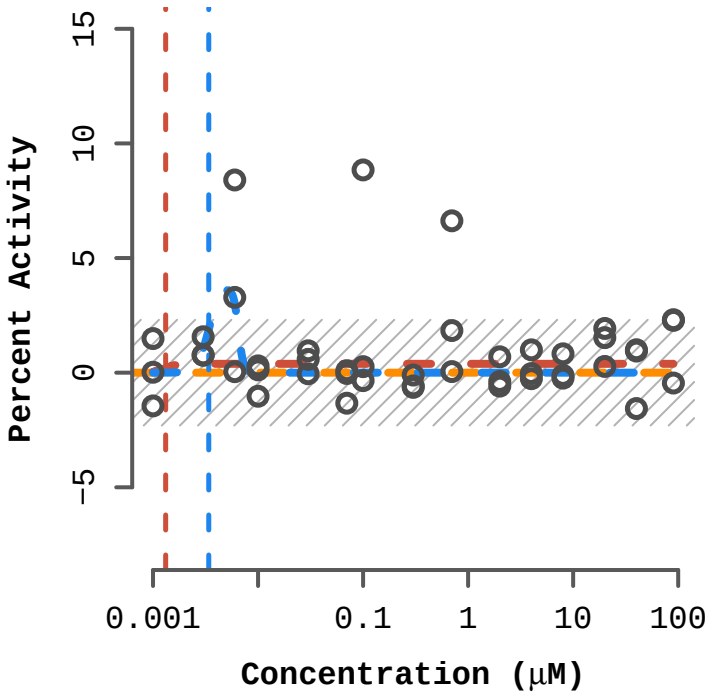
NAME: Zafirlukast
CHID: 23746 **CASRN:** 107753-78-6
SPID(S): Tox21_112176_1
M4ID: 12483259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.137 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2',3'−Dideoxycytidine
CHID: 23747 CASRN: 7481−89−2
SPID(S): Tox21_303169
M4ID: 12475964

HILL MODEL (in red):

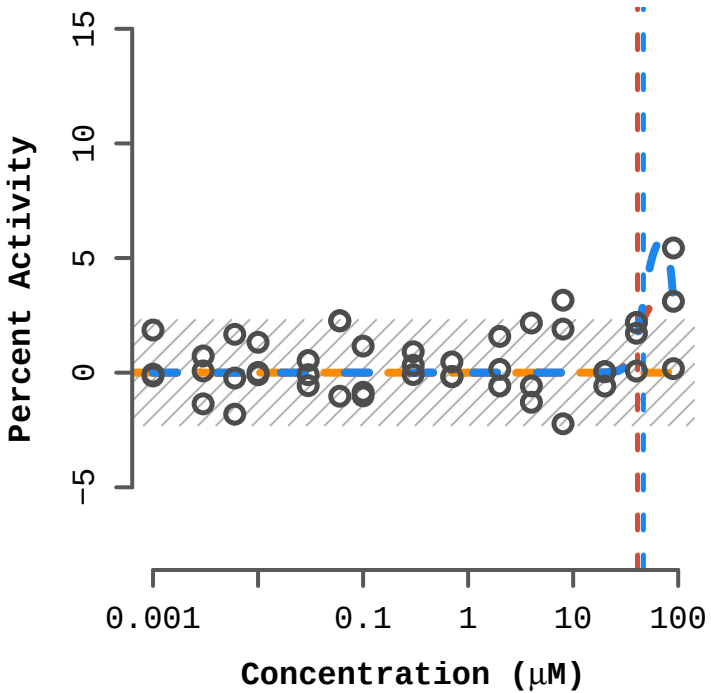
	tp	ga	gw
val:	0.386	−2.88	8
sd:	0.19	0.894	33.9

GAIN−LOSS MODEL (in blue):

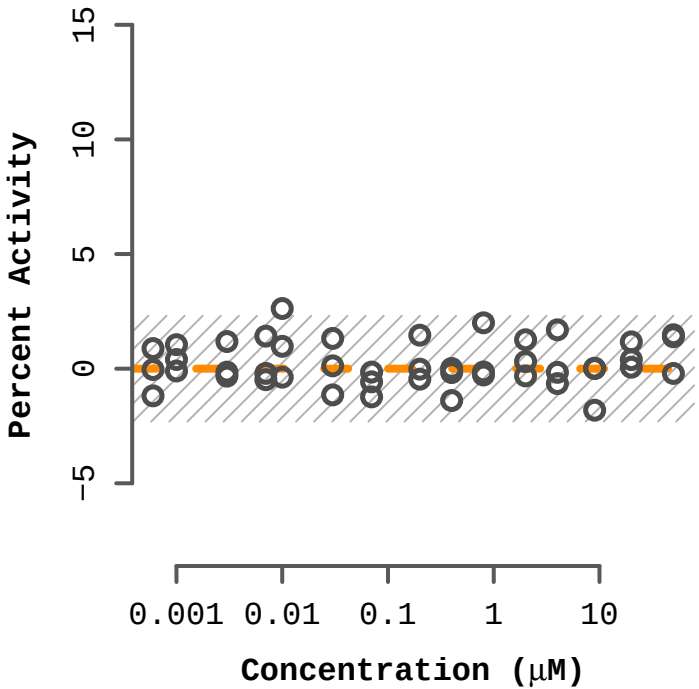
	tp	ga	gw	la	lw
val:	3.78	−2.47	8	−2.19	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	177.58	179.35	179.96
PROB:	0.58	0.24	0.18
RMSE:	2.33	2.21	2.09

MAX_MEAN: 3.91 MAX_MED: 3.29 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2',3'-Dideoxycytidine
CHID:    23747   CASRN: 7481-89-2
SPID(S): Tox21_201655
M4ID:    12480597

HILL MODEL (in red):
      tp       ga       gw
val:  3.18     1.61     8
sd:   1.02     0.0644   18.8

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.14     1.67     7.79     1.96     16.1
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  164.17      159.97      163.97
PROB: 0.1         0.79        0.11
RMSE: 1.53        1.29        1.29

MAX_MEAN: 2.91      MAX_MED: 3.11      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

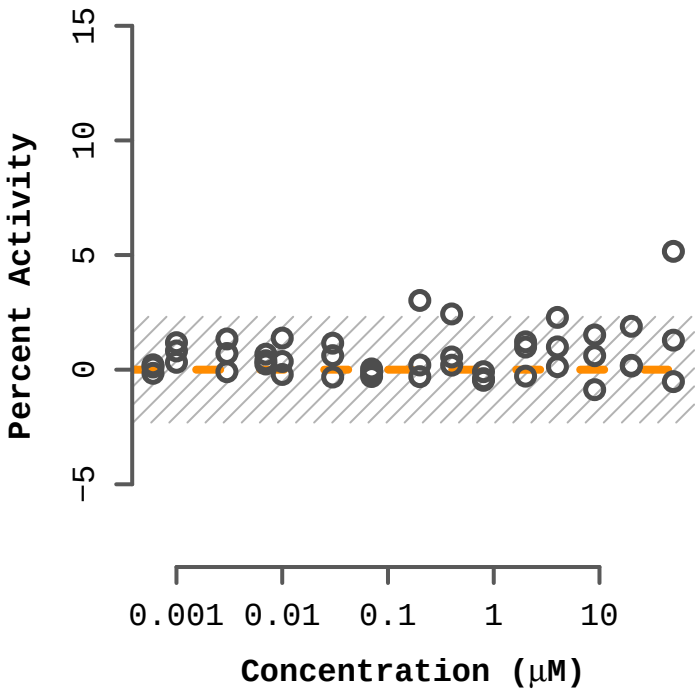
NAME: 2',3'−Dideoxycytidine
CHID: 23747 **CASRN:** 7481−89−2
SPID(S): Tox21_113491_1
M4ID: 12482632

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

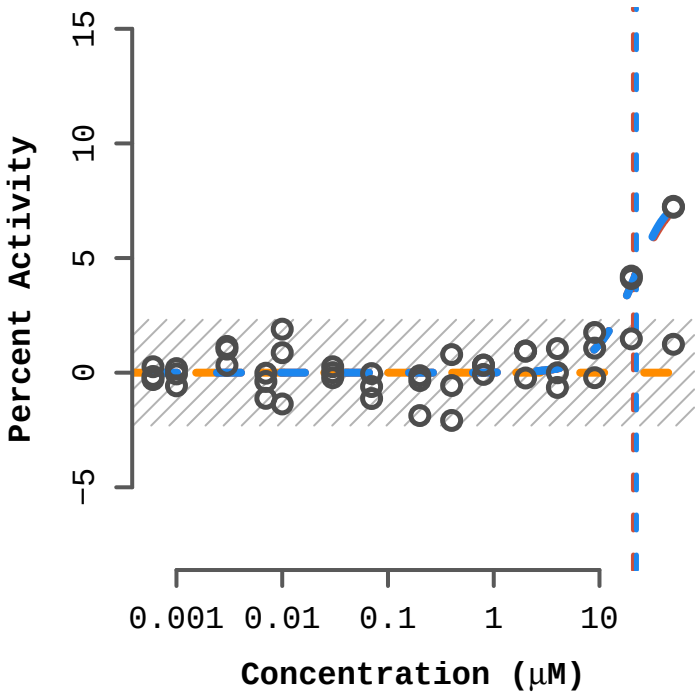
NAME: Zaleplon
CHID: 23748 **CASRN:** 151319-34-5
SPID(S): Tox21_111872_1
M4ID: 12483439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.98 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zanamivir
CHID: 23749 **CASRN:** 139110-80-8
SPID(S): Tox21_112190_1
M4ID: 12483248

HILL MODEL (in red):

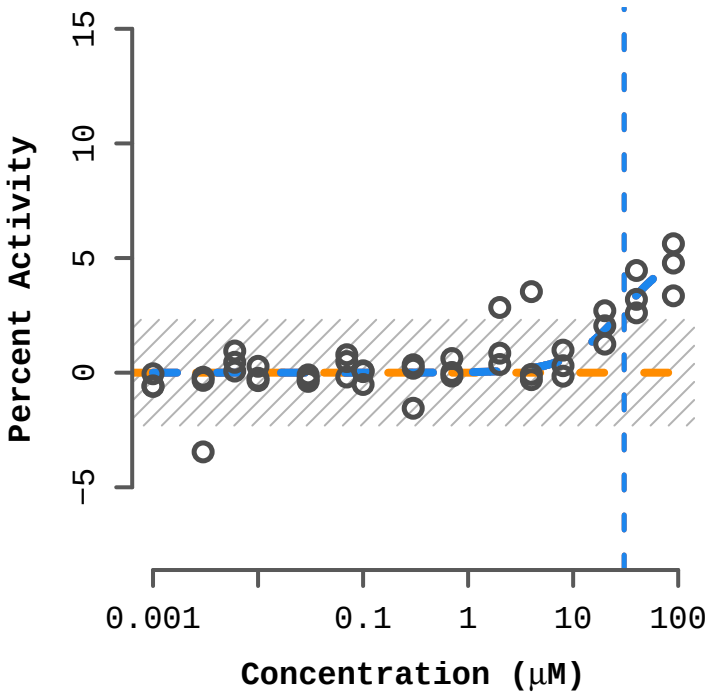
	tp	ga	gw
val:	8.05	1.32	2.28
sd:	1.49	0.109	0.937

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.71	1.35	2.22	1.94	5.23
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	166.47	134.06	138.05
PROB:	0	0.88	0.12
RMSE:	1.96	1.22	1.22

MAX_MEAN: 5.24 **MAX_MED:** 7.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zileuton
CHID: 23752 CASRN: 111406-87-2
SPID(S): Tox21_301148
M4ID: 12477985

HILL MODEL (in red):

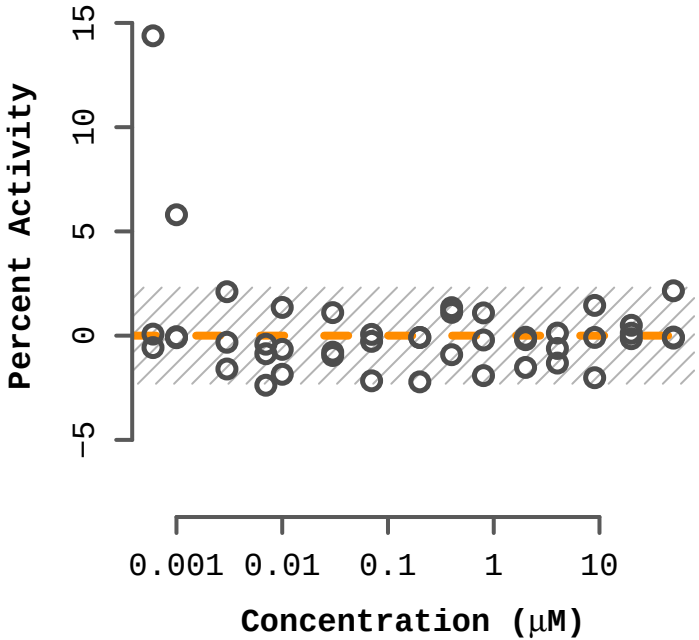
	tp	ga	gw
val:	5.56	1.49	1.63
sd:	1.63	0.213	0.729

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.56	1.49	1.63	2.71	10.1
sd:	1.63	0.213	0.729	1110	14900

	CNST	HILL	GNLS
AIC:	176.56	119.02	123.02
PROB:	0	0.88	0.12
RMSE:	1.87	1	1

MAX_MEAN: 4.59 MAX_MED: 4.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

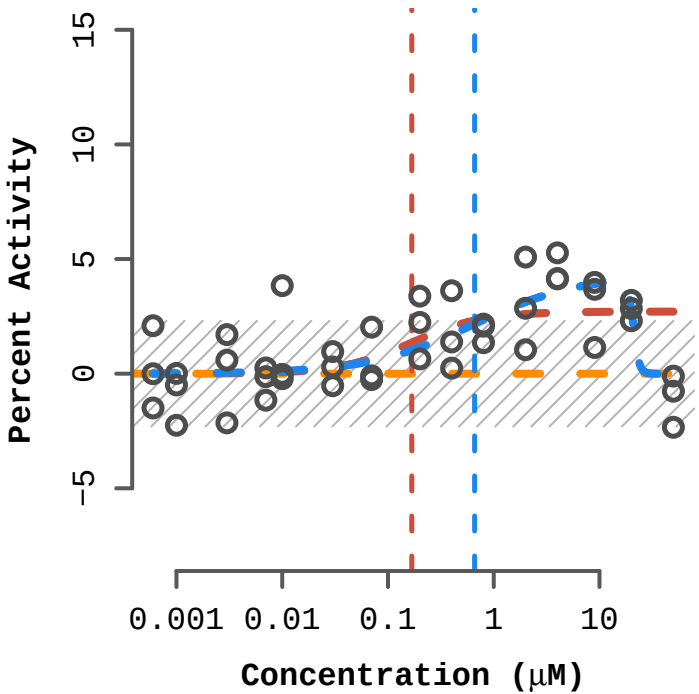
NAME: Zileuton
CHID: 23752 CASRN: 111406-87-2
SPID(S): Tox21_111680_1
M4ID: 12483539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.57	NA	NA

MAX_MEAN: 4.63 MAX_MED: 1.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ziprasidone
CHID: 23753 CASRN: 146939-27-7
SPID(S): Tox21_112194_1
M4ID: 12483246

HILL MODEL (in red):

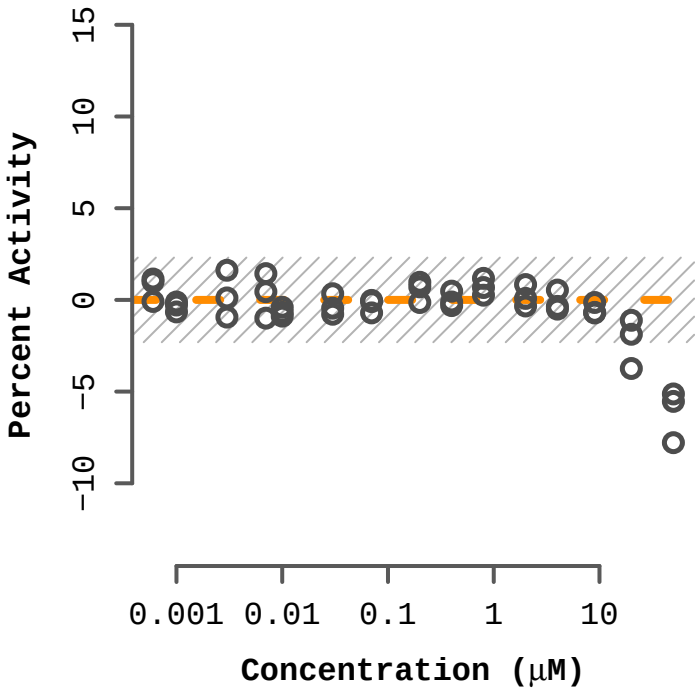
	tp	ga	gw
val:	2.71	−0.775	1.29
sd:	0.504	0.356	0.771

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.34	−0.181	0.857	1.32	16.1
sd:	1.08	0.374	0.365	0.0402	32.9

	CNST	HILL	GNLS
AIC:	208.2	180.36	165.54
PROB:	0	0	1
RMSE:	2.32	1.65	1.33

MAX_MEAN: 4.52 **MAX_MED:** 4.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

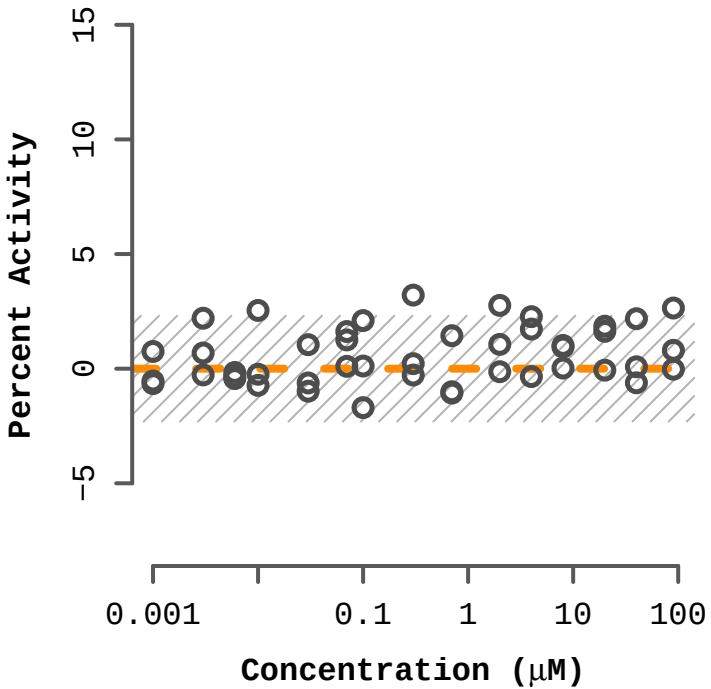
NAME: Zotepine
CHID: 23756 **CASRN:** 26615-21-4
SPID(S): Tox21_113135_1
M4ID: 12482794

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 0.703 **MAX_MED:** 0.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

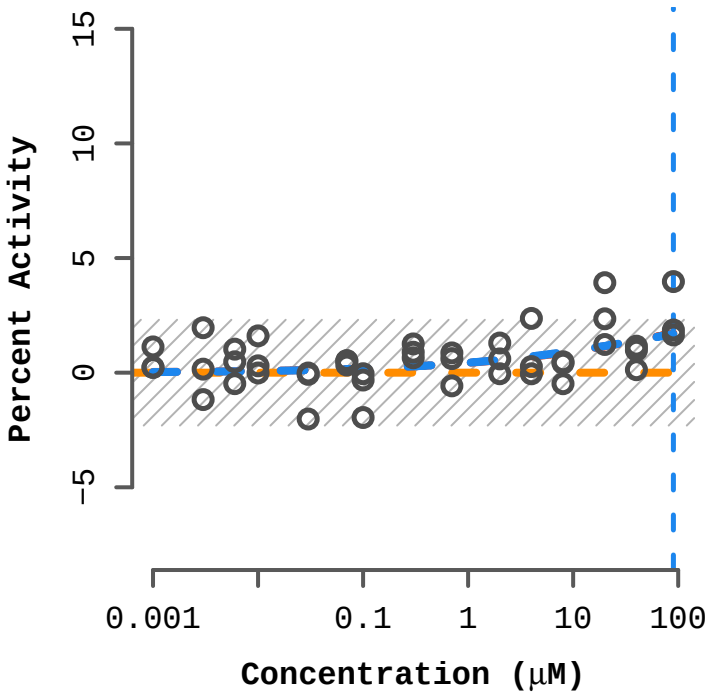
NAME: Benzo(e)pyrene
CHID: 23764 **CASRN:** 192-97-2
SPID(S): Tox21_303185
M4ID: 12475948

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzo(e)pyrene
CHID: 23764 CASRN: 192-97-2
SPID(S): Tox21_201724
M4ID: 12480528

HILL MODEL (in red):

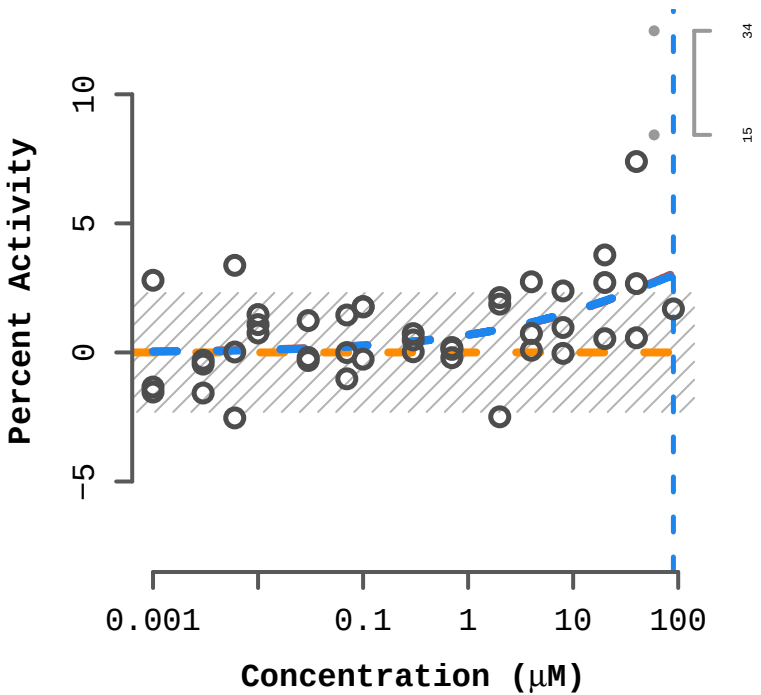
	tp	ga	gw
val:	4.44	2.45	0.396
sd:	6.86	2.71	0.215

GAIN-LOSS MODEL (in blue):

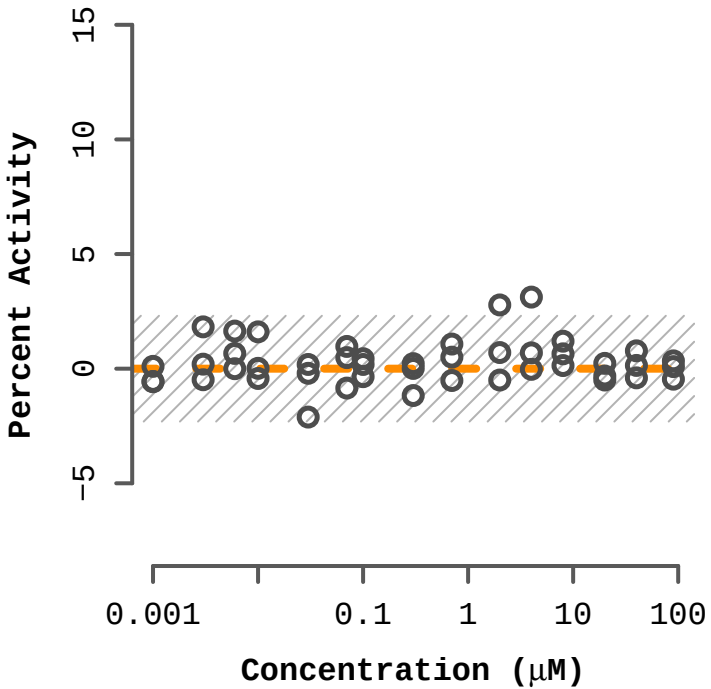
	tp	ga	gw	la	lw
val:	3.37	1.95	0.424	3.88	3.97
sd:	3.9	2.07	0.236	1300	2720

	CNST	HILL	GNLS
AIC:	151.04	134.33	138.55
PROB:	0	0.89	0.11
RMSE:	1.32	1	1.01

MAX_MEAN: 2.5 MAX_MED: 2.35 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2',3'-Dideoxyadenosine
CHID:    23771   CASRN: 4097-22-7
SPID(S): Tox21_201121
M4ID:    12481131  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  8.03     2.45     0.419
sd:   30.3     6.33     0.414

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.99     1.95     0.457    3.74     13.8
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  222.69      211.88      215.89
PROB: 0           0.88        0.12
RMSE: 5.9         5.21        5.23

MAX_MEAN: 17        MAX_MED: 14.8      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

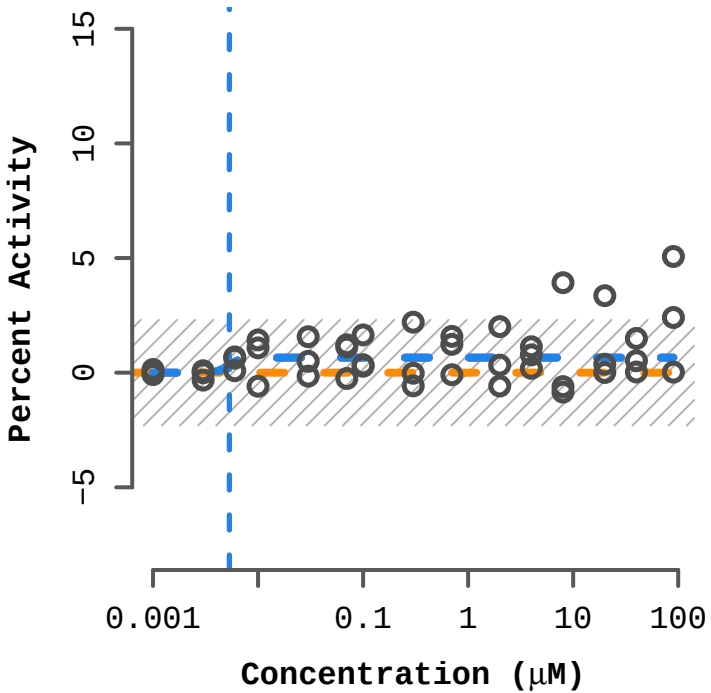
NAME: Diphenylhydantoin sodium
CHID: 23775 CASRN: 630-93-3
SPID(S): Tox21_302338
M4ID: 12476795

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.705 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl isocyanate
CHID: 23786 **CASRN:** 624-83-9
SPID(S): Tox21_201060
M4ID: 12481192

HILL MODEL (in red):

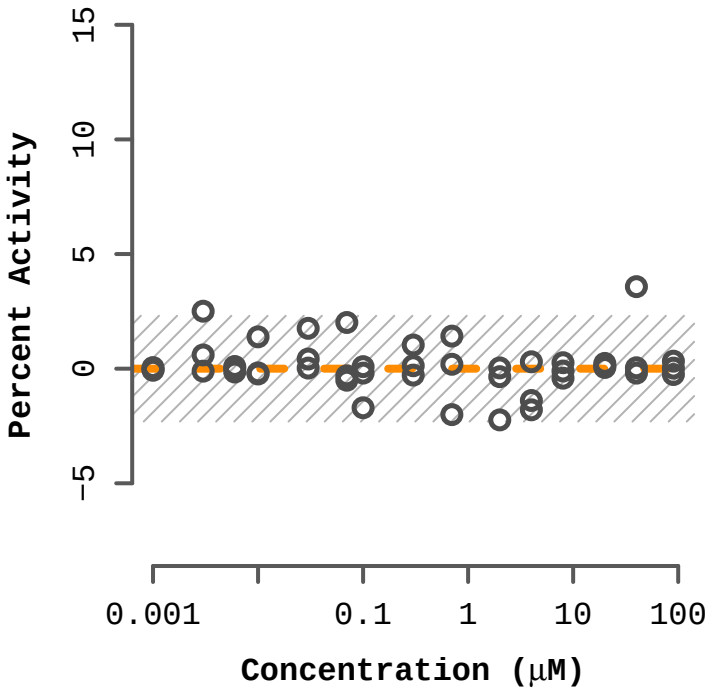
	tp	ga	gw
val:	0.656	−2.27	8
sd:	0.174	0.217	21.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.656	−2.27	8	3.26	6.25
sd:	0.174	0.217	21.7	2650	12700

	CNST	HILL	GNLS
AIC:	151.22	142.18	146.18
PROB:	0.01	0.87	0.12
RMSE:	1.42	1.19	1.19

MAX_MEAN: 2.5 **MAX_MED:** 2.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

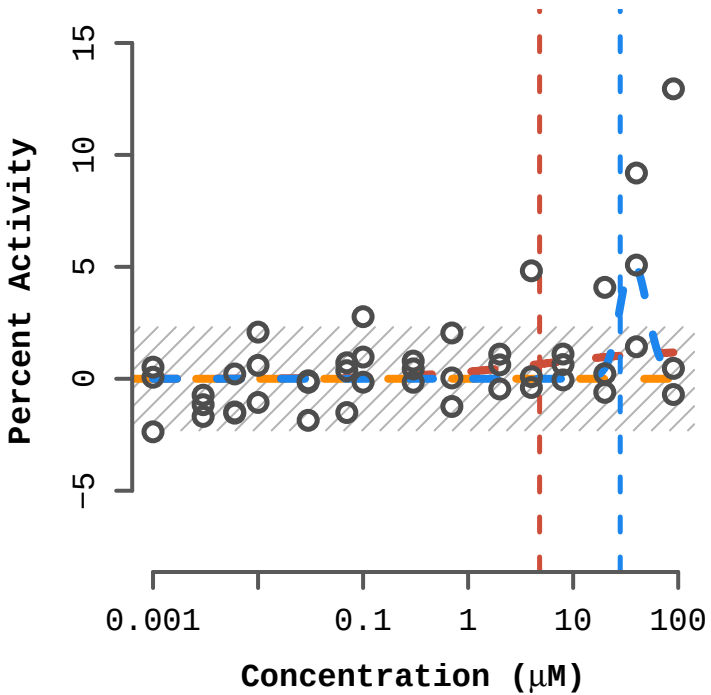
NAME: 4-Nitrotoluene
CHID: 23792 **CASRN:** 99-99-0
SPID(S): Tox21_300017
M4ID: 12479113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.601 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitrotoluene
CHID: 23792 CASRN: 99-99-0
SPID(S): Tox21_201464
M4ID: 12480788

HILL MODEL (in red):

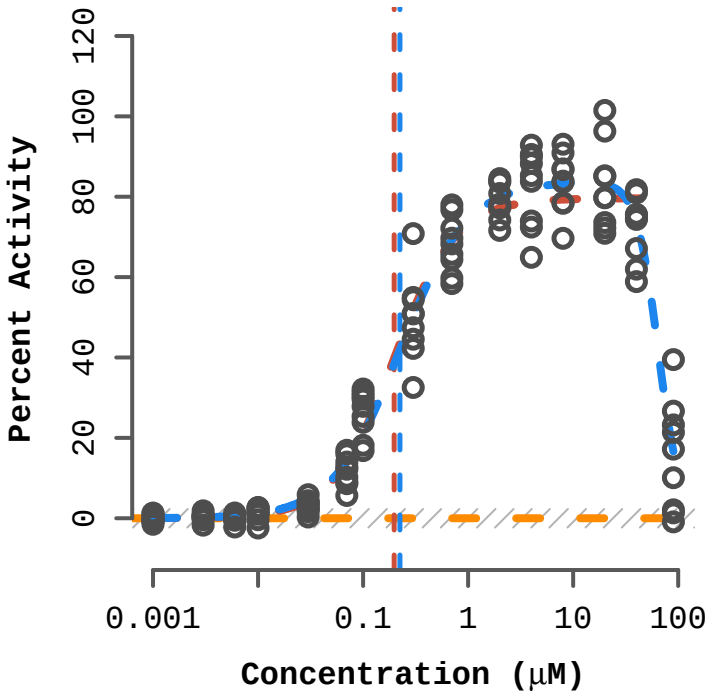
	tp	ga	gw
val:	1.31	0.68	0.732
sd:	1.38	1.6	0.845

GAIN-LOSS MODEL (in blue):

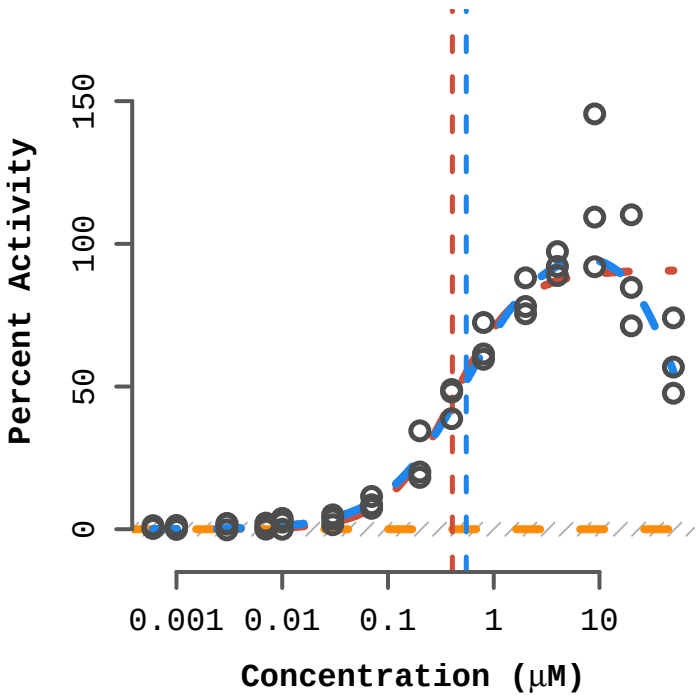
	tp	ga	gw	la	lw
val:	6.64	1.45	7.47	1.7	6.32
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	194.5	195.76	193.6
PROB:	0.32	0.17	0.51
RMSE:	2.86	2.58	2.49

MAX_MEAN: 5.24 MAX_MED: 5.08 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Oxymetholone
CHID:    23794   CASRN: 434-07-1
SPID(S): Tox21_200071
M4ID:    12482181

HILL MODEL (in red):
      tp       ga       gw
val:  79.6     -0.704   1.48
sd:   1.34     0.031    0.101

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  83.9     -0.649   1.37     1.81     4.17
sd:   1.43     0.0291   0.0818   0.0206   0.484

      CNST        HILL        GNLS
AIC:  1465.31     1037.28     900.69
PROB: 0           0           1
RMSE: 52.25       18.05       6.82

MAX_MEAN: 83.5      MAX_MED: 85.3      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxymetholone
CHID: 23794 CASRN: 434-07-1
SPID(S): Tox21_111131_1
M4ID: 12483888

HILL MODEL (in red):

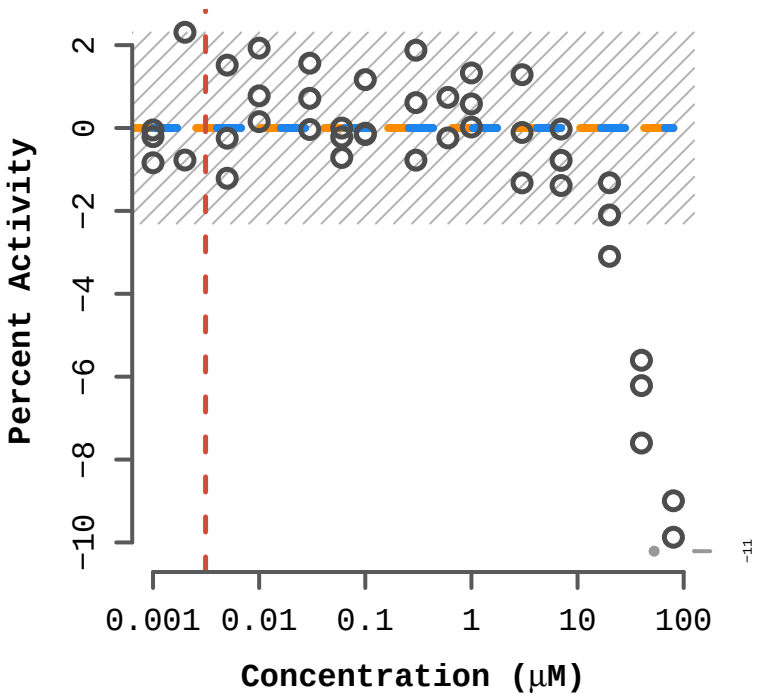
	tp	ga	gw
val:	90.7	-0.391	1.38
sd:	4.03	0.052	0.182

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	104	-0.26	1.11	1.74	1.63
sd:	7.39	0.0796	0.13	0.0547	0.49

	CNST	HILL	GNLS
AIC:	493.75	341.36	314.76
PROB:	0	0	1
RMSE:	56.46	13.5	10.13

MAX_MEAN: 116 MAX_MED: 109 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentamidine isethionate
CHID: 23796 CASRN: 140-64-7
SPID(S): Tox21_300312
M4ID: 12478818 BRK

HILL MODEL (in red):

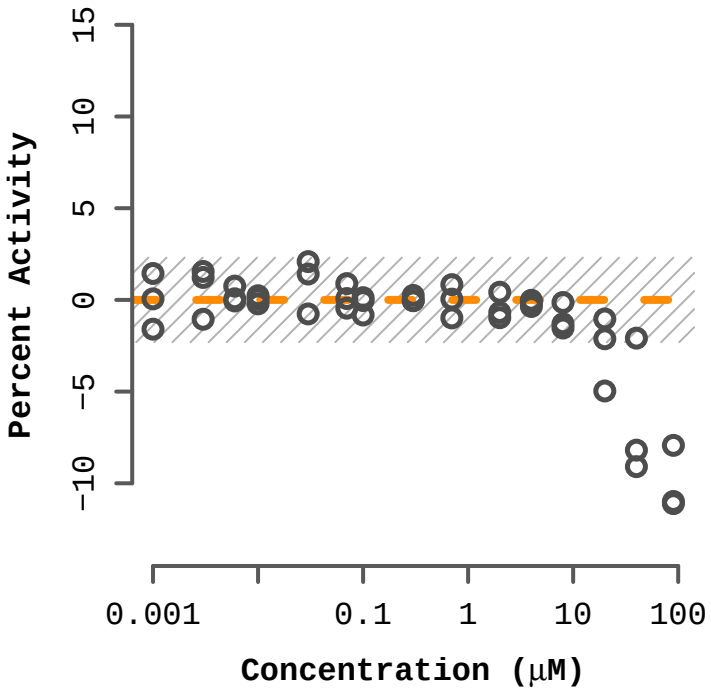
	tp	ga	gw
val:	1.23e-09	-2.5	1.91
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.23	-4.55	0.929	-4.13	6.64
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	219.37	225.37	229.37
PROB:	0.95	0.05	0.01
RMSE:	3.32	3.32	3.32

MAX_MEAN: 1.51 MAX_MED: 2.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

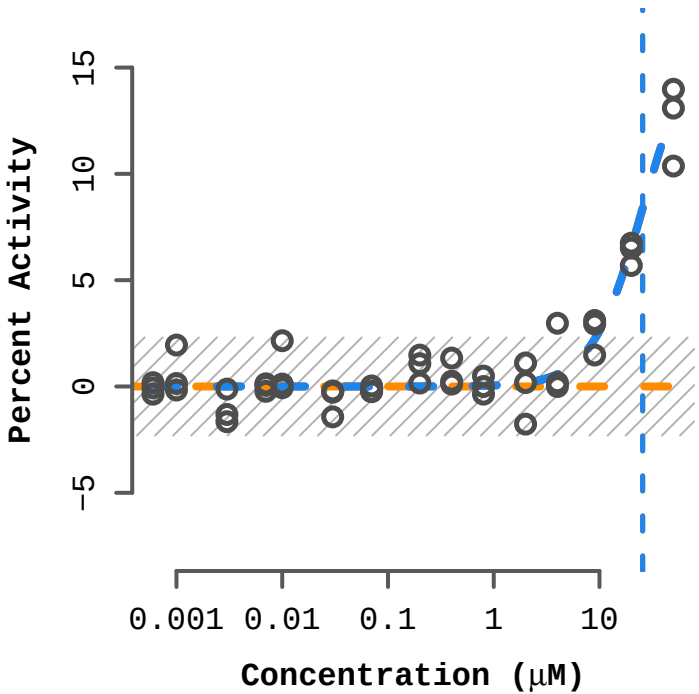
NAME: Pentamidine isethionate
CHID: 23796 CASRN: 140-64-7
SPID(S): Tox21_201722
M4ID: 12480530

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.38	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 0.913 MAX_MED: 1.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentamidine isethionate
CHID: 23796 CASRN: 140-64-7
SPID(S): Tox21_110742_1
M4ID: 12484139

HILL MODEL (in red):

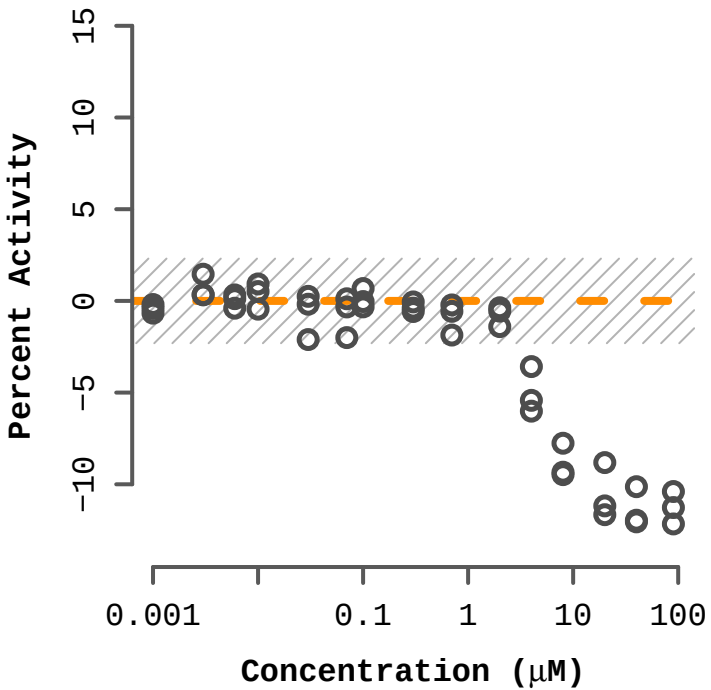
	tp	ga	gw
val:	16.8	1.41	1.8
sd:	2.44	0.0848	0.325

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.8	1.41	1.8	3.7	4.83
sd:	2.43	0.0846	0.324	6650	16100

	CNST	HILL	GNLS
AIC:	219.41	129.16	133.16
PROB:	0	0.88	0.12
RMSE:	3.8	0.97	0.97

MAX_MEAN: 12.5 **MAX_MED:** 13.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

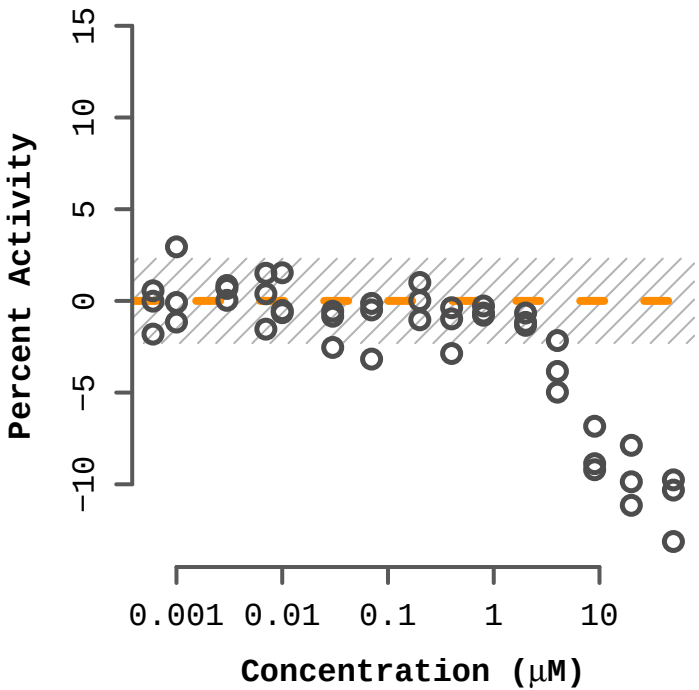
NAME: Benzethonium chloride
CHID: 23810 **CASRN:** 121-54-0
SPID(S): Tox21_202488
M4ID: 12479764

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	281.62	NA	NA
PROB:	1	NA	NA
RMSE:	5.67	NA	NA

MAX_MEAN: 0.71 **MAX_MED:** 0.513 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

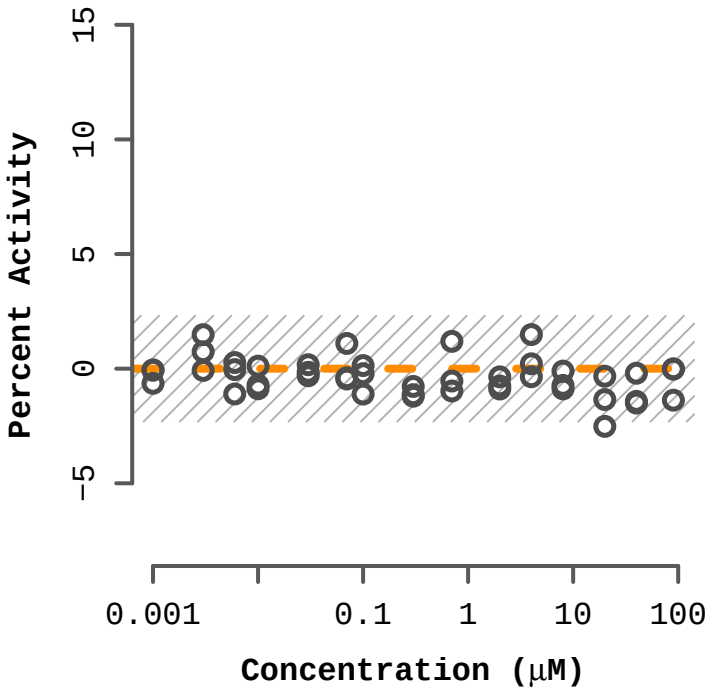
NAME: Benzethonium chloride
CHID: 23810 **CASRN:** 121-54-0
SPID(S): Tox21_110403_1
M4ID: 12484389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.39	NA	NA
PROB:	1	NA	NA
RMSE:	4.64	NA	NA

MAX_MEAN: 0.57 **MAX_MED:** 0.681 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

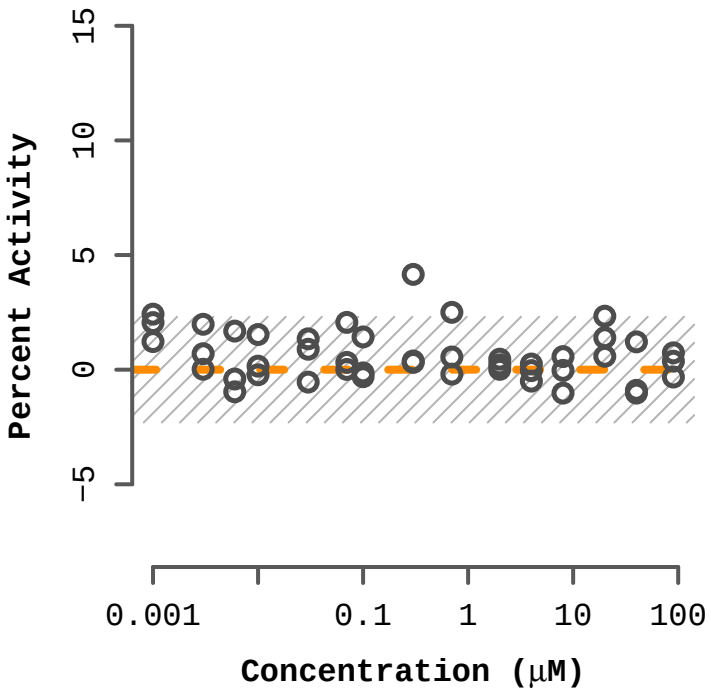
NAME: Dibromoacetic acid
CHID: 23815 CASRN: 631-64-1
SPID(S): Tox21_303291
M4ID: 12475842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.741 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

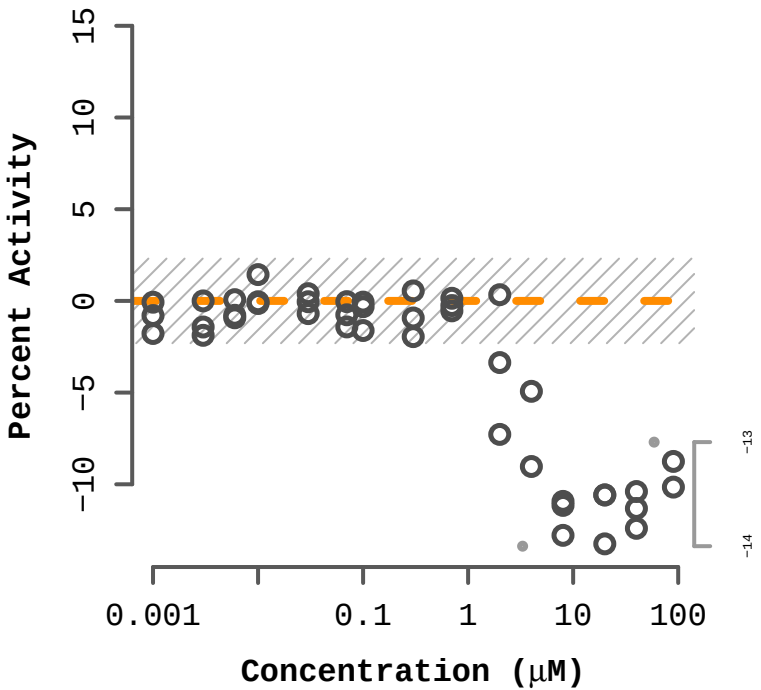
NAME: Dibromoacetic acid
CHID: 23815 **CASRN:** 631-64-1
SPID(S): Tox21_202297
M4ID: 12479955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

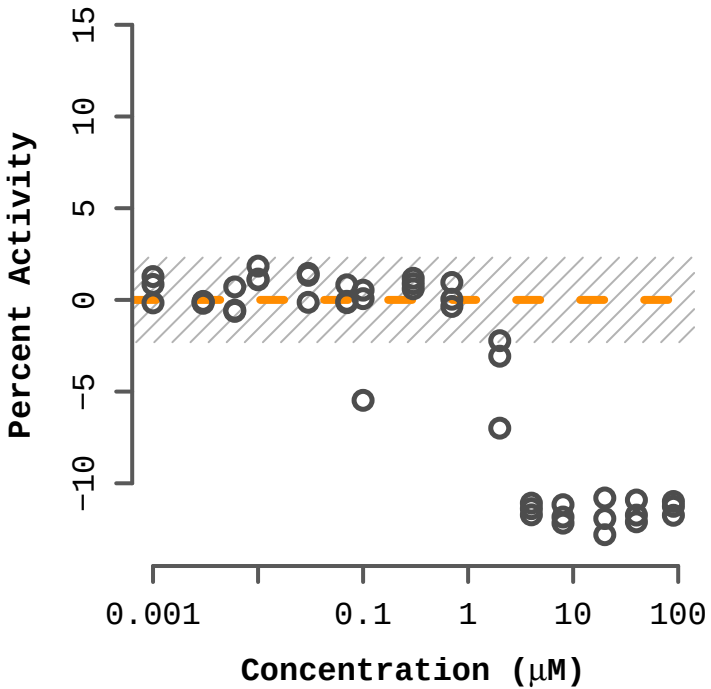
NAME: Dicyclohexylcarbodiimide
CHID: 23817 **CASRN:** 538-75-0
SPID(S): Tox21_303237
M4ID: 12475896 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	297.71	NA	NA
PROB:	1	NA	NA
RMSE:	6.57	NA	NA

MAX_MEAN: 0.418 **MAX_MED:** −0.0436 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

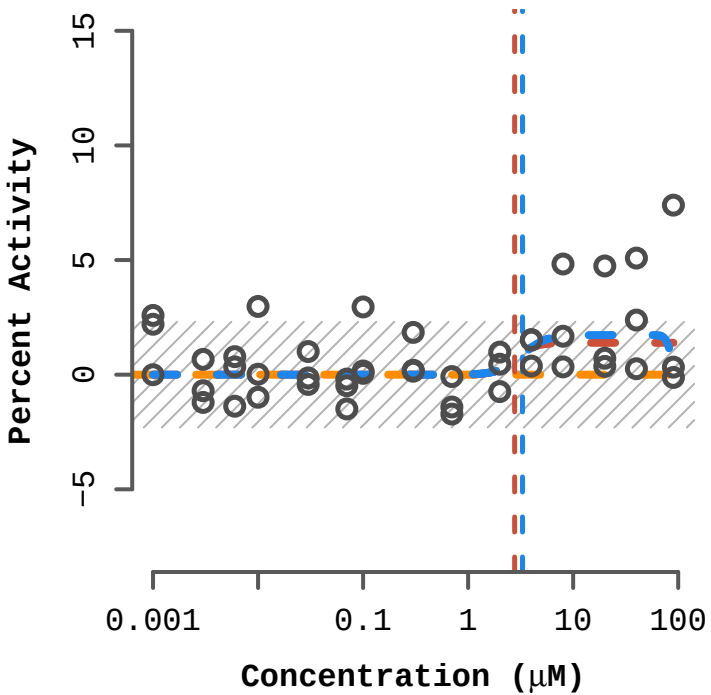
NAME: Dicyclohexylcarbodiimide
CHID: 23817 CASRN: 538-75-0
SPID(S): Tox21_203000
M4ID: 12479252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.62	NA	NA
PROB:	1	NA	NA
RMSE:	6.87	NA	NA

MAX_MEAN: 1.36 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Stavudine
CHID: 23819 CASRN: 3056-17-5
SPID(S): Tox21_300583
M4ID: 12478550

HILL MODEL (in red):

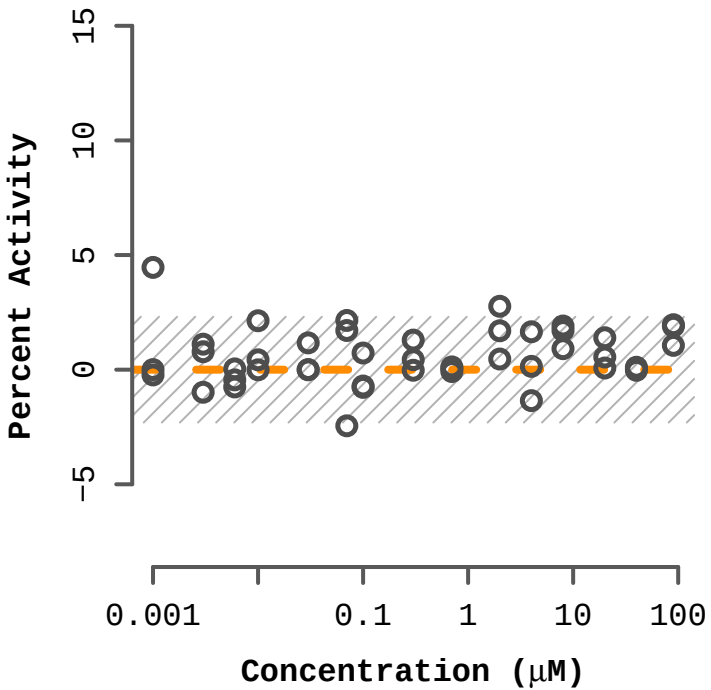
	tp	ga	gw
val:	1.39	0.443	4.87
sd:	0.534	0.286	6.75

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.73	0.518	3.96	1.93	17.3
sd:	0.655	0.215	4.93	0.0864	62.4

	CNST	HILL	GNLS
AIC:	183.56	177.9	180.54
PROB:	0.04	0.75	0.2
RMSE:	2.05	1.71	1.74

MAX_MEAN: 2.58 **MAX_MED:** 2.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

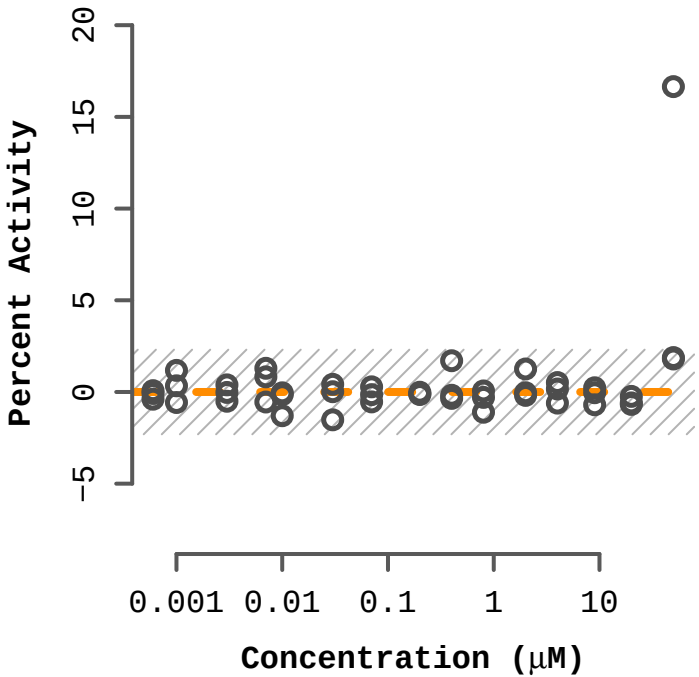
NAME: Stavudine
CHID: 23819 **CASRN:** 3056-17-5
SPID(S): Tox21_201393
M4ID: 12480859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

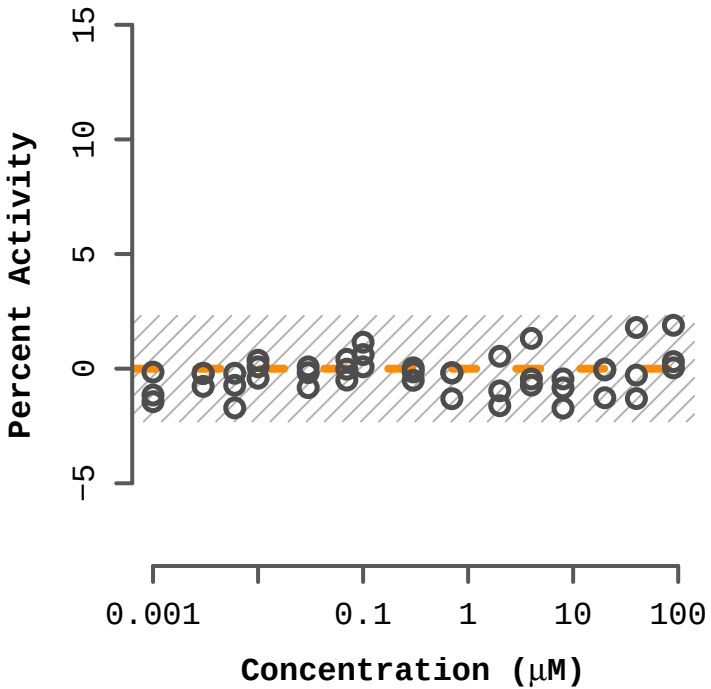
NAME: Stavudine
CHID: 23819 CASRN: 3056-17-5
SPID(S): Tox21_110886_1
M4ID: 12484041

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.33	NA	NA
PROB:	1	NA	NA
RMSE:	2.59	NA	NA

MAX_MEAN: 6.78 MAX_MED: 1.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

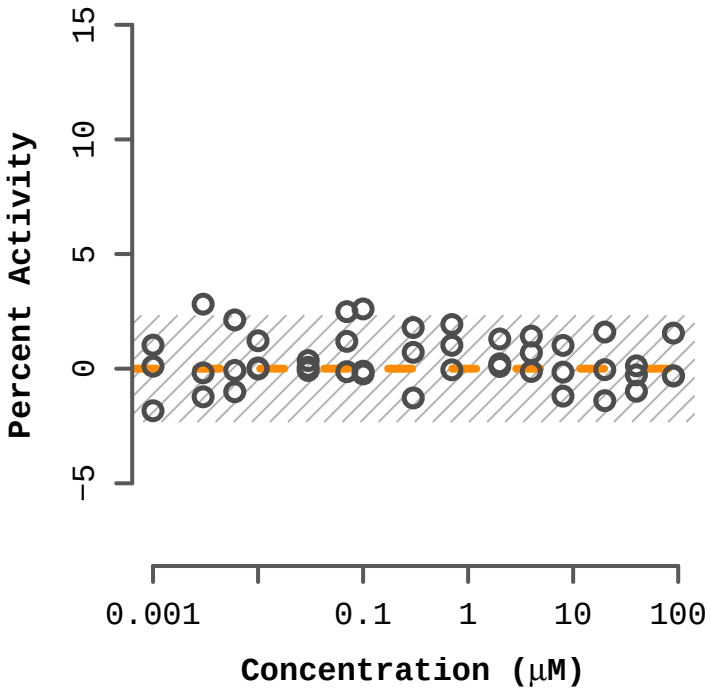
NAME: Indium arsenide
CHID: 23825 CASRN: 1303-11-3
SPID(S): Tox21_300528
M4ID: 12478604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.747 **MAX_MED:** 0.617 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

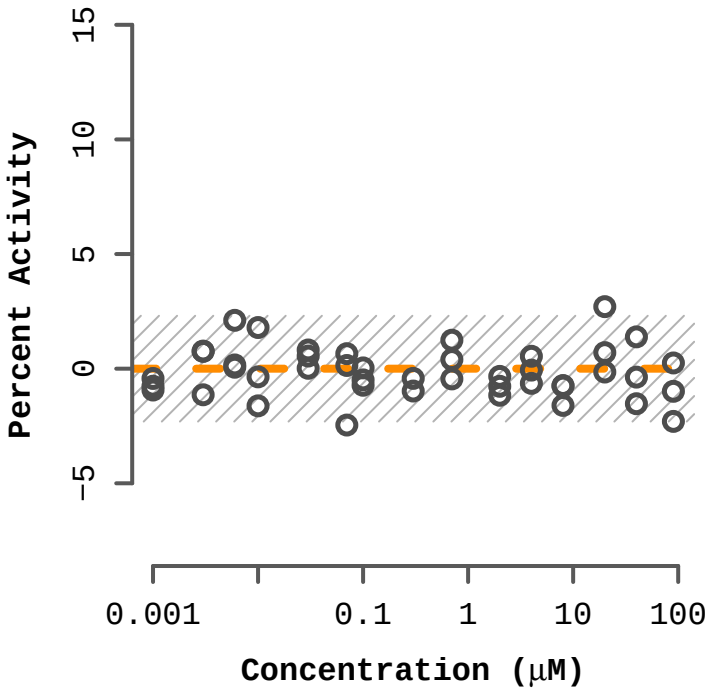
NAME: Isophorone diisocyanate
CHID: 23826 **CASRN:** 4098-71-9
SPID(S): Tox21_300298
M4ID: 12478832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

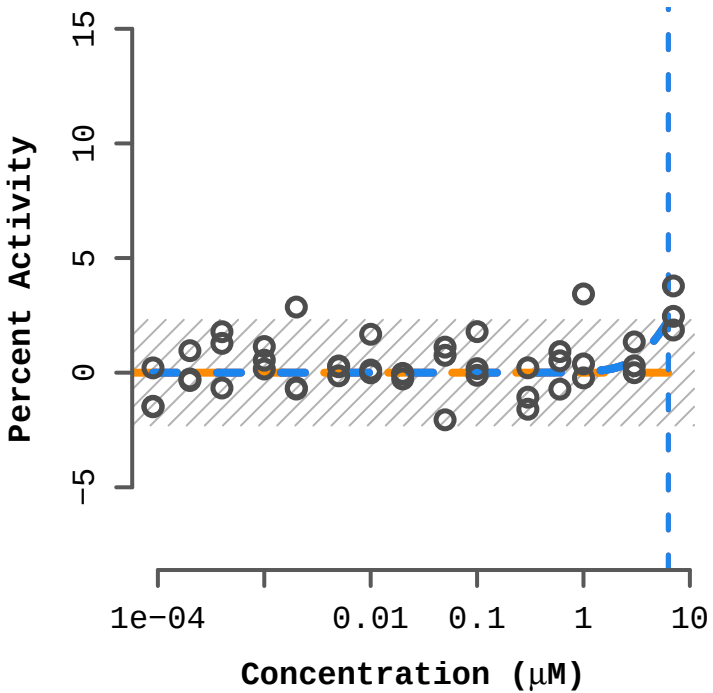
NAME: Isophorone diisocyanate
CHID: 23826 CASRN: 4098-71-9
SPID(S): Tox21_201520
M4ID: 12480732

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.758 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Polydimethylsiloxane
CHID: 23833 **CASRN:** 9016-00-6
SPID(S): Tox21_302437
M4ID: 12476696

HILL MODEL (in red):

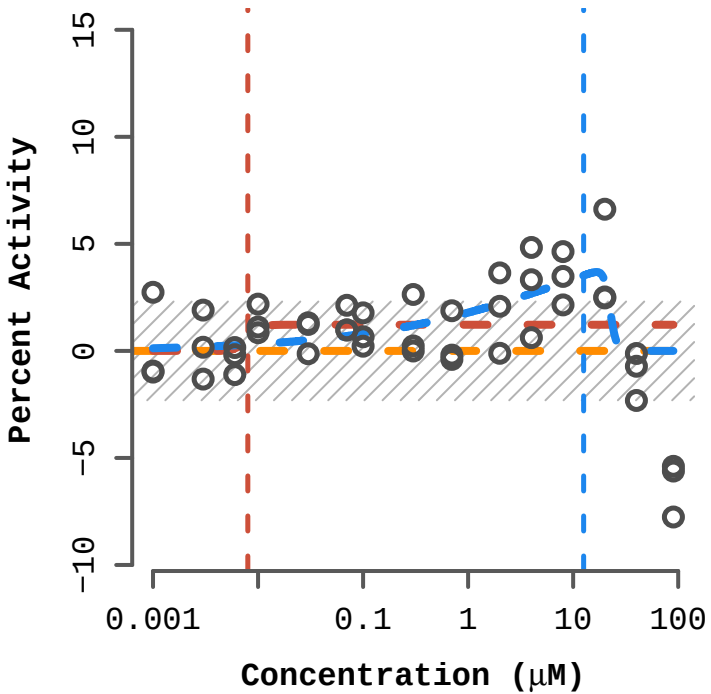
	tp	ga	gw
val:	4.54	0.798	2.63
sd:	11.5	0.907	4.34

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.54	0.798	2.63	2.8	2.62
sd:	11.4	0.903	4.32	396	542

	CNST	HILL	GNLS
AIC:	151.3	141.47	145.47
PROB:	0.01	0.88	0.12
RMSE:	1.31	1.1	1.1

MAX_MEAN: 2.7 **MAX_MED:** 2.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Saquinavir mesylate
CHID: 23835 CASRN: 149845-06-7
SPID(S): Tox21_202533
M4ID: 12479719

HILL MODEL (in red):

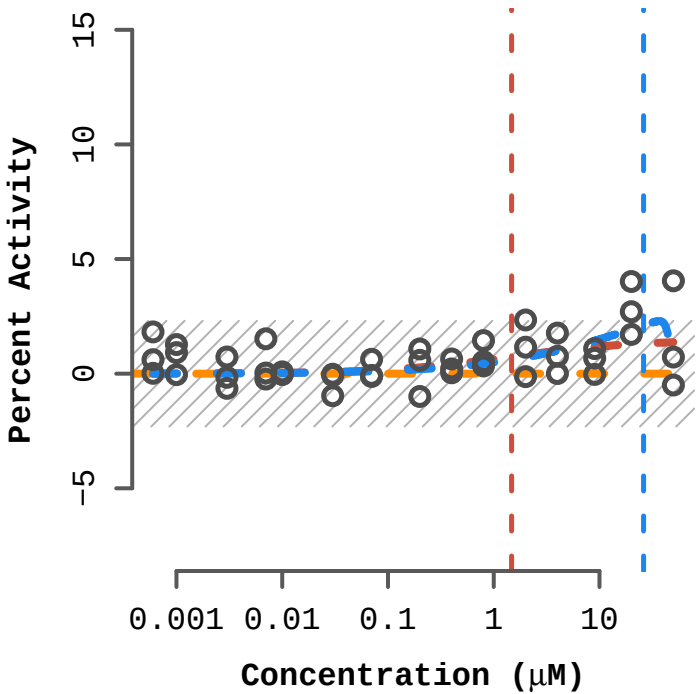
	tp	ga	gw
val:	1.22	−2.1	8
sd:	0.339	0.151	10.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.05	1.1	0.426	1.35	14.6
sd:	9.06	2.21	0.204	0.236	60.6

	CNST	HILL	GNLS
AIC:	215.47	210.2	196.15
PROB:	0	0	1
RMSE:	2.67	2.57	2.09

MAX_MEAN: 3.87 **MAX_MED:** 3.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium bromate
CHID: 23837 CASRN: 7789-38-0
SPID(S): Tox21_202534
M4ID: 12479718

HILL MODEL (in red):

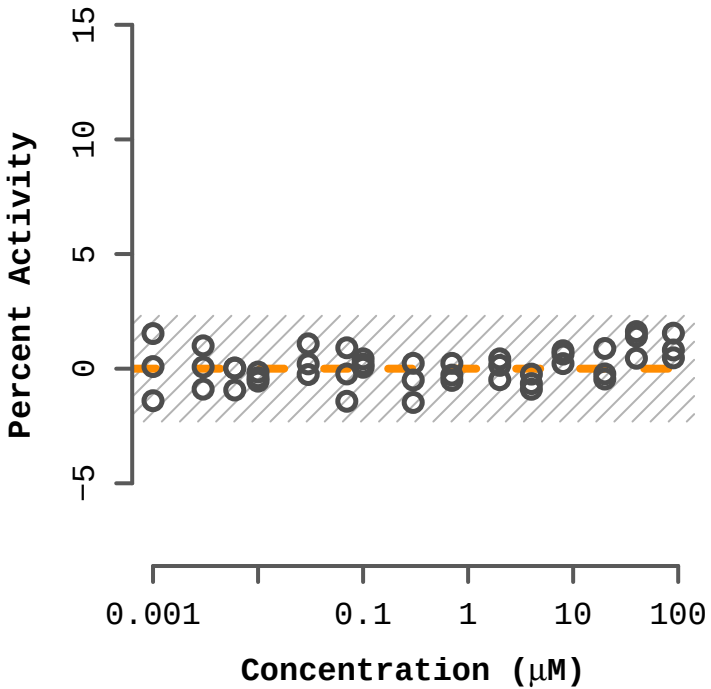
	tp	ga	gw
val:	1.47	0.169	0.745
sd:	1.49	1.62	1.04

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.21	1.42	0.62	1.67	18
sd:	6.55	1.68	0.264	0.0758	41.6

	CNST	HILL	GNLS
AIC:	142.42	129.65	130.01
PROB:	0	0.54	0.45
RMSE:	1.27	0.96	0.95

MAX_MEAN: 2.81 **MAX_MED:** 2.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

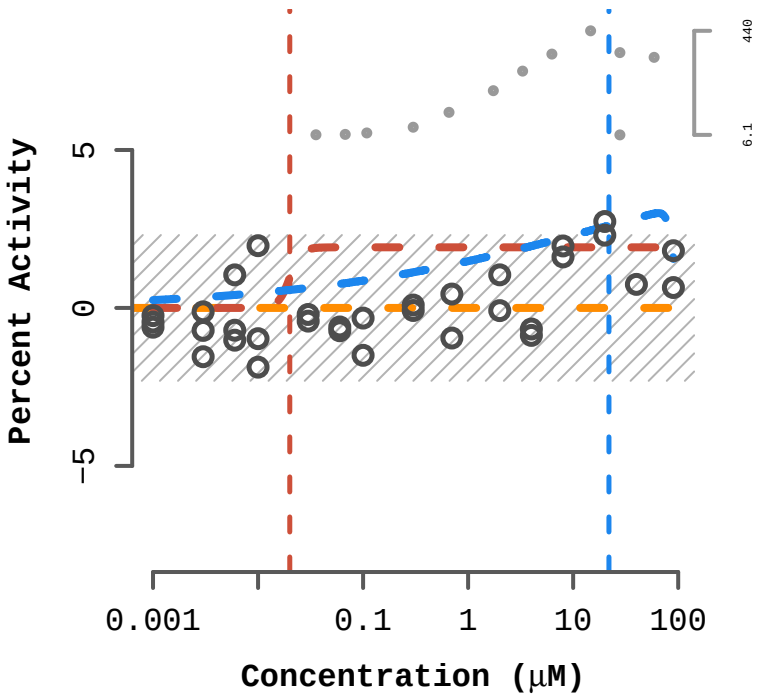
NAME: Acenaphthylene
CHID: 23845 CASRN: 208-96-8
SPID(S): Tox21_300587
M4ID: 12478546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 1.16 MAX_MED: 1.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acenaphthylene
CHID: 23845 CASRN: 208-96-8
SPID(S): Tox21_201825
M4ID: 12480427 BRK

HILL MODEL (in red):

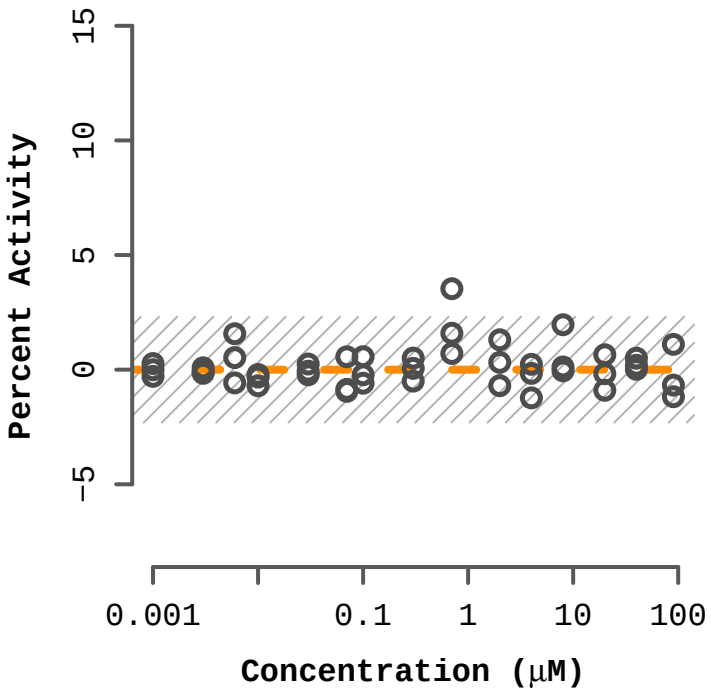
	tp	ga	gw
val:	1.92	-1.7	8
sd:	1.52	2.32	83.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.22	1.34	0.3	1.95	14.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	489.7	493.83	498.16
PROB:	0.88	0.11	0.01
RMSE:	121.16	120.43	120.35

MAX_MEAN: 148 MAX_MED: 6.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

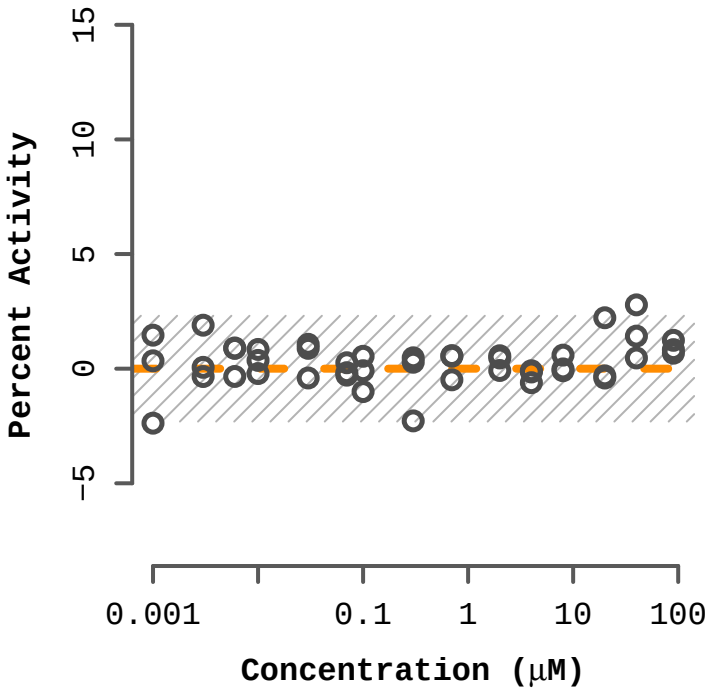
NAME: Acephate
CHID: 23846 CASRN: 30560-19-1
SPID(S): Tox21_300874
M4ID: 12478259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.94 MAX_MED: 1.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

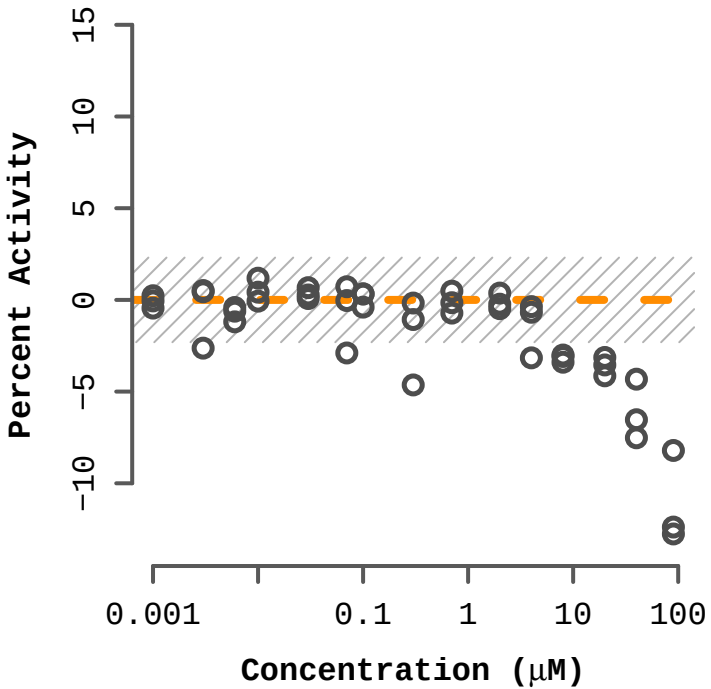
NAME: Acephate
CHID: 23846 CASRN: 30560-19-1
SPID(S): Tox21_202204
M4ID: 12480048

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.56 MAX_MED: 1.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

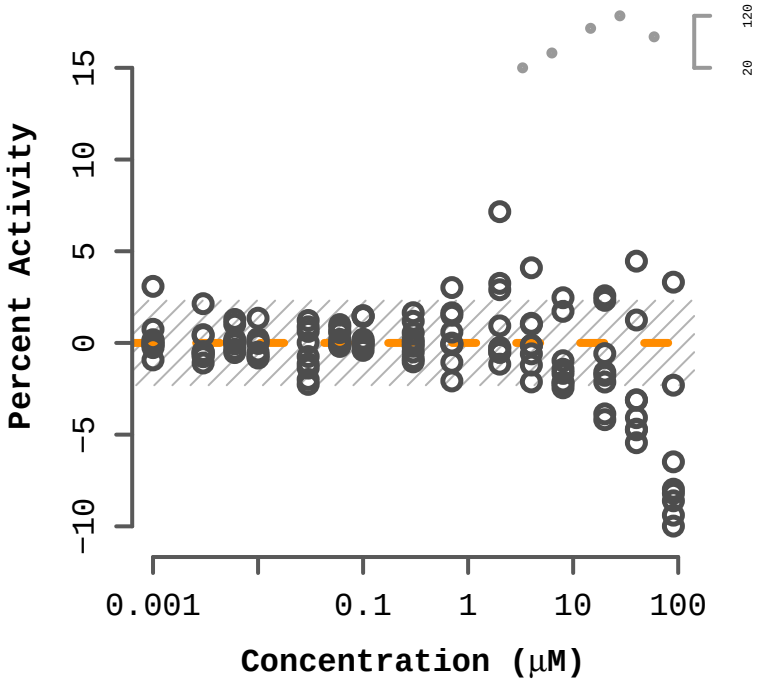
NAME: Acetochlor
CHID: 23848 **CASRN:** 34256-82-1
SPID(S): Tox21_300889
M4ID: 12478244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.07	NA	NA
PROB:	1	NA	NA
RMSE:	3.73	NA	NA

MAX_MEAN: 0.514 **MAX_MED:** 0.444 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

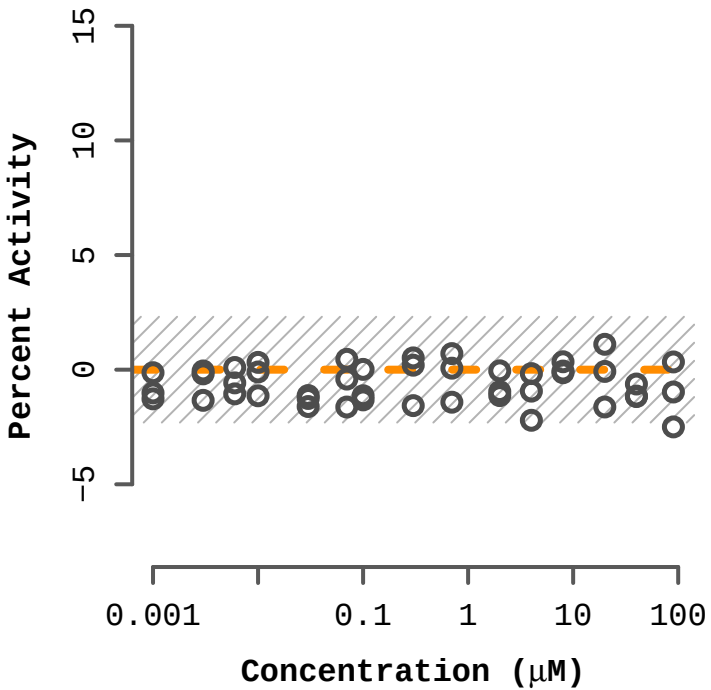
NAME: Acetochlor
CHID: 23848 **CASRN:** 34256-82-1
SPID(S): Tox21_202445
M4ID: 12479807 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	733.45	NA	NA
PROB:	1	NA	NA
RMSE:	16.22	NA	NA

MAX_MEAN: 11.6 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

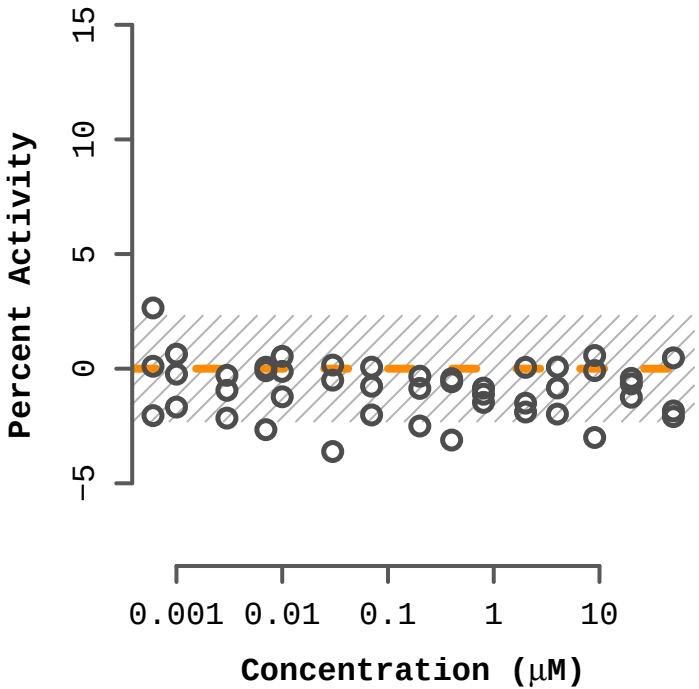
NAME: Acifluorfen-sodium
CHID: 23853 **CASRN:** 62476-59-9
SPID(S): Tox21_200391
M4ID: 12481861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.0521 **MAX_MED:** 0.196 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

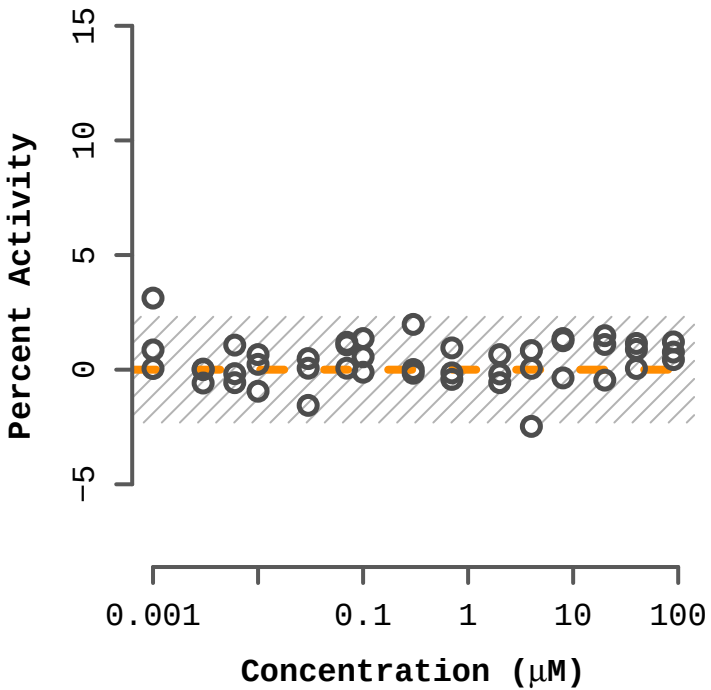
NAME: Acifluorfen-sodium
CHID: 23853 **CASRN:** 62476-59-9
SPID(S): Tox21_112903
M4ID: 12482883

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.237 **MAX_MED:** 0.106 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

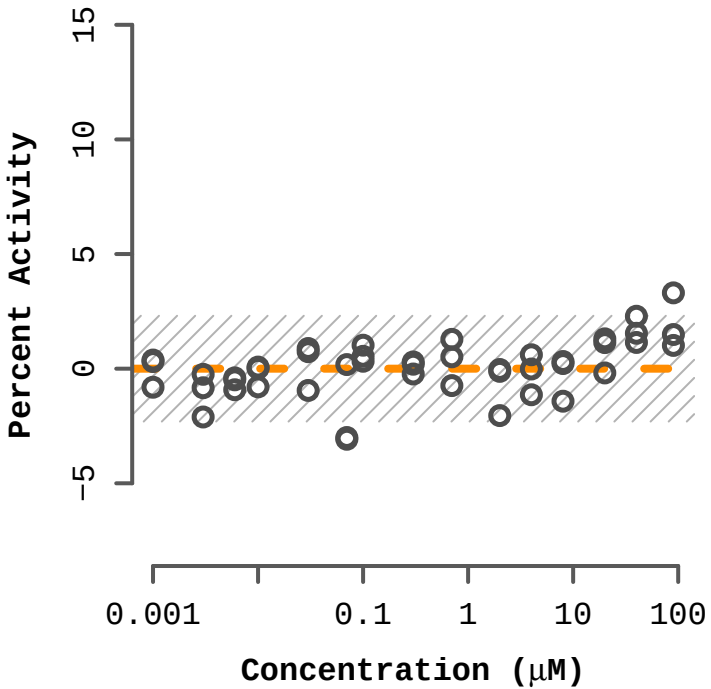
NAME: Aldoxycarb
CHID: 23862 **CASRN:** 1646-88-4
SPID(S): Tox21_303266
M4ID: 12475867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.25	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

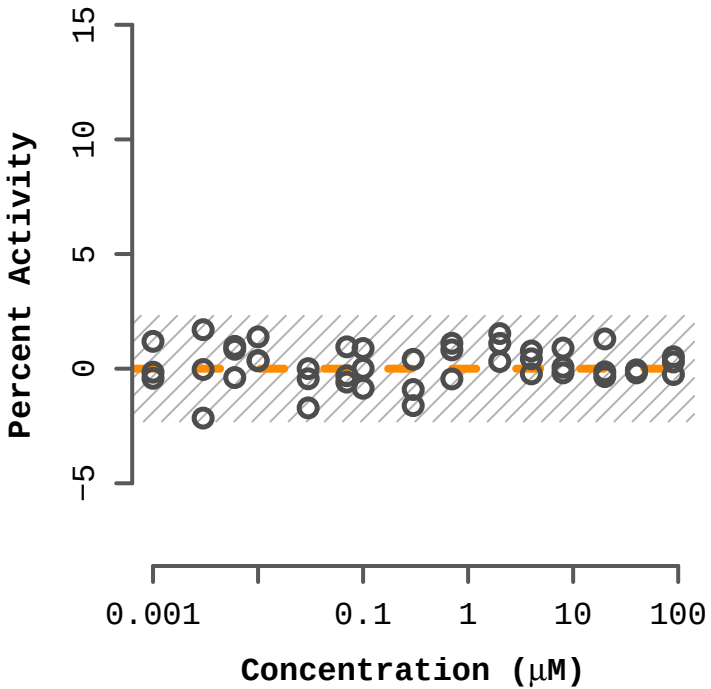
NAME: Aldoxycarb
CHID: 23862 **CASRN:** 1646-88-4
SPID(S): Tox21_201338
M4ID: 12480914

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

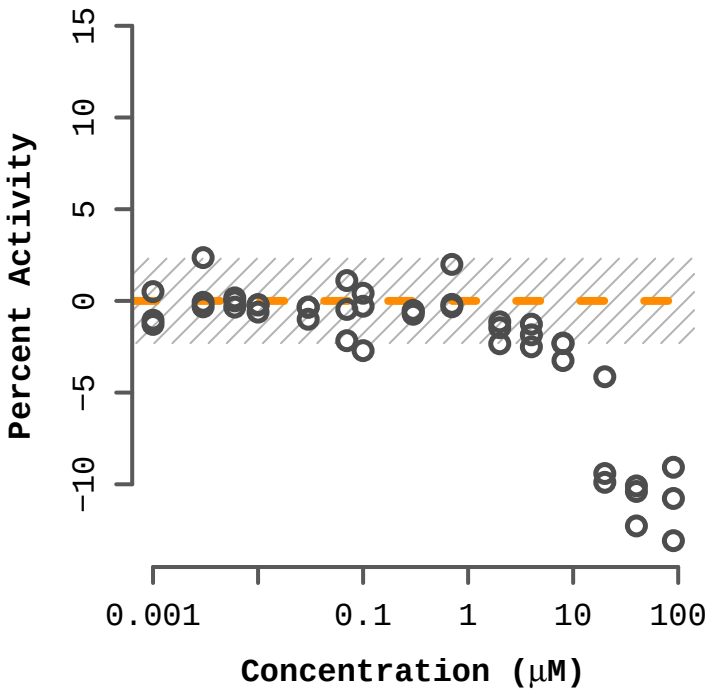
NAME: Metsulfuron-methyl
CHID: 23864 **CASRN:** 74223-64-6
SPID(S): Tox21_200856
M4ID: 12481396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.984 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

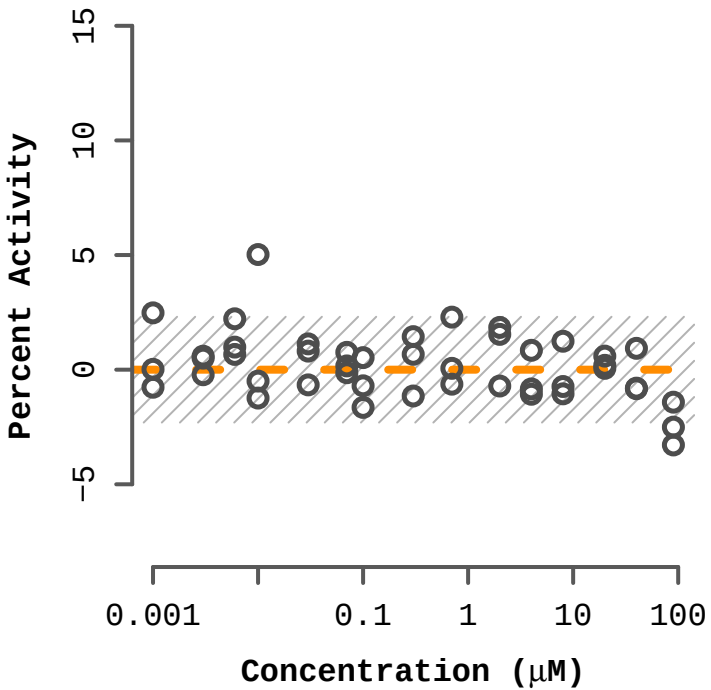
NAME: Hydramethylnon
CHID: 23868 **CASRN:** 67485-29-4
SPID(S): Tox21_303161
M4ID: 12475972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	256.13	NA	NA
PROB:	1	NA	NA
RMSE:	4.72	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 0.00139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

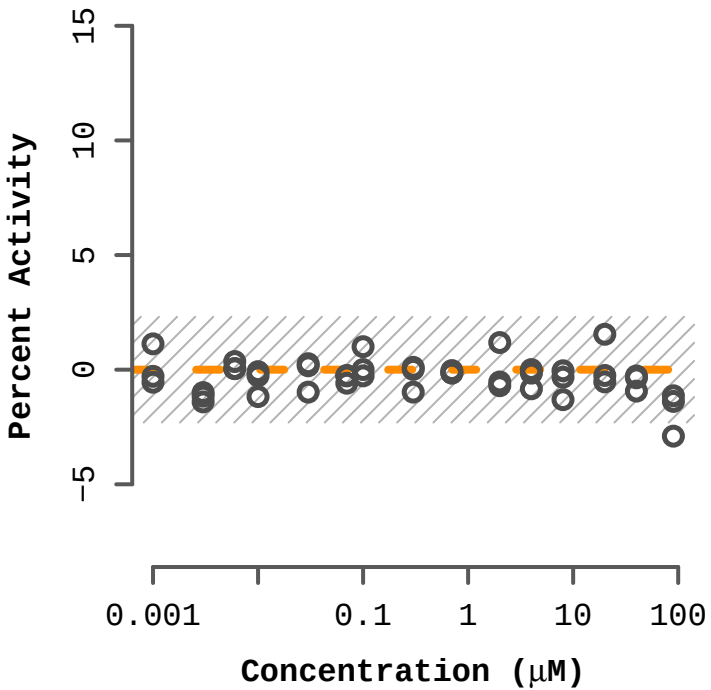
NAME: Ametryn
CHID: 23869 **CASRN:** 834-12-8
SPID(S): Tox21_300666
M4ID: 12478467

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

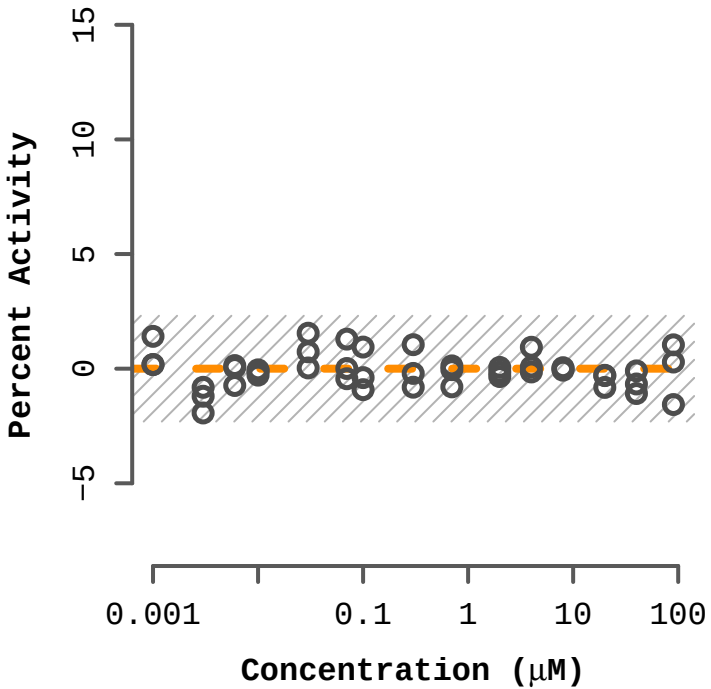
NAME: Ametryn
CHID: 23869 **CASRN:** 834-12-8
SPID(S): Tox21_201414
M4ID: 12480838

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.254 **MAX_MED:** 0.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

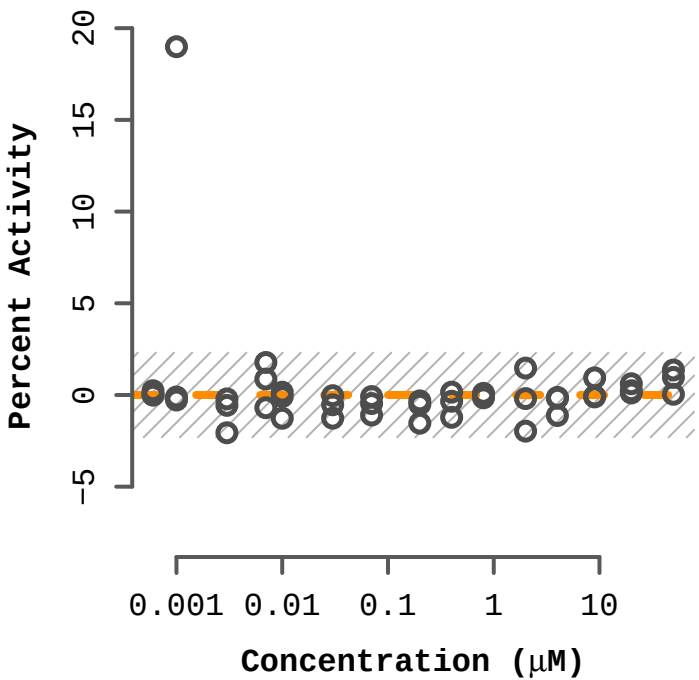
NAME: 4-Aminopyridine
CHID: 23870 **CASRN:** 504-24-5
SPID(S): Tox21_200793
M4ID: 12481459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.773 **MAX_MED:** 0.738 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

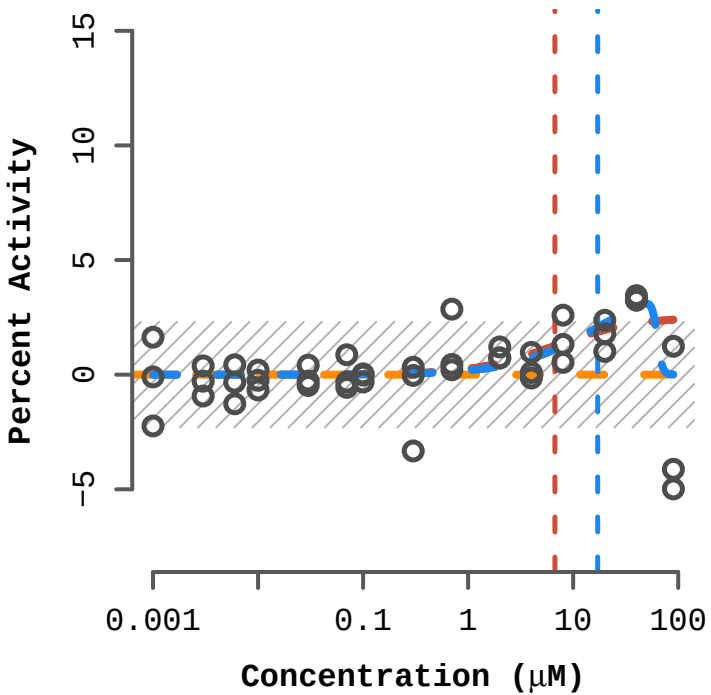
NAME: 4-Aminopyridine
CHID: 23870 CASRN: 504-24-5
SPID(S): Tox21_110065_1
M4ID: 12484685

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.95	NA	NA

MAX_MEAN: 6.2 MAX_MED: 0.961 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amitraz
CHID: 23871 CASRN: 33089-61-1
SPID(S): Tox21_300930
M4ID: 12478203

HILL MODEL (in red):

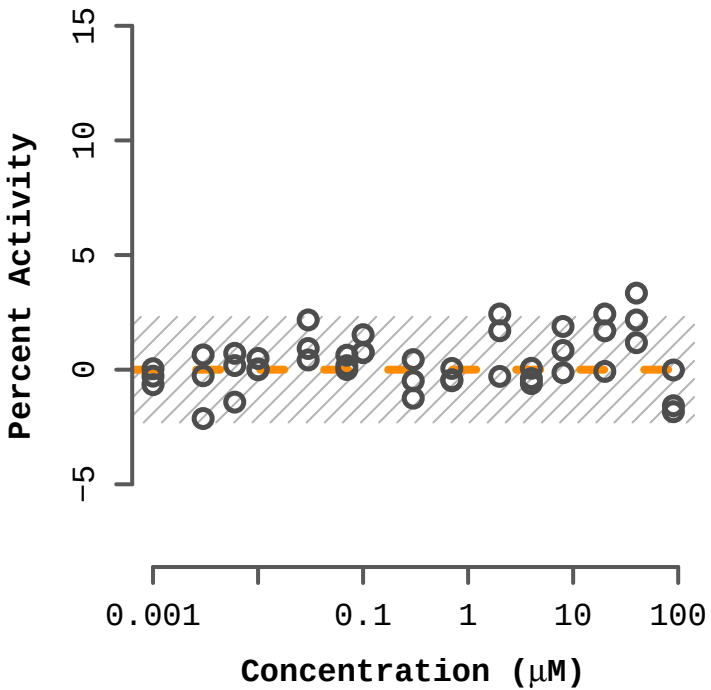
	tp	ga	gw
val:	2.52	0.826	1.15
sd:	0.84	0.344	0.661

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.14	1.23	1.08	1.8	18
sd:	1.48	0.337	0.421	0.39	39.5

	CNST	HILL	GNLS
AIC:	173.25	156.84	149.07
PROB:	0	0.02	0.98
RMSE:	1.71	1.76	1.35

MAX_MEAN: 3.32 MAX_MED: 3.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

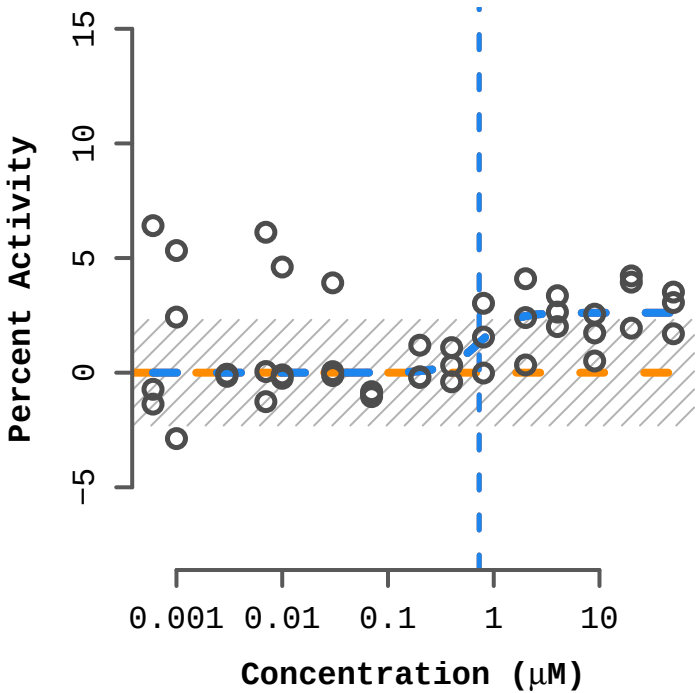
NAME: Amitraz
CHID: 23871 **CASRN:** 33089-61-1
SPID(S): Tox21_201357
M4ID: 12480895

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amitraz
CHID: 23871 **CASRN:** 33089-61-1
SPID(S): Tox21_111299_1
M4ID: 12483782

HILL MODEL (in red):

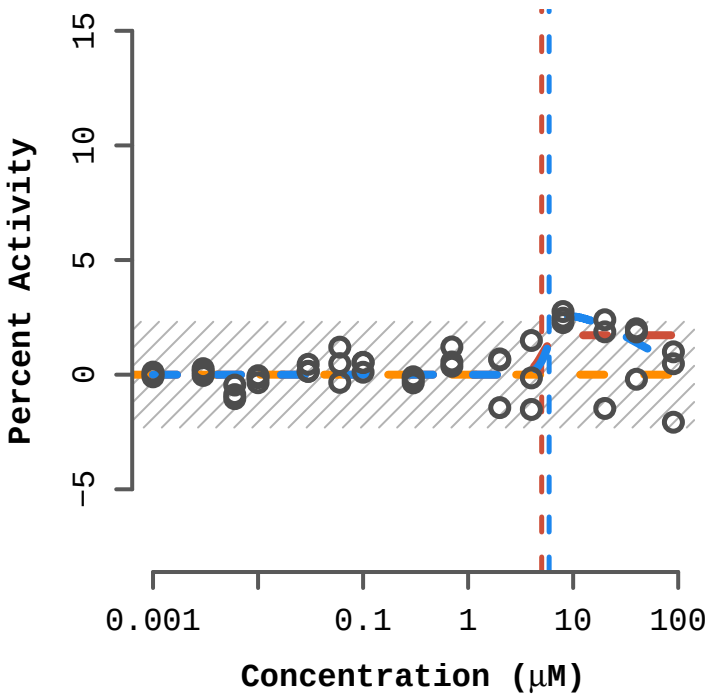
	tp	ga	gw
val:	2.61	−0.138	2.82
sd:	0.401	0.199	3.41

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.61	−0.138	2.82	3.67	3.6
sd:	0.401	0.199	3.41	1220	2180

	CNST	HILL	GNLS
AIC:	214.92	189.12	193.12
PROB:	0	0.88	0.12
RMSE:	2.56	2.06	2.06

MAX_MEAN: 3.37 **MAX_MED:** 3.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ammonium sulfamate
CHID: 23875 CASRN: 7773-06-0
SPID(S): Tox21_303063
M4ID: 12476070

HILL MODEL (in red):

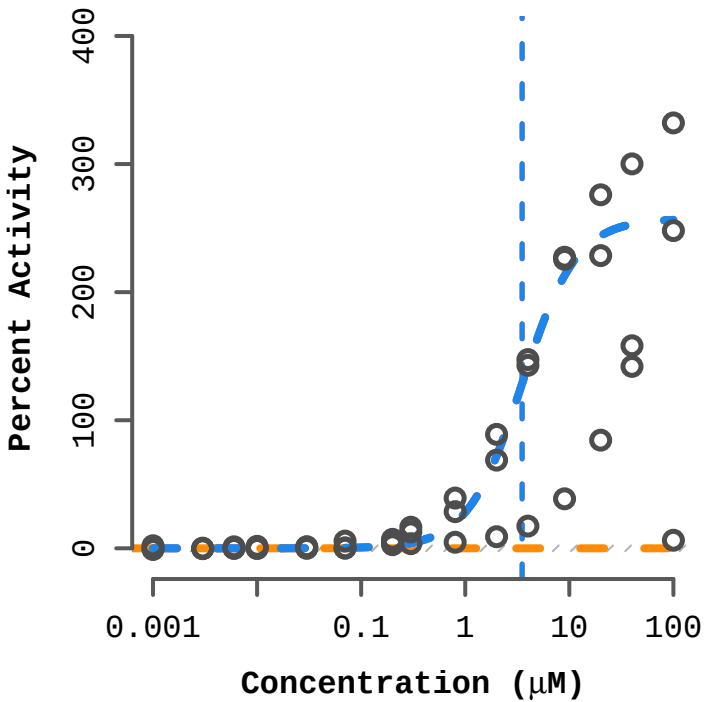
	tp	ga	gw
val:	1.72	0.7	8
sd:	0.294	0.0882	4.64

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.92	0.771	8	1.58	1.52
sd:	2.02	0.146	6.47	0.538	1.6

	CNST	HILL	GNLS
AIC:	140.44	127.57	118.99
PROB:	0	0.01	0.99
RMSE:	1.13	1.03	0.92

MAX_MEAN: 2.5 **MAX_MED:** 2.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ammonium sulfamate
CHID: 23875 CASRN: 7773-06-0
SPID(S): Tox21_201674
M4ID: 12480578

HILL MODEL (in red):

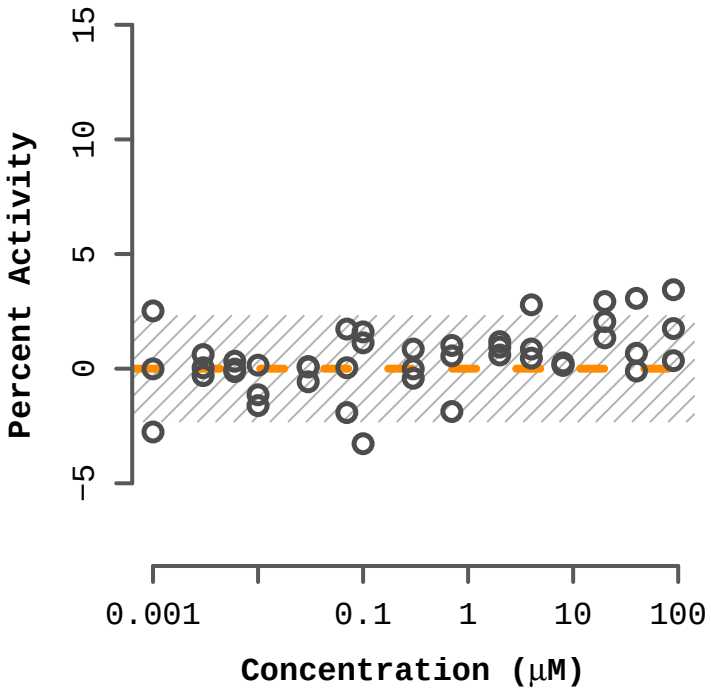
	tp	ga	gw
val:	257	0.547	1.67
sd:	18.8	0.0614	0.334

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	257	0.547	1.67	2.66	17.9
sd:	18.8	0.0614	0.334	14900	387000

	CNST	HILL	GNLS
AIC:	545.37	472.08	476.08
PROB:	0	0.88	0.12
RMSE:	115.95	61.5	61.5

MAX_MEAN: 200 MAX_MED: 248 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

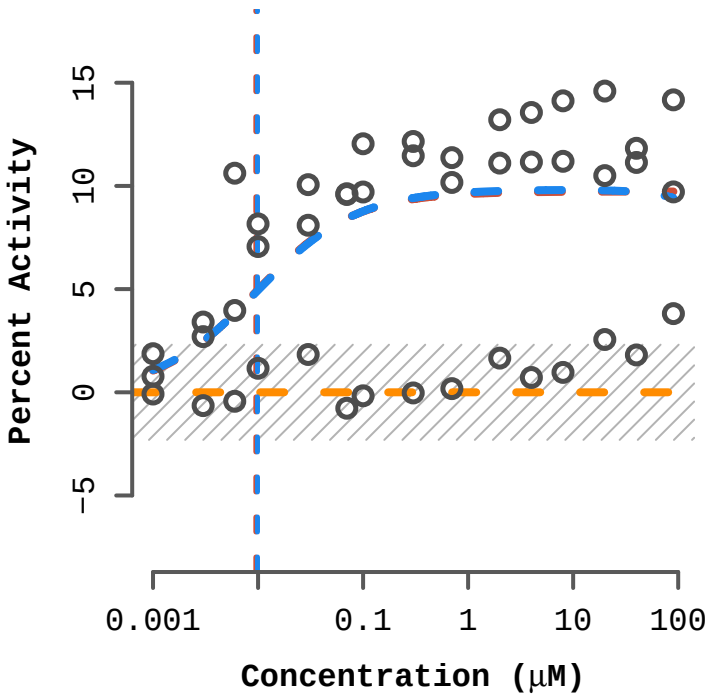
NAME: 2-Anisidine
CHID: 23877 **CASRN:** 90-04-0
SPID(S): Tox21_300053
M4ID: 12479077

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Anisidine
CHID: 23877 CASRN: 90-04-0
SPID(S): Tox21_201460
M4ID: 12480792

HILL MODEL (in red):

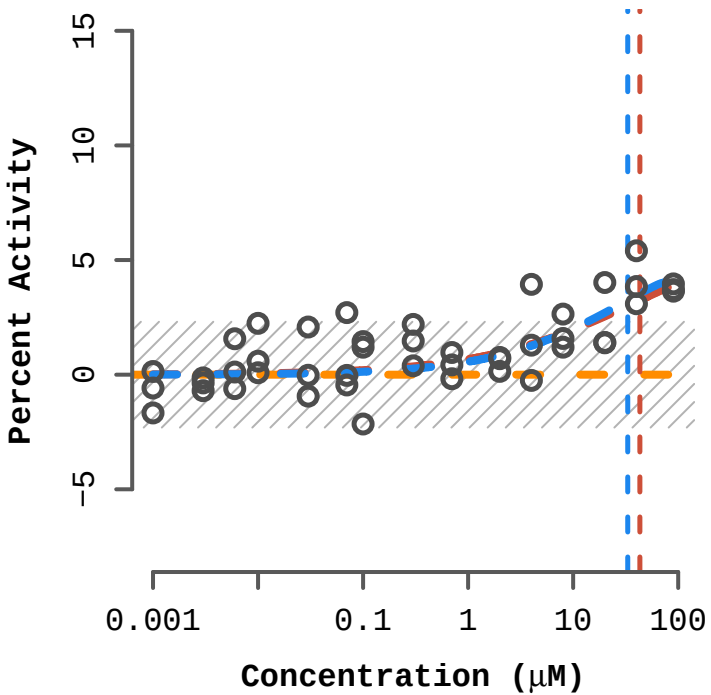
	tp	ga	gw
val:	9.73	−2.02	0.937
sd:	1.16	0.311	0.562

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.83	−2.01	0.913	2.8	1.6
sd:	1.48	0.345	0.58	7.29	13.3

	CNST	HILL	GNLS
AIC:	327.85	276.85	280.83
PROB:	0	0.88	0.12
RMSE:	8.46	4.69	4.69

MAX_MEAN: 9.23 MAX_MED: 11.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Anthracene
CHID: 23878 **CASRN:** 120-12-7
SPID(S): Tox21_300014
M4ID: 12479116

HILL MODEL (in red):

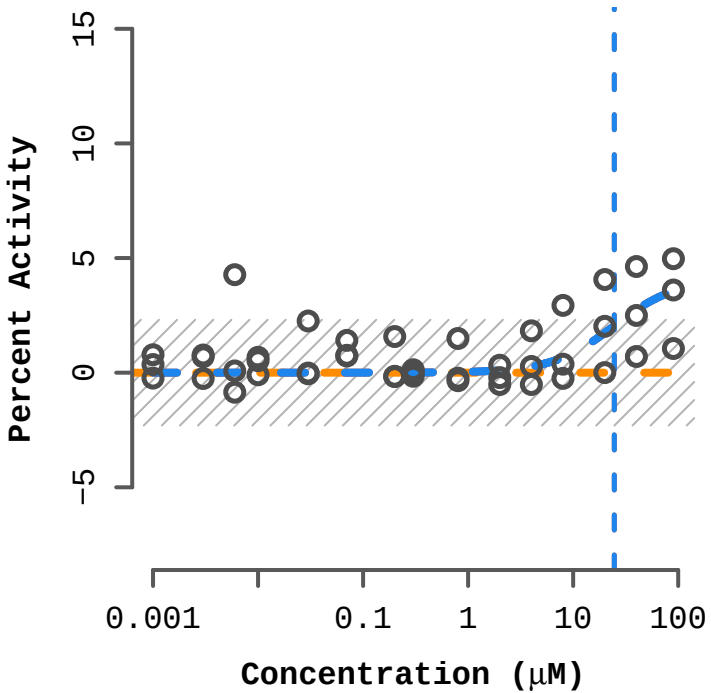
	tp	ga	gw
val:	6.49	1.64	0.571
sd:	4.37	1.09	0.289

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.49	1.52	0.673	2.04	10
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	193.94	148.49	152.15
PROB:	0	0.86	0.14
RMSE:	2.04	1.14	1.14

MAX_MEAN: 4.12 **MAX_MED:** 3.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Anthracene
CHID: 23878 **CASRN:** 120-12-7
SPID(S): Tox21_202226
M4ID: 12480026

HILL MODEL (in red):

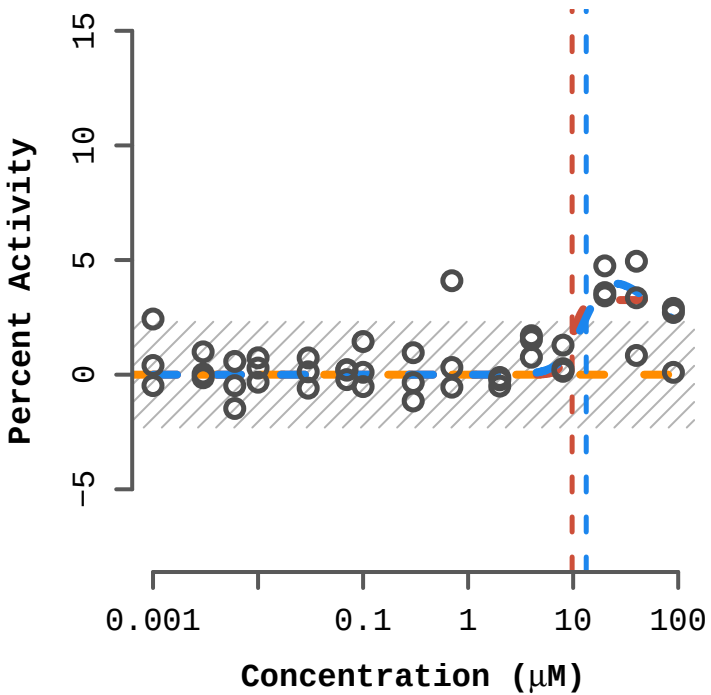
	tp	ga	gw
val:	4.09	1.39	1.46
sd:	2.23	0.489	1.14

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.09	1.39	1.46	2.88	8.31
sd:	2.23	0.489	1.14	1630	14600

	CNST	HILL	GNLS
AIC:	169.55	150.17	154.17
PROB:	0	0.88	0.12
RMSE:	1.74	1.24	1.24

MAX_MEAN: 3.21 **MAX_MED:** 3.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clofentezine
CHID: 23881 CASRN: 74115-24-5
SPID(S): Tox21_300904
M4ID: 12478229

HILL MODEL (in red):

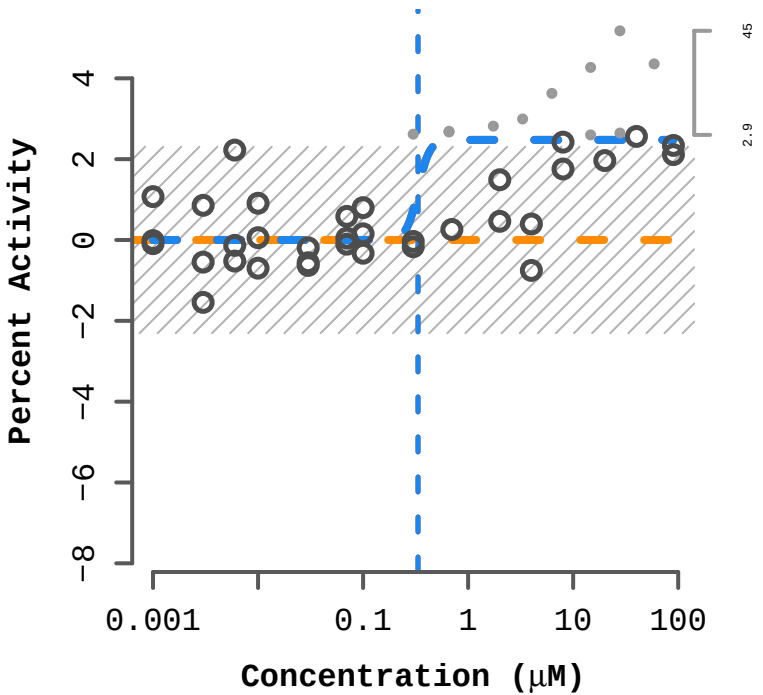
	tp	ga	gw
val:	3.25	0.99	8
sd:	0.349	0.0892	7.73

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.94	1.12	3.75	1.8	1.08
sd:	7.59	0.199	2.92	1.06	1.49

	CNST	HILL	GNLS
AIC:	173.83	142.01	141.39
PROB:	0	0.42	0.58
RMSE:	1.77	1.17	1.12

MAX_MEAN: 3.92 MAX_MED: 3.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clofentezine
CHID: 23881 **CASRN:** 74115-24-5
SPID(S): Tox21_201688
M4ID: 12480564 **BRK**

HILL MODEL (in red):

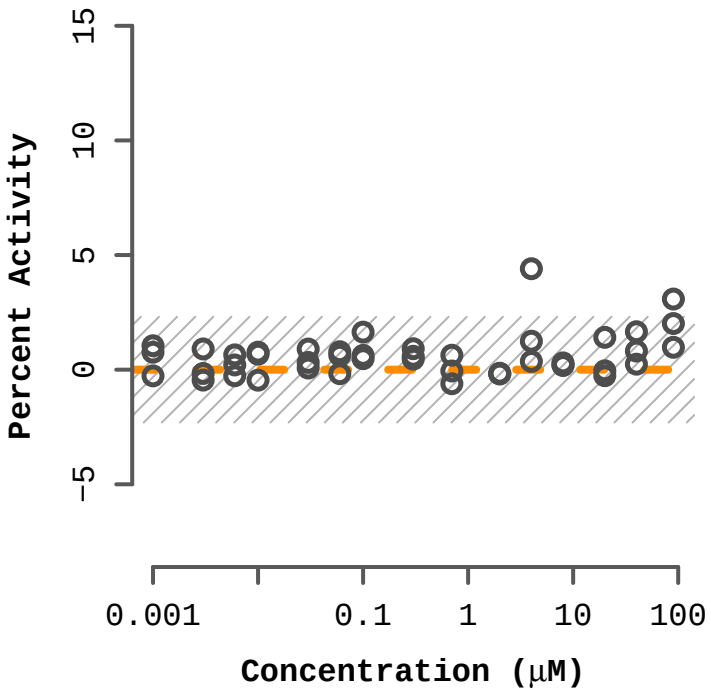
	tp	ga	gw
val:	2.48	−0.477	8
sd:	0.475	0.149	19.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.48	−0.477	8	3.72	3.08
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	276.7	260.19	264.19
PROB:	0	0.88	0.12
RMSE:	10.02	9.18	9.18

MAX_MEAN: 17 **MAX_MED:** 4.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

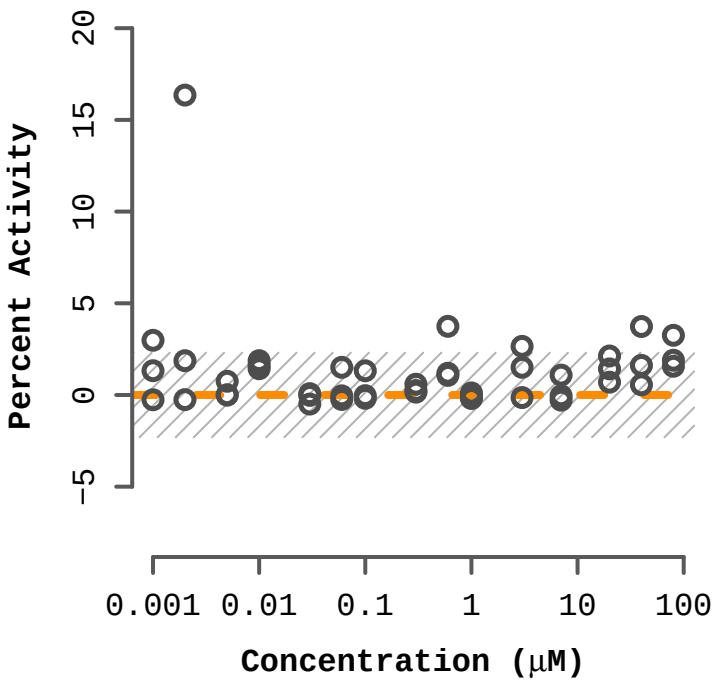
NAME: Aroclor 1016
CHID: 23883 **CASRN:** 12674-11-2
SPID(S): Tox21_202248
M4ID: 12480004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

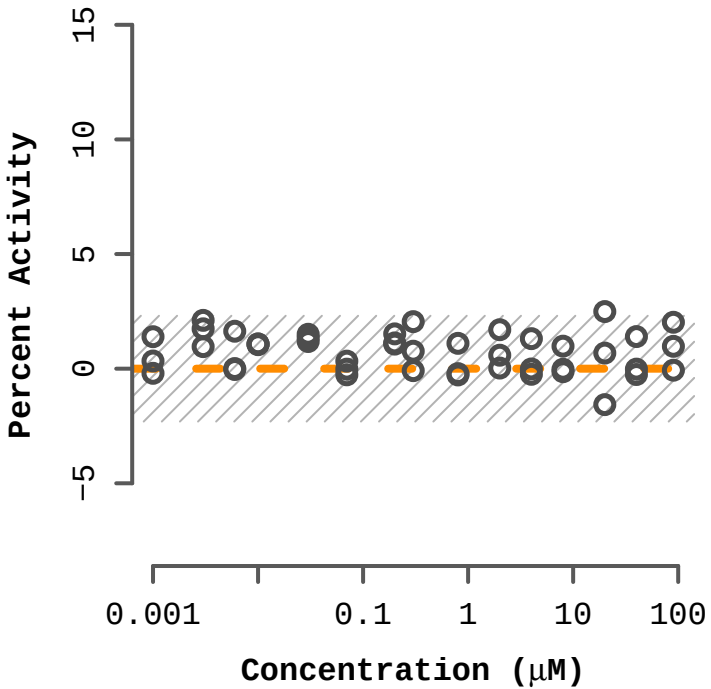
NAME: Quizalofop-ethyl
CHID: 23889 **CASRN:** 76578-14-8
SPID(S): Tox21_301040
M4ID: 12478093

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.76	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 5.99 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

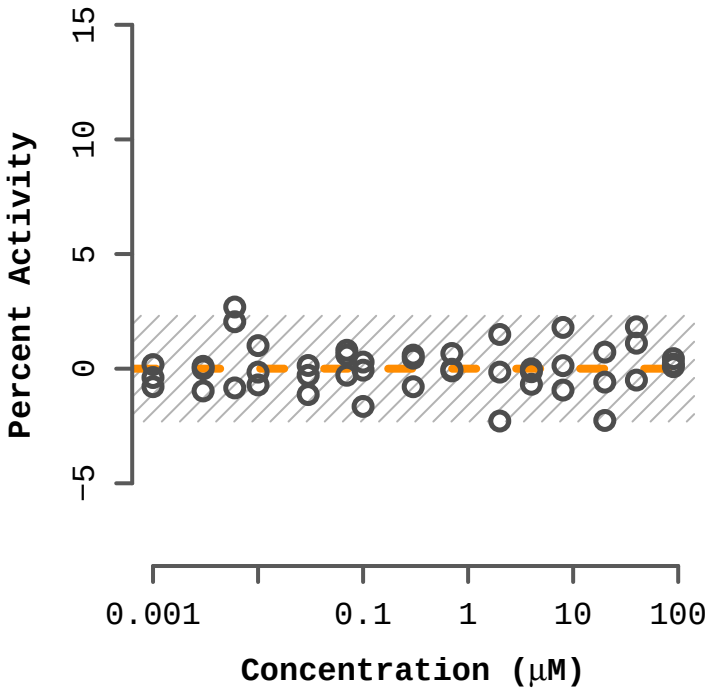
NAME: Quizalofop-ethyl
CHID: 23889 **CASRN:** 76578-14-8
SPID(S): Tox21_202007
M4ID: 12480245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

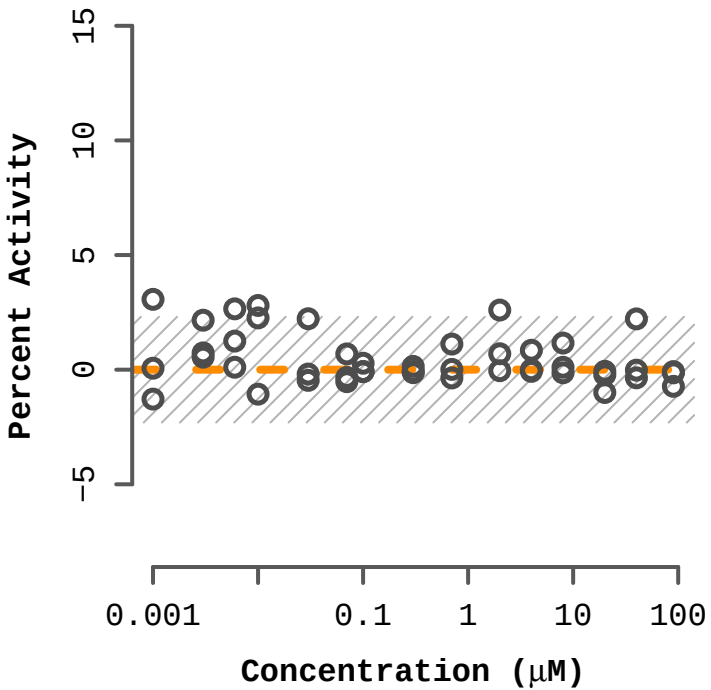
NAME: Asulam
CHID: 23890 **CASRN:** 3337-71-1
SPID(S): Tox21_300851
M4ID: 12478282

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.6	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

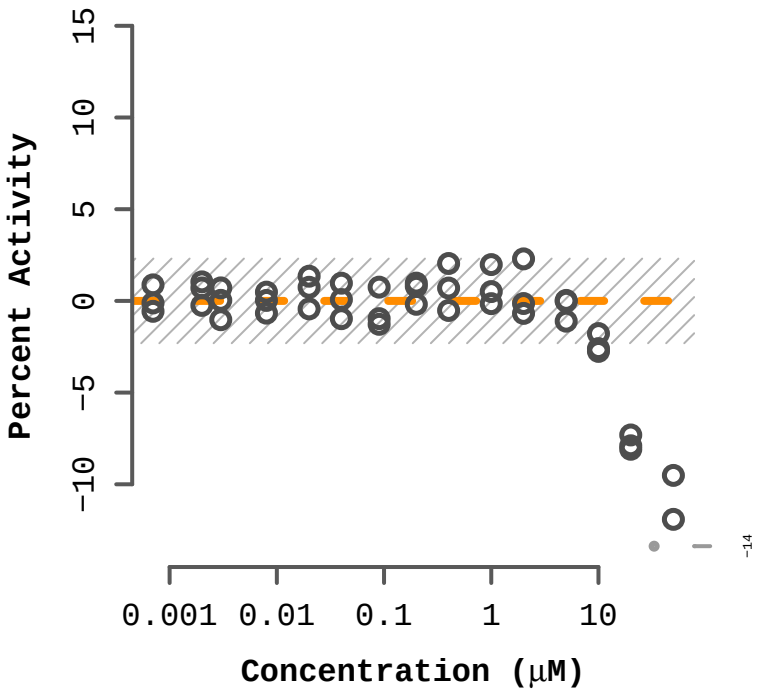
NAME: Asulam
CHID: 23890 **CASRN:** 3337-71-1
SPID(S): Tox21_201642
M4ID: 12480610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

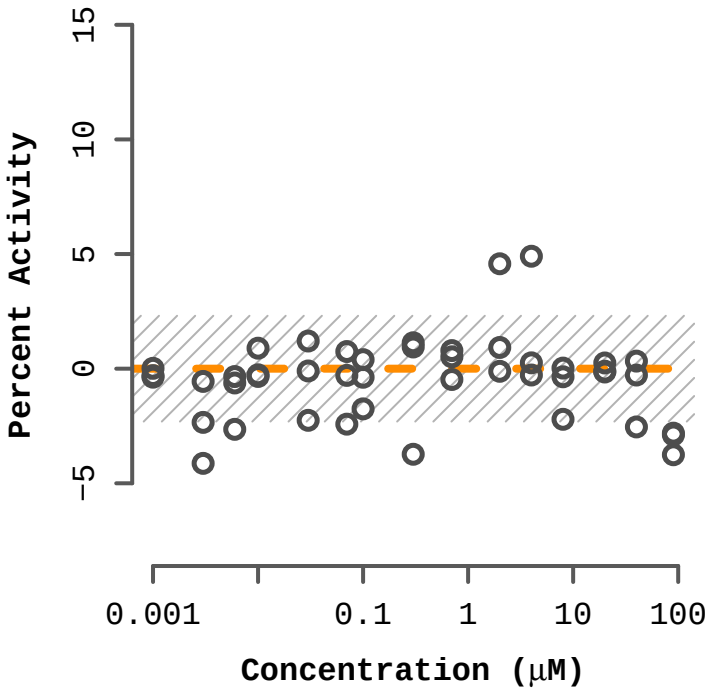
NAME: Abamectin
CHID: 23892 **CASRN:** 71751-41-2
SPID(S): Tox21_300841
M4ID: 12478292 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.55	NA	NA
PROB:	1	NA	NA
RMSE:	3.85	NA	NA

MAX_MEAN: 0.782 **MAX_MED:** 0.797 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

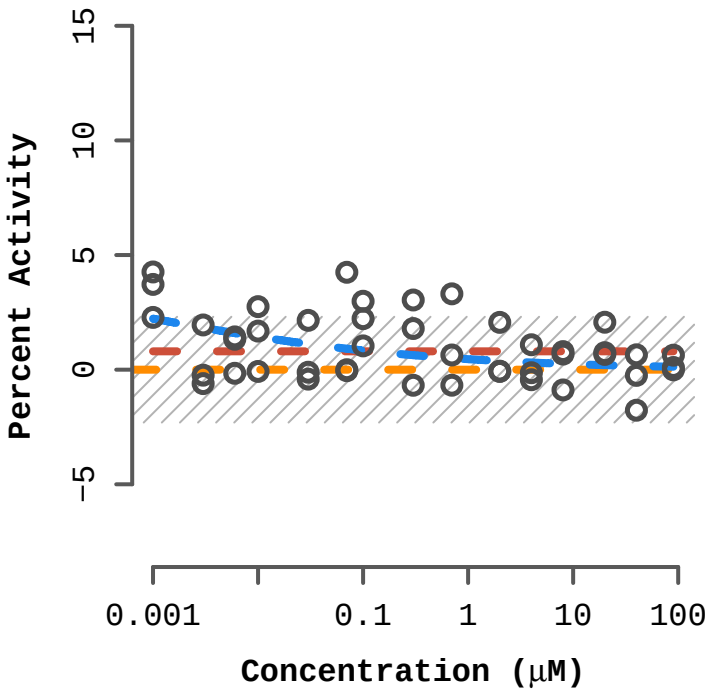
NAME: Triadimefon
CHID: 23897 **CASRN:** 43121-43-3
SPID(S): Tox21_300886
M4ID: 12478247

HILL MODEL: Not applicable.

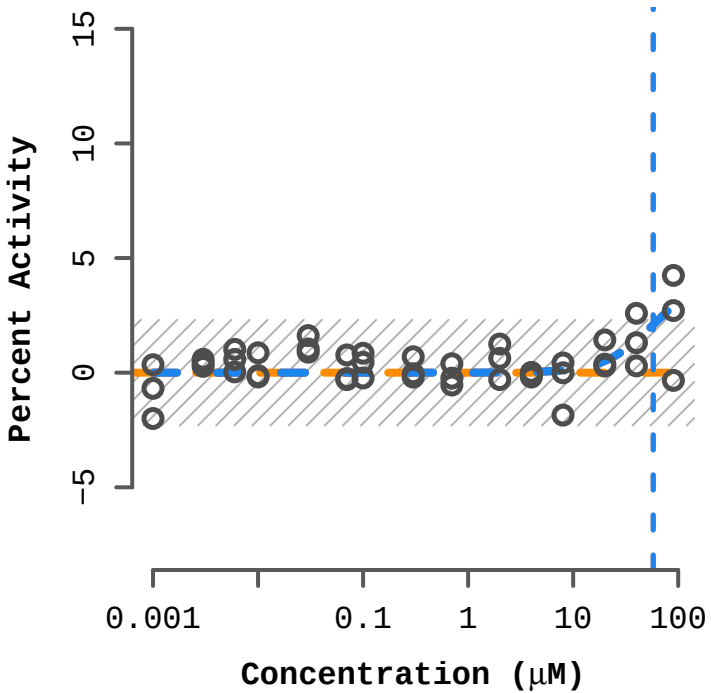
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

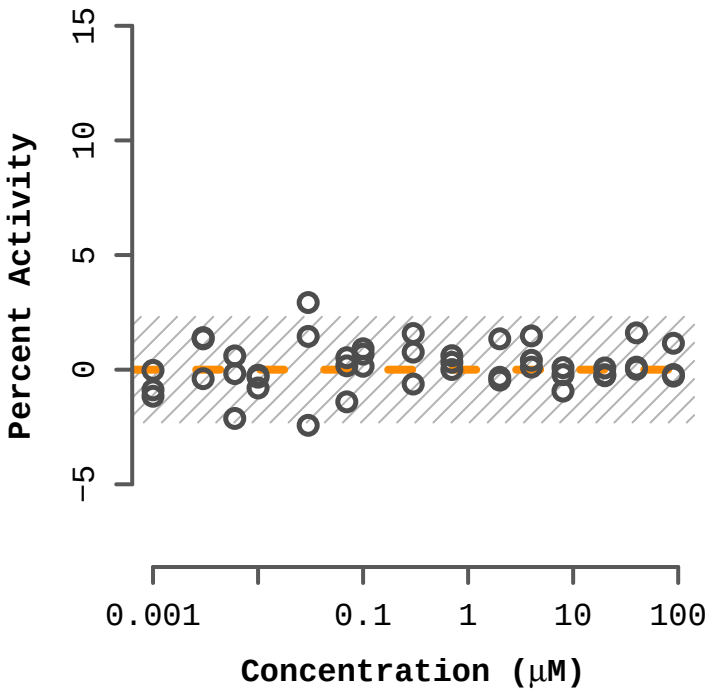
MAX_MEAN: 1.8 **MAX_MED:** 0.947 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benfluralin
CHID:    23899   CASRN: 1861-40-1
SPID(S): Tox21_300774
M4ID:    12478359

HILL MODEL (in red):
      tp       ga       gw
val:  0.8      -5       3.62
sd:   0.221    966      1750

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.01     -4.39    5.19     -3.32    0.3
sd:   12.8     444      1660     5.81     0.189

      CNST        HILL        GNLS
AIC:  178.77      171.63      169.4
PROB: 0.01        0.25        0.75
RMSE: 1.73        1.45        1.34

MAX_MEAN: 3.42      MAX_MED: 3.72      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benfluralin
CHID:    23899   CASRN: 1861-40-1
SPID(S): Tox21_202270
M4ID:    12479982

HILL MODEL (in red):
      tp       ga       gw
val:  4.18     1.76     1.85
sd:   4.44     0.595    1.55

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.18     1.76     1.85     3.12     5.63
sd:   4.44     0.595    1.55     1270     6200

      CNST        HILL        GNLS
AIC:  129.87      120.96      124.96
PROB: 0.01        0.87        0.12
RMSE: 1.12        0.9         0.9

MAX_MEAN: 2.21      MAX_MED: 2.71      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

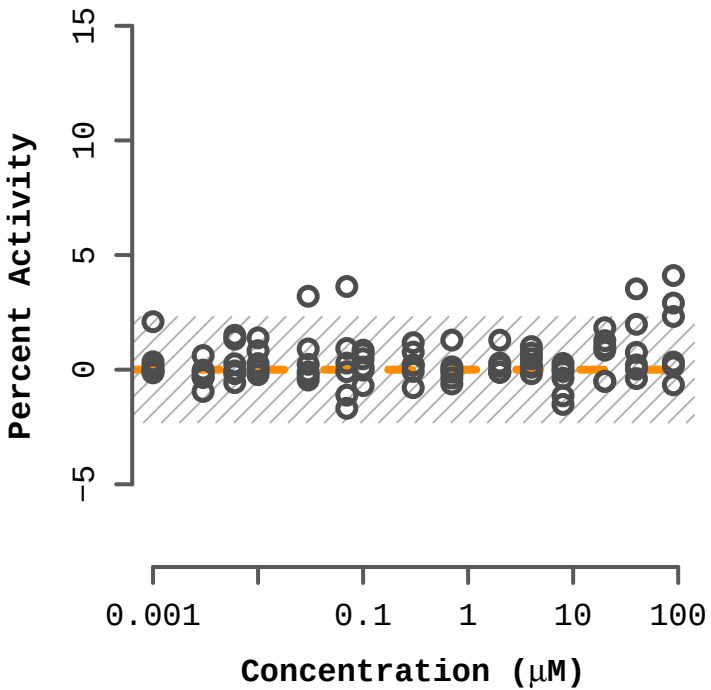
NAME: Benomyl
CHID: 23900 **CASRN:** 17804-35-2
SPID(S): Tox21_301170
M4ID: 12477963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.784 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

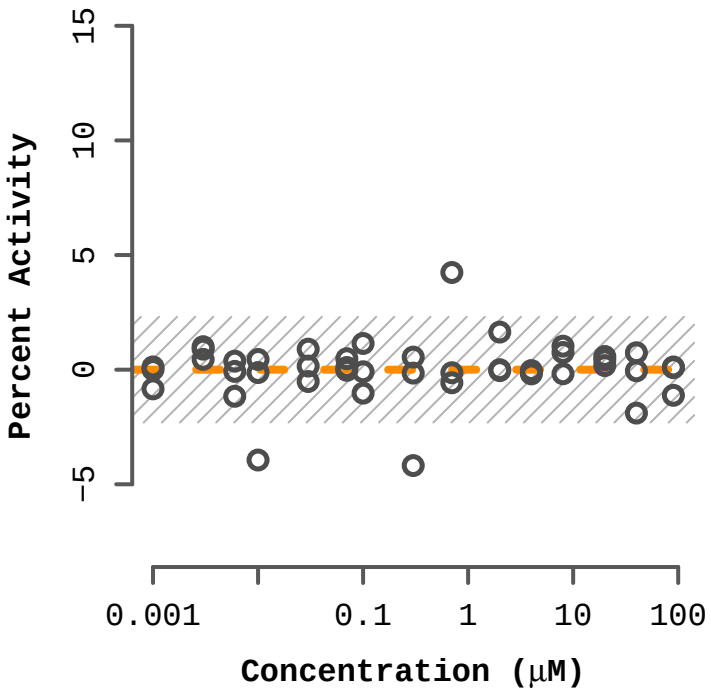
NAME: Benomyl
CHID: 23900 CASRN: 17804-35-2
SPID(S): Tox21_201234
M4ID: 12481018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.53 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

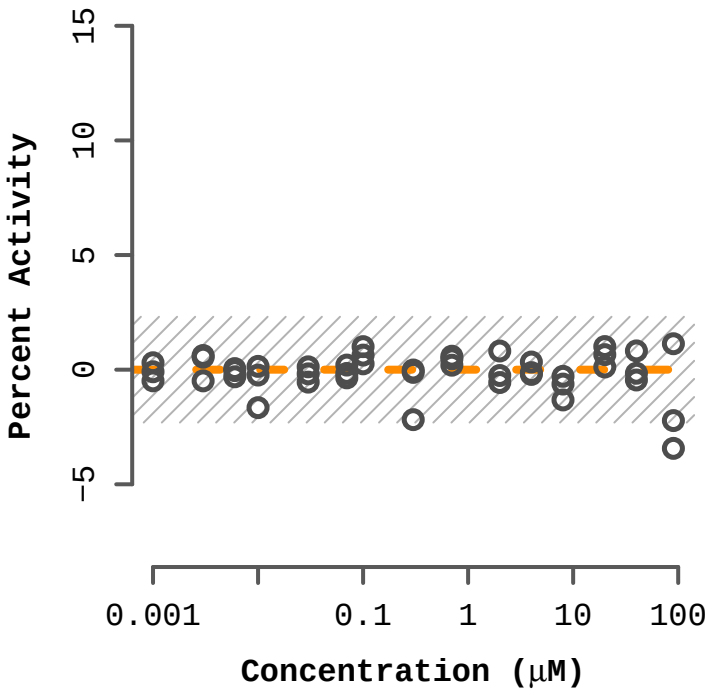
NAME: Bentazone
CHID: 23901 **CASRN:** 25057-89-0
SPID(S): Tox21_300742
M4ID: 12478391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.896 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

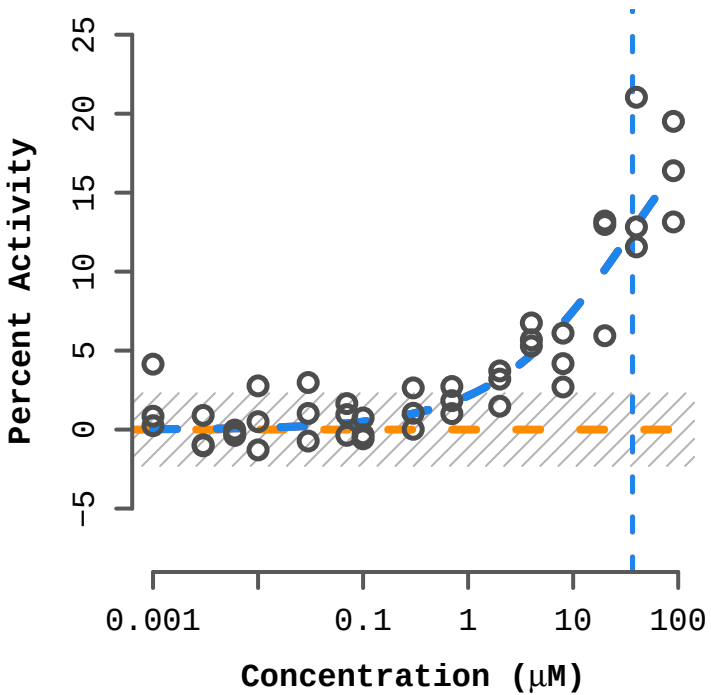
NAME: Bentazone
CHID: 23901 **CASRN:** 25057-89-0
SPID(S): Tox21_201951
M4ID: 12480301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.634 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benz(a)anthracene
CHID: 23902 CASRN: 56-55-3
SPID(S): Tox21_300499
M4ID: 12478633

HILL MODEL (in red):

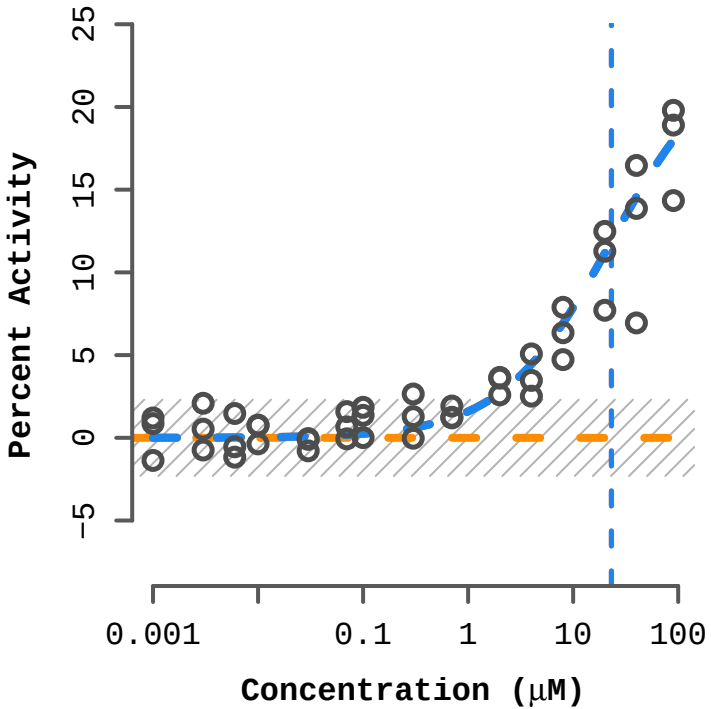
	tp	ga	gw
val:	25.2	1.56	0.661
sd:	9.38	0.53	0.149

GAIN-LOSS MODEL (in blue):

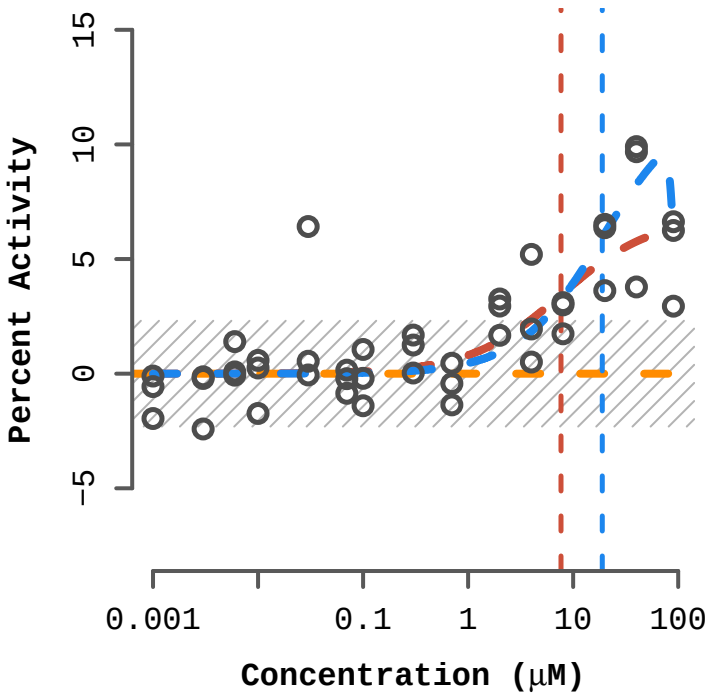
	tp	ga	gw	la	lw
val:	25.2	1.57	0.661	3.6	5.24
sd:	9.35	0.529	0.149	4950	15800

	CNST	HILL	GNLS
AIC:	294.25	196.5	200.5
PROB:	0	0.88	0.12
RMSE:	7	2.13	2.13

MAX_MEAN: 16.4 MAX_MED: 16.4 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benz(a)anthracene
CHID:    23902   CASRN: 56-55-3
SPID(S): Tox21_202060
M4ID:    12480192

HILL MODEL (in red):
      tp       ga       gw
val:  23.8     1.36     0.838
sd:   3.66     0.178    0.114

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  23.8     1.36     0.838    3.95     4.12
sd:   3.66     0.178    0.114    1080     2240

      CNST        HILL        GNLS
AIC:  290.11      171.86      175.86
PROB: 0           0.88        0.12
RMSE: 6.75        1.72        1.72

MAX_MEAN: 17.7      MAX_MED: 18.9      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzo(b)fluoranthene
CHID: 23907 CASRN: 205-99-2
SPID(S): Tox21_300289
M4ID: 12478841

HILL MODEL (in red):

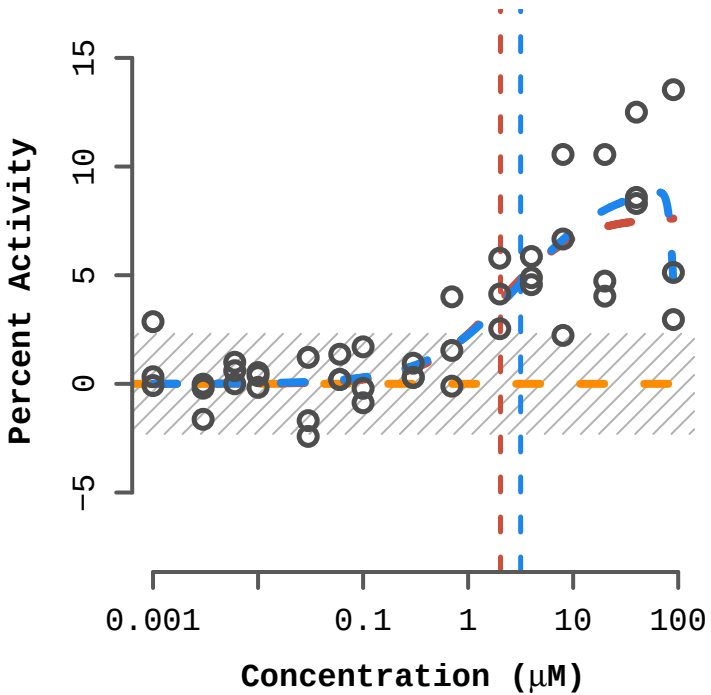
	tp	ga	gw
val:	6.88	0.884	0.994
sd:	1.29	0.243	0.38

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.9	1.28	1.09	1.96	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	235.62	181.98	181.13
PROB:	0	0.4	0.6
RMSE:	3.45	1.79	1.73

MAX_MEAN: 7.79 MAX_MED: 9.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzo(b)fluoranthene
CHID: 23907 CASRN: 205-99-2
SPID(S): Tox21_202381
M4ID: 12479871

HILL MODEL (in red):

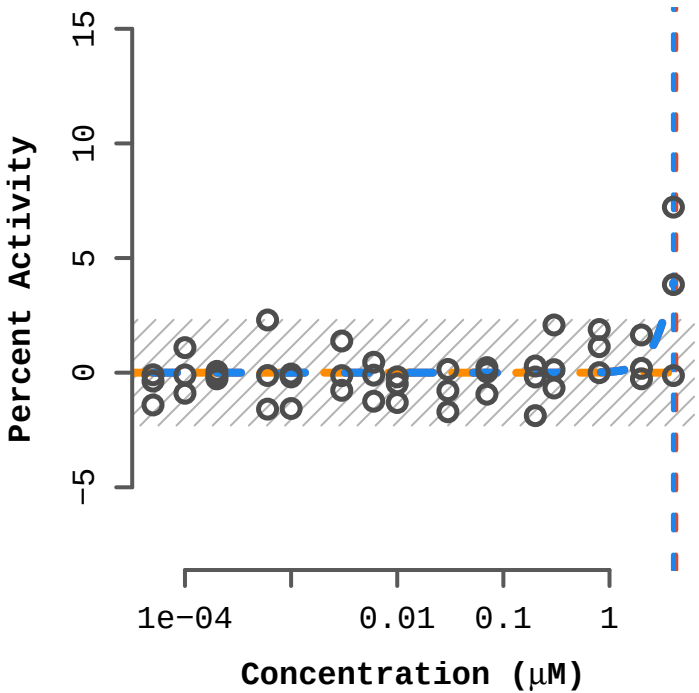
	tp	ga	gw
val:	7.69	0.308	1.2
sd:	1.45	0.21	0.447

GAIN-LOSS MODEL (in blue):

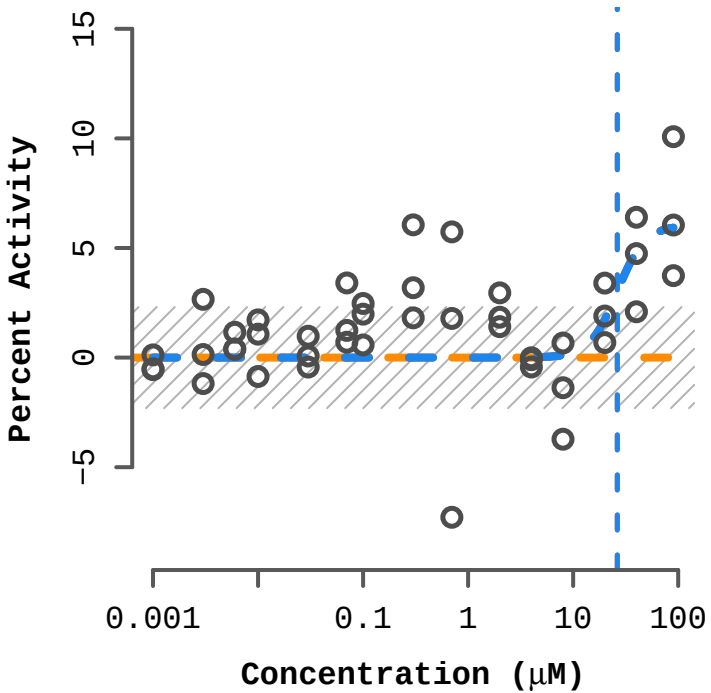
	tp	ga	gw	la	lw
val:	9.3	0.5	0.987	1.96	17.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	264.31	198.59	197.19
PROB:	0	0.33	0.67
RMSE:	4.74	2.09	2.16

MAX_MEAN: 9.8 MAX_MED: 8.58 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzo(g,h,i)perylene
CHID:    23908   CASRN: 191-24-2
SPID(S): Tox21_202732
M4ID:    12479520

HILL MODEL (in red):
      tp       ga       gw
val:  8.67     0.625    3.75
sd:   32.5     0.826    5.66

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.85     0.602    3.91     2.51     2.95
sd:   63.3     1.8      13.2     1190     1930

      CNST        HILL        GNLS
AIC:  150.32      149.26      153.27
PROB: 0.34        0.58        0.08
RMSE: 1.55        1.23        1.23

MAX_MEAN: 3.65      MAX_MED: 3.85      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzo(k)fluoranthene
CHID: 23909 CASRN: 207-08-9
SPID(S): Tox21_200721
M4ID: 12481531

HILL MODEL (in red):

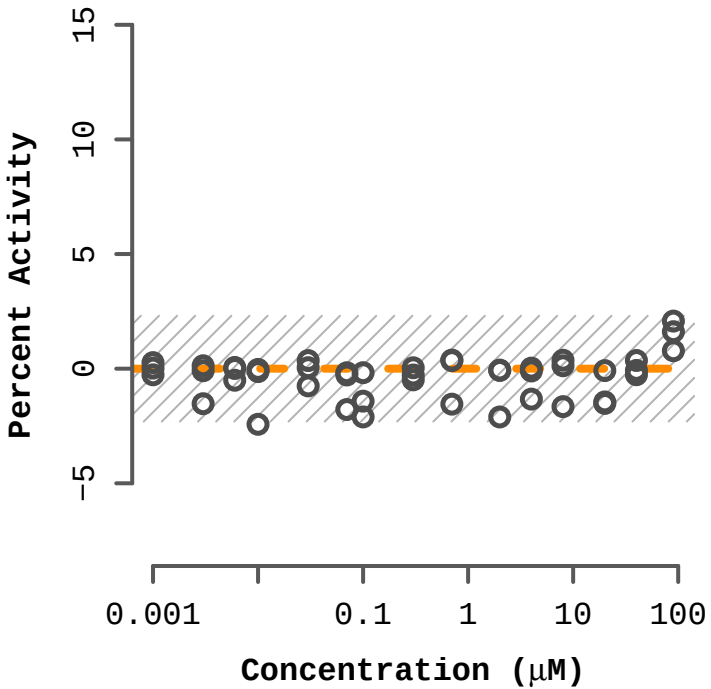
	tp	ga	gw
val:	6.03	1.42	3.3
sd:	1.78	0.165	2.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.03	1.42	3.3	2.4	16.9
sd:	1.78	0.165	2.3	400	15100

	CNST	HILL	GNLS
AIC:	228.48	207.88	211.88
PROB:	0	0.88	0.12
RMSE:	3.15	2.35	2.35

MAX_MEAN: 6.62 **MAX_MED:** 6.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

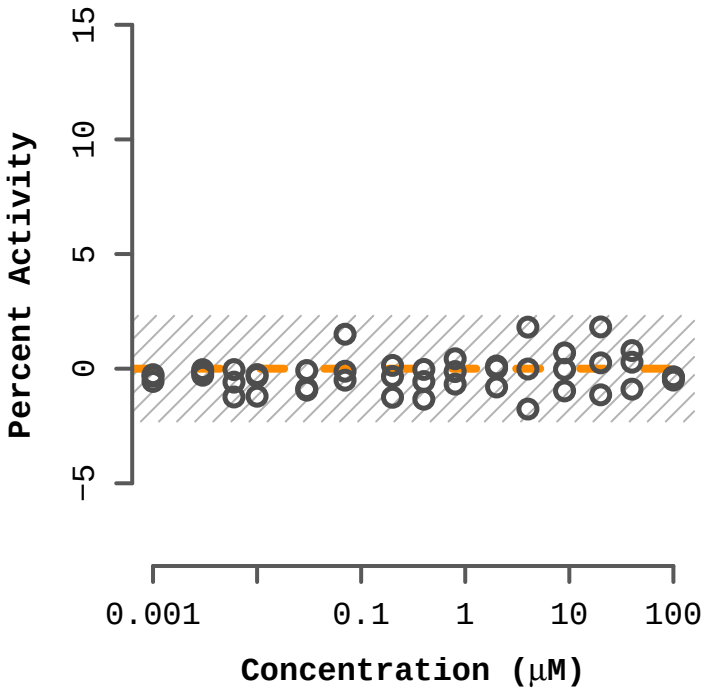
NAME: Dicrotophos
CHID: 23914 CASRN: 141-66-2
SPID(S): Tox21_301078
M4ID: 12478055

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.49 MAX_MED: 1.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

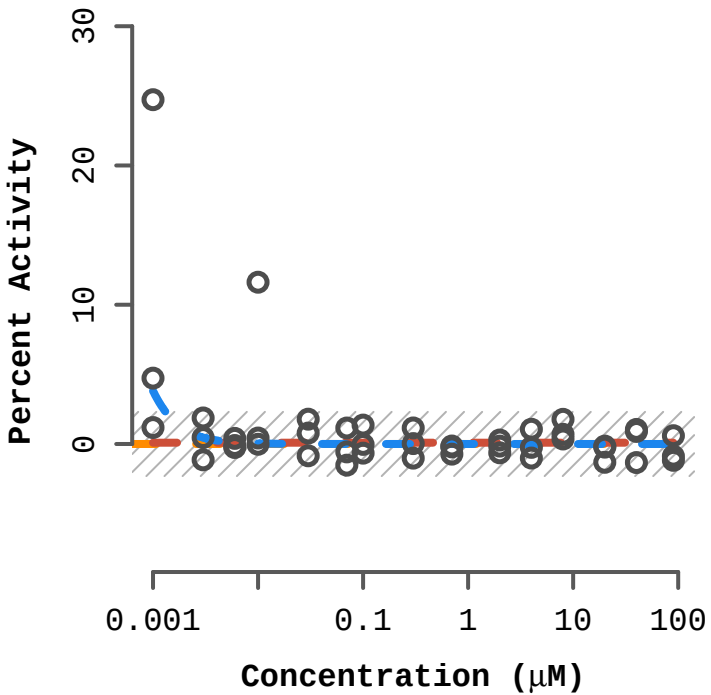
NAME: Bis(2-chloroethoxy)methane
CHID: 23917 **CASRN:** 111-91-1
SPID(S): Tox21_200284
M4ID: 12481968

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.313 **MAX_MED:** 0.284 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: p-Bromodiphenyl ether
CHID: 23927 CASRN: 101-55-3
SPID(S): Tox21_300512
M4ID: 12478620

HILL MODEL (in red):

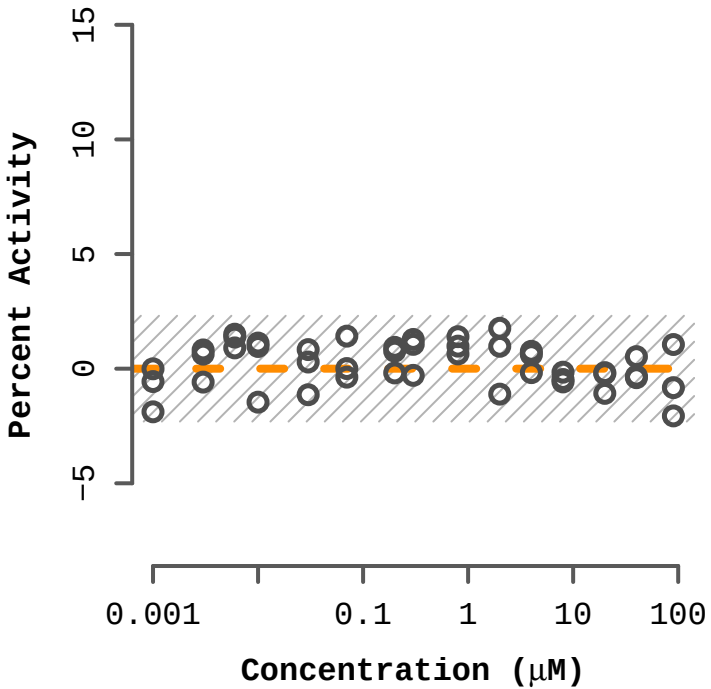
	tp	ga	gw
val:	0.0915	-4.84	6.05
sd:	0.174	141000	436000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27.1	-3.63	7.63	-3.38	2.05
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	179.01	184.73	181.98
PROB:	0.78	0.04	0.18
RMSE:	4.23	4.21	3.69

MAX_MEAN: 10.2 MAX_MED: 4.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

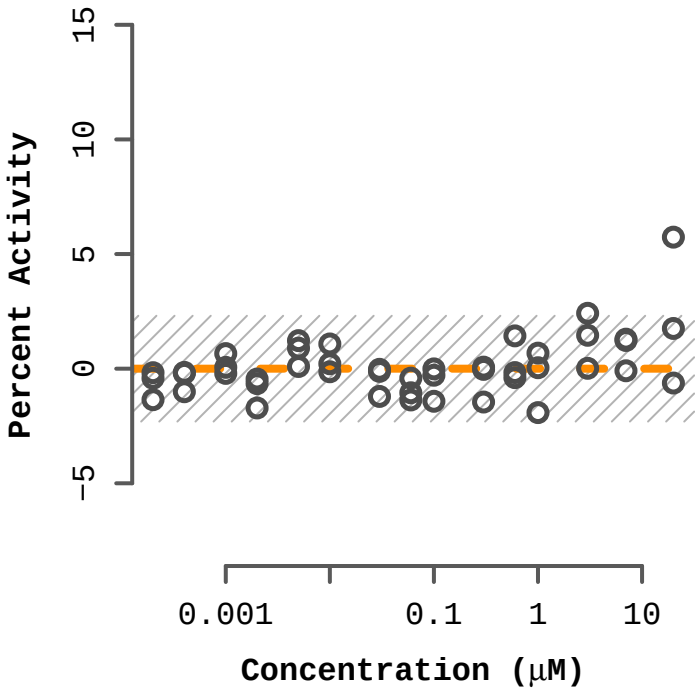
NAME: p-Bromodiphenyl ether
CHID: 23927 **CASRN:** 101-55-3
SPID(S): Tox21_201269
M4ID: 12480983

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

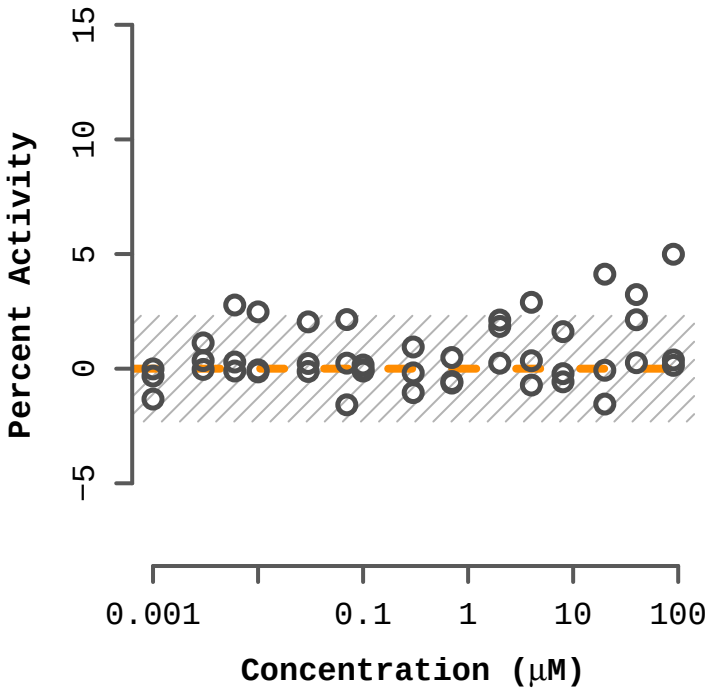
NAME: Bromotrichloromethane
CHID: 23930 **CASRN:** 75-62-7
SPID(S): Tox21_303534
M4ID: 12475610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.29 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

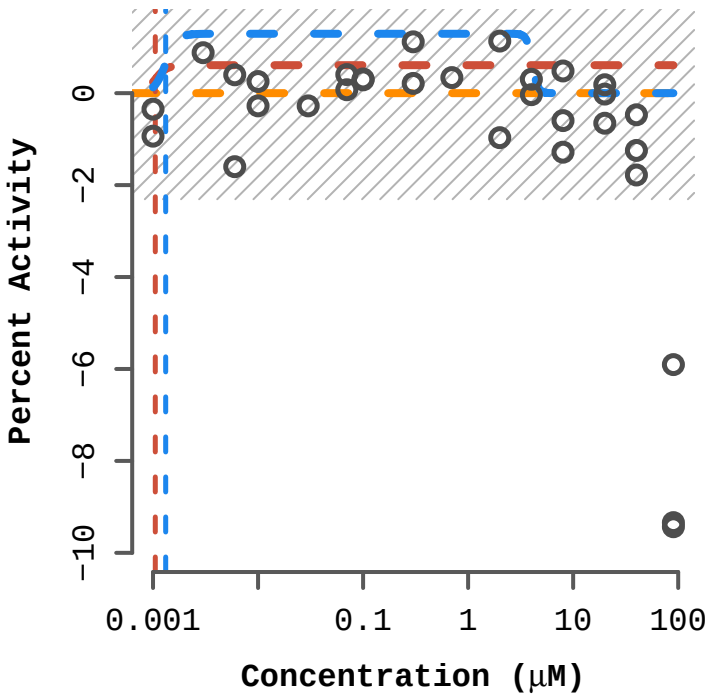
NAME: Bromotrichloromethane
CHID: 23930 CASRN: 75-62-7
SPID(S): Tox21_202292
M4ID: 12479960

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.88 MAX_MED: 2.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bromoxynil octanoate
CHID: 23932 CASRN: 1689-99-2
SPID(S): Tox21_201068
M4ID: 12481184

HILL MODEL (in red):

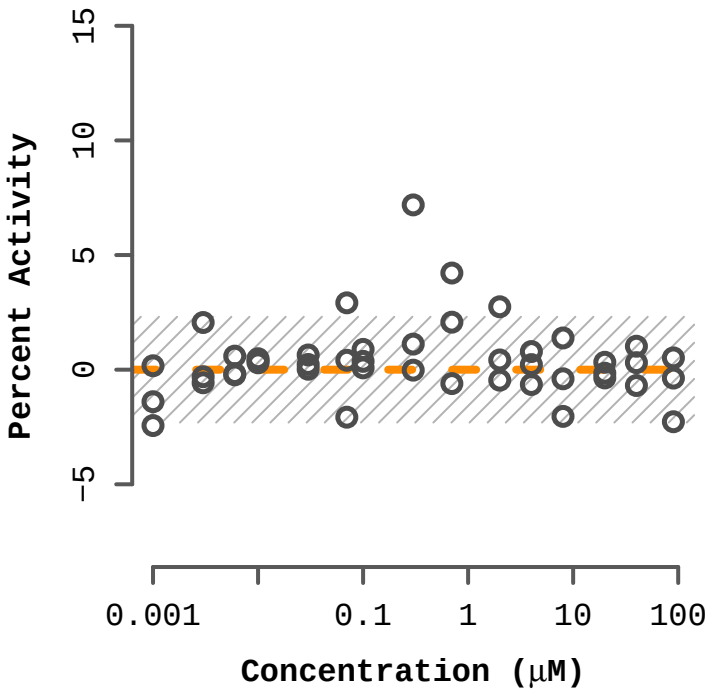
	tp	ga	gw
val:	0.609	−2.98	8
sd:	0.308	0.48	63.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.29	−2.88	8	0.611	16.5
sd:	0.348	0.478	21.2	0.327	581

	CNST	HILL	GNLS
AIC:	213.33	215.5	210.05
PROB:	0.15	0.05	0.79
RMSE:	2.85	2.86	2.63

MAX_MEAN: 2.43 **MAX_MED:** 3.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

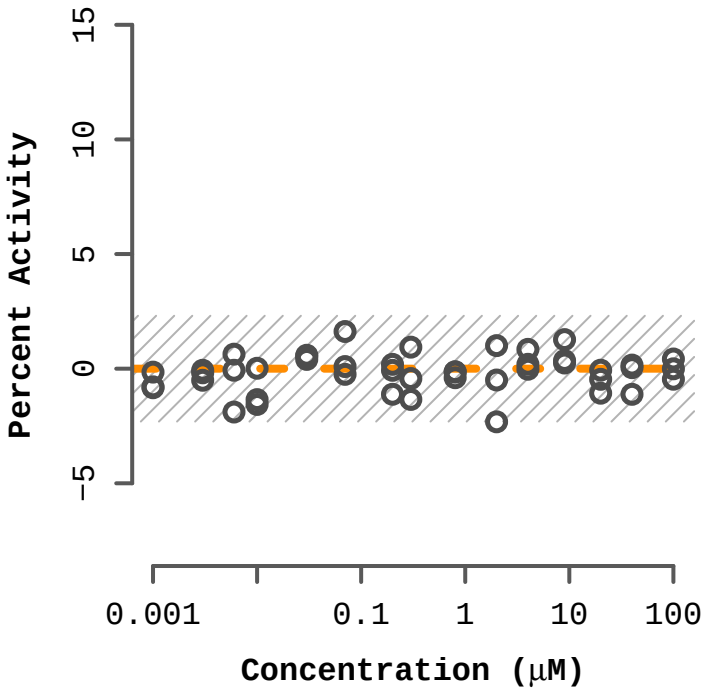
NAME: Butylate
CHID: 23936 **CASRN:** 2008-41-5
SPID(S): Tox21_300762
M4ID: 12478371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 2.76 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

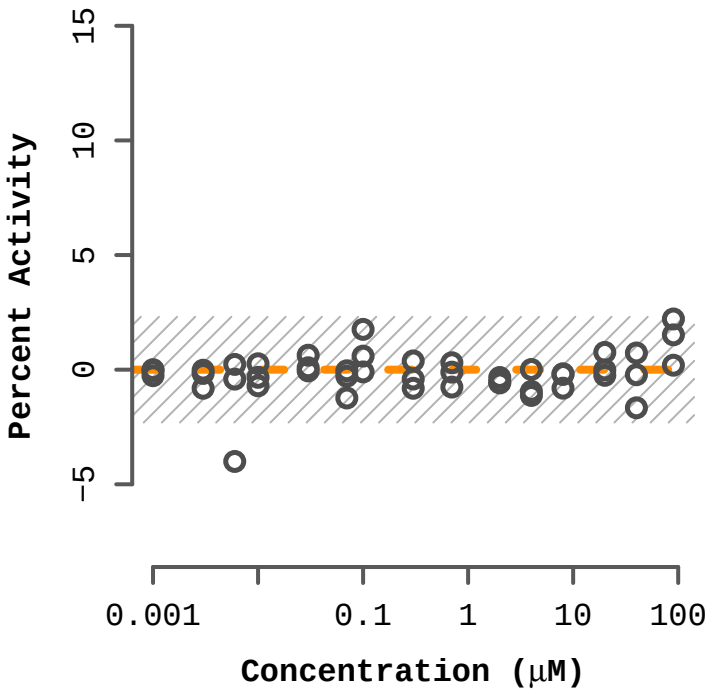
NAME: t-Butylchloride
CHID: 23937 **CASRN:** 507-20-0
SPID(S): Tox21_200192
M4ID: 12482060

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.625 **MAX_MED:** 0.546 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

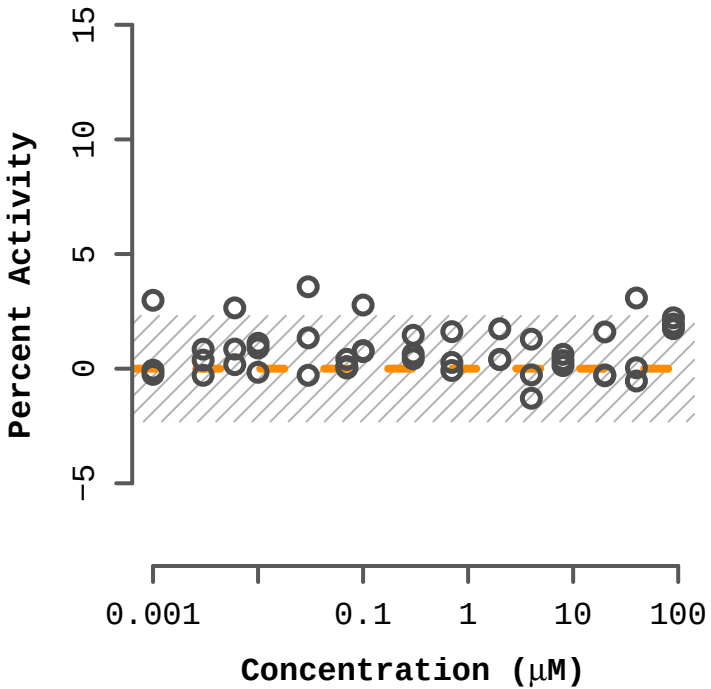
NAME: Butylphthalyl butylglycolate
CHID: 23938 CASRN: 85-70-1
SPID(S): Tox21_303276
M4ID: 12475857

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.31 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

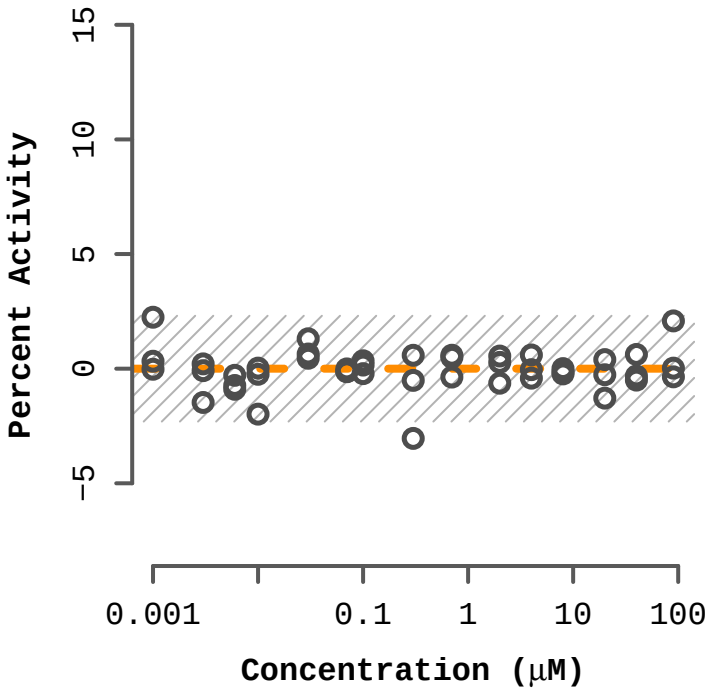
NAME: Butylphthalyl butylglycolate
CHID: 23938 **CASRN:** 85-70-1
SPID(S): Tox21_202314
M4ID: 12479938

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

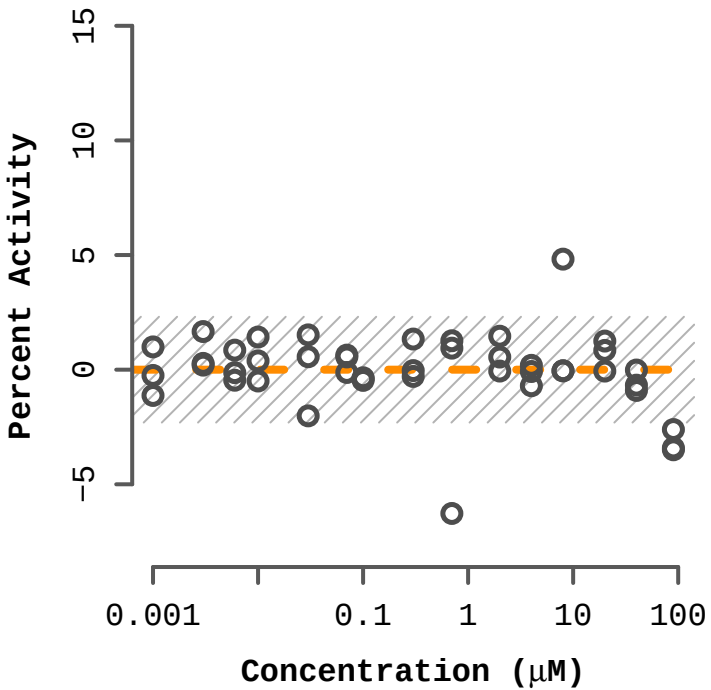
NAME: Carbon disulfide
CHID: 23947 **CASRN:** 75-15-0
SPID(S): Tox21_201168
M4ID: 12481084

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 0.642 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

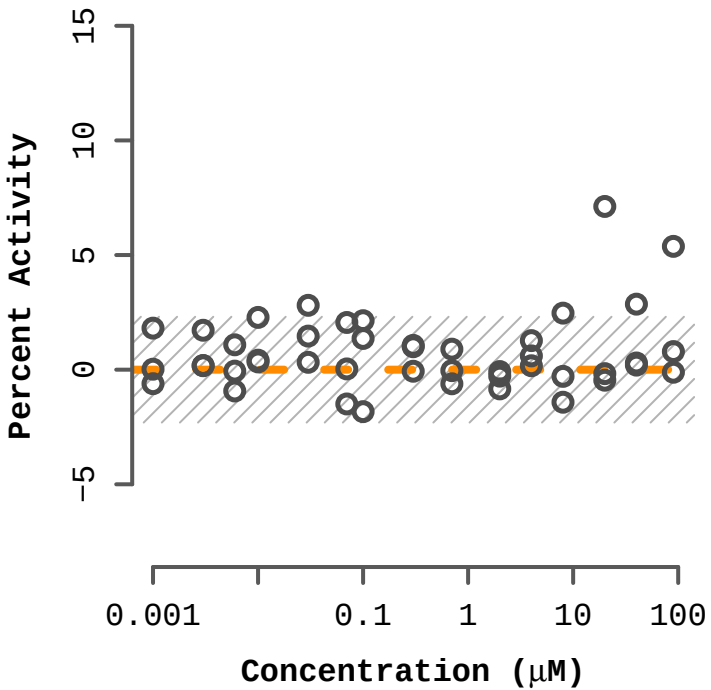
NAME: Carbosulfan
CHID: 23950 **CASRN:** 55285-14-8
SPID(S): Tox21_300473
M4ID: 12478659

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

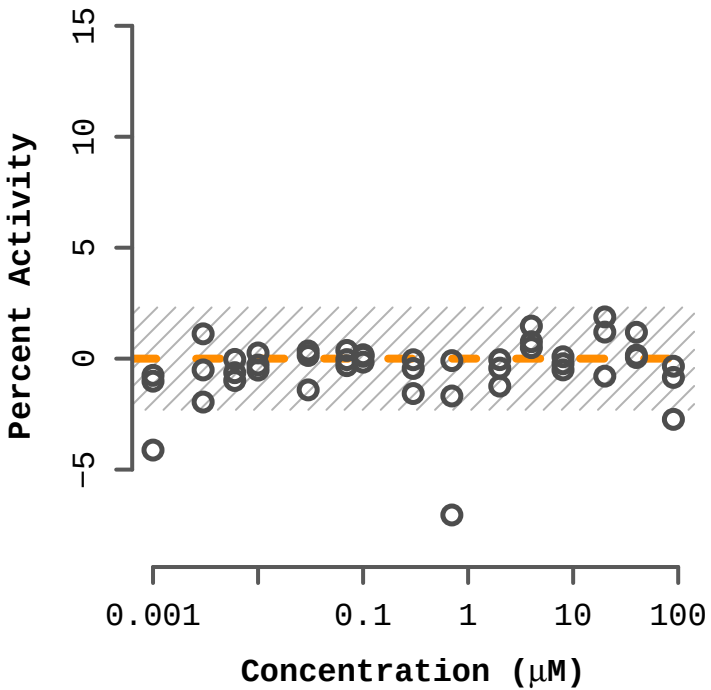
NAME: Carbosulfan
CHID: 23950 **CASRN:** 55285-14-8
SPID(S): Tox21_202336
M4ID: 12479916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

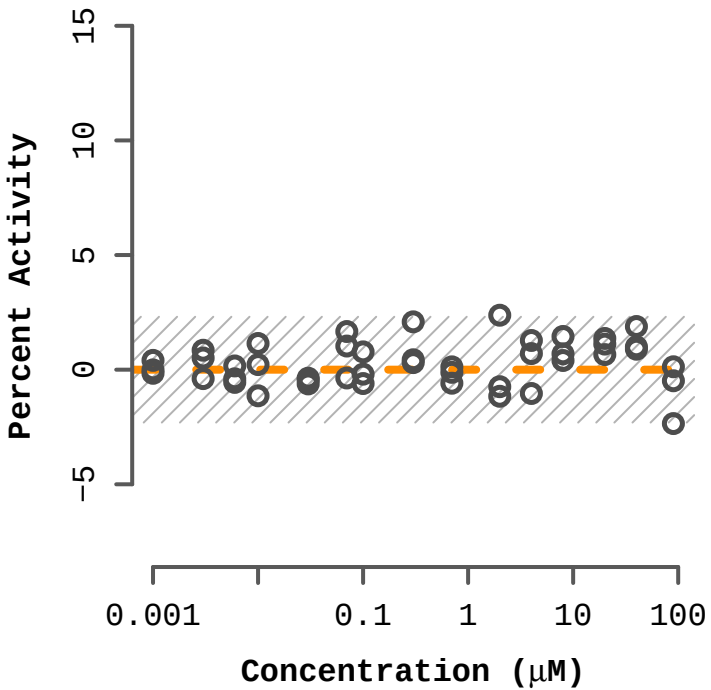
NAME: Carboxin
CHID: 23951 CASRN: 5234-68-4
SPID(S): Tox21_300706
M4ID: 12478427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.911 MAX_MED: 1.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

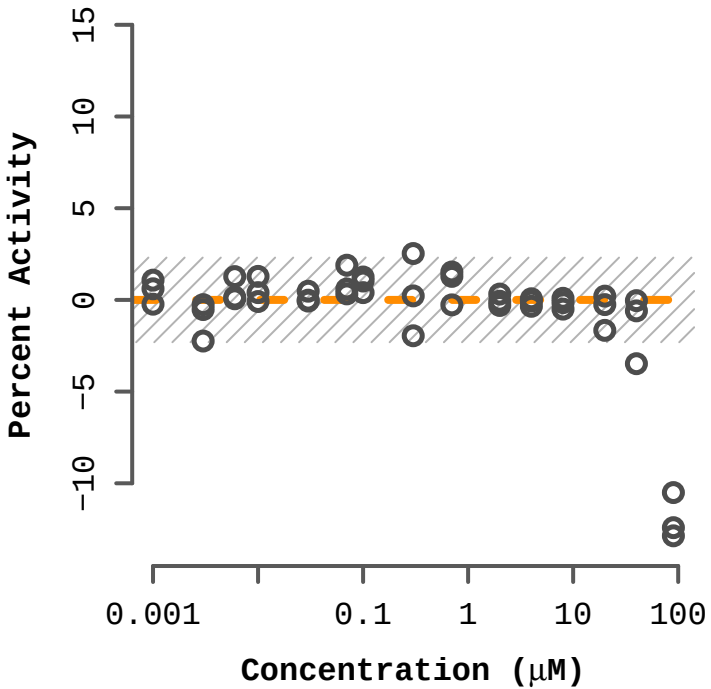
NAME: Carboxin
CHID: 23951 CASRN: 5234-68-4
SPID(S): Tox21_201988
M4ID: 12480264

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.26 MAX_MED: 1.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

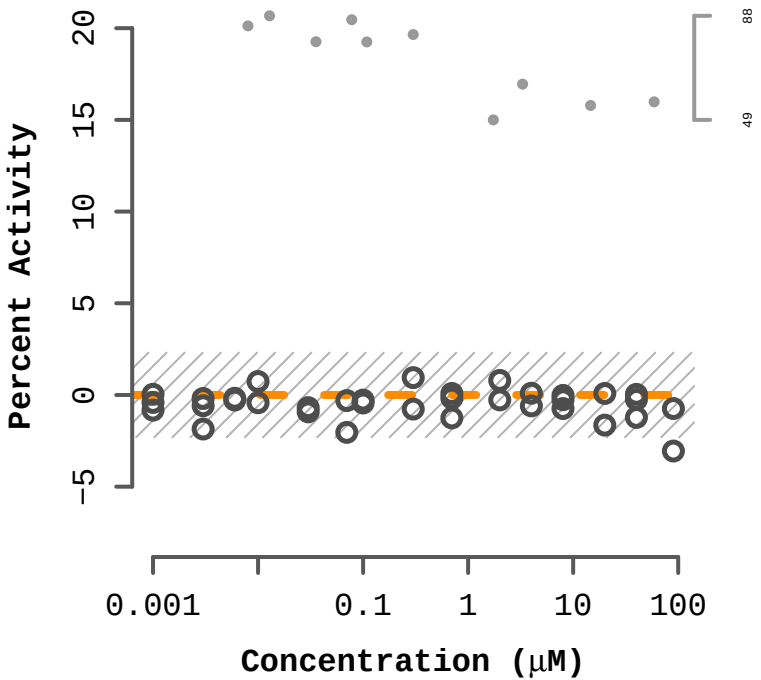
NAME: Technical chlordane
CHID: 23954 **CASRN:** 12789-03-6
SPID(S): Tox21_200290
M4ID: 12481962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.32	NA	NA
PROB:	1	NA	NA
RMSE:	3.26	NA	NA

MAX_MEAN: 0.941 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

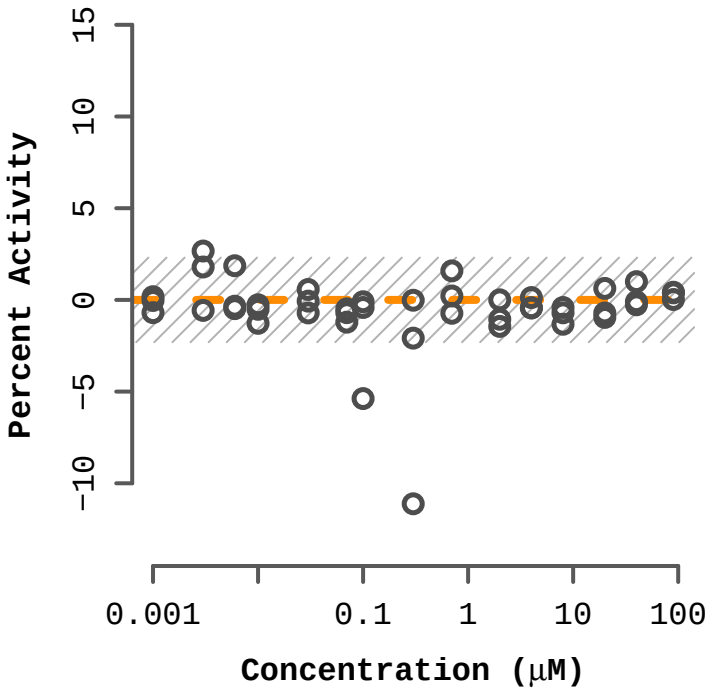
NAME: Chlorimuron-ethyl
CHID: 23955 **CASRN:** 90982-32-4
SPID(S): Tox21_303806
M4ID: 12475382 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	431.54	NA	NA
PROB:	1	NA	NA
RMSE:	34.41	NA	NA

MAX_MEAN: 29.4 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

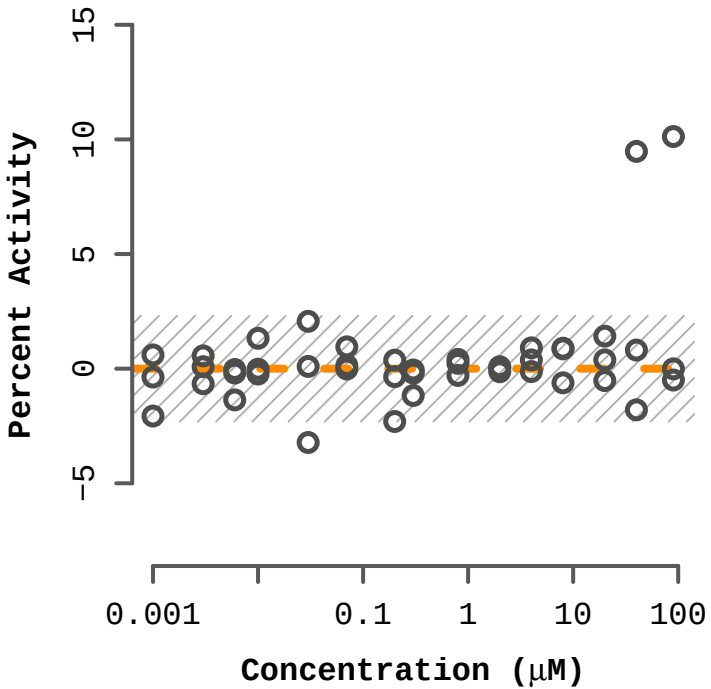
NAME: 2-Chlorobutane
CHID: 23966 **CASRN:** 78-86-4
SPID(S): Tox21_200404
M4ID: 12481848

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

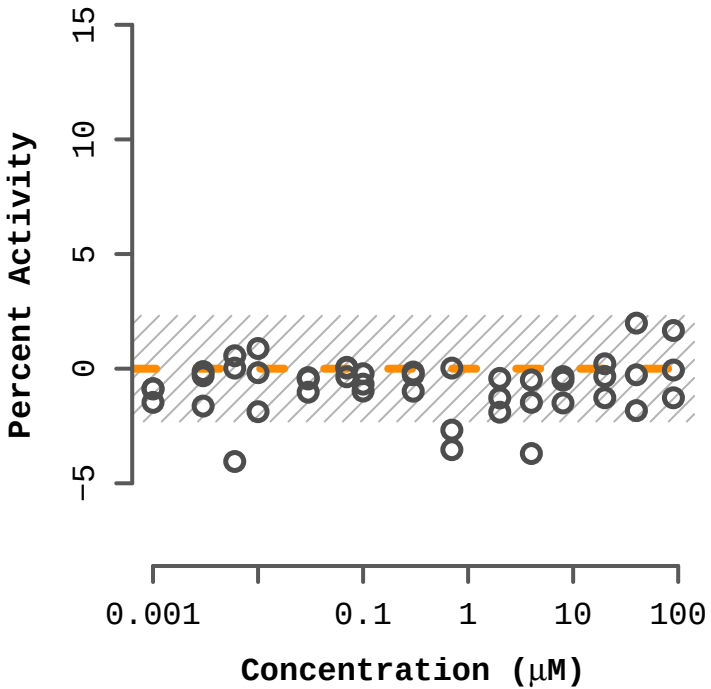
NAME: 2-Chloronaphthalene
CHID: 23971 **CASRN:** 91-58-7
SPID(S): Tox21_200981
M4ID: 12481271

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.28	NA	NA

MAX_MEAN: 3.21 **MAX_MED:** 0.864 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

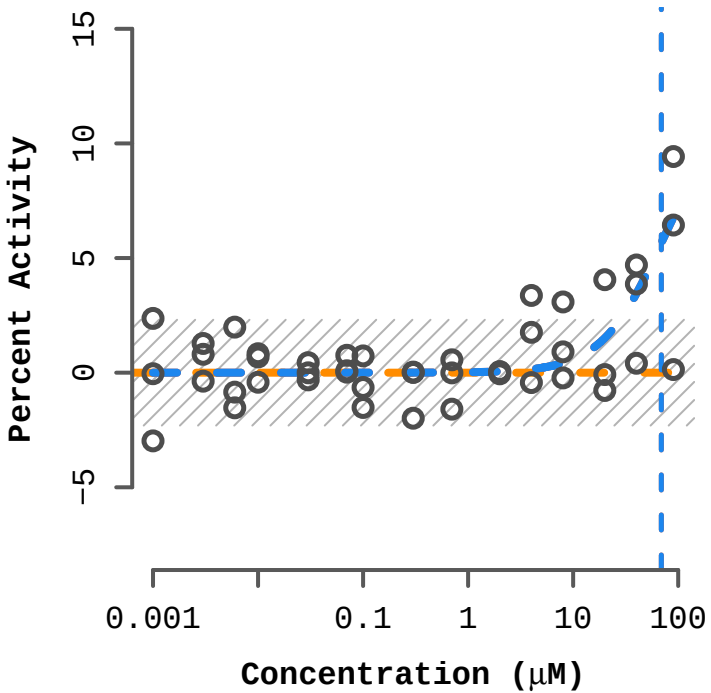
NAME: 4-Chlorophenyl methyl sulfide
CHID: 23973 **CASRN:** 123-09-1
SPID(S): Tox21_303311
M4ID: 12475822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.114 **MAX_MED:** 0.0262 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chlorophenyl methyl sulfide
CHID: 23973 **CASRN:** 123-09-1
SPID(S): Tox21_202358
M4ID: 12479894

HILL MODEL (in red):

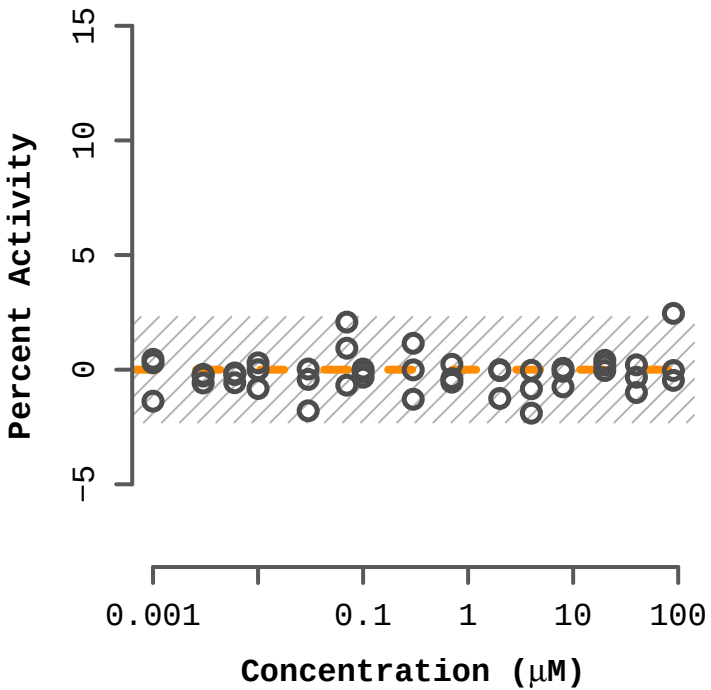
	tp	ga	gw
val:	11.3	1.84	1.51
sd:	13.1	0.727	1.79

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.3	1.84	1.51	3.95	3.39
sd:	13.1	0.725	1.79	1130	1900

	CNST	HILL	GNLS
AIC:	189.72	178.26	182.26
PROB:	0	0.88	0.12
RMSE:	2.34	1.72	1.72

MAX_MEAN: 5.34 **MAX_MED:** 6.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

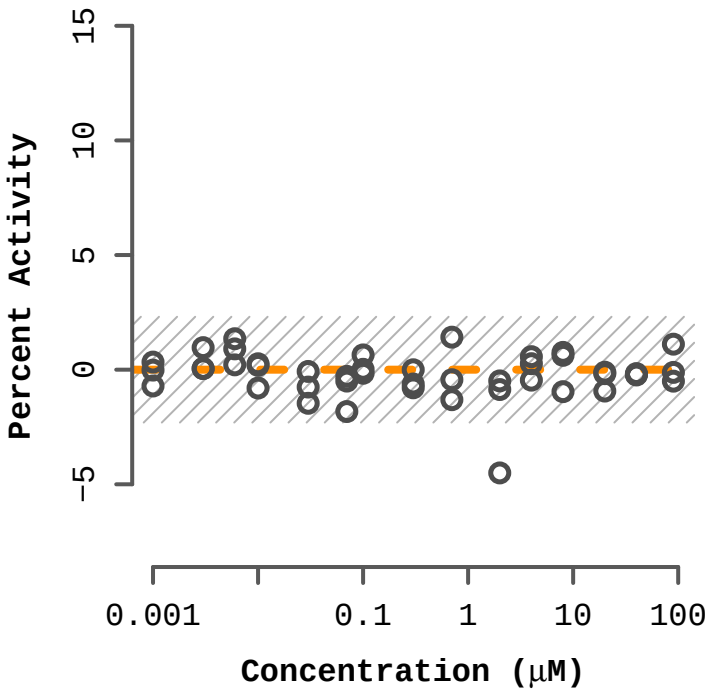
NAME: 4-Chlorophenyl methyl sulfone
CHID: 23974 **CASRN:** 98-57-7
SPID(S): Tox21_303181
M4ID: 12475952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.779 **MAX_MED:** 0.936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

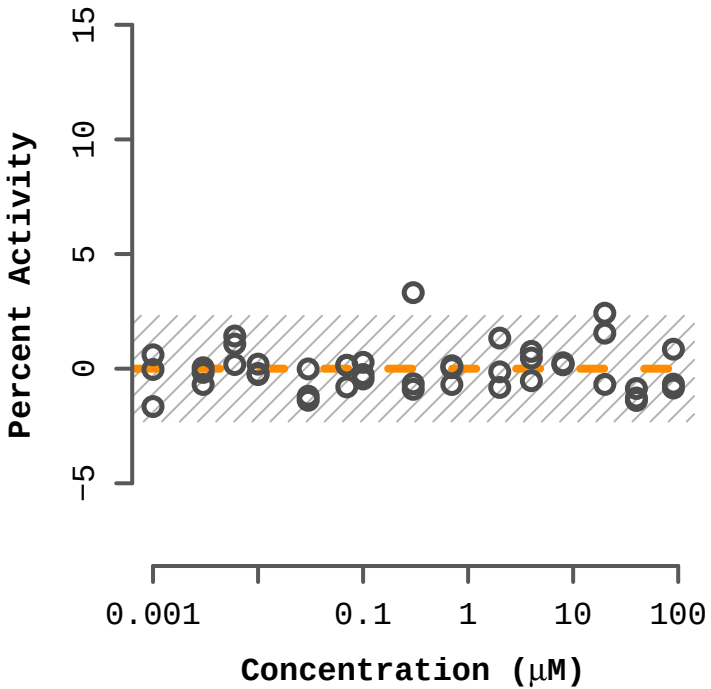
NAME: 4-Chlorophenyl methyl sulfone
CHID: 23974 **CASRN:** 98-57-7
SPID(S): Tox21_201867
M4ID: 12480385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.824 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

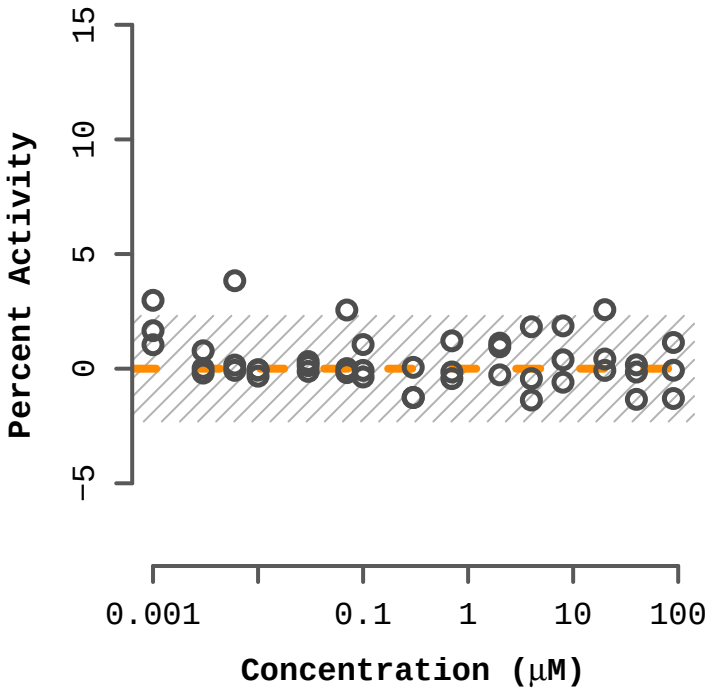
NAME: 2-Chlorotoluene
CHID: 23977 CASRN: 95-49-8
SPID(S): Tox21_300329
M4ID: 12478803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.09 MAX_MED: 1.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

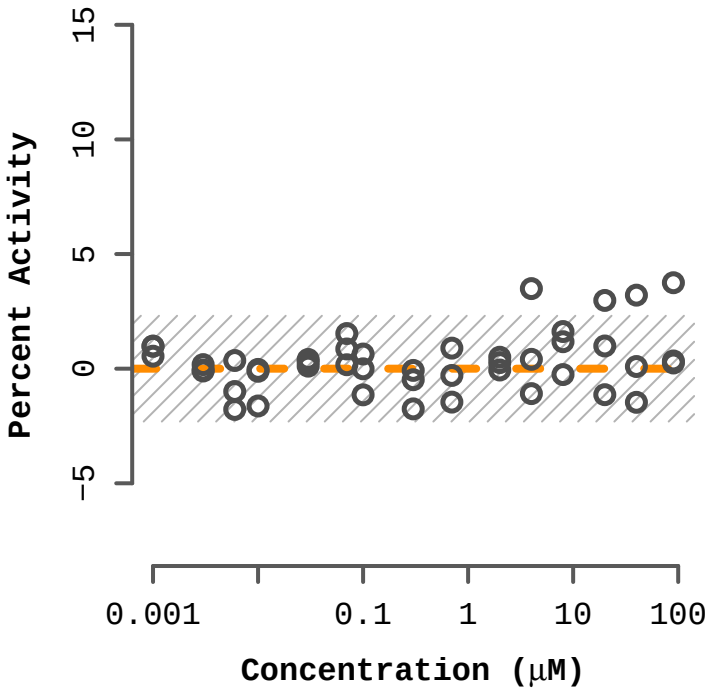
NAME: 2-Chlorotoluene
CHID: 23977 **CASRN:** 95-49-8
SPID(S): Tox21_201251
M4ID: 12481001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

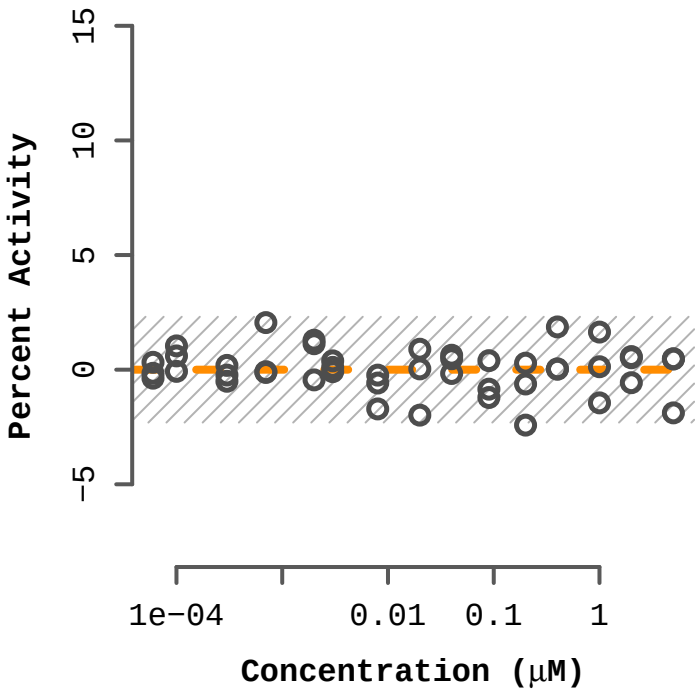
NAME: Chlorsulfuron
CHID: 23980 CASRN: 64902-72-3
SPID(S): Tox21_200255
M4ID: 12481997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.45 MAX_MED: 1.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

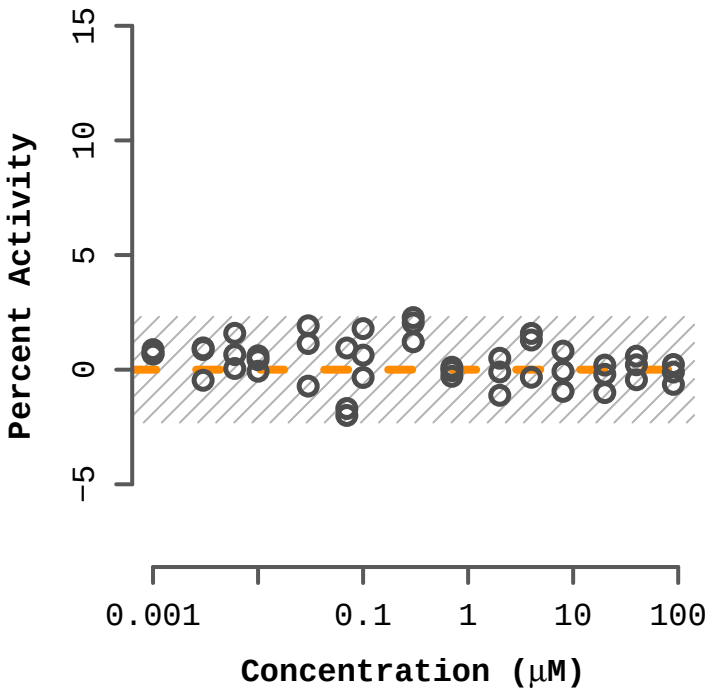
NAME: Copper cyanide
CHID: 23986 **CASRN:** 544-92-3
SPID(S): Tox21_202733
M4ID: 12479519

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.659 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

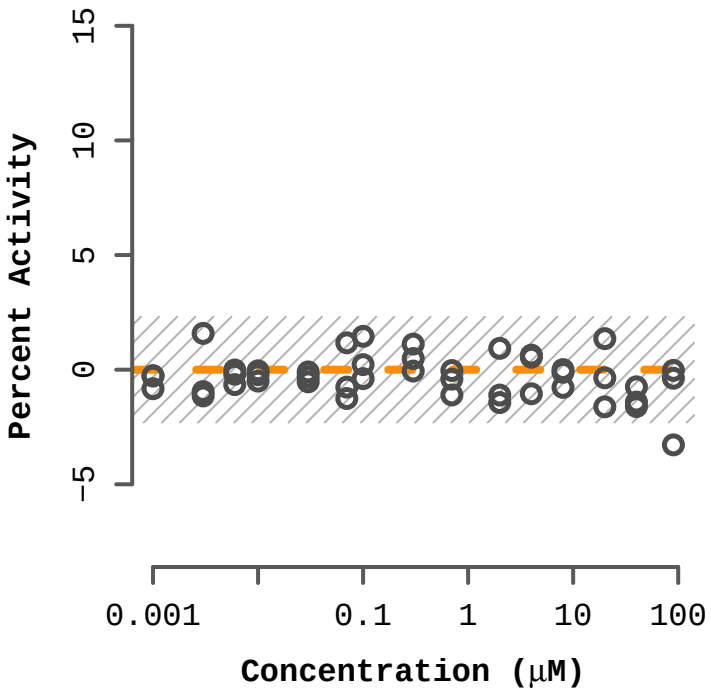
NAME: Cyanazine
CHID: 23990 **CASRN:** 21725-46-2
SPID(S): Tox21_301032
M4ID: 12478101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

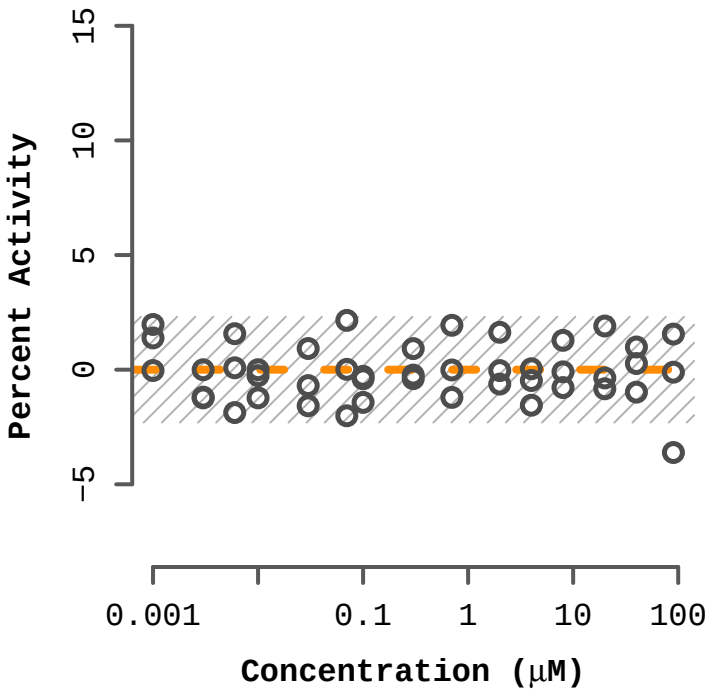
NAME: Cyanazine
CHID: 23990 **CASRN:** 21725-46-2
SPID(S): Tox21_201619
M4ID: 12480633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.515 **MAX_MED:** 0.544 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

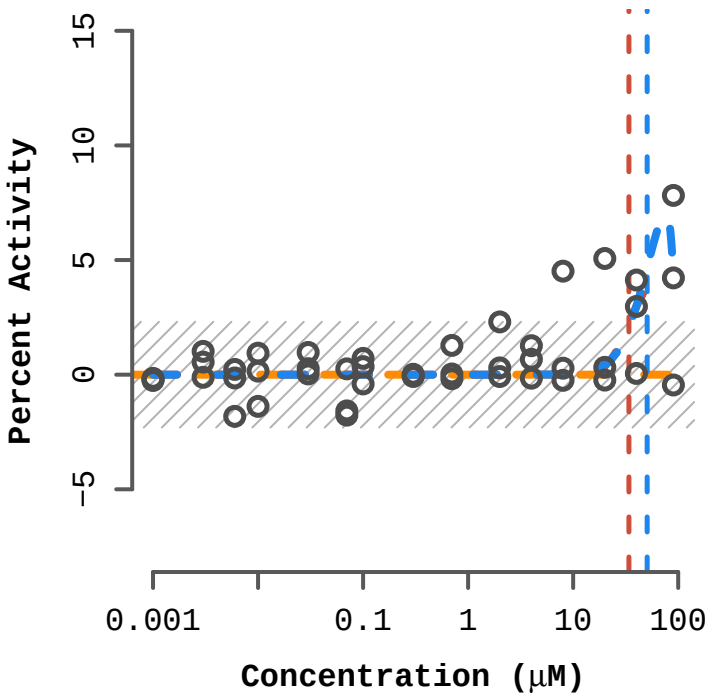
NAME: Cyclohexylamine
CHID: 23996 **CASRN:** 108-91-8
SPID(S): Tox21_300038
M4ID: 12479092

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclohexylamine
CHID: 23996 **CASRN:** 108-91-8
SPID(S): Tox21_202380
M4ID: 12479872

HILL MODEL (in red):

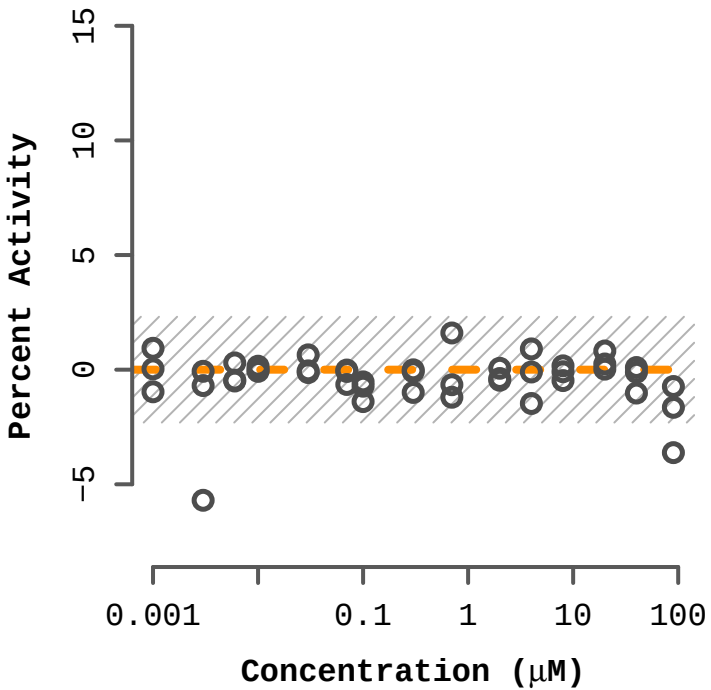
	tp	ga	gw
val:	4.43	1.53	4.41
sd:	1.02	0.0911	3.21

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.38	1.7	3.24	1.96	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	170.12	162.04	166.01
PROB:	0.02	0.87	0.12
RMSE:	1.98	1.58	1.57

MAX_MEAN: 3.86 **MAX_MED:** 4.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

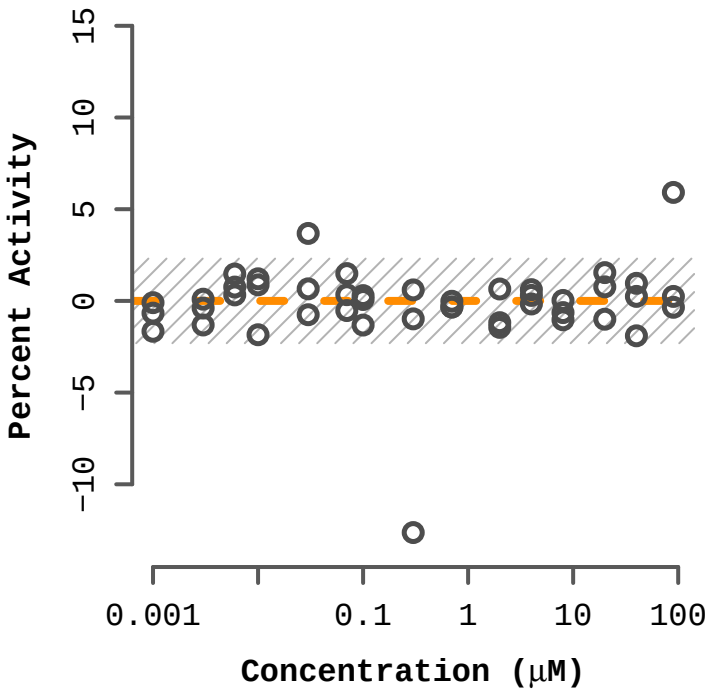
NAME: Cyhalothrin
CHID: 23997 CASRN: 68085-85-8
SPID(S): Tox21_200107
M4ID: 12482145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.364 MAX_MED: 0.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

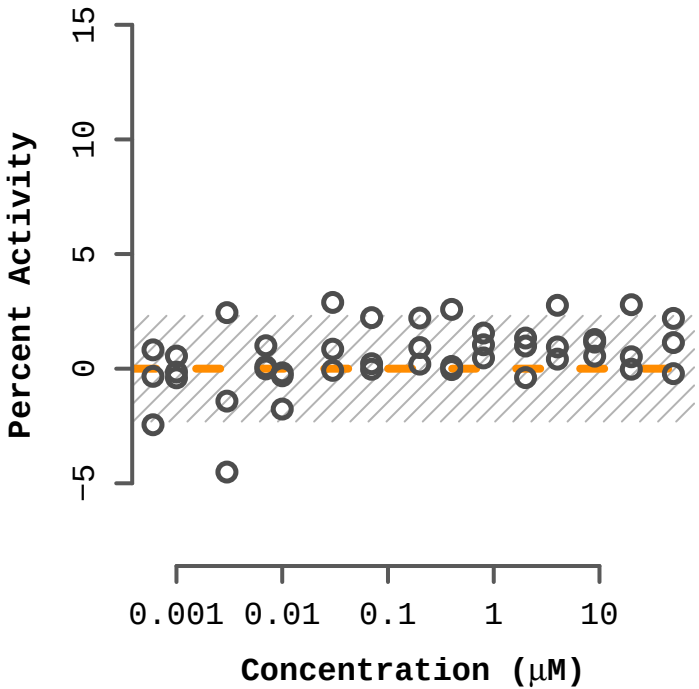
NAME: Cypermethrin
CHID: 23998 **CASRN:** 52315-07-8
SPID(S): Tox21_300892
M4ID: 12478241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.32	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 0.877 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

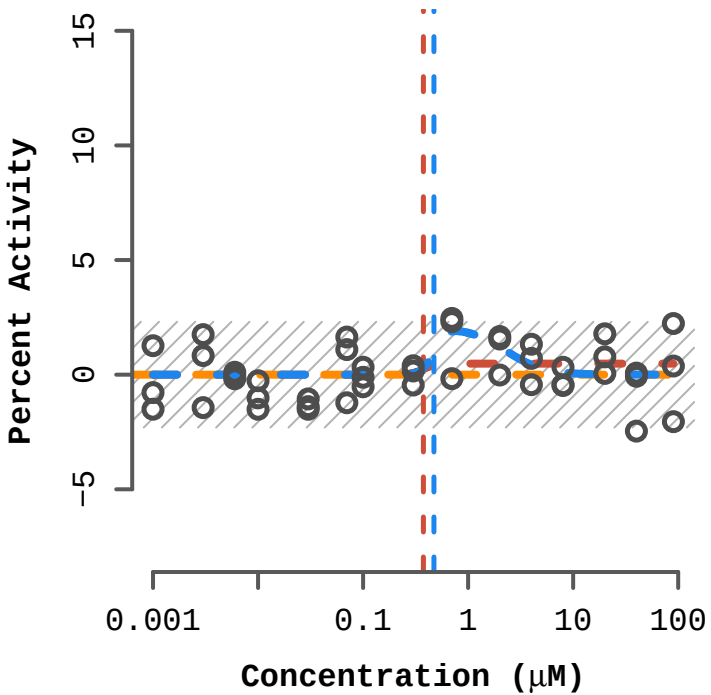
NAME: Cypermethrin
CHID: 23998 **CASRN:** 52315-07-8
SPID(S): Tox21_113579_1
M4ID: 12482599

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyromazine
CHID: 23999 CASRN: 66215-27-8
SPID(S): Tox21_300784
M4ID: 12478349

HILL MODEL (in red):

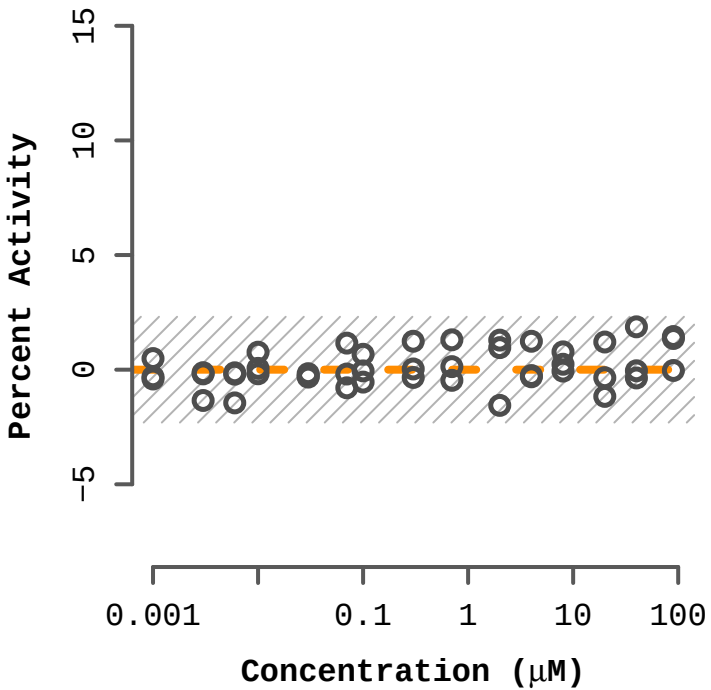
	tp	ga	gw
val:	0.481	−0.426	8
sd:	0.266	0.363	18.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.08	−0.326	8	0.362	2.41
sd:	2.68	0.693	26.2	0.576	3.39

	CNST	HILL	GNLS
AIC:	149.3	152	150.54
PROB:	0.56	0.14	0.3
RMSE:	1.19	1.15	1.09

MAX_MEAN: 1.53 **MAX_MED:** 2.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

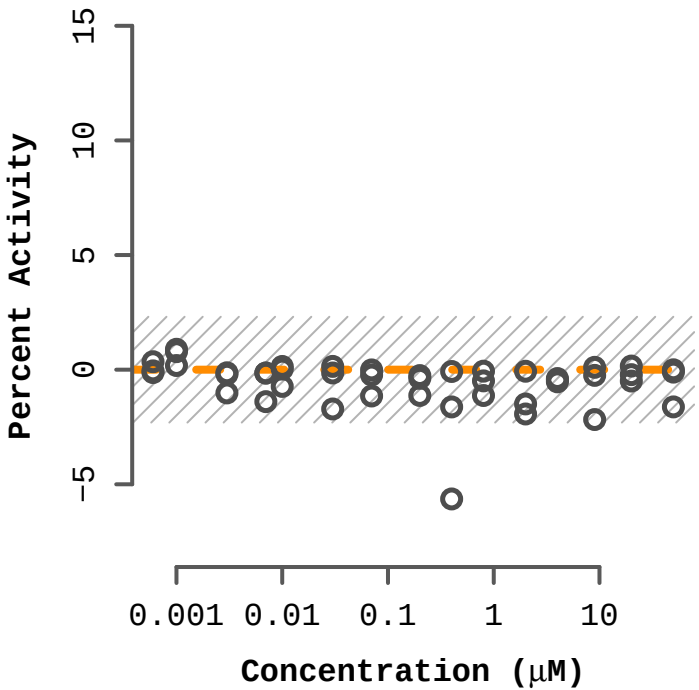
NAME: Cyromazine
CHID: 23999 **CASRN:** 66215-27-8
SPID(S): Tox21_201846
M4ID: 12480406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.925 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

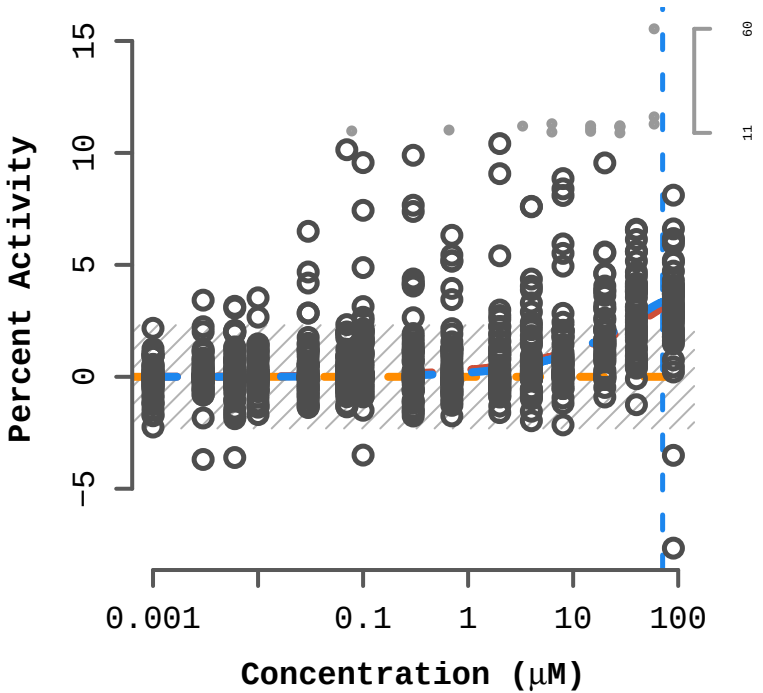
NAME: Cyromazine
CHID: 23999 **CASRN:** 66215-27-8
SPID(S): Tox21_112074_1
M4ID: 12483336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.62 **MAX_MED:** 0.787 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorthal-dimethyl
CHID: 24000 CASRN: 1861-32-1
SPID(S): Tox21_400071
M4ID: 12475066 BRK

HILL MODEL (in red):

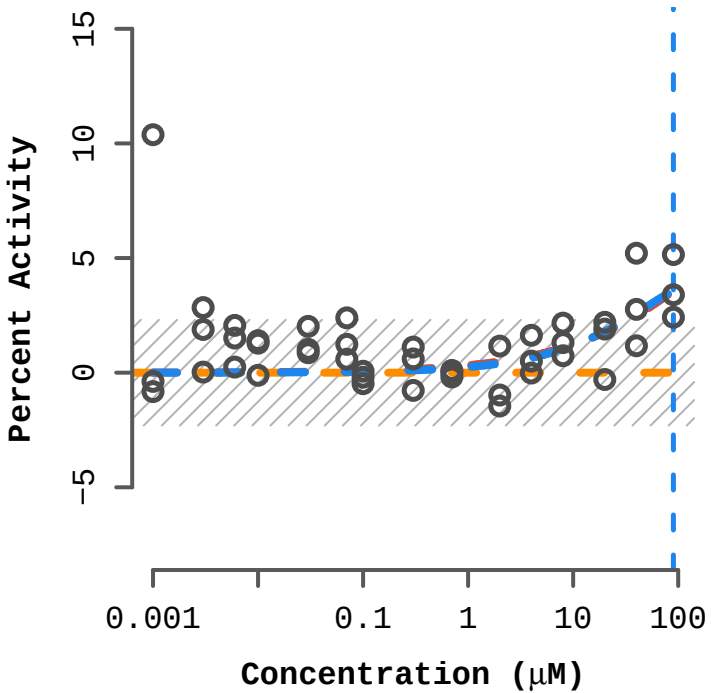
	tp	ga	gw
val:	10.4	2.45	0.615
sd:	14.3	1.62	0.233

GAIN-LOSS MODEL (in blue):

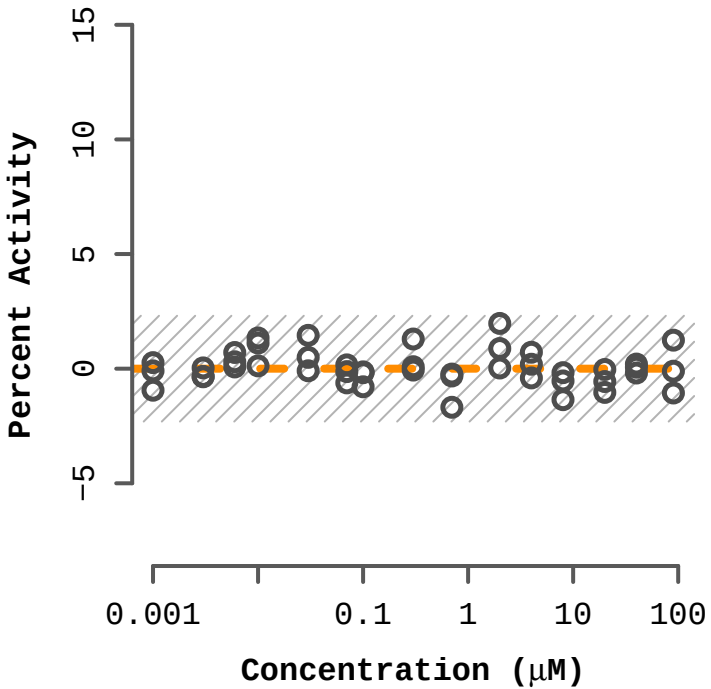
	tp	ga	gw	la	lw
val:	6.98	1.85	0.843	2.1	5.43
sd:	4.93	0.619	0.223	0.499	16.8

	CNST	HILL	GNLS
AIC:	3240.64	2914.29	2917.76
PROB:	0	0.85	0.15
RMSE:	3.7	3.27	3.28

MAX_MEAN: 4.79 MAX_MED: 3.47 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Chlorthal-dimethyl
CHID:    24000   CASRN: 1861-32-1
SPID(S): Tox21_300379
M4ID:    12478753

HILL MODEL (in red):
      tp       ga       gw
val:  10.9     2.45     0.618
sd:   101      11.2     1.76

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.34     1.95     0.748    2.23     5.35
sd:   28.1     4.1      1.25     2.88     50.1

      CNST        HILL        GNLS
AIC:  192.52      170.31      174.38
PROB: 0           0.88        0.12
RMSE: 2.35        1.96        1.96

MAX_MEAN: 3.66      MAX_MED: 3.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

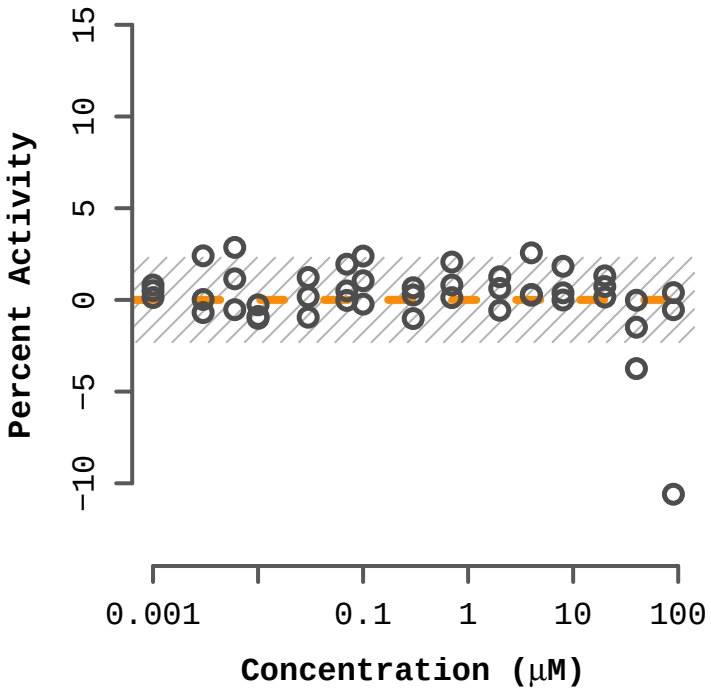
NAME: Dalapon−sodium
CHID: 24001 **CASRN:** 127−20−8
SPID(S): Tox21_201112
M4ID: 12481140

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.962 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

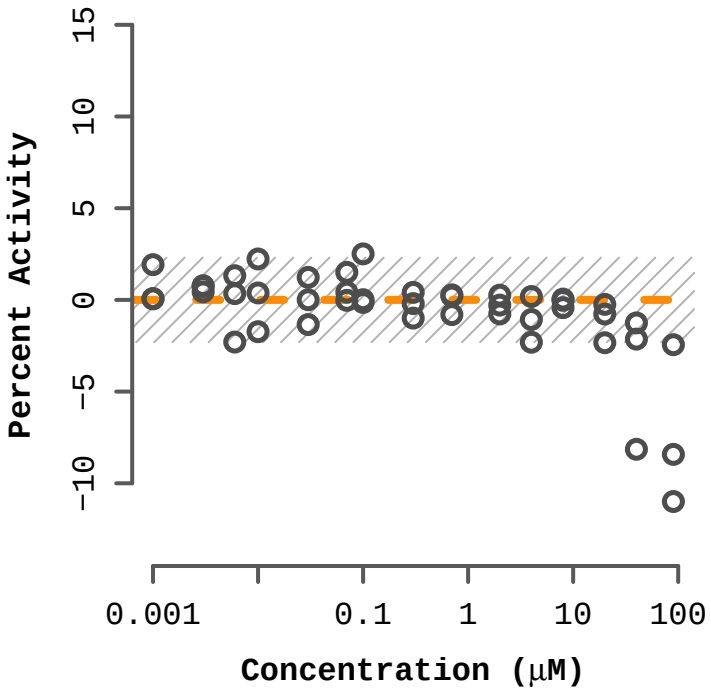
NAME: Fenpropathrin
CHID: 24002 **CASRN:** 39515-41-8
SPID(S): Tox21_300882
M4ID: 12478251

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.38	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

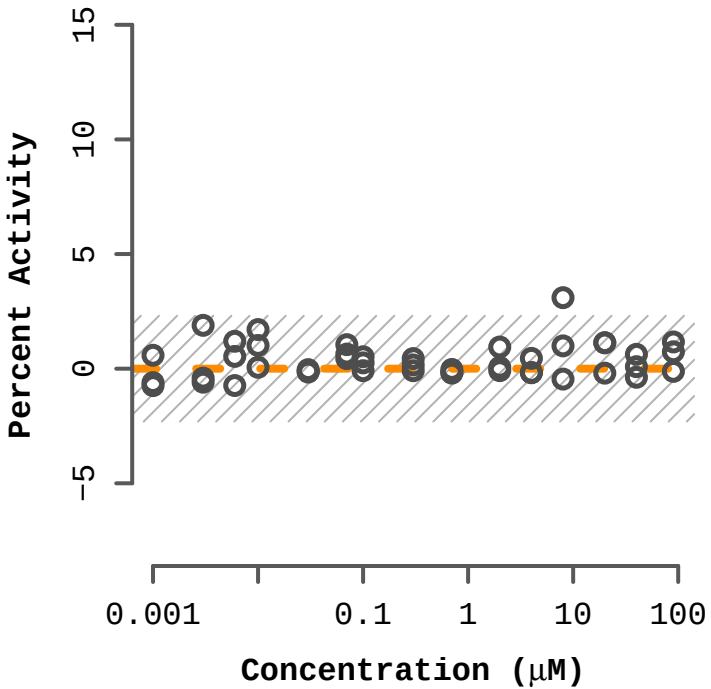
NAME: Fenpropathrin
CHID: 24002 **CASRN:** 39515-41-8
SPID(S): Tox21_201531
M4ID: 12480721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.66	NA	NA

MAX_MEAN: 0.796 **MAX_MED:** 0.733 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

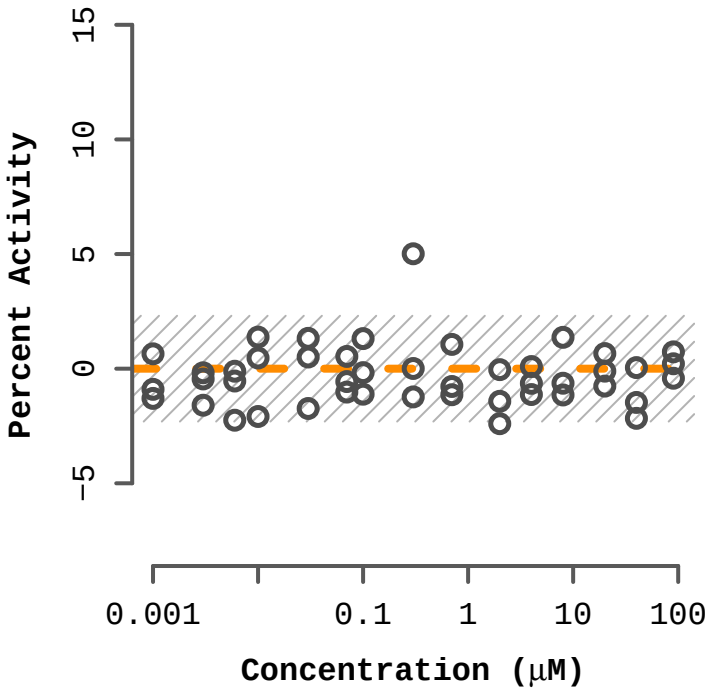
NAME: 1,4−Dibromobenzene
CHID: 24012 **CASRN:** 106−37−6
SPID(S): Tox21_303156
M4ID: 12475977

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

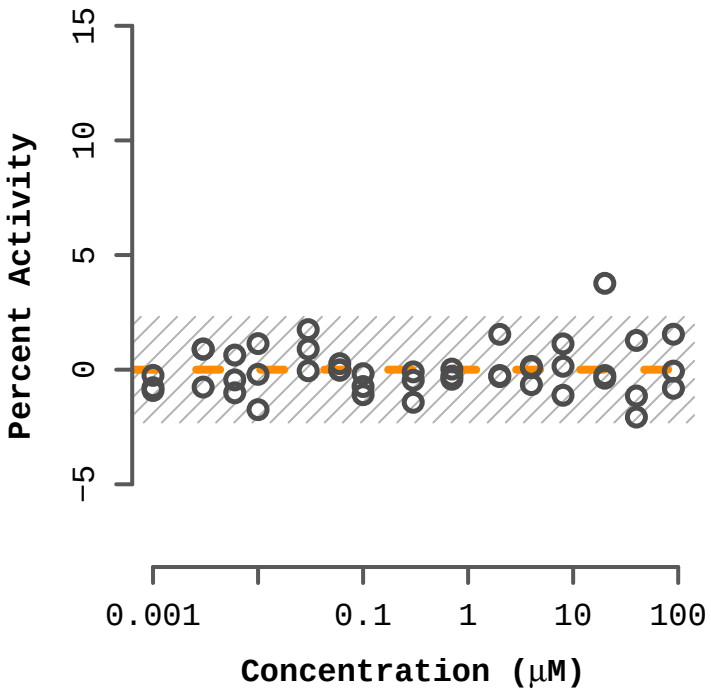
NAME: 1,4−Dibromobenzene
CHID: 24012 **CASRN:** 106−37−6
SPID(S): Tox21_201288
M4ID: 12480964

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

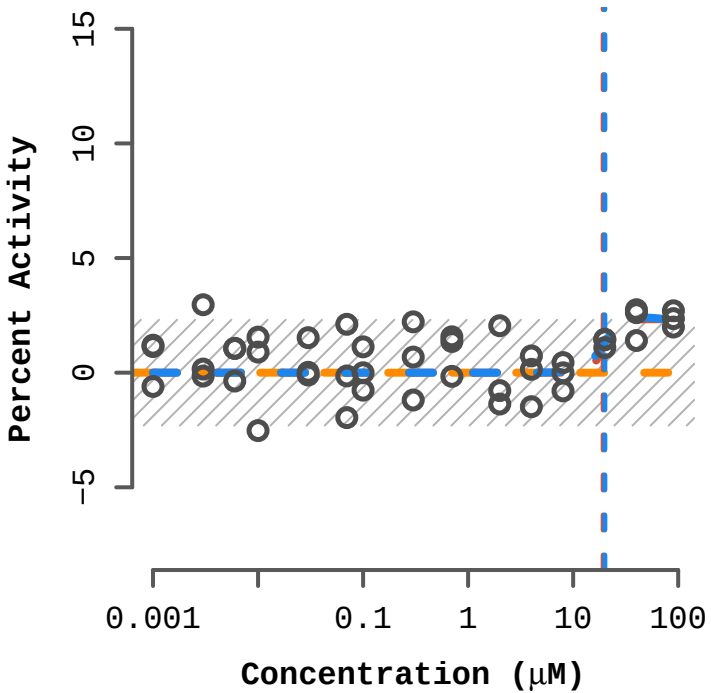
NAME: Dibromodichloromethane
CHID: 24014 **CASRN:** 594-18-3
SPID(S): Tox21_200392
M4ID: 12481860

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.901 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Dibromodiphenyl ether
CHID: 24015 CASRN: 2050−47−7
SPID(S): Tox21_303162
M4ID: 12475971

HILL MODEL (in red):

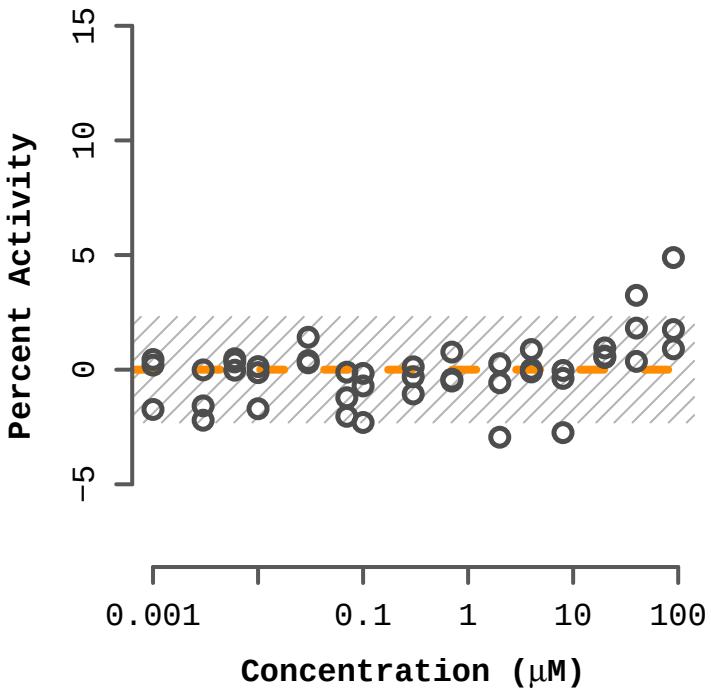
	tp	ga	gw
val:	2.33	1.29	8
sd:	0.386	0.0964	46.8

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.55	1.3	4.68	2.83	0.3
sd:	1.07	0.218	15.2	9.78	1.28

	CNST	HILL	GNLS
AIC:	169.08	149.58	153.65
PROB:	0	0.88	0.12
RMSE:	1.46	1.15	1.15

MAX_MEAN: 2.35 MAX_MED: 2.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

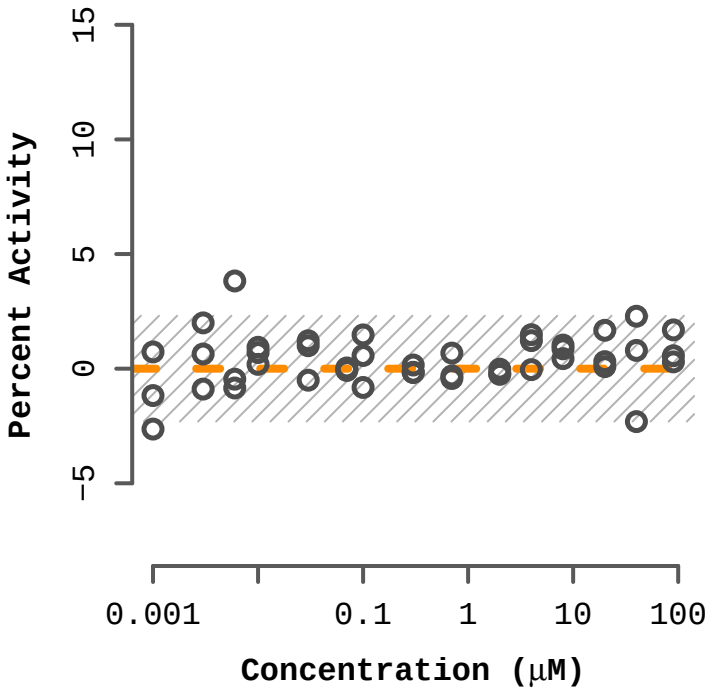
NAME: 4,4'−Dibromodiphenyl ether
CHID: 24015 **CASRN:** 2050−47−7
SPID(S): Tox21_202033
M4ID: 12480219

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.52 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

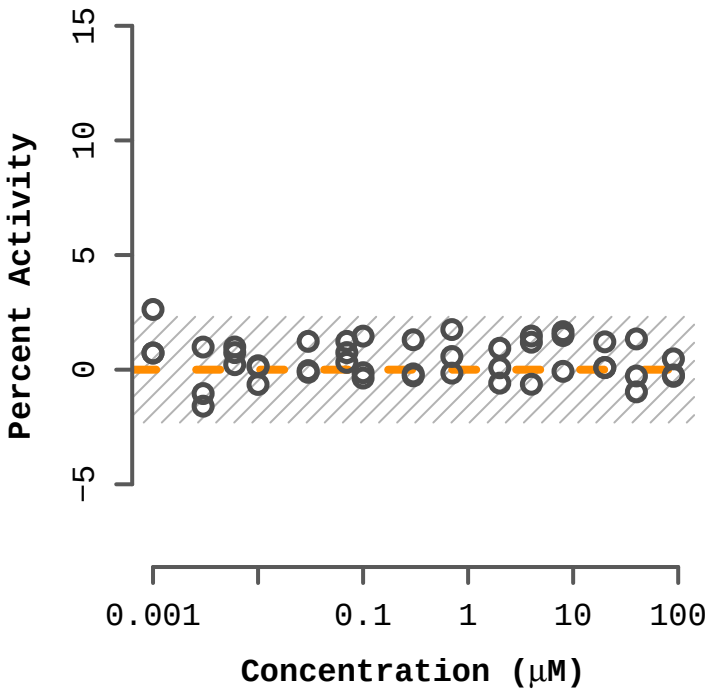
NAME: Dicamba
CHID: 24018 **CASRN:** 1918-00-9
SPID(S): Tox21_300661
M4ID: 12478472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

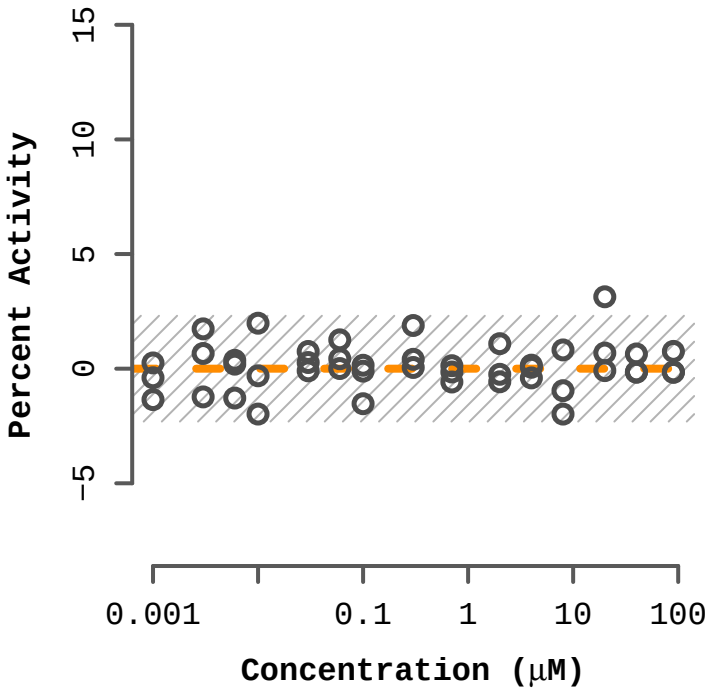
NAME: Dicamba
CHID: 24018 **CASRN:** 1918-00-9
SPID(S): Tox21_201356
M4ID: 12480896

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

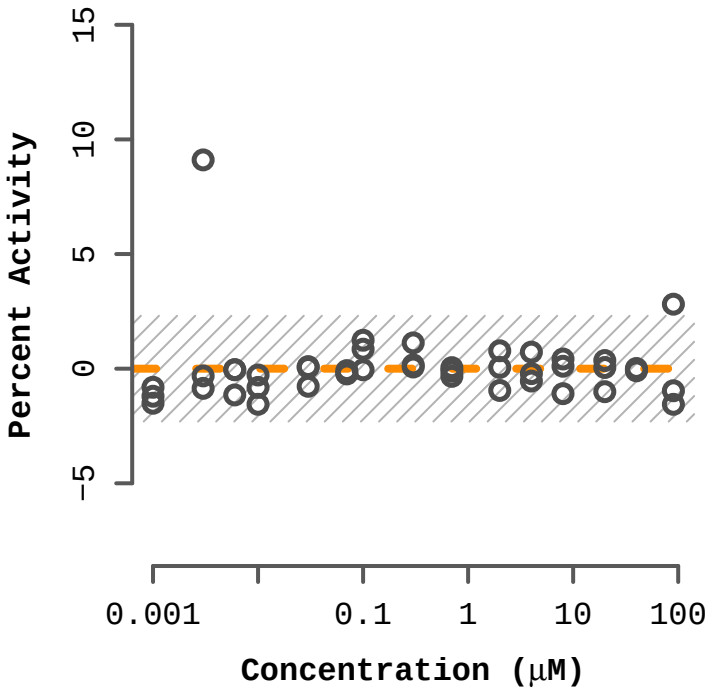
NAME: (Z)−1,2−Dichloroethylene
CHID: 24030 **CASRN:** 156−59−2
SPID(S): Tox21_200003
M4ID: 12482249

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

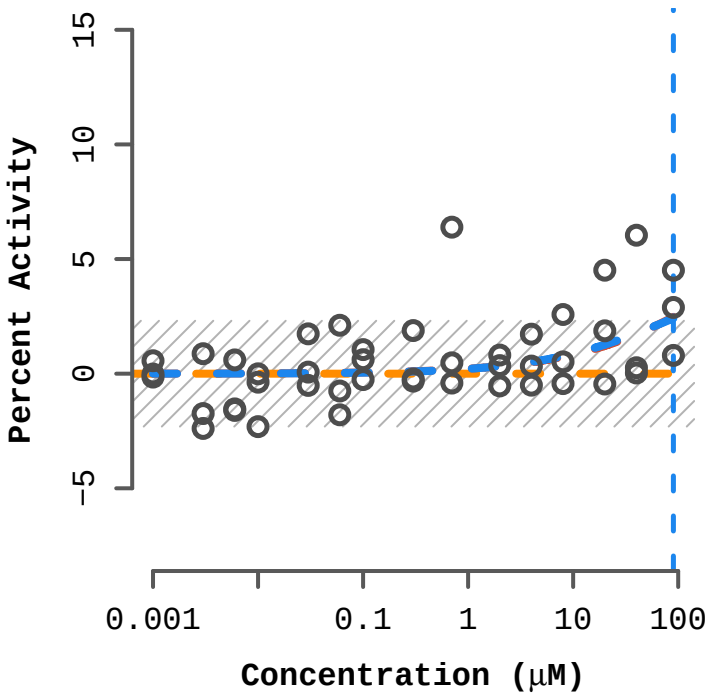
NAME: (E)−1,2−Dichloroethylene
CHID: 24031 **CASRN:** 156−60−5
SPID(S): Tox21_303130
M4ID: 12476003

HILL MODEL: Not applicable.

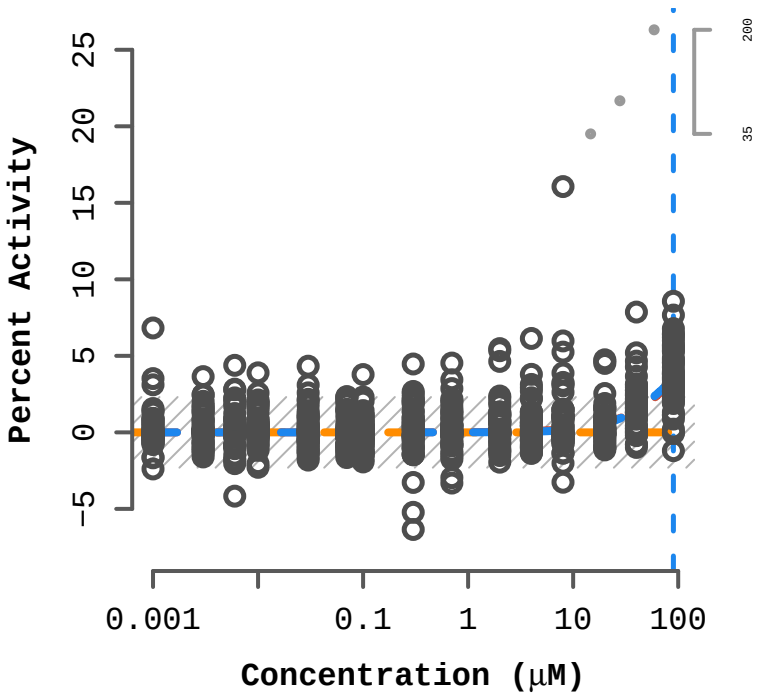
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 2.65 **MAX_MED:** 0.85 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (E)-1,2-Dichloroethylene
CHID:    24031   CASRN: 156-60-5
SPID(S): Tox21_202419
M4ID:    12479833

HILL MODEL (in red):
      tp       ga       gw
val:  7.57     2.45     0.625
sd:   25.7     3.61     0.452

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.83     1.95     0.687    3.55     5.02
sd:   9.95     2.34     0.525    2600     8240

      CNST        HILL        GNLS
AIC:  182.76      178         182.09
PROB: 0.08        0.82        0.11
RMSE: 2           1.7         1.69

MAX_MEAN: 2.73      MAX_MED: 2.89      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-DB
CHID: 24035 CASRN: 94-82-6
SPID(S): Tox21_400080
M4ID: 12475057 BRK

HILL MODEL (in red):

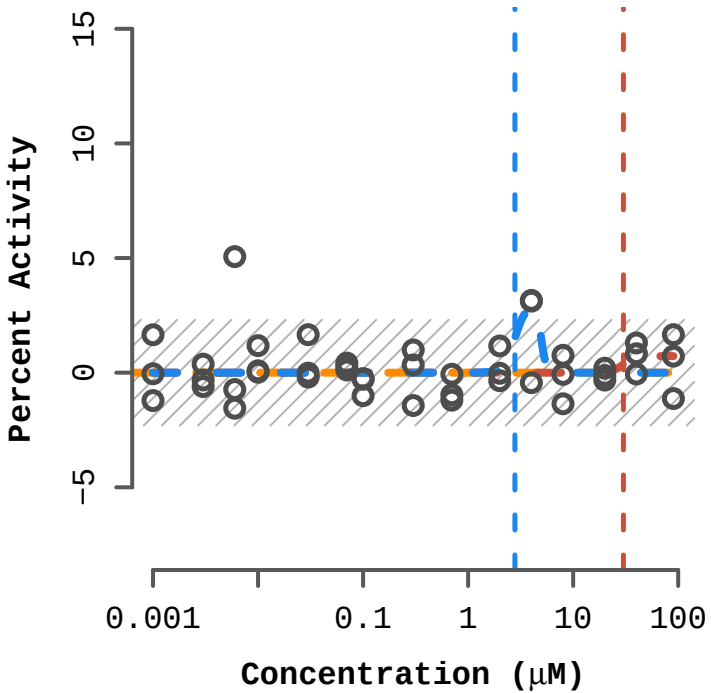
	tp	ga	gw
val:	18.6	2.45	1.26
sd:	34	0.891	0.325

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.02	1.95	1.63	3.94	3.52
sd:	5.3	0.399	0.621	943	1680

	CNST	HILL	GNLS
AIC:	2827.2	2587.04	2592.09
PROB:	0	0.93	0.07
RMSE:	8.47	8.27	8.27

MAX_MEAN: 7.69 MAX_MED: 3.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dichloro-1-propanol
CHID: 24038 CASRN: 616-23-9
SPID(S): Tox21_200342
M4ID: 12481910

HILL MODEL (in red):

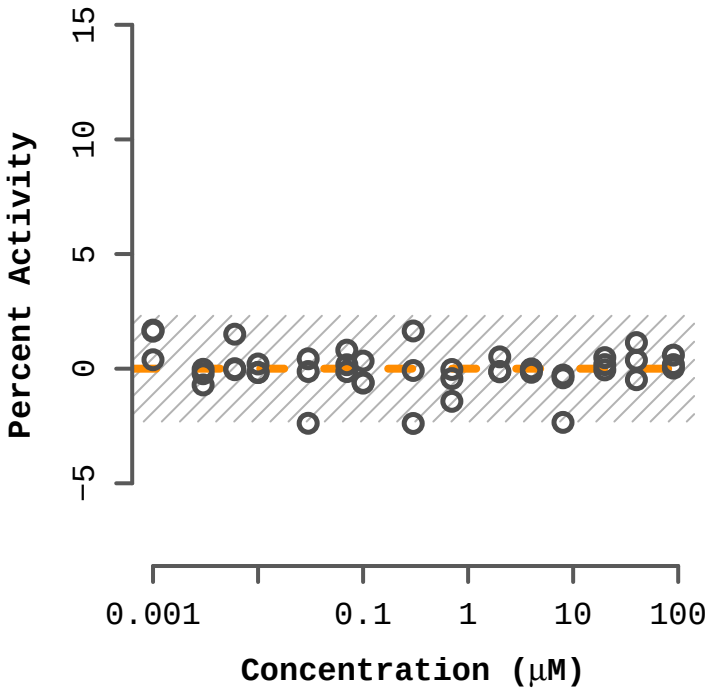
	tp	ga	gw
val:	0.722	1.48	8
sd:	0.488	0.291	14.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.03	0.445	8	0.695	18
sd:	13	1.38	66.6	2.76	238

	CNST	HILL	GNLS
AIC:	143.02	146.39	145.56
PROB:	0.68	0.13	0.19
RMSE:	1.29	1.28	1.21

MAX_MEAN: 1.95 MAX_MED: 3.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

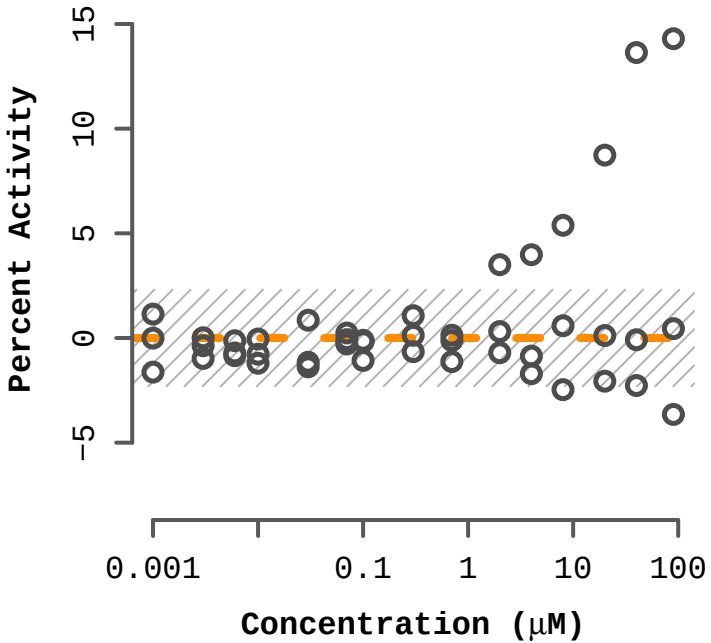
NAME: Diethyl sulfate
CHID: 24045 CASRN: 64-67-5
SPID(S): Tox21_300169
M4ID: 12478961

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.24 MAX_MED: 1.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

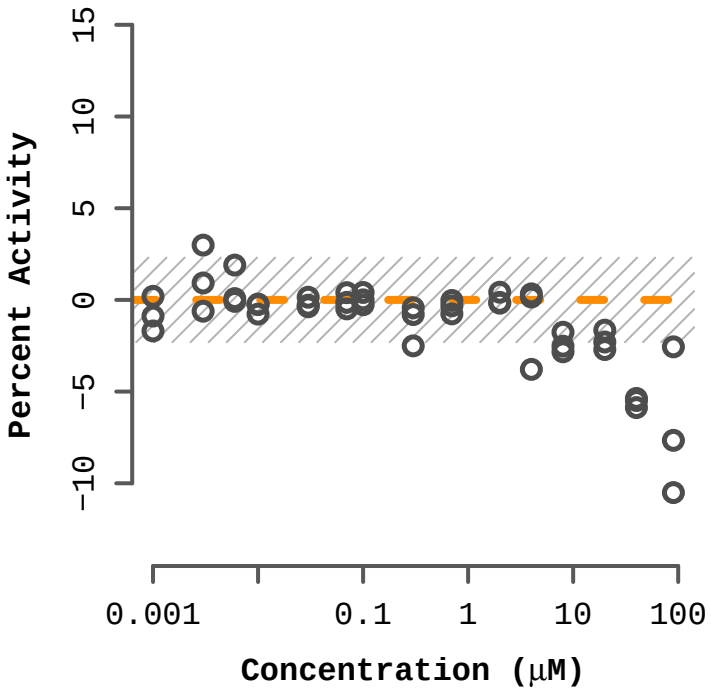
NAME: Diethyl sulfate
CHID: 24045 **CASRN:** 64-67-5
SPID(S): Tox21_202402
M4ID: 12479850

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 3.76 **MAX_MED:** 0.588 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

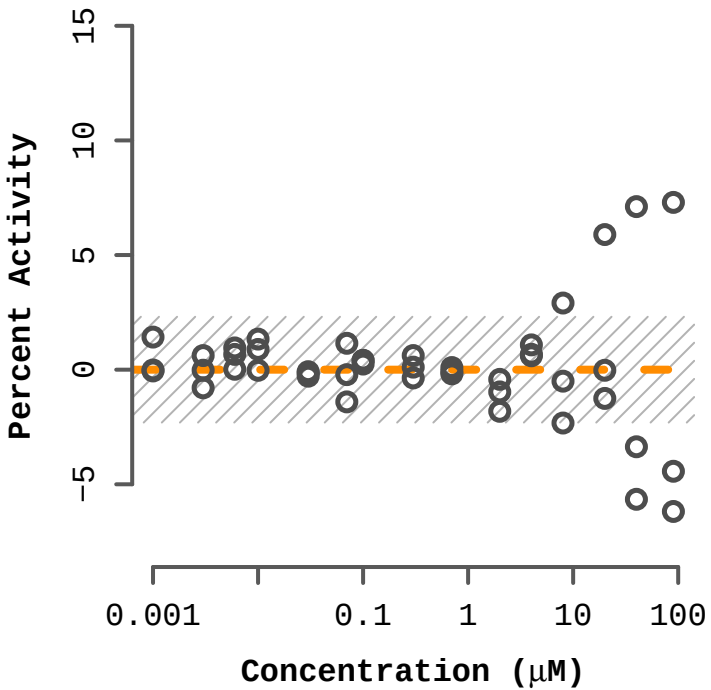
NAME: Paraoxon
CHID: 24046 **CASRN:** 311-45-5
SPID(S): Tox21_303047
M4ID: 12476086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.66	NA	NA
PROB:	1	NA	NA
RMSE:	2.76	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.925 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

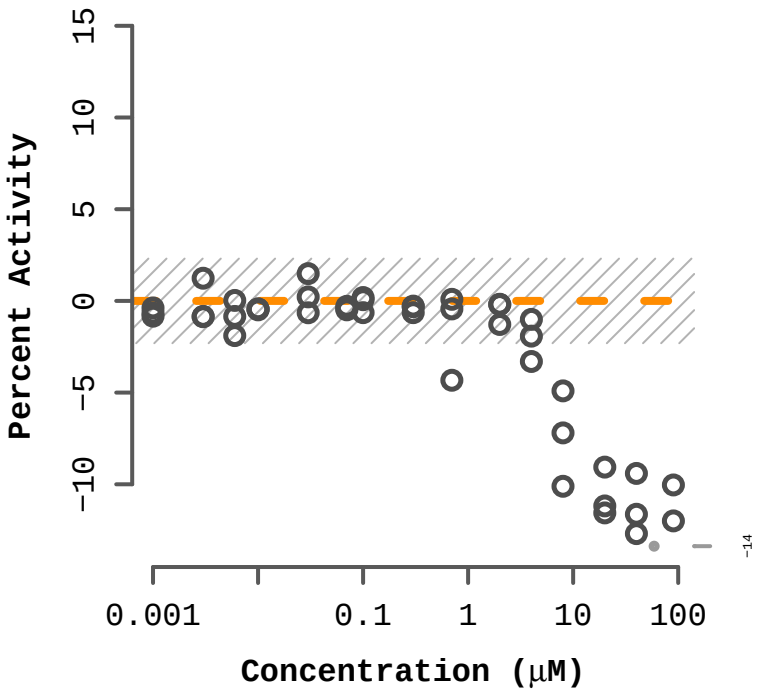
NAME: Paraoxon
CHID: 24046 **CASRN:** 311-45-5
SPID(S): Tox21_202424
M4ID: 12479828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.56	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

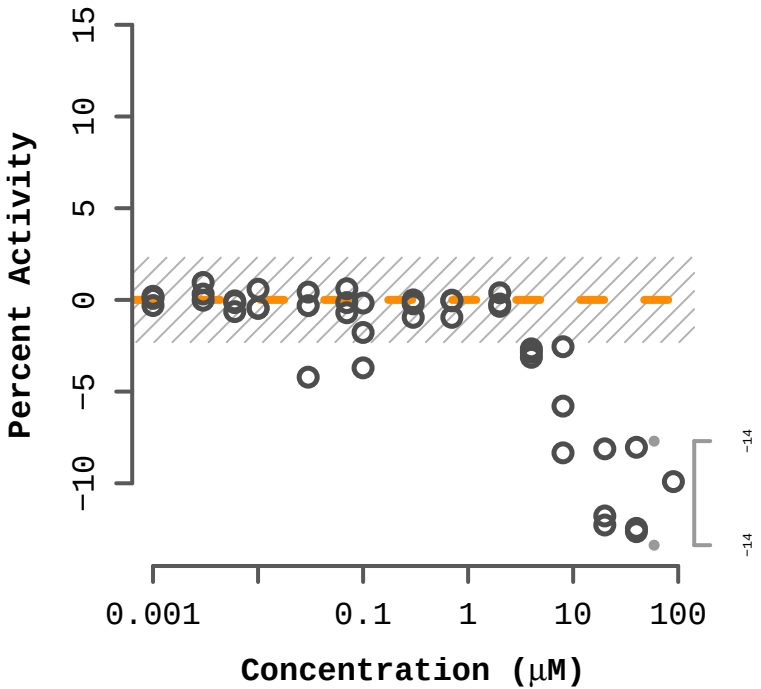
NAME: Difenzoquat metilsulfate
CHID: 24048 **CASRN:** 43222-48-6
SPID(S): Tox21_300708
M4ID: 12478425 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.08	NA	NA
PROB:	1	NA	NA
RMSE:	5.55	NA	NA

MAX_MEAN: 0.356 **MAX_MED:** 0.221 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

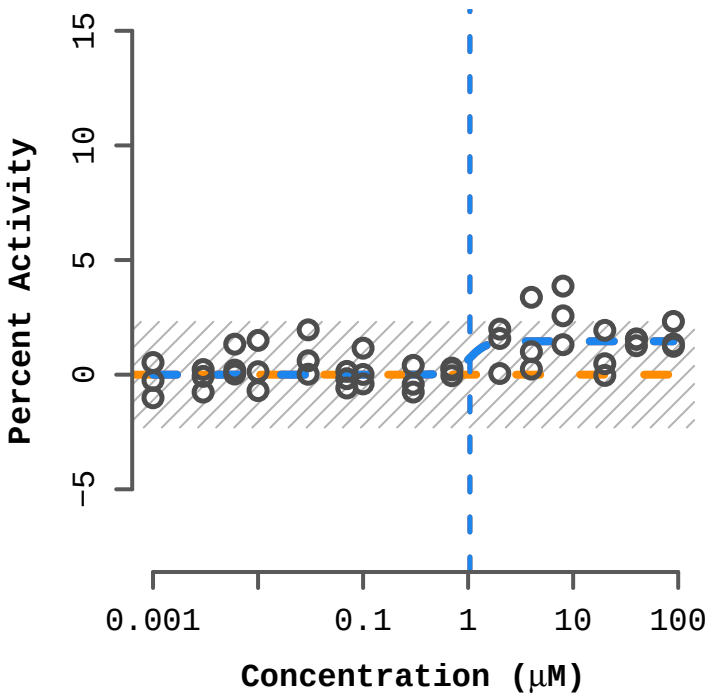
NAME: Difenzoquat metilsulfate
CHID: 24048 **CASRN:** 43222-48-6
SPID(S): Tox21_201486
M4ID: 12480766 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	274.78	NA	NA
PROB:	1	NA	NA
RMSE:	5.58	NA	NA

MAX_MEAN: 0.42 **MAX_MED:** 0.321 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diflubenzuron
CHID: 24049 CASRN: 35367-38-5
SPID(S): Tox21_303138
M4ID: 12475995

HILL MODEL (in red):

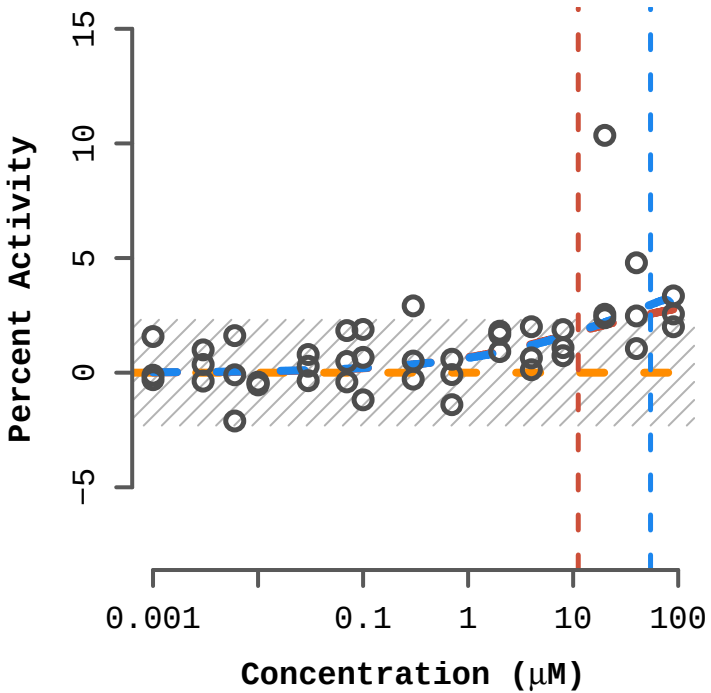
	tp	ga	gw
val:	1.46	0.0169	5.49
sd:	0.221	0.519	15.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.46	0.0168	5.49	2.61	13.3
sd:	0.221	0.52	15.4	1740	35300

	CNST	HILL	GNLS
AIC:	150.35	119.27	123.27
PROB:	0	0.88	0.12
RMSE:	1.29	0.85	0.85

MAX_MEAN: 2.58 MAX_MED: 2.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diflubenzuron
CHID: 24049 CASRN: 35367-38-5
SPID(S): Tox21_201969
M4ID: 12480283

HILL MODEL (in red):

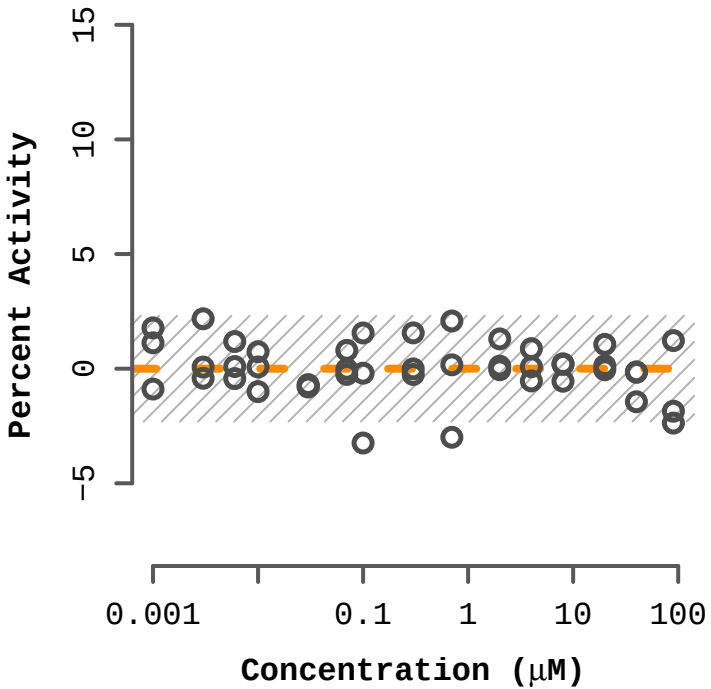
	tp	ga	gw
val:	3.55	1.05	0.606
sd:	2.06	1	0.433

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.93	1.74	0.526	1.99	17.3
sd:	11.4	2.77	0.364	0.0408	28.6

	CNST	HILL	GNLS
AIC:	185.8	152.15	155.76
PROB:	0	0.86	0.14
RMSE:	2.22	1.59	1.57

MAX_MEAN: 5.1 MAX_MED: 2.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

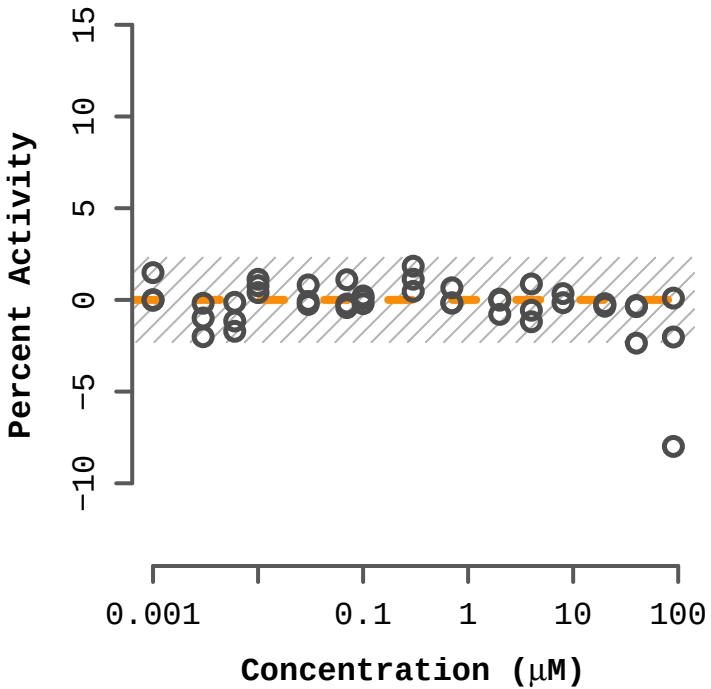
NAME: Diisopropyl methylphosphonate
CHID: 24051 **CASRN:** 1445-75-6
SPID(S): Tox21_300474
M4ID: 12478658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.674 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

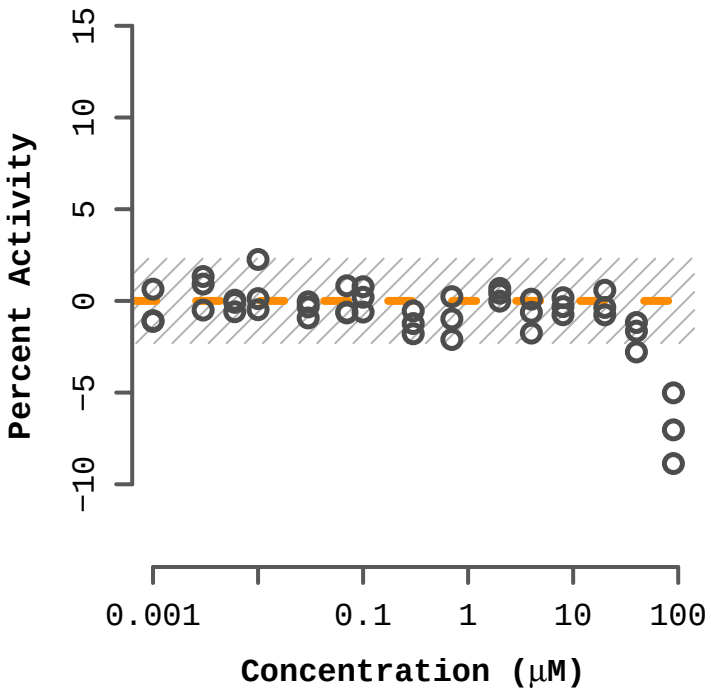
NAME: Diisopropyl methylphosphonate
CHID: 24051 **CASRN:** 1445-75-6
SPID(S): Tox21_201712
M4ID: 12480540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

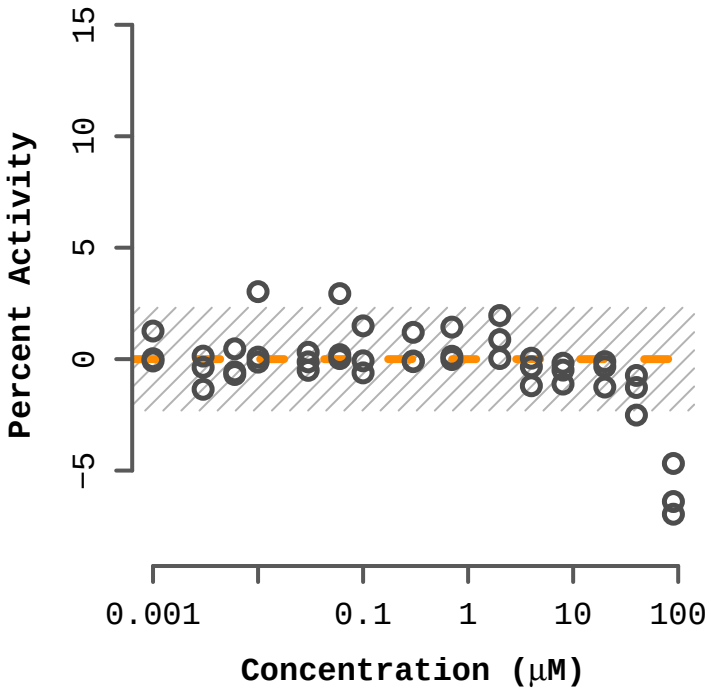
NAME: Dimethipin
CHID: 24052 **CASRN:** 55290-64-7
SPID(S): Tox21_300423
M4ID: 12478709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.75	NA	NA
PROB:	1	NA	NA
RMSE:	2.09	NA	NA

MAX_MEAN: 0.637 **MAX_MED:** 0.918 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

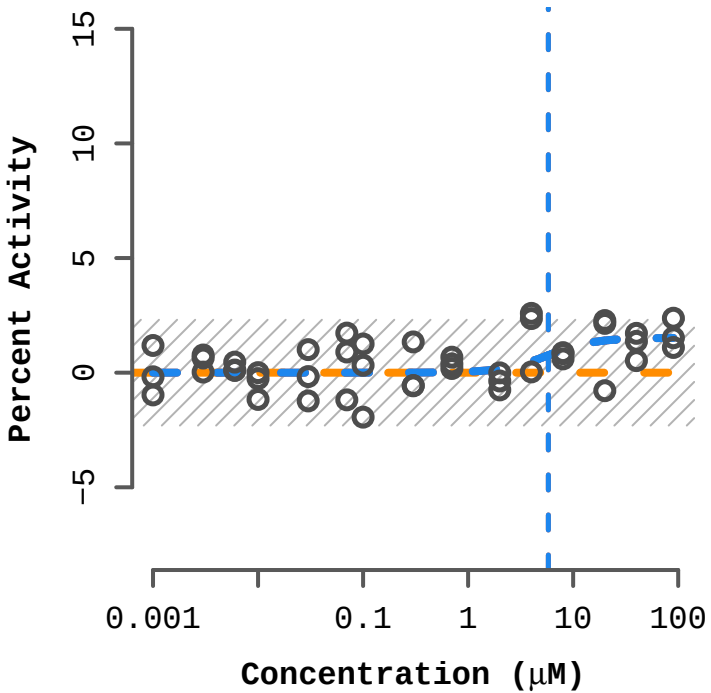
NAME: Dimethipin
CHID: 24052 **CASRN:** 55290-64-7
SPID(S): Tox21_201644
M4ID: 12480608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.87	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.879 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethyl sulfate
CHID: 24055 CASRN: 77-78-1
SPID(S): Tox21_300636
M4ID: 12478497

HILL MODEL (in red):

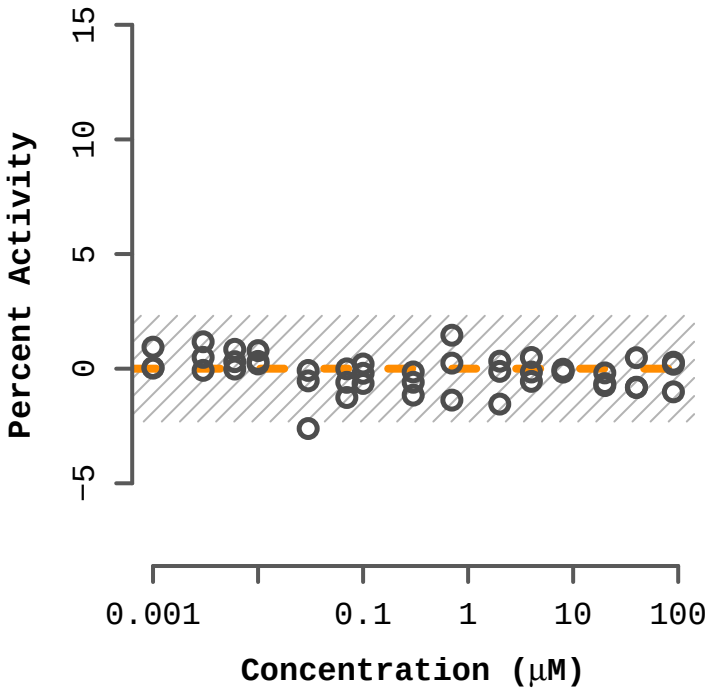
	tp	ga	gw
val:	1.52	0.764	1.98
sd:	0.365	0.288	1.73

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.52	0.764	1.99	3.47	4.35
sd:	0.365	0.288	1.73	586	1710

	CNST	HILL	GNLS
AIC:	146.31	130.74	134.74
PROB:	0	0.88	0.12
RMSE:	1.16	0.93	0.93

MAX_MEAN: 1.67 MAX_MED: 2.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

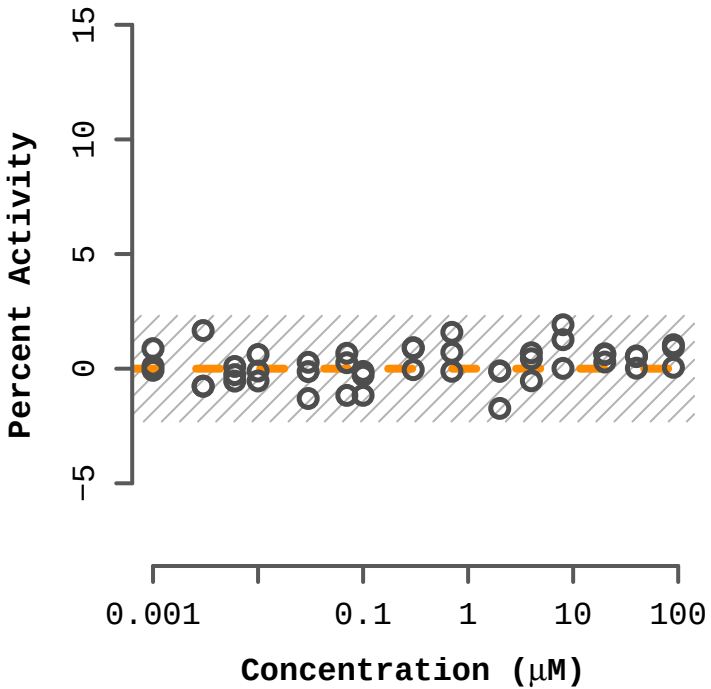
NAME: Dimethyl sulfate
CHID: 24055 **CASRN:** 77-78-1
SPID(S): Tox21_202032
M4ID: 12480220

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.532 **MAX_MED:** 0.494 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

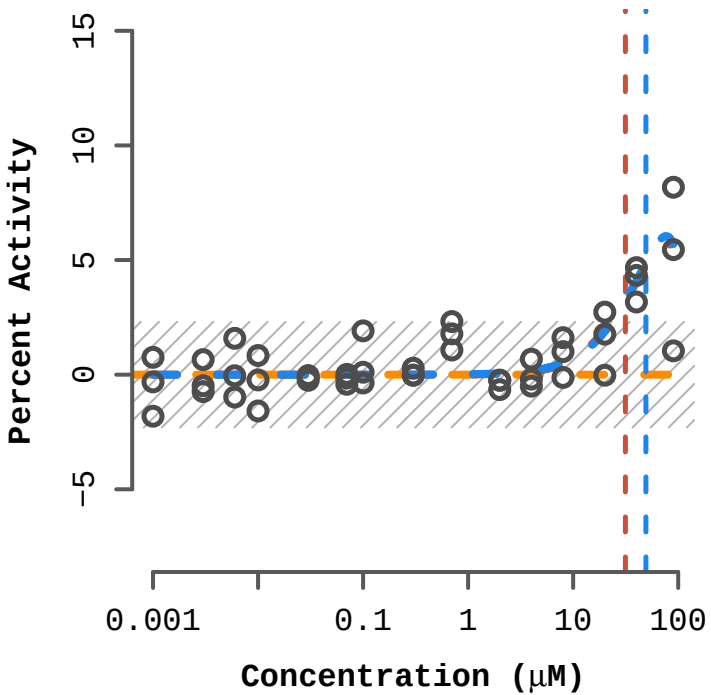
NAME: Dimethylamine
CHID: 24057 **CASRN:** 124-40-3
SPID(S): Tox21_302439
M4ID: 12476694

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−Dimethylbenzidine
CHID: 24059 CASRN: 119−93−7
SPID(S): Tox21_300278
M4ID: 12478852

HILL MODEL (in red):

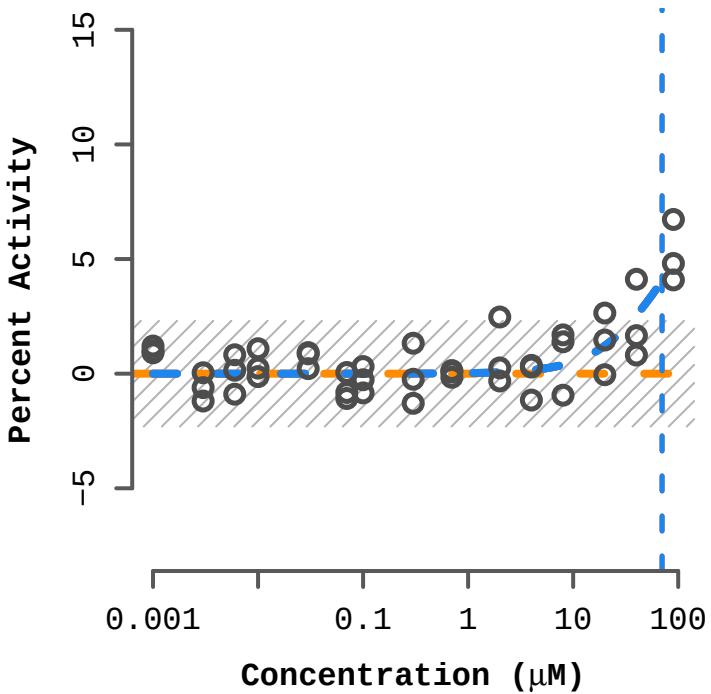
	tp	ga	gw
val:	6.58	1.5	1.87
sd:	1.82	0.164	0.794

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.81	1.69	1.6	2.05	6.44
sd:	47.7	2.18	2.11	5.85	453

	CNST	HILL	GNLS
AIC:	177.6	141.62	145.46
PROB:	0	0.87	0.13
RMSE:	2.05	1.19	1.18

MAX_MEAN: 4.89 MAX_MED: 5.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−Dimethylbenzidine
CHID: 24059 CASRN: 119−93−7
SPID(S): Tox21_201292
M4ID: 12480960

HILL MODEL (in red):

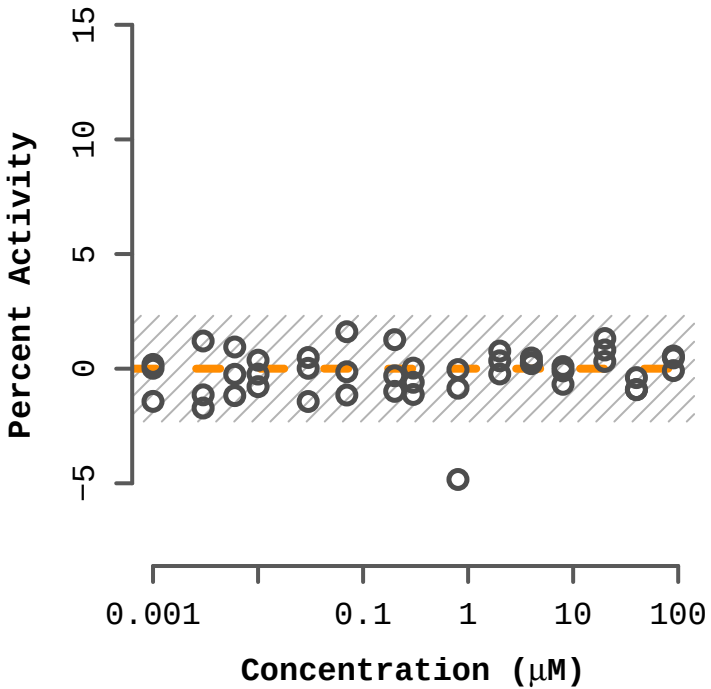
	tp	ga	gw
val:	8.07	1.85	1.38
sd:	4.49	0.374	0.612

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.07	1.85	1.38	3.44	5.61
sd:	4.49	0.374	0.612	2040	7730

	CNST	HILL	GNLS
AIC:	168.7	136.98	140.98
PROB:	0	0.88	0.12
RMSE:	1.79	0.97	0.97

MAX_MEAN: 5.21 MAX_MED: 4.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

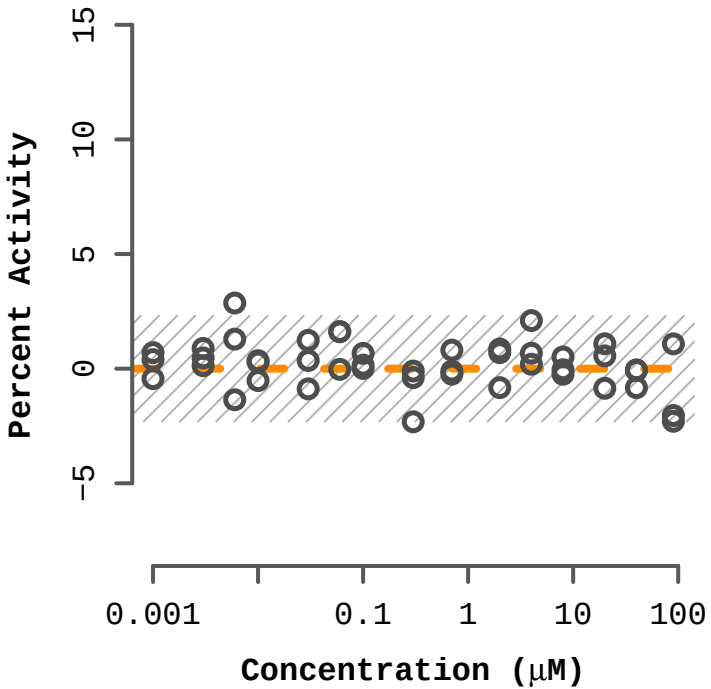
NAME: 3,4-Dimethylphenol
CHID: 24062 **CASRN:** 95-65-8
SPID(S): Tox21_300185
M4ID: 12478945

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.817 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

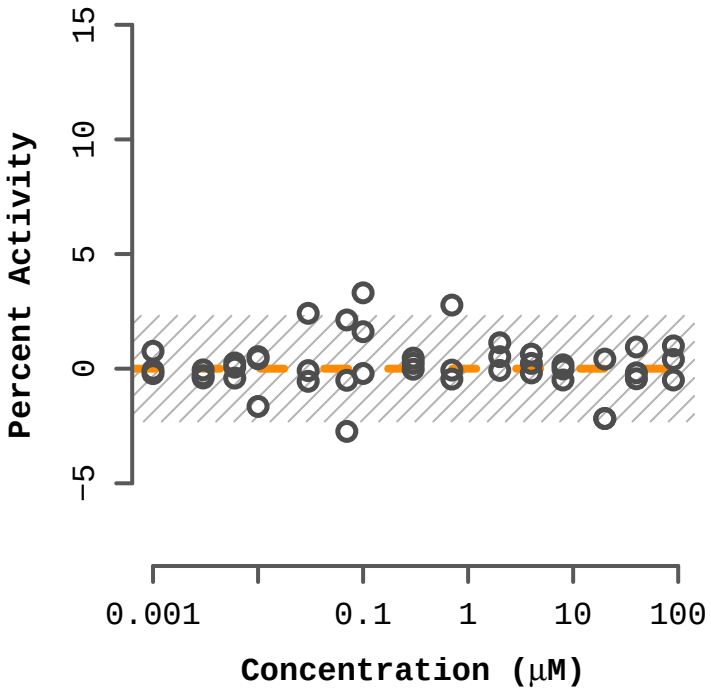
NAME: 3,4-Dimethylphenol
CHID: 24062 **CASRN:** 95-65-8
SPID(S): Tox21_201523
M4ID: 12480729

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

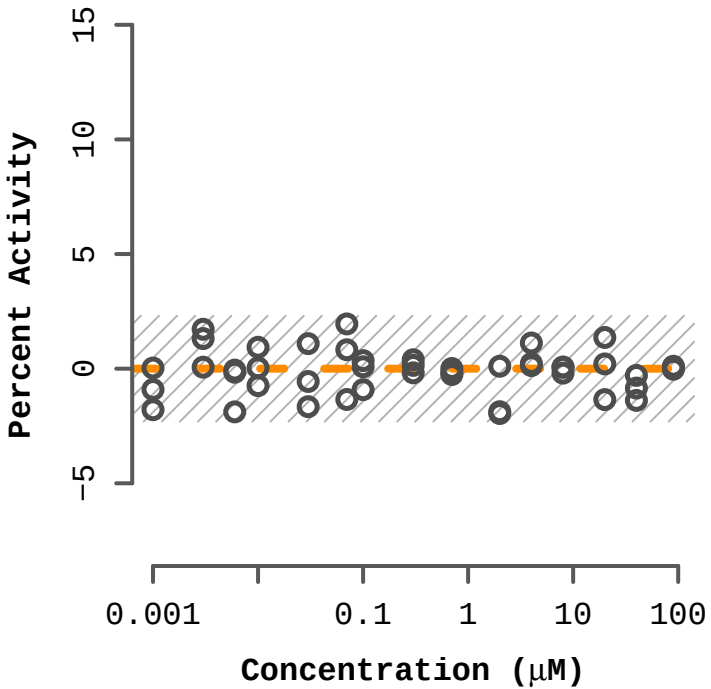
NAME: 2,6-Dimethylphenol
CHID: 24063 **CASRN:** 576-26-1
SPID(S): Tox21_300157
M4ID: 12478973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

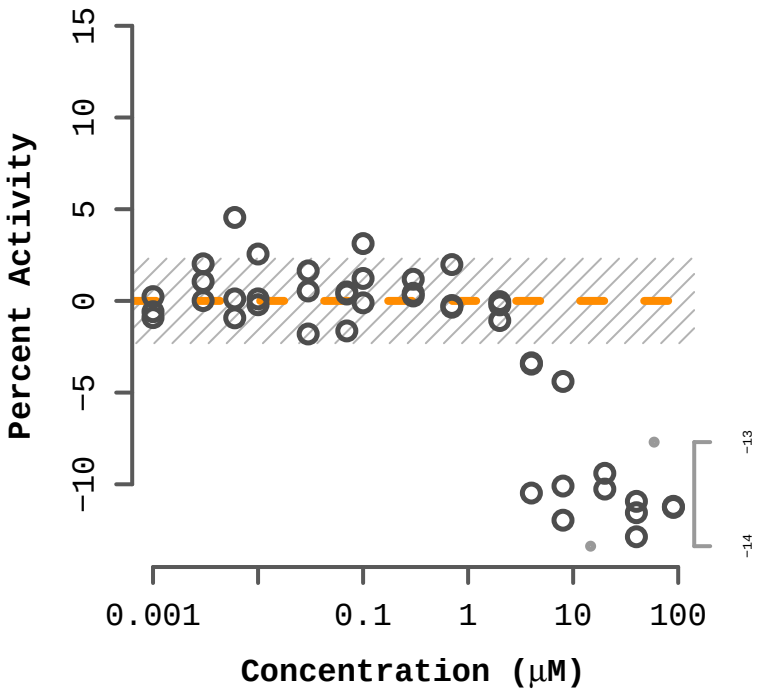
NAME: 2,6-Dimethylphenol
CHID: 24063 **CASRN:** 576-26-1
SPID(S): Tox21_201274
M4ID: 12480978

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

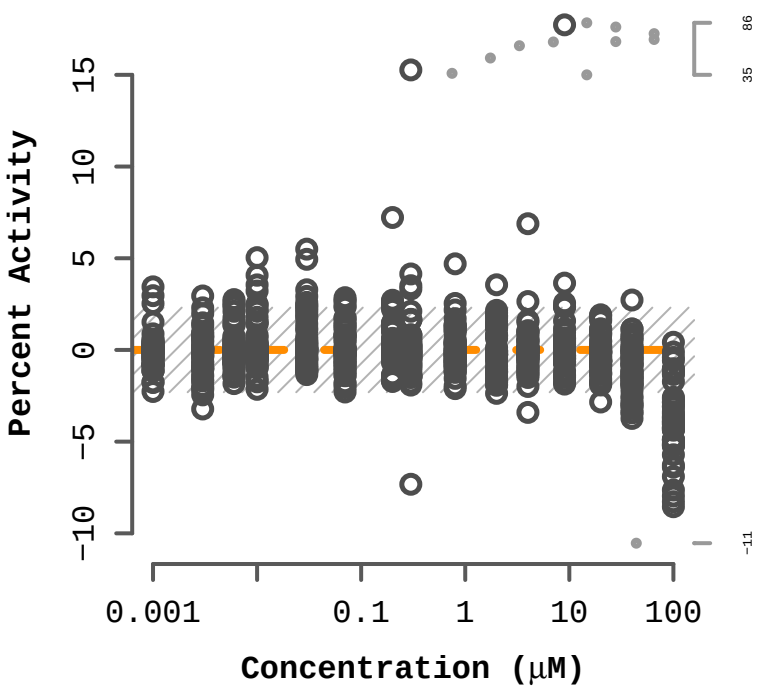
NAME: Dinex
CHID: 24064 **CASRN:** 131-89-5
SPID(S): Tox21_200872
M4ID: 12481380 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.06	NA	NA
PROB:	1	NA	NA
RMSE:	6.14	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

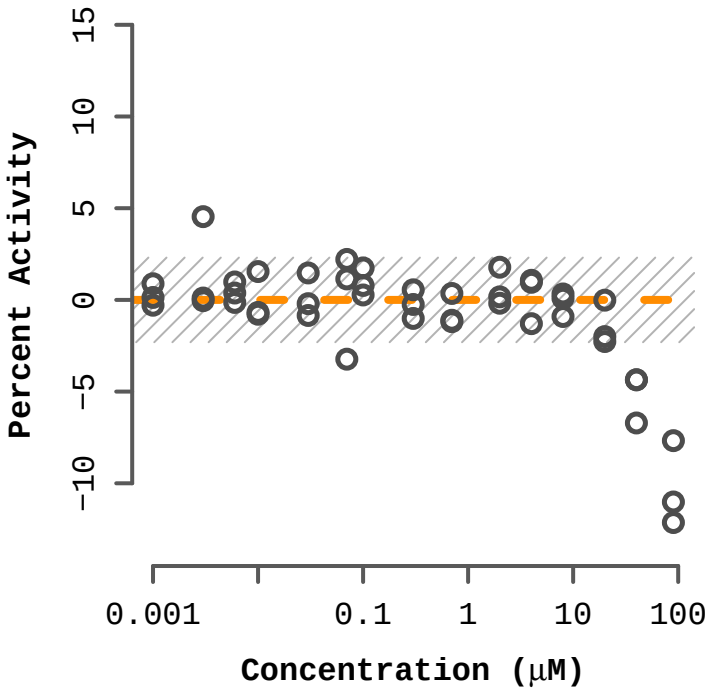
NAME: 1,3-Dinitrobenzene
CHID: 24065 **CASRN:** 99-65-0
SPID(S): Tox21_400032
M4ID: 12475105 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3157.19	NA	NA
PROB:	1	NA	NA
RMSE:	7.69	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 0.0639 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

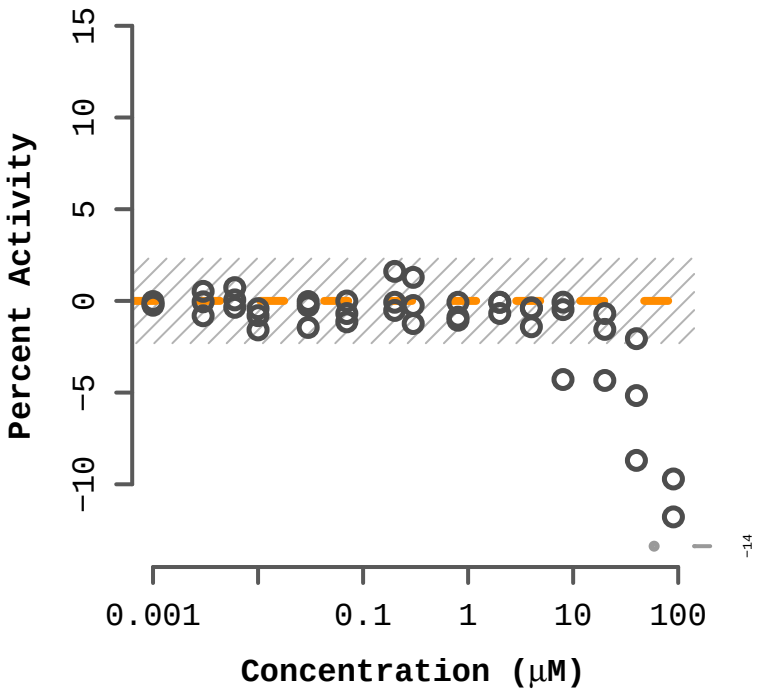
NAME: 1,2-Dinitrobenzene
CHID: 24066 **CASRN:** 528-29-0
SPID(S): Tox21_300418
M4ID: 12478714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.65	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

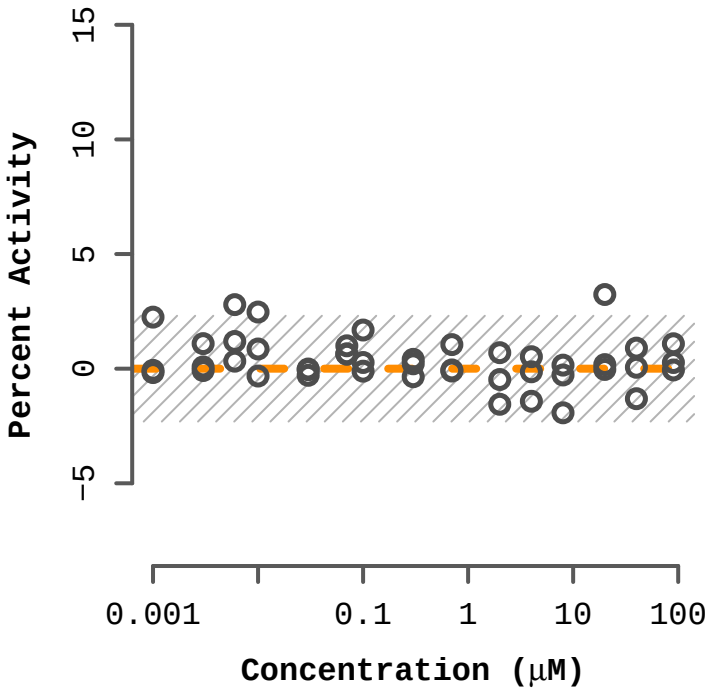
NAME: 1,2-Dinitrobenzene
CHID: 24066 **CASRN:** 528-29-0
SPID(S): Tox21_201580
M4ID: 12480672 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.3	NA	NA
PROB:	1	NA	NA
RMSE:	3.68	NA	NA

MAX_MEAN: 0.34 **MAX_MED:** 0.0574 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

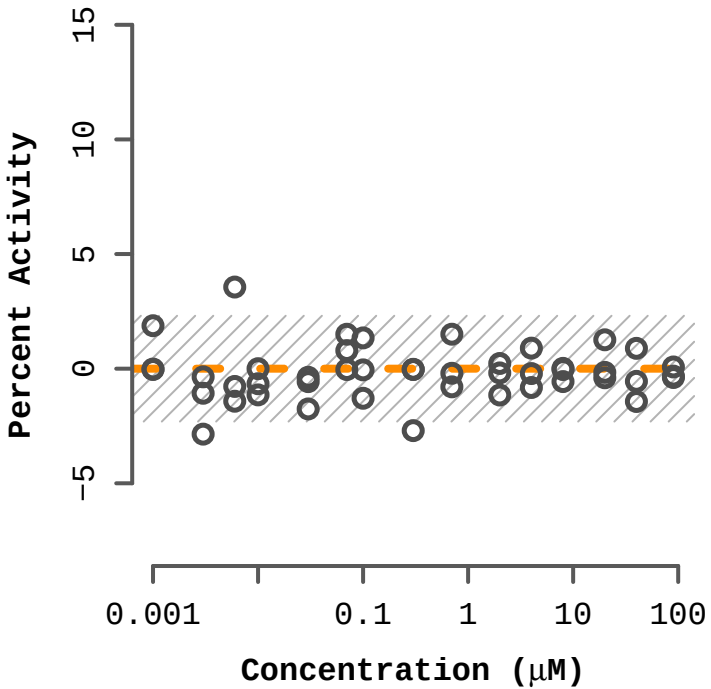
NAME: Diphenamid
CHID: 24072 CASRN: 957-51-7
SPID(S): Tox21_303077
M4ID: 12476056

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.44 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

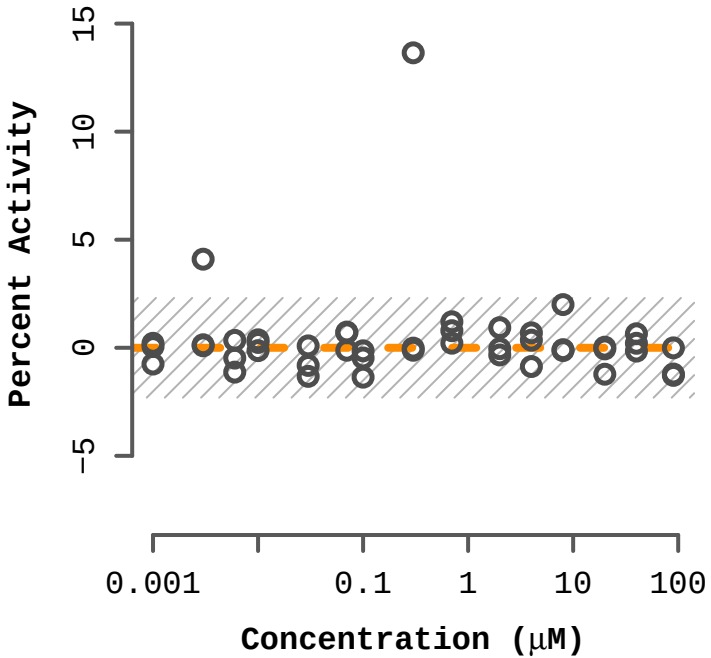
NAME: Diphenamid
CHID: 24072 CASRN: 957-51-7
SPID(S): Tox21_201282
M4ID: 12480970

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.752 MAX_MED: 0.791 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

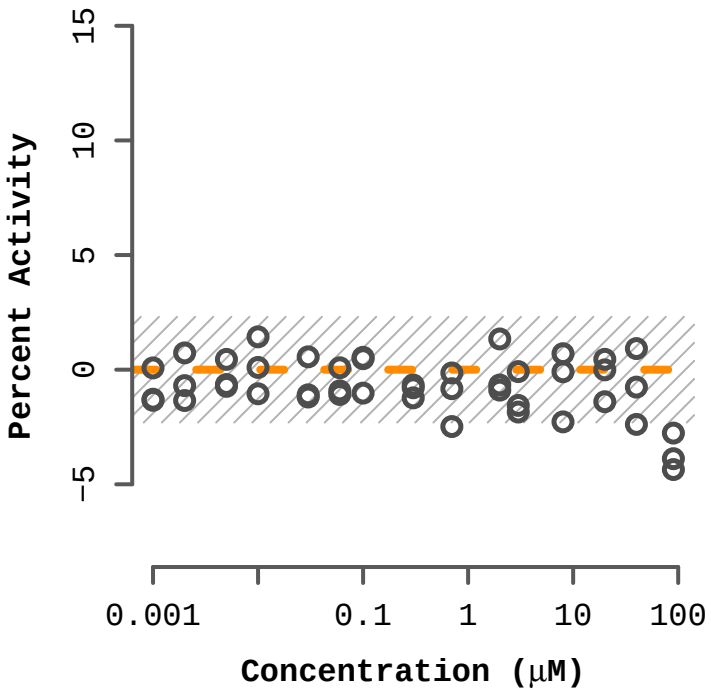
NAME: 1,4-Dithiane
CHID: 24077 CASRN: 505-29-3
SPID(S): Tox21_200405
M4ID: 12481847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 4.51 MAX_MED: 0.792 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

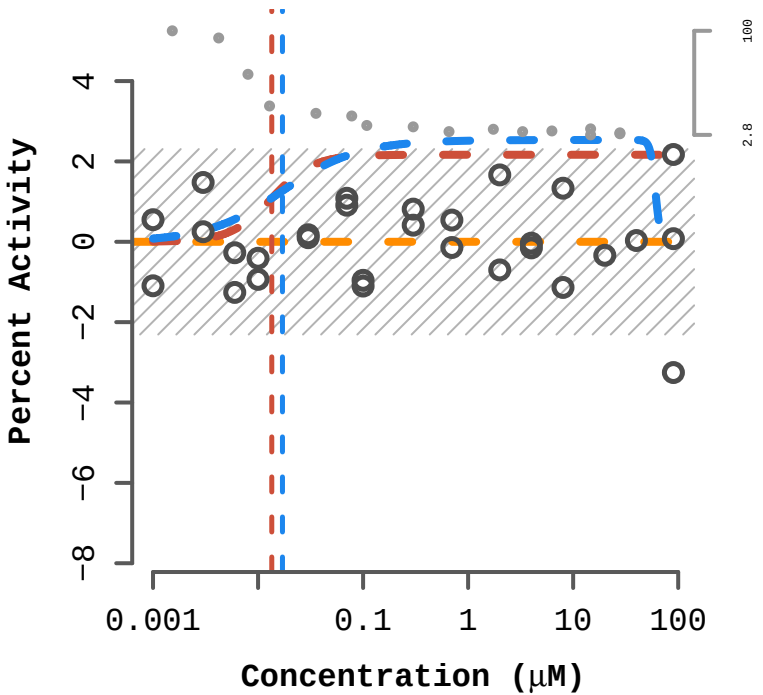
NAME: Endothal
CHID: 24081 **CASRN:** 145-73-3
SPID(S): Tox21_300094
M4ID: 12479036

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 0.161 **MAX_MED:** 0.481 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Endothal
CHID: 24081 **CASRN:** 145-73-3
SPID(S): Tox21_202446
M4ID: 12479806 **BRK**

HILL MODEL (in red):

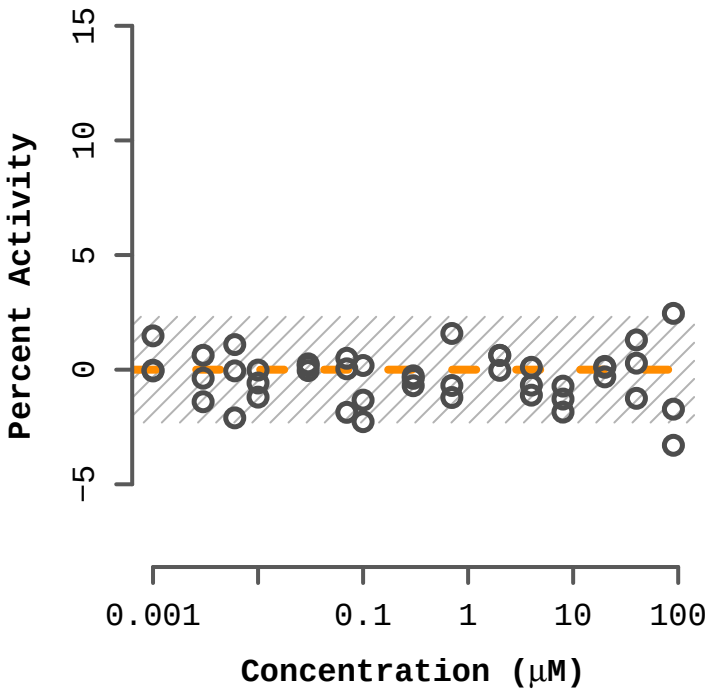
	tp	ga	gw
val:	2.17	−1.87	2.22
sd:	0.944	1.03	15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.53	−1.77	1.2	1.78	18
sd:	1.15	1.15	5.12	1.76	179

	CNST	HILL	GNLS
AIC:	350.6	350.57	353.57
PROB:	0.45	0.45	0.1
RMSE:	23.97	23.77	23.72

MAX_MEAN: 34 **MAX_MED:** 3.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

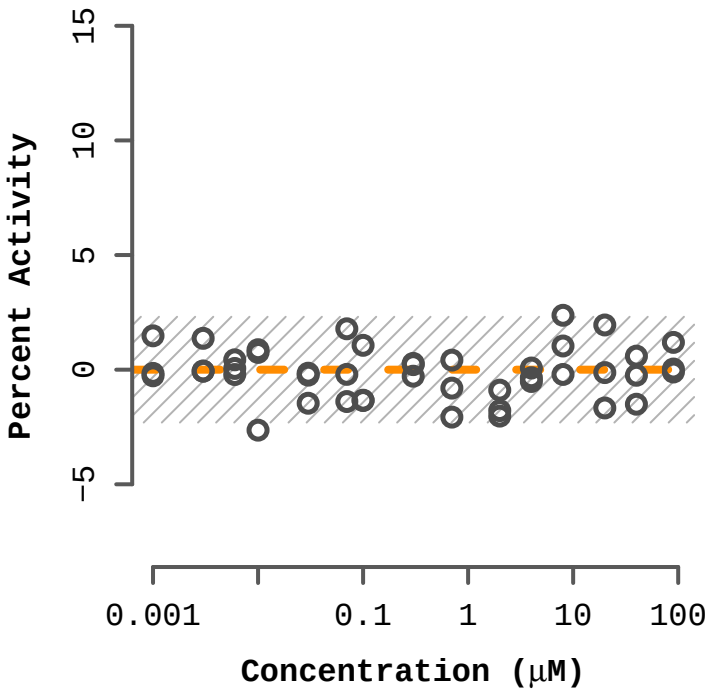
NAME: Ethephon
CHID: 24085 **CASRN:** 16672-87-0
SPID(S): Tox21_301134
M4ID: 12477999

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.467 **MAX_MED:** 0.623 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

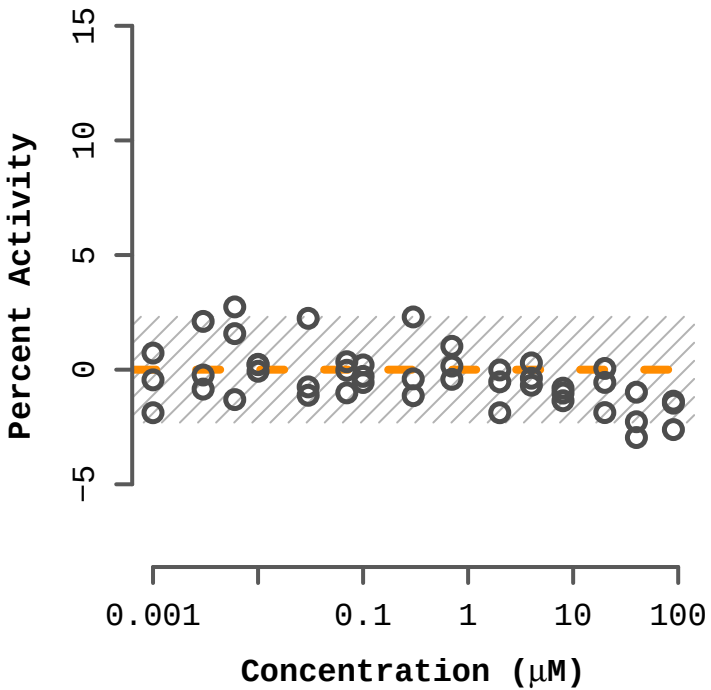
NAME: Ethephon
CHID: 24085 CASRN: 16672-87-0
SPID(S): Tox21_202118
M4ID: 12480134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.07 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

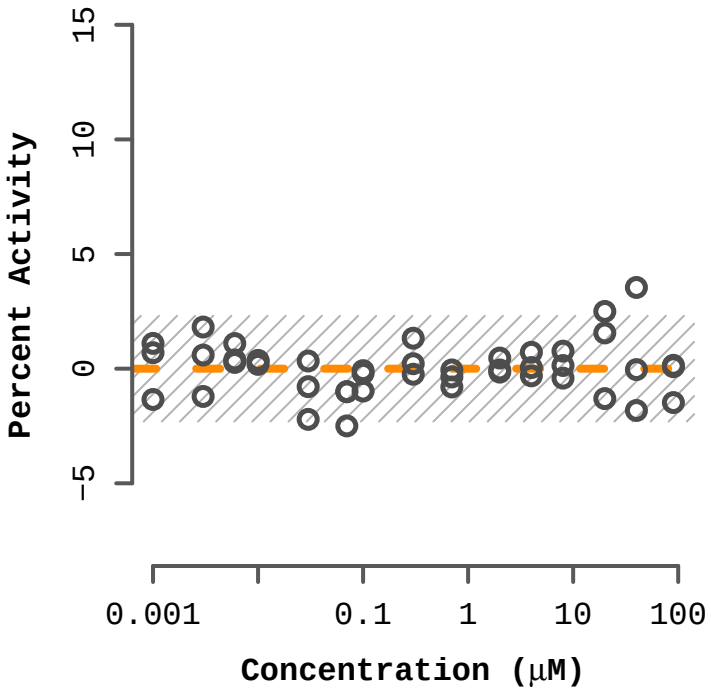
NAME: Ethion
CHID: 24086 **CASRN:** 563-12-2
SPID(S): Tox21_300175
M4ID: 12478955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

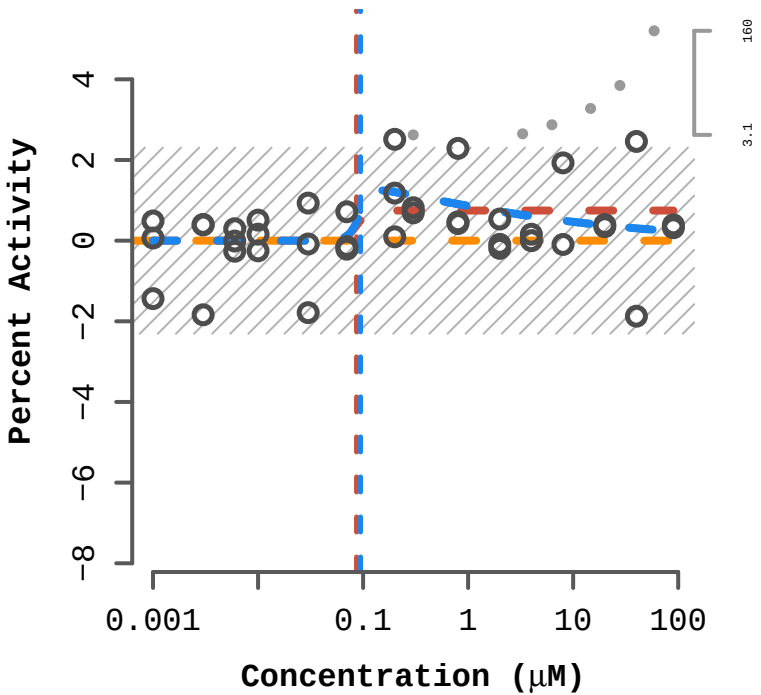
NAME: 2-Ethoxyethanol
CHID: 24087 CASRN: 110-80-5
SPID(S): Tox21_300031
M4ID: 12479099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.918 MAX_MED: 1.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethoxyethanol
CHID: 24087 **CASRN:** 110-80-5
SPID(S): Tox21_201697
M4ID: 12480555 **BRK**

HILL MODEL (in red):

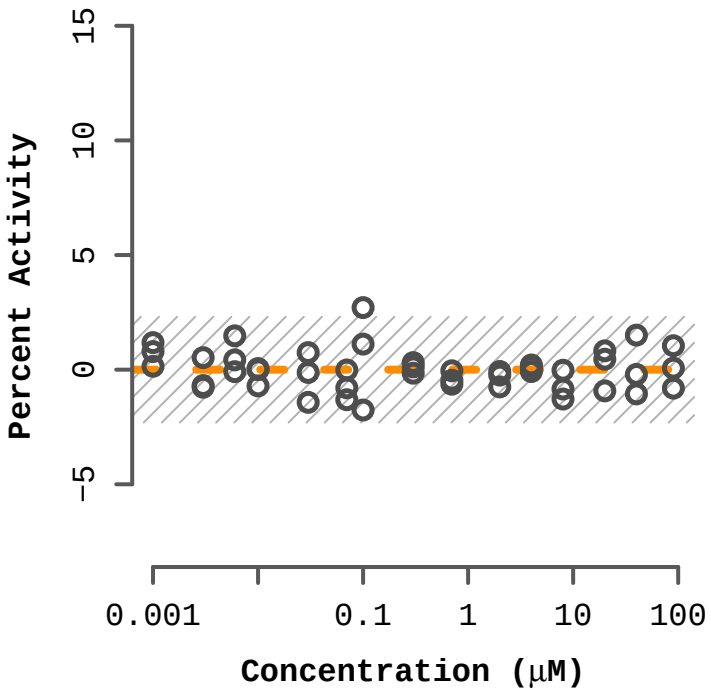
	tp	ga	gw
val:	0.746	-1.06	8
sd:	0.284	0.477	32.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.5	-1.02	7.99	-0.774	0.36
sd:	7.11	0.767	44.8	6.01	0.465

	CNST	HILL	GNLS
AIC:	271.95	270.96	273.79
PROB:	0.33	0.54	0.13
RMSE:	27.38	27.19	27.3

MAX_MEAN: 53.4 **MAX_MED:** 2.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

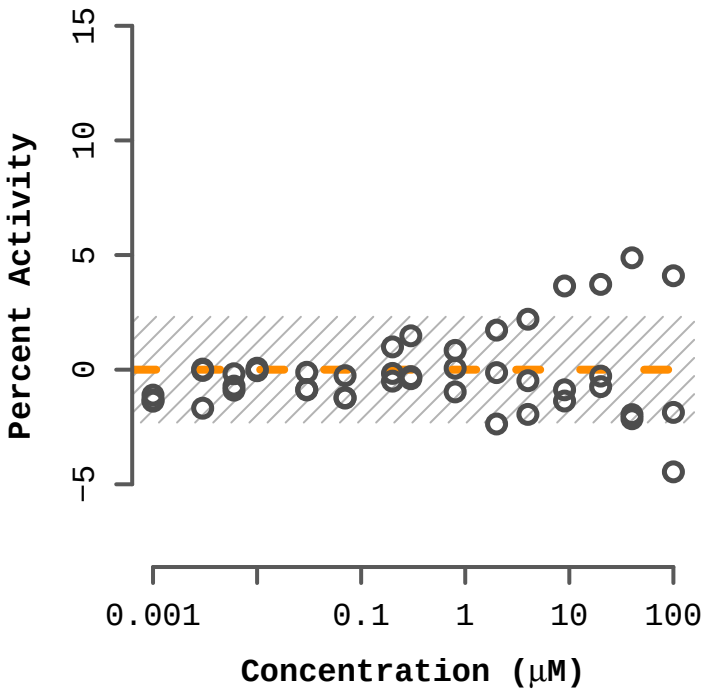
NAME: EPTC
CHID: 24091 **CASRN:** 759-94-4
SPID(S): Tox21_300727
M4ID: 12478406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.708 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

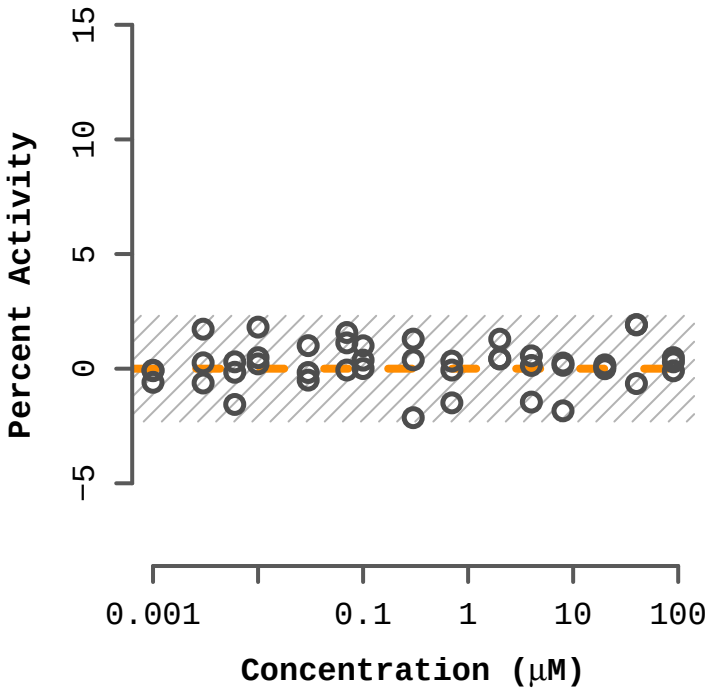
NAME: EPTC
CHID: 24091 **CASRN:** 759-94-4
SPID(S): Tox21_201962
M4ID: 12480290

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.0646 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

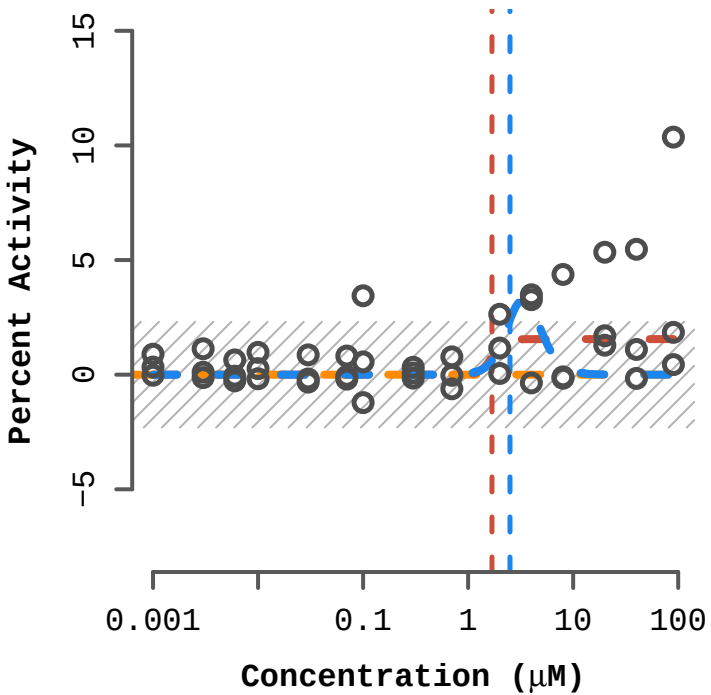
NAME: 2-Butoxyethanol
CHID: 24097 **CASRN:** 111-76-2
SPID(S): Tox21_300123
M4ID: 12479007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Butoxyethanol
CHID: 24097 CASRN: 111-76-2
SPID(S): Tox21_202399
M4ID: 12479853

HILL MODEL (in red):

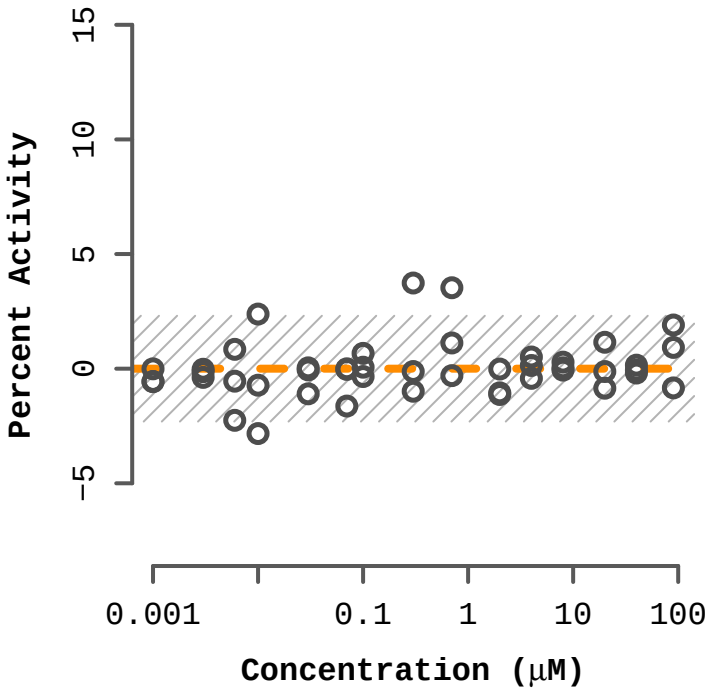
	tp	ga	gw
val:	1.55	0.227	8
sd:	0.456	0.418	37.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.17	0.398	5.01	0.648	4.36
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	181.92	171.29	182.64
PROB:	0	0.99	0
RMSE:	2.34	1.88	2.24

MAX_MEAN: 4.22 MAX_MED: 3.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

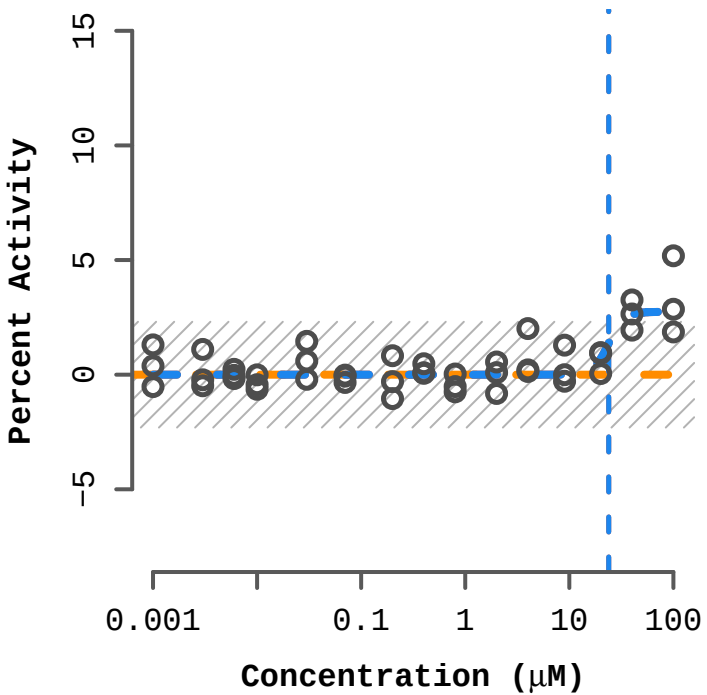
NAME: Ethyl phthalyl ethyl glycolate
CHID: 24100 CASRN: 84-72-0
SPID(S): Tox21_301488
M4ID: 12477645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.45 MAX_MED: 1.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tribenuron-methyl
CHID: 24101 **CASRN:** 101200-48-0
SPID(S): Tox21_202549
M4ID: 12479703

HILL MODEL (in red):

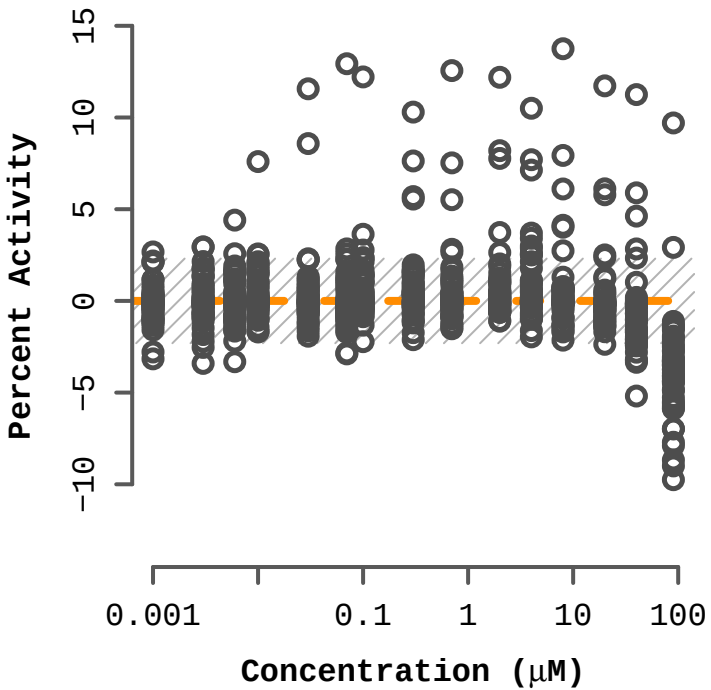
	tp	ga	gw
val:	2.74	1.38	5.96
sd:	0.492	0.112	7.43

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.74	1.38	5.96	3.89	7.27
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	141.56	104.15	108.15
PROB:	0	0.88	0.12
RMSE:	1.32	0.74	0.74

MAX_MEAN: 3.3 **MAX_MED:** 2.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

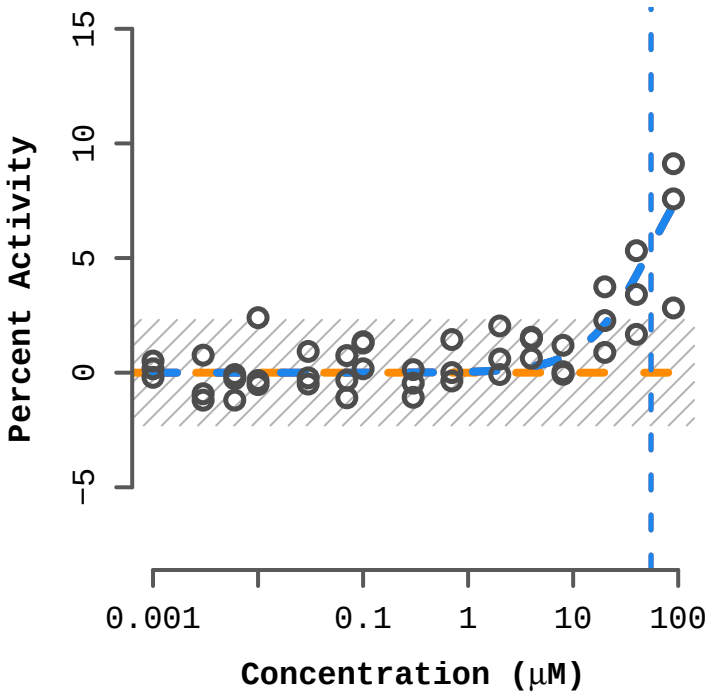
NAME: Fenamiphos
CHID: 24102 **CASRN:** 22224-92-6
SPID(S): Tox21_400081
M4ID: 12475056

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2909.1	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 0.977 **MAX_MED:** 0.327 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluoranthene
CHID: 24104 CASRN: 206-44-0
SPID(S): Tox21_300480
M4ID: 12478652

HILL MODEL (in red):

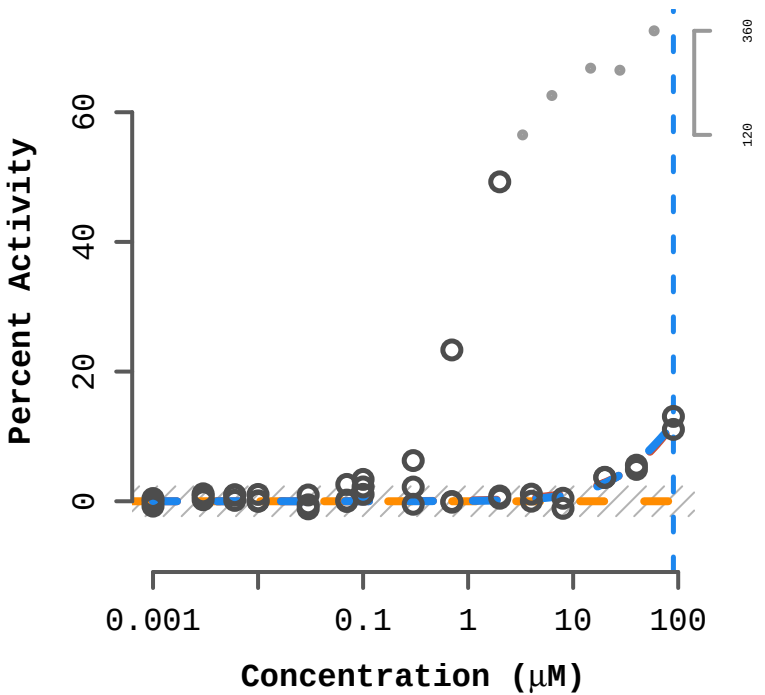
	tp	ga	gw
val:	10.9	1.74	1.41
sd:	3.72	0.231	0.469

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.9	1.74	1.41	3.37	5.46
sd:	3.73	0.231	0.469	702	2720

	CNST	HILL	GNLS
AIC:	186.21	148.53	152.53
PROB:	0	0.88	0.12
RMSE:	2.33	1.21	1.21

MAX_MEAN: 6.51 MAX_MED: 7.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluoranthene
CHID: 24104 CASRN: 206-44-0
SPID(S): Tox21_201835
M4ID: 12480417 BRK

HILL MODEL (in red):

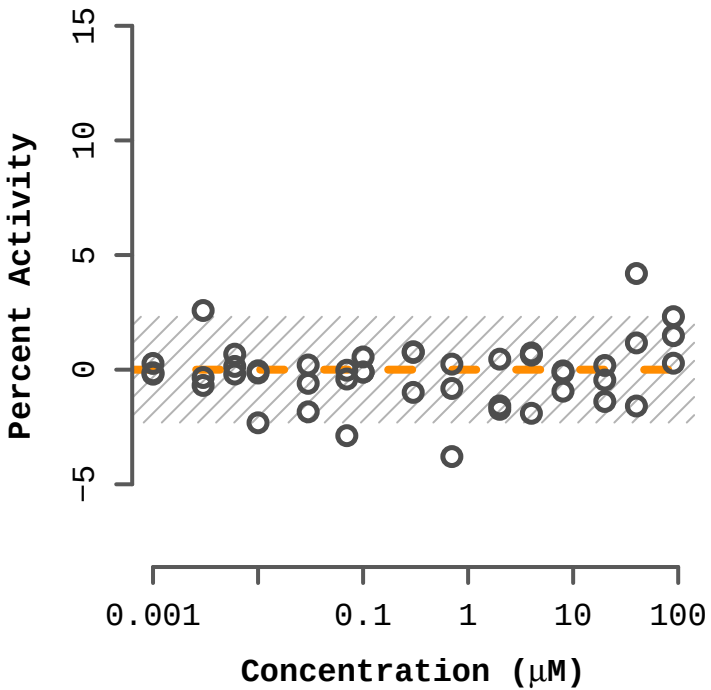
	tp	ga	gw
val:	53.8	2.45	1.08
sd:	240	2.64	0.803

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.9	1.95	1.35	3.4	4.53
sd:	32.8	0.858	0.906	605	1920

	CNST	HILL	GNLS
AIC:	433.74	421.36	425.51
PROB:	0	0.89	0.11
RMSE:	86.89	85.06	85.08

MAX_MEAN: 129 MAX_MED: 13.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

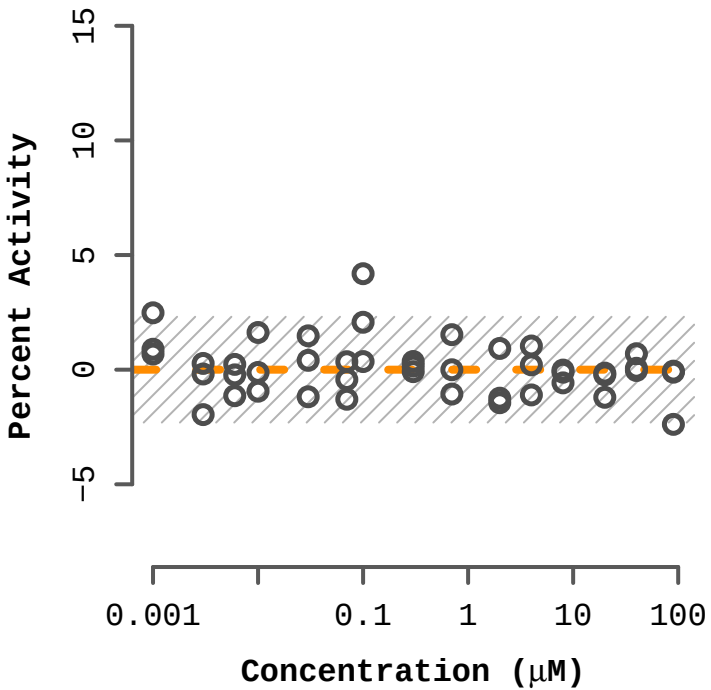
NAME: Fluorene
CHID: 24105 CASRN: 86-73-7
SPID(S): Tox21_300572
M4ID: 12478561

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.36 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

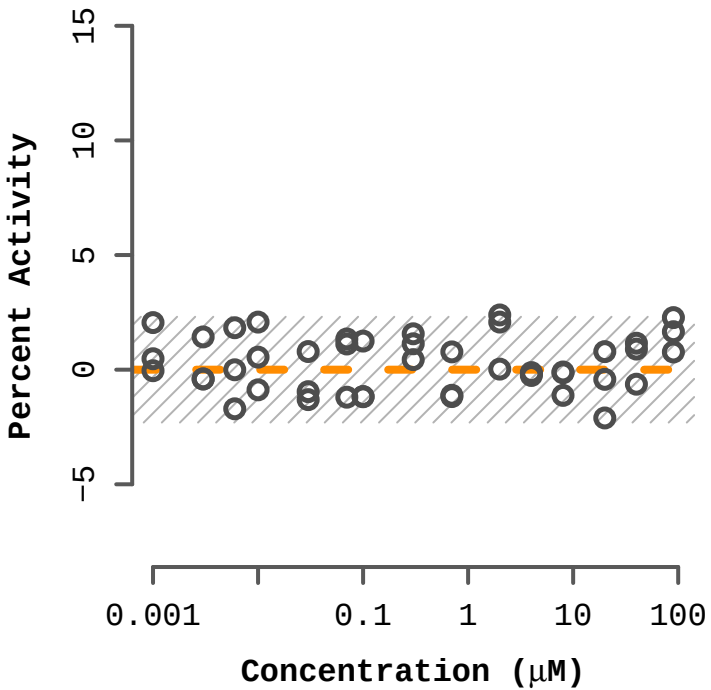
NAME: Fluorene
CHID: 24105 CASRN: 86-73-7
SPID(S): Tox21_202140
M4ID: 12480112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 2.2 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

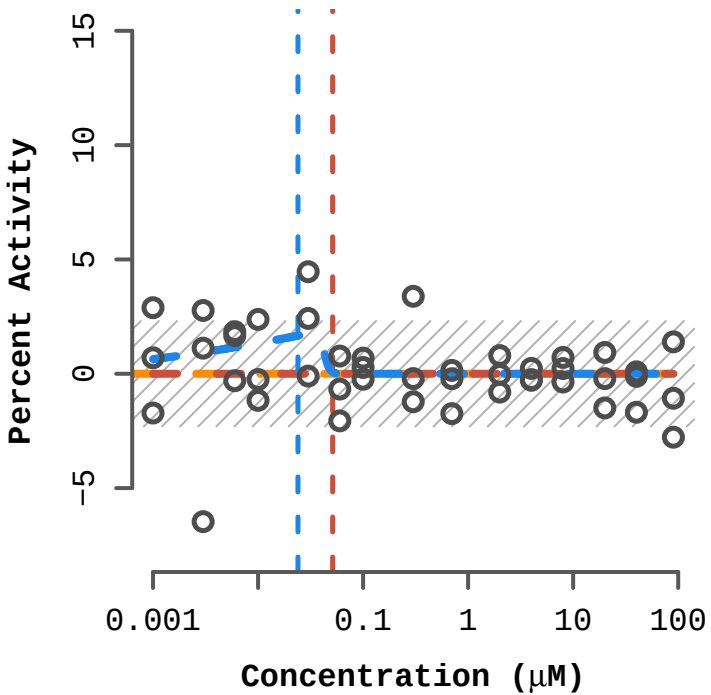
NAME: Fluridone
CHID: 24107 **CASRN:** 59756-60-4
SPID(S): Tox21_300200
M4ID: 12478930

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluridone
CHID: 24107 CASRN: 59756-60-4
SPID(S): Tox21_202162
M4ID: 12480090

HILL MODEL (in red):

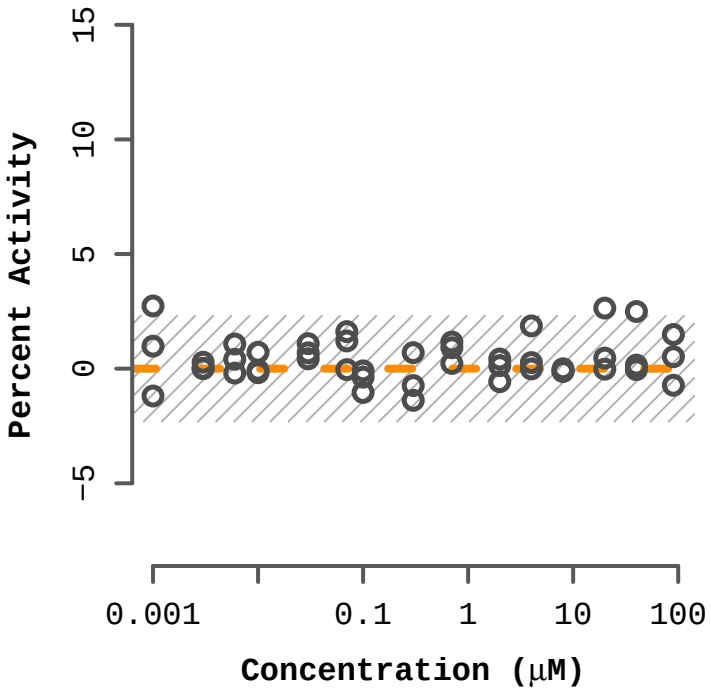
	tp	ga	gw
val:	7.42e-11	−1.29	1.8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.33	−1.62	0.45	−1.37	18
sd:	12	5.88	0.633	0.326	39.1

	CNST	HILL	GNLS
AIC:	175.05	181.05	178.43
PROB:	0.81	0.04	0.15
RMSE:	1.78	1.78	1.72

MAX_MEAN: 2.26 **MAX_MED:** 2.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

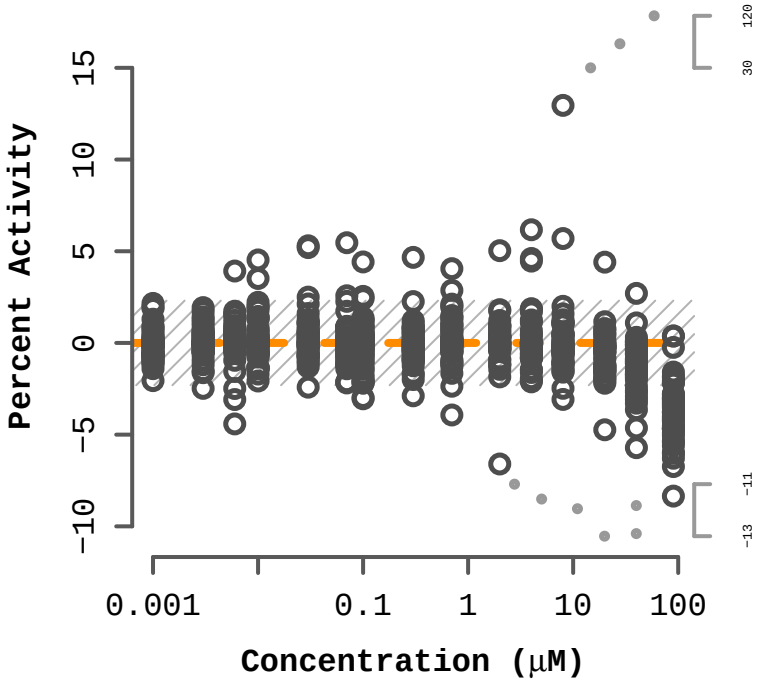
NAME: Flurprimidol
CHID: 24108 **CASRN:** 56425-91-3
SPID(S): Tox21_201156
M4ID: 12481096

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.29	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

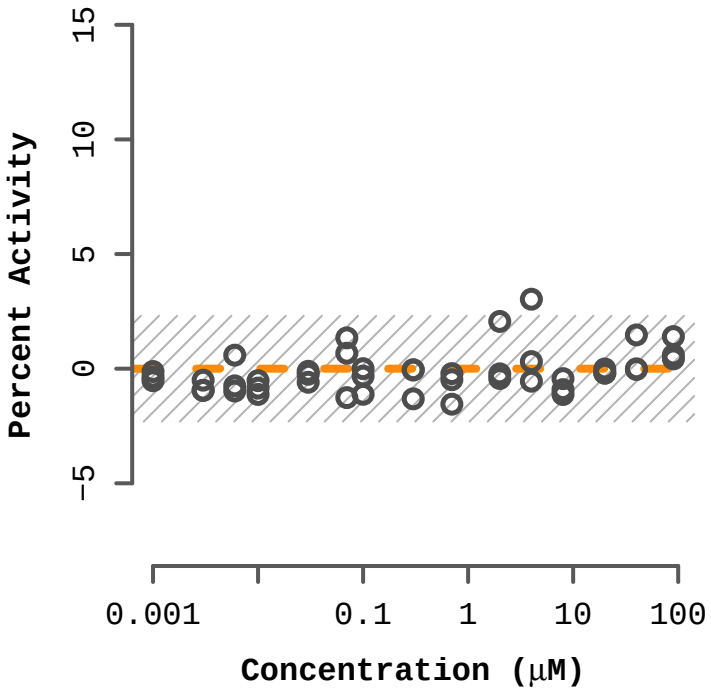
NAME: Flutolanil
CHID: 24109 **CASRN:** 66332-96-5
SPID(S): Tox21_400085
M4ID: 12475052 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2770.83	NA	NA
PROB:	1	NA	NA
RMSE:	5.79	NA	NA

MAX_MEAN: 0.348 **MAX_MED:** 0.116 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

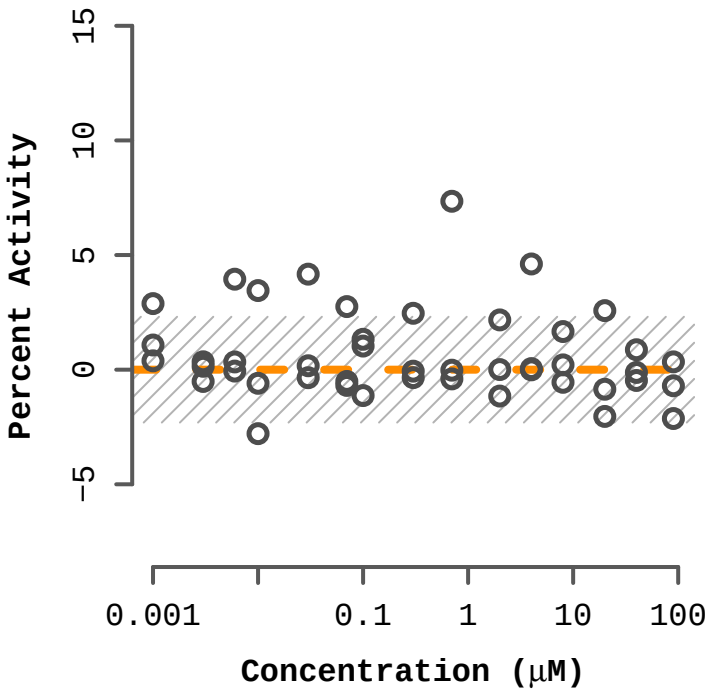
NAME: Fluvalinate
CHID: 24110 **CASRN:** 69409-94-5
SPID(S): Tox21_200245
M4ID: 12482007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 0.674 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

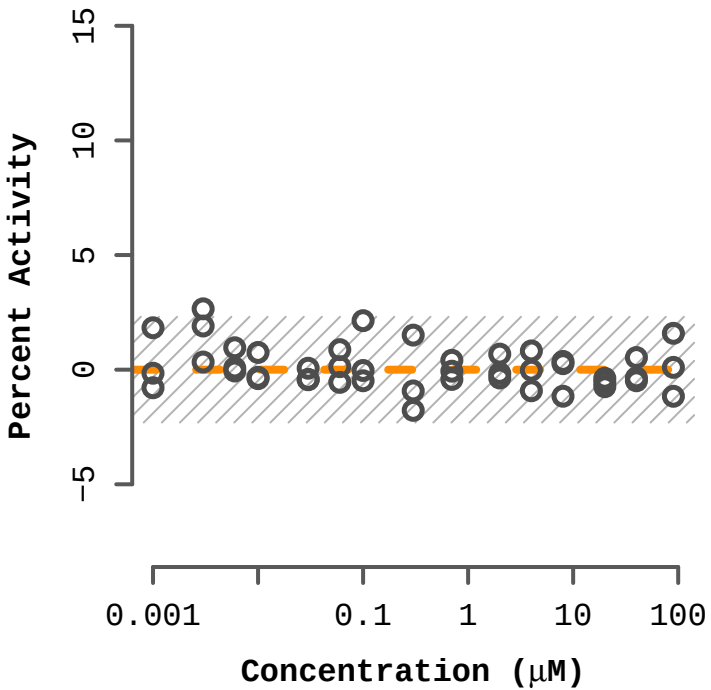
NAME: Fomesafen
CHID: 24112 **CASRN:** 72178-02-0
SPID(S): Tox21_300518
M4ID: 12478614

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.84	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 2.31 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

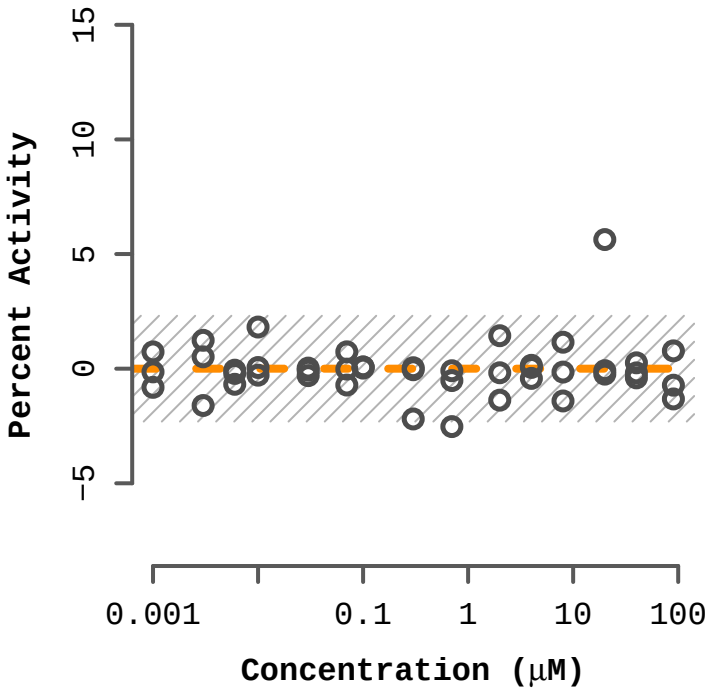
NAME: Fomesafen
CHID: 24112 **CASRN:** 72178-02-0
SPID(S): Tox21_201395
M4ID: 12480857

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

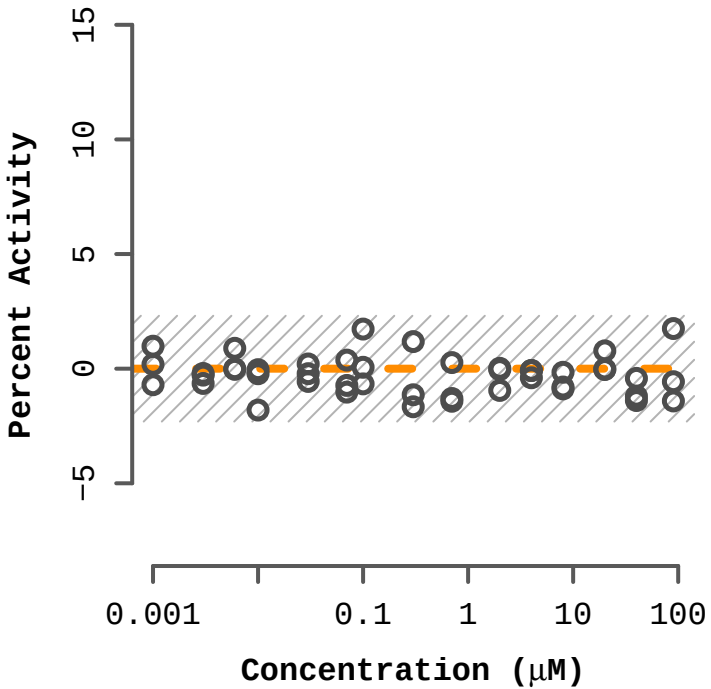
NAME: Fonofos
CHID: 24113 CASRN: 944-22-9
SPID(S): Tox21_200009
M4ID: 12482243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

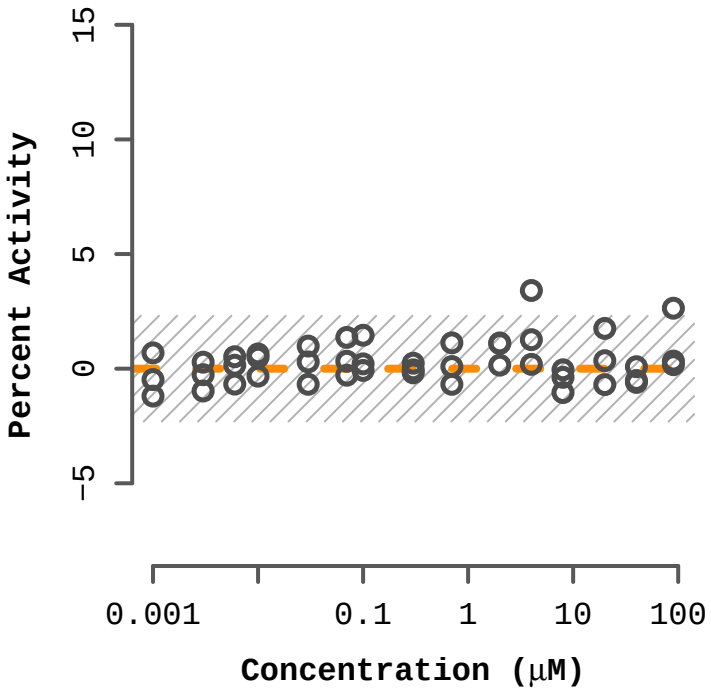
NAME: Haloxyfop-methyl
CHID: 24123 **CASRN:** 69806-40-2
SPID(S): Tox21_303113
M4ID: 12476020

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.377 **MAX_MED:** 0.189 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

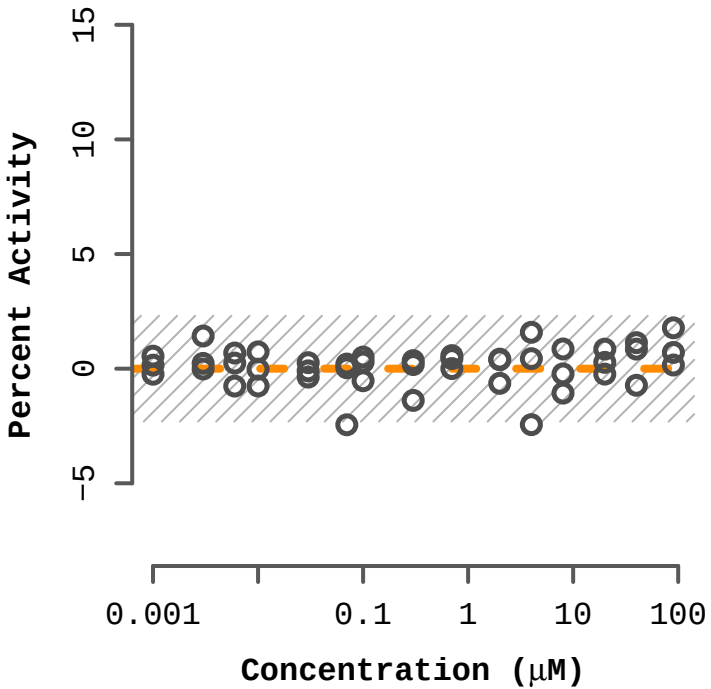
NAME: Haloxyfop-methyl
CHID: 24123 **CASRN:** 69806-40-2
SPID(S): Tox21_201797
M4ID: 12480455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

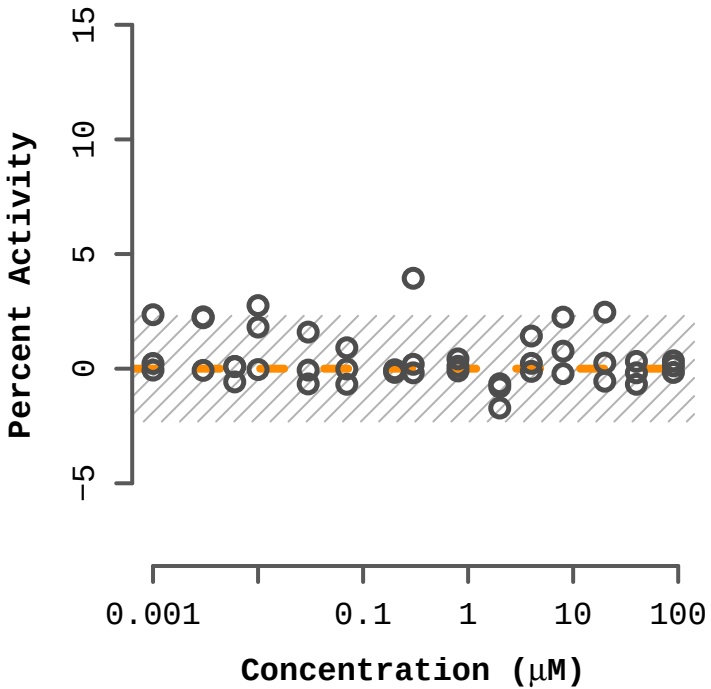
NAME: Thifensulfuron-methyl
CHID: 24124 **CASRN:** 79277-27-3
SPID(S): Tox21_303088
M4ID: 12476045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 0.856 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

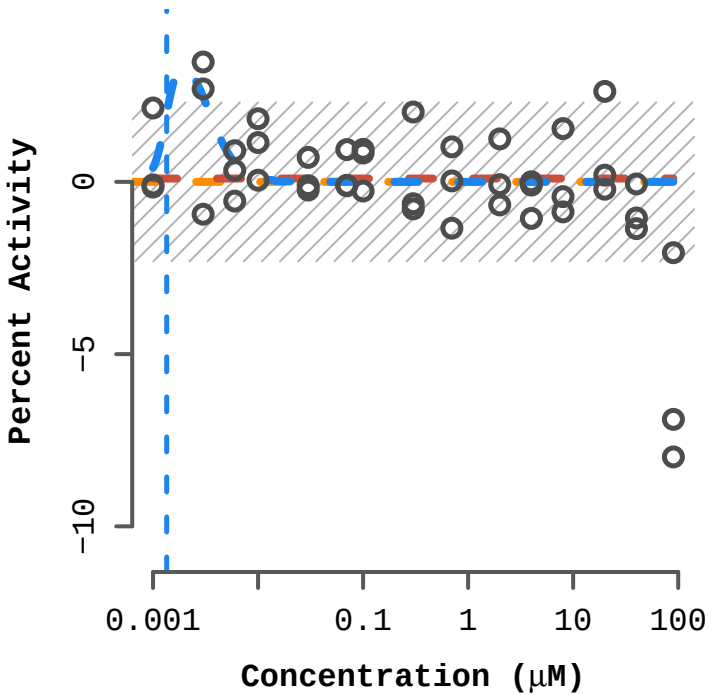
NAME: Thifensulfuron-methyl
CHID: 24124 **CASRN:** 79277-27-3
SPID(S): Tox21_202184
M4ID: 12480068

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Heptachlor epoxide
CHID: 24126 CASRN: 1024-57-3
SPID(S): Tox21_300621
M4ID: 12478512

HILL MODEL (in red):

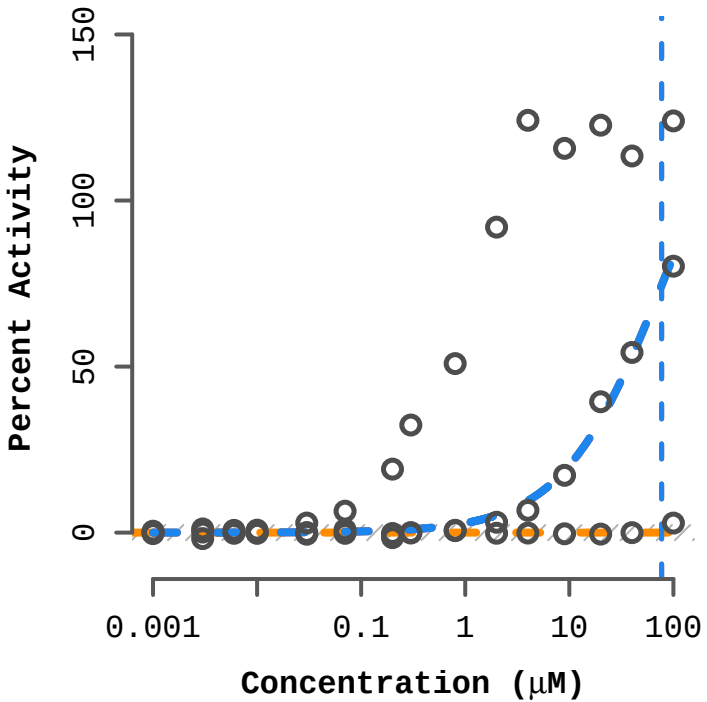
	tp	ga	gw
val:	0.097	−4.72	3.63
sd:	0.188	1610	3370

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.18	−2.87	7.34	−2.47	3.23
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	169.88	175.61	174.22
PROB:	0.85	0.05	0.1
RMSE:	1.97	1.97	1.91

MAX_MEAN: 1.75 MAX_MED: 2.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Heptane
CHID: 24127 CASRN: 142-82-5
SPID(S): Tox21_201213
M4ID: 12481039

HILL MODEL (in red):

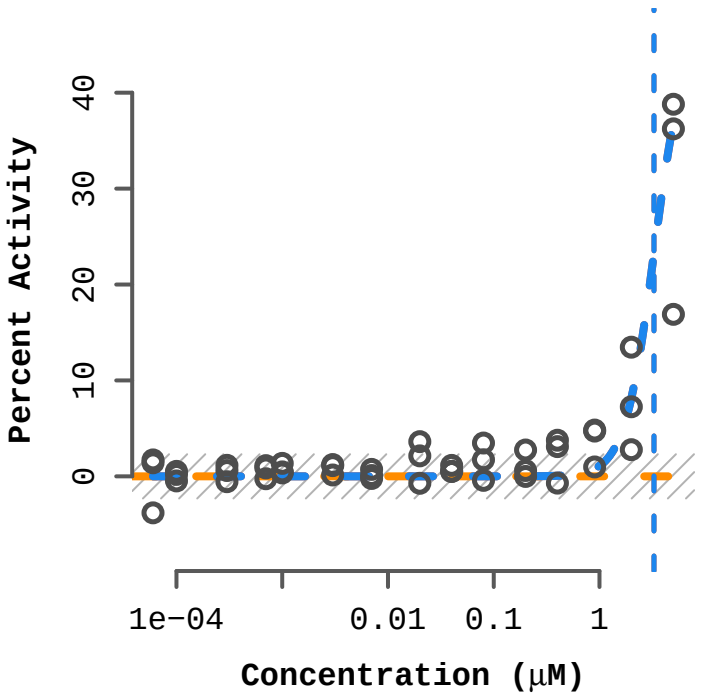
	tp	ga	gw
val:	149	1.89	0.905
sd:	146	0.959	0.561

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	149	1.89	0.904	2.86	17.8
sd:	145	0.954	0.557	0.00683	2020000

	CNST	HILL	GNLS
AIC:	457.51	438.23	442.23
PROB:	0	0.88	0.12
RMSE:	46.17	35.9	35.9

MAX_MEAN: 69 MAX_MED: 80.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexabromobenzene
CHID: 24128 CASRN: 87-82-1
SPID(S): Tox21_203003
M4ID: 12479249

HILL MODEL (in red):

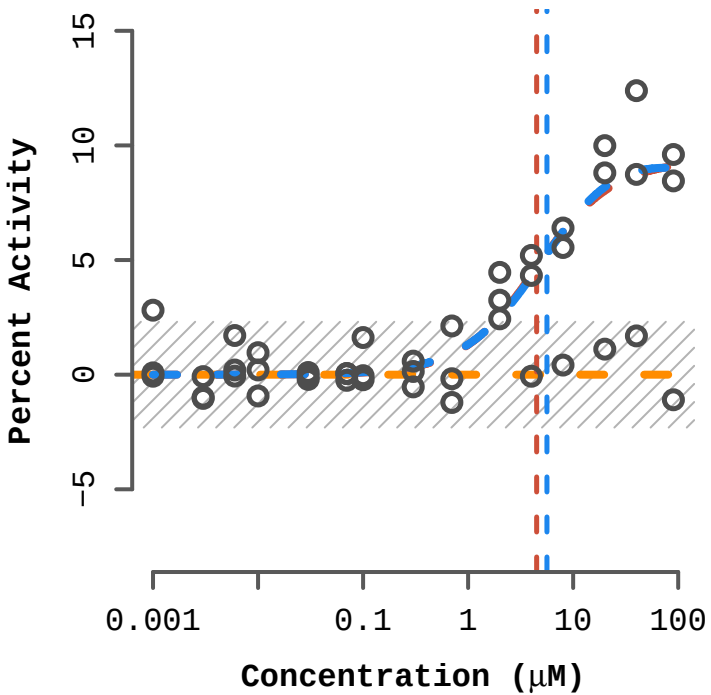
	tp	ga	gw
val:	46.6	0.515	3.15
sd:	14.9	0.128	1.54

GAIN-LOSS MODEL (in blue):

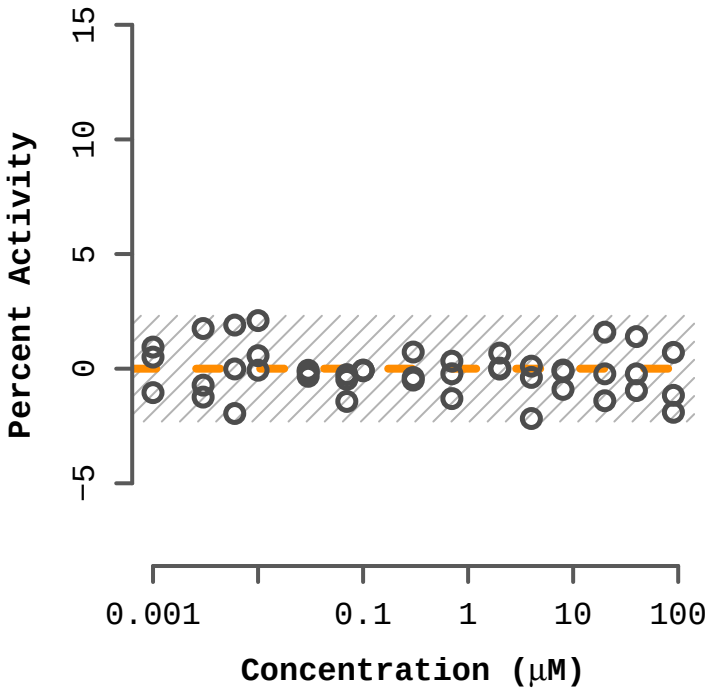
	tp	ga	gw	la	lw
val:	46.6	0.515	3.15	1.94	7.08
sd:	14.9	0.128	1.54	1970	11300

	CNST	HILL	GNLS
AIC:	266.48	216.1	220.1
PROB:	0	0.88	0.12
RMSE:	8.81	3.61	3.61

MAX_MEAN: 30.6 MAX_MED: 36.2 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    delta-Hexachlorocyclohexane
CHID:    24134   CASRN: 319-86-8
SPID(S): Tox21_303873
M4ID:    12475315

HILL MODEL (in red):
      tp       ga       gw
val:  9.34     0.652    1.21
sd:   0.89     0.123    0.297

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  11.4     0.75     1.15     3.95     0.333
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  245.74      197.54      201.25
PROB: 0           0.86        0.14
RMSE: 4.1         2.6         2.6

MAX_MEAN: 7.61      MAX_MED: 8.81      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

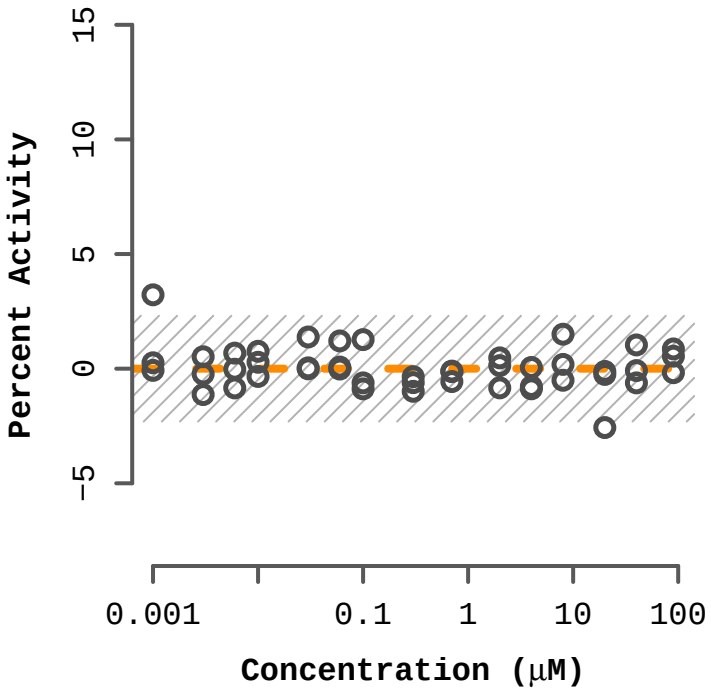
NAME: 1,6-Diisocyanatohexane
CHID: 24143 **CASRN:** 822-06-0
SPID(S): Tox21_300161
M4ID: 12478969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.868 **MAX_MED:** 0.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

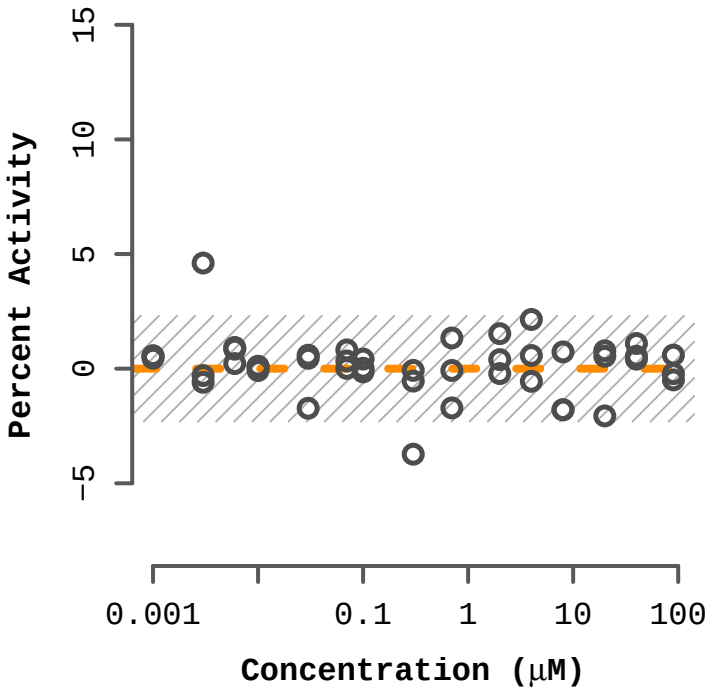
NAME: 1,6-Diisocyanatohexane
CHID: 24143 **CASRN:** 822-06-0
SPID(S): Tox21_202206
M4ID: 12480046

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.547 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

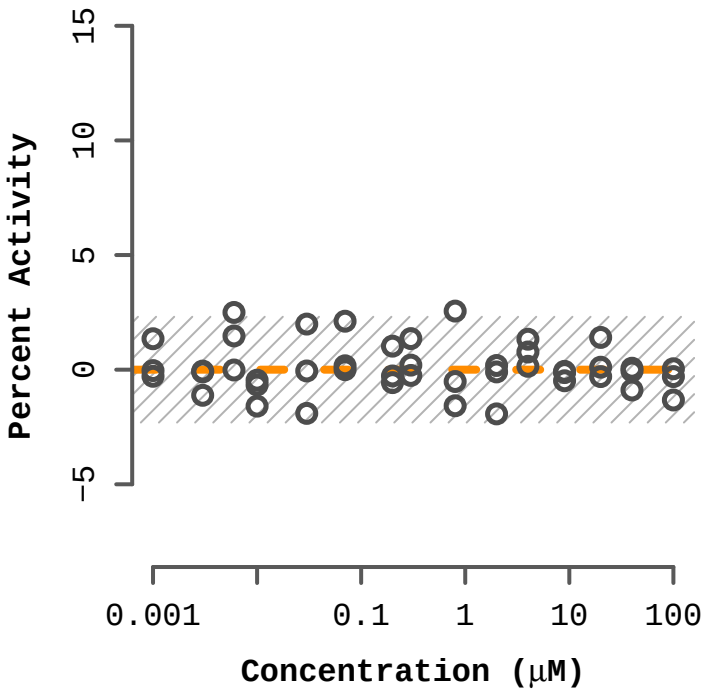
NAME: Hexazinone
CHID: 24145 **CASRN:** 51235-04-2
SPID(S): Tox21_300745
M4ID: 12478388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

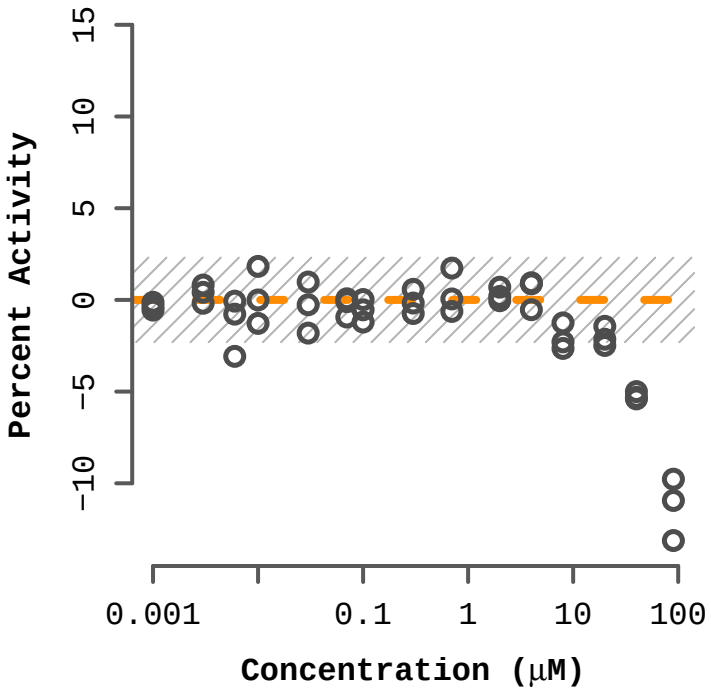
NAME: Hexazinone
CHID: 24145 CASRN: 51235-04-2
SPID(S): Tox21_201665
M4ID: 12480587

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.32 MAX_MED: 1.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

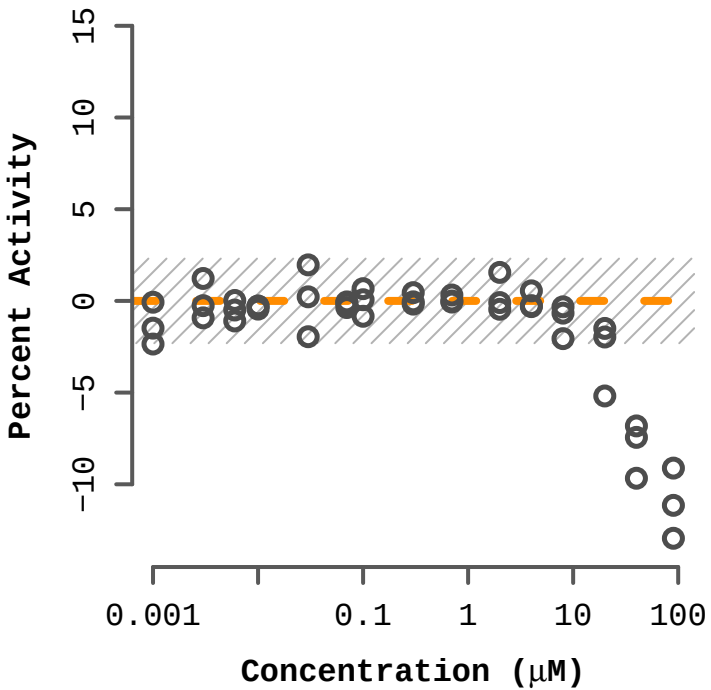
NAME: Imazalil
CHID: 24151 **CASRN:** 35554-44-0
SPID(S): Tox21_300720
M4ID: 12478413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.42	NA	NA

MAX_MEAN: 0.427 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

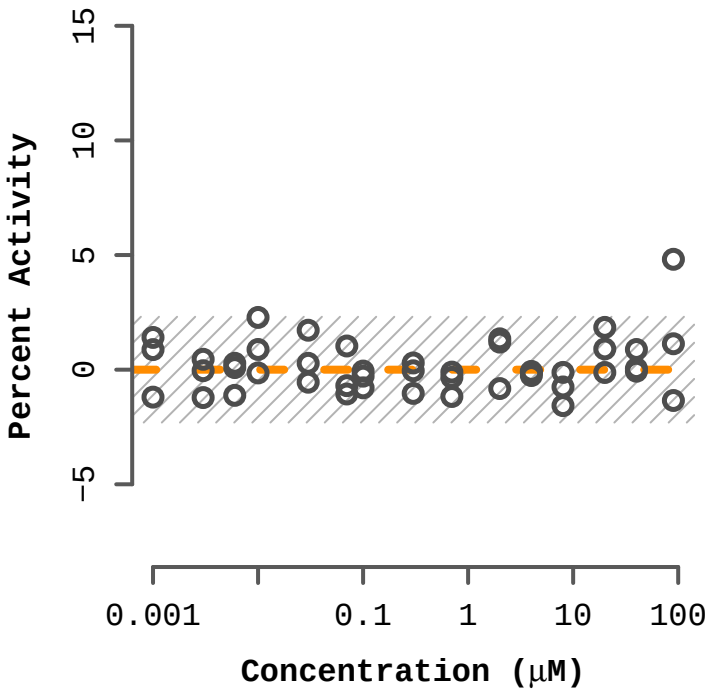
NAME: Imazalil
CHID: 24151 **CASRN:** 35554-44-0
SPID(S): Tox21_201551
M4ID: 12480701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.6	NA	NA
PROB:	1	NA	NA
RMSE:	3.75	NA	NA

MAX_MEAN: 0.338 **MAX_MED:** 0.225 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

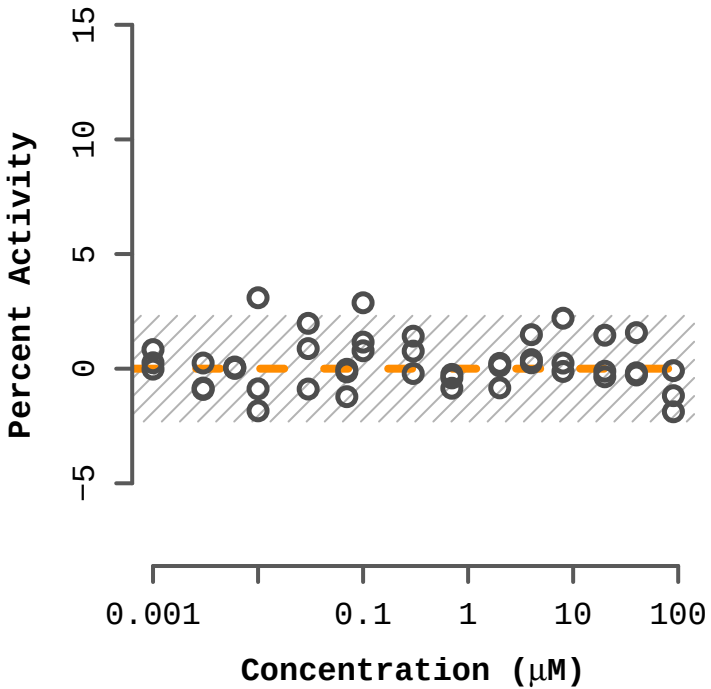
NAME: Imazaquin
CHID: 24152 CASRN: 81335-37-7
SPID(S): Tox21_300796
M4ID: 12478337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

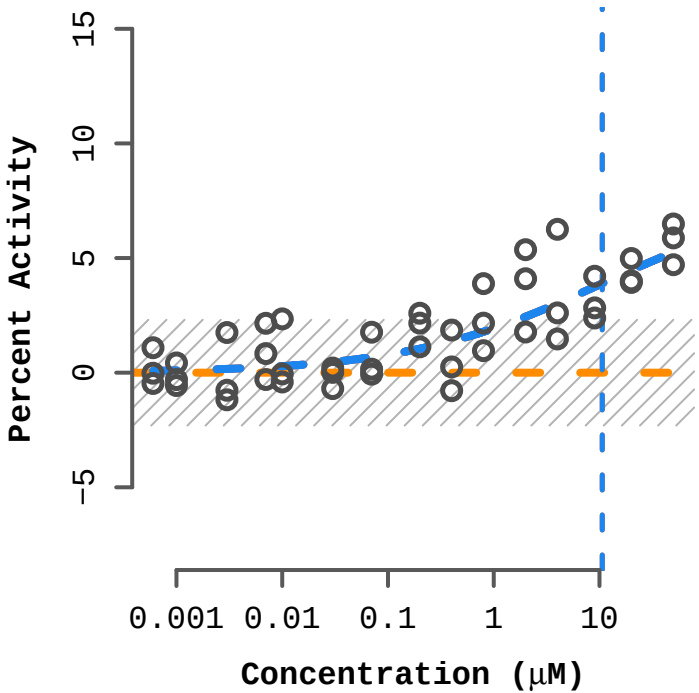
NAME: Imazaquin
CHID: 24152 **CASRN:** 81335-37-7
SPID(S): Tox21_202008
M4ID: 12480244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indeno(1,2,3-cd)pyrene
CHID: 24153 **CASRN:** 193-39-5
SPID(S): Tox21_304020
M4ID: 12475168

HILL MODEL (in red):

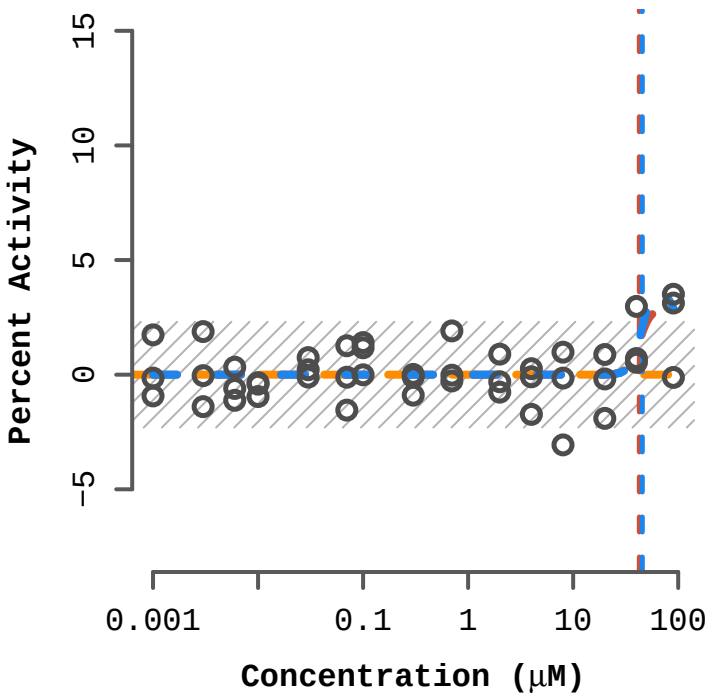
	tp	ga	gw
val:	7.79	1.03	0.469
sd:	3.67	0.96	0.144

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.79	1.03	0.469	2.48	10.9
sd:	3.67	0.961	0.144	918	12800

	CNST	HILL	GNLS
AIC:	221.58	154.53	158.53
PROB:	0	0.88	0.12
RMSE:	2.76	1.21	1.21

MAX_MEAN: 5.69 **MAX_MED:** 5.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iprodione
CHID: 24154 CASRN: 36734-19-7
SPID(S): Tox21_300865
M4ID: 12478268

HILL MODEL (in red):

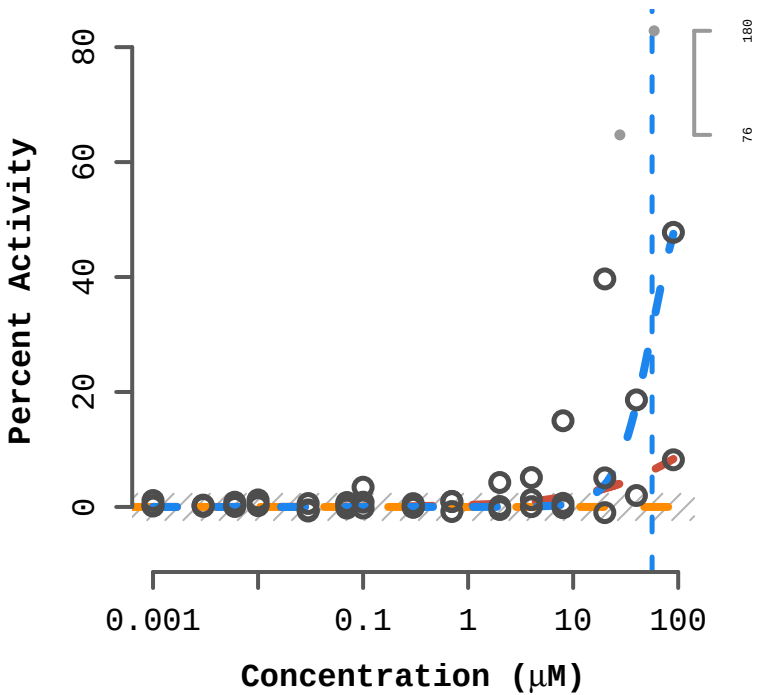
	tp	ga	gw
val:	2.91	1.63	8
sd:	0.662	0.0998	22.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.21	1.66	8	2.03	4.83
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	150.9	146.3	150.3
PROB:	0.08	0.81	0.11
RMSE:	1.3	1.13	1.13

MAX_MEAN: 2.17 MAX_MED: 3.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iprodione
CHID: 24154 CASRN: 36734-19-7
SPID(S): Tox21_201676
M4ID: 12480576 BRK

HILL MODEL (in red):

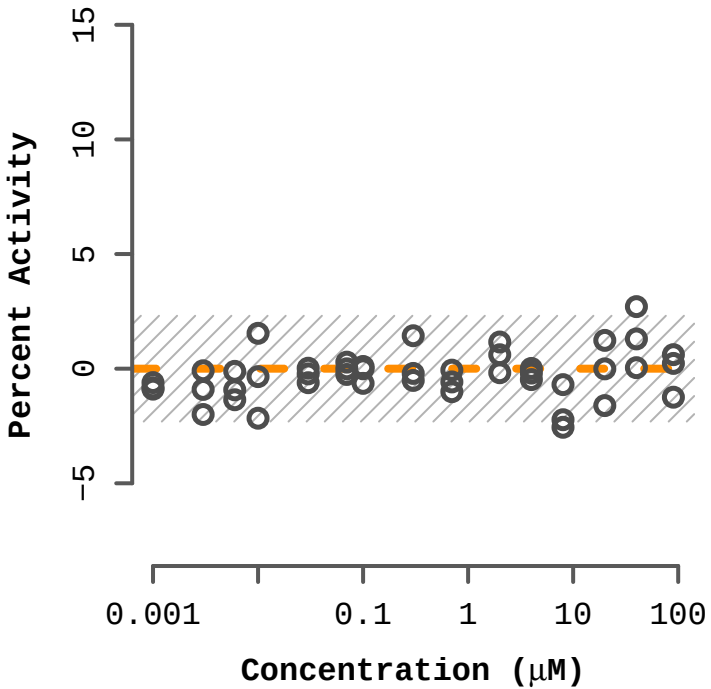
	tp	ga	gw
val:	28.9	2.45	0.783
sd:	68	2	0.428

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	61.6	1.75	2.6	3.68	4.26
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	325.68	316.12	316.53
PROB:	0	0.55	0.45
RMSE:	30.52	28.67	22.94

MAX_MEAN: 77.8 MAX_MED: 47.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

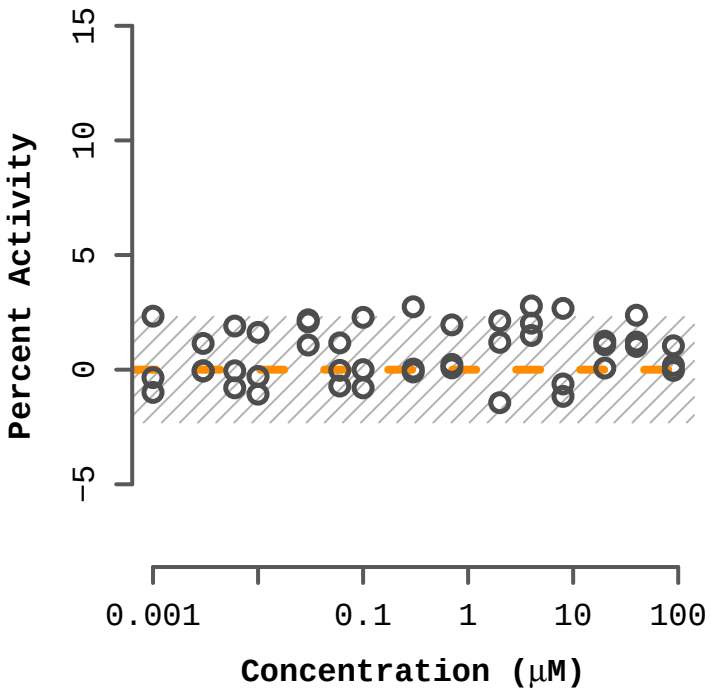
NAME: Isopropalin
CHID: 24157 CASRN: 33820-53-0
SPID(S): Tox21_300422
M4ID: 12478710

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.35 MAX_MED: 1.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

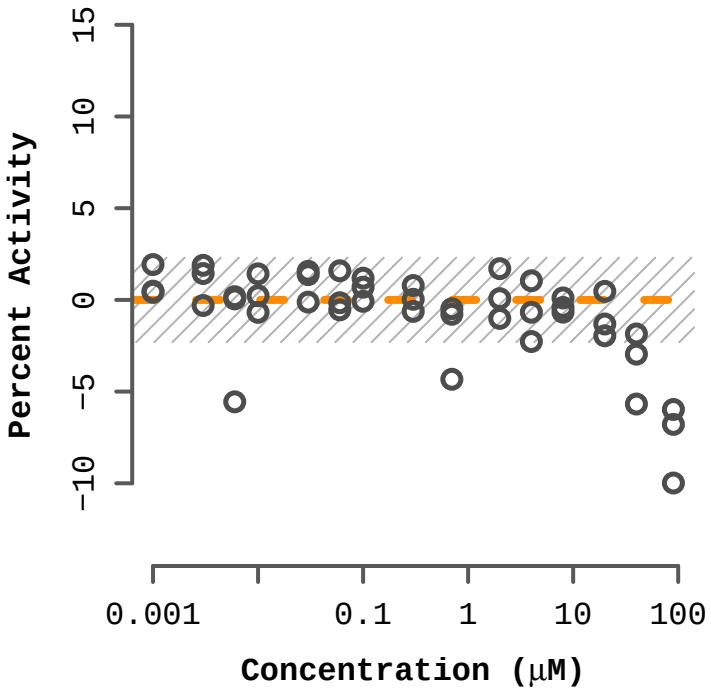
NAME: Isopropalin
CHID: 24157 CASRN: 33820-53-0
SPID(S): Tox21_202228
M4ID: 12480024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

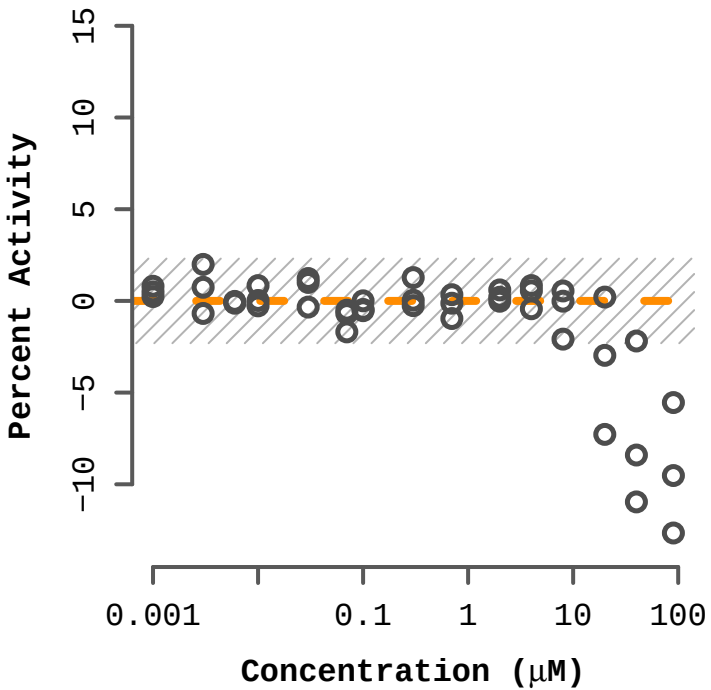
NAME: Isoxaben
CHID: 24159 CASRN: 82558-50-7
SPID(S): Tox21_300696
M4ID: 12478437

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 1.01 MAX_MED: 1.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

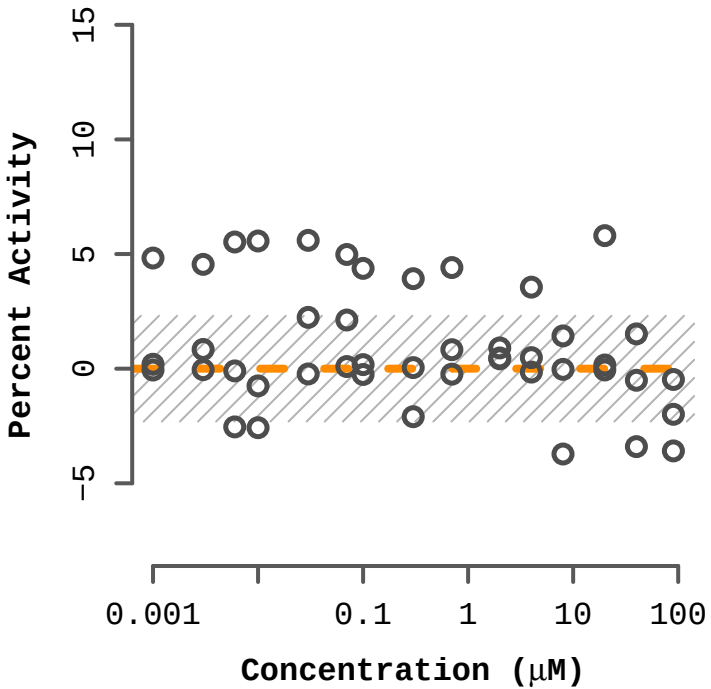
NAME: Isoxaben
CHID: 24159 CASRN: 82558-50-7
SPID(S): Tox21_201574
M4ID: 12480678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.82	NA	NA
PROB:	1	NA	NA
RMSE:	3.53	NA	NA

MAX_MEAN: 0.684 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

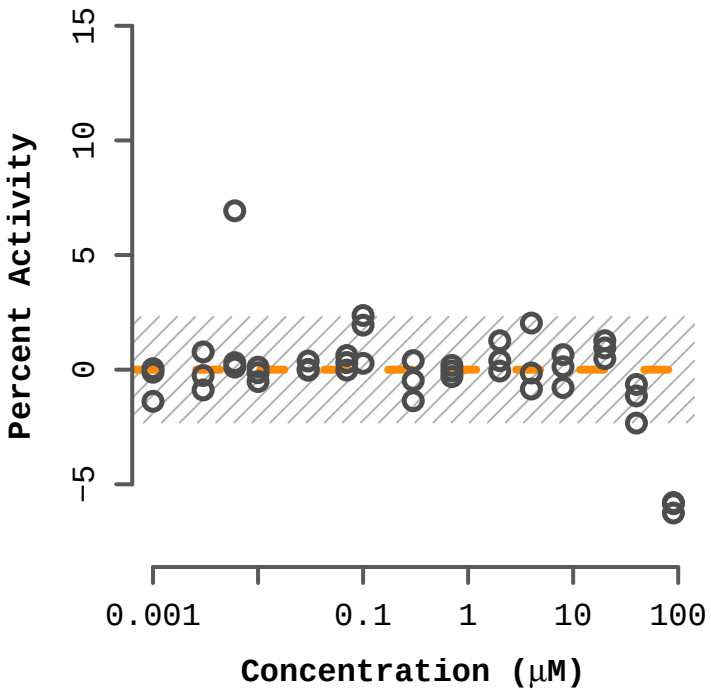
NAME: Lactofen
CHID: 24160 CASRN: 77501-63-4
SPID(S): Tox21_300868
M4ID: 12478265

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 2.54 MAX_MED: 2.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

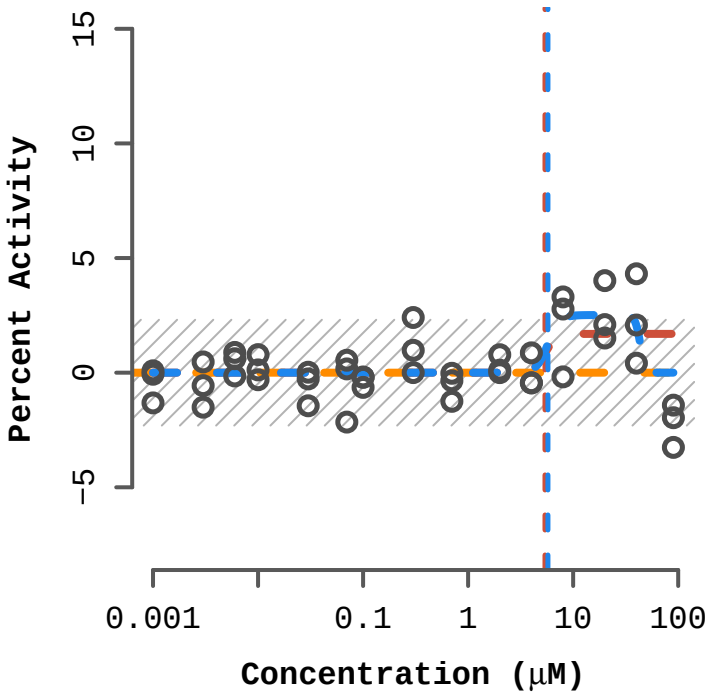
NAME: Lactofen
CHID: 24160 CASRN: 77501-63-4
SPID(S): Tox21_201300
M4ID: 12480952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 2.45 MAX_MED: 1.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linuron
CHID: 24163 **CASRN:** 330-55-2
SPID(S): Tox21_300732
M4ID: 12478401

HILL MODEL (in red):

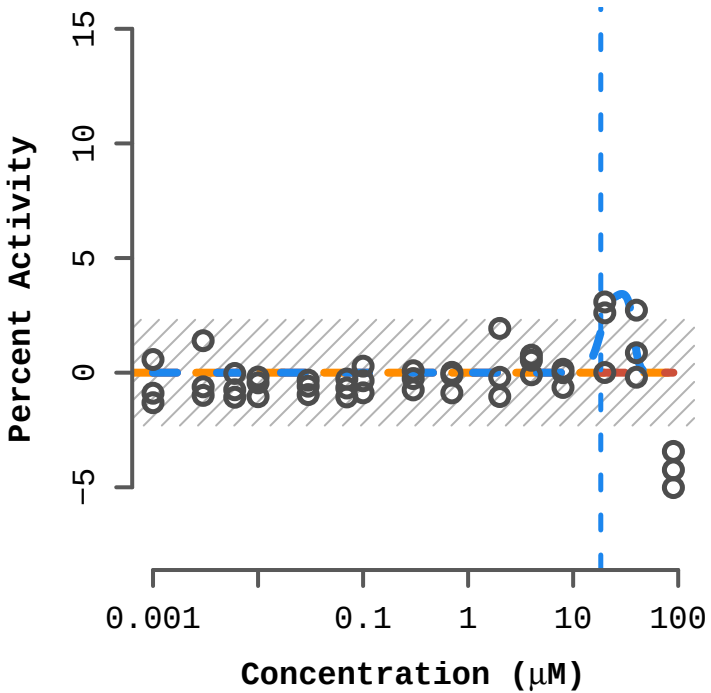
	tp	ga	gw
val:	1.69	0.732	8
sd:	0.518	0.129	7.11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.51	0.76	8	1.64	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.79	161.54	151.09
PROB:	0	0.01	0.99
RMSE:	1.53	1.44	1.15

MAX_MEAN: 2.54 **MAX_MED:** 2.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linuron
CHID: 24163 CASRN: 330-55-2
SPID(S): Tox21_201281
M4ID: 12480971

HILL MODEL (in red):

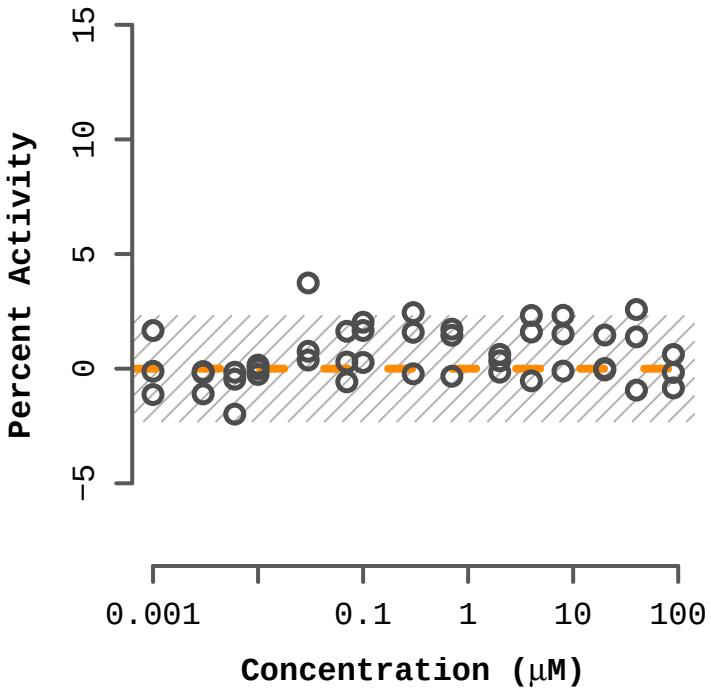
	tp	ga	gw
val:	7.36e-09	2.32	1.64
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.56	1.26	7.99	1.58	17.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.01	161.01	156.42
PROB:	0.65	0.03	0.32
RMSE:	1.49	1.49	1.38

MAX_MEAN: 1.9 MAX_MED: 2.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

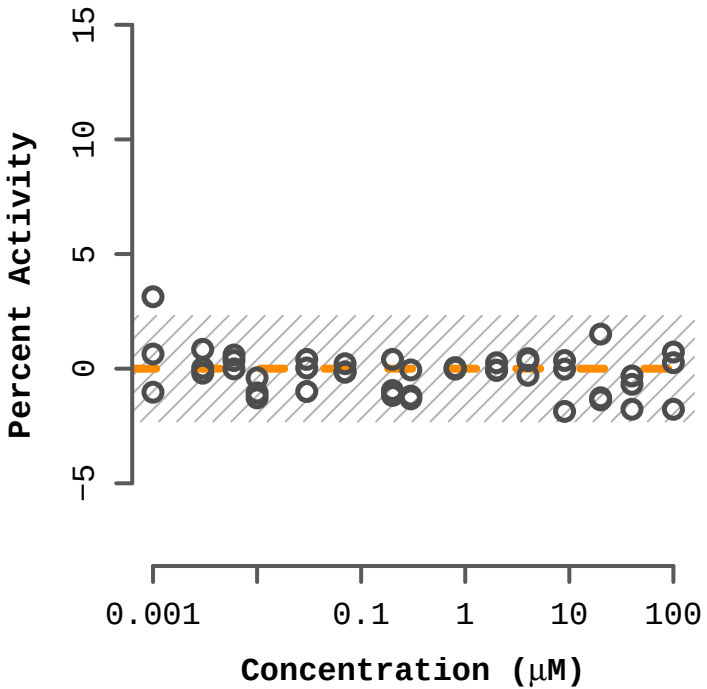
NAME: Bensulfuron-methyl
CHID: 24164 **CASRN:** 83055-99-6
SPID(S): Tox21_200393
M4ID: 12481859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

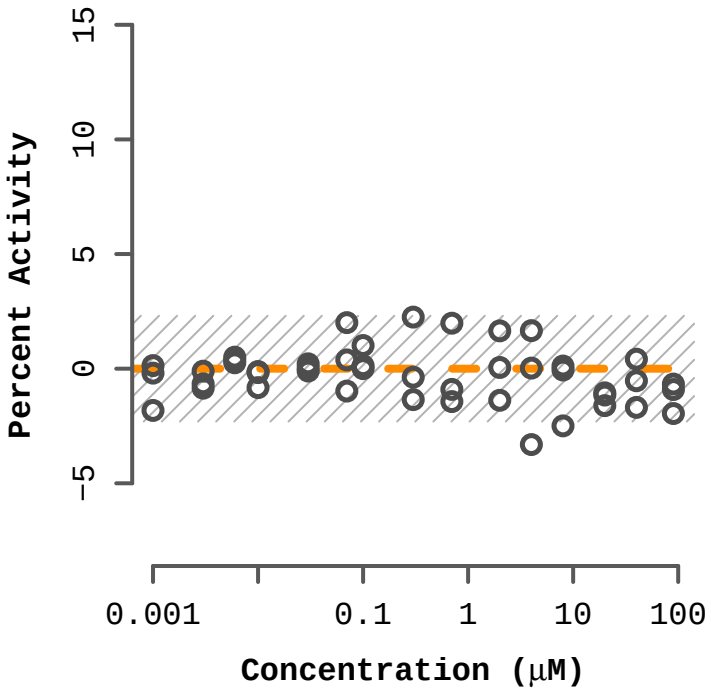
NAME: 2,5-Furandione
CHID: 24166 **CASRN:** 108-31-6
SPID(S): Tox21_200406
M4ID: 12481846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 0.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

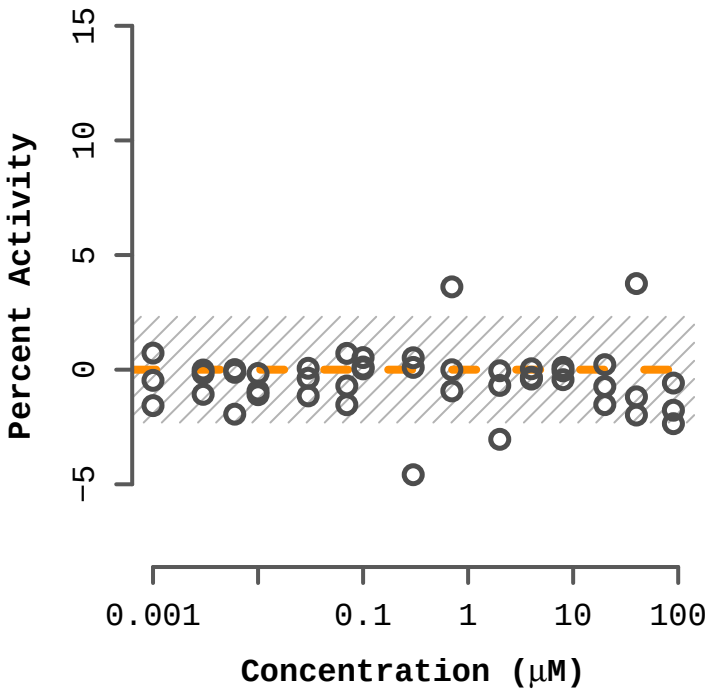
NAME: Mepiquat chloride
CHID: 24170 CASRN: 24307-26-4
SPID(S): Tox21_300773
M4ID: 12478360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.473 MAX_MED: 0.385 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

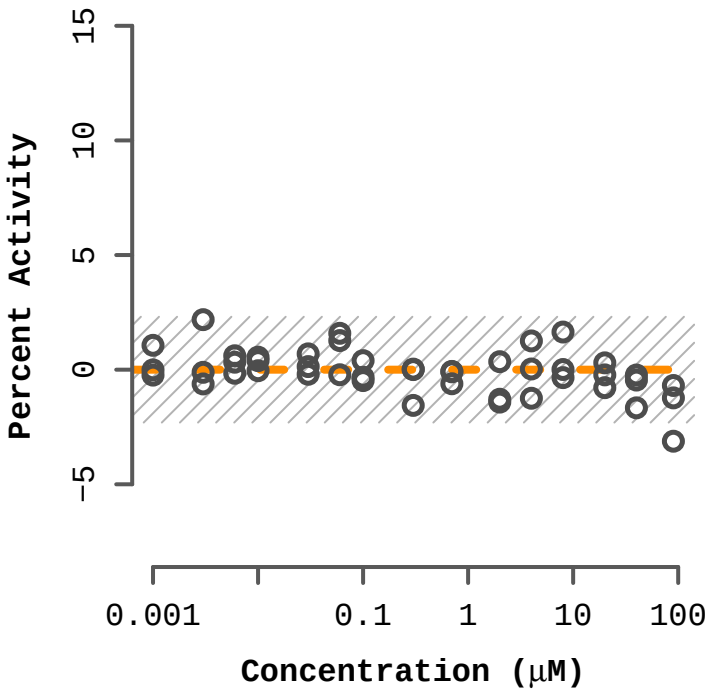
NAME: Tribufos
CHID: 24174 CASRN: 78-48-8
SPID(S): Tox21_300642
M4ID: 12478491

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 0.896 MAX_MED: 0.118 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

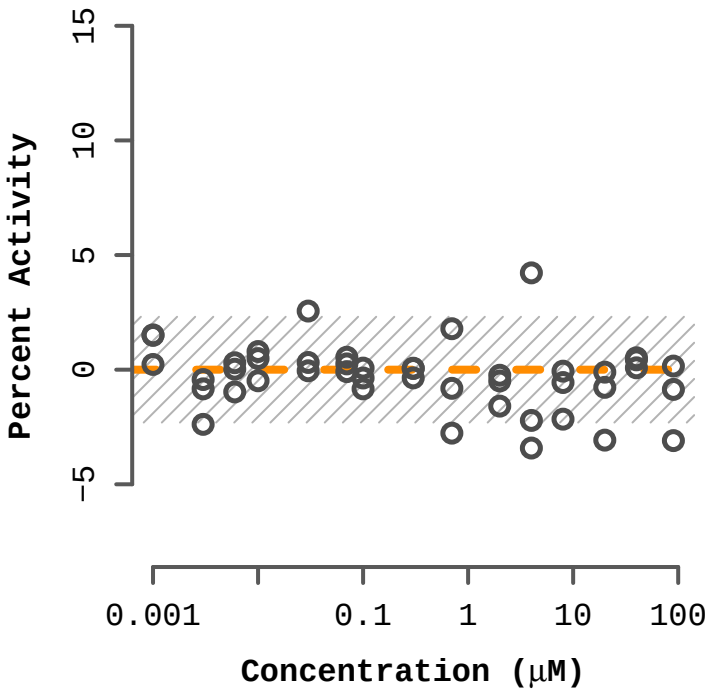
NAME: Tribufos
CHID: 24174 CASRN: 78-48-8
SPID(S): Tox21_201934
M4ID: 12480318

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.88 MAX_MED: 1.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

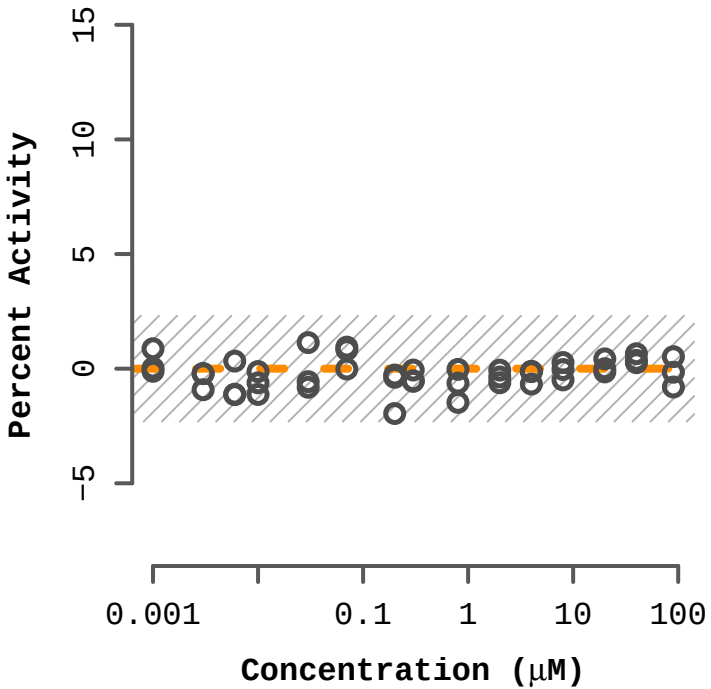
NAME: Metalaxyl
CHID: 24175 CASRN: 57837-19-1
SPID(S): Tox21_300790
M4ID: 12478343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.08 MAX_MED: 1.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

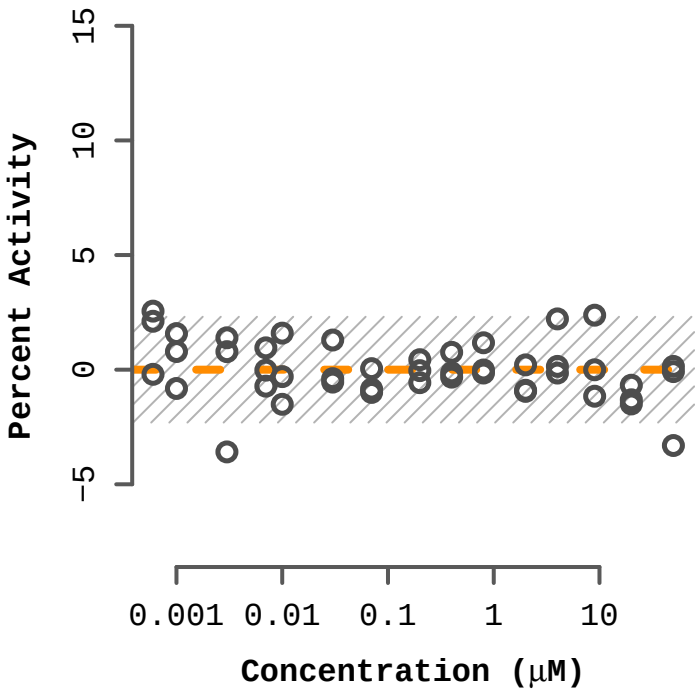
NAME: Metalaxyl
CHID: 24175 **CASRN:** 57837-19-1
SPID(S): Tox21_202061
M4ID: 12480191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.832 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

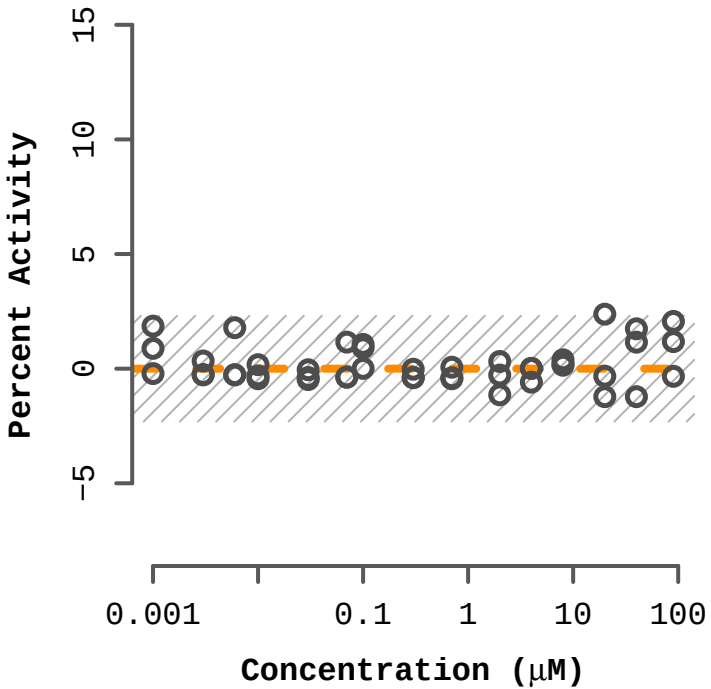
NAME: Metalaxyl
CHID: 24175 **CASRN:** 57837-19-1
SPID(S): Tox21_112070_1
M4ID: 12483339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

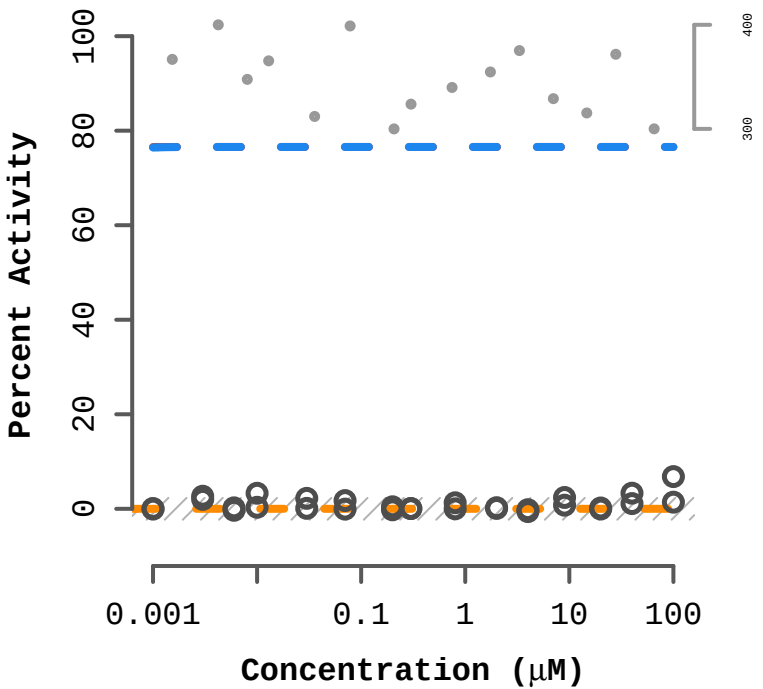
NAME: Methacrylonitrile
CHID: 24176 **CASRN:** 126-98-7
SPID(S): Tox21_303172
M4ID: 12475961

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methacrylonitrile
CHID: 24176 CASRN: 126-98-7
SPID(S): Tox21_201354
M4ID: 12480898 BRK

HILL MODEL (in red):

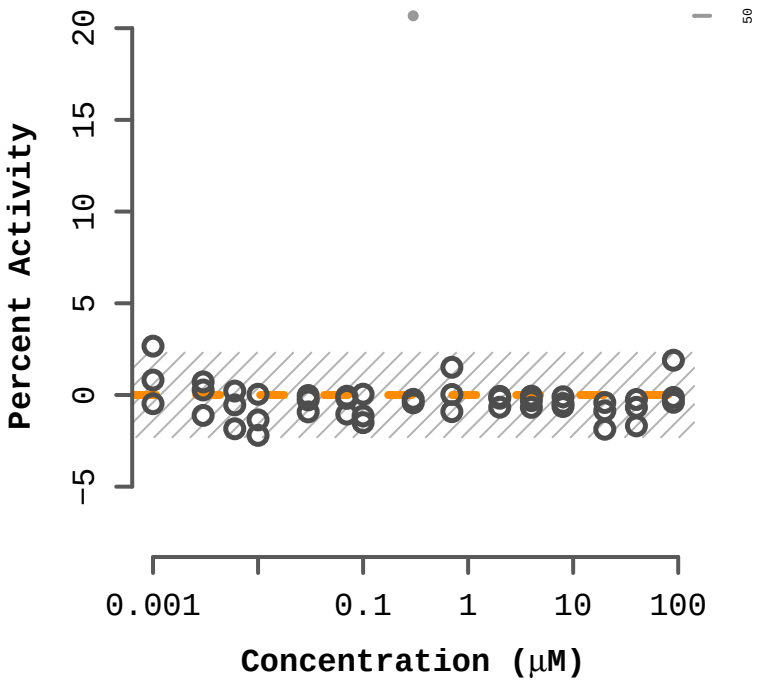
	tp	ga	gw
val:	76.6	-4.86	6.38
sd:	NA	NA	NA

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	76.6	-3.88	3.16	2.69	6.23
sd:	28.4	434	1270	232	2080

	CNST	HILL	GNLS
AIC:	685.29	600.77	604.77
PROB:	0	0.88	0.12
RMSE:	200.76	168.53	168.53

MAX_MEAN: 135 MAX_MED: 6.82 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

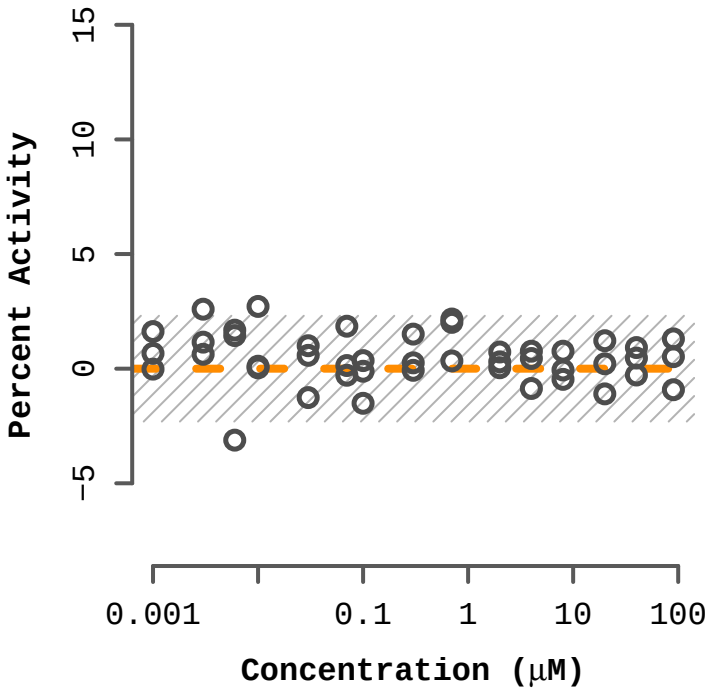
NAME: Methamidophos
CHID: 24177 **CASRN:** 10265-92-6
SPID(S): Tox21_300740
M4ID: 12478393 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.66	NA	NA
PROB:	1	NA	NA
RMSE:	7.54	NA	NA

MAX_MEAN: 16.5 **MAX_MED:** 0.815 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

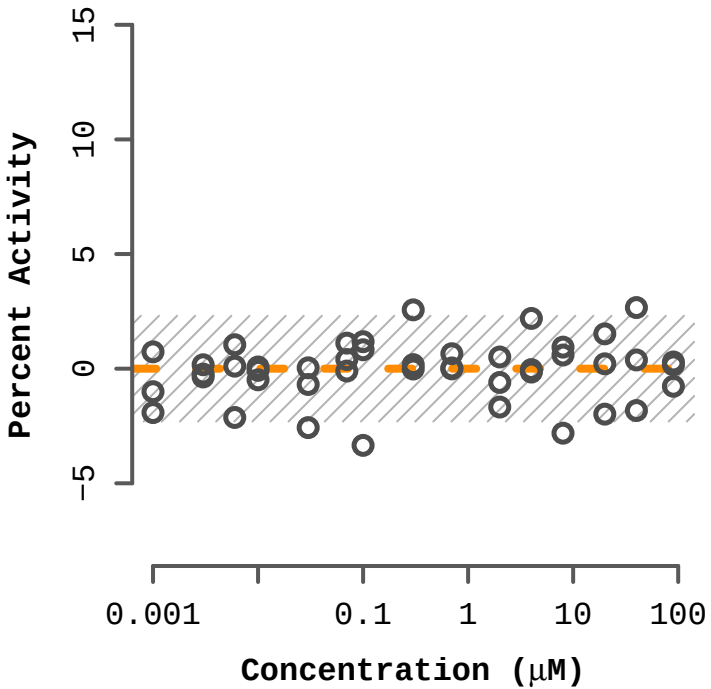
NAME: Methamidophos
CHID: 24177 CASRN: 10265-92-6
SPID(S): Tox21_202250
M4ID: 12480002

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.51 MAX_MED: 2.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

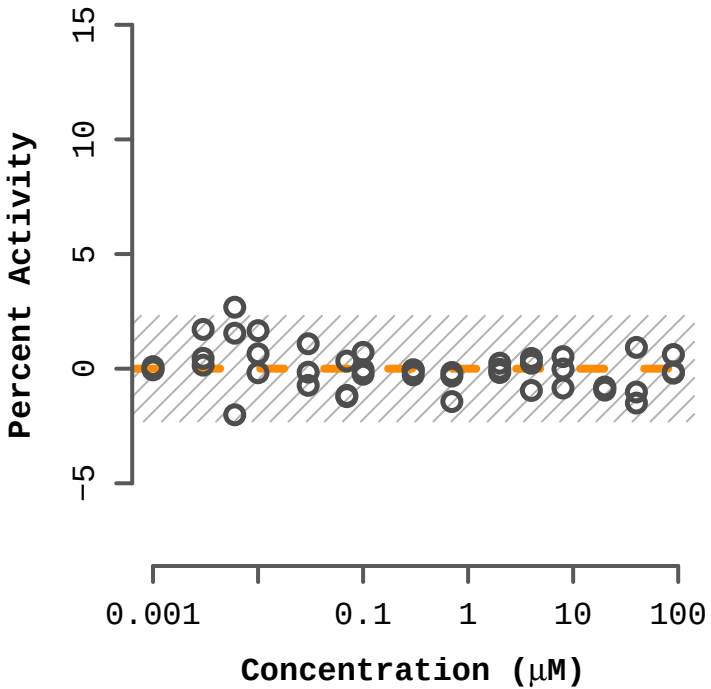
NAME: 2-Methoxyethanol
CHID: 24182 **CASRN:** 109-86-4
SPID(S): Tox21_301080
M4ID: 12478053

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 0.826 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

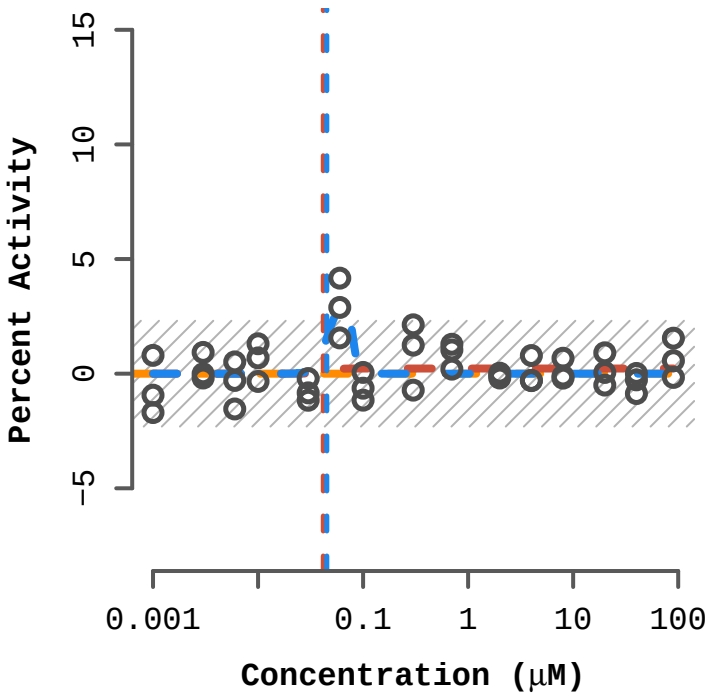
NAME: Methyl acrylate
CHID: 24183 **CASRN:** 96-33-3
SPID(S): Tox21_201000
M4ID: 12481252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.773 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl chlorocarbonate
CHID: 24185 **CASRN:** 79-22-1
SPID(S): Tox21_200841
M4ID: 12481411

HILL MODEL (in red):

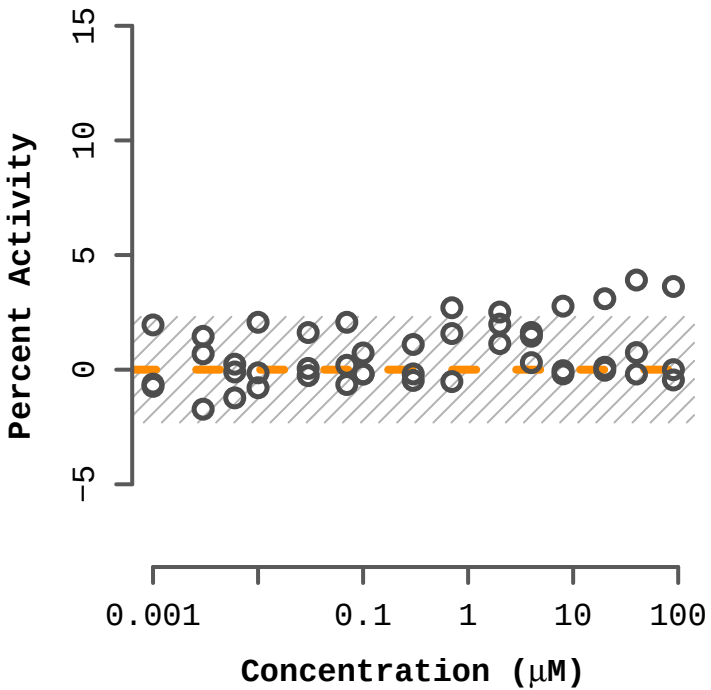
	tp	ga	gw
val:	0.225	−1.38	8
sd:	0.184	0.196	11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.11	−1.35	8	−1.1	18
sd:	1.09	0.106	4.2	0.0817	15.1

	CNST	HILL	GNLS
AIC:	135.08	139.43	129.92
PROB:	0.07	0.01	0.92
RMSE:	1.13	1.09	0.87

MAX_MEAN: 2.87 **MAX_MED:** 2.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

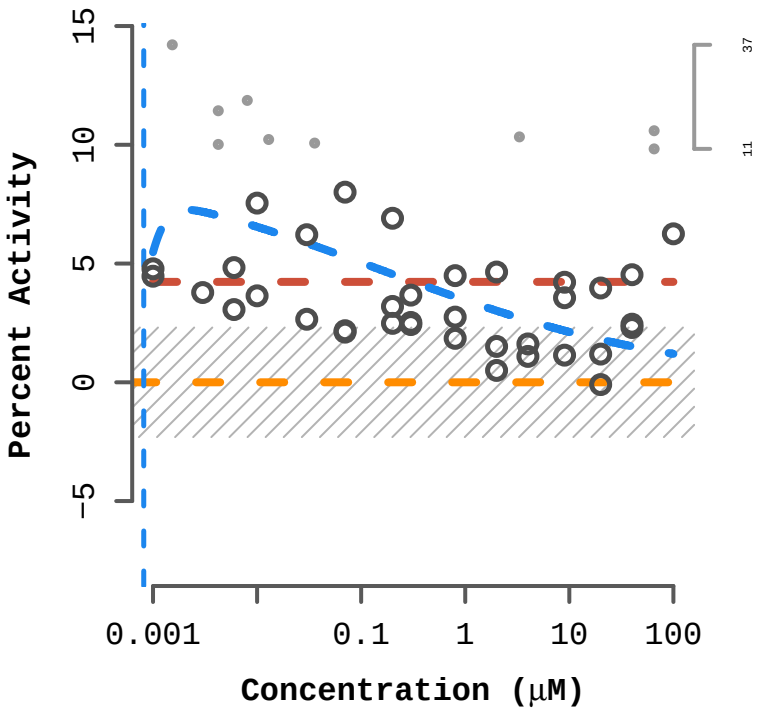
NAME: MCPB
CHID: 24193 **CASRN:** 94-81-5
SPID(S): Tox21_303338
M4ID: 12475795

HILL MODEL: Not applicable.

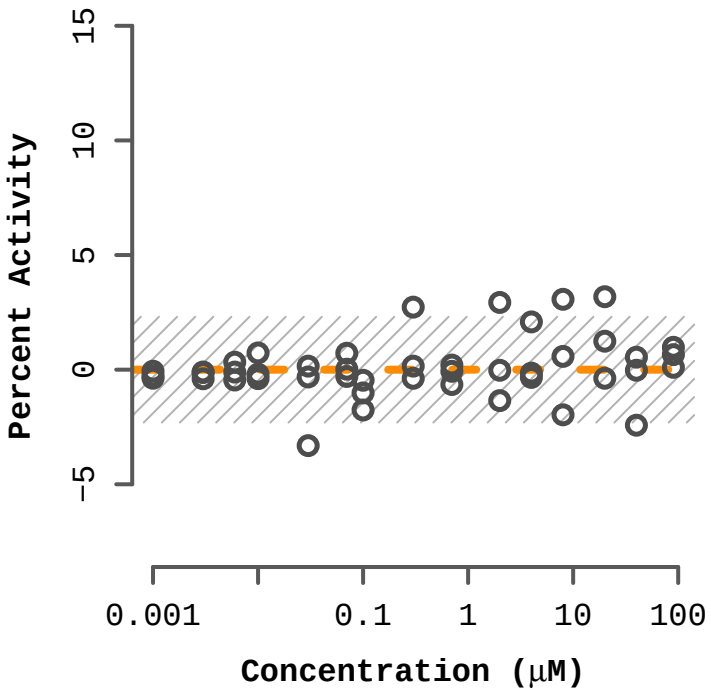
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 1.99 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    MCPB
CHID:    24193   CASRN: 94-81-5
SPID(S): Tox21_201319
M4ID:    12480933  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  4.23     -4.96    3.79
sd:   0.608    1790     3420

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.36     -3.09    4.39     -0.778   0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  317.45      285.86      287.76
PROB: 0           0.72        0.28
RMSE: 9.19        7.07        6.78

MAX_MEAN: 15.3      MAX_MED: 11.8      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

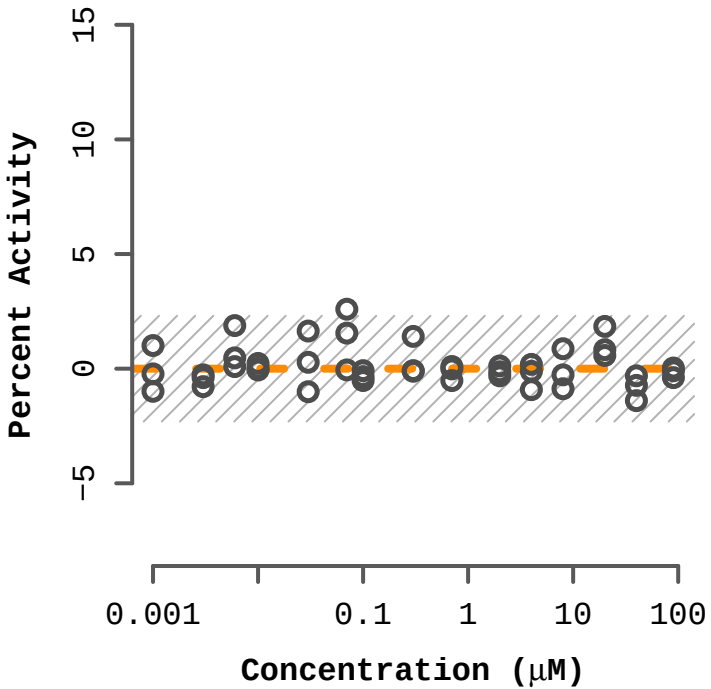
NAME: Mecoprop
CHID: 24194 CASRN: 93-65-2
SPID(S): Tox21_303335
M4ID: 12475798

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.35 MAX_MED: 1.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

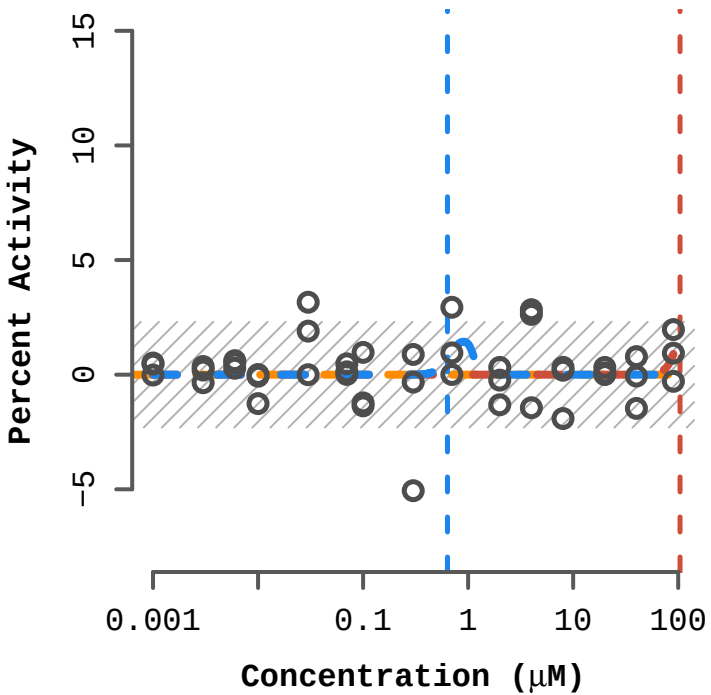
NAME: Mecoprop
CHID: 24194 **CASRN:** 93-65-2
SPID(S): Tox21_201667
M4ID: 12480585

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: MCPA
CHID: 24195 CASRN: 94-74-6
SPID(S): Tox21_300746
M4ID: 12478387

HILL MODEL (in red):

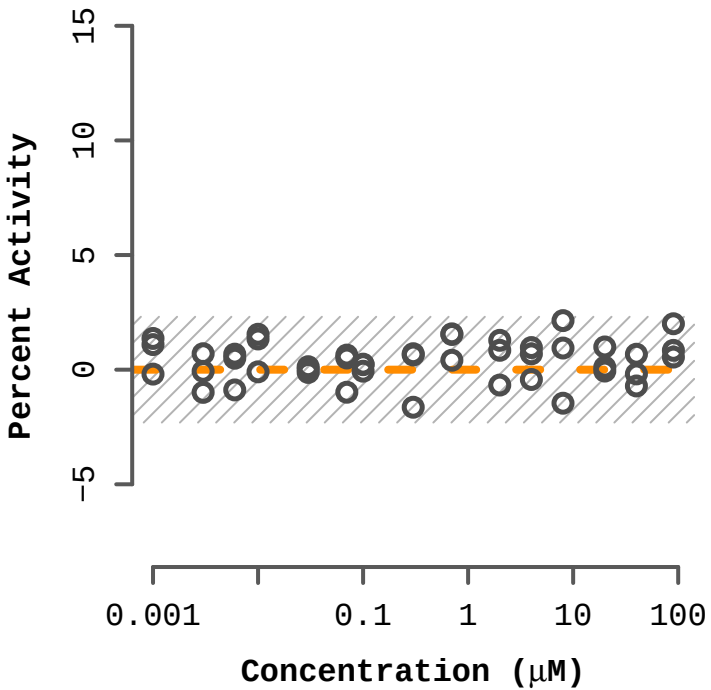
	tp	ga	gw
val:	3.78	2.02	7.98
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.56	−0.197	8	0.0535	16
sd:	23.4	2.39	50	4.06	262

	CNST	HILL	GNLS
AIC:	151.15	155.23	158.61
PROB:	0.87	0.11	0.02
RMSE:	1.4	1.38	1.36

MAX_MEAN: 1.69 MAX_MED: 2.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

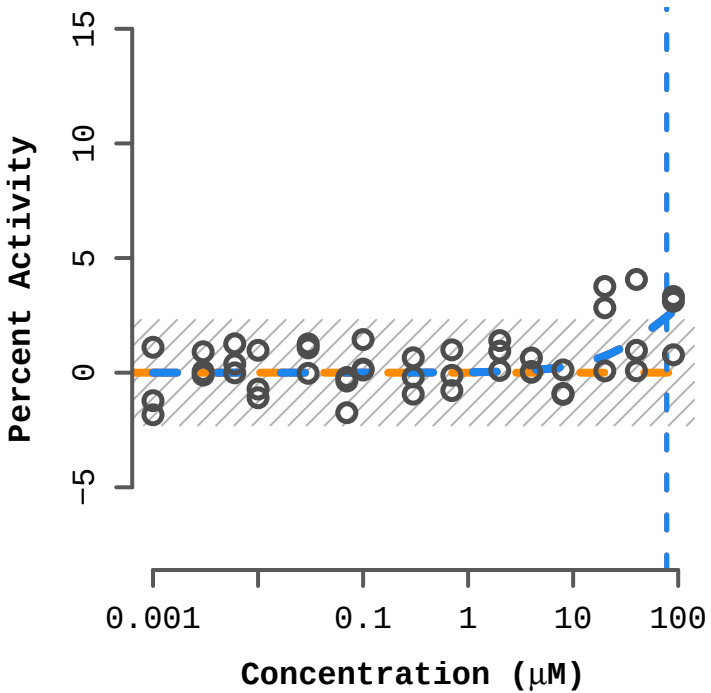
NAME: MCPA
CHID: 24195 **CASRN:** 94-74-6
SPID(S): Tox21_202272
M4ID: 12479980

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: m-Cresol
CHID: 24200 CASRN: 108-39-4
SPID(S): Tox21_302645
M4ID: 12476488

HILL MODEL (in red):

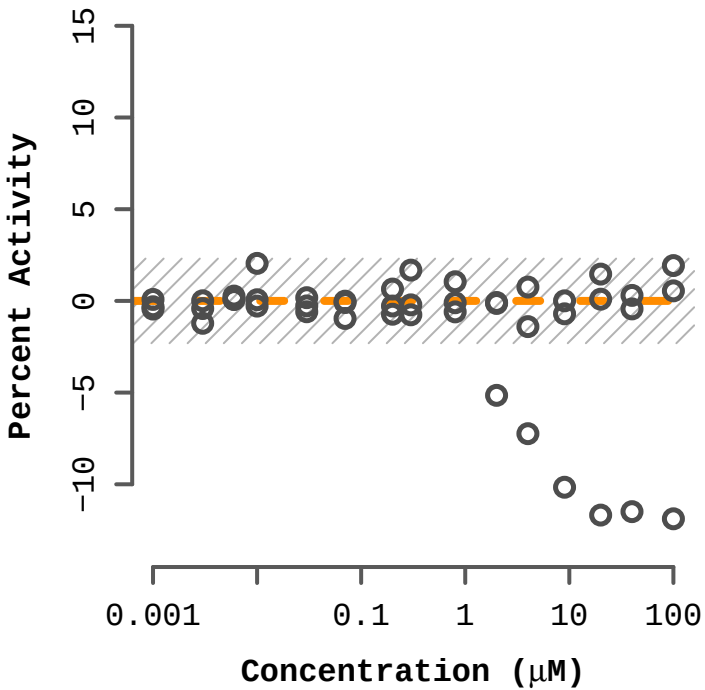
	tp	ga	gw
val:	4.88	1.89	1.28
sd:	12.3	1.76	1.67

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.88	1.89	1.28	3.32	4.9
sd:	12.3	1.76	1.67	943	3420

	CNST	HILL	GNLS
AIC:	154.84	146.52	150.52
PROB:	0.01	0.87	0.12
RMSE:	1.4	1.11	1.11

MAX_MEAN: 2.41 MAX_MED: 3.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

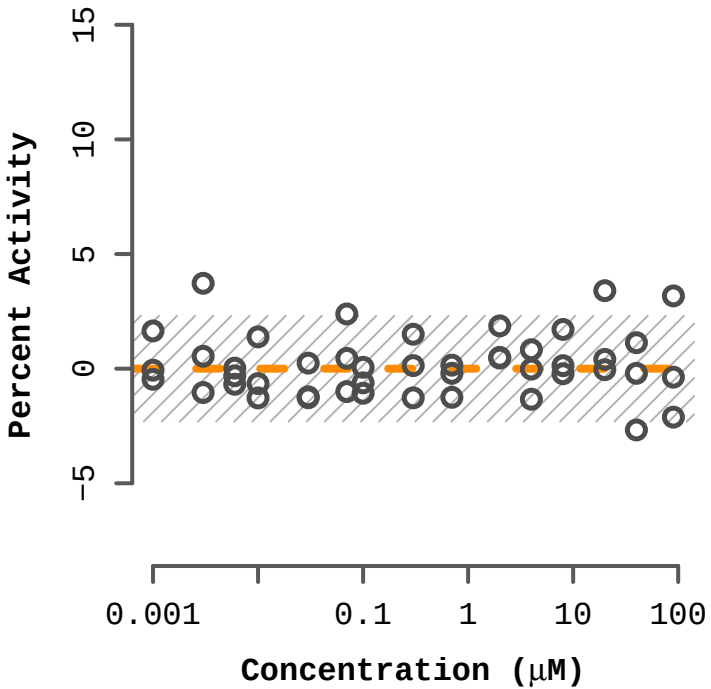
NAME: m-Cresol
CHID: 24200 CASRN: 108-39-4
SPID(S): Tox21_201941
M4ID: 12480311

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.7	NA	NA

MAX_MEAN: 0.611 **MAX_MED:** 0.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

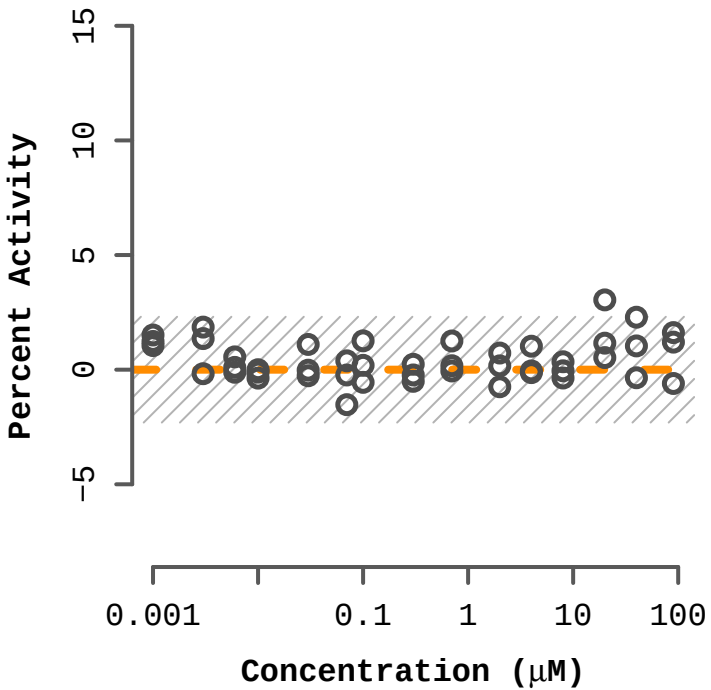
NAME: Metribuzin
CHID: 24204 **CASRN:** 21087-64-9
SPID(S): Tox21_300731
M4ID: 12478402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.542 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

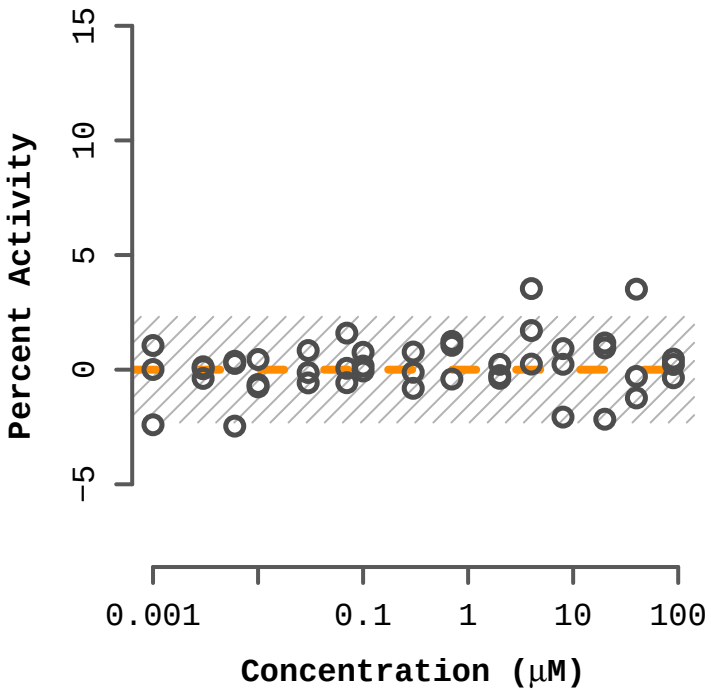
NAME: Metribuzin
CHID: 24204 **CASRN:** 21087-64-9
SPID(S): Tox21_202006
M4ID: 12480246

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

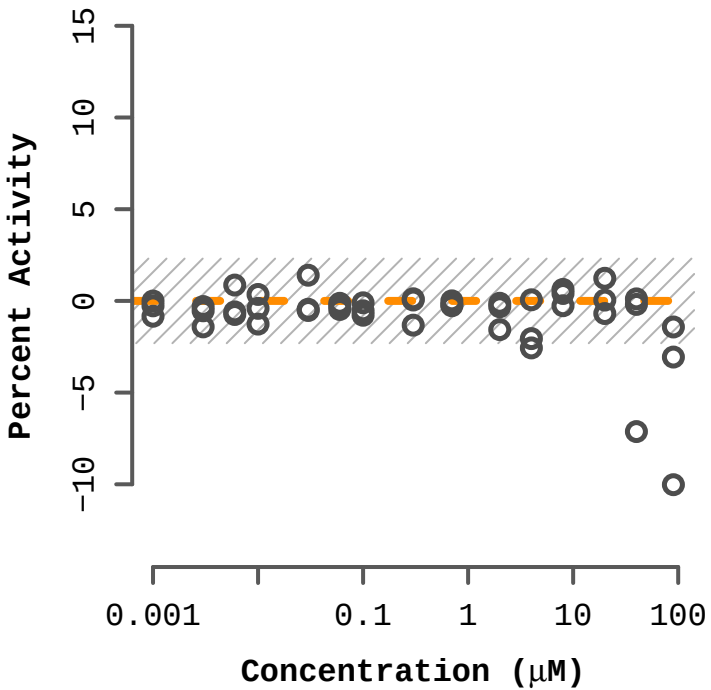
NAME: Molinate
CHID: 24206 **CASRN:** 2212-67-1
SPID(S): Tox21_300817
M4ID: 12478316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

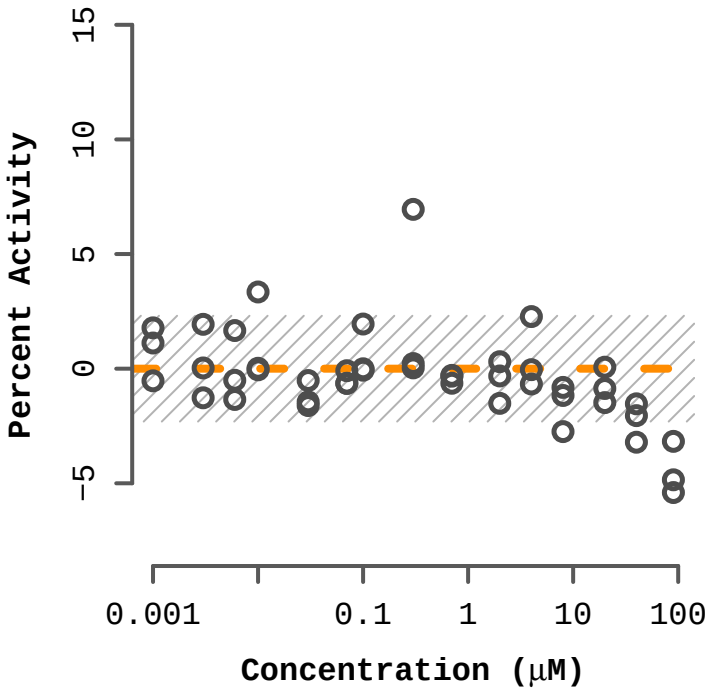
NAME: Molinate
CHID: 24206 **CASRN:** 2212-67-1
SPID(S): Tox21_201572
M4ID: 12480680

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.29	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 0.257 **MAX_MED:** 0.406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

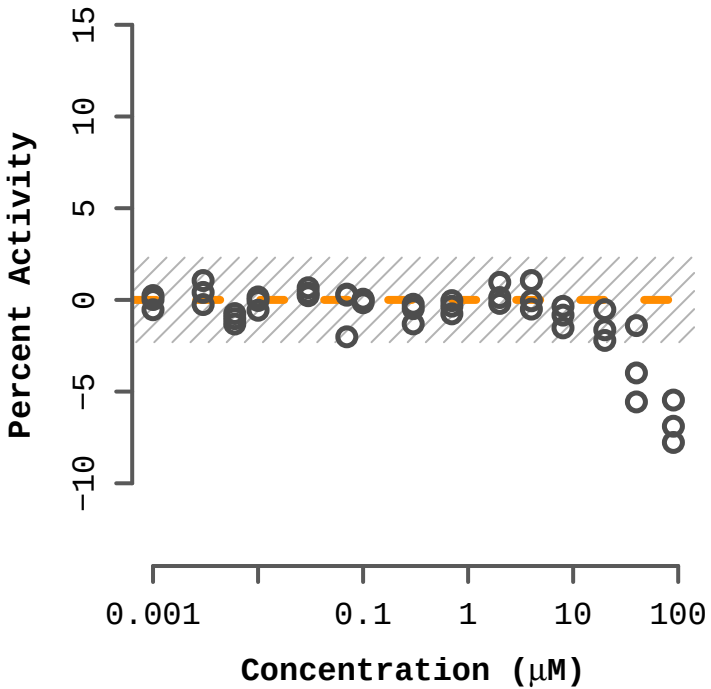
NAME: Naled
CHID: 24209 **CASRN:** 300-76-5
SPID(S): Tox21_300845
M4ID: 12478288

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.63	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 2.4 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

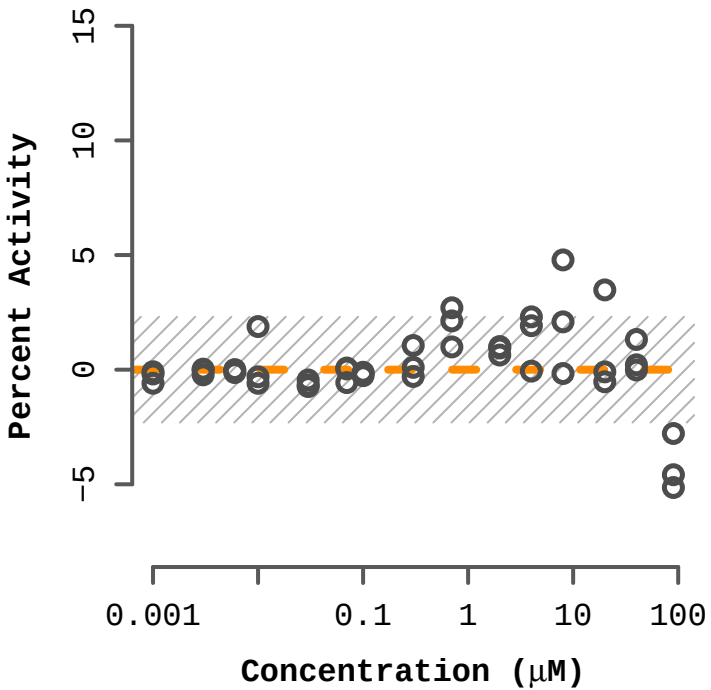
NAME: Naled
CHID: 24209 **CASRN:** 300-76-5
SPID(S): Tox21_201641
M4ID: 12480611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 0.423 **MAX_MED:** 0.411 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

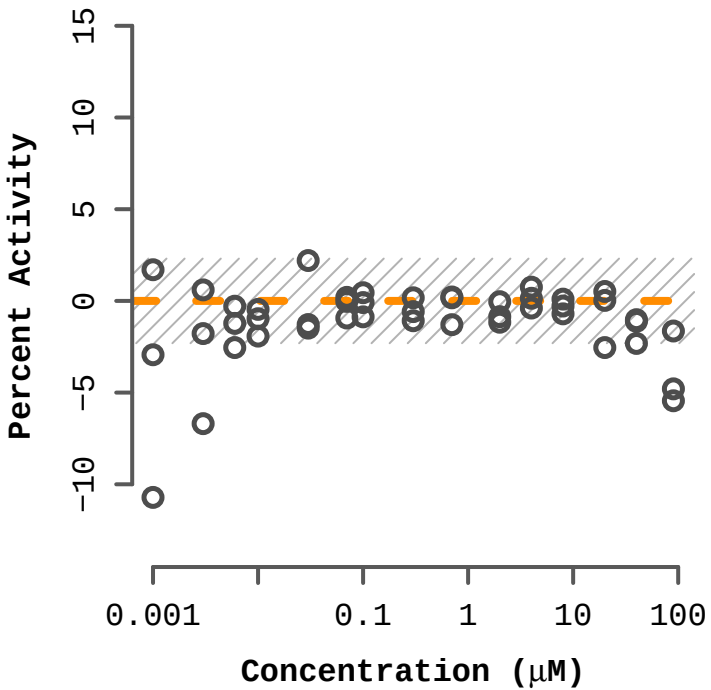
NAME: Napropamide
CHID: 24211 CASRN: 15299-99-7
SPID(S): Tox21_300655
M4ID: 12478478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

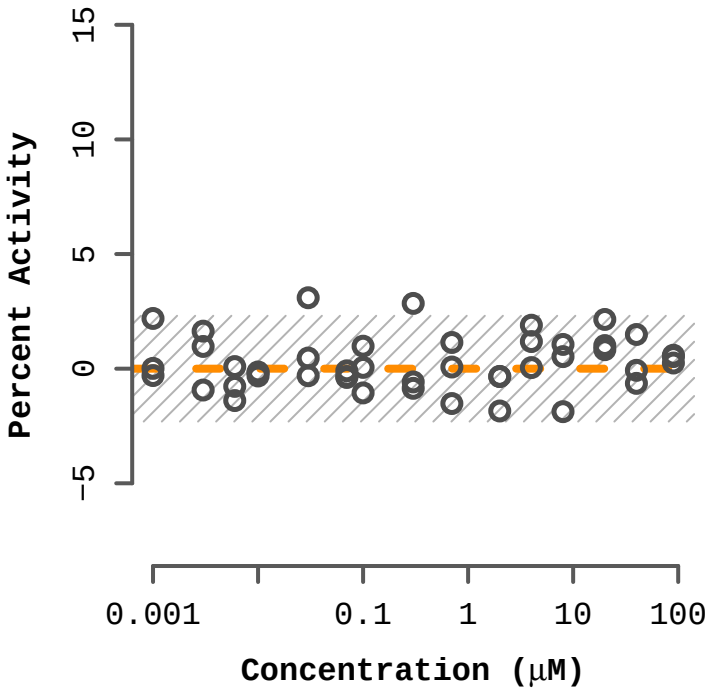
NAME: Napropamide
CHID: 24211 **CASRN:** 15299-99-7
SPID(S): Tox21_201824
M4ID: 12480428

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.47	NA	NA

MAX_MEAN: 0.169 **MAX_MED:** 0.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

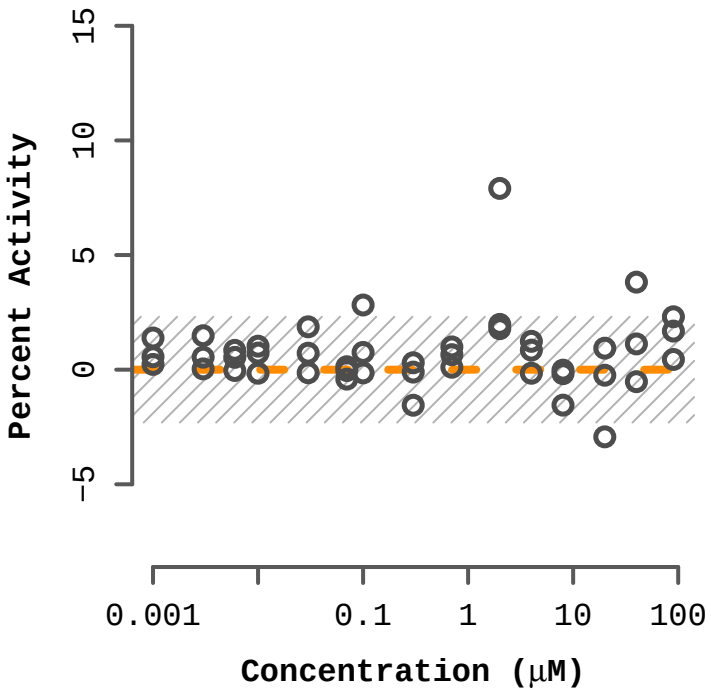
NAME: Nitrapyrin
CHID: 24216 **CASRN:** 1929-82-4
SPID(S): Tox21_300916
M4ID: 12478217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

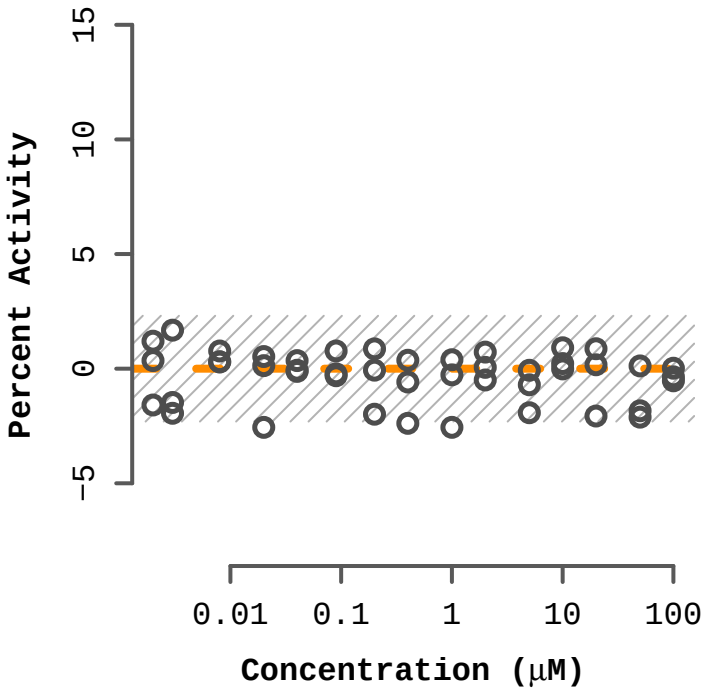
NAME: Nitrapyrin
CHID: 24216 **CASRN:** 1929-82-4
SPID(S): Tox21_202036
M4ID: 12480216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 3.89 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

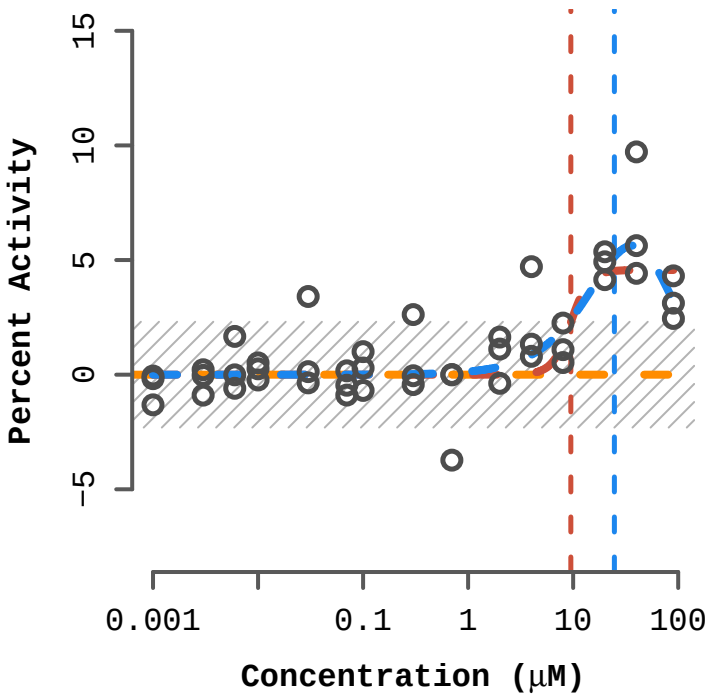
NAME: Nitroguanidine
CHID: 24222 **CASRN:** 556-88-7
SPID(S): Tox21_200886
M4ID: 12481366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.457 **MAX_MED:** 0.355 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norflurazon
CHID: 24234 CASRN: 27314-13-2
SPID(S): Tox21_300701
M4ID: 12478432

HILL MODEL (in red):

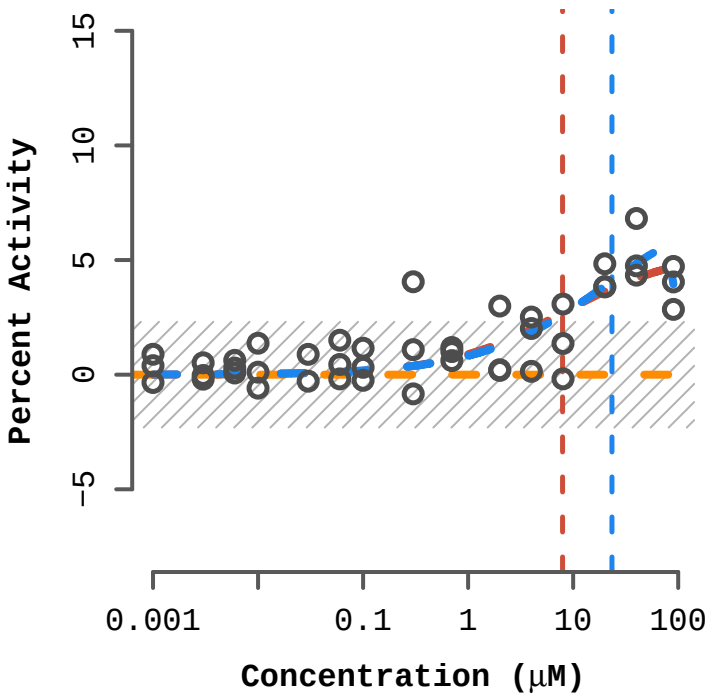
	tp	ga	gw
val:	4.57	0.978	4.93
sd:	0.447	0.0685	6.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.7	1.39	1.39	1.8	2.13
sd:	11.8	0.504	0.573	0.29	1.21

	CNST	HILL	GNLS
AIC:	210.85	161.28	154.96
PROB:	0	0.04	0.96
RMSE:	2.7	1.54	1.37

MAX_MEAN: 6.59 MAX_MED: 5.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norflurazon
CHID: 24234 CASRN: 27314-13-2
SPID(S): Tox21_202043
M4ID: 12480209

HILL MODEL (in red):

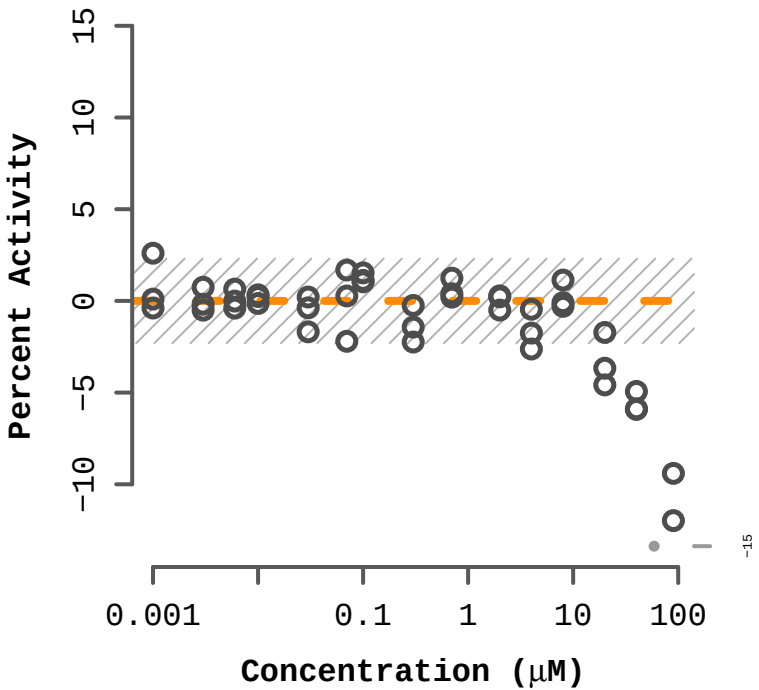
	tp	ga	gw
val:	5.39	0.899	0.784
sd:	1.44	0.354	0.462

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.18	1.37	0.694	1.98	11
sd:	3.39	0.532	0.244	0.0432	16.7

	CNST	HILL	GNLS
AIC:	199.91	138.02	136.42
PROB:	0	0.31	0.69
RMSE:	2.38	1.12	1.06

MAX_MEAN: 5.3 MAX_MED: 4.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

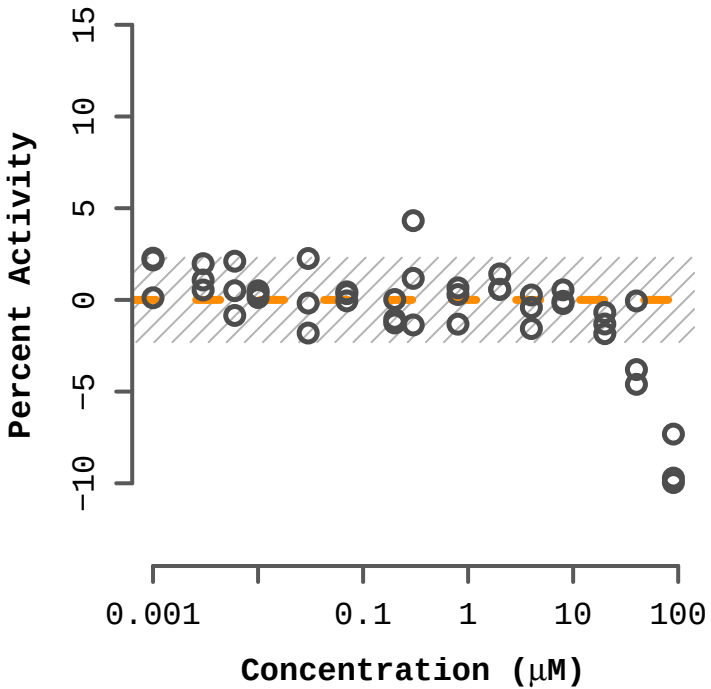
NAME: Flusilazole
CHID: 24235 CASRN: 85509-19-9
SPID(S): Tox21_300761
M4ID: 12478372 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.71	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

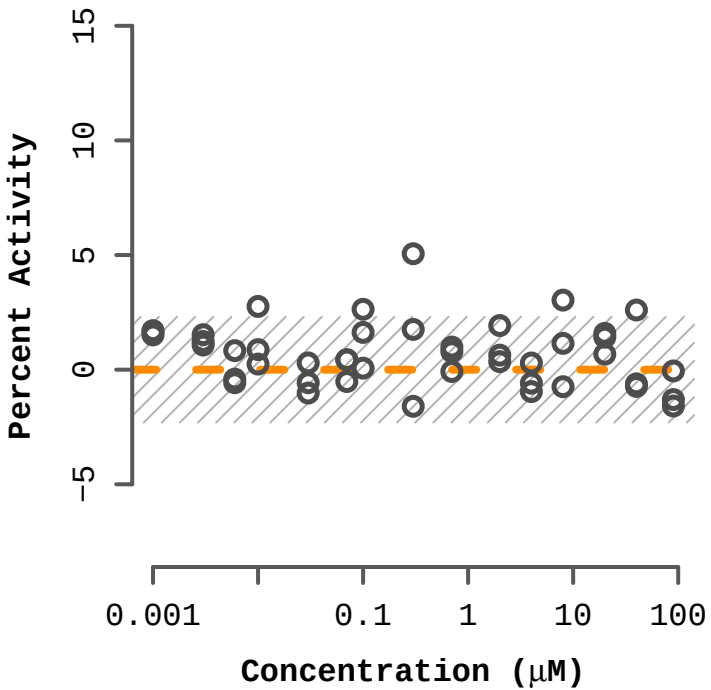
NAME: Flusilazole
CHID: 24235 CASRN: 85509-19-9
SPID(S): Tox21_201484
M4ID: 12480768

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.08	NA	NA
PROB:	1	NA	NA
RMSE:	2.79	NA	NA

MAX_MEAN: 1.53 MAX_MED: 2.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

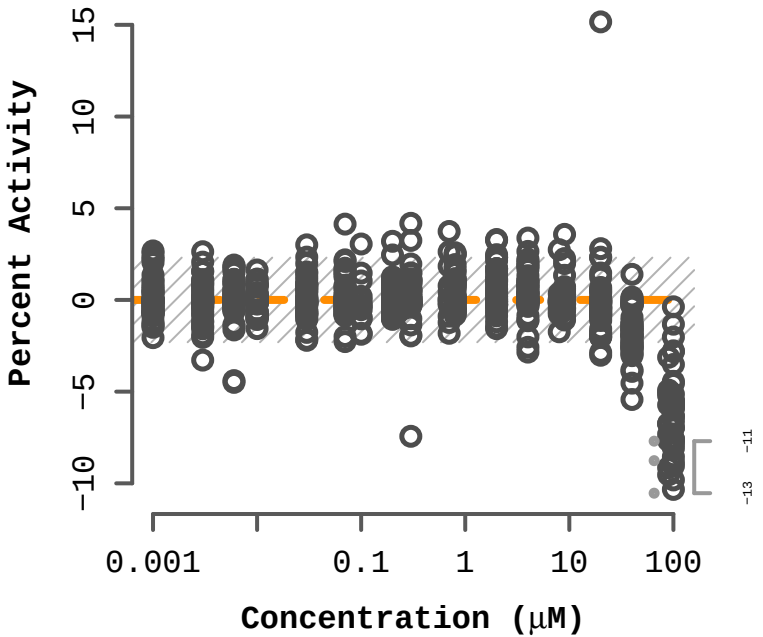
NAME: Octabromodiphenyl ether
CHID: 24236 **CASRN:** 32536-52-0
SPID(S): Tox21_200312
M4ID: 12481940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

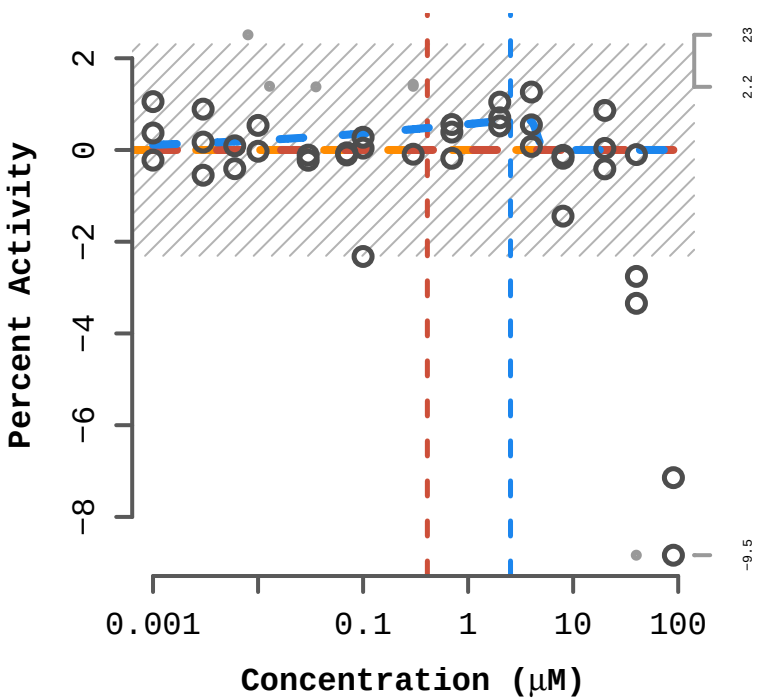
NAME: Oryzalin
CHID: 24238 **CASRN:** 19044-88-3
SPID(S): Tox21_400078
M4ID: 12475059 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2758.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 0.463 **MAX_MED:** 0.214 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxadiazon
CHID: 24239 CASRN: 19666-30-9
SPID(S): Tox21_300668
M4ID: 12478465 BRK

HILL MODEL (in red):

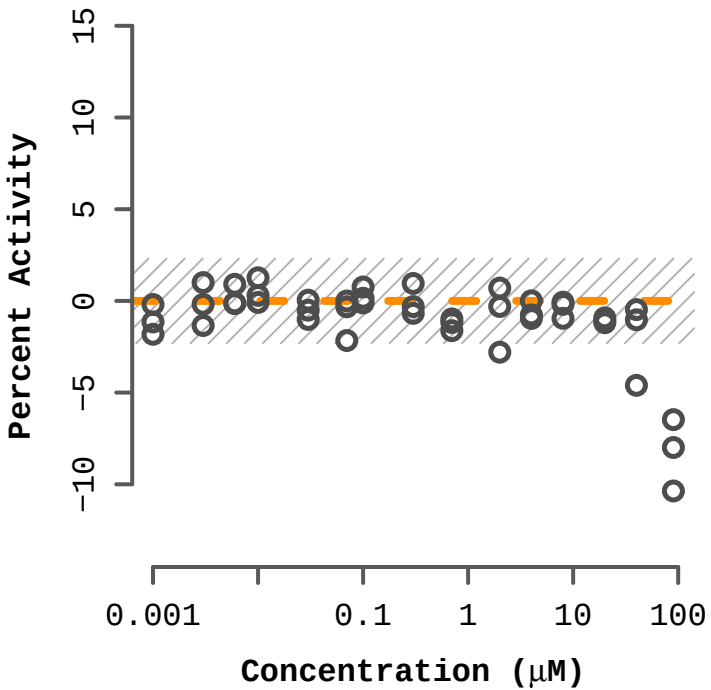
	tp	ga	gw
val:	4.76e-09	-0.388	1.64
sd:	2.02e-05	1830	21800

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.31	0.403	0.3	0.654	18
sd:	5.86	11.1	0.645	0.936	300

	CNST	HILL	GNLS
AIC:	204.89	210.89	211.2
PROB:	0.92	0.05	0.04
RMSE:	4.26	4.26	4.22

MAX_MEAN: 7.62 **MAX_MED:** 2.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

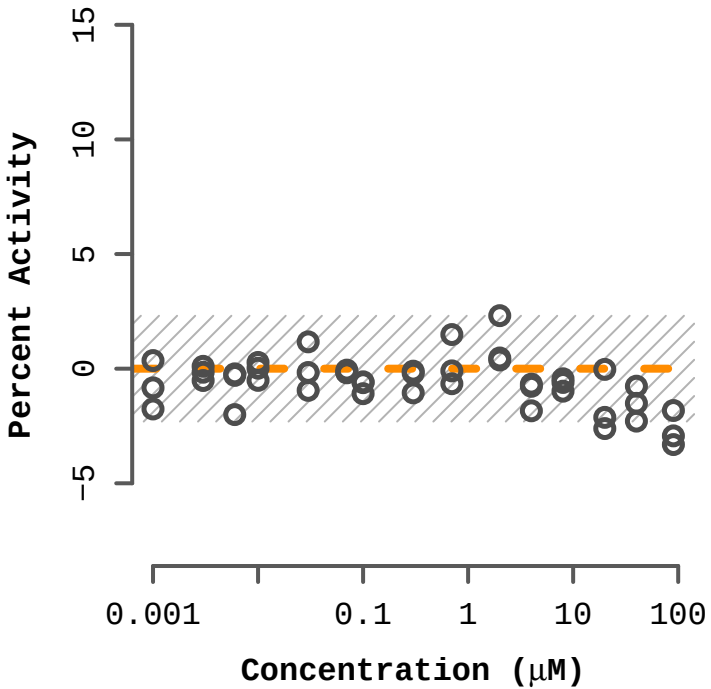
NAME: Oxadiazon
CHID: 24239 **CASRN:** 19666-30-9
SPID(S): Tox21_201877
M4ID: 12480375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 0.494 **MAX_MED:** 0.301 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

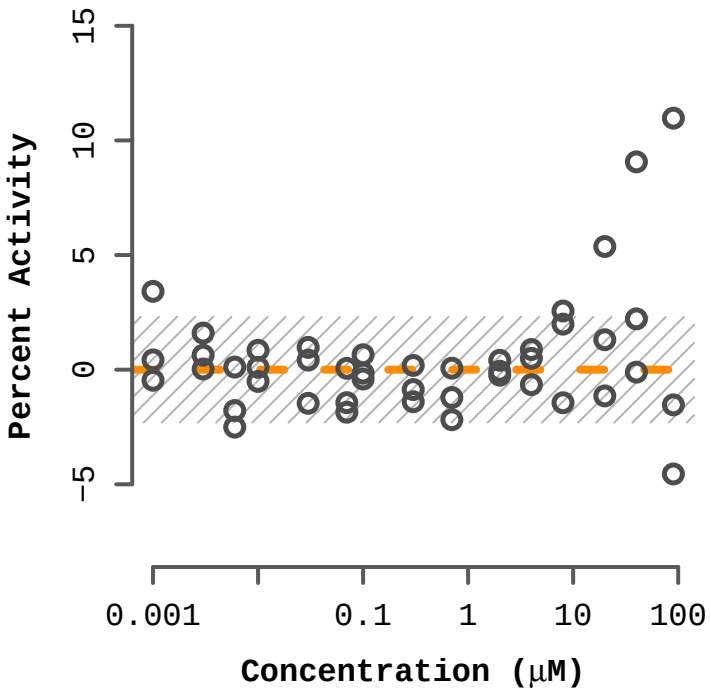
NAME: Oxyfluorfen
CHID: 24241 **CASRN:** 42874-03-3
SPID(S): Tox21_300827
M4ID: 12478306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.468 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

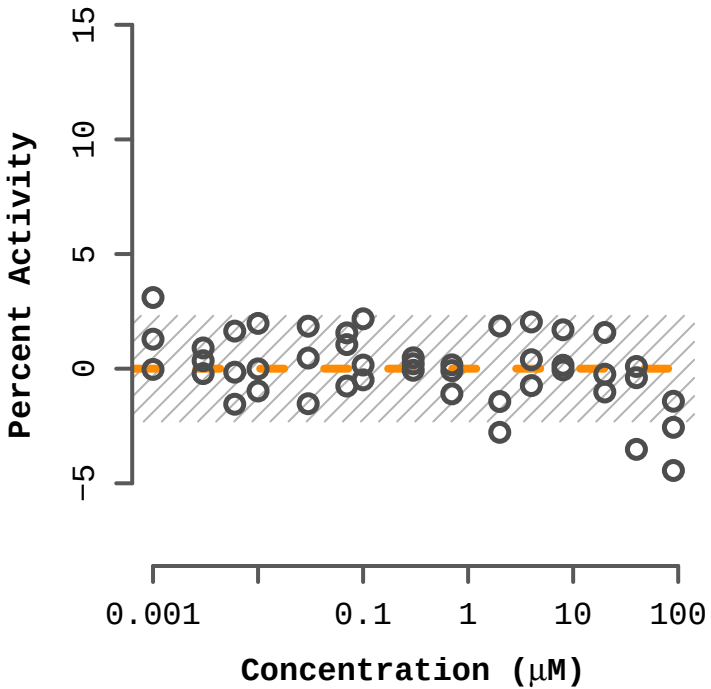
NAME: Oxyfluorfen
CHID: 24241 **CASRN:** 42874-03-3
SPID(S): Tox21_201448
M4ID: 12480804

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 3.73 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

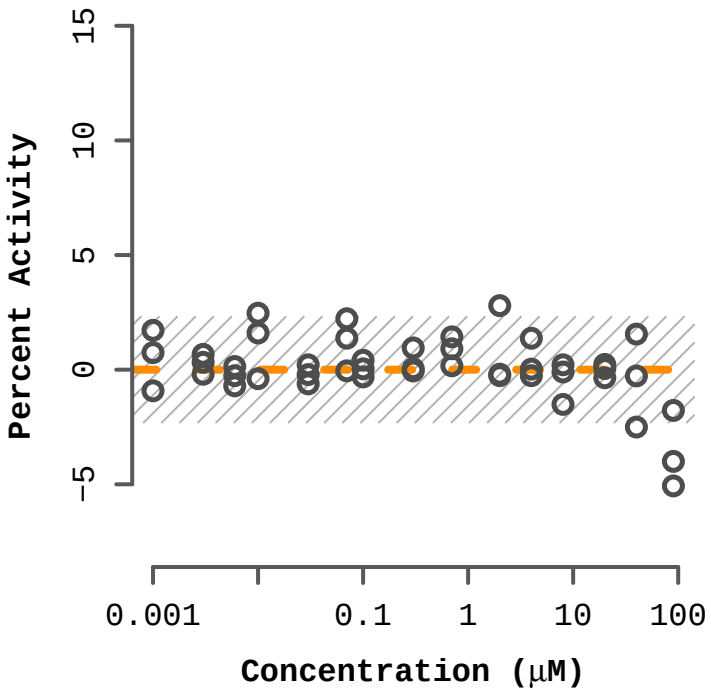
NAME: Paclobutrazol
CHID: 24242 **CASRN:** 76738-62-0
SPID(S): Tox21_300925
M4ID: 12478208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

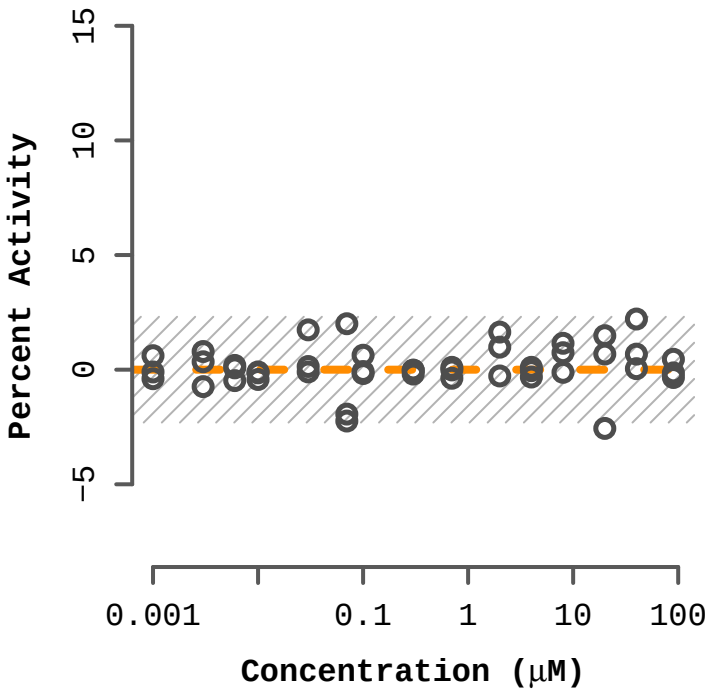
NAME: Paclobutrazol
CHID: 24242 **CASRN:** 76738-62-0
SPID(S): Tox21_202079
M4ID: 12480173

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

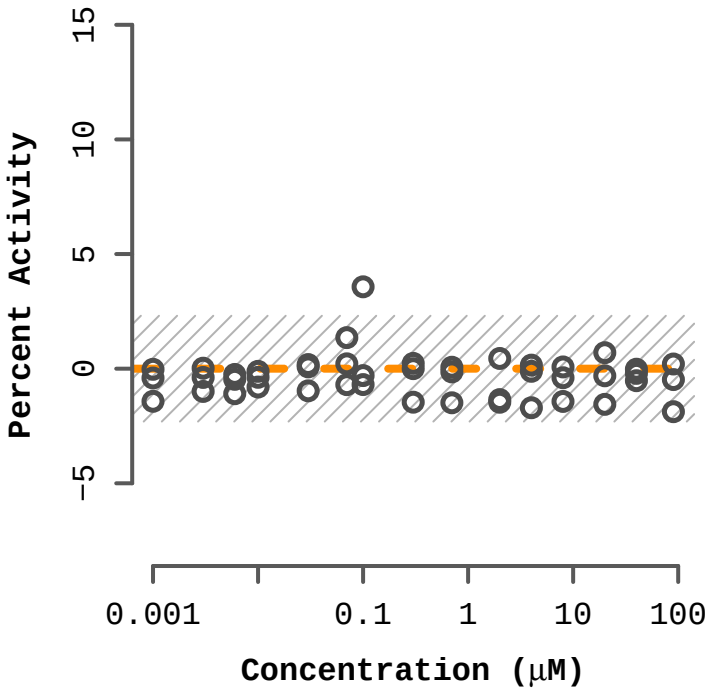
NAME: Pendimethalin
CHID: 24245 **CASRN:** 40487-42-1
SPID(S): Tox21_300867
M4ID: 12478266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.978 **MAX_MED:** 0.984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

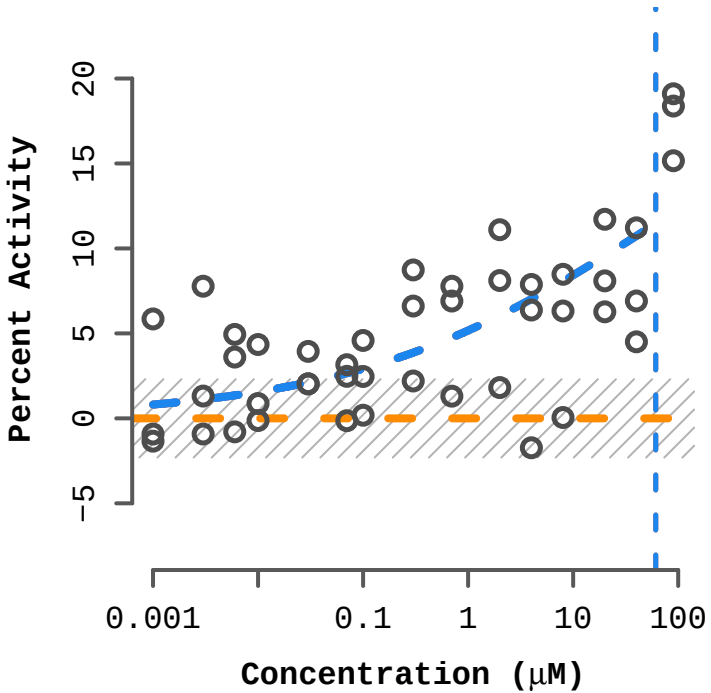
NAME: Pendimethalin
CHID: 24245 **CASRN:** 40487-42-1
SPID(S): Tox21_201896
M4ID: 12480356

HILL MODEL: Not applicable.

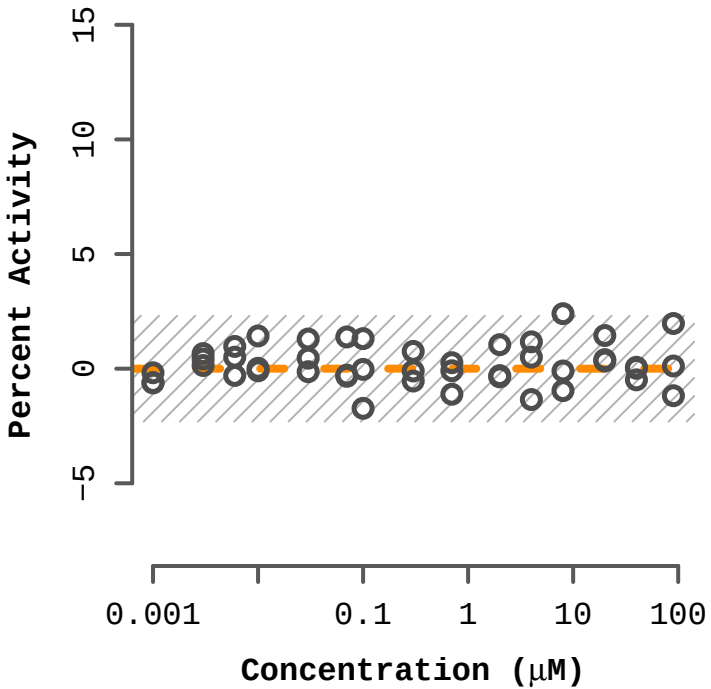
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 0.213 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pentabromodiphenyl ether
CHID:    24246   CASRN: 32534-81-9
SPID(S): Tox21_201143
M4ID:    12481109

HILL MODEL (in red):
      tp       ga       gw
val:  22.9     1.79     0.3
sd:   13.8     1.51     0.0757

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  22.9     1.79     0.3      3.75     7.25
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  305.49      250.71      254.71
PROB: 0           0.88        0.12
RMSE: 7.05        3.52        3.52

MAX_MEAN: 17.5      MAX_MED: 18.4      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

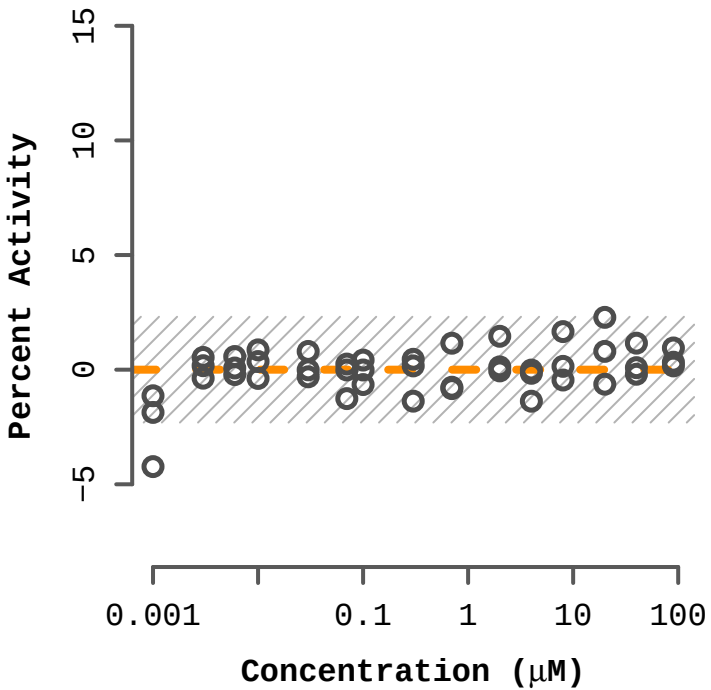
NAME: Pentachlorobenzene
CHID: 24247 **CASRN:** 608-93-5
SPID(S): Tox21_303179
M4ID: 12475954

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.726 **MAX_MED:** 0.504 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

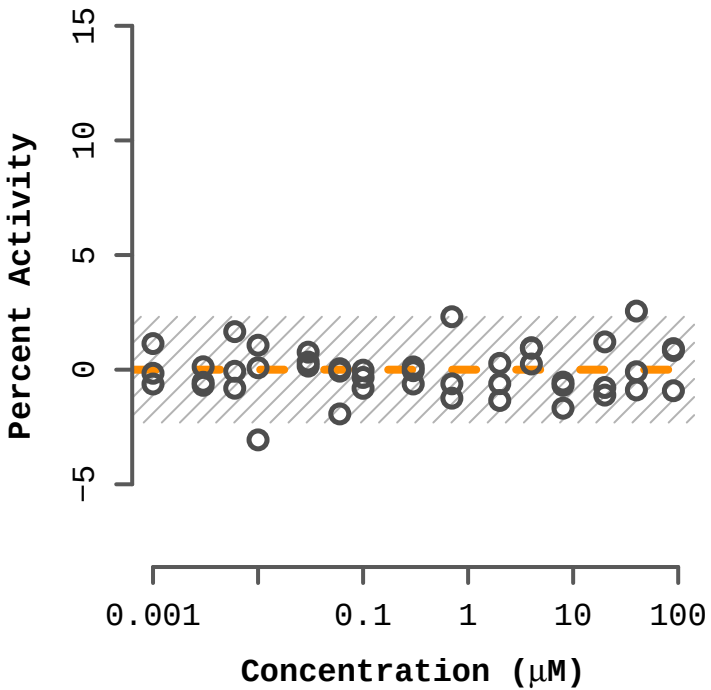
NAME: Phenanthrene
CHID: 24254 **CASRN:** 85-01-8
SPID(S): Tox21_300573
M4ID: 12478560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.817 **MAX_MED:** 0.799 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

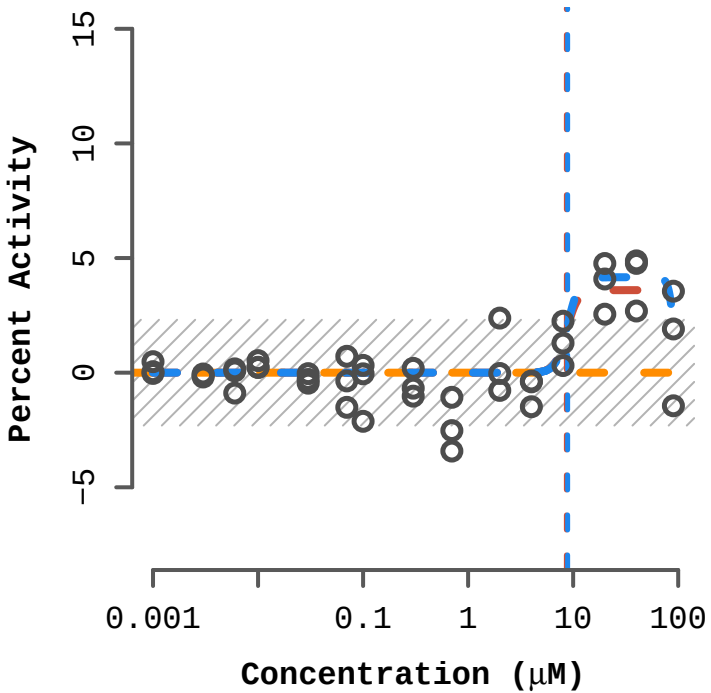
NAME: Phenanthrene
CHID: 24254 **CASRN:** 85-01-8
SPID(S): Tox21_201638
M4ID: 12480614

HILL MODEL: Not applicable.

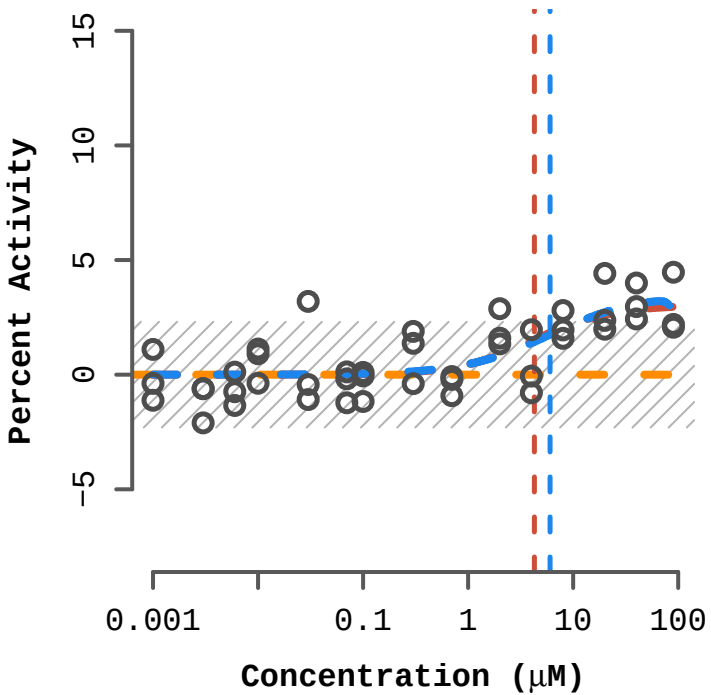
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.714 **MAX_MED:** 0.932 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenmedipham
CHID:    24255   CASRN: 13684-63-4
SPID(S): Tox21_303044
M4ID:    12476089

HILL MODEL (in red):
      tp       ga       gw
val:  3.6      0.935    8
sd:   0.43     0.0537   8.58

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.16     0.947    8        1.95     17.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  183.21      148.04      146.81
PROB: 0           0.35        0.65
RMSE: 1.91        1.3         1.17

MAX_MEAN: 4.11      MAX_MED: 4.77      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenmedipham
CHID: 24255 CASRN: 13684-63-4
SPID(S): Tox21_201295
M4ID: 12480957

HILL MODEL (in red):

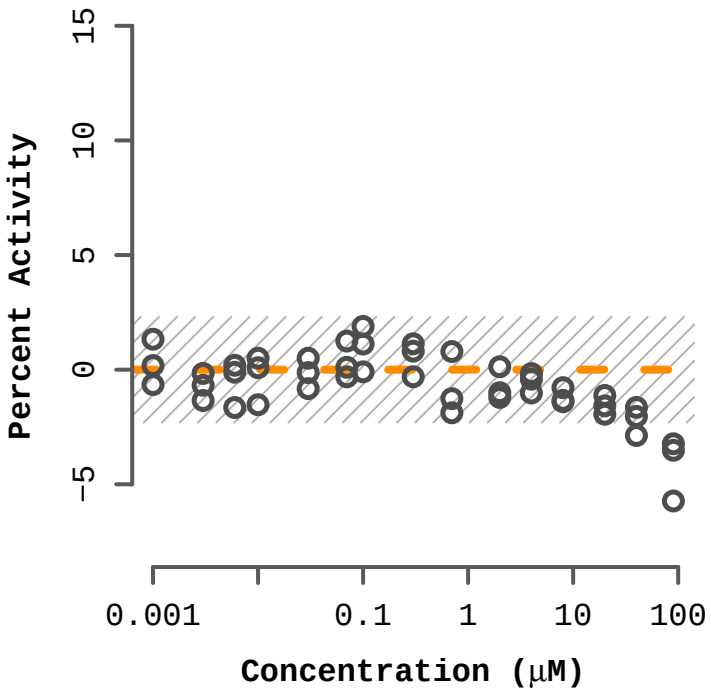
	tp	ga	gw
val:	3.03	0.631	1.2
sd:	0.607	0.292	0.568

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.49	0.78	1.05	2	12
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	186.77	147.46	151.01
PROB:	0	0.85	0.15
RMSE:	1.85	1.11	1.11

MAX_MEAN: 3.13 MAX_MED: 2.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

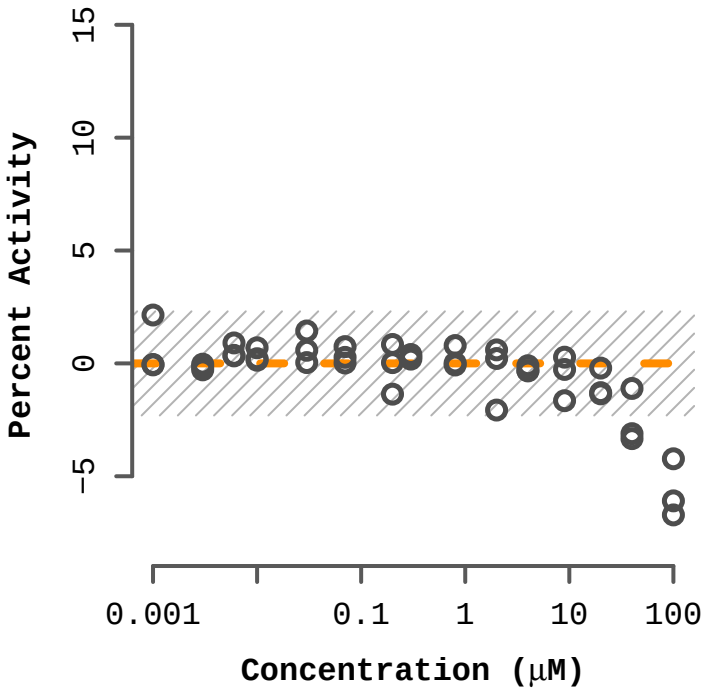
NAME: Phosalone
CHID: 24259 **CASRN:** 2310-17-0
SPID(S): Tox21_300811
M4ID: 12478322

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

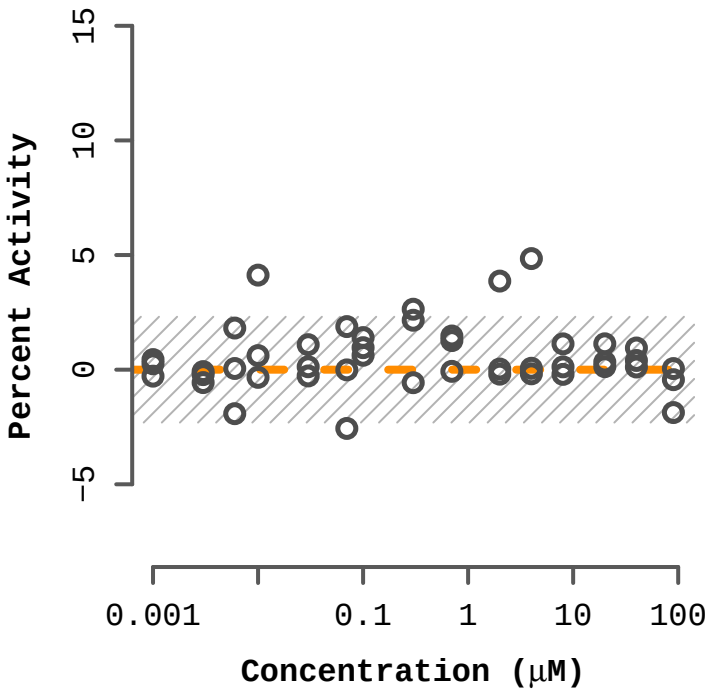
NAME: Phosalone
CHID: 24259 **CASRN:** 2310-17-0
SPID(S): Tox21_202294
M4ID: 12479958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 0.583 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

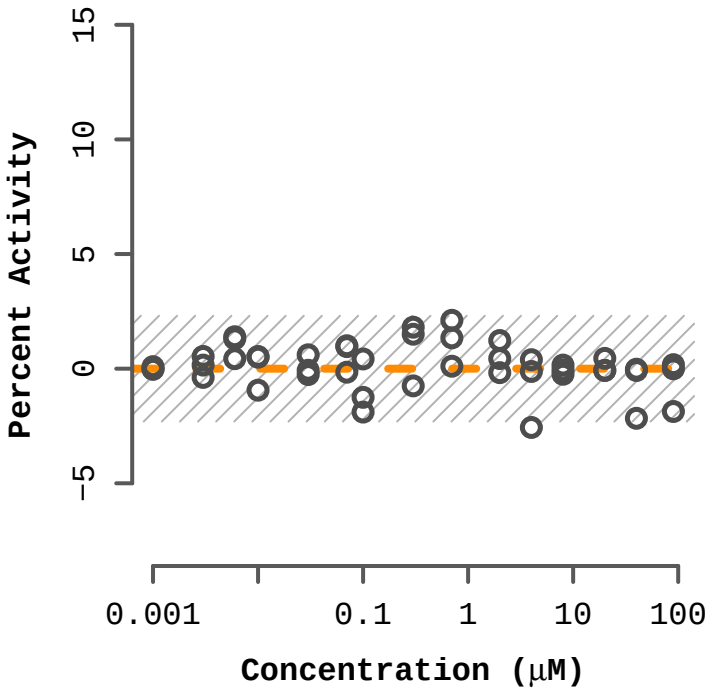
NAME: Phosmet
CHID: 24261 CASRN: 732-11-6
SPID(S): Tox21_300093
M4ID: 12479037

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

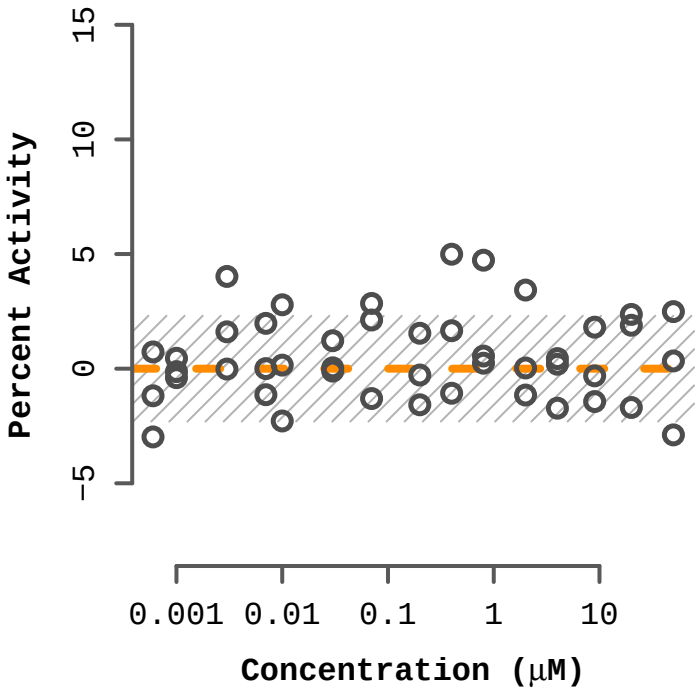
NAME: Phosmet
CHID: 24261 CASRN: 732-11-6
SPID(S): Tox21_202316
M4ID: 12479936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.19 MAX_MED: 1.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

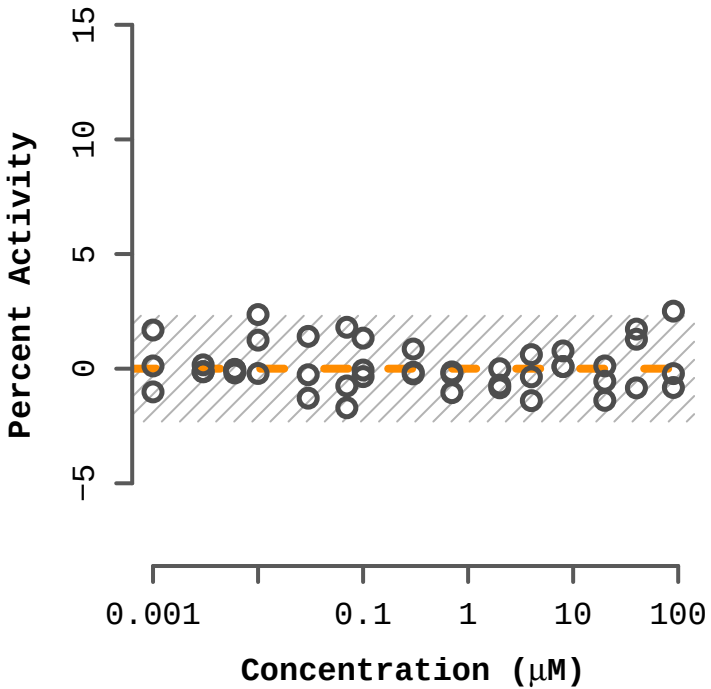
NAME: Phosmet
CHID: 24261 CASRN: 732-11-6
SPID(S): Tox21_110993_1
M4ID: 12483960

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.94	NA	NA

MAX_MEAN: 1.87 MAX_MED: 2.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

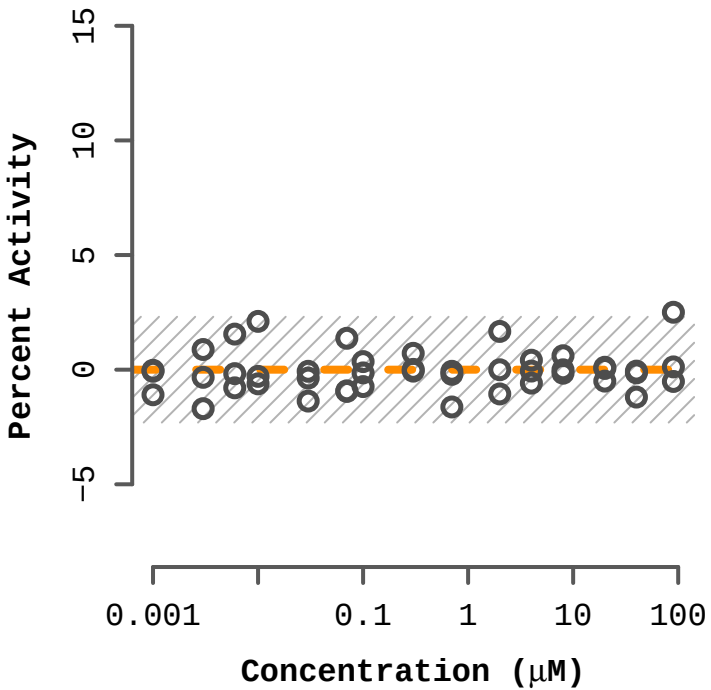
NAME: Phosphoric acid
CHID: 24263 CASRN: 7664-38-2
SPID(S): Tox21_303246
M4ID: 12475887

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.13 MAX_MED: 1.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

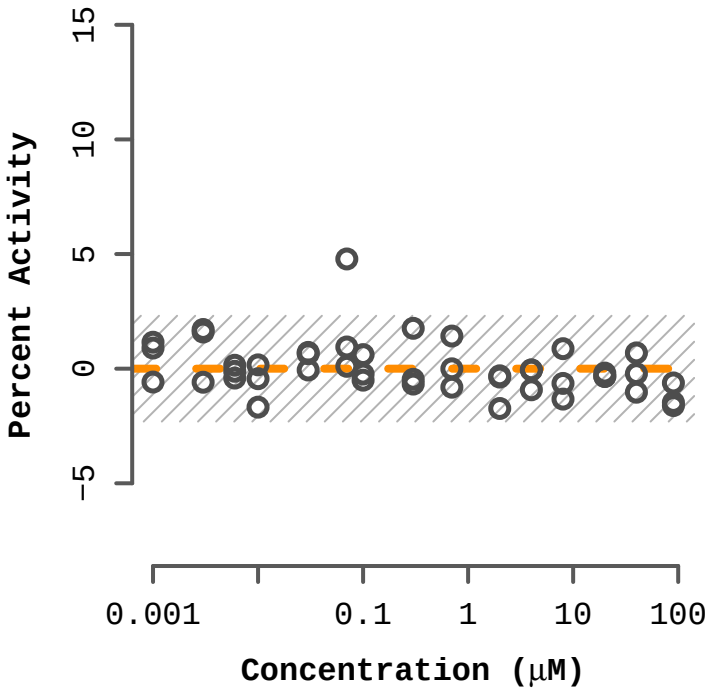
NAME: Phosphoric acid
CHID: 24263 CASRN: 7664-38-2
SPID(S): Tox21_202285
M4ID: 12479967

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.705 MAX_MED: 0.123 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

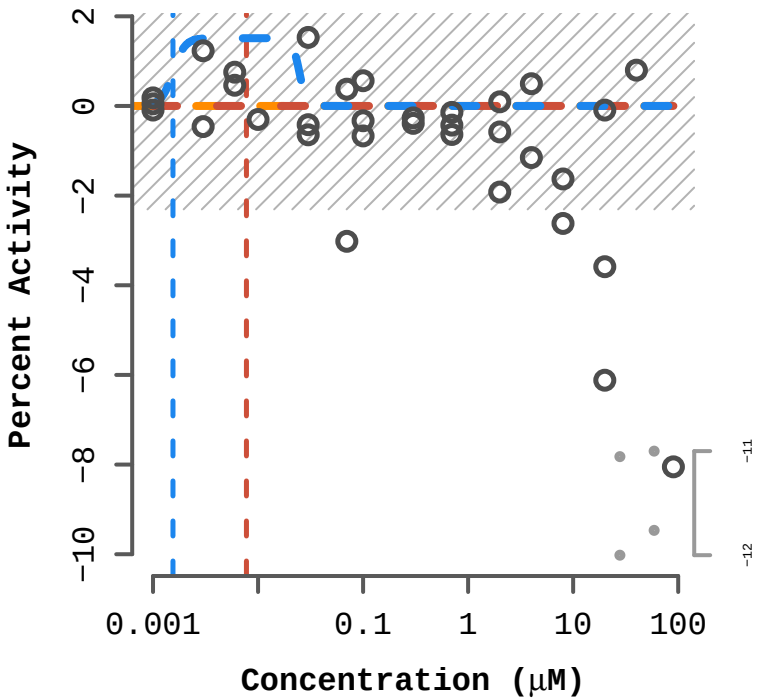
NAME: Pirimiphos-methyl
CHID: 24266 **CASRN:** 29232-93-7
SPID(S): Tox21_300718
M4ID: 12478415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Potassium silver cyanide
CHID: 24269 CASRN: 506-61-6
SPID(S): Tox21_200240
M4ID: 12482012 BRK

HILL MODEL (in red):

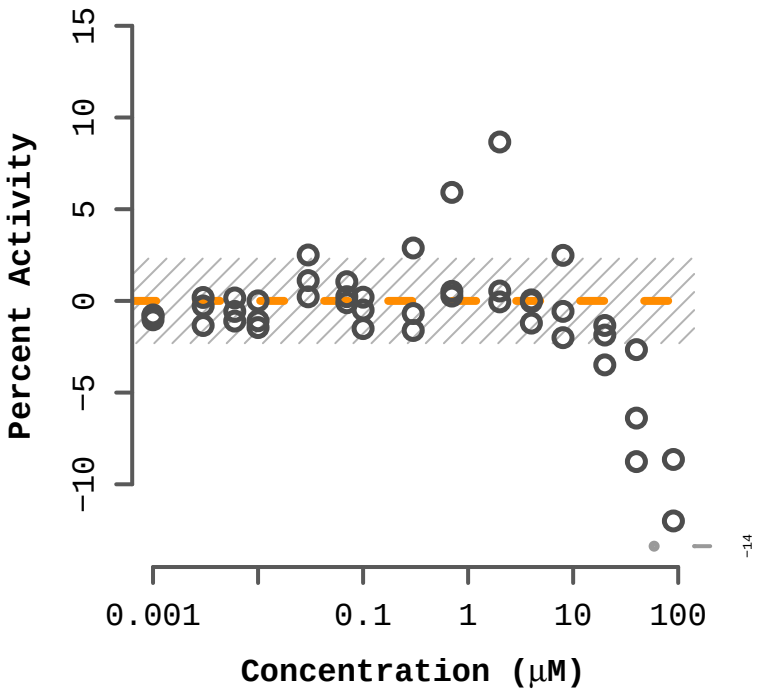
	tp	ga	gw
val:	2.44e-09	-2.11	2.11
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.51	-2.81	7.71	-1.61	12.8
sd:	0.736	1.66	64.7	4.54	687

	CNST	HILL	GNLS
AIC:	238.12	244.12	243.98
PROB:	0.91	0.05	0.05
RMSE:	4	4	3.94

MAX_MEAN: 1.74 MAX_MED: 2.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

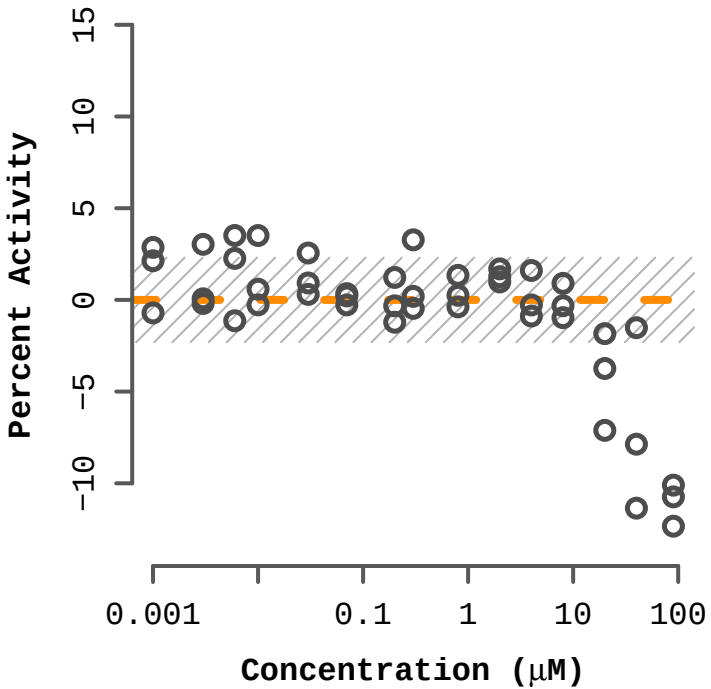
NAME: Prochloraz
CHID: 24270 CASRN: 67747-09-5
SPID(S): Tox21_301179
M4ID: 12477954 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233.77	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 3.05 MAX_MED: 1.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

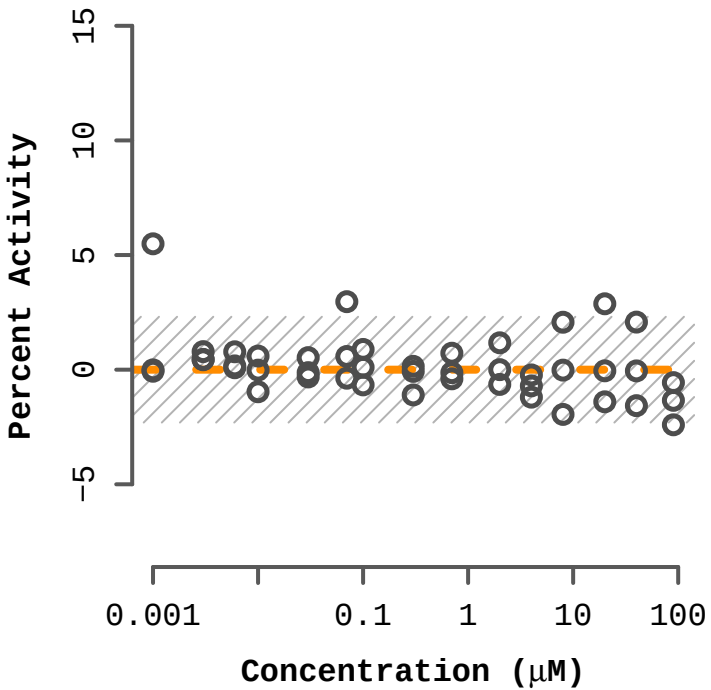
NAME: Prochloraz
CHID: 24270 **CASRN:** 67747-09-5
SPID(S): Tox21_201466
M4ID: 12480786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	238.24	NA	NA
PROB:	1	NA	NA
RMSE:	4	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

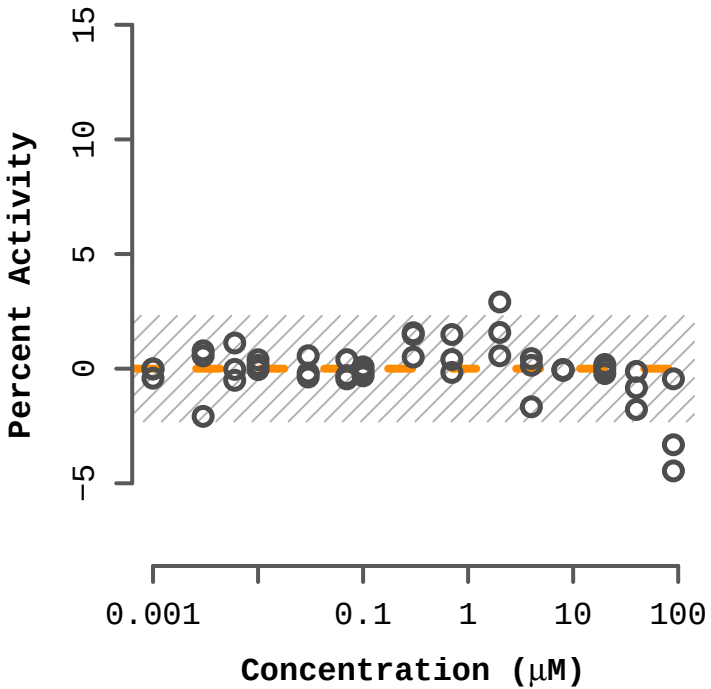
NAME: Prometryn
CHID: 24272 **CASRN:** 7287-19-6
SPID(S): Tox21_300807
M4ID: 12478326

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 0.578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

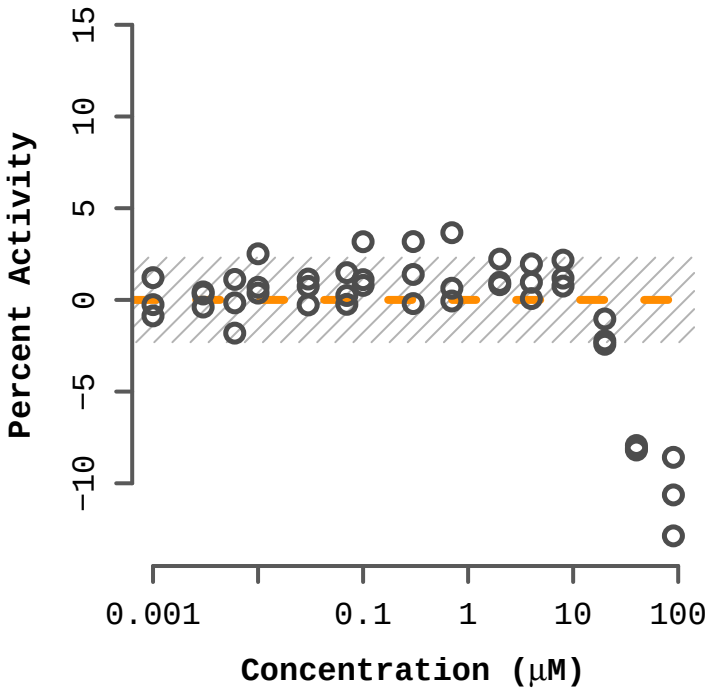
NAME: Prometryn
CHID: 24272 **CASRN:** 7287-19-6
SPID(S): Tox21_202338
M4ID: 12479914

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

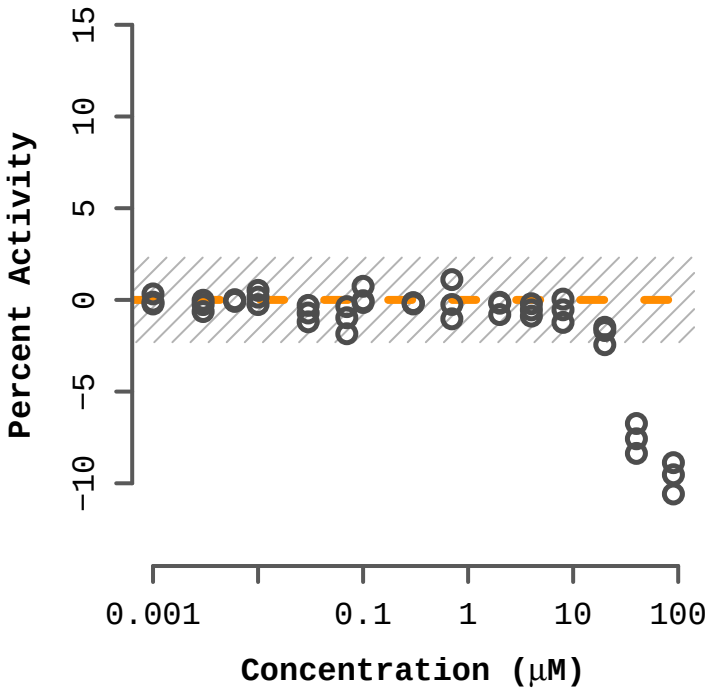
NAME: Propachlor
CHID: 24274 **CASRN:** 1918-16-7
SPID(S): Tox21_303036
M4ID: 12476097

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.75	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

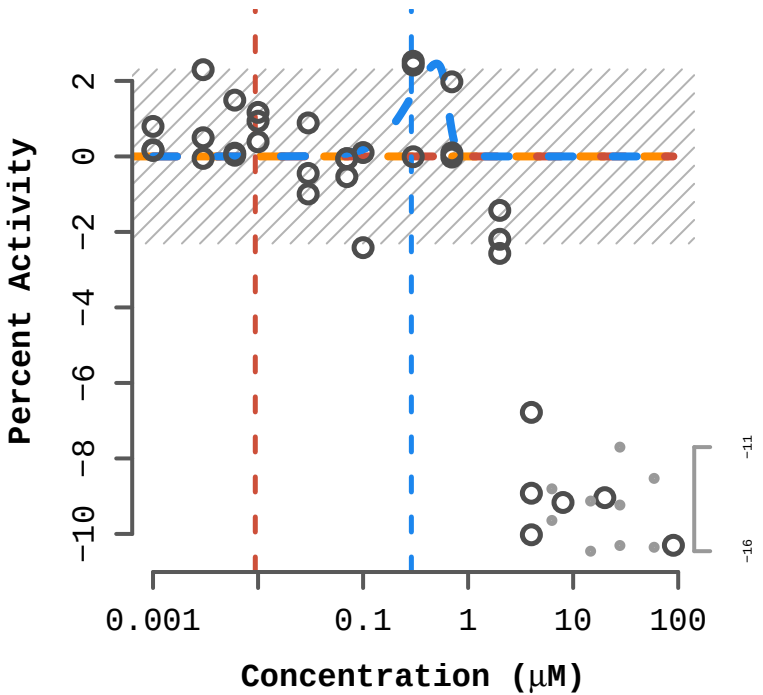
NAME: Propachlor
CHID: 24274 **CASRN:** 1918-16-7
SPID(S): Tox21_201734
M4ID: 12480518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.08	NA	NA
PROB:	1	NA	NA
RMSE:	3.26	NA	NA

MAX_MEAN: 0.188 **MAX_MED:** 0.151 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propargite
CHID: 24276 CASRN: 2312-35-8
SPID(S): Tox21_300805
M4ID: 12478328 BRK

HILL MODEL (in red):

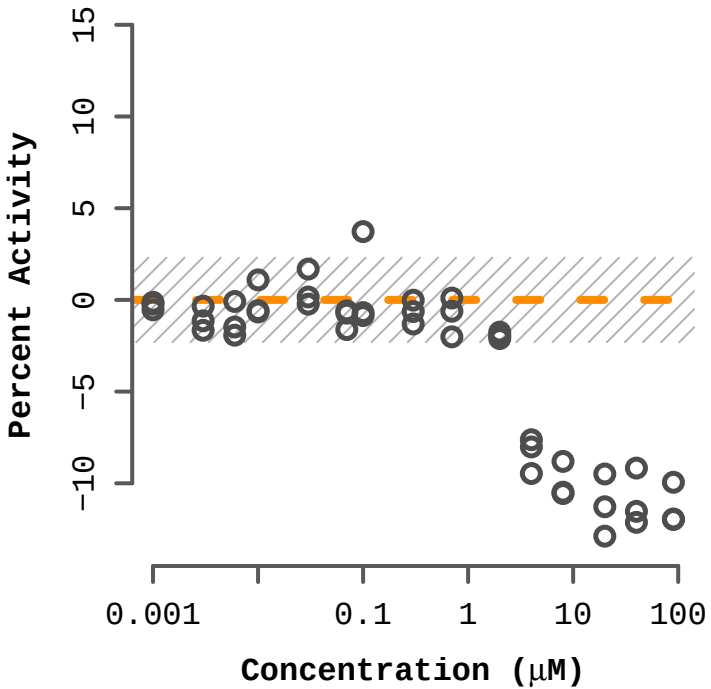
	tp	ga	gw
val:	2.29e-09	-2.03	2.78
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.17	-0.54	2.59	-0.194	13.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	303.08	309.08	312.61
PROB:	0.94	0.05	0.01
RMSE:	7.07	7.07	7.05

MAX_MEAN: 1.64 MAX_MED: 2.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

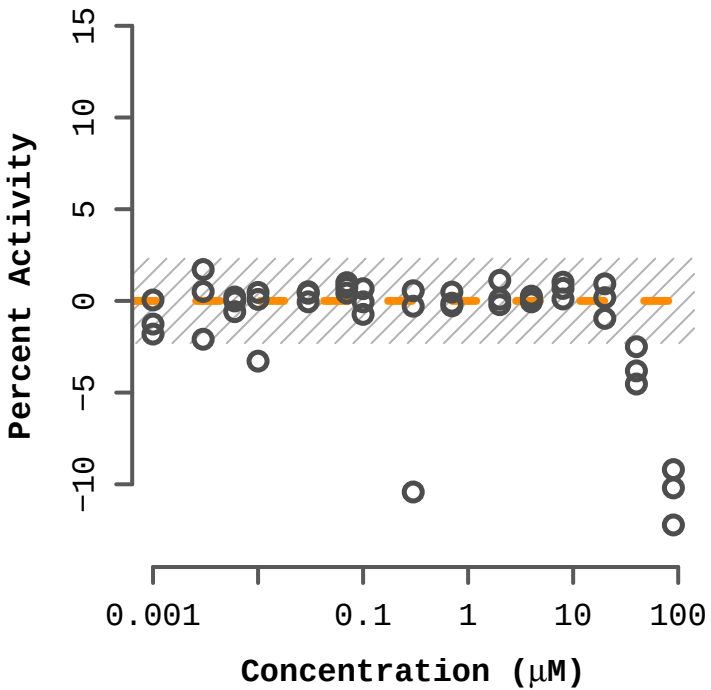
NAME: Propargite
CHID: 24276 **CASRN:** 2312-35-8
SPID(S): Tox21_202046
M4ID: 12480206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	291.83	NA	NA
PROB:	1	NA	NA
RMSE:	6.14	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 0.161 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

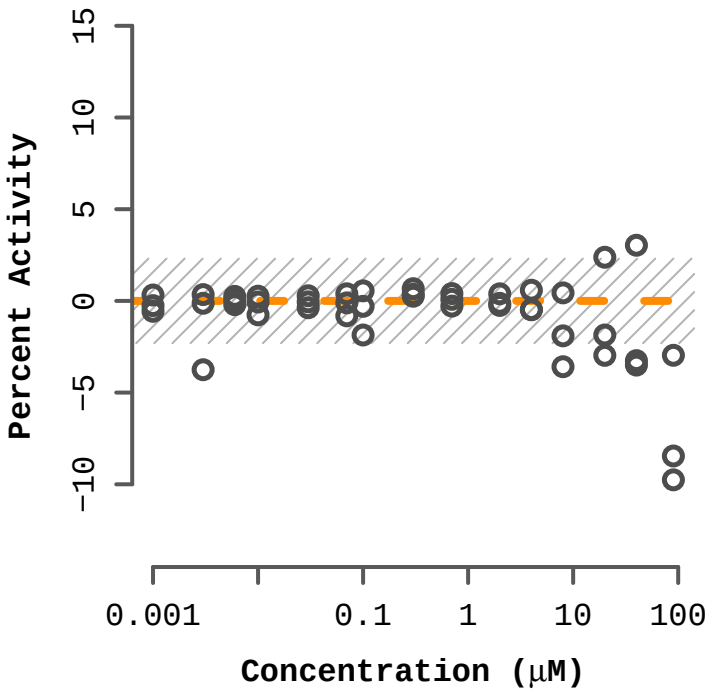
NAME: Propiconazole
CHID: 24280 **CASRN:** 60207-90-1
SPID(S): Tox21_300859
M4ID: 12478274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.44	NA	NA
PROB:	1	NA	NA
RMSE:	3.4	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 0.738 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

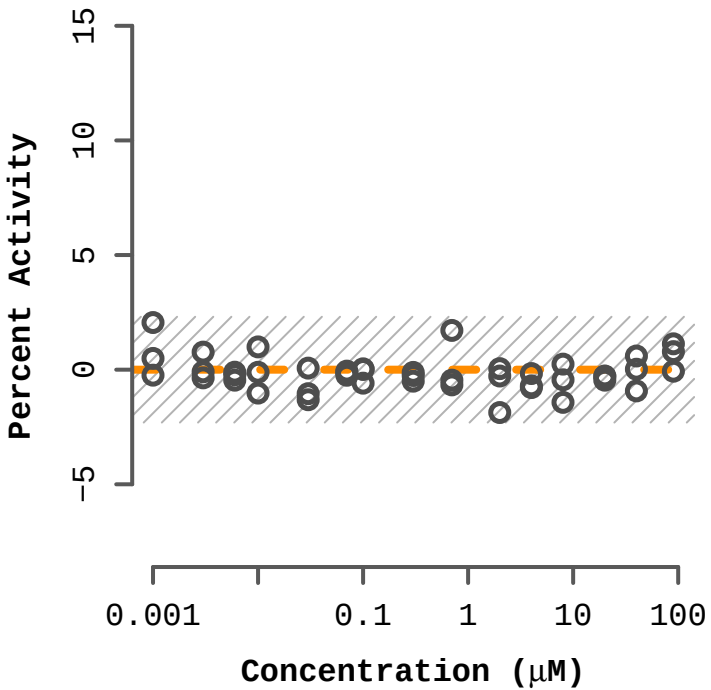
NAME: Propiconazole
CHID: 24280 **CASRN:** 60207-90-1
SPID(S): Tox21_201469
M4ID: 12480783

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.7	NA	NA
PROB:	1	NA	NA
RMSE:	2.42	NA	NA

MAX_MEAN: 0.429 **MAX_MED:** 0.362 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

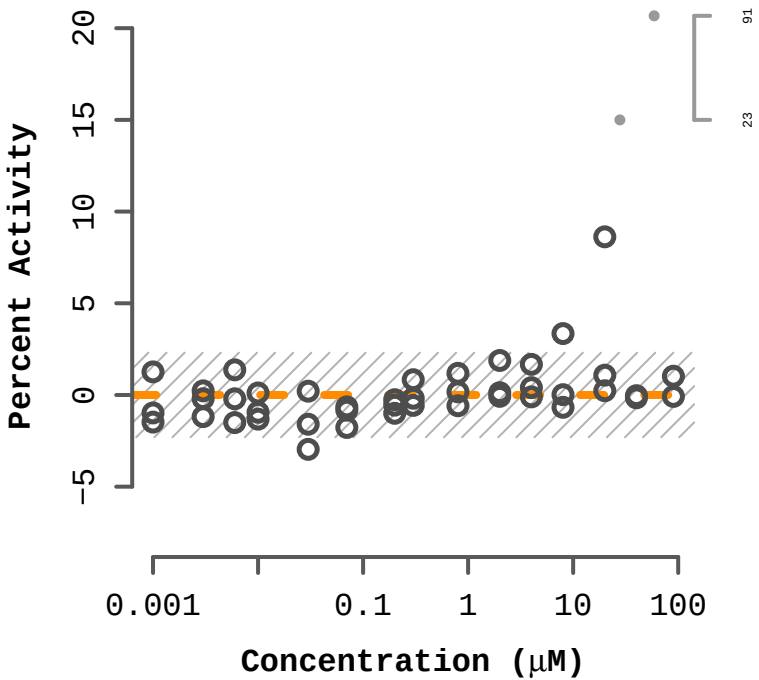
NAME: 1-Methoxy-2-propanol
CHID: 24284 **CASRN:** 107-98-2
SPID(S): Tox21_303269
M4ID: 12475864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.771 **MAX_MED:** 0.789 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

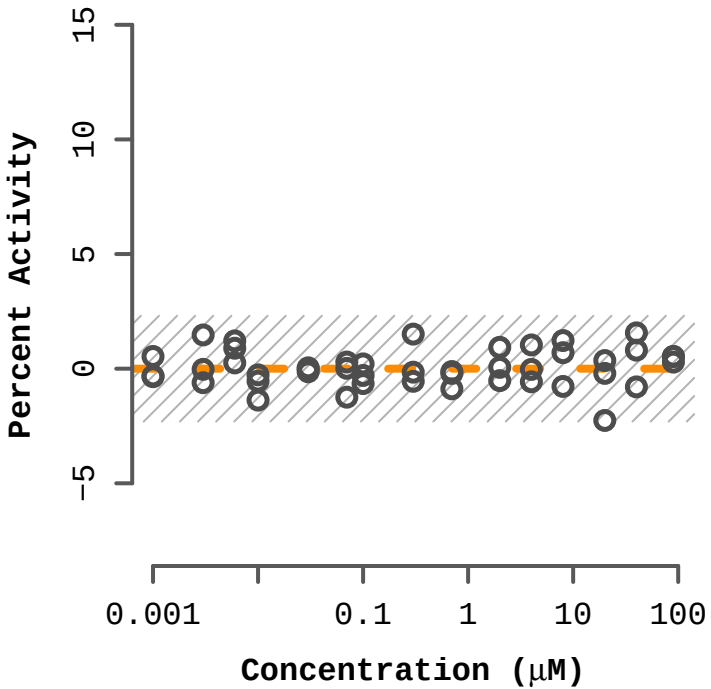
NAME: 1-Methoxy-2-propanol
CHID: 24284 **CASRN:** 107-98-2
SPID(S): Tox21_201803
M4ID: 12480449 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.87	NA	NA
PROB:	1	NA	NA
RMSE:	14.1	NA	NA

MAX_MEAN: 30.6 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

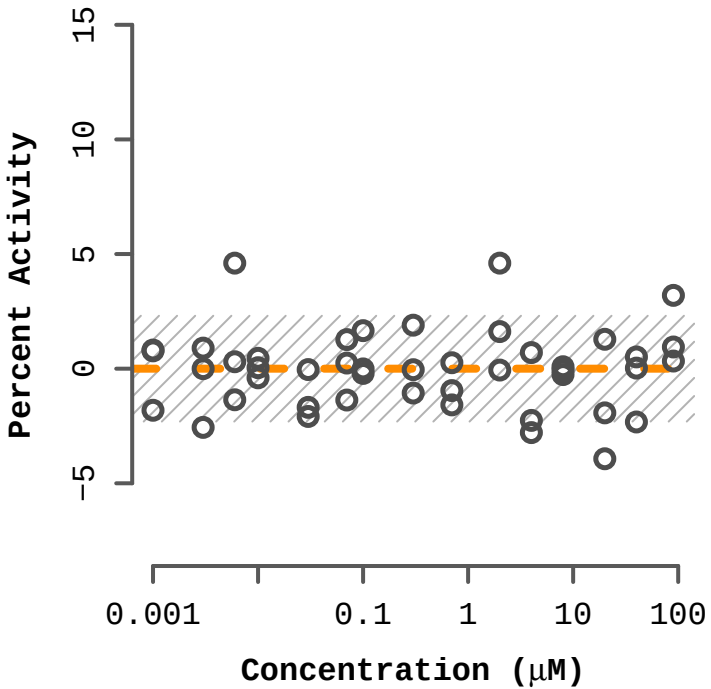
NAME: Propyleneimine
CHID: 24286 **CASRN:** 75-55-8
SPID(S): Tox21_202944
M4ID: 12479308

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.787 **MAX_MED:** 0.893 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

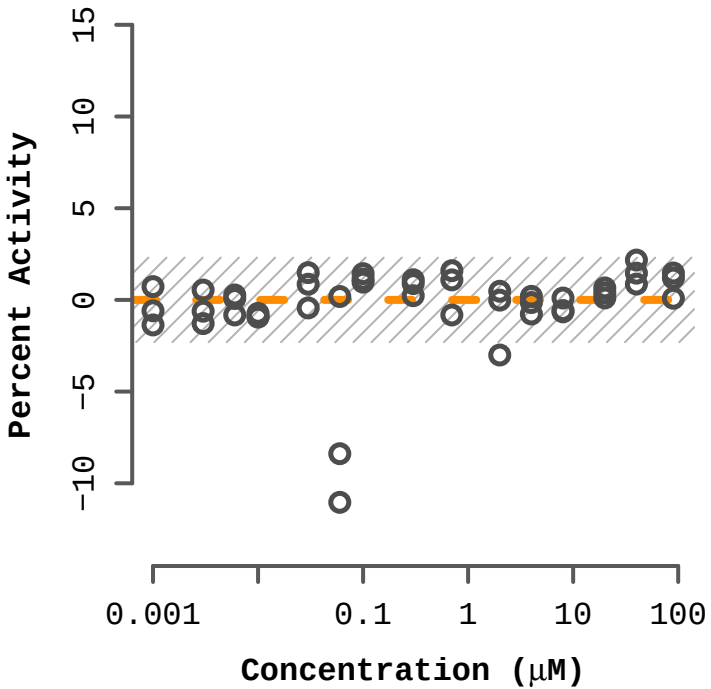
NAME: Imazethapyr
CHID: 24287 **CASRN:** 81335-77-5
SPID(S): Tox21_301012
M4ID: 12478121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

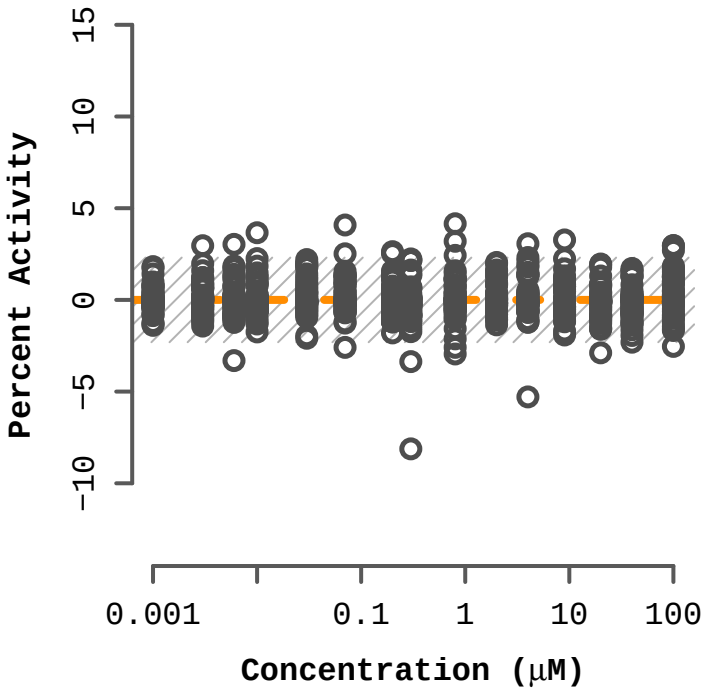
NAME: Imazethapyr
CHID: 24287 **CASRN:** 81335-77-5
SPID(S): Tox21_201339
M4ID: 12480913

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.84	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

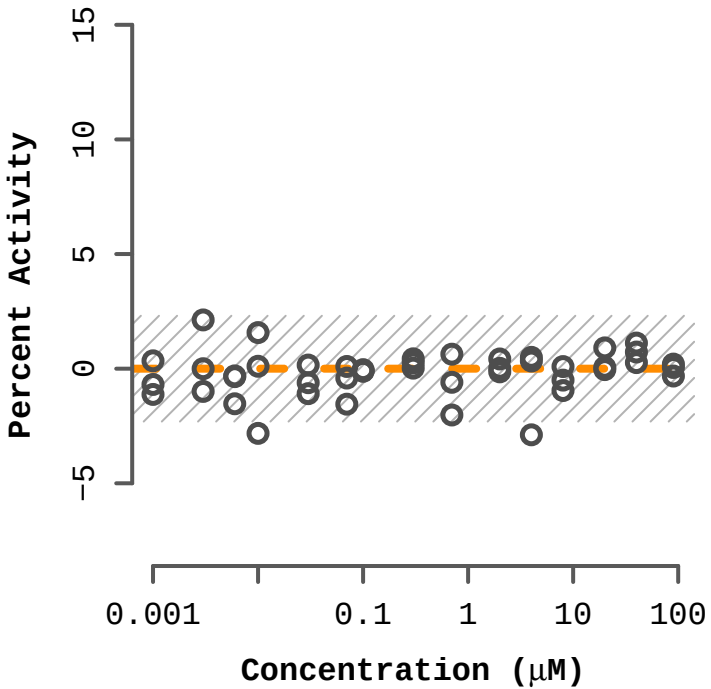
NAME: Pyrene
CHID: 24289 **CASRN:** 129-00-0
SPID(S): Tox21_400063
M4ID: 12475074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	1950.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.332 **MAX_MED:** 0.181 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

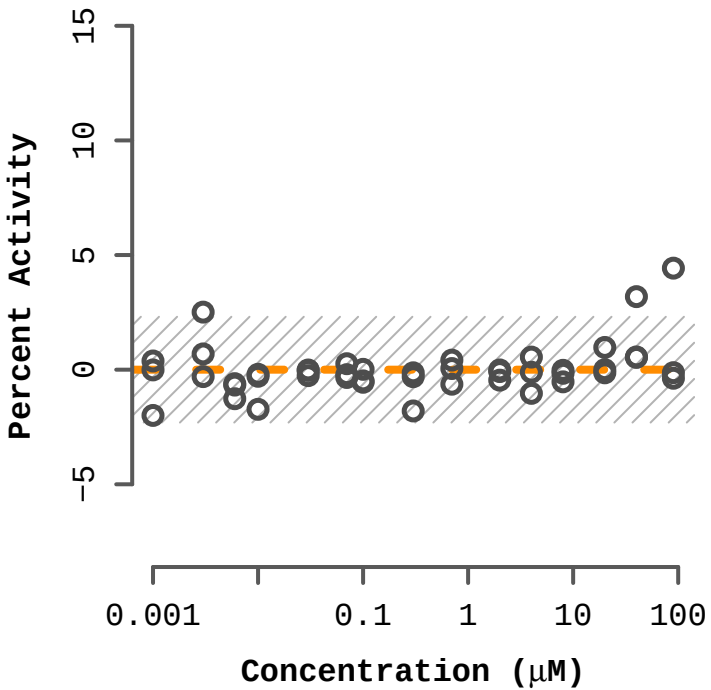
NAME: Quinalphos
CHID: 24291 **CASRN:** 13593-03-8
SPID(S): Tox21_303270
M4ID: 12475863

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.704 **MAX_MED:** 0.727 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

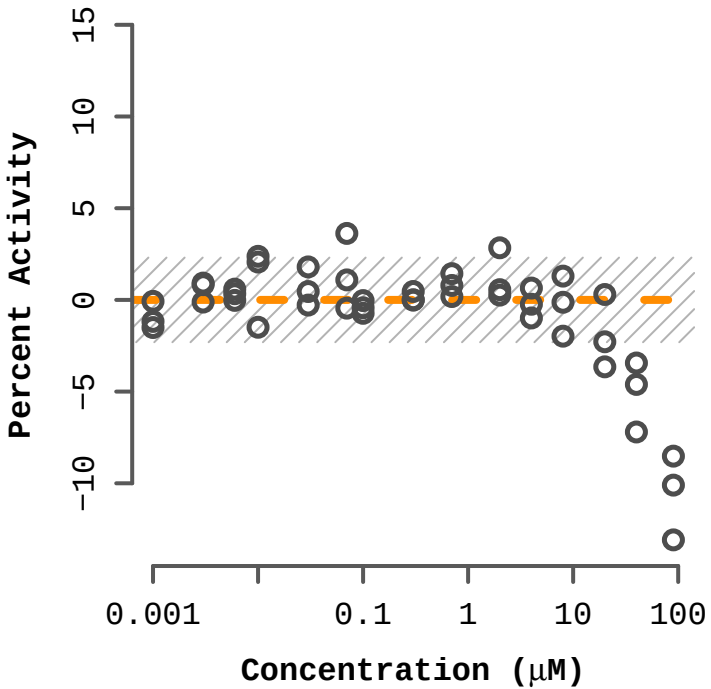
NAME: Quinalphos
CHID: 24291 **CASRN:** 13593-03-8
SPID(S): Tox21_202028
M4ID: 12480224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.689 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

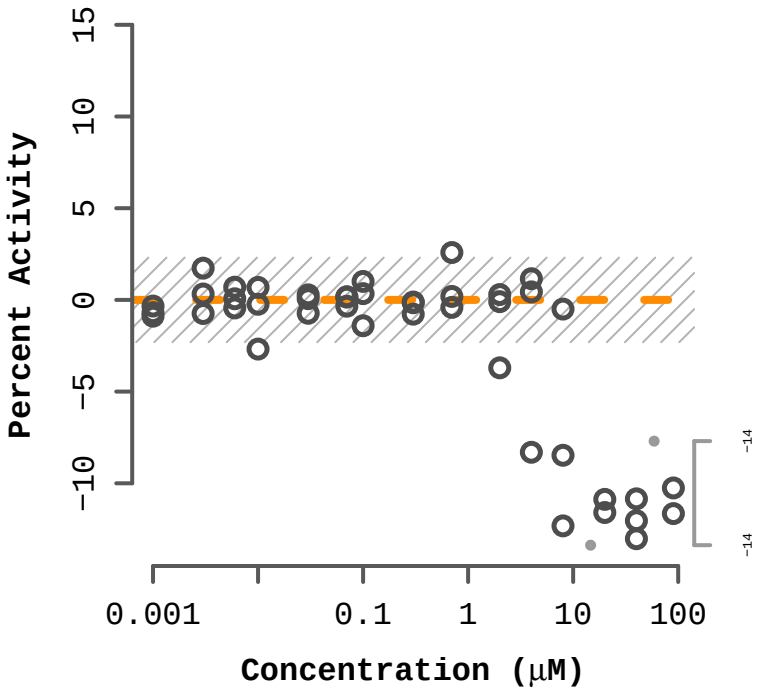
NAME: Hexythiazox
CHID: 24299 **CASRN:** 78587-05-0
SPID(S): Tox21_301050
M4ID: 12478083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.66	NA	NA
PROB:	1	NA	NA
RMSE:	3.35	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

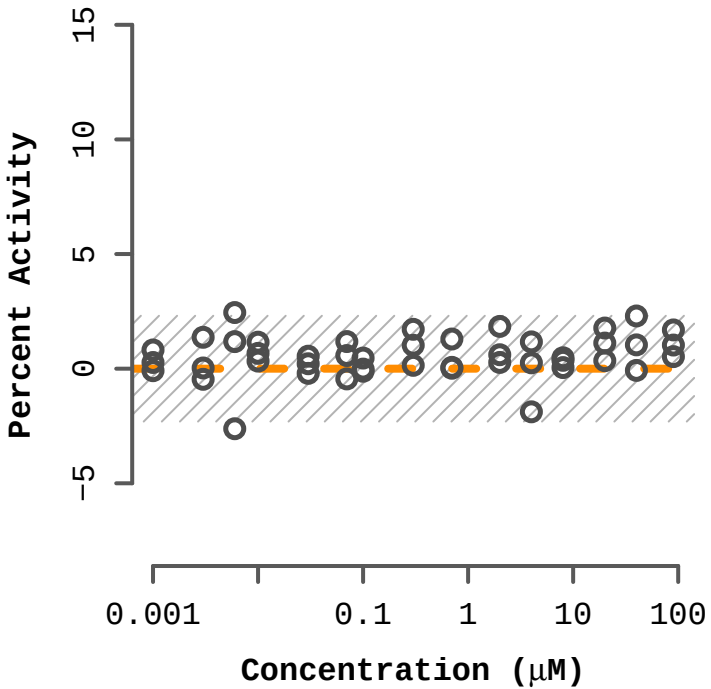
NAME: Selenious acid
CHID: 24300 **CASRN:** 7783-00-8
SPID(S): Tox21_200407
M4ID: 12481845 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	284.47	NA	NA
PROB:	1	NA	NA
RMSE:	6.06	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

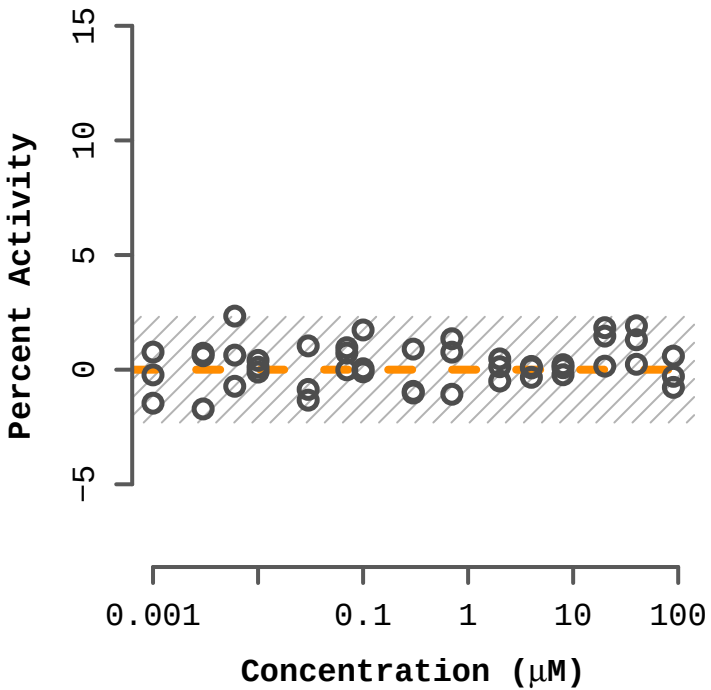
NAME: Selenourea
CHID: 24303 **CASRN:** 630-10-4
SPID(S): Tox21_200857
M4ID: 12481395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

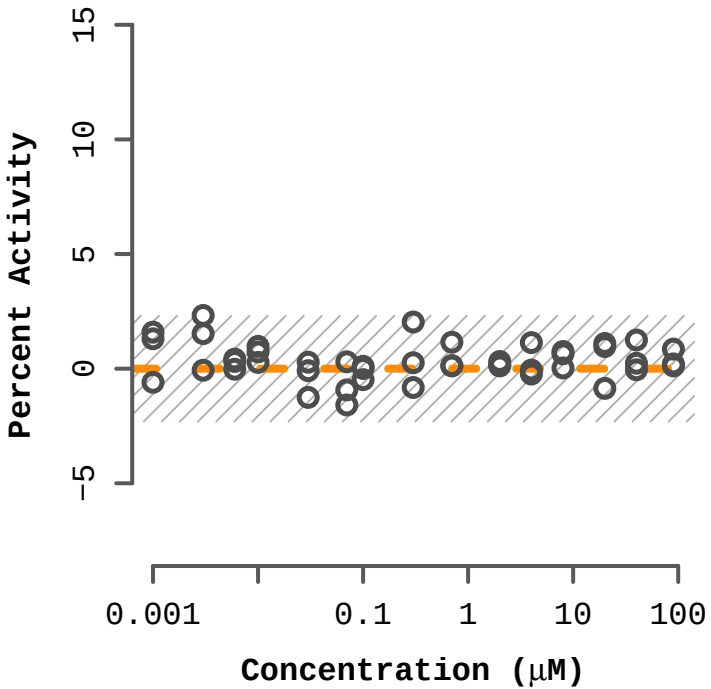
NAME: Sethoxydim
CHID: 24304 **CASRN:** 74051-80-2
SPID(S): Tox21_301052
M4ID: 12478081

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

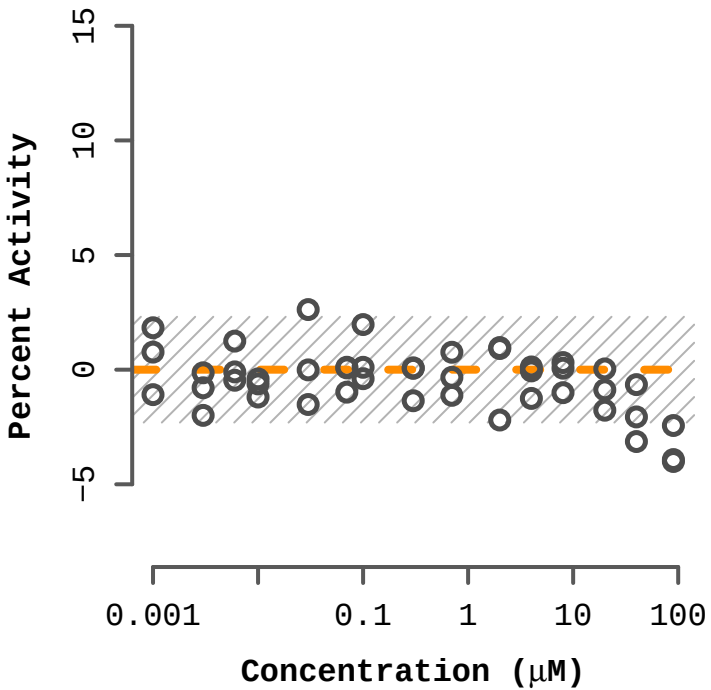
NAME: Sodium fluoroacetate
CHID: 24311 CASRN: 62-74-8
SPID(S): Tox21_301420
M4ID: 12477713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.26 MAX_MED: 1.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

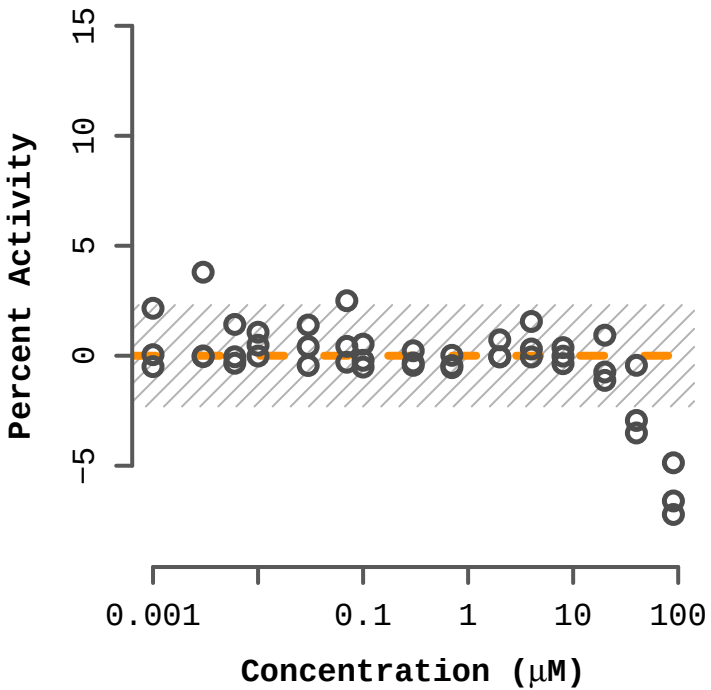
NAME: Myclobutanil
CHID: 24315 **CASRN:** 88671-89-0
SPID(S): Tox21_301135
M4ID: 12477998

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.561 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

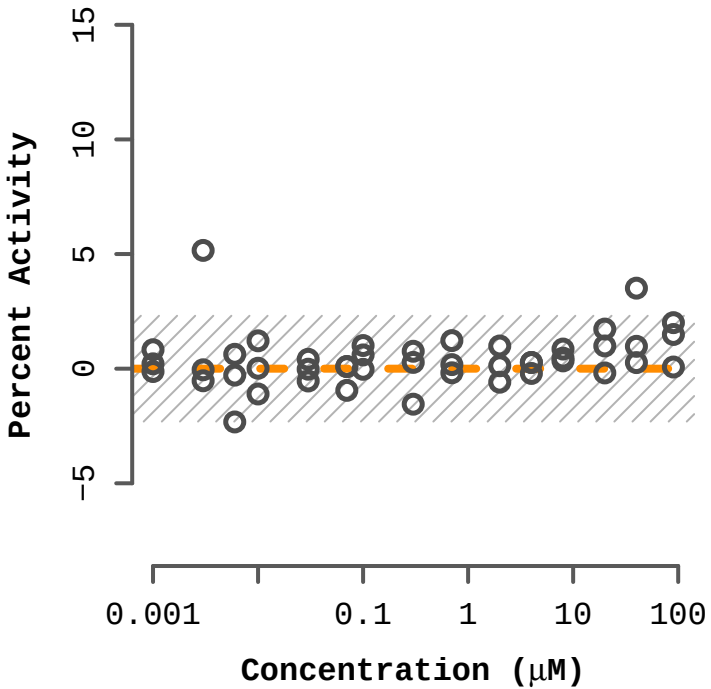
NAME: Myclobutanil
CHID: 24315 **CASRN:** 88671-89-0
SPID(S): Tox21_201915
M4ID: 12480337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.69	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.481 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

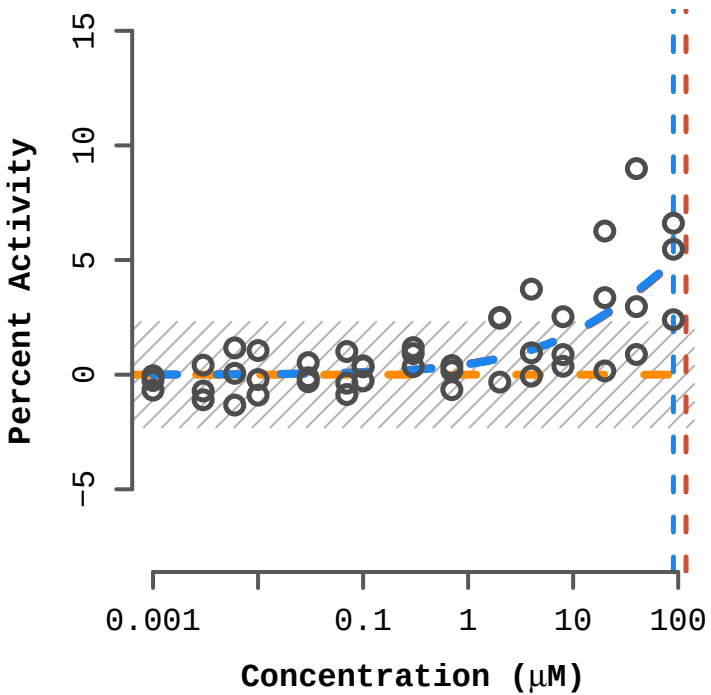
NAME: Tebuthiuron
CHID: 24316 **CASRN:** 34014-18-1
SPID(S): Tox21_300802
M4ID: 12478331

HILL MODEL: Not applicable.

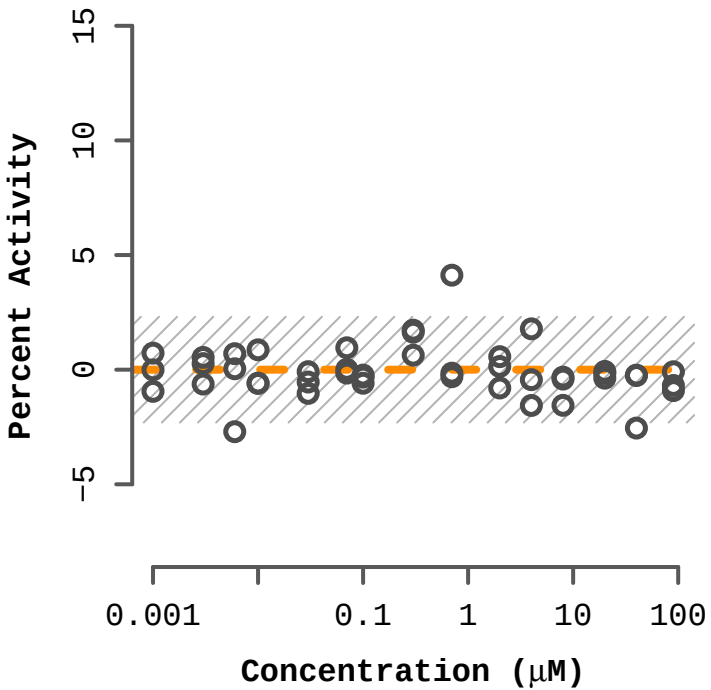
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.49 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tebuthiuron
CHID:    24316   CASRN: 34014-18-1
SPID(S): Tox21_201451
M4ID:    12480801

HILL MODEL (in red):
      tp       ga       gw
val:  10.8     2.07     0.645
sd:   9.88     1.09     0.236

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.89     1.95     0.672    2.96     17.8
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  193.25      163.69      167.78
PROB: 0           0.89        0.11
RMSE: 2.44        1.47        1.47

MAX_MEAN: 4.83      MAX_MED: 5.47      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

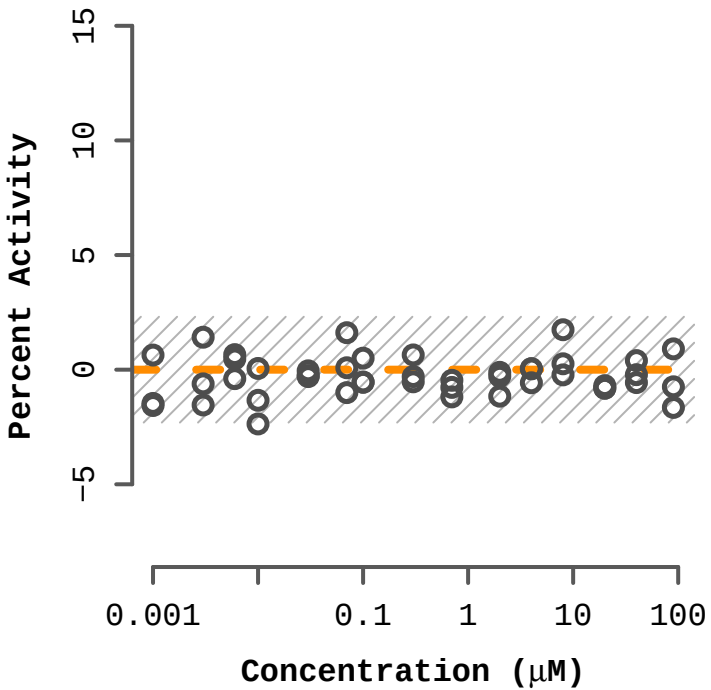
NAME: Terbacil
CHID: 24317 CASRN: 5902-51-2
SPID(S): Tox21_300831
M4ID: 12478302

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.33 MAX_MED: 1.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

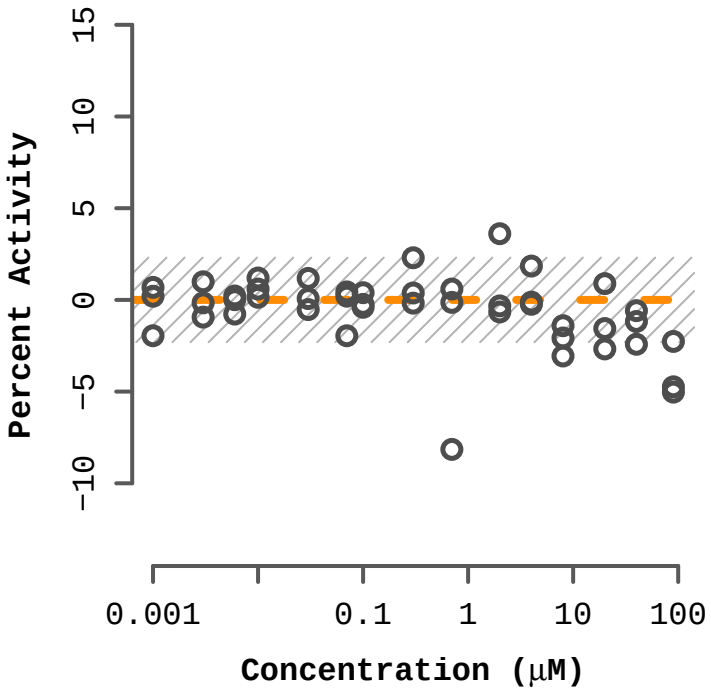
NAME: Terbacil
CHID: 24317 CASRN: 5902-51-2
SPID(S): Tox21_201244
M4ID: 12481008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.592 MAX_MED: 0.469 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

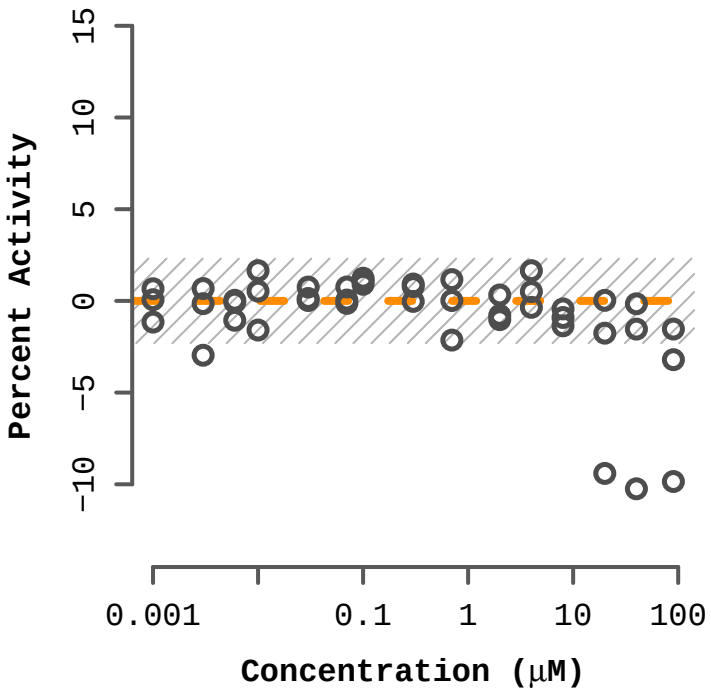
NAME: Terbutryn
CHID: 24318 **CASRN:** 886-50-0
SPID(S): Tox21_303141
M4ID: 12475992

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 0.877 **MAX_MED:** 0.592 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

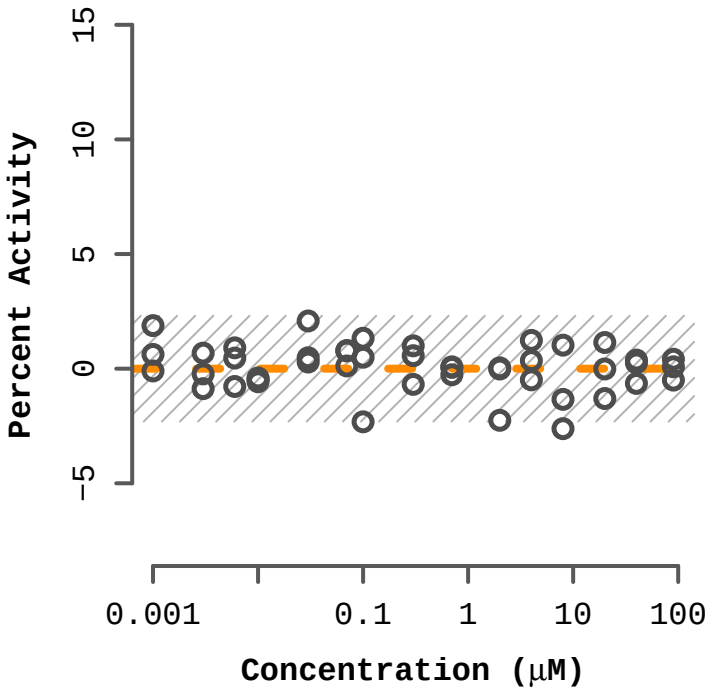
NAME: Terbutryn
CHID: 24318 **CASRN:** 886-50-0
SPID(S): Tox21_202082
M4ID: 12480170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.7	NA	NA
PROB:	1	NA	NA
RMSE:	2.77	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

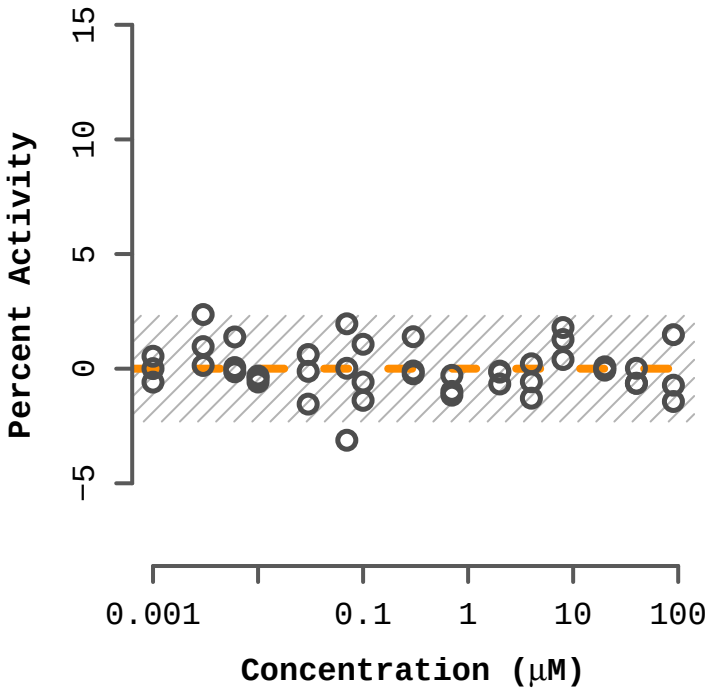
NAME: 1,2,4,5-Tetrachlorobenzene
CHID: 24320 **CASRN:** 95-94-3
SPID(S): Tox21_300505
M4ID: 12478627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 0.775 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

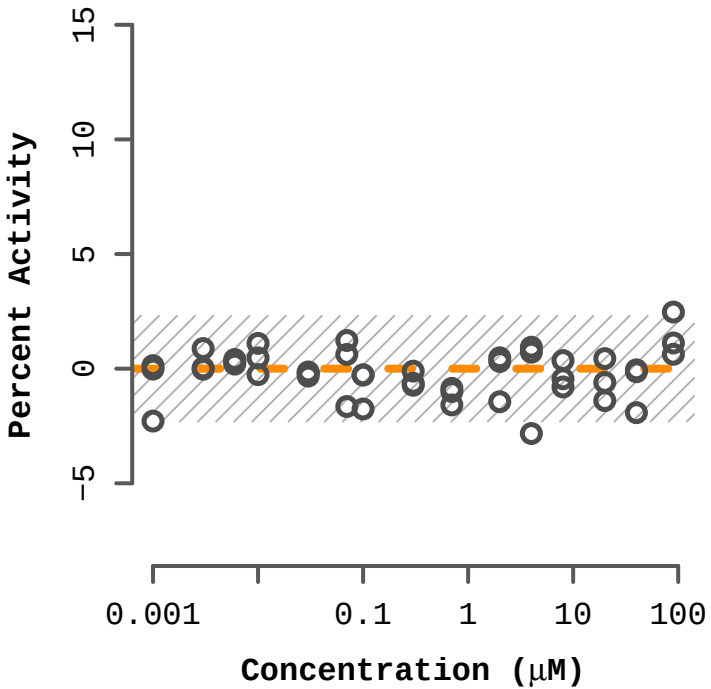
NAME: 1,2,4,5−Tetrachlorobenzene
CHID: 24320 CASRN: 95−94−3
SPID(S): Tox21_201707
M4ID: 12480545

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

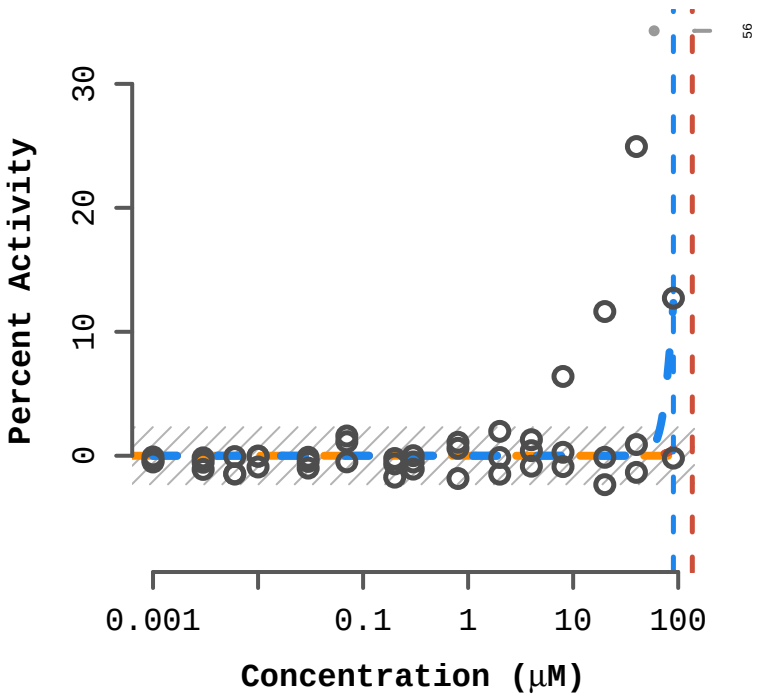
NAME: Sulfotepp
CHID: 24328 CASRN: 3689-24-5
SPID(S): Tox21_303135
M4ID: 12475998

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.41 MAX_MED: 1.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfotepp
CHID: 24328 CASRN: 3689-24-5
SPID(S): Tox21_201756
M4ID: 12480496 BRK

HILL MODEL (in red):

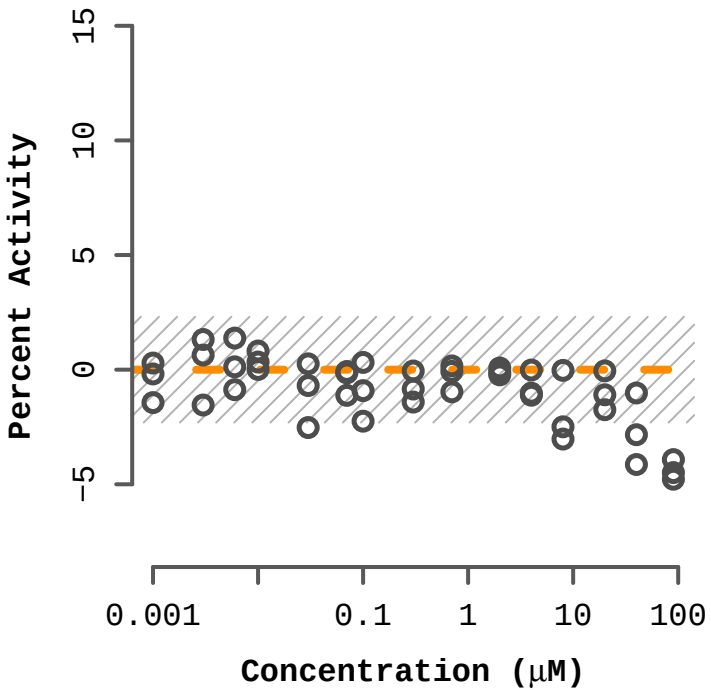
	tp	ga	gw
val:	7.93	2.13	6.25
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.7	1.95	7.89	3.92	5.58
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	233.47	239.29	240.92
PROB:	0.93	0.05	0.02
RMSE:	9.59	9.5	8.03

MAX_MEAN: 22.9 MAX_MED: 12.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

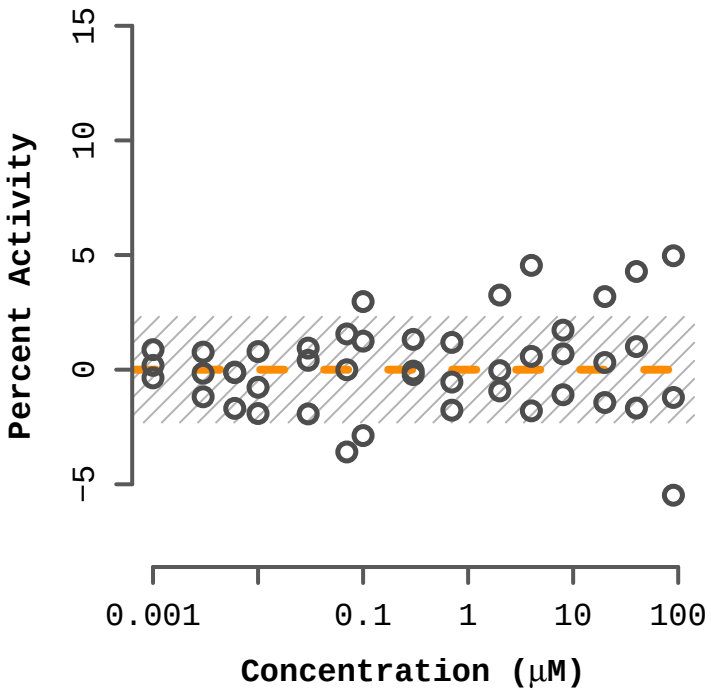
NAME: Thallium acetate
CHID: 24331 CASRN: 563-68-8
SPID(S): Tox21_201001
M4ID: 12481251

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 0.387 **MAX_MED:** 0.639 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

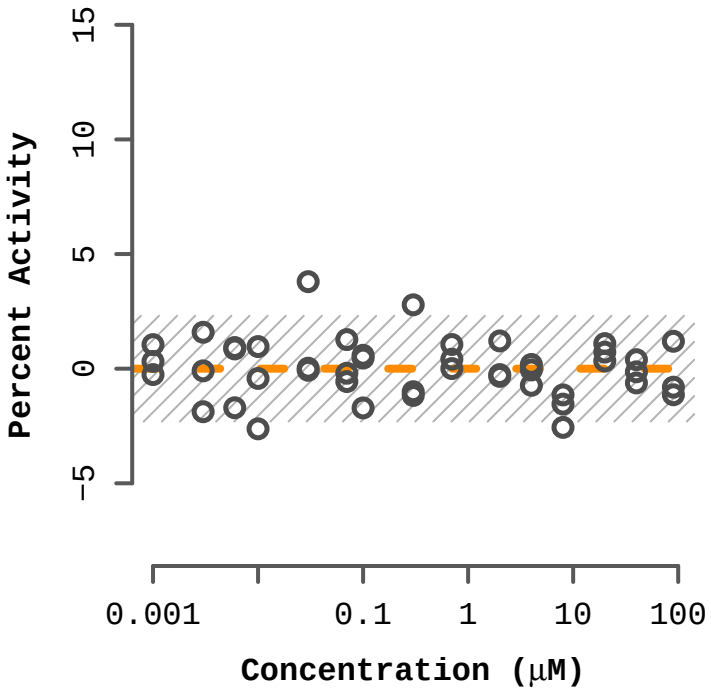
NAME: Thallium nitrate
CHID: 24334 **CASRN:** 10102-45-1
SPID(S): Tox21_200256
M4ID: 12481996

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.05	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

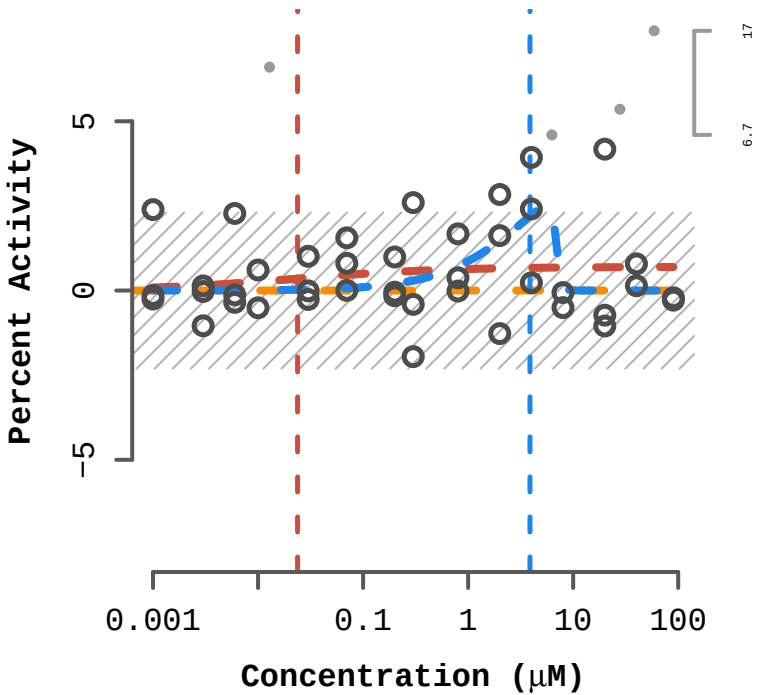
NAME: Thiobencarb
CHID: 24337 **CASRN:** 28249-77-6
SPID(S): Tox21_301155
M4ID: 12477978

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.862 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiobencarb
CHID: 24337 CASRN: 28249-77-6
SPID(S): Tox21_202360
M4ID: 12479892 BRK

HILL MODEL (in red):

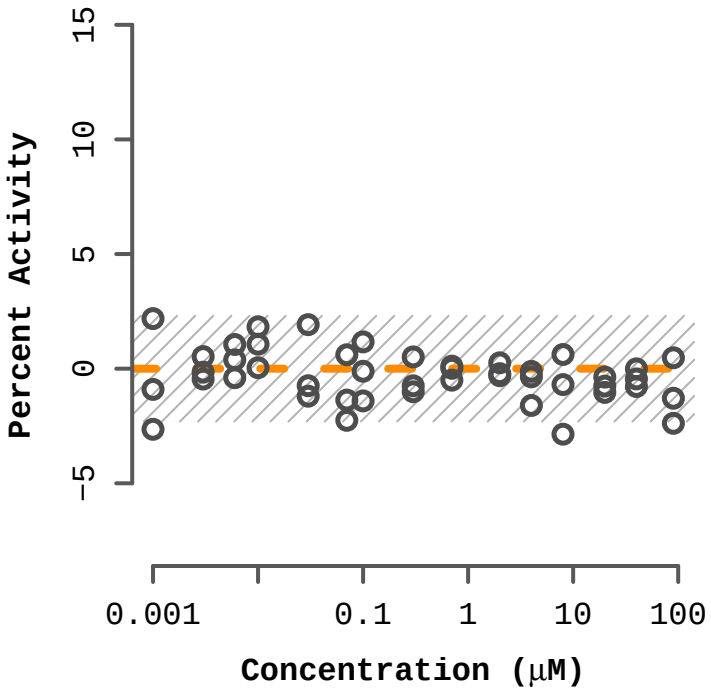
	tp	ga	gw
val:	0.699	−1.62	0.613
sd:	0.508	2.14	1.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.38	0.589	1.03	0.839	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	214.39	216.26	217.48
PROB:	0.62	0.24	0.13
RMSE:	3.91	3.72	3.84

MAX_MEAN: 5.51 MAX_MED: 2.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

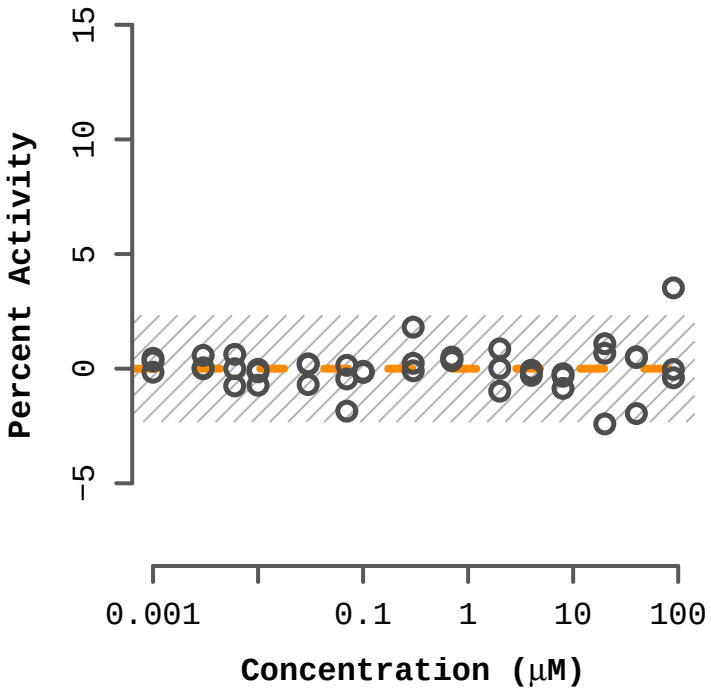
NAME: Thiophanate-methyl
CHID: 24338 **CASRN:** 23564-05-8
SPID(S): Tox21_300830
M4ID: 12478303

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.98 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

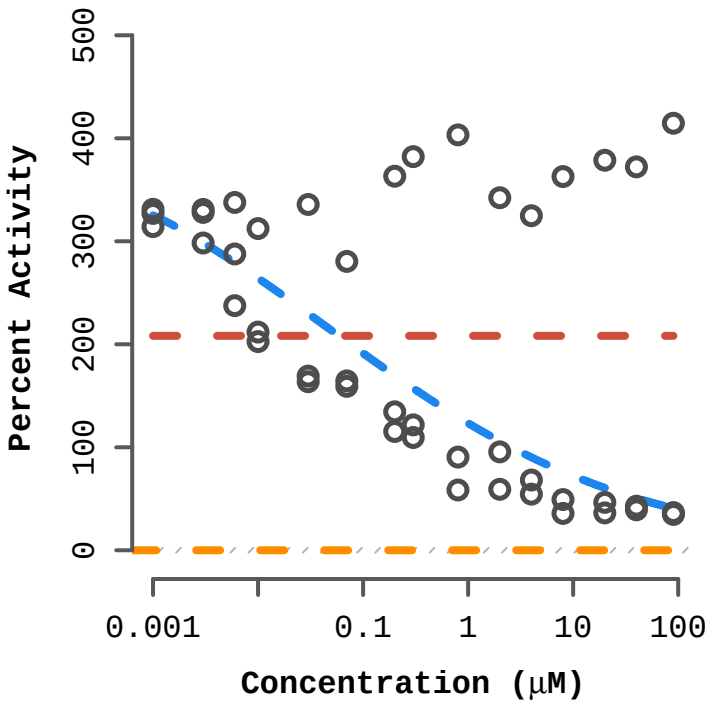
NAME: Thiophanate-methyl
CHID: 24338 **CASRN:** 23564-05-8
SPID(S): Tox21_201679
M4ID: 12480573

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.673 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Toluene diisocyanate
CHID: 24341 CASRN: 26471-62-5
SPID(S): Tox21_200144
M4ID: 12482108

HILL MODEL (in red):

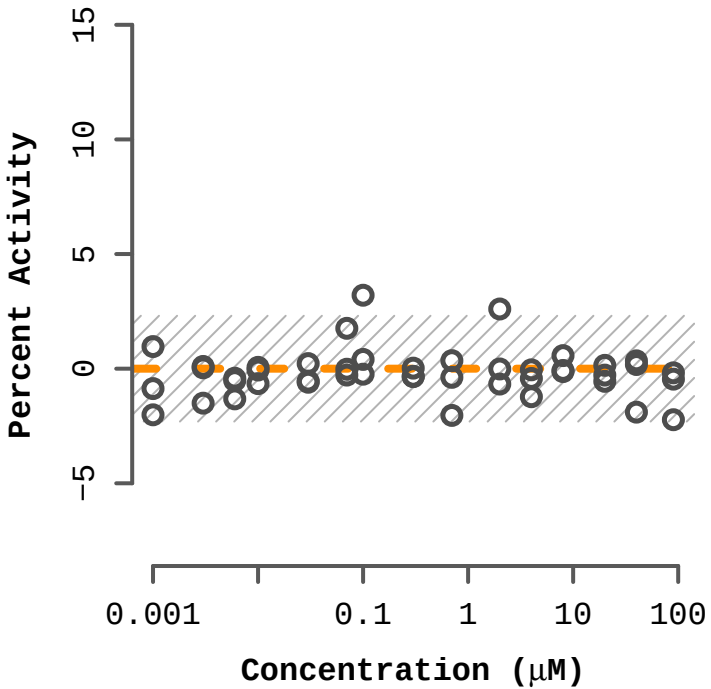
	tp	ga	gw
val:	208	-4.52	7.08
sd:	23.3	25000	117000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	428	-3.78	3.07	-1.31	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	631.41	582.55	567.58
PROB:	0	0	1
RMSE:	245.39	129.99	130.57

MAX_MEAN: 324 MAX_MED: 328 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

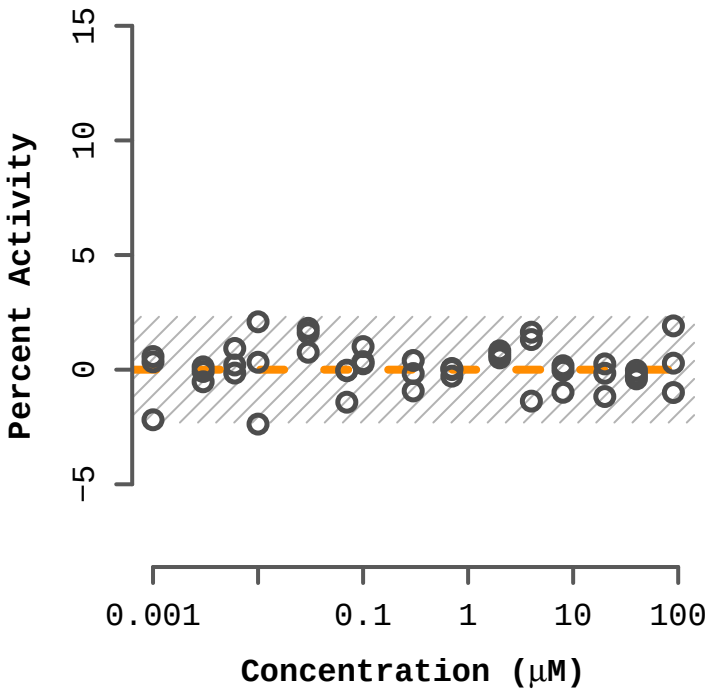
NAME: Tri-allate
CHID: 24344 **CASRN:** 2303-17-5
SPID(S): Tox21_300671
M4ID: 12478462

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.404 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

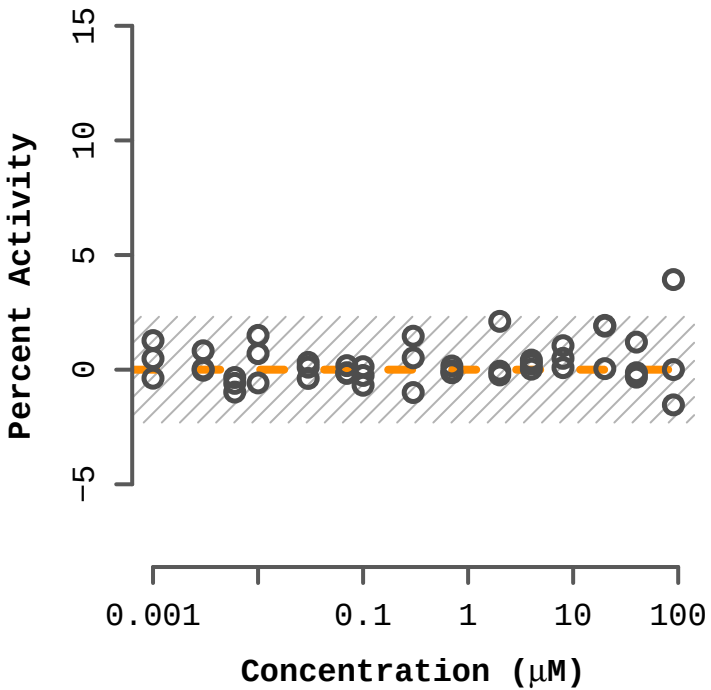
NAME: Tri-allate
CHID: 24344 **CASRN:** 2303-17-5
SPID(S): Tox21_201817
M4ID: 12480435

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

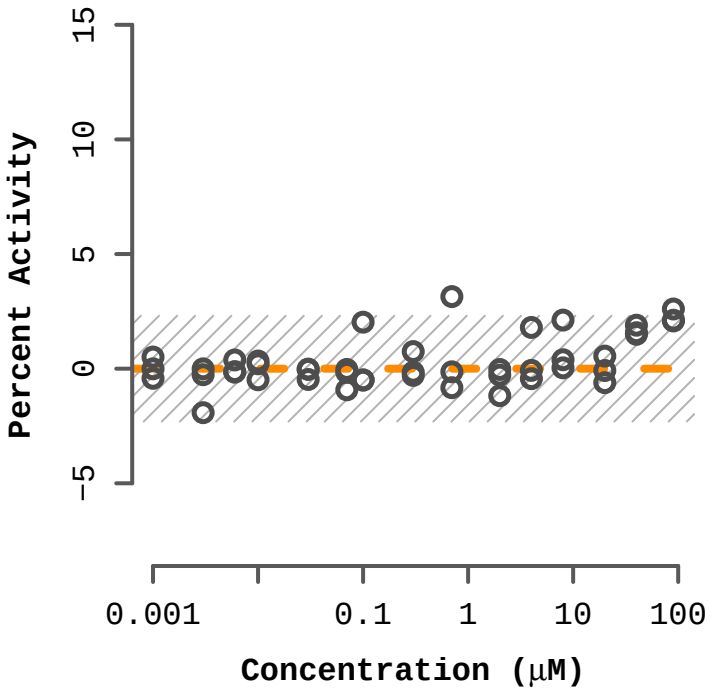
NAME: Triasulfuron
CHID: 24345 CASRN: 82097-50-5
SPID(S): Tox21_201200
M4ID: 12481052

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

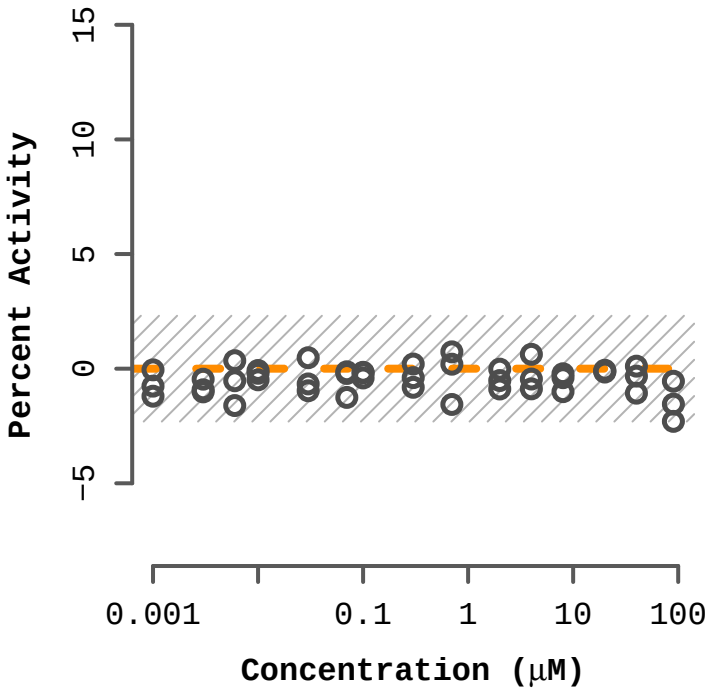
NAME: 1,2,4−Tribromobenzene
CHID: 24346 **CASRN:** 615−54−3
SPID(S): Tox21_303231
M4ID: 12475902

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 2.27 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

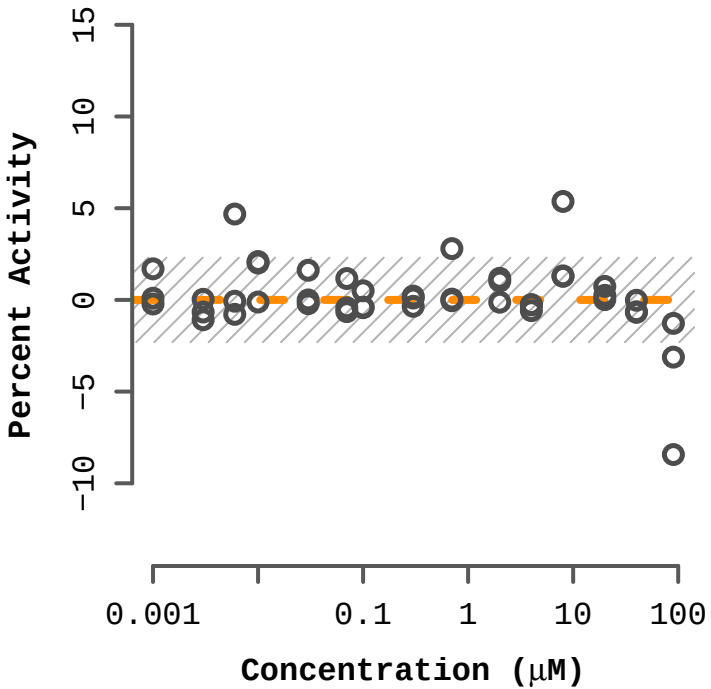
NAME: 1,2,4−Tribromobenzene
CHID: 24346 **CASRN:** 615−54−3
SPID(S): Tox21_201862
M4ID: 12480390

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: −0.108 **MAX_MED:** 0.197 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

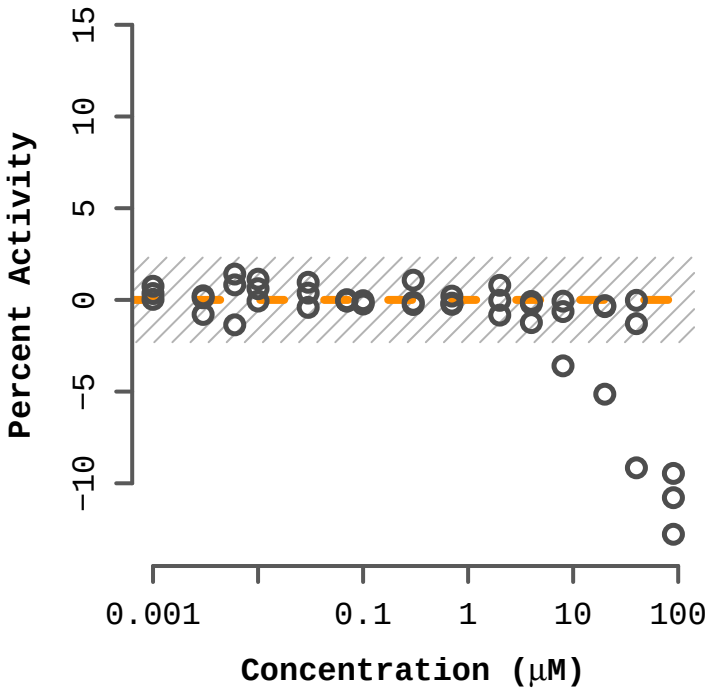
NAME: 2,4,5-Trichlorophenol
CHID: 24359 **CASRN:** 95-95-4
SPID(S): Tox21_300186
M4ID: 12478944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 2.66 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

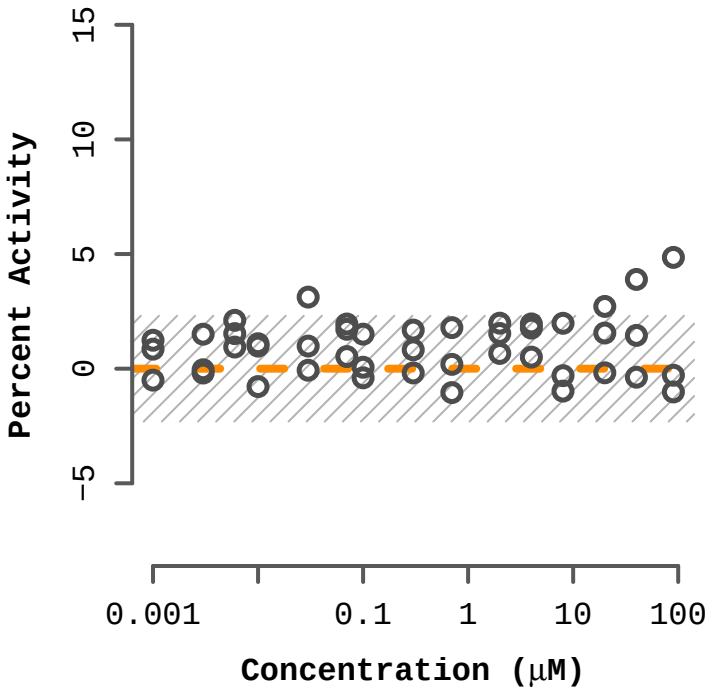
NAME: 2,4,5-Trichlorophenol
CHID: 24359 **CASRN:** 95-95-4
SPID(S): Tox21_201545
M4ID: 12480707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.2	NA	NA
PROB:	1	NA	NA
RMSE:	3.36	NA	NA

MAX_MEAN: 0.561 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

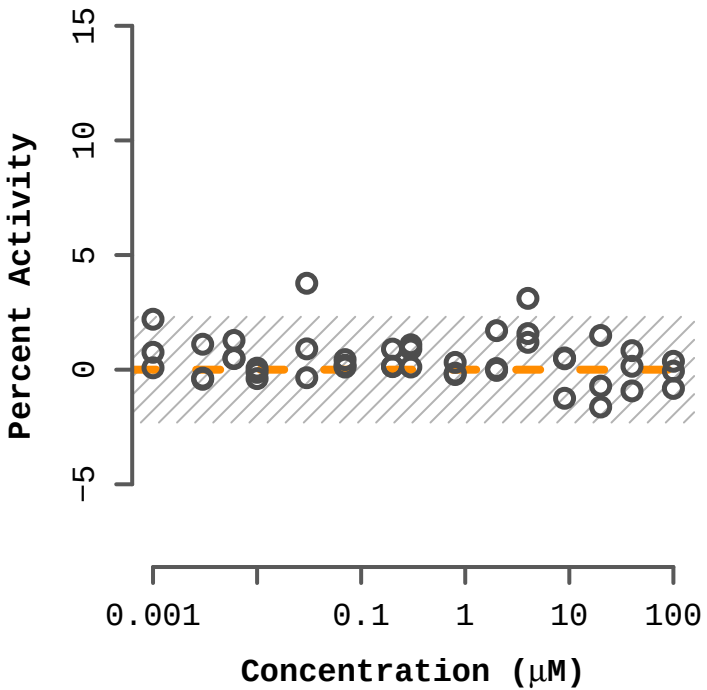
NAME: 1,1,2−Trichloropropane
CHID: 24362 **CASRN:** 598−77−6
SPID(S): Tox21_200408
M4ID: 12481844

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

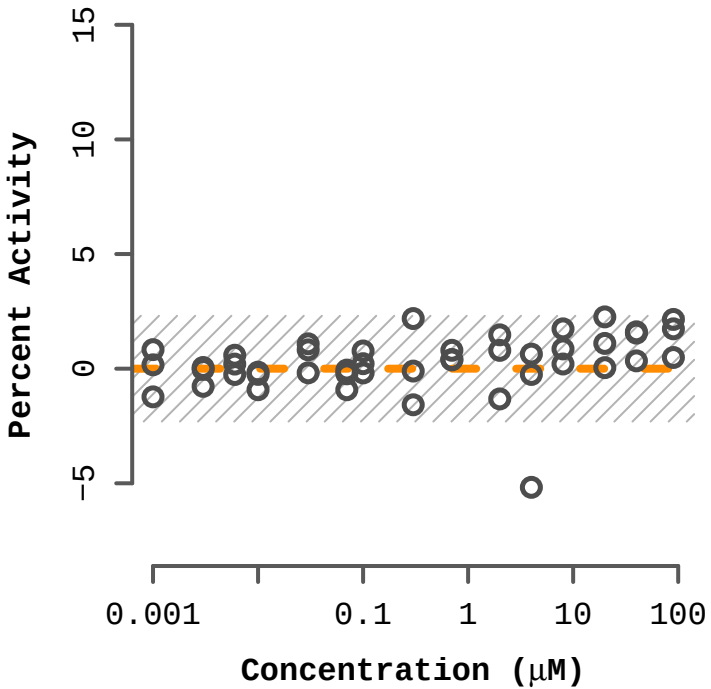
NAME: Triethylamine
CHID: 24366 **CASRN:** 121-44-8
SPID(S): Tox21_200873
M4ID: 12481379

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

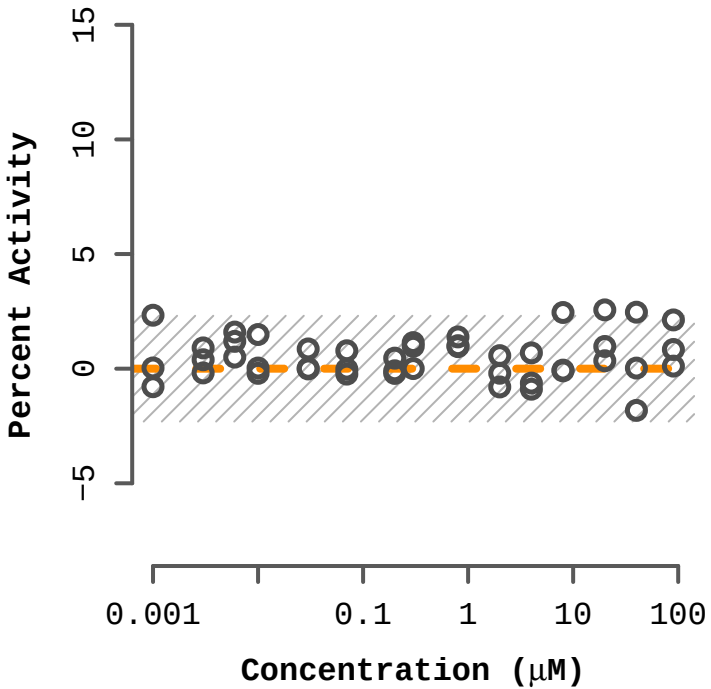
NAME: 2-[2-(2-Ethoxyethoxy)ethoxy]ethanol
CHID: 24368 **CASRN:** 112-50-5
SPID(S): Tox21_300369
M4ID: 12478763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

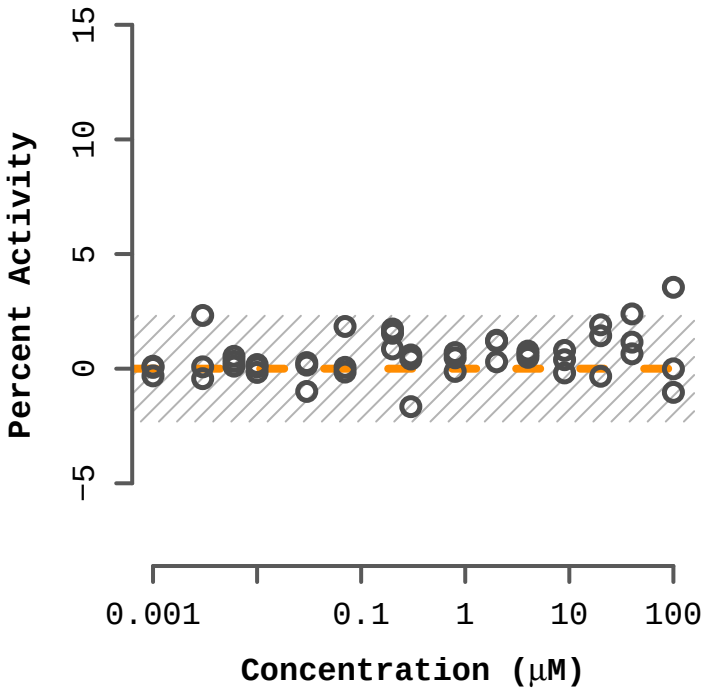
NAME: 2-[2-(2-Ethoxyethoxy)ethoxy]ethanol
CHID: 24368 **CASRN:** 112-50-5
SPID(S): Tox21_201320
M4ID: 12480932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

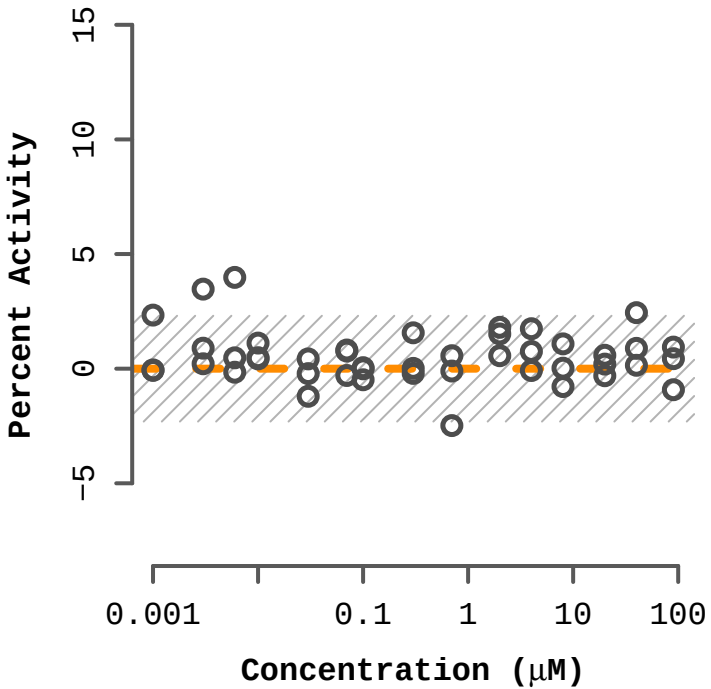
NAME: 2,2,4−Trimethylpentane
CHID: 24370 **CASRN:** 540−84−1
SPID(S): Tox21_201127
M4ID: 12481125

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

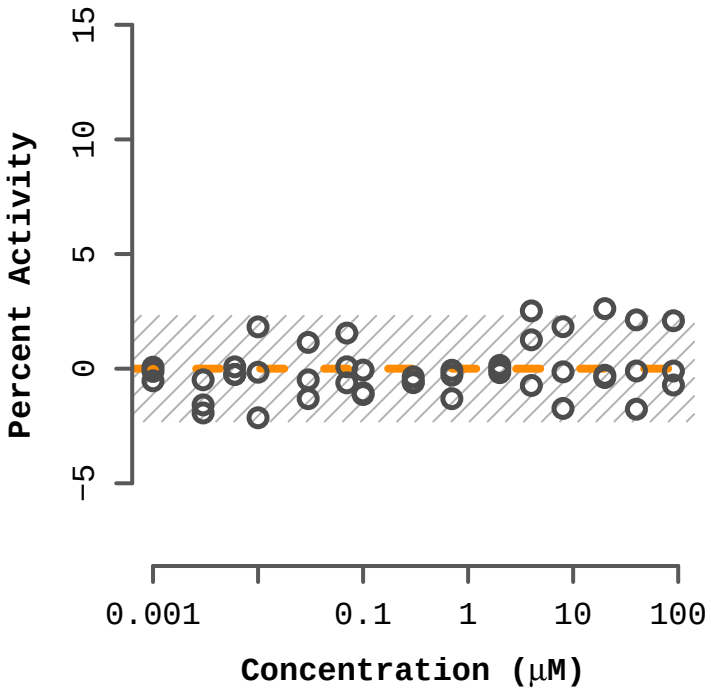
NAME: Vernolate
CHID: 24376 CASRN: 1929-77-7
SPID(S): Tox21_300173
M4ID: 12478957

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.53 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

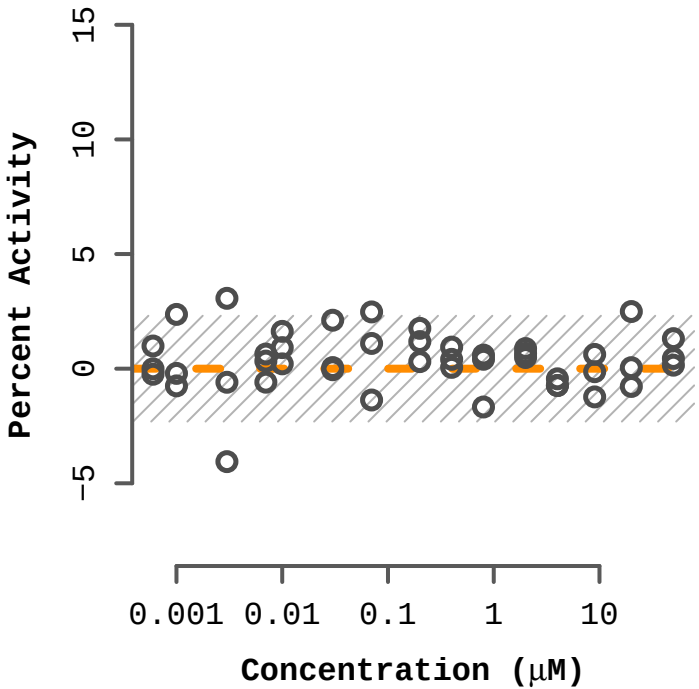
NAME: 4-Acetamidobenzoic acid
CHID: 24392 **CASRN:** 556-08-1
SPID(S): Tox21_200330
M4ID: 12481922

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

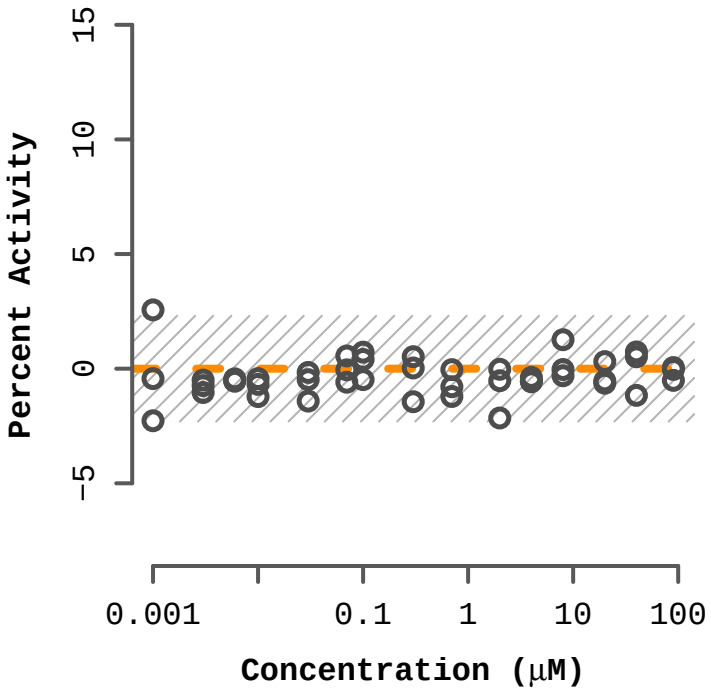
NAME: 4-Acetamidobenzoic acid
CHID: 24392 **CASRN:** 556-08-1
SPID(S): Tox21_111029_1
M4ID: 12483941

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

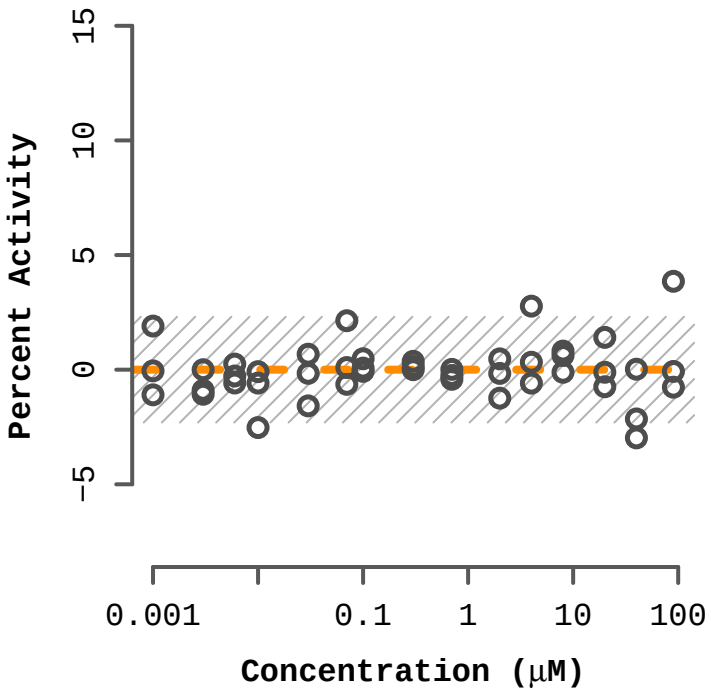
NAME: Acetic acid
CHID: 24394 **CASRN:** 64-19-7
SPID(S): Tox21_301453
M4ID: 12477680

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.308 **MAX_MED:** 0.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

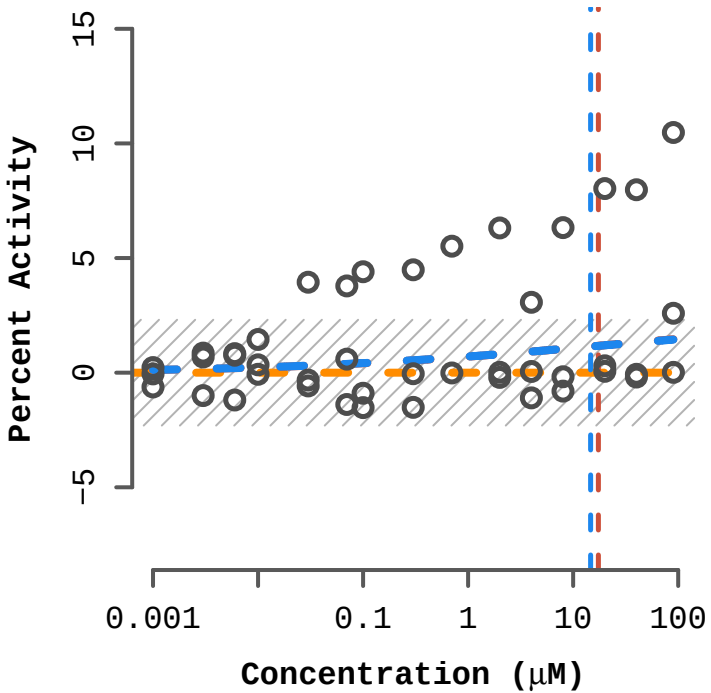
NAME: Acetic anhydride
CHID: 24395 CASRN: 108-24-7
SPID(S): Tox21_200278
M4ID: 12481974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acetoacetanilide
CHID: 24397 CASRN: 102-01-2
SPID(S): Tox21_303279
M4ID: 12475854

HILL MODEL (in red):

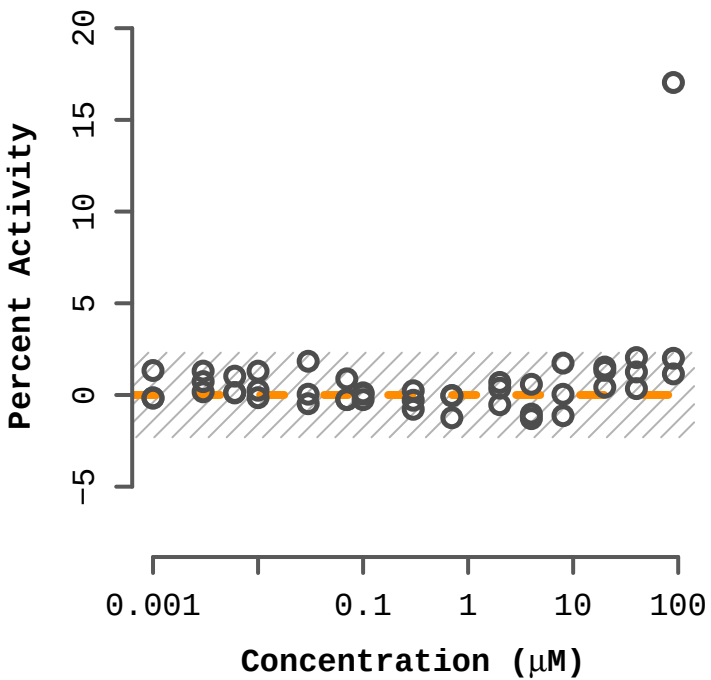
	tp	ga	gw
val:	2.35	1.24	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.28	1.17	0.3	3.8	3.49
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	217.42	219.04	223.04
PROB:	0.66	0.3	0.04
RMSE:	3.2	2.85	2.85

MAX_MEAN: 4.36 MAX_MED: 2.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

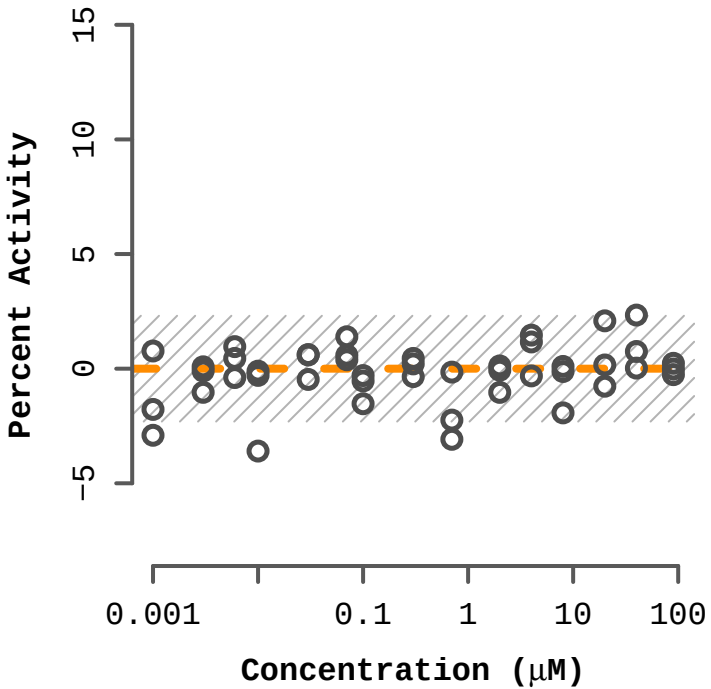
NAME: Acetoacetanilide
CHID: 24397 CASRN: 102-01-2
SPID(S): Tox21_201405
M4ID: 12480847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.7	NA	NA

MAX_MEAN: 6.73 MAX_MED: 2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

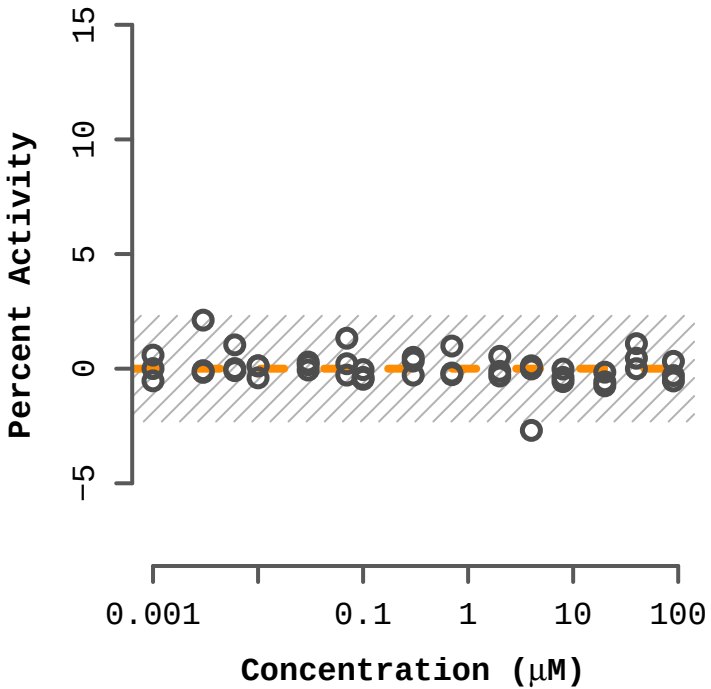
NAME: Acetoin
CHID: 24399 **CASRN:** 513-86-0
SPID(S): Tox21_302518
M4ID: 12476615

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

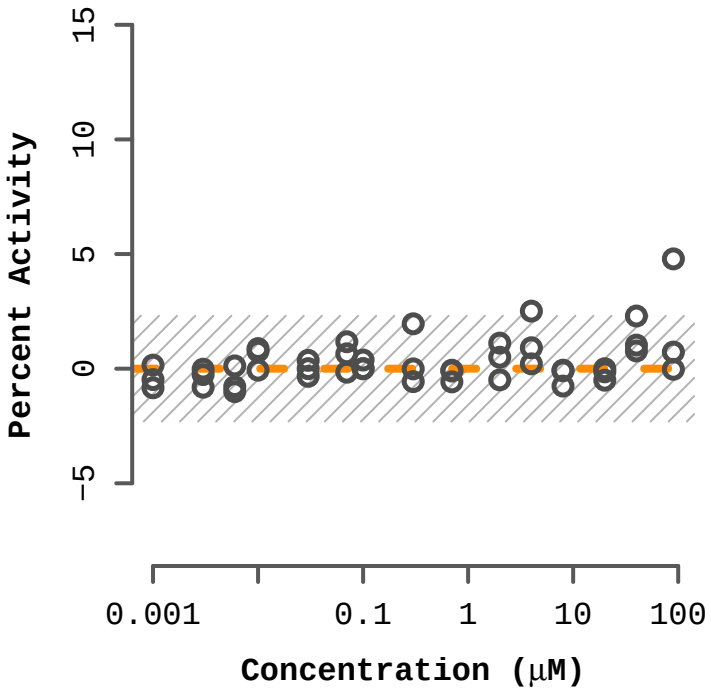
NAME: 2-Acetylpyridine
CHID: 24409 **CASRN:** 1122-62-9
SPID(S): Tox21_303104
M4ID: 12476029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	81.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.625 **MAX_MED:** 0.456 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

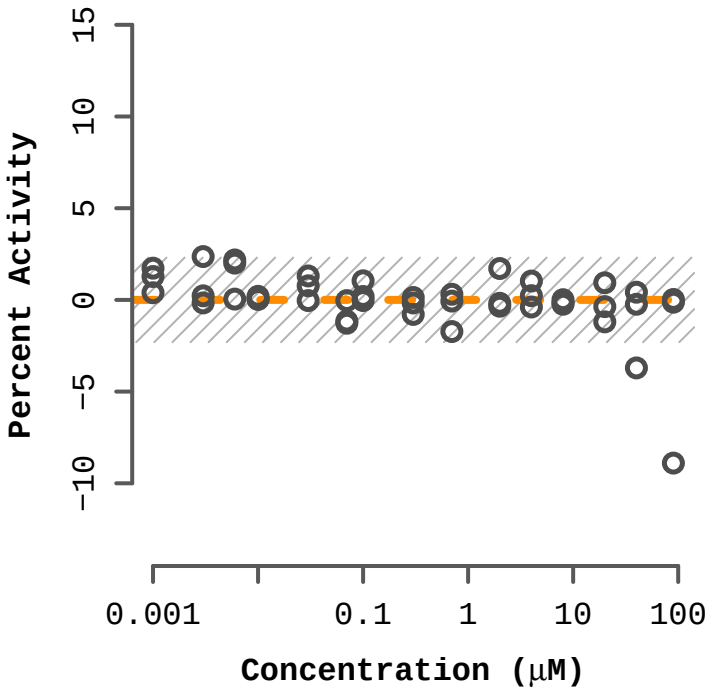
NAME: 2-Acetylpyridine
CHID: 24409 **CASRN:** 1122-62-9
SPID(S): Tox21_201499
M4ID: 12480753

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

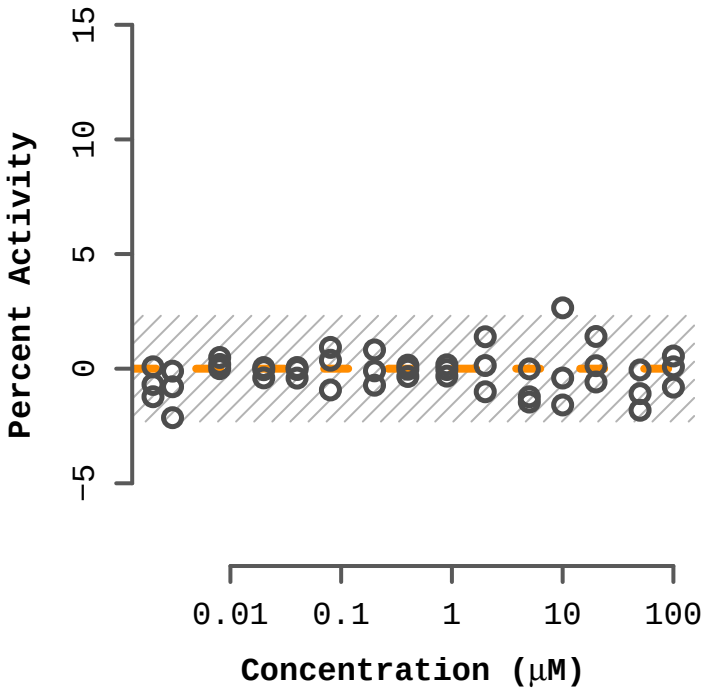
NAME: N-Acetyl-m-toluidine
CHID: 24412 **CASRN:** 537-92-8
SPID(S): Tox21_200887
M4ID: 12481365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

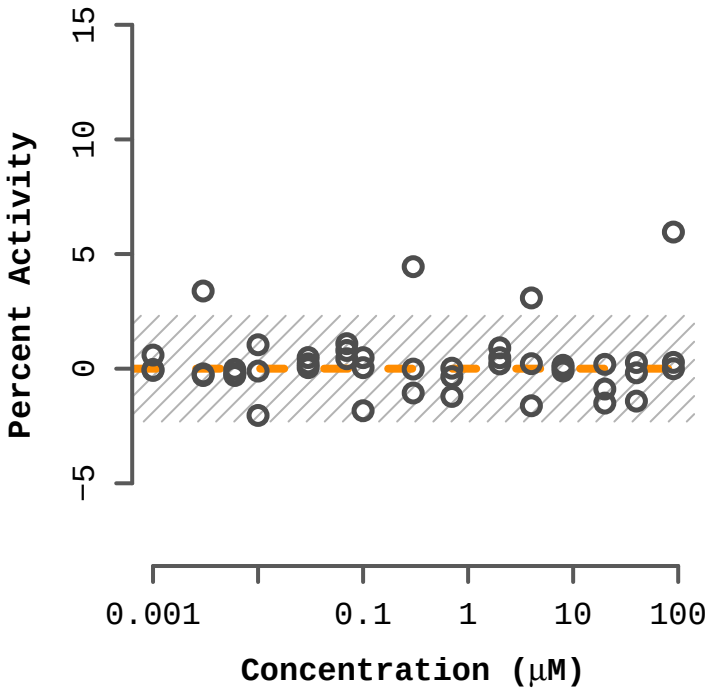
NAME: N-Acetyl-o-toluidine
CHID: 24413 **CASRN:** 120-66-1
SPID(S): Tox21_200288
M4ID: 12481964

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.319 **MAX_MED:** 0.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

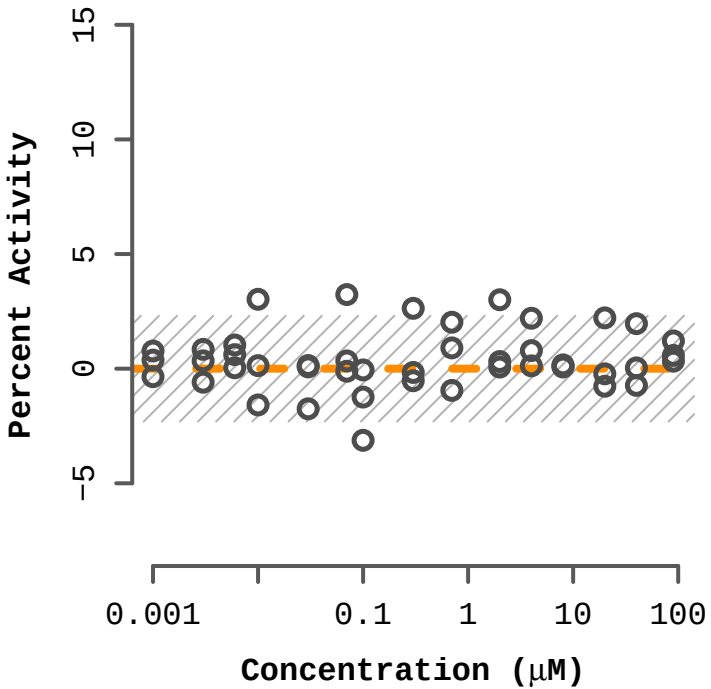
NAME: N-Acetyl-p-toluidine
CHID: 24414 **CASRN:** 103-89-9
SPID(S): Tox21_200119
M4ID: 12482133

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 0.795 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

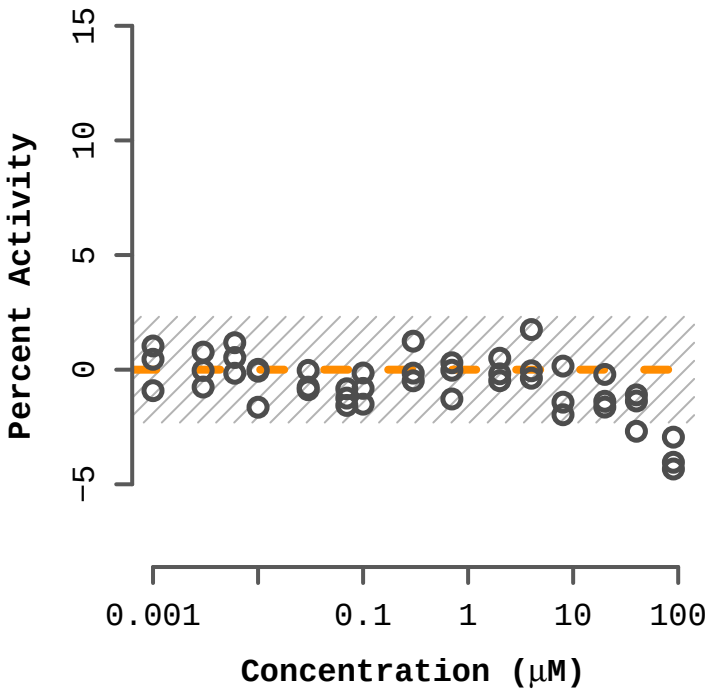
NAME: Aldicarb oxime
CHID: 24431 **CASRN:** 1646-75-9
SPID(S): Tox21_300408
M4ID: 12478724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

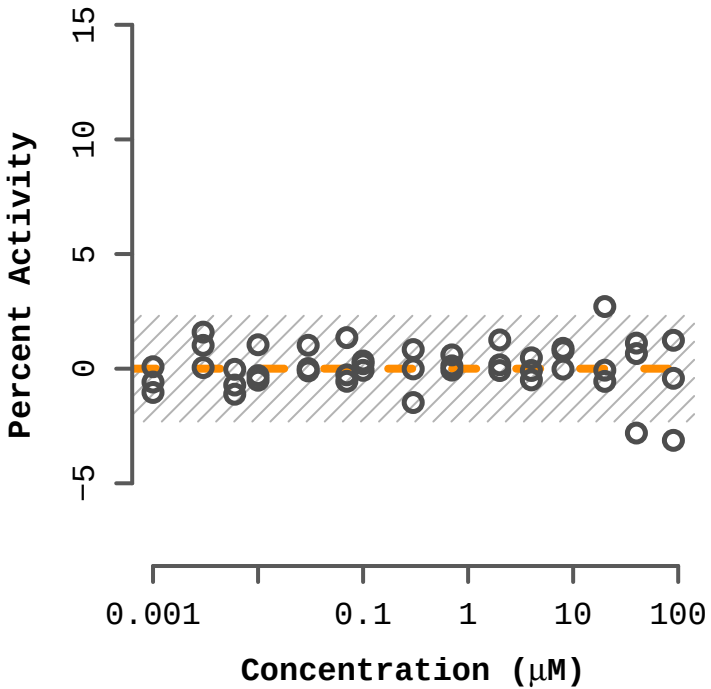
NAME: Allura Red C.I.16035
CHID: 24436 CASRN: 25956-17-6
SPID(S): Tox21_300393
M4ID: 12478739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.518 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

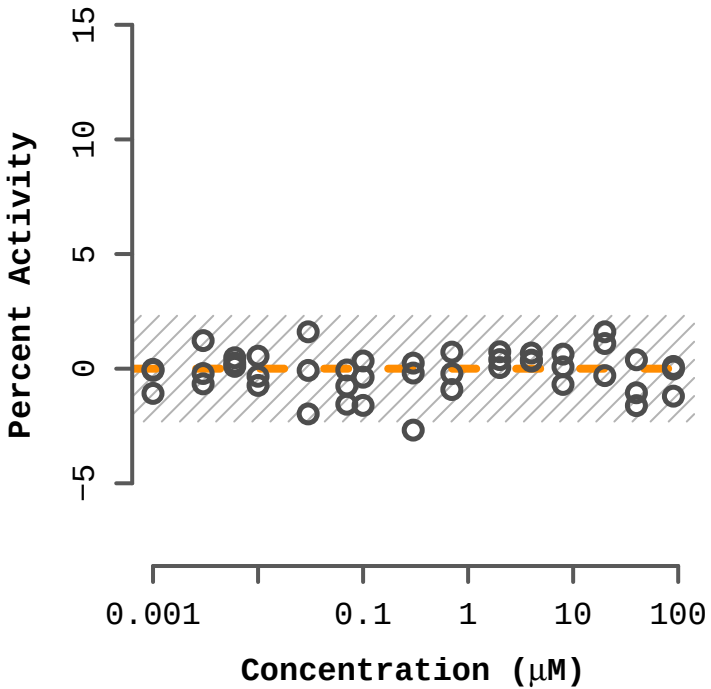
NAME: Allyl acetate
CHID: 24437 **CASRN:** 591-87-7
SPID(S): Tox21_200335
M4ID: 12481917

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.888 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

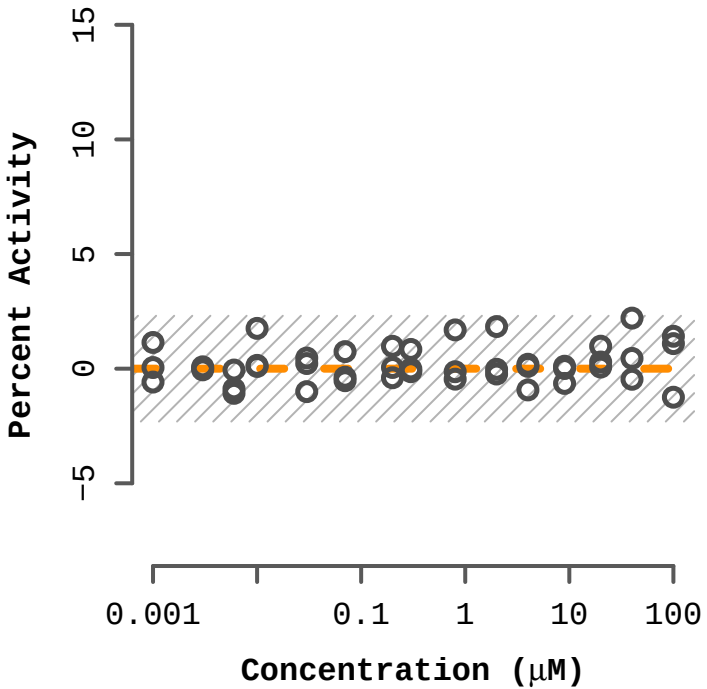
NAME: Allyl anthranilate
CHID: 24441 **CASRN:** 7493-63-2
SPID(S): Tox21_201129
M4ID: 12481123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

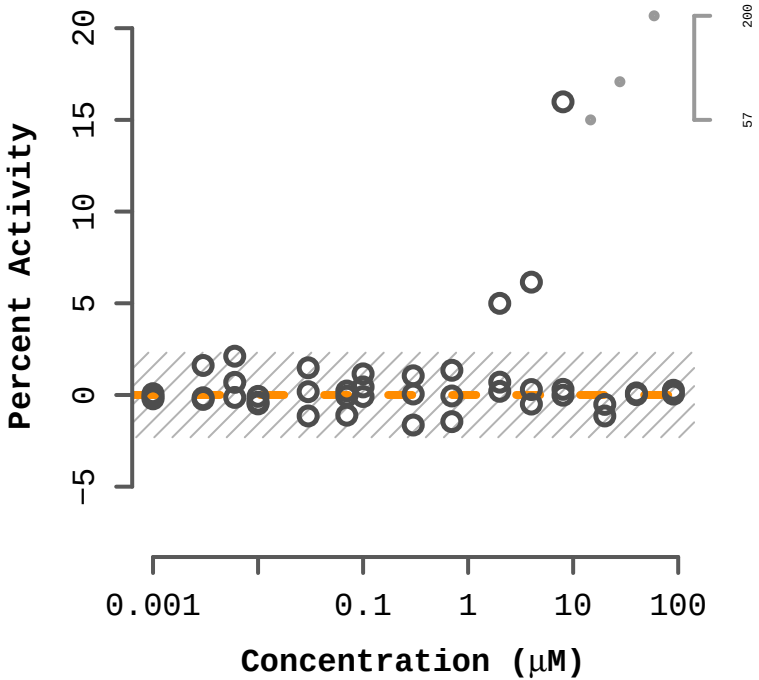
NAME: Allyl bromide
CHID: 24442 **CASRN:** 106-95-6
SPID(S): Tox21_200801
M4ID: 12481451

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.731 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

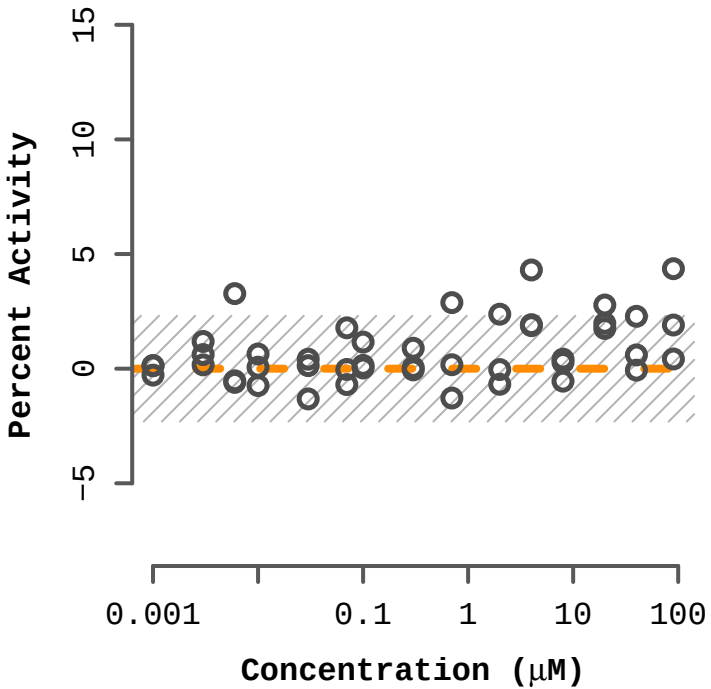
NAME: Allyl nonanoate
CHID: 24447 CASRN: 7493-72-3
SPID(S): Tox21_200173
M4ID: 12482079 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.55	NA	NA
PROB:	1	NA	NA
RMSE:	34.82	NA	NA

MAX_MEAN: 66 **MAX_MED:** 0.701 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

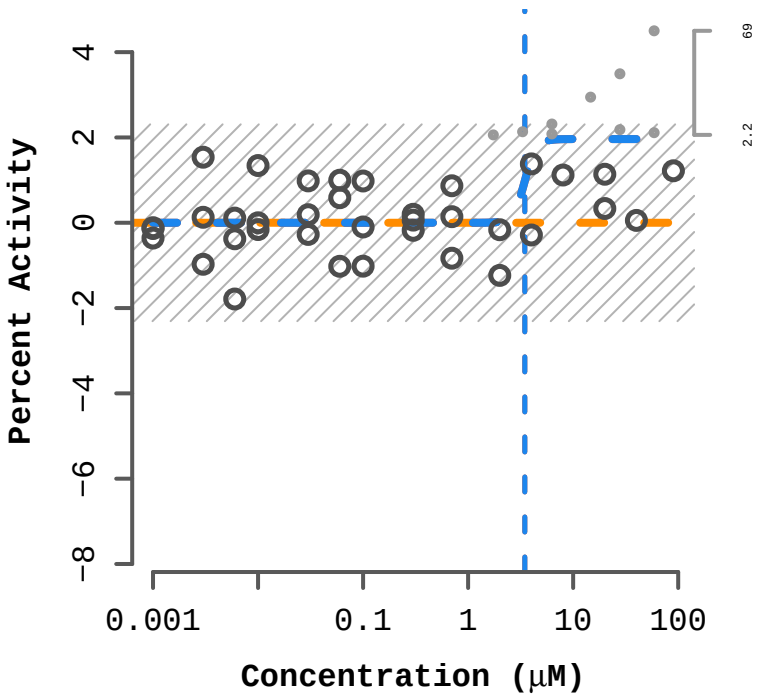
NAME: Allyl propyl disulfide
CHID: 24448 **CASRN:** 2179-59-1
SPID(S): Tox21_202612
M4ID: 12479640

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Allylthiourea
CHID: 24449 CASRN: 109-57-9
SPID(S): Tox21_200898
M4ID: 12481354 BRK

HILL MODEL (in red):

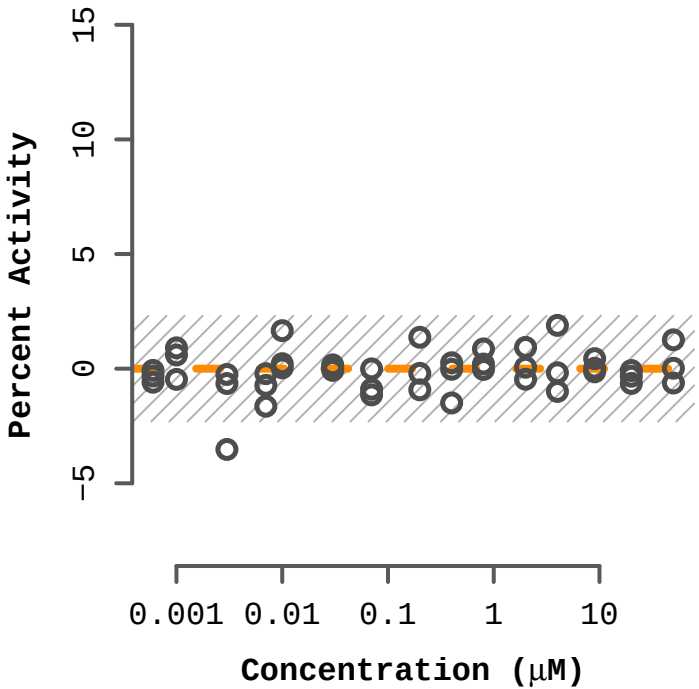
	tp	ga	gw
val:	1.96	0.54	7.99
sd:	0.639	0.516	56.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.96	0.54	8	3.72	4.01
sd:	0.639	0.521	56.6	1170	2650

	CNST	HILL	GNLS
AIC:	252.3	245.1	249.1
PROB:	0.02	0.86	0.12
RMSE:	12.71	12.18	12.18

MAX_MEAN: 24.5 MAX_MED: 5.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

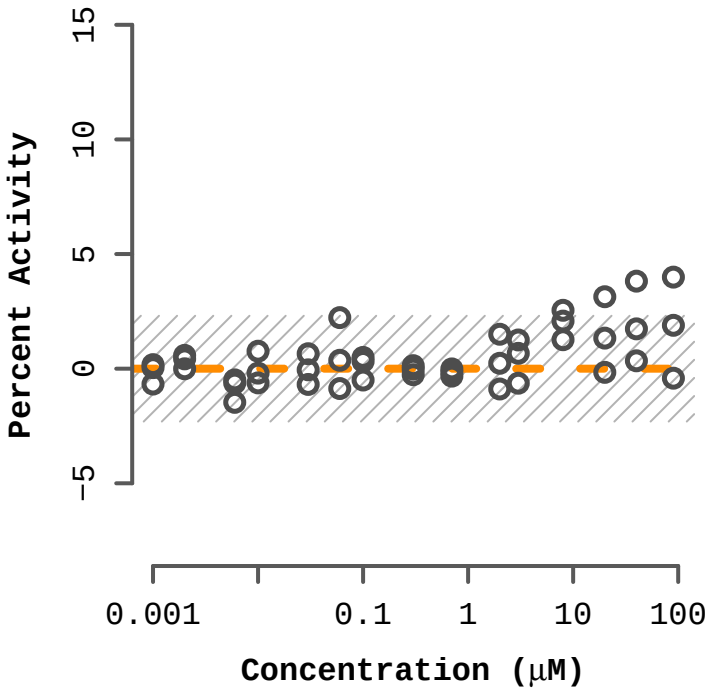
NAME: Allylthiourea
CHID: 24449 **CASRN:** 109-57-9
SPID(S): Tox21_111128_1
M4ID: 12483891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.639 **MAX_MED:** 0.599 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

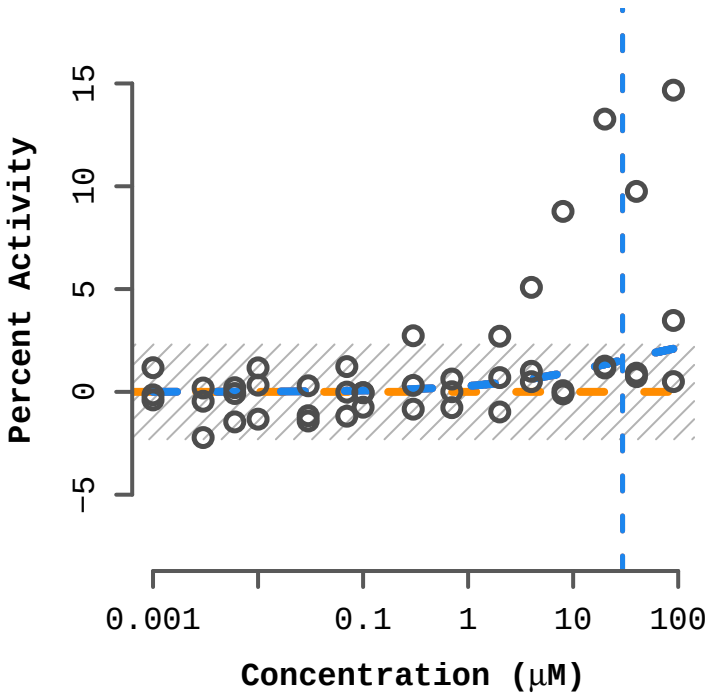
NAME: Amiloride hydrochloride
CHID: 24452 **CASRN:** 2016-88-8
SPID(S): Tox21_303068
M4ID: 12476065

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amiloride hydrochloride
CHID: 24452 CASRN: 2016-88-8
SPID(S): Tox21_201386
M4ID: 12480866

HILL MODEL (in red):

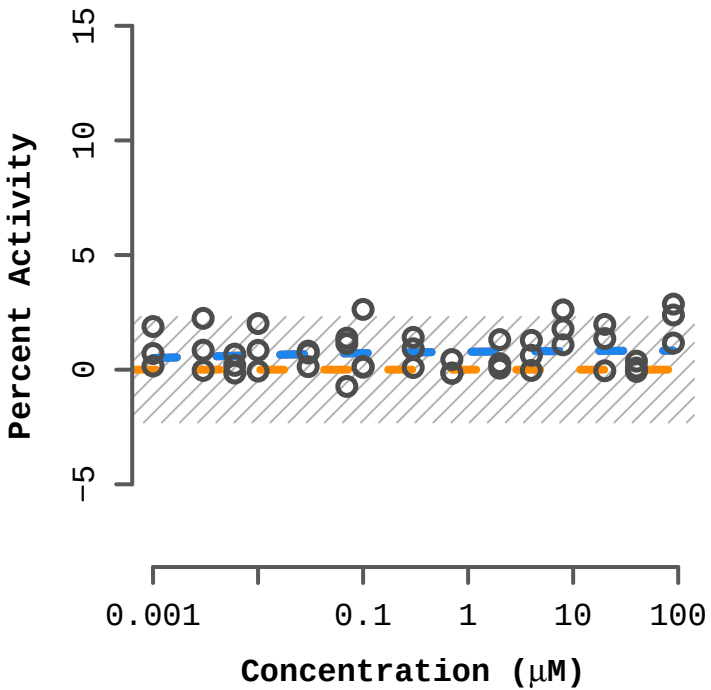
	tp	ga	gw
val:	3.09	1.47	0.673
sd:	9.77	4.24	0.89

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.09	1.47	0.673	3.43	4.95
sd:	9.78	4.24	0.89	1470	4950

	CNST	HILL	GNLS
AIC:	212.57	208.3	212.3
PROB:	0.09	0.8	0.11
RMSE:	3.78	3.3	3.3

MAX_MEAN: 6.22 **MAX_MED:** 3.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Aminoacetanilide
CHID: 24454 **CASRN:** 102-28-3
SPID(S): Tox21_200881
M4ID: 12481371

HILL MODEL (in red):

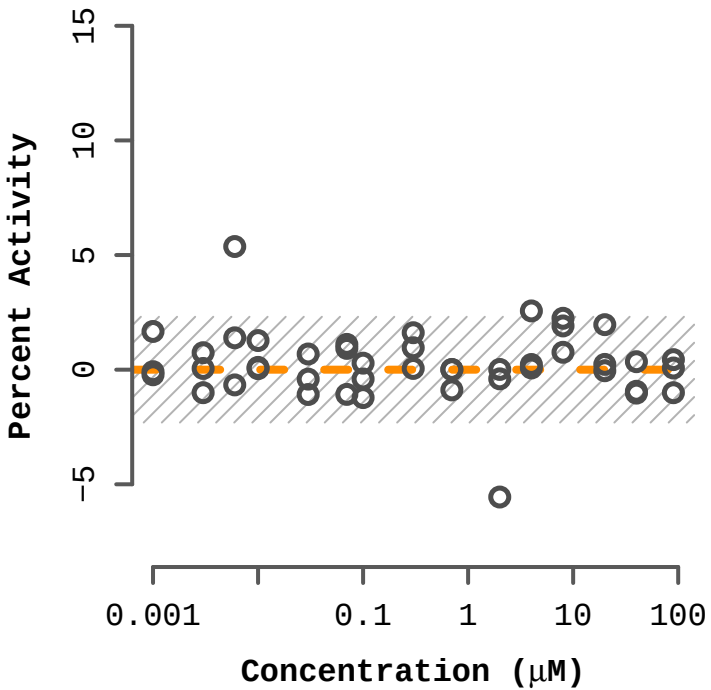
	tp	ga	gw
val:	0.848	−3.54	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.847	−3.55	0.3	3.79	4.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	147.74	128.25	132.25
PROB:	0	0.88	0.12
RMSE:	1.21	0.89	0.89

MAX_MEAN: 2.14 **MAX_MED:** 2.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

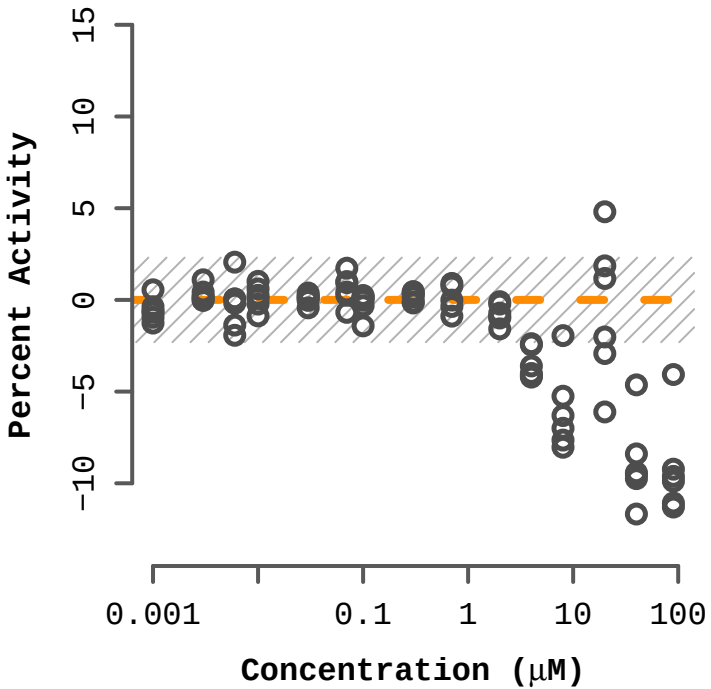
NAME: 4-Aminoacetanilide
CHID: 24455 **CASRN:** 122-80-5
SPID(S): Tox21_200754
M4ID: 12481498

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.03 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

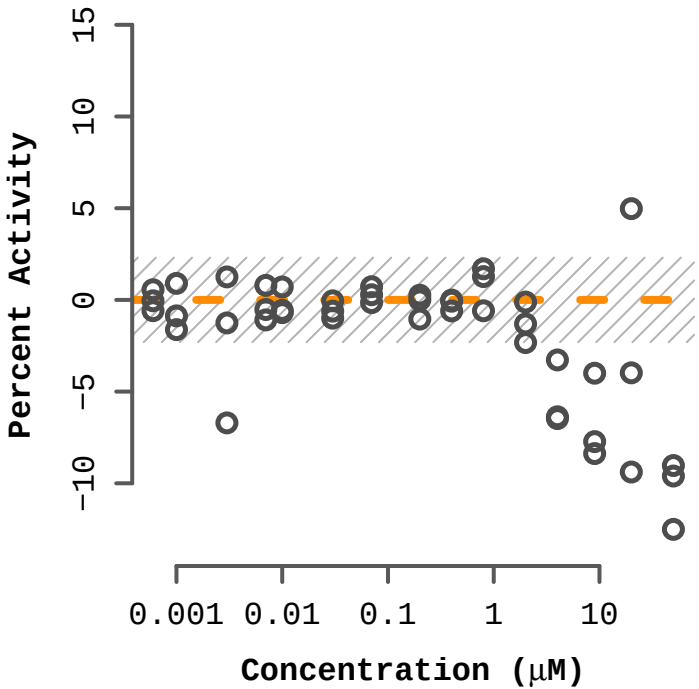
NAME: 9-Aminoacridine, monohydrochloride, monohydrat
CHID: 24457 CASRN: 52417-22-8
SPID(S): Tox21_200788
M4ID: 12481464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	481.53	NA	NA
PROB:	1	NA	NA
RMSE:	4.07	NA	NA

MAX_MEAN: 0.613 **MAX_MED:** 0.687 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

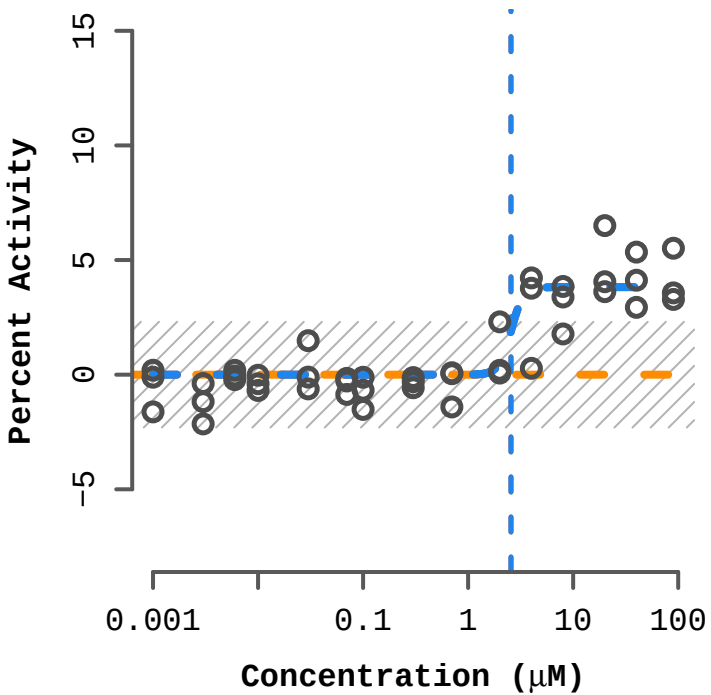
NAME: 9-Aminoacridine, monohydrochloride, monohydrat
CHID: 24457 CASRN: 52417-22-8
SPID(S): Tox21_111187_1
M4ID: 12483858

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.13	NA	NA
PROB:	1	NA	NA
RMSE:	4.14	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminoanthracene
CHID: 24458 CASRN: 613-13-8
SPID(S): Tox21_303299
M4ID: 12475834

HILL MODEL (in red):

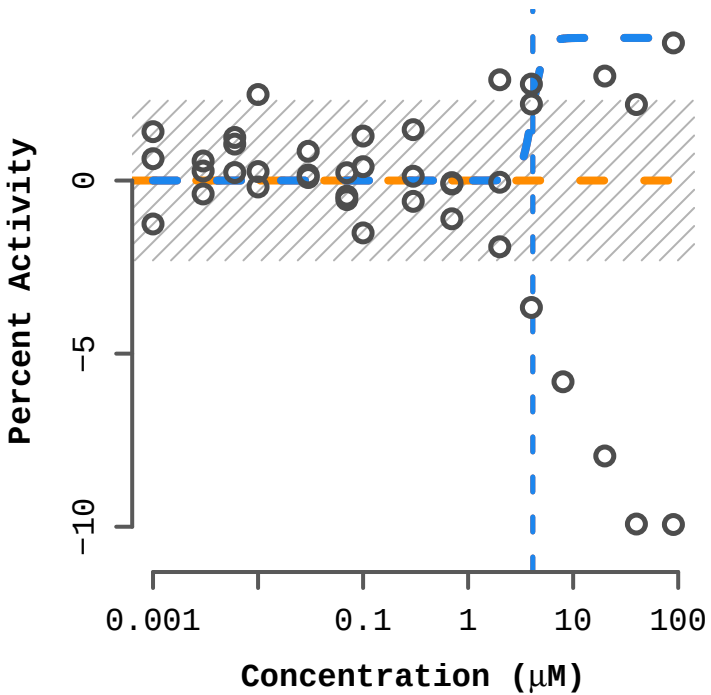
	tp	ga	gw
val:	3.82	0.408	7.47
sd:	0.272	0.112	7.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.82	0.408	7.47	3.92	3.57
sd:	0.272	0.112	7.4	1920	3130

	CNST	HILL	GNLS
AIC:	207.37	136.44	140.44
PROB:	0	0.88	0.12
RMSE:	2.43	1.07	1.07

MAX_MEAN: 4.73 MAX_MED: 4.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminoanthracene
CHID: 24458 CASRN: 613-13-8
SPID(S): Tox21_201567
M4ID: 12480685

HILL MODEL (in red):

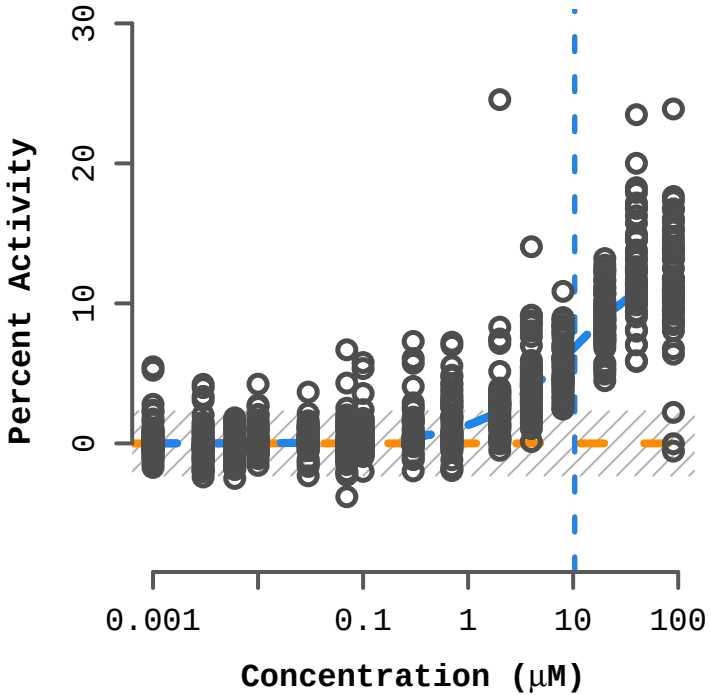
	tp	ga	gw
val:	4.12	0.616	8
sd:	0.824	0.145	73.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.12	0.616	7.96	3.95	3.22
sd:	0.822	0.143	70.8	525	855

	CNST	HILL	GNLS
AIC:	236.22	225.47	229.47
PROB:	0	0.88	0.12
RMSE:	3.53	4.03	4.03

MAX_MEAN: 1.11 MAX_MED: 4.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Aminoazobenzene
CHID: 24460 **CASRN:** 60-09-3
SPID(S): Tox21_400019
M4ID: 12475118

HILL MODEL (in red):

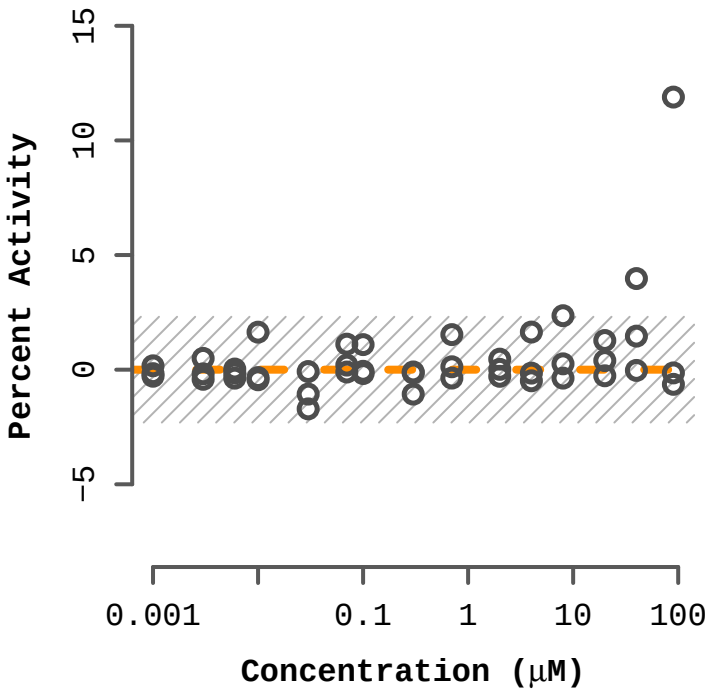
	tp	ga	gw
val:	13.7	1.01	0.961
sd:	0.683	0.0602	0.0692

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.7	1.01	0.961	3.44	6.53
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	4451.21	3027.95	3031.95
PROB:	0	0.88	0.12
RMSE:	5.83	2.38	2.38

MAX_MEAN: 12.4 **MAX_MED:** 11.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

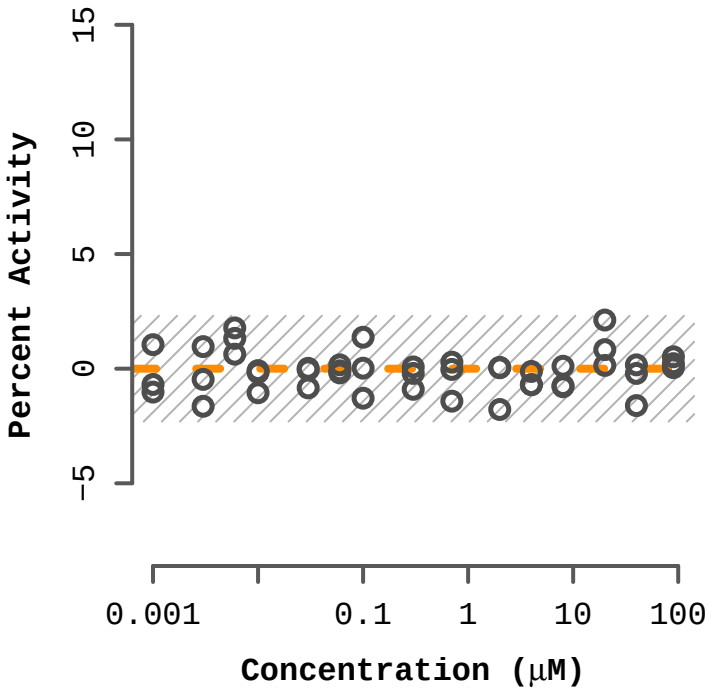
NAME: 3-Aminobenzenesulfonic acid
CHID: 24462 **CASRN:** 121-47-1
SPID(S): Tox21_201027
M4ID: 12481225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 3.7 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

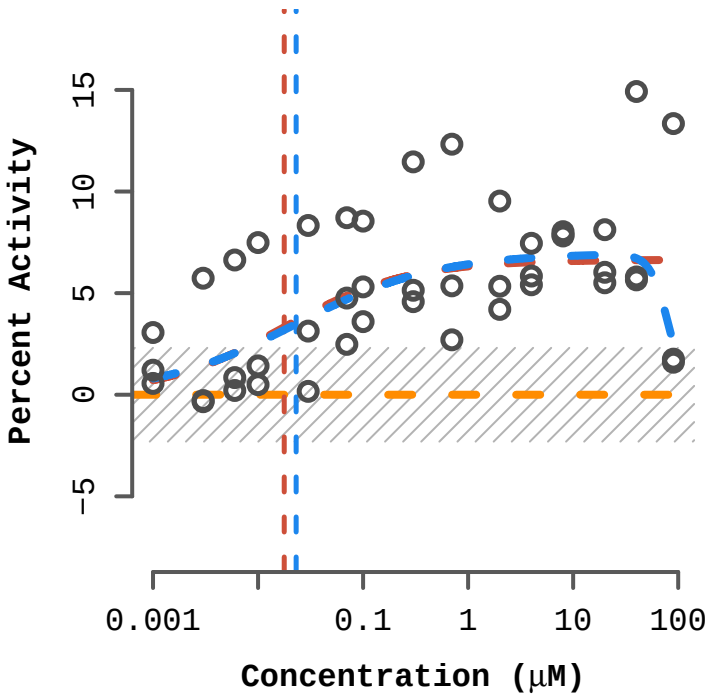
NAME: Orthanilic acid
CHID: 24463 **CASRN:** 88-21-1
SPID(S): Tox21_200956
M4ID: 12481296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminobenzimidazole
CHID: 24465 CASRN: 934-32-7
SPID(S): Tox21_303120
M4ID: 12476013

HILL MODEL (in red):

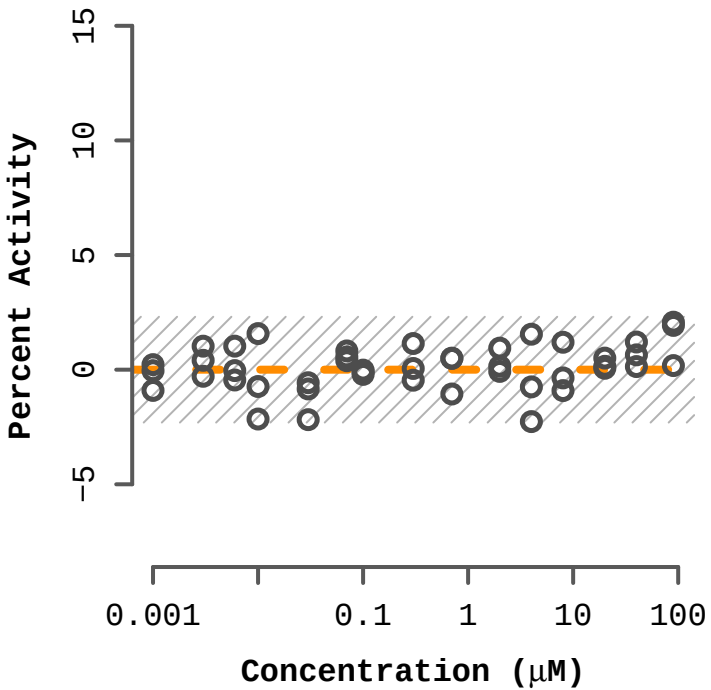
	tp	ga	gw
val:	6.64	−1.75	0.735
sd:	0.745	0.352	0.416

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.97	−1.64	0.652	1.91	5.02
sd:	0.977	0.389	0.392	0.151	12.8

	CNST	HILL	GNLS
AIC:	301.91	238.24	238.7
PROB:	0	0.56	0.44
RMSE:	6.43	3.09	3.18

MAX_MEAN: 8.79 **MAX_MED:** 7.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

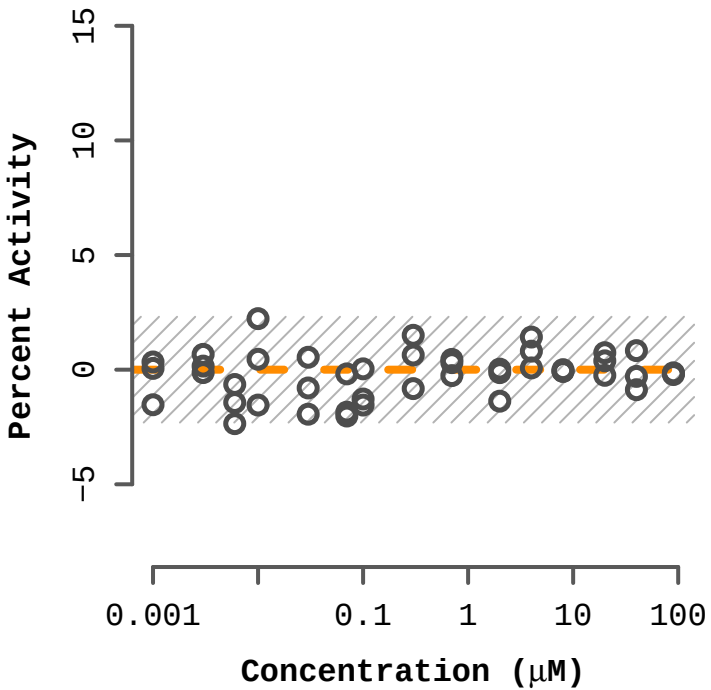
NAME: 2-Aminobenzimidazole
CHID: 24465 **CASRN:** 934-32-7
SPID(S): Tox21_201949
M4ID: 12480303

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

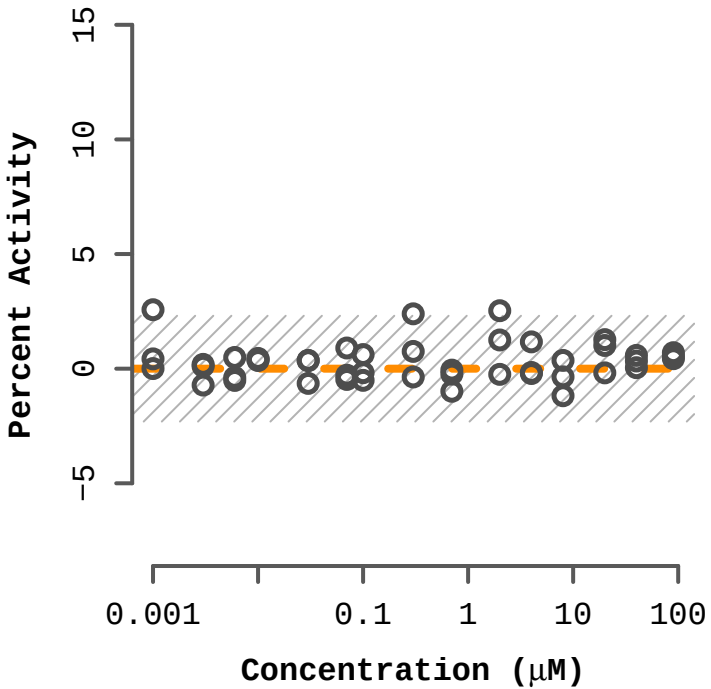
NAME: 4-Aminobenzoic acid
CHID: 24466 **CASRN:** 150-13-0
SPID(S): Tox21_300087
M4ID: 12479043

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.771 **MAX_MED:** 0.809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

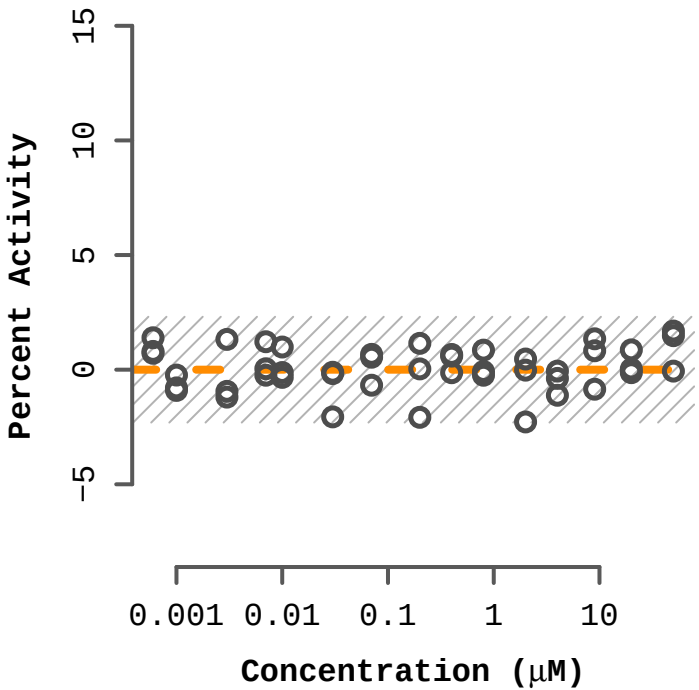
NAME: 4-Aminobenzoic acid
CHID: 24466 **CASRN:** 150-13-0
SPID(S): Tox21_201702
M4ID: 12480550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

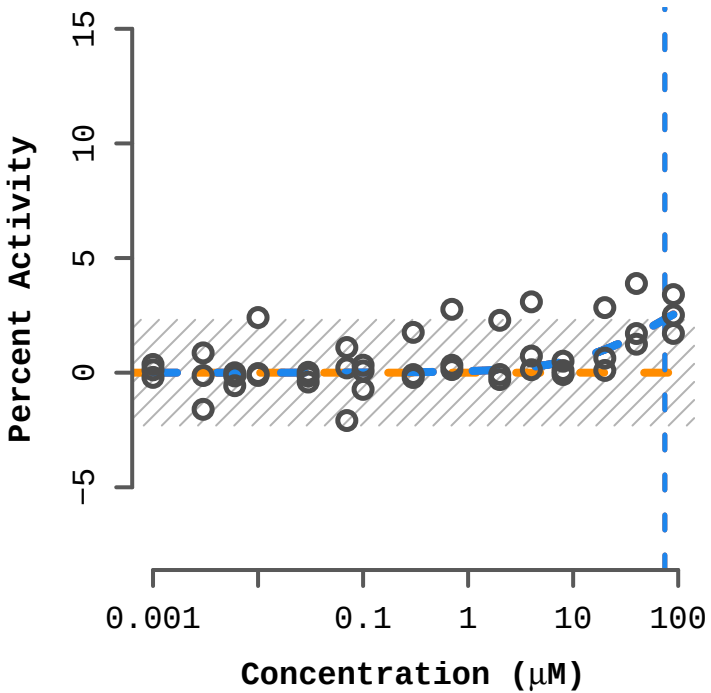
NAME: 4-Aminobenzoic acid
CHID: 24466 **CASRN:** 150-13-0
SPID(S): Tox21_111069_1
M4ID: 12483924

HILL MODEL: Not applicable.

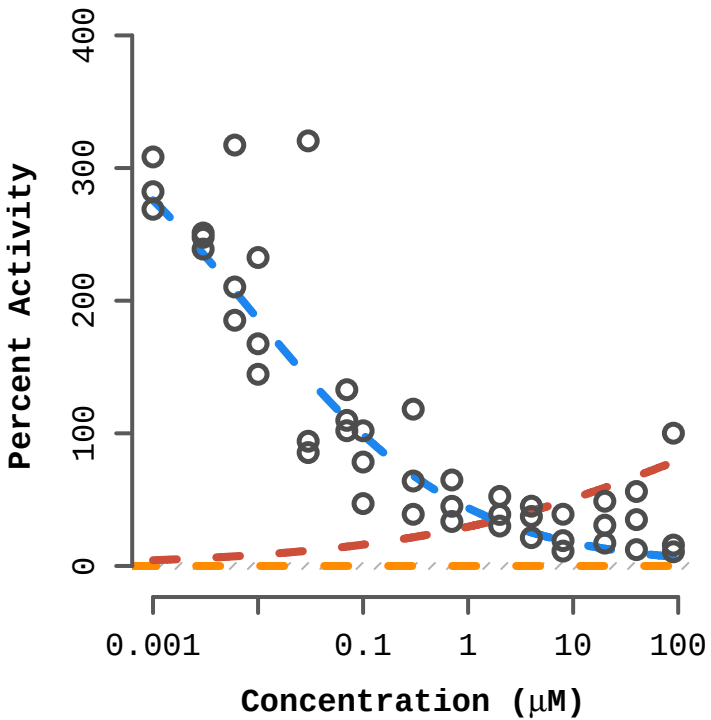
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.48 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Aminobenzothiazole
CHID:    24467   CASRN: 136-95-8
SPID(S): Tox21_200818
M4ID:    12481434

HILL MODEL (in red):
      tp       ga       gw
val:  4.67     1.87     0.98
sd:   6.21     1.21     0.883

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.67     1.87     0.98     2.2      9.36
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  157.1       134.77      138.77
PROB: 0           0.88        0.12
RMSE: 1.43        1.07        1.07

MAX_MEAN: 2.55      MAX_MED: 2.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-4-chlorobenzothiazole
CHID: 24470 CASRN: 19952-47-7
SPID(S): Tox21_200087
M4ID: 12482165

HILL MODEL (in red):

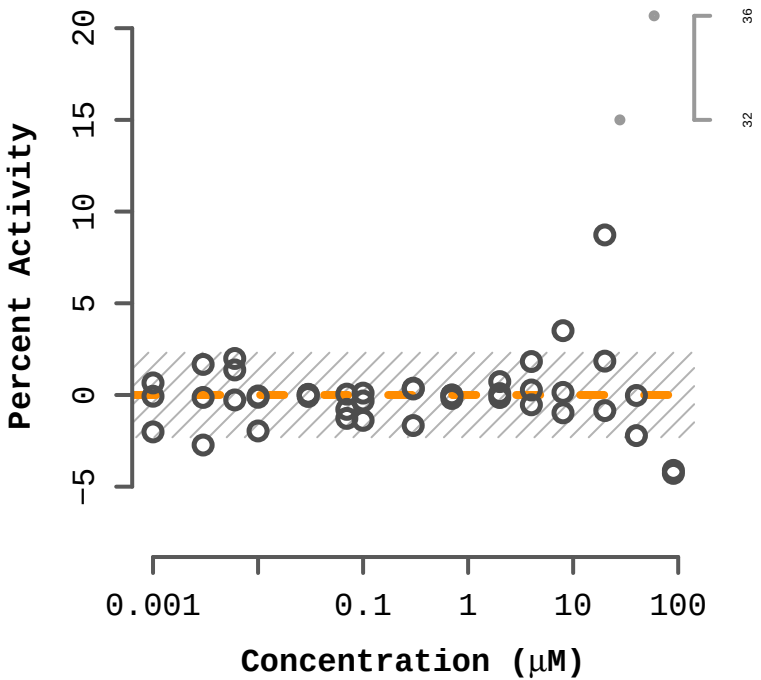
	tp	ga	gw
val:	186	2.41	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	385	-4.26	6.5	-2.07	0.432
sd:	54.7	710	3660	0.327	0.0544

	CNST	HILL	GNLS
AIC:	577.86	578.44	457.97
PROB:	0	0	1
RMSE:	144.94	138.13	41.64

MAX_MEAN: 287 MAX_MED: 282 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

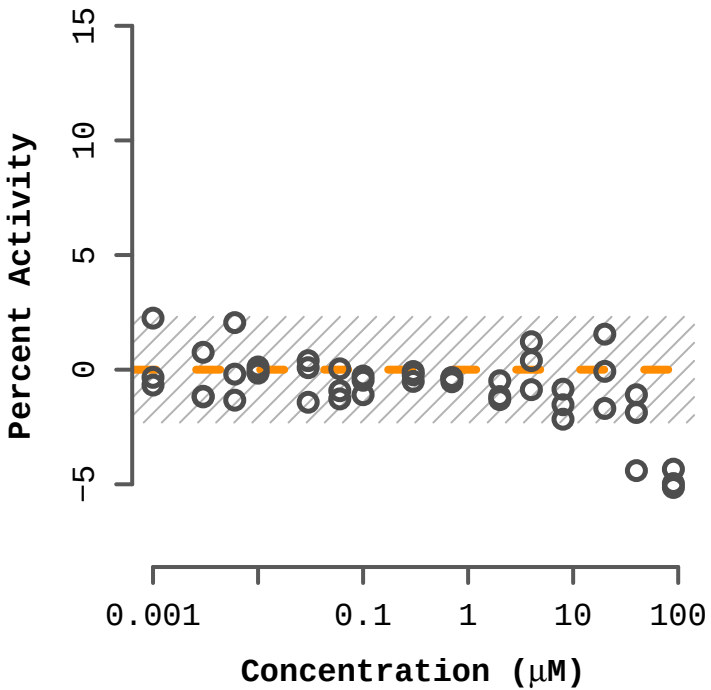
NAME: 2-Amino-4-chloro-5-nitrophenol
CHID: 24471 **CASRN:** 6358-07-2
SPID(S): Tox21_200073
M4ID: 12482179 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.86	NA	NA
PROB:	1	NA	NA
RMSE:	7.38	NA	NA

MAX_MEAN: 9.84 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

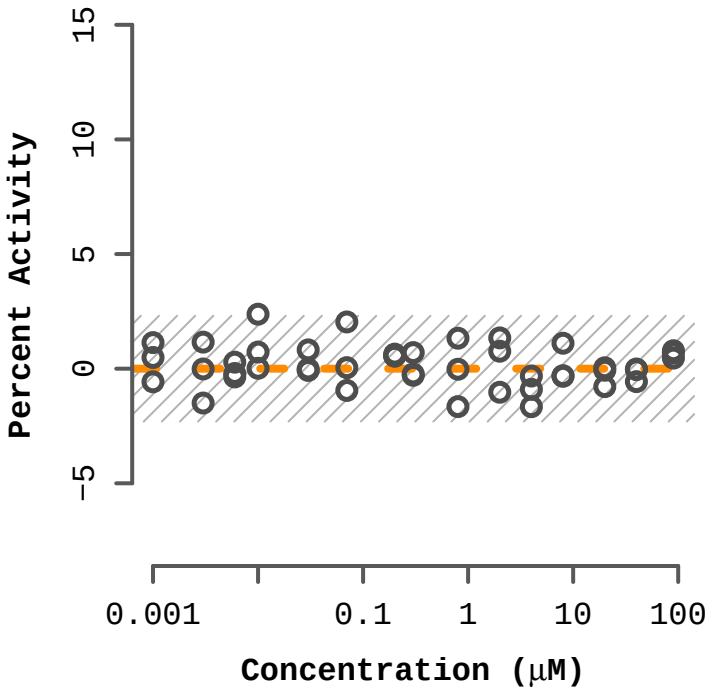
NAME: 2-Amino-4-chlorophenol
CHID: 24473 **CASRN:** 95-85-2
SPID(S): Tox21_201047
M4ID: 12481205

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.397 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

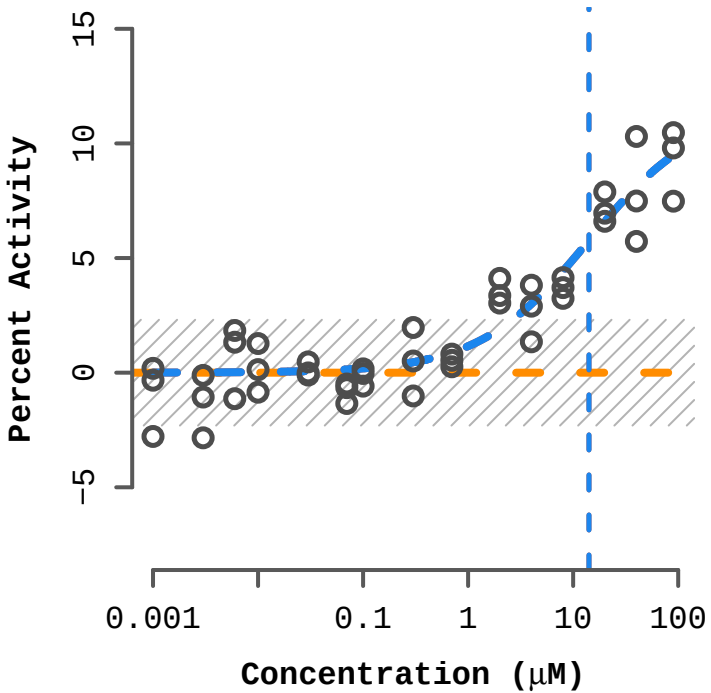
NAME: 6-Amino-4-chloro-1-phenol-2-sulfonic acid
CHID: 24474 **CASRN:** 88-23-3
SPID(S): Tox21_202892
M4ID: 12479360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.762 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-5,6-dimethylbenzothiazole
CHID: 24478 CASRN: 29927-08-0
SPID(S): Tox21_201079
M4ID: 12481173

HILL MODEL (in red):

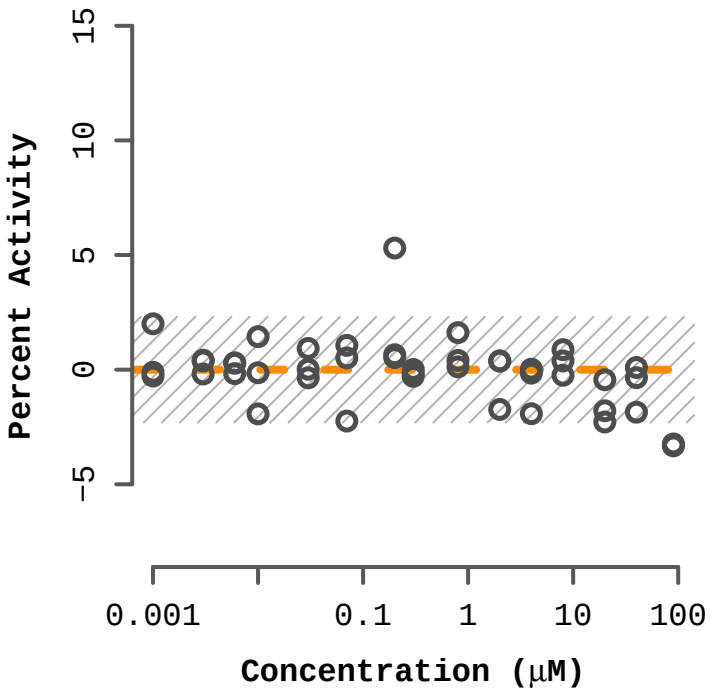
	tp	ga	gw
val:	11.5	1.15	0.829
sd:	2.1	0.238	0.175

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.5	1.15	0.828	3.12	6.27
sd:	2.1	0.238	0.175	845	4590

	CNST	HILL	GNLS
AIC:	252.2	155.46	159.46
PROB:	0	0.88	0.12
RMSE:	4.08	1.22	1.22

MAX_MEAN: 9.25 MAX_MED: 9.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

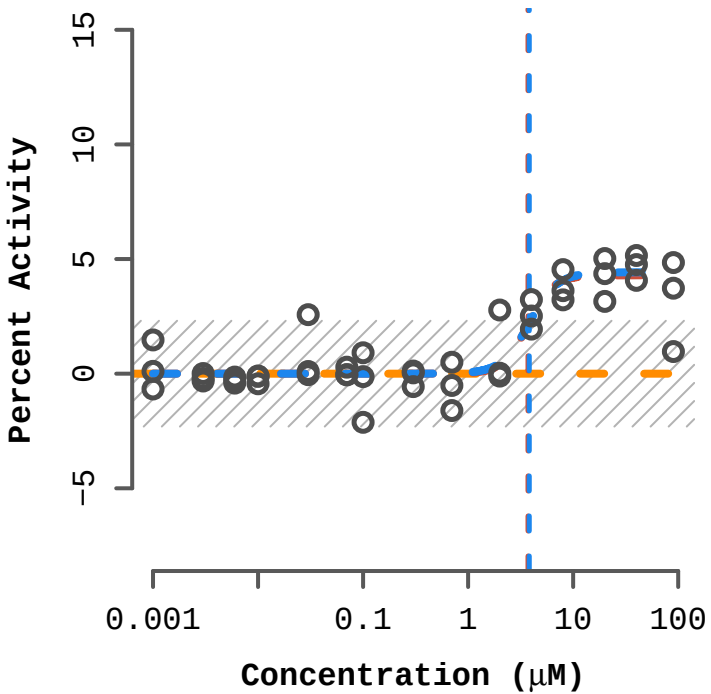
NAME: 2-Amino-4,6-dinitrophenol
CHID: 24479 CASRN: 96-91-3
SPID(S): Tox21_202887
M4ID: 12479365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.16 MAX_MED: 0.653 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-6-ethoxybenzothiazole
CHID: 24481 CASRN: 94-45-1
SPID(S): Tox21_200641
M4ID: 12481611

HILL MODEL (in red):

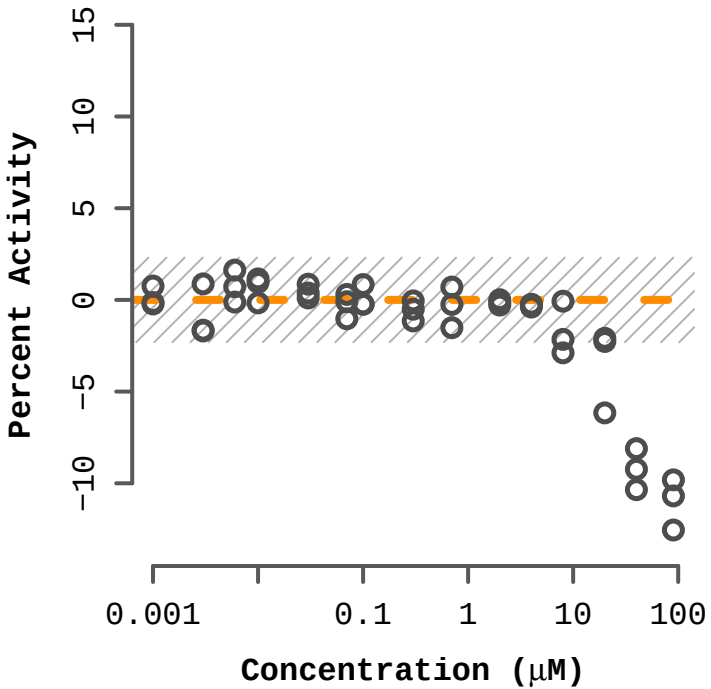
	tp	ga	gw
val:	4.29	0.57	3.7
sd:	0.269	0.0467	1.86

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.42	0.582	3.29	2.01	15.6
sd:	0.325	0.0547	1.61	0.205	62.3

	CNST	HILL	GNLS
AIC:	205.96	120.37	123.67
PROB:	0	0.84	0.16
RMSE:	2.36	0.96	0.93

MAX_MEAN: 4.66 MAX_MED: 4.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

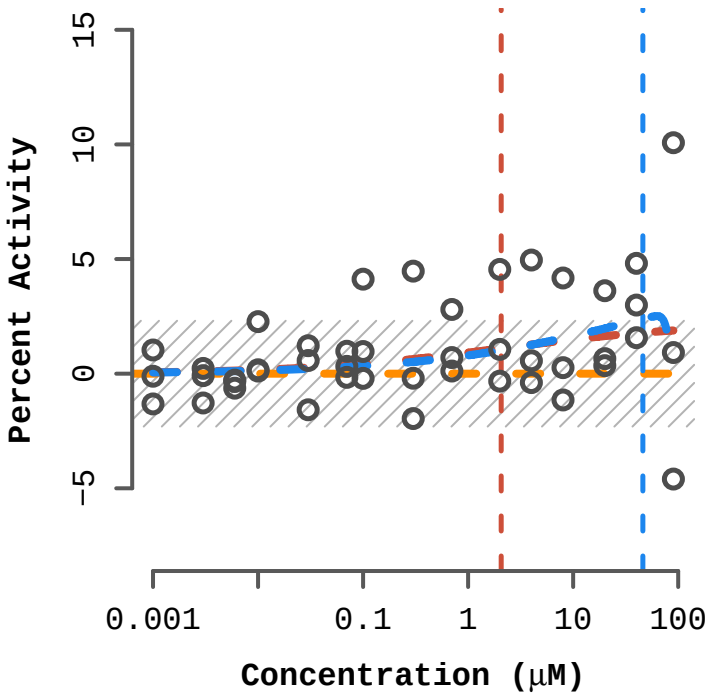
NAME: 4-Amino-4'-hydroxy-3-methyldiphenylamine
CHID: 24483 **CASRN:** 6219-89-2
SPID(S): Tox21_200344
M4ID: 12481908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-4-methoxybenzothiazole
CHID: 24484 **CASRN:** 5464-79-9
SPID(S): Tox21_200251
M4ID: 12482001

HILL MODEL (in red):

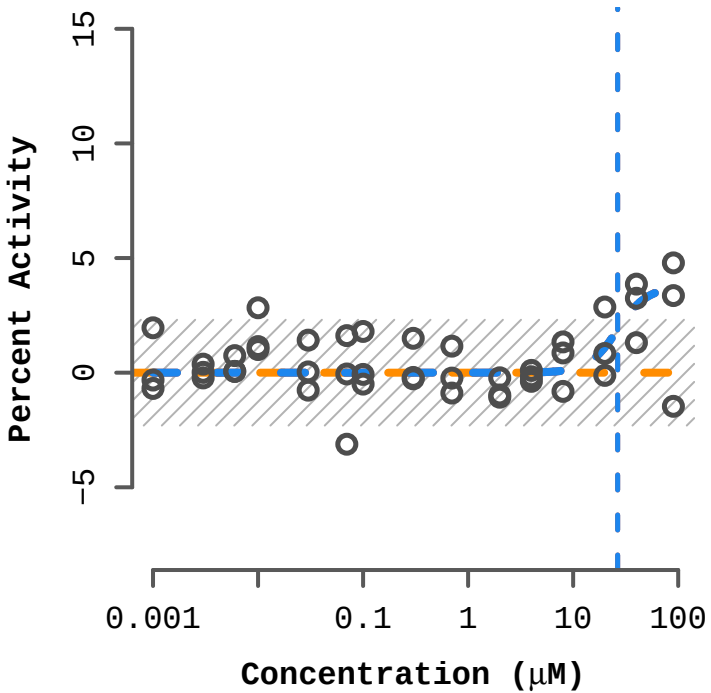
	tp	ga	gw
val:	2.2	0.315	0.468
sd:	2.71	3.02	0.535

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.77	1.66	0.42	1.91	16.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	205.36	200.61	203.19
PROB:	0.07	0.73	0.2
RMSE:	2.6	2.26	2.29

MAX_MEAN: 3.13 **MAX_MED:** 2.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-6-methoxybenzothiazole
CHID: 24485 CASRN: 1747-60-0
SPID(S): Tox21_303183
M4ID: 12475950

HILL MODEL (in red):

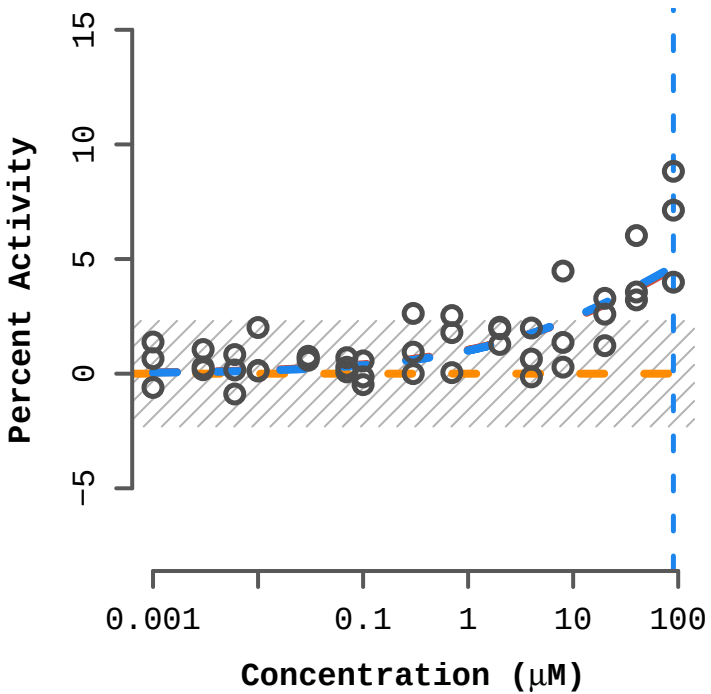
	tp	ga	gw
val:	3.75	1.42	3.11
sd:	0.984	0.135	3.11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.75	1.42	3.11	2.47	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	168.58	154.18	158.18
PROB:	0	0.88	0.12
RMSE:	1.61	1.33	1.33

MAX_MEAN: 2.81 MAX_MED: 3.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-6-methoxybenzothiazole
CHID: 24485 **CASRN:** 1747-60-0
SPID(S): Tox21_201425
M4ID: 12480827

HILL MODEL (in red):

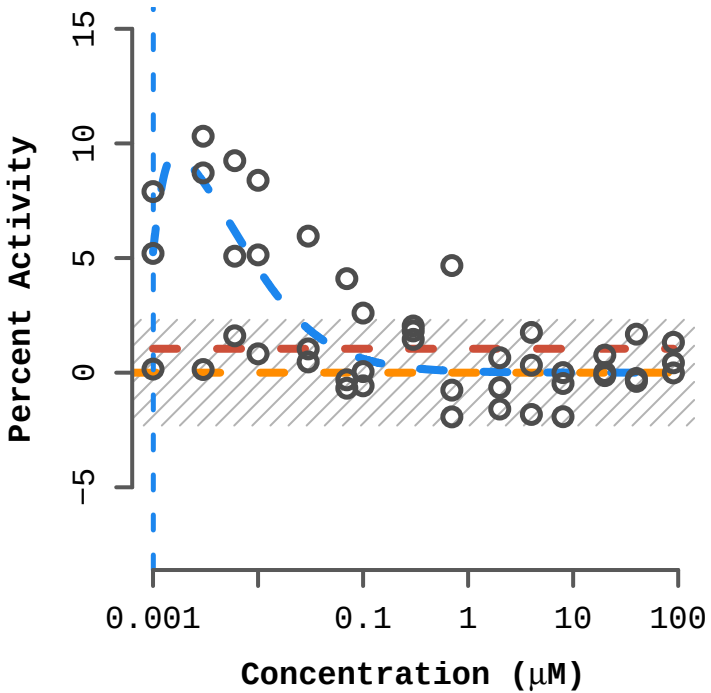
	tp	ga	gw
val:	10.6	2.22	0.434
sd:	5.88	0.912	0.119

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.34	1.95	0.471	3.41	5.38
sd:	6.79	1.06	0.128	795	2930

	CNST	HILL	GNLS
AIC:	203.25	150.49	154.93
PROB:	0	0.9	0.1
RMSE:	2.53	1.23	1.23

MAX_MEAN: 6.65 **MAX_MED:** 7.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-4-methylbenzothiazole
CHID: 24487 CASRN: 1477-42-5
SPID(S): Tox21_200233
M4ID: 12482019

HILL MODEL (in red):

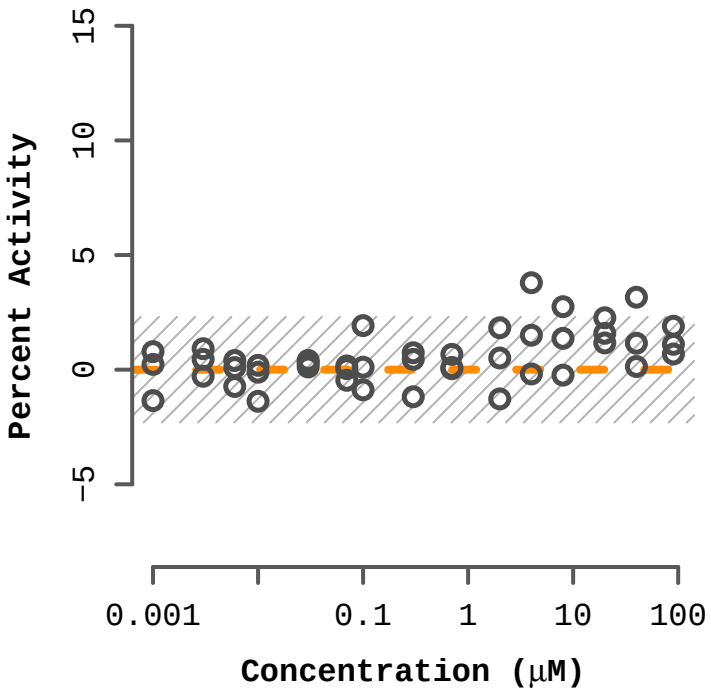
	tp	ga	gw
val:	1.04	−4.61	4.44
sd:	0.404	1140	3140

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.4	−3	6.79	−2.22	1.05
sd:	7.81	0.0573	26	0.588	0.556

	CNST	HILL	GNLS
AIC:	237.67	236.31	214.17
PROB:	0	0	1
RMSE:	3.65	3.25	2.39

MAX_MEAN: 6.39 MAX_MED: 8.72 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

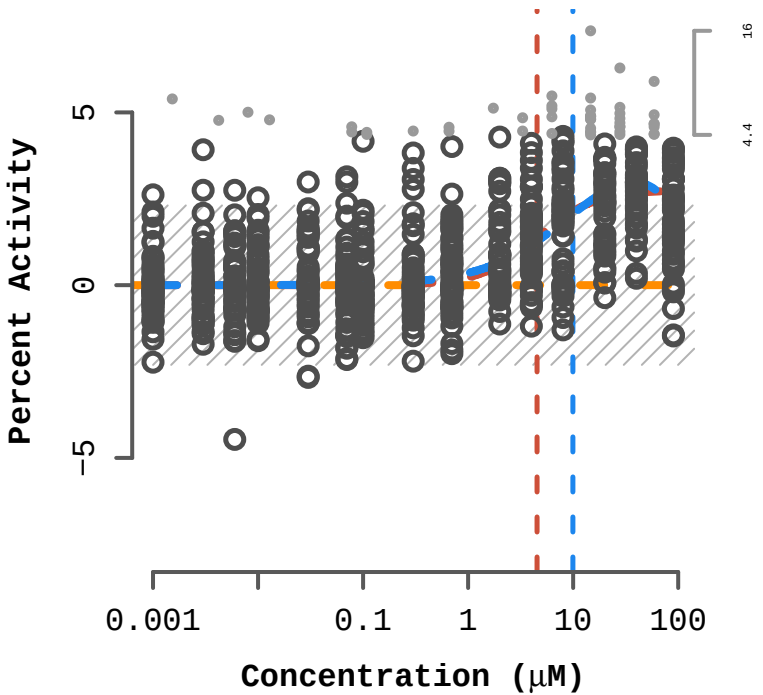
NAME: 2-Amino-4-methylphenol
CHID: 24488 **CASRN:** 95-84-1
SPID(S): Tox21_200692
M4ID: 12481560

HILL MODEL: Not applicable.

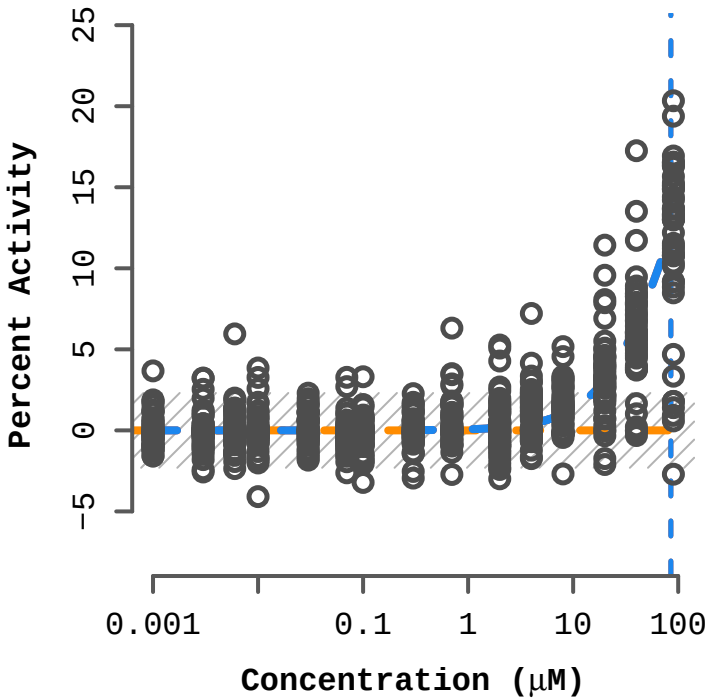
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

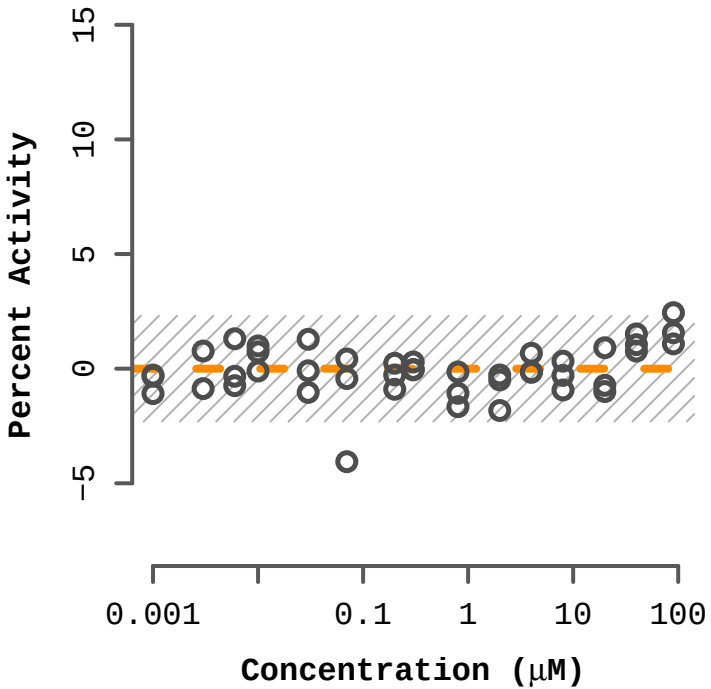
MAX_MEAN: 1.7 **MAX_MED:** 1.59 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    5-Amino-2-methylphenol
CHID:    24489   CASRN: 2835-95-2
SPID(S): Tox21_400033
M4ID:    12475104  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  2.75     0.656    1.59
sd:   0.151    0.0647   0.334

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.14     0.997    1.03     2.03     2.15
sd:   3.52     0.69     0.452    0.201    3.36

      CNST        HILL        GNLS
AIC:  3244.03     2773.67     2766.64
PROB: 0           0.03        0.97
RMSE: 2.27        1.71        1.69

MAX_MEAN: 3.31      MAX_MED: 2.96      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Amino-6-nitrobenzothiazole
CHID:    24491   CASRN: 6285-57-0
SPID(S): Tox21_400044
M4ID:    12475093

HILL MODEL (in red):
      tp       ga       gw
val:  24.4     1.93     1.33
sd:   3.23     0.0837   0.091

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  24.4     1.93     1.33     3.95     5.39
sd:   3.23     0.0837   0.0909   9260     25000

      CNST        HILL        GNLS
AIC:  3598.57     2768.18     2772.18
PROB: 0           0.88        0.12
RMSE: 4.04        2.09        2.09

MAX_MEAN: 11.4      MAX_MED: 13        BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

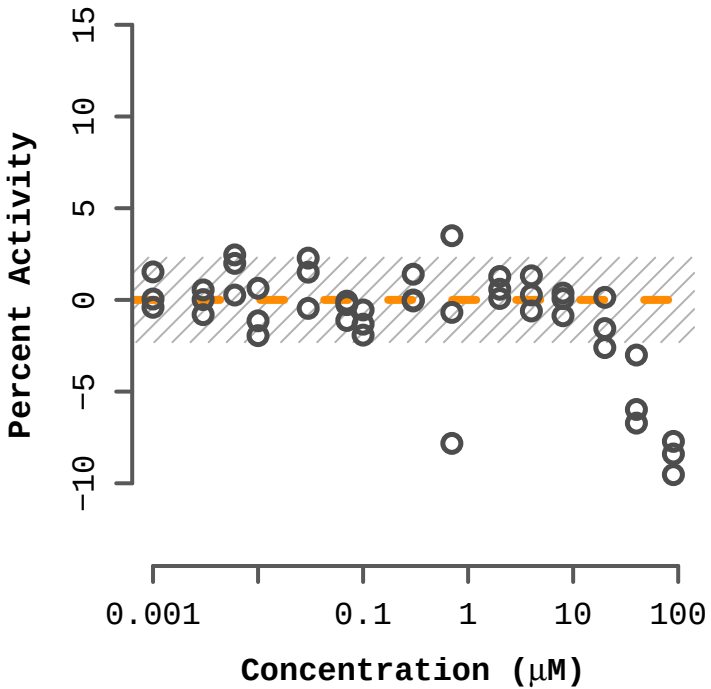
NAME: 3-Aminophenol
CHID: 24497 **CASRN:** 591-27-5
SPID(S): Tox21_200706
M4ID: 12481546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

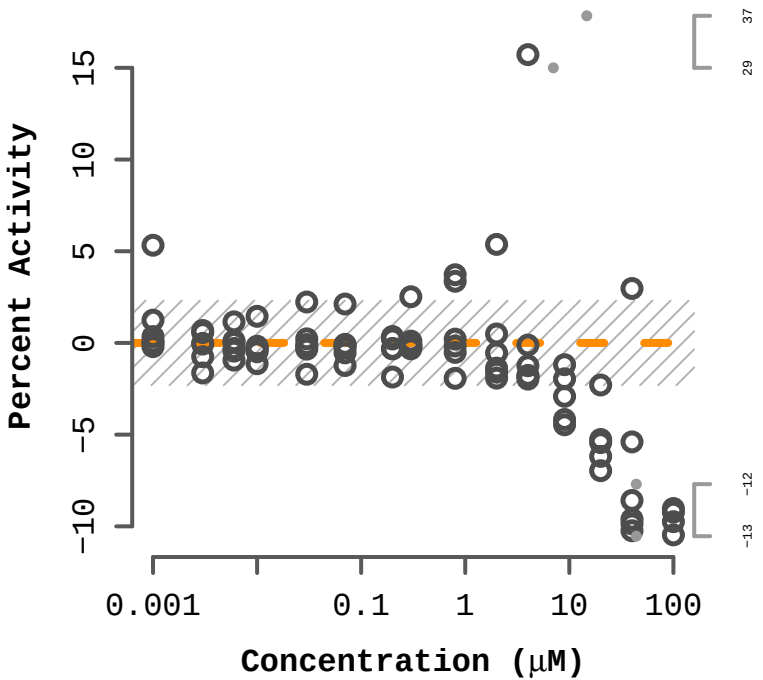
NAME: 2-Aminophenol
CHID: 24498 **CASRN:** 95-55-6
SPID(S): Tox21_200932
M4ID: 12481320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.11	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

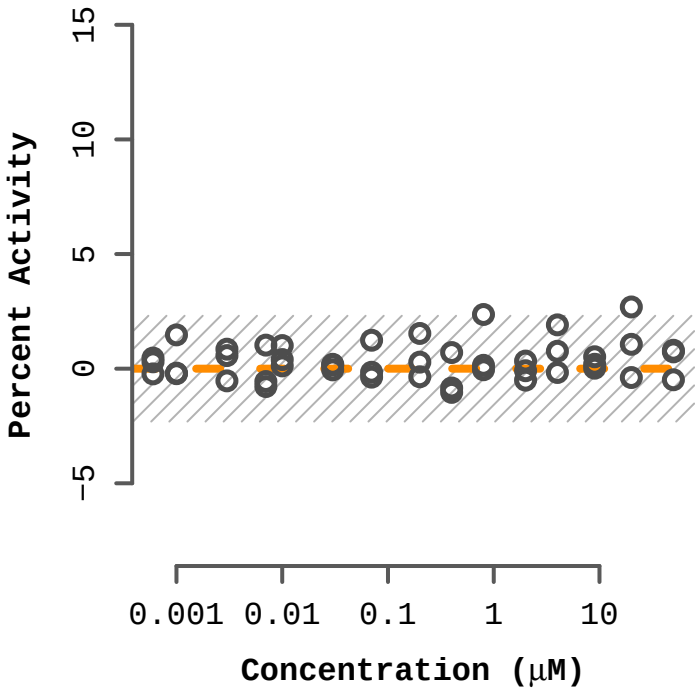
NAME: 4-Aminophenol
CHID: 24499 **CASRN:** 123-30-8
SPID(S): Tox21_201030
M4ID: 12481222 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	528.83	NA	NA
PROB:	1	NA	NA
RMSE:	6.55	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

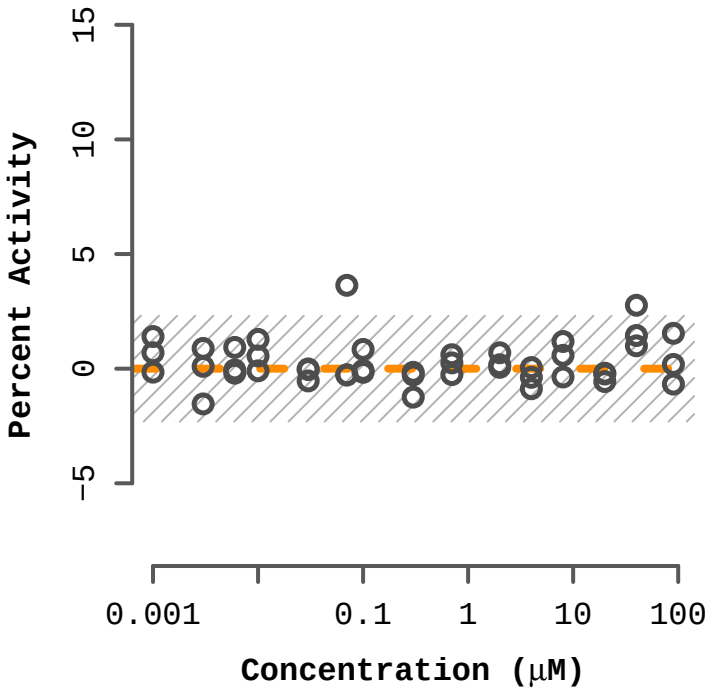
NAME: 4-Aminophenol
CHID: 24499 **CASRN:** 123-30-8
SPID(S): Tox21_113477_1
M4ID: 12482638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

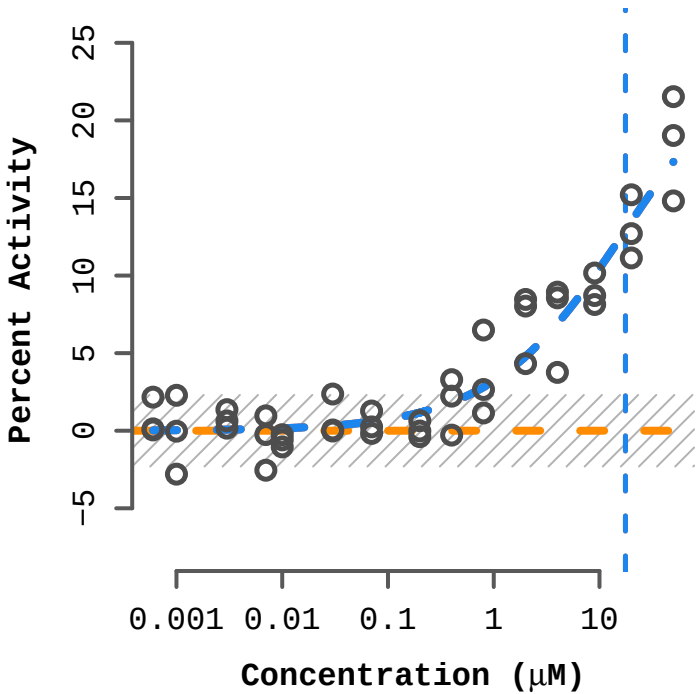
NAME: 2-Amino-1-phenol-4-sulfonic acid
CHID: 24500 **CASRN:** 98-37-3
SPID(S): Tox21_201044
M4ID: 12481208

HILL MODEL: Not applicable.

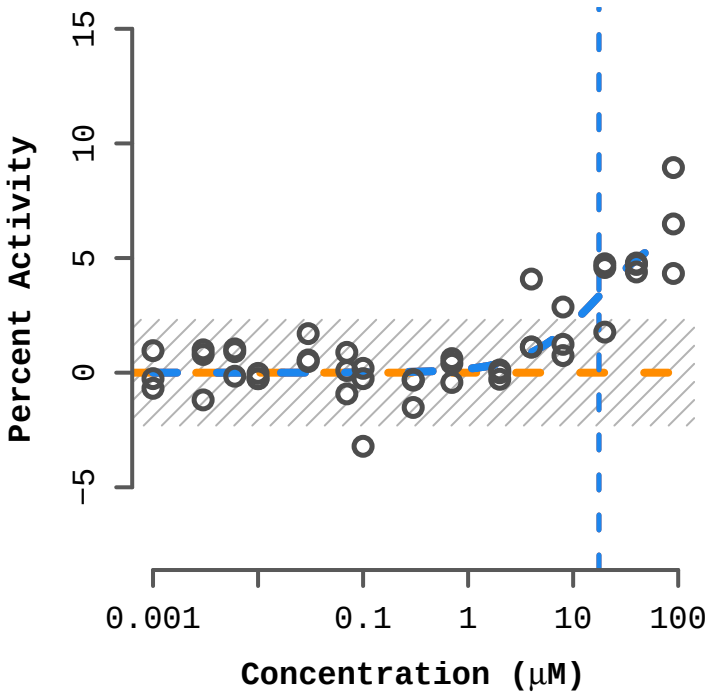
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.45 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-(4-Aminophenyl)-6-methylbenzothiazole sulfon
CHID:    24501   CASRN: 130-17-6
SPID(S): Tox21_202468
M4ID:    12479784

HILL MODEL (in red):
      tp       ga       gw
val:  25.8     1.25     0.681
sd:   8.82     0.436    0.119

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  25.8     1.25     0.681    3        9.58
sd:   8.82     0.436    0.12     59300    432000

      CNST        HILL        GNLS
AIC:  297.82      191.26      195.26
PROB: 0           0.88        0.12
RMSE: 7.04        1.79        1.79

MAX_MEAN: 18.5      MAX_MED: 19        BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-4-phenylthiazole hydrobromide hydrate
CHID: 24503 CASRN: 52253-69-7
SPID(S): Tox21_200171
M4ID: 12482081

HILL MODEL (in red):

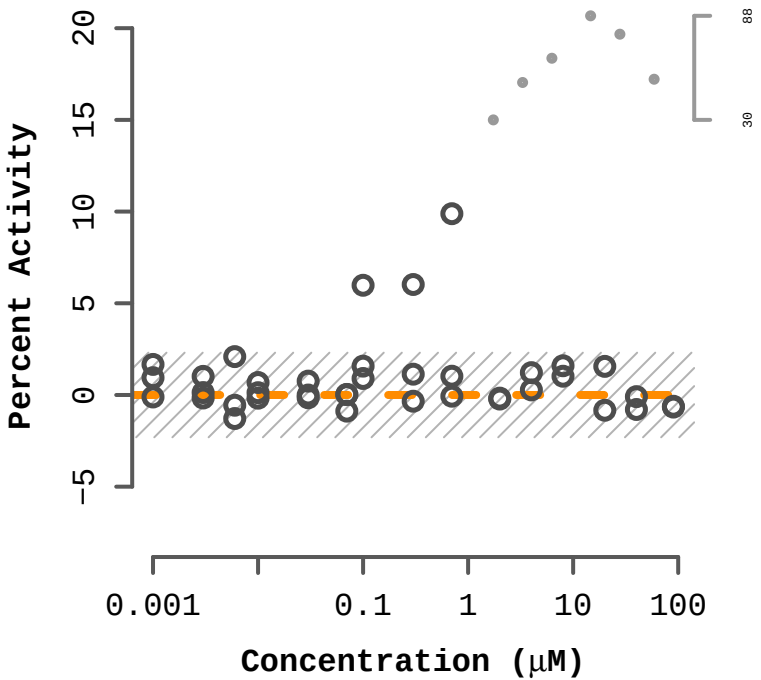
	tp	ga	gw
val:	6.68	1.25	1.27
sd:	2.34	0.352	0.509

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.68	1.25	1.27	3.38	5.86
sd:	2.34	0.352	0.509	1760	7260

	CNST	HILL	GNLS
AIC:	206.77	141.87	145.87
PROB:	0	0.88	0.12
RMSE:	2.61	1.13	1.13

MAX_MEAN: 6.59 MAX_MED: 6.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

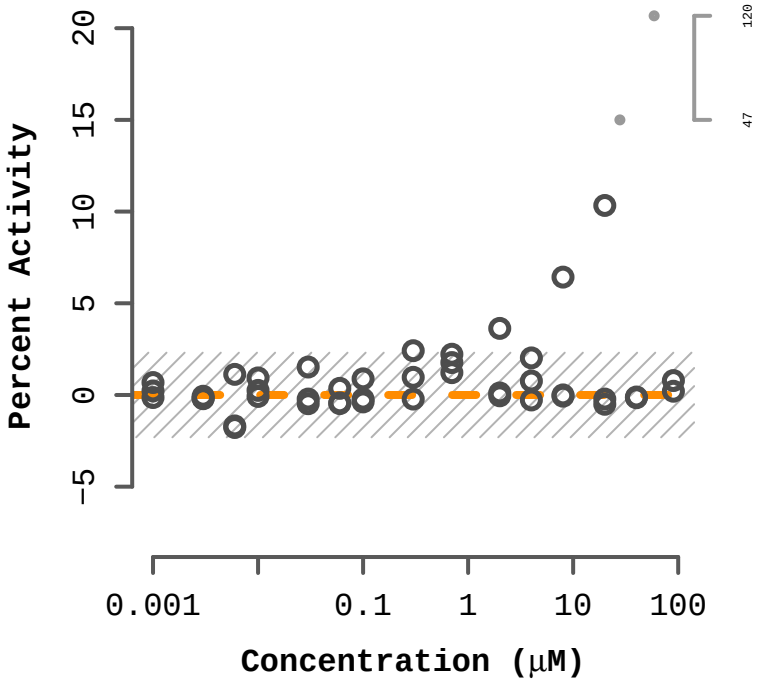
NAME: Luminol
CHID: 24504 **CASRN:** 521-31-3
SPID(S): Tox21_200940
M4ID: 12481312 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	341.59	NA	NA
PROB:	1	NA	NA
RMSE:	23.29	NA	NA

MAX_MEAN: 29.7 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

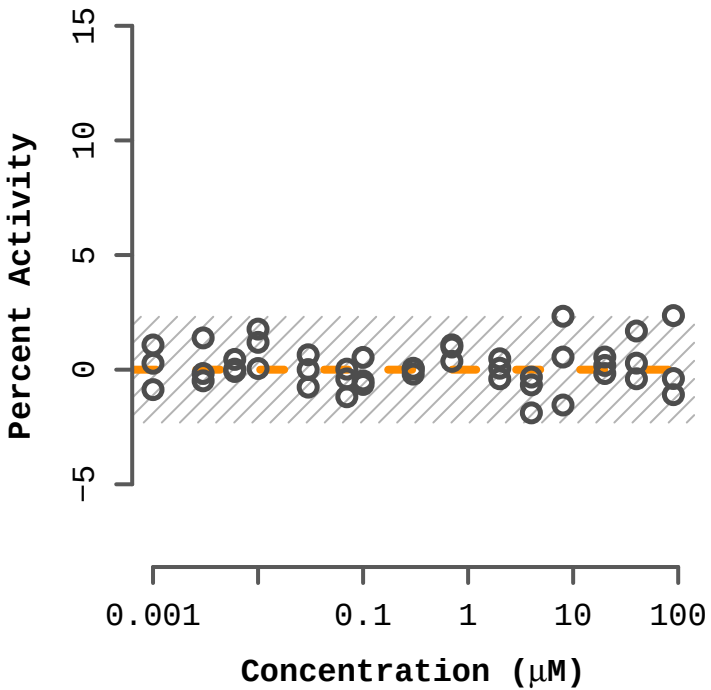
NAME: 2-Aminopyridine
CHID: 24505 **CASRN:** 504-29-0
SPID(S): Tox21_200880
M4ID: 12481372 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.03	NA	NA
PROB:	1	NA	NA
RMSE:	19.2	NA	NA

MAX_MEAN: 40.1 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

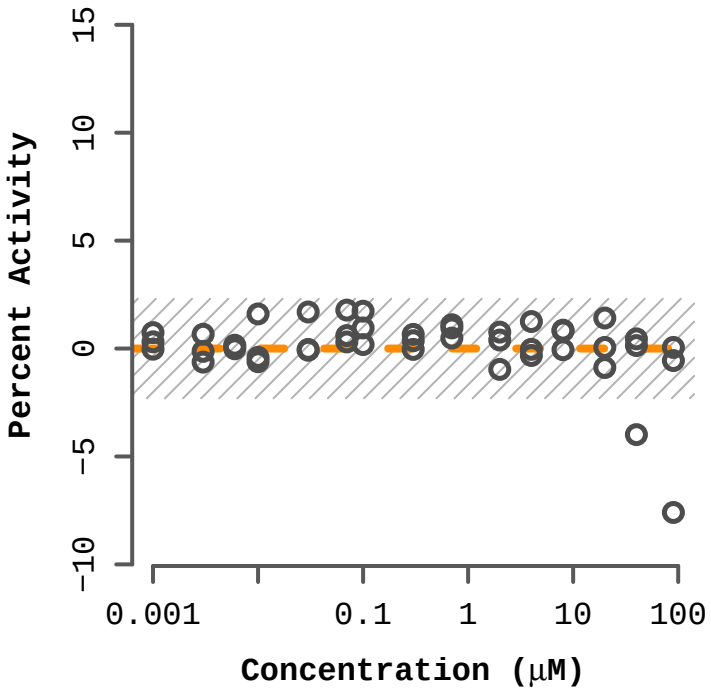
NAME: 5-Aminosalicylic acid
CHID: 24506 **CASRN:** 89-57-6
SPID(S): Tox21_303125
M4ID: 12476008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

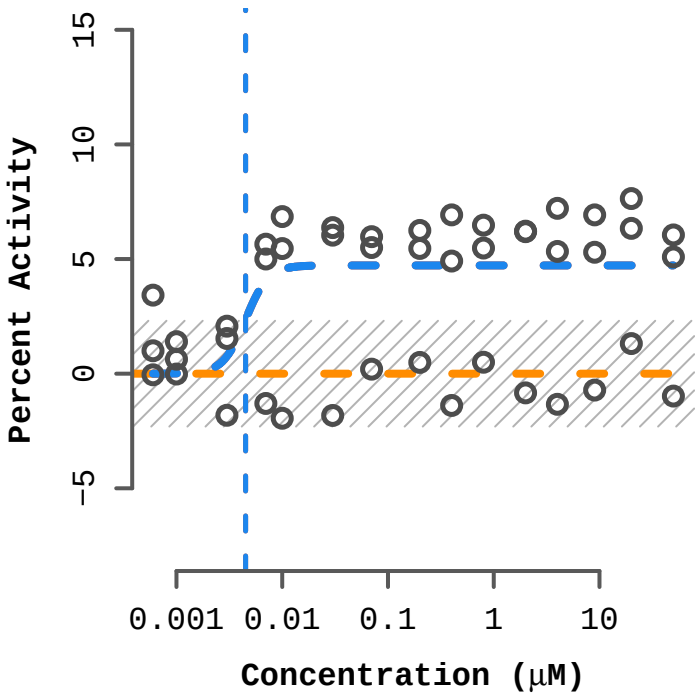
NAME: 5-Aminosalicylic acid
CHID: 24506 **CASRN:** 89-57-6
SPID(S): Tox21_201610
M4ID: 12480642

HILL MODEL: Not applicable.

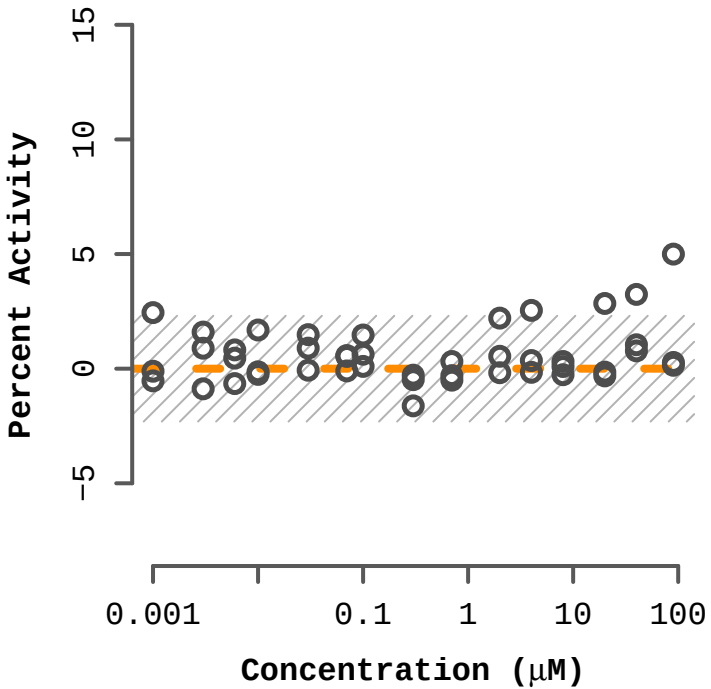
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 0.958 **MAX_MED:** 0.958 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    5-Aminosalicylic acid
CHID:    24506   CASRN: 89-57-6
SPID(S): Tox21_110384_1
M4ID:    12484406

HILL MODEL (in red):
      tp       ga       gw
val:  4.72     -2.35    4.06
sd:   0.585    0.203    4.57

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.72     -2.35    4.06     3.17     7.86
sd:   0.585    0.203    4.57     290000   1570000

      CNST        HILL        GNLS
AIC:  272.3       238.68      242.68
PROB: 0           0.88        0.12
RMSE: 4.54        3.09        3.09

MAX_MEAN: 5.1       MAX_MED: 6.34      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

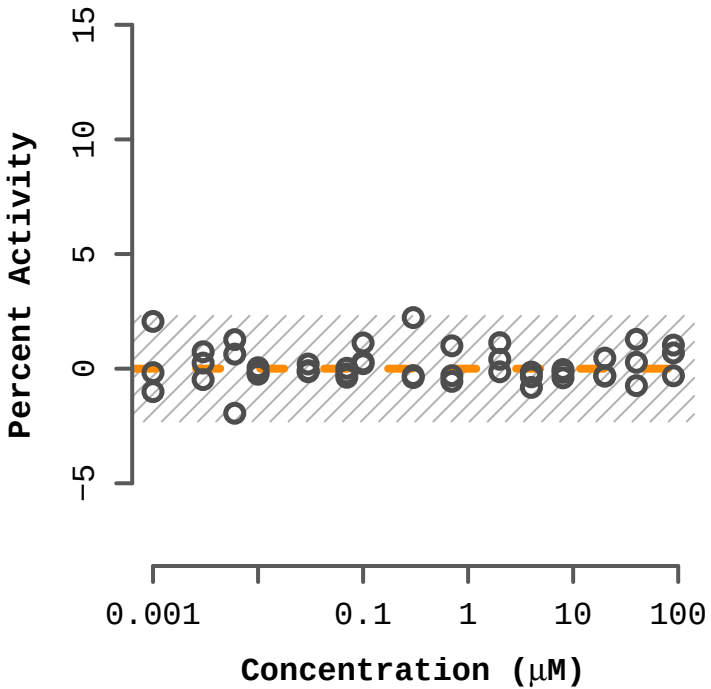
NAME: 5-Amino-3-sulfosalicylic acid
CHID: 24507 **CASRN:** 6201-87-2
SPID(S): Tox21_201016
M4ID: 12481236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

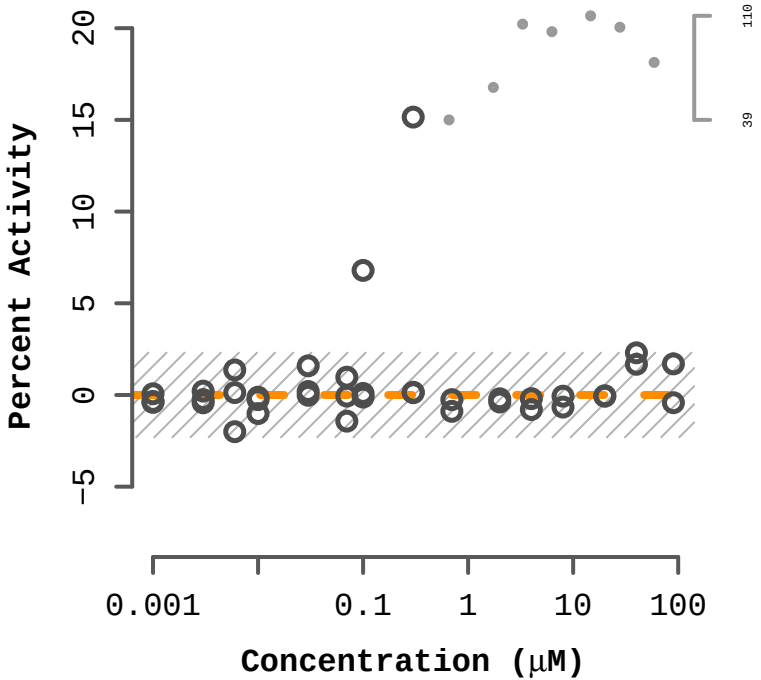
NAME: 2-Aminothiazole
CHID: 24508 CASRN: 96-50-4
SPID(S): Tox21_200726
M4ID: 12481526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.546 MAX_MED: 0.689 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

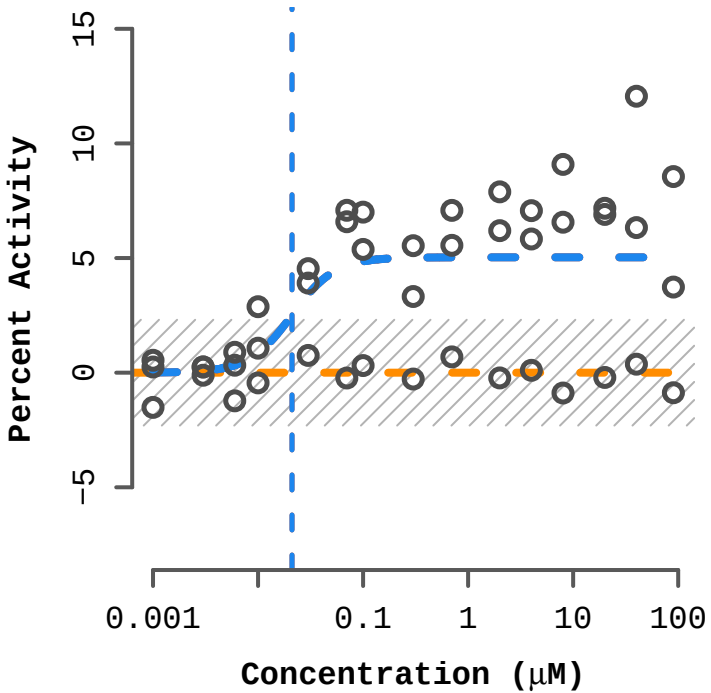
NAME: 2-Amino-4-thiazoleacetic acid
CHID: 24509 **CASRN:** 29676-71-9
SPID(S): Tox21_200900
M4ID: 12481352 **BRK**

HILL MODEL: Not applicable.

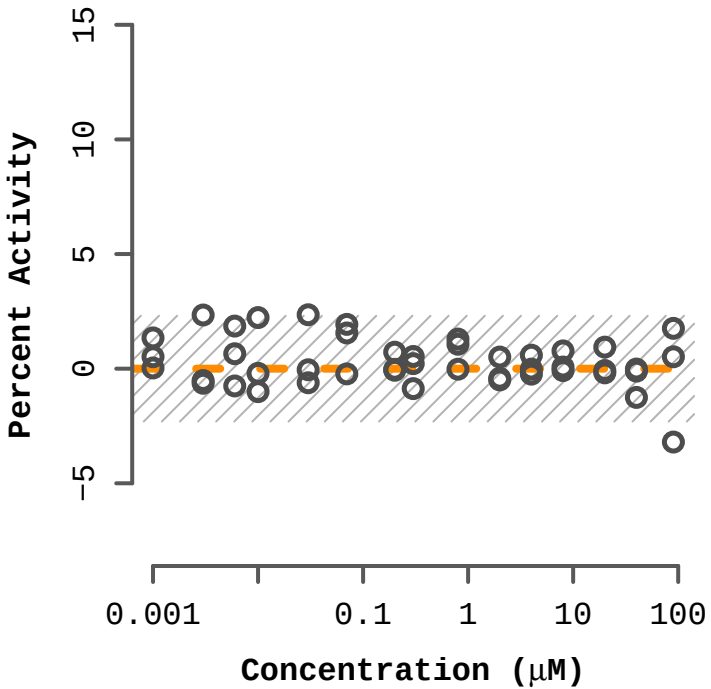
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	386.61	NA	NA
PROB:	1	NA	NA
RMSE:	33.75	NA	NA

MAX_MEAN: 35.2 **MAX_MED:** 2.3 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-(Trifluoromethyl)aniline
CHID:    24512   CASRN: 98-16-8
SPID(S): Tox21_303081
M4ID:    12476052

HILL MODEL (in red):
      tp       ga       gw
val:  5.03     -1.68    2.13
sd:   0.689    0.234    1.64

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.03     -1.68    2.13     3.65     6.71
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  273.02      237.29      241.29
PROB: 0           0.88        0.12
RMSE: 4.78        3.02        3.02

MAX_MEAN: 6.25      MAX_MED: 6.9       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

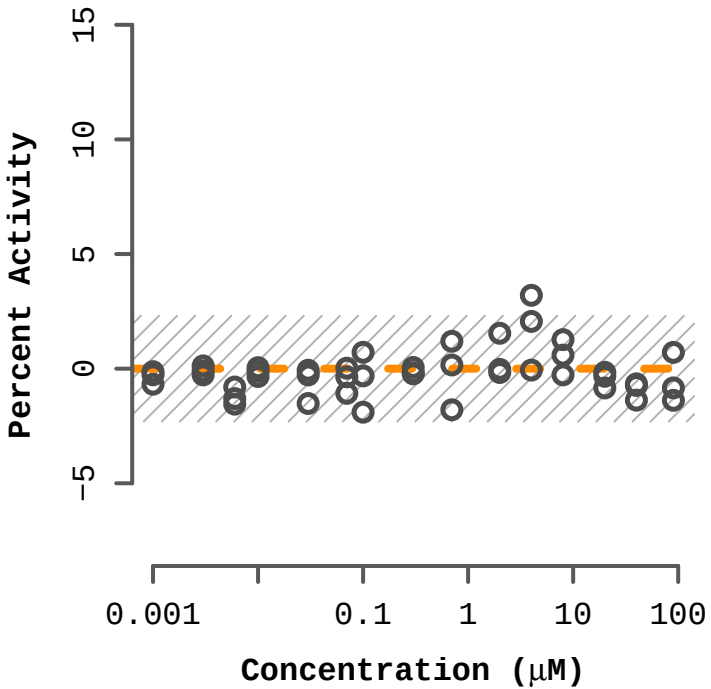
NAME: 3-(Trifluoromethyl)aniline
CHID: 24512 **CASRN:** 98-16-8
SPID(S): Tox21_201909
M4ID: 12480343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

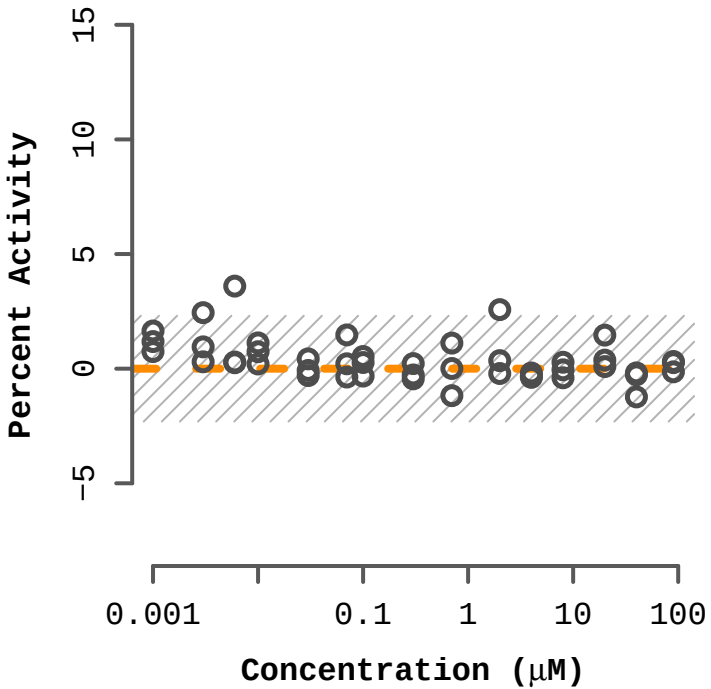
NAME: Ammonium perchlorate
CHID: 24515 **CASRN:** 7790-98-9
SPID(S): Tox21_303314
M4ID: 12475819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

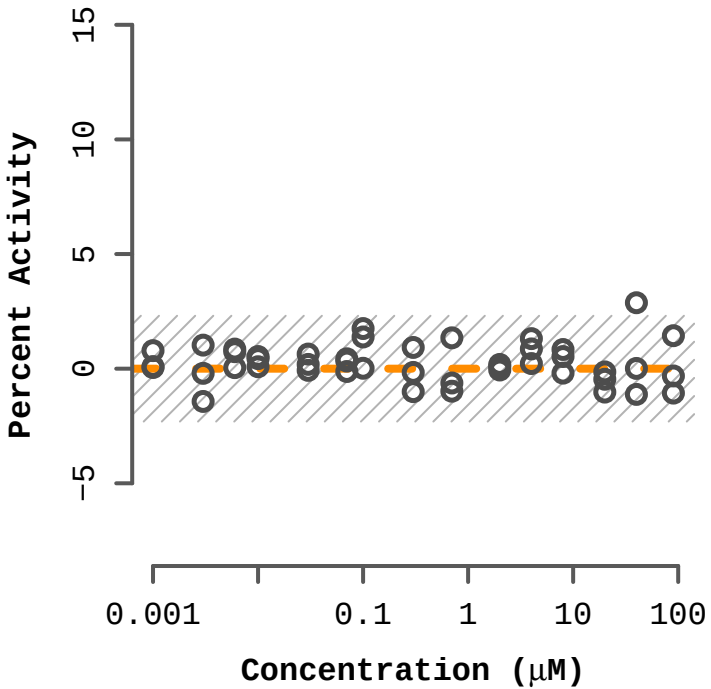
NAME: Ammonium perchlorate
CHID: 24515 **CASRN:** 7790-98-9
SPID(S): Tox21_202293
M4ID: 12479959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

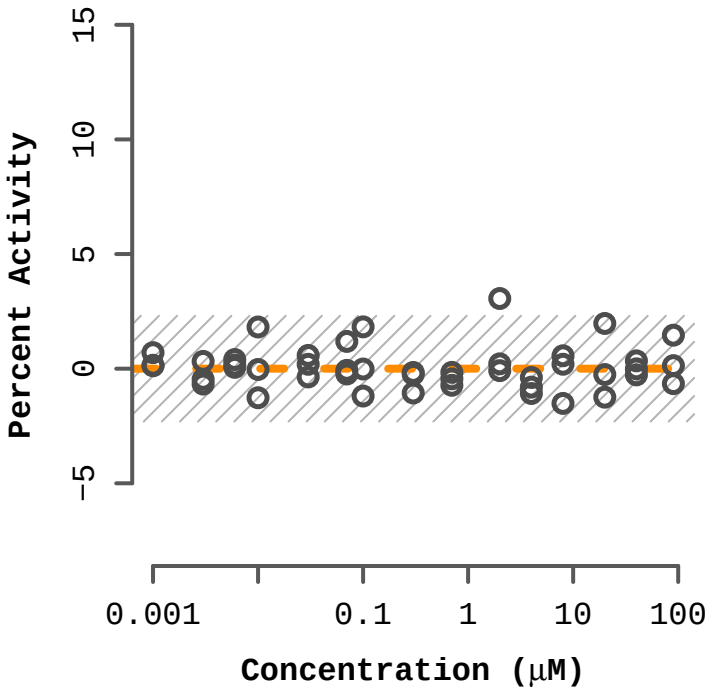
NAME: tert-Amyl methyl ether
CHID: 24521 **CASRN:** 994-05-8
SPID(S): Tox21_201154
M4ID: 12481098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

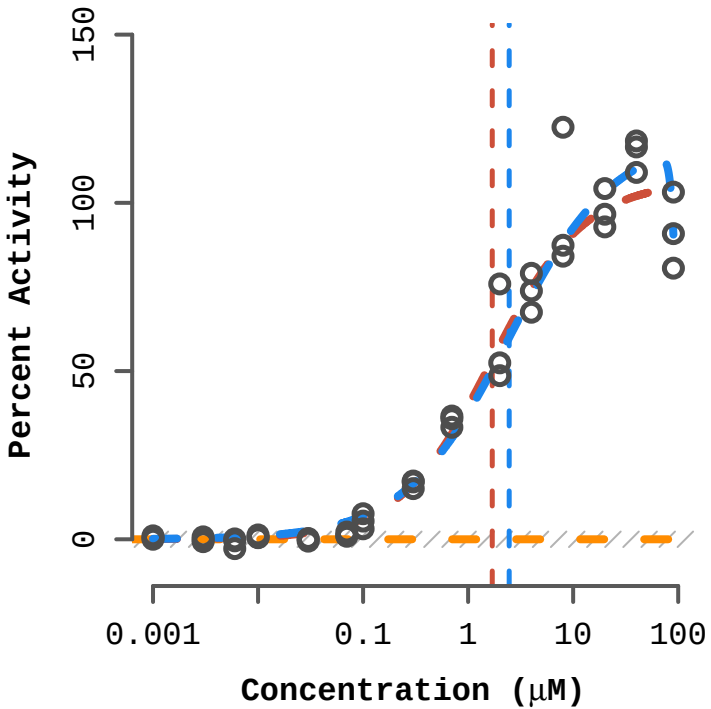
NAME: Pentyl nitrite
CHID: 24522 CASRN: 463-04-7
SPID(S): Tox21_202898
M4ID: 12479354

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.06 MAX_MED: 0.212 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Androstene-3,17-dione
CHID: 24523 CASRN: 63-05-8
SPID(S): Tox21_300579
M4ID: 12478554

HILL MODEL (in red):

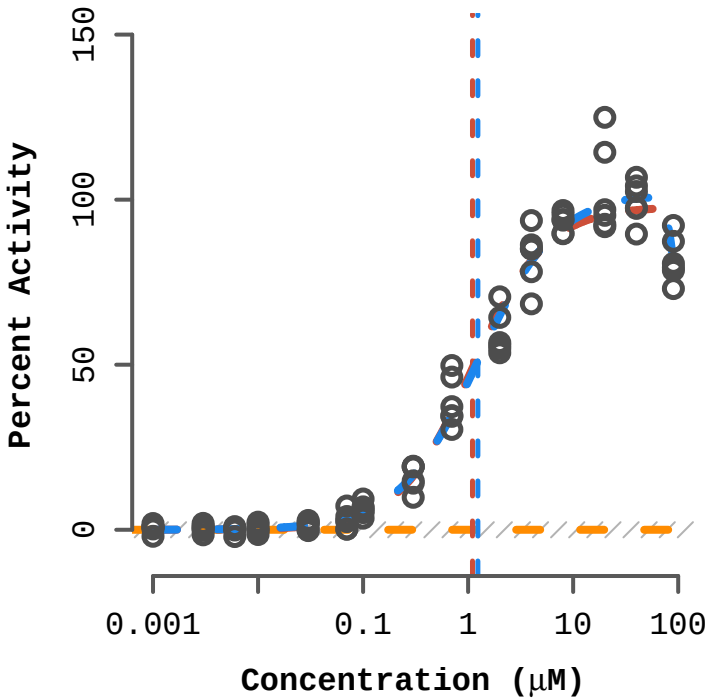
	tp	ga	gw
val:	107	0.23	0.986
sd:	4.02	0.0617	0.069

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	120	0.391	0.87	1.99	15.9
sd:	5.43	0.0703	0.0587	0.00715	3.33

	CNST	HILL	GNLS
AIC:	497.2	305.57	295.83
PROB:	0	0.01	0.99
RMSE:	58.74	8.46	7.4

MAX_MEAN: 115 MAX_MED: 117 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Androstene-3,17-dione
CHID: 24523 CASRN: 63-05-8
SPID(S): Tox21_202269
M4ID: 12479983

HILL MODEL (in red):

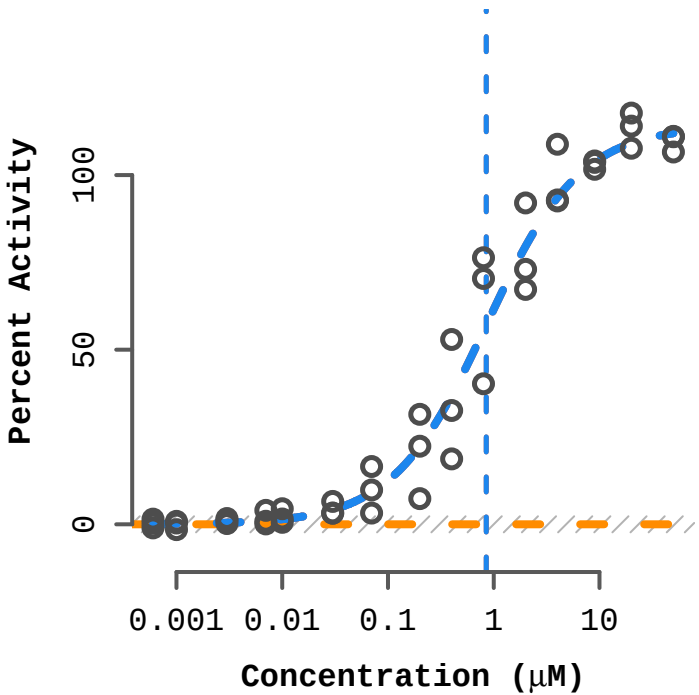
	tp	ga	gw
val:	97.9	0.0416	1.24
sd:	1.76	0.0315	0.0716

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	102	0.0927	1.16	2.03	7.93
sd:	1.88	0.0318	0.0598	0.0102	1.16

	CNST	HILL	GNLS
AIC:	988.39	589.62	552.53
PROB:	0	0	1
RMSE:	56.85	7.24	5.67

MAX_MEAN: 103 MAX_MED: 100 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Androstene-3,17-dione
CHID: 24523 CASRN: 63-05-8
SPID(S): Tox21_110893_1
M4ID: 12484034

HILL MODEL (in red):

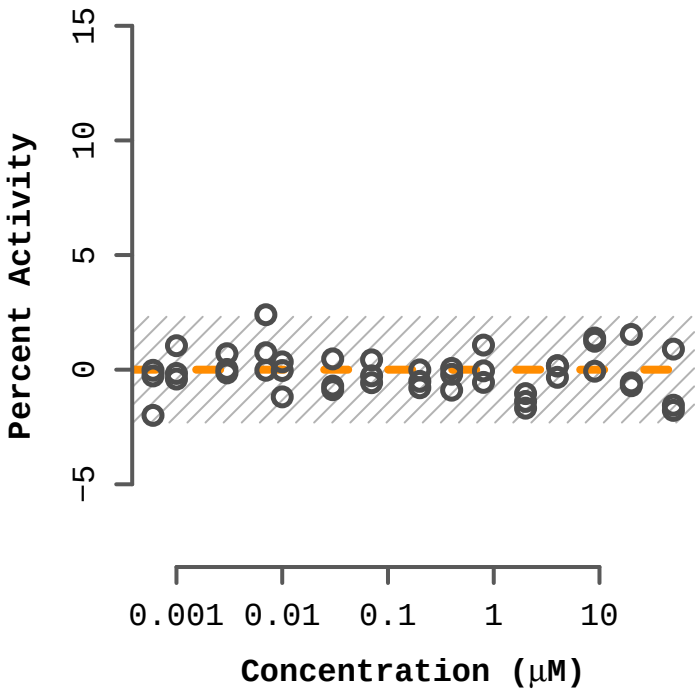
	tp	ga	gw
val:	114	-0.0707	0.979
sd:	3.16	0.0837	0.0892

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	114	-0.0707	0.979	3.09	11.4
sd:	3.16	0.0837	0.0892	214000	822000

	CNST	HILL	GNLS
AIC:	502.55	313.06	317.06
PROB:	0	0.88	0.12
RMSE:	61.9	7.68	7.68

MAX_MEAN: 113 MAX_MED: 114 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

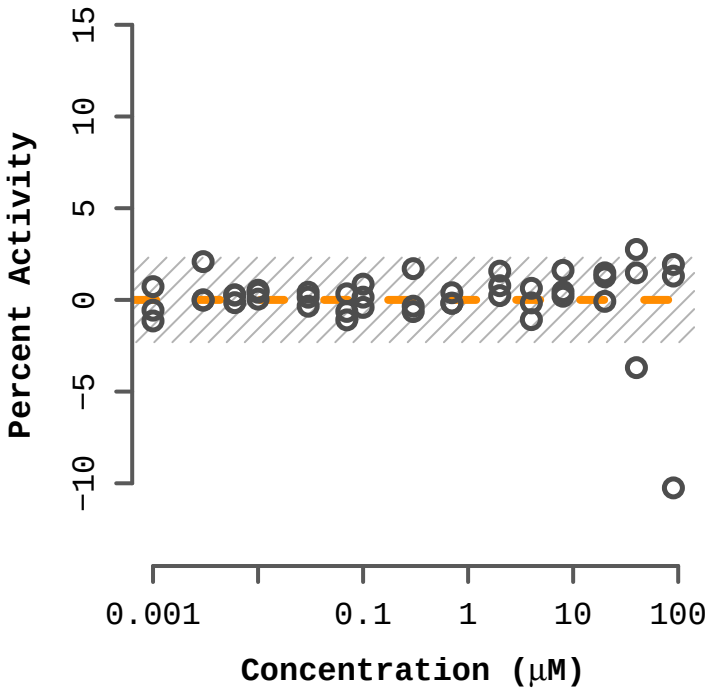
NAME: Anise oil
CHID: 24528 **CASRN:** 8007-70-3
SPID(S): Tox21_302845
M4ID: 12476288

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

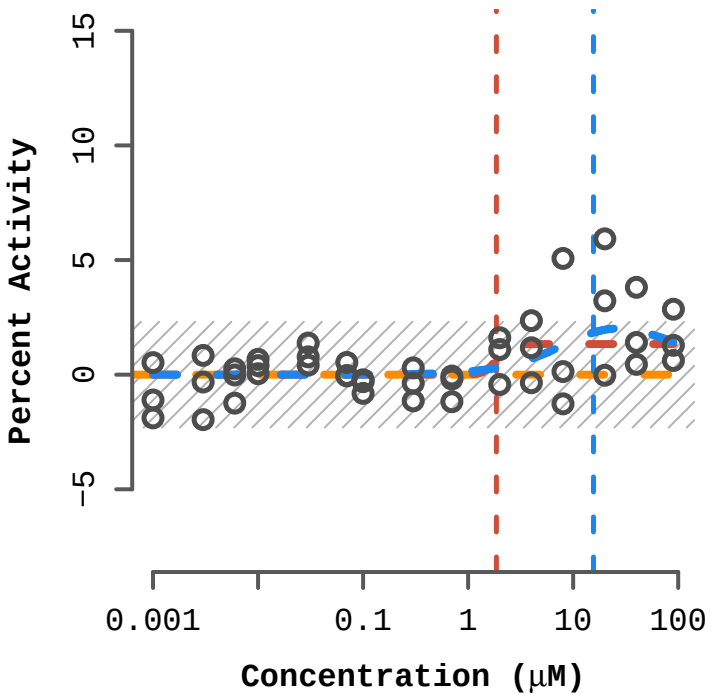
NAME: Anise oil
CHID: 24528 CASRN: 8007-70-3
SPID(S): Tox21_201615
M4ID: 12480637

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 0.886 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methoxyaniline
CHID: 24529 **CASRN:** 536-90-3
SPID(S): Tox21_200820
M4ID: 12481432

HILL MODEL (in red):

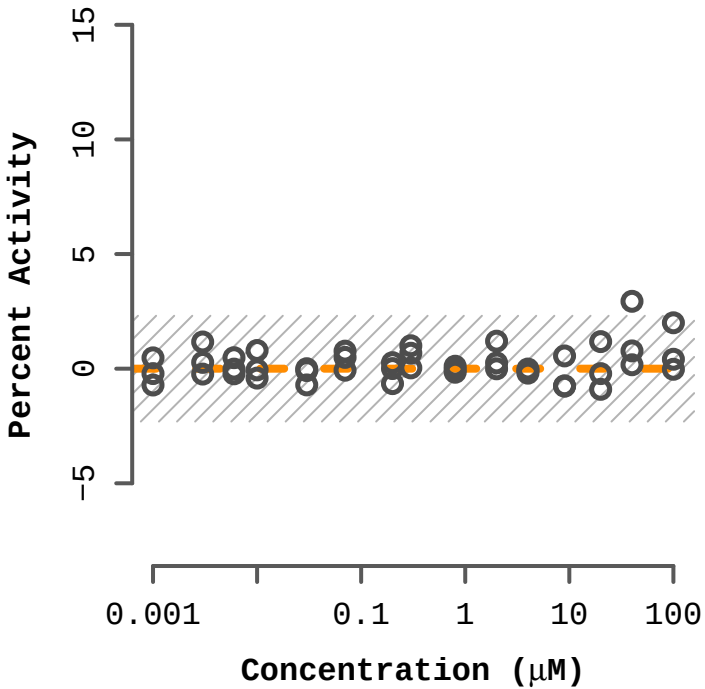
	tp	ga	gw
val:	1.33	0.269	7.73
sd:	0.403	0.22	52.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.89	1.19	1.34	1.44	0.874
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	166.23	158.28	162.3
PROB:	0.02	0.87	0.12
RMSE:	1.7	1.36	1.32

MAX_MEAN: 3.04 **MAX_MED:** 3.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

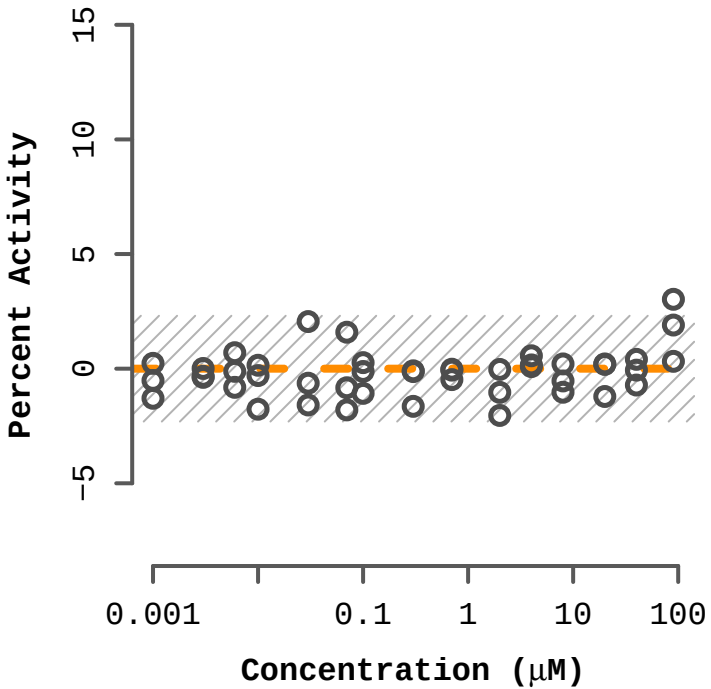
NAME: 4-Methoxyaniline
CHID: 24532 CASRN: 104-94-9
SPID(S): Tox21_303039
M4ID: 12476094

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.3 MAX_MED: 0.777 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

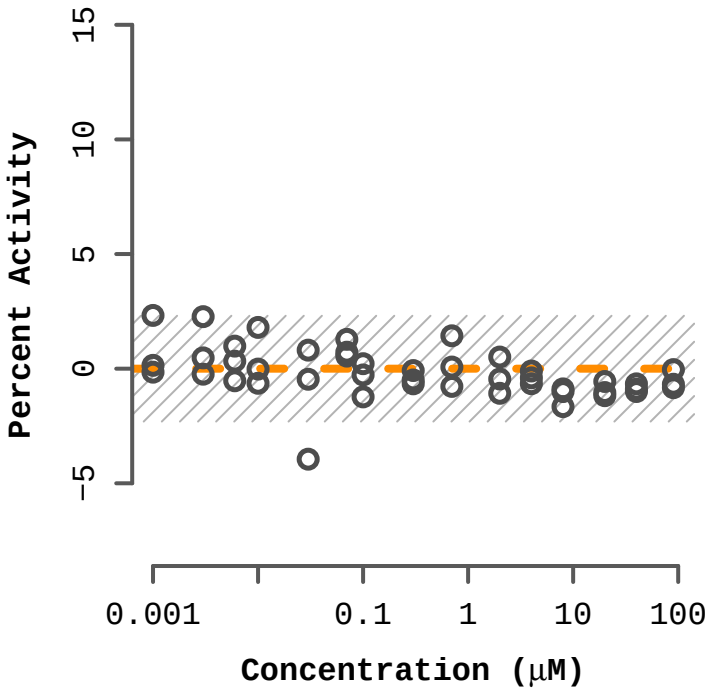
NAME: 4-Methoxyaniline
CHID: 24532 **CASRN:** 104-94-9
SPID(S): Tox21_202437
M4ID: 12479815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

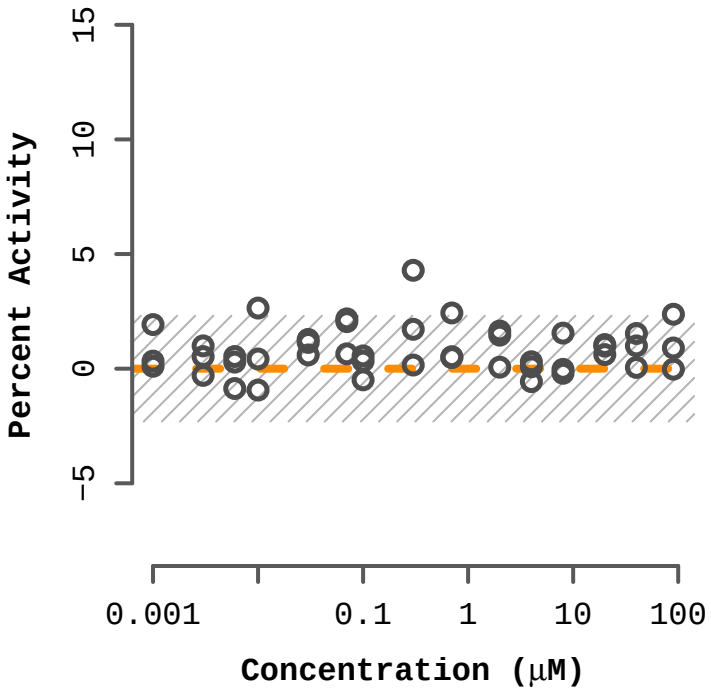
NAME: Annatto
CHID: 24534 **CASRN:** 1393-63-1
SPID(S): Tox21_202485
M4ID: 12479767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 0.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

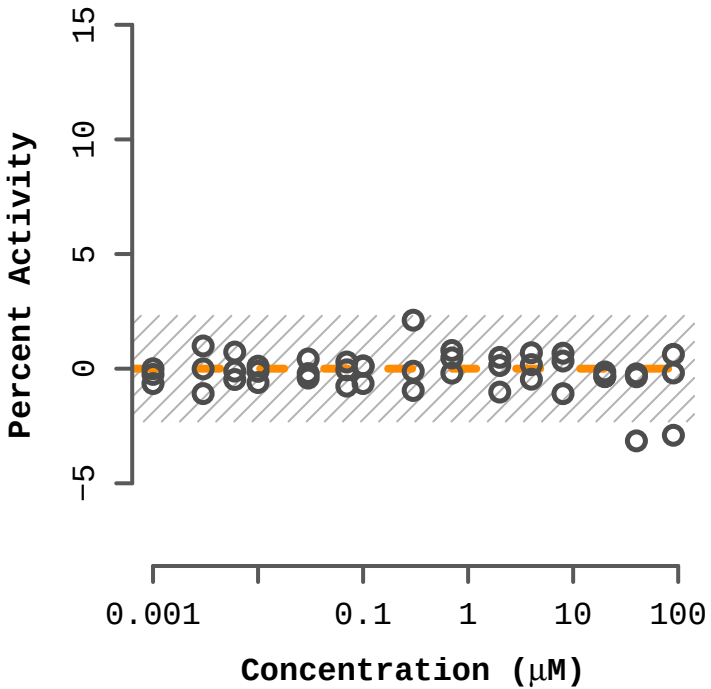
NAME: Anthralin
CHID: 24538 **CASRN:** 1143-38-0
SPID(S): Tox21_300290
M4ID: 12478840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

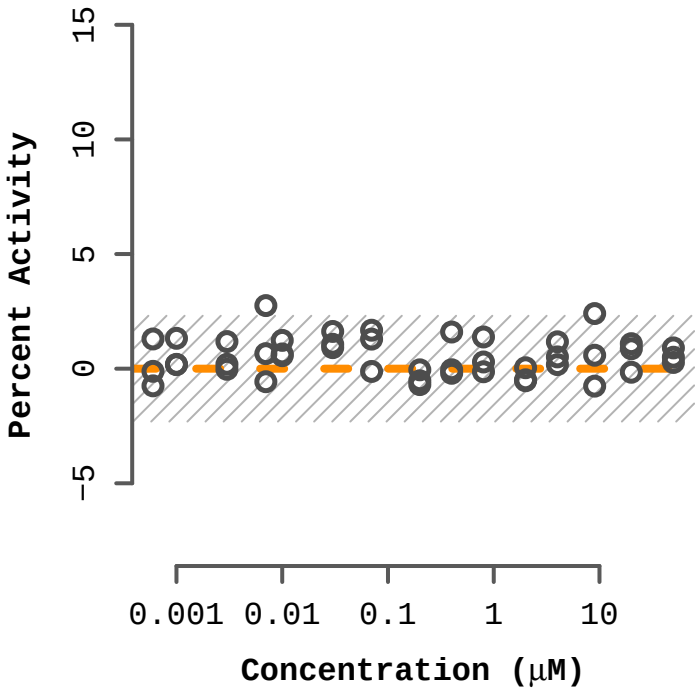
NAME: Anthralin
CHID: 24538 **CASRN:** 1143-38-0
SPID(S): Tox21_201851
M4ID: 12480401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.357 **MAX_MED:** 0.469 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

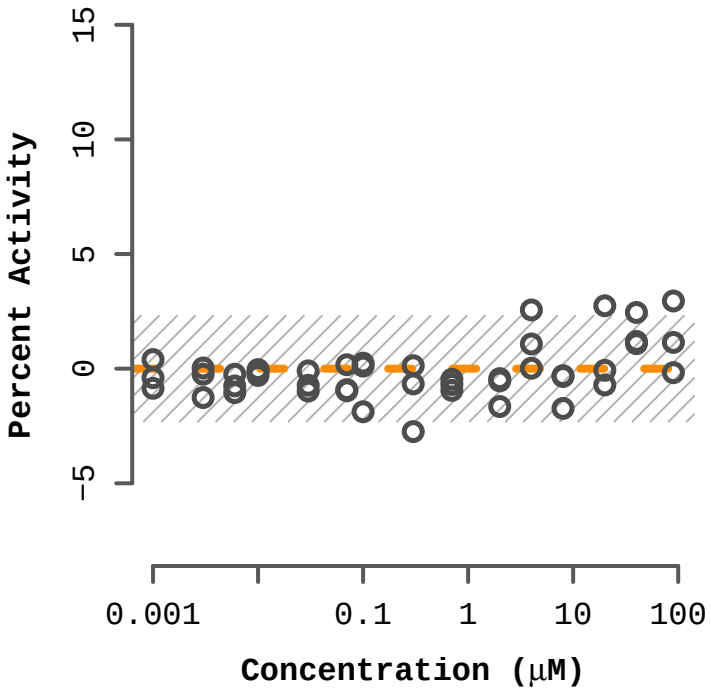
NAME: Anthralin
CHID: 24538 **CASRN:** 1143-38-0
SPID(S): Tox21_111115_1
M4ID: 12483898

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

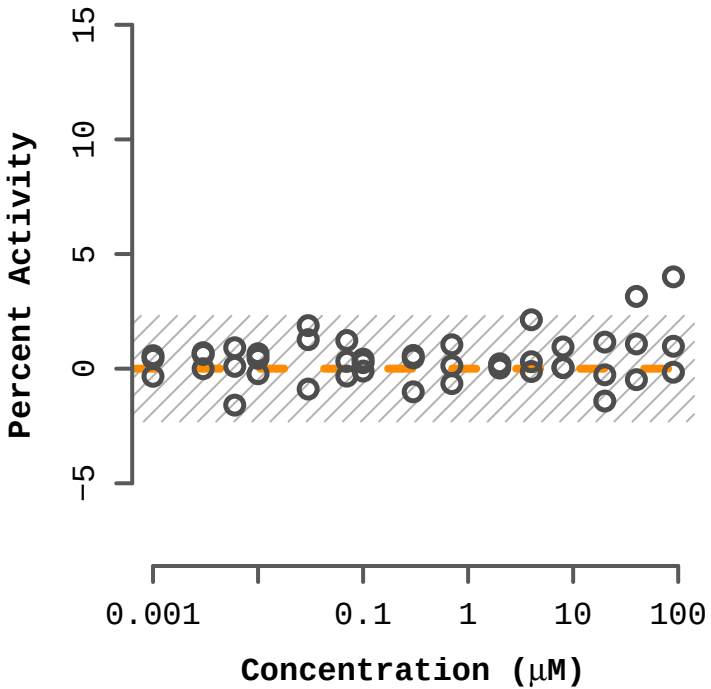
NAME: Azodicarbonamide
CHID: 24553 **CASRN:** 123-77-3
SPID(S): Tox21_303264
M4ID: 12475869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

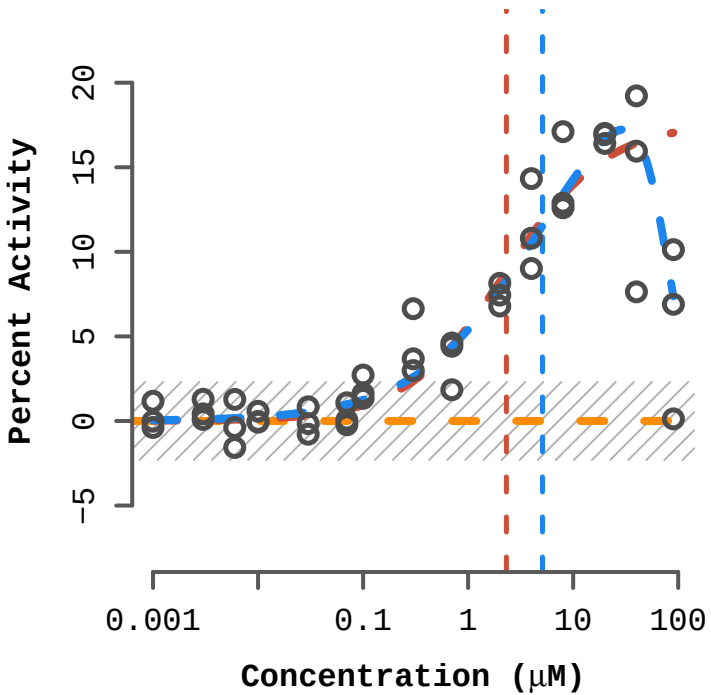
NAME: Azodicarbonamide
CHID: 24553 **CASRN:** 123-77-3
SPID(S): Tox21_201849
M4ID: 12480403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Azoxyanisole
CHID: 24554 CASRN: 1562-94-3
SPID(S): Tox21_201162
M4ID: 12481090

HILL MODEL (in red):

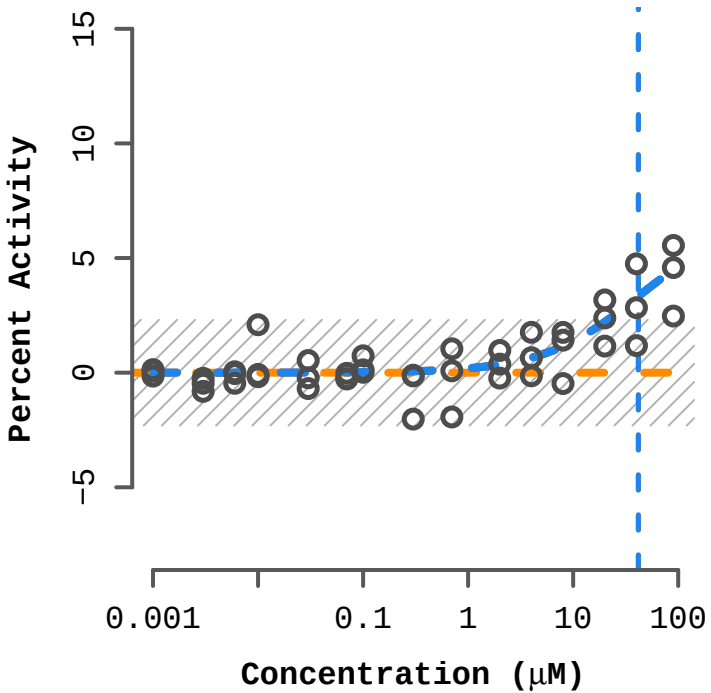
	tp	ga	gw
val:	17.6	0.364	0.914
sd:	1.72	0.131	0.158

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.1	0.708	0.728	1.88	3.26
sd:	3.79	0.224	0.103	0.0495	1.13

	CNST	HILL	GNLS
AIC:	316.99	218.47	189.23
PROB:	0	0	1
RMSE:	8.16	3.66	2.22

MAX_MEAN: 16.8 MAX_MED: 16.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Azoxybenzene
CHID: 24555 CASRN: 495-48-7
SPID(S): Tox21_201167
M4ID: 12481085

HILL MODEL (in red):

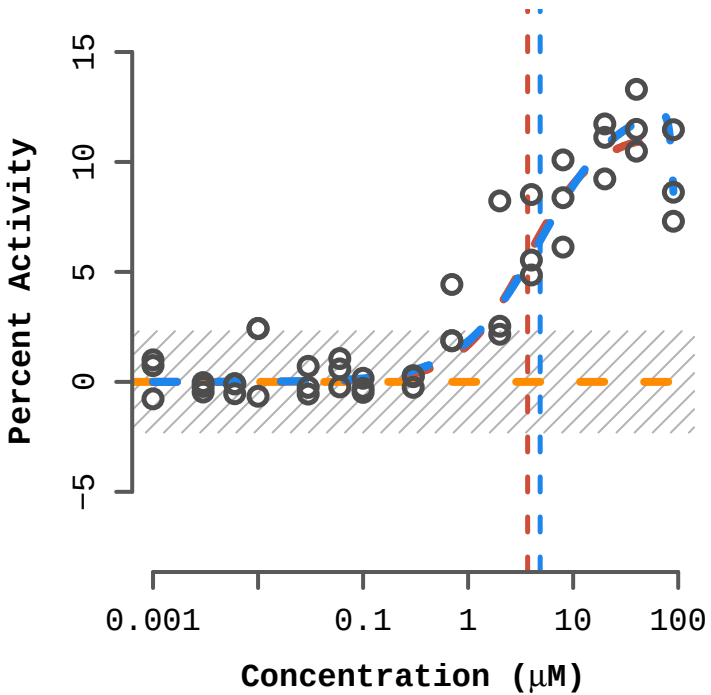
	tp	ga	gw
val:	6.66	1.62	0.946
sd:	3.78	0.584	0.366

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.66	1.62	0.946	3.18	14
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	168.23	122.73	126.73
PROB:	0	0.88	0.12
RMSE:	1.72	0.9	0.9

MAX_MEAN: 4.2 MAX_MED: 4.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Basic Oange 2
CHID: 24559 CASRN: 532-82-1
SPID(S): Tox21_202486
M4ID: 12479766

HILL MODEL (in red):

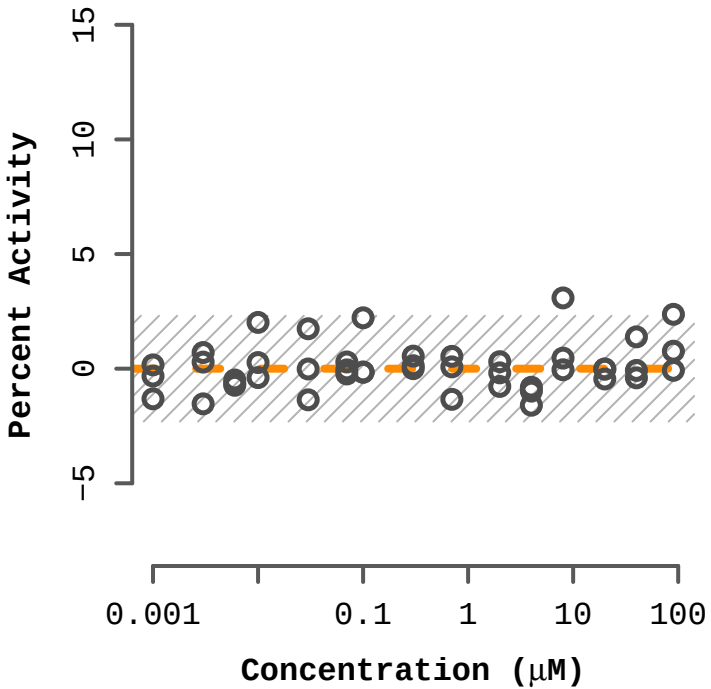
	tp	ga	gw
val:	11.4	0.567	1.34
sd:	0.707	0.0857	0.304

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.9	0.686	1.13	1.97	17.8
sd:	1.39	0.125	0.252	0.00859	8.6

	CNST	HILL	GNLS
AIC:	285.69	168	164.54
PROB:	0	0.15	0.85
RMSE:	5.74	1.52	1.4

MAX_MEAN: 11.8 MAX_MED: 11.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

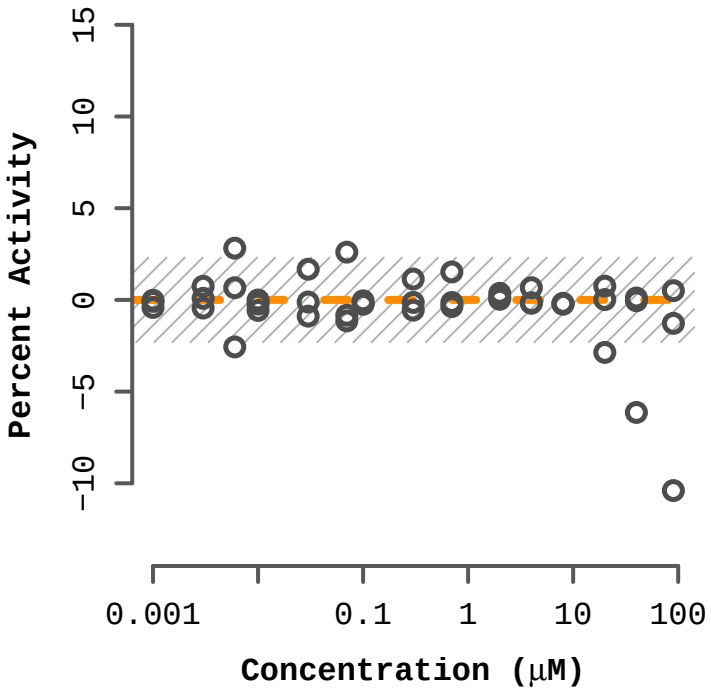
NAME: Benzenesulfonic acid
CHID: 24568 **CASRN:** 98-11-3
SPID(S): Tox21_303131
M4ID: 12476002

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.763 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

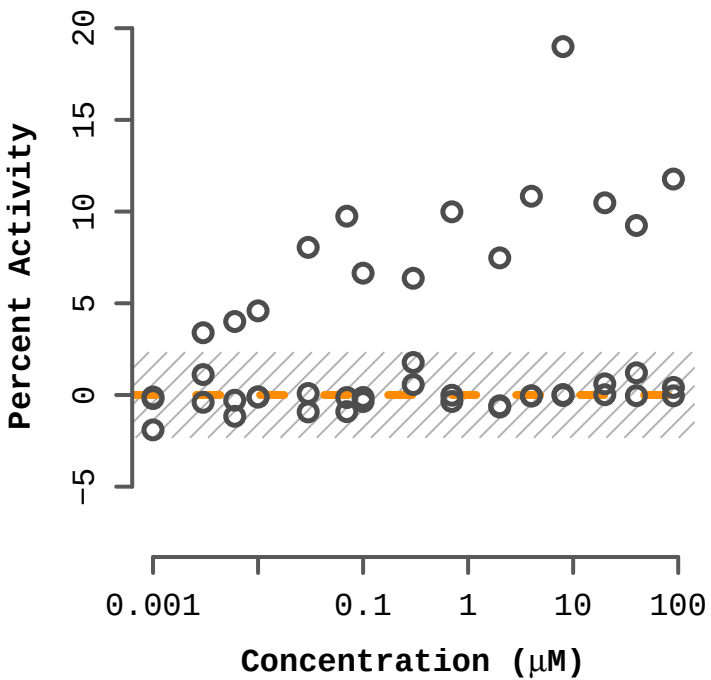
NAME: Benzenesulfonic acid
CHID: 24568 **CASRN:** 98-11-3
SPID(S): Tox21_201960
M4ID: 12480292

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.11	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 0.342 **MAX_MED:** 0.664 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

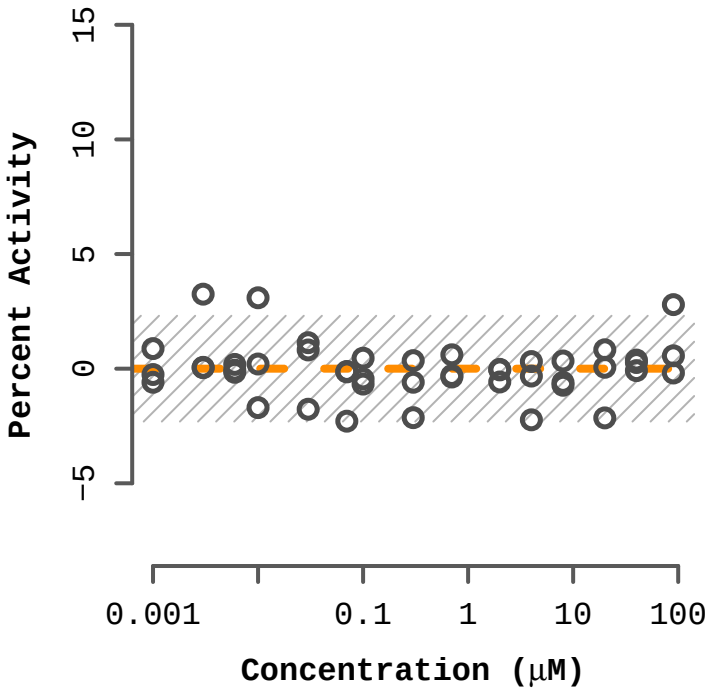
NAME: Benzimidazole
CHID: 24573 CASRN: 51-17-2
SPID(S): Tox21_303321
M4ID: 12475812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.6	NA	NA
PROB:	1	NA	NA
RMSE:	5.32	NA	NA

MAX_MEAN: 6.33 MAX_MED: 1.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

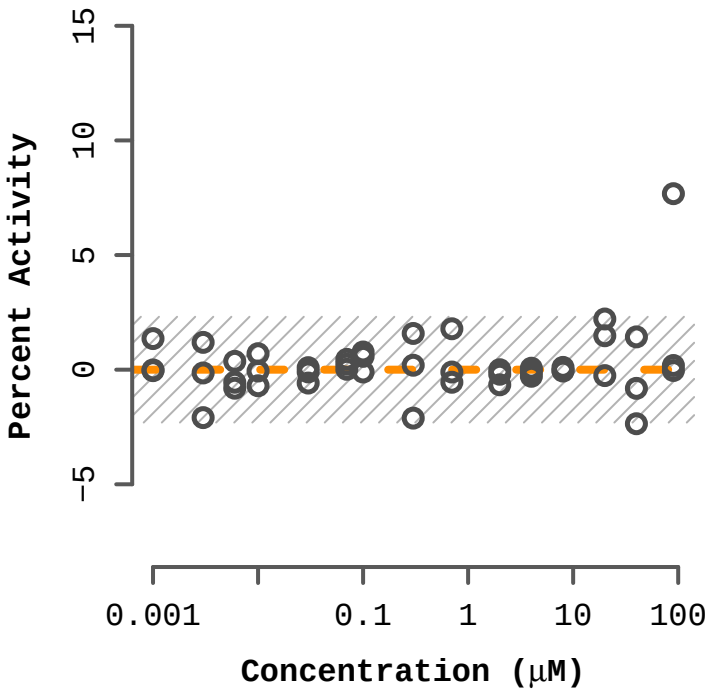
NAME: Benzimidazole
CHID: 24573 **CASRN:** 51-17-2
SPID(S): Tox21_202107
M4ID: 12480145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

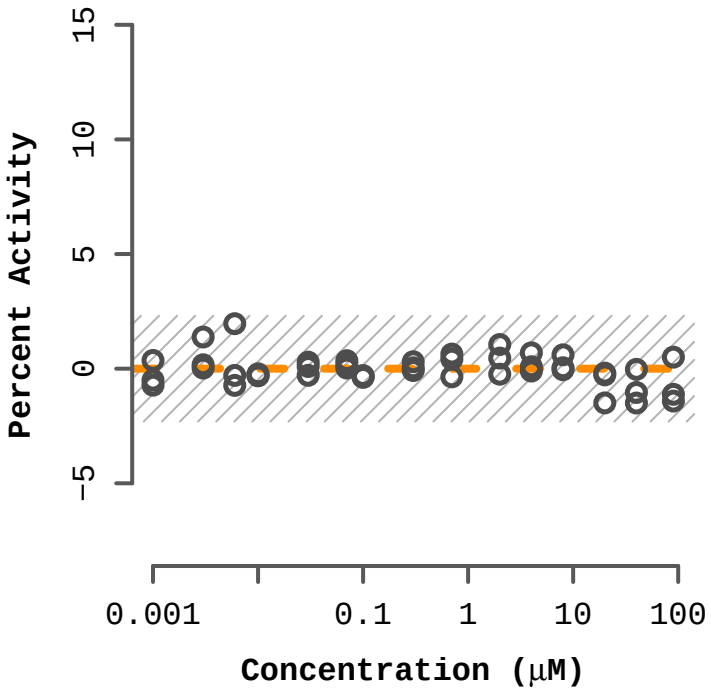
NAME: 2-Benzimidazolylurea
CHID: 24574 CASRN: 24370-25-0
SPID(S): Tox21_200170
M4ID: 12482082

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.61 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

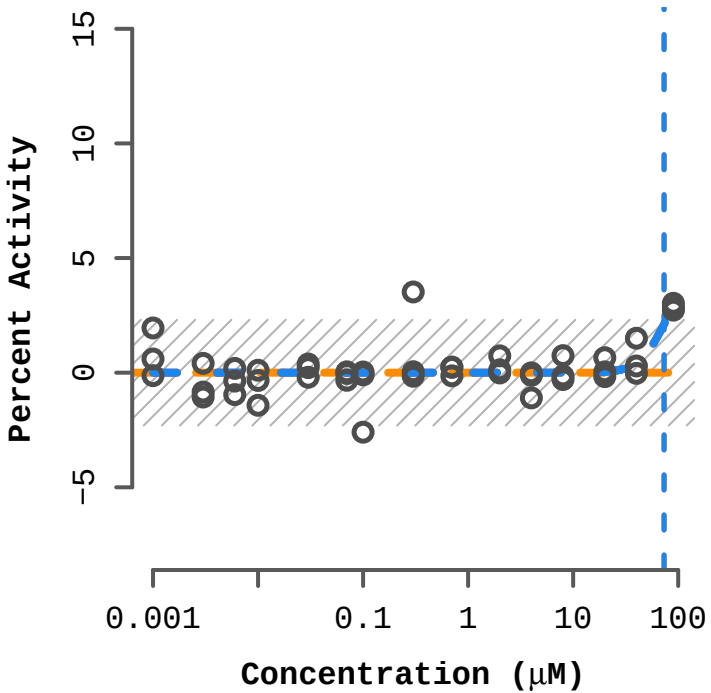
NAME: Benzoin acetate
CHID: 24580 **CASRN:** 574-06-1
SPID(S): Tox21_201080
M4ID: 12481172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.527 **MAX_MED:** 0.463 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzo(f)quinoline
CHID: 24585 CASRN: 85-02-9
SPID(S): Tox21_303188
M4ID: 12475945

HILL MODEL (in red):

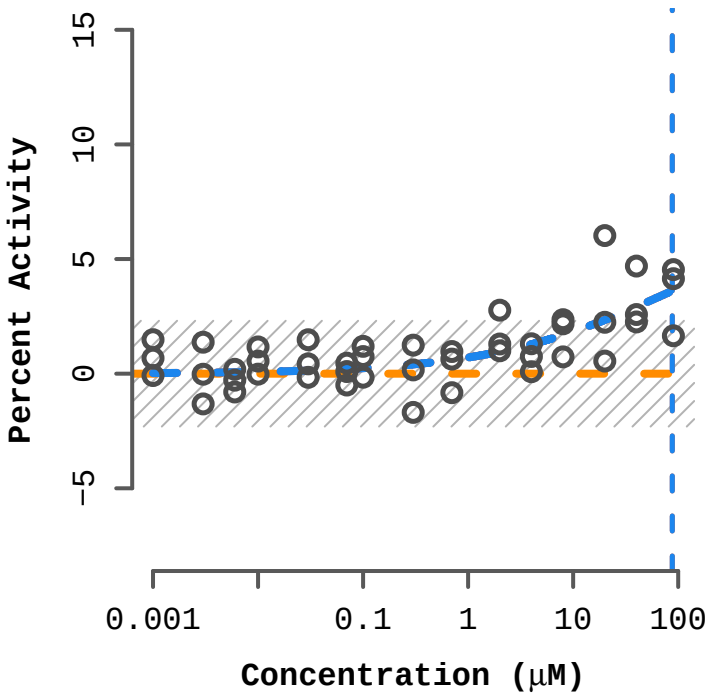
	tp	ga	gw
val:	4.23	1.87	3.61
sd:	7.8	0.572	4.87

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.23	1.87	3.61	3.48	4.03
sd:	8.11	0.594	5.04	1020	2710

	CNST	HILL	GNLS
AIC:	128.36	102.04	106.04
PROB:	0	0.88	0.12
RMSE:	1.14	0.86	0.86

MAX_MEAN: 2.86 MAX_MED: 2.84 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzo(f)quinoline
CHID: 24585 CASRN: 85-02-9
SPID(S): Tox21_201772
M4ID: 12480480

HILL MODEL (in red):

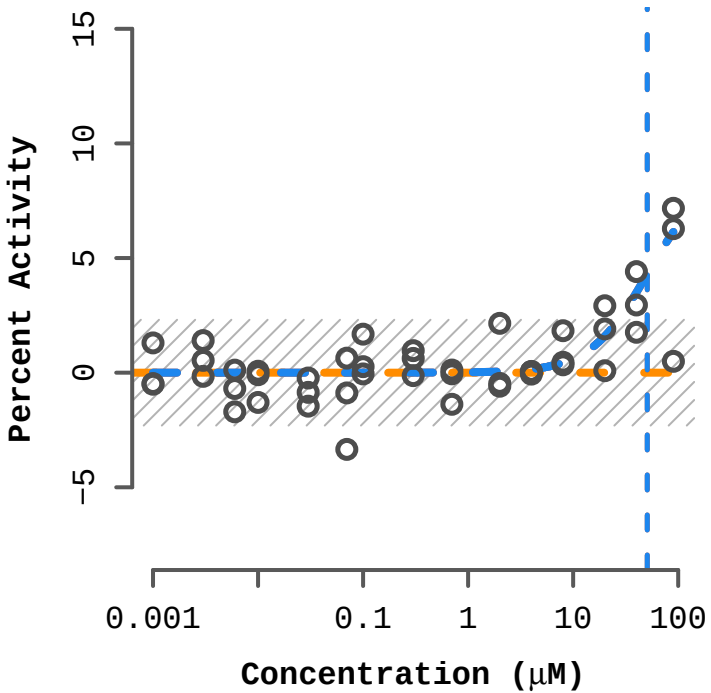
	tp	ga	gw
val:	7.23	1.94	0.497
sd:	5.48	1.23	0.184

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.23	1.94	0.497	3.88	15.5
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	181.08	139.73	143.73
PROB:	0	0.88	0.12
RMSE:	1.88	1.07	1.07

MAX_MEAN: 3.45 **MAX_MED:** 4.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzothiazole
CHID: 24586 CASRN: 95-16-9
SPID(S): Tox21_303232
M4ID: 12475901

HILL MODEL (in red):

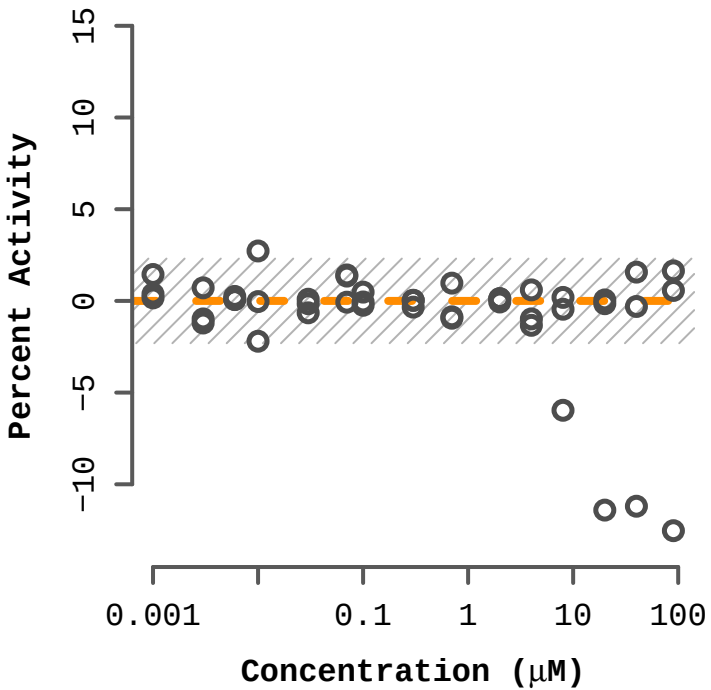
	tp	ga	gw
val:	8.61	1.71	1.59
sd:	2.85	0.214	0.521

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.61	1.71	1.59	3.95	3.68
sd:	2.85	0.214	0.521	806	1500

	CNST	HILL	GNLS
AIC:	176.15	149.57	153.57
PROB:	0	0.88	0.12
RMSE:	1.97	1.33	1.33

MAX_MEAN: 4.65 MAX_MED: 6.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

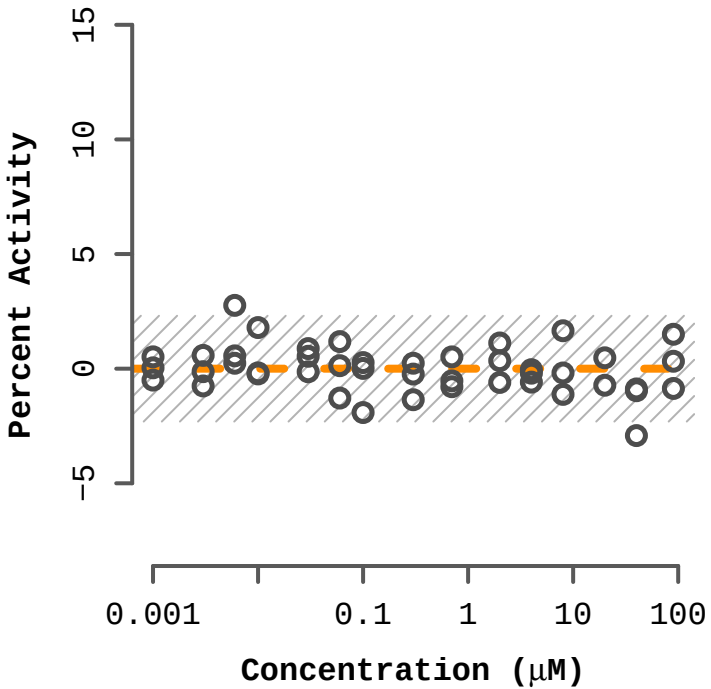
NAME: Benzothiazole
CHID: 24586 **CASRN:** 95-16-9
SPID(S): Tox21_201853
M4ID: 12480399

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.04	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

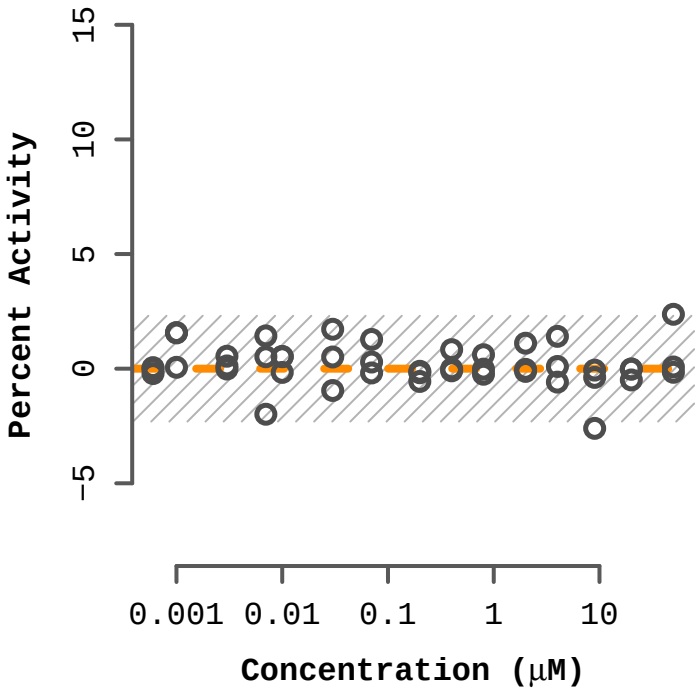
NAME: Benzotrifluoride
CHID: 24589 **CASRN:** 98-08-8
SPID(S): Tox21_200954
M4ID: 12481298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.61	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

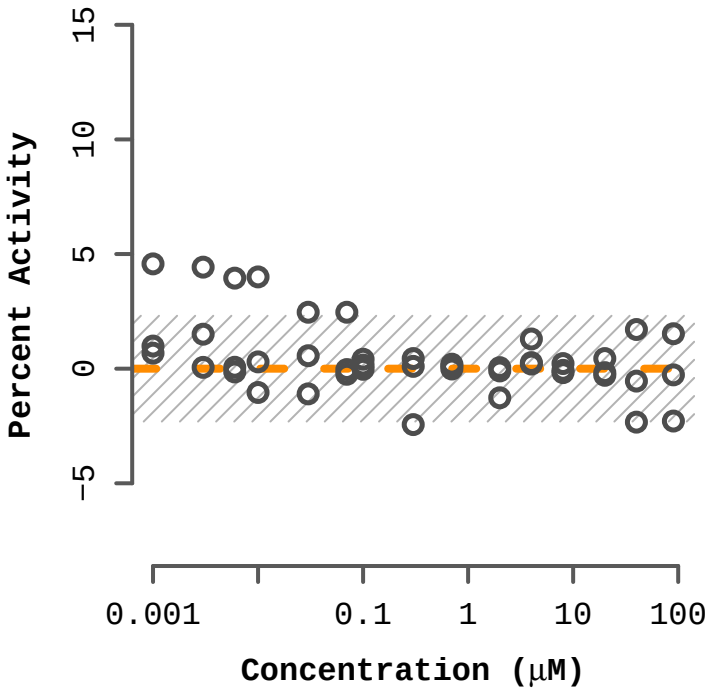
NAME: Benzoyl peroxide
CHID: 24591 **CASRN:** 94-36-0
SPID(S): Tox21_111619_1
M4ID: 12483581

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

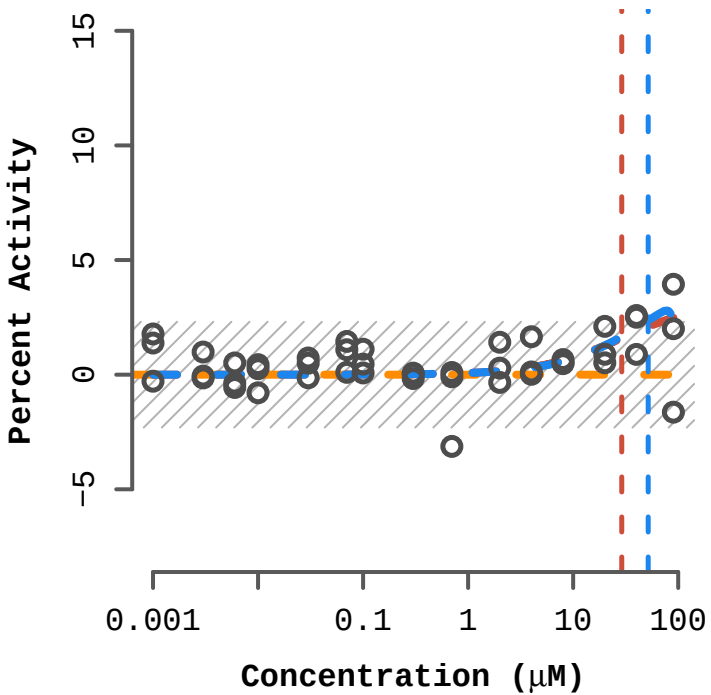
NAME: Benzyl phenylacetate
CHID: 24597 CASRN: 102-16-9
SPID(S): Tox21_200685
M4ID: 12481567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzyl salicylate
CHID: 24598 **CASRN:** 118-58-1
SPID(S): Tox21_303046
M4ID: 12476087

HILL MODEL (in red):

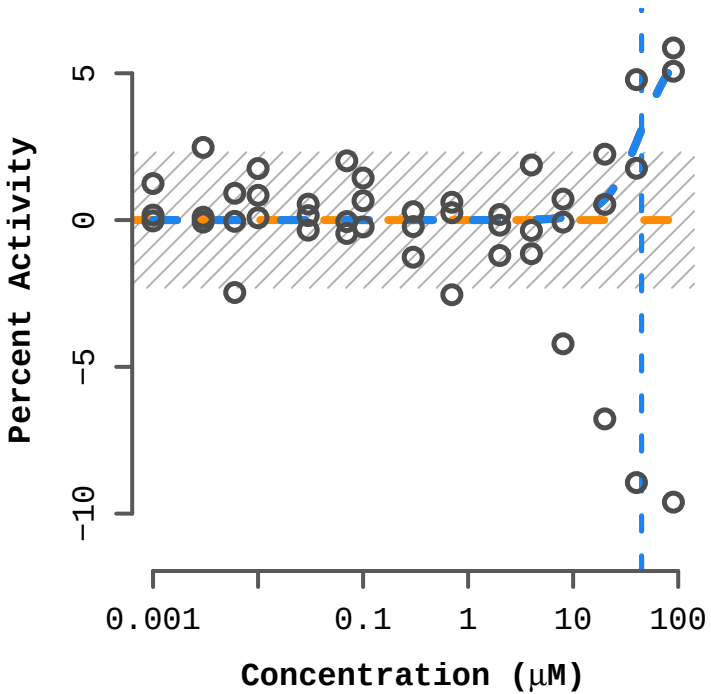
	tp	ga	gw
val:	3.19	1.46	1.11
sd:	2.72	0.787	0.986

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	1.71	1.05	1.98	18
sd:	7.04	1.07	0.651	0.0398	37.7

	CNST	HILL	GNLS
AIC:	145.44	128.4	132
PROB:	0	0.86	0.14
RMSE:	1.25	1.05	1.04

MAX_MEAN: 1.99 **MAX_MED:** 2.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzyl salicylate
CHID: 24598 CASRN: 118-58-1
SPID(S): Tox21_201869
M4ID: 12480383

HILL MODEL (in red):

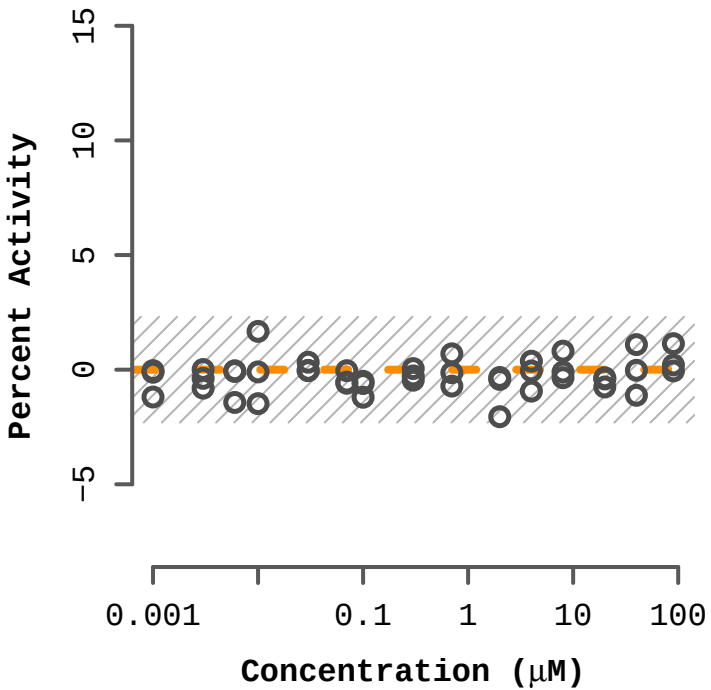
	tp	ga	gw
val:	6.17	1.65	2.51
sd:	3.19	0.305	2.24

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.17	1.65	2.51	3.47	3.86
sd:	3.19	0.305	2.24	1150	3020

	CNST	HILL	GNLS
AIC:	208.6	199.24	203.24
PROB:	0.01	0.87	0.12
RMSE:	2.86	3.26	3.26

MAX_MEAN: 0.894 MAX_MED: 5.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

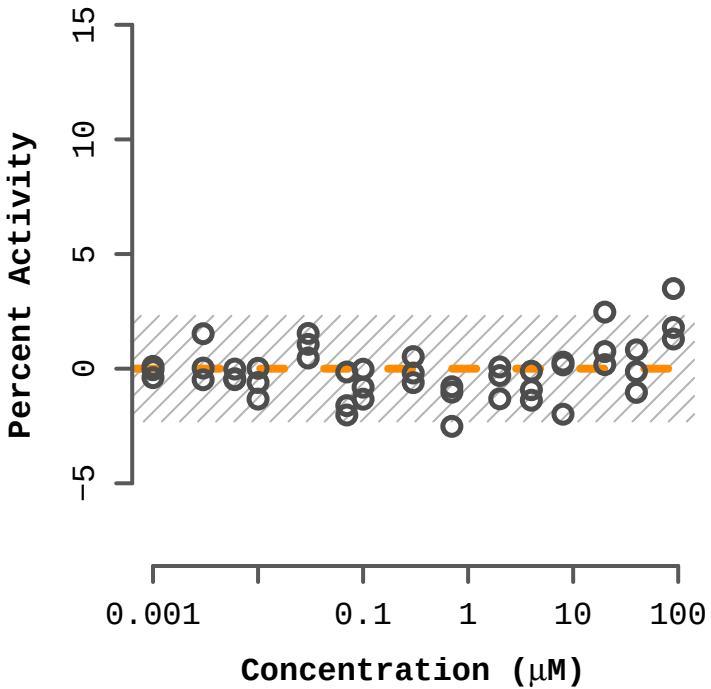
NAME: Benzyl sulfide
CHID: 24599 **CASRN:** 538-74-9
SPID(S): Tox21_200326
M4ID: 12481926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.43 **MAX_MED:** 0.206 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

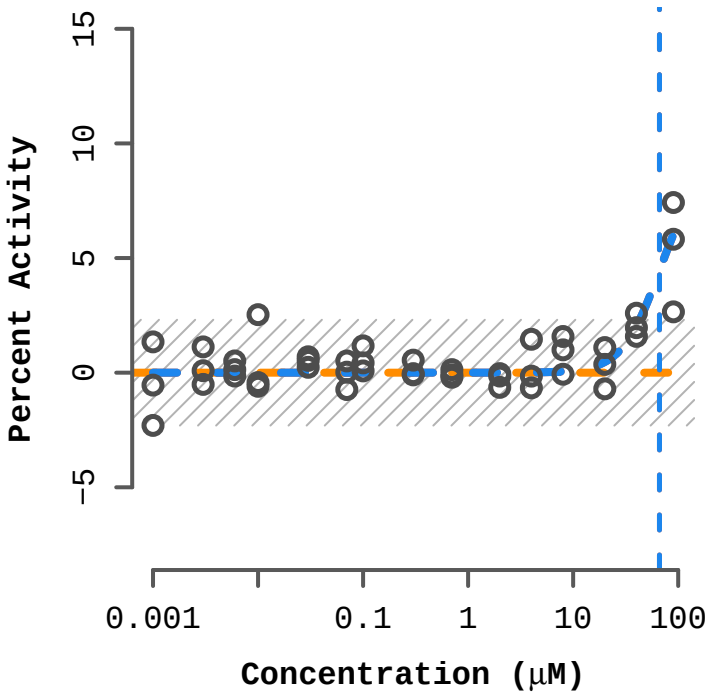
NAME: Benzyltrimethylammonium chloride
CHID: 24600 **CASRN:** 56-93-9
SPID(S): Tox21_303260
M4ID: 12475873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.2 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzyltrimethylammonium chloride
CHID: 24600 CASRN: 56-93-9
SPID(S): Tox21_201587
M4ID: 12480665

HILL MODEL (in red):

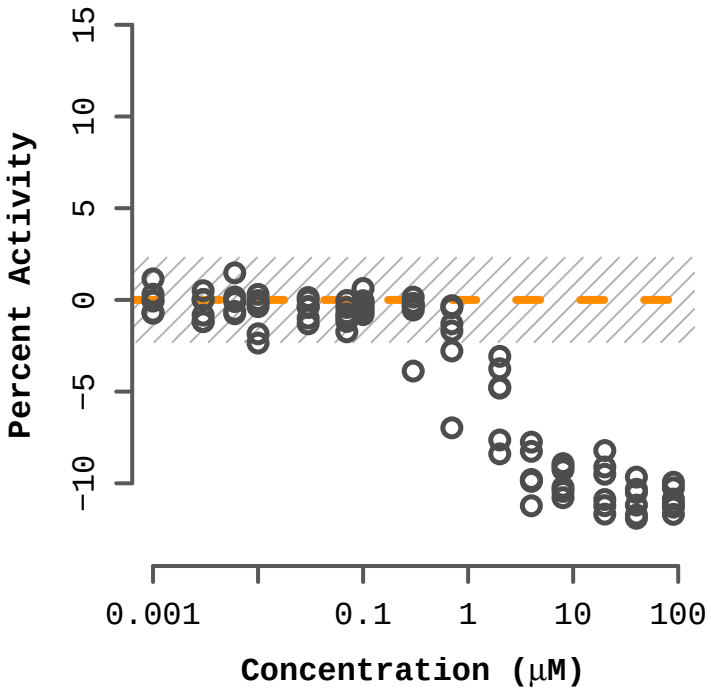
	tp	ga	gw
val:	8.91	1.82	2.41
sd:	9.45	0.462	2.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.91	1.82	2.41	3.73	4.03
sd:	9.45	0.462	2.25	2510	5700

	CNST	HILL	GNLS
AIC:	157.35	124.2	128.2
PROB:	0	0.88	0.12
RMSE:	1.75	0.96	0.96

MAX_MEAN: 5.3 **MAX_MED:** 5.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

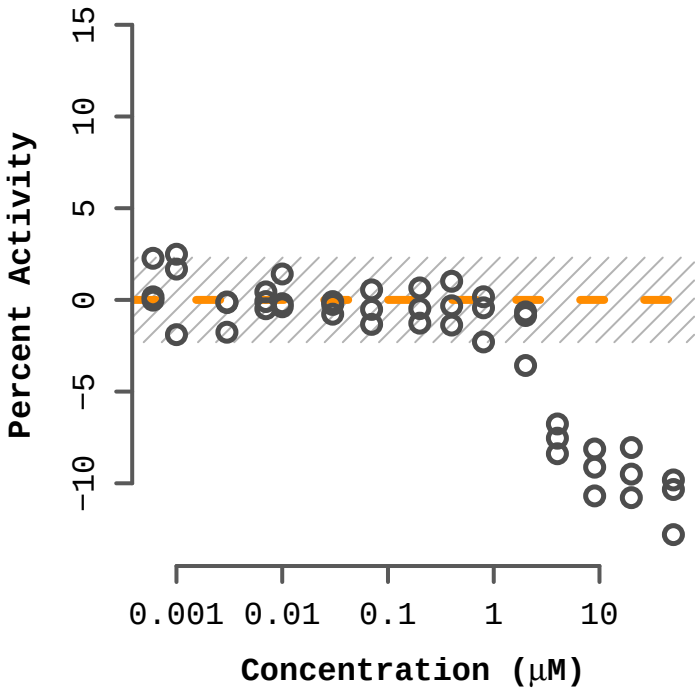
NAME: Berberine chloride
CHID: 24602 **CASRN:** 633-65-8
SPID(S): Tox21_200348
M4ID: 12481904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	588.3	NA	NA
PROB:	1	NA	NA
RMSE:	6.21	NA	NA

MAX_MEAN: 0.0337 **MAX_MED:** −0.0287 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

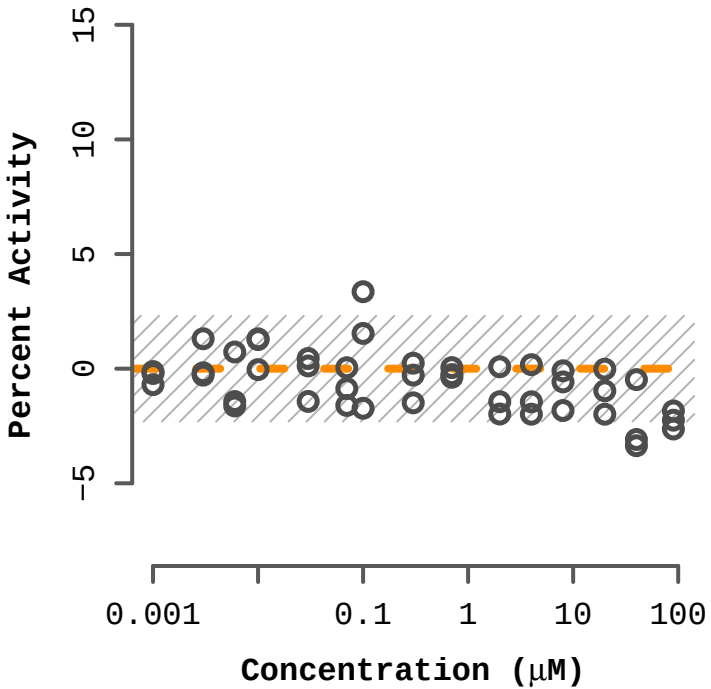
NAME: Berberine chloride
CHID: 24602 **CASRN:** 633-65-8
SPID(S): Tox21_110474_1
M4ID: 12484328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	268.7	NA	NA
PROB:	1	NA	NA
RMSE:	5	NA	NA

MAX_MEAN: 0.809 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

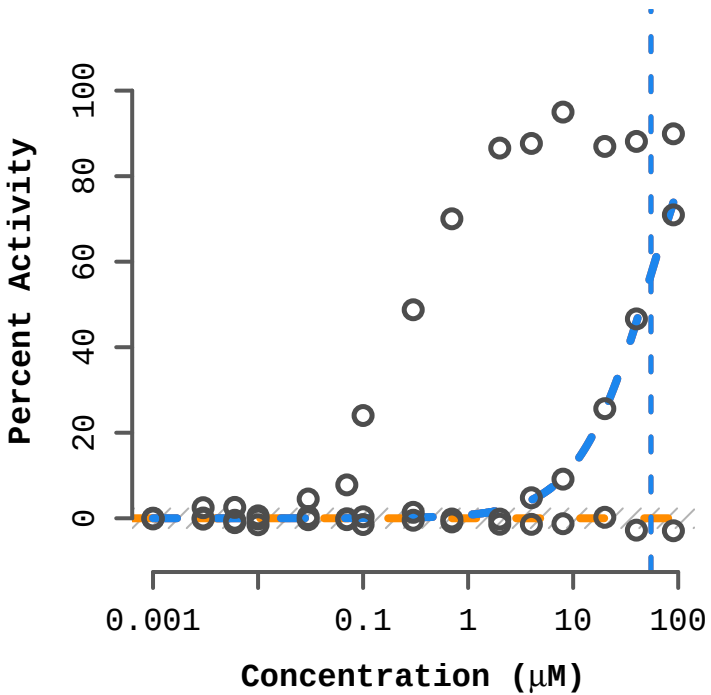
NAME: Beryllium sulfate tetrahydrate
CHID: 24603 CASRN: 7787-56-6
SPID(S): Tox21_202871
M4ID: 12479381

HILL MODEL: Not applicable.

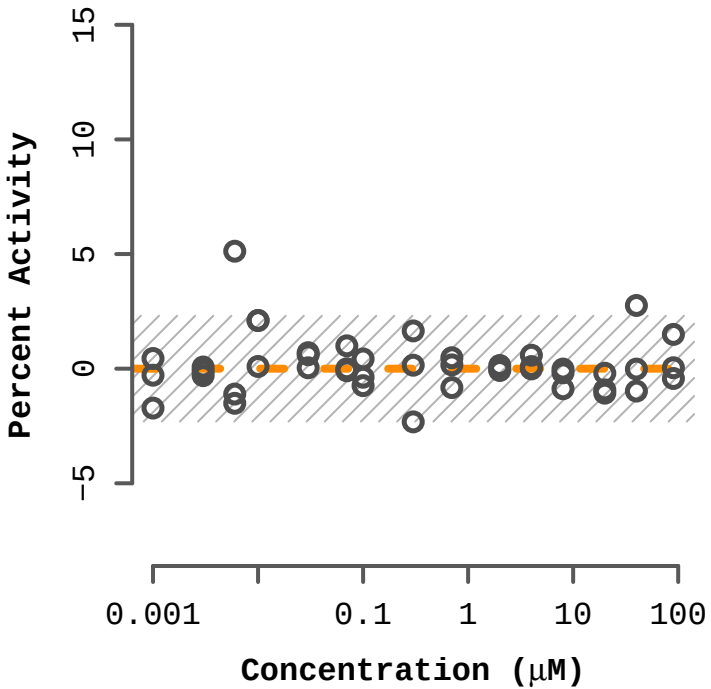
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.54 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,2-Bis[(benzoyloxy)methyl]dibenzoate propaned
CHID:    24608   CASRN: 4196-86-5
SPID(S): Tox21_200988
M4ID:    12481264

HILL MODEL (in red):
      tp       ga       gw
val:  114      1.74     1.24
sd:   103      0.723    0.938

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  114      1.74     1.24     2.72     13
sd:   103      0.721    0.936    19200    322000

      CNST        HILL        GNLS
AIC:  439.9       426.53      430.53
PROB: 0           0.88        0.12
RMSE: 37.59       31.34       31.34

MAX_MEAN: 52.7      MAX_MED: 71        BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

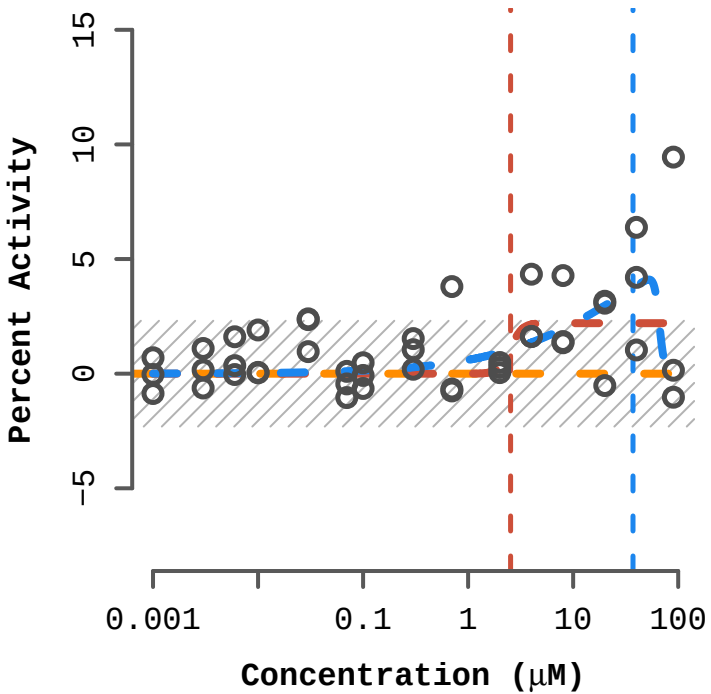
NAME: Bis(eta(5)−2,4−cyclopentadien−1−yl) chromium
CHID: 24615 **CASRN:** 1271−24−5
SPID(S): Tox21_202889
M4ID: 12479363

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(cyclopentadienyl)vanadium chloride
CHID: 24616 CASRN: 12083-48-6
SPID(S): Tox21_202489
M4ID: 12479763

HILL MODEL (in red):

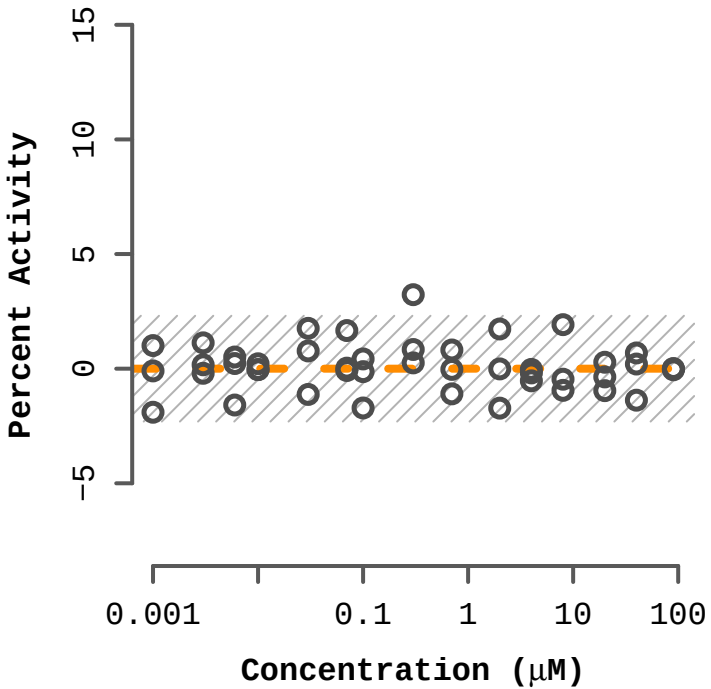
	tp	ga	gw
val:	2.2	0.404	8
sd:	0.523	0.193	13.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.47	1.57	0.675	1.82	18
sd:	14.1	2.28	0.595	0.494	65.4

	CNST	HILL	GNLS
AIC:	195.16	181.43	180
PROB:	0	0.33	0.67
RMSE:	2.4	1.84	1.96

MAX_MEAN: 3.87 MAX_MED: 4.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

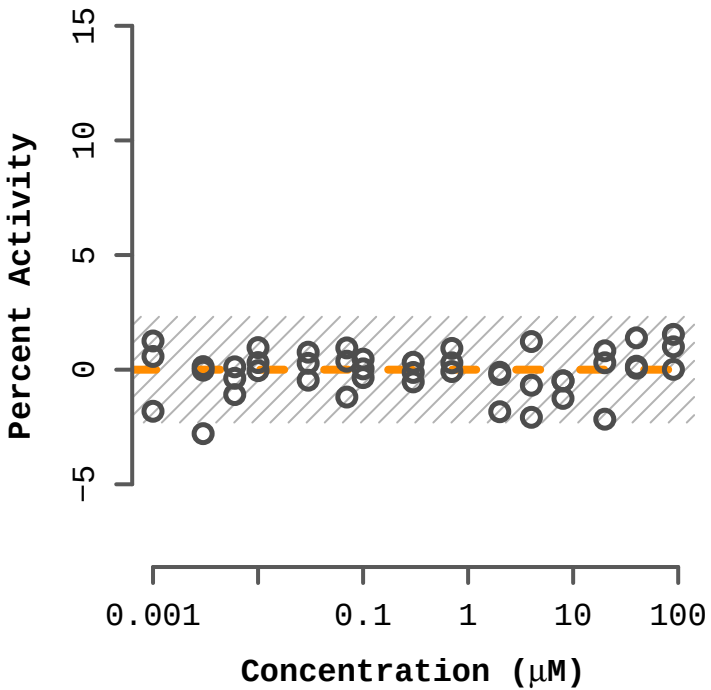
NAME: Bis(2-methoxyethyl) ether
CHID: 24621 **CASRN:** 111-96-6
SPID(S): Tox21_300077
M4ID: 12479053

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.838 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

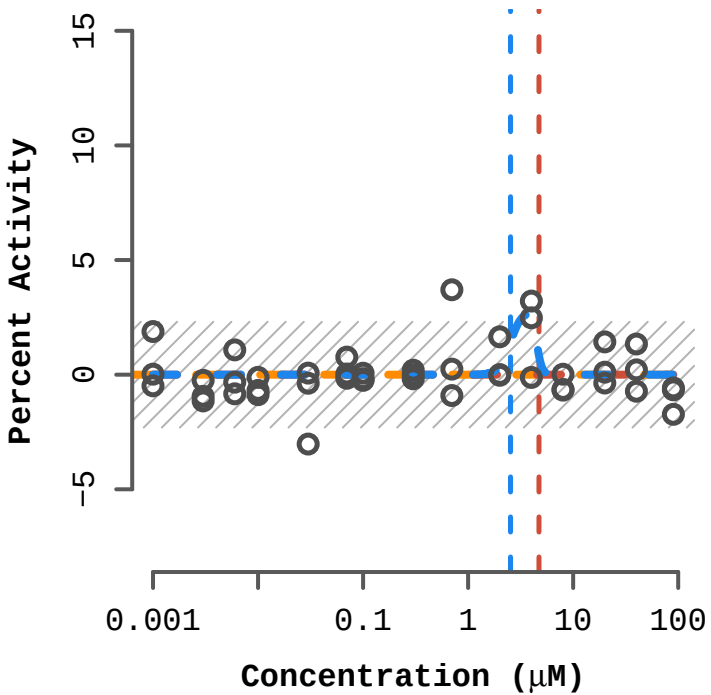
NAME: Bis(2-methoxyethyl) ether
CHID: 24621 **CASRN:** 111-96-6
SPID(S): Tox21_202340
M4ID: 12479912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 0.999 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bisphenol A diglycidyl ether
CHID: 24624 CASRN: 1675-54-3
SPID(S): Tox21_303315
M4ID: 12475818

HILL MODEL (in red):

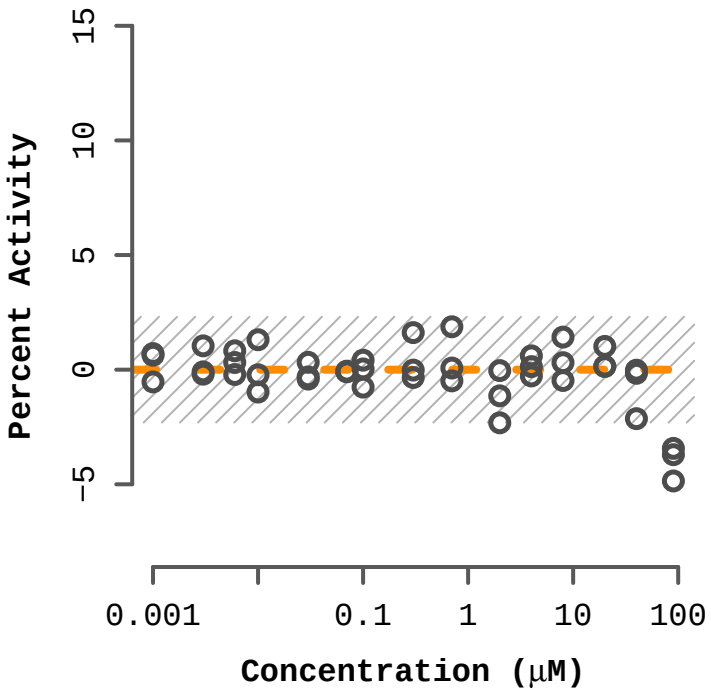
	tp	ga	gw
val:	1.09e-11	0.674	1.98
sd:	2.41e-06	29600	129000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.83	0.403	7.97	0.653	17.9
sd:	117	3.35	262	8.52	378

	CNST	HILL	GNLS
AIC:	135.66	141.66	137.76
PROB:	0.72	0.04	0.25
RMSE:	1.18	1.18	1.08

MAX_MEAN: 1.86 MAX_MED: 2.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

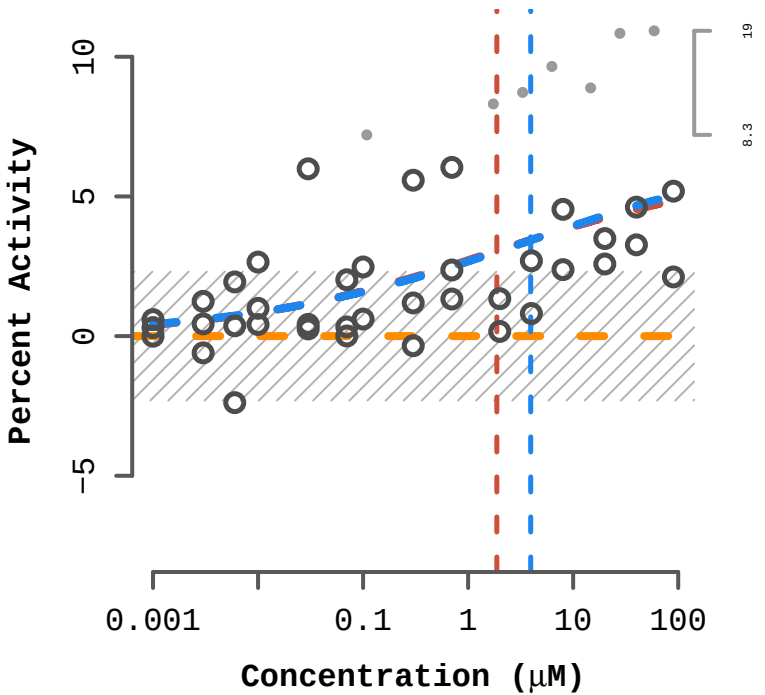
NAME: Bisphenol A diglycidyl ether
CHID: 24624 **CASRN:** 1675-54-3
SPID(S): Tox21_202141
M4ID: 12480111

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.486 **MAX_MED:** 0.631 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2−Bis(phenylthio)ethane
CHID: 24625 **CASRN:** 622−20−8
SPID(S): Tox21_201038
M4ID: 12481214 **BRK**

HILL MODEL (in red):

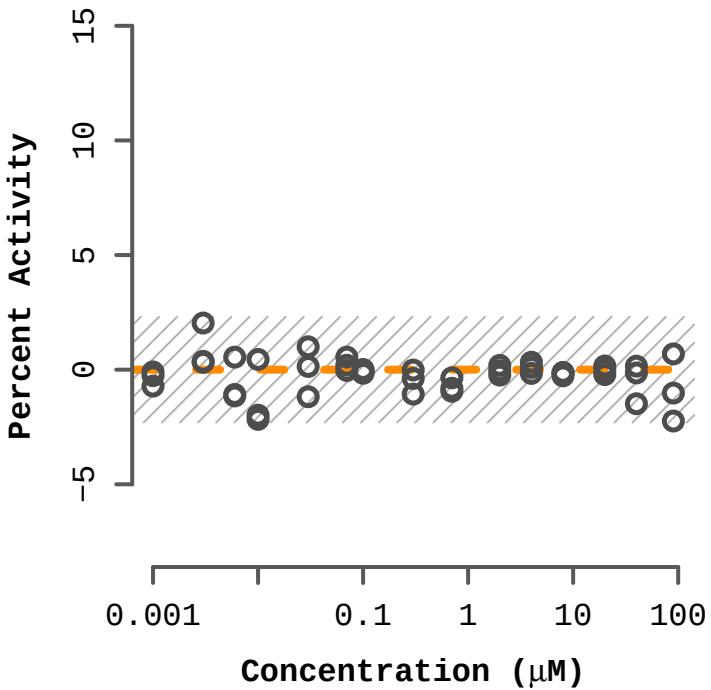
	tp	ga	gw
val:	6.1	0.273	0.35
sd:	5.4	2.7	0.303

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.86	0.596	0.327	2.06	10.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	281.5	256.39	260.37
PROB:	0	0.88	0.12
RMSE:	6.28	4.6	4.6

MAX_MEAN: 8.96 **MAX_MED:** 5.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

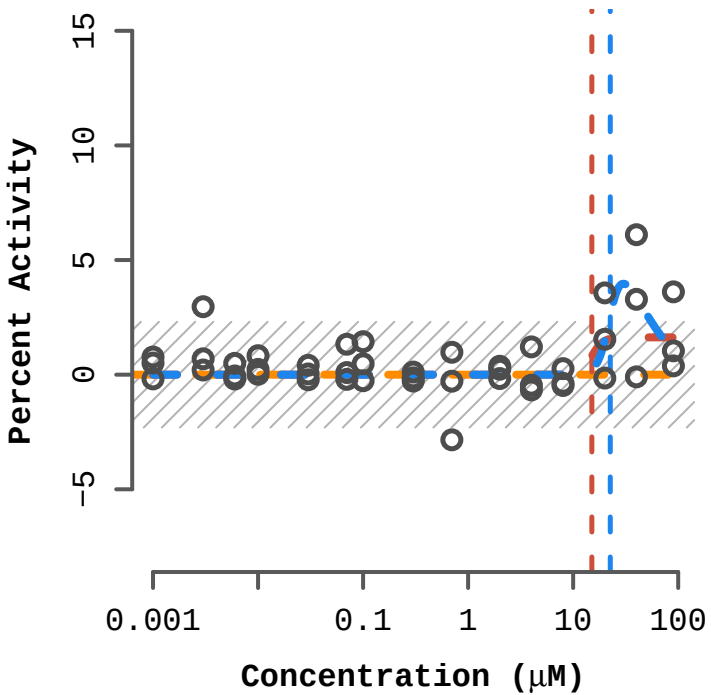
NAME: Biurea
CHID: 24628 **CASRN:** 110-21-4
SPID(S): Tox21_300989
M4ID: 12478144

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.907 **MAX_MED:** 0.364 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bixin
CHID: 24629 CASRN: 6983-79-5
SPID(S): Tox21_303095
M4ID: 12476038

HILL MODEL (in red):

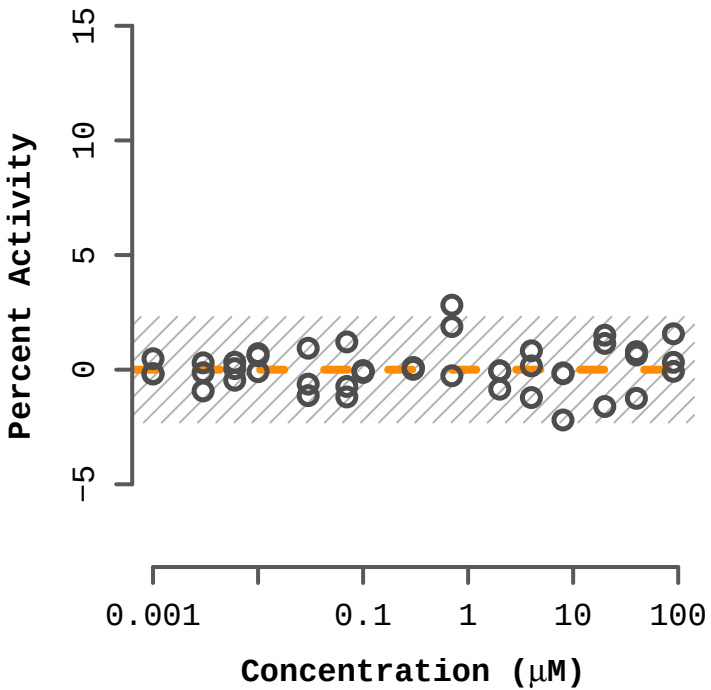
	tp	ga	gw
val:	1.63	1.18	8
sd:	0.84	0.287	11.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.74	1.35	8	1.61	2.05
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	147.8	143.02	143.21
PROB:	0.05	0.5	0.45
RMSE:	1.53	1.21	1.16

MAX_MEAN: 3.1 MAX_MED: 3.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

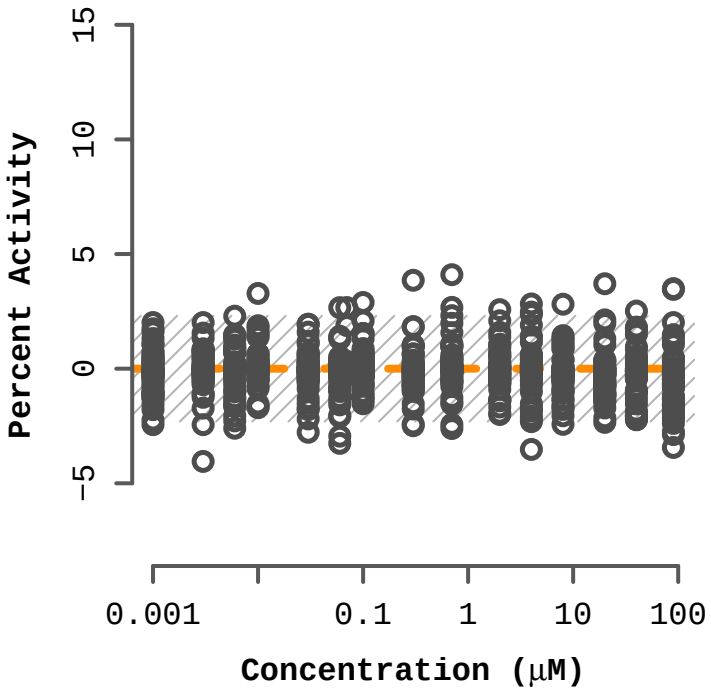
NAME: Bromobenzene
CHID: 24637 CASRN: 108-86-1
SPID(S): Tox21_200849
M4ID: 12481403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.48 MAX_MED: 1.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

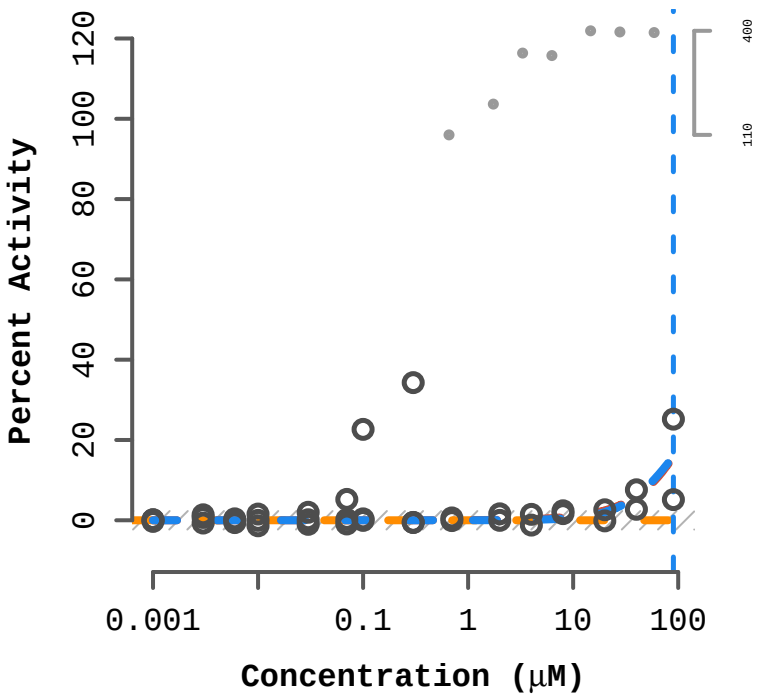
NAME: 2-Bromobiphenyl
CHID: 24638 **CASRN:** 2052-07-5
SPID(S): Tox21_400039
M4ID: 12475098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2082.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.374 **MAX_MED:** 0.0391 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Bromobiphenyl
CHID: 24639 CASRN: 2113-57-7
SPID(S): Tox21_200121
M4ID: 12482131 BRK

HILL MODEL (in red):

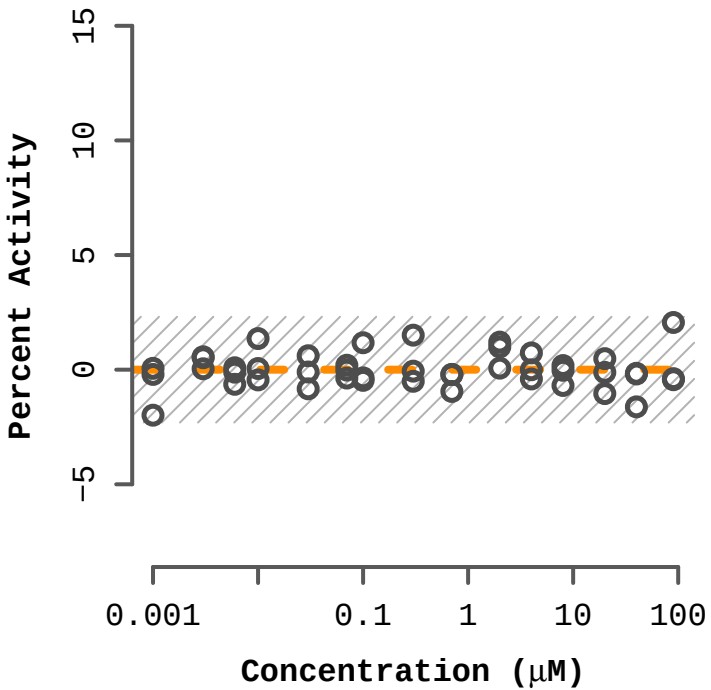
	tp	ga	gw
val:	91.4	2.45	1.35
sd:	972	4.79	2.19

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	31.9	1.95	1.79	3.94	3.41
sd:	143	2.15	4.28	3650	6370

	CNST	HILL	GNLS
AIC:	501.39	503.27	507.31
PROB:	0.69	0.27	0.04
RMSE:	129.04	127.29	127.34

MAX_MEAN: 142 MAX_MED: 25.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

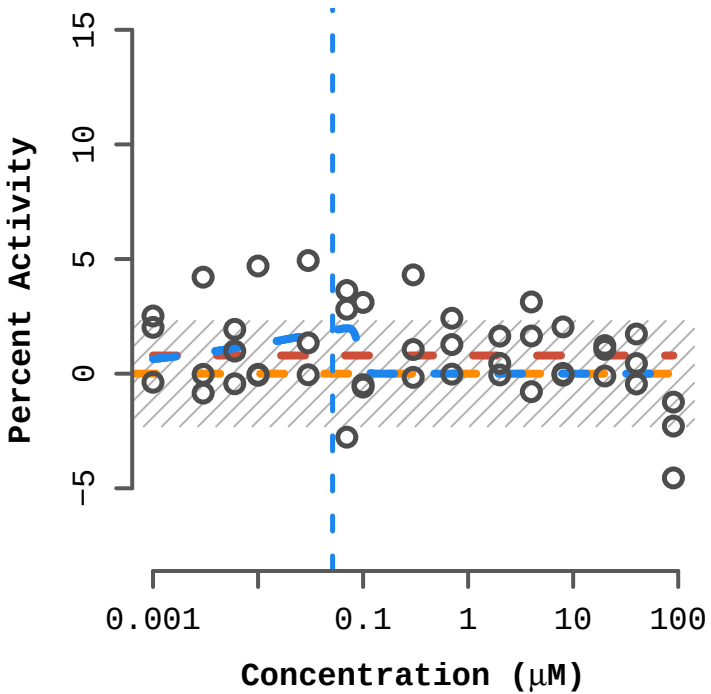
NAME: 4-Bromobiphenyl
CHID: 24640 **CASRN:** 92-66-0
SPID(S): Tox21_200254
M4ID: 12481998

HILL MODEL: Not applicable.

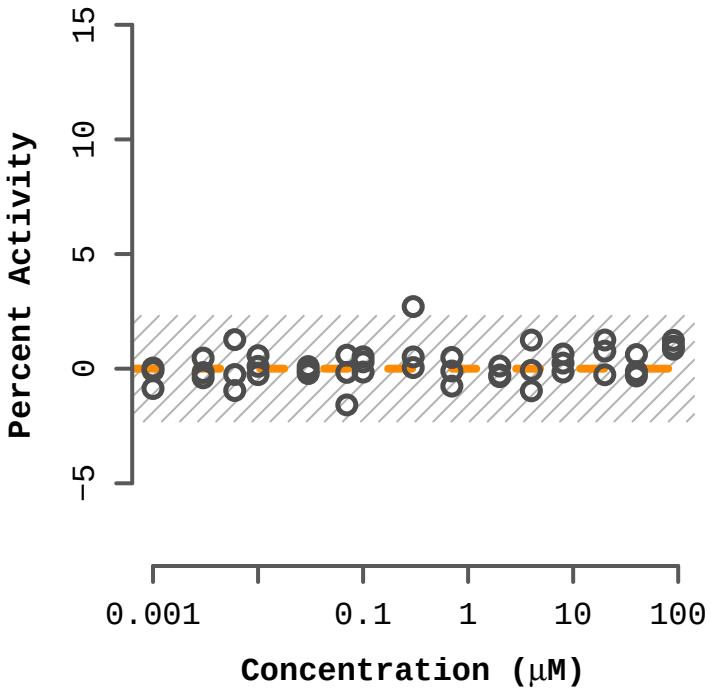
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.755 **MAX_MED:** 0.992 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-Bromo-2,2-bis(bromomethyl)propanol
CHID:    24641   CASRN: 1522-92-5
SPID(S): Tox21_200249
M4ID:    12482003

HILL MODEL (in red):
      tp       ga       gw
val:  0.792    -4.71    4.09
sd:   0.276    1320     3150

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.76     -1.29    0.405    -1.04    18
sd:   10.4     4.91     0.561    0.114    39.5

      CNST        HILL        GNLS
AIC:  197.63      195.55      200.69
PROB: 0.25        0.7         0.05
RMSE: 2.12        1.93        1.94

MAX_MEAN: 2.08      MAX_MED: 2.81      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

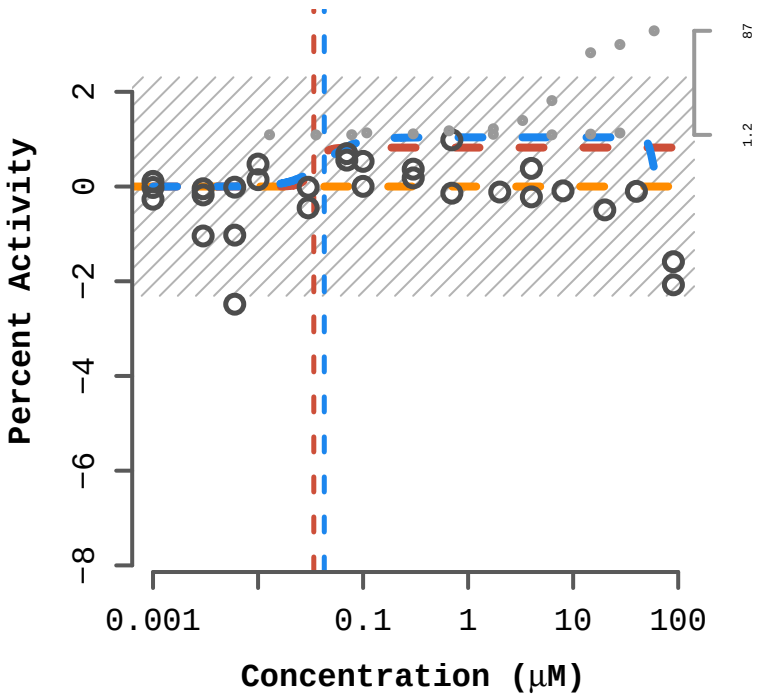
NAME: Bromochloroacetic acid
CHID: 24642 **CASRN:** 5589-96-8
SPID(S): Tox21_200894
M4ID: 12481358

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bromodichloroacetic acid
CHID: 24644 CASRN: 71133-14-7
SPID(S): Tox21_200923
M4ID: 12481329 BRK

HILL MODEL (in red):

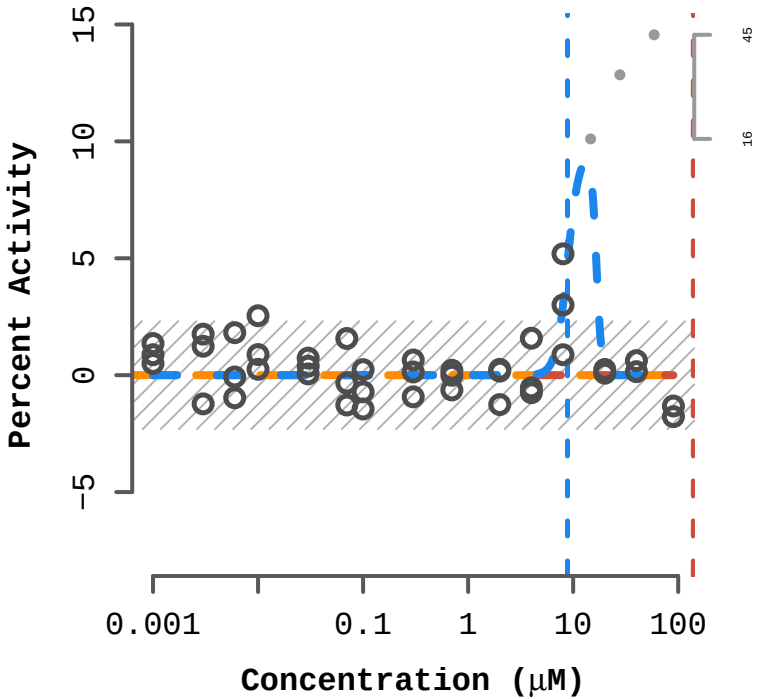
	tp	ga	gw
val:	0.822	−1.47	8
sd:	0.381	0.86	123

GAIN-LOSS MODEL (in blue):

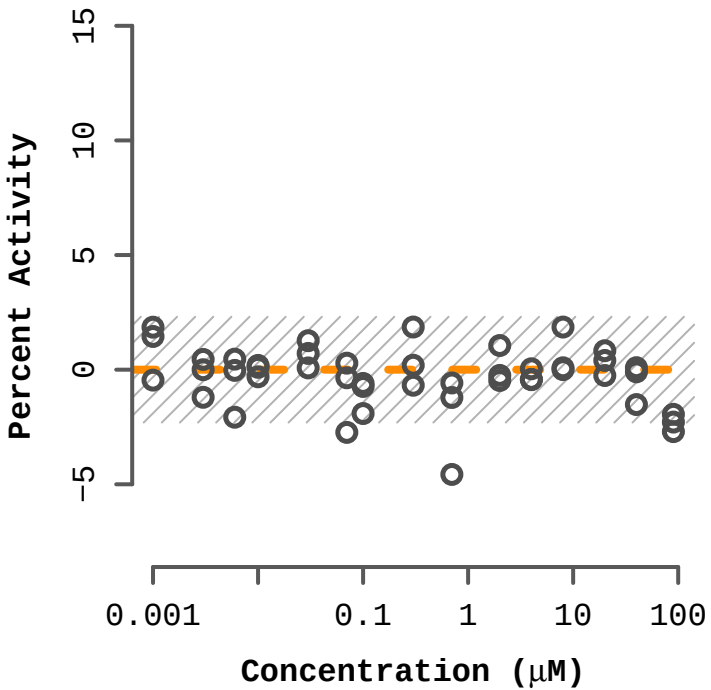
	tp	ga	gw	la	lw
val:	1.04	−1.37	2.88	1.76	18
sd:	0.448	0.547	9.31	0.914	92.8

	CNST	HILL	GNLS
AIC:	297.45	298.61	300.23
PROB:	0.55	0.31	0.14
RMSE:	20.58	20.33	20.36

MAX_MEAN: 27.7 MAX_MED: 2.72 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Bromo-4,6-dinitroaniline
CHID:    24646   CASRN: 1817-73-8
SPID(S): Tox21_200070
M4ID:    12482182  BRK

HILL MODEL (in red):
      tp        ga        gw
val:  4.88e-10  2.14      1.59
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  9.63      0.946     8         1.22      18
sd:   NaN       NaN       NaN       NaN       NaN

      CNST        HILL        GNLS
AIC:  224.87      230.87      226.68
PROB: 0.69        0.03        0.28
RMSE: 8.91        8.91        8.87

MAX_MEAN: 14.1      MAX_MED: 3          BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

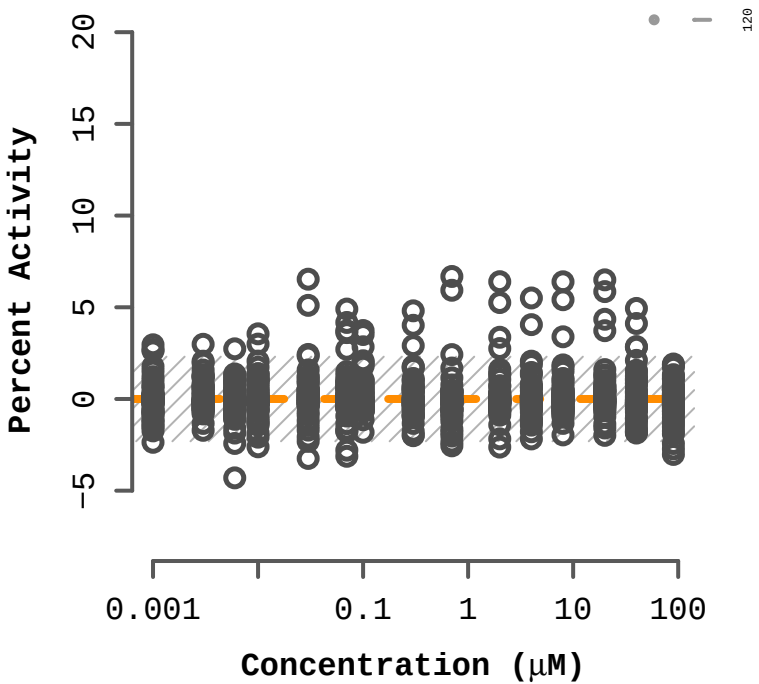
NAME: Bronopol
CHID: 24652 CASRN: 52-51-7
SPID(S): Tox21_300126
M4ID: 12479004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

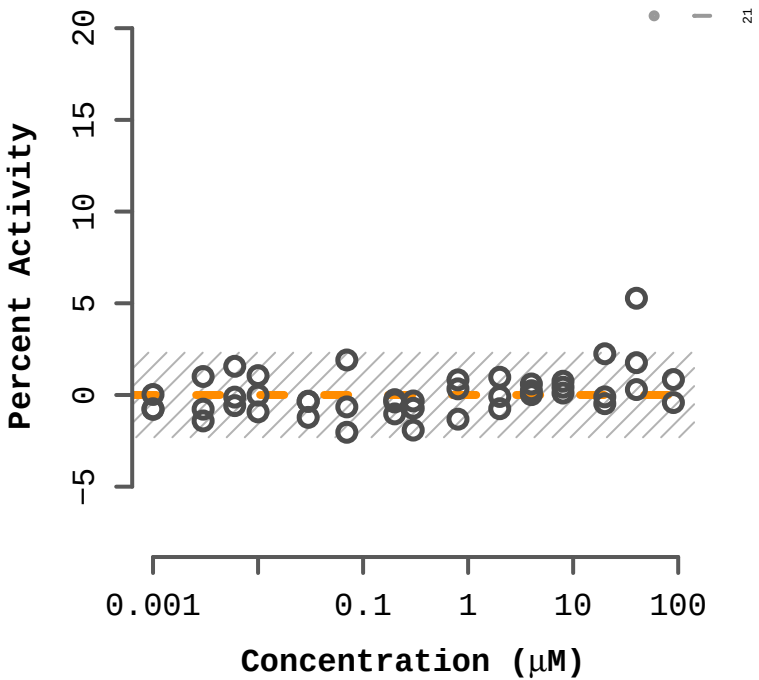
NAME: 3-Bromo-1-propanol
CHID: 24657 CASRN: 627-18-9
SPID(S): Tox21_400042
M4ID: 12475095 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2250.94	NA	NA
PROB:	1	NA	NA
RMSE:	4.7	NA	NA

MAX_MEAN: 2.42 MAX_MED: 0.052 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

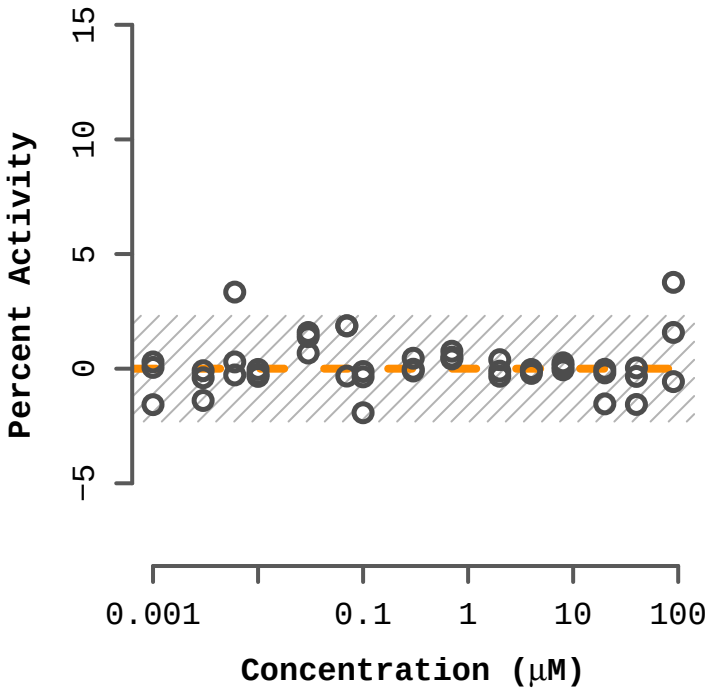
NAME: alpha-Bromotoluene
CHID: 24658 CASRN: 100-39-0
SPID(S): Tox21_200018
M4ID: 12482234 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.04	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 7.22 MAX_MED: 1.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

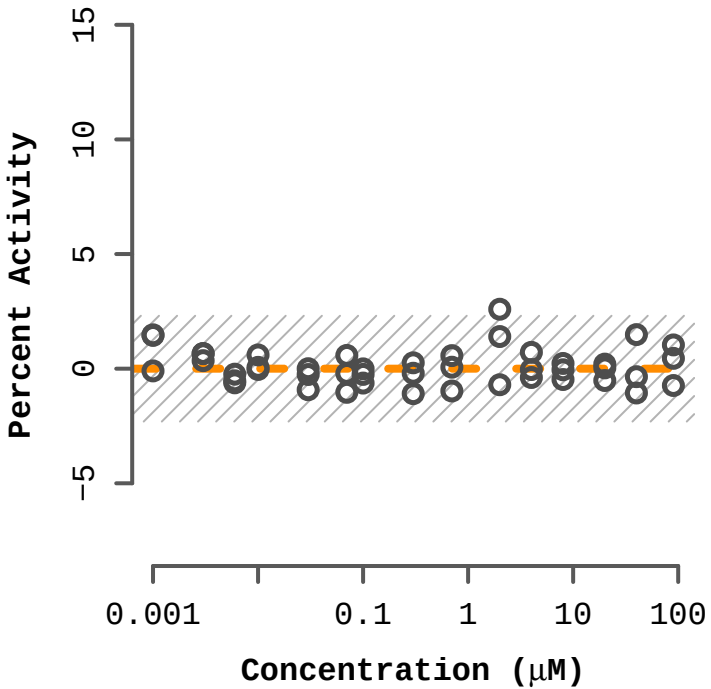
NAME: 3-Bromotoluene
CHID: 24659 **CASRN:** 591-17-3
SPID(S): Tox21_200334
M4ID: 12481918

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

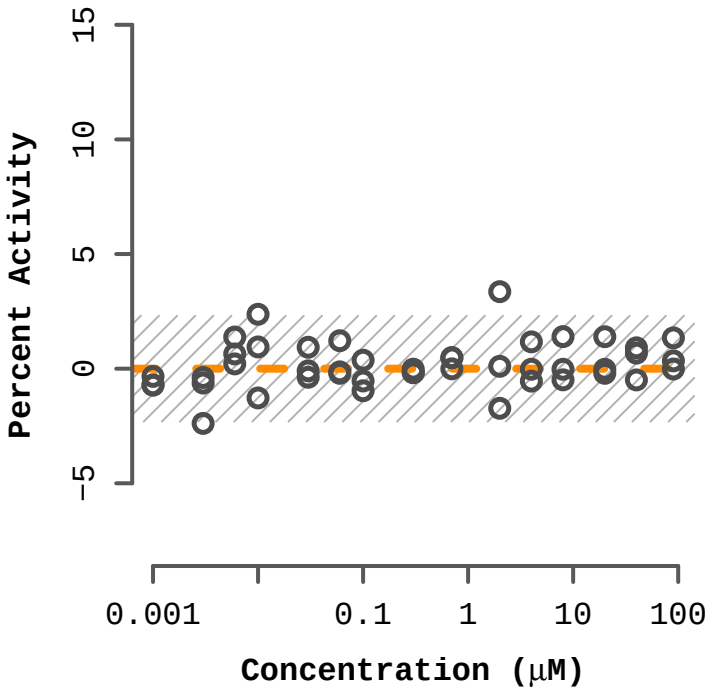
NAME: 2-Bromotoluene
CHID: 24660 **CASRN:** 95-46-5
SPID(S): Tox21_200379
M4ID: 12481873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

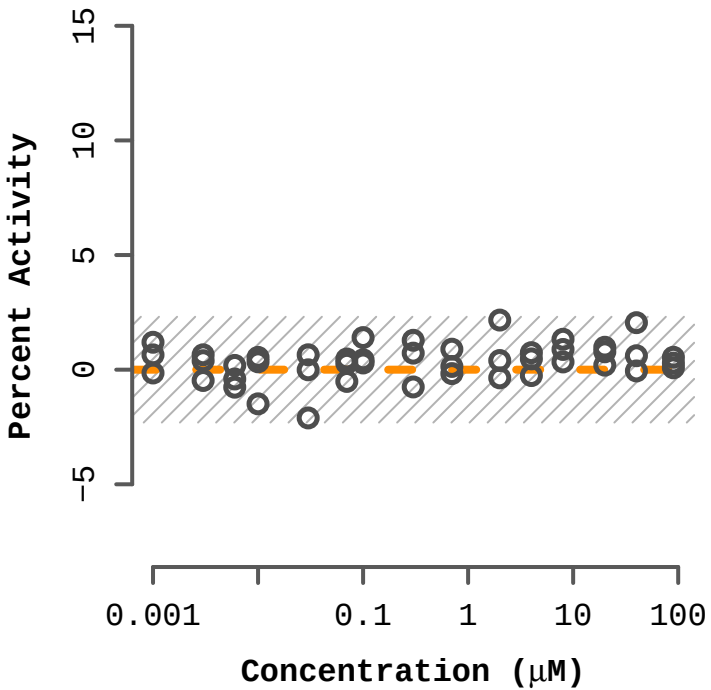
NAME: 4-Bromotoluene
CHID: 24661 **CASRN:** 106-38-7
SPID(S): Tox21_200969
M4ID: 12481283

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.744 **MAX_MED:** 0.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

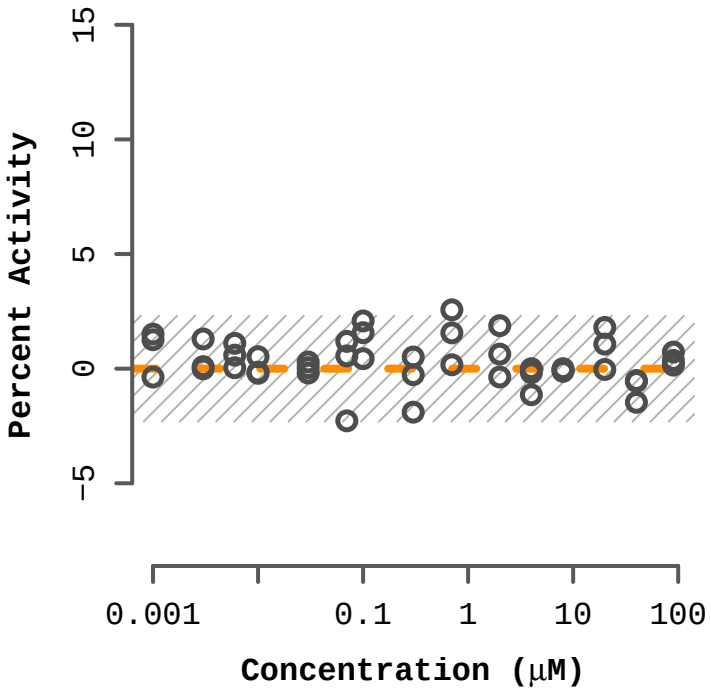
NAME: Brucine
CHID: 24662 CASRN: 357-57-3
SPID(S): Tox21_302174
M4ID: 12476959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.869 **MAX_MED:** 0.883 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

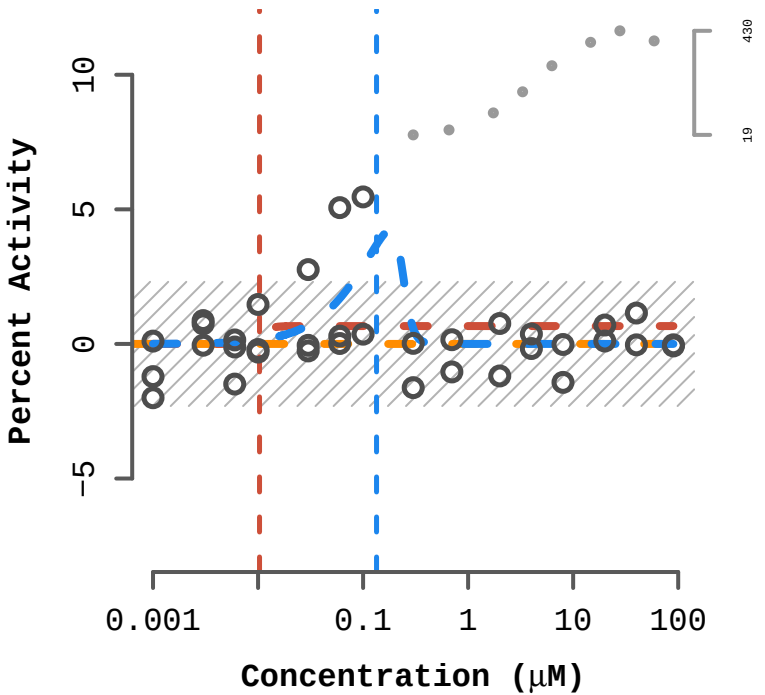
NAME: Butanal oxime
CHID: 24664 **CASRN:** 110-69-0
SPID(S): Tox21_303175
M4ID: 12475958

HILL MODEL: Not applicable.

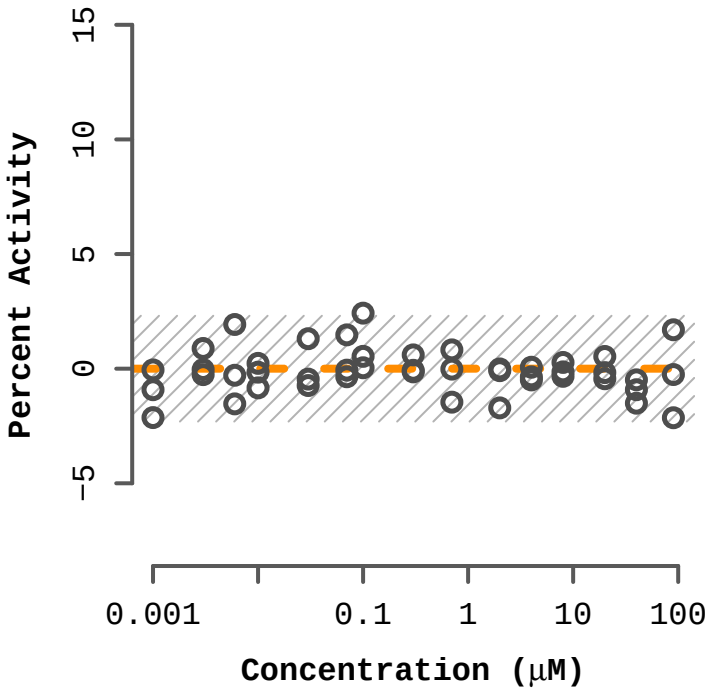
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.57 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Butanal oxime
CHID:    24664   CASRN: 110-69-0
SPID(S): Tox21_201786
M4ID:    12480466  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  0.664    -1.99    8
sd:   0.811    0.775    70.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.4      -0.872   1.51     -0.622   9.58
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  452         457.26      460.25
PROB: 0.92        0.07        0.01
RMSE: 118.33      118.1       118.33

MAX_MEAN: 143       MAX_MED: 2.91      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

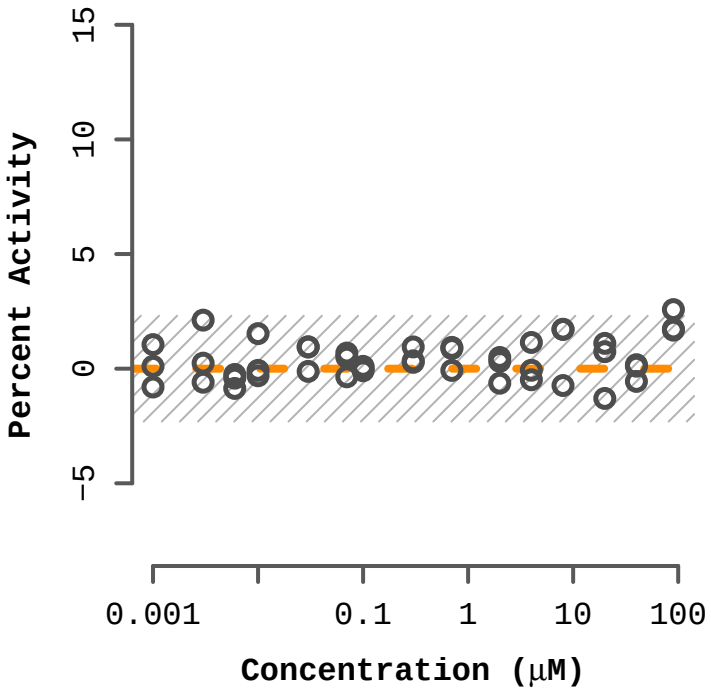
NAME: 1,4−Butanediol
CHID: 24666 **CASRN:** 110−63−4
SPID(S): Tox21_303040
M4ID: 12476093

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.539 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

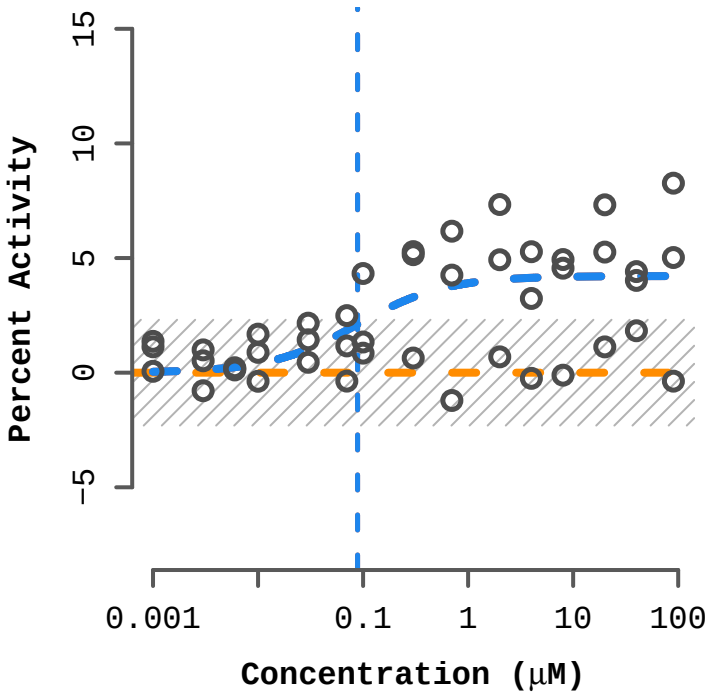
NAME: 1,4−Butanediol
CHID: 24666 **CASRN:** 110−63−4
SPID(S): Tox21_202245
M4ID: 12480007

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Butanediol diglycidyl ether
CHID: 24667 CASRN: 2425−79−8
SPID(S): Tox21_202267
M4ID: 12479985

HILL MODEL (in red):

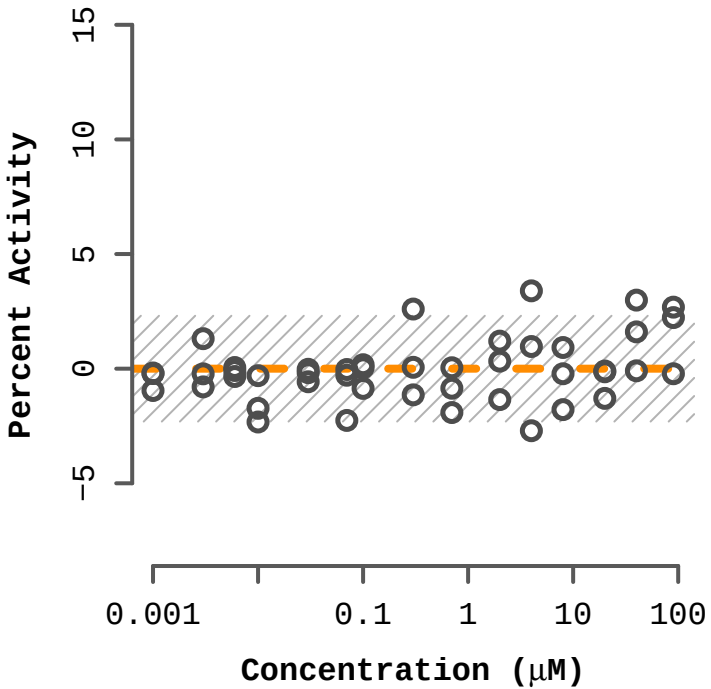
	tp	ga	gw
val:	4.22	−1.05	1.04
sd:	0.552	0.262	0.743

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.22	−1.05	1.04	3.48	5.32
sd:	0.552	0.262	0.743	2320	8120

	CNST	HILL	GNLS
AIC:	242.1	201.77	205.77
PROB:	0	0.88	0.12
RMSE:	3.45	2.08	2.08

MAX_MEAN: 4.57 MAX_MED: 5.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

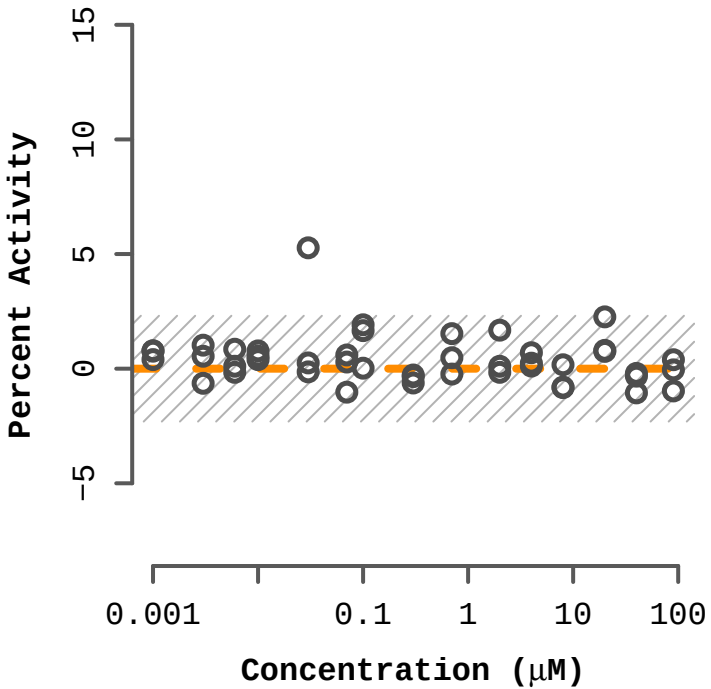
NAME: 1,2,3,4−Butanetetracarboxylic acid
CHID: 24670 **CASRN:** 1703−58−8
SPID(S): Tox21_303236
M4ID: 12475897

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

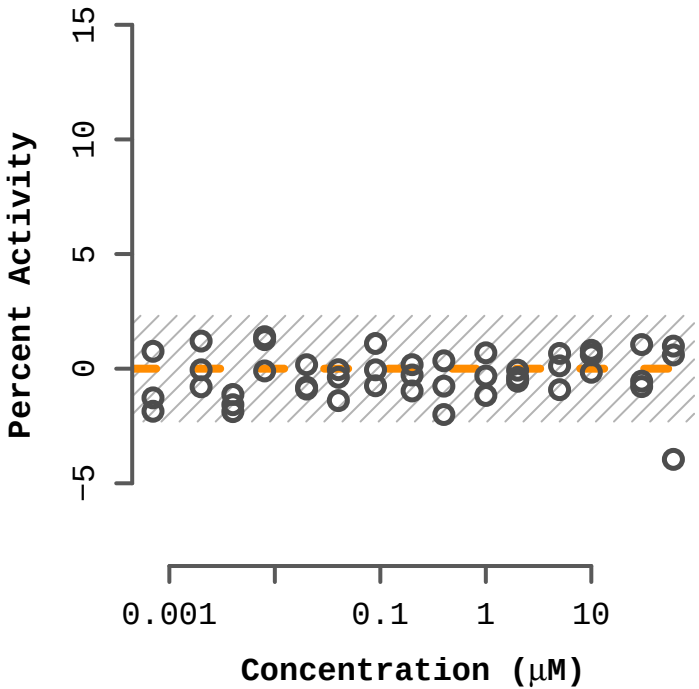
NAME: 1,2,3,4-Butanetetracarboxylic acid
CHID: 24670 **CASRN:** 1703-58-8
SPID(S): Tox21_201271
M4ID: 12480981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

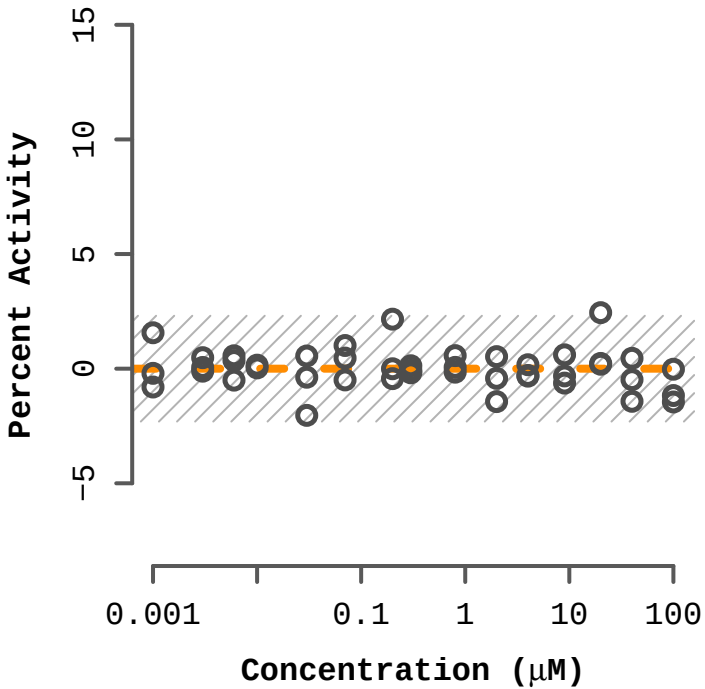
NAME: 2-(2-Butoxyethoxy)ethyl thiocyanate
CHID: 24674 **CASRN:** 112-56-1
SPID(S): Tox21_303547
M4ID: 12475598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

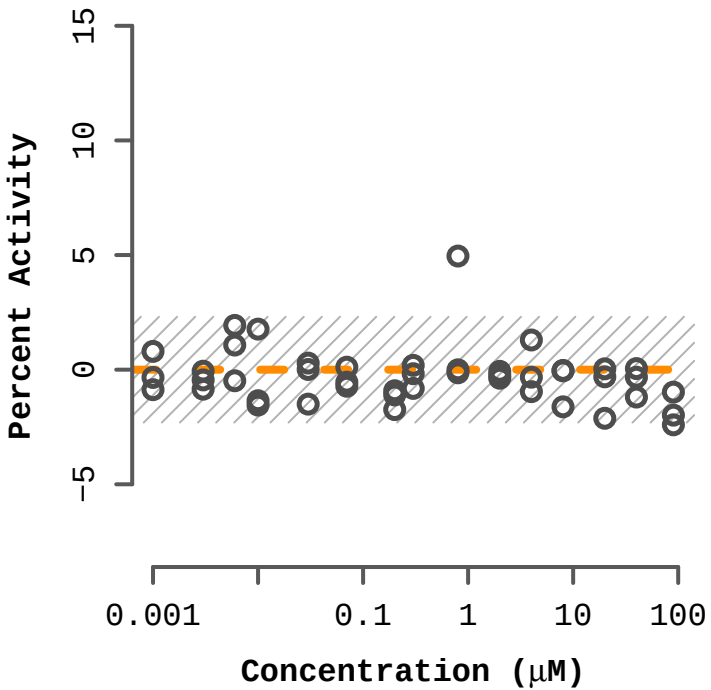
NAME: 2-(2-Butoxyethoxy)ethyl thiocyanate
CHID: 24674 **CASRN:** 112-56-1
SPID(S): Tox21_201317
M4ID: 12480935

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

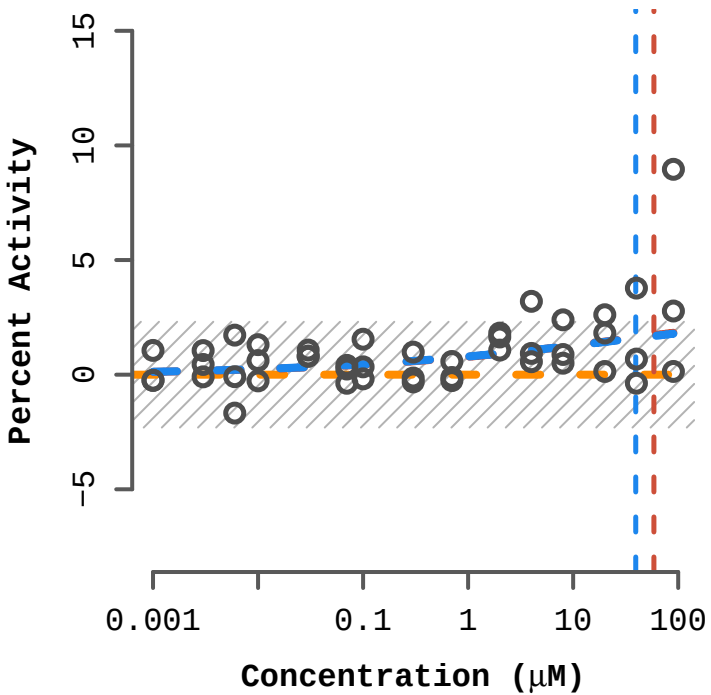
NAME: Butyl acrylate
CHID: 24676 **CASRN:** 141-32-2
SPID(S): Tox21_303296
M4ID: 12475837

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl acrylate
CHID: 24676 CASRN: 141-32-2
SPID(S): Tox21_201387
M4ID: 12480865

HILL MODEL (in red):

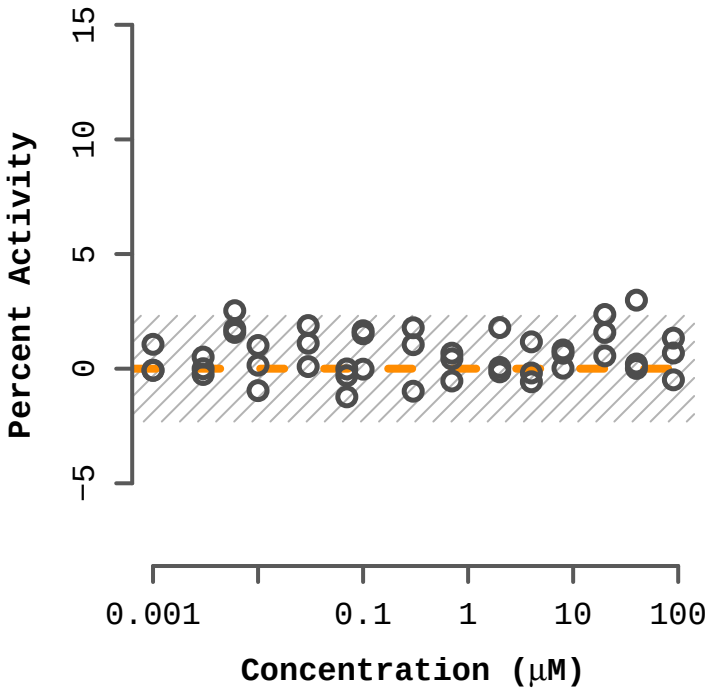
	tp	ga	gw
val:	3.43	1.77	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.18	1.6	0.3	3.53	4.71
sd:	10.1	8.64	0.442	1580	4800

	CNST	HILL	GNLS
AIC:	165.43	148.88	152.87
PROB:	0	0.88	0.12
RMSE:	1.86	1.43	1.43

MAX_MEAN: 3.96 **MAX_MED:** 2.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

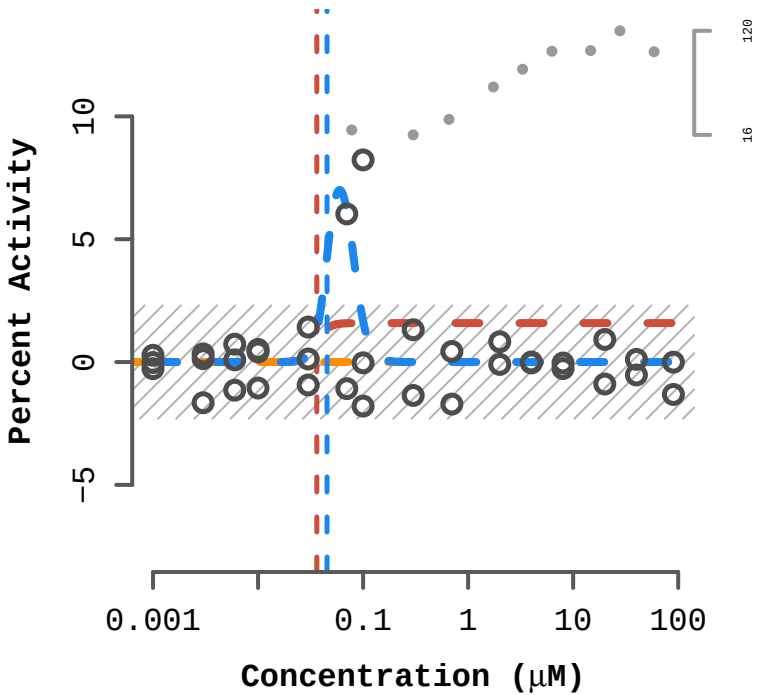
NAME: tert-Butylamine
CHID: 24681 **CASRN:** 75-64-9
SPID(S): Tox21_301289
M4ID: 12477844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl anthranilate
CHID: 24683 CASRN: 7756-96-9
SPID(S): Tox21_201173
M4ID: 12481079 BRK

HILL MODEL (in red):

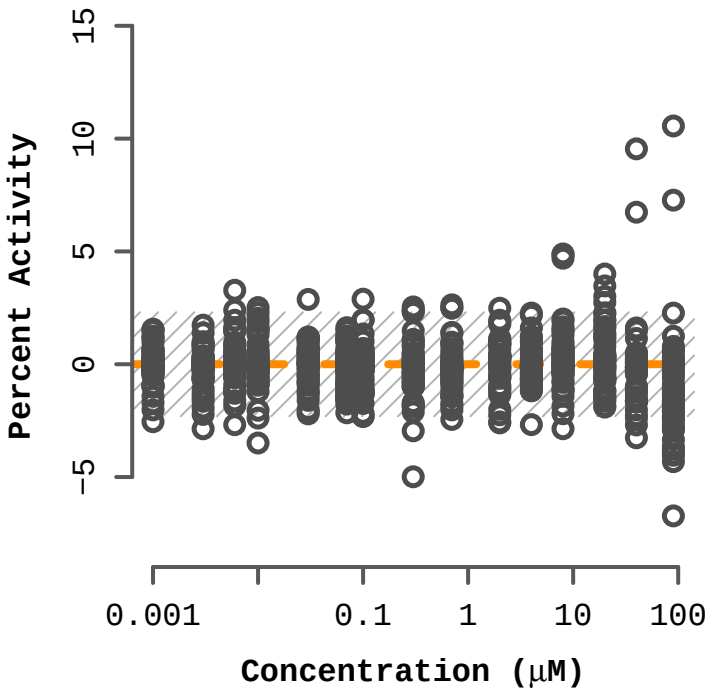
	tp	ga	gw
val:	1.59	−1.44	8
sd:	1.43	0.583	30.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.81	−1.34	8	−1.09	6.75
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	398.92	403.35	406.61
PROB:	0.88	0.1	0.02
RMSE:	34.48	33.86	34.41

MAX_MEAN: 38.6 MAX_MED: 6.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

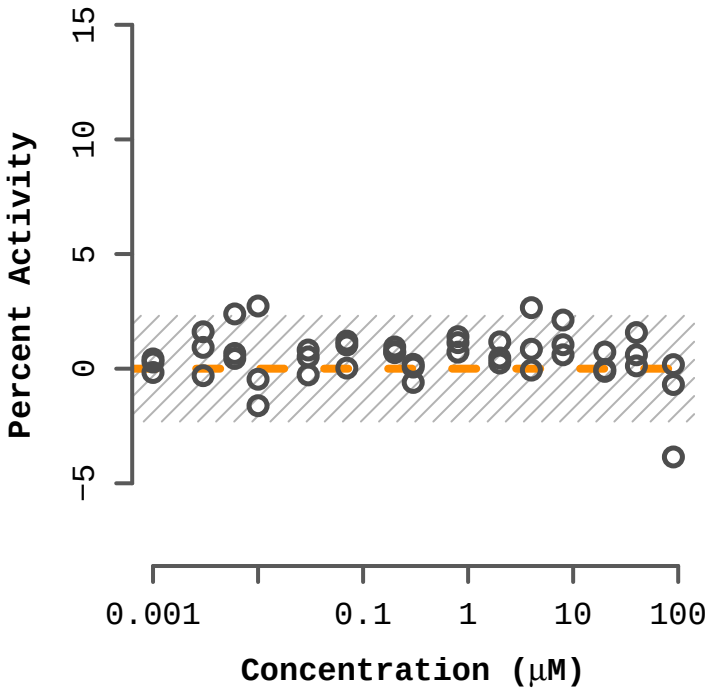
NAME: 4-tert-Butylcatechol
CHID: 24687 CASRN: 98-29-3
SPID(S): Tox21_400003
M4ID: 12475134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2310.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.344 **MAX_MED:** 0.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

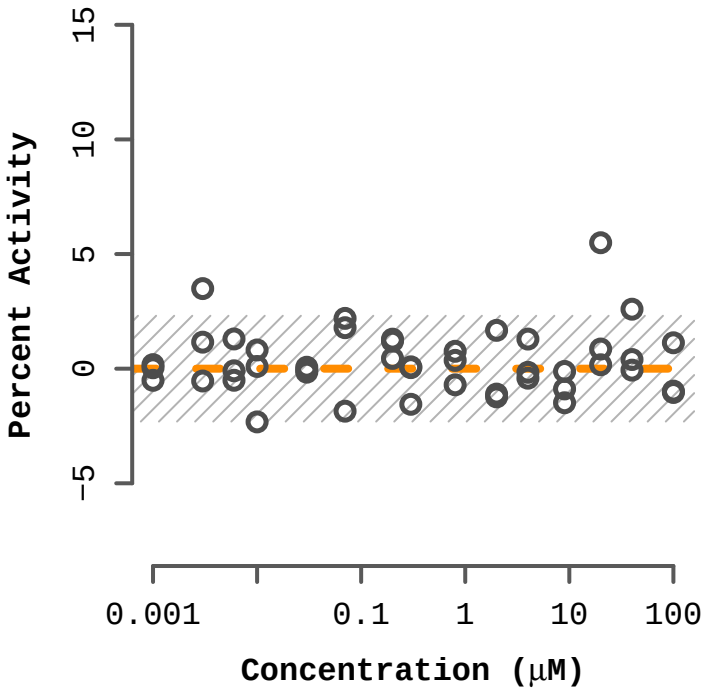
NAME: 4-tert-Butylcatechol
CHID: 24687 **CASRN:** 98-29-3
SPID(S): Tox21_202989
M4ID: 12479263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

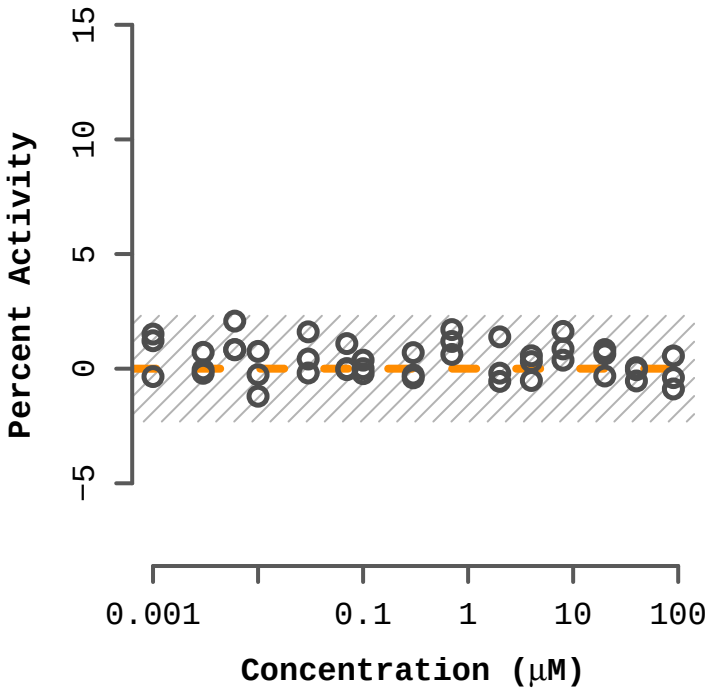
NAME: tert-Butyl formate
CHID: 24690 **CASRN:** 762-75-4
SPID(S): Tox21_200359
M4ID: 12481893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 2.18 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

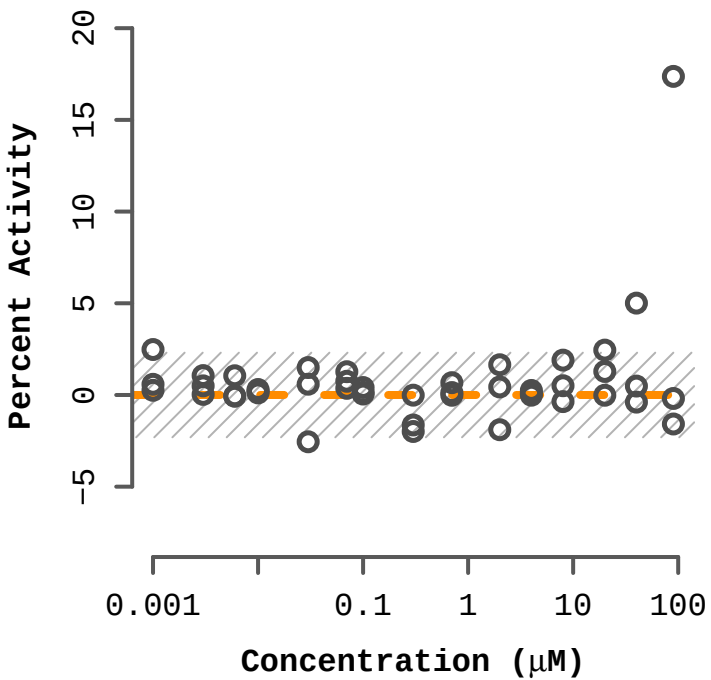
NAME: Butyl glycidyl ether
CHID: 24691 **CASRN:** 2426-08-6
SPID(S): Tox21_303211
M4ID: 12475922

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

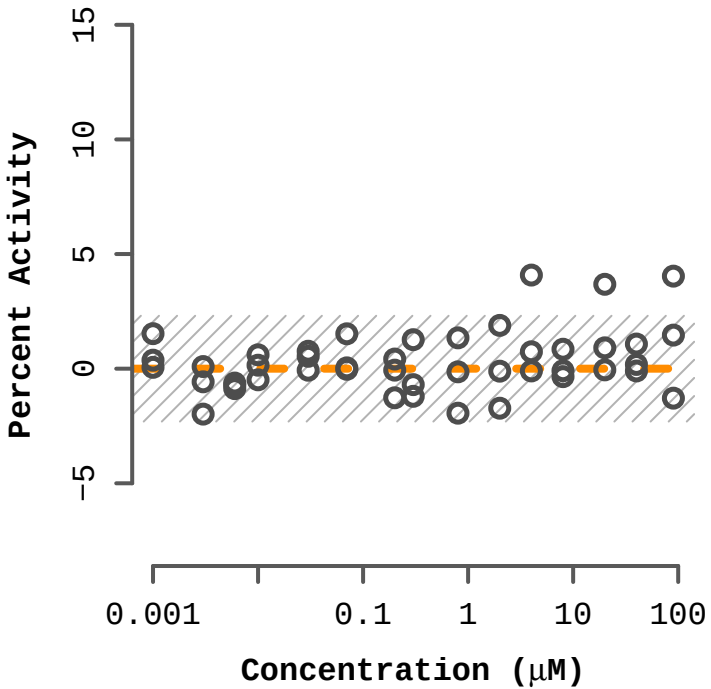
NAME: Butyl glycidyl ether
CHID: 24691 **CASRN:** 2426-08-6
SPID(S): Tox21_201746
M4ID: 12480506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 5.2 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

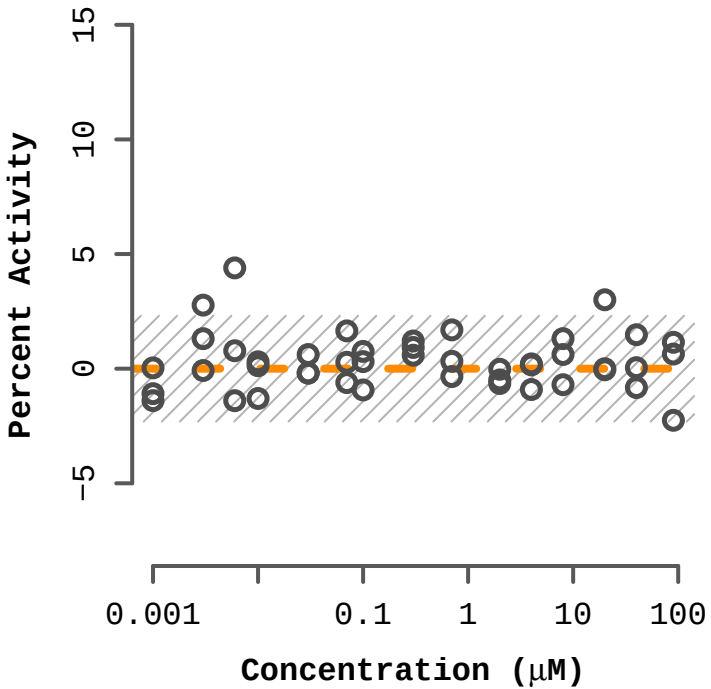
NAME: tert-Butyl glycidyl ether
CHID: 24692 CASRN: 7665-72-7
SPID(S): Tox21_200253
M4ID: 12481999

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.58 MAX_MED: 1.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

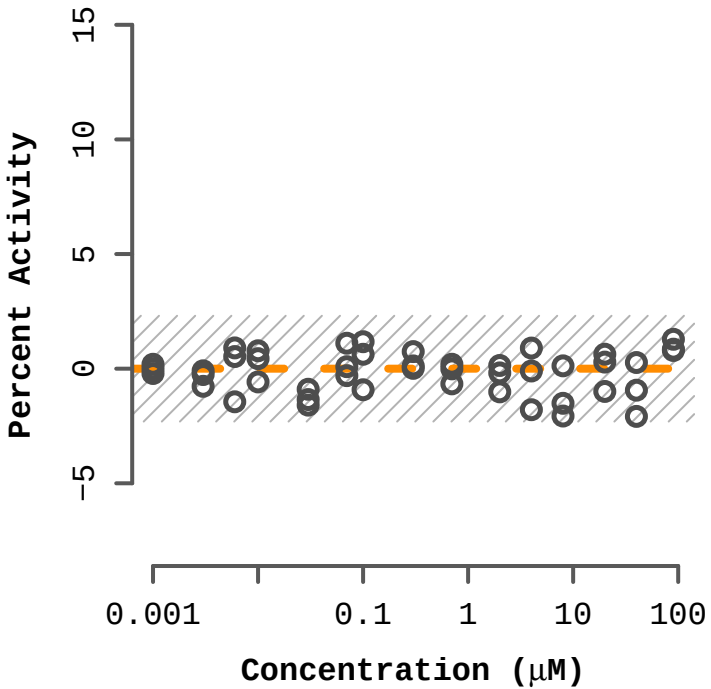
NAME: Butyl methacrylate
CHID: 24696 CASRN: 97-88-1
SPID(S): Tox21_200161
M4ID: 12482091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

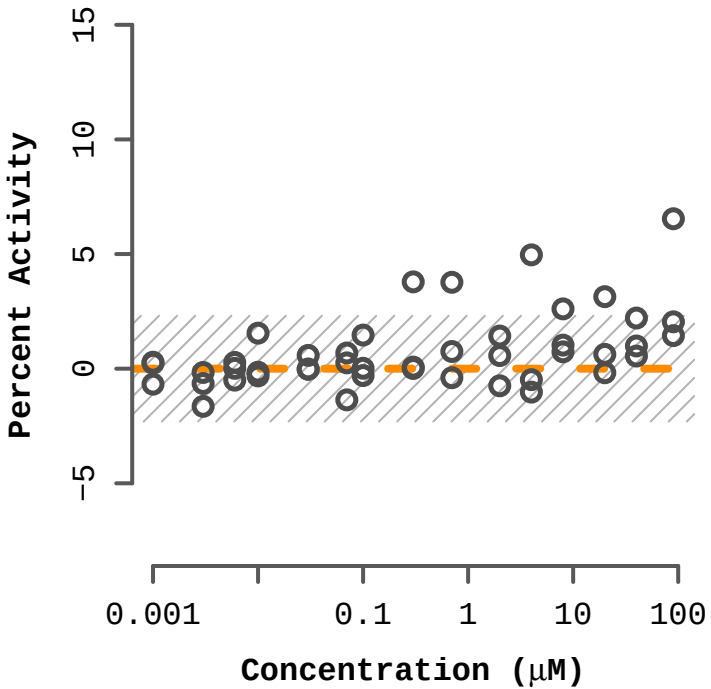
NAME: tert-Butyl perbenzoate
CHID: 24699 **CASRN:** 614-45-9
SPID(S): Tox21_300070
M4ID: 12479060

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

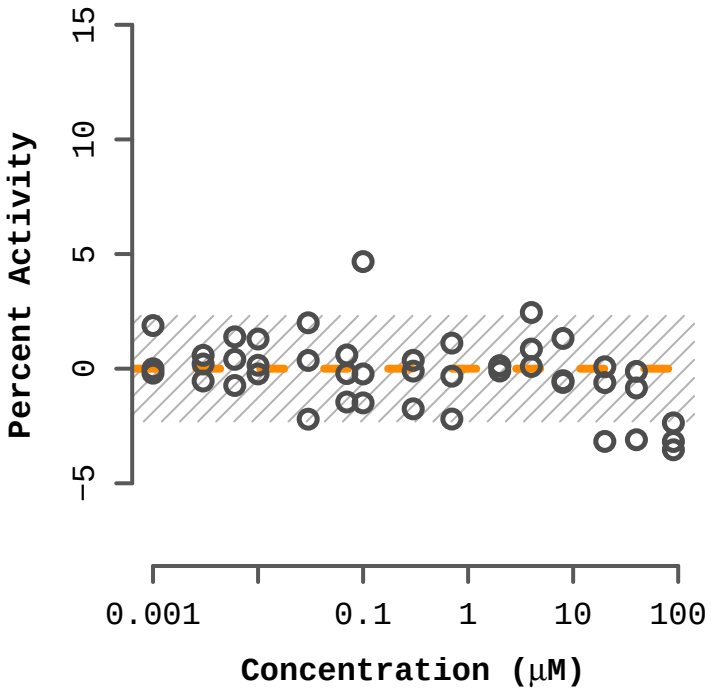
NAME: tert-Butyl perbenzoate
CHID: 24699 **CASRN:** 614-45-9
SPID(S): Tox21_202287
M4ID: 12479965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 3.34 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

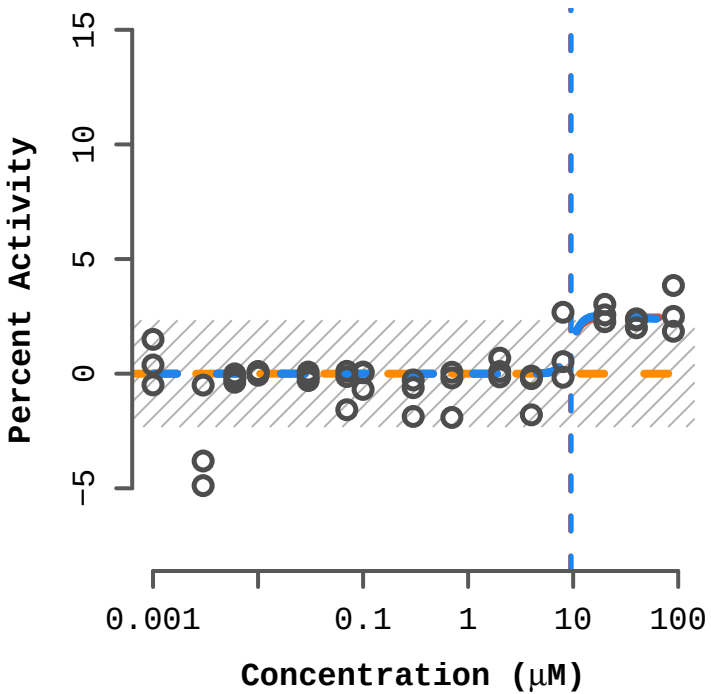
NAME: tert-Butylphenyl diphenyl phosphate
CHID: 24701 **CASRN:** 56803-37-3
SPID(S): Tox21_202980
M4ID: 12479272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.857 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: tert-Butyl phenyl glycidyl ether
CHID: 24702 CASRN: 3101-60-8
SPID(S): Tox21_200310
M4ID: 12481942

HILL MODEL (in red):

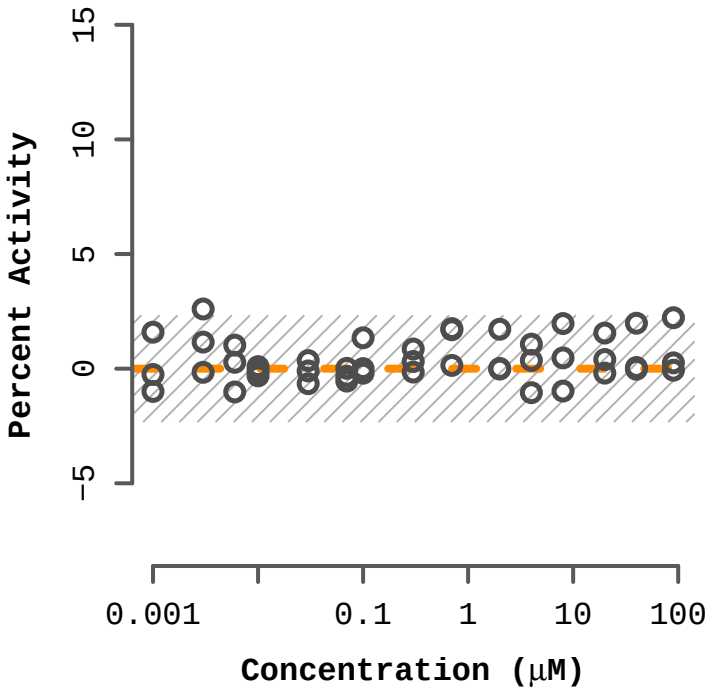
	tp	ga	gw
val:	2.45	0.976	8
sd:	0.207	0.103	9.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.93	0.98	8	3.95	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	171.56	128.31	132.3
PROB:	0	0.88	0.12
RMSE:	1.66	1.19	1.19

MAX_MEAN: 2.73 MAX_MED: 2.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

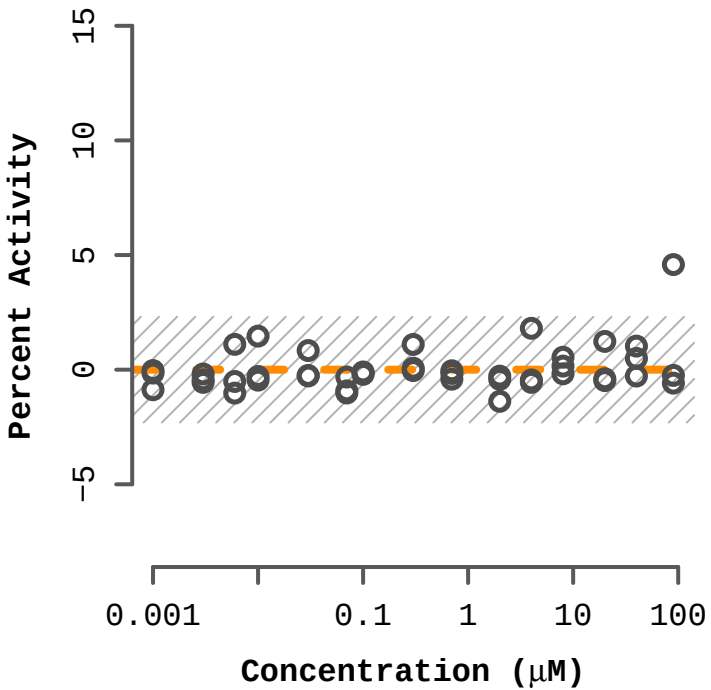
NAME: 4-tert-Butyltoluene
CHID: 24704 **CASRN:** 98-51-1
SPID(S): Tox21_303201
M4ID: 12475932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

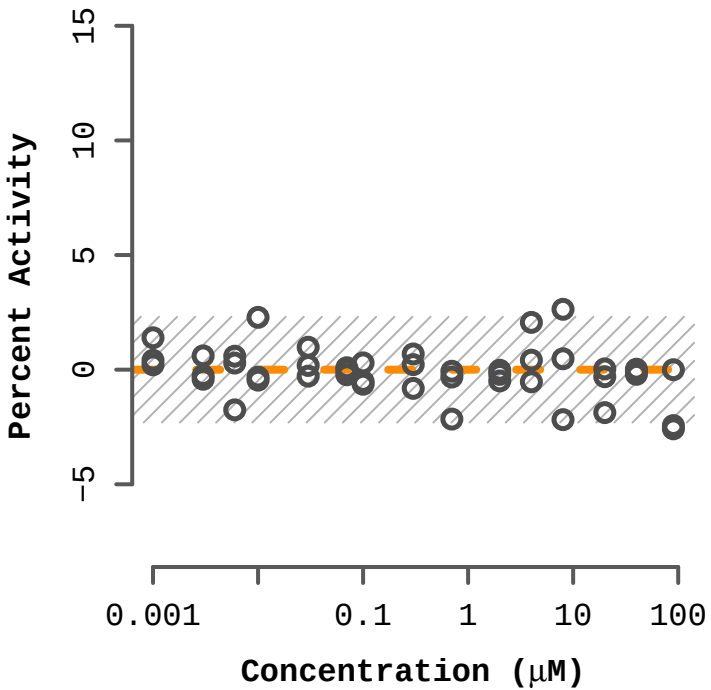
NAME: 4-tert-Butyltoluene
CHID: 24704 **CASRN:** 98-51-1
SPID(S): Tox21_202329
M4ID: 12479923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.492 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

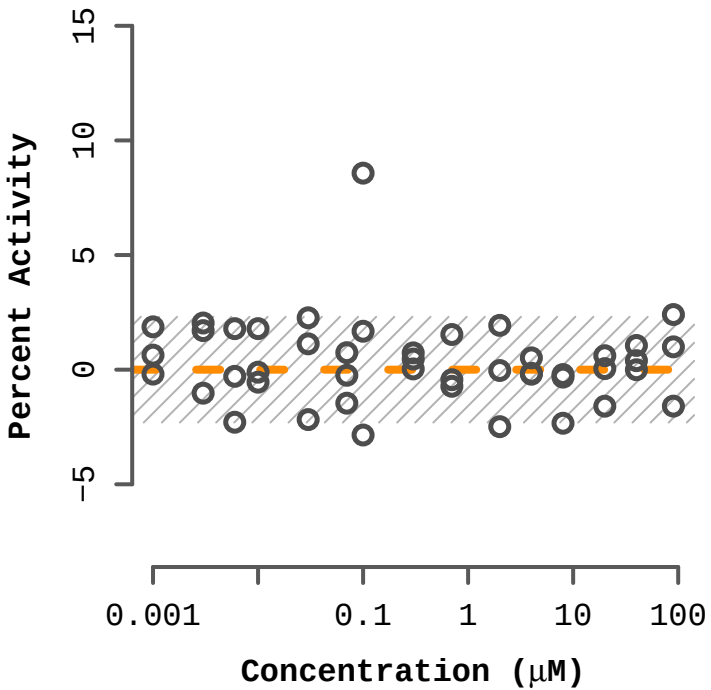
NAME: Butyryl chloride
CHID: 24710 **CASRN:** 141-75-3
SPID(S): Tox21_200294
M4ID: 12481958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.477 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

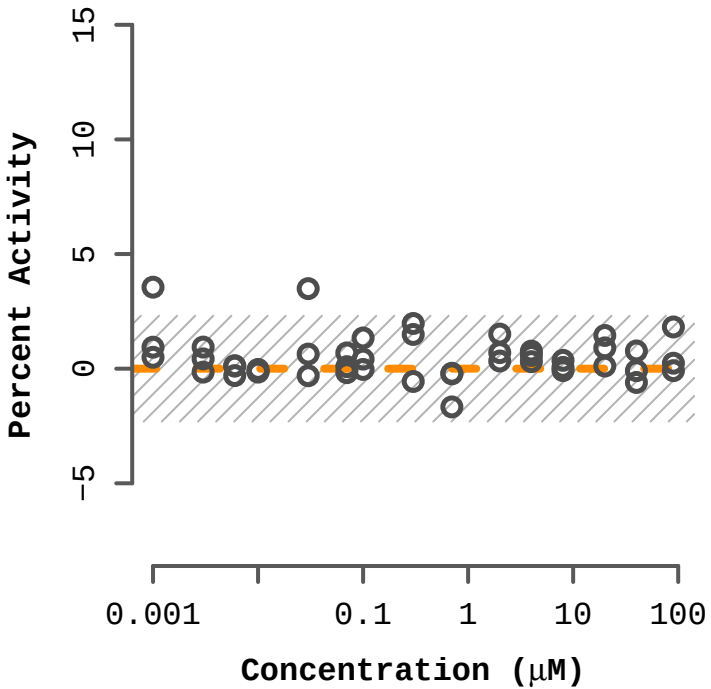
NAME: Cadmium oxide
CHID: 24715 **CASRN:** 1306-19-0
SPID(S): Tox21_202492
M4ID: 12479760

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 2.47 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

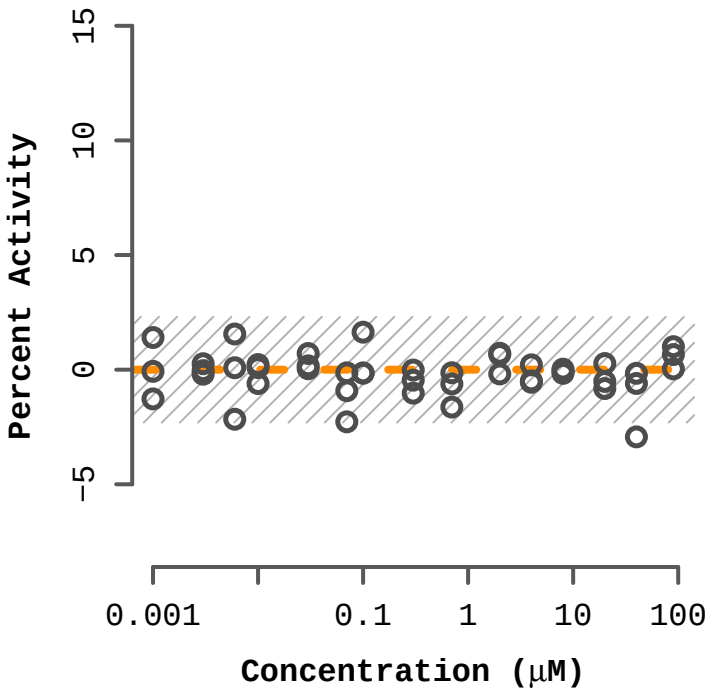
NAME: D−Camphor
CHID: 24721 CASRN: 464−49−3
SPID(S): Tox21_303052
M4ID: 12476081

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.66 MAX_MED: 1.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

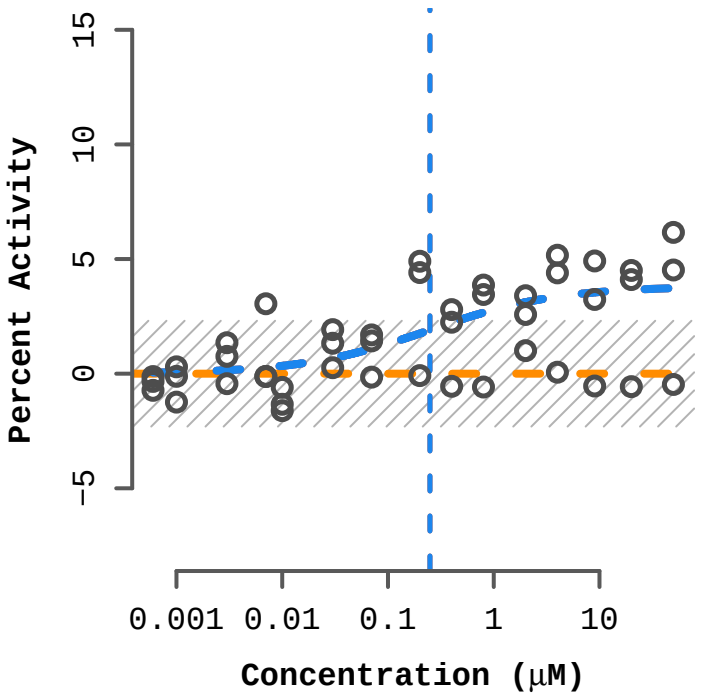
NAME: D−Camphor
CHID: 24721 **CASRN:** 464−49−3
SPID(S): Tox21_202187
M4ID: 12480065

HILL MODEL: Not applicable.

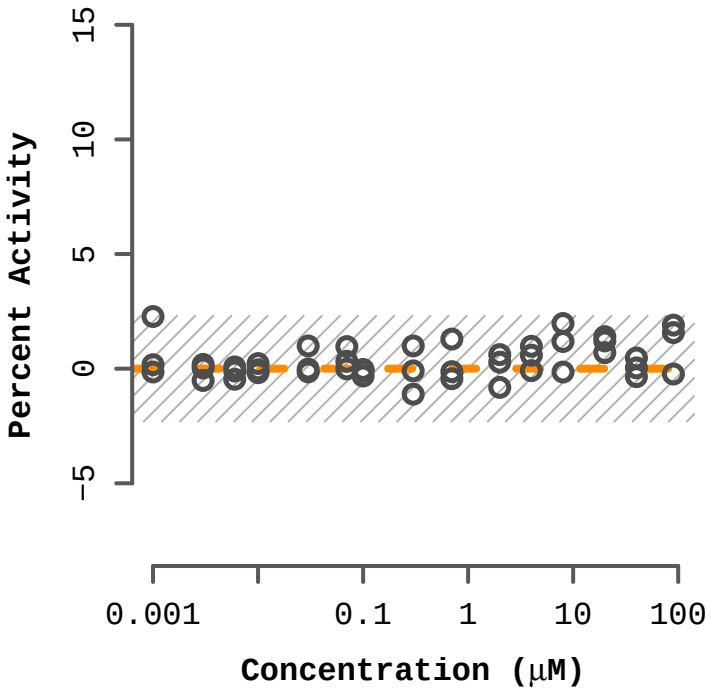
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.567 **MAX_MED:** 0.662 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    D-Camphor
CHID:    24721   CASRN: 464-49-3
SPID(S): Tox21_110995_1
M4ID:    12483958

HILL MODEL (in red):
      tp       ga       gw
val:  3.81     -0.603   0.722
sd:   1.18     0.726    0.459

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.81     -0.603   0.722    2.8      7.08
sd:   1.18     0.726    0.459    1120     7150

      CNST        HILL        GNLS
AIC:  217.86      189.34      193.34
PROB: 0           0.88        0.12
RMSE: 2.62        1.81        1.81

MAX_MEAN: 3.41      MAX_MED: 4.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

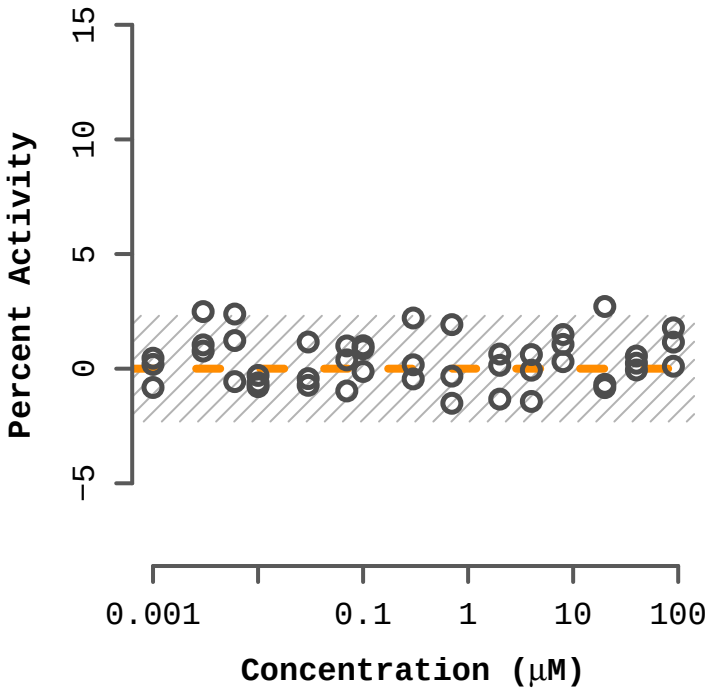
NAME: Caprylyl chloride
CHID: 24724 **CASRN:** 111-64-8
SPID(S): Tox21_202251
M4ID: 12480001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

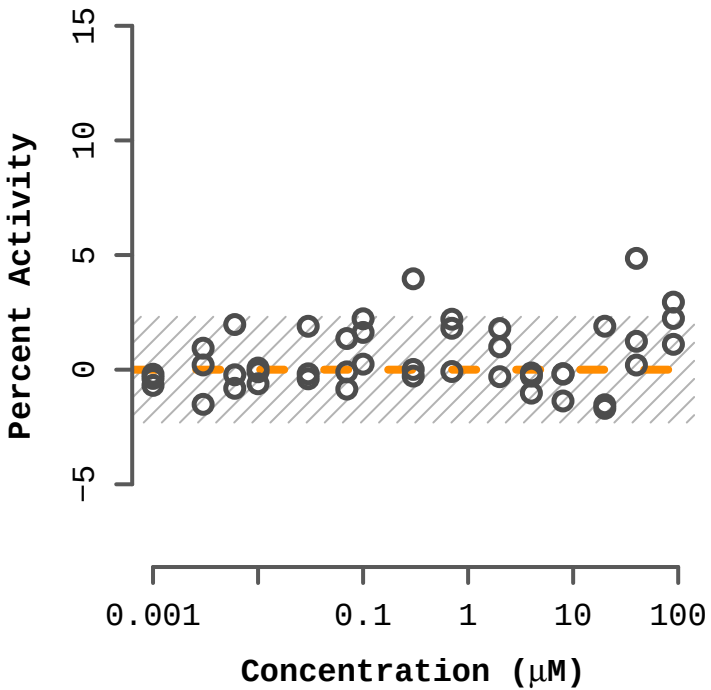
NAME: Carbamide peroxide
CHID: 24726 **CASRN:** 124-43-6
SPID(S): Tox21_302451
M4ID: 12476682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

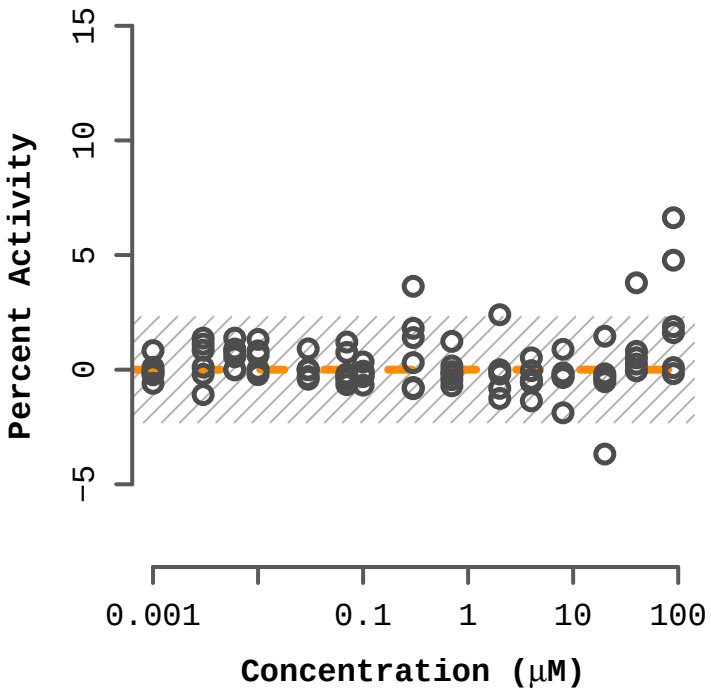
NAME: Carbendazim
CHID: 24729 **CASRN:** 10605-21-7
SPID(S): Tox21_300478
M4ID: 12478654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

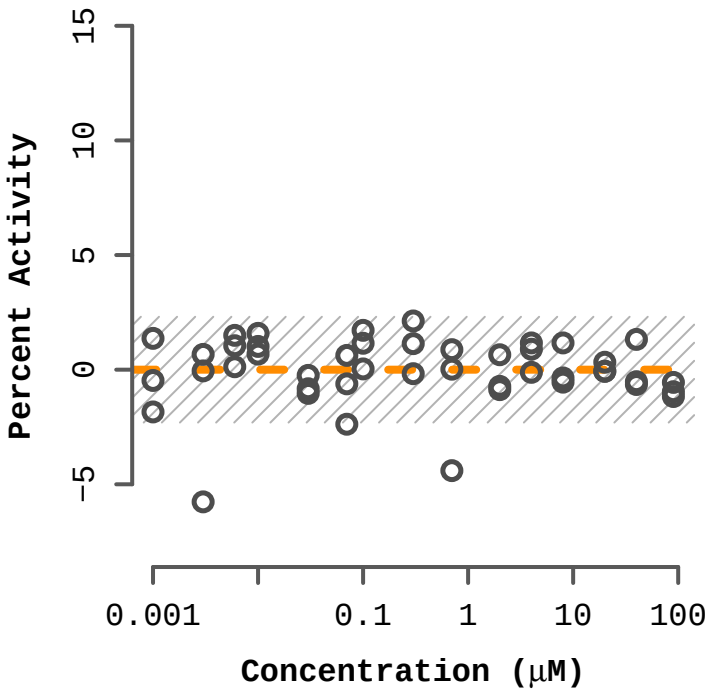
NAME: Carbendazim
CHID: 24729 **CASRN:** 10605-21-7
SPID(S): Tox21_202295
M4ID: 12479957

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	266.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.47 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

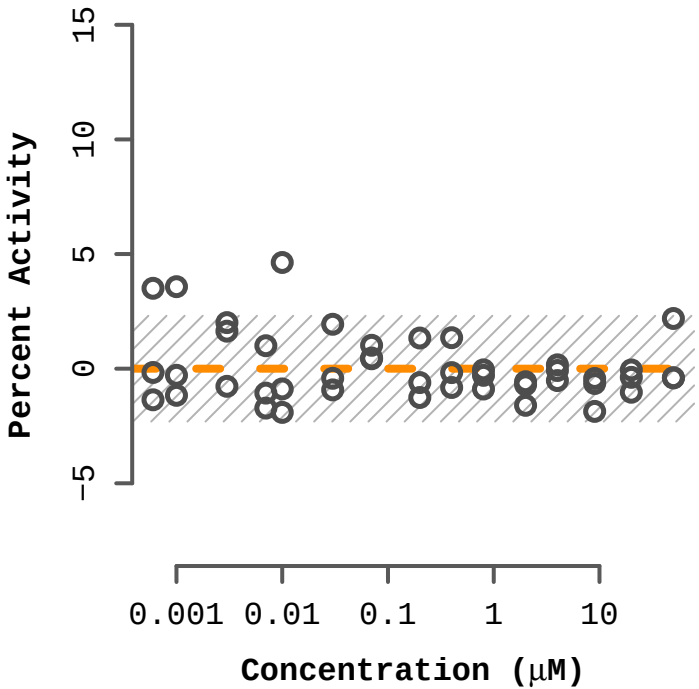
NAME: Carisoprodol
CHID: 24733 **CASRN:** 78-44-4
SPID(S): Tox21_200623
M4ID: 12481629

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

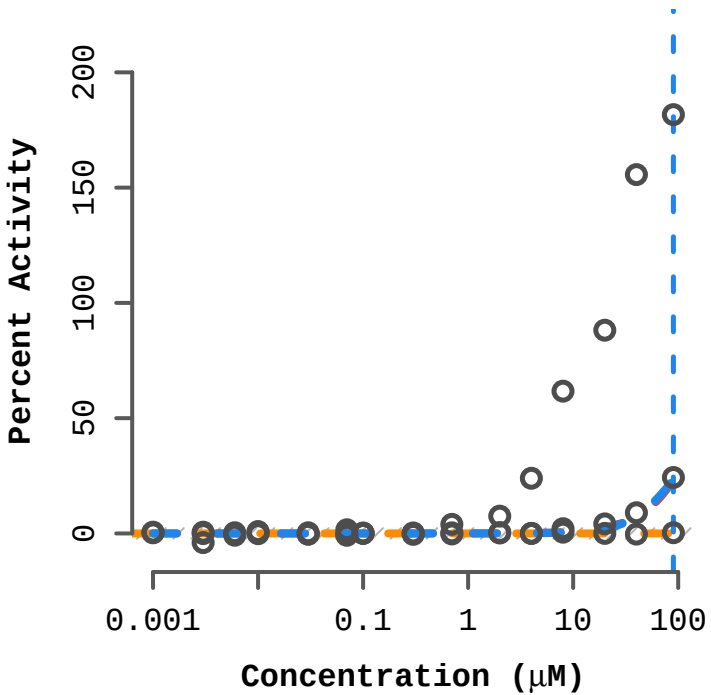
NAME: Carisoprodol
CHID: 24733 **CASRN:** 78-44-4
SPID(S): Tox21_110122_1
M4ID: 12484631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 0.96 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carveol
CHID: 24736 CASRN: 99-48-9
SPID(S): Tox21_200175
M4ID: 12482077

HILL MODEL (in red):

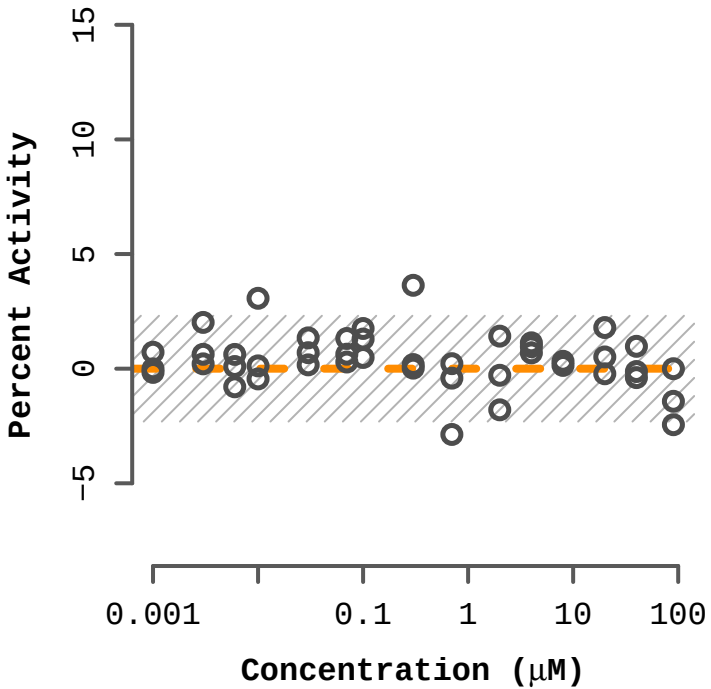
	tp	ga	gw
val:	166	2.45	1.57
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	46.6	1.95	2.04	3.02	6.14
sd:	51.6	0.466	1.1	466	2690

	CNST	HILL	GNLS
AIC:	351.63	352.64	357.03
PROB:	0.6	0.36	0.04
RMSE:	39.49	36.34	36.36

MAX_MEAN: 68.8 MAX_MED: 24.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

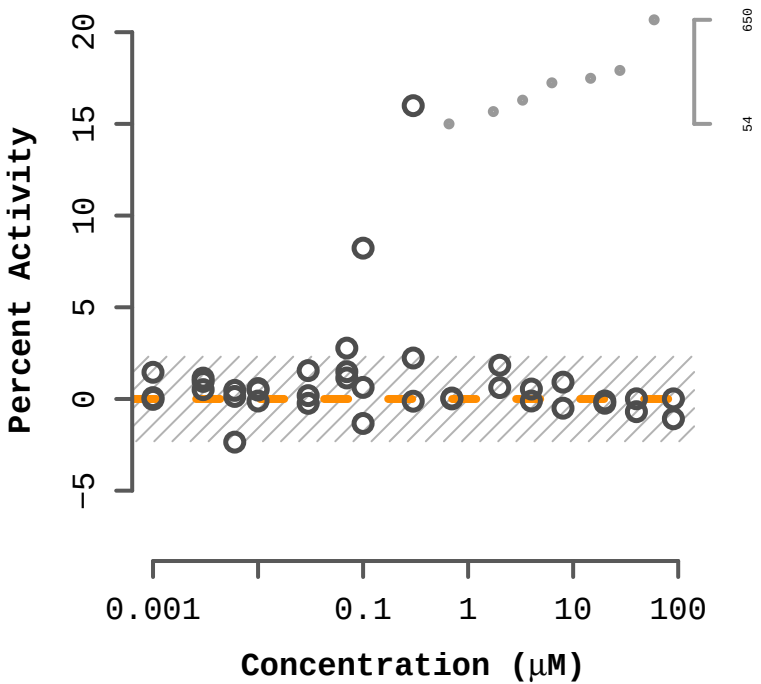
NAME: Carvyl acetate
CHID: 24738 **CASRN:** 97-42-7
SPID(S): Tox21_303105
M4ID: 12476028

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

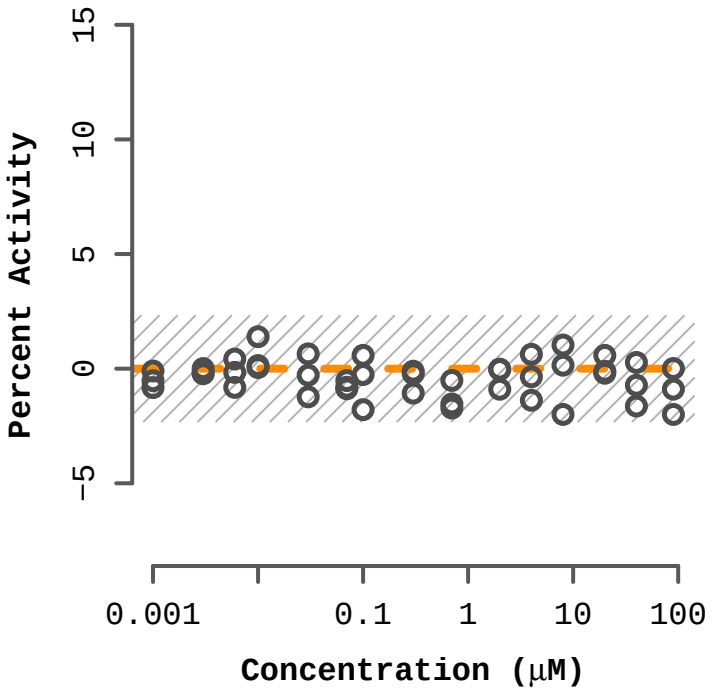
NAME: Carvyl acetate
CHID: 24738 **CASRN:** 97-42-7
SPID(S): Tox21_201728
M4ID: 12480524 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	462.76	NA	NA
PROB:	1	NA	NA
RMSE:	132.71	NA	NA

MAX_MEAN: 217 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

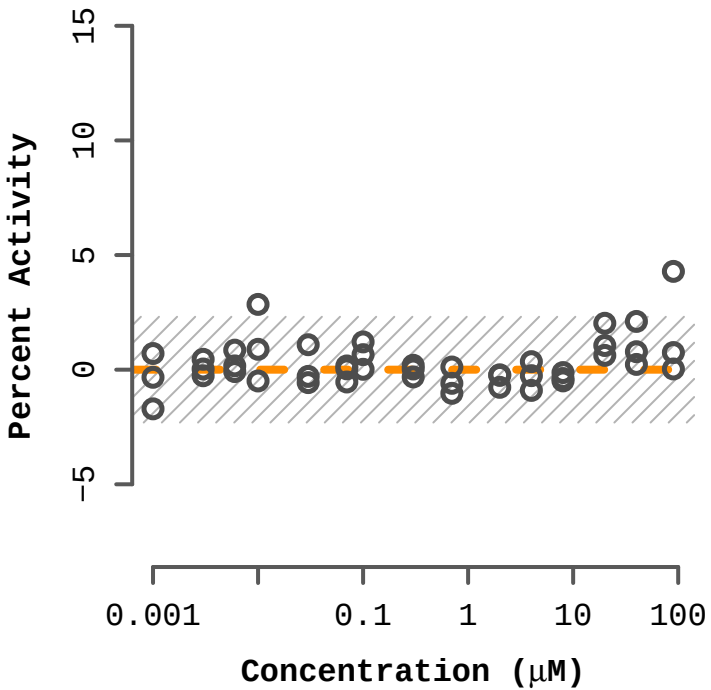
NAME: beta-Caryophyllene
CHID: 24739 CASRN: 87-44-5
SPID(S): Tox21_301497
M4ID: 12477636

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.528 MAX_MED: 0.153 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

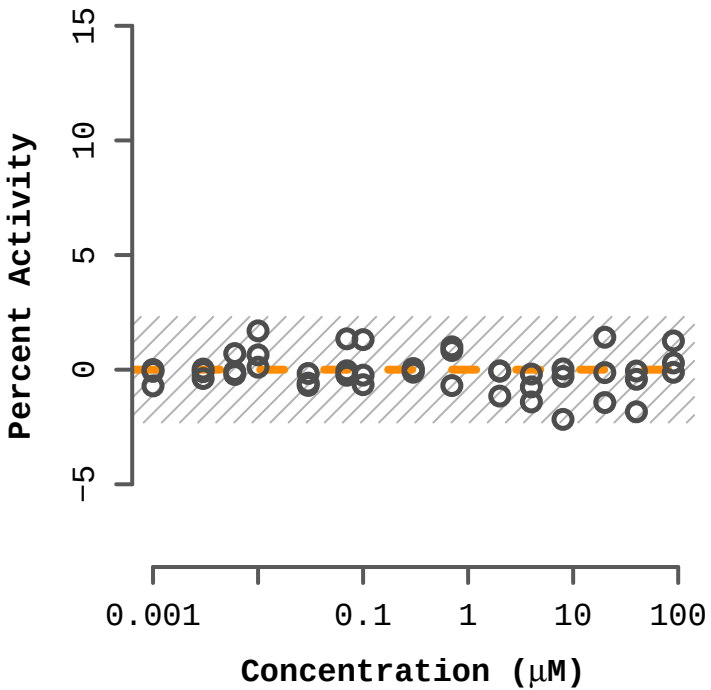
NAME: Casanthrol
CHID: 24740 **CASRN:** 8024-48-4
SPID(S): Tox21_202493
M4ID: 12479759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

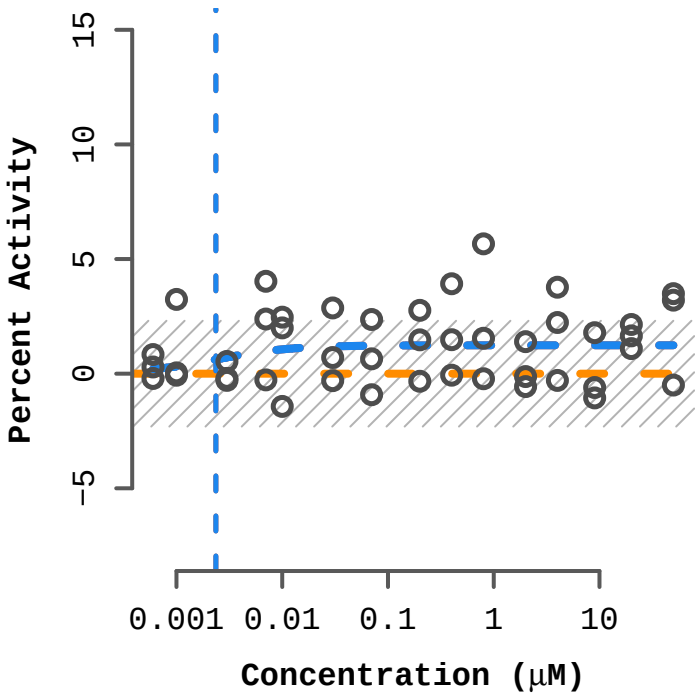
NAME: Castor oil
CHID: 24742 CASRN: 8001-79-4
SPID(S): Tox21_200934
M4ID: 12481318

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.817 MAX_MED: 0.838 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloramphenicol sodium succinate
CHID: 24747 **CASRN:** 982-57-0
SPID(S): Tox21_113484_1
M4ID: 12482635

HILL MODEL (in red):

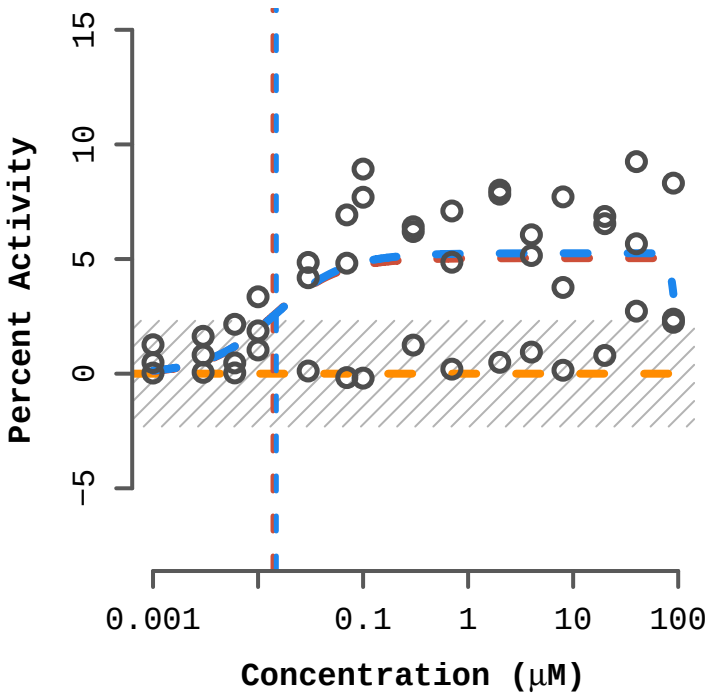
	tp	ga	gw
val:	1.24	−2.63	1.23
sd:	0.316	0.842	2.85

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.24	−2.63	1.23	3.65	3.83
sd:	0.316	0.842	2.85	1690	3310

	CNST	HILL	GNLS
AIC:	192.7	182.08	186.08
PROB:	0	0.88	0.12
RMSE:	2.01	1.61	1.61

MAX_MEAN: 2.33 **MAX_MED:** 3.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Chloroaniline
CHID: 24761 **CASRN:** 108-42-9
SPID(S): Tox21_303199
M4ID: 12475934

HILL MODEL (in red):

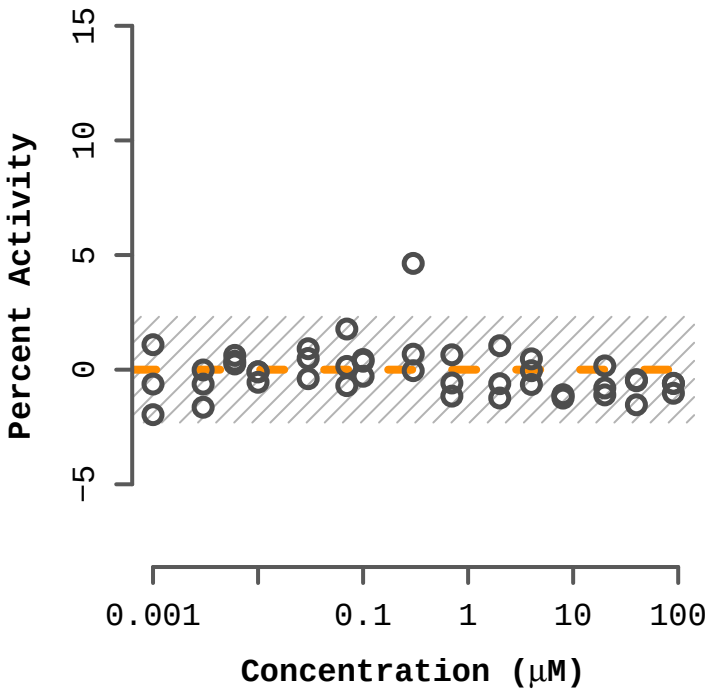
	tp	ga	gw
val:	5.04	−1.86	1.4
sd:	0.617	0.235	0.874

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.25	−1.83	1.34	1.97	14.5
sd:	0.642	0.232	0.8	0.0594	43.4

	CNST	HILL	GNLS
AIC:	272.72	226.39	229.48
PROB:	0	0.82	0.18
RMSE:	4.69	2.61	2.63

MAX_MEAN: 5.88 **MAX_MED:** 7.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

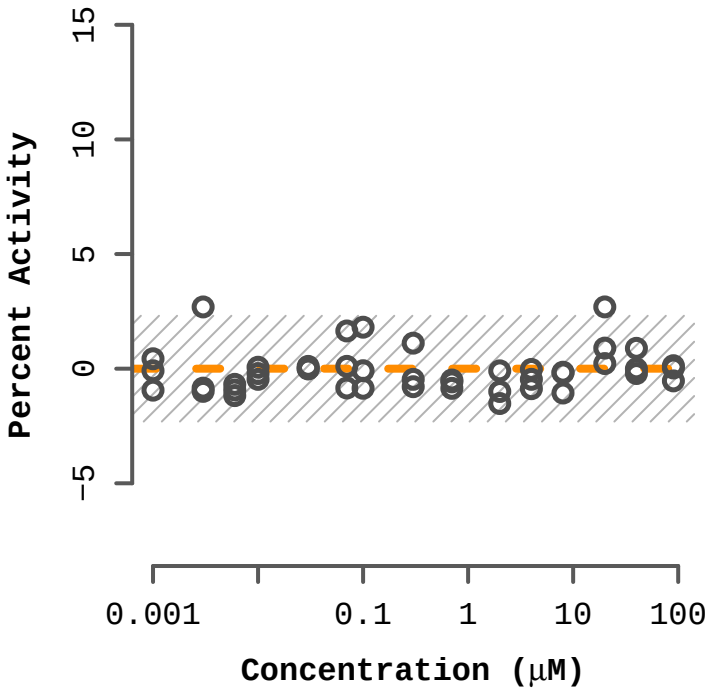
NAME: 3-Chloroaniline
CHID: 24761 **CASRN:** 108-42-9
SPID(S): Tox21_202237
M4ID: 12480015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 0.677 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

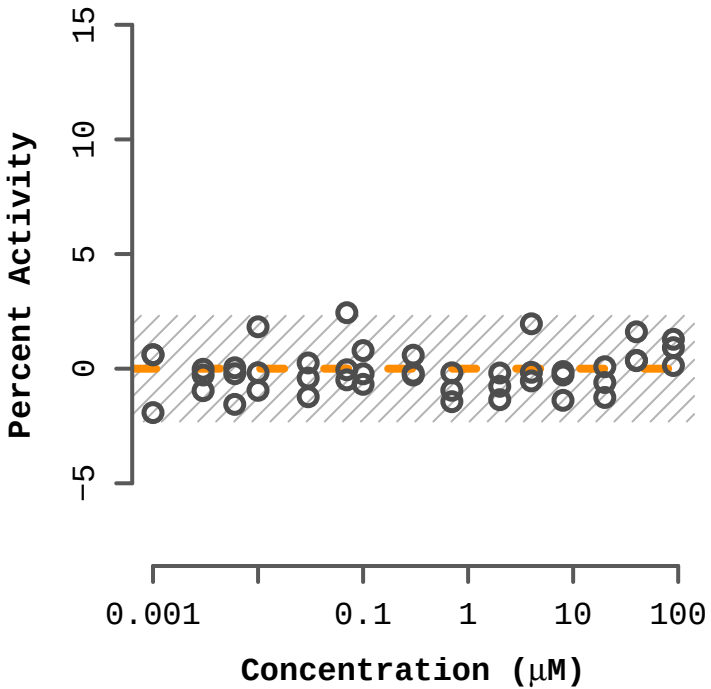
NAME: 2-Chlorobenzaldehyde
CHID: 24764 **CASRN:** 89-98-5
SPID(S): Tox21_200373
M4ID: 12481879

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

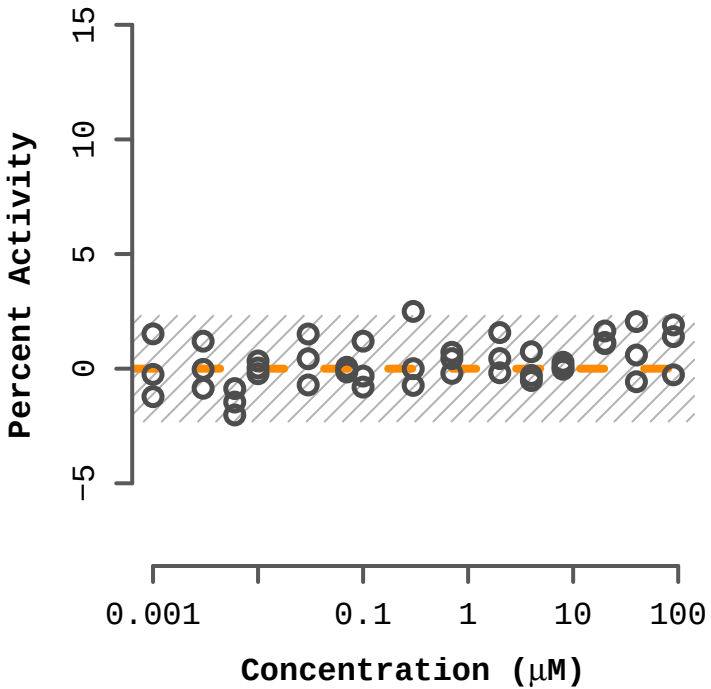
NAME: 3-Chlorobenzoic acid
CHID: 24770 **CASRN:** 535-80-8
SPID(S): Tox21_200325
M4ID: 12481927

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.78 **MAX_MED:** 0.918 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

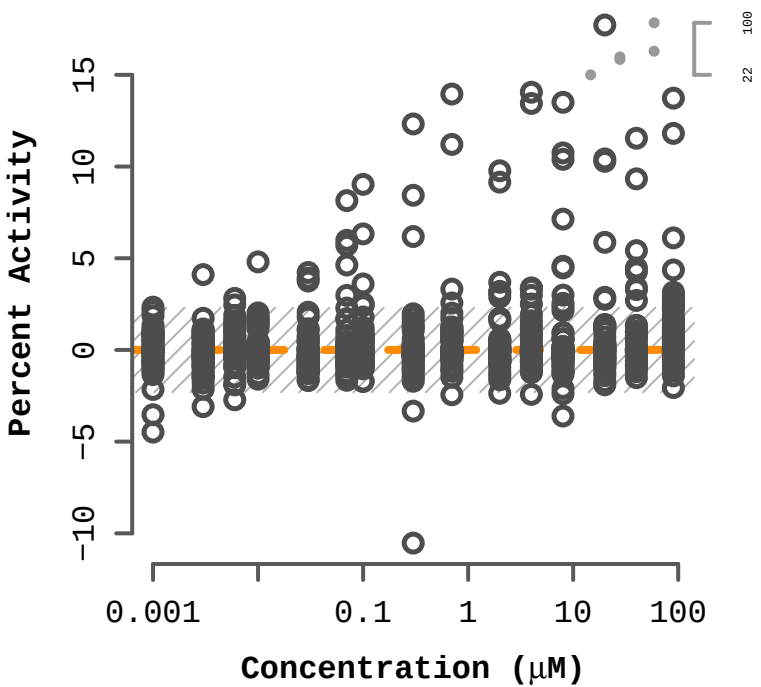
NAME: 2-Chlorobenzoic acid
CHID: 24771 **CASRN:** 118-91-2
SPID(S): Tox21_200286
M4ID: 12481966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.92	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

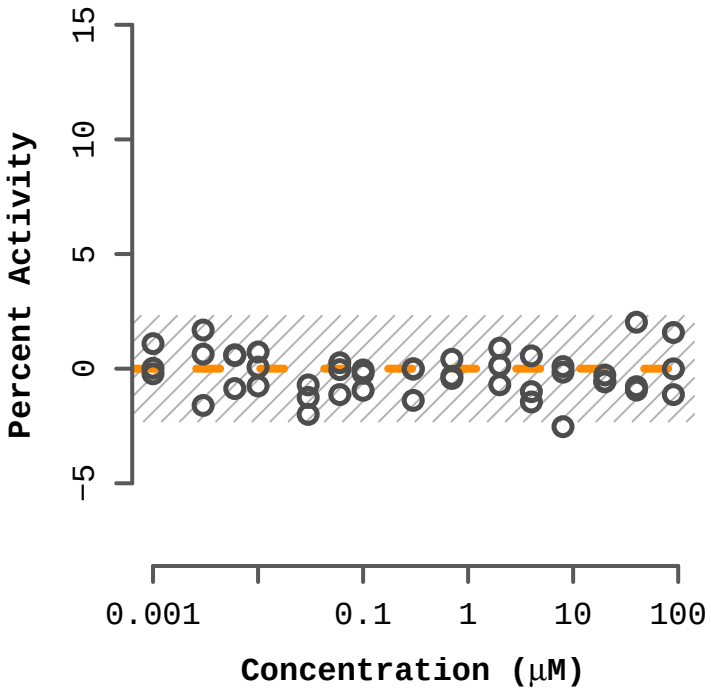
NAME: 4-Chlorobenzoic acid
CHID: 24772 **CASRN:** 74-11-3
SPID(S): Tox21_400062
M4ID: 12475075 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2805.57	NA	NA
PROB:	1	NA	NA
RMSE:	5.61	NA	NA

MAX_MEAN: 4.74 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

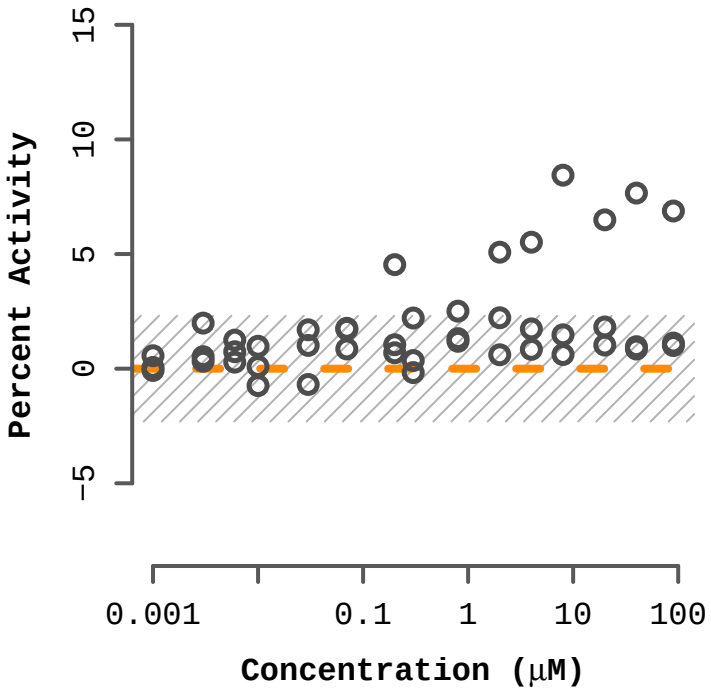
NAME: 3-Chlorobenzotrifluoride
CHID: 24773 **CASRN:** 98-15-7
SPID(S): Tox21_200385
M4ID: 12481867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.297 **MAX_MED:** 0.636 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

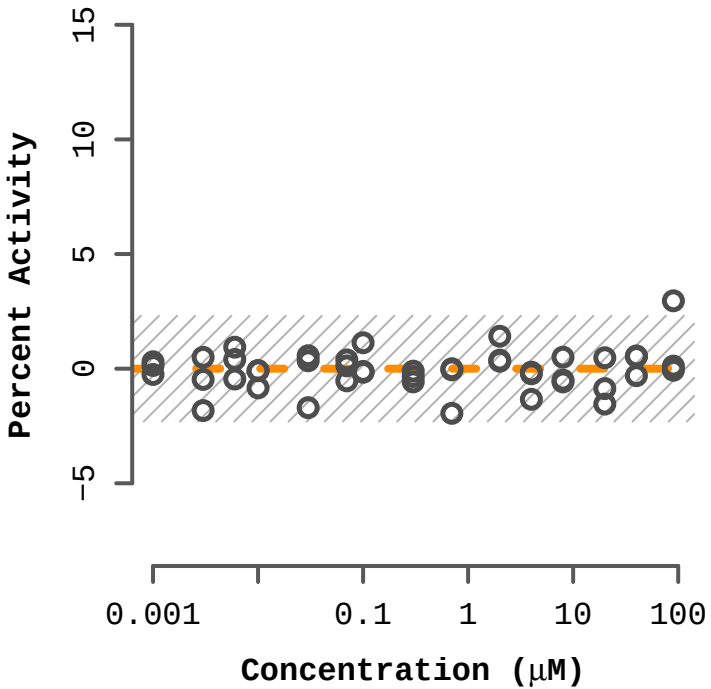
NAME: 2-Chlorobenzotrifluoride
CHID: 24774 **CASRN:** 88-16-4
SPID(S): Tox21_200751
M4ID: 12481501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.8	NA	NA

MAX_MEAN: 3.51 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

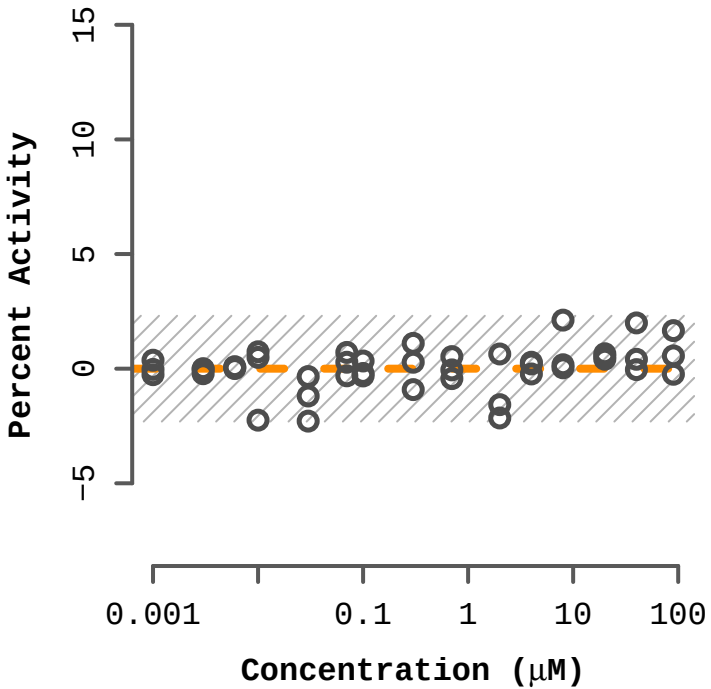
NAME: 1-Chloro-2-bromoethane
CHID: 24775 **CASRN:** 107-04-0
SPID(S): Tox21_303193
M4ID: 12475940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.533 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

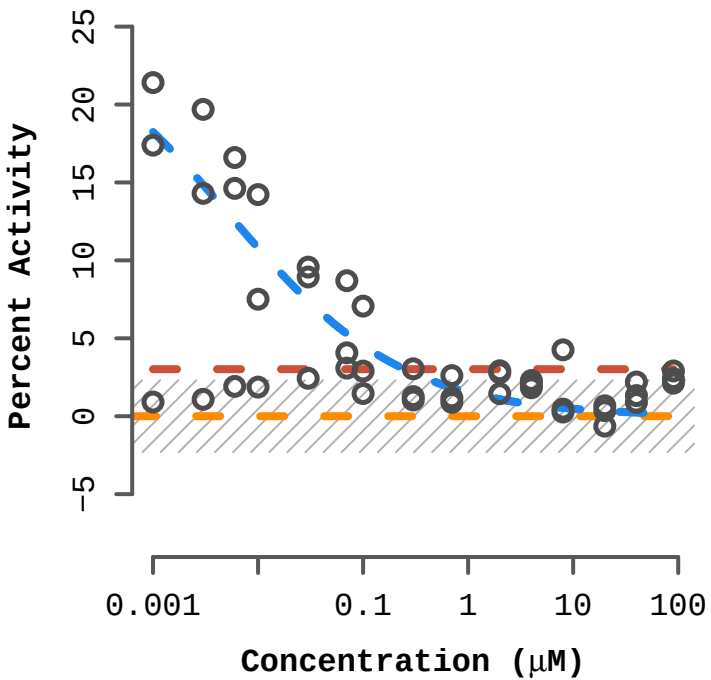
NAME: 1-Chloro-2-bromoethane
CHID: 24775 **CASRN:** 107-04-0
SPID(S): Tox21_201726
M4ID: 12480526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.789 **MAX_MED:** 0.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloropropyldimethylamine hydrochloride
CHID: 24780 CASRN: 4584-49-0
SPID(S): Tox21_303897
M4ID: 12475291

HILL MODEL (in red):

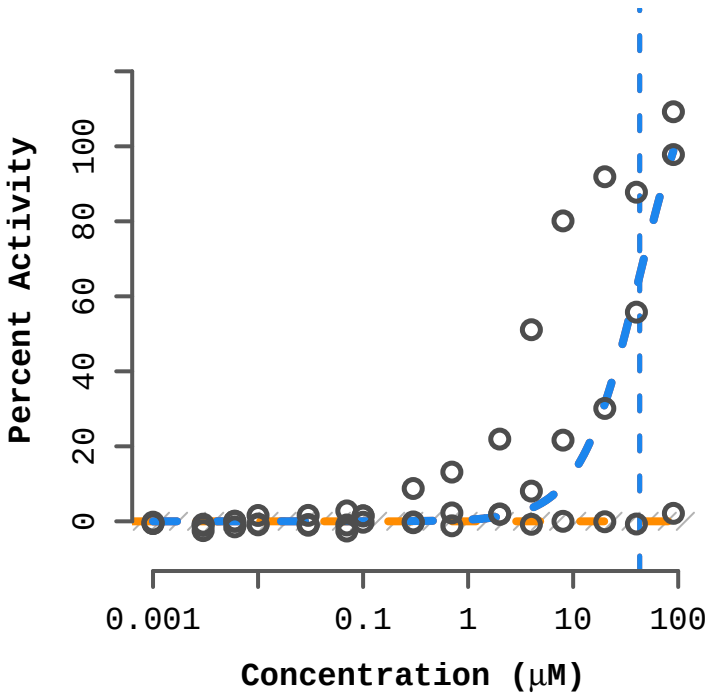
	tp	ga	gw
val:	3.02	-4.99	3.82
sd:	0.62	2230	4260

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	25.7	-4.13	5.48	-2.26	0.528
sd:	8.74	429	2070	0.644	0.157

	CNST	HILL	GNLS
AIC:	302.33	284.12	255.38
PROB:	0	0	1
RMSE:	7.52	6.02	4.43

MAX_MEAN: 13.2 MAX_MED: 17.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-1,3-dinitro-5-(trifluoromethyl)benzen
CHID: 24781 CASRN: 393-75-9
SPID(S): Tox21_200966
M4ID: 12481286

HILL MODEL (in red):

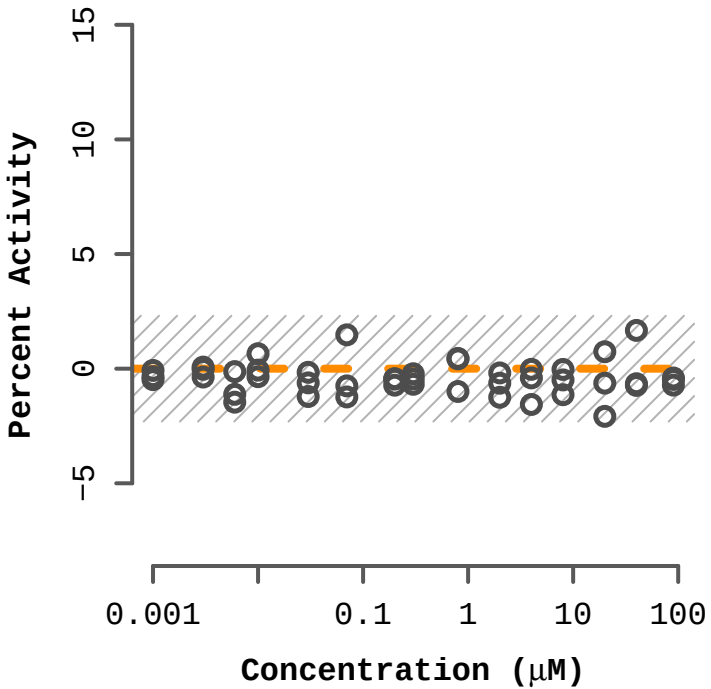
	tp	ga	gw
val:	131	1.63	1.51
sd:	29.7	0.164	0.489

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	131	1.63	1.51	3.35	7.63
sd:	29.7	0.164	0.488	14800	80800

	CNST	HILL	GNLS
AIC:	414.28	386.61	390.61
PROB:	0	0.88	0.12
RMSE:	34	24.49	24.49

MAX_MEAN: 69.7 MAX_MED: 97.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

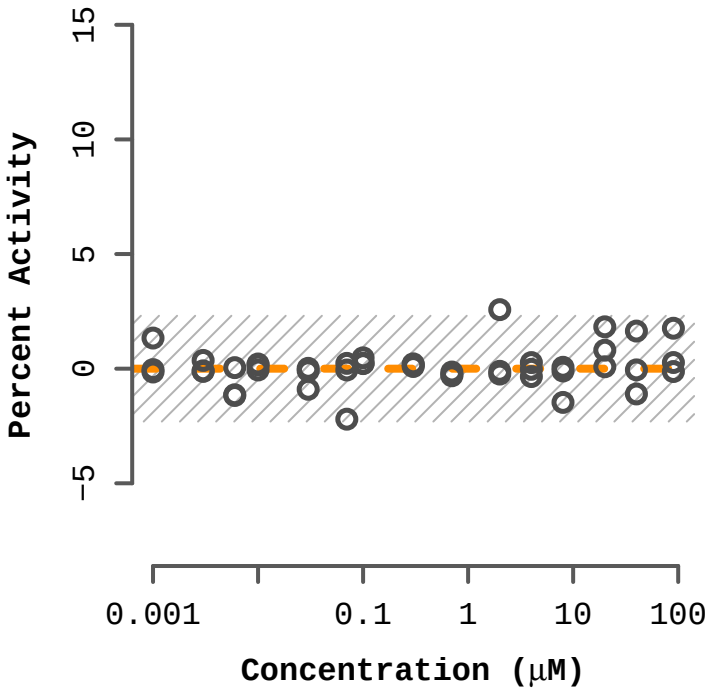
NAME: 2-Chloroethyl acrylate
CHID: 24783 CASRN: 2206-89-5
SPID(S): Tox21_202897
M4ID: 12479355

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.0955 MAX_MED: 0.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

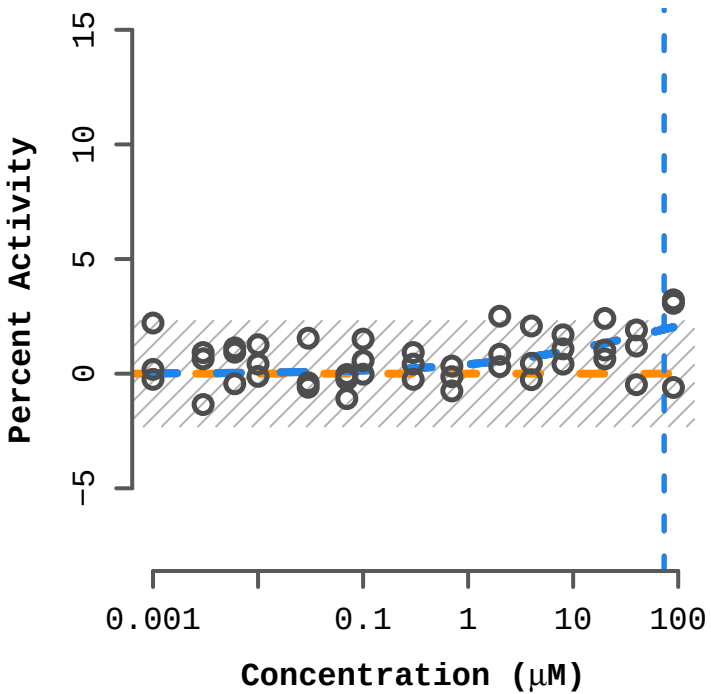
NAME: Chlorogenic acid
CHID: 24786 CASRN: 327-97-9
SPID(S): Tox21_202495
M4ID: 12479757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.907 MAX_MED: 0.807 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Chloro-2-methyl-1H-benzimidazole
CHID: 24787 **CASRN:** 2818-69-1
SPID(S): Tox21_200803
M4ID: 12481449

HILL MODEL (in red):

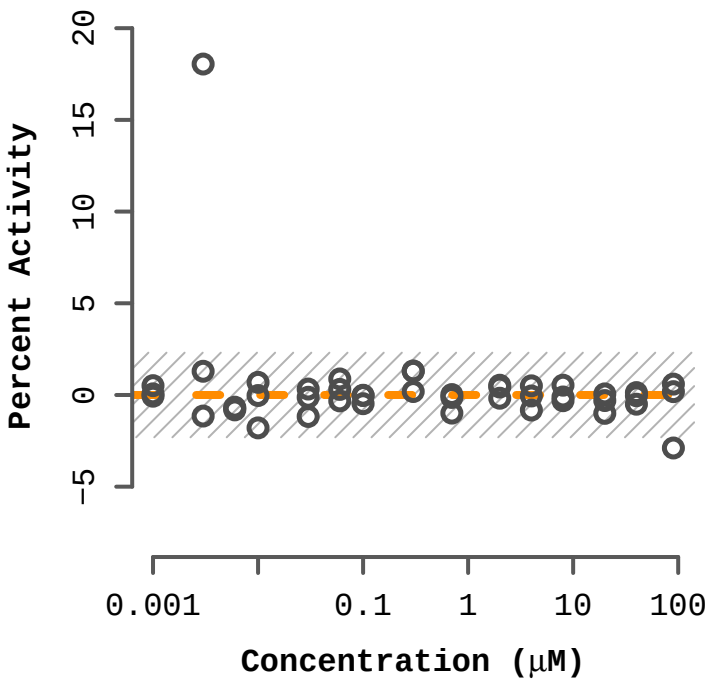
	tp	ga	gw
val:	3.87	1.87	0.497
sd:	4.27	1.68	0.294

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.87	1.87	0.497	3.71	4.41
sd:	4.26	1.68	0.294	1310	3310

	CNST	HILL	GNLS
AIC:	149.26	136.31	140.31
PROB:	0	0.88	0.12
RMSE:	1.24	0.99	0.99

MAX_MEAN: 1.9 **MAX_MED:** 3.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

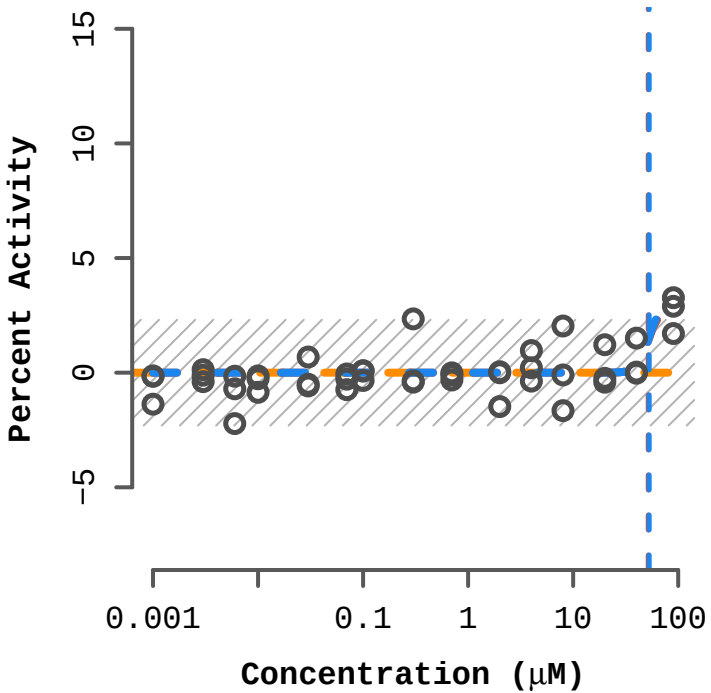
NAME: 1-Chloronaphthalene
CHID: 24791 **CASRN:** 90-13-1
SPID(S): Tox21_200823
M4ID: 12481429

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.8	NA	NA

MAX_MEAN: 6.06 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chloroneb
CHID: 24793 CASRN: 2675-77-6
SPID(S): Tox21_300739
M4ID: 12478394

HILL MODEL (in red):

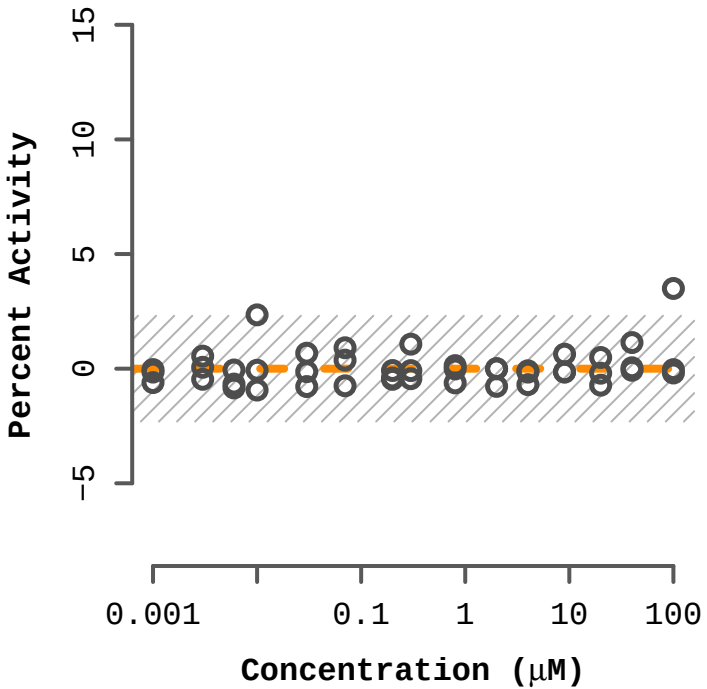
	tp	ga	gw
val:	2.79	1.71	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.28	1.72	7.94	2.33	2.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	128.97	113.31	117.31
PROB:	0	0.88	0.12
RMSE:	1.08	0.83	0.83

MAX_MEAN: 2.63 **MAX_MED:** 2.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

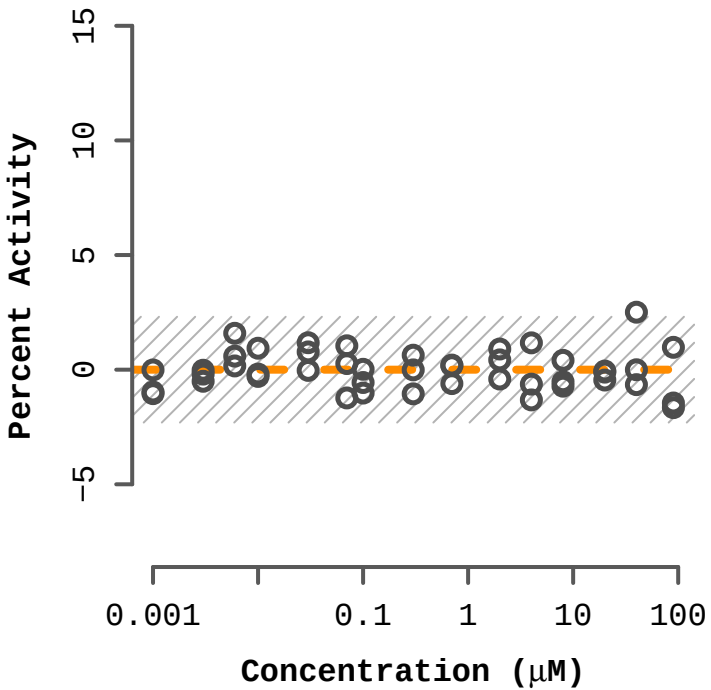
NAME: 1-Chloro-1-nitropropane
CHID: 24797 **CASRN:** 600-25-9
SPID(S): Tox21_200337
M4ID: 12481915

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.373 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

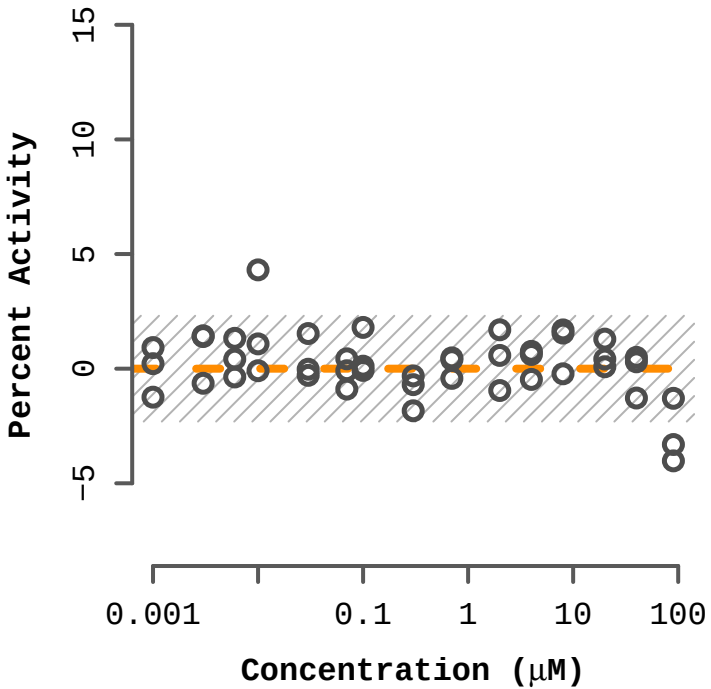
NAME: 2-Chloro-2-nitropropane
CHID: 24798 **CASRN:** 594-71-8
SPID(S): Tox21_200336
M4ID: 12481916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.776 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

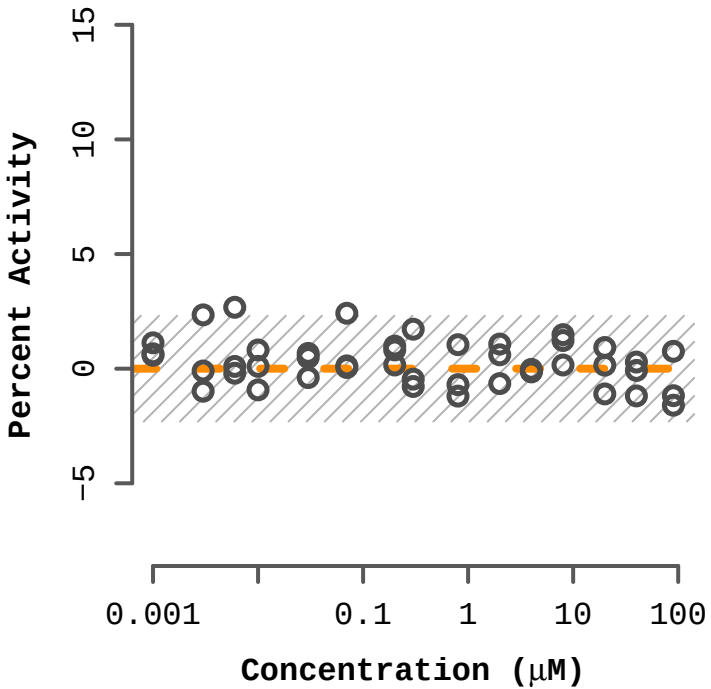
NAME: 1-Chloro-2-nitro-4-(trifluoromethyl)benzene
CHID: 24799 **CASRN:** 121-17-5
SPID(S): Tox21_303339
M4ID: 12475794

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

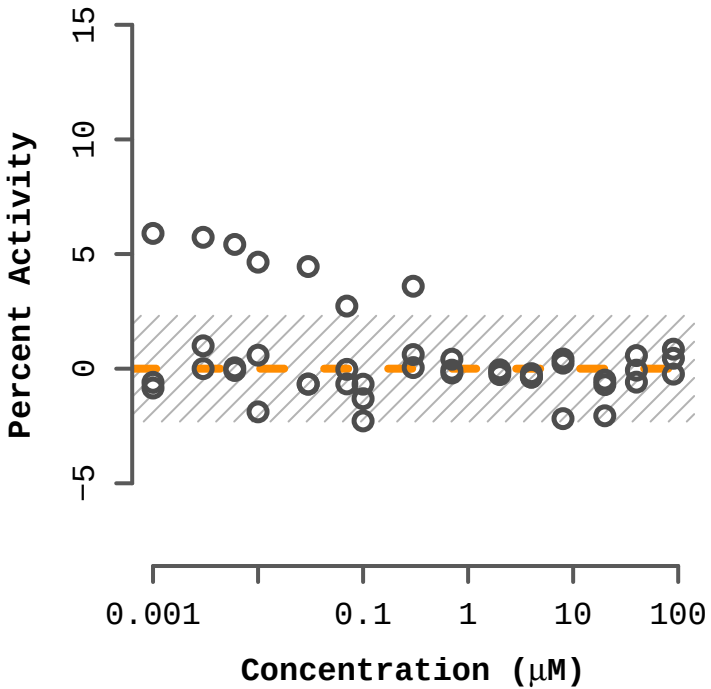
NAME: 1-Chloro-2-nitro-4-(trifluoromethyl)benzene
CHID: 24799 **CASRN:** 121-17-5
SPID(S): Tox21_201833
M4ID: 12480419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.959 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

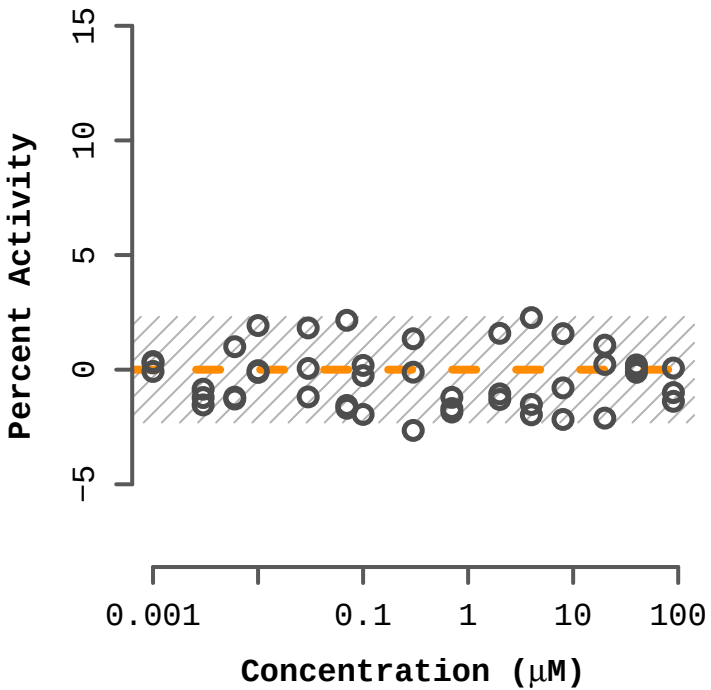
NAME: 3-Chlorophenol
CHID: 24800 **CASRN:** 108-43-0
SPID(S): Tox21_200833
M4ID: 12481419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.36	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 0.998 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

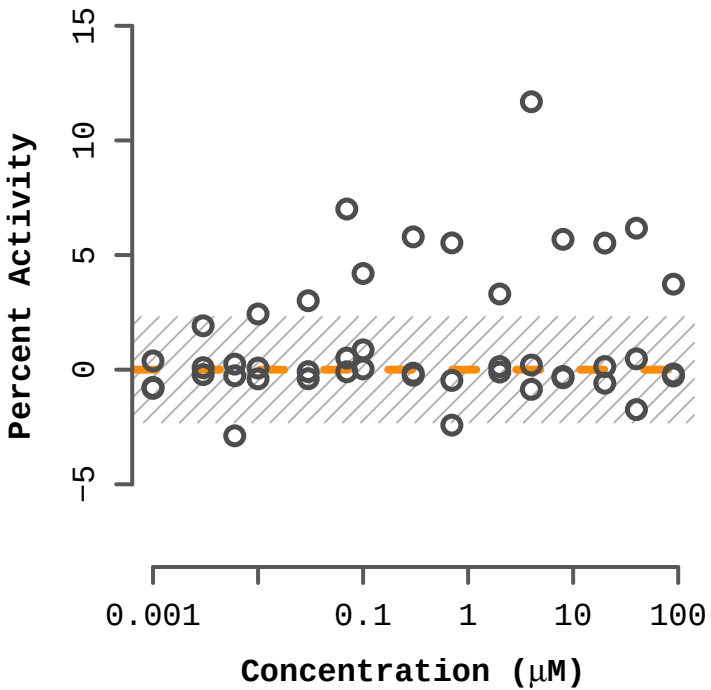
NAME: 3-Chloro-1-propanol
CHID: 24809 **CASRN:** 627-30-5
SPID(S): Tox21_303962
M4ID: 12475226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.589 **MAX_MED:** 0.298 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

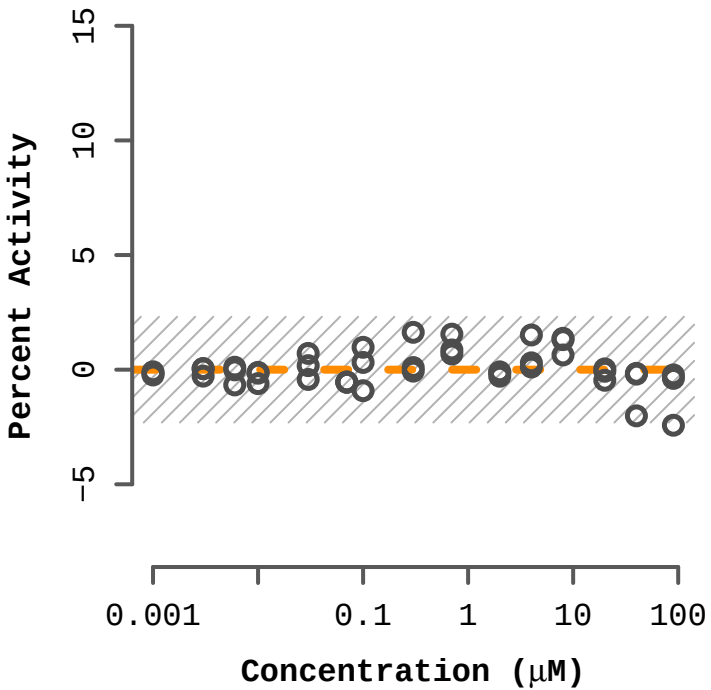
NAME: 2-Chloropyridine
CHID: 24810 **CASRN:** 109-09-1
SPID(S): Tox21_303307
M4ID: 12475826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.89	NA	NA
PROB:	1	NA	NA
RMSE:	3.11	NA	NA

MAX_MEAN: 3.68 **MAX_MED:** 0.866 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

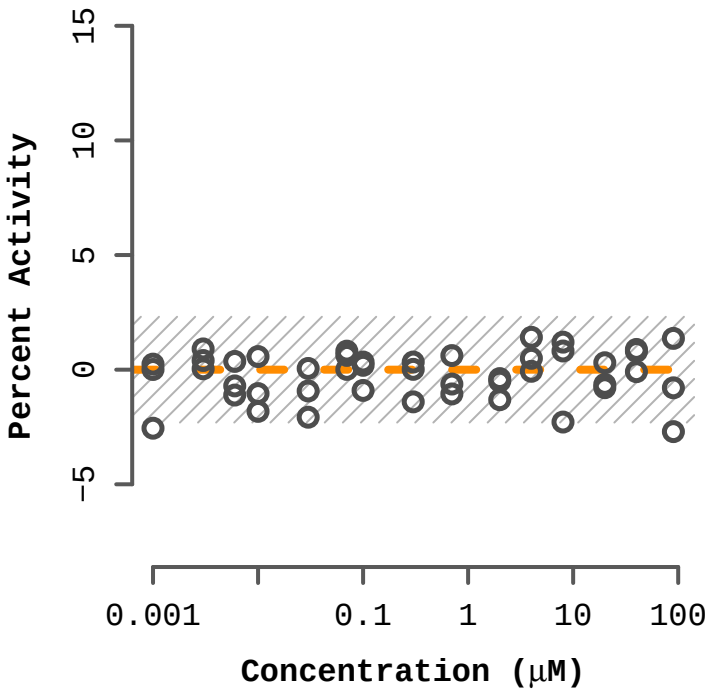
NAME: 2-Chloropyridine
CHID: 24810 **CASRN:** 109-09-1
SPID(S): Tox21_202283
M4ID: 12479969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

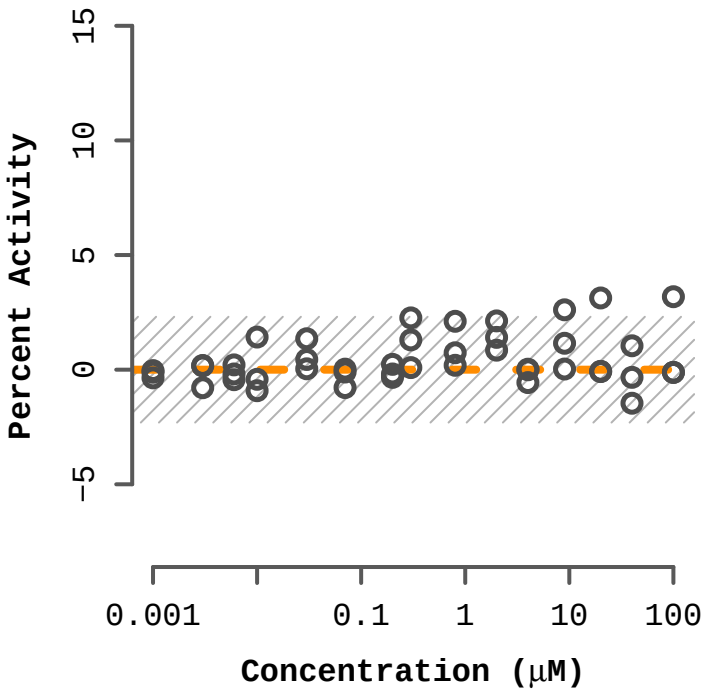
NAME: 4-Chlorotoluene
CHID: 24814 **CASRN:** 106-43-4
SPID(S): Tox21_300346
M4ID: 12478786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.613 **MAX_MED:** 0.816 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

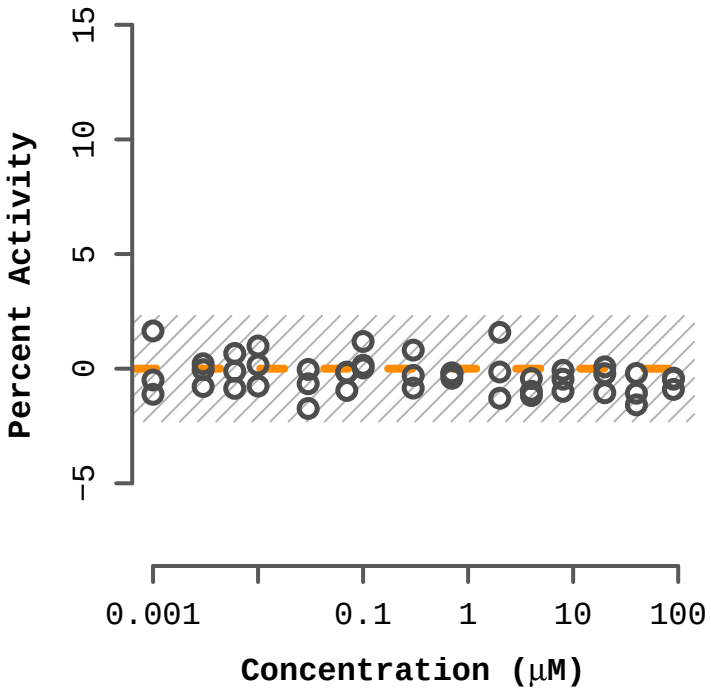
NAME: 4-Chlorotoluene
CHID: 24814 **CASRN:** 106-43-4
SPID(S): Tox21_201408
M4ID: 12480844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

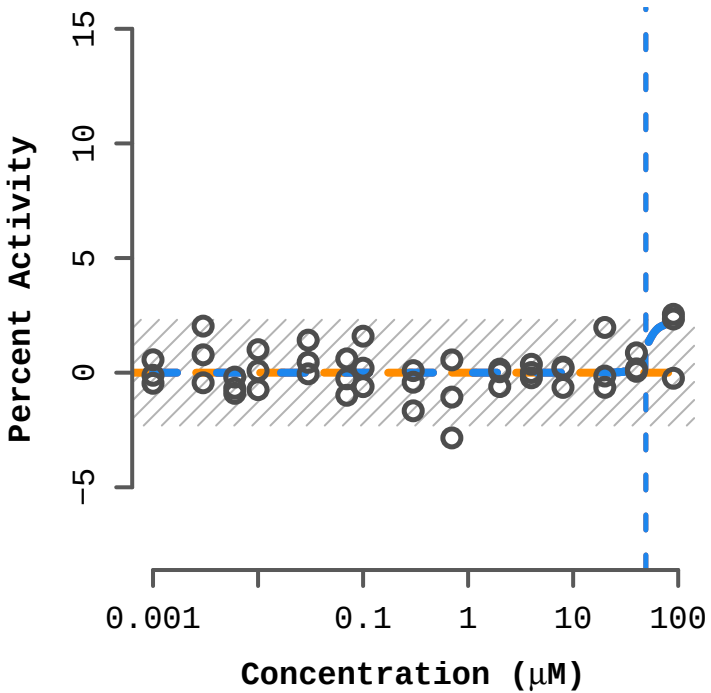
NAME: 3-Chloro-2-methylaniline
CHID: 24815 **CASRN:** 87-60-5
SPID(S): Tox21_200370
M4ID: 12481882

HILL MODEL: Not applicable.

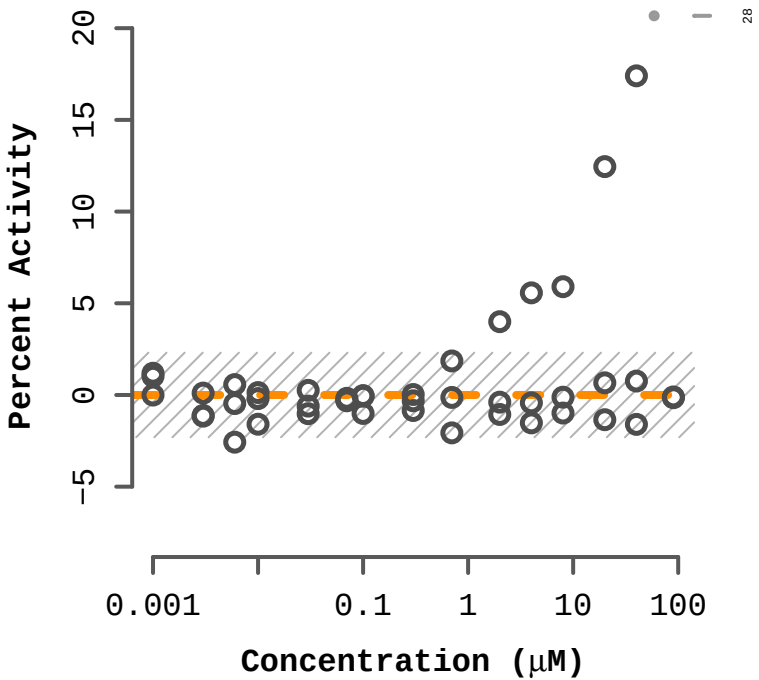
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.457 **MAX_MED:** 0.163 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Chloro-4-(trifluoromethyl)benzene
CHID:    24821   CASRN: 98-56-6
SPID(S): Tox21_303261
M4ID:    12475872

HILL MODEL (in red):
      tp       ga       gw
val:  2.16     1.69     8
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.16     1.69     8        2.37     8.83
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  126.23      124.57      128.57
PROB: 0.28        0.64        0.09
RMSE: 1.01        0.93        0.93

MAX_MEAN: 1.55      MAX_MED: 2.34      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

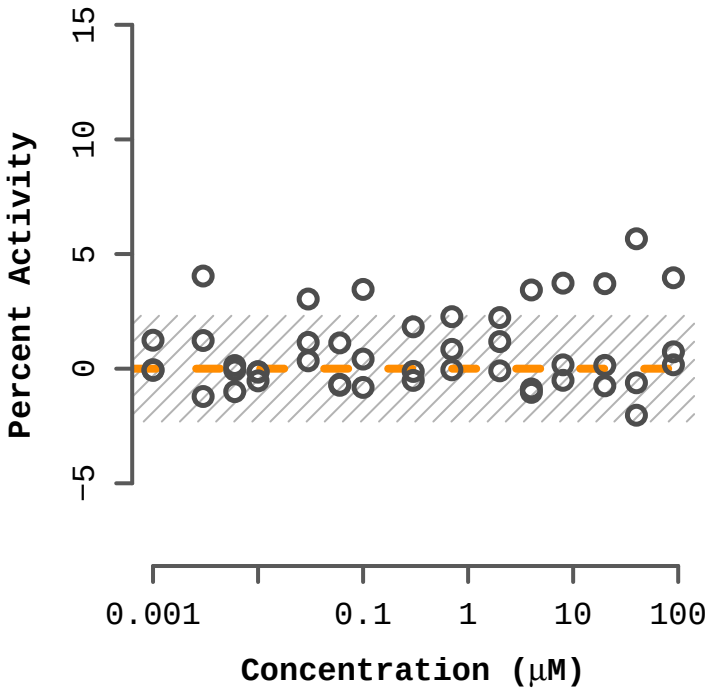
NAME: 1-Chloro-4-(trifluoromethyl)benzene
CHID: 24821 CASRN: 98-56-6
SPID(S): Tox21_201445
M4ID: 12480807 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.8	NA	NA
PROB:	1	NA	NA
RMSE:	5.44	NA	NA

MAX_MEAN: 9.09 MAX_MED: 1.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

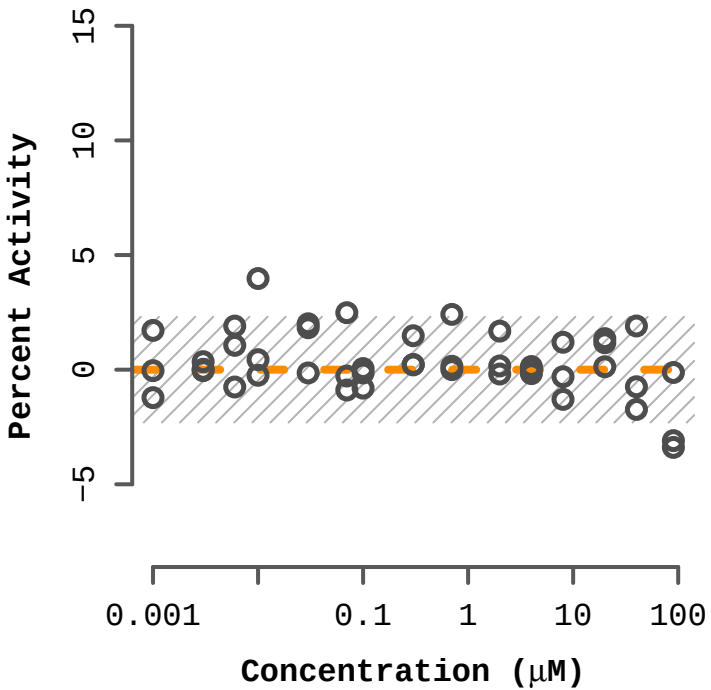
NAME: Chlorotrimethylsilane
CHID: 24822 **CASRN:** 75-77-4
SPID(S): Tox21_200221
M4ID: 12482031

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

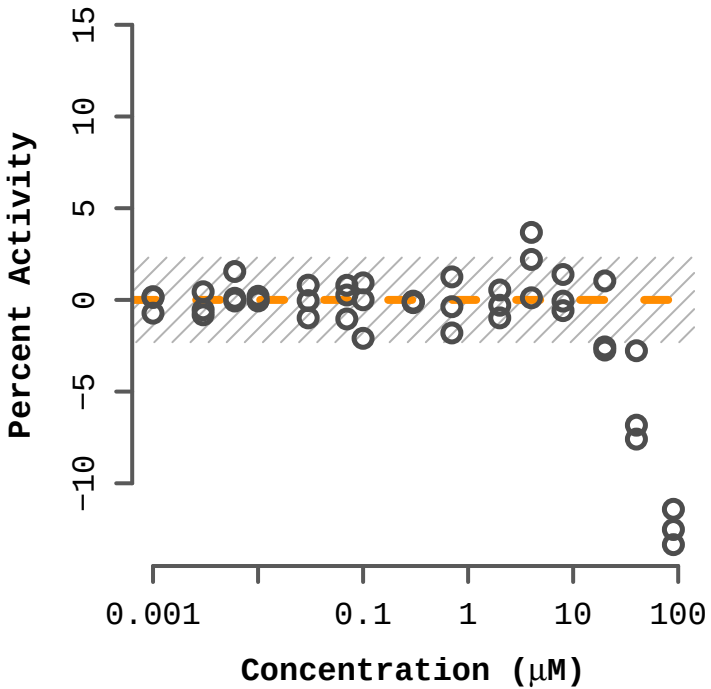
NAME: Chlorinated paraffins:C12, 60% chlorine
CHID: 24824 **CASRN:** NOCAS_24824
SPID(S): Tox21_301113
M4ID: 12478020

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

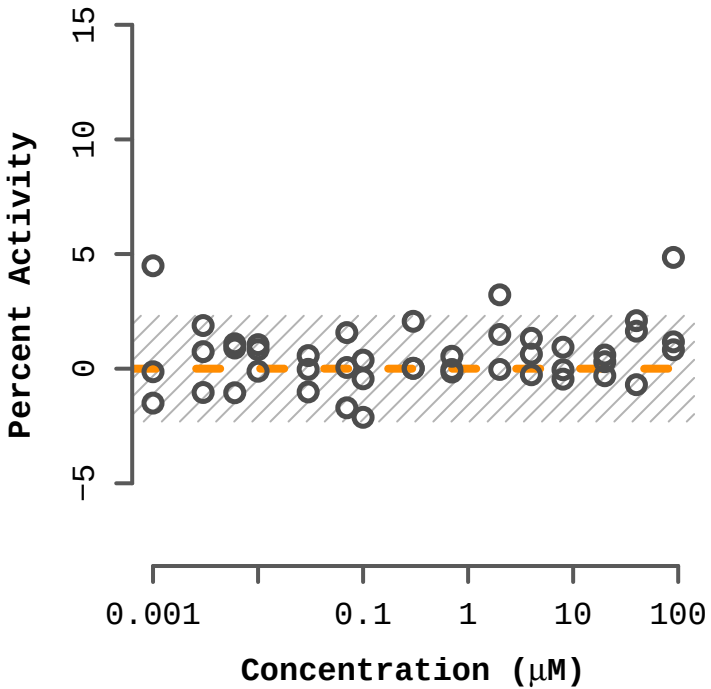
NAME: Chlorpromazine hydrochloride
CHID: 24827 **CASRN:** 69-09-0
SPID(S): Tox21_300517
M4ID: 12478615

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.75	NA	NA

MAX_MEAN: 2 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

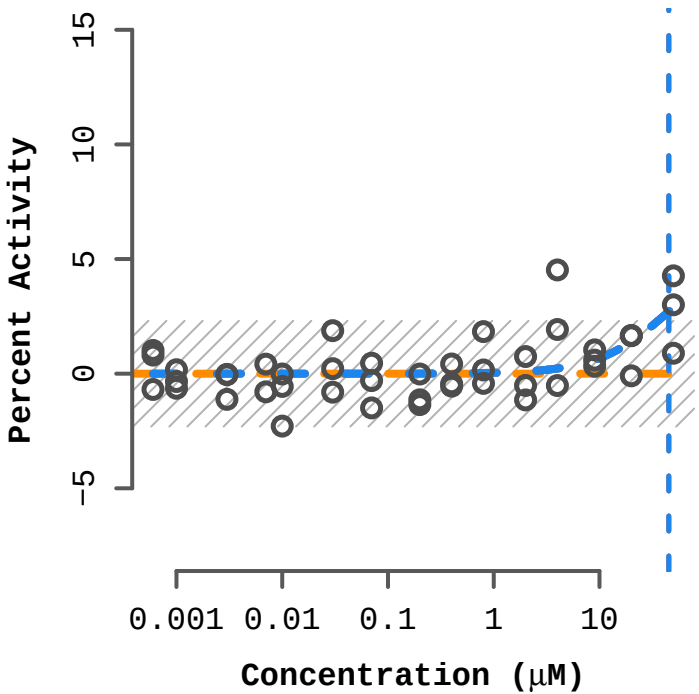
NAME: Chromium picolinate
CHID: 24831 **CASRN:** 14639-25-9
SPID(S): Tox21_200574
M4ID: 12481678

HILL MODEL: Not applicable.

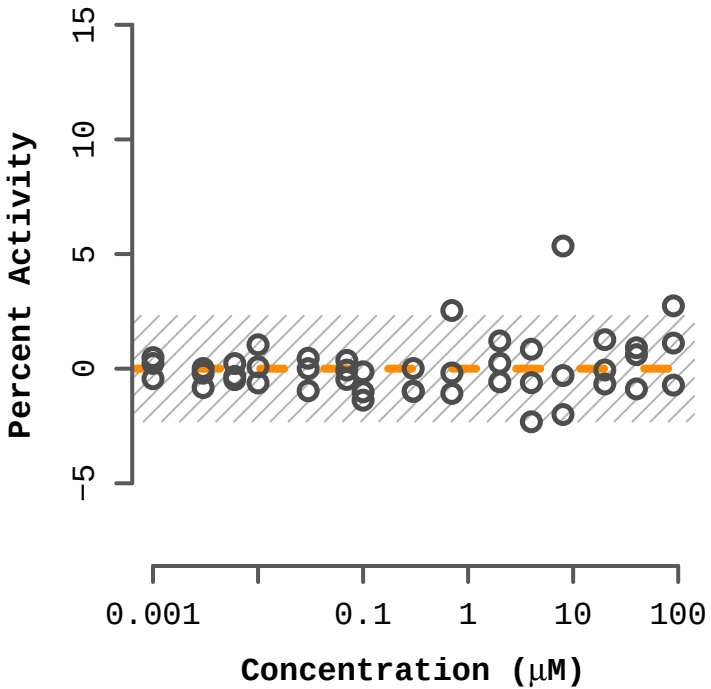
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 1.64 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Chrysophanic acid
CHID:    24832   CASRN: 481-74-3
SPID(S): Tox21_202499
M4ID:    12479753

HILL MODEL (in red):
      tp       ga       gw
val:  5.43     1.66     1.29
sd:   6.46     0.777    0.809

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.43     1.66     1.29     3.31     4.29
sd:   6.45     0.777    0.809    1090     2930

      CNST        HILL        GNLS
AIC:  149.67      139.18      143.18
PROB: 0           0.88        0.12
RMSE: 1.4         1.14        1.14

MAX_MEAN: 2.72      MAX_MED: 3.01      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

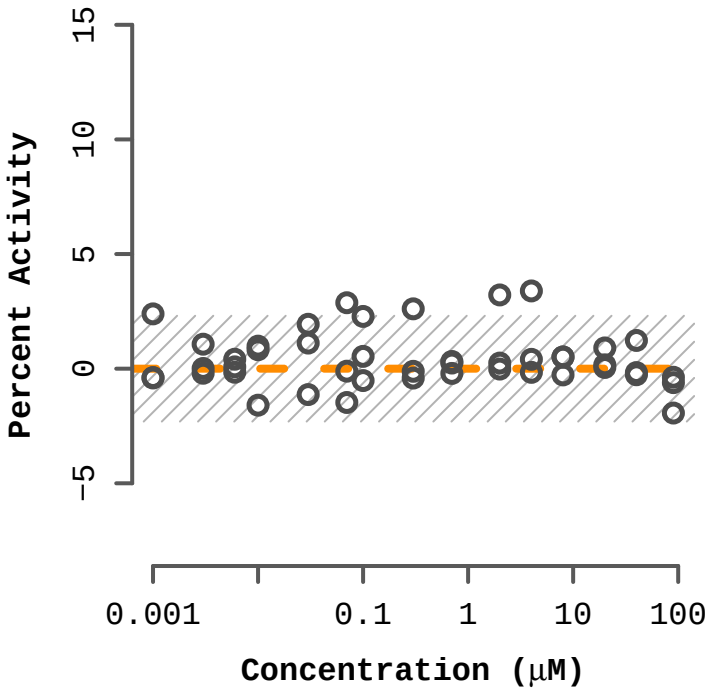
NAME: (2E)-3-Phenylprop-2-enal
CHID: 24834 **CASRN:** 14371-10-9
SPID(S): Tox21_303271
M4ID: 12475862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

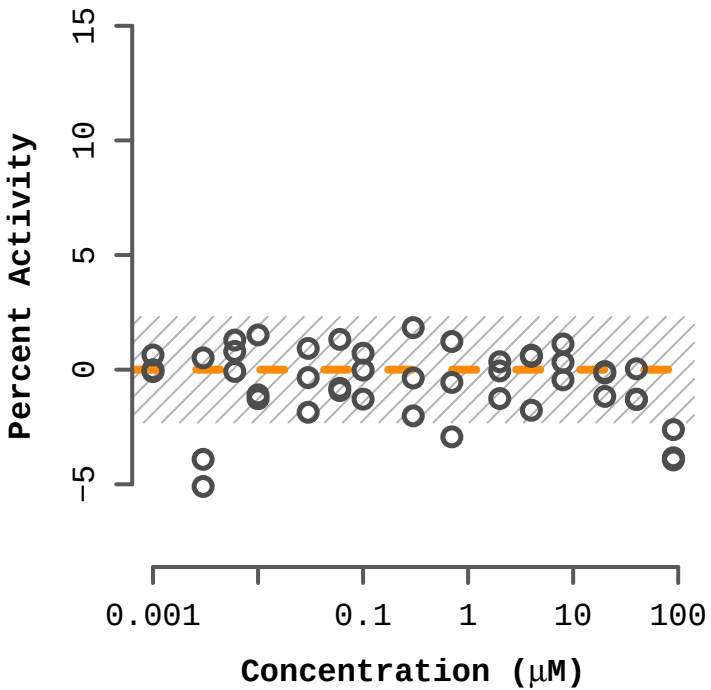
NAME: (2E)-3-Phenylprop-2-enal
CHID: 24834 **CASRN:** 14371-10-9
SPID(S): Tox21_201804
M4ID: 12480448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

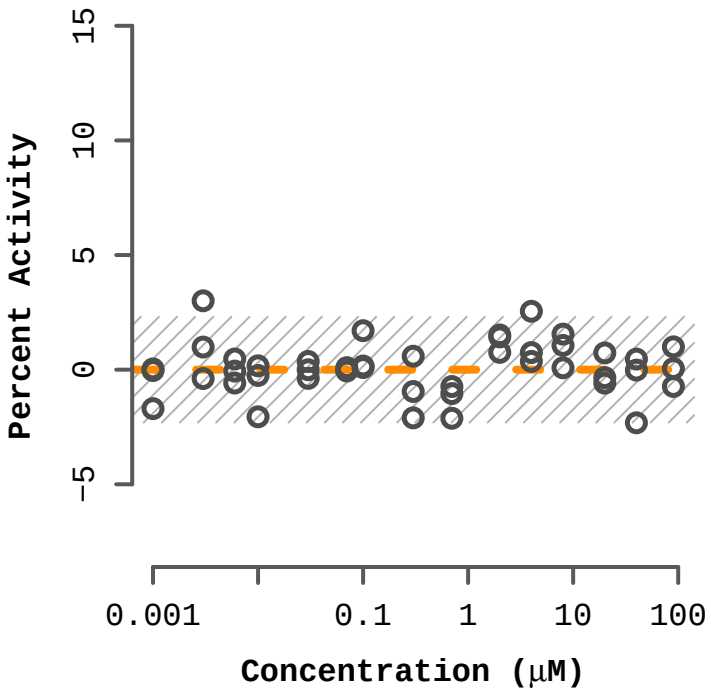
NAME: 3-Phenylprop-2-enal
CHID: 24835 **CASRN:** 104-55-2
SPID(S): Tox21_200272
M4ID: 12481980

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 0.797 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

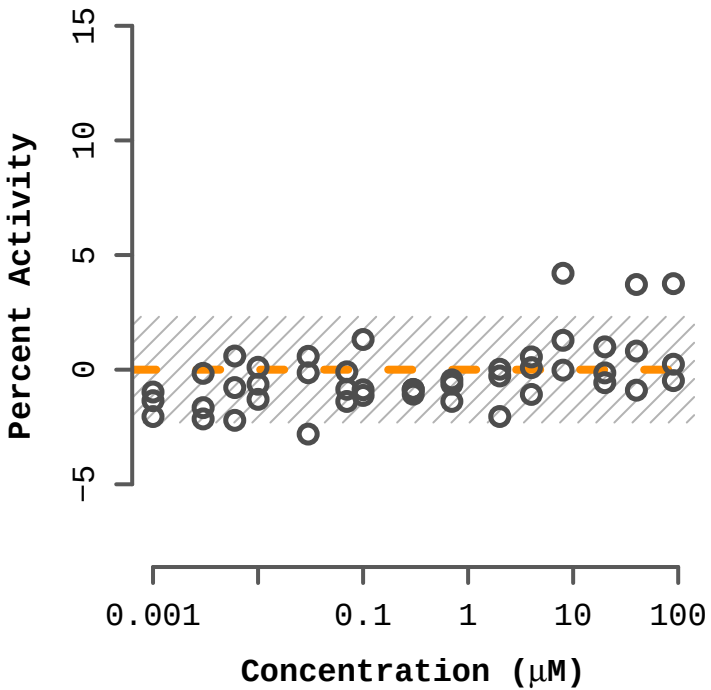
NAME: 3,7-Dimethyl-2,6-octadienal
CHID: 24836 **CASRN:** 5392-40-5
SPID(S): Tox21_300095
M4ID: 12479035

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

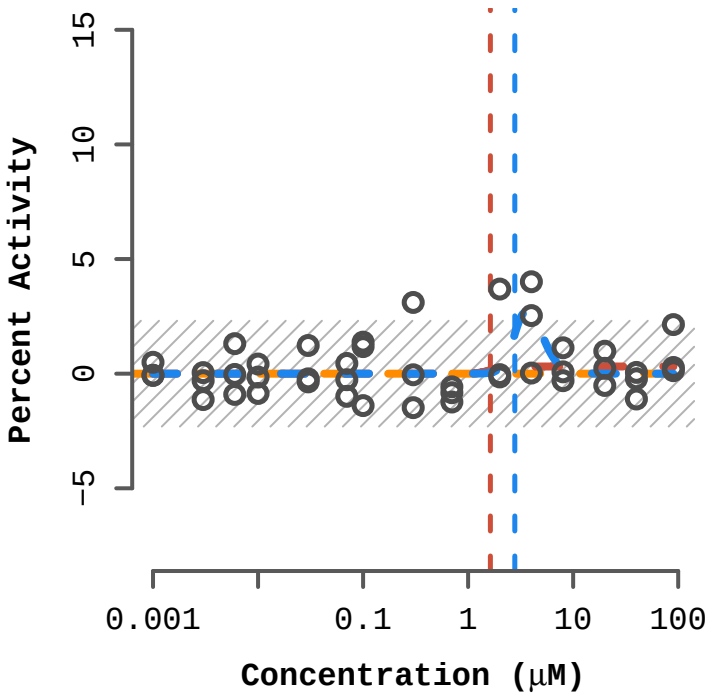
NAME: 3,7-Dimethyl-2,6-octadienal
CHID: 24836 **CASRN:** 5392-40-5
SPID(S): Tox21_202093
M4ID: 12480159

HILL MODEL: Not applicable.

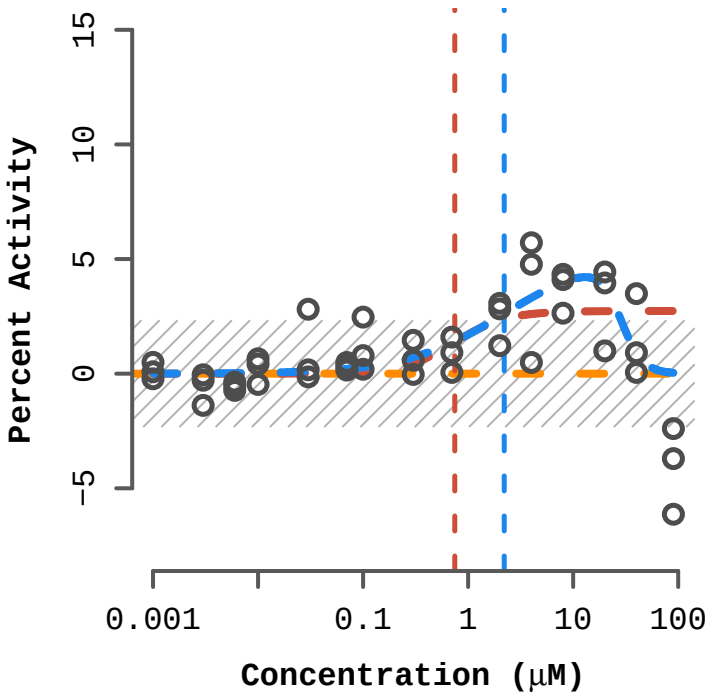
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.28 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Citral diethyl acetal
CHID:    24837   CASRN: 7492-66-2
SPID(S): Tox21_304016
M4ID:    12475172

HILL MODEL (in red):
      tp       ga       gw
val:  0.313    0.212    8
sd:   0.258    0.67     26.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.64     0.444    7.99     0.694    5.31
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  143.14      147.45      145.9
PROB: 0.73        0.08        0.18
RMSE: 1.27        1.21        1.12

MAX_MEAN: 2.19      MAX_MED: 2.54      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Solvent Red 80
CHID: 24838 CASRN: 6358-53-8
SPID(S): Tox21_303891
M4ID: 12475297

HILL MODEL (in red):

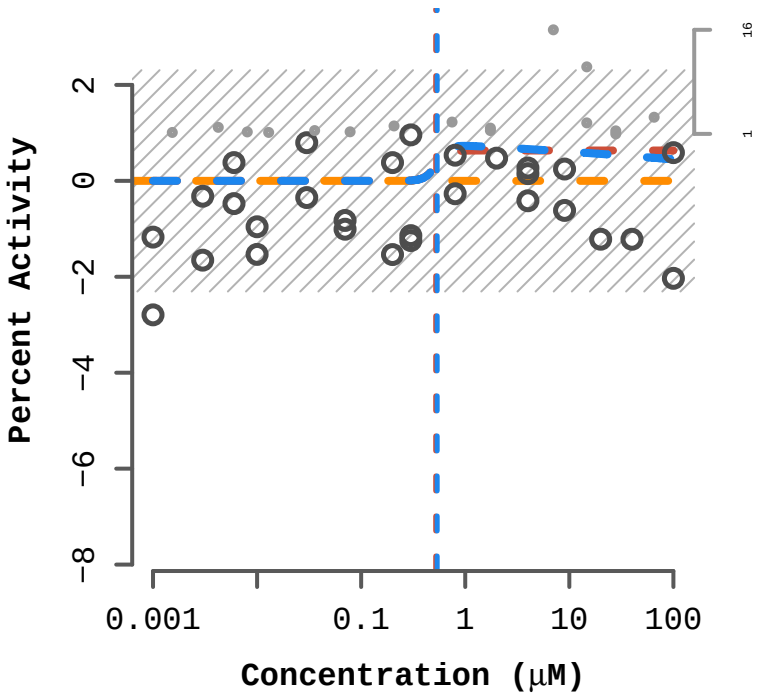
	tp	ga	gw
val:	2.73	−0.127	1.77
sd:	0.59	0.414	2.61

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.22	0.344	0.921	1.45	4.24
sd:	3.04	0.671	0.652	0.142	2.3

	CNST	HILL	GNLS
AIC:	204.16	187.22	169.72
PROB:	0	0	1
RMSE:	2.35	2.17	1.58

MAX_MEAN: 3.69 MAX_MED: 4.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cobaltocene
CHID: 24840 CASRN: 1277-43-6
SPID(S): Tox21_202502
M4ID: 12479750 BRK

HILL MODEL (in red):

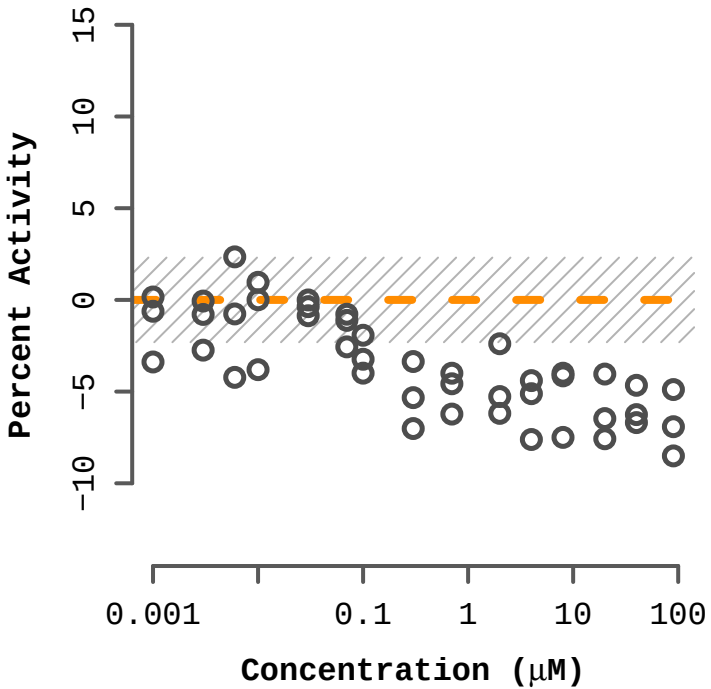
	tp	ga	gw
val:	0.632	−0.284	8
sd:	0.366	0.513	19.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.932	−0.27	8	1.9	0.3
sd:	3.82	0.559	19.8	16.8	1.4

	CNST	HILL	GNLS
AIC:	194.71	197.69	201.63
PROB:	0.8	0.18	0.02
RMSE:	3.13	2.99	3

MAX_MEAN: 5.11 MAX_MED: 2.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

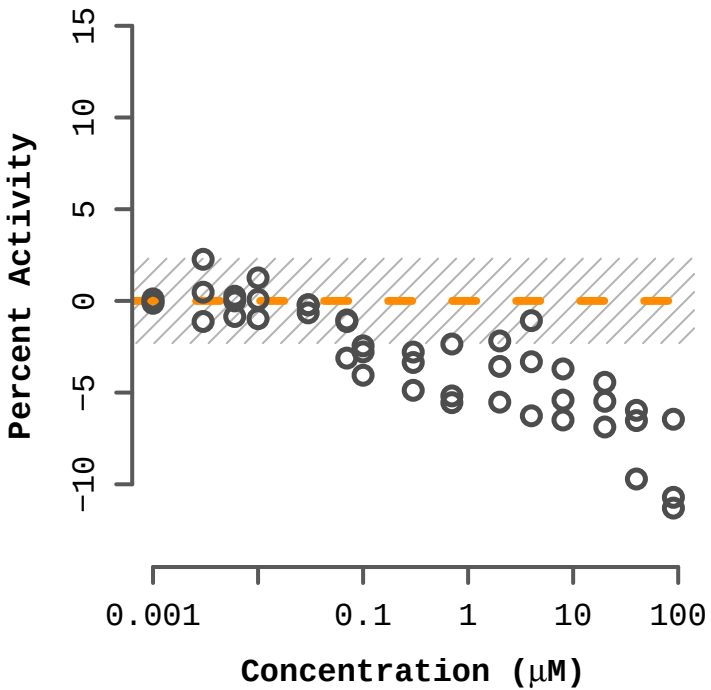
NAME: Colchicine
CHID: 24845 **CASRN:** 64-86-8
SPID(S): Tox21_300582
M4ID: 12478551

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.29	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: −0.41 **MAX_MED:** 0.00853 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

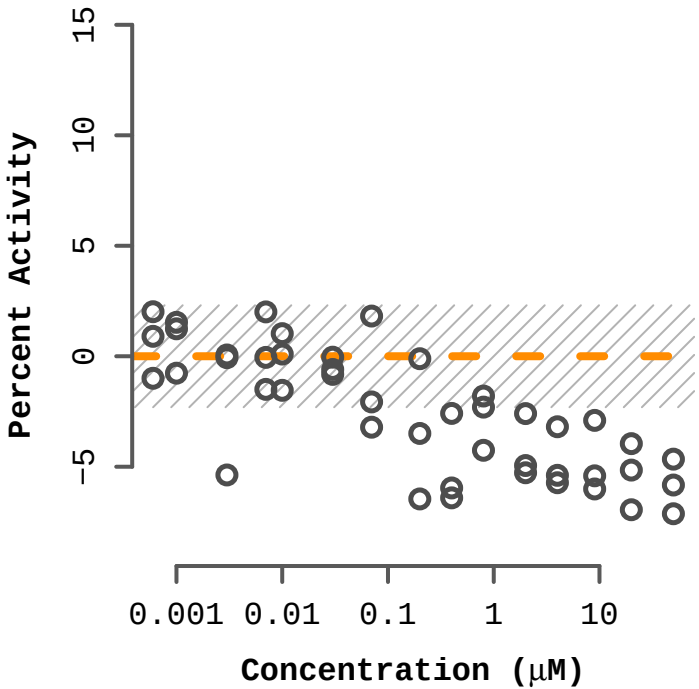
NAME: Colchicine
CHID: 24845 **CASRN:** 64-86-8
SPID(S): Tox21_201547
M4ID: 12480705

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.76	NA	NA
PROB:	1	NA	NA
RMSE:	4.46	NA	NA

MAX_MEAN: 0.541 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

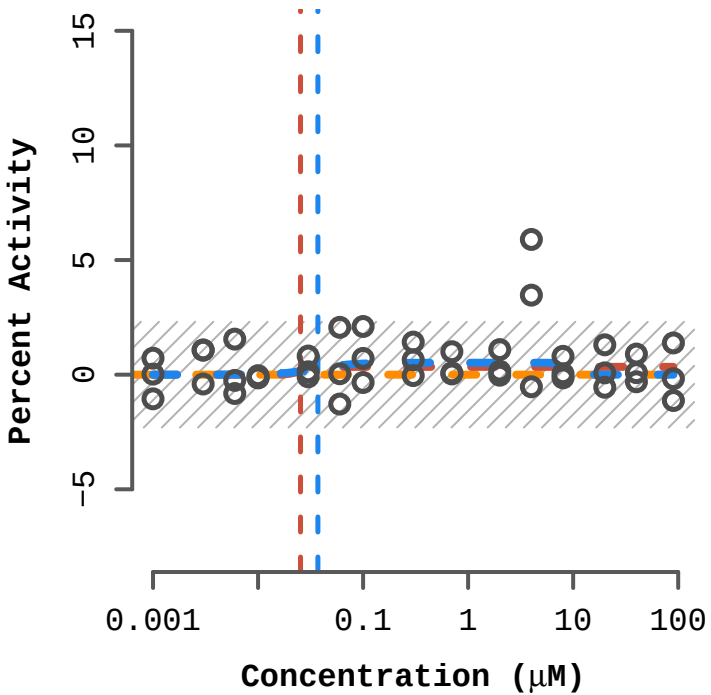
NAME: Colchicine
CHID: 24845 **CASRN:** 64-86-8
SPID(S): Tox21_110947_1
M4ID: 12483992

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253.46	NA	NA
PROB:	1	NA	NA
RMSE:	3.75	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Creosote, wood
CHID: 24853 CASRN: 8021-39-4
SPID(S): Tox21_201136
M4ID: 12481116

HILL MODEL (in red):

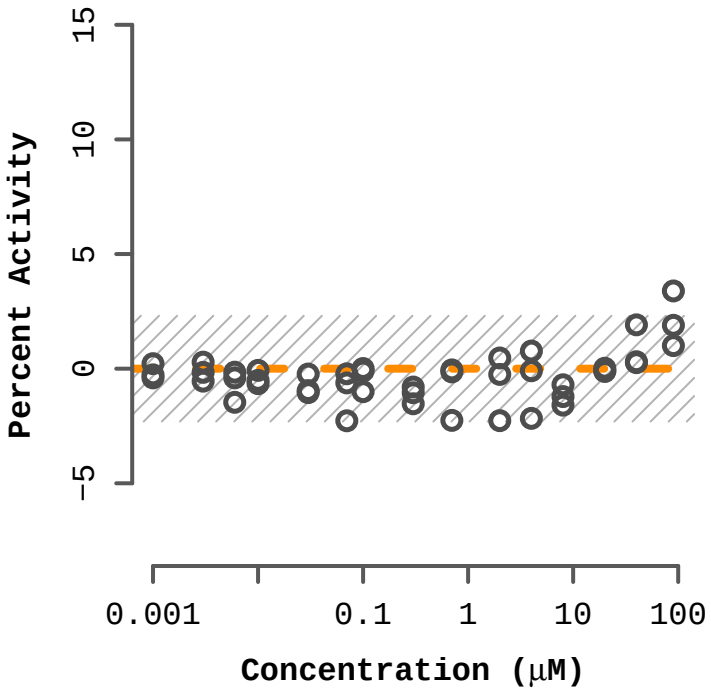
	tp	ga	gw
val:	0.34	−1.6	7.89
sd:	0.172	1.1	124

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.52	−1.43	2.56	0.895	16.9
sd:	0.262	0.661	4.96	0.313	601

	CNST	HILL	GNLS
AIC:	136.99	138.54	141.67
PROB:	0.64	0.3	0.06
RMSE:	1.31	1.23	1.2

MAX_MEAN: 2.95 MAX_MED: 3.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

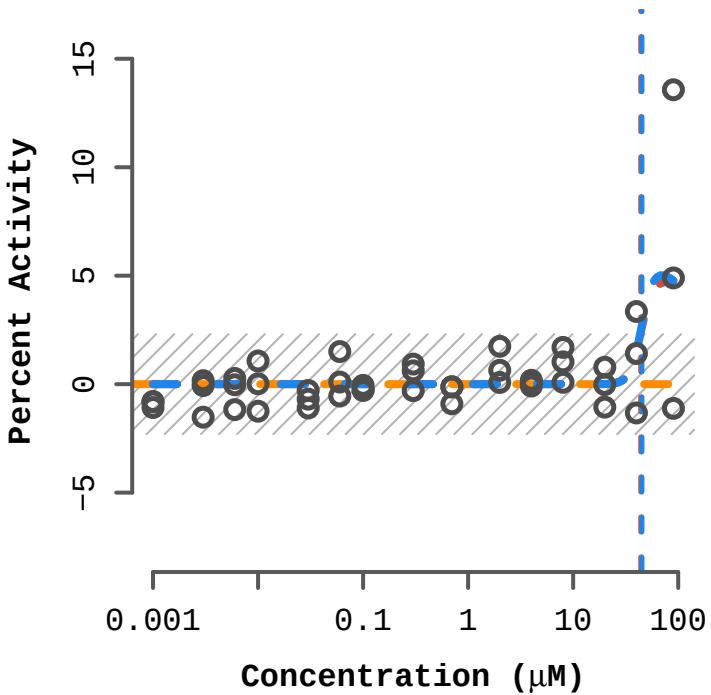
NAME: 3-Methoxy-4-methylaniline
CHID: 24855 **CASRN:** 16452-01-0
SPID(S): Tox21_202884
M4ID: 12479368

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: m,p−Cresol mixture
CHID: 24858 CASRN: NOCAS_24858
SPID(S): Tox21_201115
M4ID: 12481137

HILL MODEL (in red):

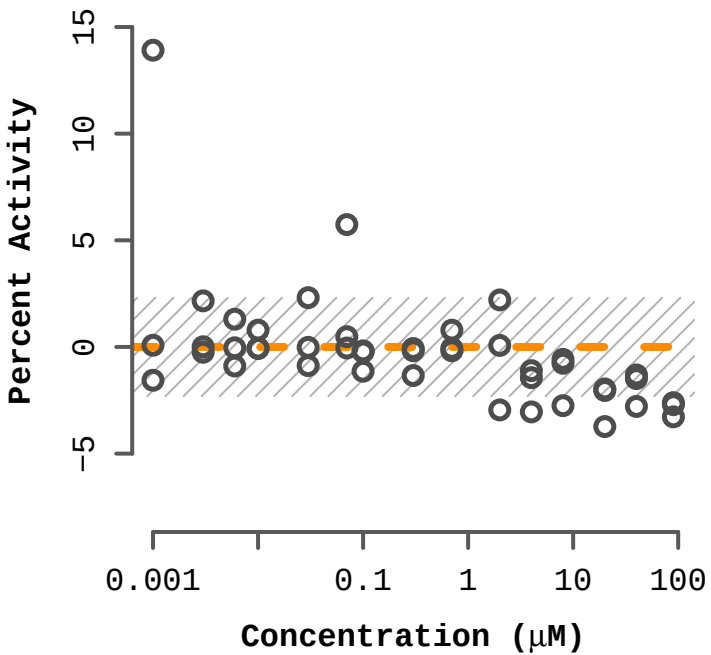
	tp	ga	gw
val:	4.78	1.64	8
sd:	0.845	0.133	23.3

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.61	1.65	8	2.23	2.8
sd:	49.7	0.418	32.5	12	111

	CNST	HILL	GNLS
AIC:	156.55	155.91	159.91
PROB:	0.39	0.54	0.07
RMSE:	2.35	1.82	1.82

MAX_MEAN: 5.79 **MAX_MED:** 4.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

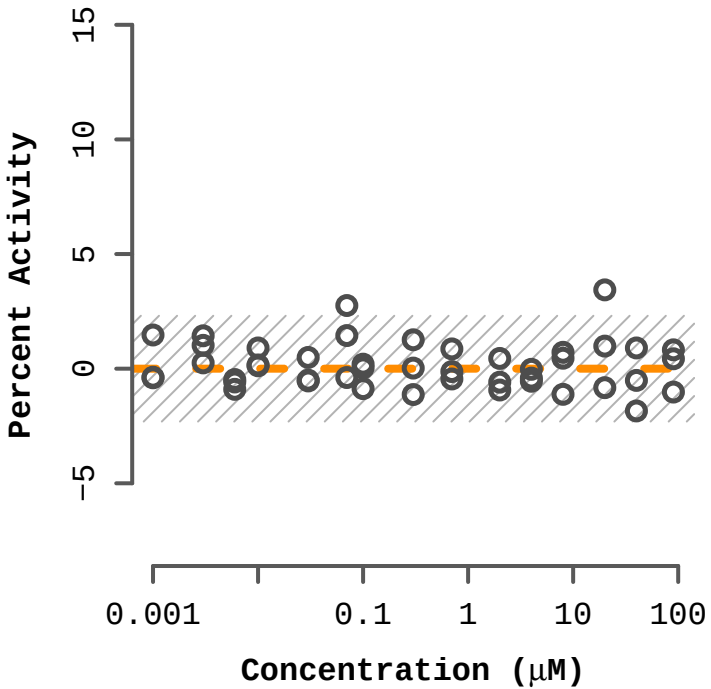
NAME: Cresyl diphenyl phosphate
CHID: 24861 CASRN: 26444-49-5
SPID(S): Tox21_202888
M4ID: 12479364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.31	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 4.14 MAX_MED: 0.483 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

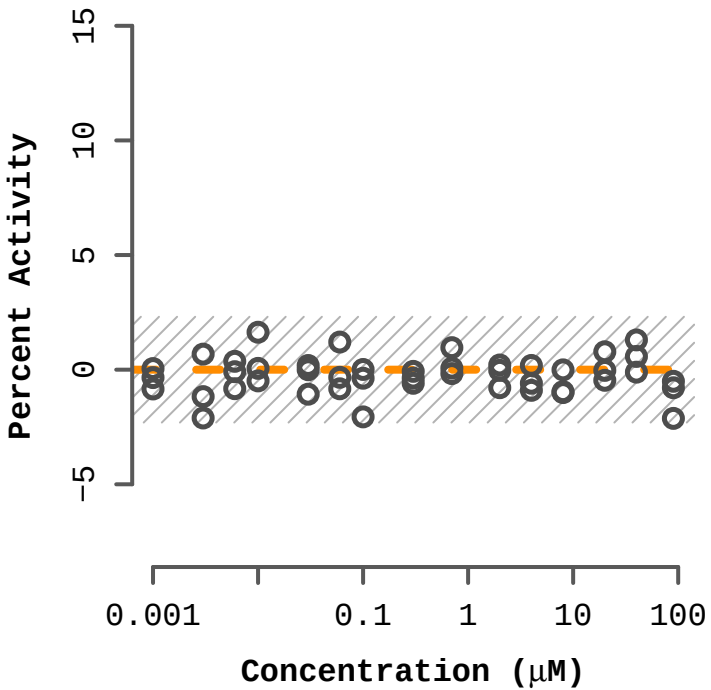
NAME: o-Cresyl glycidyl ether
CHID: 24862 **CASRN:** 2210-79-9
SPID(S): Tox21_200885
M4ID: 12481367

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

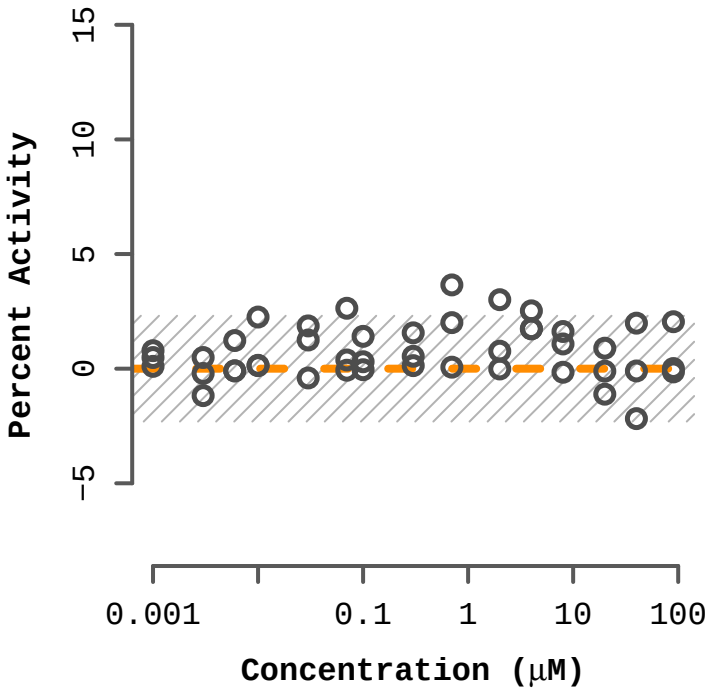
NAME: Crotonaldehyde
CHID: 24864 **CASRN:** 4170-30-3
SPID(S): Tox21_200316
M4ID: 12481936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.59 **MAX_MED:** 0.578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

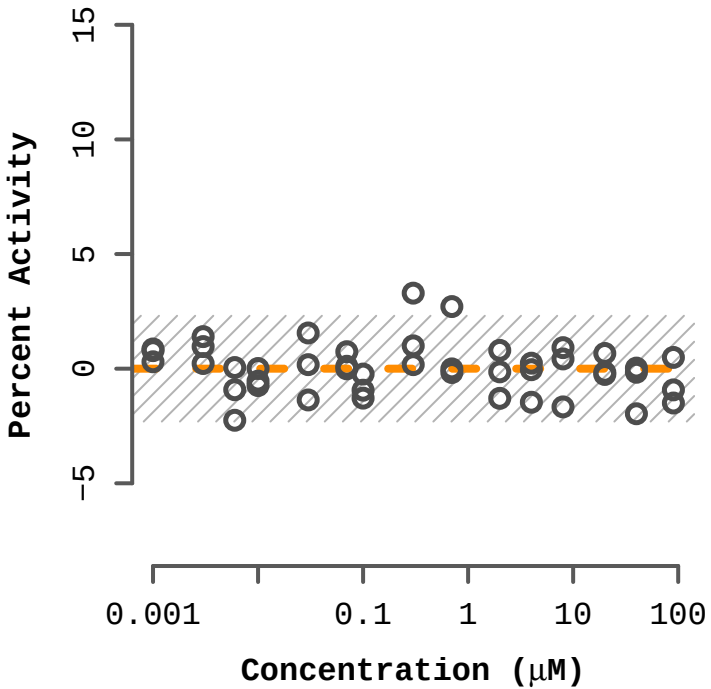
NAME: Crystal Violet lactone
CHID: 24866 **CASRN:** 1552-42-7
SPID(S): Tox21_200866
M4ID: 12481386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 2 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

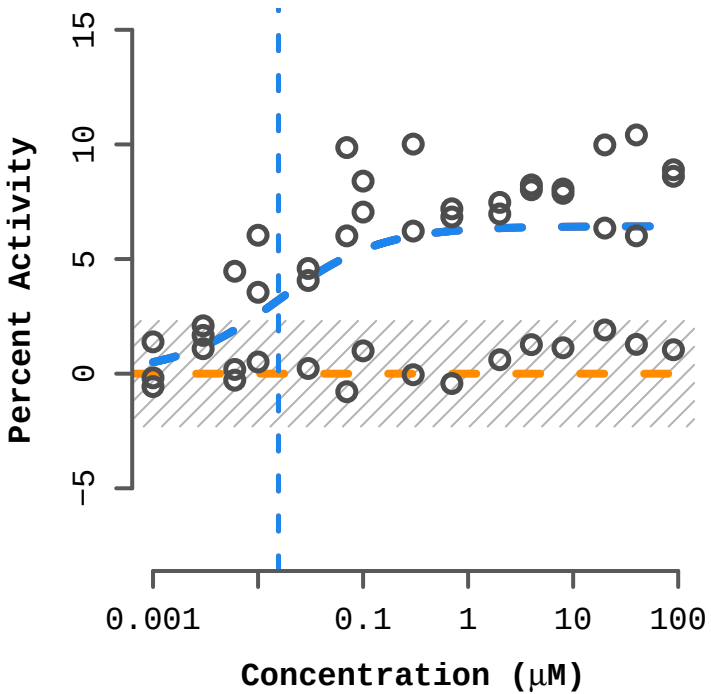
NAME: Cumene hydroperoxide
CHID: 24869 **CASRN:** 80-15-9
SPID(S): Tox21_300283
M4ID: 12478847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 0.997 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyanuric acid
CHID: 24873 CASRN: 108-80-5
SPID(S): Tox21_303192
M4ID: 12475941

HILL MODEL (in red):

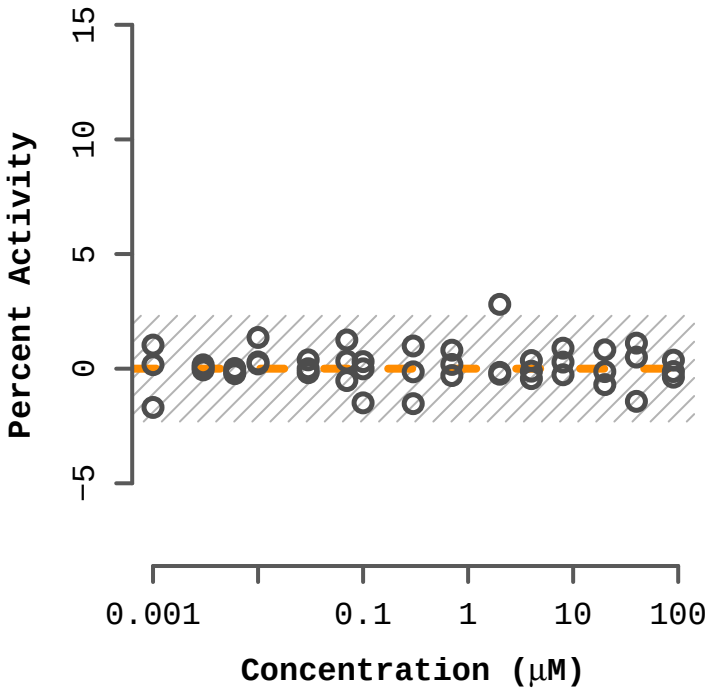
	tp	ga	gw
val:	6.43	−1.81	0.897
sd:	0.81	0.328	0.514

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.43	−1.81	0.897	3.82	4.12
sd:	0.81	0.328	0.514	1900	4220

	CNST	HILL	GNLS
AIC:	289.96	243.04	247.04
PROB:	0	0.88	0.12
RMSE:	5.62	3.17	3.17

MAX_MEAN: 6.18 MAX_MED: 8.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

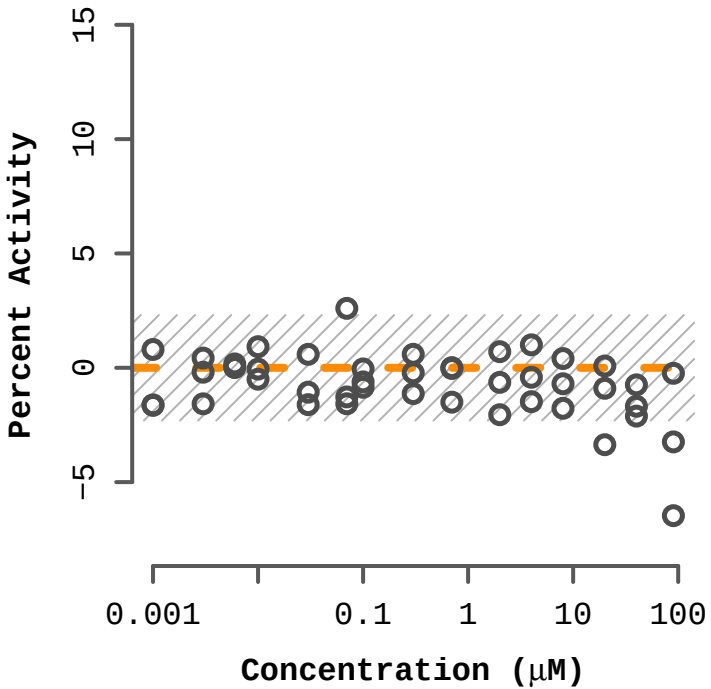
NAME: Cyanuric acid
CHID: 24873 **CASRN:** 108-80-5
SPID(S): Tox21_202362
M4ID: 12479890

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 0.507 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

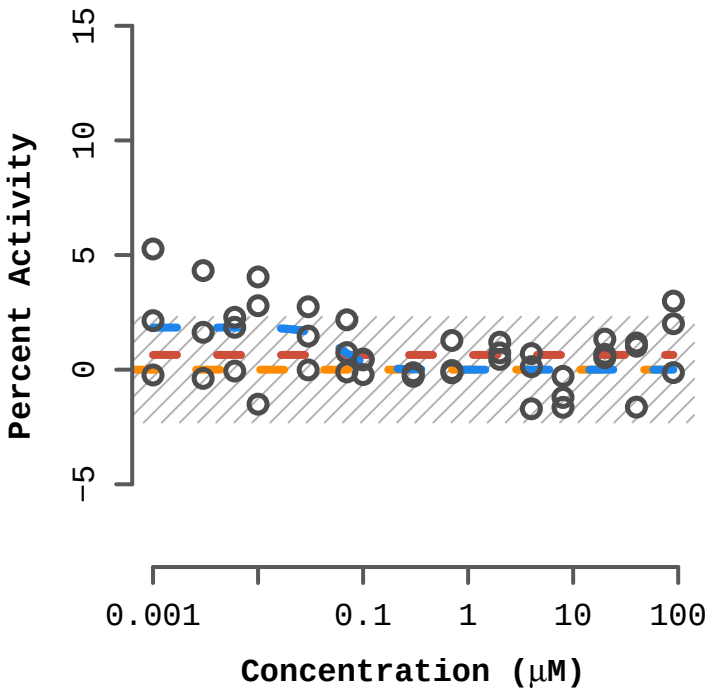
NAME: 1,2-Cyclohexanedicarboxylic acid, bis(oxiranyl
CHID: 24875 **CASRN:** 5493-45-8
SPID(S): Tox21_200005
M4ID: 12482247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 0.124 **MAX_MED:** 0.0225 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclohexanone cyanohydrin
CHID: 24878 **CASRN:** 931-97-5
SPID(S): Tox21_200377
M4ID: 12481875

HILL MODEL (in red):

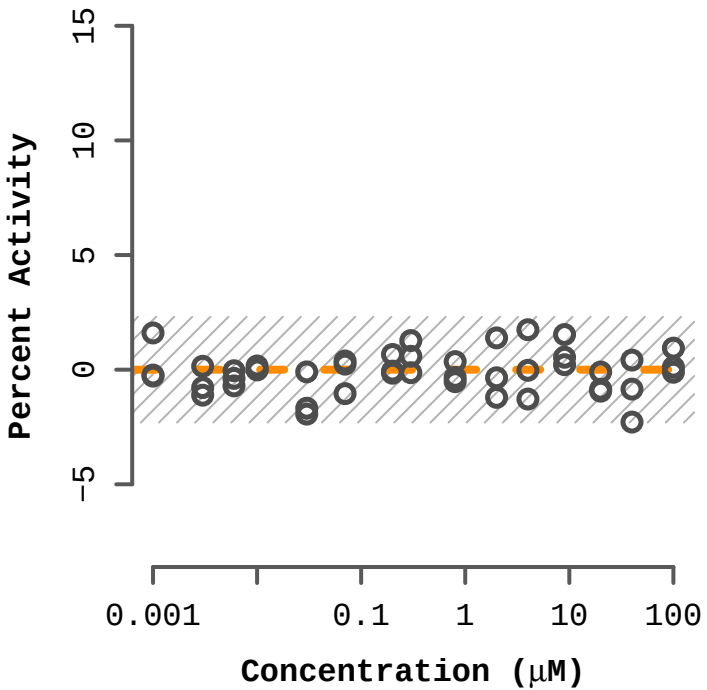
	tp	ga	gw
val:	0.643	−4.75	4.16
sd:	0.215	1580	3740

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.84	−4.95	3.29	−1.22	2.99
sd:	0.528	985	1670	0.321	4.79

	CNST	HILL	GNLS
AIC:	177.05	174.26	170.56
PROB:	0.03	0.13	0.84
RMSE:	1.74	1.55	1.39

MAX_MEAN: 2.39 **MAX_MED:** 2.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

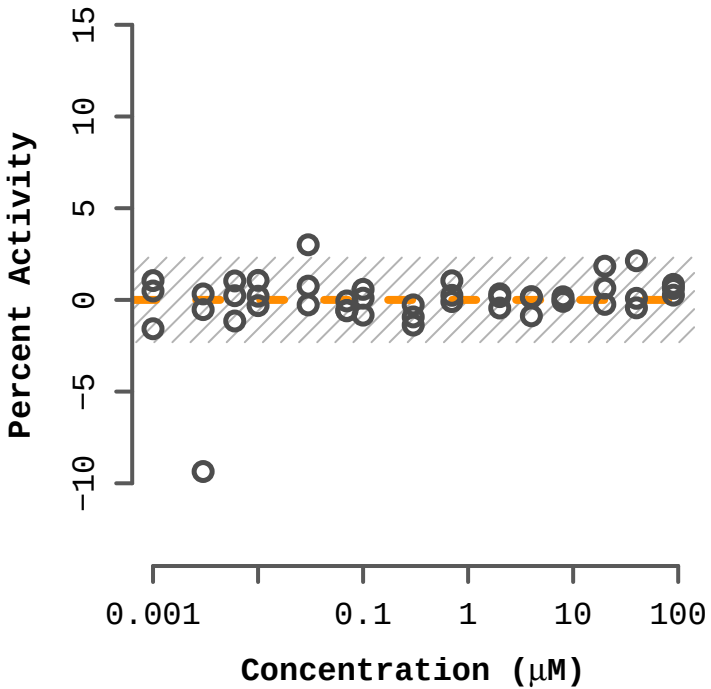
NAME: Cyclohexene oxide
CHID: 24880 **CASRN:** 286-20-4
SPID(S): Tox21_201152
M4ID: 12481100

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.766 **MAX_MED:** 0.585 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

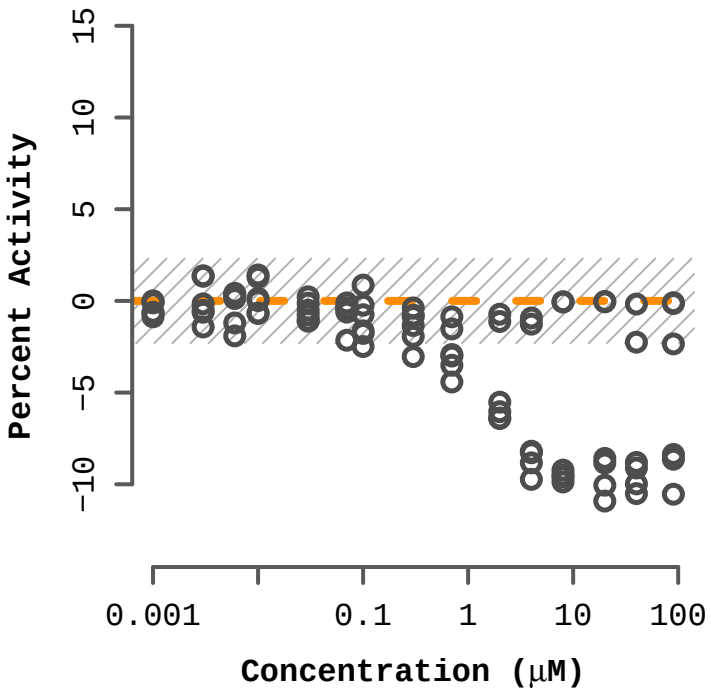
NAME: 2-Cyclohexen-1-one
CHID: 24881 **CASRN:** 930-68-7
SPID(S): Tox21_200008
M4ID: 12482244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.752 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

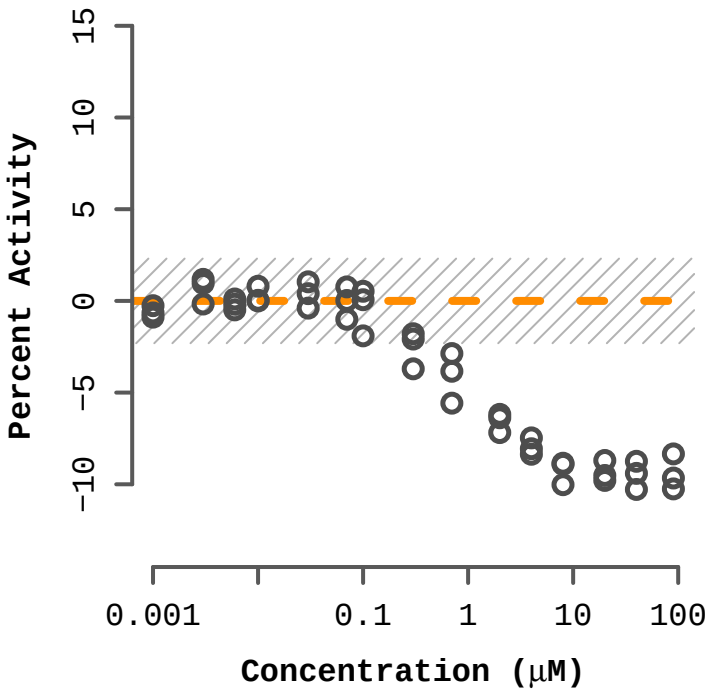
NAME: Cycloheximide
CHID: 24882 **CASRN:** 66-81-9
SPID(S): Tox21_303652
M4ID: 12475496

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	522.85	NA	NA
PROB:	1	NA	NA
RMSE:	4.65	NA	NA

MAX_MEAN: 0.254 **MAX_MED:** 0.202 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

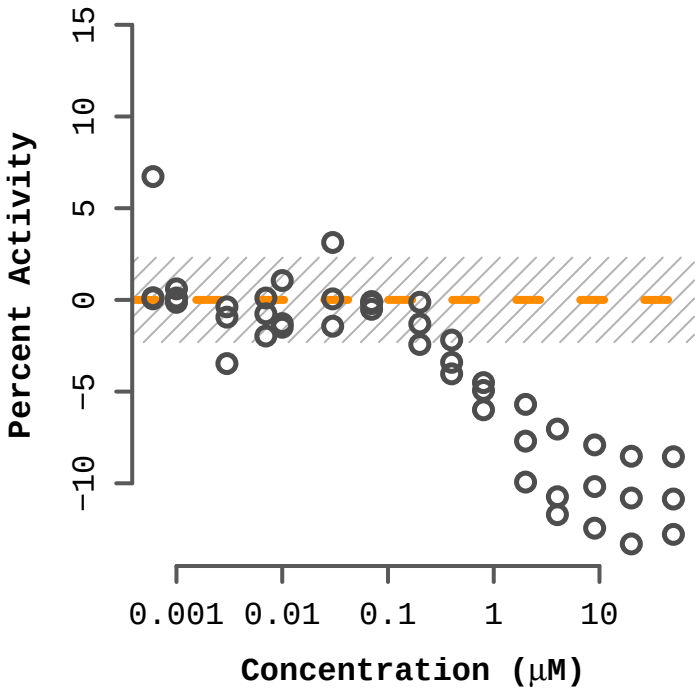
NAME: Cycloheximide
CHID: 24882 **CASRN:** 66-81-9
SPID(S): Tox21_201158
M4ID: 12481094

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.56	NA	NA
PROB:	1	NA	NA
RMSE:	5.71	NA	NA

MAX_MEAN: 0.655 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

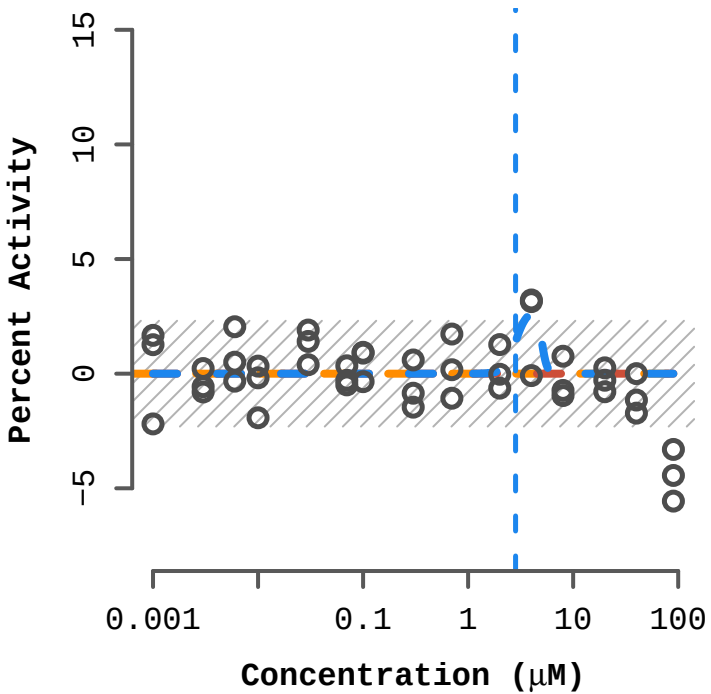
NAME: Cycloheximide
CHID: 24882 **CASRN:** 66-81-9
SPID(S): Tox21_113580_1
M4ID: 12482598

HILL MODEL: Not applicable.

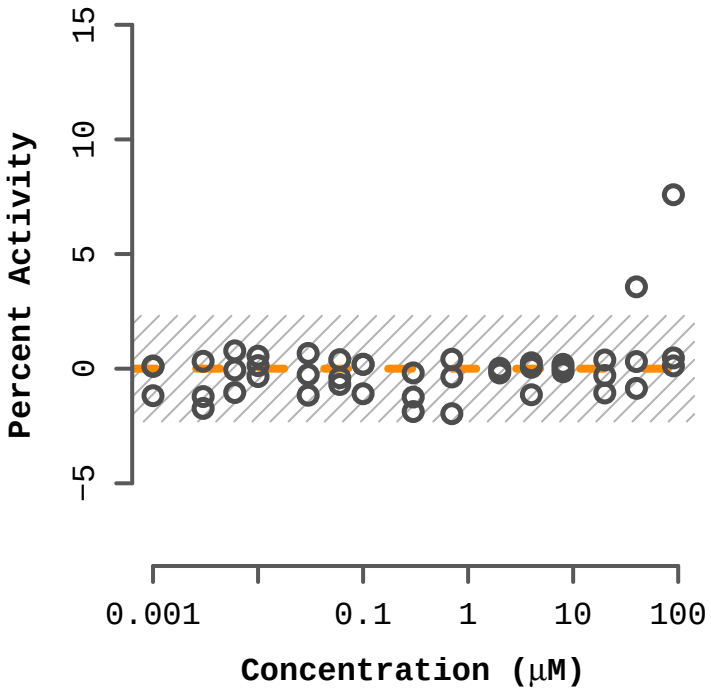
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	295.28	NA	NA
PROB:	1	NA	NA
RMSE:	6.21	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 0.122 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Cyclohexyl-4-methylbenzenesulfonamide
CHID:    24885   CASRN: 80-30-8
SPID(S): Tox21_200091
M4ID:    12482161

HILL MODEL (in red):
      tp        ga        gw
val:  3.84e-10  2.45      1.7
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  2.81      0.452     8         0.702     17.8
sd:   8.44      1.34      62.8      1.34      124

      CNST          HILL          GNLS
AIC:  169.88        175.88        173.99
PROB: 0.85          0.04          0.11
RMSE: 1.67          1.67          1.58

MAX_MEAN: 2.09      MAX_MED: 3.15      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

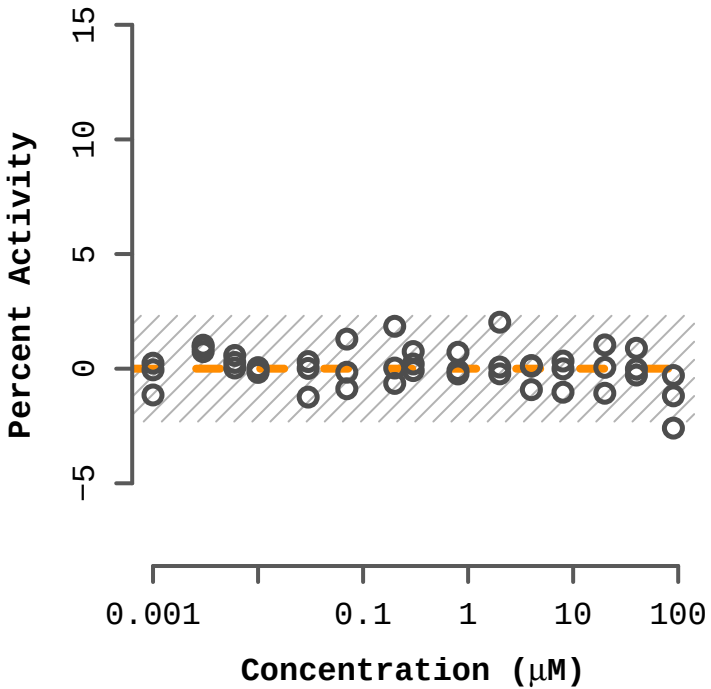
NAME: Cyclopentane
CHID: 24886 **CASRN:** 287-92-3
SPID(S): Tox21_200202
M4ID: 12482050

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 2.73 **MAX_MED:** 0.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

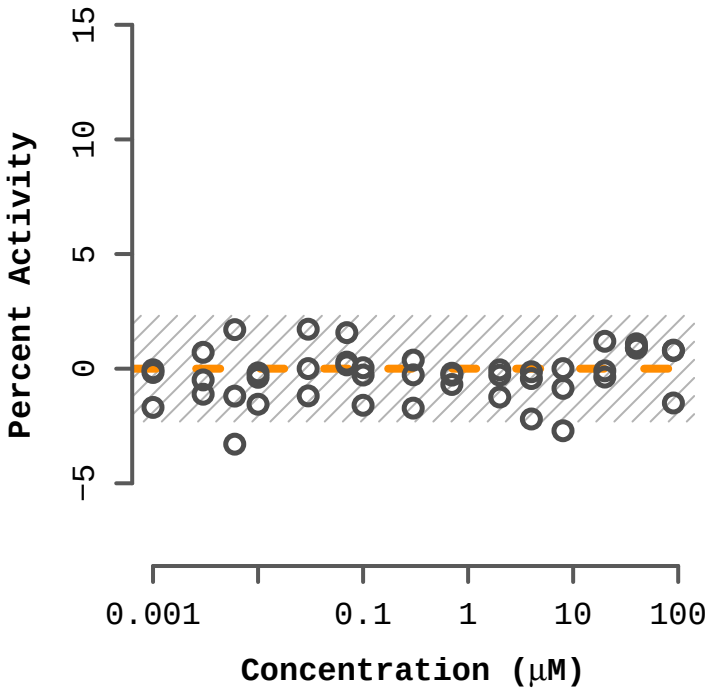
NAME: 4-H-Cyclopenta(d,e,f)phenanthrene
CHID: 24887 CASRN: 203-64-5
SPID(S): Tox21_201057
M4ID: 12481195

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

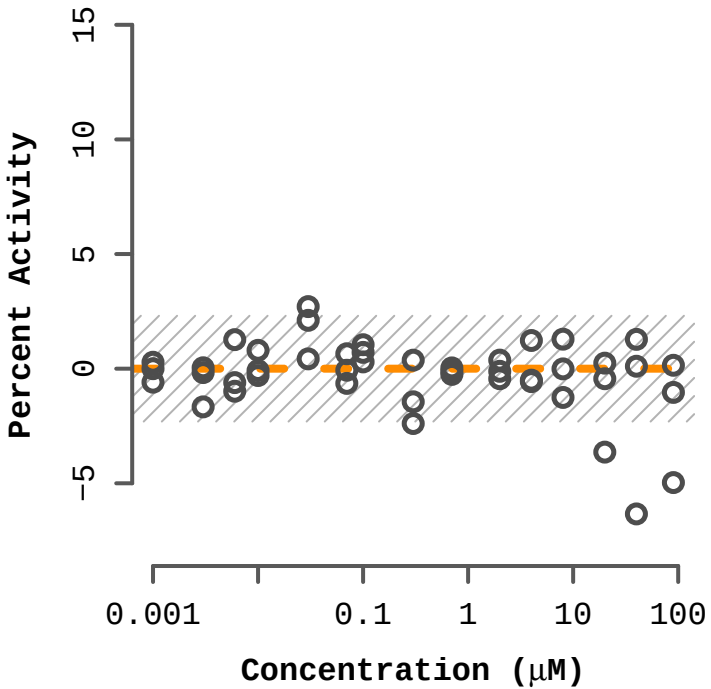
NAME: Cyclophosphamide monohydrate
CHID: 24888 **CASRN:** 6055-19-2
SPID(S): Tox21_300529
M4ID: 12478603

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.915 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

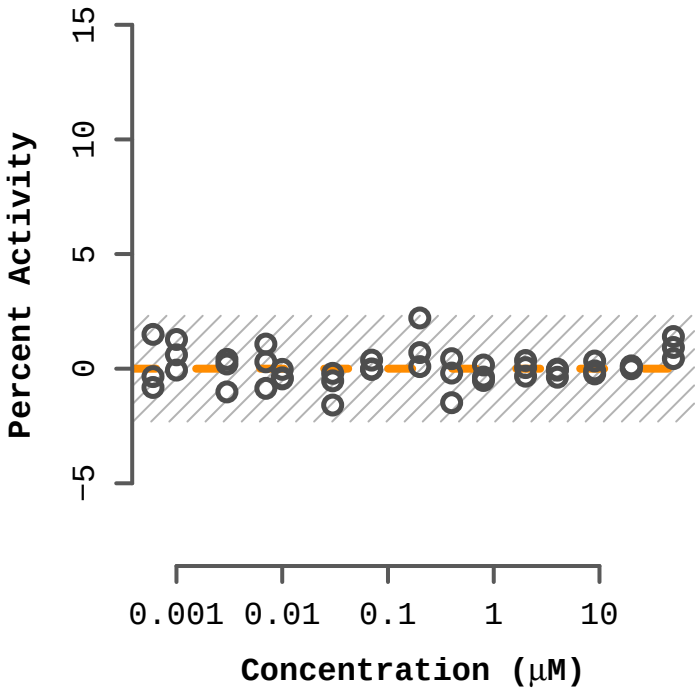
NAME: Cyclophosphamide monohydrate
CHID: 24888 **CASRN:** 6055-19-2
SPID(S): Tox21_201503
M4ID: 12480749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

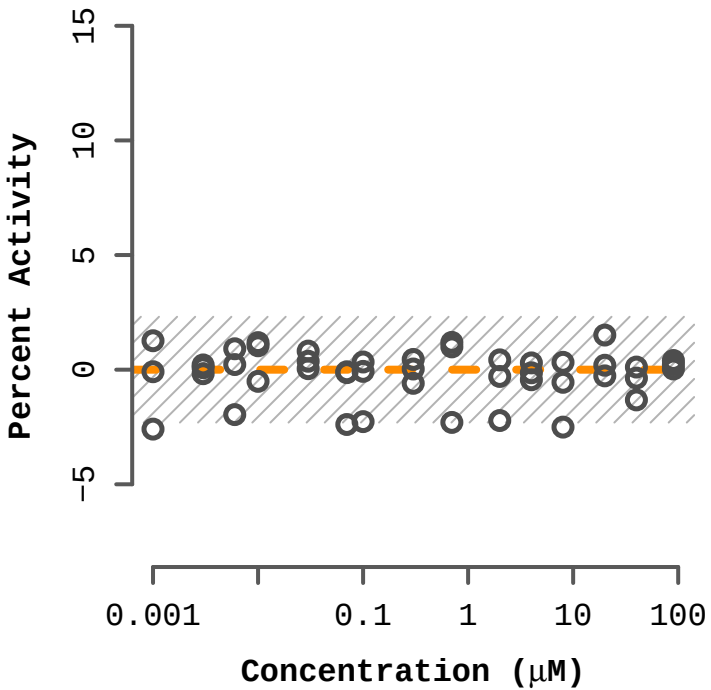
NAME: Cyclophosphamide monohydrate
CHID: 24888 CASRN: 6055-19-2
SPID(S): Tox21_110100_1
M4ID: 12484653

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

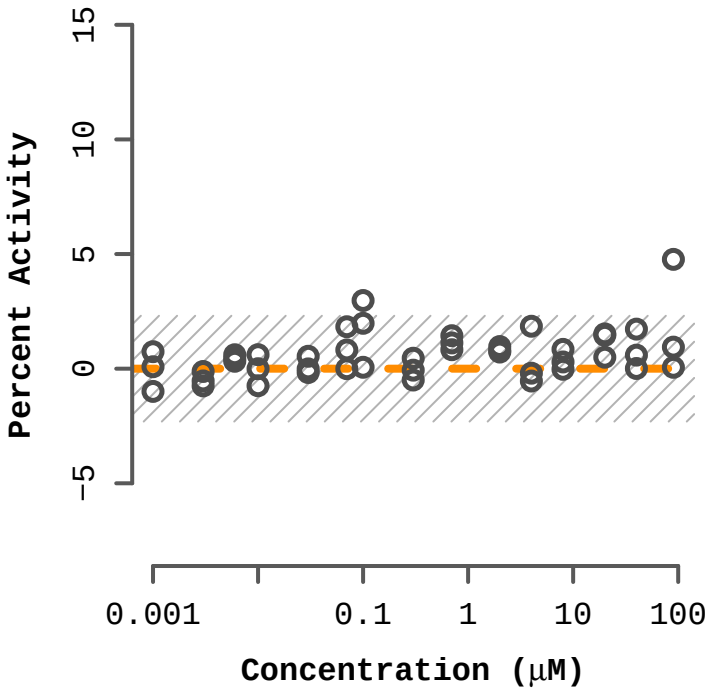
NAME: p-Cymen-8-ol
CHID: 24890 **CASRN:** 1197-01-9
SPID(S): Tox21_302135
M4ID: 12476998

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.573 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

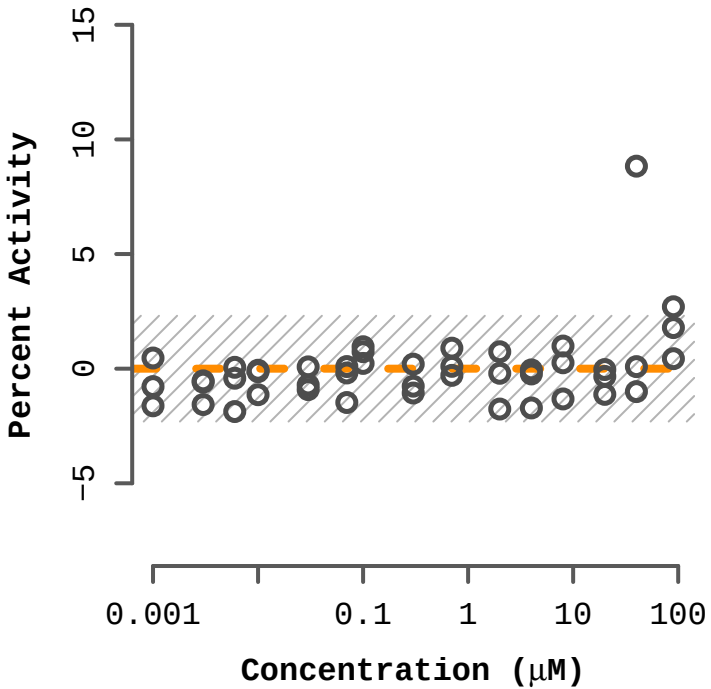
NAME: Cytarabine hydrochloride
CHID: 24891 **CASRN:** 69-74-9
SPID(S): Tox21_300488
M4ID: 12478644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

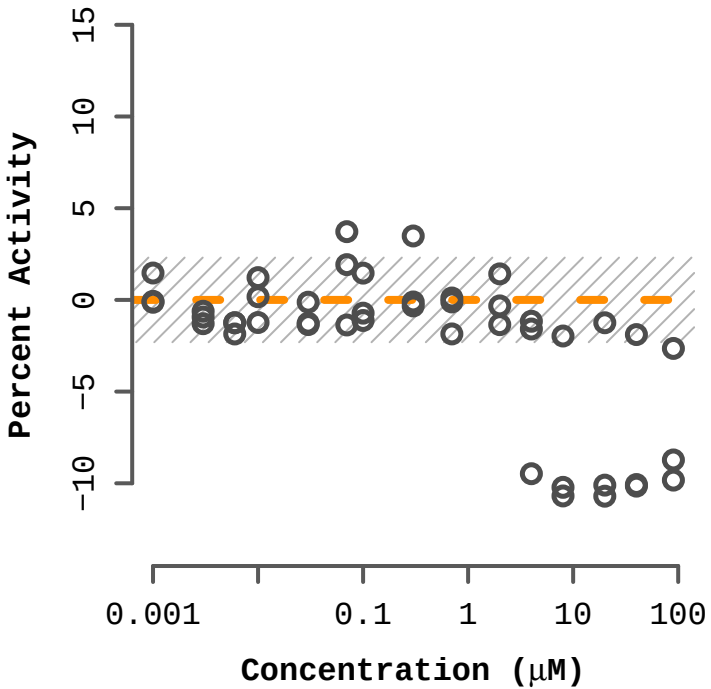
NAME: 2,4−D, Dimethylamine salt
CHID: 24896 CASRN: 2008−39−1
SPID(S): Tox21_200302
M4ID: 12481950

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.64 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

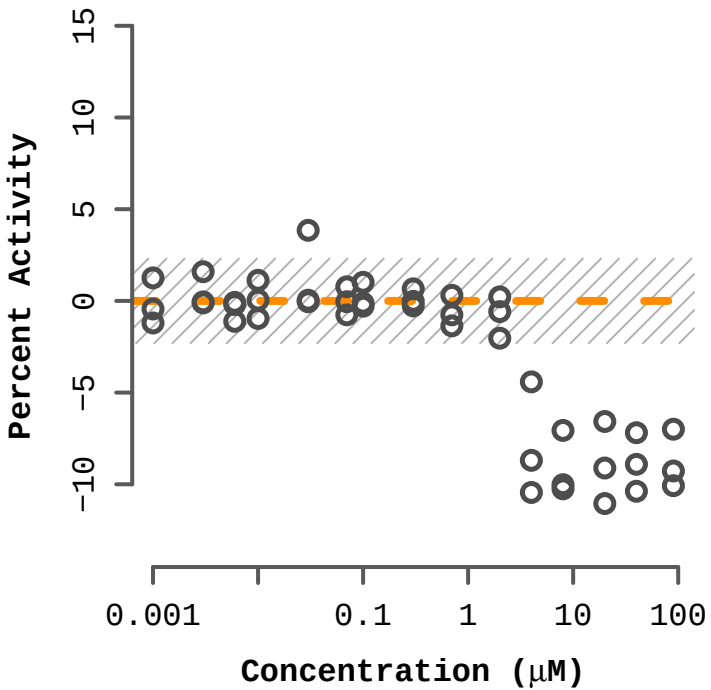
NAME: Dazomet
CHID: 24902 **CASRN:** 533-74-4
SPID(S): Tox21_300990
M4ID: 12478143

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	259.14	NA	NA
PROB:	1	NA	NA
RMSE:	4.67	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

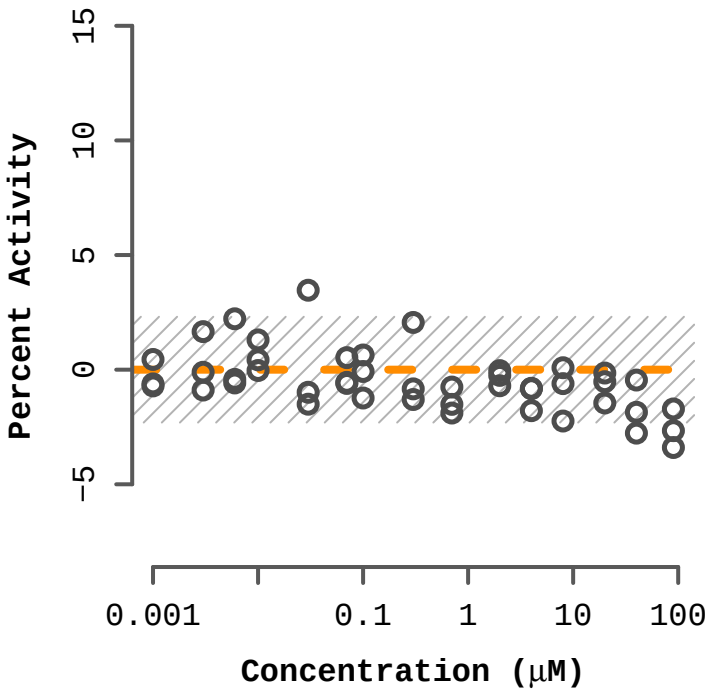
NAME: Dazomet
CHID: 24902 **CASRN:** 533-74-4
SPID(S): Tox21_201236
M4ID: 12481016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	275.84	NA	NA
PROB:	1	NA	NA
RMSE:	5.2	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.0441 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

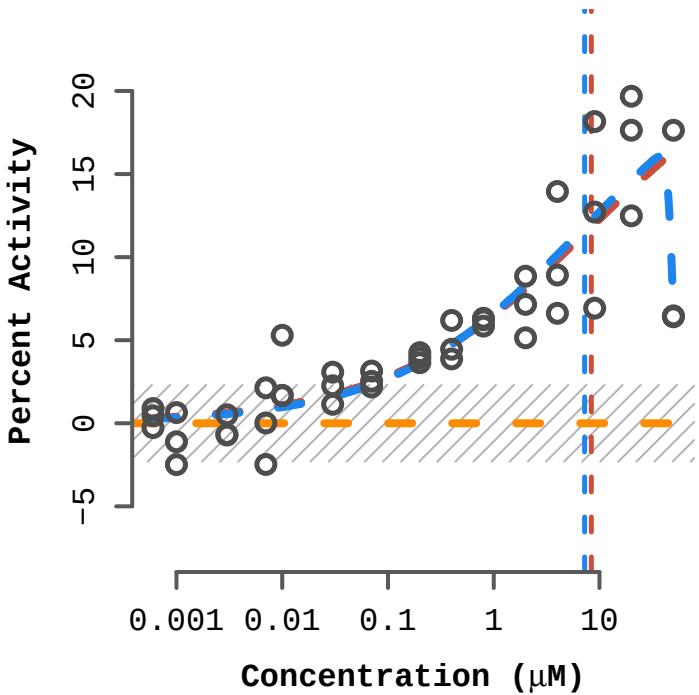
NAME: 4',5'−Dibromofluorescein
CHID: 24904 **CASRN:** 596−03−2
SPID(S): Tox21_303911
M4ID: 12475277

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 0.566 **MAX_MED:** 0.431 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D&C Yellow 11
CHID: 24906 CASRN: 8003-22-3
SPID(S): Tox21_202504
M4ID: 12479748

HILL MODEL (in red):

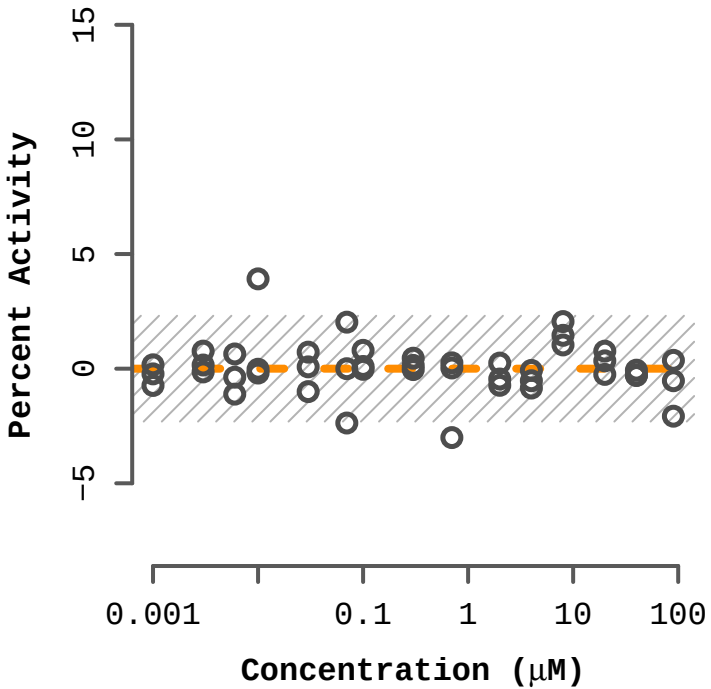
	tp	ga	gw
val:	23.6	0.923	0.453
sd:	8.28	0.687	0.0949

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.6	0.86	0.477	1.69	17.1
sd:	8.43	0.579	0.0759	0.0121	24.7

	CNST	HILL	GNLS
AIC:	309.48	220.6	213.13
PROB:	0	0.02	0.98
RMSE:	7.58	2.98	2.64

MAX_MEAN: 16.6 MAX_MED: 17.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

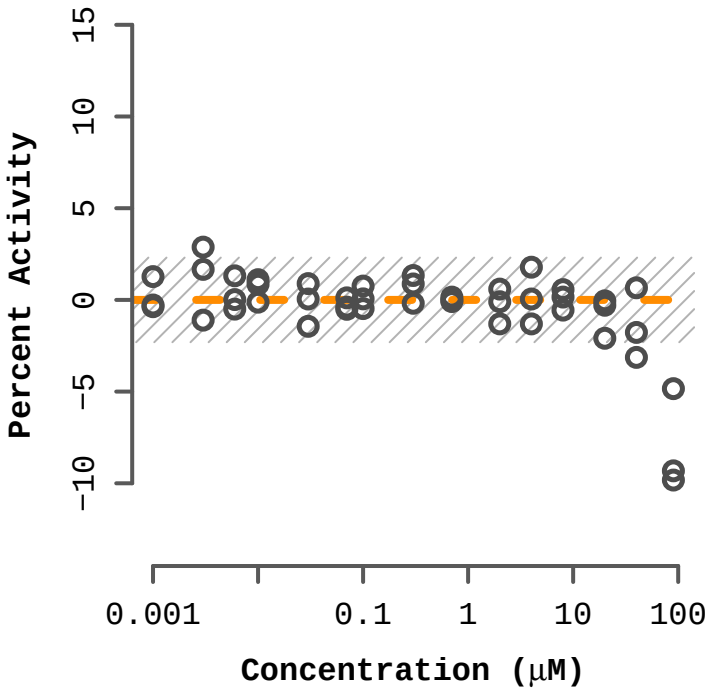
NAME: (E,E)−2,4−Decadienal
CHID: 24911 CASRN: 25152−84−5
SPID(S): Tox21_303165
M4ID: 12475968

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.52 MAX_MED: 1.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

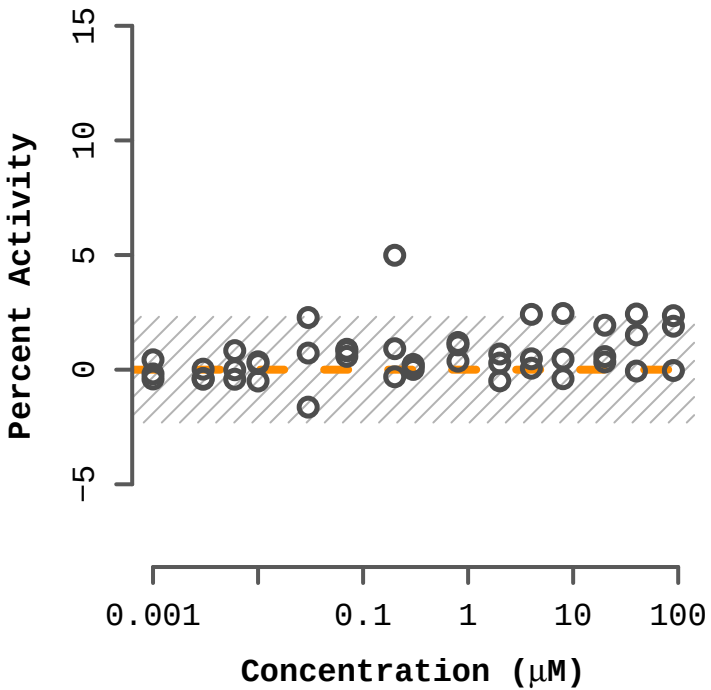
NAME: (E,E)−2,4−Decadienal
CHID: 24911 **CASRN:** 25152−84−5
SPID(S): Tox21_201894
M4ID: 12480358

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

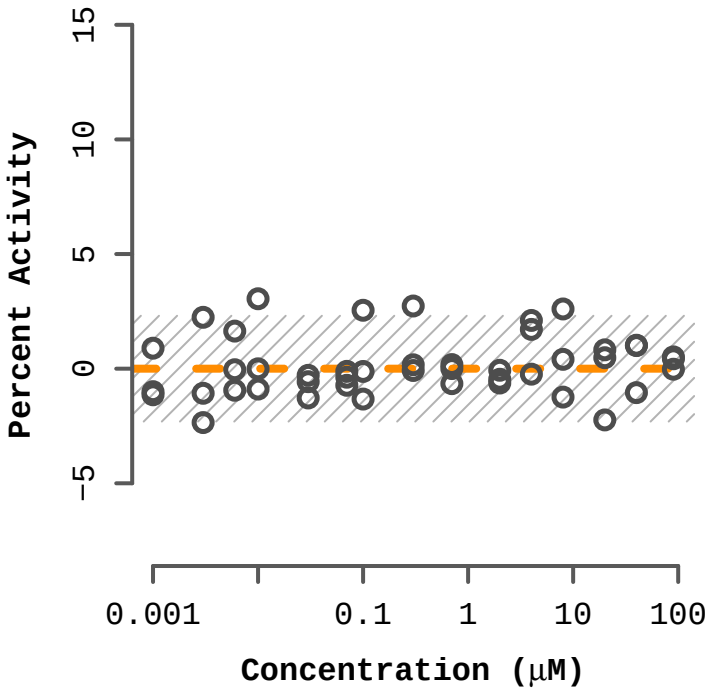
NAME: Decalin
CHID: 24912 **CASRN:** 91-17-8
SPID(S): Tox21_200222
M4ID: 12482030

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

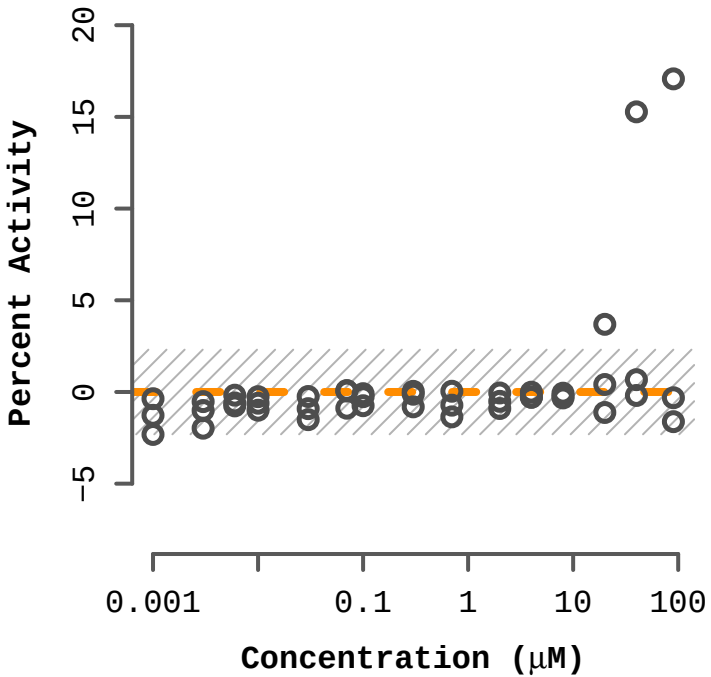
NAME: Decane
CHID: 24913 **CASRN:** 124-18-5
SPID(S): Tox21_300336
M4ID: 12478796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

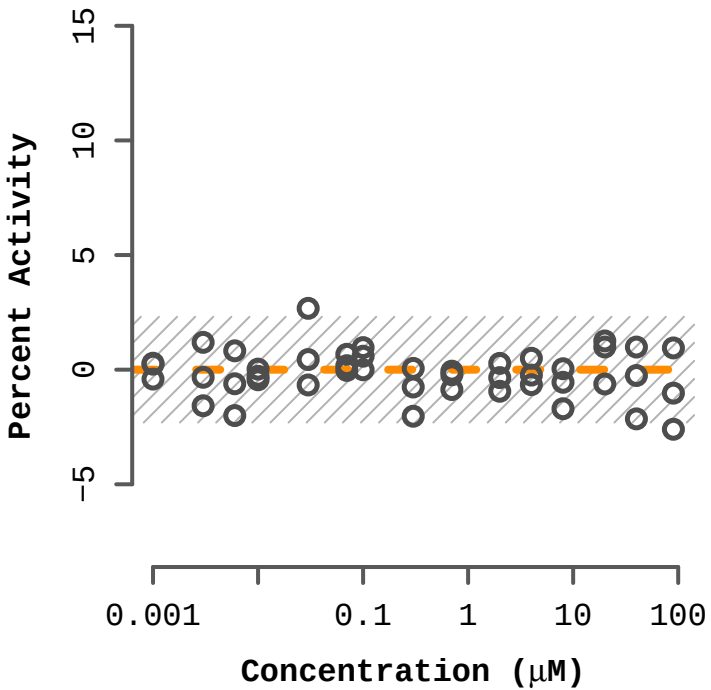
NAME: Decane
CHID: 24913 **CASRN:** 124-18-5
SPID(S): Tox21_201881
M4ID: 12480371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.34	NA	NA
PROB:	1	NA	NA
RMSE:	3.55	NA	NA

MAX_MEAN: 5.25 **MAX_MED:** 0.673 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

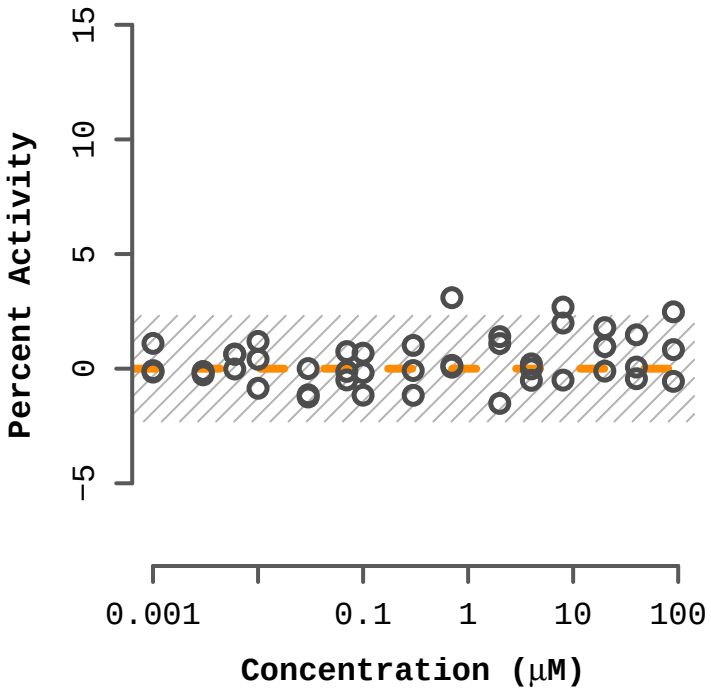
NAME: Decyl methacrylate
CHID: 24915 CASRN: 3179-47-3
SPID(S): Tox21_200311
M4ID: 12481941

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.818 MAX_MED: 0.992 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

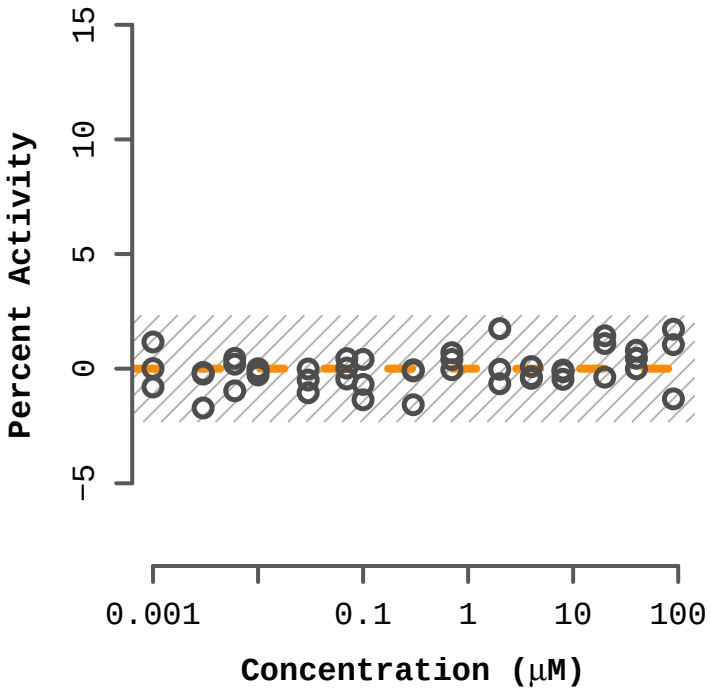
NAME: Diacetone acrylamide
CHID: 24916 CASRN: 2873-97-4
SPID(S): Tox21_302117
M4ID: 12477016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.39 MAX_MED: 1.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

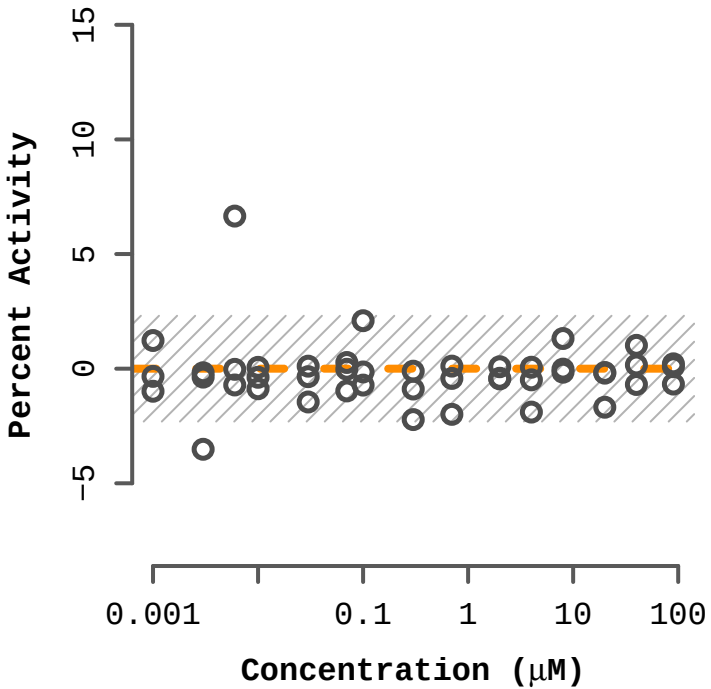
NAME: Diacetone alcohol
CHID: 24917 **CASRN:** 123-42-2
SPID(S): Tox21_303479
M4ID: 12475662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.722 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

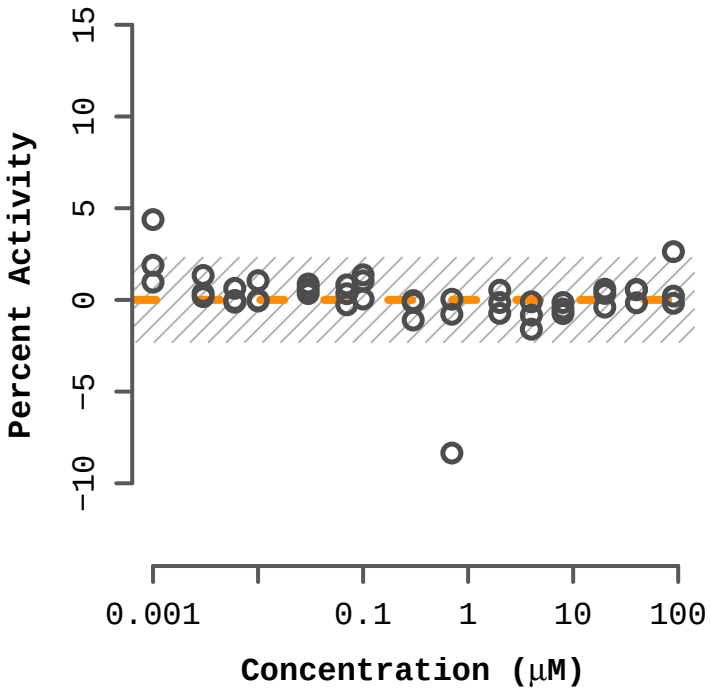
NAME: Diacetone alcohol
CHID: 24917 **CASRN:** 123-42-2
SPID(S): Tox21_201266
M4ID: 12480986

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 0.164 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

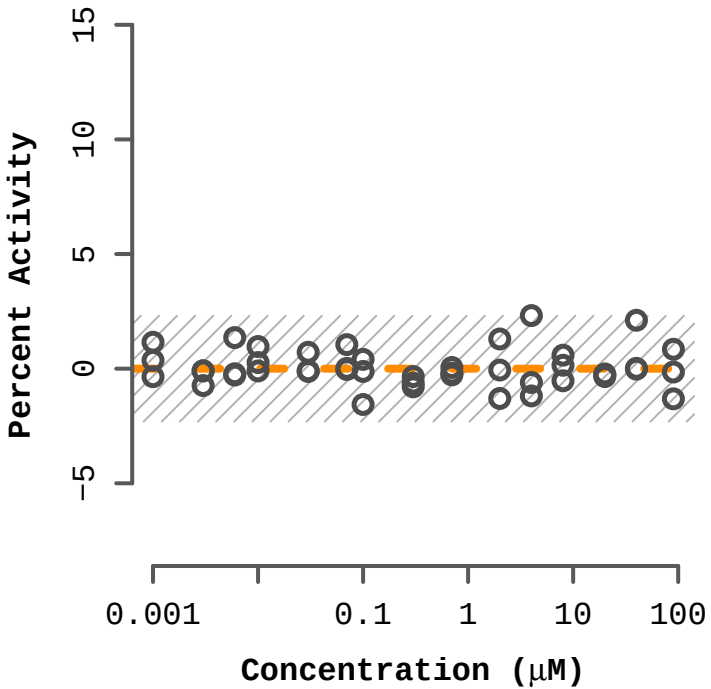
NAME: Diallylamine
CHID: 24918 **CASRN:** 124-02-7
SPID(S): Tox21_303139
M4ID: 12475994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.41 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

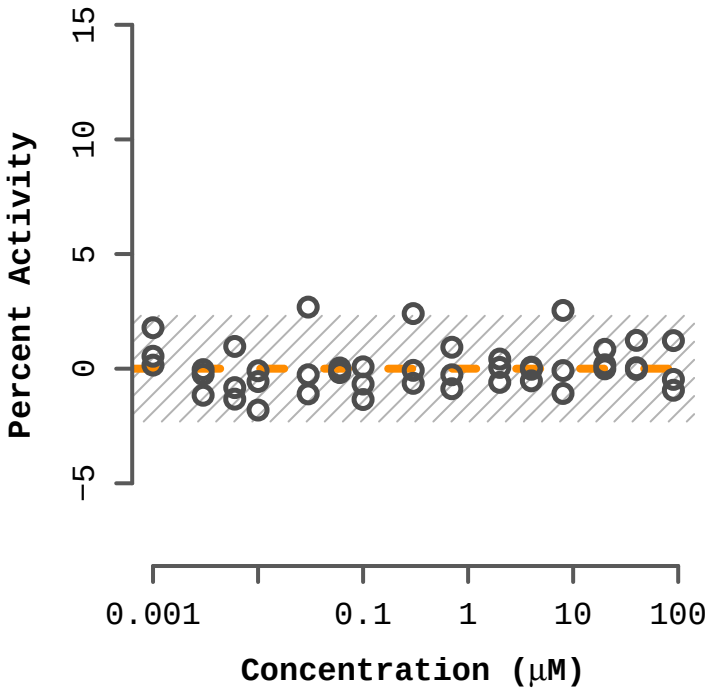
NAME: Diallylamine
CHID: 24918 **CASRN:** 124-02-7
SPID(S): Tox21_201555
M4ID: 12480697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.703 **MAX_MED:** 0.367 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

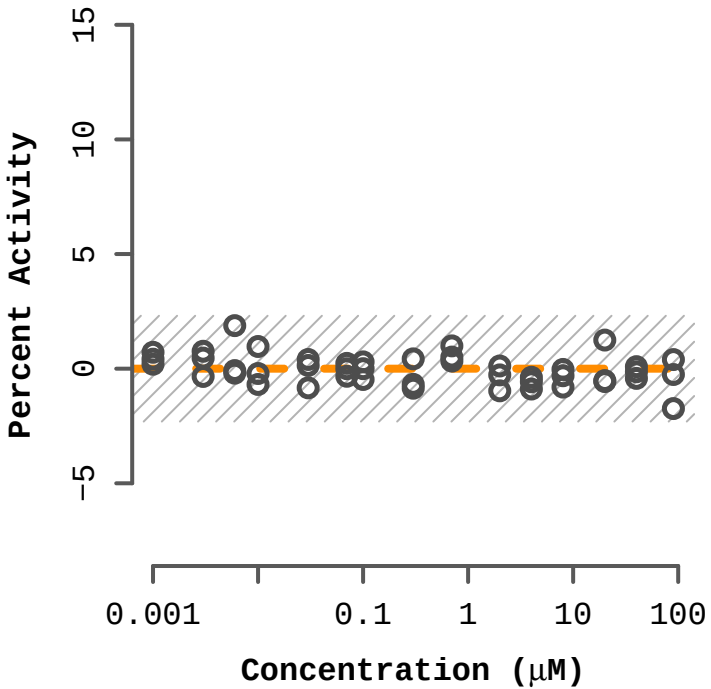
NAME: 4,4'−Diaminodicyclohexylmethane
CHID: 24921 CASRN: 1761−71−3
SPID(S): Tox21_200300
M4ID: 12481952

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.829 **MAX_MED:** 0.544 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

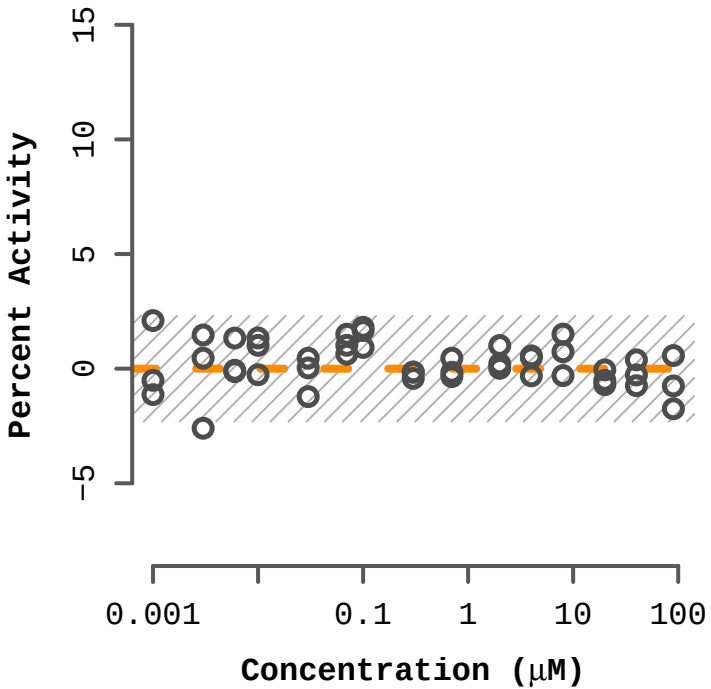
NAME: 1,6-Hexanediamine
CHID: 24922 **CASRN:** 124-09-4
SPID(S): Tox21_303123
M4ID: 12476010

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.612 **MAX_MED:** 0.508 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

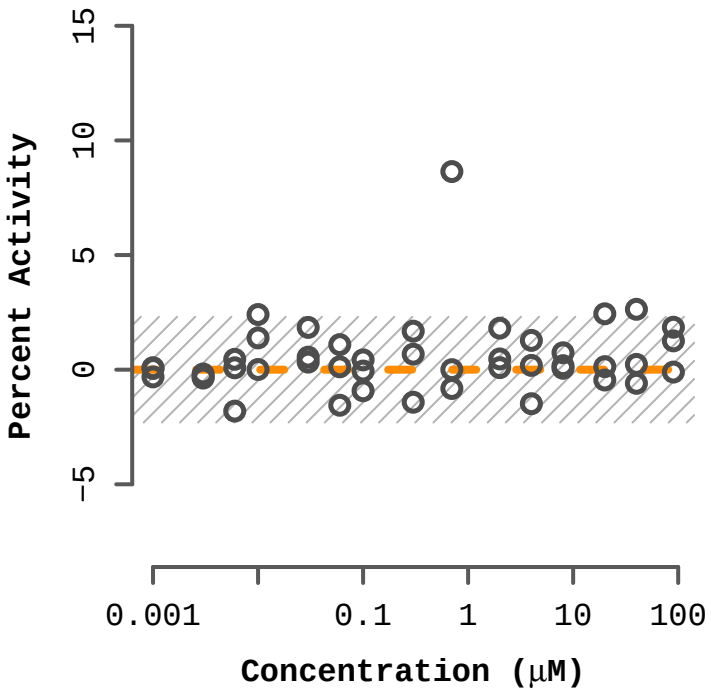
NAME: 1,6-Hexanediamine
CHID: 24922 **CASRN:** 124-09-4
SPID(S): Tox21_202088
M4ID: 12480164

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

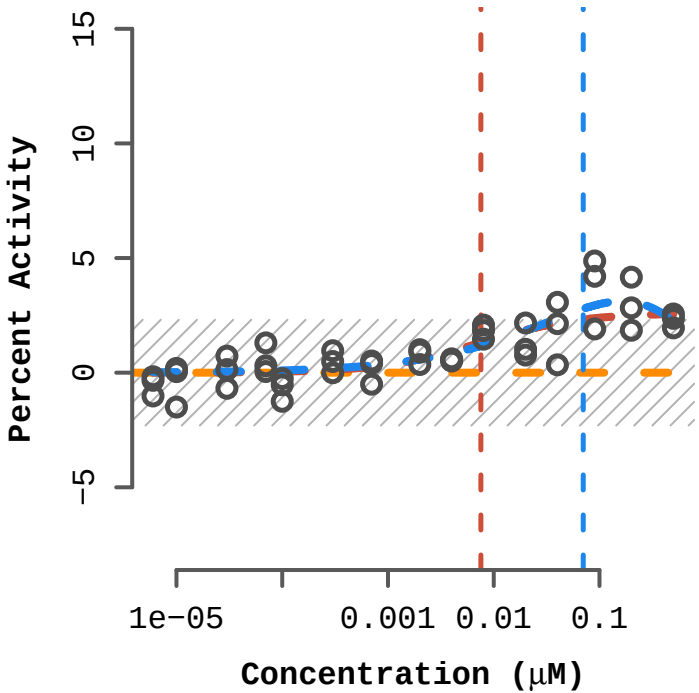
NAME: Diaminomaleonitrile
CHID: 24923 **CASRN:** 1187-42-4
SPID(S): Tox21_200991
M4ID: 12481261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2.61 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Diamino−2,2'−stilbenedisulfonic acid
CHID: 24926 **CASRN:** 81−11−8
SPID(S): Tox21_112127_1
M4ID: 12483300

HILL MODEL (in red):

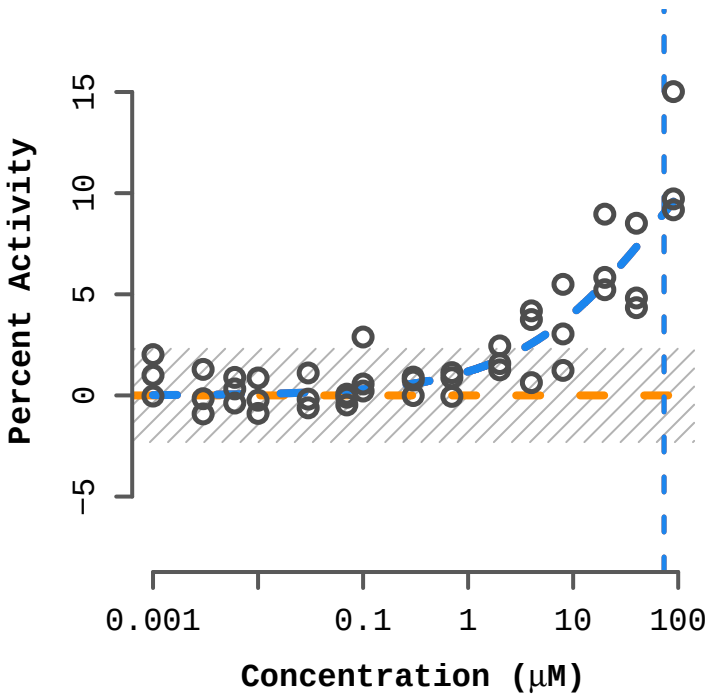
	tp	ga	gw
val:	2.61	−2.12	0.932
sd:	0.347	0.231	0.352

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.85	−1.15	0.621	−0.295	1.52
sd:	9.67	1.9	0.28	0.562	1.65

	CNST	HILL	GNLS
AIC:	176.49	116.74	118.44
PROB:	0	0.7	0.3
RMSE:	1.72	0.83	0.78

MAX_MEAN: 3.66 **MAX_MED:** 4.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,4−Diaminotoluene
CHID: 24930 CASRN: 496−72−0
SPID(S): Tox21_300507
M4ID: 12478625

HILL MODEL (in red):

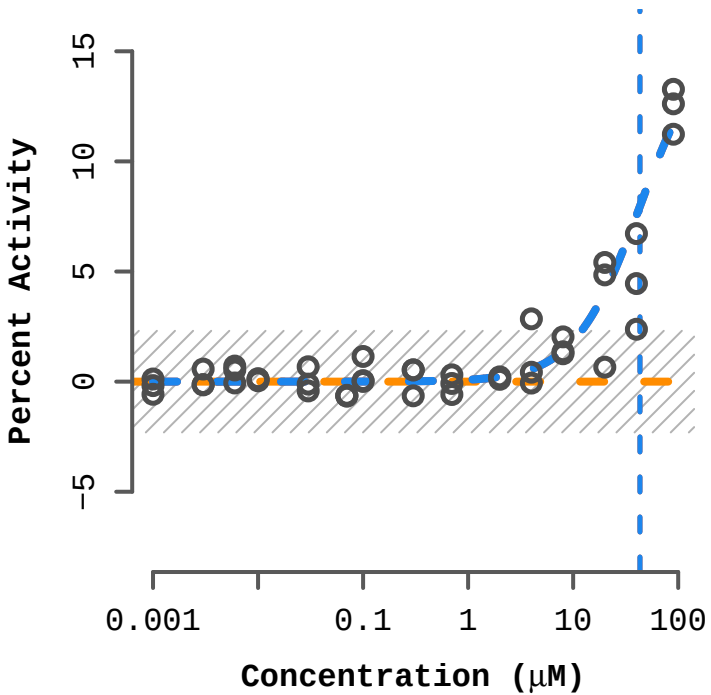
	tp	ga	gw
val:	18	1.87	0.618
sd:	10.3	0.789	0.16

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18	1.87	0.618	3.79	4.16
sd:	10.3	0.791	0.16	997	2290

	CNST	HILL	GNLS
AIC:	244.71	162.17	166.17
PROB:	0	0.88	0.12
RMSE:	4.13	1.47	1.47

MAX_MEAN: 11.3 **MAX_MED:** 9.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,4−Diaminotoluene
CHID: 24930 CASRN: 496−72−0
SPID(S): Tox21_201749
M4ID: 12480503

HILL MODEL (in red):

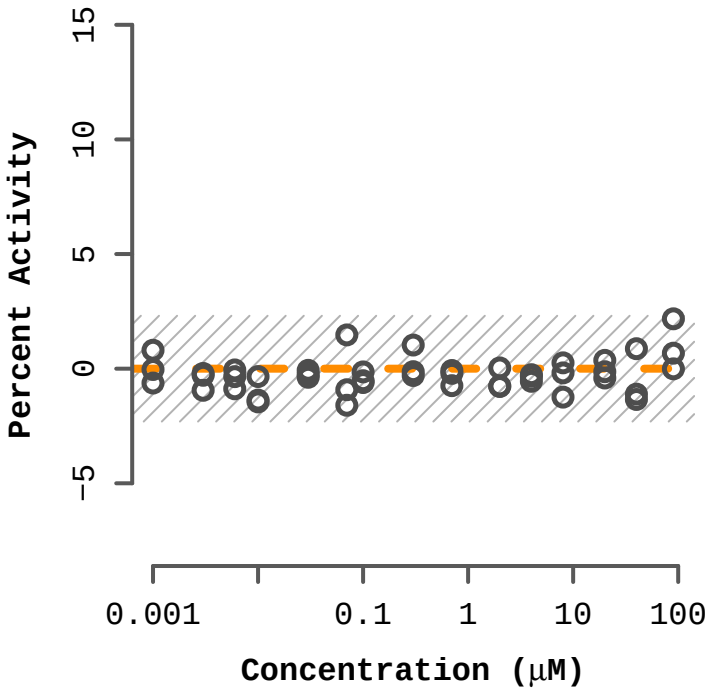
	tp	ga	gw
val:	15.9	1.64	1.39
sd:	2.48	0.133	0.175

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.9	1.64	1.39	3.3	7.89
sd:	2.48	0.133	0.175	6750	39700

	CNST	HILL	GNLS
AIC:	210.71	130.61	134.61
PROB:	0	0.88	0.12
RMSE:	3.68	1.22	1.22

MAX_MEAN: 12.4 **MAX_MED:** 12.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

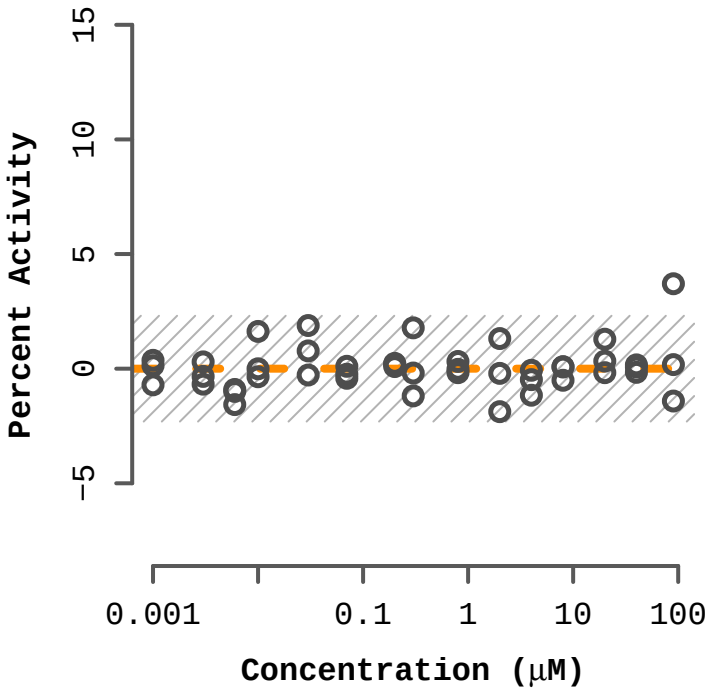
NAME: N-pentylpentan-1-amine
CHID: 24931 CASRN: 2050-92-2
SPID(S): Tox21_303290
M4ID: 12475843

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.95 MAX_MED: 0.677 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

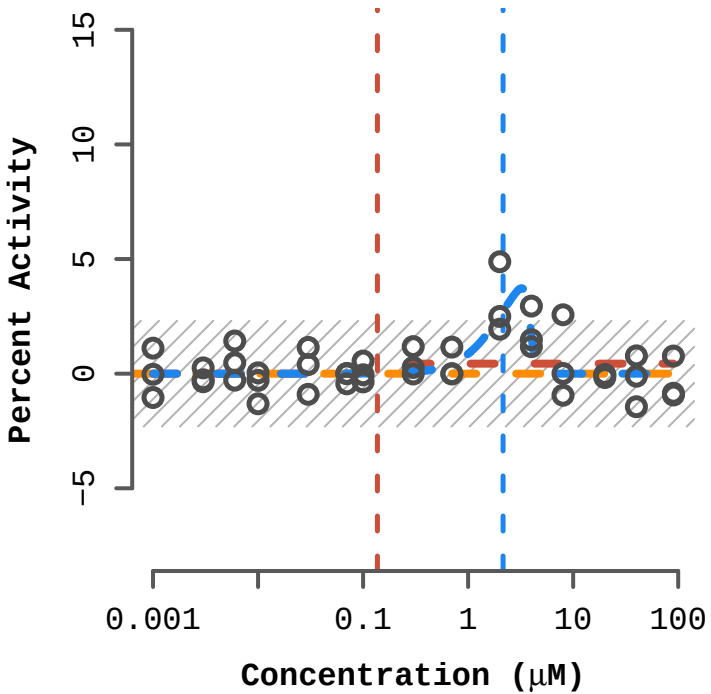
NAME: N-pentylpentan-1-amine
CHID: 24931 **CASRN:** 2050-92-2
SPID(S): Tox21_202211
M4ID: 12480041

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 0.776 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diazoaminobenzene
CHID: 24934 **CASRN:** 136-35-6
SPID(S): Tox21_303249
M4ID: 12475884

HILL MODEL (in red):

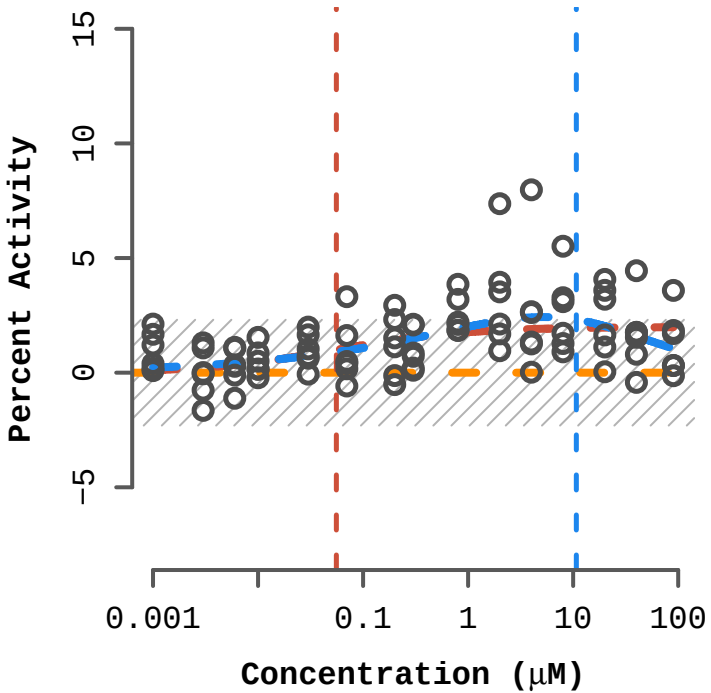
	tp	ga	gw
val:	0.438	-0.863	8
sd:	0.227	1.75	68.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.47	0.333	2.18	0.59	17.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	140.71	142.77	121.79
PROB:	0	0	1
RMSE:	1.26	1.16	0.84

MAX_MEAN: 3.11 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diazoaminobenzene
CHID: 24934 CASRN: 136-35-6
SPID(S): Tox21_202253
M4ID: 12479999

HILL MODEL (in red):

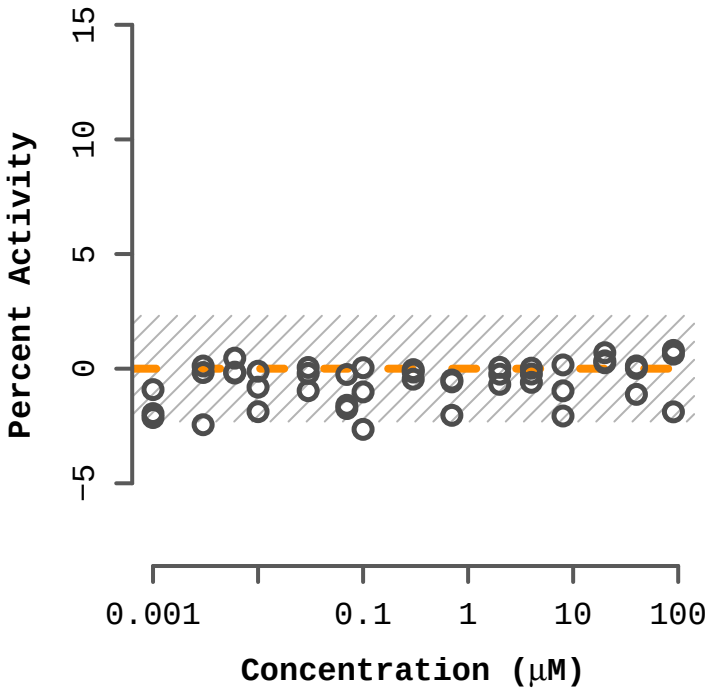
	tp	ga	gw
val:	1.99	−1.25	0.71
sd:	0.258	0.356	0.303

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.43	1.03	0.376	1.28	0.868
sd:	26	5.93	0.257	1.32	0.532

	CNST	HILL	GNLS
AIC:	392.1	319.58	316.83
PROB:	0	0.2	0.8
RMSE:	2.2	1.46	1.39

MAX_MEAN: 3.27 **MAX_MED:** 2.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

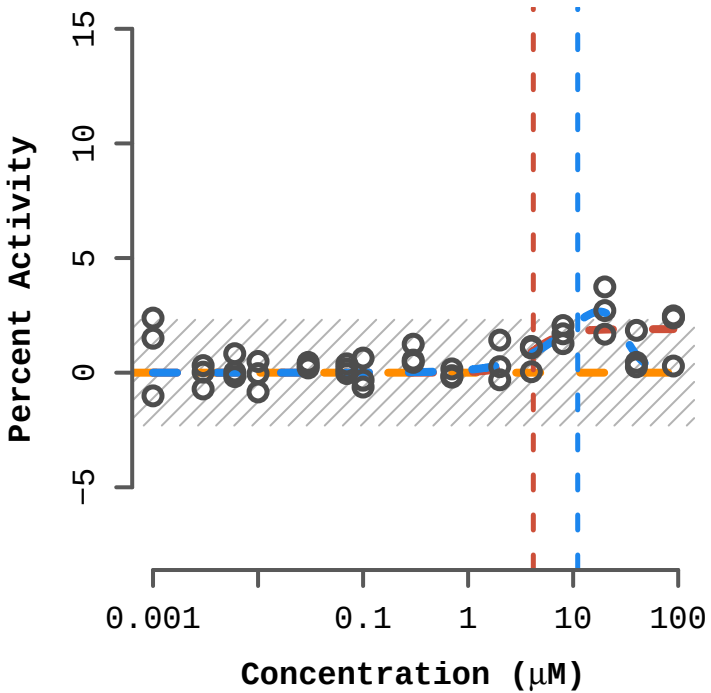
NAME: Phenoxathiin
CHID: 24937 **CASRN:** 262-20-4
SPID(S): Tox21_303241
M4ID: 12475892

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.433 **MAX_MED:** 0.635 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenoxathiin
CHID: 24937 CASRN: 262-20-4
SPID(S): Tox21_202275
M4ID: 12479977

HILL MODEL (in red):

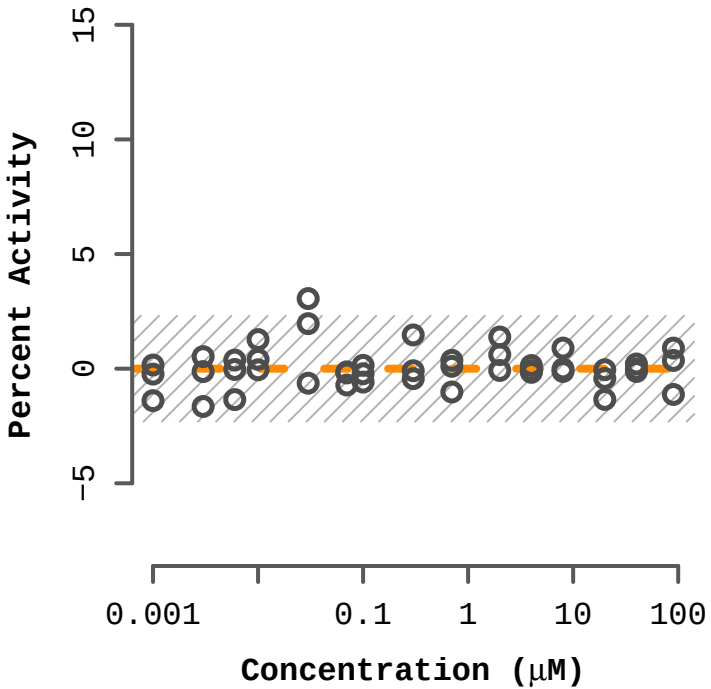
	tp	ga	gw
val:	1.9	0.621	2.93
sd:	0.304	0.123	2.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.49	1.04	1.48	1.46	4.25
sd:	5.52	0.616	0.98	0.228	5.73

	CNST	HILL	GNLS
AIC:	145.27	115.16	120.02
PROB:	0	0.92	0.08
RMSE:	1.23	0.81	0.85

MAX_MEAN: 2.71 MAX_MED: 2.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

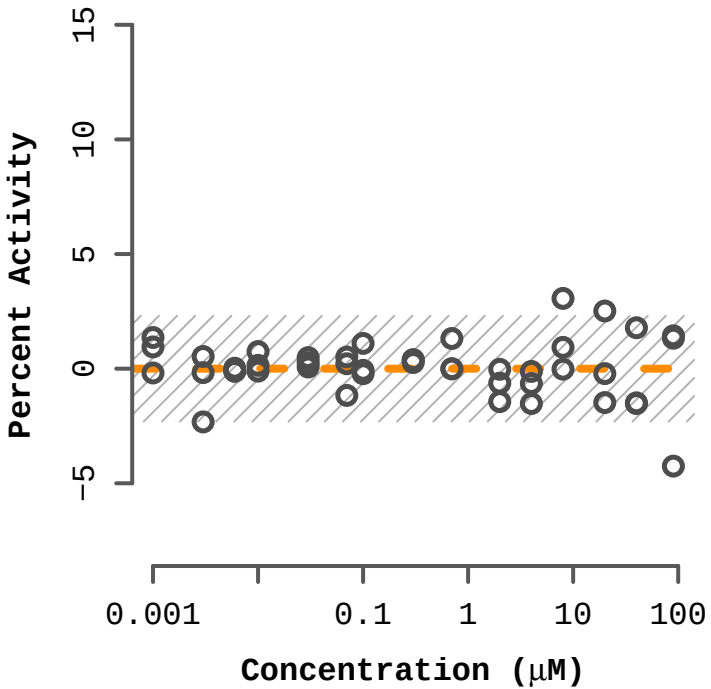
NAME: Dibromoacetonitrile
CHID: 24940 **CASRN:** 3252-43-5
SPID(S): Tox21_303041
M4ID: 12476092

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

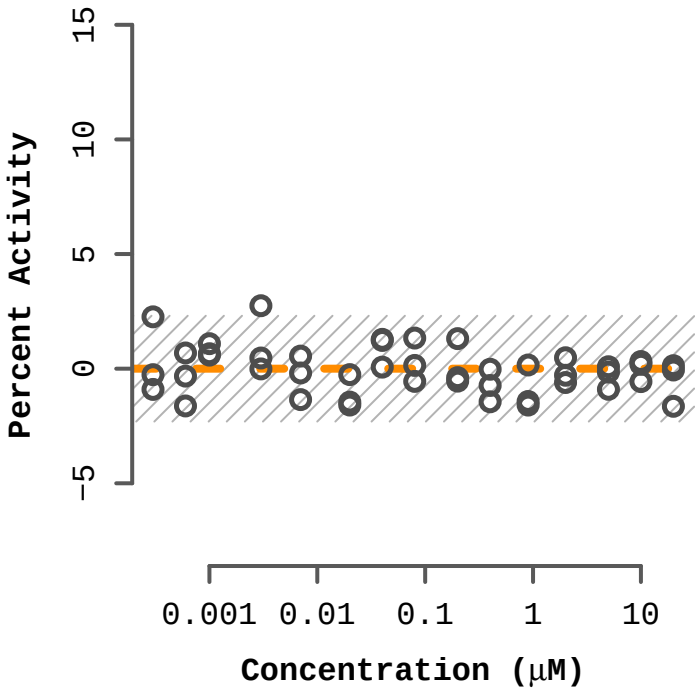
NAME: Dibromoacetonitrile
CHID: 24940 CASRN: 3252-43-5
SPID(S): Tox21_202319
M4ID: 12479933

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.33 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

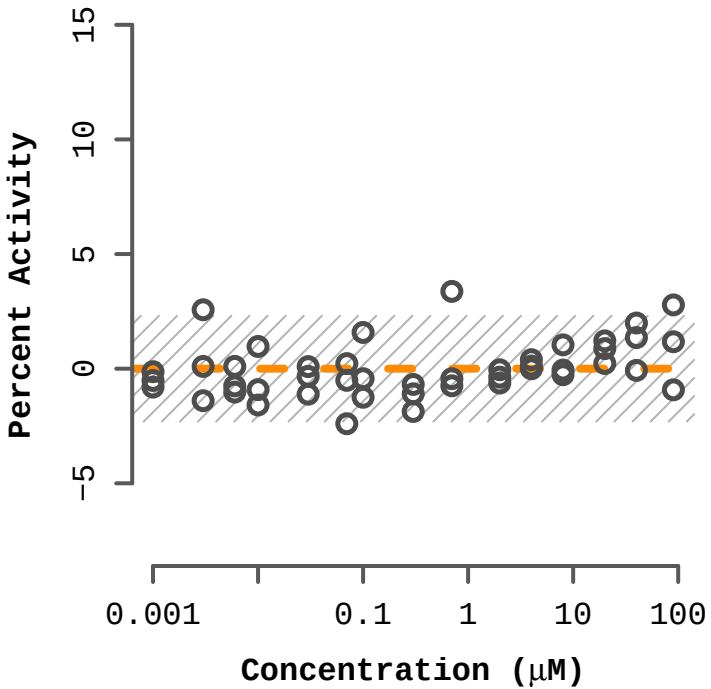
NAME: (E)−1,4−Dibromo−2−butene
CHID: 24941 **CASRN:** 821−06−7
SPID(S): Tox21_202728
M4ID: 12479524

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.21	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

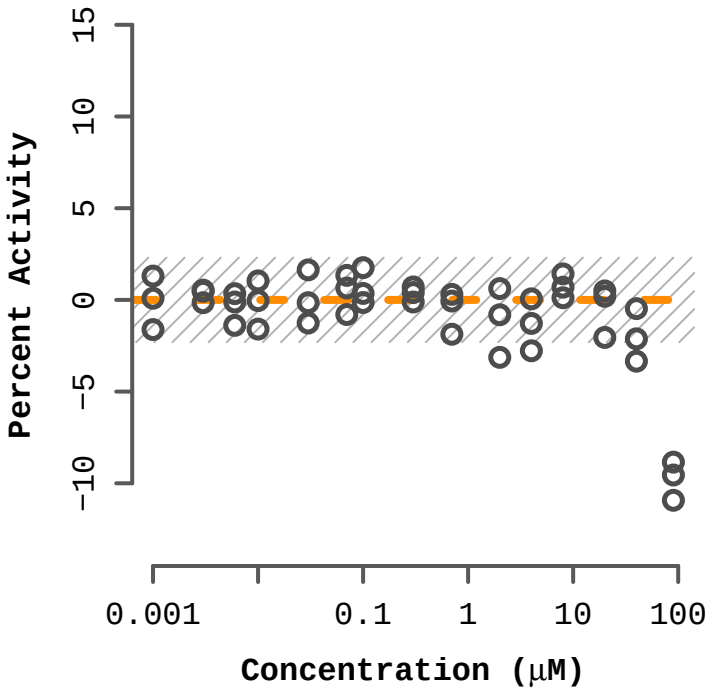
NAME: (2E)-2,3-Dibromo-2-butene-1,4-diol
CHID: 24942 **CASRN:** 21285-46-1
SPID(S): Tox21_201101
M4ID: 12481151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

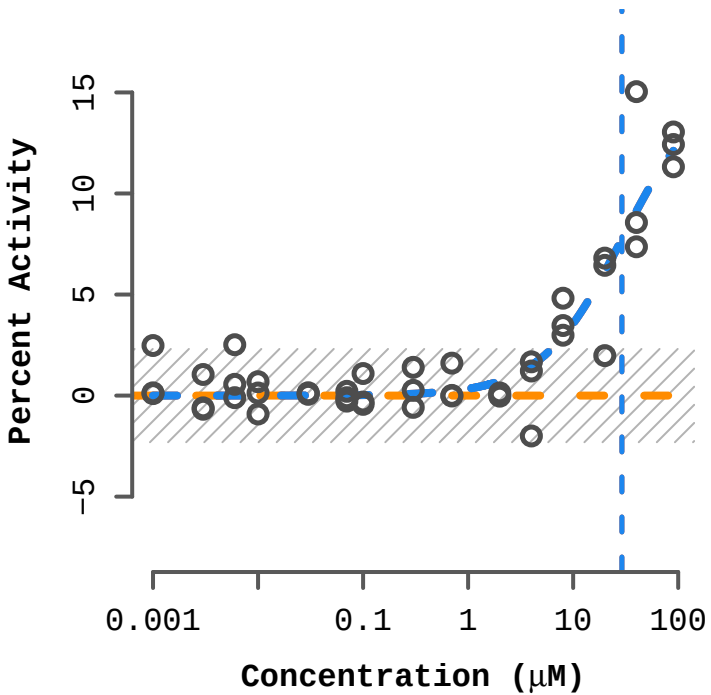
NAME: 1,2-Dibromo-2,4-dicyanobutane
CHID: 24944 **CASRN:** 35691-65-7
SPID(S): Tox21_301951
M4ID: 12477182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.82	NA	NA

MAX_MEAN: 0.745 **MAX_MED:** 0.695 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane
CHID: 24947 CASRN: 3322-93-8
SPID(S): Tox21_200970
M4ID: 12481282

HILL MODEL (in red):

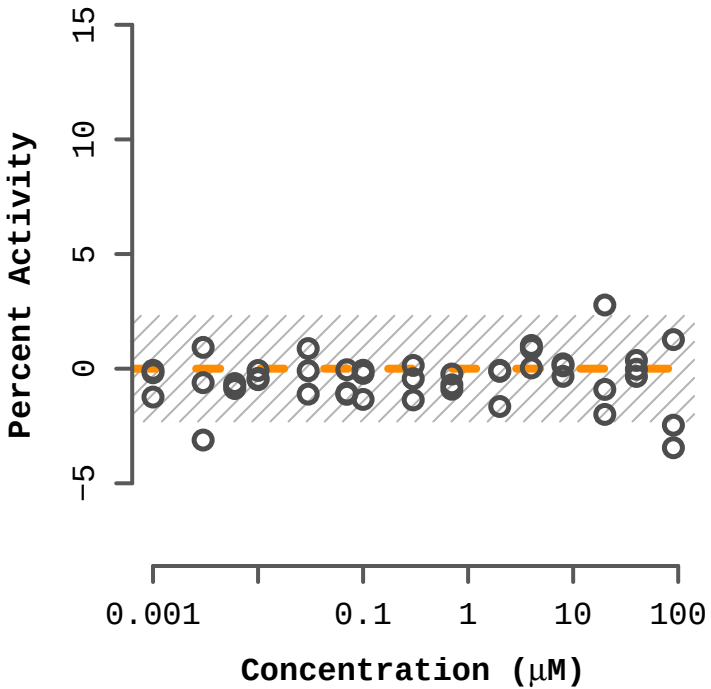
	tp	ga	gw
val:	15.5	1.46	1.13
sd:	2.74	0.183	0.214

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.5	1.46	1.13	3.56	5.18
sd:	2.74	0.183	0.214	1360	4400

	CNST	HILL	GNLS
AIC:	249.26	152.24	156.24
PROB:	0	0.88	0.12
RMSE:	4.65	1.47	1.47

MAX_MEAN: 12.3 MAX_MED: 12.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

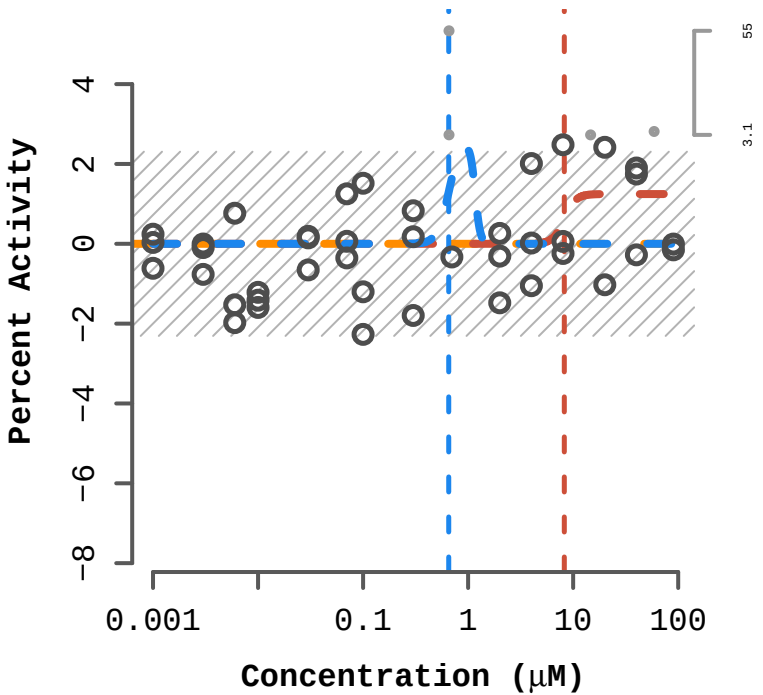
NAME: 2,3-Dibromopropyl acrylate
CHID: 24950 **CASRN:** 19660-16-3
SPID(S): Tox21_303936
M4ID: 12475252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.646 **MAX_MED:** 0.887 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Butyl-1-butanamine
CHID: 24952 **CASRN:** 111-92-2
SPID(S): Tox21_200418
M4ID: 12481834 **BRK**

HILL MODEL (in red):

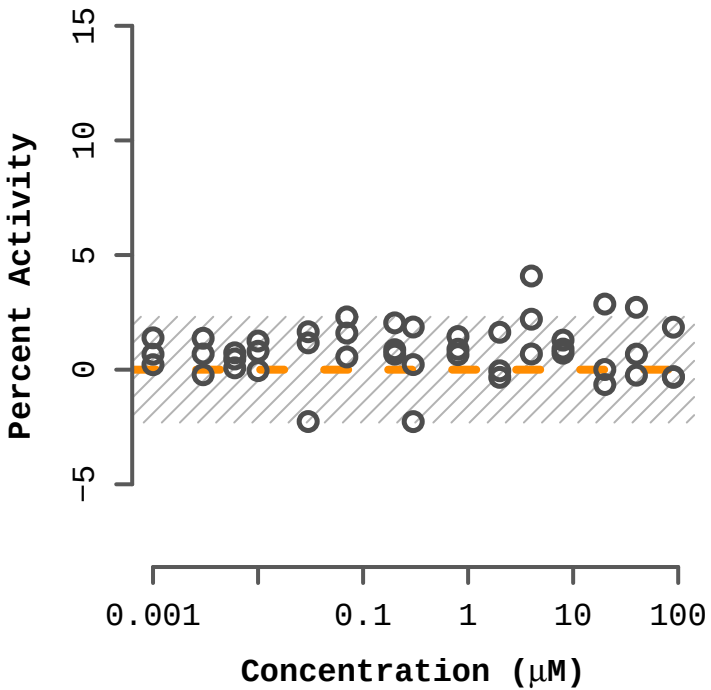
	tp	ga	gw
val:	1.25	0.916	7.99
sd:	0.589	0.168	72.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.6	−0.185	7.9	0.0665	17.9
sd:	21.6	1.17	38.8	4.34	332

	CNST	HILL	GNLS
AIC:	194.62	195.6	203.45
PROB:	0.62	0.38	0.01
RMSE:	8.34	8.32	8.09

MAX_MEAN: 19.3 **MAX_MED:** 3.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

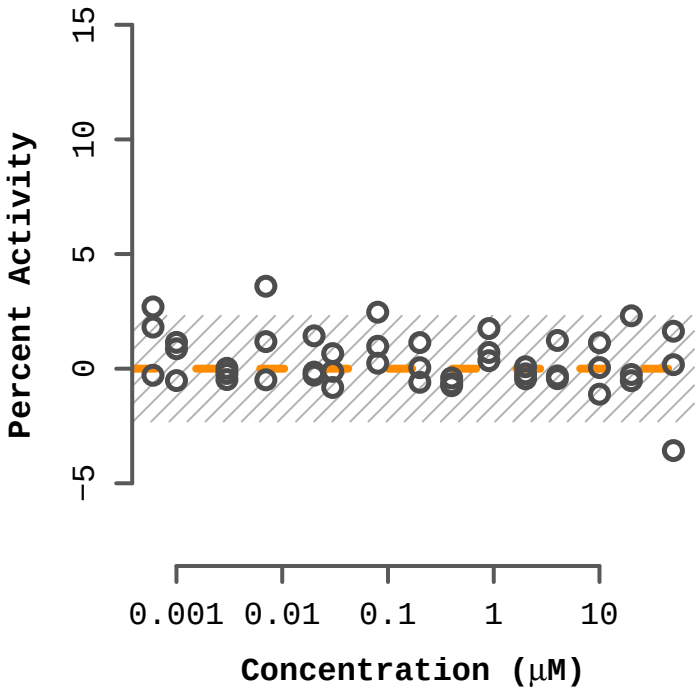
NAME: 2-(Dibutylamino)ethanol
CHID: 24953 **CASRN:** 102-81-8
SPID(S): Tox21_200702
M4ID: 12481550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 2.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

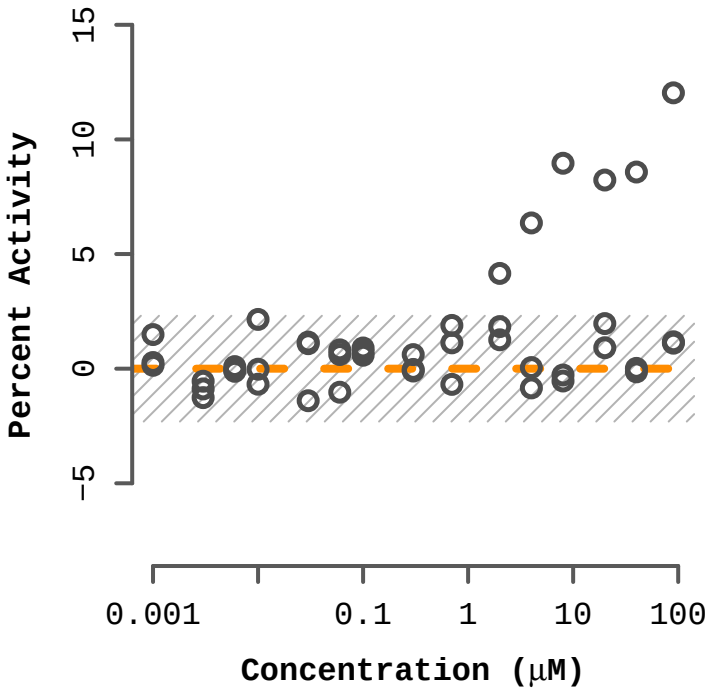
NAME: Di-tert-butyl peroxide
CHID: 24955 **CASRN:** 110-05-4
SPID(S): Tox21_300099
M4ID: 12479031

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

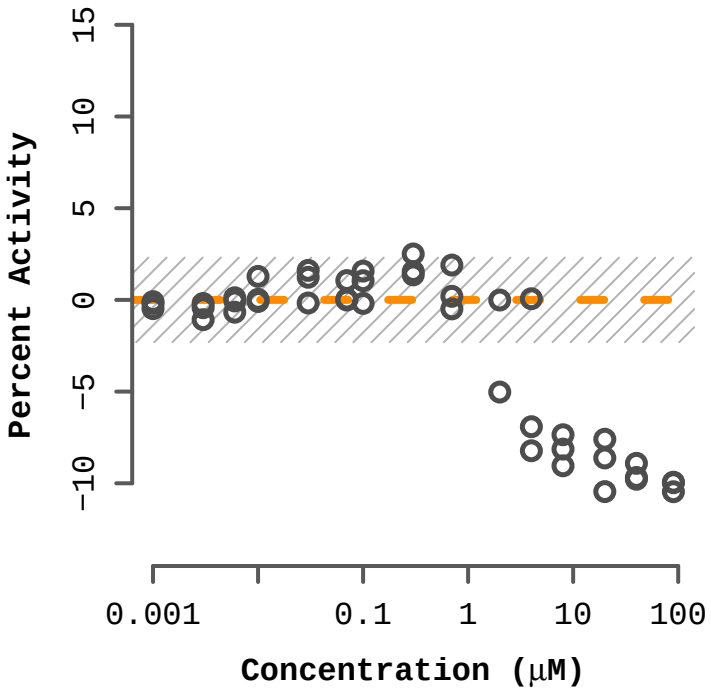
NAME: Di-tert-butyl peroxide
CHID: 24955 **CASRN:** 110-05-4
SPID(S): Tox21_201461
M4ID: 12480791

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.2	NA	NA

MAX_MEAN: 4.77 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

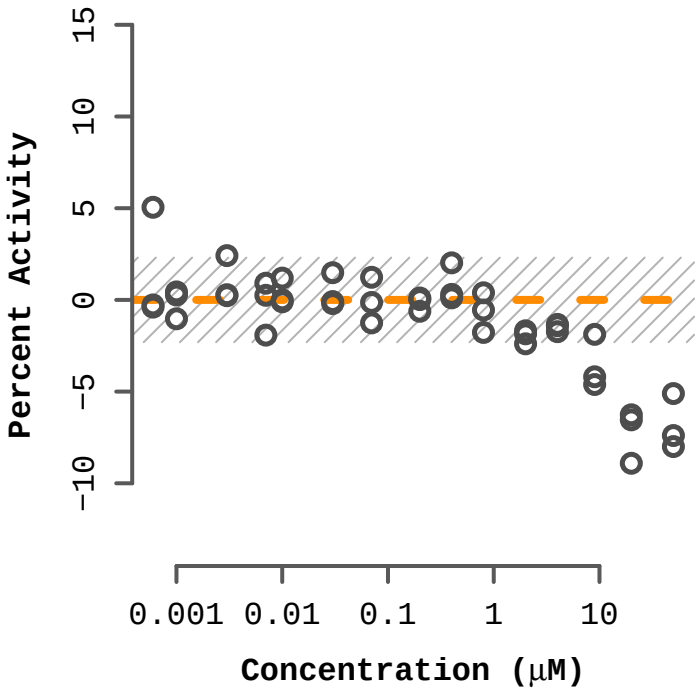
NAME: N,N'-Bis(1-methylpropyl)-1,4-benzenediamine
CHID: 24956 **CASRN:** 101-96-2
SPID(S): Tox21_200371
M4ID: 12481881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.54	NA	NA
PROB:	1	NA	NA
RMSE:	5.19	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

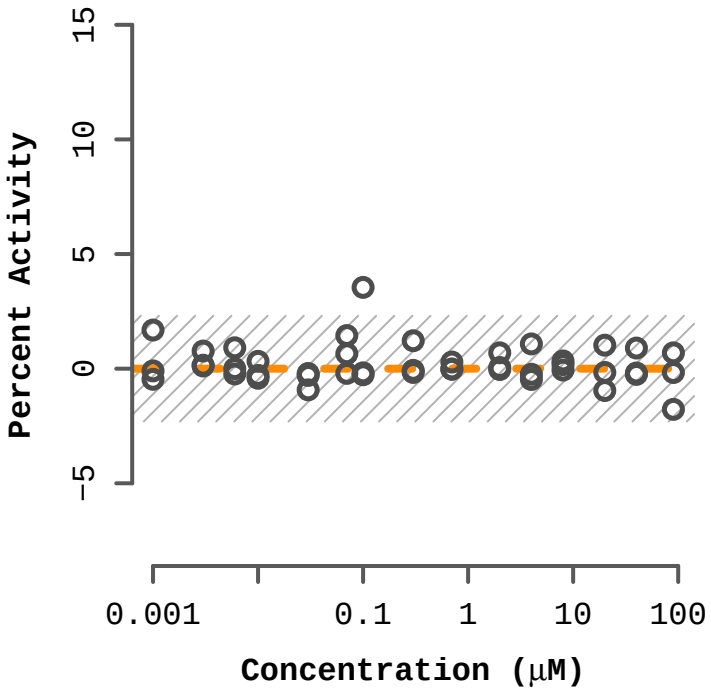
NAME: Dibutyltin dilaurate
CHID: 24961 CASRN: 77-58-7
SPID(S): Tox21_112324_1
M4ID: 12483162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.23	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 0.302 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

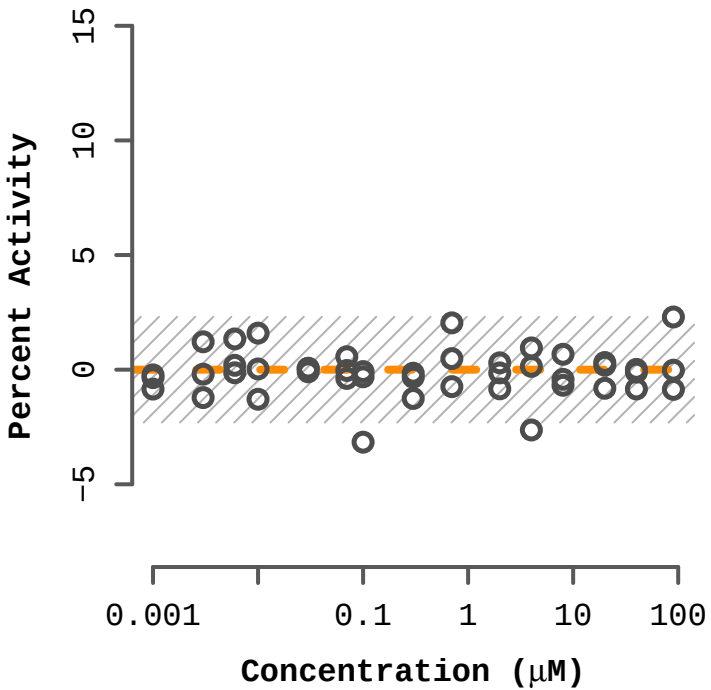
NAME: Dichloroacetyl chloride
CHID: 24965 **CASRN:** 79-36-7
SPID(S): Tox21_200778
M4ID: 12481474

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.652 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

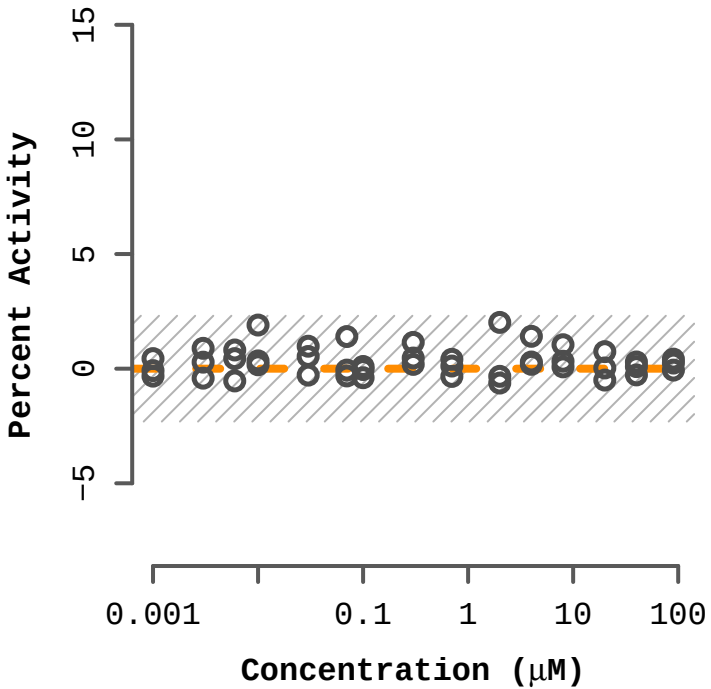
NAME: 2,4-Dichloroaniline
CHID: 24966 **CASRN:** 554-00-7
SPID(S): Tox21_303206
M4ID: 12475927

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.484 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

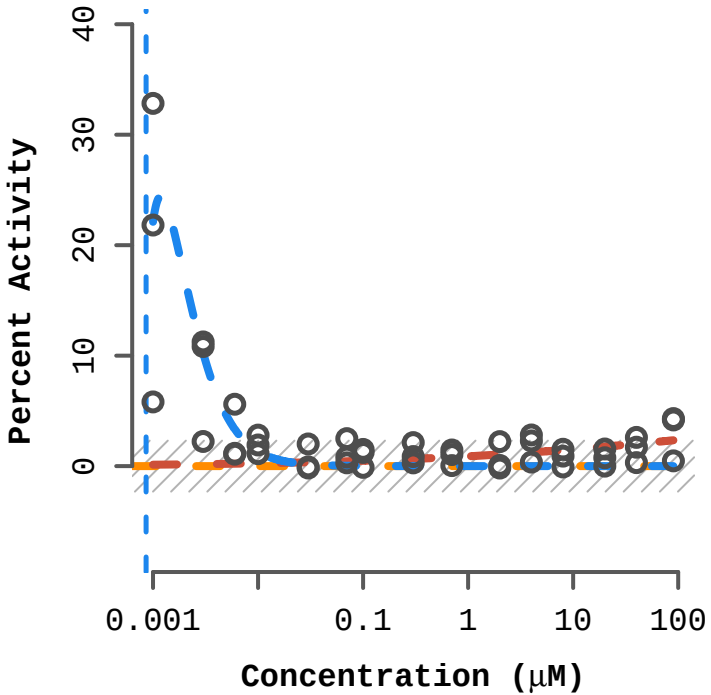
NAME: 2,4-Dichloroaniline
CHID: 24966 **CASRN:** 554-00-7
SPID(S): Tox21_201522
M4ID: 12480730

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.806 **MAX_MED:** 0.533 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,5-Dichloroaniline
CHID: 24967 CASRN: 95-82-9
SPID(S): Tox21_200381
M4ID: 12481871

HILL MODEL (in red):

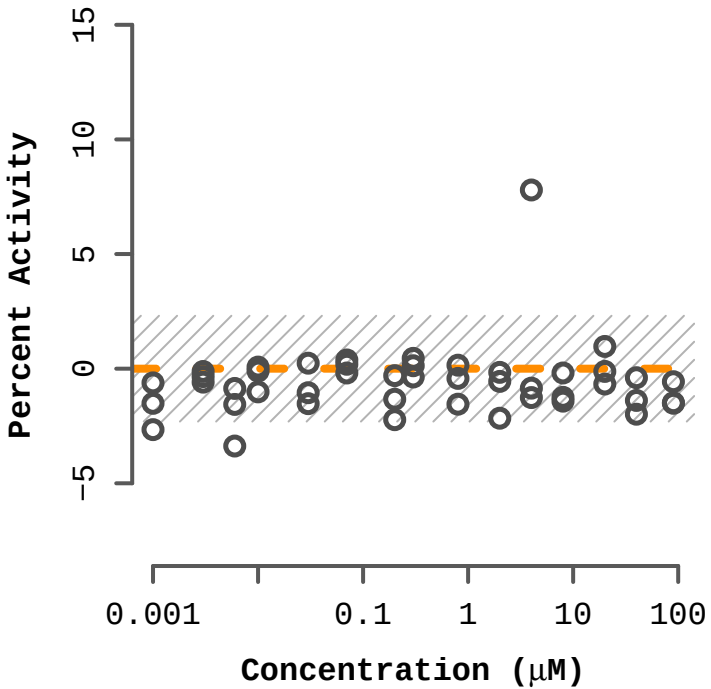
	tp	ga	gw
val:	5.47	2.37	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	39.4	-3.07	7.4	-2.76	1.92
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	252.1	244.77	222.65
PROB:	0	0	1
RMSE:	6.63	6.49	3.52

MAX_MEAN: 20.2 MAX_MED: 21.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

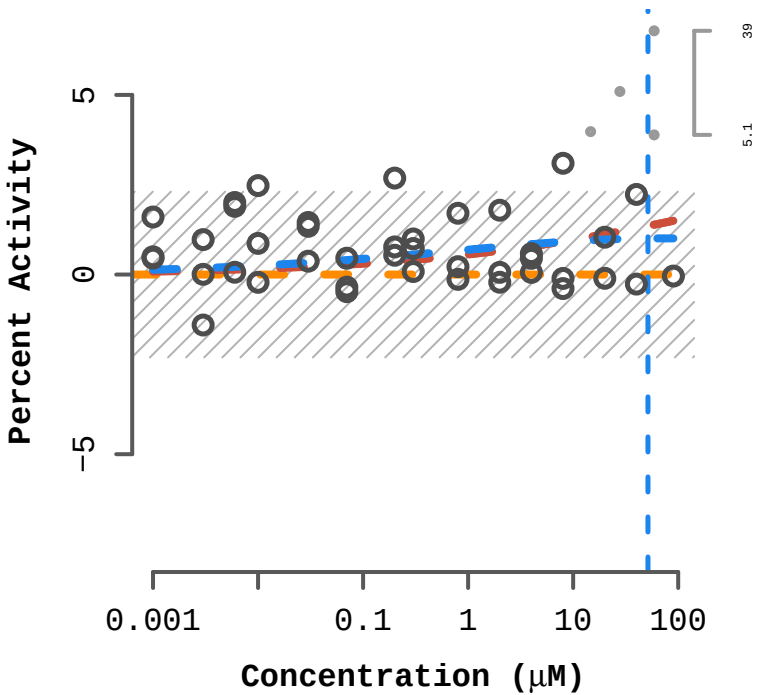
NAME: 2,6-Dichlorobenzaldehyde
CHID: 24970 **CASRN:** 83-38-5
SPID(S): Tox21_200742
M4ID: 12481510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 0.193 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,4−Dichlorobenzaldehyde
CHID: 24971 CASRN: 6287−38−3
SPID(S): Tox21_200040
M4ID: 12482212 BRK

HILL MODEL (in red):

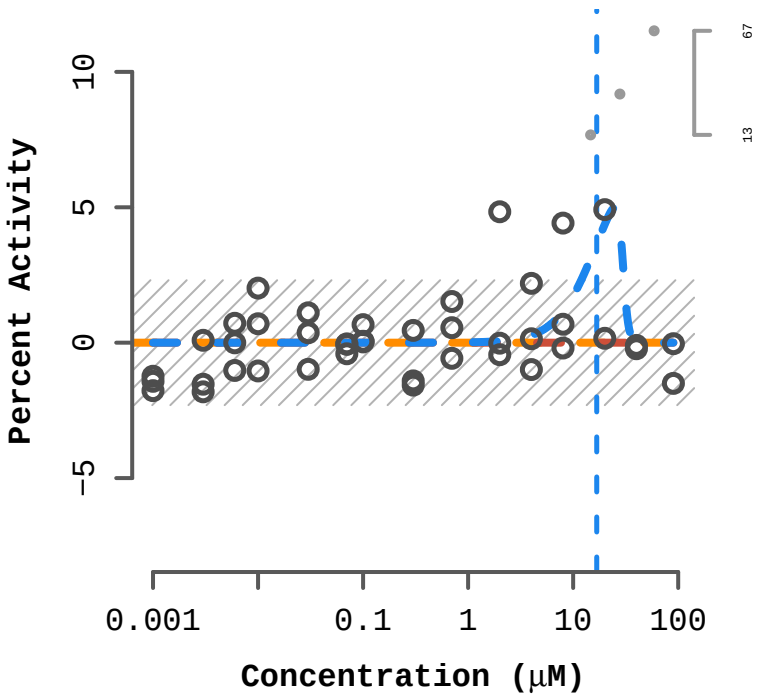
	tp	ga	gw
val:	3.61	2.45	0.3
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.7	1.71	0.3	1.96	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	210.95	208.48	211.81
PROB:	0.2	0.68	0.13
RMSE:	6.62	6.28	6.37

MAX_MEAN: 14.5 MAX_MED: 5.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dichlorobenzoic acid
CHID: 24976 CASRN: 50-45-3
SPID(S): Tox21_201189
M4ID: 12481063 BRK

HILL MODEL (in red):

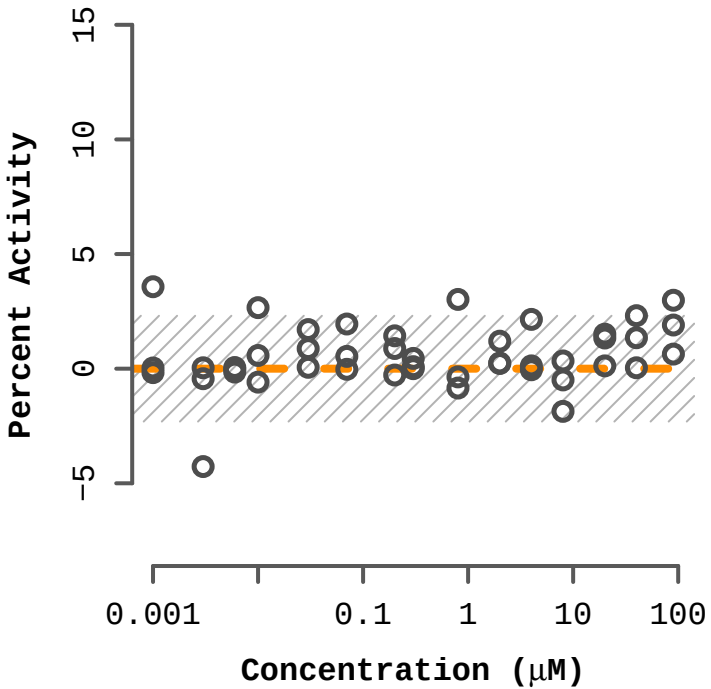
	tp	ga	gw
val:	2.16e-08	2.45	2.04
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.31	1.22	2.26	1.47	17.8
sd:	19.7	1.15	3.94	0.609	84.9

	CNST	HILL	GNLS
AIC:	235.12	241.12	239.17
PROB:	0.85	0.04	0.11
RMSE:	11.52	11.52	11.41

MAX_MEAN: 21.9 MAX_MED: 4.91 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

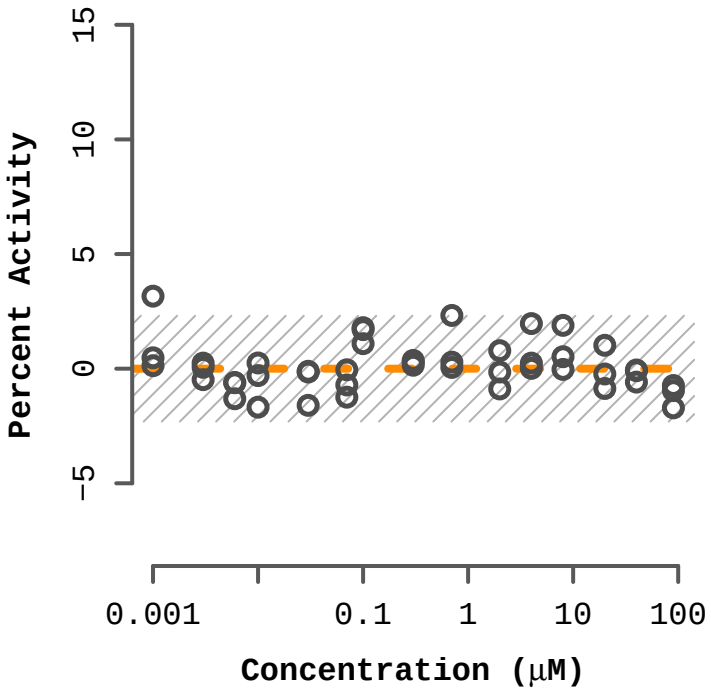
NAME: 2,4-Dichlorobenzoic acid
CHID: 24977 **CASRN:** 50-84-0
SPID(S): Tox21_200756
M4ID: 12481496

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

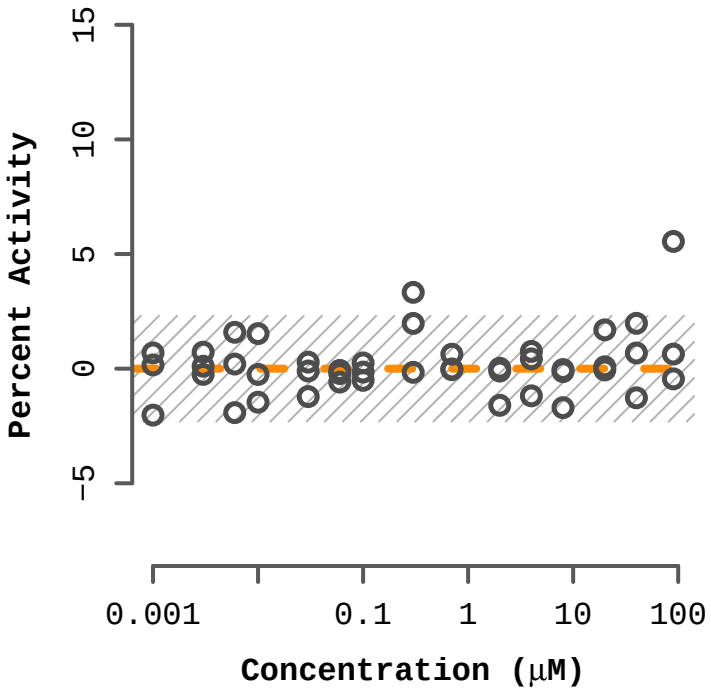
NAME: 2,5-Dichlorobenzoic acid
CHID: 24978 **CASRN:** 50-79-3
SPID(S): Tox21_200321
M4ID: 12481931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

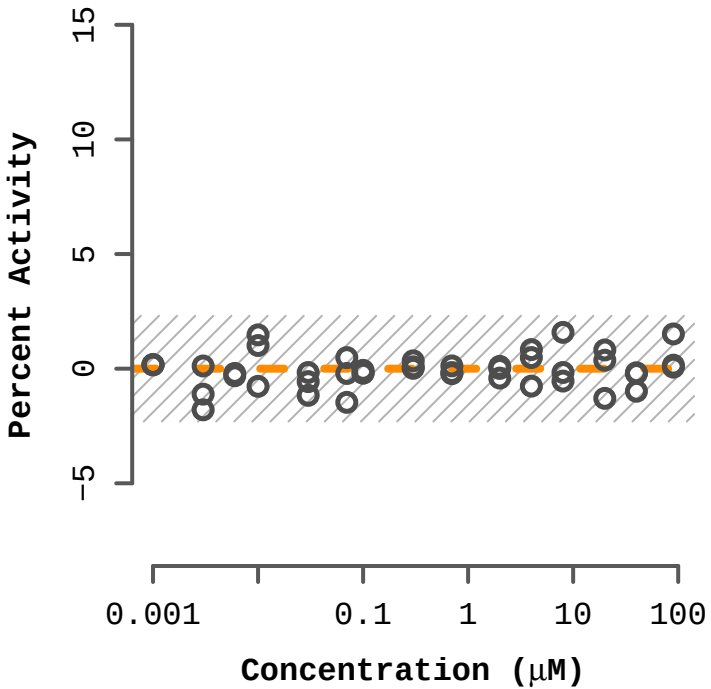
NAME: 2,6-Dichlorobenzoic acid
CHID: 24979 **CASRN:** 50-30-6
SPID(S): Tox21_200320
M4ID: 12481932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

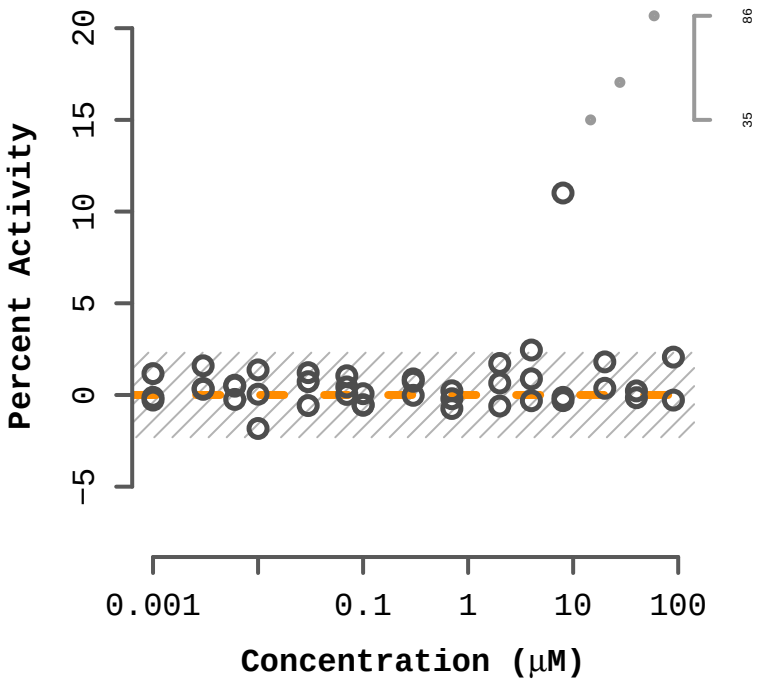
NAME: 3,4-Dichlorobenzoic acid
CHID: 24980 **CASRN:** 51-44-5
SPID(S): Tox21_200322
M4ID: 12481930

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.58 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

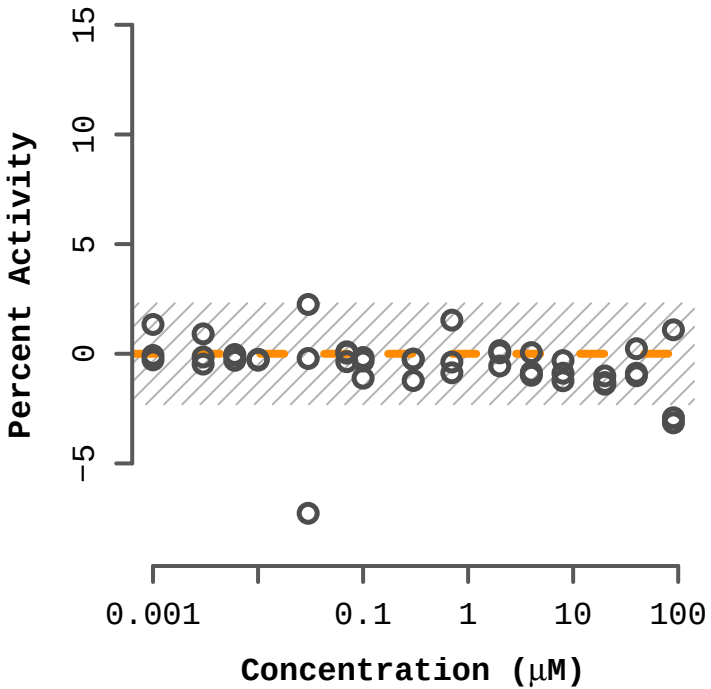
NAME: 3,5-Dichlorobenzoic acid
CHID: 24981 **CASRN:** 51-36-5
SPID(S): Tox21_200155
M4ID: 12482097 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	239.91	NA	NA
PROB:	1	NA	NA
RMSE:	16.1	NA	NA

MAX_MEAN: 29.4 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

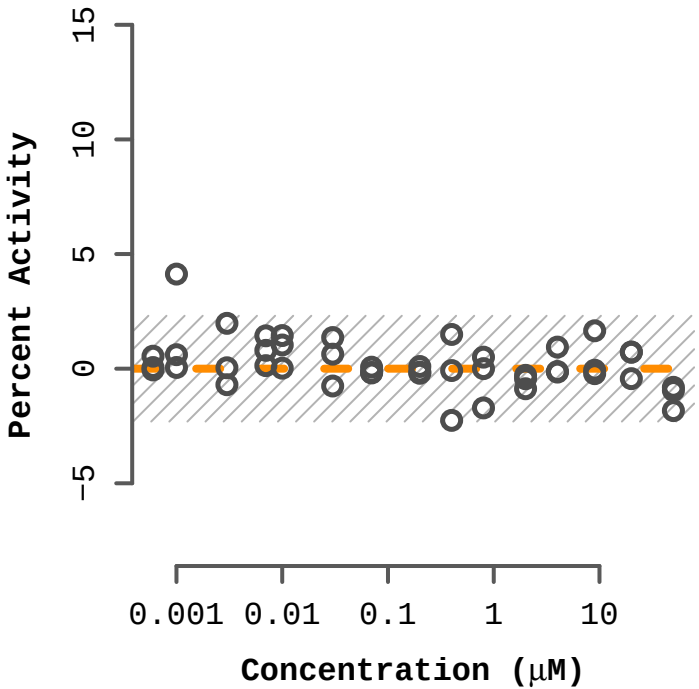
NAME: Cisplatin
CHID: 24983 **CASRN:** 15663-27-1
SPID(S): Tox21_202500
M4ID: 12479752

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.329 **MAX_MED:** 0.0448 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

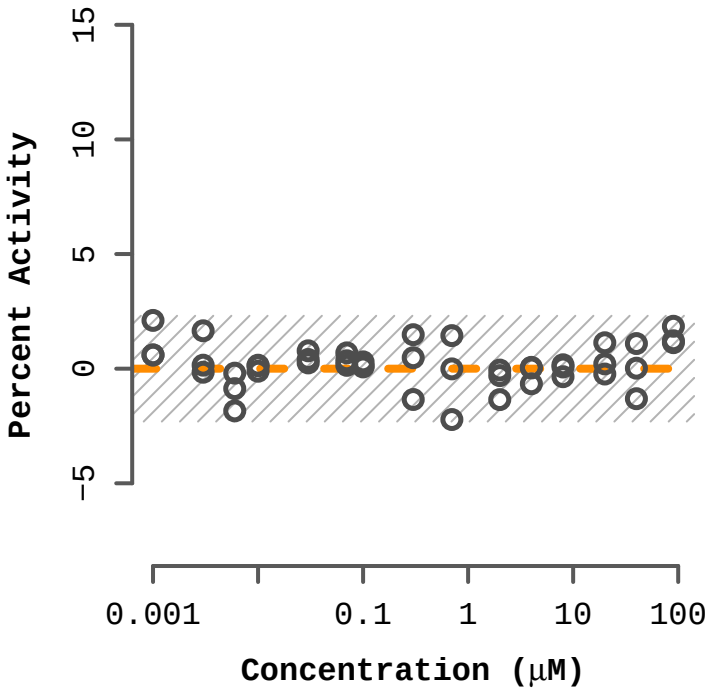
NAME: Cisplatin
CHID: 24983 **CASRN:** 15663-27-1
SPID(S): Tox21_111011_1
M4ID: 12483950

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

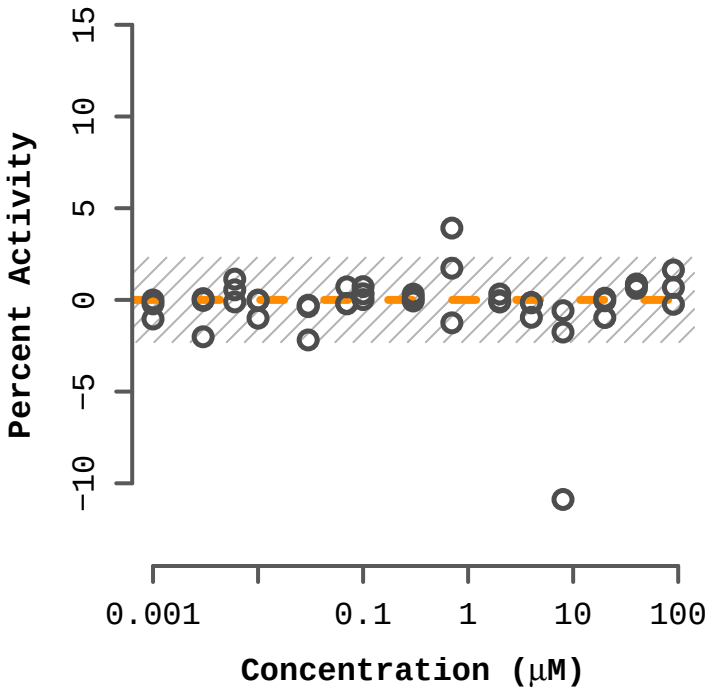
NAME: 1,3-Dichloro-5,5-dimethylhydantoin
CHID: 24985 **CASRN:** 118-52-5
SPID(S): Tox21_300184
M4ID: 12478946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

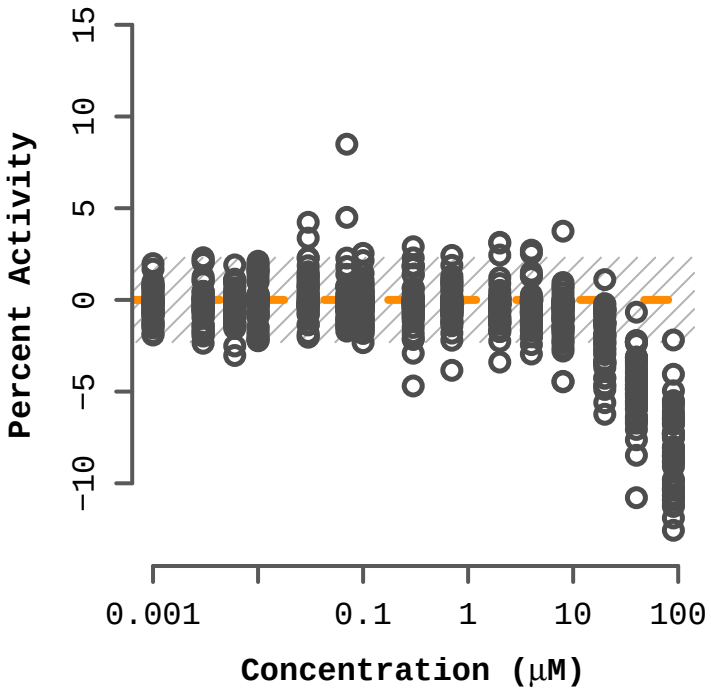
NAME: 1,3-Dichloro-5,5-dimethylhydantoin
CHID: 24985 **CASRN:** 118-52-5
SPID(S): Tox21_202384
M4ID: 12479868

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

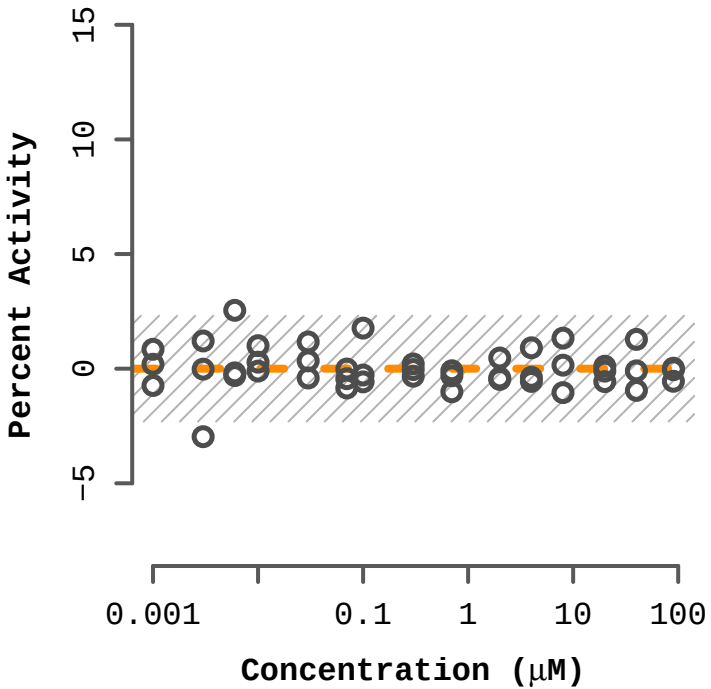
NAME: 4,4'−Dichlorodiphenyl sulfone
CHID: 24986 **CASRN:** 80−07−9
SPID(S): Tox21_400008
M4ID: 12475129

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3249.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.85	NA	NA

MAX_MEAN: 0.242 **MAX_MED:** −0.0578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

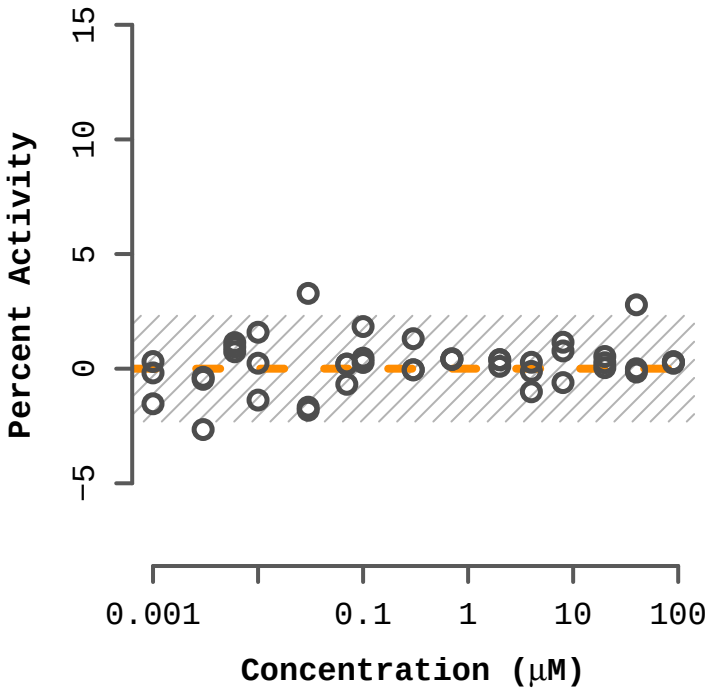
NAME: 1,2-Dichloroethylene
CHID: 24991 **CASRN:** 540-59-0
SPID(S): Tox21_200774
M4ID: 12481478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.689 **MAX_MED:** 0.341 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

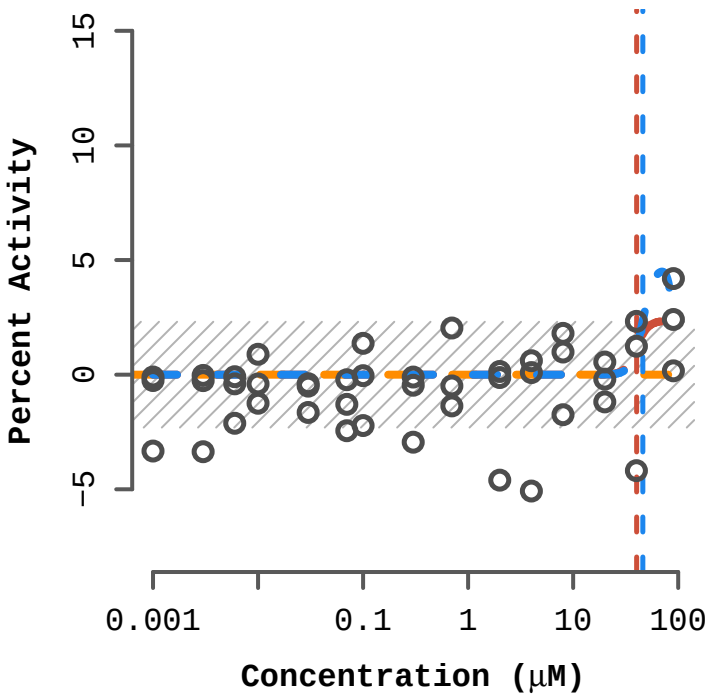
NAME: Troclosene
CHID: 24993 **CASRN:** 2782-57-2
SPID(S): Tox21_302395
M4ID: 12476738

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium dichloroisocyanurate
CHID: 24994 CASRN: 2893-78-9
SPID(S): Tox21_303262
M4ID: 12475871

HILL MODEL (in red):

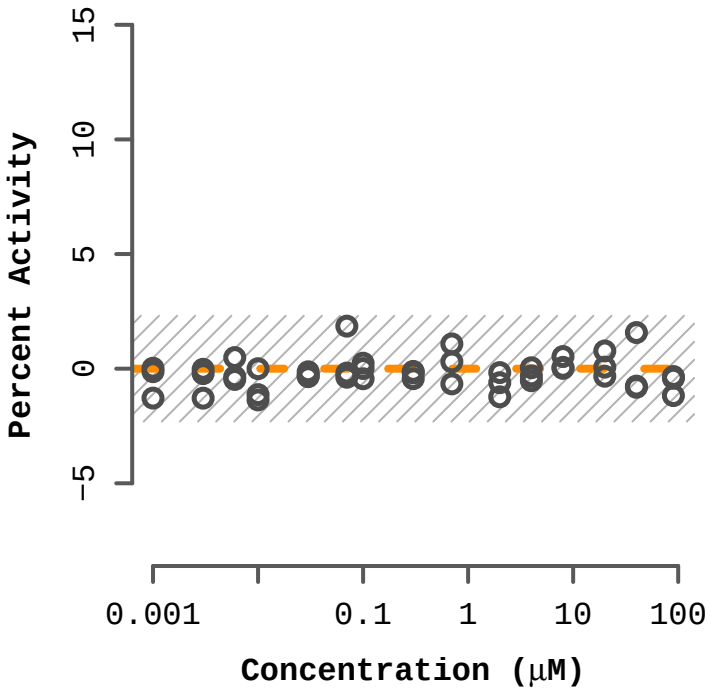
	tp	ga	gw
val:	2.36	1.6	8
sd:	1.03	0.105	22.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	1.66	8	1.95	16.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	186.74	187.26	191.26
PROB:	0.53	0.41	0.06
RMSE:	1.92	1.87	1.87

MAX_MEAN: 2.26 **MAX_MED:** 2.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

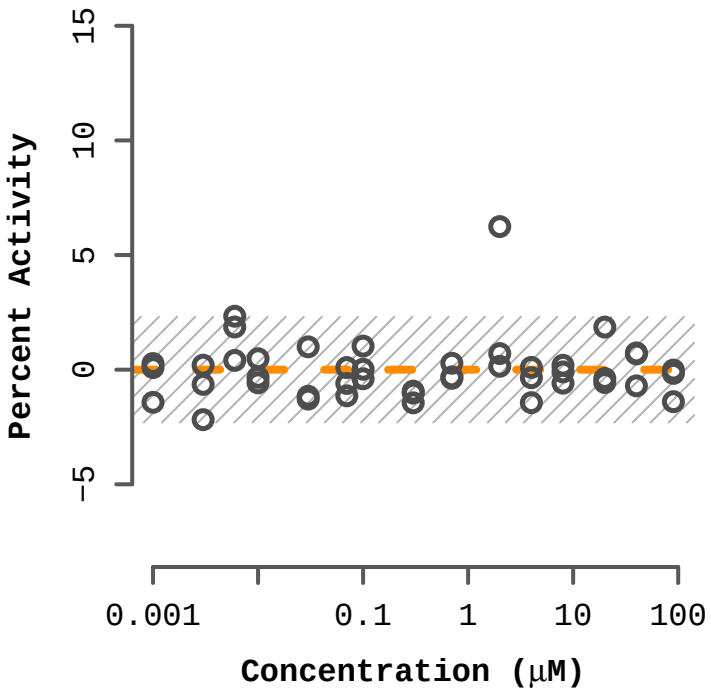
NAME: Sodium dichloroisocyanurate
CHID: 24994 CASRN: 2893-78-9
SPID(S): Tox21_201601
M4ID: 12480651

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.431 **MAX_MED:** 0.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

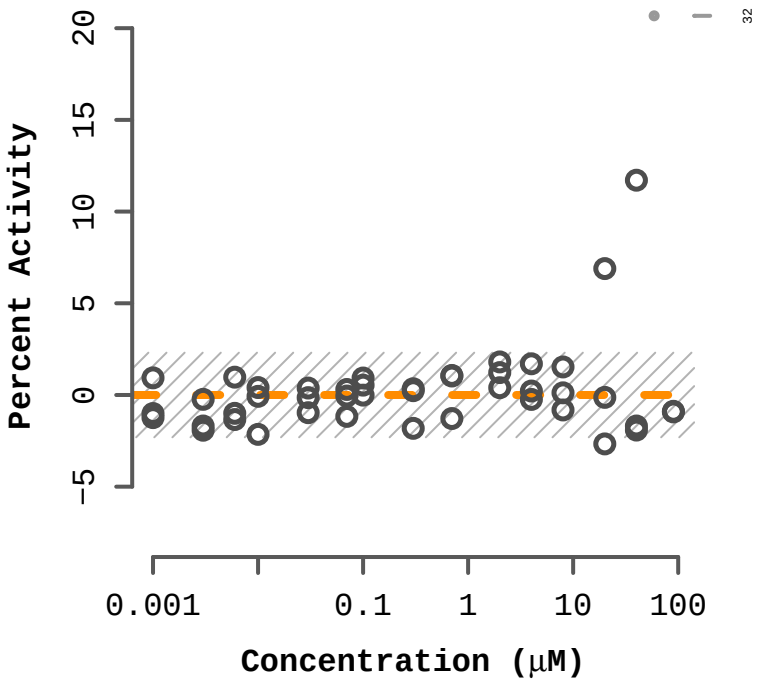
NAME: 2,3-Dichloronitrobenzene
CHID: 24997 CASRN: 3209-22-1
SPID(S): Tox21_200851
M4ID: 12481401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 2.37 MAX_MED: 1.86 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

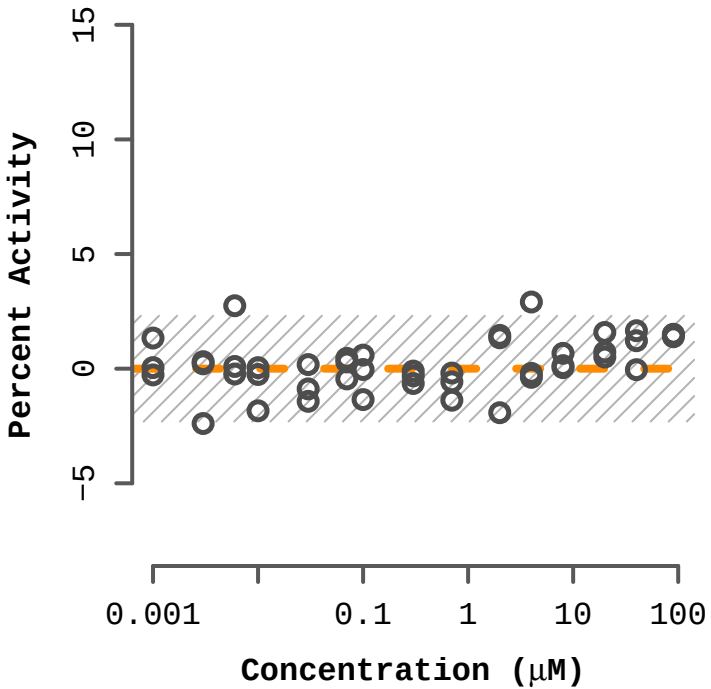
NAME: 2,4-Dichloronitrobenzene
CHID: 24998 **CASRN:** 611-06-3
SPID(S): Tox21_200204
M4ID: 12482048 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.13	NA	NA
PROB:	1	NA	NA
RMSE:	5.32	NA	NA

MAX_MEAN: 10.1 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

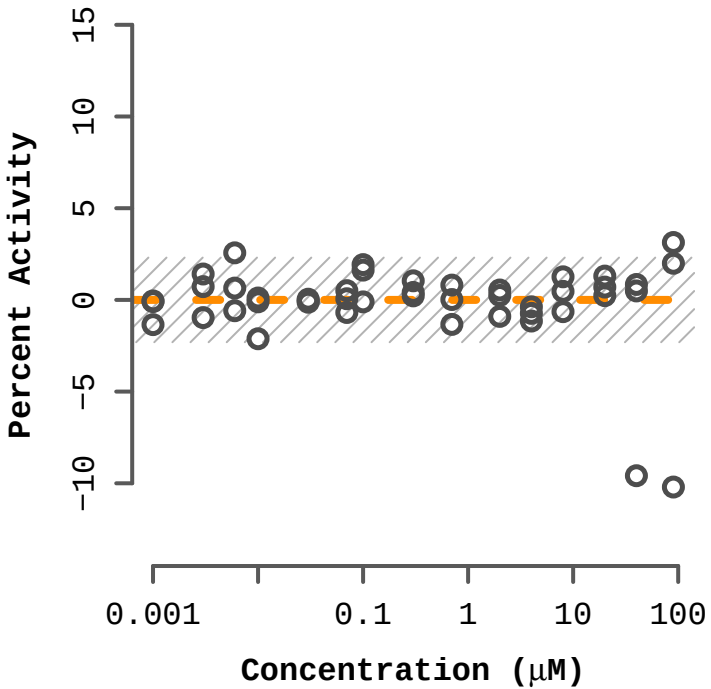
NAME: 3,4−Dichloronitrobenzene
CHID: 24999 **CASRN:** 99−54−7
SPID(S): Tox21_300293
M4ID: 12478837

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

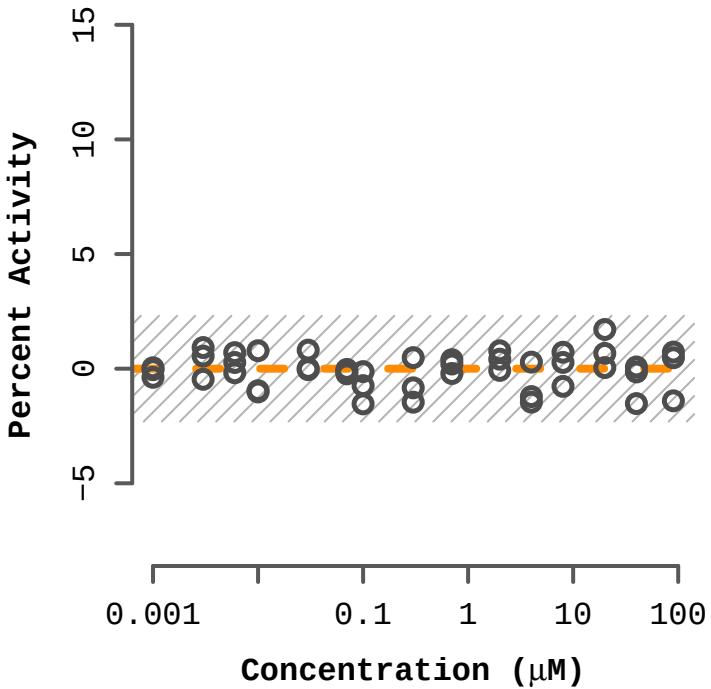
NAME: 3,4-Dichloronitrobenzene
CHID: 24999 **CASRN:** 99-54-7
SPID(S): Tox21_201613
M4ID: 12480639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.74	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

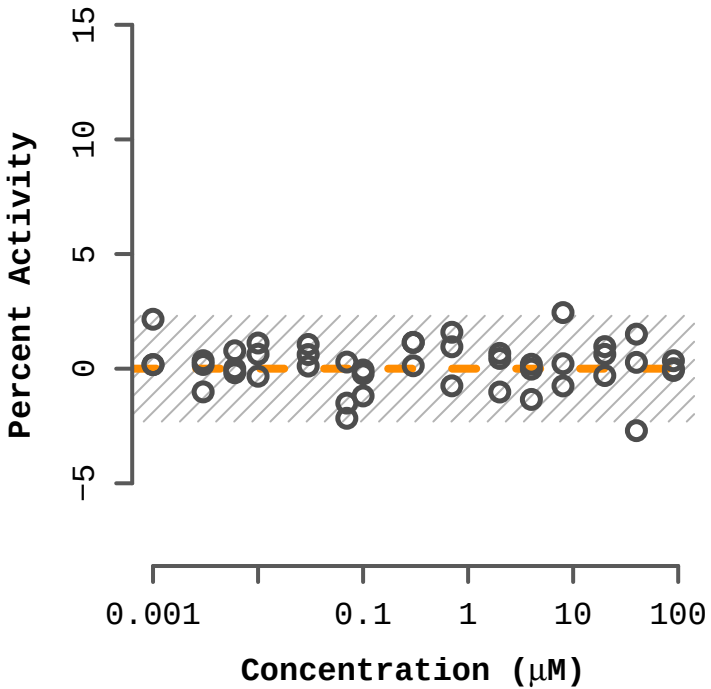
NAME: 2,3-Dichlorophenol
CHID: 25001 **CASRN:** 576-24-9
SPID(S): Tox21_200909
M4ID: 12481343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.81 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

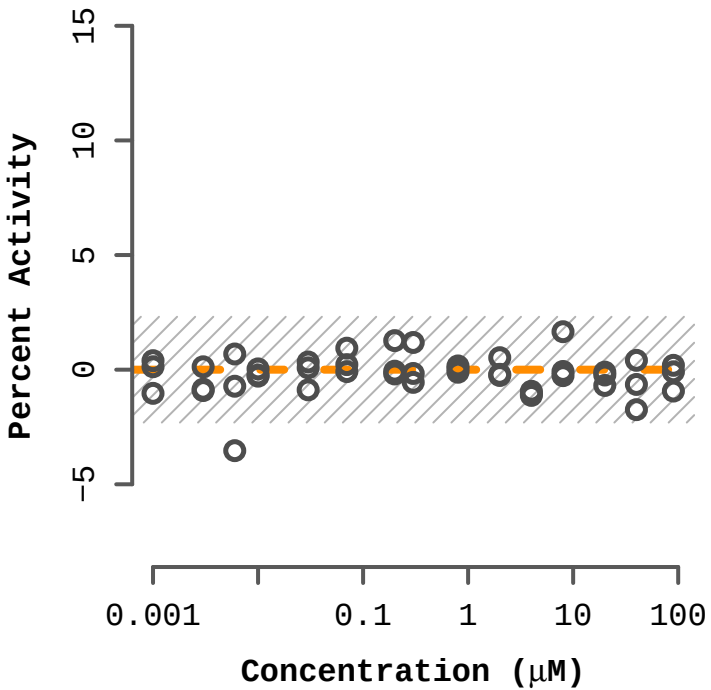
NAME: 2,5-Dichlorophenol
CHID: 25003 **CASRN:** 583-78-8
SPID(S): Tox21_303053
M4ID: 12476080

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.838 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

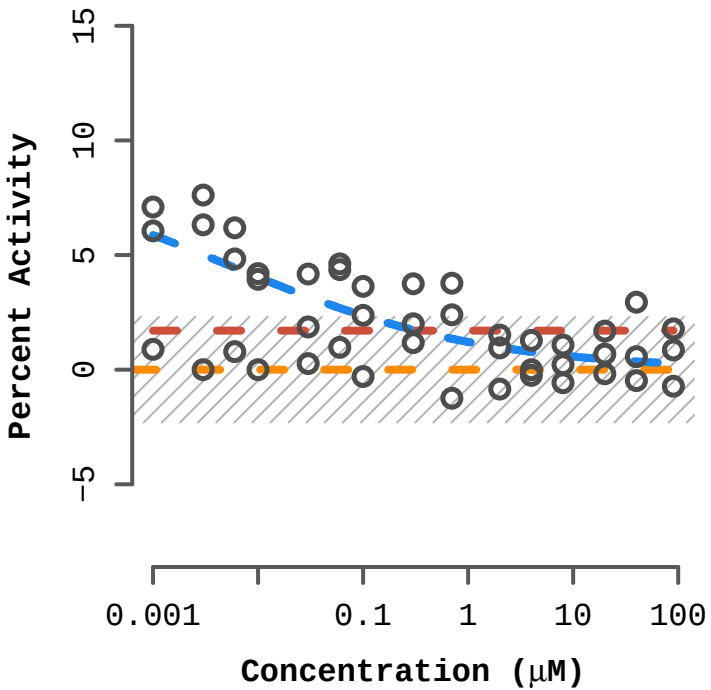
NAME: 2,5-Dichlorophenol
CHID: 25003 **CASRN:** 583-78-8
SPID(S): Tox21_201889
M4ID: 12480363

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.441 **MAX_MED:** 0.223 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6-Dichlorophenol
CHID: 25004 **CASRN:** 87-65-0
SPID(S): Tox21_200775
M4ID: 12481477

HILL MODEL (in red):

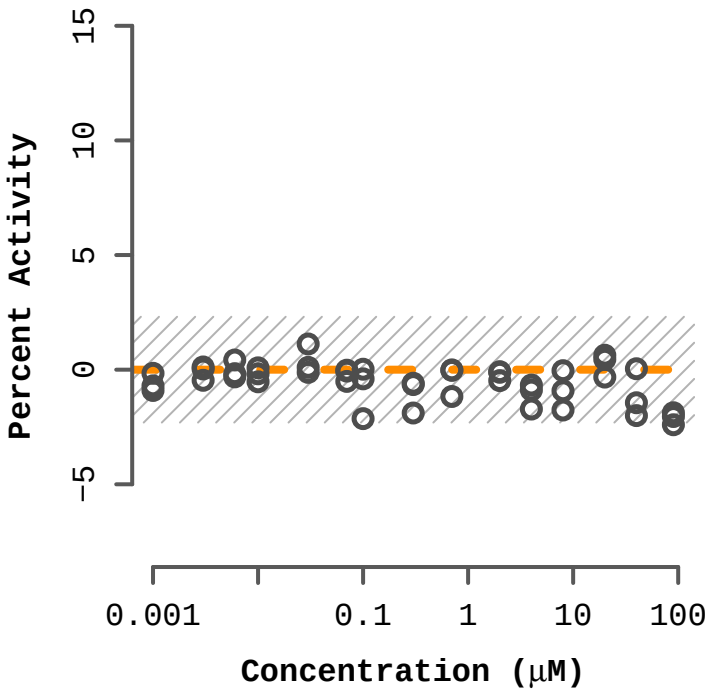
	tp	ga	gw
val:	1.7	−4.58	4.89
sd:	0.353	1520	4710

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.14	−4.23	3.24	−2.29	0.357
sd:	5.73	42.9	285	1.56	0.137

	CNST	HILL	GNLS
AIC:	230.59	213.98	196.37
PROB:	0	0	1
RMSE:	3.08	2.33	1.89

MAX_MEAN: 4.68 **MAX_MED:** 6.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

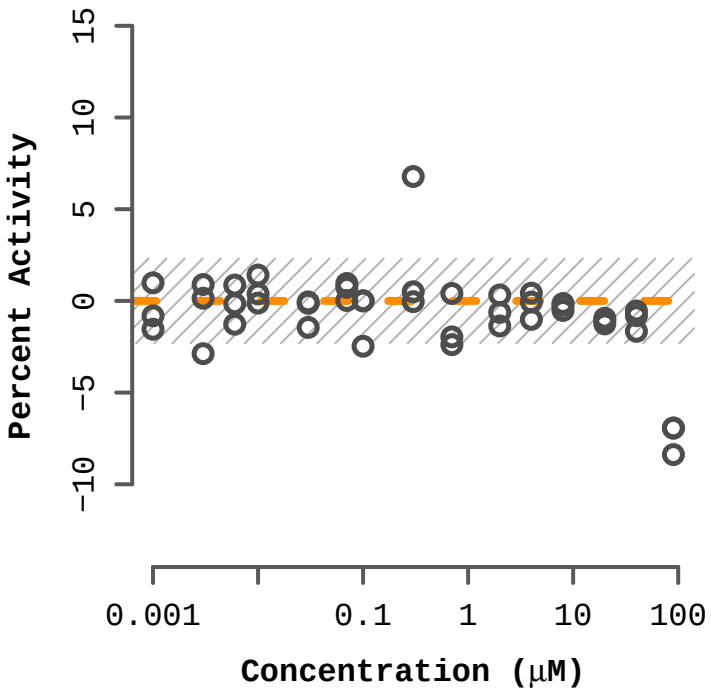
NAME: 3,4-Dichlorophenol
CHID: 25005 **CASRN:** 95-77-2
SPID(S): Tox21_200675
M4ID: 12481577

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.37 **MAX_MED:** 0.454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

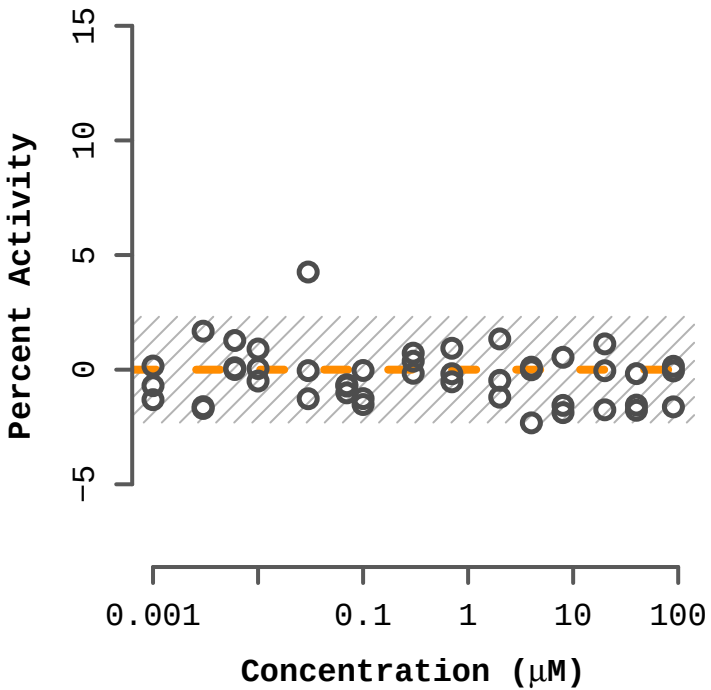
NAME: 3,5-Dichlorophenol
CHID: 25006 **CASRN:** 591-35-5
SPID(S): Tox21_200931
M4ID: 12481321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.41	NA	NA

MAX_MEAN: 2.41 **MAX_MED:** 0.743 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

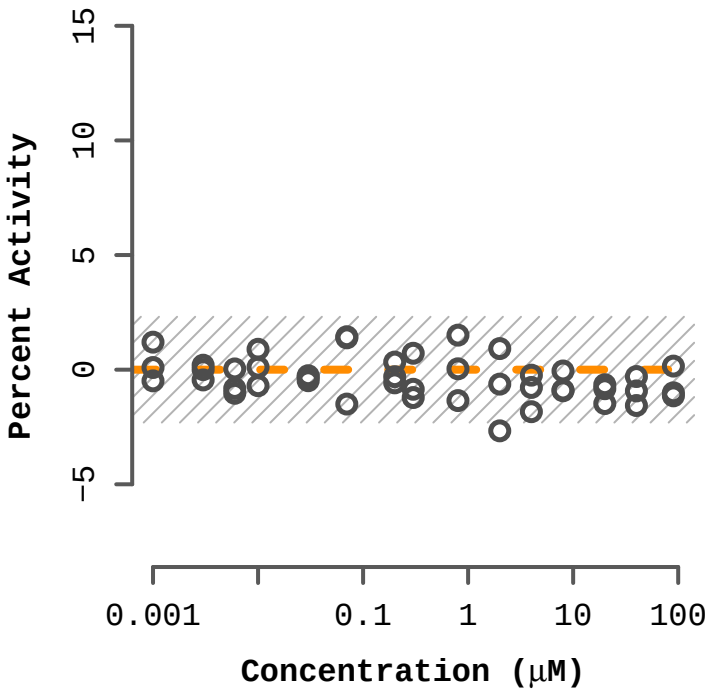
NAME: 1,3-Dichloro-2-propanol
CHID: 25010 **CASRN:** 96-23-1
SPID(S): Tox21_300284
M4ID: 12478846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.985 **MAX_MED:** 0.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

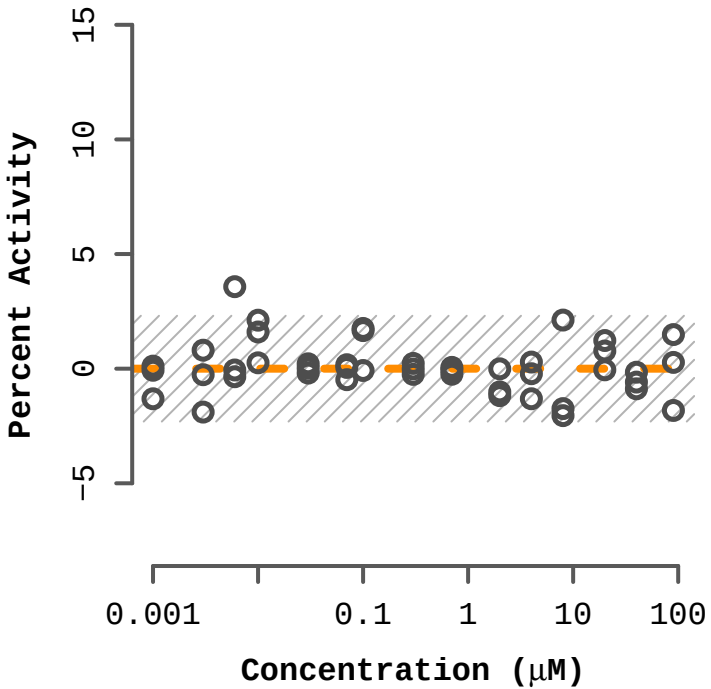
NAME: 1,3-Dichloro-2-propanol
CHID: 25010 CASRN: 96-23-1
SPID(S): Tox21_201890
M4ID: 12480362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.443 MAX_MED: 1.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

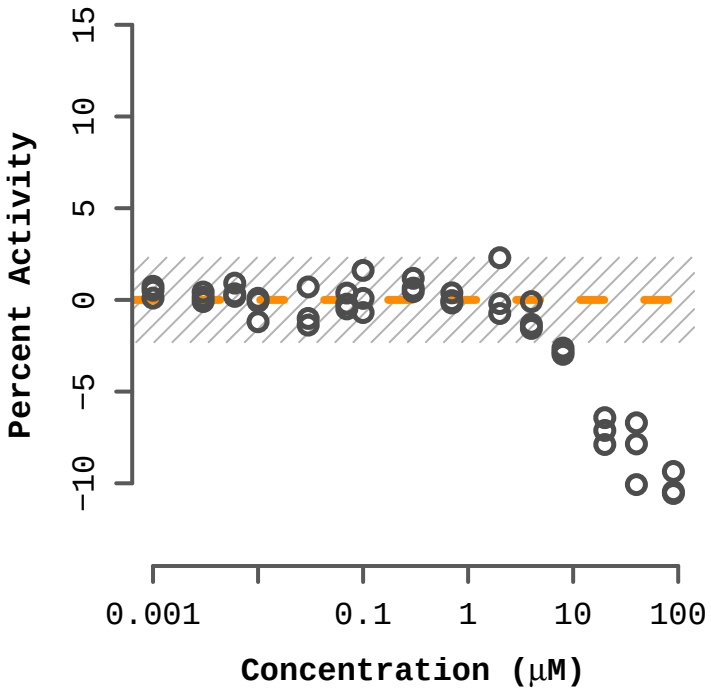
NAME: 2,3-Dichloro-1-propene
CHID: 25012 CASRN: 78-88-6
SPID(S): Tox21_200640
M4ID: 12481612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.33 MAX_MED: 1.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

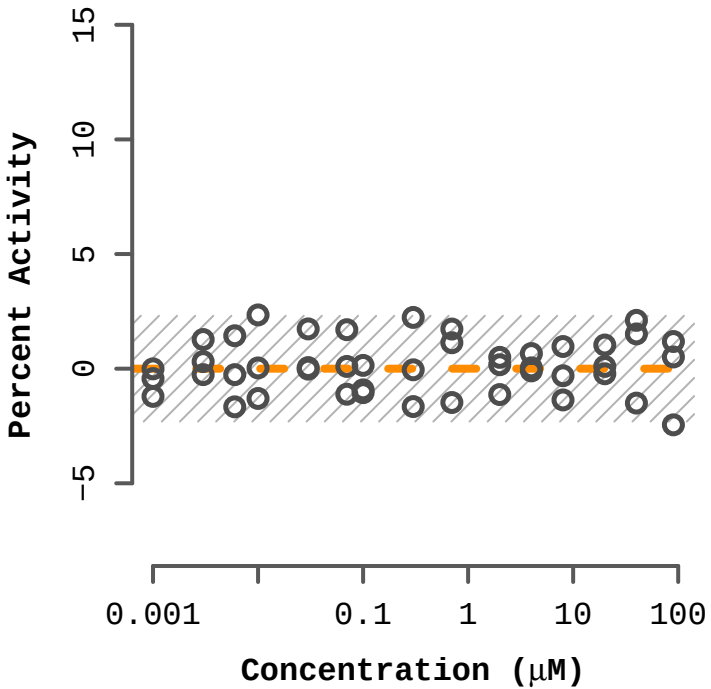
NAME: 2,3-Dichloroquinoxaline
CHID: 25013 **CASRN:** 2213-63-0
SPID(S): Tox21_200138
M4ID: 12482114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.06	NA	NA
PROB:	1	NA	NA
RMSE:	3.99	NA	NA

MAX_MEAN: 0.758 **MAX_MED:** 0.645 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

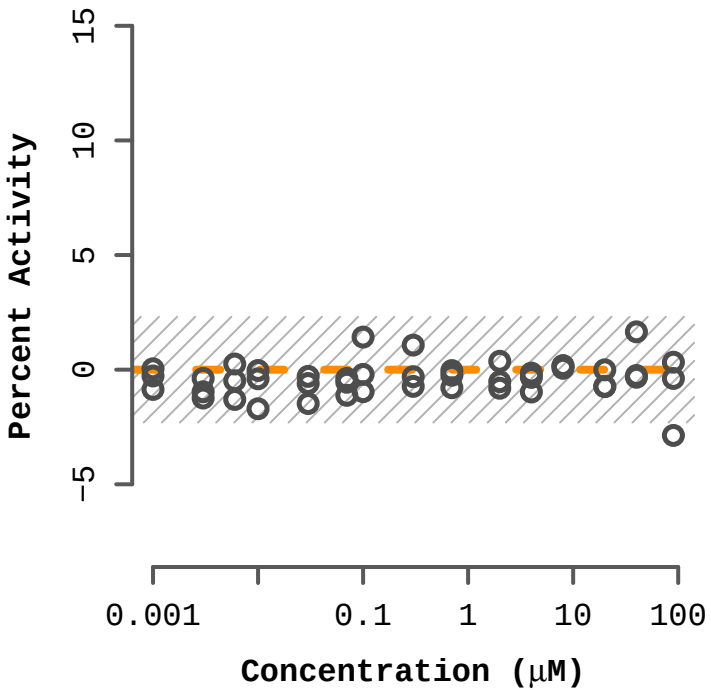
NAME: Benzal chloride
CHID: 25014 CASRN: 98-87-3
SPID(S): Tox21_300171
M4ID: 12478959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.709 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

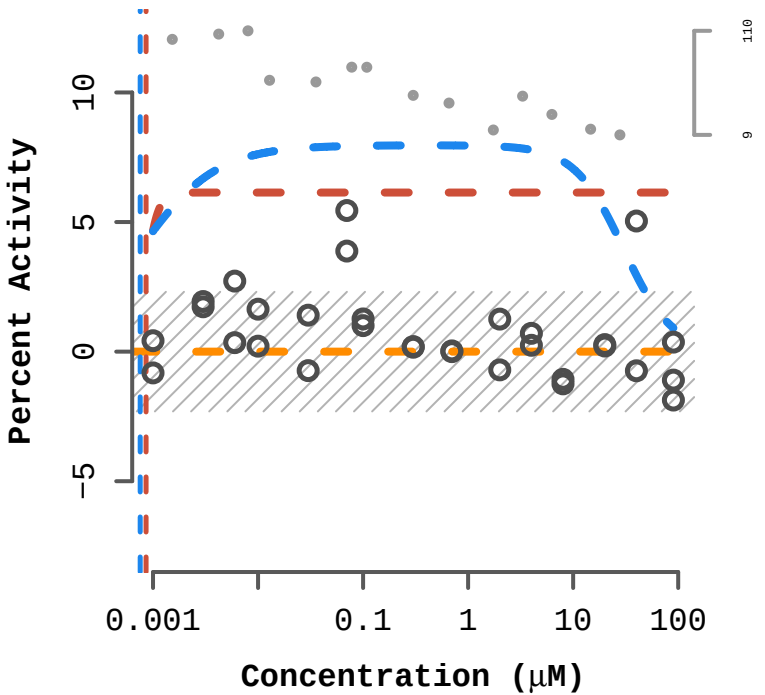
NAME: Benzal chloride
CHID: 25014 **CASRN:** 98-87-3
SPID(S): Tox21_201313
M4ID: 12480939

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.356 **MAX_MED:** 0.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dicumyl peroxide
CHID: 25017 CASRN: 80-43-3
SPID(S): Tox21_300069
M4ID: 12479061 BRK

HILL MODEL (in red):

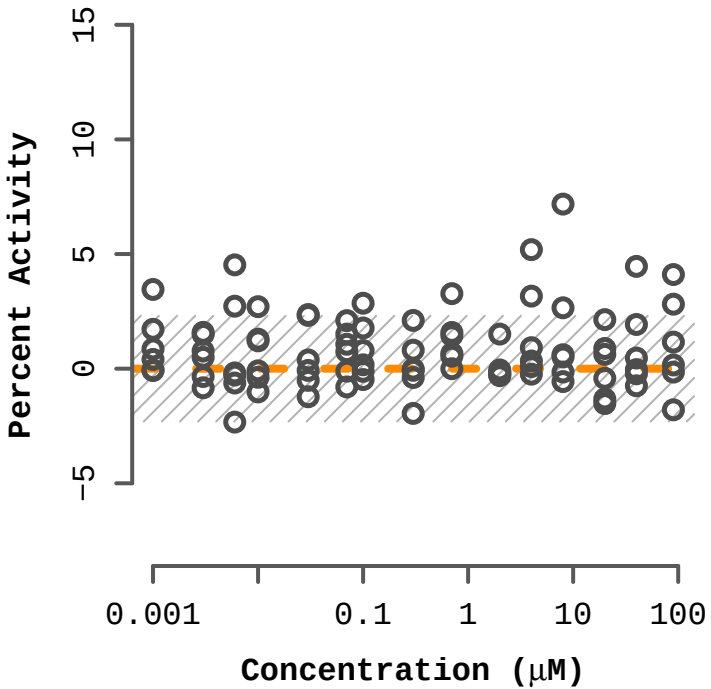
	tp	ga	gw
val:	6.14	−3.07	7.52
sd:	2.95	3.75	424

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.96	−3.12	1.2	1.48	1.86
sd:	5.12	2.26	5.92	1.07	7.41

	CNST	HILL	GNLS
AIC:	432.59	432.95	436.03
PROB:	0.5	0.42	0.09
RMSE:	36.36	33.83	33.37

MAX_MEAN: 37.6 MAX_MED: 5.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

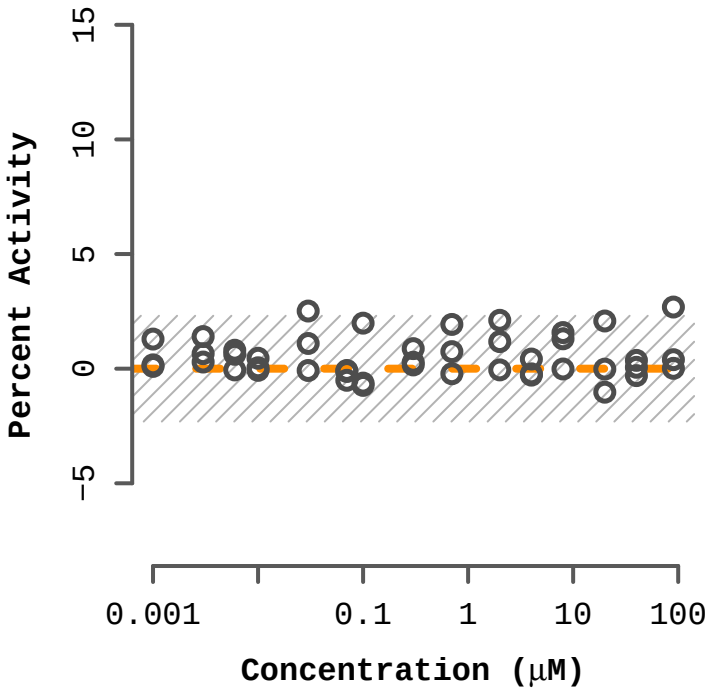
NAME: Dicumyl peroxide
CHID: 25017 **CASRN:** 80-43-3
SPID(S): Tox21_202385
M4ID: 12479867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	349.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

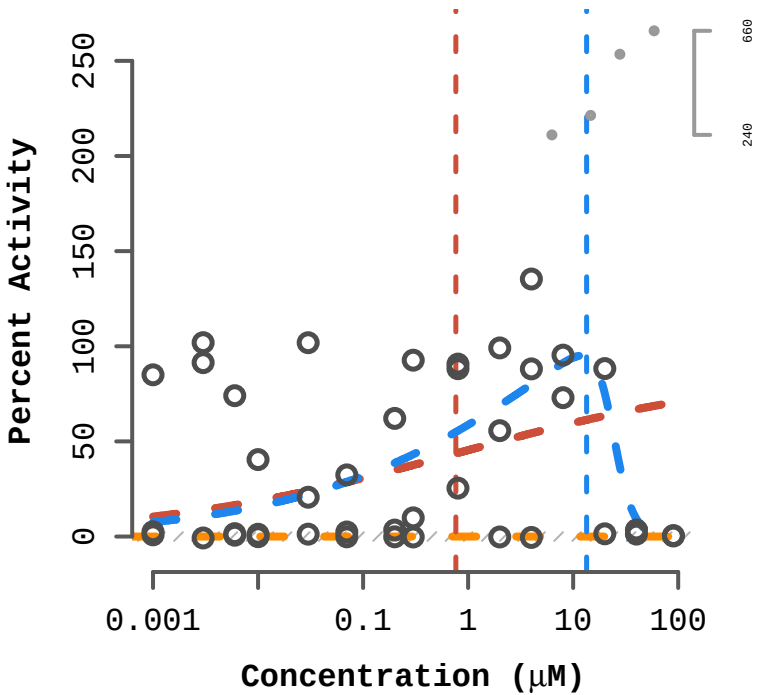
NAME: Dicyclohexylamine
CHID: 25018 **CASRN:** 101-83-7
SPID(S): Tox21_303097
M4ID: 12476036

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dicyclohexylamine
CHID: 25018 CASRN: 101-83-7
SPID(S): Tox21_201771
M4ID: 12480481 BRK

HILL MODEL (in red):

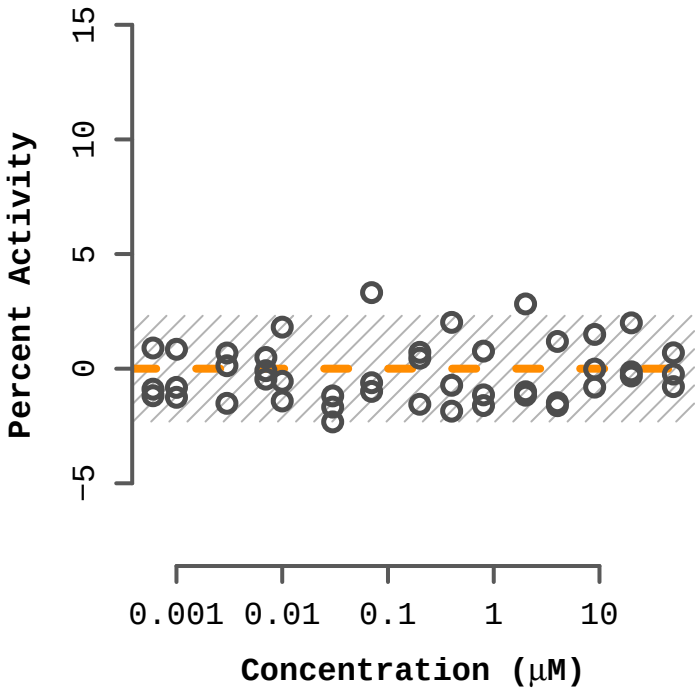
	tp	ga	gw
val:	87.3	-0.117	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	201	1.13	0.341	1.38	4.79
sd:	268	2.87	0.2	0.185	5.3

	CNST	HILL	GNLS
AIC:	546.73	535.46	531.84
PROB:	0	0.14	0.86
RMSE:	153.01	131.88	141.21

MAX_MEAN: 221 MAX_MED: 95.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

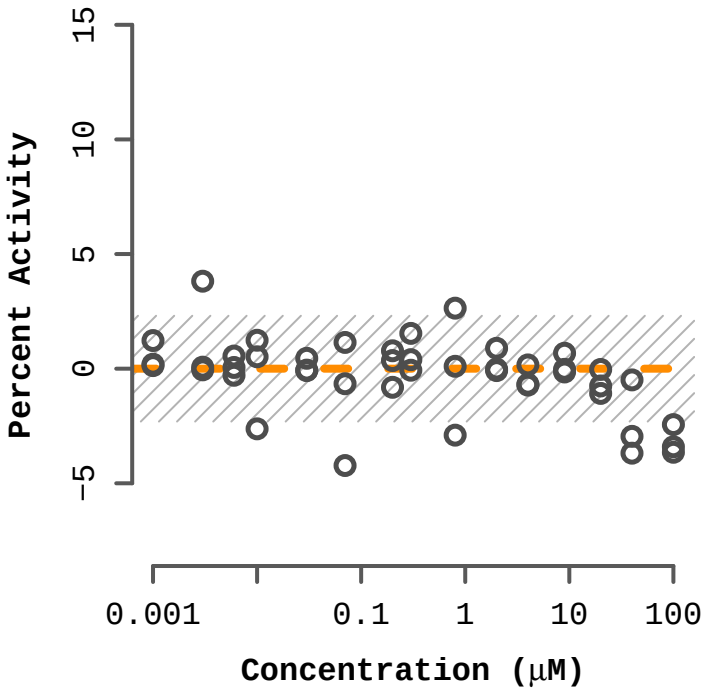
NAME: Dicyclohexylamine
CHID: 25018 **CASRN:** 101-83-7
SPID(S): Tox21_111044_1
M4ID: 12483934

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.573 **MAX_MED:** 0.458 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

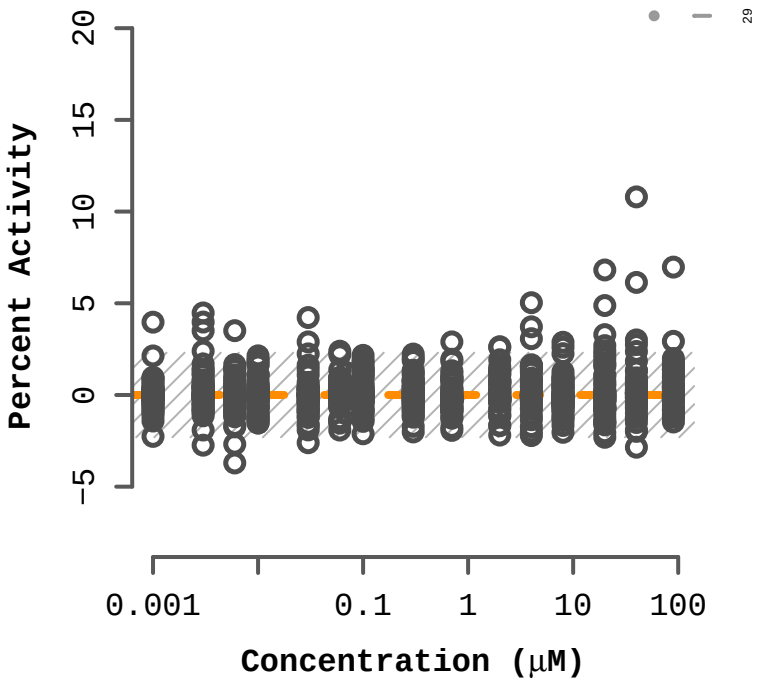
NAME: Dicyclohexyl phthalate
CHID: 25021 **CASRN:** 84-61-7
SPID(S): Tox21_303132
M4ID: 12476001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

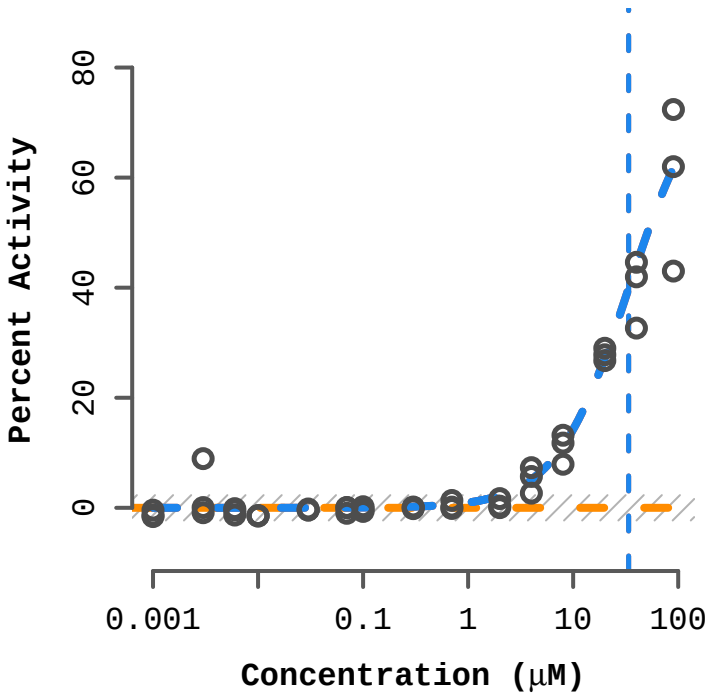
NAME: Dicyclopentadiene
CHID: 25023 **CASRN:** 77-73-6
SPID(S): Tox21_400017
M4ID: 12475120 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2103.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 7-Diethylamino-4-methylcoumarin
CHID: 25035 CASRN: 91-44-1
SPID(S): Tox21_303285
M4ID: 12475848

HILL MODEL (in red):

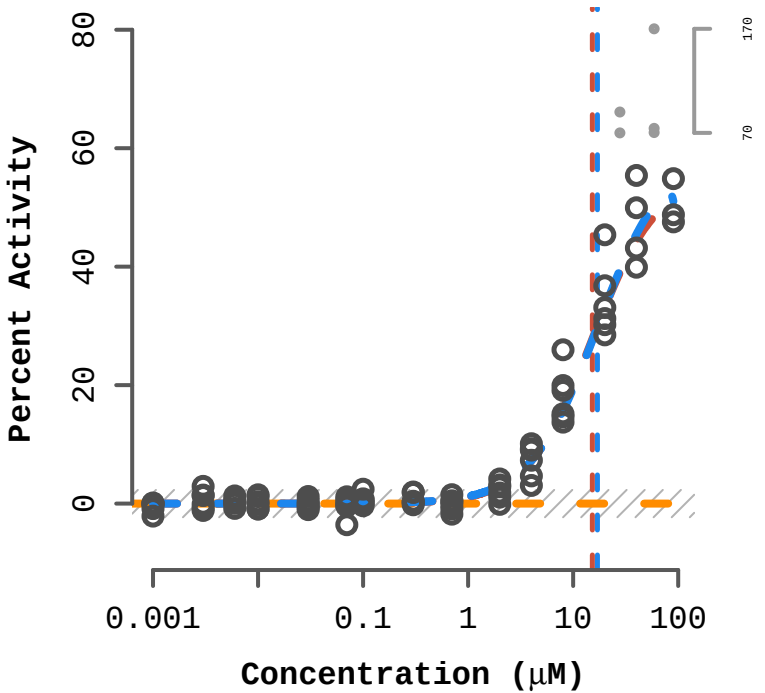
	tp	ga	gw
val:	79.8	1.53	1.25
sd:	5.02	0.0525	0.0848

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	79.8	1.53	1.25	3.32	6.31
sd:	5.02	0.0525	0.0848	973	4520

	CNST	HILL	GNLS
AIC:	376.72	216.63	220.63
PROB:	0	0.88	0.12
RMSE:	20.36	4.05	4.05

MAX_MEAN: 59.1 MAX_MED: 62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 7-Diethylamino-4-methylcoumarin
CHID: 25035 CASRN: 91-44-1
SPID(S): Tox21_201789
M4ID: 12480463 BRK

HILL MODEL (in red):

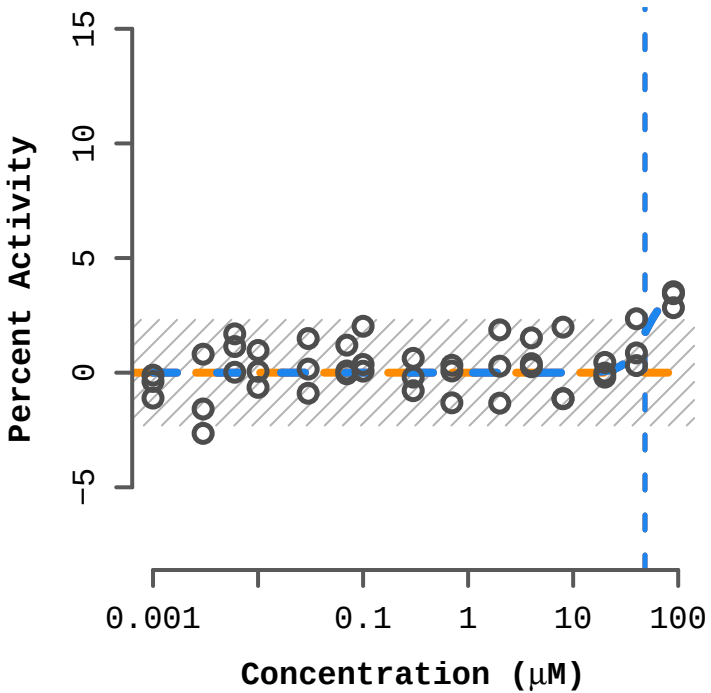
	tp	ga	gw
val:	55.5	1.18	1.42
sd:	4.33	0.0619	0.124

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	59.6	1.23	1.37	2.03	15.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	799.83	520.03	523.9
PROB:	0	0.87	0.13
RMSE:	29.25	13.8	13.77

MAX_MEAN: 76.8 MAX_MED: 62.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Diethylaminophenol
CHID: 25037 CASRN: 91-68-9
SPID(S): Tox21_200238
M4ID: 12482014

HILL MODEL (in red):

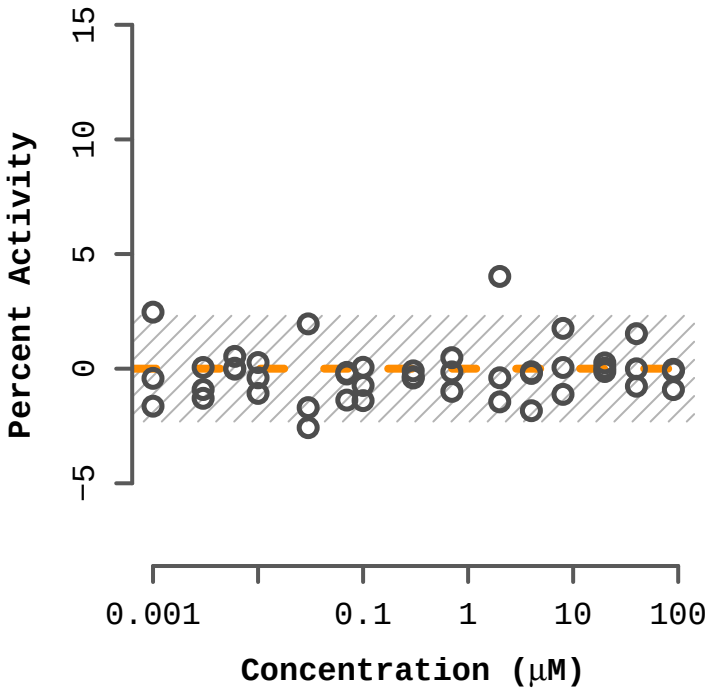
	tp	ga	gw
val:	3.48	1.68	4.46
sd:	1.77	0.259	9.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.48	1.68	4.46	3.08	6.2
sd:	1.77	0.259	9.24	25200	141000

	CNST	HILL	GNLS
AIC:	156.1	138.17	142.17
PROB:	0	0.88	0.12
RMSE:	1.35	1.01	1.01

MAX_MEAN: 3.27 **MAX_MED:** 3.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

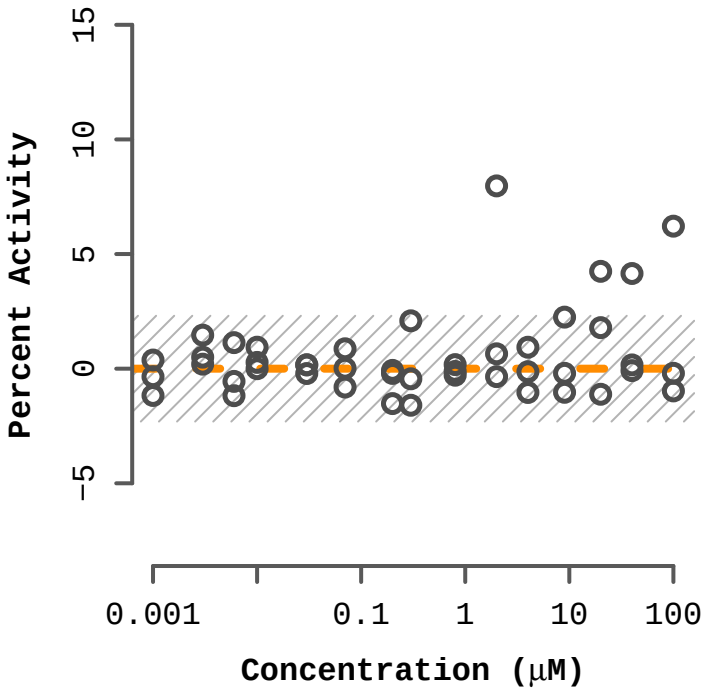
NAME: N,N'−Diethylcarbanilide
CHID: 25040 CASRN: 85−98−3
SPID(S): Tox21_200369
M4ID: 12481883

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.728 MAX_MED: 0.0526 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

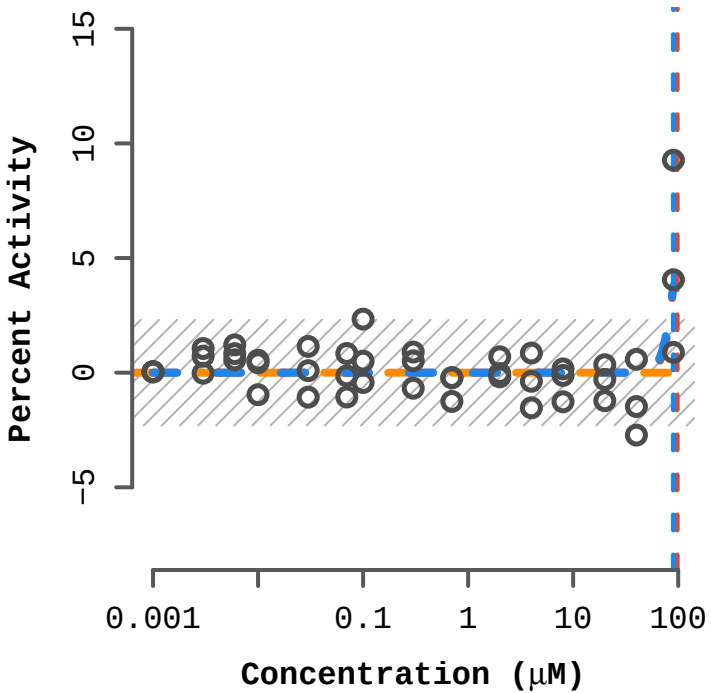
NAME: Diethyl carbonate
CHID: 25041 **CASRN:** 105-58-8
SPID(S): Tox21_200769
M4ID: 12481483

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 2.76 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethylene glycol diacrylate
CHID: 25045 CASRN: 4074-88-8
SPID(S): Tox21_201088
M4ID: 12481164

HILL MODEL (in red):

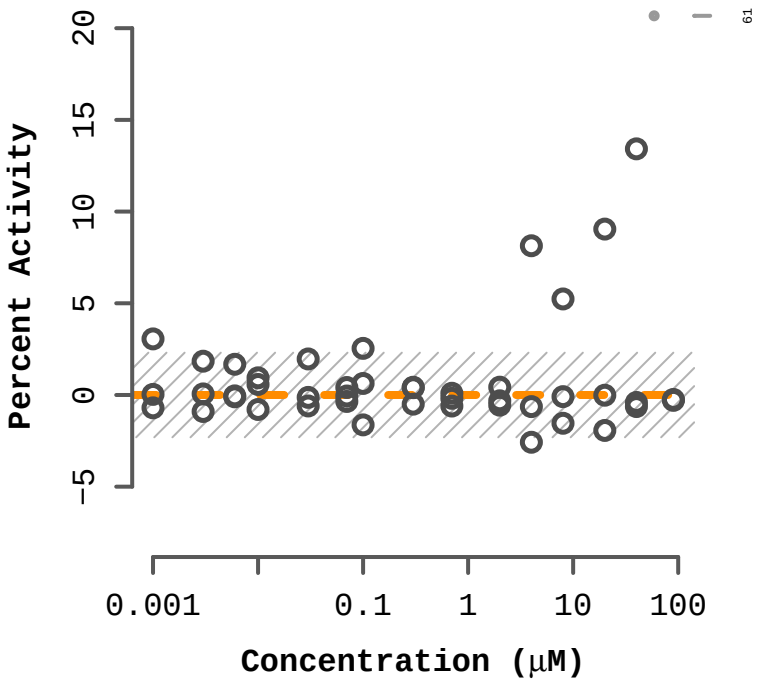
	tp	ga	gw
val:	11.1	1.99	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.58	1.95	7.85	3.61	3.56
sd:	7.14	0.106	8.51	1870	4070

	CNST	HILL	GNLS
AIC:	148.49	145.77	149.78
PROB:	0.18	0.72	0.1
RMSE:	1.76	1.29	1.29

MAX_MEAN: 4.74 **MAX_MED:** 4.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

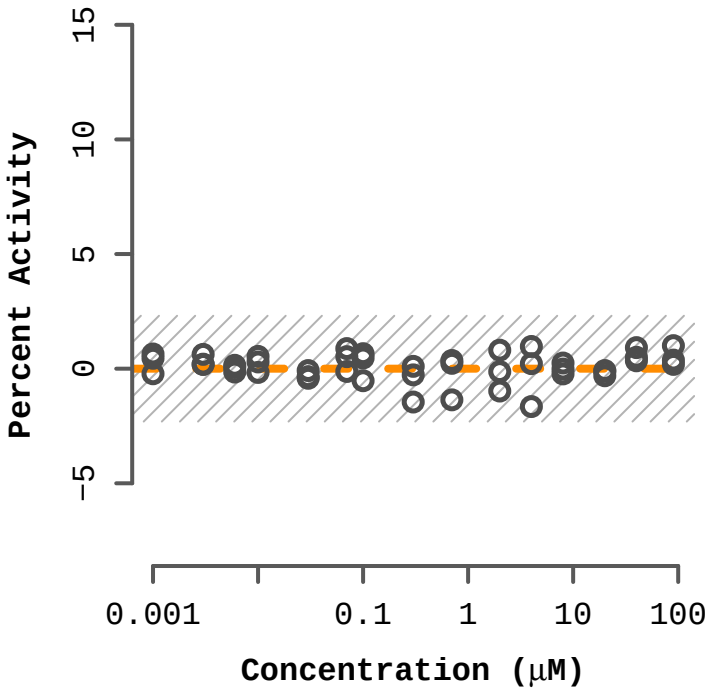
NAME: Diethylene glycol dibutyl ether
CHID: 25046 CASRN: 112-73-2
SPID(S): Tox21_200964
M4ID: 12481288 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.33	NA	NA
PROB:	1	NA	NA
RMSE:	9.54	NA	NA

MAX_MEAN: 20.1 MAX_MED: 0.629 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

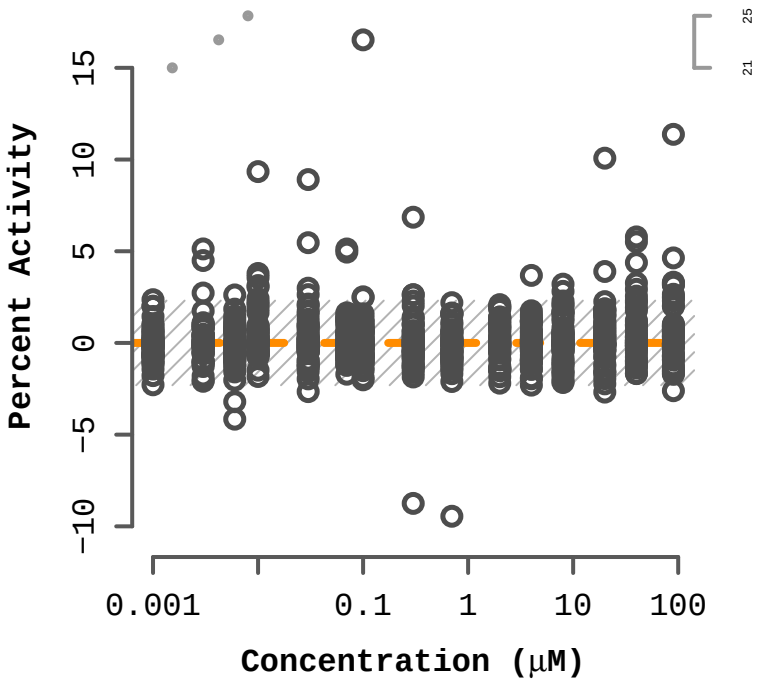
NAME: Diethylene glycol diethyl ether
CHID: 25047 CASRN: 112-36-7
SPID(S): Tox21_302050
M4ID: 12477083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	82.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.6	NA	NA

MAX_MEAN: 0.587 MAX_MED: 0.527 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

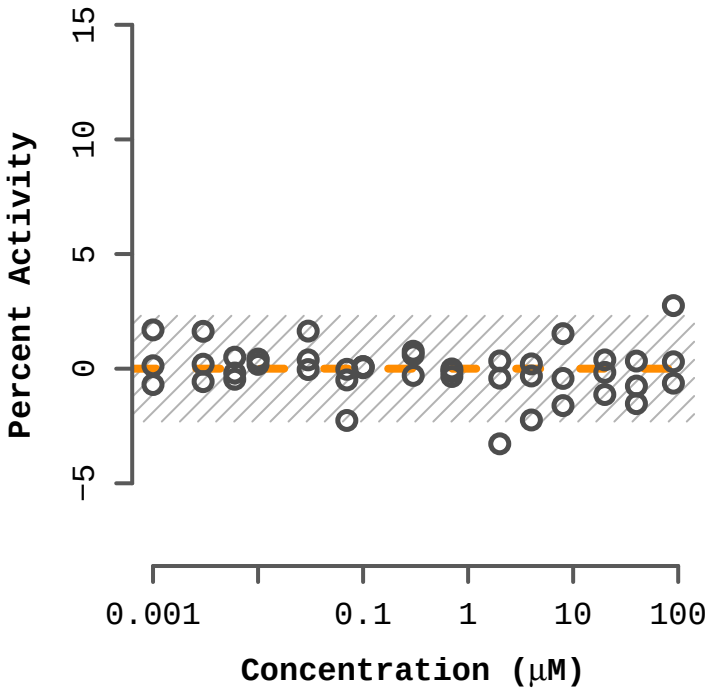
NAME: Diethylene glycol monomethyl ether
CHID: 25049 **CASRN:** 111-77-3
SPID(S): Tox21_400009
M4ID: 12475128 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2579.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 0.693 **MAX_MED:** 0.398 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

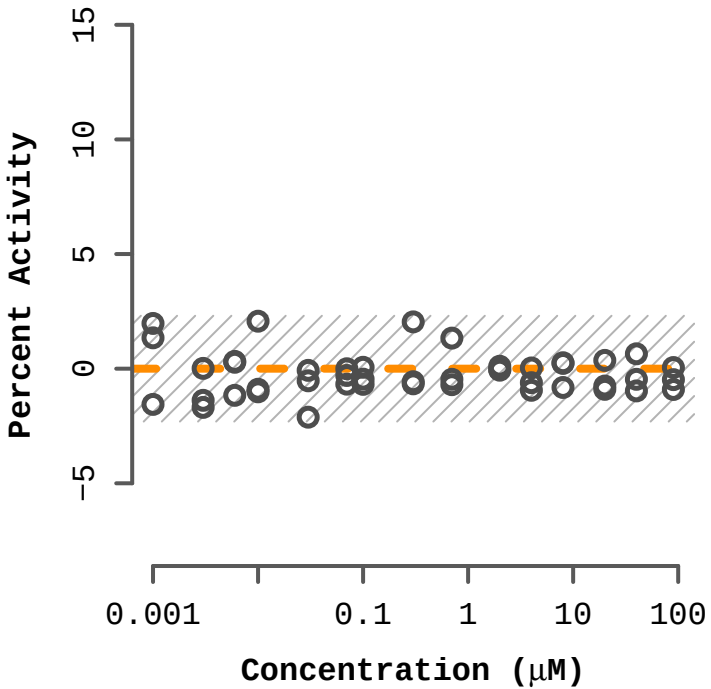
NAME: Diethylenetriamine
CHID: 25050 **CASRN:** 111-40-0
SPID(S): Tox21_303114
M4ID: 12476019

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.808 **MAX_MED:** 0.606 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

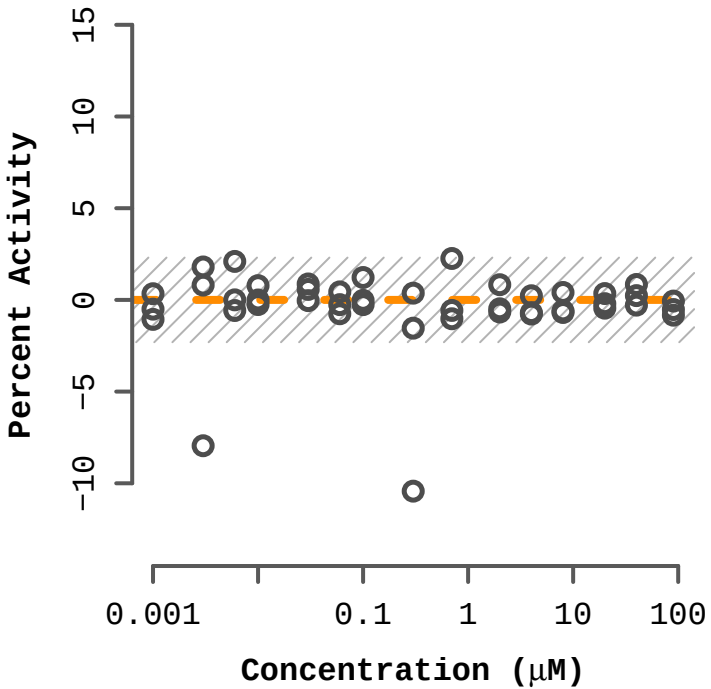
NAME: Diethylenetriamine
CHID: 25050 **CASRN:** 111-40-0
SPID(S): Tox21_201453
M4ID: 12480799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

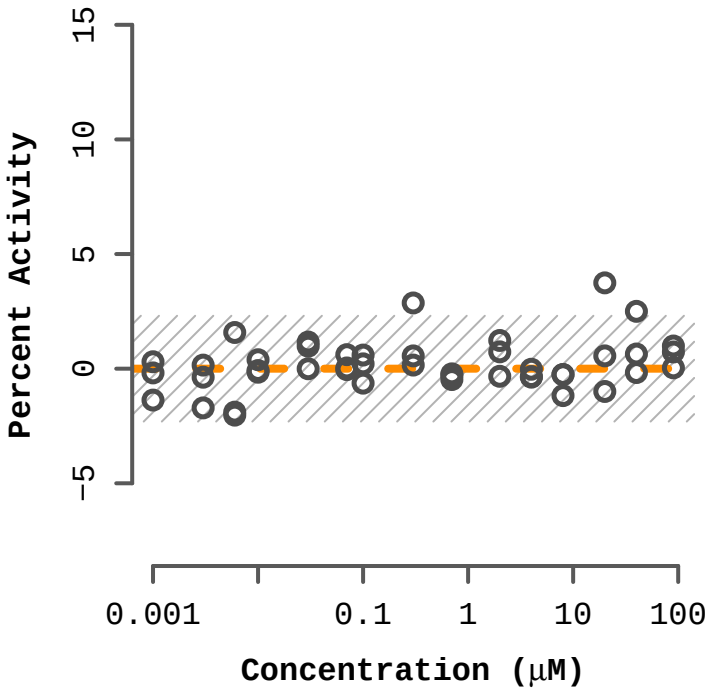
NAME: Diethyl ethylphosphonate
CHID: 25051 CASRN: 78-38-6
SPID(S): Tox21_200361
M4ID: 12481891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.01	NA	NA
PROB:	1	NA	NA
RMSE:	2.11	NA	NA

MAX_MEAN: 0.509 MAX_MED: 0.809 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

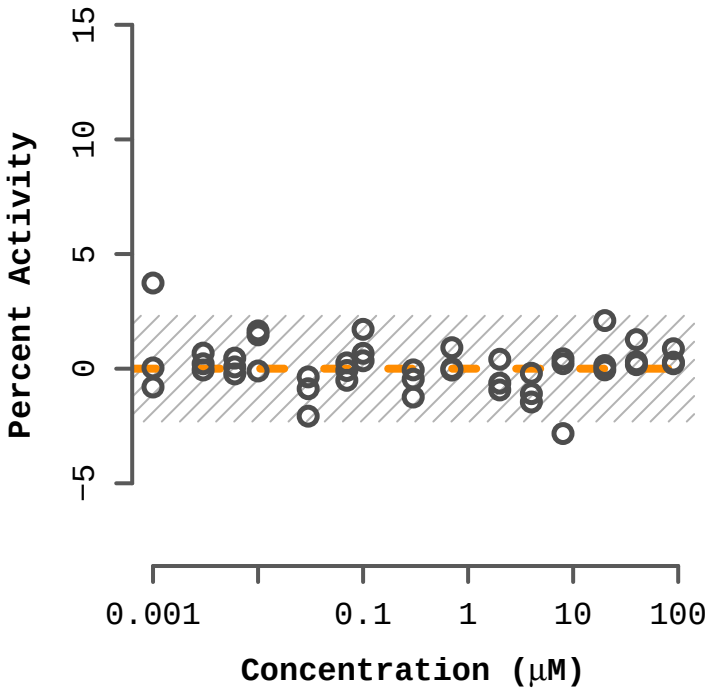
NAME: 2,2'−Diethylhexylamine
CHID: 25053 **CASRN:** 106−20−7
SPID(S): Tox21_200785
M4ID: 12481467

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

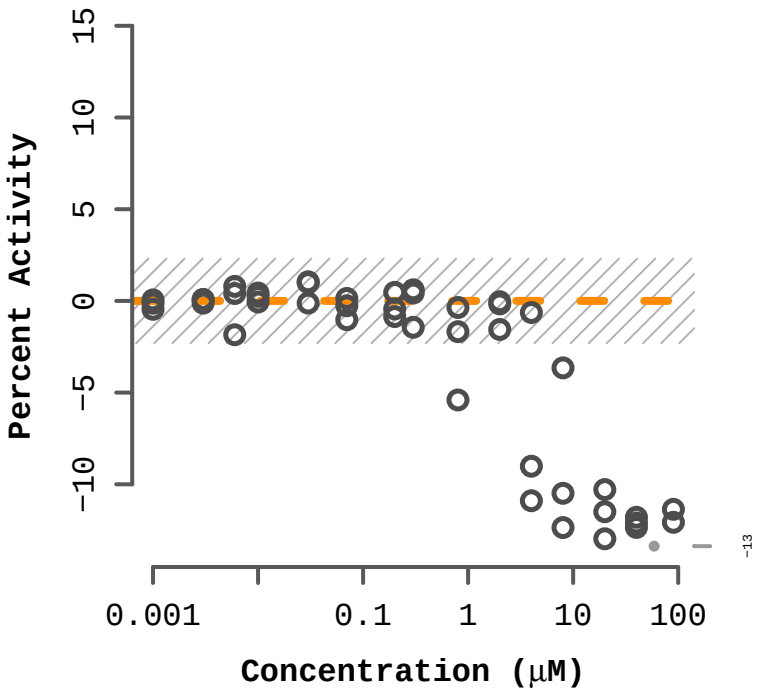
NAME: Bis(2-ethylhexyl) decanedioate
CHID: 25055 **CASRN:** 122-62-3
SPID(S): Tox21_303439
M4ID: 12475701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

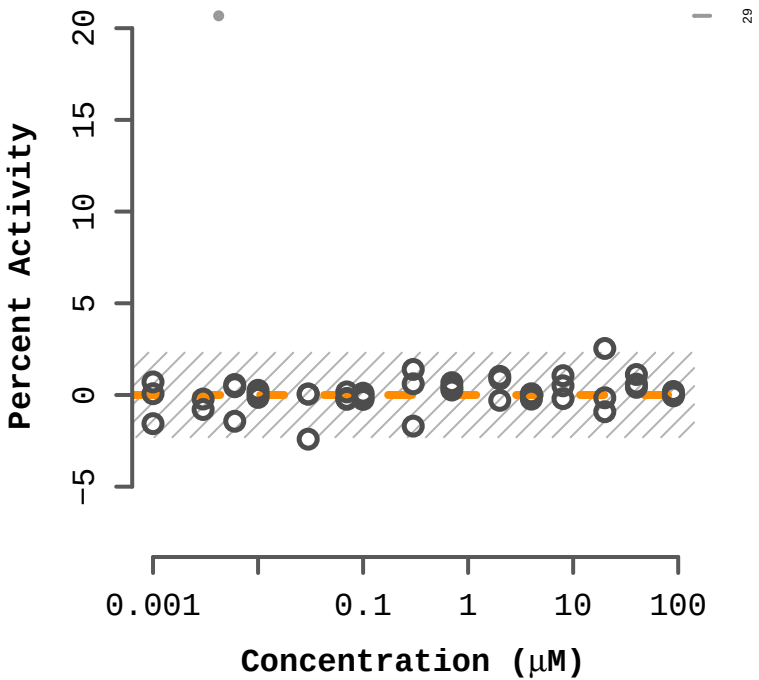
NAME: N,N−Diethylbenzene−1,4−diamine
CHID: 25058 **CASRN:** 93−05−0
SPID(S): Tox21_200888
M4ID: 12481364 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.39	NA	NA
PROB:	1	NA	NA
RMSE:	6.37	NA	NA

MAX_MEAN: 0.642 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

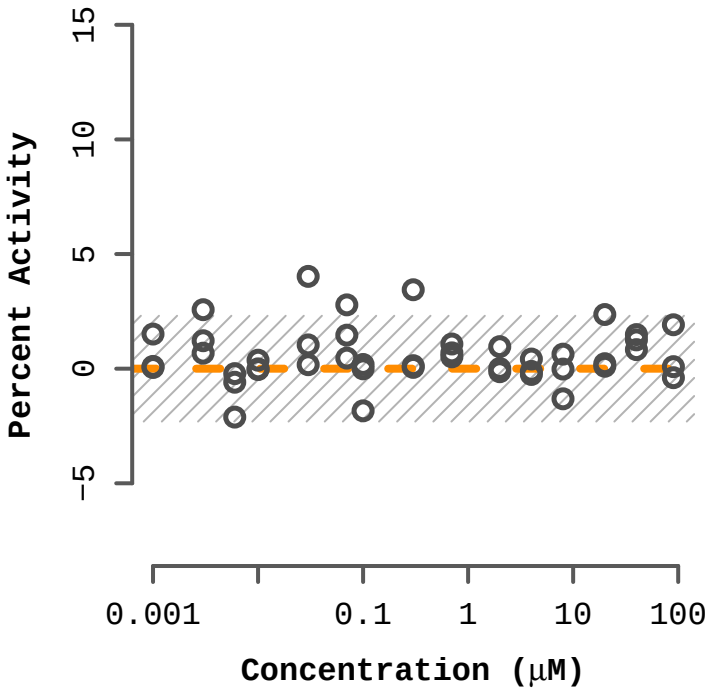
NAME: N,N−Dimethylpentanamide
CHID: 25063 CASRN: 6225−06−5
SPID(S): Tox21_200869
M4ID: 12481383 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.59	NA	NA
PROB:	1	NA	NA
RMSE:	4.35	NA	NA

MAX_MEAN: 9.22 MAX_MED: 0.879 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

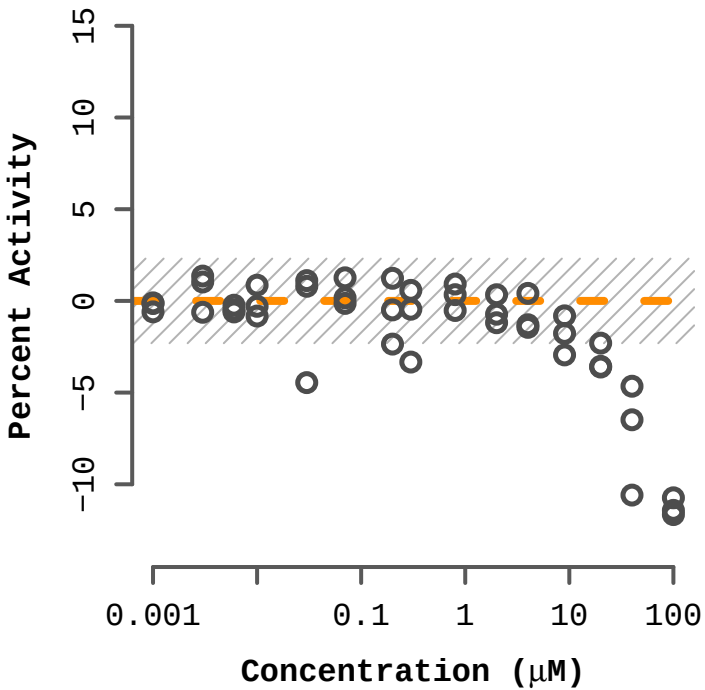
NAME: 2,4-Difluoroaniline
CHID: 25064 **CASRN:** 367-25-9
SPID(S): Tox21_200620
M4ID: 12481632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

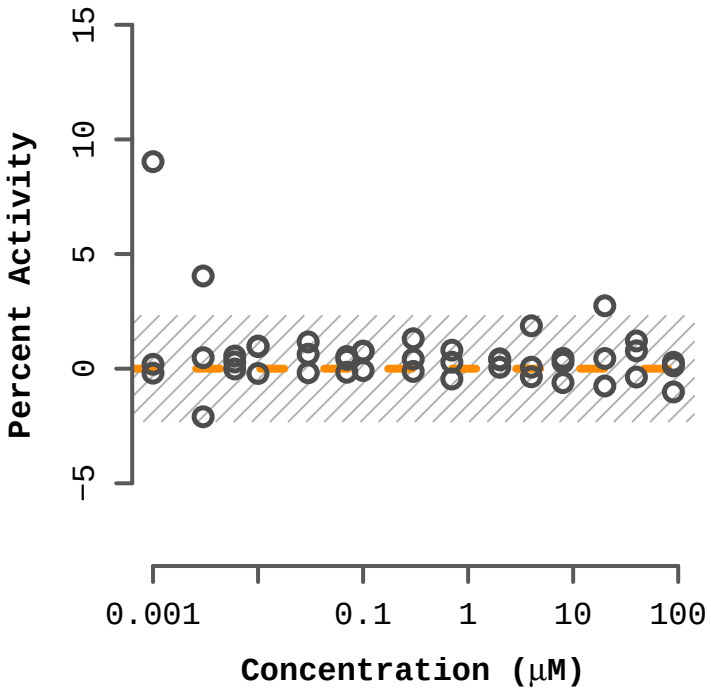
NAME: Digitonin
CHID: 25065 CASRN: 11024-24-1
SPID(S): Tox21_202507
M4ID: 12479745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.82	NA	NA

MAX_MEAN: 0.59 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

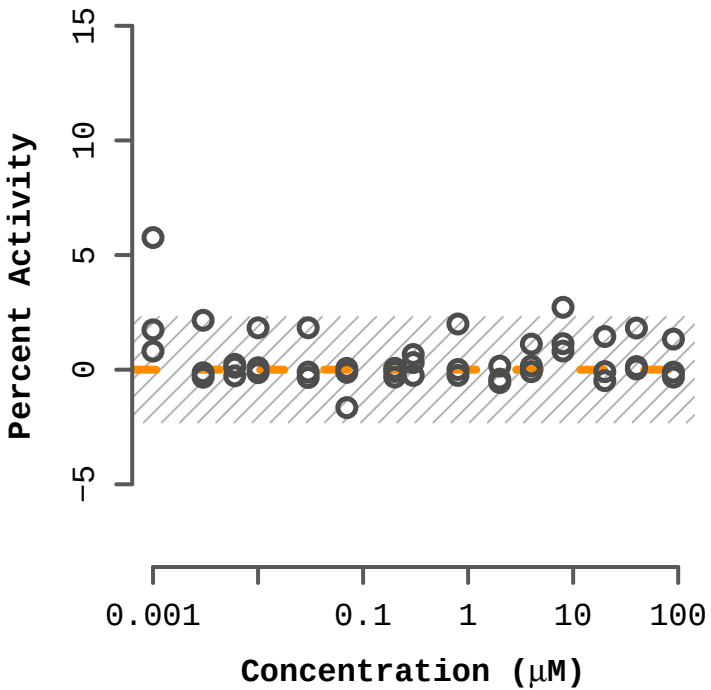
NAME: Dihexyl phthalate
CHID: 25068 **CASRN:** 84-75-3
SPID(S): Tox21_300165
M4ID: 12478965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 3.01 **MAX_MED:** 0.965 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

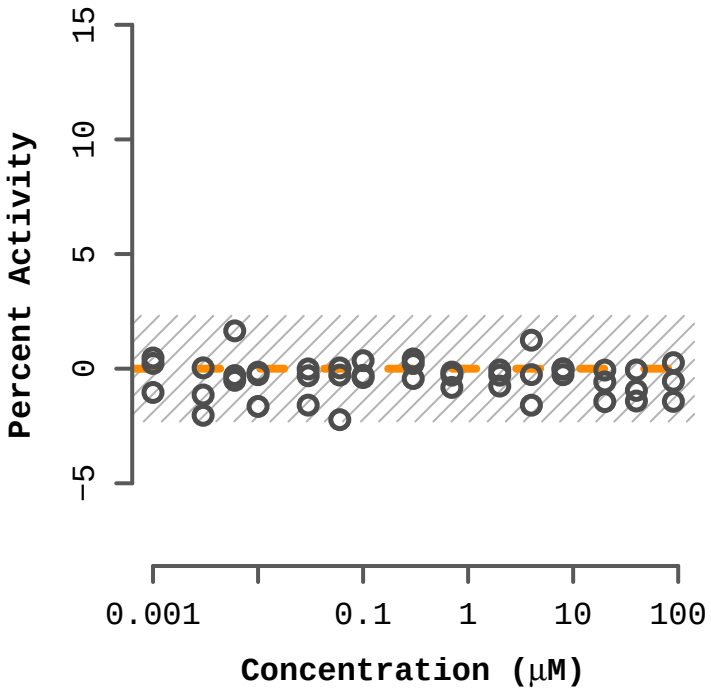
NAME: Dihexyl phthalate
CHID: 25068 **CASRN:** 84-75-3
SPID(S): Tox21_202420
M4ID: 12479832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 2.77 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

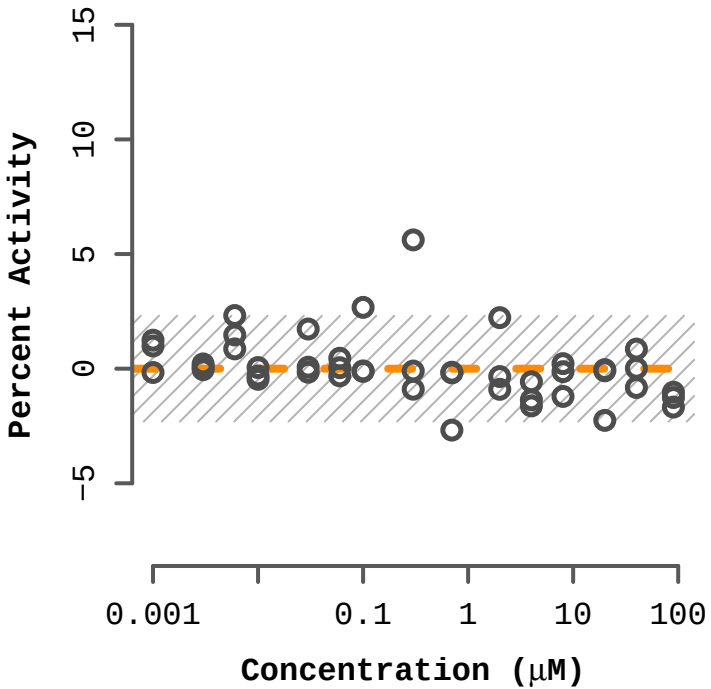
NAME: 1,2-Dihydro-2,2,4-trimethylquinoline
CHID: 25070 **CASRN:** 147-47-7
SPID(S): Tox21_201077
M4ID: 12481175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.282 **MAX_MED:** 0.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

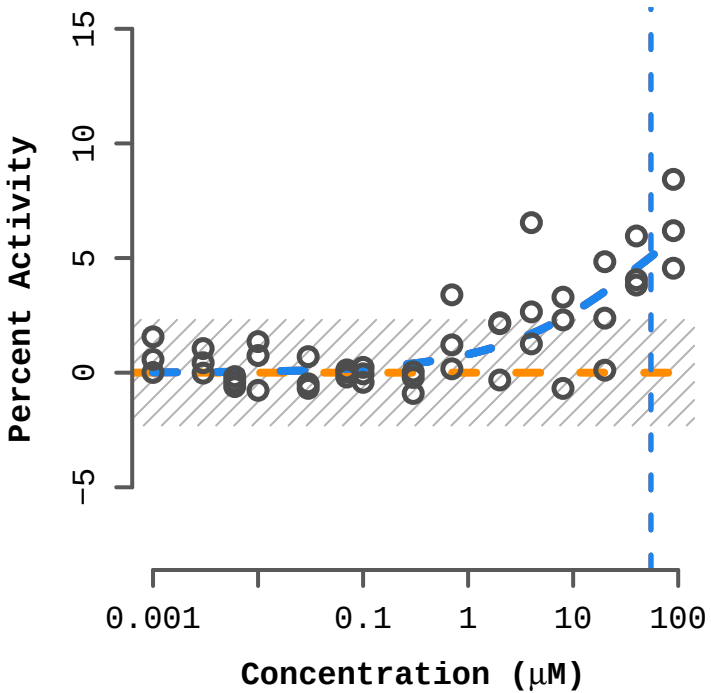
NAME: 1,2-Dihydro-2,2,4-trimethylquinoline, polymer
CHID: 25071 CASRN: 26780-96-1
SPID(S): Tox21_202467
M4ID: 12479785

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.55 MAX_MED: 1.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4−Dihydroxybenzoic acid
CHID: 25074 CASRN: 89−86−1
SPID(S): Tox21_202471
M4ID: 12479781

HILL MODEL (in red):

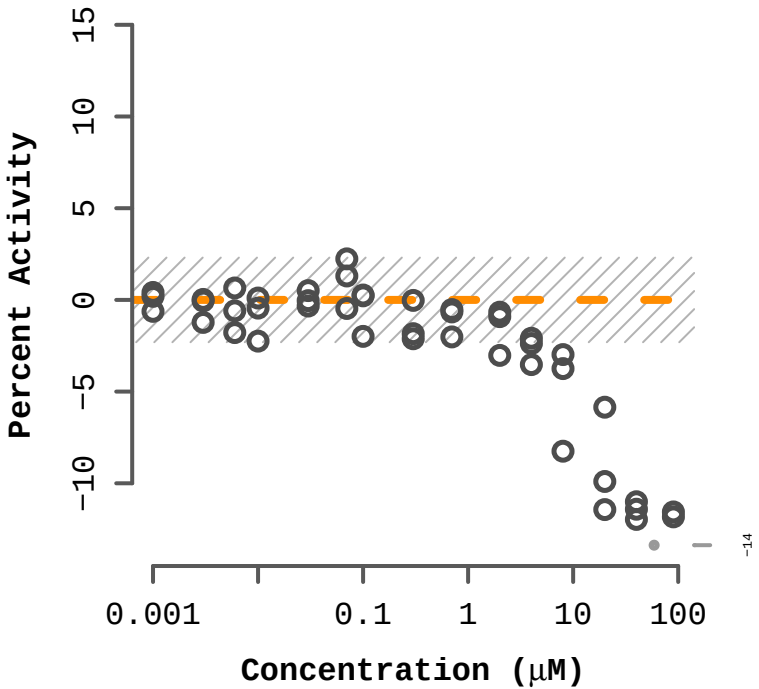
	tp	ga	gw
val:	10.1	1.74	0.612
sd:	7.51	1.04	0.204

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.1	1.74	0.612	3.55	4.57
sd:	7.5	1.04	0.204	692	1990

	CNST	HILL	GNLS
AIC:	211.13	156.96	160.96
PROB:	0	0.88	0.12
RMSE:	2.69	1.37	1.37

MAX_MEAN: 6.4 MAX_MED: 6.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

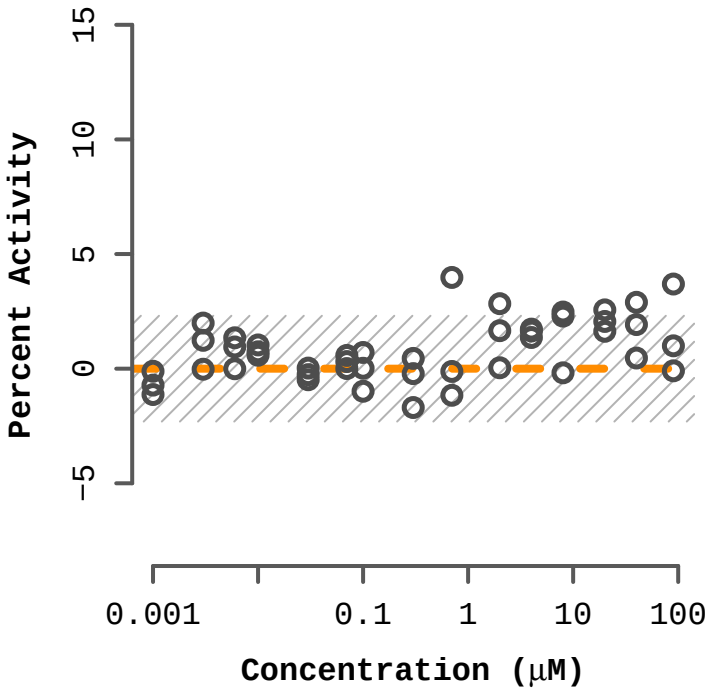
NAME: 1,8-Dihydroxy-4,5-dinitroanthraquinone
CHID: 25076 CASRN: 81-55-0
SPID(S): Tox21_200725
M4ID: 12481527 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	271.37	NA	NA
PROB:	1	NA	NA
RMSE:	5.35	NA	NA

MAX_MEAN: 1.03 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

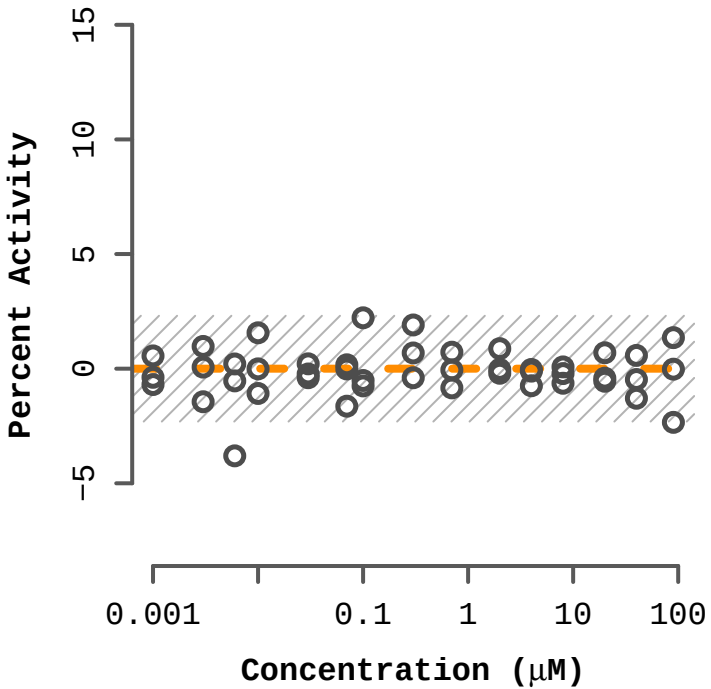
NAME: 5,7-Dihydroxy-4-methylcoumarin
CHID: 25078 **CASRN:** 2107-76-8
SPID(S): Tox21_200882
M4ID: 12481370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

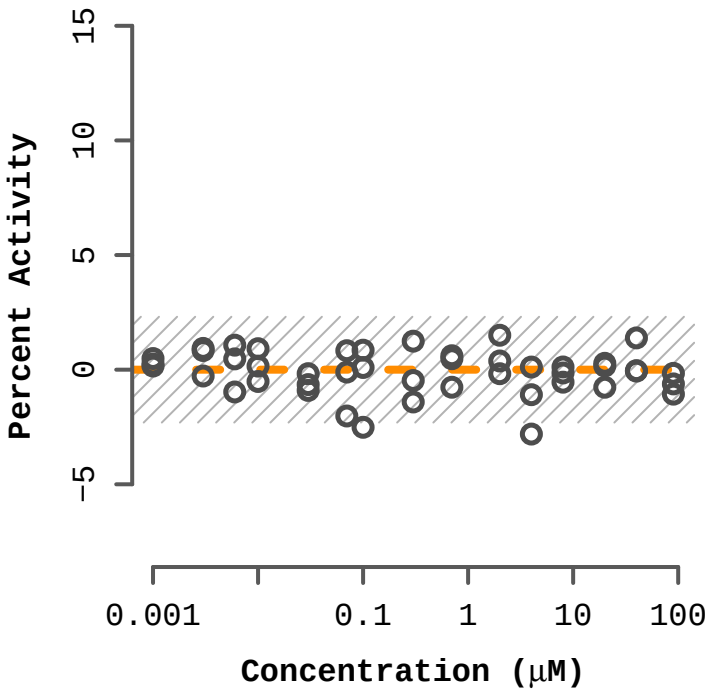
NAME: Diisobutylamine
CHID: 25079 **CASRN:** 110-96-3
SPID(S): Tox21_200177
M4ID: 12482075

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.734 **MAX_MED:** 0.686 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

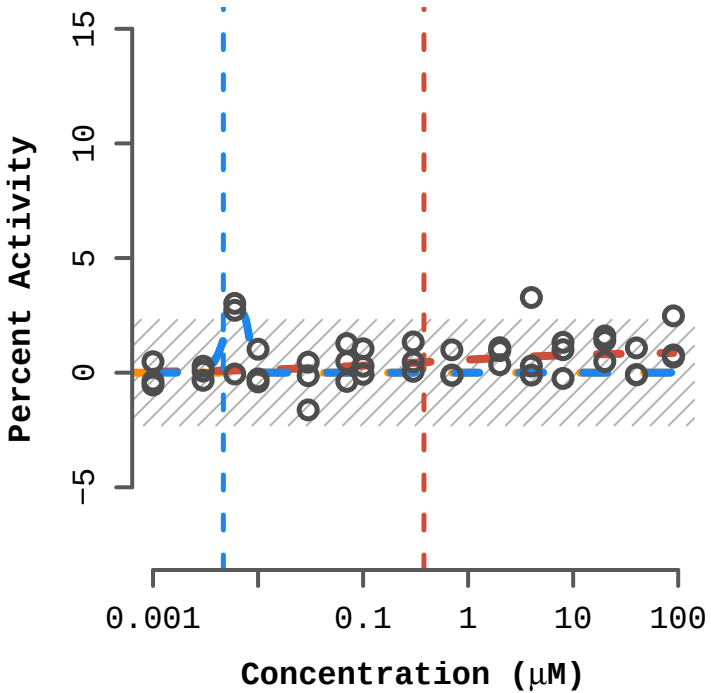
NAME: Diisobutyl ketone
CHID: 25080 CASRN: 108-83-8
SPID(S): Tox21_303091
M4ID: 12476042

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.57 MAX_MED: 0.837 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diisobutyl ketone
CHID: 25080 CASRN: 108-83-8
SPID(S): Tox21_202406
M4ID: 12479846

HILL MODEL (in red):

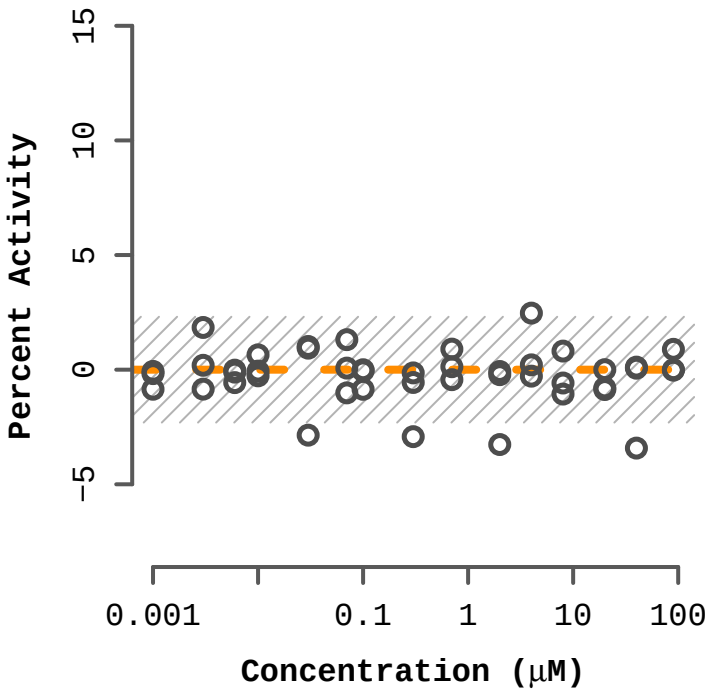
	tp	ga	gw
val:	0.914	−0.42	0.514
sd:	0.505	1.47	0.566

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.86	−2.33	8	−2.08	18
sd:	3.14	0.363	12.7	0.431	91.8

	CNST	HILL	GNLS
AIC:	135.4	123.33	137.74
PROB:	0	1	0
RMSE:	1.12	0.94	1.02

MAX_MEAN: 1.9 MAX_MED: 2.72 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

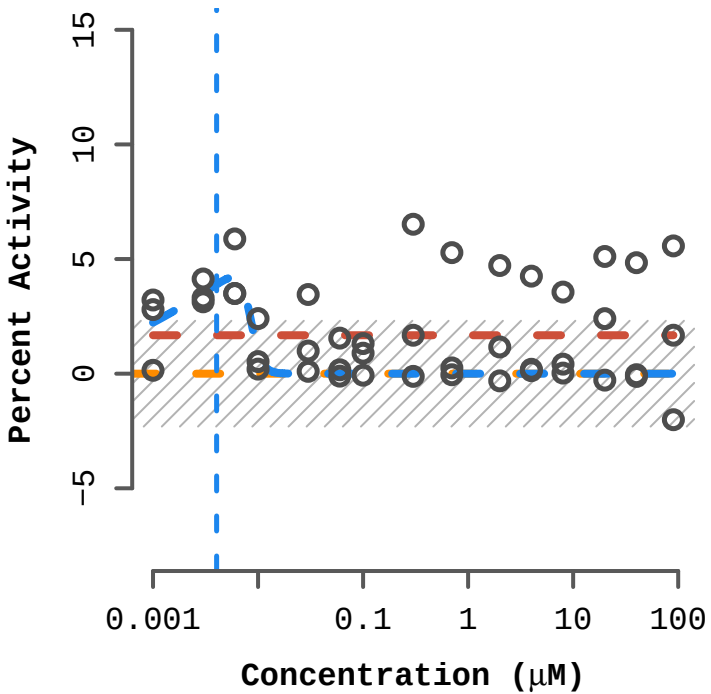
NAME: Diisodecyl phthalate
CHID: 25082 CASRN: 26761-40-0
SPID(S): Tox21_201431
M4ID: 12480821

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.8 **MAX_MED:** 0.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diisopropylamine
CHID: 25085 **CASRN:** 108-18-9
SPID(S): Tox21_200216
M4ID: 12482036

HILL MODEL (in red):

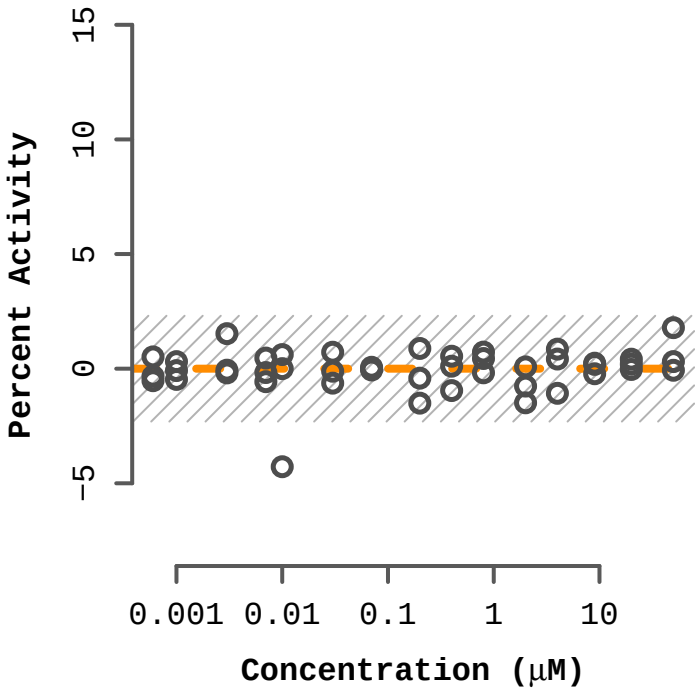
	tp	ga	gw
val:	1.68	−4.72	4.22
sd:	0.342	1570	3800

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.8	−2.39	0.657	−2.07	8.53
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	224.8	207.55	210.88
PROB:	0	0.84	0.16
RMSE:	2.83	2.1	2.37

MAX_MEAN: 4.29 **MAX_MED:** 3.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

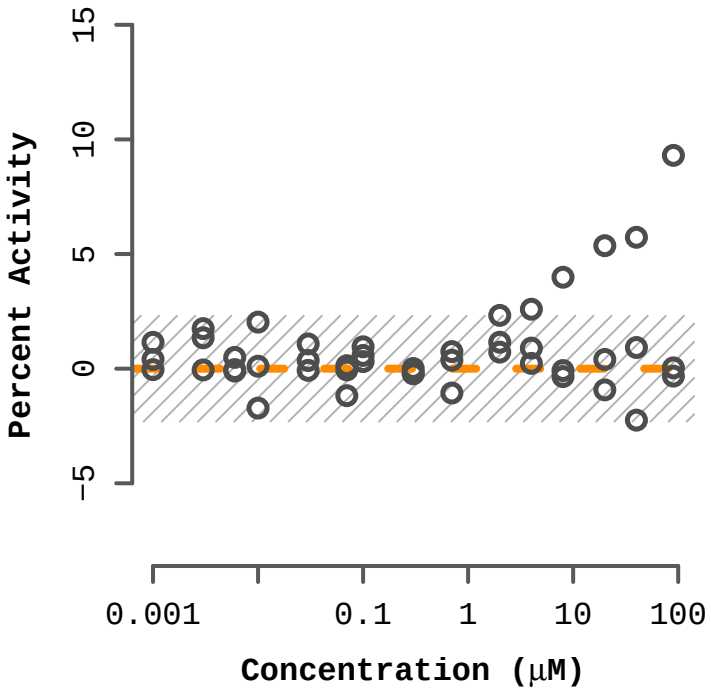
NAME: Diisopropylamine
CHID: 25085 **CASRN:** 108-18-9
SPID(S): Tox21_111075_1
M4ID: 12483921

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.678 **MAX_MED:** 0.444 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

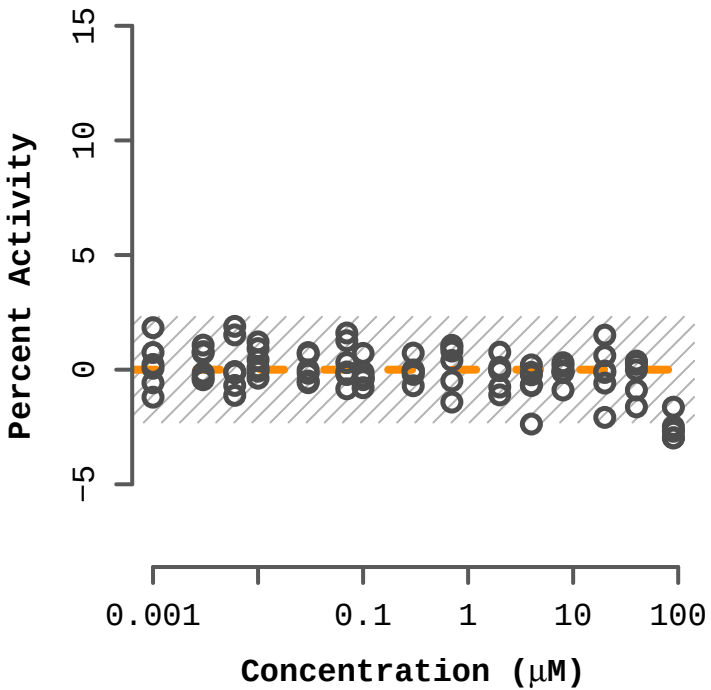
NAME: Diisopropylcarbodiimide
CHID: 25086 **CASRN:** 693-13-0
SPID(S): Tox21_202451
M4ID: 12479801

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.79	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 3.01 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

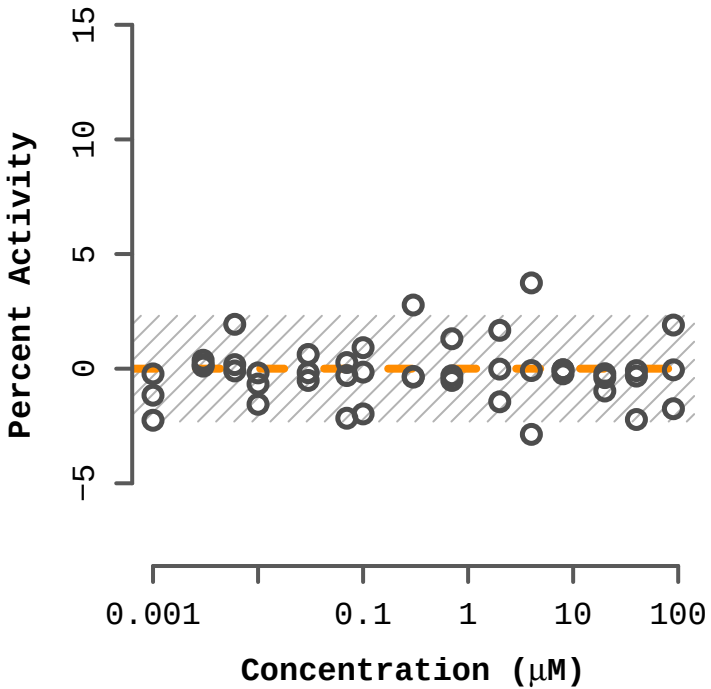
NAME: Dimenhydrinate
CHID: 25087 CASRN: 523-87-5
SPID(S): Tox21_200323
M4ID: 12481929

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.369 **MAX_MED:** 0.608 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

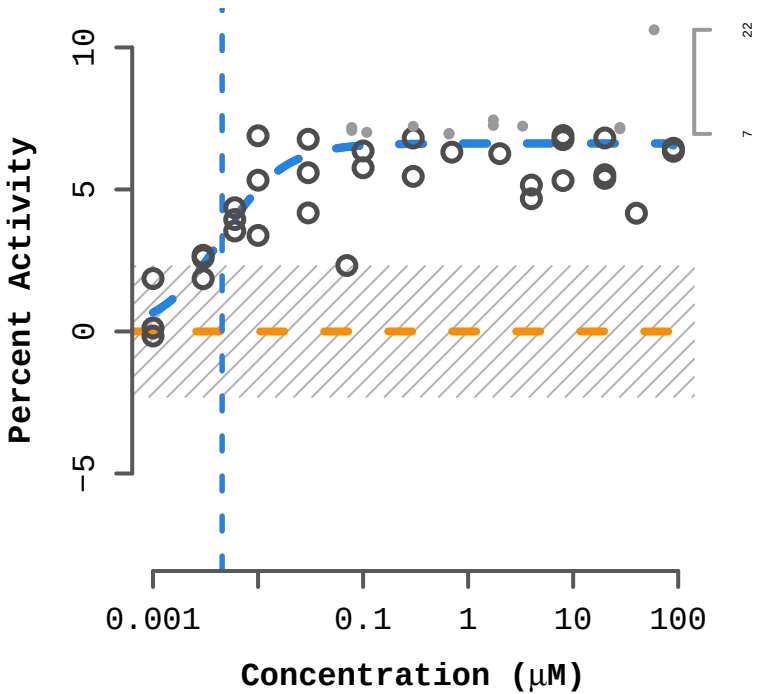
NAME: 3,3'−Dimethoxybenzidine
CHID: 25091 **CASRN:** 119−90−4
SPID(S): Tox21_300041
M4ID: 12479089

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.691 **MAX_MED:** 0.179 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−Dimethoxybenzidine
CHID: 25091 CASRN: 119−90−4
SPID(S): Tox21_202443
M4ID: 12479809 BRK

HILL MODEL (in red):

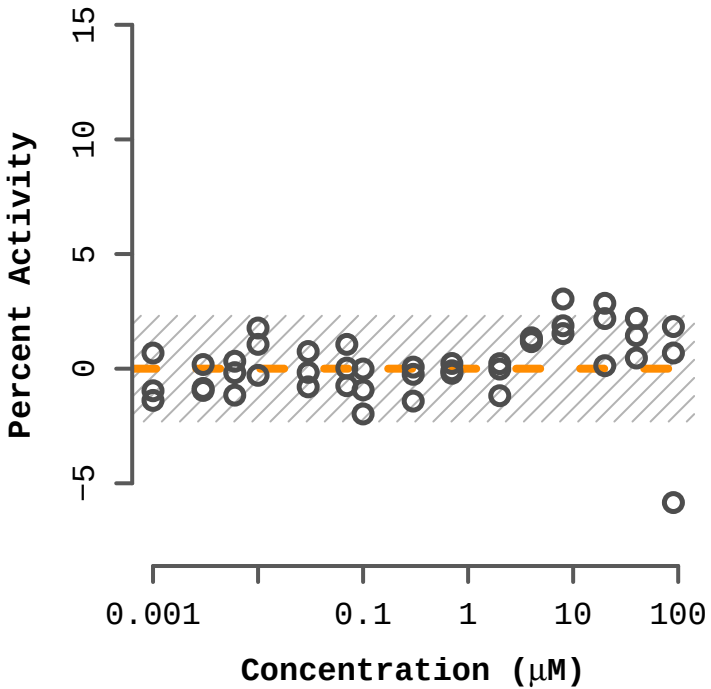
	tp	ga	gw
val:	6.61	−2.34	1.45
sd:	0.25	0.0783	0.444

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.63	−2.34	1.44	2.09	13.9
sd:	0.27	0.0794	0.445	0.383	39.6

	CNST	HILL	GNLS
AIC:	305.34	175.93	179.91
PROB:	0	0.88	0.12
RMSE:	6.74	2.68	2.69

MAX_MEAN: 11.8 MAX_MED: 8.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

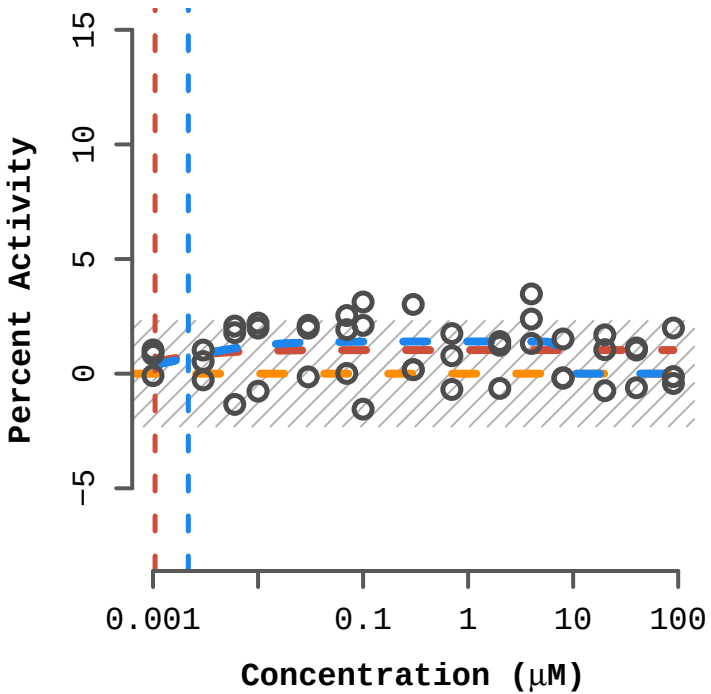
NAME: 4,4'−Dimethoxydiphenylamine
CHID: 25093 **CASRN:** 101−70−2
SPID(S): Tox21_202895
M4ID: 12479357

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Di(2-methoxyethyl) phthalate
CHID: 25094 **CASRN:** 117-82-8
SPID(S): Tox21_303033
M4ID: 12476100

HILL MODEL (in red):

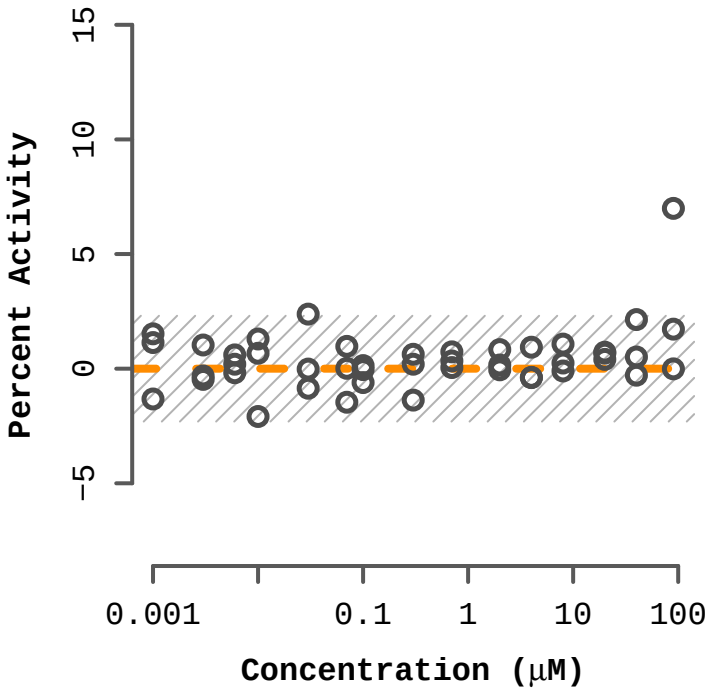
	tp	ga	gw
val:	1.03	−2.98	1.42
sd:	0.232	0.778	1.85

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.4	−2.66	1.31	0.871	17.7
sd:	0.299	0.547	1.48	0.417	224

	CNST	HILL	GNLS
AIC:	173.57	160.12	162.01
PROB:	0	0.72	0.28
RMSE:	1.55	1.23	1.22

MAX_MEAN: 2.39 **MAX_MED:** 2.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

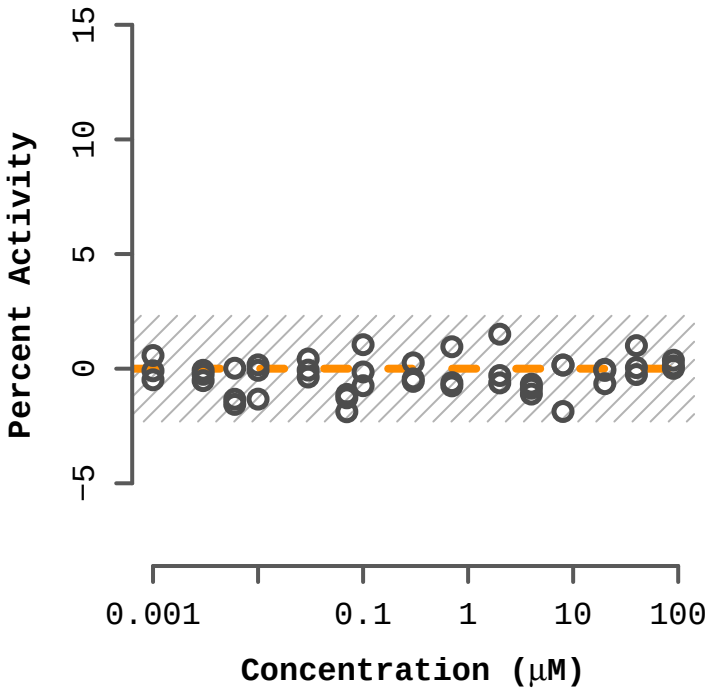
NAME: Di(2-methoxyethyl) phthalate
CHID: 25094 **CASRN:** 117-82-8
SPID(S): Tox21_201857
M4ID: 12480395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.9 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

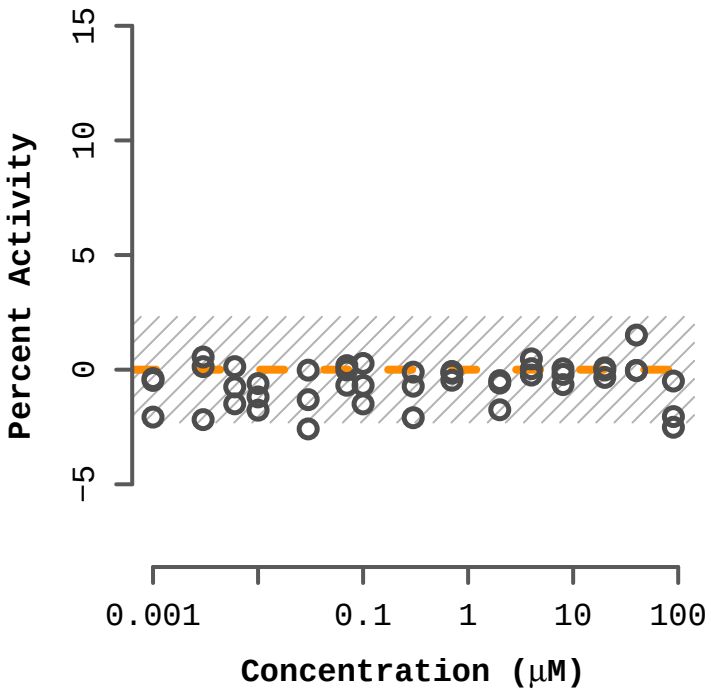
NAME: Dimethyl adipate
CHID: 25096 **CASRN:** 627-93-0
SPID(S): Tox21_300363
M4ID: 12478769

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.268 **MAX_MED:** 0.158 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

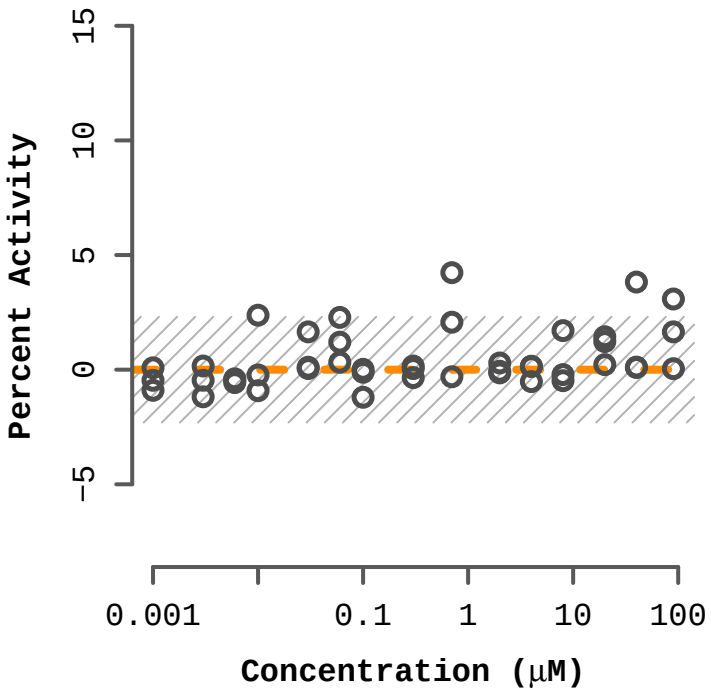
NAME: Dimethyl adipate
CHID: 25096 **CASRN:** 627-93-0
SPID(S): Tox21_201912
M4ID: 12480340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** 0.134 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

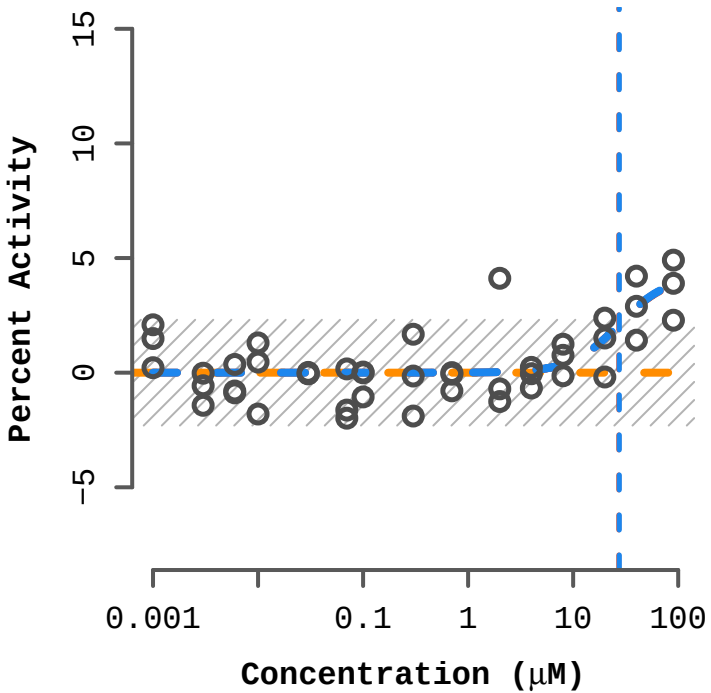
NAME: 2-(Dimethylamino)ethyl acrylate
CHID: 25100 **CASRN:** 2439-35-2
SPID(S): Tox21_200307
M4ID: 12481945

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 2 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Dimethylaminophenol
CHID: 25101 **CASRN:** 99-07-0
SPID(S): Tox21_303187
M4ID: 12475946

HILL MODEL (in red):

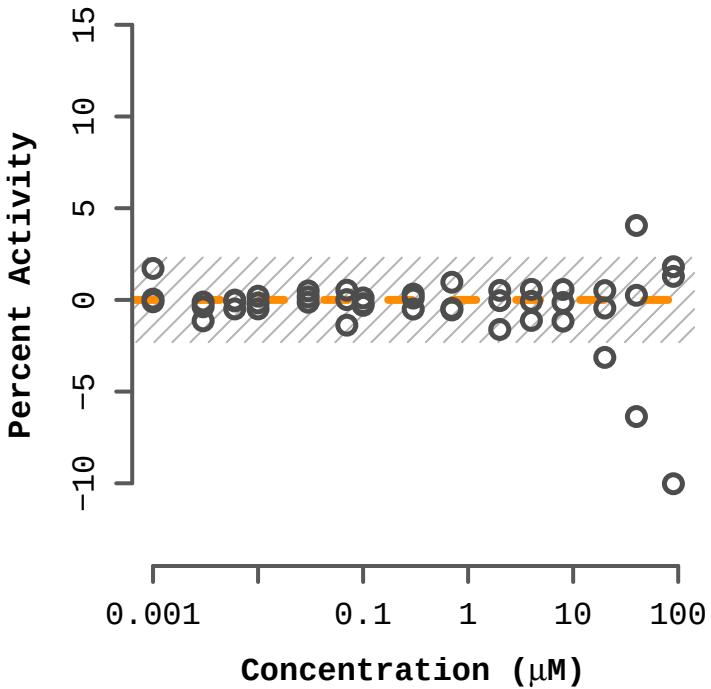
	tp	ga	gw
val:	4.19	1.43	1.93
sd:	1.26	0.216	1.07

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.24	1.44	1.92	2.24	7.17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	174.85	148.69	152.69
PROB:	0	0.88	0.12
RMSE:	1.72	1.18	1.18

MAX_MEAN: 3.7 **MAX_MED:** 3.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

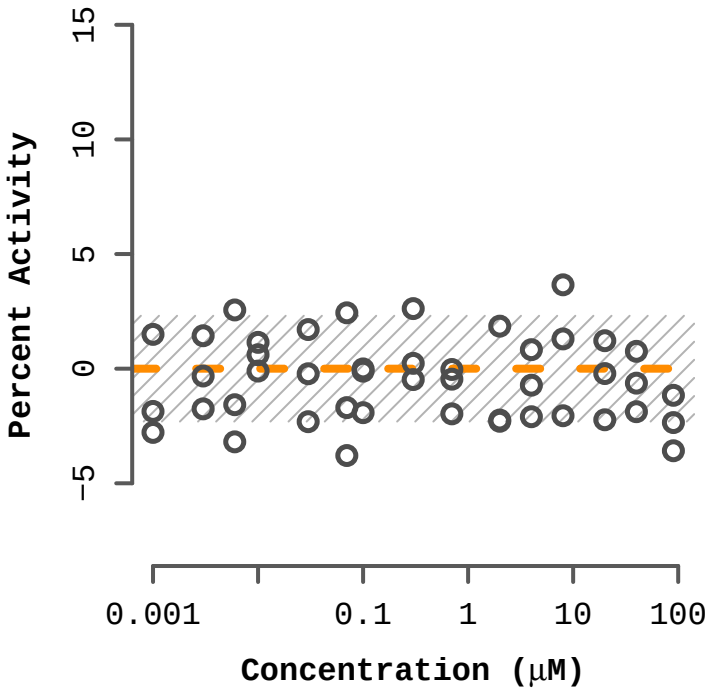
NAME: 3-Dimethylaminophenol
CHID: 25101 CASRN: 99-07-0
SPID(S): Tox21_201927
M4ID: 12480325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.03	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 0.552 MAX_MED: 1.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

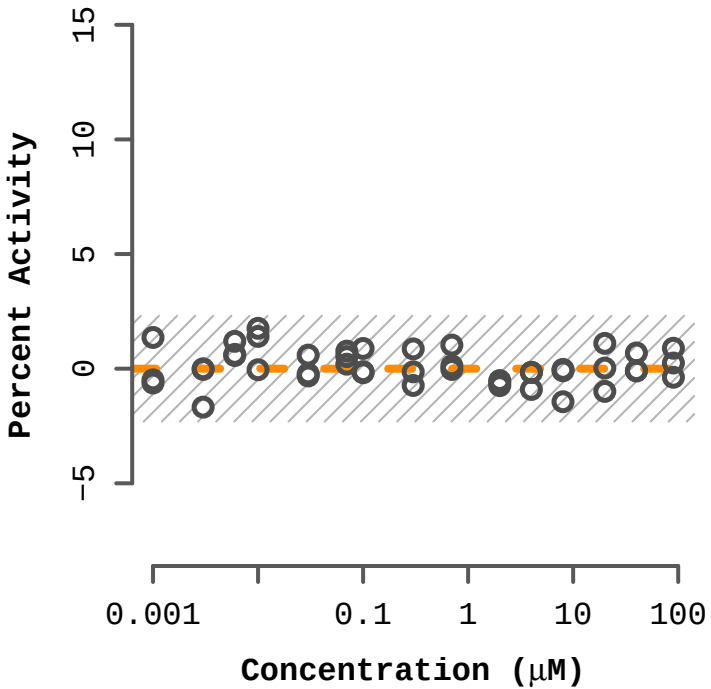
NAME: 3-(Dimethylamino)propylamine
CHID: 25102 **CASRN:** 109-55-7
SPID(S): Tox21_303328
M4ID: 12475805

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 0.97 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

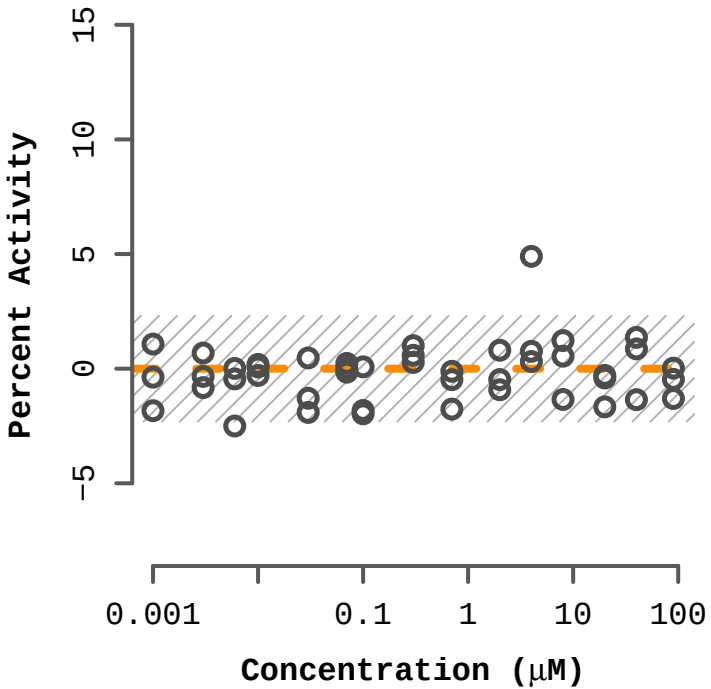
NAME: 3-(Dimethylamino)propylamine
CHID: 25102 **CASRN:** 109-55-7
SPID(S): Tox21_202048
M4ID: 12480204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

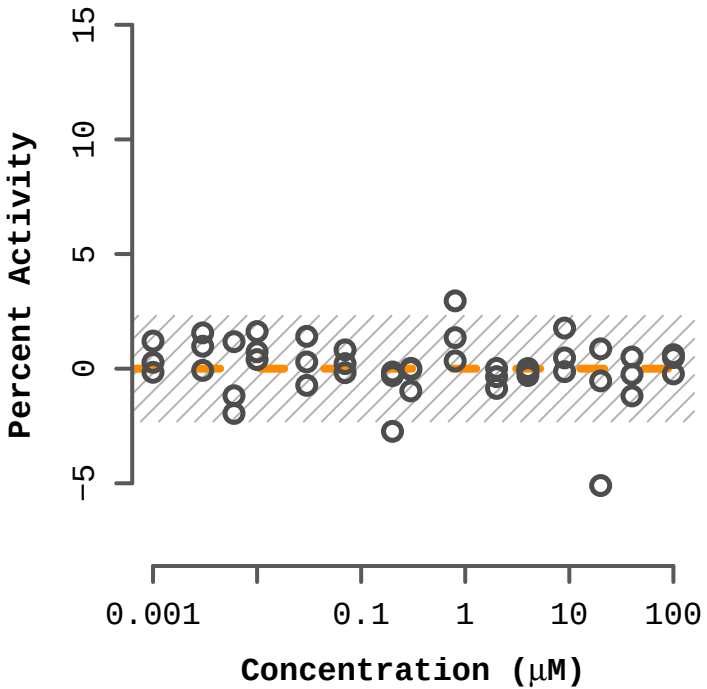
NAME: 2,5-Dimethyl-2,5-di-(tert-butylperoxy)hexane
CHID: 25110 **CASRN:** 78-63-7
SPID(S): Tox21_300177
M4ID: 12478953

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 0.863 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

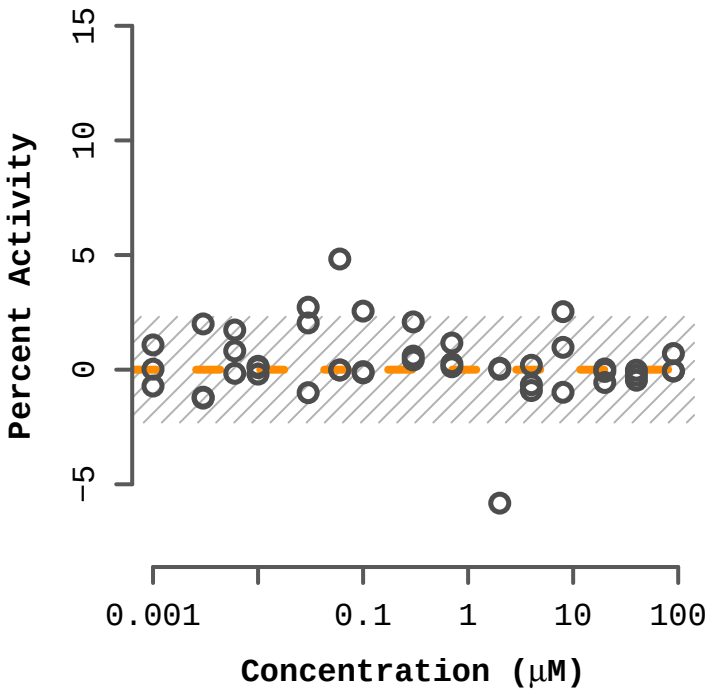
NAME: 2,2-Dimethylbutane
CHID: 25111 **CASRN:** 75-83-2
SPID(S): Tox21_200358
M4ID: 12481894

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

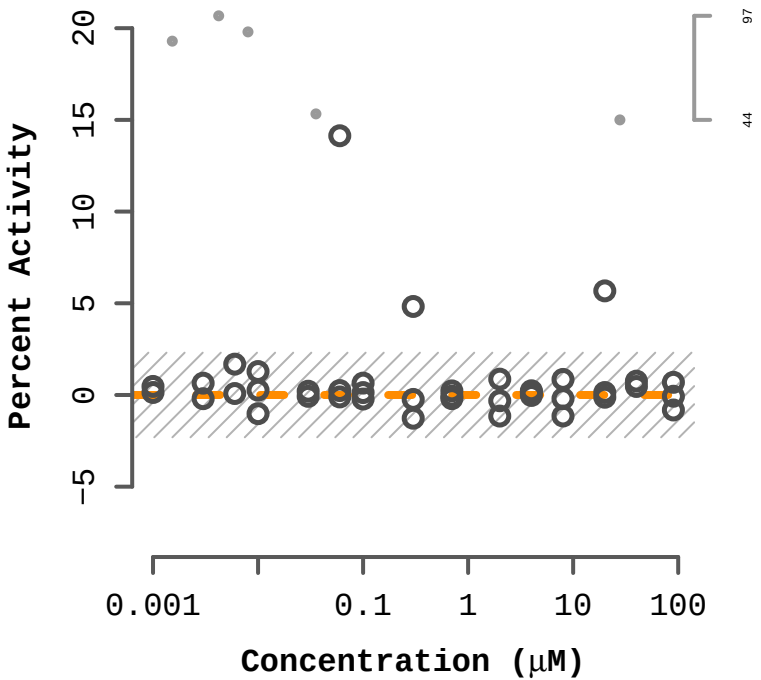
NAME: 2,3-Dimethylbutane
CHID: 25112 **CASRN:** 79-29-8
SPID(S): Tox21_200674
M4ID: 12481578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

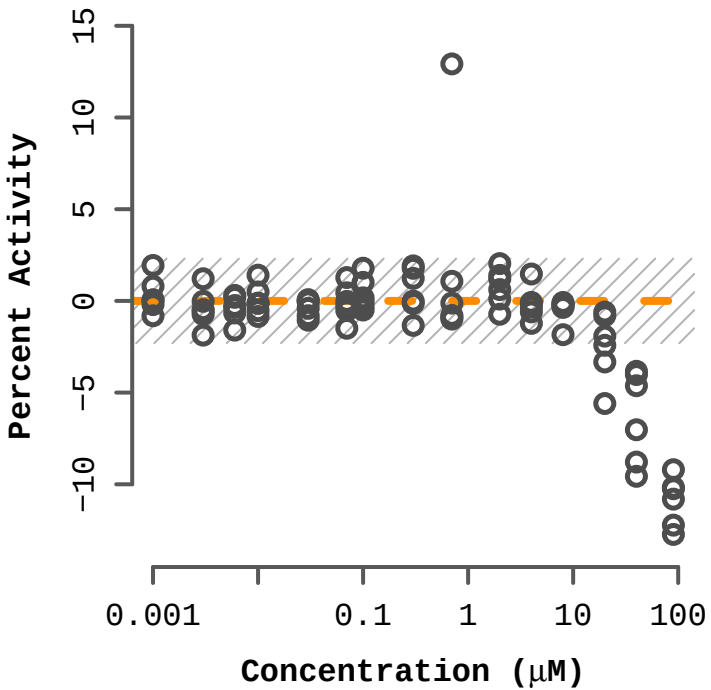
NAME: 1,3-Dimethylbutylamine
CHID: 25113 **CASRN:** 108-09-8
SPID(S): Tox21_201157
M4ID: 12481095 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	320.46	NA	NA
PROB:	1	NA	NA
RMSE:	25.27	NA	NA

MAX_MEAN: 32.5 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

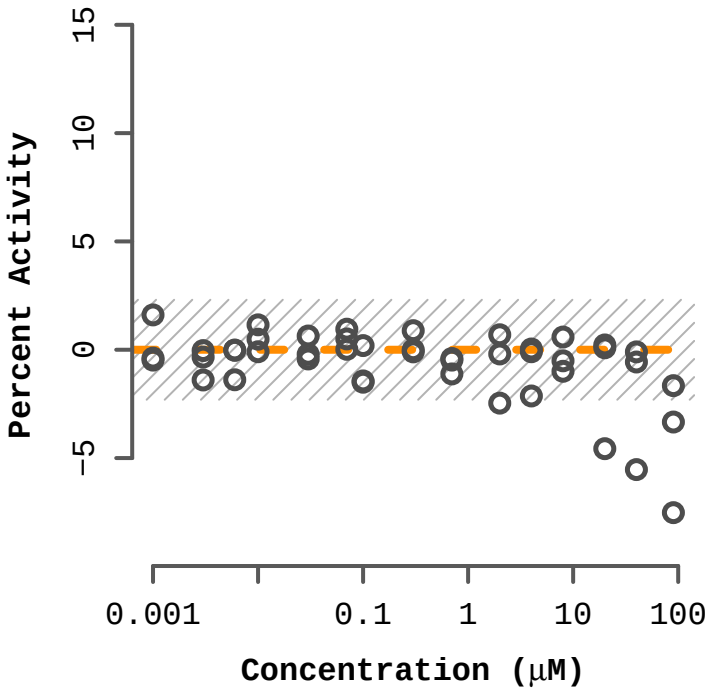
NAME: N-(1,3-Dimethylbutyl)-N'-phenyl-p-phenylenedia
CHID: 25114 **CASRN:** 793-24-8
SPID(S): Tox21_200890
M4ID: 12481362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	439.62	NA	NA
PROB:	1	NA	NA
RMSE:	3.76	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 0.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

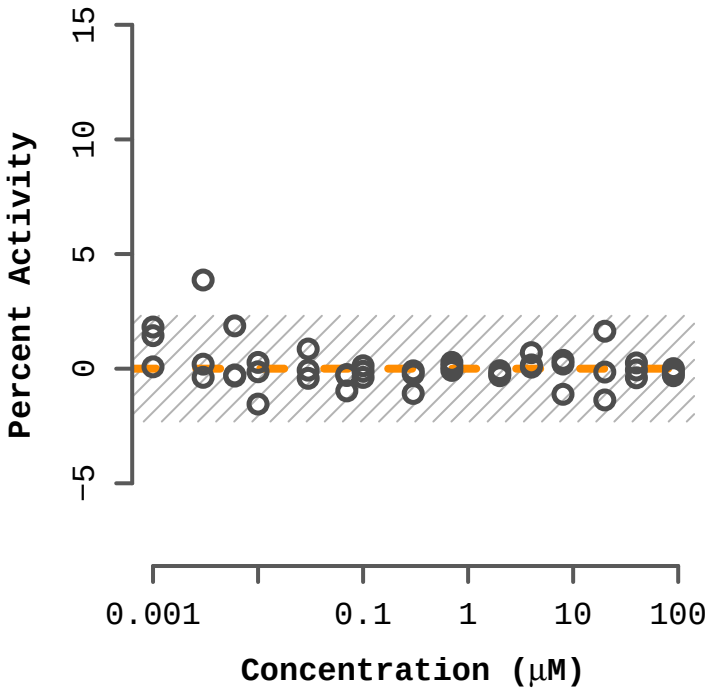
NAME: Methyl disulfide
CHID: 25117 CASRN: 624-92-0
SPID(S): Tox21_201525
M4ID: 12480727

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 0.517 MAX_MED: 0.502 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

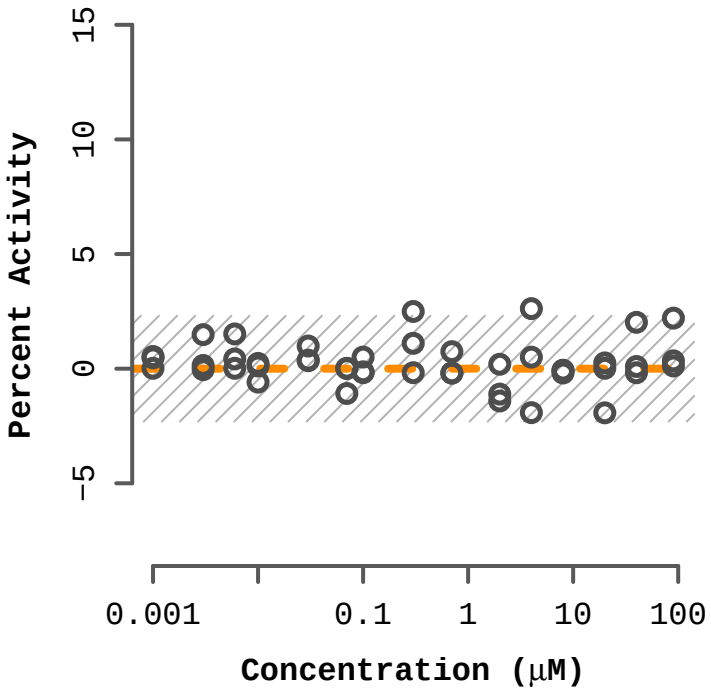
NAME: Dimethyl glutarate
CHID: 25122 **CASRN:** 1119-40-0
SPID(S): Tox21_300115
M4ID: 12479015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

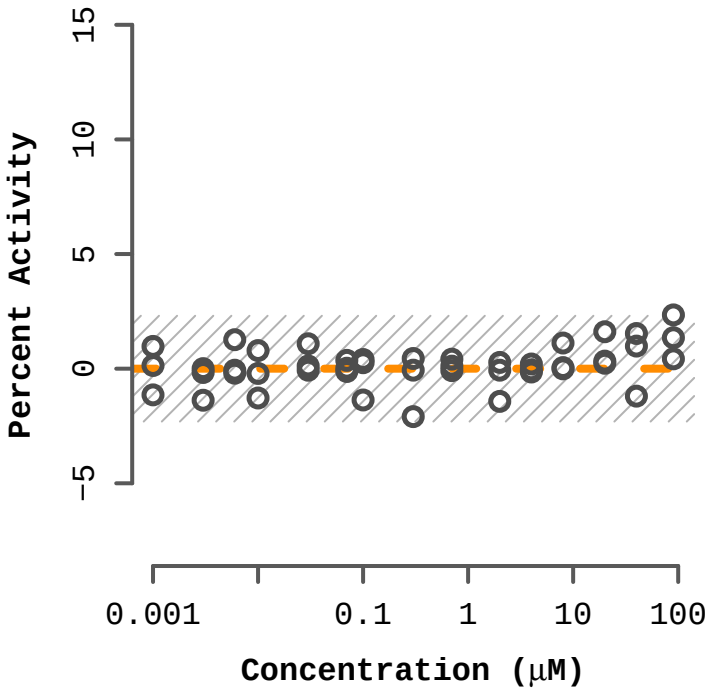
NAME: Dimethyl glutarate
CHID: 25122 **CASRN:** 1119-40-0
SPID(S): Tox21_201235
M4ID: 12481017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

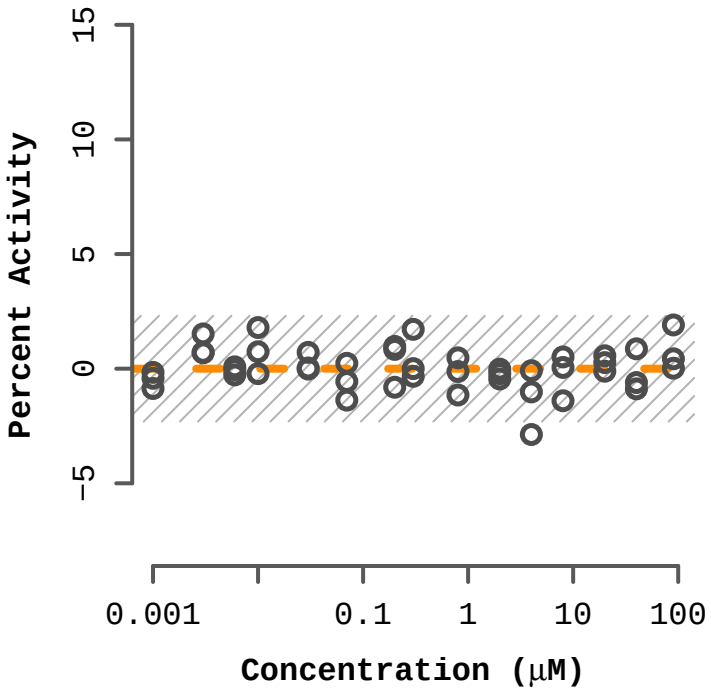
NAME: Dimethylnaphthalene
CHID: 25130 **CASRN:** 28804-88-8
SPID(S): Tox21_303140
M4ID: 12475993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

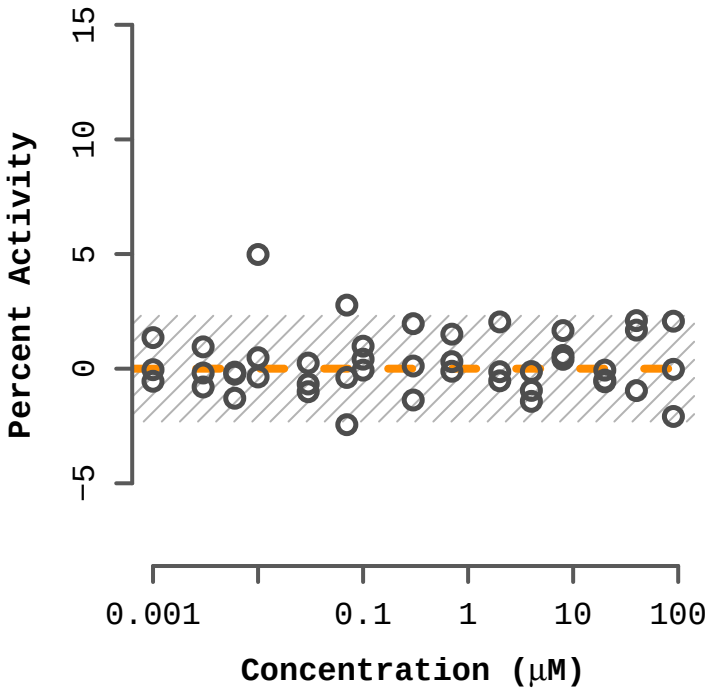
NAME: Dimethylnaphthalene
CHID: 25130 **CASRN:** 28804-88-8
SPID(S): Tox21_202167
M4ID: 12480085

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 0.842 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

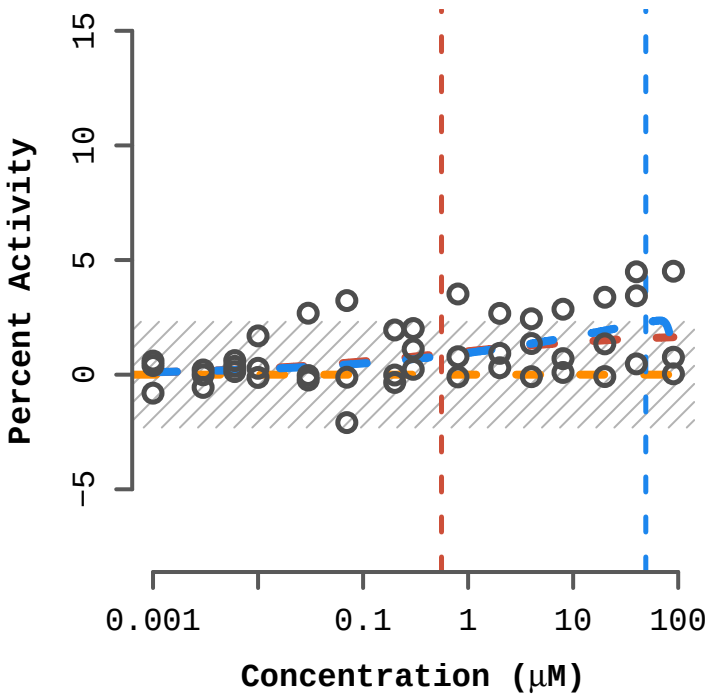
NAME: 1,2-Dimethyl-3-nitrobenzene
CHID: 25132 **CASRN:** 83-41-0
SPID(S): Tox21_300334
M4ID: 12478798

HILL MODEL: Not applicable.

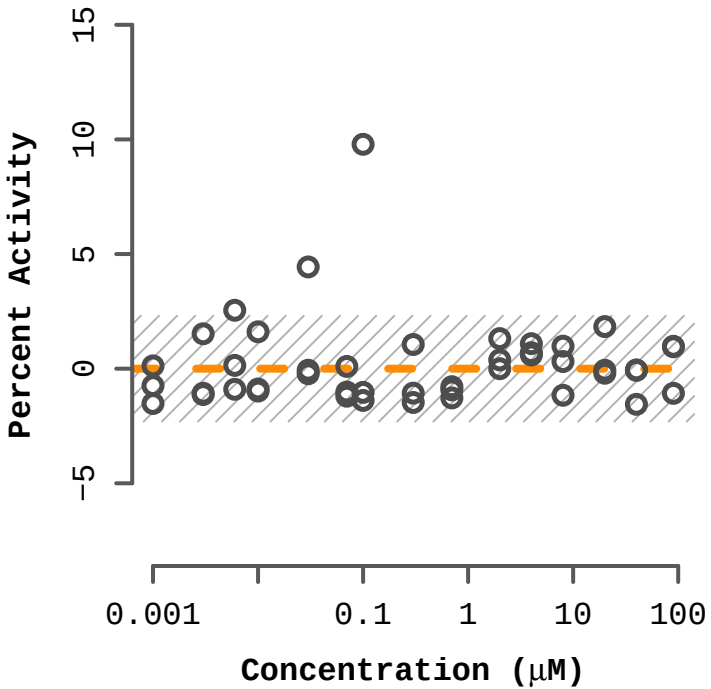
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.68 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1,2-Dimethyl-3-nitrobenzene
CHID:    25132   CASRN: 83-41-0
SPID(S): Tox21_202000
M4ID:    12480252

HILL MODEL (in red):
      tp       ga       gw
val:  1.81     -0.254   0.441
sd:   1.39     1.99     0.454

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.53     1.69     0.34     1.94     17.4
sd:   10.3     4.68     0.207    0.0512   68.6

      CNST        HILL        GNLS
AIC:  177.82      163.24      165.89
PROB: 0           0.79        0.21
RMSE: 1.77        1.32        1.32

MAX_MEAN: 2.8       MAX_MED: 3.44      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

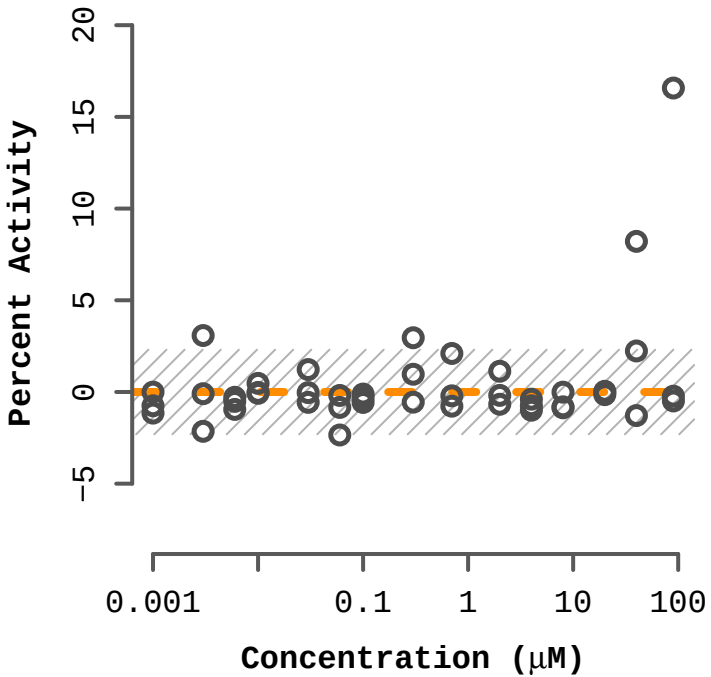
NAME: 1,2-Dimethyl-4-nitrobenzene
CHID: 25133 **CASRN:** 99-51-4
SPID(S): Tox21_300387
M4ID: 12478745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 2.46 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

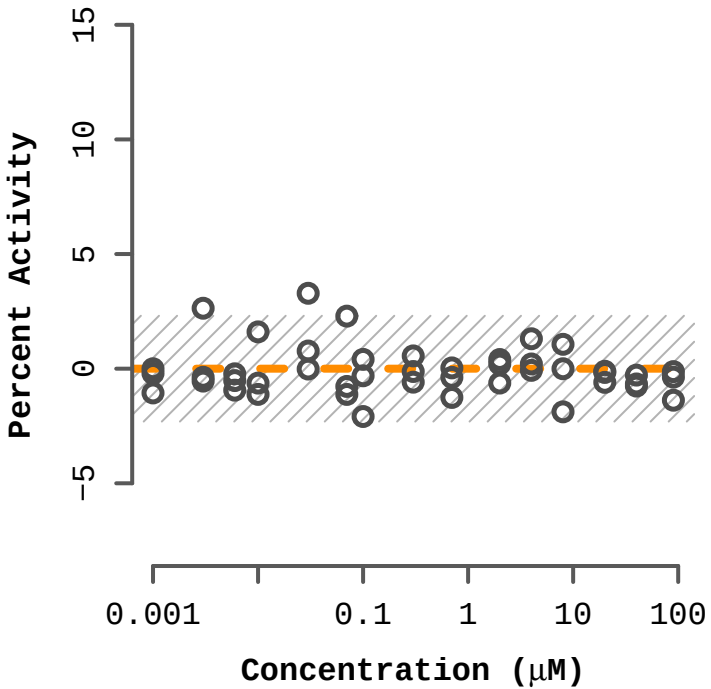
NAME: 1,2-Dimethyl-4-nitrobenzene
CHID: 25133 CASRN: 99-51-4
SPID(S): Tox21_201332
M4ID: 12480920

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.56	NA	NA
PROB:	1	NA	NA
RMSE:	2.96	NA	NA

MAX_MEAN: 5.29 MAX_MED: 2.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

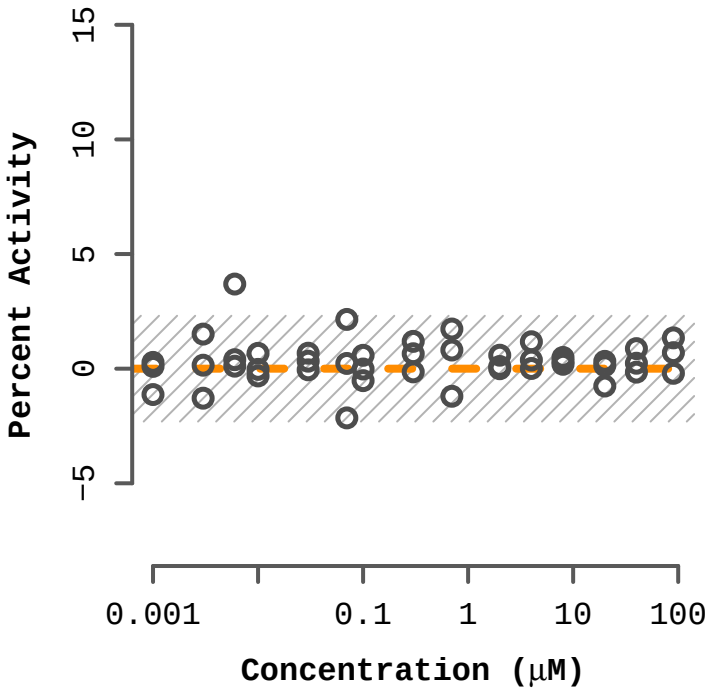
NAME: 1,3-Dimethyl-2-nitrobenzene
CHID: 25134 **CASRN:** 81-20-9
SPID(S): Tox21_303337
M4ID: 12475796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.771 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

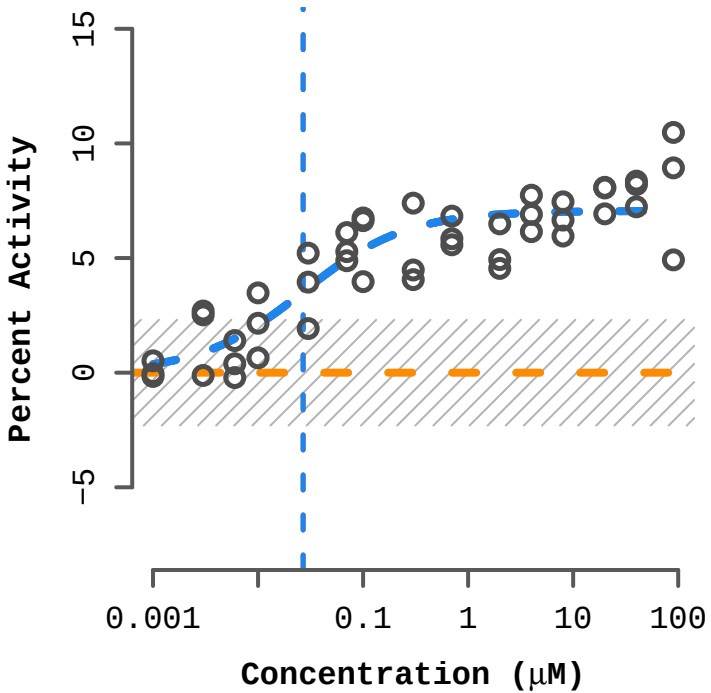
NAME: 1,3-Dimethyl-2-nitrobenzene
CHID: 25134 **CASRN:** 81-20-9
SPID(S): Tox21_201388
M4ID: 12480864

HILL MODEL: Not applicable.

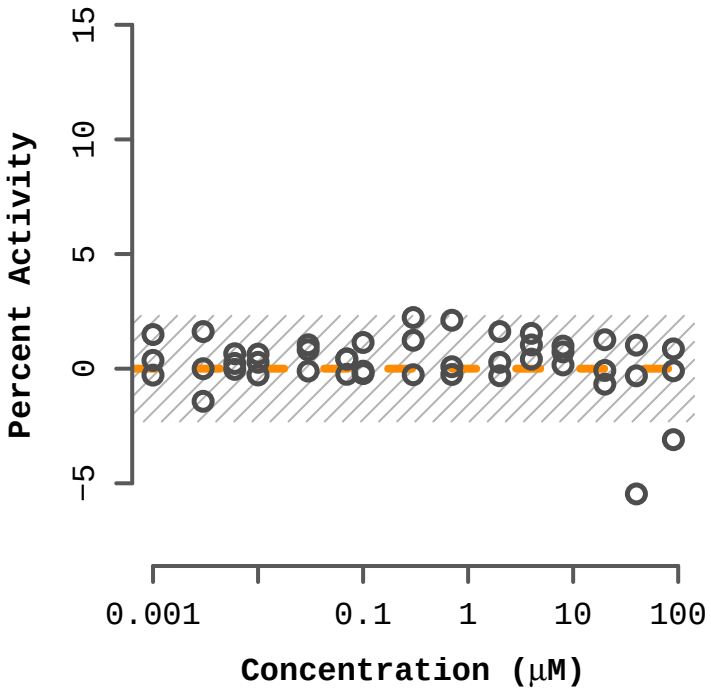
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.814 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1,3-Dimethyl-4-nitrobenzene
CHID:    25135   CASRN: 89-87-2
SPID(S): Tox21_303215
M4ID:    12475918

HILL MODEL (in red):
      tp       ga       gw
val:  7.06     -1.57    0.882
sd:   0.431    0.161    0.357

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.06     -1.57    0.882    3.45     10.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  292.91      164.21      168.21
PROB: 0           0.88        0.12
RMSE: 5.63        1.31        1.31

MAX_MEAN: 8.11      MAX_MED: 8.94      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

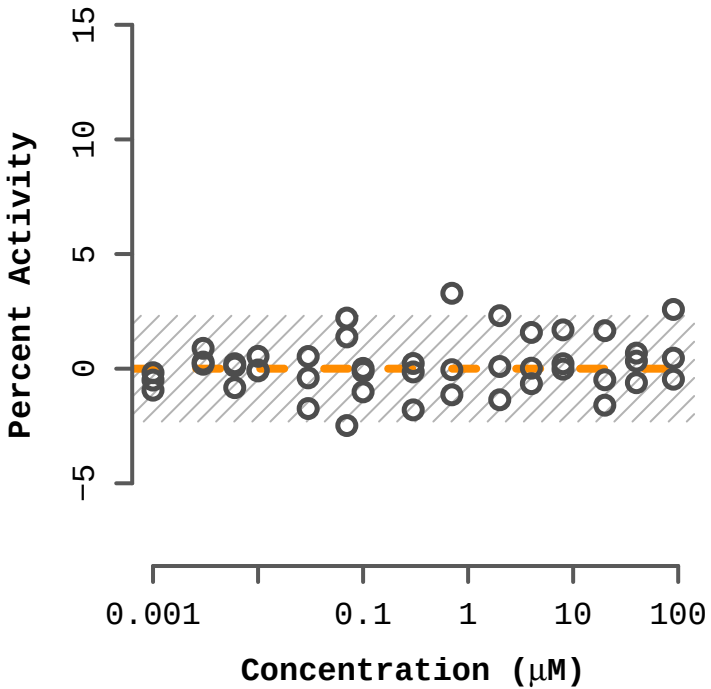
NAME: 1,3-Dimethyl-4-nitrobenzene
CHID: 25135 **CASRN:** 89-87-2
SPID(S): Tox21_202223
M4ID: 12480029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

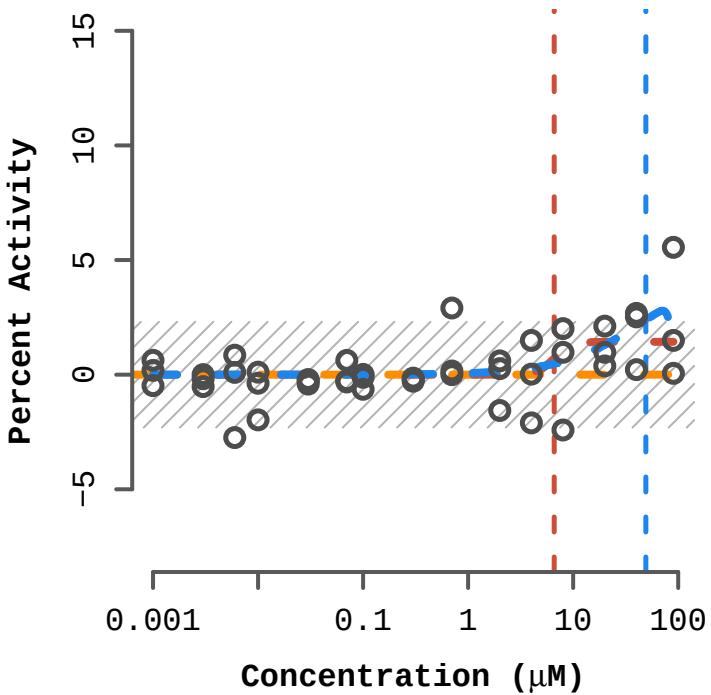
NAME: 1,3-Dimethyl-5-nitrobenzene
CHID: 25136 **CASRN:** 99-12-7
SPID(S): Tox21_200776
M4ID: 12481476

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.862 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4-Dimethyl-2-nitrobenzene
CHID: 25137 CASRN: 89-58-7
SPID(S): Tox21_200372
M4ID: 12481880

HILL MODEL (in red):

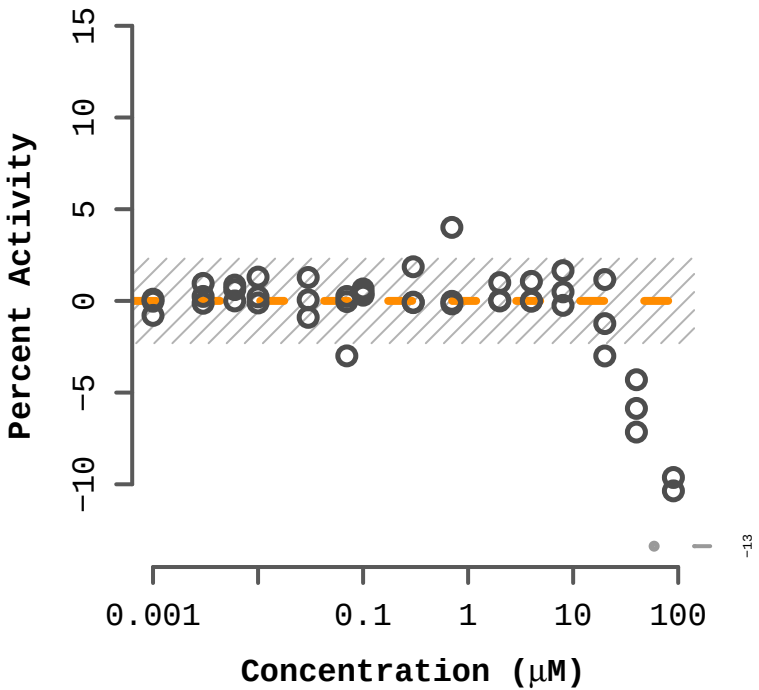
	tp	ga	gw
val:	1.43	0.819	5.44
sd:	0.413	0.234	15.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.78	1.69	1.09	1.94	17.2
sd:	50.3	7.11	2.48	0.125	162

	CNST	HILL	GNLS
AIC:	154.33	145.99	149
PROB:	0.01	0.81	0.18
RMSE:	1.46	1.25	1.25

MAX_MEAN: 2.37 MAX_MED: 2.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

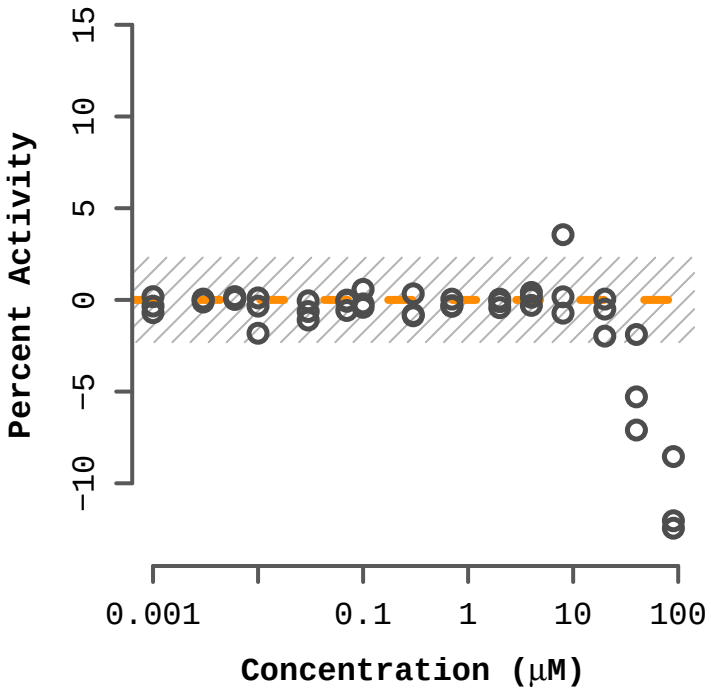
NAME: N,N-Dimethyl-4-nitrosoaniline
CHID: 25138 **CASRN:** 138-89-6
SPID(S): Tox21_303049
M4ID: 12476084 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.45	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

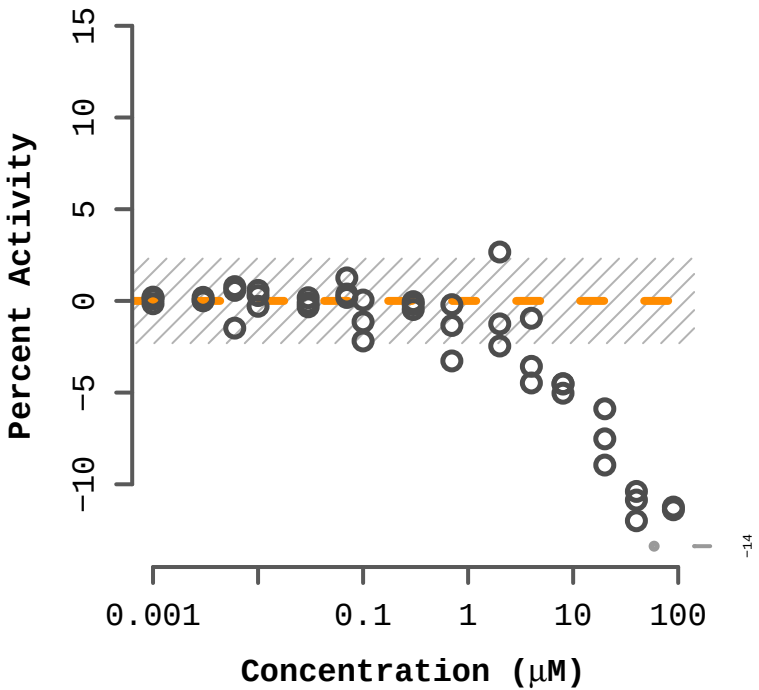
NAME: N,N-Dimethyl-4-nitrosoaniline
CHID: 25138 **CASRN:** 138-89-6
SPID(S): Tox21_202129
M4ID: 12480123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.51	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.171 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

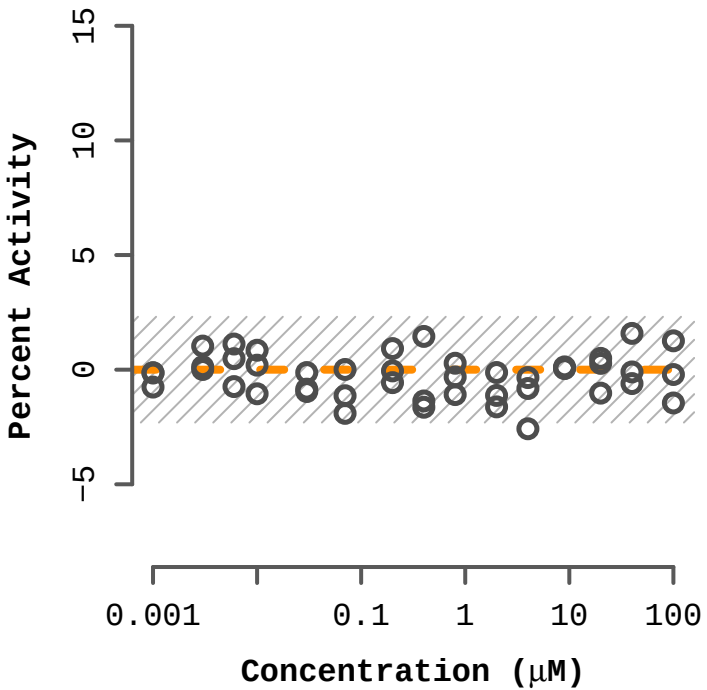
NAME: N,N−Dimethyl−N−benzyl−N−octadecylammonium chlo
CHID: 25139 CASRN: 122−19−0
SPID(S): Tox21_200419
M4ID: 12481833 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.53	NA	NA
PROB:	1	NA	NA
RMSE:	4.99	NA	NA

MAX_MEAN: 0.608 MAX_MED: 0.574 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

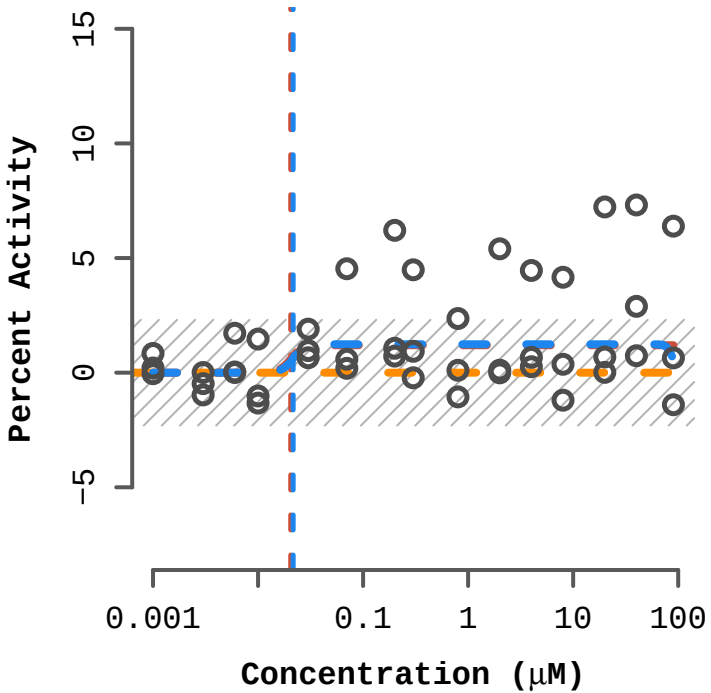
NAME: Dimethylolurea
CHID: 25141 **CASRN:** 140-95-4
SPID(S): Tox21_300714
M4ID: 12478419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.391 **MAX_MED:** 0.482 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dimethylphenol
CHID: 25143 CASRN: 526-75-0
SPID(S): Tox21_303513
M4ID: 12475629

HILL MODEL (in red):

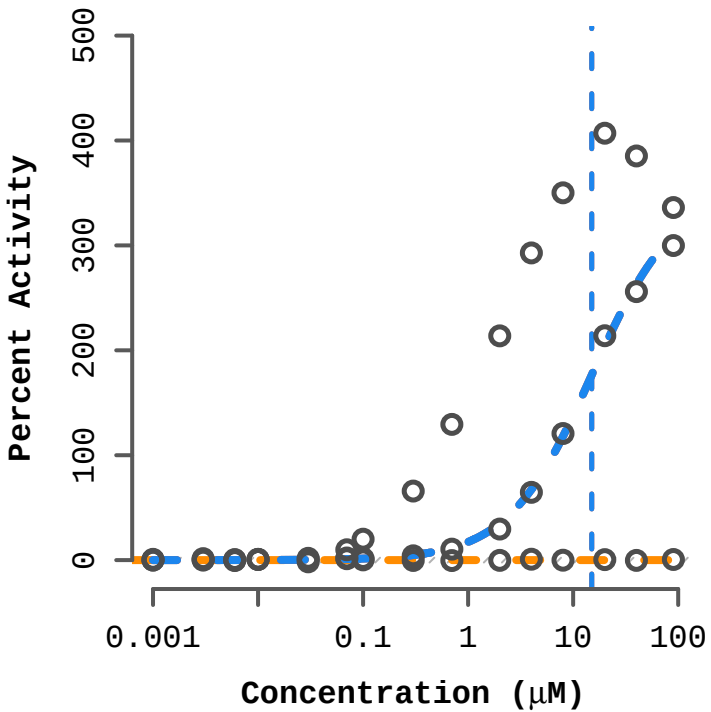
	tp	ga	gw
val:	1.2	−1.69	8
sd:	0.39	0.718	27.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.24	−1.67	7.99	1.95	16
sd:	0.41	0.662	30	0.149	390

	CNST	HILL	GNLS
AIC:	210.67	204.24	208.01
PROB:	0.03	0.84	0.13
RMSE:	2.71	2.26	2.27

MAX_MEAN: 3.65 MAX_MED: 2.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dimethylphenol
CHID: 25143 CASRN: 526-75-0
SPID(S): Tox21_201831
M4ID: 12480421

HILL MODEL (in red):

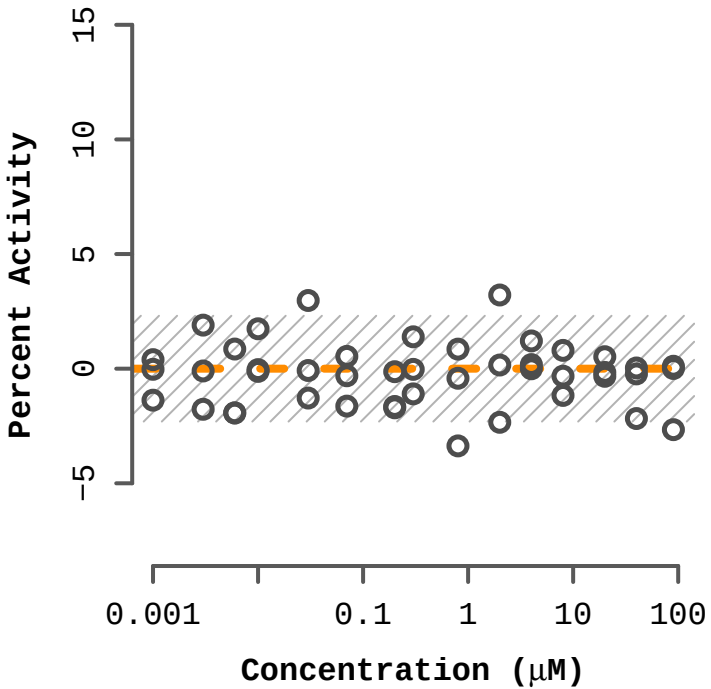
	tp	ga	gw
val:	353	1.18	1.09
sd:	93.4	0.315	0.565

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	353	1.18	1.09	3.95	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	587.82	530.02	534.02
PROB:	0	0.88	0.12
RMSE:	143.28	98.62	98.62

MAX_MEAN: 214 MAX_MED: 300 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

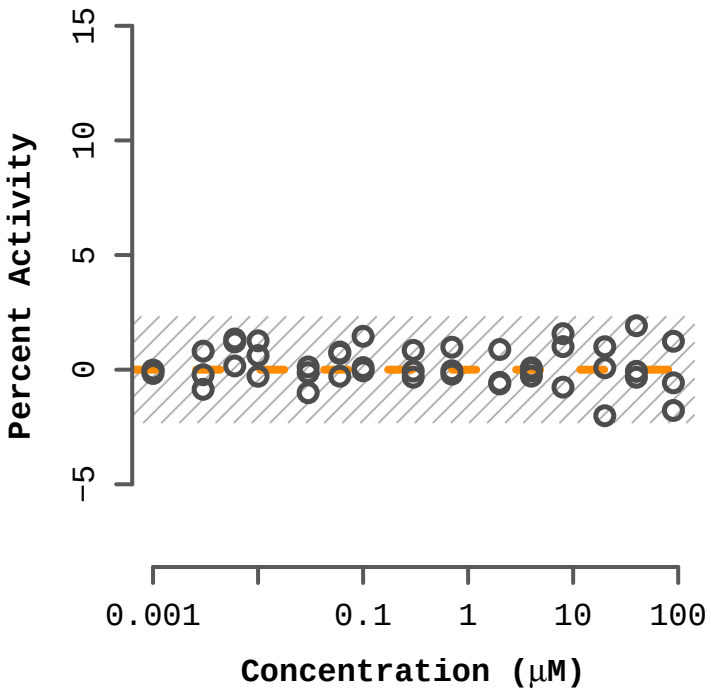
NAME: 2,5-Dimethylphenol
CHID: 25145 **CASRN:** 95-87-4
SPID(S): Tox21_300326
M4ID: 12478806

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.539 **MAX_MED:** 0.181 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

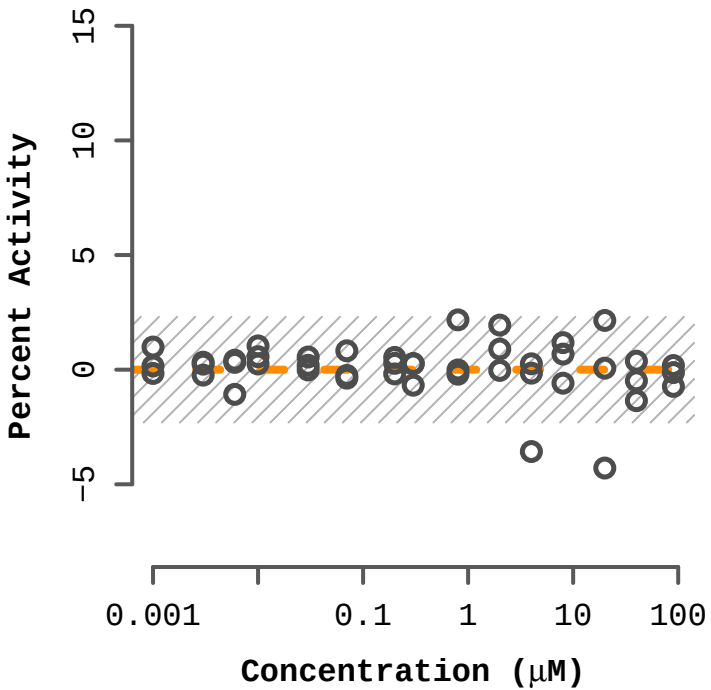
NAME: 2,5-Dimethylphenol
CHID: 25145 CASRN: 95-87-4
SPID(S): Tox21_201275
M4ID: 12480977

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.905 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

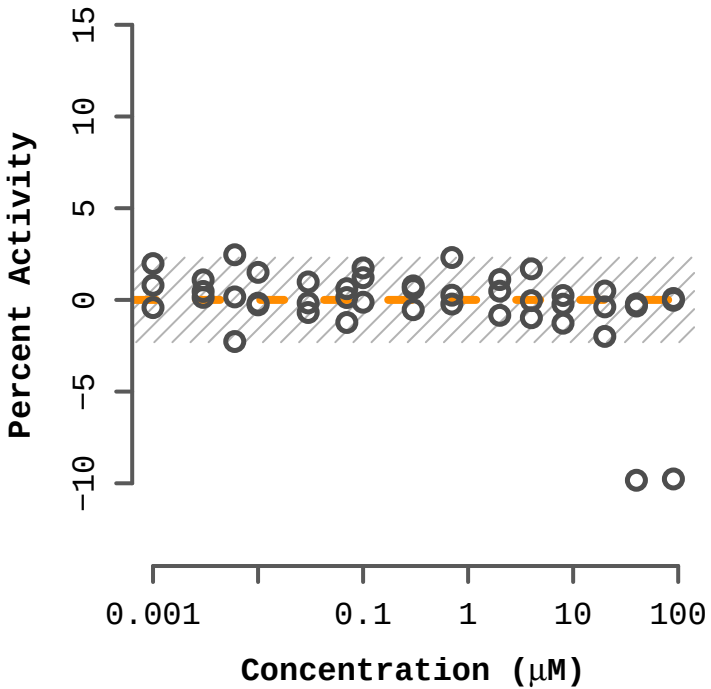
NAME: 3,5-Dimethylphenol
CHID: 25148 **CASRN:** 108-68-9
SPID(S): Tox21_303372
M4ID: 12475763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 0.901 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

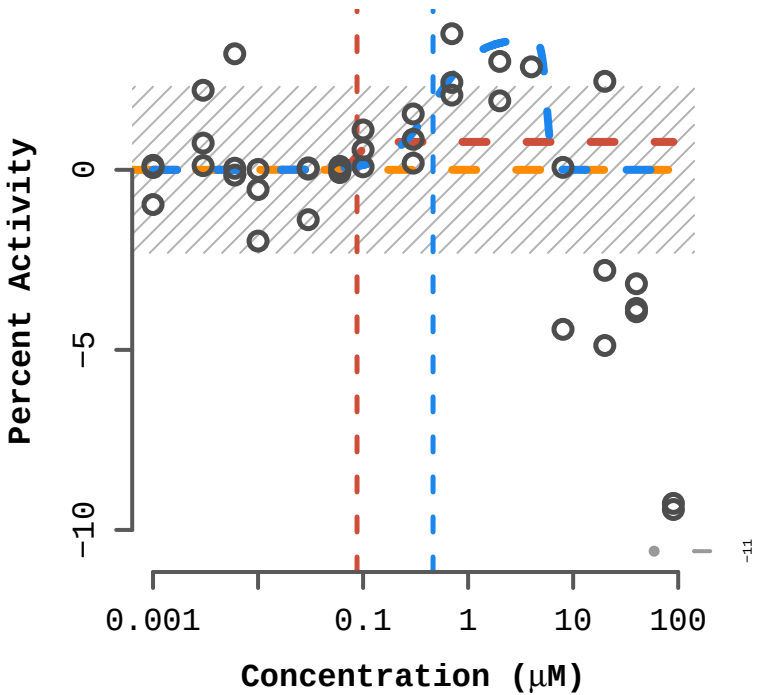
NAME: 3,5-Dimethylphenol
CHID: 25148 **CASRN:** 108-68-9
SPID(S): Tox21_202181
M4ID: 12480071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.7	NA	NA
PROB:	1	NA	NA
RMSE:	2.3	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N,N−Dimethyl−p−phenylenediamine
CHID: 25149 CASRN: 99−98−9
SPID(S): Tox21_200191
M4ID: 12482061 BRK

HILL MODEL (in red):

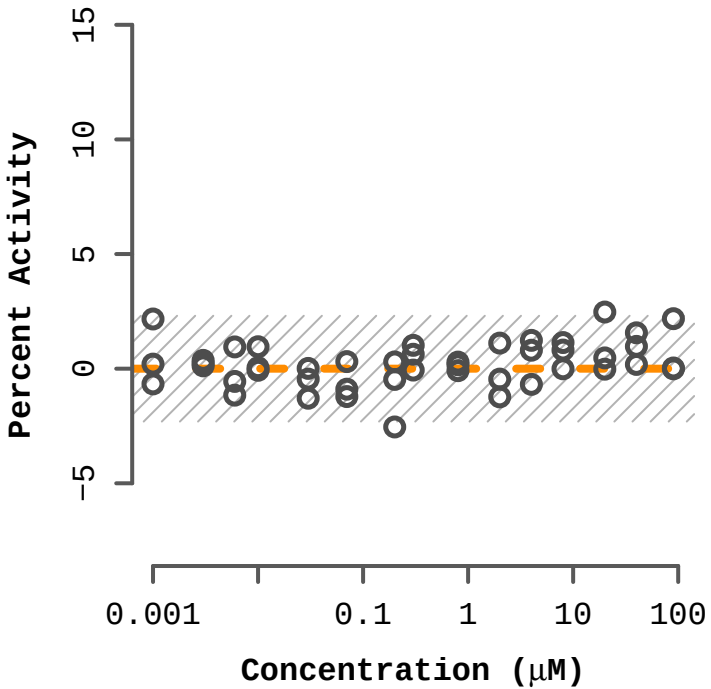
	tp	ga	gw
val:	0.775	−1.06	8
sd:	0.758	0.524	51.7

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.68	−0.334	2.12	0.748	18
sd:	0.989	0.23	2.73	0.536	64

	CNST	HILL	GNLS
AIC:	240.46	245.32	230.9
PROB:	0.01	0	0.99
RMSE:	3.67	3.76	3.36

MAX_MEAN: 3.73 MAX_MED: 3.93 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

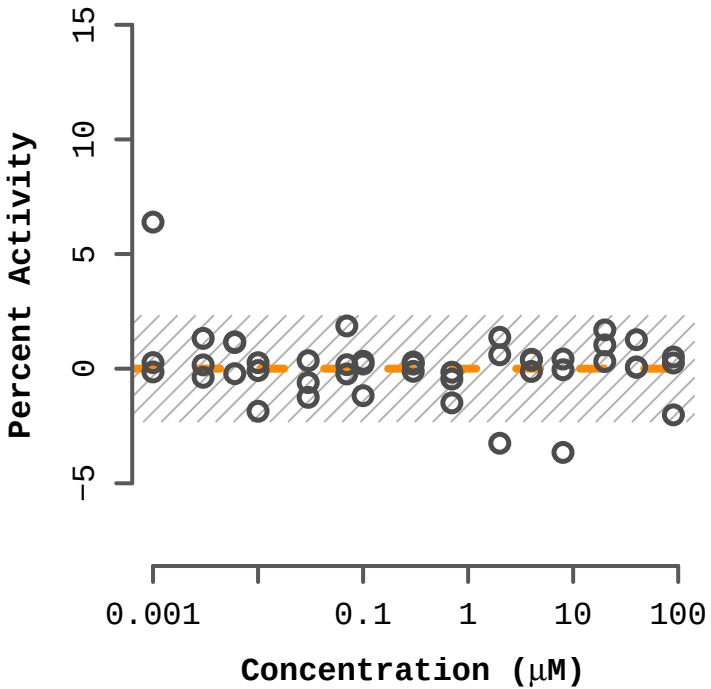
NAME: Dimethyl phosphate
CHID: 25150 **CASRN:** 813-78-5
SPID(S): Tox21_301411
M4ID: 12477722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.974 **MAX_MED:** 0.974 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

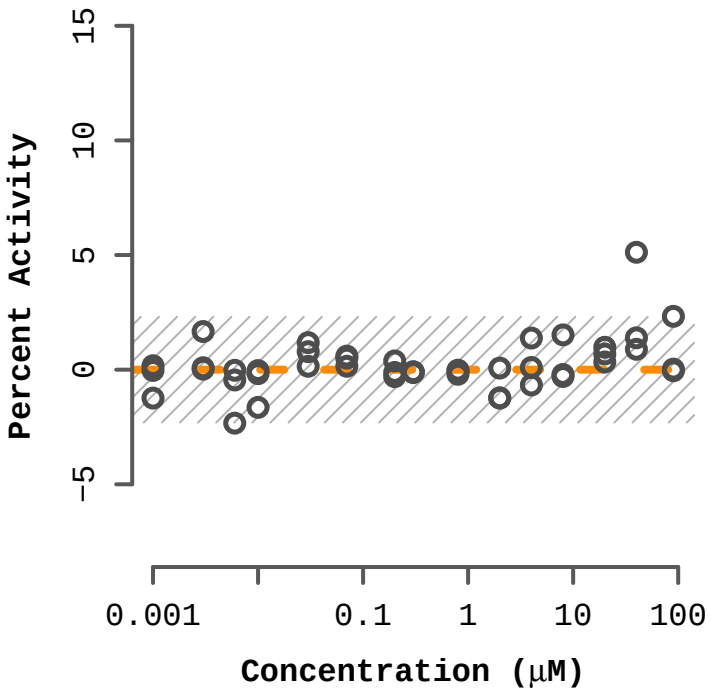
NAME: Dimethyl succinate
CHID: 25152 **CASRN:** 106-65-0
SPID(S): Tox21_300350
M4ID: 12478782

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 2.17 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

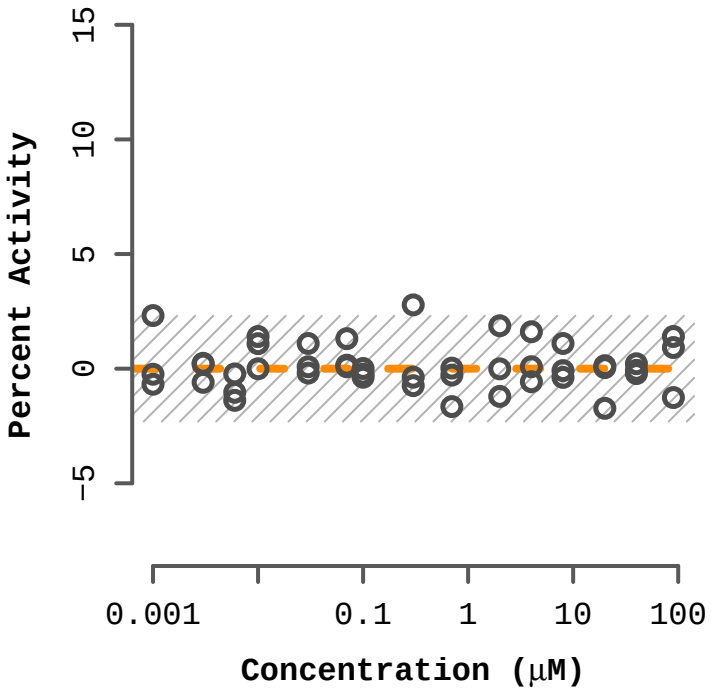
NAME: Dimethyl succinate
CHID: 25152 **CASRN:** 106-65-0
SPID(S): Tox21_202189
M4ID: 12480063

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 2.47 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

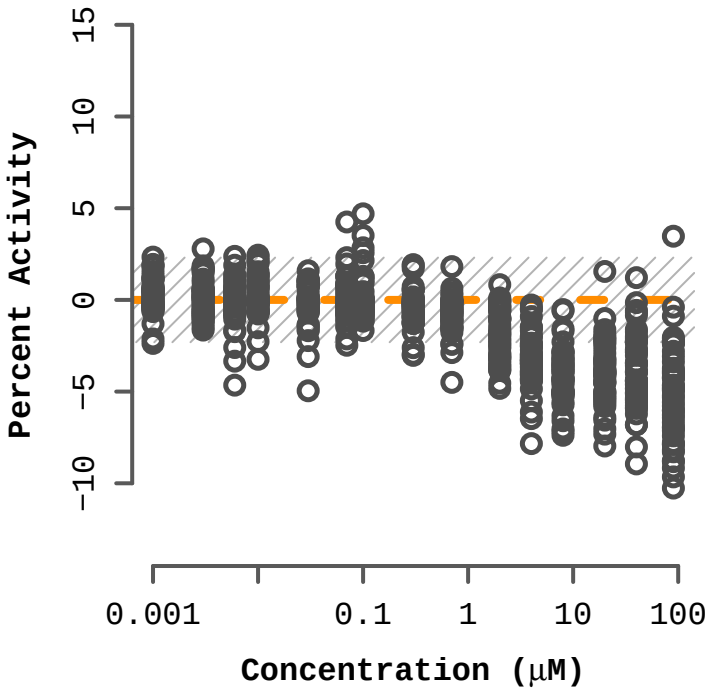
NAME: N,N'−Dimethylurea
CHID: 25156 **CASRN:** 96−31−1
SPID(S): Tox21_200794
M4ID: 12481458

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.832 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

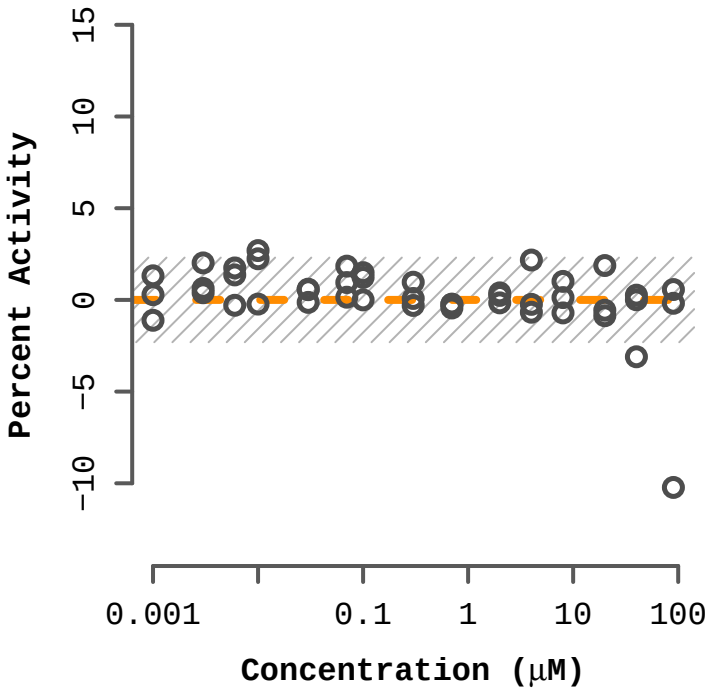
NAME: 1,3-Dinitronaphthalene
CHID: 25164 **CASRN:** 606-37-1
SPID(S): Tox21_400056
M4ID: 12475081

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3499.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 0.268 **MAX_MED:** 0.279 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

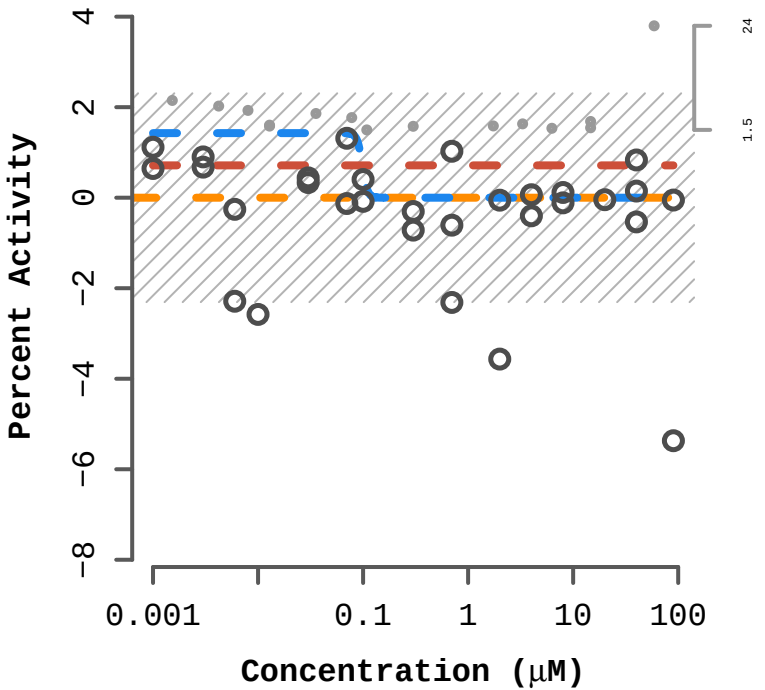
NAME: 1,5-Dinitronaphthalene
CHID: 25165 CASRN: 605-71-0
SPID(S): Tox21_200953
M4ID: 12481299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 1.57 MAX_MED: 2.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,8−Dinitronaphthalene
CHID: 25166 CASRN: 602−38−0
SPID(S): Tox21_202886
M4ID: 12479366 BRK

HILL MODEL (in red):

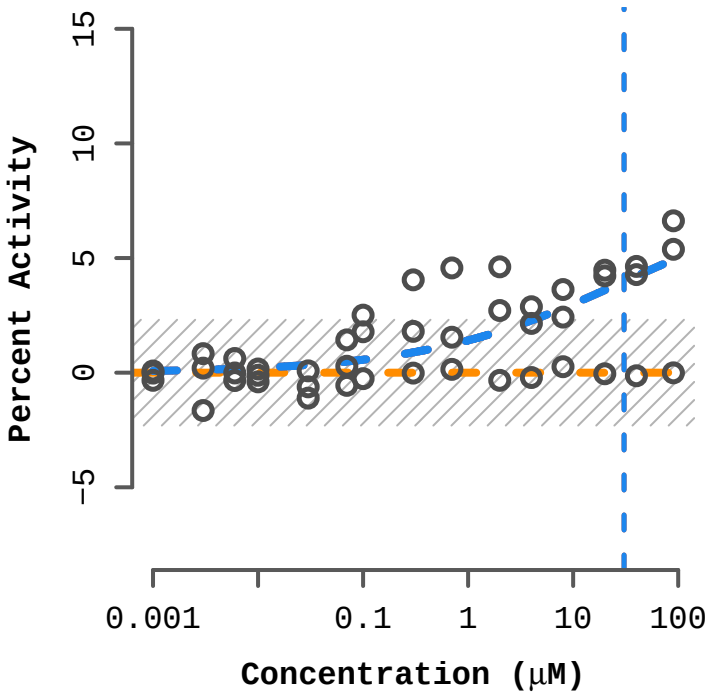
	tp	ga	gw
val:	0.714	−4.87	3.66
sd:	0.325	1290	2530

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.43	−4.99	3.13	−1.01	18
sd:	0.569	911	1420	0.0885	136

	CNST	HILL	GNLS
AIC:	228.01	229.24	231.13
PROB:	0.57	0.31	0.12
RMSE:	4.42	4.24	4.25

MAX_MEAN: 6.2 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 8-Hydroxy-5,7-dinitro-2-naphthalenesulfonic ac
CHID: 25167 CASRN: 483-84-1
SPID(S): Tox21_201142
M4ID: 12481110

HILL MODEL (in red):

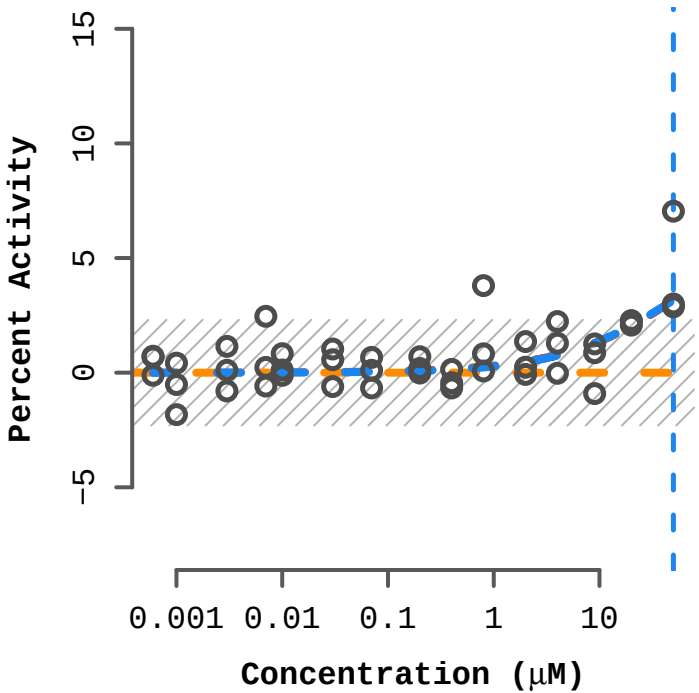
	tp	ga	gw
val:	7.95	1.48	0.449
sd:	6.03	1.46	0.168

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.95	1.48	0.449	3.9	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	208.31	178.42	182.42
PROB:	0	0.88	0.12
RMSE:	2.46	1.69	1.69

MAX_MEAN: 4 MAX_MED: 5.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Dioctyldiphenylamine
CHID: 25170 **CASRN:** 101−67−7
SPID(S): Tox21_303750
M4ID: 12475438

HILL MODEL (in red):

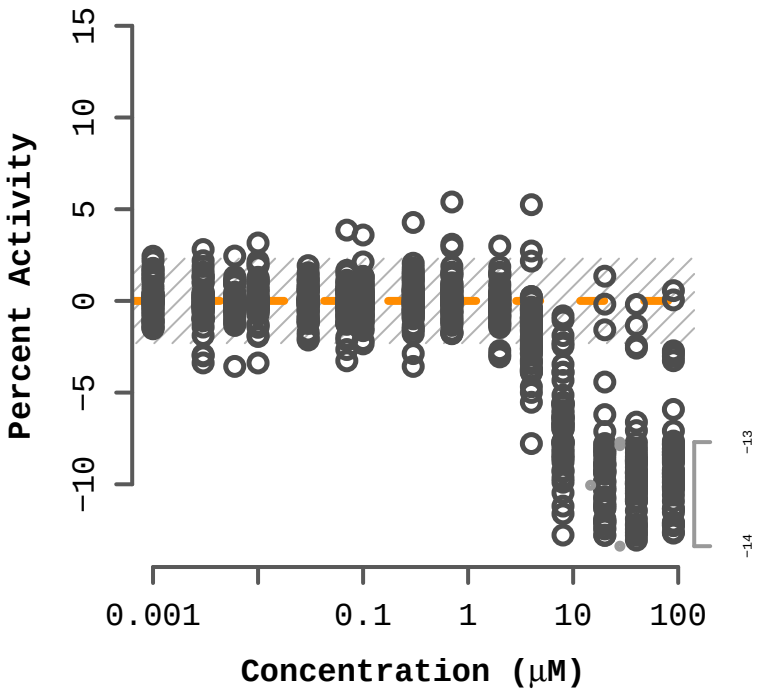
	tp	ga	gw
val:	8.45	2.01	0.709
sd:	13.3	1.65	0.377

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.32	1.7	0.793	3.29	3.26
sd:	6.67	1.1	0.422	591	941

	CNST	HILL	GNLS
AIC:	163.49	132.07	136.16
PROB:	0	0.89	0.11
RMSE:	1.67	1.11	1.11

MAX_MEAN: 4.31 **MAX_MED:** 3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

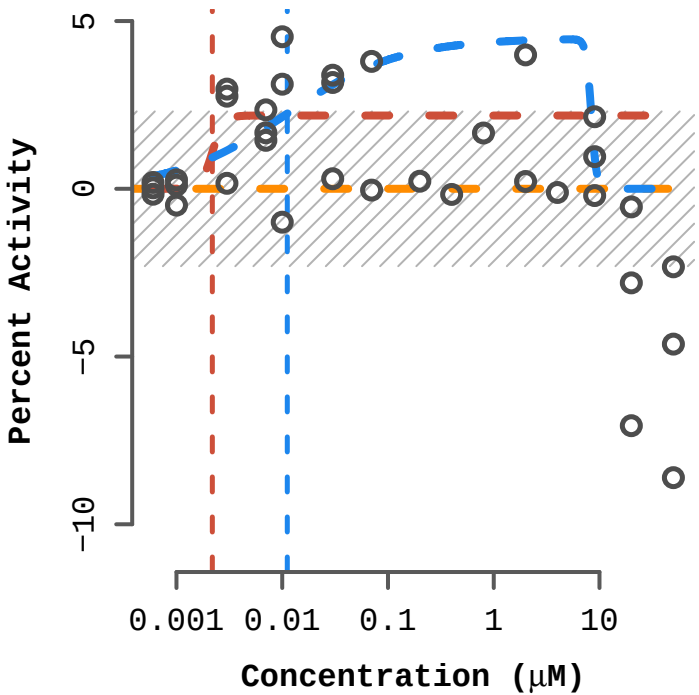
NAME: 1,3-Diphenylguanidine
CHID: 25178 **CASRN:** 102-06-7
SPID(S): Tox21_400041
M4ID: 12475096 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	4426.9	NA	NA
PROB:	1	NA	NA
RMSE:	4.83	NA	NA

MAX_MEAN: 0.202 **MAX_MED:** 0.0707 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3-Diphenylguanidine
CHID: 25178 CASRN: 102-06-7
SPID(S): Tox21_110998_1
M4ID: 12483956

HILL MODEL (in red):

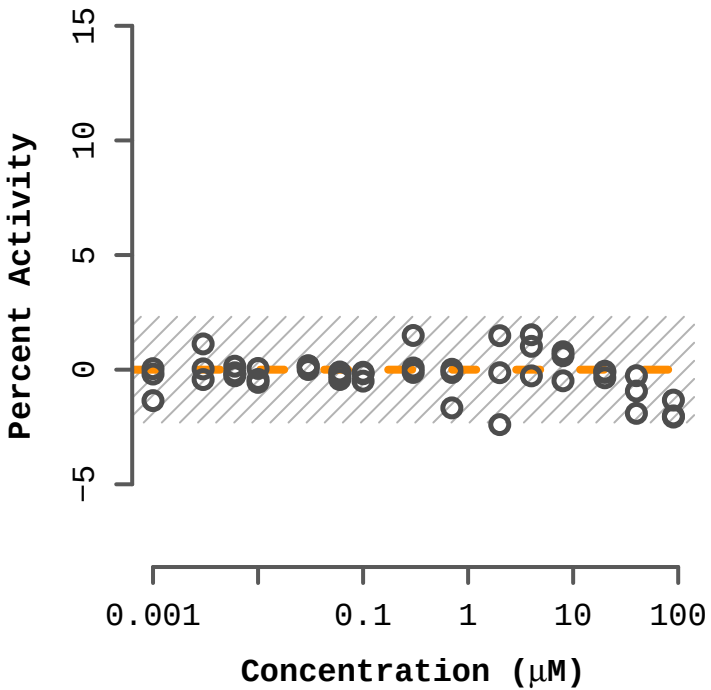
	tp	ga	gw
val:	2.18	−2.66	8
sd:	0.537	1.75	101

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.49	−1.95	0.818	0.922	17.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	249.41	239.7	222.63
PROB:	0	0	1
RMSE:	3.66	3.3	2.64

MAX_MEAN: 4.08 MAX_MED: 5.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

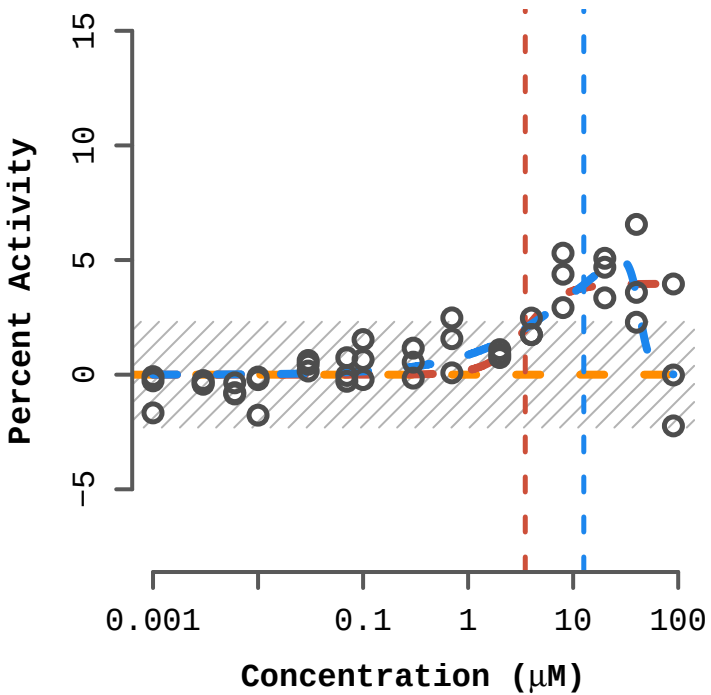
NAME: 4,4'−Diphenylmethane diisocyanate
CHID: 25180 CASRN: 101−68−8
SPID(S): Tox21_200268
M4ID: 12481984

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.759 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diphenylurea
CHID: 25183 CASRN: 102-07-8
SPID(S): Tox21_200068
M4ID: 12482184

HILL MODEL (in red):

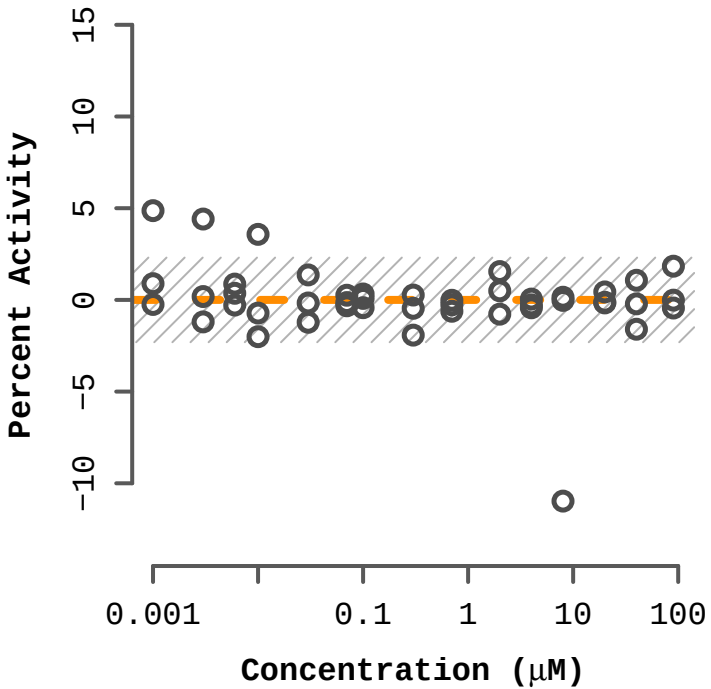
	tp	ga	gw
val:	3.96	0.544	2.38
sd:	0.409	0.0835	1.11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.86	1.1	0.824	1.63	8.26
sd:	6.28	0.88	0.456	0.0837	33.7

	CNST	HILL	GNLS
AIC:	199.88	150.65	142.63
PROB:	0	0.02	0.98
RMSE:	2.28	1.44	1.13

MAX_MEAN: 4.37 MAX_MED: 4.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

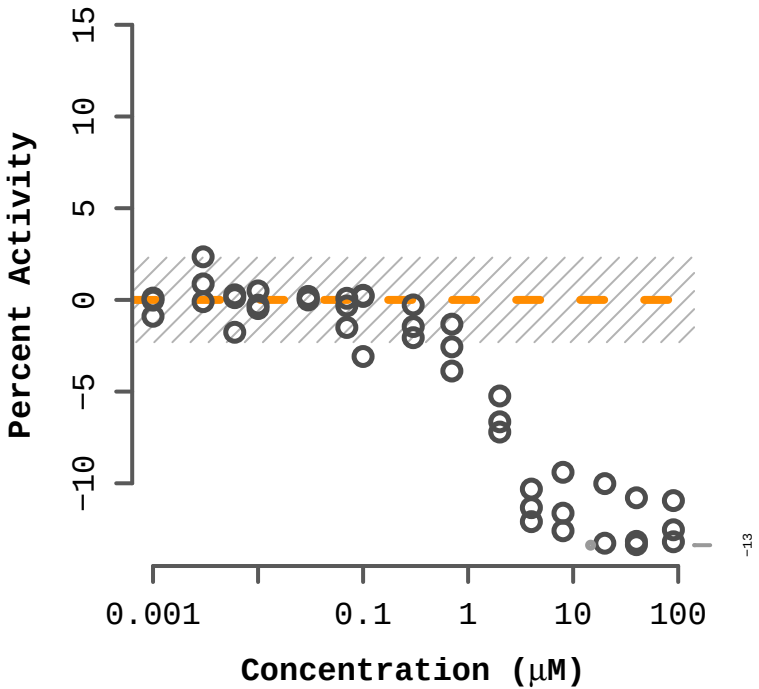
NAME: Dipropylamine
CHID: 25185 **CASRN:** 142-84-7
SPID(S): Tox21_202085
M4ID: 12480167

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 0.887 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

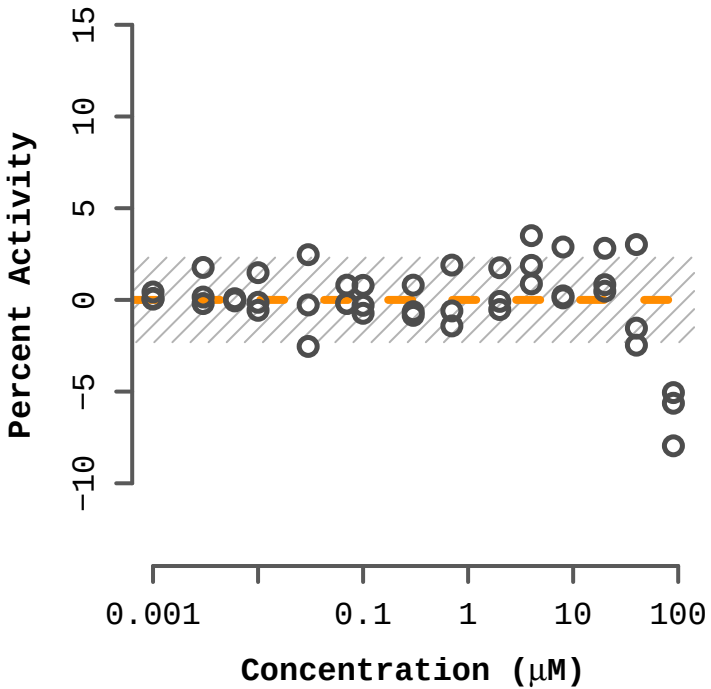
NAME: C.I. Direct Red 2
CHID: 25203 CASRN: 992-59-6
SPID(S): Tox21_202508
M4ID: 12479744 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	308.01	NA	NA
PROB:	1	NA	NA
RMSE:	7.17	NA	NA

MAX_MEAN: 1.04 MAX_MED: 0.874 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

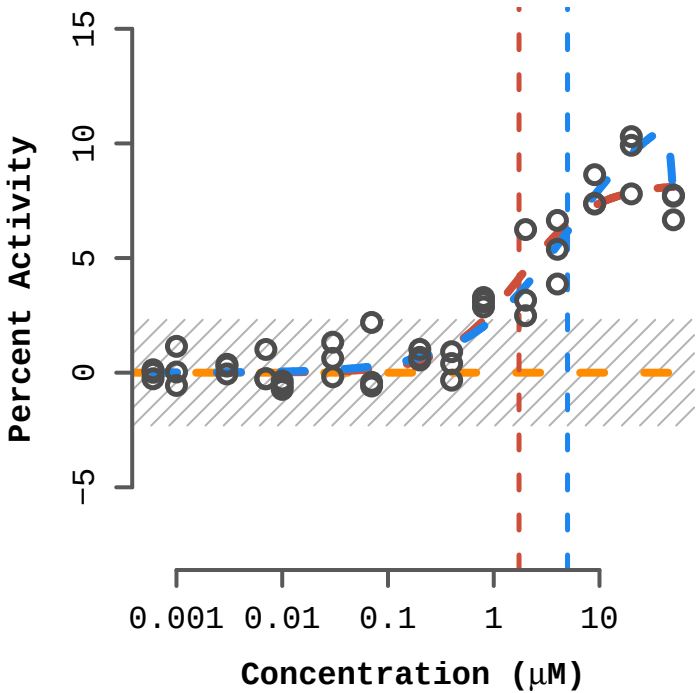
NAME: C.I. Disperse Blue 27
CHID: 25209 **CASRN:** 15791-78-3
SPID(S): Tox21_301887
M4ID: 12477246

HILL MODEL: Not applicable.

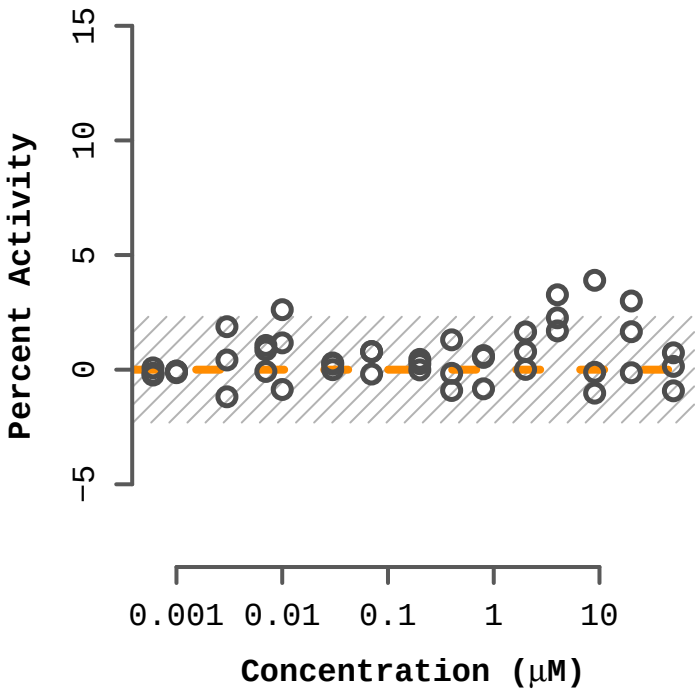
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 1.89 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    C.I. Disperse Red 60
CHID:    25210   CASRN: 17418-58-5
SPID(S): Tox21_303924
M4ID:    12475264

HILL MODEL (in red):
      tp       ga       gw
val:  8.24     0.239    1.24
sd:   0.514    0.112    0.204

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.3     0.698    0.891    1.72     17.1
sd:   2.27     0.222    0.154    0.00608  8.25

      CNST        HILL        GNLS
AIC:  256.01      136.06      129.7
PROB: 0           0.04        0.96
RMSE: 4.21        1           0.88

MAX_MEAN: 9.34      MAX_MED: 9.92      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

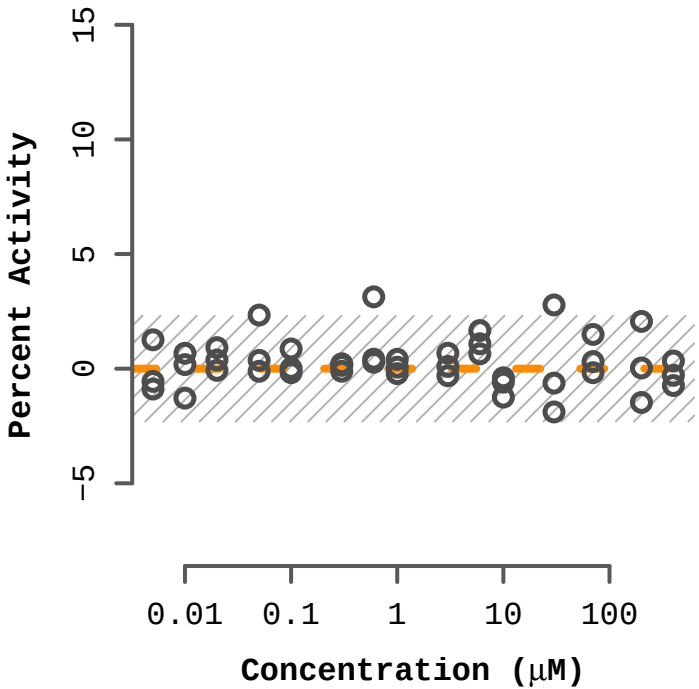
NAME: Diundecyl phthalate
CHID: 25215 **CASRN:** 3648-20-2
SPID(S): Tox21_202509
M4ID: 12479743

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 2.41 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

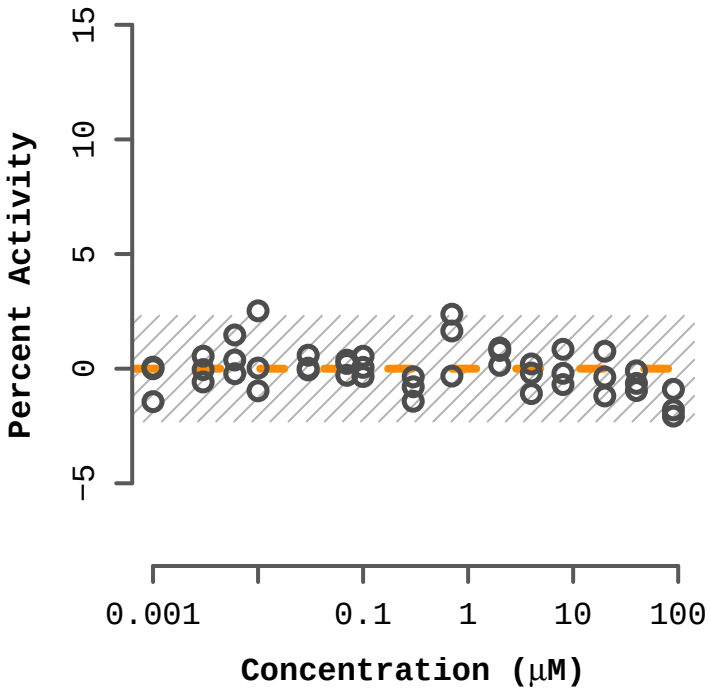
NAME: Divinylbenzene
CHID: 25216 **CASRN:** 1321-74-0
SPID(S): Tox21_302792
M4ID: 12476341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

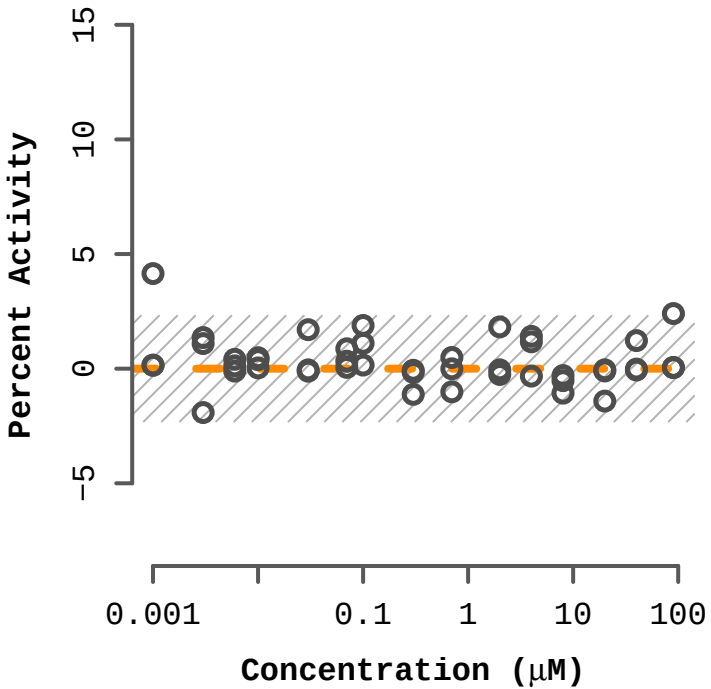
NAME: (2-Dodecenyl)succinic anhydride
CHID: 25217 **CASRN:** 19780-11-1
SPID(S): Tox21_303400
M4ID: 12475739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

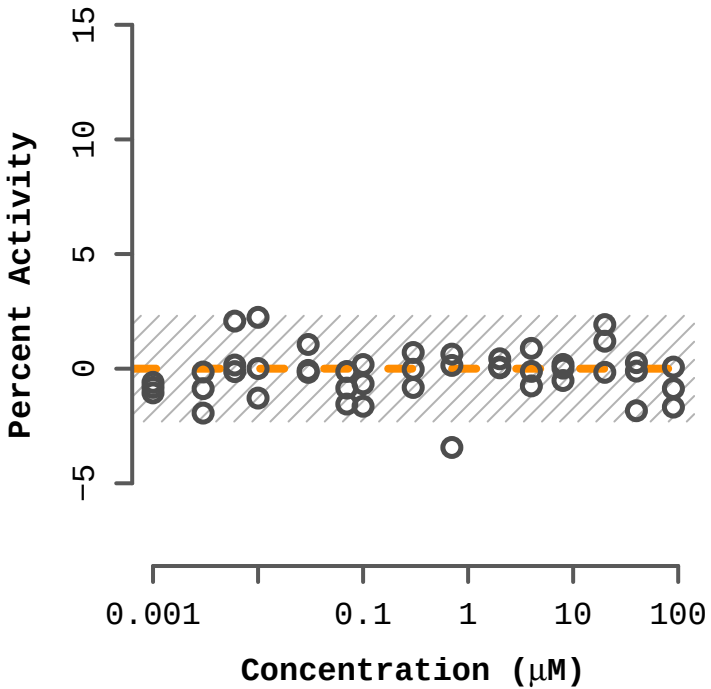
NAME: (2-Dodecenyl)succinic anhydride
CHID: 25217 **CASRN:** 19780-11-1
SPID(S): Tox21_202473
M4ID: 12479779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

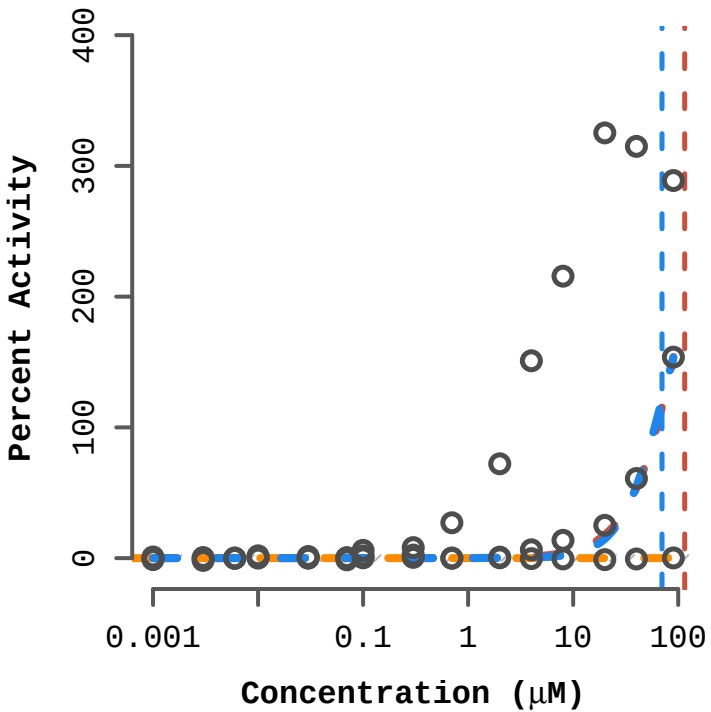
NAME: Sodium dodecylbenzenesulfonate
CHID: 25219 **CASRN:** 25155-30-0
SPID(S): Tox21_300506
M4ID: 12478626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.988 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium dodecylbenzenesulfonate
CHID: 25219 CASRN: 25155-30-0
SPID(S): Tox21_201718
M4ID: 12480534

HILL MODEL (in red):

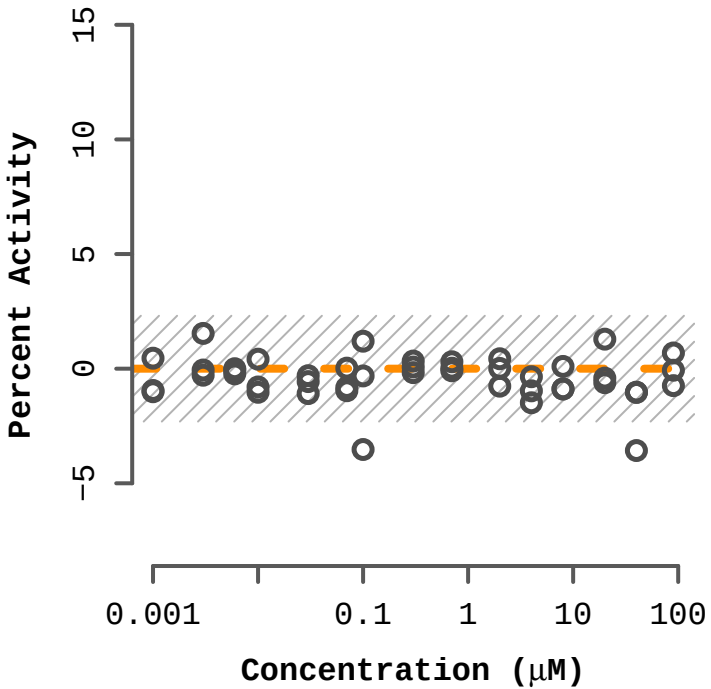
	tp	ga	gw
val:	390	2.06	1.74
sd:	158	0.179	0.358

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	242	1.85	2.18	3.95	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	482.16	475.88	480.17
PROB:	0.04	0.86	0.1
RMSE:	93.33	79.1	79.42

MAX_MEAN: 148 MAX_MED: 154 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

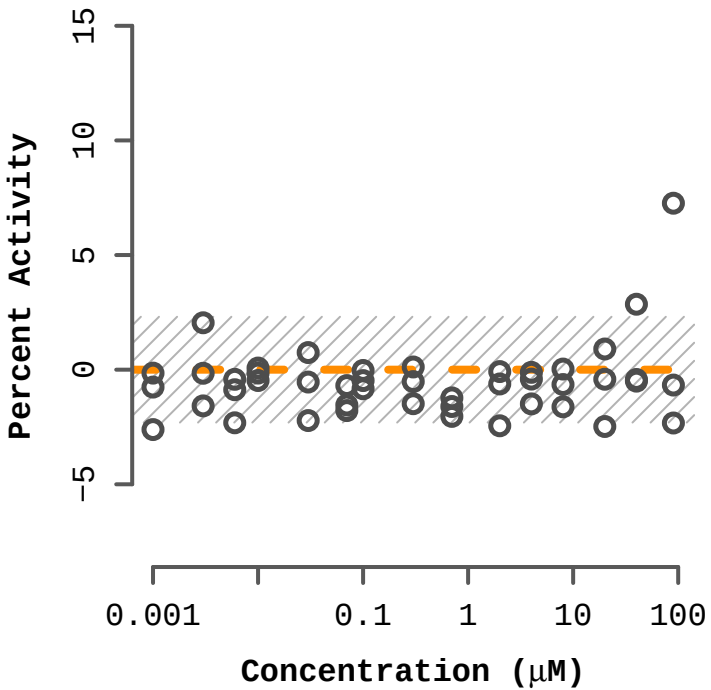
NAME: 1-Dodecanethiol
CHID: 25220 **CASRN:** 112-55-0
SPID(S): Tox21_303101
M4ID: 12476032

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.399 **MAX_MED:** 0.0739 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

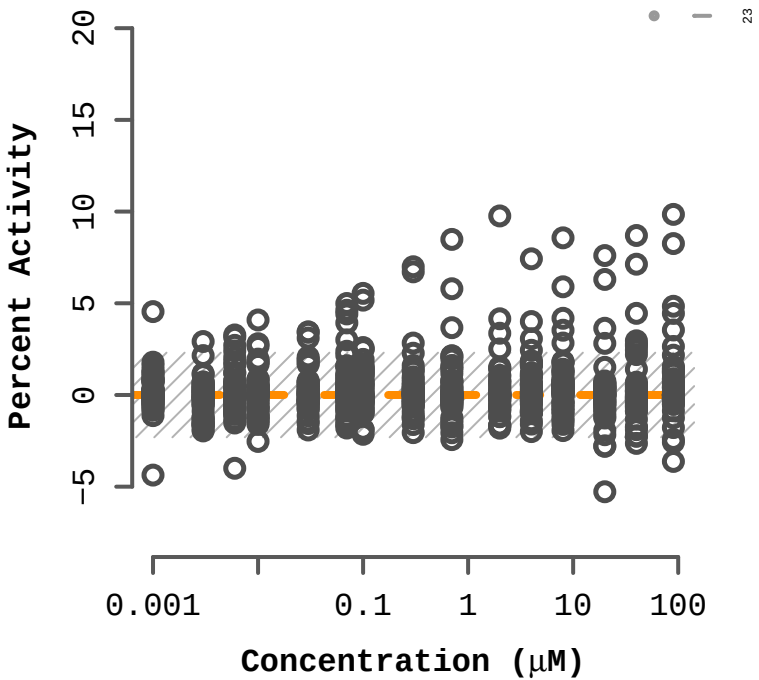
NAME: 1-Dodecanethiol
CHID: 25220 **CASRN:** 112-55-0
SPID(S): Tox21_201758
M4ID: 12480494

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** −0.146 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

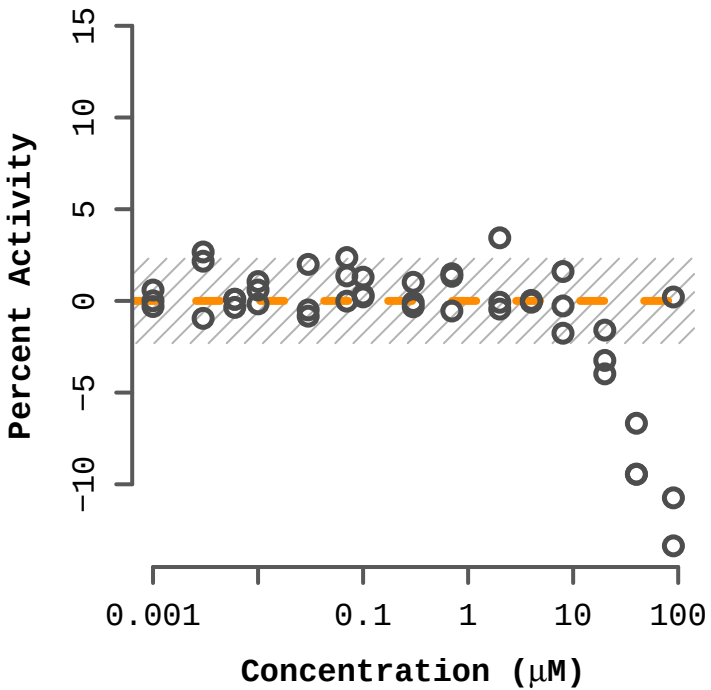
NAME: tert-Dodecanethiol
CHID: 25221 **CASRN:** 25103-58-6
SPID(S): Tox21_400018
M4ID: 12475119 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2486.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.407 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

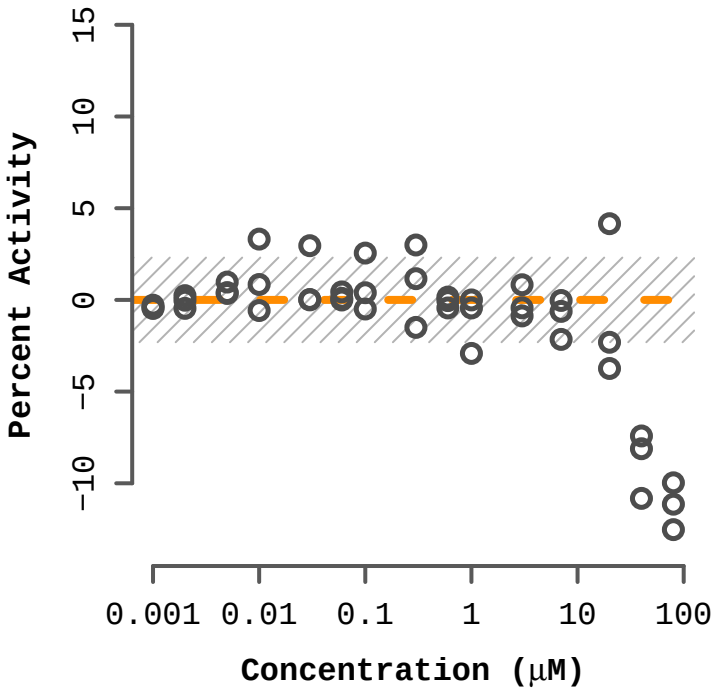
NAME: Econazole nitrate
CHID: 25226 **CASRN:** 24169-02-6
SPID(S): Tox21_303391
M4ID: 12475747

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.82	NA	NA
PROB:	1	NA	NA
RMSE:	3.65	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

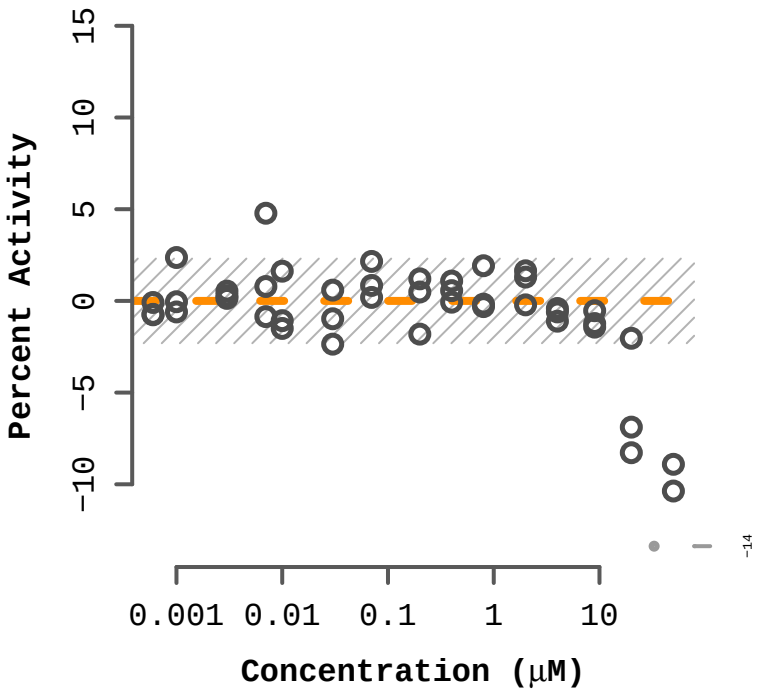
NAME: Econazole nitrate
CHID: 25226 **CASRN:** 24169-02-6
SPID(S): Tox21_200771
M4ID: 12481481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.77	NA	NA
PROB:	1	NA	NA
RMSE:	3.98	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

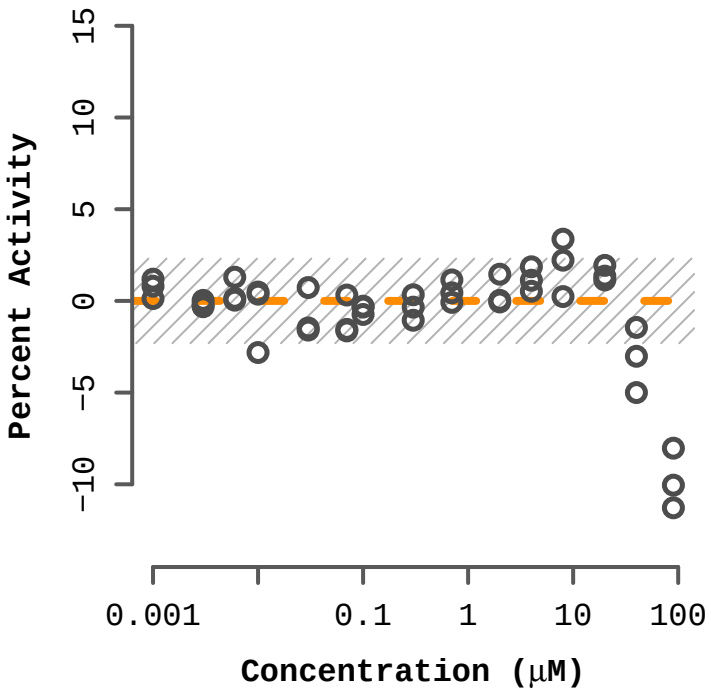
NAME: Econazole nitrate
CHID: 25226 **CASRN:** 24169-02-6
SPID(S): Tox21_110852_1
M4ID: 12484068 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.35	NA	NA
PROB:	1	NA	NA
RMSE:	3.56	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

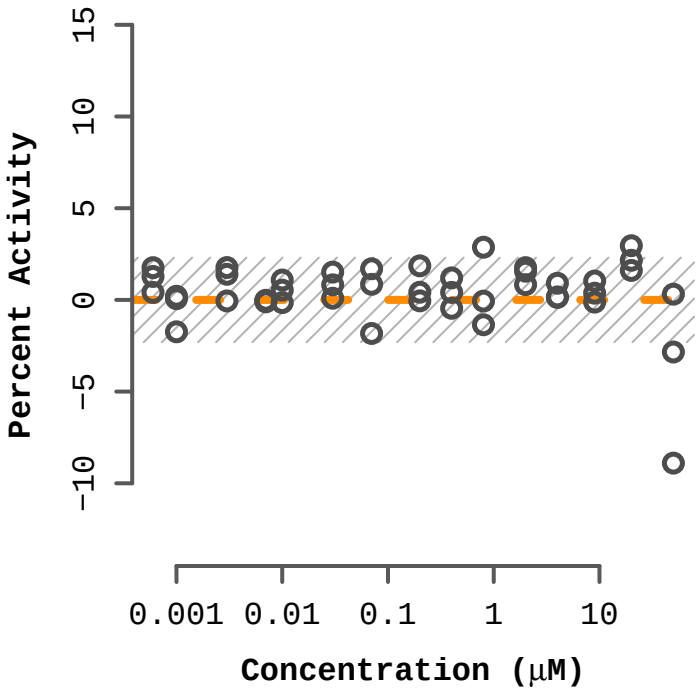
NAME: Emodin
CHID: 25231 **CASRN:** 518-82-1
SPID(S): Tox21_303218
M4ID: 12475915

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

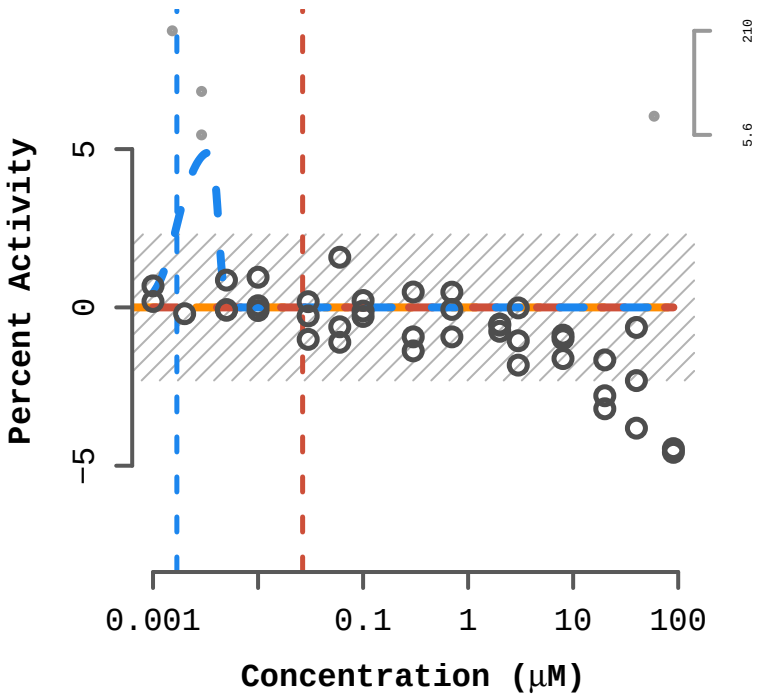
NAME: Emodin
CHID: 25231 **CASRN:** 518-82-1
SPID(S): Tox21_202999
M4ID: 12479253

HILL MODEL: Not applicable.

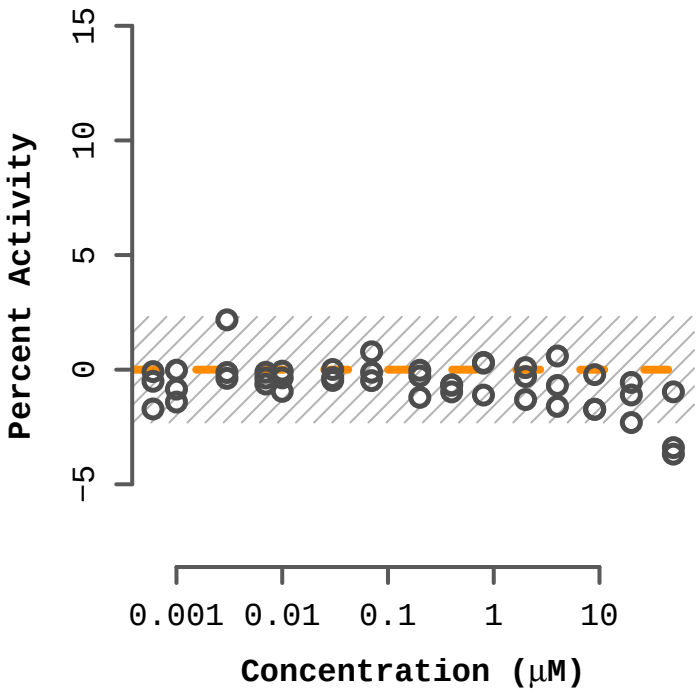
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 2.16 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Eosin
CHID:    25234   CASRN: 17372-87-1
SPID(S): Tox21_302152
M4ID:    12476981  BRK

HILL MODEL (in red):
      tp        ga        gw
val:  2.72e-10 -1.58     1.99
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  5.19      -2.77     4.46      -2.38     17.9
sd:   NaN       NaN       NaN       NaN       NaN

      CNST         HILL         GNLS
AIC:  275.19       281.19       283.52
PROB: 0.94         0.05         0.01
RMSE: 34.07        34.07        33.8

MAX_MEAN: 68.9      MAX_MED: 5.64      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

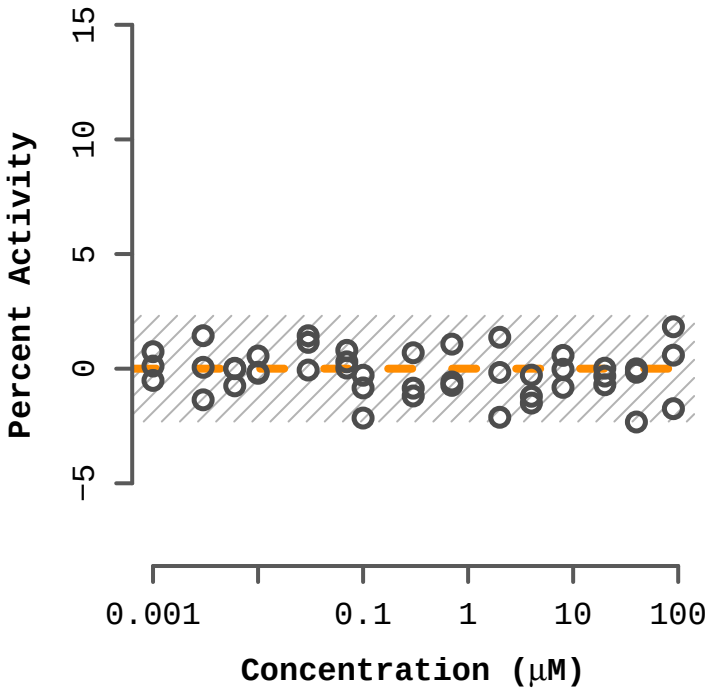
NAME: Eosin
CHID: 25234 **CASRN:** 17372-87-1
SPID(S): Tox21_112323_1
M4ID: 12483163

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.559 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

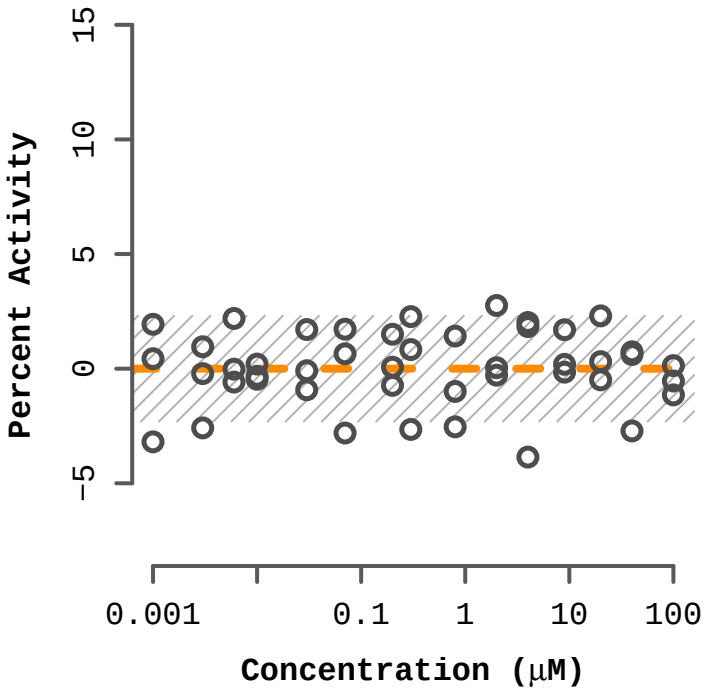
NAME: Epibromohydrin
CHID: 25237 **CASRN:** 3132-64-7
SPID(S): Tox21_202607
M4ID: 12479645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.843 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

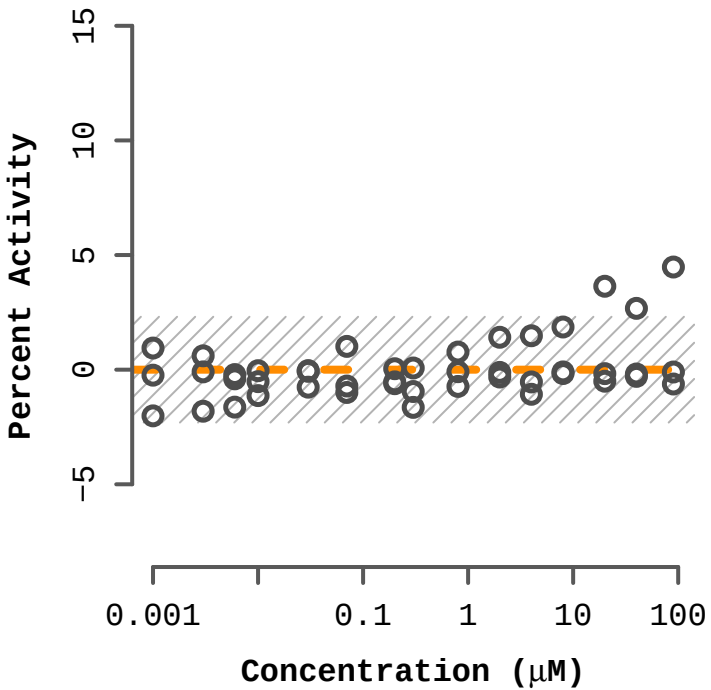
NAME: 1,2-Epoxy-3-butene
CHID: 25240 **CASRN:** 930-22-3
SPID(S): Tox21_200871
M4ID: 12481381

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 0.84 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

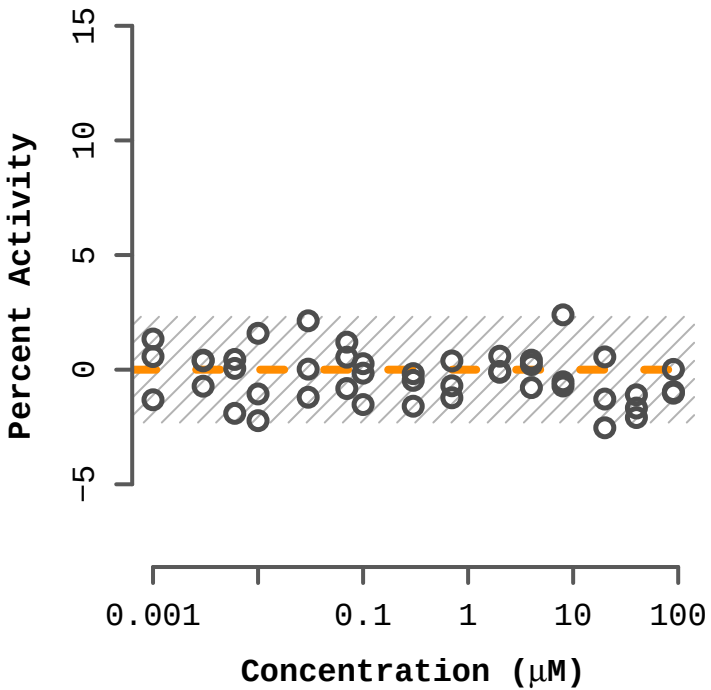
NAME: 1,2-Epoxydecane
CHID: 25242 **CASRN:** 2404-44-6
SPID(S): Tox21_200306
M4ID: 12481946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** −0.0709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

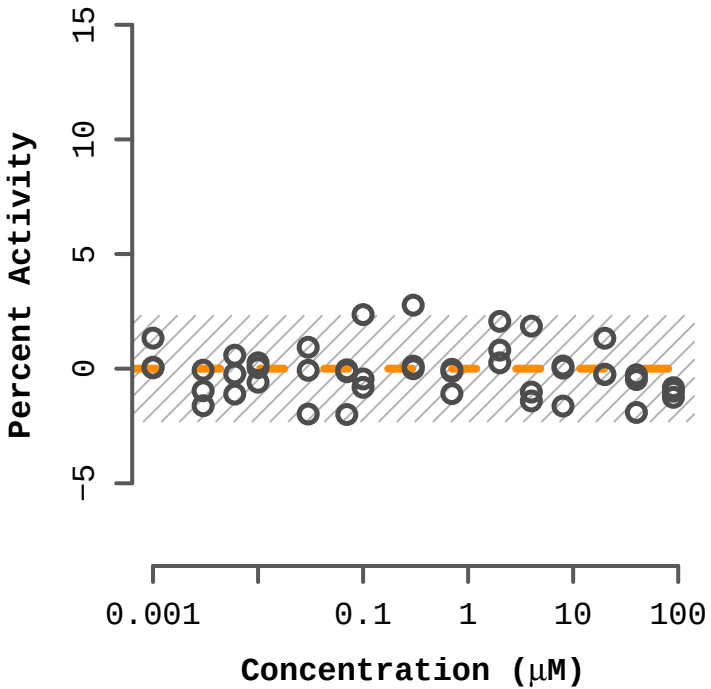
NAME: 1,2-Epoxydodecane
CHID: 25243 **CASRN:** 2855-19-8
SPID(S): Tox21_301660
M4ID: 12477473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.386 **MAX_MED:** 0.574 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

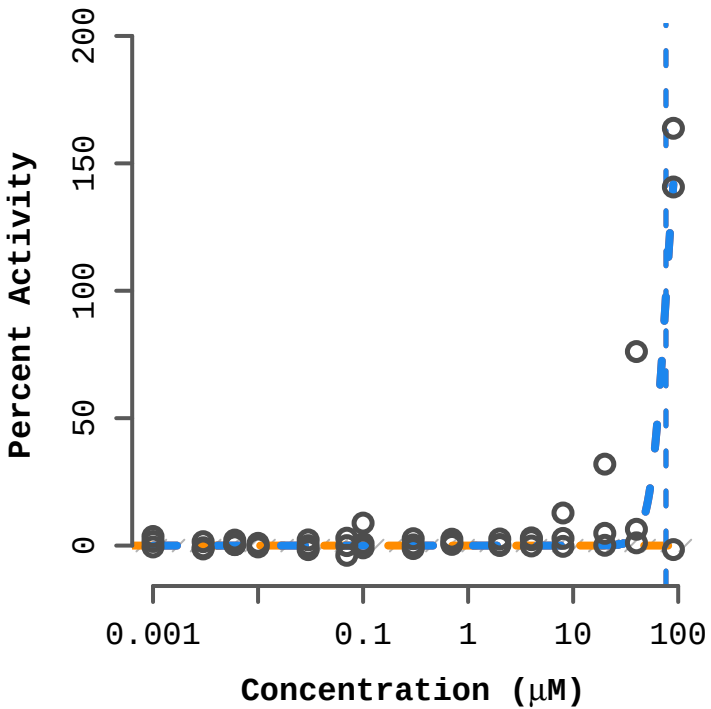
NAME: 1,2-Epoxyhexadecane
CHID: 25245 **CASRN:** 7320-37-8
SPID(S): Tox21_201042
M4ID: 12481210

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Epoxytetradecane
CHID: 25249 CASRN: 3234-28-4
SPID(S): Tox21_200250
M4ID: 12482002

HILL MODEL (in red):

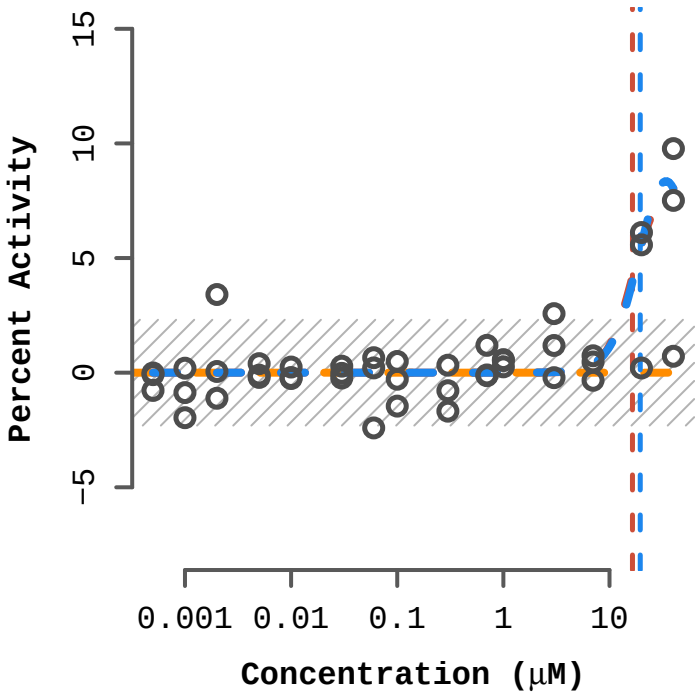
	tp	ga	gw
val:	197	1.88	5.87
sd:	9.83	0.0091	0.935

GAIN-LOSS MODEL (in blue):

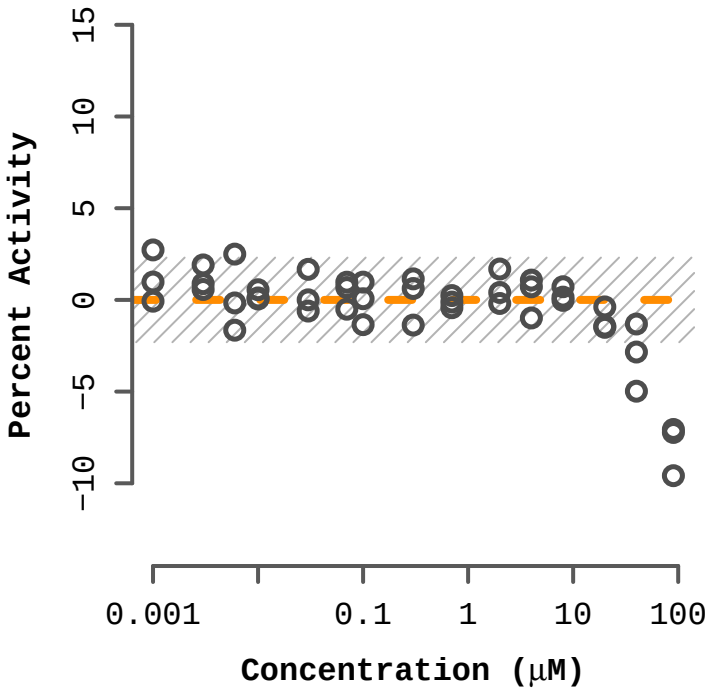
	tp	ga	gw	la	lw
val:	196	1.88	5.87	3.95	10.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	330.45	313.78	317.78
PROB:	0	0.88	0.12
RMSE:	34.6	24.78	24.78

MAX_MEAN: 101 MAX_MED: 141 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ergotamine D-tartrate
CHID:    25253   CASRN: 379-79-3
SPID(S): Tox21_303182
M4ID:    12475951

HILL MODEL (in red):
      tp       ga       gw
val:  8.36     1.22     3.62
sd:   1.2      0.0588   1.54

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.9     1.29     3.24     1.75     4.21
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  177.88      156.31      160.28
PROB: 0           0.88        0.12
RMSE: 2.42        1.69        1.68

MAX_MEAN: 6         MAX_MED: 7.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

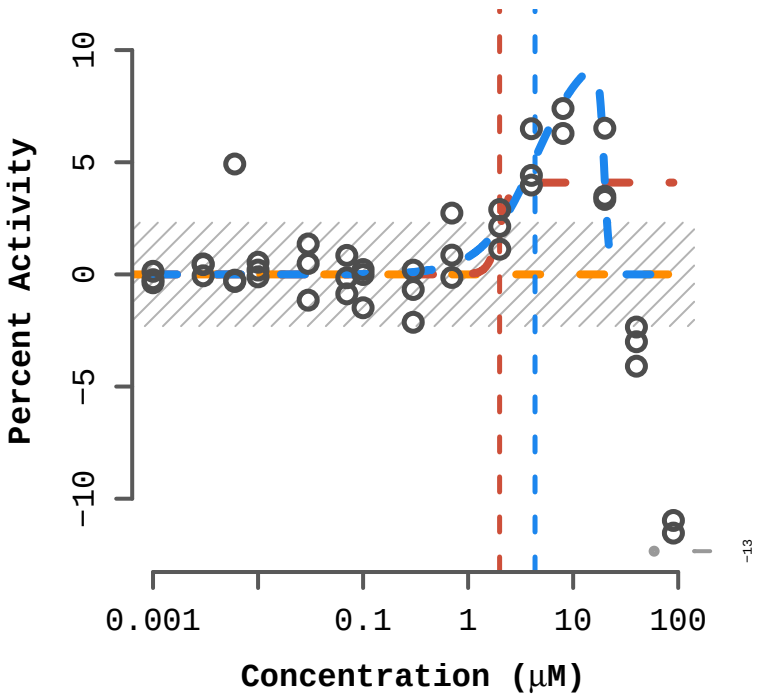
NAME: Ergotamine D−tartrate
CHID: 25253 **CASRN:** 379−79−3
SPID(S): Tox21_201705
M4ID: 12480547

HILL MODEL: Not applicable.

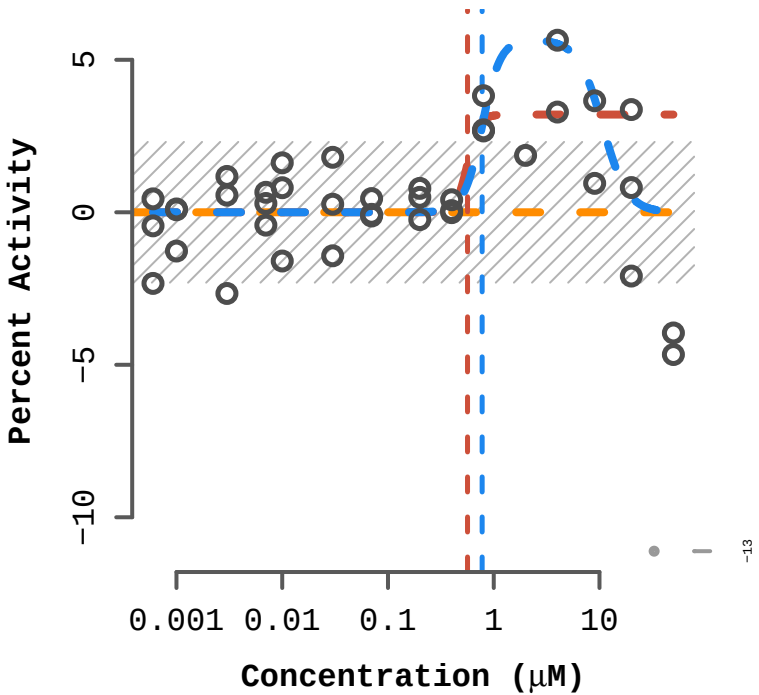
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.57	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.976 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ethacrynic acid
CHID:    25257   CASRN: 58-54-8
SPID(S): Tox21_201102
M4ID:    12481150  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  4.09     0.3      8
sd:   0.892    0.0619   15.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.3     0.637    1.71     1.29     17.8
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  253.86      248.08      216.39
PROB: 0           0           1
RMSE: 4.39        4.8         3.39

MAX_MEAN: 8.26      MAX_MED: 7.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethacrynic acid
CHID: 25257 CASRN: 58-54-8
SPID(S): Tox21_110335_1
M4ID: 12484445 BRK

HILL MODEL (in red):

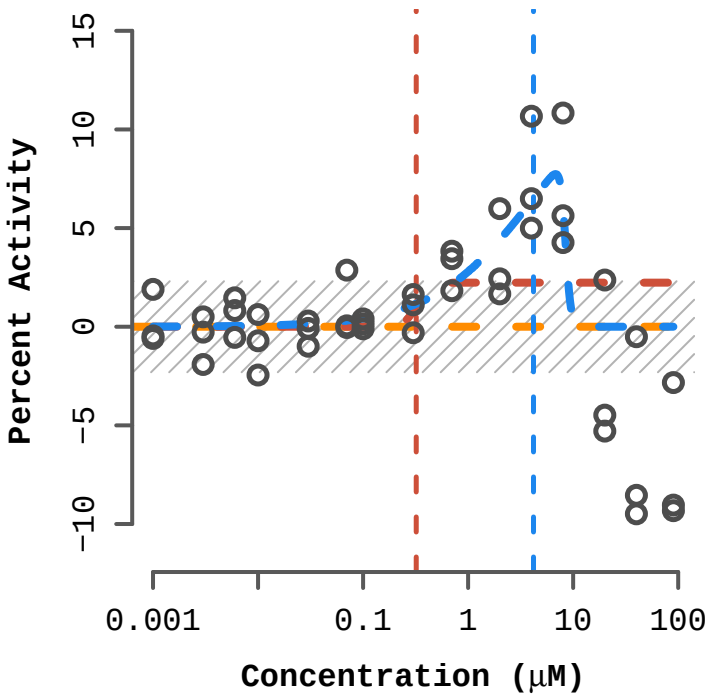
	tp	ga	gw
val:	3.2	−0.248	8
sd:	0.716	0.193	10

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.67	−0.11	5.12	1.03	3.71
sd:	0.85	0.052	6.28	0.125	2.61

	CNST	HILL	GNLS
AIC:	231.12	217.28	199.93
PROB:	0	0	1
RMSE:	3.42	3.33	2.53

MAX_MEAN: 5.75 MAX_MED: 6.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethidium bromide
CHID: 25258 CASRN: 1239-45-8
SPID(S): Tox21_202511
M4ID: 12479741

HILL MODEL (in red):

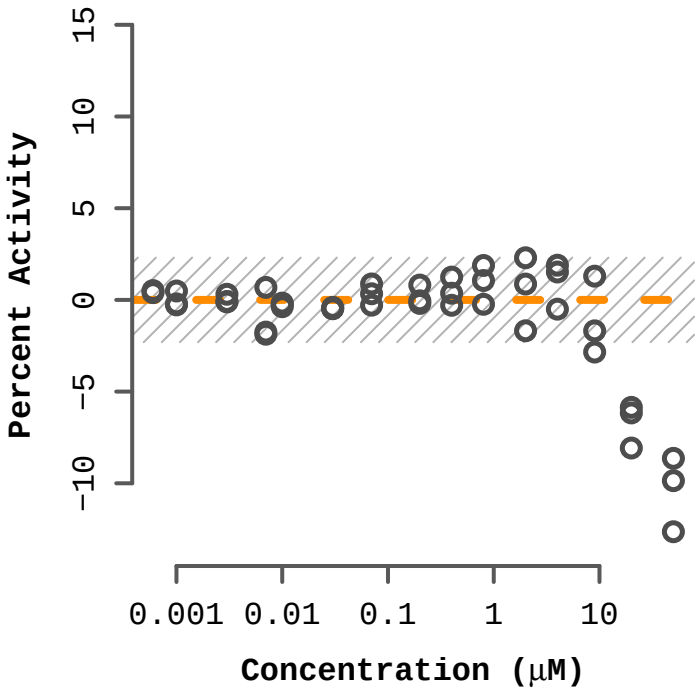
	tp	ga	gw
val:	2.23	-0.494	8
sd:	0.945	0.177	29.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13	0.622	0.904	0.927	17.7
sd:	18.4	1.26	0.483	0.294	214

	CNST	HILL	GNLS
AIC:	258.22	259.63	234.78
PROB:	0	0	1
RMSE:	4.34	4.43	3.29

MAX_MEAN: 7.39 MAX_MED: 6.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

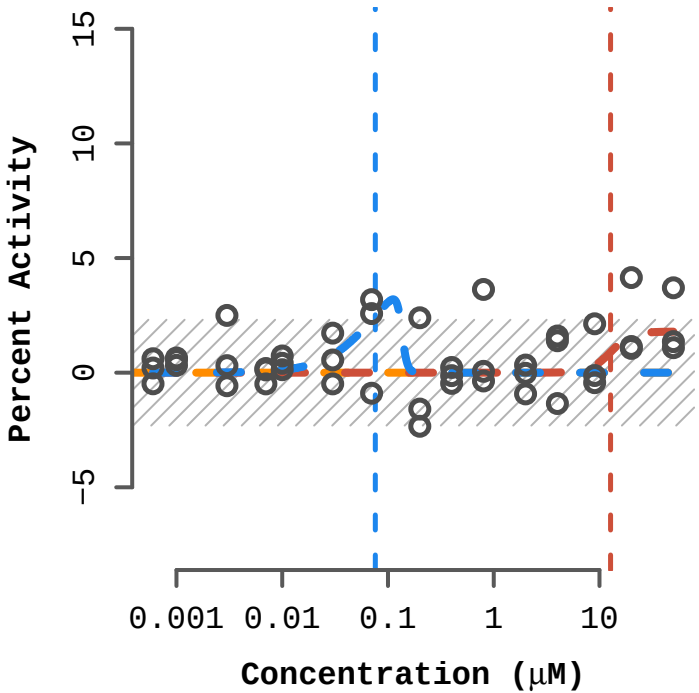
NAME: Ethidium bromide
CHID: 25258 **CASRN:** 1239-45-8
SPID(S): Tox21_111410_1
M4ID: 12483706

HILL MODEL: Not applicable.

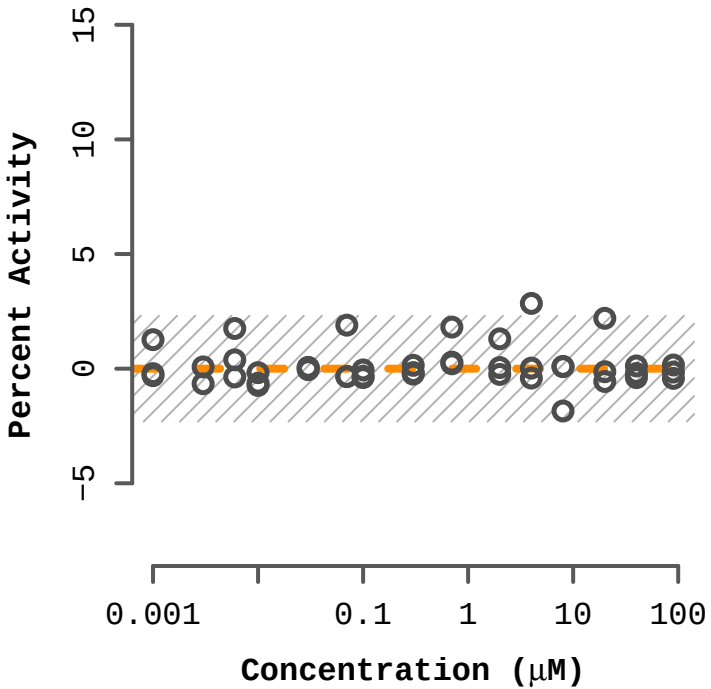
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.65	NA	NA
PROB:	1	NA	NA
RMSE:	3.42	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.52 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cinoxate
CHID:    25264   CASRN: 104-28-9
SPID(S): Tox21_113675
M4ID:    12482539

HILL MODEL (in red):
      tp       ga       gw
val:  1.79     1.1      4.53
sd:   0.751    0.26     9.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.95     -1.12    1.82     -0.87    17.9
sd:   13.6     1.26     2.79     0.719    75.3

      CNST        HILL        GNLS
AIC:  165.46      159.85      170.28
PROB: 0.06        0.94        0.01
RMSE: 1.54        1.34        1.48

MAX_MEAN: 2.12      MAX_MED: 2.58      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

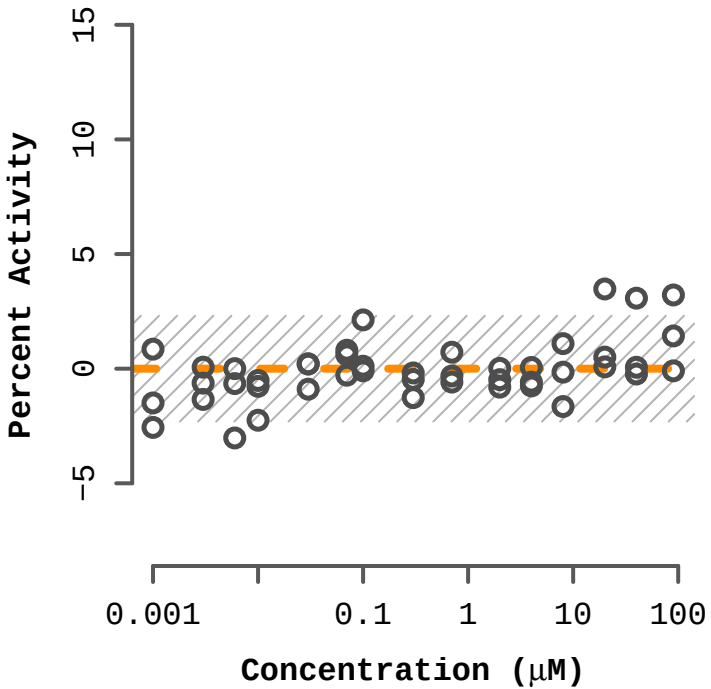
NAME: 3-Ethylamino-4-methylphenol
CHID: 25269 **CASRN:** 120-37-6
SPID(S): Tox21_201008
M4ID: 12481244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.822 **MAX_MED:** 0.387 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

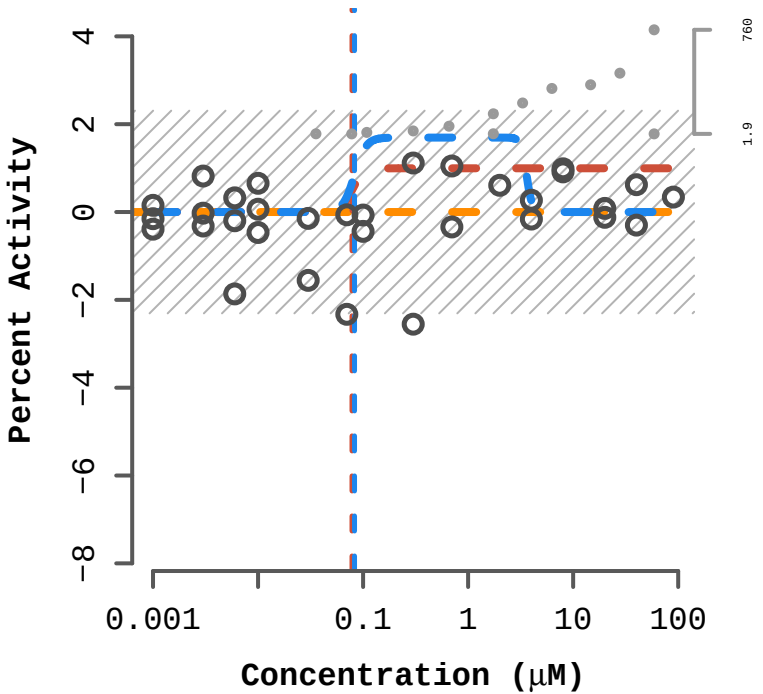
NAME: N-Ethylaniline
CHID: 25271 **CASRN:** 103-69-5
SPID(S): Tox21_300605
M4ID: 12478528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Ethylaniline
CHID: 25271 **CASRN:** 103-69-5
SPID(S): Tox21_201766
M4ID: 12480486 **BRK**

HILL MODEL (in red):

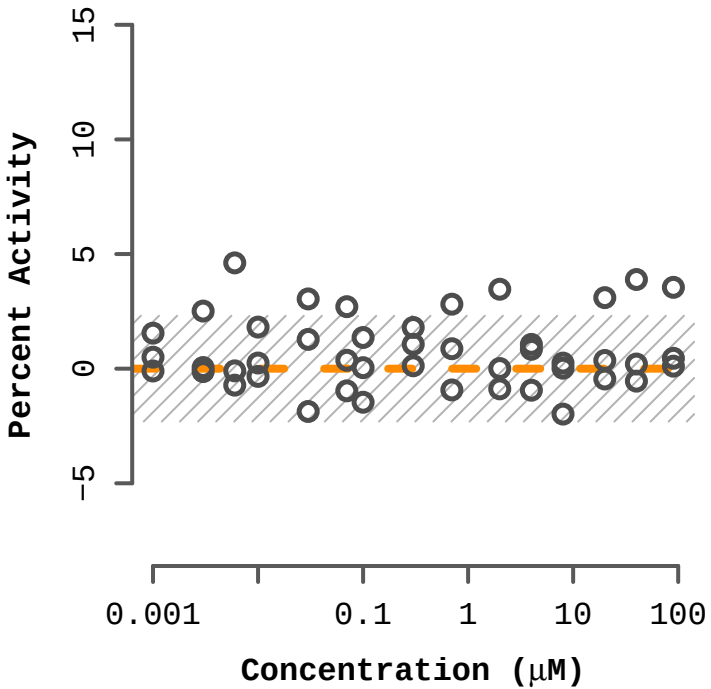
	tp	ga	gw
val:	0.996	−1.11	8
sd:	1.09	0.37	36.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.69	−1.08	8	0.556	16.4
sd:	1.86	0.268	27.4	2.27	807

	CNST	HILL	GNLS
AIC:	479.74	484.76	488.69
PROB:	0.92	0.07	0.01
RMSE:	156.24	155.9	156.17

MAX_MEAN: 255 **MAX_MED:** 2.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

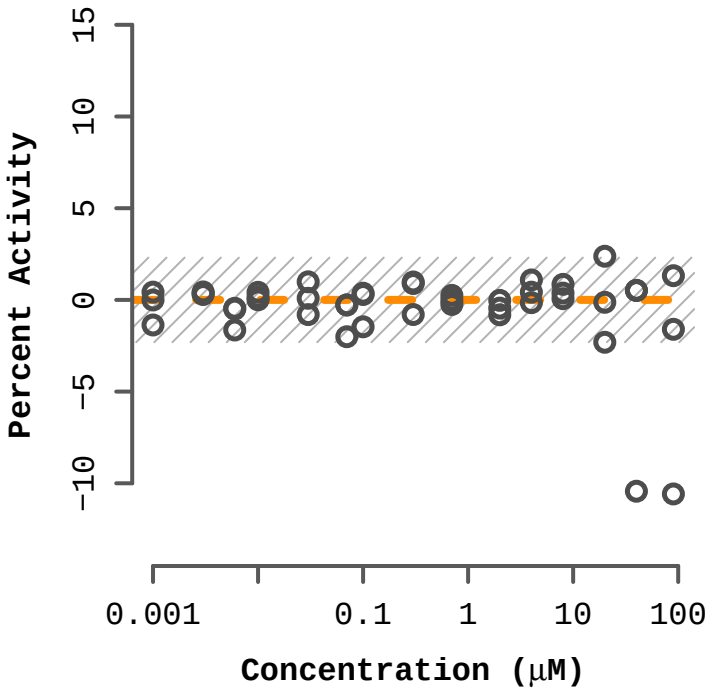
NAME: Ethyl anthranilate
CHID: 25272 **CASRN:** 87-25-2
SPID(S): Tox21_303197
M4ID: 12475936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

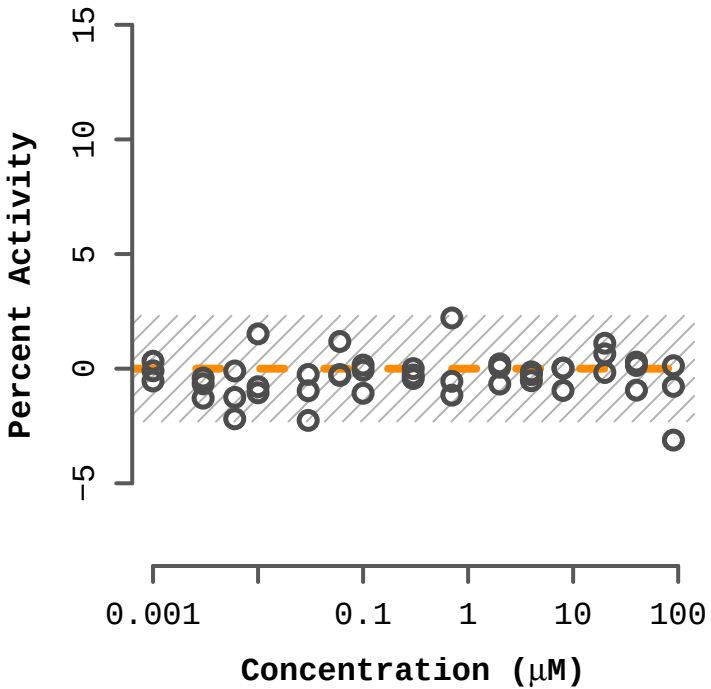
NAME: Ethyl anthranilate
CHID: 25272 **CASRN:** 87-25-2
SPID(S): Tox21_202019
M4ID: 12480233

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.1	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 0.454 **MAX_MED:** 0.894 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

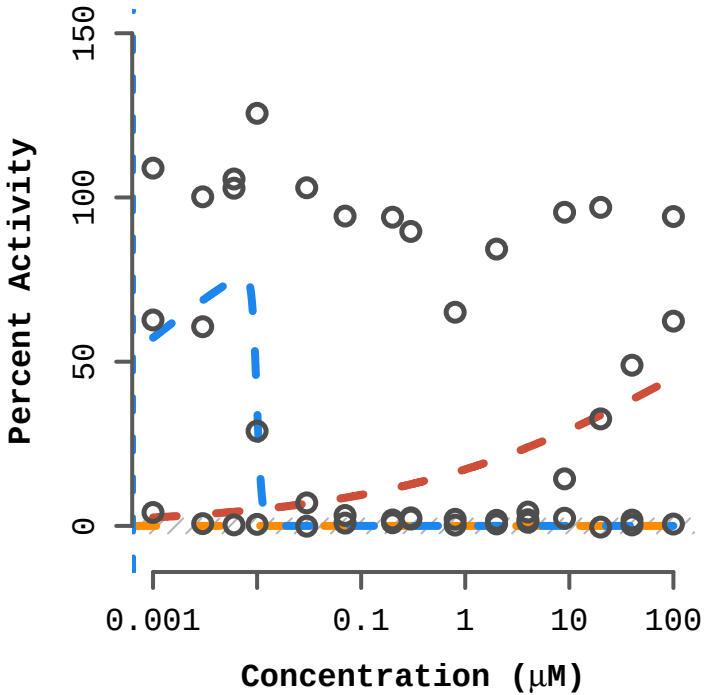
NAME: N-Ethyl-N-butylamine
CHID: 25276 CASRN: 13360-63-9
SPID(S): Tox21_201096
M4ID: 12481156

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.531 MAX_MED: 0.647 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: S-Ethyl chlorothioformic acid
CHID: 25278 CASRN: 2941-64-2
SPID(S): Tox21_201225
M4ID: 12481027

HILL MODEL (in red):

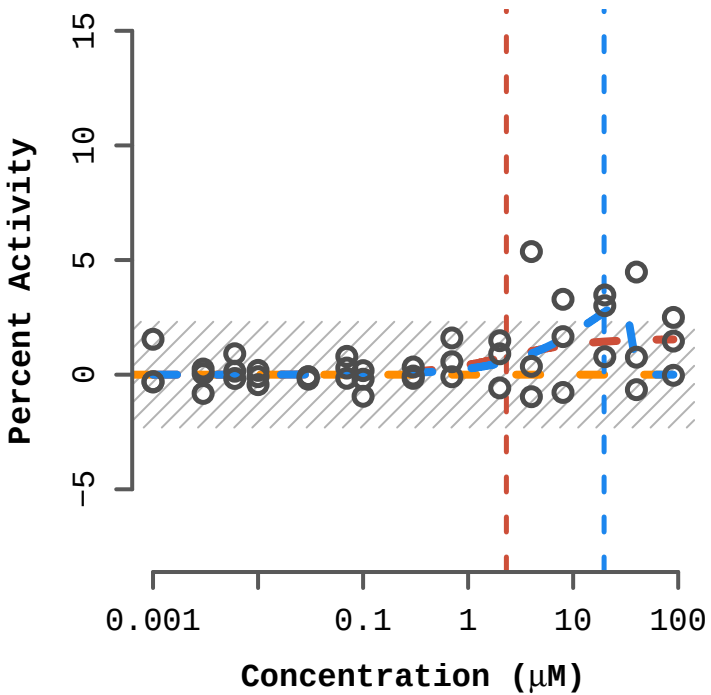
	tp	ga	gw
val:	98.9	2.25	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	105	-3.19	0.411	-2	18
sd:	223	5.29	1.27	0.0627	205

	CNST	HILL	GNLS
AIC:	495.34	491.42	490.79
PROB:	0.06	0.4	0.55
RMSE:	57.86	51.6	49.57

MAX_MEAN: 69.6 MAX_MED: 103 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl cyanoacrylate
CHID: 25279 CASRN: 7085-85-0
SPID(S): Tox21_303235
M4ID: 12475898

HILL MODEL (in red):

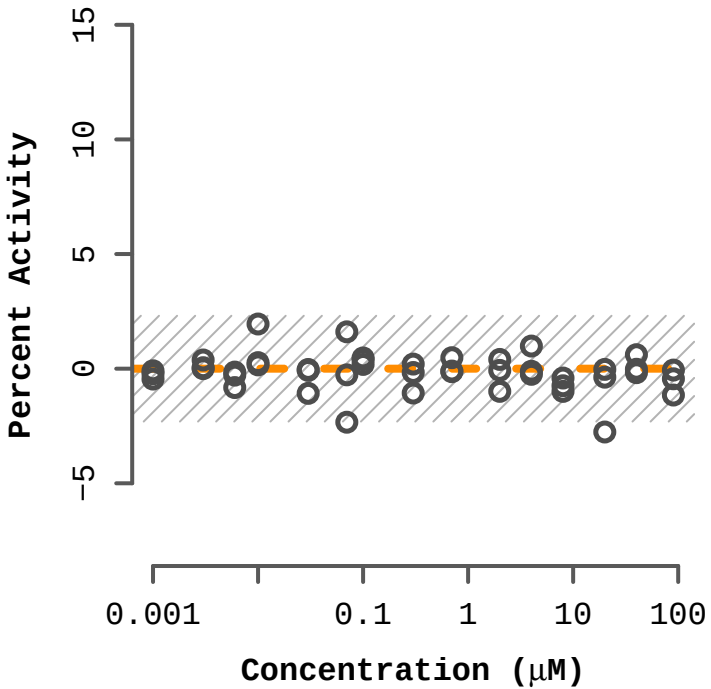
	tp	ga	gw
val:	1.56	0.364	1.16
sd:	0.539	0.514	0.842

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.44	1.29	1	1.55	14.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.48	146.45	149.85
PROB:	0.01	0.84	0.15
RMSE:	1.55	1.22	1.27

MAX_MEAN: 2.42 **MAX_MED:** 3.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

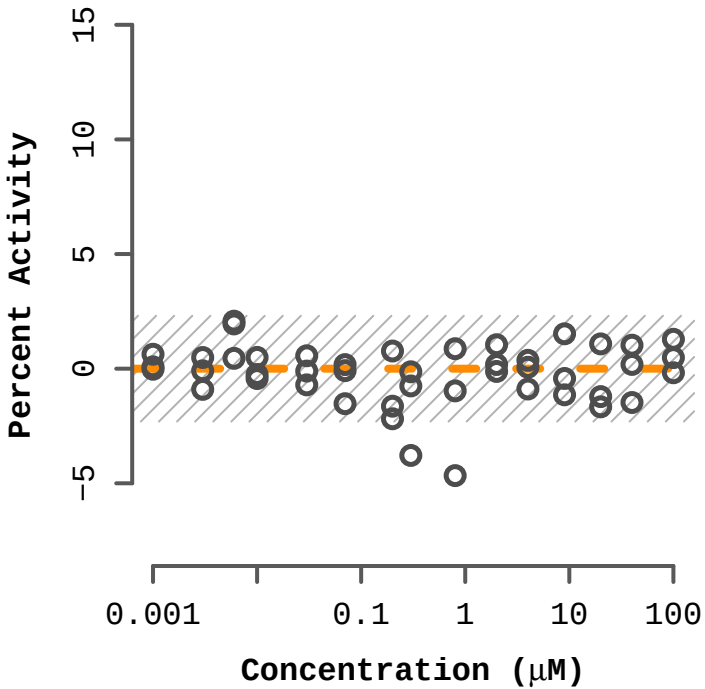
NAME: Ethyl cyanoacrylate
CHID: 25279 **CASRN:** 7085-85-0
SPID(S): Tox21_202453
M4ID: 12479799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.794 **MAX_MED:** 0.395 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

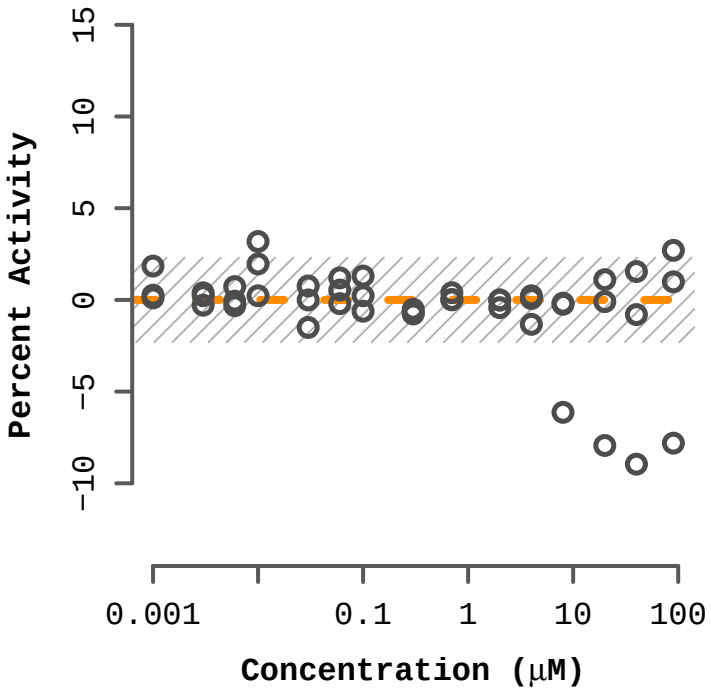
NAME: Ethylene glycol diethyl ether
CHID: 25285 CASRN: 629-14-1
SPID(S): Tox21_200656
M4ID: 12481596

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.49 MAX_MED: 1.95 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

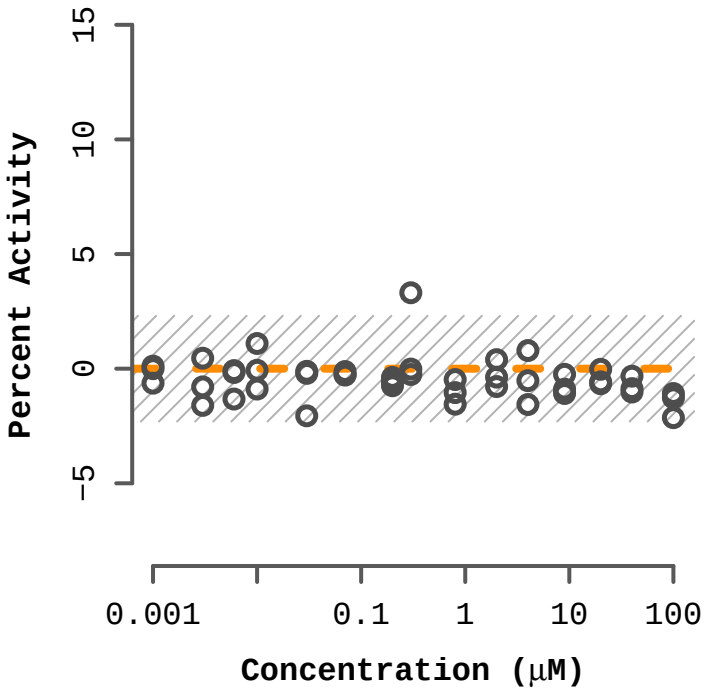
NAME: Ethylene glycol dimethyl ether
CHID: 25286 **CASRN:** 110-71-4
SPID(S): Tox21_200420
M4ID: 12481832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.08	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

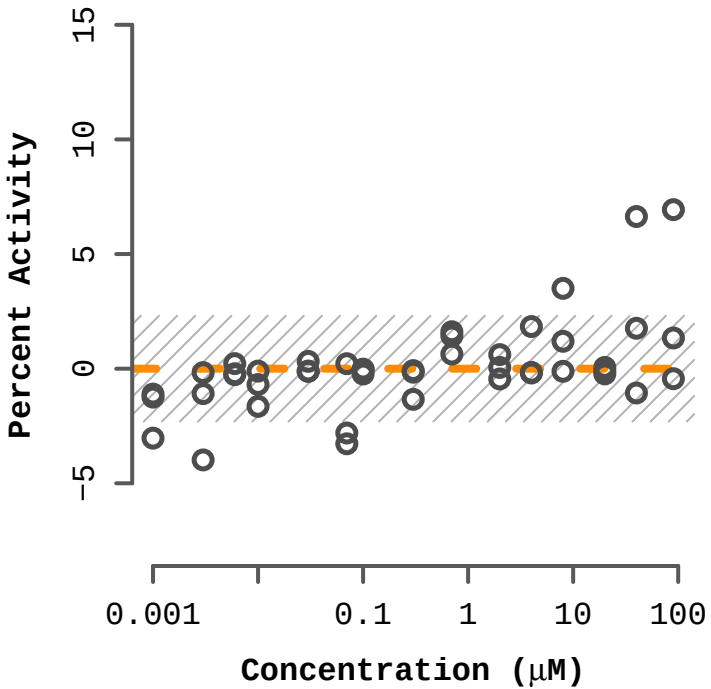
NAME: 2-Ethylhexanal
CHID: 25291 CASRN: 123-05-7
SPID(S): Tox21_303326
M4ID: 12475807

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.01 MAX_MED: 0.00178 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

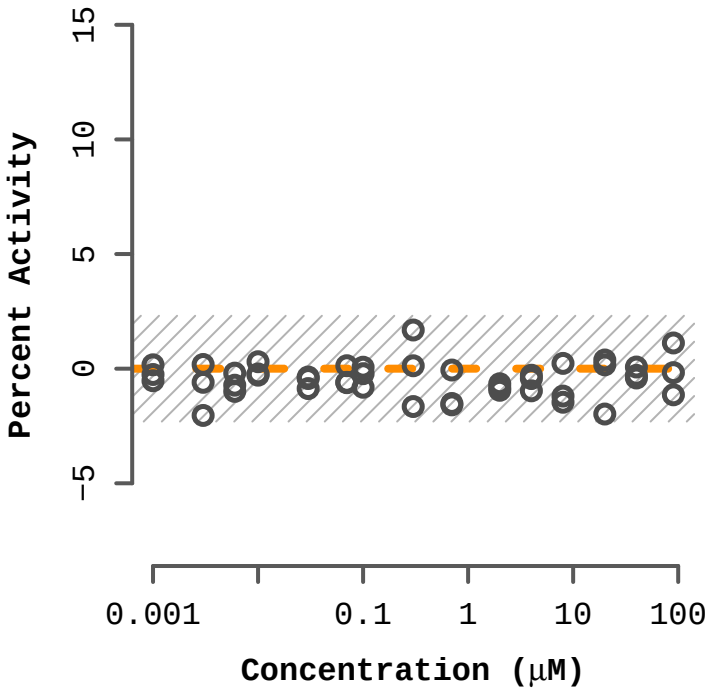
NAME: 2-Ethylhexanal
CHID: 25291 **CASRN:** 123-05-7
SPID(S): Tox21_202095
M4ID: 12480157

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 2.61 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

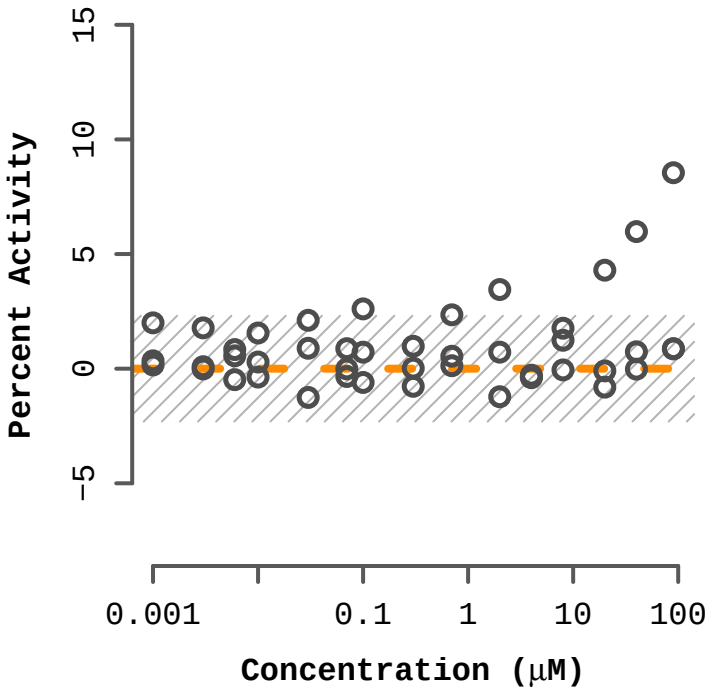
NAME: 2-Ethyl-1,3-hexanediol
CHID: 25292 **CASRN:** 94-96-2
SPID(S): Tox21_303253
M4ID: 12475880

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.0557 **MAX_MED:** 0.167 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

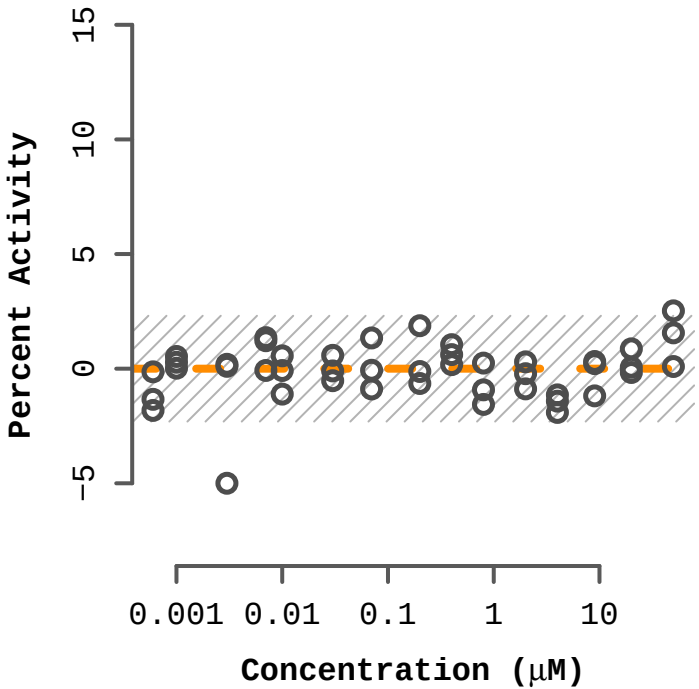
NAME: 2-Ethyl-1,3-hexanediol
CHID: 25292 **CASRN:** 94-96-2
SPID(S): Tox21_202003
M4ID: 12480249

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 3.43 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

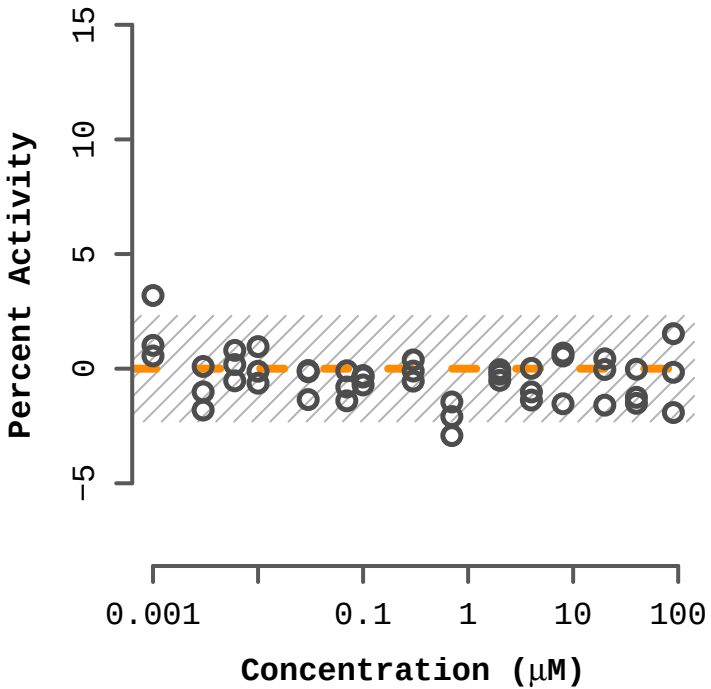
NAME: 2-Ethyl-1,3-hexanediol
CHID: 25292 **CASRN:** 94-96-2
SPID(S): Tox21_111152_1
M4ID: 12483876

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

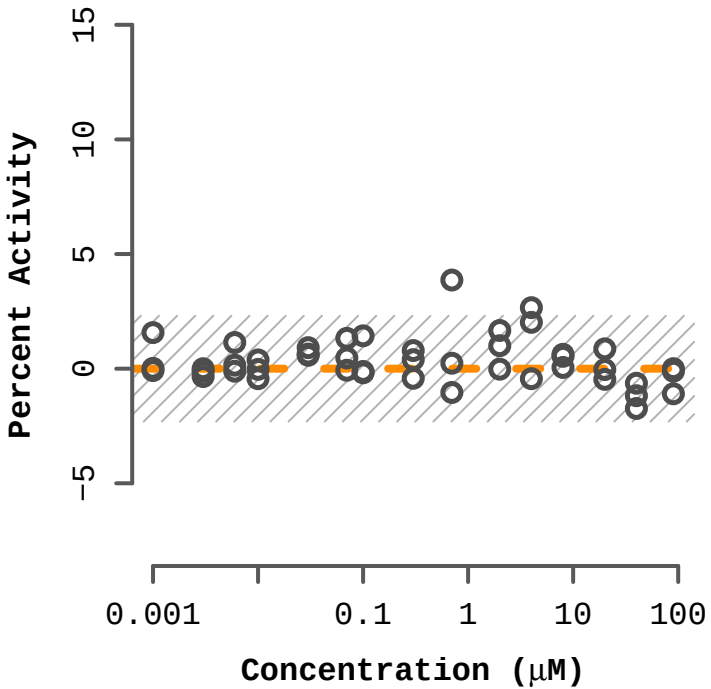
NAME: 2-Ethylhexanoic acid
CHID: 25293 **CASRN:** 149-57-5
SPID(S): Tox21_300108
M4ID: 12479022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

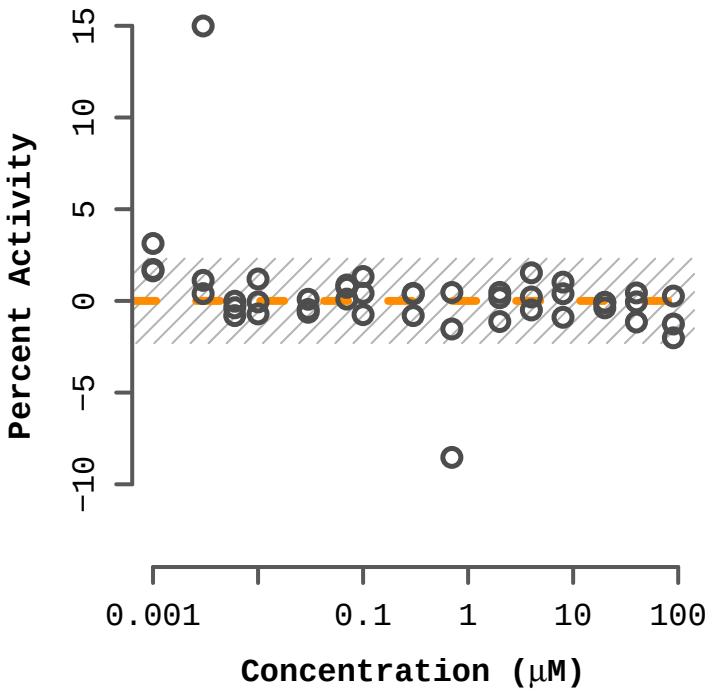
NAME: 2-Ethylhexanoic acid
CHID: 25293 **CASRN:** 149-57-5
SPID(S): Tox21_201406
M4ID: 12480846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 2.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

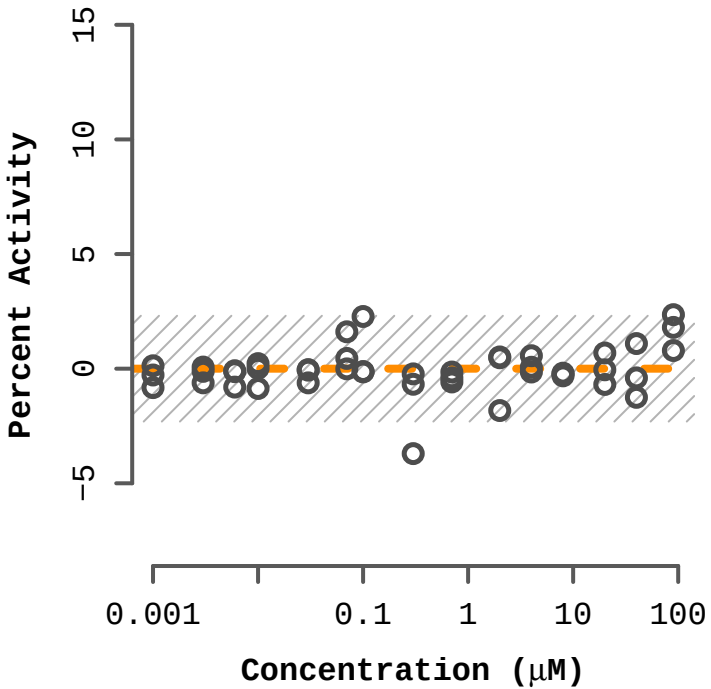
NAME: 2-Ethyl-2-hexenal
CHID: 25296 **CASRN:** 645-62-5
SPID(S): Tox21_303143
M4ID: 12475990

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.31	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 5.5 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

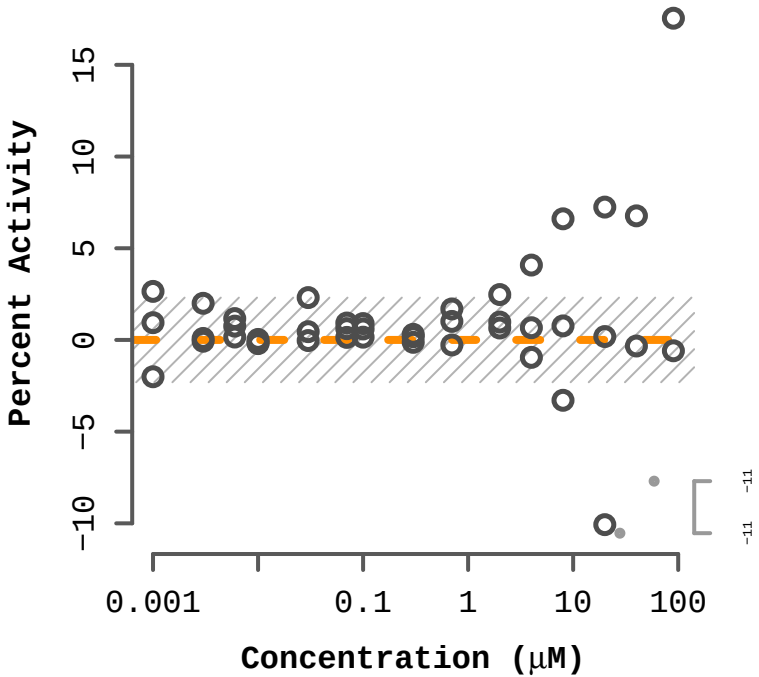
NAME: 2-Ethylhexyl acrylate
CHID: 25297 **CASRN:** 103-11-7
SPID(S): Tox21_303227
M4ID: 12475906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

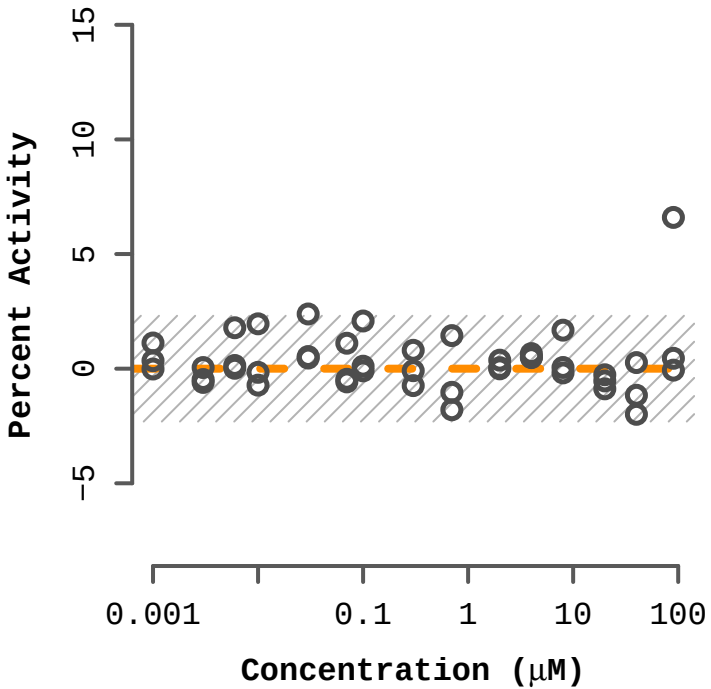
NAME: 2-Ethylhexyl acrylate
CHID: 25297 **CASRN:** 103-11-7
SPID(S): Tox21_202053
M4ID: 12480199 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.03	NA	NA
PROB:	1	NA	NA
RMSE:	4.37	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

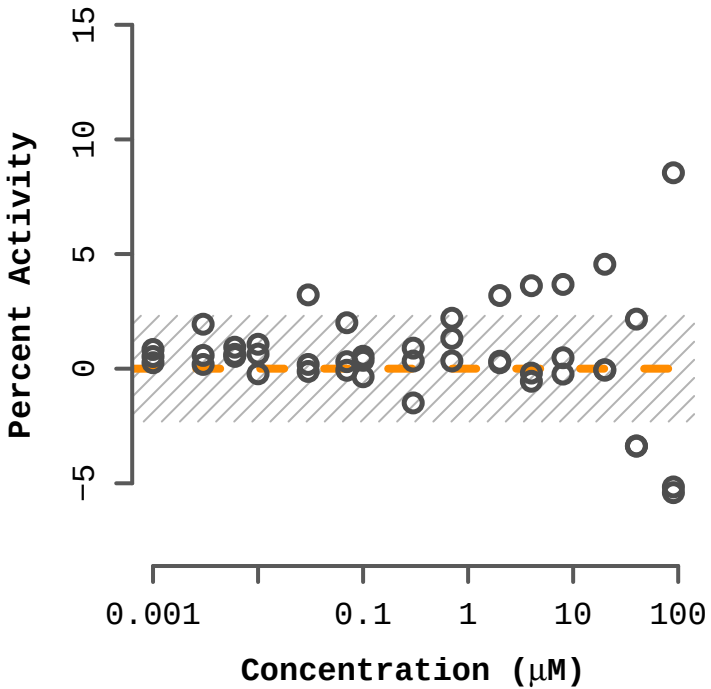
NAME: 2-Ethylhexylamine
CHID: 25298 **CASRN:** 104-75-6
SPID(S): Tox21_200736
M4ID: 12481516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 0.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

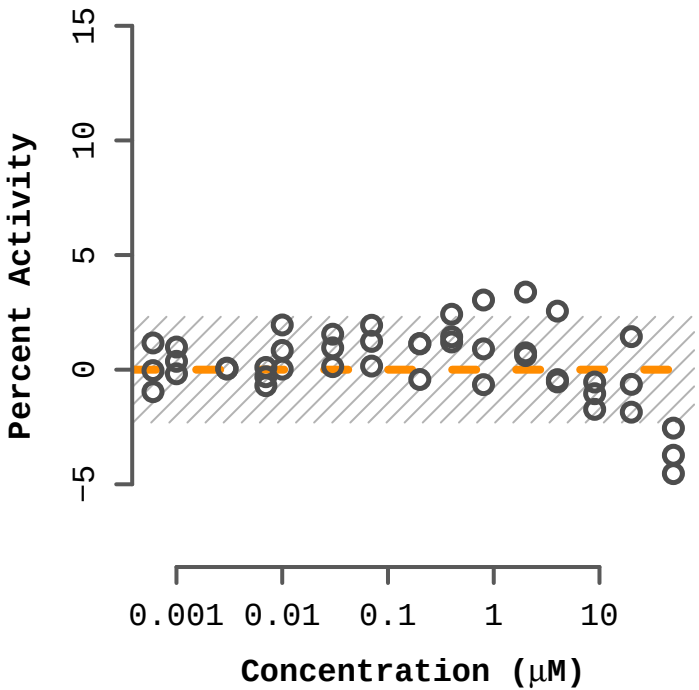
NAME: 2-Ethylhexyl-2-cyano-3,3-diphenylacrylate
CHID: 25299 **CASRN:** 6197-30-4
SPID(S): Tox21_200236
M4ID: 12482016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.42	NA	NA
PROB:	1	NA	NA
RMSE:	2.35	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

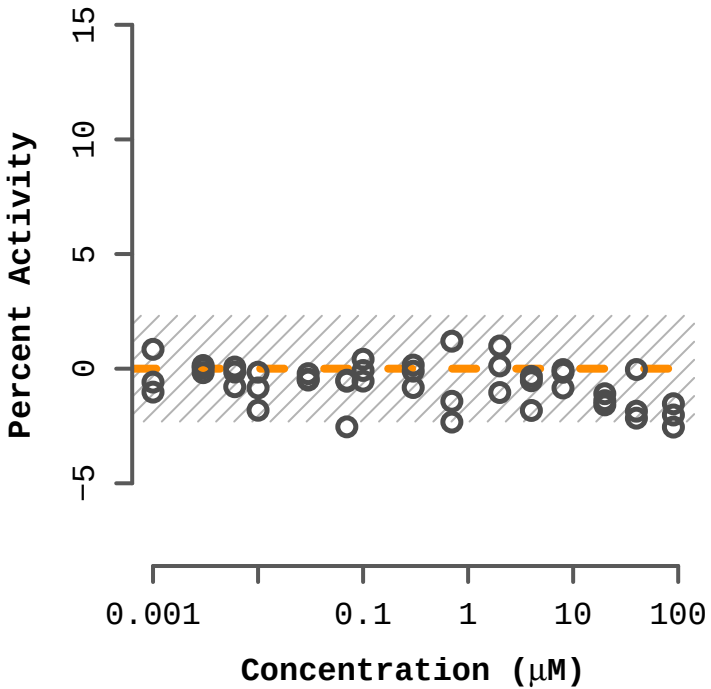
NAME: 2-Ethylhexyl-2-cyano-3,3-diphenylacrylate
CHID: 25299 **CASRN:** 6197-30-4
SPID(S): Tox21_111153_1
M4ID: 12483875

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

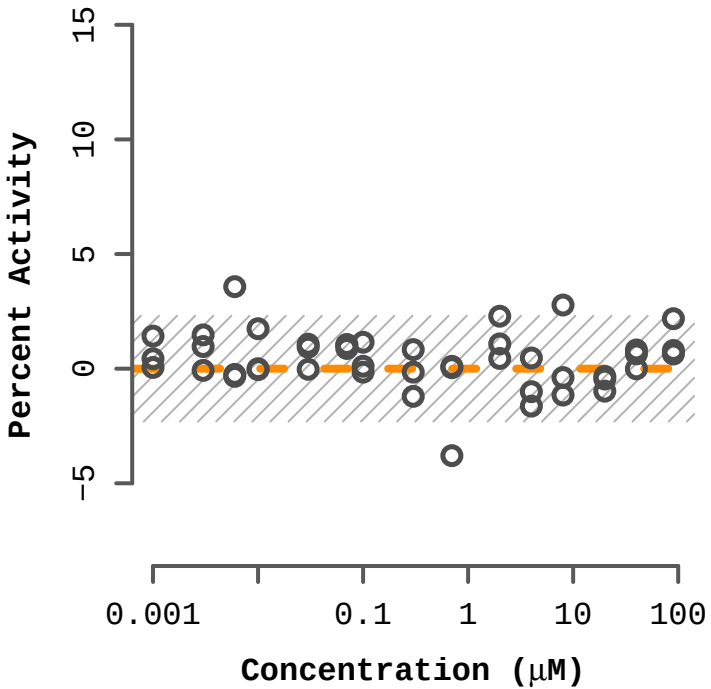
NAME: 2-Ethylhexyl diphenyl phosphate
CHID: 25300 CASRN: 1241-94-7
SPID(S): Tox21_303313
M4ID: 12475820

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.0247 **MAX_MED:** 0.121 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

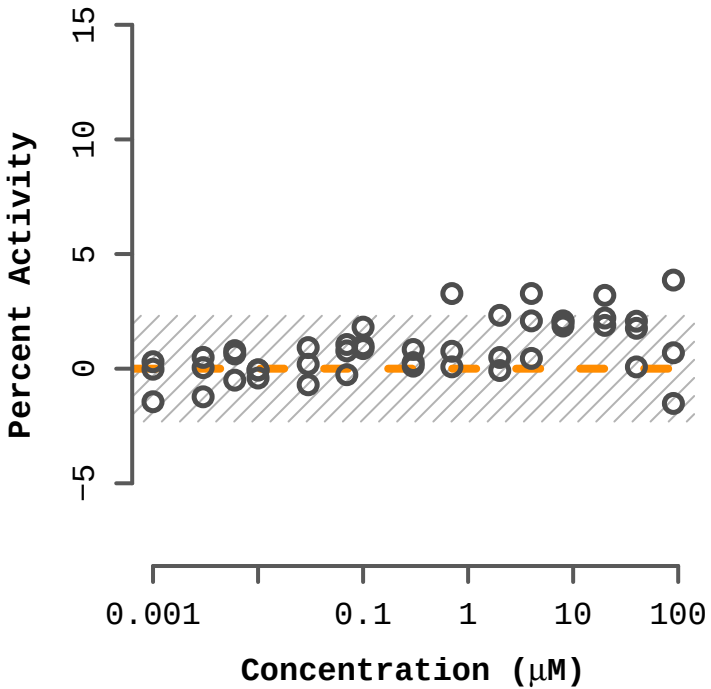
NAME: 2-Ethylhexyl glycidyl ether
CHID: 25301 **CASRN:** 2461-15-6
SPID(S): Tox21_303126
M4ID: 12476007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

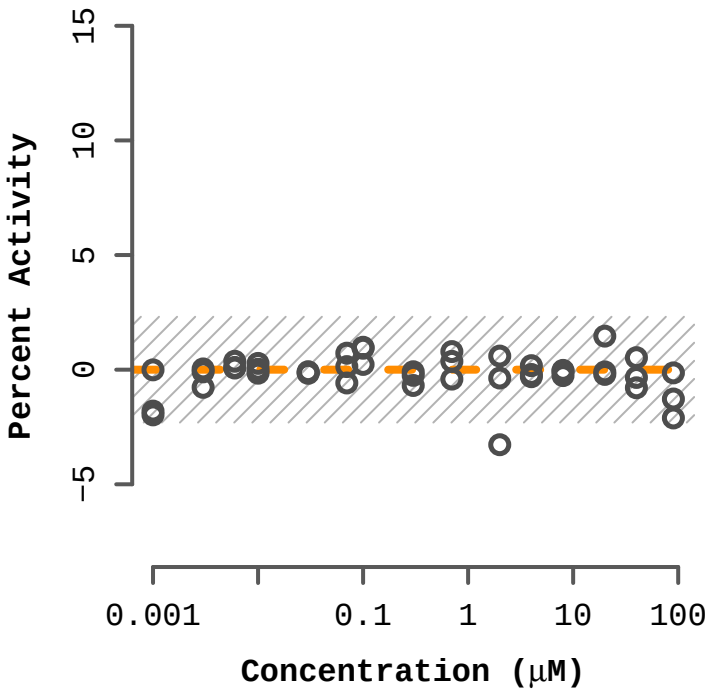
NAME: 2-Ethylhexyl glycidyl ether
CHID: 25301 **CASRN:** 2461-15-6
SPID(S): Tox21_201983
M4ID: 12480269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.43 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

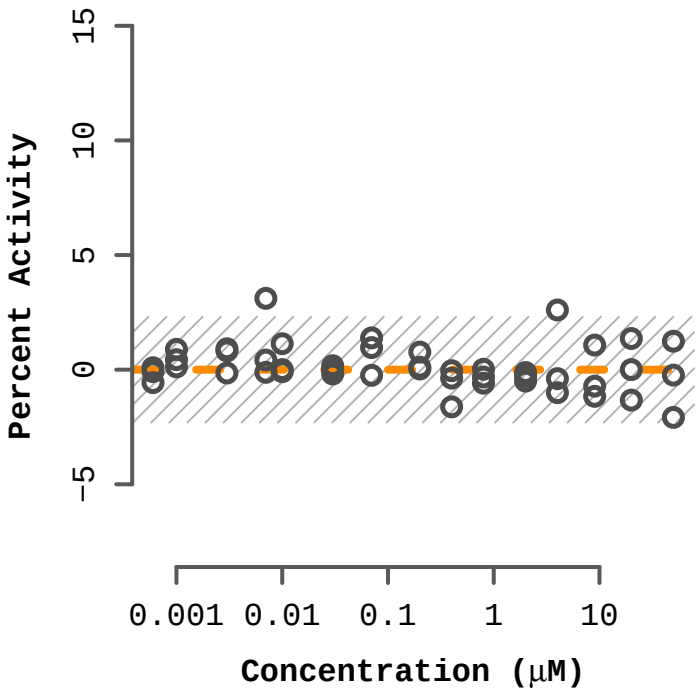
NAME: Octinoxate
CHID: 25302 **CASRN:** 5466-77-3
SPID(S): Tox21_201327
M4ID: 12480925

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.715 **MAX_MED:** 0.935 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

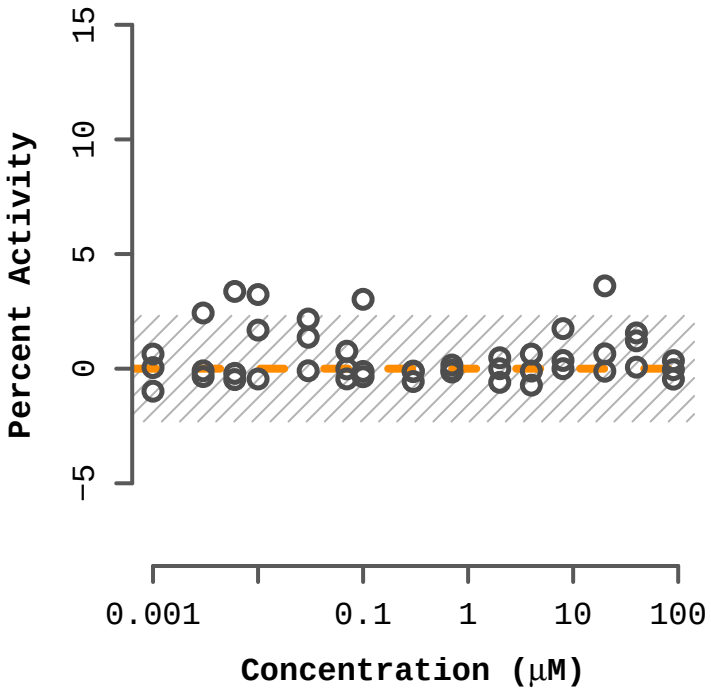
NAME: Octinoxate
CHID: 25302 **CASRN:** 5466-77-3
SPID(S): Tox21_111942_1
M4ID: 12483419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

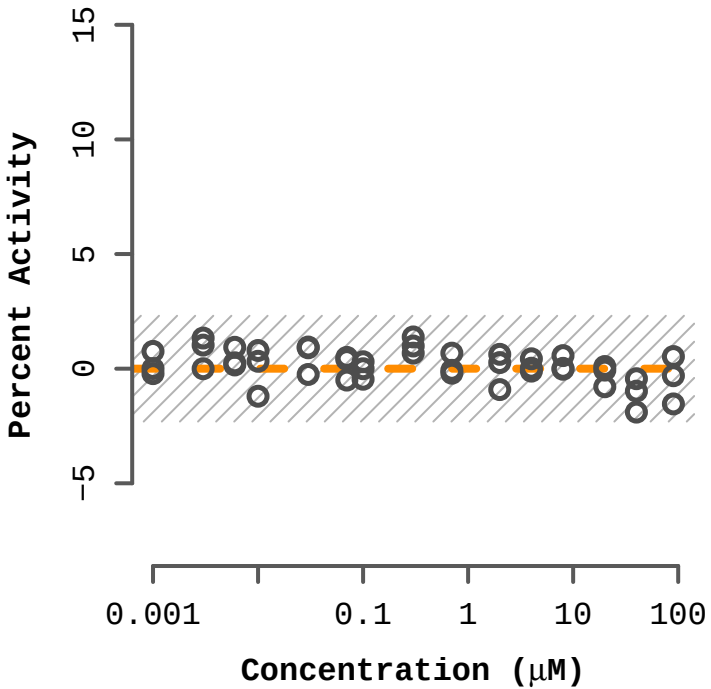
NAME: 3-((2-Ethylhexyl)oxy)propionitrile
CHID: 25303 **CASRN:** 10213-75-9
SPID(S): Tox21_300885
M4ID: 12478248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

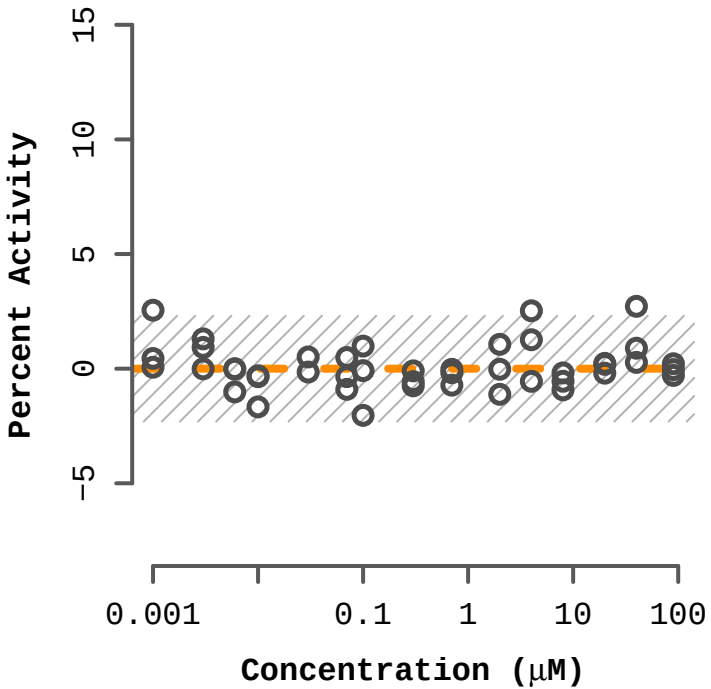
NAME: 3-((2-Ethylhexyl)oxy)propylamine
CHID: 25304 CASRN: 5397-31-9
SPID(S): Tox21_200836
M4ID: 12481416

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

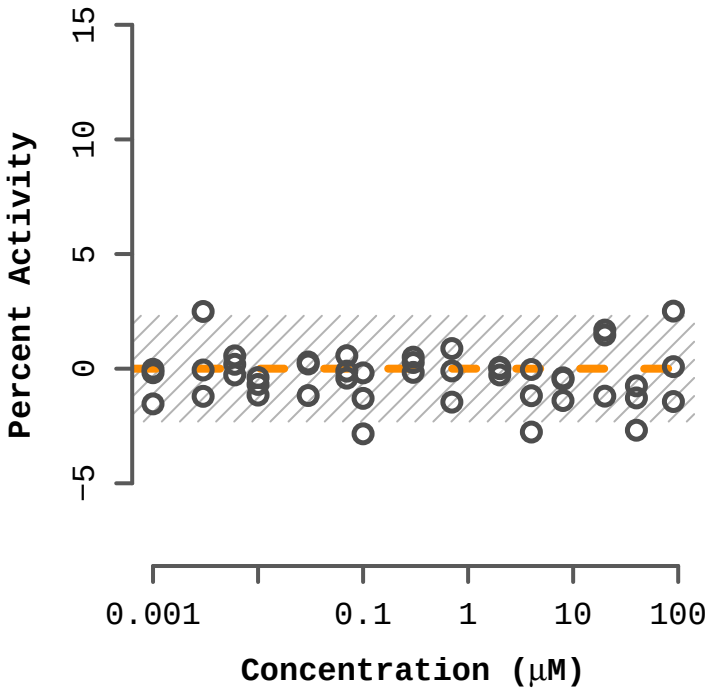
NAME: Ethyl 3-hydroxybutyrate
CHID: 25305 **CASRN:** 5405-41-4
SPID(S): Tox21_303950
M4ID: 12475238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

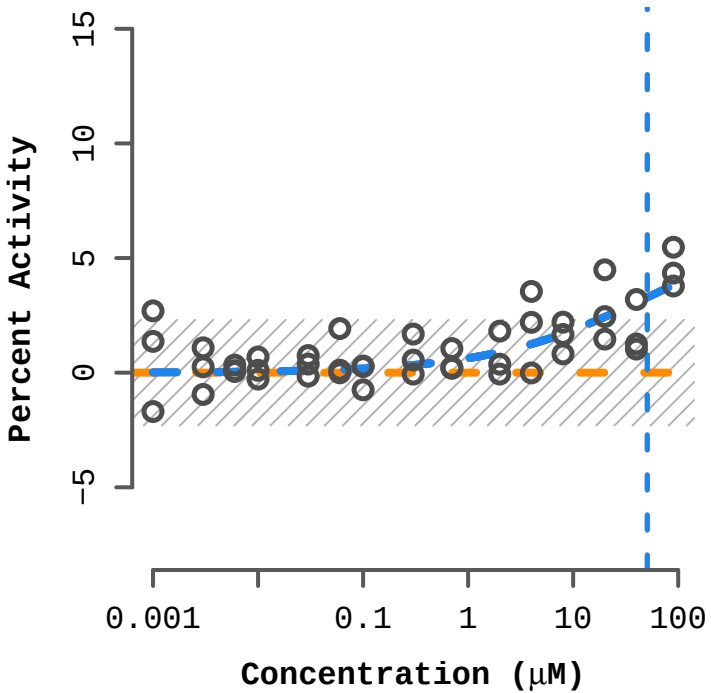
NAME: 5-Ethylidene-2-norbornene
CHID: 25306 **CASRN:** 16219-75-3
SPID(S): Tox21_303067
M4ID: 12476066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.653 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Ethylidene-2-norbornene
CHID: 25306 **CASRN:** 16219-75-3
SPID(S): Tox21_201637
M4ID: 12480615

HILL MODEL (in red):

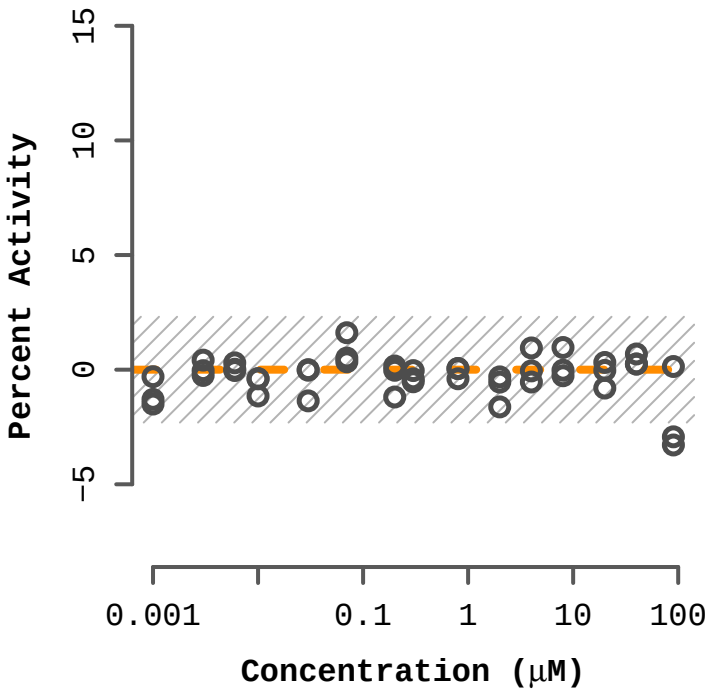
	tp	ga	gw
val:	6.57	1.71	0.571
sd:	3.08	0.707	0.177

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.57	1.71	0.571	3.78	6.75
sd:	3.09	0.708	0.177	139000	522000

	CNST	HILL	GNLS
AIC:	182.06	138.91	142.91
PROB:	0	0.88	0.12
RMSE:	1.87	1.04	1.04

MAX_MEAN: 4.53 **MAX_MED:** 4.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

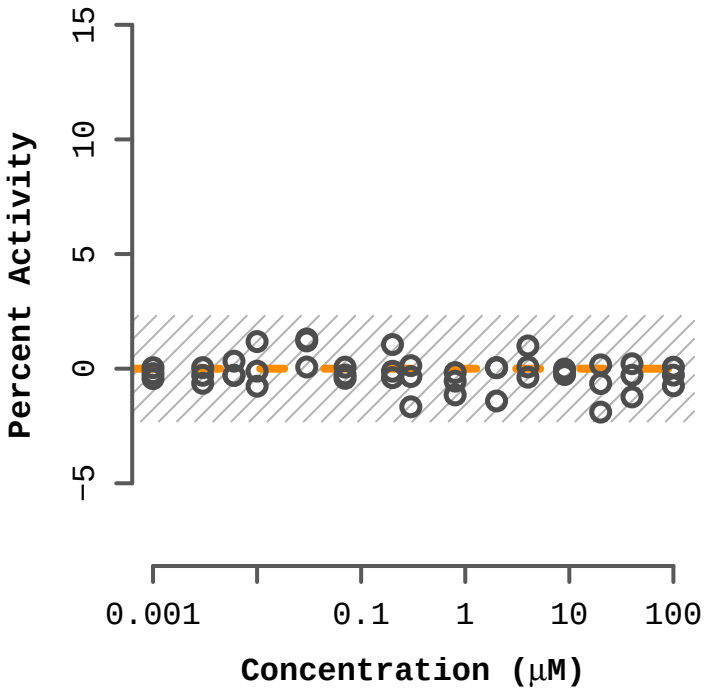
NAME: Ethyl linolenate
CHID: 25307 CASRN: 1191-41-9
SPID(S): Tox21_201013
M4ID: 12481239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.823 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

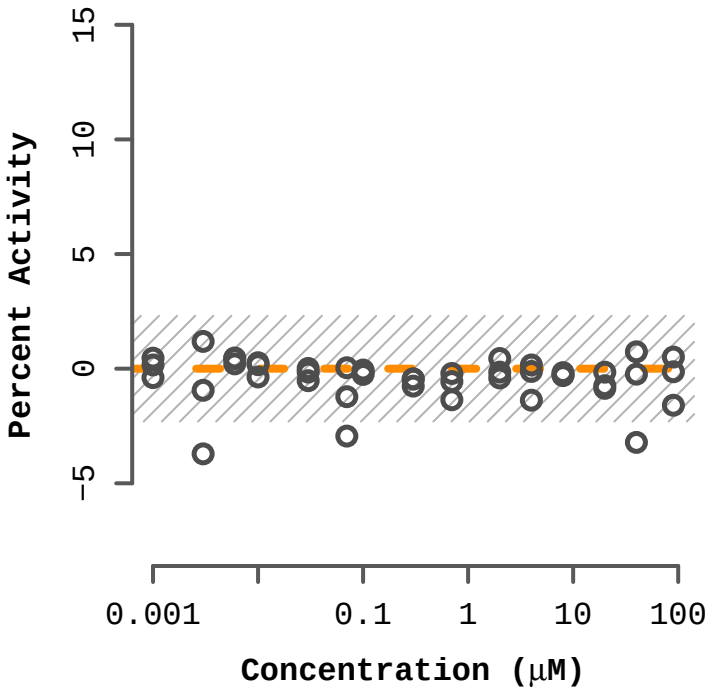
NAME: Ethyl methacrylate
CHID: 25308 CASRN: 97-63-2
SPID(S): Tox21_200810
M4ID: 12481442

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

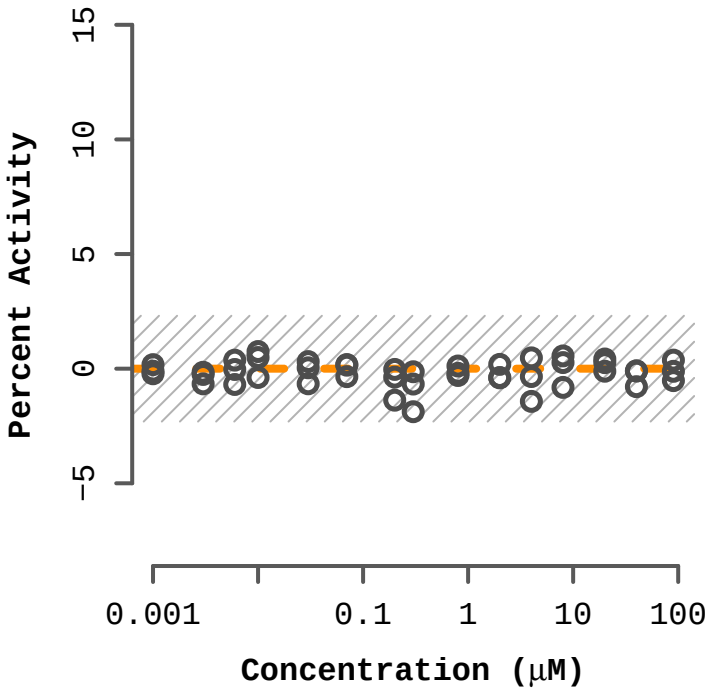
NAME: Ethyl methanesulfonate
CHID: 25309 **CASRN:** 62-50-0
SPID(S): Tox21_200006
M4ID: 12482246

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

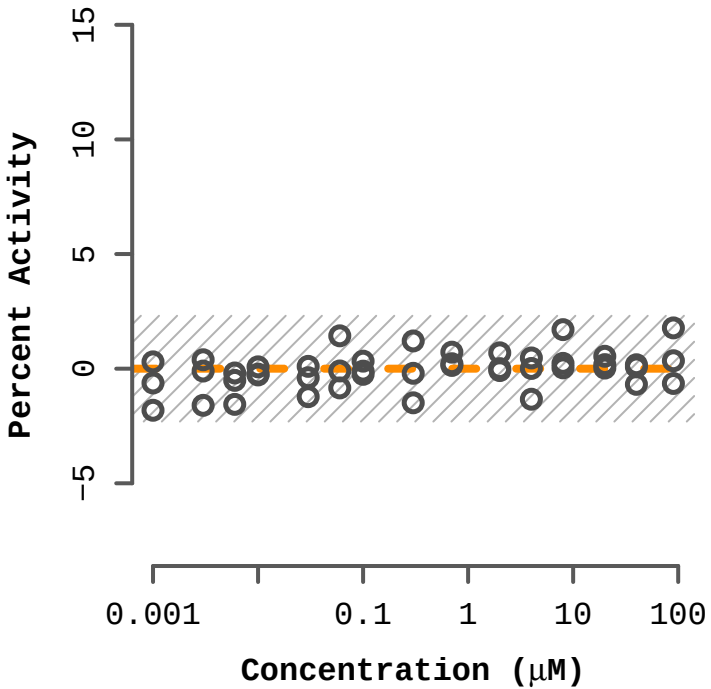
NAME: N-Ethyl-4-methylbenzenesulfonamide
CHID: 25310 **CASRN:** 80-39-7
SPID(S): Tox21_200366
M4ID: 12481886

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	73.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.56	NA	NA

MAX_MEAN: 0.284 **MAX_MED:** 0.487 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

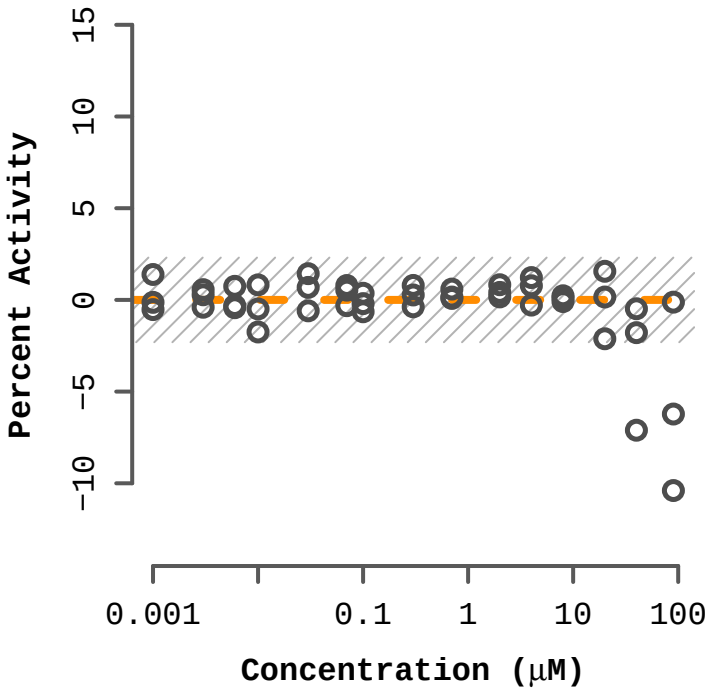
NAME: N-Ethylmorpholine
CHID: 25312 **CASRN:** 100-74-3
SPID(S): Tox21_201103
M4ID: 12481149

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.658 **MAX_MED:** 0.349 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

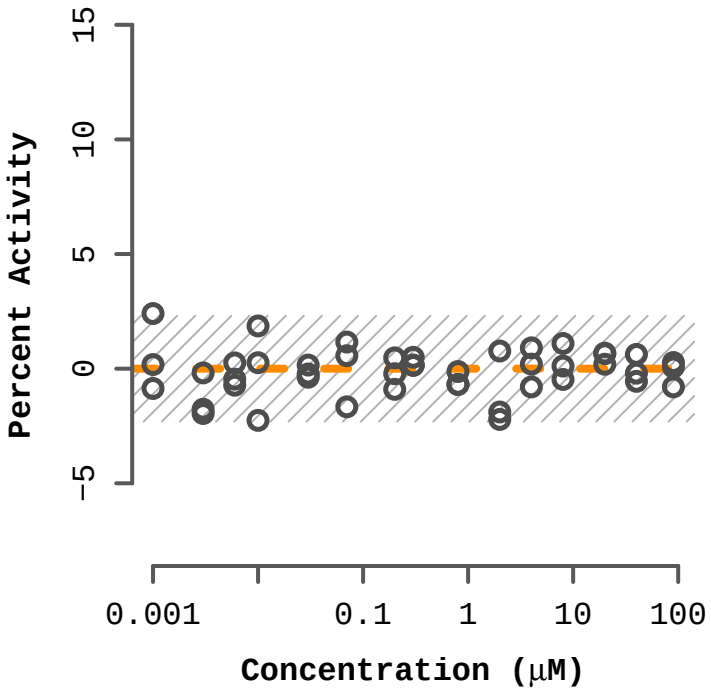
NAME: N-Ethyl-N-phenyl benzylamine
CHID: 25315 **CASRN:** 92-59-1
SPID(S): Tox21_200375
M4ID: 12481877

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 0.57 **MAX_MED:** 0.772 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

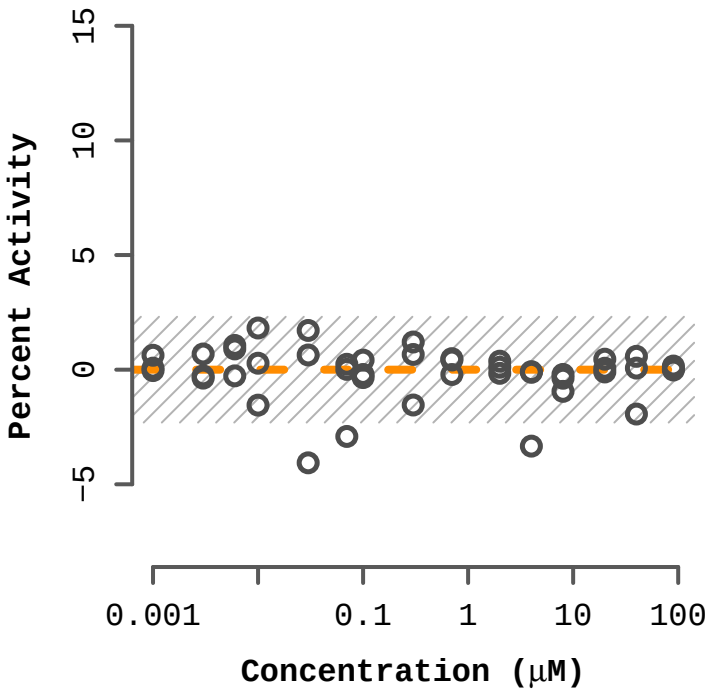
NAME: Ethyl vinyl ketone
CHID: 25318 **CASRN:** 1629-58-9
SPID(S): Tox21_200636
M4ID: 12481616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.575 **MAX_MED:** 0.654 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

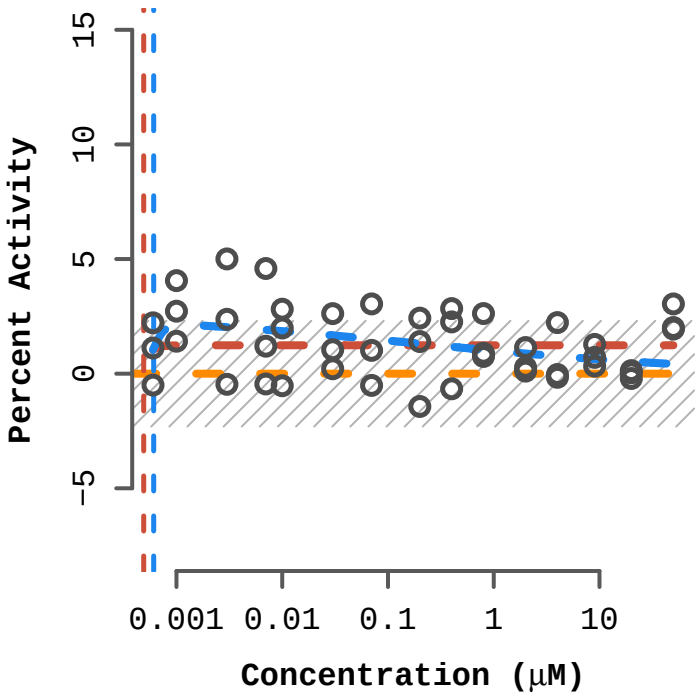
NAME: Ferrocene
CHID: 25326 **CASRN:** 102-54-5
SPID(S): Tox21_202514
M4ID: 12479738

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.565 **MAX_MED:** 0.906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluorescein sodium
CHID: 25328 CASRN: 518-47-8
SPID(S): Tox21_111592_1
M4ID: 12483600

HILL MODEL (in red):

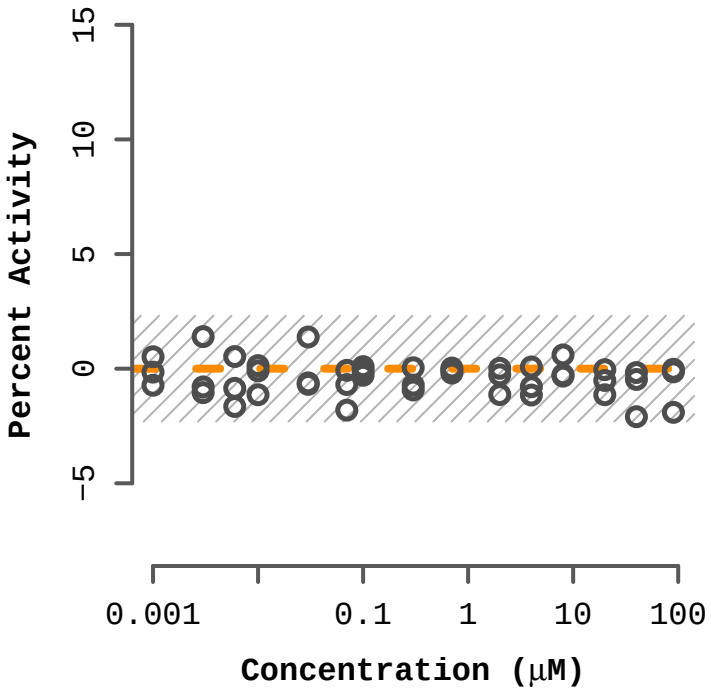
	tp	ga	gw
val:	1.24	−3.31	8
sd:	0.242	0.51	26.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.6	−3.22	8	−0.672	0.3
sd:	8.46	0.143	10.4	11.2	1.17

	CNST	HILL	GNLS
AIC:	192.62	174.06	174.94
PROB:	0	0.61	0.39
RMSE:	1.97	1.47	1.41

MAX_MEAN: 2.74 **MAX_MED:** 2.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

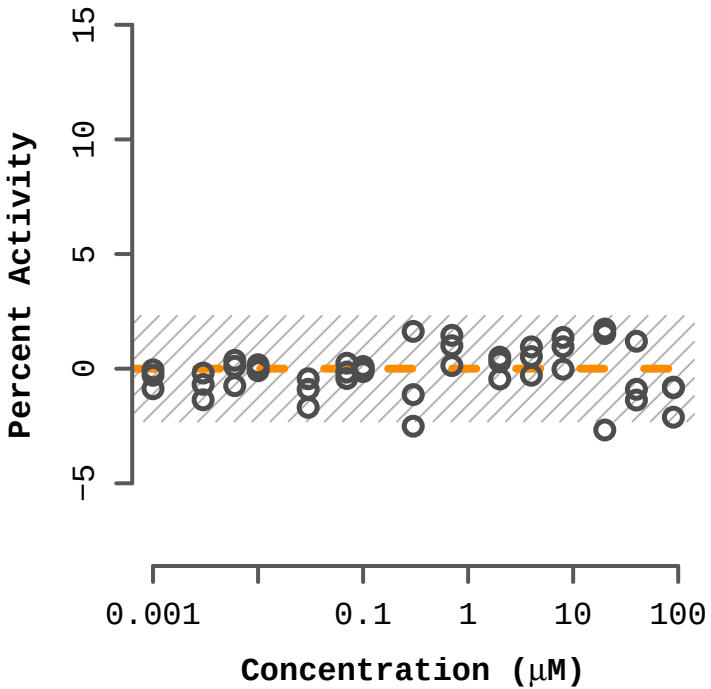
NAME: Fluorobenzene
CHID: 25329 **CASRN:** 462-06-6
SPID(S): Tox21_201054
M4ID: 12481198

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.0274 **MAX_MED:** −0.0702 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

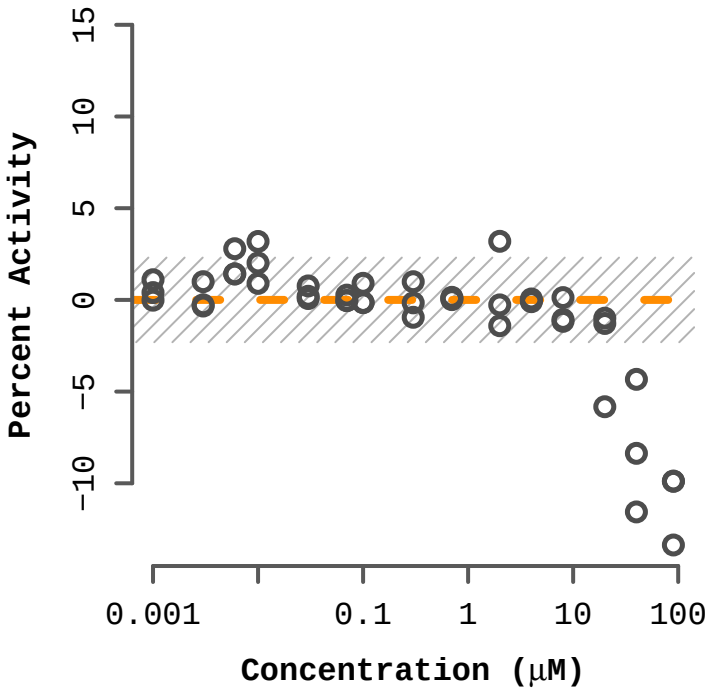
NAME: 2-Fluorobenzoyl chloride
CHID: 25330 **CASRN:** 393-52-2
SPID(S): Tox21_200637
M4ID: 12481615

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.865 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

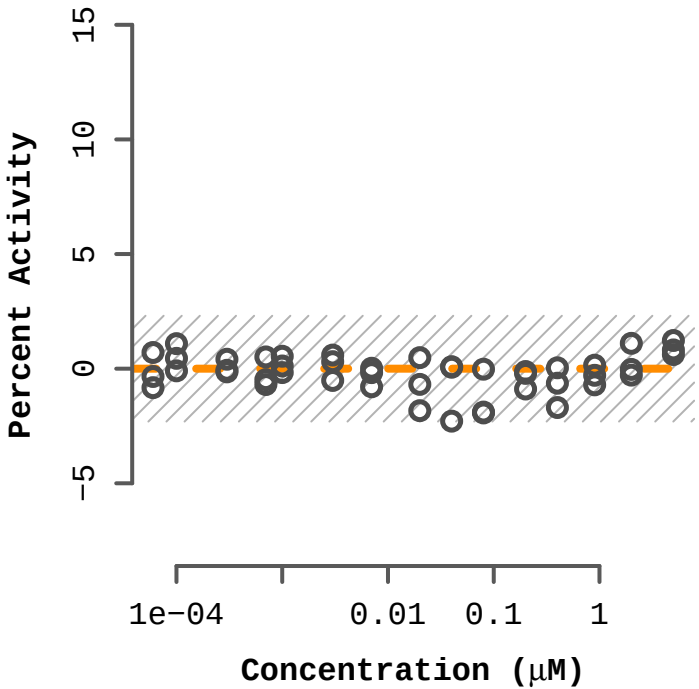
NAME: 1-Fluoro-2,4-dinitrobenzene
CHID: 25331 **CASRN:** 70-34-8
SPID(S): Tox21_200352
M4ID: 12481900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.37	NA	NA
PROB:	1	NA	NA
RMSE:	3.89	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 2.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

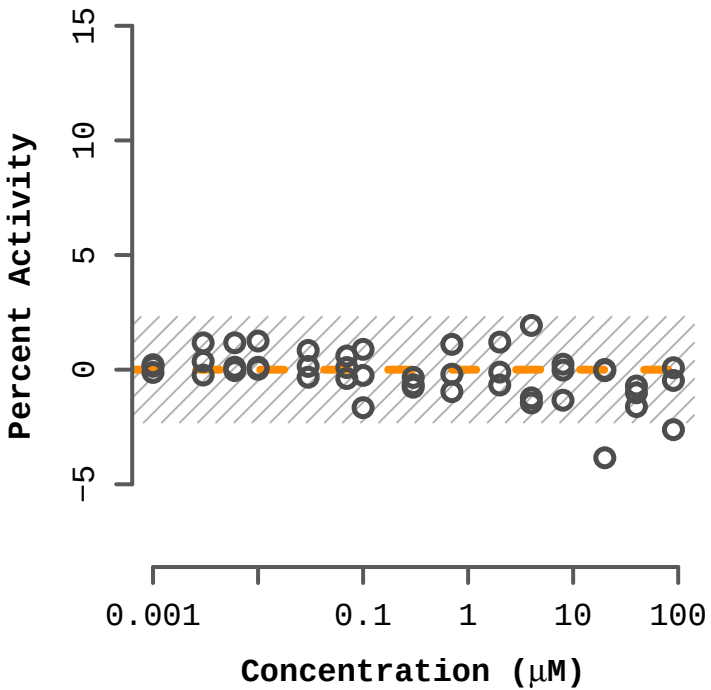
NAME: 4-Fluoro-dl-phenylalanine
CHID: 25332 **CASRN:** 51-65-0
SPID(S): Tox21_202890
M4ID: 12479362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.889 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

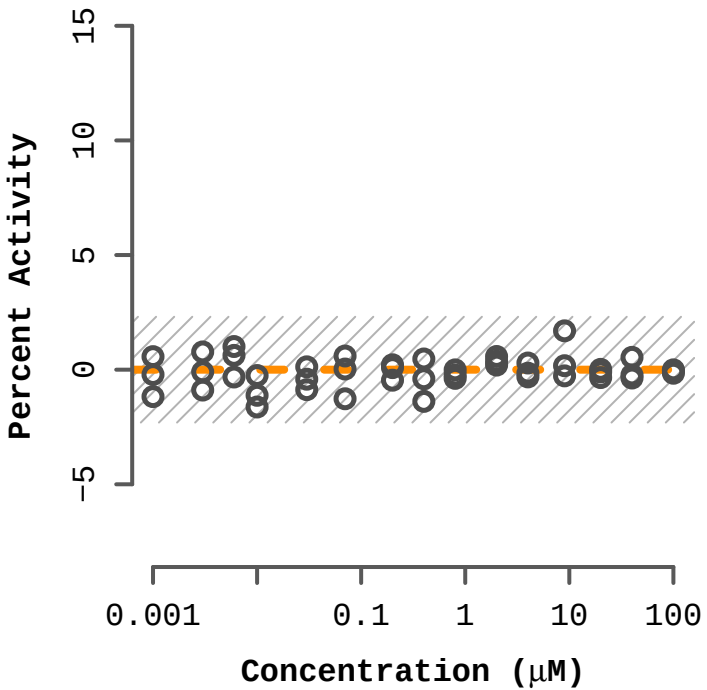
NAME: Formamide
CHID: 25337 **CASRN:** 75-12-7
SPID(S): Tox21_302824
M4ID: 12476309

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.458 **MAX_MED:** 0.364 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

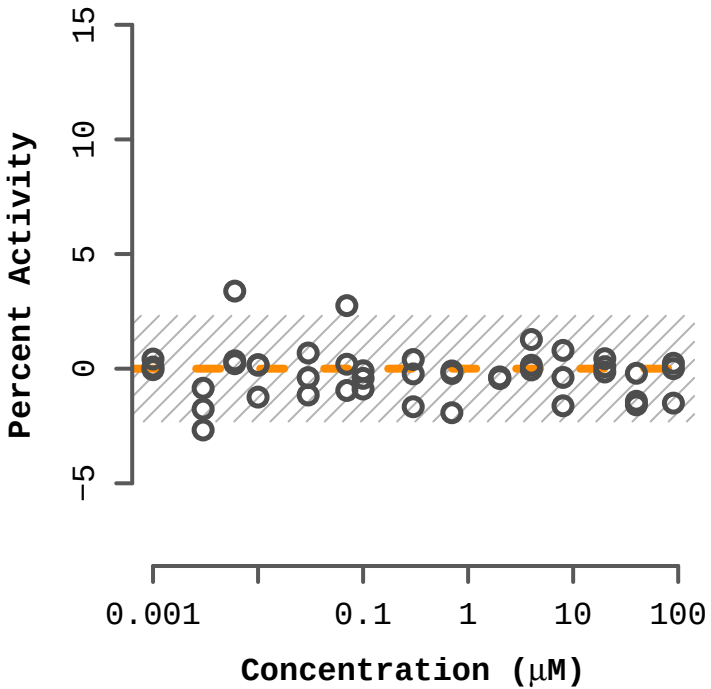
NAME: Formamide
CHID: 25337 CASRN: 75-12-7
SPID(S): Tox21_201942
M4ID: 12480310

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.534 MAX_MED: 0.624 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

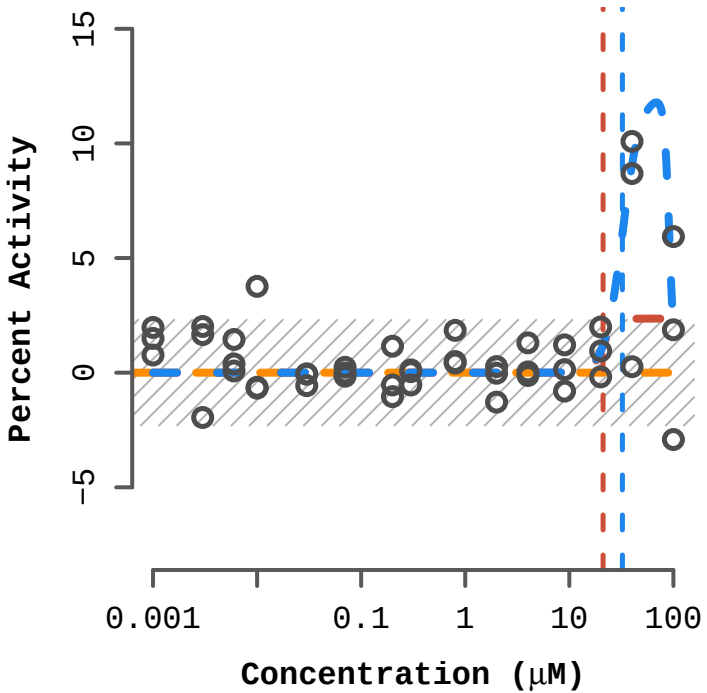
NAME: Formanilide
CHID: 25338 **CASRN:** 103-70-8
SPID(S): Tox21_200271
M4ID: 12481981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.345 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fumaronitrile
CHID: 25342 **CASRN:** 764-42-1
SPID(S): Tox21_201151
M4ID: 12481101

HILL MODEL (in red):

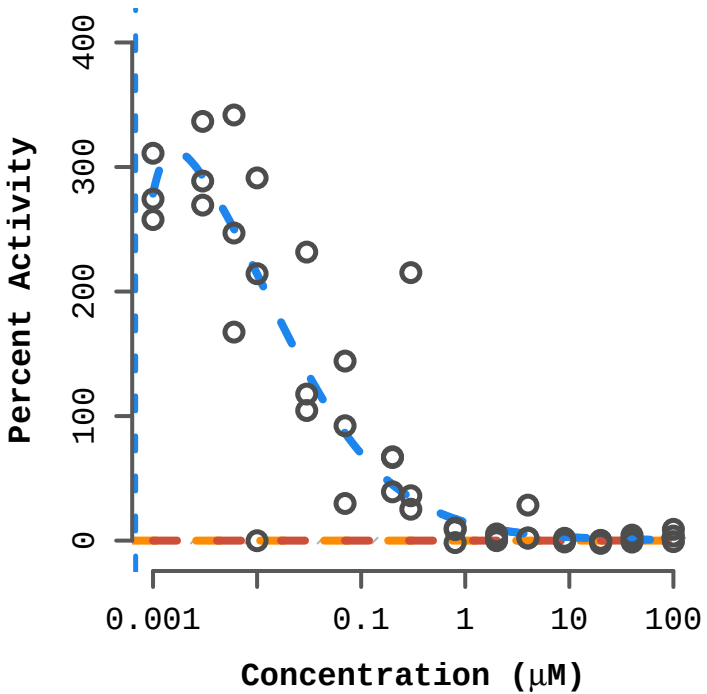
	tp	ga	gw
val:	2.36	1.32	8
sd:	1.5	0.117	32.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.1	1.51	5.15	1.96	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	184.96	185.02	176.97
PROB:	0.02	0.02	0.97
RMSE:	2.48	2.08	1.93

MAX_MEAN: 6.35 **MAX_MED:** 8.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Furfural acetone
CHID: 25345 CASRN: 623-15-4
SPID(S): Tox21_200569
M4ID: 12481683

HILL MODEL (in red):

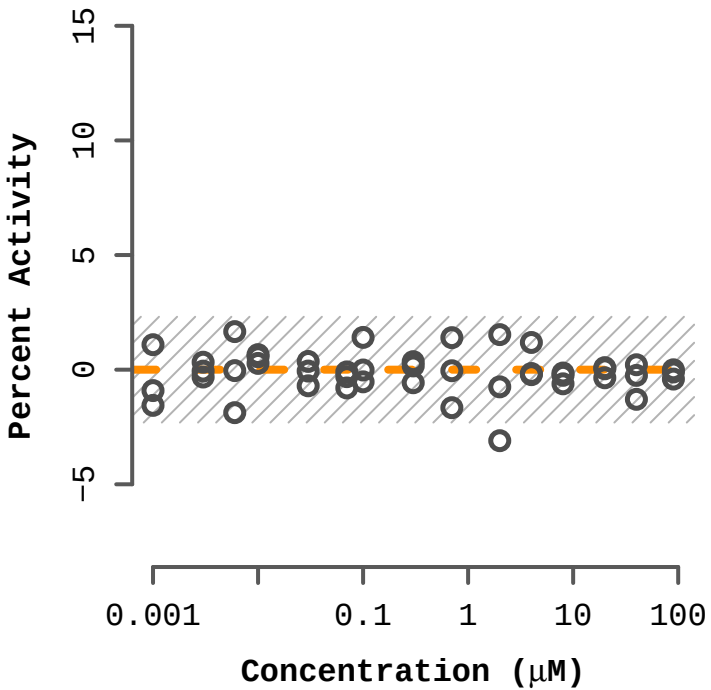
	tp	ga	gw
val:	295	2.5	3.72
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	396	-3.17	3.8	-1.91	0.74
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	577.7	583.69	467.12
PROB:	0	0	1
RMSE:	150.03	150.03	52.34

MAX_MEAN: 298 MAX_MED: 289 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

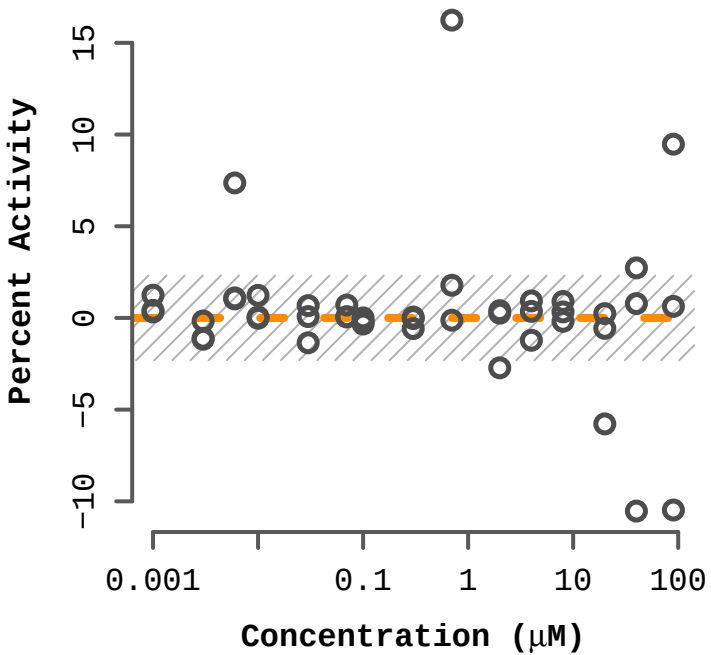
NAME: Furfuryl acetate
CHID: 25346 CASRN: 623-17-6
SPID(S): Tox21_303142
M4ID: 12475991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.5 MAX_MED: 0.567 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

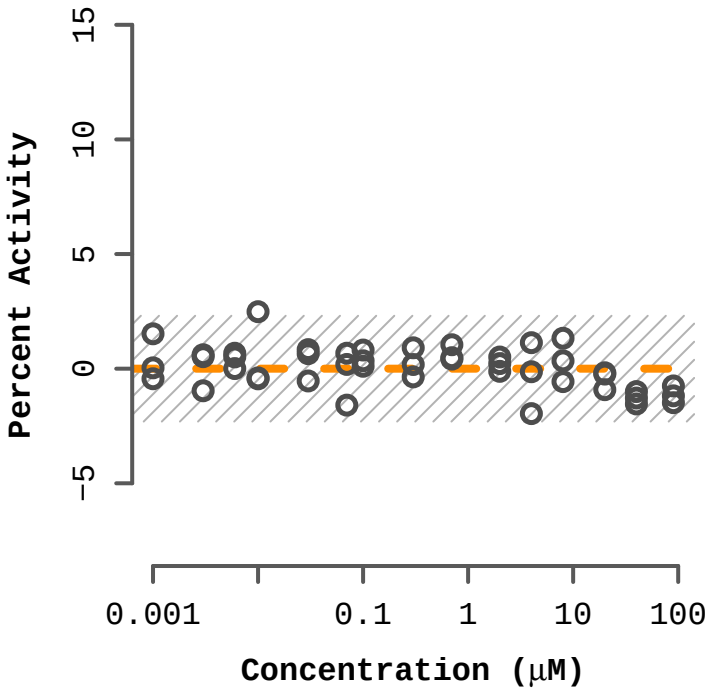
NAME: Furfuryl acetate
CHID: 25346 CASRN: 623-17-6
SPID(S): Tox21_201590
M4ID: 12480662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.72	NA	NA
PROB:	1	NA	NA
RMSE:	3.93	NA	NA

MAX_MEAN: 5.97 MAX_MED: 1.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

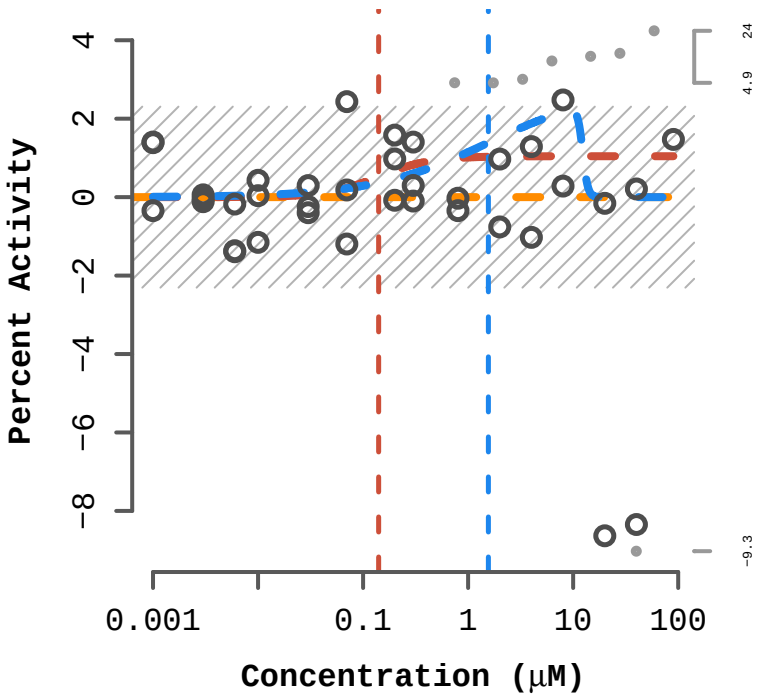
NAME: Furfuryl alcohol
CHID: 25347 **CASRN:** 98-00-0
SPID(S): Tox21_303093
M4ID: 12476040

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.648 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Furfuryl alcohol
CHID: 25347 CASRN: 98-00-0
SPID(S): Tox21_202102
M4ID: 12480150 BRK

HILL MODEL (in red):

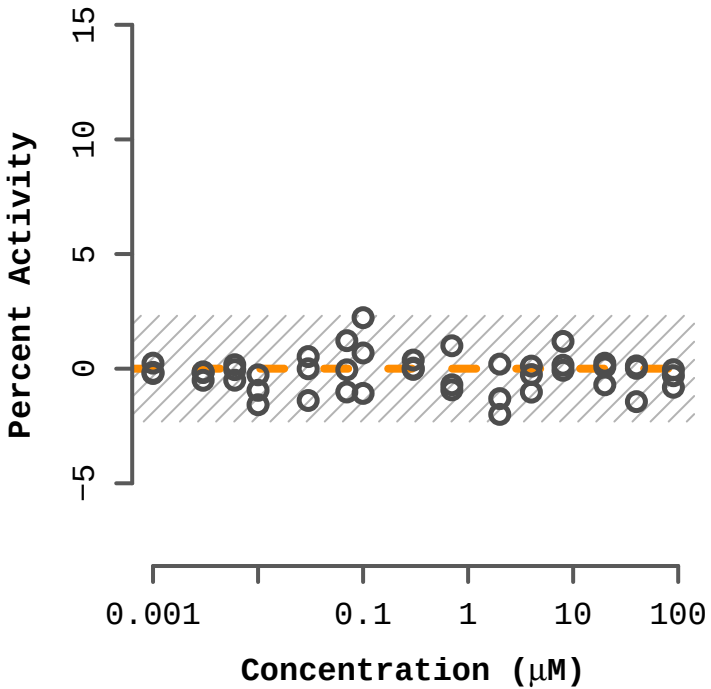
	tp	ga	gw
val:	1.04	−0.852	1.77
sd:	0.791	1.18	3.63

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.78	0.193	0.783	1.09	17.9
sd:	6.53	3.24	1.43	1.99	179

	CNST	HILL	GNLS
AIC:	261.62	264.63	266.9
PROB:	0.77	0.17	0.06
RMSE:	5.94	5.73	5.78

MAX_MEAN: 5.49 **MAX_MED:** 2.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

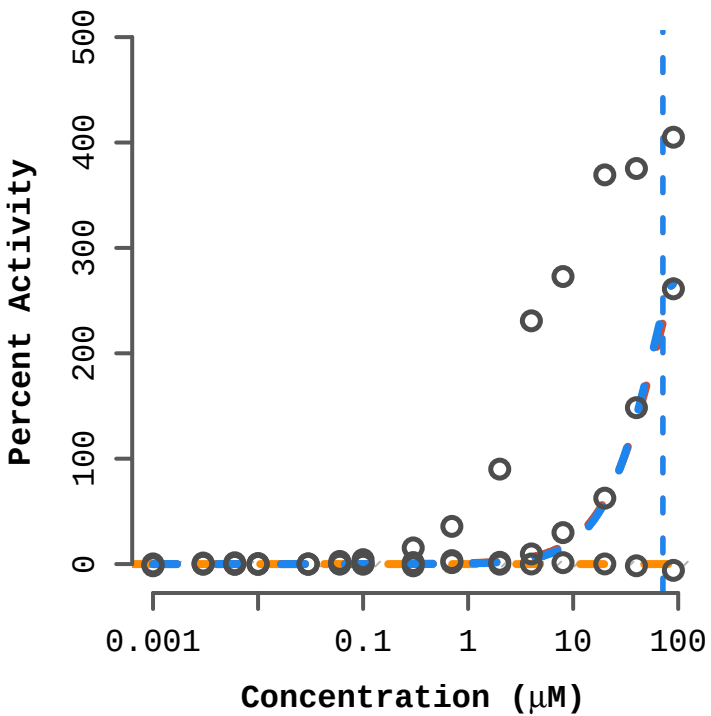
NAME: Glutaraldehyde
CHID: 25355 **CASRN:** 111-30-8
SPID(S): Tox21_303295
M4ID: 12475838

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.612 **MAX_MED:** 0.687 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glutaraldehyde
CHID: 25355 CASRN: 111-30-8
SPID(S): Tox21_201742
M4ID: 12480510

HILL MODEL (in red):

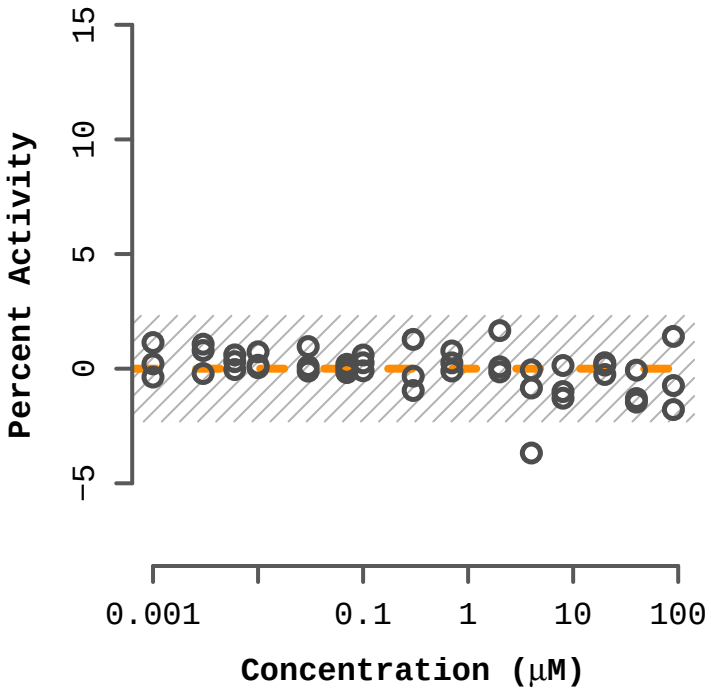
	tp	ga	gw
val:	461	1.86	1.48
sd:	477	0.653	0.938

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	486	1.85	1.57	2.1	7.54
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	527.97	505.67	509.61
PROB:	0	0.88	0.12
RMSE:	122.39	93.65	93.81

MAX_MEAN: 220 MAX_MED: 261 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

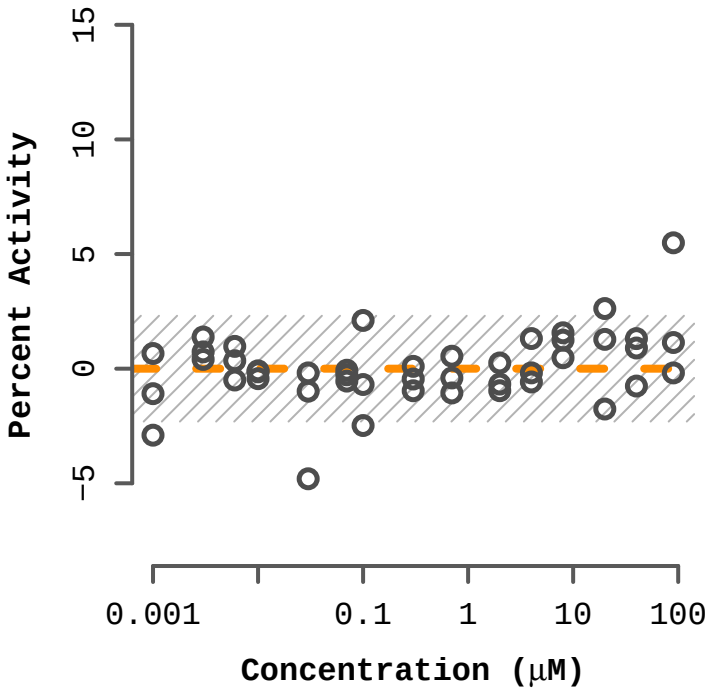
NAME: Glycidyl methacrylate
CHID: 25361 CASRN: 106-91-2
SPID(S): Tox21_303145
M4ID: 12475988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.552 MAX_MED: 0.795 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

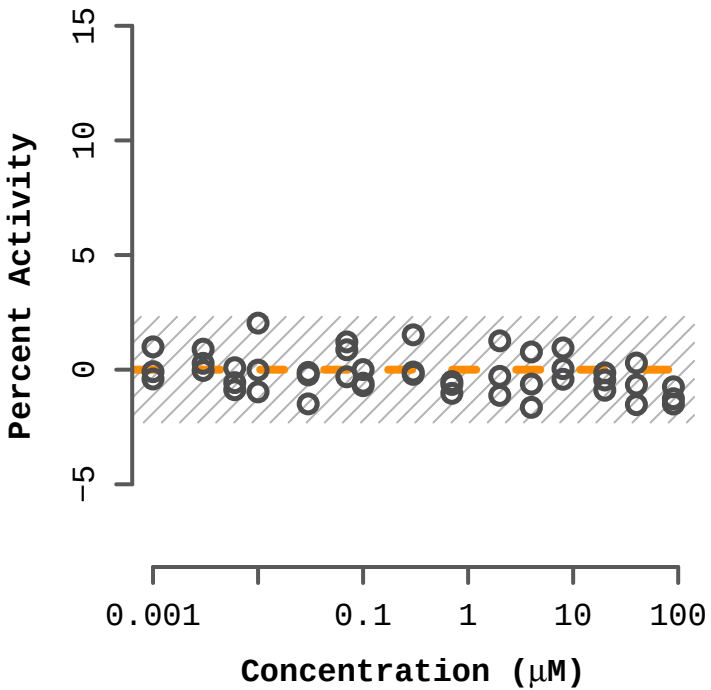
NAME: Glycidyl methacrylate
CHID: 25361 **CASRN:** 106-91-2
SPID(S): Tox21_201494
M4ID: 12480758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

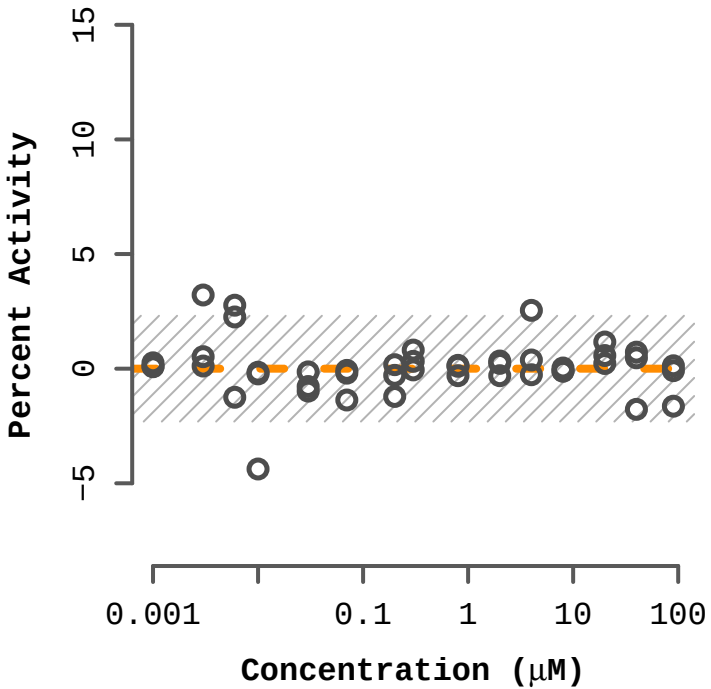
NAME: Glycolic acid
CHID: 25363 CASRN: 79-14-1
SPID(S): Tox21_301298
M4ID: 12477835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.591 MAX_MED: 0.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

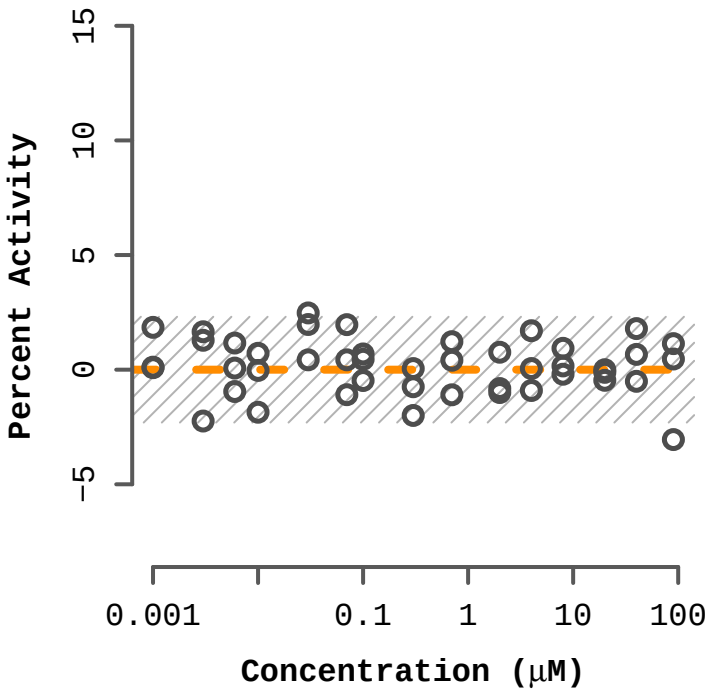
NAME: Glyoxal
CHID: 25364 CASRN: 107-22-2
SPID(S): Tox21_202517
M4ID: 12479735

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.29 MAX_MED: 2.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

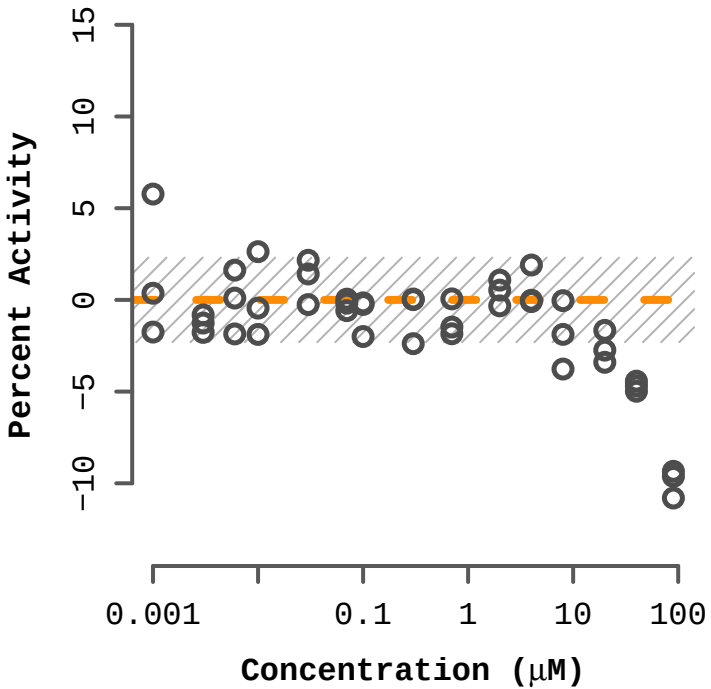
NAME: Guanazole
CHID: 25367 **CASRN:** 1455-77-2
SPID(S): Tox21_202973
M4ID: 12479279

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

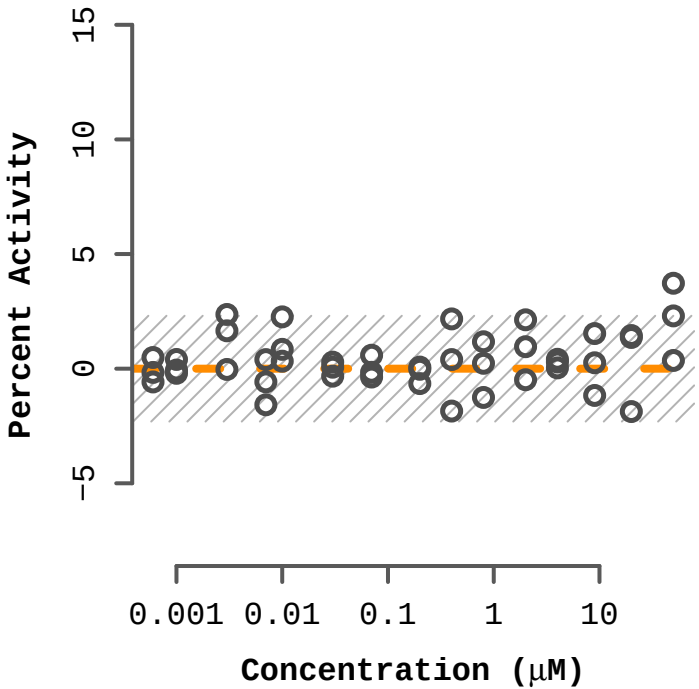
NAME: Halazone
CHID: 25370 CASRN: 80-13-7
SPID(S): Tox21_202519
M4ID: 12479733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.22	NA	NA
PROB:	1	NA	NA
RMSE:	3.3	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

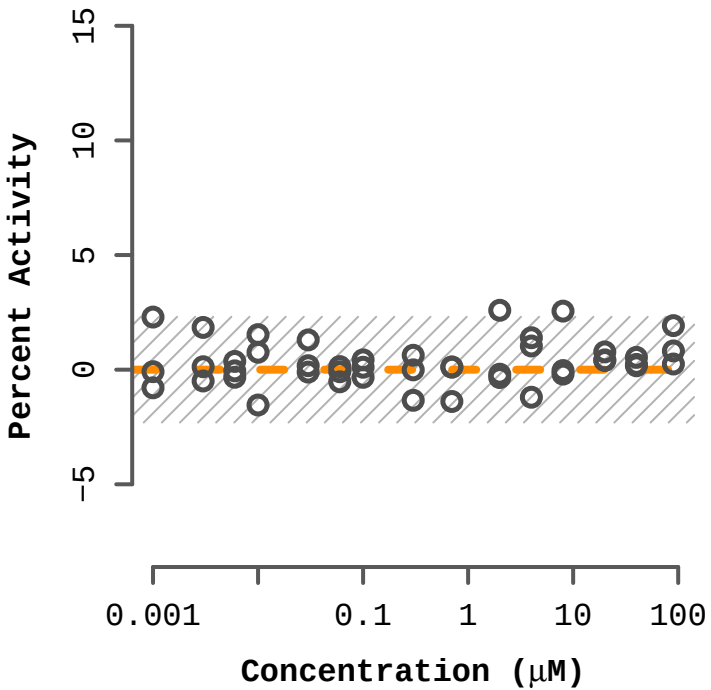
NAME: Halazone
CHID: 25370 CASRN: 80-13-7
SPID(S): Tox21_111104_1
M4ID: 12483905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

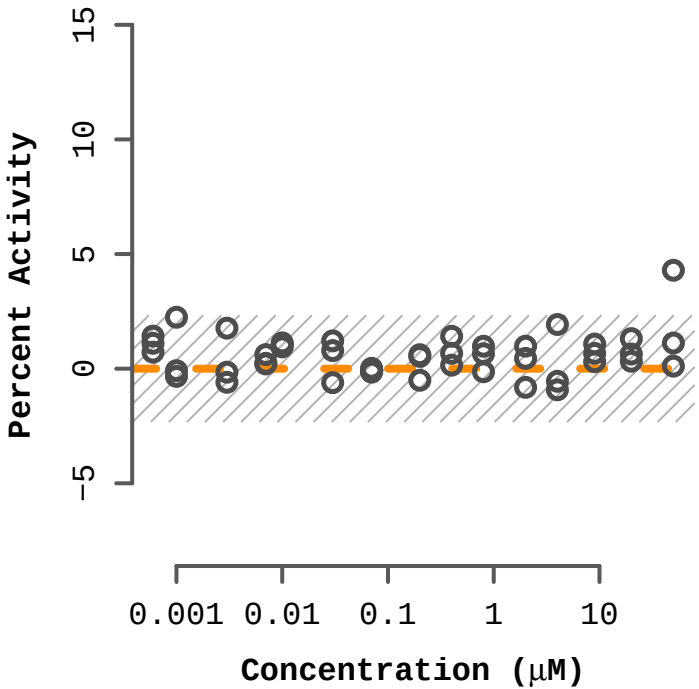
NAME: Halothane
CHID: 25371 CASRN: 151-67-7
SPID(S): Tox21_200850
M4ID: 12481402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.4	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.997 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

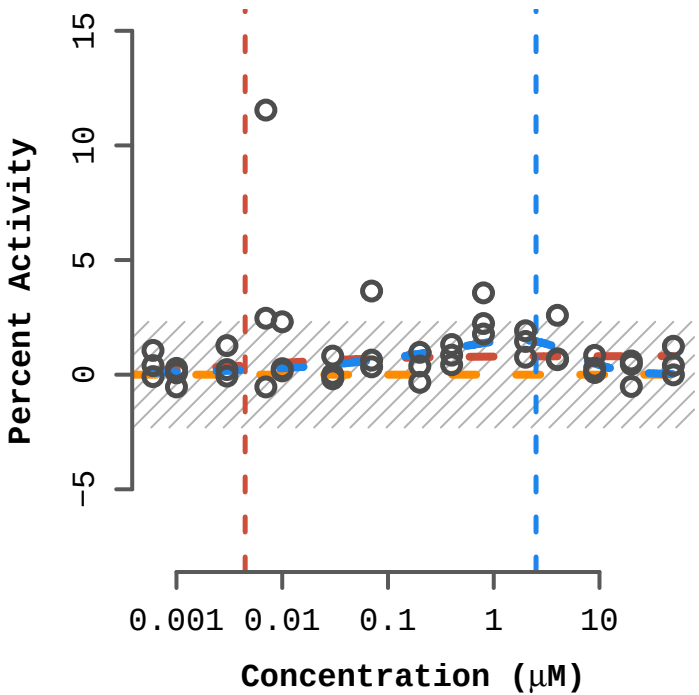
NAME: Halothane
CHID: 25371 **CASRN:** 151-67-7
SPID(S): Tox21_111033_1
M4ID: 12483939

HILL MODEL: Not applicable.

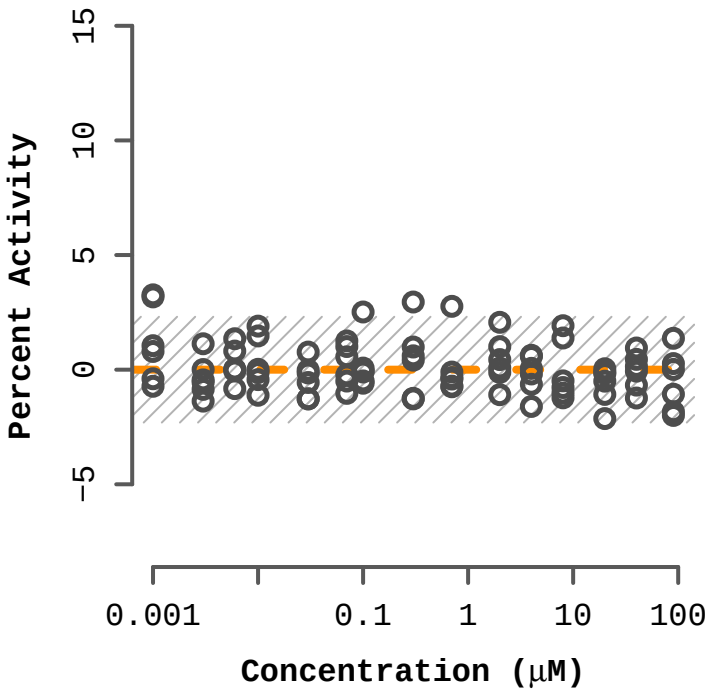
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.12 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hexadecylamine
CHID:    25390   CASRN: 143-27-1
SPID(S): Tox21_112293_1
M4ID:    12483178

HILL MODEL (in red):
      tp       ga       gw
val:  0.81     -2.35    0.666
sd:   0.2      0.963    0.582

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.82     0.4      0.458    0.65     1.99
sd:   10.1     3.84     0.338    0.509    1.2

      CNST        HILL        GNLS
AIC:  163.83      147.87      144.1
PROB: 0           0.13        0.87
RMSE: 2.13        1.91        1.91

MAX_MEAN: 4.49      MAX_MED: 2.46      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

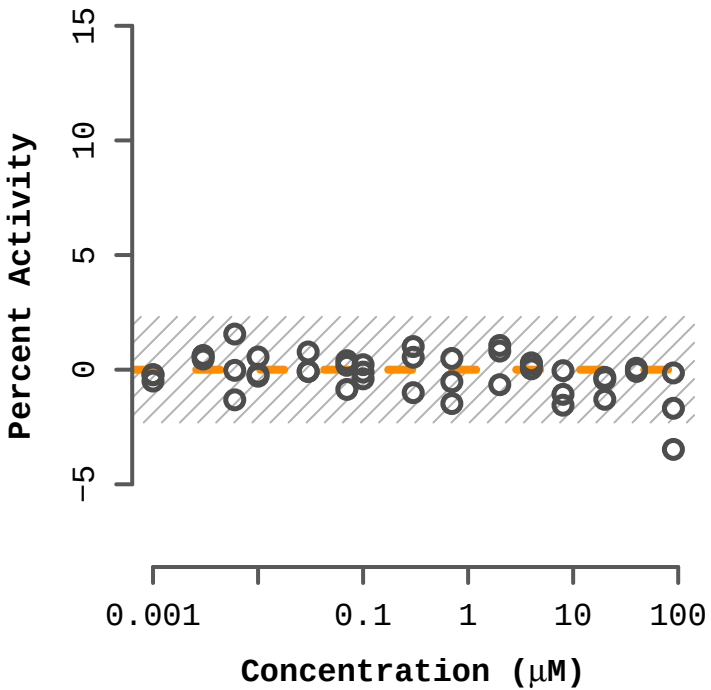
NAME: (2E,4E)-2,4-Hexadienal
CHID: 25391 **CASRN:** 142-83-6
SPID(S): Tox21_200834
M4ID: 12481418

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	278.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.922 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

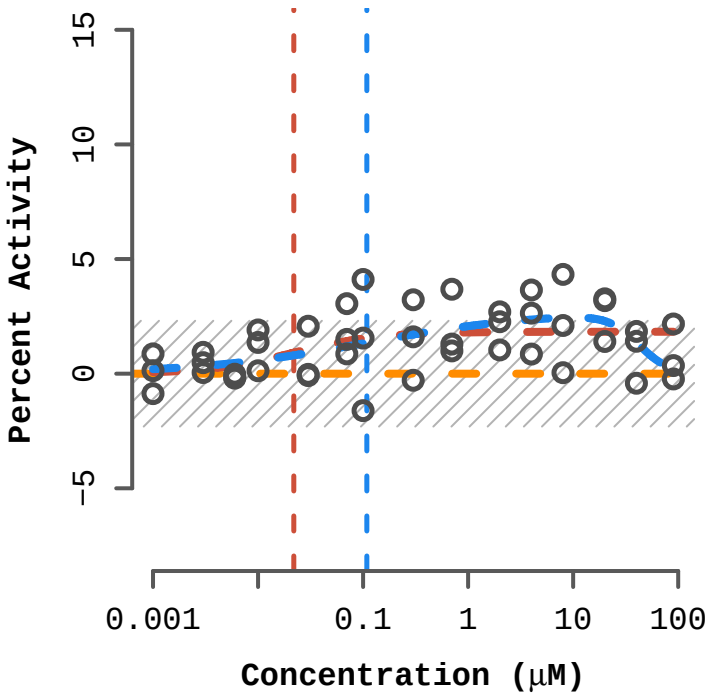
NAME: 1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol
CHID: 25394 **CASRN:** 4719-04-4
SPID(S): Tox21_303727
M4ID: 12475461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.553 **MAX_MED:** 0.812 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexamethyldisilazane
CHID: 25395 CASRN: 999-97-3
SPID(S): Tox21_303281
M4ID: 12475852

HILL MODEL (in red):

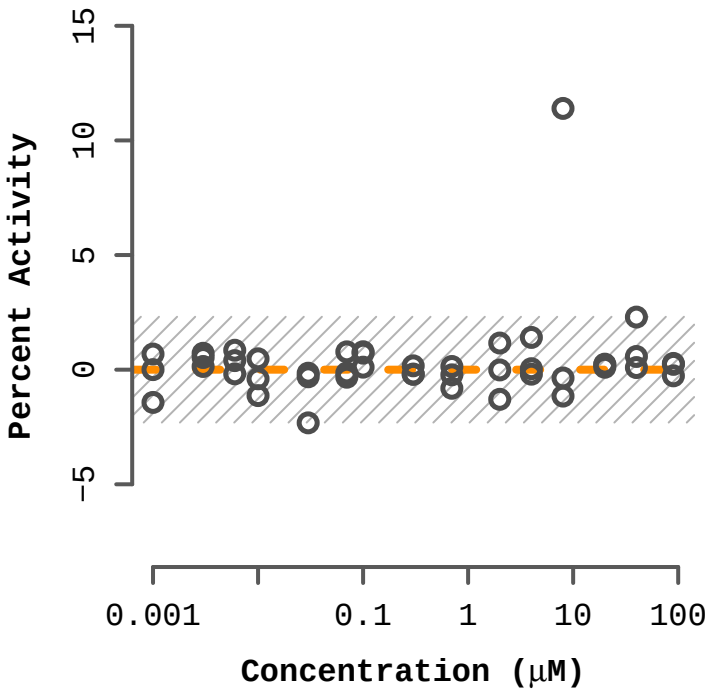
	tp	ga	gw
val:	1.83	−1.66	1.07
sd:	0.292	0.407	0.758

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.7	−0.964	0.541	1.62	3.03
sd:	1.41	1.33	0.495	0.233	4.43

	CNST	HILL	GNLS
AIC:	191.34	159.16	158.21
PROB:	0	0.38	0.62
RMSE:	1.93	1.26	1.2

MAX_MEAN: 2.62 MAX_MED: 3.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

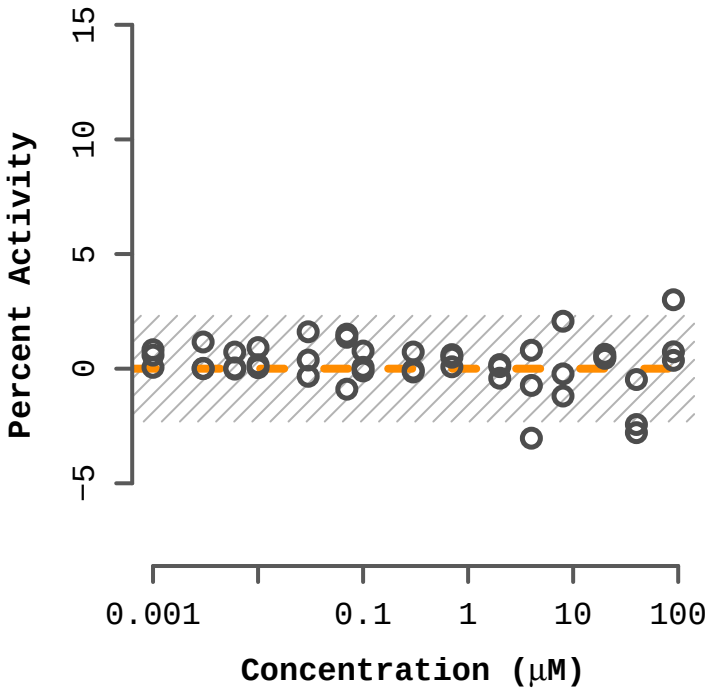
NAME: Hexamethyldisilazane
CHID: 25395 **CASRN:** 999-97-3
SPID(S): Tox21_202428
M4ID: 12479824

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 3.29 **MAX_MED:** 0.721 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

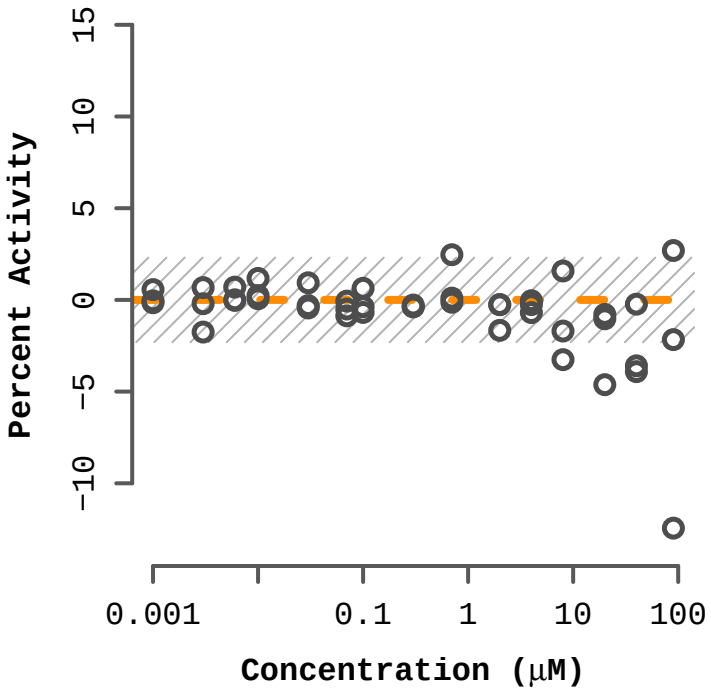
NAME: 1,6-Hexanediol diacrylate
CHID: 25401 **CASRN:** 13048-33-4
SPID(S): Tox21_303168
M4ID: 12475965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

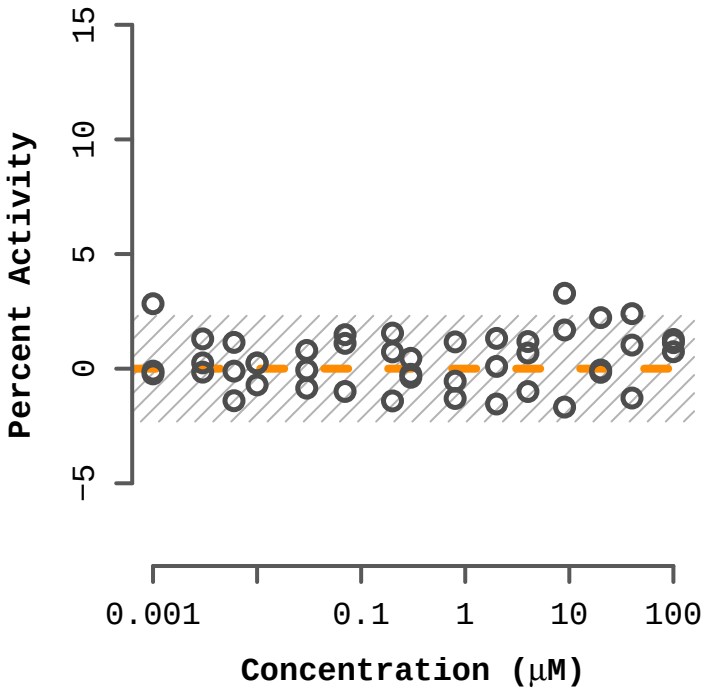
NAME: 1,6-Hexanediol diacrylate
CHID: 25401 **CASRN:** 13048-33-4
SPID(S): Tox21_201349
M4ID: 12480903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 0.813 **MAX_MED:** 0.238 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

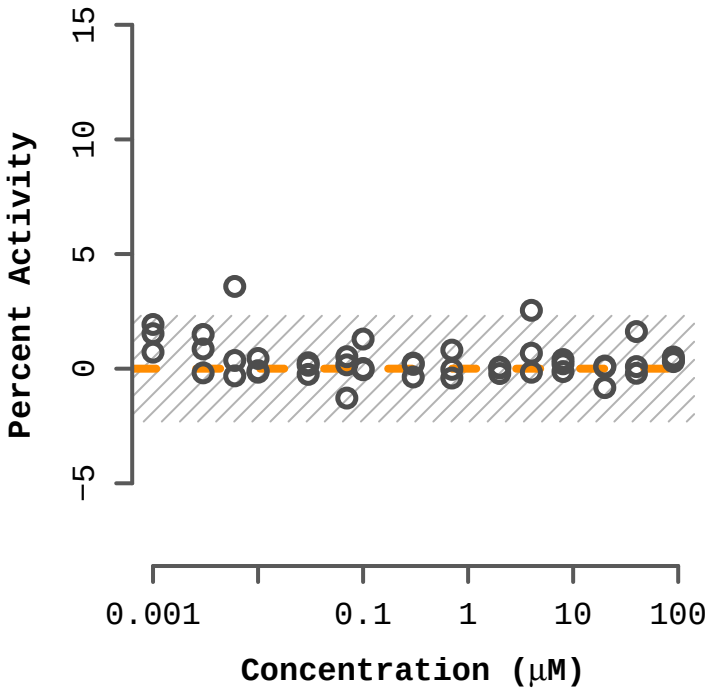
NAME: 1-Hexene
CHID: 25402 **CASRN:** 592-41-6
SPID(S): Tox21_200723
M4ID: 12481529

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

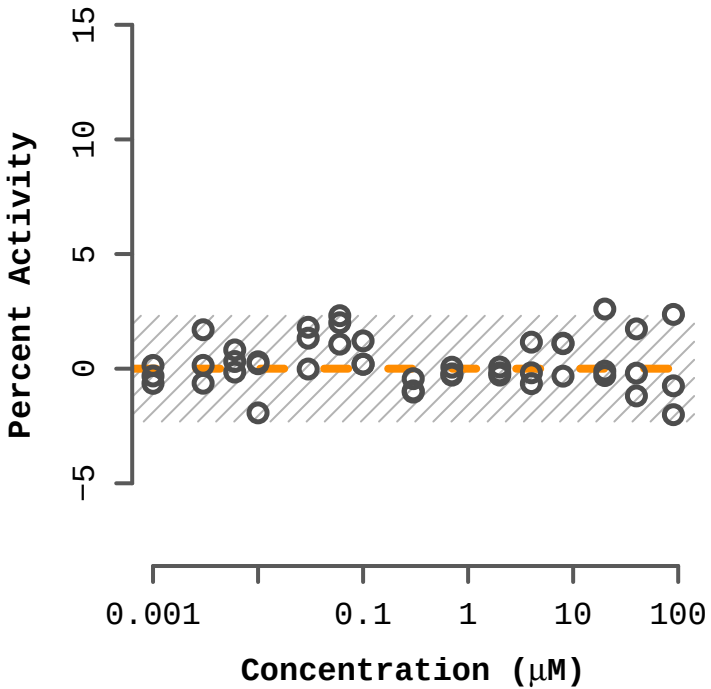
NAME: Hexyl benzoate
CHID: 25403 **CASRN:** 6789-88-4
SPID(S): Tox21_302347
M4ID: 12476786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

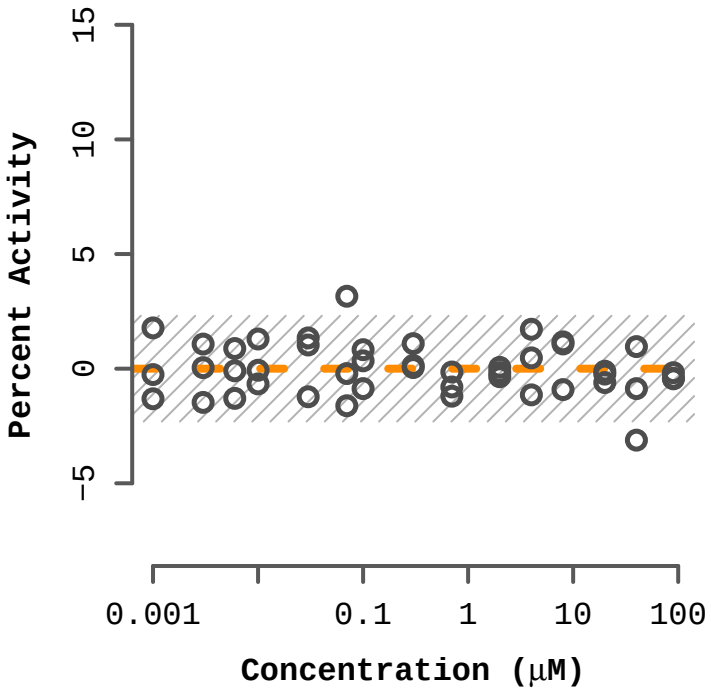
NAME: 4-Hexyl-4'-cyanobiphenyl
CHID: 25404 **CASRN:** 41122-70-7
SPID(S): Tox21_201123
M4ID: 12481129

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

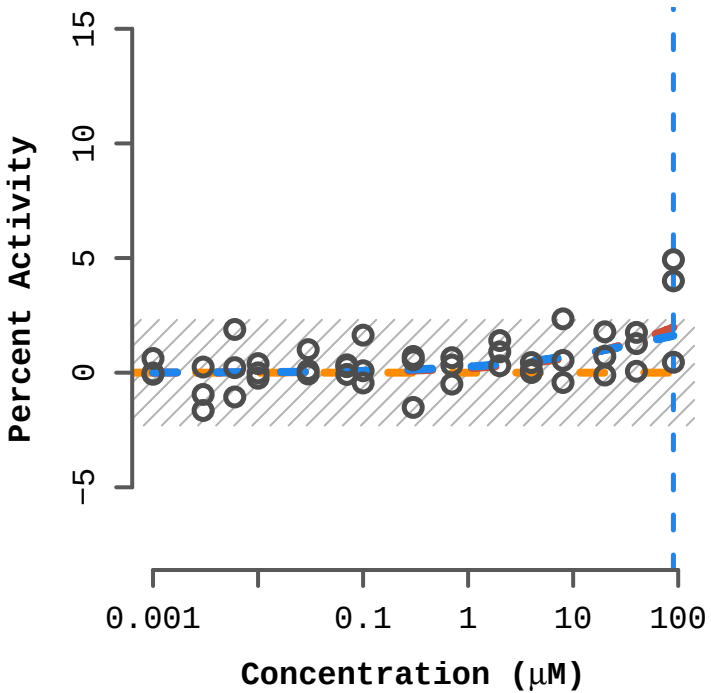
NAME: Hexyl methacrylate
CHID: 25406 **CASRN:** 142-09-6
SPID(S): Tox21_303323
M4ID: 12475810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.447 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexyl methacrylate
CHID: 25406 CASRN: 142-09-6
SPID(S): Tox21_201680
M4ID: 12480572

HILL MODEL (in red):

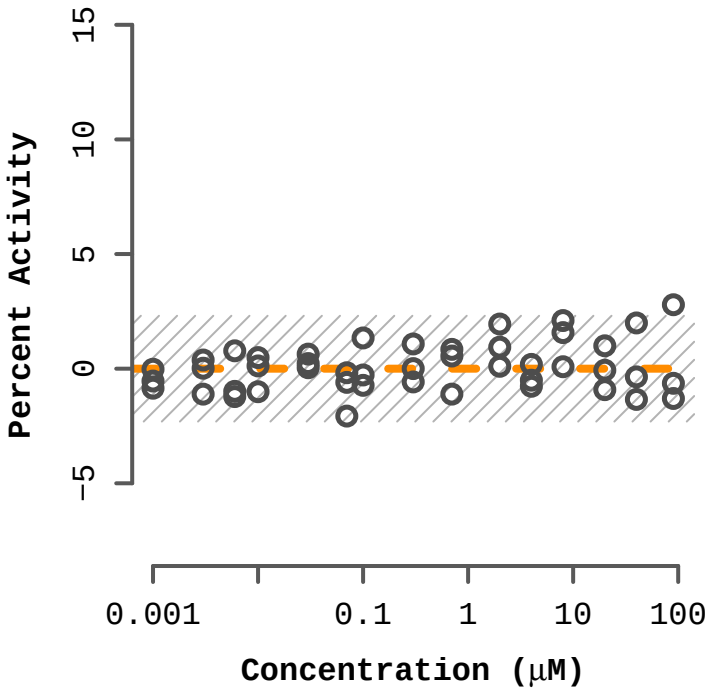
	tp	ga	gw
val:	5.92	2.45	0.6
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.23	1.95	0.54	3.95	5.21
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	139.89	130.46	134.77
PROB:	0.01	0.89	0.1
RMSE:	1.29	0.96	0.99

MAX_MEAN: 3.13 MAX_MED: 4.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

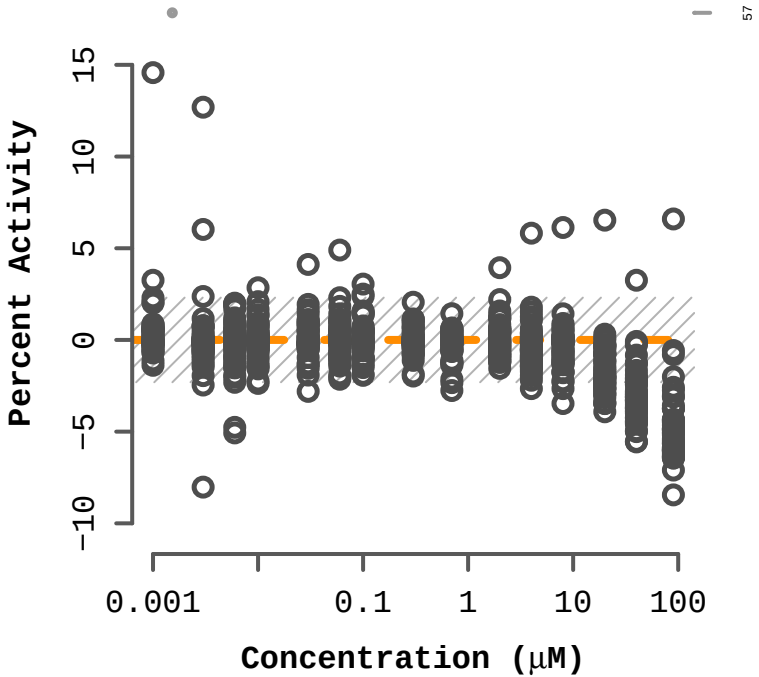
NAME: Hydrastine
CHID: 25409 CASRN: 118-08-1
SPID(S): Tox21_200686
M4ID: 12481566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.25 MAX_MED: 1.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

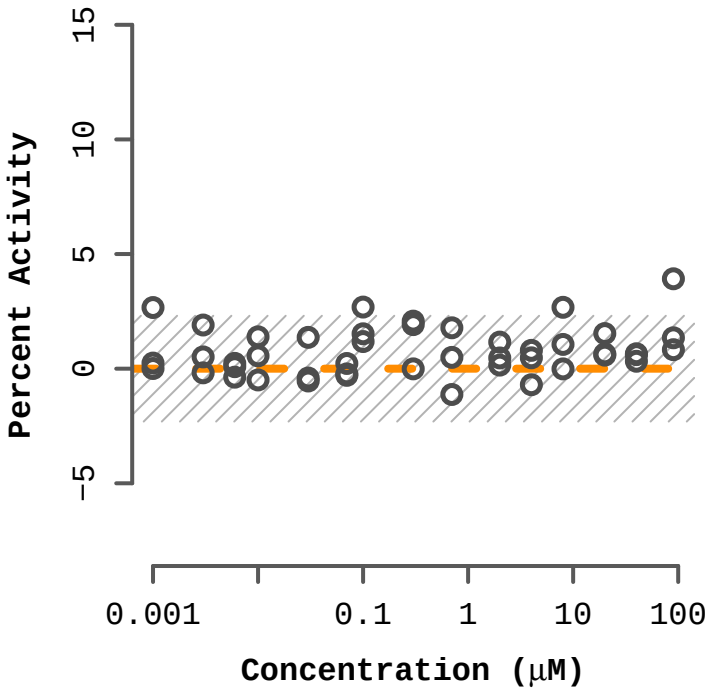
NAME: N-Hydroxybenzamide
CHID: 25421 **CASRN:** 495-18-1
SPID(S): Tox21_400060
M4ID: 12475077 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2900.31	NA	NA
PROB:	1	NA	NA
RMSE:	3	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 0.0511 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

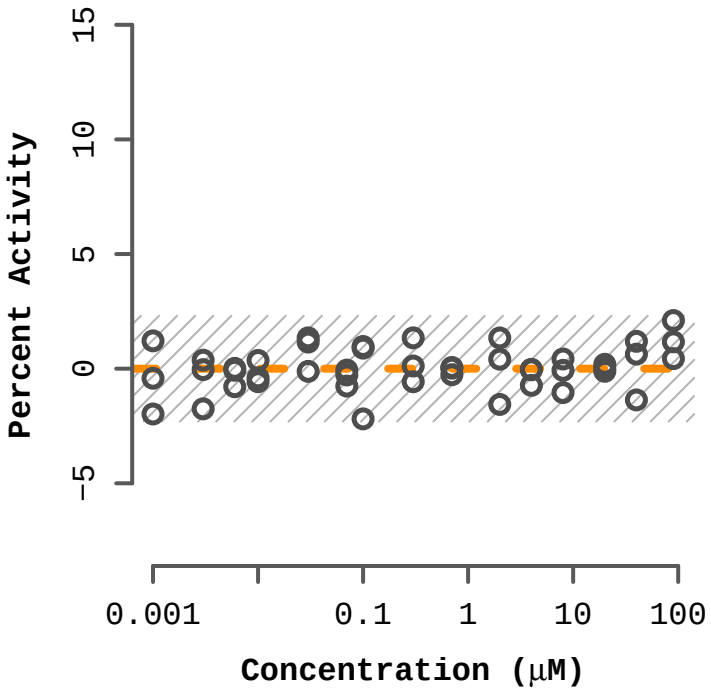
NAME: alpha−Hydroxybenzeneacetonitrile
CHID: 25422 **CASRN:** 532−28−5
SPID(S): Tox21_200804
M4ID: 12481448

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 2.03 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

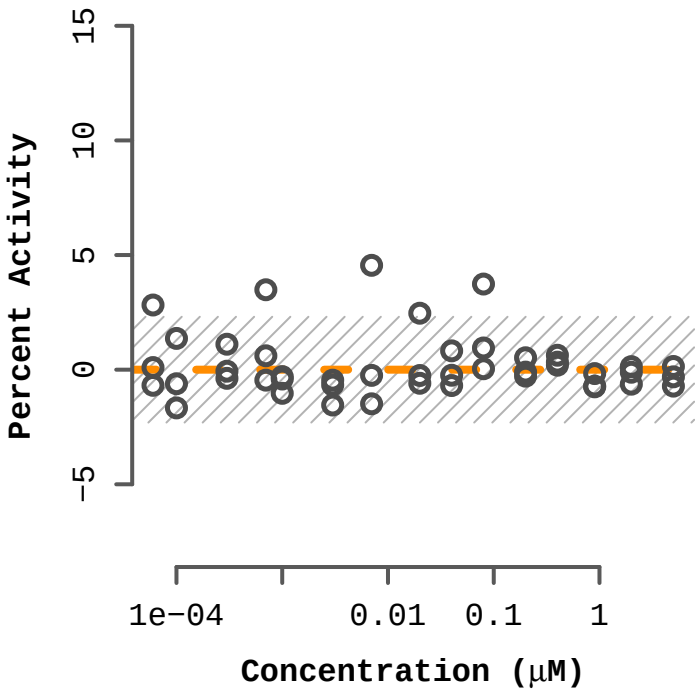
NAME: N−(Hydroxyethyl)ethylenediamine
CHID: 25423 **CASRN:** 111−41−1
SPID(S): Tox21_200209
M4ID: 12482043

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

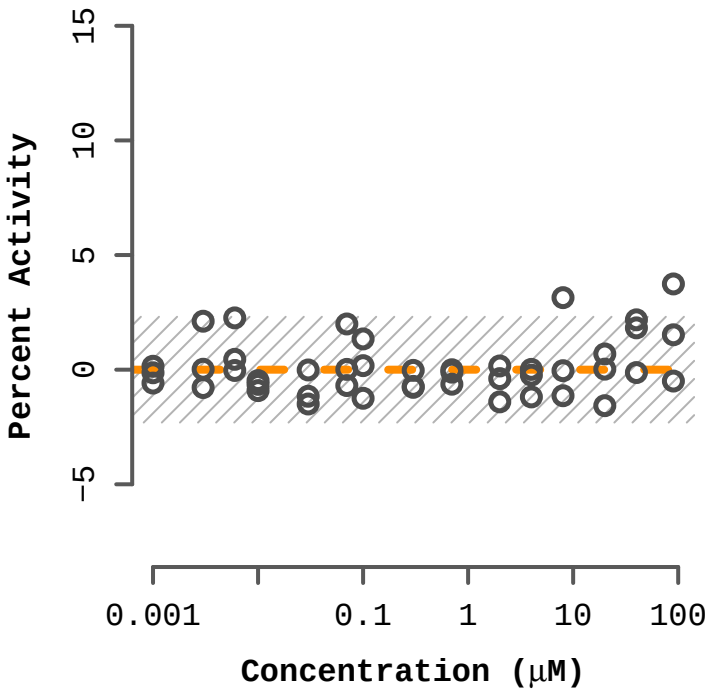
NAME: Hydroxylamine sulfate (2:1)
CHID: 25424 **CASRN:** 10039-54-0
SPID(S): Tox21_202730
M4ID: 12479522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

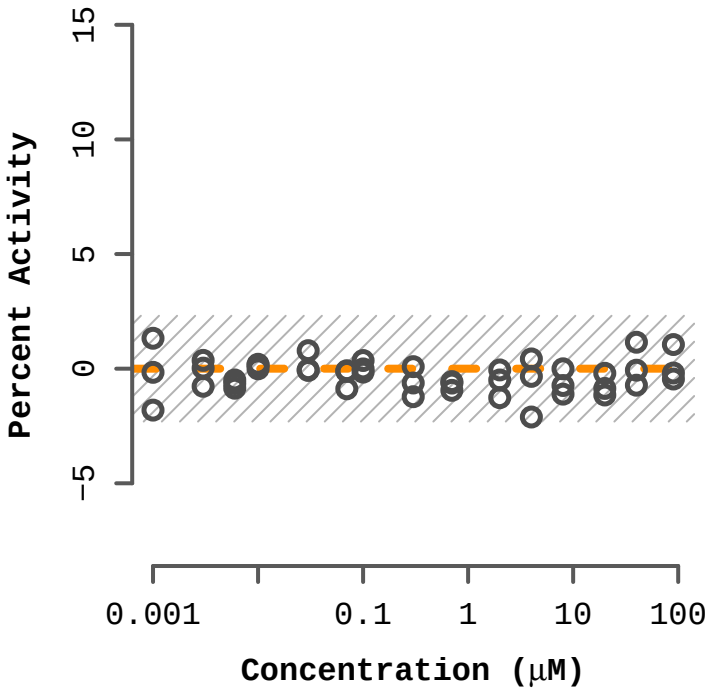
NAME: Hydroxylamine hydrochloride
CHID: 25425 **CASRN:** 5470-11-1
SPID(S): Tox21_202970
M4ID: 12479282

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

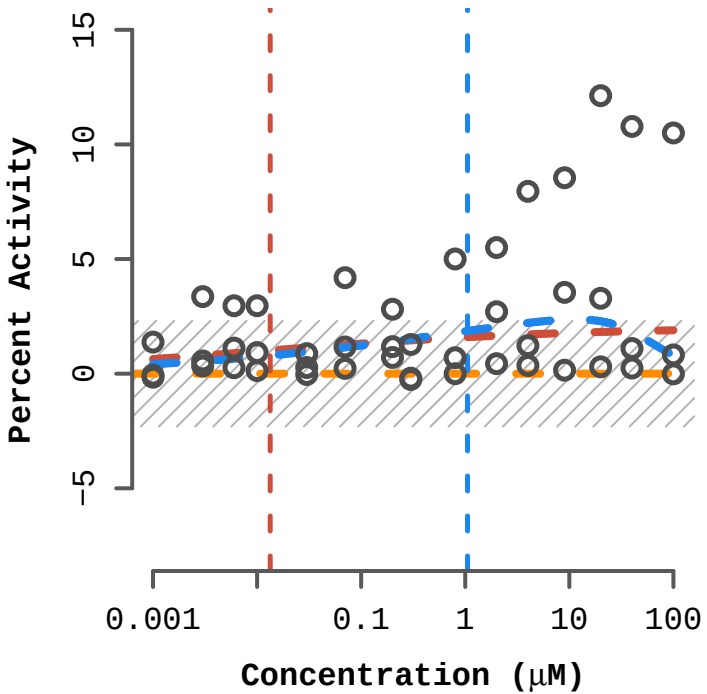
NAME: 2-Hydroxy-2-methylpropanenitrile
CHID: 25427 CASRN: 75-86-5
SPID(S): Tox21_303256
M4ID: 12475877

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.223 MAX_MED: 0.155 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxy-2-methylpropanenitrile
CHID: 25427 **CASRN:** 75-86-5
SPID(S): Tox21_201490
M4ID: 12480762

HILL MODEL (in red):

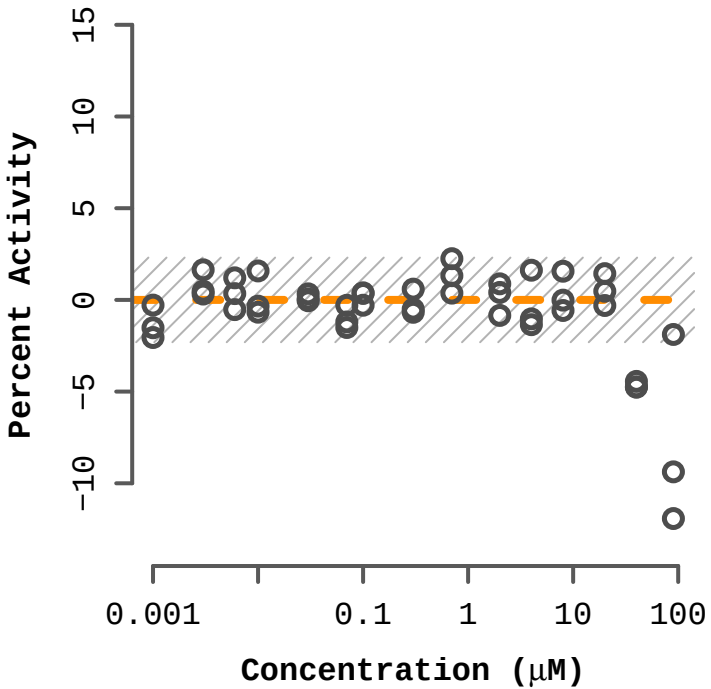
	tp	ga	gw
val:	2.02	−1.87	0.3
sd:	1.46	2.69	0.458

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.73	0.022	0.3	1.76	1.78
sd:	30.9	24.2	1.32	2.01	2.37

	CNST	HILL	GNLS
AIC:	236.16	223.05	226.17
PROB:	0	0.83	0.17
RMSE:	3.84	3.11	3.1

MAX_MEAN: 5.24 **MAX_MED:** 3.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

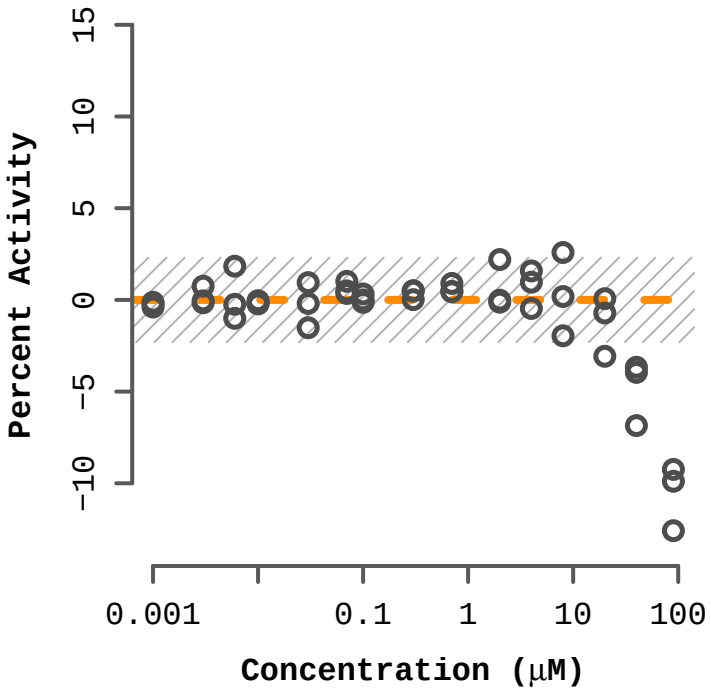
NAME: 6-Hydroxy-2-naphthyl disulfide
CHID: 25429 **CASRN:** 6088-51-3
SPID(S): Tox21_303354
M4ID: 12475779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

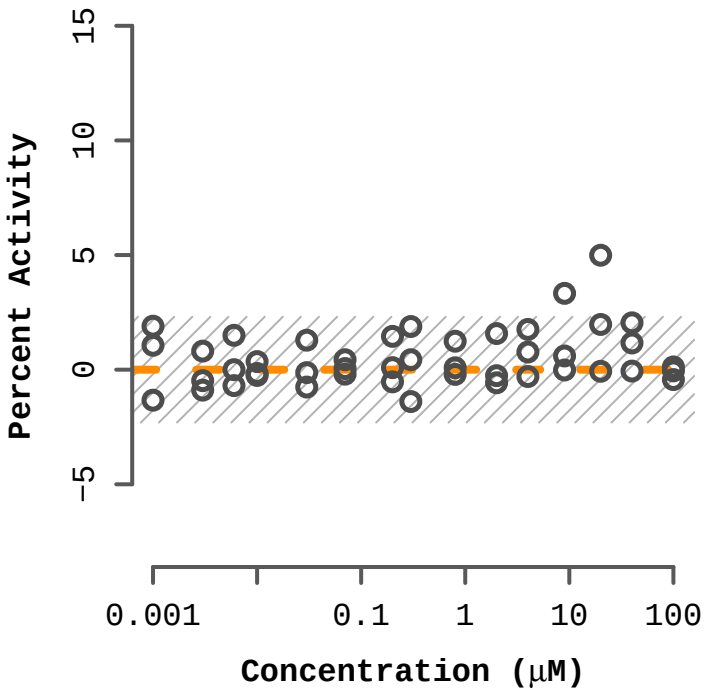
NAME: 6-Hydroxy-2-naphthyl disulfide
CHID: 25429 **CASRN:** 6088-51-3
SPID(S): Tox21_200789
M4ID: 12481463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.75	NA	NA
PROB:	1	NA	NA
RMSE:	3.19	NA	NA

MAX_MEAN: 0.694 **MAX_MED:** 0.967 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

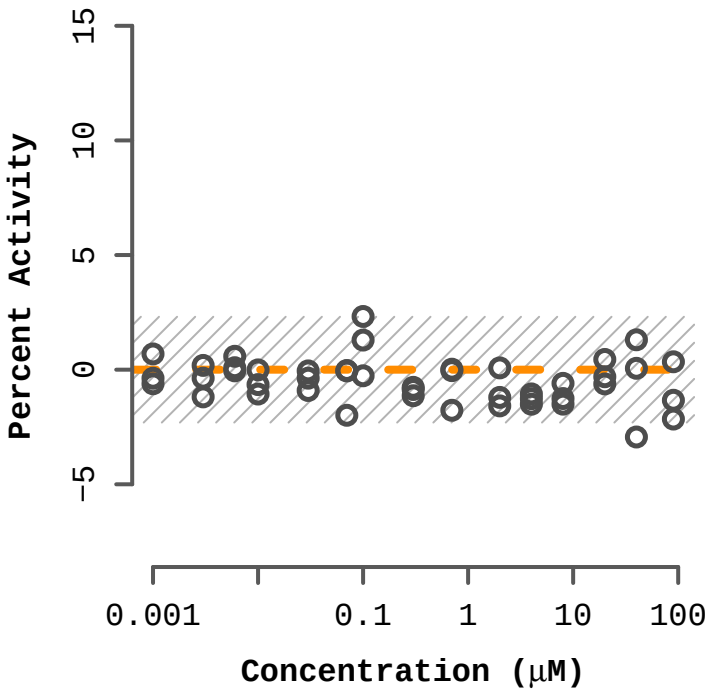
NAME: 3-Hydroxy-N-phenylaniline
CHID: 25431 **CASRN:** 101-18-8
SPID(S): Tox21_200308
M4ID: 12481944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

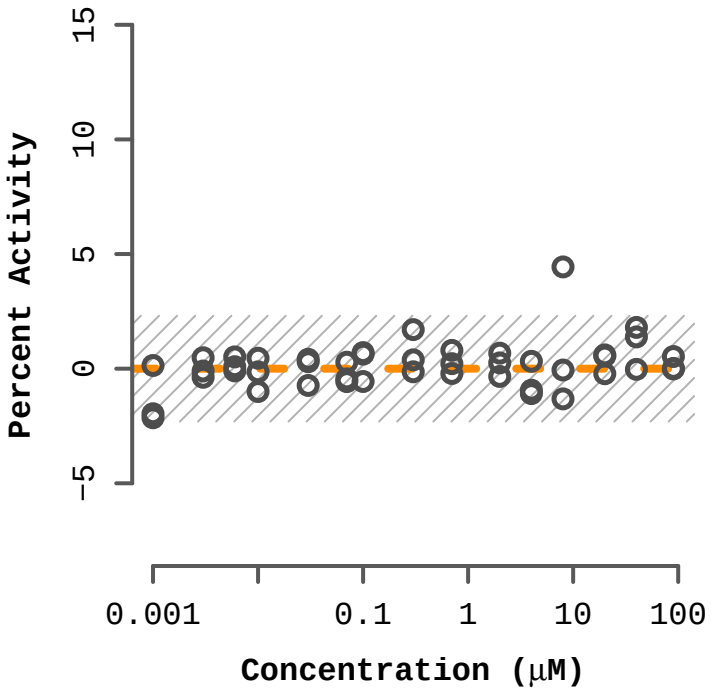
NAME: Lactonitrile
CHID: 25432 **CASRN:** 78-97-7
SPID(S): Tox21_303777
M4ID: 12475411

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

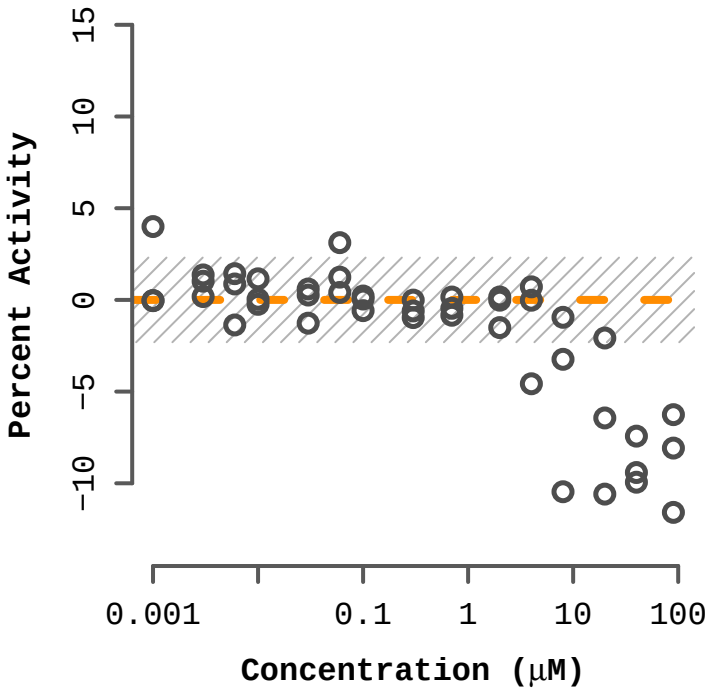
NAME: 3-Hydroxypropanenitrile
CHID: 25433 **CASRN:** 109-78-4
SPID(S): Tox21_303822
M4ID: 12475366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

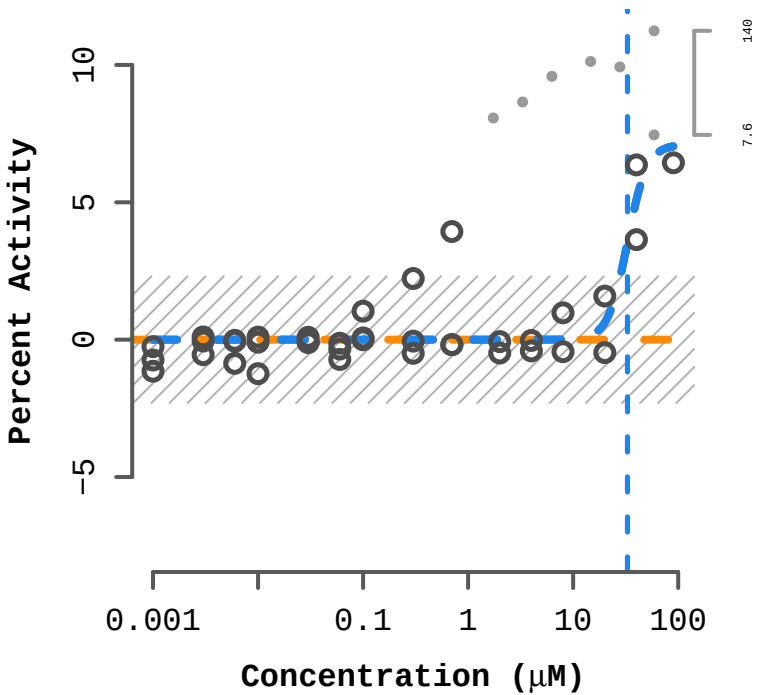
NAME: 8-Hydroxyquinoline sulfate
CHID: 25436 **CASRN:** 134-31-6
SPID(S): Tox21_303537
M4ID: 12475607

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.73	NA	NA
PROB:	1	NA	NA
RMSE:	4.28	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: L-5-Hydroxytryptophan
CHID: 25437 CASRN: 4350-09-8
SPID(S): Tox21_201032
M4ID: 12481220 BRK

HILL MODEL (in red):

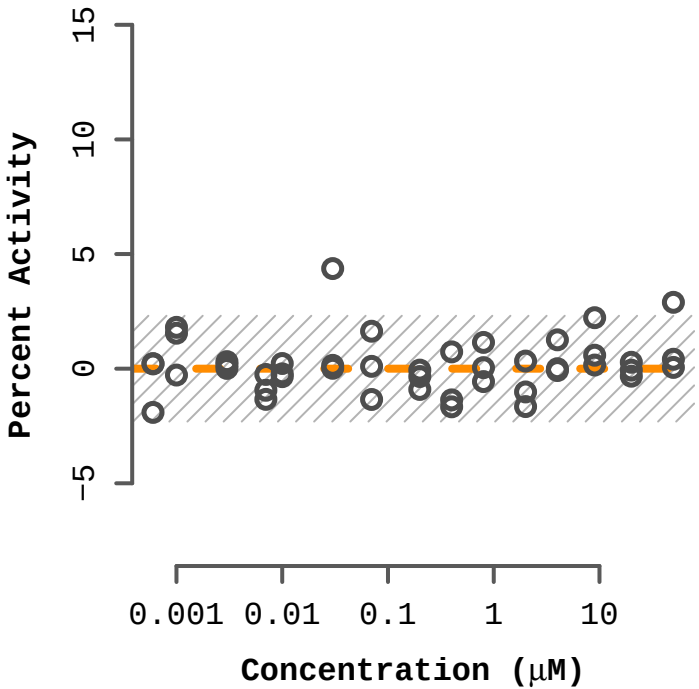
	tp	ga	gw
val:	7.1	1.52	4.7
sd:	0.954	0.0814	3.07

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.1	1.52	4.7	3.89	8.58
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	356.87	337.46	341.46
PROB:	0	0.88	0.12
RMSE:	32.65	31.58	31.58

MAX_MEAN: 50.9 MAX_MED: 7.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

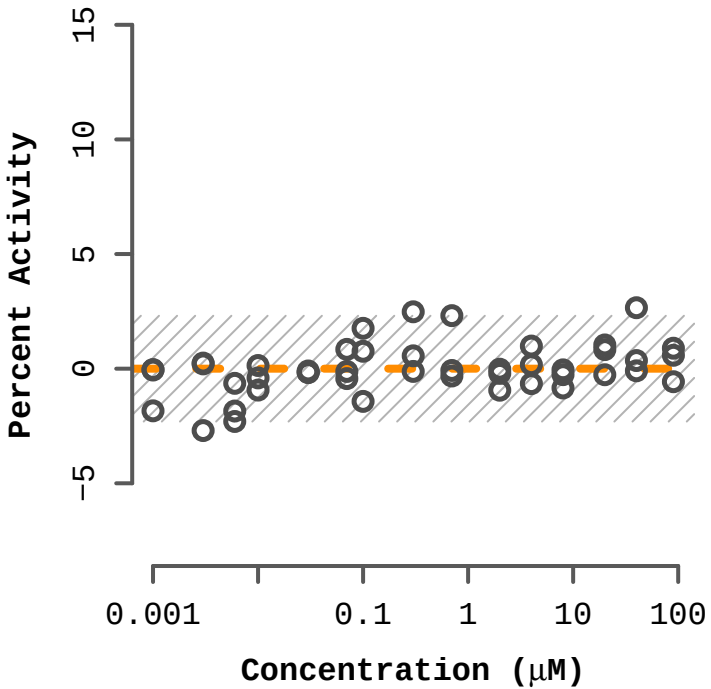
NAME: L−5−Hydroxytryptophan
CHID: 25437 CASRN: 4350−09−8
SPID(S): Tox21_111073_1
M4ID: 12483922

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

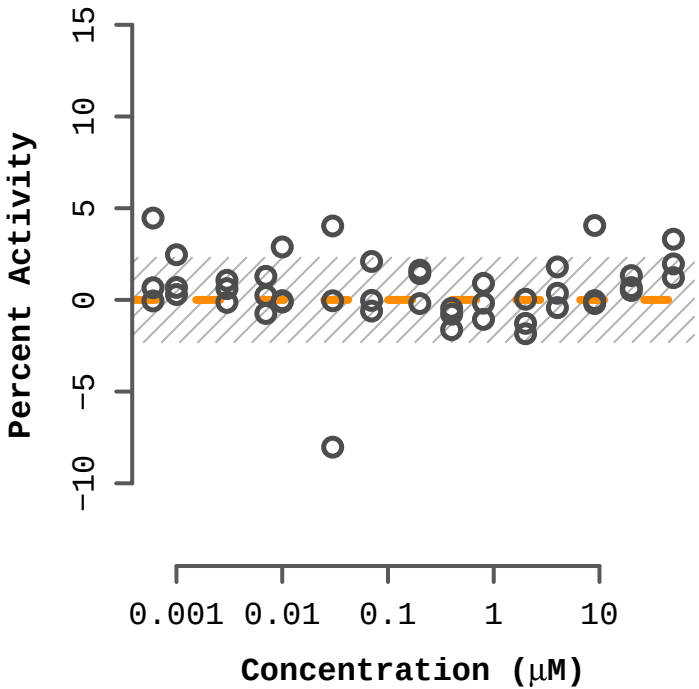
NAME: Hydroxyurea
CHID: 25438 CASRN: 127-07-1
SPID(S): Tox21_300319
M4ID: 12478812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.976 MAX_MED: 0.833 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

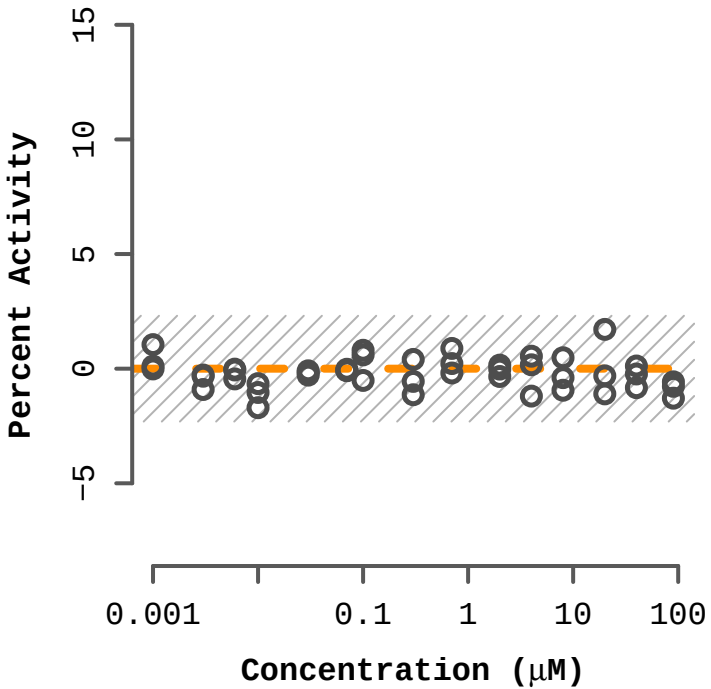
NAME: Hydroxyurea
CHID: 25438 **CASRN:** 127-07-1
SPID(S): Tox21_110168_1
M4ID: 12484589

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

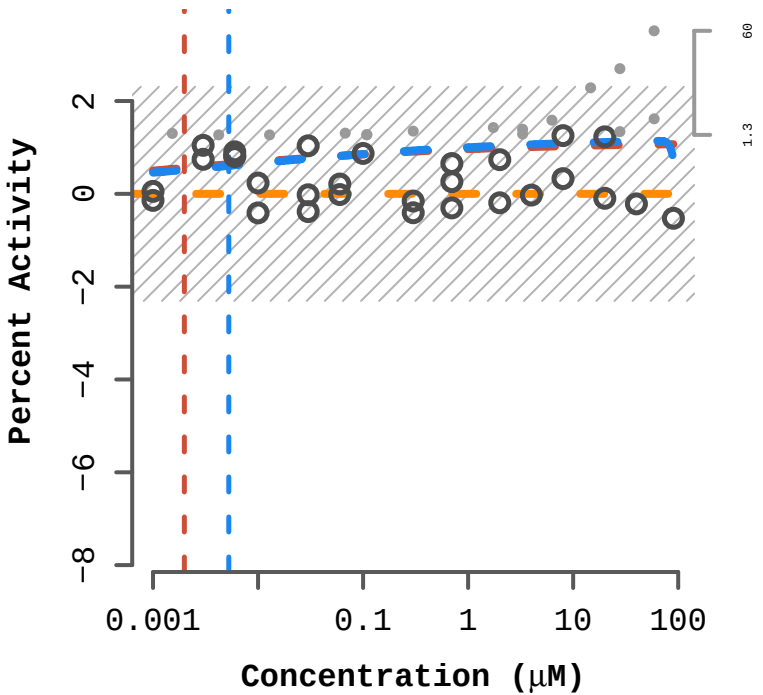
NAME: Iminobis−3−propylamine
CHID: 25440 **CASRN:** 56−18−8
SPID(S): Tox21_202847
M4ID: 12479405

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.385 **MAX_MED:** 0.602 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Iodoethylbenzene
CHID: 25447 CASRN: 17376-04-4
SPID(S): Tox21_200053
M4ID: 12482199 BRK

HILL MODEL (in red):

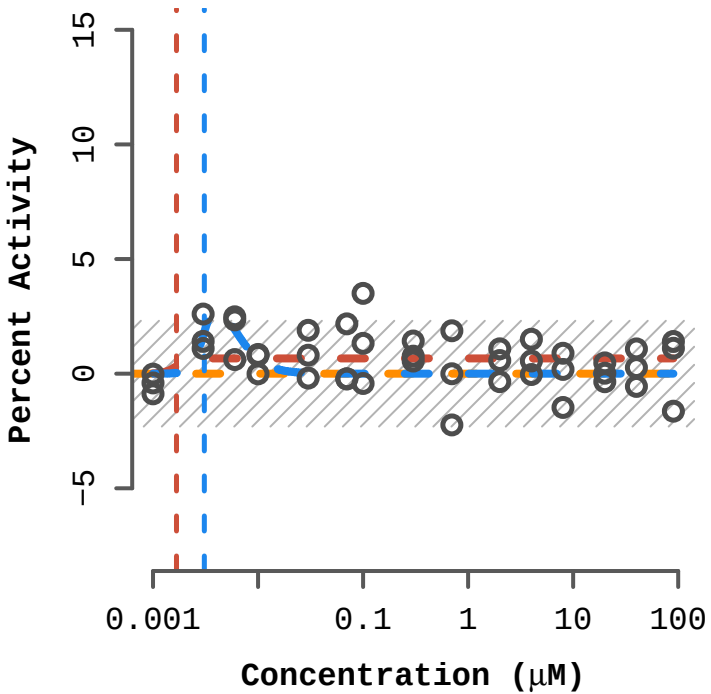
	tp	ga	gw
val:	1.11	−2.7	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.21	−2.28	0.3	1.97	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	264.63	260.38	264.35
PROB:	0.09	0.8	0.11
RMSE:	11.66	11.33	11.36

MAX_MEAN: 23.2 MAX_MED: 10.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Iodo-3-nitrobenzene
CHID: 25449 CASRN: 645-00-1
SPID(S): Tox21_201085
M4ID: 12481167

HILL MODEL (in red):

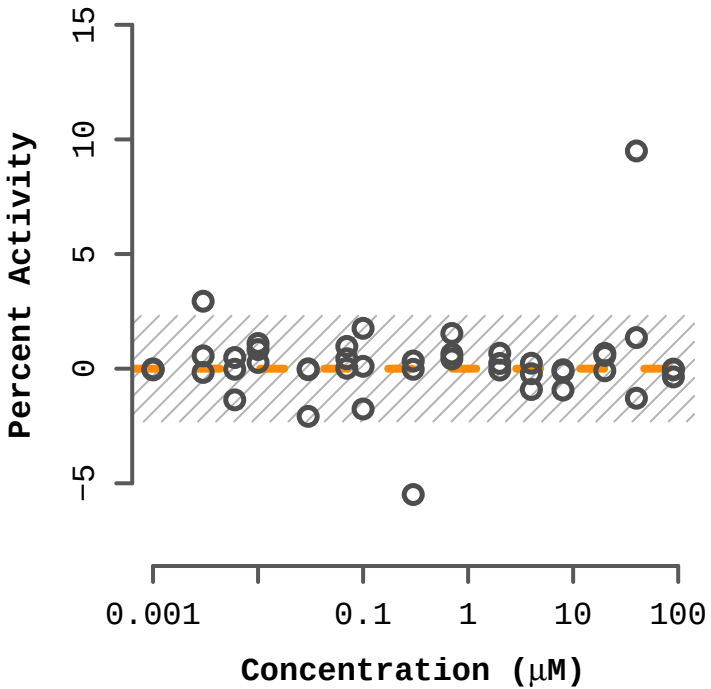
	tp	ga	gw
val:	0.666	−2.78	8
sd:	0.163	0.279	9.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.21	−2.51	8	−2.25	3.03
sd:	12.6	0.17	24.8	0.891	7.12

	CNST	HILL	GNLS
AIC:	153.58	144.97	147.52
PROB:	0.01	0.77	0.22
RMSE:	1.28	1.11	1.1

MAX_MEAN: 1.82 MAX_MED: 2.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

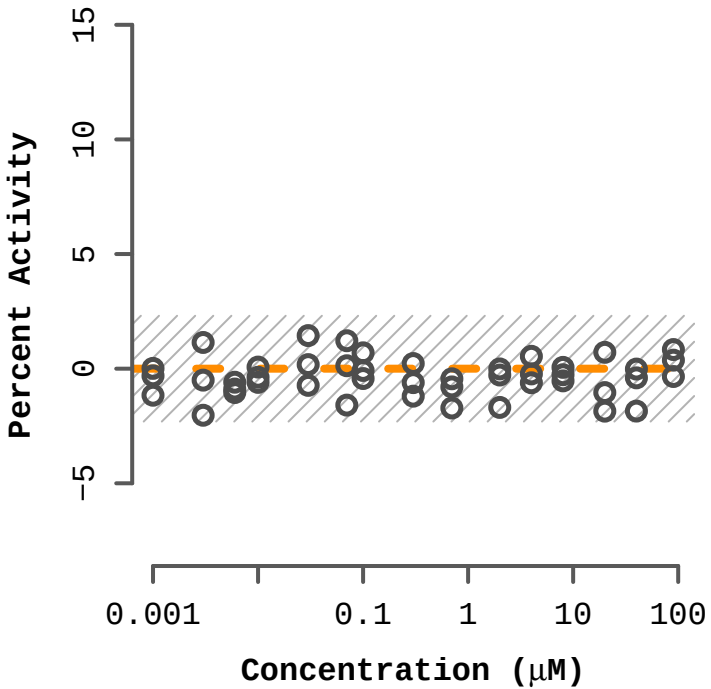
NAME: 4-(2,6,6-Trimethyl-cyclohex-1-enyl)-but-3-en-2-
CHID: 25451 CASRN: 14901-07-6
SPID(S): Tox21_300709
M4ID: 12478424

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 3.19 MAX_MED: 1.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

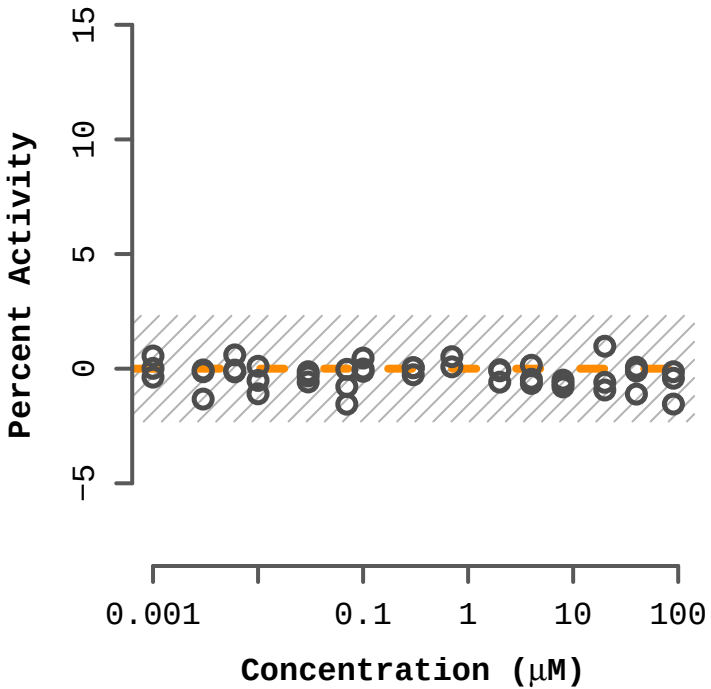
NAME: 3-Methylbutyl acetate
CHID: 25453 **CASRN:** 123-92-2
SPID(S): Tox21_300373
M4ID: 12478759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.299 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

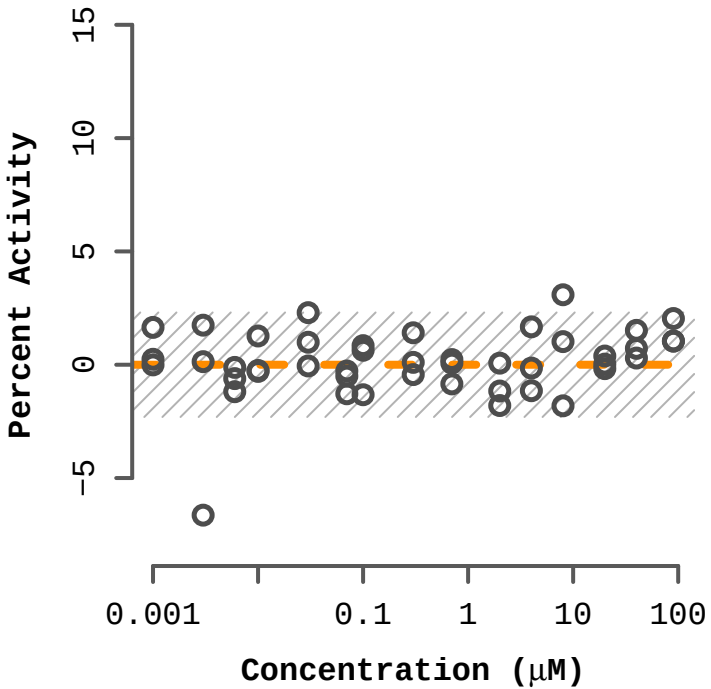
NAME: 3-Methylbutyl acetate
CHID: 25453 **CASRN:** 123-92-2
SPID(S): Tox21_201257
M4ID: 12480995

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	82.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.303 **MAX_MED:** 0.303 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

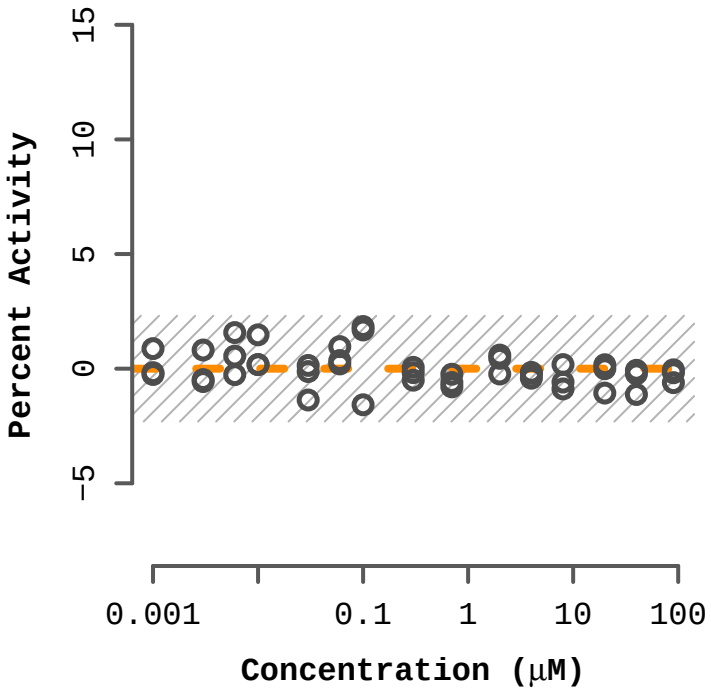
NAME: 3-Methylbutyl cinnamate
CHID: 25454 **CASRN:** 7779-65-9
SPID(S): Tox21_200007
M4ID: 12482245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

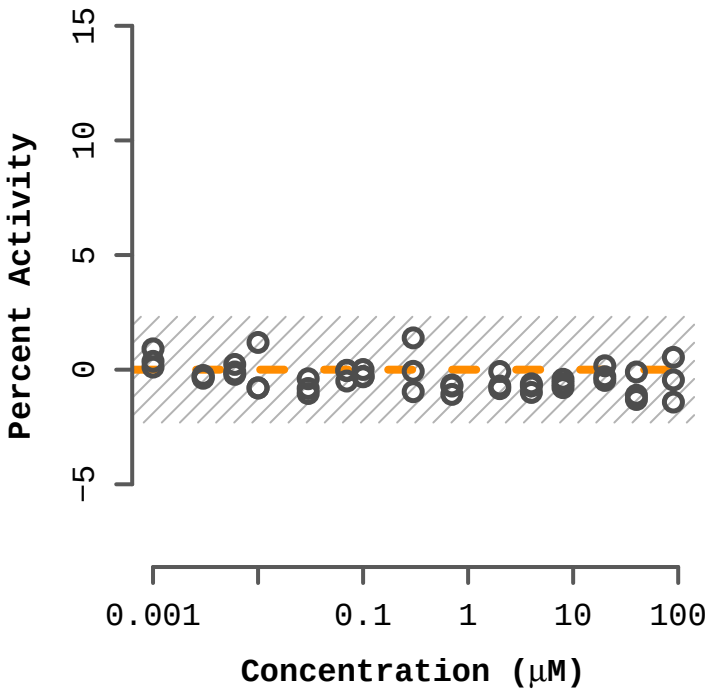
NAME: 3-Methylbutyl nitrite
CHID: 25455 **CASRN:** 110-46-3
SPID(S): Tox21_200983
M4ID: 12481269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.652 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

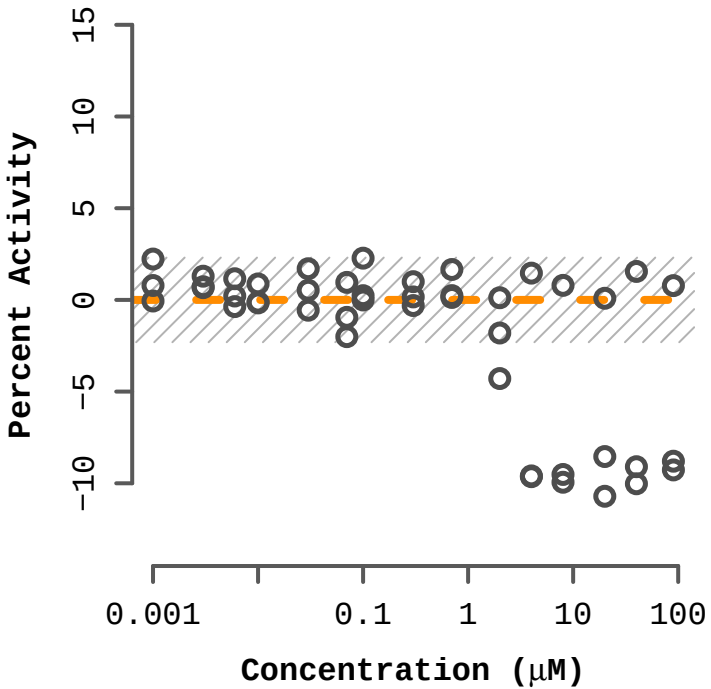
NAME: Isobutyl methacrylate
CHID: 25461 **CASRN:** 97-86-9
SPID(S): Tox21_303327
M4ID: 12475806

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.462 **MAX_MED:** 0.364 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

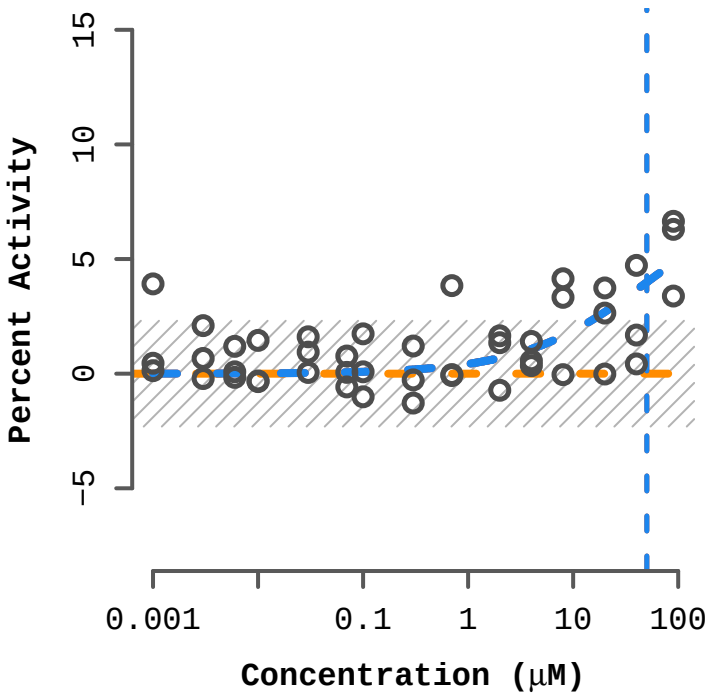
NAME: Isobutyl methacrylate
CHID: 25461 **CASRN:** 97-86-9
SPID(S): Tox21_201568
M4ID: 12480684

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.82	NA	NA
PROB:	1	NA	NA
RMSE:	4.63	NA	NA

MAX_MEAN: 0.985 **MAX_MED:** 0.787 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isocyanatocyclohexane
CHID: 25464 CASRN: 3173-53-3
SPID(S): Tox21_200234
M4ID: 12482018

HILL MODEL (in red):

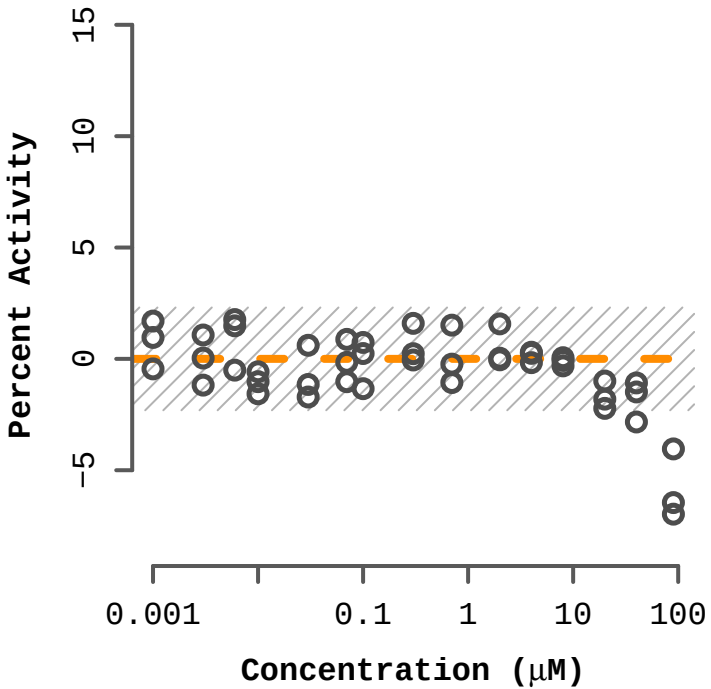
	tp	ga	gw
val:	7.98	1.7	0.734
sd:	4.96	0.717	0.298

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.98	1.7	0.734	3.33	6.18
sd:	4.97	0.718	0.297	1740	7840

	CNST	HILL	GNLS
AIC:	196.57	170.13	174.13
PROB:	0	0.88	0.12
RMSE:	2.25	1.46	1.46

MAX_MEAN: 5.44 MAX_MED: 6.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

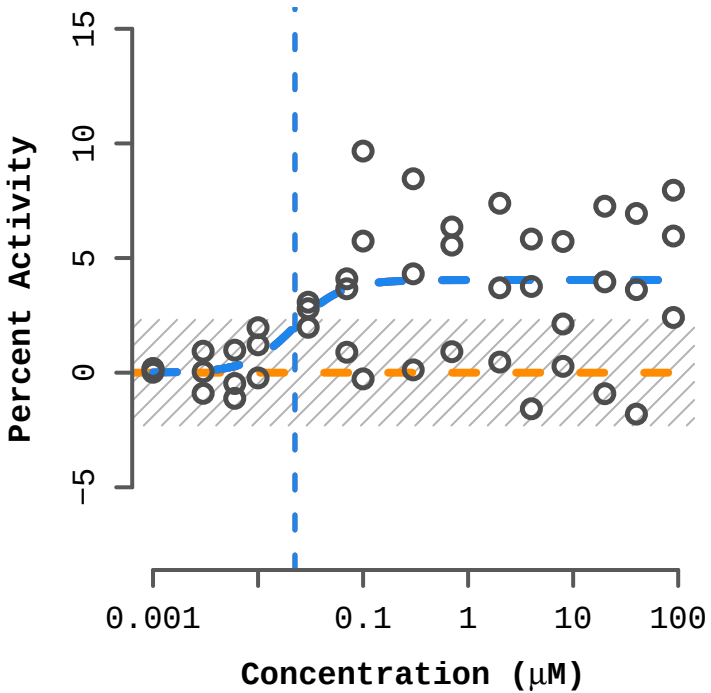
NAME: Isodecyl diphenyl phosphate
CHID: 25465 **CASRN:** 29761-21-5
SPID(S): Tox21_202981
M4ID: 12479271

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.916 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isodecyl methacrylate
CHID: 25466 CASRN: 29964-84-9
SPID(S): Tox21_200421
M4ID: 12481831

HILL MODEL (in red):

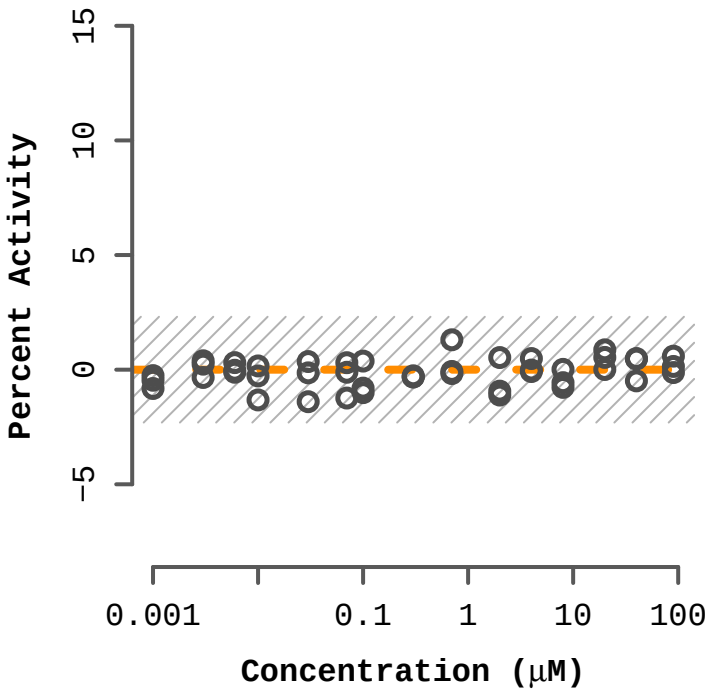
	tp	ga	gw
val:	4.04	−1.65	1.96
sd:	0.592	0.236	1.36

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.04	−1.65	1.96	3.95	3.11
sd:	0.592	0.236	1.36	307	480

	CNST	HILL	GNLS
AIC:	257.79	222.51	226.51
PROB:	0	0.88	0.12
RMSE:	4.07	2.59	2.59

MAX_MEAN: 5.44 **MAX_MED:** 5.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

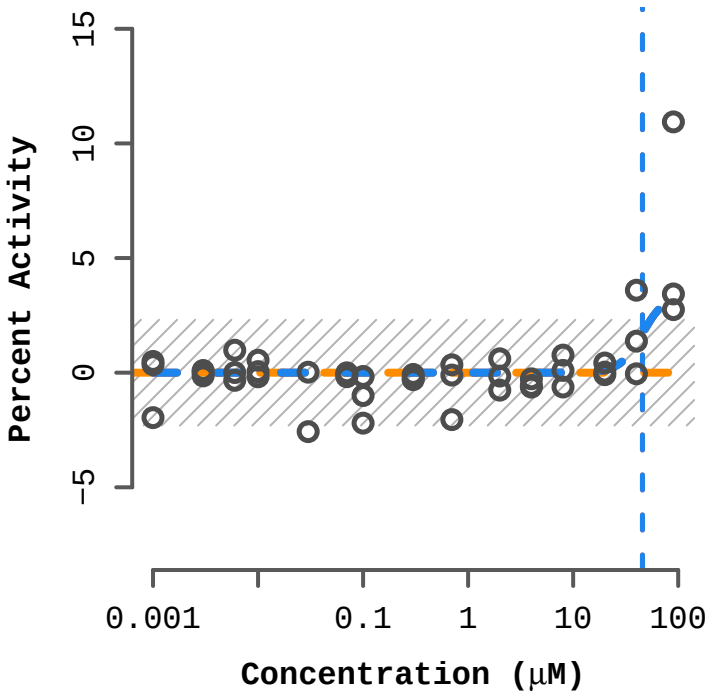
NAME: Isopentyl alcohol
CHID: 25469 CASRN: 123-51-3
SPID(S): Tox21_302359
M4ID: 12476774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	85.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.6	NA	NA

MAX_MEAN: 0.471 **MAX_MED:** 0.536 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isophytol
CHID: 25474 **CASRN:** 505-32-8
SPID(S): Tox21_200139
M4ID: 12482113

HILL MODEL (in red):

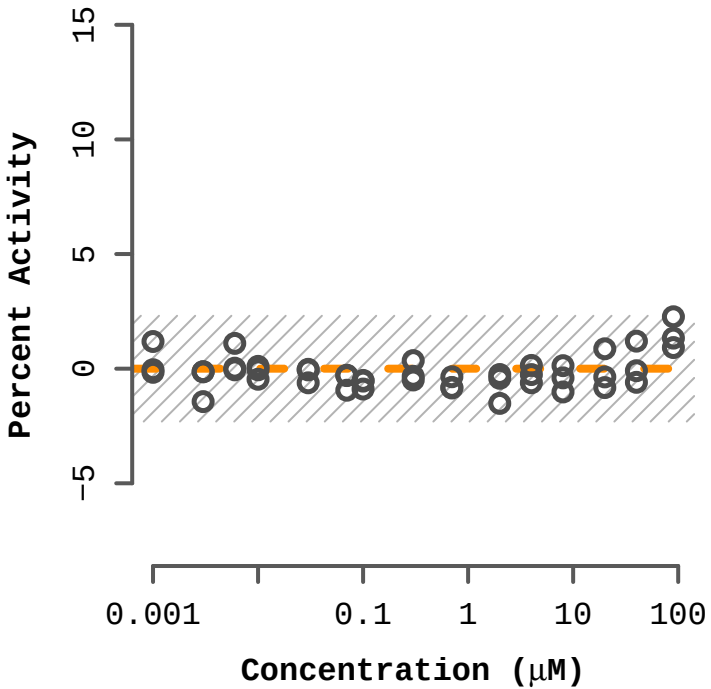
	tp	ga	gw
val:	3.41	1.66	4.04
sd:	1.01	0.154	4.34

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.41	1.66	4.04	2.92	6.67
sd:	0.978	0.153	4.34	41600	293000

	CNST	HILL	GNLS
AIC:	147	127.84	131.84
PROB:	0	0.88	0.12
RMSE:	2.02	1.45	1.45

MAX_MEAN: 5.71 **MAX_MED:** 3.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

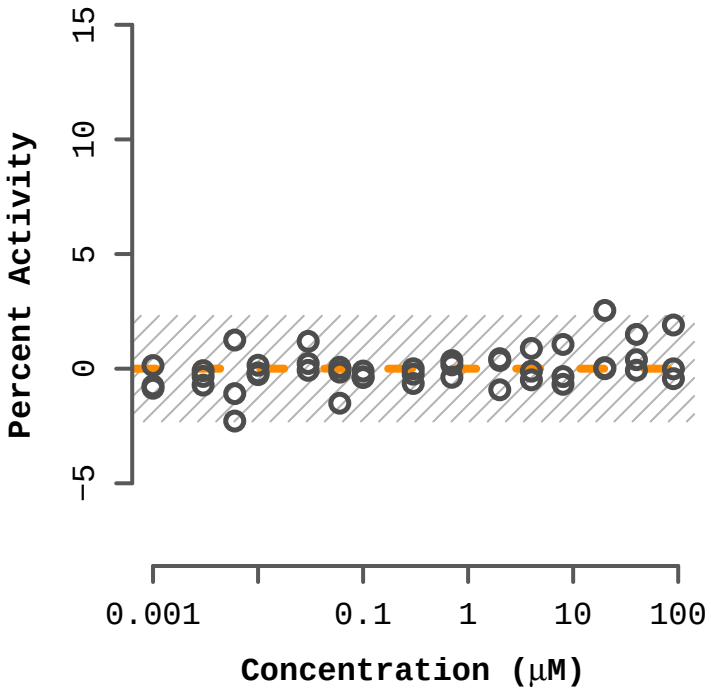
NAME: Isopropyl acetate
CHID: 25478 CASRN: 108-21-4
SPID(S): Tox21_303287
M4ID: 12475846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.51 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

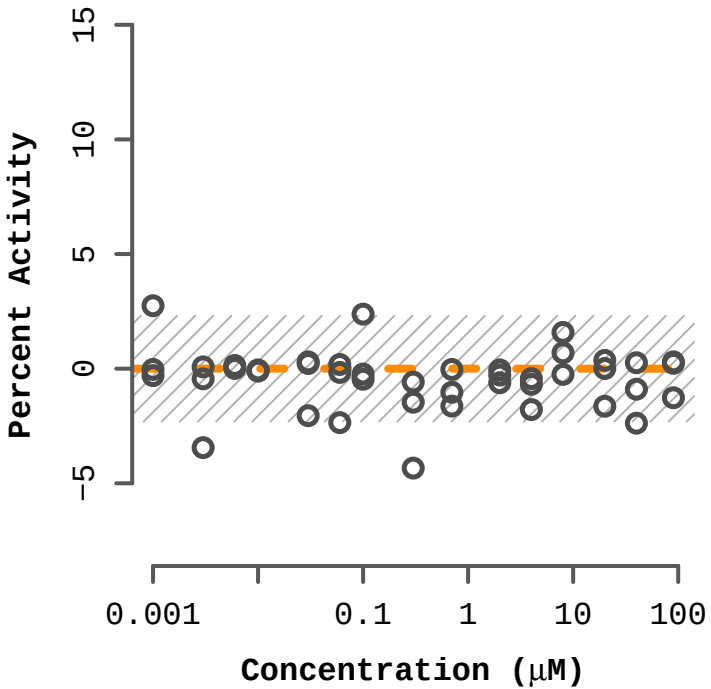
NAME: Isopropyl acetate
CHID: 25478 **CASRN:** 108-21-4
SPID(S): Tox21_201443
M4ID: 12480809

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.863 **MAX_MED:** 0.393 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

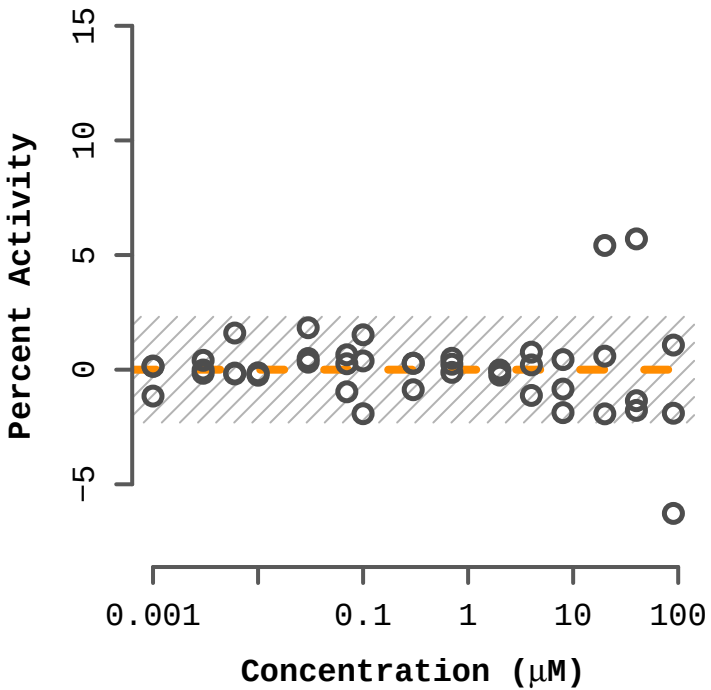
NAME: N-Isopropylaniline
CHID: 25479 **CASRN:** 768-52-5
SPID(S): Tox21_200360
M4ID: 12481892

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 0.694 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

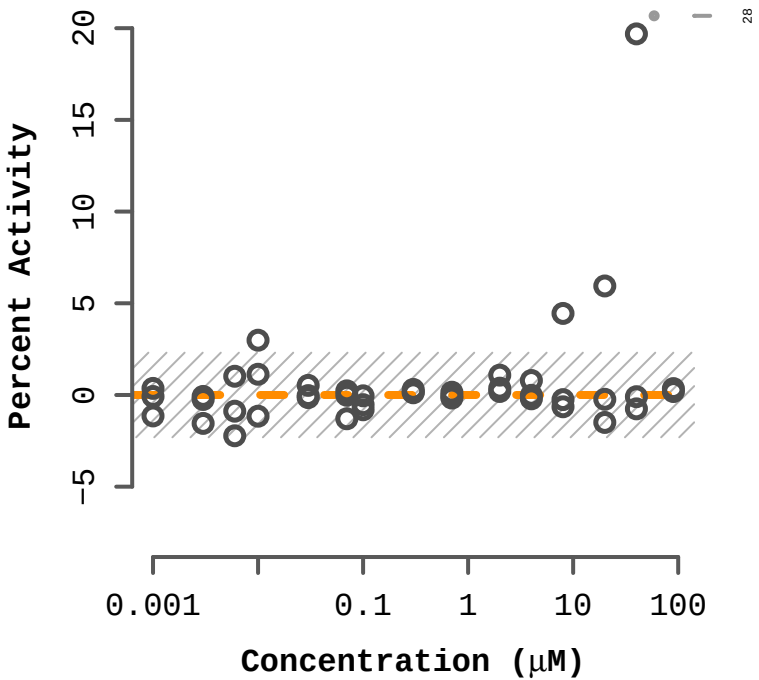
NAME: Isopropyl glycidyl ether
CHID: 25480 CASRN: 4016-14-2
SPID(S): Tox21_200038
M4ID: 12482214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.591 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

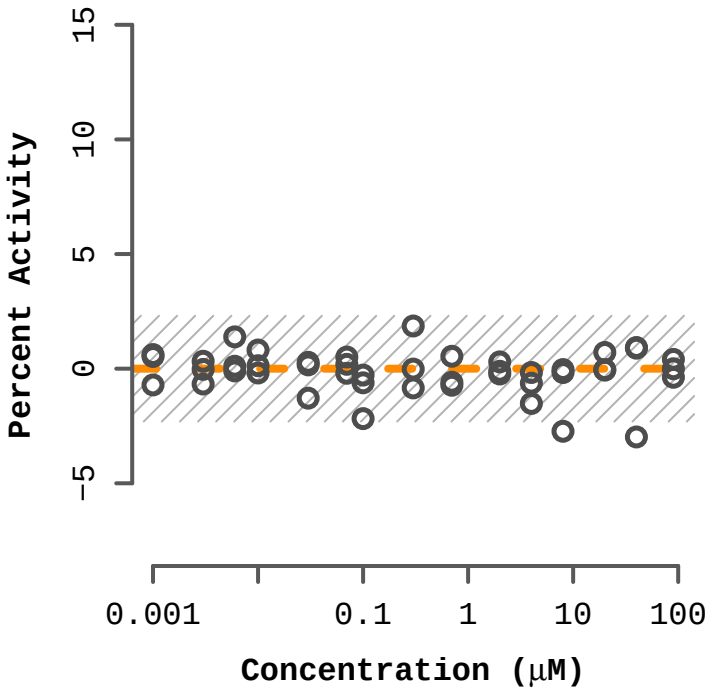
NAME: Isopropyl mercaptan
CHID: 25481 CASRN: 75-33-2
SPID(S): Tox21_201170
M4ID: 12481082 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.85	NA	NA
PROB:	1	NA	NA
RMSE:	5.32	NA	NA

MAX_MEAN: 9.62 MAX_MED: 1.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

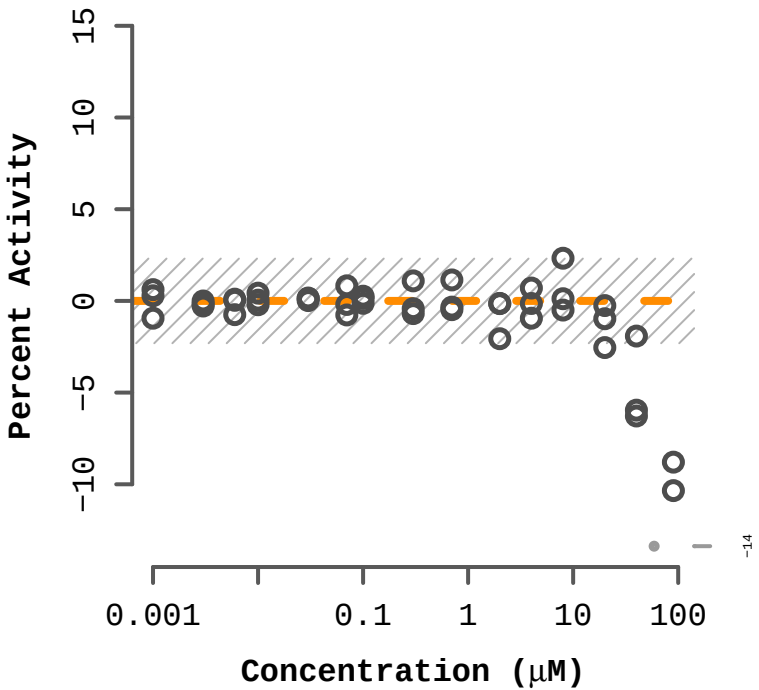
NAME: Isopropyl phenylacetate
CHID: 25483 CASRN: 4861-85-2
SPID(S): Tox21_201145
M4ID: 12481107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.467 **MAX_MED:** 0.895 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

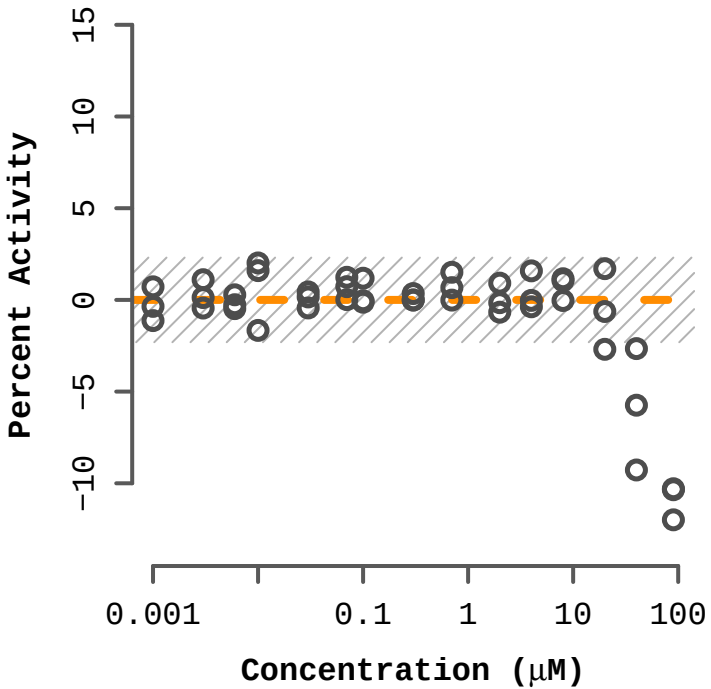
NAME: N-Isopropyl-N'-phenyl-p-phenylenediamine
CHID: 25485 CASRN: 101-72-4
SPID(S): Tox21_303202
M4ID: 12475931 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.26	NA	NA
PROB:	1	NA	NA
RMSE:	3.29	NA	NA

MAX_MEAN: 0.651 MAX_MED: 0.283 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

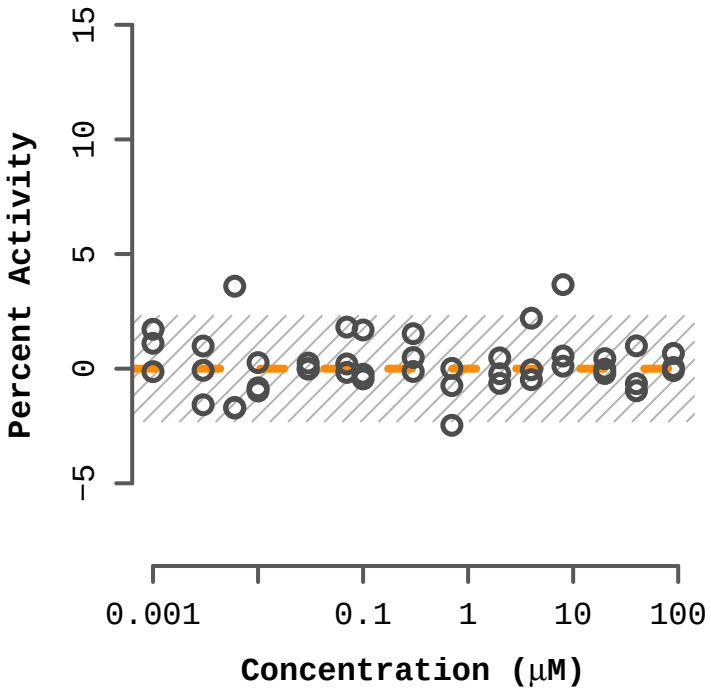
NAME: N-Isopropyl-N'-phenyl-p-phenylenediamine
CHID: 25485 **CASRN:** 101-72-4
SPID(S): Tox21_201424
M4ID: 12480828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.84	NA	NA
PROB:	1	NA	NA
RMSE:	3.4	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

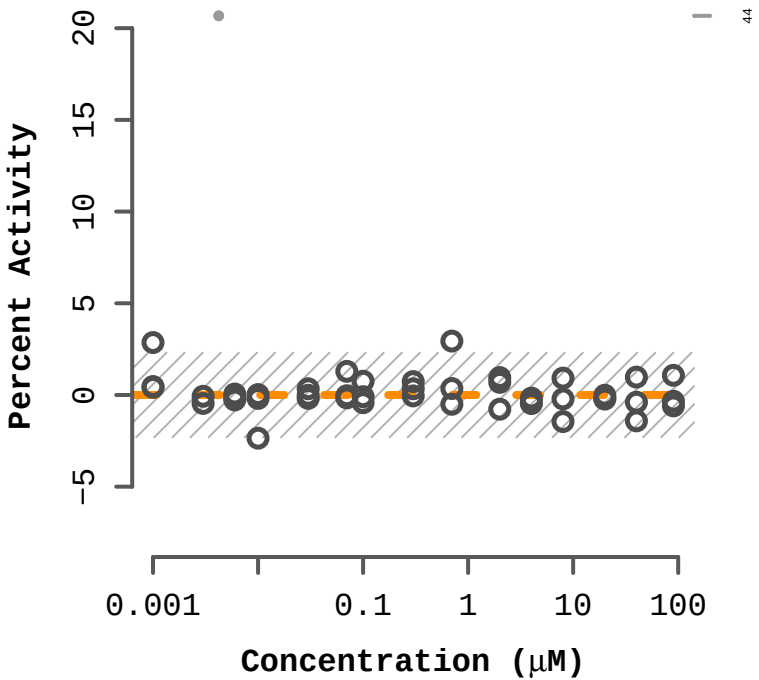
NAME: Isoproterenol hydrochloride
CHID: 25486 **CASRN:** 51-30-9
SPID(S): Tox21_300308
M4ID: 12478822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

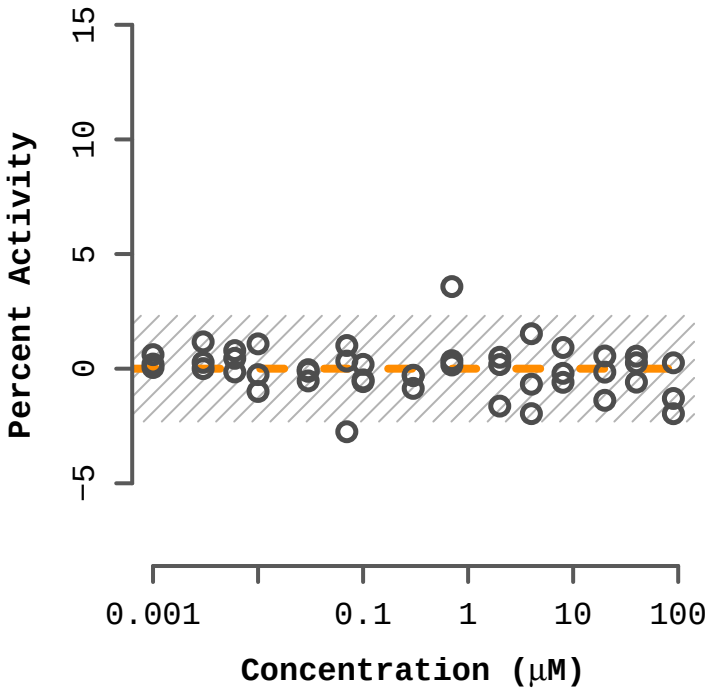
NAME: Isoproterenol hydrochloride
CHID: 25486 CASRN: 51-30-9
SPID(S): Tox21_201272
M4ID: 12480980 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.59	NA	NA
PROB:	1	NA	NA
RMSE:	6.65	NA	NA

MAX_MEAN: 14.6 MAX_MED: 0.691 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

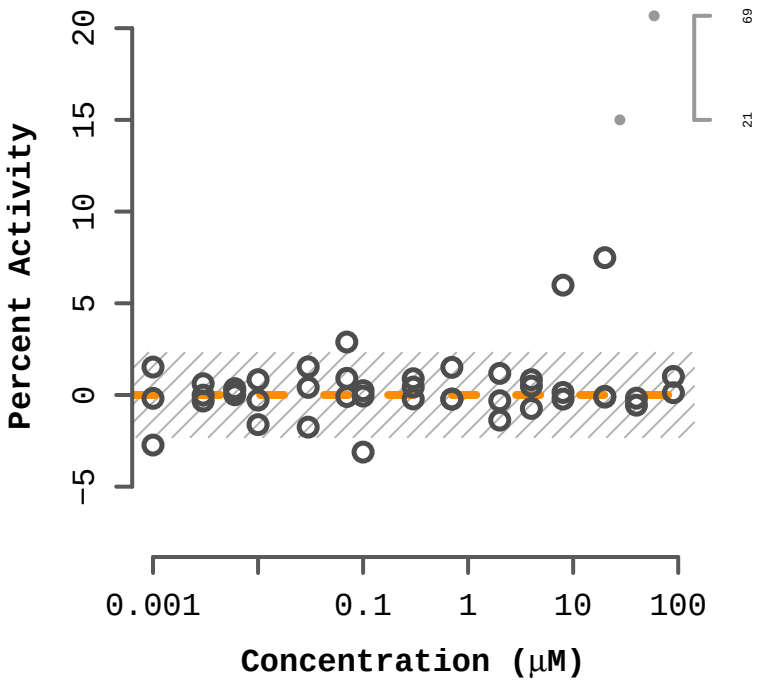
NAME: 1-Chlorododecane
CHID: 25492 **CASRN:** 112-52-7
SPID(S): Tox21_303224
M4ID: 12475909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.452 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

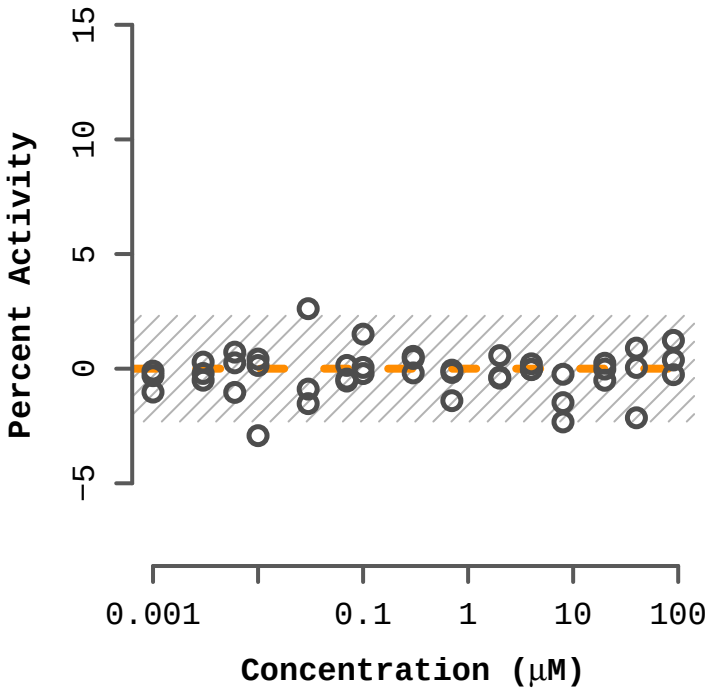
NAME: 1-Chlorododecane
CHID: 25492 **CASRN:** 112-52-7
SPID(S): Tox21_201790
M4ID: 12480462 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.33	NA	NA
PROB:	1	NA	NA
RMSE:	10.85	NA	NA

MAX_MEAN: 23.3 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

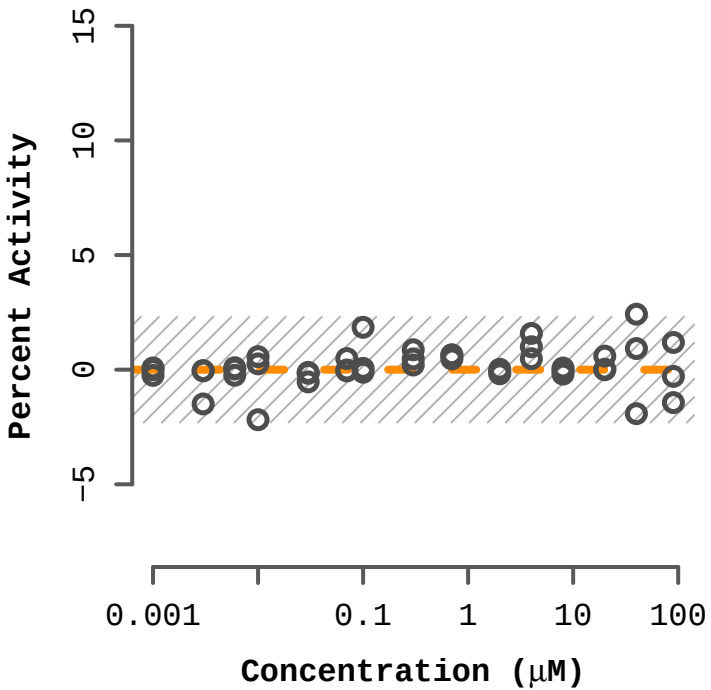
NAME: Dodecyl glycidyl ether
CHID: 25494 **CASRN:** 2461-18-9
SPID(S): Tox21_200787
M4ID: 12481465

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.453 **MAX_MED:** 0.445 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

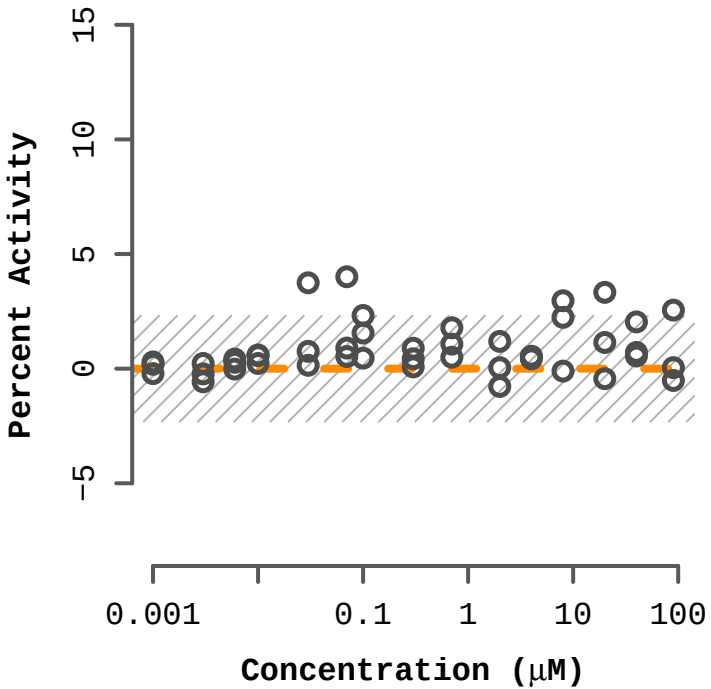
NAME: Dipentenedimercaptan
CHID: 25501 **CASRN:** 4802-20-4
SPID(S): Tox21_301895
M4ID: 12477238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

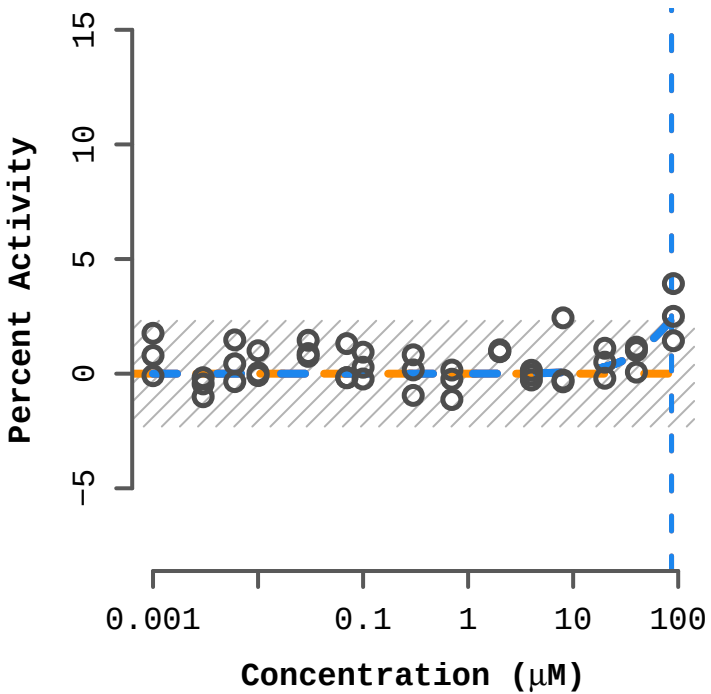
NAME: Linalool
CHID: 25502 CASRN: 78-70-6
SPID(S): Tox21_303037
M4ID: 12476096

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.81 MAX_MED: 2.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linalool
CHID: 25502 **CASRN:** 78-70-6
SPID(S): Tox21_201658
M4ID: 12480594

HILL MODEL (in red):

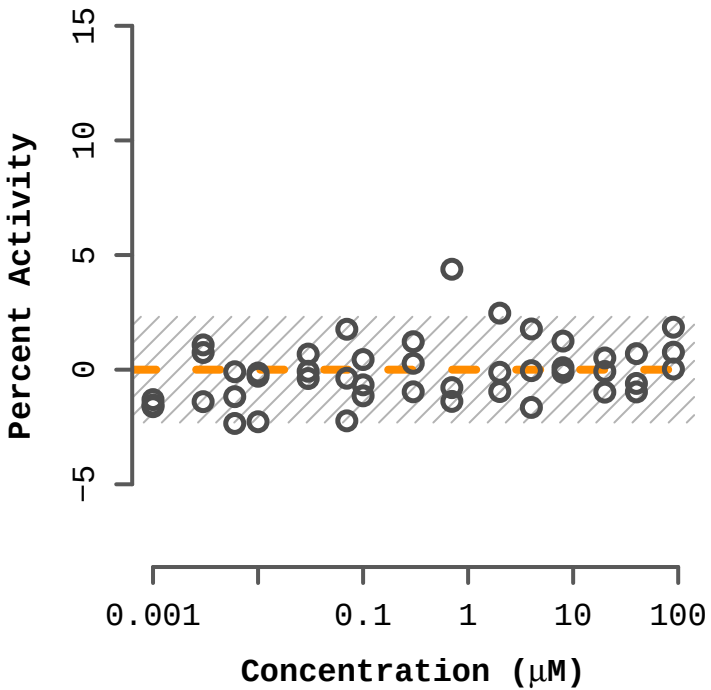
	tp	ga	gw
val:	4.72	1.94	1.86
sd:	6.37	0.634	1.49

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.72	1.94	1.86	3.9	3.15
sd:	6.42	0.639	1.51	619	1020

	CNST	HILL	GNLS
AIC:	134.04	121.34	125.34
PROB:	0	0.88	0.12
RMSE:	1.1	0.84	0.84

MAX_MEAN: 2.62 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

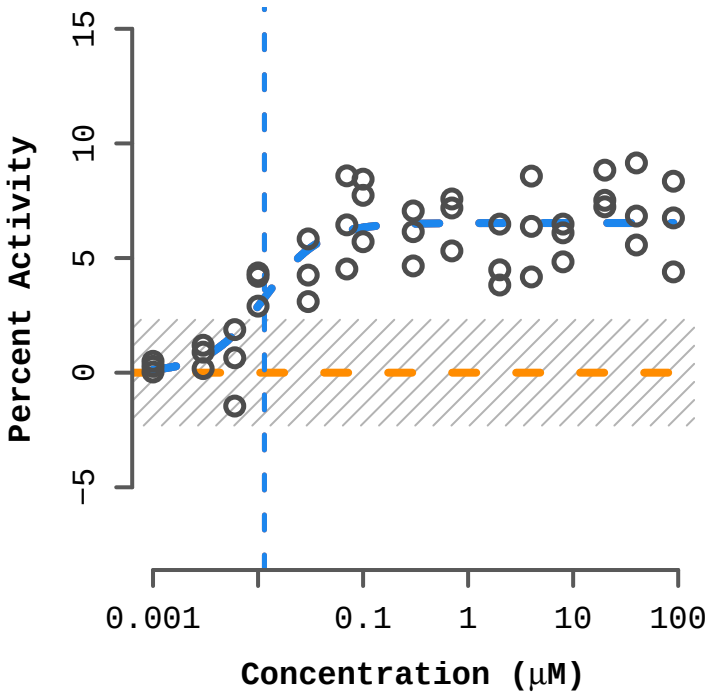
NAME: Linalyl anthranilate
CHID: 25503 **CASRN:** 7149-26-0
SPID(S): Tox21_200570
M4ID: 12481682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.883 **MAX_MED:** 0.765 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linoleic acid
CHID: 25505 CASRN: 60-33-3
SPID(S): Tox21_303080
M4ID: 12476053

HILL MODEL (in red):

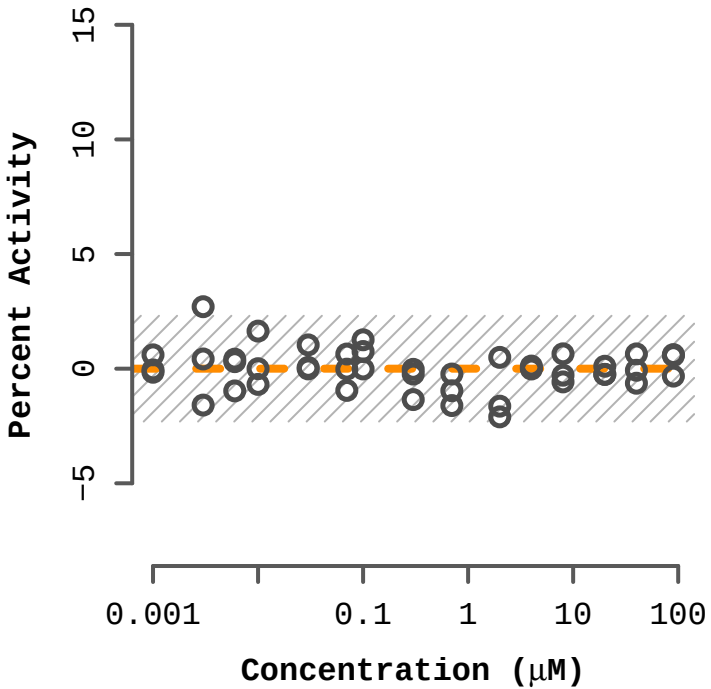
	tp	ga	gw
val:	6.53	−1.94	1.6
sd:	0.304	0.114	0.535

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.53	−1.94	1.6	3.17	6.54
sd:	0.304	0.114	0.535	1850	9880

	CNST	HILL	GNLS
AIC:	294.17	171.2	175.2
PROB:	0	0.88	0.12
RMSE:	5.69	1.42	1.42

MAX_MEAN: 7.86 MAX_MED: 7.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

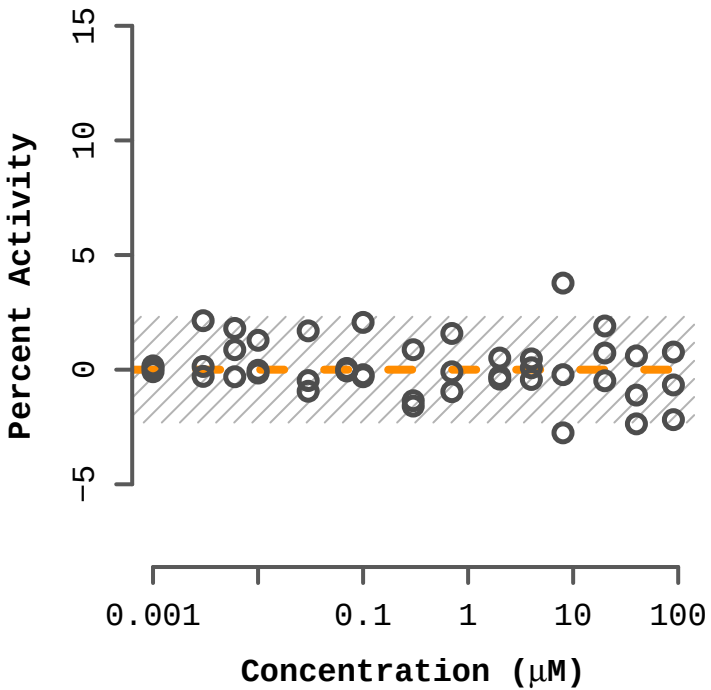
NAME: Linoleic acid
CHID: 25505 CASRN: 60-33-3
SPID(S): Tox21_202171
M4ID: 12480081

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.667 MAX_MED: 0.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

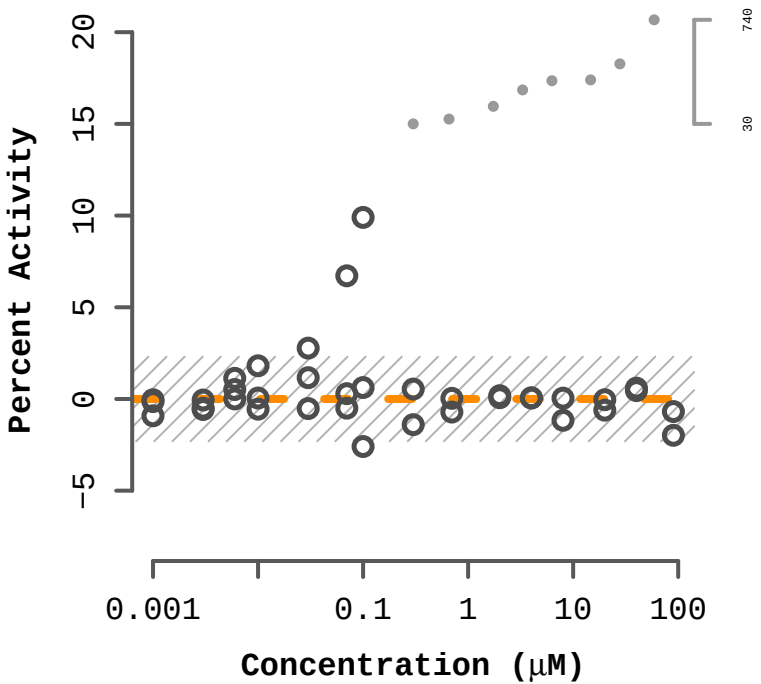
NAME: Linolenic acid
CHID: 25506 **CASRN:** 463-40-1
SPID(S): Tox21_303322
M4ID: 12475811

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.789 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

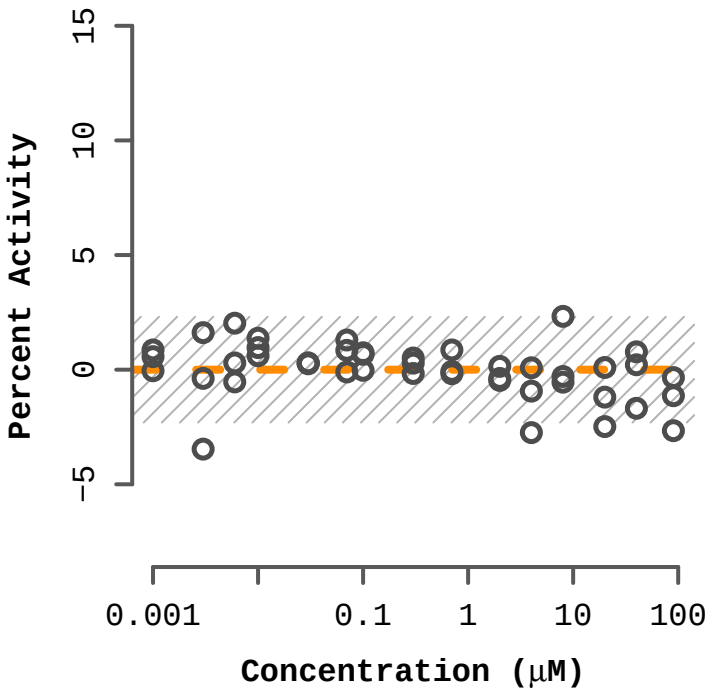
NAME: Linolenic acid
CHID: 25506 **CASRN:** 463-40-1
SPID(S): Tox21_201727
M4ID: 12480525 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	481.92	NA	NA
PROB:	1	NA	NA
RMSE:	151.79	NA	NA

MAX_MEAN: 244 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

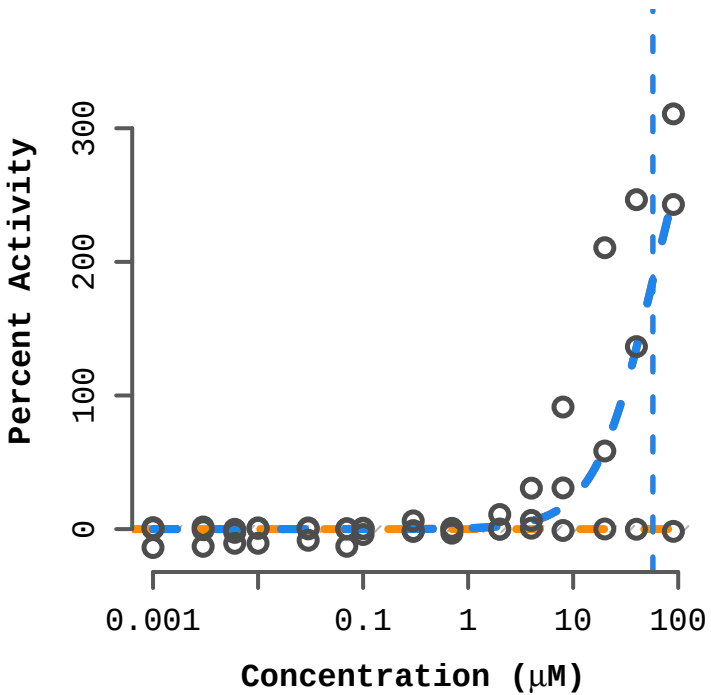
NAME: alpha−Lipoic acid
CHID: 25508 **CASRN:** 1077−28−7
SPID(S): Tox21_303092
M4ID: 12476041

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: alpha-Lipoic acid
CHID: 25508 CASRN: 1077-28-7
SPID(S): Tox21_201808
M4ID: 12480444

HILL MODEL (in red):

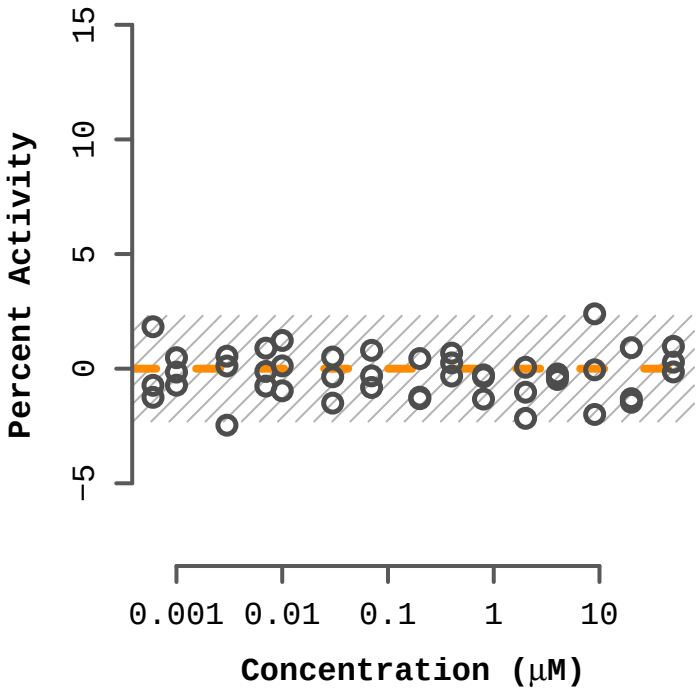
	tp	ga	gw
val:	373	1.76	1.55
sd:	103	0.175	0.377

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	373	1.76	1.55	2.39	17.8
sd:	103	0.175	0.377	297	12000

	CNST	HILL	GNLS
AIC:	466.56	442.46	446.46
PROB:	0	0.88	0.12
RMSE:	80.85	54	54

MAX_MEAN: 184 MAX_MED: 243 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

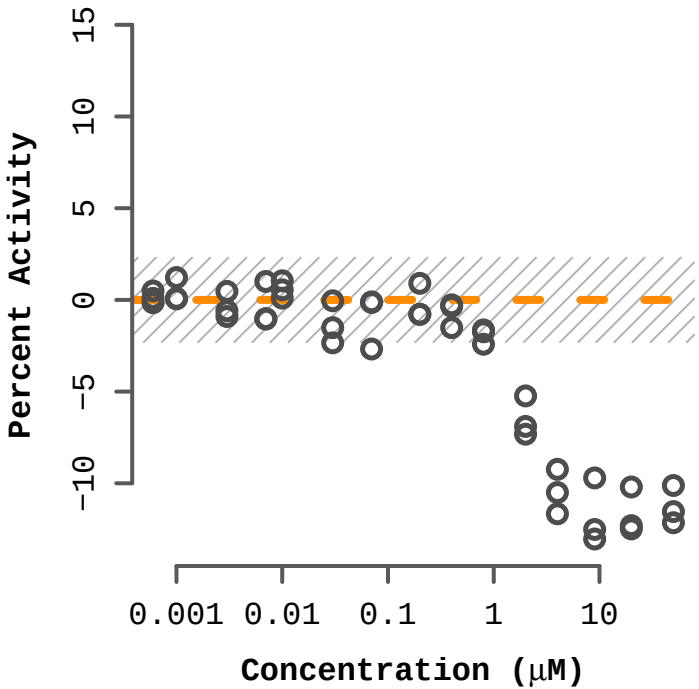
NAME: alpha−Lipoic acid
CHID: 25508 **CASRN:** 1077−28−7
SPID(S): Tox21_110285_1
M4ID: 12484483

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.286 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

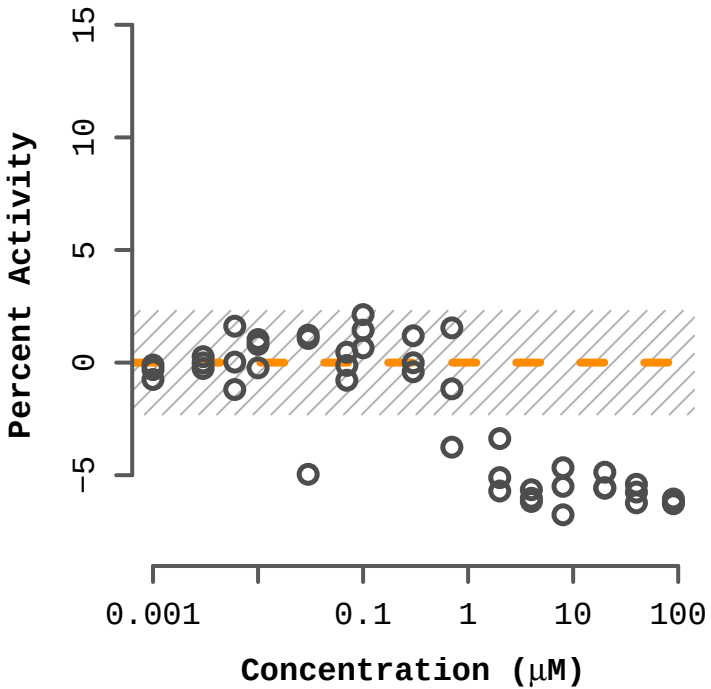
NAME: Malachite green
CHID: 25512 **CASRN:** 569-64-2
SPID(S): Tox21_303977
M4ID: 12475211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.86	NA	NA
PROB:	1	NA	NA
RMSE:	6.17	NA	NA

MAX_MEAN: 0.564 **MAX_MED:** 0.549 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

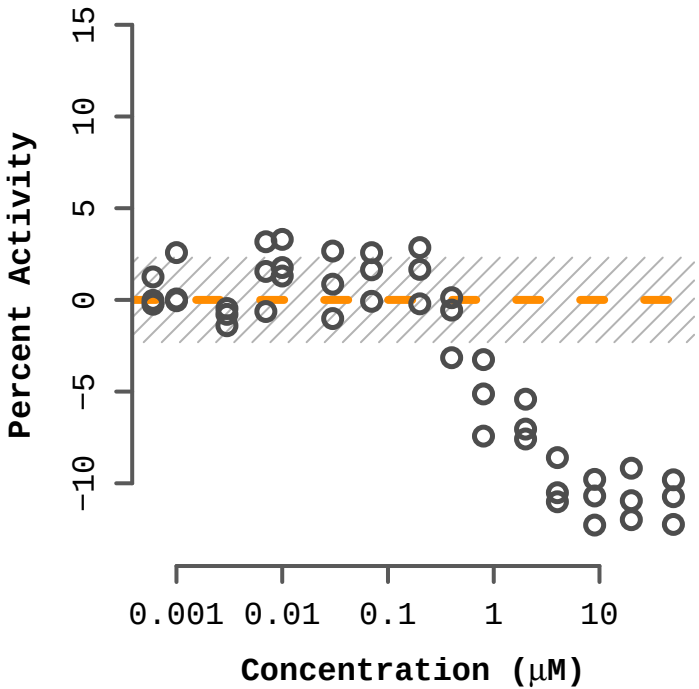
NAME: Malachite green oxalate
CHID: 25513 **CASRN:** 2437-29-8
SPID(S): Tox21_202521
M4ID: 12479731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	252.81	NA	NA
PROB:	1	NA	NA
RMSE:	3.76	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

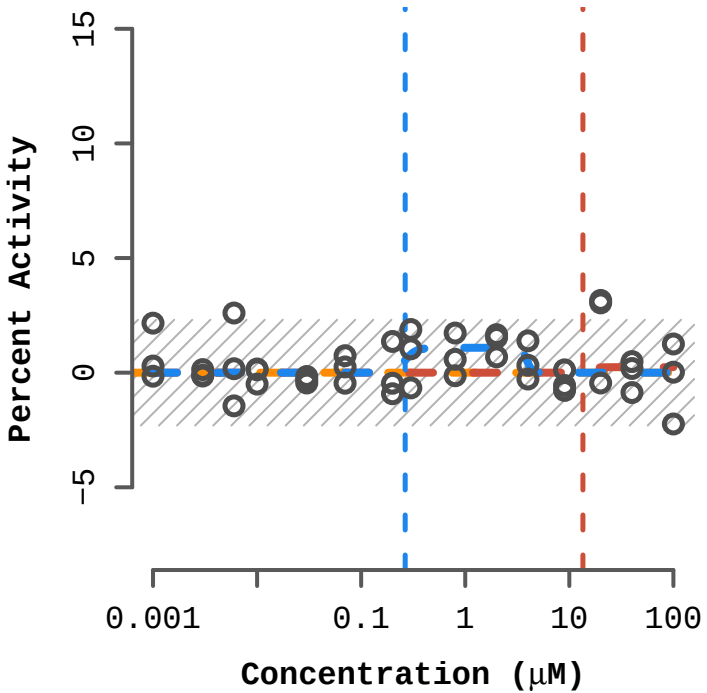
NAME: Malachite green oxalate
CHID: 25513 **CASRN:** 2437-29-8
SPID(S): Tox21_110008_1
M4ID: 12484714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	293.76	NA	NA
PROB:	1	NA	NA
RMSE:	6.11	NA	NA

MAX_MEAN: 2.12 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Maltol
CHID: 25523 CASRN: 118-71-8
SPID(S): Tox21_300118
M4ID: 12479012

HILL MODEL (in red):

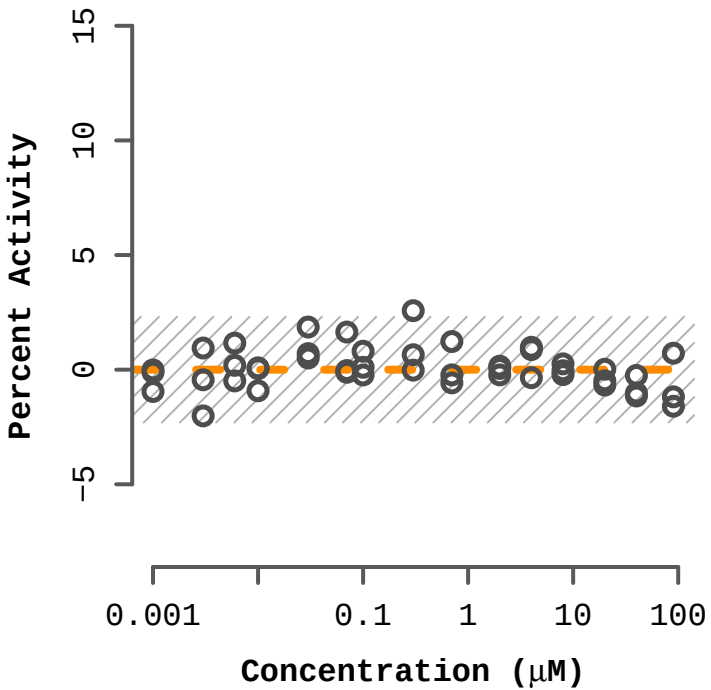
	tp	ga	gw
val:	0.24	1.13	8
sd:	0.417	0.325	15.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.09	−0.577	8	0.592	17.9
sd:	0.342	0.114	10.5	0.269	469

	CNST	HILL	GNLS
AIC:	141.69	147.33	141.99
PROB:	0.52	0.03	0.45
RMSE:	1.18	1.16	1.09

MAX_MEAN: 1.92 MAX_MED: 3.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

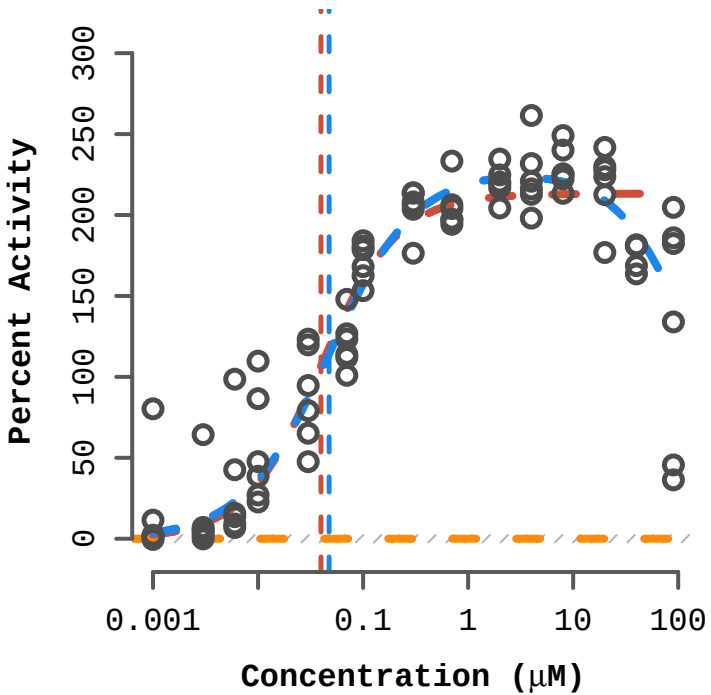
NAME: Maltol
CHID: 25523 **CASRN:** 118-71-8
SPID(S): Tox21_202215
M4ID: 12480037

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.879 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Medroxyprogesterone acetate
CHID: 25527 CASRN: 71-58-9
SPID(S): Tox21_200141
M4ID: 12482111

HILL MODEL (in red):

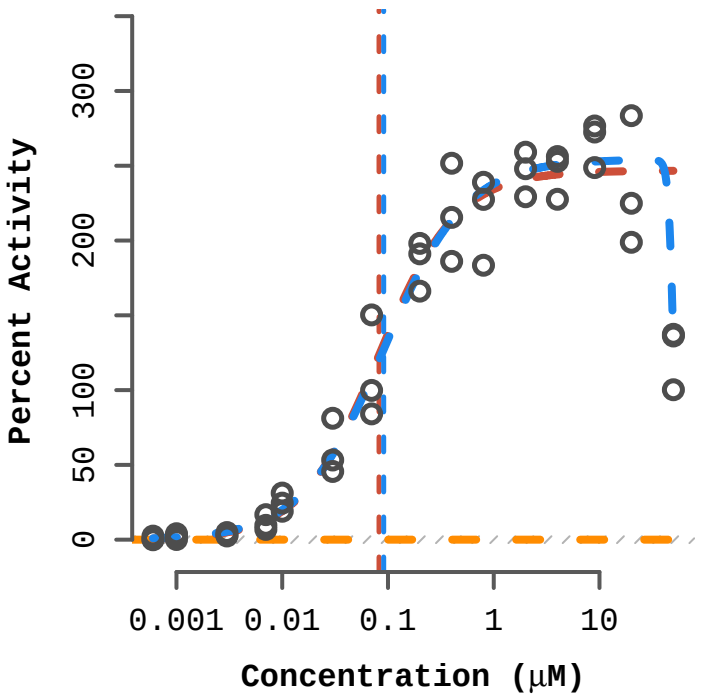
	tp	ga	gw
val:	213	-1.4	1.19
sd:	4.2	0.0495	0.121

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	228	-1.32	1.06	2.18	1.19
sd:	6.4	0.0506	0.109	0.194	0.404

	CNST	HILL	GNLS
AIC:	1189.55	874.91	851.36
PROB:	0	0	1
RMSE:	162.79	36.88	28.61

MAX_MEAN: 229 MAX_MED: 226 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Medroxyprogesterone acetate
CHID: 25527 CASRN: 71-58-9
SPID(S): Tox21_111319_1
M4ID: 12483772

HILL MODEL (in red):

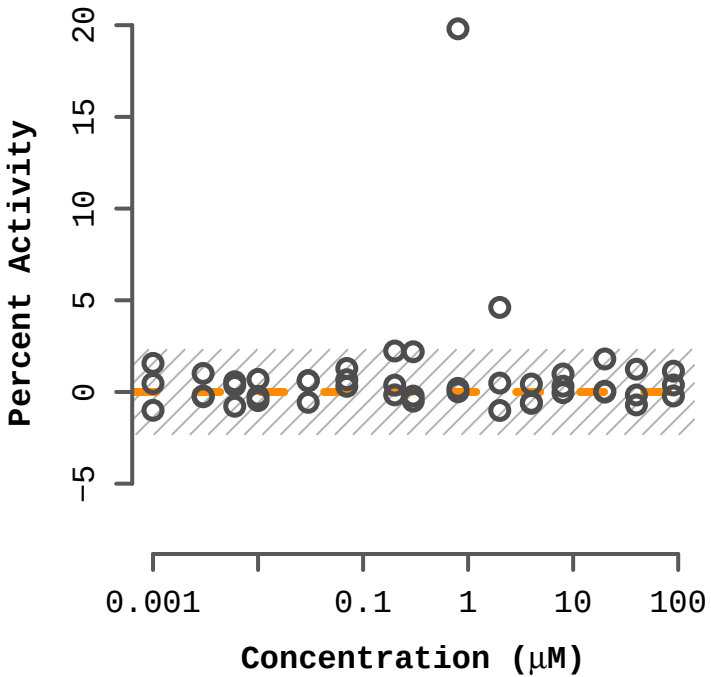
	tp	ga	gw
val:	247	-1.08	1.18
sd:	7.66	0.0636	0.137

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	254	-1.04	1.12	1.7	18
sd:	6.68	0.0563	0.107	0.00462	80

	CNST	HILL	GNLS
AIC:	595.27	436.25	401.75
PROB:	0	0	1
RMSE:	165.81	36.76	19.16

MAX_MEAN: 266 **MAX_MED:** 273 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

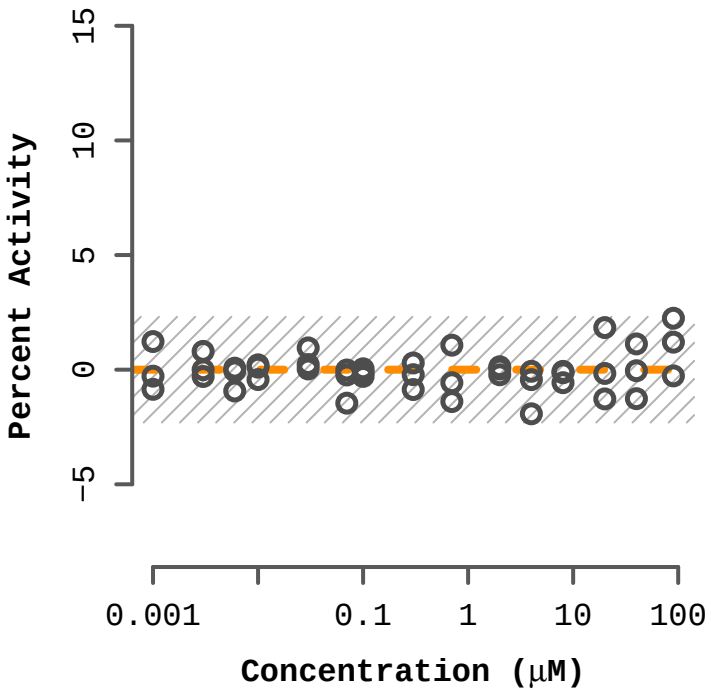
NAME: Menthofuran
CHID: 25534 CASRN: 494-90-6
SPID(S): Tox21_200722
M4ID: 12481530

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.14	NA	NA

MAX_MEAN: 6.67 MAX_MED: 0.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

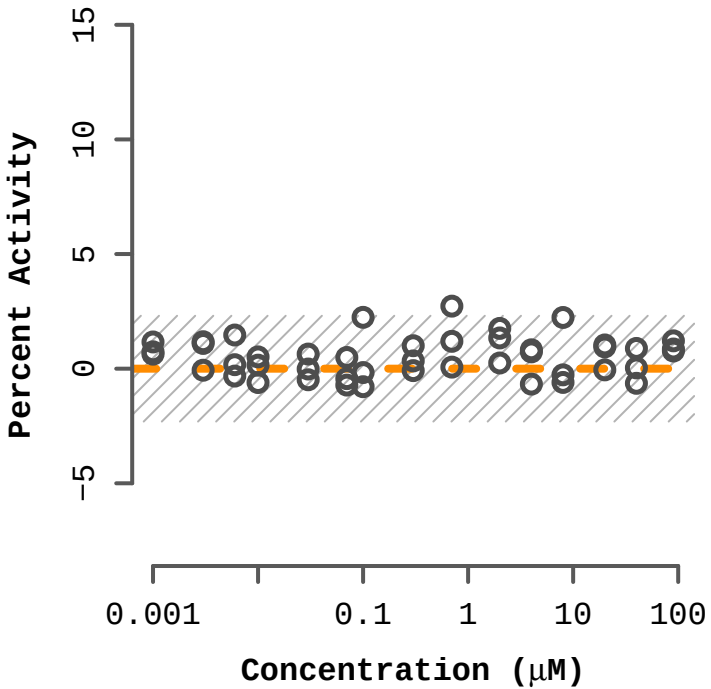
NAME: 2-Mercaptobenzimidazole
CHID: 25536 **CASRN:** 583-39-1
SPID(S): Tox21_303274
M4ID: 12475859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

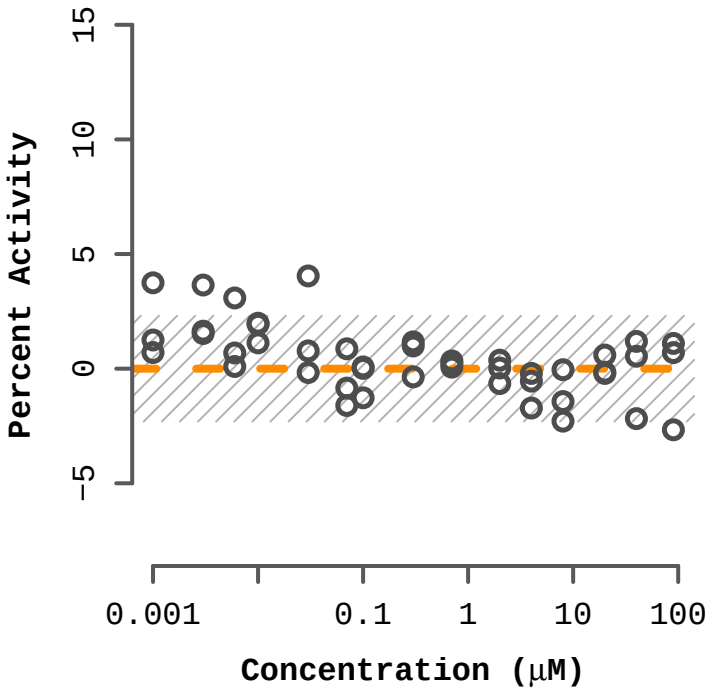
NAME: 2-Mercaptobenzimidazole
CHID: 25536 **CASRN:** 583-39-1
SPID(S): Tox21_201828
M4ID: 12480424

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

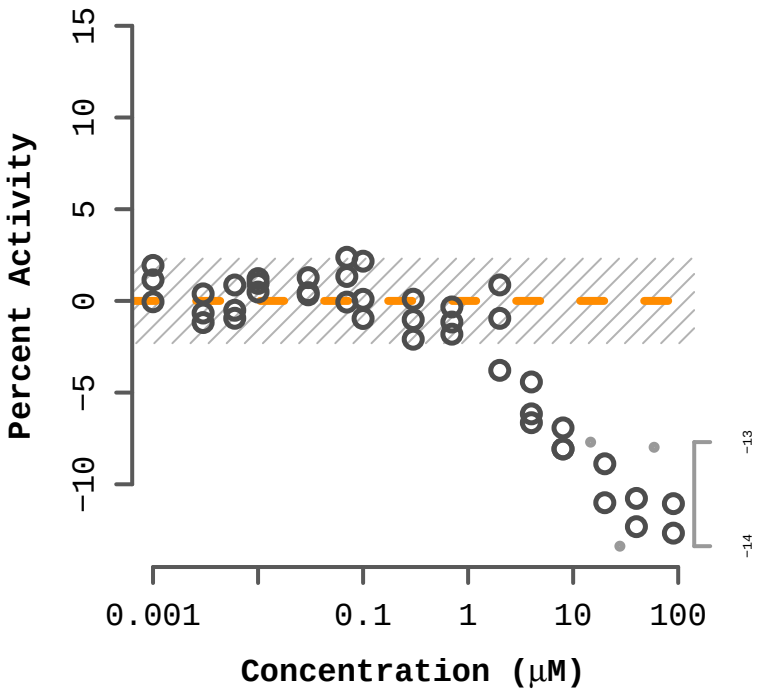
NAME: 6-Mercaptopurine monohydrate
CHID: 25538 CASRN: 6112-76-1
SPID(S): Tox21_200994
M4ID: 12481258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 2.27 MAX_MED: 1.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

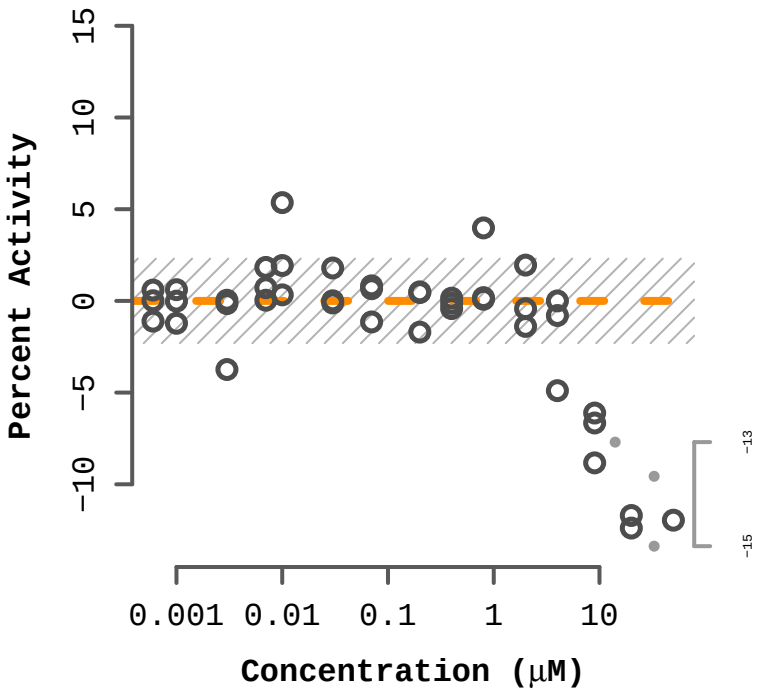
NAME: Thimerosal
CHID: 25540 **CASRN:** 54-64-8
SPID(S): Tox21_302176
M4ID: 12476957 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	287.81	NA	NA
PROB:	1	NA	NA
RMSE:	6.06	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

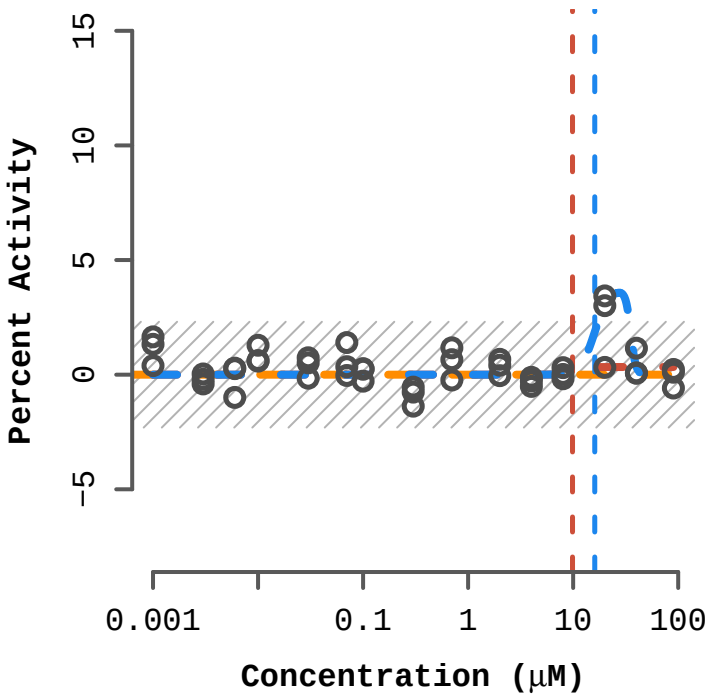
NAME: Thimerosal
CHID: 25540 **CASRN:** 54-64-8
SPID(S): Tox21_111331_1
M4ID: 12483761 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.03	NA	NA
PROB:	1	NA	NA
RMSE:	5.35	NA	NA

MAX_MEAN: 2.54 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methacrylic acid
CHID: 25542 **CASRN:** 79-41-4
SPID(S): Tox21_200826
M4ID: 12481426

HILL MODEL (in red):

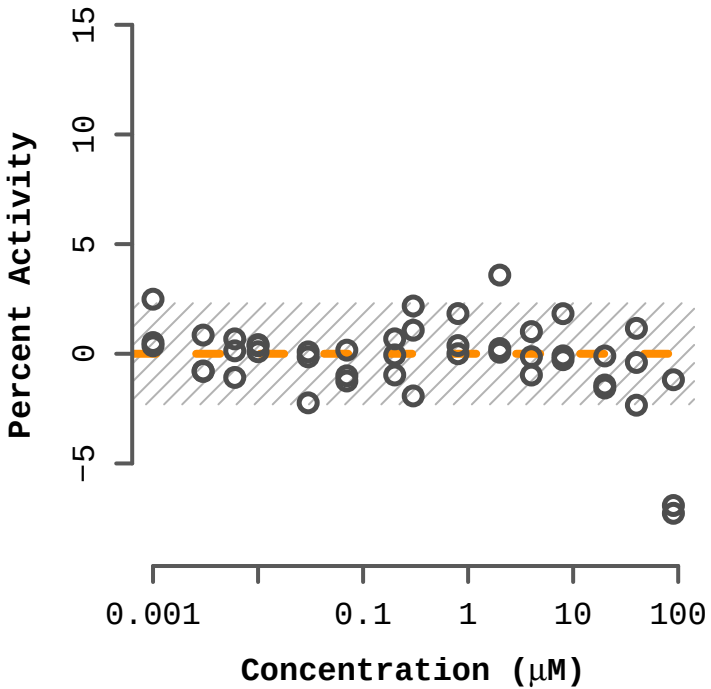
	tp	ga	gw
val:	0.333	0.994	8
sd:	0.249	0.363	18.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.73	1.21	6.47	1.55	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	113.05	117.11	109.91
PROB:	0.17	0.02	0.81
RMSE:	0.94	0.89	0.76

MAX_MEAN: 2.26 **MAX_MED:** 3.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

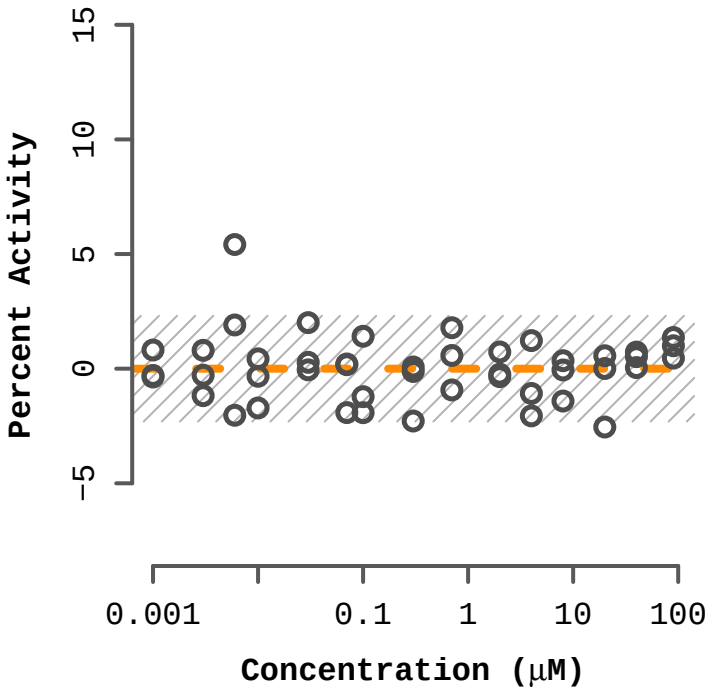
NAME: 2-Methoxycinnamaldehyde
CHID: 25551 **CASRN:** 1504-74-1
SPID(S): Tox21_202885
M4ID: 12479367

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.91	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

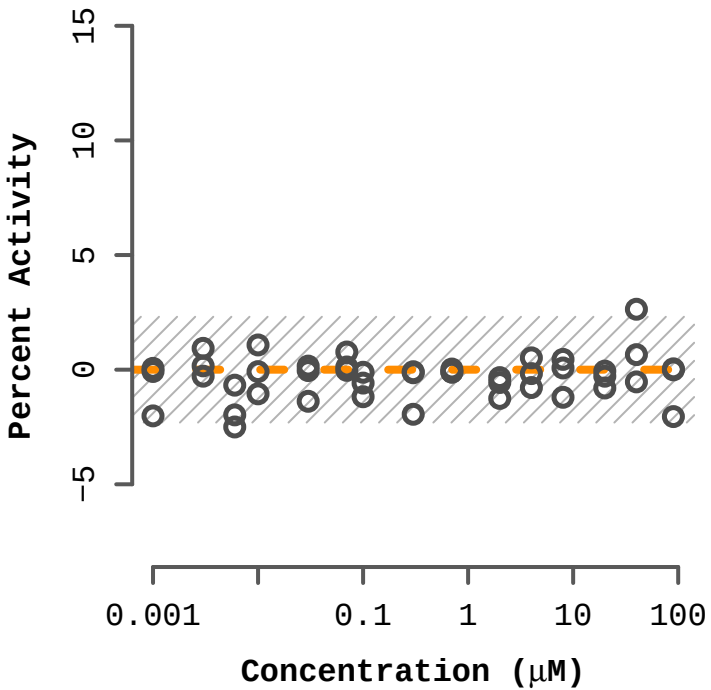
NAME: 4-Methoxy-4-methyl-2-pentanone
CHID: 25557 **CASRN:** 107-70-0
SPID(S): Tox21_300873
M4ID: 12478260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

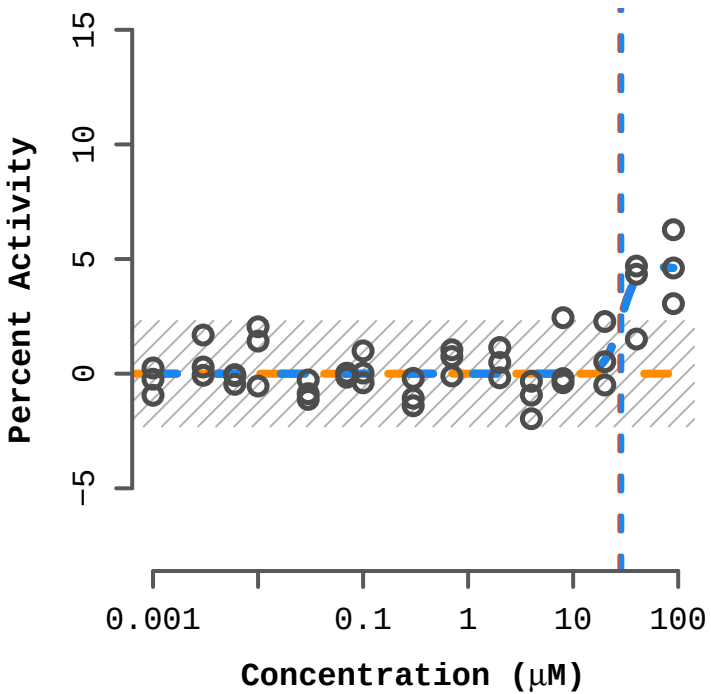
NAME: 4-Methoxy-3-nitro-N-phenylbenzamide
CHID: 25558 **CASRN:** 97-32-5
SPID(S): Tox21_200743
M4ID: 12481509

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.921 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Methoxypsoralen
CHID: 25560 CASRN: 484-20-8
SPID(S): Tox21_303255
M4ID: 12475878

HILL MODEL (in red):

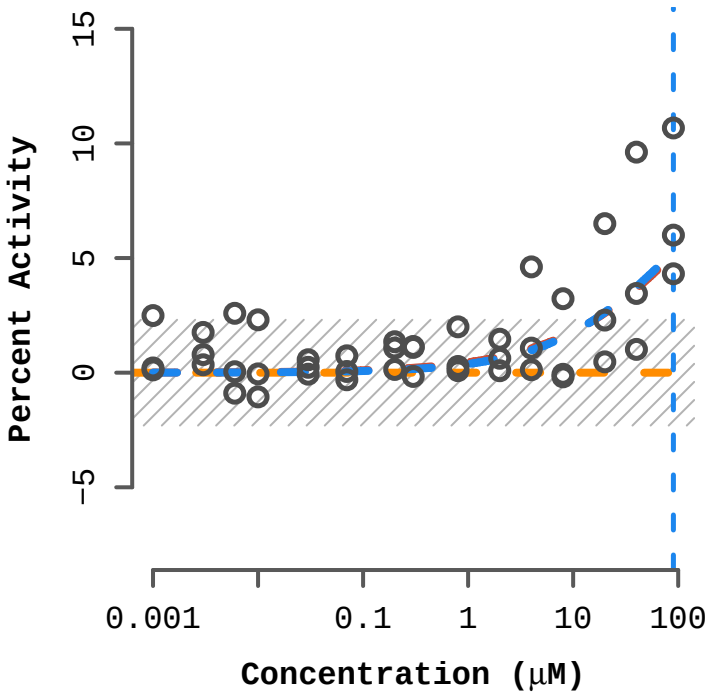
	tp	ga	gw
val:	4.62	1.44	5.84
sd:	0.737	0.0911	3.32

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.89	1.46	5.42	3.82	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	172.07	138.57	142.57
PROB:	0	0.88	0.12
RMSE:	1.83	1.03	1.03

MAX_MEAN: 4.65 MAX_MED: 4.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Methoxypsoralen
CHID: 25560 CASRN: 484-20-8
SPID(S): Tox21_202357
M4ID: 12479895

HILL MODEL (in red):

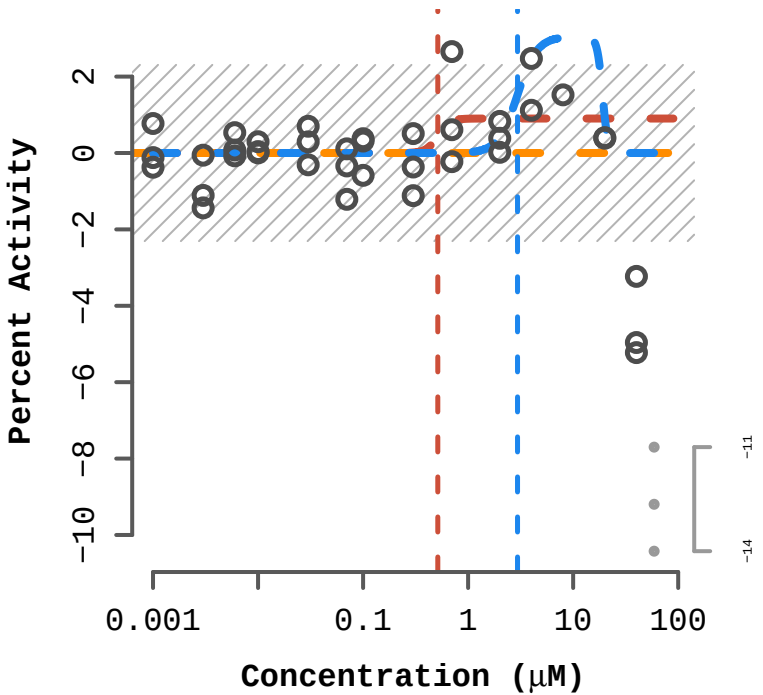
	tp	ga	gw
val:	12.8	2.22	0.648
sd:	9.45	0.882	0.283

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.95	0.731	3.29	5.5
sd:	8.24	0.848	0.326	611	2510

	CNST	HILL	GNLS
AIC:	209.16	180.68	185.05
PROB:	0	0.9	0.1
RMSE:	2.95	1.82	1.81

MAX_MEAN: 7 MAX_MED: 6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Methyl-p-aminophenol sulfate
CHID: 25565 CASRN: 55-55-0
SPID(S): Tox21_200906
M4ID: 12481346 BRK

HILL MODEL (in red):

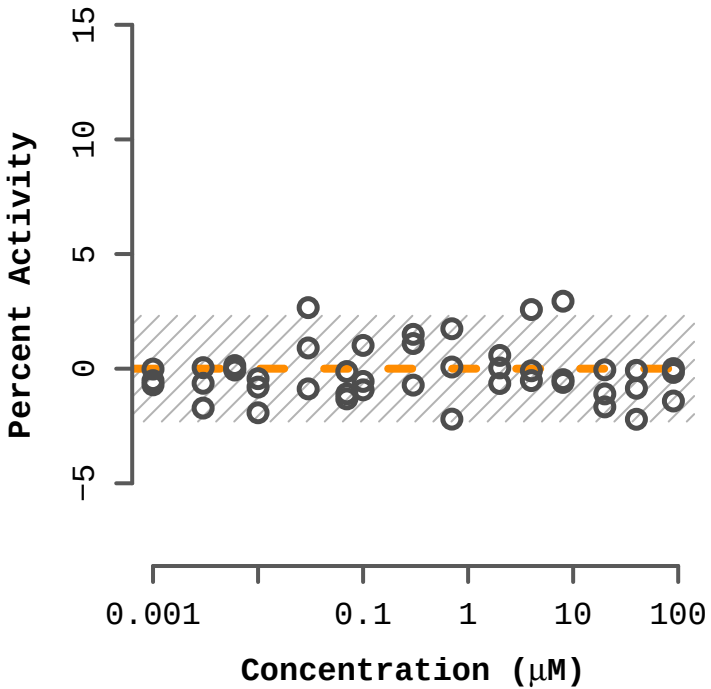
	tp	ga	gw
val:	0.902	−0.289	8
sd:	0.487	0.445	19.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.05	0.47	4.68	1.28	16.9
sd:	0.845	0.143	4.19	0.091	72.2

	CNST	HILL	GNLS
AIC:	220	222.75	212.17
PROB:	0.02	0	0.98
RMSE:	3.68	3.86	3.52

MAX_MEAN: 2.9 **MAX_MED:** 3.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

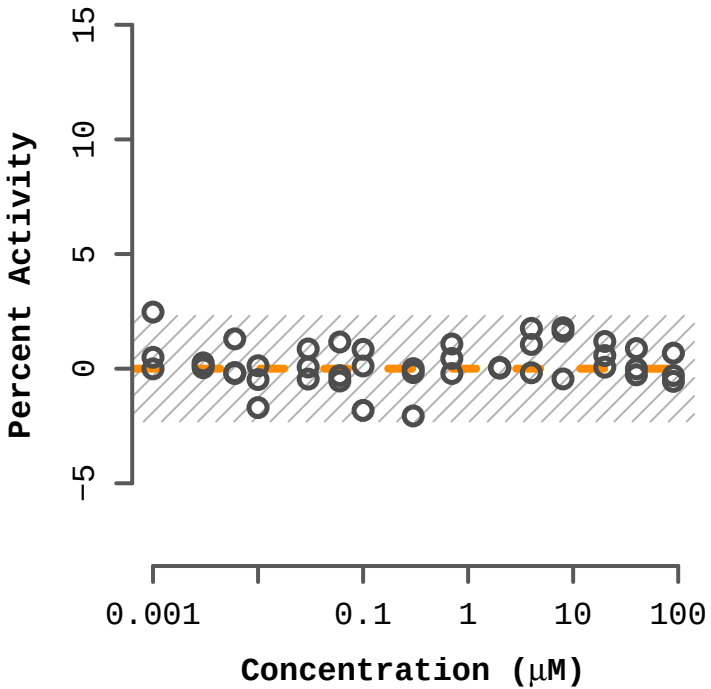
NAME: Methyl 2-aminobenzoate
CHID: 25567 **CASRN:** 134-20-3
SPID(S): Tox21_300347
M4ID: 12478785

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.897 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

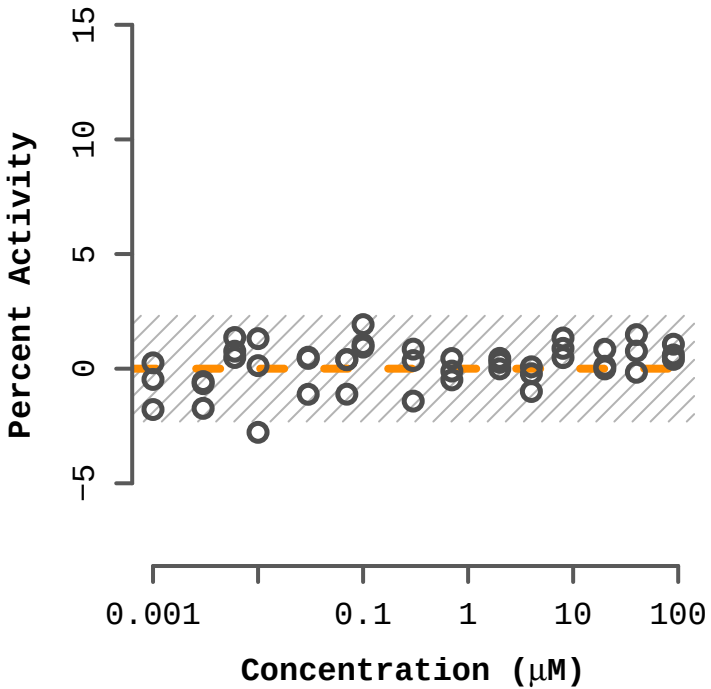
NAME: Methyl 2-aminobenzoate
CHID: 25567 **CASRN:** 134-20-3
SPID(S): Tox21_201657
M4ID: 12480595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.991 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

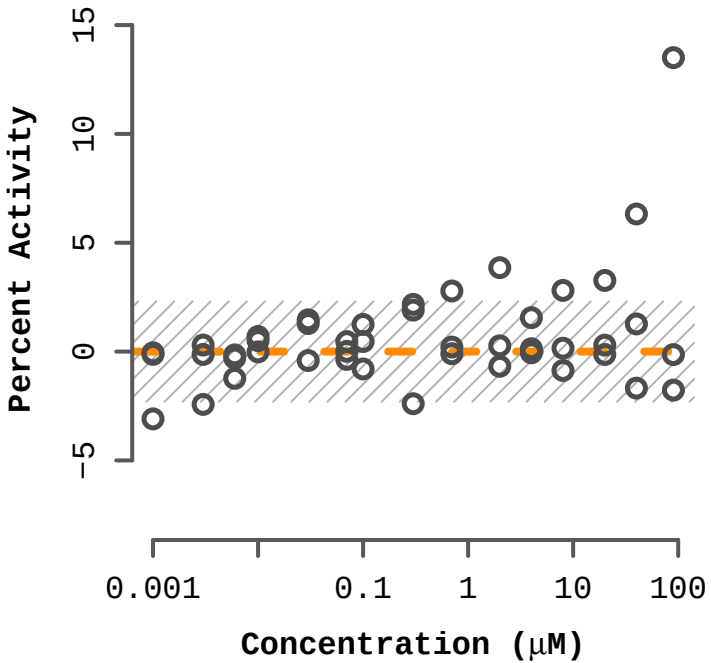
NAME: 2-Methylbenzamide
CHID: 25569 **CASRN:** 527-85-5
SPID(S): Tox21_200187
M4ID: 12482065

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

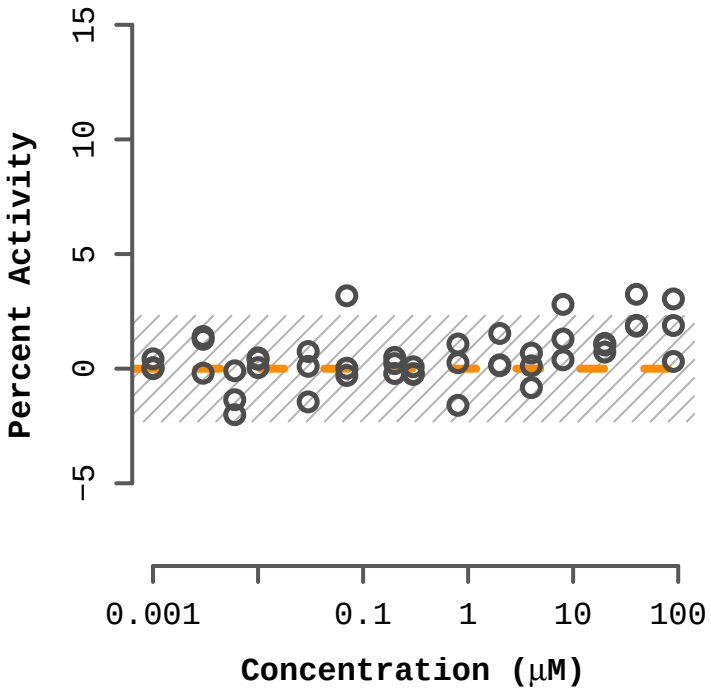
NAME: N-Methylbenzamide
CHID: 25570 CASRN: 613-93-4
SPID(S): Tox21_200220
M4ID: 12482032

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.38	NA	NA
PROB:	1	NA	NA
RMSE:	2.64	NA	NA

MAX_MEAN: 3.87 MAX_MED: 1.91 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

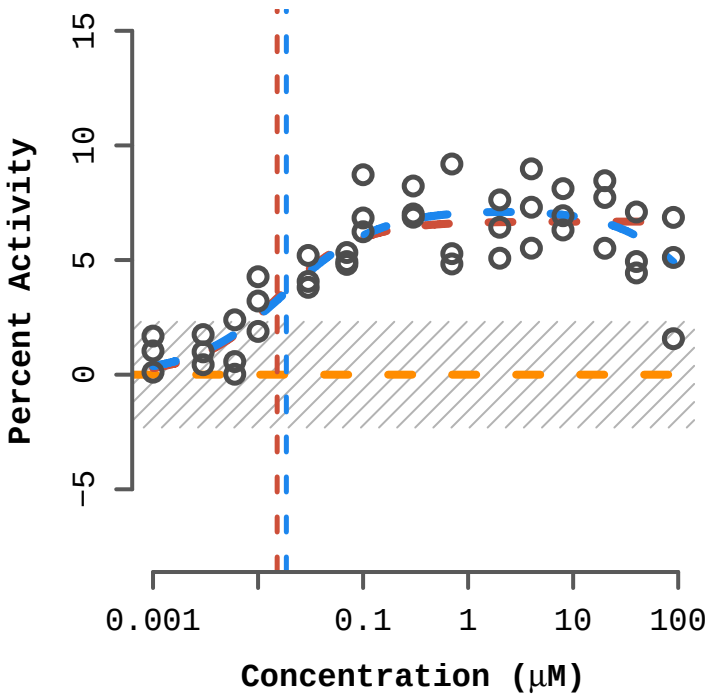
NAME: 2-Methyl-1,3-benzenediol
CHID: 25571 **CASRN:** 608-25-3
SPID(S): Tox21_301973
M4ID: 12477160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl benzoate
CHID: 25572 CASRN: 93-58-3
SPID(S): Tox21_303198
M4ID: 12475935

HILL MODEL (in red):

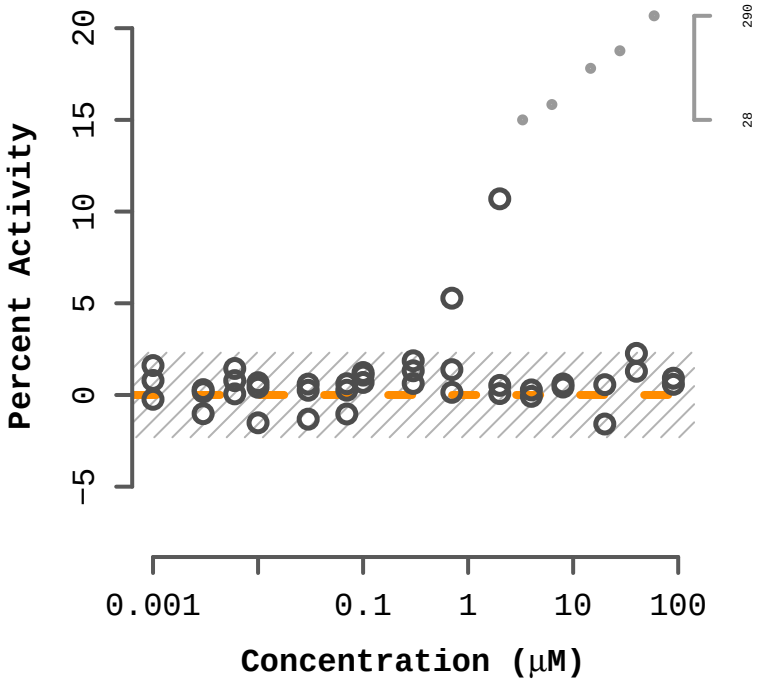
	tp	ga	gw
val:	6.68	−1.82	1.14
sd:	0.315	0.111	0.256

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.21	−1.73	0.994	2.25	1.11
sd:	0.57	0.132	0.235	0.415	0.997

	CNST	HILL	GNLS
AIC:	292.83	167.28	166.34
PROB:	0	0.39	0.61
RMSE:	5.61	1.44	1.29

MAX_MEAN: 7.37 **MAX_MED:** 7.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

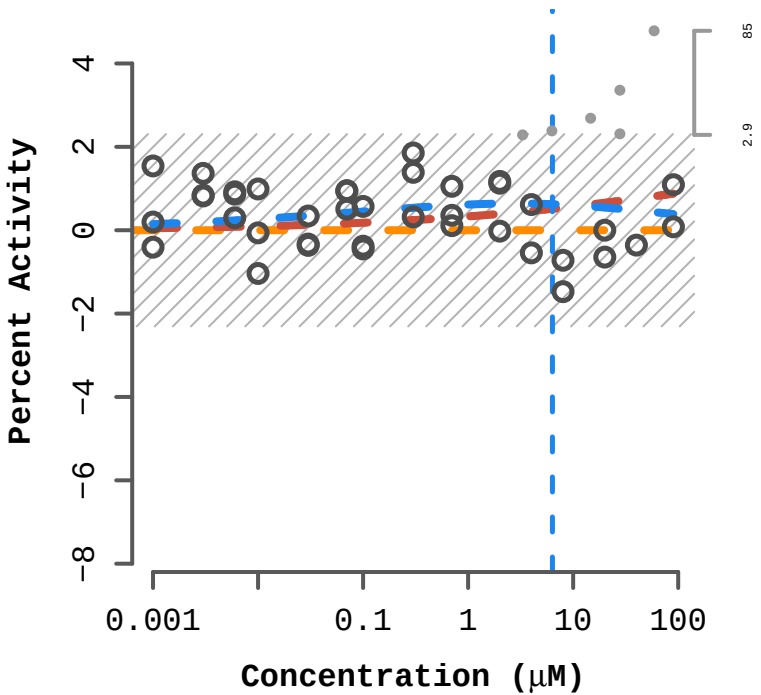
NAME: Methyl benzoate
CHID: 25572 **CASRN:** 93-58-3
SPID(S): Tox21_201832
M4ID: 12480420 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	344.3	NA	NA
PROB:	1	NA	NA
RMSE:	57.84	NA	NA

MAX_MEAN: 95.7 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylbenzyl alcohol
CHID: 25574 CASRN: 589-18-4
SPID(S): Tox21_200089
M4ID: 12482163 BRK

HILL MODEL (in red):

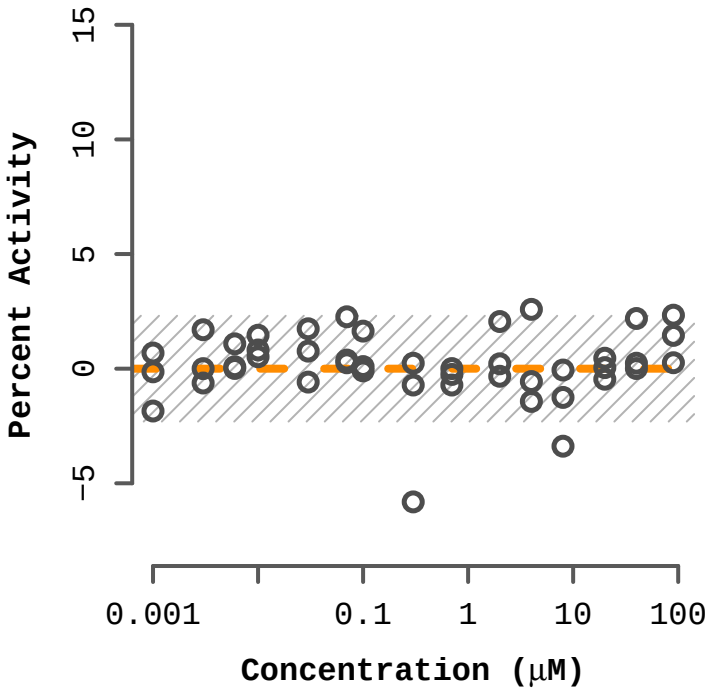
	tp	ga	gw
val:	2.1	2.43	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.18	0.803	0.3	1.05	0.509
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	231.04	233.69	235.59
PROB:	0.73	0.19	0.08
RMSE:	14.19	14	14.08

MAX_MEAN: 28.8 MAX_MED: 3.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

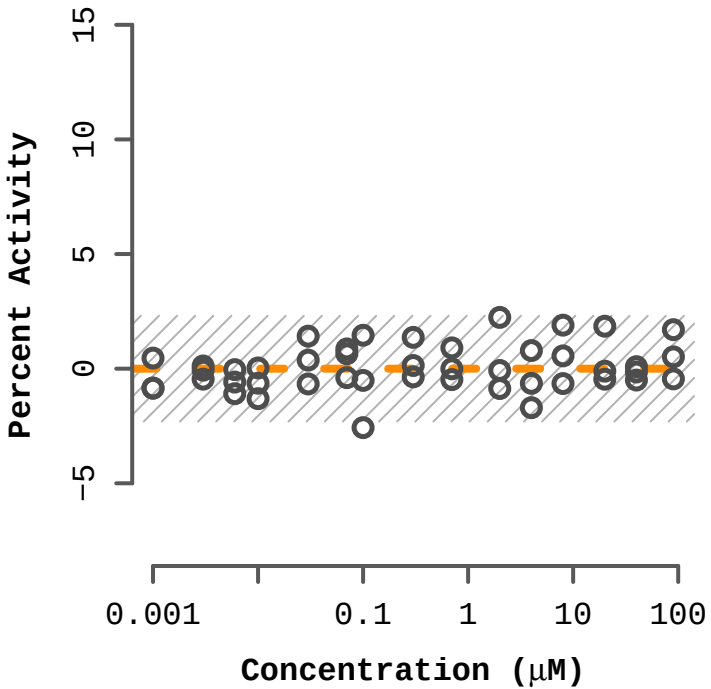
NAME: 2-Methyl-2-butenenitrile
CHID: 25577 **CASRN:** 4403-61-6
SPID(S): Tox21_200317
M4ID: 12481935

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

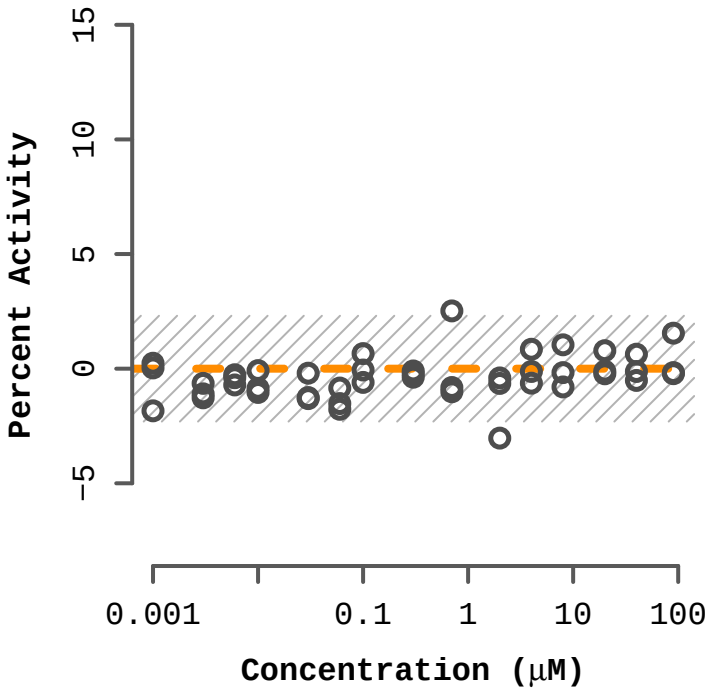
NAME: 2-Methyl-3-butenenitrile
CHID: 25578 **CASRN:** 16529-56-9
SPID(S): Tox21_303720
M4ID: 12475468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.604 **MAX_MED:** 0.651 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

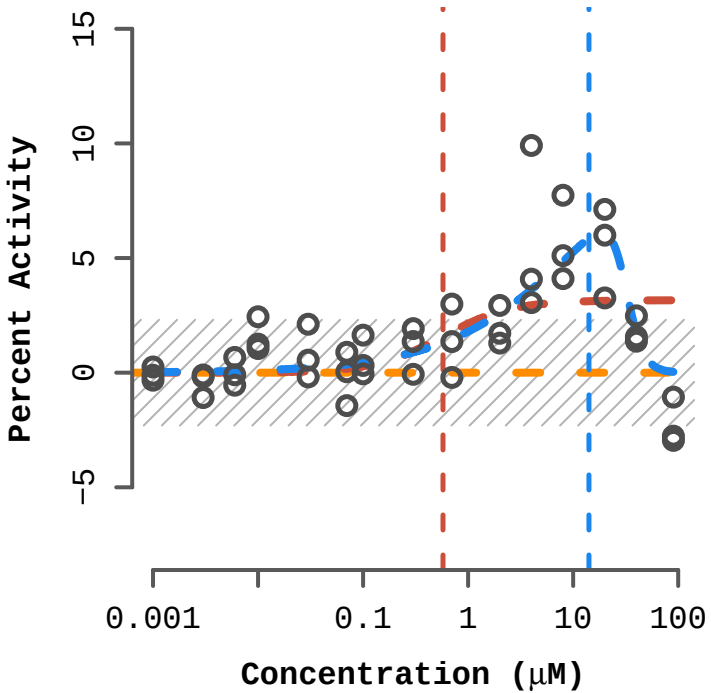
NAME: Prop-2-en-1-yl (3-methylbutoxy)acetate
CHID: 25580 **CASRN:** 67634-00-8
SPID(S): Tox21_200351
M4ID: 12481901

HILL MODEL: Not applicable.

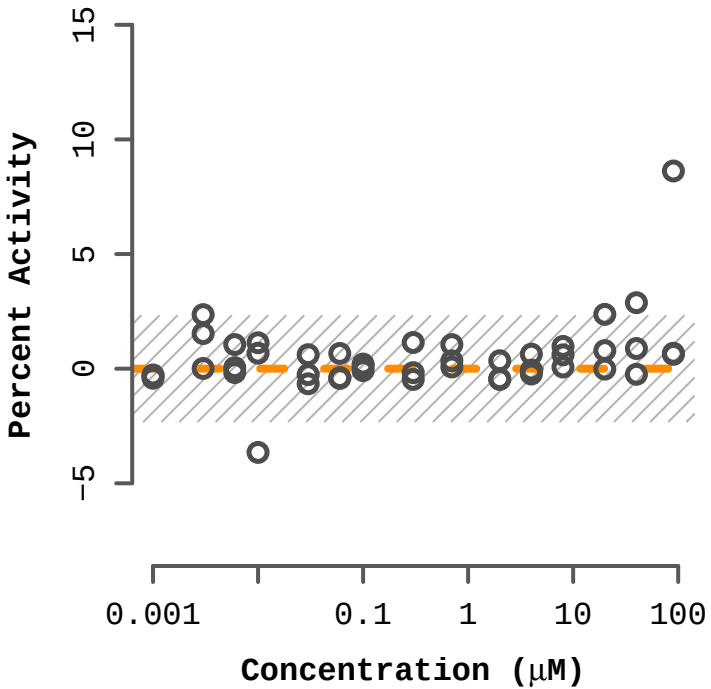
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.388 **MAX_MED:** 0.0345 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (+)-2-Methylbutyl-4-methoxybenzyladine-4'-amin
CHID:    25581   CASRN: 24140-30-5
SPID(S): Tox21_202606
M4ID:    12479646

HILL MODEL (in red):
      tp       ga       gw
val:  3.16     -0.239   1.34
sd:   0.637    0.343    0.782

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  11.9     1.15     0.653    1.5      5.36
sd:   12.5     1.21     0.269    0.14     4.6

      CNST        HILL        GNLS
AIC:  221.39      199.11      167.78
PROB: 0           0           1
RMSE: 2.99        2.25        1.53

MAX_MEAN: 5.68      MAX_MED: 6         BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

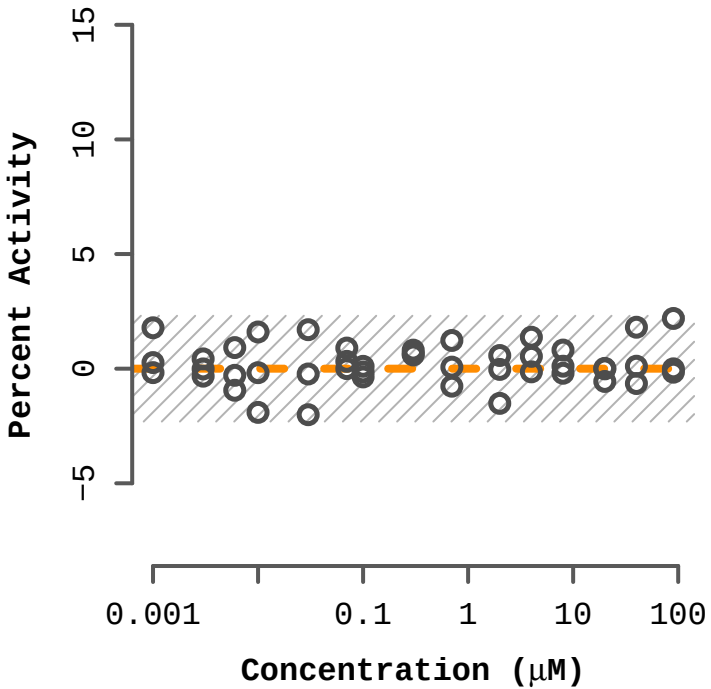
NAME: alpha−Methyl cinnamaldehyde
CHID: 25587 **CASRN:** 101−39−3
SPID(S): Tox21_200051
M4ID: 12482201

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 3.31 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

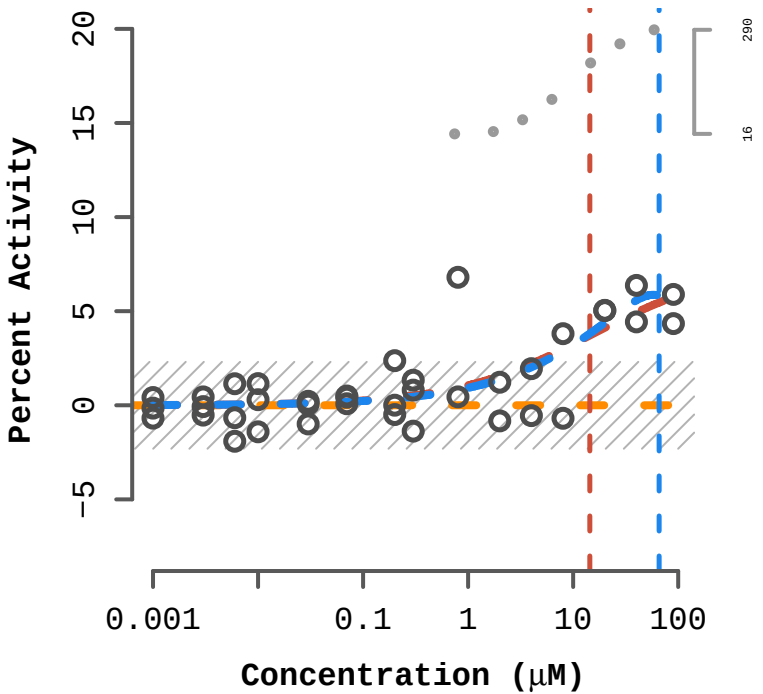
NAME: 6-Methyl coumarin
CHID: 25588 **CASRN:** 92-48-8
SPID(S): Tox21_303180
M4ID: 12475953

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.691 **MAX_MED:** 0.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Methyl coumarin
CHID: 25588 **CASRN:** 92-48-8
SPID(S): Tox21_201810
M4ID: 12480442 **BRK**

HILL MODEL (in red):

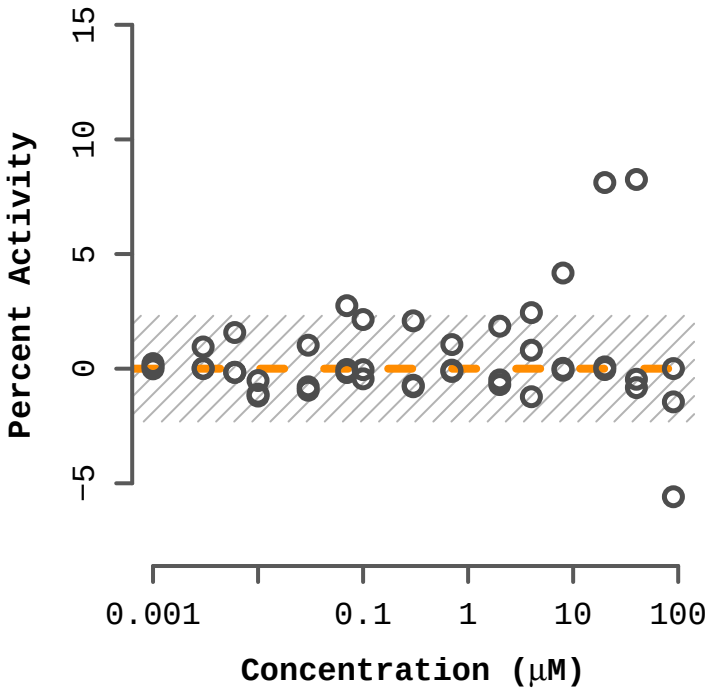
	tp	ga	gw
val:	7.42	1.16	0.673
sd:	5.65	1.18	0.59

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.7	1.82	0.628	2.07	2.98
sd:	32	2.55	0.458	0.395	11.3

	CNST	HILL	GNLS
AIC:	397.12	387.79	391.35
PROB:	0.01	0.85	0.14
RMSE:	66.75	65.32	65.31

MAX_MEAN: 99.1 **MAX_MED:** 6.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

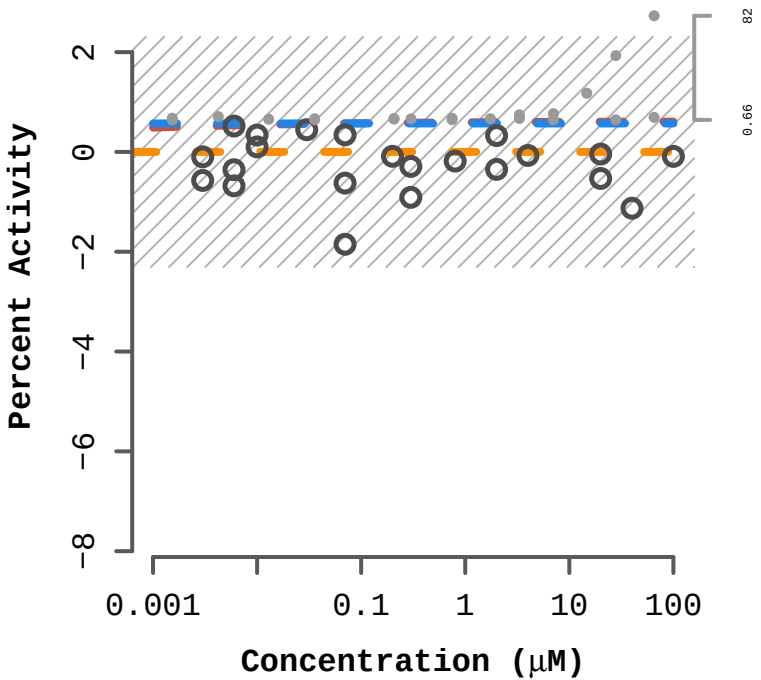
NAME: Methylcyclopentane
CHID: 25590 CASRN: 96-37-7
SPID(S): Tox21_202882
M4ID: 12479370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.38	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 2.72 MAX_MED: 0.806 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Methyldiethanolamine
CHID: 25591 CASRN: 105-59-9
SPID(S): Tox21_201199
M4ID: 12481053 BRK

HILL MODEL (in red):

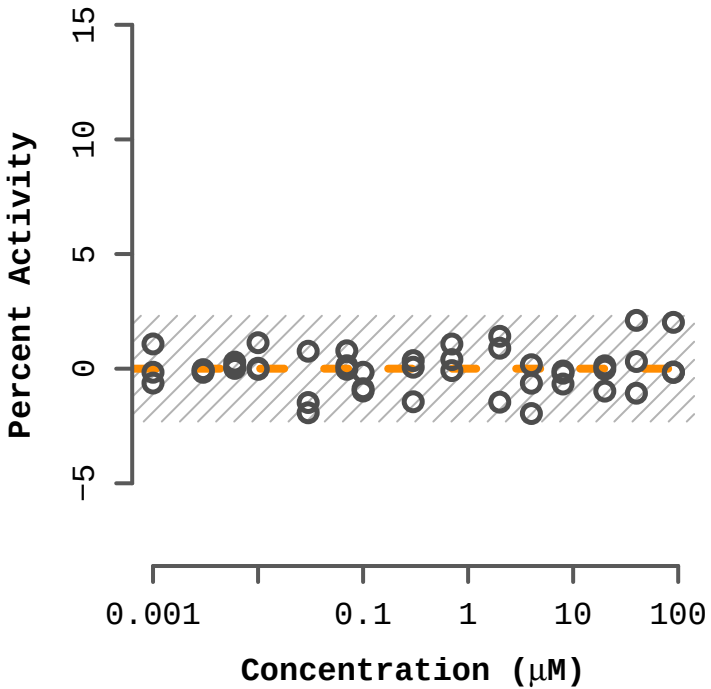
	tp	ga	gw
val:	0.612	-5	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.571	-4.98	3.62	3.26	8.18
sd:	0.224	1600	2930	48200	312000

	CNST	HILL	GNLS
AIC:	246.05	245.74	249.7
PROB:	0.43	0.5	0.07
RMSE:	14.77	14.61	14.62

MAX_MEAN: 28.1 MAX_MED: 2.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

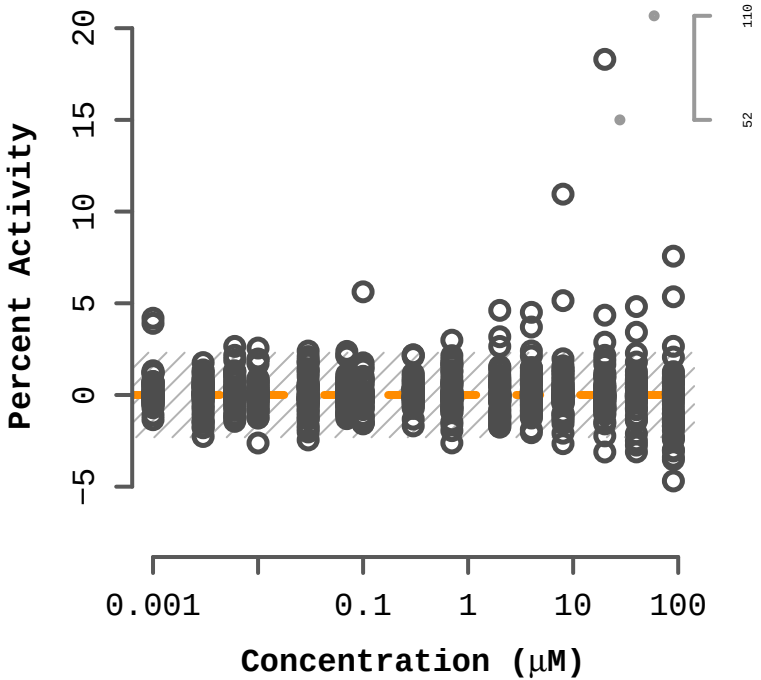
NAME: N'-Methyl-N,N-diphenylurea
CHID: 25593 **CASRN:** 13114-72-2
SPID(S): Tox21_200786
M4ID: 12481466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.573 **MAX_MED:** 0.894 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

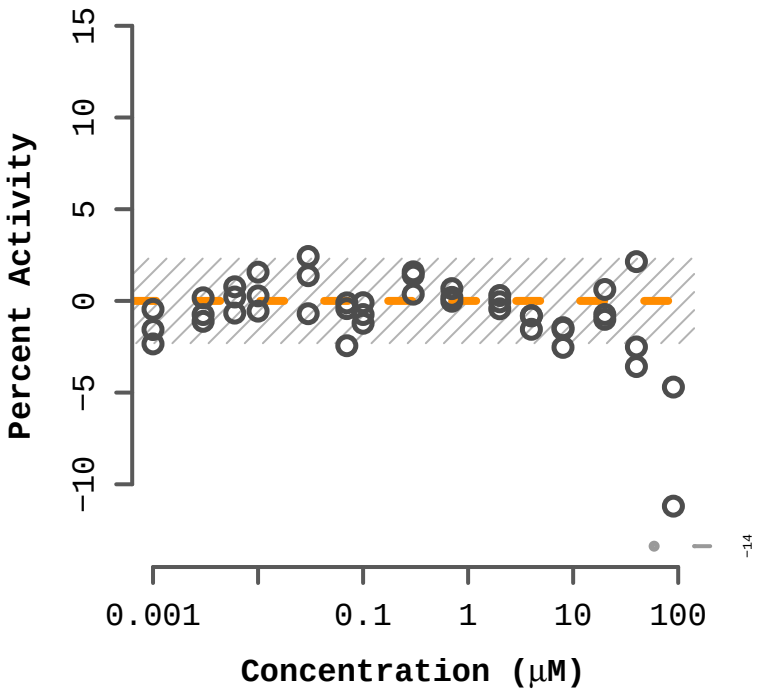
NAME: N,N'−Methylenebisacrylamide
CHID: 25595 **CASRN:** 110−26−9
SPID(S): Tox21_400038
M4ID: 12475099 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2190.48	NA	NA
PROB:	1	NA	NA
RMSE:	4.66	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 0.136 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

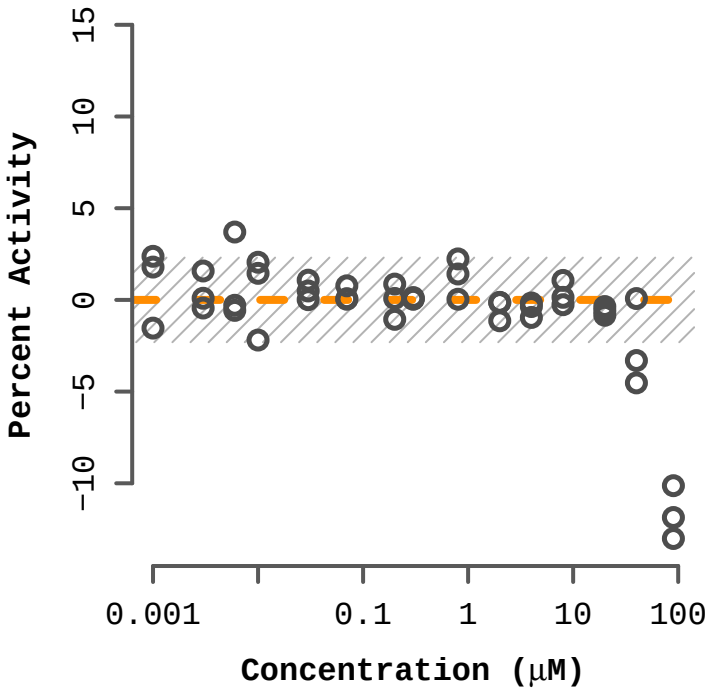
NAME: Methylene bis(thiocyanate)
CHID: 25599 CASRN: 6317-18-6
SPID(S): Tox21_301058
M4ID: 12478075 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.7	NA	NA
PROB:	1	NA	NA
RMSE:	3.08	NA	NA

MAX_MEAN: 1.12 MAX_MED: 1.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

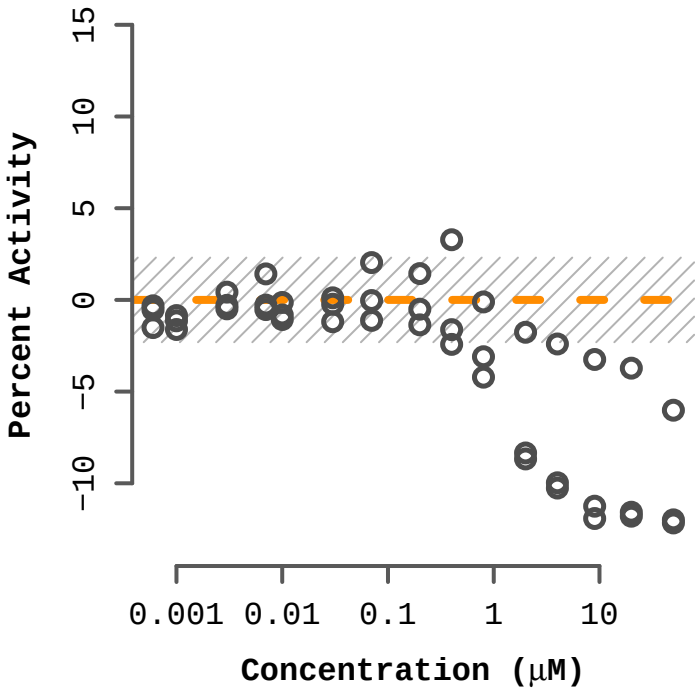
NAME: Methylene bis(thiocyanate)
CHID: 25599 CASRN: 6317-18-6
SPID(S): Tox21_202325
M4ID: 12479927

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.33	NA	NA

MAX_MEAN: 1.23 MAX_MED: 1.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

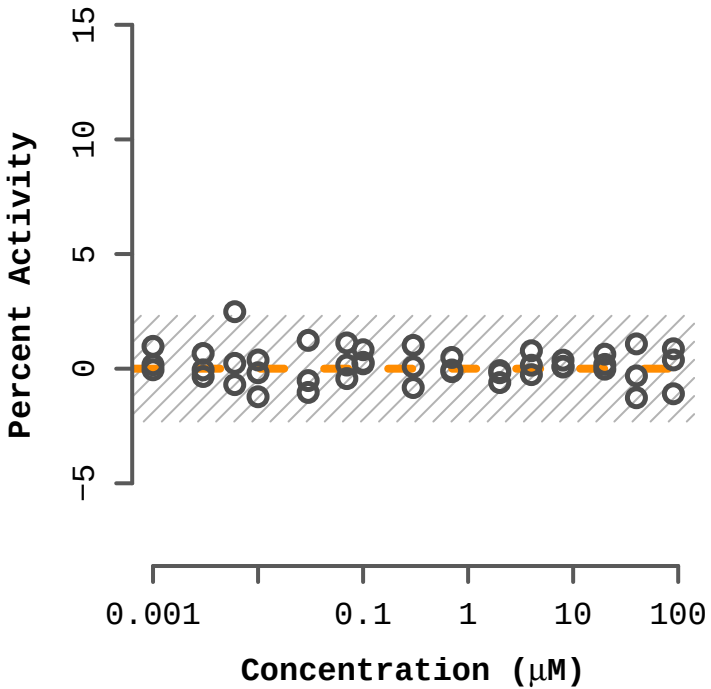
NAME: Methylene Blue trihydrate
CHID: 25600 **CASRN:** 7220-79-3
SPID(S): Tox21_202525
M4ID: 12479727

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.05	NA	NA
PROB:	1	NA	NA
RMSE:	5.42	NA	NA

MAX_MEAN: 0.297 **MAX_MED:** −0.0321 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

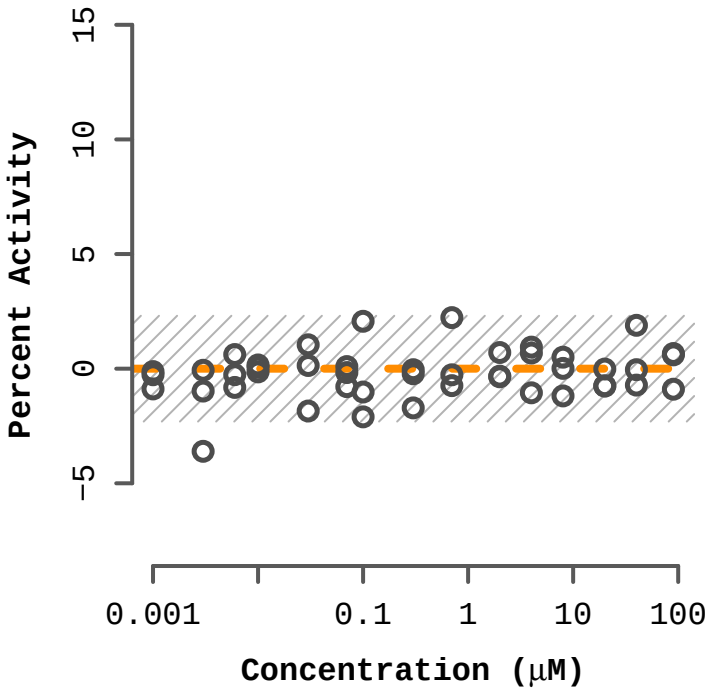
NAME: N-Methylethanolamine
CHID: 25603 CASRN: 109-83-1
SPID(S): Tox21_301013
M4ID: 12478120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.675 MAX_MED: 0.383 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

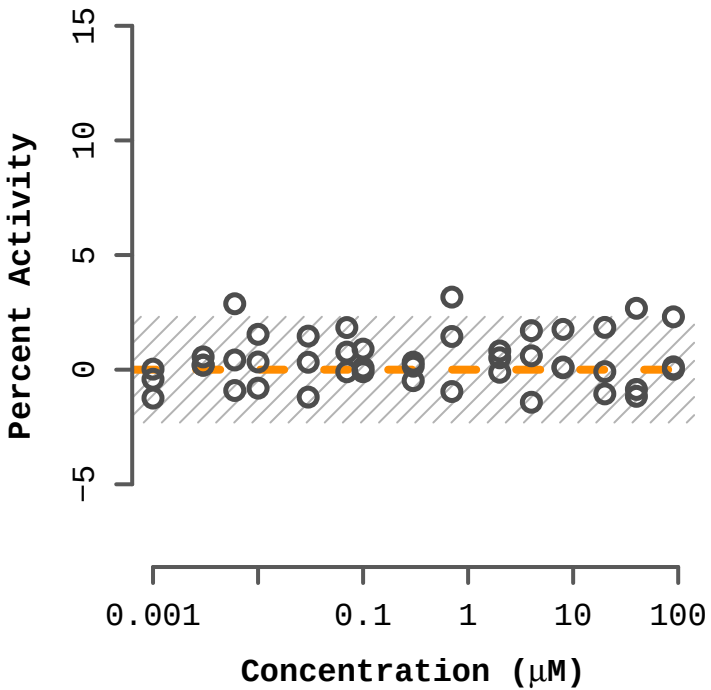
NAME: 2-Methyl-2-ethoxypropane
CHID: 25604 **CASRN:** 637-92-3
SPID(S): Tox21_200349
M4ID: 12481903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.408 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

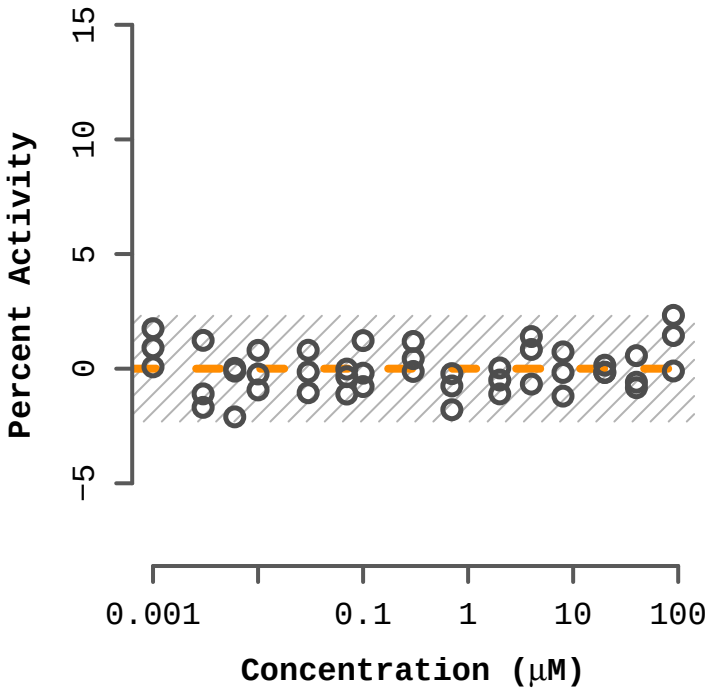
NAME: Methyleugenol
CHID: 25607 **CASRN:** 93-15-2
SPID(S): Tox21_300071
M4ID: 12479059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

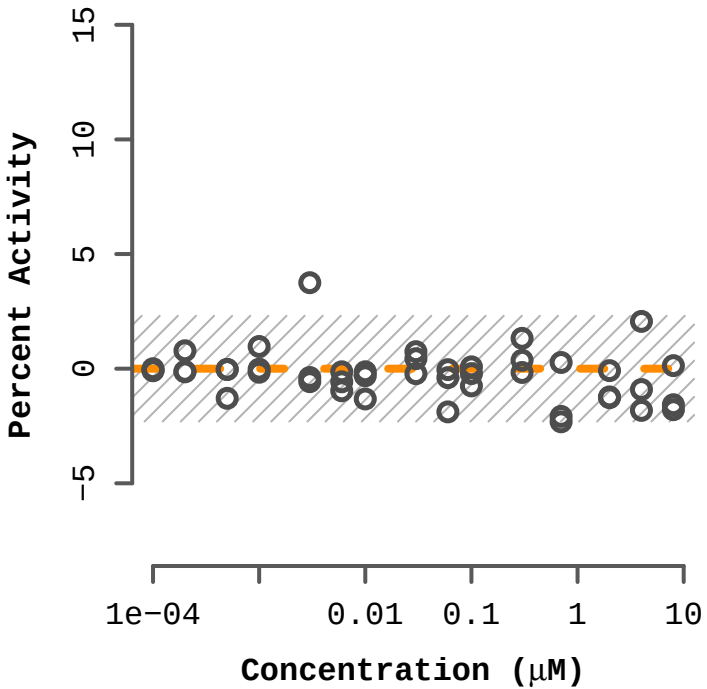
NAME: Methyleugenol
CHID: 25607 **CASRN:** 93-15-2
SPID(S): Tox21_202347
M4ID: 12479905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

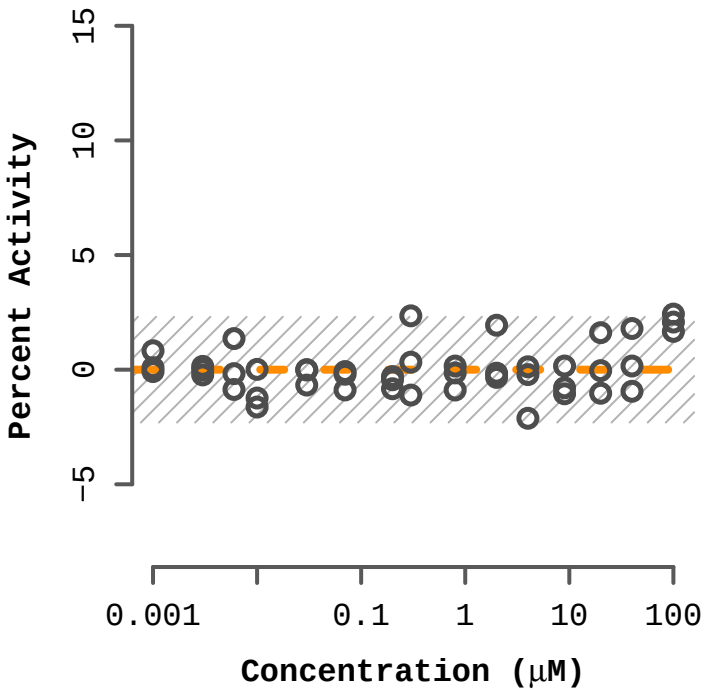
NAME: Methyl formate
CHID: 25609 **CASRN:** 107-31-3
SPID(S): Tox21_300962
M4ID: 12478171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.934 **MAX_MED:** 0.438 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

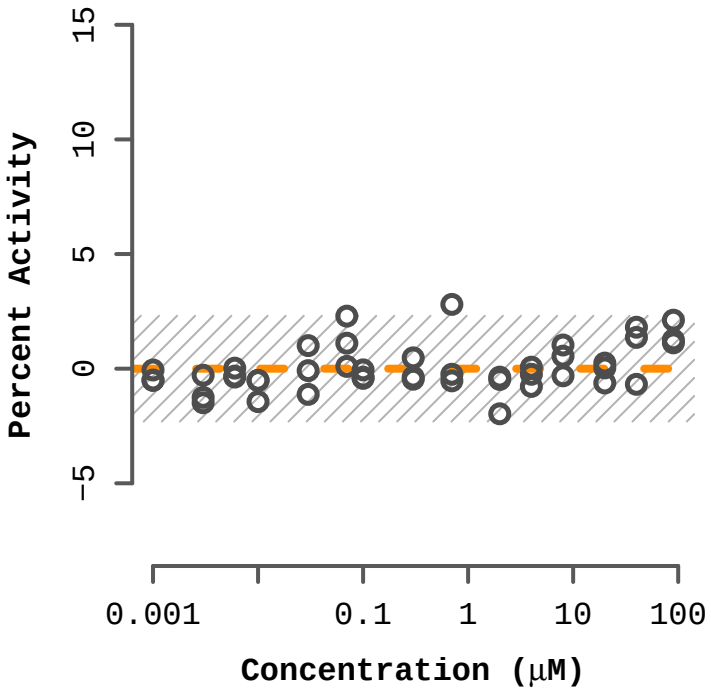
NAME: Methyl 4-formylbenzoate
CHID: 25610 **CASRN:** 1571-08-0
SPID(S): Tox21_303302
M4ID: 12475831

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

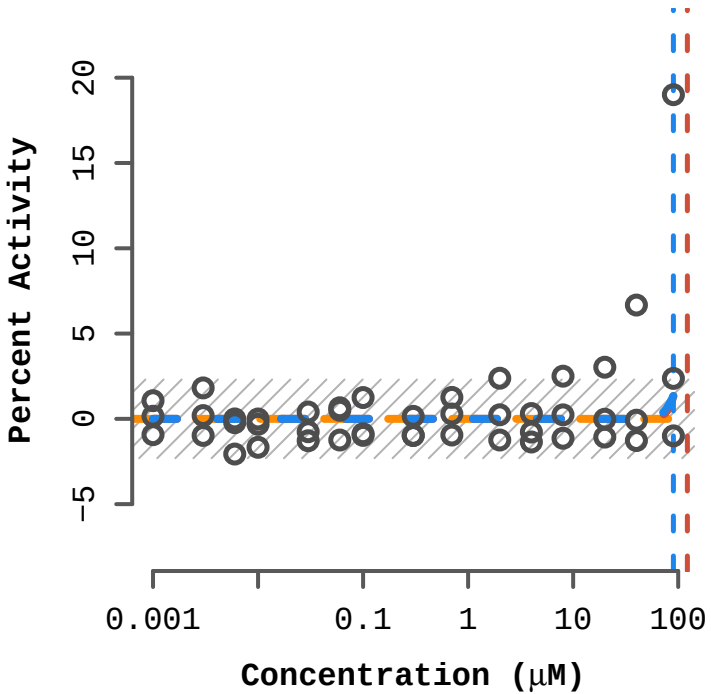
NAME: Methyl 4-formylbenzoate
CHID: 25610 **CASRN:** 1571-08-0
SPID(S): Tox21_202369
M4ID: 12479883

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.59	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylfuran
CHID: 25611 CASRN: 534-22-5
SPID(S): Tox21_200203
M4ID: 12482049

HILL MODEL (in red):

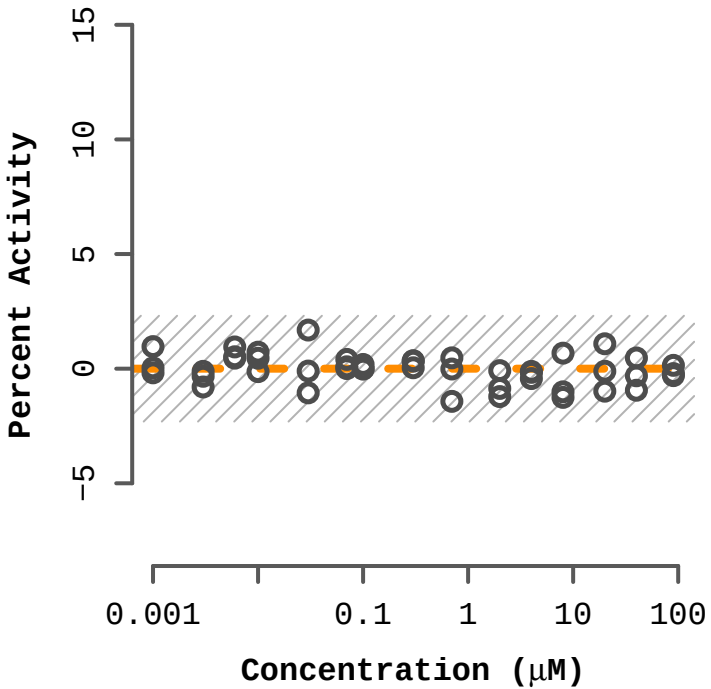
	tp	ga	gw
val:	16.9	2.09	7.99
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.69	1.95	8	3.92	1.23
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	179.96	185.22	189.23
PROB:	0.92	0.07	0.01
RMSE:	3.22	3.05	3.05

MAX_MEAN: 6.79 MAX_MED: 2.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

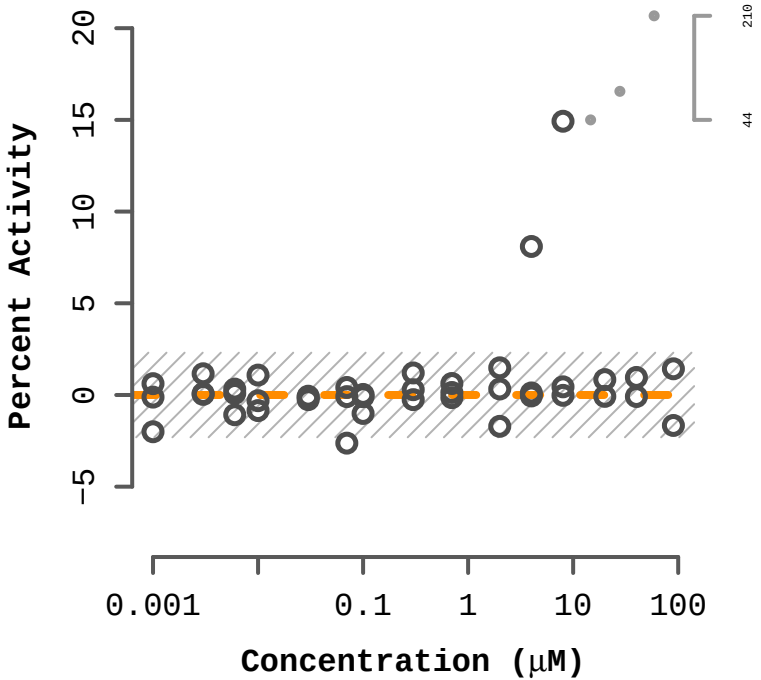
NAME: 2-Methylpentanedinitrile
CHID: 25612 **CASRN:** 4553-62-2
SPID(S): Tox21_303174
M4ID: 12475959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.644 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

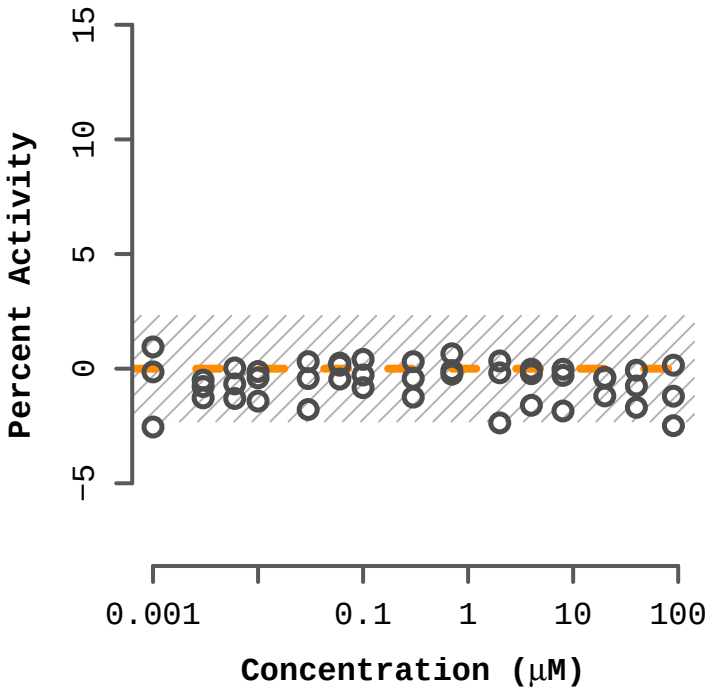
NAME: 2-Methylpentanedinitrile
CHID: 25612 **CASRN:** 4553-62-2
SPID(S): Tox21_201788
M4ID: 12480464 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	269.97	NA	NA
PROB:	1	NA	NA
RMSE:	35.42	NA	NA

MAX_MEAN: 71.3 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

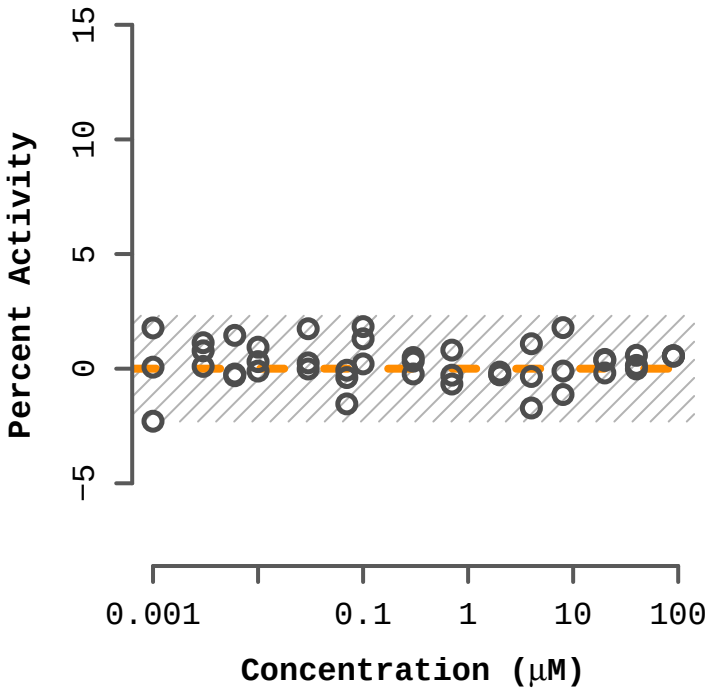
NAME: 4-Methylimidazole
CHID: 25617 **CASRN:** 822-36-6
SPID(S): Tox21_201048
M4ID: 12481204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.111 **MAX_MED:** 0.152 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

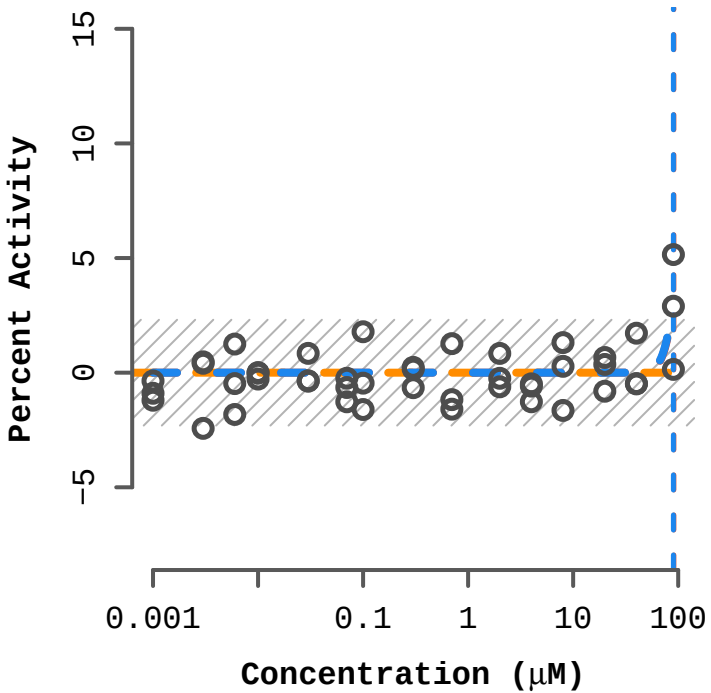
NAME: 2-Methyl-3-nitroaniline
CHID: 25628 **CASRN:** 603-83-8
SPID(S): Tox21_200773
M4ID: 12481479

HILL MODEL: Not applicable.

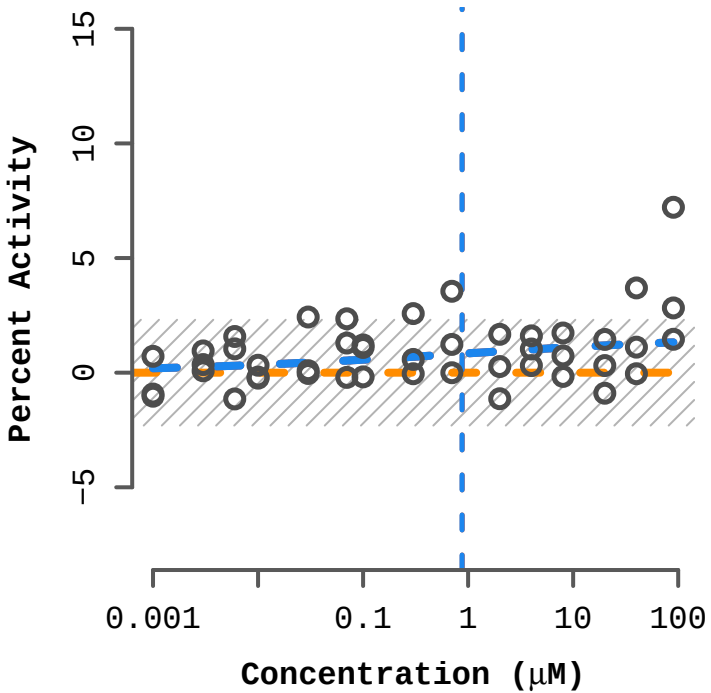
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

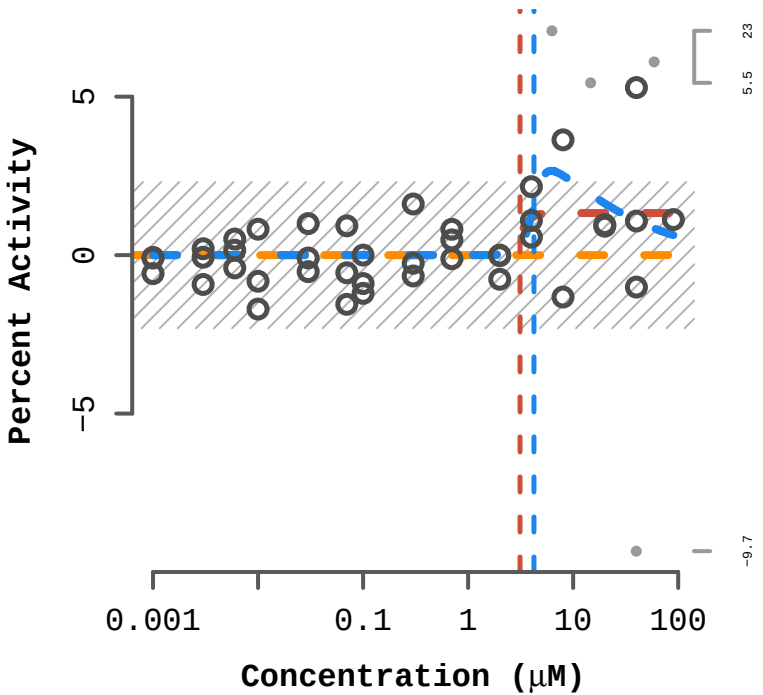
MAX_MEAN: 1.12 **MAX_MED:** 1.3 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Methyl-4-nitroaniline
CHID:    25629   CASRN: 99-52-5
SPID(S): Tox21_200387
M4ID:    12481865

HILL MODEL (in red):
      tp       ga       gw
val:  6.17     1.96     7.95
sd:   6.78     0.13     76.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.93     1.95     7.81     2.27     15.6
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  146.79      146.06      150.06
PROB: 0.38        0.55        0.07
RMSE: 1.3         1.1         1.1

MAX_MEAN: 2.73      MAX_MED: 2.9       BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Methyl-2-nitroaniline
CHID:    25632   CASRN: 89-62-3
SPID(S): Tox21_303189
M4ID:    12475944

HILL MODEL (in red):
      tp       ga       gw
val:  1.65     -0.0561  0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.65     -0.0579  0.3      3.94     17.2
sd:   NA       NA       NA       NA       NA

      CNST       HILL       GNLS
AIC:  169.96     157.86     161.86
PROB: 0          0.88       0.12
RMSE: 1.75       1.41       1.41

MAX_MEAN: 3.83      MAX_MED: 2.83      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methyl-2-nitroaniline
CHID: 25632 **CASRN:** 89-62-3
SPID(S): Tox21_202055
M4ID: 12480197 **BRK**

HILL MODEL (in red):

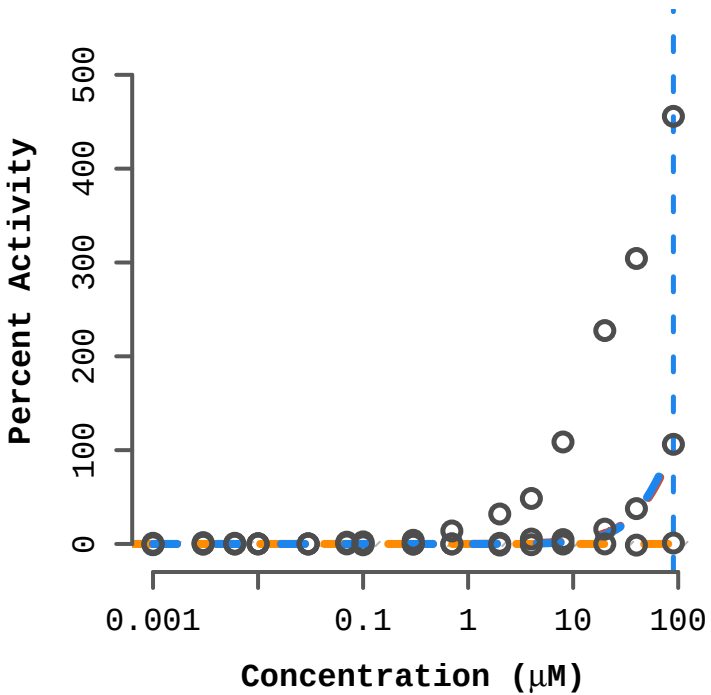
	tp	ga	gw
val:	1.33	0.494	8
sd:	0.511	0.193	10.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.18	0.627	7.98	0.877	0.795
sd:	15.9	0.133	14.6	2.76	1.05

	CNST	HILL	GNLS
AIC:	207.25	204.75	208.16
PROB:	0.2	0.68	0.12
RMSE:	4.4	4.15	4.03

MAX_MEAN: 8.37 **MAX_MED:** 3.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methyl-3-nitroaniline
CHID: 25633 CASRN: 119-32-4
SPID(S): Tox21_200103
M4ID: 12482149

HILL MODEL (in red):

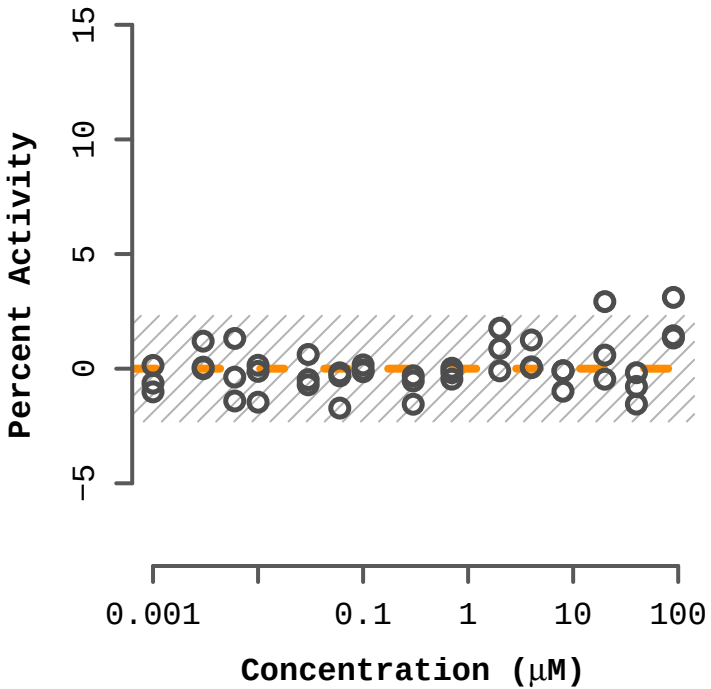
	tp	ga	gw
val:	547	2.34	1.6
sd:	169	0.059	0.248

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	210	1.95	2.01	3.88	15.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	442.04	441.21	445.47
PROB:	0.37	0.56	0.07
RMSE:	91.95	77.5	77.58

MAX_MEAN: 188 MAX_MED: 106 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

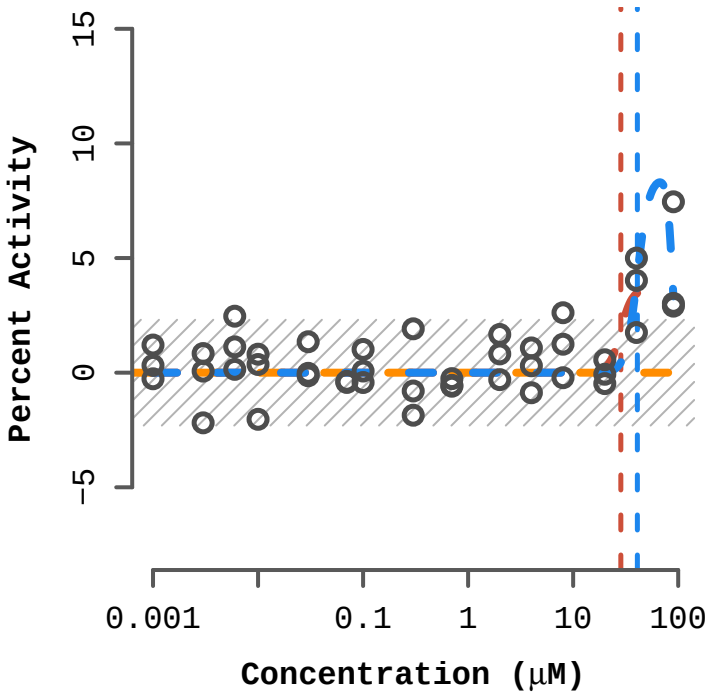
NAME: 5-Methyl-2-nitroaniline
CHID: 25634 **CASRN:** 578-46-1
SPID(S): Tox21_200333
M4ID: 12481919

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Methyl-4-nitroaniline
CHID: 25635 CASRN: 100-15-2
SPID(S): Tox21_200001
M4ID: 12482251

HILL MODEL (in red):

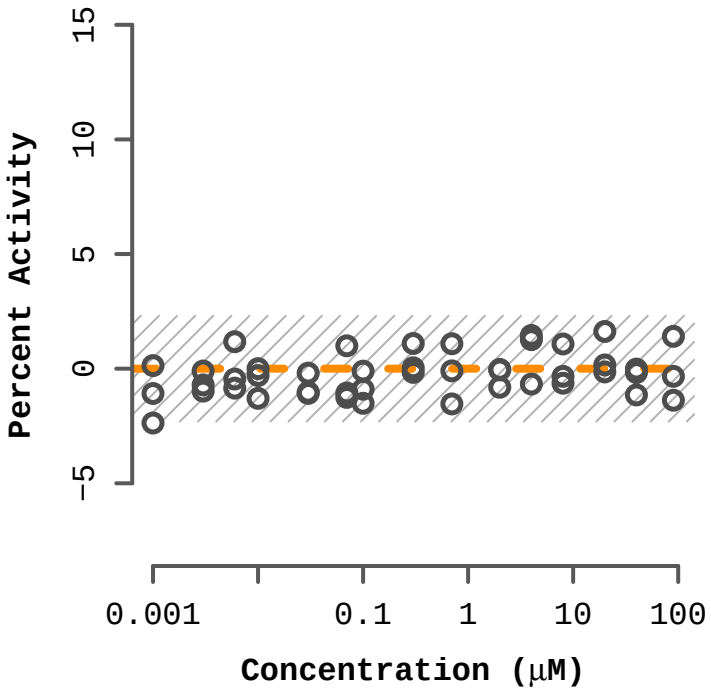
	tp	ga	gw
val:	3.67	1.45	8
sd:	0.633	0.0864	4.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.54	1.61	7.96	1.94	17.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	173.87	150.38	153.64
PROB:	0	0.84	0.16
RMSE:	1.93	1.23	1.25

MAX_MEAN: 4.46 MAX_MED: 4.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

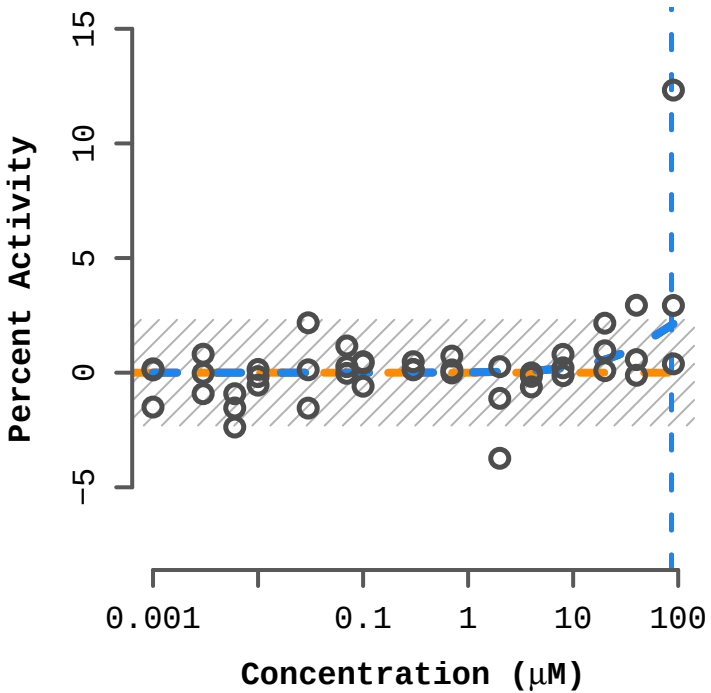
NAME: 2-Methyl-3-nitrobenzoic acid
CHID: 25637 **CASRN:** 1975-50-4
SPID(S): Tox21_201228
M4ID: 12481024

HILL MODEL: Not applicable.

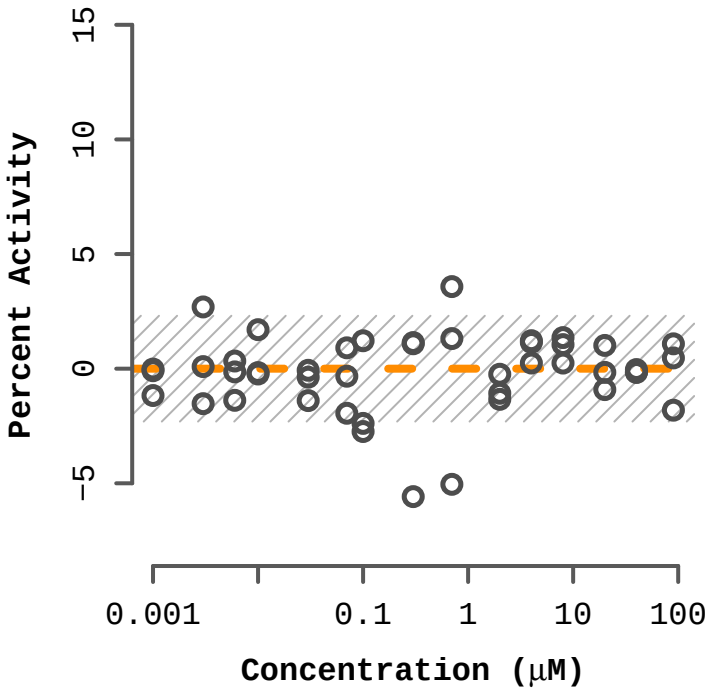
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.683 **MAX_MED:** 1.27 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Methyl-6-nitrobenzoic acid
CHID:    25639   CASRN: 13506-76-8
SPID(S): Tox21_200201
M4ID:    12482051

HILL MODEL (in red):
      tp       ga       gw
val:  4.15     1.94     1.26
sd:   17.2     2.6      1.55

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.15     1.94     1.26     3.79     3.37
sd:   17.2     2.6      1.55     879      1680

      CNST        HILL        GNLS
AIC:  156.84      155.06      159.06
PROB: 0.27        0.65        0.09
RMSE: 2.18        1.86        1.86

MAX_MEAN: 5.22      MAX_MED: 2.93      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

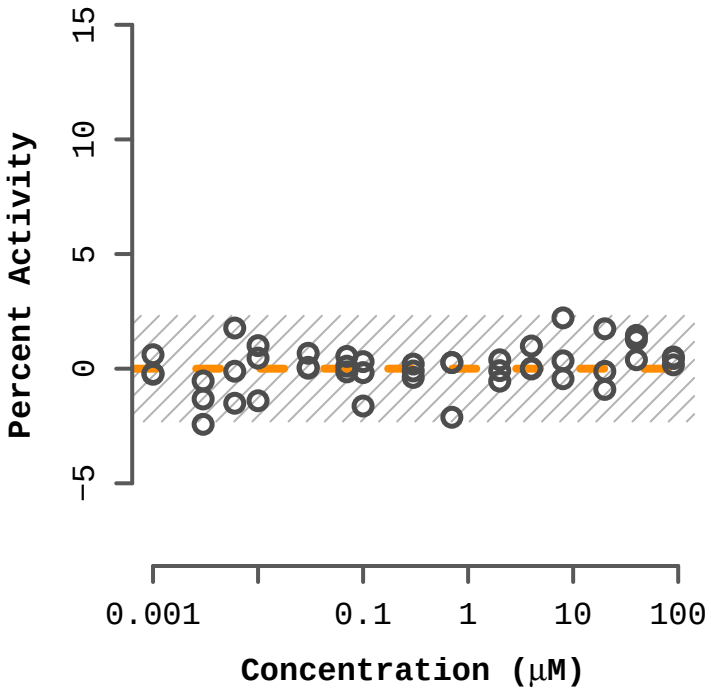
NAME: 3-Methyl-2-nitrobenzoic acid
CHID: 25640 **CASRN:** 5437-38-7
SPID(S): Tox21_200852
M4ID: 12481400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 0.885 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

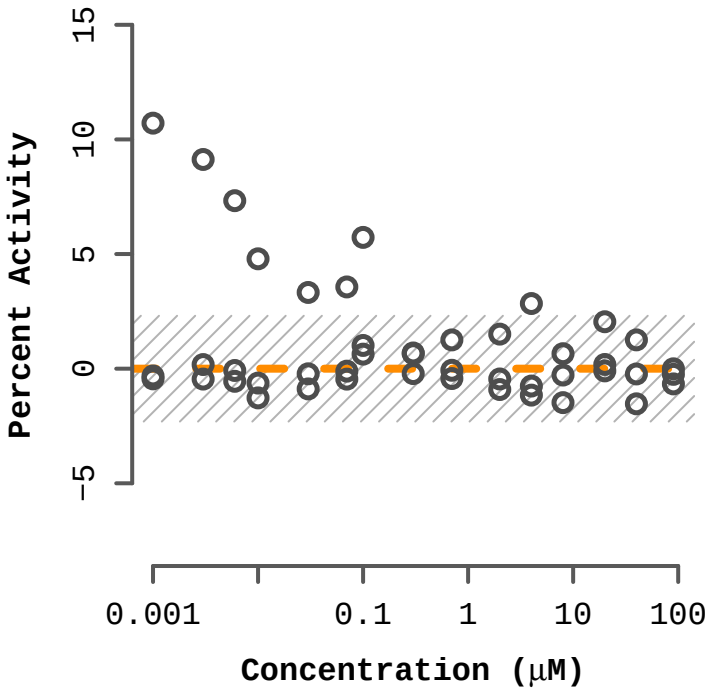
NAME: 3-Methyl-4-nitrobenzoic acid
CHID: 25641 **CASRN:** 3113-71-1
SPID(S): Tox21_200835
M4ID: 12481417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

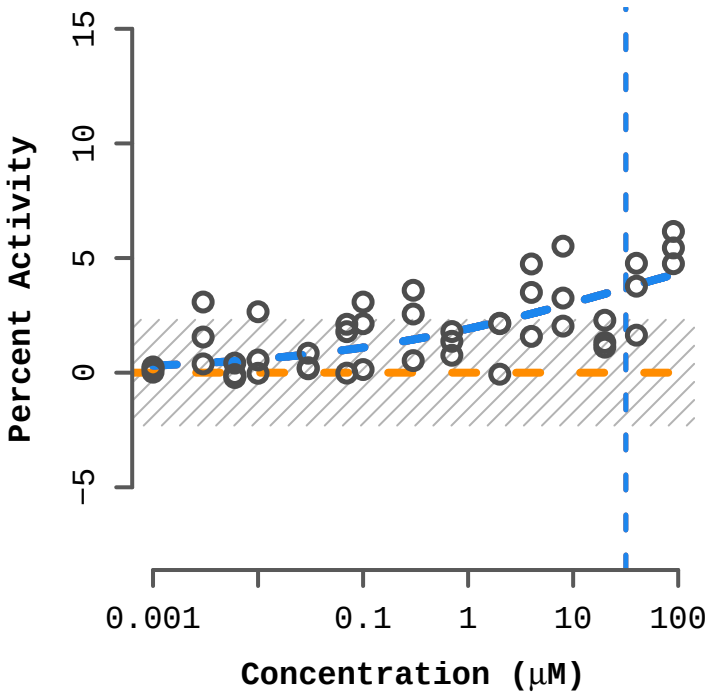
NAME: 4-Methyl-3-nitrobenzoic acid
CHID: 25642 **CASRN:** 96-98-0
SPID(S): Tox21_201069
M4ID: 12481183

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.75	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 3.32 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Methyl phenanthrene
CHID: 25648 CASRN: 832-69-9
SPID(S): Tox21_303752
M4ID: 12475436

HILL MODEL (in red):

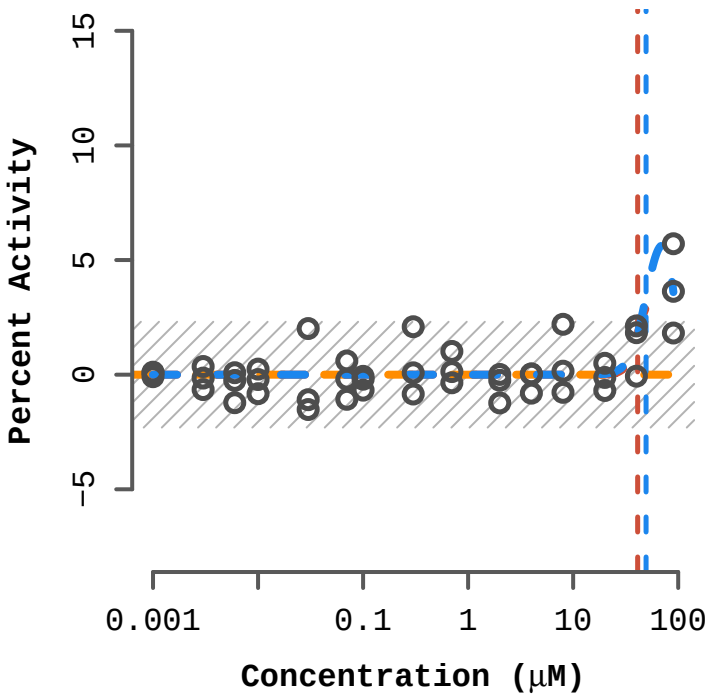
	tp	ga	gw
val:	7.39	1.5	0.303
sd:	3.67	1.35	0.0817

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.39	1.5	0.303	3.01	8.32
sd:	3.67	1.35	0.0817	1190	9410

	CNST	HILL	GNLS
AIC:	216.02	160.54	164.54
PROB:	0	0.88	0.12
RMSE:	2.57	1.27	1.27

MAX_MEAN: 5.45 MAX_MED: 5.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylphenanthrene
CHID: 25649 CASRN: 2531-84-2
SPID(S): Tox21_200567
M4ID: 12481685

HILL MODEL (in red):

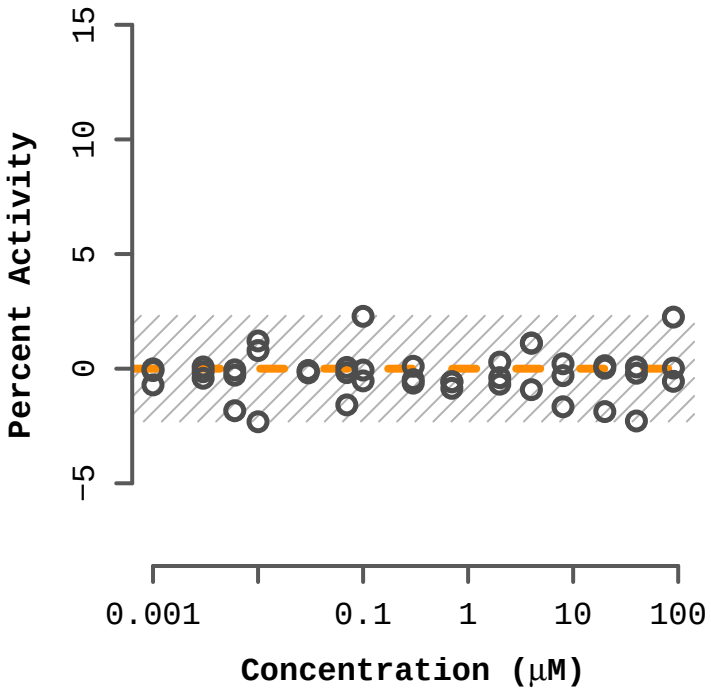
	tp	ga	gw
val:	3.61	1.61	8
sd:	0.702	0.0438	15.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.85	1.69	5.7	1.96	9.89
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	143.54	126.24	130.28
PROB:	0	0.88	0.12
RMSE:	1.37	0.92	0.92

MAX_MEAN: 3.72 MAX_MED: 3.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

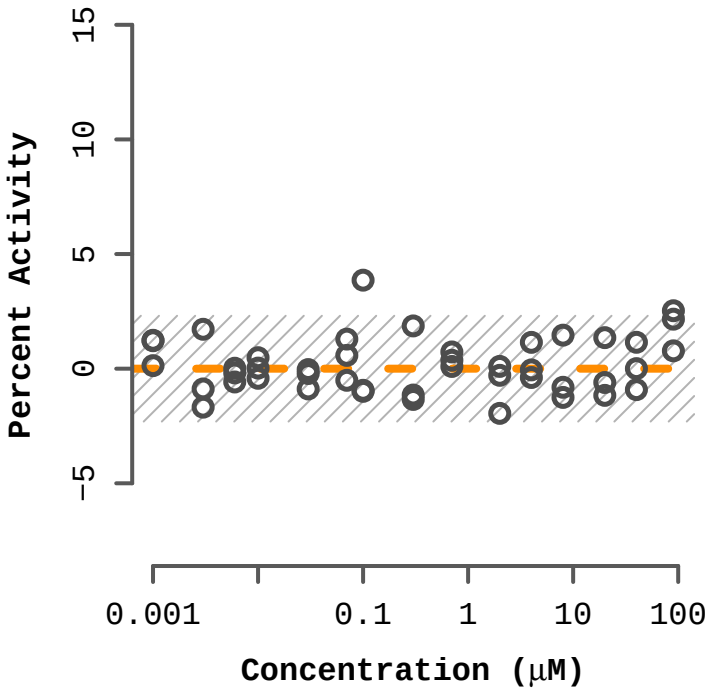
NAME: 2-(2-Methylpropyl)thiazole
CHID: 25653 CASRN: 18640-74-9
SPID(S): Tox21_200301
M4ID: 12481951

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.576 MAX_MED: 1.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

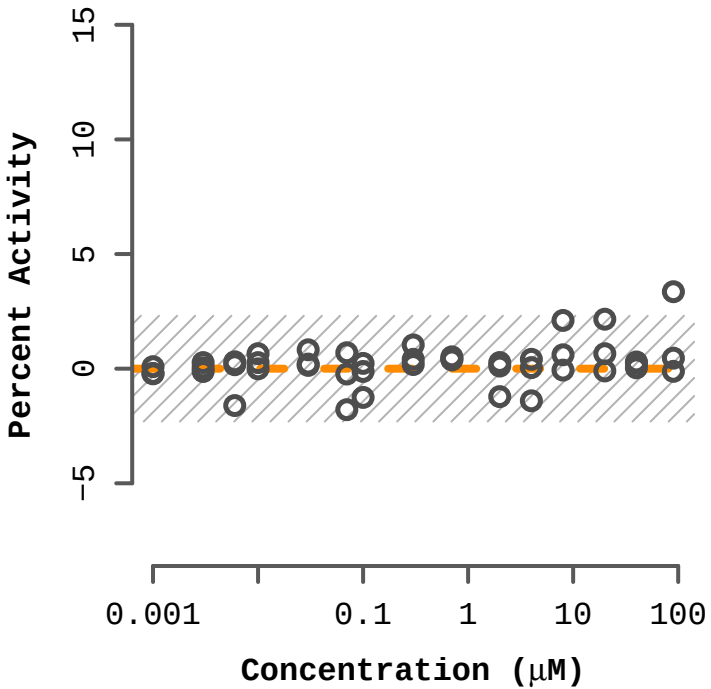
NAME: 1-Methylpyrene
CHID: 25654 **CASRN:** 2381-21-7
SPID(S): Tox21_200154
M4ID: 12482098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

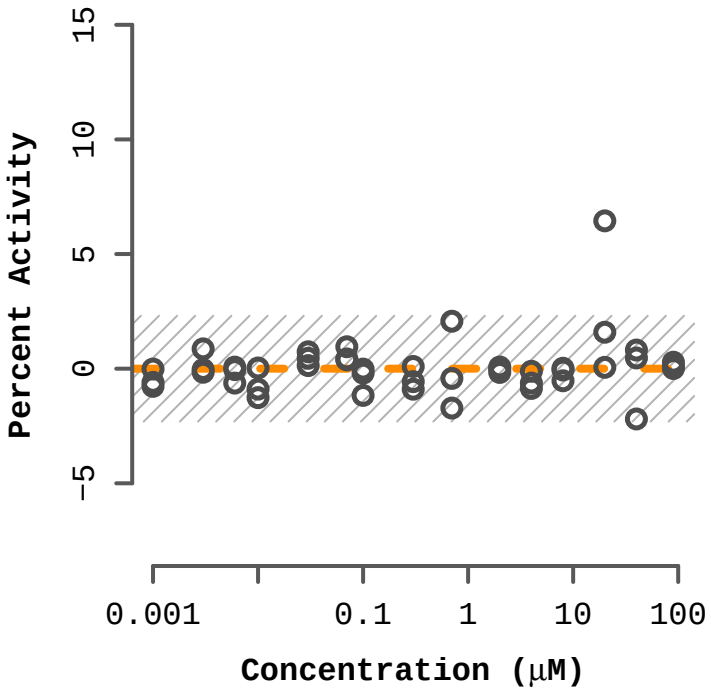
NAME: 7-Methylquinoline
CHID: 25657 **CASRN:** 612-60-2
SPID(S): Tox21_201146
M4ID: 12481106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.655 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

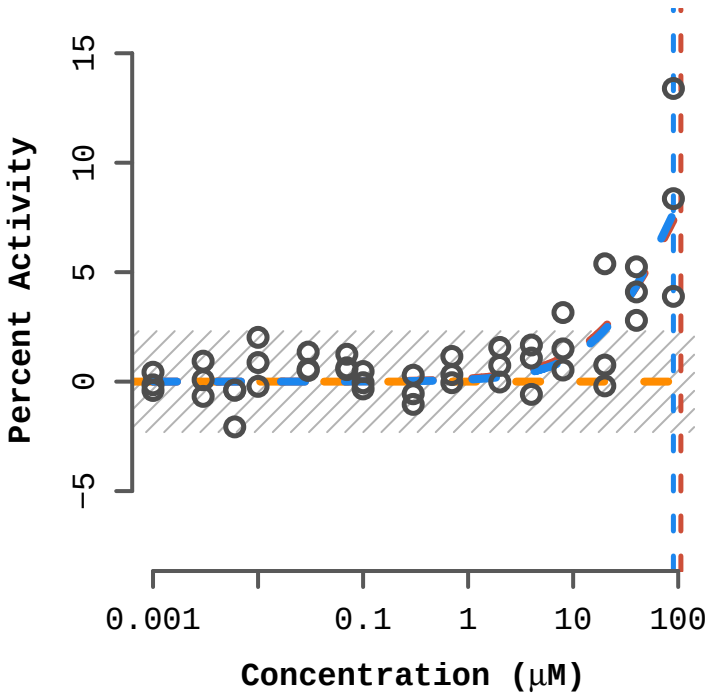
NAME: Methyl salicylate
CHID: 25659 **CASRN:** 119-36-8
SPID(S): Tox21_300137
M4ID: 12478993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl salicylate
CHID: 25659 CASRN: 119-36-8
SPID(S): Tox21_201543
M4ID: 12480709

HILL MODEL (in red):

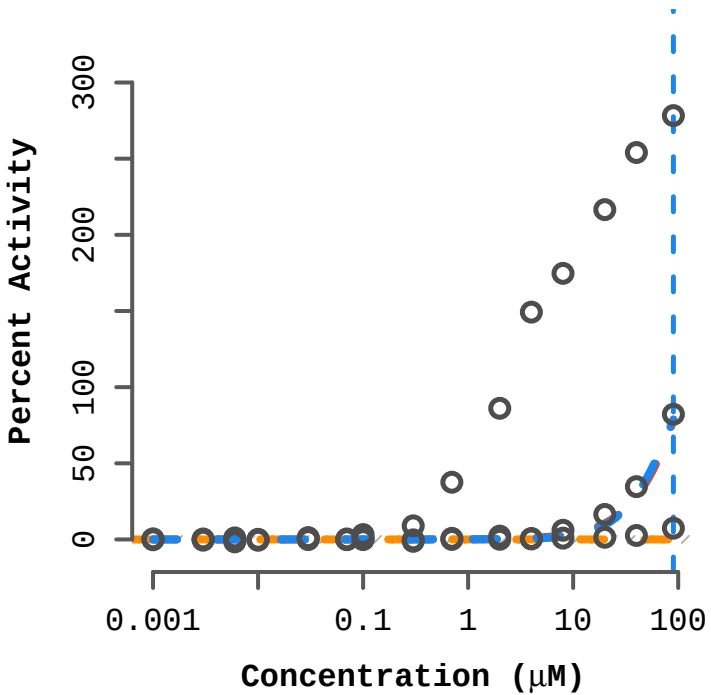
	tp	ga	gw
val:	16.1	2.03	1.02
sd:	9.55	0.421	0.422

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.4	1.95	1.13	2.97	8.02
sd:	9.99	0.432	0.472	973	7700

	CNST	HILL	GNLS
AIC:	198.46	161.18	165.36
PROB:	0	0.89	0.11
RMSE:	2.93	1.49	1.48

MAX_MEAN: 8.55 **MAX_MED:** 8.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: alpha-Methylstyrene
CHID: 25661 CASRN: 98-83-9
SPID(S): Tox21_200159
M4ID: 12482093

HILL MODEL (in red):

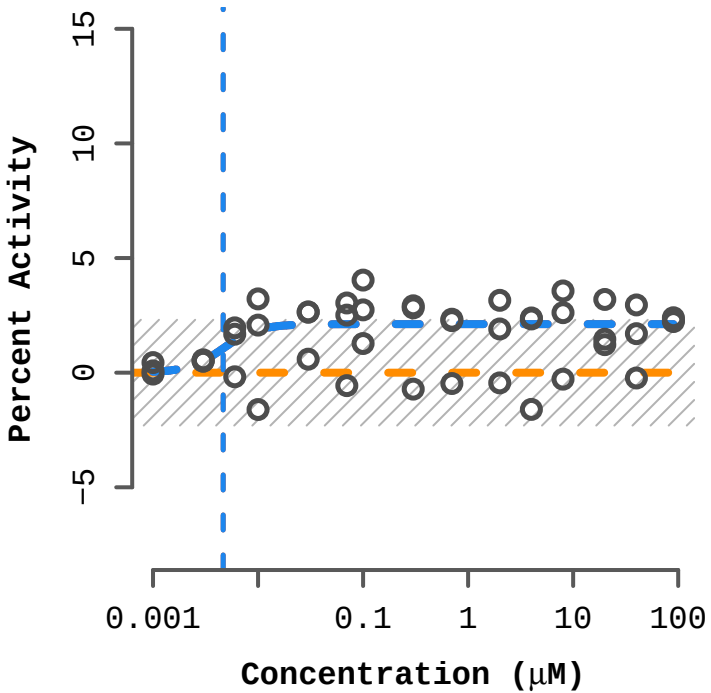
	tp	ga	gw
val:	334	2.3	1.49
sd:	1330	1.66	0.775

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	157	1.95	1.82	3.56	15.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	464.26	459.57	463.81
PROB:	0.08	0.82	0.1
RMSE:	75.86	66.61	66.68

MAX_MEAN: 123 MAX_MED: 82.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl styryl ketone
CHID: 25662 CASRN: 122-57-6
SPID(S): Tox21_303222
M4ID: 12475911

HILL MODEL (in red):

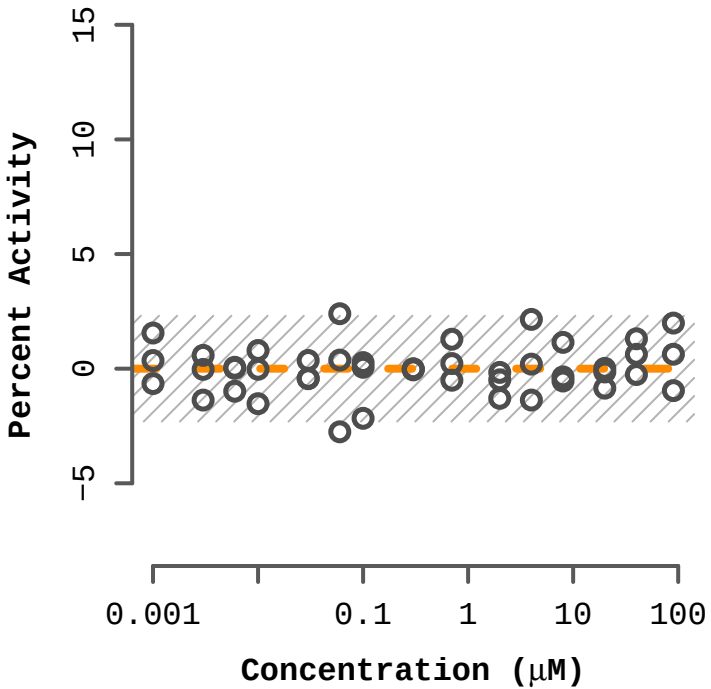
	tp	ga	gw
val:	2.12	−2.33	2.6
sd:	0.222	0.163	2.28

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.12	−2.33	2.6	3.73	3.83
sd:	0.222	0.163	2.28	706	1540

	CNST	HILL	GNLS
AIC:	203.01	162.76	166.76
PROB:	0	0.88	0.12
RMSE:	2.09	1.39	1.39

MAX_MEAN: 2.68 MAX_MED: 2.83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

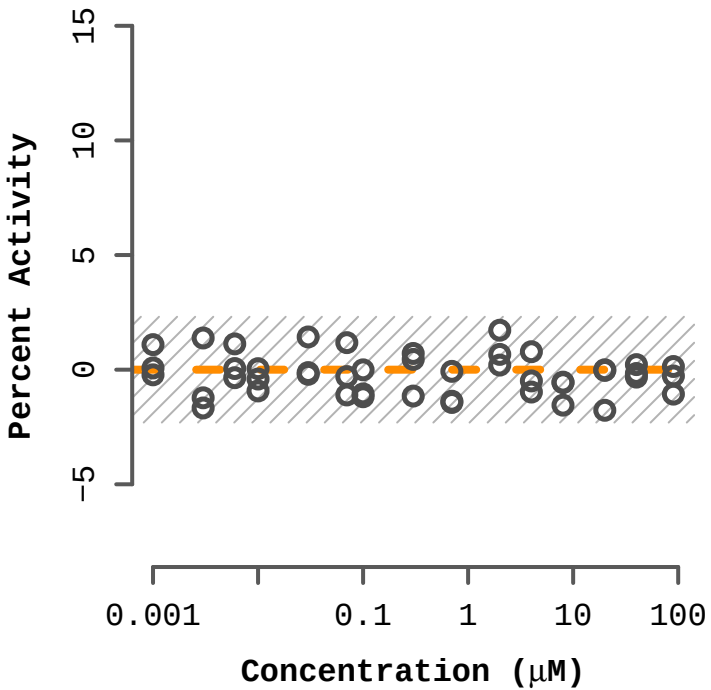
NAME: Methyl styryl ketone
CHID: 25662 **CASRN:** 122-57-6
SPID(S): Tox21_201502
M4ID: 12480750

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.56 **MAX_MED:** 0.631 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

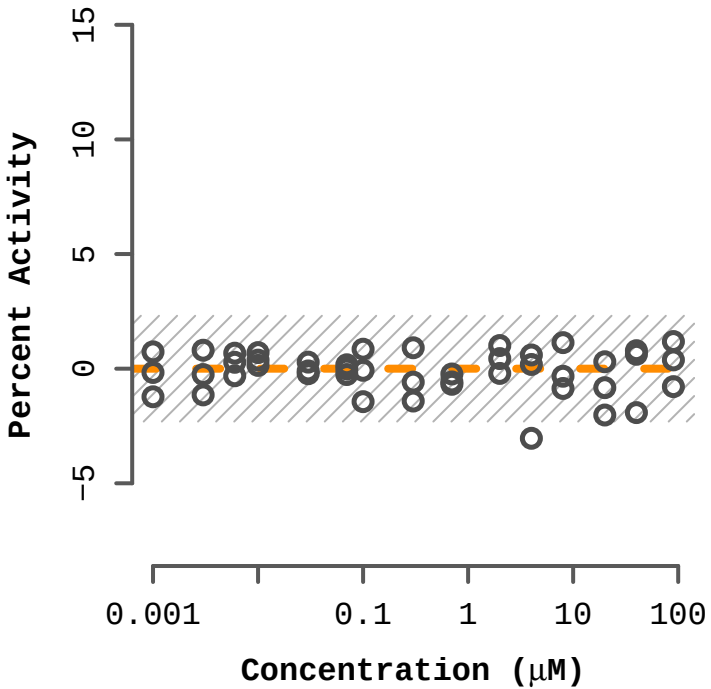
NAME: 5-Methyl-2-thiouracil
CHID: 25665 **CASRN:** 636-26-0
SPID(S): Tox21_202899
M4ID: 12479353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.864 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

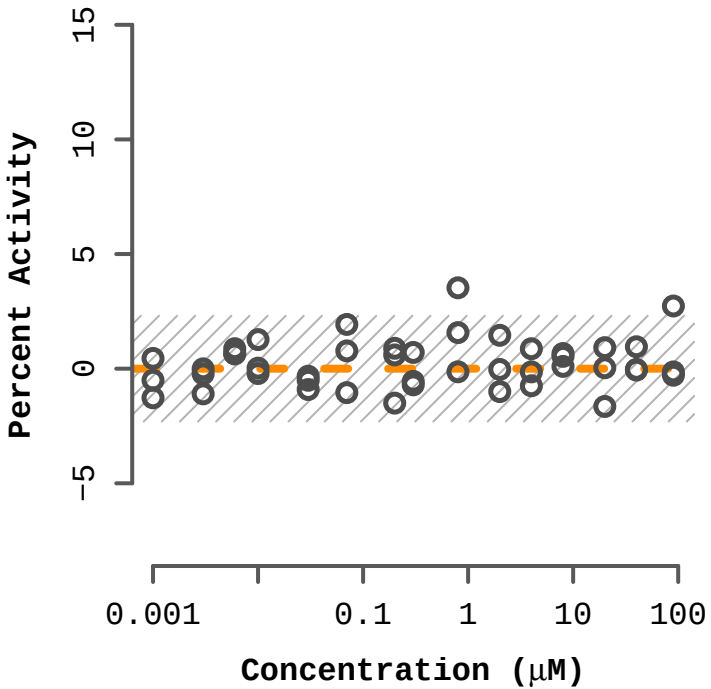
NAME: Methyl 4-methylbenzoate
CHID: 25668 **CASRN:** 99-75-2
SPID(S): Tox21_303124
M4ID: 12476009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

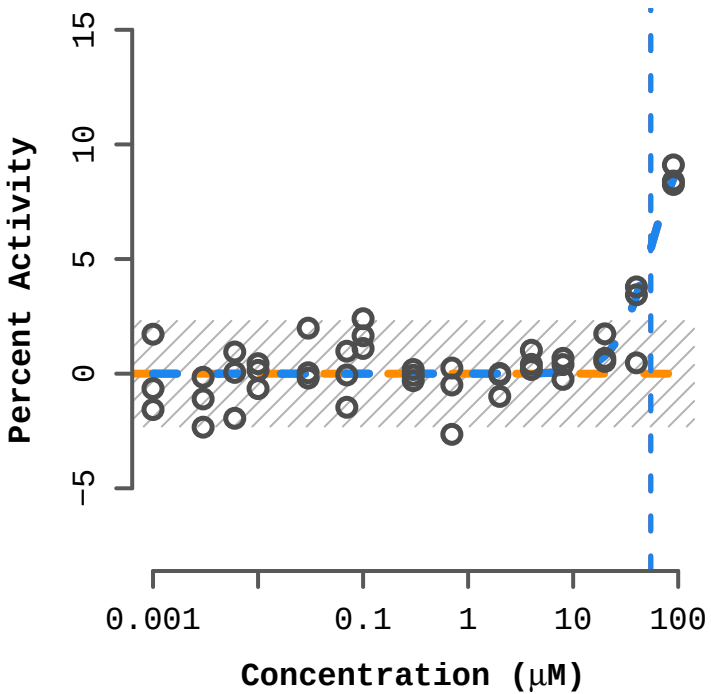
NAME: Methyl 4-methylbenzoate
CHID: 25668 CASRN: 99-75-2
SPID(S): Tox21_202391
M4ID: 12479861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.66 MAX_MED: 1.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylumbelliferone
CHID: 25670 CASRN: 90-33-5
SPID(S): Tox21_300915
M4ID: 12478218

HILL MODEL (in red):

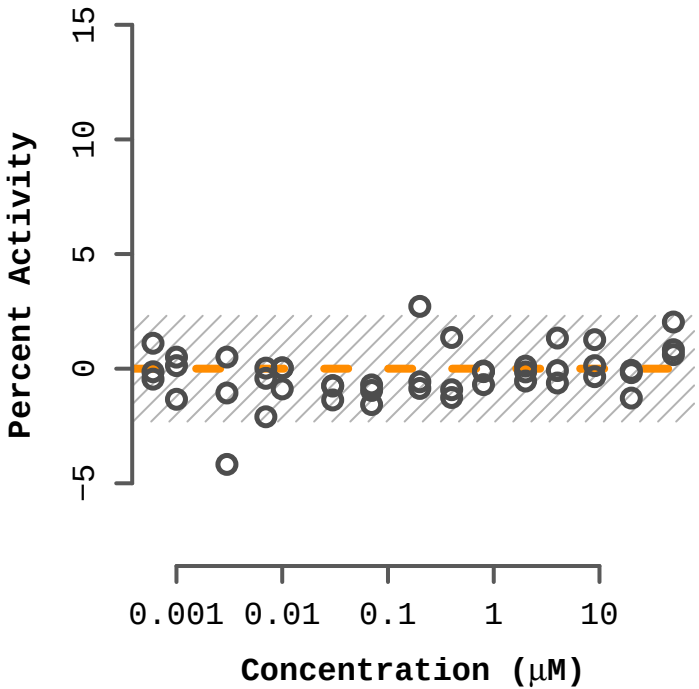
	tp	ga	gw
val:	10.9	1.74	2.53
sd:	2.82	0.123	0.894

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.9	1.74	2.53	3.37	5.25
sd:	2.86	0.125	0.908	772	2870

	CNST	HILL	GNLS
AIC:	190.96	142.08	146.07
PROB:	0	0.88	0.12
RMSE:	2.57	1.1	1.1

MAX_MEAN: 8.59 MAX_MED: 8.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

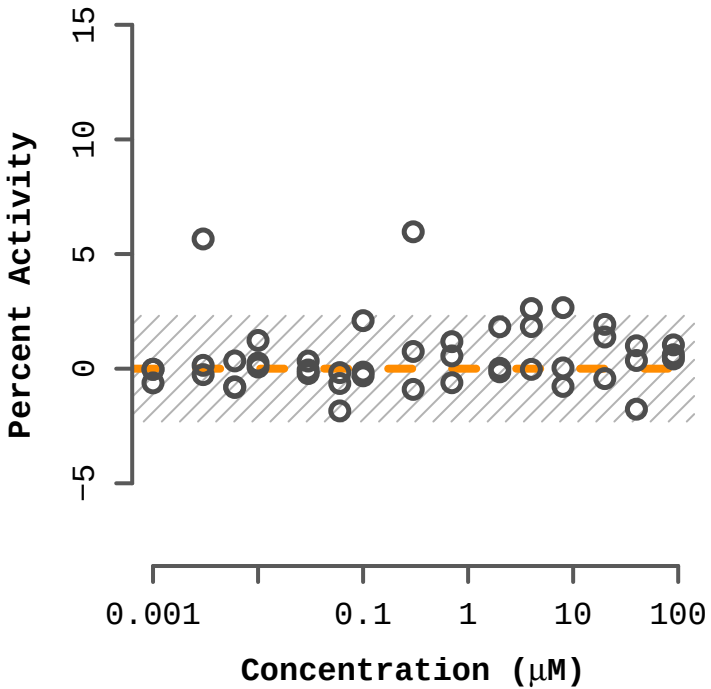
NAME: 4-Methylumbelliferone
CHID: 25670 **CASRN:** 90-33-5
SPID(S): Tox21_110385_1
M4ID: 12484405

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

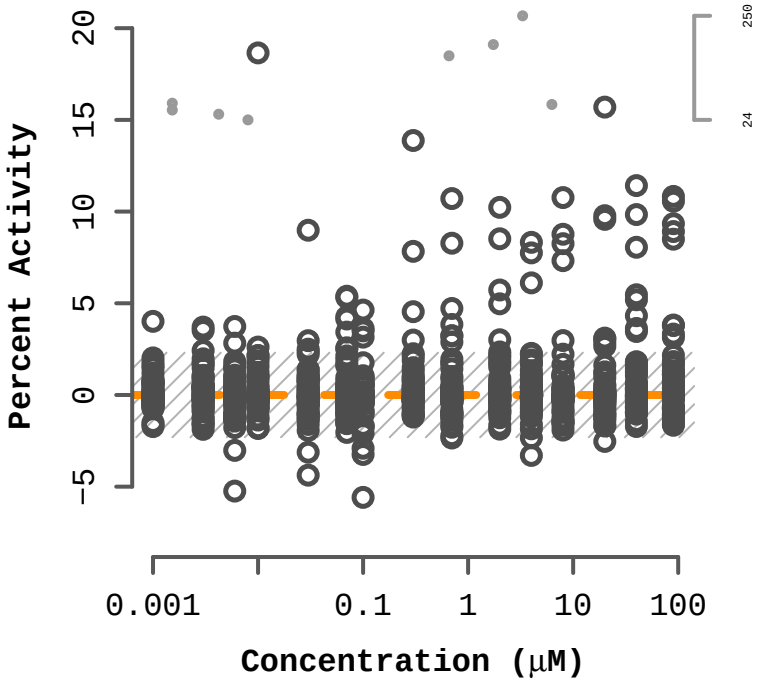
NAME: Methyl vinyl ketone
CHID: 25671 **CASRN:** 78-94-4
SPID(S): Tox21_200363
M4ID: 12481889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

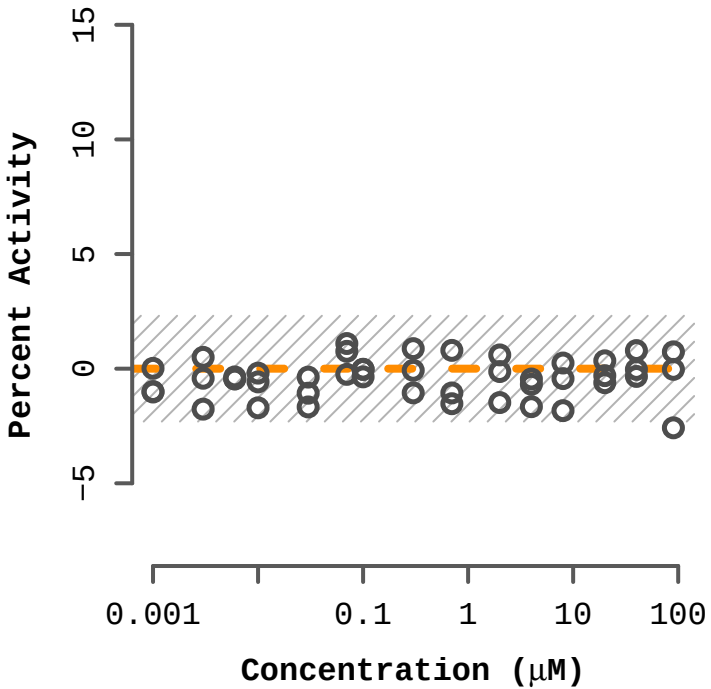
NAME: MEHP
CHID: 25680 **CASRN:** 4376-20-9
SPID(S): Tox21_400076
M4ID: 12475061 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2996.4	NA	NA
PROB:	1	NA	NA
RMSE:	13.66	NA	NA

MAX_MEAN: 5.63 **MAX_MED:** 0.246 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

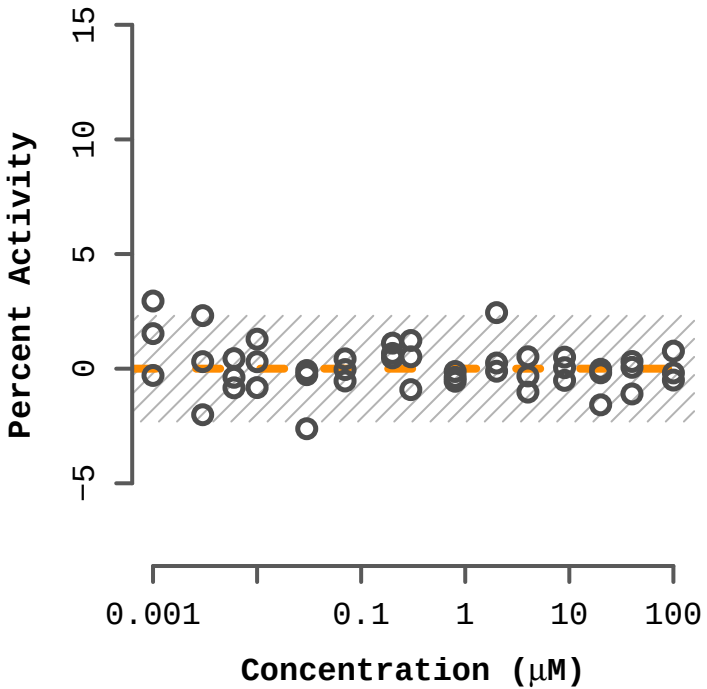
NAME: Morpholine
CHID: 25688 CASRN: 110-91-8
SPID(S): Tox21_303240
M4ID: 12475893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.537 MAX_MED: 0.758 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

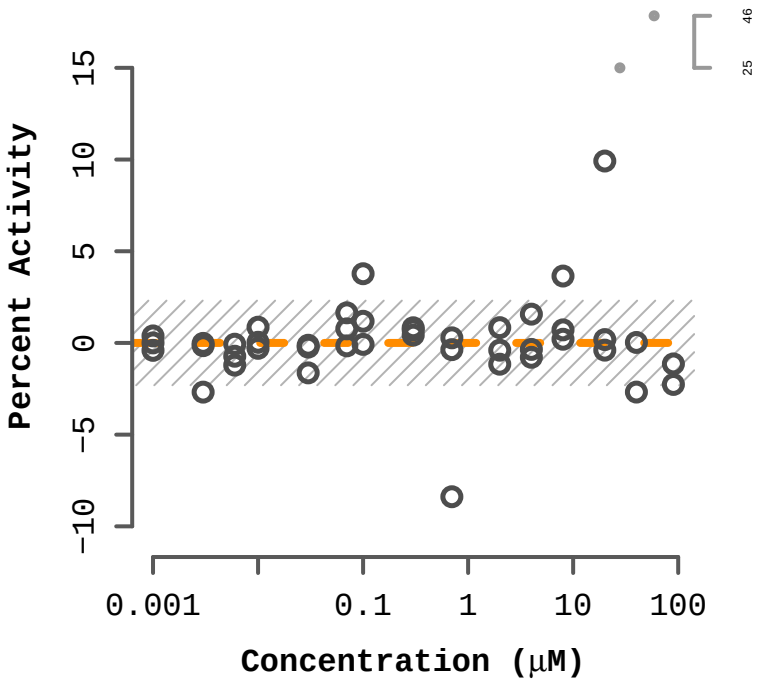
NAME: Morpholine
CHID: 25688 **CASRN:** 110-91-8
SPID(S): Tox21_202450
M4ID: 12479802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

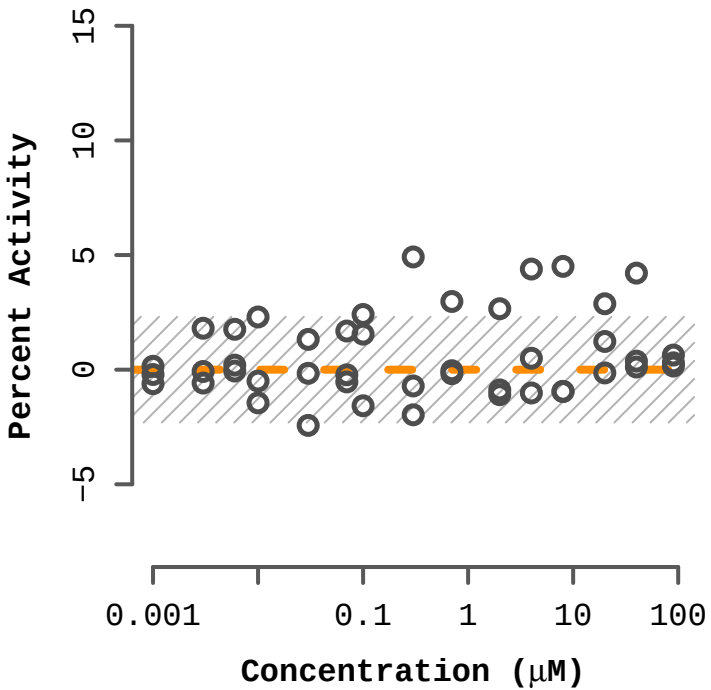
NAME: Musk ambrette
CHID: 25689 **CASRN:** 83-66-9
SPID(S): Tox21_201195
M4ID: 12481057 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.43	NA	NA
PROB:	1	NA	NA
RMSE:	8.09	NA	NA

MAX_MEAN: 14.1 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

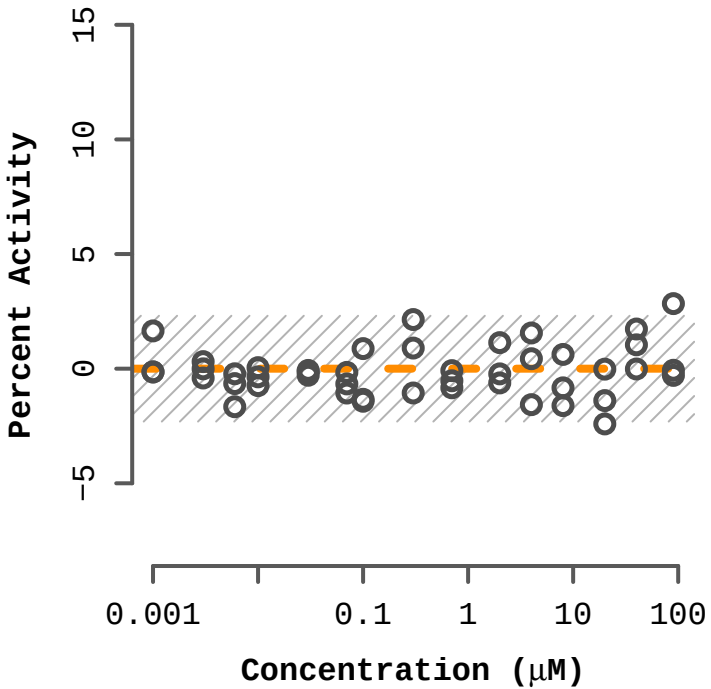
NAME: Musk ketone
CHID: 25690 **CASRN:** 81-14-1
SPID(S): Tox21_301627
M4ID: 12477506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

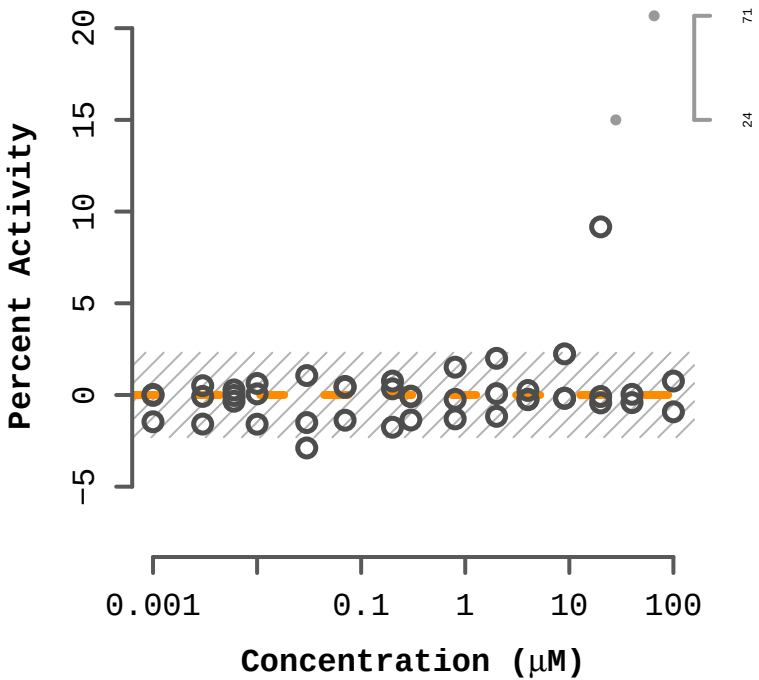
NAME: Myrcene
CHID: 25692 CASRN: 123-35-3
SPID(S): Tox21_300351
M4ID: 12478781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.921 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

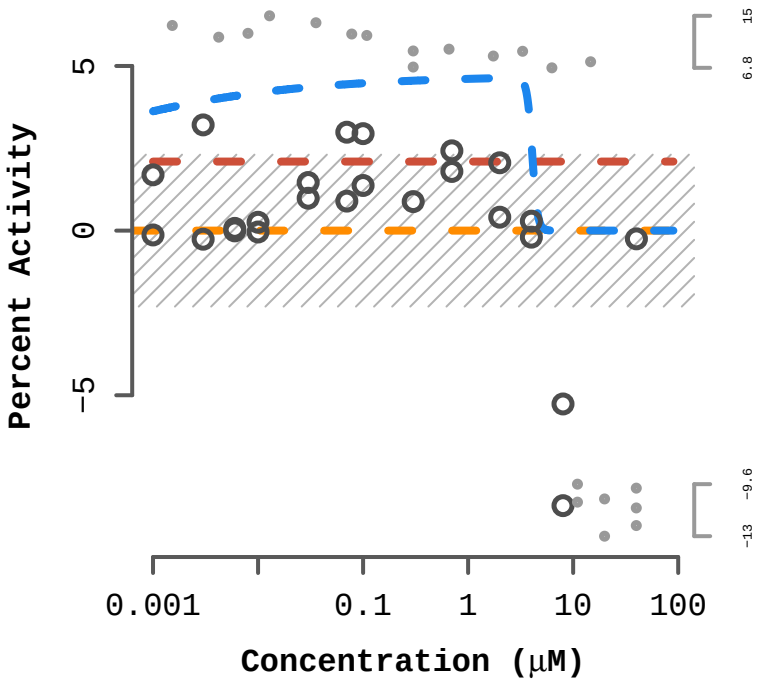
NAME: Myristicin
CHID: 25693 **CASRN:** 607-91-0
SPID(S): Tox21_200172
M4ID: 12482080 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.8	NA	NA
PROB:	1	NA	NA
RMSE:	11.25	NA	NA

MAX_MEAN: 23.5 **MAX_MED:** 0.763 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Naphthalenediamine
CHID: 25696 CASRN: 2243−61−0
SPID(S): Tox21_202900
M4ID: 12479352 BRK

HILL MODEL (in red):

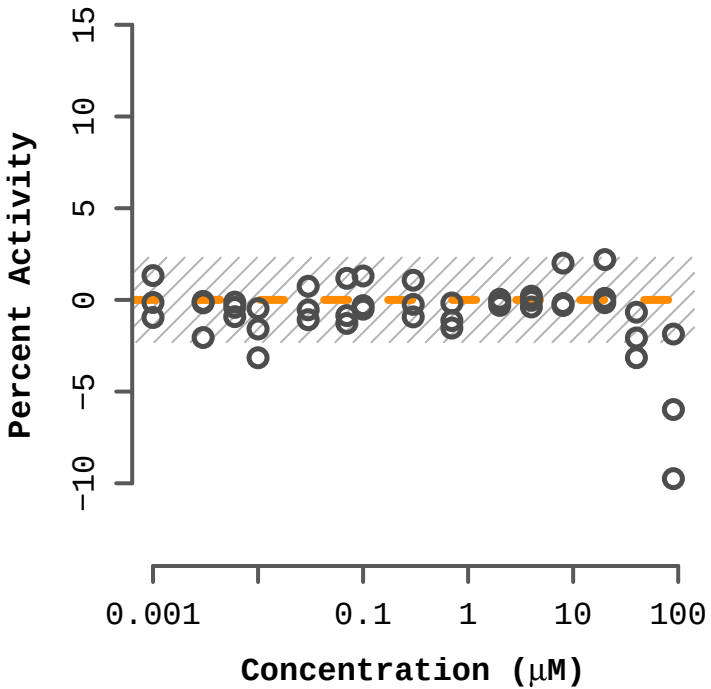
	tp	ga	gw
val:	2.1	−4.25	5.51
sd:	1.12	1250	5500

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.71	−4.38	0.381	0.61	17.6
sd:	2.9	9.51	2.24	0.332	682

	CNST	HILL	GNLS
AIC:	317.9	320.51	314.57
PROB:	0.15	0.04	0.81
RMSE:	7.72	7.5	6.55

MAX_MEAN: 5.79 MAX_MED: 6.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

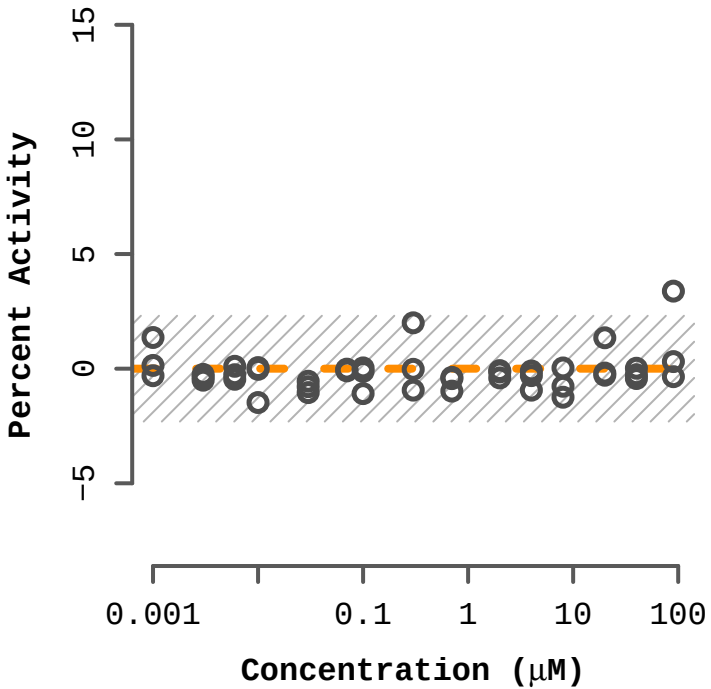
NAME: alpha−Naphylisothiocyanate
CHID: 25703 **CASRN:** 551−06−4
SPID(S): Tox21_200329
M4ID: 12481923

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 0.712 **MAX_MED:** 0.0858 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

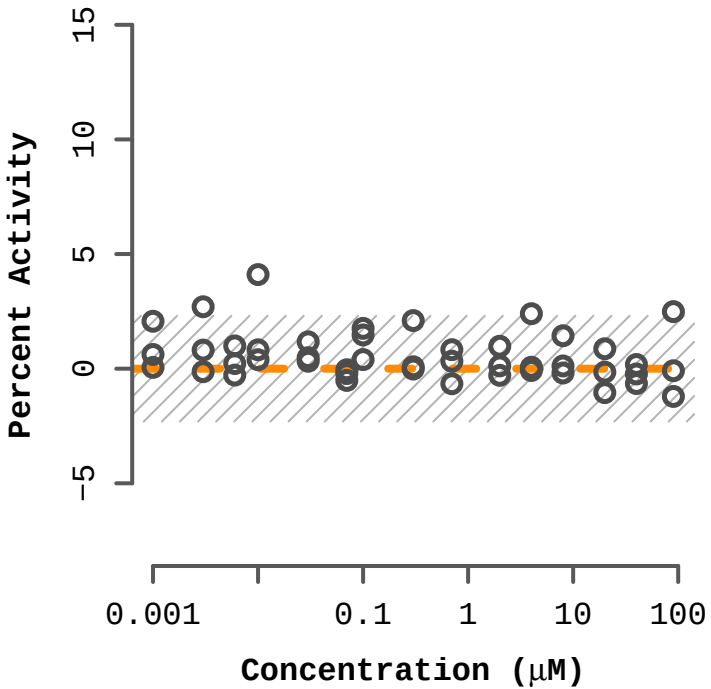
NAME: Neohesperidin dihydrochalcone
CHID: 25706 **CASRN:** 20702-77-6
SPID(S): Tox21_200303
M4ID: 12481949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.311 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

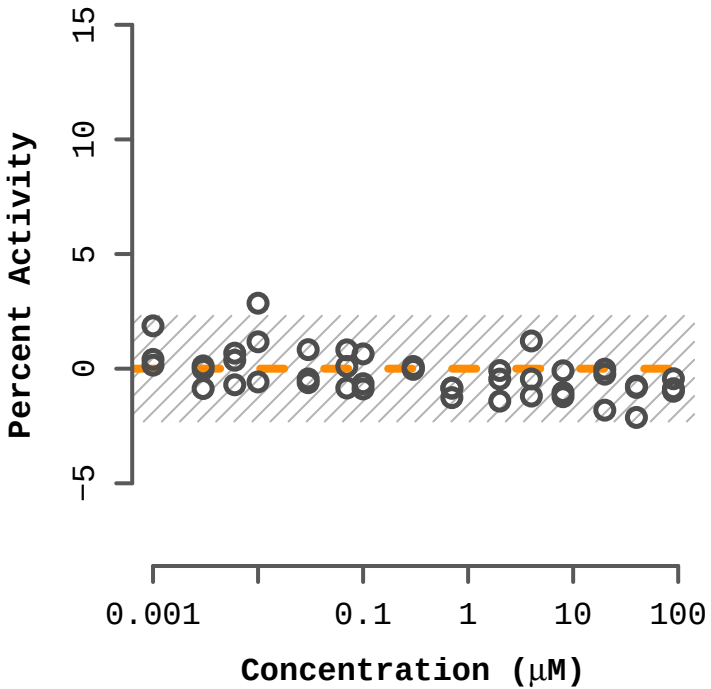
NAME: Neopentyl glycol diglycidyl ether
CHID: 25707 **CASRN:** 17557-23-2
SPID(S): Tox21_303734
M4ID: 12475454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

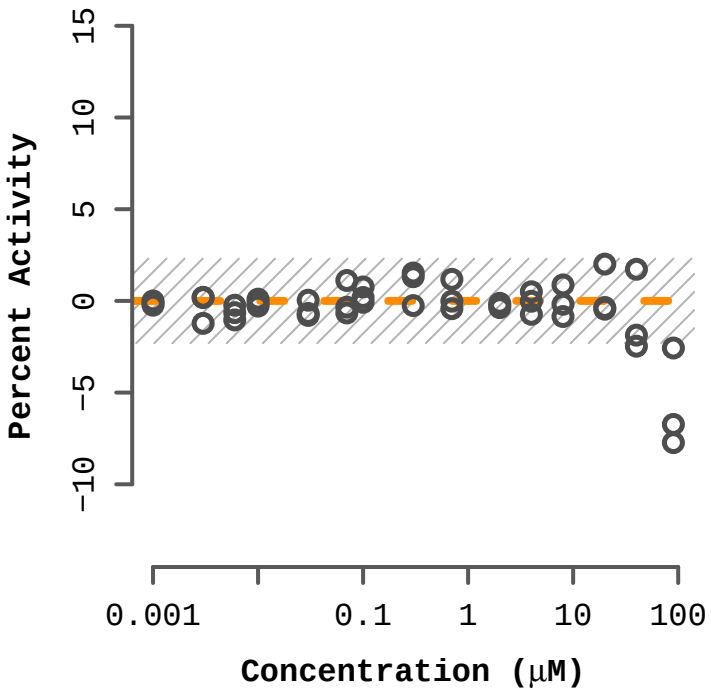
NAME: Nickelocene
CHID: 25709 **CASRN:** 1271-28-9
SPID(S): Tox21_202527
M4ID: 12479725

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

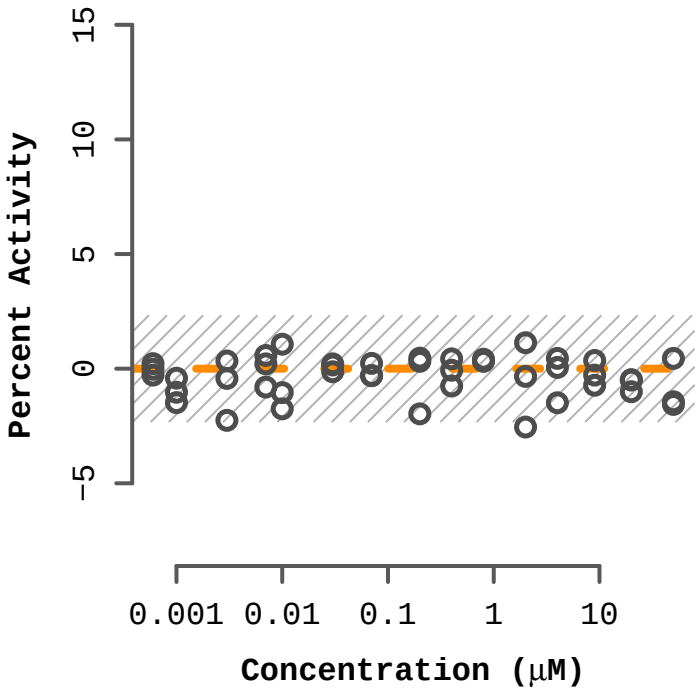
NAME: Nifedipine
CHID: 25715 **CASRN:** 21829-25-4
SPID(S): Tox21_200304
M4ID: 12481948

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 0.863 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

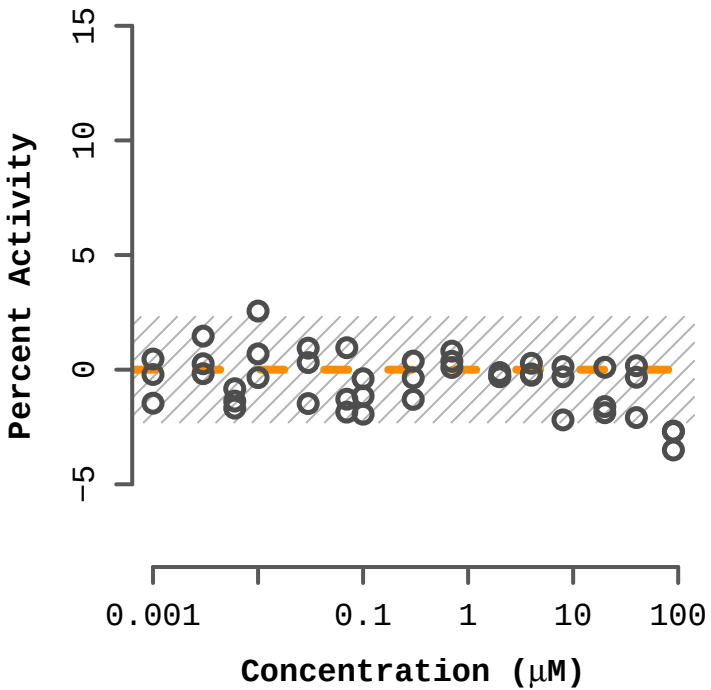
NAME: Nifedipine
CHID: 25715 **CASRN:** 21829-25-4
SPID(S): Tox21_110212_1
M4ID: 12484548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.359 **MAX_MED:** 0.343 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

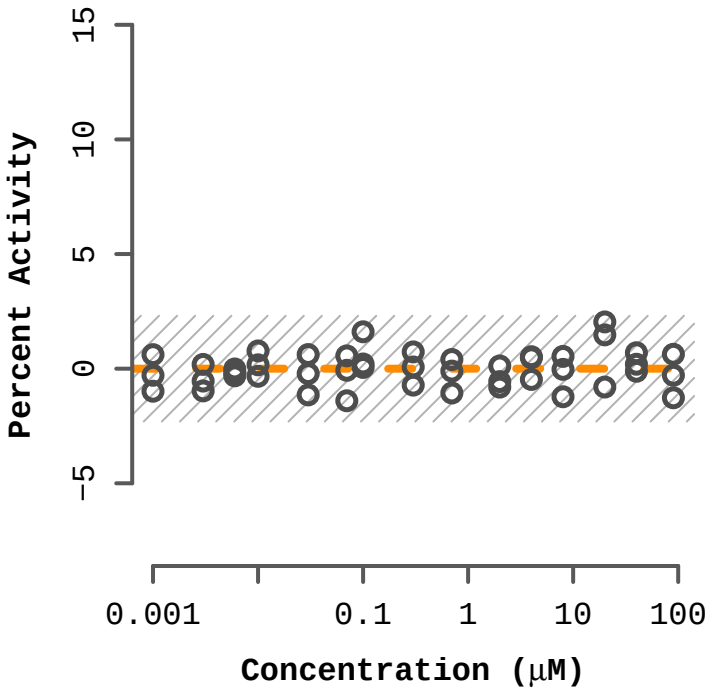
NAME: Ninhydrin
CHID: 25716 **CASRN:** 485-47-2
SPID(S): Tox21_200705
M4ID: 12481547

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.969 **MAX_MED:** 0.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

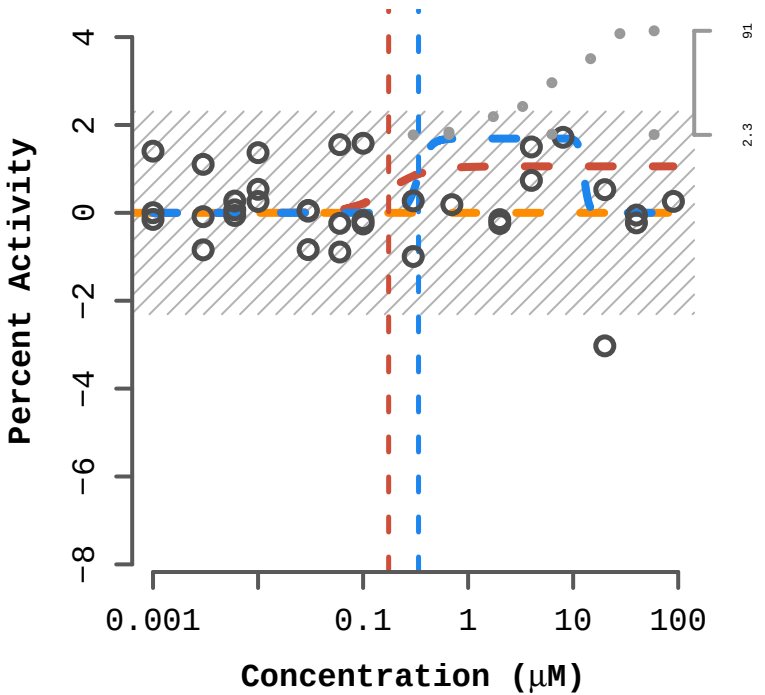
NAME: 3-Nitroacetophenone
CHID: 25722 **CASRN:** 121-89-1
SPID(S): Tox21_200737
M4ID: 12481515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Nitroacetophenone
CHID: 25723 CASRN: 577-59-3
SPID(S): Tox21_200072
M4ID: 12482180 BRK

HILL MODEL (in red):

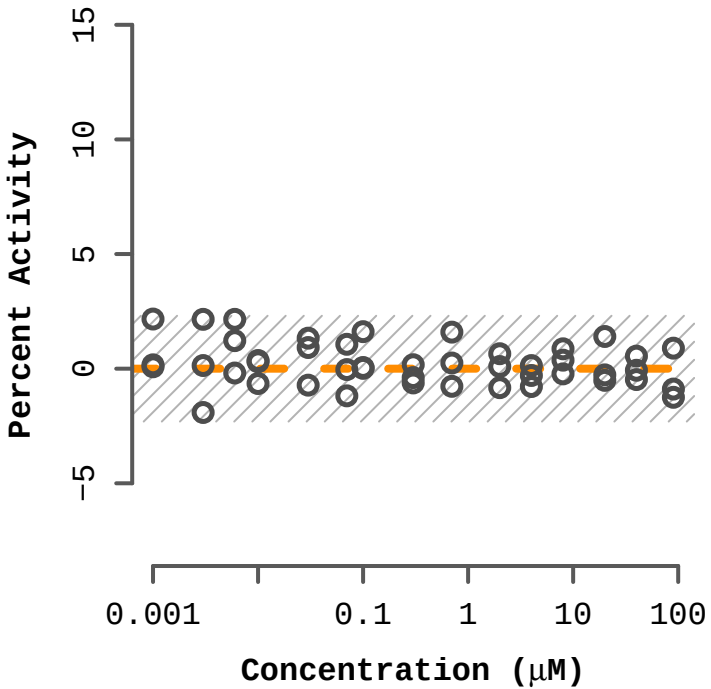
	tp	ga	gw
val:	1.06	−0.757	2.47
sd:	0.555	1.06	4.63

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.69	−0.472	8	1.1	18
sd:	0.681	0.219	24.7	1.2	109

	CNST	HILL	GNLS
AIC:	321.33	323.03	325.09
PROB:	0.63	0.27	0.1
RMSE:	23.08	22.73	22.92

MAX_MEAN: 31.3 MAX_MED: 2.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

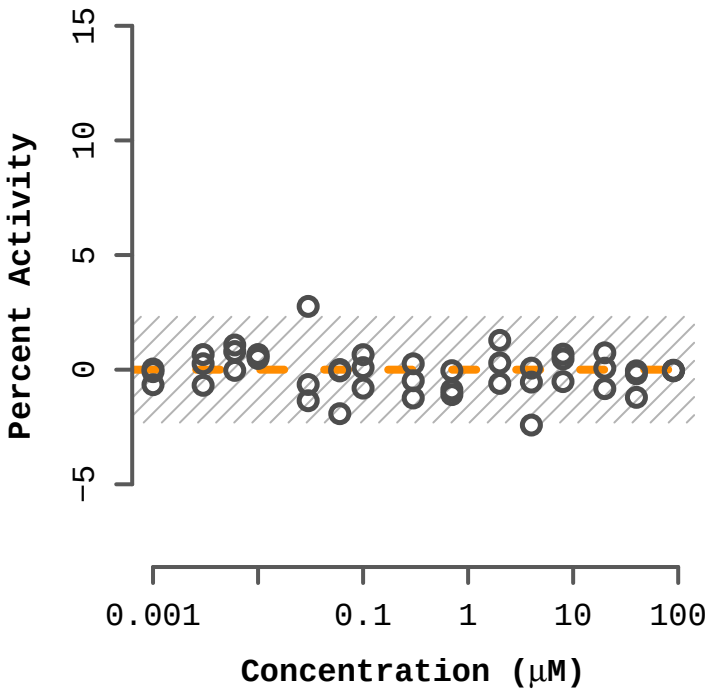
NAME: 4-Nitroacetophenone
CHID: 25724 **CASRN:** 100-19-6
SPID(S): Tox21_200265
M4ID: 12481987

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

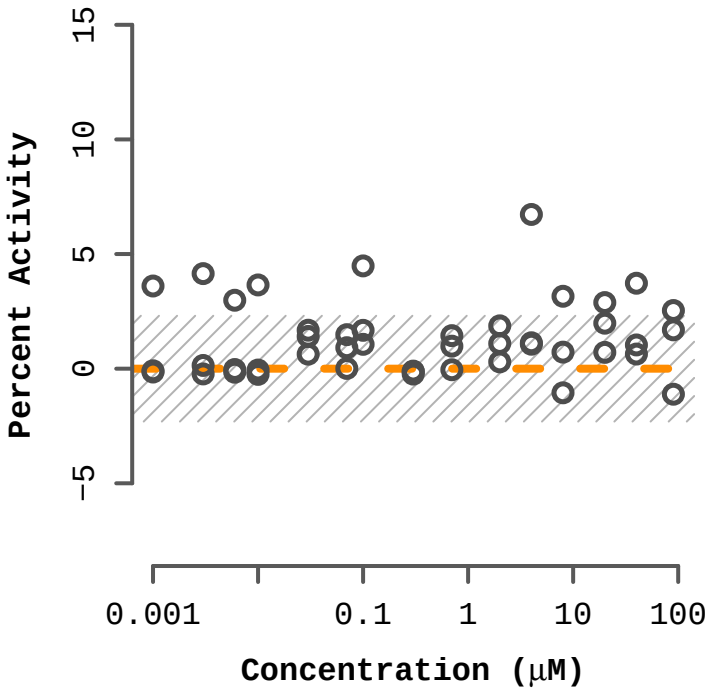
NAME: 3-Nitroaniline
CHID: 25725 CASRN: 99-09-2
SPID(S): Tox21_200386
M4ID: 12481866

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.614 MAX_MED: 0.794 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

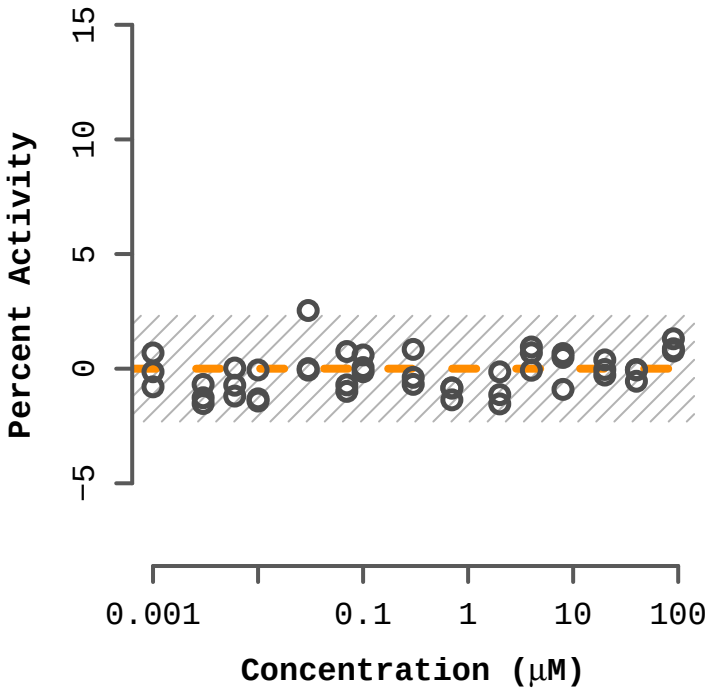
NAME: 2-Nitroaniline
CHID: 25726 **CASRN:** 88-74-4
SPID(S): Tox21_303292
M4ID: 12475841

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 2.98 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

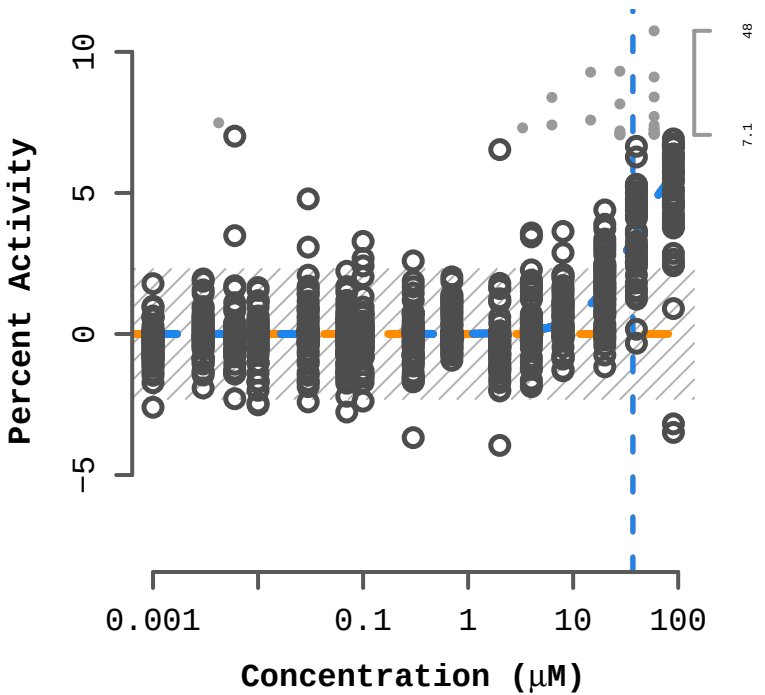
NAME: 2-Nitroaniline
CHID: 25726 **CASRN:** 88-74-4
SPID(S): Tox21_202371
M4ID: 12479881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9−Nitroanthracene
CHID: 25730 **CASRN:** 602−60−8
SPID(S): Tox21_400025
M4ID: 12475112 **BRK**

HILL MODEL (in red):

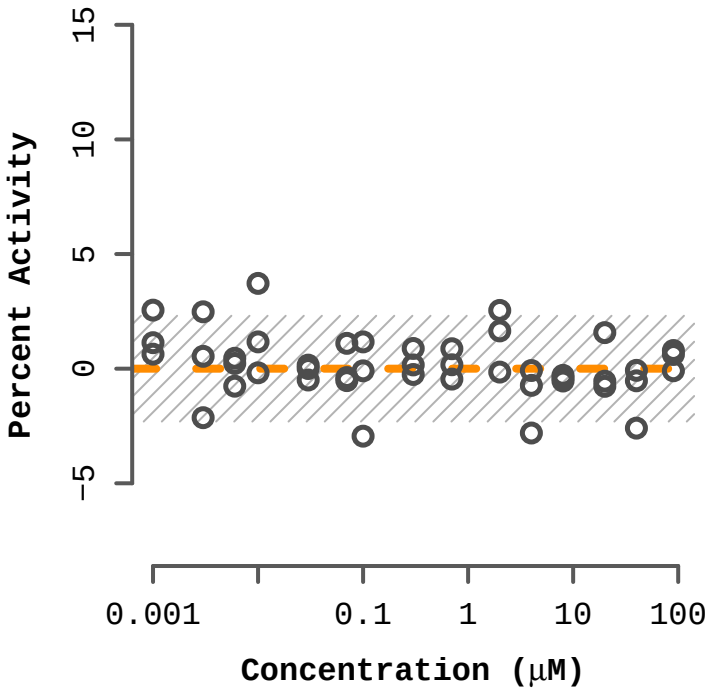
	tp	ga	gw
val:	6.72	1.57	1.82
sd:	0.727	0.0701	0.287

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.72	1.57	1.82	3.93	5.91
sd:	0.727	0.0701	0.287	32500	112000

	CNST	HILL	GNLS
AIC:	3112.87	2544.56	2548.56
PROB:	0	0.88	0.12
RMSE:	3.81	3.08	3.08

MAX_MEAN: 7.13 **MAX_MED:** 5.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

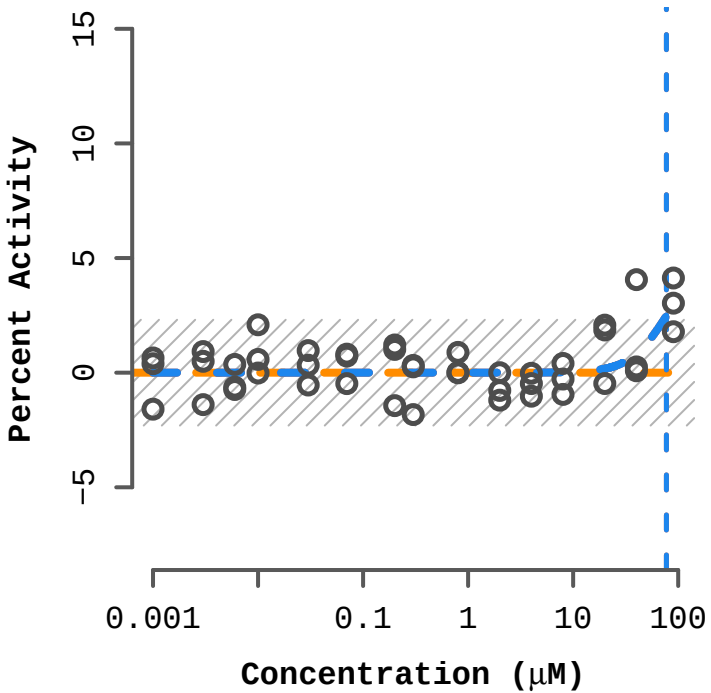
NAME: 3-Nitrobenzamide
CHID: 25732 **CASRN:** 645-09-0
SPID(S): Tox21_200090
M4ID: 12482162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Nitrobenzamide
CHID: 25733 CASRN: 610-15-1
SPID(S): Tox21_200805
M4ID: 12481447

HILL MODEL (in red):

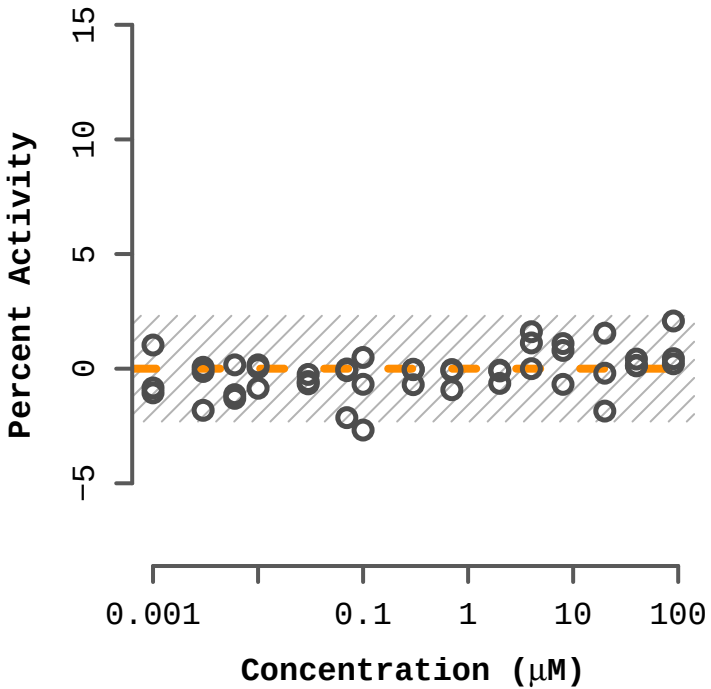
	tp	ga	gw
val:	4.96	1.89	2.46
sd:	5.52	0.427	2.57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.96	1.89	2.46	3.95	3.88
sd:	5.52	0.428	2.57	3590	7040

	CNST	HILL	GNLS
AIC:	151.54	140.56	144.56
PROB:	0	0.88	0.12
RMSE:	1.35	1.04	1.04

MAX_MEAN: 2.98 MAX_MED: 3.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

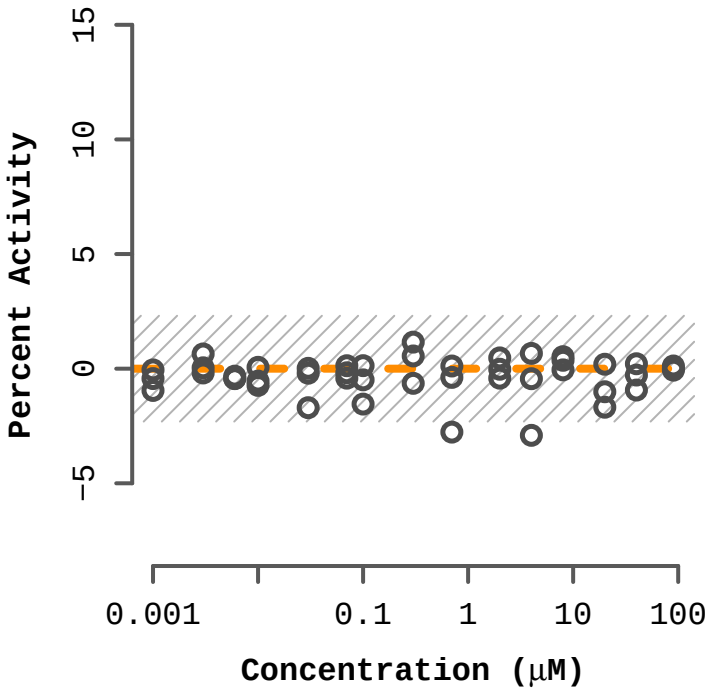
NAME: 3-Nitrobenzoic acid
CHID: 25737 **CASRN:** 121-92-6
SPID(S): Tox21_303250
M4ID: 12475883

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

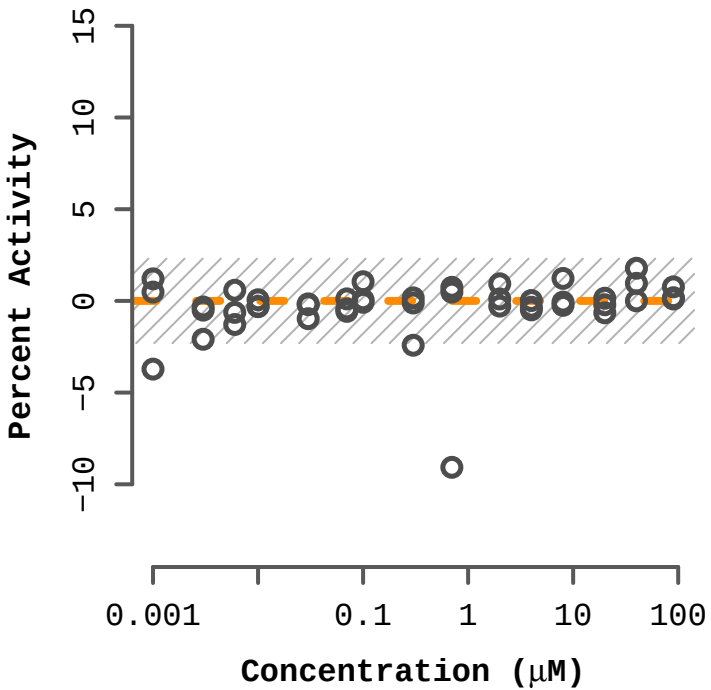
NAME: 3-Nitrobenzoic acid
CHID: 25737 **CASRN:** 121-92-6
SPID(S): Tox21_201238
M4ID: 12481014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.359 **MAX_MED:** 0.556 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

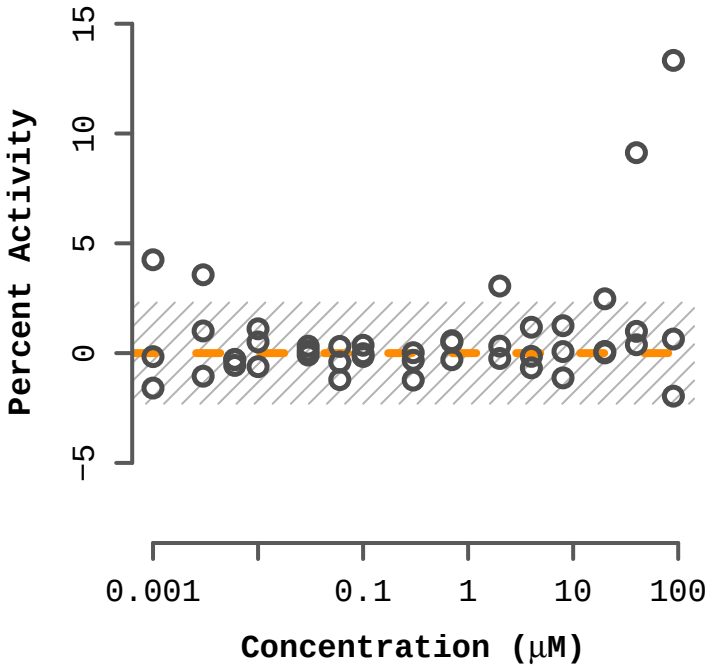
NAME: 2-Nitrobenzoic acid
CHID: 25738 **CASRN:** 552-16-9
SPID(S): Tox21_201020
M4ID: 12481232

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 0.914 **MAX_MED:** 0.959 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

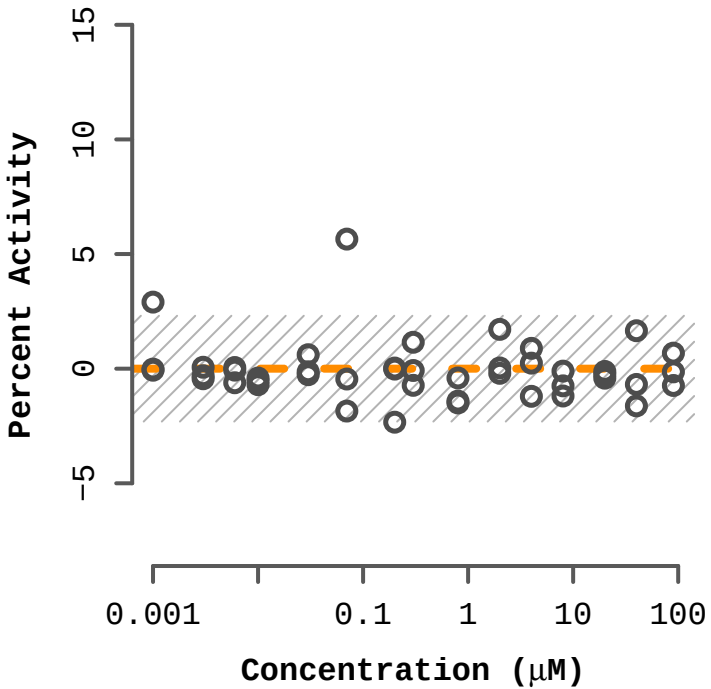
NAME: 3-Nitrobenzoyl chloride
CHID: 25740 **CASRN:** 121-90-4
SPID(S): Tox21_201094
M4ID: 12481158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.7	NA	NA

MAX_MEAN: 4.01 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

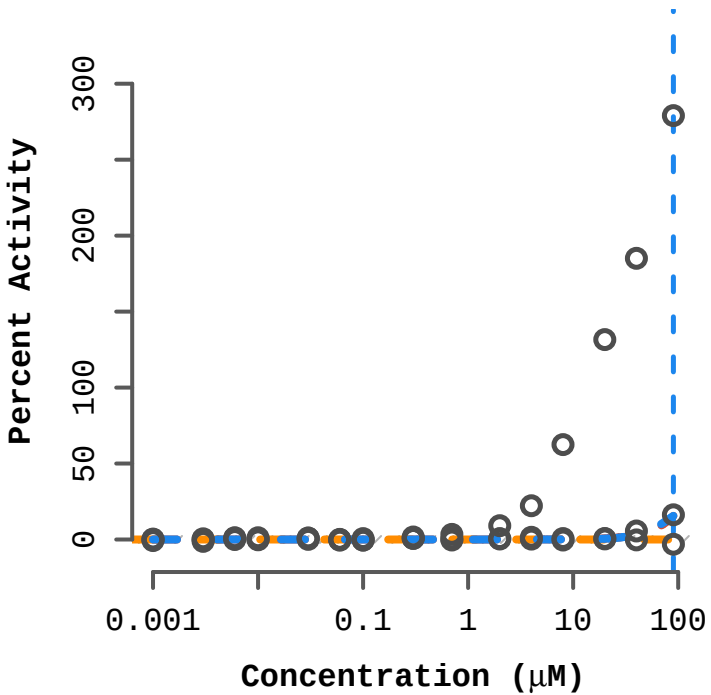
NAME: 2-Nitrobenzoyl chloride
CHID: 25741 **CASRN:** 610-14-0
SPID(S): Tox21_200340
M4ID: 12481912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.243 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitrobenzoyl chloride
CHID: 25742 CASRN: 122-04-3
SPID(S): Tox21_200137
M4ID: 12482115

HILL MODEL (in red):

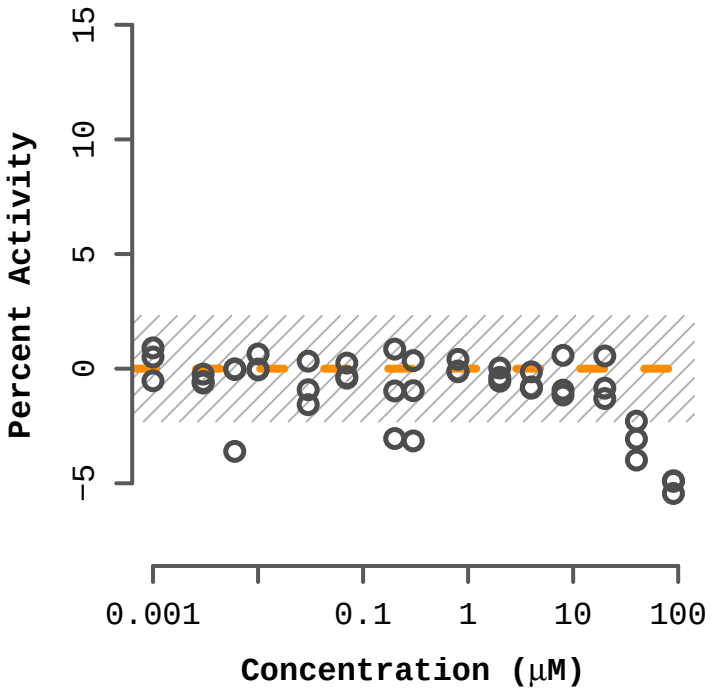
	tp	ga	gw
val:	191	2.45	2.11
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	31.1	1.95	2.68	3.85	4.36
sd:	48	0.498	1.71	17700	41100

	CNST	HILL	GNLS
AIC:	352.16	355.06	359.1
PROB:	0.79	0.19	0.02
RMSE:	54.62	52.61	52.61

MAX_MEAN: 97.4 MAX_MED: 16.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

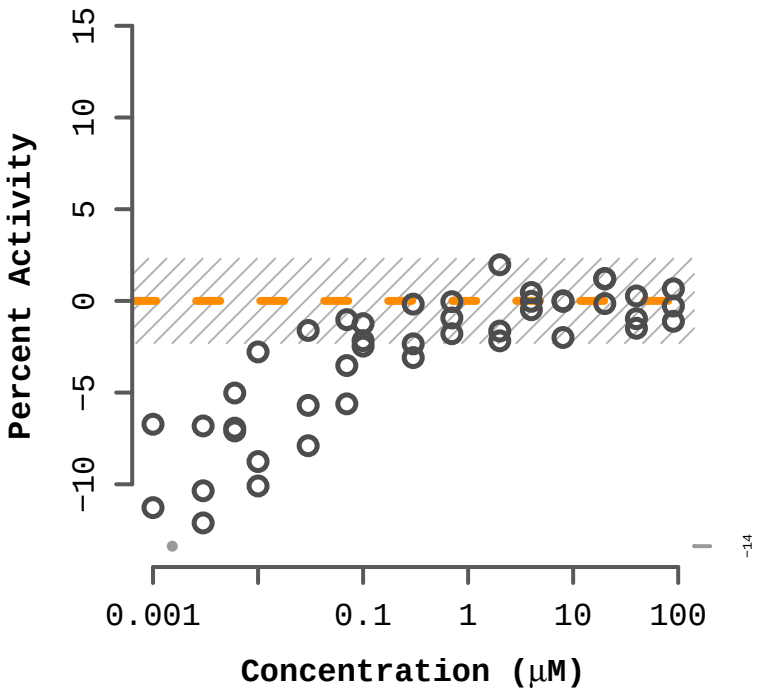
NAME: 3-Nitrobenzyl chloride
CHID: 25743 **CASRN:** 619-23-8
SPID(S): Tox21_200837
M4ID: 12481415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.87	NA	NA

MAX_MEAN: 0.297 **MAX_MED:** 0.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

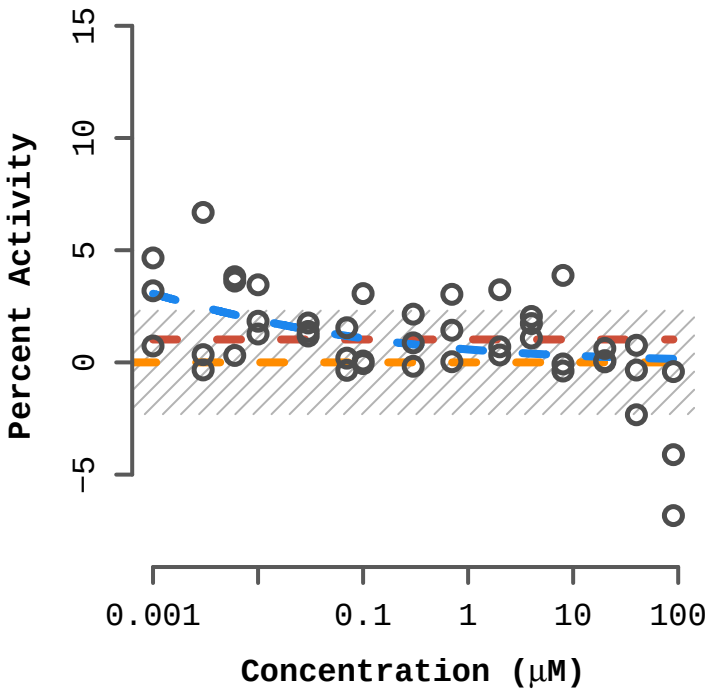
NAME: 2-Nitrobenzyl chloride
CHID: 25744 **CASRN:** 612-23-7
SPID(S): Tox21_200821
M4ID: 12481431 **BRK**

HILL MODEL: Not applicable.

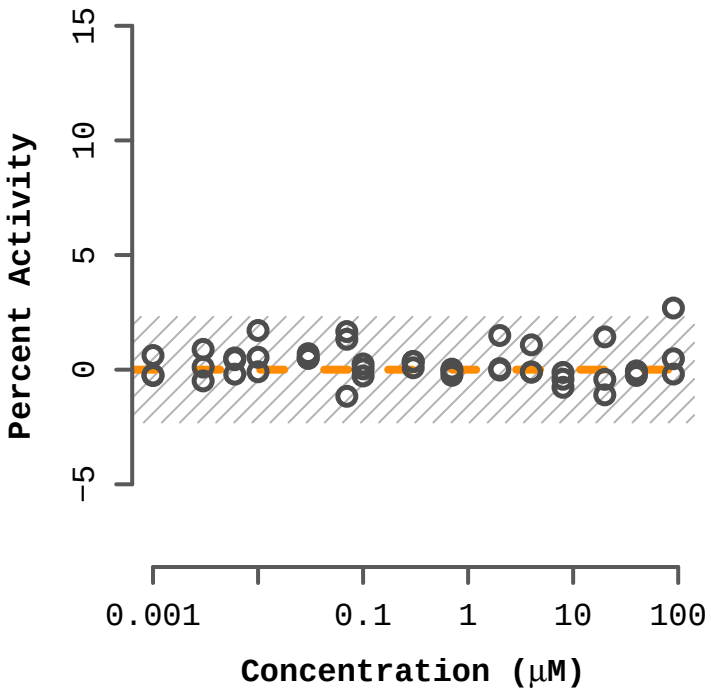
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	272.51	NA	NA
PROB:	1	NA	NA
RMSE:	5.08	NA	NA

MAX_MEAN: 0.759 **MAX_MED:** 1.2 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Nitrobenzyl chloride
CHID:    25745   CASRN: 100-14-1
SPID(S): Tox21_200572
M4ID:    12481680

HILL MODEL (in red):
      tp       ga       gw
val:  1.02     -4.95    3.76
sd:   0.264    1310     2530

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.02     -4.14    7.9      -3.7     0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  206.23      198.49      194.01
PROB: 0           0.1         0.9
RMSE: 2.41        2.19        1.94

MAX_MEAN: 2.86      MAX_MED: 3.63      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

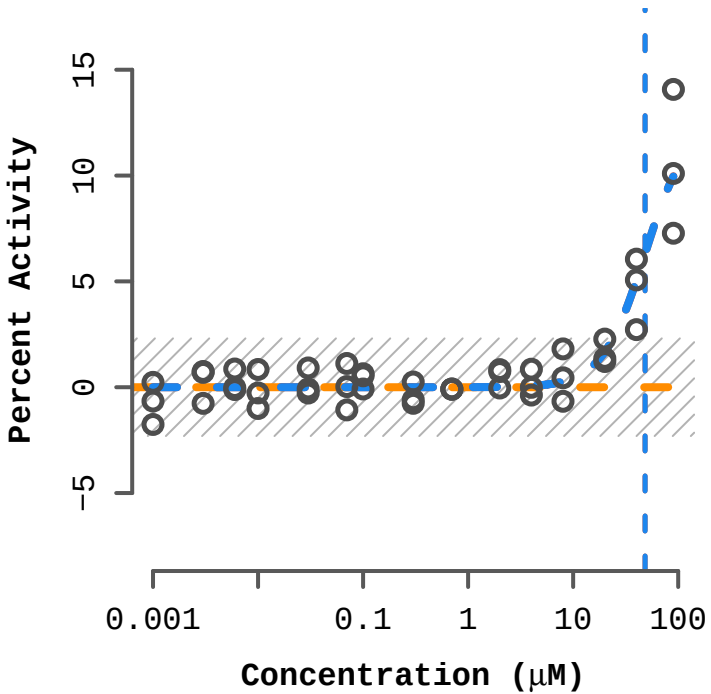
NAME: 2-Nitro-1,1'-biphenyl
CHID: 25746 **CASRN:** 86-00-0
SPID(S): Tox21_200759
M4ID: 12481493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Nitrodiphenylamine
CHID: 25749 **CASRN:** 119-75-5
SPID(S): Tox21_200720
M4ID: 12481532

HILL MODEL (in red):

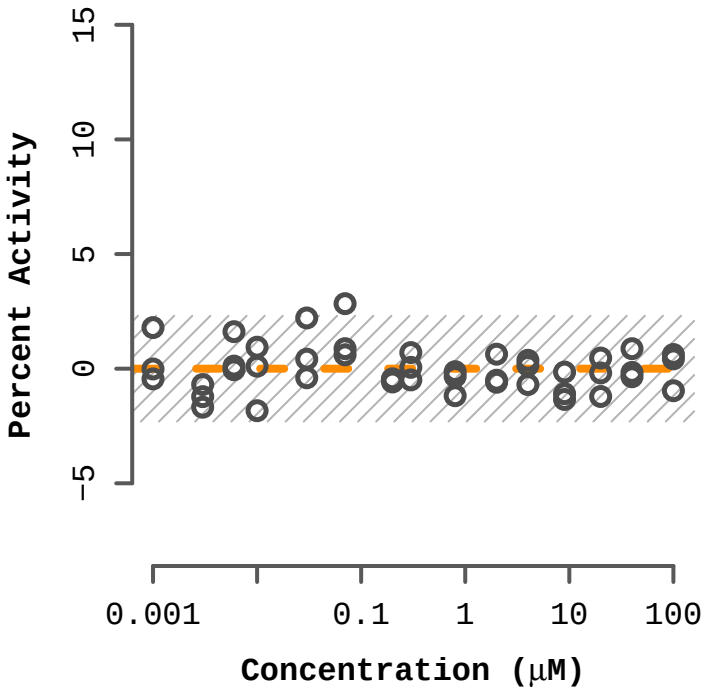
	tp	ga	gw
val:	12.6	1.68	2.14
sd:	3.3	0.144	0.689

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.6	1.68	2.13	2.22	9.66
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	193.61	129.68	133.68
PROB:	0	0.88	0.12
RMSE:	3.16	1.05	1.05

MAX_MEAN: 10.5 **MAX_MED:** 10.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

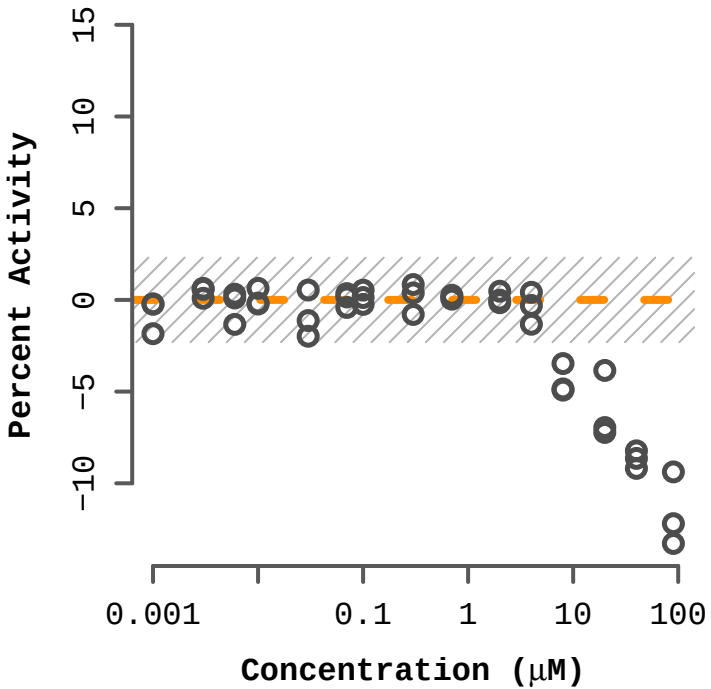
NAME: 2-Nitroethanol
CHID: 25751 **CASRN:** 625-48-9
SPID(S): Tox21_200622
M4ID: 12481630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

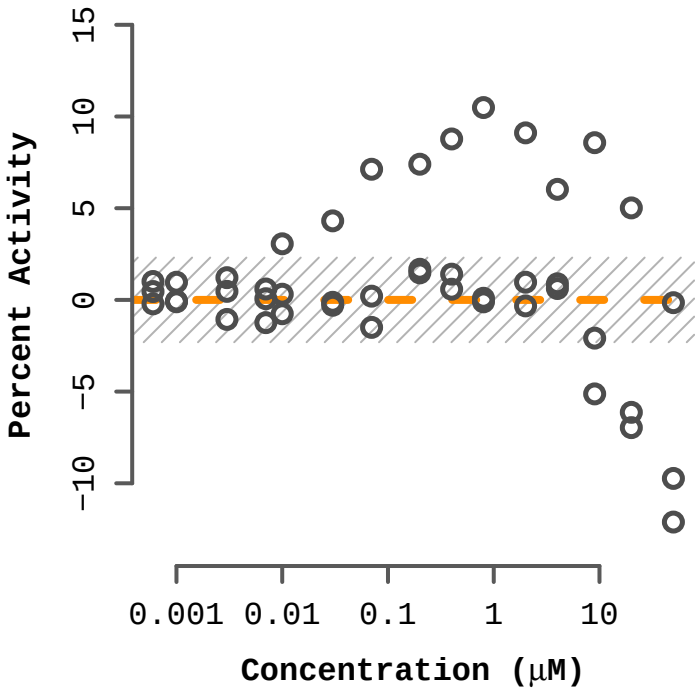
NAME: Nitrogen mustard hydrochloride
CHID: 25757 CASRN: 55-86-7
SPID(S): Tox21_200638
M4ID: 12481614

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.12	NA	NA
PROB:	1	NA	NA
RMSE:	4.3	NA	NA

MAX_MEAN: 0.433 **MAX_MED:** 0.576 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

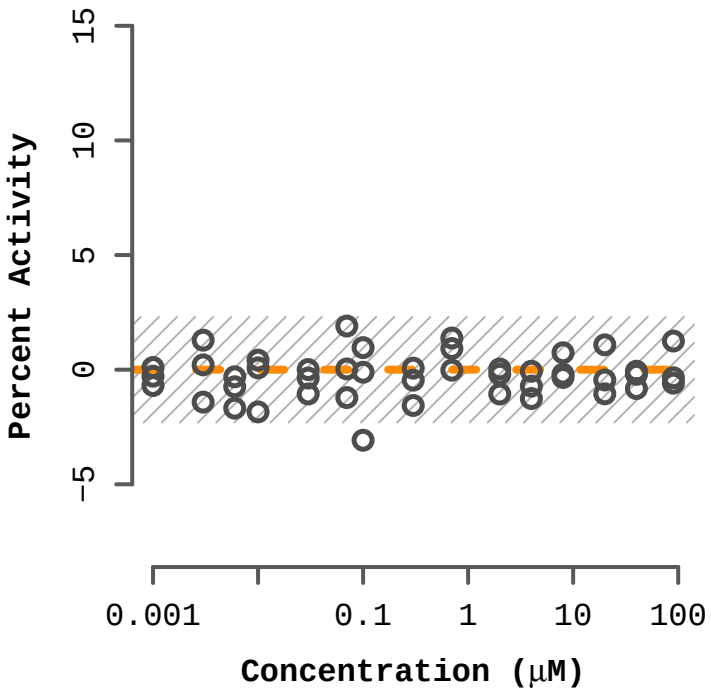
NAME: Nitrogen mustard hydrochloride
CHID: 25757 **CASRN:** 55-86-7
SPID(S): Tox21_111170_1
M4ID: 12483865

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	260.17	NA	NA
PROB:	1	NA	NA
RMSE:	4.51	NA	NA

MAX_MEAN: 3.59 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

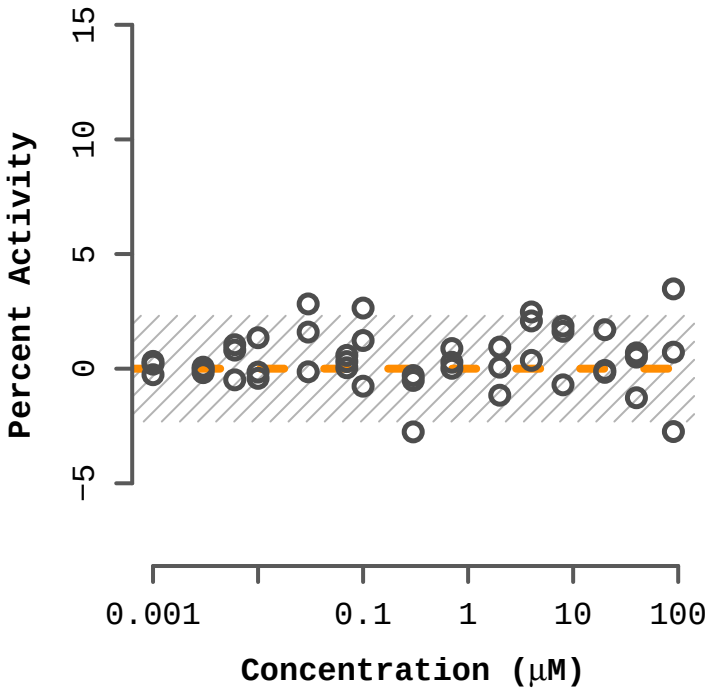
NAME: 1-Nitrohexane
CHID: 25758 **CASRN:** 646-14-0
SPID(S): Tox21_200707
M4ID: 12481545

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.762 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

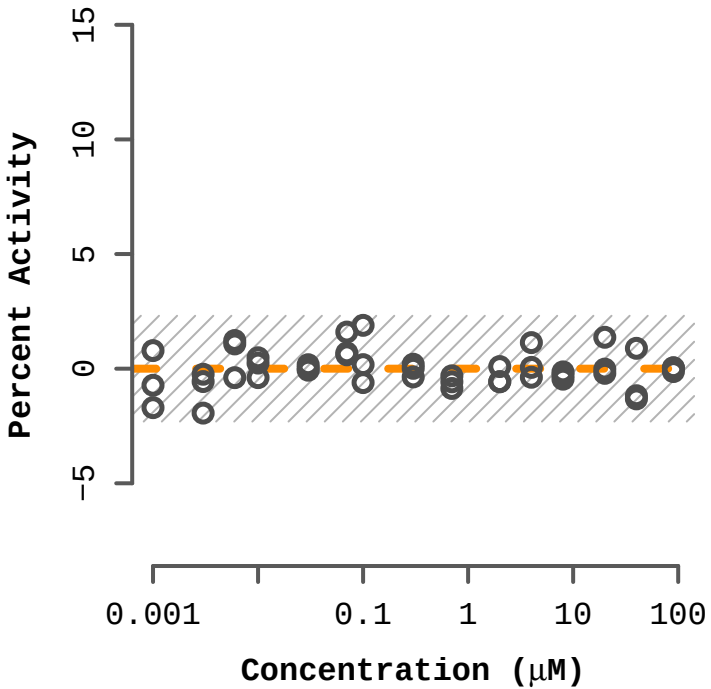
NAME: 4-Nitrohippuric acid
CHID: 25759 **CASRN:** 2645-07-0
SPID(S): Tox21_201181
M4ID: 12481071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

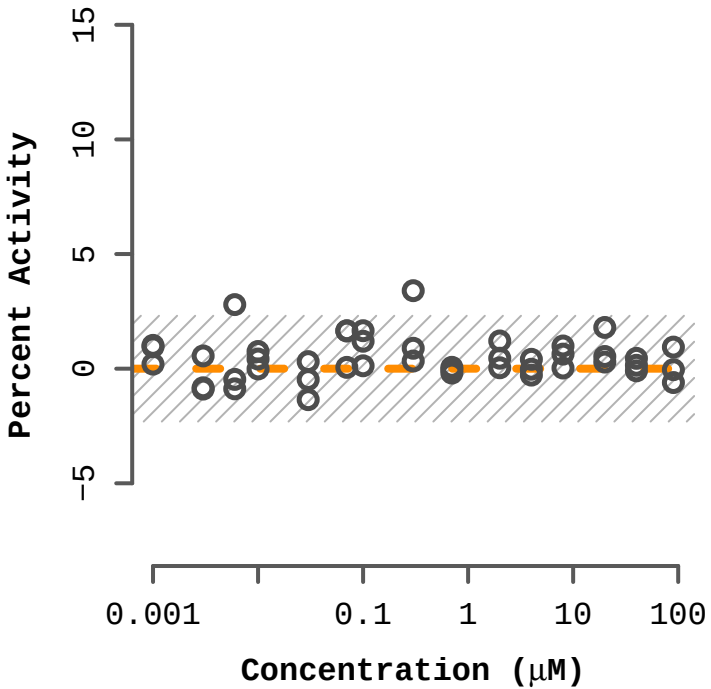
NAME: 1-Nitro-2-methylnaphthalene
CHID: 25761 **CASRN:** 881-03-8
SPID(S): Tox21_200174
M4ID: 12482078

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

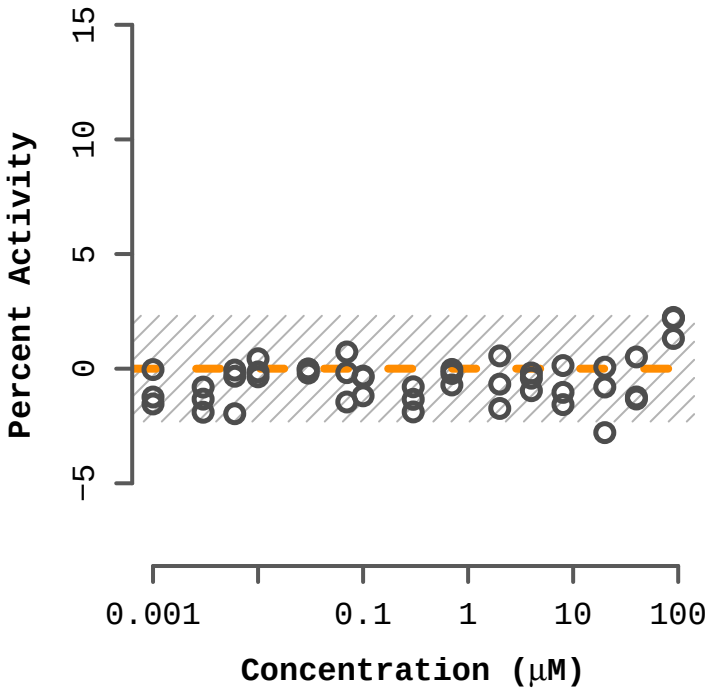
NAME: 2-(2-Nitrophenyl)ethanol
CHID: 25763 **CASRN:** 15121-84-3
SPID(S): Tox21_200295
M4ID: 12481957

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

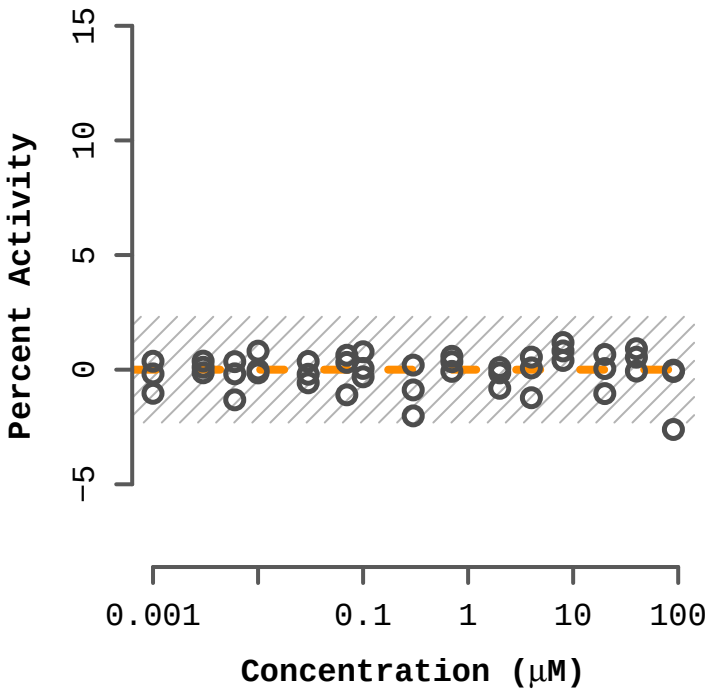
NAME: 2-(4-Nitrophenyl)ethanol
CHID: 25764 **CASRN:** 100-27-6
SPID(S): Tox21_200285
M4ID: 12481967

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

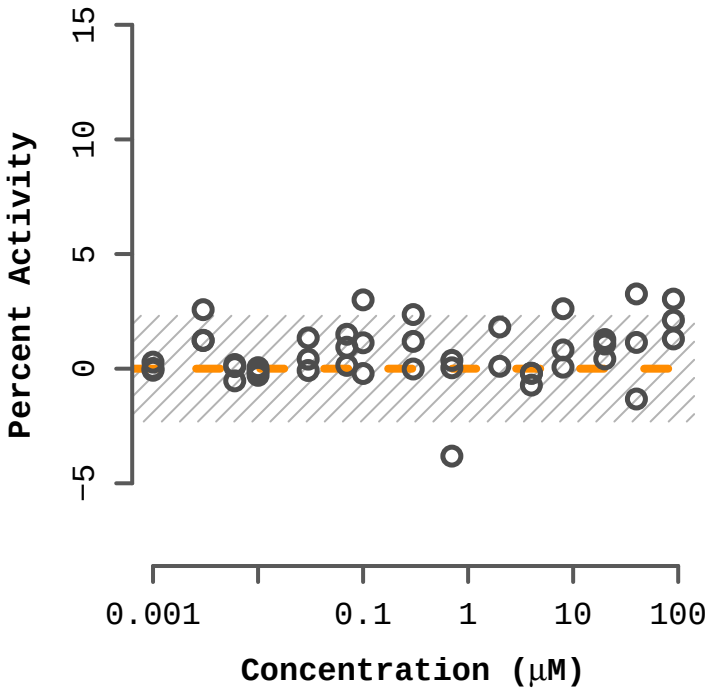
NAME: 3-Nitrophenol
CHID: 25765 **CASRN:** 554-84-7
SPID(S): Tox21_200022
M4ID: 12482230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

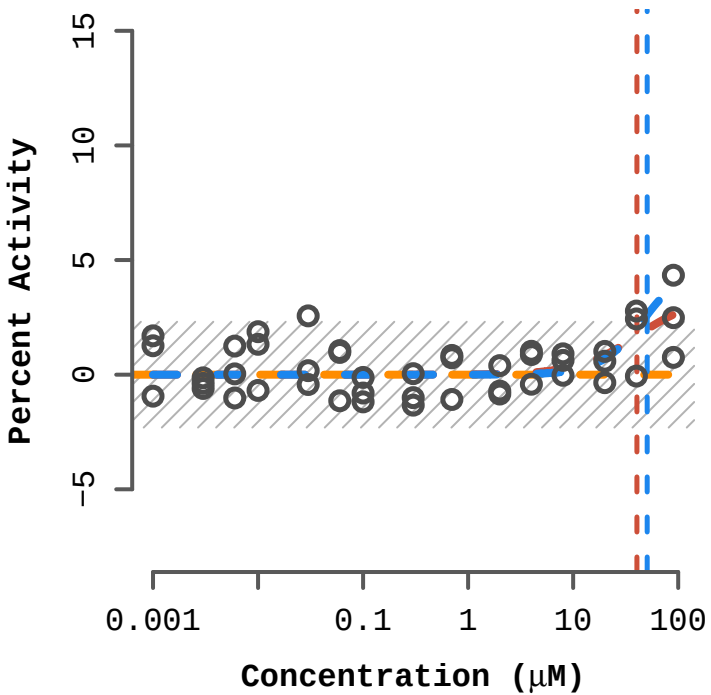
NAME: (2-Nitrophenyl)acetonitrile
CHID: 25768 **CASRN:** 610-66-2
SPID(S): Tox21_200975
M4ID: 12481277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitro-1,3-benzenediamine
CHID: 25770 **CASRN:** 5131-58-8
SPID(S): Tox21_200992
M4ID: 12481260

HILL MODEL (in red):

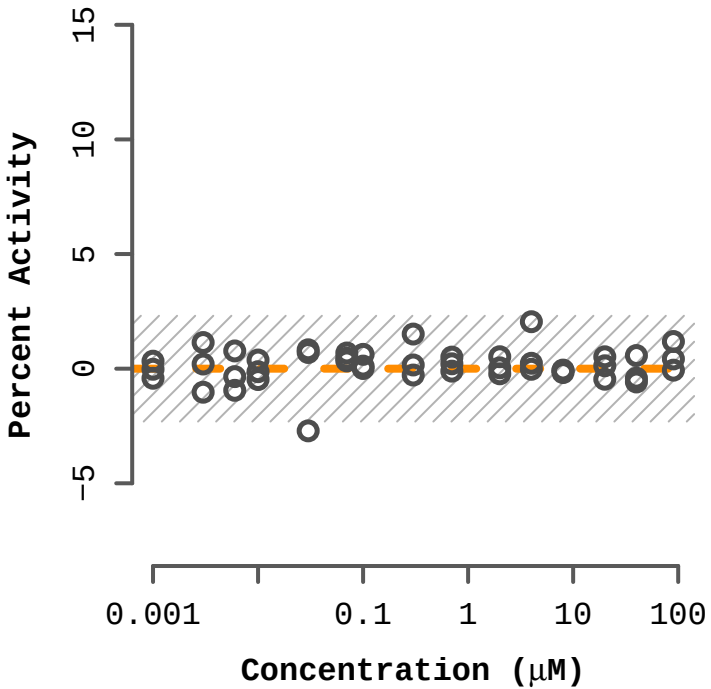
	tp	ga	gw
val:	3.38	1.61	1.55
sd:	3.75	0.795	2.37

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.21	1.7	2	1.97	13.3
sd:	12.6	0.927	3.06	0.0721	73.6

	CNST	HILL	GNLS
AIC:	152.3	143.68	147.37
PROB:	0.01	0.85	0.13
RMSE:	1.31	1.04	1.04

MAX_MEAN: 2.53 **MAX_MED:** 2.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

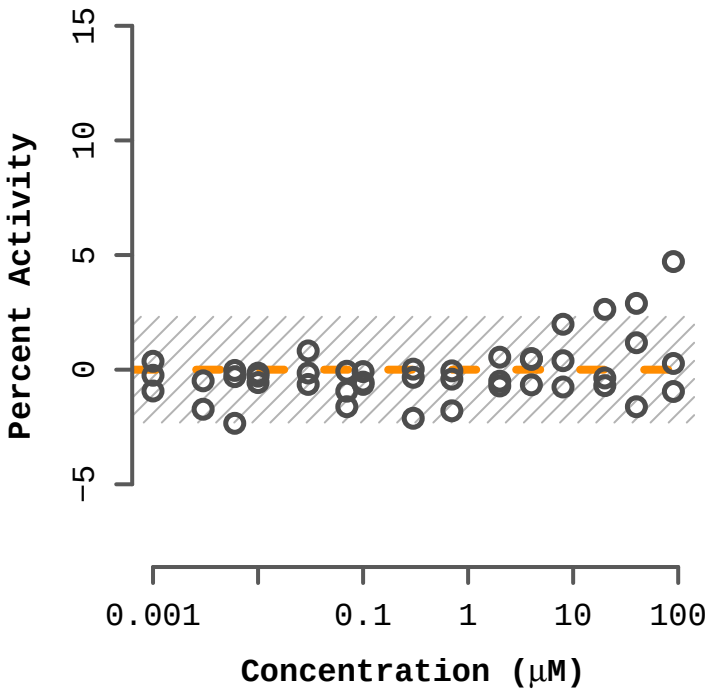
NAME: 6-Nitrophthalhydrazide
CHID: 25774 **CASRN:** 3682-19-7
SPID(S): Tox21_200021
M4ID: 12482231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.753 **MAX_MED:** 0.708 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

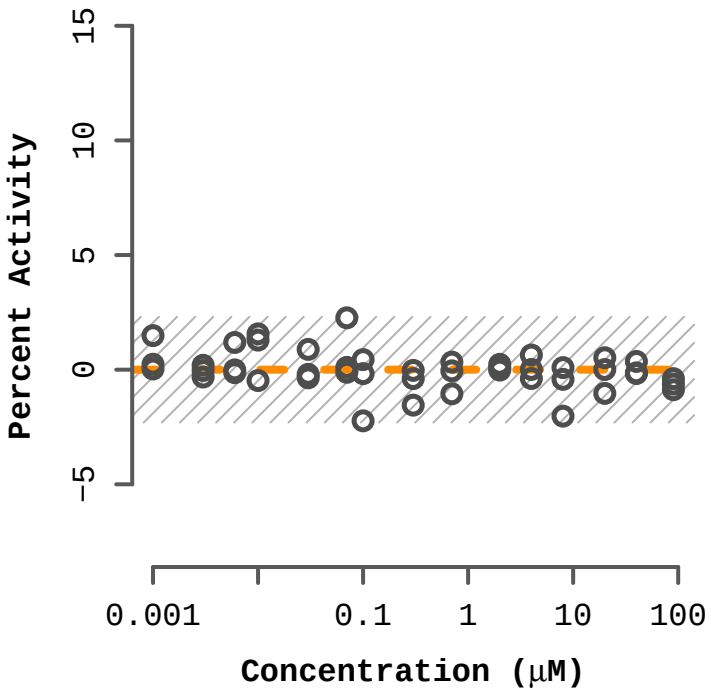
NAME: 4-Nitrophthalic anhydride
CHID: 25775 **CASRN:** 5466-84-2
SPID(S): Tox21_200328
M4ID: 12481924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

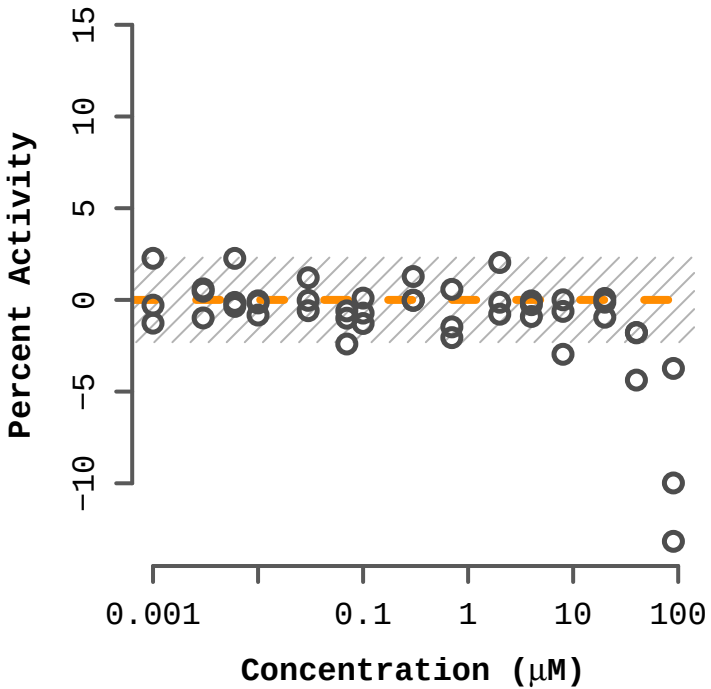
NAME: 4-Nitrophthalimide
CHID: 25776 **CASRN:** 89-40-7
SPID(S): Tox21_200190
M4ID: 12482062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

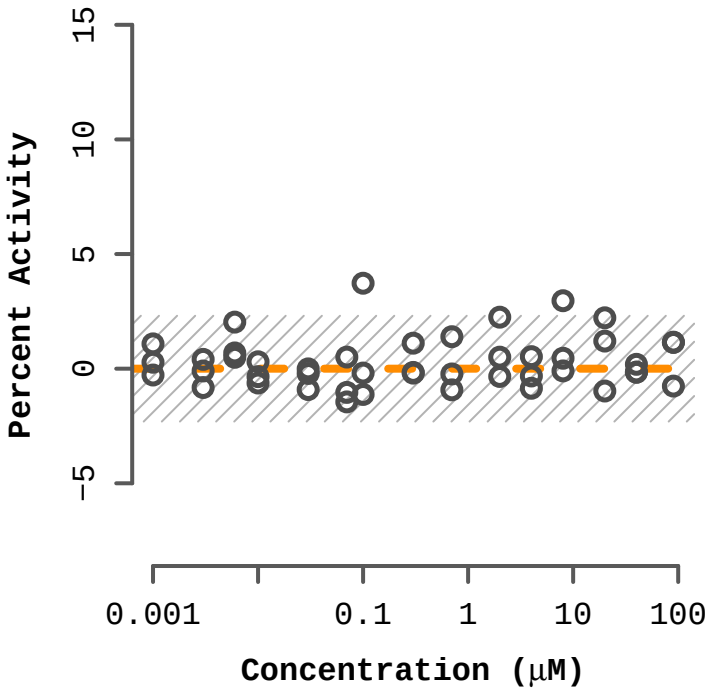
NAME: beta-Nitrostyrene
CHID: 25789 **CASRN:** 102-96-5
SPID(S): Tox21_300677
M4ID: 12478456

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 0.592 **MAX_MED:** 0.473 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

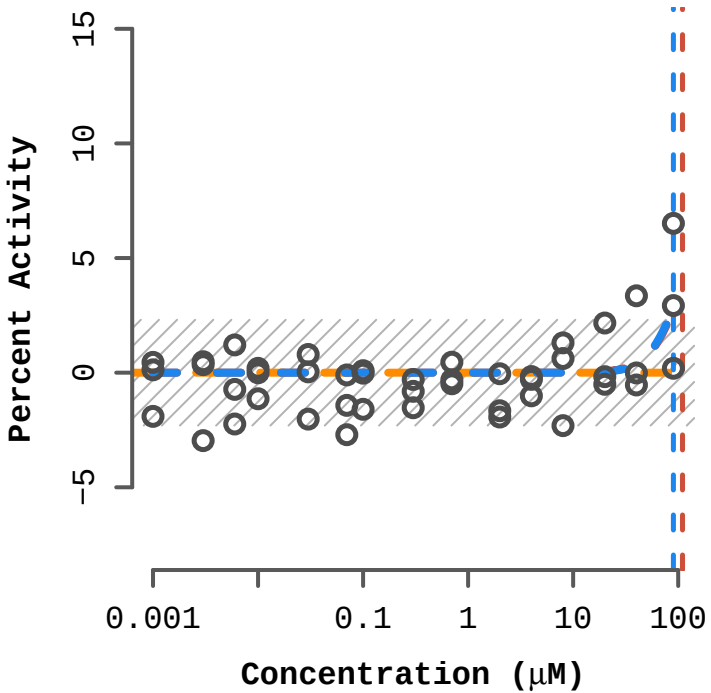
NAME: 2-Nitrotoluene
CHID: 25791 CASRN: 88-72-2
SPID(S): Tox21_300032
M4ID: 12479098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.11 MAX_MED: 1.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Nitrotoluene
CHID: 25791 **CASRN:** 88-72-2
SPID(S): Tox21_202393
M4ID: 12479859

HILL MODEL (in red):

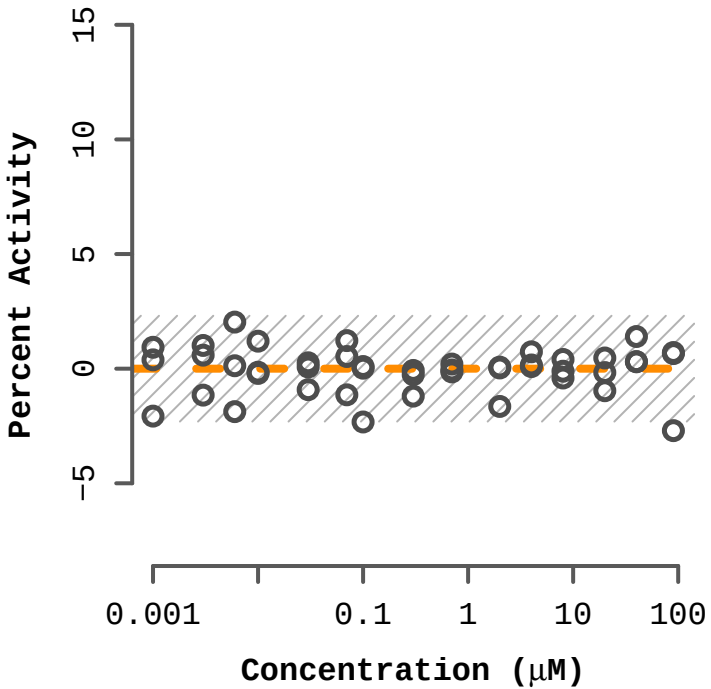
	tp	ga	gw
val:	7.82	2.04	2.91
sd:	56.4	1.83	5.71

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.67	1.95	3.23	3.95	0.995
sd:	42	1.96	9.68	74.8	47.7

	CNST	HILL	GNLS
AIC:	167.66	168.12	172.13
PROB:	0.53	0.42	0.06
RMSE:	1.66	1.43	1.43

MAX_MEAN: 3.21 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

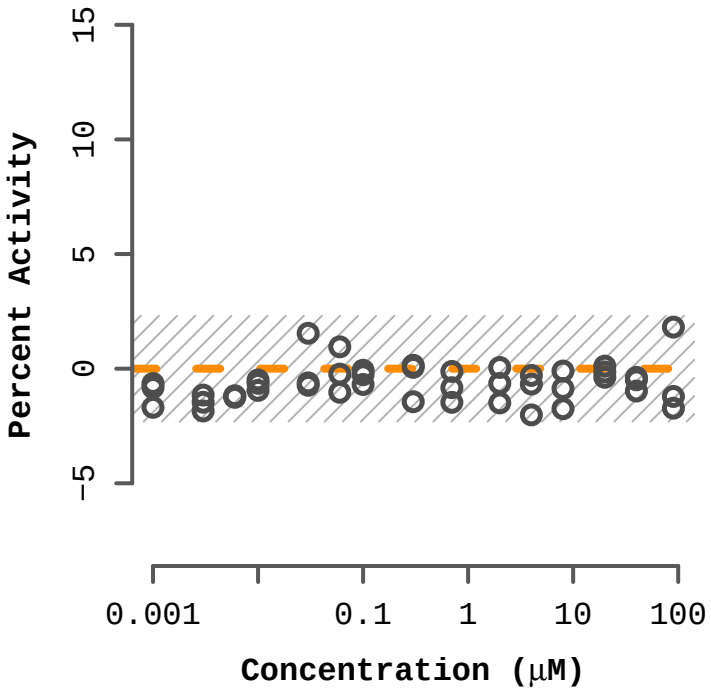
NAME: 1-Nitro-2-(trifluoromethyl)benzene
CHID: 25793 **CASRN:** 384-22-5
SPID(S): Tox21_303057
M4ID: 12476076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.671 **MAX_MED:** 0.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

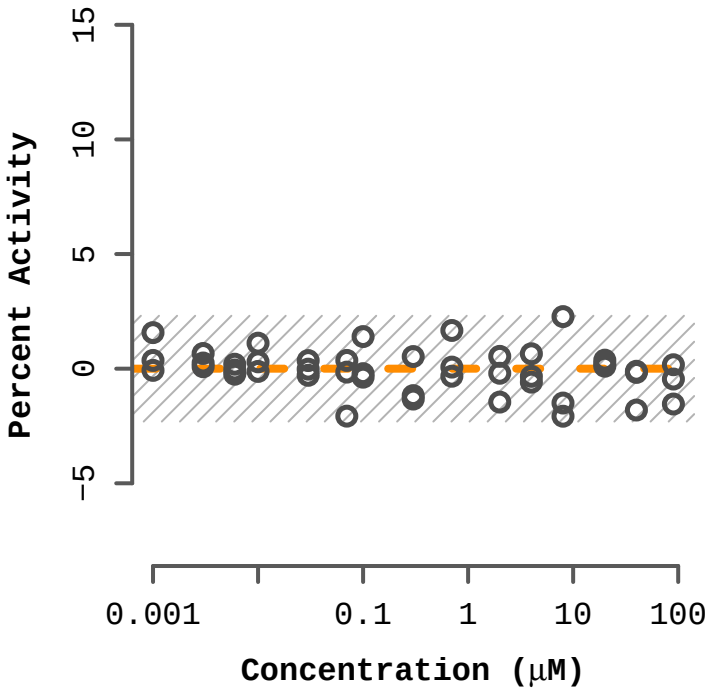
NAME: 1-Nitro-2-(trifluoromethyl)benzene
CHID: 25793 **CASRN:** 384-22-5
SPID(S): Tox21_201264
M4ID: 12480988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.0672 **MAX_MED:** 0.0601 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

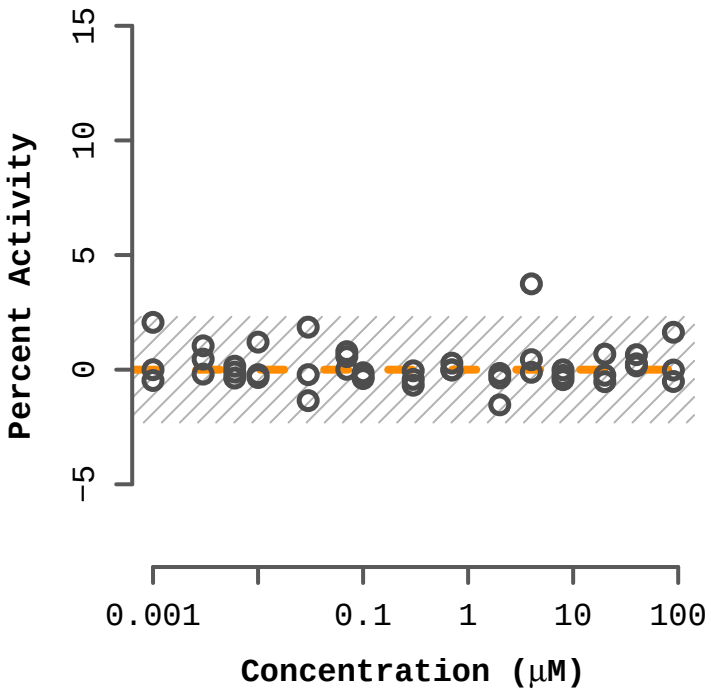
NAME: 1-Nitro-3-(trifluoromethyl)benzene
CHID: 25794 **CASRN:** 98-46-4
SPID(S): Tox21_200760
M4ID: 12481492

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.621 **MAX_MED:** 0.363 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

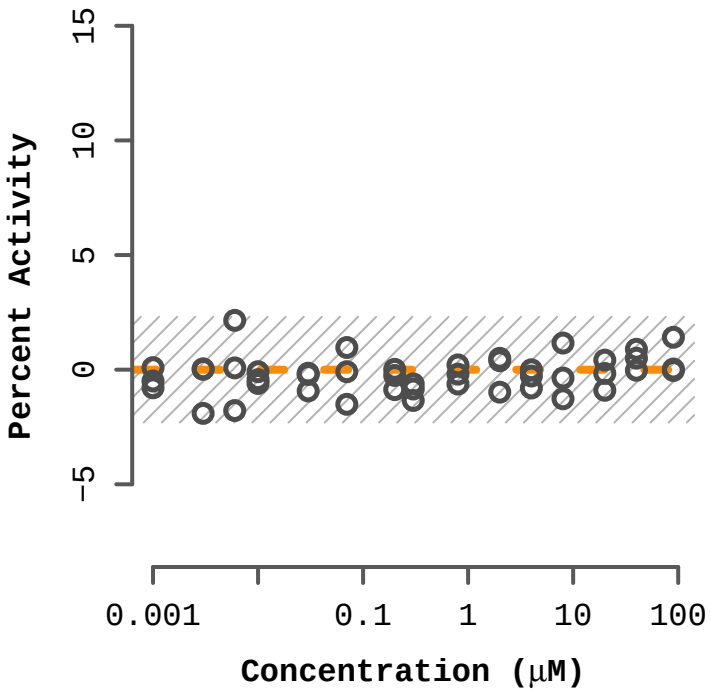
NAME: Nonane
CHID: 25796 **CASRN:** 111-84-2
SPID(S): Tox21_303148
M4ID: 12475985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.572 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

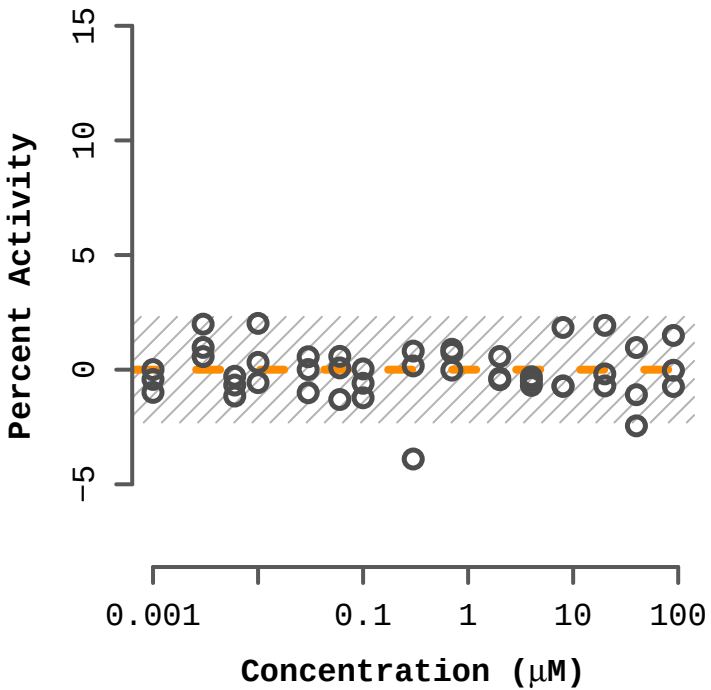
NAME: Nonane
CHID: 25796 **CASRN:** 111-84-2
SPID(S): Tox21_201479
M4ID: 12480773

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.47 **MAX_MED:** 0.501 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

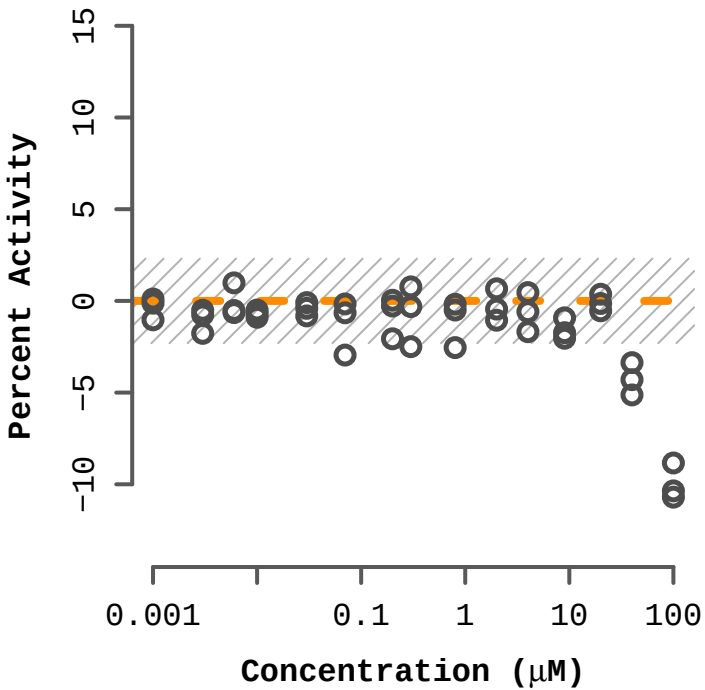
NAME: 1-Octene
CHID: 25804 **CASRN:** 111-66-0
SPID(S): Tox21_200652
M4ID: 12481600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.973 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

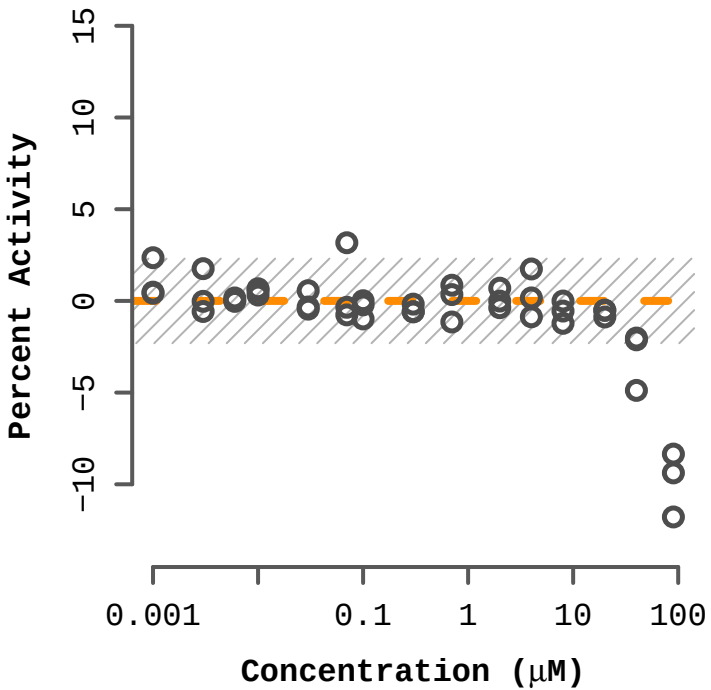
NAME: Octhilinone
CHID: 25805 **CASRN:** 26530-20-1
SPID(S): Tox21_300566
M4ID: 12478567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.09	NA	NA
PROB:	1	NA	NA
RMSE:	3	NA	NA

MAX_MEAN: −0.0577 **MAX_MED:** −0.122 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

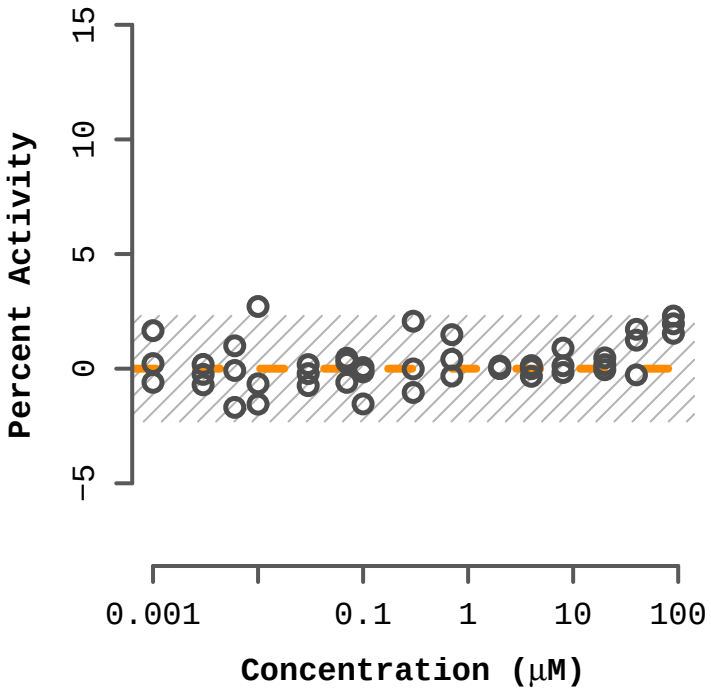
NAME: Octhilinone
CHID: 25805 **CASRN:** 26530-20-1
SPID(S): Tox21_201459
M4ID: 12480793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.69	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.573 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

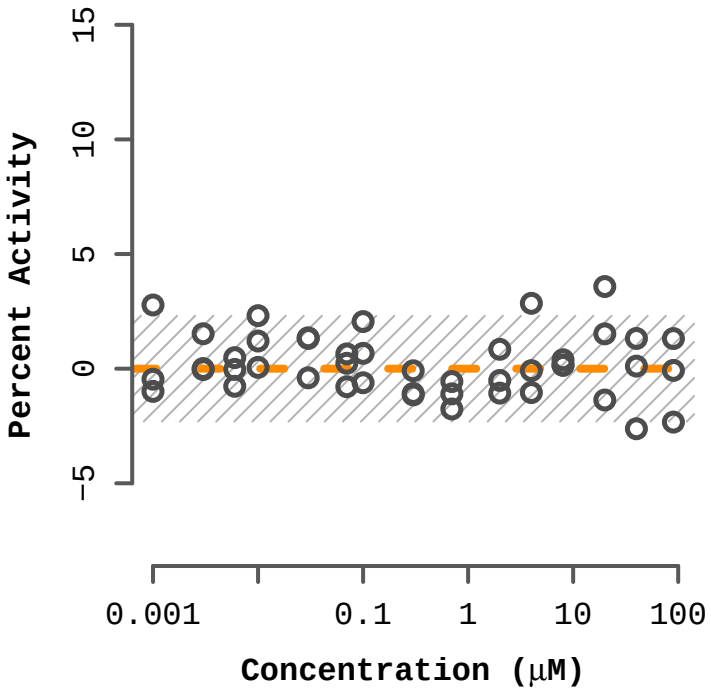
NAME: 4-Octyloxybenzoic acid
CHID: 25807 **CASRN:** 2493-84-7
SPID(S): Tox21_200904
M4ID: 12481348

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

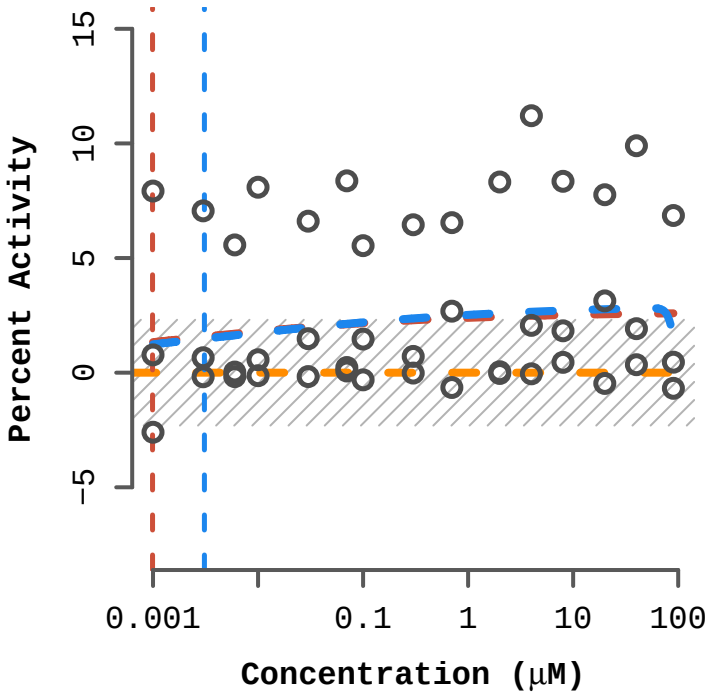
NAME: Oleic acid
CHID: 25809 **CASRN:** 112-80-1
SPID(S): Tox21_303324
M4ID: 12475809

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oleic acid
CHID: 25809 CASRN: 112-80-1
SPID(S): Tox21_201967
M4ID: 12480285

HILL MODEL (in red):

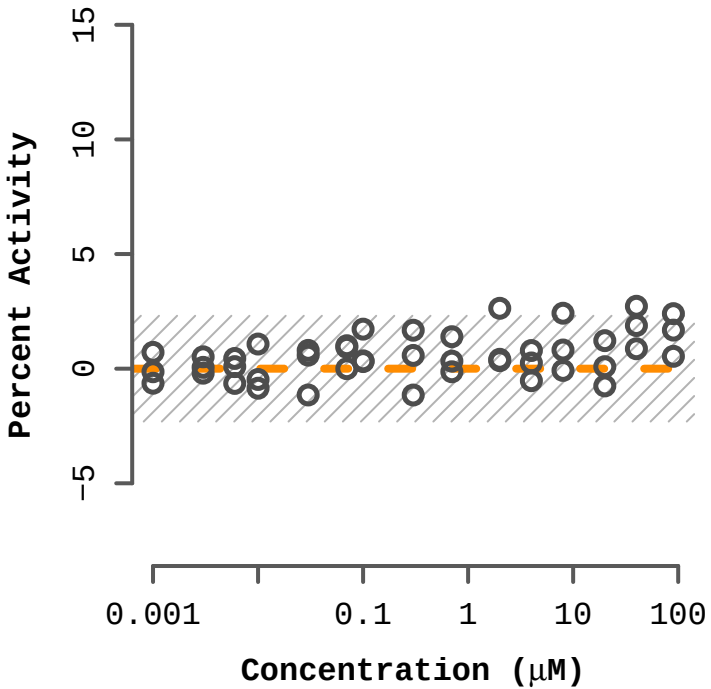
	tp	ga	gw
val:	2.66	-3	0.319
sd:	1.88	3.03	1.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.97	-2.51	0.3	1.96	13.4
sd:	5.43	4.98	1.76	0.16	304

	CNST	HILL	GNLS
AIC:	265.83	255.97	259.71
PROB:	0.01	0.86	0.13
RMSE:	4.6	3.65	3.64

MAX_MEAN: 4.41 MAX_MED: 3.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

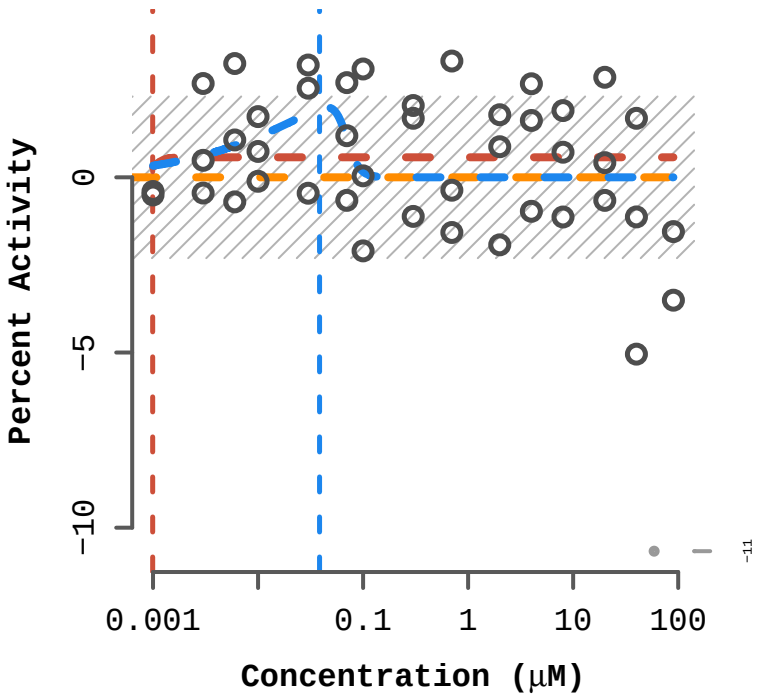
NAME: Methyl (9Z)-octadec-9-enoate
CHID: 25811 **CASRN:** 112-62-9
SPID(S): Tox21_200225
M4ID: 12482027

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Olivetol
CHID: 25812 **CASRN:** 500-66-3
SPID(S): Tox21_303332
M4ID: 12475801 **BRK**

HILL MODEL (in red):

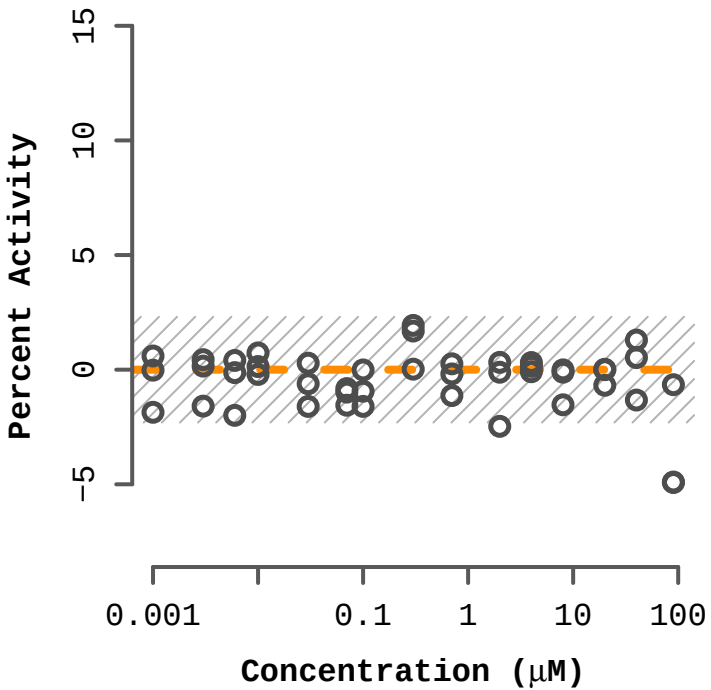
	tp	ga	gw
val:	0.572	−3	7.99
sd:	0.331	0.498	215

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.98	−1.41	0.657	−1.16	7.25
sd:	18.2	5.39	1.25	0.189	24.4

	CNST	HILL	GNLS
AIC:	211.32	214.38	216.03
PROB:	0.76	0.16	0.07
RMSE:	2.75	2.74	2.64

MAX_MEAN: 2.23 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

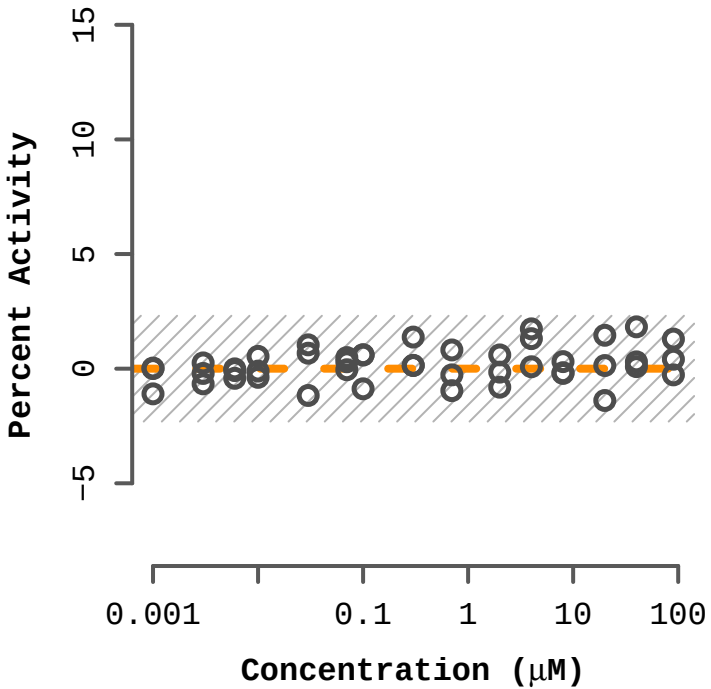
NAME: Olivetol
CHID: 25812 **CASRN:** 500-66-3
SPID(S): Tox21_202349
M4ID: 12479903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

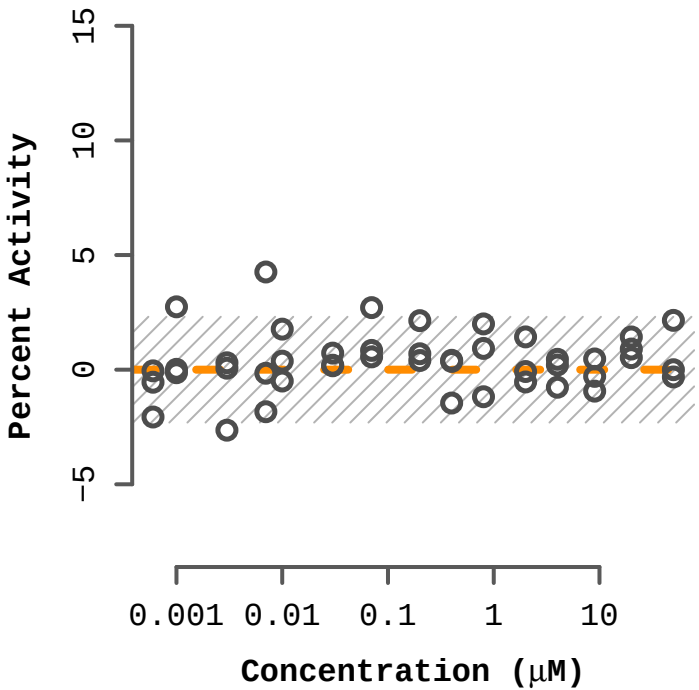
NAME: Orotic acid
CHID: 25814 **CASRN:** 65-86-1
SPID(S): Tox21_201104
M4ID: 12481148

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

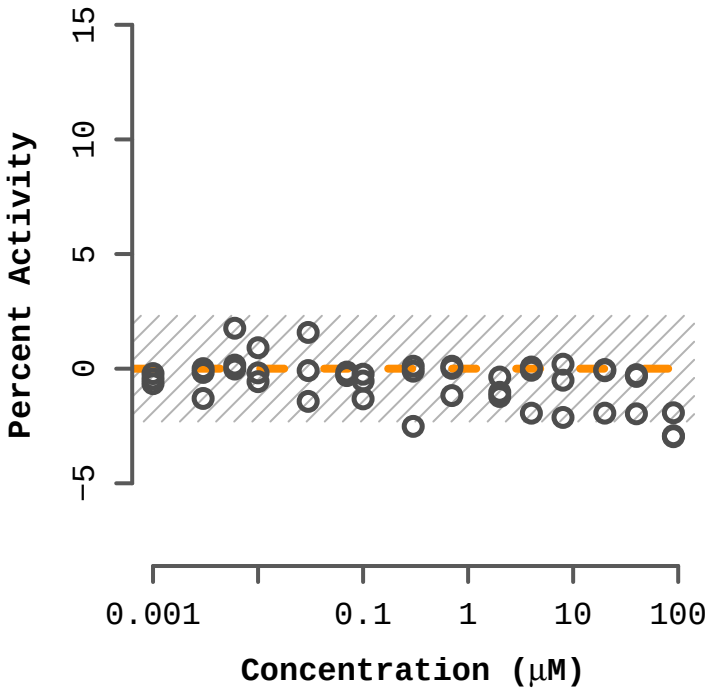
NAME: Orotic acid
CHID: 25814 **CASRN:** 65-86-1
SPID(S): Tox21_111121_1
M4ID: 12483895

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.929 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

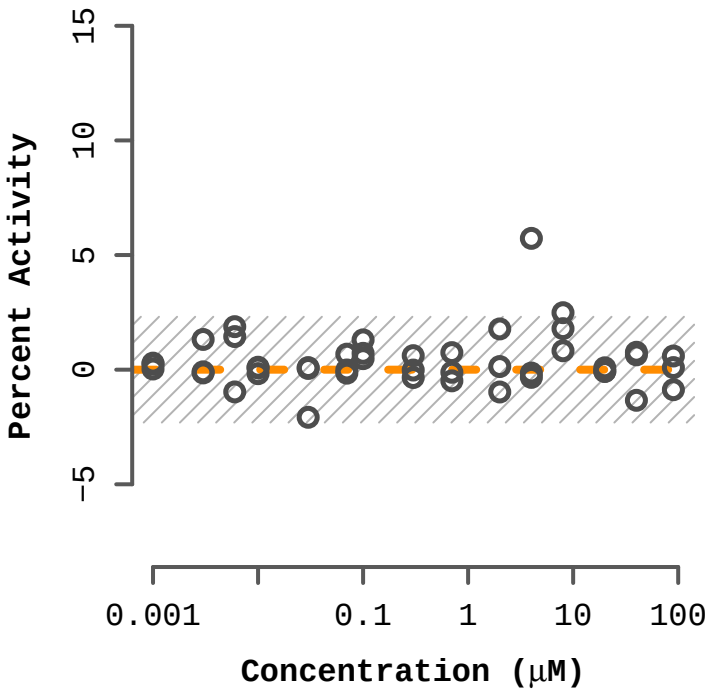
NAME: Orphenadrine hydrochloride
CHID: 25815 **CASRN:** 341-69-5
SPID(S): Tox21_301927
M4ID: 12477206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 0.159 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

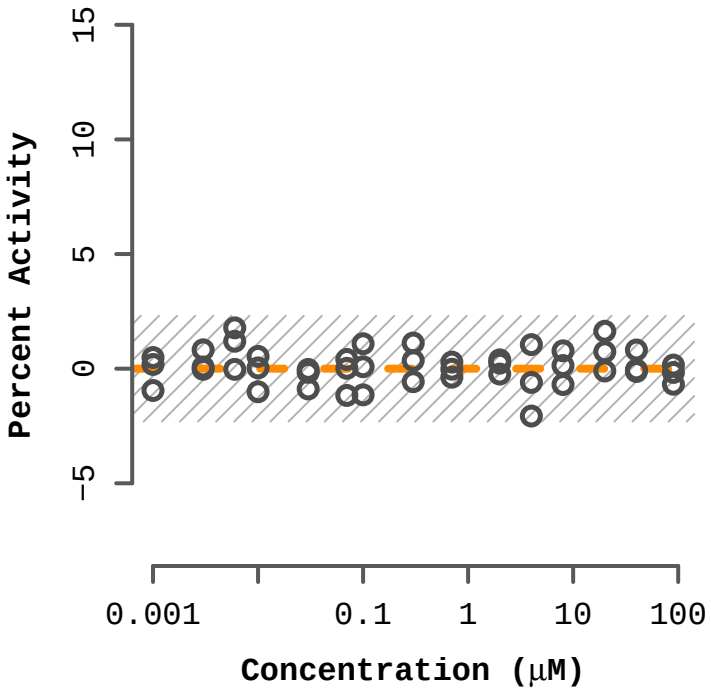
NAME: Oxalic acid
CHID: 25816 **CASRN:** 144-62-7
SPID(S): Tox21_303346
M4ID: 12475787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

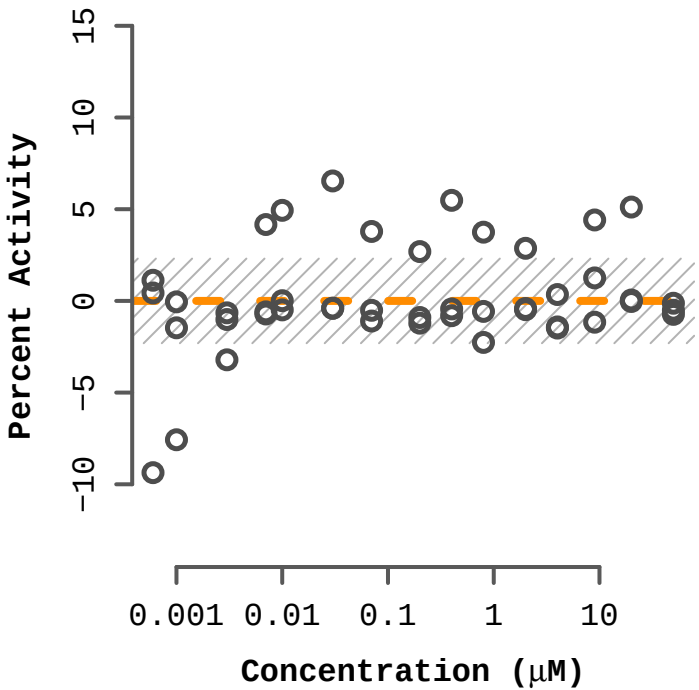
NAME: Oxalic acid
CHID: 25816 **CASRN:** 144-62-7
SPID(S): Tox21_202122
M4ID: 12480130

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.984 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

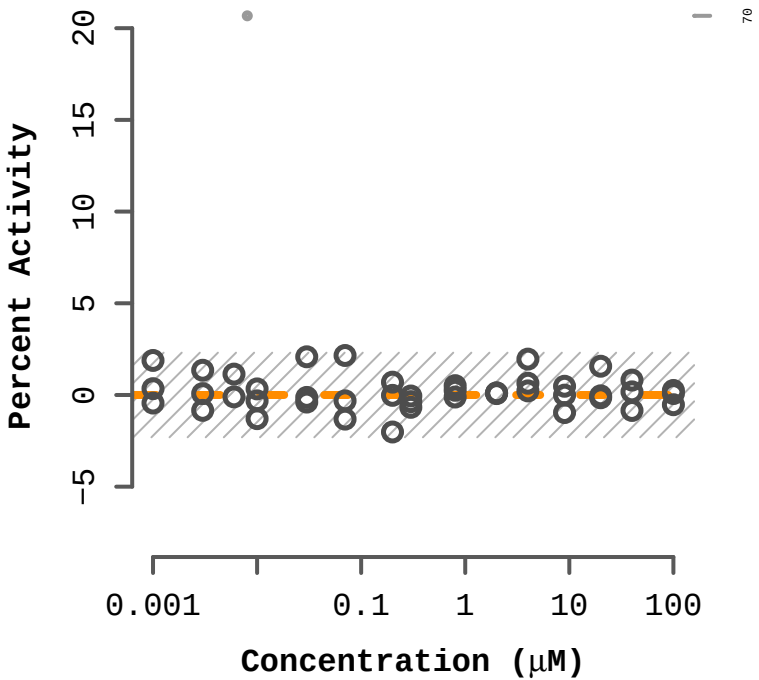
NAME: Oxethazaine
CHID: 25818 **CASRN:** 126-27-2
SPID(S): Tox21_110407_1
M4ID: 12484385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.92	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

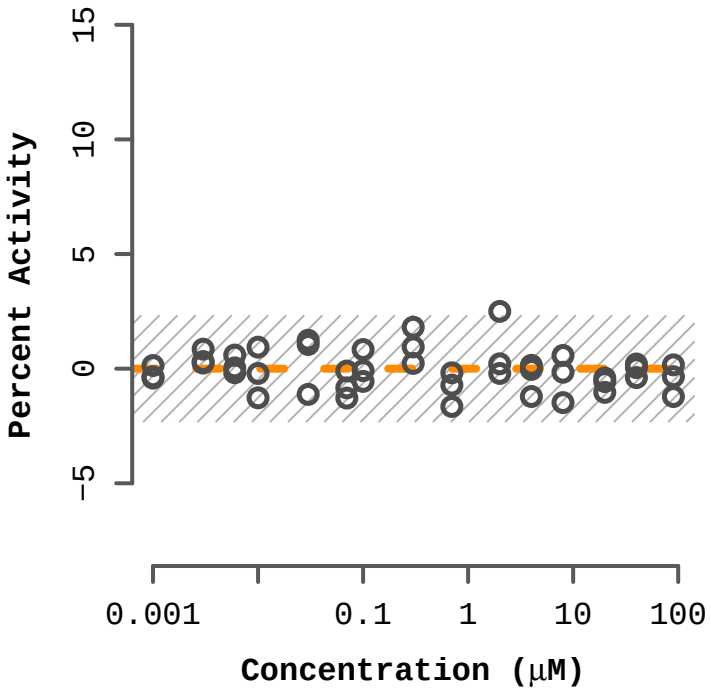
NAME: Dibenzyl ether
CHID: 25819 **CASRN:** 103-50-4
SPID(S): Tox21_200903
M4ID: 12481349 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.93	NA	NA
PROB:	1	NA	NA
RMSE:	10.49	NA	NA

MAX_MEAN: 23.7 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

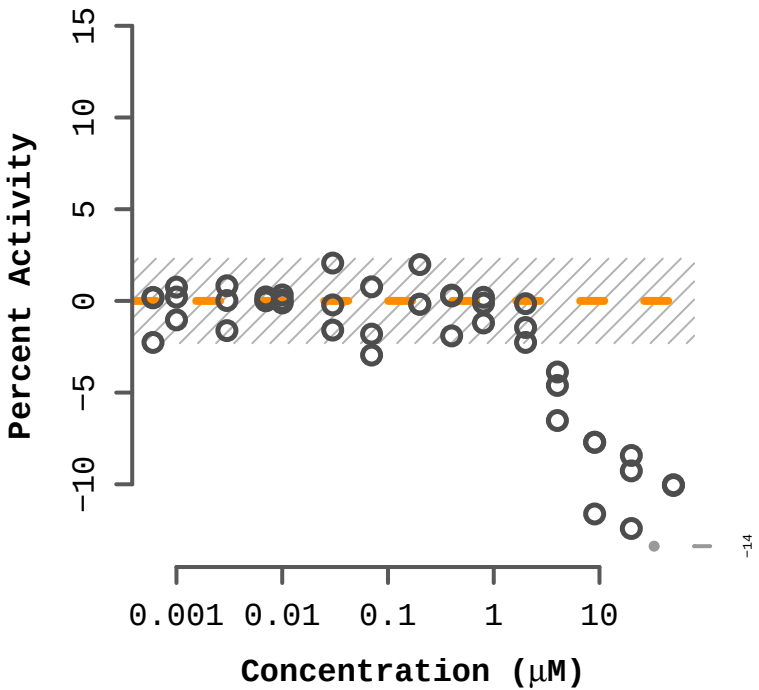
NAME: Palladium(II) chloride
CHID: 25824 **CASRN:** 7647-10-1
SPID(S): Tox21_301366
M4ID: 12477767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.997 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

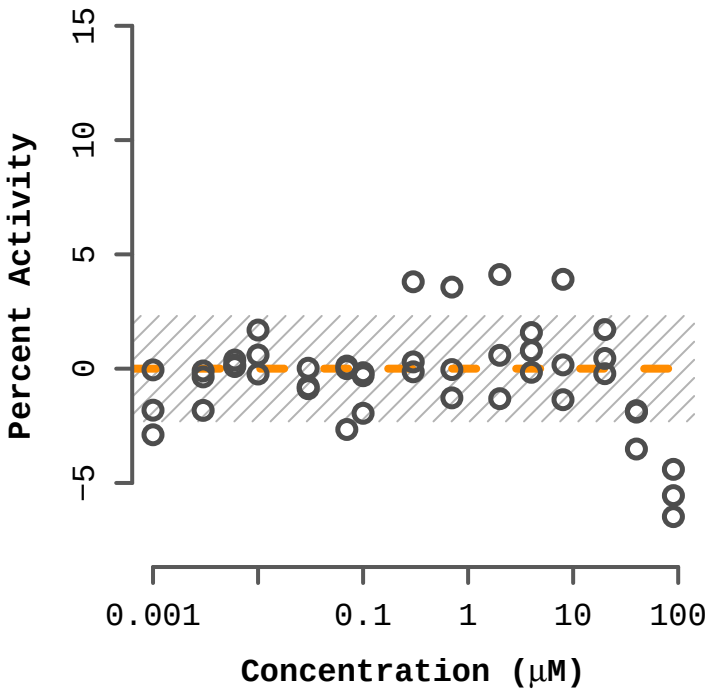
NAME: Papaverine hydrochloride
CHID: 25825 **CASRN:** 61-25-6
SPID(S): Tox21_110226_1
M4ID: 12484535 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	263.01	NA	NA
PROB:	1	NA	NA
RMSE:	4.89	NA	NA

MAX_MEAN: 0.542 **MAX_MED:** 0.269 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

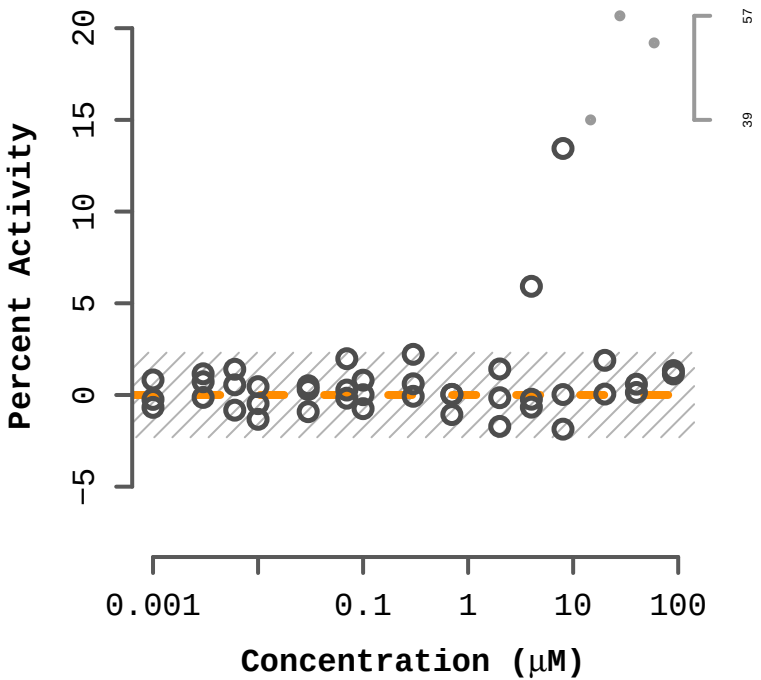
NAME: Pentabromoethane
CHID: 25830 **CASRN:** 75-95-6
SPID(S): Tox21_200571
M4ID: 12481681

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.33	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.789 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

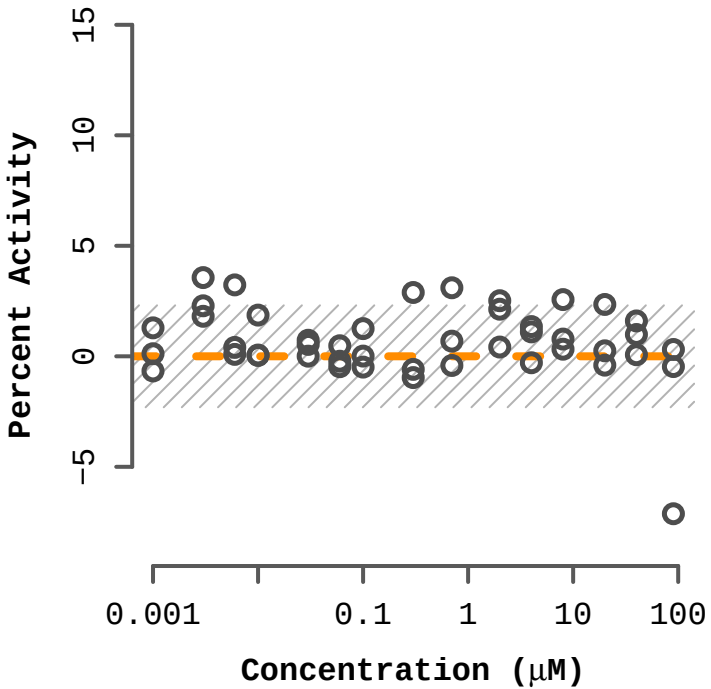
NAME: 2,4-Dichloro-1-(trichloromethyl)benzene
CHID: 25839 **CASRN:** 13014-18-1
SPID(S): Tox21_200939
M4ID: 12481313 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.08	NA	NA
PROB:	1	NA	NA
RMSE:	13.17	NA	NA

MAX_MEAN: 19.4 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

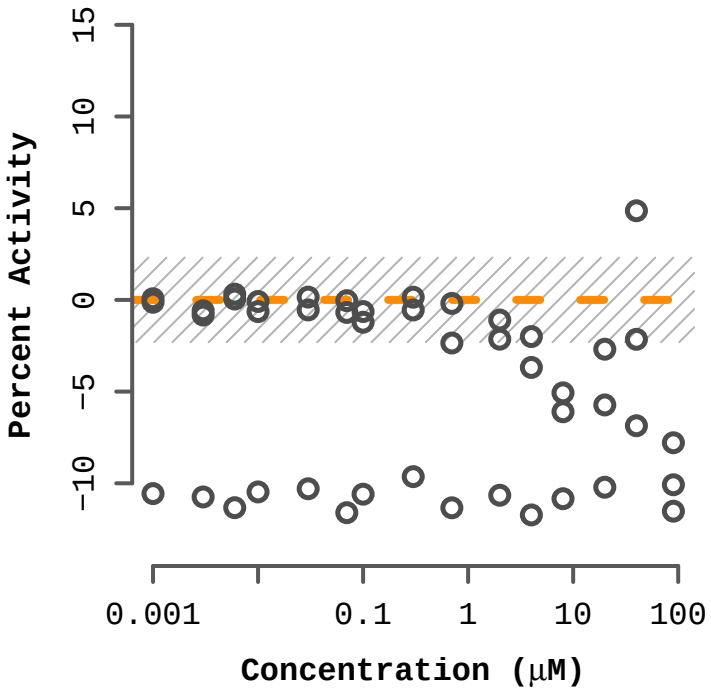
NAME: 1,2-Dichloro-4-(trichloromethyl)benzene
CHID: 25840 **CASRN:** 13014-24-9
SPID(S): Tox21_200169
M4ID: 12482083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.78	NA	NA

MAX_MEAN: 2.55 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

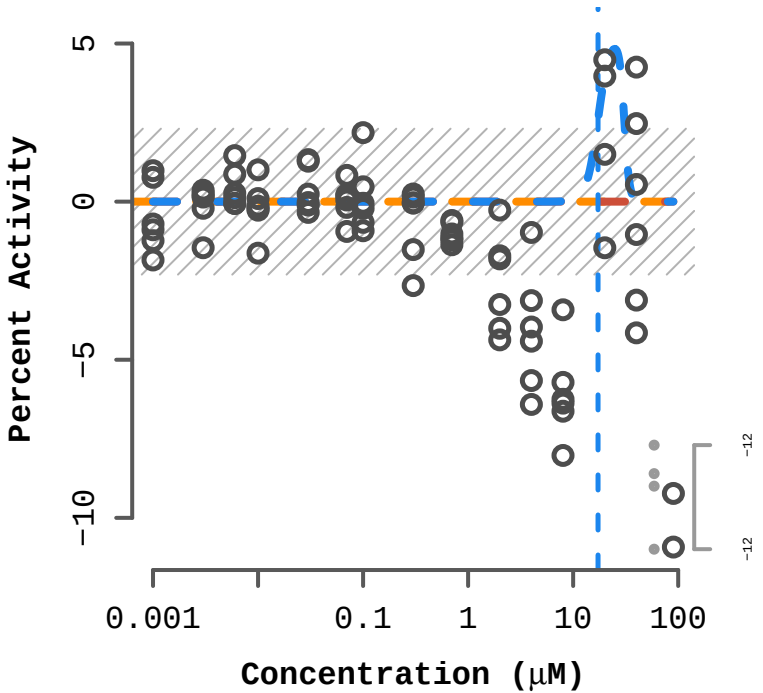
NAME: Pentaerythritol triacrylate
CHID: 25842 **CASRN:** 3524-68-3
SPID(S): Tox21_303252
M4ID: 12475881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	304.02	NA	NA
PROB:	1	NA	NA
RMSE:	6.7	NA	NA

MAX_MEAN: −1.38 **MAX_MED:** 0.0477 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentaerythritol triacrylate
CHID: 25842 CASRN: 3524-68-3
SPID(S): Tox21_202024
M4ID: 12480228 BRK

HILL MODEL (in red):

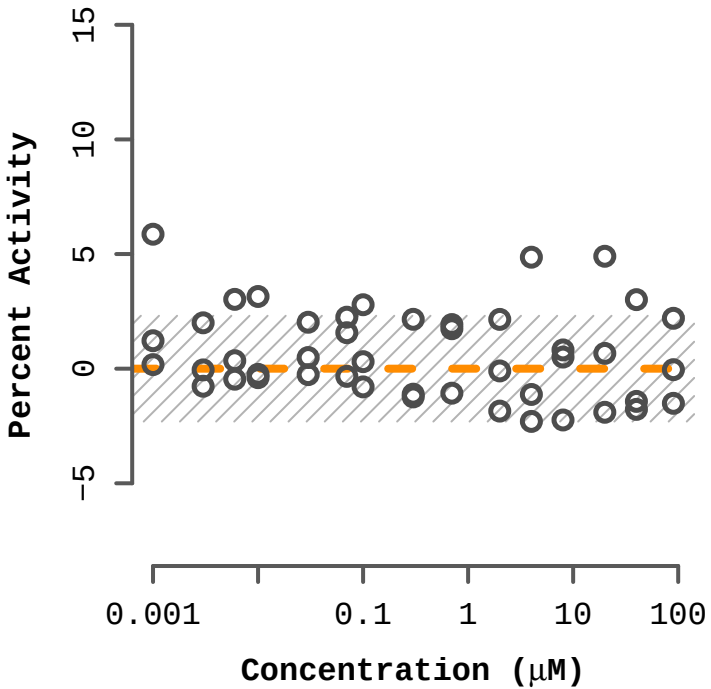
	tp	ga	gw
val:	4.76e-10	2.42	2.09
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.21	1.24	7.98	1.49	18
sd:	11.2	0.441	8.97	0.422	65.9

	CNST	HILL	GNLS
AIC:	481.61	487.61	482.14
PROB:	0.55	0.03	0.42
RMSE:	3.93	3.93	3.82

MAX_MEAN: 3.58 MAX_MED: 4.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

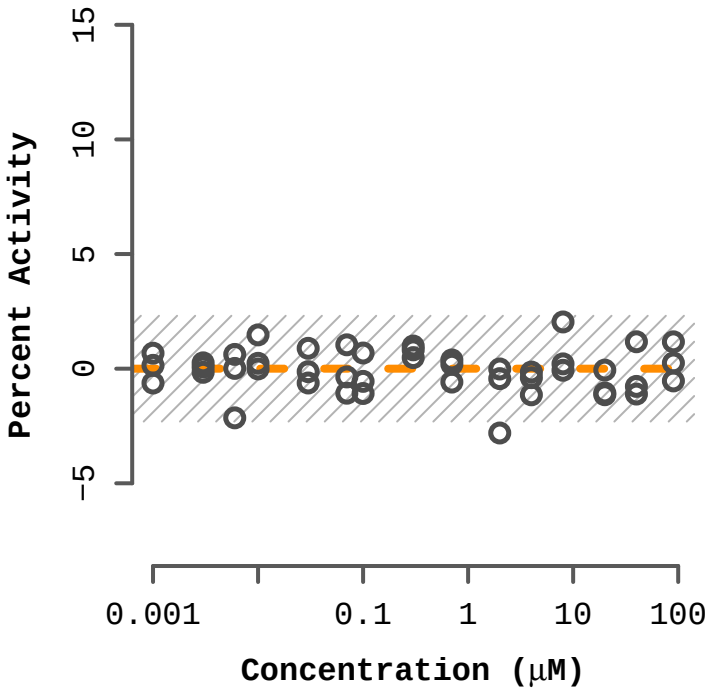
NAME: Pentane
CHID: 25846 **CASRN:** 109-66-0
SPID(S): Tox21_200248
M4ID: 12482004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 2.42 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

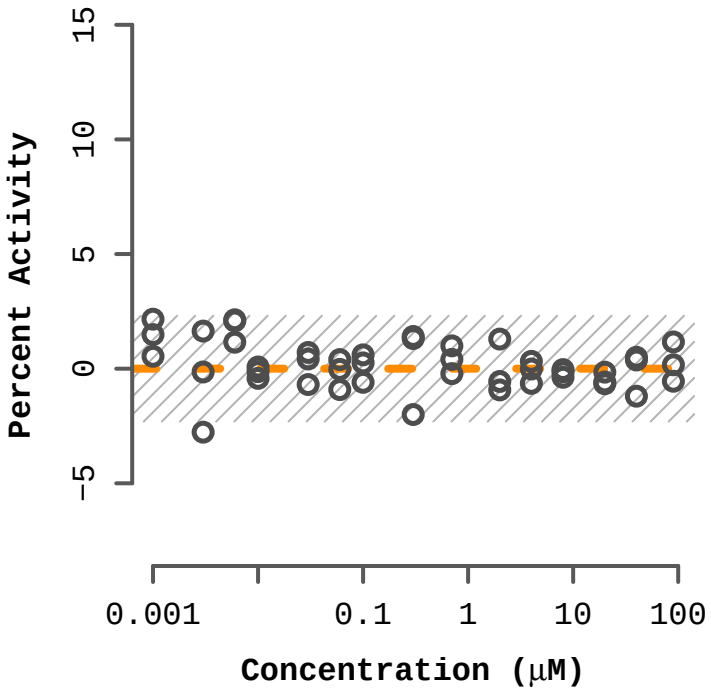
NAME: 1-Pentene
CHID: 25849 CASRN: 109-67-1
SPID(S): Tox21_200280
M4ID: 12481972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.765 MAX_MED: 0.823 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

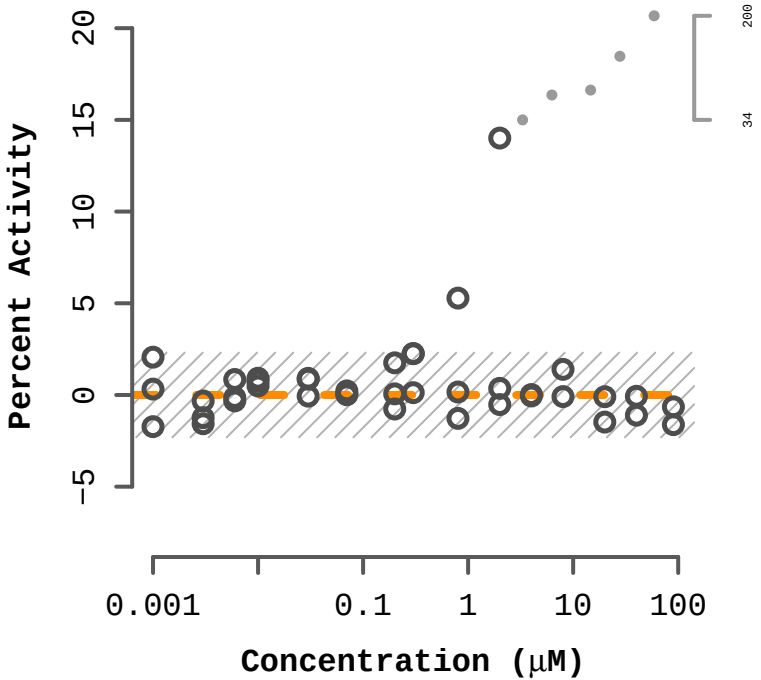
NAME: 2-Pentenenitrile
CHID: 25850 **CASRN:** 13284-42-9
SPID(S): Tox21_200185
M4ID: 12482067

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

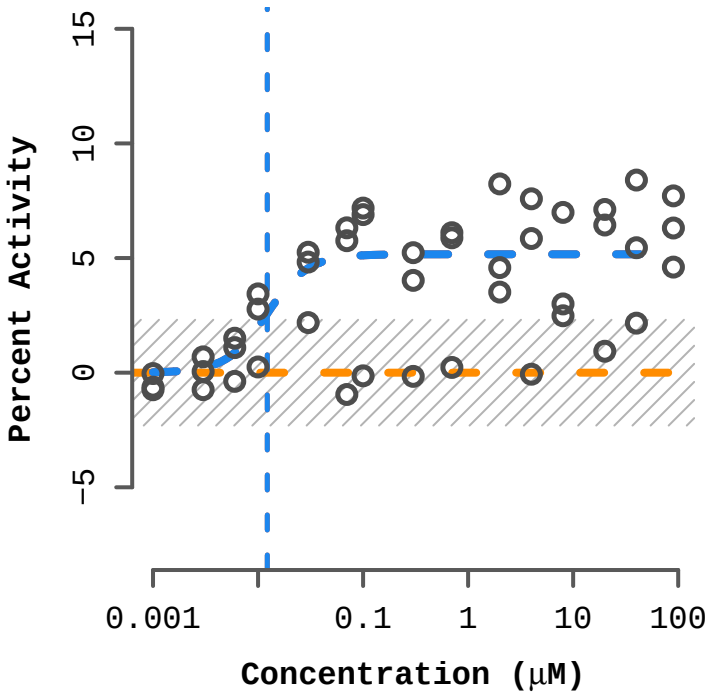
NAME: 3-Pentenenitrile
CHID: 25851 **CASRN:** 4635-87-4
SPID(S): Tox21_200088
M4ID: 12482164 **BRK**

HILL MODEL: Not applicable.

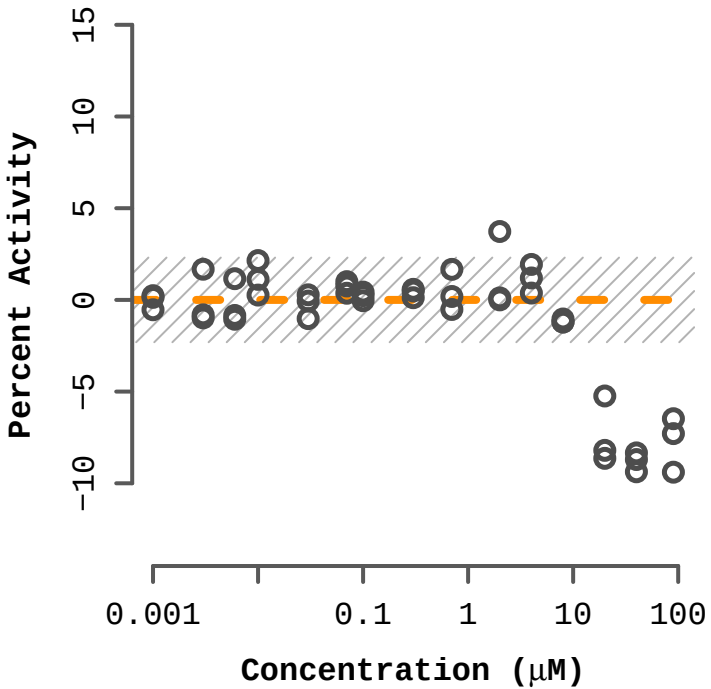
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	336.65	NA	NA
PROB:	1	NA	NA
RMSE:	39.35	NA	NA

MAX_MEAN: 64.7 **MAX_MED:** 2.25 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Perchloromethylmercaptan
CHID:    25854   CASRN: 594-42-3
SPID(S): Tox21_200422
M4ID:    12481830

HILL MODEL (in red):
      tp       ga       gw
val:  5.17     -1.91    2.24
sd:   0.479    0.181    1.44

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.16     -1.91    2.24     3.78     6.58
sd:   0.479    0.181    1.44     111000   399000

      CNST        HILL        GNLS
AIC:  272.11      213.38      217.38
PROB: 0           0.88        0.12
RMSE: 4.58        2.39        2.39

MAX_MEAN: 6.21      MAX_MED: 6.9       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

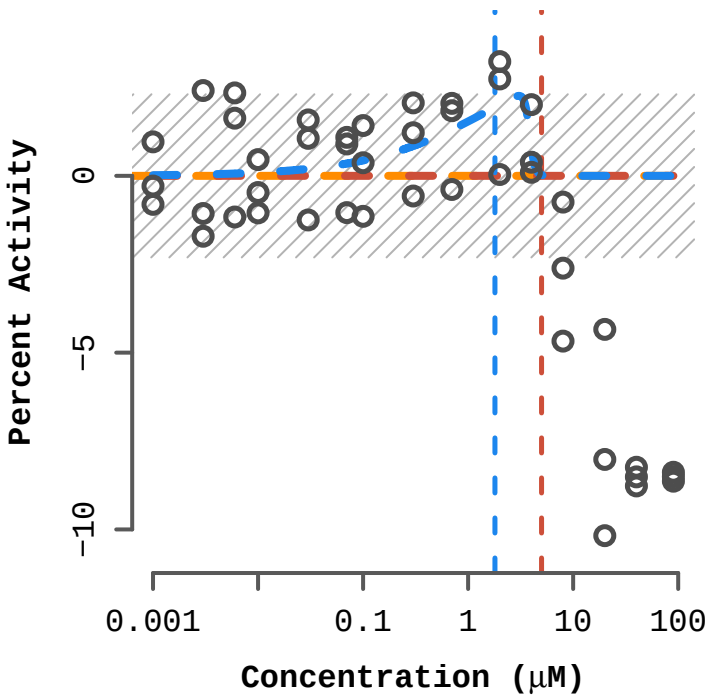
NAME: 1,10-Phenanthroline
CHID: 25857 **CASRN:** 66-71-7
SPID(S): Tox21_303111
M4ID: 12476022

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	236.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.74	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,10-Phenanthroline
CHID: 25857 CASRN: 66-71-7
SPID(S): Tox21_201998
M4ID: 12480254

HILL MODEL (in red):

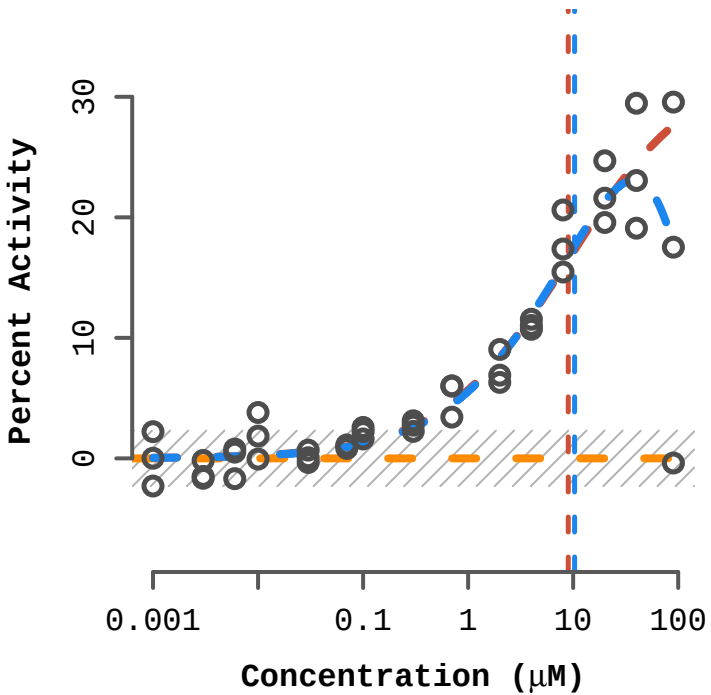
	tp	ga	gw
val:	7.74e-11	0.699	1.65
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.88	0.255	0.715	0.584	17.5
sd:	15.4	4.65	1.45	0.422	415

	CNST	HILL	GNLS
AIC:	248.11	254.11	254.61
PROB:	0.92	0.05	0.04
RMSE:	4	4	3.94

MAX_MEAN: 2 MAX_MED: 2.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenethyl anthranilate
CHID: 25861 CASRN: 133-18-6
SPID(S): Tox21_303500
M4ID: 12475642

HILL MODEL (in red):

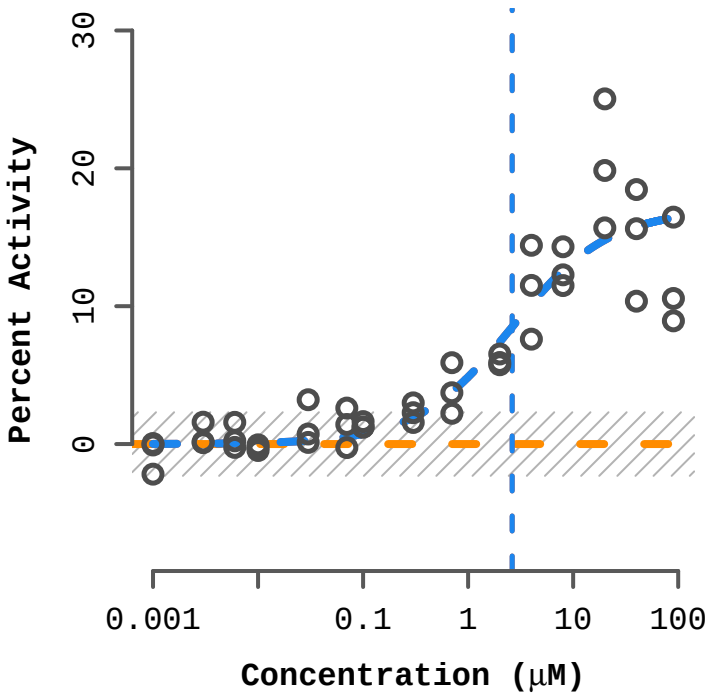
	tp	ga	gw
val:	32.9	0.953	0.715
sd:	5.1	0.214	0.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	35.5	1.01	0.721	2.04	2.13
sd:	9.04	0.288	0.0976	0.0718	1.17

	CNST	HILL	GNLS
AIC:	346.06	221.63	219.64
PROB:	0	0.27	0.73
RMSE:	11.62	4.81	3.7

MAX_MEAN: 23.9 MAX_MED: 23.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenethyl anthranilate
CHID: 25861 CASRN: 133-18-6
SPID(S): Tox21_202175
M4ID: 12480077

HILL MODEL (in red):

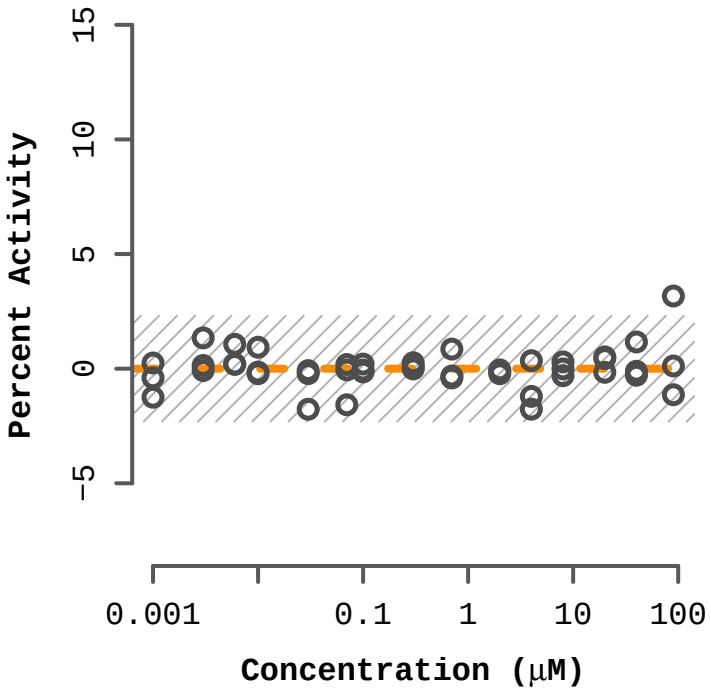
	tp	ga	gw
val:	17	0.419	0.946
sd:	1.36	0.115	0.175

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17	0.419	0.946	3.66	9.48
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	323.07	210.14	214.14
PROB:	0	0.88	0.12
RMSE:	8.85	2.7	2.7

MAX_MEAN: 20.2 MAX_MED: 19.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

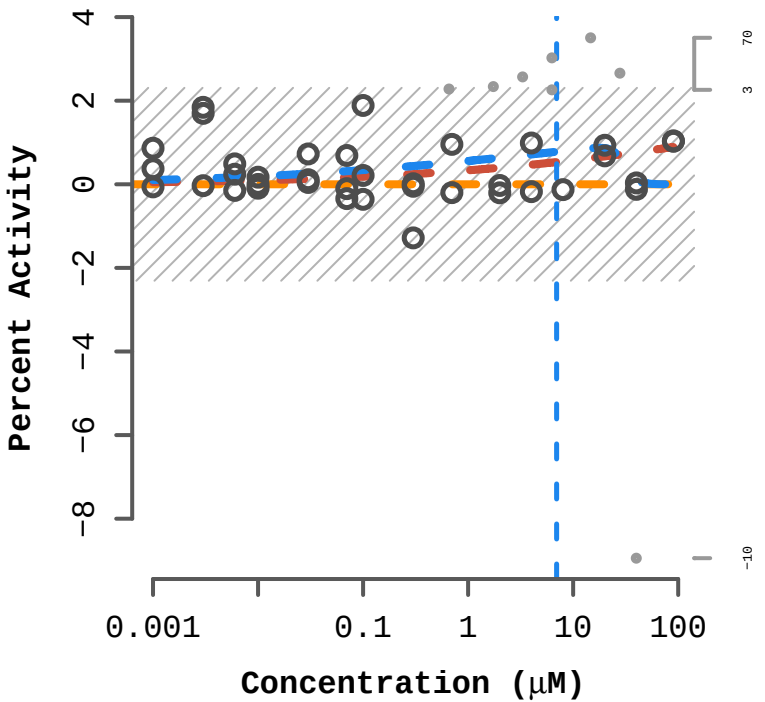
NAME: 3-Ethoxyaniline
CHID: 25862 **CASRN:** 621-33-0
SPID(S): Tox21_200997
M4ID: 12481255

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.443 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethoxyaniline
CHID: 25863 **CASRN:** 94-70-2
SPID(S): Tox21_201003
M4ID: 12481249 **BRK**

HILL MODEL (in red):

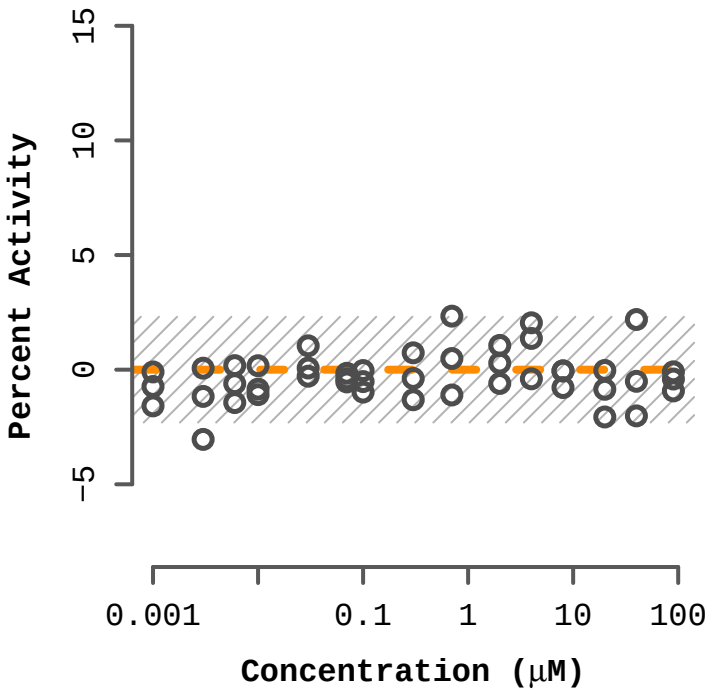
	tp	ga	gw
val:	2.15	2.45	0.3
sd:	3.65	0.444	0.285

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.56	0.842	0.3	1.48	7.51
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	265.81	268.59	272.11
PROB:	0.77	0.19	0.03
RMSE:	13.37	13.21	13.17

MAX_MEAN: 23.9 **MAX_MED:** 3.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

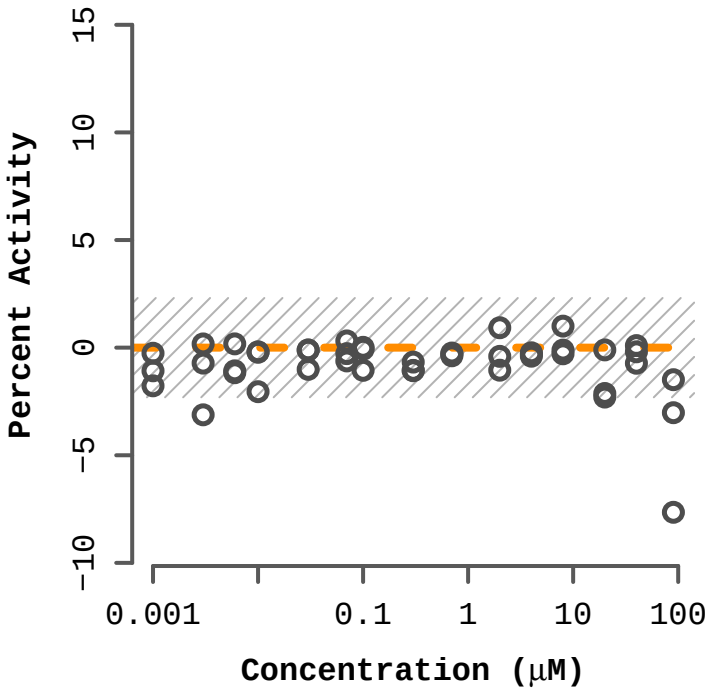
NAME: 4-Ethoxyaniline
CHID: 25864 **CASRN:** 156-43-4
SPID(S): Tox21_303334
M4ID: 12475799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

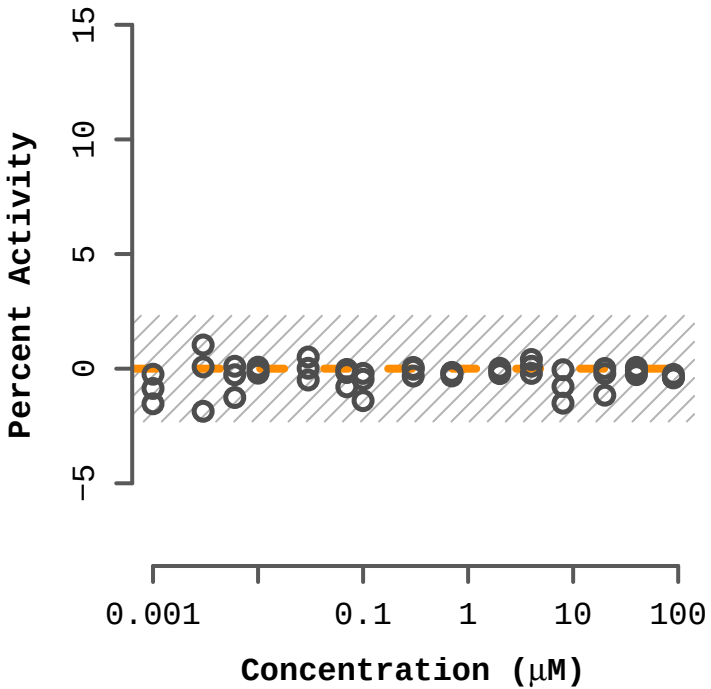
NAME: 4-Ethoxyaniline
CHID: 25864 **CASRN:** 156-43-4
SPID(S): Tox21_201946
M4ID: 12480306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 0.201 **MAX_MED:** −0.0732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

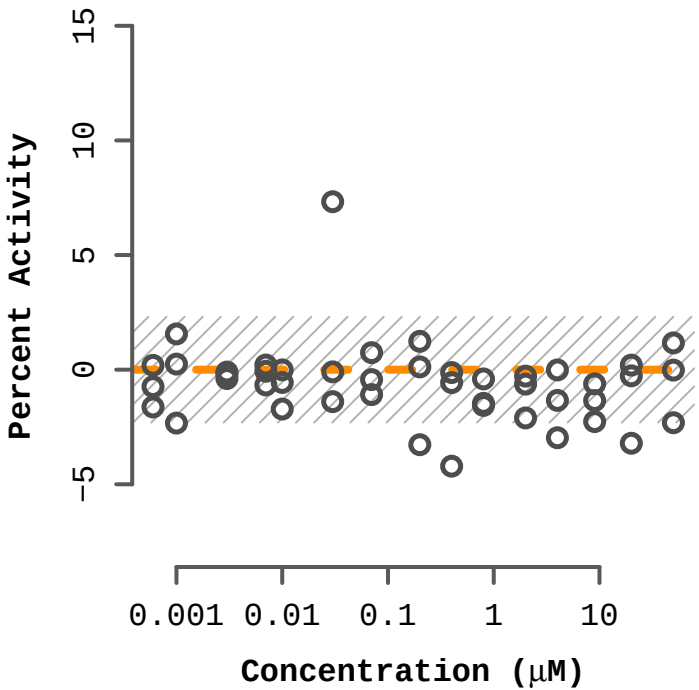
NAME: Pheniramine maleate
CHID: 25866 **CASRN:** 132-20-7
SPID(S): Tox21_201074
M4ID: 12481178

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	80.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 0.102 **MAX_MED:** 0.109 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

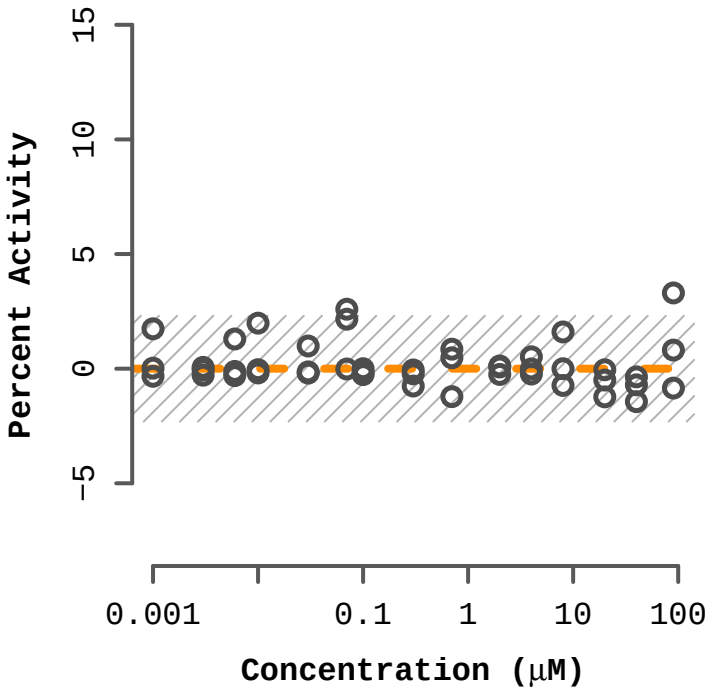
NAME: Pheniramine maleate
CHID: 25866 CASRN: 132-20-7
SPID(S): Tox21_111188_1
M4ID: 12483857

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.95 MAX_MED: 0.245 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

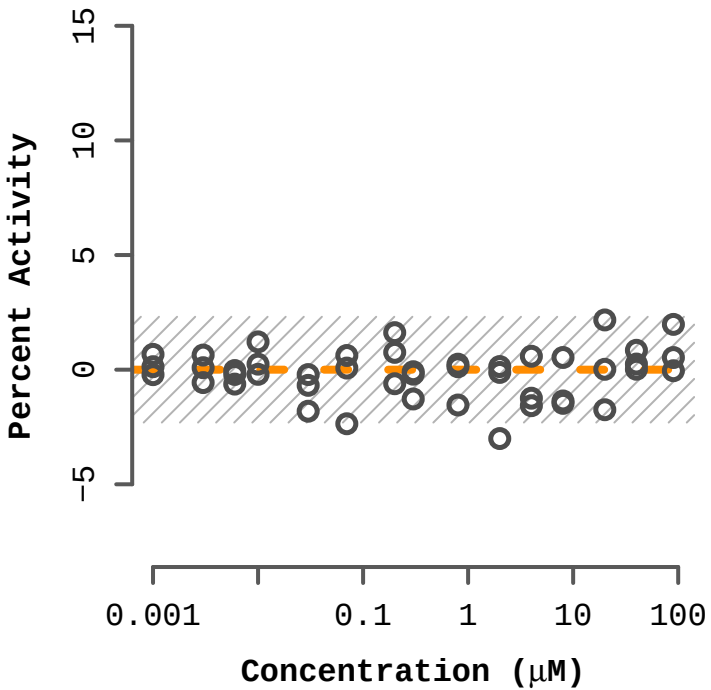
NAME: Phenoxyacetic acid
CHID: 25873 **CASRN:** 122-59-8
SPID(S): Tox21_303164
M4ID: 12475969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.74	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

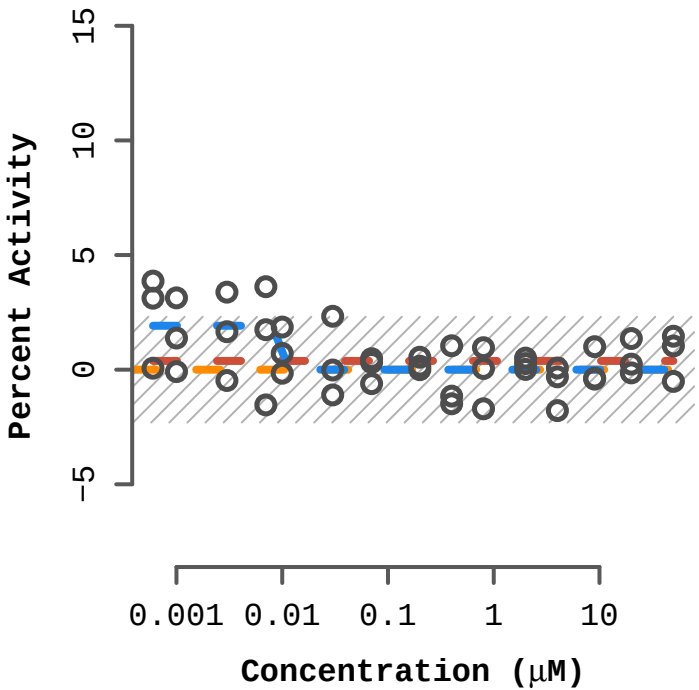
NAME: Phenoxyacetic acid
CHID: 25873 **CASRN:** 122-59-8
SPID(S): Tox21_201854
M4ID: 12480398

HILL MODEL: Not applicable.

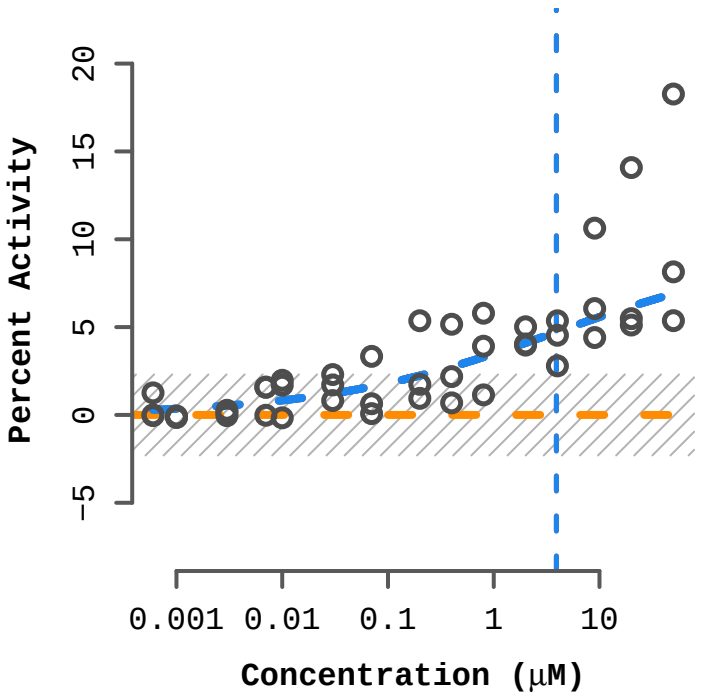
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.821 **MAX_MED:** 0.757 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenoxyacetic acid
CHID:    25873   CASRN: 122-59-8
SPID(S): Tox21_111092_1
M4ID:    12483911

HILL MODEL (in red):
      tp       ga       gw
val:  0.382    -4.96    4.12
sd:   0.194    1310     3060

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.92     -5.08    6.33     -2.01    11.5
sd:   0.521    190000   660000   0.0841   53.8

      CNST        HILL        GNLS
AIC:  163.57      165.64      158.25
PROB: 0.06        0.02        0.91
RMSE: 1.49        1.39        1.21

MAX_MEAN: 2.35      MAX_MED: 3.12      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−(1,4−Phenylene)bis−2−propenoic acid
CHID: 25879 **CASRN:** 16323−43−6
SPID(S): Tox21_202476
M4ID: 12479776

HILL MODEL (in red):

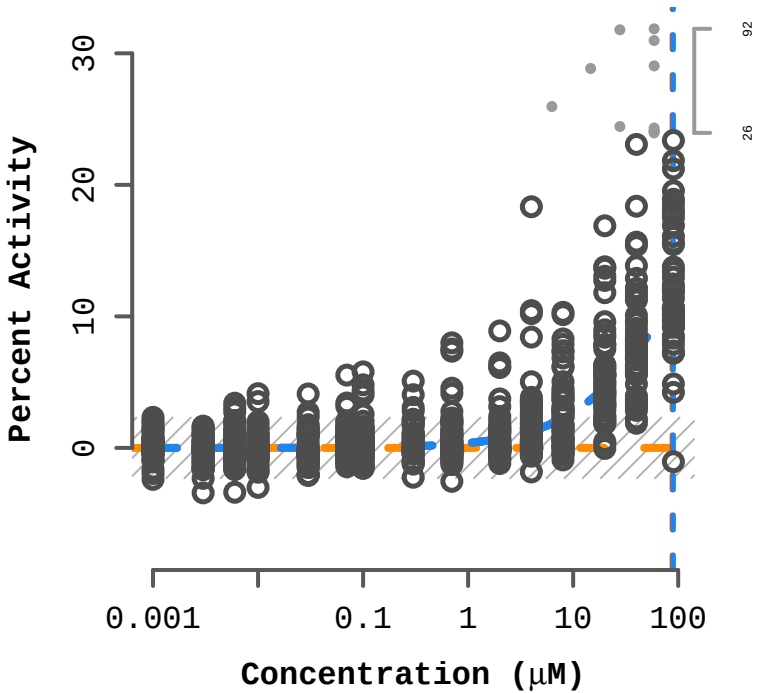
	tp	ga	gw
val:	9.43	0.593	0.392
sd:	4.5	1.15	0.131

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.43	0.592	0.392	3.38	4.51
sd:	4.5	1.15	0.131	1160	3150

	CNST	HILL	GNLS
AIC:	265.36	190.11	194.11
PROB:	0	0.88	0.12
RMSE:	4.98	2.49	2.49

MAX_MEAN: 10.6 **MAX_MED:** 8.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Phenylenediamine
CHID: 25881 CASRN: 95-54-5
SPID(S): Tox21_400014
M4ID: 12475123 BRK

HILL MODEL (in red):

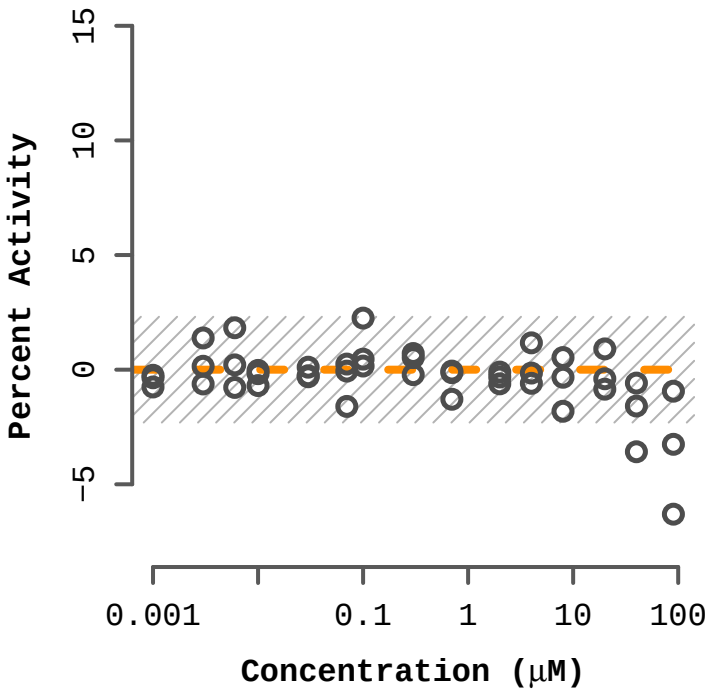
	tp	ga	gw
val:	22.3	1.94	0.91
sd:	6.35	0.257	0.108

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.8	1.95	0.911	2.93	1.94
sd:	31.7	0.982	0.214	11.3	23.8

	CNST	HILL	GNLS
AIC:	4397.08	3519.38	3523.37
PROB:	0	0.88	0.12
RMSE:	8.52	6.67	6.67

MAX_MEAN: 17.5 MAX_MED: 12.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

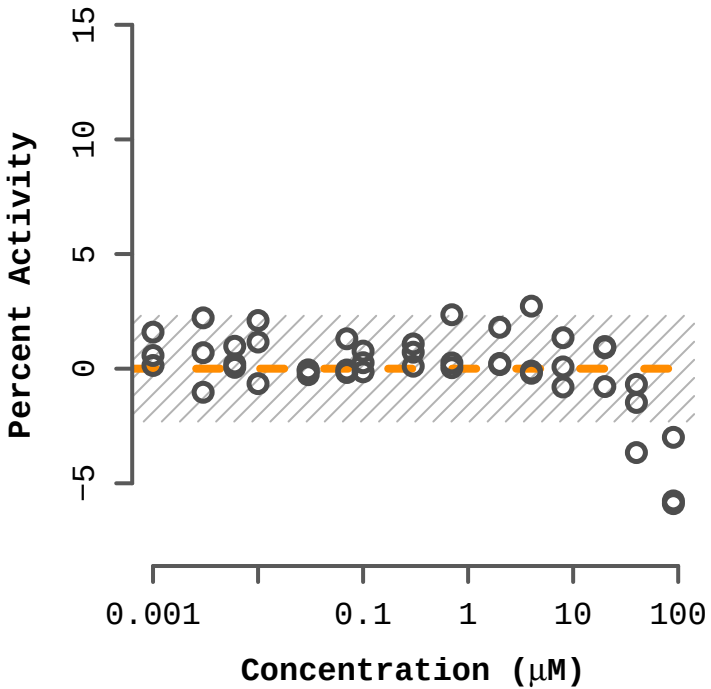
NAME: Ethyl 3-phenylglycidate
CHID: 25886 **CASRN:** 121-39-1
SPID(S): Tox21_303367
M4ID: 12475768

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 0.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

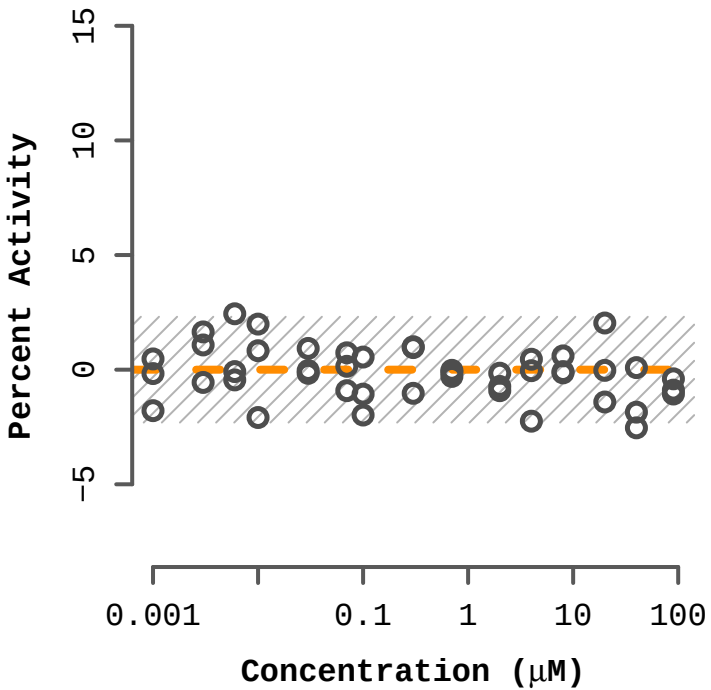
NAME: Ethyl 3-phenylglycidate
CHID: 25886 **CASRN:** 121-39-1
SPID(S): Tox21_202247
M4ID: 12480005

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

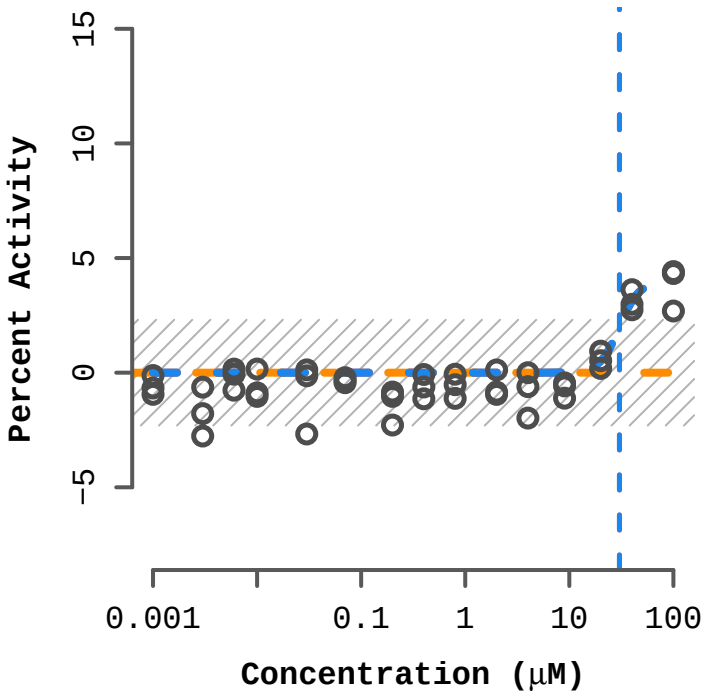
NAME: Phenylglyoxal
CHID: 25888 **CASRN:** 1074-12-0
SPID(S): Tox21_200277
M4ID: 12481975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Phenylhydroxylamine
CHID: 25889 CASRN: 100-65-2
SPID(S): Tox21_202727
M4ID: 12479525

HILL MODEL (in red):

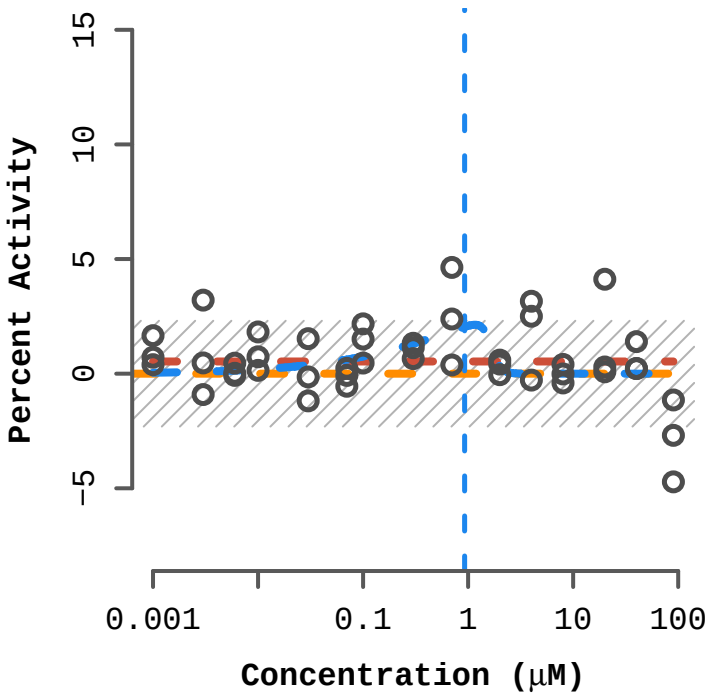
	tp	ga	gw
val:	3.98	1.48	4.64
sd:	0.528	0.0641	1.6

GAIN-LOSS MODEL (in blue):

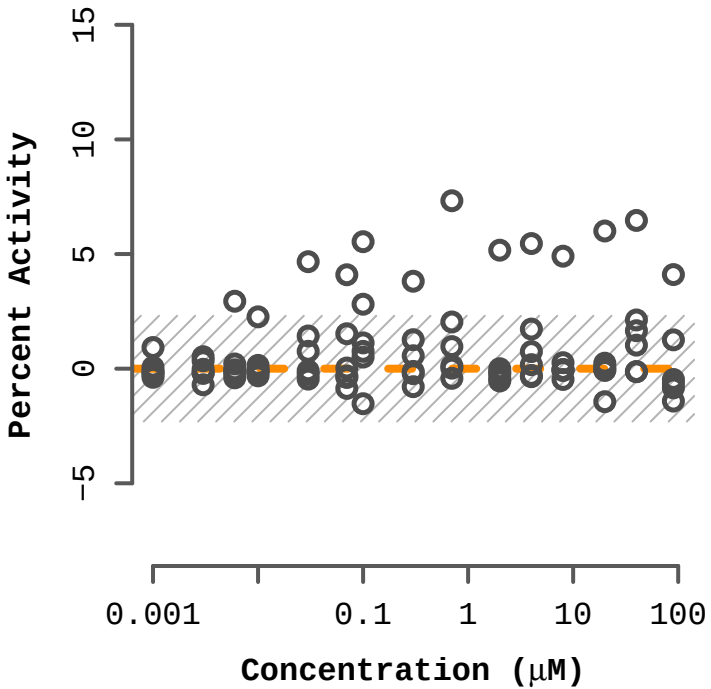
	tp	ga	gw	la	lw
val:	3.98	1.48	4.64	3.9	4.58
sd:	0.528	0.0641	1.6	14700	35600

	CNST	HILL	GNLS
AIC:	168.11	130.63	134.63
PROB:	0	0.88	0.12
RMSE:	1.61	0.98	0.98

MAX_MEAN: 3.81 MAX_MED: 4.33 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Phenyl-1-naphthylamine
CHID:    25892   CASRN: 90-30-2
SPID(S): Tox21_303075
M4ID:    12476058

HILL MODEL (in red):
      tp       ga       gw
val:  0.531    -5       3.38
sd:   0.183    1170     1980

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.09     -0.0333  0.672    0.217    9.86
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  171.09      168.97      169.9
PROB: 0.18        0.51        0.32
RMSE: 1.69        1.58        1.52

MAX_MEAN: 2.47      MAX_MED: 2.51      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

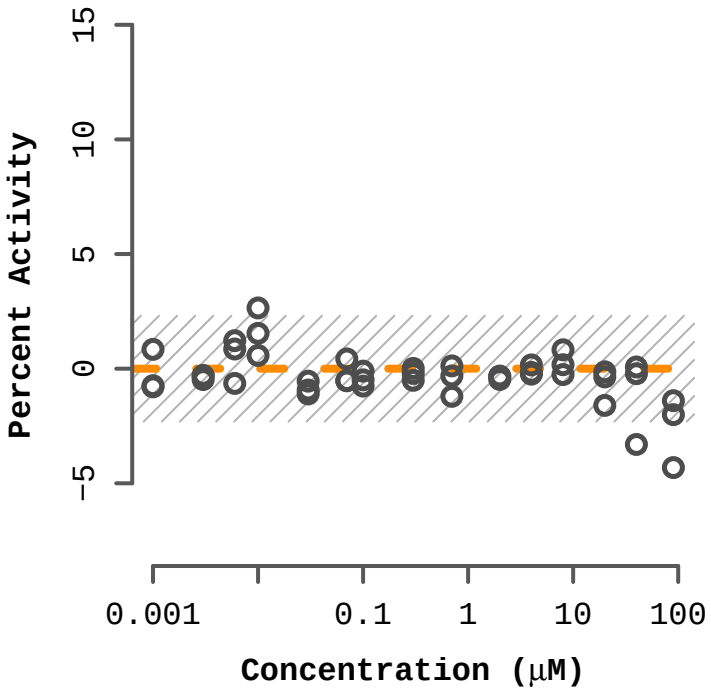
NAME: N-Phenyl-1-naphthylamine
CHID: 25892 CASRN: 90-30-2
SPID(S): Tox21_202073
M4ID: 12480179

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	347.4	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 1.84 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

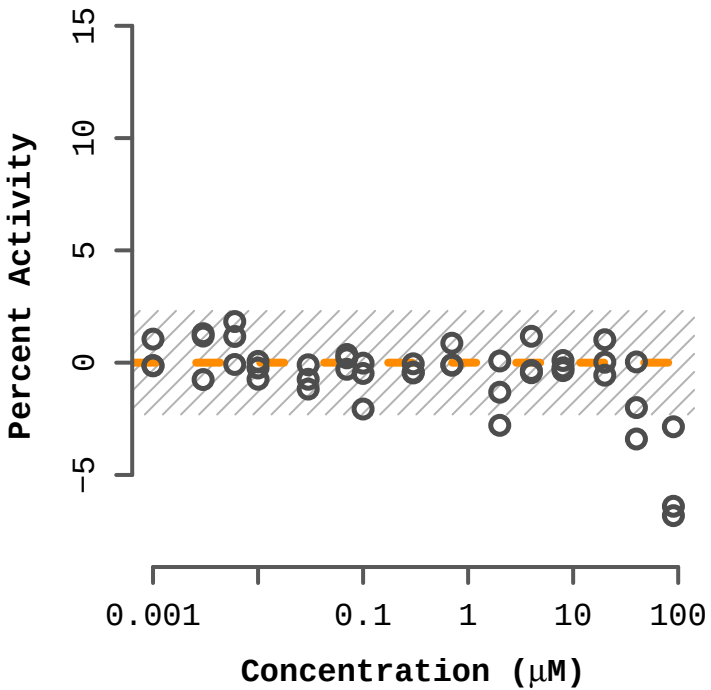
NAME: N-Phenyl-1,4-benzenediamine
CHID: 25895 **CASRN:** 101-54-2
SPID(S): Tox21_300027
M4ID: 12479103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

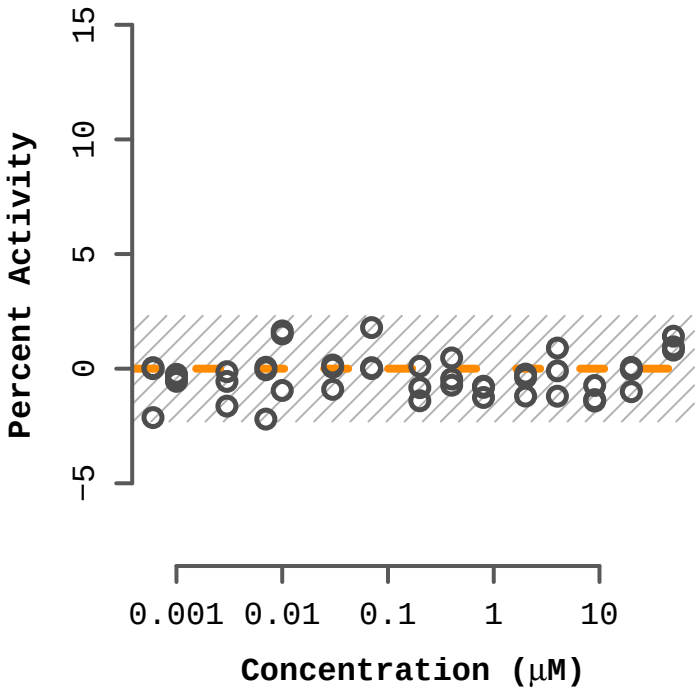
NAME: N-Phenyl-1,4-benzenediamine
CHID: 25895 **CASRN:** 101-54-2
SPID(S): Tox21_202144
M4ID: 12480108

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 0.974 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

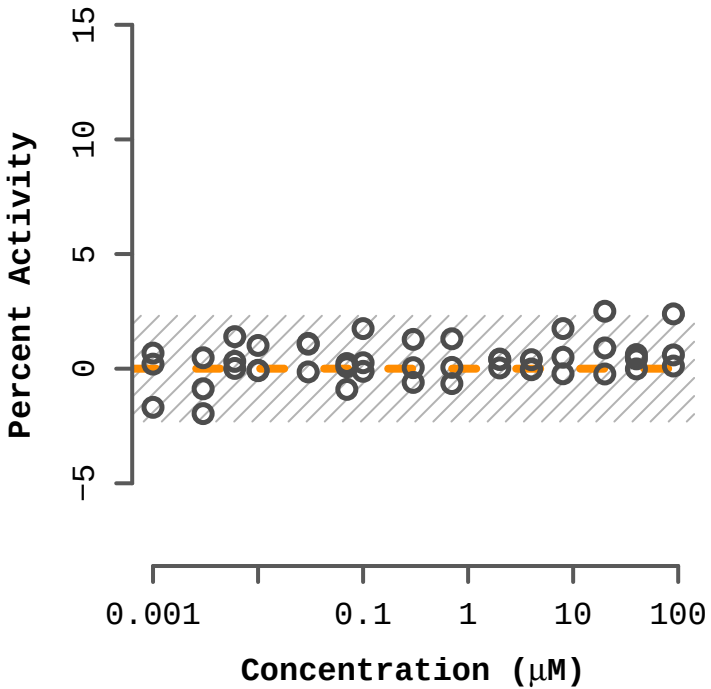
NAME: Phenylpropanolamine hydrochloride
CHID: 25896 **CASRN:** 154-41-6
SPID(S): Tox21_110431_1
M4ID: 12484363

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

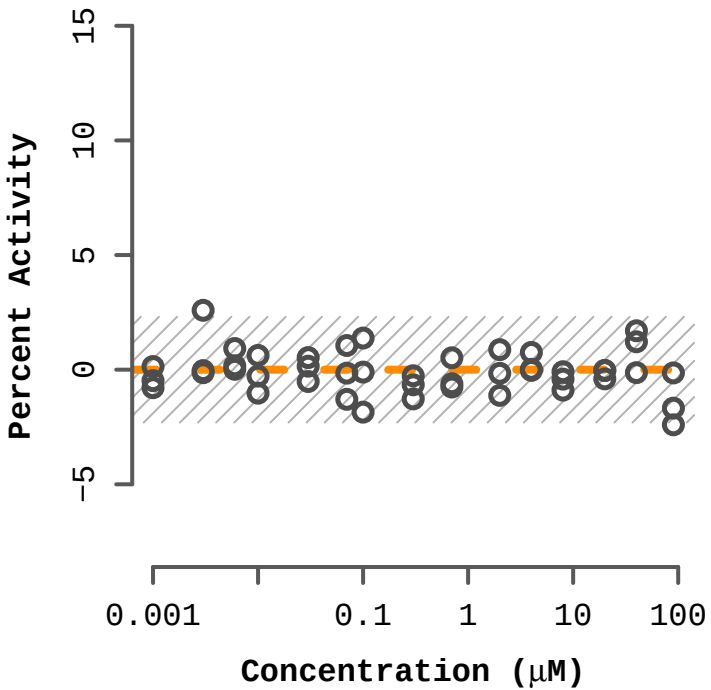
NAME: 1(2H)−Phthalazinone
CHID: 25903 **CASRN:** 119−39−1
SPID(S): Tox21_200287
M4ID: 12481965

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

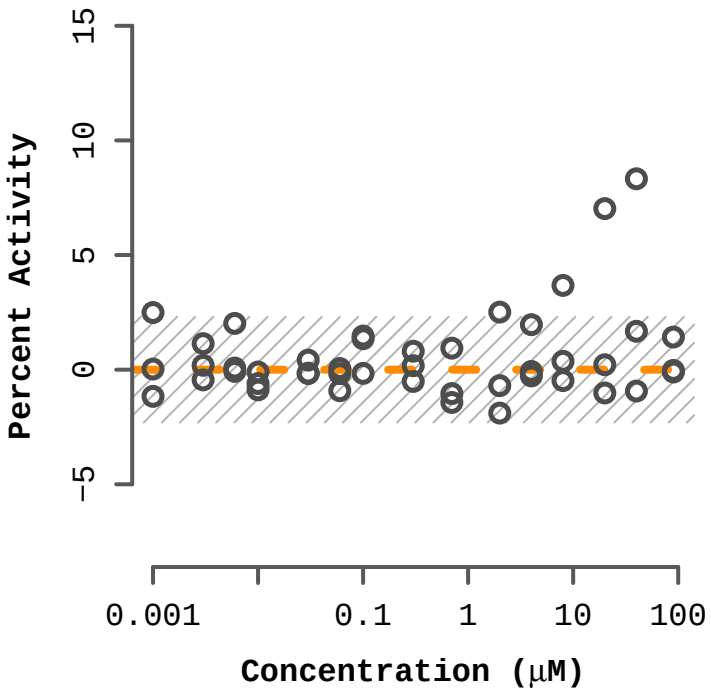
NAME: Pinane
CHID: 25922 **CASRN:** 473-55-2
SPID(S): Tox21_303280
M4ID: 12475853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

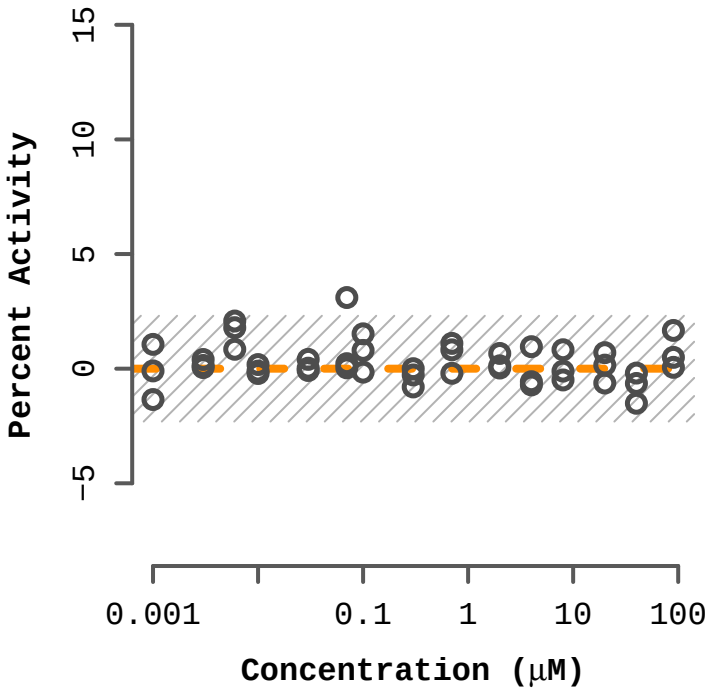
NAME: Pinane
CHID: 25922 **CASRN:** 473-55-2
SPID(S): Tox21_202039
M4ID: 12480213

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 3.02 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

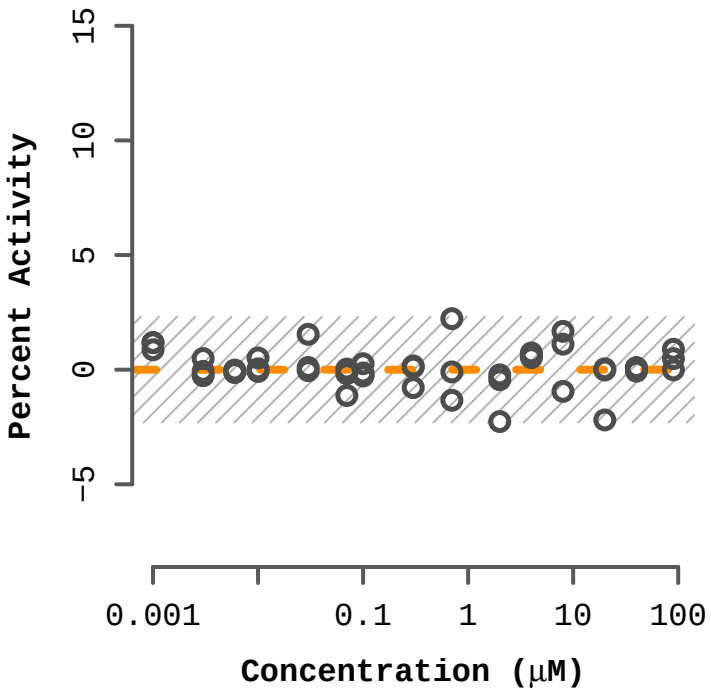
NAME: Piperonal
CHID: 25924 **CASRN:** 120-57-0
SPID(S): Tox21_200120
M4ID: 12482132

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

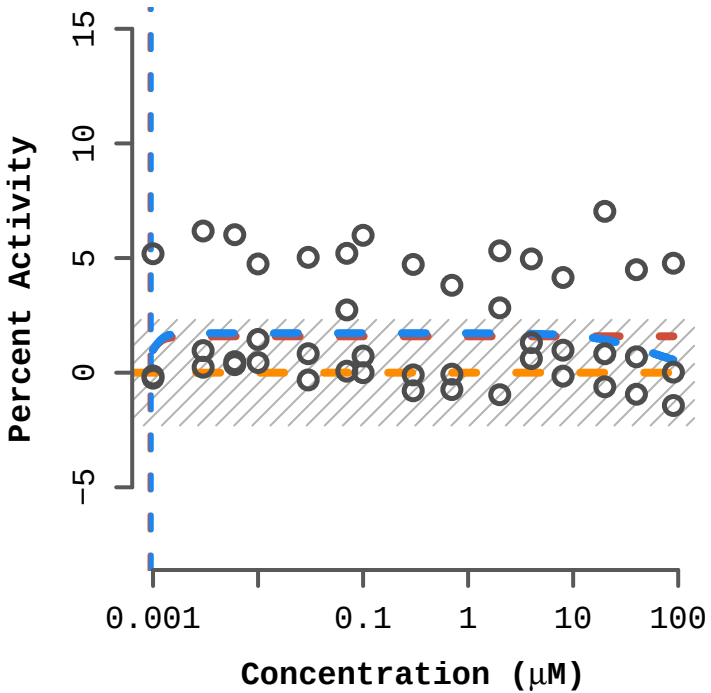
NAME: Piperonyl acetate
CHID: 25925 **CASRN:** 326-61-4
SPID(S): Tox21_303086
M4ID: 12476047

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piperonyl acetate
CHID: 25925 CASRN: 326-61-4
SPID(S): Tox21_201683
M4ID: 12480569

HILL MODEL (in red):

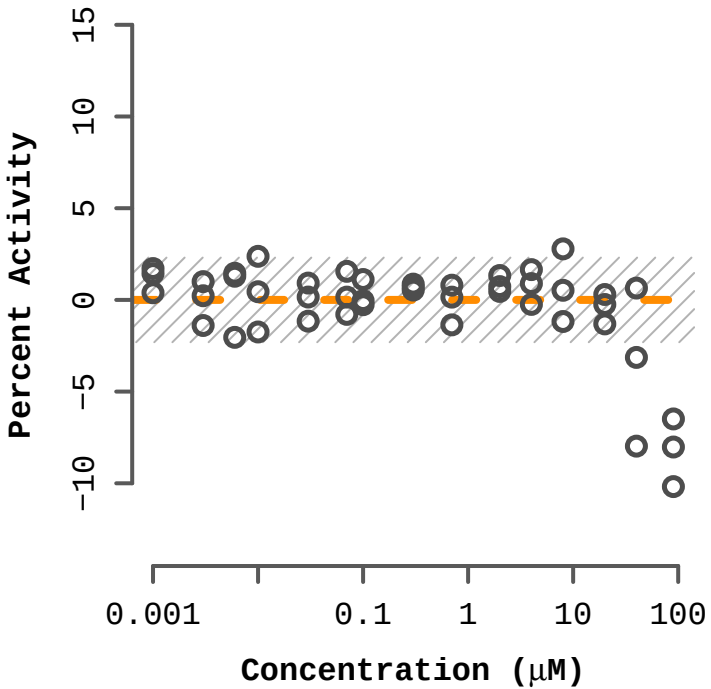
	tp	ga	gw
val:	1.59	−3.03	7.98
sd:	0.428	0.438	119

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.72	−3.02	7.64	1.75	1.56
sd:	0.498	0.372	162	0.784	3.91

	CNST	HILL	GNLS
AIC:	232.85	223.55	227
PROB:	0.01	0.84	0.15
RMSE:	3.13	2.5	2.49

MAX_MEAN: 2.67 **MAX_MED:** 2.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

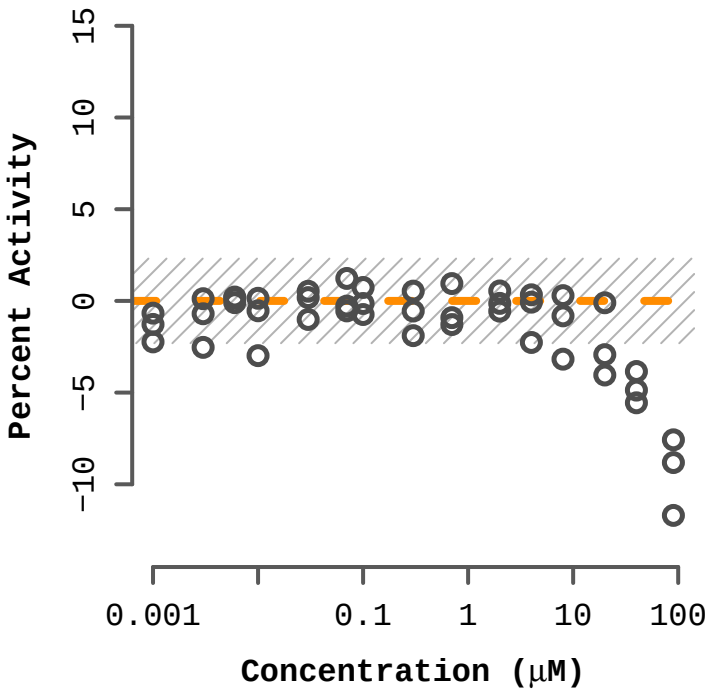
NAME: Piperonal acetone
CHID: 25926 **CASRN:** 3160-37-0
SPID(S): Tox21_202464
M4ID: 12479788

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

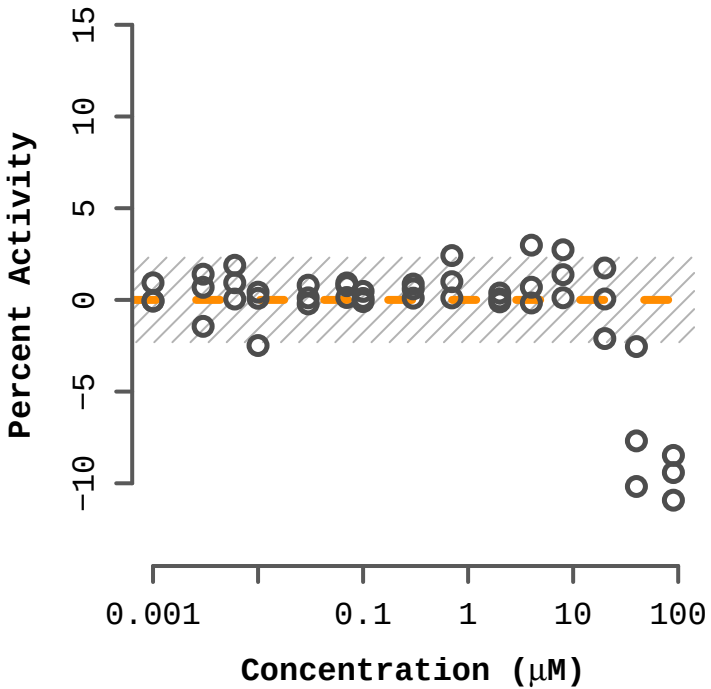
NAME: Pindone
CHID: 25930 **CASRN:** 83-26-1
SPID(S): Tox21_303317
M4ID: 12475816

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.73	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 0.134 **MAX_MED:** 0.181 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

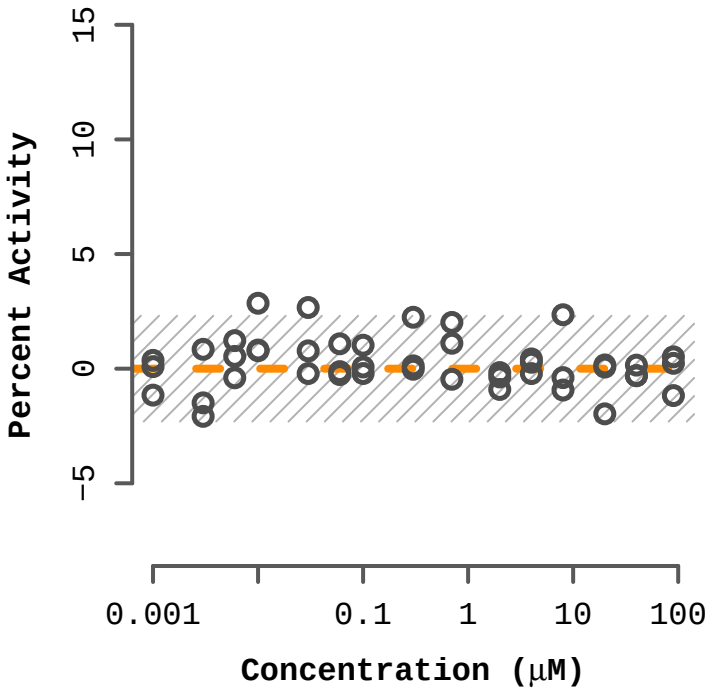
NAME: Pindone
CHID: 25930 **CASRN:** 83-26-1
SPID(S): Tox21_201353
M4ID: 12480899

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.34	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

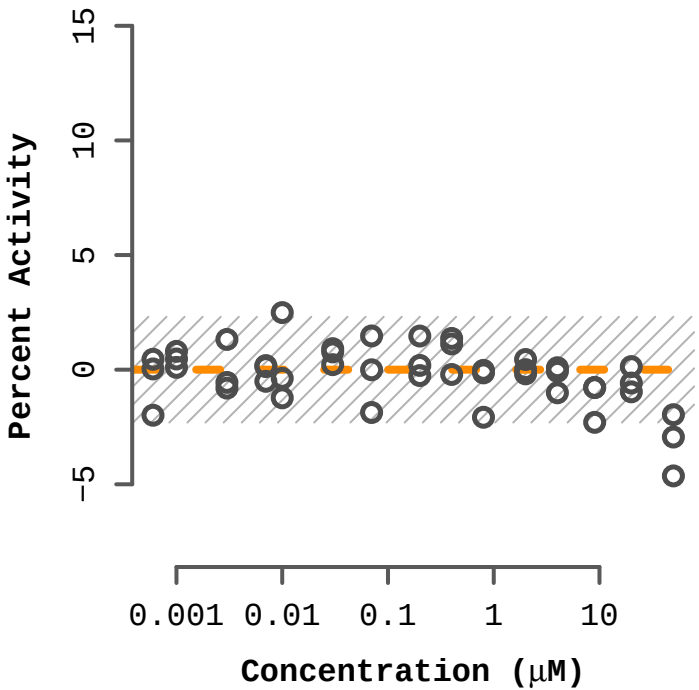
NAME: Poly(2-hydroxypropyl methacrylate)
CHID: 25934 **CASRN:** 25703-79-1
SPID(S): Tox21_202531
M4ID: 12479721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

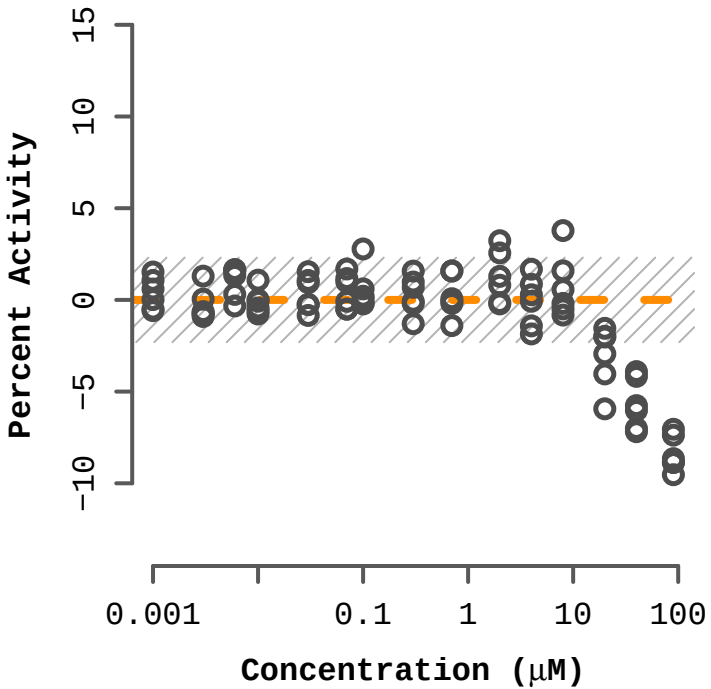
NAME: Polythiazide
CHID: 25939 **CASRN:** 346-18-9
SPID(S): Tox21_113137_1
M4ID: 12482792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.76 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

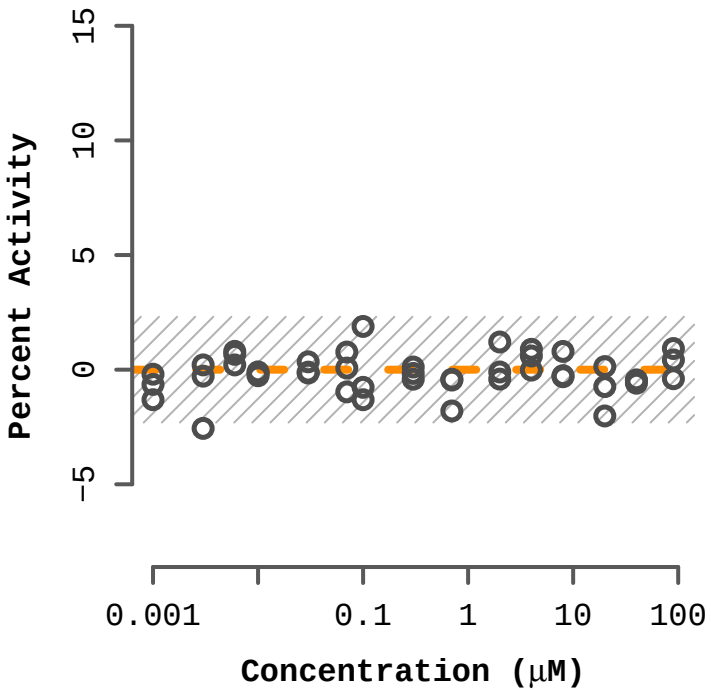
NAME: Potassium dichromate
CHID: 25948 **CASRN:** 7778-50-9
SPID(S): Tox21_202307
M4ID: 12479945

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	426.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.98	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

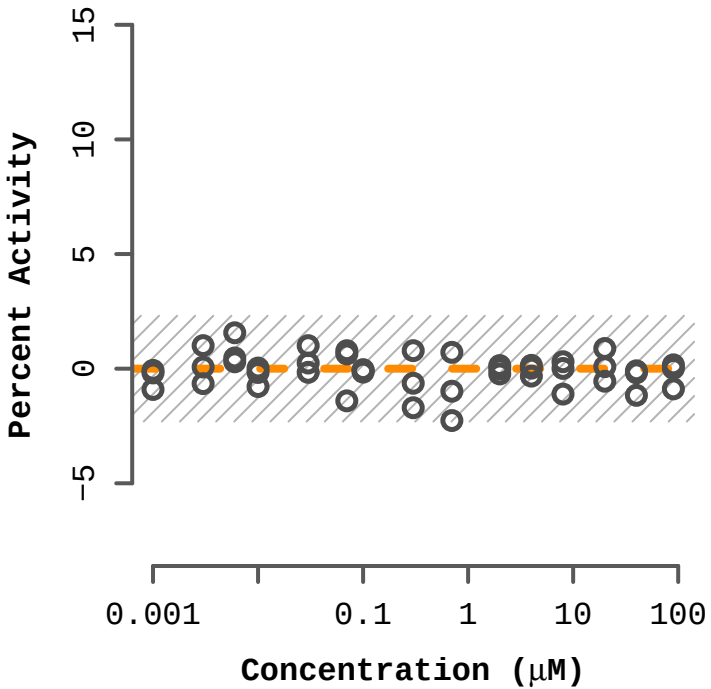
NAME: Propionic acid
CHID: 25961 CASRN: 79-09-4
SPID(S): Tox21_304030
M4ID: 12475158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.559 MAX_MED: 0.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

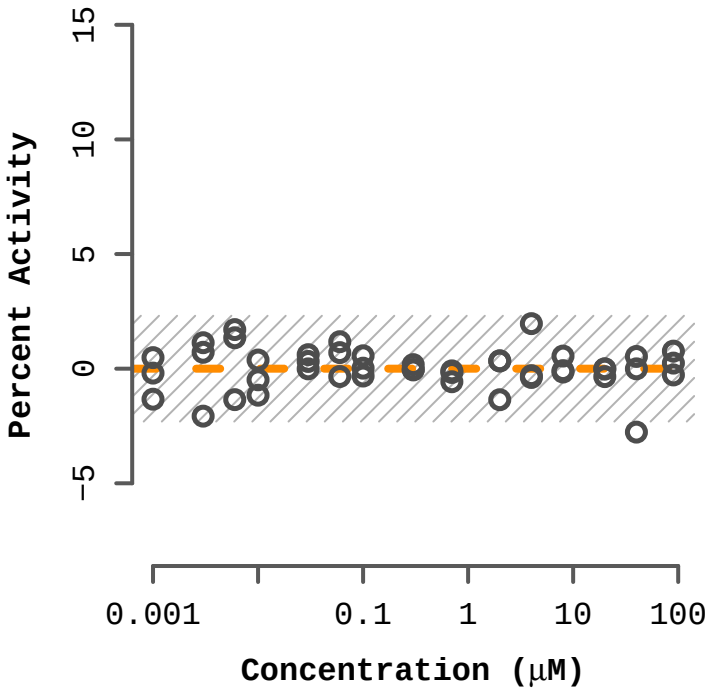
NAME: S−(Propyl) chlorothioformate
CHID: 25963 CASRN: 13889−92−4
SPID(S): Tox21_202532
M4ID: 12479720

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.779 **MAX_MED:** 0.645 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

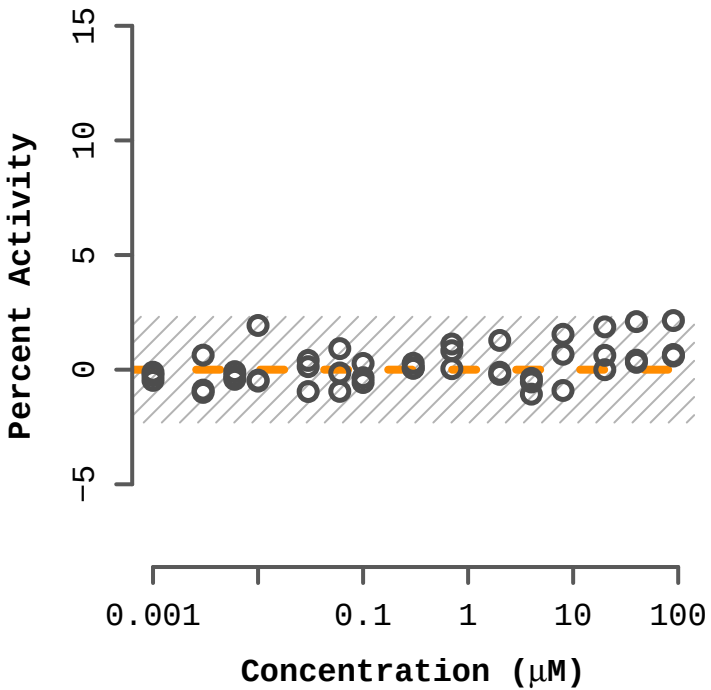
NAME: 1-tert-Butoxy-2-propanol
CHID: 25967 **CASRN:** 57018-52-7
SPID(S): Tox21_200655
M4ID: 12481597

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.569 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

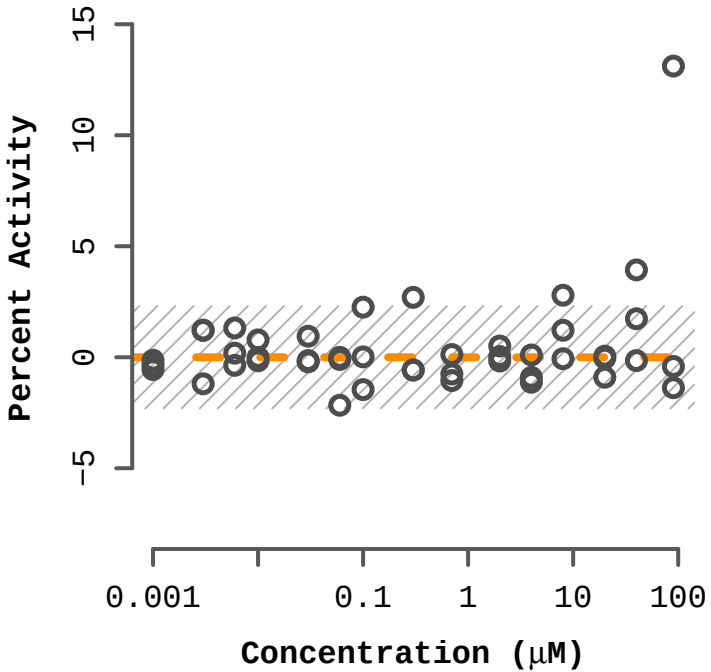
NAME: 1,3-Propylene oxide
CHID: 25969 **CASRN:** 503-30-0
SPID(S): Tox21_200739
M4ID: 12481513

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

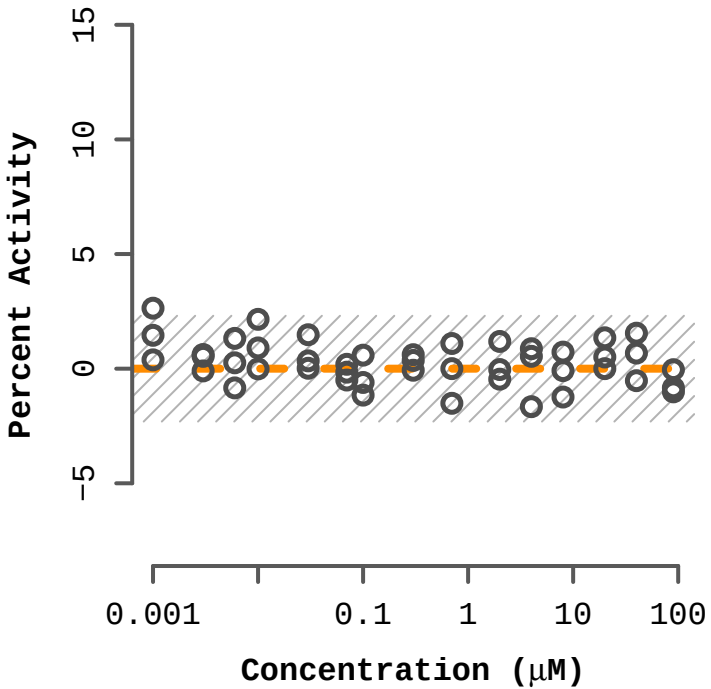
NAME: 3-Propylidenephthalide
CHID: 25972 **CASRN:** 17369-59-4
SPID(S): Tox21_201206
M4ID: 12481046

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 3.78 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

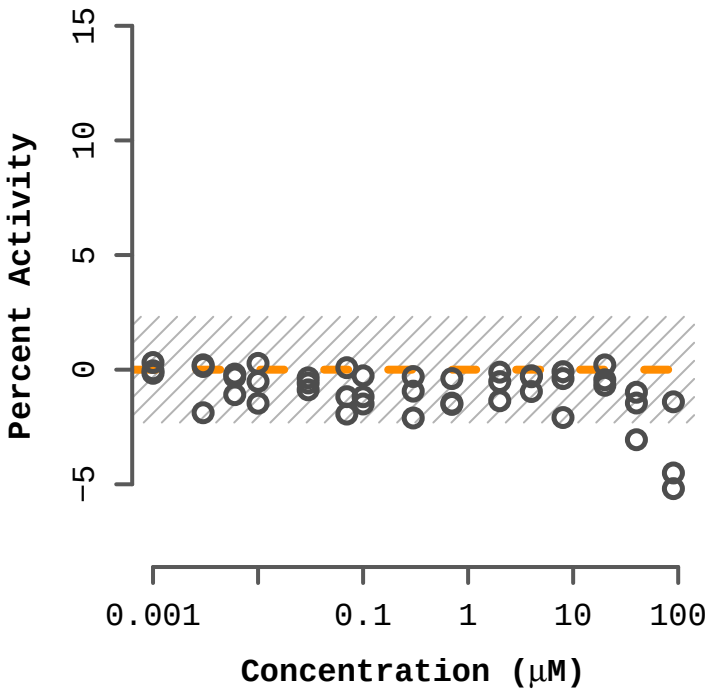
NAME: R−(+)−Pulegone
CHID: 25975 CASRN: 89−82−7
SPID(S): Tox21_200206
M4ID: 12482046

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.49 MAX_MED: 1.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

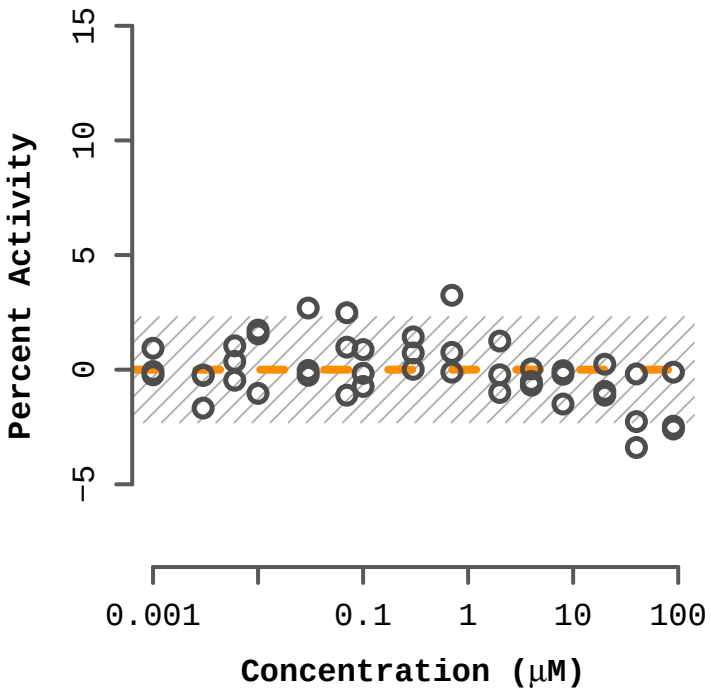
NAME: Pyrazineethanethiol
CHID: 25977 **CASRN:** 35250-53-4
SPID(S): Tox21_302691
M4ID: 12476442

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.0365 **MAX_MED:** 0.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

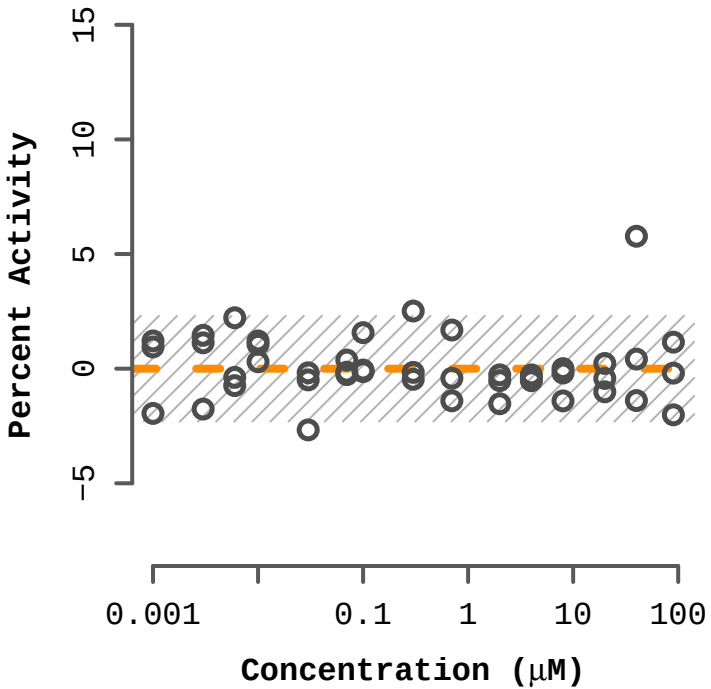
NAME: Pyrogallol
CHID: 25983 **CASRN:** 87-66-1
SPID(S): Tox21_202373
M4ID: 12479879

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

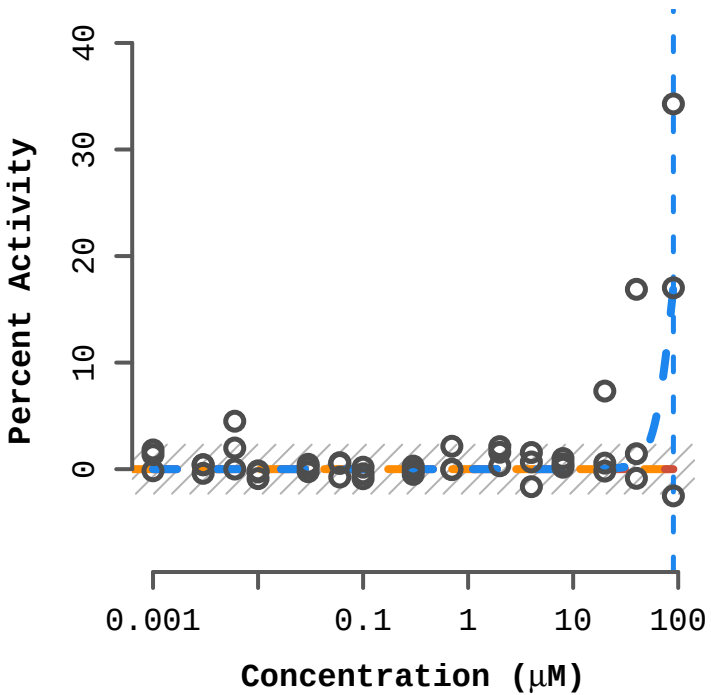
NAME: 4-Nitrosophenol
CHID: 25991 **CASRN:** 104-91-6
SPID(S): Tox21_303059
M4ID: 12476074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitrosophenol
CHID: 25991 CASRN: 104-91-6
SPID(S): Tox21_201754
M4ID: 12480498

HILL MODEL (in red):

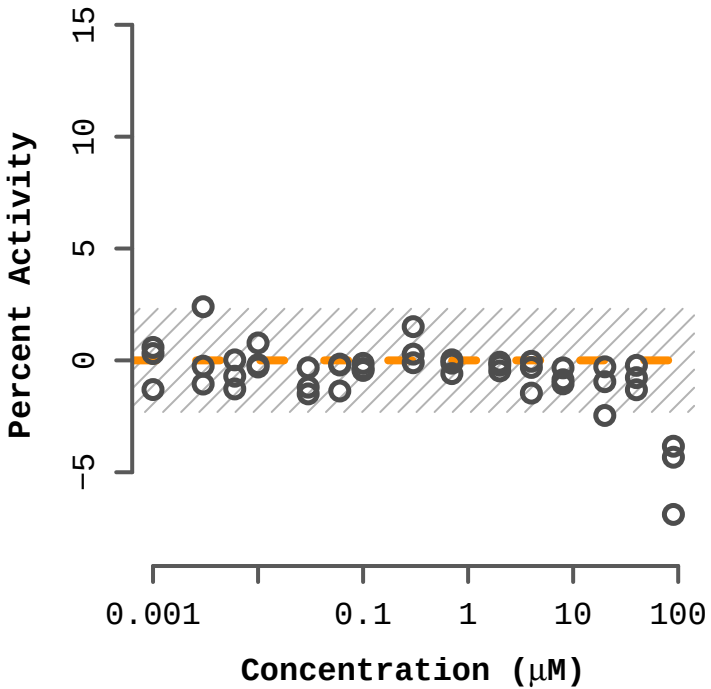
	tp	ga	gw
val:	0.12	2.45	7.99
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	34.1	1.95	4.75	3.82	3.43
sd:	3.22	0.0191	1.99	3840	7270

	CNST	HILL	GNLS
AIC:	220.55	226.55	221.13
PROB:	0.56	0.03	0.42
RMSE:	6.44	6.44	4.83

MAX_MEAN: 16.3 MAX_MED: 17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

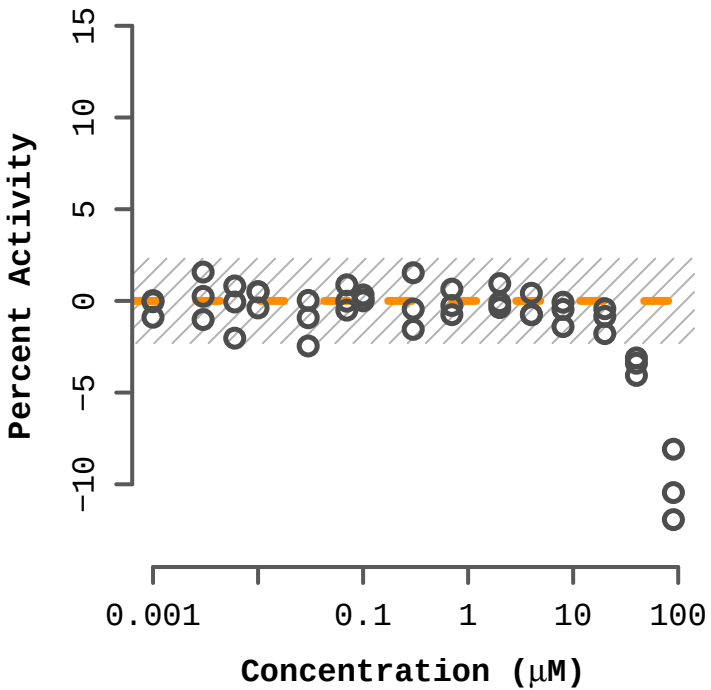
NAME: 13-cis-Retinal
CHID: 25997 **CASRN:** 472-86-6
SPID(S): Tox21_201076
M4ID: 12481176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 0.563 **MAX_MED:** 0.307 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

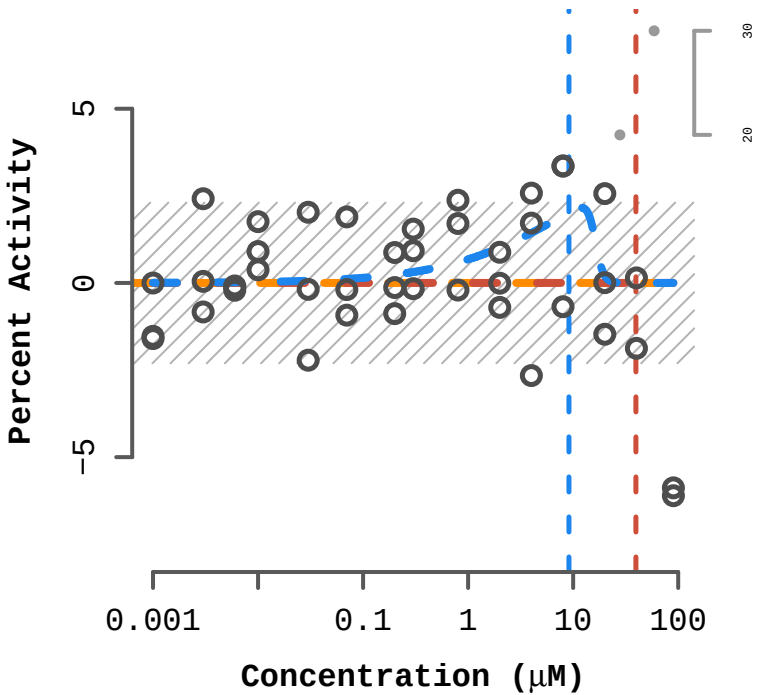
NAME: Retinal
CHID: 25998 **CASRN:** 116-31-4
SPID(S): Tox21_201005
M4ID: 12481247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 0.269 **MAX_MED:** 0.497 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Rhein
CHID: 26000 CASRN: 478-43-3
SPID(S): Tox21_201098
M4ID: 12481154 BRK

HILL MODEL (in red):

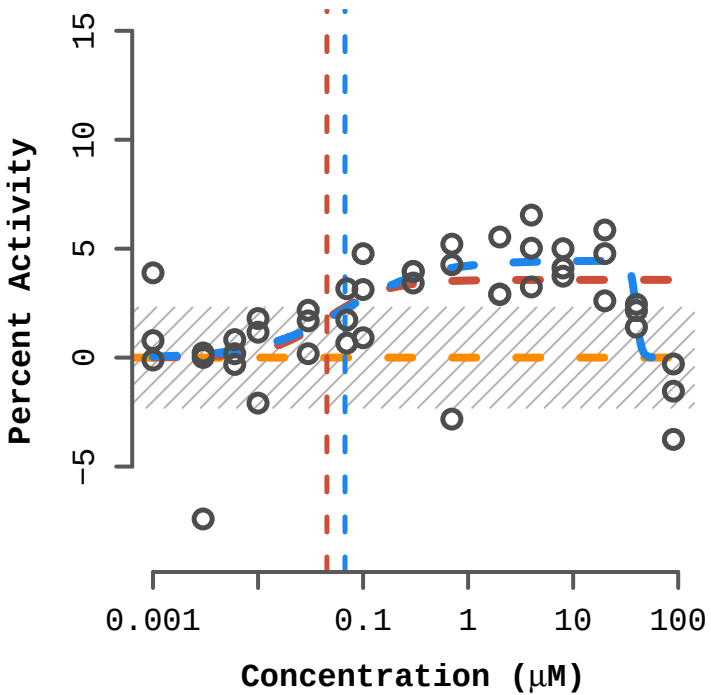
	tp	ga	gw
val:	1.36e-09	1.6	1.76
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

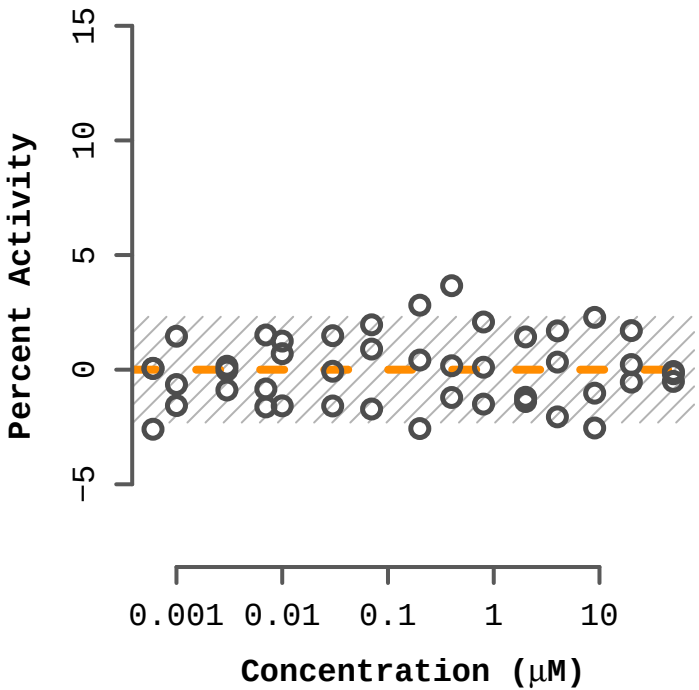
	tp	ga	gw	la	lw
val:	4.05	0.96	0.726	1.21	11.6
sd:	13.6	2.86	0.904	0.657	78.7

	CNST	HILL	GNLS
AIC:	225.78	231.78	231.26
PROB:	0.9	0.04	0.06
RMSE:	5.76	5.76	5.74

MAX_MEAN: 6.14 MAX_MED: 3.35 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Silybin
CHID:    26018   CASRN: 22888-70-6
SPID(S): Tox21_200755
M4ID:    12481497

HILL MODEL (in red):
      tp       ga       gw
val:  3.57     -1.34    1.54
sd:   0.419    0.233    0.921

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.45     -1.17    1.07     1.6      17
sd:   0.44     0.194    0.459    0.0199   66.4

      CNST        HILL        GNLS
AIC:  243.77      205.97      185.01
PROB: 0           0           1
RMSE: 3.35        2.44        2

MAX_MEAN: 4.94      MAX_MED: 5.02      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

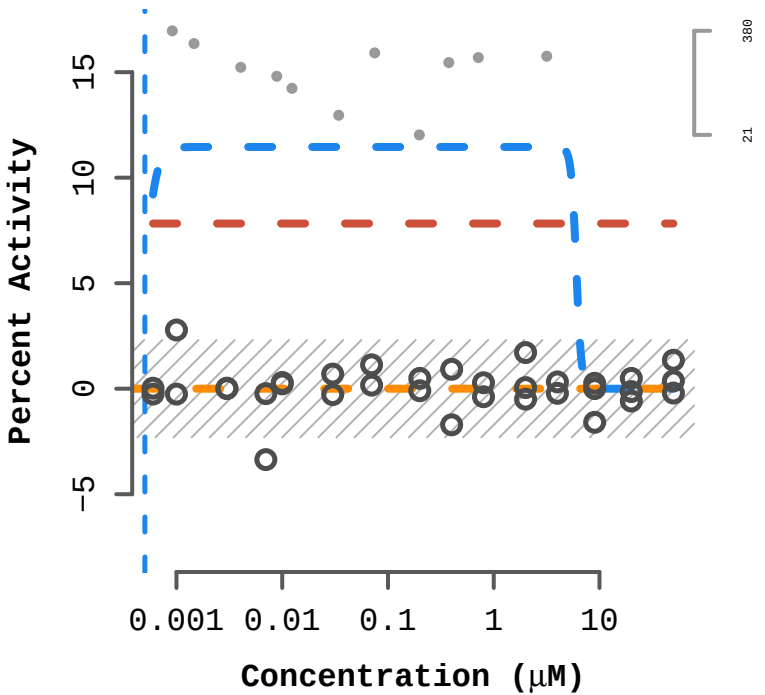
NAME: Silybin
CHID: 26018 CASRN: 22888-70-6
SPID(S): Tox21_111070_1
M4ID: 12483923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 0.875 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium arsanilate
CHID: 26022 CASRN: 127-85-5
SPID(S): Tox21_202893
M4ID: 12479359 BRK

HILL MODEL (in red):

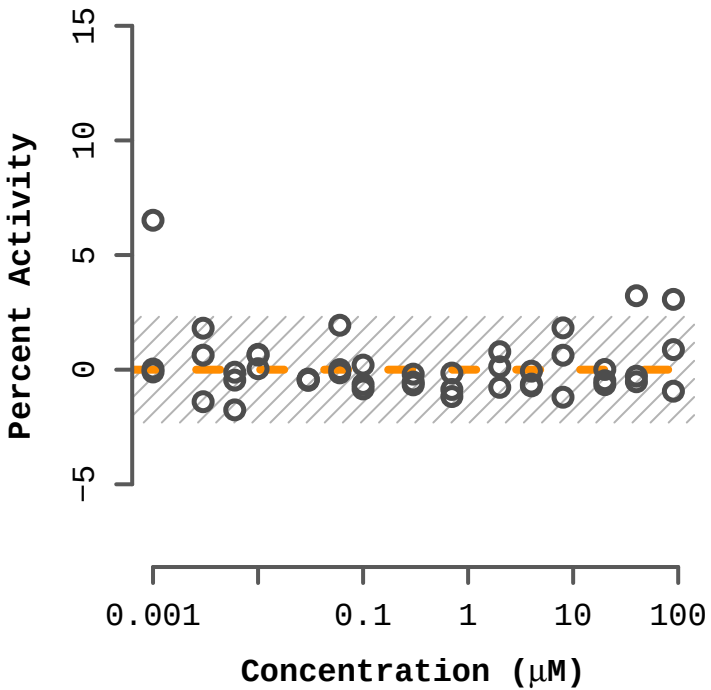
	tp	ga	gw
val:	7.83	−5.17	3
sd:	7.53	2550	3680

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.5	−3.3	7.92	0.781	18
sd:	9.98	8.26	820	6.72	687

	CNST	HILL	GNLS
AIC:	561.8	546.87	550.3
PROB:	0	0.85	0.15
RMSE:	129.67	126.3	124.91

MAX_MEAN: 127 **MAX_MED:** 2.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

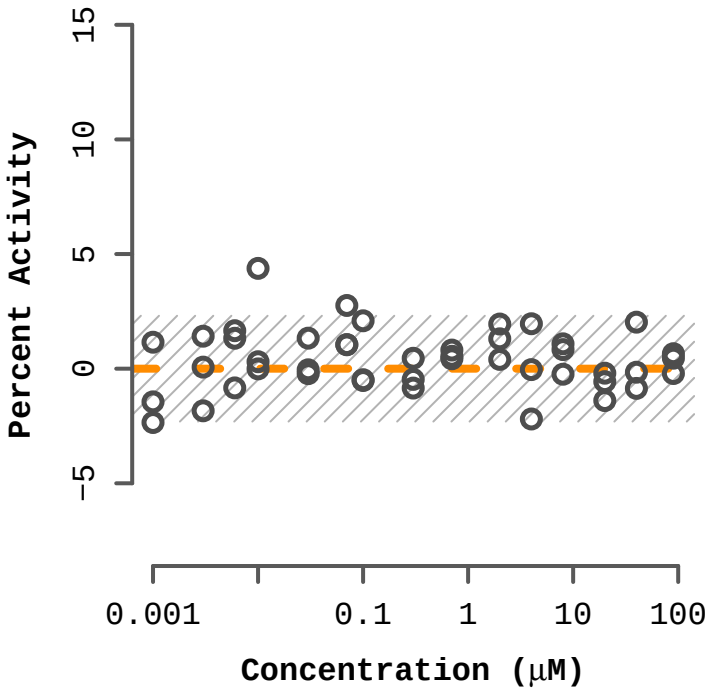
NAME: Sodium chlorate
CHID: 26025 **CASRN:** 7775-09-9
SPID(S): Tox21_202133
M4ID: 12480119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

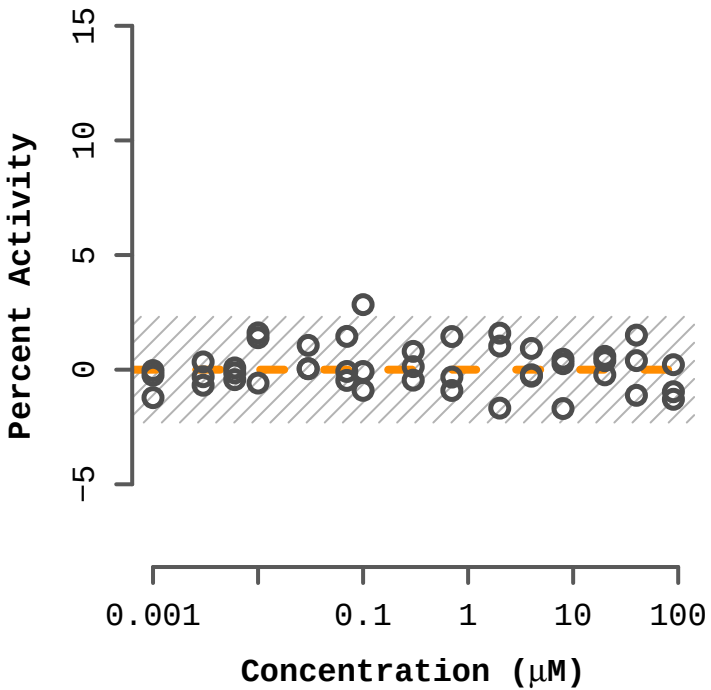
NAME: Sodium dehydroacetate
CHID: 26029 **CASRN:** 4418-26-2
SPID(S): Tox21_300075
M4ID: 12479055

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

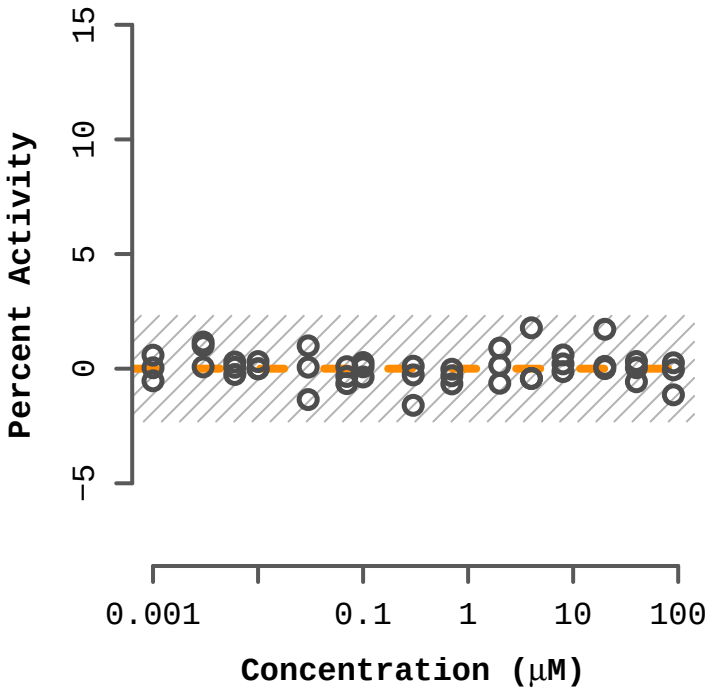
NAME: Sodium dodecyl sulfate
CHID: 26031 **CASRN:** 151-21-3
SPID(S): Tox21_300149
M4ID: 12478981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

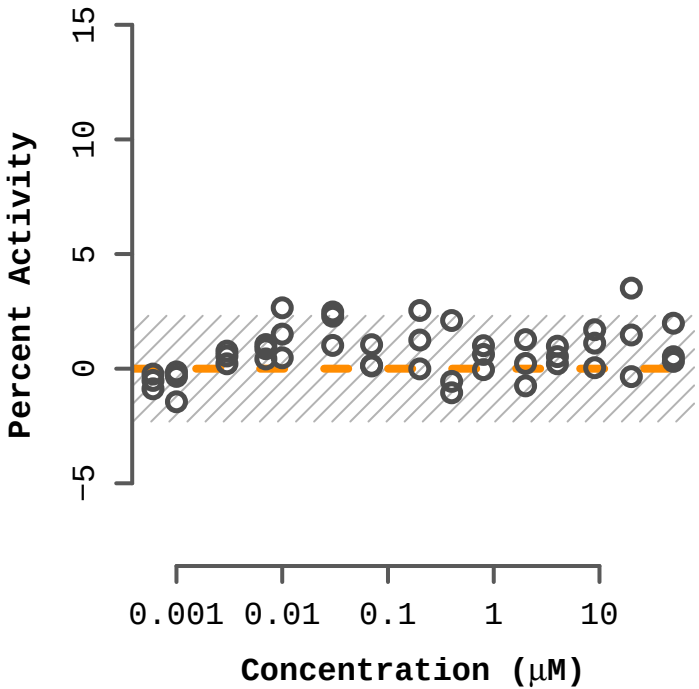
NAME: Sodium dodecyl sulfate
CHID: 26031 CASRN: 151-21-3
SPID(S): Tox21_201614
M4ID: 12480638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.751 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

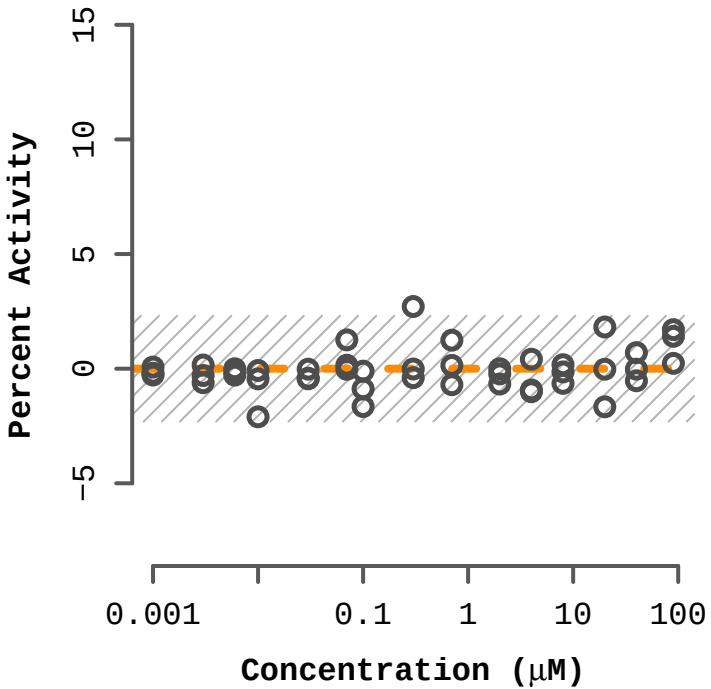
NAME: Sodium dodecyl sulfate
CHID: 26031 CASRN: 151-21-3
SPID(S): Tox21_111059_1
M4ID: 12483928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

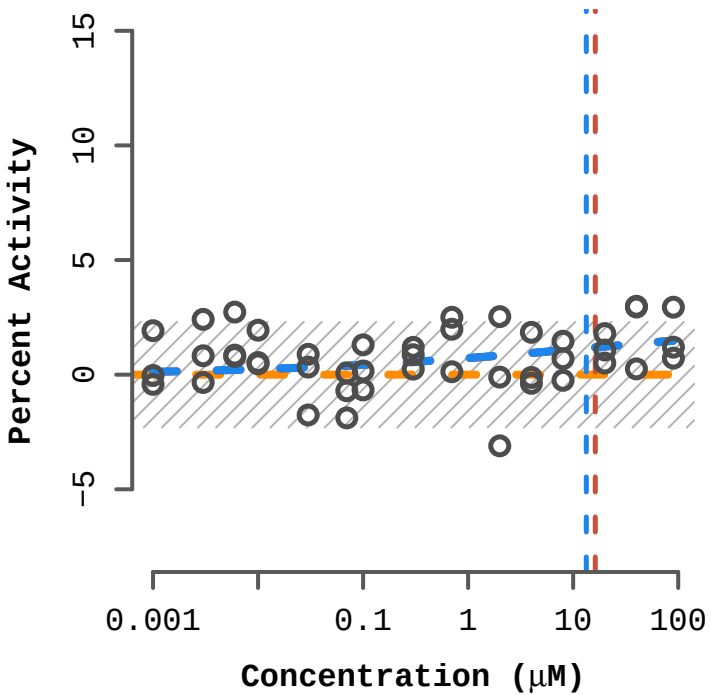
NAME: Sodium ethasulfate
CHID: 26033 **CASRN:** 126-92-1
SPID(S): Tox21_303207
M4ID: 12475926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium 2-mercaptobenzothiolate
CHID: 26035 CASRN: 2492-26-4
SPID(S): Tox21_301502
M4ID: 12477631

HILL MODEL (in red):

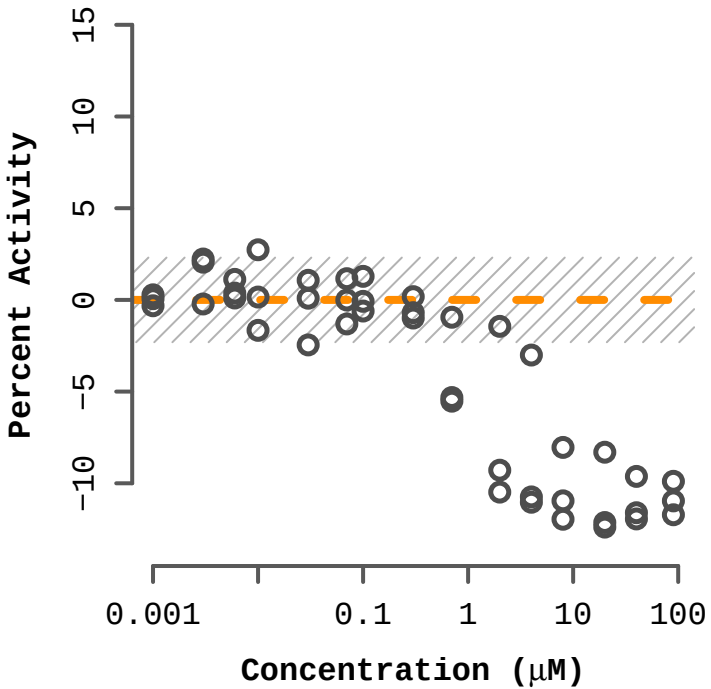
	tp	ga	gw
val:	2.38	1.21	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.31	1.13	0.3	3.33	4.82
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	169.05	158.9	162.9
PROB:	0.01	0.88	0.12
RMSE:	1.5	1.28	1.28

MAX_MEAN: 2.06 **MAX_MED:** 2.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

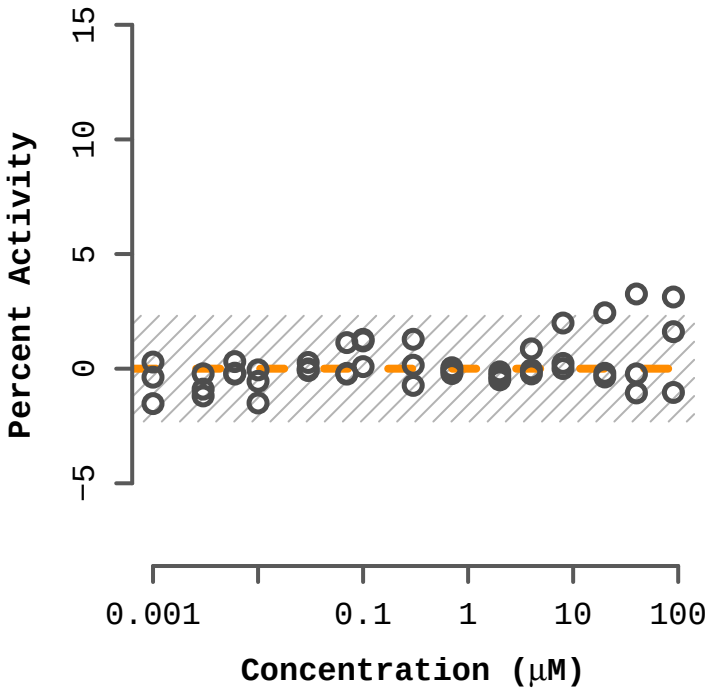
NAME: C.I. Solvent Black 5
CHID: 26040 **CASRN:** 11099-03-9
SPID(S): Tox21_202538
M4ID: 12479714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.86	NA	NA
PROB:	1	NA	NA
RMSE:	6.6	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

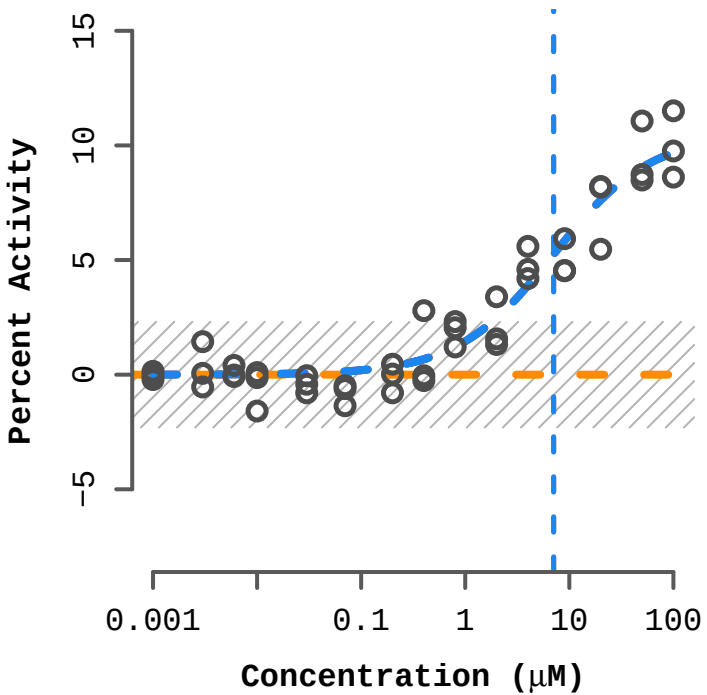
NAME: cis-Stilbene
CHID: 26049 **CASRN:** 645-49-8
SPID(S): Tox21_200350
M4ID: 12481902

HILL MODEL: Not applicable.

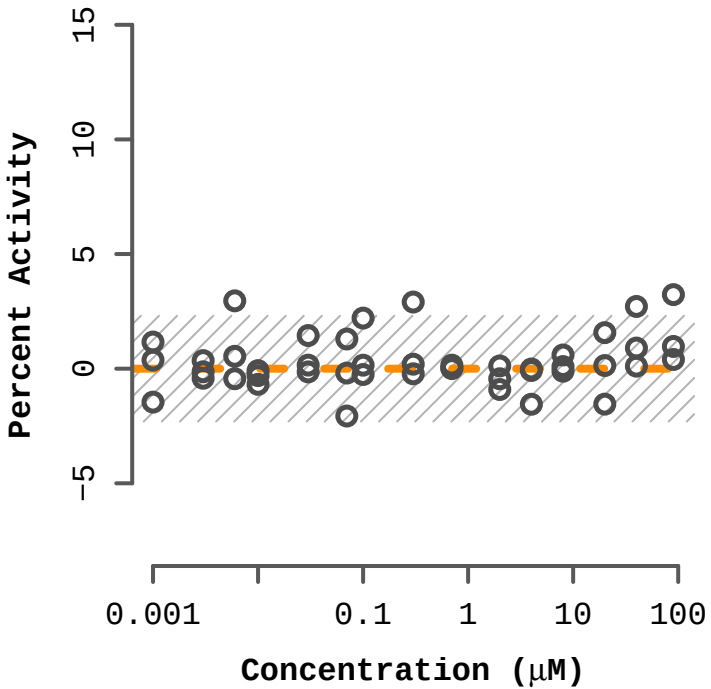
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.62 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    trans-Stilbene
CHID:    26050   CASRN: 103-30-0
SPID(S): Tox21_202726
M4ID:    12479526

HILL MODEL (in red):
      tp       ga       gw
val:  10.5     0.849    0.933
sd:   0.99     0.14     0.151

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.5     0.849    0.933    3.16     6.27
sd:   0.99     0.14     0.151    552      2980

      CNST        HILL        GNLS
AIC:  261.95      135.93      139.93
PROB: 0           0.88        0.12
RMSE: 4.54        0.97        0.97

MAX_MEAN: 9.96      MAX_MED: 9.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

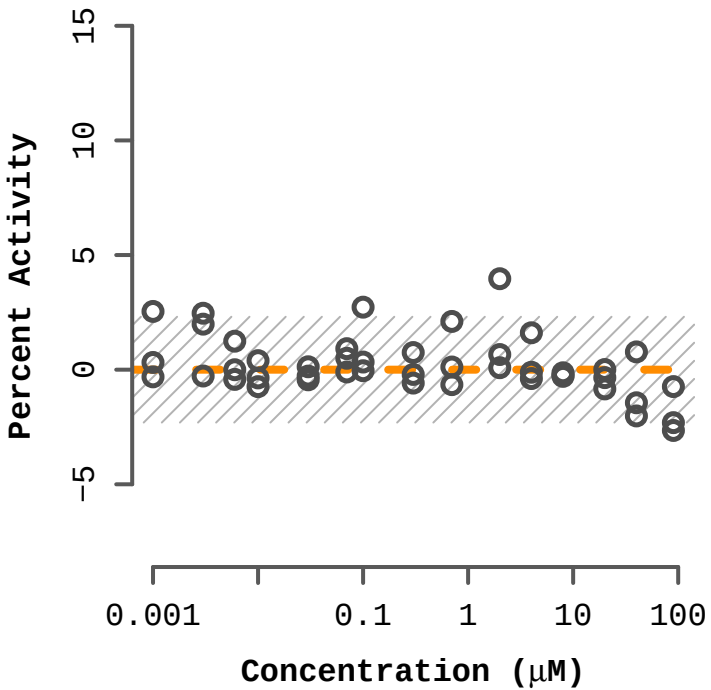
NAME: Stoddard solvent
CHID: 26051 **CASRN:** 8052-41-3
SPID(S): Tox21_202611
M4ID: 12479641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 0.971 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

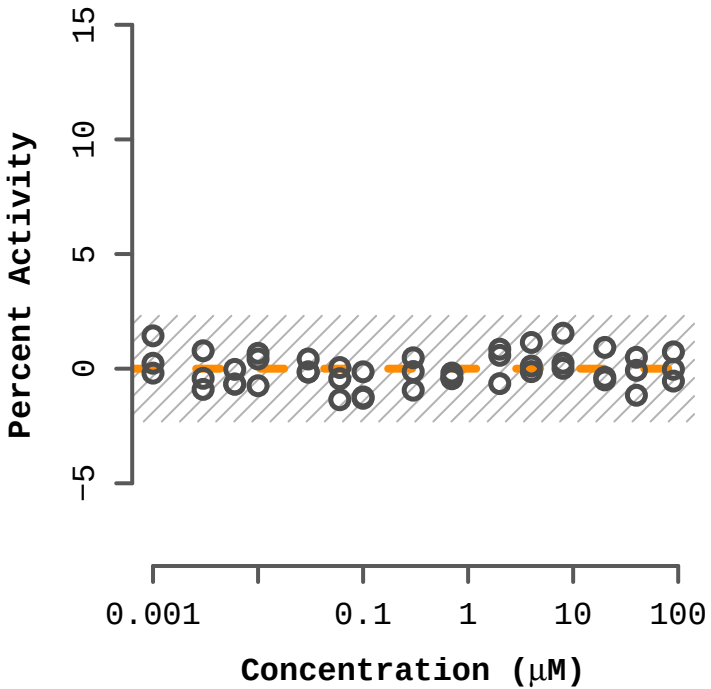
NAME: Styrax balsam
CHID: 26054 CASRN: 8046-19-3
SPID(S): Tox21_202539
M4ID: 12479713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.57 MAX_MED: 1.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

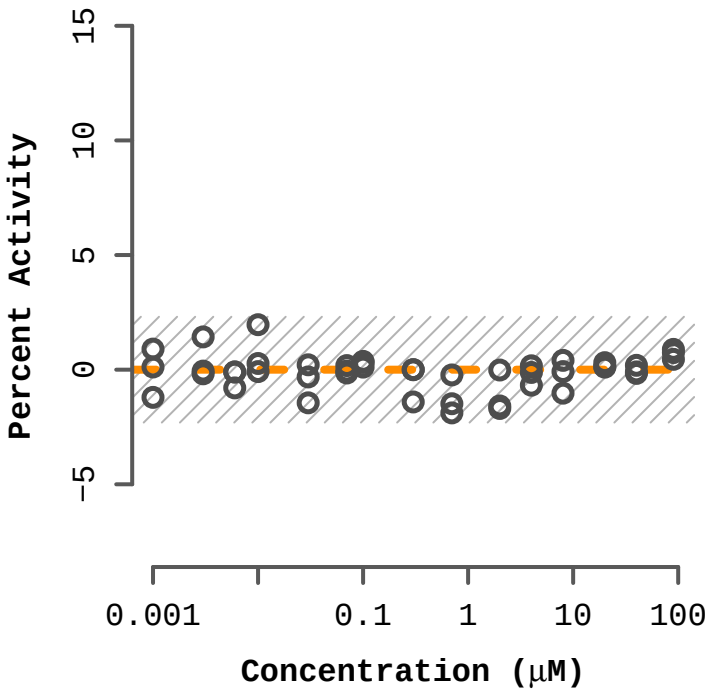
NAME: Succinonitrile
CHID: 26059 CASRN: 110-61-2
SPID(S): Tox21_200635
M4ID: 12481617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.602 MAX_MED: 0.583 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

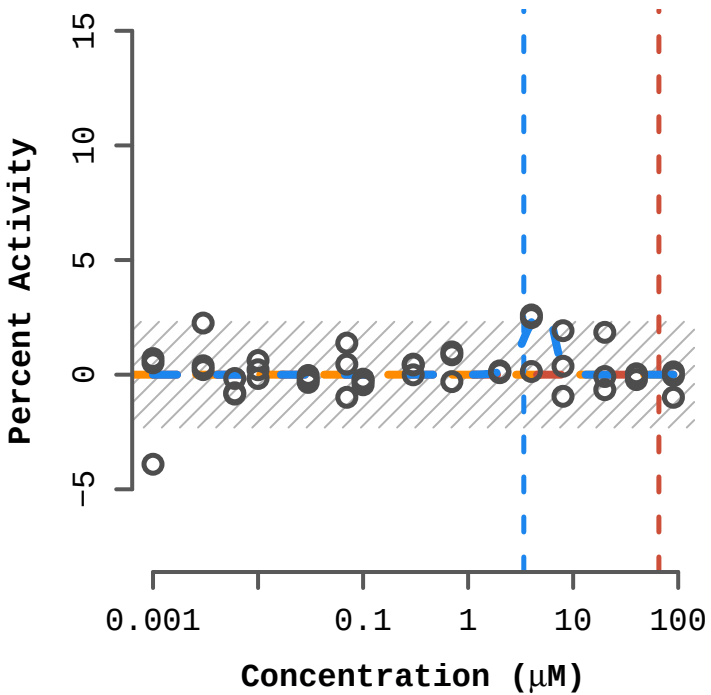
NAME: Sulfacetamide
CHID: 26060 **CASRN:** 144-80-9
SPID(S): Tox21_303100
M4ID: 12476033

HILL MODEL: Not applicable.

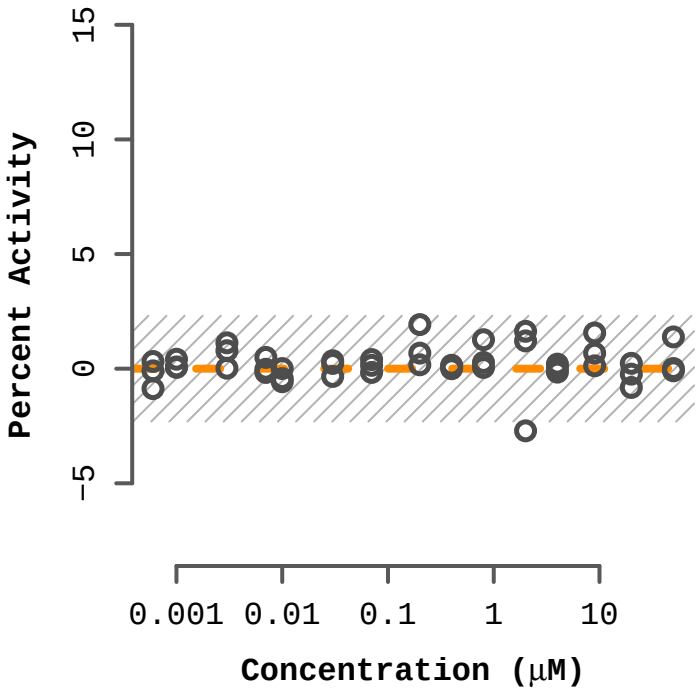
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.748 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Sulfacetamide
CHID:    26060   CASRN: 144-80-9
SPID(S): Tox21_201999
M4ID:    12480253

HILL MODEL (in red):
      tp        ga        gw
val:  4.04e-10  1.82      1.81
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.13      0.53      5.97      0.83      12.3
sd:   NaN       NaN       NaN       NaN       NaN

      CNST         HILL         GNLS
AIC:  124.06       130.06       124.45
PROB: 0.53         0.03         0.44
RMSE: 1.07         1.07         0.97

MAX_MEAN: 1.75      MAX_MED: 2.49      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

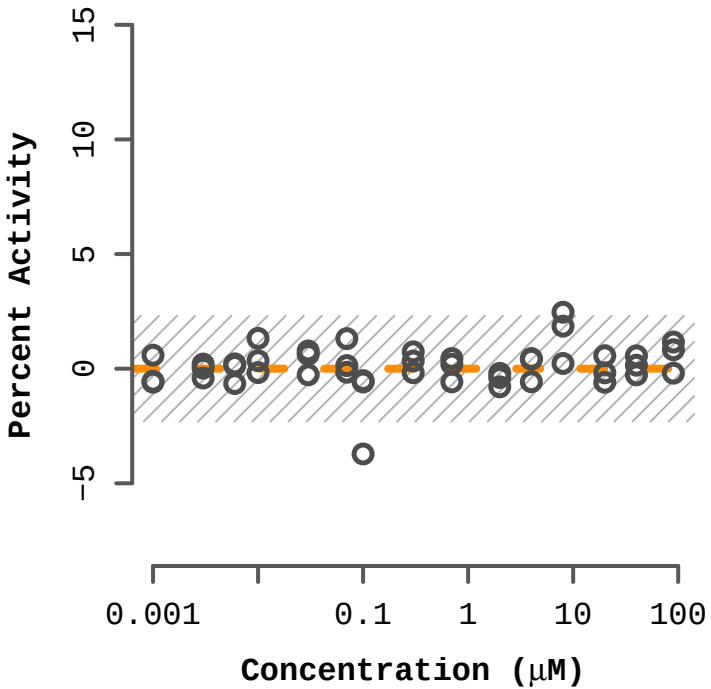
NAME: Sulfacetamide
CHID: 26060 **CASRN:** 144-80-9
SPID(S): Tox21_110846_1
M4ID: 12484073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.925 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

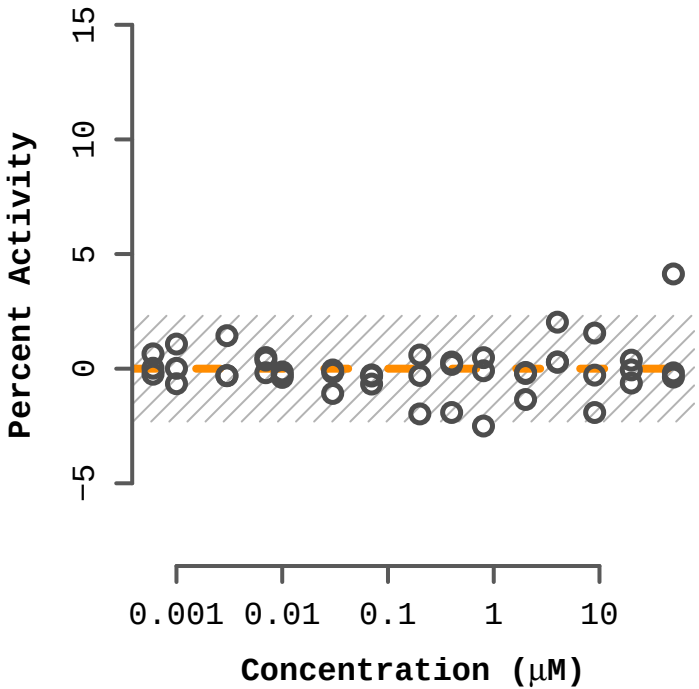
NAME: Sulfamethoxazole
CHID: 26064 **CASRN:** 723-46-6
SPID(S): Tox21_200353
M4ID: 12481899

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

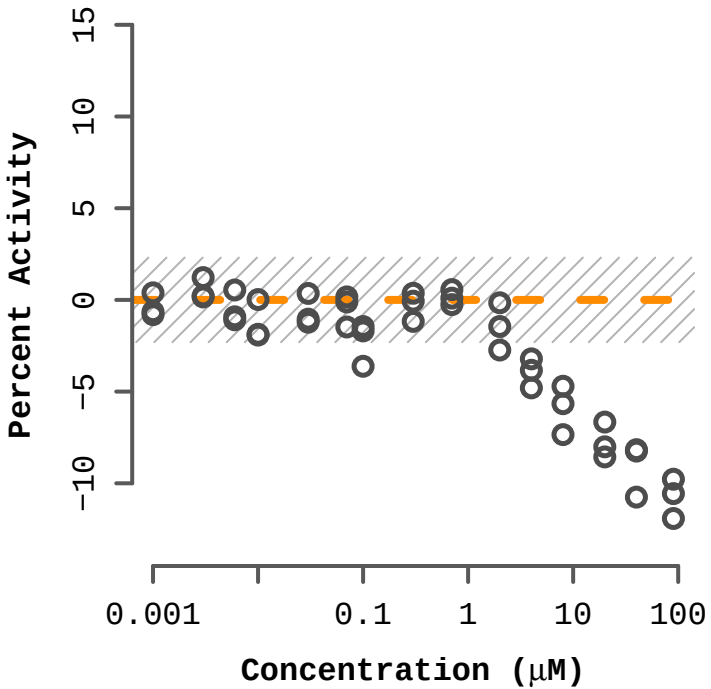
NAME: Sulfamethoxazole
CHID: 26064 **CASRN:** 723-46-6
SPID(S): Tox21_110480_1
M4ID: 12484323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.378 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

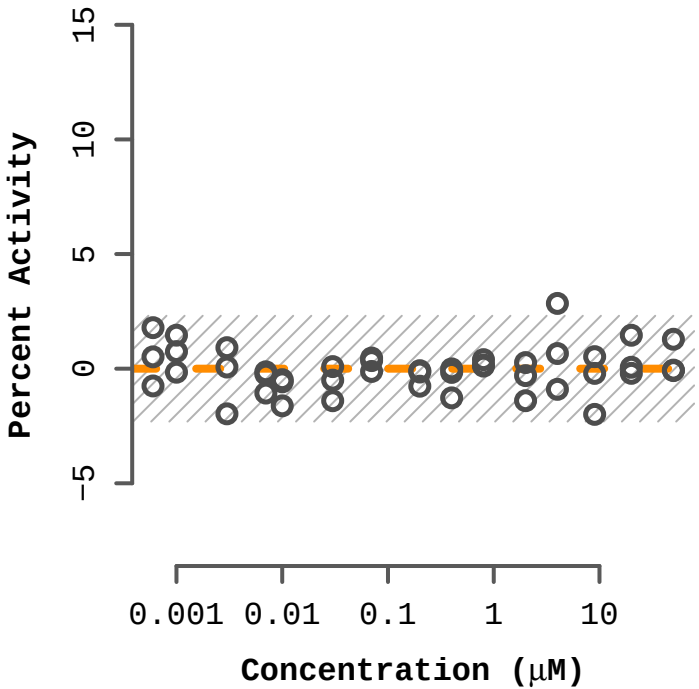
NAME: Sulfan blue
CHID: 26065 **CASRN:** 129-17-9
SPID(S): Tox21_302151
M4ID: 12476982

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.42	NA	NA
PROB:	1	NA	NA
RMSE:	4.68	NA	NA

MAX_MEAN: 0.535 **MAX_MED:** 0.221 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

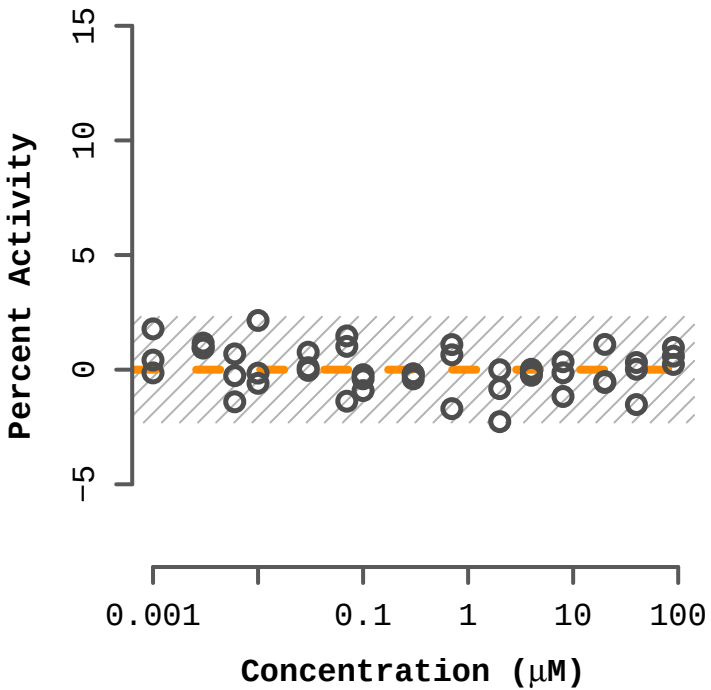
NAME: Sulfapyridine
CHID: 26067 **CASRN:** 144-83-2
SPID(S): Tox21_110426_1
M4ID: 12484368

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.87 **MAX_MED:** 0.747 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

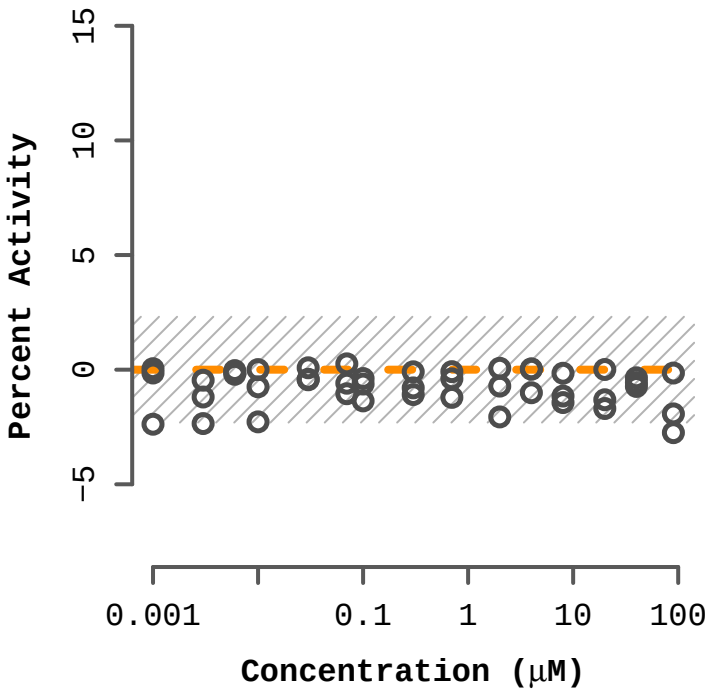
NAME: Sulfathiazole
CHID: 26068 CASRN: 72-14-0
SPID(S): Tox21_303238
M4ID: 12475895

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.02 MAX_MED: 1.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

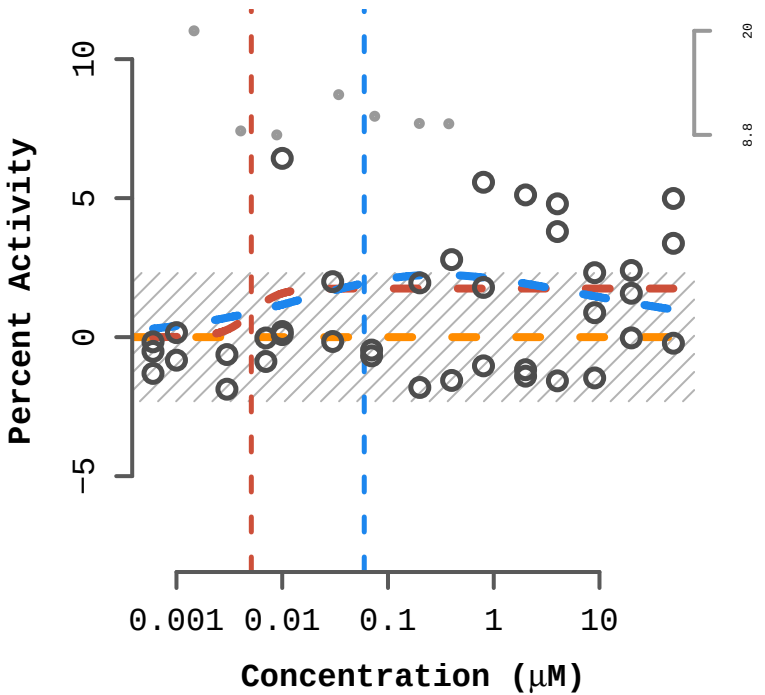
NAME: Sulfathiazole
CHID: 26068 **CASRN:** 72-14-0
SPID(S): Tox21_202243
M4ID: 12480009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: −0.116 **MAX_MED:** 0.0218 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfathiazole
CHID: 26068 **CASRN:** 72-14-0
SPID(S): Tox21_110363_1
M4ID: 12484425 **BRK**

HILL MODEL (in red):

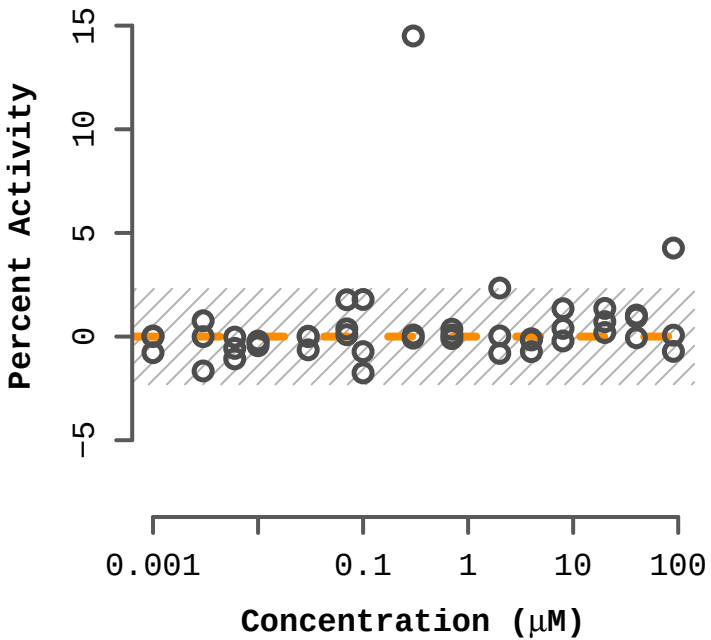
	tp	ga	gw
val:	1.75	−2.29	3.28
sd:	0.655	0.85	12.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.93	−1.22	0.628	−0.867	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	267.85	265.7	270.33
PROB:	0.24	0.69	0.07
RMSE:	5.35	4.9	4.86

MAX_MEAN: 6.49 **MAX_MED:** 3.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

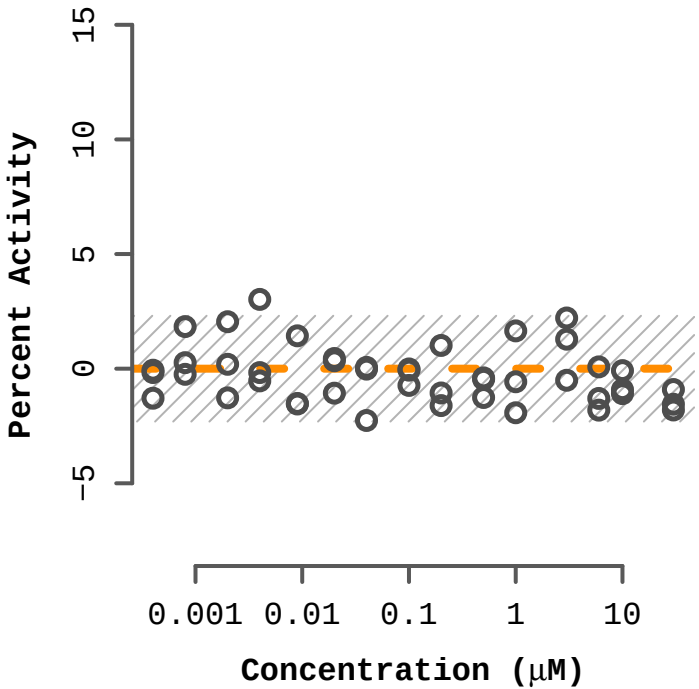
NAME: Isobutyl (2,4,5−trichlorophenoxy)acetate
CHID: 26074 CASRN: 4938−72−1
SPID(S): Tox21_200319
M4ID: 12481933

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.31	NA	NA
PROB:	1	NA	NA
RMSE:	2.4	NA	NA

MAX_MEAN: 4.84 MAX_MED: 0.939 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

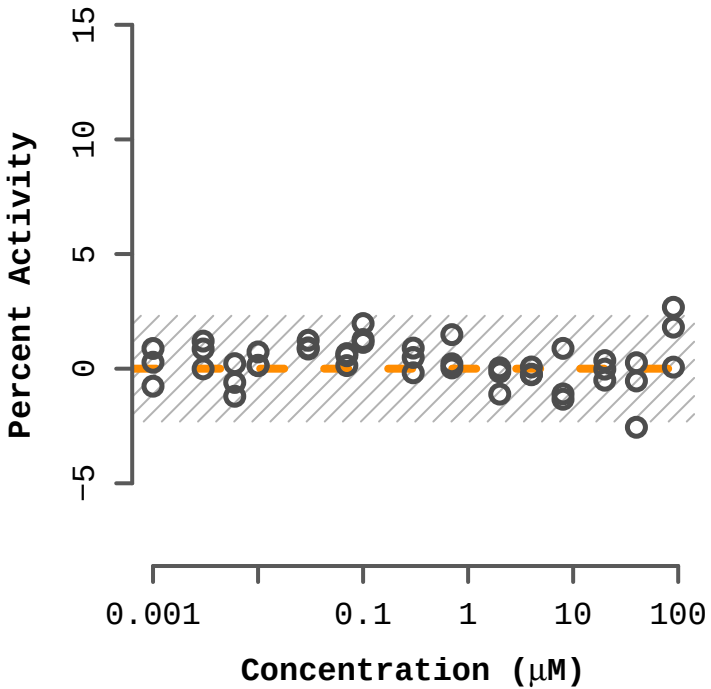
NAME: Tannic acid
CHID: 26076 **CASRN:** 1401-55-4
SPID(S): Tox21_300079
M4ID: 12479051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.998 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

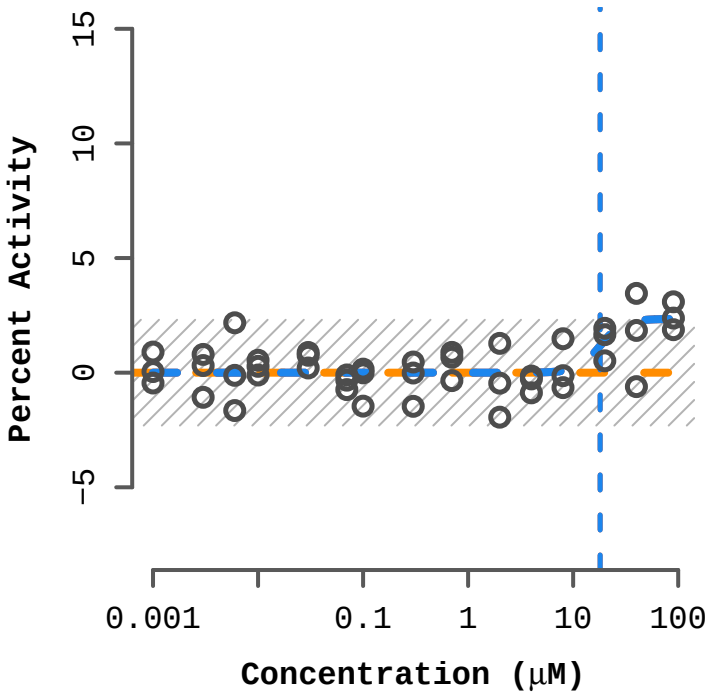
NAME: Terephthalic acid
CHID: 26080 **CASRN:** 100-21-0
SPID(S): Tox21_303229
M4ID: 12475904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Terephthalic acid
CHID: 26080 CASRN: 100-21-0
SPID(S): Tox21_201659
M4ID: 12480593

HILL MODEL (in red):

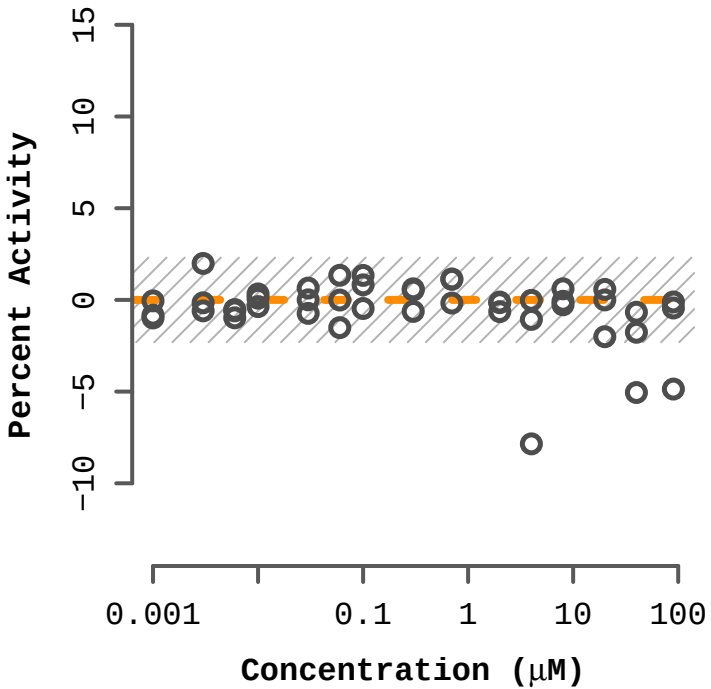
	tp	ga	gw
val:	2.34	1.26	4.06
sd:	0.422	0.101	4.98

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.34	1.26	4.06	2.5	15.3
sd:	0.422	0.101	4.98	913	25300

	CNST	HILL	GNLS
AIC:	148.41	128.66	132.66
PROB:	0	0.88	0.12
RMSE:	1.24	0.94	0.94

MAX_MEAN: 2.45 MAX_MED: 2.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

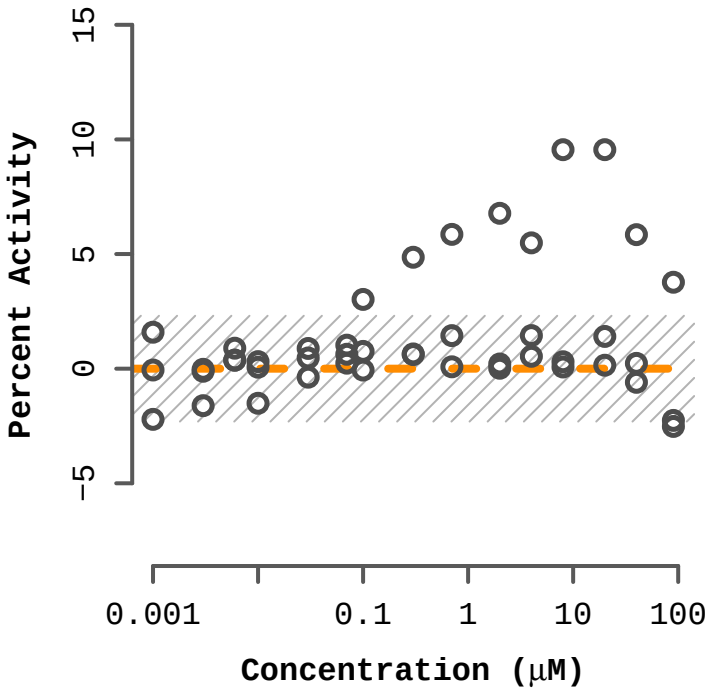
NAME: 3,3',5,5'−Tetrabromobisphenol A
CHID: 26081 **CASRN:** 79−94−7
SPID(S): Tox21_300561
M4ID: 12478572

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 0.698 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

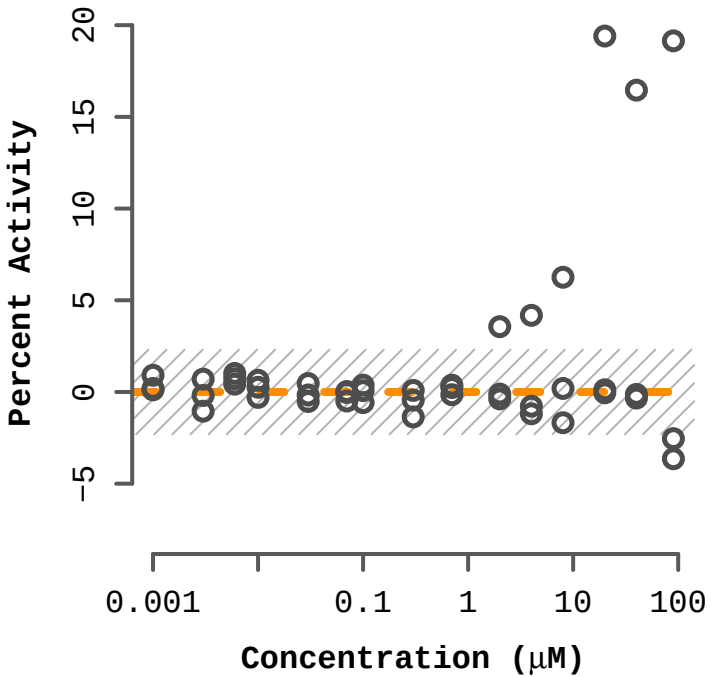
NAME: 3,3',5,5'−Tetrabromobisphenol A
CHID: 26081 **CASRN:** 79−94−7
SPID(S): Tox21_201981
M4ID: 12480271

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.27	NA	NA
PROB:	1	NA	NA
RMSE:	3.02	NA	NA

MAX_MEAN: 3.7 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

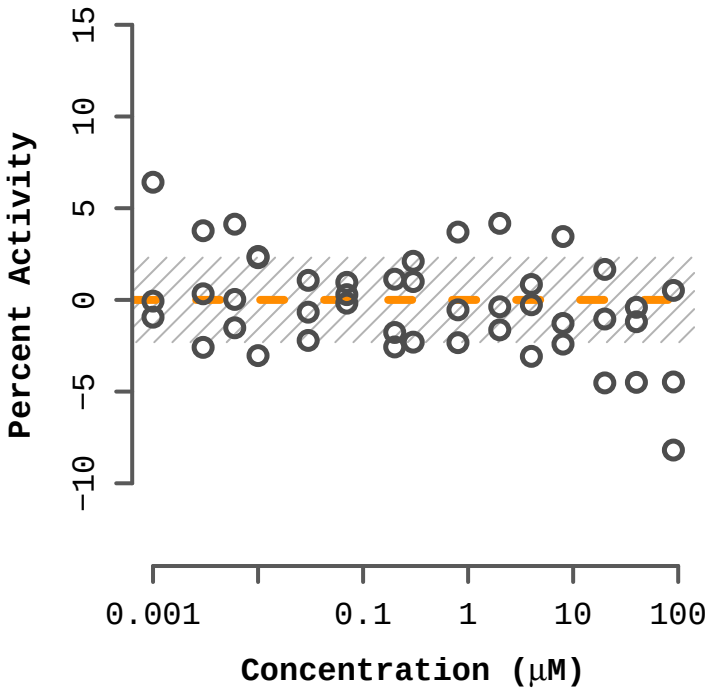
NAME: 3,3',5,5'−Tetrabromobisphenol A
CHID: 26081 CASRN: 79−94−7
SPID(S): Tox21_201182
M4ID: 12481070

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.94	NA	NA
PROB:	1	NA	NA
RMSE:	4.98	NA	NA

MAX_MEAN: 6.5 MAX_MED: 0.727 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

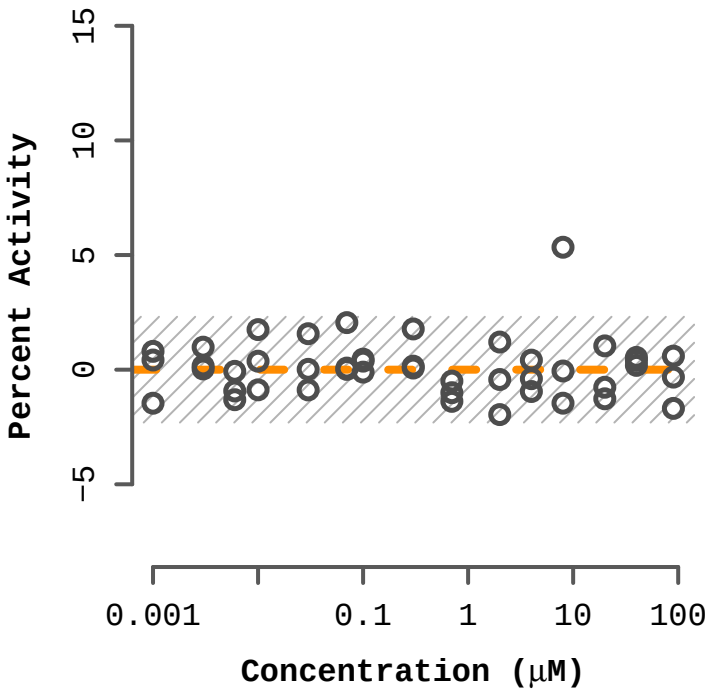
NAME: 1,1,1,2-Tetrabromoethane
CHID: 26082 **CASRN:** 630-16-0
SPID(S): Tox21_201187
M4ID: 12481065

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.19	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

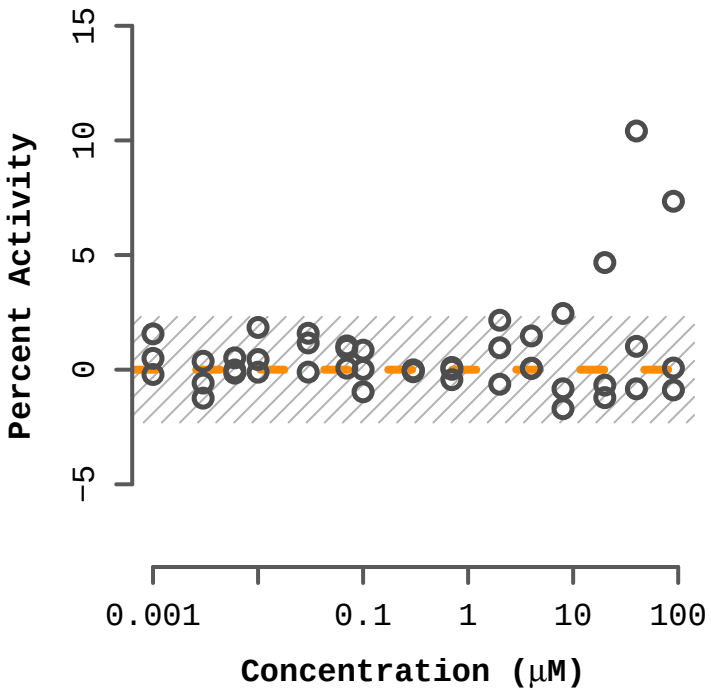
NAME: 1,1,2,2-Tetrabromoethane
CHID: 26083 **CASRN:** 79-27-6
SPID(S): Tox21_200364
M4ID: 12481888

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.422 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

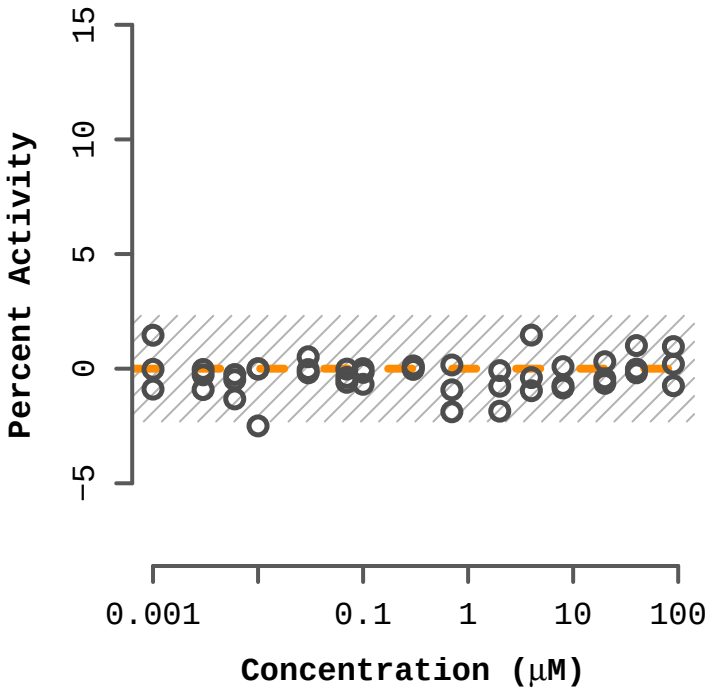
NAME: Tetrabromophthalic anhydride
CHID: 26084 **CASRN:** 632-79-1
SPID(S): Tox21_200056
M4ID: 12482196

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.12	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 3.53 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

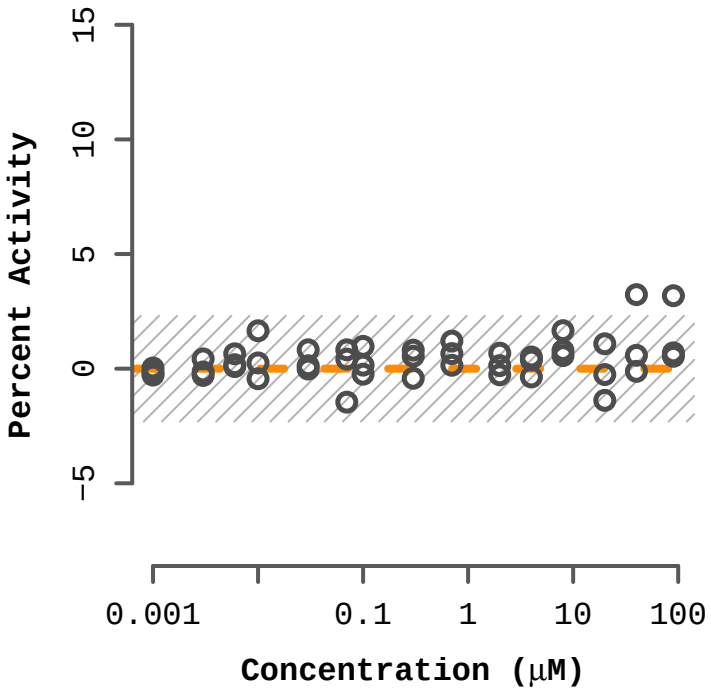
NAME: 1,2,3,4-Tetrachlorobenzene
CHID: 26088 **CASRN:** 634-66-2
SPID(S): Tox21_303272
M4ID: 12475861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.271 **MAX_MED:** 0.198 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

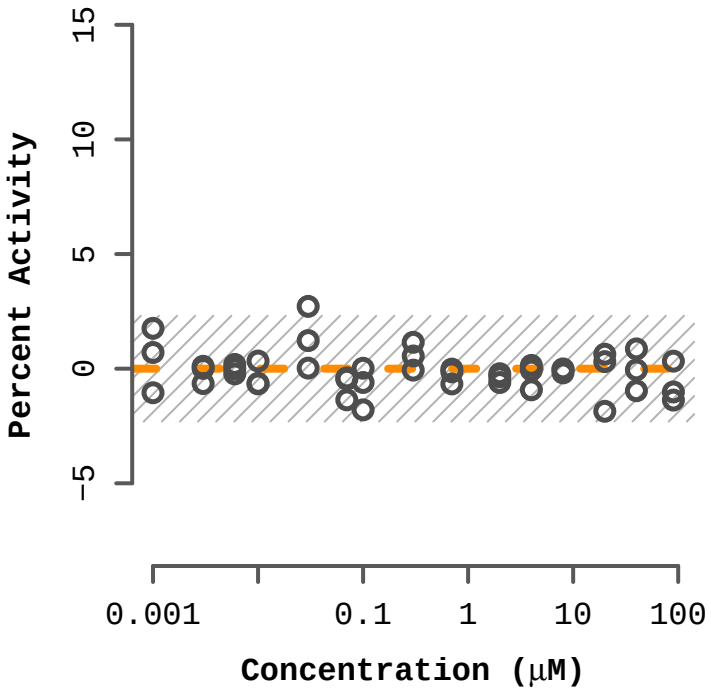
NAME: 1,2,3,4-Tetrachlorobenzene
CHID: 26088 **CASRN:** 634-66-2
SPID(S): Tox21_201497
M4ID: 12480755

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

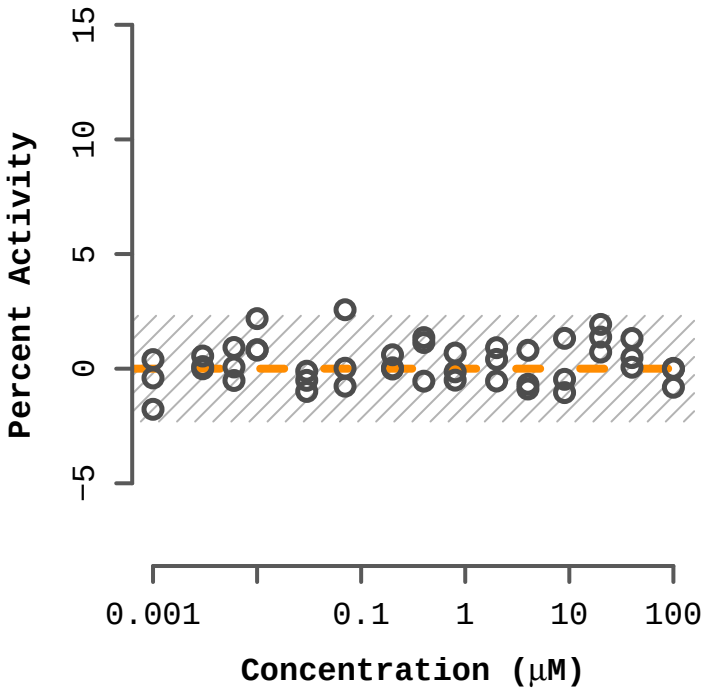
NAME: 1,2,3,5-Tetrachlorobenzene
CHID: 26089 **CASRN:** 634-90-2
SPID(S): Tox21_200673
M4ID: 12481579

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

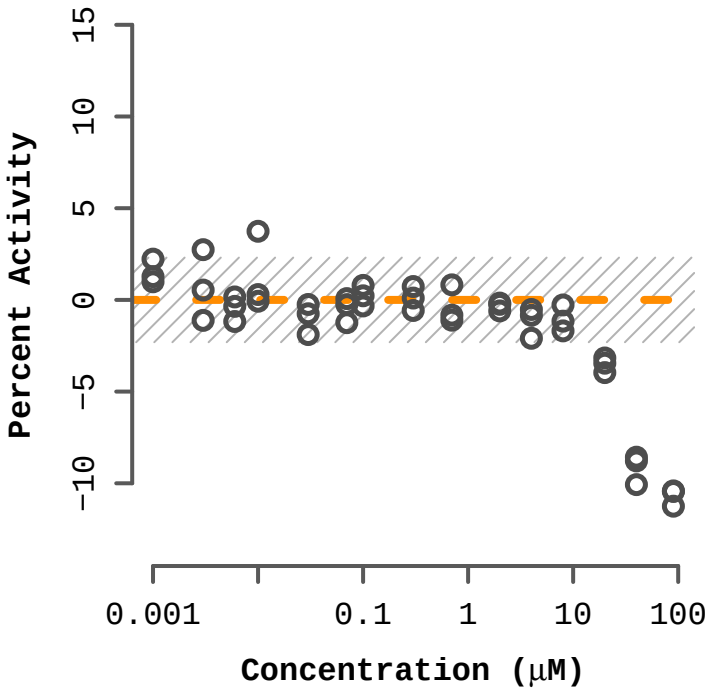
NAME: 1,2-Difluoro-1,1,2,2-tetrachloroethane
CHID: 26091 **CASRN:** 76-12-0
SPID(S): Tox21_200566
M4ID: 12481686

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

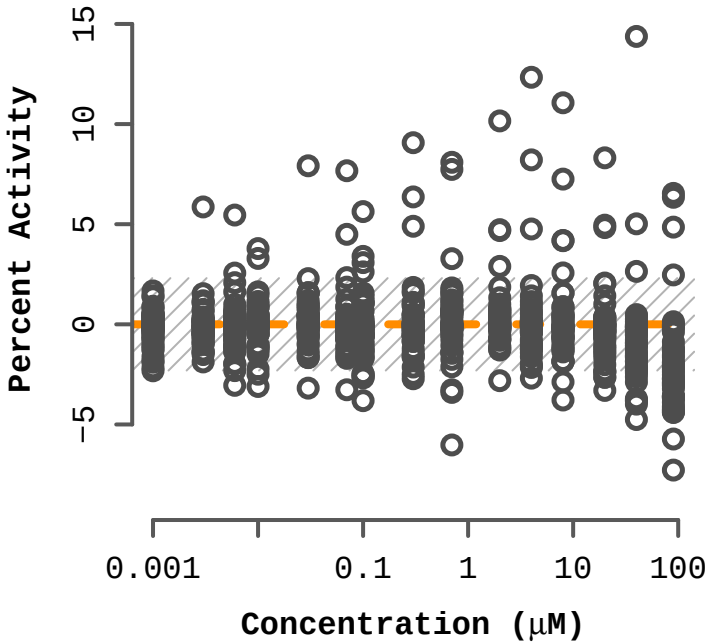
NAME: 2,3,4,5-Tetrachloronitrobenzene
CHID: 26097 **CASRN:** 879-39-0
SPID(S): Tox21_200893
M4ID: 12481359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.9	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

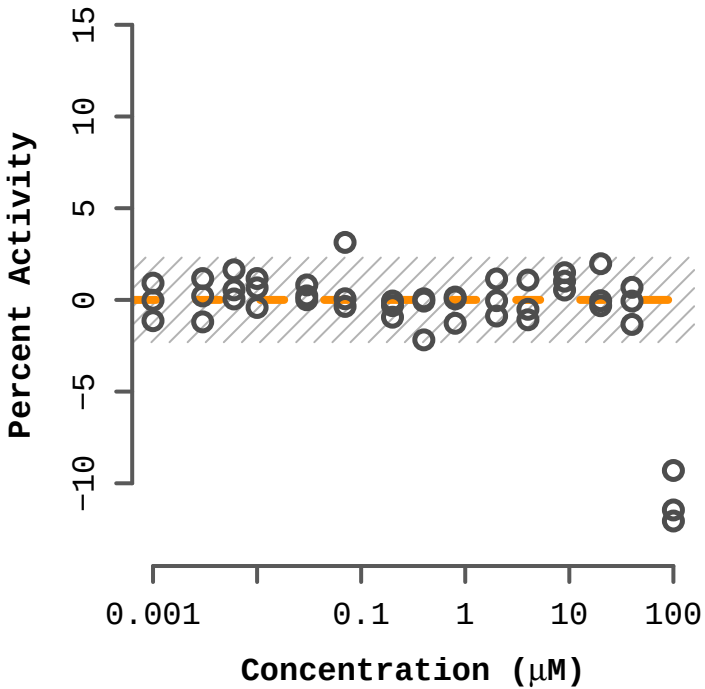
NAME: 2,3,5,6-Tetrachloronitrobenzene
CHID: 26098 **CASRN:** 117-18-0
SPID(S): Tox21_400013
M4ID: 12475124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2701.36	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 0.426 **MAX_MED:** 0.0473 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

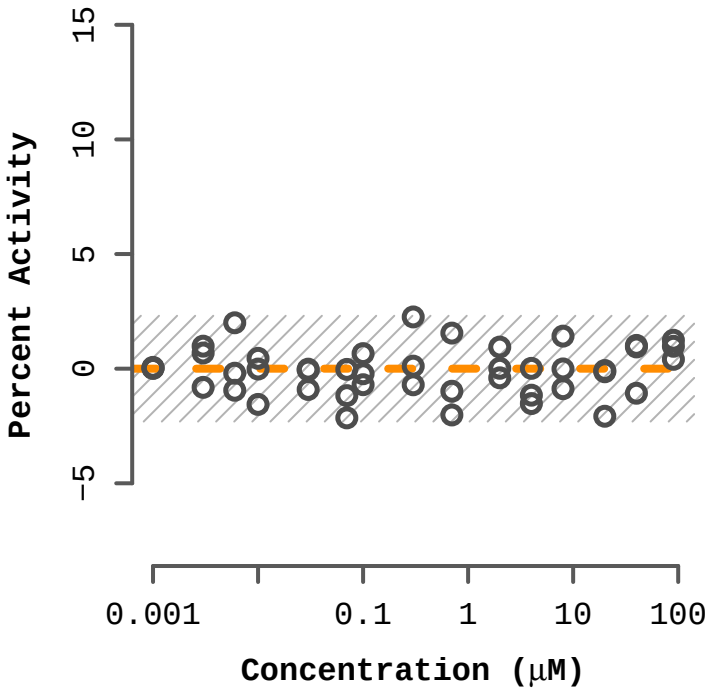
NAME: 2,3,5,6-Tetrachlorophenol
CHID: 26101 **CASRN:** 935-95-5
SPID(S): Tox21_200910
M4ID: 12481342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.91	NA	NA
PROB:	1	NA	NA
RMSE:	3	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

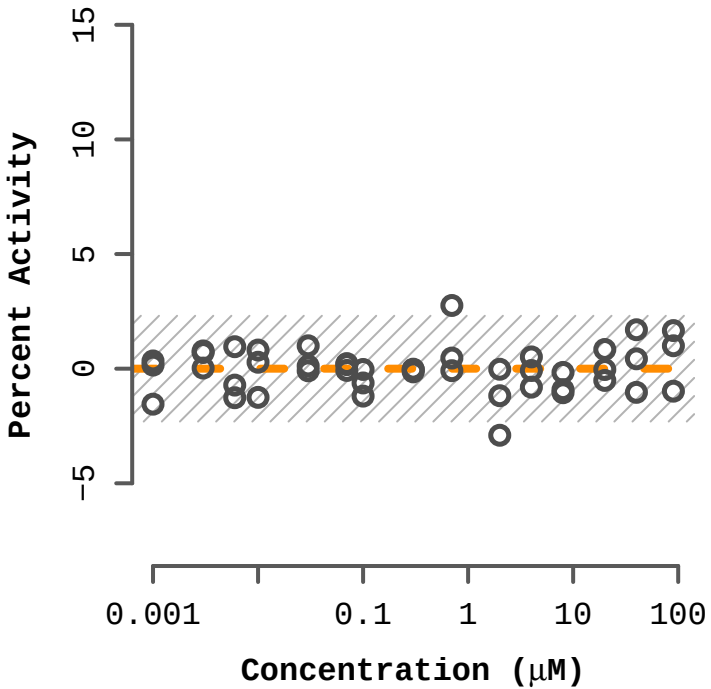
NAME: Tetrachlorophthalic anhydride
CHID: 26102 **CASRN:** 117-08-8
SPID(S): Tox21_303212
M4ID: 12475921

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

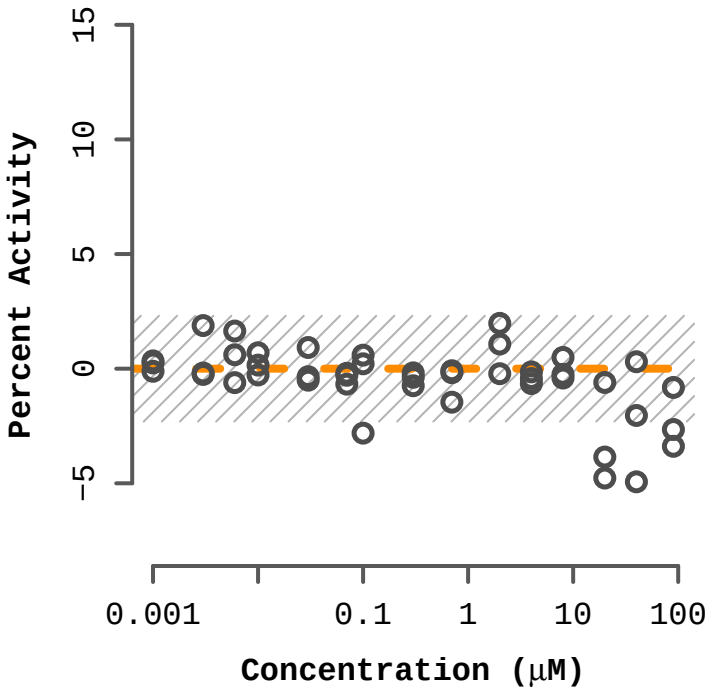
NAME: Tetrachlorophthalic anhydride
CHID: 26102 **CASRN:** 117-08-8
SPID(S): Tox21_201740
M4ID: 12480512

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

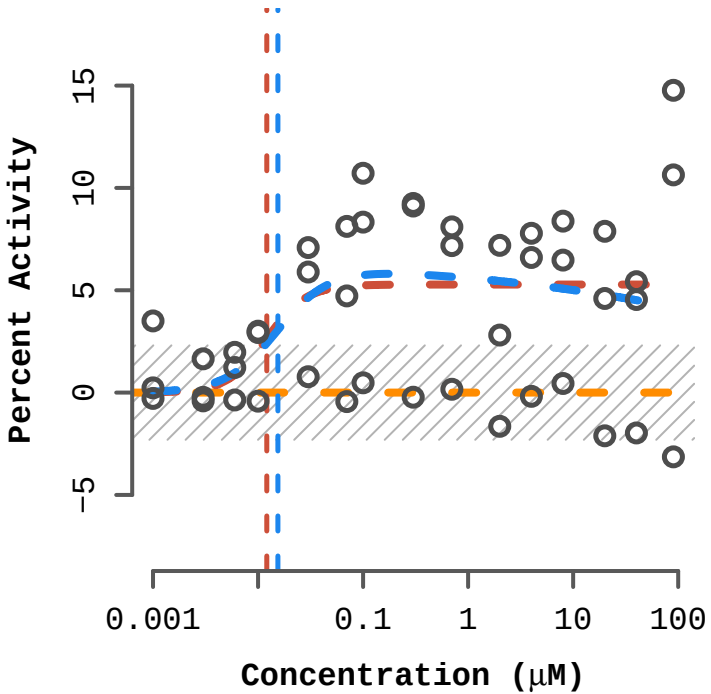
NAME: Tetraethylene glycol diacrylate
CHID: 26107 **CASRN:** 17831-71-9
SPID(S): Tox21_202993
M4ID: 12479259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 0.946 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetraethylene glycol diacrylate
CHID: 26107 CASRN: 17831-71-9
SPID(S): Tox21_202541
M4ID: 12479711

HILL MODEL (in red):

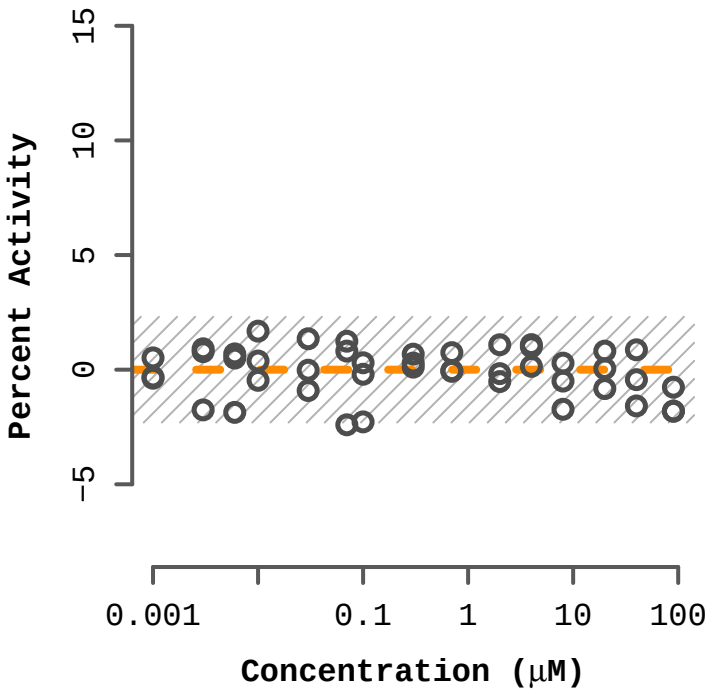
	tp	ga	gw
val:	5.28	−1.92	2.31
sd:	0.828	0.249	2.65

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.35	−1.81	1.78	2.91	0.3
sd:	6.13	0.468	1.95	4.34	1.01

	CNST	HILL	GNLS
AIC:	288.3	260.67	264.43
PROB:	0	0.87	0.13
RMSE:	5.67	3.9	3.91

MAX_MEAN: 7.42 MAX_MED: 10.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

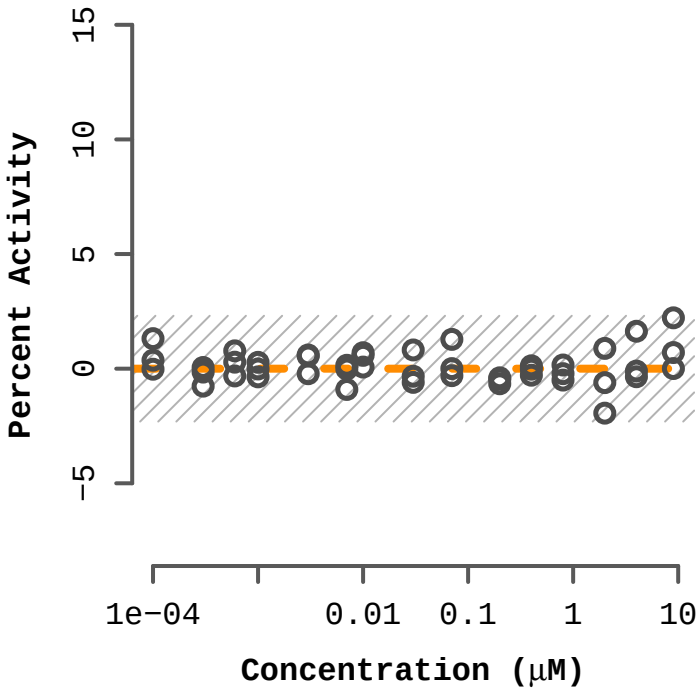
NAME: Tetraethylenepentamine
CHID: 26108 **CASRN:** 112-57-2
SPID(S): Tox21_200669
M4ID: 12481583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.747 **MAX_MED:** 0.999 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

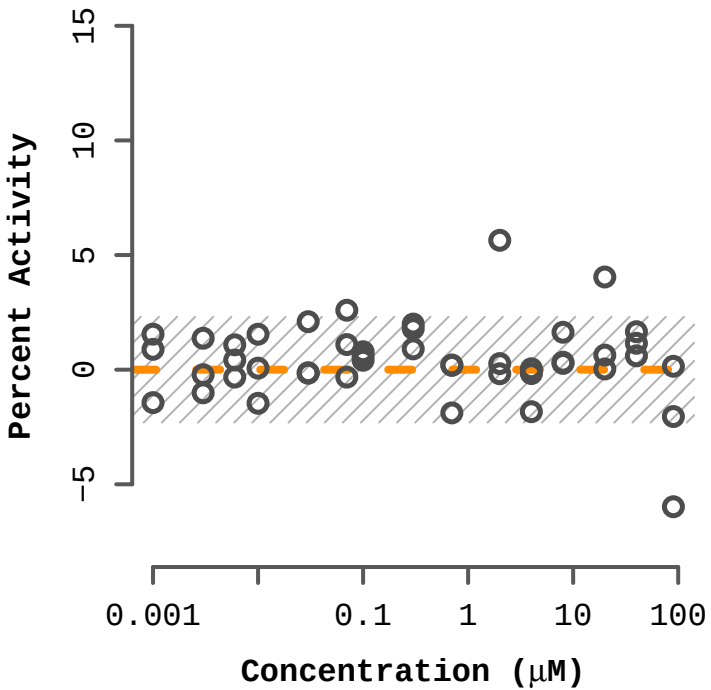
NAME: Tetraethylenepentamine
CHID: 26108 **CASRN:** 112-57-2
SPID(S): Tox21_111047_1
M4ID: 12483933

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.978 **MAX_MED:** 0.705 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

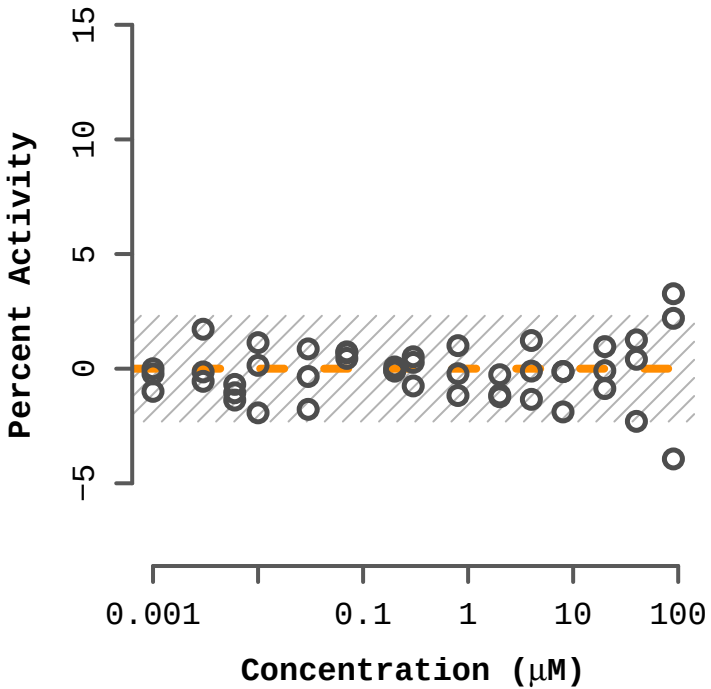
NAME: 1,2,3,4−Tetrahydro−9−acridinamine hydrochlorid
CHID: 26112 CASRN: 1684−40−8
SPID(S): Tox21_200299
M4ID: 12481953

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

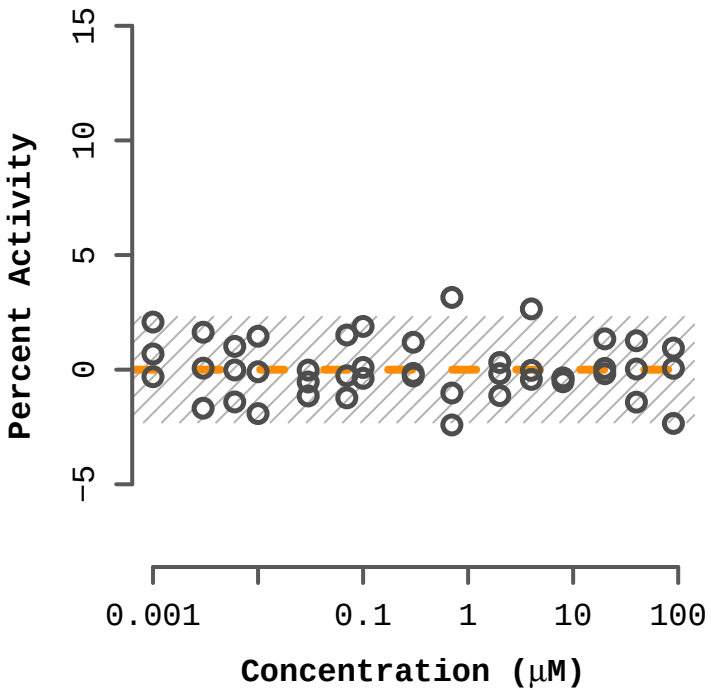
NAME: 1,2,3,4−Tetrahydroisoquinoline
CHID: 26115 **CASRN:** 91−21−4
SPID(S): Tox21_200374
M4ID: 12481878

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.624 **MAX_MED:** 2.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

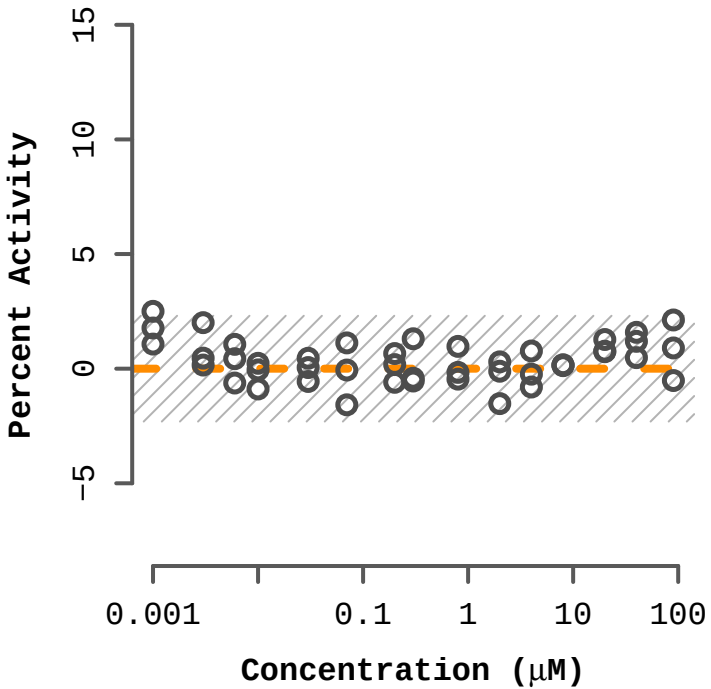
NAME: Tetralin
CHID: 26118 **CASRN:** 119-64-2
SPID(S): Tox21_303325
M4ID: 12475808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.82 **MAX_MED:** 0.686 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

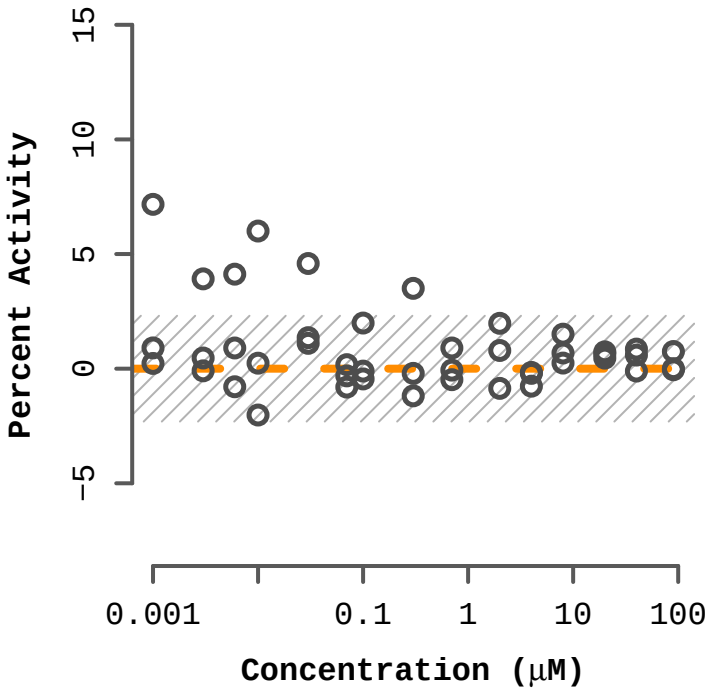
NAME: Tetralin
CHID: 26118 **CASRN:** 119-64-2
SPID(S): Tox21_201793
M4ID: 12480459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

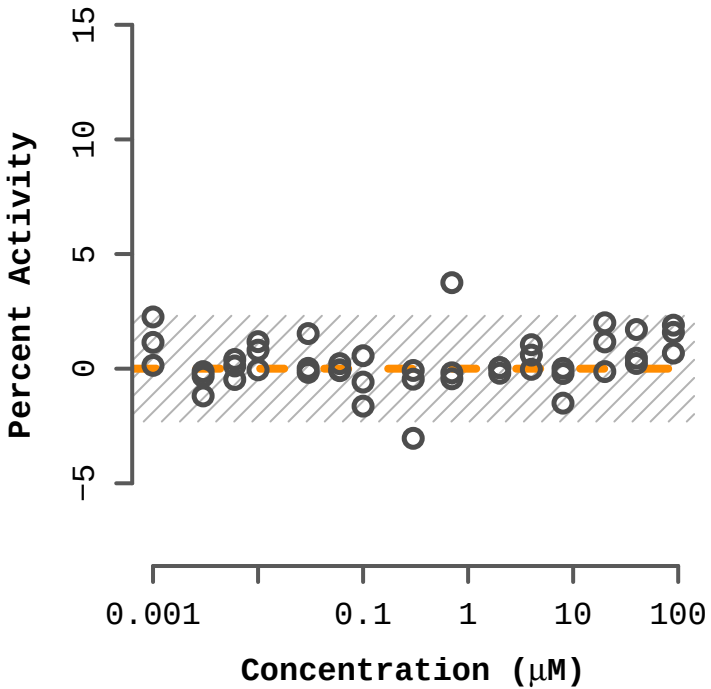
NAME: 1,2,3,5-Tetramethylbenzene
CHID: 26119 **CASRN:** 527-53-7
SPID(S): Tox21_302230
M4ID: 12476903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 2.77 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

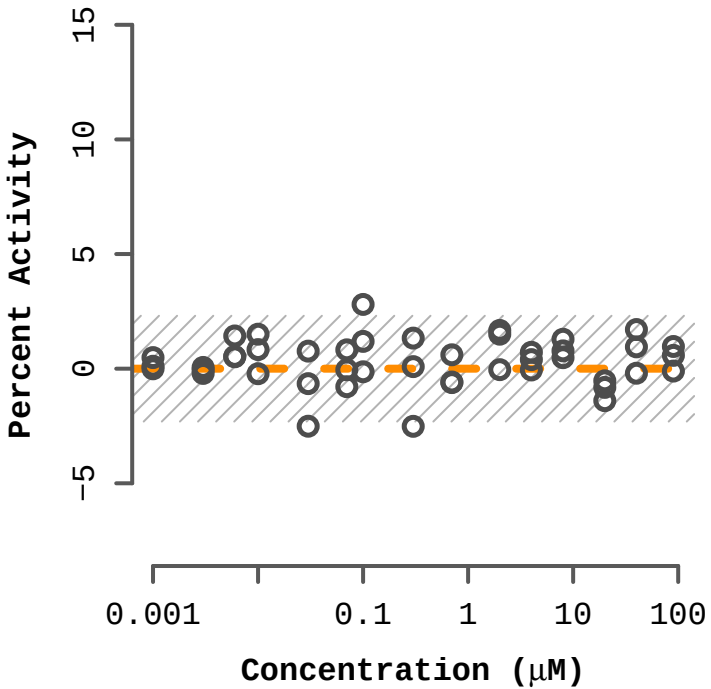
NAME: 3,3',5,5'−Tetramethylbenzidine
CHID: 26120 **CASRN:** 54827−17−7
SPID(S): Tox21_303150
M4ID: 12475983

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

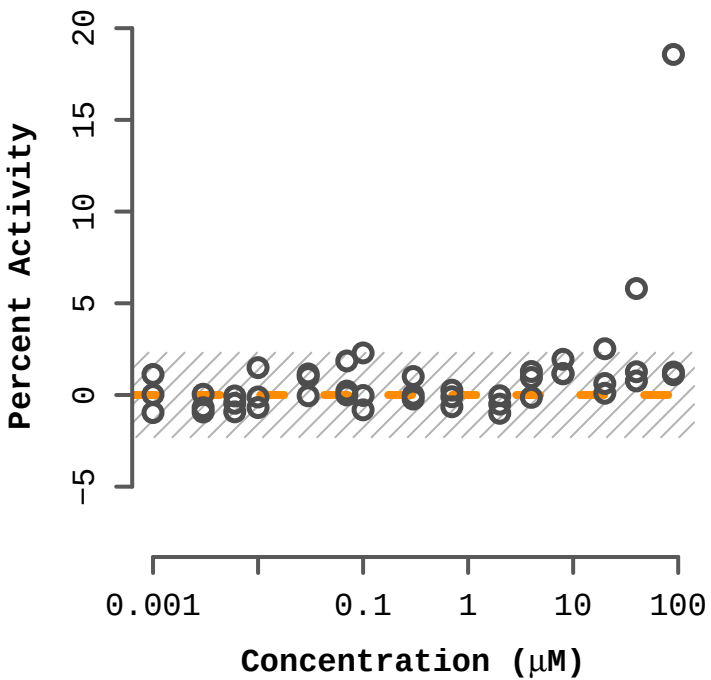
NAME: 3,3',5,5'−Tetramethylbenzidine
CHID: 26120 **CASRN:** 54827−17−7
SPID(S): Tox21_201500
M4ID: 12480752

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

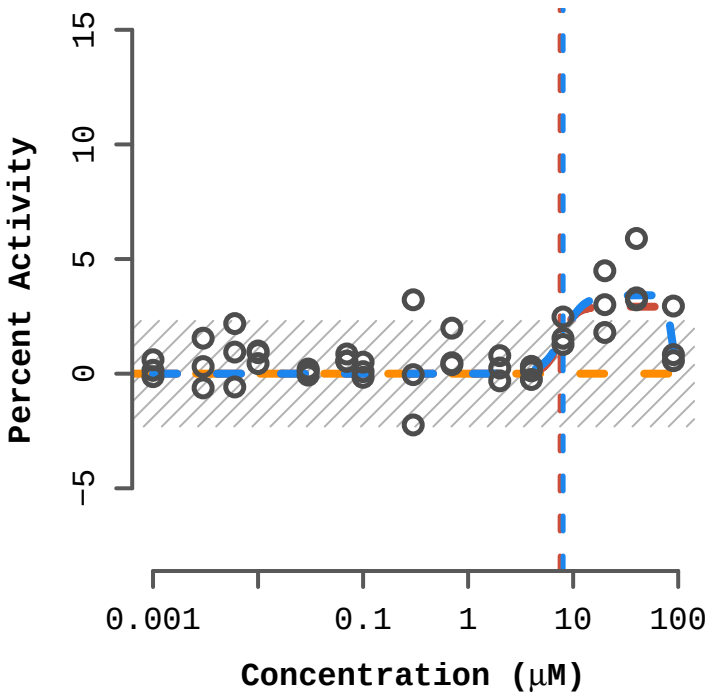
NAME: N,N,N',N'−Tetramethylethylenediamine
CHID: 26122 CASRN: 110−18−9
SPID(S): Tox21_200241
M4ID: 12482011

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.06	NA	NA

MAX_MEAN: 6.98 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N,N,N',N'−Tetramethyl−p−phenylenediamine
CHID: 26124 CASRN: 100−22−1
SPID(S): Tox21_200617
M4ID: 12481635

HILL MODEL (in red):

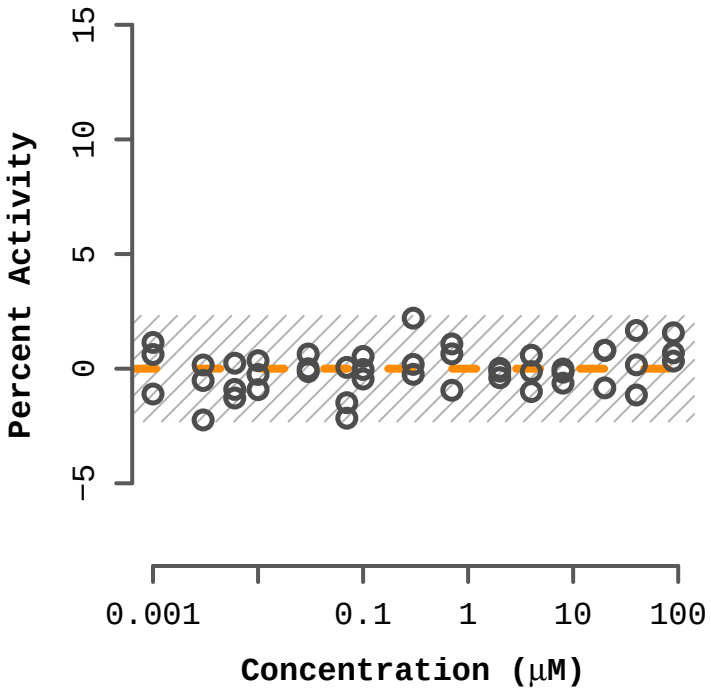
	tp	ga	gw
val:	2.92	0.876	6.05
sd:	0.372	0.0655	9.83

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.42	0.904	4.44	1.93	16.4
sd:	0.429	0.0624	4.99	0.0324	25.3

	CNST	HILL	GNLS
AIC:	175.03	141.04	137.27
PROB:	0	0.13	0.87
RMSE:	1.78	1.13	1.04

MAX_MEAN: 4.14 MAX_MED: 3.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

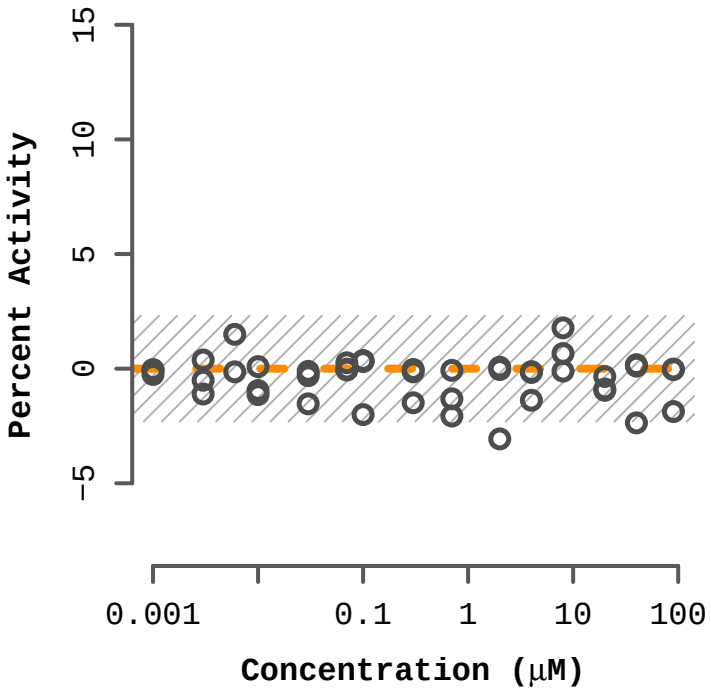
NAME: Tetramethylsuccinonitrile
CHID: 26125 **CASRN:** 3333-52-6
SPID(S): Tox21_200573
M4ID: 12481679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.864 **MAX_MED:** 0.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

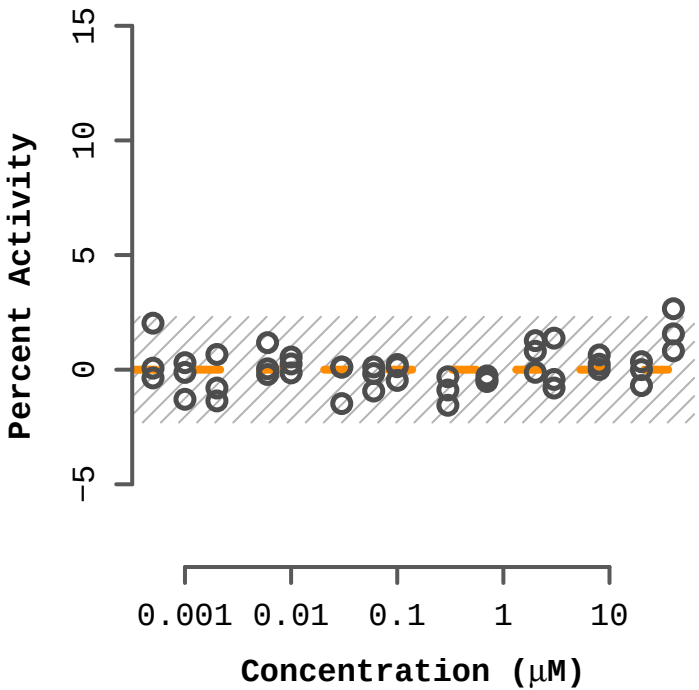
NAME: Tetrapropylammonium bromide
CHID: 26130 **CASRN:** 1941-30-6
SPID(S): Tox21_301504
M4ID: 12477629

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.78 **MAX_MED:** 0.682 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

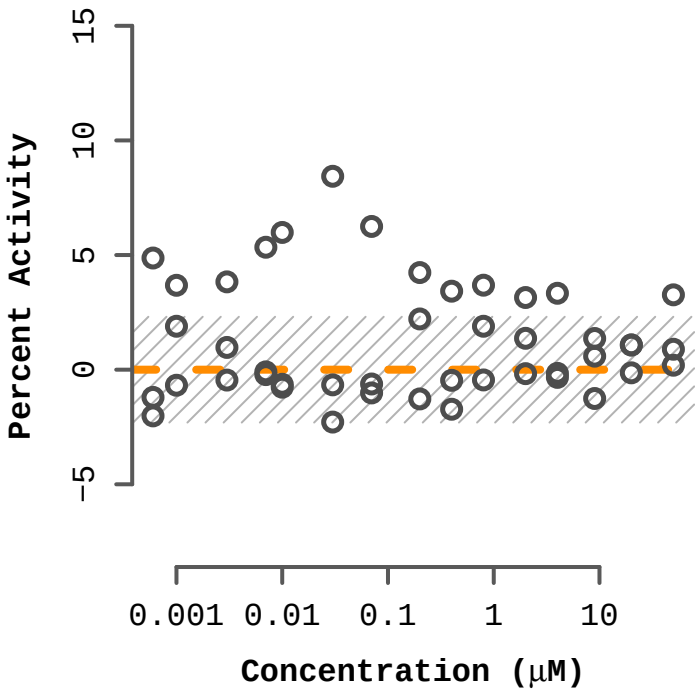
NAME: Theobromine
CHID: 26132 **CASRN:** 83-67-0
SPID(S): Tox21_300016
M4ID: 12479114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

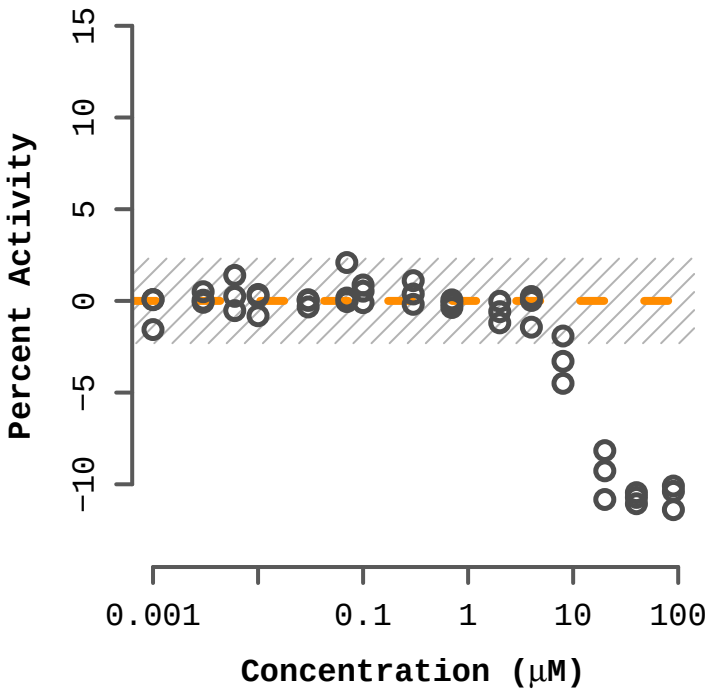
NAME: Theobromine
CHID: 26132 **CASRN:** 83-67-0
SPID(S): Tox21_110284_1
M4ID: 12484484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.76	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

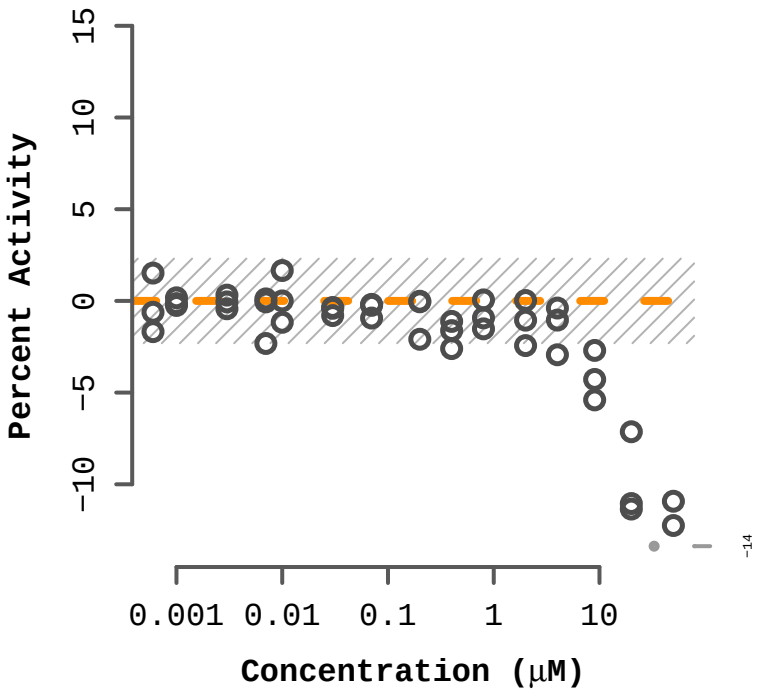
NAME: Fenticlor
CHID: 26137 **CASRN:** 97-24-5
SPID(S): Tox21_200961
M4ID: 12481291

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	255.43	NA	NA
PROB:	1	NA	NA
RMSE:	4.73	NA	NA

MAX_MEAN: 0.74 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

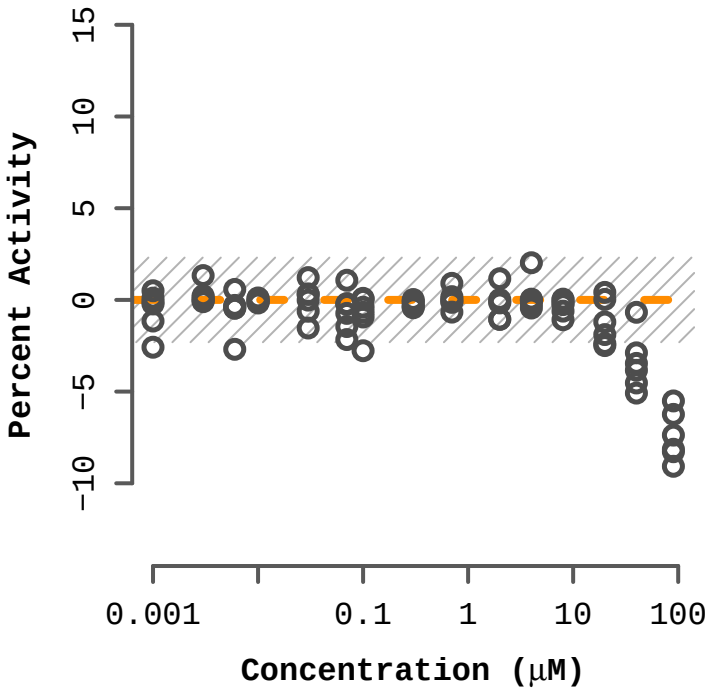
NAME: Fenticlor
CHID: 26137 **CASRN:** 97-24-5
SPID(S): Tox21_110031_1
M4ID: 12484702 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.85	NA	NA
PROB:	1	NA	NA
RMSE:	4.38	NA	NA

MAX_MEAN: 0.164 **MAX_MED:** 9e-06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

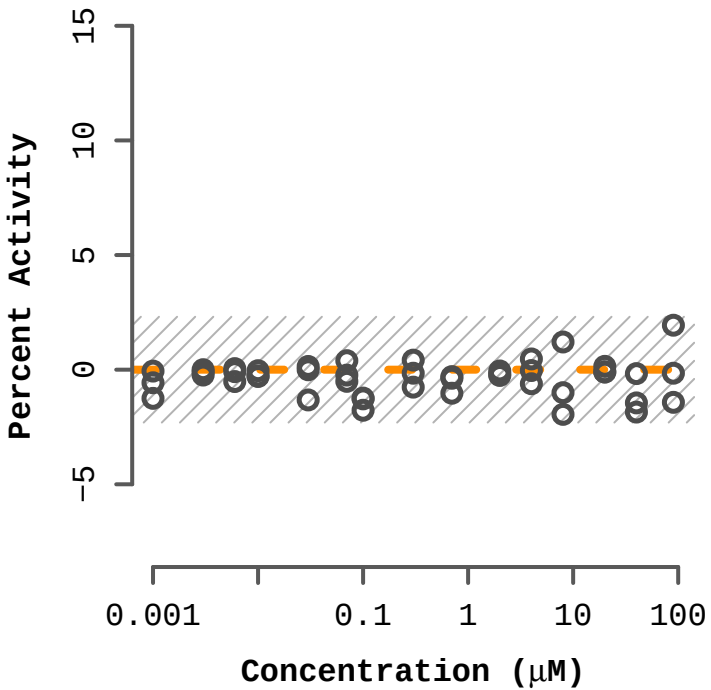
NAME: Thiocarbanilide
CHID: 26139 **CASRN:** 102-08-9
SPID(S): Tox21_200269
M4ID: 12481983

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	358.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 0.264 **MAX_MED:** 0.144 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

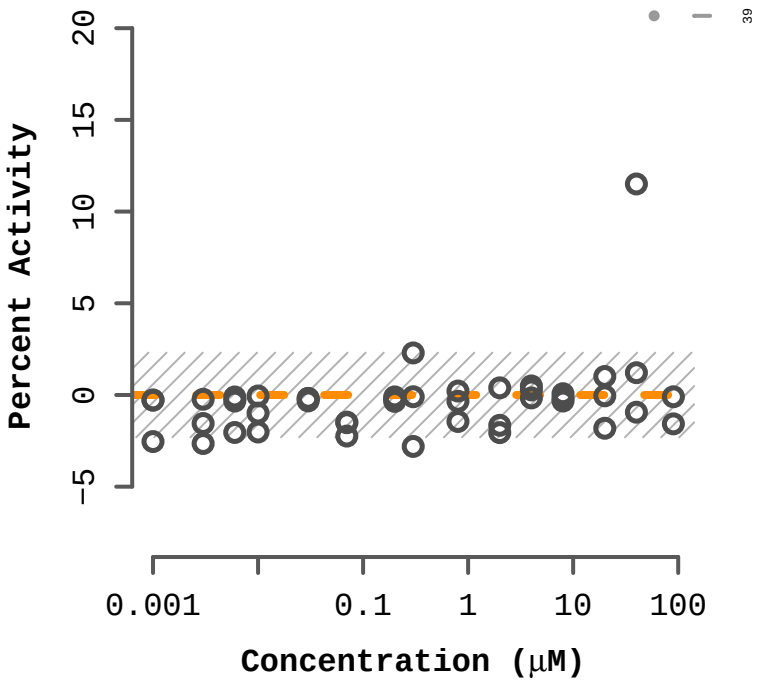
NAME: Thioglycolic acid
CHID: 26141 **CASRN:** 68-11-1
SPID(S): Tox21_303306
M4ID: 12475827

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.121 **MAX_MED:** −0.00301 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

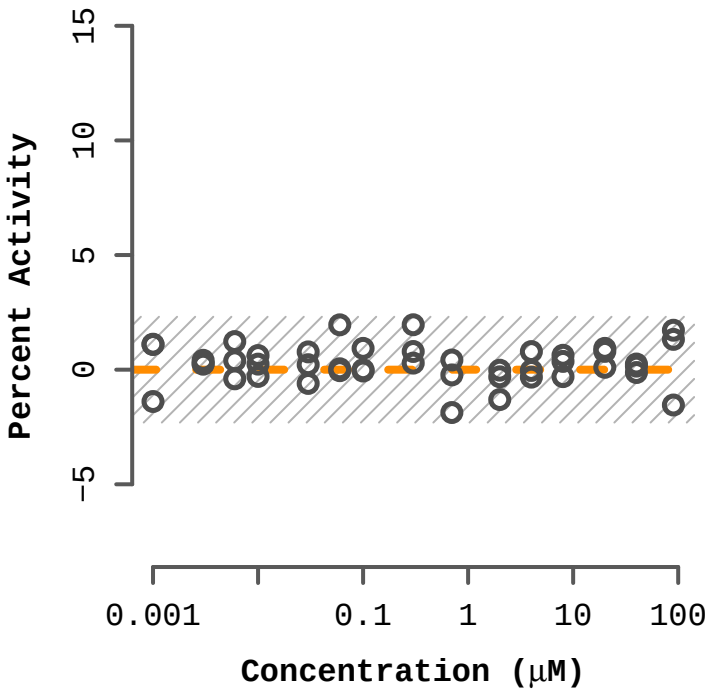
NAME: Thioglycolic acid
CHID: 26141 CASRN: 68-11-1
SPID(S): Tox21_201717
M4ID: 12480535 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.32	NA	NA
PROB:	1	NA	NA
RMSE:	6.2	NA	NA

MAX_MEAN: 12.5 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

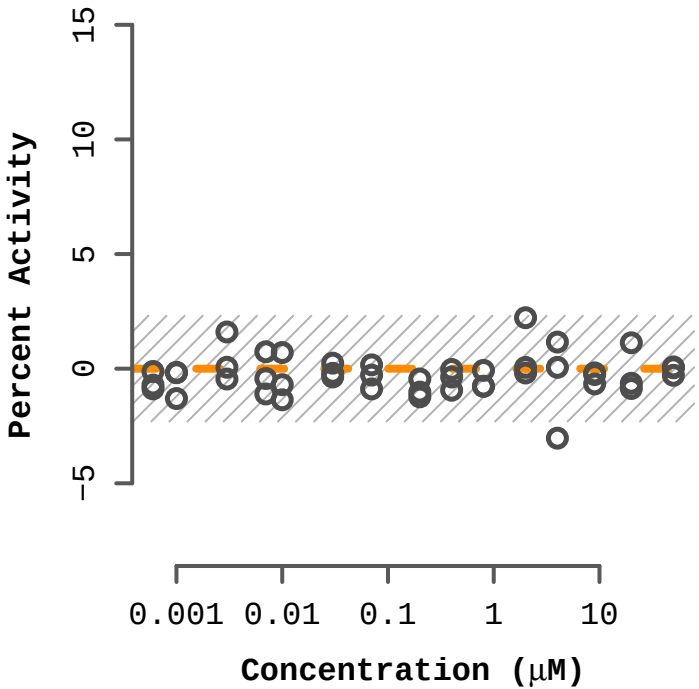
NAME: Thiophene
CHID: 26145 **CASRN:** 110-02-1
SPID(S): Tox21_200002
M4ID: 12482250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

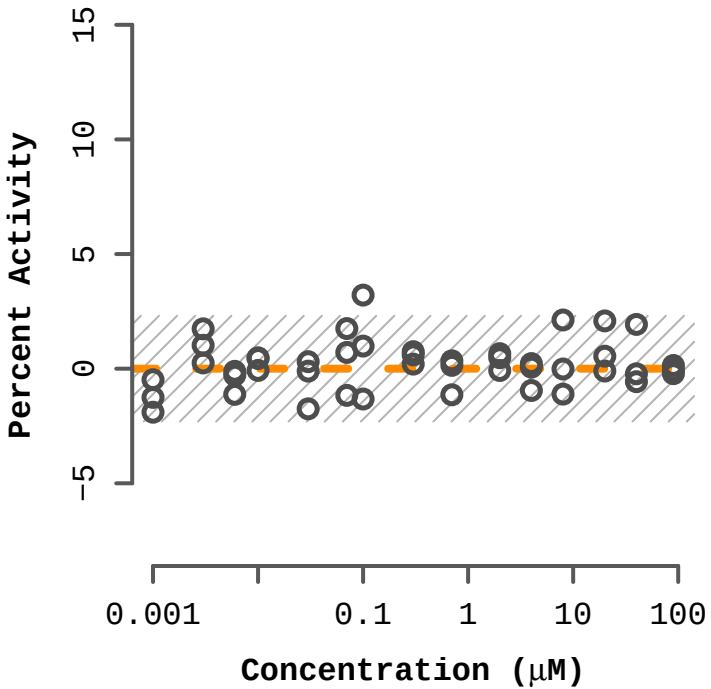
NAME: Thonzylamine hydrochloride
CHID: 26147 CASRN: 63-56-9
SPID(S): Tox21_111387_1
M4ID: 12483719

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.698 **MAX_MED:** 0.0625 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

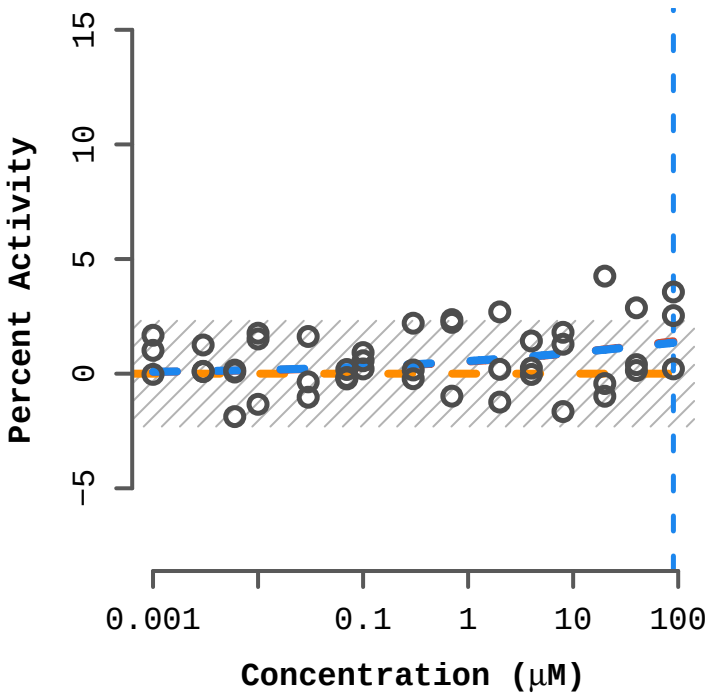
NAME: alpha−Thujone
CHID: 26148 **CASRN:** 546−80−5
SPID(S): Tox21_200868
M4ID: 12481384

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: d-alpha-Tocopheryl succinate
CHID: 26151 CASRN: 4345-03-3
SPID(S): Tox21_200568
M4ID: 12481684

HILL MODEL (in red):

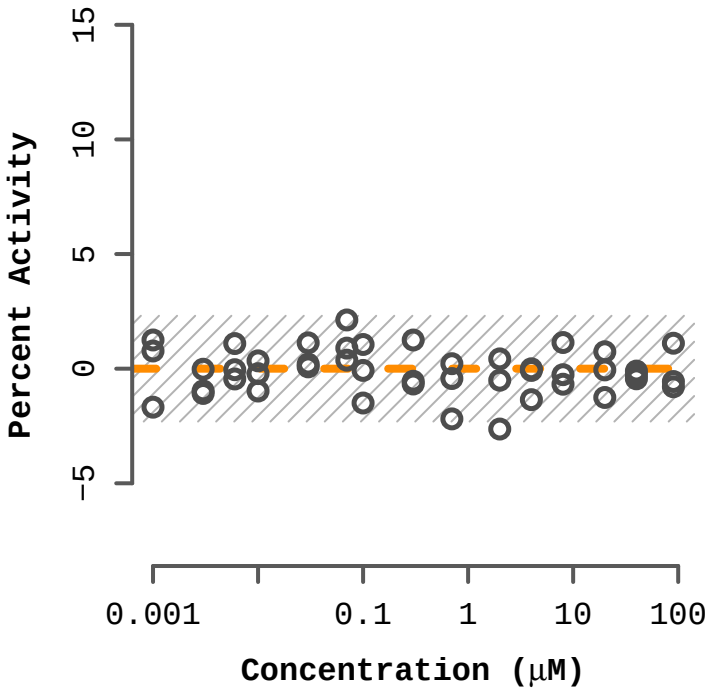
	tp	ga	gw
val:	3.41	2.45	0.3
sd:	16.8	10.7	0.343

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.69	1.95	0.301	3.57	3.97
sd:	11.1	9.82	0.358	397	983

	CNST	HILL	GNLS
AIC:	167.2	165.03	169.06
PROB:	0.23	0.68	0.09
RMSE:	1.51	1.32	1.32

MAX_MEAN: 2.1 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

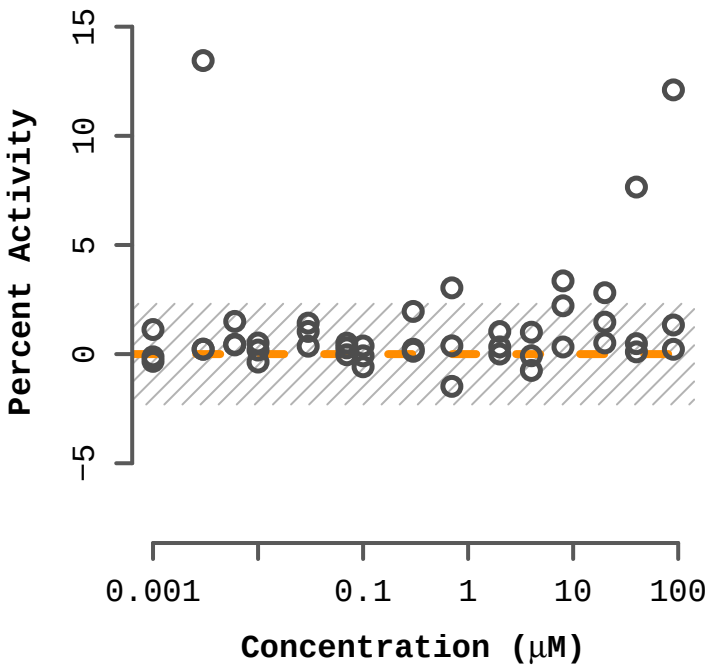
NAME: Toluene−2,4−diisocyanate
CHID: 26156 **CASRN:** 584−84−9
SPID(S): Tox21_300160
M4ID: 12478970

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.898 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

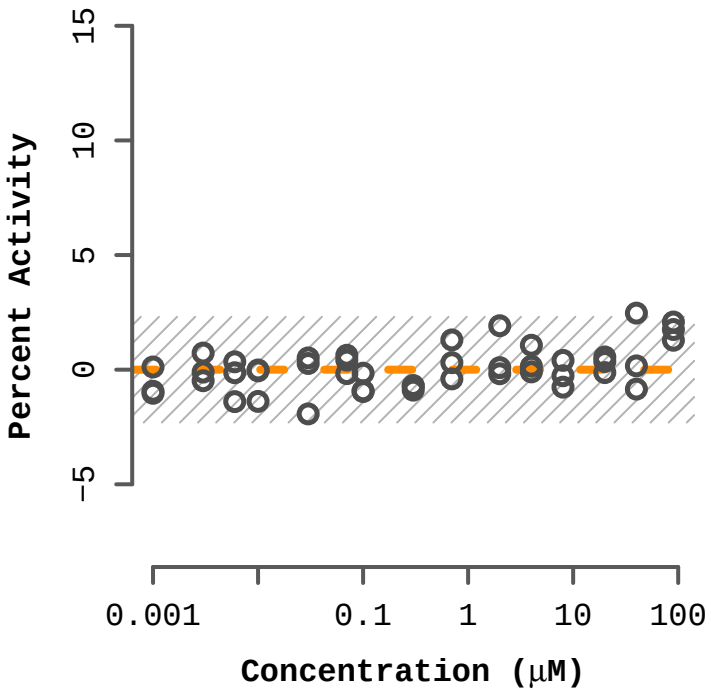
NAME: Toluene−2,4−diisocyanate
CHID: 26156 CASRN: 584−84−9
SPID(S): Tox21_202058
M4ID: 12480194

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.34	NA	NA
PROB:	1	NA	NA
RMSE:	3.13	NA	NA

MAX_MEAN: 4.64 MAX_MED: 2.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

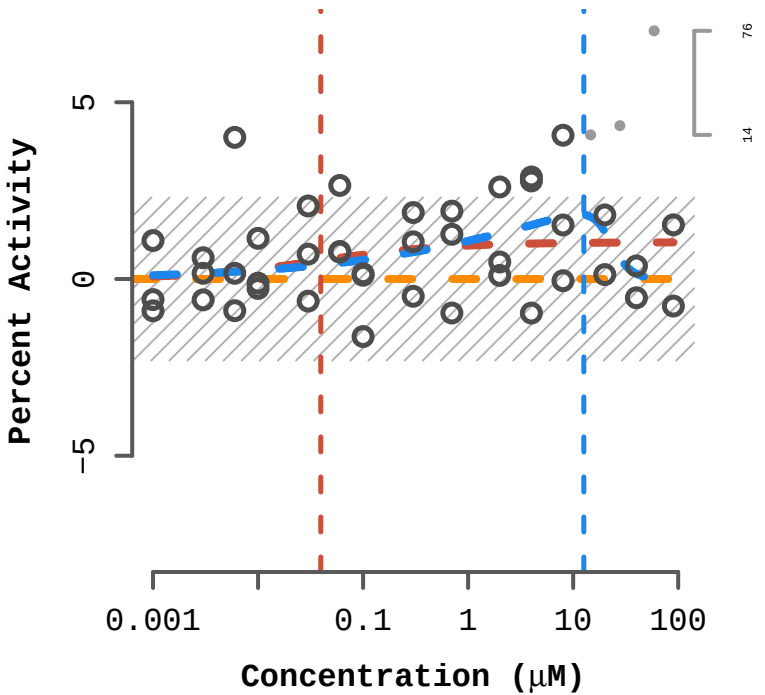
NAME: Toluene−2,6−diisocyanate
CHID: 26157 **CASRN:** 91−08−7
SPID(S): Tox21_201661
M4ID: 12480591

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylbenzoic acid
CHID: 26161 **CASRN:** 118-90-1
SPID(S): Tox21_200086
M4ID: 12482166 **BRK**

HILL MODEL (in red):

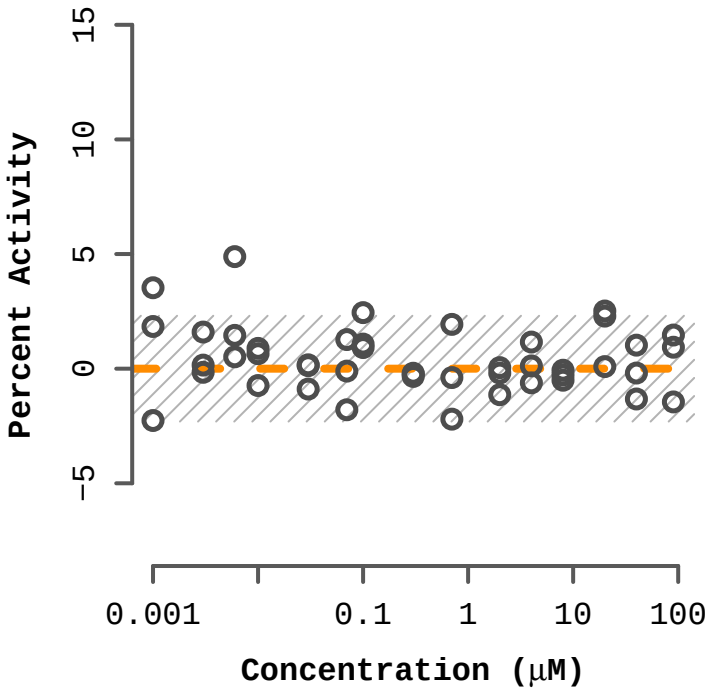
	tp	ga	gw
val:	1.04	−1.4	0.713
sd:	0.499	1.32	0.855

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.88	1.1	0.377	1.35	4.7
sd:	13.8	7.08	0.44	0.262	11.5

	CNST	HILL	GNLS
AIC:	233.29	230.63	232.65
PROB:	0.16	0.61	0.22
RMSE:	11.94	11.71	11.87

MAX_MEAN: 25.5 **MAX_MED:** 2.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

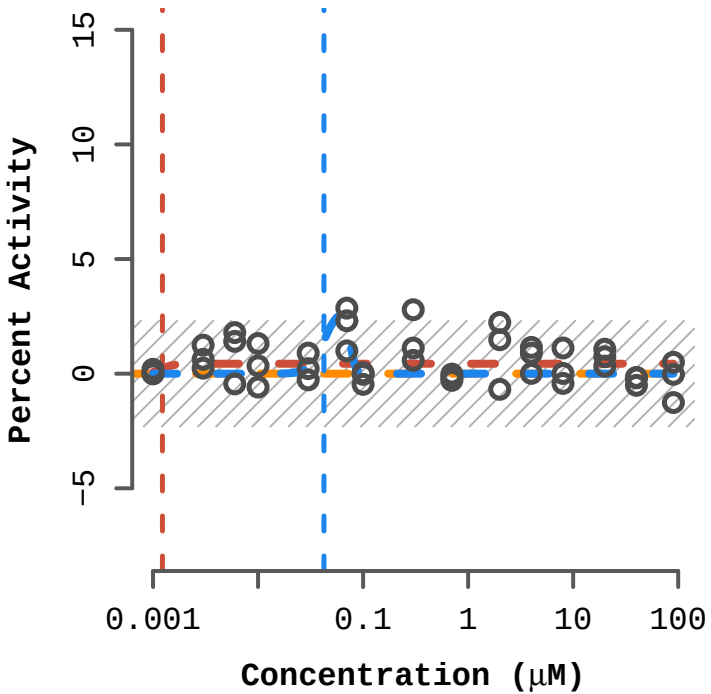
NAME: 2-Methylaniline
CHID: 26164 **CASRN:** 95-53-4
SPID(S): Tox21_300179
M4ID: 12478951

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.29 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylaniline
CHID: 26164 CASRN: 95-53-4
SPID(S): Tox21_201256
M4ID: 12480996

HILL MODEL (in red):

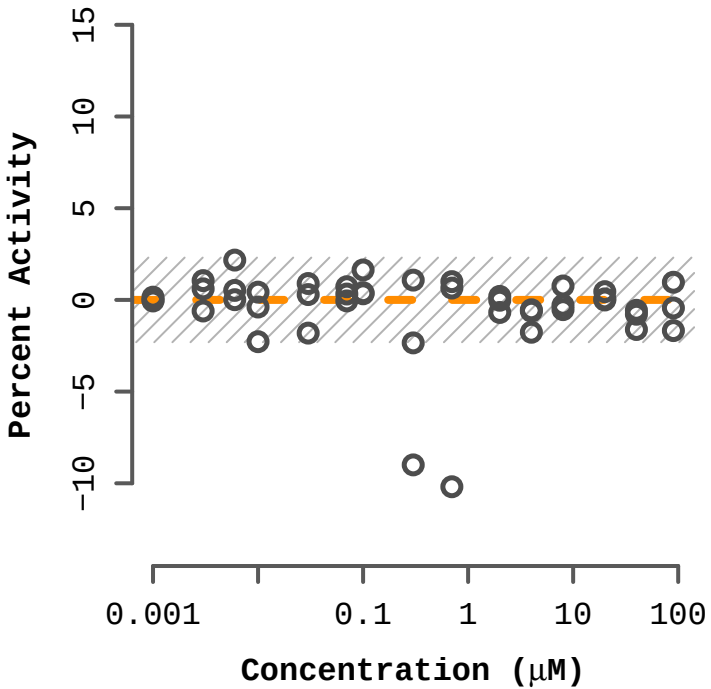
	tp	ga	gw
val:	0.433	−2.91	8
sd:	0.141	0.571	43.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.85	−1.37	6.51	−1.12	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	132.06	128.61	129.36
PROB:	0.1	0.54	0.37
RMSE:	1.05	0.92	0.91

MAX_MEAN: 2.06 MAX_MED: 2.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

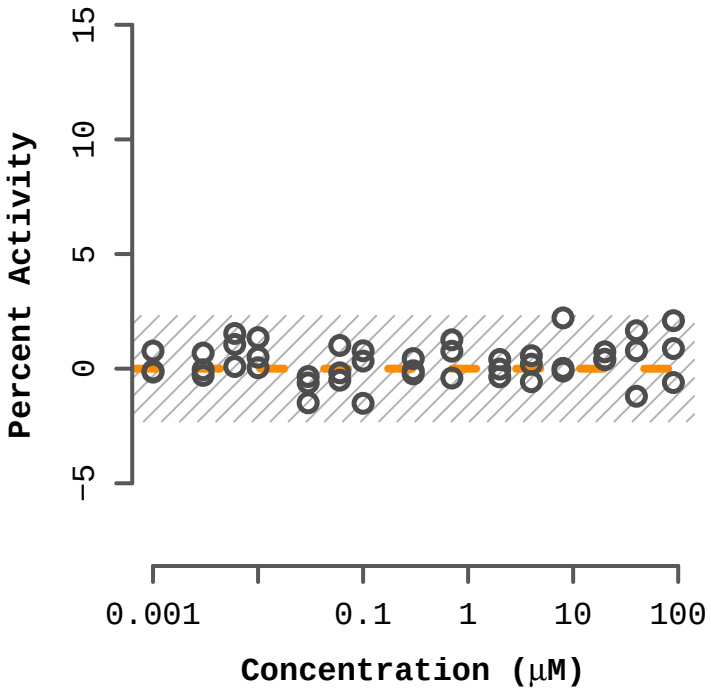
NAME: 3-Methylbenzonitrile
CHID: 26167 **CASRN:** 620-22-4
SPID(S): Tox21_200853
M4ID: 12481399

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.48	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.648 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

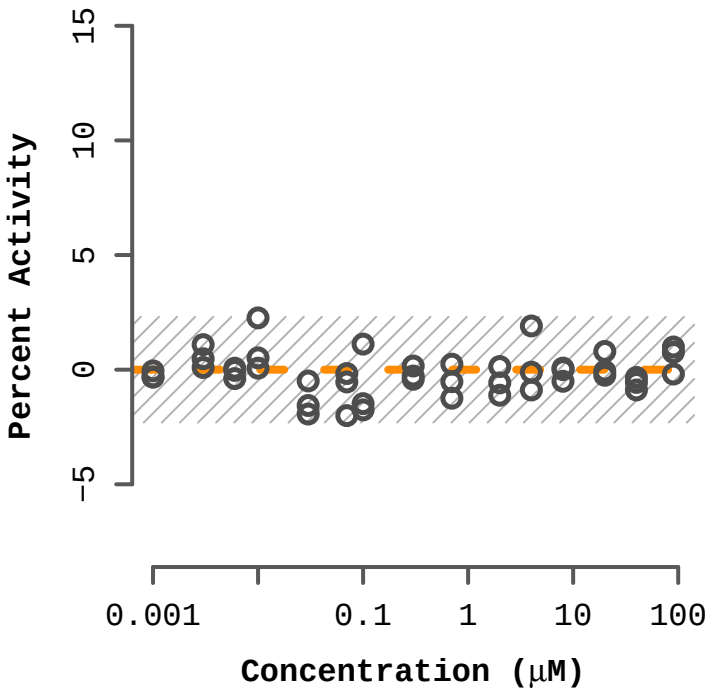
NAME: 4-Methylbenzonitrile
CHID: 26169 **CASRN:** 104-85-8
SPID(S): Tox21_200947
M4ID: 12481305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

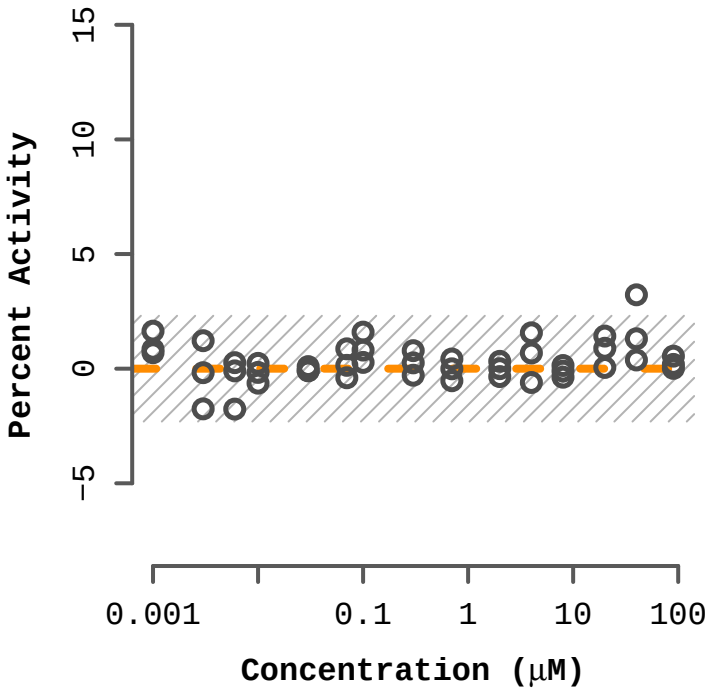
NAME: Tolyltriazole
CHID: 26171 **CASRN:** 29385-43-1
SPID(S): Tox21_303186
M4ID: 12475947

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.948 **MAX_MED:** 0.758 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

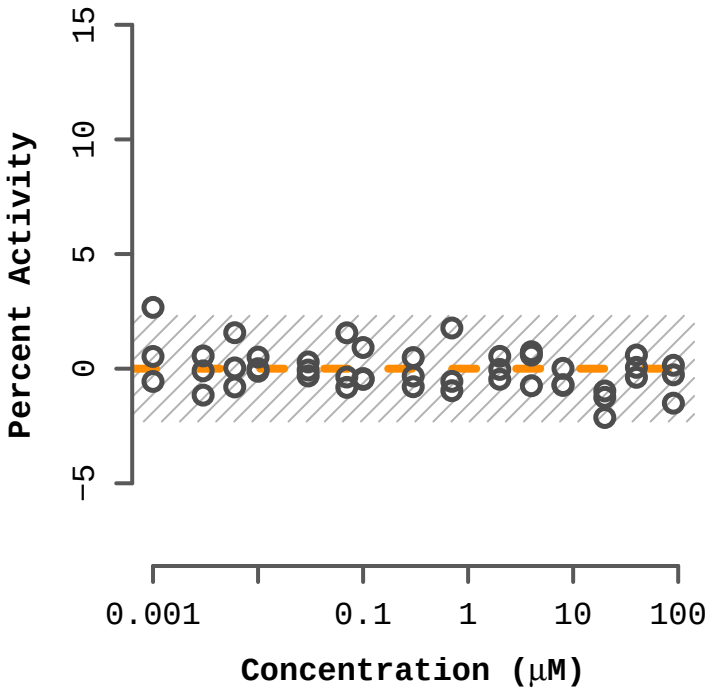
NAME: Tolyltriazole
CHID: 26171 **CASRN:** 29385-43-1
SPID(S): Tox21_201321
M4ID: 12480931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

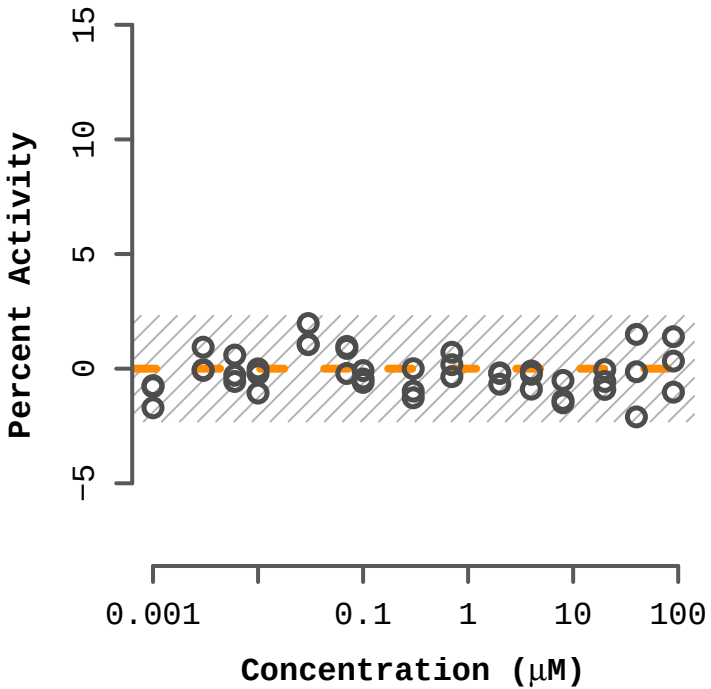
NAME: Triallylamine
CHID: 26174 **CASRN:** 102-70-5
SPID(S): Tox21_300670
M4ID: 12478463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 0.593 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

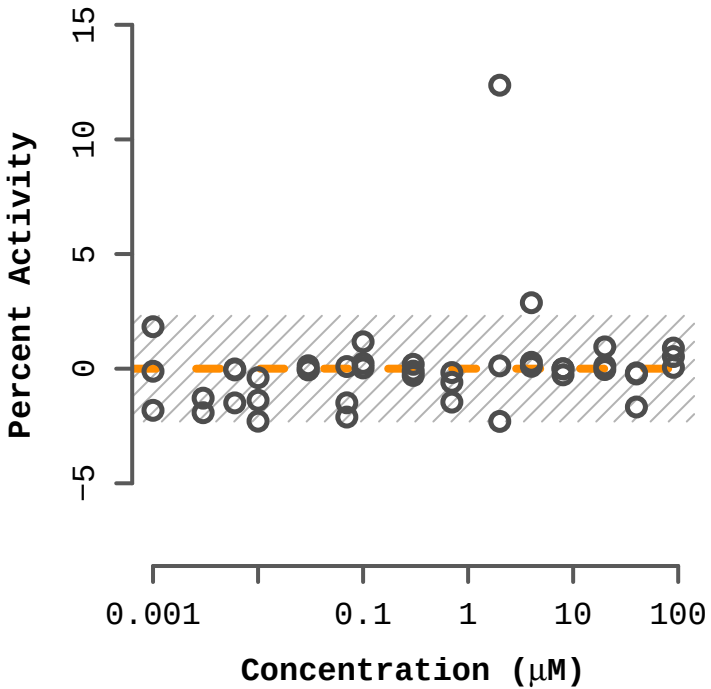
NAME: Triallyl isocyanurate
CHID: 26175 **CASRN:** 1025-15-6
SPID(S): Tox21_200270
M4ID: 12481982

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

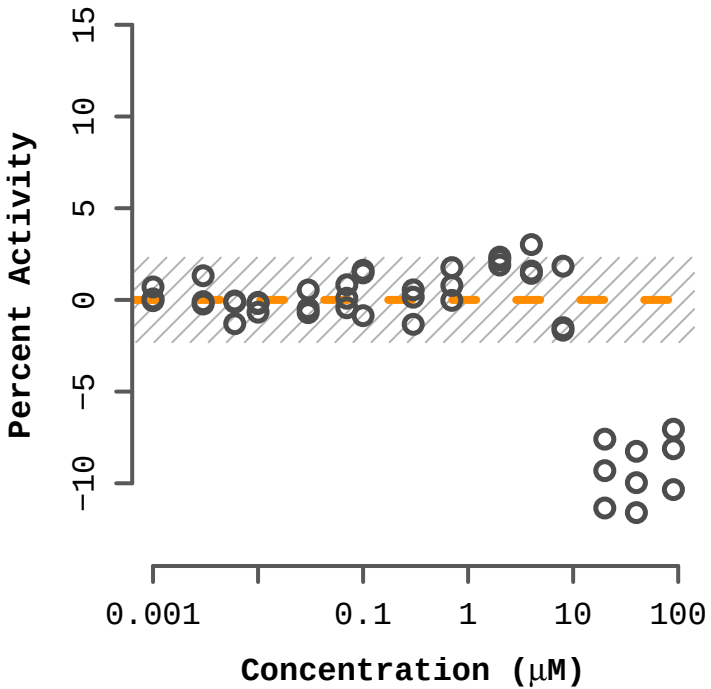
NAME: Potassium dichloroisocyanurate
CHID: 26178 **CASRN:** 2244-21-5
SPID(S): Tox21_302423
M4ID: 12476710

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.88	NA	NA
PROB:	1	NA	NA
RMSE:	2.15	NA	NA

MAX_MEAN: 3.4 **MAX_MED:** 0.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

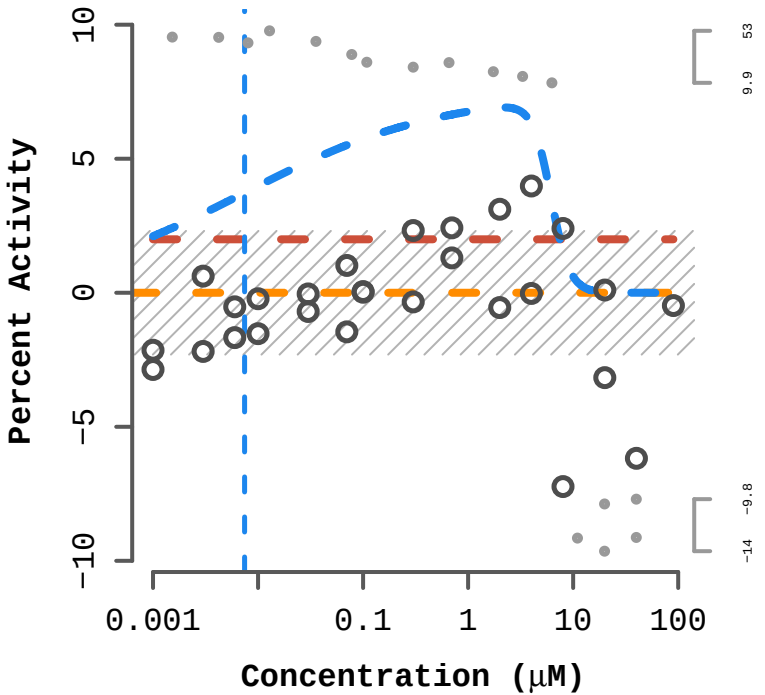
NAME: Tribromsalan
CHID: 26181 **CASRN:** 87-10-5
SPID(S): Tox21_303223
M4ID: 12475910

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.31	NA	NA
PROB:	1	NA	NA
RMSE:	4.35	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tribromsalan
CHID: 26181 CASRN: 87-10-5
SPID(S): Tox21_202442
M4ID: 12479810 BRK

HILL MODEL (in red):

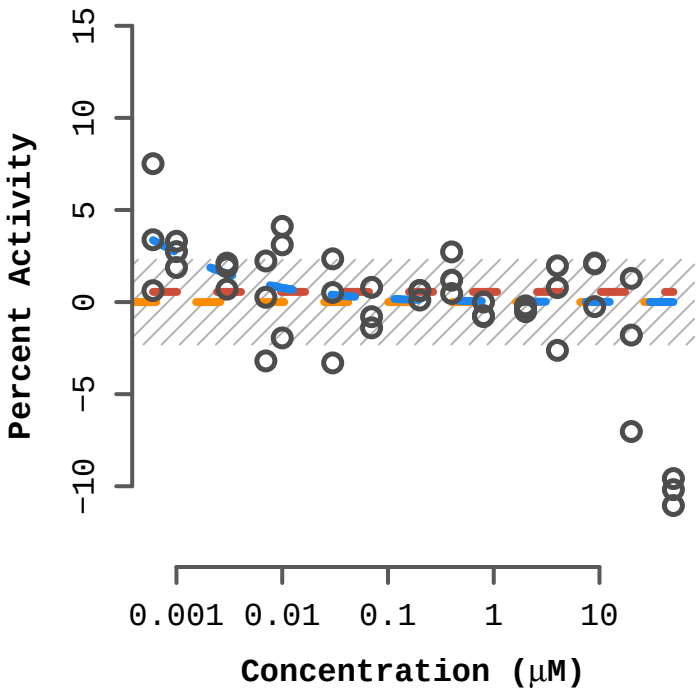
	tp	ga	gw
val:	1.99	−4.43	3.71
sd:	1.97	1830	4320

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.46	−2.13	0.463	0.789	4.89
sd:	11.5	3.77	1.72	0.688	15.8

	CNST	HILL	GNLS
AIC:	381.29	386.18	385.11
PROB:	0.81	0.07	0.12
RMSE:	18.64	17.99	17.03

MAX_MEAN: 16.9 MAX_MED: 3.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tribromsalan
CHID: 26181 CASRN: 87-10-5
SPID(S): Tox21_111700_1
M4ID: 12483530

HILL MODEL (in red):

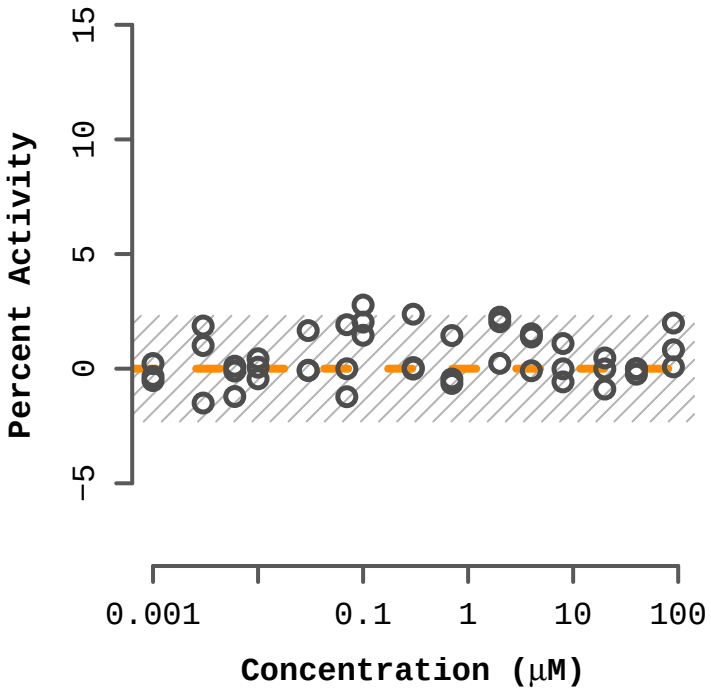
	tp	ga	gw
val:	0.553	−5.2	3.47
sd:	0.373	1180	2030

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.02	−5.22	4.17	−3.57	0.655
sd:	37	13700	28900	4.53	0.807

	CNST	HILL	GNLS
AIC:	233.62	237.57	231.75
PROB:	0.27	0.04	0.69
RMSE:	3.55	3.61	3.32

MAX_MEAN: 3.84 **MAX_MED:** 3.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

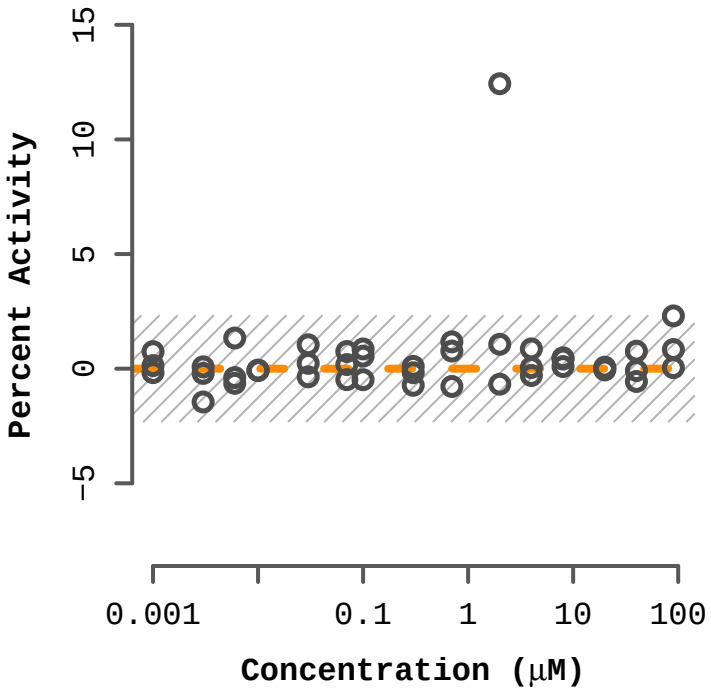
NAME: Tributylamine
CHID: 26183 **CASRN:** 102-82-9
SPID(S): Tox21_300020
M4ID: 12479110

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

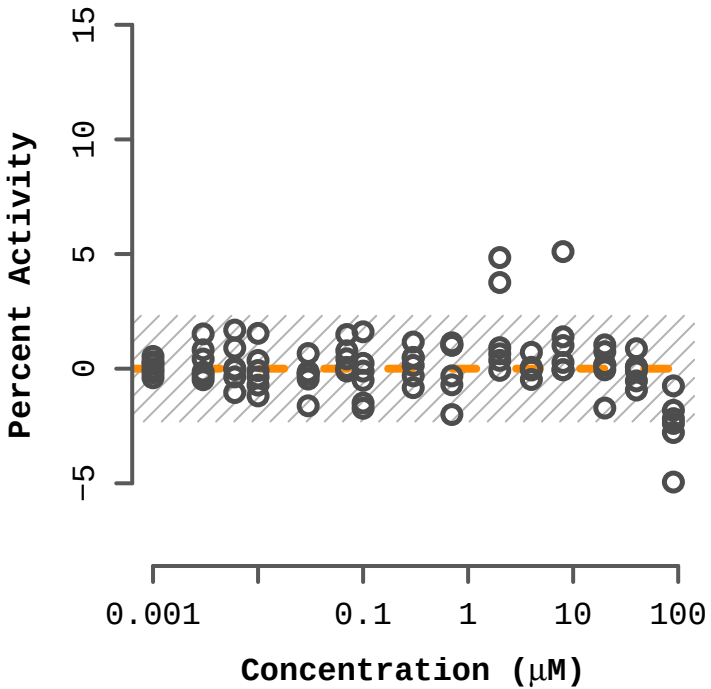
NAME: Tributylamine
CHID: 26183 **CASRN:** 102-82-9
SPID(S): Tox21_200423
M4ID: 12481829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 4.27 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

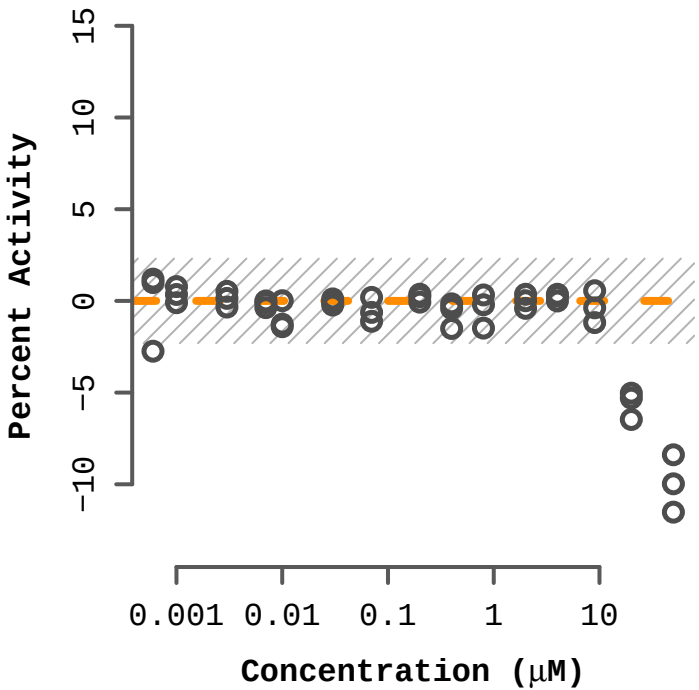
NAME: 2,2',4'−Trichloroacetophenone
CHID: 26190 **CASRN:** 4252−78−2
SPID(S): Tox21_200671
M4ID: 12481581

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	281.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 0.784 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

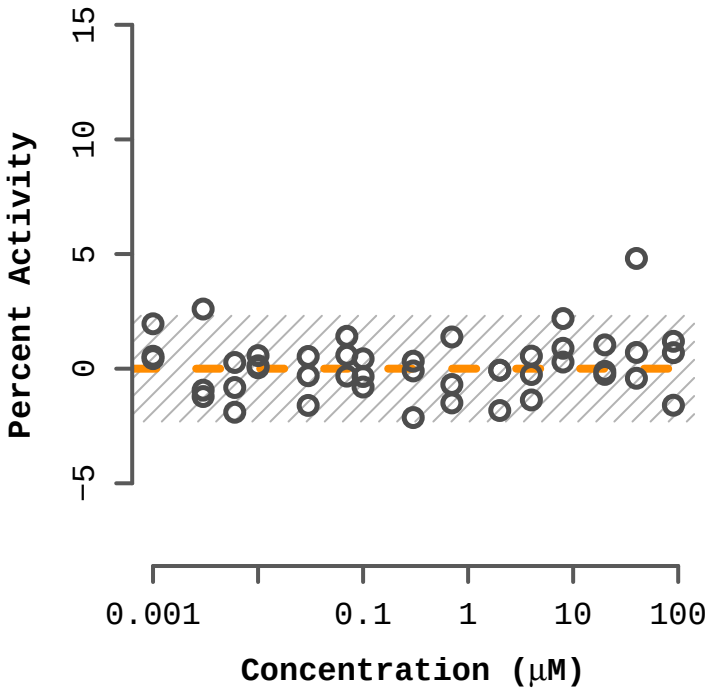
NAME: 2,2',4'−Trichloroacetophenone
CHID: 26190 **CASRN:** 4252−78−2
SPID(S): Tox21_113461_1
M4ID: 12482645

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.17	NA	NA
PROB:	1	NA	NA
RMSE:	3.06	NA	NA

MAX_MEAN: 0.346 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

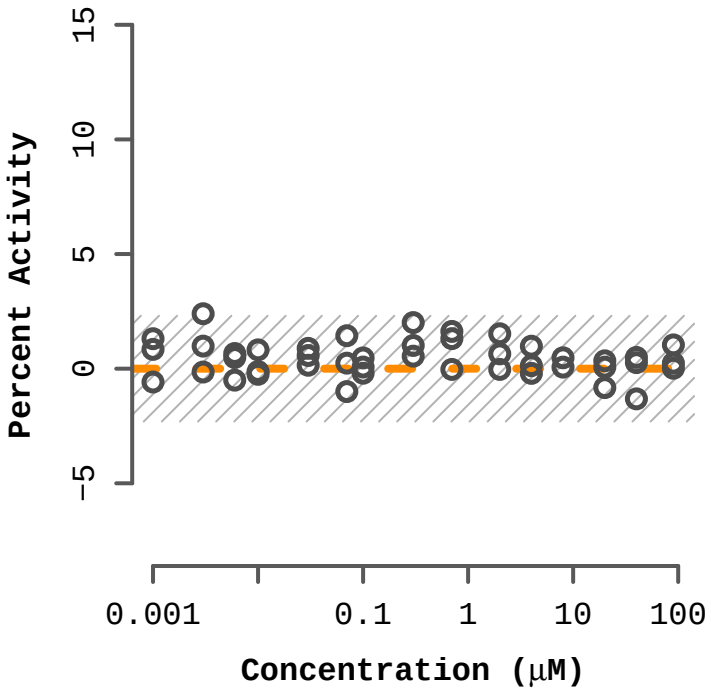
NAME: 1,2,3-Trichlorobenzene
CHID: 26193 **CASRN:** 87-61-6
SPID(S): Tox21_300501
M4ID: 12478631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 0.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

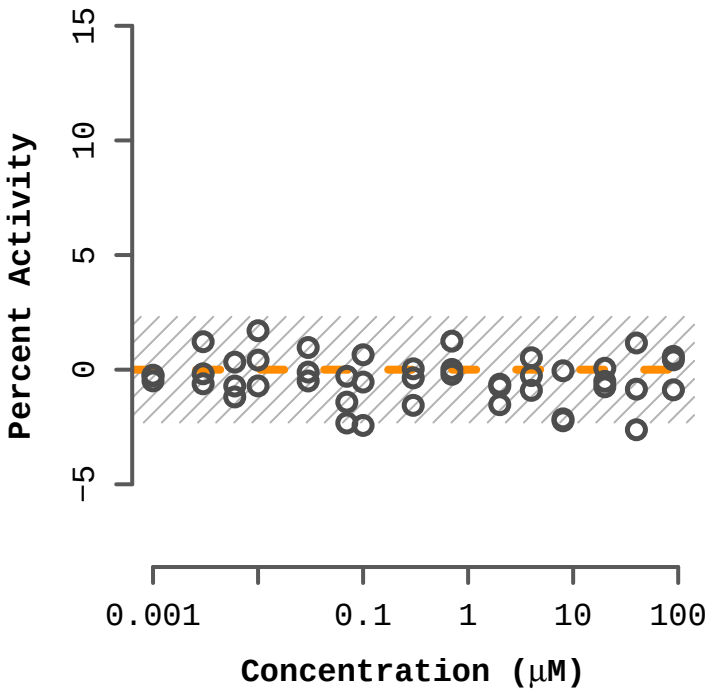
NAME: 1,2,3-Trichlorobenzene
CHID: 26193 CASRN: 87-61-6
SPID(S): Tox21_202113
M4ID: 12480139

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.19 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

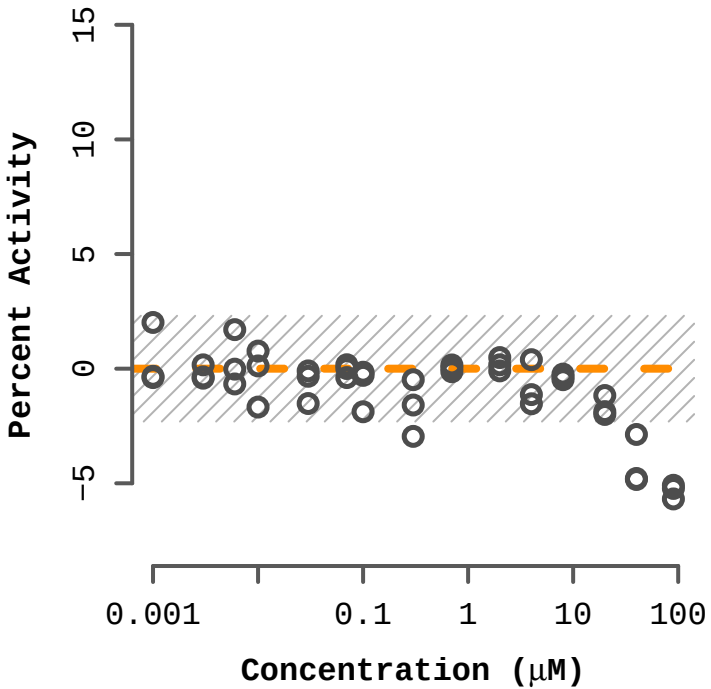
NAME: 1,3,5-Trichlorobenzene
CHID: 26195 **CASRN:** 108-70-3
SPID(S): Tox21_200279
M4ID: 12481973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.471 **MAX_MED:** 0.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

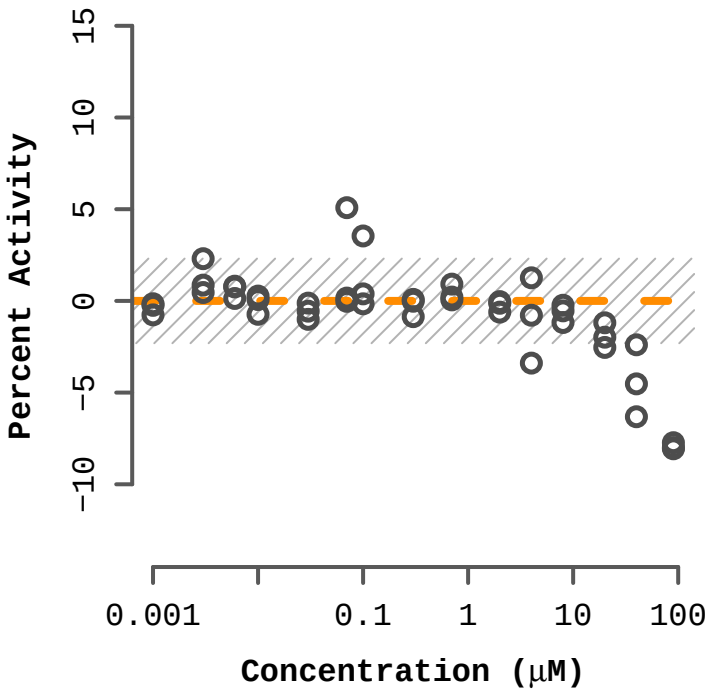
NAME: 2,3,4-Trichloronitrobenzene
CHID: 26202 CASRN: 17700-09-3
SPID(S): Tox21_200670
M4ID: 12481582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.5	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 0.433 MAX_MED: 0.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

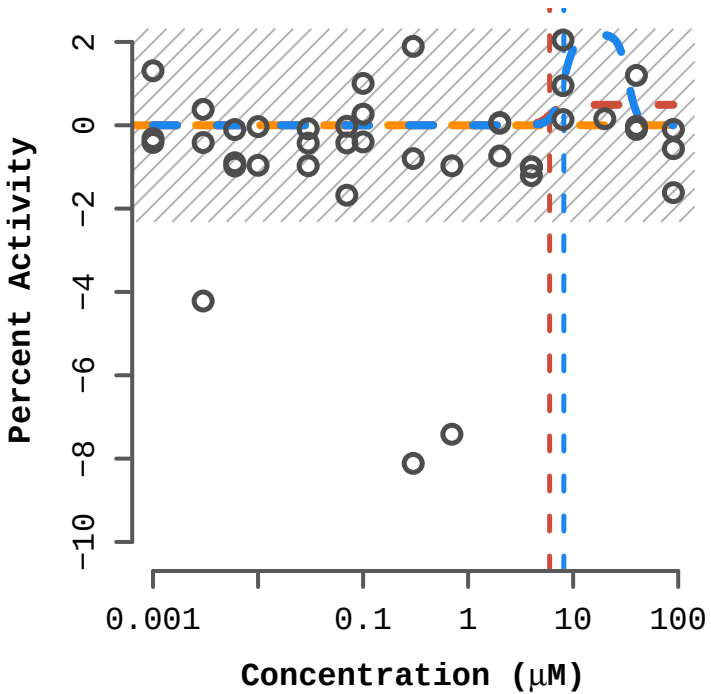
NAME: 2,4,5-Trichloronitrobenzene
CHID: 26203 **CASRN:** 89-69-0
SPID(S): Tox21_200937
M4ID: 12481315

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.72	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 0.862 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,6-Trichloronitrobenzene
CHID: 26204 **CASRN:** 18708-70-8
SPID(S): Tox21_200687
M4ID: 12481565

HILL MODEL (in red):

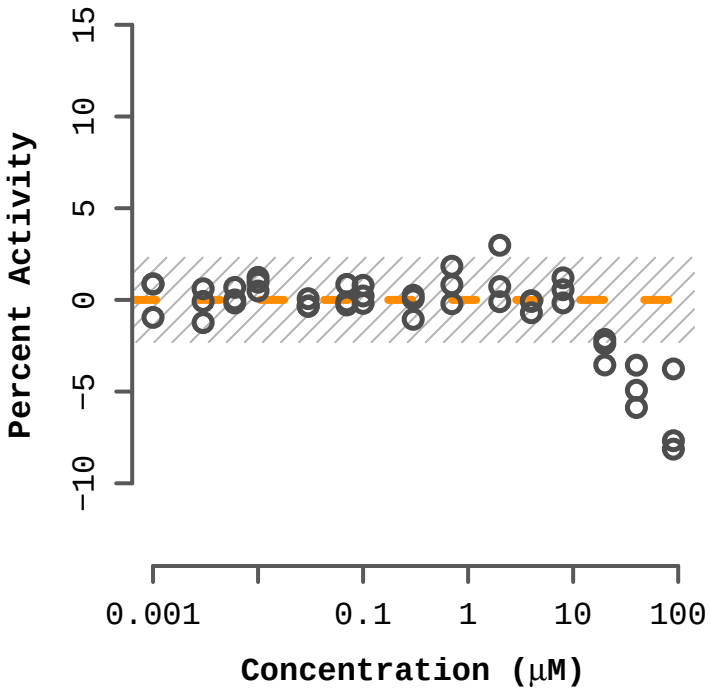
	tp	ga	gw
val:	0.491	0.776	8
sd:	0.406	0.187	9.88

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.18	0.911	8	1.52	9.53
sd:	1.2	0.0869	9.94	0.698	78.8

	CNST	HILL	GNLS
AIC:	175.65	180.1	177.45
PROB:	0.66	0.07	0.27
RMSE:	2.09	2.06	2.01

MAX_MEAN: 1.89 **MAX_MED:** 2.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

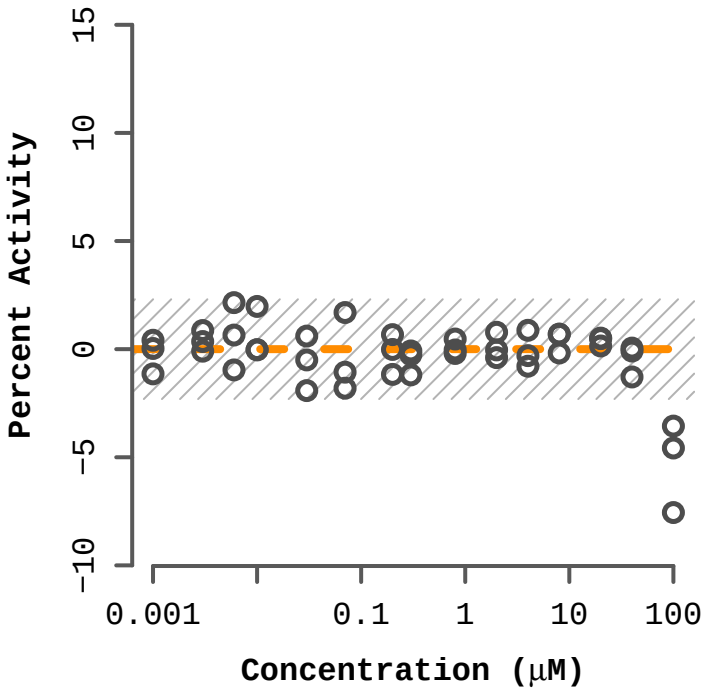
NAME: 3,4,5-Trichloronitrobenzene
CHID: 26205 **CASRN:** 20098-48-0
SPID(S): Tox21_200704
M4ID: 12481548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.4	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.968 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

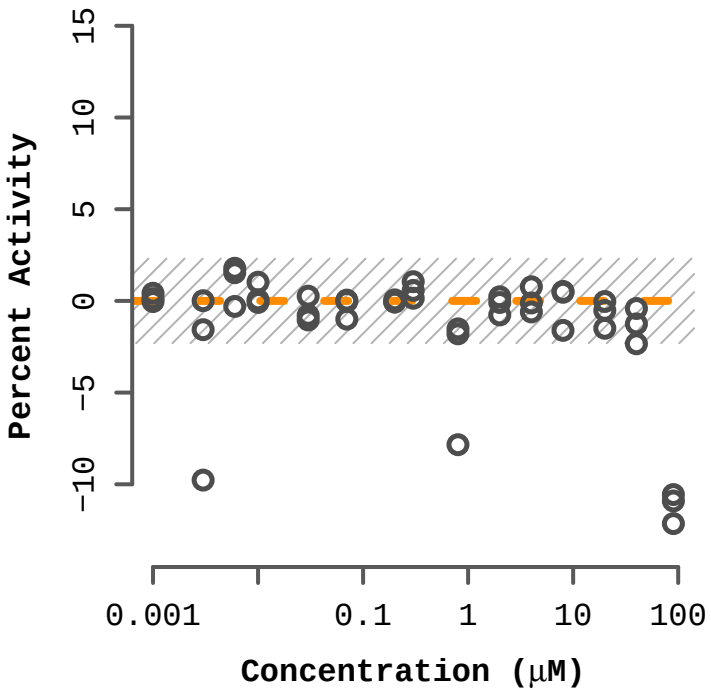
NAME: 2,3,4-Trichlorophenol
CHID: 26207 **CASRN:** 15950-66-0
SPID(S): Tox21_200297
M4ID: 12481955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 0.641 **MAX_MED:** 0.692 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

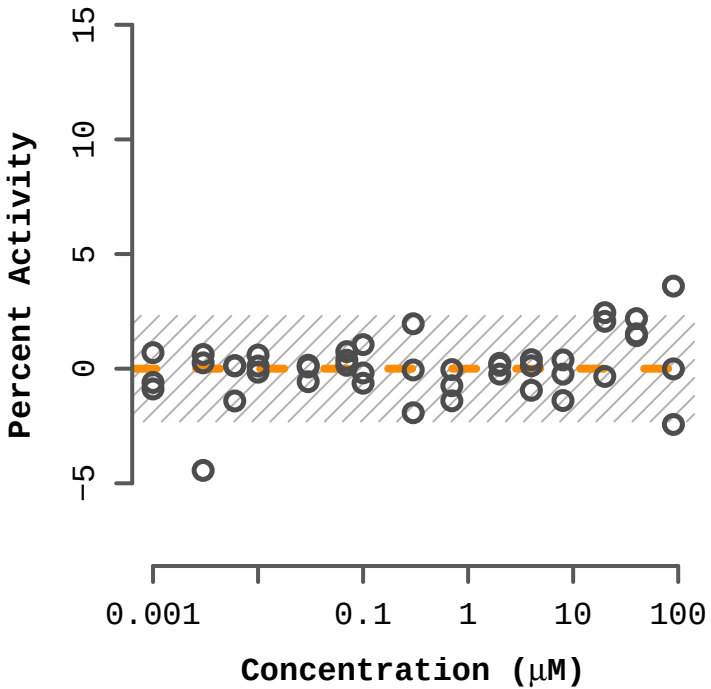
NAME: 2,3,5-Trichlorophenol
CHID: 26208 CASRN: 933-78-8
SPID(S): Tox21_200624
M4ID: 12481628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.55	NA	NA

MAX_MEAN: 1.01 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

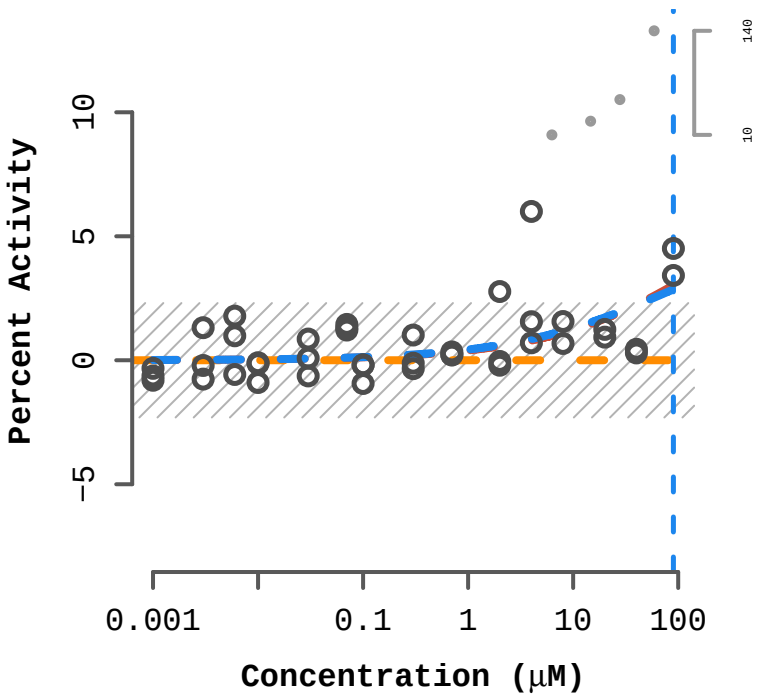
NAME: 2,3,6-Trichlorophenol
CHID: 26209 CASRN: 933-75-5
SPID(S): Tox21_303116
M4ID: 12476017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.72 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,6-Trichlorophenol
CHID: 26209 CASRN: 933-75-5
SPID(S): Tox21_201763
M4ID: 12480489 BRK

HILL MODEL (in red):

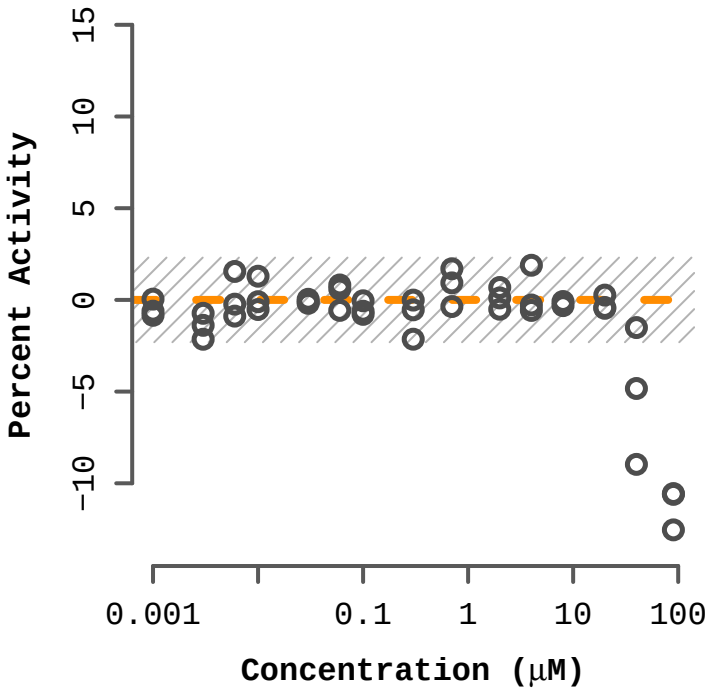
	tp	ga	gw
val:	8.66	2.45	0.538
sd:	17.6	2.3	0.249

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.71	1.95	0.556	3.48	4.95
sd:	10.4	2.24	0.262	765	2500

	CNST	HILL	GNLS
AIC:	263.06	254.4	258.69
PROB:	0.01	0.88	0.1
RMSE:	22.16	21.55	21.58

MAX_MEAN: 47.8 MAX_MED: 4.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

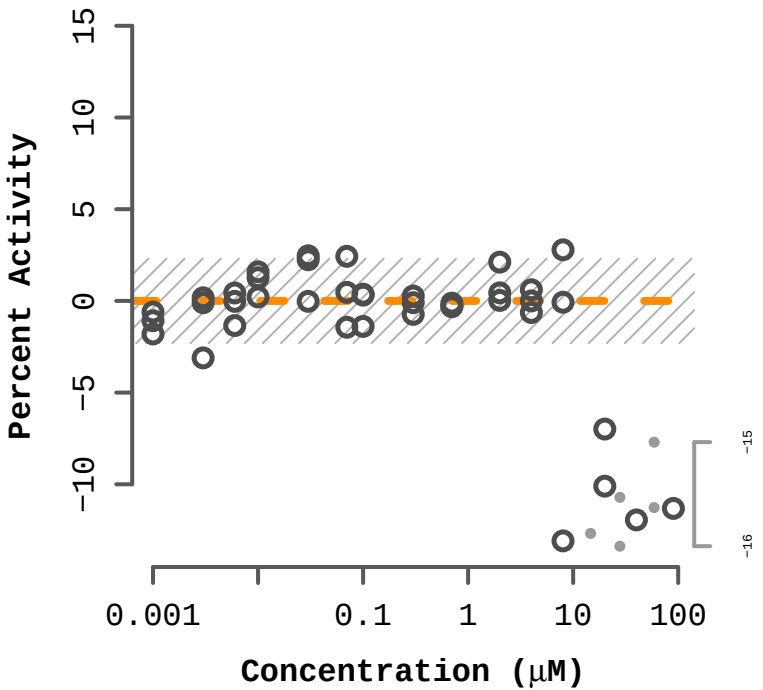
NAME: 3,4,5-Trichlorophenol
CHID: 26212 CASRN: 609-19-8
SPID(S): Tox21_200188
M4ID: 12482064

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 0.756 MAX_MED: 0.929 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

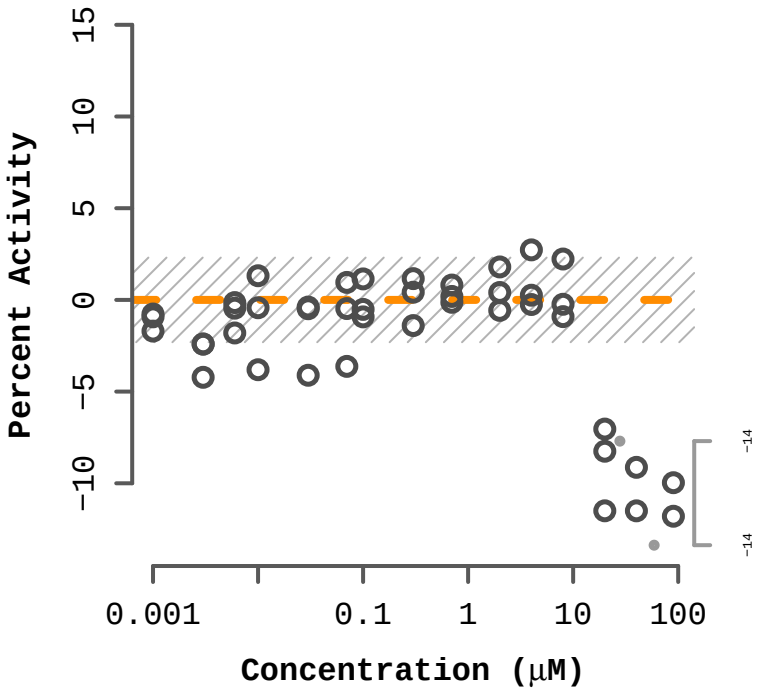
NAME: Triclocarban
CHID: 26214 **CASRN:** 101-20-2
SPID(S): Tox21_300481
M4ID: 12478651 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.34	NA	NA
PROB:	1	NA	NA
RMSE:	6.39	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

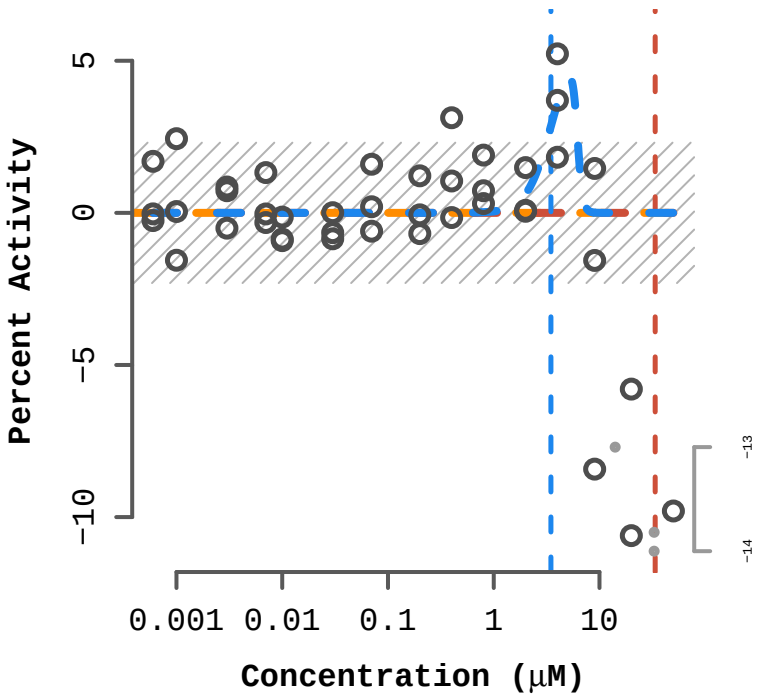
NAME: Triclocarban
CHID: 26214 **CASRN:** 101-20-2
SPID(S): Tox21_202030
M4ID: 12480222 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	266.69	NA	NA
PROB:	1	NA	NA
RMSE:	5.18	NA	NA

MAX_MEAN: 0.912 **MAX_MED:** 0.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triclocarban
CHID: 26214 CASRN: 101-20-2
SPID(S): Tox21_112078_1
M4ID: 12483333 BRK

HILL MODEL (in red):

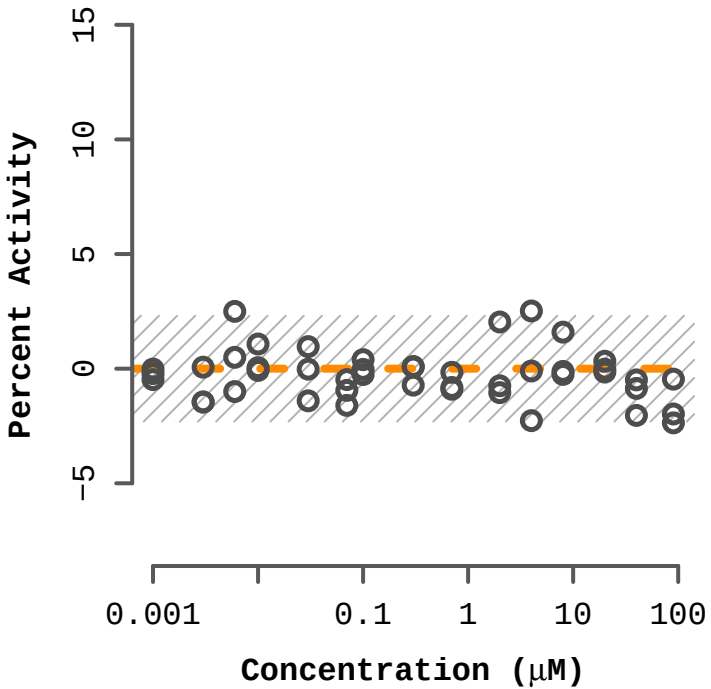
	tp	ga	gw
val:	8.7e-10	1.53	1.71
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.7	0.541	3.81	0.791	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	245.78	251.78	248.1
PROB:	0.73	0.04	0.23
RMSE:	4.59	4.59	4.49

MAX_MEAN: 3.59 MAX_MED: 3.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

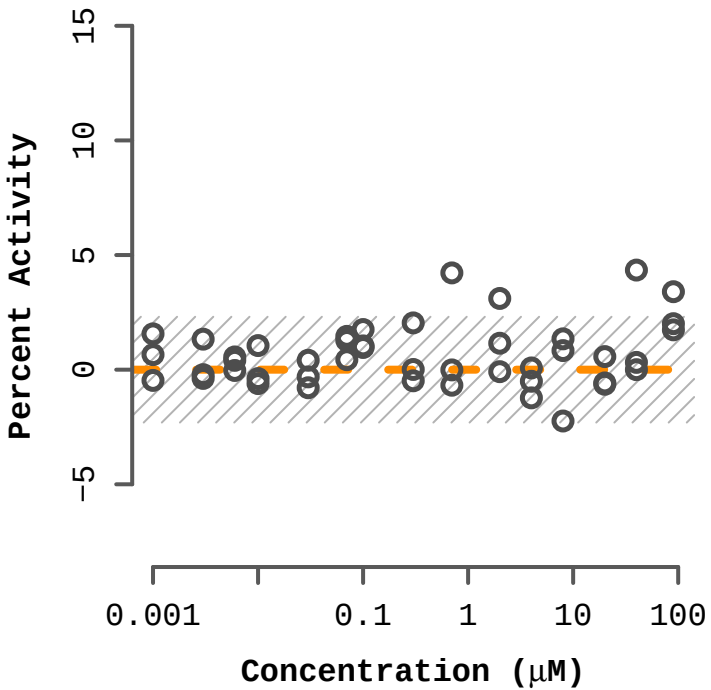
NAME: Tri-m-tolyl phosphate
CHID: 26216 **CASRN:** 563-04-2
SPID(S): Tox21_303758
M4ID: 12475430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.667 **MAX_MED:** 0.495 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

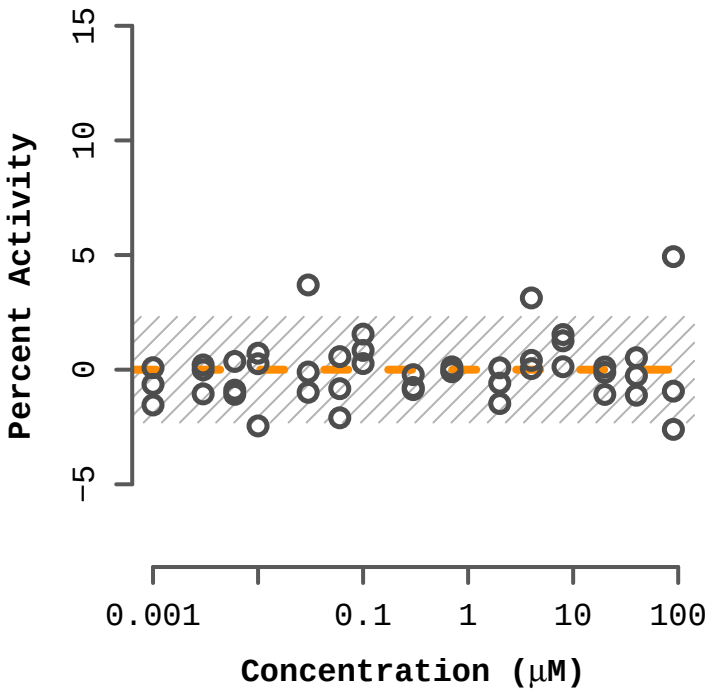
NAME: Triethanolamine stearate
CHID: 26219 **CASRN:** 4568-28-9
SPID(S): Tox21_200858
M4ID: 12481394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

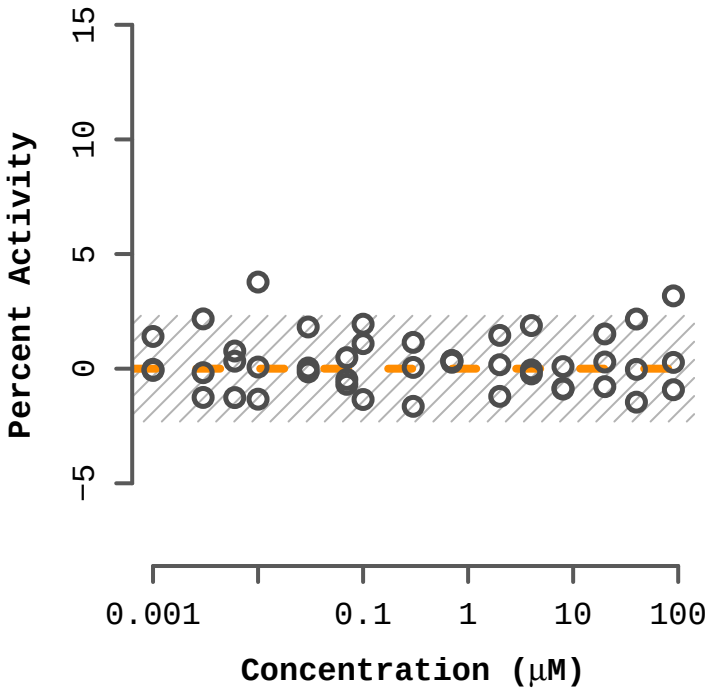
NAME: 2,4,5-Triethoxyacetophenone
CHID: 26220 **CASRN:** 63213-29-6
SPID(S): Tox21_201041
M4ID: 12481211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

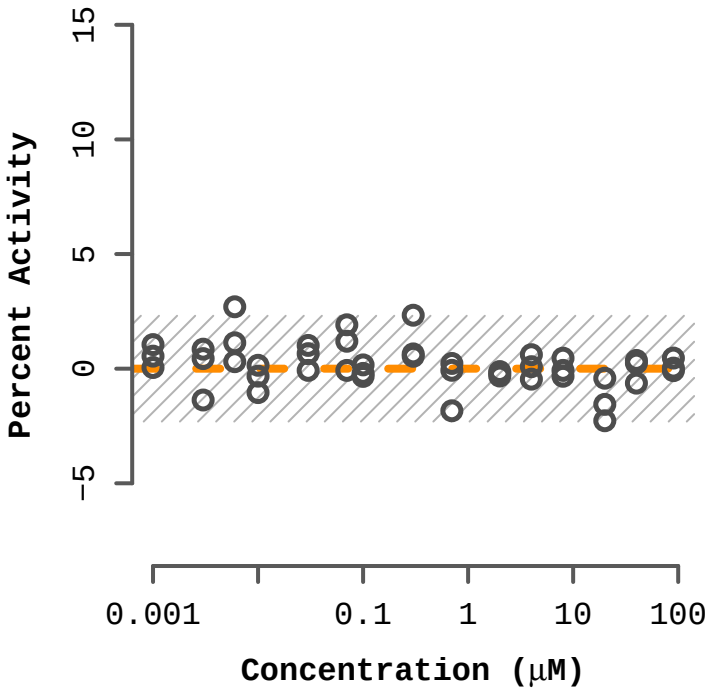
NAME: Triethylene glycol diacetate
CHID: 26223 **CASRN:** 111-21-7
SPID(S): Tox21_300597
M4ID: 12478536

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.845 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

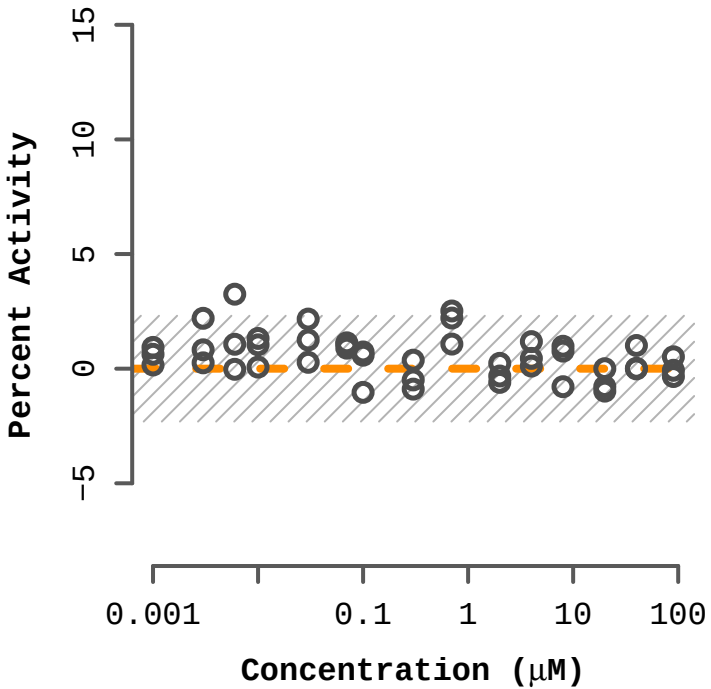
NAME: Triethylene glycol diacetate
CHID: 26223 **CASRN:** 111-21-7
SPID(S): Tox21_201270
M4ID: 12480982

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

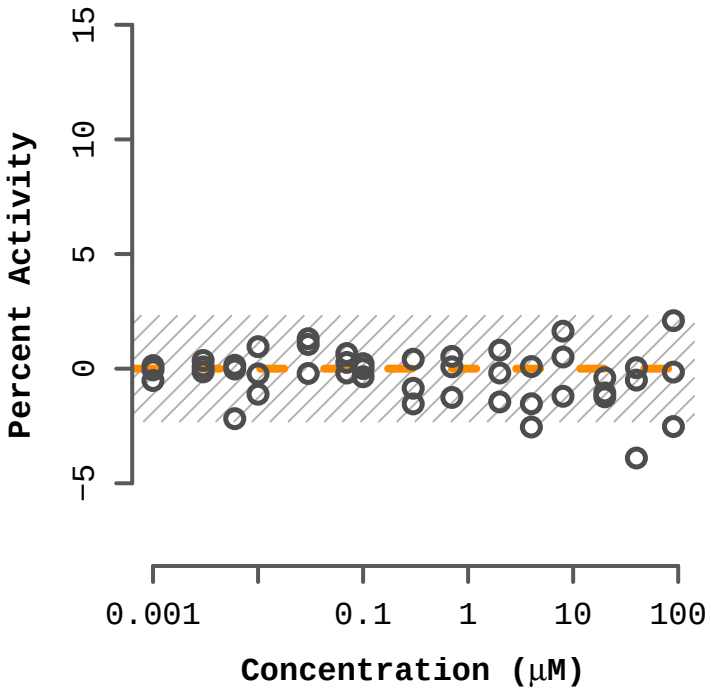
NAME: Triethylene glycol dimethyl ether
CHID: 26224 CASRN: 112-49-2
SPID(S): Tox21_300509
M4ID: 12478623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

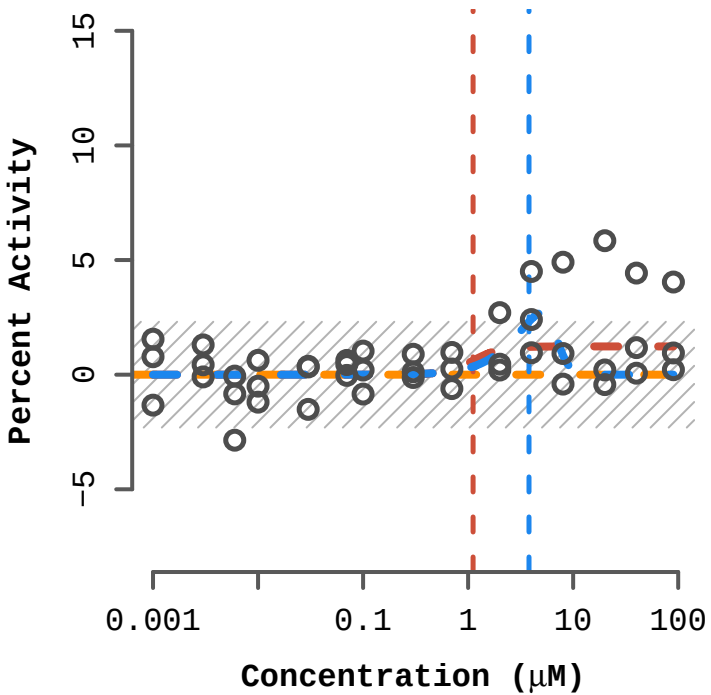
NAME: Triethyl phosphate
CHID: 26228 CASRN: 78-40-0
SPID(S): Tox21_303106
M4ID: 12476027

HILL MODEL: Not applicable.

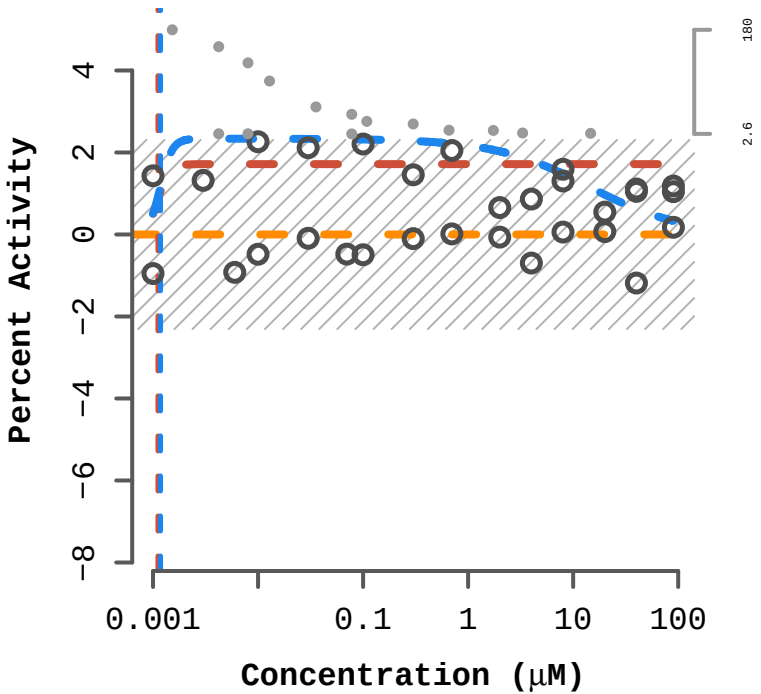
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.72 **MAX_MED:** 1.06 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Triethyl phosphate
CHID:    26228   CASRN: 78-40-0
SPID(S): Tox21_202463
M4ID:    12479789

HILL MODEL (in red):
      tp       ga       gw
val:  1.23     0.0472   3.3
sd:   0.424    0.45     4.97

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.69     0.579    2.04     0.829    7.47
sd:   13.3     1.19     4.25     0.663    59.6

      CNST        HILL        GNLS
AIC:  174.96      168.74      174.07
PROB: 0.04        0.9         0.06
RMSE: 1.87        1.51        1.67

MAX_MEAN: 2.62      MAX_MED: 2.41      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,8,9−Trihydroxyanthracene
CHID: 26231 CASRN: 480−22−8
SPID(S): Tox21_202894
M4ID: 12479358 BRK

HILL MODEL (in red):

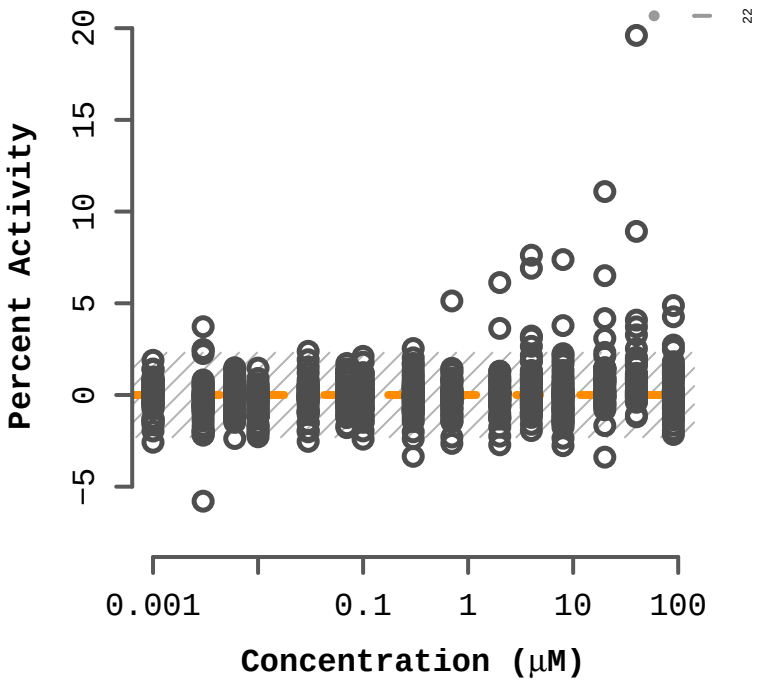
	tp	ga	gw
val:	1.72	−2.95	8
sd:	0.8	0.791	119

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.34	−2.93	7.78	1.15	0.967
sd:	1.24	3.31	361	1.31	1.87

	CNST	HILL	GNLS
AIC:	394.16	395.25	398.5
PROB:	0.59	0.34	0.07
RMSE:	42.59	42.09	41.93

MAX_MEAN: 59.3 **MAX_MED:** 2.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

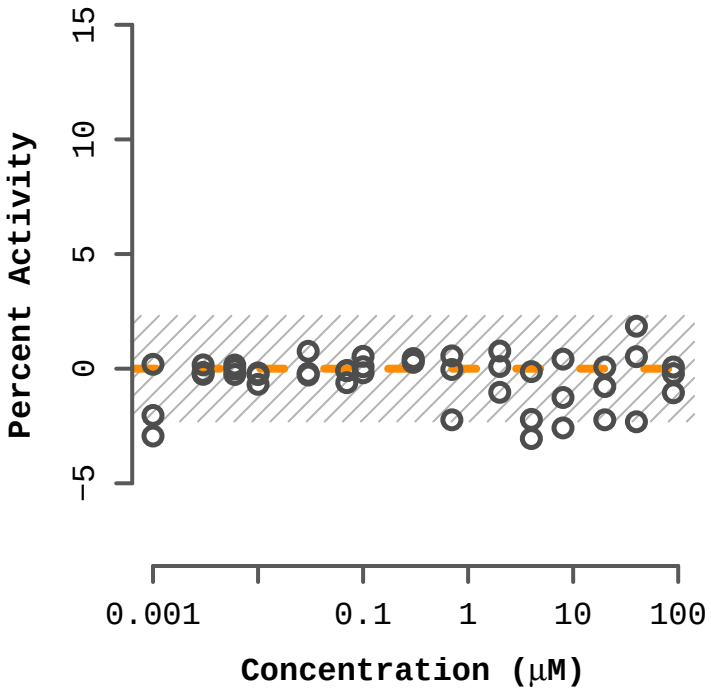
NAME: 2',4',5'−Trihydroxybutyrophenone
CHID: 26232 CASRN: 1421−63−2
SPID(S): Tox21_400052
M4ID: 12475085 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2257.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 1.33 MAX_MED: 0.724 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

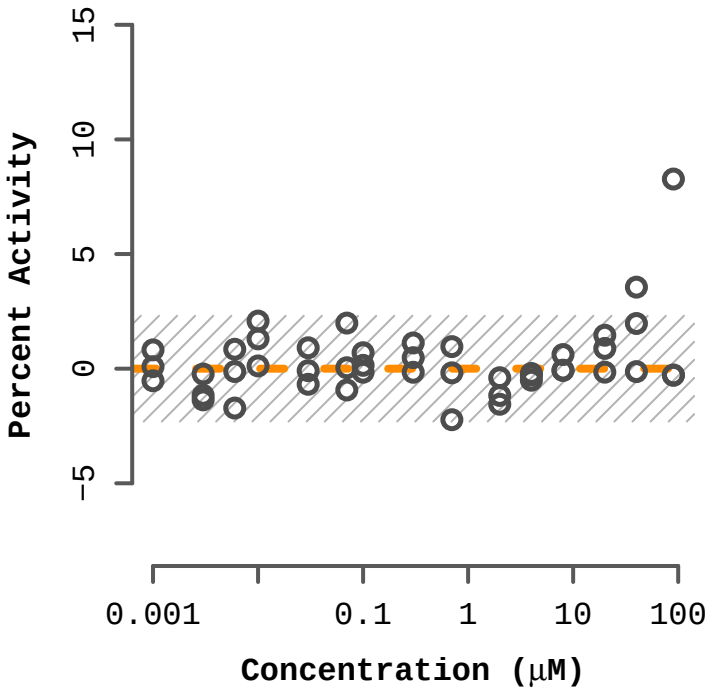
NAME: Trimellitic anhydride
CHID: 26235 CASRN: 552-30-7
SPID(S): Tox21_303117
M4ID: 12476016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.363 MAX_MED: 0.526 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

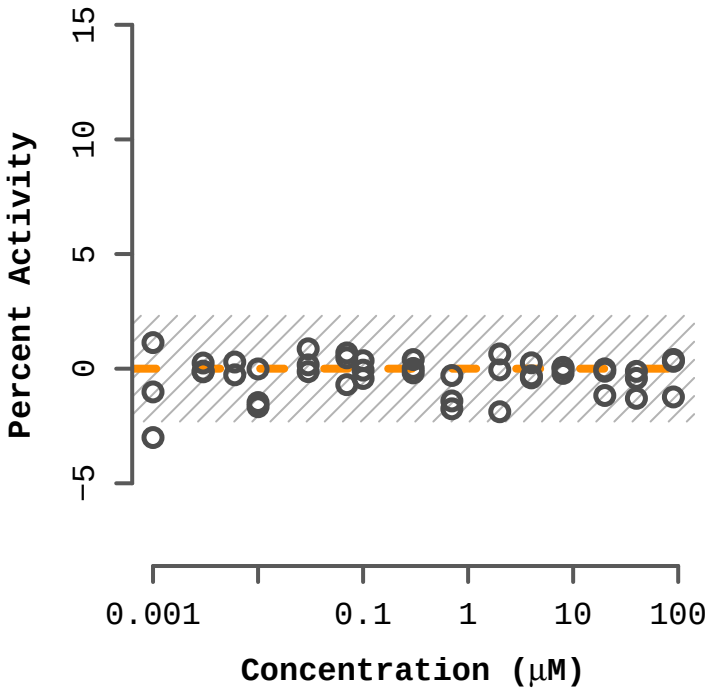
NAME: Trimellitic anhydride
CHID: 26235 **CASRN:** 552-30-7
SPID(S): Tox21_202066
M4ID: 12480186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 2.57 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

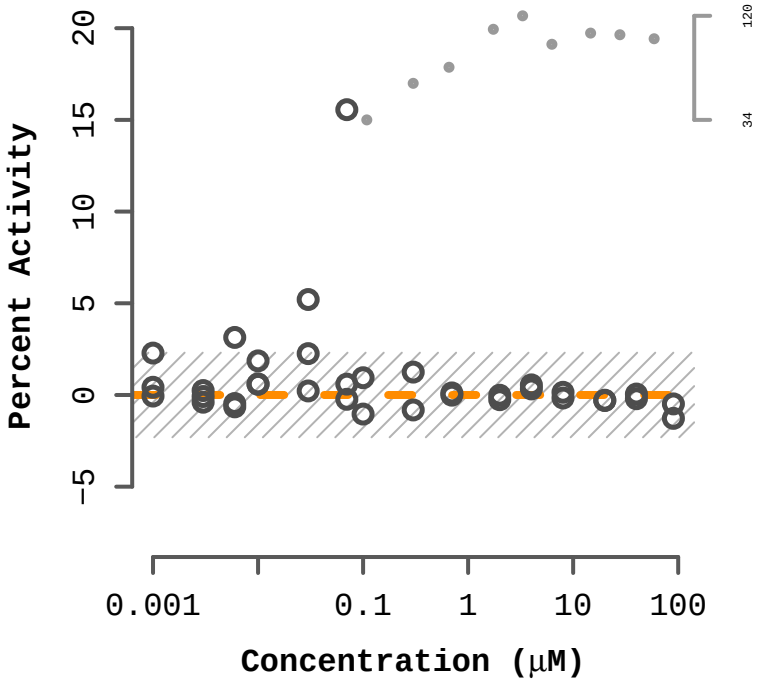
NAME: Trimethylamine
CHID: 26238 **CASRN:** 75-50-3
SPID(S): Tox21_302355
M4ID: 12476778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.304 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

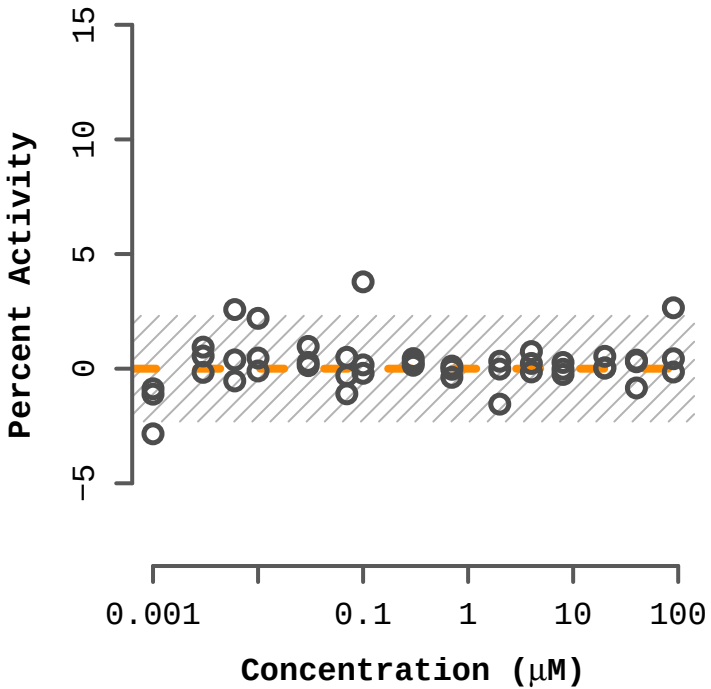
NAME: 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1-penten-
CHID: 26240 CASRN: 7779-30-8
SPID(S): Tox21_201192
M4ID: 12481060 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	432.52	NA	NA
PROB:	1	NA	NA
RMSE:	40.83	NA	NA

MAX_MEAN: 39 MAX_MED: 2.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

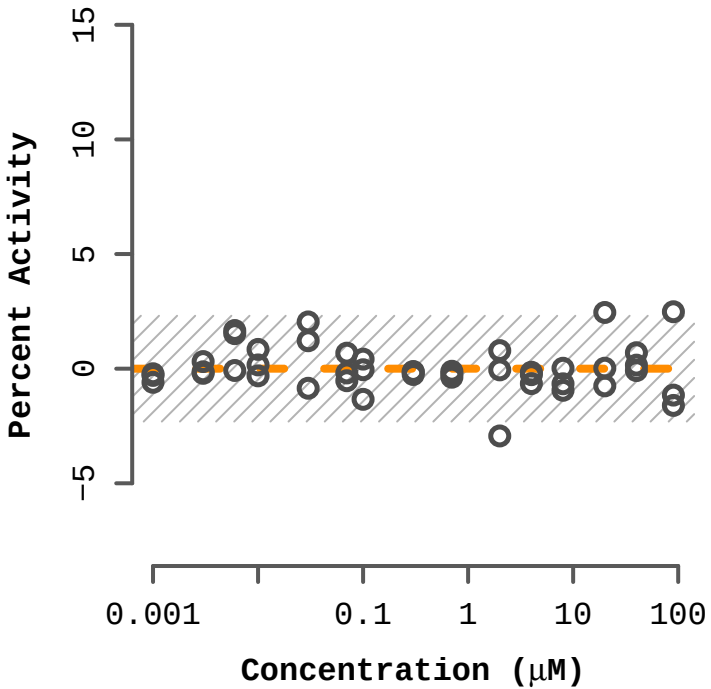
NAME: 3,3,5-Trimethylcyclohexyl salicylate
CHID: 26241 CASRN: 118-56-9
SPID(S): Tox21_303082
M4ID: 12476051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.553 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

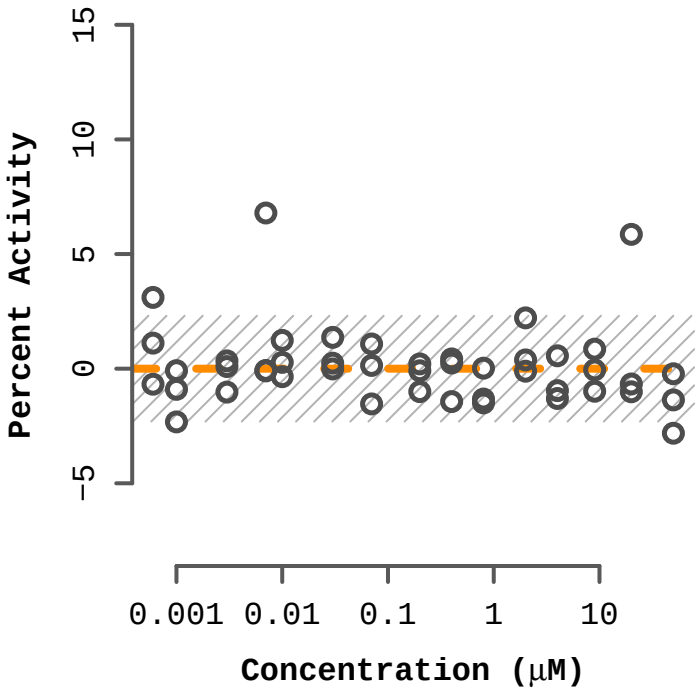
NAME: 3,3,5-Trimethylcyclohexyl salicylate
CHID: 26241 CASRN: 118-56-9
SPID(S): Tox21_202109
M4ID: 12480143

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

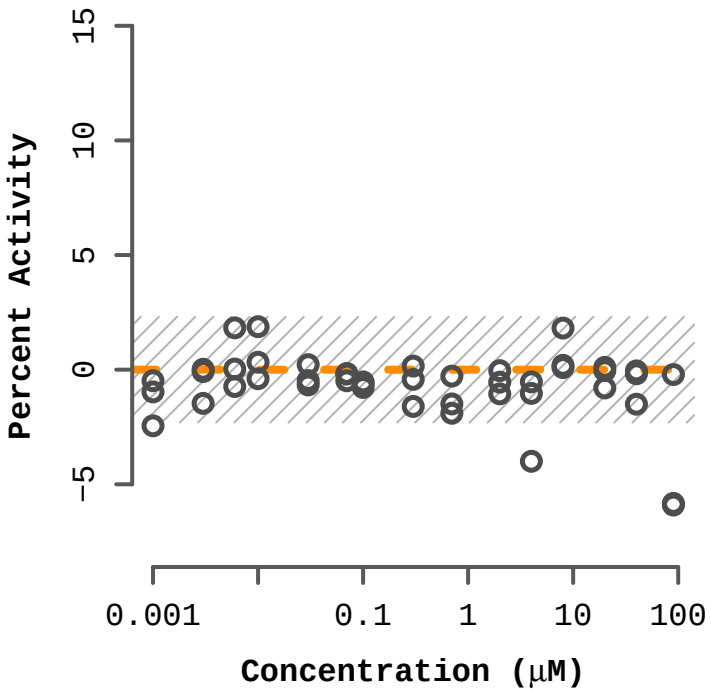
NAME: 3,3,5-Trimethylcyclohexyl salicylate
CHID: 26241 **CASRN:** 118-56-9
SPID(S): Tox21_111174_1
M4ID: 12483863

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

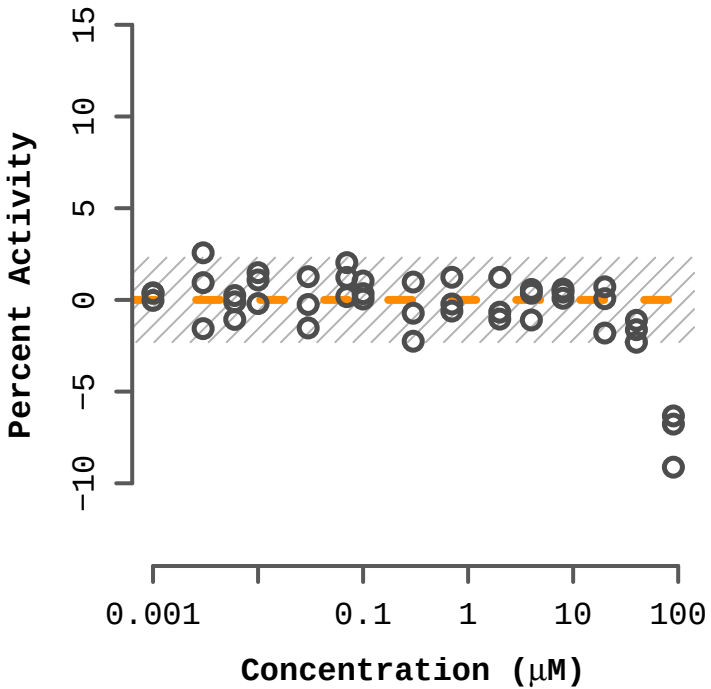
NAME: Triphenylphosphine
CHID: 26251 **CASRN:** 603-35-0
SPID(S): Tox21_303294
M4ID: 12475839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 0.7 **MAX_MED:** 0.327 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

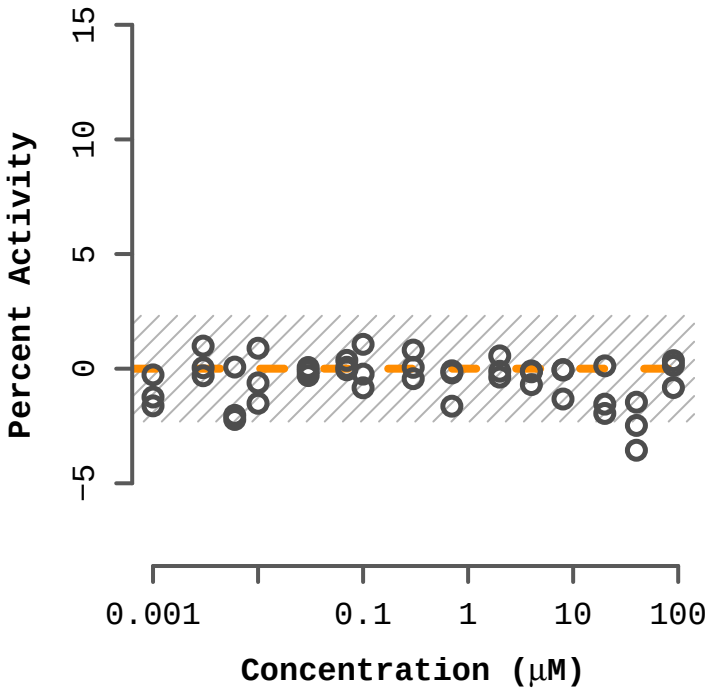
NAME: Triphenylphosphine
CHID: 26251 **CASRN:** 603-35-0
SPID(S): Tox21_202114
M4ID: 12480138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.5	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

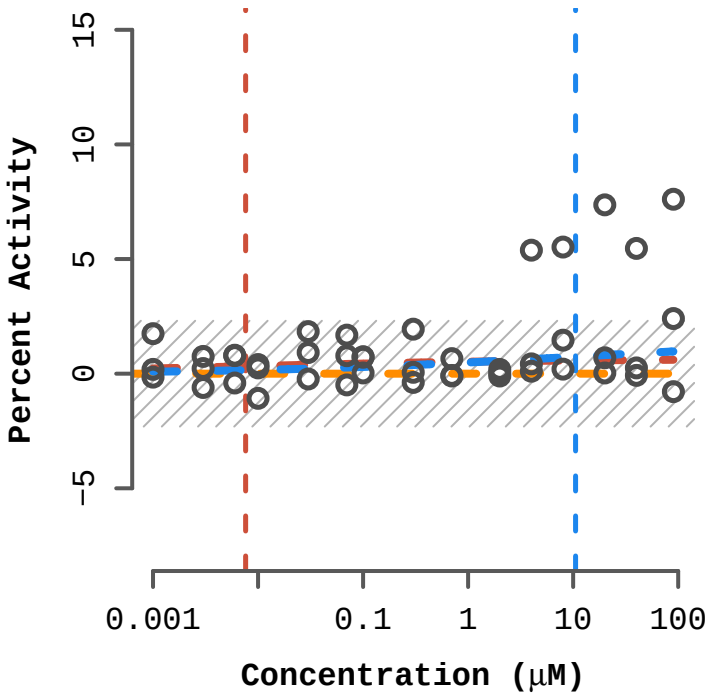
NAME: Triphenyl phosphite
CHID: 26252 **CASRN:** 101-02-0
SPID(S): Tox21_300002
M4ID: 12479128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.242 **MAX_MED:** 0.145 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triphenyl phosphite
CHID: 26252 CASRN: 101-02-0
SPID(S): Tox21_202034
M4ID: 12480218

HILL MODEL (in red):

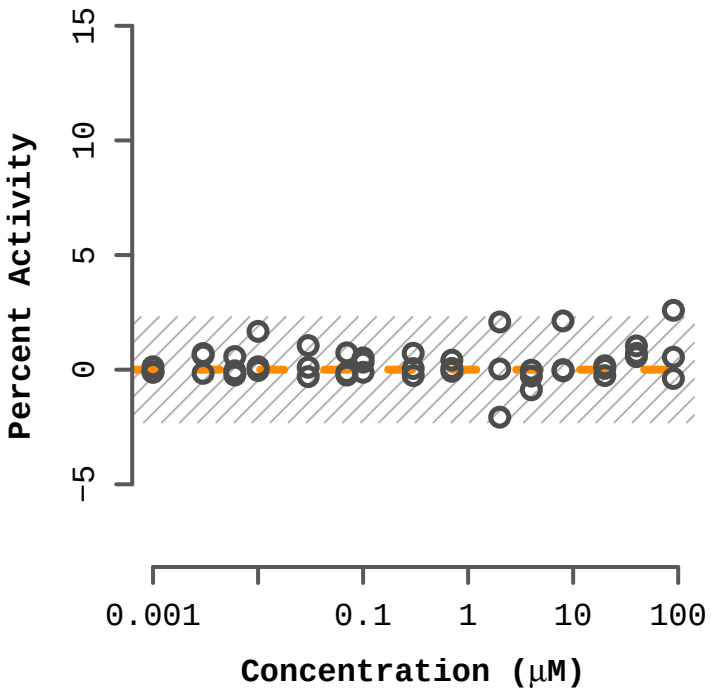
	tp	ga	gw
val:	0.642	−2.12	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.48	1.02	0.3	2.52	13.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	178.06	176.24	180.56
PROB:	0.27	0.66	0.08
RMSE:	2.27	2.06	2

MAX_MEAN: 3.08 MAX_MED: 2.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

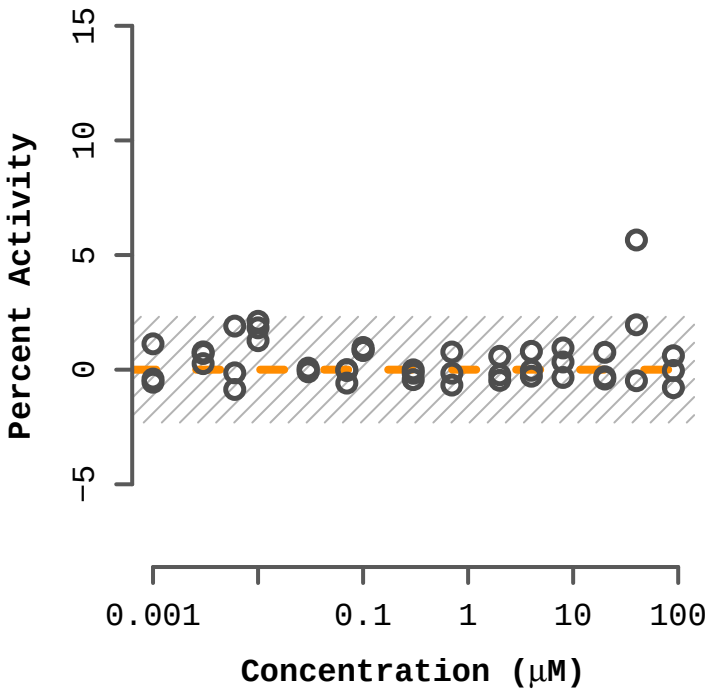
NAME: Tris(2-chloroethyl) phosphite
CHID: 26258 CASRN: 140-08-9
SPID(S): Tox21_303066
M4ID: 12476067

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.918 MAX_MED: 0.713 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

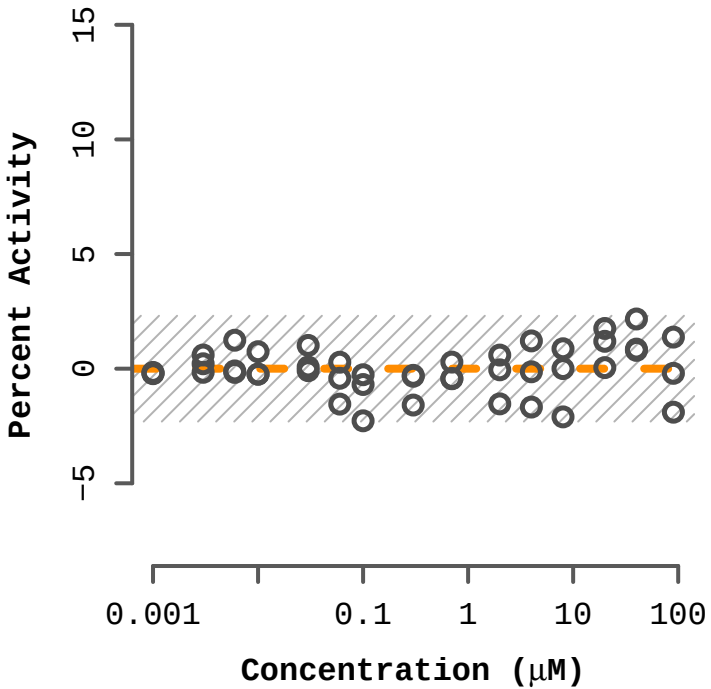
NAME: Tris(2-chloroethyl) phosphite
CHID: 26258 **CASRN:** 140-08-9
SPID(S): Tox21_202136
M4ID: 12480116

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

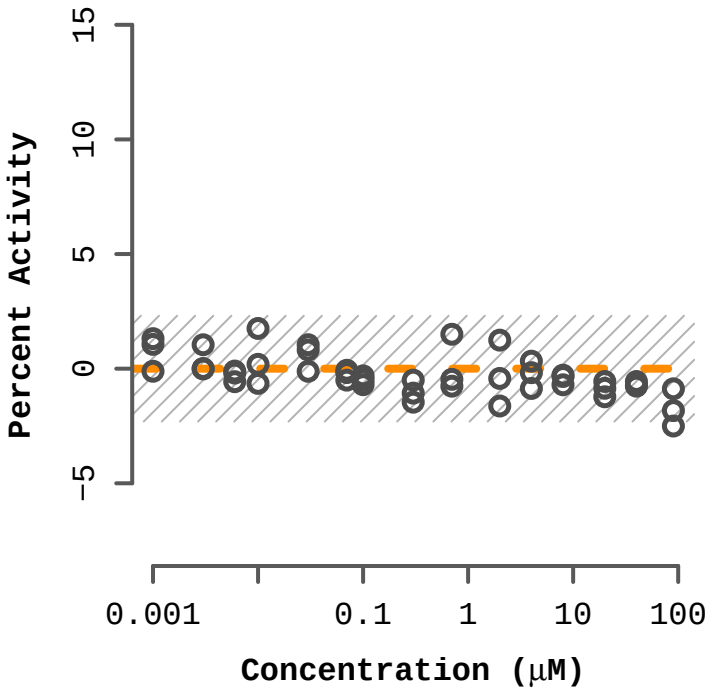
NAME: Tris(2-chloroisopropyl)phosphate
CHID: 26259 **CASRN:** 13674-84-5
SPID(S): Tox21_303533
M4ID: 12475611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

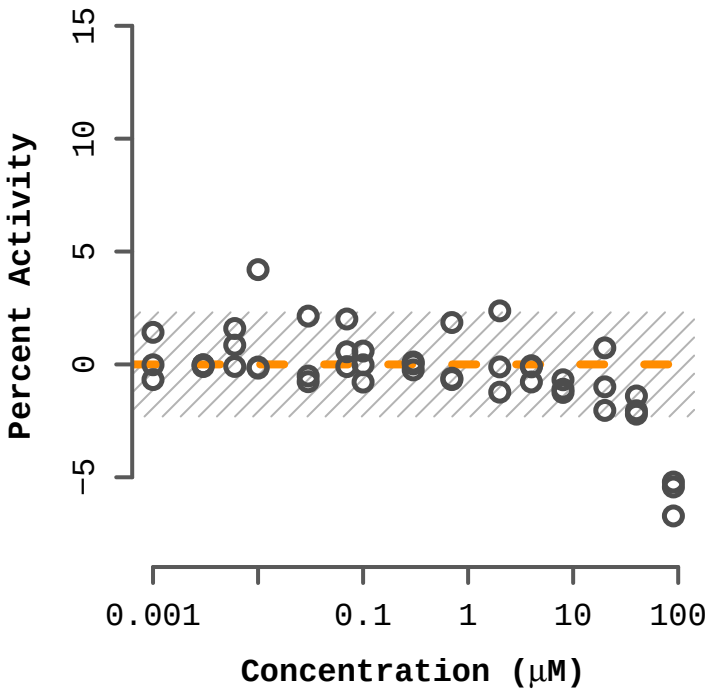
NAME: Tris(2-chloroisopropyl)phosphate
CHID: 26259 **CASRN:** 13674-84-5
SPID(S): Tox21_202982
M4ID: 12479270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

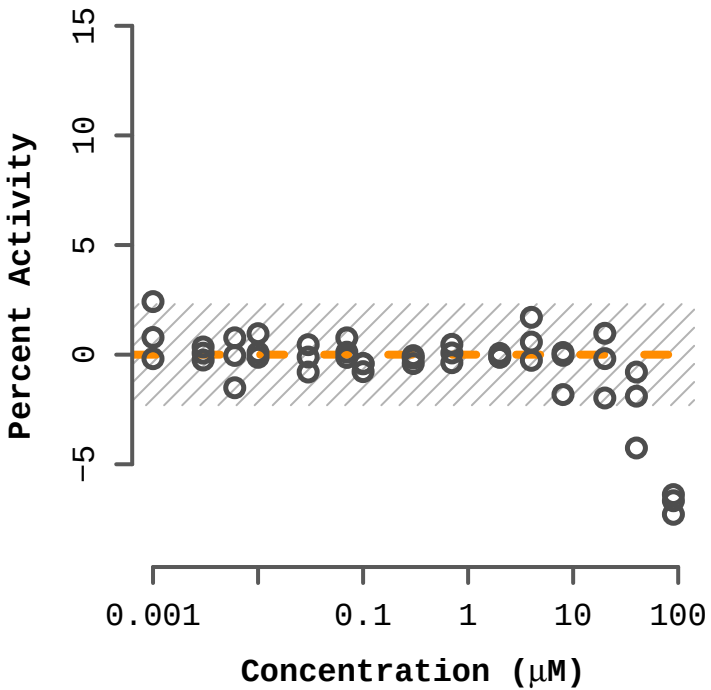
NAME: TDCPP
CHID: 26261 **CASRN:** 13674-87-8
SPID(S): Tox21_300194
M4ID: 12478936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

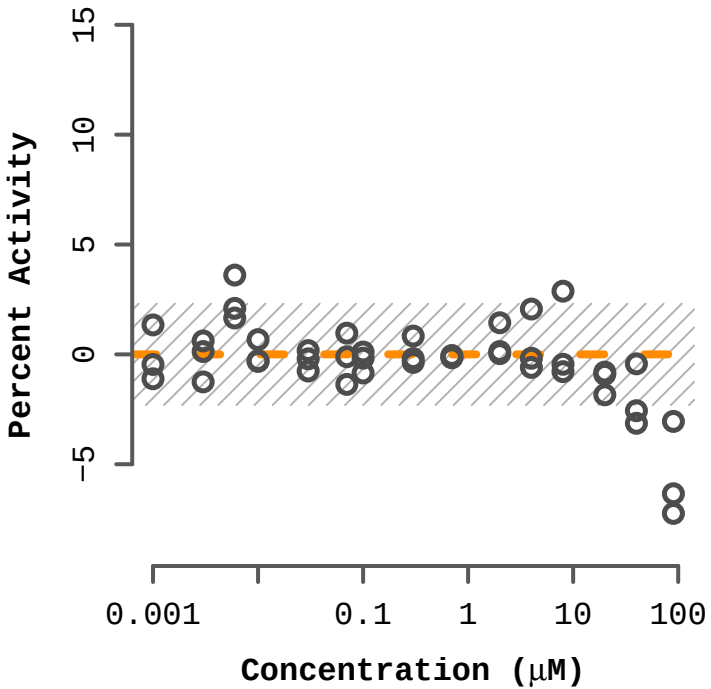
NAME: TDCPP
CHID: 26261 **CASRN:** 13674-87-8
SPID(S): Tox21_202166
M4ID: 12480086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

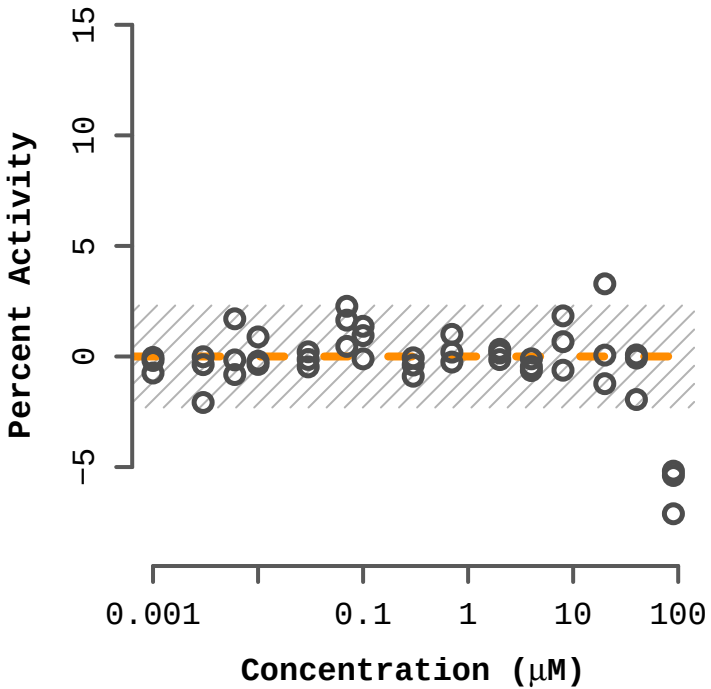
NAME: Triglycidyl isocyanurate
CHID: 26262 **CASRN:** 2451-62-9
SPID(S): Tox21_300119
M4ID: 12479011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 2.45 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

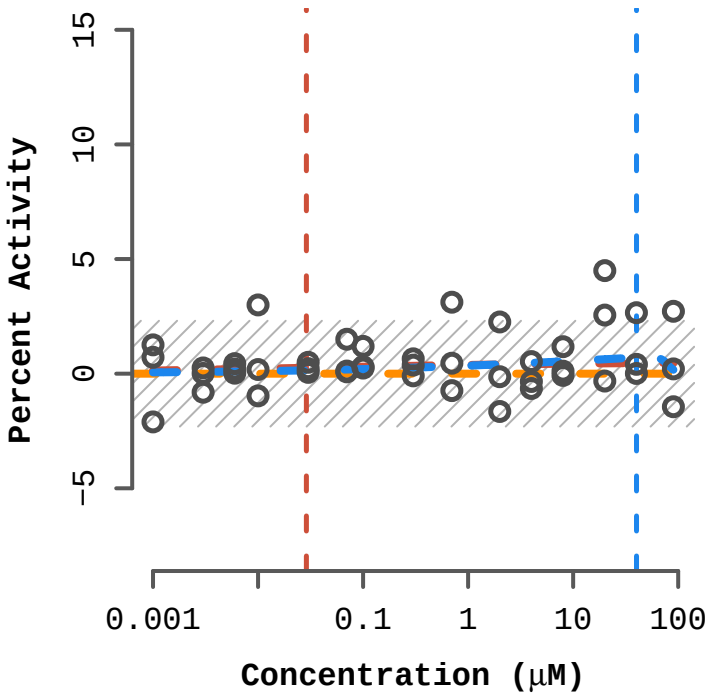
NAME: Triglycidyl isocyanurate
CHID: 26262 **CASRN:** 2451-62-9
SPID(S): Tox21_201660
M4ID: 12480592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tris(2-ethylhexyl) trimellitate
CHID: 26265 CASRN: 3319-31-1
SPID(S): Tox21_300614
M4ID: 12478519

HILL MODEL (in red):

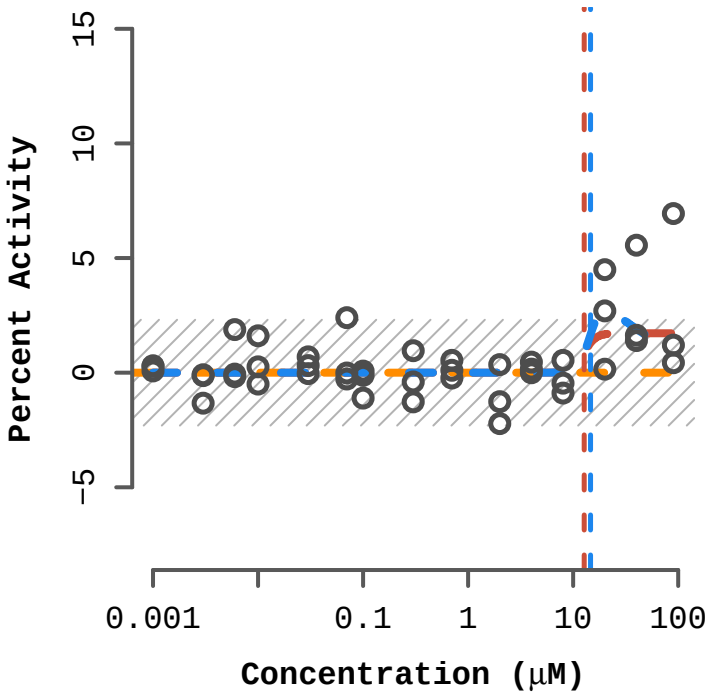
	tp	ga	gw
val:	0.513	-1.54	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.41	1.6	0.3	1.9	10.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	152.08	153.77	157.81
PROB:	0.67	0.29	0.04
RMSE:	1.39	1.28	1.27

MAX_MEAN: 2.24 MAX_MED: 2.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tris(2-ethylhexyl) trimellitate
CHID: 26265 **CASRN:** 3319-31-1
SPID(S): Tox21_202002
M4ID: 12480250

HILL MODEL (in red):

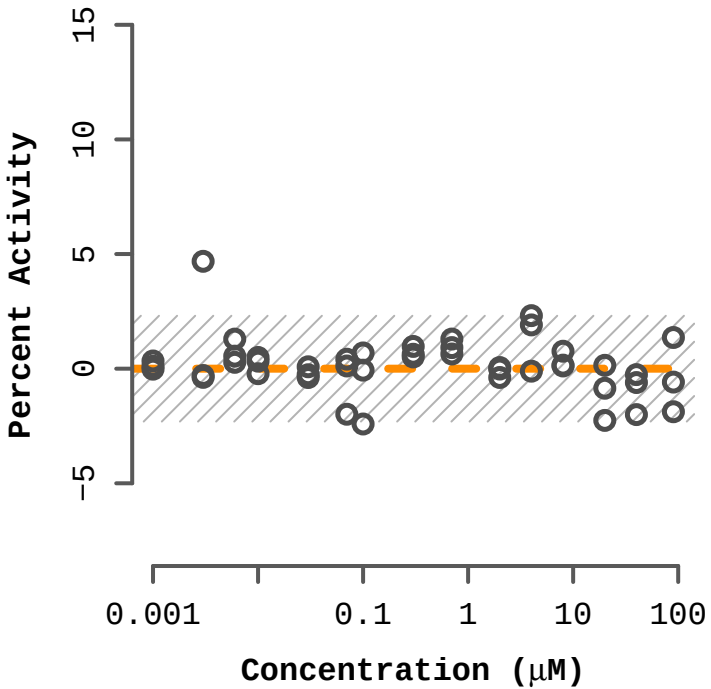
	tp	ga	gw
val:	1.72	1.11	8
sd:	0.449	0.168	6.78

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.05	1.17	7.98	1.42	1.15
sd:	10.6	0.207	6.88	1.5	1.33

	CNST	HILL	GNLS
AIC:	160.06	149.58	150.79
PROB:	0	0.64	0.35
RMSE:	1.77	1.36	1.39

MAX_MEAN: 2.87 **MAX_MED:** 2.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

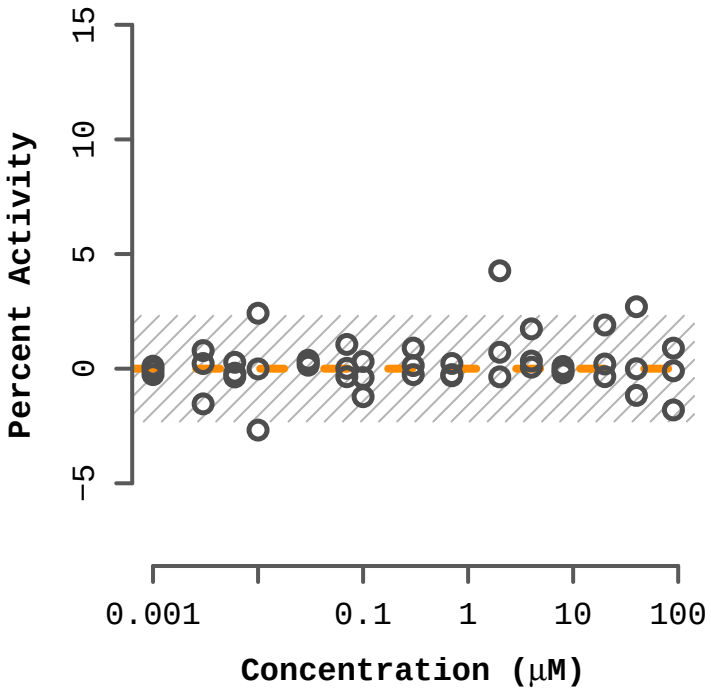
NAME: Tris(2-hydroxyethyl) isocyanurate
CHID: 26266 **CASRN:** 839-90-7
SPID(S): Tox21_303239
M4ID: 12475894

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

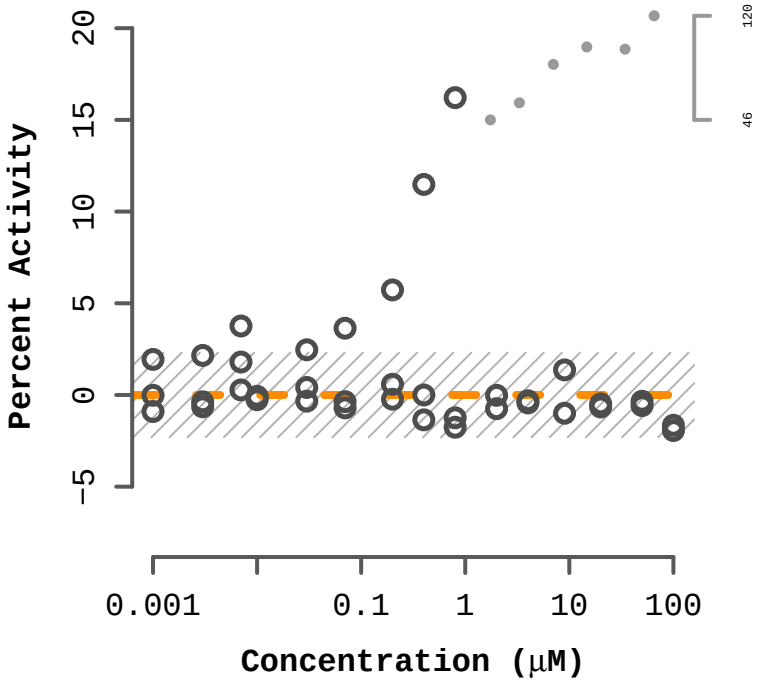
NAME: Tris(2-hydroxyethyl) isocyanurate
CHID: 26266 CASRN: 839-90-7
SPID(S): Tox21_201489
M4ID: 12480763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.54 MAX_MED: 0.717 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

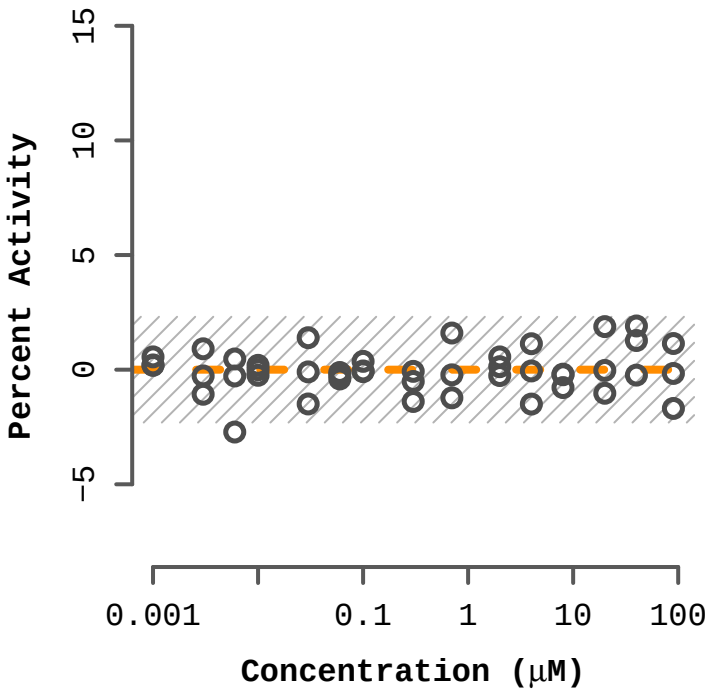
NAME: TXP
CHID: 26267 CASRN: 25155-23-1
SPID(S): Tox21_201099
M4ID: 12481153 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	372.32	NA	NA
PROB:	1	NA	NA
RMSE:	31.1	NA	NA

MAX_MEAN: 37.2 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

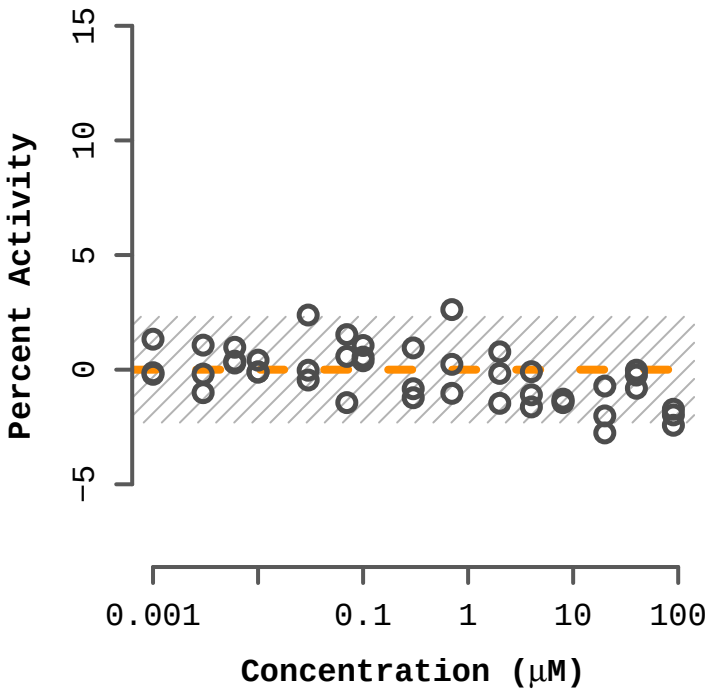
NAME: Valeronitrile
CHID: 26275 **CASRN:** 110-59-8
SPID(S): Tox21_200282
M4ID: 12481970

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

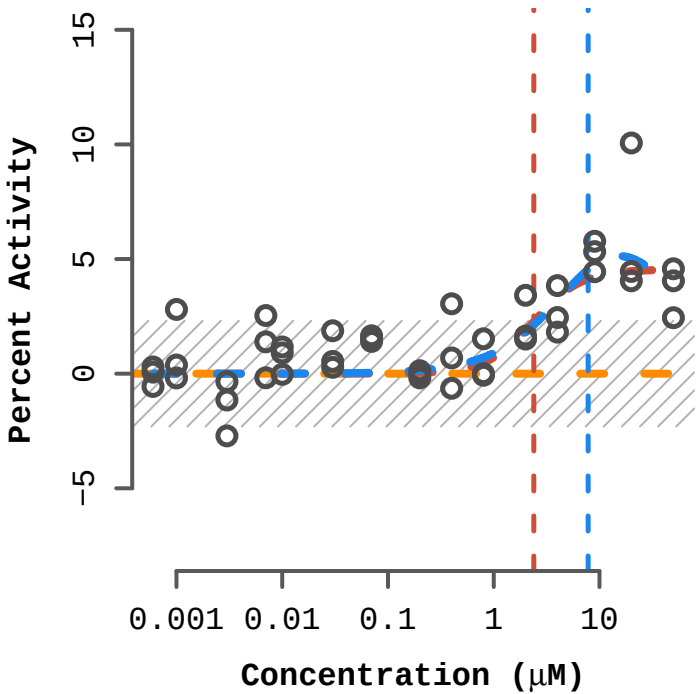
NAME: Indigo
CHID: 26279 **CASRN:** 482-89-3
SPID(S): Tox21_202545
M4ID: 12479707

HILL MODEL: Not applicable.

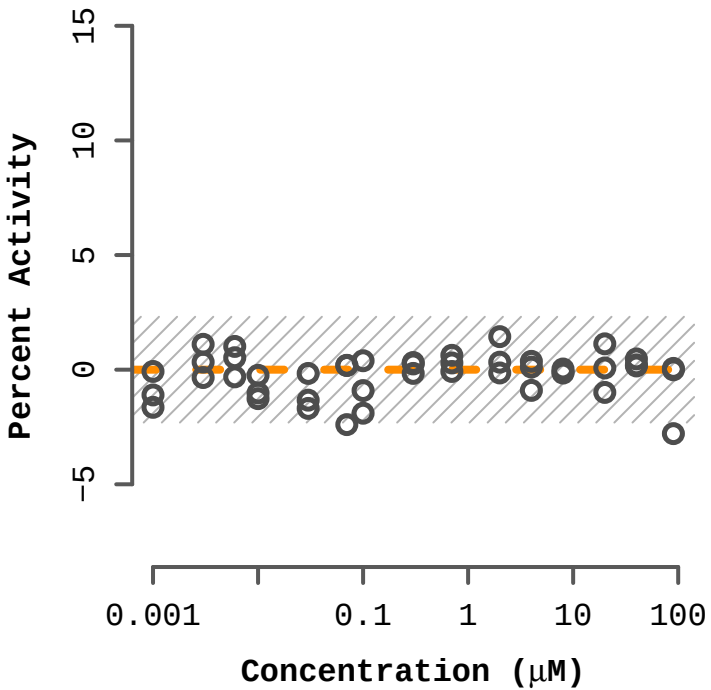
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.666 **MAX_MED:** 0.579 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Indigo
CHID:    26279   CASRN: 482-89-3
SPID(S): Tox21_112052_1
M4ID:    12483345

HILL MODEL (in red):
      tp       ga       gw
val:  4.54     0.379    1.94
sd:   0.454    0.116    0.789

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.1     0.893    1.2      1.39     0.962
sd:   18.7     0.813    0.845    1.11     1.1

      CNST        HILL        GNLS
AIC:  218.08      162.42      162.75
PROB: 0           0.54        0.46
RMSE: 2.81        1.46        1.37

MAX_MEAN: 6.19      MAX_MED: 5.33      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

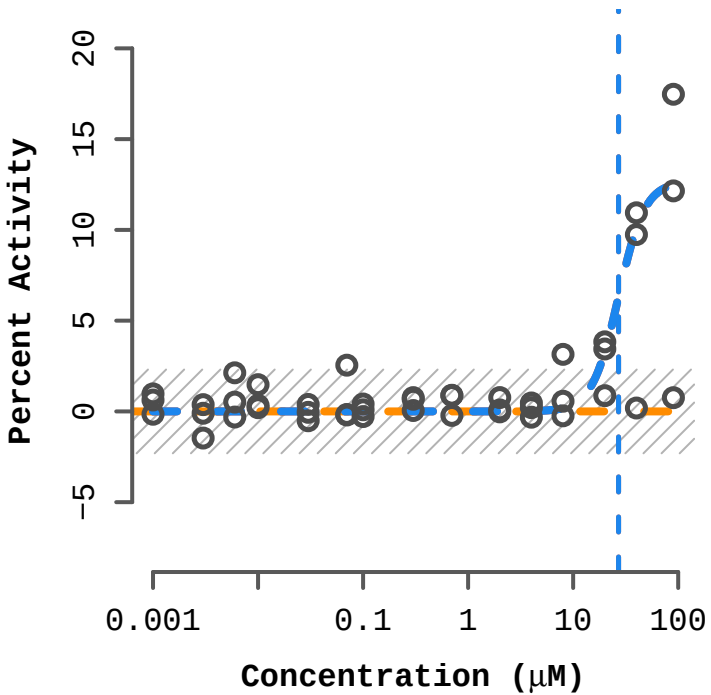
NAME: Veratraldehyde
CHID: 26285 **CASRN:** 120-14-9
SPID(S): Tox21_303074
M4ID: 12476059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.543 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Veratraldehyde
CHID: 26285 CASRN: 120-14-9
SPID(S): Tox21_201566
M4ID: 12480686

HILL MODEL (in red):

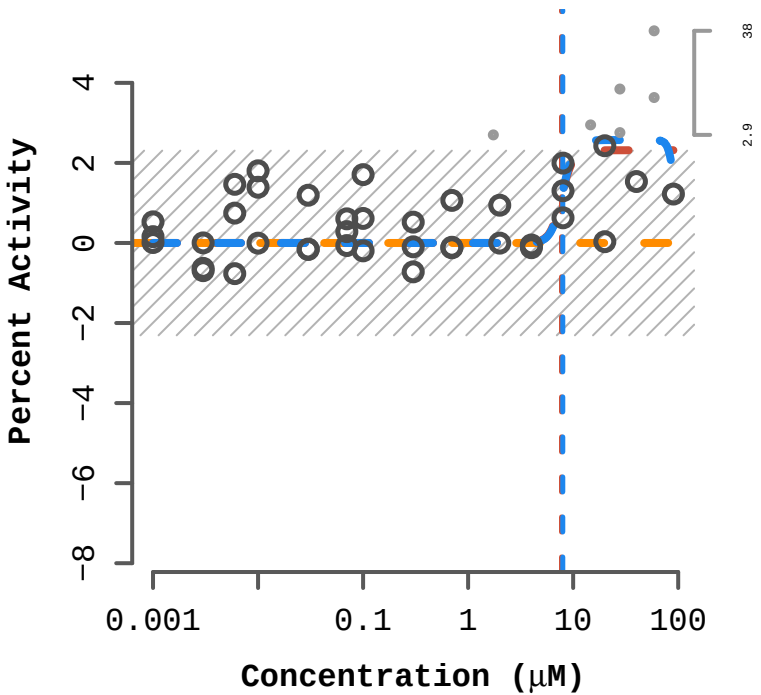
	tp	ga	gw
val:	12.7	1.43	3.47
sd:	0.992	0.0382	0.765

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.7	1.43	3.47	3.89	4.28
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	206.18	171.52	175.52
PROB:	0	0.88	0.12
RMSE:	4.02	2.57	2.57

MAX_MEAN: 10.1 MAX_MED: 12.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vinyltoluene
CHID: 26292 **CASRN:** 25013-15-4
SPID(S): Tox21_200186
M4ID: 12482066 **BRK**

HILL MODEL (in red):

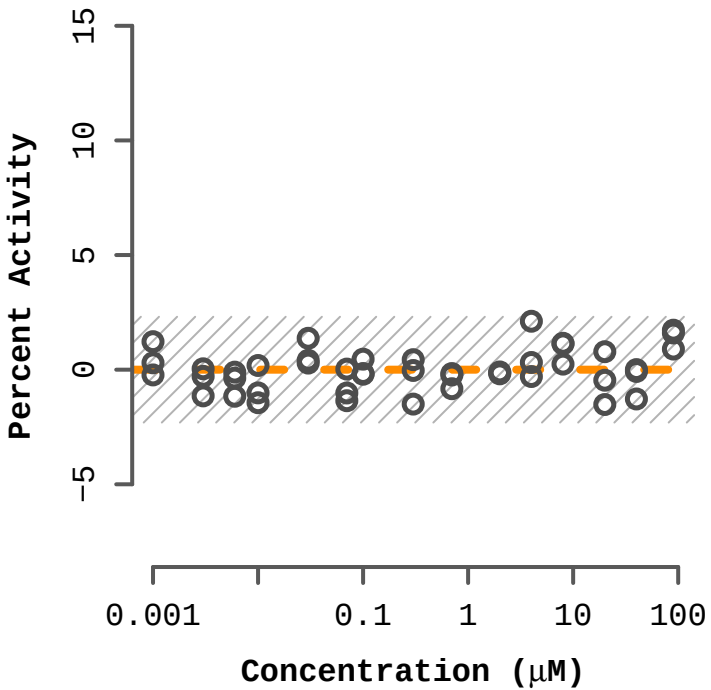
	tp	ga	gw
val:	2.32	0.889	8
sd:	0.638	0.074	23.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.57	0.901	7.97	1.97	15.6
sd:	0.724	0.0573	28.2	0.055	59.4

	CNST	HILL	GNLS
AIC:	218.93	206.85	210.28
PROB:	0	0.85	0.15
RMSE:	6.91	6.3	6.41

MAX_MEAN: 18.4 **MAX_MED:** 15.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

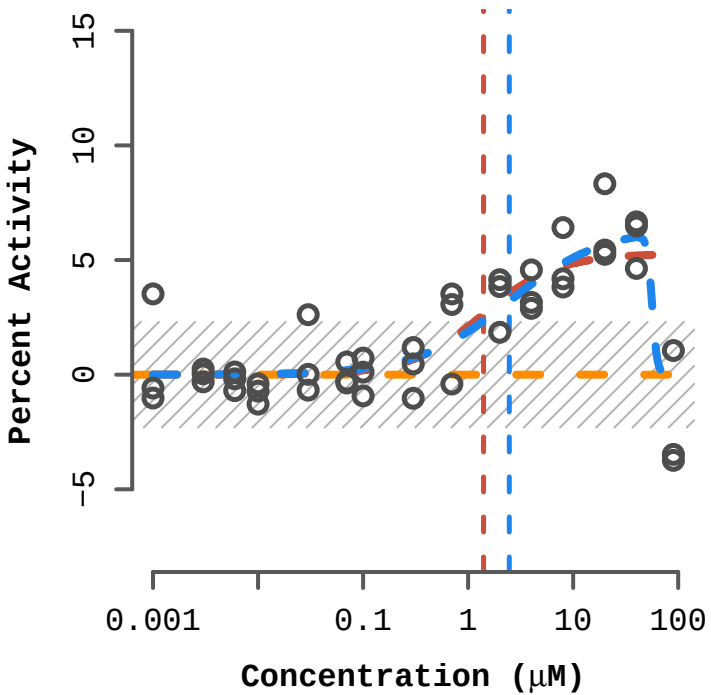
NAME: D&C Violet 2
CHID: 26293 **CASRN:** 81-48-1
SPID(S): Tox21_202902
M4ID: 12479350

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vitamin D3
CHID: 26294 CASRN: 67-97-0
SPID(S): Tox21_202546
M4ID: 12479706

HILL MODEL (in red):

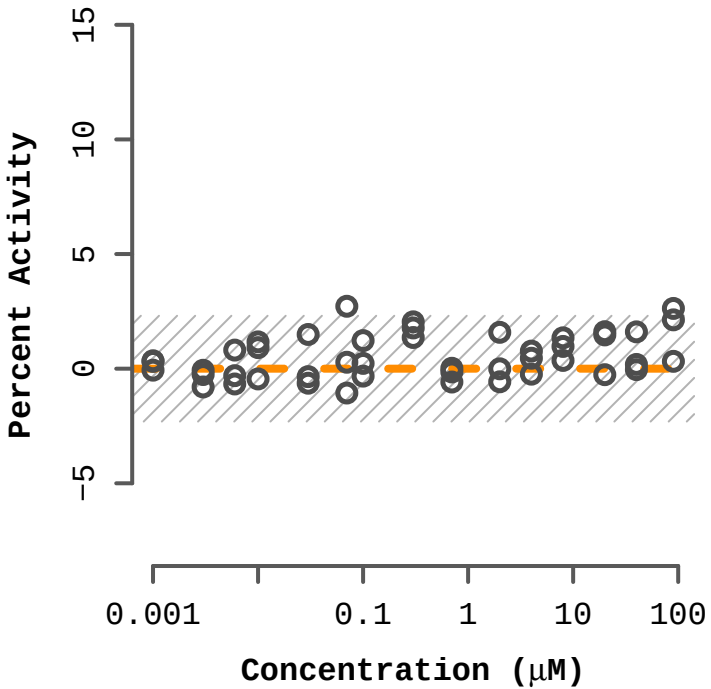
	tp	ga	gw
val:	5.28	0.147	1.24
sd:	0.731	0.226	0.421

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.41	0.392	0.974	1.75	18
sd:	1.03	0.249	0.288	0.422	43.5

	CNST	HILL	GNLS
AIC:	234.84	186.82	167.05
PROB:	0	0	1
RMSE:	3.2	2.3	1.39

MAX_MEAN: 6.34 MAX_MED: 6.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

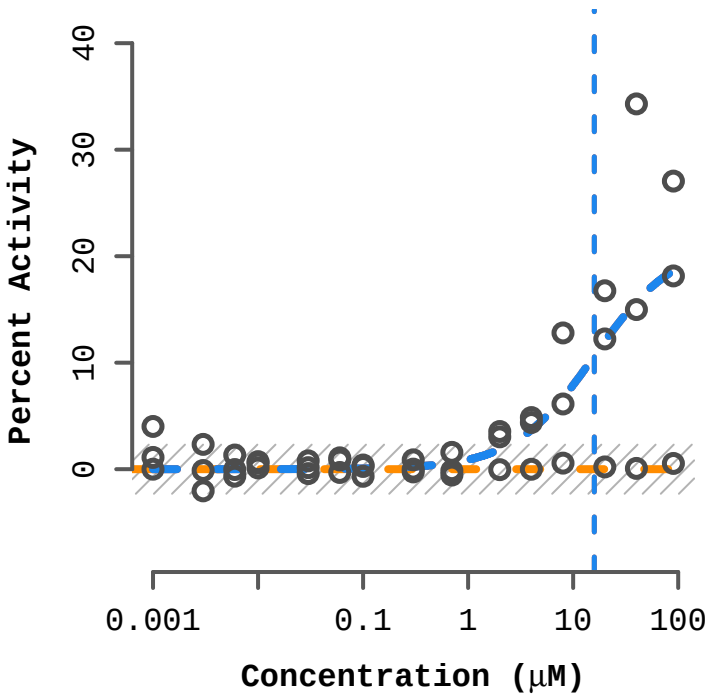
NAME: m-Xylene
CHID: 26298 **CASRN:** 108-38-3
SPID(S): Tox21_303203
M4ID: 12475930

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: m-Xylene
CHID: 26298 **CASRN:** 108-38-3
SPID(S): Tox21_202056
M4ID: 12480196

HILL MODEL (in red):

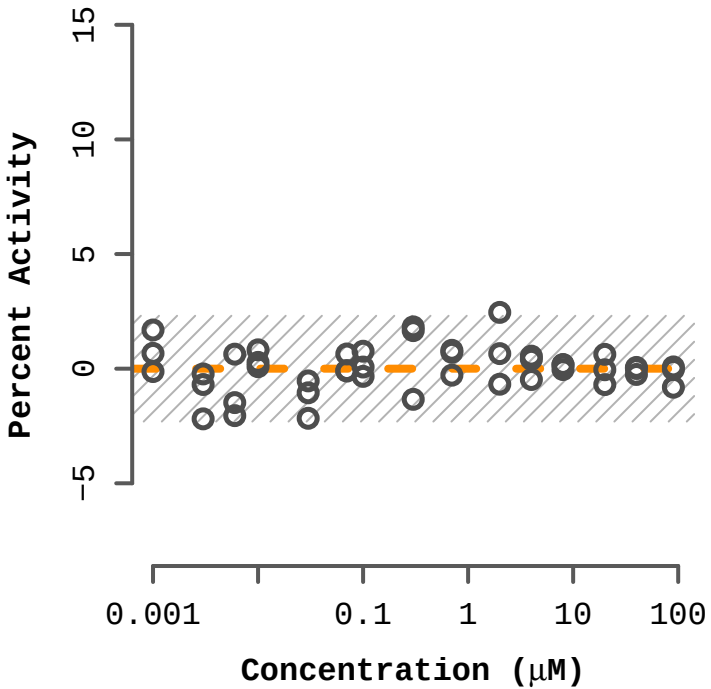
	tp	ga	gw
val:	21.3	1.2	1.13
sd:	4.89	0.258	0.352

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.3	1.2	1.13	3.56	4.52
sd:	4.89	0.258	0.352	1050	3010

	CNST	HILL	GNLS
AIC:	286.74	255.48	259.48
PROB:	0	0.88	0.12
RMSE:	8.43	5.35	5.35

MAX_MEAN: 16.5 **MAX_MED:** 18.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

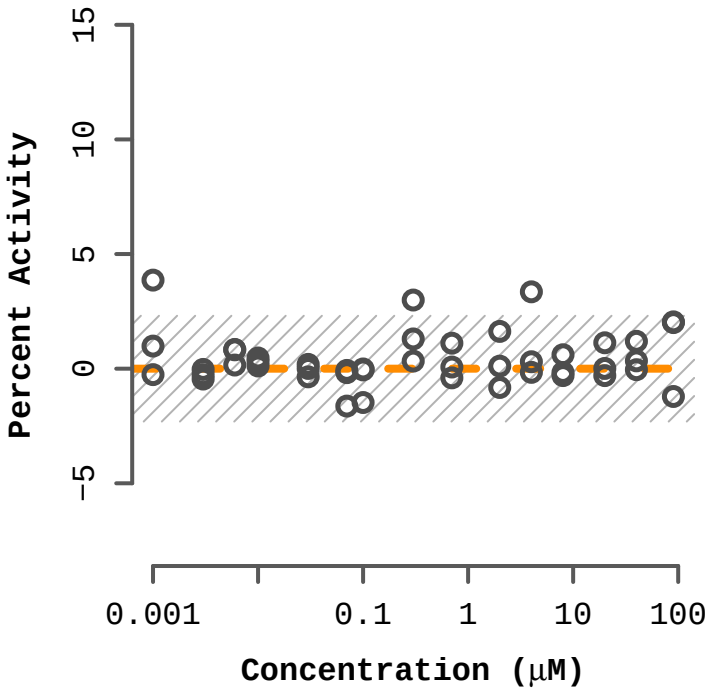
NAME: Sodium xylenesulfonate
CHID: 26302 **CASRN:** 1300-72-7
SPID(S): Tox21_300072
M4ID: 12479058

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.813 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

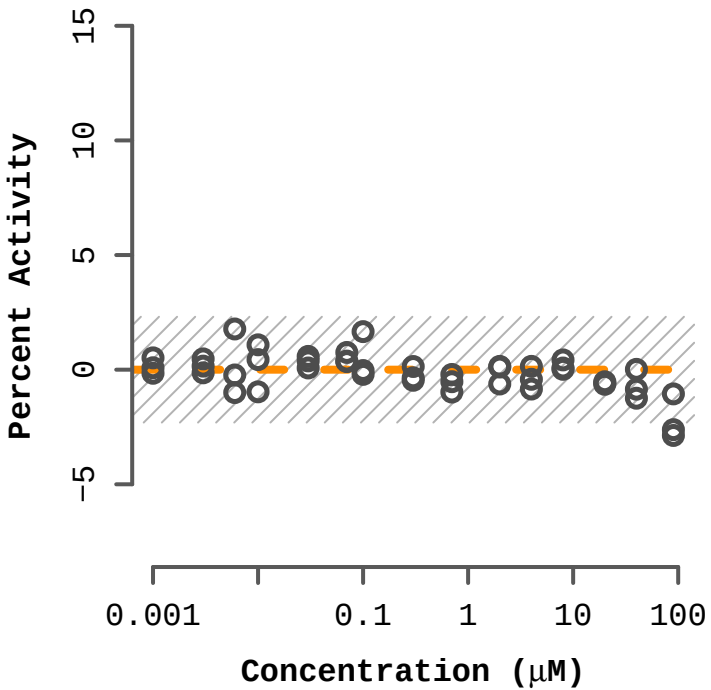
NAME: Sodium xylenesulfonate
CHID: 26302 CASRN: 1300-72-7
SPID(S): Tox21_202016
M4ID: 12480236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

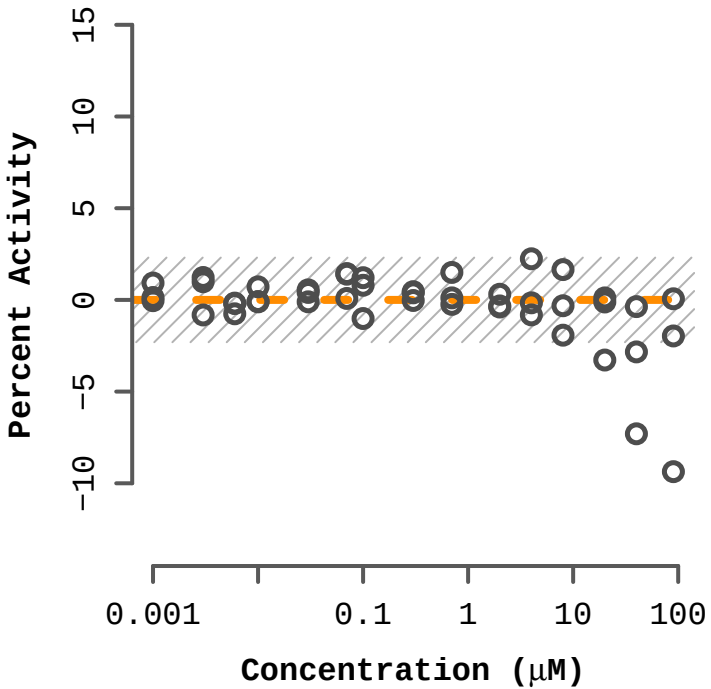
NAME: p-Xylenol blue
CHID: 26303 CASRN: 125-31-5
SPID(S): Tox21_303062
M4ID: 12476071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.495 MAX_MED: 0.441 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

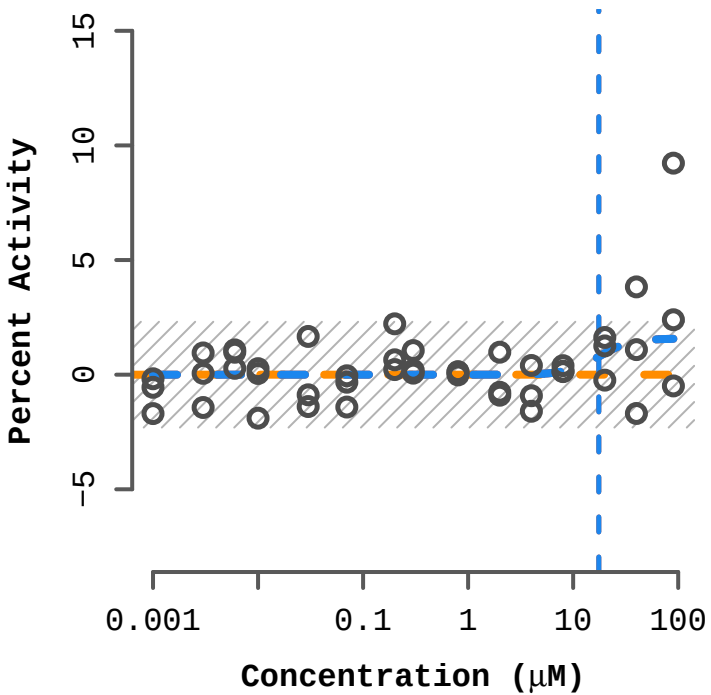
NAME: p-Xylenol blue
CHID: 26303 **CASRN:** 125-31-5
SPID(S): Tox21_201524
M4ID: 12480728

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 0.973 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dimethylaniline
CHID: 26304 **CASRN:** 87-59-2
SPID(S): Tox21_200158
M4ID: 12482094

HILL MODEL (in red):

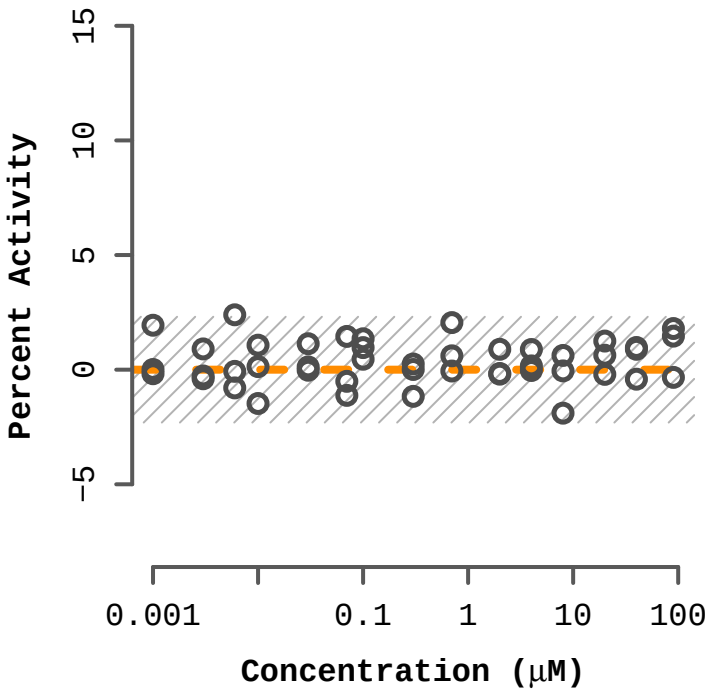
	tp	ga	gw
val:	1.58	1.24	2.93
sd:	1.21	0.416	3.92

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.58	1.24	2.93	3.01	6.99
sd:	1.21	0.416	3.92	1350	8960

	CNST	HILL	GNLS
AIC:	158.54	159.2	163.2
PROB:	0.55	0.4	0.05
RMSE:	1.8	1.59	1.59

MAX_MEAN: 3.71 **MAX_MED:** 2.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

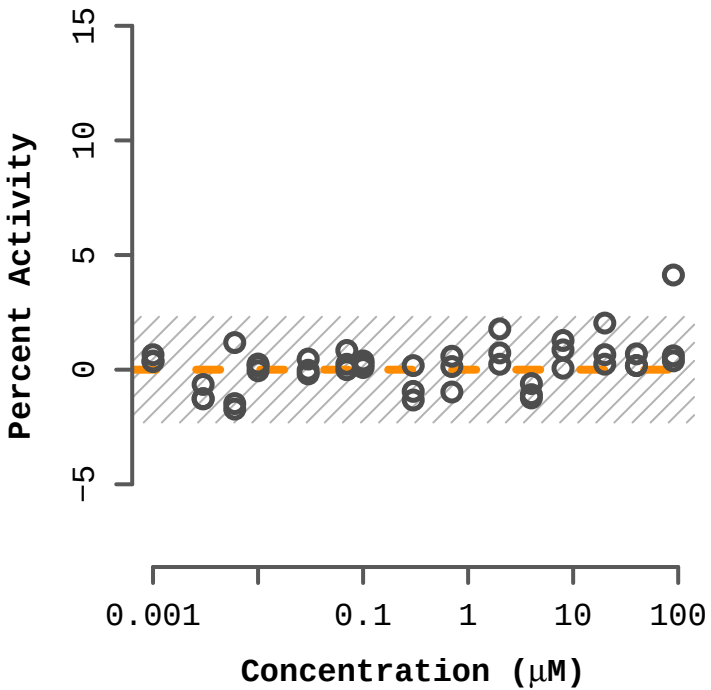
NAME: 2,4−Dimethylaniline
CHID: 26305 **CASRN:** 95−68−1
SPID(S): Tox21_200380
M4ID: 12481872

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.975 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

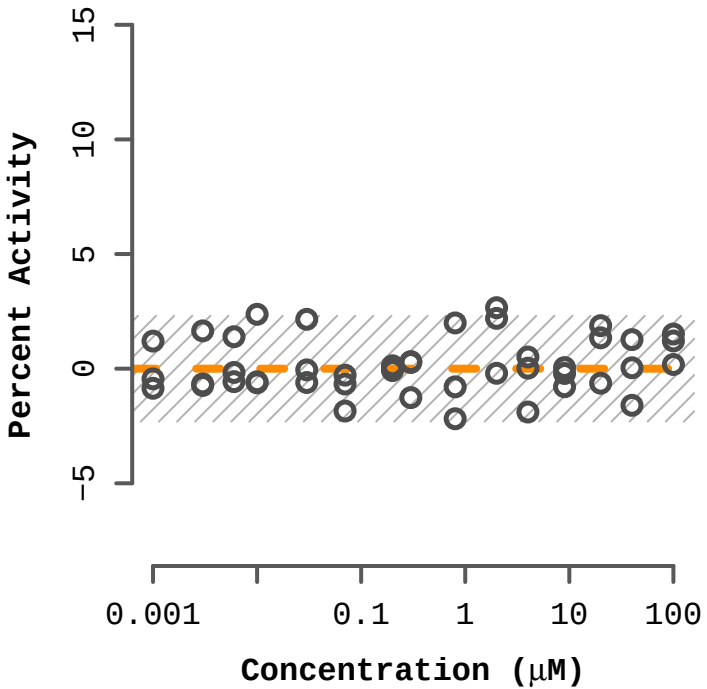
NAME: 2,5-Dimethylaniline
CHID: 26306 **CASRN:** 95-78-3
SPID(S): Tox21_201025
M4ID: 12481227

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 0.864 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

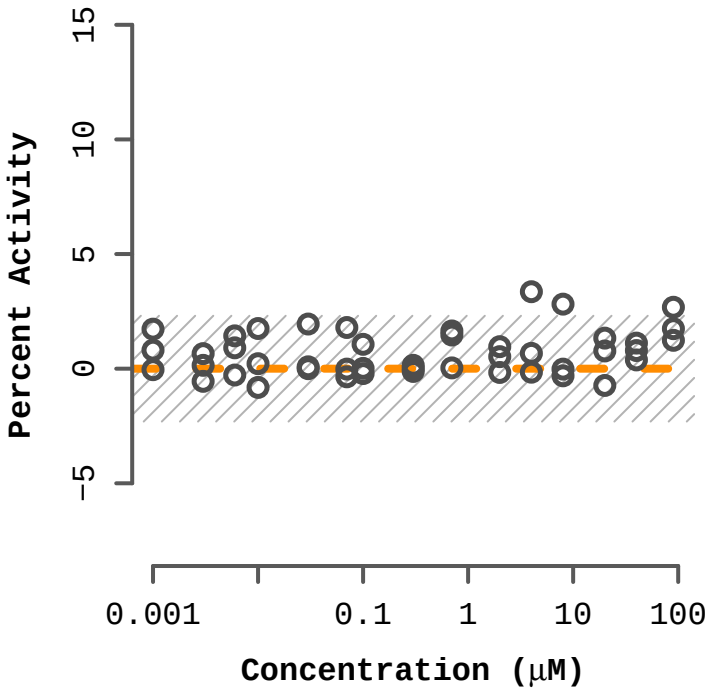
NAME: 2,6-Dimethylaniline
CHID: 26307 **CASRN:** 87-62-7
SPID(S): Tox21_300055
M4ID: 12479075

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 2.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

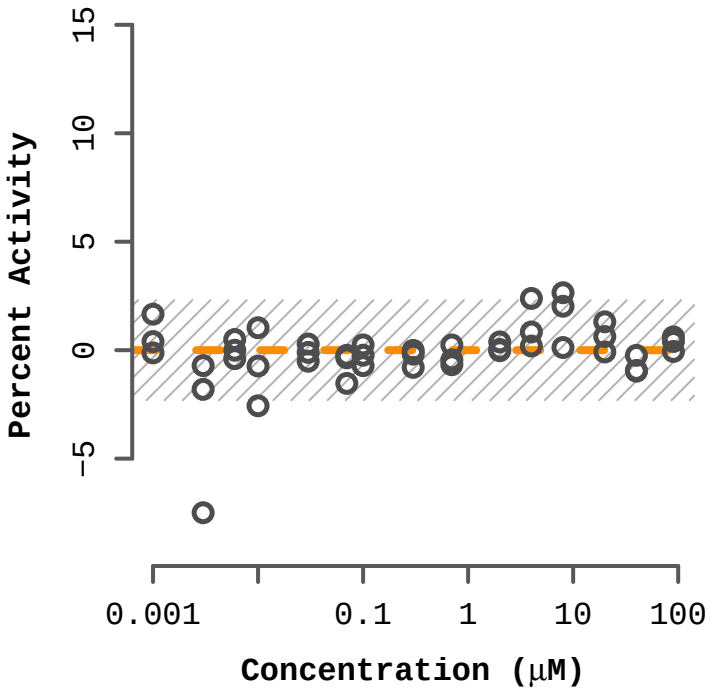
NAME: 2,6-Dimethylaniline
CHID: 26307 **CASRN:** 87-62-7
SPID(S): Tox21_201426
M4ID: 12480826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

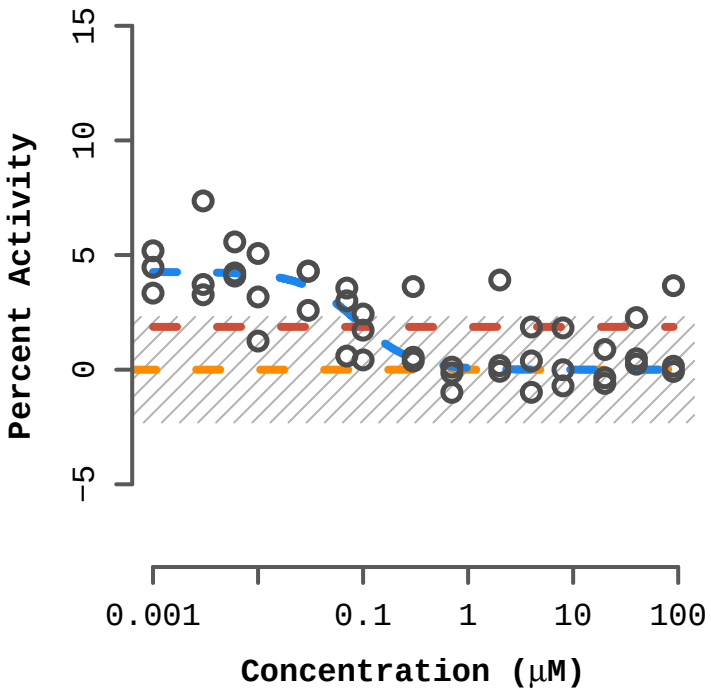
NAME: 3,4-Dimethylaniline
CHID: 26308 CASRN: 95-64-7
SPID(S): Tox21_200058
M4ID: 12482194

HILL MODEL: Not applicable.

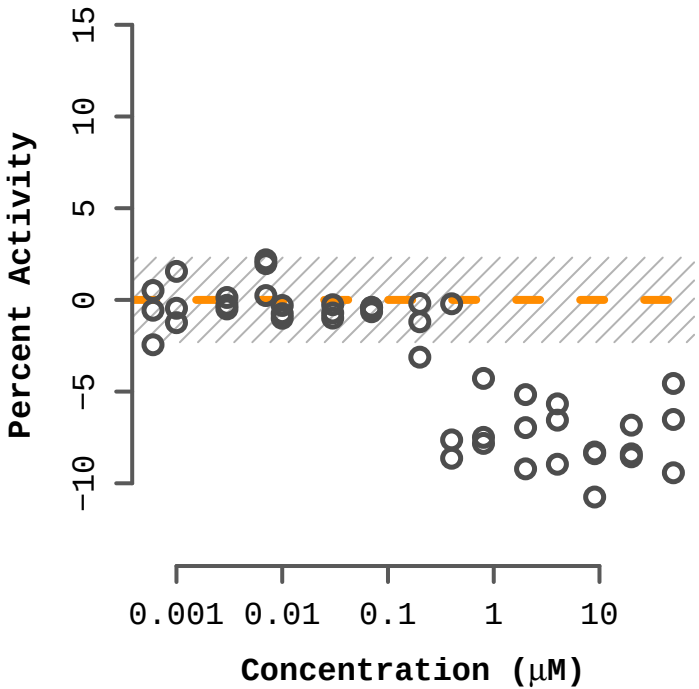
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.6 MAX_MED: 2.03 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3,5-Dimethylaniline
CHID:    26309   CASRN: 108-69-0
SPID(S): Tox21_200232
M4ID:    12482020

HILL MODEL (in red):
      tp       ga       gw
val:  1.87     -5       3.7
sd:   0.346    956      1760

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.26     -4.57    5.29     -1.06    1.64
sd:   0.385    3470     11700    0.127    0.861

      CNST        HILL        GNLS
AIC:  227.44      207         165.87
PROB: 0           0           1
RMSE: 2.88        2.07        1.41

MAX_MEAN: 4.78      MAX_MED: 4.47      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

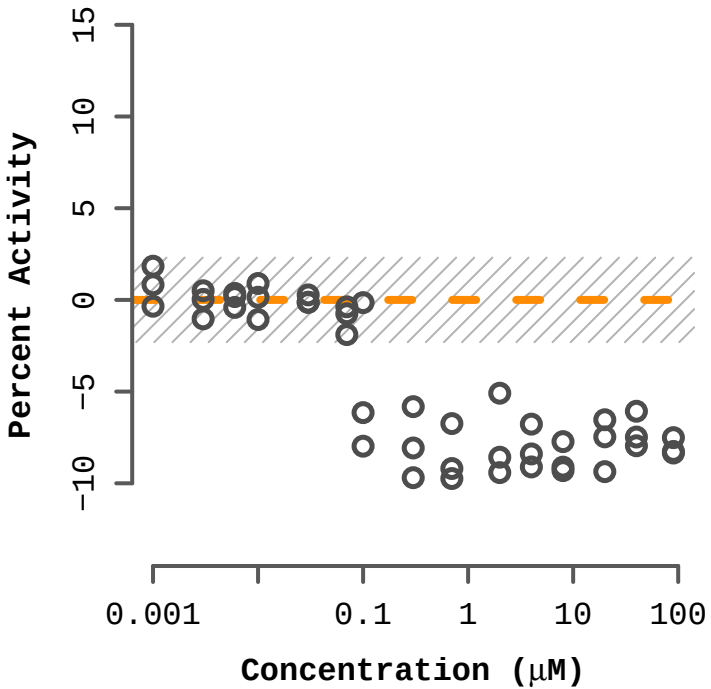
NAME: Zinc pyrithione
CHID: 26314 **CASRN:** 13463-41-7
SPID(S): Tox21_303205
M4ID: 12475928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	280.83	NA	NA
PROB:	1	NA	NA
RMSE:	5.2	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

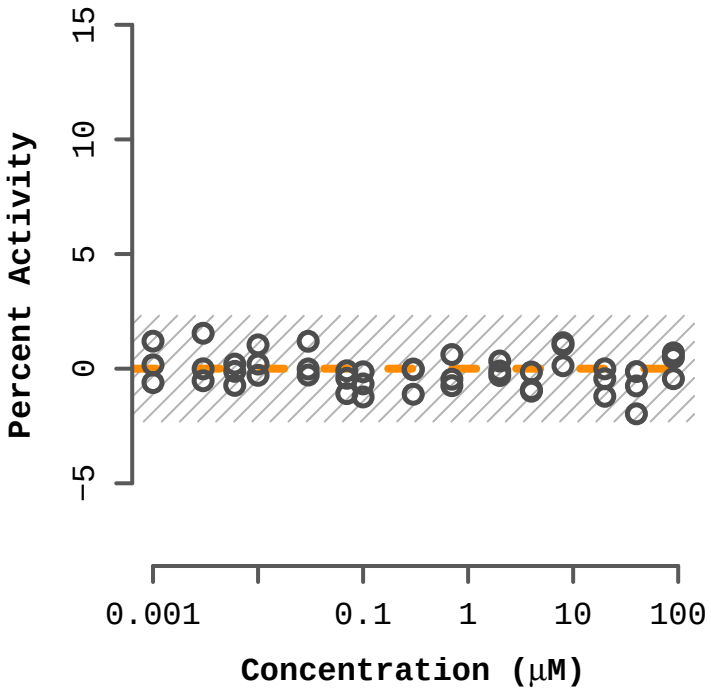
NAME: Zinc pyrithione
CHID: 26314 **CASRN:** 13463-41-7
SPID(S): Tox21_202180
M4ID: 12480072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	298.87	NA	NA
PROB:	1	NA	NA
RMSE:	6.12	NA	NA

MAX_MEAN: 0.775 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

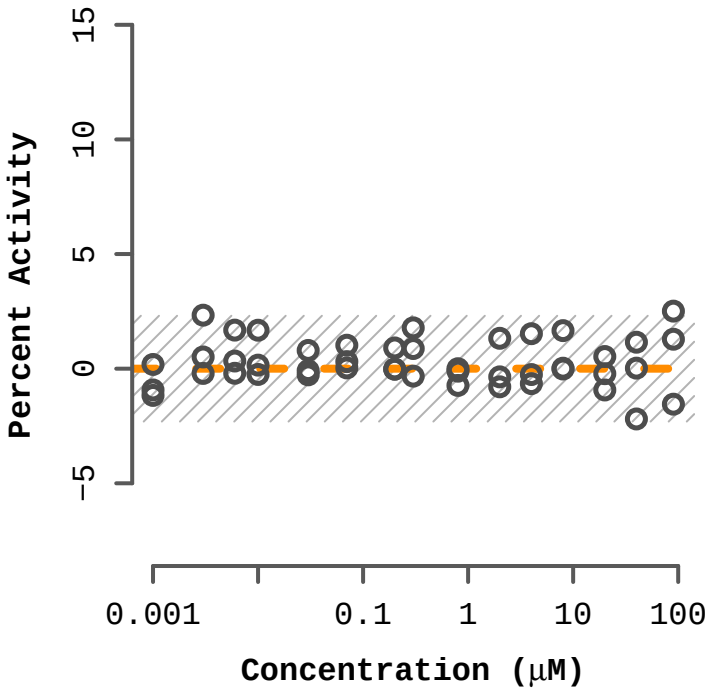
NAME: Zirconocene dichloride
CHID: 26318 CASRN: 1291-32-3
SPID(S): Tox21_202891
M4ID: 12479361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.766 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

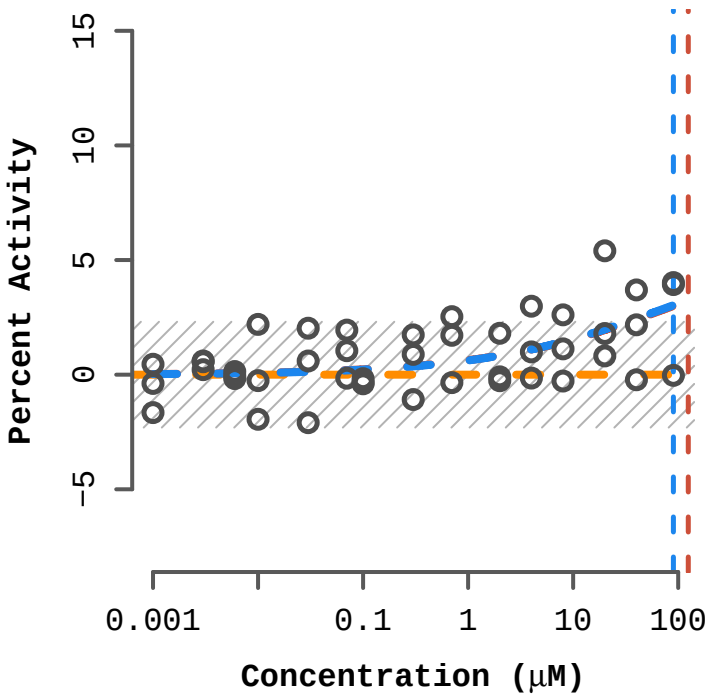
NAME: N-(4-Methoxyphenyl)acetamide
CHID: 26325 **CASRN:** 51-66-1
SPID(S): Tox21_201131
M4ID: 12481121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.88 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vitamin E
CHID: 26339 **CASRN:** 59-02-9
SPID(S): Tox21_202081
M4ID: 12480171

HILL MODEL (in red):

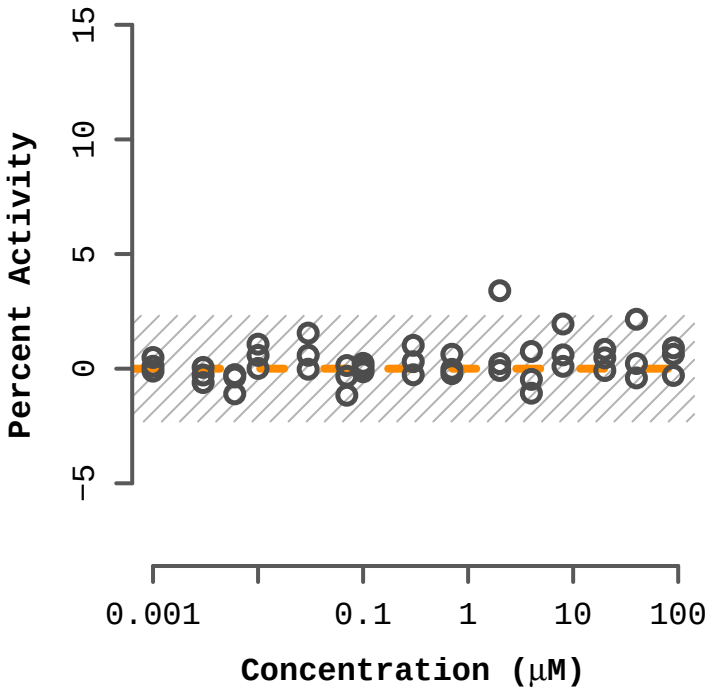
	tp	ga	gw
val:	6.48	2.1	0.462
sd:	7.25	1.83	0.244

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.06	1.95	0.483	3.71	4.33
sd:	8	2.07	0.259	1550	3840

	CNST	HILL	GNLS
AIC:	180.47	165.19	169.23
PROB:	0	0.88	0.12
RMSE:	1.8	1.35	1.35

MAX_MEAN: 2.67 **MAX_MED:** 3.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

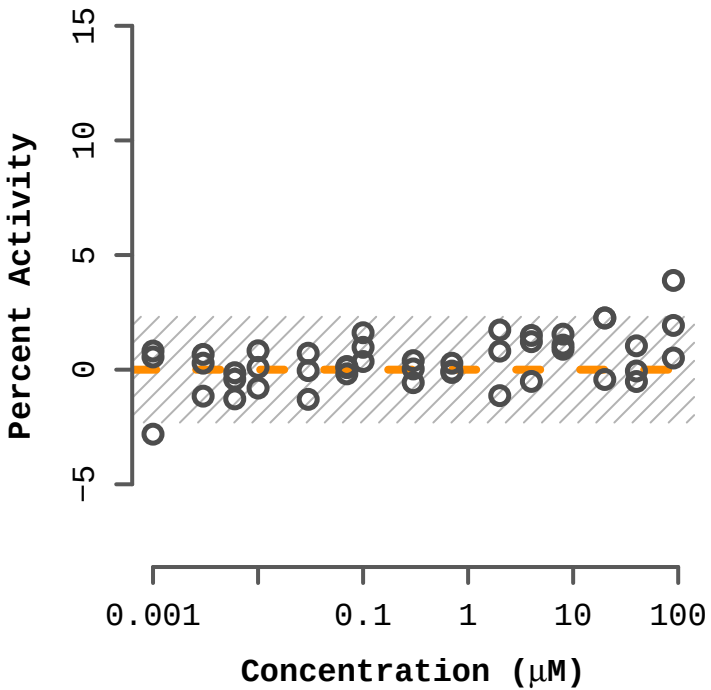
NAME: 2-Phenylethanol
CHID: 26342 **CASRN:** 60-12-8
SPID(S): Tox21_303383
M4ID: 12475755

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

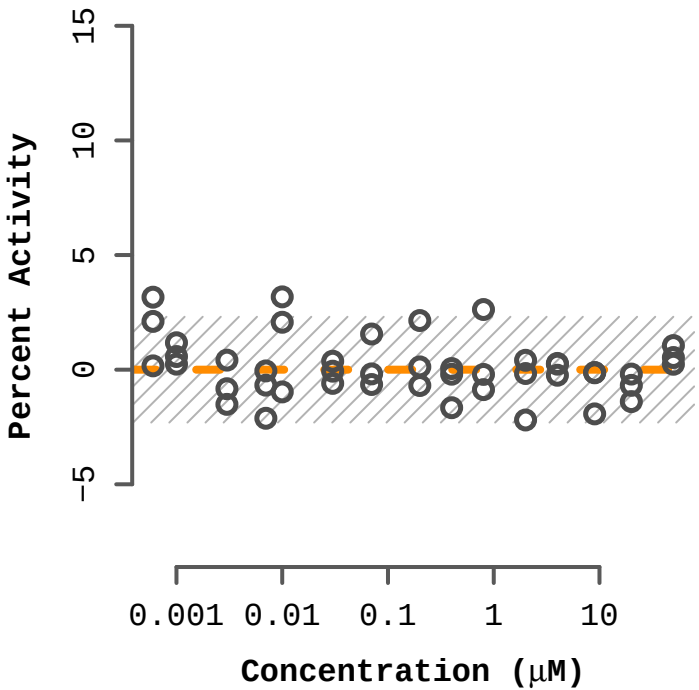
NAME: 2-Phenylethanol
CHID: 26342 CASRN: 60-12-8
SPID(S): Tox21_201322
M4ID: 12480930

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 2.11 MAX_MED: 2.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

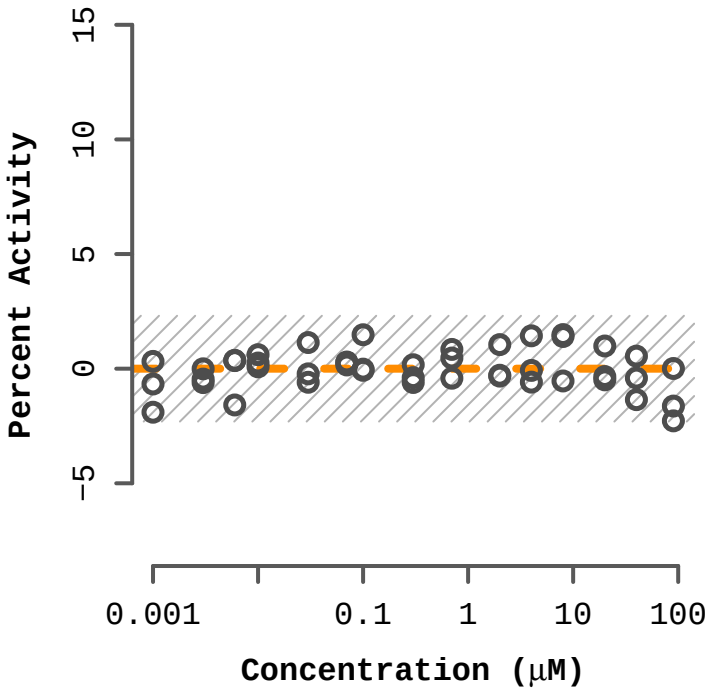
NAME: 2-Phenylethanol
CHID: 26342 **CASRN:** 60-12-8
SPID(S): Tox21_113544_1
M4ID: 12482615

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

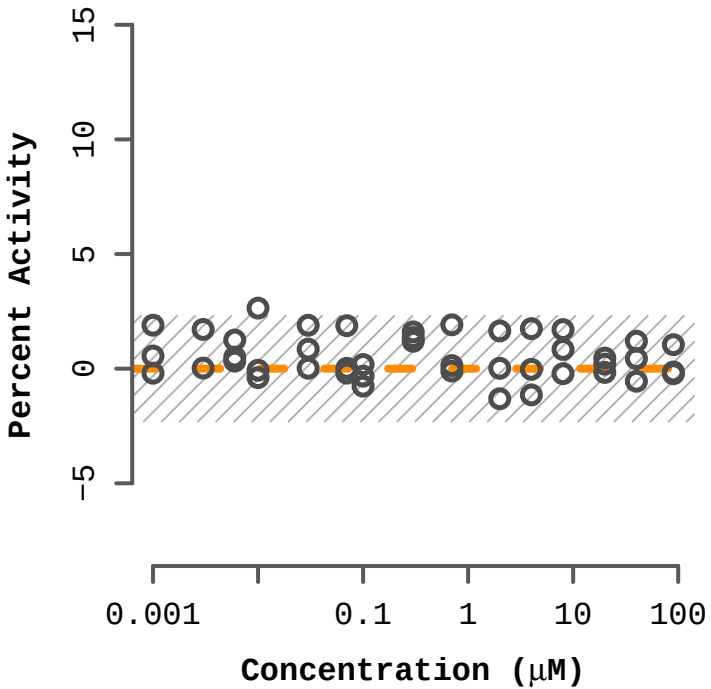
NAME: 1,4-Bis(trichloromethyl)benzene
CHID: 26366 **CASRN:** 68-36-0
SPID(S): Tox21_200257
M4ID: 12481995

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.786 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

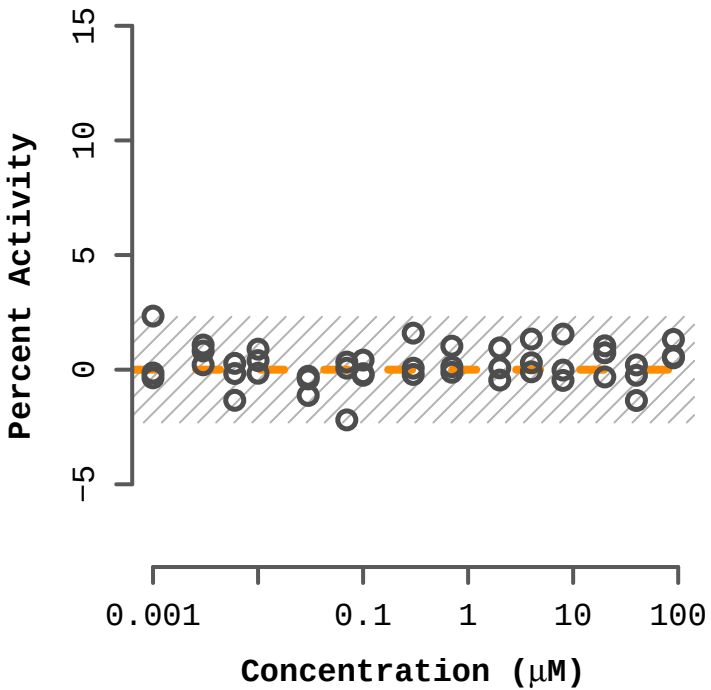
NAME: Salicylic acid
CHID: 26368 **CASRN:** 69-72-7
SPID(S): Tox21_303109
M4ID: 12476024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

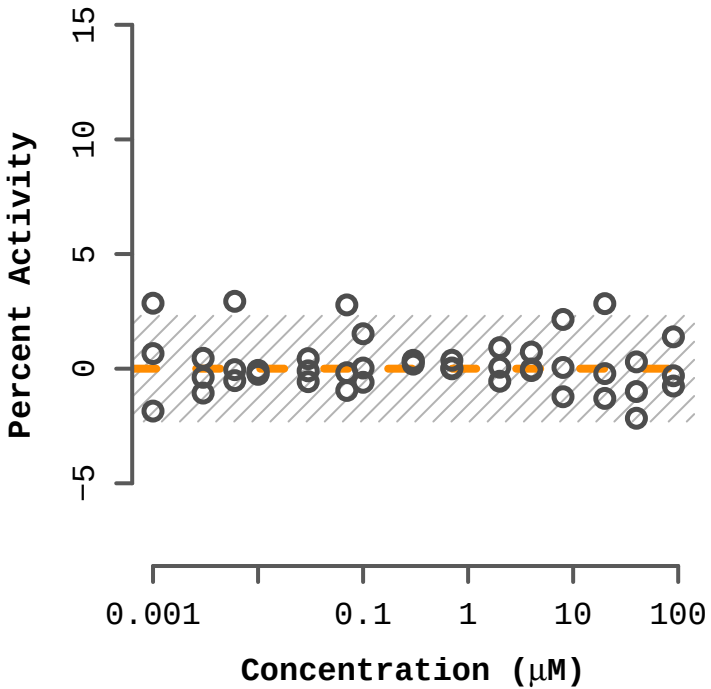
NAME: Salicylic acid
CHID: 26368 **CASRN:** 69-72-7
SPID(S): Tox21_201471
M4ID: 12480781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.806 **MAX_MED:** 0.818 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

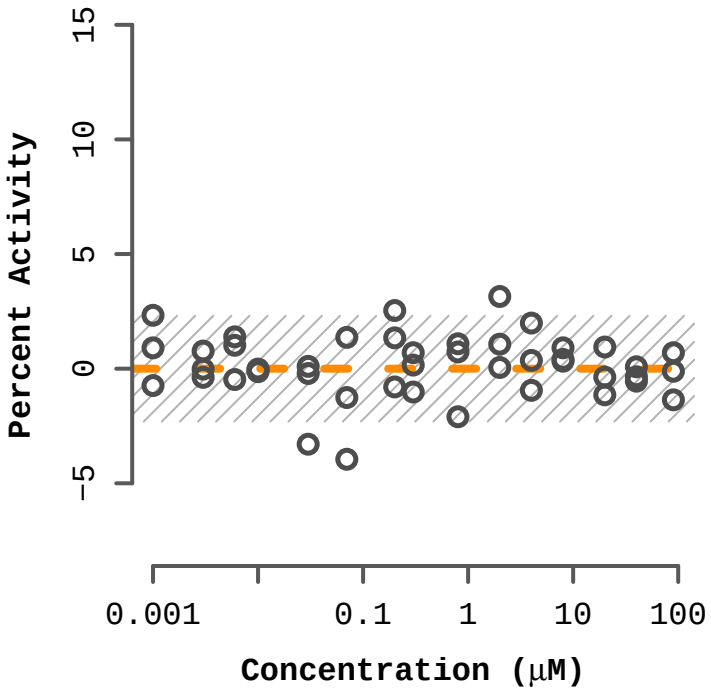
NAME: Cobalt(II) acetate
CHID: 26373 **CASRN:** 71-48-7
SPID(S): Tox21_200424
M4ID: 12481828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 0.661 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

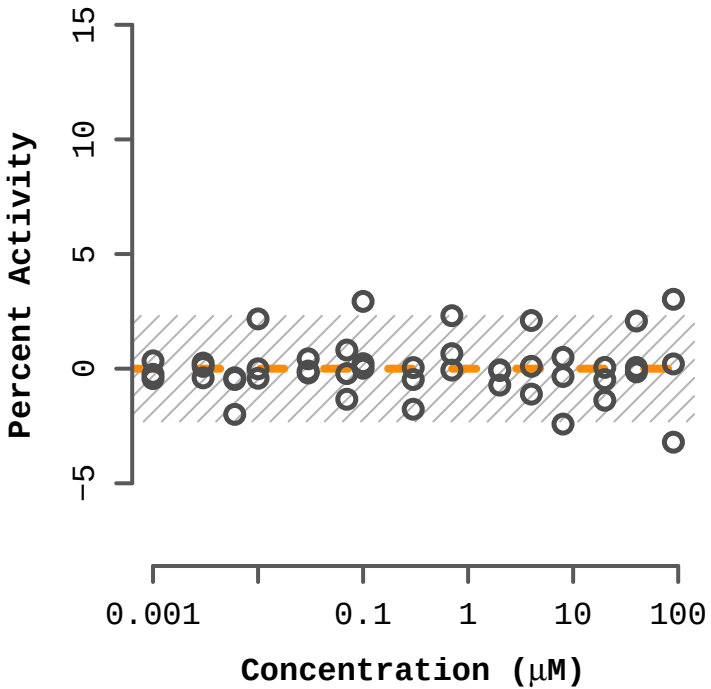
NAME: 2-Methyl-2-propanethiol
CHID: 26418 **CASRN:** 75-66-1
SPID(S): Tox21_200874
M4ID: 12481378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

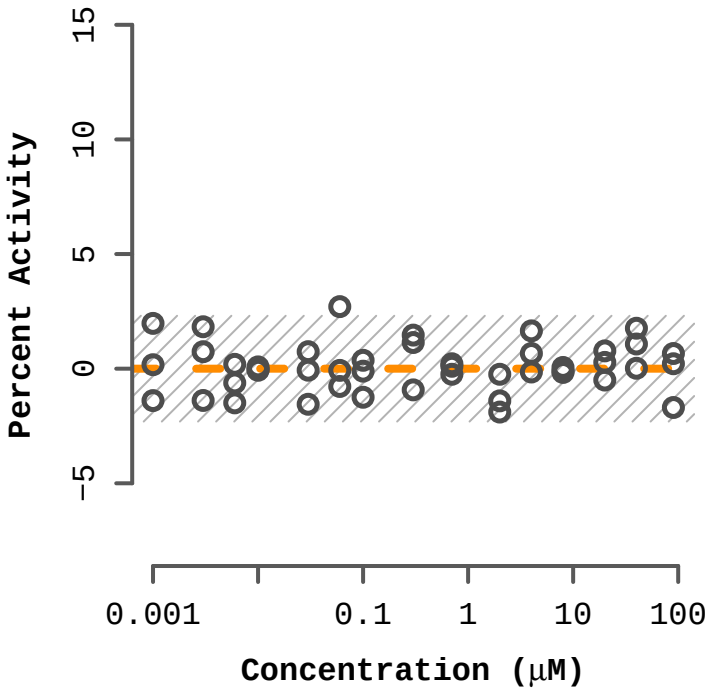
NAME: Methanesulfonic acid
CHID: 26422 **CASRN:** 75-75-2
SPID(S): Tox21_201073
M4ID: 12481179

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

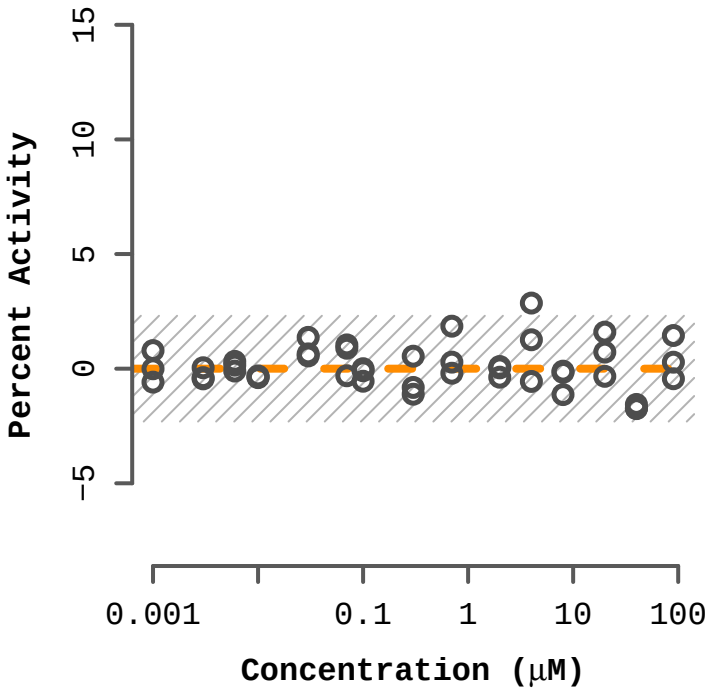
NAME: Tetramethylsilane
CHID: 26423 **CASRN:** 75-76-3
SPID(S): Tox21_200011
M4ID: 12482241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.954 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

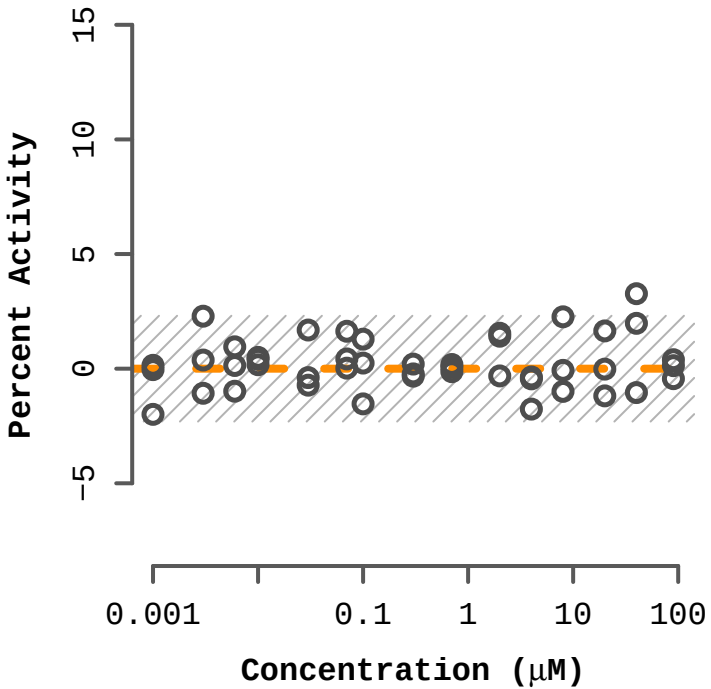
NAME: 2,2−Dimethylpropanoic acid
CHID: 26432 **CASRN:** 75−98−9
SPID(S): Tox21_200425
M4ID: 12481827

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

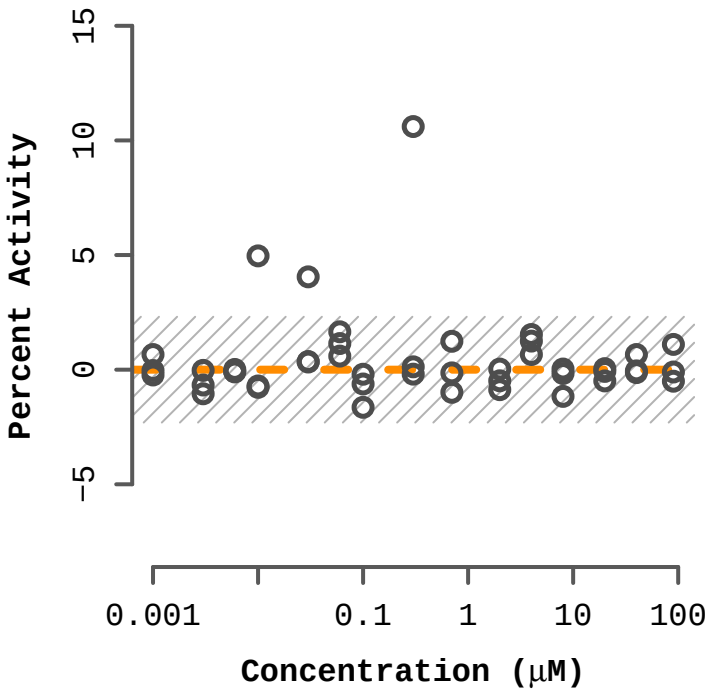
NAME: 2-Methyl-2-nitro-1-propanol
CHID: 26436 **CASRN:** 76-39-1
SPID(S): Tox21_301911
M4ID: 12477222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

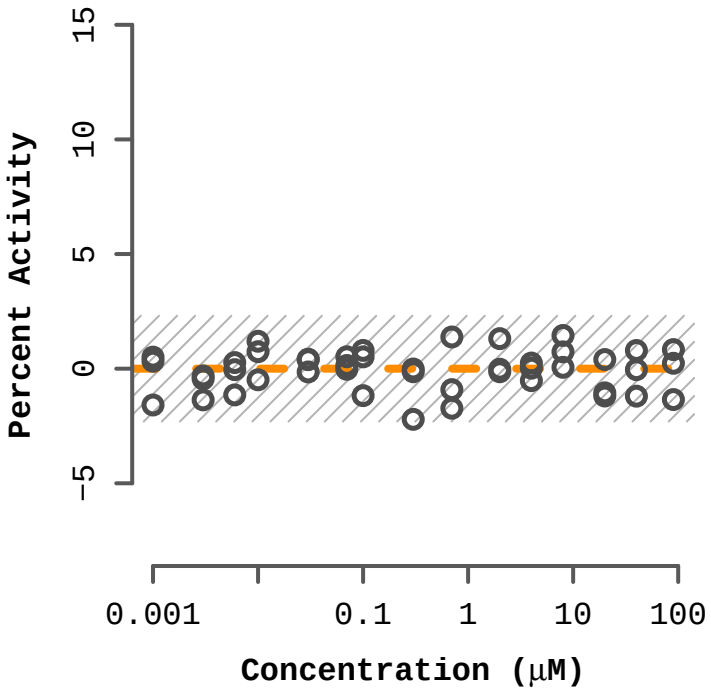
NAME: 2,2−Dimethoxypropane
CHID: 26441 **CASRN:** 77−76−9
SPID(S): Tox21_200627
M4ID: 12481625

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 3.51 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

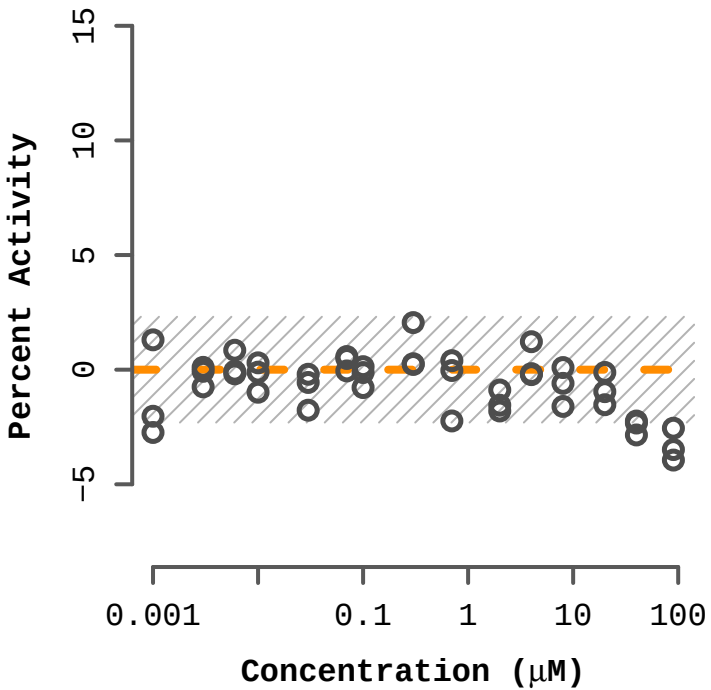
NAME: 2-(Hydroxymethyl)-2-methyl-1,3-propanediol
CHID: 26444 **CASRN:** 77-85-0
SPID(S): Tox21_201125
M4ID: 12481127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.749 **MAX_MED:** 0.743 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

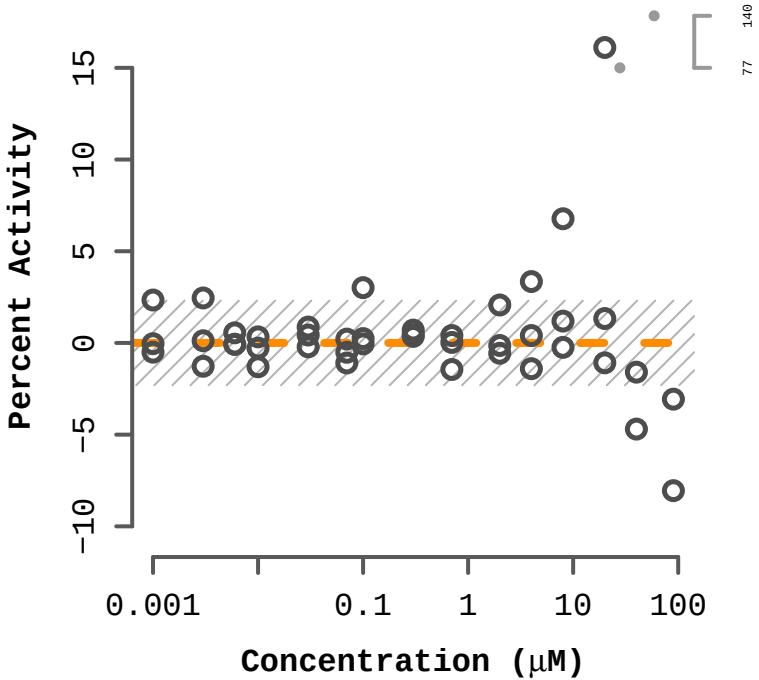
NAME: Acetyl tributyl citrate
CHID: 26446 **CASRN:** 77-90-7
SPID(S): Tox21_303128
M4ID: 12476005

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 0.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

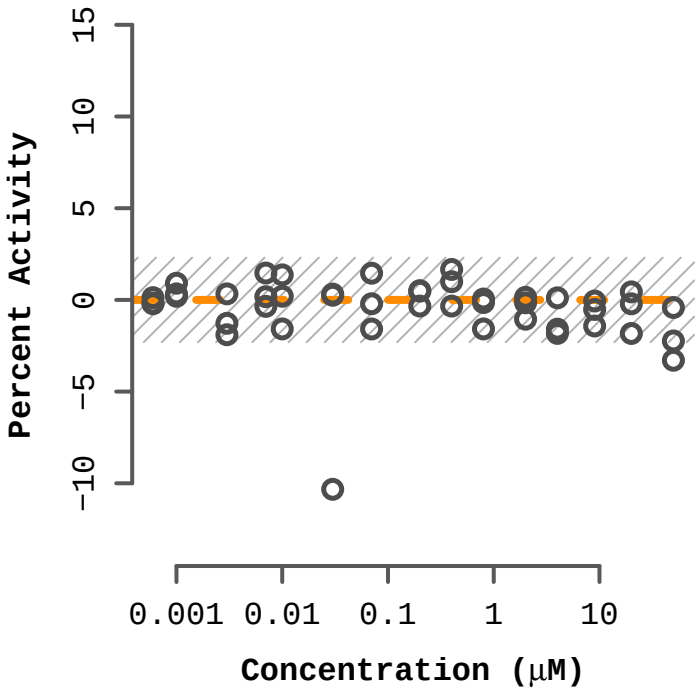
NAME: Acetyl tributyl citrate
CHID: 26446 **CASRN:** 77-90-7
SPID(S): Tox21_201779
M4ID: 12480473 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.32	NA	NA
PROB:	1	NA	NA
RMSE:	23.46	NA	NA

MAX_MEAN: 41.5 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

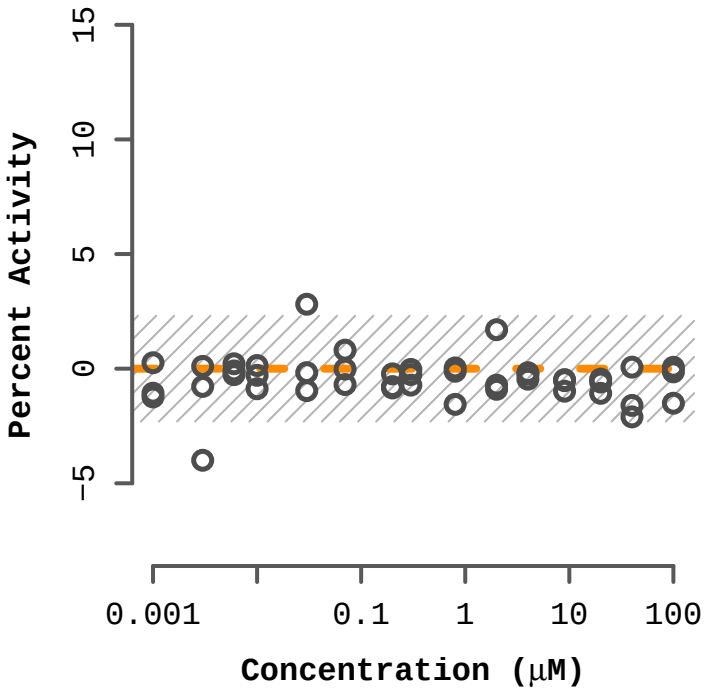
NAME: Acetyl tributyl citrate
CHID: 26446 **CASRN:** 77-90-7
SPID(S): Tox21_112777
M4ID: 12482956

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.773 **MAX_MED:** 0.993 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

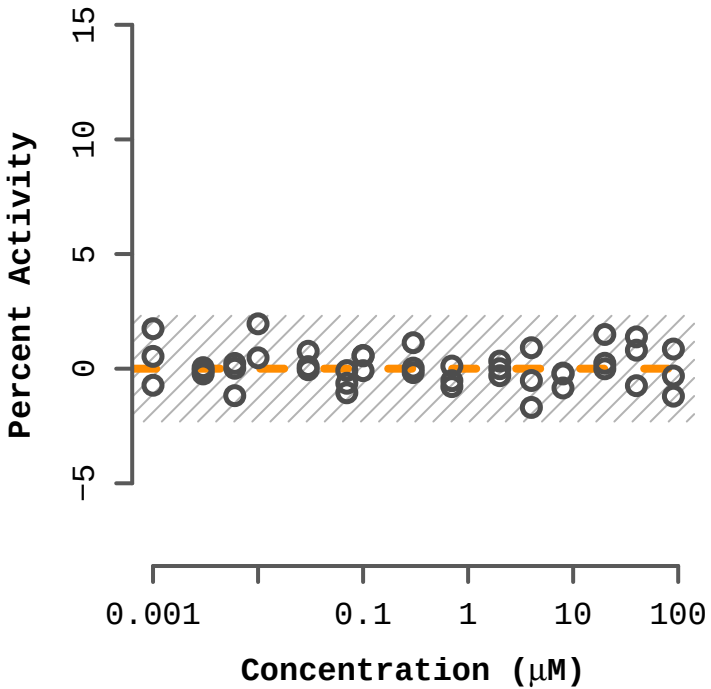
NAME: 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol
CHID: 26448 **CASRN:** 77-99-6
SPID(S): Tox21_200028
M4ID: 12482224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.562 **MAX_MED:** −0.0171 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

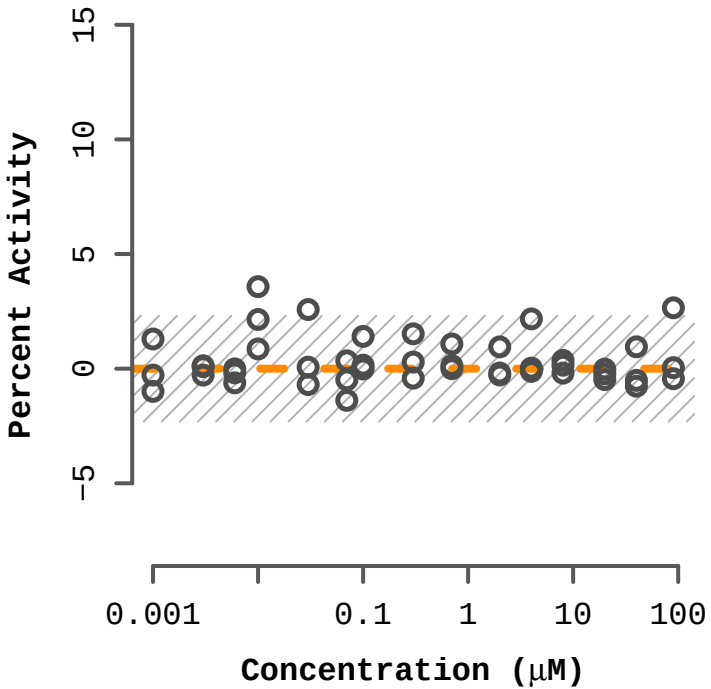
NAME: Tetraethyl orthosilicate
CHID: 26450 CASRN: 78-10-4
SPID(S): Tox21_200426
M4ID: 12481826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

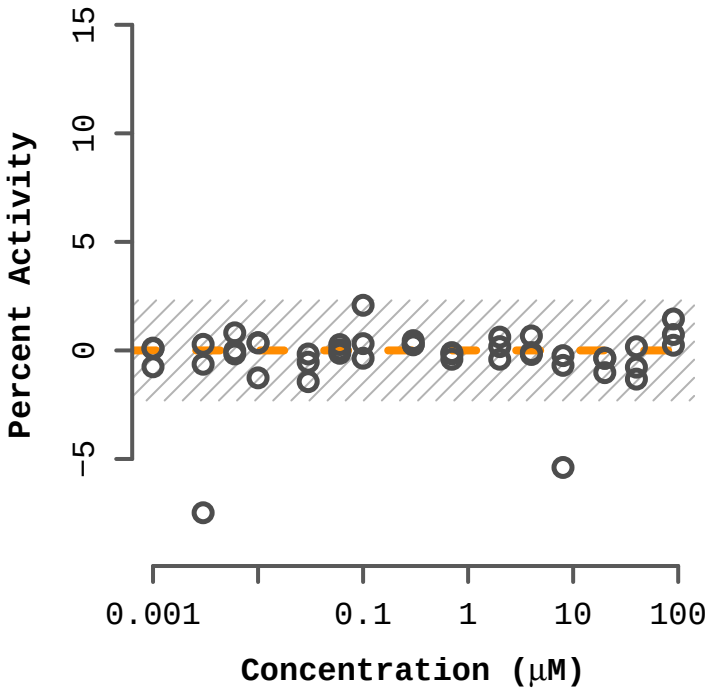
NAME: 2,2'−Azobis(2−methylpropanenitrile)
CHID: 26457 **CASRN:** 78−67−1
SPID(S): Tox21_303177
M4ID: 12475956

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 2.2 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

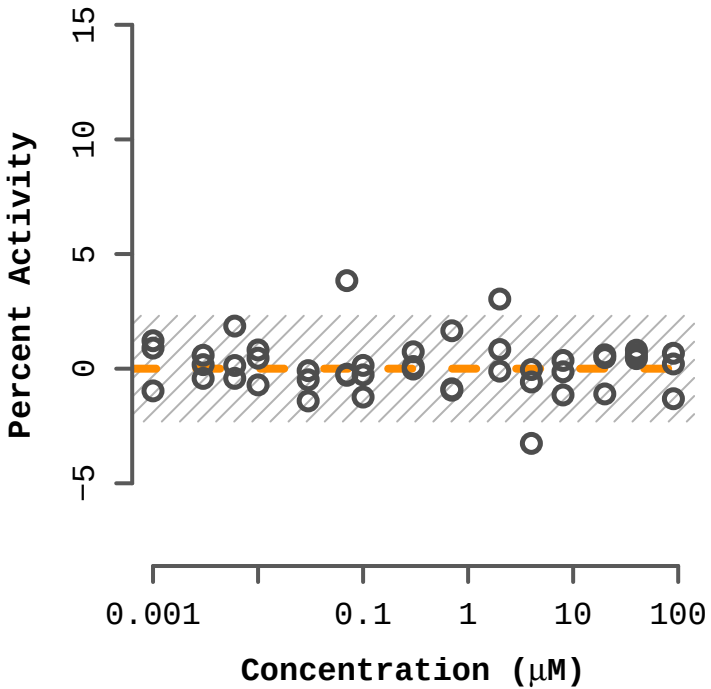
NAME: 2,2'−Azobis(2−methylpropanenitrile)
CHID: 26457 CASRN: 78−67−1
SPID(S): Tox21_202084
M4ID: 12480168

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.808 MAX_MED: 0.736 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

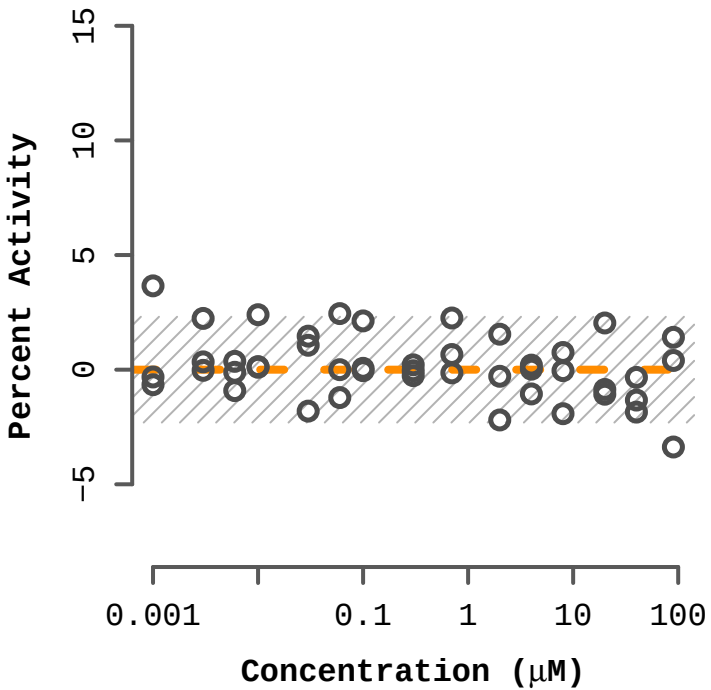
NAME: 2-Methylpropanenitrile
CHID: 26461 **CASRN:** 78-82-0
SPID(S): Tox21_303042
M4ID: 12476091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

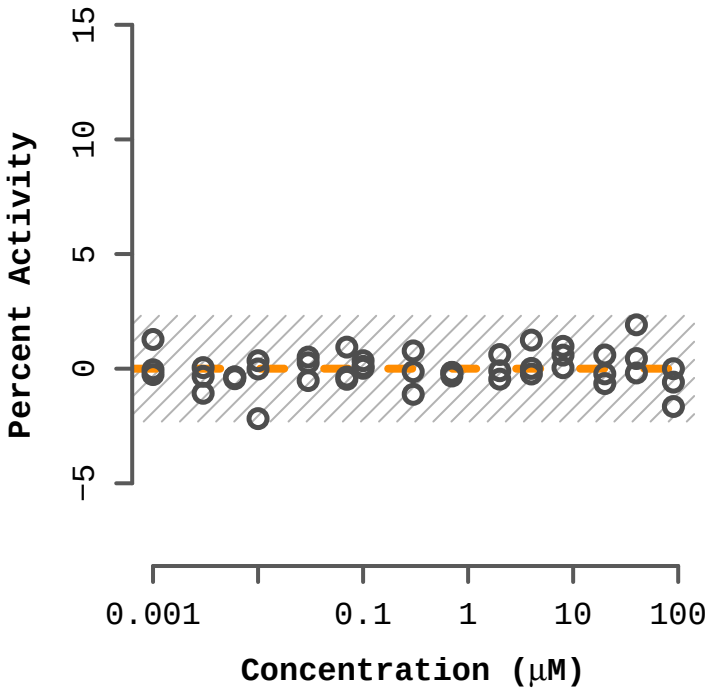
NAME: 2-Methylpropanenitrile
CHID: 26461 **CASRN:** 78-82-0
SPID(S): Tox21_201929
M4ID: 12480323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.927 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

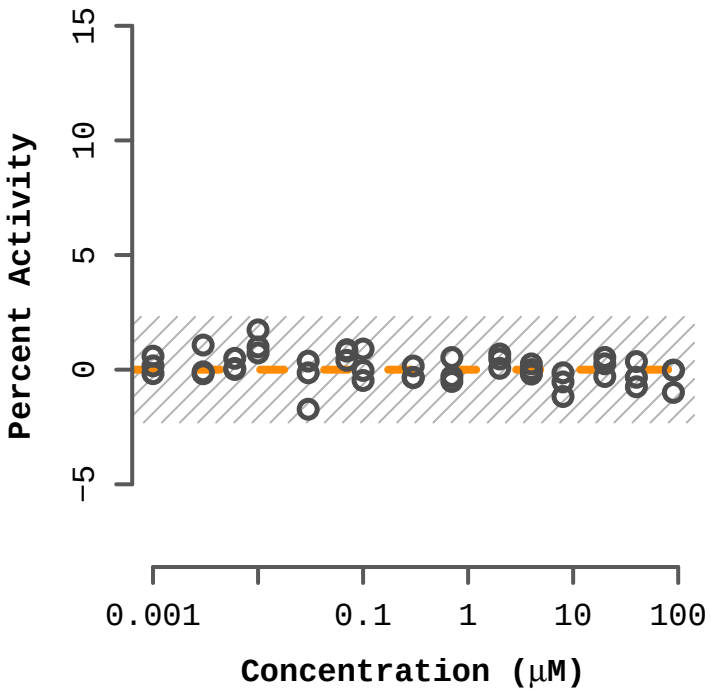
NAME: Chloroacetyl chloride
CHID: 26472 **CASRN:** 79-04-9
SPID(S): Tox21_200644
M4ID: 12481608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.724 **MAX_MED:** 0.592 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

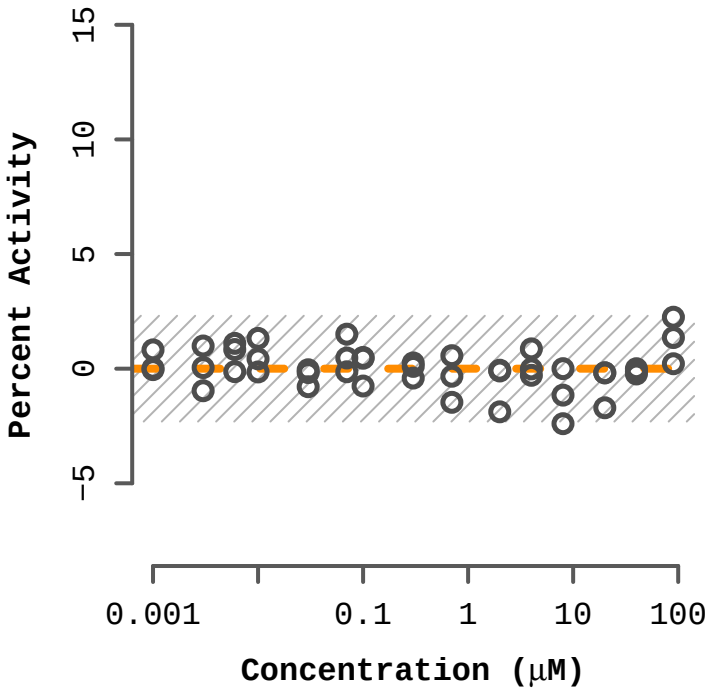
NAME: Camphene
CHID: 26488 **CASRN:** 79-92-5
SPID(S): Tox21_303152
M4ID: 12475981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.994 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

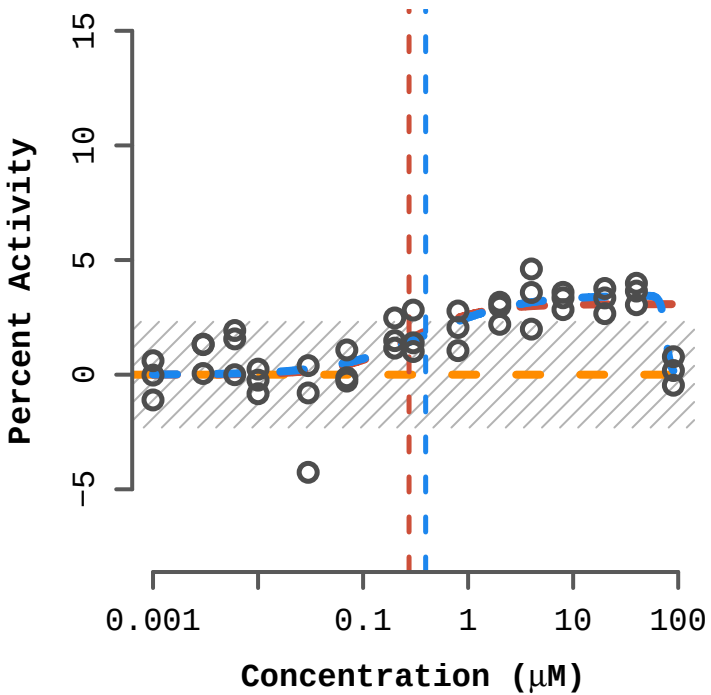
NAME: Camphene
CHID: 26488 **CASRN:** 79-92-5
SPID(S): Tox21_202014
M4ID: 12480238

HILL MODEL: Not applicable.

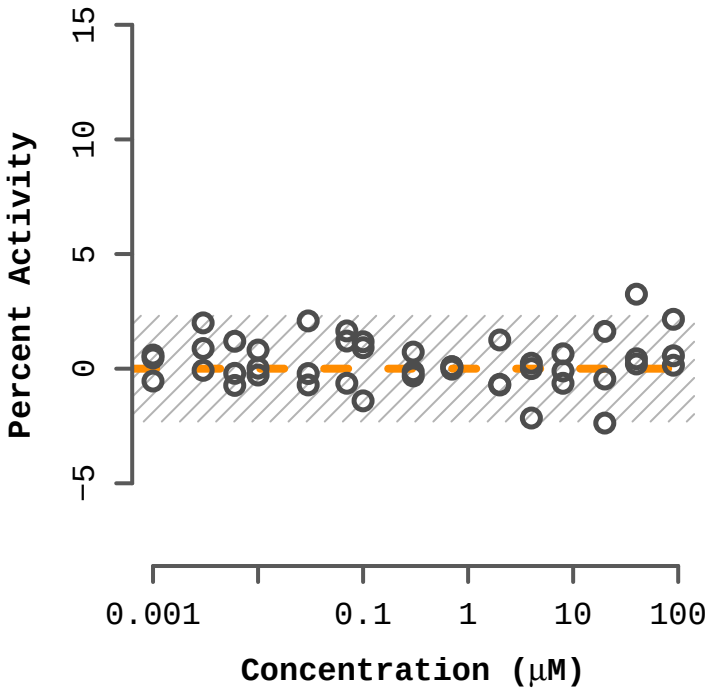
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.36 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dichlorodiphenylsilane
CHID:    26494   CASRN: 80-10-4
SPID(S): Tox21_202552
M4ID:    12479700

HILL MODEL (in red):
      tp       ga       gw
val:  3.08     -0.563   1.32
sd:   0.307    0.19     0.583

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.47     -0.404   1        1.88     17.6
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  208.23      149.24      130.52
PROB: 0           0           1
RMSE: 2.27        1.27        1.02

MAX_MEAN: 3.56      MAX_MED: 3.65      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

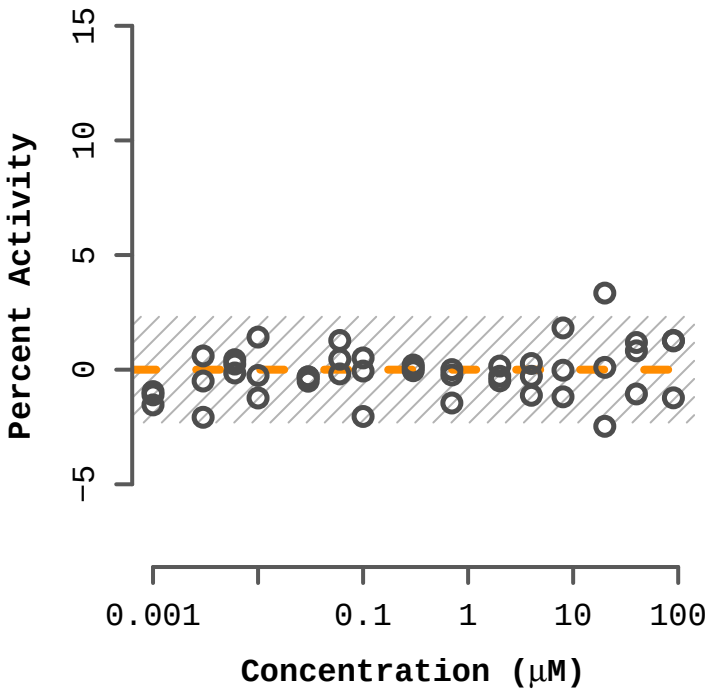
NAME: alpha-Terpinyl acetate
CHID: 26496 **CASRN:** 80-26-2
SPID(S): Tox21_303242
M4ID: 12475891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

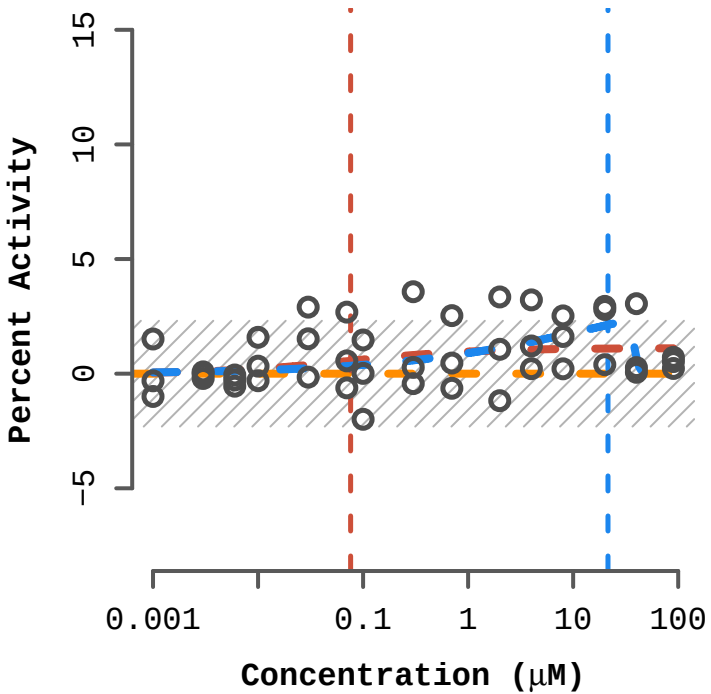
NAME: alpha-Terpinyl acetate
CHID: 26496 **CASRN:** 80-26-2
SPID(S): Tox21_202188
M4ID: 12480064

HILL MODEL: Not applicable.

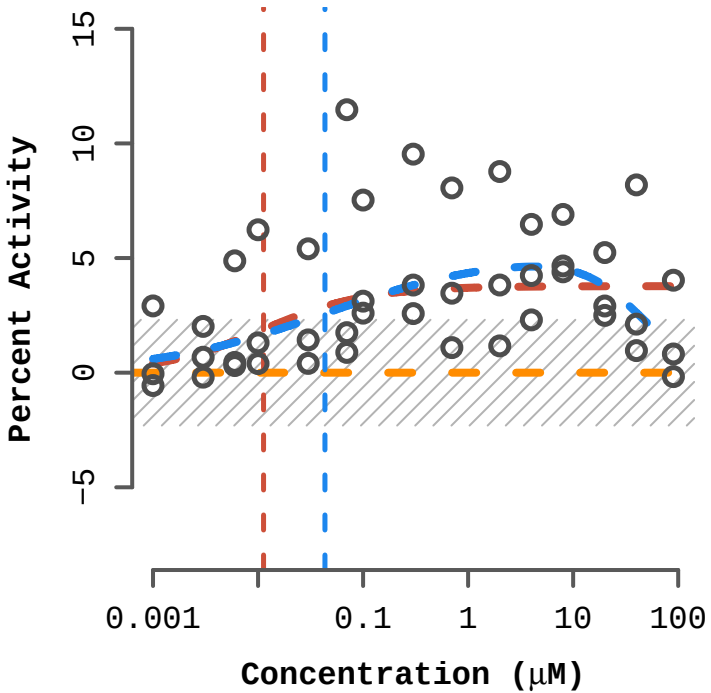
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.517 **MAX_MED:** 1.26 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4,4'-Oxybis(benzenesulfonhydrazide)
CHID:    26499   CASRN: 80-51-3
SPID(S): Tox21_301976
M4ID:    12477157

HILL MODEL (in red):
      tp       ga       gw
val:  1.11     -1.12    0.72
sd:   0.406    1.17     0.633

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.26     1.33     0.432    1.58     17.9
sd:   8.08     3.37     0.302    0.0672   57.4

      CNST        HILL        GNLS
AIC:  170.92      162.51      163.38
PROB: 0.01        0.6         0.39
RMSE: 1.58        1.29        1.27

MAX_MEAN: 2.04      MAX_MED: 2.8       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-(4-tert-Butylphenyl)-2-methylpropanal
CHID: 26500 CASRN: 80-54-6
SPID(S): Tox21_303107
M4ID: 12476026

HILL MODEL (in red):

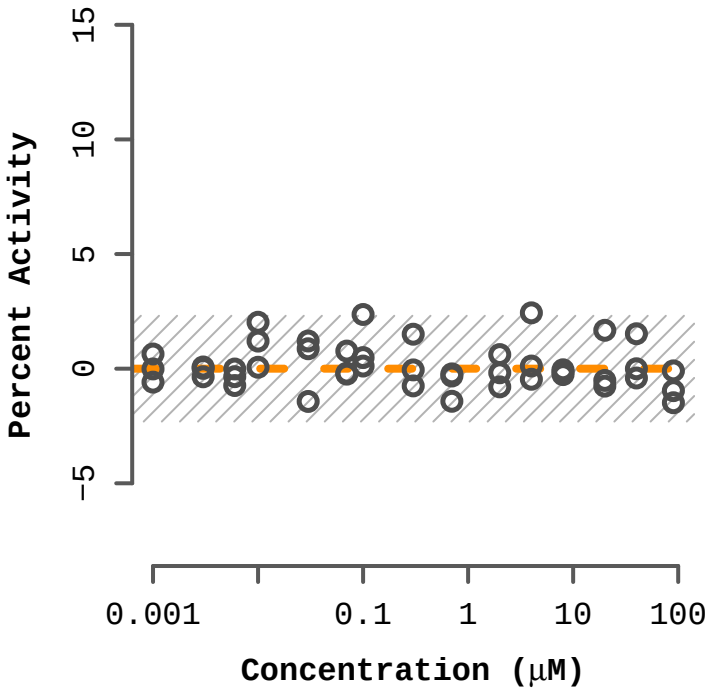
	tp	ga	gw
val:	3.77	−1.95	0.876
sd:	0.561	0.444	0.562

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.16	−1.36	0.539	1.62	1.55
sd:	2.15	0.974	0.431	0.318	1.28

	CNST	HILL	GNLS
AIC:	265.08	224.78	224.02
PROB:	0	0.41	0.59
RMSE:	4.44	2.71	2.63

MAX_MEAN: 5.32 MAX_MED: 4.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

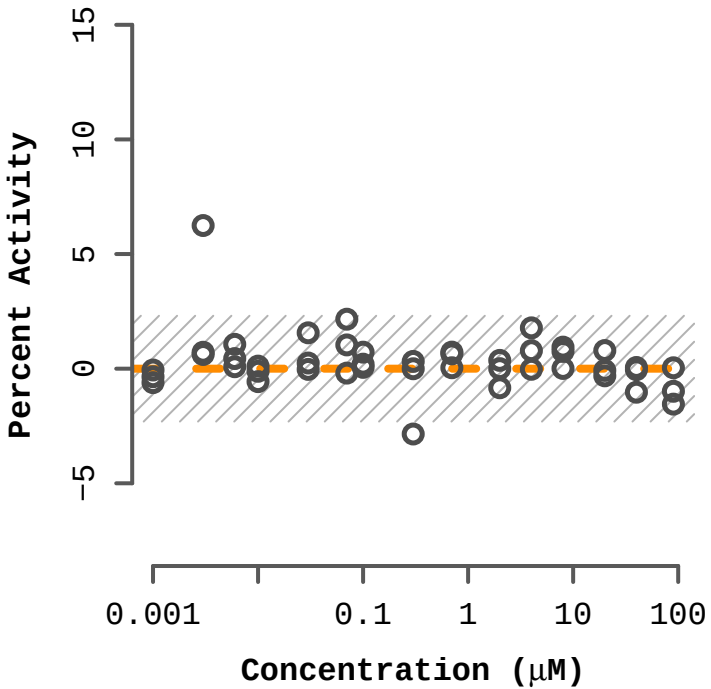
NAME: 3-(4-tert-Butylphenyl)-2-methylpropanal
CHID: 26500 **CASRN:** 80-54-6
SPID(S): Tox21_201412
M4ID: 12480840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

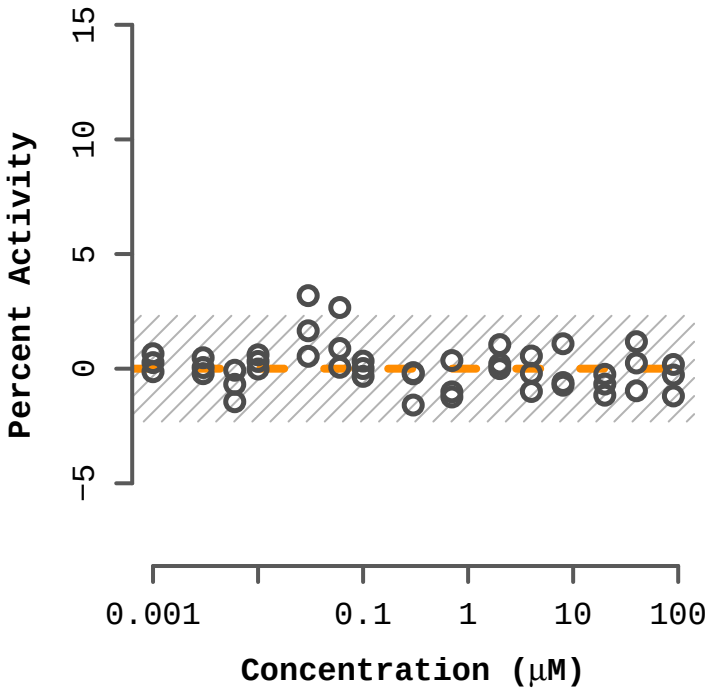
NAME: alpha-Pinene
CHID: 26501 **CASRN:** 80-56-8
SPID(S): Tox21_303385
M4ID: 12475753

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 2.53 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

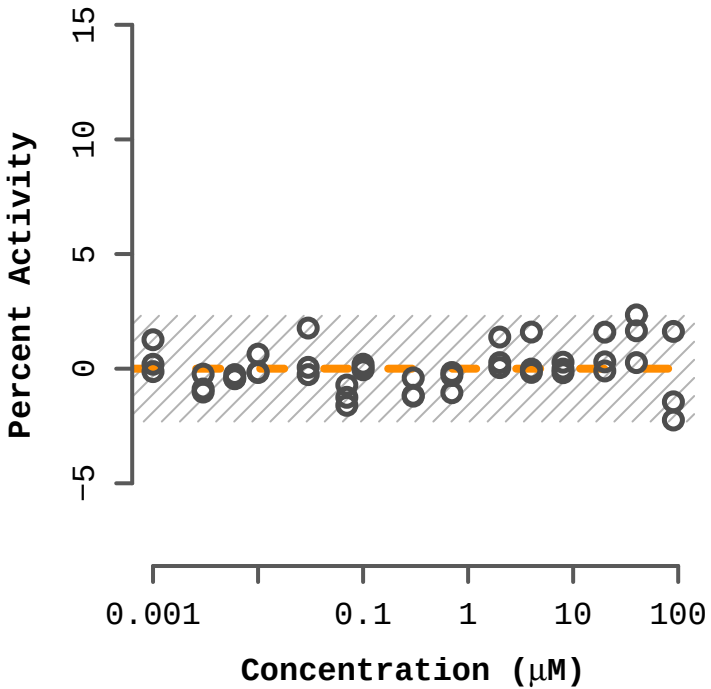
NAME: alpha-Pinene
CHID: 26501 **CASRN:** 80-56-8
SPID(S): Tox21_200108
M4ID: 12482144

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

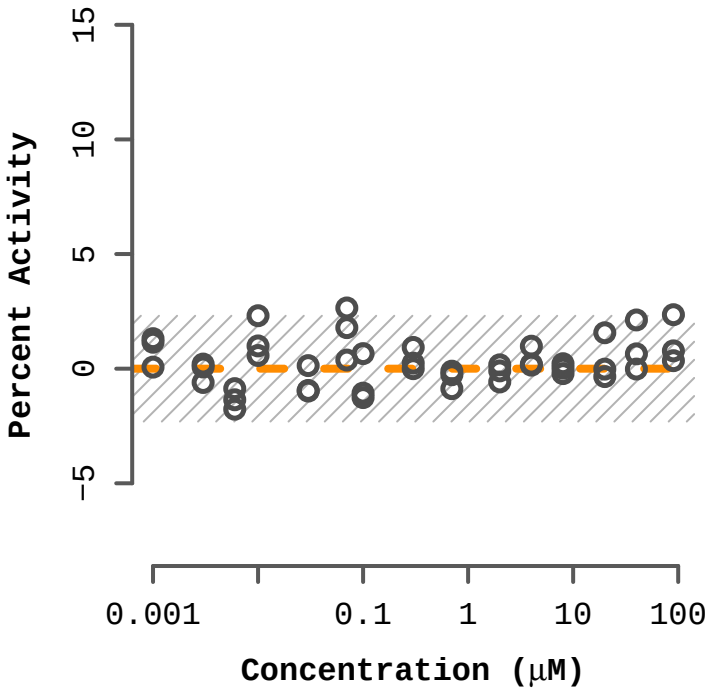
NAME: 1H,3H−Naphtho(1,8−cd)pyran−1,3−dione
CHID: 26505 **CASRN:** 81−84−5
SPID(S): Tox21_200045
M4ID: 12482207

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

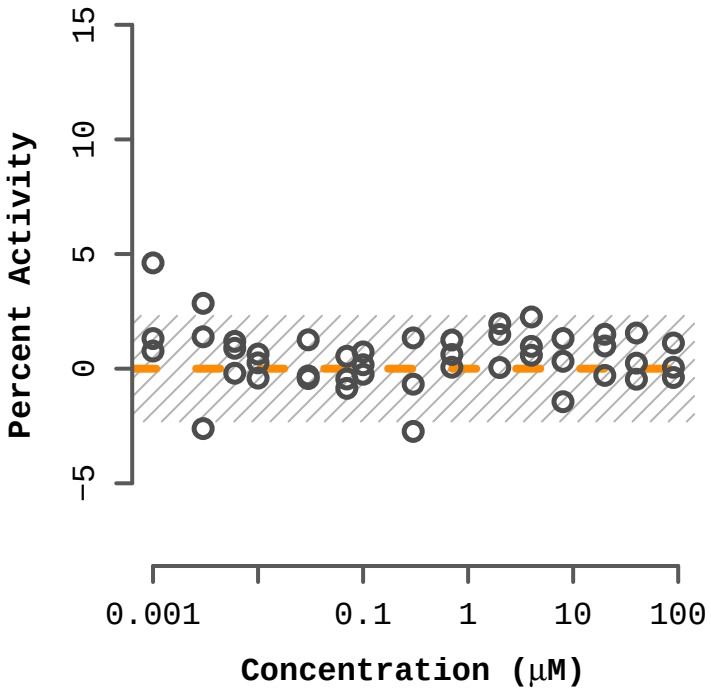
NAME: Didecyl phthalate
CHID: 26512 **CASRN:** 84-77-5
SPID(S): Tox21_200427
M4ID: 12481825

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

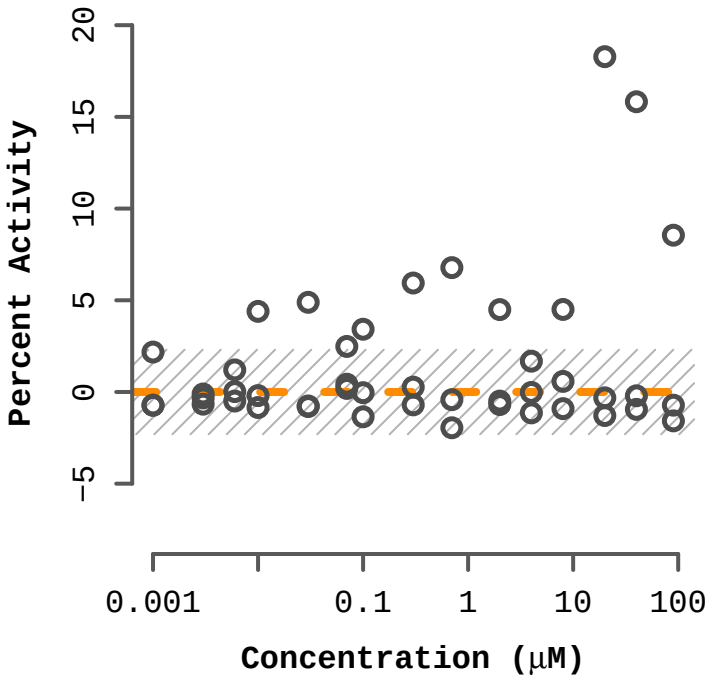
NAME: 1,2,3,6−Tetrahydrophthalimide
CHID: 26513 **CASRN:** 85−40−5
SPID(S): Tox21_301178
M4ID: 12477955

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

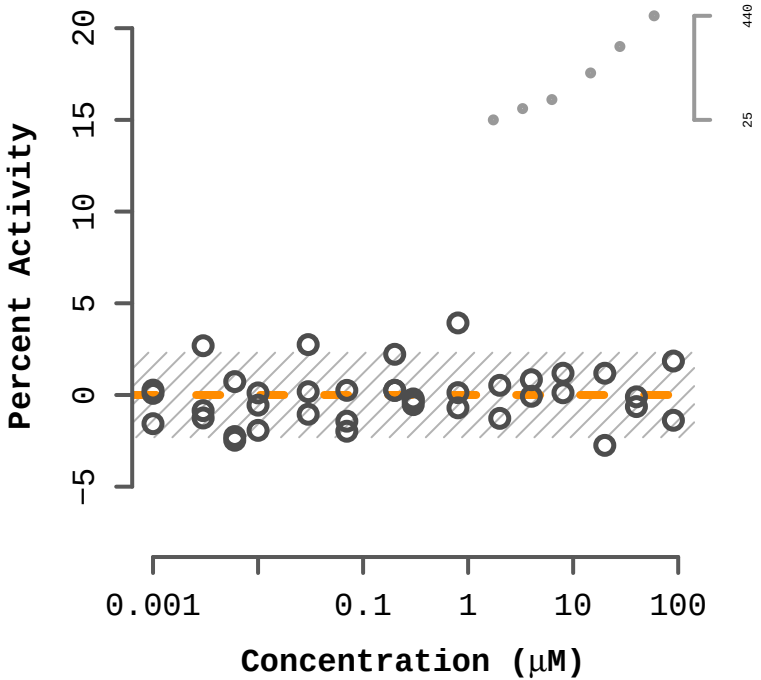
NAME: Phthalimide
CHID: 26514 CASRN: 85-41-6
SPID(S): Tox21_303319
M4ID: 12475814

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.6	NA	NA
PROB:	1	NA	NA
RMSE:	4.39	NA	NA

MAX_MEAN: 5.56 MAX_MED: 0.579 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

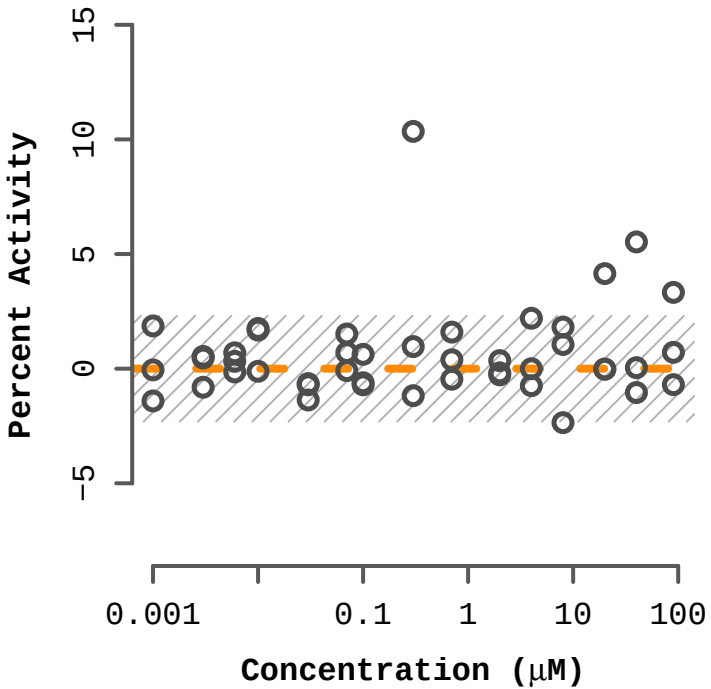
NAME: Phthalimide
CHID: 26514 **CASRN:** 85-41-6
SPID(S): Tox21_201800
M4ID: 12480452 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	383.93	NA	NA
PROB:	1	NA	NA
RMSE:	88.04	NA	NA

MAX_MEAN: 145 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

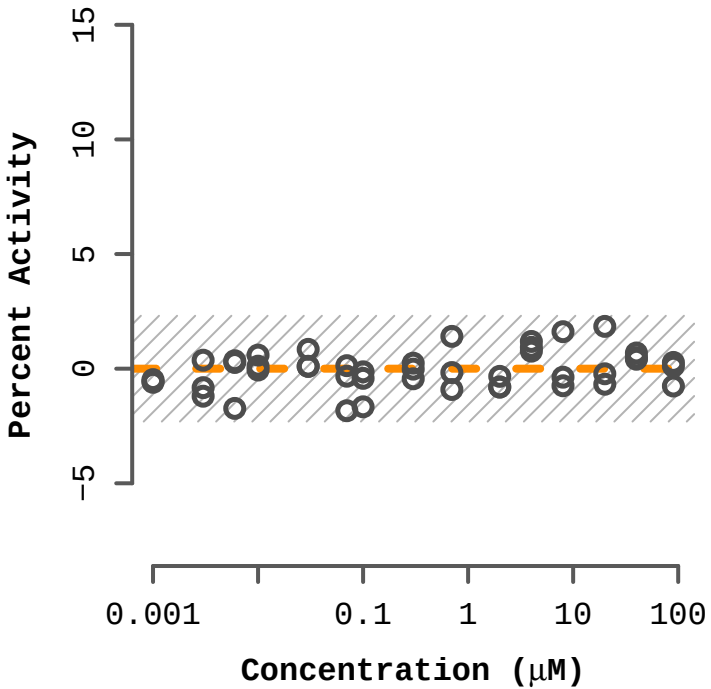
NAME: Hexahydrophthalic anhydride
CHID: 26515 **CASRN:** 85-42-7
SPID(S): Tox21_200661
M4ID: 12481591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.48	NA	NA
PROB:	1	NA	NA
RMSE:	2.15	NA	NA

MAX_MEAN: 3.38 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

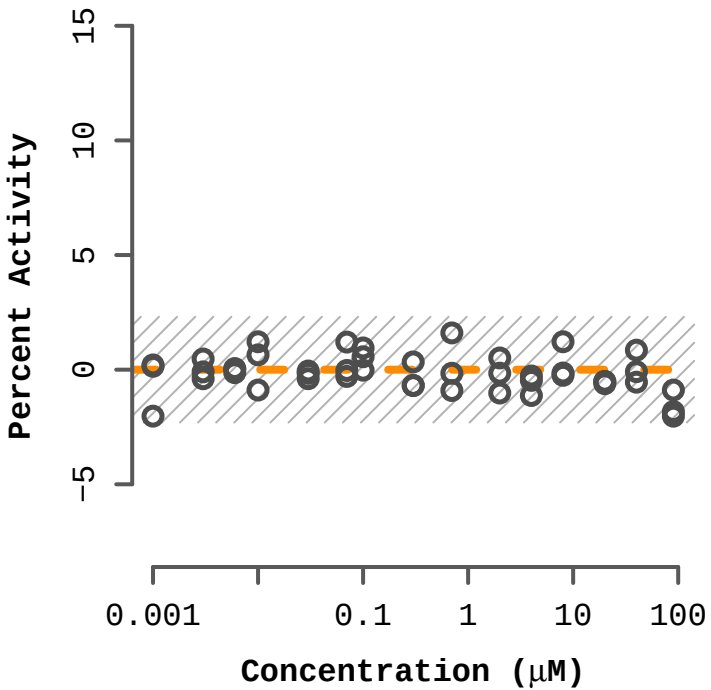
NAME: Tetrahydrophthalic anhydride
CHID: 26516 **CASRN:** 85-43-8
SPID(S): Tox21_202210
M4ID: 12480042

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 0.934 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

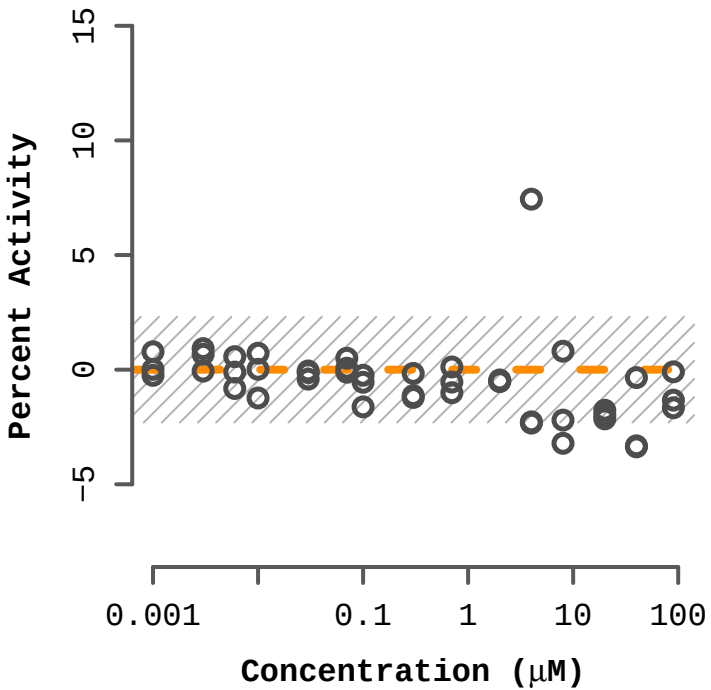
NAME: Butyl 2-ethylhexyl phthalate
CHID: 26519 CASRN: 85-69-8
SPID(S): Tox21_200061
M4ID: 12482191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.498 **MAX_MED:** 0.649 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

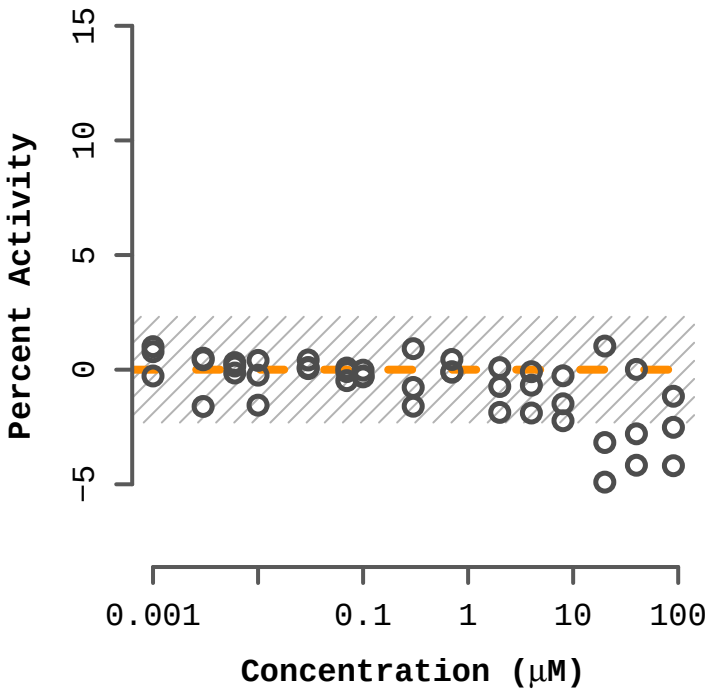
NAME: 7-Amino-4-hydroxynaphthalene-2-sulfonic acid
CHID: 26520 **CASRN:** 87-02-5
SPID(S): Tox21_303310
M4ID: 12475823

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 0.945 **MAX_MED:** 0.673 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

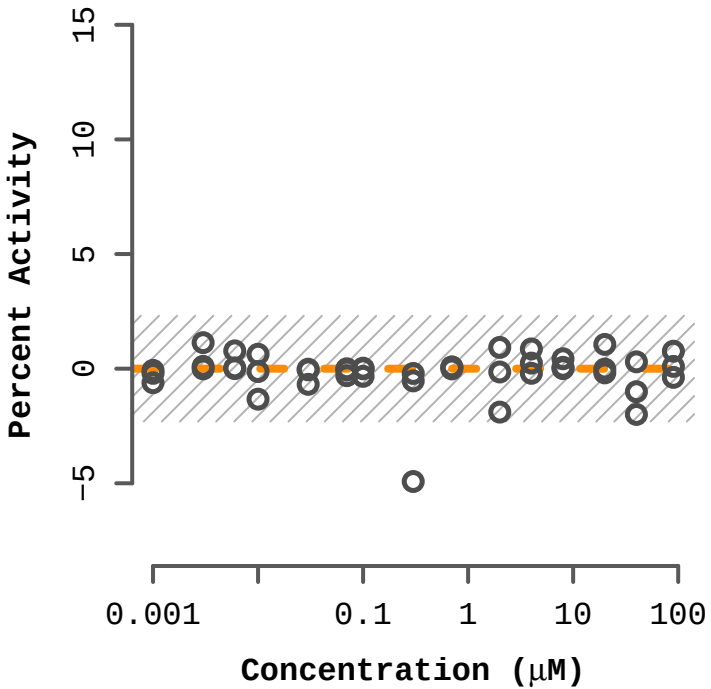
NAME: 7-Amino-4-hydroxynaphthalene-2-sulfonic acid
CHID: 26520 **CASRN:** 87-02-5
SPID(S): Tox21_202232
M4ID: 12480020

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 0.506 **MAX_MED:** 0.785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

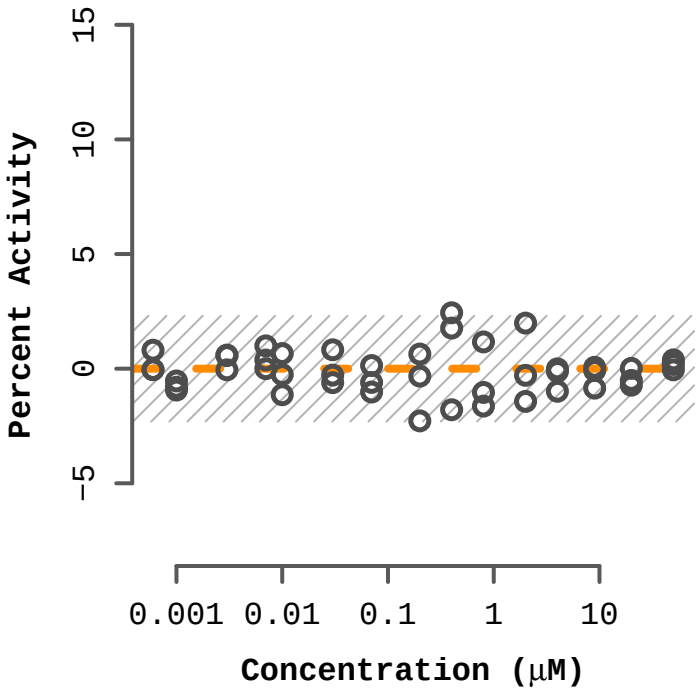
NAME: Symclosene
CHID: 26523 CASRN: 87-90-1
SPID(S): Tox21_300858
M4ID: 12478275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.411 MAX_MED: 0.245 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

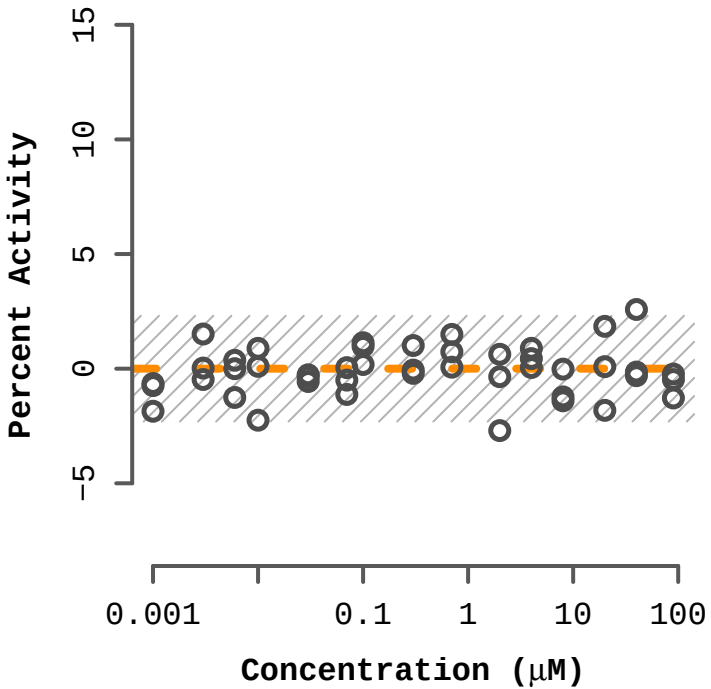
NAME: Symclosene
CHID: 26523 **CASRN:** 87-90-1
SPID(S): Tox21_112103_1
M4ID: 12483318

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

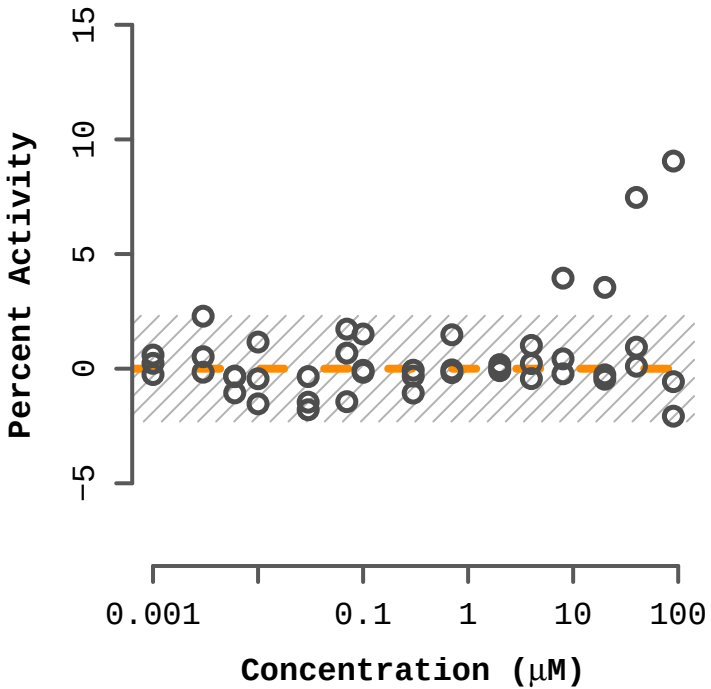
NAME: 2-tert-Butylphenol
CHID: 26525 CASRN: 88-18-6
SPID(S): Tox21_300011
M4ID: 12479119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.767 MAX_MED: 0.974 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

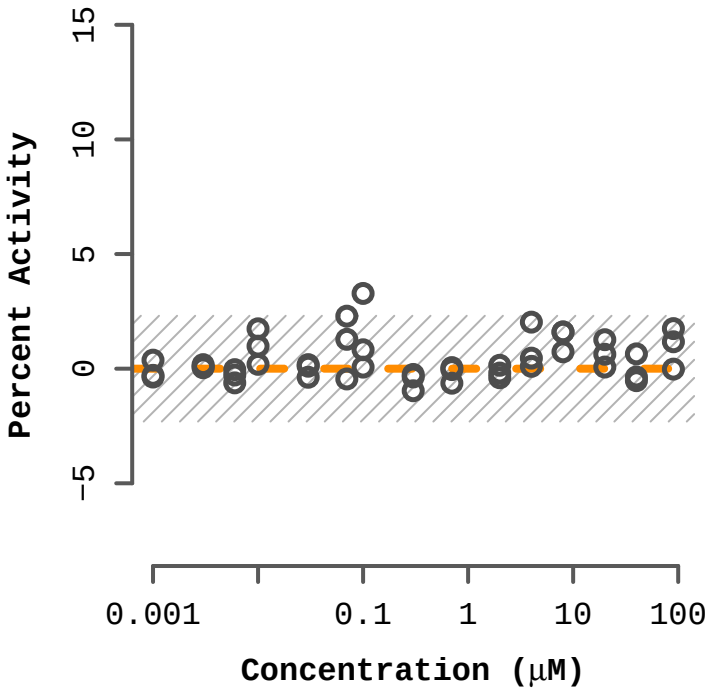
NAME: 2-tert-Butylphenol
CHID: 26525 CASRN: 88-18-6
SPID(S): Tox21_202041
M4ID: 12480211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.12	NA	NA

MAX_MEAN: 2.84 MAX_MED: 0.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

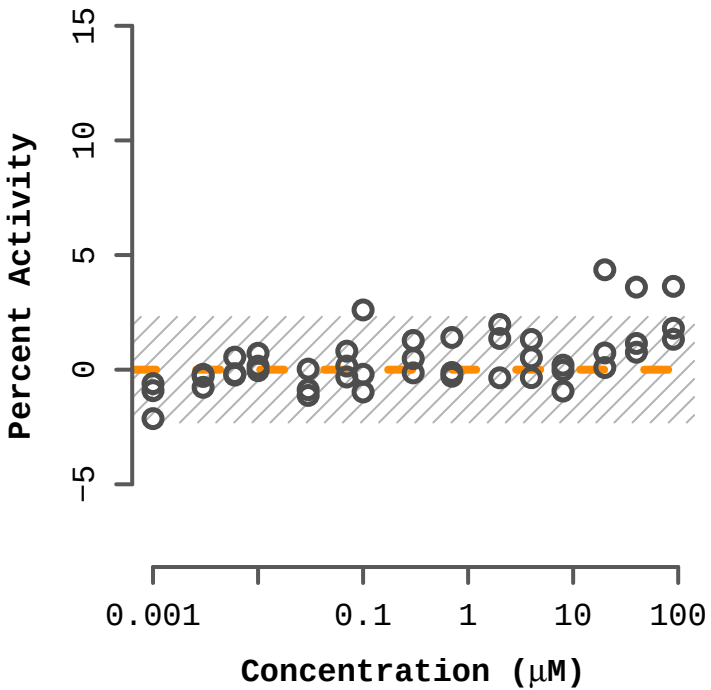
NAME: 2-Amino-5-methylbenzenesulfonic acid
CHID: 26526 **CASRN:** 88-44-8
SPID(S): Tox21_303178
M4ID: 12475955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

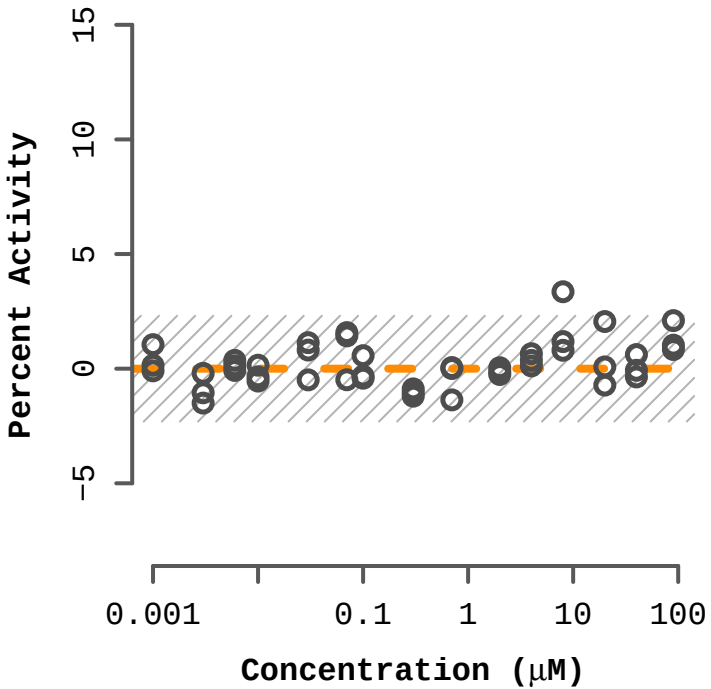
NAME: 2-Amino-5-methylbenzenesulfonic acid
CHID: 26526 **CASRN:** 88-44-8
SPID(S): Tox21_202254
M4ID: 12479998

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 2.26 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

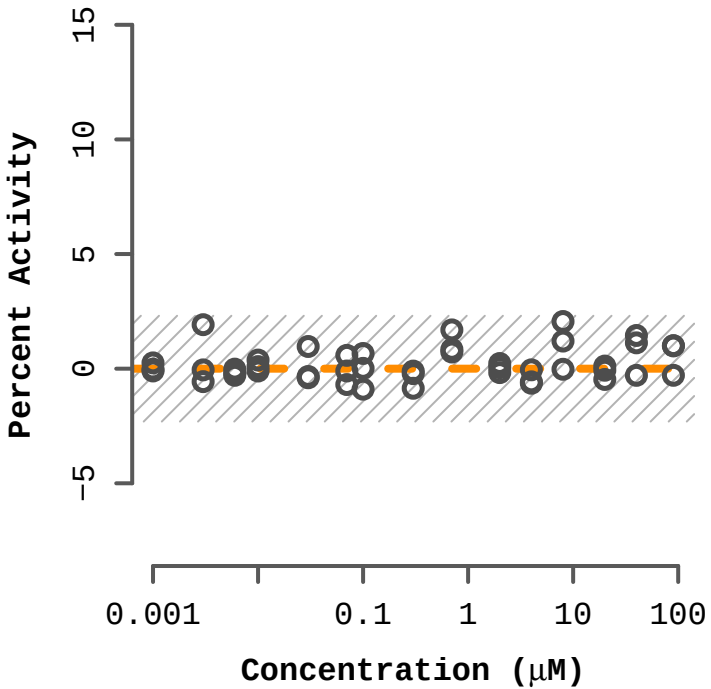
NAME: 2-Amino-4-chloro-5-methylbenzenesulfonic acid
CHID: 26527 **CASRN:** 88-51-7
SPID(S): Tox21_200428
M4ID: 12481824

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

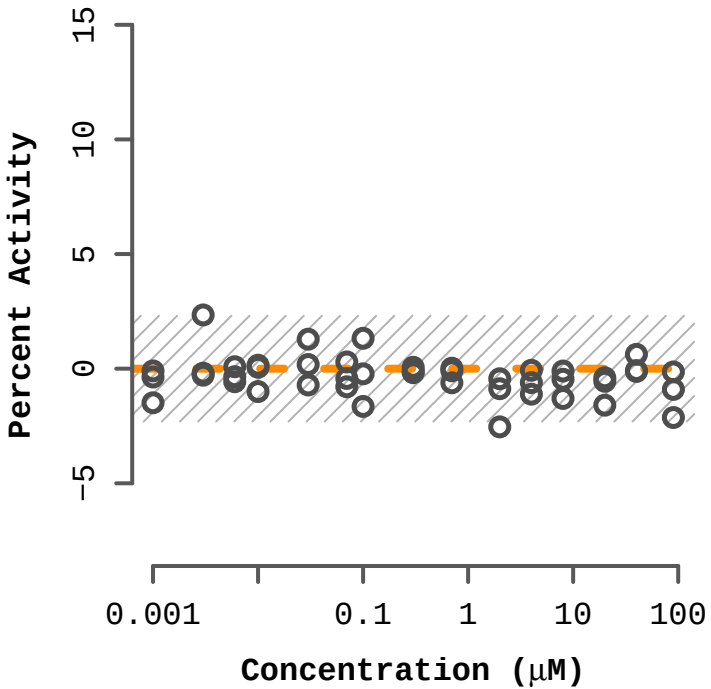
NAME: 2-Amino-5-chloro-4-methylbenzenesulfonic acid
CHID: 26528 CASRN: 88-53-9
SPID(S): Tox21_200678
M4ID: 12481574

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 1.09 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

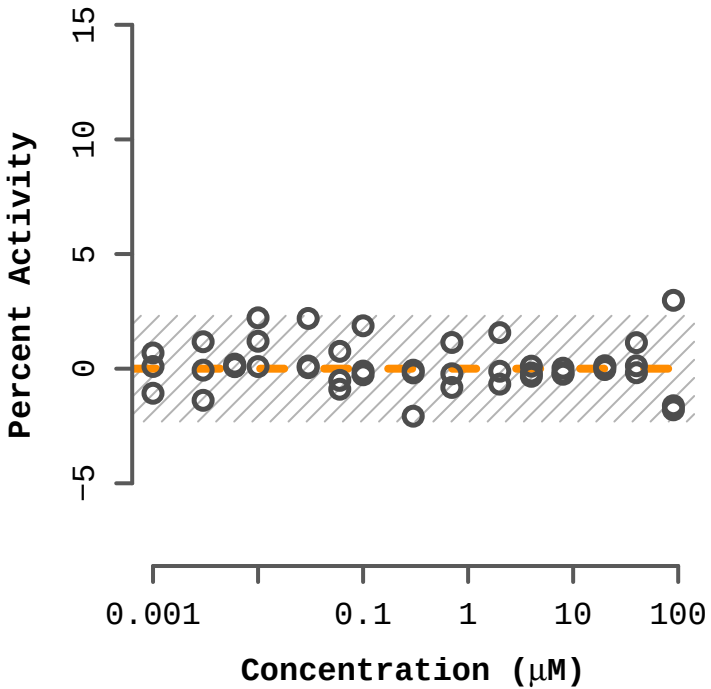
NAME: 2-tert-Butyl-5-methylphenol
CHID: 26529 **CASRN:** 88-60-8
SPID(S): Tox21_300486
M4ID: 12478646

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.623 **MAX_MED:** 0.183 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

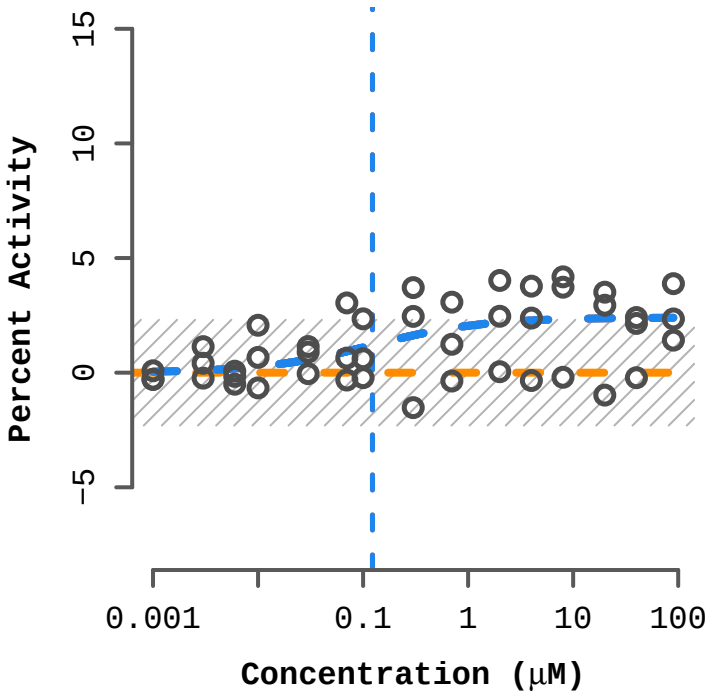
NAME: 2-tert-Butyl-5-methylphenol
CHID: 26529 **CASRN:** 88-60-8
SPID(S): Tox21_201418
M4ID: 12480834

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Sulfophthalic acid
CHID: 26535 CASRN: 89-08-7
SPID(S): Tox21_202553
M4ID: 12479699

HILL MODEL (in red):

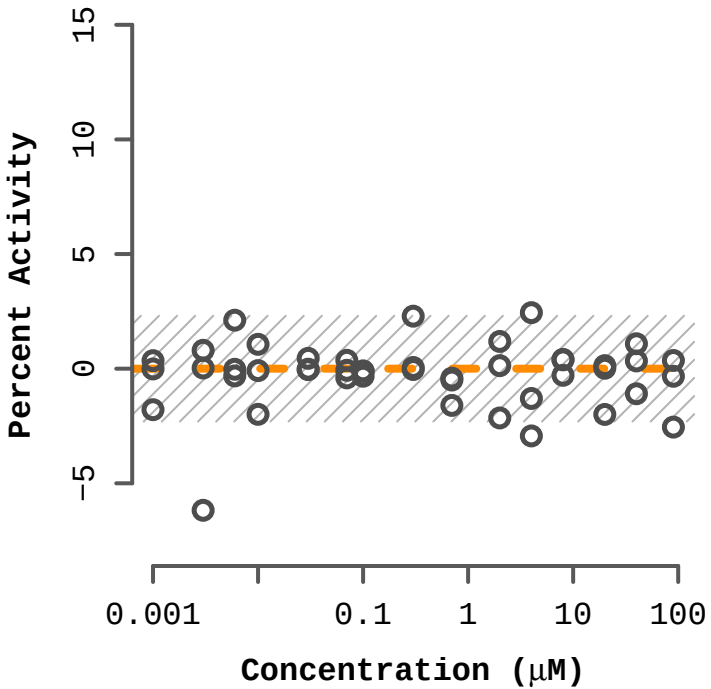
	tp	ga	gw
val:	2.41	−0.911	0.826
sd:	0.445	0.481	0.554

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.41	−0.911	0.826	3.24	5.23
sd:	0.445	0.481	0.554	921	3910

	CNST	HILL	GNLS
AIC:	196.17	169.5	173.5
PROB:	0	0.88	0.12
RMSE:	2.04	1.42	1.42

MAX_MEAN: 2.57 MAX_MED: 3.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

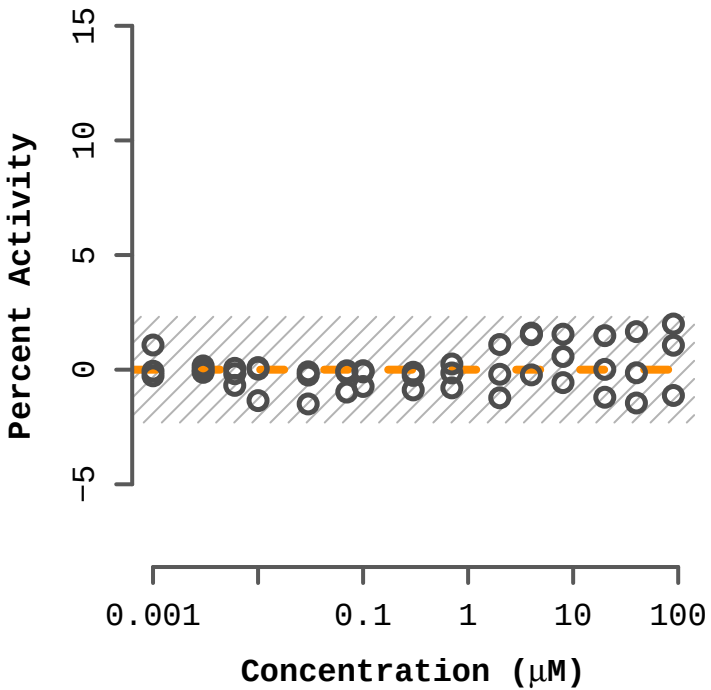
NAME: 1H,3H-Benzo(1,2-c:4,5-c')difuran-1,3,5,7-tetro
CHID: 26536 CASRN: 89-32-7
SPID(S): Tox21_303118
M4ID: 12476015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.77 MAX_MED: 0.386 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

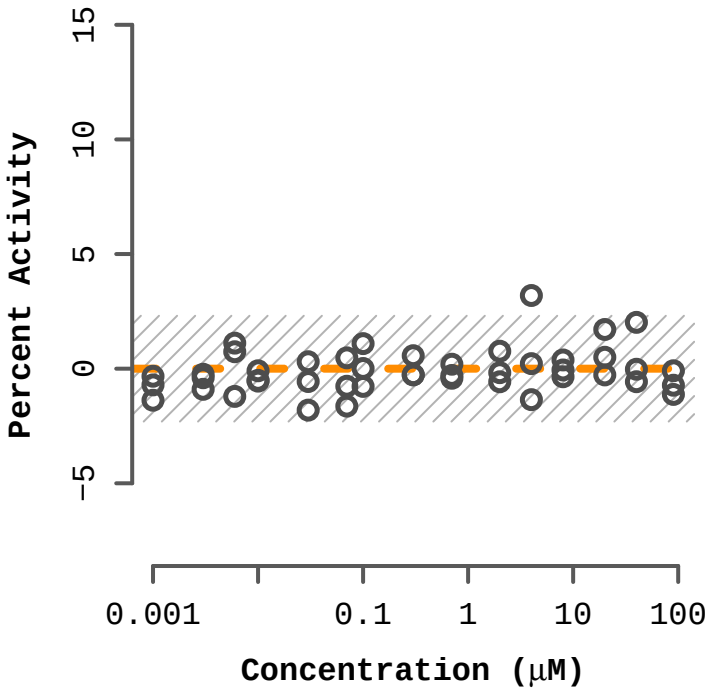
NAME: 1H,3H-Benzo(1,2-c:4,5-c')difuran-1,3,5,7-tetro
CHID: 26536 **CASRN:** 89-32-7
SPID(S): Tox21_201714
M4ID: 12480538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

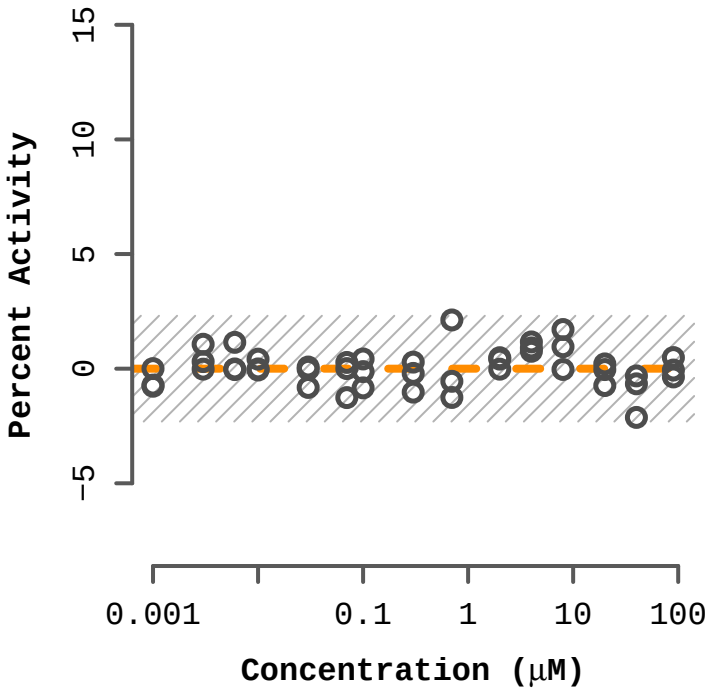
NAME: Isoascorbic acid
CHID: 26537 **CASRN:** 89-65-6
SPID(S): Tox21_201111
M4ID: 12481141

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

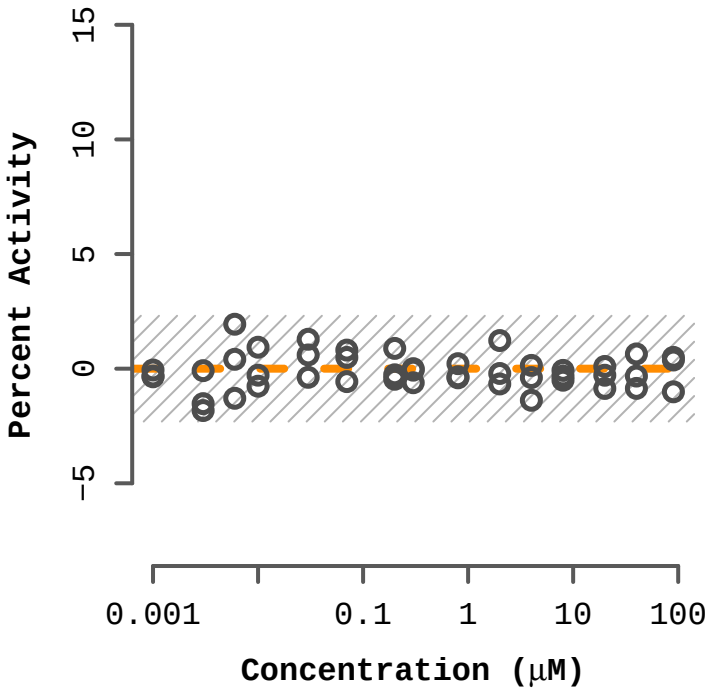
NAME: 1,2,3−Benzotriazin−4(1H)−one
CHID: 26544 **CASRN:** 90−16−4
SPID(S): Tox21_303160
M4ID: 12475973

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.945 **MAX_MED:** 0.959 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

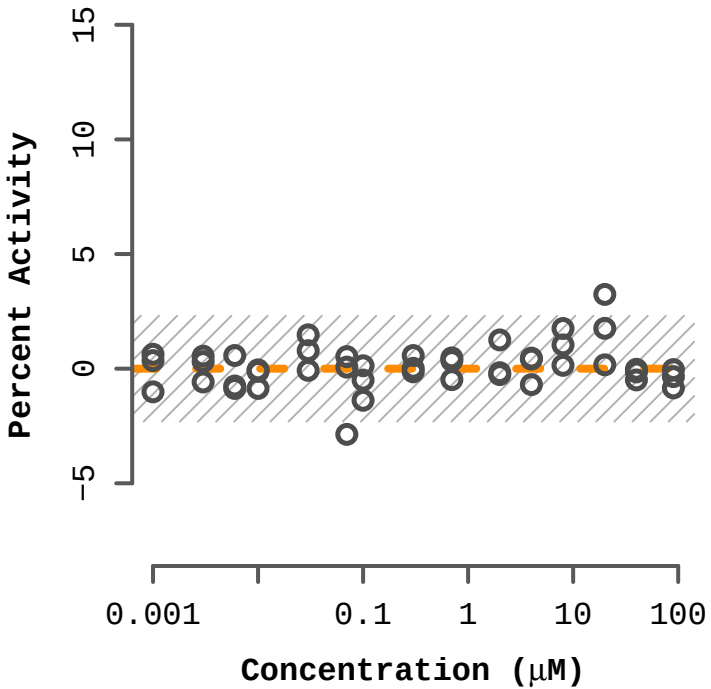
NAME: 1,2,3−Benzotriazin−4(1H)−one
CHID: 26544 **CASRN:** 90−16−4
SPID(S): Tox21_201876
M4ID: 12480376

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.503 **MAX_MED:** 0.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

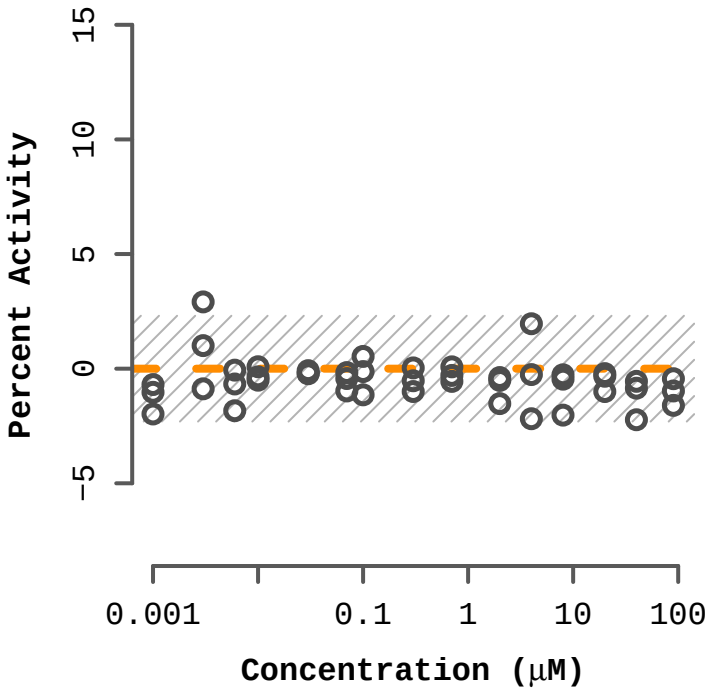
NAME: 6-Amino-4-hydroxynaphthalene-2-sulfonic acid
CHID: 26547 **CASRN:** 90-51-7
SPID(S): Tox21_200078
M4ID: 12482174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

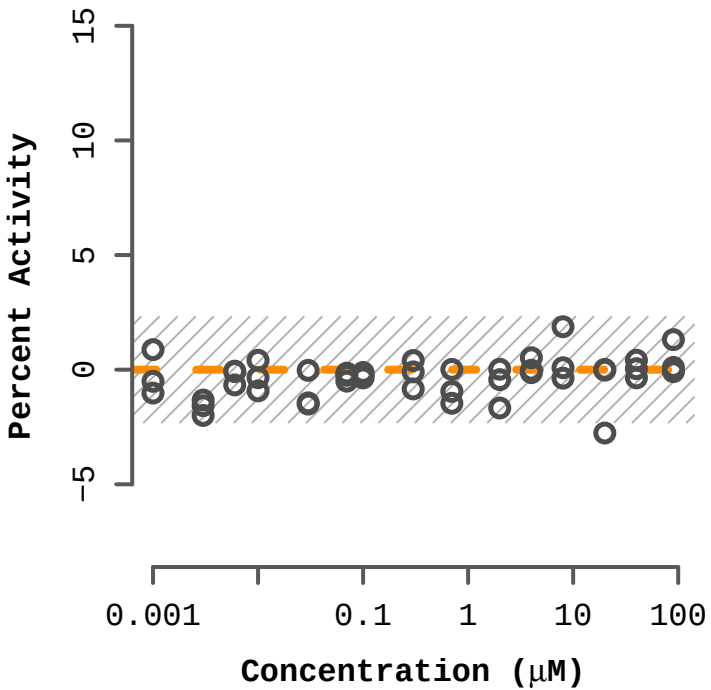
NAME: 2,4,6-Tris(dimethylaminomethyl)phenol
CHID: 26548 **CASRN:** 90-72-2
SPID(S): Tox21_303329
M4ID: 12475804

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

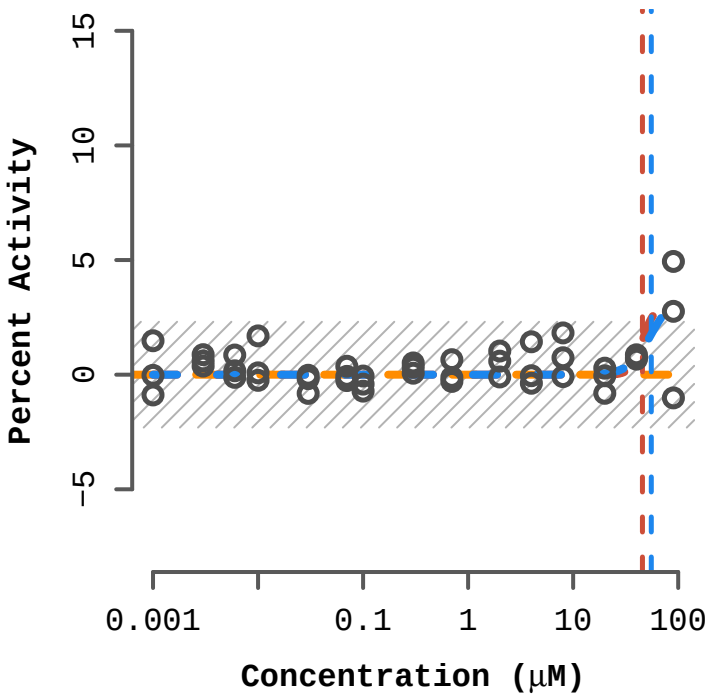
NAME: 2,4,6-Tris(dimethylaminomethyl)phenol
CHID: 26548 **CASRN:** 90-72-2
SPID(S): Tox21_201895
M4ID: 12480357

HILL MODEL: Not applicable.

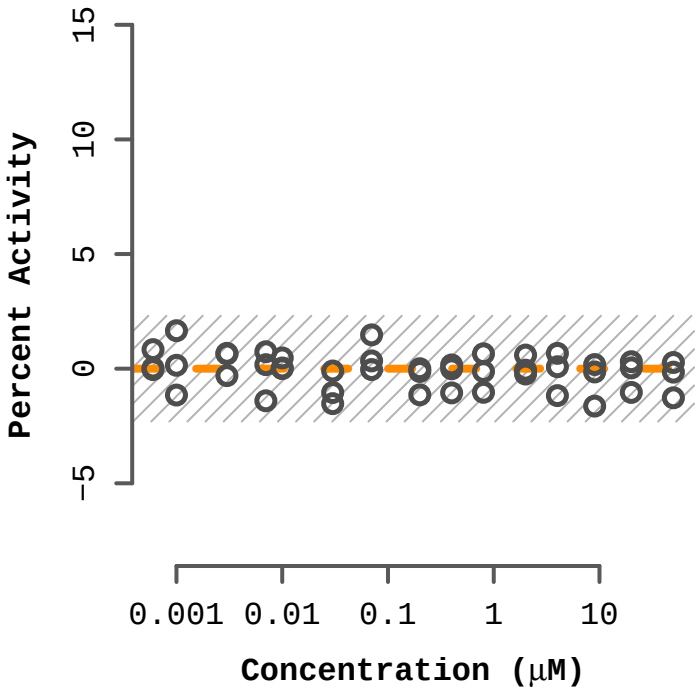
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.531 **MAX_MED:** 0.0989 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Gluconolactone
CHID:    26549   CASRN: 90-80-2
SPID(S): Tox21_200429
M4ID:    12481823

HILL MODEL (in red):
      tp       ga       gw
val:  2.97     1.66     8
sd:   0.617    0.125    16.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.29     1.74     4.12     3.95     0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  120.13      113.91      118.07
PROB: 0.04        0.86        0.11
RMSE: 1.09        0.92        0.93

MAX_MEAN: 2.23      MAX_MED: 2.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

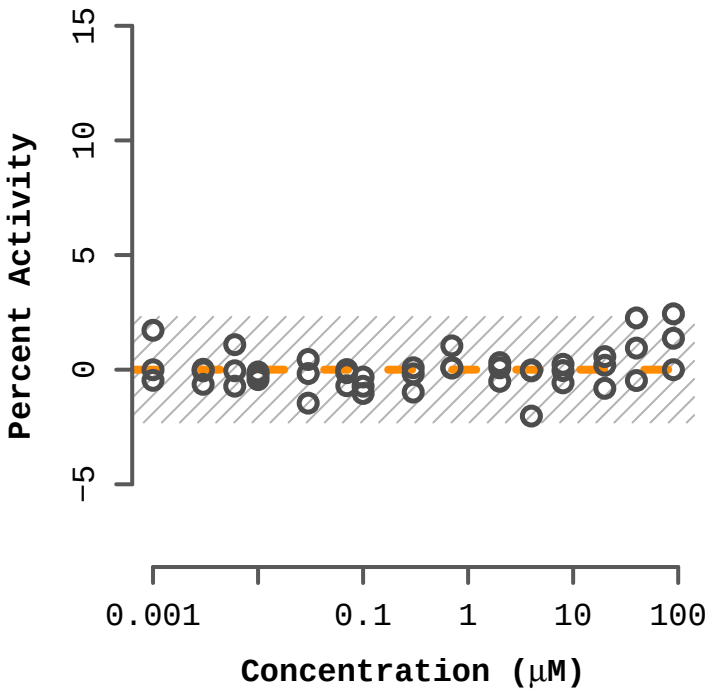
NAME: Gluconolactone
CHID: 26549 **CASRN:** 90-80-2
SPID(S): Tox21_111383_1
M4ID: 12483722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.593 **MAX_MED:** 0.642 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

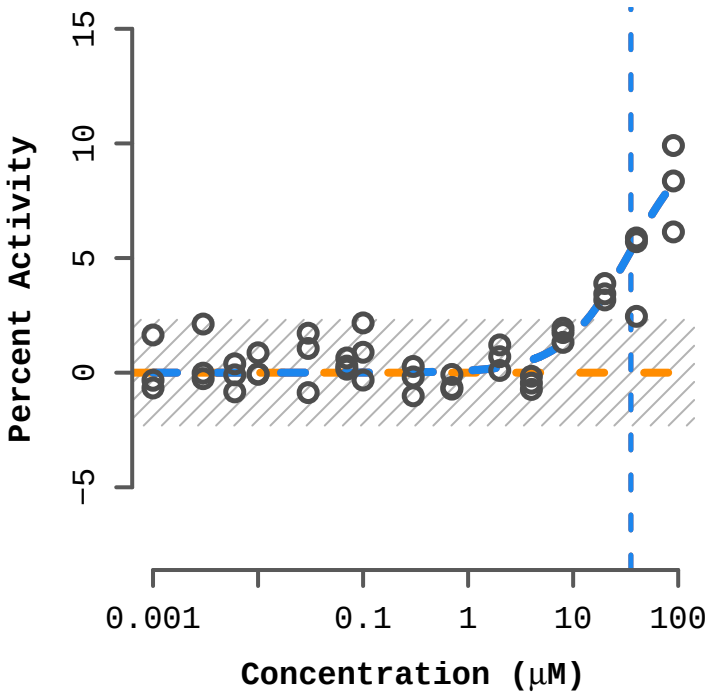
NAME: 2,2'−(3−Chlorophenylimino)diethanol
CHID: 26557 CASRN: 92−00−2
SPID(S): Tox21_303219
M4ID: 12475914

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(2-Methoxyphenyl)-3-oxobutanamide
CHID: 26558 CASRN: 92-15-9
SPID(S): Tox21_303221
M4ID: 12475912

HILL MODEL (in red):

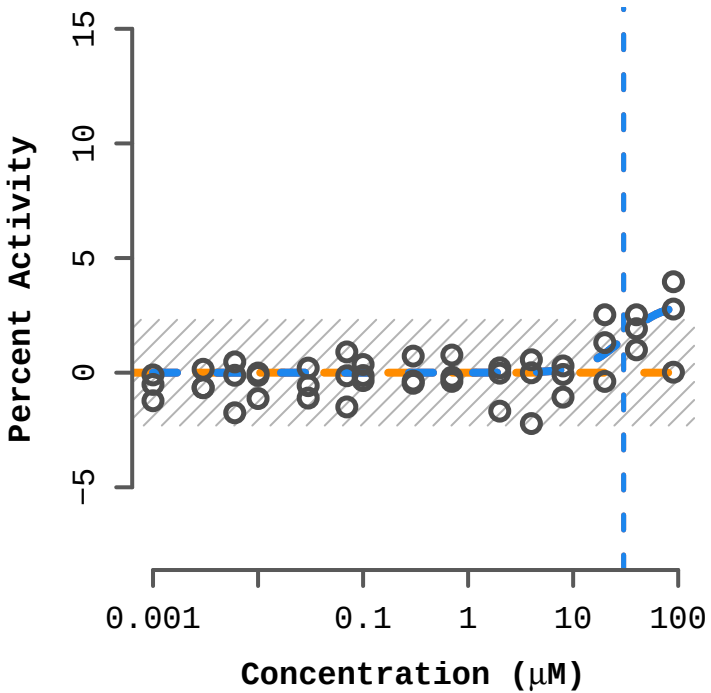
	tp	ga	gw
val:	10.6	1.55	1.33
sd:	2.74	0.195	0.316

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.6	1.55	1.33	3.79	4.02
sd:	2.74	0.195	0.316	984	2190

	CNST	HILL	GNLS
AIC:	205.69	132.92	136.92
PROB:	0	0.88	0.12
RMSE:	2.79	1.01	1.01

MAX_MEAN: 8.14 MAX_MED: 8.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(2-Methoxyphenyl)-3-oxobutanamide
CHID: 26558 CASRN: 92-15-9
SPID(S): Tox21_201280
M4ID: 12480972

HILL MODEL (in red):

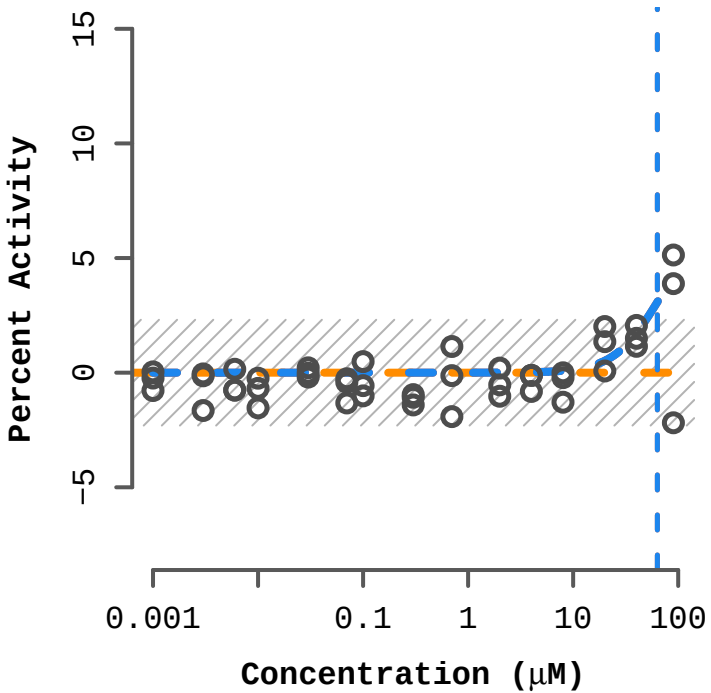
	tp	ga	gw
val:	3.02	1.48	2.35
sd:	1.14	0.234	1.35

GAIN-LOSS MODEL (in blue):

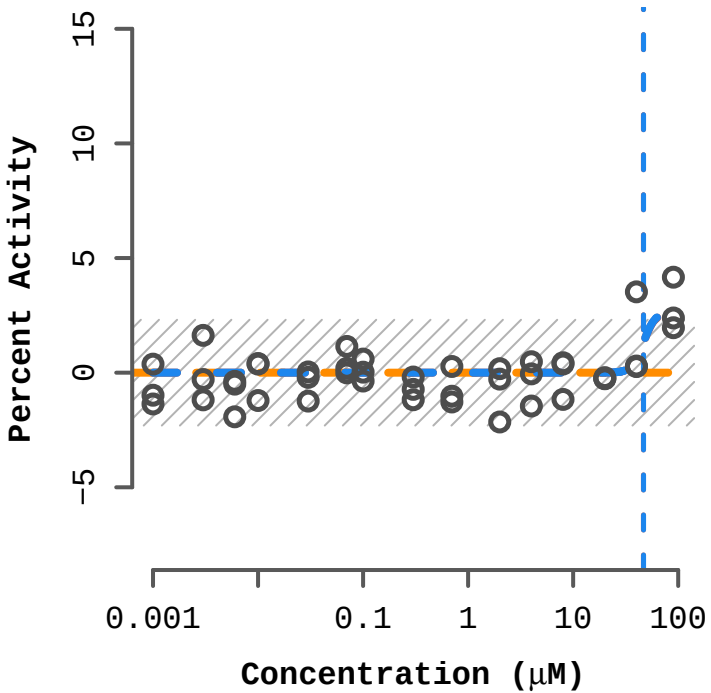
	tp	ga	gw	la	lw
val:	3.02	1.48	2.35	3.04	7.21
sd:	1.14	0.234	1.35	1840	12200

	CNST	HILL	GNLS
AIC:	141.48	126.59	130.59
PROB:	0	0.88	0.12
RMSE:	1.21	0.92	0.92

MAX_MEAN: 2.26 MAX_MED: 2.78 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-Hydroxy-2-naphthoic acid
CHID:    26560   CASRN: 92-70-6
SPID(S): Tox21_303283
M4ID:    12475850

HILL MODEL (in red):
      tp       ga       gw
val:  6.16     1.8      2.07
sd:   3.43     0.267    0.956

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.16     1.8      2.07     3.23     6.78
sd:   3.44     0.267    0.957    4200     22400

      CNST       HILL       GNLS
AIC:  149.48     133.47     137.47
PROB: 0          0.88       0.12
RMSE: 1.37       1.24       1.24

MAX_MEAN: 2.28      MAX_MED: 3.88      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Hydroxy-2-naphthoic acid
CHID: 26560 **CASRN:** 92-70-6
SPID(S): Tox21_201550
M4ID: 12480702

HILL MODEL (in red):

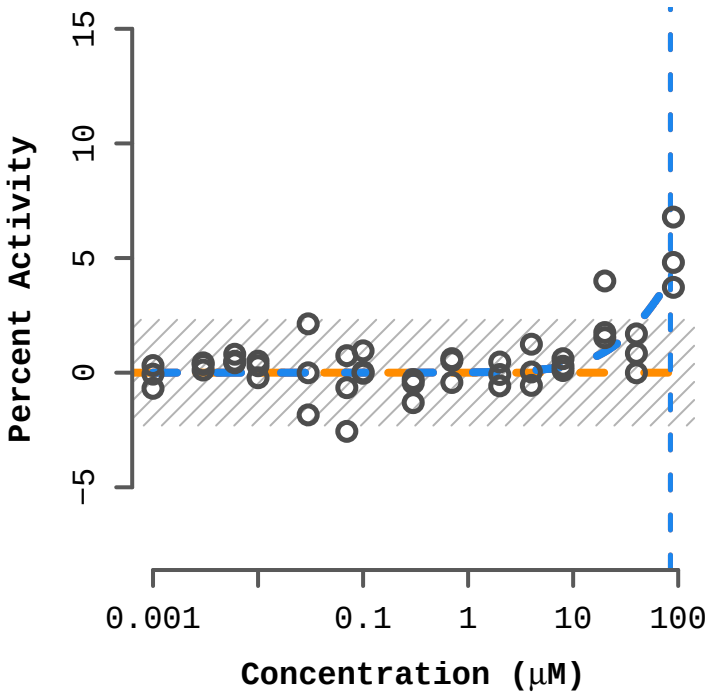
	tp	ga	gw
val:	2.61	1.67	8
sd:	0.596	0.189	20.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.65	1.67	8	2.53	3.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	143.15	131.3	135.3
PROB:	0	0.88	0.12
RMSE:	1.24	0.96	0.96

MAX_MEAN: 2.84 **MAX_MED:** 2.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(2-Methylphenyl)-3-oxobutanamide
CHID: 26562 **CASRN:** 93-68-5
SPID(S): Tox21_303146
M4ID: 12475987

HILL MODEL (in red):

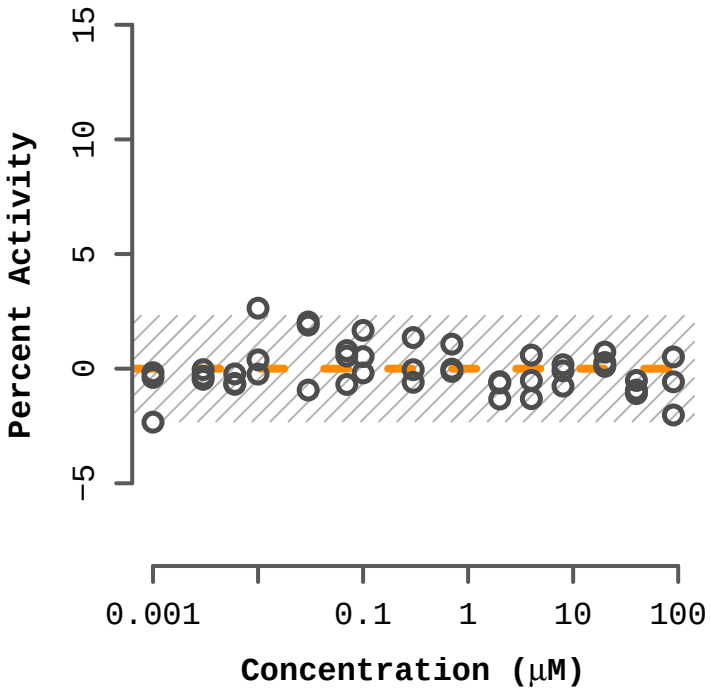
	tp	ga	gw
val:	8.14	1.93	1.44
sd:	3.77	0.265	0.568

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.14	1.93	1.44	3.33	9.5
sd:	3.77	0.265	0.568	103000	686000

	CNST	HILL	GNLS
AIC:	159.59	132.3	136.3
PROB:	0	0.88	0.12
RMSE:	1.72	1.03	1.03

MAX_MEAN: 5.11 **MAX_MED:** 4.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

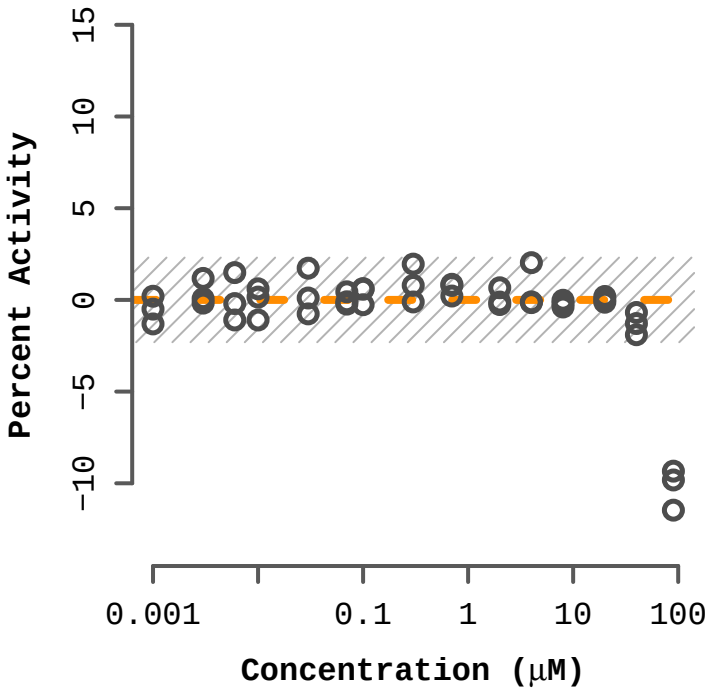
NAME: N-(2-Methylphenyl)-3-oxobutanamide
CHID: 26562 **CASRN:** 93-68-5
SPID(S): Tox21_201308
M4ID: 12480944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

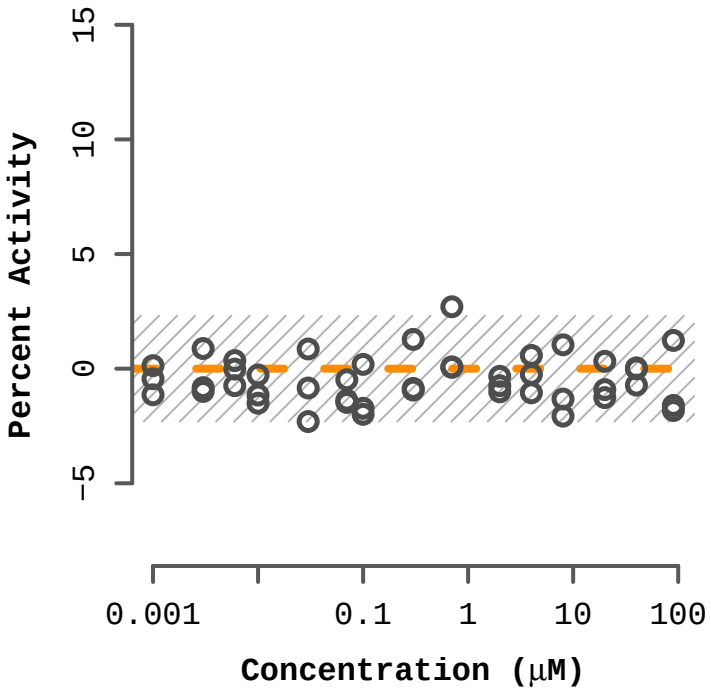
NAME: (9Z)-N,N-Bis(2-hydroxyethyl)octadec-9-enamide
CHID: 26563 **CASRN:** 93-83-4
SPID(S): Tox21_202528
M4ID: 12479724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.96	NA	NA
PROB:	1	NA	NA
RMSE:	2.77	NA	NA

MAX_MEAN: 0.879 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

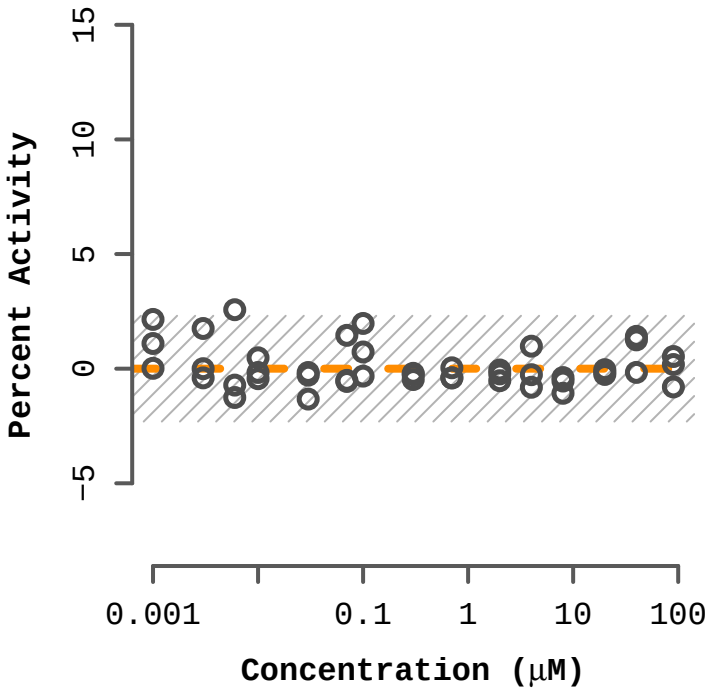
NAME: Triethylene glycol bis(2-ethylhexanoate)
CHID: 26564 **CASRN:** 94-28-0
SPID(S): Tox21_300309
M4ID: 12478821

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.947 **MAX_MED:** 0.0791 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

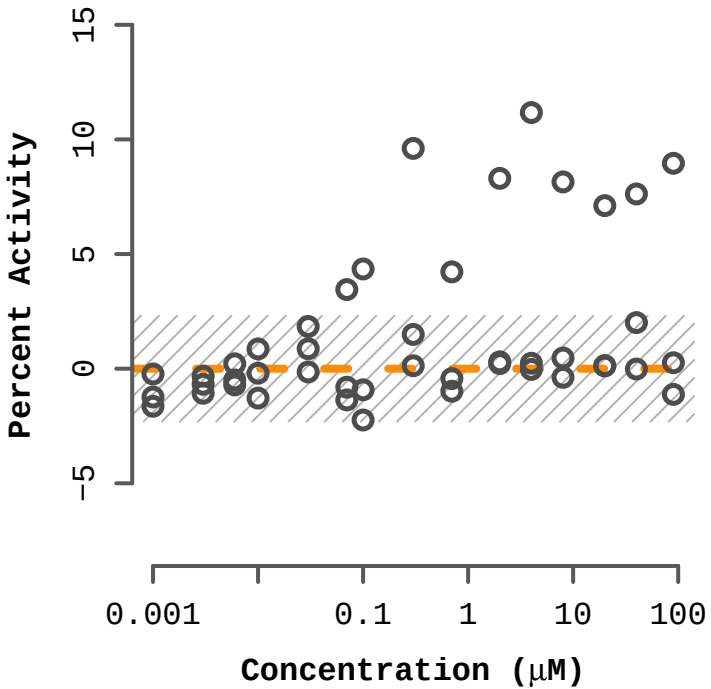
NAME: Triethylene glycol bis(2-ethylhexanoate)
CHID: 26564 **CASRN:** 94-28-0
SPID(S): Tox21_202276
M4ID: 12479976

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

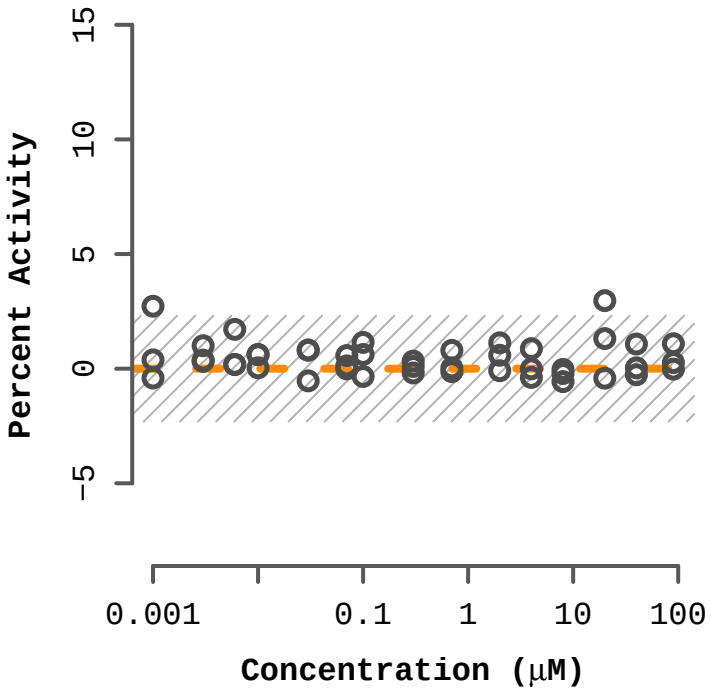
NAME: Dimethyl hexahydroterephthalate
CHID: 26566 **CASRN:** 94-60-0
SPID(S): Tox21_303293
M4ID: 12475840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.86	NA	NA
PROB:	1	NA	NA
RMSE:	3.72	NA	NA

MAX_MEAN: 3.79 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

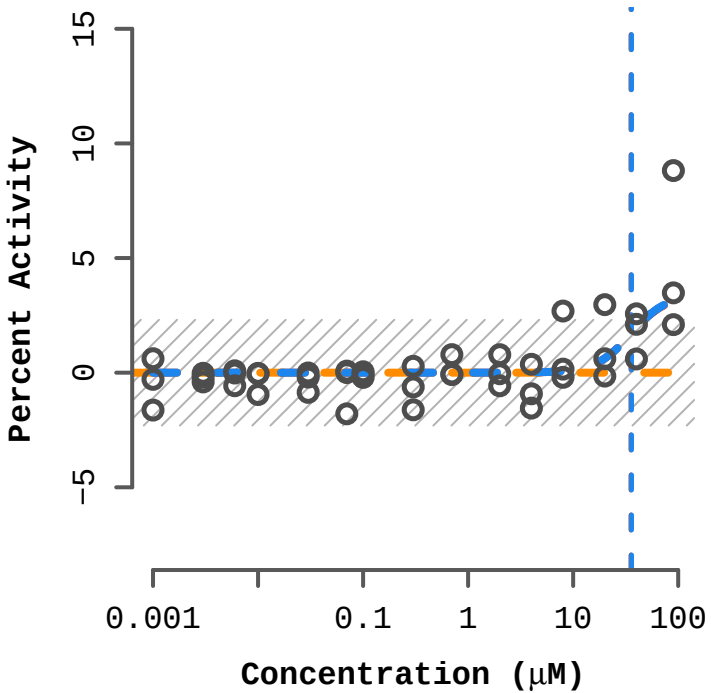
NAME: Dimethyl hexahydroterephthalate
CHID: 26566 CASRN: 94-60-0
SPID(S): Tox21_202298
M4ID: 12479954

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.29 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-tert-Butyl-2-benzothiazolesulfenamide
CHID: 26572 **CASRN:** 95-31-8
SPID(S): Tox21_200895
M4ID: 12481357

HILL MODEL (in red):

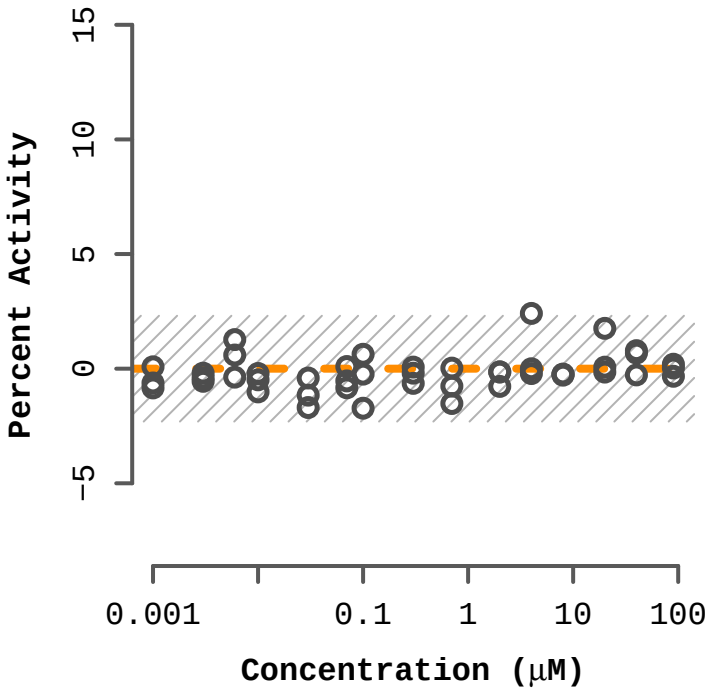
	tp	ga	gw
val:	3.39	1.55	2.58
sd:	1.14	0.168	1.89

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.43	1.55	2.57	2.07	16.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	152.66	131	135
PROB:	0	0.88	0.12
RMSE:	1.76	1.21	1.21

MAX_MEAN: 4.8 **MAX_MED:** 3.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

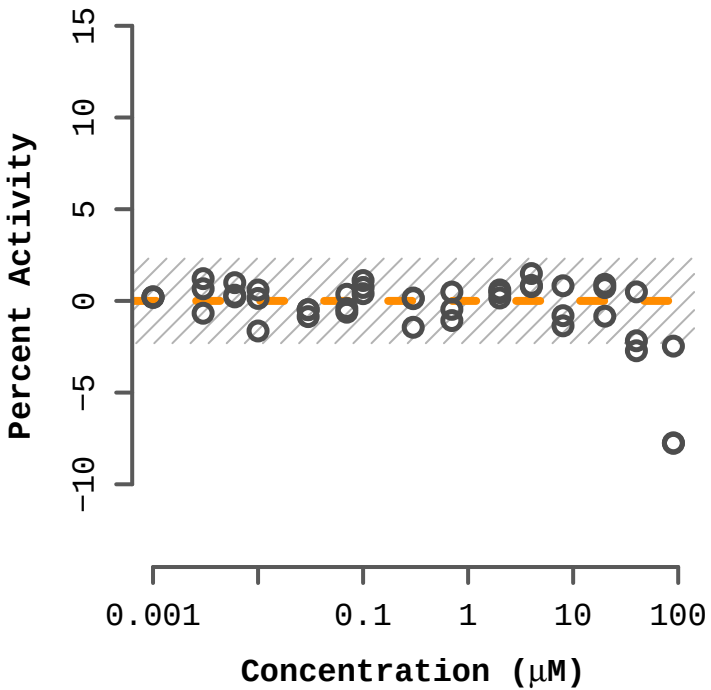
NAME: 2-(Morpholin-4-yldithio)-1,3-benzothiazole
CHID: 26573 **CASRN:** 95-32-9
SPID(S): Tox21_303278
M4ID: 12475855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.733 **MAX_MED:** 0.681 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

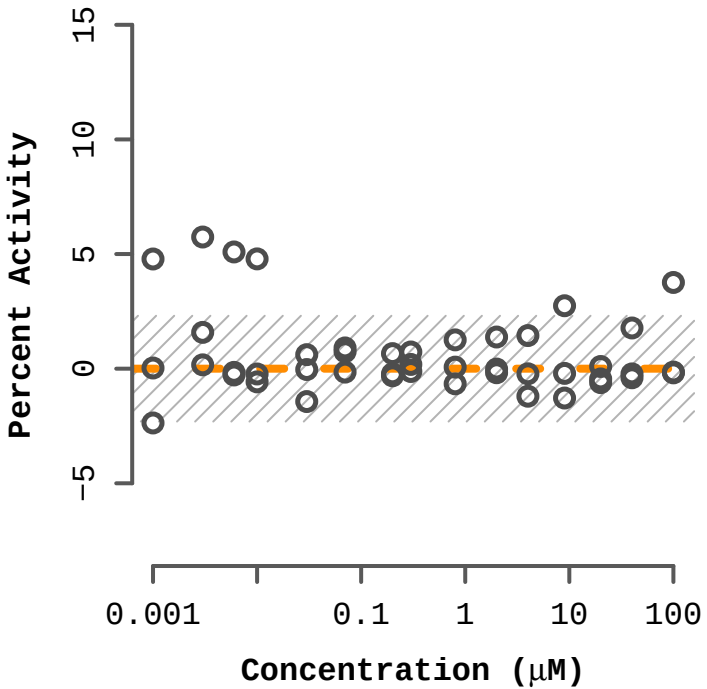
NAME: 2-(Morpholin-4-yldithio)-1,3-benzothiazole
CHID: 26573 **CASRN:** 95-32-9
SPID(S): Tox21_201340
M4ID: 12480912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.848 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

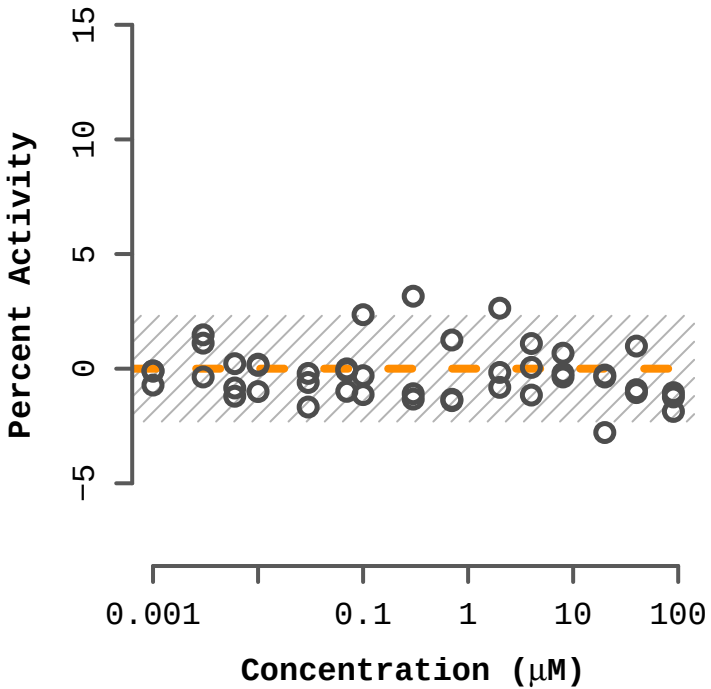
NAME: 1,3-Dioxolan-2-one
CHID: 26600 **CASRN:** 96-49-1
SPID(S): Tox21_201075
M4ID: 12481177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 2.5 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

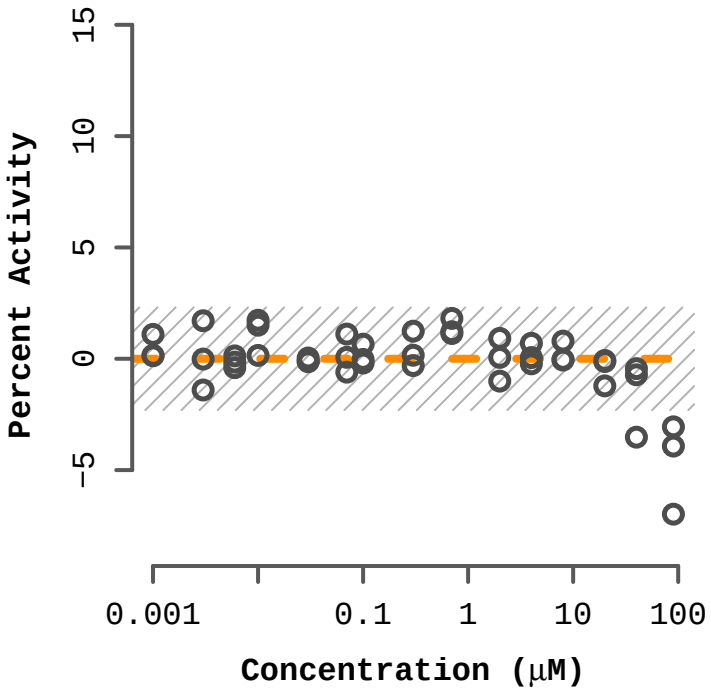
NAME: 2,4-Di-tert-butylphenol
CHID: 26602 **CASRN:** 96-76-4
SPID(S): Tox21_300114
M4ID: 12479016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.744 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

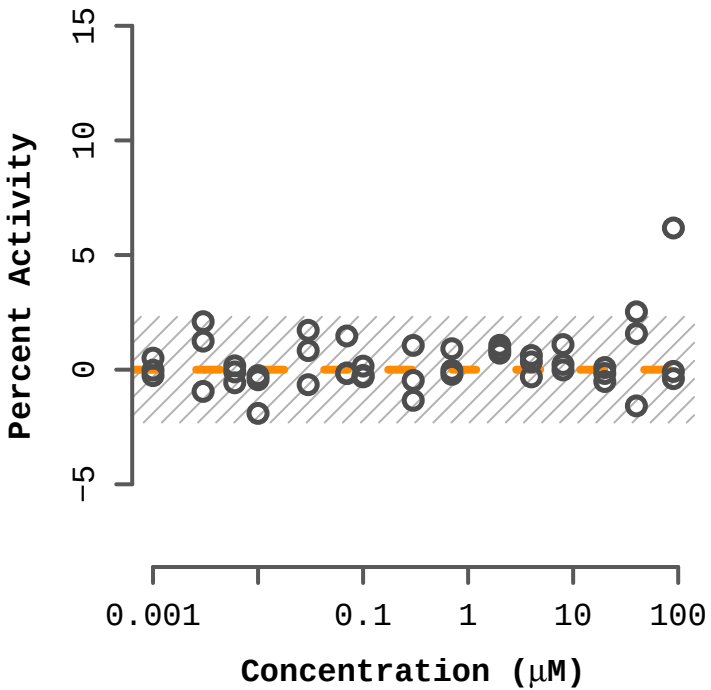
NAME: 2,4-Di-tert-butylphenol
CHID: 26602 **CASRN:** 96-76-4
SPID(S): Tox21_202320
M4ID: 12479932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

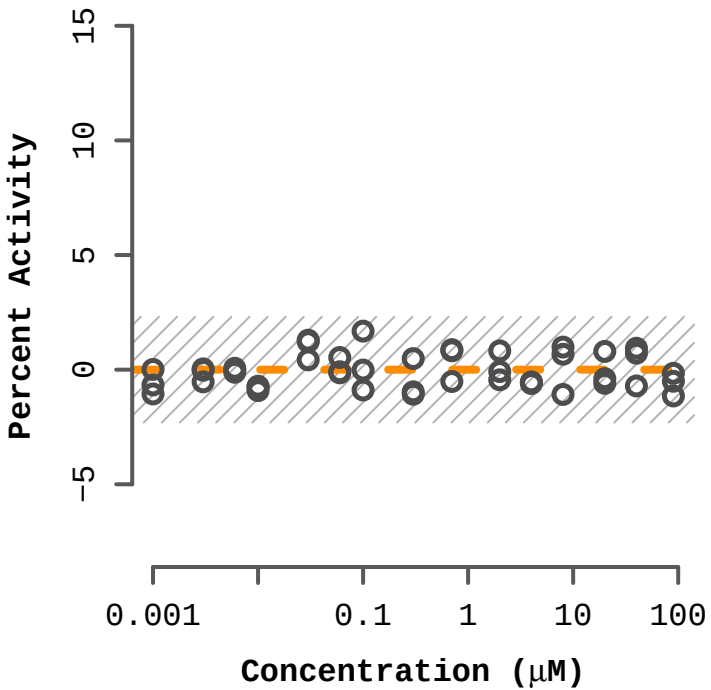
NAME: Methyl alpha-D-glucopyranoside
CHID: 26605 **CASRN:** 97-30-3
SPID(S): Tox21_200430
M4ID: 12481822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

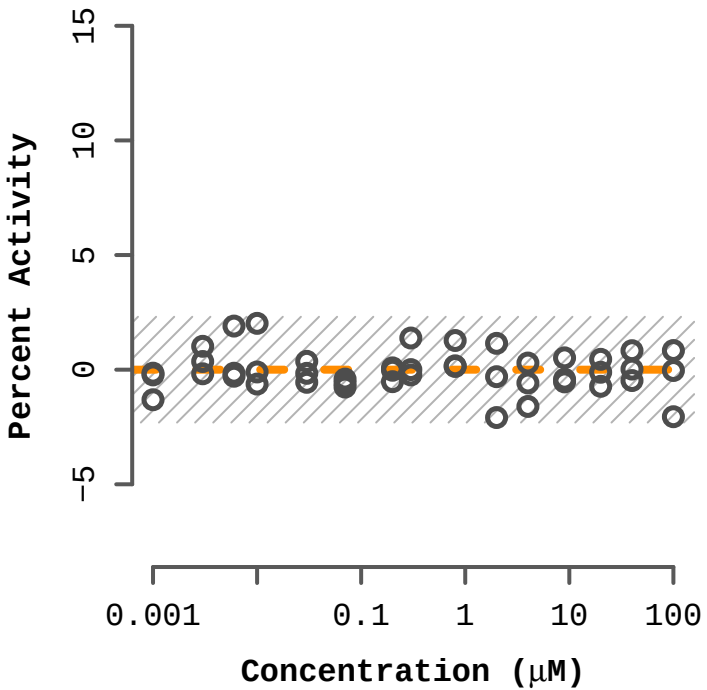
NAME: 1,3-Bis(2-methylphenyl)guanidine
CHID: 26606 **CASRN:** 97-39-2
SPID(S): Tox21_200712
M4ID: 12481540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.98 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

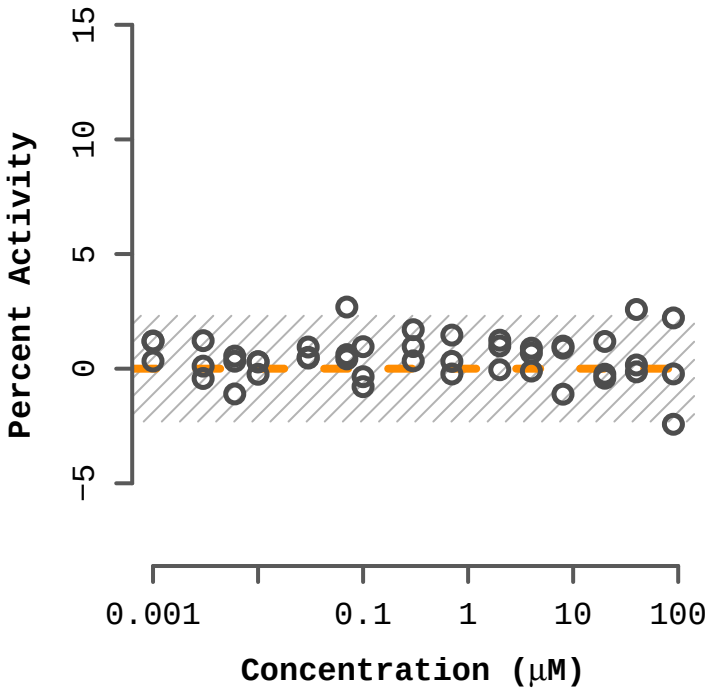
NAME: Methylenebutanedioic acid
CHID: 26608 CASRN: 97-65-4
SPID(S): Tox21_303071
M4ID: 12476062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.359 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

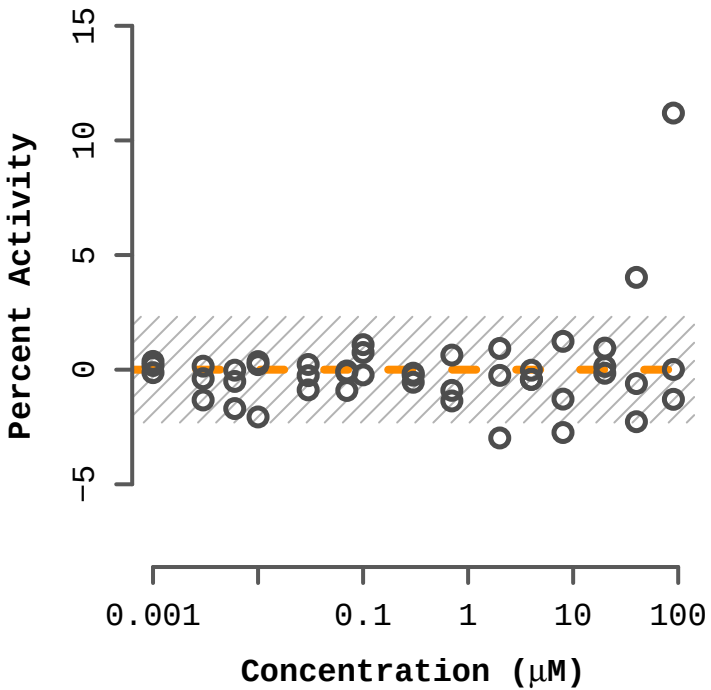
NAME: Methylenebutanedioic acid
CHID: 26608 CASRN: 97-65-4
SPID(S): Tox21_201299
M4ID: 12480953

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

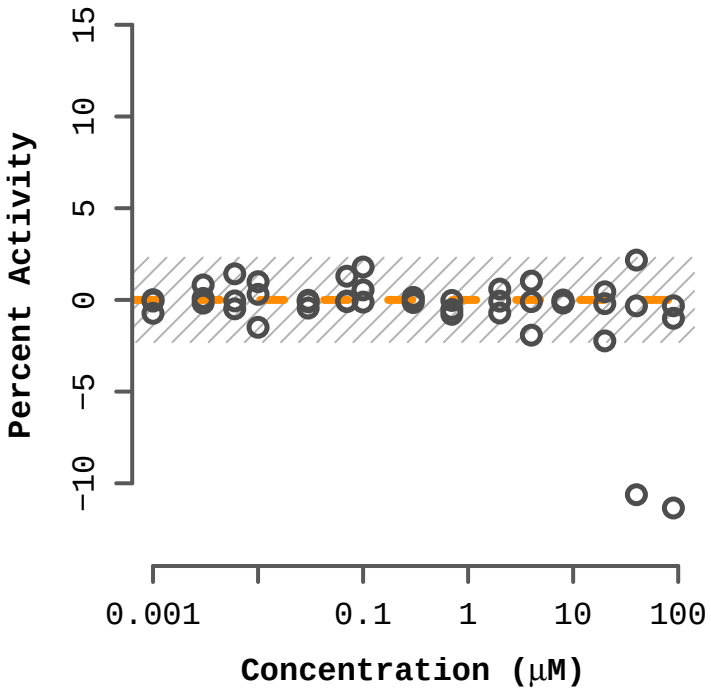
NAME: Isobutyric anhydride
CHID: 26609 CASRN: 97-72-3
SPID(S): Tox21_201002
M4ID: 12481250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.28	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 3.31 **MAX_MED:** 0.751 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

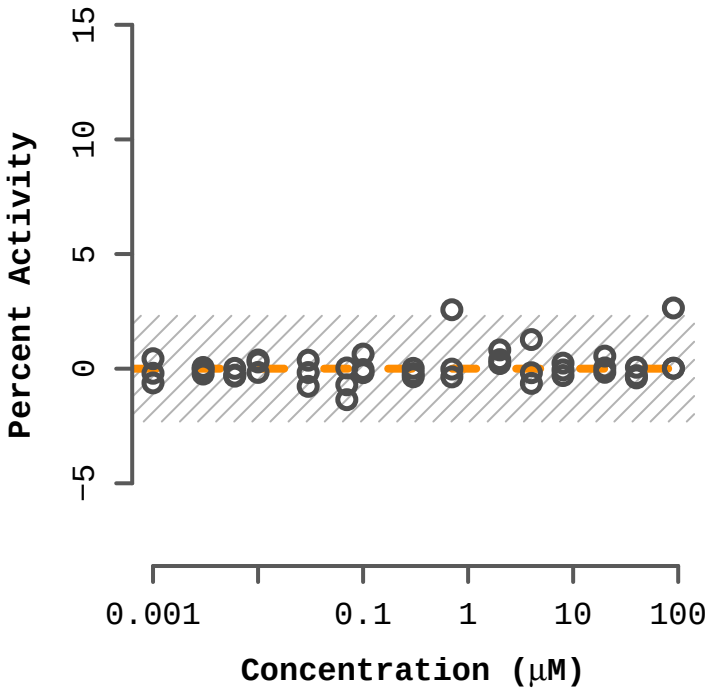
NAME: Isobutyl isobutyrate
CHID: 26612 **CASRN:** 97-85-8
SPID(S): Tox21_201573
M4ID: 12480679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.01	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 0.741 **MAX_MED:** 0.548 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

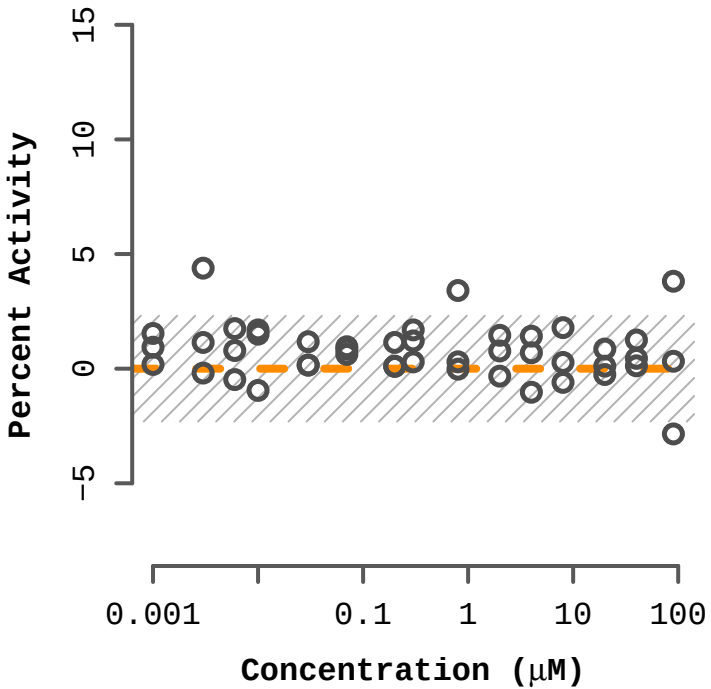
NAME: Ethylene glycol dimethacrylate
CHID: 26615 CASRN: 97-90-5
SPID(S): Tox21_303153
M4ID: 12475980

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	77.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.897 MAX_MED: 0.395 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

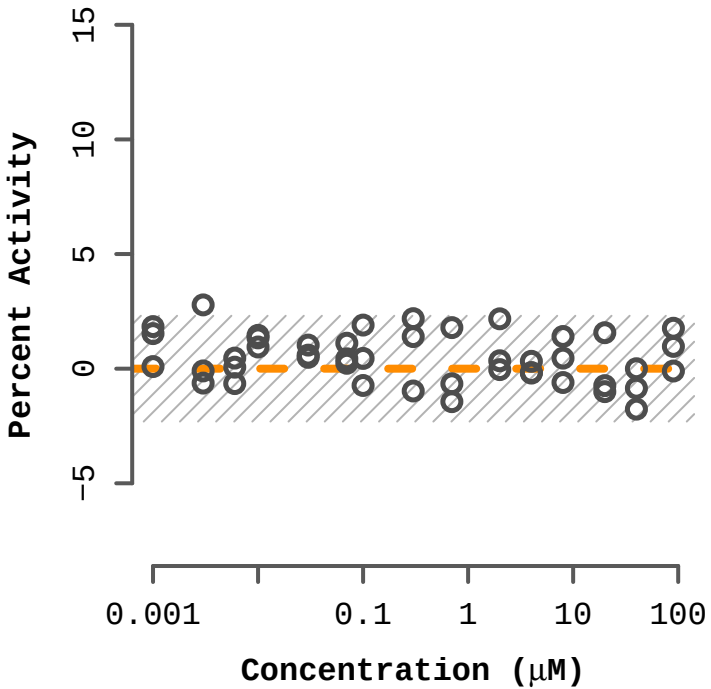
NAME: Ethylene glycol dimethacrylate
CHID: 26615 CASRN: 97-90-5
SPID(S): Tox21_201914
M4ID: 12480338

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

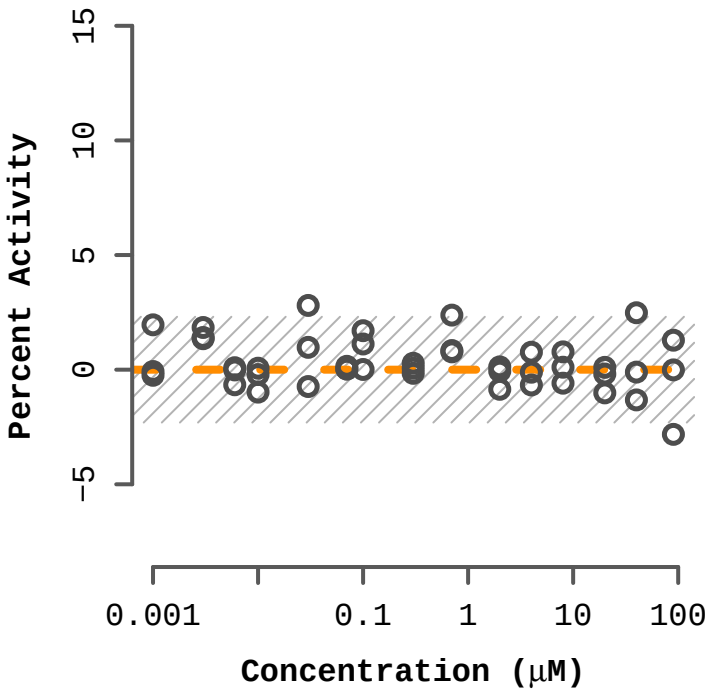
NAME: Benzenesulfonyl chloride
CHID: 26619 CASRN: 98-09-9
SPID(S): Tox21_200143
M4ID: 12482109

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.25 MAX_MED: 1.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

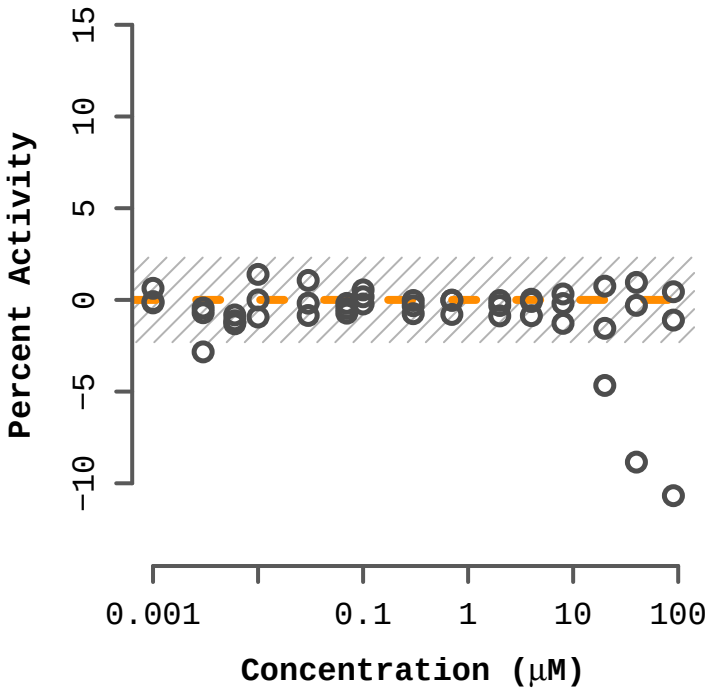
NAME: 4-tert-Butylcyclohexanol
CHID: 26623 **CASRN:** 98-52-2
SPID(S): Tox21_303090
M4ID: 12476043

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

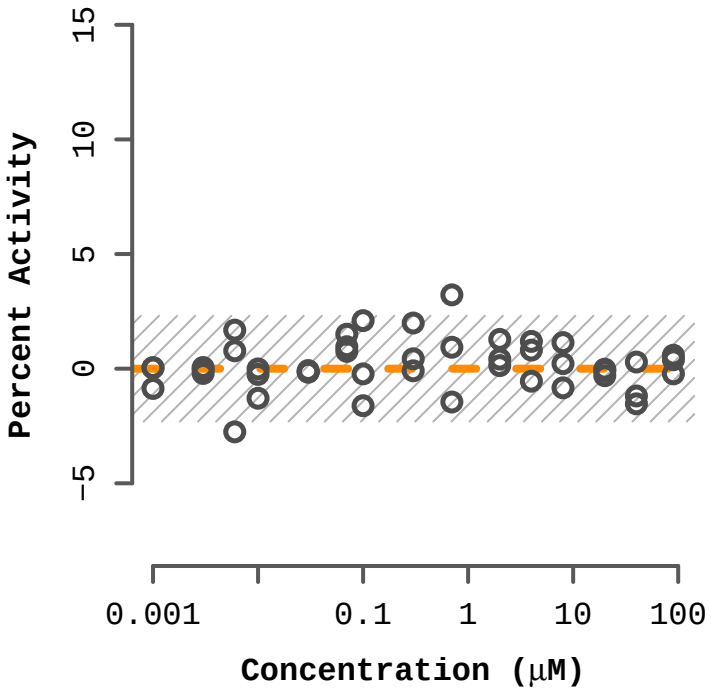
NAME: 4-tert-Butylcyclohexanol
CHID: 26623 **CASRN:** 98-52-2
SPID(S): Tox21_201515
M4ID: 12480737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.32	NA	NA

MAX_MEAN: 0.166 **MAX_MED:** 0.172 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

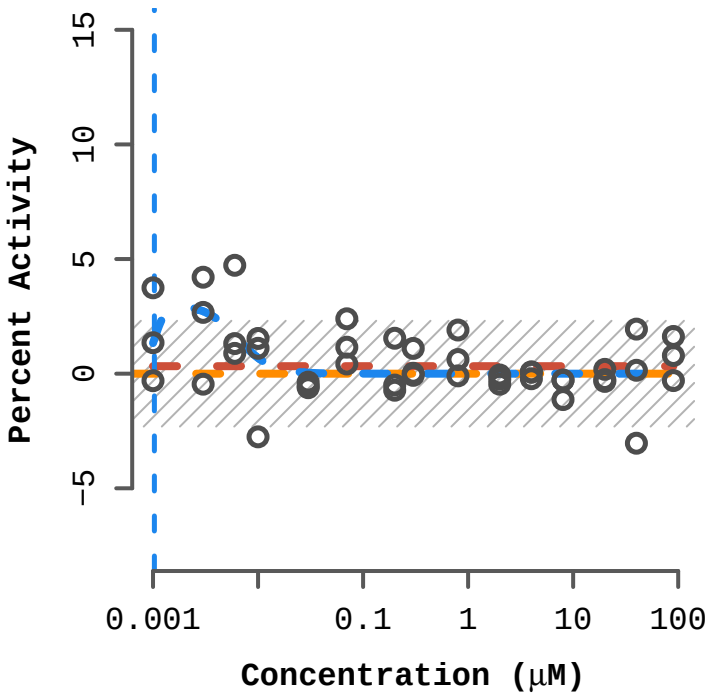
NAME: alpha-Terpineol
CHID: 26625 **CASRN:** 98-55-5
SPID(S): Tox21_200112
M4ID: 12482140

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzoyl chloride
CHID: 26631 CASRN: 98-88-4
SPID(S): Tox21_200431
M4ID: 12481821

HILL MODEL (in red):

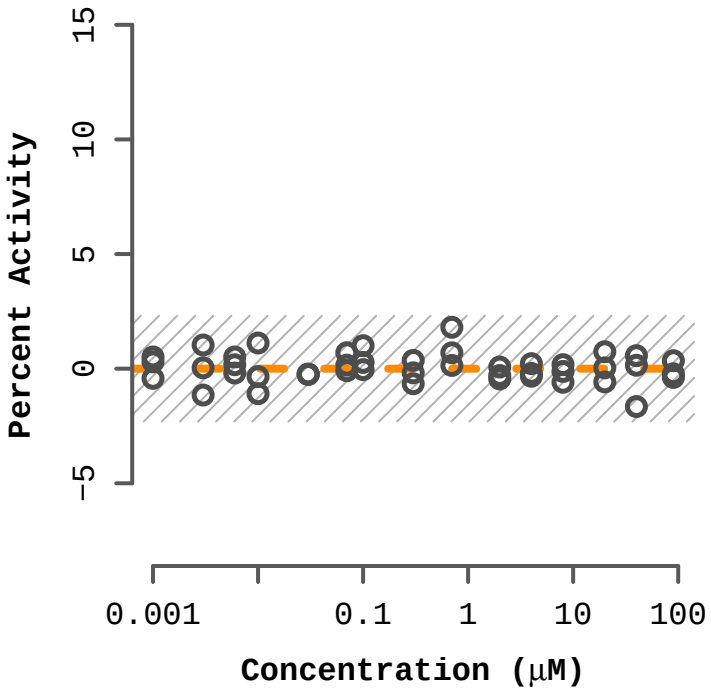
	tp	ga	gw
val:	0.326	−4.99	3.27
sd:	0.19	999	1630

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.04	−2.99	7.87	−2.19	2.8
sd:	1.81	0.141	78.2	0.279	2.73

	CNST	HILL	GNLS
AIC:	164.73	167.69	160.95
PROB:	0.13	0.03	0.84
RMSE:	1.58	1.51	1.32

MAX_MEAN: 2.31 MAX_MED: 2.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

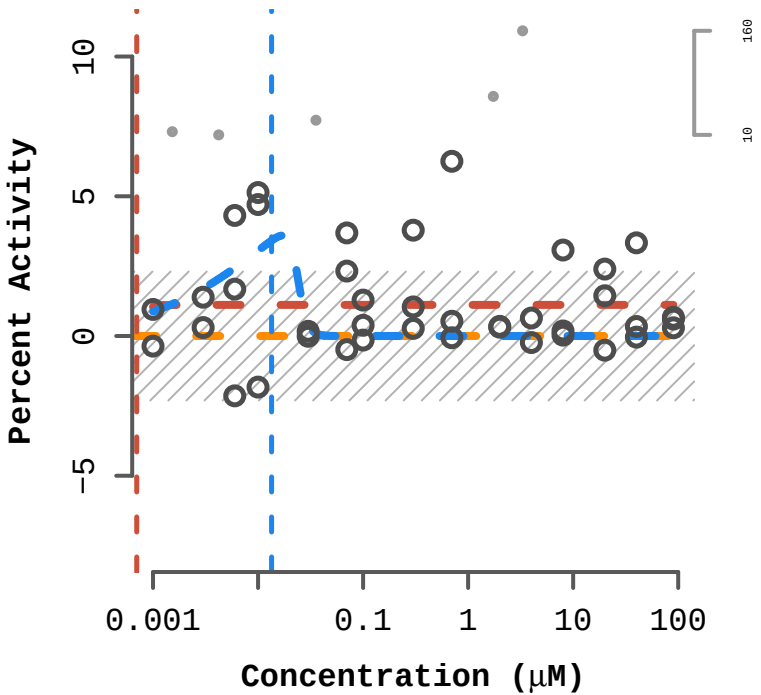
NAME: N,N−Dimethylcyclohexylamine
CHID: 26633 **CASRN:** 98−94−2
SPID(S): Tox21_201360
M4ID: 12480892

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	83.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.62	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 0.695 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3−Diisopropylbenzene
CHID: 26640 CASRN: 99−62−7
SPID(S): Tox21_300362
M4ID: 12478770 BRK

HILL MODEL (in red):

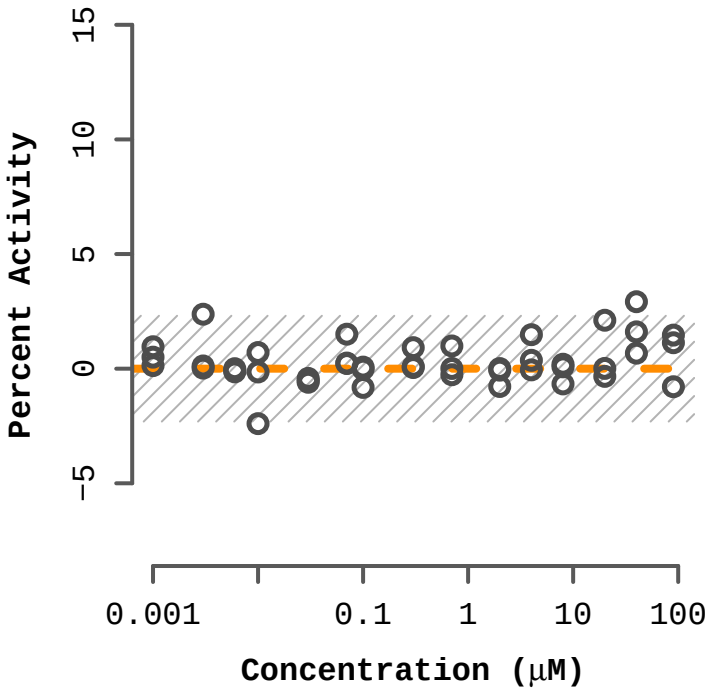
	tp	ga	gw
val:	1.11	−3.16	7.65
sd:	0.399	7.23	345

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.85	−1.87	0.739	−1.62	9.73
sd:	29.9	4.35	1.2	2.03	202

	CNST	HILL	GNLS
AIC:	299.11	296.85	304.01
PROB:	0.24	0.74	0.02
RMSE:	25.86	25.57	25.81

MAX_MEAN: 52.3 MAX_MED: 4.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

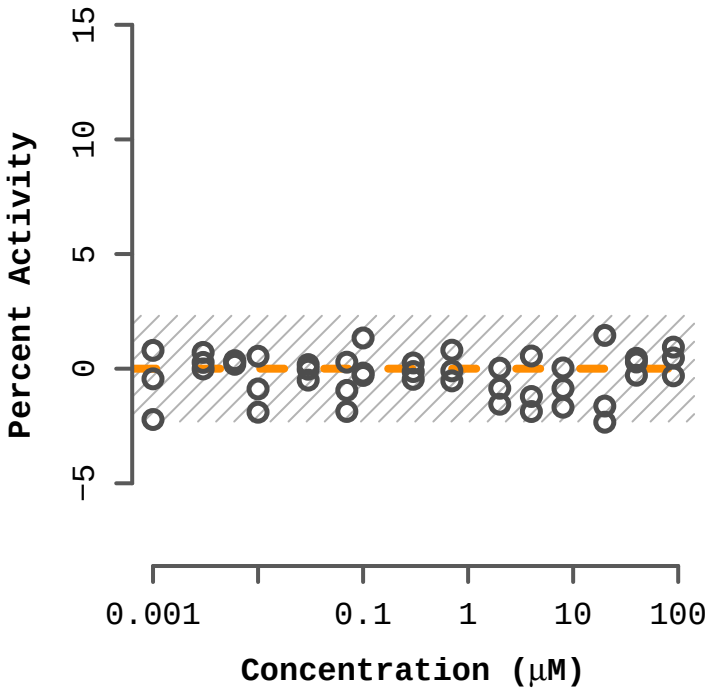
NAME: 1,3-Diisopropylbenzene
CHID: 26640 **CASRN:** 99-62-7
SPID(S): Tox21_201318
M4ID: 12480934

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

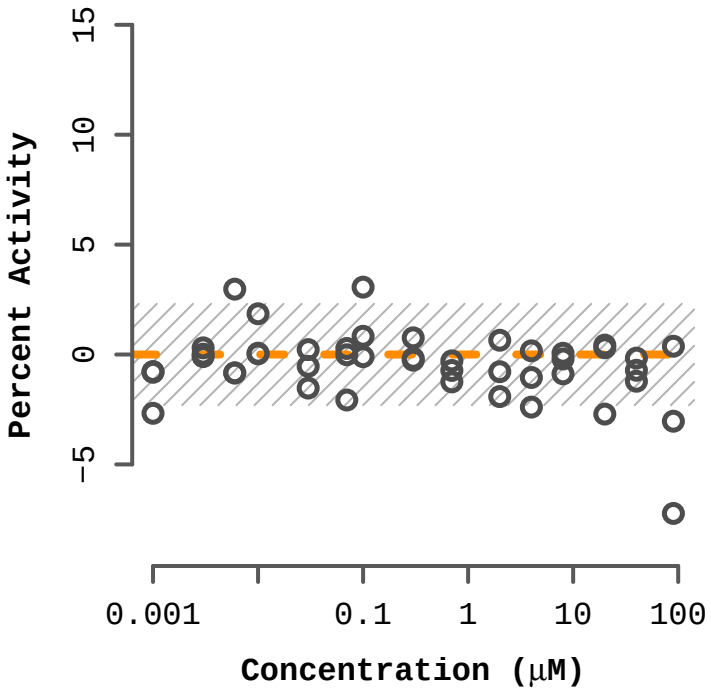
NAME: 1,3−Benzenedicarbonyl dichloride
CHID: 26641 **CASRN:** 99−63−8
SPID(S): Tox21_303056
M4ID: 12476077

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.367 **MAX_MED:** 0.469 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

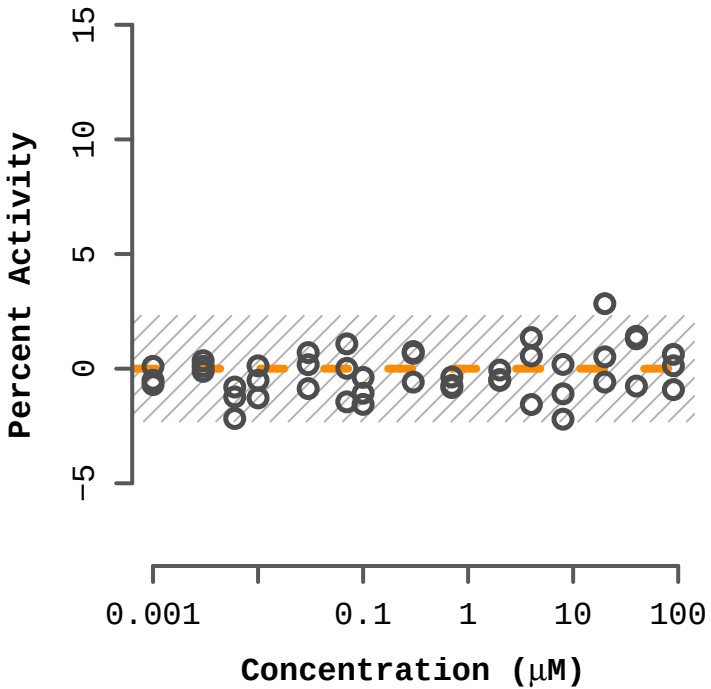
NAME: 1,3−Benzenedicarbonyl dichloride
CHID: 26641 CASRN: 99−63−8
SPID(S): Tox21_201596
M4ID: 12480656

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.831 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

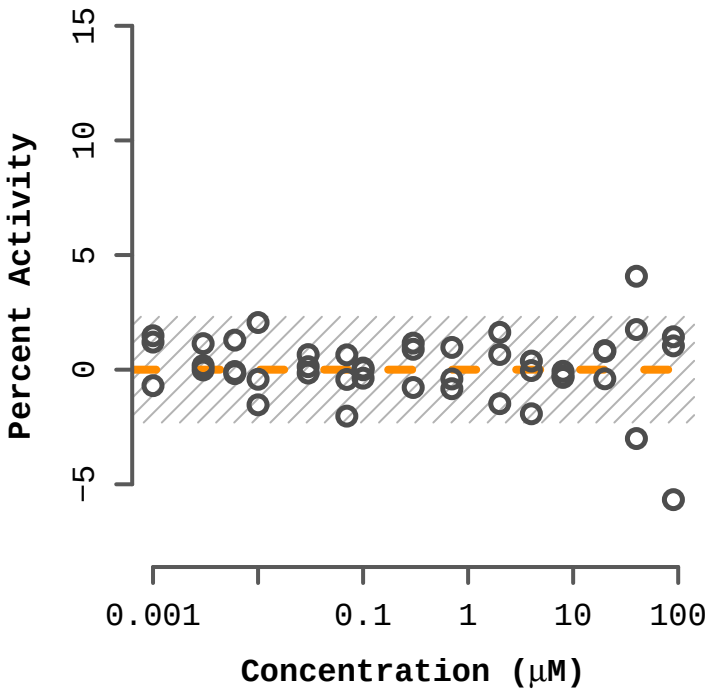
NAME: p-Cymene
CHID: 26645 **CASRN:** 99-87-6
SPID(S): Tox21_300338
M4ID: 12478794

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.924 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

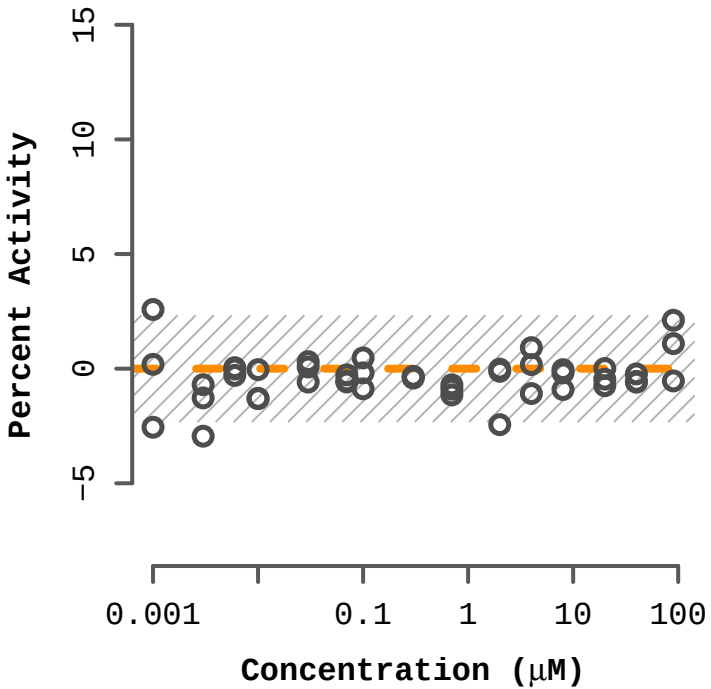
NAME: p-Cymene
CHID: 26645 **CASRN:** 99-87-6
SPID(S): Tox21_201932
M4ID: 12480320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

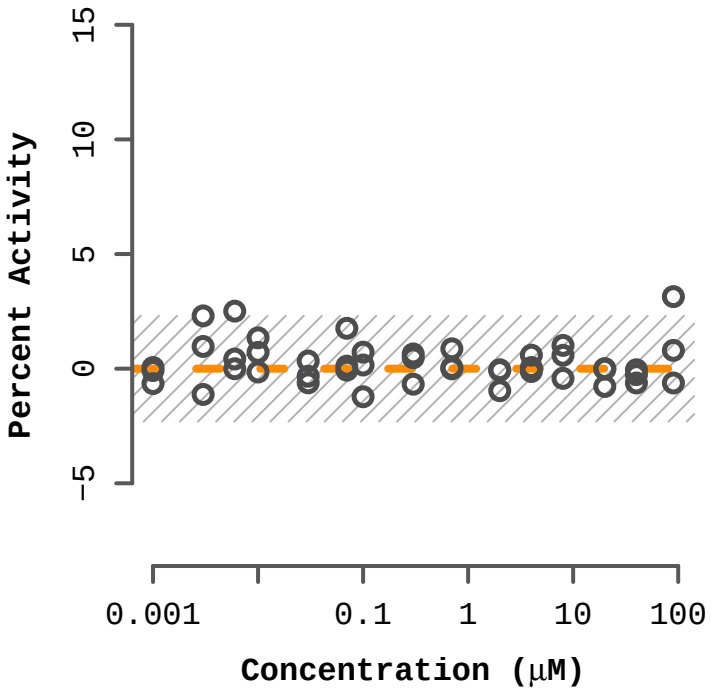
NAME: 4-Hydroxybenzoic acid
CHID: 26647 CASRN: 99-96-7
SPID(S): Tox21_303301
M4ID: 12475832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

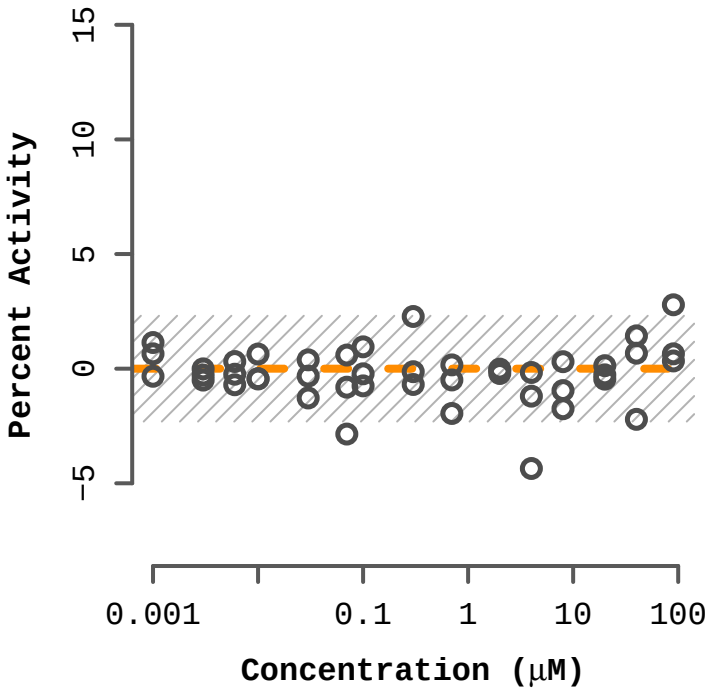
NAME: 4-Hydroxybenzoic acid
CHID: 26647 CASRN: 99-96-7
SPID(S): Tox21_202342
M4ID: 12479910

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.11 MAX_MED: 0.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

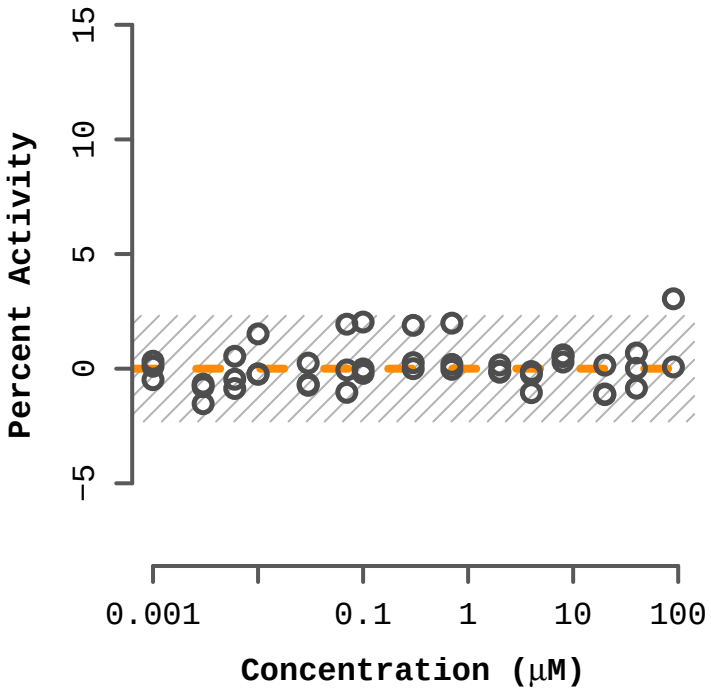
NAME: 1,4-Diisopropylbenzene
CHID: 26652 **CASRN:** 100-18-5
SPID(S): Tox21_303217
M4ID: 12475916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.677 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

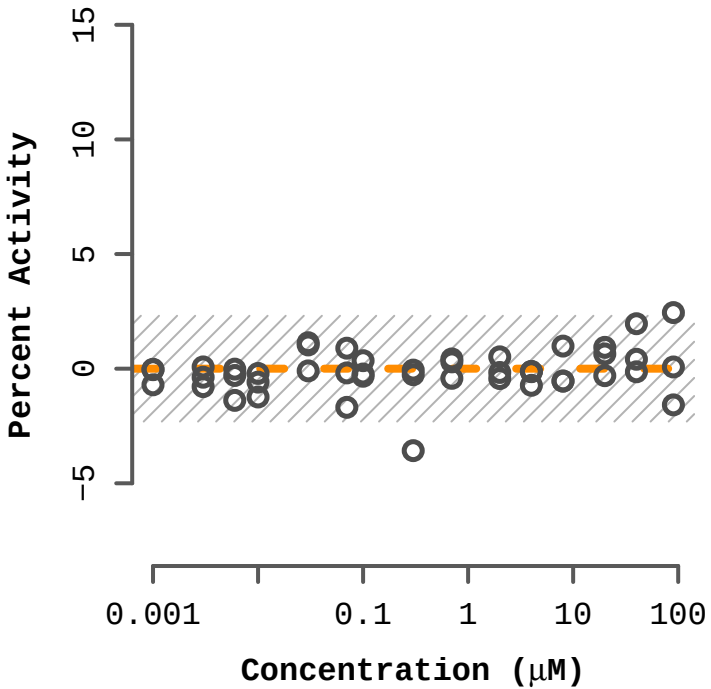
NAME: 1,4-Diisopropylbenzene
CHID: 26652 CASRN: 100-18-5
SPID(S): Tox21_201380
M4ID: 12480872

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.56 MAX_MED: 1.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

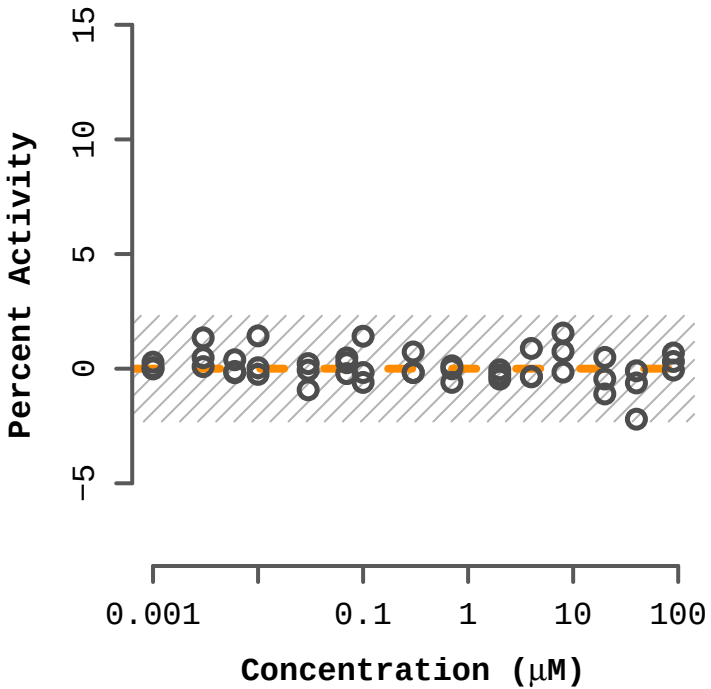
NAME: 1,4−Benzenedicarbonyl dichloride
CHID: 26653 **CASRN:** 100−20−9
SPID(S): Tox21_303166
M4ID: 12475967

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.747 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

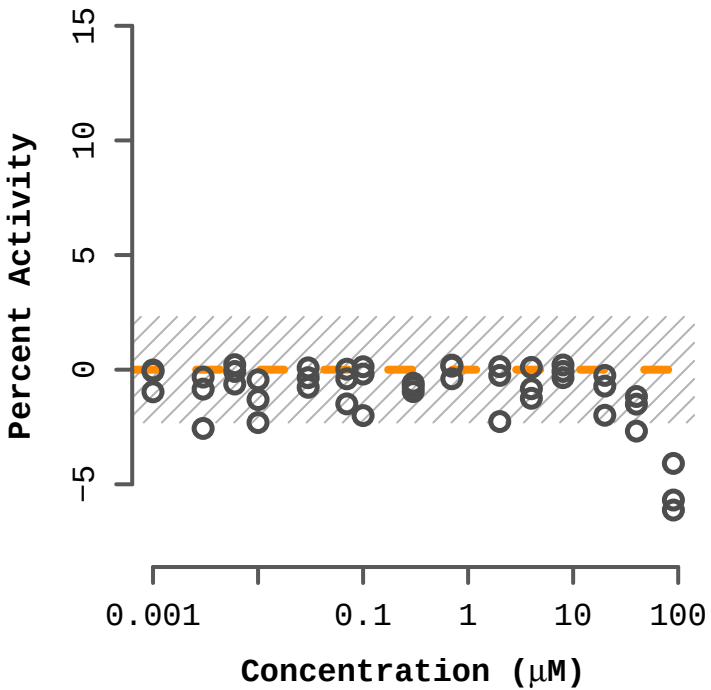
NAME: 1,4−Benzenedicarbonyl dichloride
CHID: 26653 CASRN: 100−20−9
SPID(S): Tox21_201899
M4ID: 12480353

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.72 MAX_MED: 0.752 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

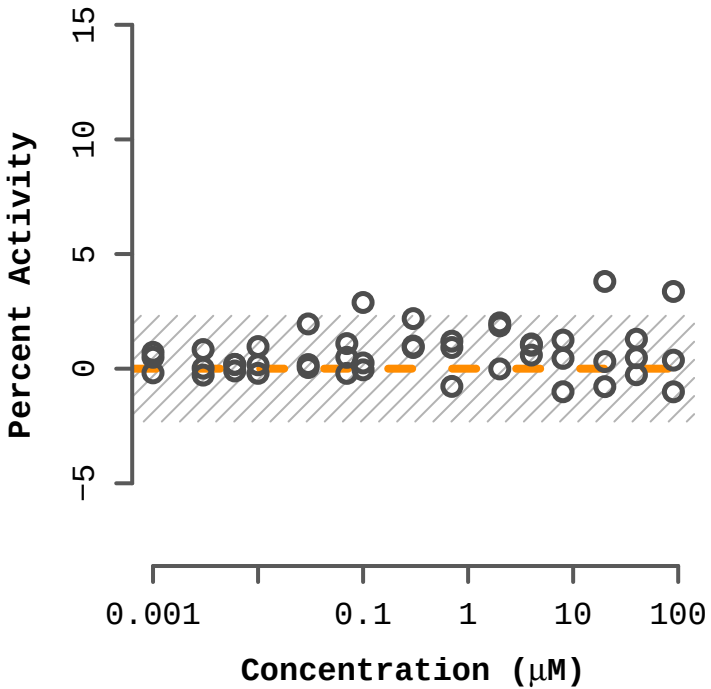
NAME: 1-Ethoxy-4-nitrobenzene
CHID: 26655 **CASRN:** 100-29-8
SPID(S): Tox21_200729
M4ID: 12481523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: −0.0142 **MAX_MED:** 0.152 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

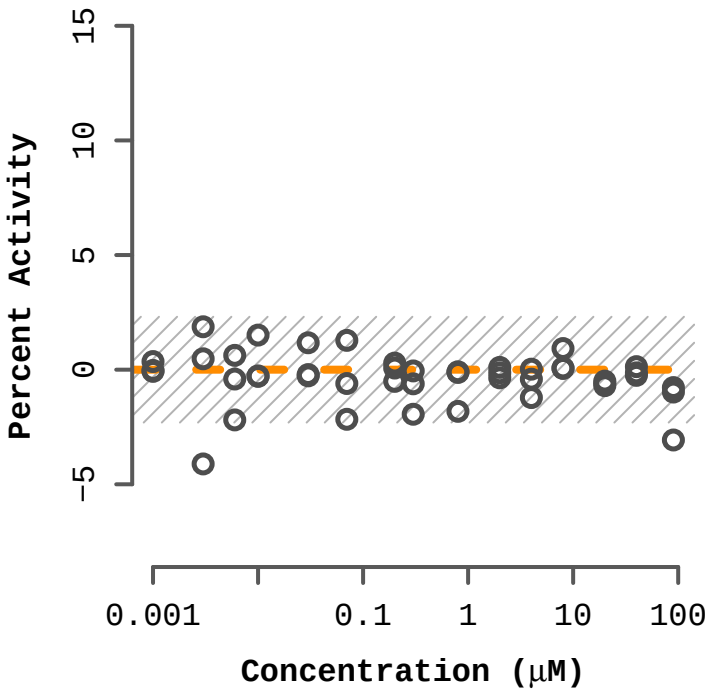
NAME: 3-Cyclohexene-1-carboxaldehyde
CHID: 26661 **CASRN:** 100-50-5
SPID(S): Tox21_201059
M4ID: 12481193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

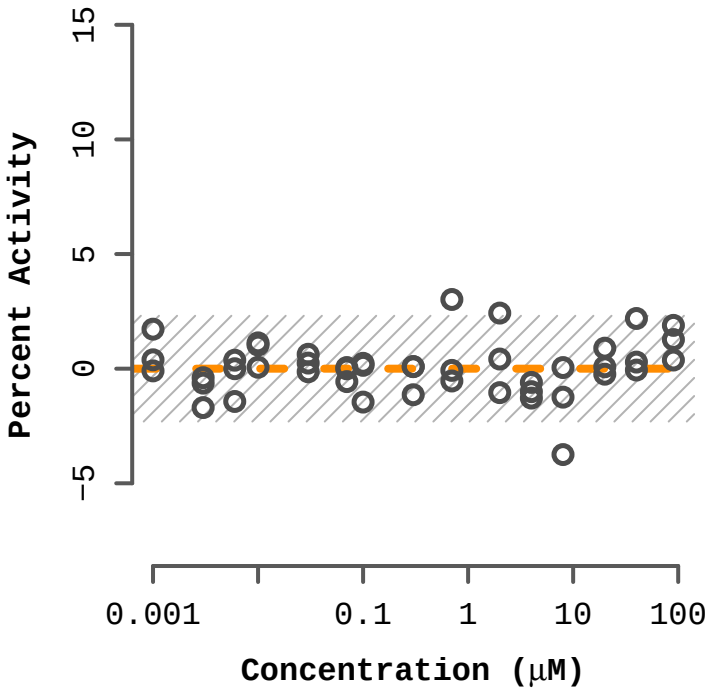
NAME: Benzenemethanethiol
CHID: 26664 **CASRN:** 100-53-8
SPID(S): Tox21_200129
M4ID: 12482123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.352 **MAX_MED:** 0.476 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

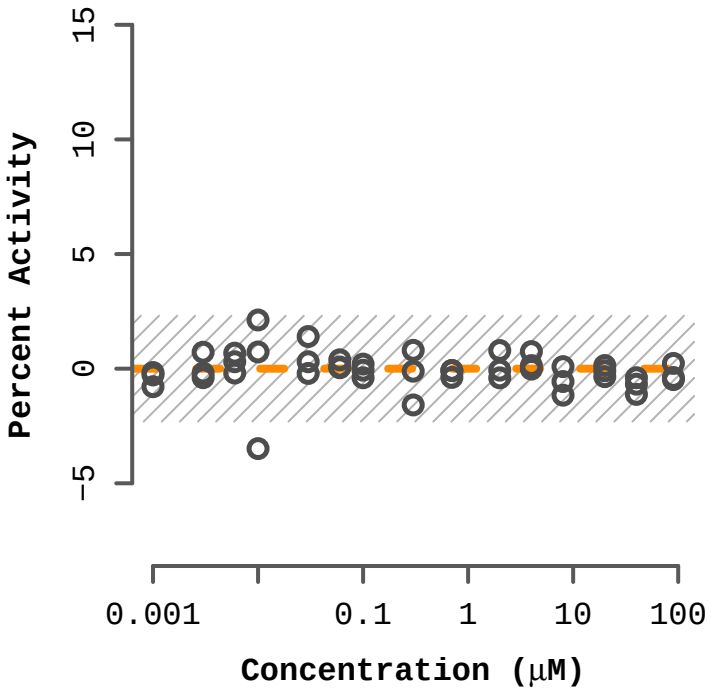
NAME: 3-Pyridinecarbonitrile
CHID: 26665 CASRN: 100-54-9
SPID(S): Tox21_300354
M4ID: 12478778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.18 MAX_MED: 1.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

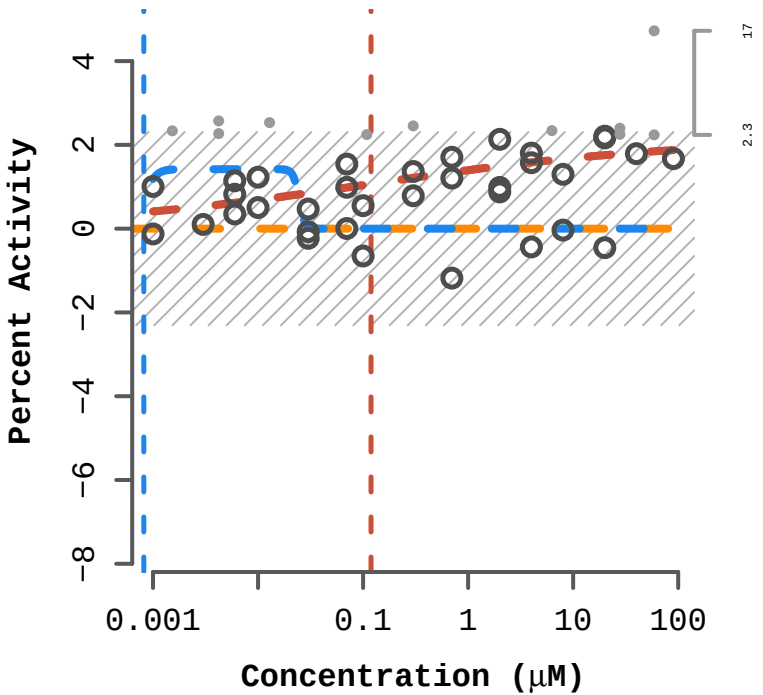
NAME: 3-Pyridinecarbonitrile
CHID: 26665 **CASRN:** 100-54-9
SPID(S): Tox21_201669
M4ID: 12480583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.501 **MAX_MED:** 0.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Vinylpyridine
CHID: 26667 CASRN: 100-69-6
SPID(S): Tox21_200035
M4ID: 12482217 BRK

HILL MODEL (in red):

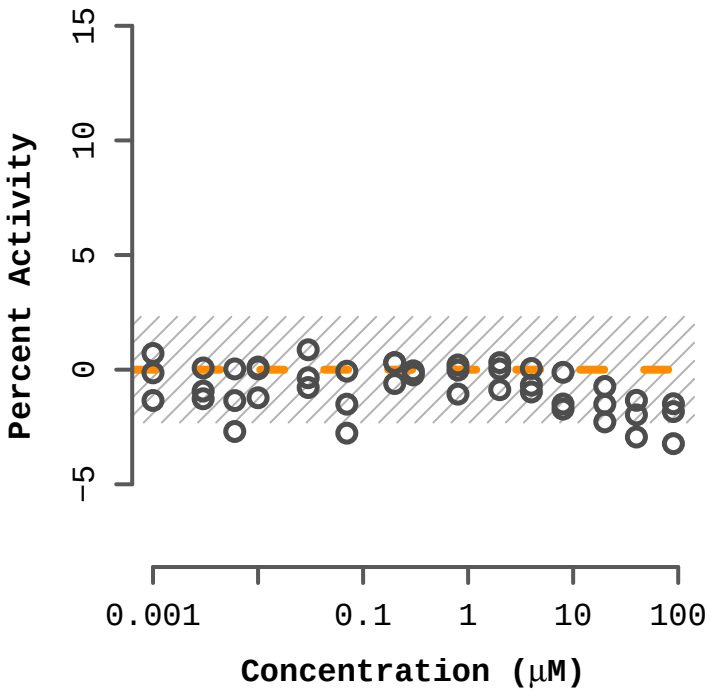
	tp	ga	gw
val:	2.13	−0.925	0.3
sd:	4.77	8.11	0.994

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.42	−3.09	7.99	−1.61	15.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	202.09	175.28	204.45
PROB:	0	1	0
RMSE:	3.15	2.65	3.05

MAX_MEAN: 7.12 MAX_MED: 2.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

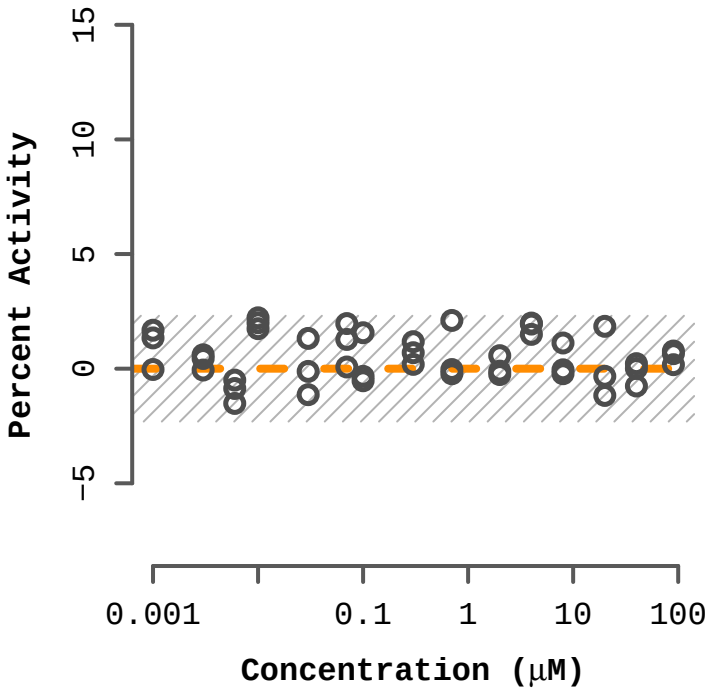
NAME: 1,1'−Oxybis(4−nitrobenzene)
CHID: 26676 **CASRN:** 101−63−3
SPID(S): Tox21_200432
M4ID: 12481820

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.00372 **MAX_MED:** 0.303 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

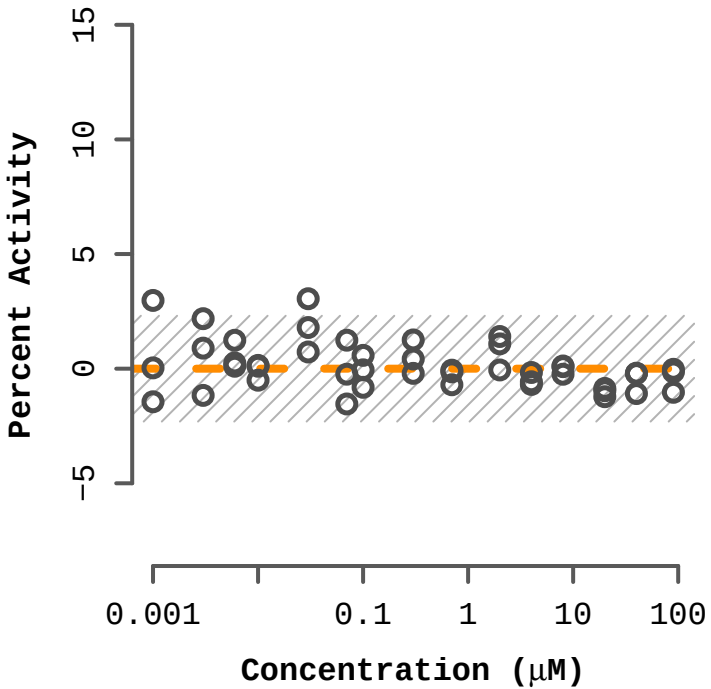
NAME: 2-Benzylideneoctanal
CHID: 26684 CASRN: 101-86-0
SPID(S): Tox21_300142
M4ID: 12478988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.99 MAX_MED: 2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

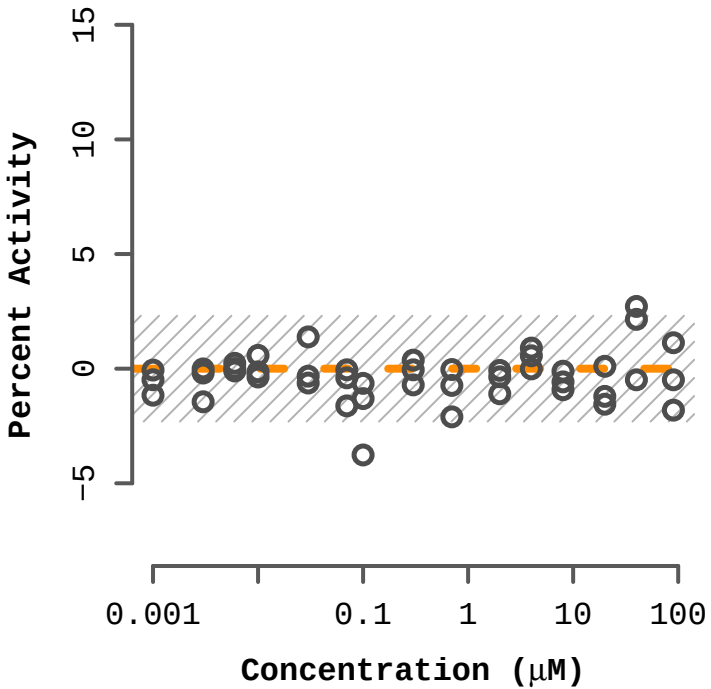
NAME: 2-Benzylideneoctanal
CHID: 26684 CASRN: 101-86-0
SPID(S): Tox21_202301
M4ID: 12479951

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.86 MAX_MED: 1.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

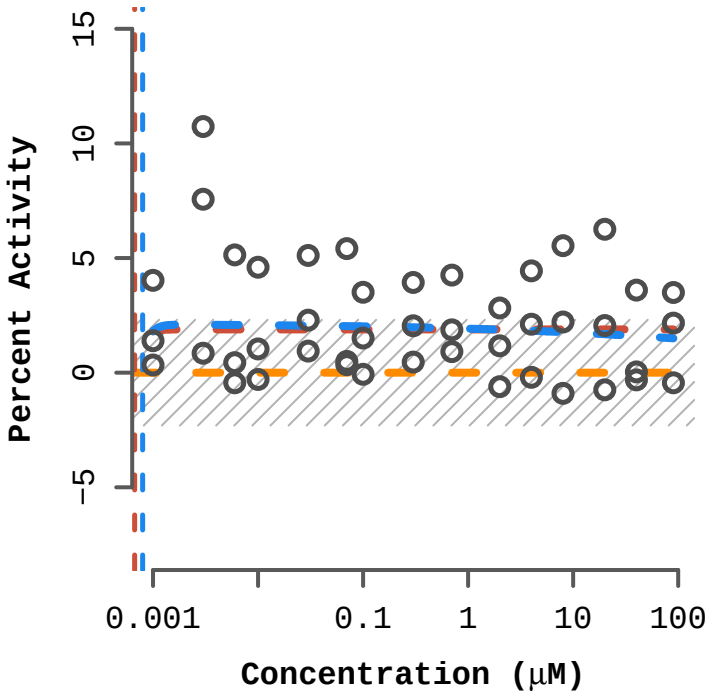
NAME: N,N,N',N'−Tetrakis(2−Hydroxypropyl)ethylenedia
CHID: 26689 **CASRN:** 102−60−3
SPID(S): Tox21_300552
M4ID: 12478581

HILL MODEL: Not applicable.

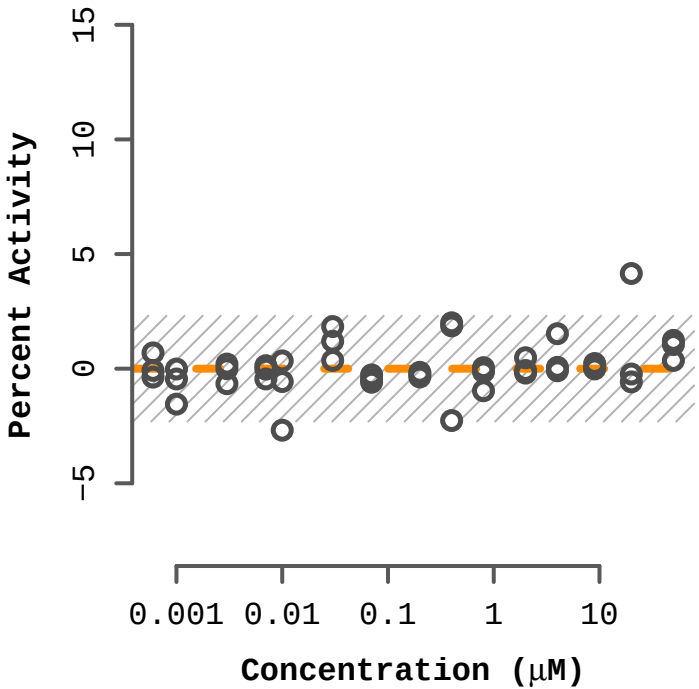
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 2.15 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N,N,N',N'−Tetrakis(2−Hydroxypropyl)ethylenedia
CHID:    26689   CASRN: 102−60−3
SPID(S): Tox21_201973
M4ID:    12480279

HILL MODEL (in red):
      tp       ga       gw
val:  1.89     −3.17    7.61
sd:   0.375    2.87     121

GAIN−LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.13     −3.1     7.89     3.2      0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  236.34      216.99      220.77
PROB: 0           0.87        0.13
RMSE: 3.35        2.51        2.48

MAX_MEAN: 6.39      MAX_MED: 7.57      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

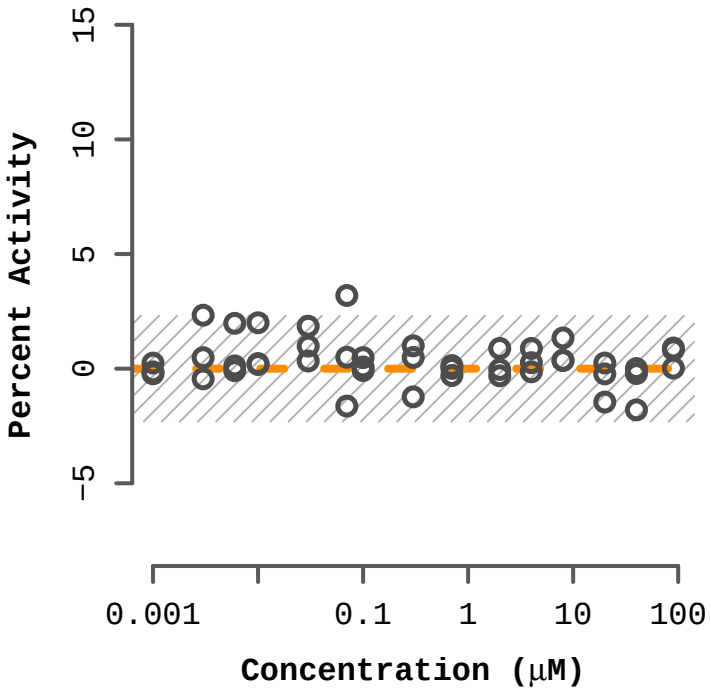
NAME: N,N,N',N'−Tetrakis(2−Hydroxypropyl)ethylenedia
CHID: 26689 CASRN: 102−60−3
SPID(S): Tox21_112102_1
M4ID: 12483319

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.13 MAX_MED: 1.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

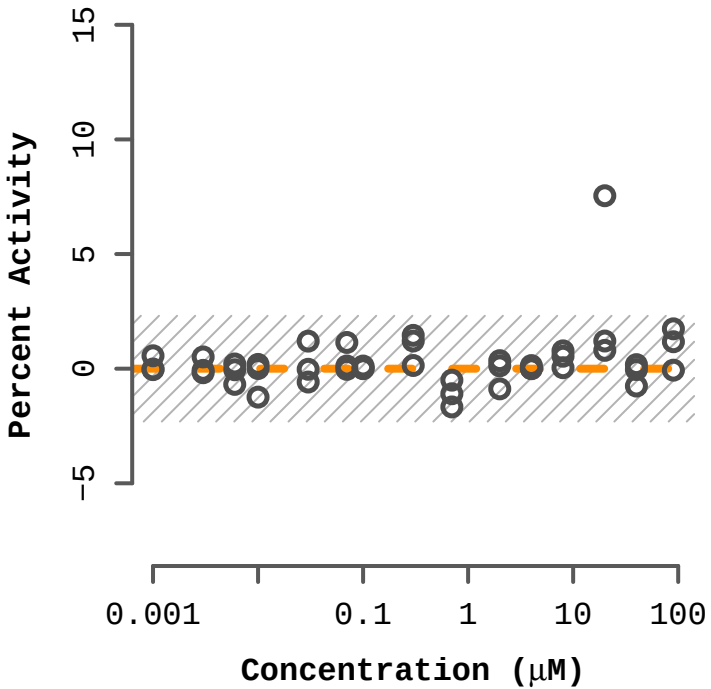
NAME: Triacetin
CHID: 26691 **CASRN:** 102-76-1
SPID(S): Tox21_300111
M4ID: 12479019

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.985 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

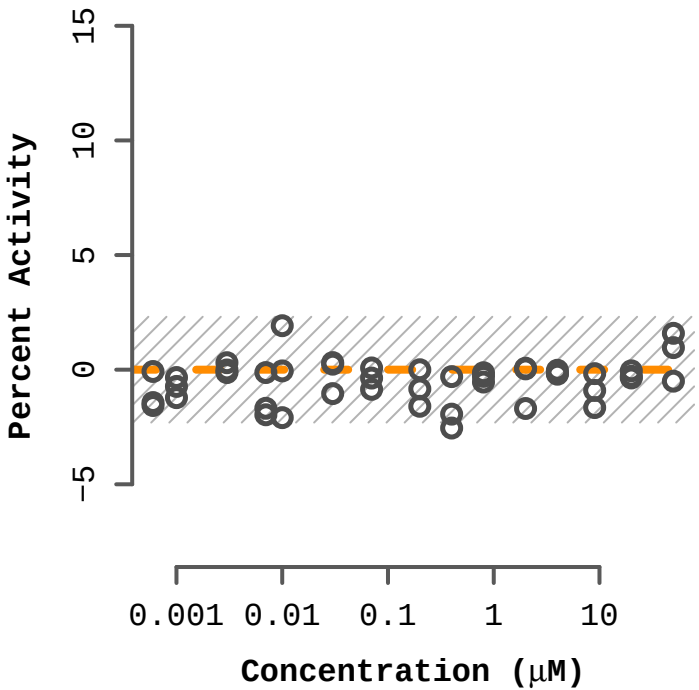
NAME: Triacetin
CHID: 26691 CASRN: 102-76-1
SPID(S): Tox21_201745
M4ID: 12480507

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 3.18 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

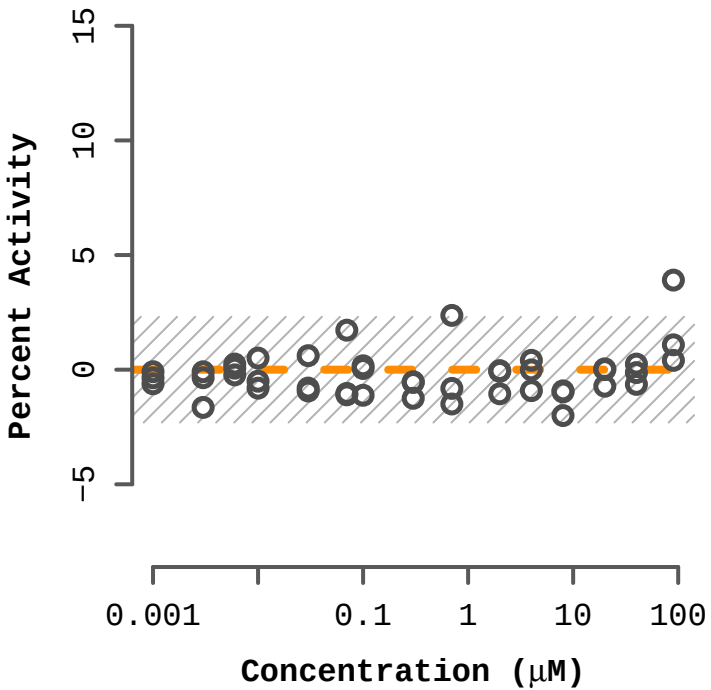
NAME: Triacetin
CHID: 26691 **CASRN:** 102-76-1
SPID(S): Tox21_111155_1
M4ID: 12483873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.683 **MAX_MED:** 0.963 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

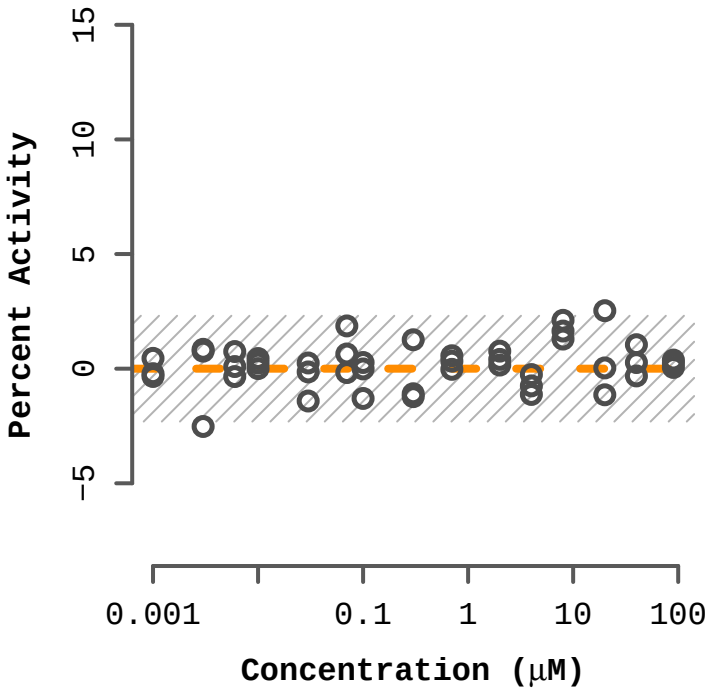
NAME: 2-Ethylhexyl acetate
CHID: 26694 **CASRN:** 103-09-3
SPID(S): Tox21_303318
M4ID: 12475815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

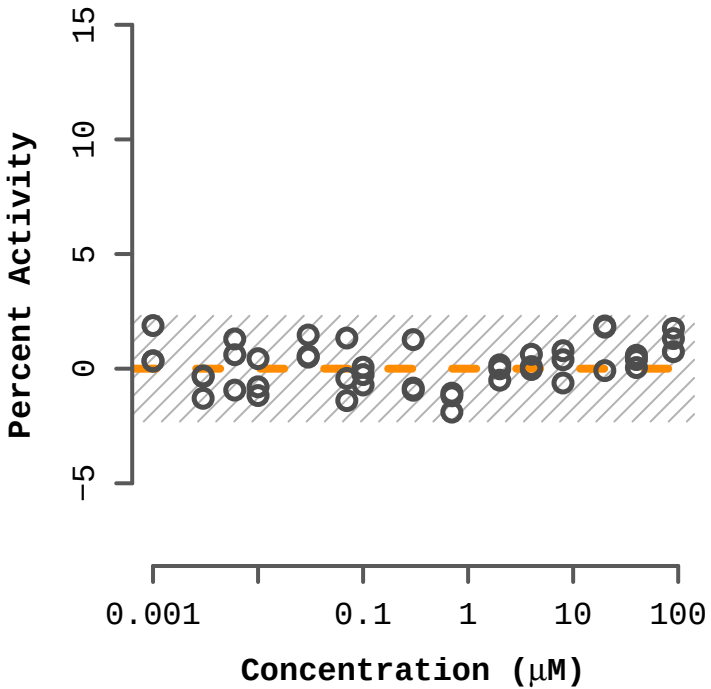
NAME: 2-Ethylhexyl acetate
CHID: 26694 **CASRN:** 103-09-3
SPID(S): Tox21_201992
M4ID: 12480260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

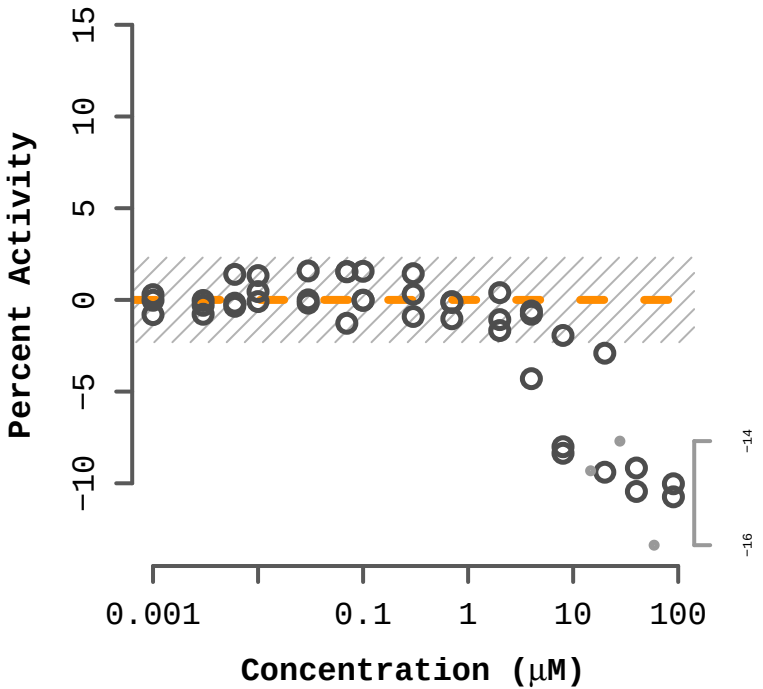
NAME: Bis(2-ethylhexyl) nonanedioate
CHID: 26697 **CASRN:** 103-24-2
SPID(S): Tox21_300600
M4ID: 12478533

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

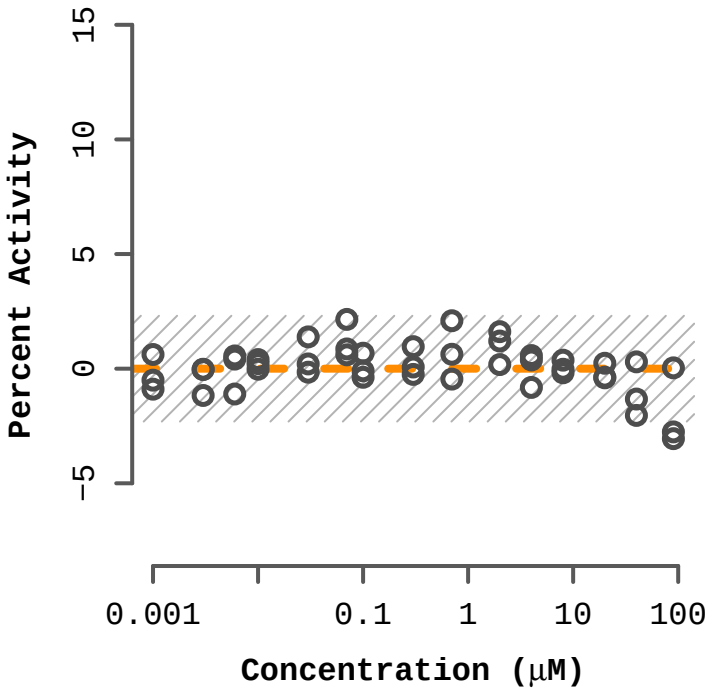
NAME: Bis(2-ethylhexyl) nonanedioate
CHID: 26697 **CASRN:** 103-24-2
SPID(S): Tox21_201553
M4ID: 12480699 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	268.44	NA	NA
PROB:	1	NA	NA
RMSE:	5.4	NA	NA

MAX_MEAN: 0.603 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

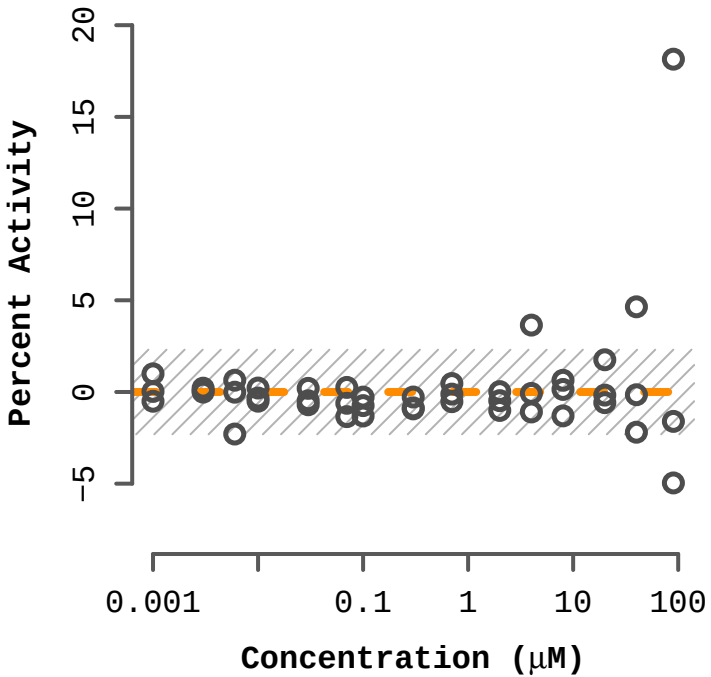
NAME: 4,4'−Dithiodimorpholine
CHID: 26698 **CASRN:** 103−34−4
SPID(S): Tox21_303110
M4ID: 12476023

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

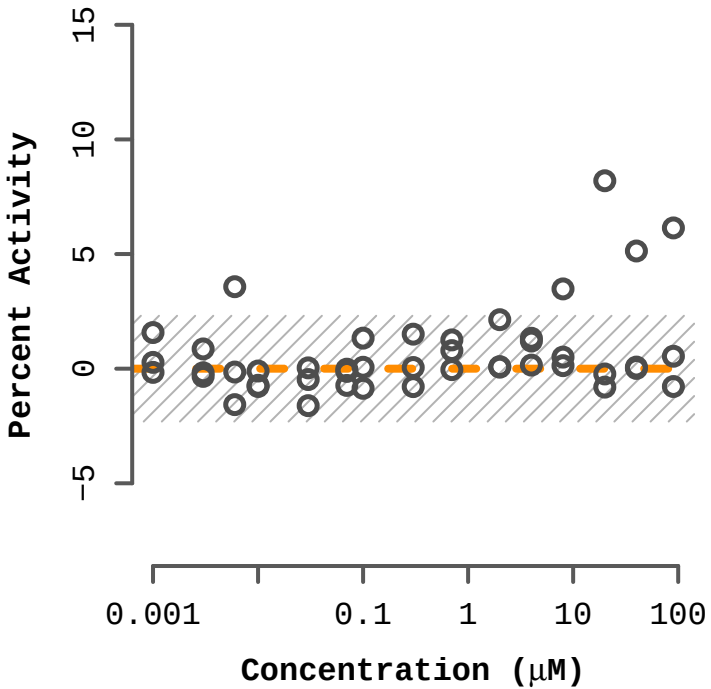
NAME: 4,4'−Dithiodimorpholine
CHID: 26698 CASRN: 103−34−4
SPID(S): Tox21_201775
M4ID: 12480477

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.23	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 3.86 MAX_MED: 0.139 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

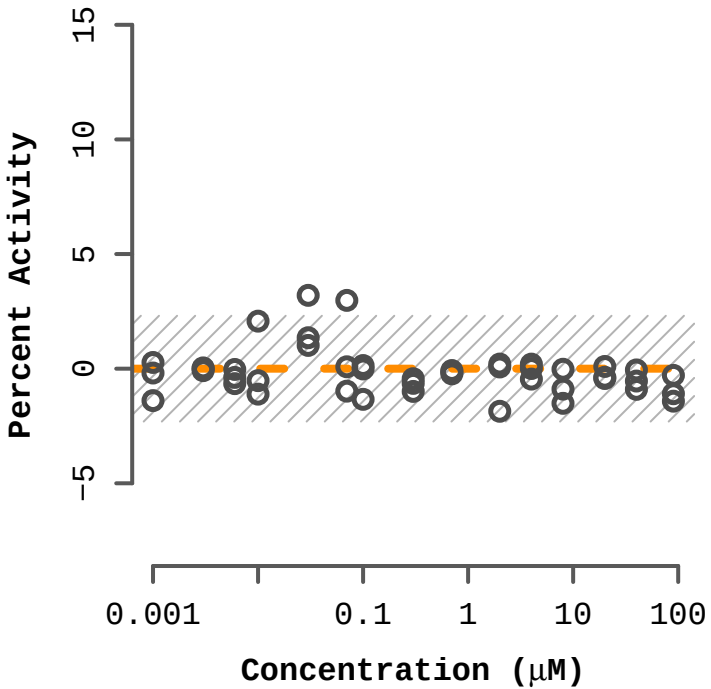
NAME: 4-Methylbenzenesulfonic acid
CHID: 26701 **CASRN:** 104-15-4
SPID(S): Tox21_202364
M4ID: 12479888

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.89	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 2.39 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

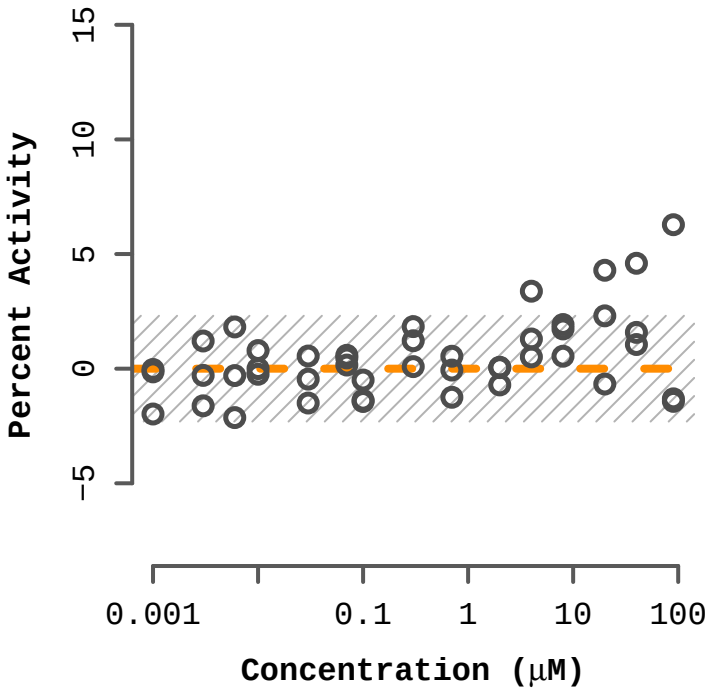
NAME: 2,2'−[1,4−Phenylenebis(oxy)]diethanol
CHID: 26702 **CASRN:** 104−38−1
SPID(S): Tox21_200746
M4ID: 12481506

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

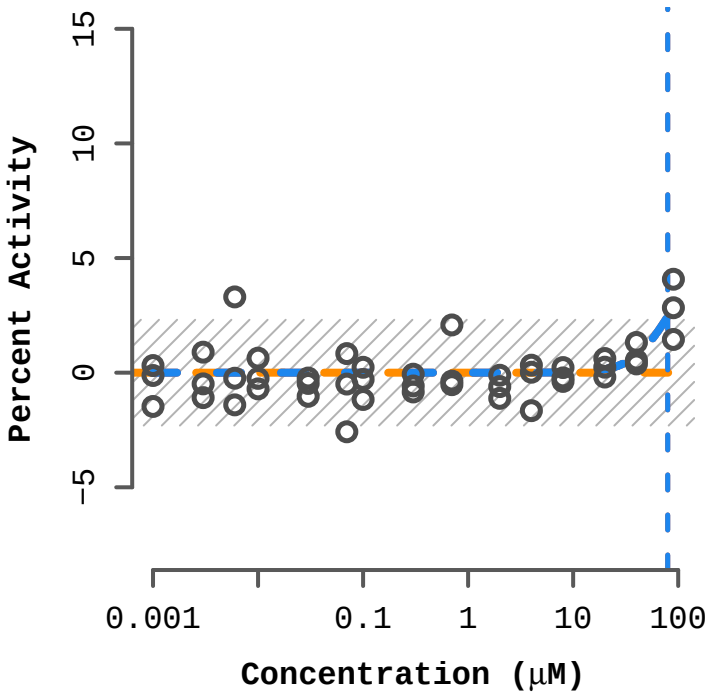
NAME: 1,2−Diphenoxyethane
CHID: 26706 **CASRN:** 104−66−5
SPID(S): Tox21_303309
M4ID: 12475824

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 2.41 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Diphenoxyethane
CHID: 26706 **CASRN:** 104-66-5
SPID(S): Tox21_201399
M4ID: 12480853

HILL MODEL (in red):

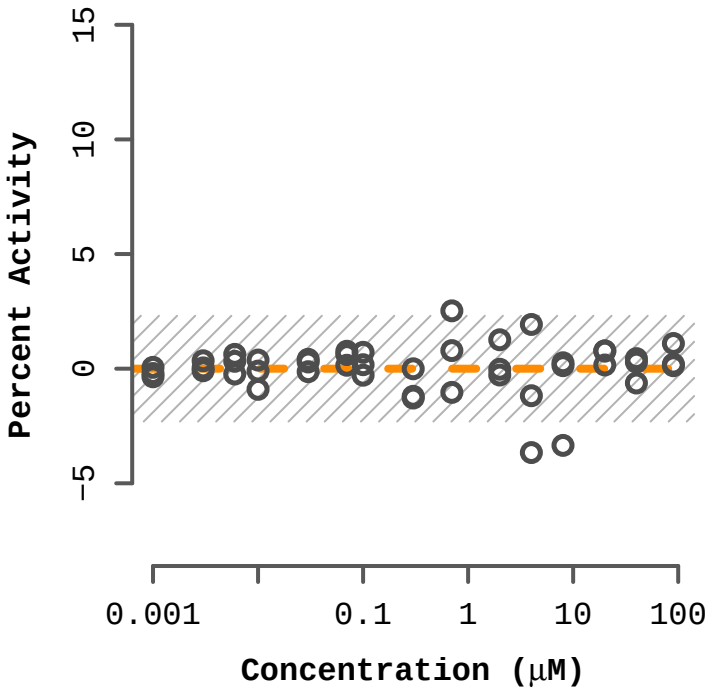
	tp	ga	gw
val:	4.89	1.9	2.5
sd:	11.1	0.853	3.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.89	1.9	2.5	3.59	2.57
sd:	11.1	0.854	3.06	294	492

	CNST	HILL	GNLS
AIC:	141.79	129.57	133.57
PROB:	0	0.88	0.12
RMSE:	1.24	0.99	0.99

MAX_MEAN: 2.79 **MAX_MED:** 2.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

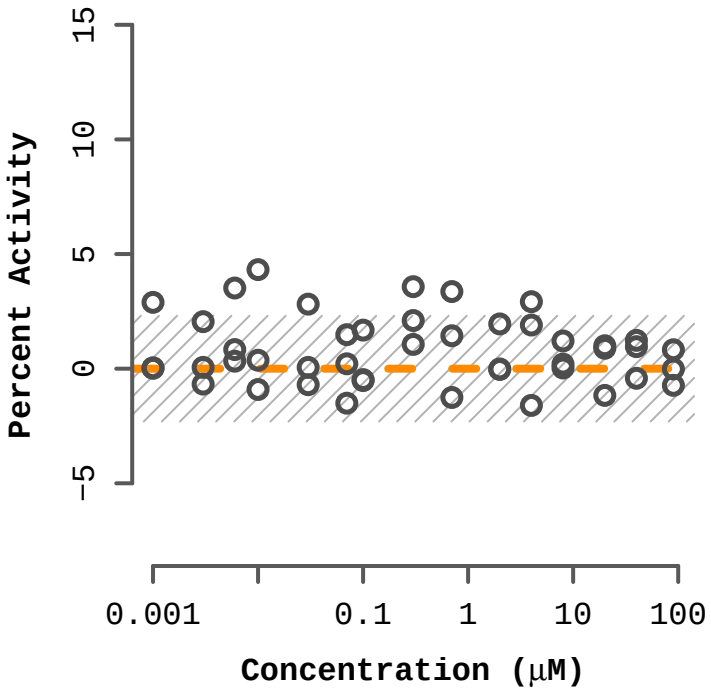
NAME: 1-Methoxy-4-methylbenzene
CHID: 26710 **CASRN:** 104-93-8
SPID(S): Tox21_201081
M4ID: 12481171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.761 **MAX_MED:** 0.791 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

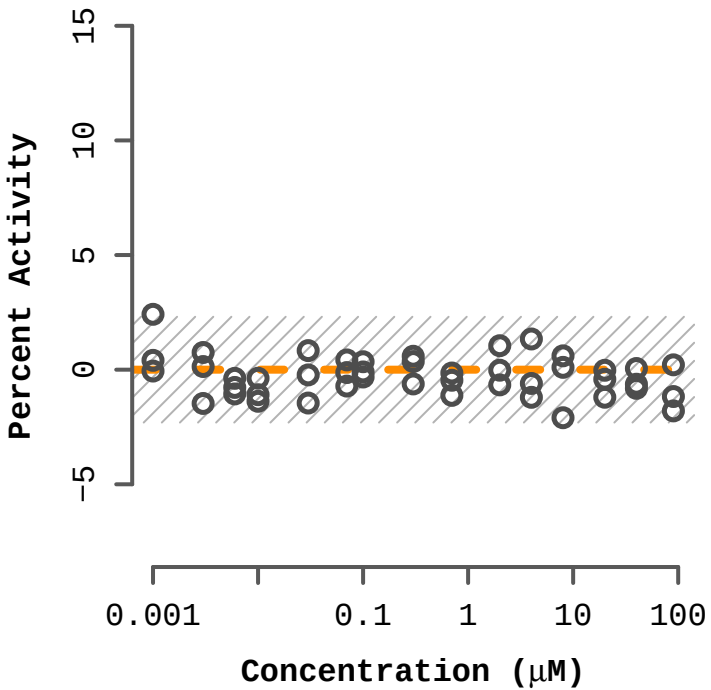
NAME: 1,4-Diethylbenzene
CHID: 26711 **CASRN:** 105-05-5
SPID(S): Tox21_200146
M4ID: 12482106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

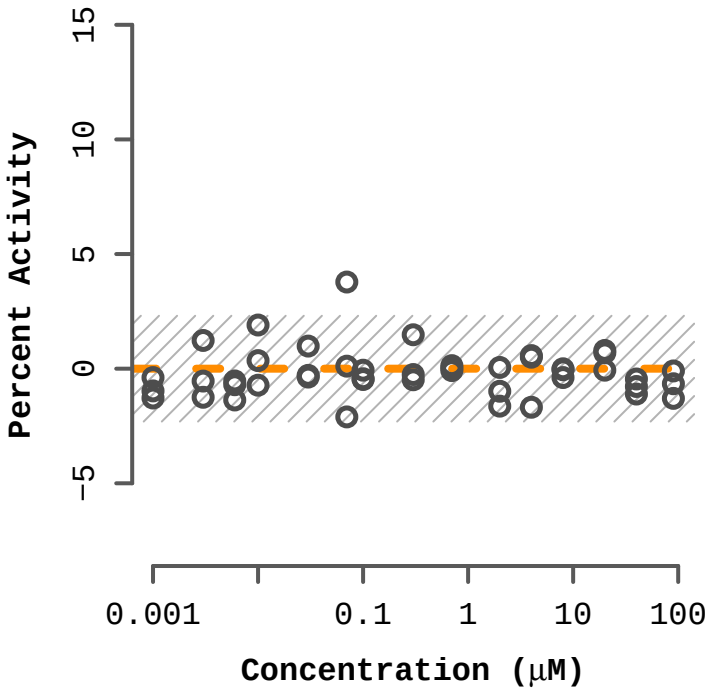
NAME: 1,4-Cyclohexanedimethanol
CHID: 26712 **CASRN:** 105-08-8
SPID(S): Tox21_200433
M4ID: 12481819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.922 **MAX_MED:** 0.409 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

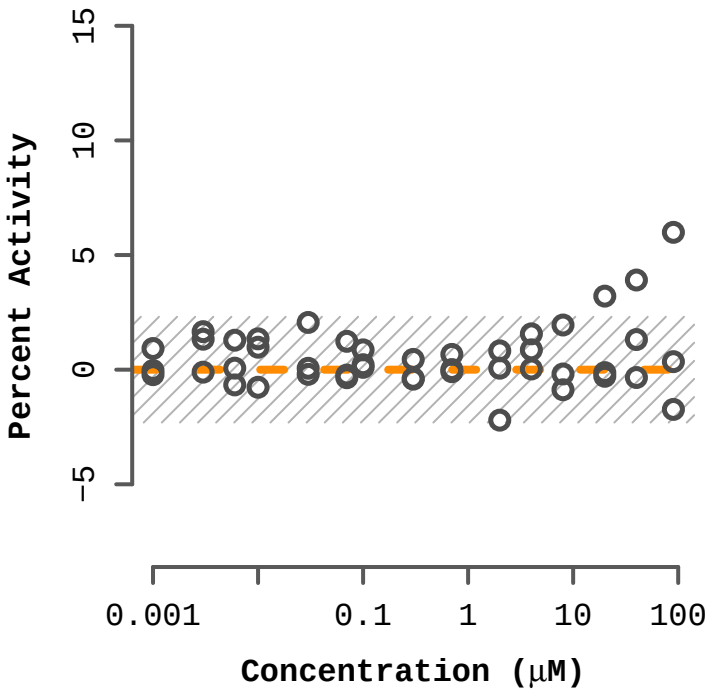
NAME: 2-(Diethylamino)ethyl methacrylate
CHID: 26713 **CASRN:** 105-16-8
SPID(S): Tox21_200763
M4ID: 12481489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.691 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

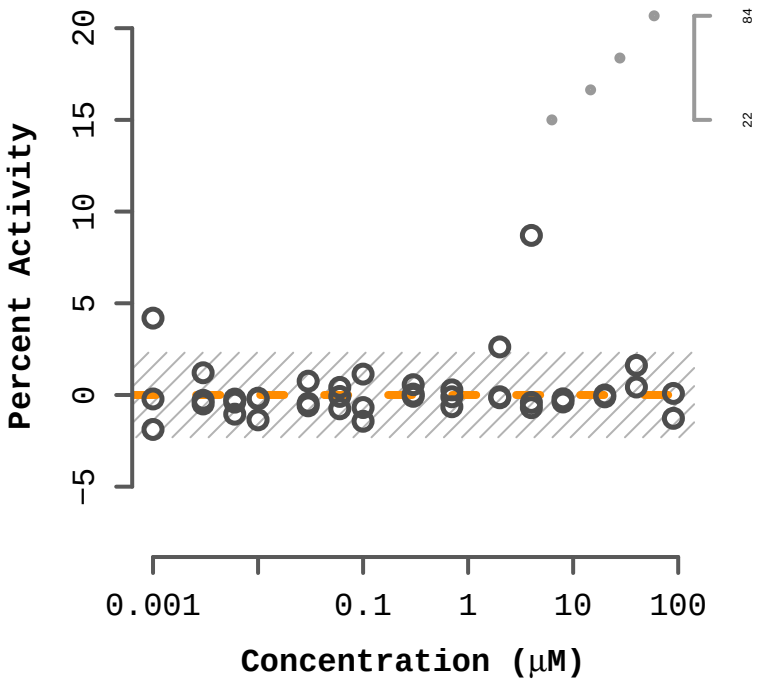
NAME: 2-Methyl-1-pentanol
CHID: 26714 **CASRN:** 105-30-6
SPID(S): Tox21_200753
M4ID: 12481499

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

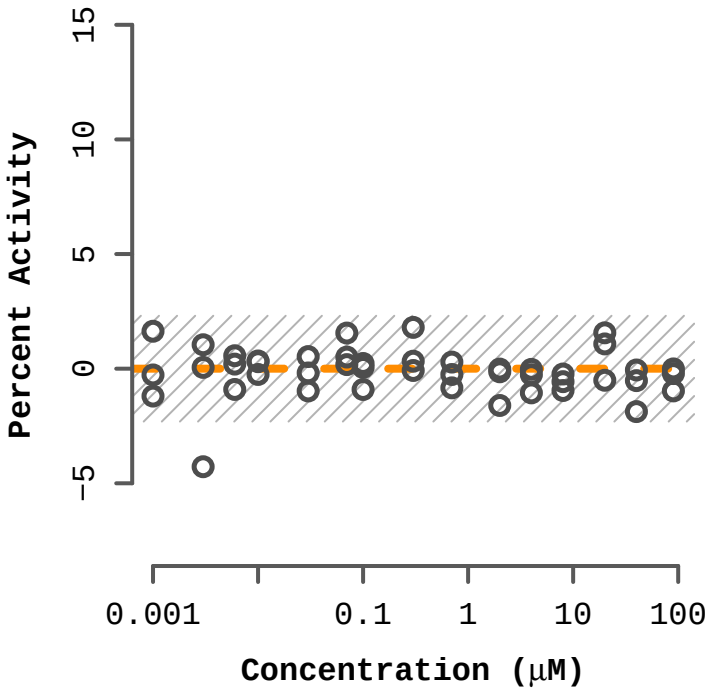
NAME: Ethyl chloroacetate
CHID: 26715 **CASRN:** 105-39-5
SPID(S): Tox21_201053
M4ID: 12481199 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.27	NA	NA
PROB:	1	NA	NA
RMSE:	16.79	NA	NA

MAX_MEAN: 27.6 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

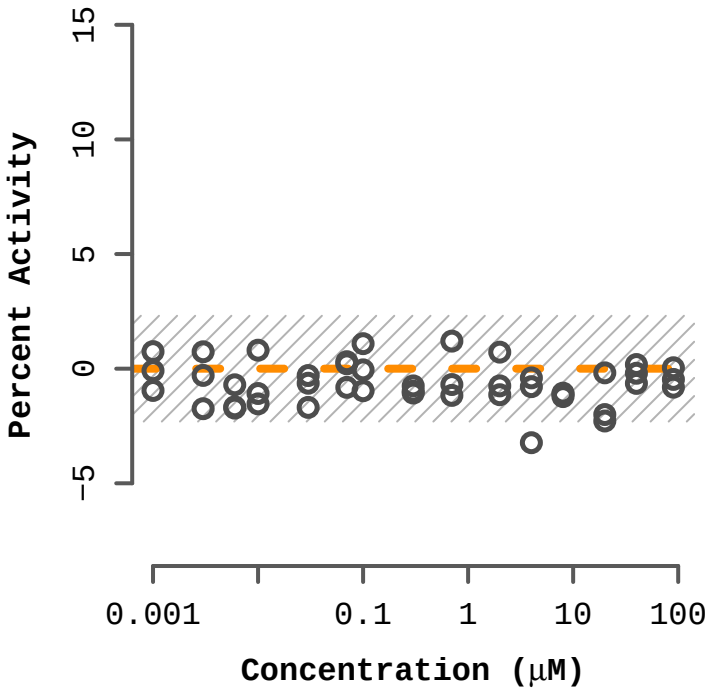
NAME: Methyl acetoacetate
CHID: 26716 CASRN: 105-45-3
SPID(S): Tox21_200162
M4ID: 12482090

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.748 MAX_MED: 1.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

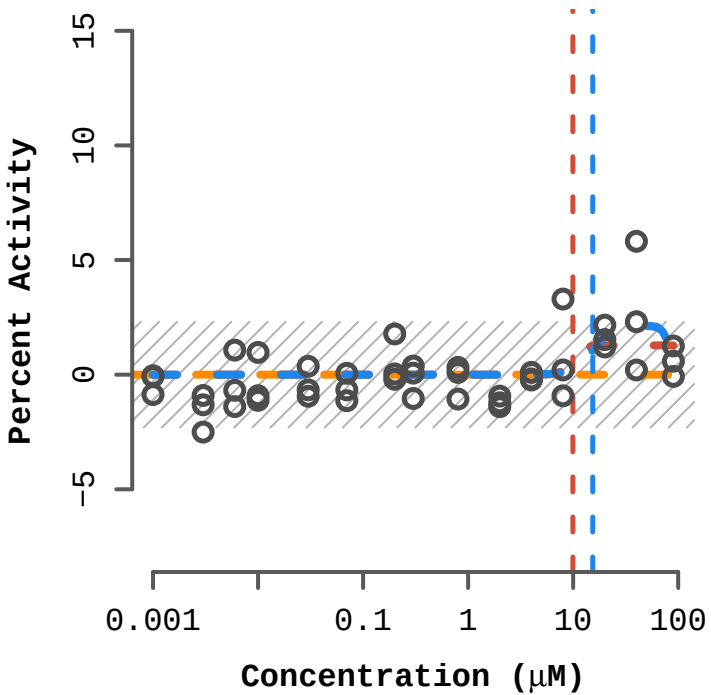
NAME: Ethyl cyanoacetate
CHID: 26718 **CASRN:** 105-56-6
SPID(S): Tox21_200434
M4ID: 12481818

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.0276 **MAX_MED:** 0.214 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dibutyl maleate
CHID: 26724 **CASRN:** 105-76-0
SPID(S): Tox21_200779
M4ID: 12481473

HILL MODEL (in red):

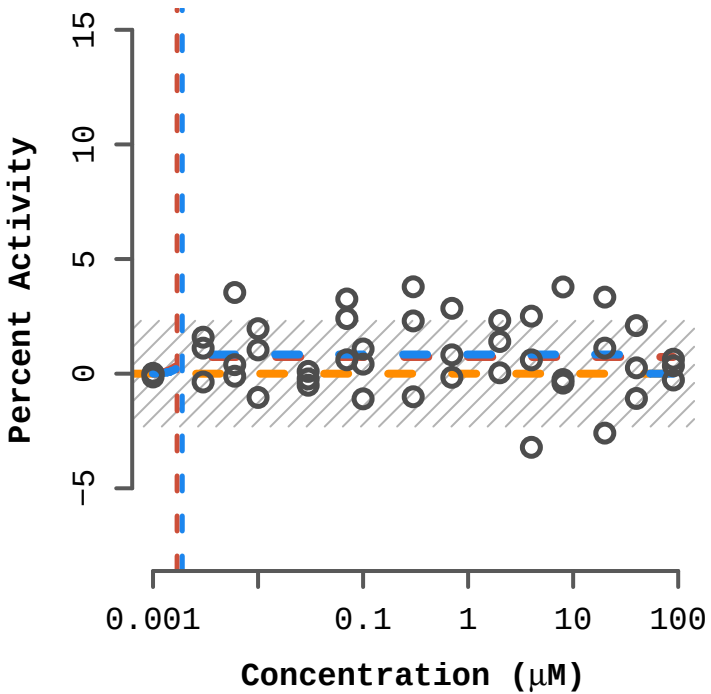
	tp	ga	gw
val:	1.28	0.997	8
sd:	0.361	0.237	13.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.13	1.19	4.43	1.92	12.4
sd:	0.969	0.23	6.43	0.125	45.8

	CNST	HILL	GNLS
AIC:	152.66	147.38	148.27
PROB:	0.04	0.58	0.37
RMSE:	1.42	1.21	1.15

MAX_MEAN: 2.78 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 12−Hydroxyoctadecanoic acid
CHID: 26725 CASRN: 106−14−9
SPID(S): Tox21_303035
M4ID: 12476098

HILL MODEL (in red):

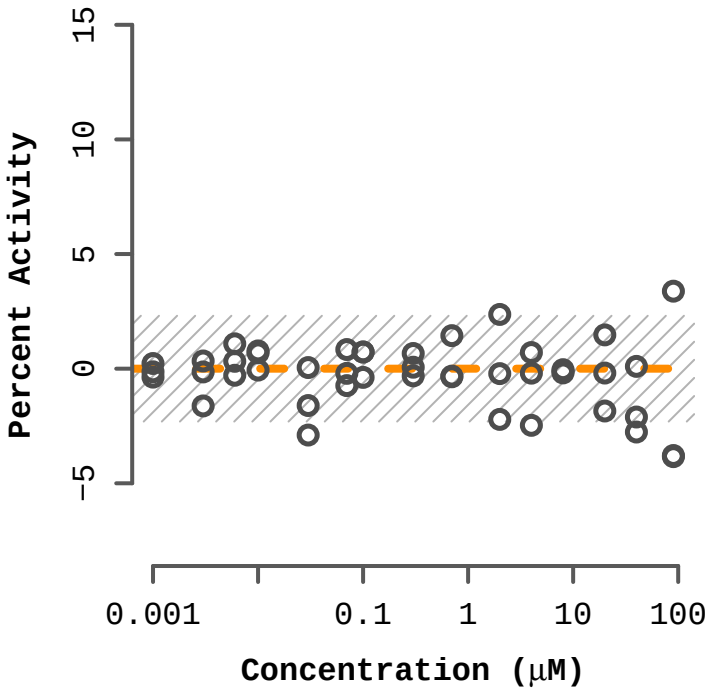
	tp	ga	gw
val:	0.728	−2.77	8
sd:	0.243	0.977	32.7

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.836	−2.72	8	1.59	18
sd:	0.278	1.26	43.9	0.156	368

	CNST	HILL	GNLS
AIC:	180.38	177.46	180.73
PROB:	0.16	0.7	0.14
RMSE:	1.74	1.56	1.55

MAX_MEAN: 2.09 **MAX_MED:** 2.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

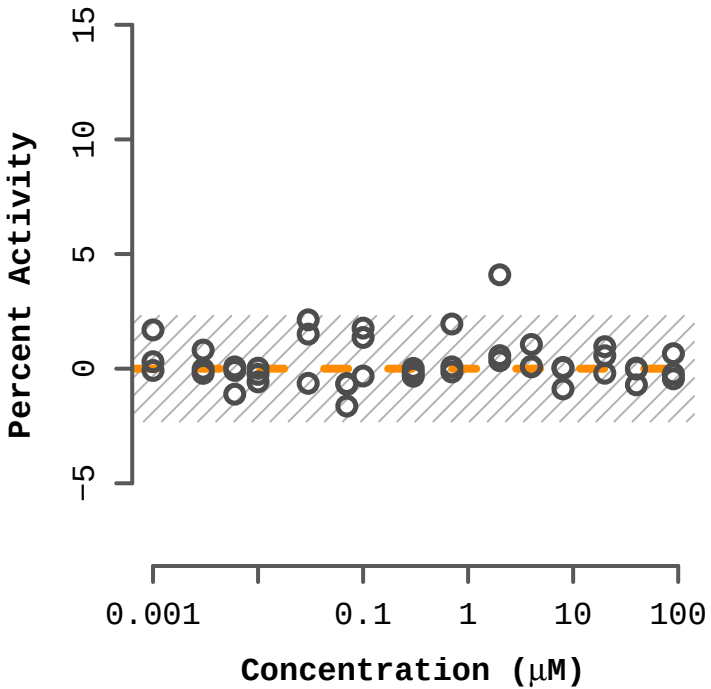
NAME: 12-Hydroxyoctadecanoic acid
CHID: 26725 **CASRN:** 106-14-9
SPID(S): Tox21_201492
M4ID: 12480760

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.469 **MAX_MED:** 0.726 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

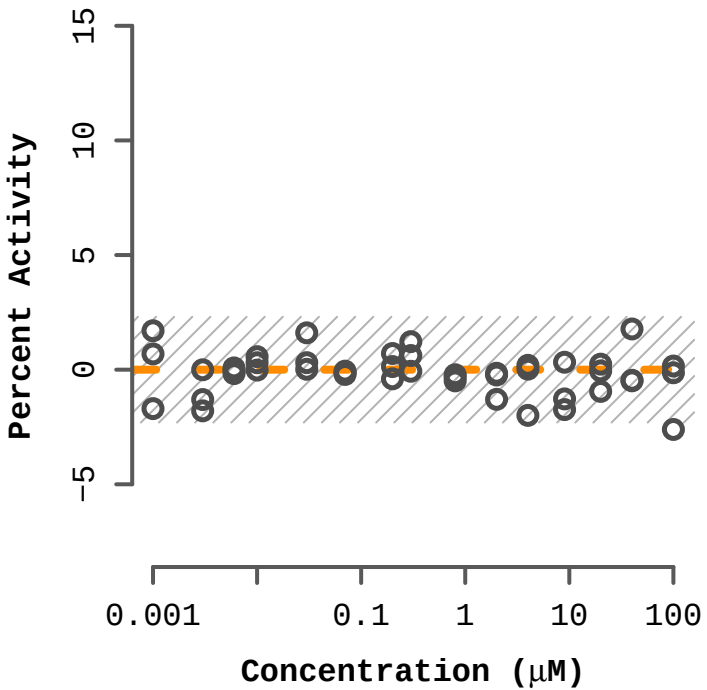
NAME: Citronellol
CHID: 26726 CASRN: 106-22-9
SPID(S): Tox21_300003
M4ID: 12479127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.67 MAX_MED: 1.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

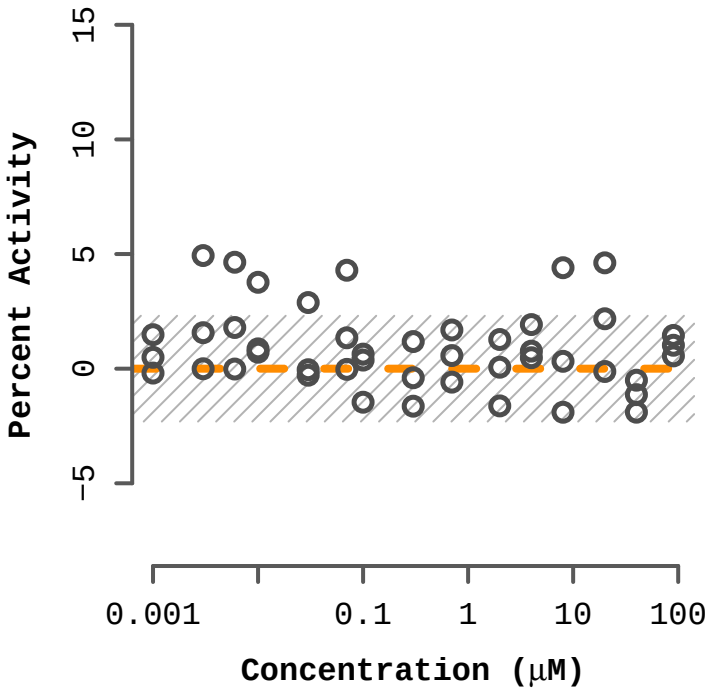
NAME: Citronellol
CHID: 26726 **CASRN:** 106-22-9
SPID(S): Tox21_202119
M4ID: 12480133

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.645 **MAX_MED:** 0.689 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

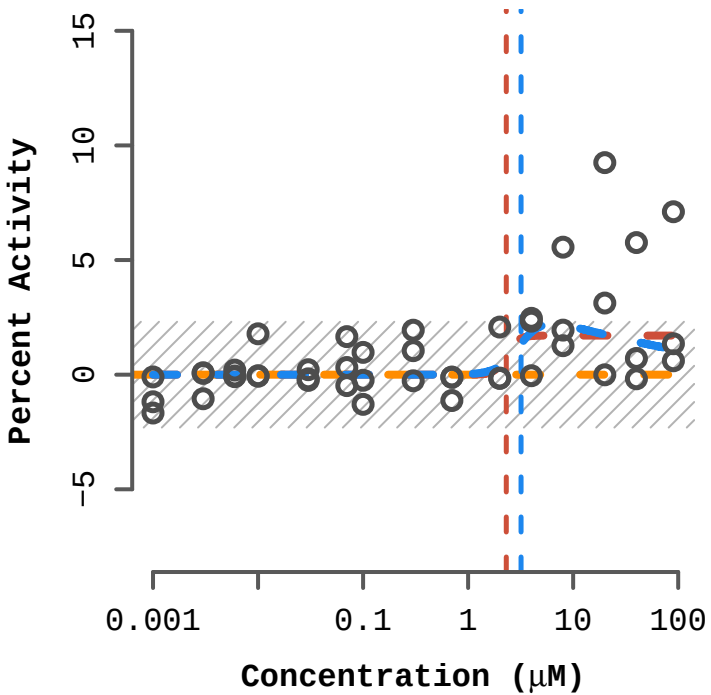
NAME: Geraniol
CHID: 26727 **CASRN:** 106-24-1
SPID(S): Tox21_300136
M4ID: 12478994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Geraniol
CHID: 26727 CASRN: 106-24-1
SPID(S): Tox21_202386
M4ID: 12479866

HILL MODEL (in red):

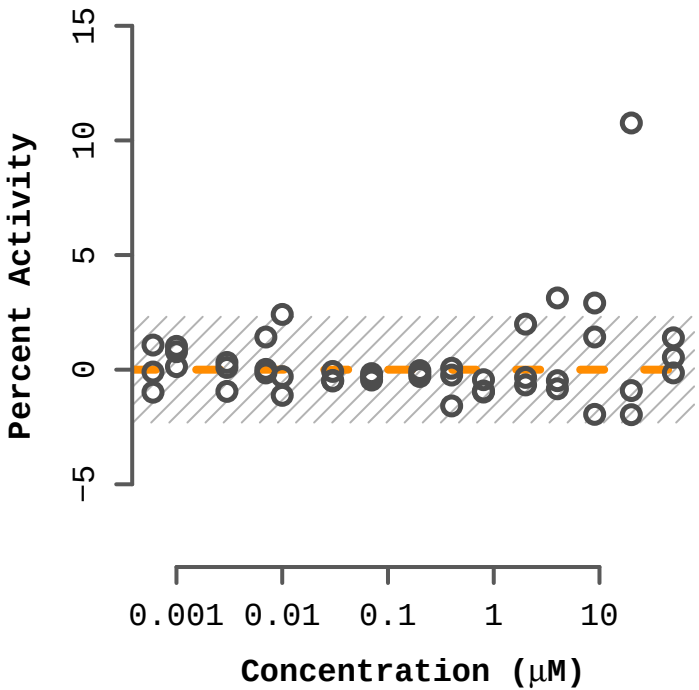
	tp	ga	gw
val:	1.71	0.363	8
sd:	0.43	0.179	18.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.78	0.504	4.16	0.754	0.434
sd:	28	0.283	4.22	11	1.29

	CNST	HILL	GNLS
AIC:	186.42	174.87	177.84
PROB:	0	0.81	0.18
RMSE:	2.38	1.87	1.89

MAX_MEAN: 4.12 MAX_MED: 3.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

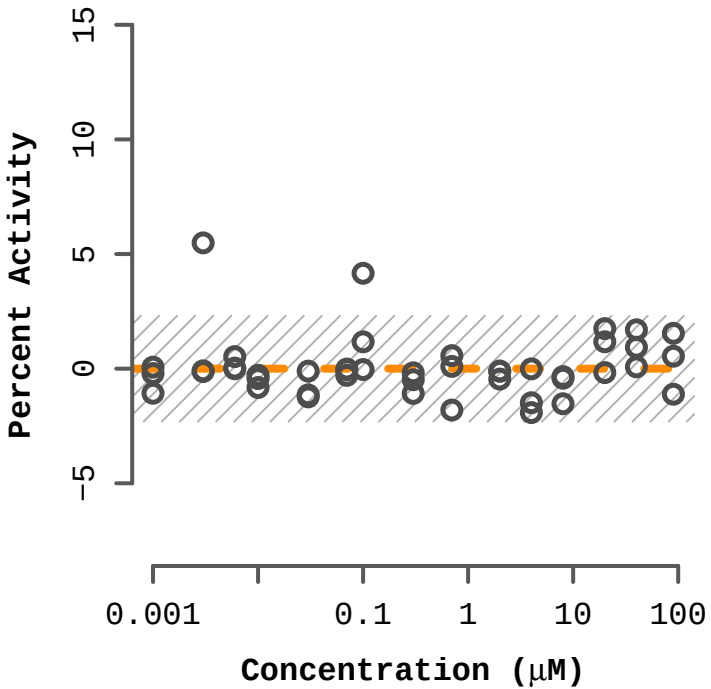
NAME: Geraniol
CHID: 26727 CASRN: 106-24-1
SPID(S): Tox21_110010_1
M4ID: 12484713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 2.63 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

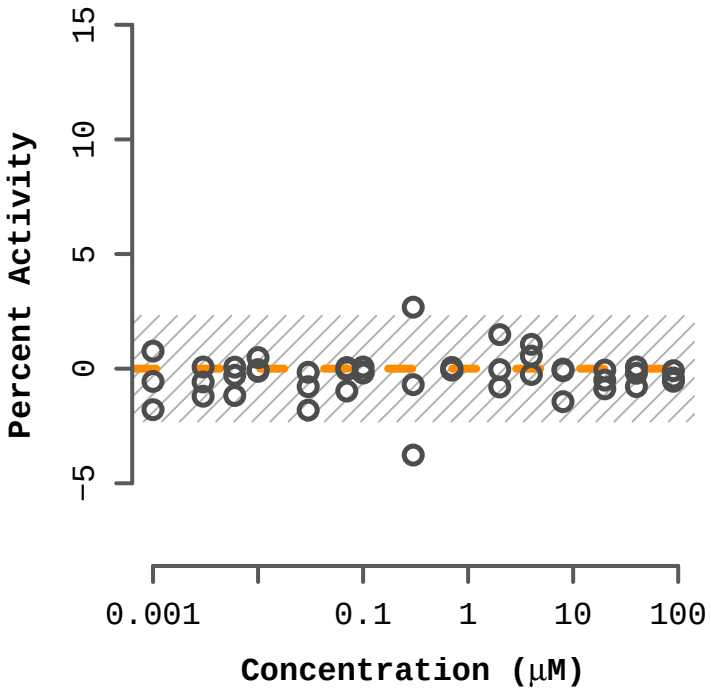
NAME: (2Z)-3,7-Dimethylocta-2,6-dien-1-ol
CHID: 26728 **CASRN:** 106-25-2
SPID(S): Tox21_300542
M4ID: 12478590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

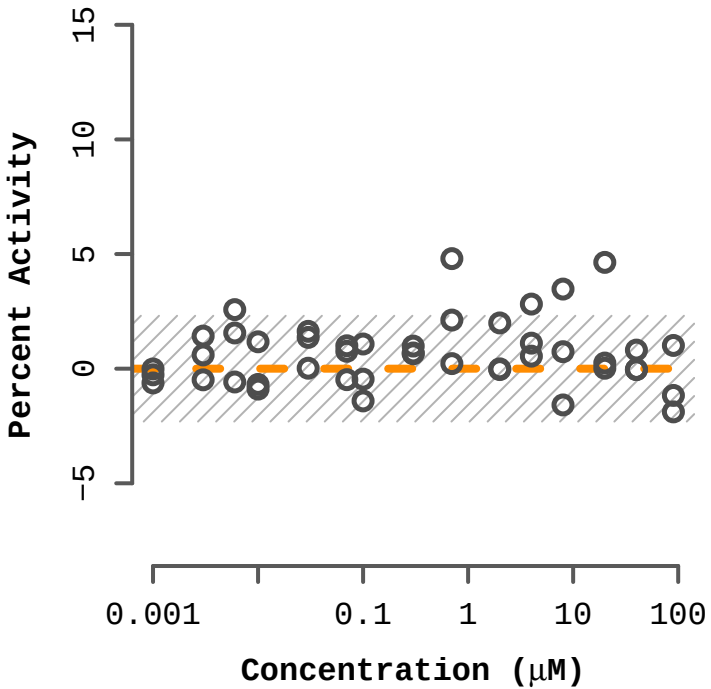
NAME: (2Z)-3,7-Dimethylocta-2,6-dien-1-ol
CHID: 26728 CASRN: 106-25-2
SPID(S): Tox21_202029
M4ID: 12480223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.454 MAX_MED: 0.551 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

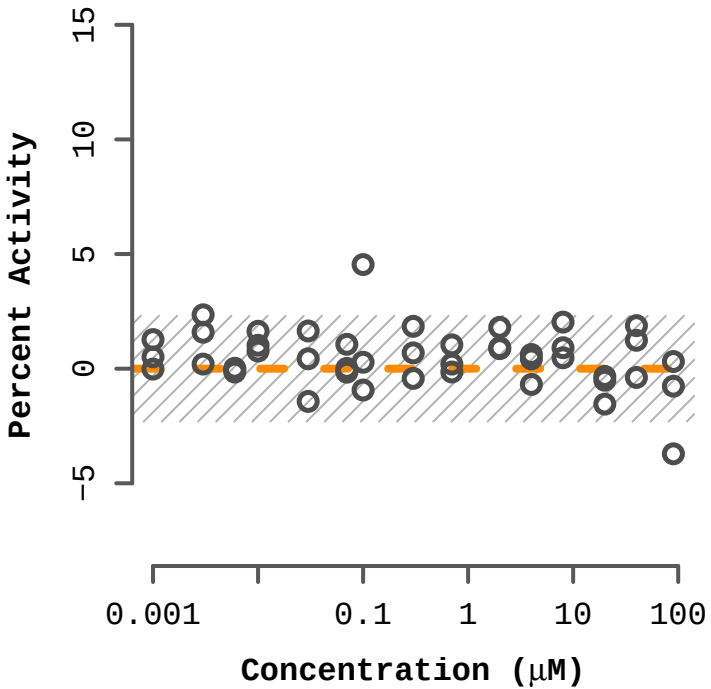
NAME: Butanoic anhydride
CHID: 26729 **CASRN:** 106-31-0
SPID(S): Tox21_201086
M4ID: 12481166

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

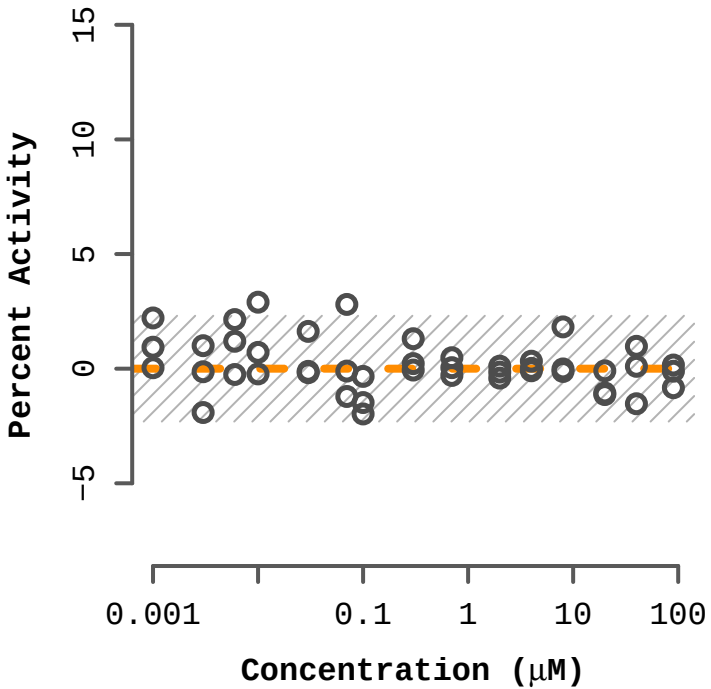
NAME: Carbonochloridic acid, oxydi−2,1−ethanediyl est
CHID: 26739 **CASRN:** 106−75−2
SPID(S): Tox21_301037
M4ID: 12478096

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

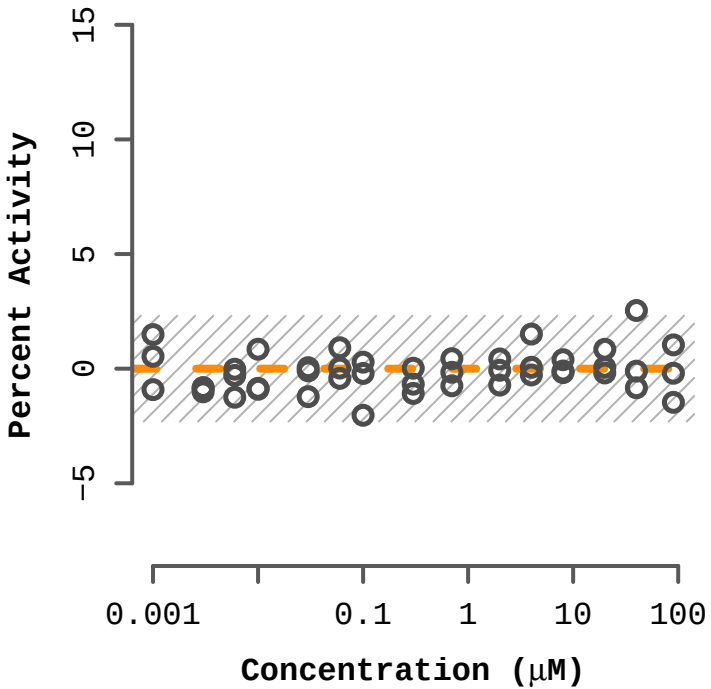
NAME: Dimethyl decanedioate
CHID: 26740 CASRN: 106-79-6
SPID(S): Tox21_200178
M4ID: 12482074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.13 MAX_MED: 1.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

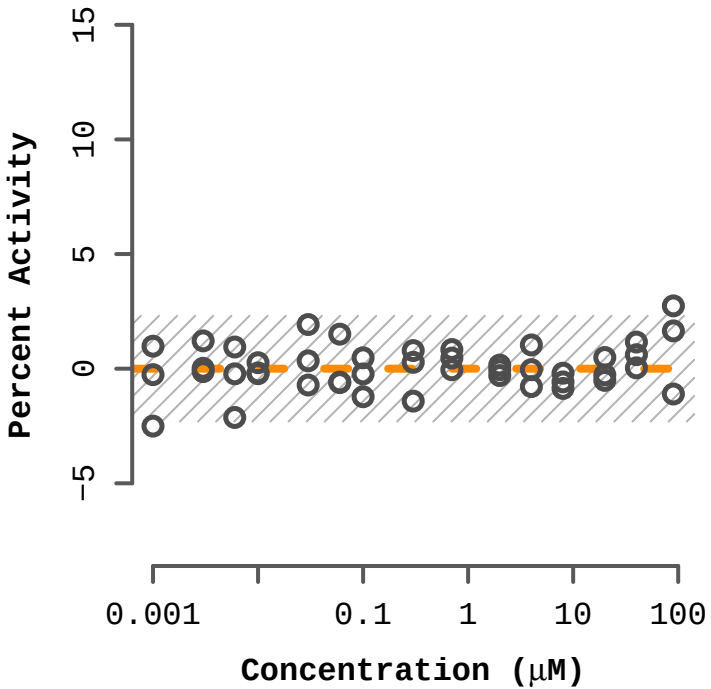
NAME: 2,4,4−Trimethyl−1−pentene
CHID: 26765 **CASRN:** 107−39−1
SPID(S): Tox21_200435
M4ID: 12481817

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.535 **MAX_MED:** 0.538 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

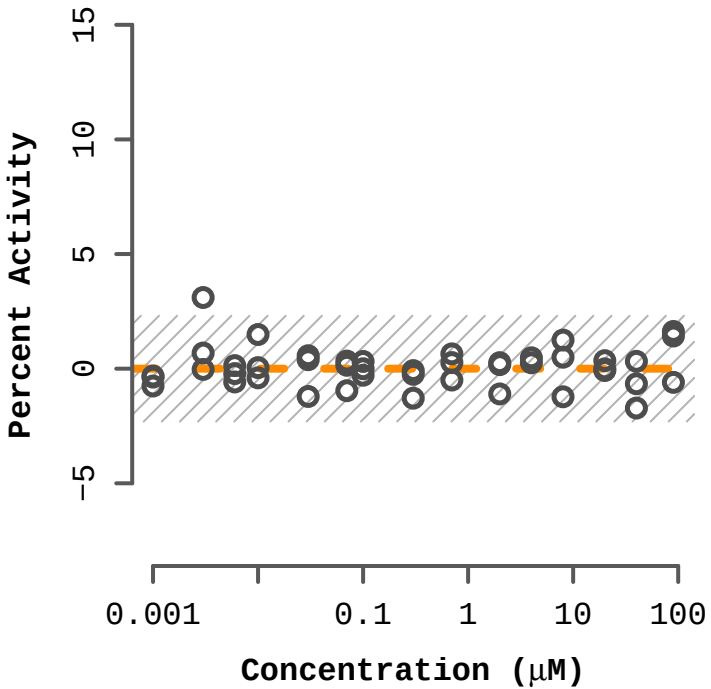
NAME: 2,4,4−Trimethyl−2−pentene
CHID: 26766 **CASRN:** 107−40−4
SPID(S): Tox21_200795
M4ID: 12481457

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

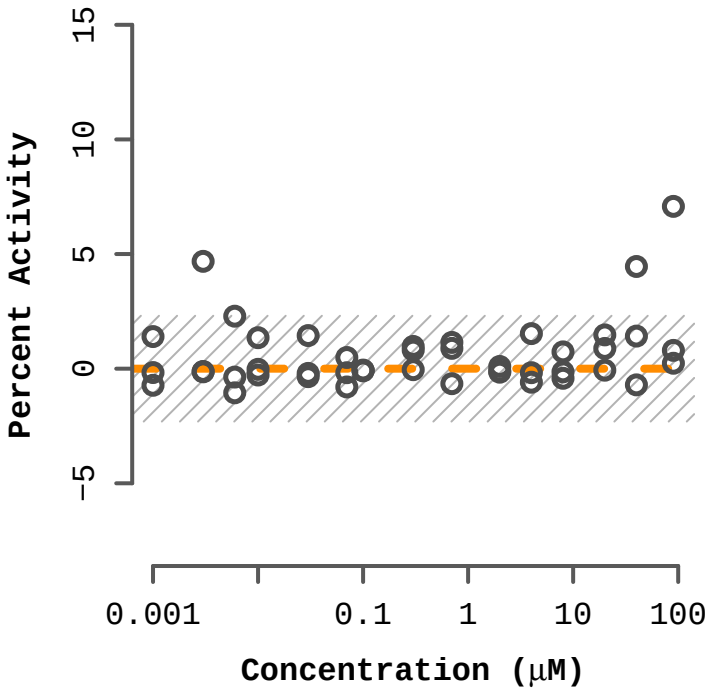
NAME: Hexamethyldisiloxane
CHID: 26769 **CASRN:** 107-46-0
SPID(S): Tox21_303119
M4ID: 12476014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

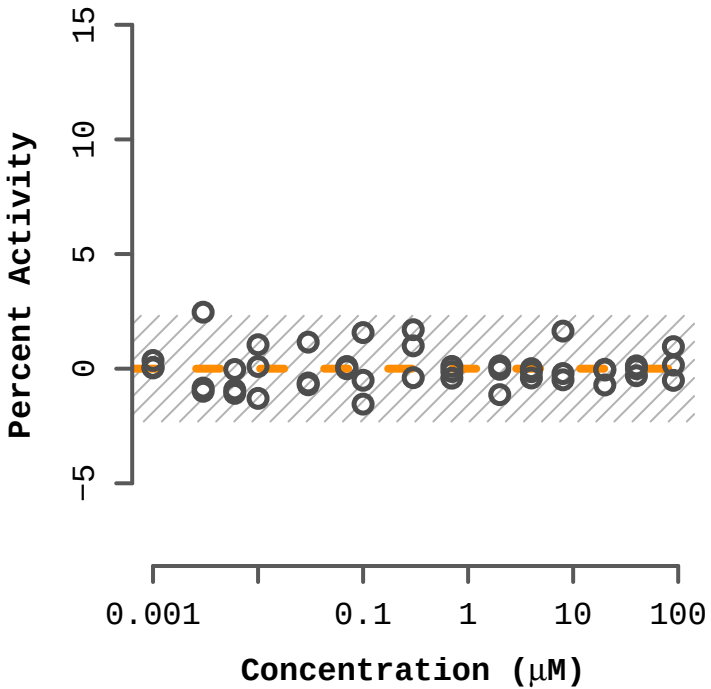
NAME: Hexamethyldisiloxane
CHID: 26769 **CASRN:** 107-46-0
SPID(S): Tox21_201713
M4ID: 12480539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.71 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

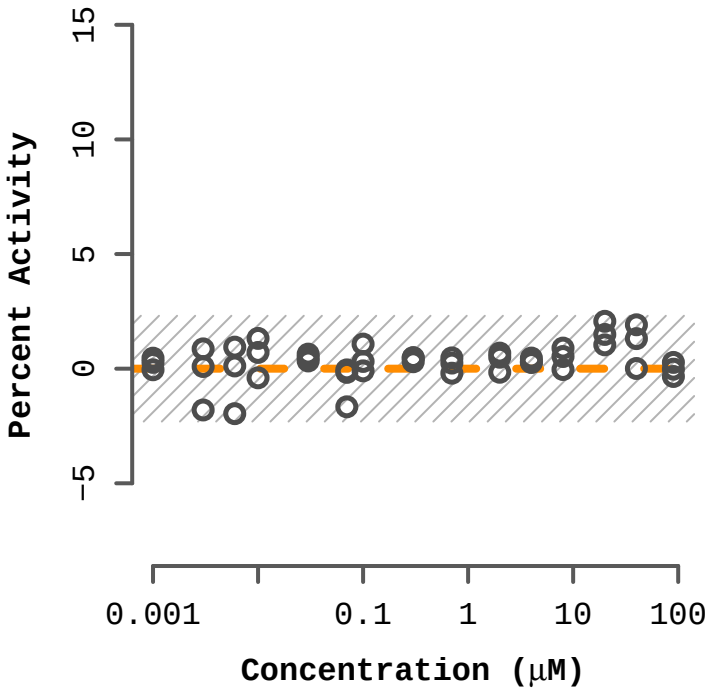
NAME: 1,3-Butanediol
CHID: 26773 CASRN: 107-88-0
SPID(S): Tox21_300085
M4ID: 12479045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.77 MAX_MED: 0.997 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

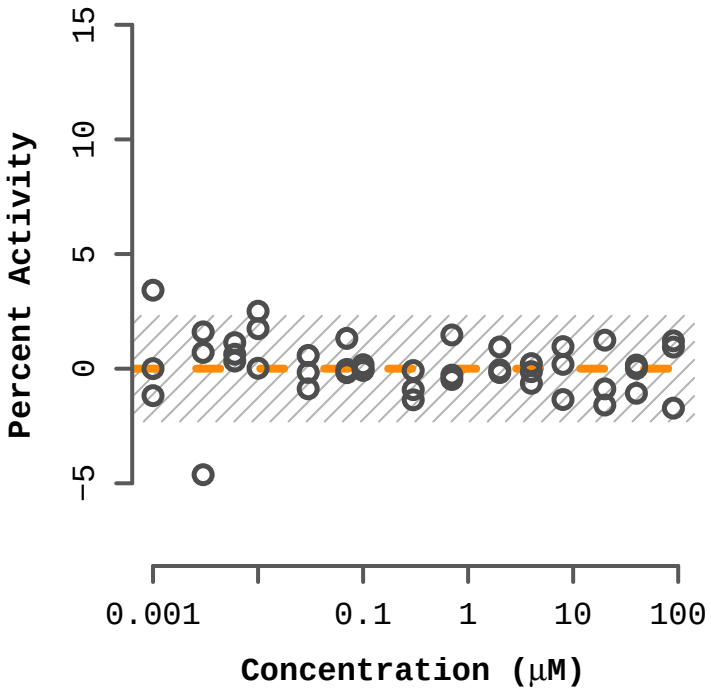
NAME: 1,3-Butanediol
CHID: 26773 **CASRN:** 107-88-0
SPID(S): Tox21_202408
M4ID: 12479844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

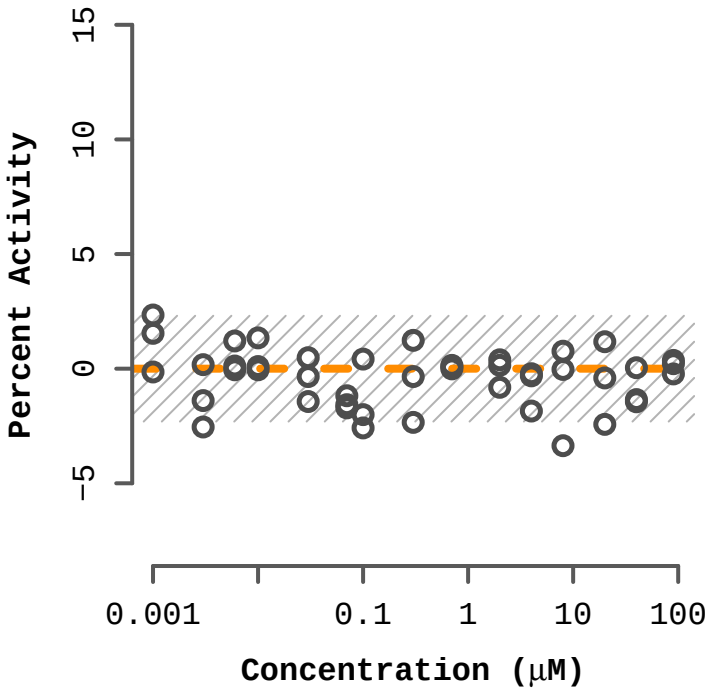
NAME: 3-Mercaptopropanoic acid
CHID: 26775 CASRN: 107-96-0
SPID(S): Tox21_200194
M4ID: 12482058

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.42 MAX_MED: 1.75 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

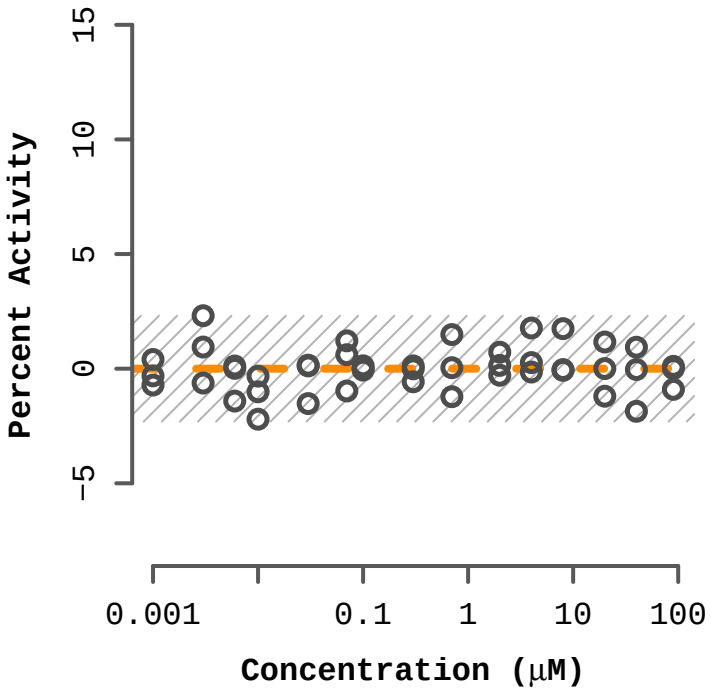
NAME: 4-Methyl-2-pentanol
CHID: 26781 **CASRN:** 108-11-2
SPID(S): Tox21_300083
M4ID: 12479047

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

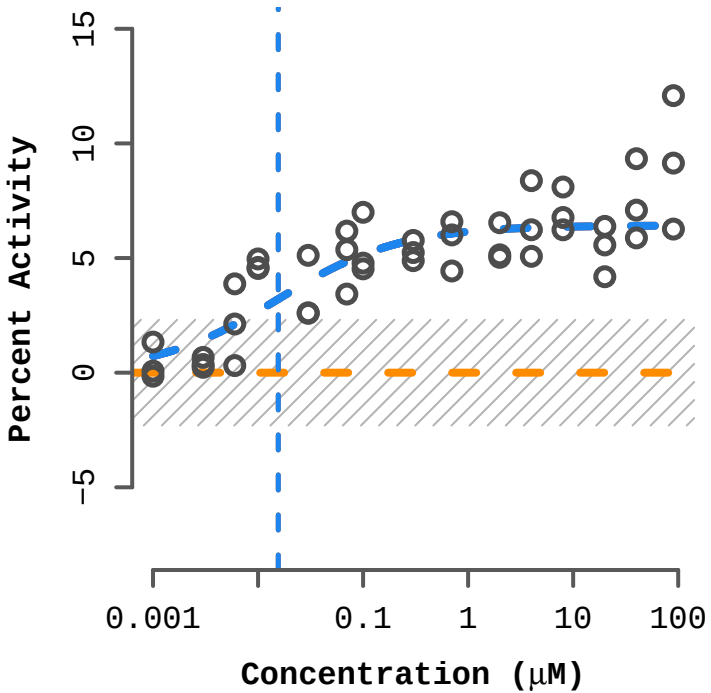
NAME: 4-Methyl-2-pentanol
CHID: 26781 **CASRN:** 108-11-2
SPID(S): Tox21_200436
M4ID: 12481816

HILL MODEL: Not applicable.

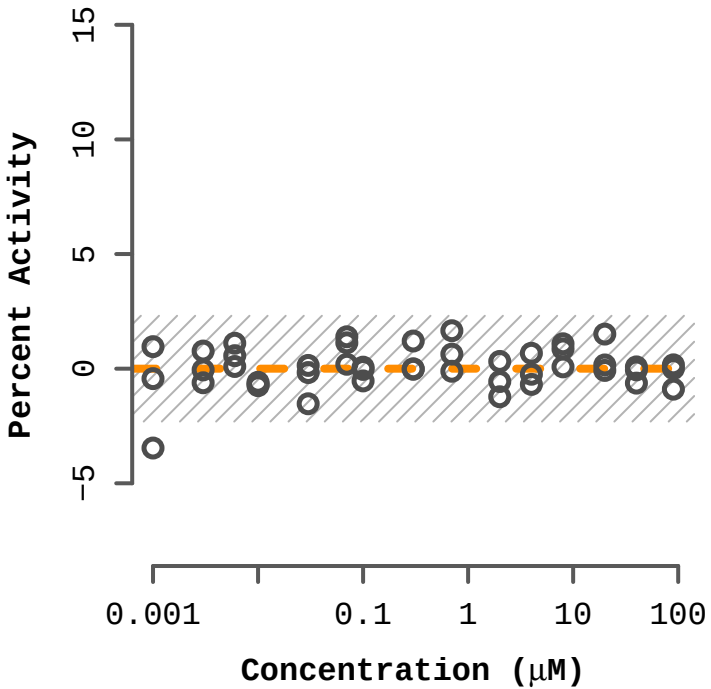
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.877 **MAX_MED:** 0.945 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Imidodicarbonic diamide
CHID:    26783   CASRN: 108-19-0
SPID(S): Tox21_303191
M4ID:    12475942

HILL MODEL (in red):
      tp       ga       gw
val:  6.42     -1.81    0.75
sd:   0.453    0.228    0.25

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.42     -1.81    0.75     3.9      17.4
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  291.58      172.55      176.55
PROB: 0           0.88        0.12
RMSE: 5.56        1.54        1.54

MAX_MEAN: 9.17      MAX_MED: 9.14      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

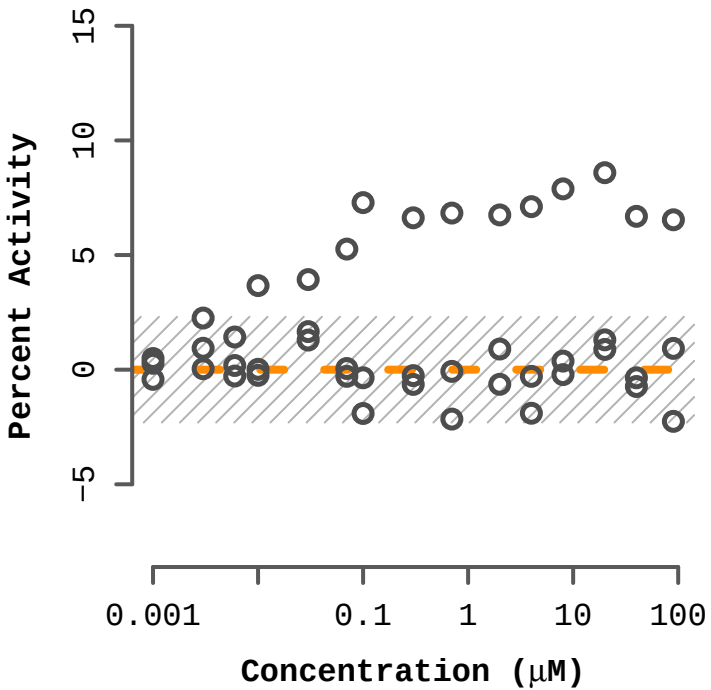
NAME: Imidodicarbonic diamide
CHID: 26783 **CASRN:** 108-19-0
SPID(S): Tox21_202163
M4ID: 12480089

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

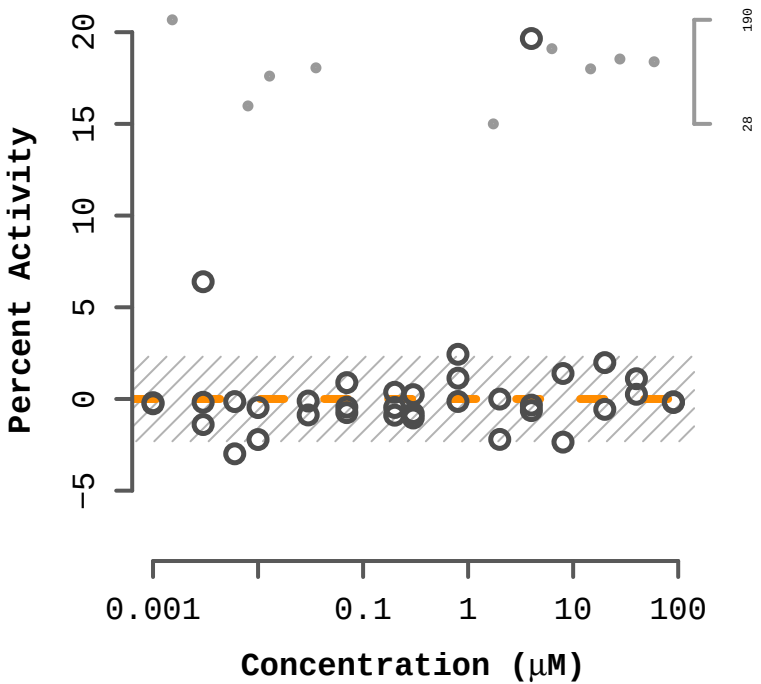
NAME: Propylene carbonate
CHID: 26789 **CASRN:** 108-32-7
SPID(S): Tox21_303214
M4ID: 12475919

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.71	NA	NA
PROB:	1	NA	NA
RMSE:	3.52	NA	NA

MAX_MEAN: 3.59 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

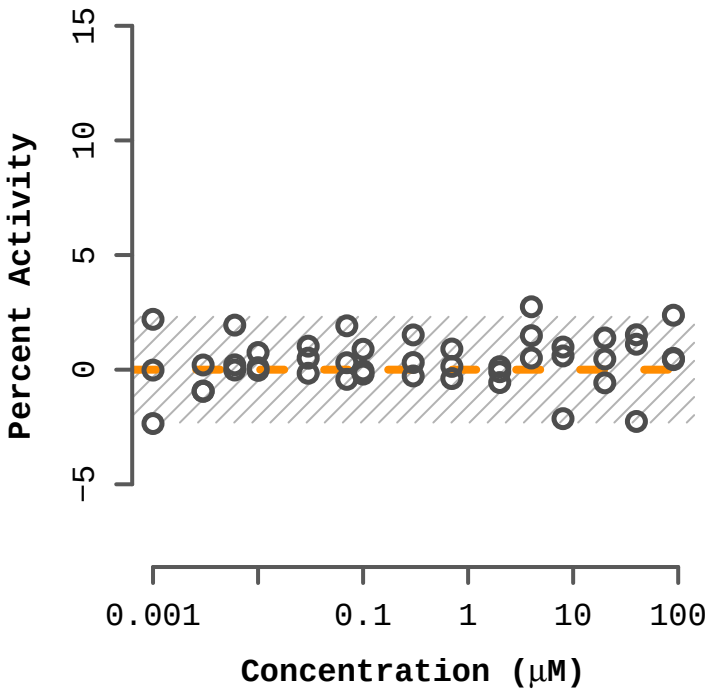
NAME: Propylene carbonate
CHID: 26789 **CASRN:** 108-32-7
SPID(S): Tox21_202047
M4ID: 12480205 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	450.21	NA	NA
PROB:	1	NA	NA
RMSE:	54.33	NA	NA

MAX_MEAN: 63.9 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

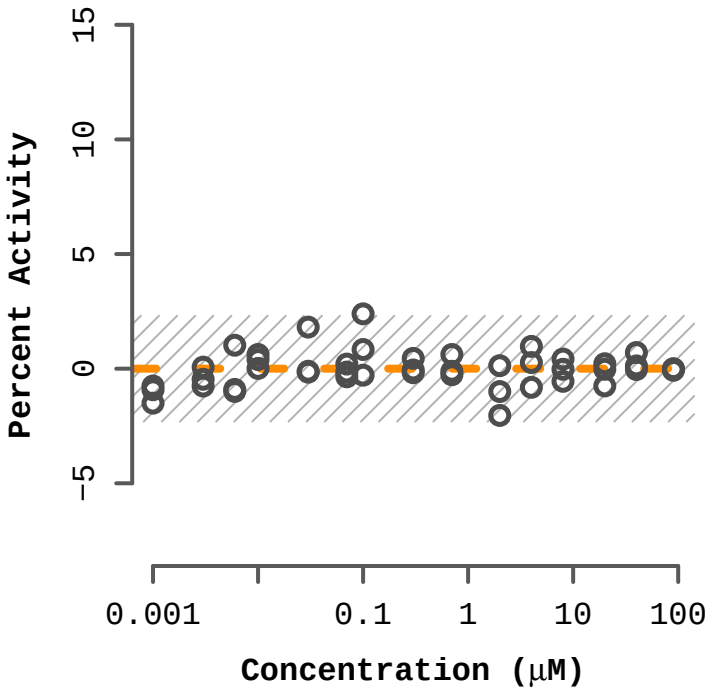
NAME: 3-Methylaniline
CHID: 26792 **CASRN:** 108-44-1
SPID(S): Tox21_300568
M4ID: 12478565

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

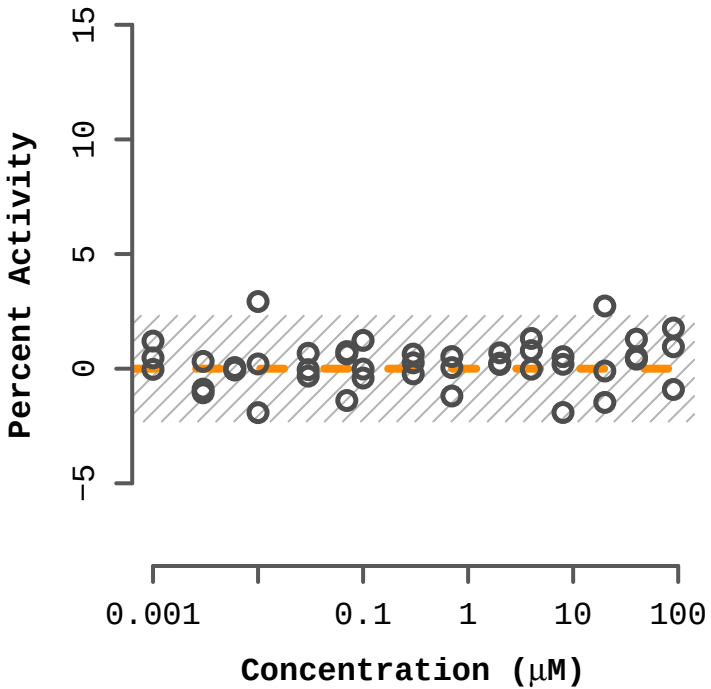
NAME: 3-Methylaniline
CHID: 26792 **CASRN:** 108-44-1
SPID(S): Tox21_201265
M4ID: 12480987

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

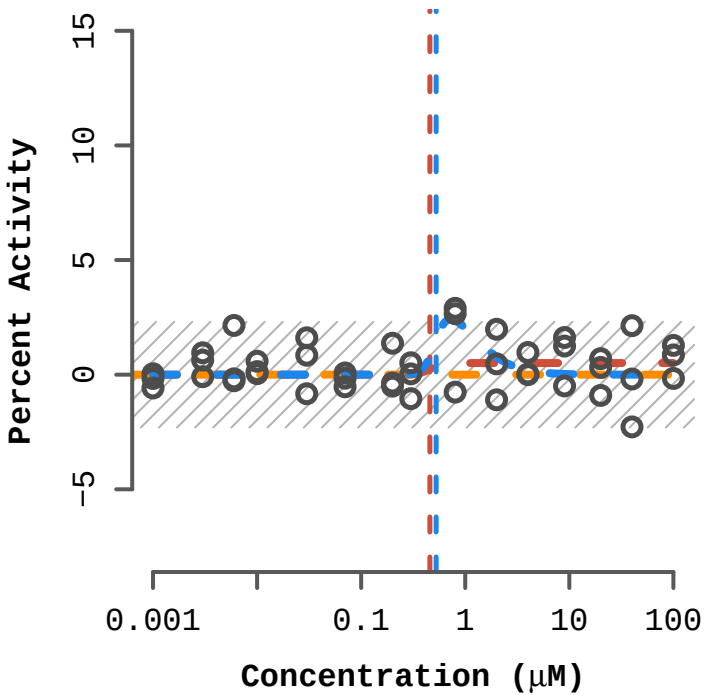
NAME: 1-Methoxy-2-propyl acetate
CHID: 26796 **CASRN:** 108-65-6
SPID(S): Tox21_201436
M4ID: 12480816

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.738 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3,5-Trimethylbenzene
CHID: 26797 **CASRN:** 108-67-8
SPID(S): Tox21_300341
M4ID: 12478791

HILL MODEL (in red):

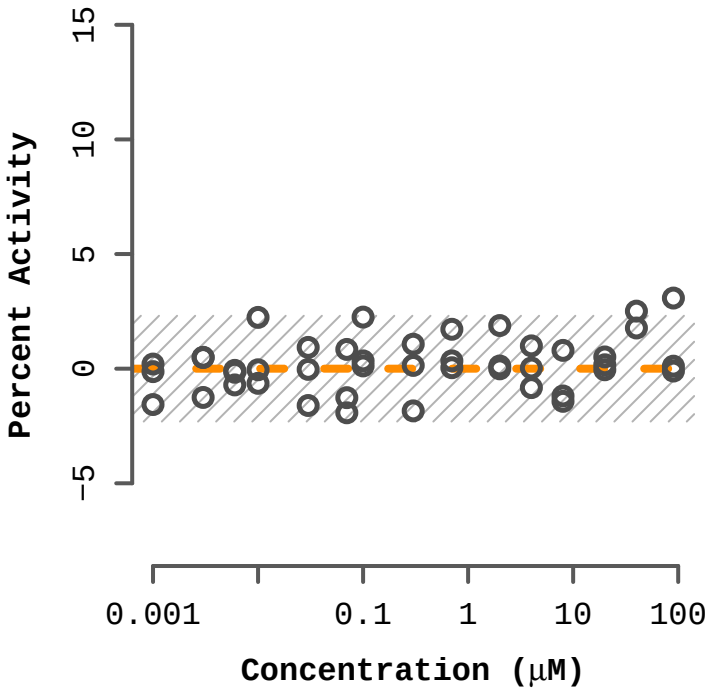
	tp	ga	gw
val:	0.507	−0.34	8
sd:	0.247	0.428	16

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.47	−0.28	8	0.0653	2.31
sd:	3.51	0.265	9.47	0.455	3.52

	CNST	HILL	GNLS
AIC:	138.03	139.82	141.12
PROB:	0.62	0.25	0.13
RMSE:	1.11	1.04	1.04

MAX_MEAN: 1.6 **MAX_MED:** 2.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

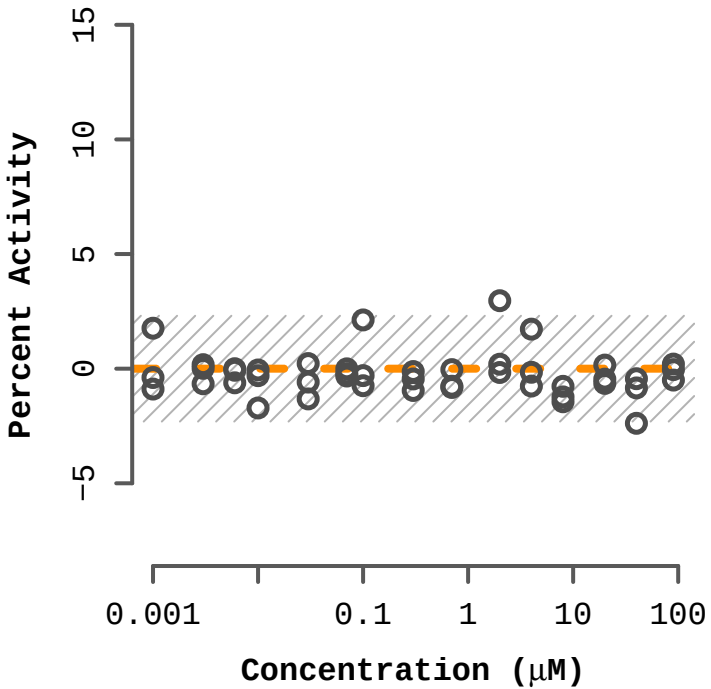
NAME: 1,3,5-Trimethylbenzene
CHID: 26797 **CASRN:** 108-67-8
SPID(S): Tox21_201452
M4ID: 12480800

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

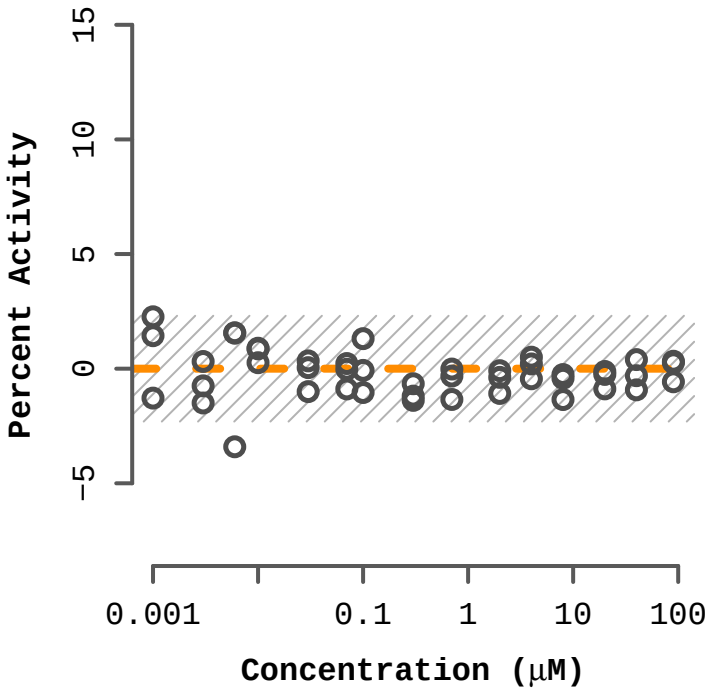
NAME: 2,4,6-Trichloro-s-triazine
CHID: 26799 **CASRN:** 108-77-0
SPID(S): Tox21_303286
M4ID: 12475847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.999 **MAX_MED:** 0.196 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

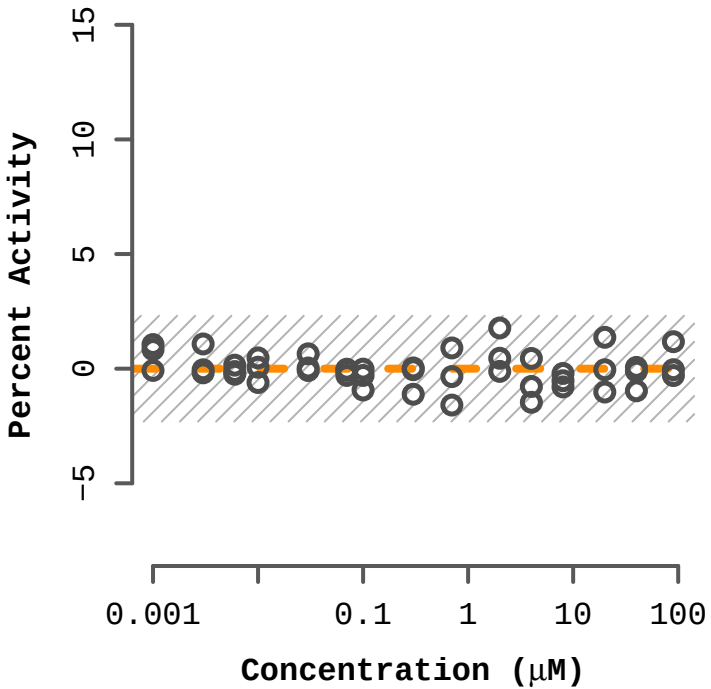
NAME: 2,4,6-Trichloro-s-triazine
CHID: 26799 **CASRN:** 108-77-0
SPID(S): Tox21_202449
M4ID: 12479803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

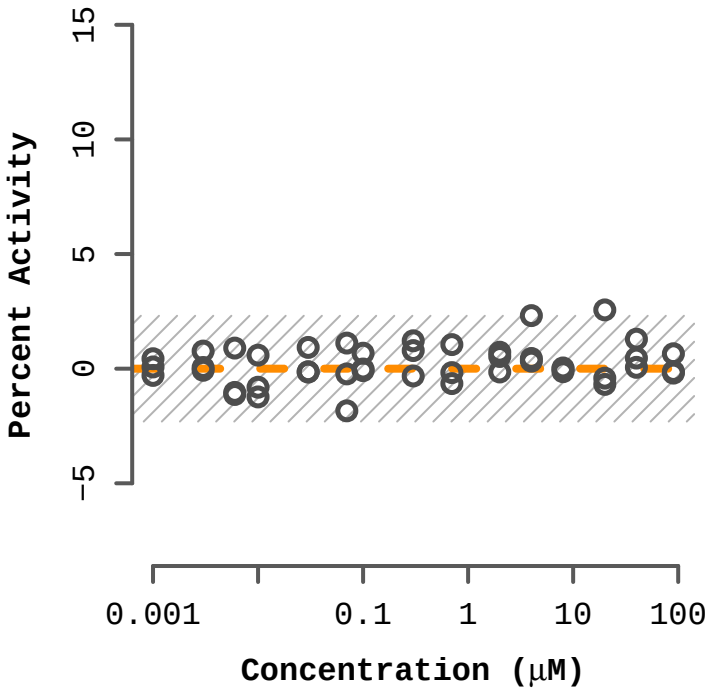
NAME: 2,6-Dimethyl-4-heptanol
CHID: 26802 **CASRN:** 108-82-7
SPID(S): Tox21_202737
M4ID: 12479515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.704 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

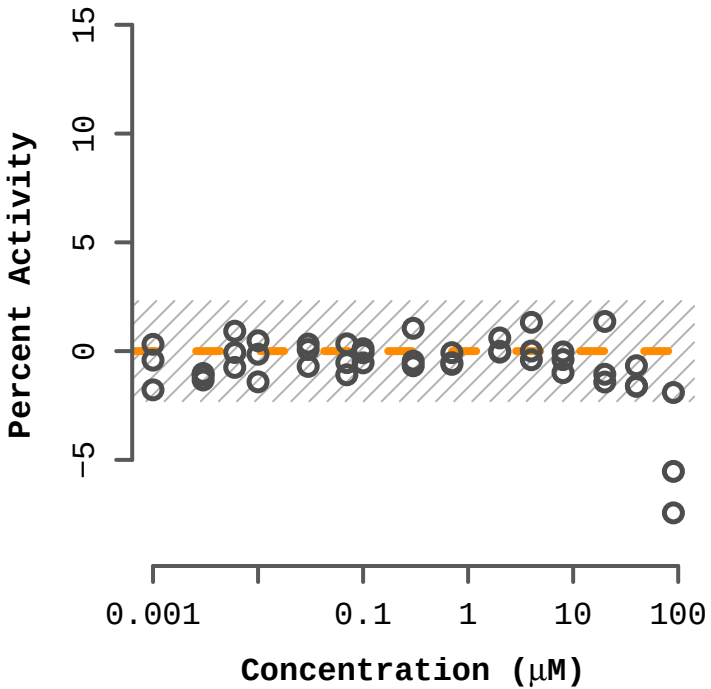
NAME: Benzenethiol
CHID: 26811 **CASRN:** 108-98-5
SPID(S): Tox21_303257
M4ID: 12475876

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.791 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

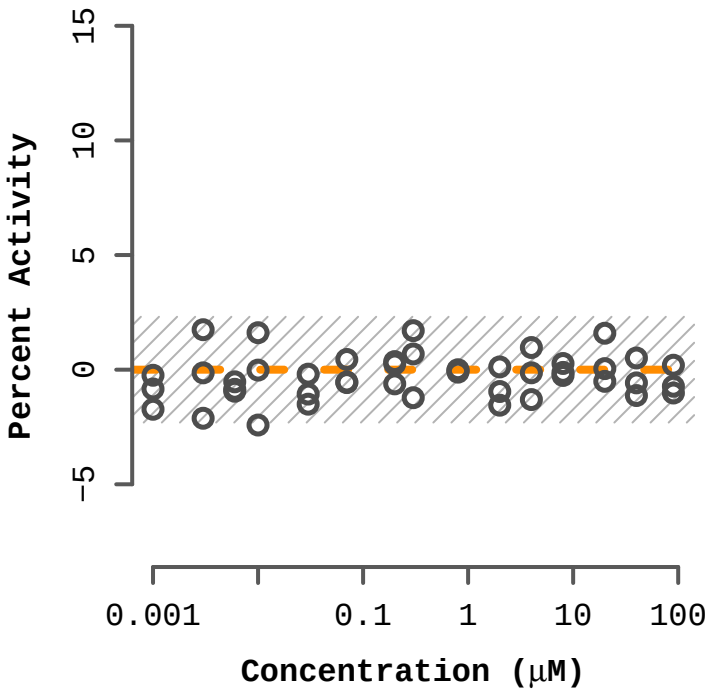
NAME: Benzenethiol
CHID: 26811 **CASRN:** 108-98-5
SPID(S): Tox21_201577
M4ID: 12480675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 0.312 **MAX_MED:** 0.0744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

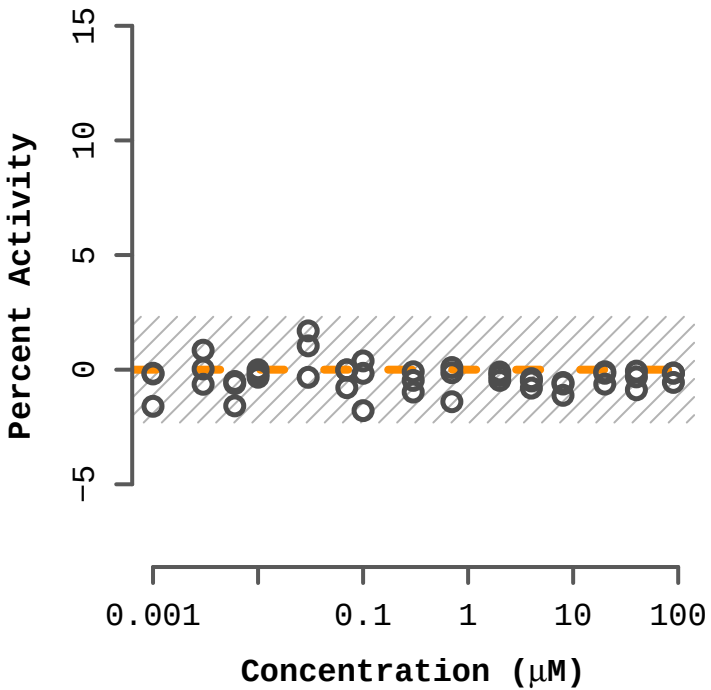
NAME: 1-Butanethiol
CHID: 26824 **CASRN:** 109-79-5
SPID(S): Tox21_200811
M4ID: 12481441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.39 **MAX_MED:** 0.687 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

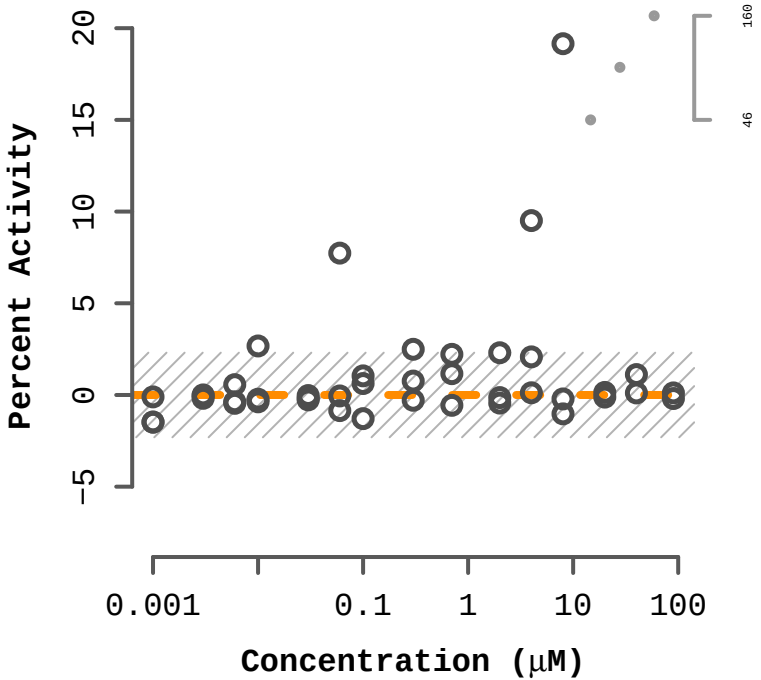
NAME: 2,5-Dimethylhexane-2,5-diol
CHID: 26830 **CASRN:** 110-03-2
SPID(S): Tox21_200281
M4ID: 12481971

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.8 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

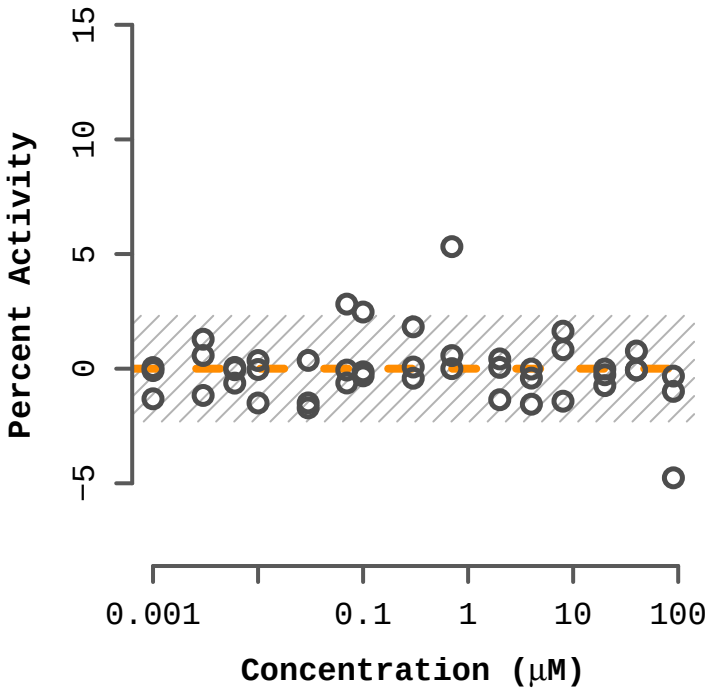
NAME: Isobutyl acetate
CHID: 26837 CASRN: 110-19-0
SPID(S): Tox21_201735
M4ID: 12480517 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.89	NA	NA
PROB:	1	NA	NA
RMSE:	30	NA	NA

MAX_MEAN: 54.5 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

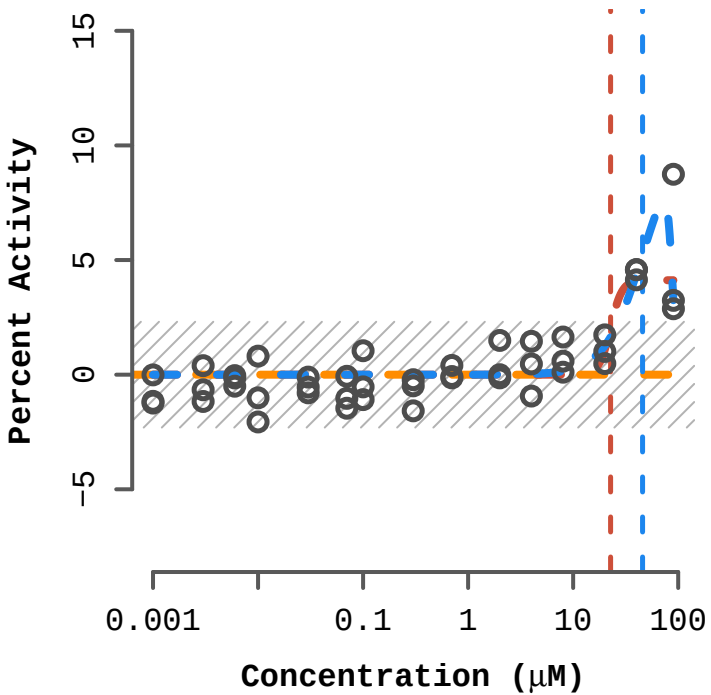
NAME: Isopropyl tetradecanoic acid
CHID: 26838 **CASRN:** 110-27-0
SPID(S): Tox21_303171
M4ID: 12475962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 0.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isopropyl tetradecanoic acid
CHID: 26838 CASRN: 110-27-0
SPID(S): Tox21_202065
M4ID: 12480187

HILL MODEL (in red):

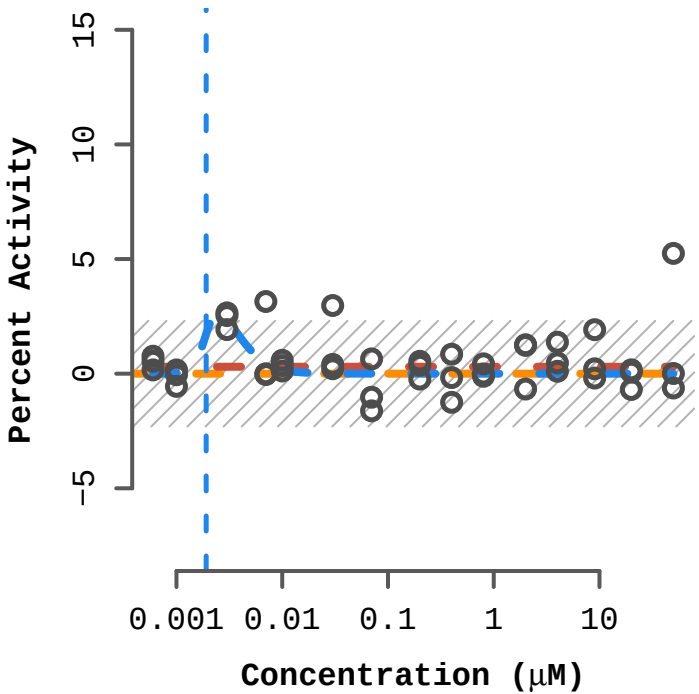
	tp	ga	gw
val:	4.12	1.36	8
sd:	0.43	0.0445	5.05

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.66	2.41	1.94	18
sd:	12.6	0.403	1.35	0.00953	42.2

	CNST	HILL	GNLS
AIC:	176.91	136.54	136.81
PROB:	0	0.53	0.47
RMSE:	2.04	1.1	1.15

MAX_MEAN: 4.95 MAX_MED: 4.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isopropyl tetradecanoic acid
CHID: 26838 **CASRN:** 110-27-0
SPID(S): Tox21_112080_1
M4ID: 12483332

HILL MODEL (in red):

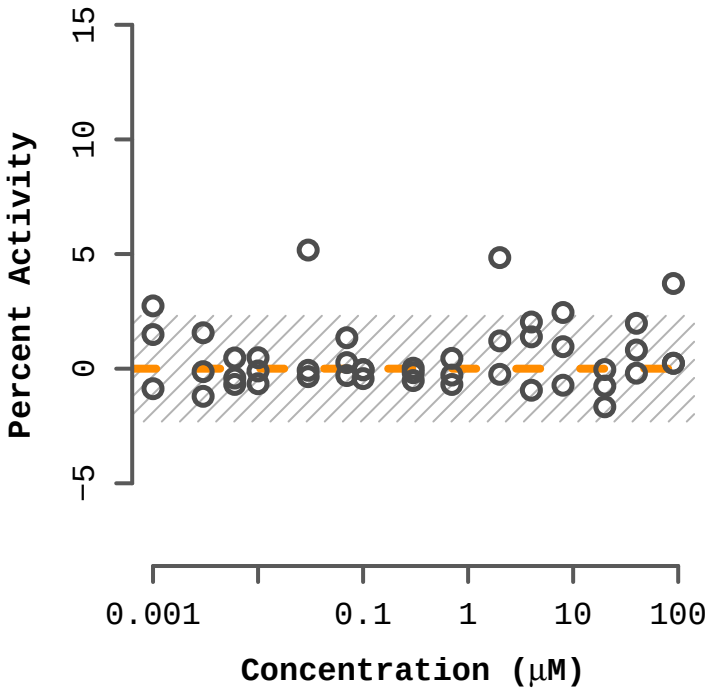
	tp	ga	gw
val:	0.301	−4.9	4.06
sd:	0.139	1630	4140

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.15	−2.72	7.99	−2.47	2.83
sd:	7.7	0.4	12.1	0.625	3.17

	CNST	HILL	GNLS
AIC:	144.71	145.9	135.57
PROB:	0.01	0.01	0.98
RMSE:	1.36	1.27	1.19

MAX_MEAN: 2.37 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

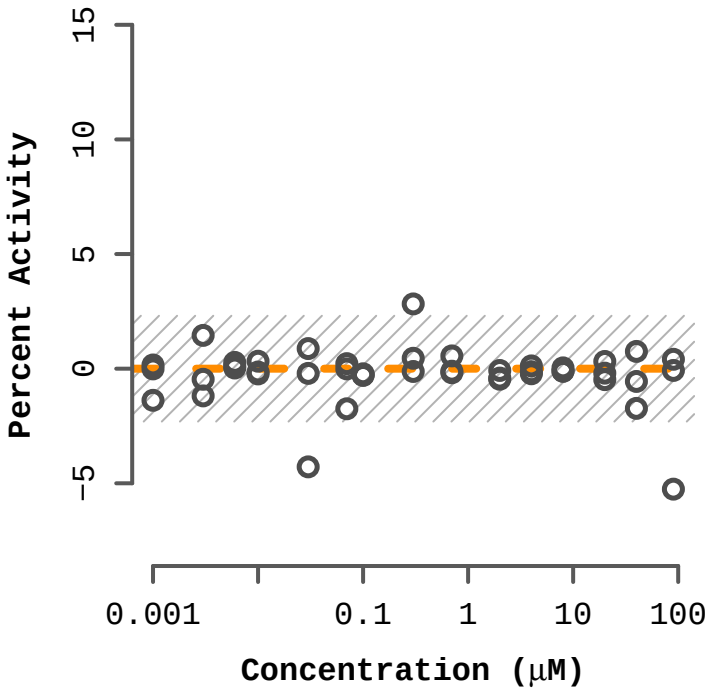
NAME: Dihexyl hexanedioate
CHID: 26841 **CASRN:** 110-33-8
SPID(S): Tox21_301005
M4ID: 12478128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

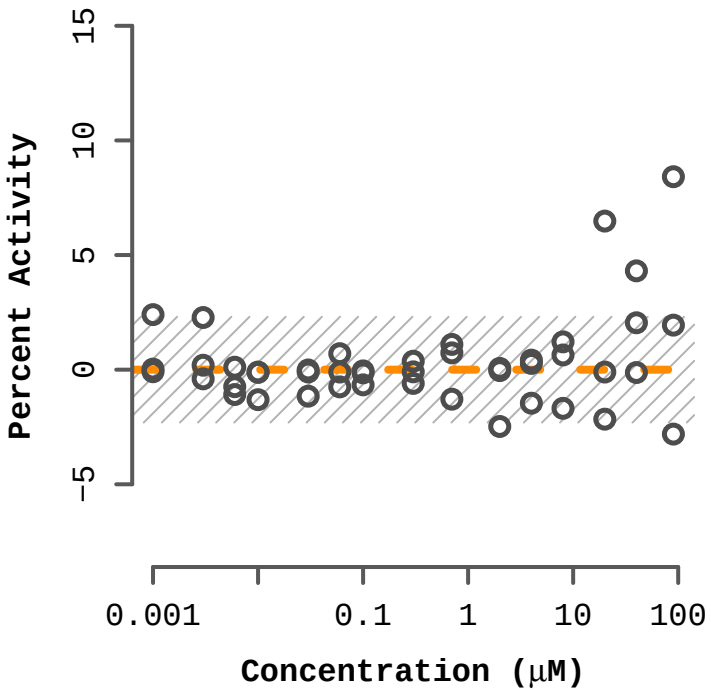
NAME: Methyl decanoate
CHID: 26842 **CASRN:** 110-42-9
SPID(S): Tox21_303060
M4ID: 12476073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.456 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

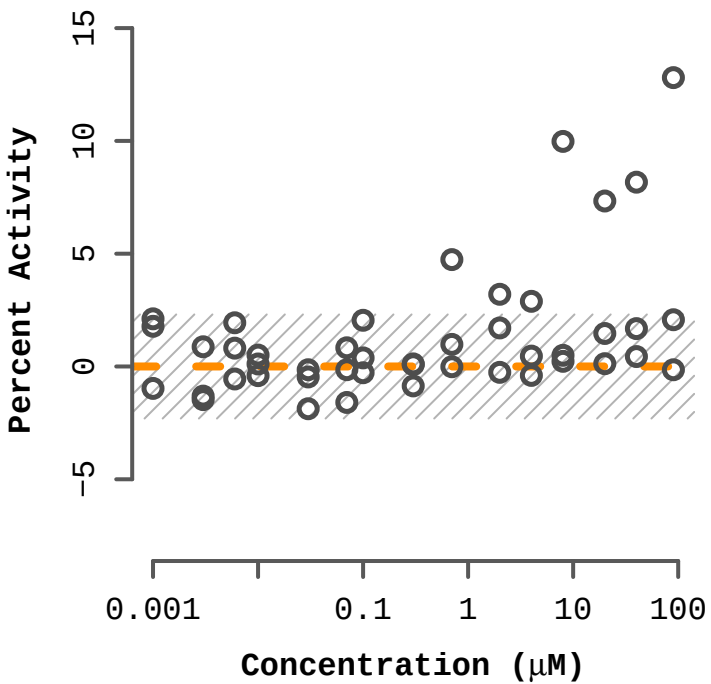
NAME: Methyl decanoate
CHID: 26842 **CASRN:** 110-42-9
SPID(S): Tox21_201757
M4ID: 12480495

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 2.52 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

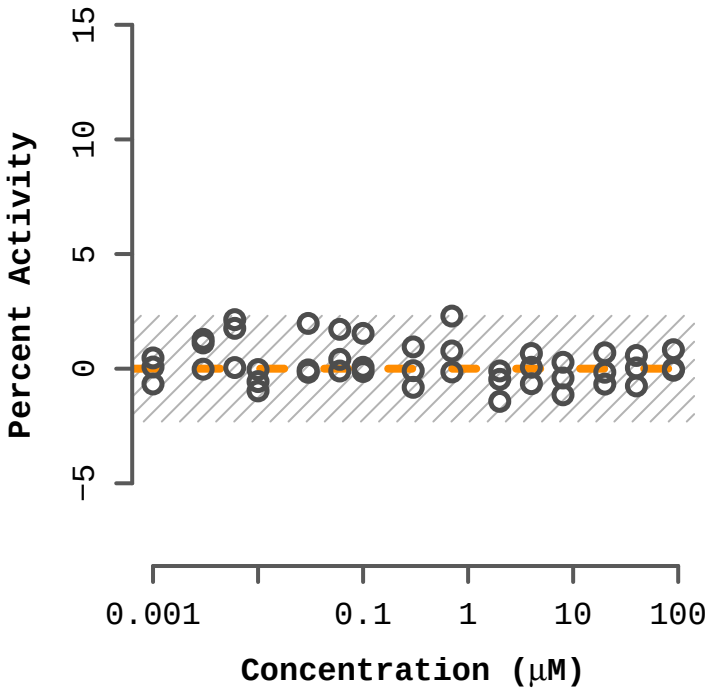
NAME: 2-Butene-1,4-diol
CHID: 26849 CASRN: 110-64-5
SPID(S): Tox21_202430
M4ID: 12479822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.26	NA	NA
PROB:	1	NA	NA
RMSE:	3.23	NA	NA

MAX_MEAN: 4.91 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

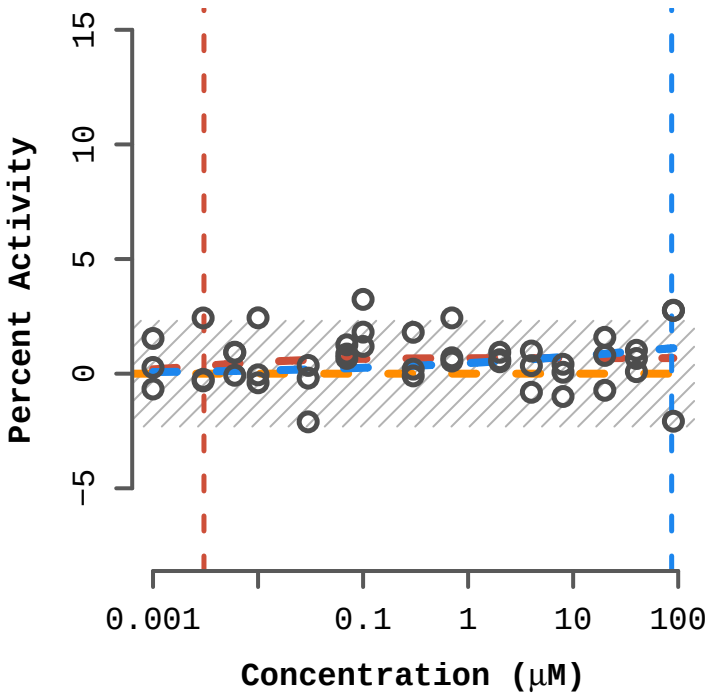
NAME: 3-Methoxypropionitrile
CHID: 26851 **CASRN:** 110-67-8
SPID(S): Tox21_200210
M4ID: 12482042

HILL MODEL: Not applicable.

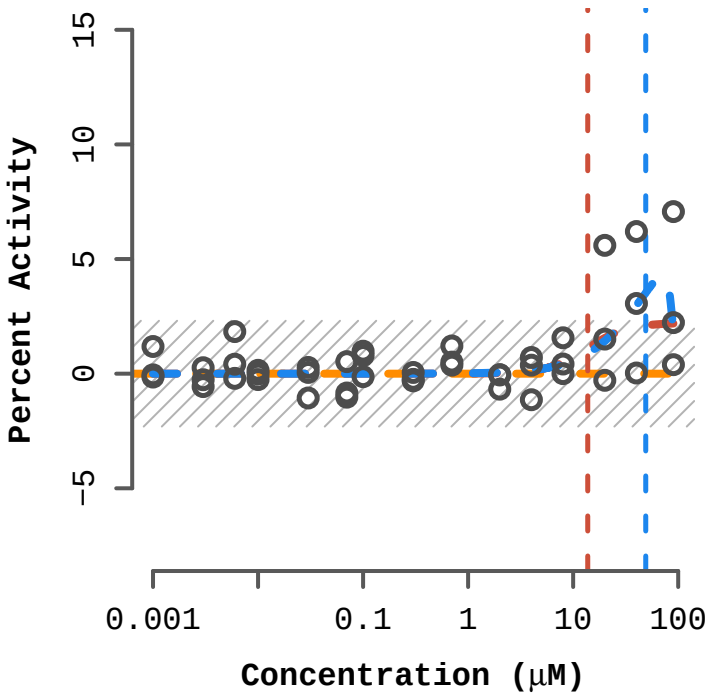
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.76 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1,1'-Oxybis-2-propanol
CHID:    26863   CASRN: 110-98-5
SPID(S): Tox21_303094
M4ID:    12476039

HILL MODEL (in red):
      tp       ga       gw
val:  0.679    -2.51    0.856
sd:   0.204    1.37     1.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.22     1.94     0.3      3.49     5.05
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  155.84      149.05      156.79
PROB: 0.03        0.95        0.02
RMSE: 1.32        1.16        1.22

MAX_MEAN: 2.08      MAX_MED: 2.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1'−Oxybis−2−propanol
CHID: 26863 **CASRN:** 110−98−5
SPID(S): Tox21_201485
M4ID: 12480767

HILL MODEL (in red):

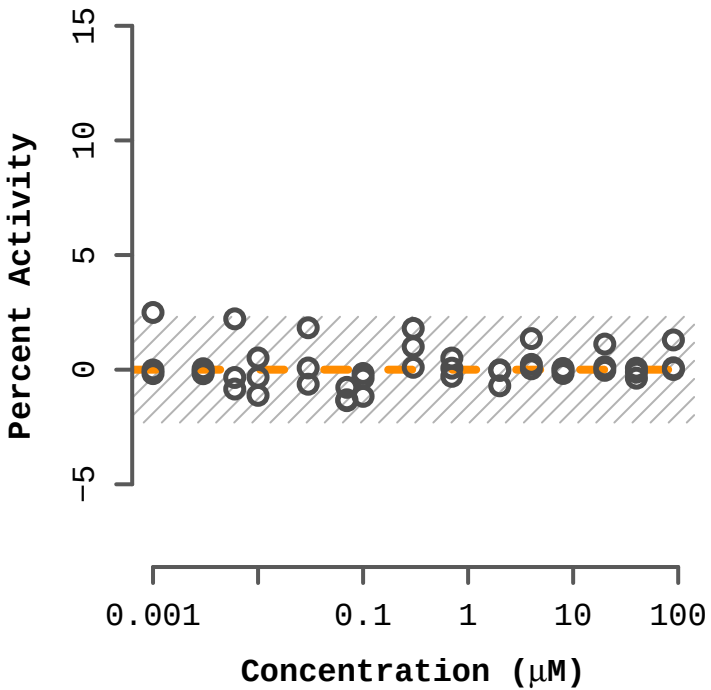
	tp	ga	gw
val:	2.22	1.14	2.3
sd:	0.78	0.266	1.65

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.06	1.69	1.53	1.94	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.83	148.53	151.14
PROB:	0.02	0.77	0.21
RMSE:	1.85	1.38	1.38

MAX_MEAN: 3.23 **MAX_MED:** 3.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

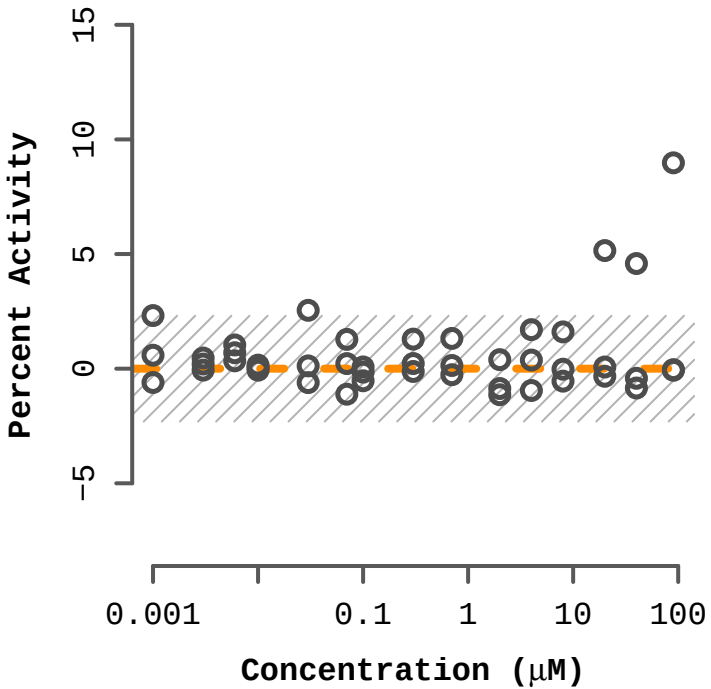
NAME: Methyl octanoate
CHID: 26864 **CASRN:** 111-11-5
SPID(S): Tox21_300557
M4ID: 12478576

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.968 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

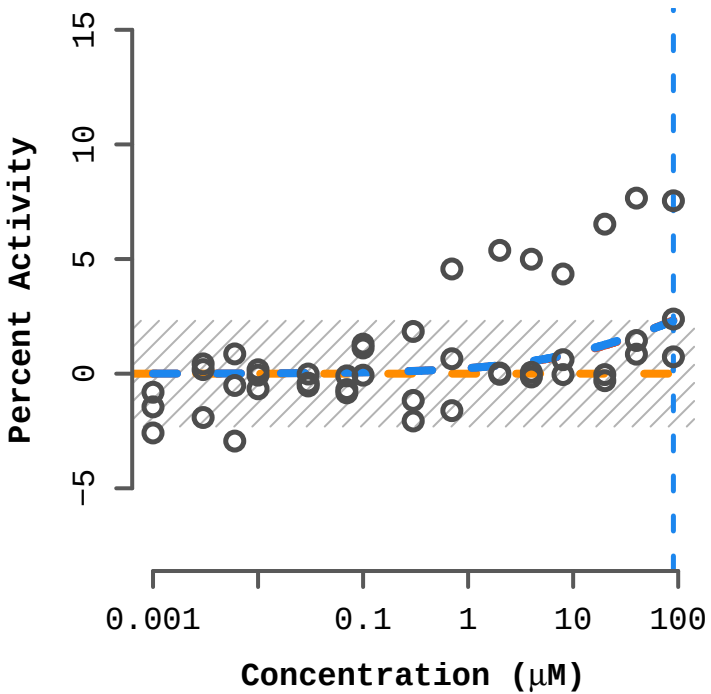
NAME: Methyl octanoate
CHID: 26864 **CASRN:** 111-11-5
SPID(S): Tox21_201470
M4ID: 12480782

HILL MODEL: Not applicable.

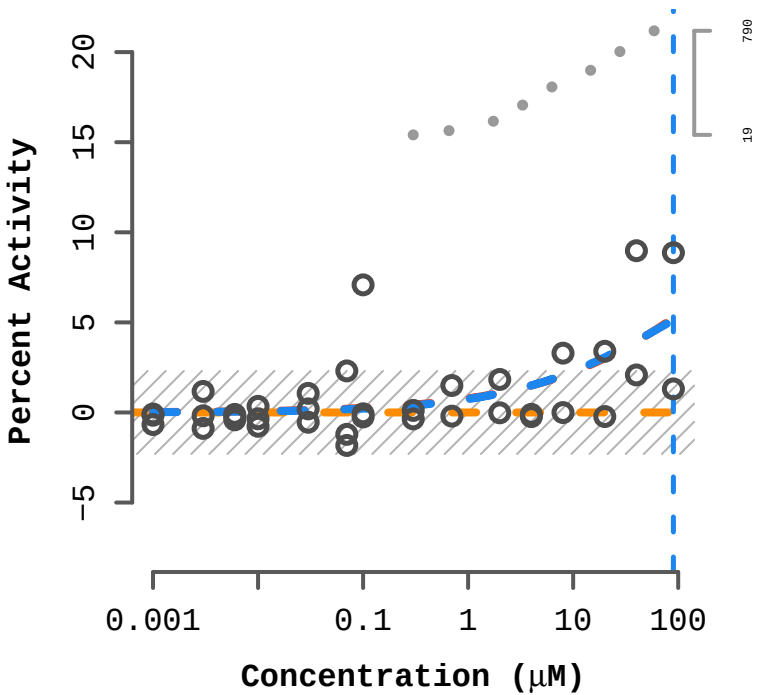
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 2.96 **MAX_MED:** 0.697 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Decanedioic acid
CHID:    26867   CASRN: 111-20-6
SPID(S): Tox21_303263
M4ID:    12475870

HILL MODEL (in red):
      tp       ga       gw
val:  5.92     2.26     0.606
sd:   29.6     5.82     0.668

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.58     1.95     0.642    3.93     3.76
sd:   14.5     3.84     0.639    4050     7680

      CNST        HILL        GNLS
AIC:  203.7       200.57      204.57
PROB: 0.16        0.74        0.1
RMSE: 2.59        2.2         2.2

MAX_MEAN: 3.55      MAX_MED: 2.38      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Decanedioic acid
CHID: 26867 CASRN: 111-20-6
SPID(S): Tox21_201778
M4ID: 12480474 BRK

HILL MODEL (in red):

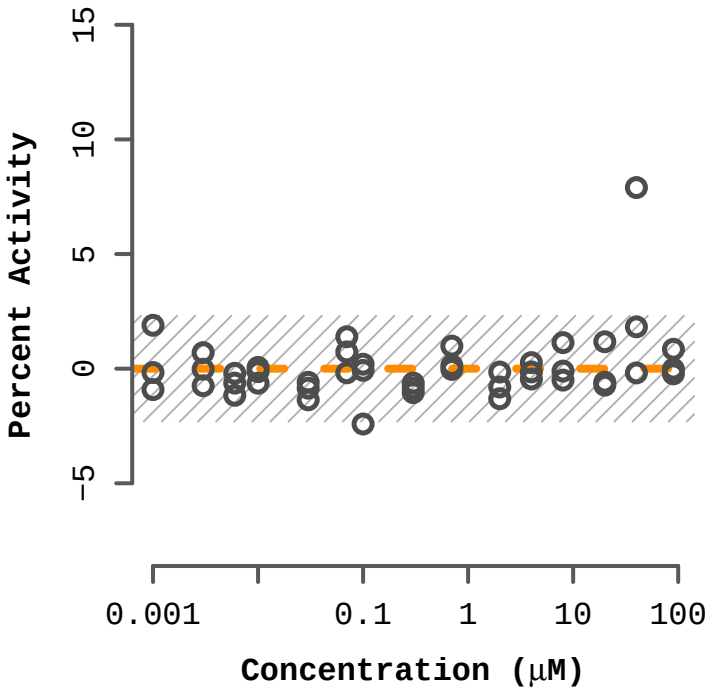
	tp	ga	gw
val:	14.7	2.45	0.51
sd:	58.7	5.41	0.706

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.3	1.95	0.568	3.01	5.15
sd:	26.7	3.5	0.866	695	3080

	CNST	HILL	GNLS
AIC:	486.33	488.24	492.28
PROB:	0.7	0.27	0.04
RMSE:	182.93	181.77	181.77

MAX_MEAN: 268 MAX_MED: 8.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

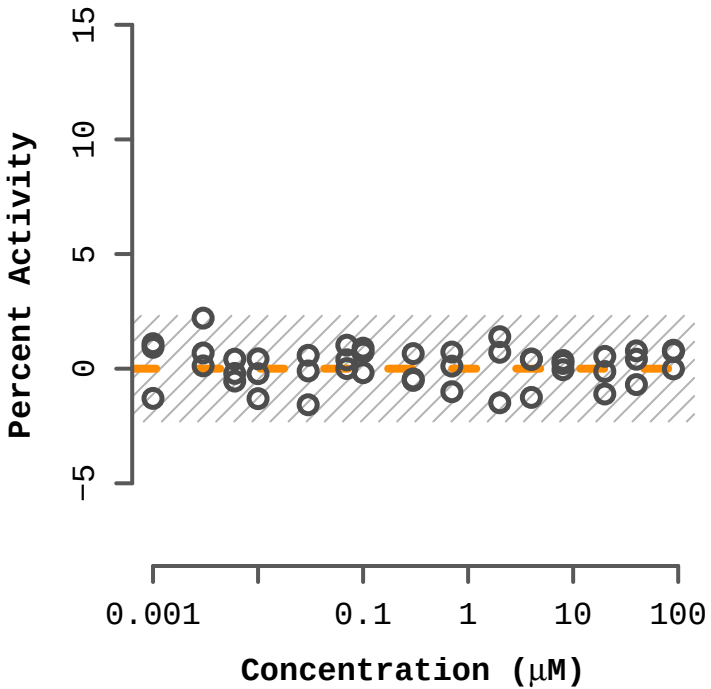
NAME: Butyl isocyanate
CHID: 26872 CASRN: 111-36-4
SPID(S): Tox21_200437
M4ID: 12481815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 3.18 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

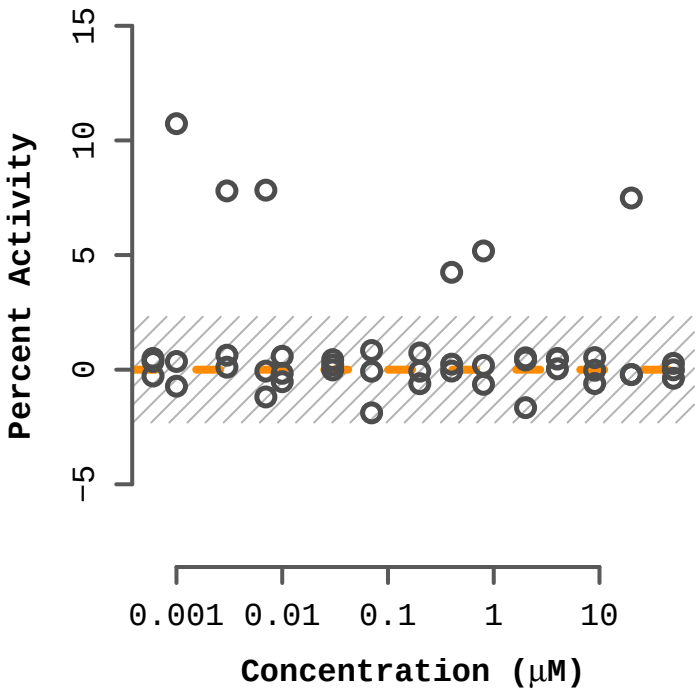
NAME: 2,2'−Thiobisethanol
CHID: 26878 **CASRN:** 111−48−8
SPID(S): Tox21_200827
M4ID: 12481425

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

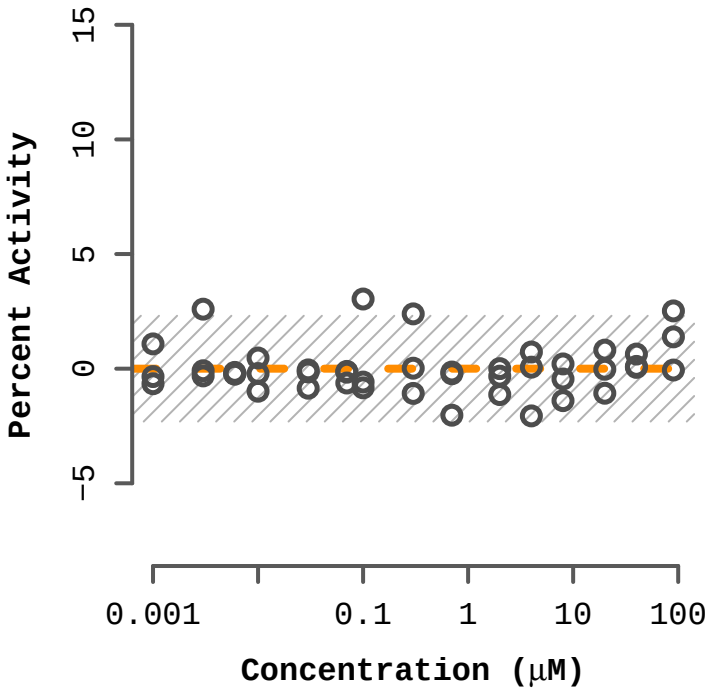
NAME: 2,2'−Thiobisethanol
CHID: 26878 **CASRN:** 111−48−8
SPID(S): Tox21_111413_1
M4ID: 12483704

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.8	NA	NA

MAX_MEAN: 3.46 **MAX_MED:** 0.633 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

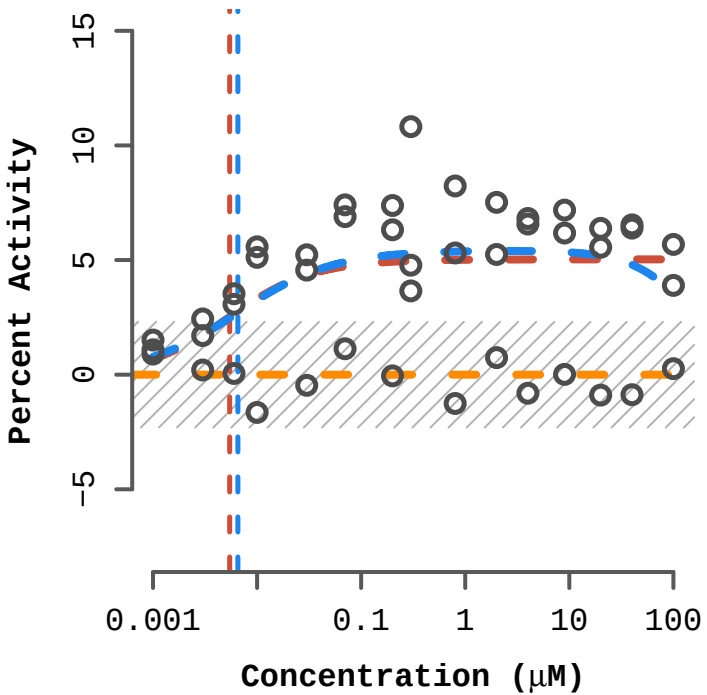
NAME: Hexamethyleneimine
CHID: 26879 **CASRN:** 111-49-9
SPID(S): Tox21_303304
M4ID: 12475829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexamethyleneimine
CHID: 26879 **CASRN:** 111-49-9
SPID(S): Tox21_201482
M4ID: 12480770

HILL MODEL (in red):

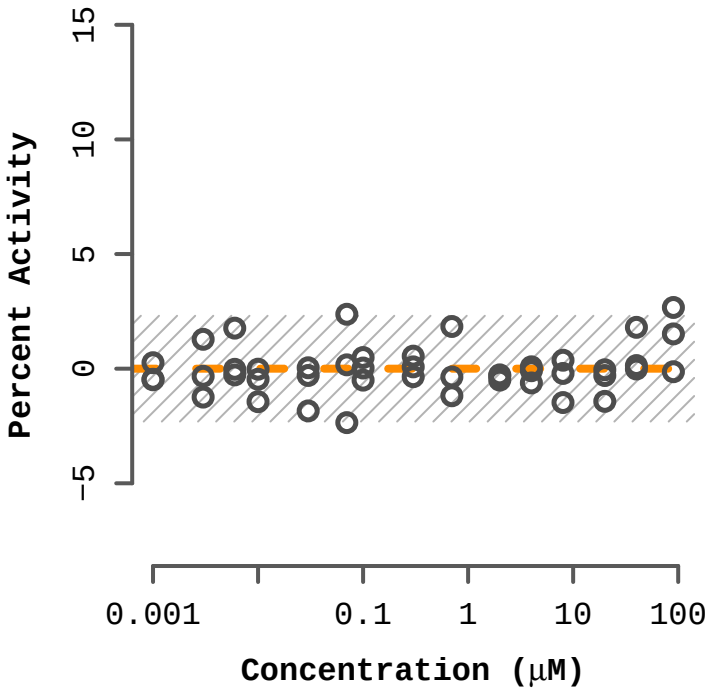
	tp	ga	gw
val:	5.03	−2.26	1.08
sd:	0.61	0.298	0.751

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.42	−2.18	0.951	2.19	1.52
sd:	1.16	0.377	0.716	0.961	6.6

	CNST	HILL	GNLS
AIC:	277.48	236.78	239.65
PROB:	0	0.81	0.19
RMSE:	4.86	3.01	3

MAX_MEAN: 6.42 **MAX_MED:** 6.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

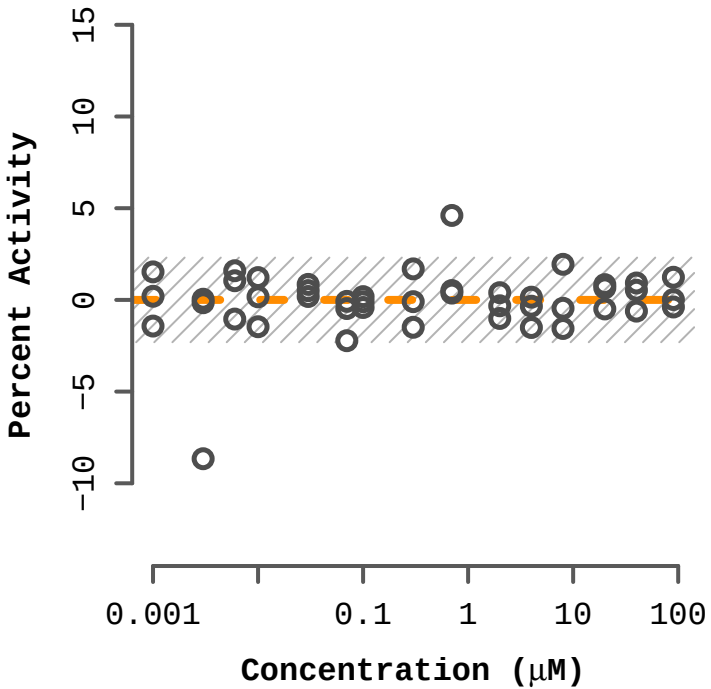
NAME: 1,2−Ethanediol diacetate
CHID: 26880 **CASRN:** 111−55−7
SPID(S): Tox21_303428
M4ID: 12475711

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

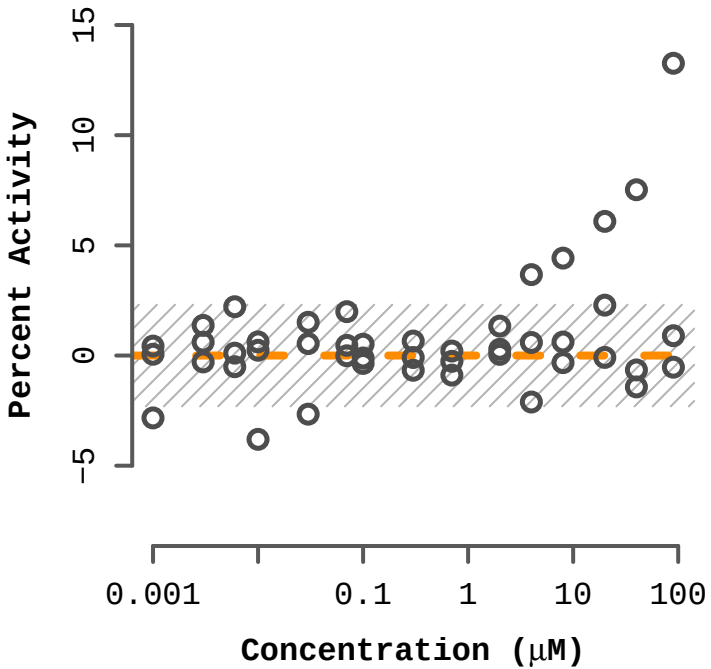
NAME: 1,2-Ethanediol diacetate
CHID: 26880 CASRN: 111-55-7
SPID(S): Tox21_202083
M4ID: 12480169

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 1.83 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

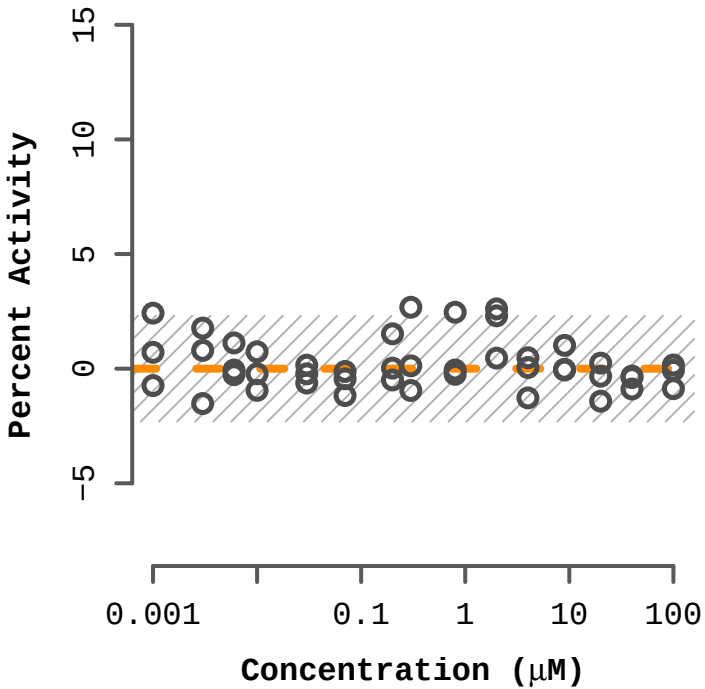
NAME: Octane
CHID: 26882 **CASRN:** 111-65-9
SPID(S): Tox21_202452
M4ID: 12479800

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.85	NA	NA

MAX_MEAN: 4.55 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

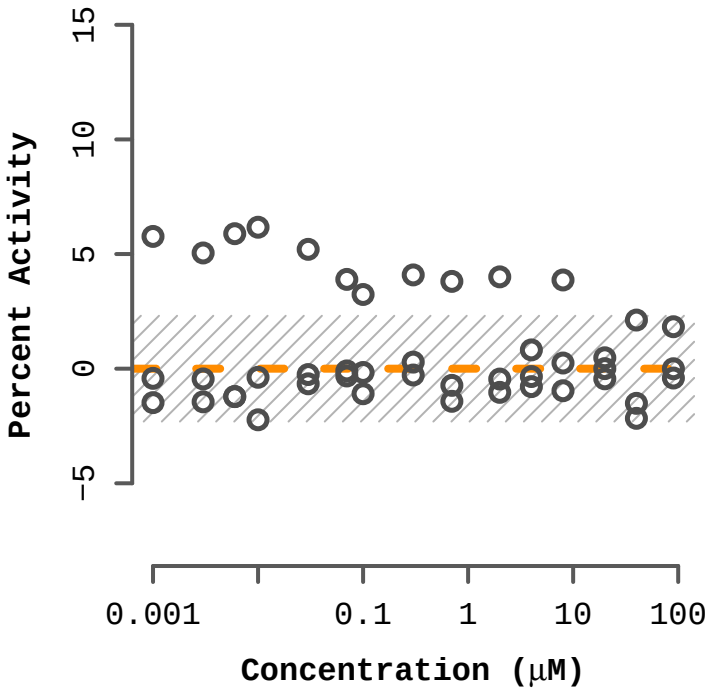
NAME: 1,5-Cyclooctadiene
CHID: 26888 **CASRN:** 111-78-4
SPID(S): Tox21_201015
M4ID: 12481237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

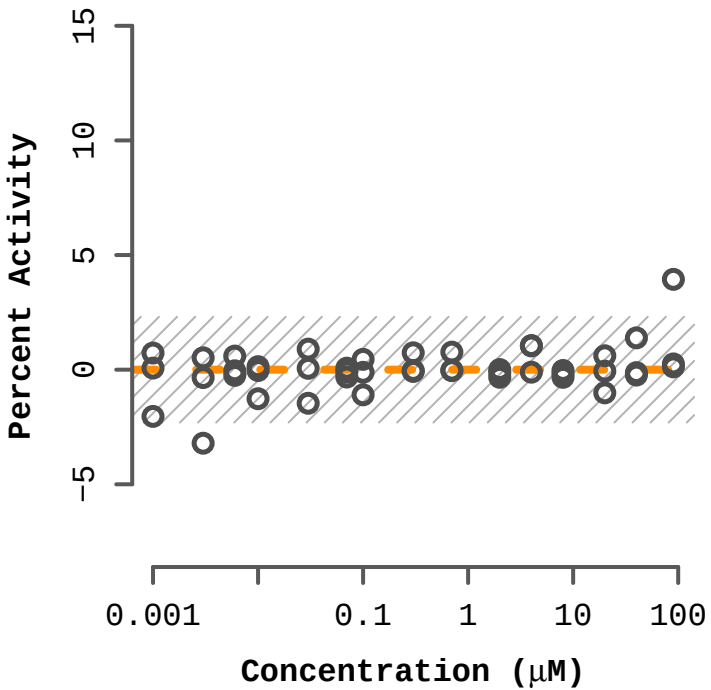
NAME: Methyl dodecanoate
CHID: 26889 **CASRN:** 111-82-0
SPID(S): Tox21_300555
M4ID: 12478578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.28	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.287 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

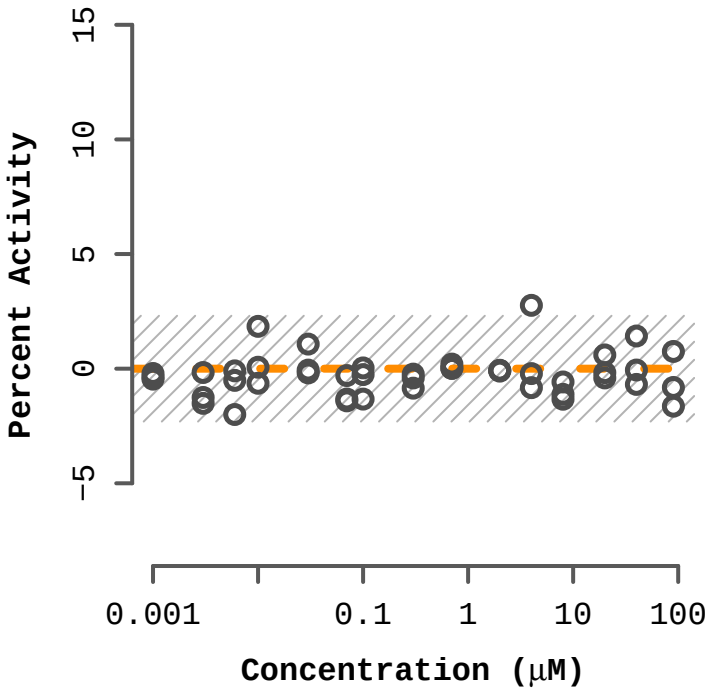
NAME: Methyl dodecanoate
CHID: 26889 CASRN: 111-82-0
SPID(S): Tox21_201488
M4ID: 12480764

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.44 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

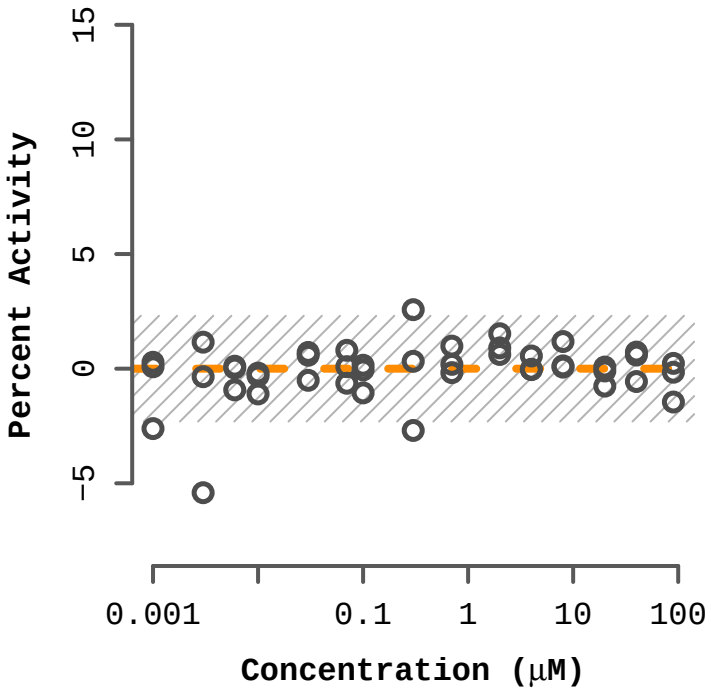
NAME: 1-Octanethiol
CHID: 26894 **CASRN:** 111-88-6
SPID(S): Tox21_201799
M4ID: 12480453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.575 **MAX_MED:** 0.0644 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

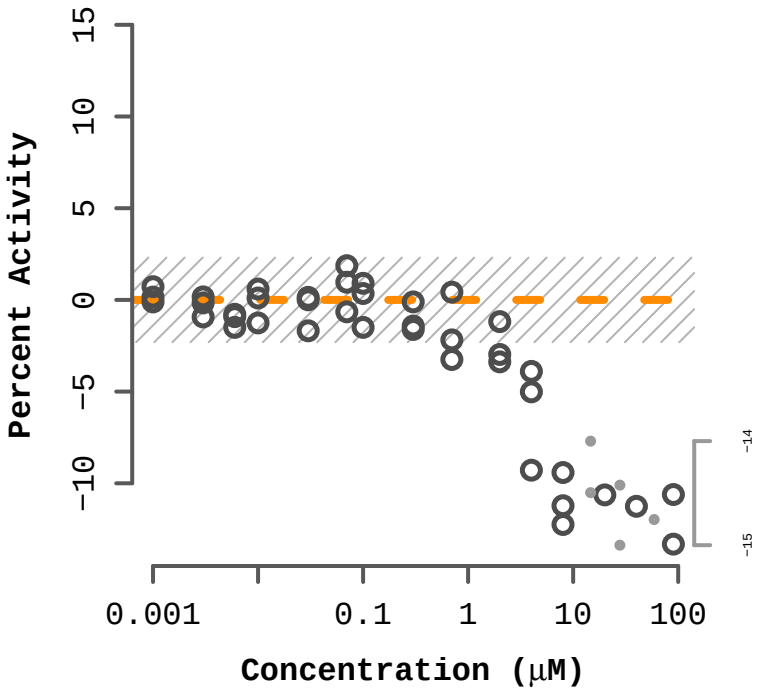
NAME: 3,3'−Thiodipropionitrile
CHID: 26899 **CASRN:** 111−97−7
SPID(S): Tox21_200226
M4ID: 12482026

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

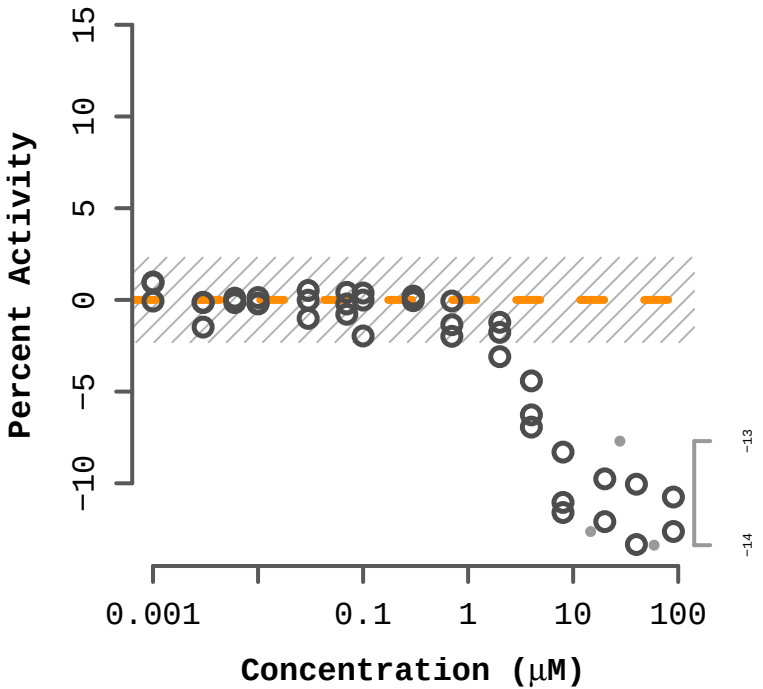
NAME: Dodecyltrimethylammonium chloride
CHID: 26900 **CASRN:** 112-00-5
SPID(S): Tox21_300356
M4ID: 12478776 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	299.96	NA	NA
PROB:	1	NA	NA
RMSE:	6.91	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

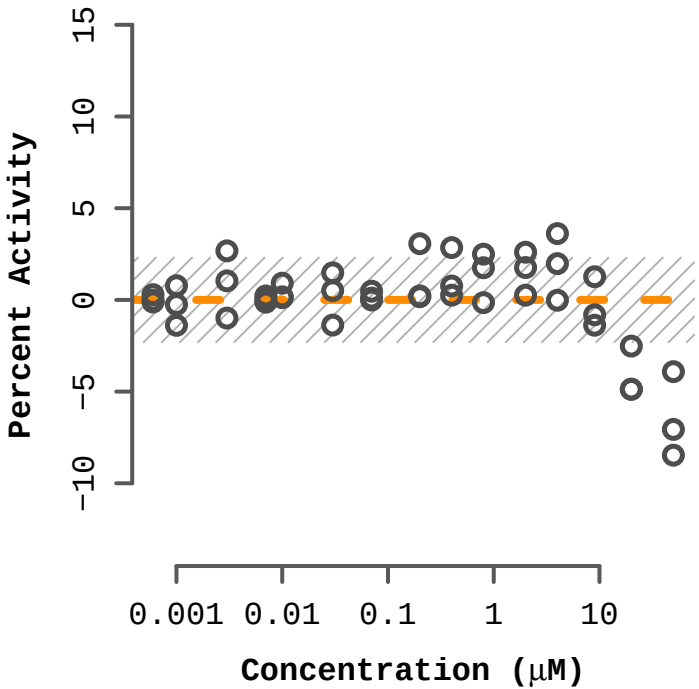
NAME: Dodecyltrimethylammonium chloride
CHID: 26900 CASRN: 112-00-5
SPID(S): Tox21_202101
M4ID: 12480151 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.34	NA	NA
PROB:	1	NA	NA
RMSE:	6.38	NA	NA

MAX_MEAN: 0.615 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

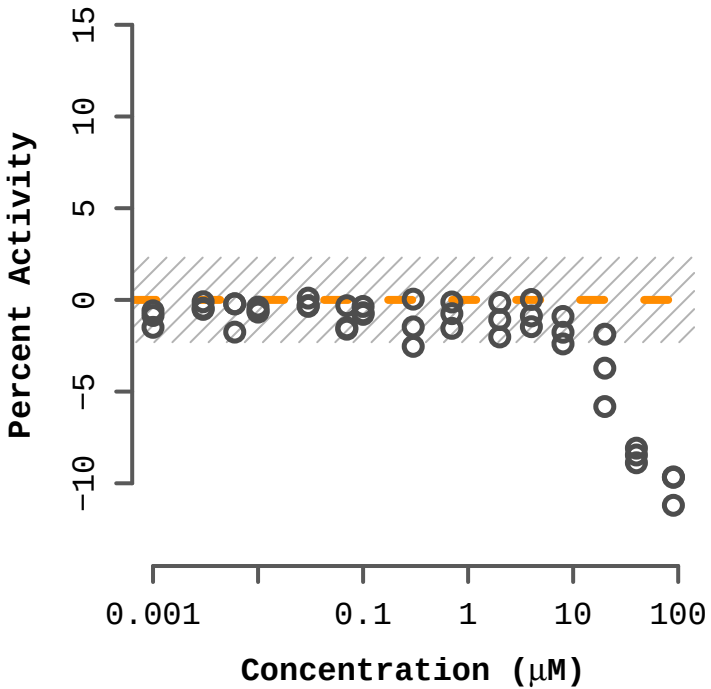
NAME: Hexadecyl trimethyl ammonium chloride
CHID: 26901 **CASRN:** 112-02-7
SPID(S): Tox21_202555
M4ID: 12479697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.83	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

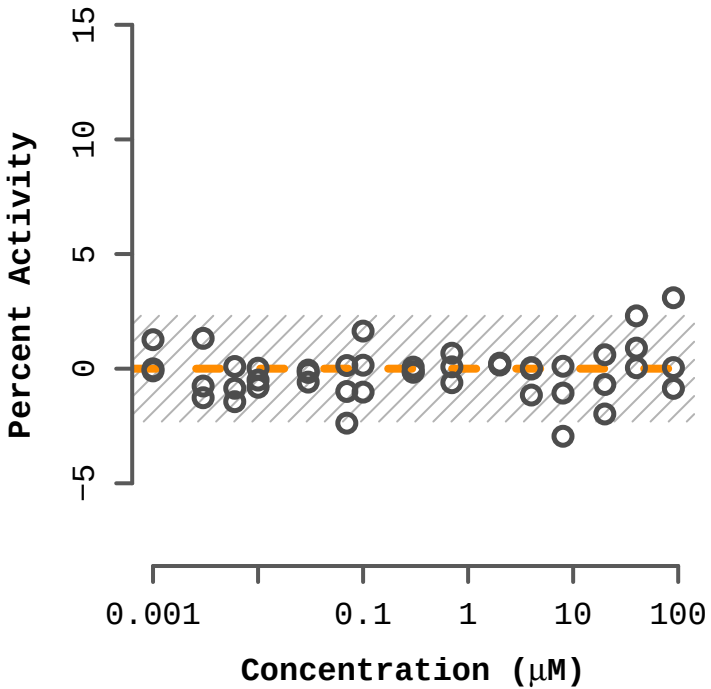
NAME: N,N,N−Trimethyloctadecan−1−aminium chloride
CHID: 26902 **CASRN:** 112−03−8
SPID(S): Tox21_200438
M4ID: 12481814

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.41	NA	NA
PROB:	1	NA	NA
RMSE:	3.72	NA	NA

MAX_MEAN: −0.187 **MAX_MED:** −0.219 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

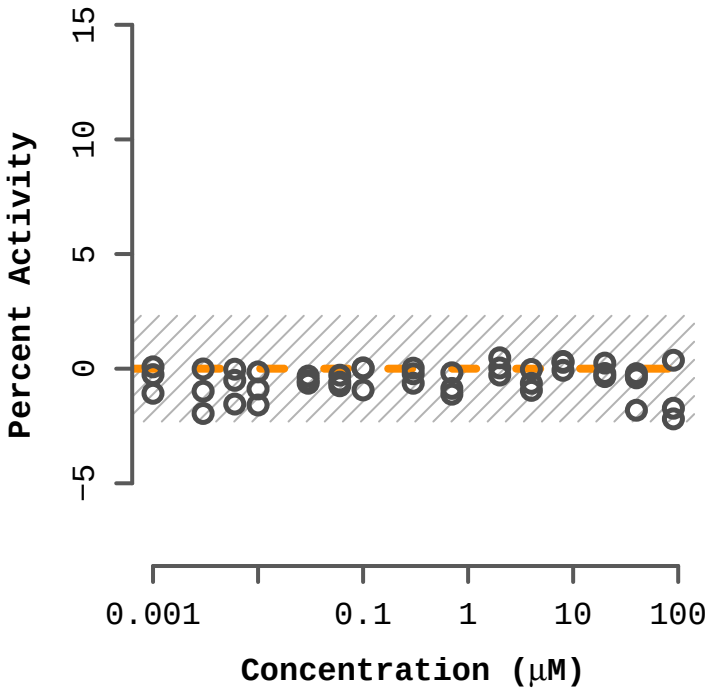
NAME: 2-Butoxyethyl acetate
CHID: 26904 CASRN: 112-07-2
SPID(S): Tox21_303230
M4ID: 12475903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.08 MAX_MED: 0.898 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

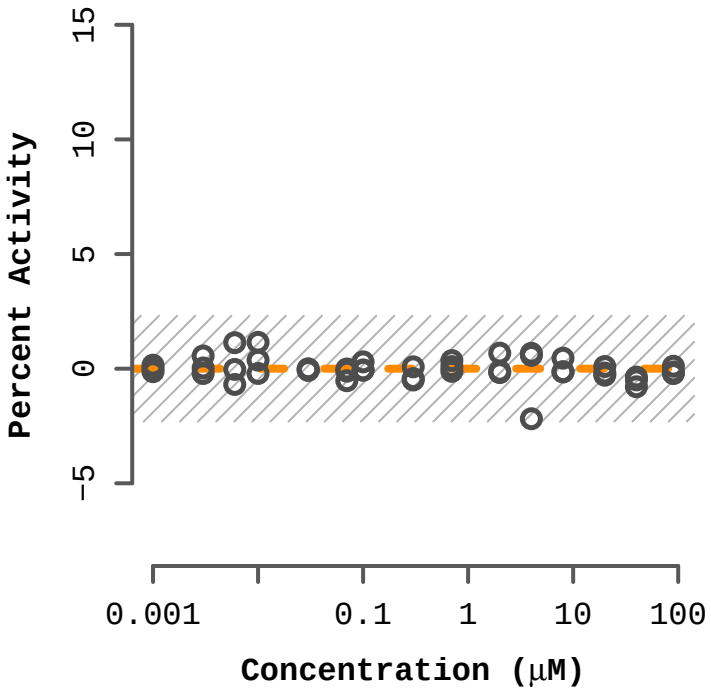
NAME: 2-Butoxyethyl acetate
CHID: 26904 **CASRN:** 112-07-2
SPID(S): Tox21_201583
M4ID: 12480669

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.174 **MAX_MED:** 0.277 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

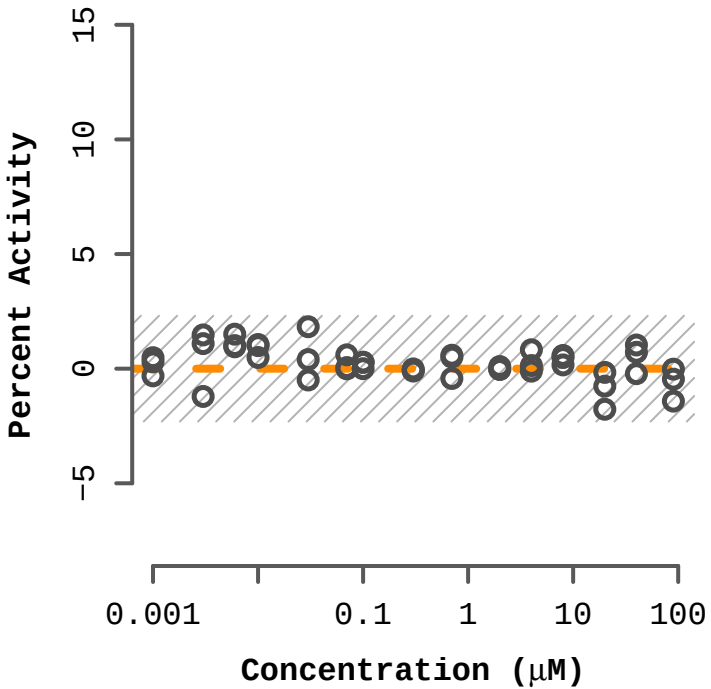
NAME: 2-(2-Ethoxyethoxy)ethyl acetate
CHID: 26905 CASRN: 112-15-2
SPID(S): Tox21_200843
M4ID: 12481409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	58.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.52	NA	NA

MAX_MEAN: 0.439 **MAX_MED:** 0.579 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

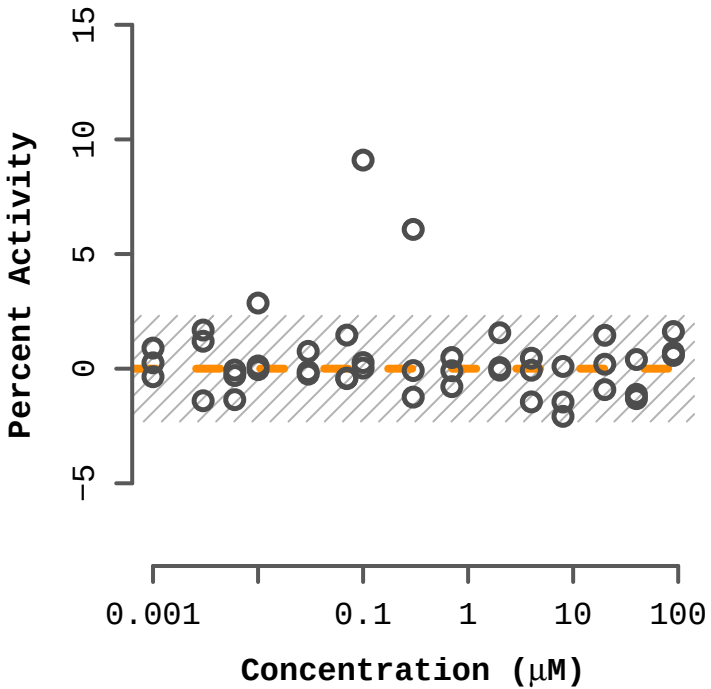
NAME: N,N−Dimethyldodecan−1−amine
CHID: 26906 **CASRN:** 112−18−5
SPID(S): Tox21_303073
M4ID: 12476060

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

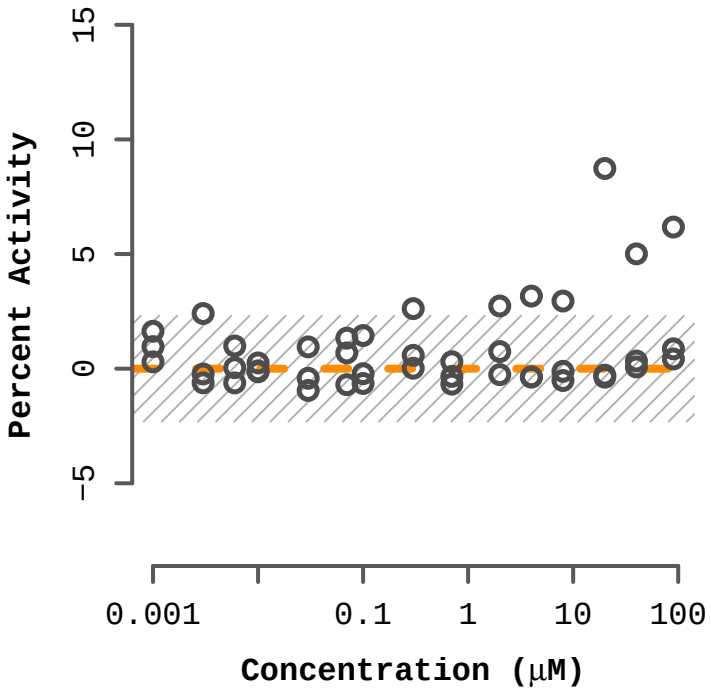
NAME: 2-(Hexyloxy)ethanol
CHID: 26908 **CASRN:** 112-25-4
SPID(S): Tox21_300545
M4ID: 12478587

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.91	NA	NA

MAX_MEAN: 3.13 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

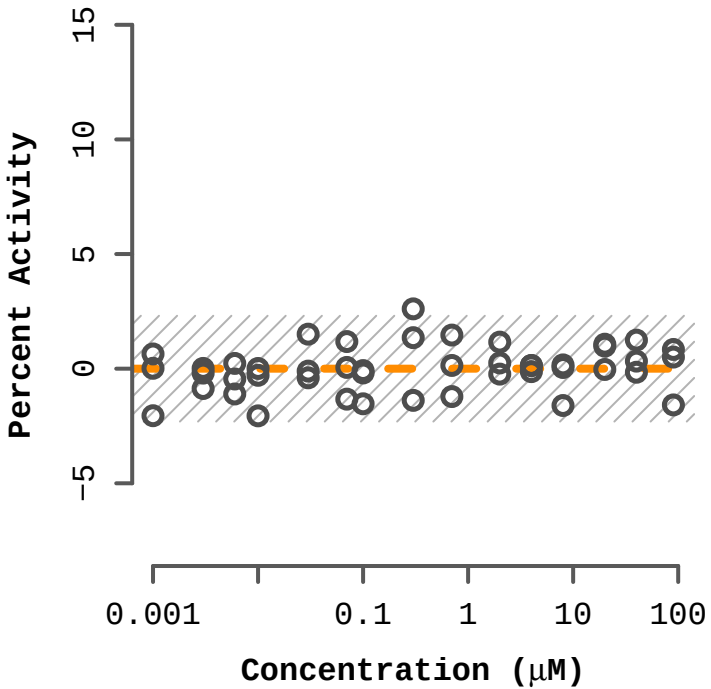
NAME: 2-(Hexyloxy)ethanol
CHID: 26908 **CASRN:** 112-25-4
SPID(S): Tox21_202105
M4ID: 12480147

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 2.69 **MAX_MED:** 0.963 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

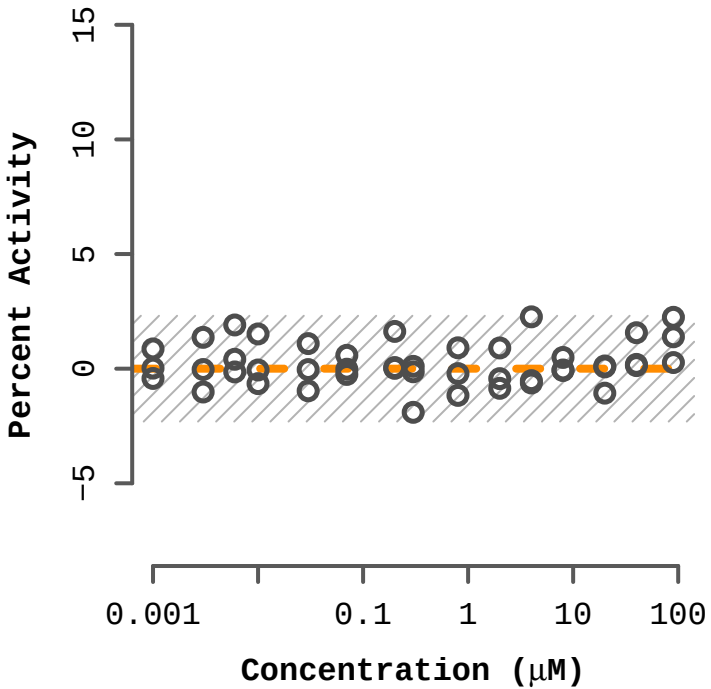
NAME: 2-[2-(2-Methoxyethoxy)ethoxy]ethanol
CHID: 26912 **CASRN:** 112-35-6
SPID(S): Tox21_303115
M4ID: 12476018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.76	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

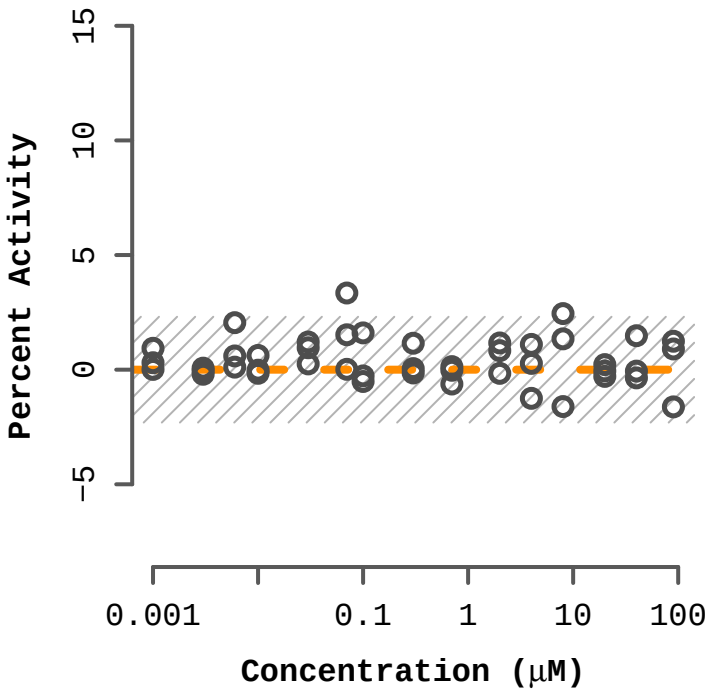
NAME: 2-[2-(2-Methoxyethoxy)ethoxy]ethanol
CHID: 26912 **CASRN:** 112-35-6
SPID(S): Tox21_201820
M4ID: 12480432

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

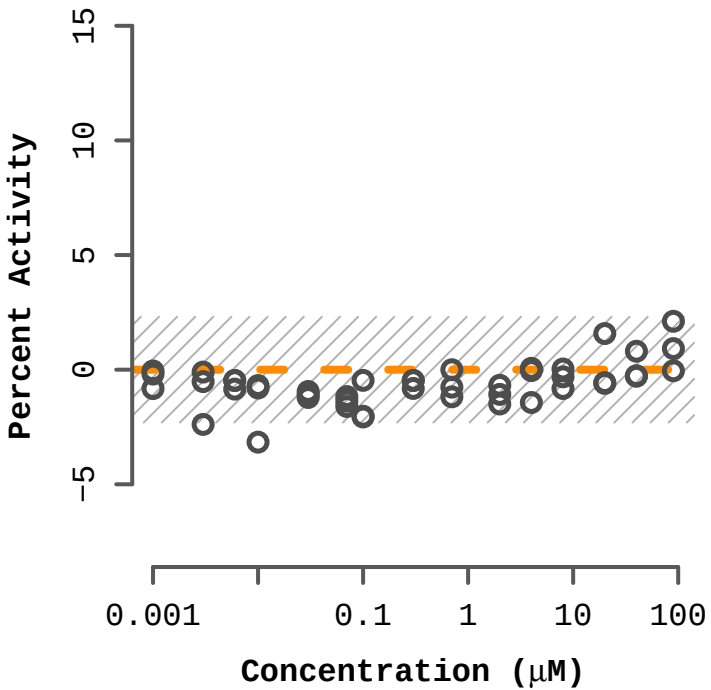
NAME: Dodecane
CHID: 26913 CASRN: 112-40-3
SPID(S): Tox21_303615
M4ID: 12475530

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.63 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

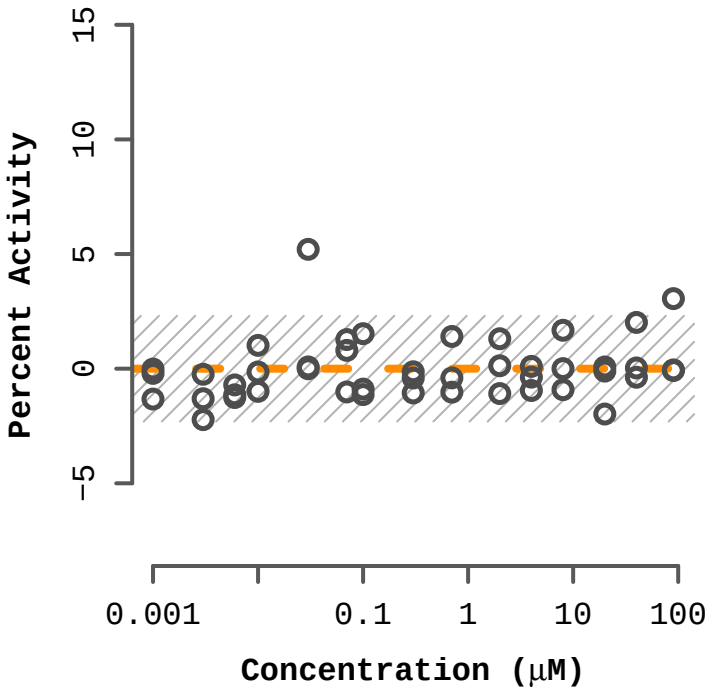
NAME: 1-Dodecene
CHID: 26914 **CASRN:** 112-41-4
SPID(S): Tox21_303303
M4ID: 12475830

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.995 **MAX_MED:** 0.921 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

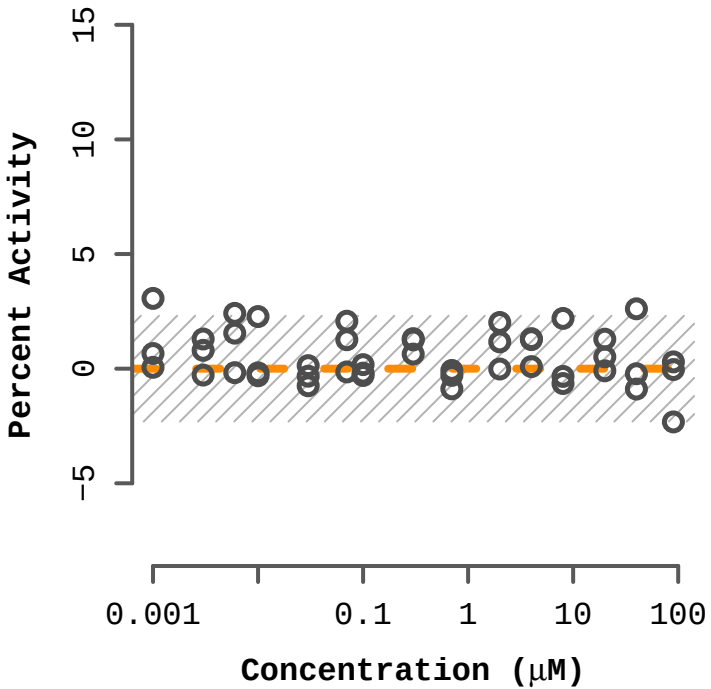
NAME: 1-Dodecene
CHID: 26914 **CASRN:** 112-41-4
SPID(S): Tox21_201382
M4ID: 12480870

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 0.799 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

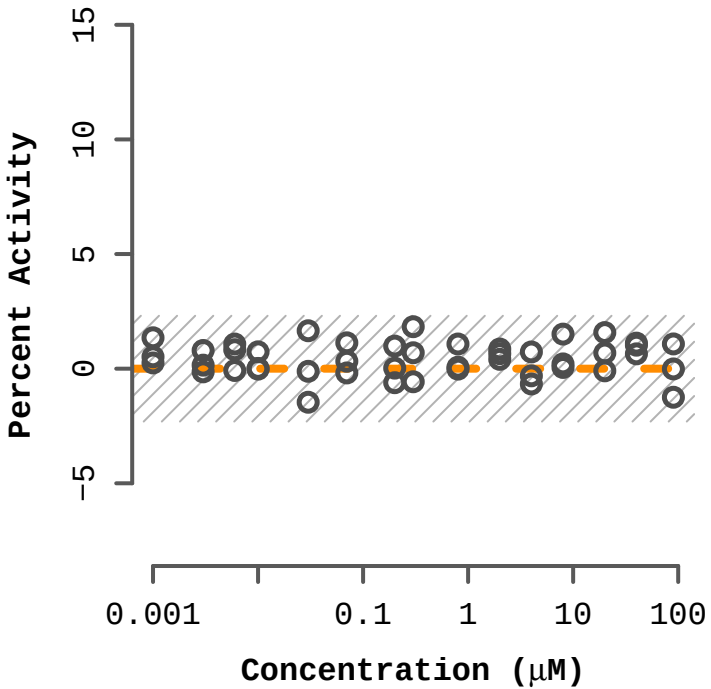
NAME: 1-Undecanol
CHID: 26915 **CASRN:** 112-42-5
SPID(S): Tox21_300548
M4ID: 12478584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

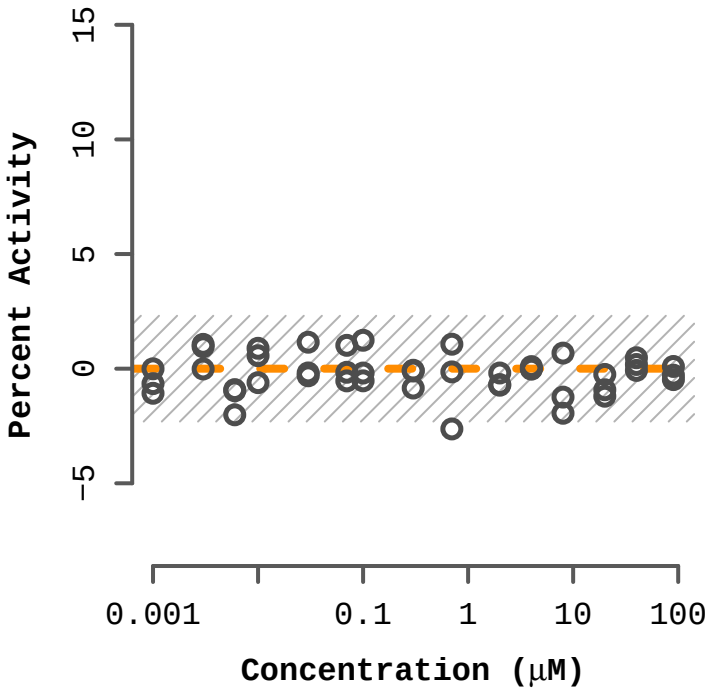
NAME: 1-Undecanol
CHID: 26915 **CASRN:** 112-42-5
SPID(S): Tox21_201585
M4ID: 12480667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

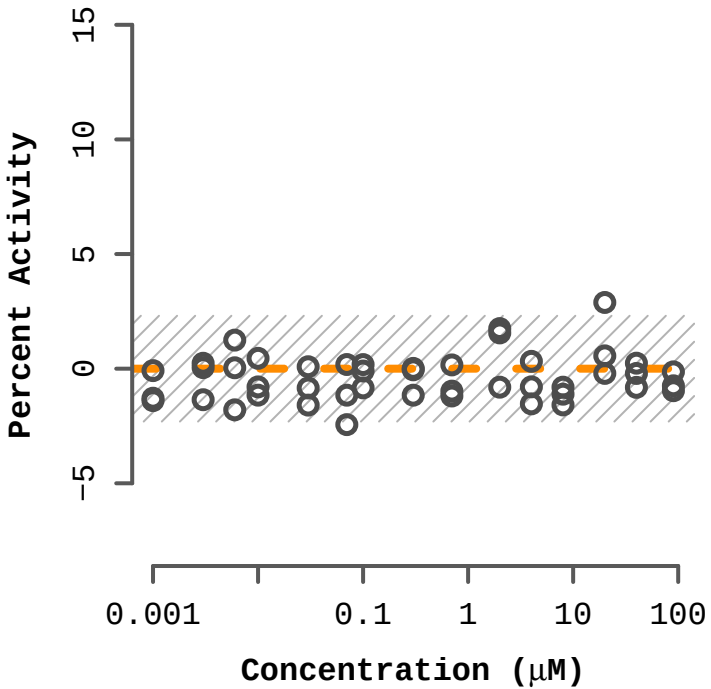
NAME: 1-Dodecanol
CHID: 26918 **CASRN:** 112-53-8
SPID(S): Tox21_300120
M4ID: 12479010

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.67 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

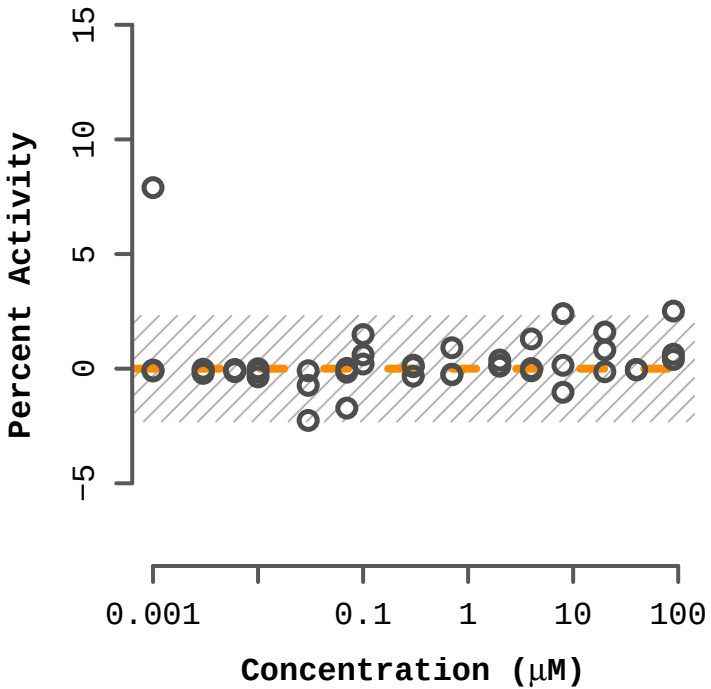
NAME: 1-Dodecanol
CHID: 26918 **CASRN:** 112-53-8
SPID(S): Tox21_202124
M4ID: 12480128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

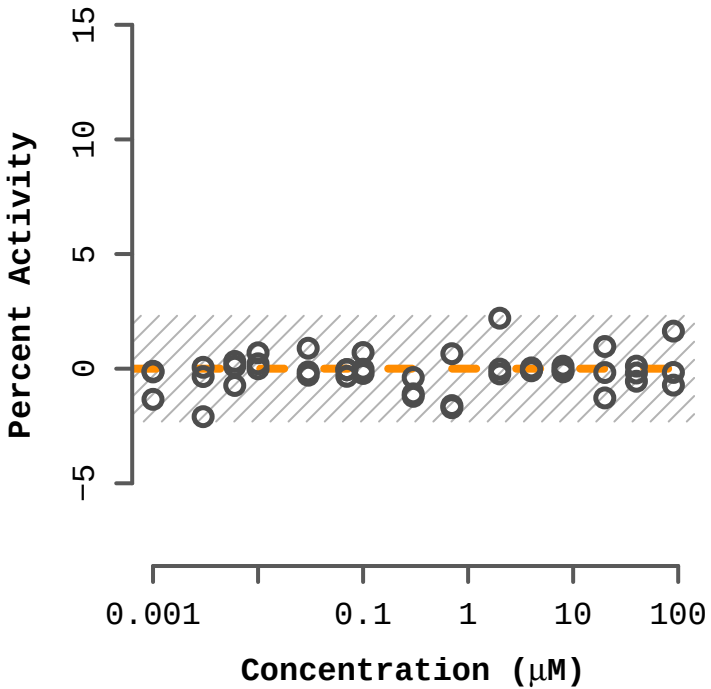
NAME: 2-[2-(Hexyloxy)ethoxy]ethanol
CHID: 26921 **CASRN:** 112-59-4
SPID(S): Tox21_303108
M4ID: 12476025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.58 **MAX_MED:** 0.815 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

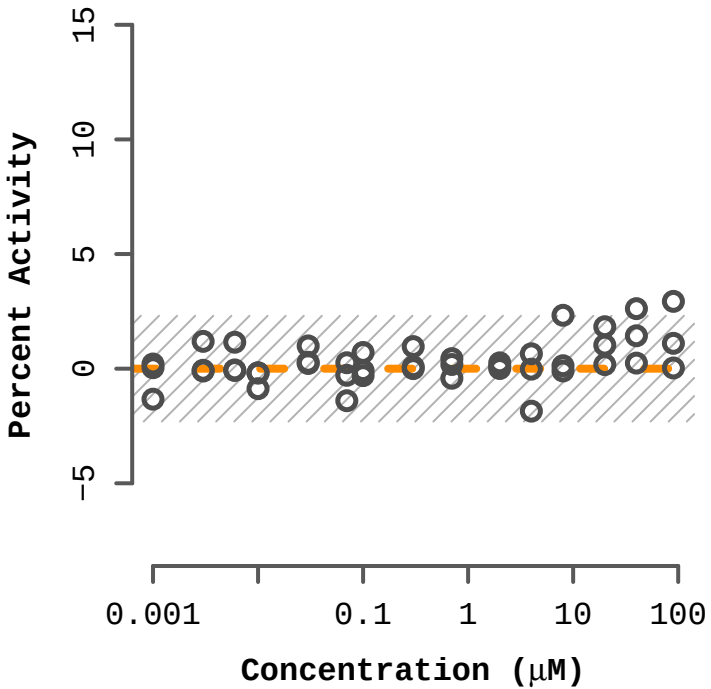
NAME: 2-[2-(Hexyloxy)ethoxy]ethanol
CHID: 26921 **CASRN:** 112-59-4
SPID(S): Tox21_202146
M4ID: 12480106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.653 **MAX_MED:** 0.214 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

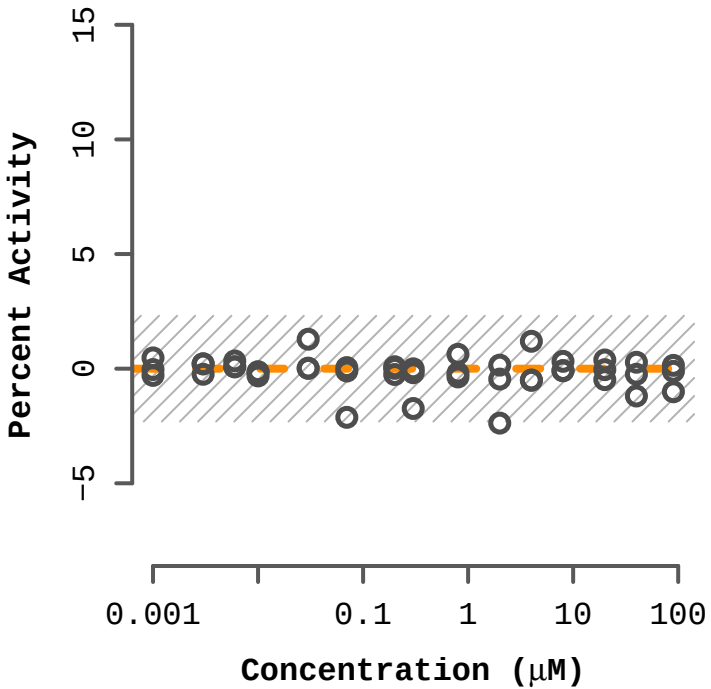
NAME: Tetraethylene glycol
CHID: 26922 **CASRN:** 112-60-7
SPID(S): Tox21_303245
M4ID: 12475888

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

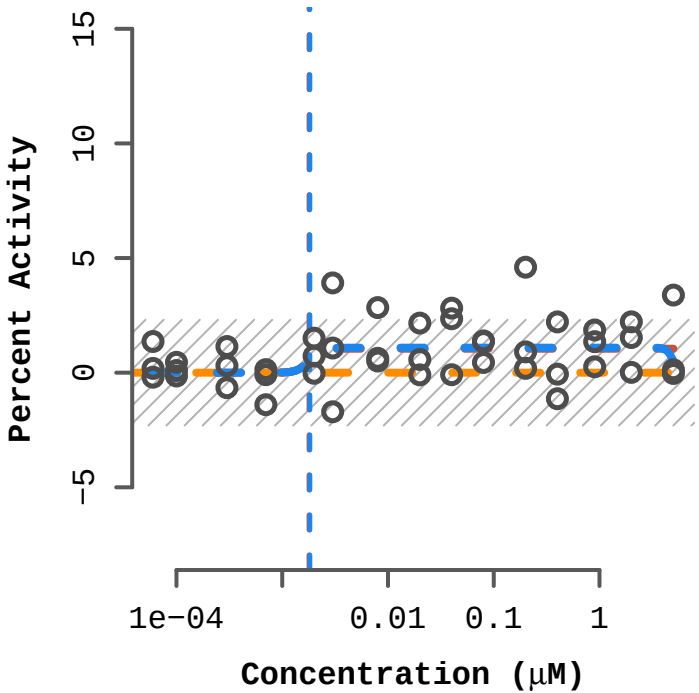
NAME: Tetraethylene glycol
CHID: 26922 **CASRN:** 112-60-7
SPID(S): Tox21_201629
M4ID: 12480623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	80.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.442 **MAX_MED:** 0.211 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethylcetylamine
CHID: 26924 **CASRN:** 112-69-6
SPID(S): Tox21_202994
M4ID: 12479258

HILL MODEL (in red):

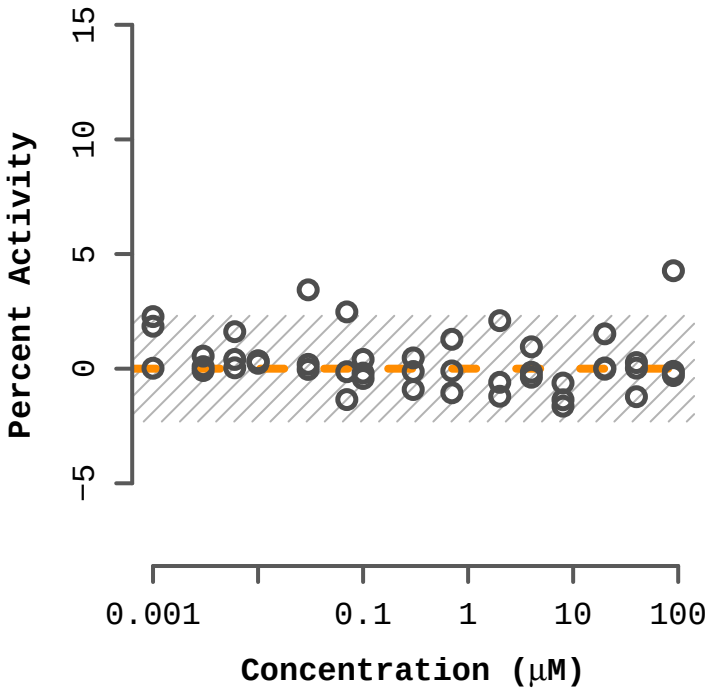
	tp	ga	gw
val:	1.04	−2.75	8
sd:	0.234	0.228	31.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.09	−2.74	7.79	0.695	14.6
sd:	0.239	0.199	31.1	0.267	1010

	CNST	HILL	GNLS
AIC:	168.32	153.95	157.42
PROB:	0	0.85	0.15
RMSE:	1.58	1.23	1.24

MAX_MEAN: 1.9 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

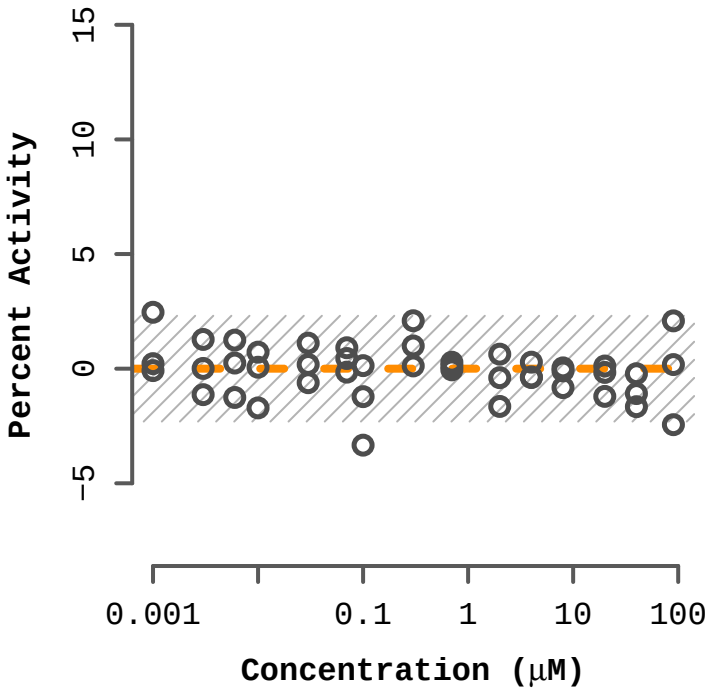
NAME: 1-Tetradecanol
CHID: 26926 **CASRN:** 112-72-1
SPID(S): Tox21_300538
M4ID: 12478594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

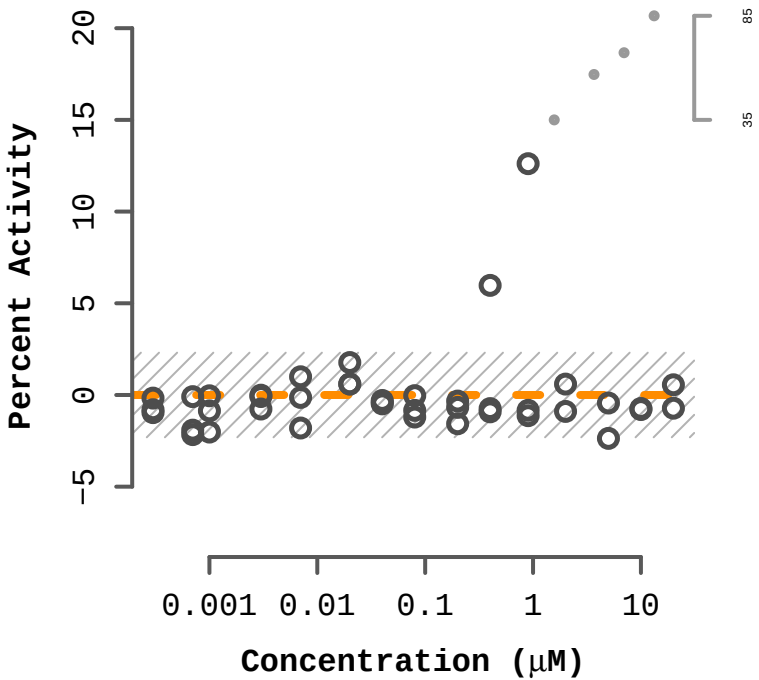
NAME: 1-Tetradecanol
CHID: 26926 **CASRN:** 112-72-1
SPID(S): Tox21_201842
M4ID: 12480410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

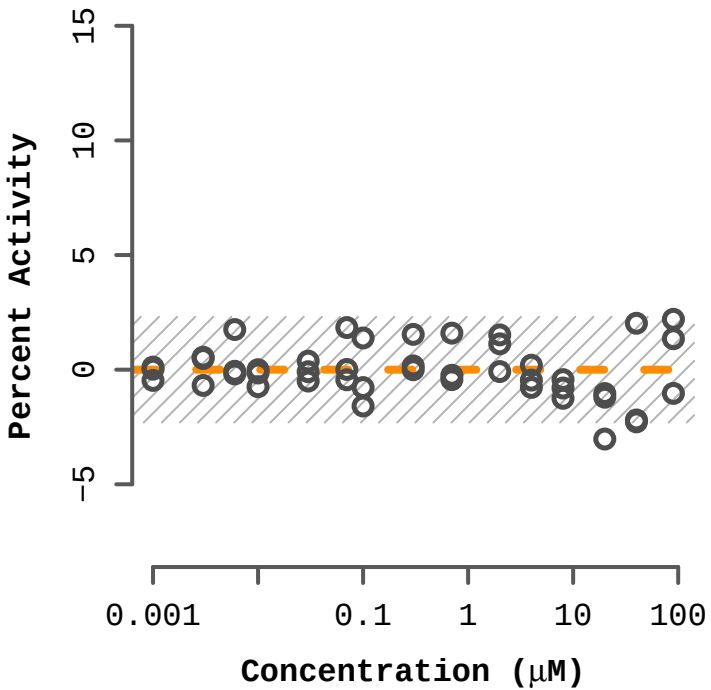
NAME: N,N−Dimethyltetradecylamine
CHID: 26927 **CASRN:** 112−75−4
SPID(S): Tox21_202738
M4ID: 12479514 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	287.98	NA	NA
PROB:	1	NA	NA
RMSE:	19.13	NA	NA

MAX_MEAN: 28.4 **MAX_MED:** 0.601 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

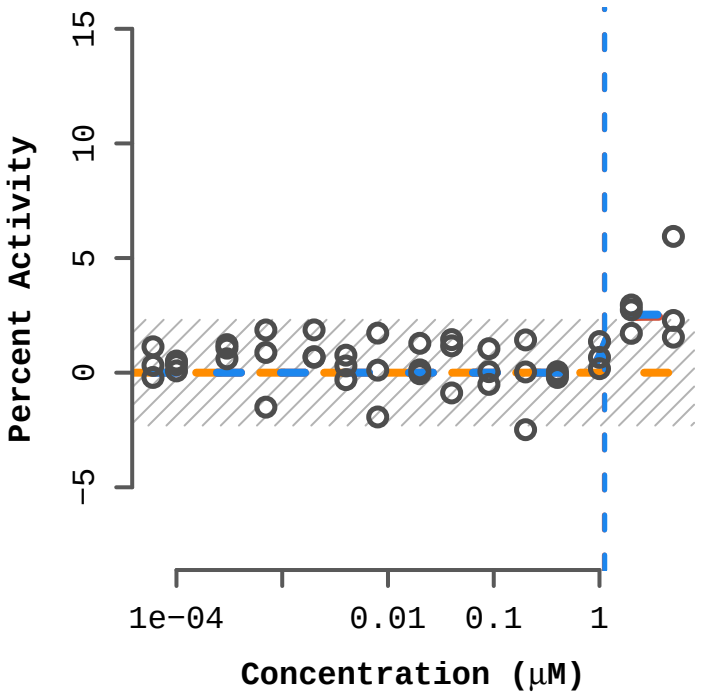
NAME: (13Z)-Docos-13-enoic acid
CHID: 26931 **CASRN:** 112-86-7
SPID(S): Tox21_200242
M4ID: 12482010

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Octadecene
CHID: 26932 CASRN: 112-88-9
SPID(S): Tox21_202739
M4ID: 12479513

HILL MODEL (in red):

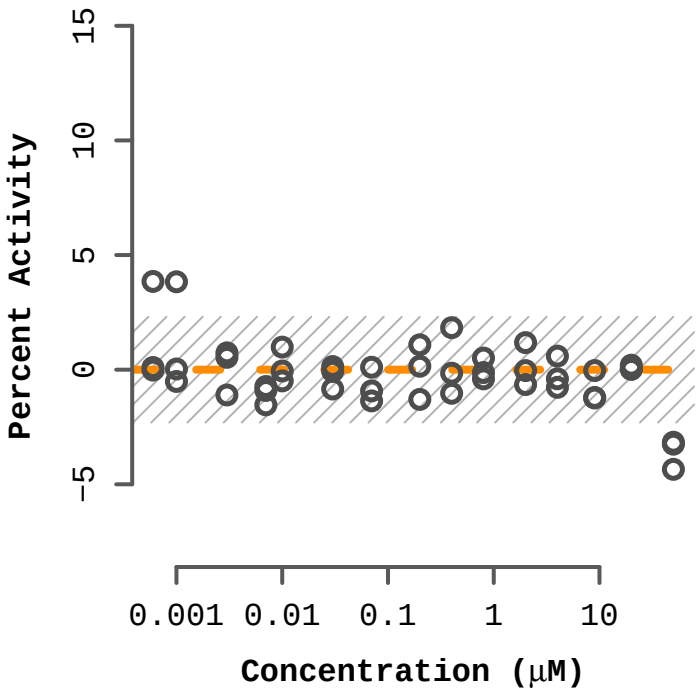
	tp	ga	gw
val:	2.44	0.0463	8
sd:	0.428	0.102	15.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.53	0.0496	8	0.753	17.9
sd:	1.23	0.44	64.9	8.67	2860

	CNST	HILL	GNLS
AIC:	161.42	141.98	145.9
PROB:	0	0.88	0.12
RMSE:	1.51	1.09	1.1

MAX_MEAN: 3.26 MAX_MED: 2.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

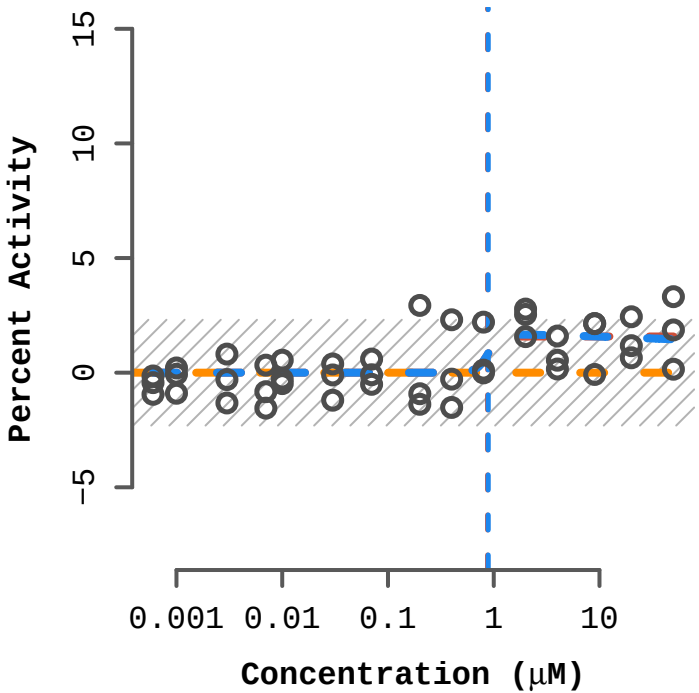
NAME: (Z)−9−Octadecenylamine
CHID: 26933 CASRN: 112−90−3
SPID(S): Tox21_112099_1
M4ID: 12483321

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Octadecanol
CHID: 26935 **CASRN:** 112-92-5
SPID(S): Tox21_111610_1
M4ID: 12483589

HILL MODEL (in red):

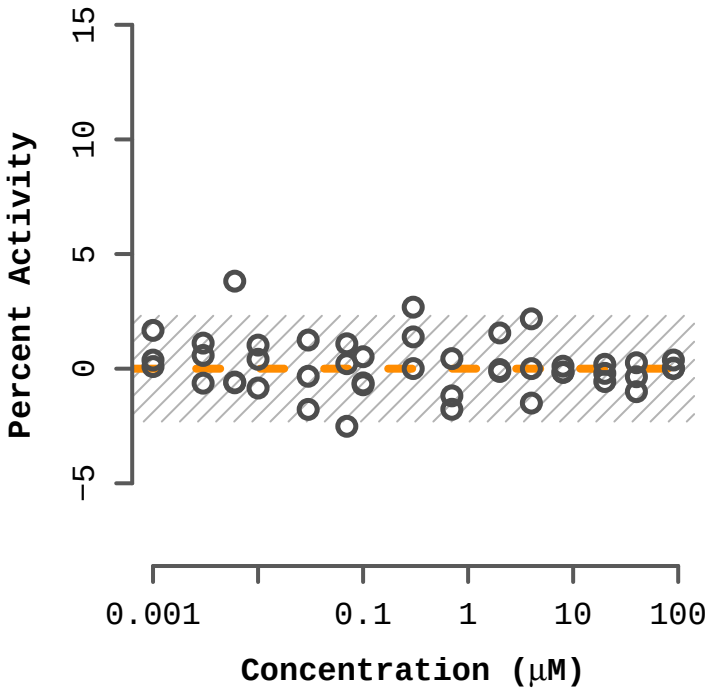
	tp	ga	gw
val:	1.58	−0.0578	8
sd:	0.284	0.111	13.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.82	−0.052	8	3.69	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	159.8	141.03	144.98
PROB:	0	0.88	0.12
RMSE:	1.38	1.04	1.04

MAX_MEAN: 2.3 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

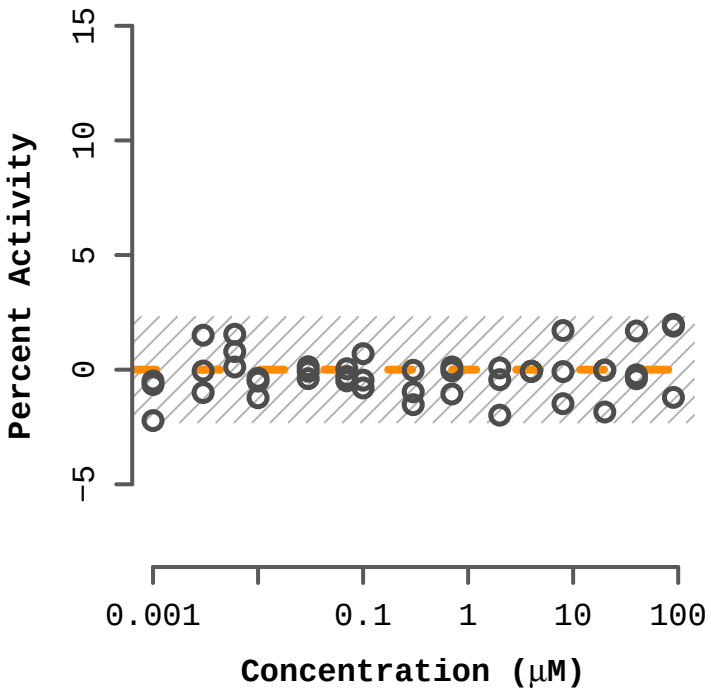
NAME: Chlorendic anhydride
CHID: 26941 **CASRN:** 115-27-5
SPID(S): Tox21_200439
M4ID: 12481813

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

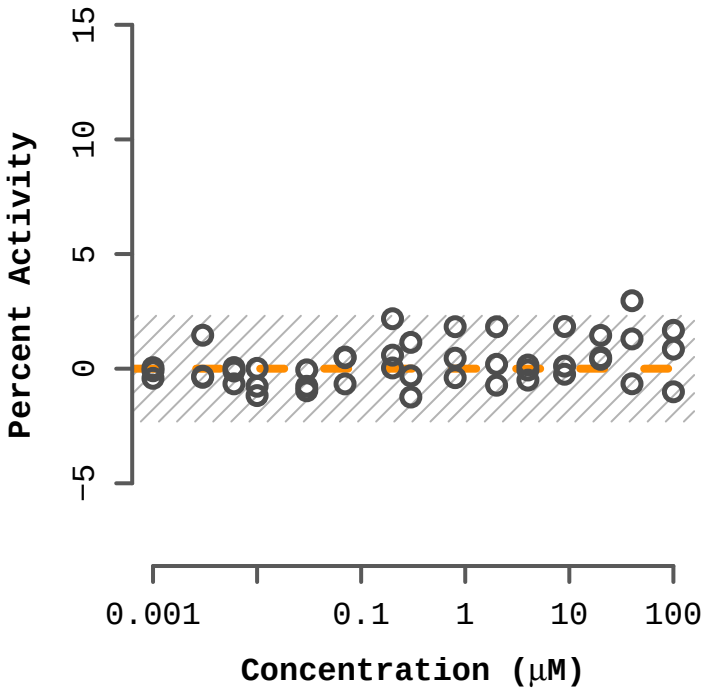
NAME: Pentaerythritol
CHID: 26943 **CASRN:** 115-77-5
SPID(S): Tox21_303573
M4ID: 12475572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.6	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

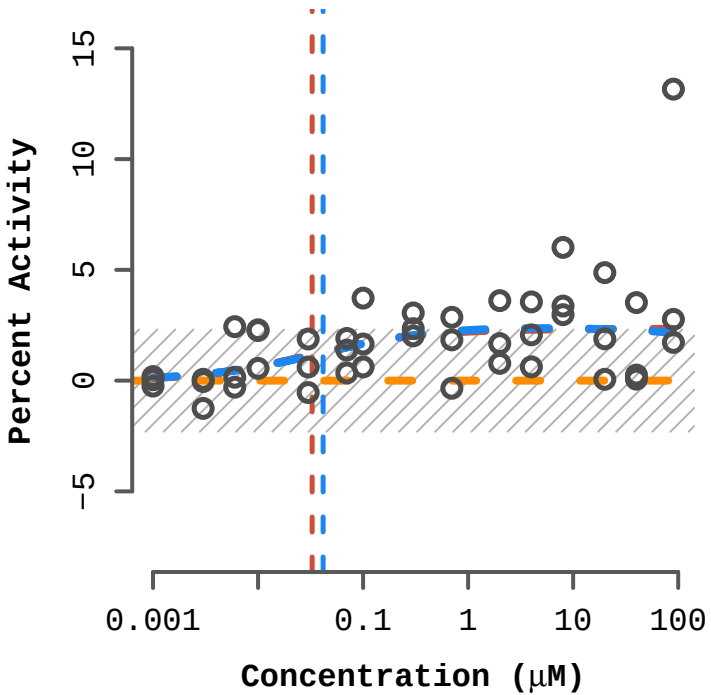
NAME: Pentaerythritol
CHID: 26943 **CASRN:** 115-77-5
SPID(S): Tox21_201921
M4ID: 12480331

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.83	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linalyl acetate
CHID: 26946 CASRN: 115-95-7
SPID(S): Tox21_303134
M4ID: 12475999

HILL MODEL (in red):

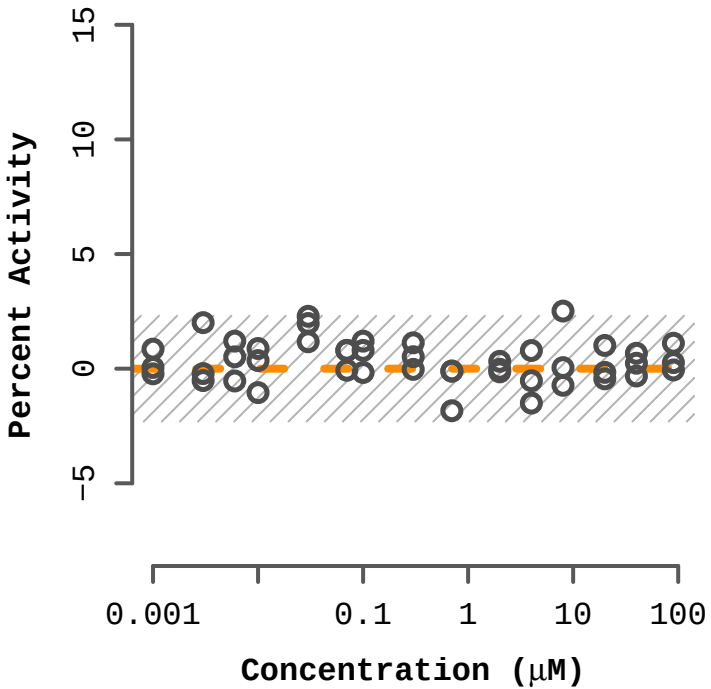
	tp	ga	gw
val:	2.34	−1.48	0.838
sd:	0.401	0.436	0.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.51	−1.38	0.771	3.55	0.505
sd:	1.22	0.726	0.539	7.62	2.56

	CNST	HILL	GNLS
AIC:	215.09	178.12	182.06
PROB:	0	0.88	0.12
RMSE:	2.94	2.09	2.1

MAX_MEAN: 5.88 MAX_MED: 3.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

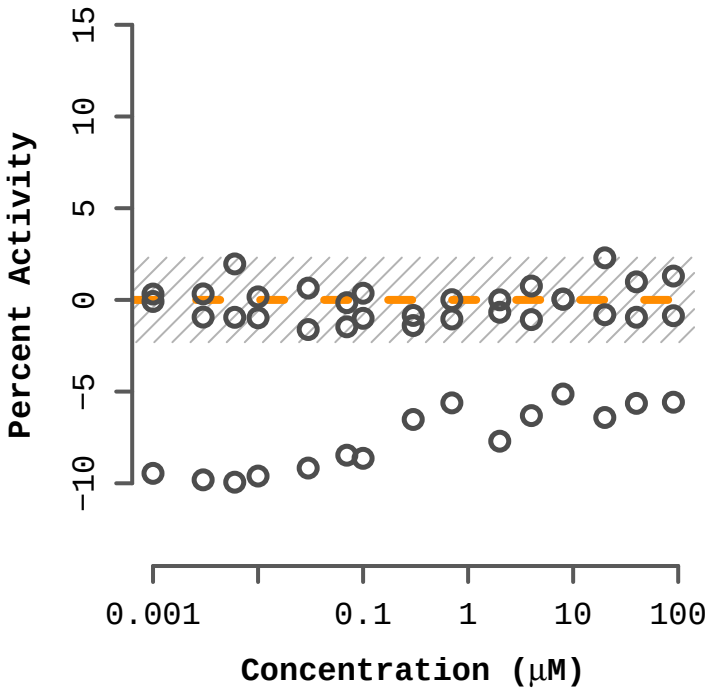
NAME: Linalyl acetate
CHID: 26946 **CASRN:** 115-95-7
SPID(S): Tox21_201306
M4ID: 12480946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

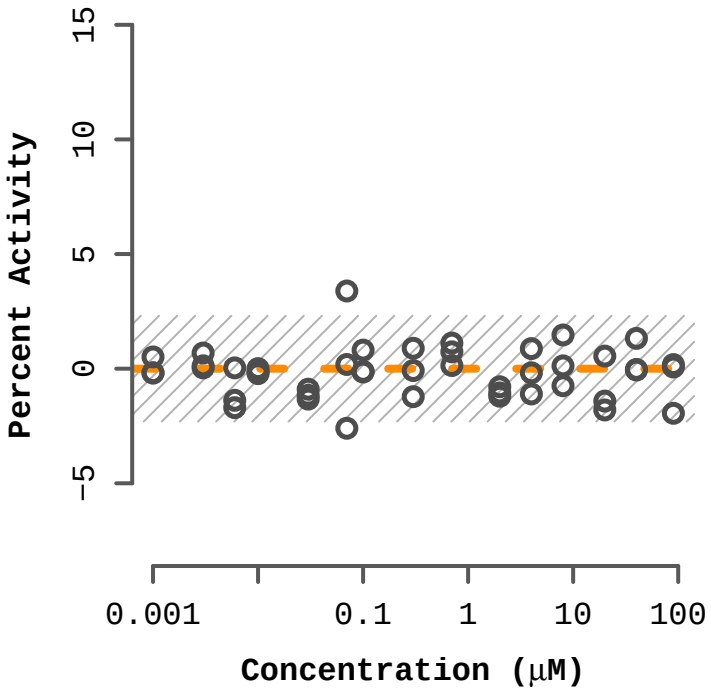
NAME: 2-(Hydroxymethyl)-1H-Isoindole-1,3(2H)-dione
CHID: 26954 **CASRN:** 118-29-6
SPID(S): Tox21_200859
M4ID: 12481393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.03	NA	NA
PROB:	1	NA	NA
RMSE:	4.57	NA	NA

MAX_MEAN: −1.64 **MAX_MED:** 0.0346 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

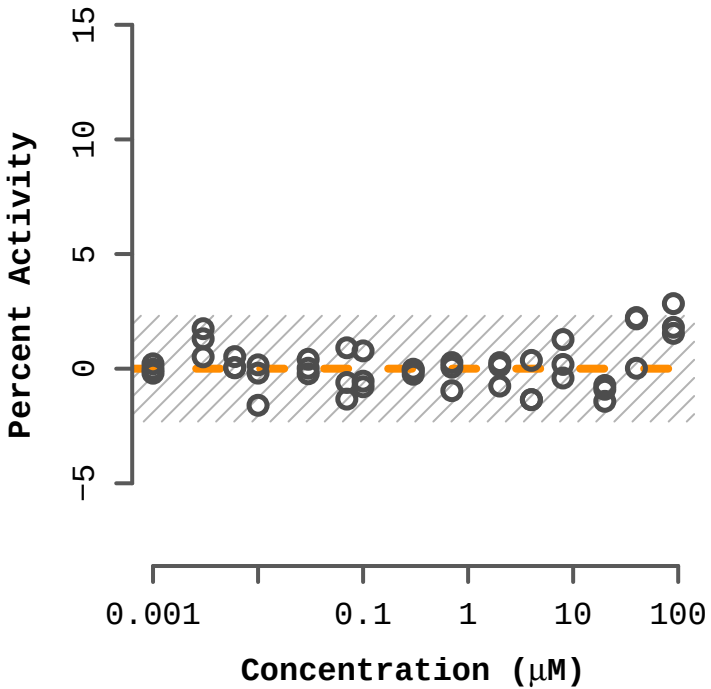
NAME: 2H-3,1-Benzoxazine-2,4(1H)-dione
CHID: 26955 CASRN: 118-48-9
SPID(S): Tox21_303058
M4ID: 12476075

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.664 MAX_MED: 0.737 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

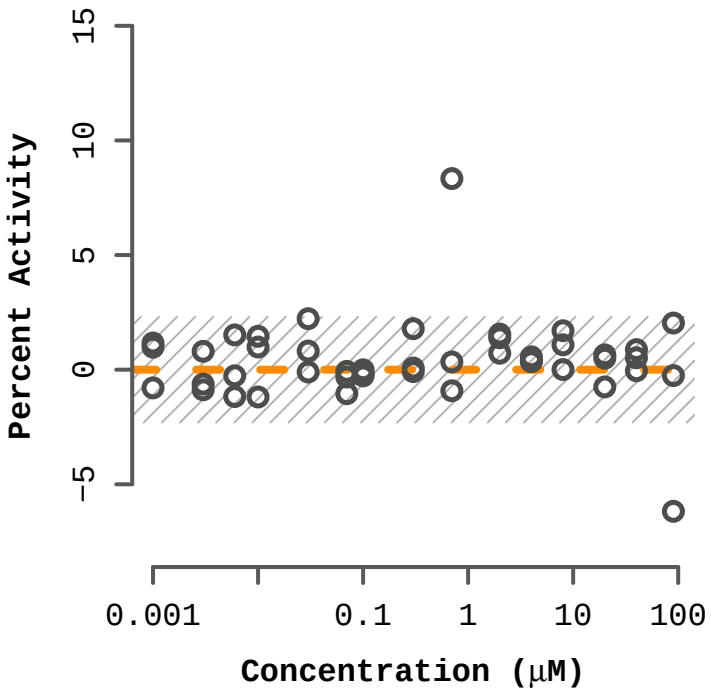
NAME: 2H-3,1-Benzoxazine-2,4(1H)-dione
CHID: 26955 **CASRN:** 118-48-9
SPID(S): Tox21_201325
M4ID: 12480927

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

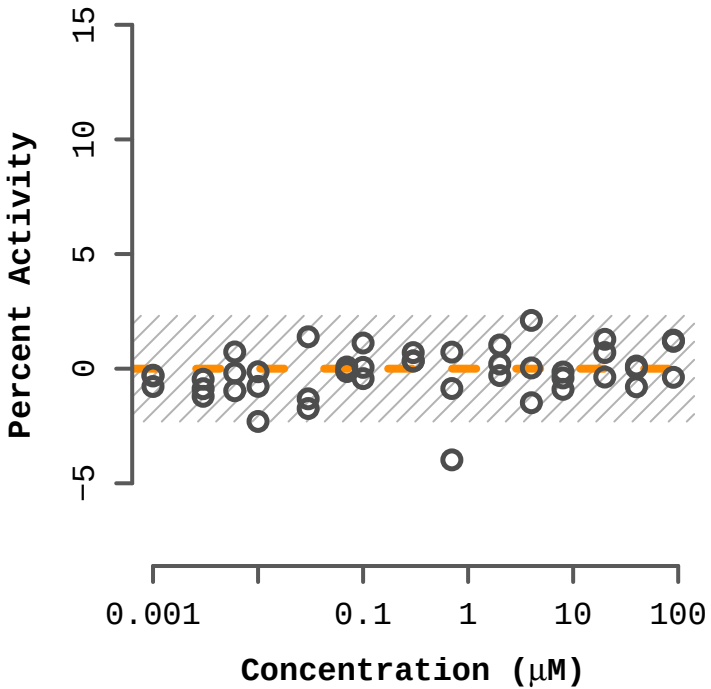
NAME: 4-Methyl-2-nitrophenol
CHID: 26961 **CASRN:** 119-33-5
SPID(S): Tox21_200933
M4ID: 12481319

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 2.59 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

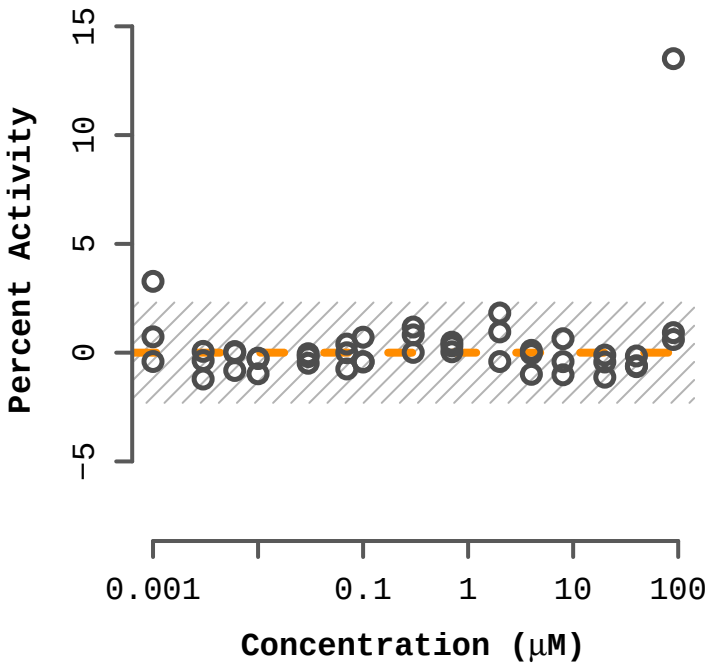
NAME: Diethylene glycol dibenzoate
CHID: 26967 CASRN: 120-55-8
SPID(S): Tox21_300522
M4ID: 12478610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

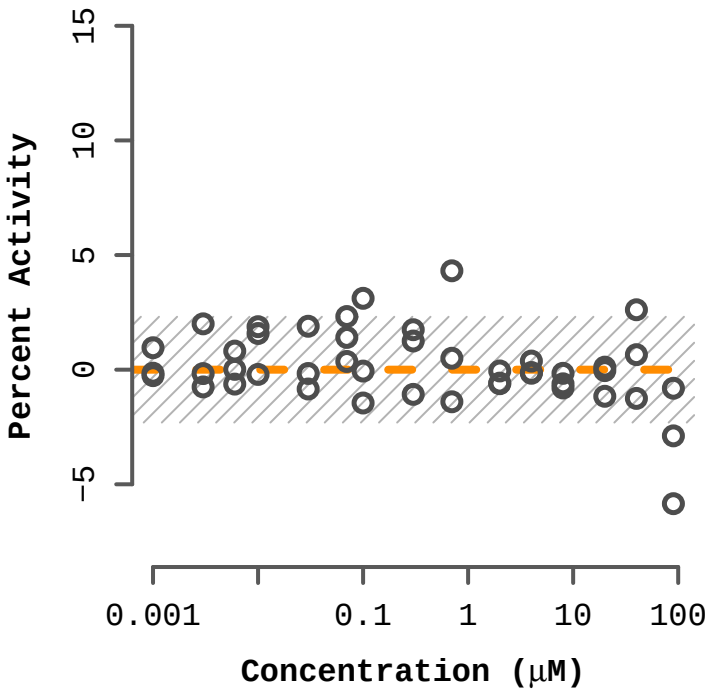
NAME: Diethylene glycol dibenzoate
CHID: 26967 CASRN: 120-55-8
SPID(S): Tox21_201732
M4ID: 12480520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 5.01 MAX_MED: 0.956 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

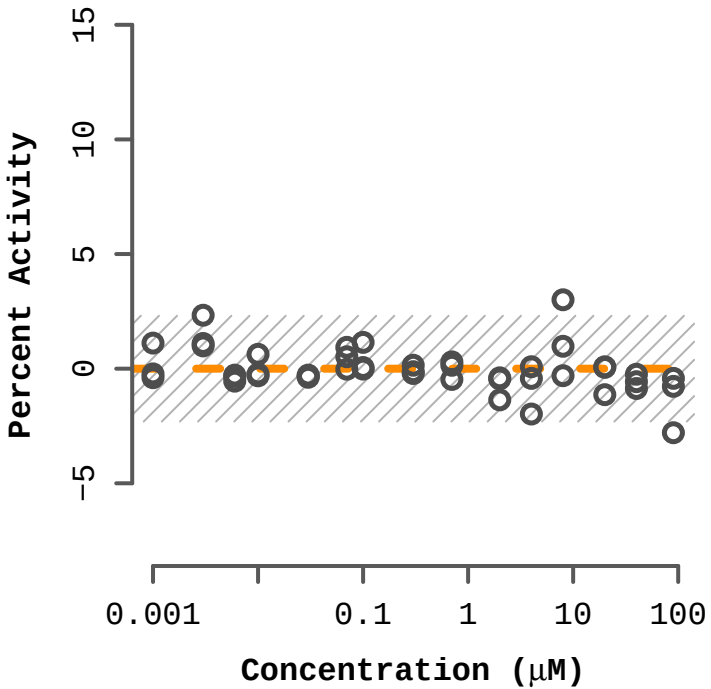
NAME: 2,4-Bis(2-methylbutan-2-yl)phenol
CHID: 26974 **CASRN:** 120-95-6
SPID(S): Tox21_300090
M4ID: 12479040

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

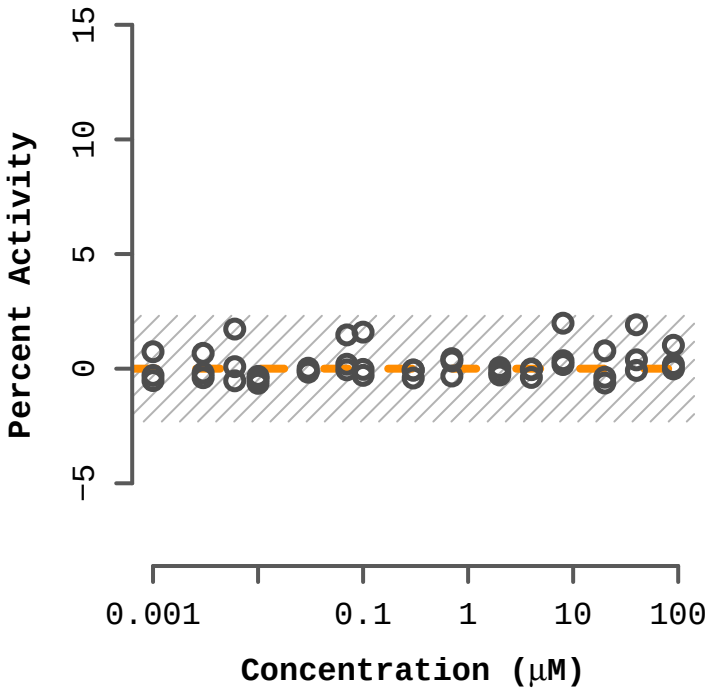
NAME: 2,4-Bis(2-methylbutan-2-yl)phenol
CHID: 26974 **CASRN:** 120-95-6
SPID(S): Tox21_202168
M4ID: 12480084

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

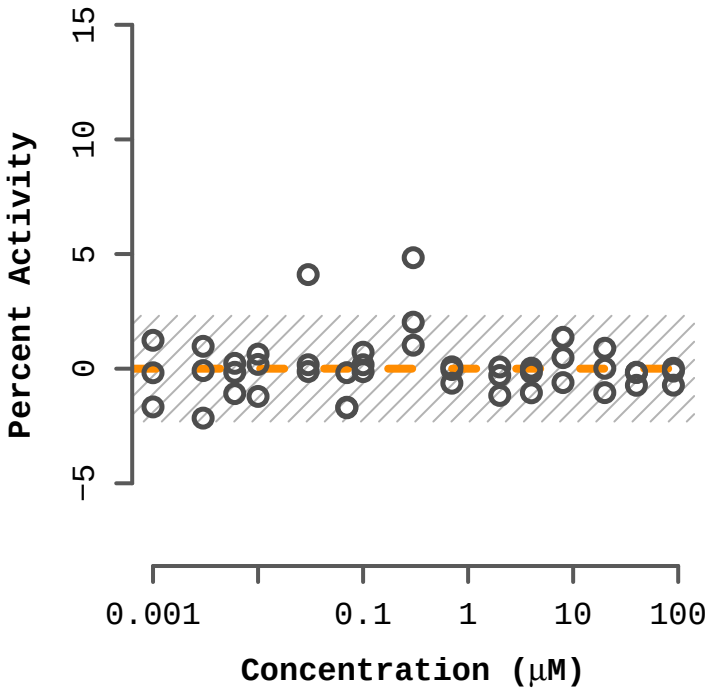
NAME: 2-Methyl-5-nitrobenzenesulfonic acid
CHID: 26975 **CASRN:** 121-03-9
SPID(S): Tox21_303151
M4ID: 12475982

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.839 **MAX_MED:** 0.388 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

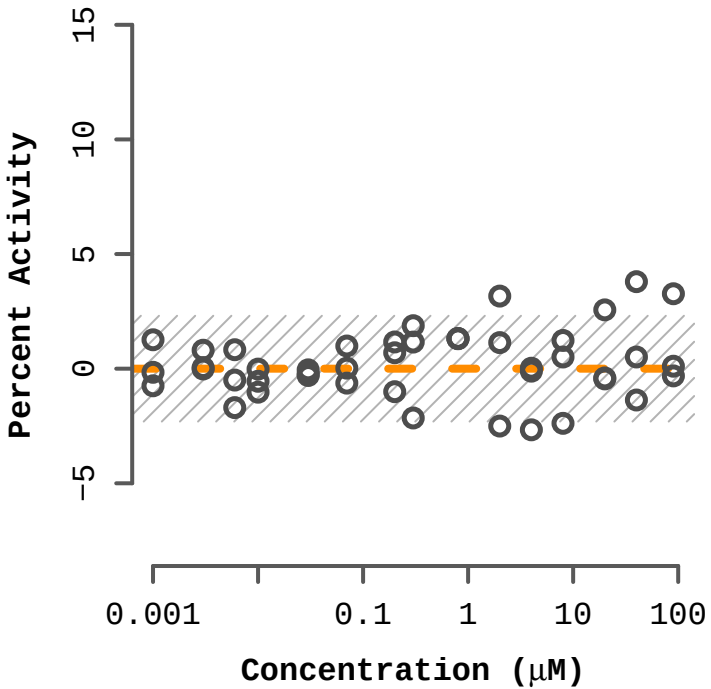
NAME: 2-Methyl-5-nitrobenzenesulfonic acid
CHID: 26975 **CASRN:** 121-03-9
SPID(S): Tox21_202190
M4ID: 12480062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.63 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

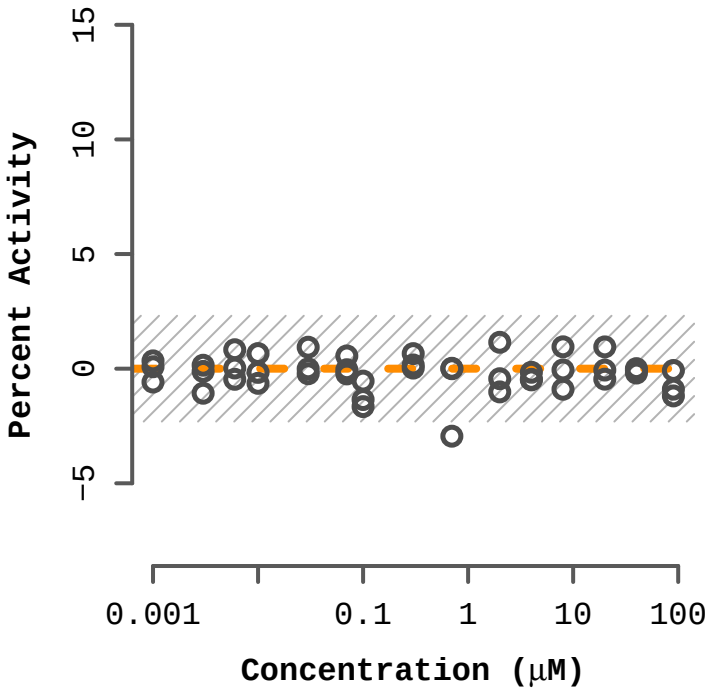
NAME: Trimethyl phosphite
CHID: 26979 **CASRN:** 121-45-9
SPID(S): Tox21_200440
M4ID: 12481812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

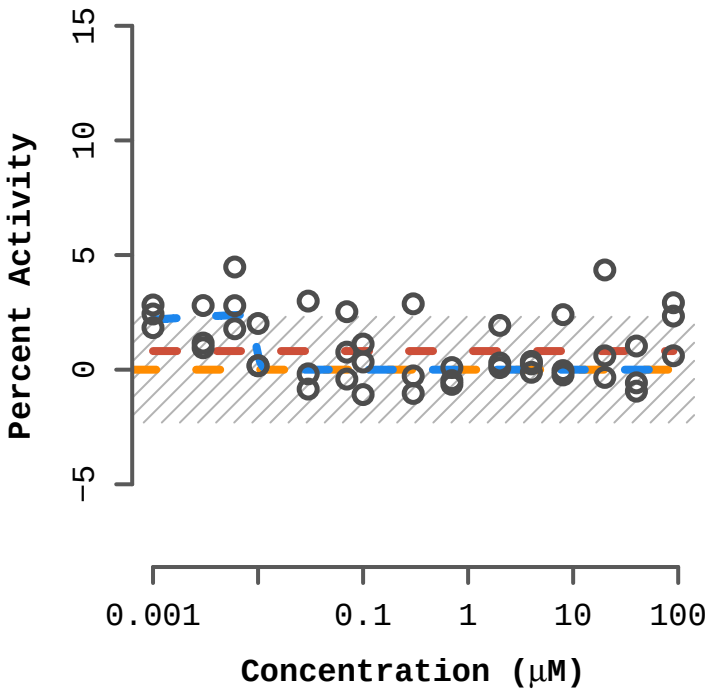
NAME: 4-(Acetylamino)benzenesulfonyl chloride
CHID: 26981 **CASRN:** 121-60-8
SPID(S): Tox21_202556
M4ID: 12479696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.283 **MAX_MED:** 0.163 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-1-methyl-4-nitrobenzene
CHID: 26984 **CASRN:** 121-86-8
SPID(S): Tox21_200875
M4ID: 12481377

HILL MODEL (in red):

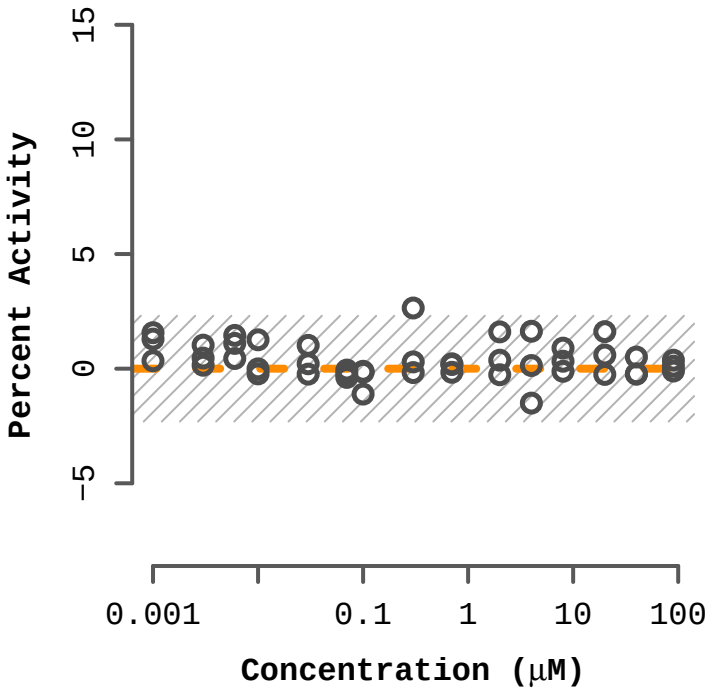
	tp	ga	gw
val:	0.812	−4.6	4.79
sd:	0.233	1260	3770

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.73	−5	0.3	−2.02	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	180.31	173.84	164.8
PROB:	0	0.01	0.99
RMSE:	1.75	1.46	1.39

MAX_MEAN: 3.02 **MAX_MED:** 2.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

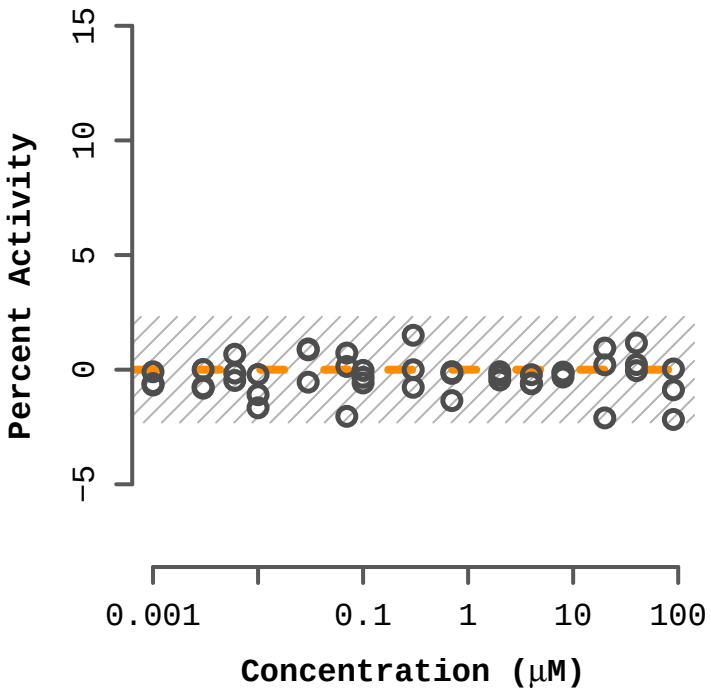
NAME: Triethyl phosphite
CHID: 26991 **CASRN:** 122-52-1
SPID(S): Tox21_303083
M4ID: 12476050

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

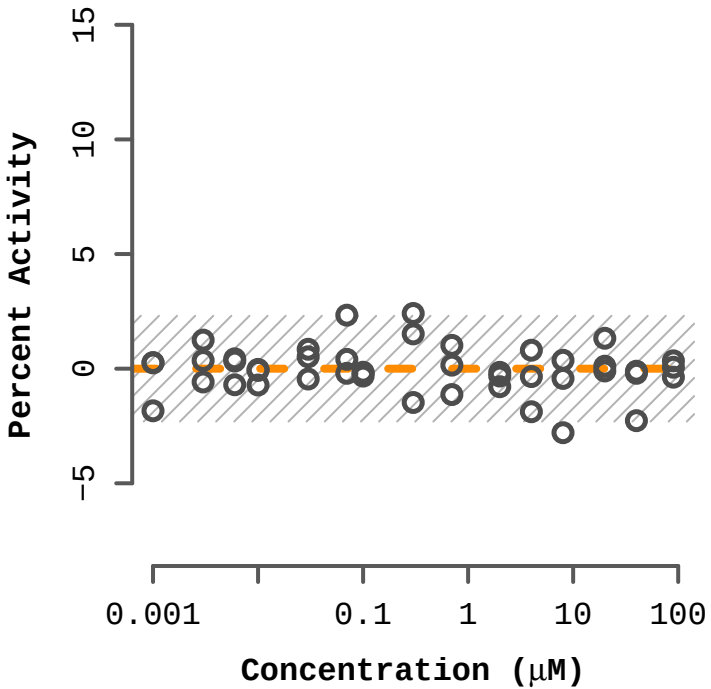
NAME: Triethyl phosphite
CHID: 26991 CASRN: 122-52-1
SPID(S): Tox21_201603
M4ID: 12480649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.452 MAX_MED: 0.866 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

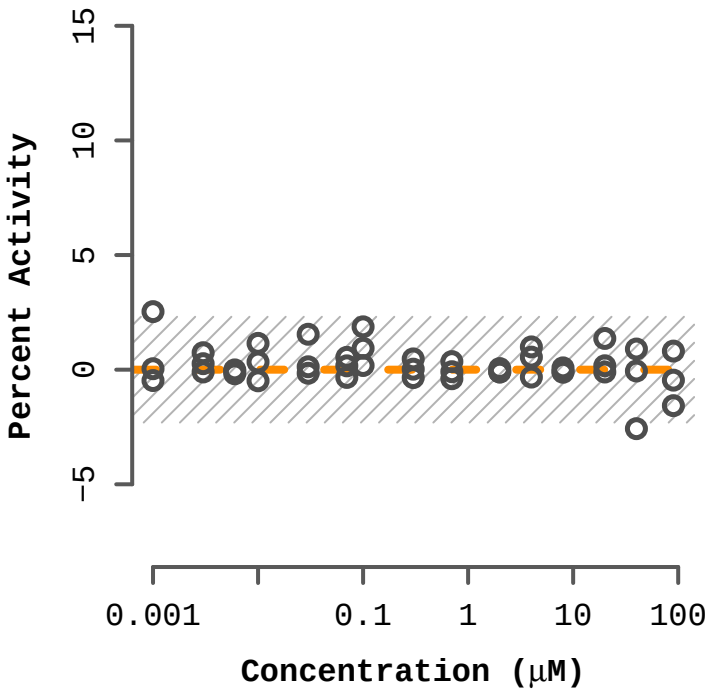
NAME: Dodecylbenzene
CHID: 26994 CASRN: 123-01-3
SPID(S): Tox21_303061
M4ID: 12476072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.847 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

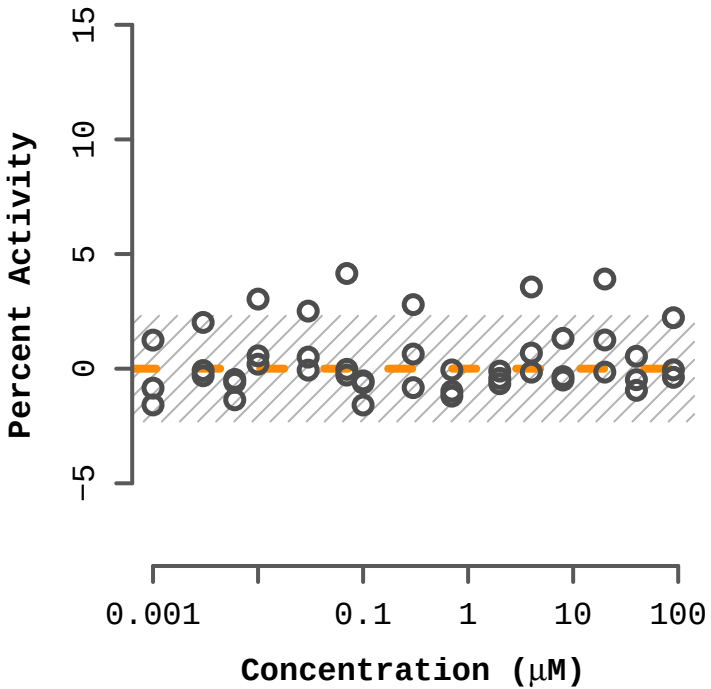
NAME: Dodecylbenzene
CHID: 26994 **CASRN:** 123-01-3
SPID(S): Tox21_201344
M4ID: 12480908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.996 **MAX_MED:** 0.936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

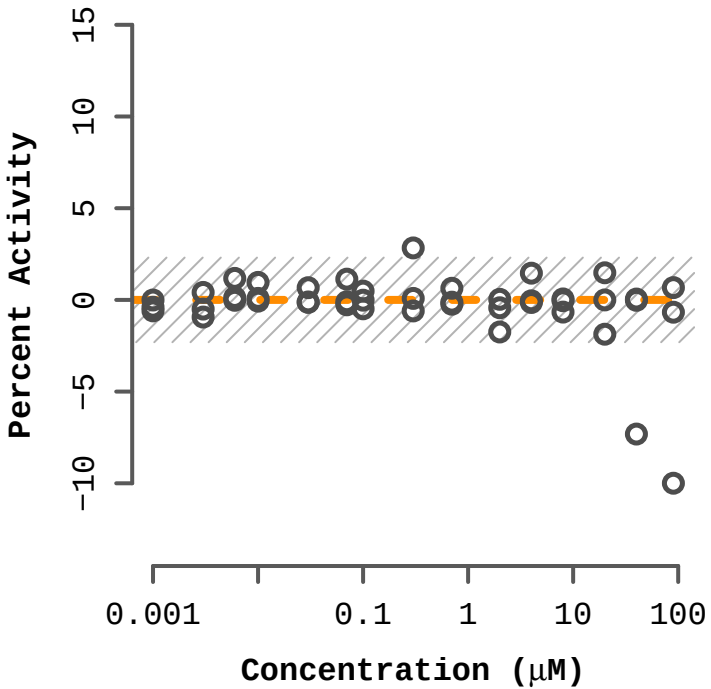
NAME: 4-Methoxybenzaldehyde
CHID: 26997 **CASRN:** 123-11-5
SPID(S): Tox21_303331
M4ID: 12475802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

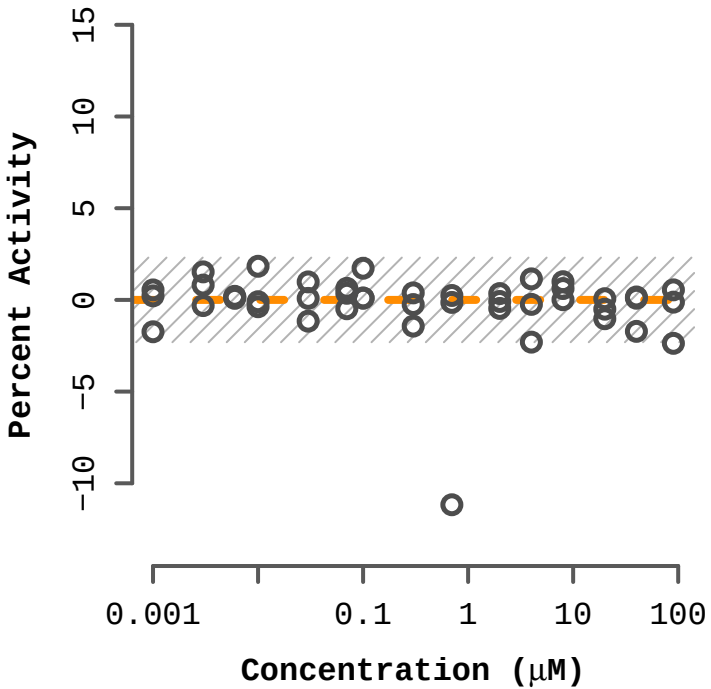
NAME: 4-Methoxybenzaldehyde
CHID: 26997 **CASRN:** 123-11-5
SPID(S): Tox21_201943
M4ID: 12480309

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.05	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 0.772 **MAX_MED:** 0.133 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

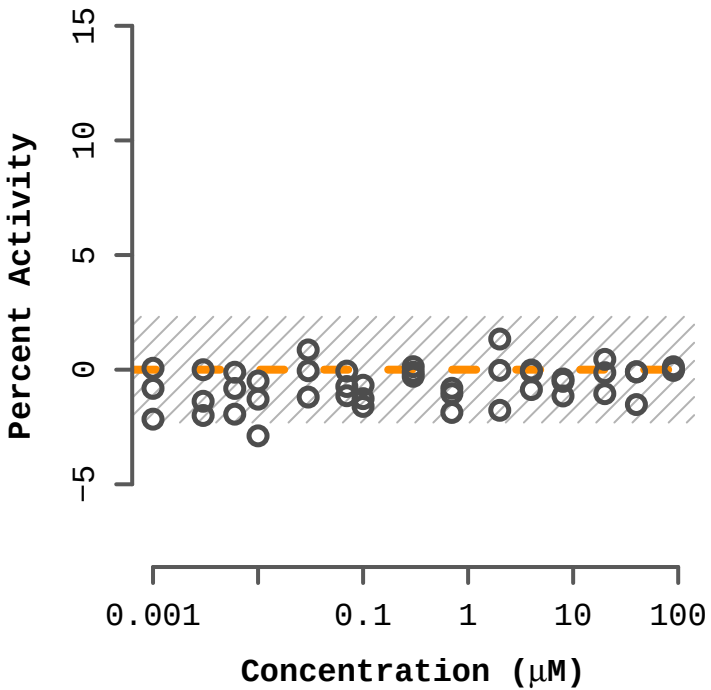
NAME: 2,6,8-Trimethyl-4-nonanone
CHID: 26998 CASRN: 123-18-2
SPID(S): Tox21_303158
M4ID: 12475975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 0.677 MAX_MED: 0.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

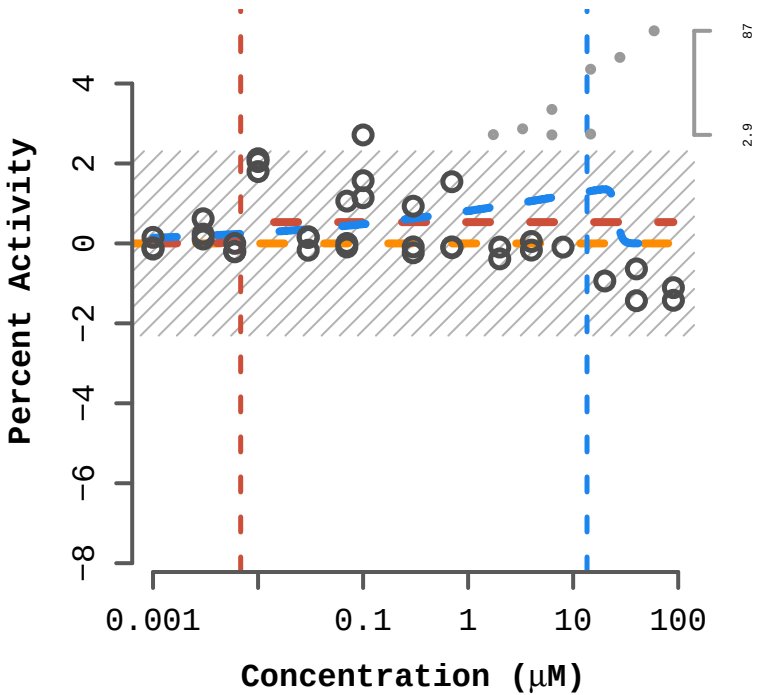
NAME: 2,6,8-Trimethyl-4-nonanone
CHID: 26998 **CASRN:** 123-18-2
SPID(S): Tox21_201537
M4ID: 12480715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.0413 **MAX_MED:** 0.0256 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propanoic anhydride
CHID: 27007 CASRN: 123-62-6
SPID(S): Tox21_201029
M4ID: 12481223 BRK

HILL MODEL (in red):

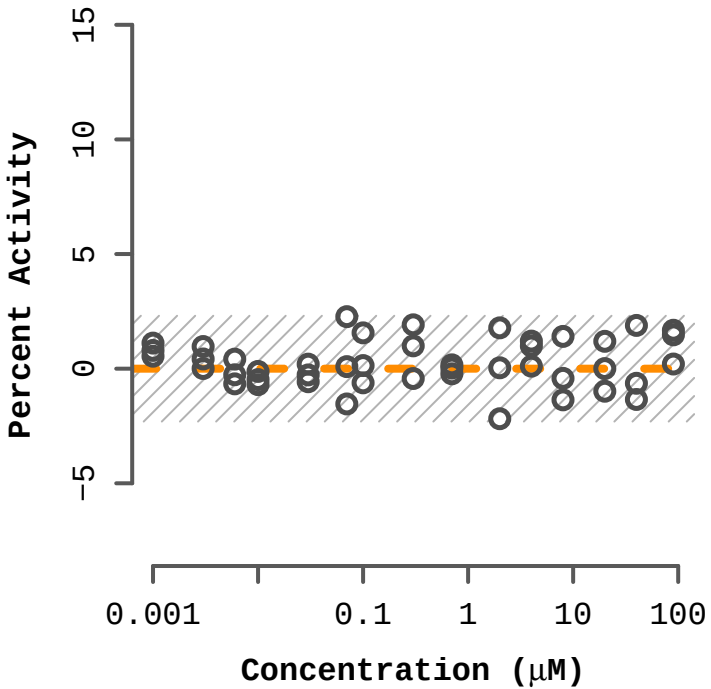
	tp	ga	gw
val:	0.533	−2.17	8
sd:	0.315	0.228	15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.59	1.13	0.3	1.41	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	278.97	281.84	283.92
PROB:	0.76	0.18	0.06
RMSE:	18.58	18.42	18.44

MAX_MEAN: 28 MAX_MED: 3.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

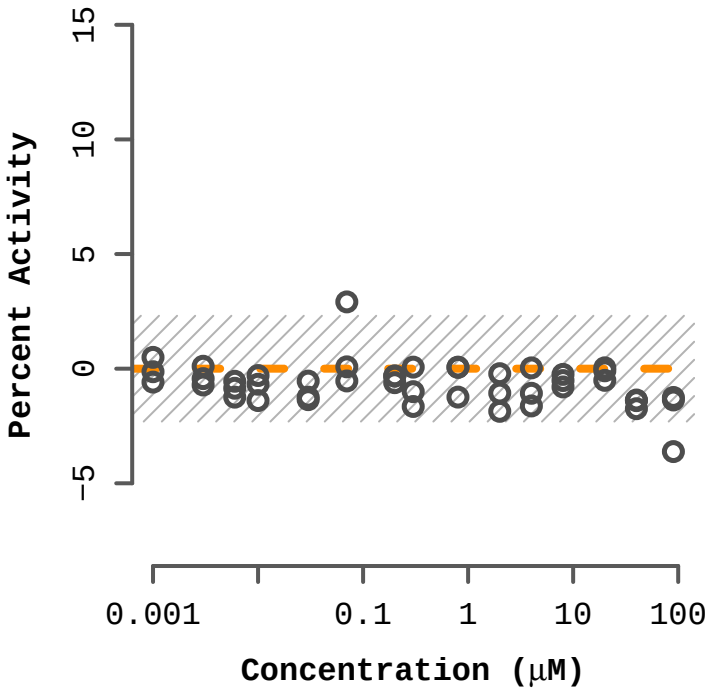
NAME: 2-Octanol
CHID: 27014 **CASRN:** 123-96-6
SPID(S): Tox21_303347
M4ID: 12475786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

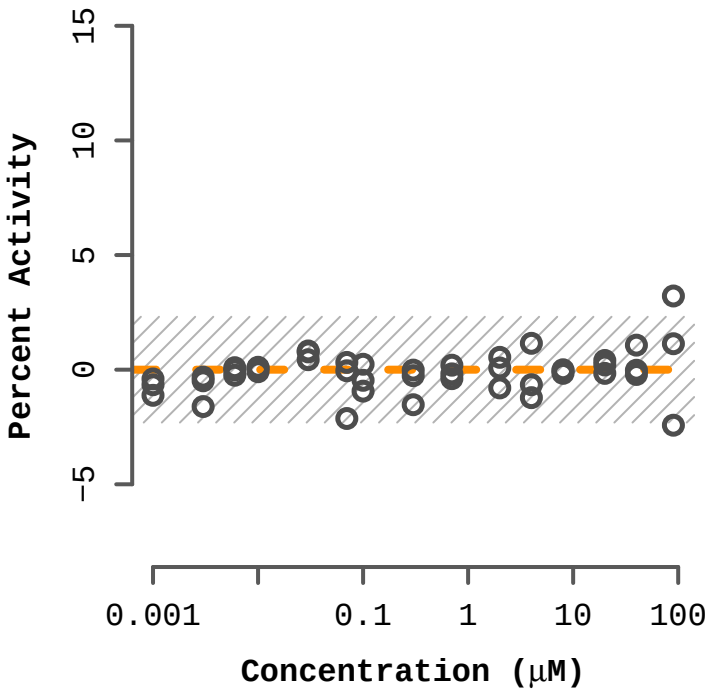
NAME: 2-Octanol
CHID: 27014 **CASRN:** 123-96-6
SPID(S): Tox21_201625
M4ID: 12480627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.82 **MAX_MED:** 0.0815 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

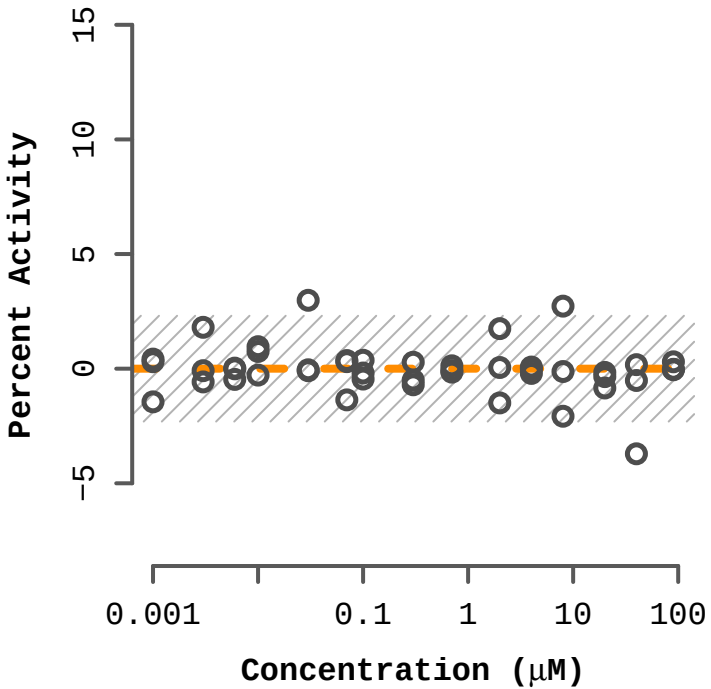
NAME: Methyl tetradecanoate
CHID: 27019 **CASRN:** 124-10-7
SPID(S): Tox21_200012
M4ID: 12482240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.677 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

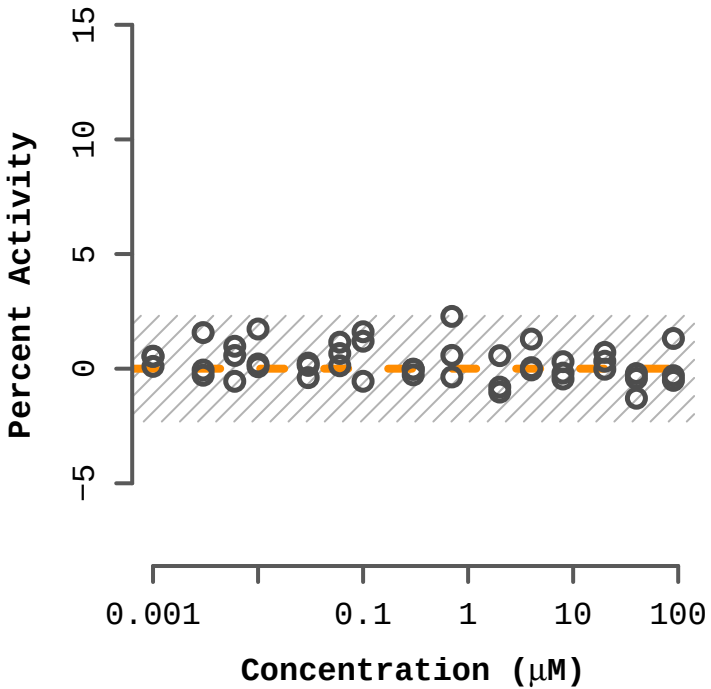
NAME: 2-(2-Butoxyethoxy)ethyl acetate
CHID: 27021 CASRN: 124-17-4
SPID(S): Tox21_303055
M4ID: 12476078

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.95 MAX_MED: 0.753 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

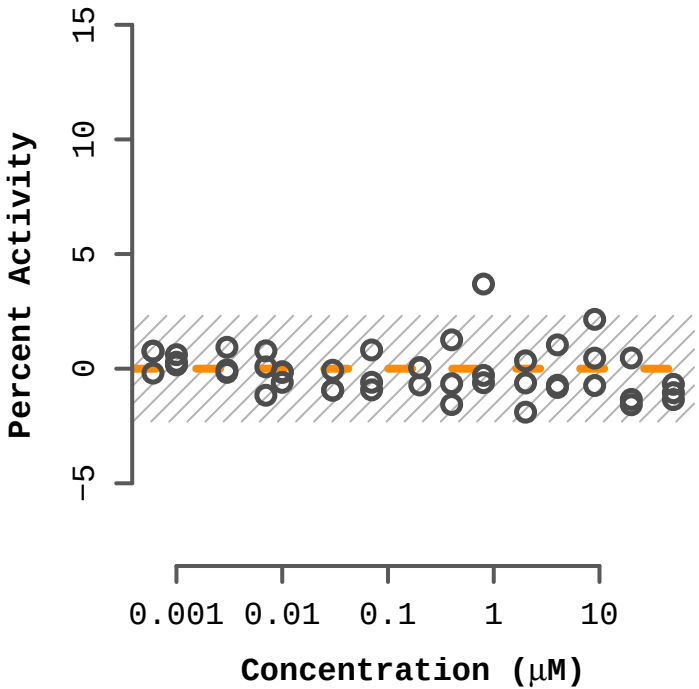
NAME: 2-(2-Butoxyethoxy)ethyl acetate
CHID: 27021 **CASRN:** 124-17-4
SPID(S): Tox21_201957
M4ID: 12480295

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.834 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

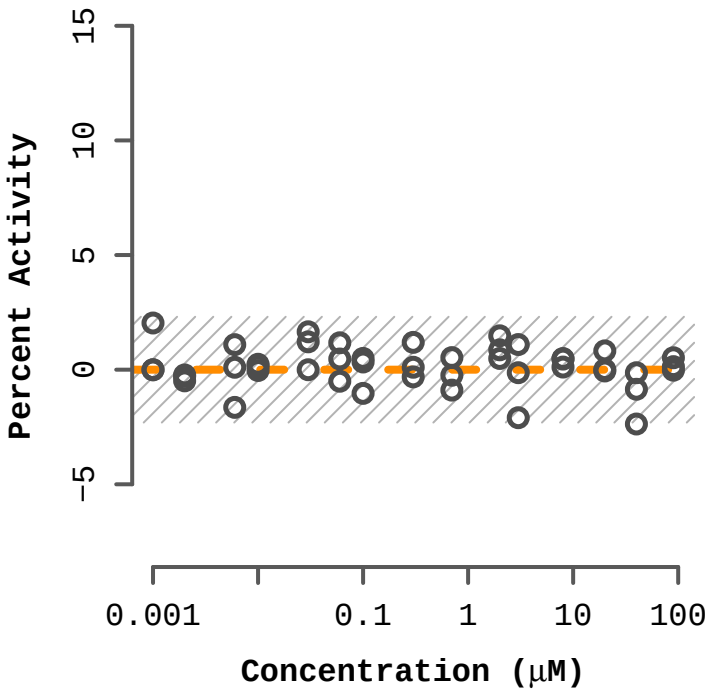
NAME: N,N−Dimethyl−1−octadecanamine
CHID: 27026 **CASRN:** 124−28−7
SPID(S): Tox21_113870
M4ID: 12482355

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.931 **MAX_MED:** 0.764 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

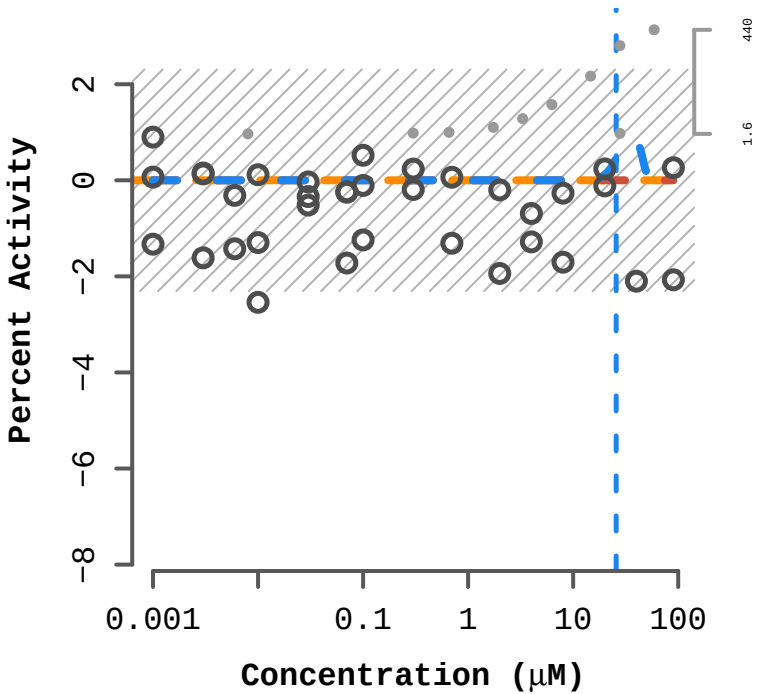
NAME: 2-Amino-2-methylpropan-1-ol
CHID: 27032 **CASRN:** 124-68-5
SPID(S): Tox21_303149
M4ID: 12475984

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-2-methylpropan-1-ol
CHID: 27032 **CASRN:** 124-68-5
SPID(S): Tox21_201780
M4ID: 12480472 **BRK**

HILL MODEL (in red):

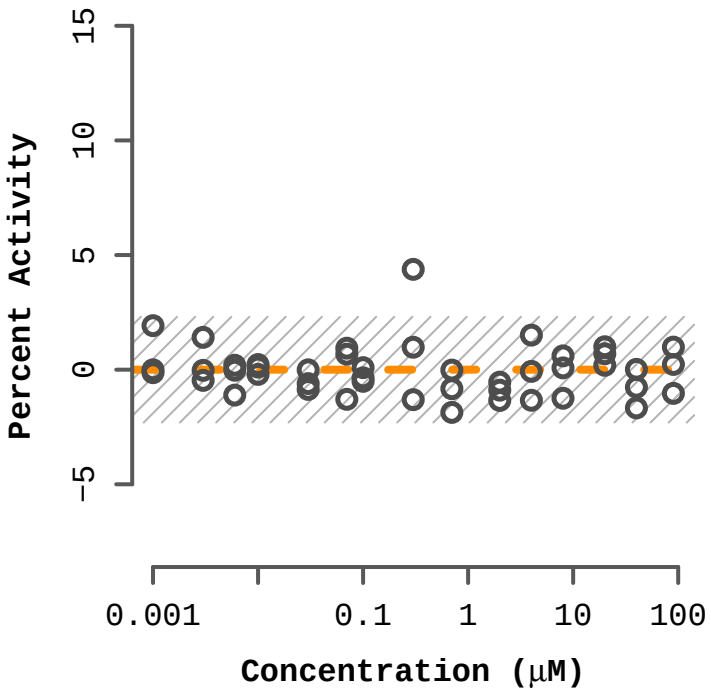
	tp	ga	gw
val:	5e-04	2.43	7.26
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.92	1.41	7.91	1.66	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	395.72	401.72	405.61
PROB:	0.95	0.05	0.01
RMSE:	96.48	96.48	96.41

MAX_MEAN: 147 **MAX_MED:** 3.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

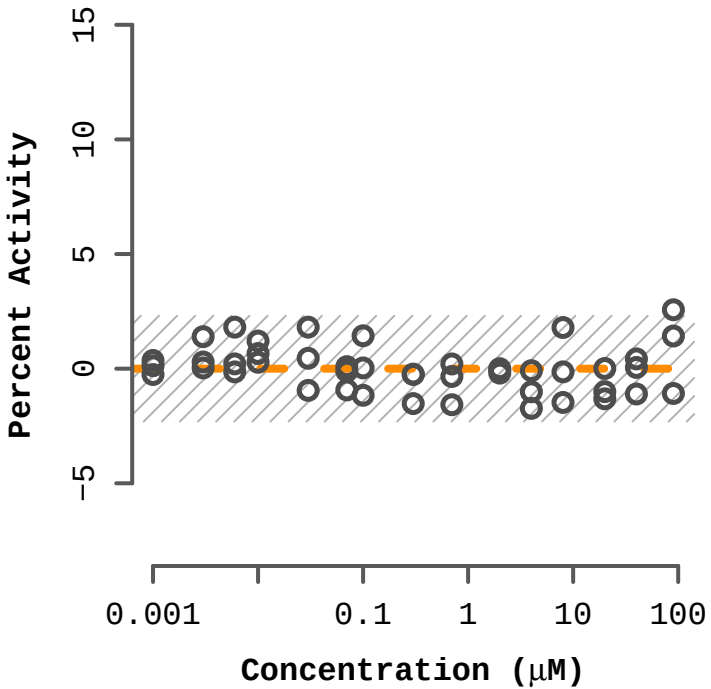
NAME: 2-(Hydroxymethyl)-2-nitro-1,3-propanediol
CHID: 27034 CASRN: 126-11-4
SPID(S): Tox21_300295
M4ID: 12478835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.35 MAX_MED: 0.979 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

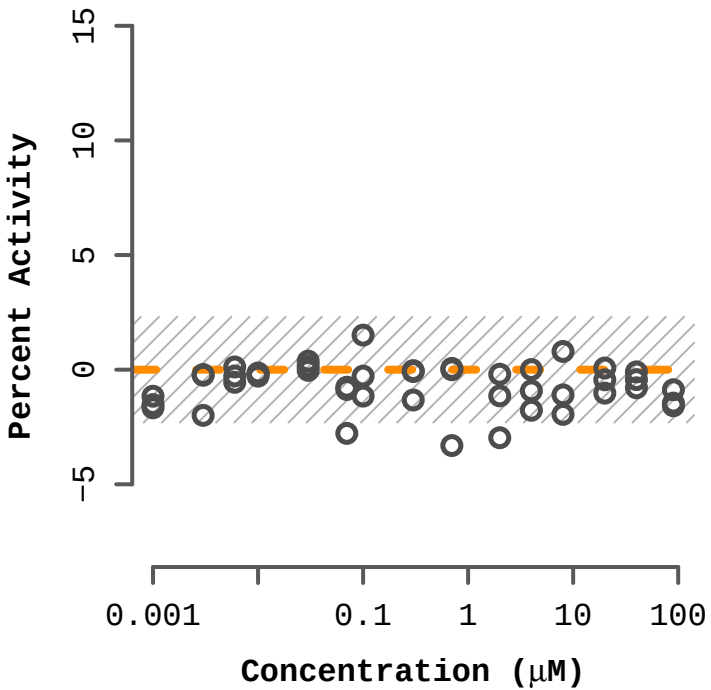
NAME: 2-(Hydroxymethyl)-2-nitro-1,3-propanediol
CHID: 27034 **CASRN:** 126-11-4
SPID(S): Tox21_200441
M4ID: 12481811

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.25	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

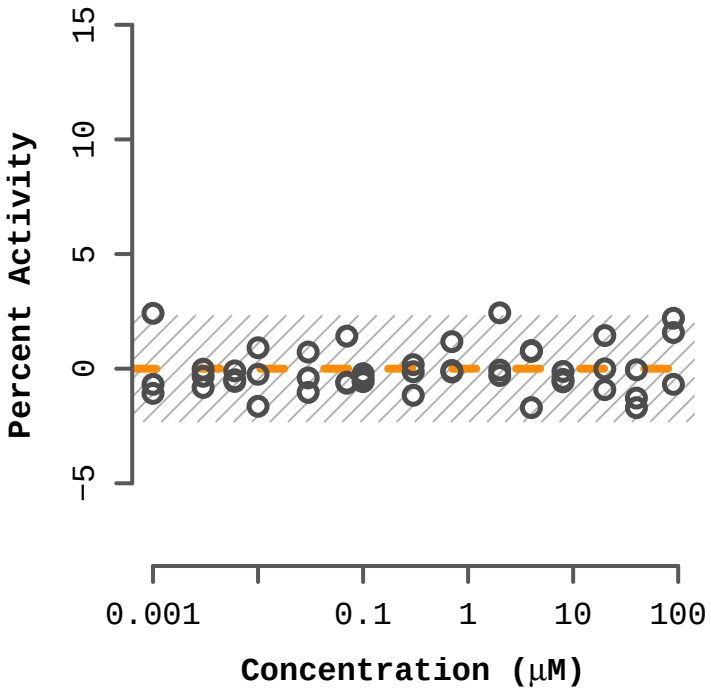
NAME: 2,2-Dimethylpropane-1,3-diol
CHID: 27036 **CASRN:** 126-30-7
SPID(S): Tox21_303298
M4ID: 12475835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.168 **MAX_MED:** 0.158 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

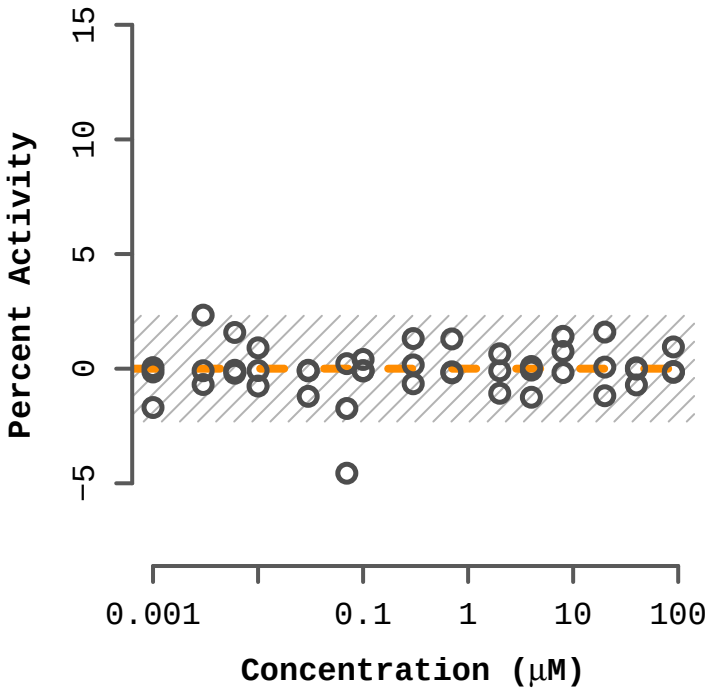
NAME: 2,2-Dimethylpropane-1,3-diol
CHID: 27036 **CASRN:** 126-30-7
SPID(S): Tox21_201363
M4ID: 12480889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

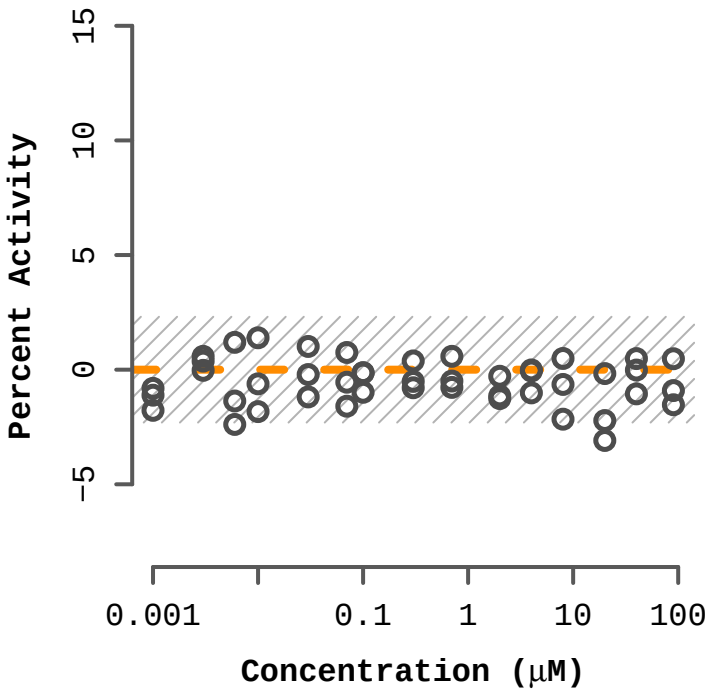
NAME: Sulfolane
CHID: 27037 CASRN: 126-33-0
SPID(S): Tox21_200628
M4ID: 12481624

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.666 MAX_MED: 0.752 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

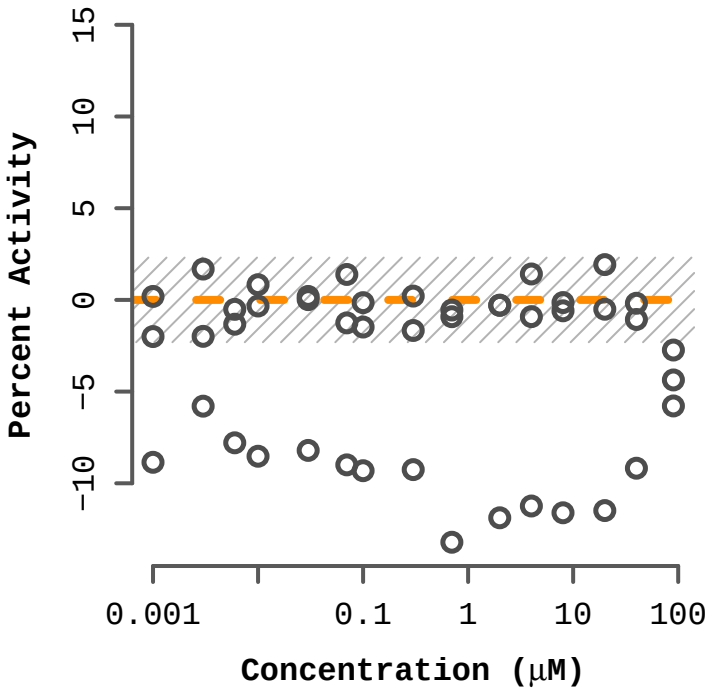
NAME: Dipentaerythritol
CHID: 27039 **CASRN:** 126-58-9
SPID(S): Tox21_301606
M4ID: 12477527

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.31 **MAX_MED:** 0.375 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

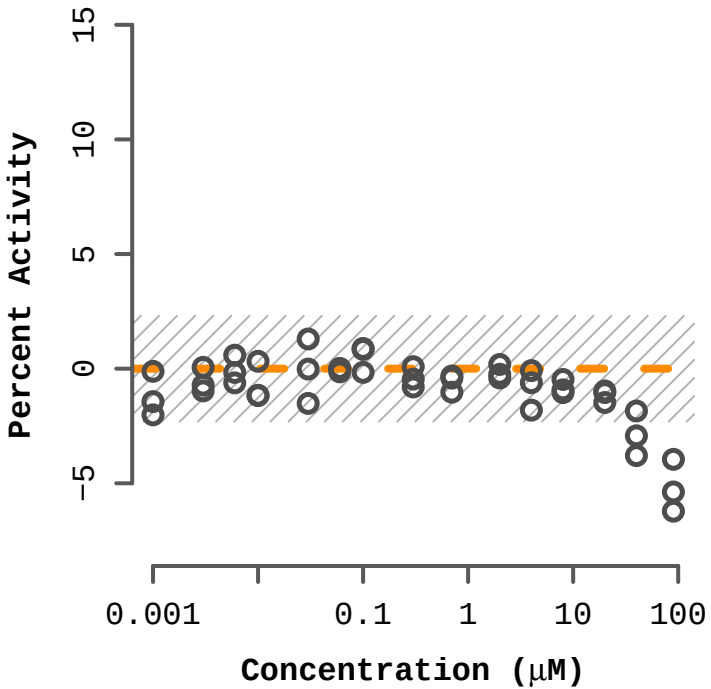
NAME: 2,4,7,9−Tetramethyl−5−decyne−4,7−diol
CHID: 27041 **CASRN:** 126−86−3
SPID(S): Tox21_300559
M4ID: 12478574

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	284.13	NA	NA
PROB:	1	NA	NA
RMSE:	5.68	NA	NA

MAX_MEAN: −2.03 **MAX_MED:** 0.0163 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

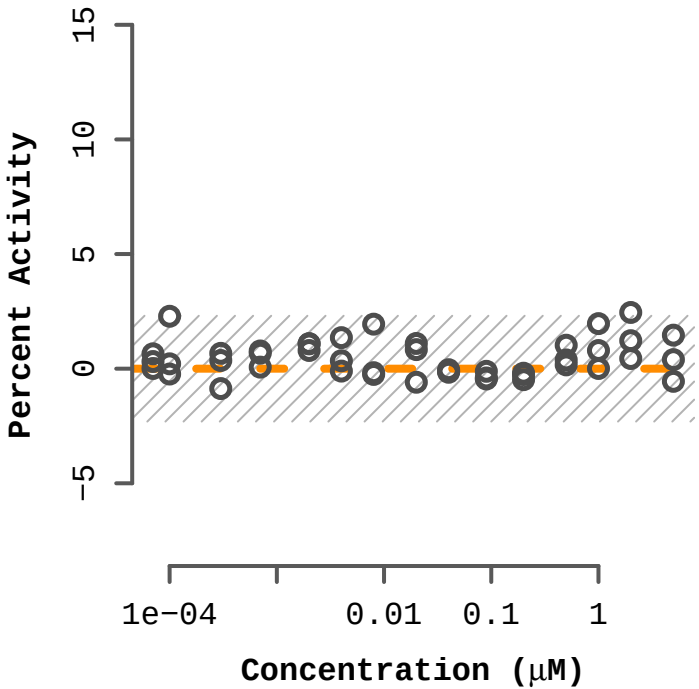
NAME: 2,4,7,9-Tetramethyl-5-decyne-4,7-diol
CHID: 27041 **CASRN:** 126-86-3
SPID(S): Tox21_201648
M4ID: 12480604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 0.521 **MAX_MED:** 0.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

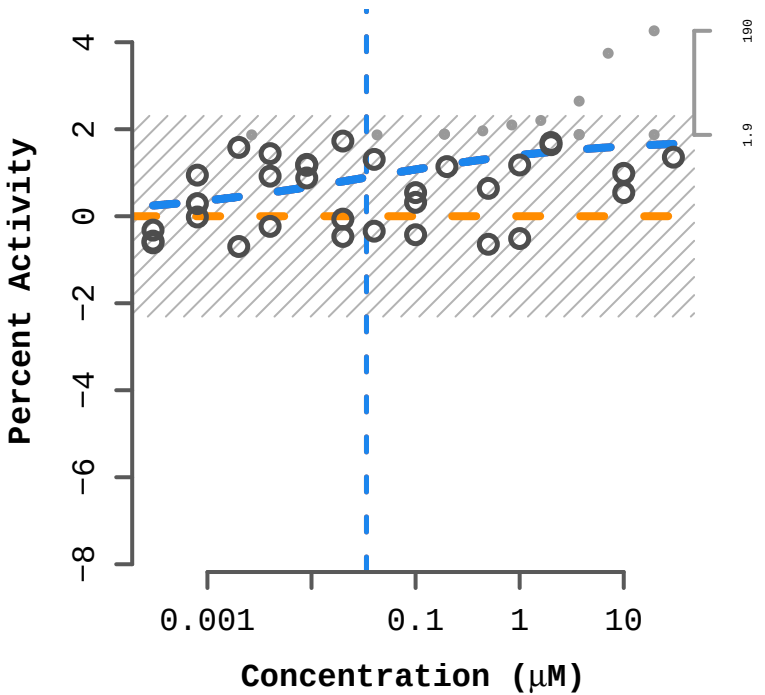
NAME: Potassium acetate
CHID: 27043 **CASRN:** 127-08-2
SPID(S): Tox21_202740
M4ID: 12479512

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium acetate
CHID: 27044 **CASRN:** 127-09-3
SPID(S): Tox21_202741
M4ID: 12479511 **BRK**

HILL MODEL (in red):

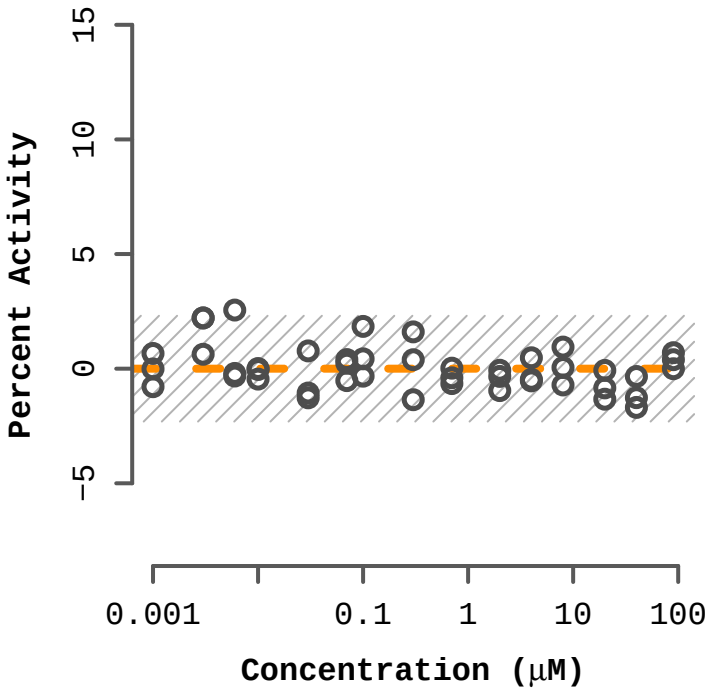
	tp	ga	gw
val:	1.78	−1.47	0.388
sd:	1.25	2.28	0.483

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.78	−1.47	0.388	2.64	6.27
sd:	1.25	2.28	0.483	1820	9820

	CNST	HILL	GNLS
AIC:	318.38	310.8	314.8
PROB:	0.02	0.86	0.12
RMSE:	36.7	36.25	36.25

MAX_MEAN: 63 **MAX_MED:** 2.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

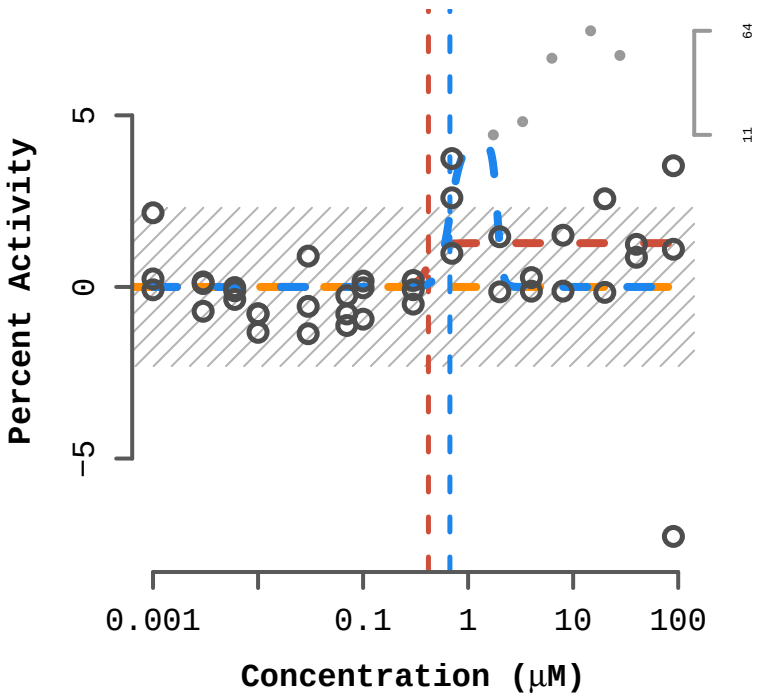
NAME: alpha-Isomethylionone
CHID: 27047 **CASRN:** 127-51-5
SPID(S): Tox21_300152
M4ID: 12478978

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium 3-nitrobenzenesulfonate
CHID: 27048 CASRN: 127-68-4
SPID(S): Tox21_200902
M4ID: 12481350 BRK

HILL MODEL (in red):

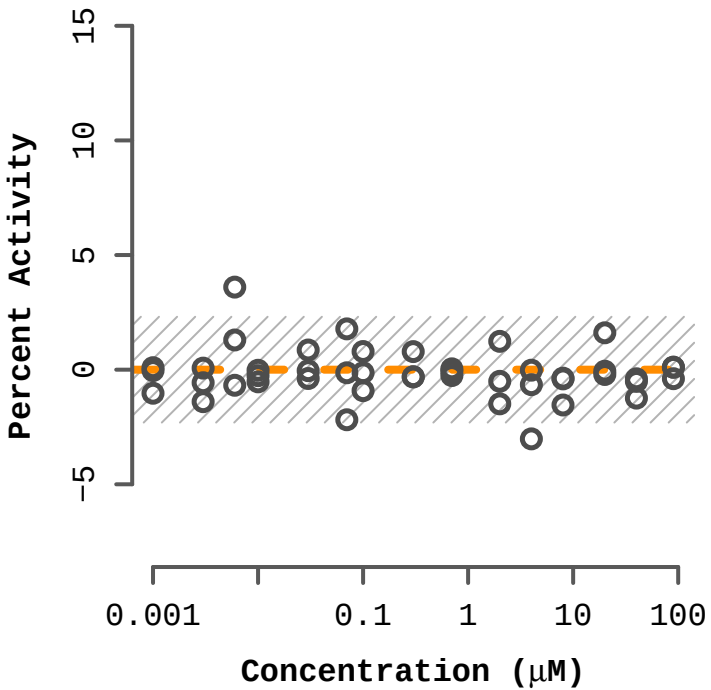
	tp	ga	gw
val:	1.28	−0.378	8
sd:	0.434	0.228	9.94

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.22	−0.174	7.99	0.279	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	280.76	278.62	284.3
PROB:	0.24	0.71	0.04
RMSE:	14.77	14.39	14.74

MAX_MEAN: 22.1 MAX_MED: 2.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

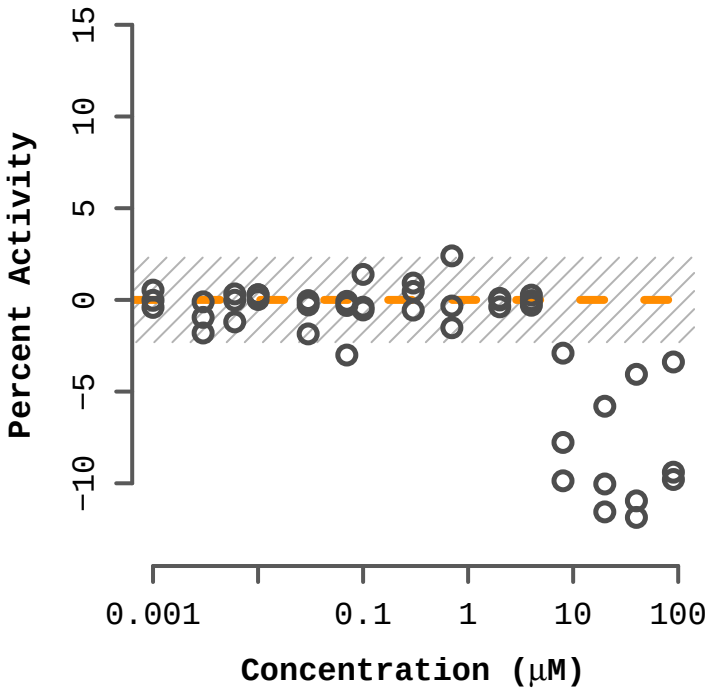
NAME: beta−Pinene
CHID: 27049 **CASRN:** 127−91−3
SPID(S): Tox21_200029
M4ID: 12482223

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

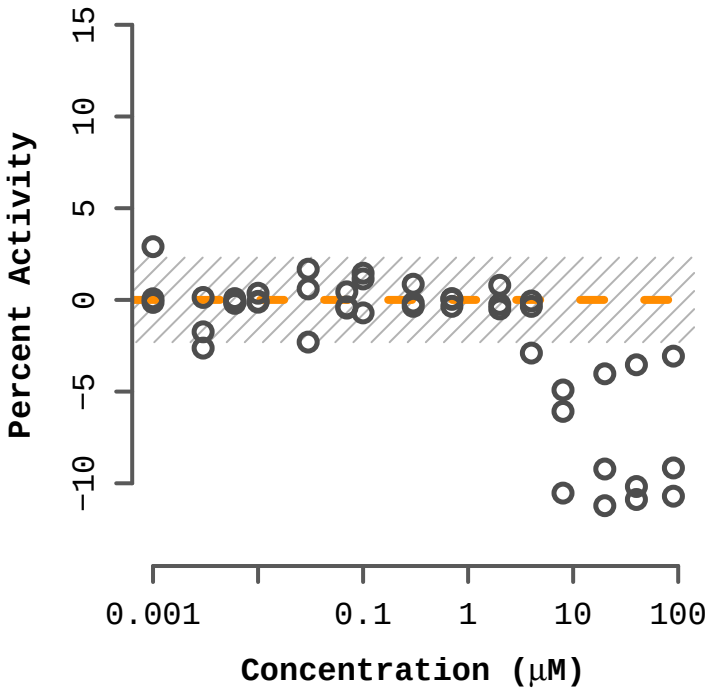
NAME: Sodium dimethyldithiocarbamate
CHID: 27050 **CASRN:** 128-04-1
SPID(S): Tox21_300391
M4ID: 12478741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253.66	NA	NA
PROB:	1	NA	NA
RMSE:	4.57	NA	NA

MAX_MEAN: 0.277 **MAX_MED:** 0.465 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

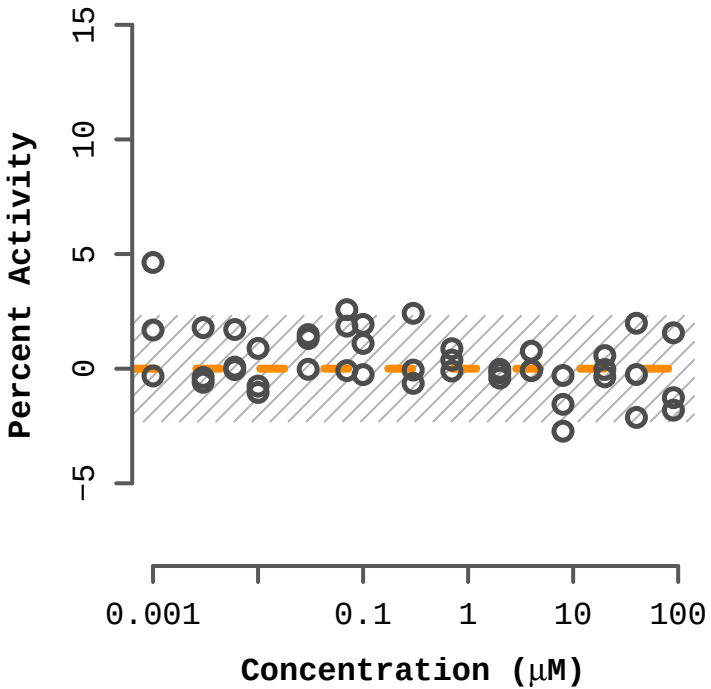
NAME: Sodium dimethyldithiocarbamate
CHID: 27050 **CASRN:** 128-04-1
SPID(S): Tox21_201971
M4ID: 12480281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	252.09	NA	NA
PROB:	1	NA	NA
RMSE:	4.43	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

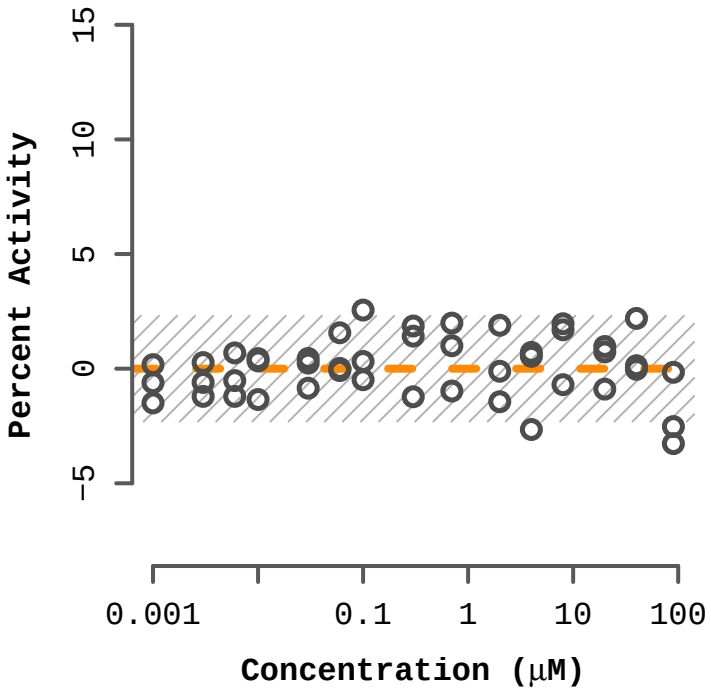
NAME: 2,6-Di-tert-butylphenol
CHID: 27052 **CASRN:** 128-39-2
SPID(S): Tox21_300091
M4ID: 12479039

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

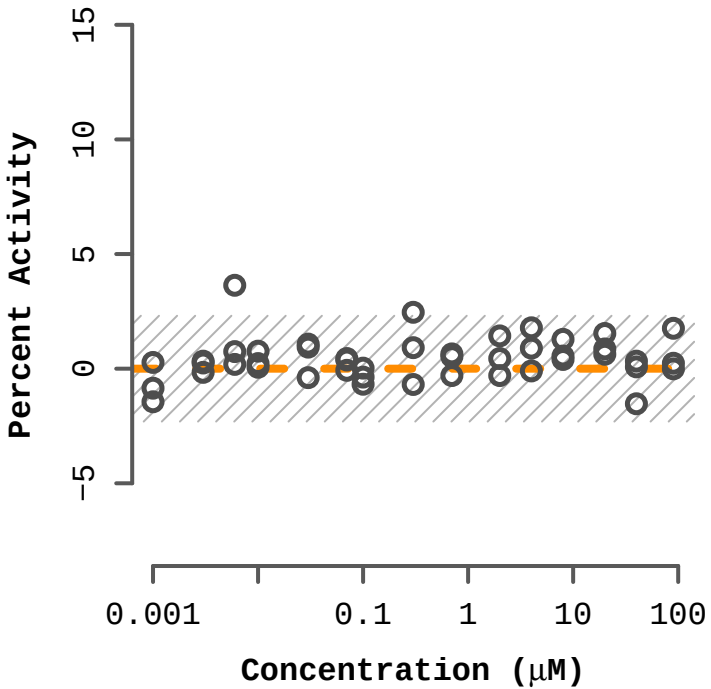
NAME: 2,6-Di-tert-butylphenol
CHID: 27052 **CASRN:** 128-39-2
SPID(S): Tox21_200442
M4ID: 12481810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.988 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

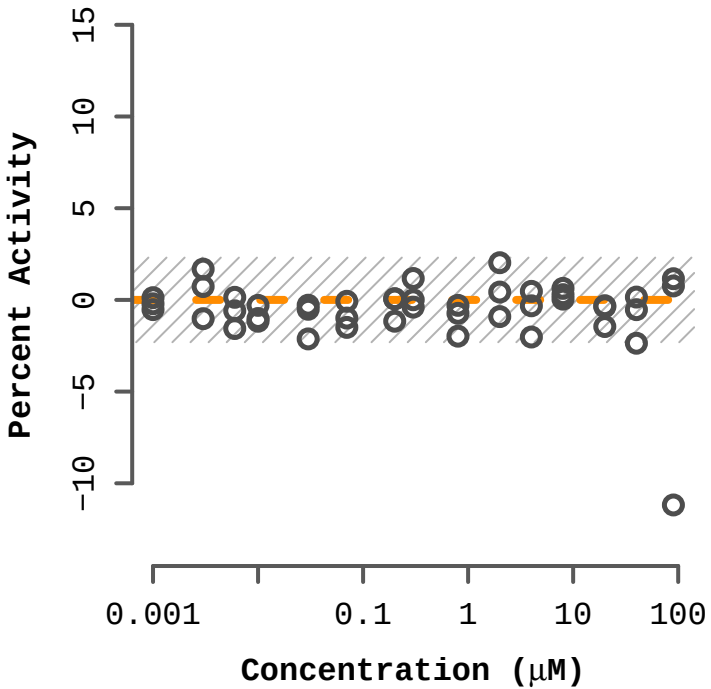
NAME: 2-Naphthalenol
CHID: 27061 **CASRN:** 135-19-3
SPID(S): Tox21_303038
M4ID: 12476095

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 0.942 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

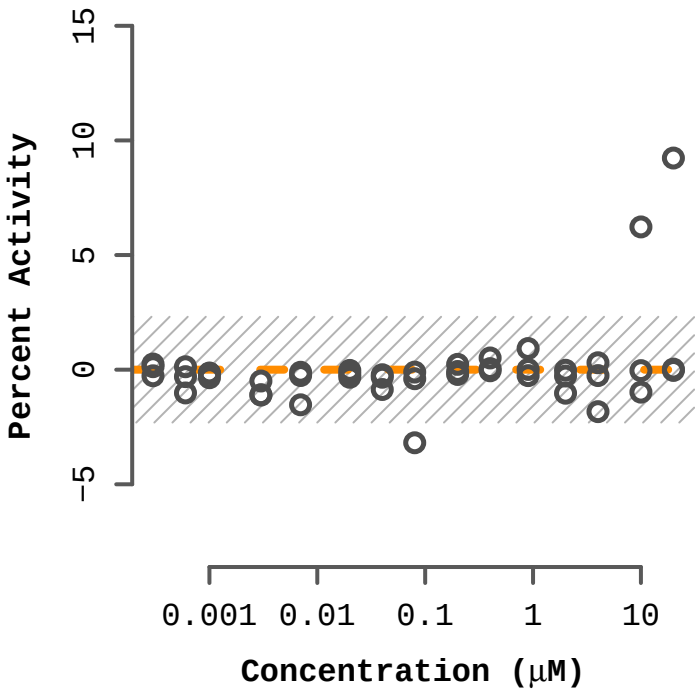
NAME: 2-Naphthalenol
CHID: 27061 **CASRN:** 135-19-3
SPID(S): Tox21_201884
M4ID: 12480368

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 0.517 **MAX_MED:** 0.762 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

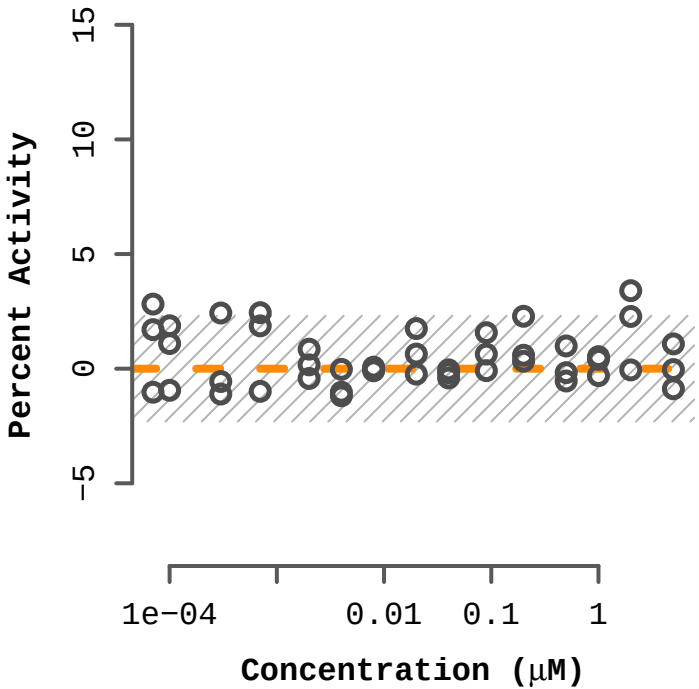
NAME: Calcium 2-ethylhexanoate
CHID: 27063 **CASRN:** 136-51-6
SPID(S): Tox21_202742
M4ID: 12479510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 3.08 **MAX_MED:** 0.132 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

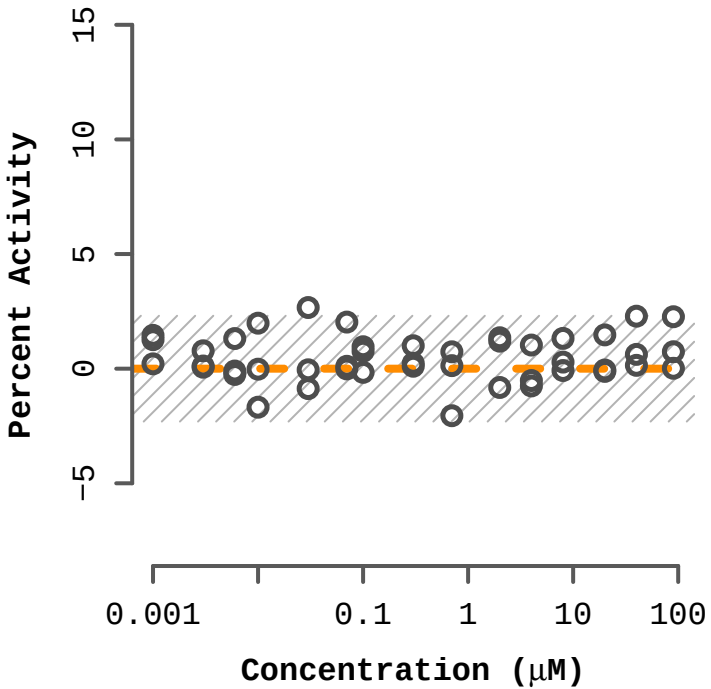
NAME: Sodium [dodecanoyl(methyl)amino]acetate
CHID: 27066 **CASRN:** 137-16-6
SPID(S): Tox21_202996
M4ID: 12479256

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

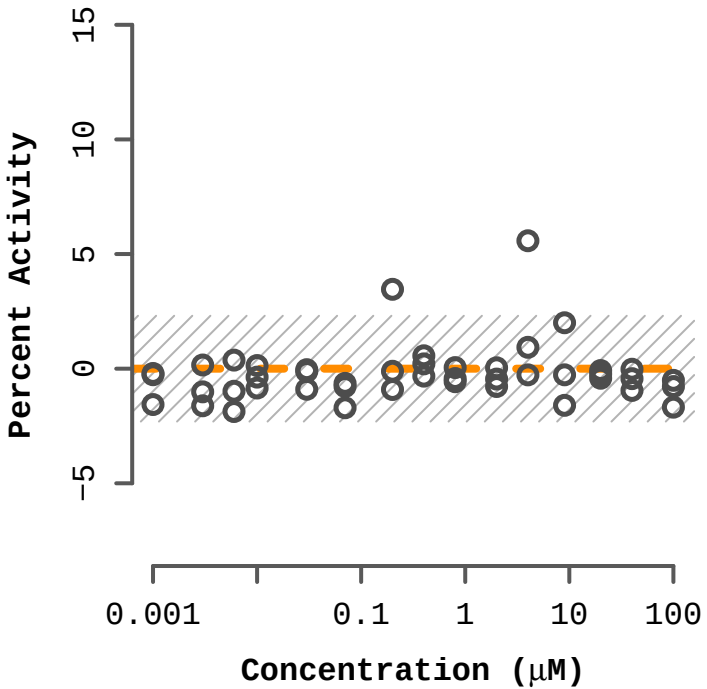
NAME: 2-Methyl-1-butanol
CHID: 27069 **CASRN:** 137-32-6
SPID(S): Tox21_303200
M4ID: 12475933

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

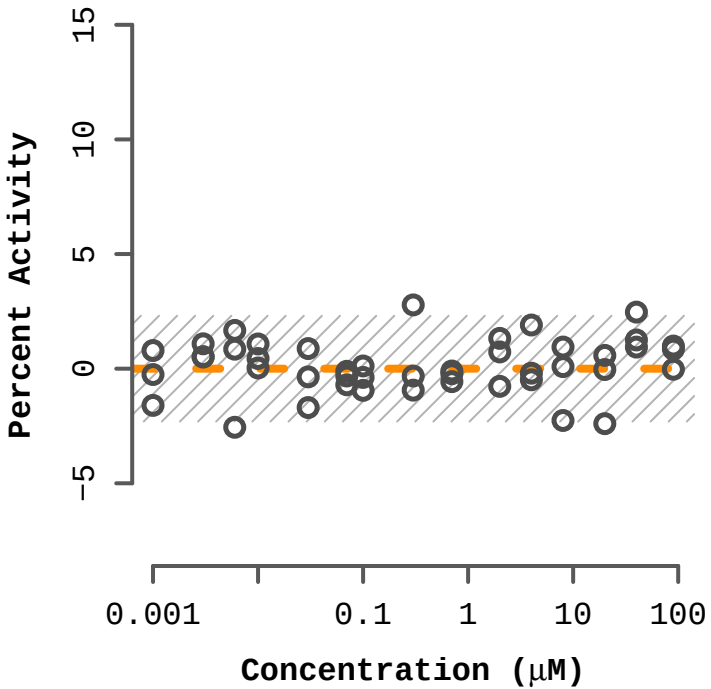
NAME: 2-Methyl-1-butanol
CHID: 27069 **CASRN:** 137-32-6
SPID(S): Tox21_201558
M4ID: 12480694

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

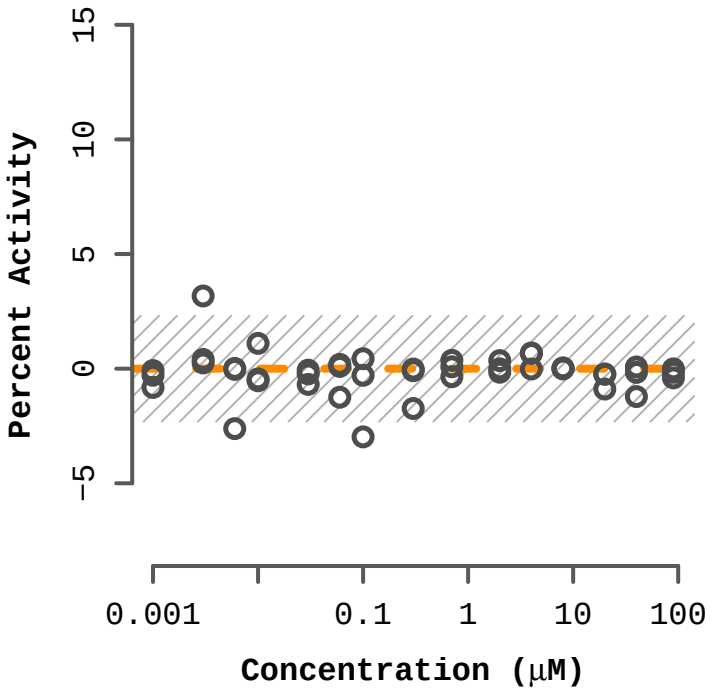
NAME: Sodium phenolate
CHID: 27072 **CASRN:** 139-02-6
SPID(S): Tox21_303251
M4ID: 12475882

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

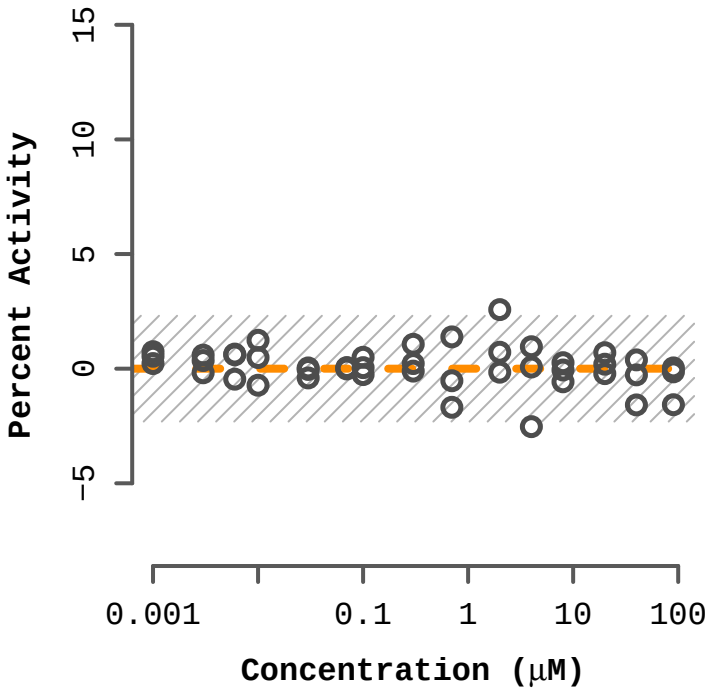
NAME: Sodium phenolate
CHID: 27072 **CASRN:** 139-02-6
SPID(S): Tox21_202212
M4ID: 12480040

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.664 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

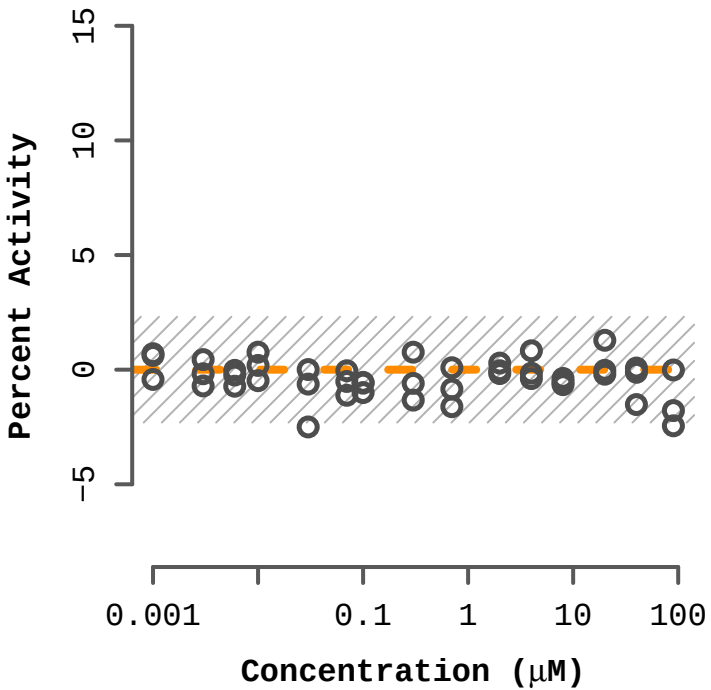
NAME: Dodecyl sulfate triethanolamine
CHID: 27076 **CASRN:** 139-96-8
SPID(S): Tox21_303076
M4ID: 12476057

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.719 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

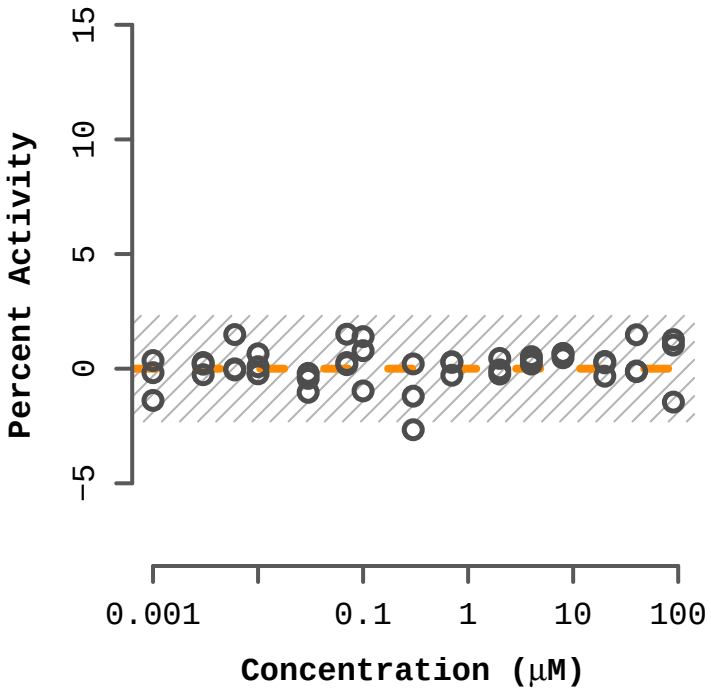
NAME: Proxan-sodium
CHID: 27084 **CASRN:** 140-93-2
SPID(S): Tox21_301325
M4ID: 12477808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.353 **MAX_MED:** 0.623 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

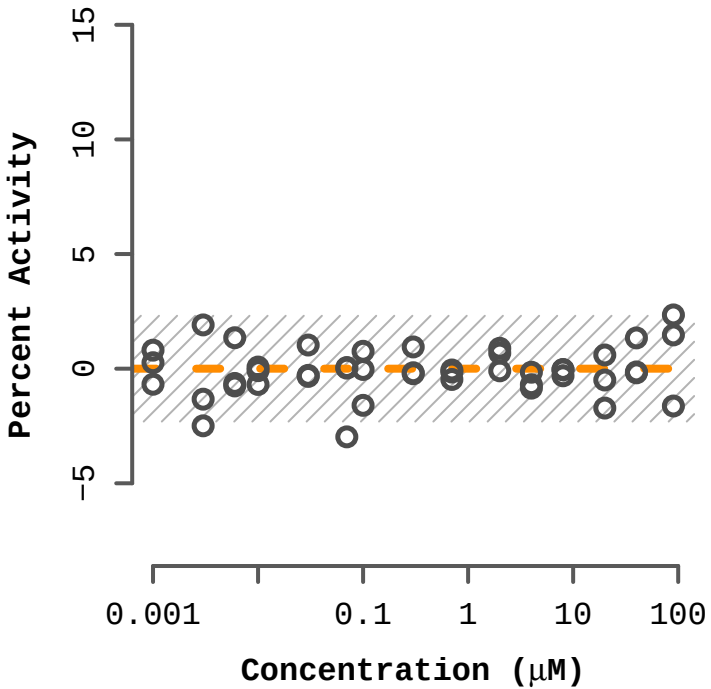
NAME: Bis[2−(2−butoxyethoxy)ethyl] hexandioate
CHID: 27085 **CASRN:** 141−17−3
SPID(S): Tox21_303084
M4ID: 12476049

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.65 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

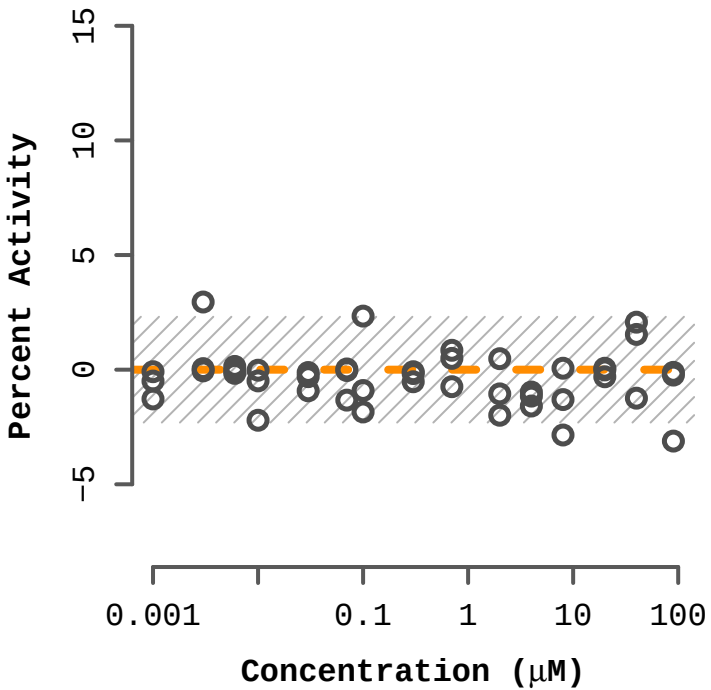
NAME: Bis[2−(2−butoxyethoxy)ethyl] hexandioate
CHID: 27085 **CASRN:** 141−17−3
SPID(S): Tox21_202042
M4ID: 12480210

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.731 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

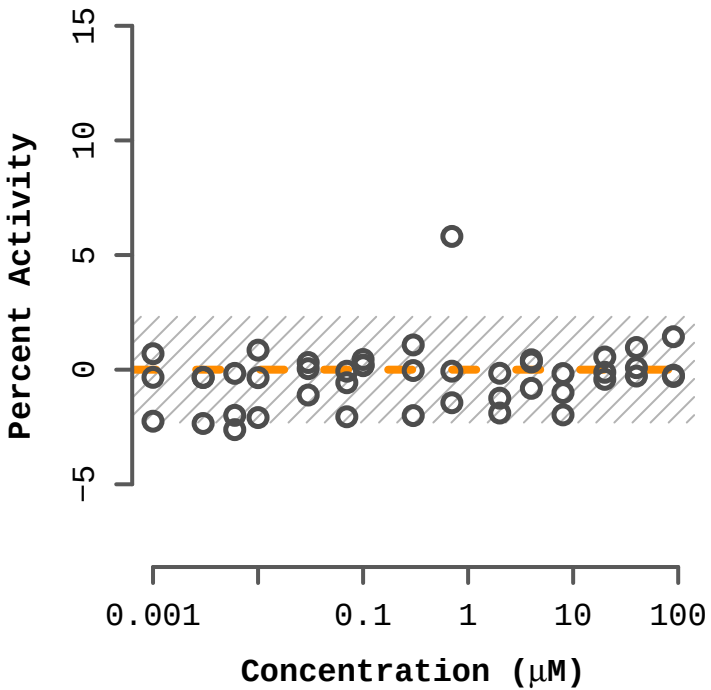
NAME: Methyl 12-hydroxyoctadecanoate
CHID: 27086 CASRN: 141-23-1
SPID(S): Tox21_303267
M4ID: 12475866

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.983 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

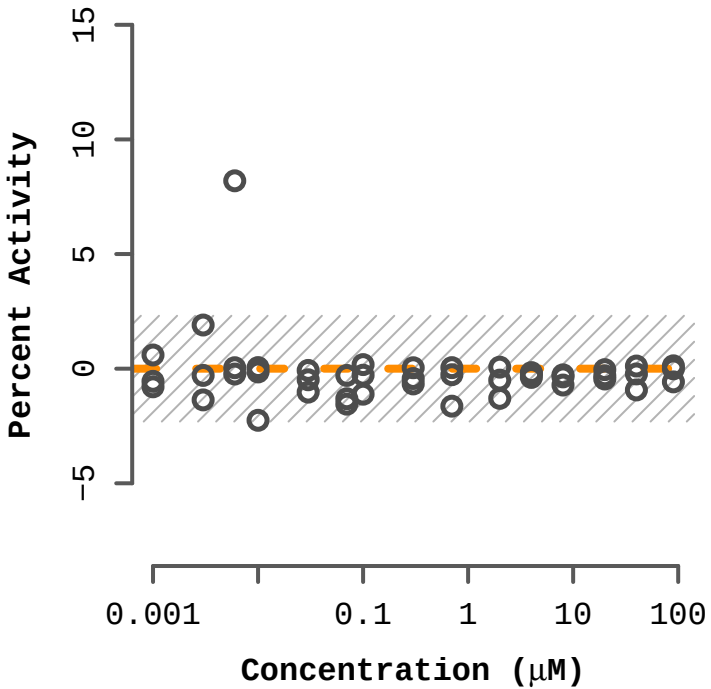
NAME: Ethyl acetoacetate
CHID: 27092 **CASRN:** 141-97-9
SPID(S): Tox21_200645
M4ID: 12481607

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.336 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

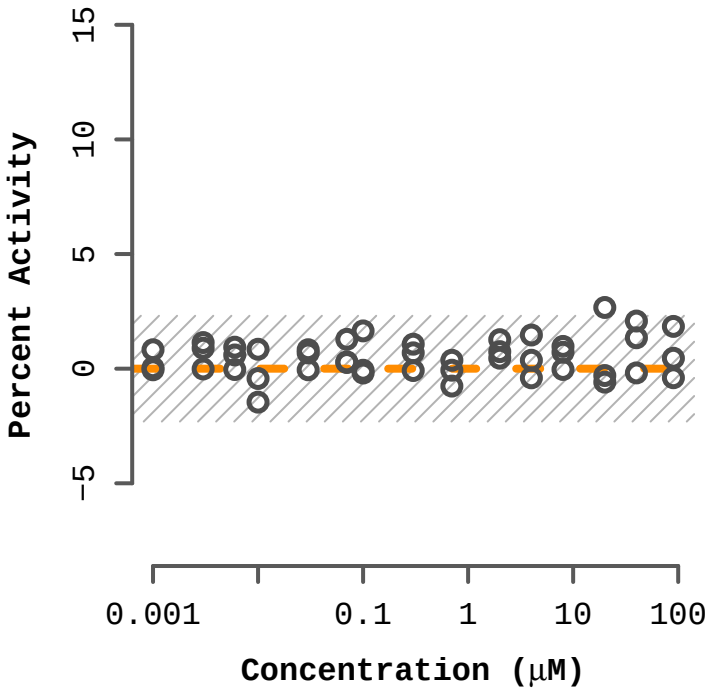
NAME: Bis(2-ethylhexyl) maleate
CHID: 27094 **CASRN:** 142-16-5
SPID(S): Tox21_303254
M4ID: 12475879

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.67 **MAX_MED:** 0.0432 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

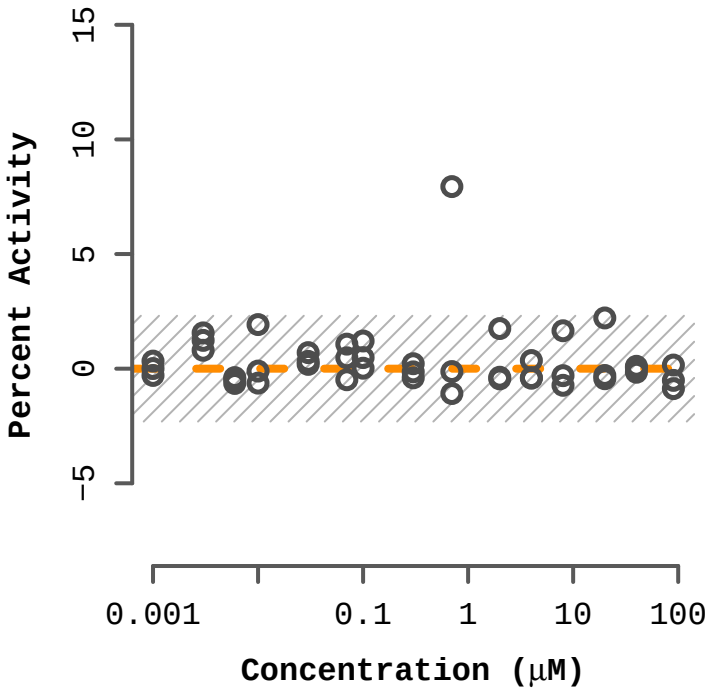
NAME: Bis(2-ethylhexyl) maleate
CHID: 27094 **CASRN:** 142-16-5
SPID(S): Tox21_201422
M4ID: 12480830

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

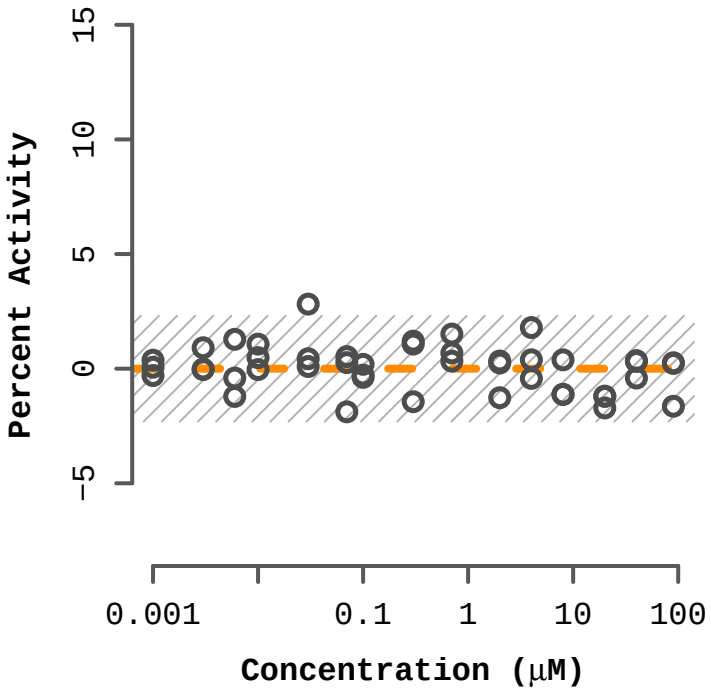
NAME: 2,5-Dimethyl-3-hexyne-2,5-diol
CHID: 27096 **CASRN:** 142-30-3
SPID(S): Tox21_201021
M4ID: 12481231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

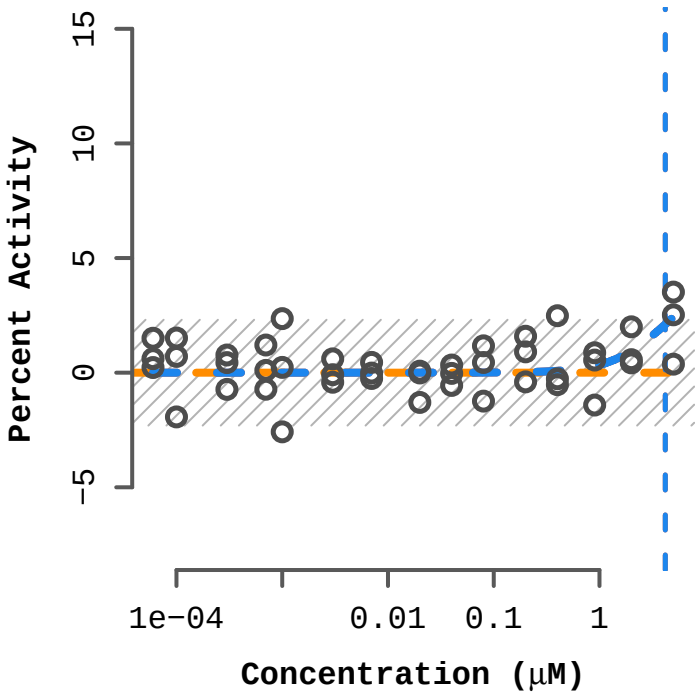
NAME: Magnesium acetate
CHID: 27097 **CASRN:** 142-72-3
SPID(S): Tox21_202557
M4ID: 12479695

HILL MODEL: Not applicable.

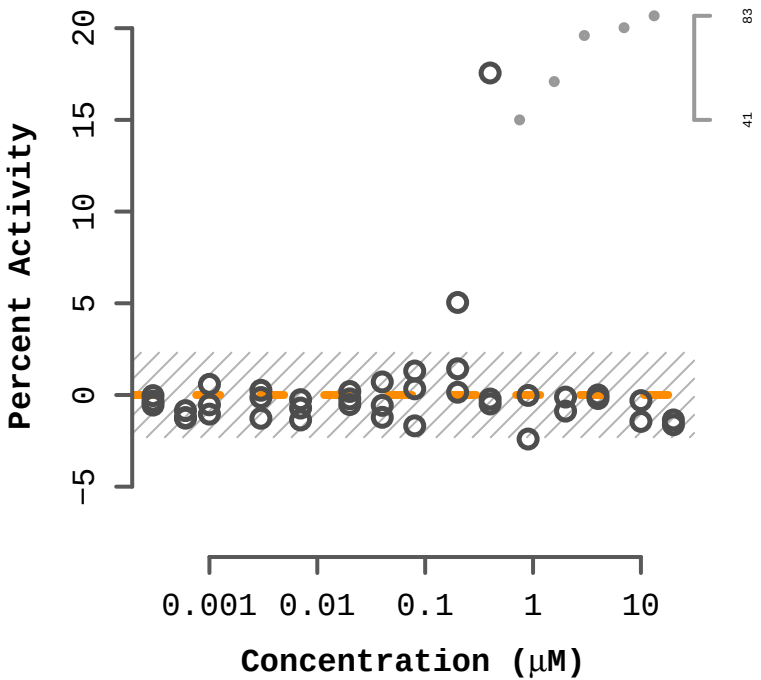
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.07 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Iminodiacetic acid
CHID:    27098   CASRN: 142-73-4
SPID(S): Tox21_202743
M4ID:    12479509

HILL MODEL (in red):
      tp       ga       gw
val:  4.22     0.622    1.68
sd:   9.16     1.2      2.63

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.22     0.622    1.68     2.7      6.1
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  146.61      141.83      145.83
PROB: 0.07        0.82        0.11
RMSE: 1.22        1.06        1.06

MAX_MEAN: 2.14      MAX_MED: 2.53      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

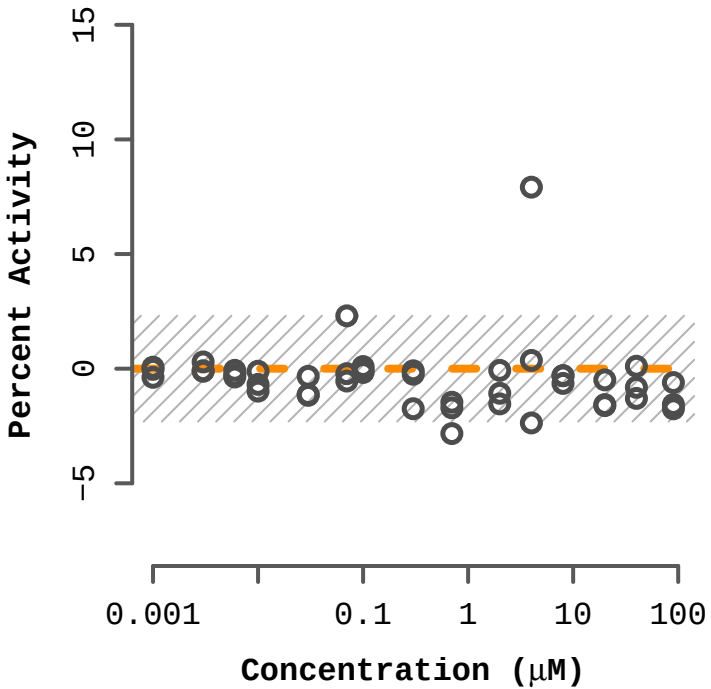
NAME: 9-Octadecenoic acid (9Z)-, butyl ester
CHID: 27099 **CASRN:** 142-77-8
SPID(S): Tox21_202744
M4ID: 12479508 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	320.83	NA	NA
PROB:	1	NA	NA
RMSE:	23.03	NA	NA

MAX_MEAN: 26.6 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

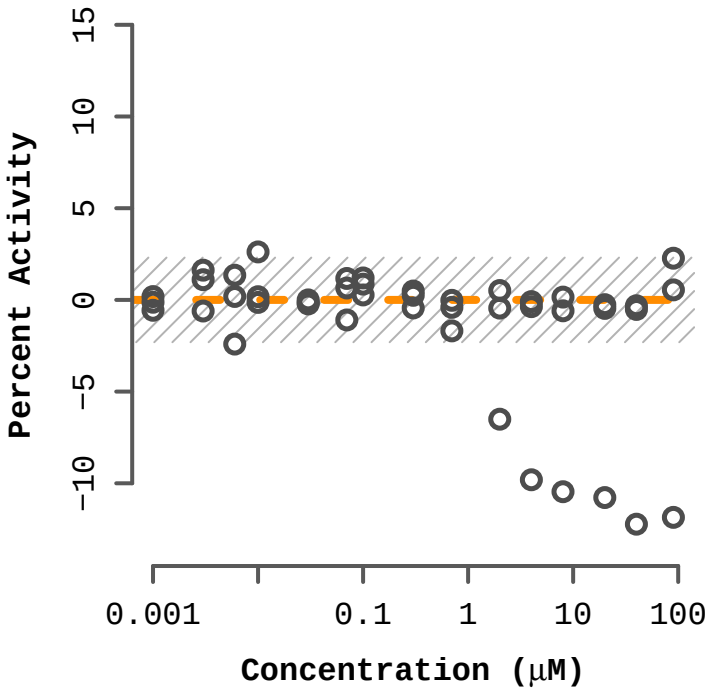
NAME: Dodecyl 2-methylacrylate
CHID: 27103 CASRN: 142-90-5
SPID(S): Tox21_303316
M4ID: 12475817

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.97 MAX_MED: 0.362 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

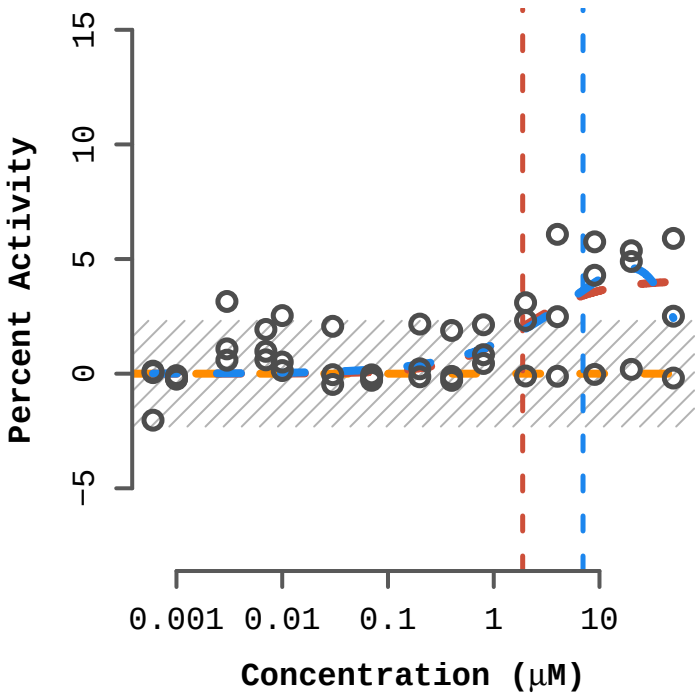
NAME: Dodecyl 2-methylacrylate
CHID: 27103 **CASRN:** 142-90-5
SPID(S): Tox21_201903
M4ID: 12480349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.2	NA	NA
PROB:	1	NA	NA
RMSE:	3.91	NA	NA

MAX_MEAN: 0.886 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexadecanoic acid, 1-methylethyl ester
CHID: 27104 CASRN: 142-91-6
SPID(S): Tox21_202558
M4ID: 12479694

HILL MODEL (in red):

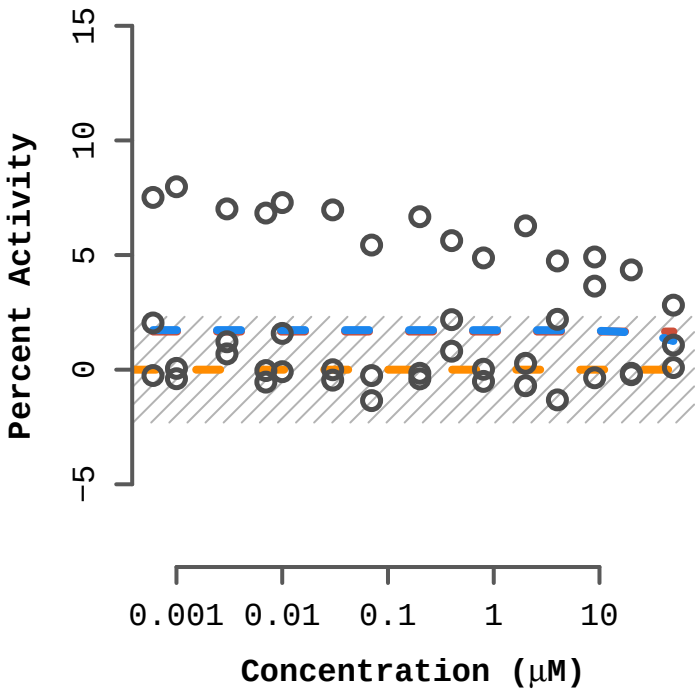
	tp	ga	gw
val:	4.08	0.274	1.24
sd:	1.11	0.301	0.778

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.29	0.844	0.801	1.64	2.89
sd:	8.68	1.28	0.601	0.268	4.3

	CNST	HILL	GNLS
AIC:	201.16	181.07	182.51
PROB:	0	0.67	0.33
RMSE:	2.35	1.66	1.65

MAX_MEAN: 3.48 MAX_MED: 4.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexadecanoic acid, 1-methylethyl ester
CHID: 27104 **CASRN:** 142-91-6
SPID(S): Tox21_112085_1
M4ID: 12483330

HILL MODEL (in red):

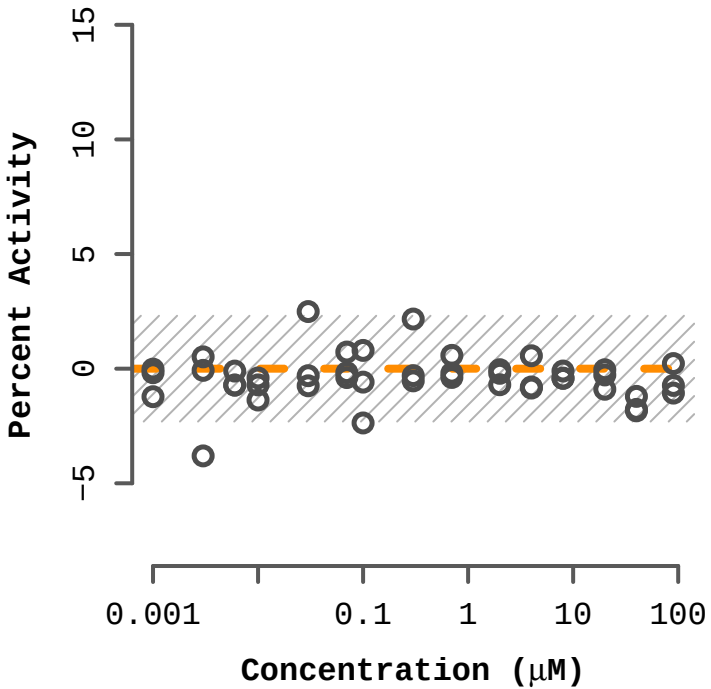
	tp	ga	gw
val:	1.66	−4.95	3.76
sd:	0.479	930	2050

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.73	−4.99	3.87	1.93	1.86
sd:	0.532	1440	3200	1.42	7.22

	CNST	HILL	GNLS
AIC:	245.36	238.04	241.94
PROB:	0.02	0.86	0.12
RMSE:	3.65	2.97	2.96

MAX_MEAN: 3.1 **MAX_MED:** 3.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

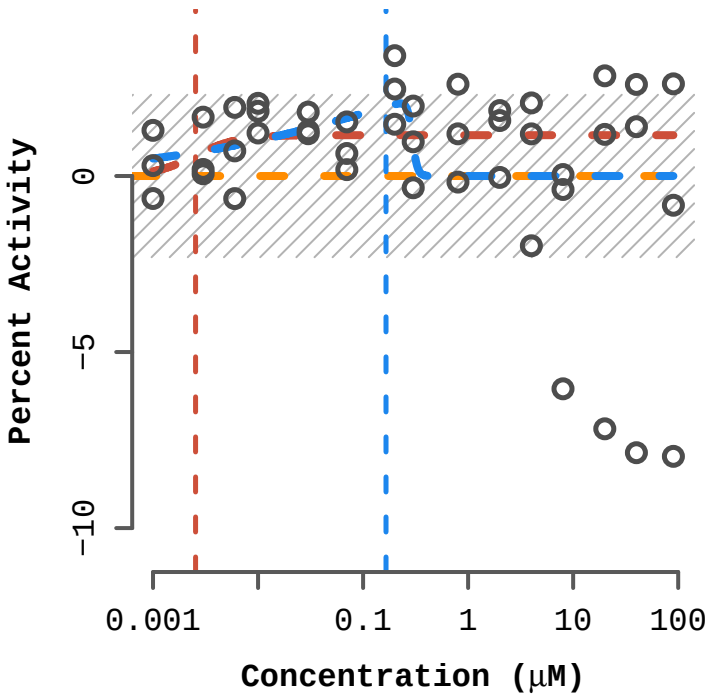
NAME: N-(6-Aminohexyl)hexane-1,6-diamine
CHID: 27109 **CASRN:** 143-23-7
SPID(S): Tox21_200046
M4ID: 12482206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** −0.0713 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2,4−Trimethyl−1,3−pentanediol
CHID: 27113 CASRN: 144−19−4
SPID(S): Tox21_200443
M4ID: 12481809

HILL MODEL (in red):

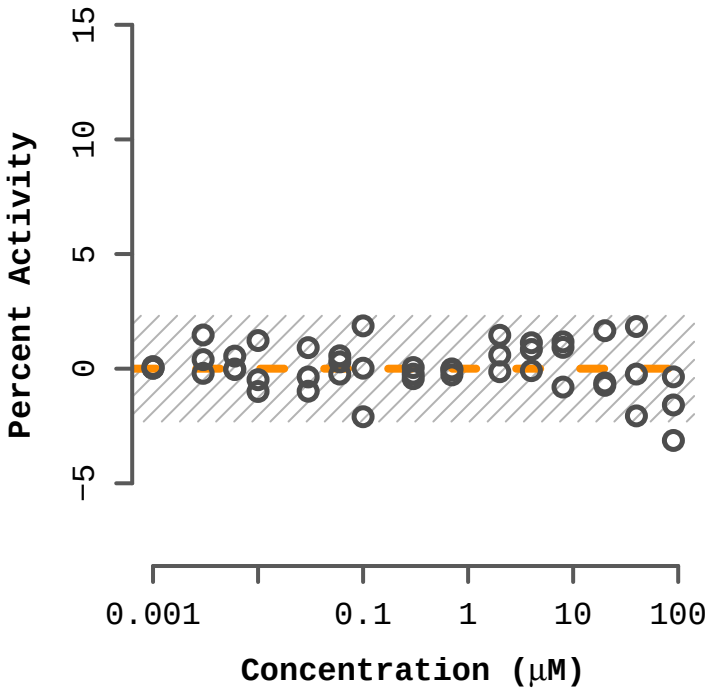
	tp	ga	gw
val:	1.16	−2.59	2.18
sd:	0.26	0.699	4.09

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.93	−0.782	0.379	−0.532	18
sd:	14	7.74	0.63	0.0558	70.7

	CNST	HILL	GNLS
AIC:	209.16	199.92	206.01
PROB:	0.01	0.95	0.04
RMSE:	2.65	2.74	2.5

MAX_MEAN: 2.45 MAX_MED: 2.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

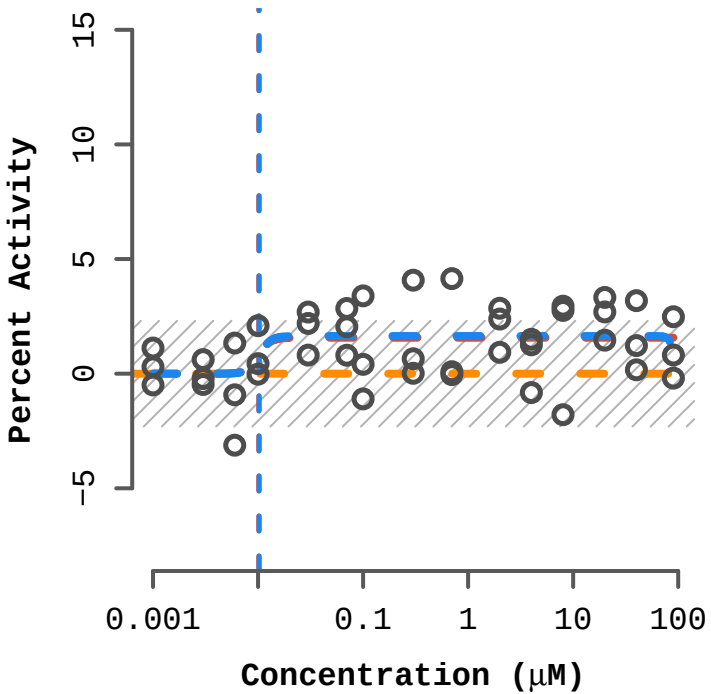
NAME: Chloro(methyl)diphenylsilane
CHID: 27116 **CASRN:** 144-79-6
SPID(S): Tox21_200662
M4ID: 12481590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.931 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium hydroxymethanesulfinate
CHID: 27120 **CASRN:** 149-44-0
SPID(S): Tox21_201133
M4ID: 12481119

HILL MODEL (in red):

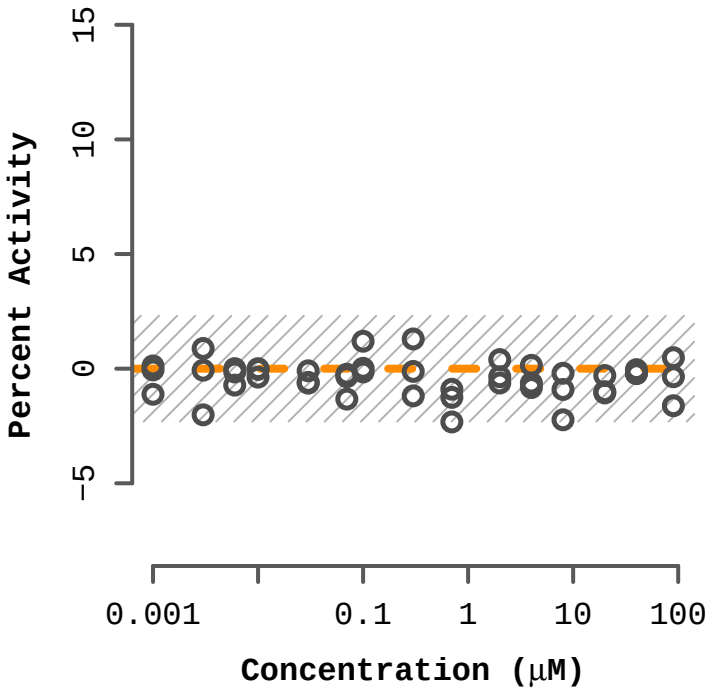
	tp	ga	gw
val:	1.57	−1.99	8
sd:	0.273	0.109	14.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.64	−1.99	8	1.96	17.8
sd:	0.288	0.108	14.6	0.0588	120

	CNST	HILL	GNLS
AIC:	193.13	171.44	174.84
PROB:	0	0.85	0.15
RMSE:	1.94	1.42	1.42

MAX_MEAN: 2.49 **MAX_MED:** 2.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

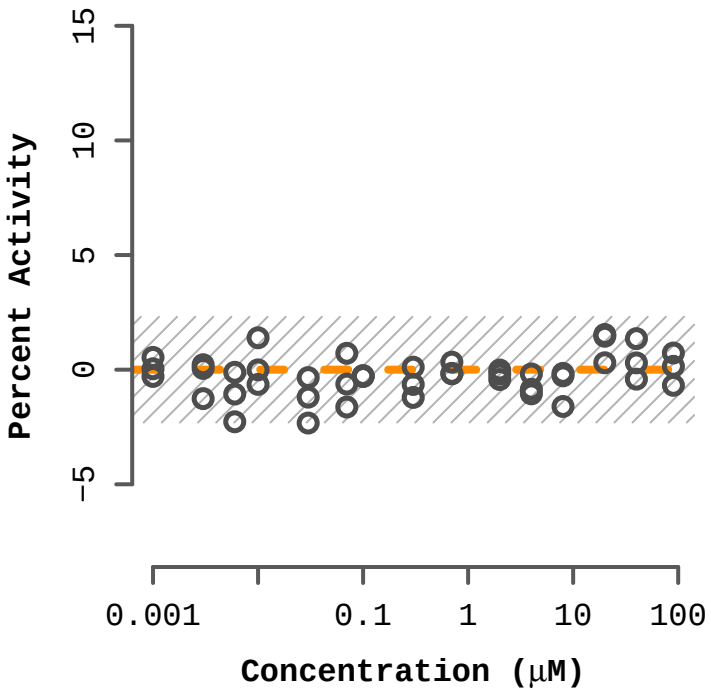
NAME: Trimethoxymethane
CHID: 27122 **CASRN:** 149-73-5
SPID(S): Tox21_200062
M4ID: 12482190

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.358 **MAX_MED:** 0.0171 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

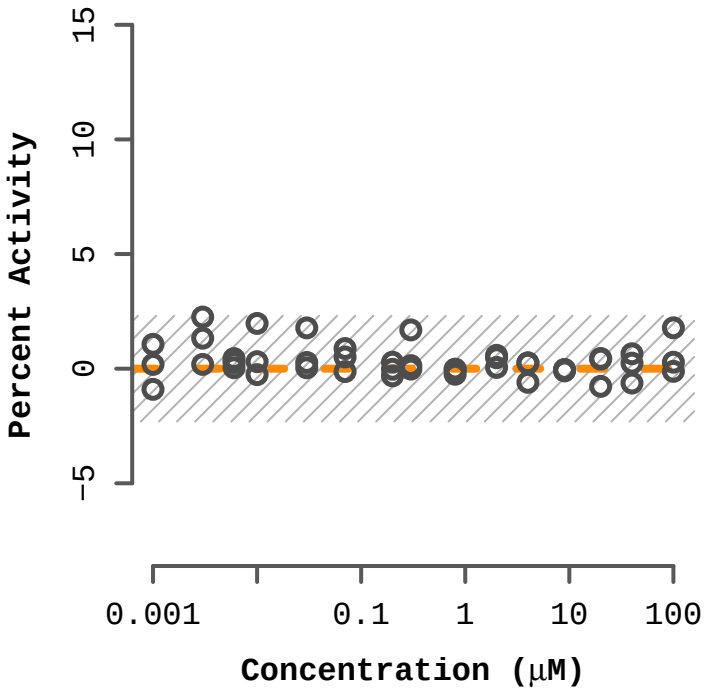
NAME: 1H-1,2,4-Triazole
CHID: 27131 **CASRN:** 288-88-0
SPID(S): Tox21_300113
M4ID: 12479017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

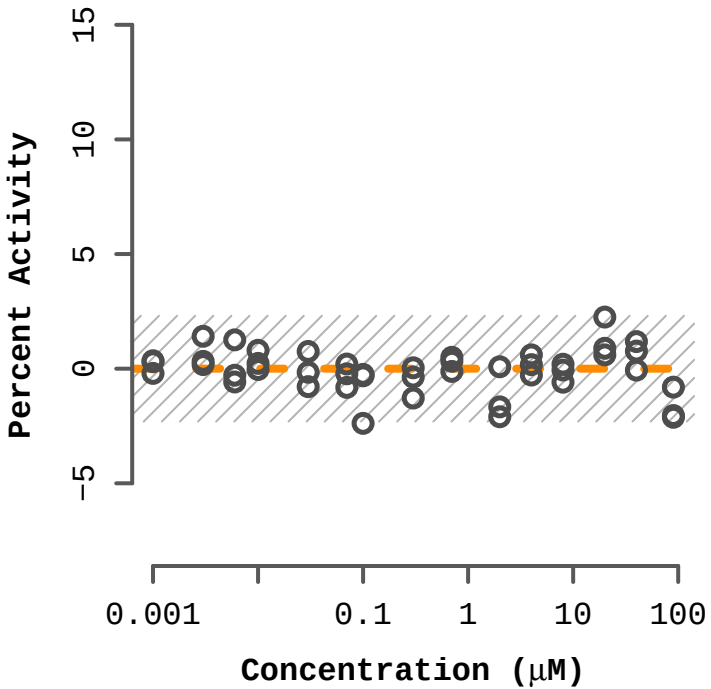
NAME: O,O−Diethyl dithiophosphate
CHID: 27133 **CASRN:** 298−06−6
SPID(S): Tox21_301493
M4ID: 12477640

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

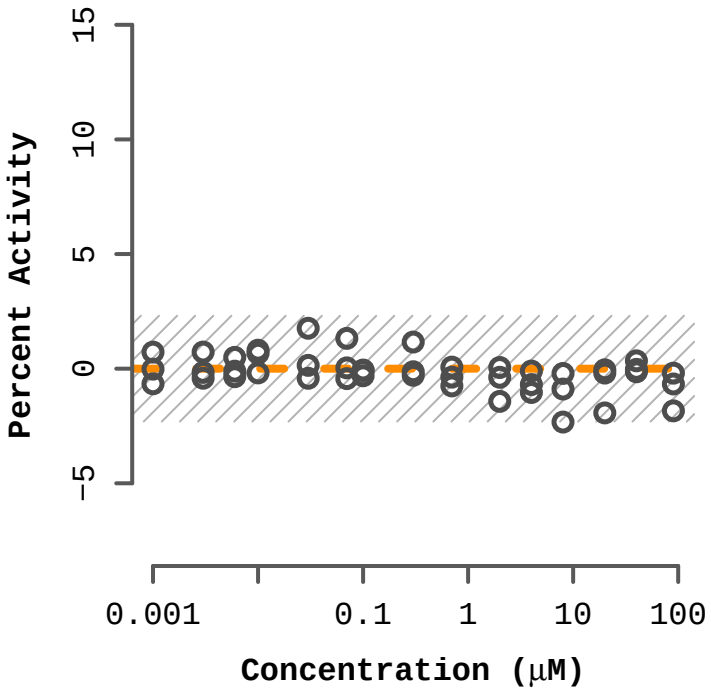
NAME: Bis(2-ethylhexyl) phosphate
CHID: 27134 **CASRN:** 298-07-7
SPID(S): Tox21_303087
M4ID: 12476046

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

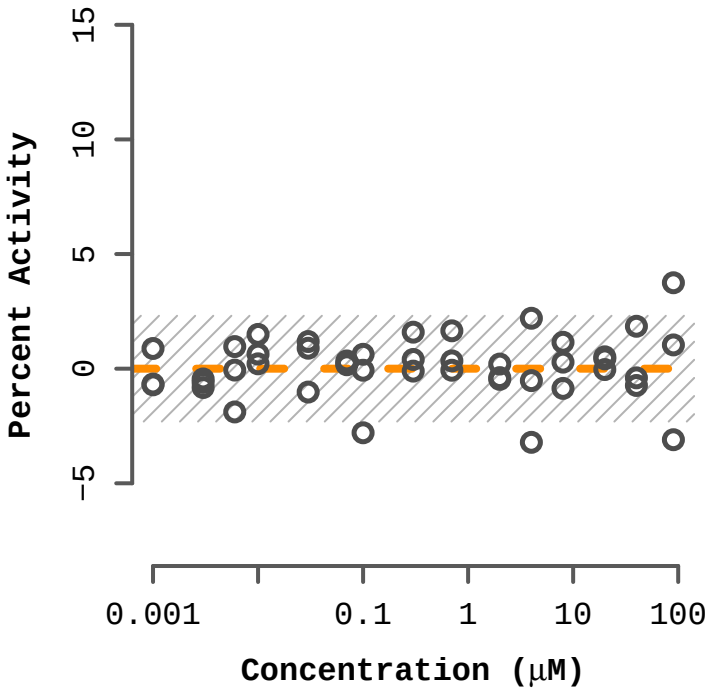
NAME: Bis(2-ethylhexyl) phosphate
CHID: 27134 **CASRN:** 298-07-7
SPID(S): Tox21_201622
M4ID: 12480630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.497 **MAX_MED:** 0.674 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

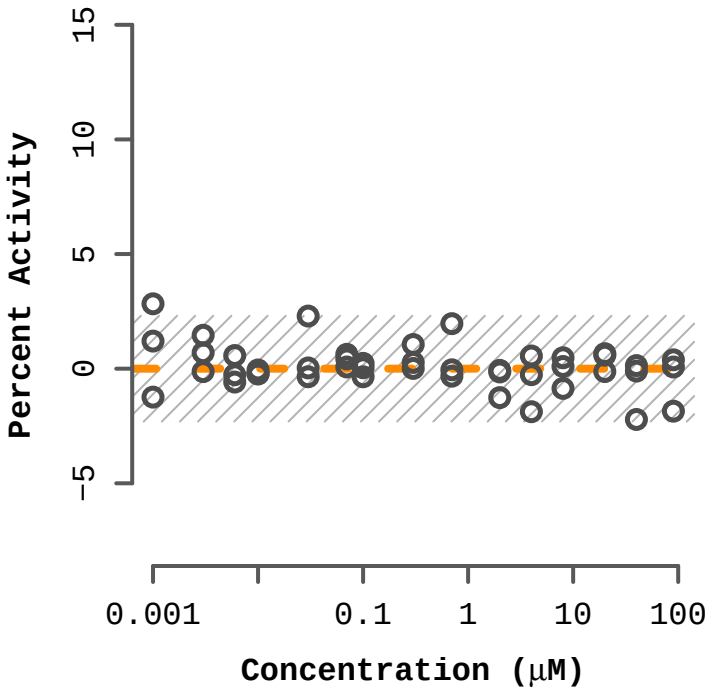
NAME: (9Z)-Octadec-9-enamide
CHID: 27137 **CASRN:** 301-02-0
SPID(S): Tox21_200444
M4ID: 12481808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.782 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

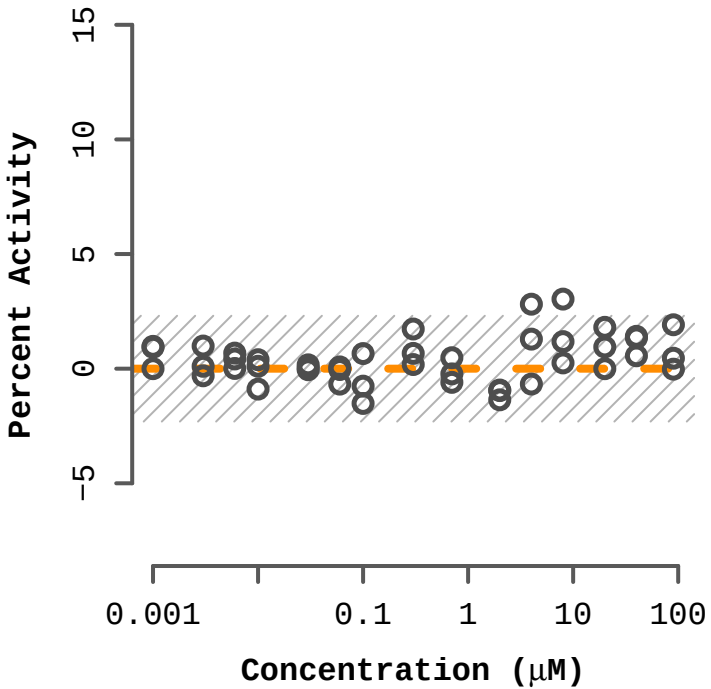
NAME: 1,2-Dichloro-4-(trifluoromethyl)benzene
CHID: 27142 **CASRN:** 328-84-7
SPID(S): Tox21_303089
M4ID: 12476044

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

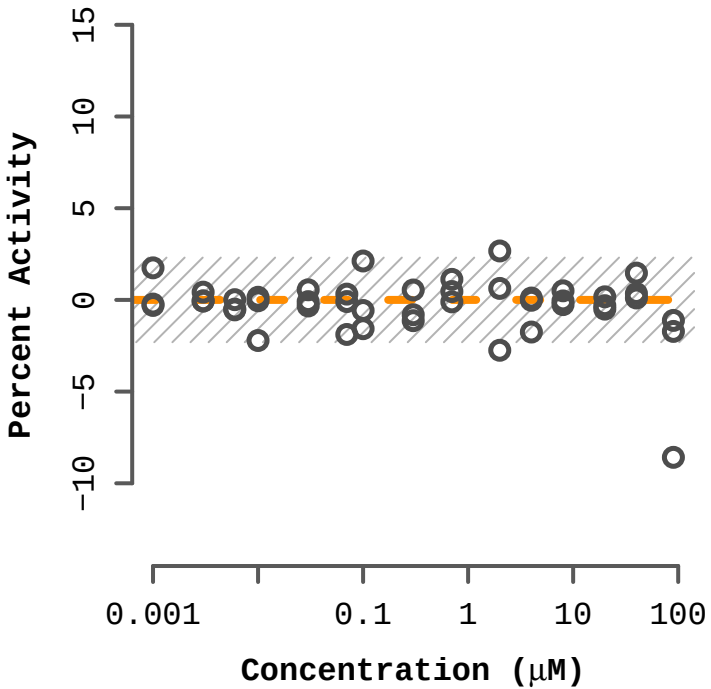
NAME: 1,2-Dichloro-4-(trifluoromethyl)benzene
CHID: 27142 **CASRN:** 328-84-7
SPID(S): Tox21_201972
M4ID: 12480280

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

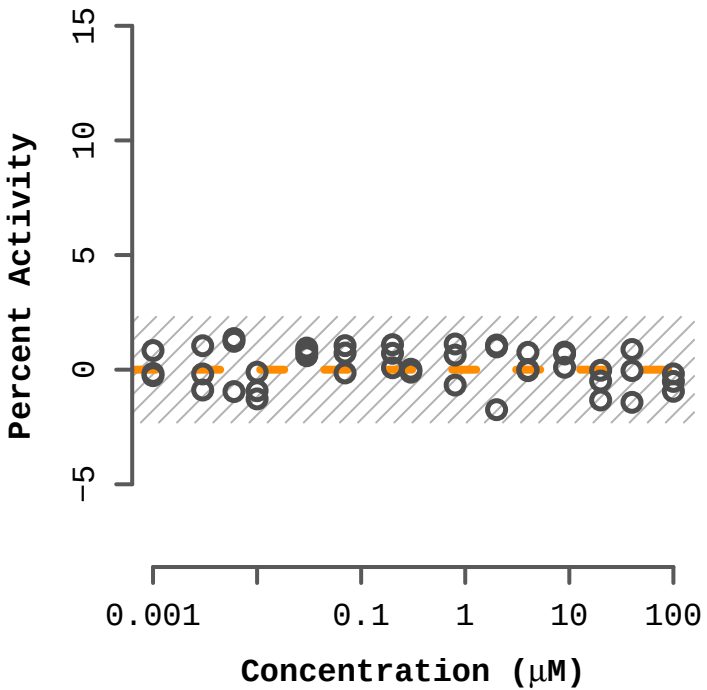
NAME: 1-Isocyanato-3-(trifluoromethyl)benzene
CHID: 27143 **CASRN:** 329-01-1
SPID(S): Tox21_200679
M4ID: 12481573

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

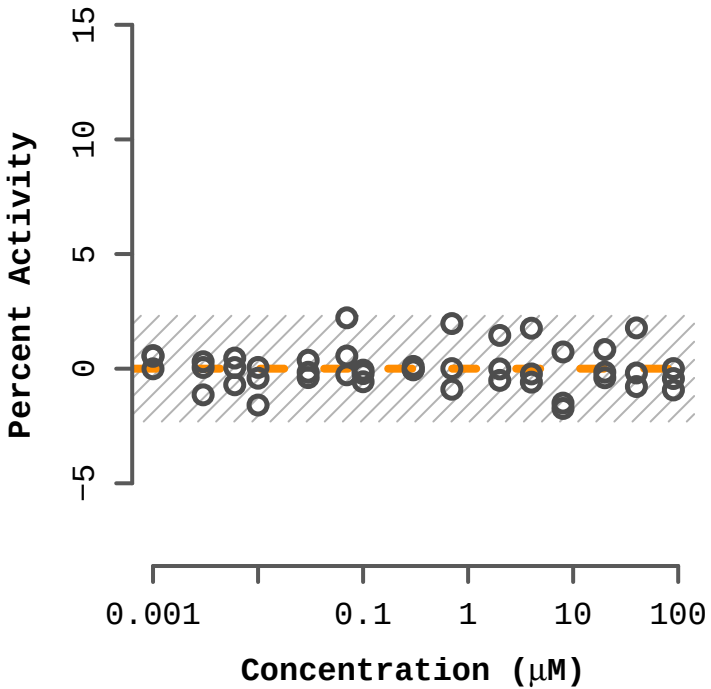
NAME: Diethyl sulfide
CHID: 27146 CASRN: 352-93-2
SPID(S): Tox21_200927
M4ID: 12481325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.782 MAX_MED: 1.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

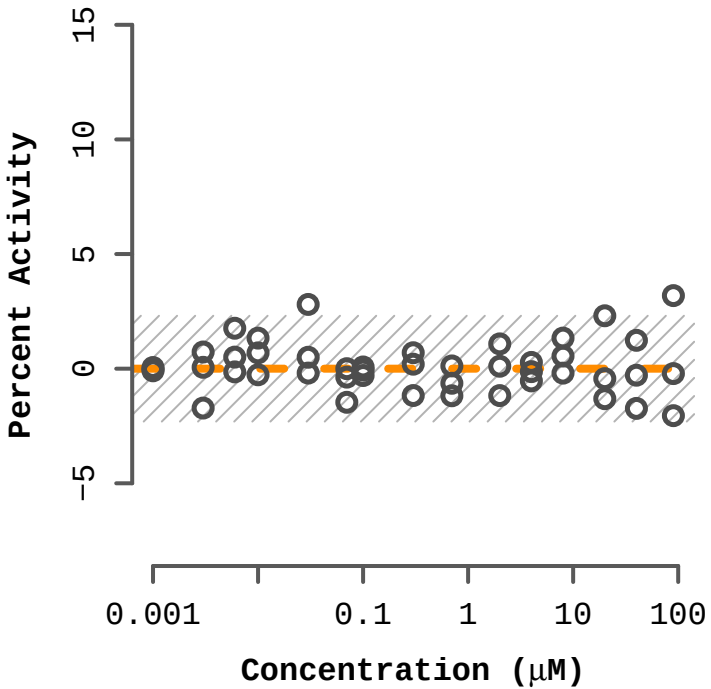
NAME: 1,1,1−Trichloro−2,2,2−trifluoroethane
CHID: 27148 CASRN: 354−58−5
SPID(S): Tox21_200079
M4ID: 12482173

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.836 **MAX_MED:** 0.555 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

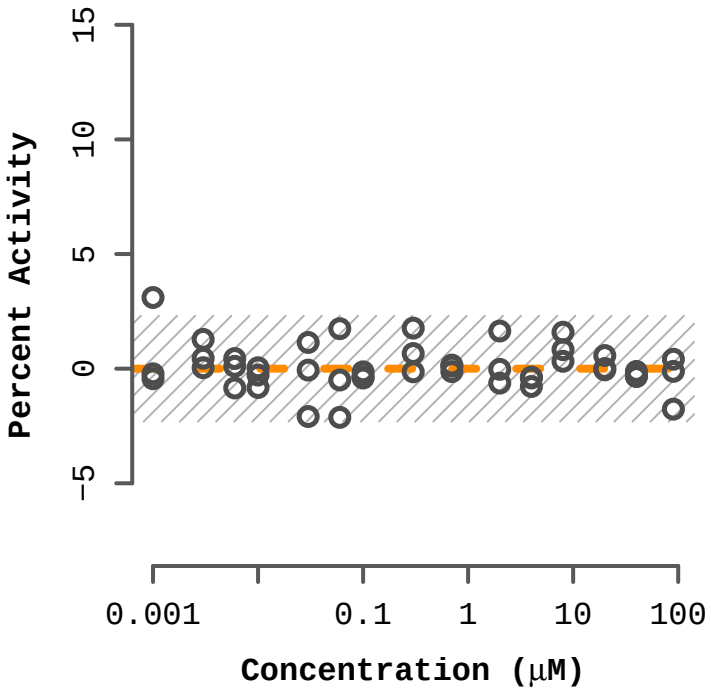
NAME: Cyanoacetic acid
CHID: 27149 **CASRN:** 372-09-8
SPID(S): Tox21_303155
M4ID: 12475978

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.691 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

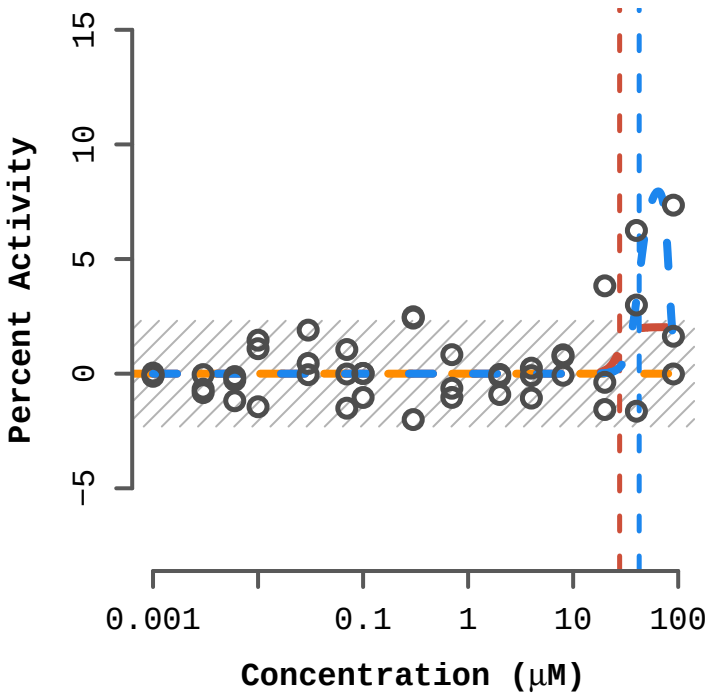
NAME: Cyanoacetic acid
CHID: 27149 **CASRN:** 372-09-8
SPID(S): Tox21_201645
M4ID: 12480607

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.916 **MAX_MED:** 0.831 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Bromo-4-fluorobenzene
CHID: 27153 CASRN: 460-00-4
SPID(S): Tox21_303305
M4ID: 12475828

HILL MODEL (in red):

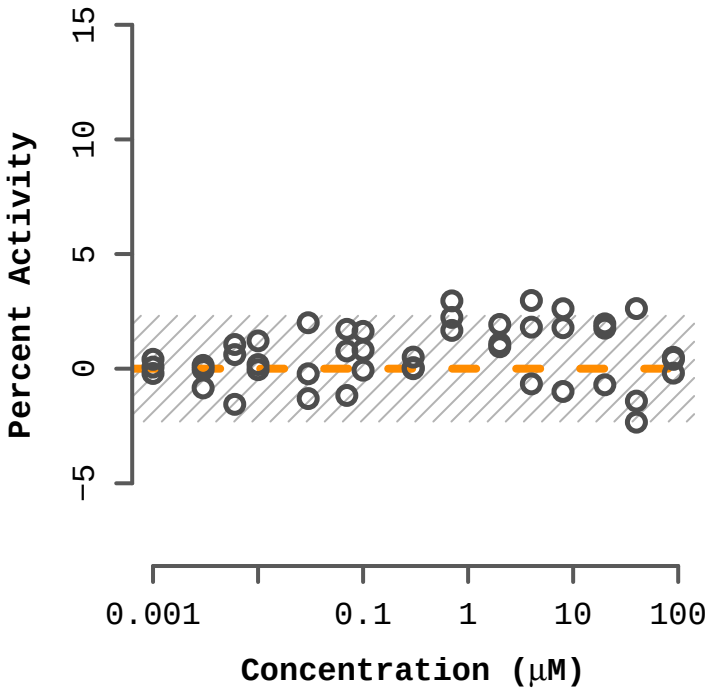
	tp	ga	gw
val:	2.03	1.44	8
sd:	0.968	0.141	7.68

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.38	1.63	7.88	1.91	17.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	171.6	172.89	175.04
PROB:	0.59	0.31	0.11
RMSE:	1.9	1.63	1.67

MAX_MEAN: 2.99 MAX_MED: 3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

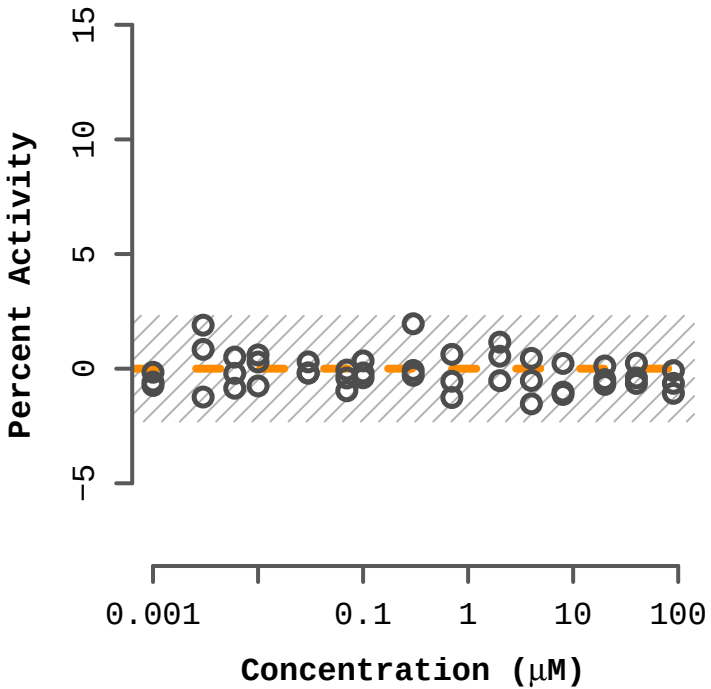
NAME: 1-Bromo-4-fluorobenzene
CHID: 27153 **CASRN:** 460-00-4
SPID(S): Tox21_201379
M4ID: 12480873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.29 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

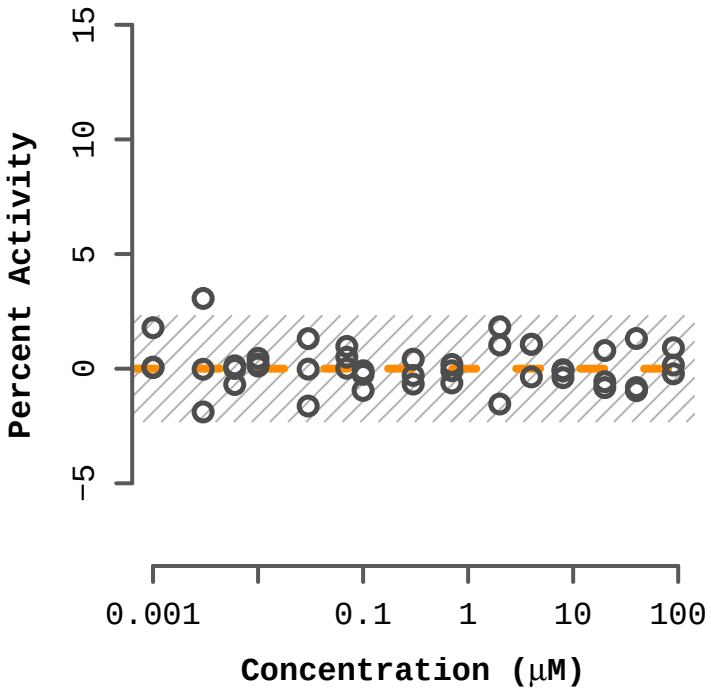
NAME: Benzyl chloroformate
CHID: 27158 **CASRN:** 501-53-1
SPID(S): Tox21_201072
M4ID: 12481180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.533 **MAX_MED:** 0.844 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

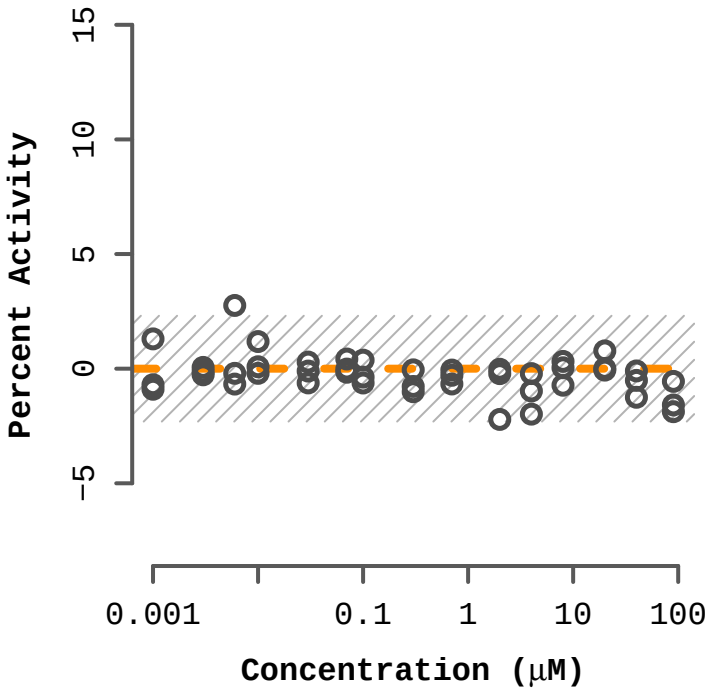
NAME: 2-Oxepanone
CHID: 27159 **CASRN:** 502-44-3
SPID(S): Tox21_200445
M4ID: 12481807

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

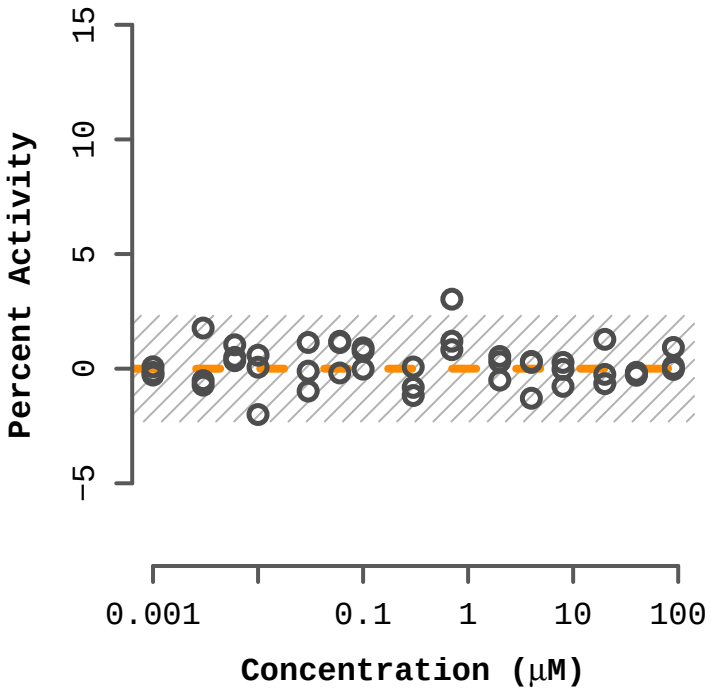
NAME: N-Methylmethanamine hydrochloride
CHID: 27163 **CASRN:** 506-59-2
SPID(S): Tox21_200696
M4ID: 12481556

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.629 **MAX_MED:** 0.0851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

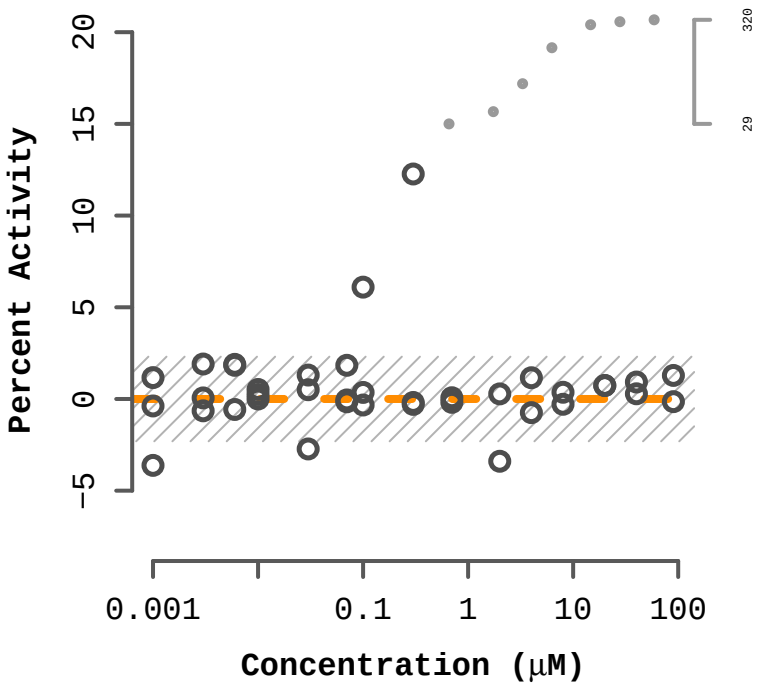
NAME: (1-Chloro-2-methylpropan-2-yl)benzene
CHID: 27167 **CASRN:** 515-40-2
SPID(S): Tox21_200949
M4ID: 12481303

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

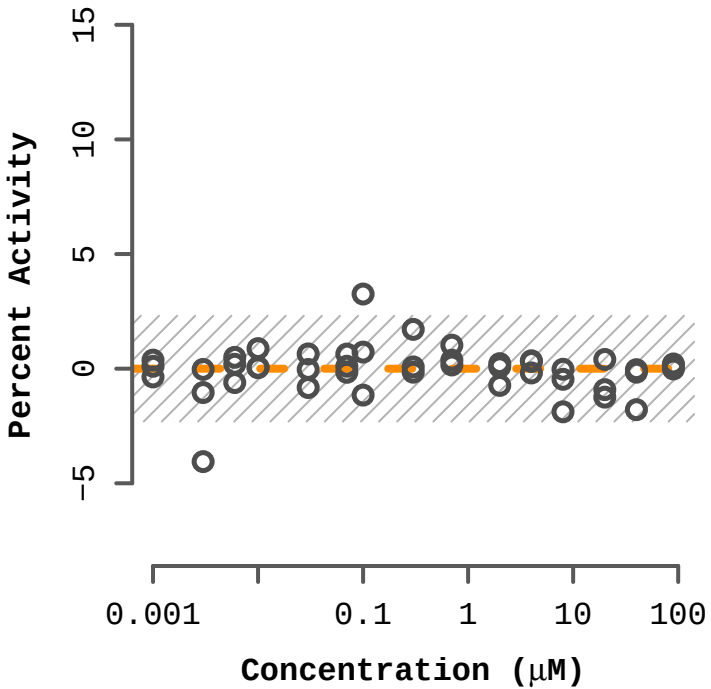
NAME: D-Gluconic acid
CHID: 27169 **CASRN:** 526-95-4
SPID(S): Tox21_202745
M4ID: 12479507 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	435.02	NA	NA
PROB:	1	NA	NA
RMSE:	92.45	NA	NA

MAX_MEAN: 108 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

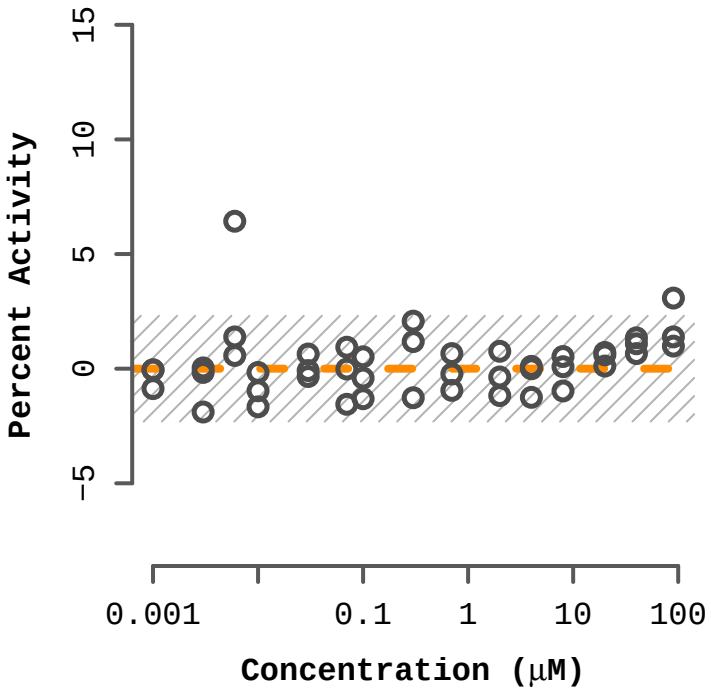
NAME: 1,2,3,4-Tetrahydronaphthalen-1-ol
CHID: 27174 **CASRN:** 529-33-9
SPID(S): Tox21_200096
M4ID: 12482156

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 0.725 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

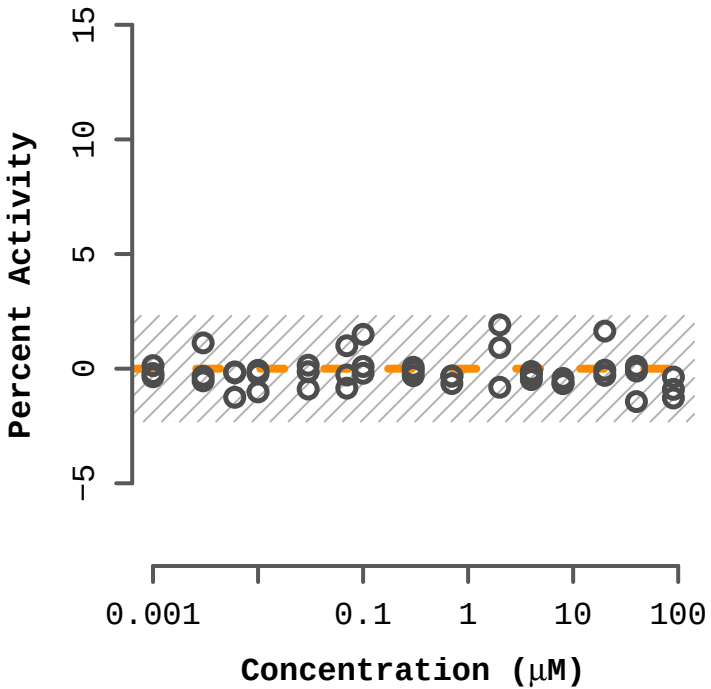
NAME: 1,2,3,4−Tetrahydronaphthalen−1−one
CHID: 27175 **CASRN:** 529−34−0
SPID(S): Tox21_200446
M4ID: 12481806

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.8 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

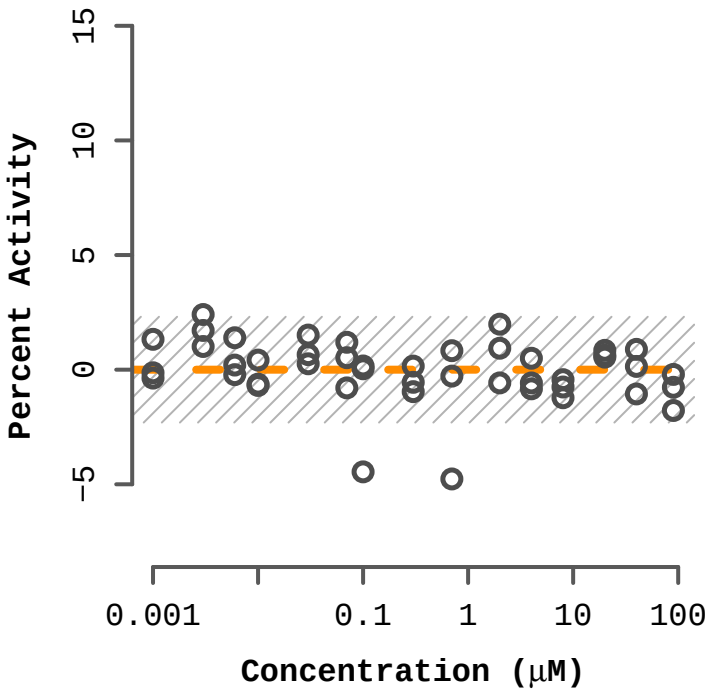
NAME: 1,1−Dimethoxyethane
CHID: 27178 **CASRN:** 534−15−6
SPID(S): Tox21_200713
M4ID: 12481539

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.677 **MAX_MED:** 0.926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

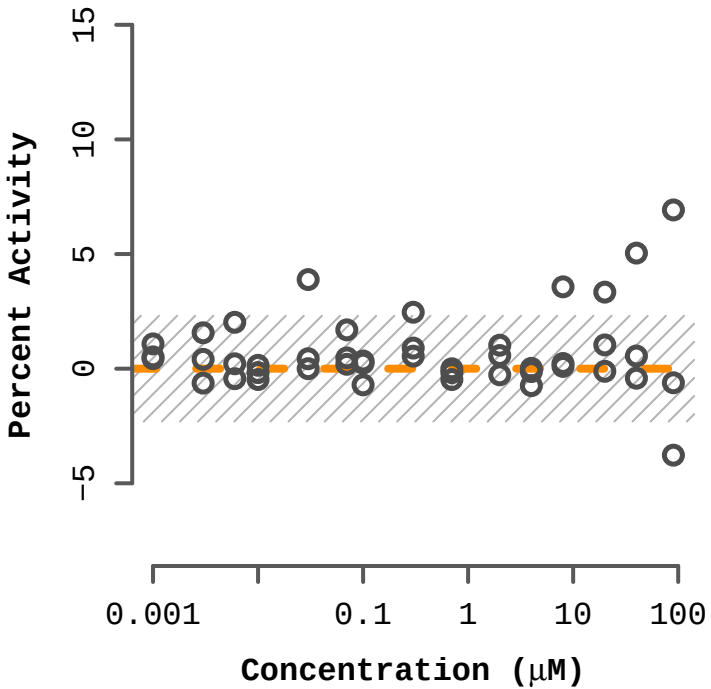
NAME: Isobutylbenzene
CHID: 27181 **CASRN:** 538-93-2
SPID(S): Tox21_303054
M4ID: 12476079

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

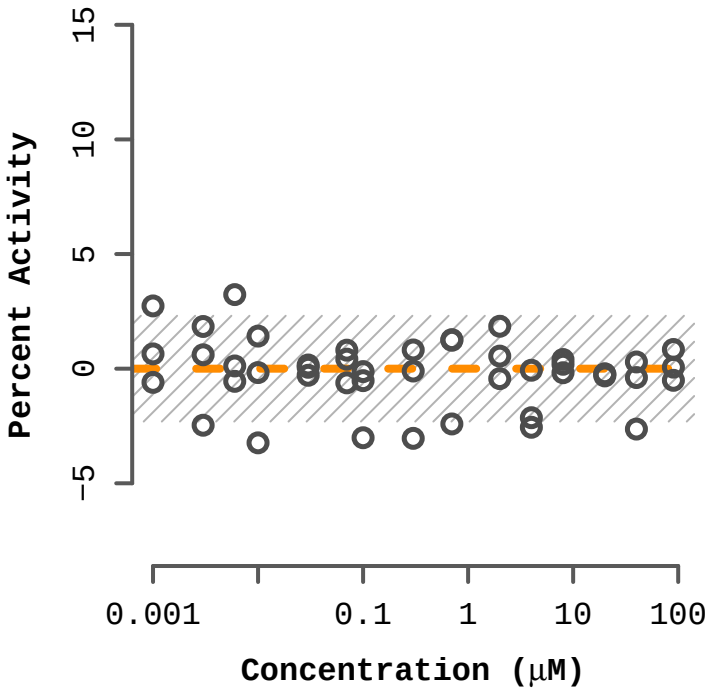
NAME: Isobutylbenzene
CHID: 27181 **CASRN:** 538-93-2
SPID(S): Tox21_201991
M4ID: 12480261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

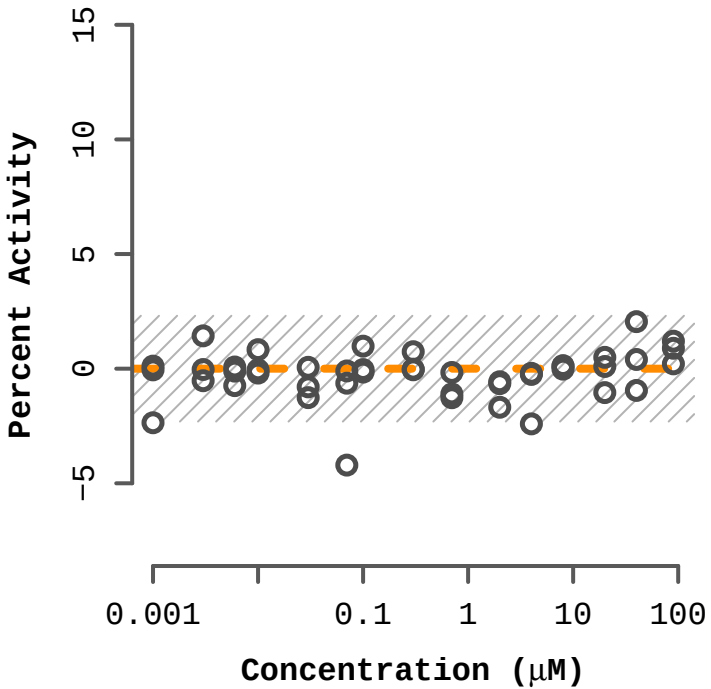
NAME: Decamethylcyclopentasiloxane
CHID: 27184 **CASRN:** 541-02-6
SPID(S): Tox21_303170
M4ID: 12475963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 0.934 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

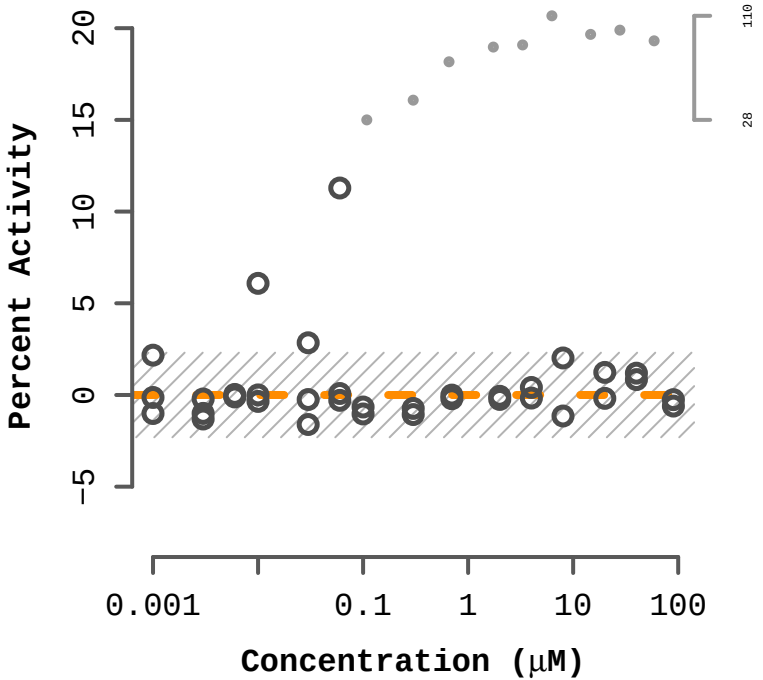
NAME: Hexamethylcyclotrisiloxane
CHID: 27185 **CASRN:** 541-05-9
SPID(S): Tox21_303233
M4ID: 12475900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.768 **MAX_MED:** 0.891 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

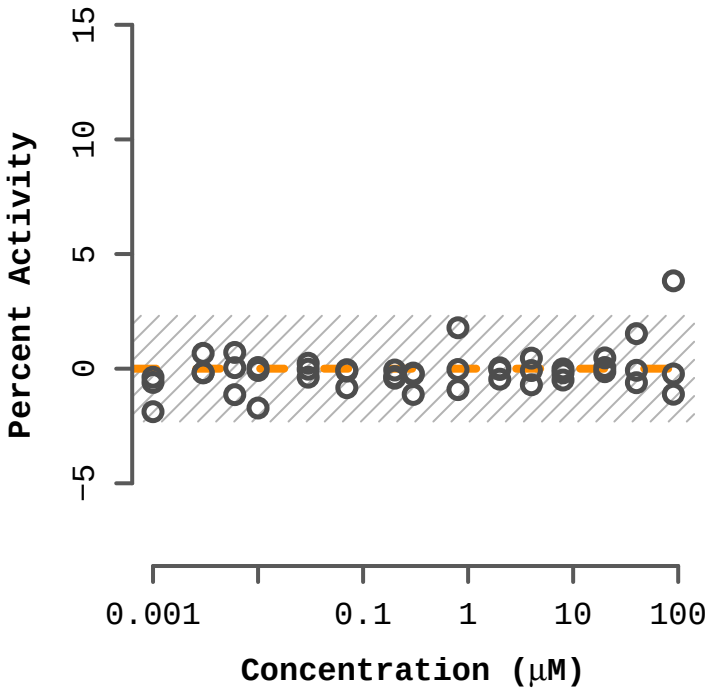
NAME: Ethyl chloroformate
CHID: 27186 **CASRN:** 541-41-3
SPID(S): Tox21_201034
M4ID: 12481218 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	423.36	NA	NA
PROB:	1	NA	NA
RMSE:	38.4	NA	NA

MAX_MEAN: 38.3 **MAX_MED:** 2.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

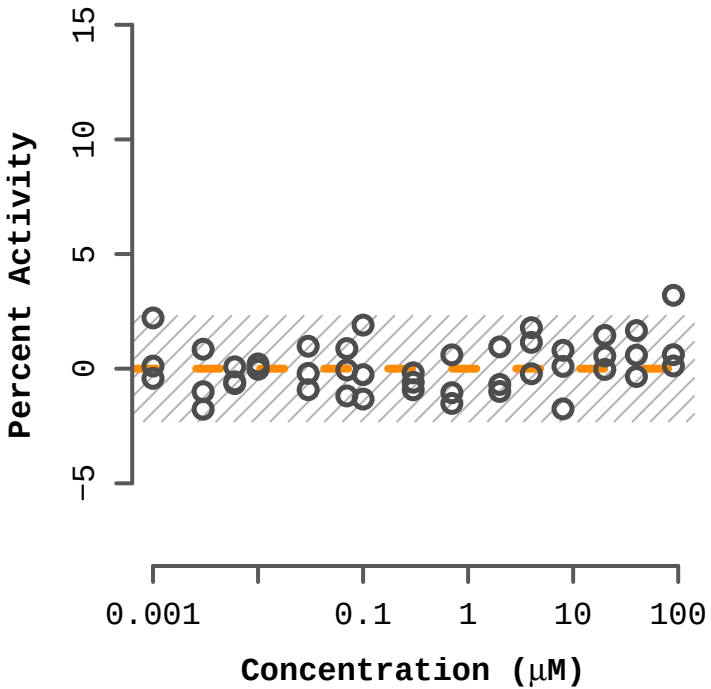
NAME: 1,1-Ethanediol diacetate
CHID: 27188 **CASRN:** 542-10-9
SPID(S): Tox21_200113
M4ID: 12482139

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.83 **MAX_MED:** 0.053 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

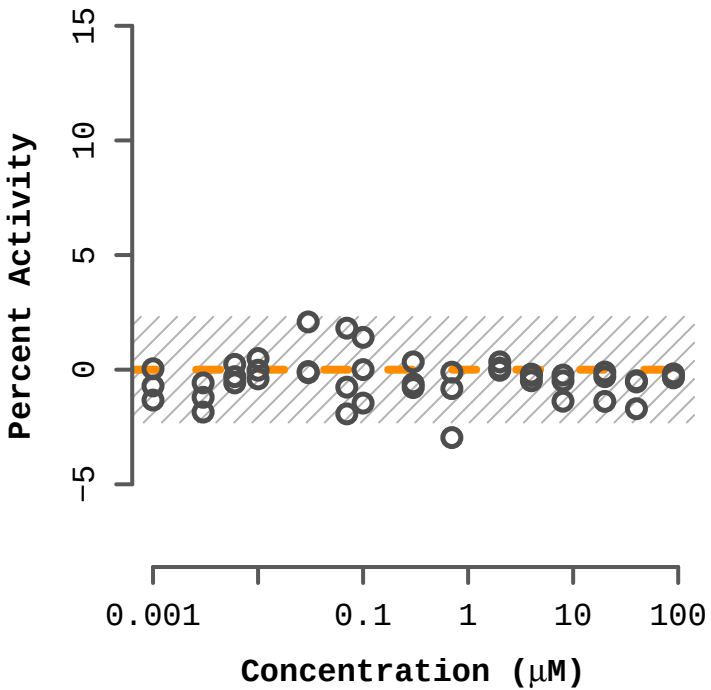
NAME: 1,3-Cyclopentadiene
CHID: 27191 **CASRN:** 542-92-7
SPID(S): Tox21_302134
M4ID: 12476999

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

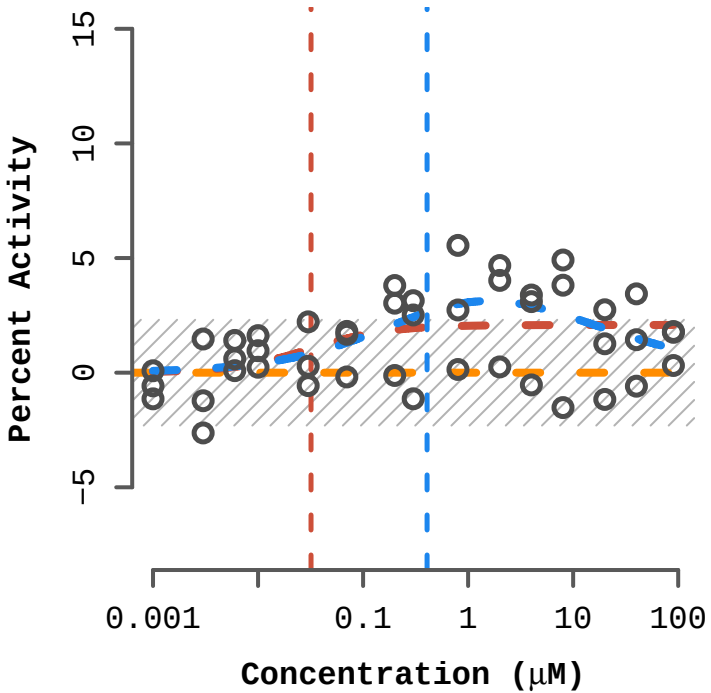
NAME: Hexadecane
CHID: 27195 **CASRN:** 544-76-3
SPID(S): Tox21_300485
M4ID: 12478647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.625 **MAX_MED:** 0.0655 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl 2-hydroxypropanoate
CHID: 27197 CASRN: 547-64-8
SPID(S): Tox21_200447
M4ID: 12481805

HILL MODEL (in red):

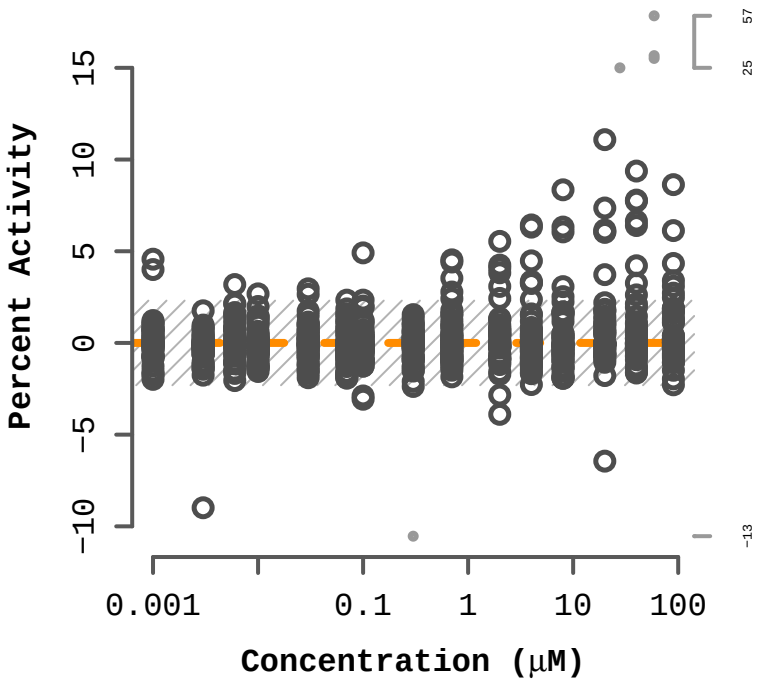
	tp	ga	gw
val:	2.08	−1.5	1.18
sd:	0.425	0.497	0.749

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.66	−0.391	0.734	0.658	0.552
sd:	19.1	1.98	0.441	3.77	0.673

	CNST	HILL	GNLS
AIC:	207.78	188.61	188.7
PROB:	0	0.51	0.49
RMSE:	2.31	1.71	1.69

MAX_MEAN: 2.99 **MAX_MED:** 4.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

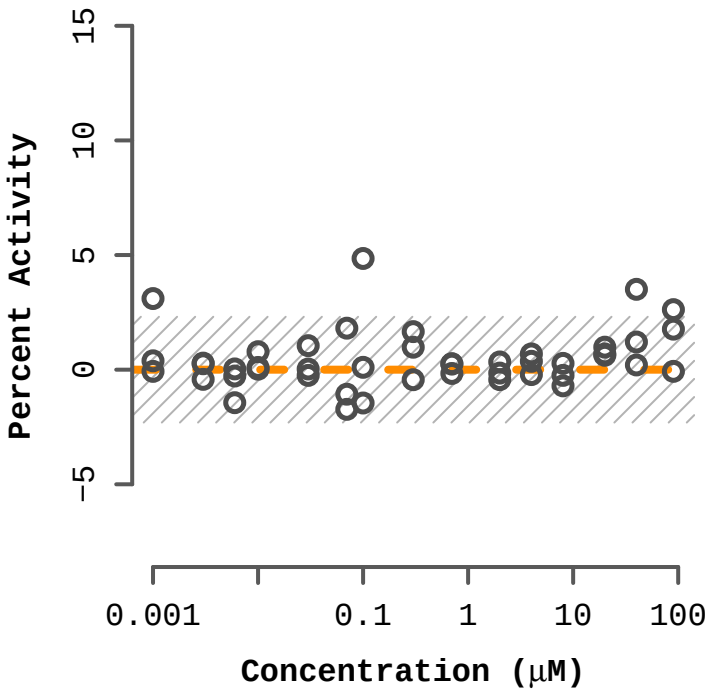
NAME: N-Methylphthalimide
CHID: 27198 **CASRN:** 550-44-7
SPID(S): Tox21_400053
M4ID: 12475084 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2560.39	NA	NA
PROB:	1	NA	NA
RMSE:	3.35	NA	NA

MAX_MEAN: 3.26 **MAX_MED:** 0.224 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

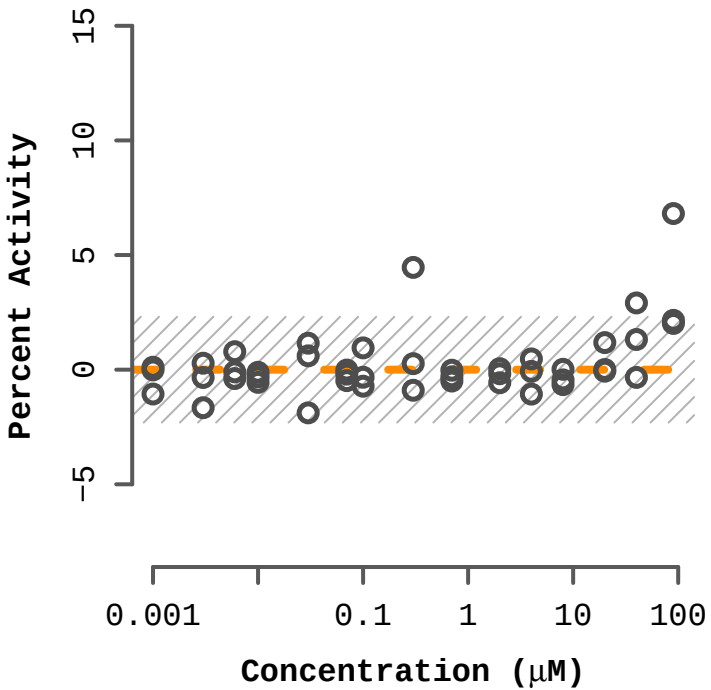
NAME: 4,4'−Bipyridine
CHID: 27200 **CASRN:** 553−26−4
SPID(S): Tox21_300577
M4ID: 12478556

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

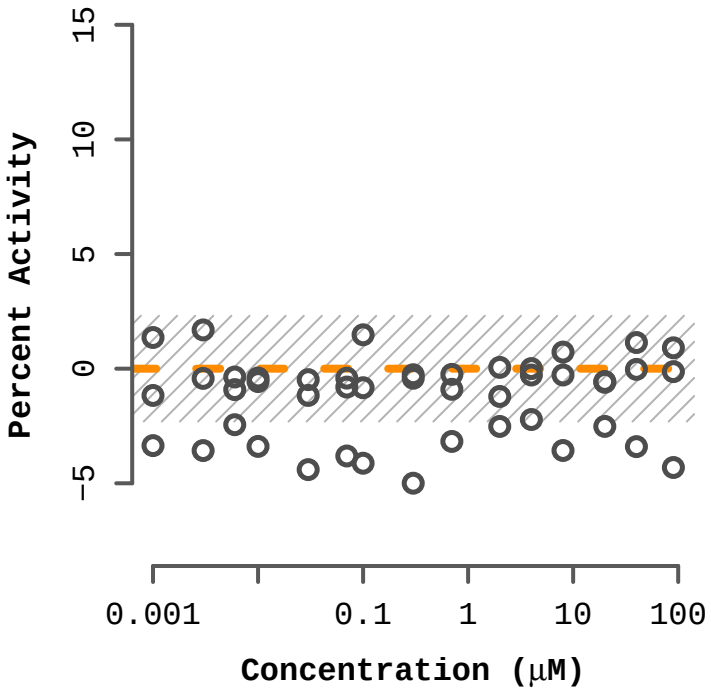
NAME: 4,4'−Bipyridine
CHID: 27200 **CASRN:** 553−26−4
SPID(S): Tox21_201668
M4ID: 12480584

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 3.66 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

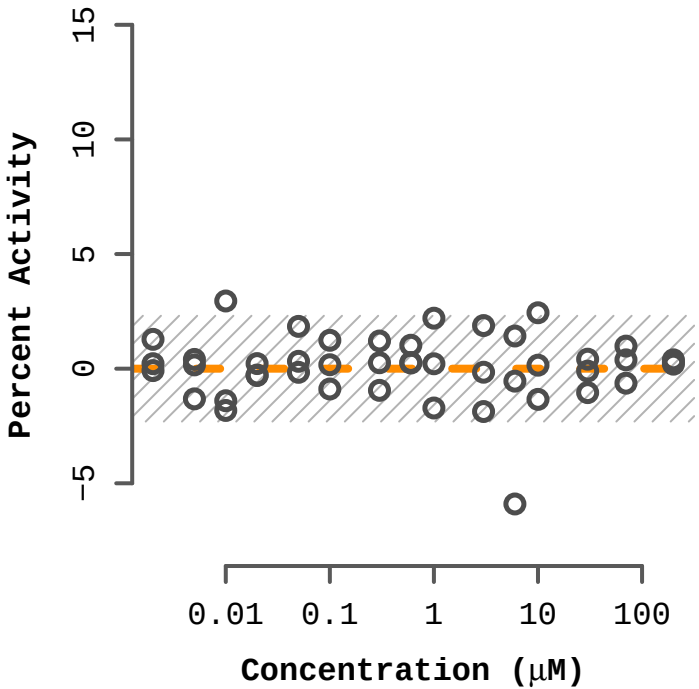
NAME: Methyl propanoate
CHID: 27201 CASRN: 554-12-1
SPID(S): Tox21_200730
M4ID: 12481522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: −0.762 **MAX_MED:** −0.0299 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

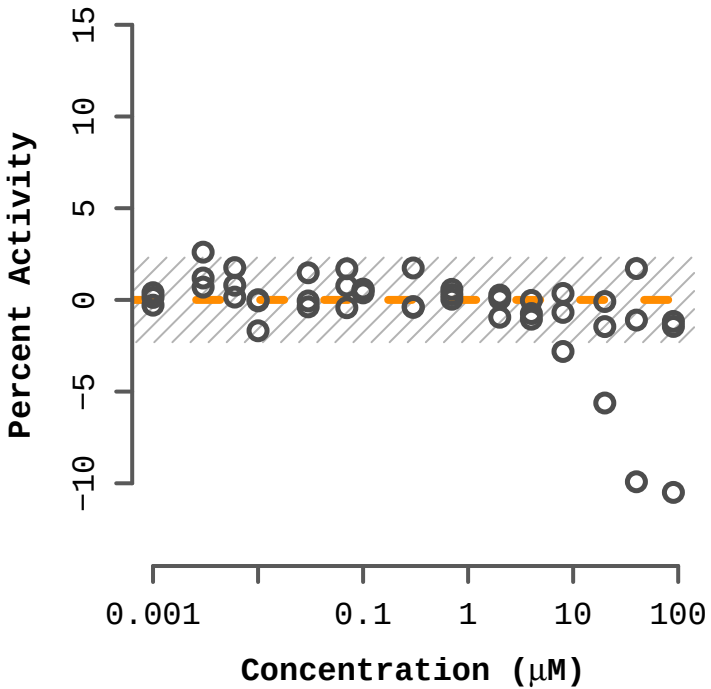
NAME: Methyl isothiocyanate
CHID: 27204 **CASRN:** 556-61-6
SPID(S): Tox21_300912
M4ID: 12478221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 0.67 **MAX_MED:** 0.386 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

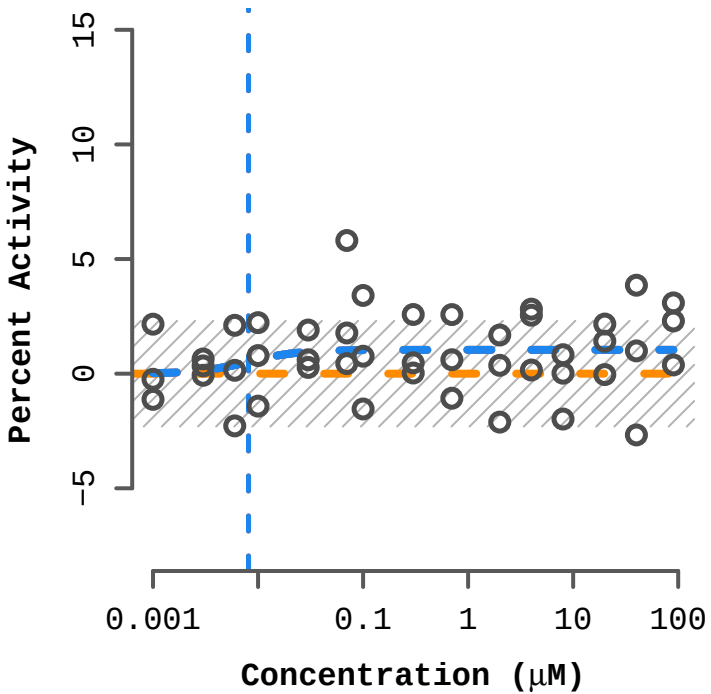
NAME: Methyl isothiocyanate
CHID: 27204 **CASRN:** 556-61-6
SPID(S): Tox21_201548
M4ID: 12480704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.53	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Octamethylcyclotetrasiloxane
CHID: 27205 **CASRN:** 556-67-2
SPID(S): Tox21_300547
M4ID: 12478585

HILL MODEL (in red):

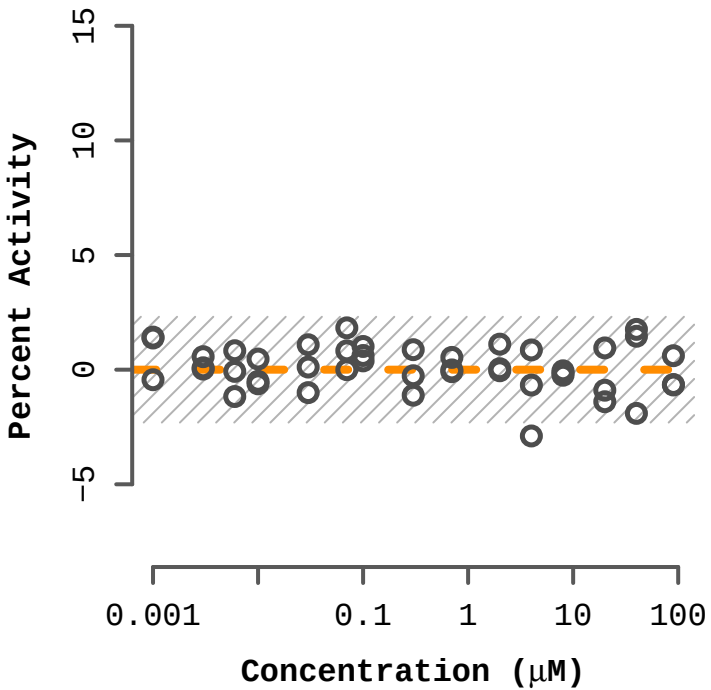
	tp	ga	gw
val:	1.04	−2.09	1.84
sd:	0.305	0.655	3.82

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.04	−2.09	1.84	3.69	17.6
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	189.94	184.24	188.24
PROB:	0.05	0.84	0.11
RMSE:	1.92	1.69	1.69

MAX_MEAN: 2.68 **MAX_MED:** 2.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

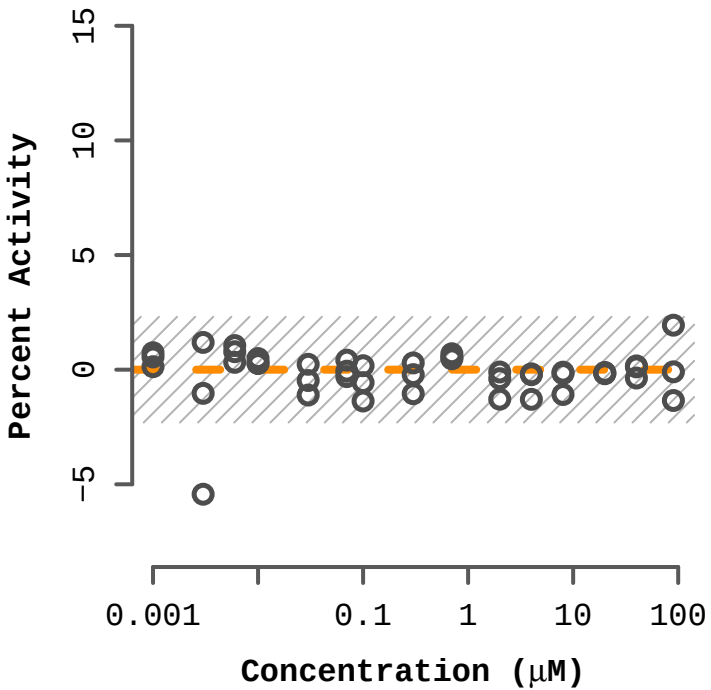
NAME: Octamethylcyclotetrasiloxane
CHID: 27205 **CASRN:** 556-67-2
SPID(S): Tox21_201398
M4ID: 12480854

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.883 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

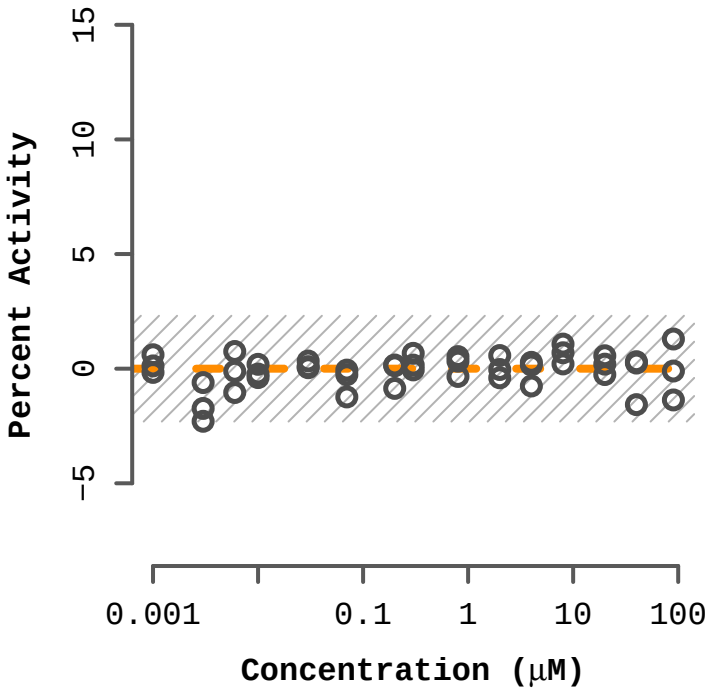
NAME: 3-Methyl-2-buten-1-ol
CHID: 27206 **CASRN:** 556-82-1
SPID(S): Tox21_303419
M4ID: 12475720

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.72 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

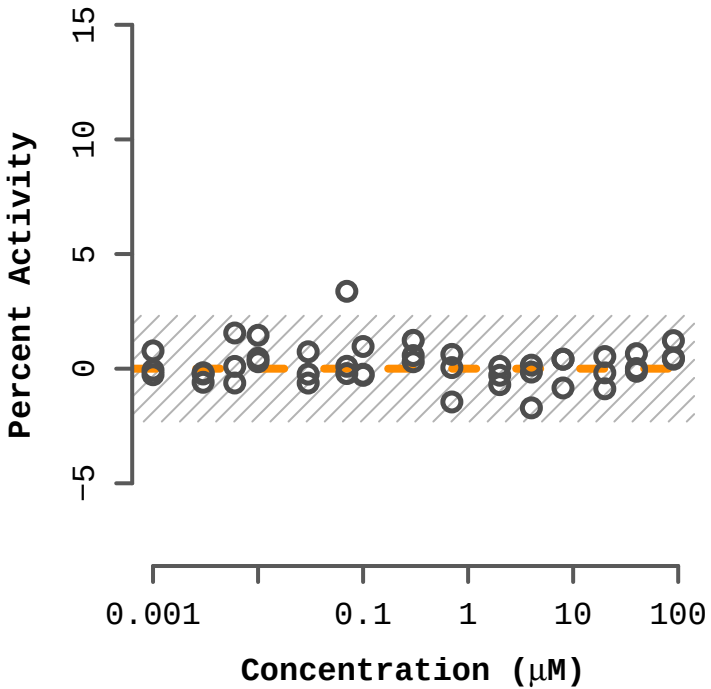
NAME: 3-Methyl-2-buten-1-ol
CHID: 27206 CASRN: 556-82-1
SPID(S): Tox21_202234
M4ID: 12480018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.659 MAX_MED: 0.695 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

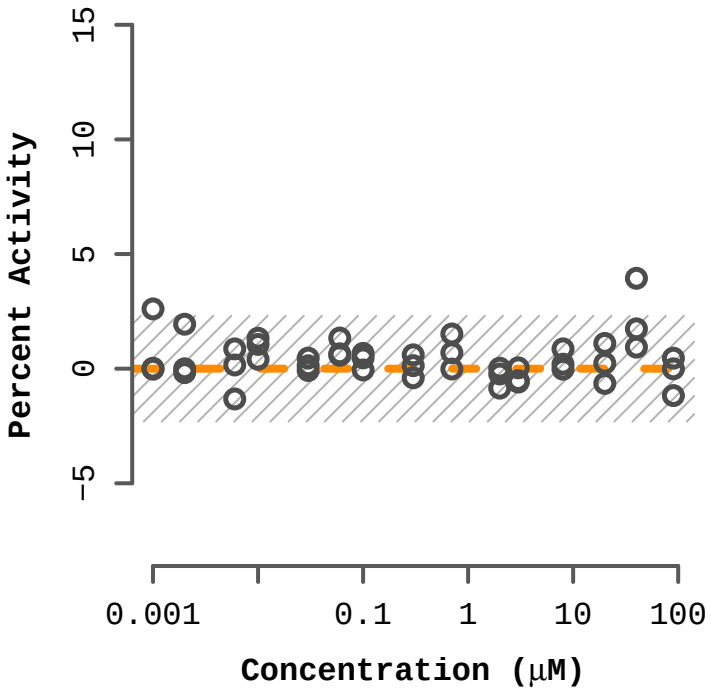
NAME: 3,3-Dimethyl-1-butene
CHID: 27211 CASRN: 558-37-2
SPID(S): Tox21_303243
M4ID: 12475890

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.09 MAX_MED: 0.575 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

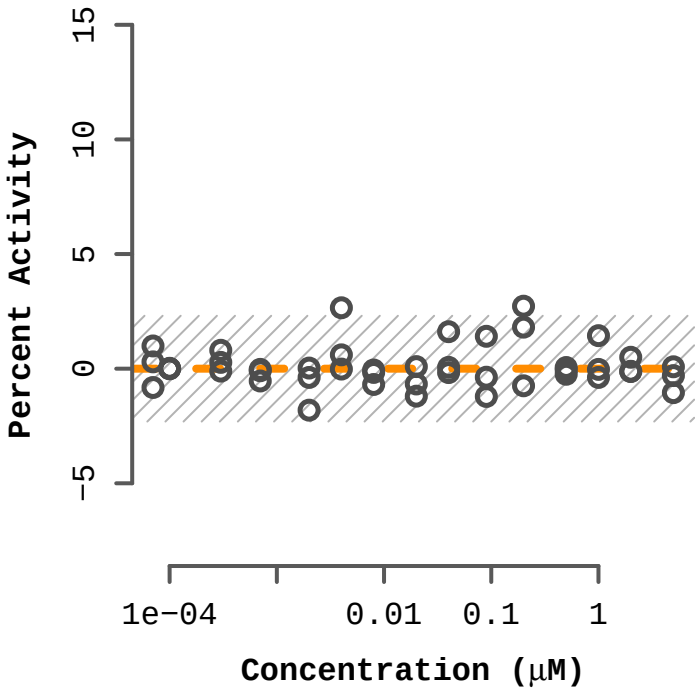
NAME: 3,3-Dimethyl-1-butene
CHID: 27211 CASRN: 558-37-2
SPID(S): Tox21_202256
M4ID: 12479996

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 2.21 MAX_MED: 1.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

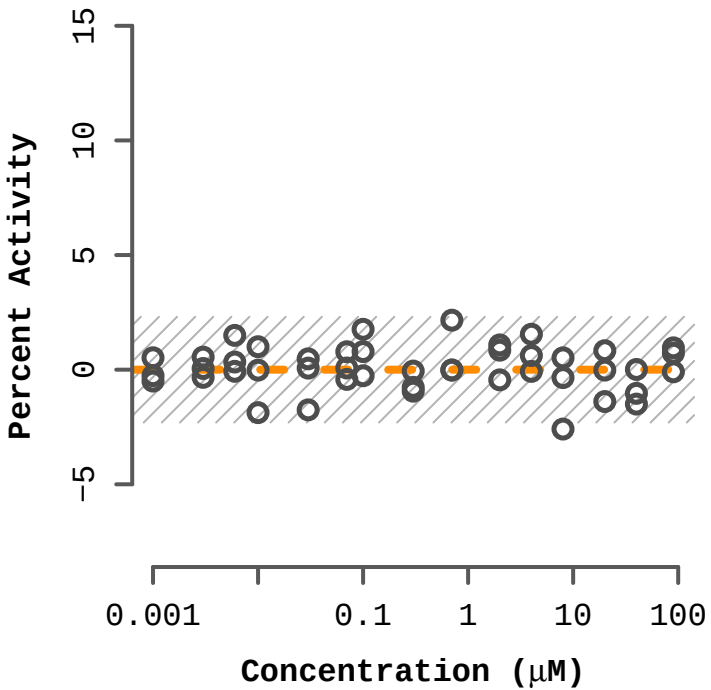
NAME: Ethanedioic acid, calcium salt (1:1)
CHID: 27214 **CASRN:** 563-72-4
SPID(S): Tox21_202746
M4ID: 12479506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

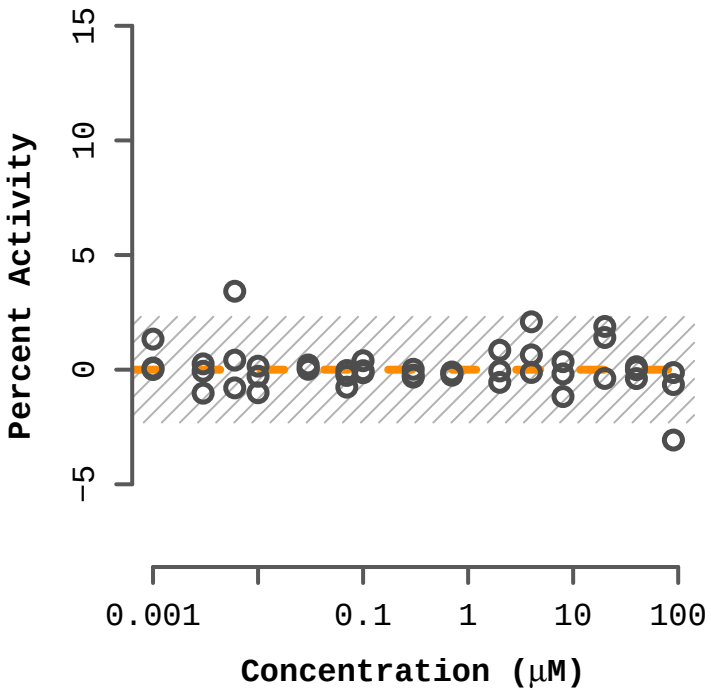
NAME: 2,6-Diethylaniline
CHID: 27218 **CASRN:** 579-66-8
SPID(S): Tox21_300333
M4ID: 12478799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.763 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

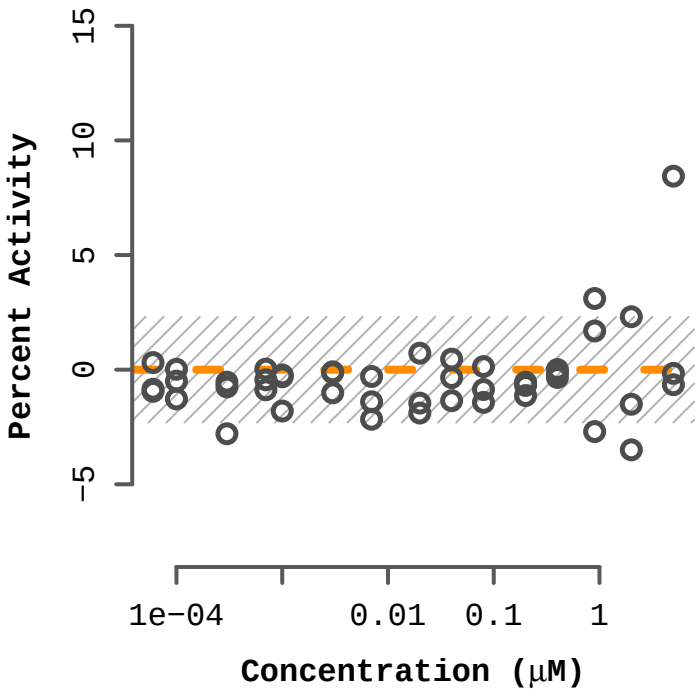
NAME: 2,6-Diethylaniline
CHID: 27218 **CASRN:** 579-66-8
SPID(S): Tox21_202010
M4ID: 12480242

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

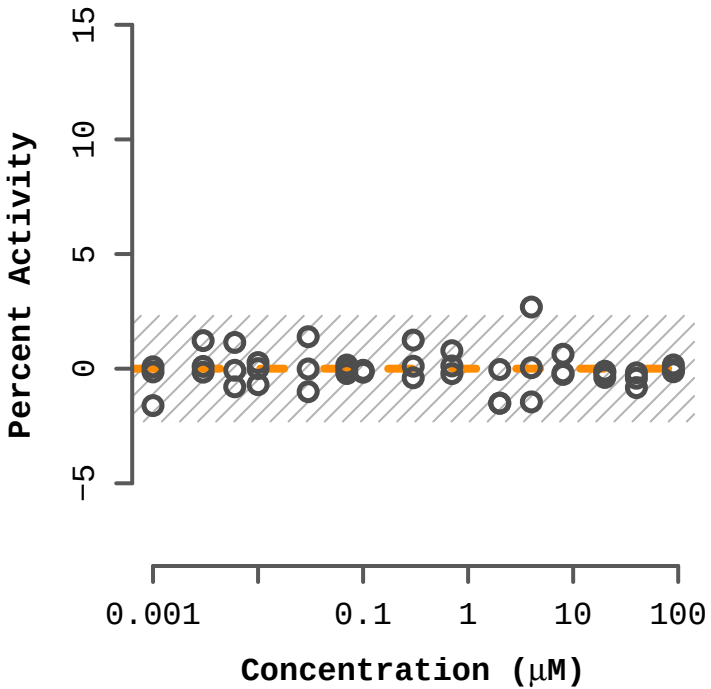
NAME: Potassium benzoate
CHID: 27219 **CASRN:** 582-25-2
SPID(S): Tox21_202747
M4ID: 12479505

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 2.54 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

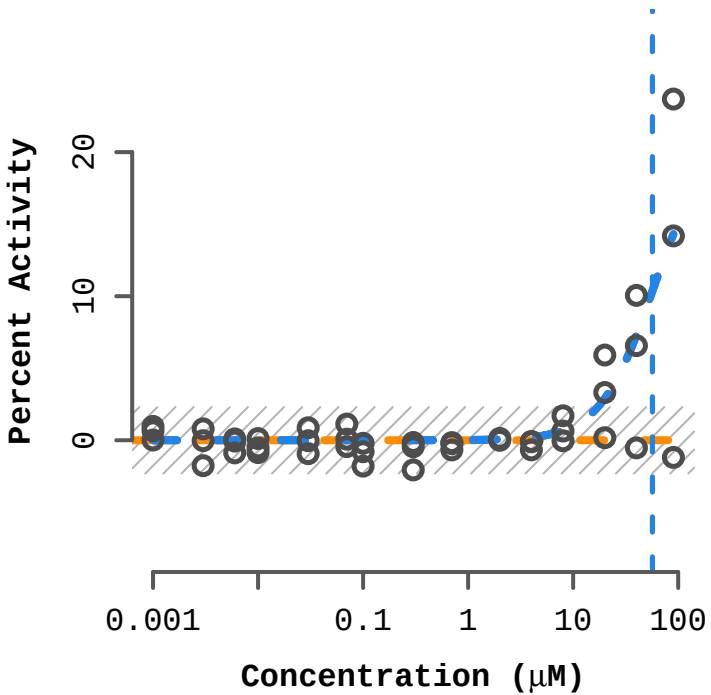
NAME: Terpinolene
CHID: 27222 CASRN: 586-62-9
SPID(S): Tox21_303268
M4ID: 12475865

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.429 MAX_MED: 0.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl propionate
CHID: 27223 CASRN: 590-01-2
SPID(S): Tox21_201691
M4ID: 12480561

HILL MODEL (in red):

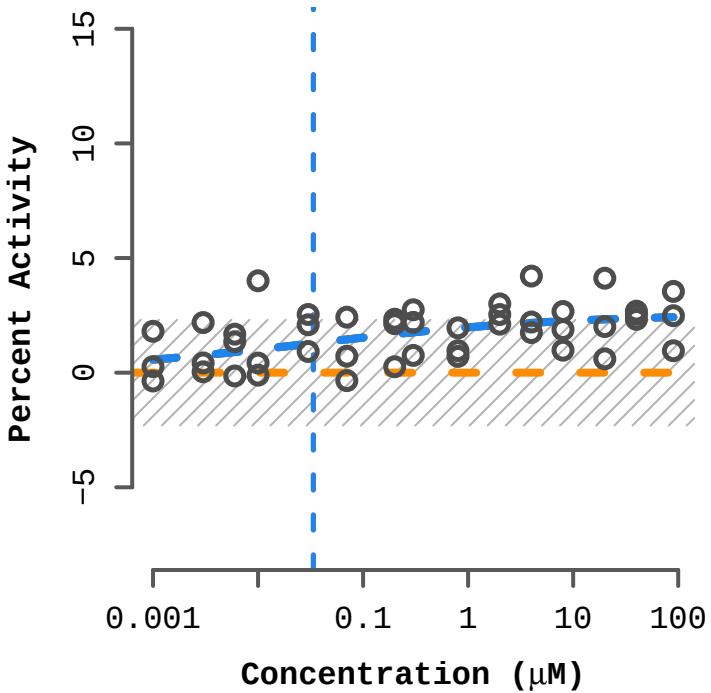
	tp	ga	gw
val:	20.7	1.75	1.74
sd:	7.72	0.231	0.507

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	20.7	1.75	1.74	2.39	17.6
sd:	7.72	0.231	0.507	422	16600

	CNST	HILL	GNLS
AIC:	205.77	185.61	189.61
PROB:	0	0.88	0.12
RMSE:	4.66	3.11	3.11

MAX_MEAN: 12.2 MAX_MED: 14.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Hexadiene
CHID: 27227 CASRN: 592−45−0
SPID(S): Tox21_201155
M4ID: 12481097

HILL MODEL (in red):

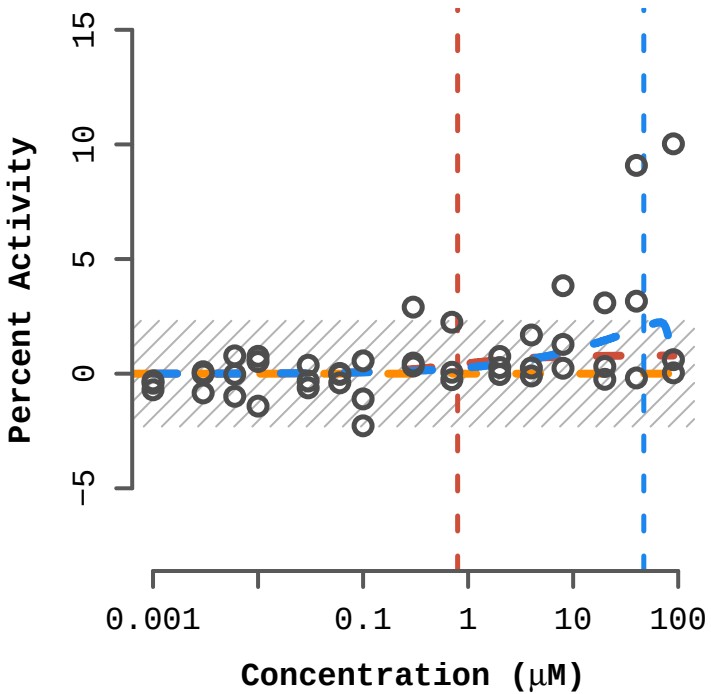
	tp	ga	gw
val:	2.56	−1.47	0.357
sd:	0.719	0.979	0.257

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.56	−1.47	0.357	3.91	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	201.08	142.58	146.58
PROB:	0	0.88	0.12
RMSE:	2.07	1.05	1.05

MAX_MEAN: 2.73 MAX_MED: 2.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Pentenenitrile
CHID: 27228 **CASRN:** 592-51-8
SPID(S): Tox21_201124
M4ID: 12481128

HILL MODEL (in red):

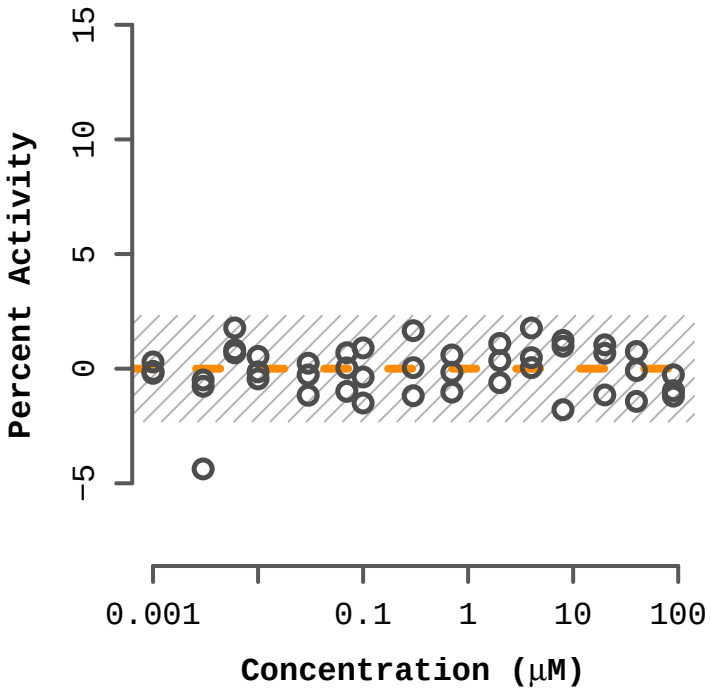
	tp	ga	gw
val:	0.794	−0.0999	1.16
sd:	0.772	2.07	1.78

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.08	1.67	0.688	1.92	18
sd:	51.4	11.6	0.949	0.165	41.4

	CNST	HILL	GNLS
AIC:	171.59	170.18	173.4
PROB:	0.29	0.59	0.12
RMSE:	2.36	2.14	2.07

MAX_MEAN: 4.02 **MAX_MED:** 3.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

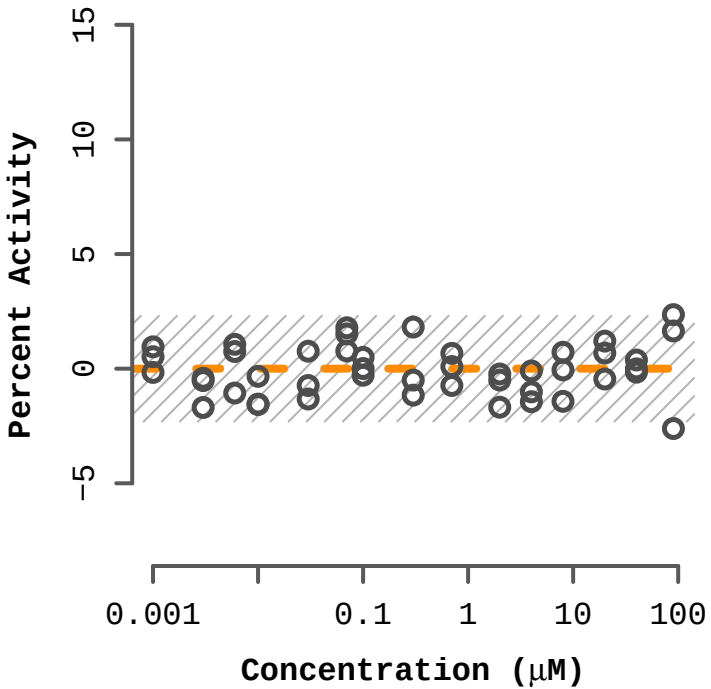
NAME: N,N−Dimethylmethanamine hydrochloride
CHID: 27229 **CASRN:** 593−81−7
SPID(S): Tox21_200130
M4ID: 12482122

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

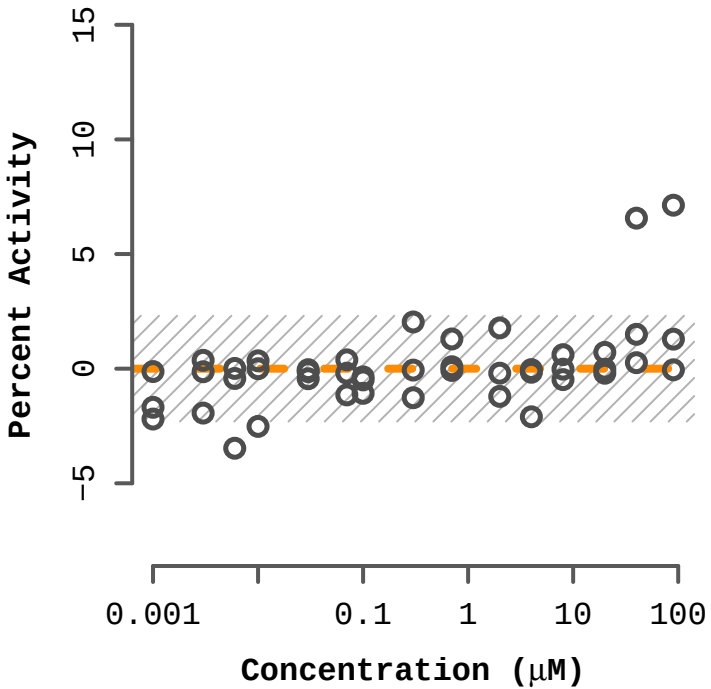
NAME: 2-Bromopropionic acid
CHID: 27233 **CASRN:** 598-72-1
SPID(S): Tox21_303226
M4ID: 12475907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

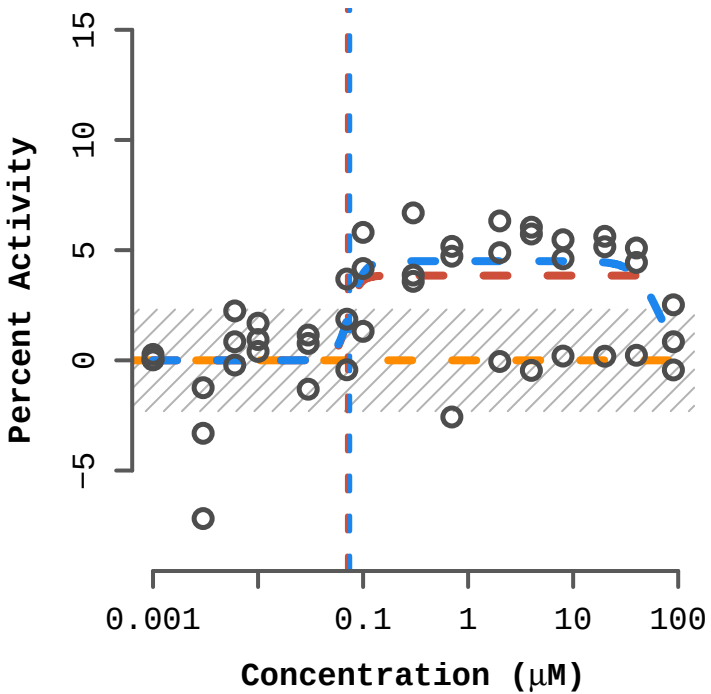
NAME: 2-Bromopropionic acid
CHID: 27233 **CASRN:** 598-72-1
SPID(S): Tox21_201417
M4ID: 12480835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 2.79 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl pivalate
CHID: 27234 **CASRN:** 598-98-1
SPID(S): Tox21_200448
M4ID: 12481804

HILL MODEL (in red):

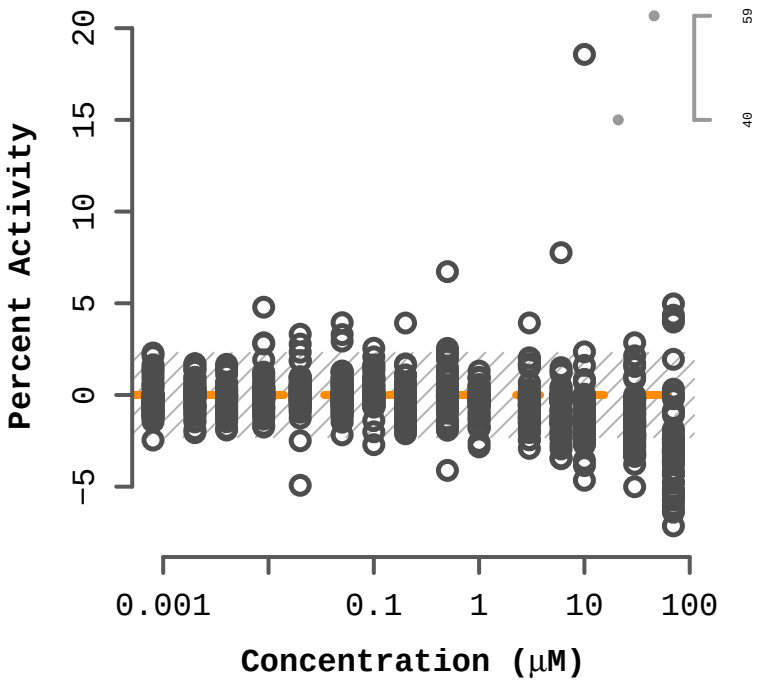
	tp	ga	gw
val:	3.85	−1.15	8
sd:	0.522	0.0718	12.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.5	−1.13	6.58	1.8	3.79
sd:	0.529	0.0688	8.24	0.149	3.28

	CNST	HILL	GNLS
AIC:	248.06	217.17	214.01
PROB:	0	0.17	0.83
RMSE:	3.57	2.48	2.42

MAX_MEAN: 4.72 **MAX_MED:** 5.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

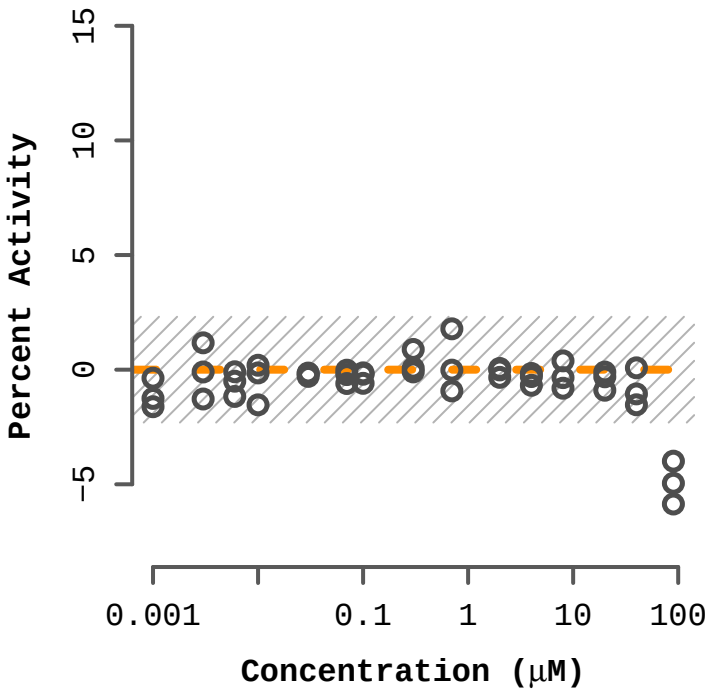
NAME: 2,3-Dinitrotoluene
CHID: 27236 **CASRN:** 602-01-7
SPID(S): Tox21_400034
M4ID: 12475103 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2808.96	NA	NA
PROB:	1	NA	NA
RMSE:	3.1	NA	NA

MAX_MEAN: 0.171 **MAX_MED:** 0.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

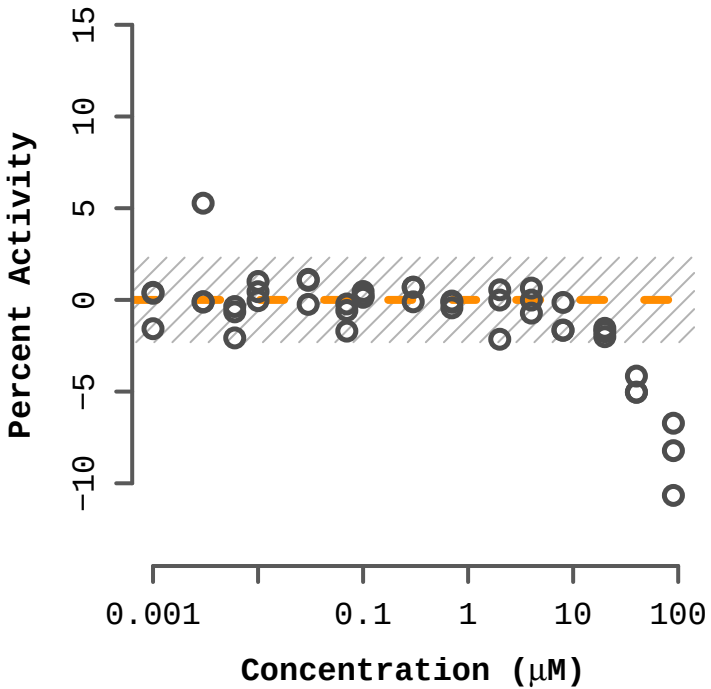
NAME: 4-Methyl-2,6-dinitrophenol
CHID: 27239 CASRN: 609-93-8
SPID(S): Tox21_200747
M4ID: 12481505

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.285 MAX_MED: 0.0668 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

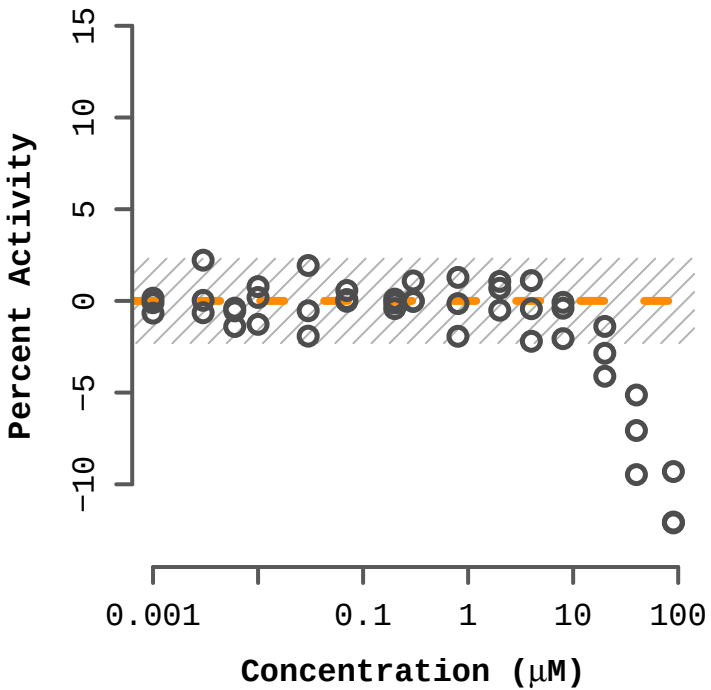
NAME: 3,4-Dinitrotoluene
CHID: 27240 **CASRN:** 610-39-9
SPID(S): Tox21_303210
M4ID: 12475923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.03	NA	NA
PROB:	1	NA	NA
RMSE:	2.82	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

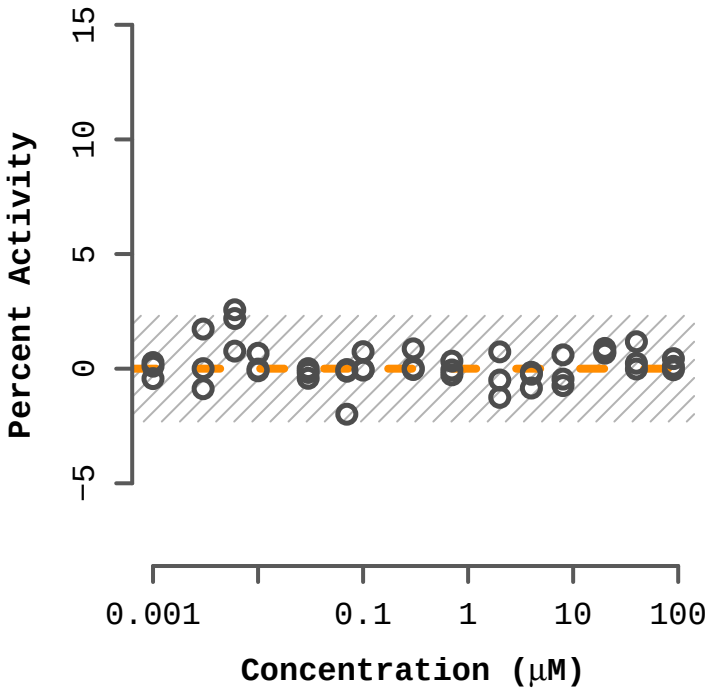
NAME: 3,4-Dinitrotoluene
CHID: 27240 CASRN: 610-39-9
SPID(S): Tox21_202159
M4ID: 12480093

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.4	NA	NA
PROB:	1	NA	NA
RMSE:	3.68	NA	NA

MAX_MEAN: 0.537 MAX_MED: 0.693 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

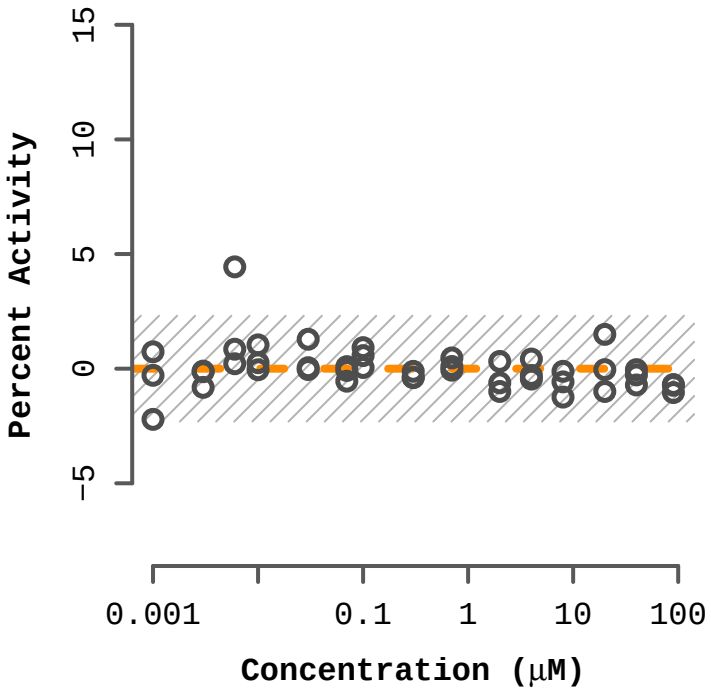
NAME: 2-Chlorobenzyl chloride
CHID: 27241 **CASRN:** 611-19-8
SPID(S): Tox21_201089
M4ID: 12481163

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

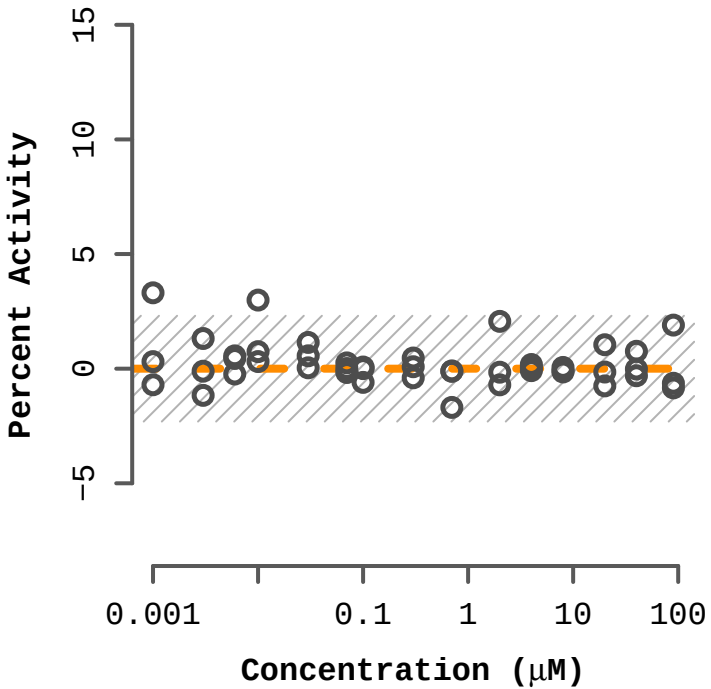
NAME: 1,2-Dichlorobutane
CHID: 27244 **CASRN:** 616-21-7
SPID(S): Tox21_200147
M4ID: 12482105

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

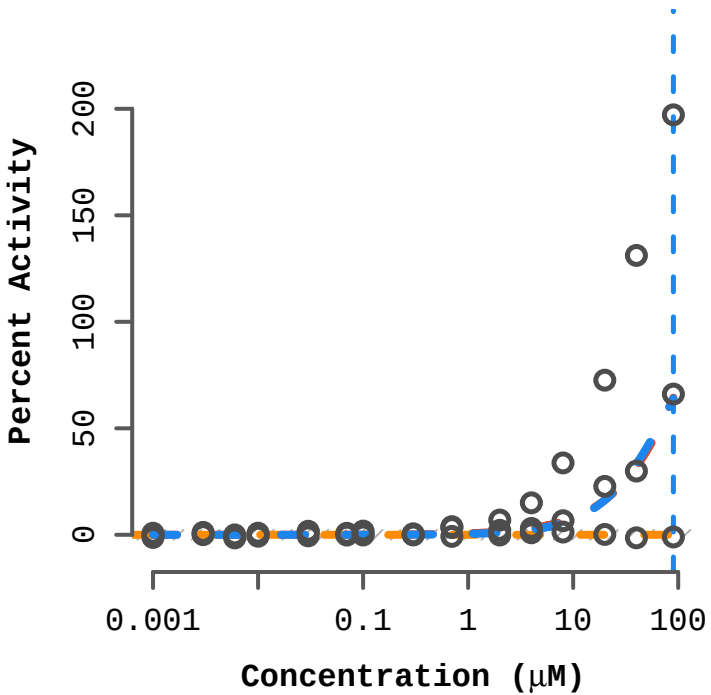
NAME: 2-Pyrrolidinone
CHID: 27246 **CASRN:** 616-45-5
SPID(S): Tox21_303259
M4ID: 12475874

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.745 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Pyrrolidinone
CHID: 27246 CASRN: 616-45-5
SPID(S): Tox21_201630
M4ID: 12480622

HILL MODEL (in red):

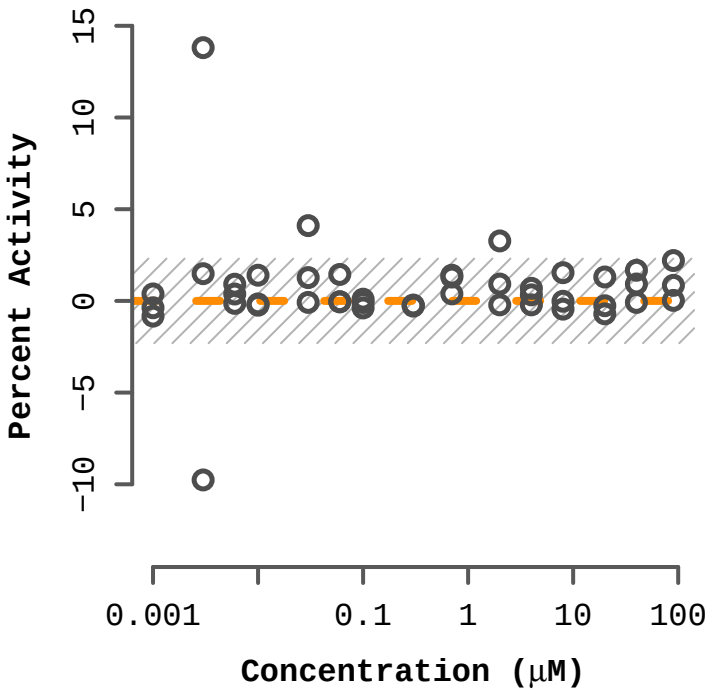
	tp	ga	gw
val:	237	2.35	1.08
sd:	115	0.268	0.136

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	128	1.95	1.28	3.68	5.15
sd:	61.5	0.311	0.297	2970	8910

	CNST	HILL	GNLS
AIC:	375.16	366.33	371.82
PROB:	0.01	0.93	0.06
RMSE:	39.06	28.81	28.79

MAX_MEAN: 87.4 MAX_MED: 66.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

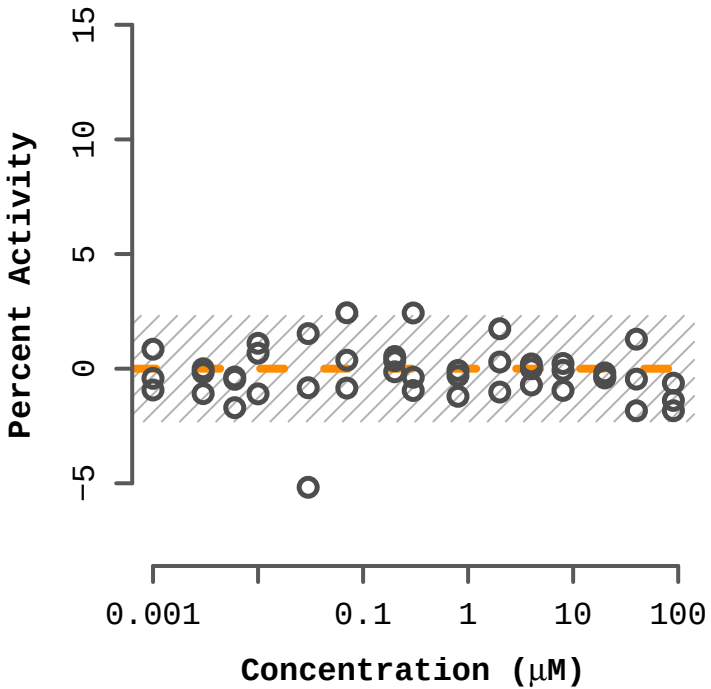
NAME: 2-Phenylpropan-2-ol
CHID: 27247 **CASRN:** 617-94-7
SPID(S): Tox21_200449
M4ID: 12481803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.76	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

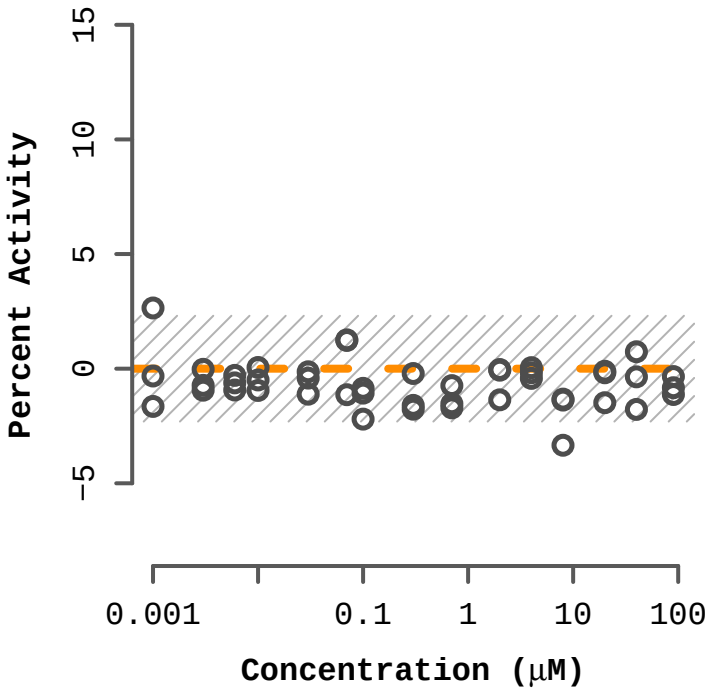
NAME: 4-Carboxybenzaldehyde
CHID: 27249 **CASRN:** 619-66-9
SPID(S): Tox21_202478
M4ID: 12479774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 0.675 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

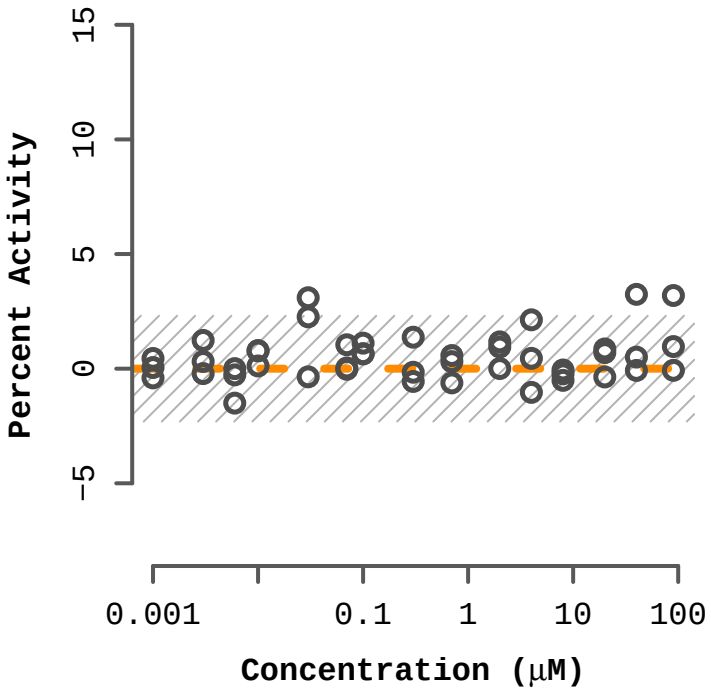
NAME: Diethyl (2E)−but−2−enedioate
CHID: 27253 **CASRN:** 623−91−6
SPID(S): Tox21_200764
M4ID: 12481488

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.453 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

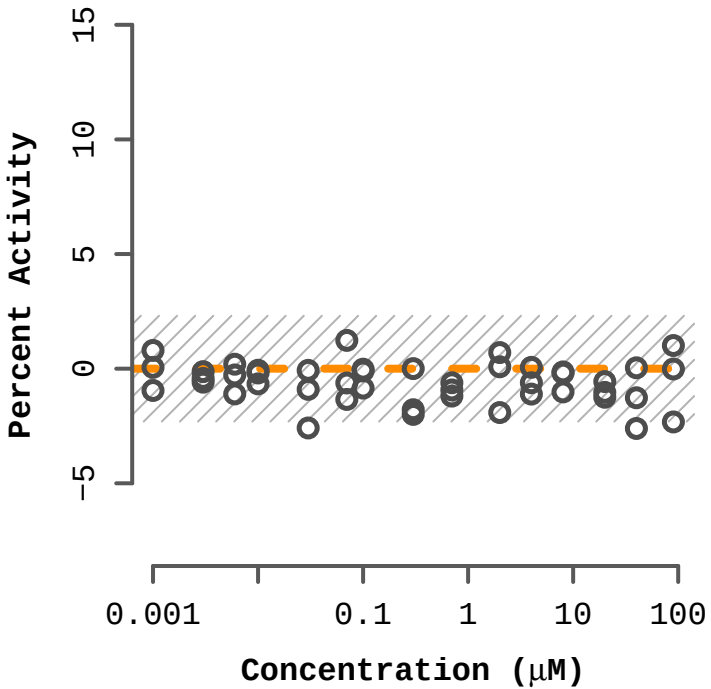
NAME: 2-Methylbutyl acetate
CHID: 27254 **CASRN:** 624-41-9
SPID(S): Tox21_200883
M4ID: 12481369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

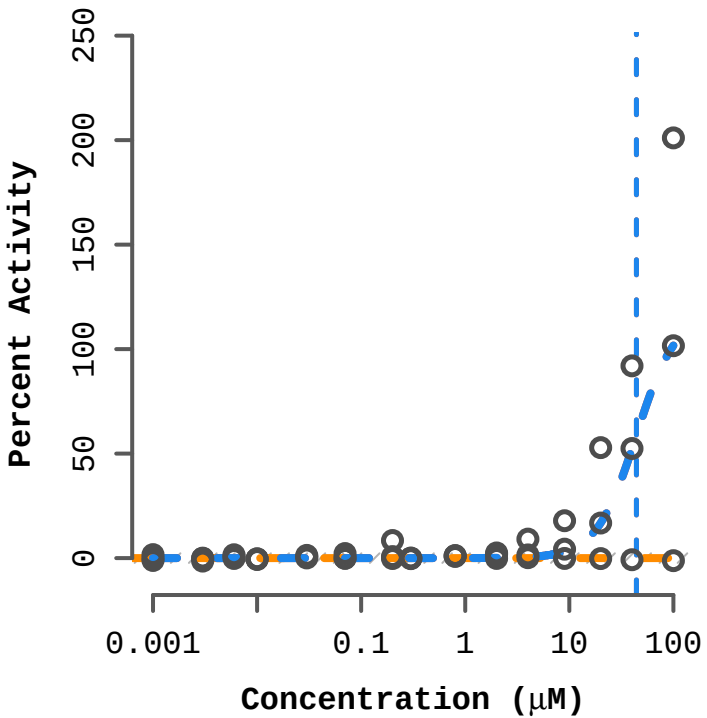
NAME: Isopropyl formate
CHID: 27258 **CASRN:** 625-55-8
SPID(S): Tox21_303282
M4ID: 12475851

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: −0.0313 **MAX_MED:** 0.0836 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isopropyl formate
CHID: 27258 CASRN: 625-55-8
SPID(S): Tox21_201844
M4ID: 12480408

HILL MODEL (in red):

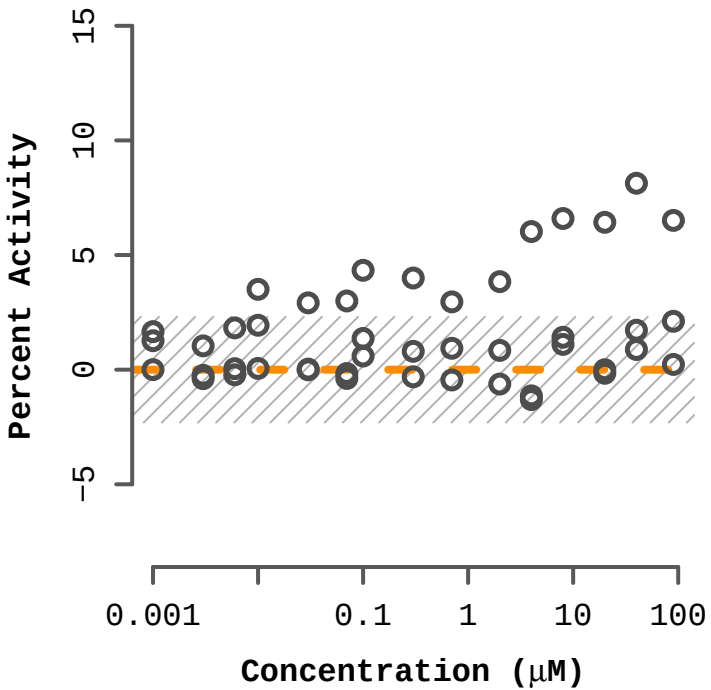
	tp	ga	gw
val:	118	1.64	2.26
sd:	8.08	0.0402	0.314

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	118	1.64	2.26	3.81	5.52
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	363.85	348.05	352.05
PROB:	0	0.88	0.12
RMSE:	38.18	24.43	24.43

MAX_MEAN: 101 MAX_MED: 102 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

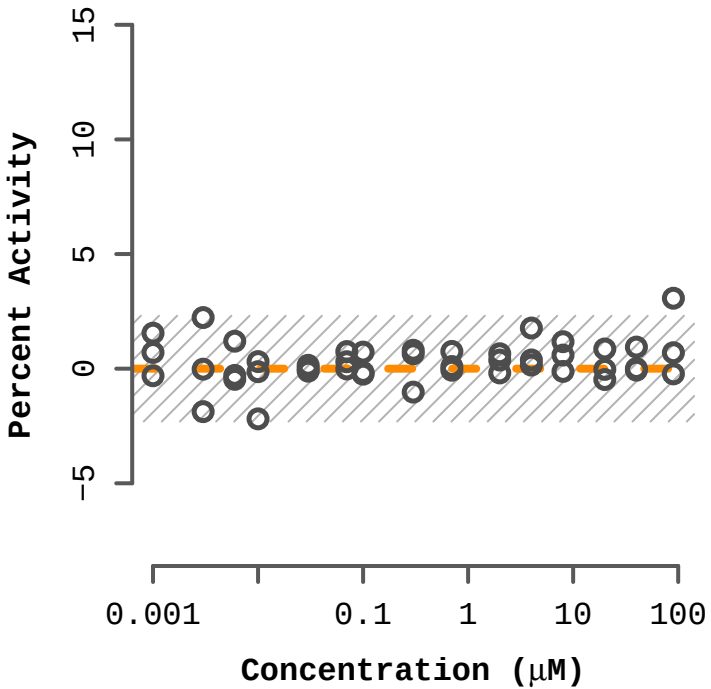
NAME: 1,3-Benzenedicarbonitrile
CHID: 27259 **CASRN:** 626-17-5
SPID(S): Tox21_303190
M4ID: 12475943

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.79	NA	NA

MAX_MEAN: 3.58 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

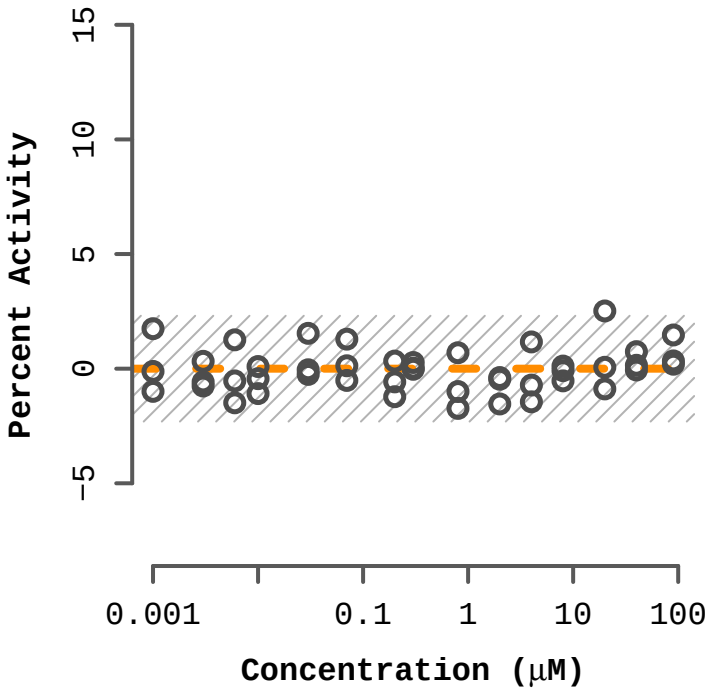
NAME: 1,3-Benzenedicarbonitrile
CHID: 27259 **CASRN:** 626-17-5
SPID(S): Tox21_201474
M4ID: 12480778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

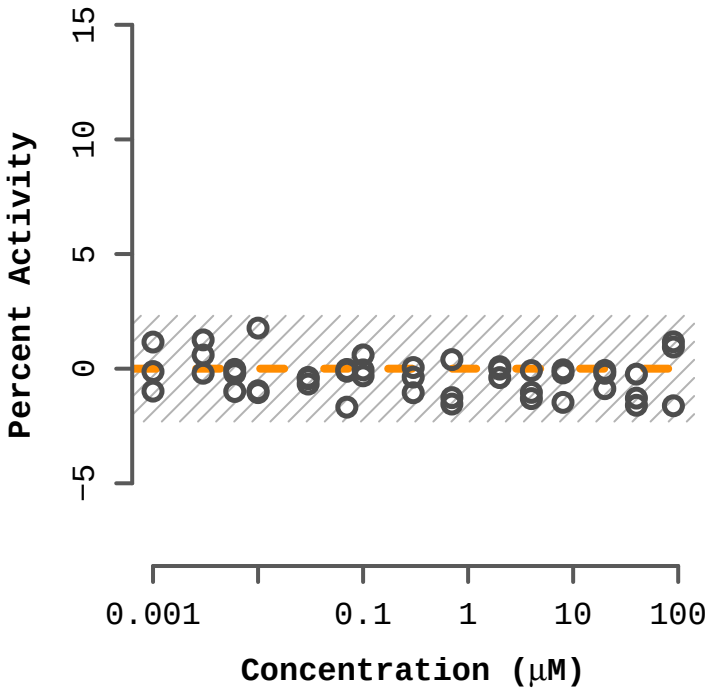
NAME: Pyridine hydrochloride
CHID: 27262 **CASRN:** 628-13-7
SPID(S): Tox21_200163
M4ID: 12482089

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.669 **MAX_MED:** 0.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

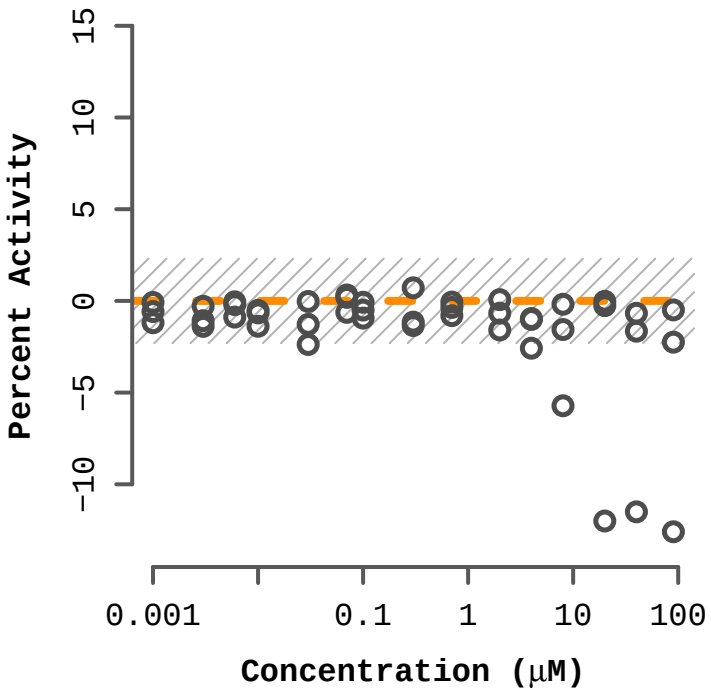
NAME: Pentyl acetate
CHID: 27263 **CASRN:** 628-63-7
SPID(S): Tox21_300360
M4ID: 12478772

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.552 **MAX_MED:** 0.945 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

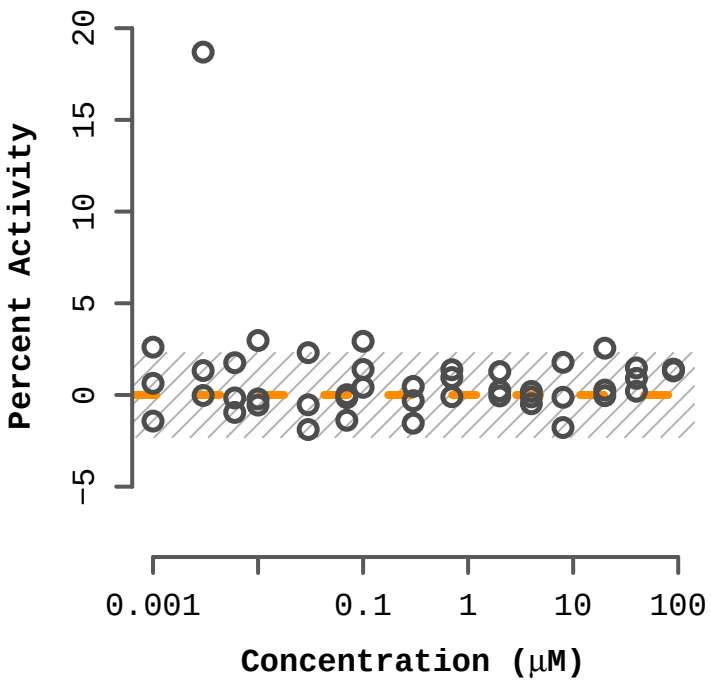
NAME: Pentyl acetate
CHID: 27263 **CASRN:** 628-63-7
SPID(S): Tox21_201628
M4ID: 12480624

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.2	NA	NA
PROB:	1	NA	NA
RMSE:	3.37	NA	NA

MAX_MEAN: −0.0355 **MAX_MED:** 0.193 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

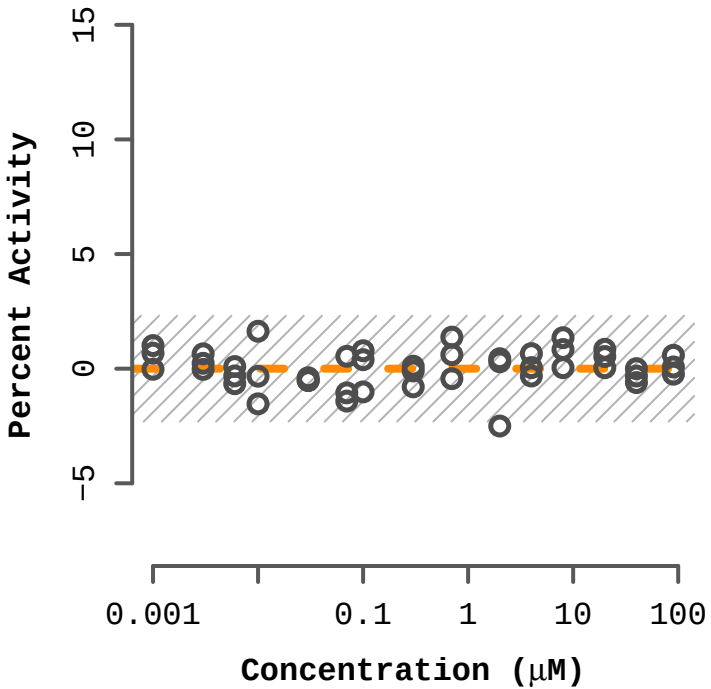
NAME: 1,6-Hexanediol
CHID: 27265 CASRN: 629-11-8
SPID(S): Tox21_200450
M4ID: 12481802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.07	NA	NA

MAX_MEAN: 6.67 MAX_MED: 1.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

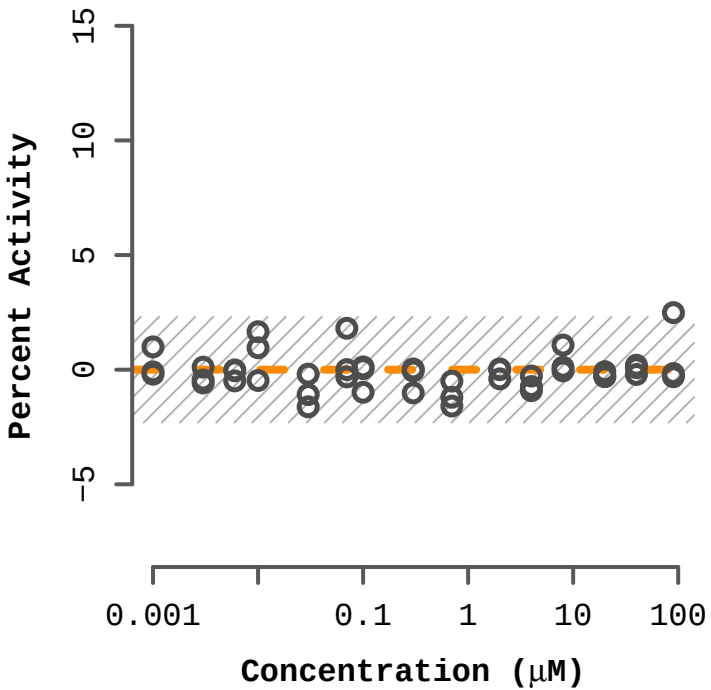
NAME: Tridecane
CHID: 27266 **CASRN:** 629-50-5
SPID(S): Tox21_303043
M4ID: 12476090

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.745 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

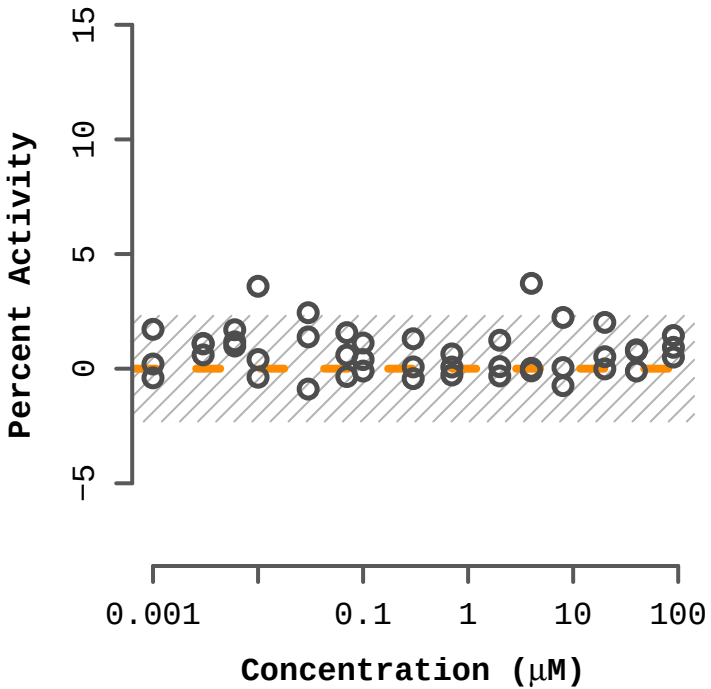
NAME: Tetradecane
CHID: 27267 **CASRN:** 629-59-4
SPID(S): Tox21_303277
M4ID: 12475856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.714 **MAX_MED:** 0.956 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

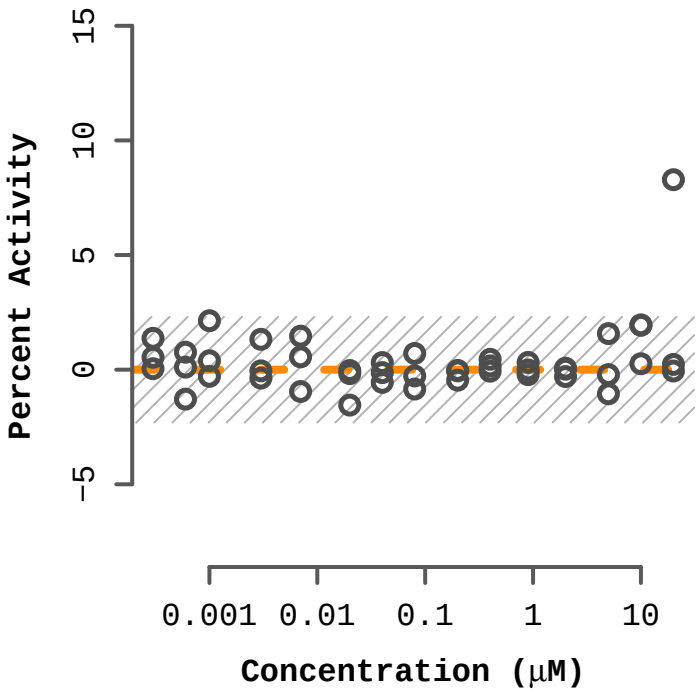
NAME: Pentadecane
CHID: 27268 **CASRN:** 629-62-9
SPID(S): Tox21_300535
M4ID: 12478597

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

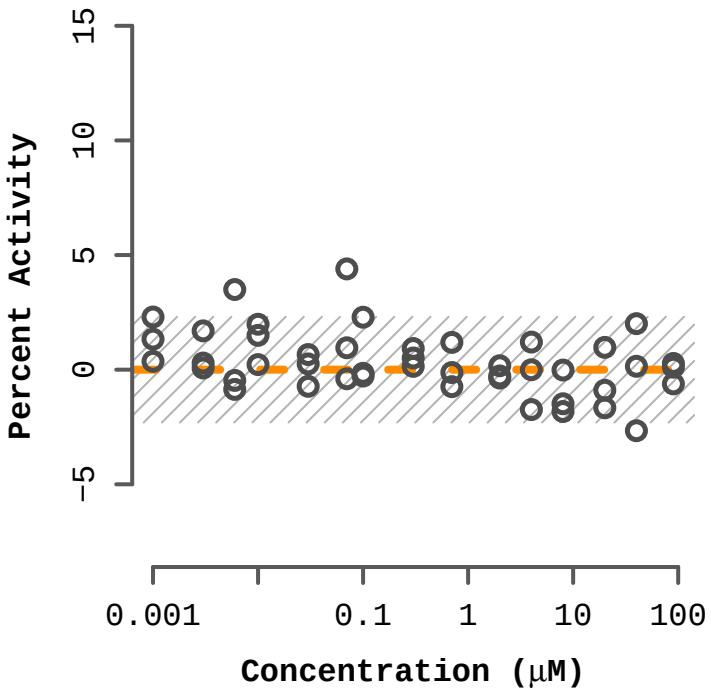
NAME: 1-Hexadecene
CHID: 27269 **CASRN:** 629-73-2
SPID(S): Tox21_202748
M4ID: 12479504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.82 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

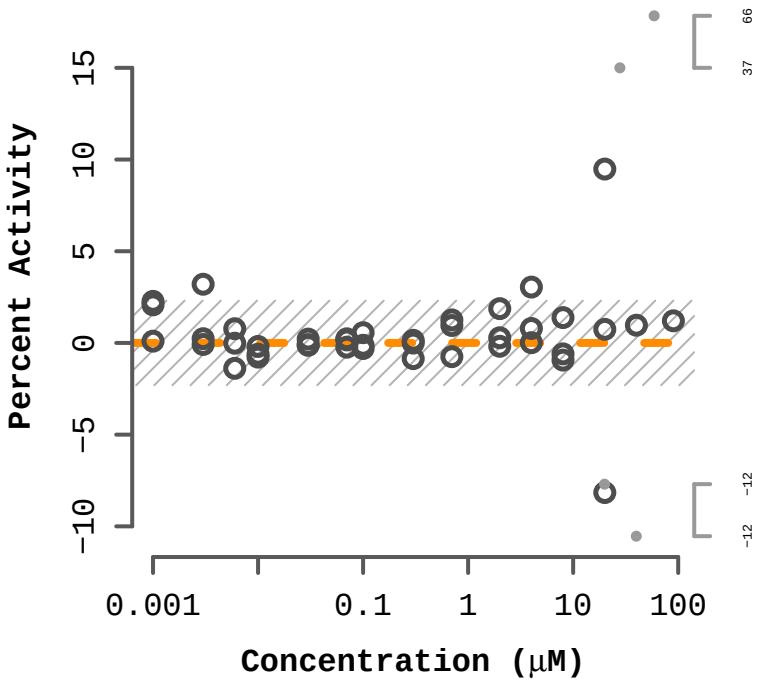
NAME: 1-Pentadecanol
CHID: 27270 **CASRN:** 629-76-5
SPID(S): Tox21_300553
M4ID: 12478580

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

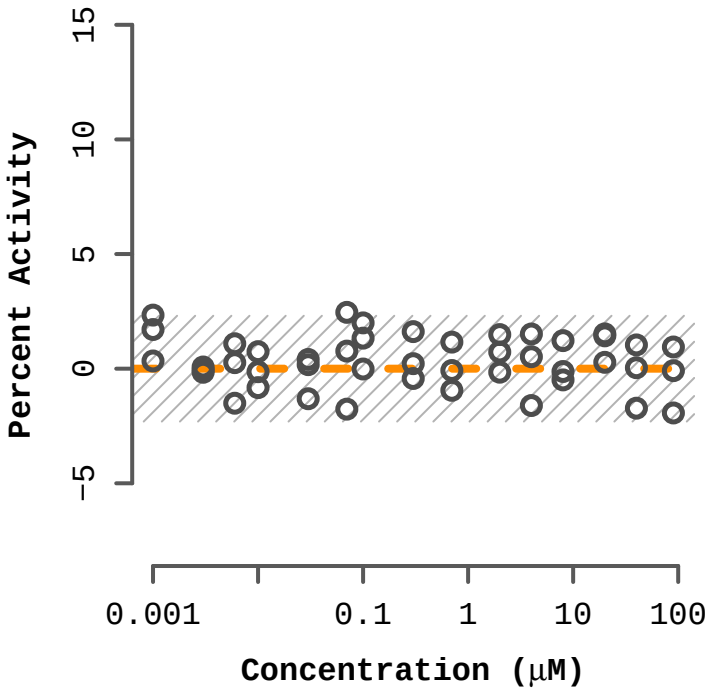
NAME: 1-Pentadecanol
CHID: 27270 **CASRN:** 629-76-5
SPID(S): Tox21_201699
M4ID: 12480553 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	255.15	NA	NA
PROB:	1	NA	NA
RMSE:	11.8	NA	NA

MAX_MEAN: 18.4 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

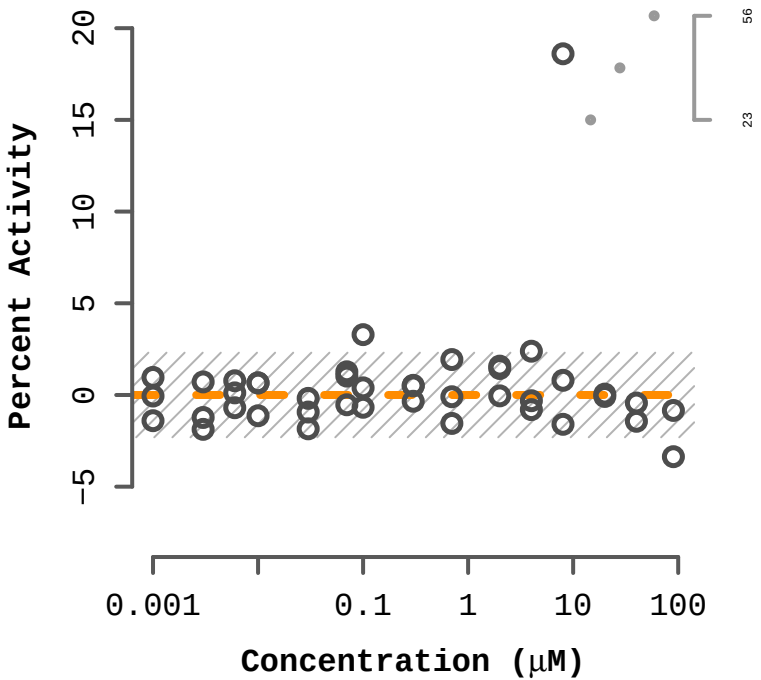
NAME: Manganese(II) acetate
CHID: 27279 **CASRN:** 638-38-0
SPID(S): Tox21_303412
M4ID: 12475727

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

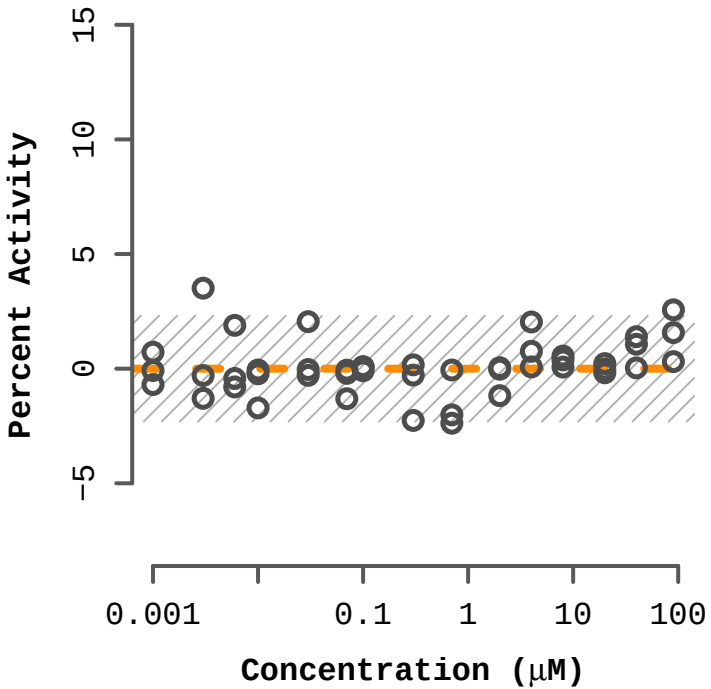
NAME: Manganese(II) acetate
CHID: 27279 **CASRN:** 638-38-0
SPID(S): Tox21_201865
M4ID: 12480387 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.7	NA	NA
PROB:	1	NA	NA
RMSE:	11.12	NA	NA

MAX_MEAN: 17.2 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

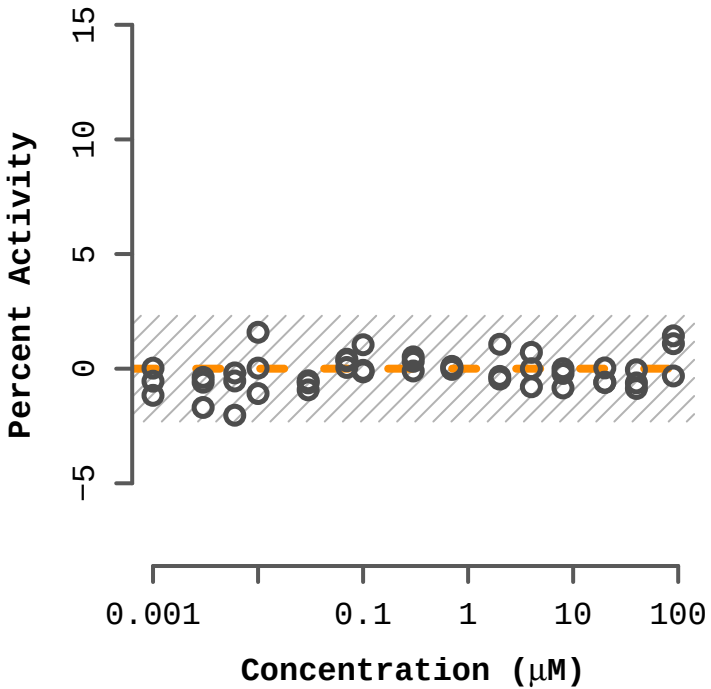
NAME: Octadecanenitrile
CHID: 27280 **CASRN:** 638-65-3
SPID(S): Tox21_202559
M4ID: 12479693

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

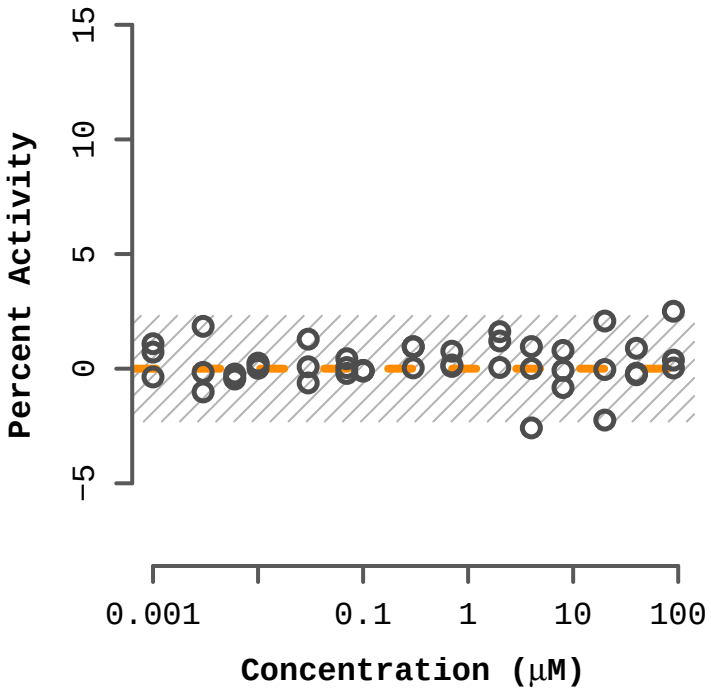
NAME: 2,3-Quinolinedicarboxylic acid
CHID: 27281 CASRN: 643-38-9
SPID(S): Tox21_301230
M4ID: 12477903

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.737 MAX_MED: 1.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

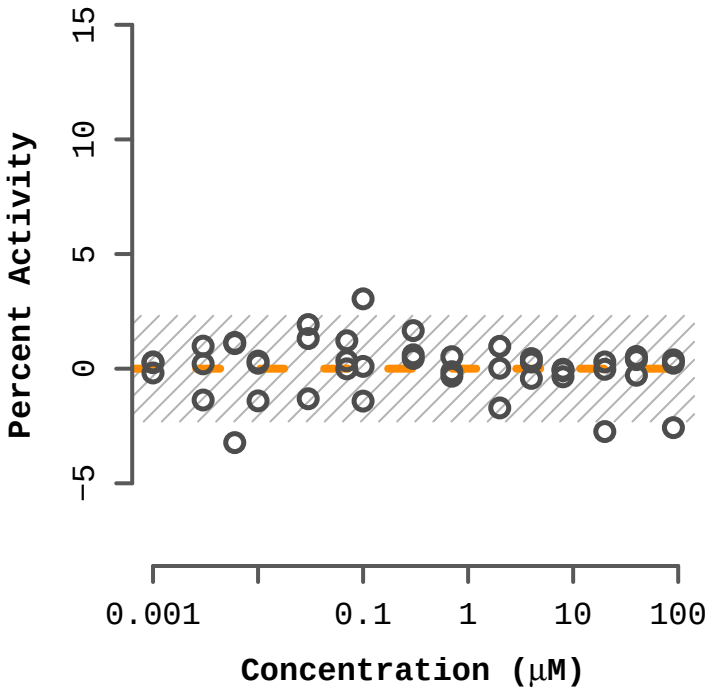
NAME: Phenyl phosphorus dichloride
CHID: 27282 **CASRN:** 644-97-3
SPID(S): Tox21_303070
M4ID: 12476063

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

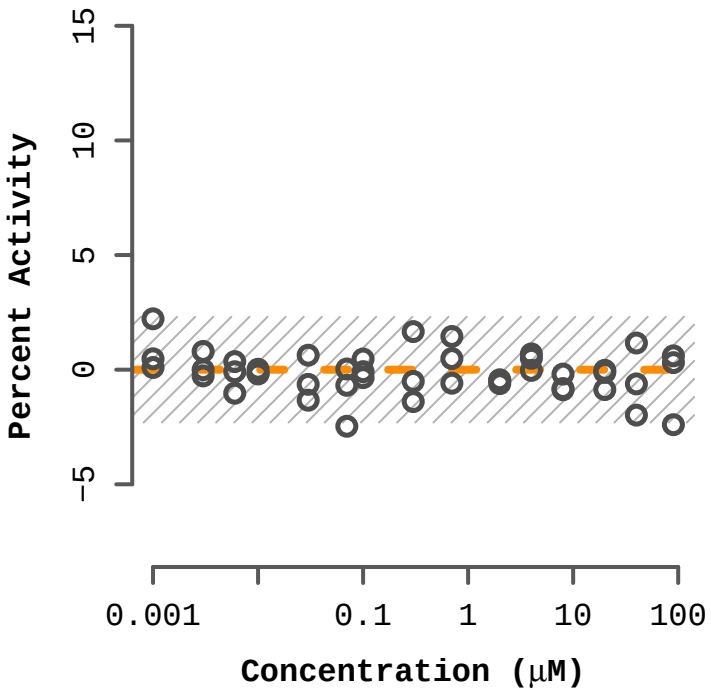
NAME: 1,3-Dioxolane
CHID: 27284 **CASRN:** 646-06-0
SPID(S): Tox21_300693
M4ID: 12478440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

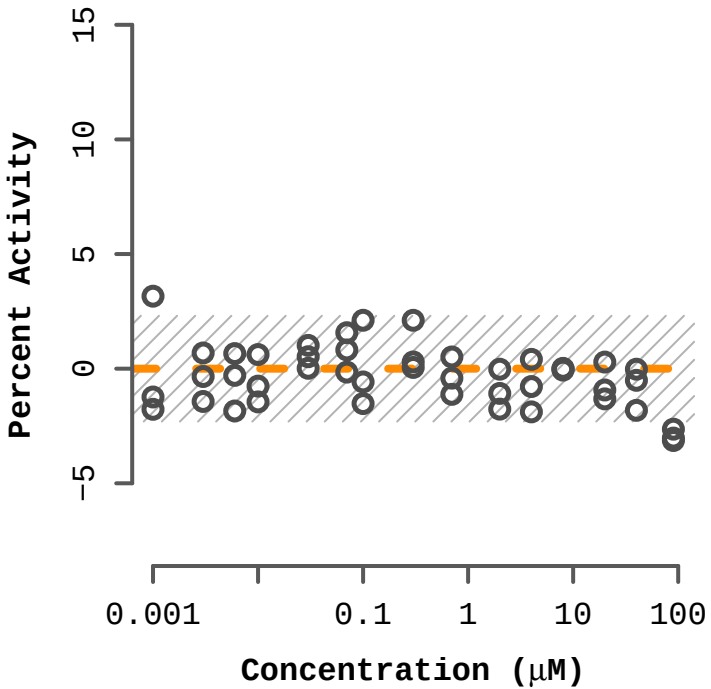
NAME: 2,6-Dimethyl-2,4,6-octatriene
CHID: 27288 **CASRN:** 673-84-7
SPID(S): Tox21_303244
M4ID: 12475889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 0.496 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

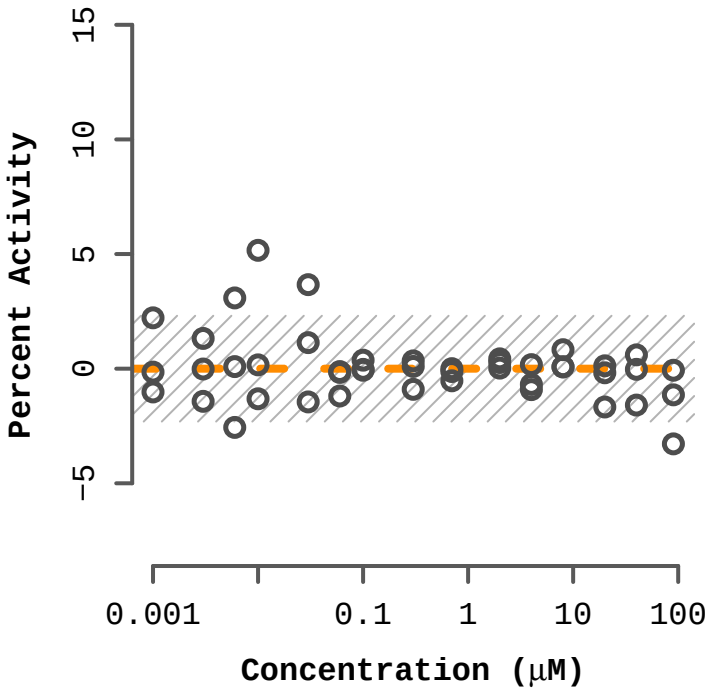
NAME: 2,6-Dimethyl-2,4,6-octatriene
CHID: 27288 **CASRN:** 673-84-7
SPID(S): Tox21_202278
M4ID: 12479974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.82 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

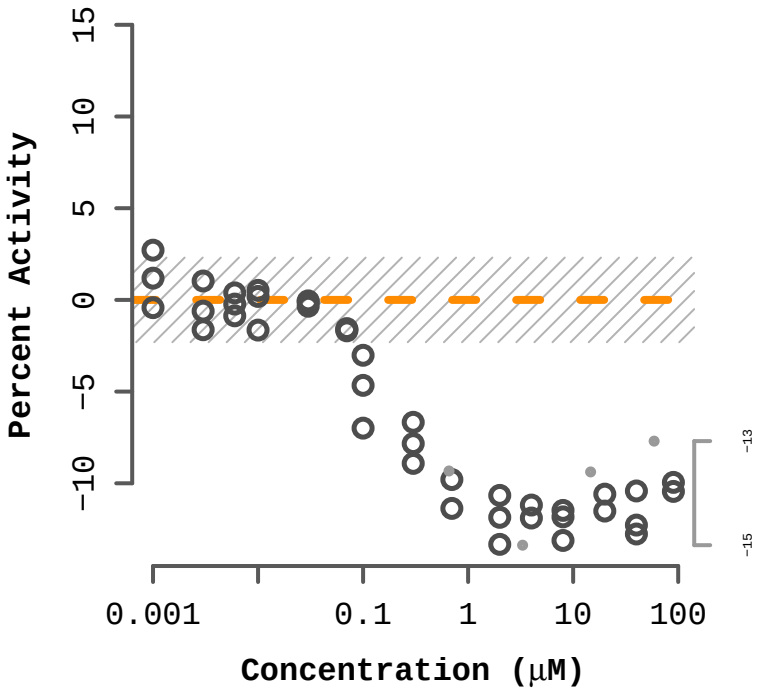
NAME: Tetramethyl orthosilicate
CHID: 27291 **CASRN:** 681-84-5
SPID(S): Tox21_200780
M4ID: 12481472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

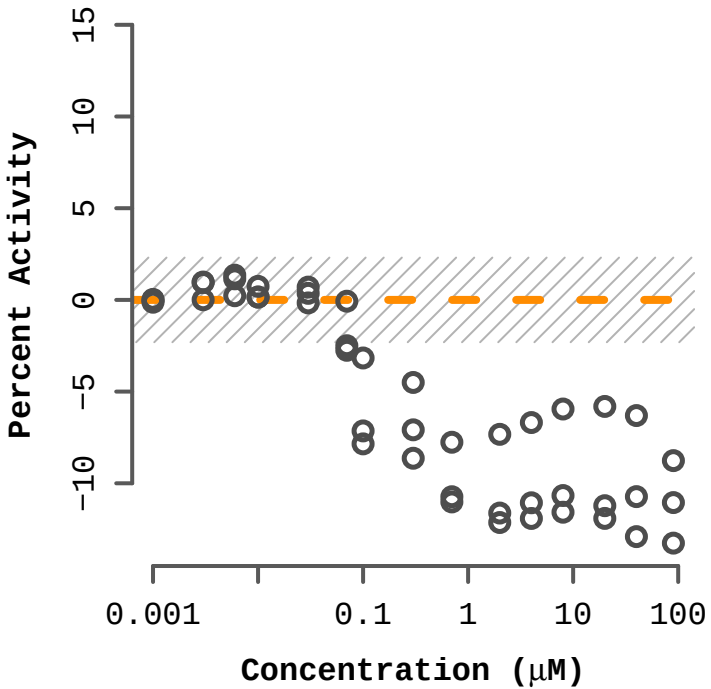
NAME: Dibutyltin dichloride
CHID: 27292 **CASRN:** 683-18-1
SPID(S): Tox21_303112
M4ID: 12476021 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	329.03	NA	NA
PROB:	1	NA	NA
RMSE:	8.59	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

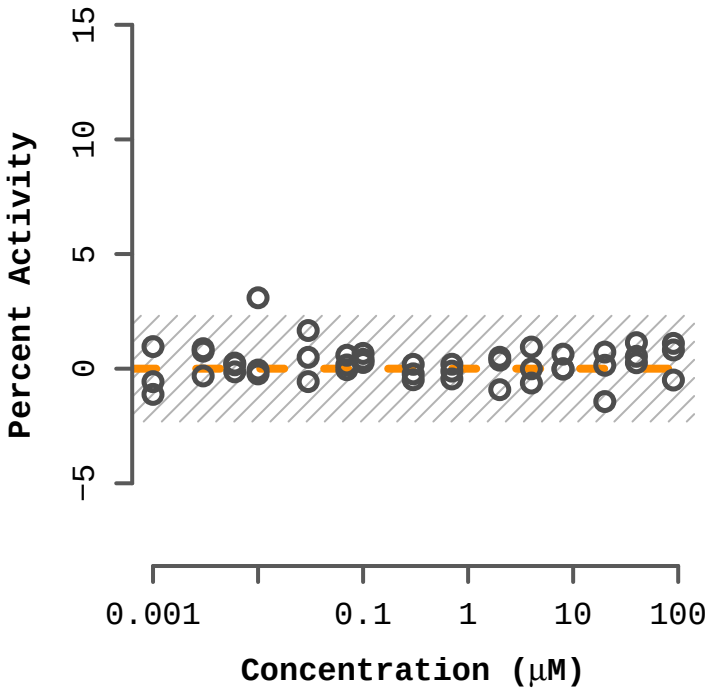
NAME: Dibutyltin dichloride
CHID: 27292 **CASRN:** 683-18-1
SPID(S): Tox21_201675
M4ID: 12480577

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	315.82	NA	NA
PROB:	1	NA	NA
RMSE:	7.47	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

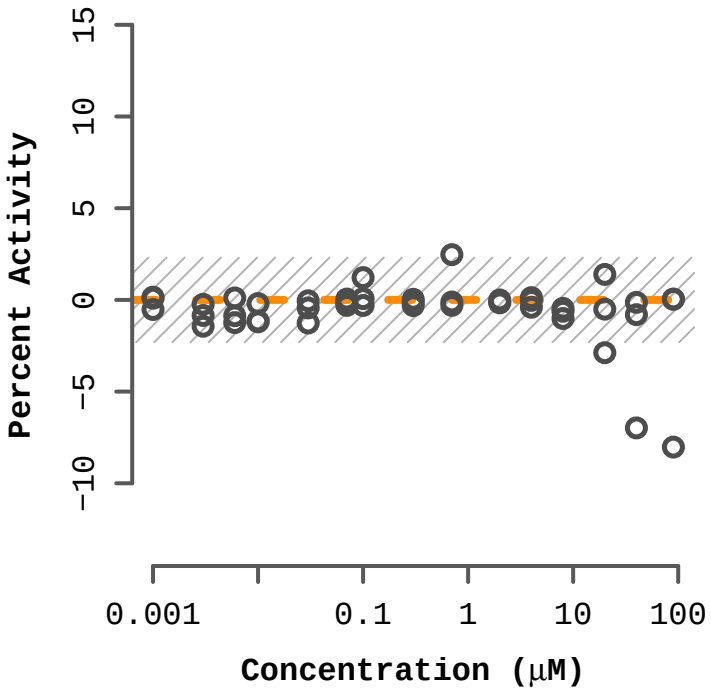
NAME: 2-Ethylhexyl methacrylate
CHID: 27293 CASRN: 688-84-6
SPID(S): Tox21_303072
M4ID: 12476061

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.937 MAX_MED: 0.818 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

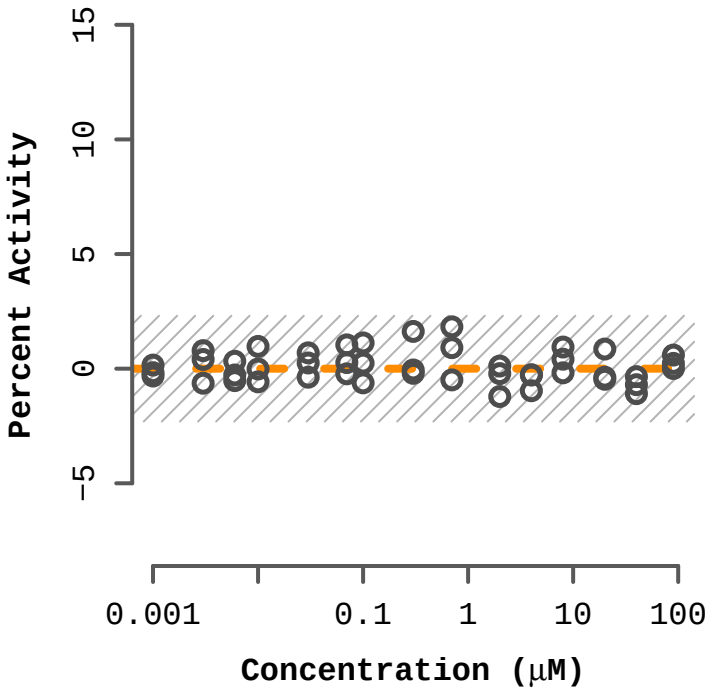
NAME: 2-Ethylhexyl methacrylate
CHID: 27293 **CASRN:** 688-84-6
SPID(S): Tox21_201535
M4ID: 12480717

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 0.687 **MAX_MED:** 0.0926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

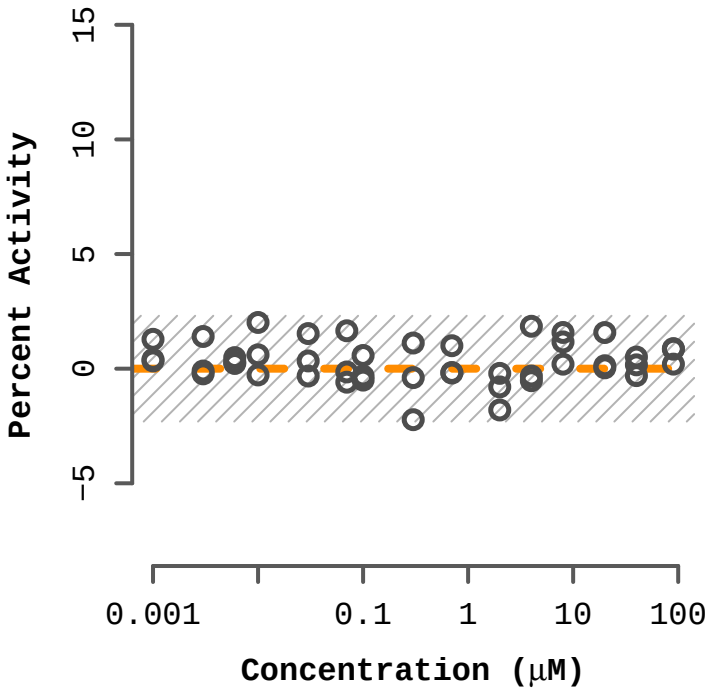
NAME: sec−Butylurea
CHID: 27294 **CASRN:** 689−11−2
SPID(S): Tox21_301703
M4ID: 12477430

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.752 **MAX_MED:** 0.918 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

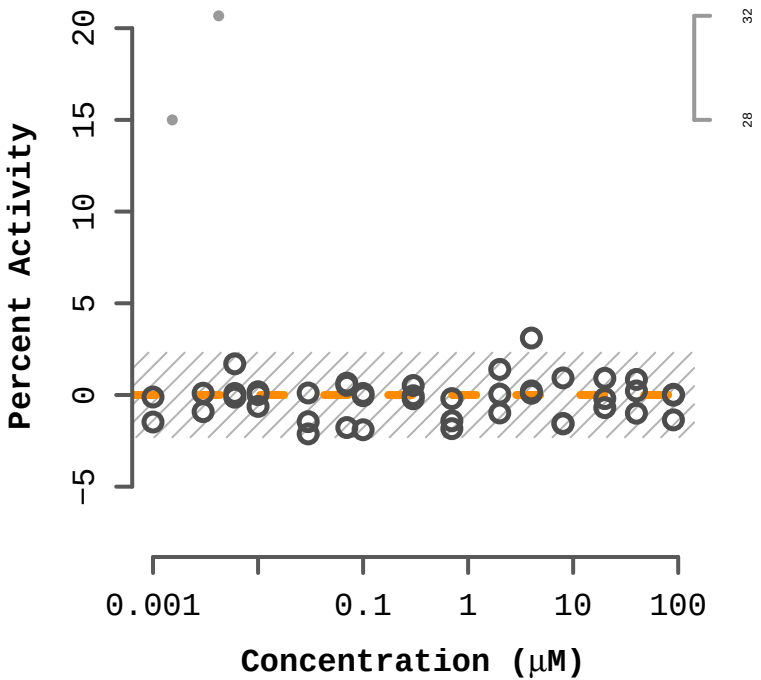
NAME: 1-Chloro-2-(ethylthio)ethane
CHID: 27295 **CASRN:** 693-07-2
SPID(S): Tox21_200911
M4ID: 12481341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

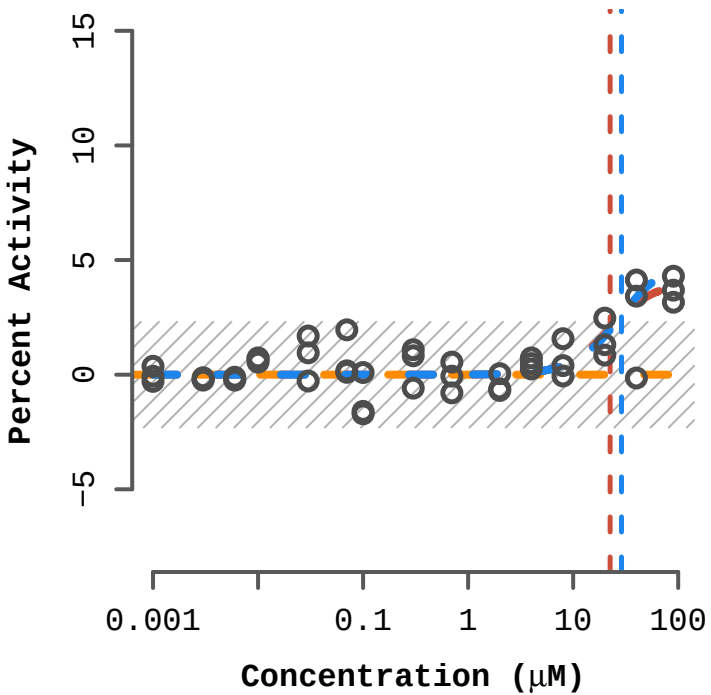
NAME: Dodecanedioic acid
CHID: 27297 **CASRN:** 693-23-2
SPID(S): Tox21_303308
M4ID: 12475825 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.67	NA	NA
PROB:	1	NA	NA
RMSE:	6.44	NA	NA

MAX_MEAN: 10.5 **MAX_MED:** 0.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dodecanedioic acid
CHID: 27297 CASRN: 693-23-2
SPID(S): Tox21_201954
M4ID: 12480298

HILL MODEL (in red):

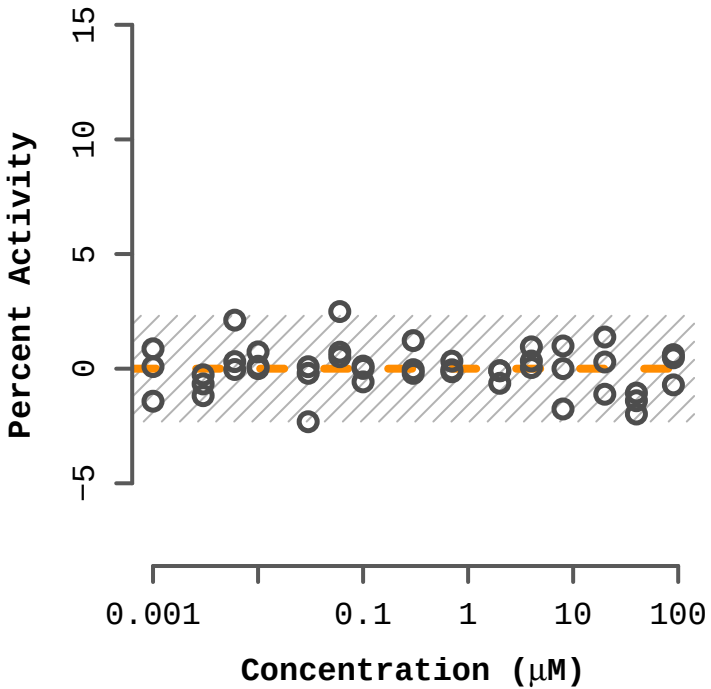
	tp	ga	gw
val:	4.02	1.35	2.12
sd:	0.618	0.111	1.27

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.16	1.46	1.96	2.05	6.53
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.69	118.64	121.77
PROB:	0	0.83	0.17
RMSE:	1.5	0.88	0.9

MAX_MEAN: 3.72 MAX_MED: 3.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

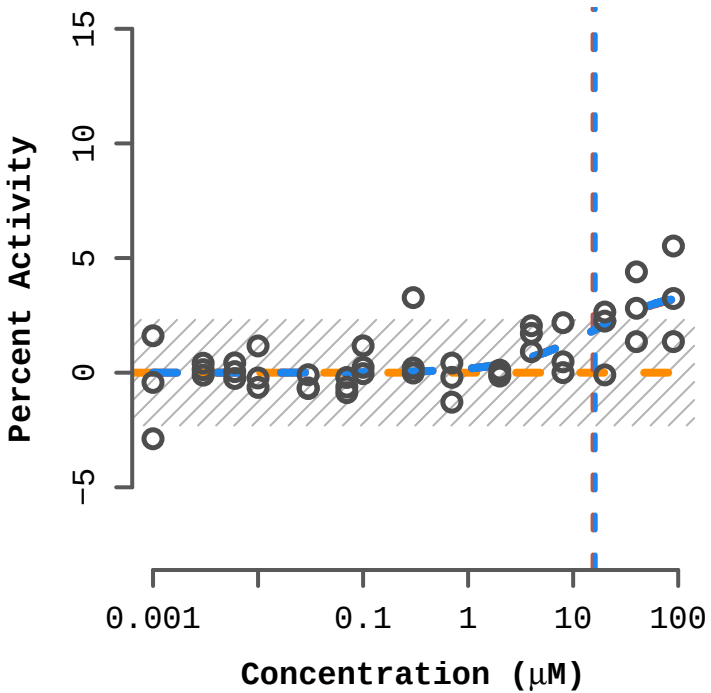
NAME: 4-Methylthiazole
CHID: 27300 **CASRN:** 693-95-8
SPID(S): Tox21_200124
M4ID: 12482128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.722 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2-Cyclohexanediamine
CHID: 27301 **CASRN:** 694-83-7
SPID(S): Tox21_303220
M4ID: 12475913

HILL MODEL (in red):

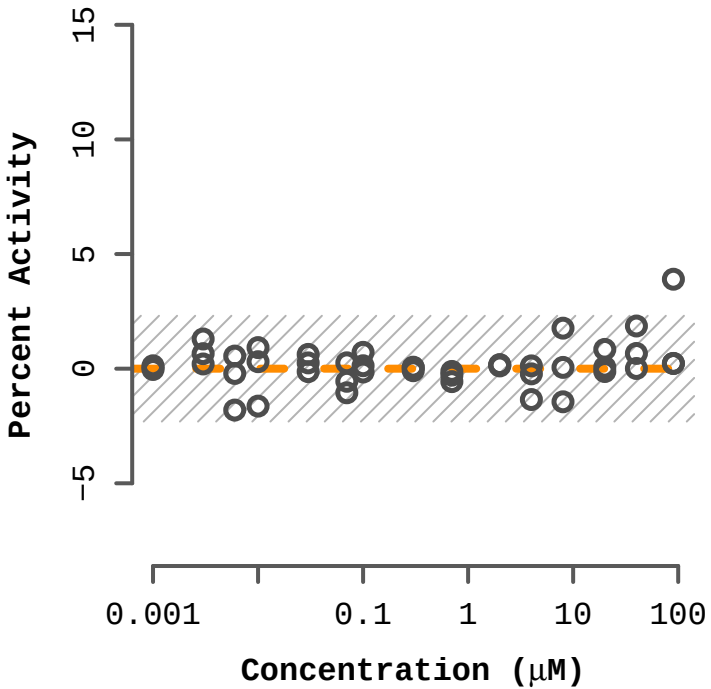
	tp	ga	gw
val:	3.67	1.19	1.09
sd:	1.66	0.494	0.564

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.75	1.21	1.08	2.1	12.6
sd:	4.57	1.15	0.873	1.35	133

	CNST	HILL	GNLS
AIC:	169.15	141.09	145.09
PROB:	0	0.88	0.12
RMSE:	1.68	1.1	1.1

MAX_MEAN: 3.37 **MAX_MED:** 3.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

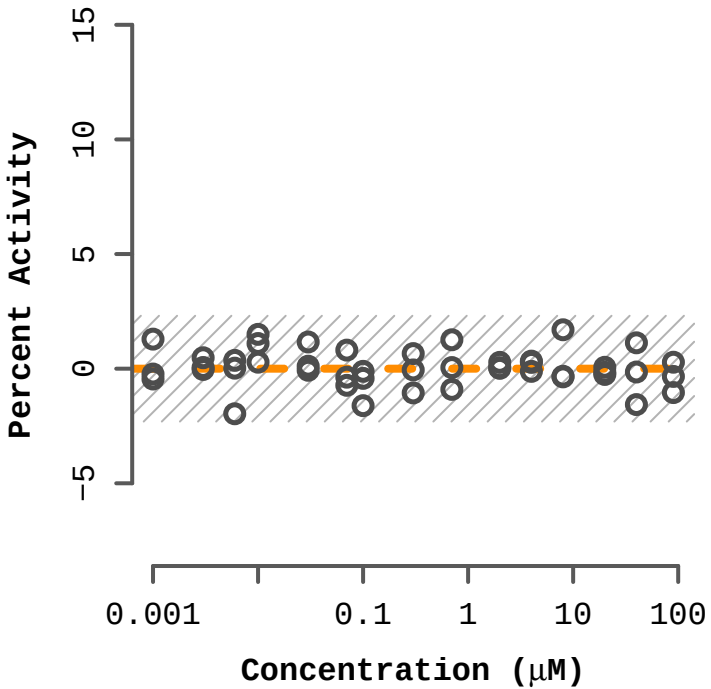
NAME: 1,2-Cyclohexanediamine
CHID: 27301 **CASRN:** 694-83-7
SPID(S): Tox21_201883
M4ID: 12480369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 0.666 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

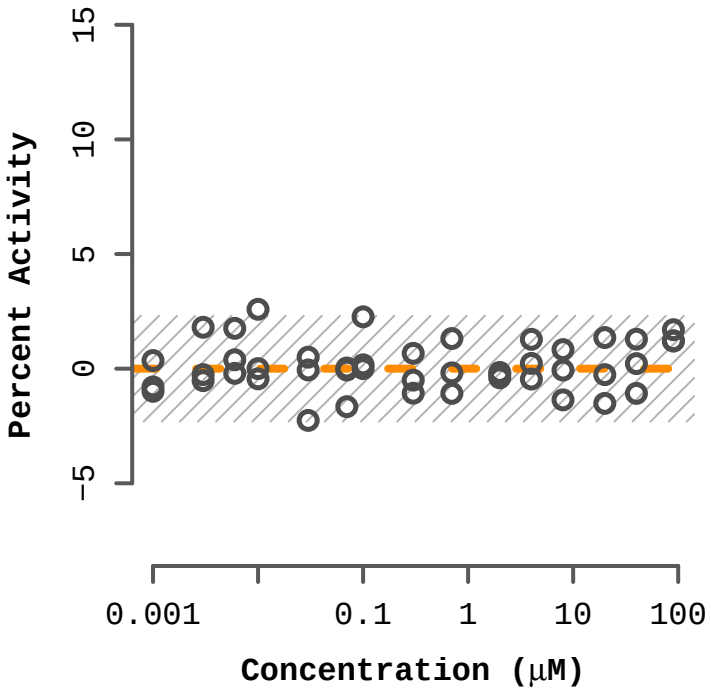
NAME: 2,3,5,6−Tetrachlorobenzene−1,4−dicarbonyl dich
CHID: 27302 CASRN: 719−32−4
SPID(S): Tox21_303098
M4ID: 12476035

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.961 MAX_MED: 1.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

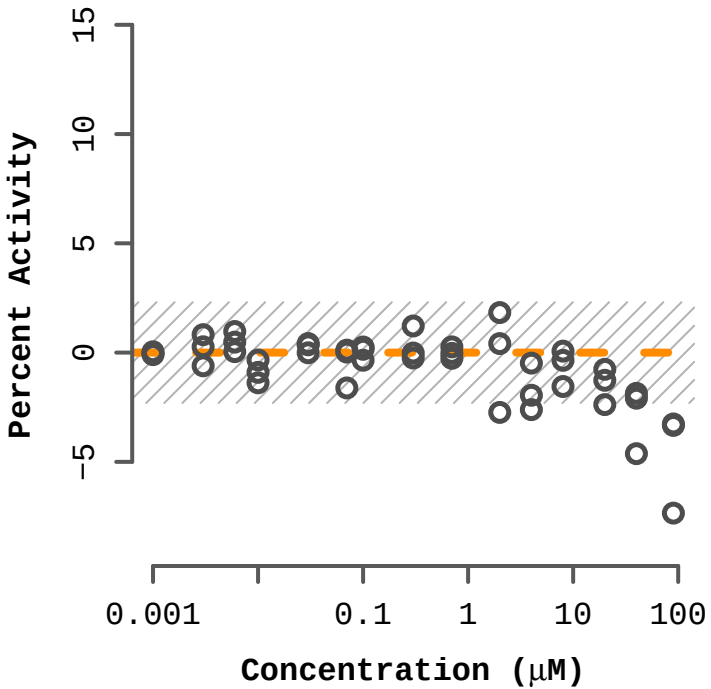
NAME: 2,3,5,6-Tetrachlorobenzene-1,4-dicarbonyl dich
CHID: 27302 CASRN: 719-32-4
SPID(S): Tox21_201449
M4ID: 12480803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.38 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

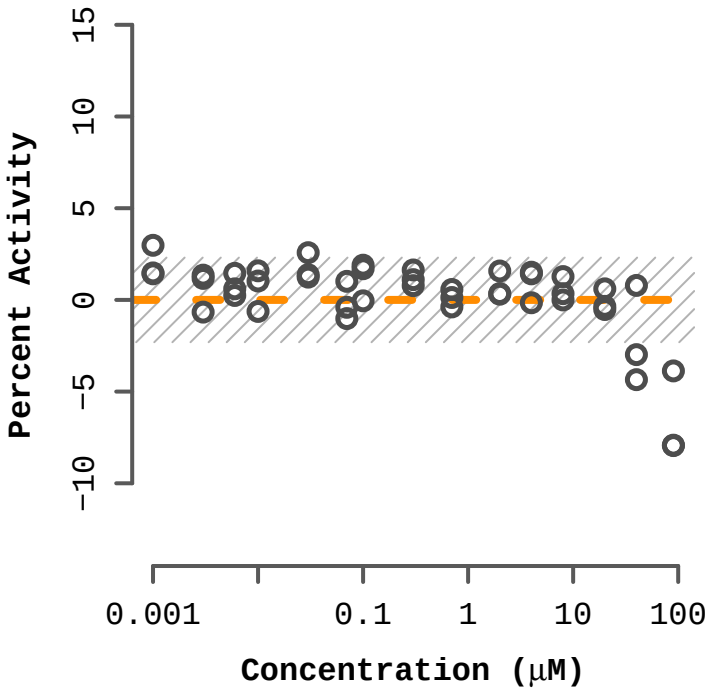
NAME: Dimethyltin dichloride
CHID: 27304 **CASRN:** 753-73-1
SPID(S): Tox21_303137
M4ID: 12475996

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 0.497 **MAX_MED:** 0.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

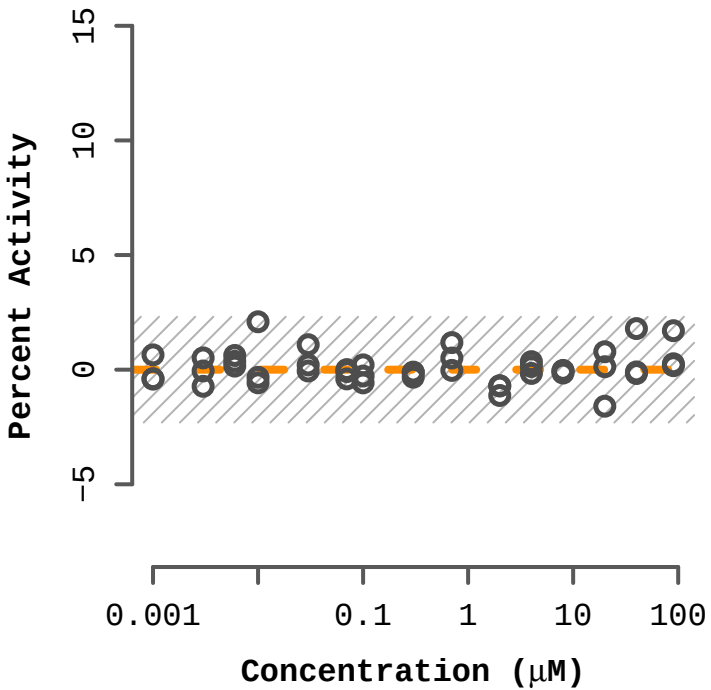
NAME: Dimethyltin dichloride
CHID: 27304 **CASRN:** 753-73-1
SPID(S): Tox21_201249
M4ID: 12481003

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

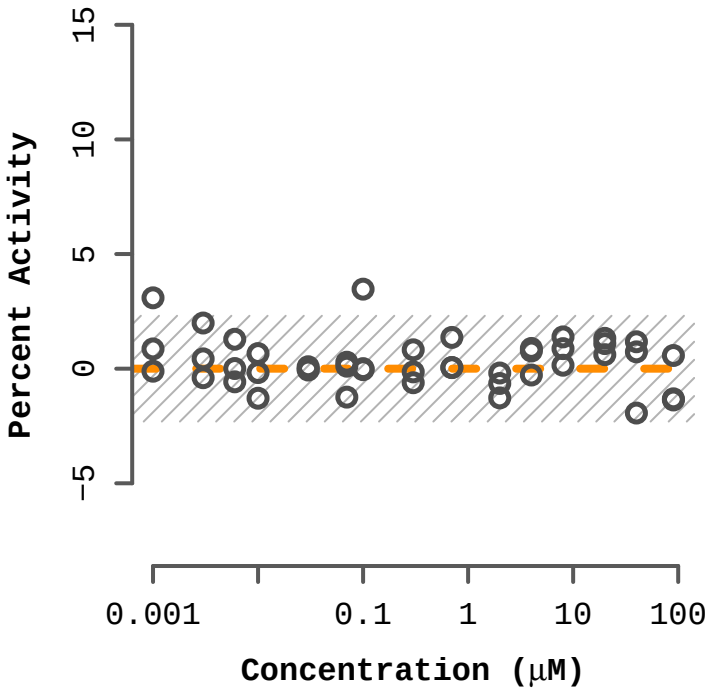
NAME: 2-Ethylhexanoyl chloride
CHID: 27308 **CASRN:** 760-67-8
SPID(S): Tox21_303258
M4ID: 12475875

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.713 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

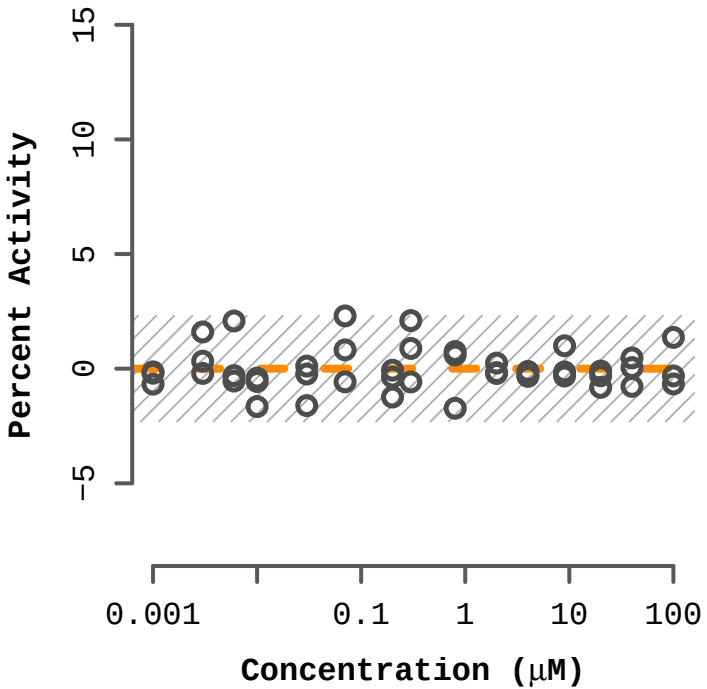
NAME: 2-Ethylhexanoyl chloride
CHID: 27308 **CASRN:** 760-67-8
SPID(S): Tox21_201268
M4ID: 12480984

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

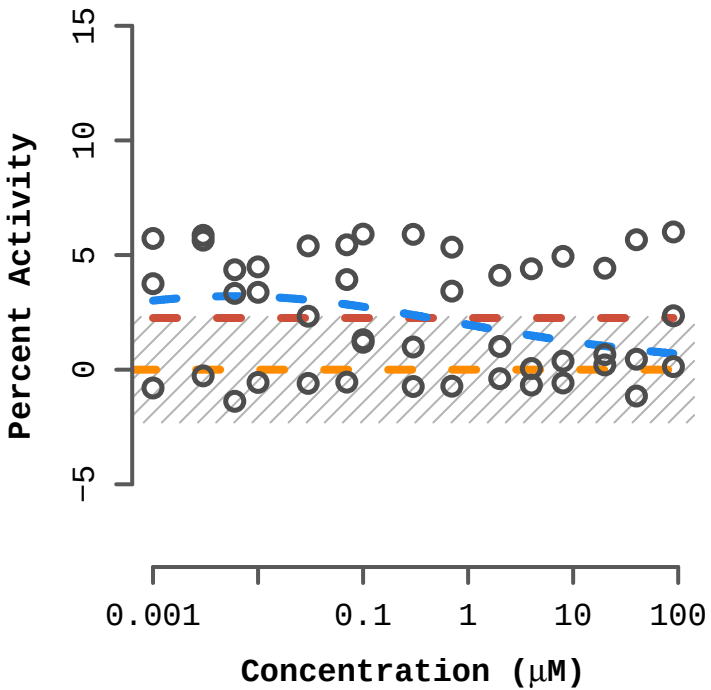
NAME: Ethyl 3-ethoxypropionate
CHID: 27309 **CASRN:** 763-69-9
SPID(S): Tox21_200179
M4ID: 12482073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.851 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4-Dichloro-2-butene
CHID: 27310 **CASRN:** 764-41-0
SPID(S): Tox21_200451
M4ID: 12481801

HILL MODEL (in red):

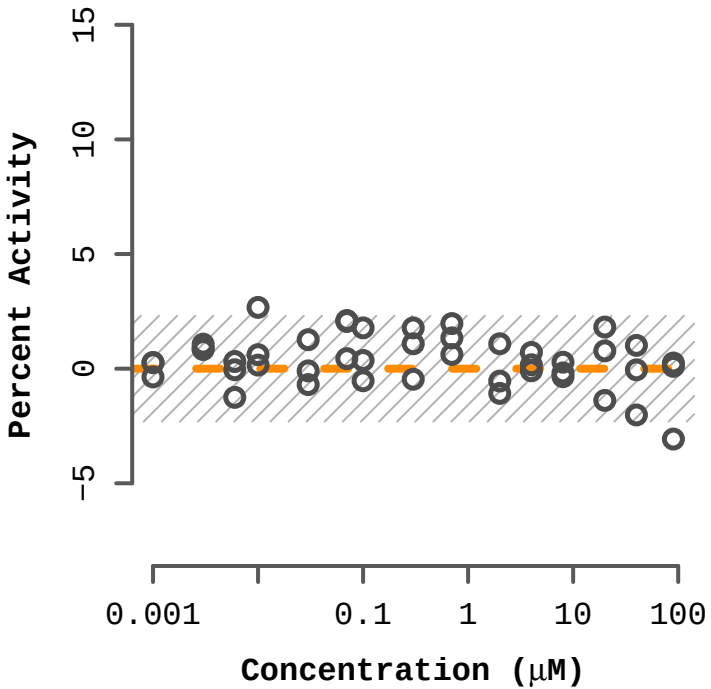
	tp	ga	gw
val:	2.25	−4.9	3.65
sd:	0.455	1180	2250

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.16	−3.24	0.3	−1.21	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	245.16	228.39	230.96
PROB:	0	0.78	0.22
RMSE:	3.44	2.54	2.57

MAX_MEAN: 3.75 **MAX_MED:** 5.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

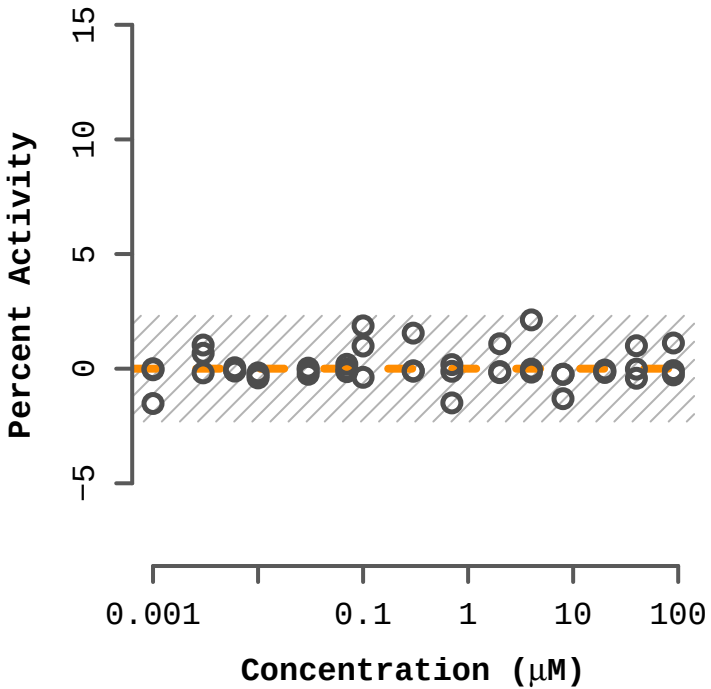
NAME: 1-Phenoxy-2-propanol
CHID: 27312 **CASRN:** 770-35-4
SPID(S): Tox21_303078
M4ID: 12476055

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

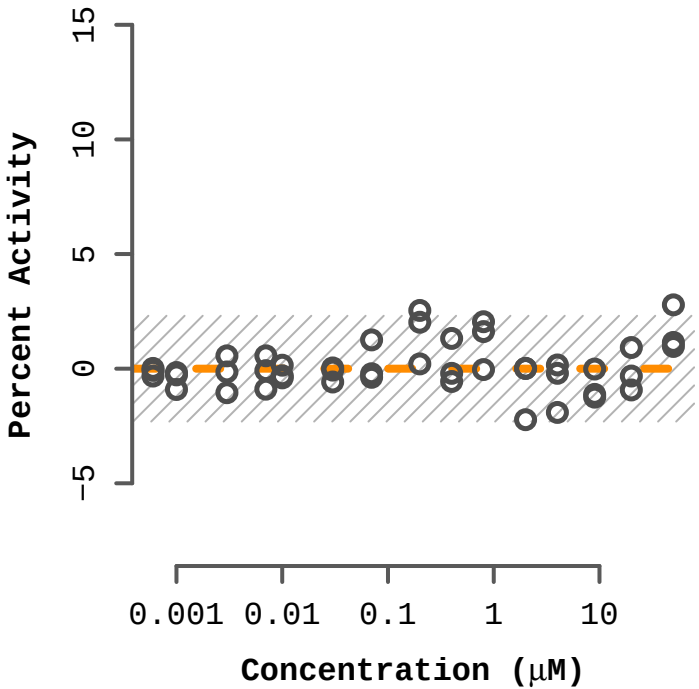
NAME: 1-Phenoxy-2-propanol
CHID: 27312 **CASRN:** 770-35-4
SPID(S): Tox21_201710
M4ID: 12480542

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.827 **MAX_MED:** 0.989 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

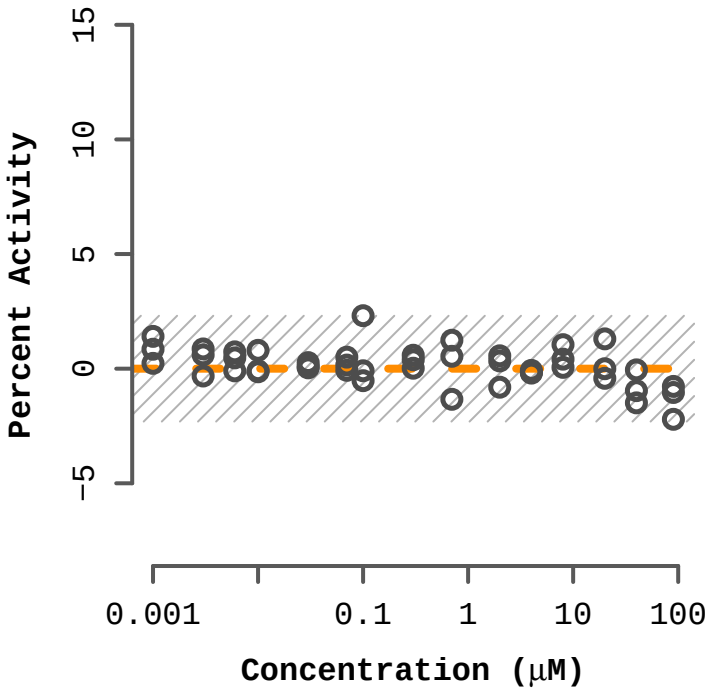
NAME: 1-Phenoxy-2-propanol
CHID: 27312 **CASRN:** 770-35-4
SPID(S): Tox21_112108_1
M4ID: 12483315

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

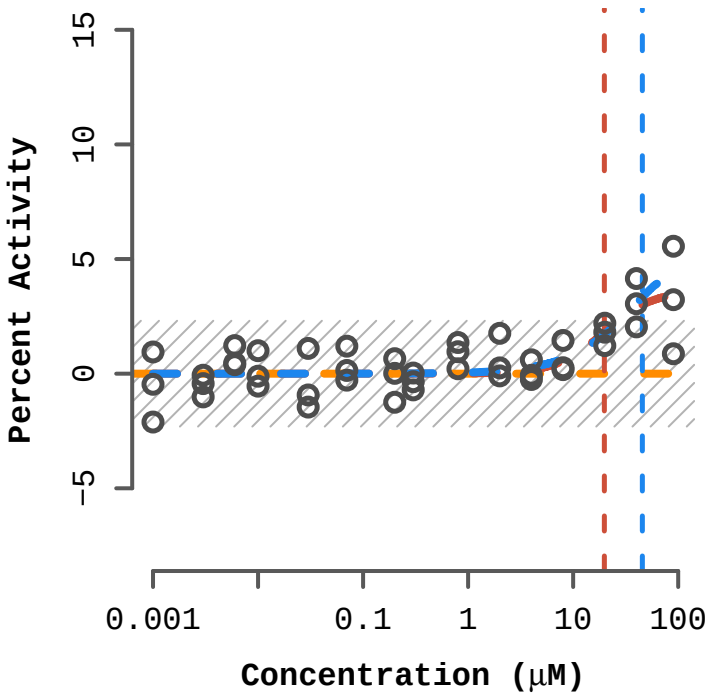
NAME: 3,3-Dimethyl-2-oxobutyric acid
CHID: 27314 **CASRN:** 815-17-8
SPID(S): Tox21_301454
M4ID: 12477679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.831 **MAX_MED:** 0.849 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6-Toluenediamine
CHID: 27319 **CASRN:** 823-40-5
SPID(S): Tox21_200125
M4ID: 12482127

HILL MODEL (in red):

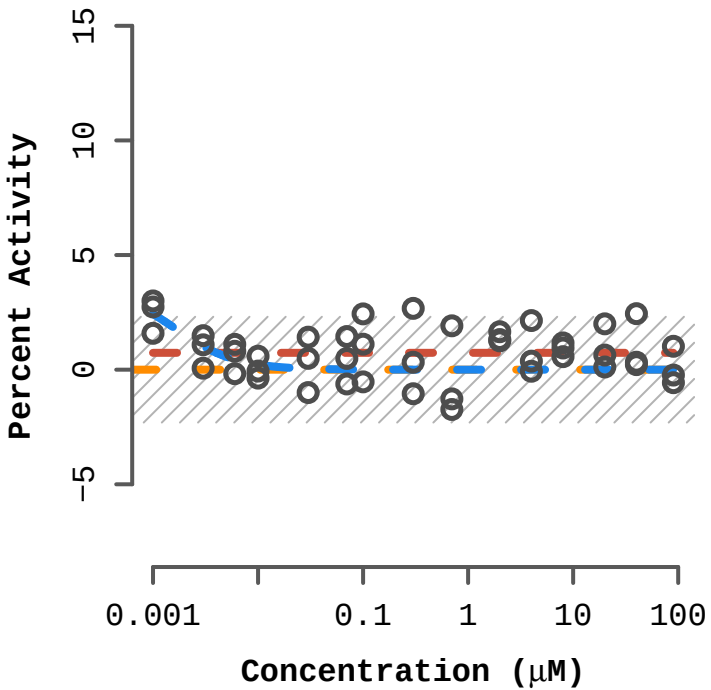
	tp	ga	gw
val:	3.63	1.3	1.89
sd:	1.06	0.183	1.19

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.67	1.66	1.28	1.99	8.54
sd:	12.3	1.17	1.06	0.0909	27.4

	CNST	HILL	GNLS
AIC:	162.25	130.3	133.88
PROB:	0	0.86	0.14
RMSE:	1.56	0.94	0.93

MAX_MEAN: 3.22 **MAX_MED:** 3.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium 4-nitrophenolate
CHID: 27320 CASRN: 824-78-2
SPID(S): Tox21_300477
M4ID: 12478655

HILL MODEL (in red):

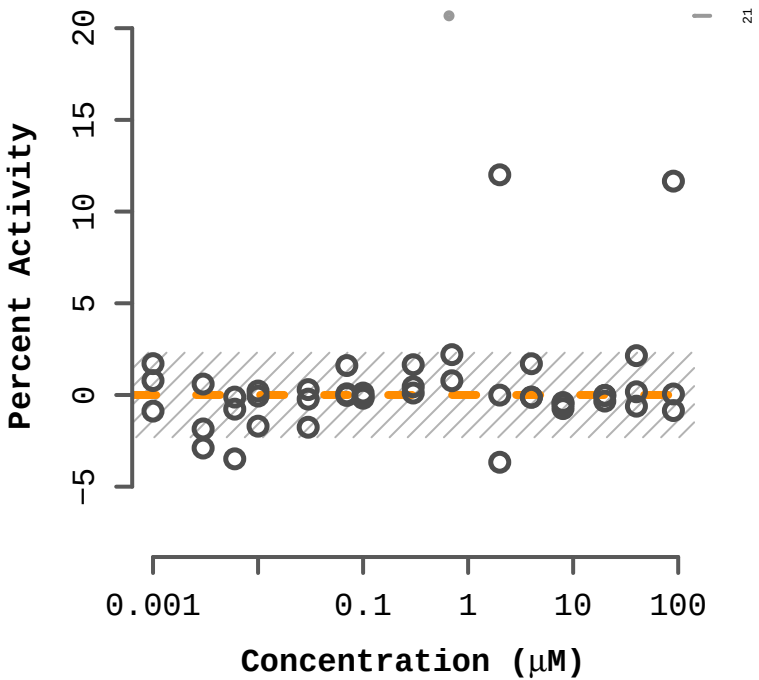
	tp	ga	gw
val:	0.735	−4.94	3.93
sd:	0.17	1310	2660

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.6	−3.95	7.89	−2.79	1.5
sd:	4.23	1440	11900	0.808	1.67

	CNST	HILL	GNLS
AIC:	159.27	148.99	154.56
PROB:	0.01	0.94	0.06
RMSE:	1.34	1.11	1.15

MAX_MEAN: 2.44 **MAX_MED:** 2.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

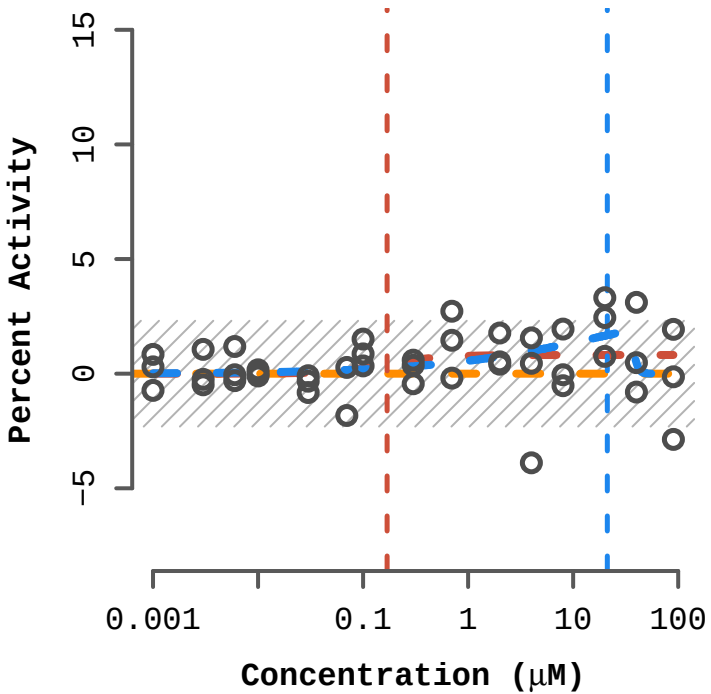
NAME: Monosodium 4-phenolsulfonate
CHID: 27321 **CASRN:** 825-90-1
SPID(S): Tox21_202560
M4ID: 12479692 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.15	NA	NA
PROB:	1	NA	NA
RMSE:	4.23	NA	NA

MAX_MEAN: 8.1 **MAX_MED:** 2.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclododecanone
CHID: 27322 CASRN: 830-13-7
SPID(S): Tox21_303048
M4ID: 12476085

HILL MODEL (in red):

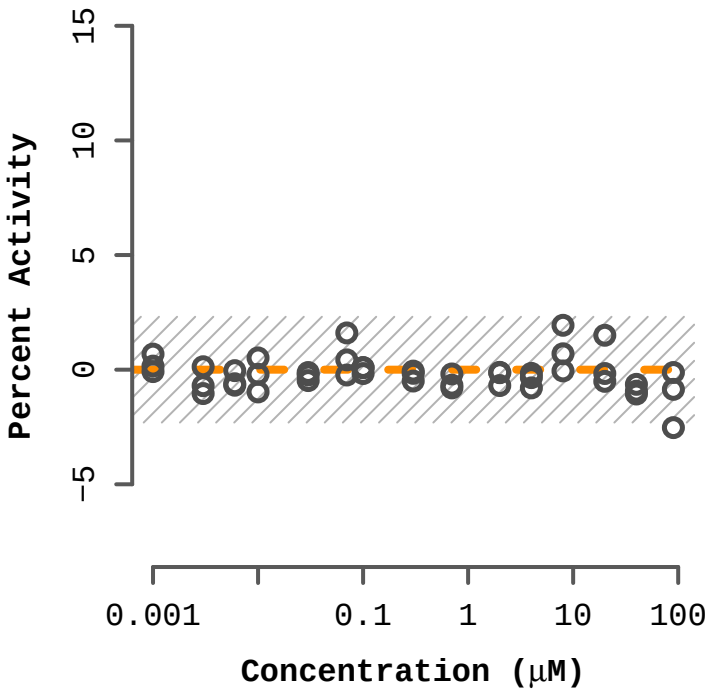
	tp	ga	gw
val:	0.815	−0.771	1.69
sd:	0.344	0.902	2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.36	1.33	0.527	1.58	18
sd:	8.09	3.18	0.321	0.106	69.7

	CNST	HILL	GNLS
AIC:	154.12	151.26	153.09
PROB:	0.15	0.61	0.24
RMSE:	1.41	1.33	1.3

MAX_MEAN: 2.17 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

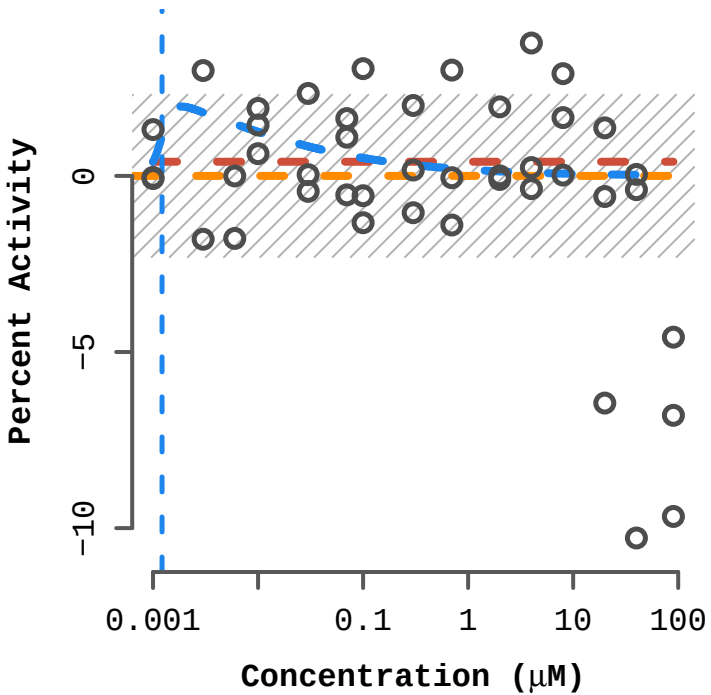
NAME: Cyclododecanone
CHID: 27322 **CASRN:** 830-13-7
SPID(S): Tox21_201557
M4ID: 12480695

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 0.695 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitro-N-phenylaniline
CHID: 27323 CASRN: 836-30-6
SPID(S): Tox21_303333
M4ID: 12475800

HILL MODEL (in red):

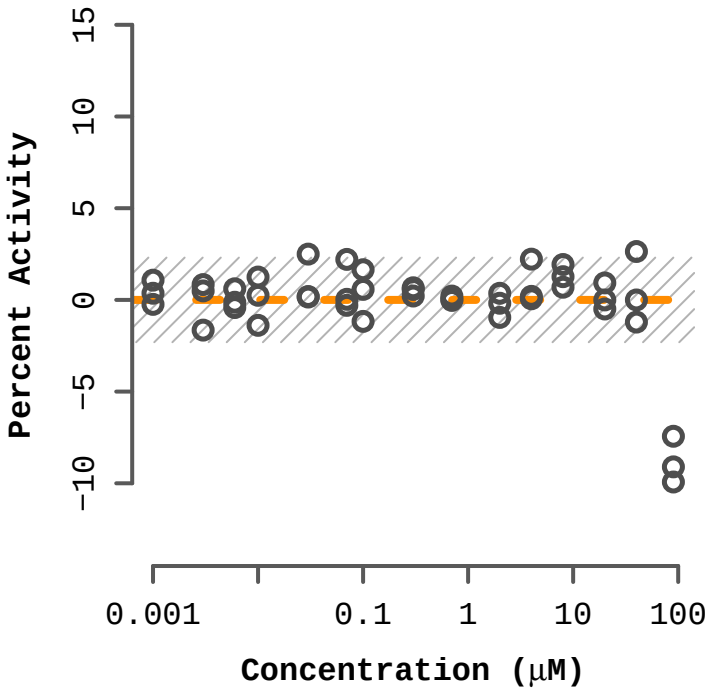
	tp	ga	gw
val:	0.402	−4.73	3.1
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.92	−2.91	7.99	−2.66	0.496
sd:	15	0.502	44.2	4.98	0.57

	CNST	HILL	GNLS
AIC:	223.02	227.63	228.88
PROB:	0.87	0.09	0.05
RMSE:	3.15	3.19	3.07

MAX_MEAN: 1.99 MAX_MED: 2.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

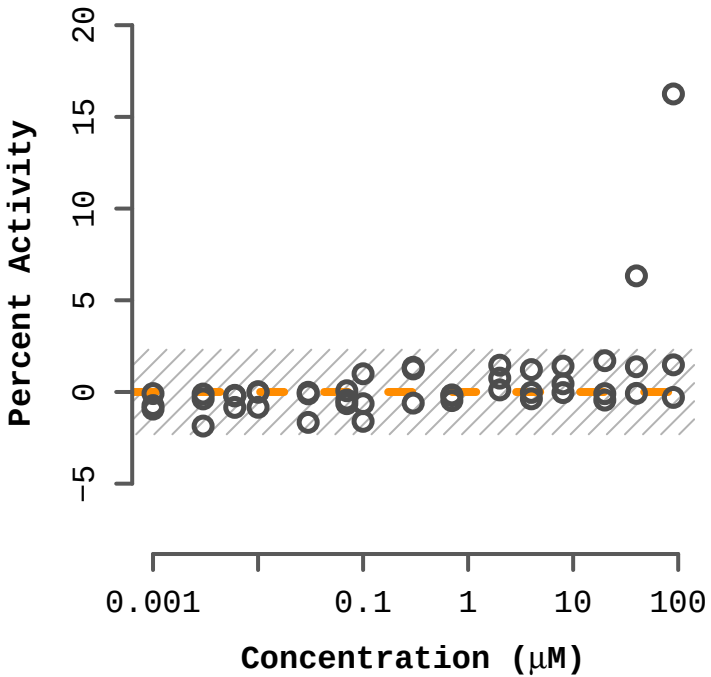
NAME: 4-Nitro-N-phenylaniline
CHID: 27323 **CASRN:** 836-30-6
SPID(S): Tox21_202300
M4ID: 12479952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

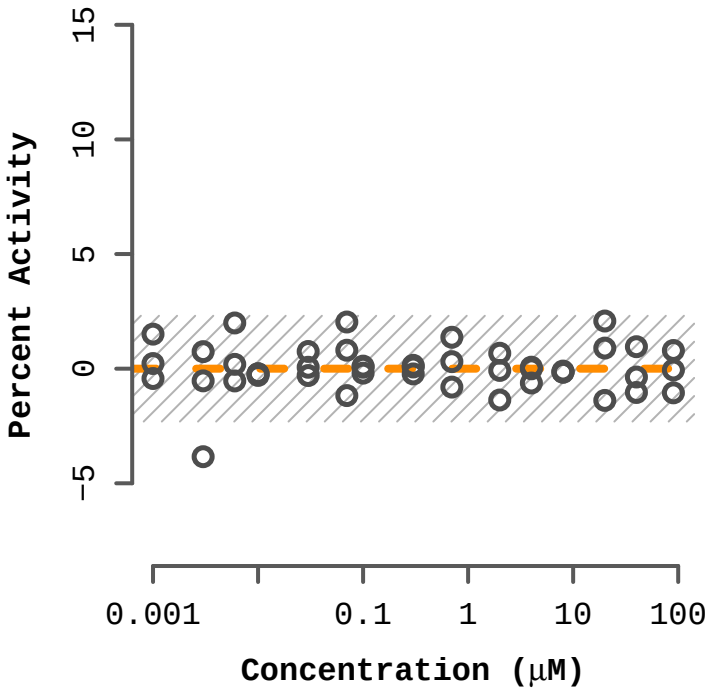
NAME: Sodium hydroxymethanesulfonate
CHID: 27328 CASRN: 870-72-4
SPID(S): Tox21_201095
M4ID: 12481157

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.03	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 5.81 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

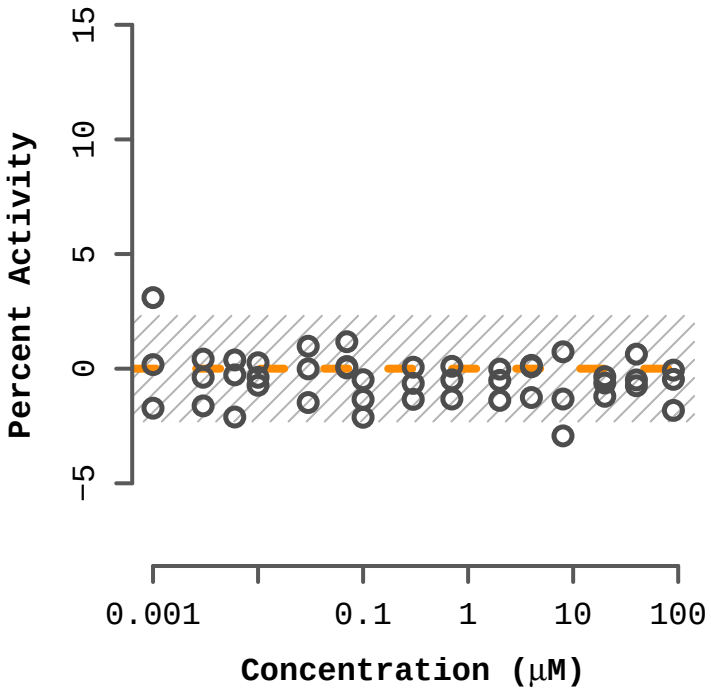
NAME: 1-Decene
CHID: 27329 **CASRN:** 872-05-9
SPID(S): Tox21_200195
M4ID: 12482057

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.557 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

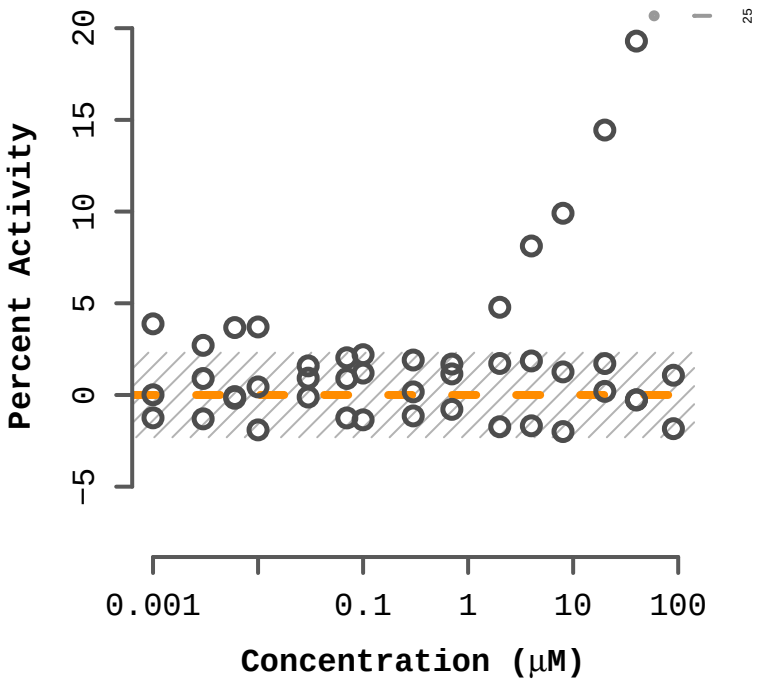
NAME: 3-Aminopropyltriethoxysilane
CHID: 27333 **CASRN:** 919-30-2
SPID(S): Tox21_303330
M4ID: 12475803

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.52 **MAX_MED:** 0.179 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

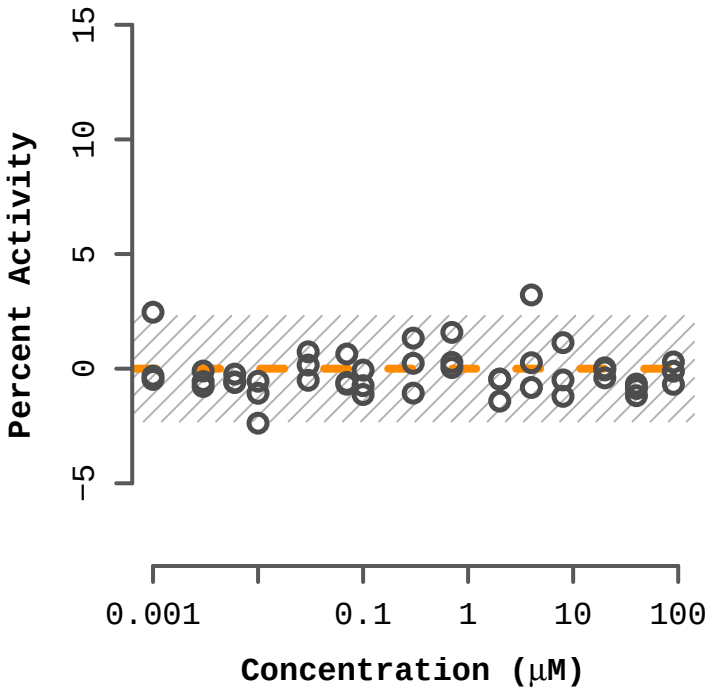
NAME: 3-Aminopropyltriethoxysilane
CHID: 27333 CASRN: 919-30-2
SPID(S): Tox21_201446
M4ID: 12480806 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	250.99	NA	NA
PROB:	1	NA	NA
RMSE:	5.79	NA	NA

MAX_MEAN: 8.11 MAX_MED: 1.86 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

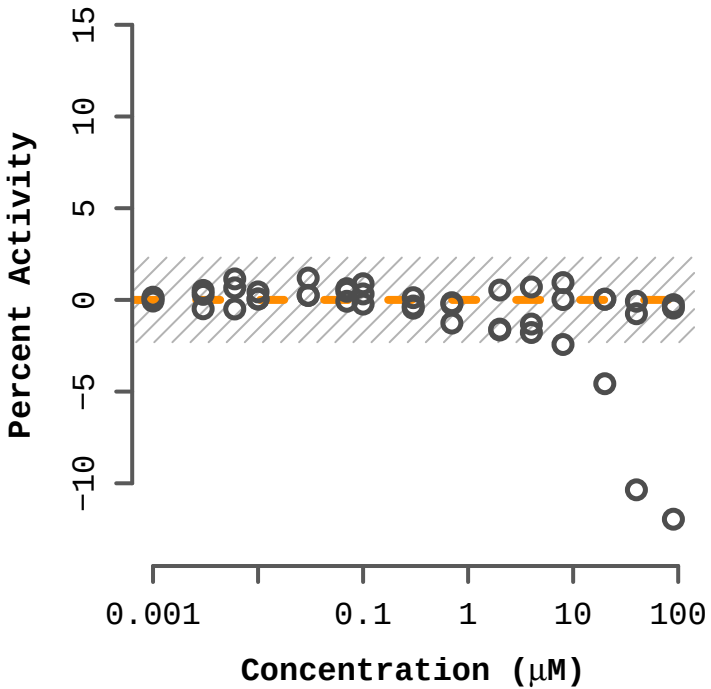
NAME: 3-(Triethoxysilyl)propionitrile
CHID: 27334 **CASRN:** 919-31-3
SPID(S): Tox21_303320
M4ID: 12475813

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.887 **MAX_MED:** 0.272 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

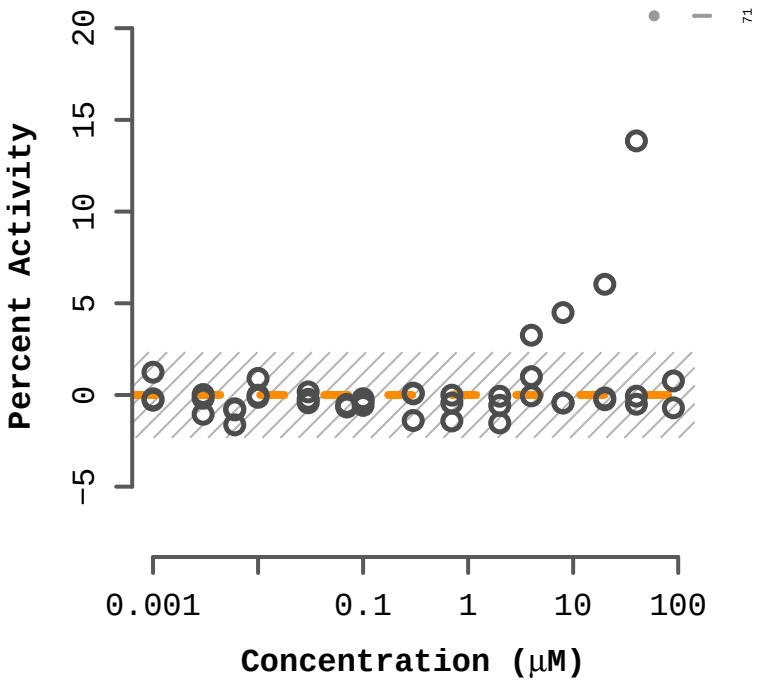
NAME: 3-(Triethoxysilyl)propionitrile
CHID: 27334 **CASRN:** 919-31-3
SPID(S): Tox21_201902
M4ID: 12480350

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.46	NA	NA
PROB:	1	NA	NA
RMSE:	2.57	NA	NA

MAX_MEAN: 0.562 **MAX_MED:** 0.658 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

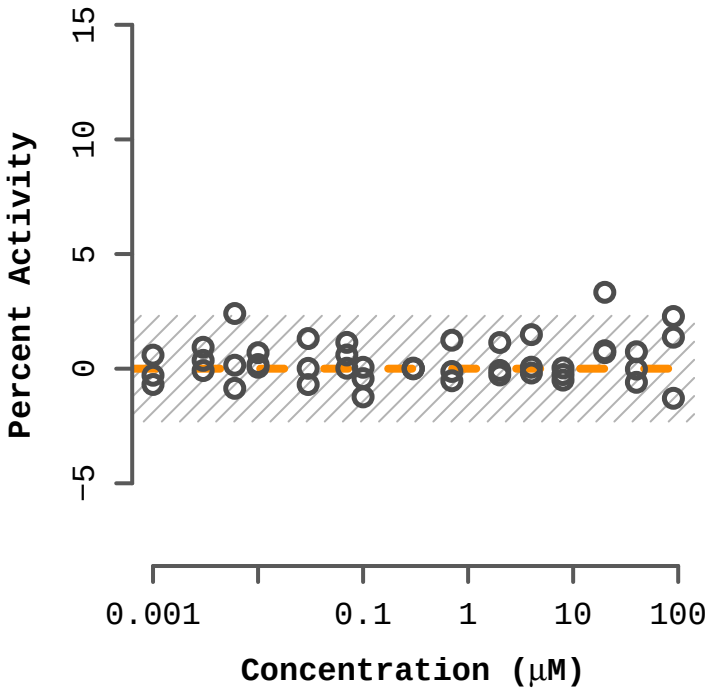
NAME: 1,3-Dichloro-2-butene
CHID: 27338 **CASRN:** 926-57-8
SPID(S): Tox21_200965
M4ID: 12481287 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.02	NA	NA
PROB:	1	NA	NA
RMSE:	10.82	NA	NA

MAX_MEAN: 23.6 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

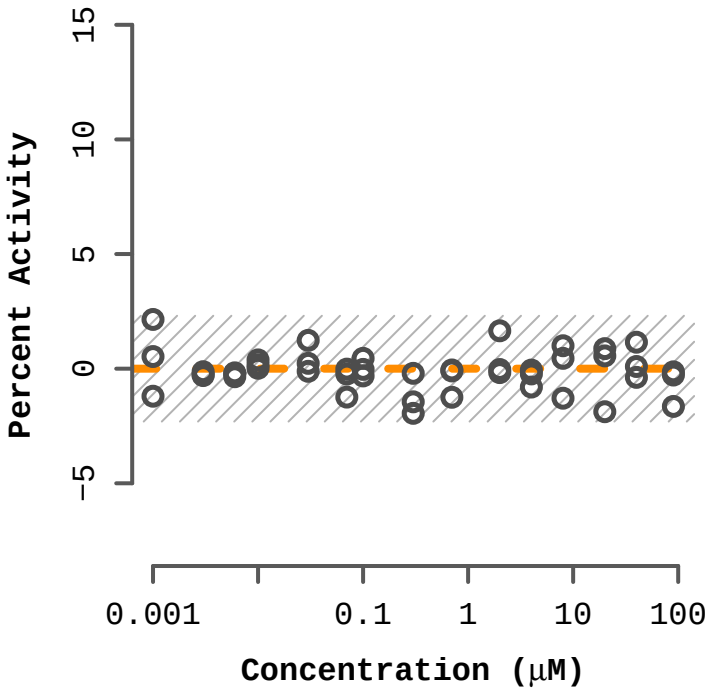
NAME: 2-(2-Aminoethoxy)ethanol
CHID: 27341 **CASRN:** 929-06-6
SPID(S): Tox21_303163
M4ID: 12475970

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

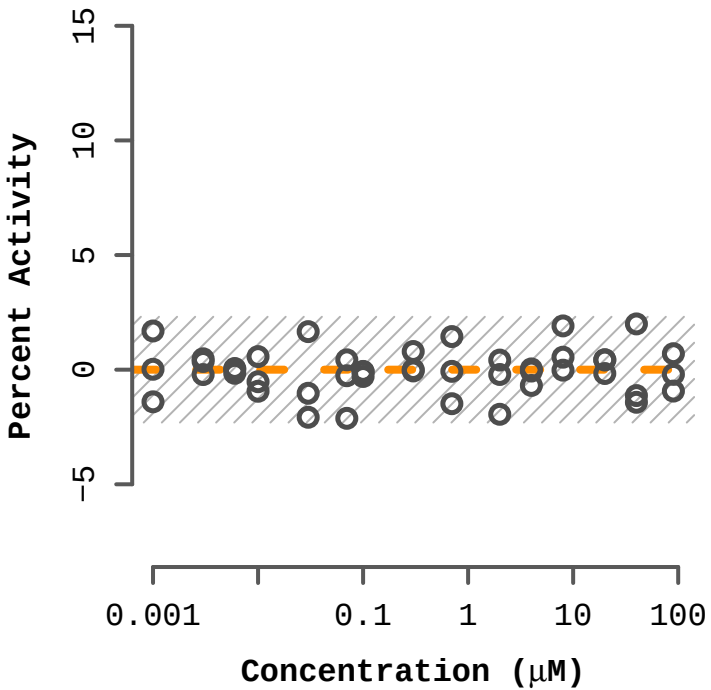
NAME: 2-(2-Aminoethoxy)ethanol
CHID: 27341 **CASRN:** 929-06-6
SPID(S): Tox21_201287
M4ID: 12480965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.493 **MAX_MED:** 0.558 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

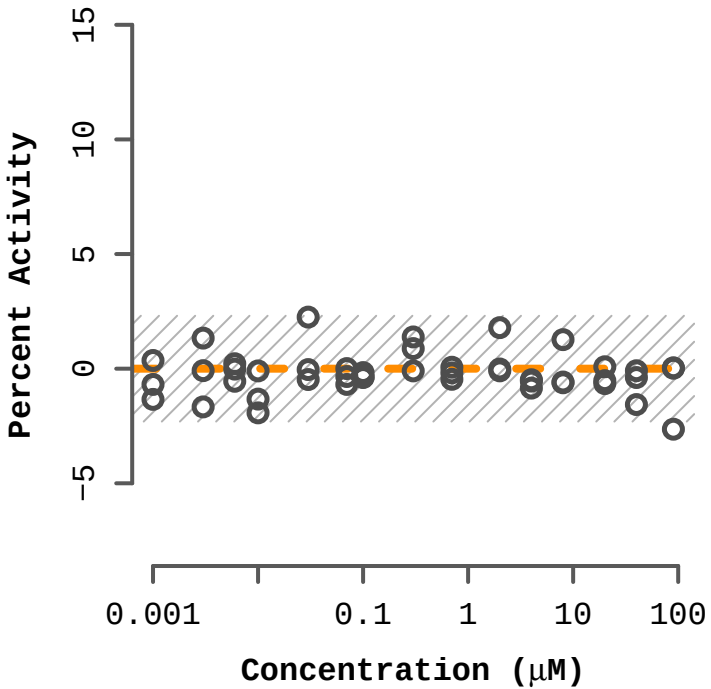
NAME: Sodium benzenethiolate
CHID: 27342 **CASRN:** 930-69-8
SPID(S): Tox21_303102
M4ID: 12476031

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.812 **MAX_MED:** 0.545 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

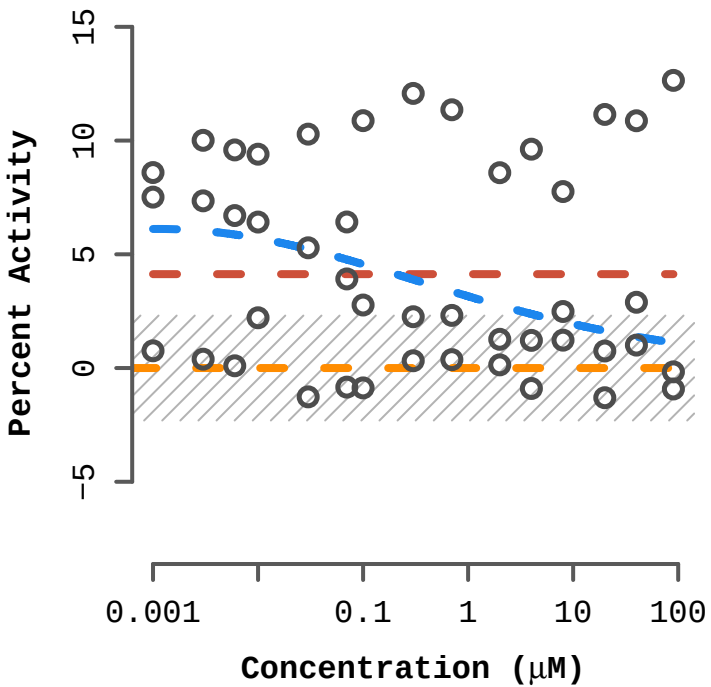
NAME: Sodium benzenethiolate
CHID: 27342 CASRN: 930-69-8
SPID(S): Tox21_201620
M4ID: 12480632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.723 MAX_MED: 0.879 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-tert-Butylbenzaldehyde
CHID: 27343 CASRN: 939-97-9
SPID(S): Tox21_200452
M4ID: 12481800

HILL MODEL (in red):

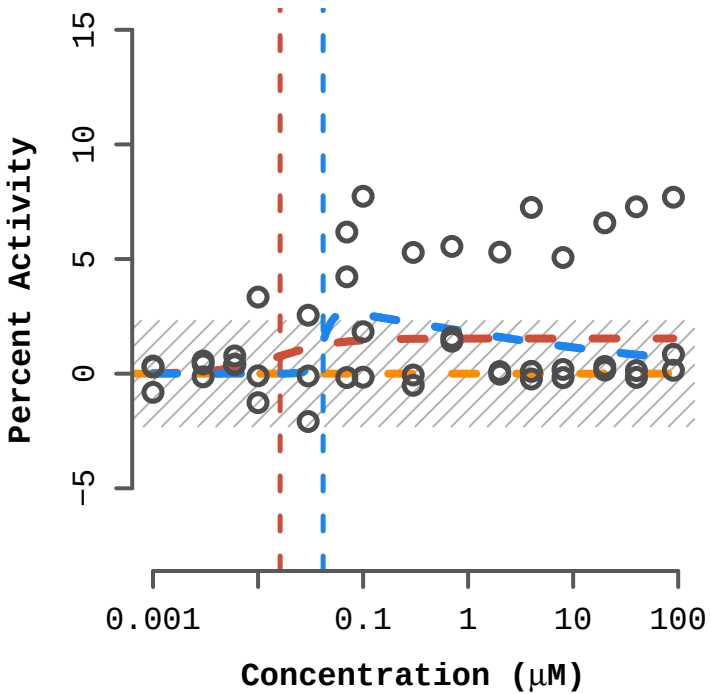
	tp	ga	gw
val:	4.13	-4.78	4.17
sd:	0.781	1550	3630

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.62	-4.93	0.3	-0.968	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	299.08	278.45	280.17
PROB:	0	0.7	0.3
RMSE:	6.35	4.49	4.63

MAX_MEAN: 6.01 MAX_MED: 7.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Azacyclotridecan-2-one
CHID: 27344 CASRN: 947-04-6
SPID(S): Tox21_303079
M4ID: 12476054

HILL MODEL (in red):

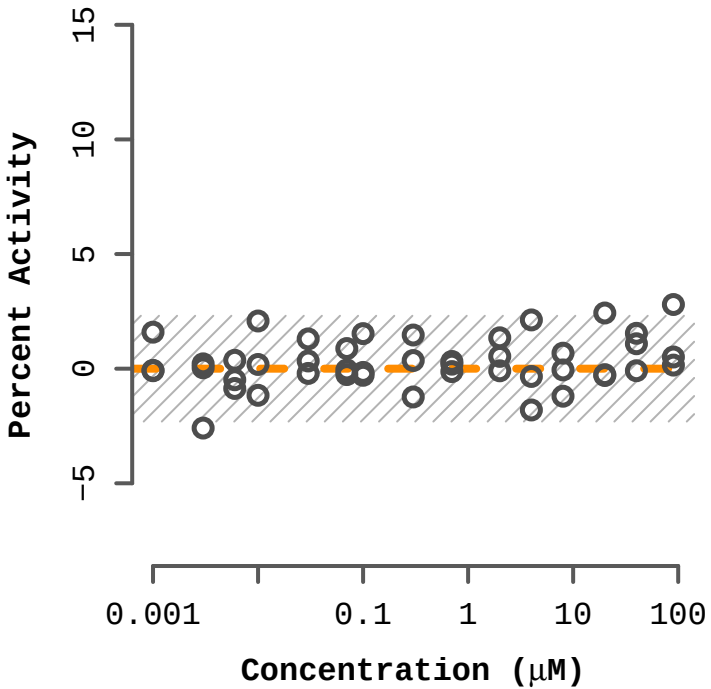
	tp	ga	gw
val:	1.53	−1.79	1.61
sd:	0.56	0.99	2.57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.43	−1.38	8	−0.526	0.3
sd:	23.6	0.249	11.2	15.5	0.939

	CNST	HILL	GNLS
AIC:	228.84	223.72	226.17
PROB:	0.06	0.73	0.21
RMSE:	3.24	2.67	2.66

MAX_MEAN: 3.41 MAX_MED: 4.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

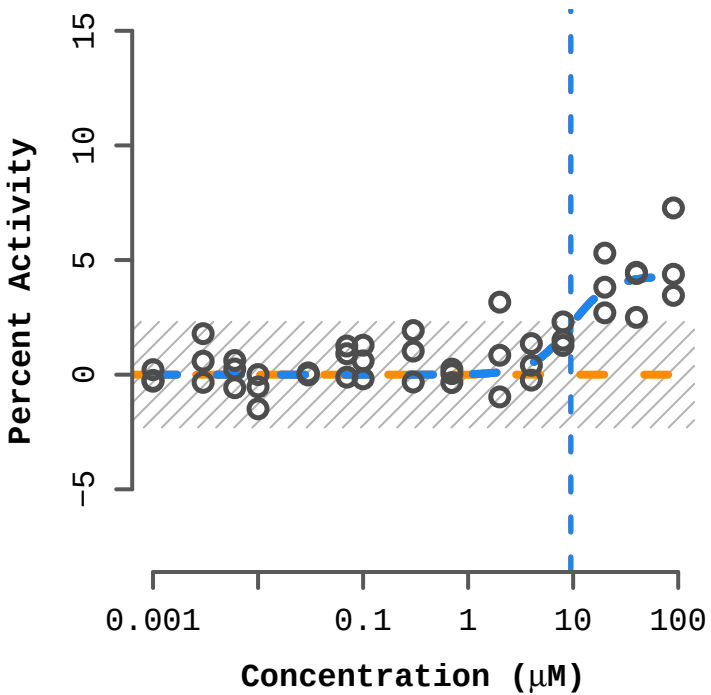
NAME: Azacyclotridecan-2-one
CHID: 27344 **CASRN:** 947-04-6
SPID(S): Tox21_202067
M4ID: 12480185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triphenylborane
CHID: 27345 **CASRN:** 960-71-4
SPID(S): Tox21_303213
M4ID: 12475920

HILL MODEL (in red):

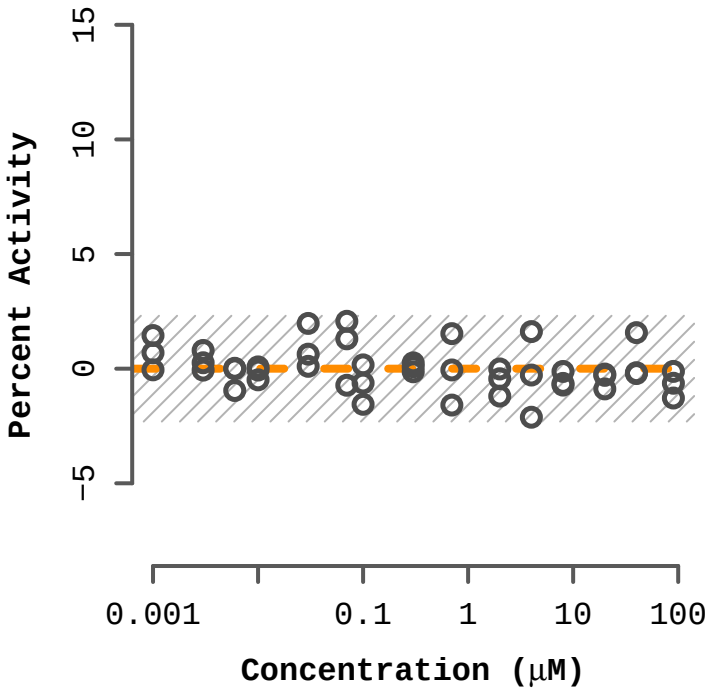
	tp	ga	gw
val:	4.3	0.978	2.36
sd:	0.474	0.0944	1.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.3	0.978	2.36	3.67	3.74
sd:	0.474	0.0944	1.23	867	1980

	CNST	HILL	GNLS
AIC:	193.71	131.5	135.5
PROB:	0	0.88	0.12
RMSE:	2.21	1.01	1.01

MAX_MEAN: 5.04 **MAX_MED:** 4.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

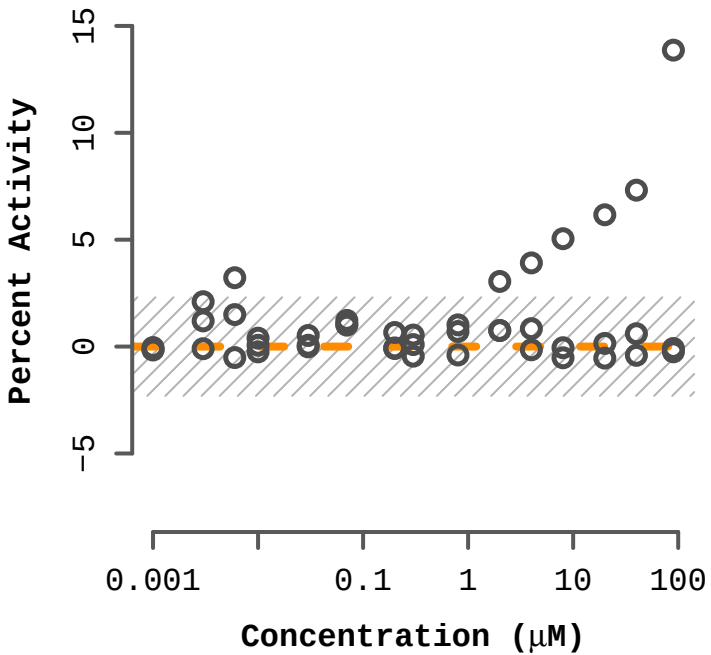
NAME: Trichloromethylstannane
CHID: 27346 **CASRN:** 993-16-8
SPID(S): Tox21_303173
M4ID: 12475960

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.905 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

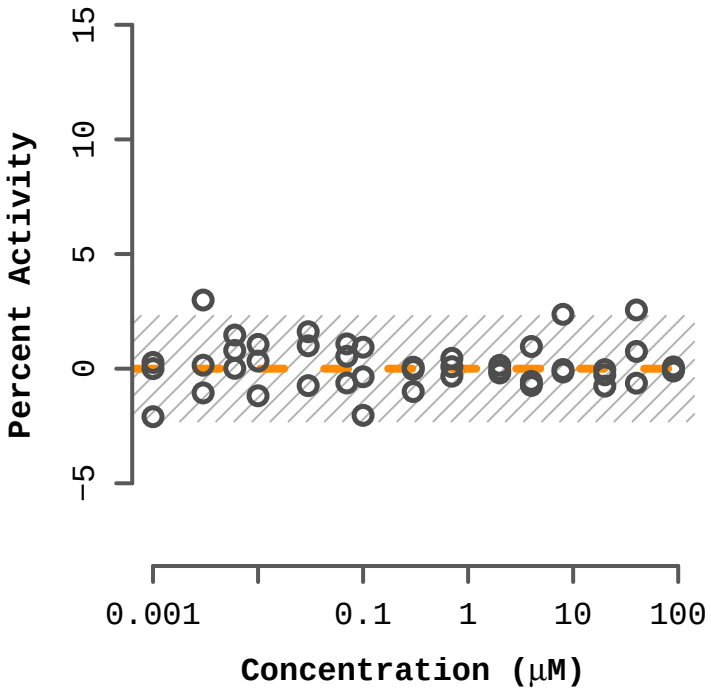
NAME: Trichloromethylstannane
CHID: 27346 **CASRN:** 993-16-8
SPID(S): Tox21_202322
M4ID: 12479930

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 4.51 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

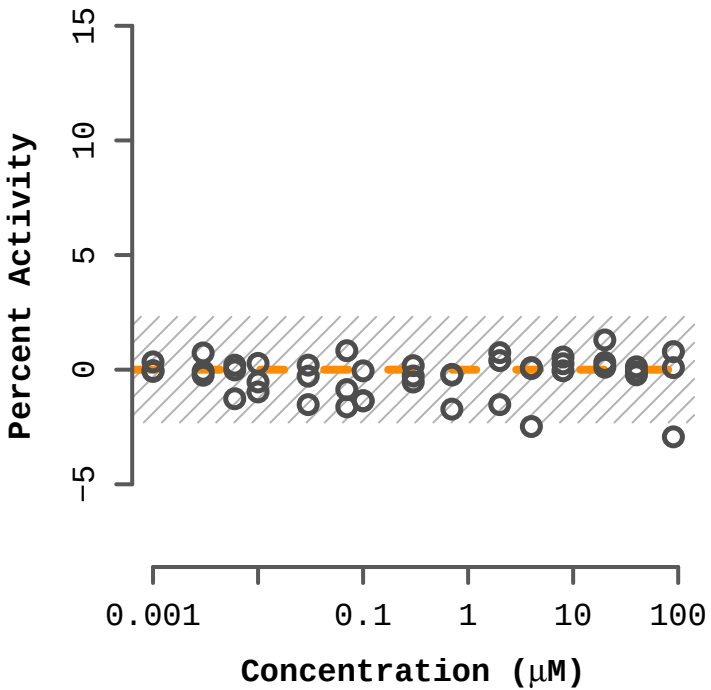
NAME: 1-Chlorodecane
CHID: 27352 **CASRN:** 1002-69-3
SPID(S): Tox21_200812
M4ID: 12481440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

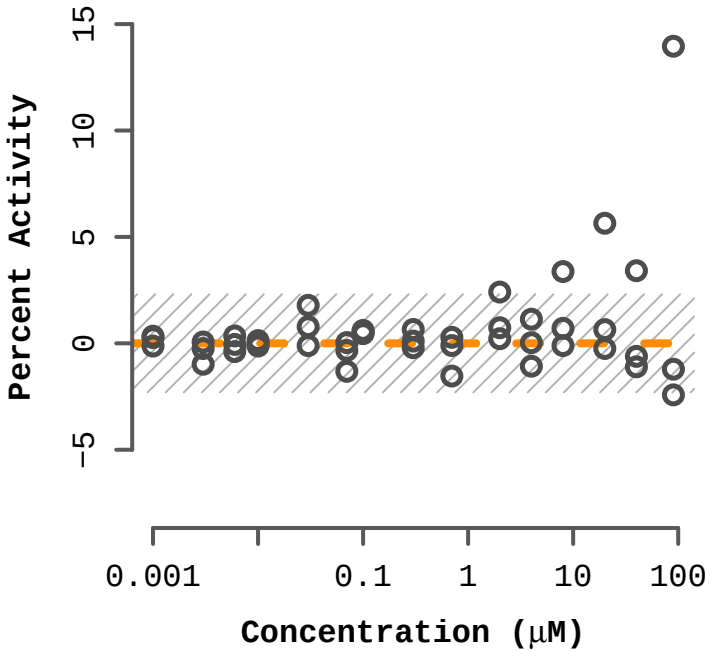
NAME: Tris(2-methoxyethoxy)vinylsilane
CHID: 27356 **CASRN:** 1067-53-4
SPID(S): Tox21_303099
M4ID: 12476034

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.573 **MAX_MED:** 0.399 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

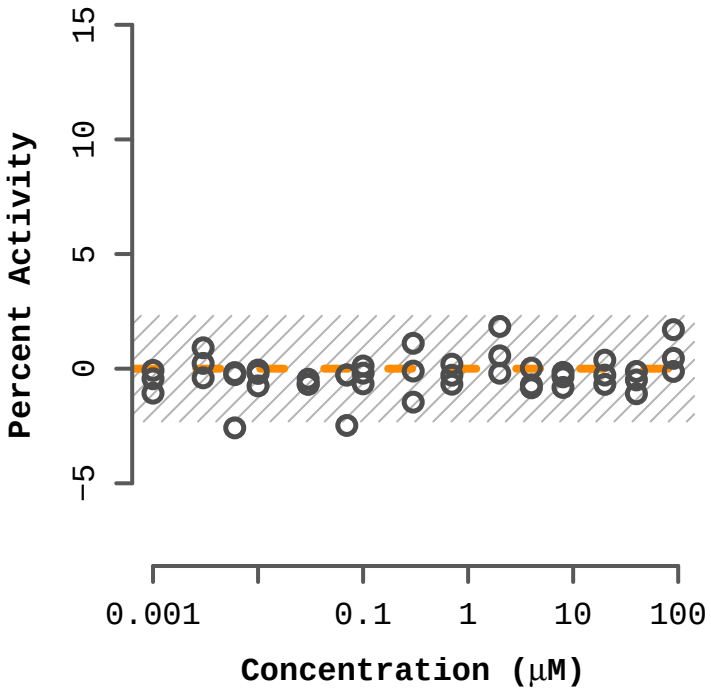
NAME: Tris(2-methoxyethoxy)vinylsilane
CHID: 27356 **CASRN:** 1067-53-4
SPID(S): Tox21_202344
M4ID: 12479908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 3.44 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

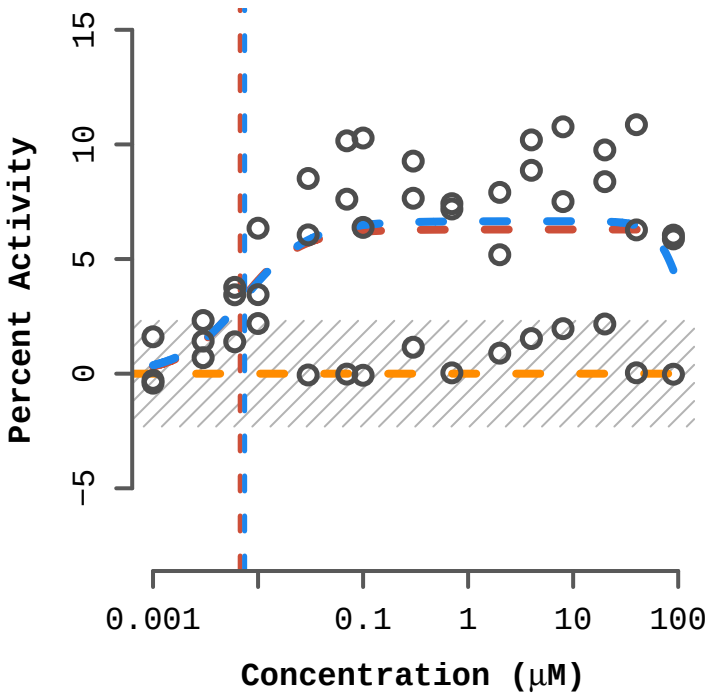
NAME: Potassium 1,3-dioxo-1,3-dihydroisoindol-2-ide
CHID: 27358 **CASRN:** 1074-82-4
SPID(S): Tox21_201007
M4ID: 12481245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.736 **MAX_MED:** 0.561 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ammonium carbamate
CHID: 27360 CASRN: 1111-78-0
SPID(S): Tox21_302509
M4ID: 12476624

HILL MODEL (in red):

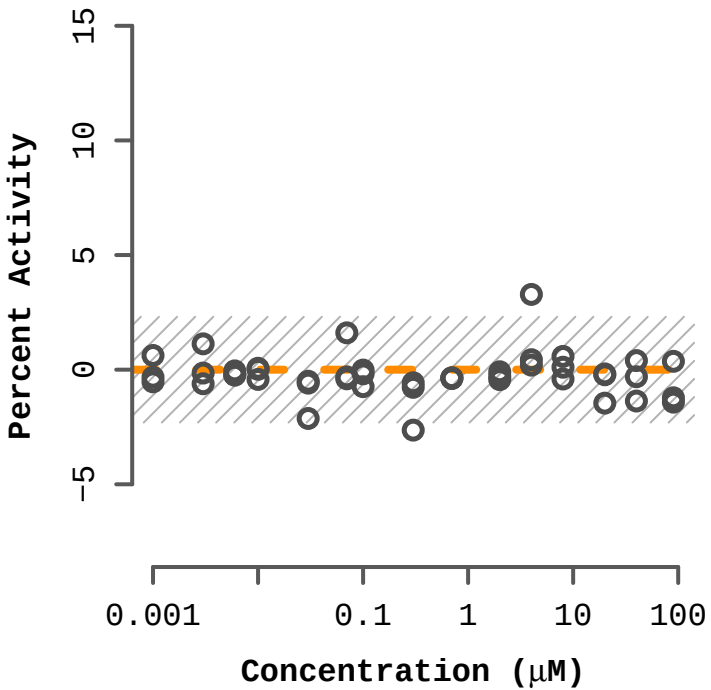
	tp	ga	gw
val:	6.29	−2.17	1.54
sd:	0.713	0.199	1.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.65	−2.13	1.41	2.05	3.49
sd:	0.808	0.21	0.952	0.351	11.6

	CNST	HILL	GNLS
AIC:	295.88	247.48	250.32
PROB:	0	0.8	0.2
RMSE:	5.99	3.33	3.31

MAX_MEAN: 6.87 **MAX_MED:** 8.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

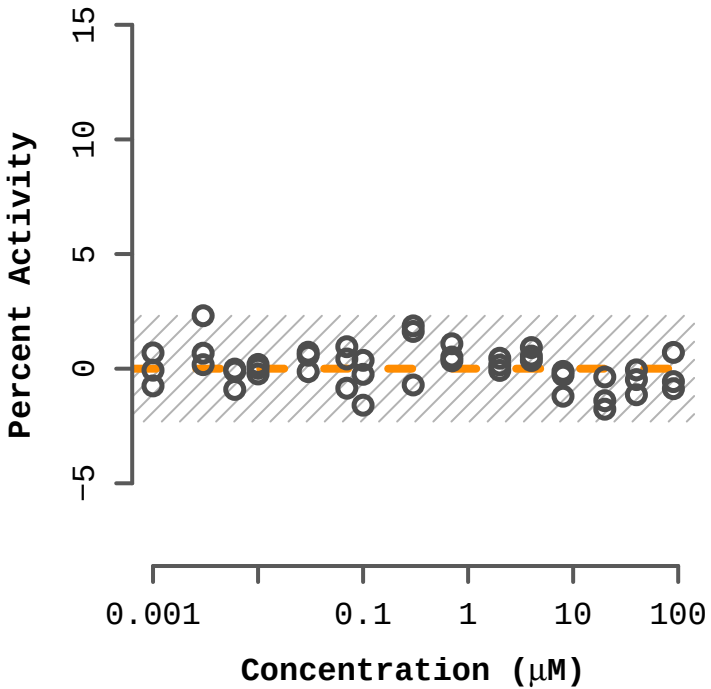
NAME: 3-Hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dim
CHID: 27361 **CASRN:** 1115-20-4
SPID(S): Tox21_303300
M4ID: 12475833

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.436 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

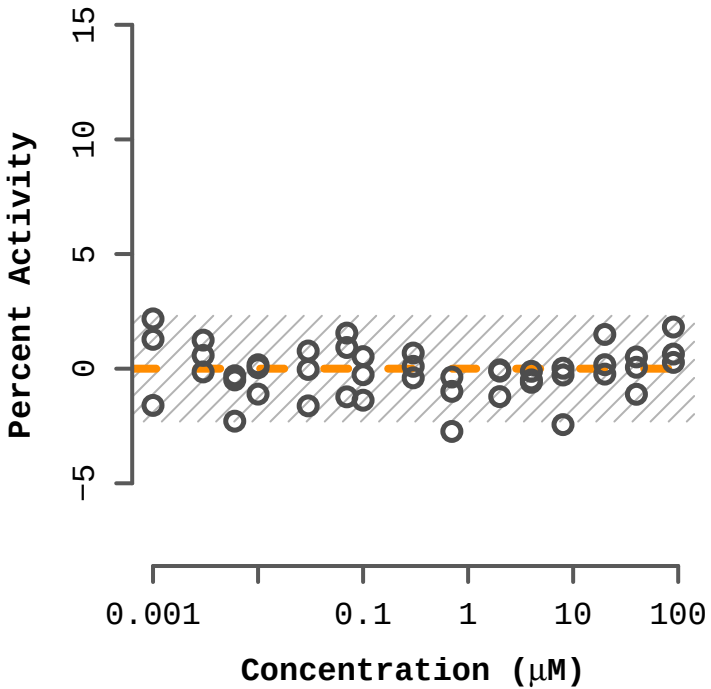
NAME: 3-Hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dim
CHID: 27361 **CASRN:** 1115-20-4
SPID(S): Tox21_201302
M4ID: 12480950

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

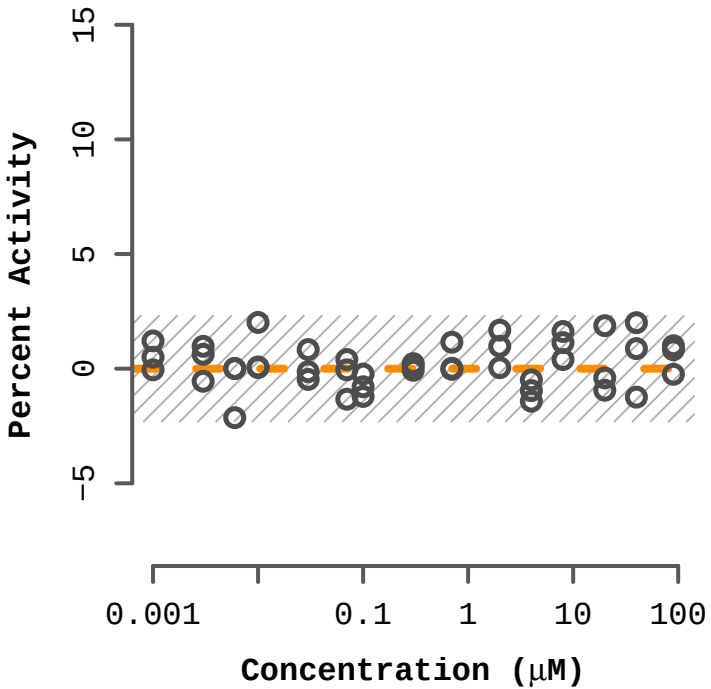
NAME: N,N−Dimethyloctanamide
CHID: 27364 **CASRN:** 1118−92−9
SPID(S): Tox21_301930
M4ID: 12477203

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

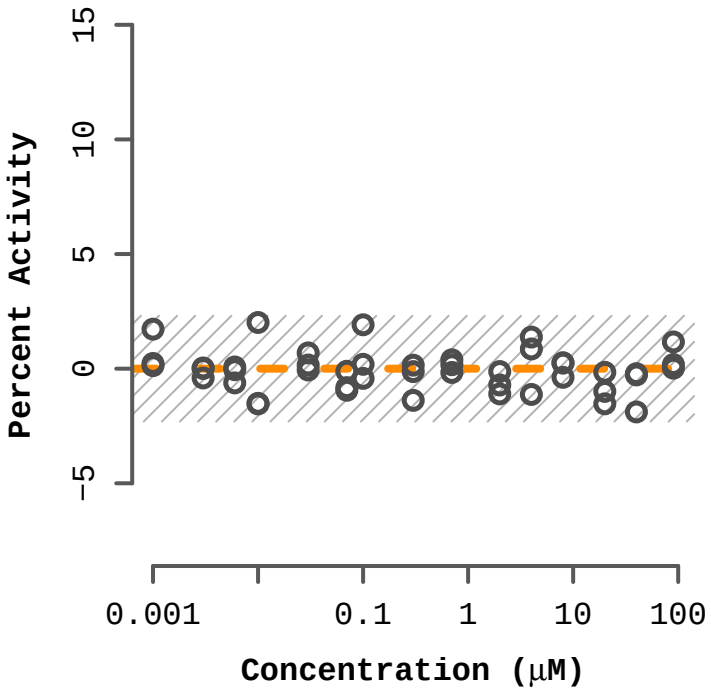
NAME: 1-Tetradecene
CHID: 27367 **CASRN:** 1120-36-1
SPID(S): Tox21_303051
M4ID: 12476082

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

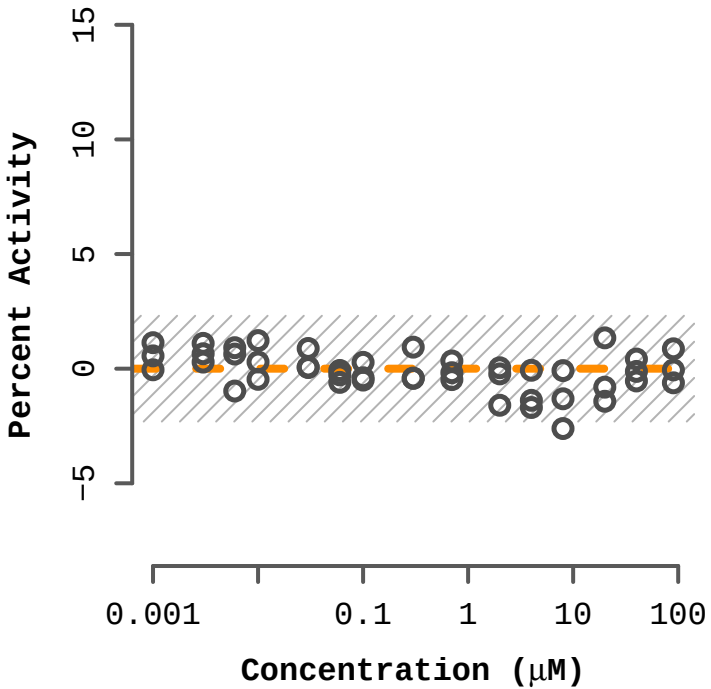
NAME: N−[(Benzyloxy)carbonyl]−L−aspartic acid
CHID: 27368 **CASRN:** 1152−61−0
SPID(S): Tox21_200211
M4ID: 12482041

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.696 **MAX_MED:** 0.863 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

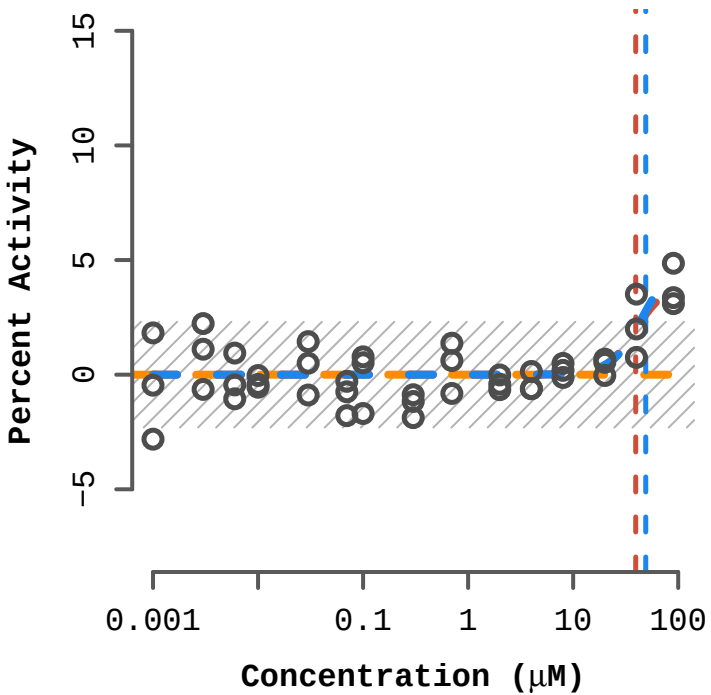
NAME: Trimethoxymethylsilane
CHID: 27370 **CASRN:** 1185-55-3
SPID(S): Tox21_200453
M4ID: 12481799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.682 **MAX_MED:** 0.652 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethylaniline
CHID: 27377 CASRN: 1300-73-8
SPID(S): Tox21_301836
M4ID: 12477297

HILL MODEL (in red):

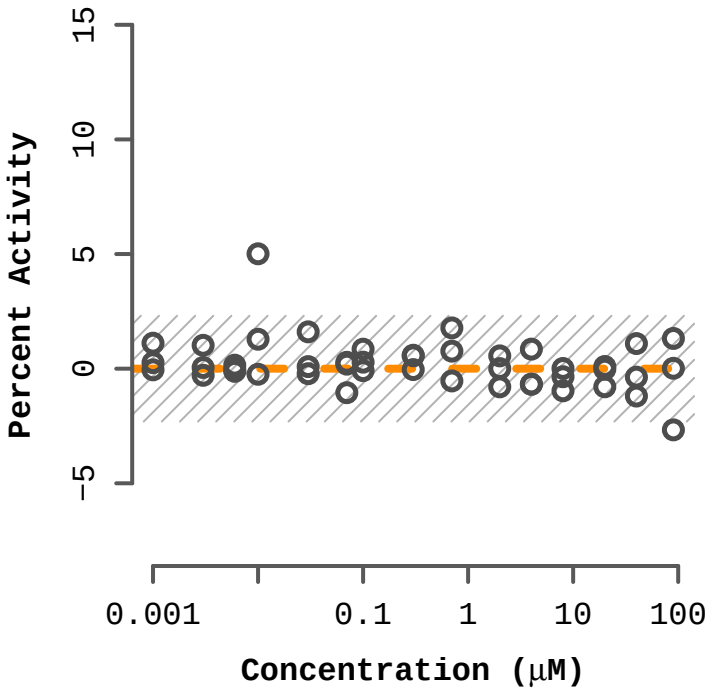
	tp	ga	gw
val:	3.94	1.6	3.14
sd:	1.05	0.144	2.29

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.66	1.69	2.82	2.07	4.57
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.32	140.05	144.05
PROB:	0	0.88	0.12
RMSE:	1.52	1.03	1.03

MAX_MEAN: 3.77 MAX_MED: 3.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

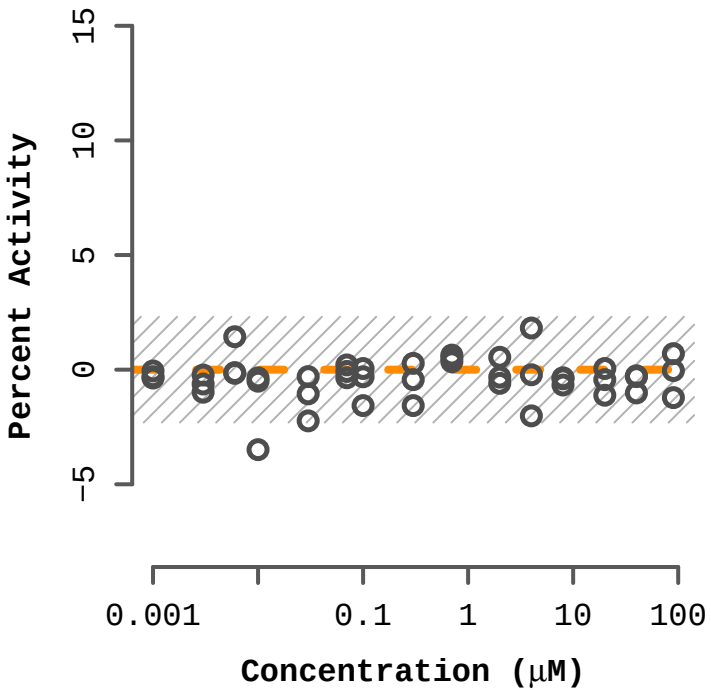
NAME: Isodecyl acrylate
CHID: 27386 **CASRN:** 1330-61-6
SPID(S): Tox21_303085
M4ID: 12476048

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

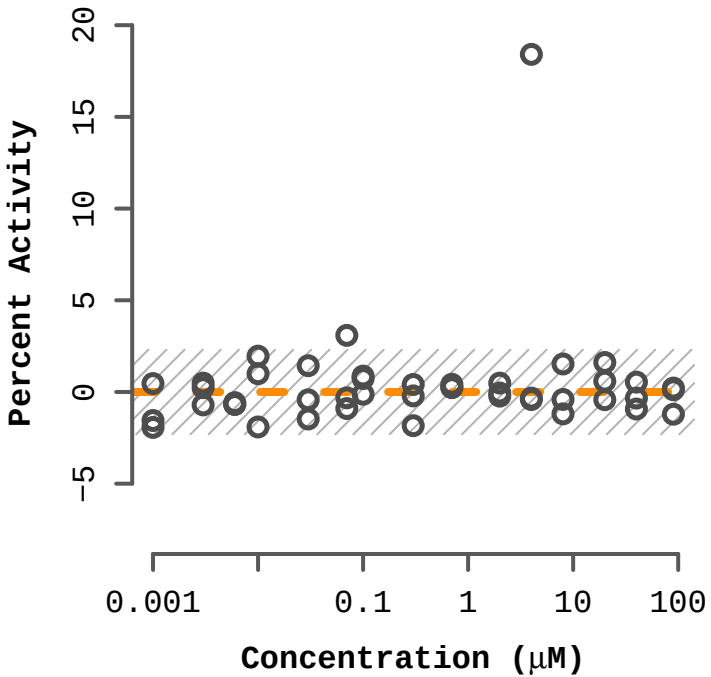
NAME: Isodecyl acrylate
CHID: 27386 **CASRN:** 1330-61-6
SPID(S): Tox21_201861
M4ID: 12480391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.503 **MAX_MED:** 0.526 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

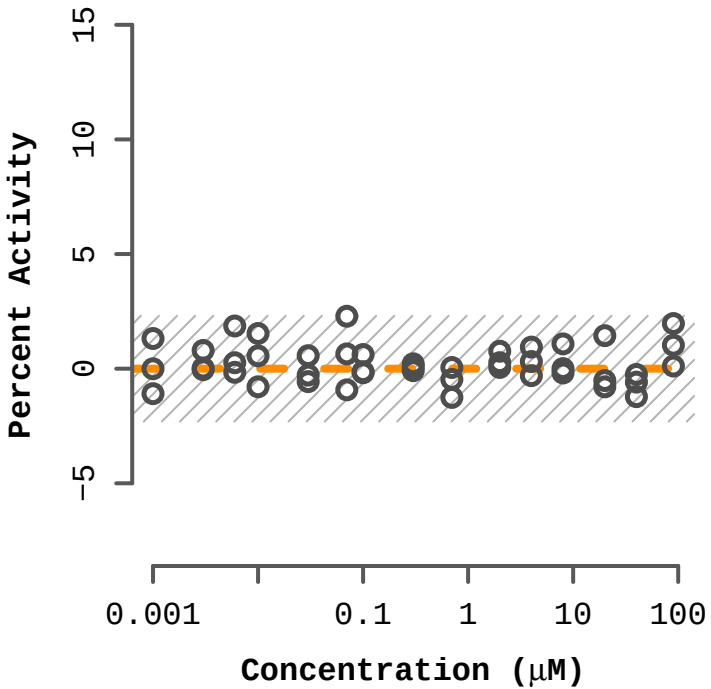
NAME: Diisooctyl adipate
CHID: 27388 CASRN: 1330-86-5
SPID(S): Tox21_302422
M4ID: 12476711

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.66	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 5.89 MAX_MED: 0.996 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

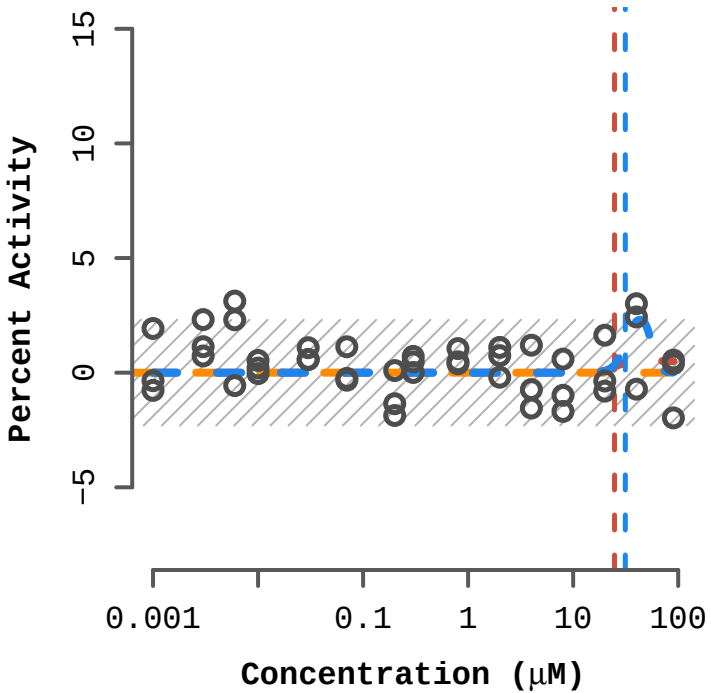
NAME: Phenolsulfonic acid
CHID: 27390 **CASRN:** 1333-39-7
SPID(S): Tox21_303096
M4ID: 12476037

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Naphthenic acids
CHID: 27394 **CASRN:** 1338-24-5
SPID(S): Tox21_200828
M4ID: 12481424

HILL MODEL (in red):

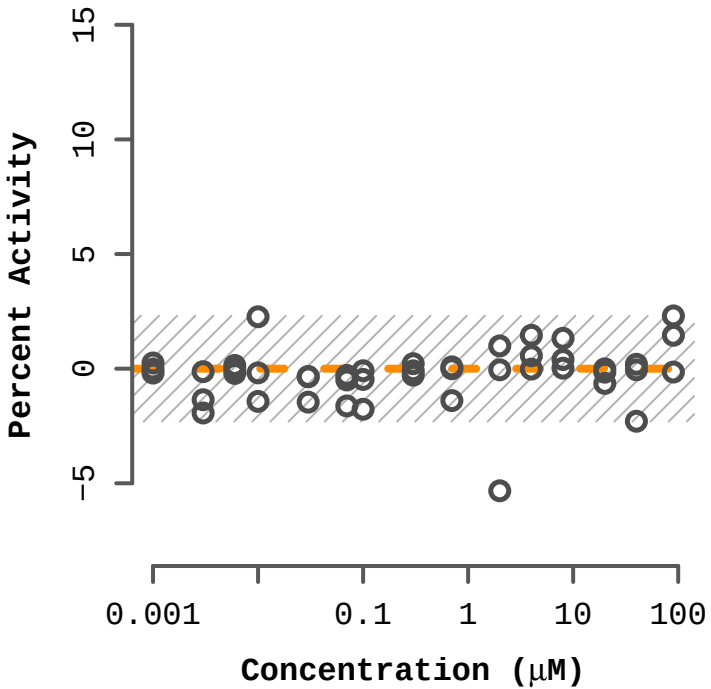
	tp	ga	gw
val:	0.506	1.39	8
sd:	0.633	0.318	16.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.6	1.5	8	1.75	12.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	152.32	157.62	157.83
PROB:	0.88	0.06	0.06
RMSE:	1.26	1.24	1.21

MAX_MEAN: 1.62 **MAX_MED:** 2.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

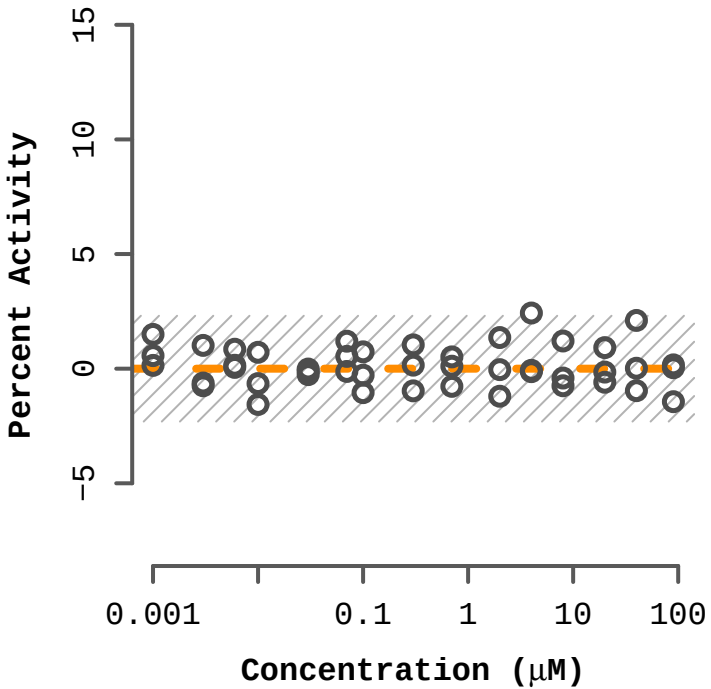
NAME: Sorbitan, mono-(9Z)-9-octadecenoate
CHID: 27397 CASRN: 1338-43-8
SPID(S): Tox21_300389
M4ID: 12478743

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.2 MAX_MED: 1.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

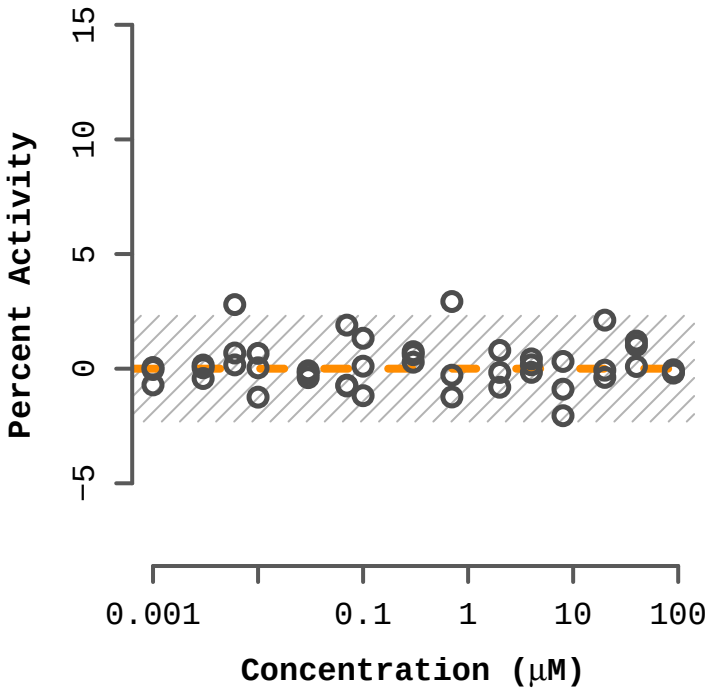
NAME: 1,1,1−Trimethoxyethane
CHID: 27400 **CASRN:** 1445−45−0
SPID(S): Tox21_200955
M4ID: 12481297

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.743 **MAX_MED:** 0.571 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

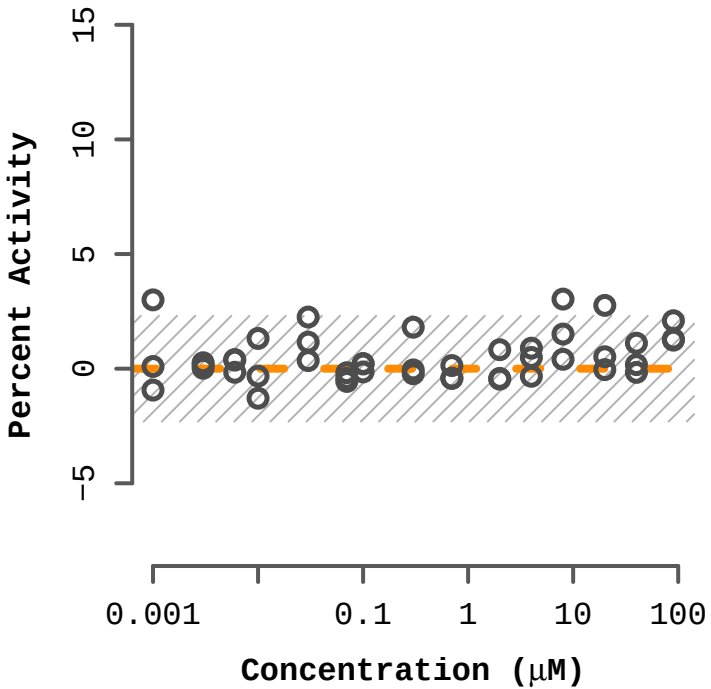
NAME: 4-Thiazolecarbonitrile
CHID: 27401 CASRN: 1452-15-9
SPID(S): Tox21_301240
M4ID: 12477893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

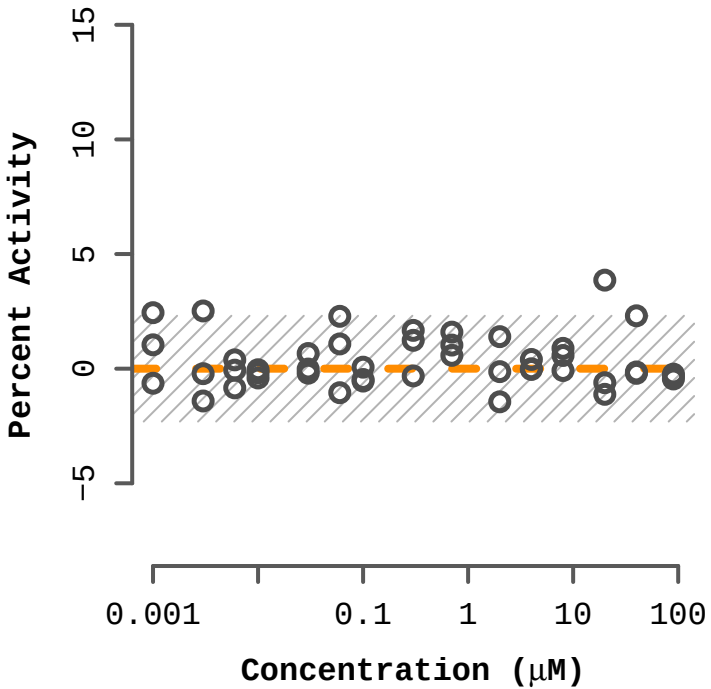
NAME: Dimethyl isophthalate
CHID: 27402 **CASRN:** 1459-93-4
SPID(S): Tox21_303209
M4ID: 12475924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

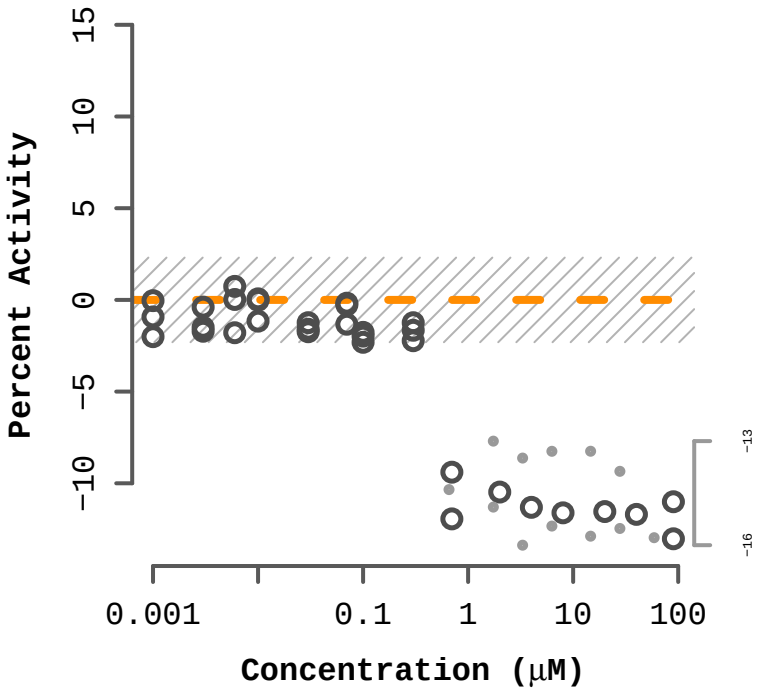
NAME: Dimethyl isophthalate
CHID: 27402 **CASRN:** 1459-93-4
SPID(S): Tox21_201345
M4ID: 12480907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

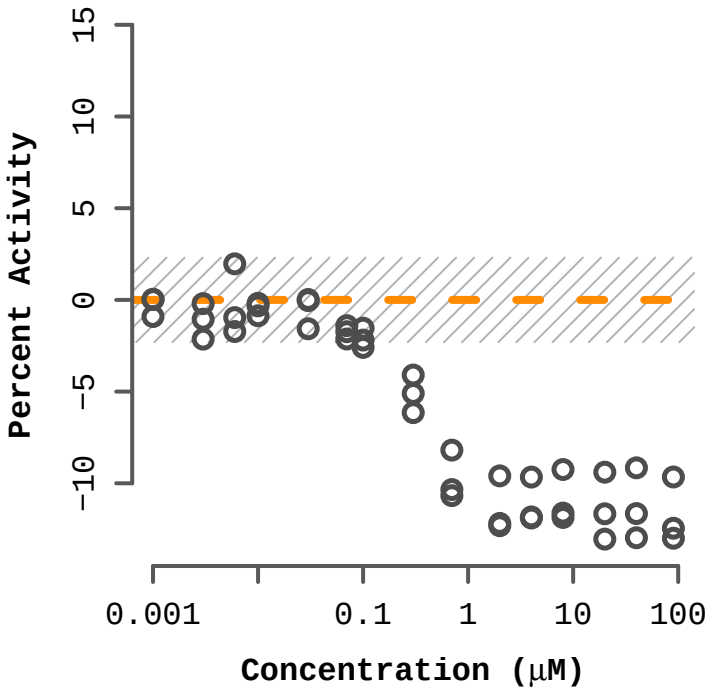
NAME: Tributyltin chloride
CHID: 27403 **CASRN:** 1461-22-9
SPID(S): Tox21_300543
M4ID: 12478589 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	332.76	NA	NA
PROB:	1	NA	NA
RMSE:	9.14	NA	NA

MAX_MEAN: −0.341 **MAX_MED:** 0.0257 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

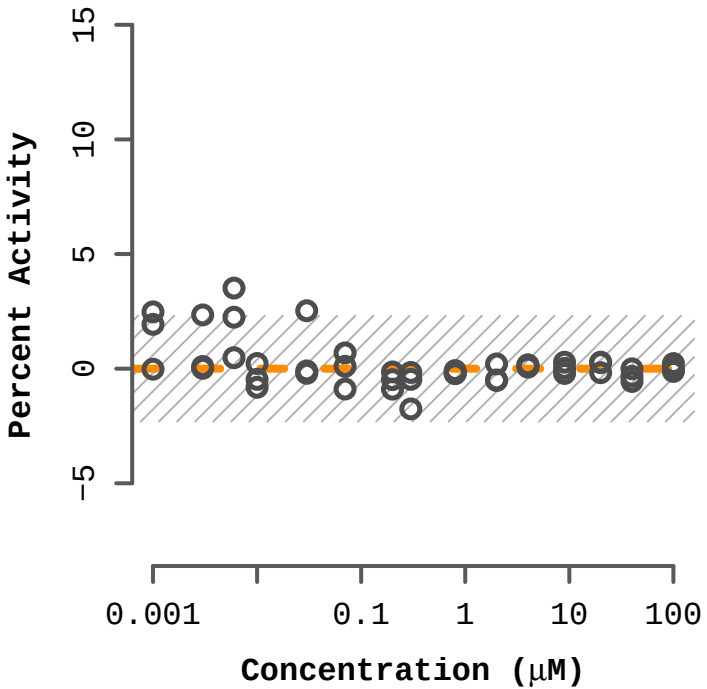
NAME: Tributyltin chloride
CHID: 27403 **CASRN:** 1461-22-9
SPID(S): Tox21_201626
M4ID: 12480626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	319.41	NA	NA
PROB:	1	NA	NA
RMSE:	7.8	NA	NA

MAX_MEAN: −0.24 **MAX_MED:** 0.0208 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

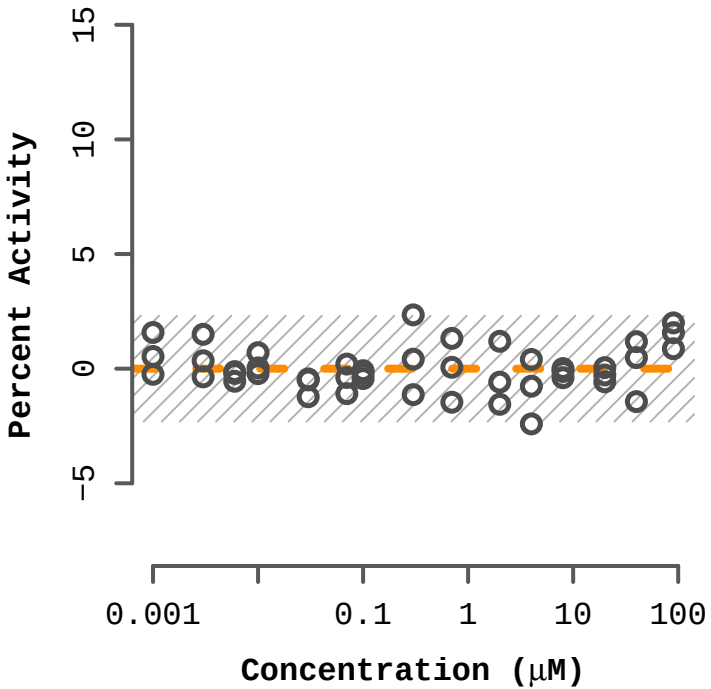
NAME: (2Z)-1,4-Dichlorobut-2-ene
CHID: 27405 **CASRN:** 1476-11-5
SPID(S): Tox21_200796
M4ID: 12481456

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

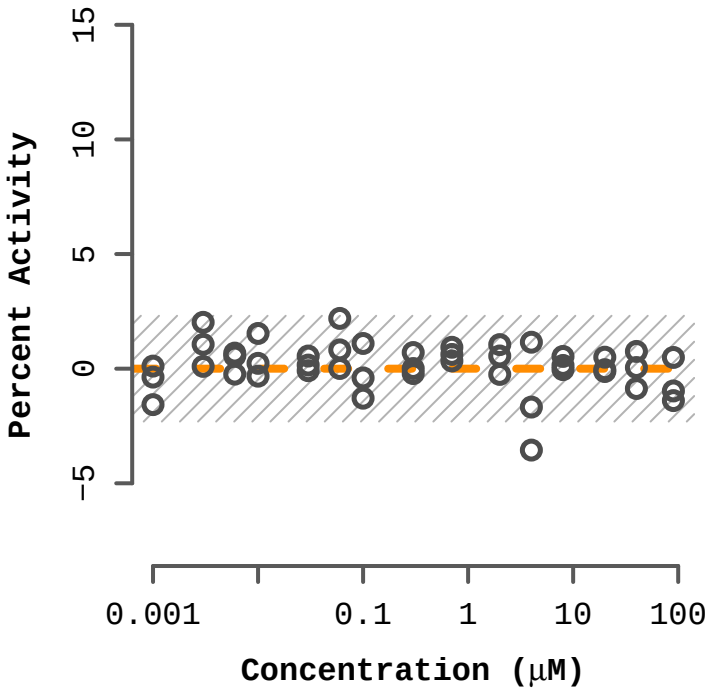
NAME: Ethyl dichlorophosphate
CHID: 27407 CASRN: 1498-51-7
SPID(S): Tox21_303159
M4ID: 12475974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

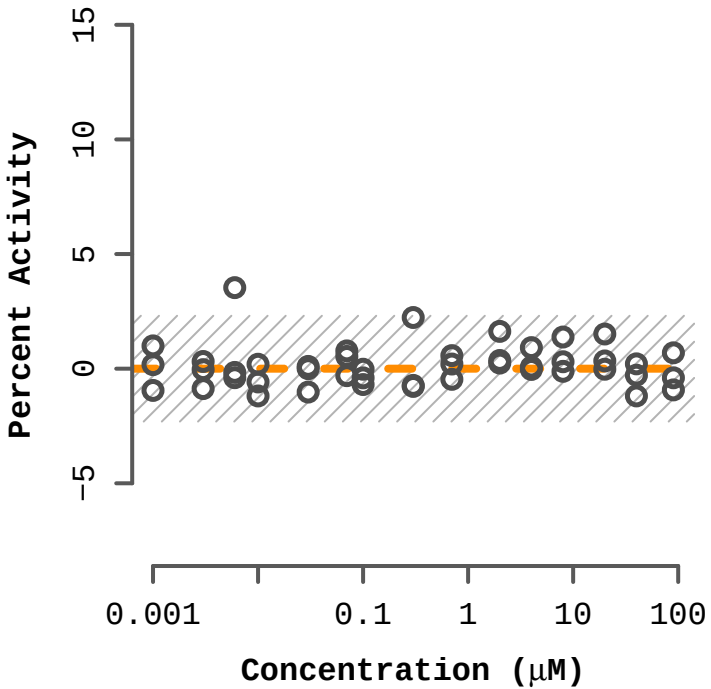
NAME: Ethyl dichlorophosphate
CHID: 27407 **CASRN:** 1498-51-7
SPID(S): Tox21_201328
M4ID: 12480924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.76	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

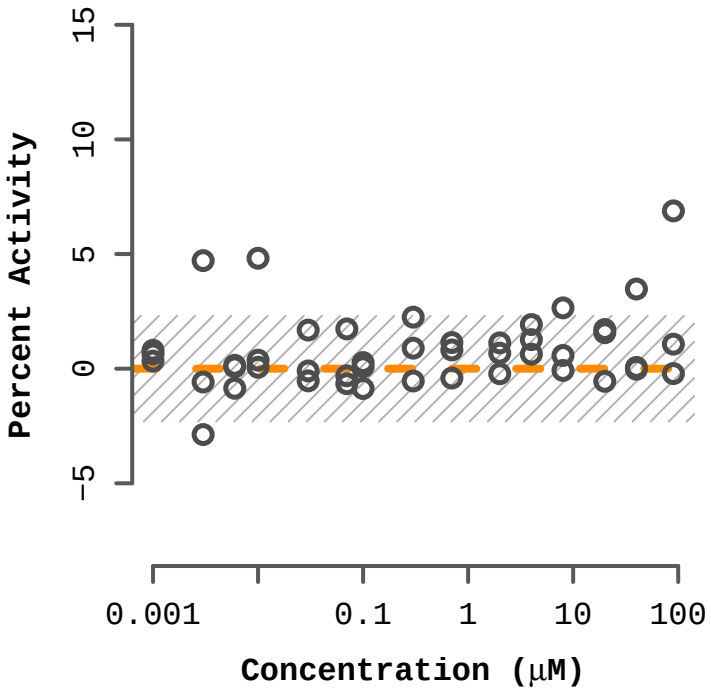
NAME: 3,6,9,12-Tetraoxahexadecan-1-ol
CHID: 27412 **CASRN:** 1559-34-8
SPID(S): Tox21_301342
M4ID: 12477791

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.995 **MAX_MED:** 0.536 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

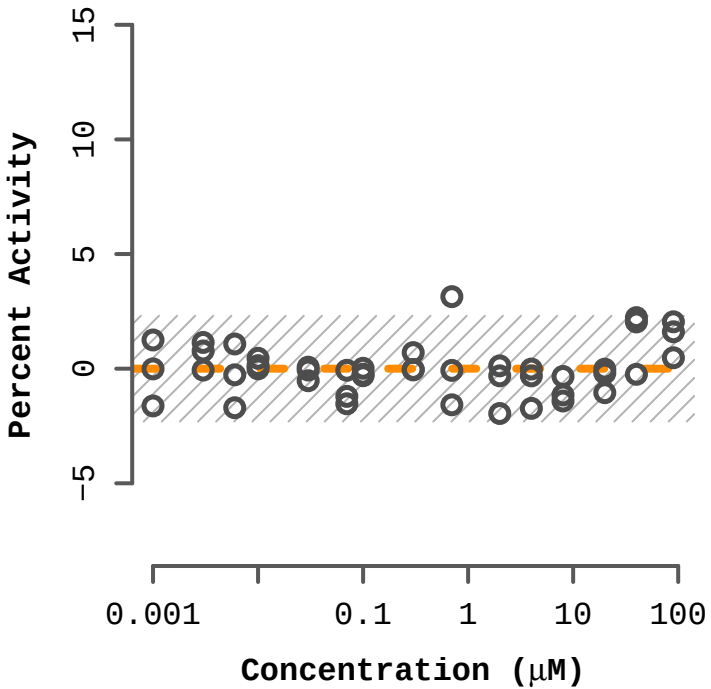
NAME: Sodium 2-hydroxyethanesulfonate
CHID: 27413 **CASRN:** 1562-00-1
SPID(S): Tox21_200227
M4ID: 12482025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 2.58 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

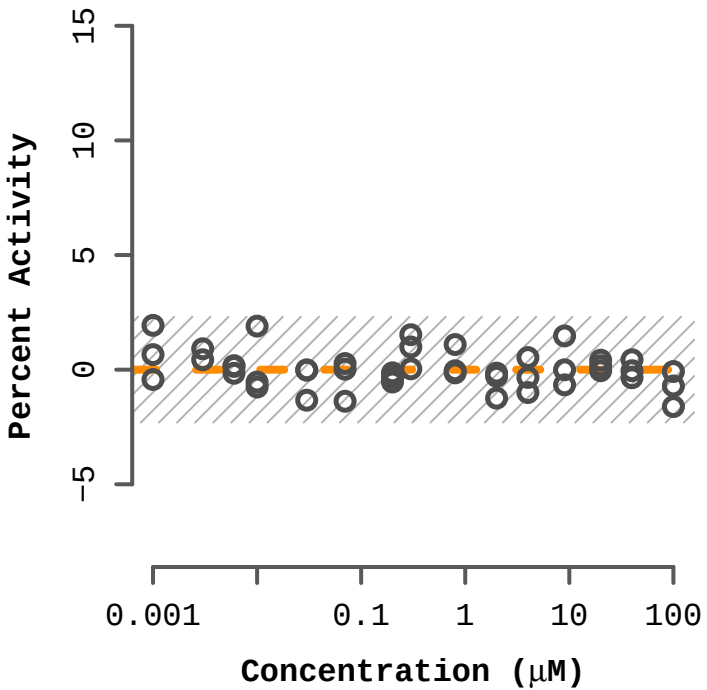
NAME: 2,3-Dihydro-2,2-dimethyl-7-benzofuranol
CHID: 27414 **CASRN:** 1563-38-8
SPID(S): Tox21_303234
M4ID: 12475899

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

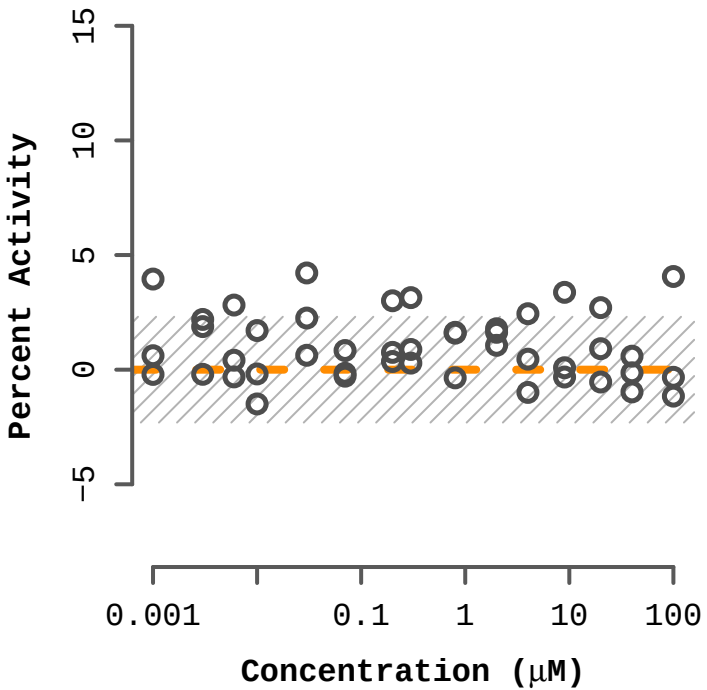
NAME: 2,3-Dihydro-2,2-dimethyl-7-benzofuranol
CHID: 27414 **CASRN:** 1563-38-8
SPID(S): Tox21_201958
M4ID: 12480294

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 0.991 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

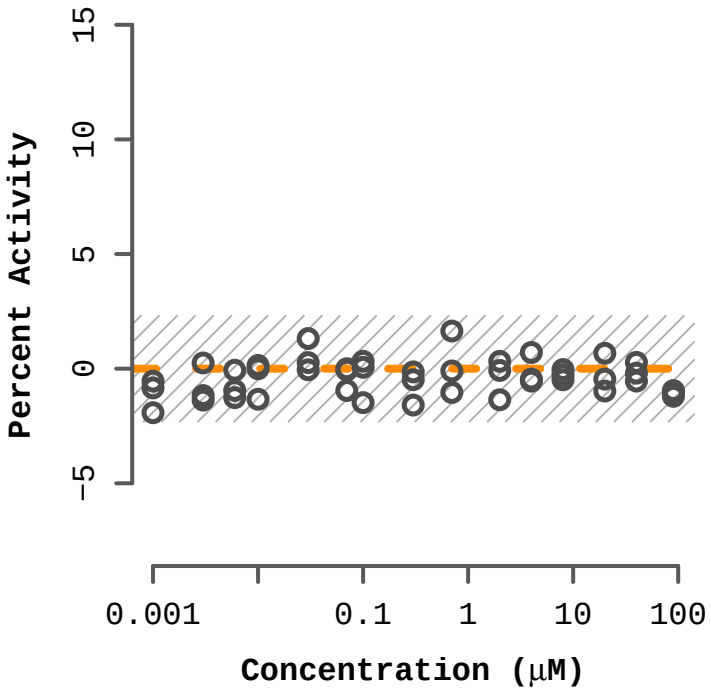
NAME: Cyclohexanethiol
CHID: 27416 **CASRN:** 1569-69-3
SPID(S): Tox21_200454
M4ID: 12481798

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 2.37 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

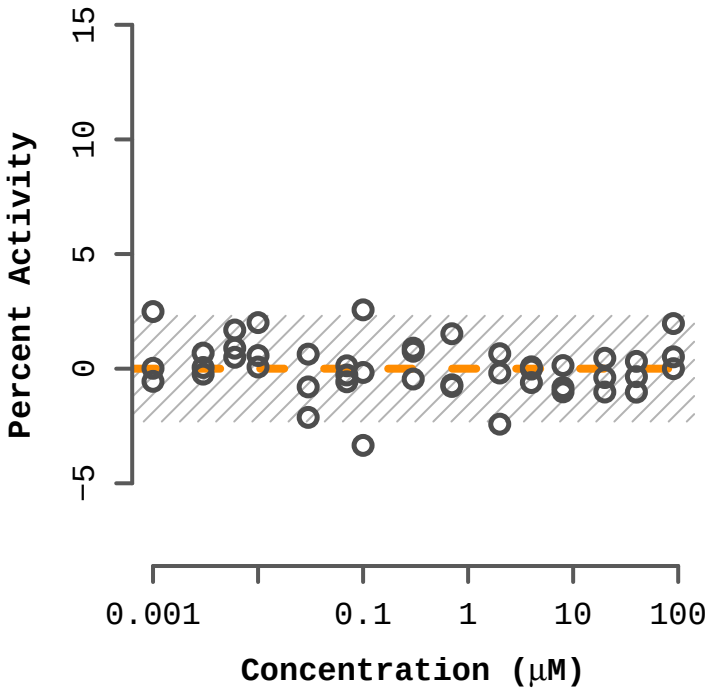
NAME: 2-Methylenepentanedinitrile
CHID: 27418 **CASRN:** 1572-52-7
SPID(S): Tox21_200844
M4ID: 12481408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.512 **MAX_MED:** 0.265 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

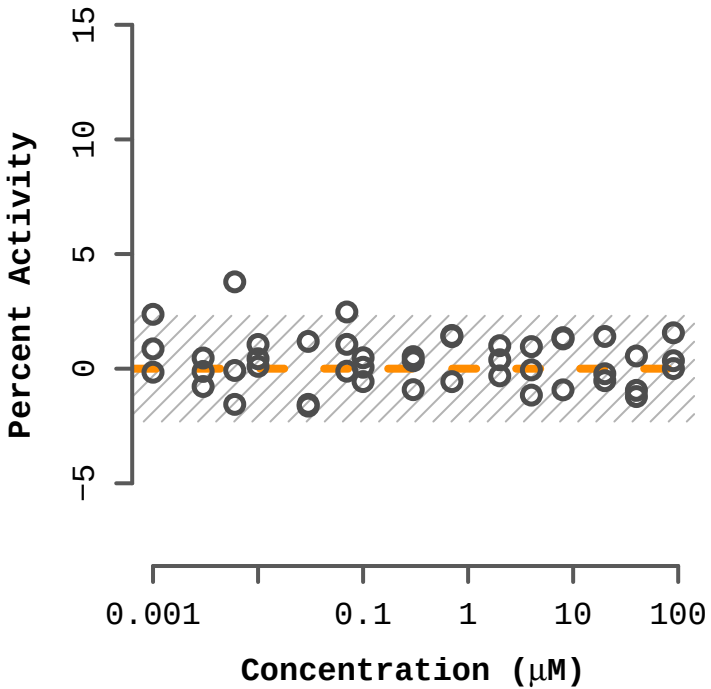
NAME: 1,4−Benzenedicarboxylic acid, monomethyl ester
CHID: 27425 **CASRN:** 1679−64−7
SPID(S): Tox21_200990
M4ID: 12481262

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.895 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

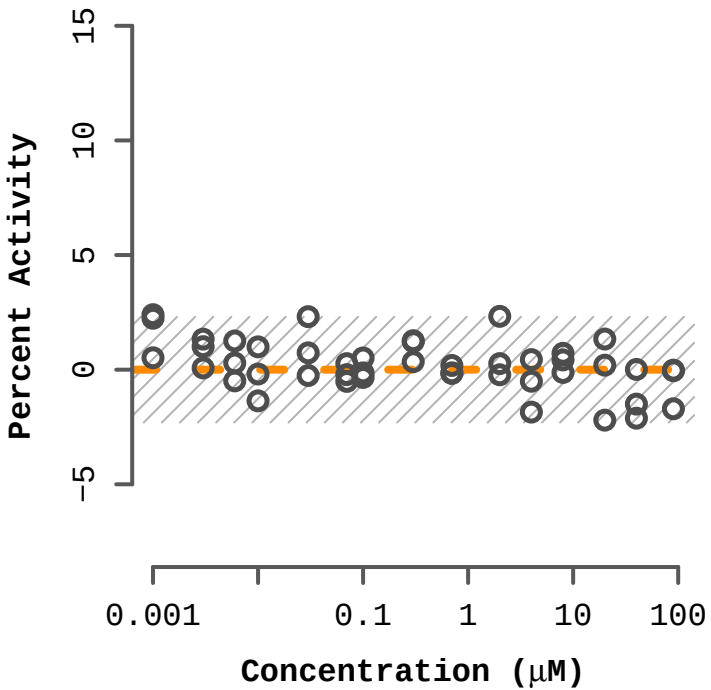
NAME: 2-[2-(Dimethylamino)ethoxy]ethanol
CHID: 27427 **CASRN:** 1704-62-7
SPID(S): Tox21_200243
M4ID: 12482009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

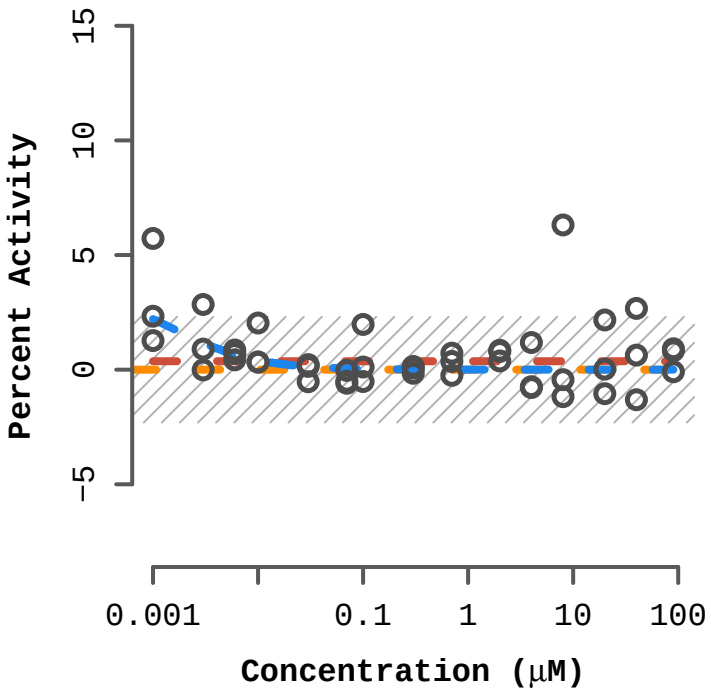
NAME: Cyclododecanol
CHID: 27429 **CASRN:** 1724-39-6
SPID(S): Tox21_303196
M4ID: 12475937

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclododecanol
CHID: 27429 **CASRN:** 1724-39-6
SPID(S): Tox21_201801
M4ID: 12480451

HILL MODEL (in red):

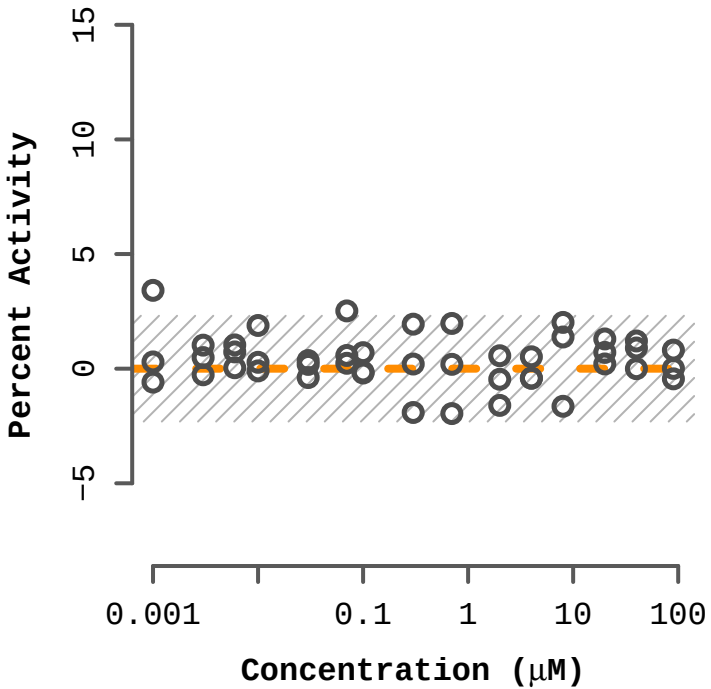
	tp	ga	gw
val:	0.368	−5	3.51
sd:	0.16	1030	1810

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.54	−4.65	3.95	−2.8	1.1
sd:	6.33	1380	3330	1.54	1.16

	CNST	HILL	GNLS
AIC:	157.51	158.18	151.82
PROB:	0.05	0.04	0.91
RMSE:	1.65	1.54	1.4

MAX_MEAN: 3.11 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

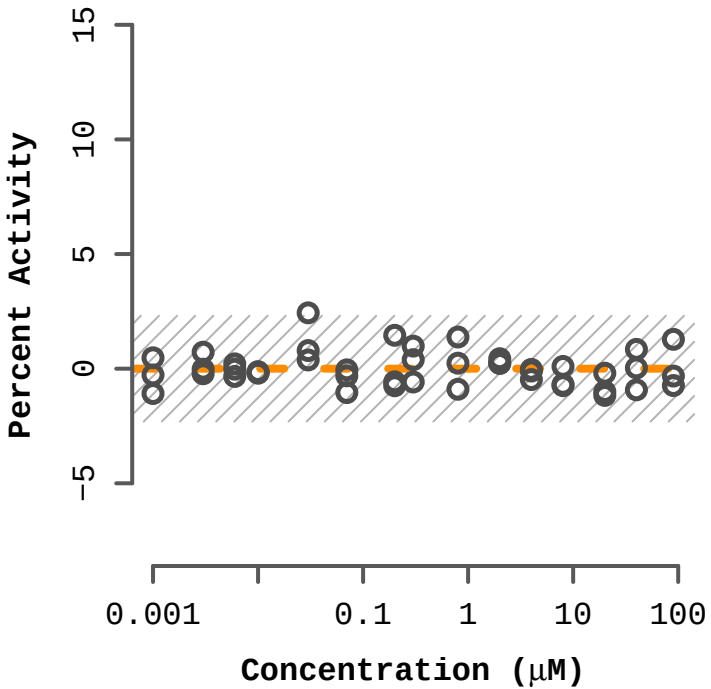
NAME: 3-Dimethylaminopropionitrile
CHID: 27432 **CASRN:** 1738-25-6
SPID(S): Tox21_303032
M4ID: 12476101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

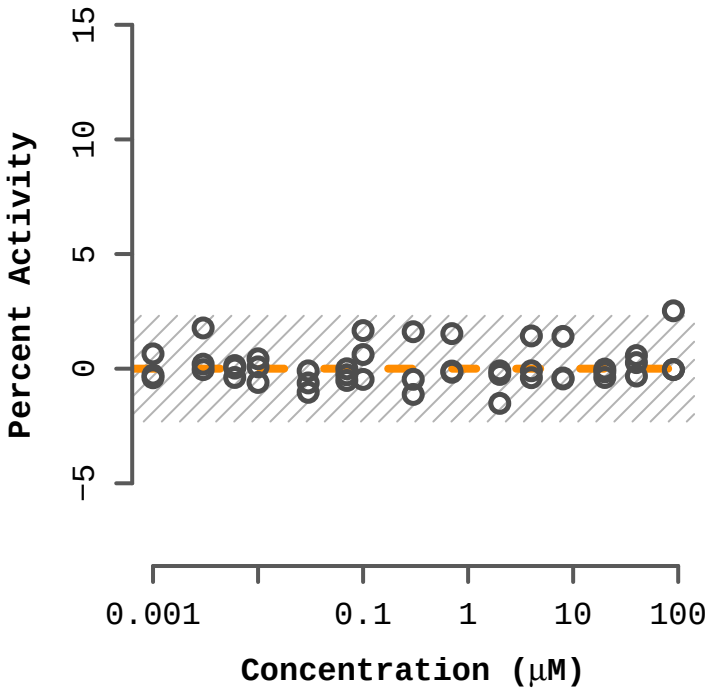
NAME: 3-Dimethylaminopropionitrile
CHID: 27432 **CASRN:** 1738-25-6
SPID(S): Tox21_201364
M4ID: 12480888

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.791 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

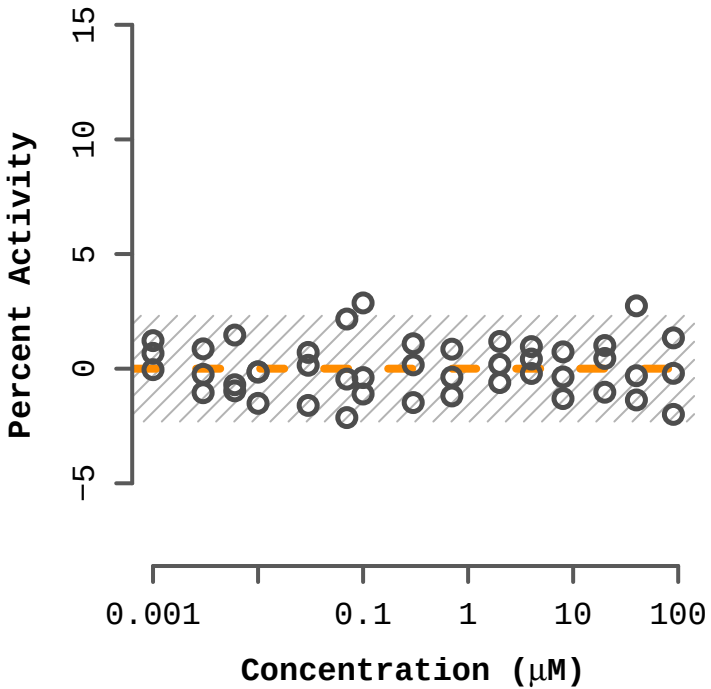
NAME: N−[3−(Trimethoxysilyl)propyl]ethane−1,2−diamin
CHID: 27433 **CASRN:** 1760−24−3
SPID(S): Tox21_303228
M4ID: 12475905

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.817 **MAX_MED:** 0.619 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

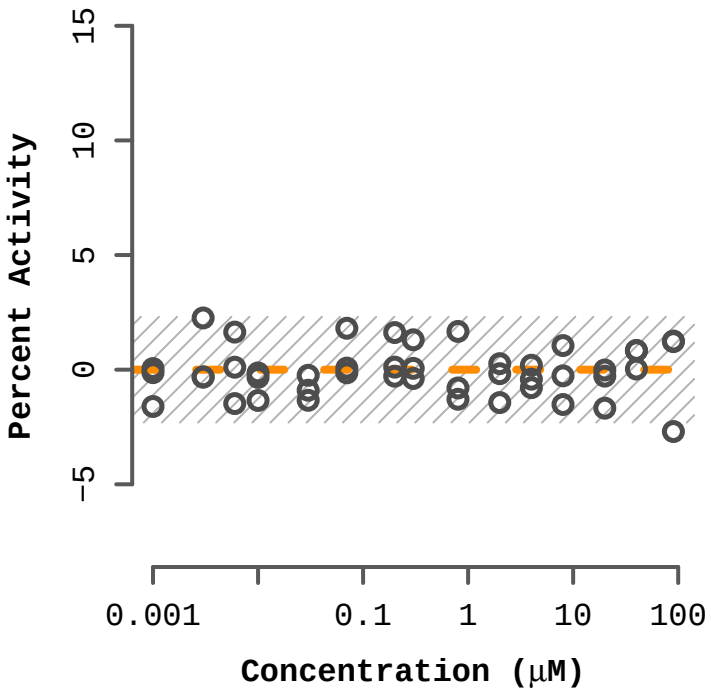
NAME: N−[3−(Trimethoxysilyl)propyl]ethane−1,2−diamin
CHID: 27433 **CASRN:** 1760−24−3
SPID(S): Tox21_201649
M4ID: 12480603

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.617 **MAX_MED:** 0.669 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

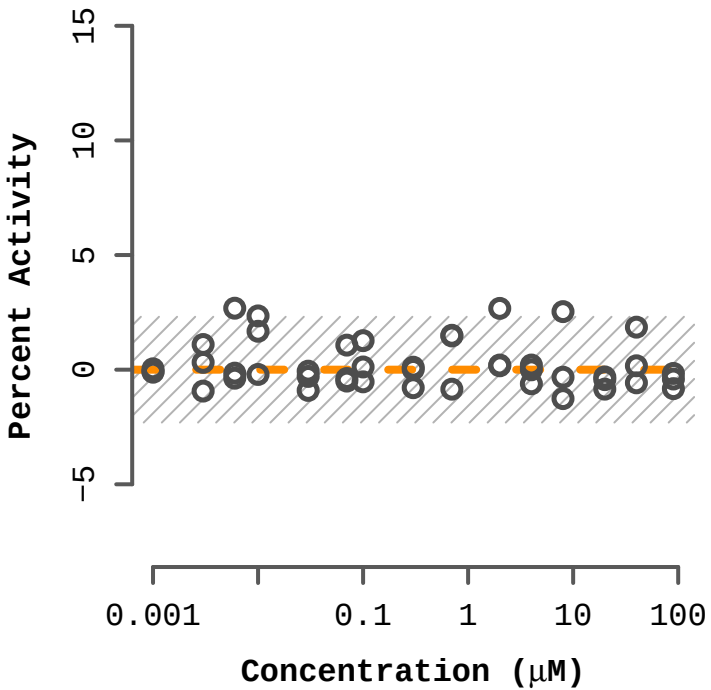
NAME: Phenylphosphinic acid
CHID: 27436 CASRN: 1779-48-2
SPID(S): Tox21_200455
M4ID: 12481797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.58 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

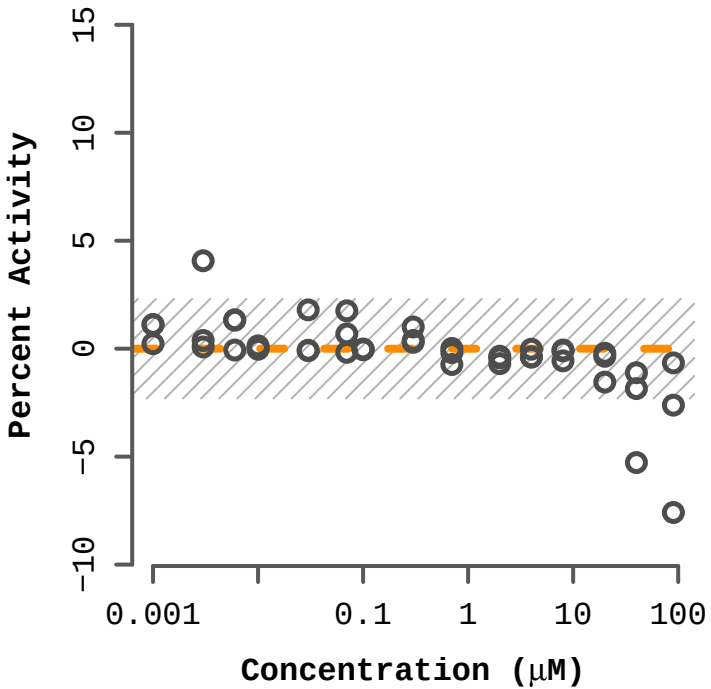
NAME: Dibutyl phosphite
CHID: 27438 **CASRN:** 1809-19-4
SPID(S): Tox21_303064
M4ID: 12476069

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

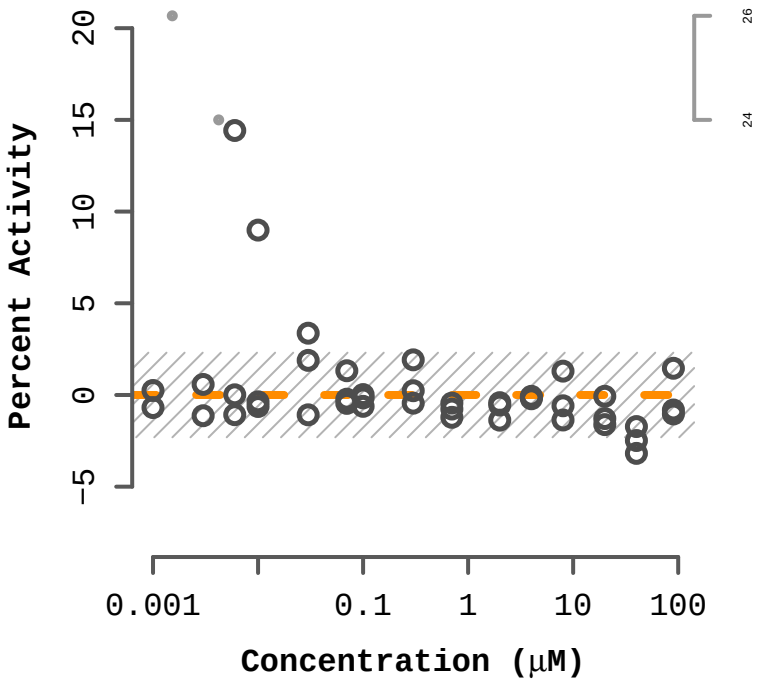
NAME: Dibutyl phosphite
CHID: 27438 **CASRN:** 1809-19-4
SPID(S): Tox21_201976
M4ID: 12480276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

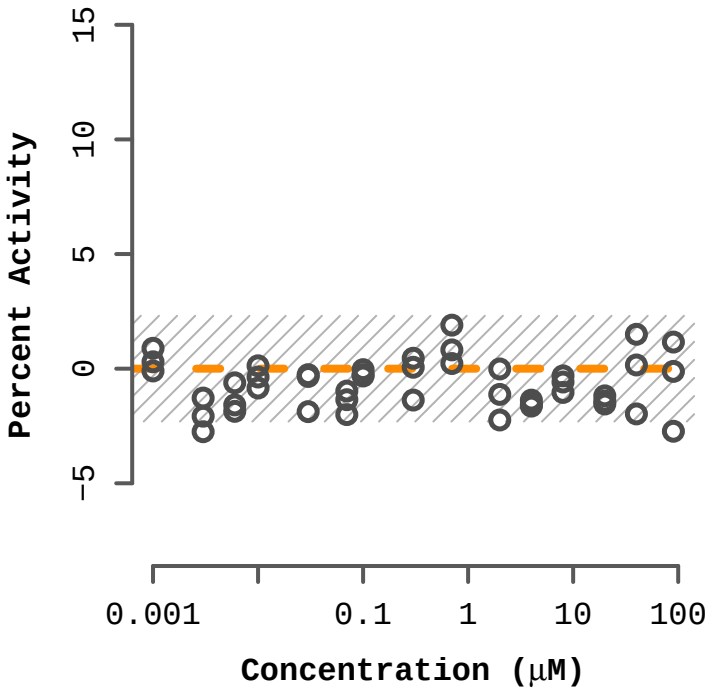
NAME: Octabenzone
CHID: 27441 **CASRN:** 1843-05-6
SPID(S): Tox21_300484
M4ID: 12478648 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.36	NA	NA
PROB:	1	NA	NA
RMSE:	5.98	NA	NA

MAX_MEAN: 8.58 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

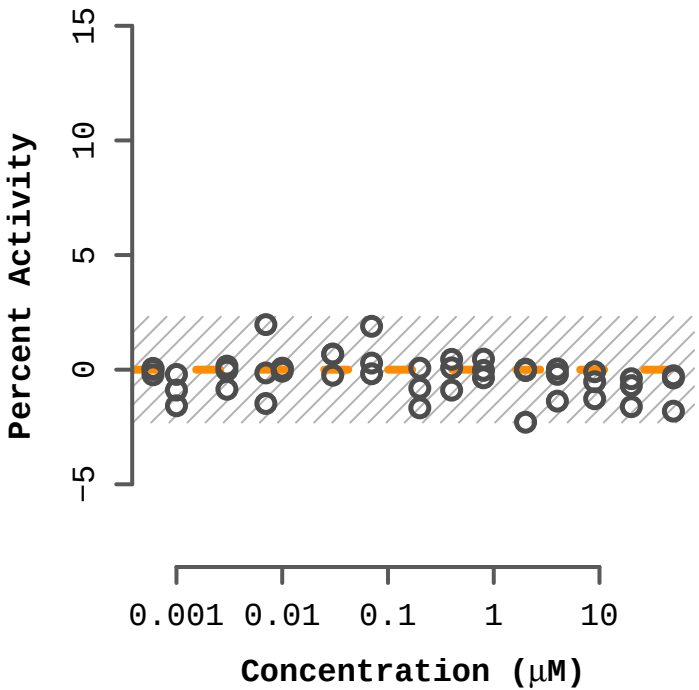
NAME: Octabenzone
CHID: 27441 **CASRN:** 1843-05-6
SPID(S): Tox21_201383
M4ID: 12480869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

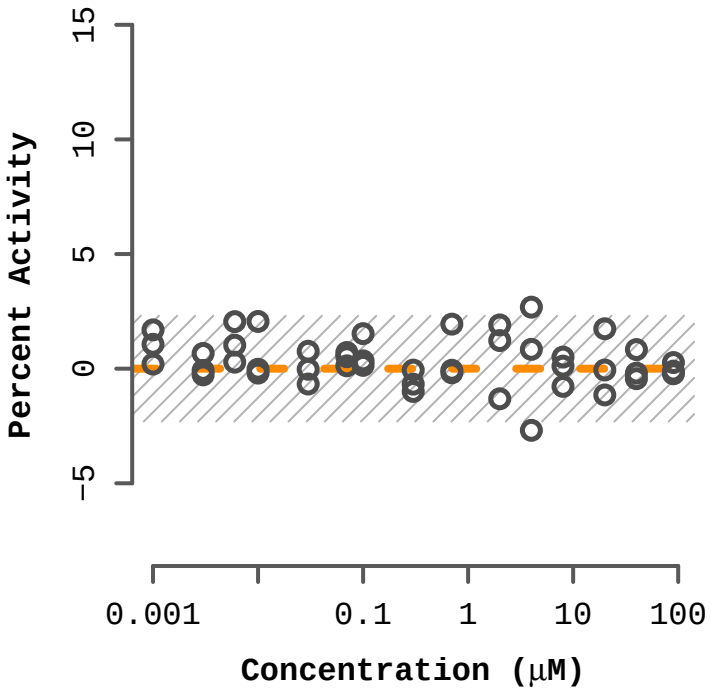
NAME: Octabenzone
CHID: 27441 **CASRN:** 1843-05-6
SPID(S): Tox21_112089_1
M4ID: 12483327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.669 **MAX_MED:** 0.677 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

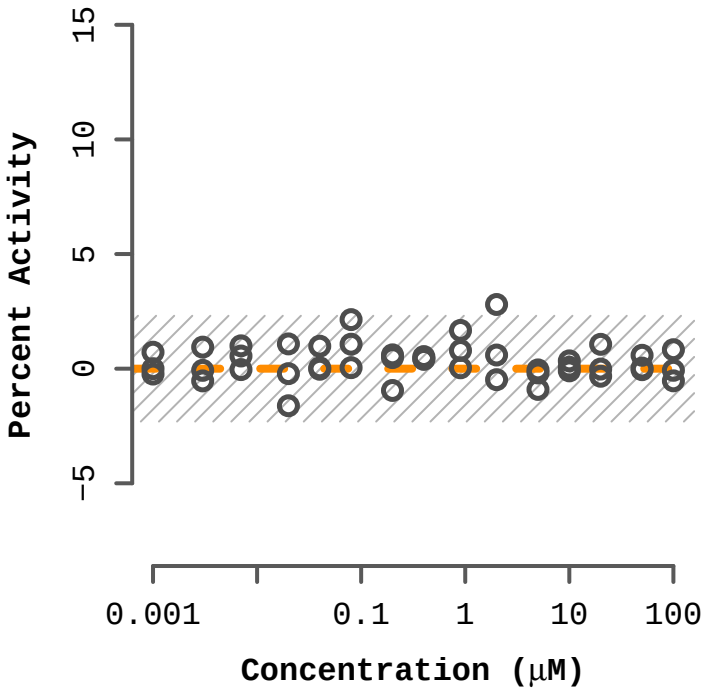
NAME: N−(Butoxymethyl)acrylamide
CHID: 27443 **CASRN:** 1852−16−0
SPID(S): Tox21_303121
M4ID: 12476012

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

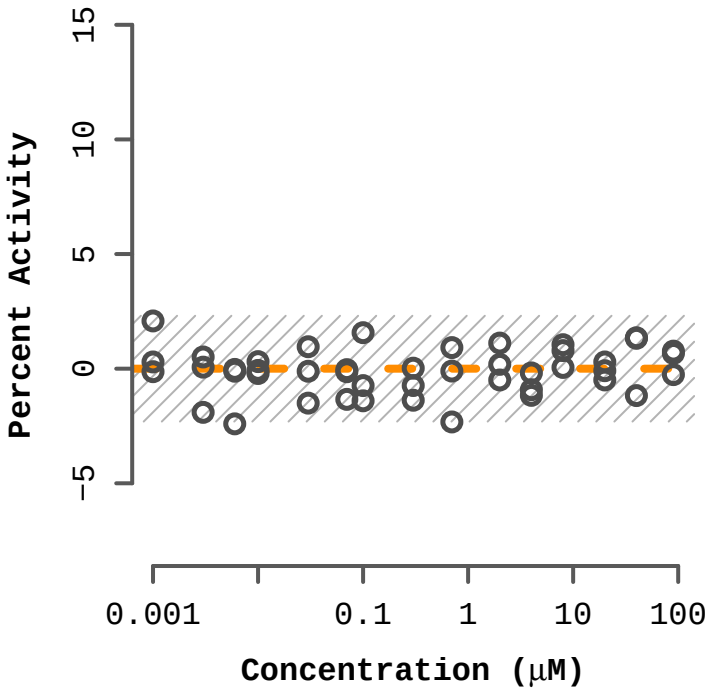
NAME: N−(Butoxymethyl)acrylamide
CHID: 27443 **CASRN:** 1852−16−0
SPID(S): Tox21_202366
M4ID: 12479886

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

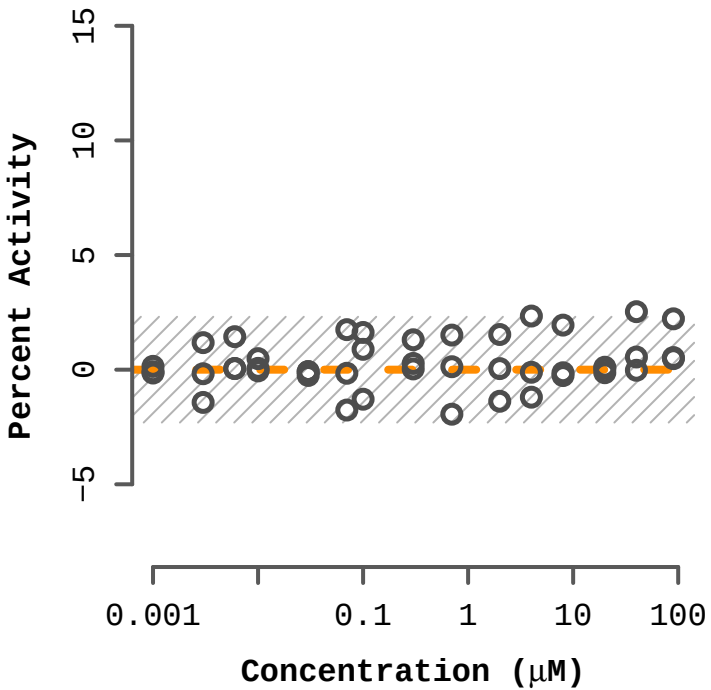
NAME: Decanenitrile
CHID: 27449 **CASRN:** 1975-78-6
SPID(S): Tox21_200860
M4ID: 12481392

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.95	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.749 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

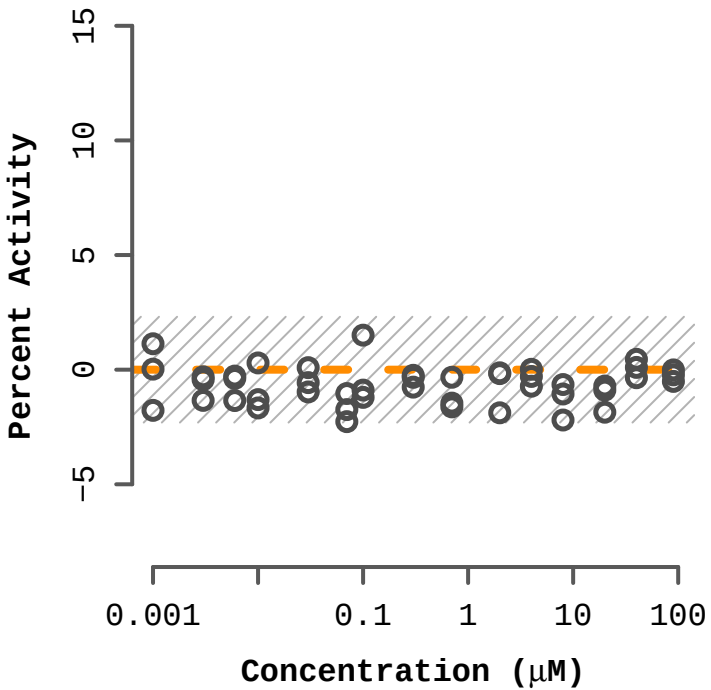
NAME: 2,5-Dichloroanisole
CHID: 27452 **CASRN:** 1984-58-3
SPID(S): Tox21_200952
M4ID: 12481300

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.888 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

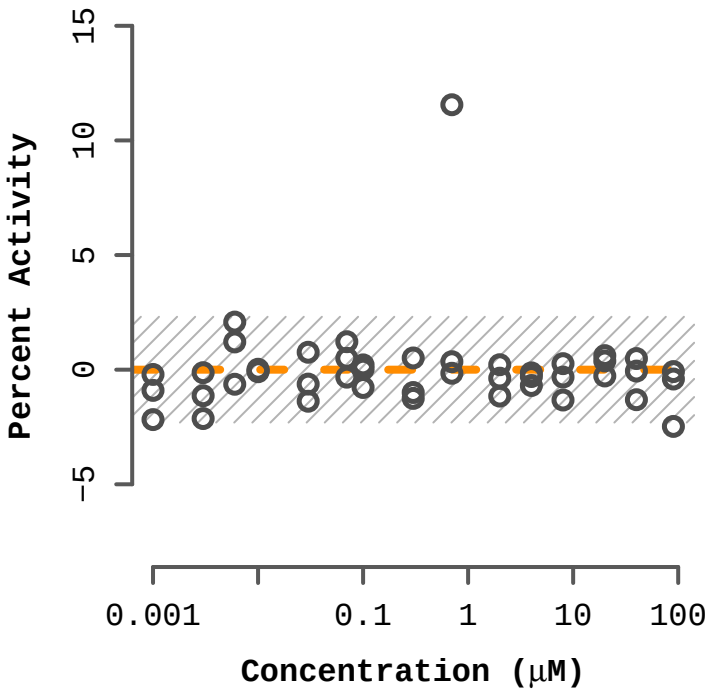
NAME: N,N−Dimethylacetoacetamide
CHID: 27454 **CASRN:** 2044−64−6
SPID(S): Tox21_303265
M4ID: 12475868

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.0682 **MAX_MED:** 0.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

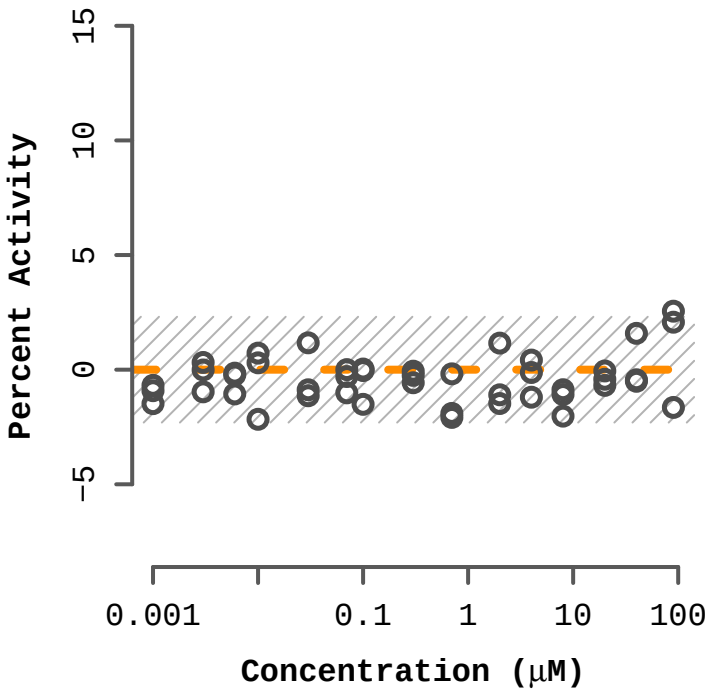
NAME: N,N−Dimethylacetoacetamide
CHID: 27454 CASRN: 2044−64−6
SPID(S): Tox21_201898
M4ID: 12480354

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 3.92 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

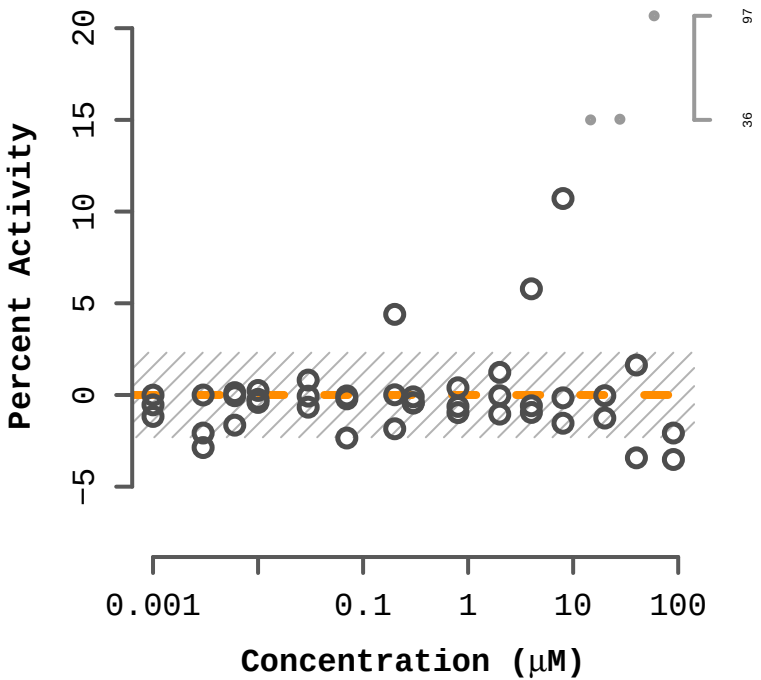
NAME: Thiocarbazide
CHID: 27461 **CASRN:** 2231-57-4
SPID(S): Tox21_303273
M4ID: 12475860

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.992 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

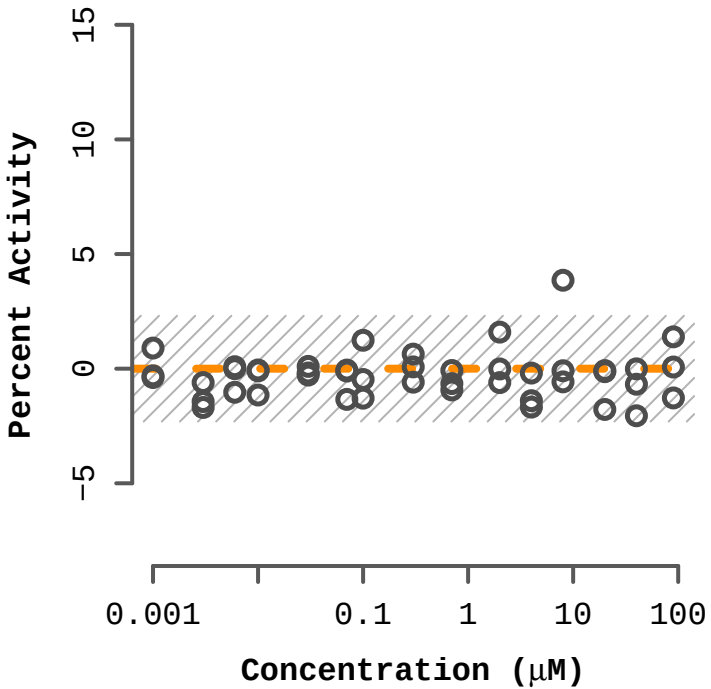
NAME: Thiocarbazide
CHID: 27461 **CASRN:** 2231-57-4
SPID(S): Tox21_201365
M4ID: 12480887 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	266.31	NA	NA
PROB:	1	NA	NA
RMSE:	16.5	NA	NA

MAX_MEAN: 30.4 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

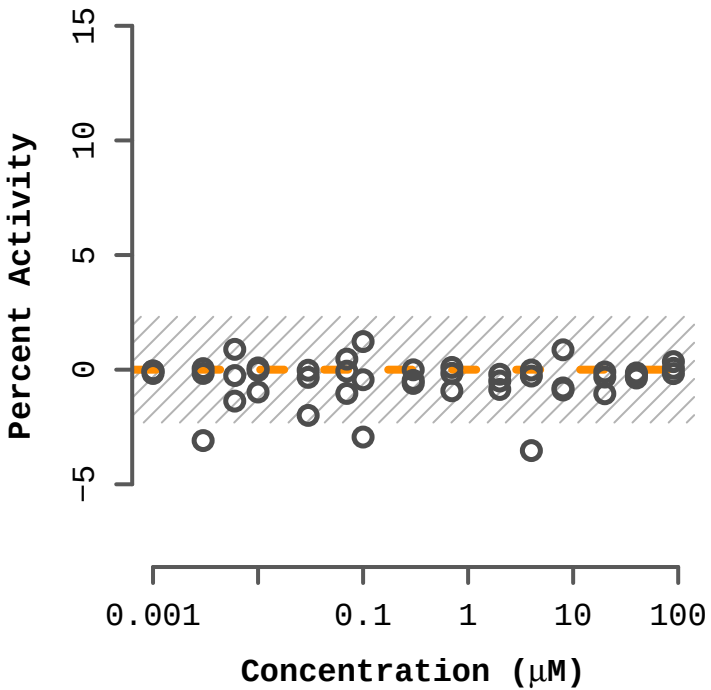
NAME: Ammonium dodecyl sulfate
CHID: 27462 CASRN: 2235-54-3
SPID(S): Tox21_202561
M4ID: 12479691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.07 MAX_MED: 0.0792 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

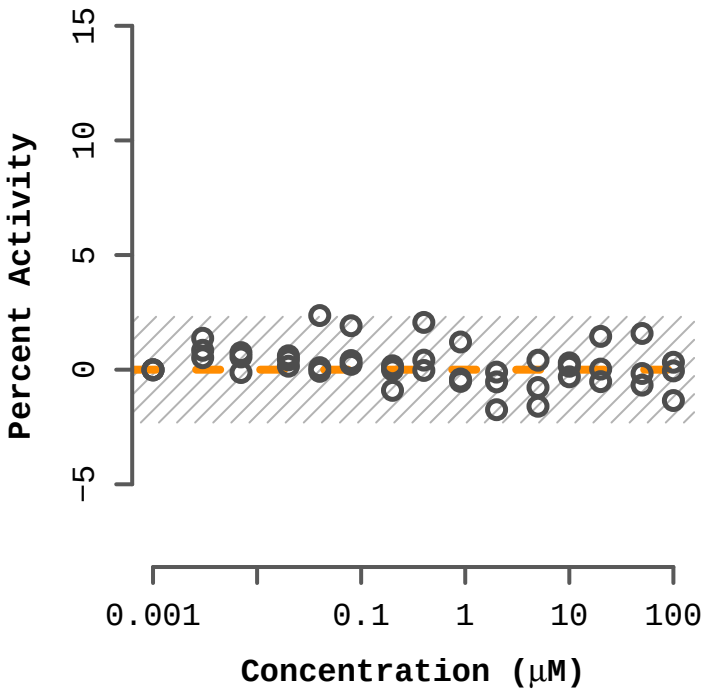
NAME: UT-632
CHID: 27466 CASRN: 2386-87-0
SPID(S): Tox21_303312
M4ID: 12475821

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.0807 MAX_MED: 0.0602 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

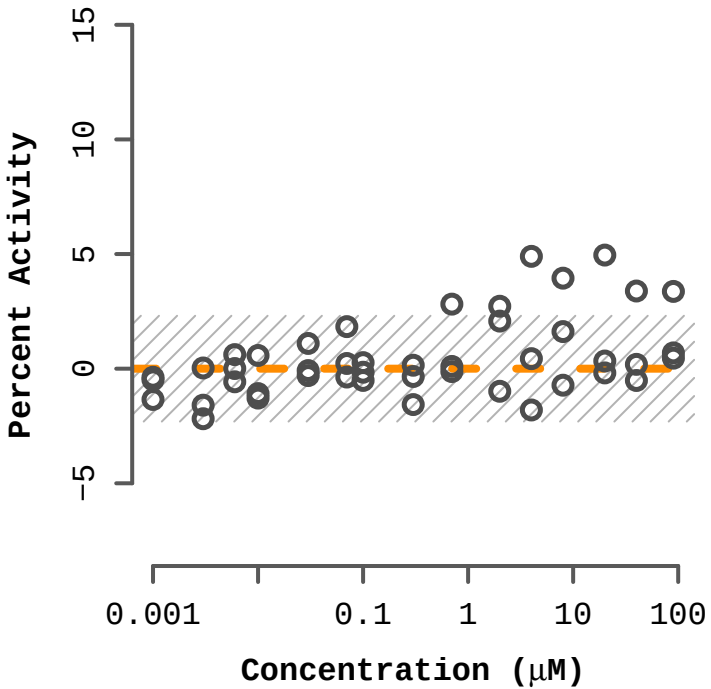
NAME: UT-632
CHID: 27466 **CASRN:** 2386-87-0
SPID(S): Tox21_202388
M4ID: 12479864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.914 **MAX_MED:** 0.847 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

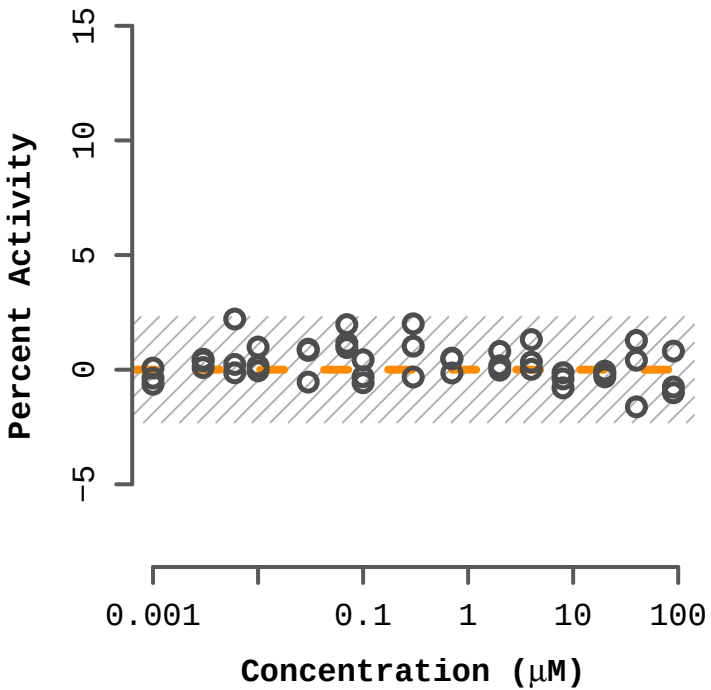
NAME: 2,3,5,6-Tetrachloropyridine
CHID: 27467 **CASRN:** 2402-79-1
SPID(S): Tox21_200259
M4ID: 12481993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

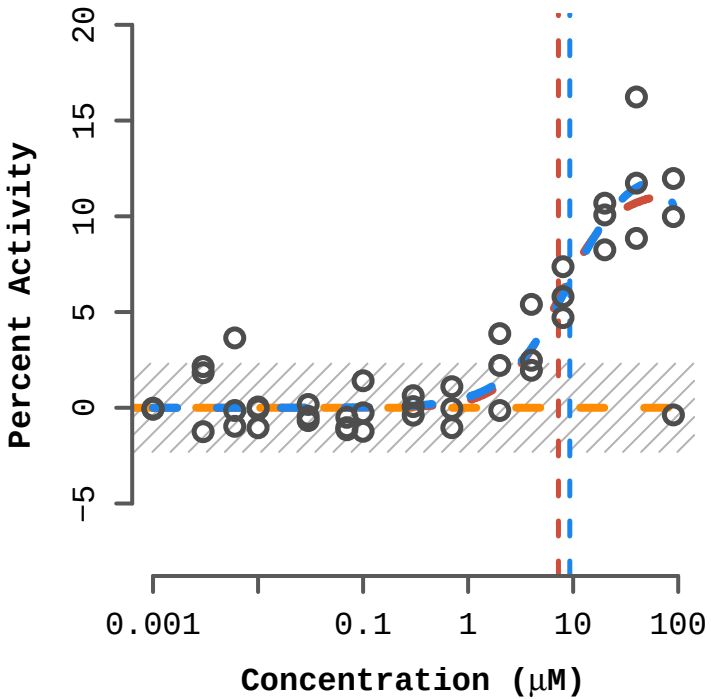
NAME: 1-Chlorotetradecane
CHID: 27471 **CASRN:** 2425-54-9
SPID(S): Tox21_200456
M4ID: 12481796

HILL MODEL: Not applicable.

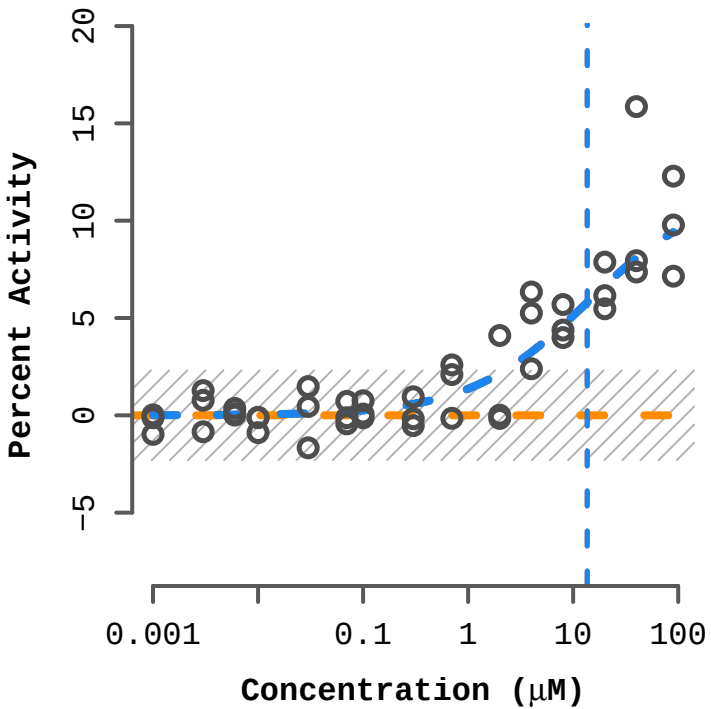
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.16 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-(2H-Benzotriazol-2-yl)-4-methylphenol
CHID:    27479   CASRN: 2440-22-4
SPID(S): Tox21_303578
M4ID:    12475567

HILL MODEL (in red):
      tp       ga       gw
val:  11.3     0.86     1.68
sd:   0.912    0.0765   0.419

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.2     0.968    1.39     2.16     3.48
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  268.48      180.5       183.42
PROB: 0           0.81        0.19
RMSE: 5.19        2.25        2.16

MAX_MEAN: 12.3      MAX_MED: 11.7      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(2H-Benzotriazol-2-yl)-4-methylphenol
CHID: 27479 **CASRN:** 2440-22-4
SPID(S): Tox21_200876
M4ID: 12481376

HILL MODEL (in red):

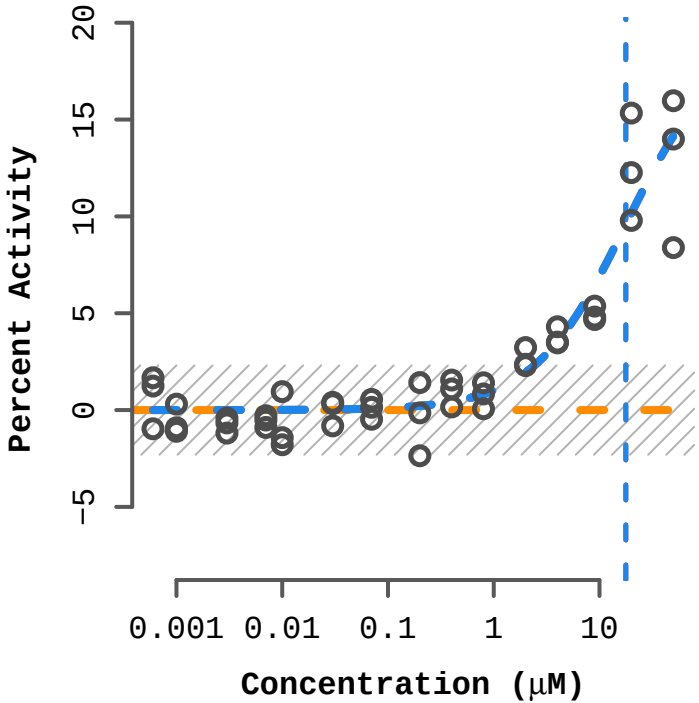
	tp	ga	gw
val:	11.6	1.13	0.772
sd:	3.13	0.366	0.217

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.6	1.13	0.772	3.11	7.72
sd:	3.13	0.366	0.217	2770	18600

	CNST	HILL	GNLS
AIC:	259.55	166.7	170.7
PROB:	0	0.88	0.12
RMSE:	4.66	1.67	1.67

MAX_MEAN: 10.4 **MAX_MED:** 9.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(2H-Benzotriazol-2-yl)-4-methylphenol
CHID: 27479 **CASRN:** 2440-22-4
SPID(S): Tox21_112369_1
M4ID: 12483131

HILL MODEL (in red):

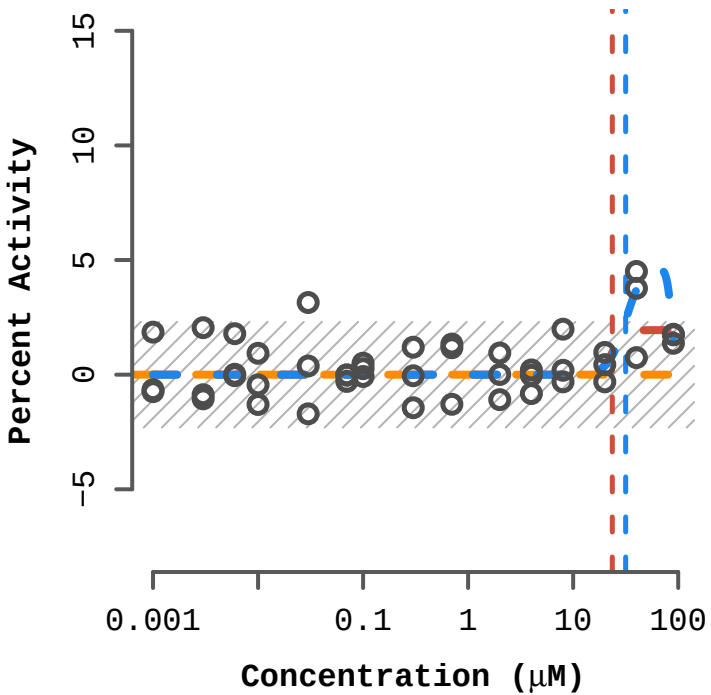
	tp	ga	gw
val:	19.2	1.25	1
sd:	3.27	0.178	0.154

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.2	1.25	1	3.66	3.92
sd:	3.27	0.178	0.154	1120	2200

	CNST	HILL	GNLS
AIC:	258.43	162.94	166.94
PROB:	0	0.88	0.12
RMSE:	5.11	1.54	1.54

MAX_MEAN: 12.8 **MAX_MED:** 14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: O,O−Dimethyl chlorothiophosphate
CHID: 27486 CASRN: 2524−03−0
SPID(S): Tox21_202562
M4ID: 12479690

HILL MODEL (in red):

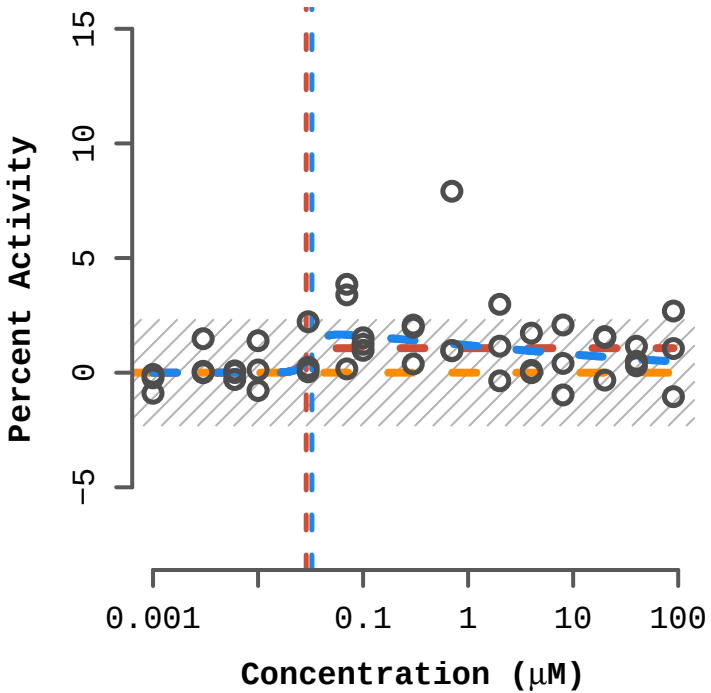
	tp	ga	gw
val:	1.94	1.37	8
sd:	0.487	0.0938	7.88

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.75	1.5	5.31	1.94	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.39	147.71	147.55
PROB:	0	0.48	0.52
RMSE:	1.41	1.13	1.11

MAX_MEAN: 3.01 MAX_MED: 3.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: O,O−Diethyl chlorothiophosphate
CHID: 27487 CASRN: 2524−04−1
SPID(S): Tox21_200977
M4ID: 12481275

HILL MODEL (in red):

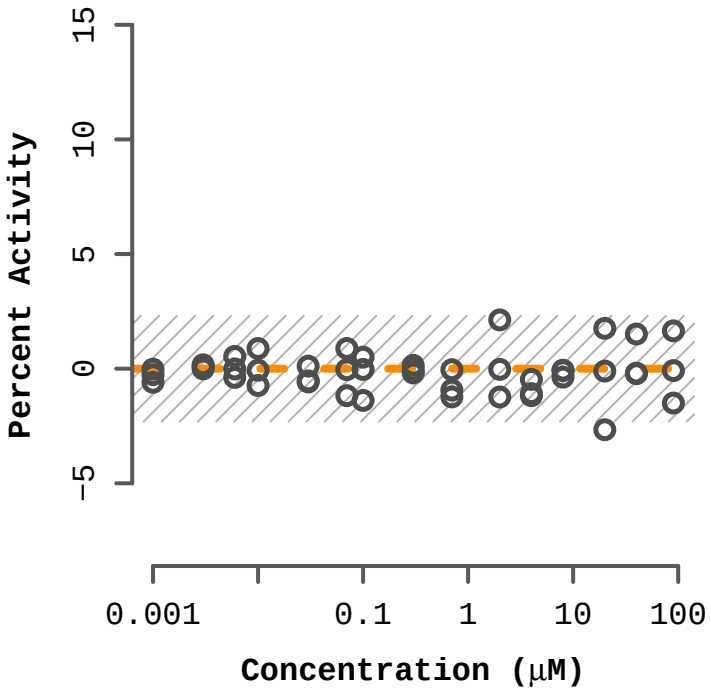
	tp	ga	gw
val:	1.07	−1.54	8
sd:	0.209	0.165	34.7

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.42	−1.49	7.5	−0.0395	0.3
sd:	7.88	0.122	15.6	10.1	0.816

	CNST	HILL	GNLS
AIC:	171.48	154.49	155.95
PROB:	0	0.67	0.32
RMSE:	1.82	1.46	1.41

MAX_MEAN: 3.28 **MAX_MED:** 3.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

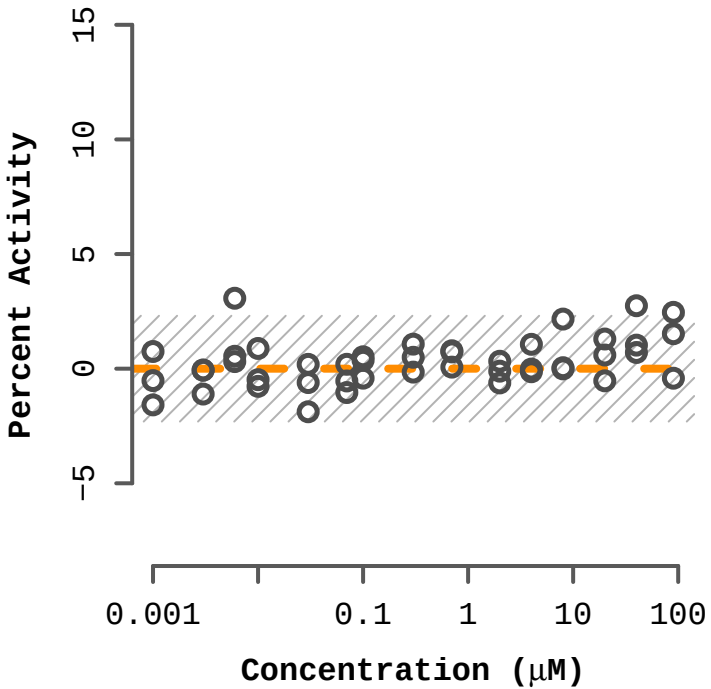
NAME: Trimethoxy[3-(oxiran-2-ylmethoxy)propyl]silane
CHID: 27489 **CASRN:** 2530-83-8
SPID(S): Tox21_303288
M4ID: 12475845

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.367 **MAX_MED:** 0.0992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

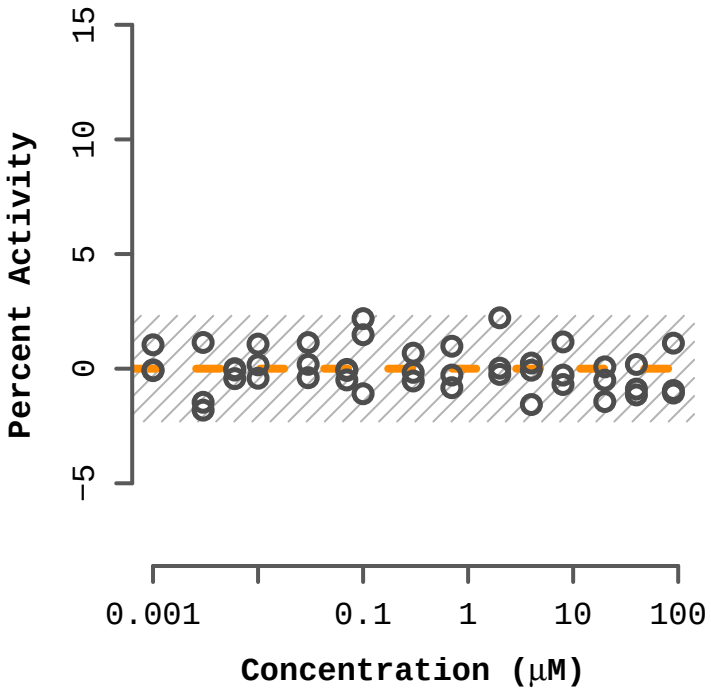
NAME: Trimethoxy[3-(oxiran-2-ylmethoxy)propyl]silane
CHID: 27489 **CASRN:** 2530-83-8
SPID(S): Tox21_201672
M4ID: 12480580

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

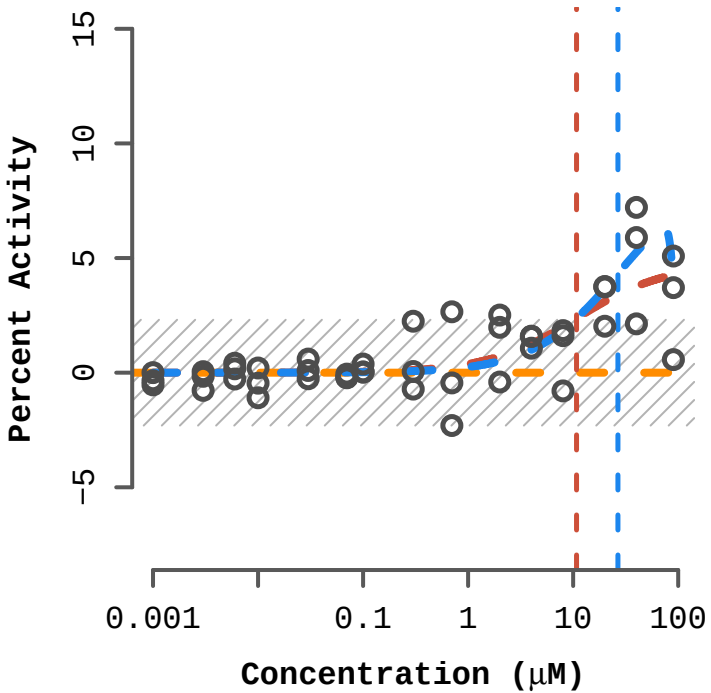
NAME: (3-Chloropropyl)trimethoxysilane
CHID: 27490 **CASRN:** 2530-87-2
SPID(S): Tox21_200013
M4ID: 12482239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.859 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Diaminotoluene
CHID: 27494 CASRN: 2687-25-4
SPID(S): Tox21_300092
M4ID: 12479038

HILL MODEL (in red):

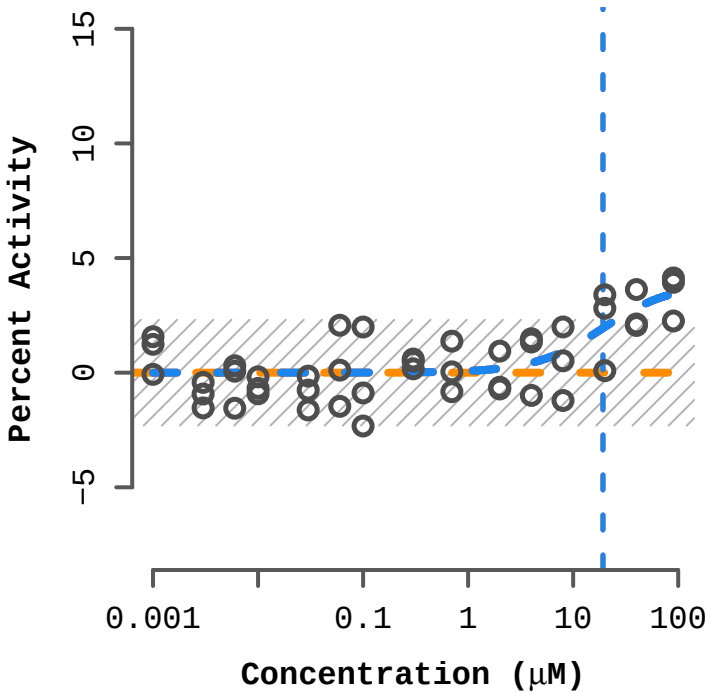
	tp	ga	gw
val:	4.74	1.03	1.03
sd:	1.23	0.286	0.481

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.65	1.43	1.07	1.96	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	189.42	149.62	150.12
PROB:	0	0.56	0.44
RMSE:	2.15	1.26	1.2

MAX_MEAN: 5.08 MAX_MED: 5.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Diaminotoluene
CHID: 27494 CASRN: 2687-25-4
SPID(S): Tox21_200457
M4ID: 12481795

HILL MODEL (in red):

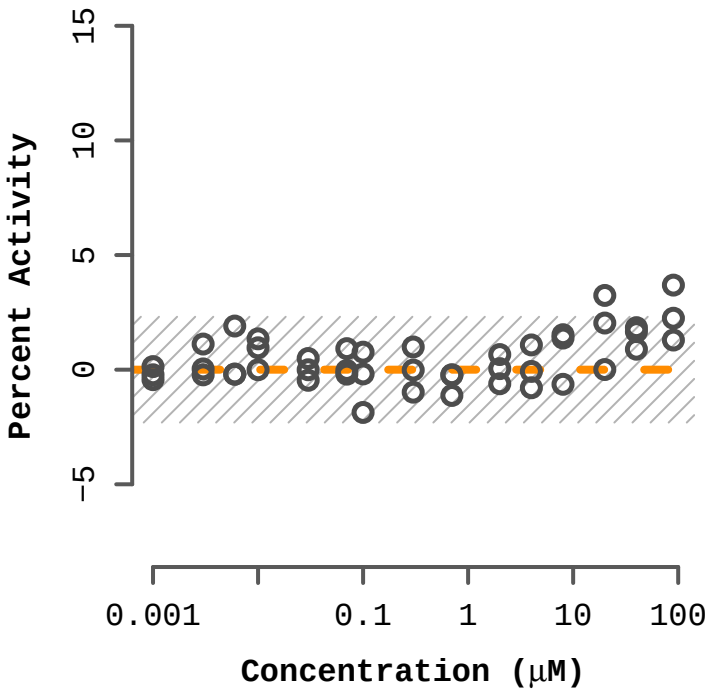
	tp	ga	gw
val:	3.88	1.28	1.33
sd:	1.93	0.501	1.12

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.88	1.28	1.33	3.43	5.04
sd:	1.93	0.501	1.12	1390	4830

	CNST	HILL	GNLS
AIC:	177.38	151.14	155.14
PROB:	0	0.88	0.12
RMSE:	1.67	1.12	1.12

MAX_MEAN: 3.44 MAX_MED: 3.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

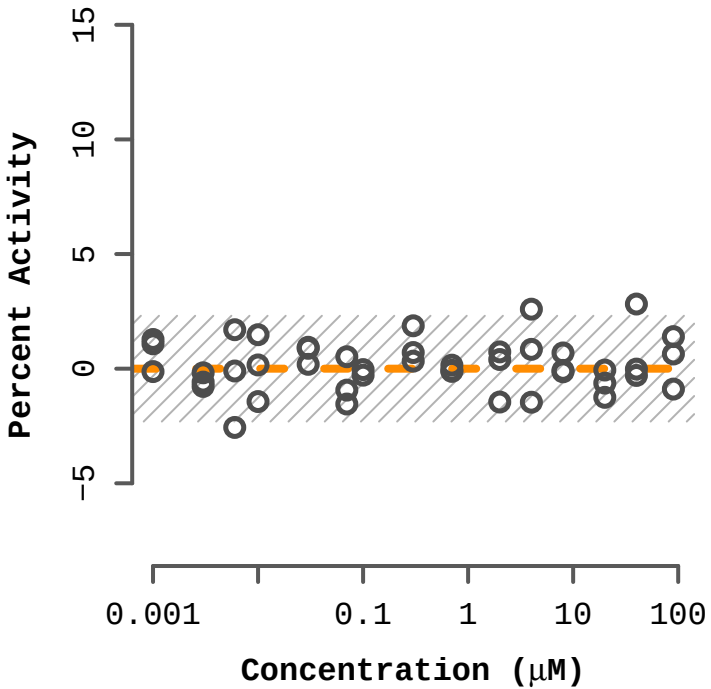
NAME: 2,4−D sodium salt
CHID: 27496 CASRN: 2702−72−9
SPID(S): Tox21_303248
M4ID: 12475885

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.41 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

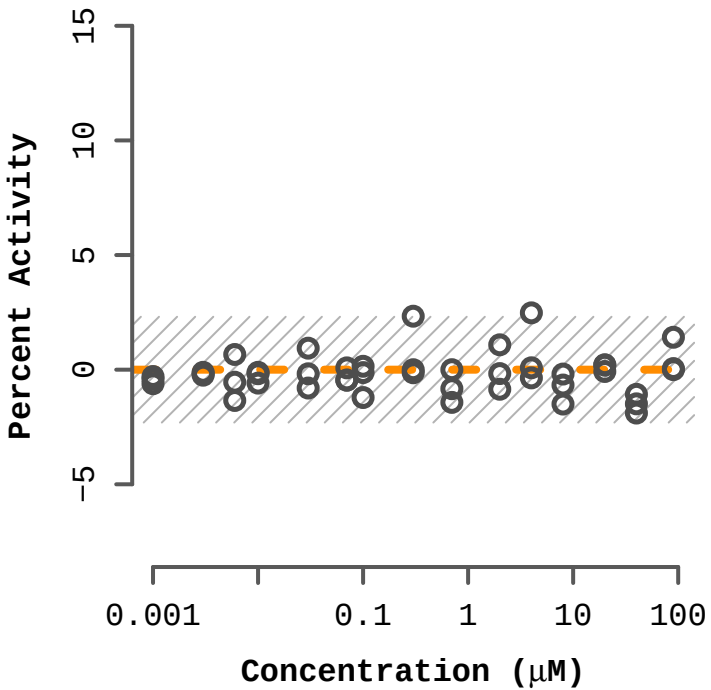
NAME: 2,4−D sodium salt
CHID: 27496 CASRN: 2702−72−9
SPID(S): Tox21_201377
M4ID: 12480875

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.969 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

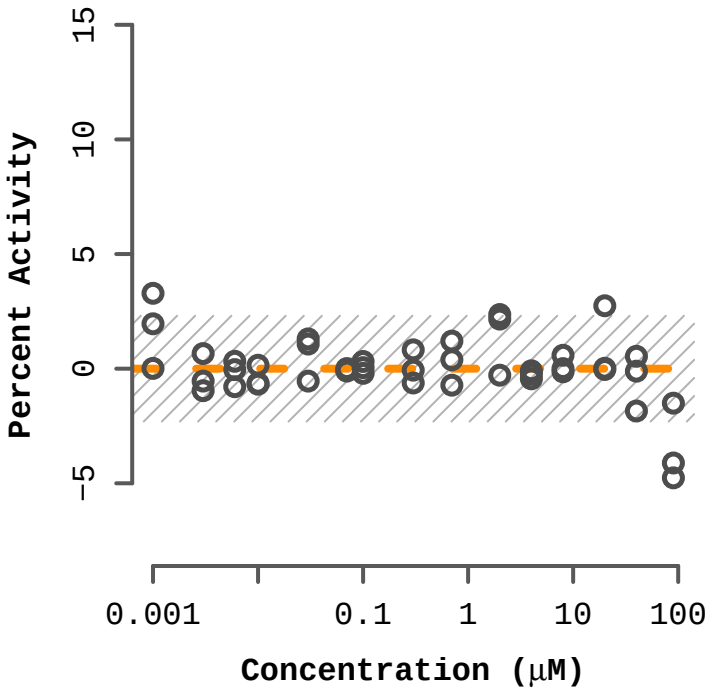
NAME: 1,3-Bis(2-isocyanatopropan-2-yl)benzene
CHID: 27498 **CASRN:** 2778-42-9
SPID(S): Tox21_303289
M4ID: 12475844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.735 **MAX_MED:** 0.198 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

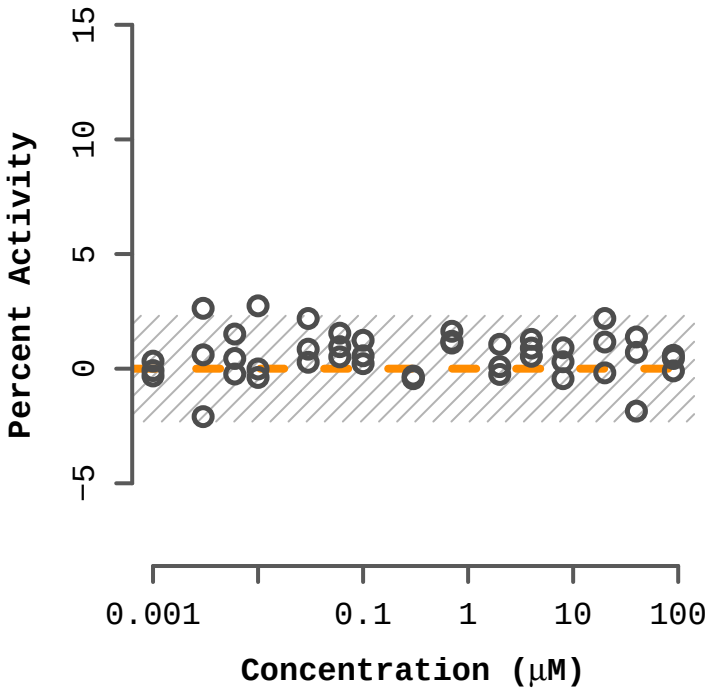
NAME: 1,3-Bis(2-isocyanatopropan-2-yl)benzene
CHID: 27498 **CASRN:** 2778-42-9
SPID(S): Tox21_202410
M4ID: 12479842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

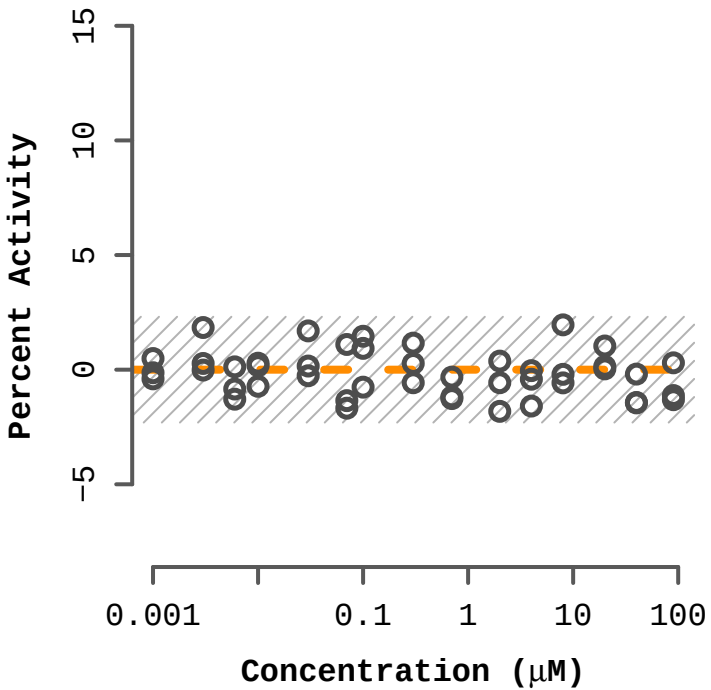
NAME: 2-Propoxyethanol
CHID: 27500 **CASRN:** 2807-30-9
SPID(S): Tox21_303034
M4ID: 12476099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

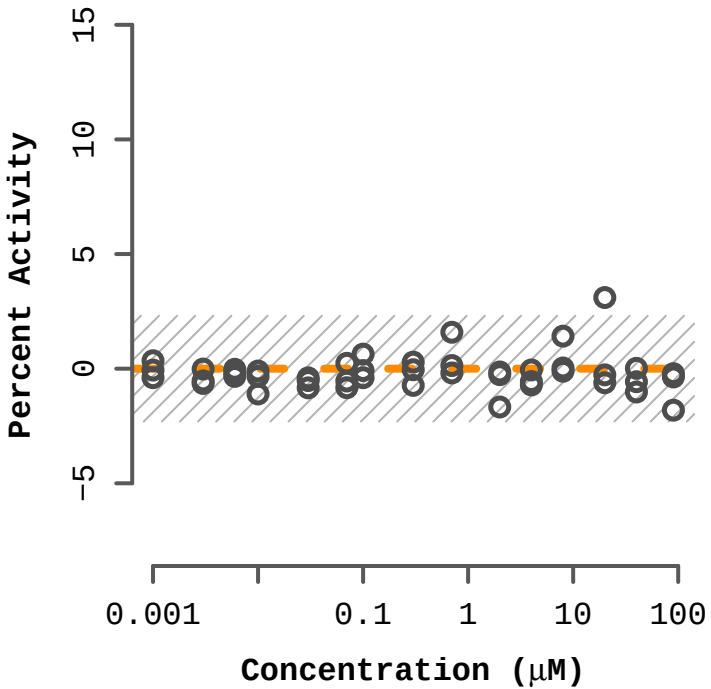
NAME: 2-Propoxyethanol
CHID: 27500 **CASRN:** 2807-30-9
SPID(S): Tox21_201994
M4ID: 12480258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.699 **MAX_MED:** 0.931 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

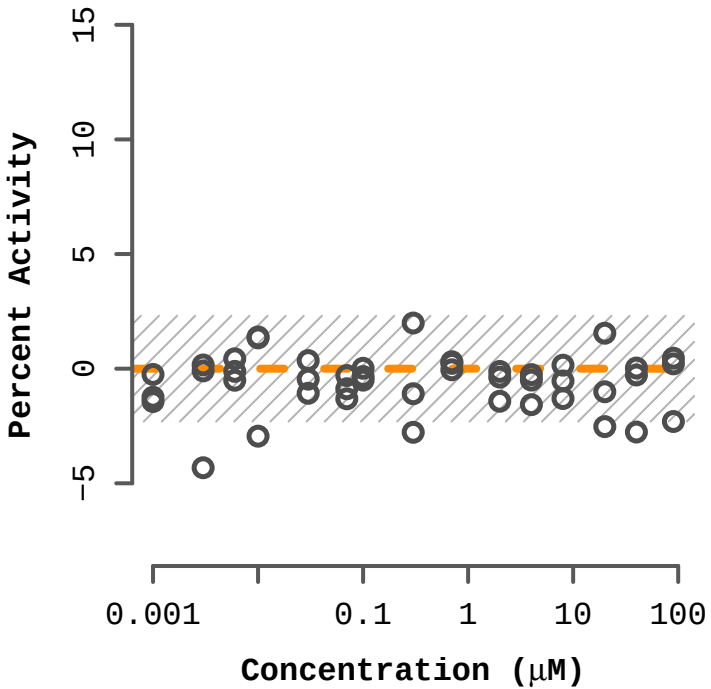
NAME: 2-Isopropyl-6-methyl-4-pyrimidone
CHID: 27502 **CASRN:** 2814-20-2
SPID(S): Tox21_303297
M4ID: 12475836

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.138 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

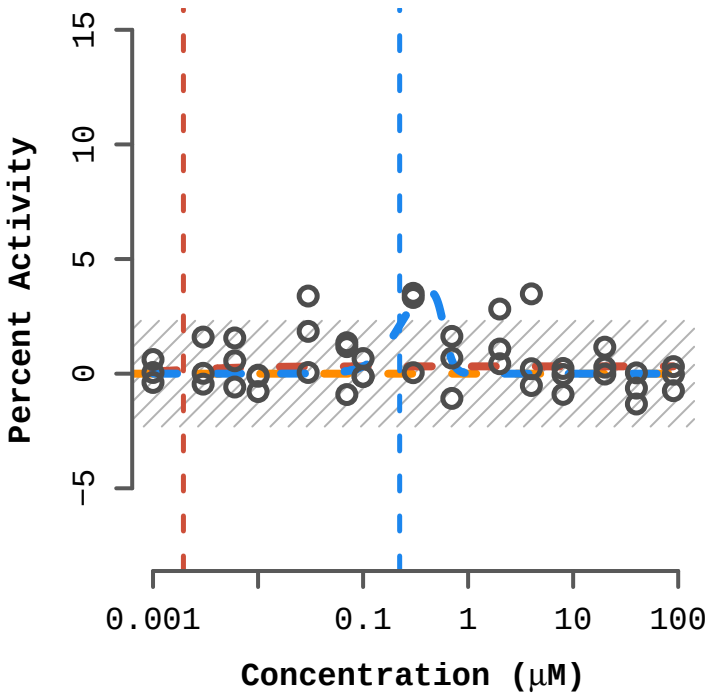
NAME: 2-Isopropyl-6-methyl-4-pyrimidone
CHID: 27502 CASRN: 2814-20-2
SPID(S): Tox21_201995
M4ID: 12480257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.163 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isophorone diamine
CHID: 27503 CASRN: 2855-13-2
SPID(S): Tox21_303122
M4ID: 12476011

HILL MODEL (in red):

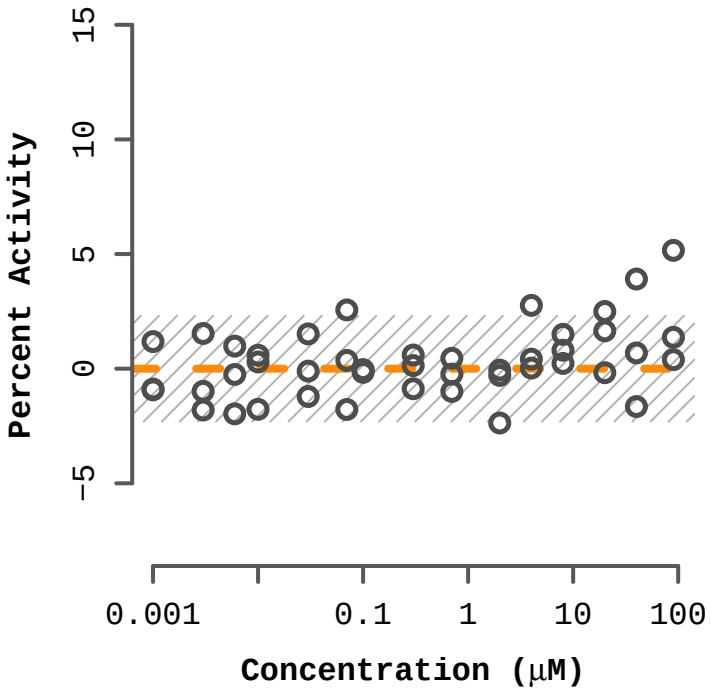
	tp	ga	gw
val:	0.319	−2.71	1.24
sd:	0.198	2.05	2.99

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.21	−0.652	3.12	−0.231	10.2
sd:	6.88	0.611	5.2	0.94	126

	CNST	HILL	GNLS
AIC:	149.87	152.58	150.52
PROB:	0.51	0.13	0.36
RMSE:	1.34	1.25	1.21

MAX_MEAN: 2.29 MAX_MED: 3.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

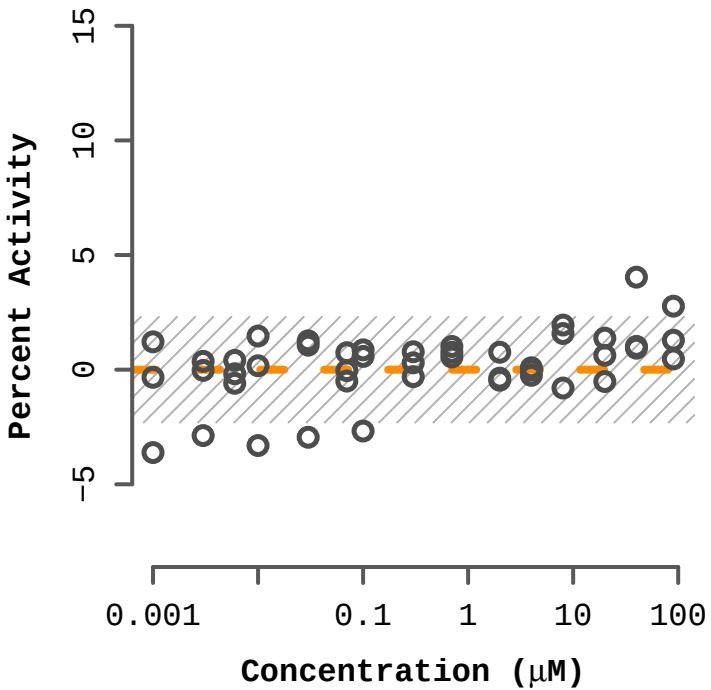
NAME: Isophorone diamine
CHID: 27503 **CASRN:** 2855-13-2
SPID(S): Tox21_201401
M4ID: 12480851

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 2.31 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

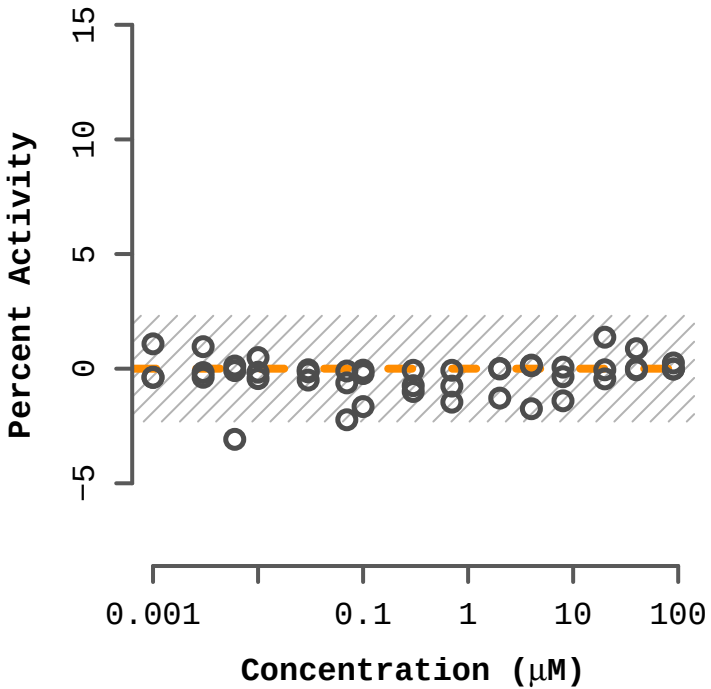
NAME: 2-(Dimethylamino)ethyl methacrylate
CHID: 27504 **CASRN:** 2867-47-2
SPID(S): Tox21_201694
M4ID: 12480558

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

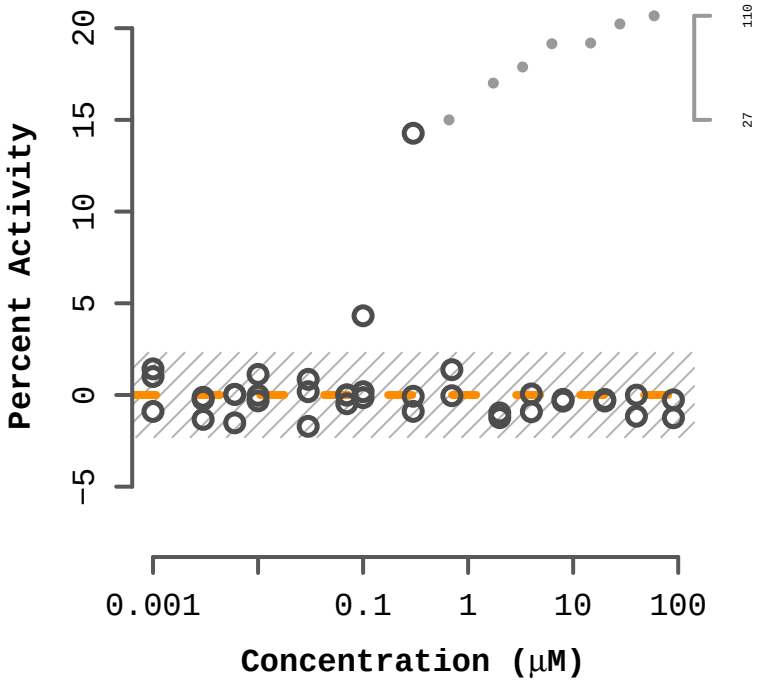
NAME: 3,5-Dichlorobenzoyl chloride
CHID: 27506 **CASRN:** 2905-62-6
SPID(S): Tox21_200629
M4ID: 12481623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.295 **MAX_MED:** 0.128 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

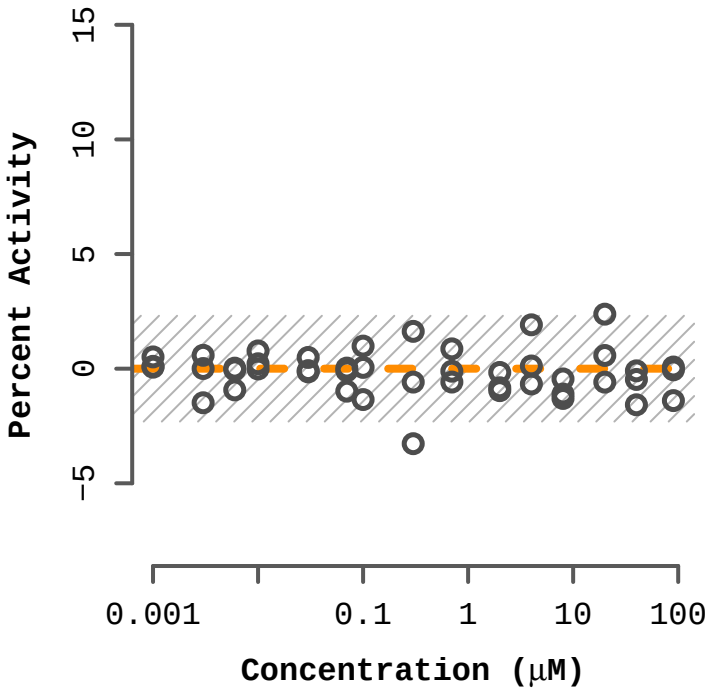
NAME: Methyl 3-chlorobenzoate
CHID: 27507 **CASRN:** 2905-65-9
SPID(S): Tox21_201012
M4ID: 12481240 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	377.41	NA	NA
PROB:	1	NA	NA
RMSE:	32.43	NA	NA

MAX_MEAN: 36.1 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

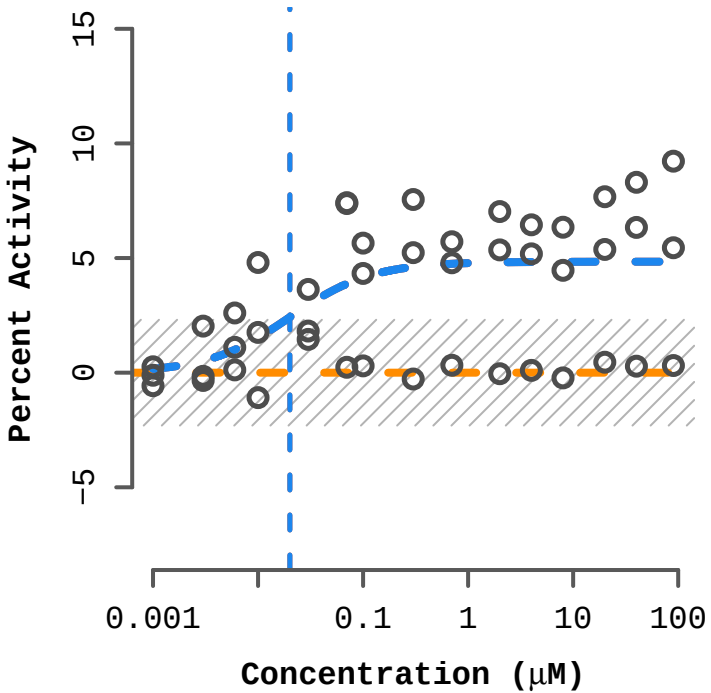
NAME: Methyl 3-sulfanylpropanoate
CHID: 27509 **CASRN:** 2935-90-2
SPID(S): Tox21_200030
M4ID: 12482222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis[2−(dimethylamino)ethyl]ether
CHID: 27512 CASRN: 3033−62−3
SPID(S): Tox21_303216
M4ID: 12475917

HILL MODEL (in red):

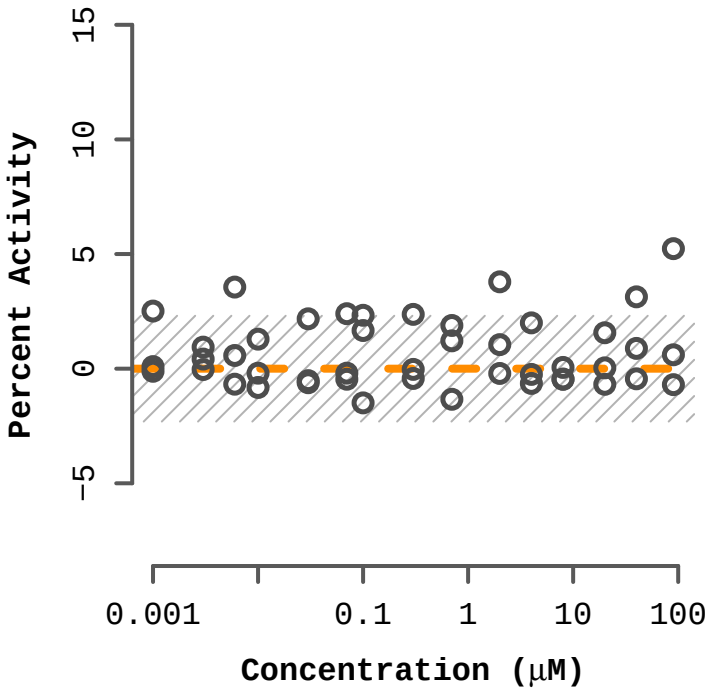
	tp	ga	gw
val:	4.84	−1.7	1.11
sd:	0.665	0.319	0.703

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.84	−1.7	1.11	3.32	5.56
sd:	0.665	0.319	0.703	1770	7160

	CNST	HILL	GNLS
AIC:	267.21	227.95	231.95
PROB:	0	0.88	0.12
RMSE:	4.42	2.68	2.68

MAX_MEAN: 5.01 MAX_MED: 7.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

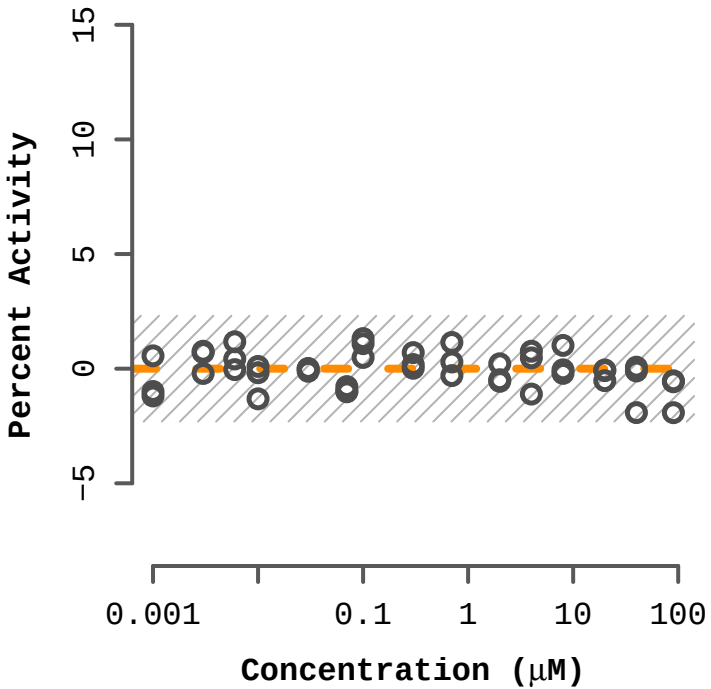
NAME: Bis[2−(dimethylamino)ethyl]ether
CHID: 27512 **CASRN:** 3033−62−3
SPID(S): Tox21_202013
M4ID: 12480239

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

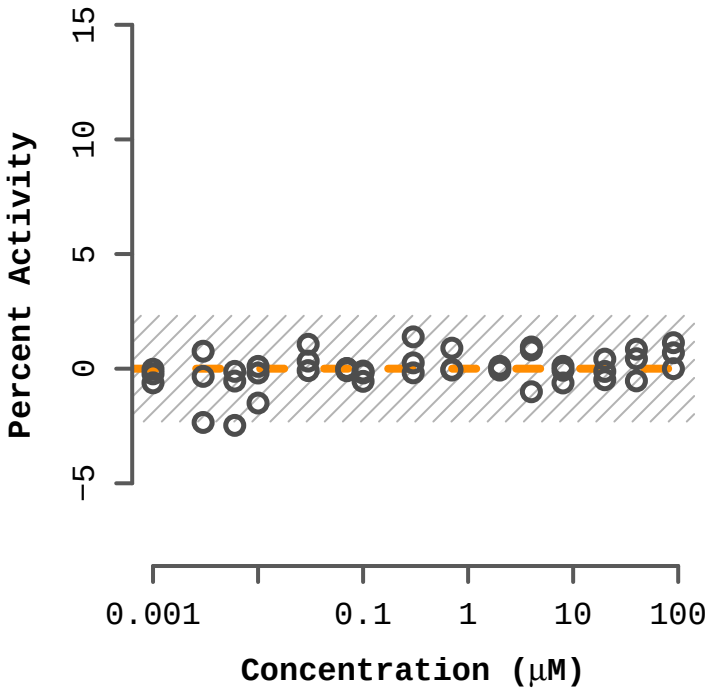
NAME: Sodium ethenesulfonate
CHID: 27513 **CASRN:** 3039-83-6
SPID(S): Tox21_301466
M4ID: 12477667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

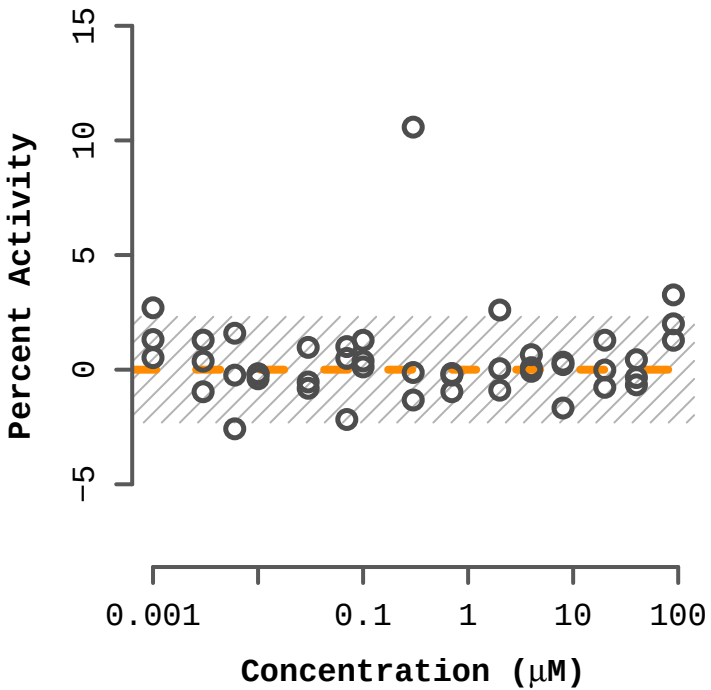
NAME: 3a,4,7,7a−Tetrahydroindene
CHID: 27515 CASRN: 3048−65−5
SPID(S): Tox21_200458
M4ID: 12481794

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.611 MAX_MED: 0.819 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

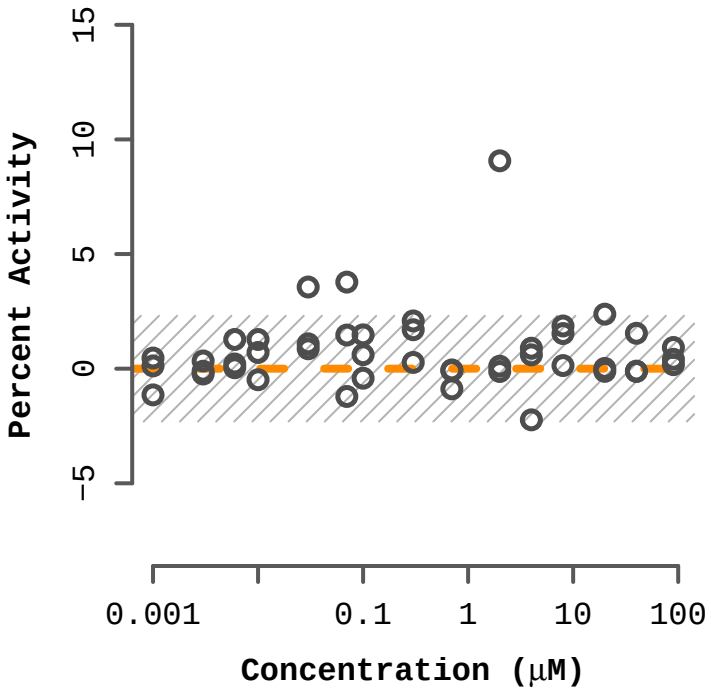
NAME: Aluminum tributoxide
CHID: 27518 **CASRN:** 3085-30-1
SPID(S): Tox21_303204
M4ID: 12475929

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 3.05 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

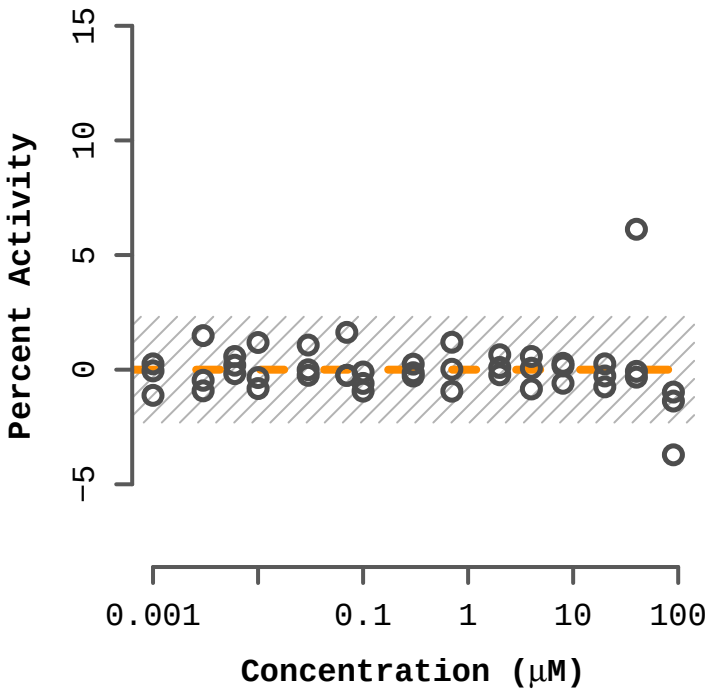
NAME: N,N,N',N',N'',N''−Hexakis(methoxymethyl)−1,3,5·
CHID: 27520 **CASRN:** 3089−11−0
SPID(S): Tox21_303133
M4ID: 12476000

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 3.02 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

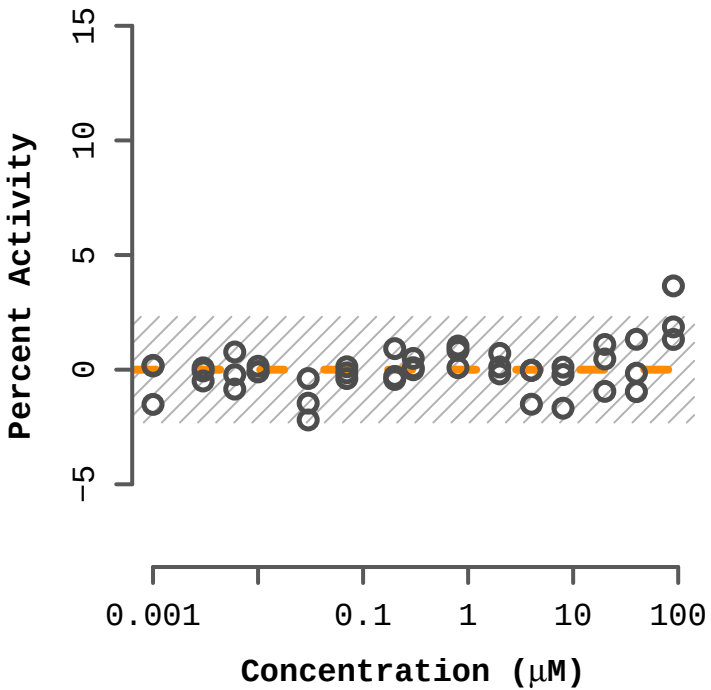
NAME: N,N,N',N',N'',N''−Hexakis(methoxymethyl)−1,3,5·
CHID: 27520 **CASRN:** 3089−11−0
SPID(S): Tox21_201599
M4ID: 12480653

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

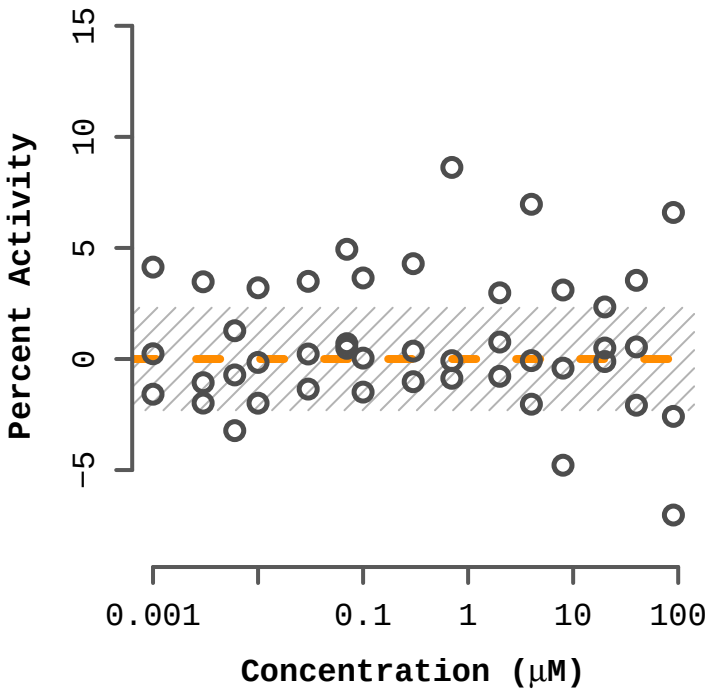
NAME: 3-Bromobenzaldehyde
CHID: 27521 **CASRN:** 3132-99-8
SPID(S): Tox21_200948
M4ID: 12481304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

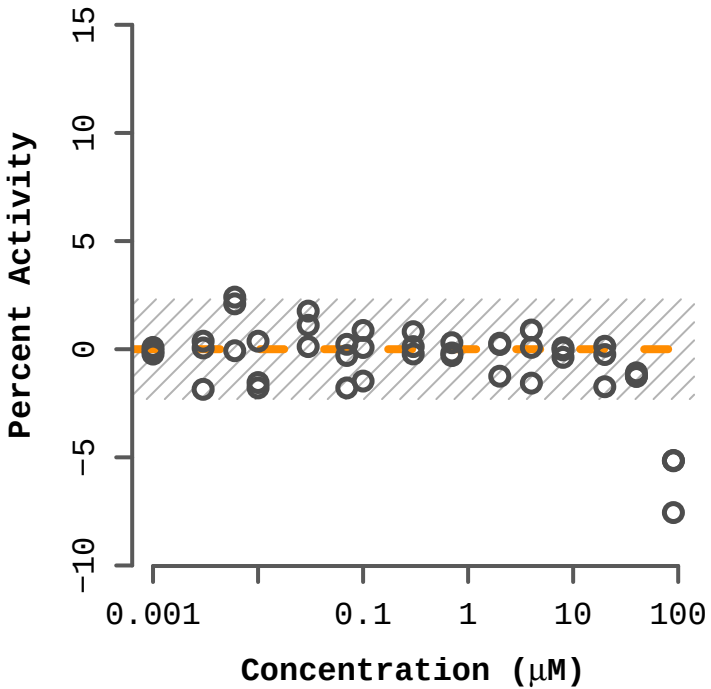
NAME: Octrizole
CHID: 27522 **CASRN:** 3147-75-9
SPID(S): Tox21_300498
M4ID: 12478634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 2.56 **MAX_MED:** 0.764 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

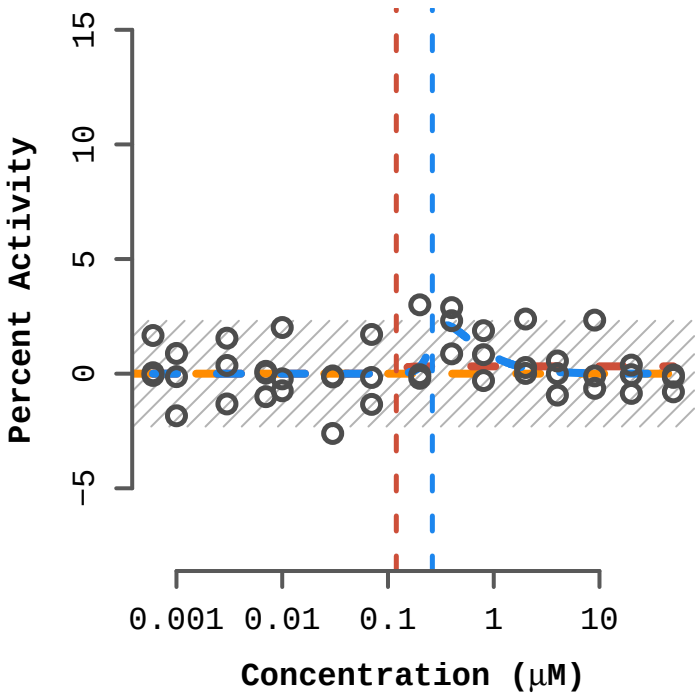
NAME: Octrizole
CHID: 27522 CASRN: 3147-75-9
SPID(S): Tox21_201456
M4ID: 12480796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.48 MAX_MED: 2.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Octrizole
CHID: 27522 **CASRN:** 3147-75-9
SPID(S): Tox21_112086_1
M4ID: 12483329

HILL MODEL (in red):

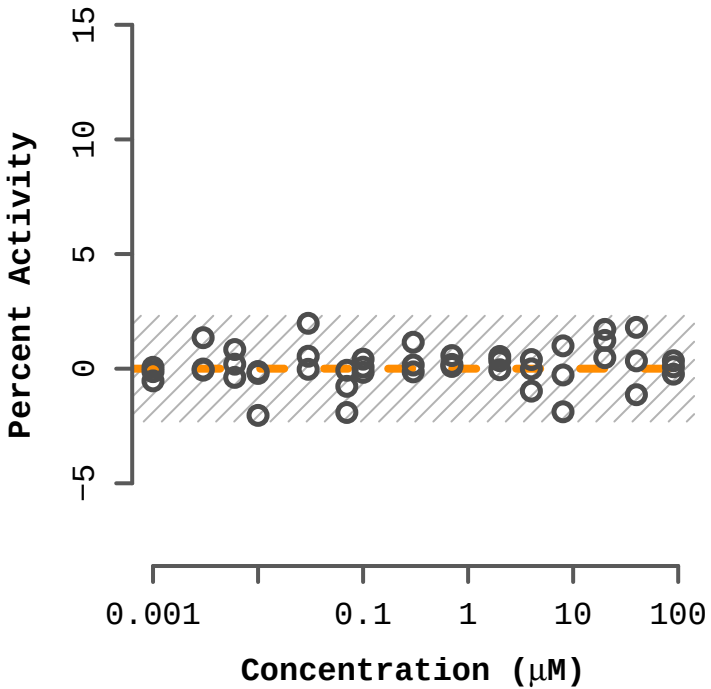
	tp	ga	gw
val:	0.319	−0.921	8
sd:	0.238	1.47	46.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.61	−0.58	7.99	−0.316	1.83
sd:	4.56	0.188	10.8	0.605	1.67

	CNST	HILL	GNLS
AIC:	149.3	153.38	147.41
PROB:	0.27	0.04	0.69
RMSE:	1.25	1.2	1.1

MAX_MEAN: 2.02 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

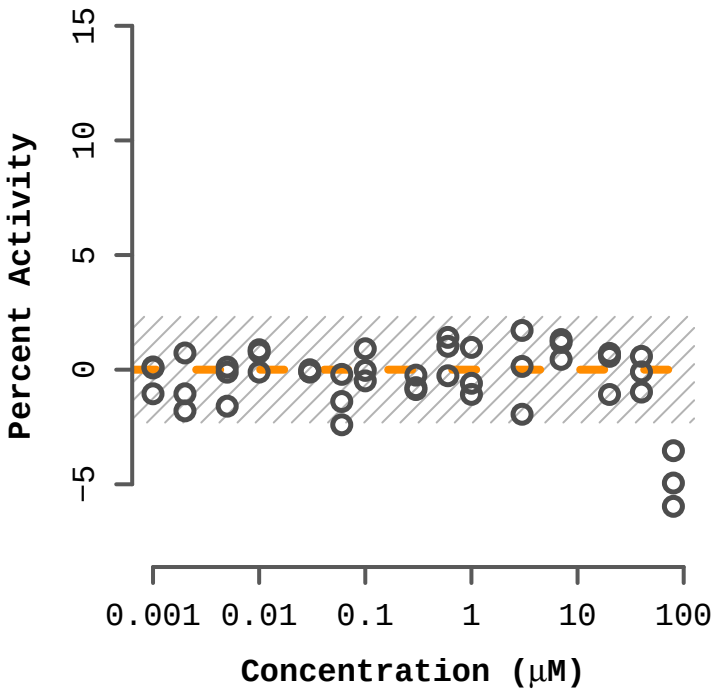
NAME: Potassium 2-ethylhexanoate
CHID: 27525 **CASRN:** 3164-85-0
SPID(S): Tox21_303103
M4ID: 12476030

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

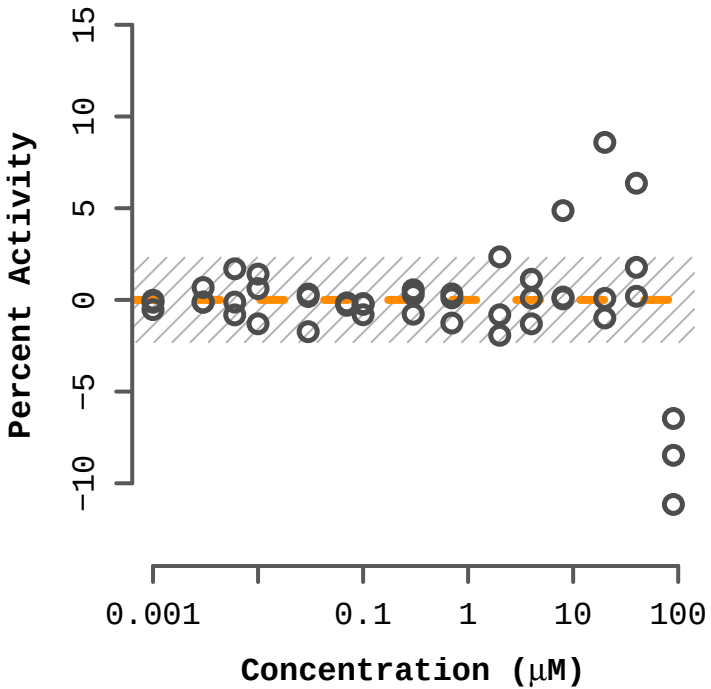
NAME: 1,2,5,6,9,10−Hexabromocyclododecane
CHID: 27527 **CASRN:** 3194−55−6
SPID(S): Tox21_303176
M4ID: 12475957

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 0.986 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

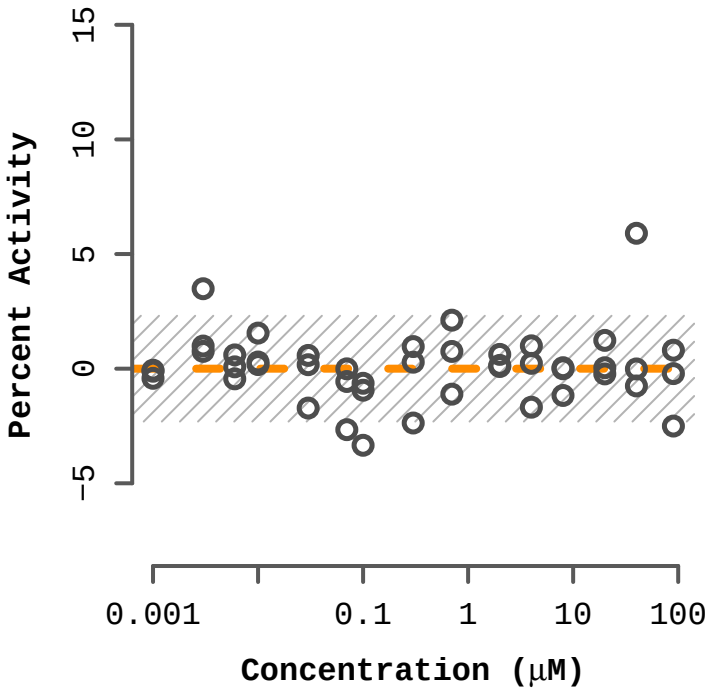
NAME: 1,2,5,6,9,10−Hexabromocyclododecane
CHID: 27527 **CASRN:** 3194−55−6
SPID(S): Tox21_201402
M4ID: 12480850

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.61	NA	NA
PROB:	1	NA	NA
RMSE:	3.01	NA	NA

MAX_MEAN: 2.78 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

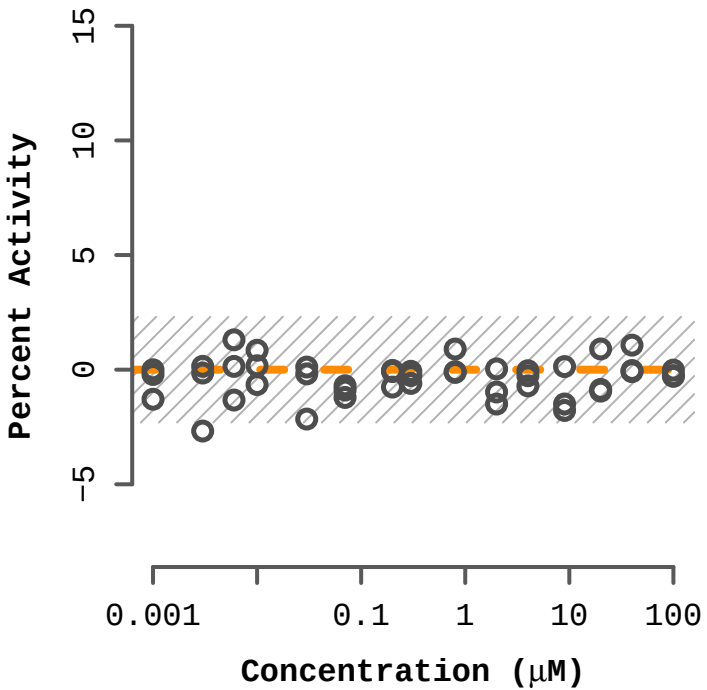
NAME: 3-(Methylthio)propanal
CHID: 27528 **CASRN:** 3268-49-3
SPID(S): Tox21_303157
M4ID: 12475976

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 0.989 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

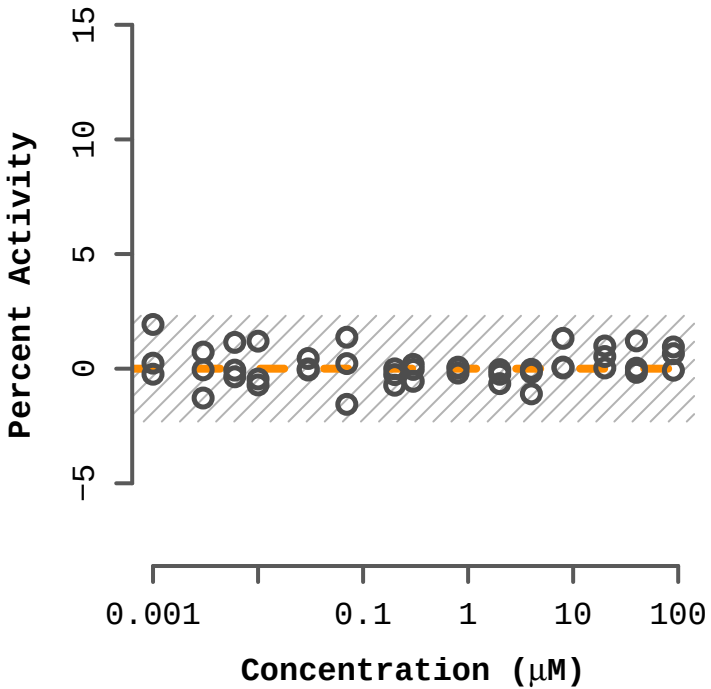
NAME: 3-(Methylthio)propanal
CHID: 27528 **CASRN:** 3268-49-3
SPID(S): Tox21_201978
M4ID: 12480274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.317 **MAX_MED:** 0.174 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

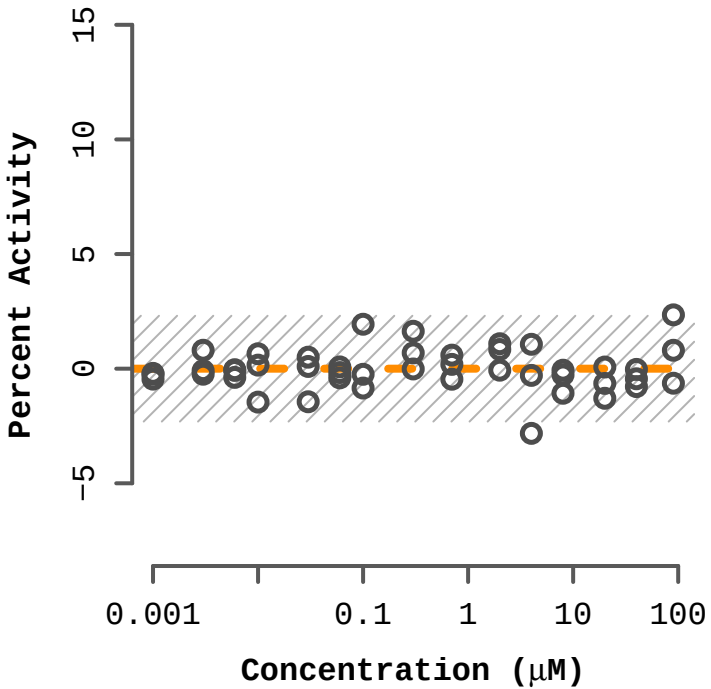
NAME: 2,2−Dimethylpropanoyl chloride
CHID: 27529 CASRN: 3282−30−2
SPID(S): Tox21_200646
M4ID: 12481606

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.644 MAX_MED: 0.655 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

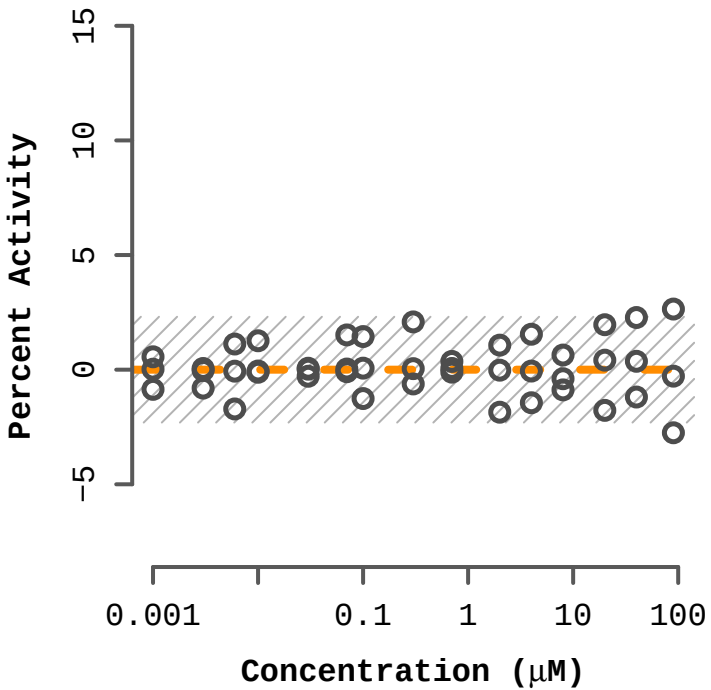
NAME: Trimethylolpropane trimethacrylate
CHID: 27530 **CASRN:** 3290-92-4
SPID(S): Tox21_303195
M4ID: 12475938

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.84 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

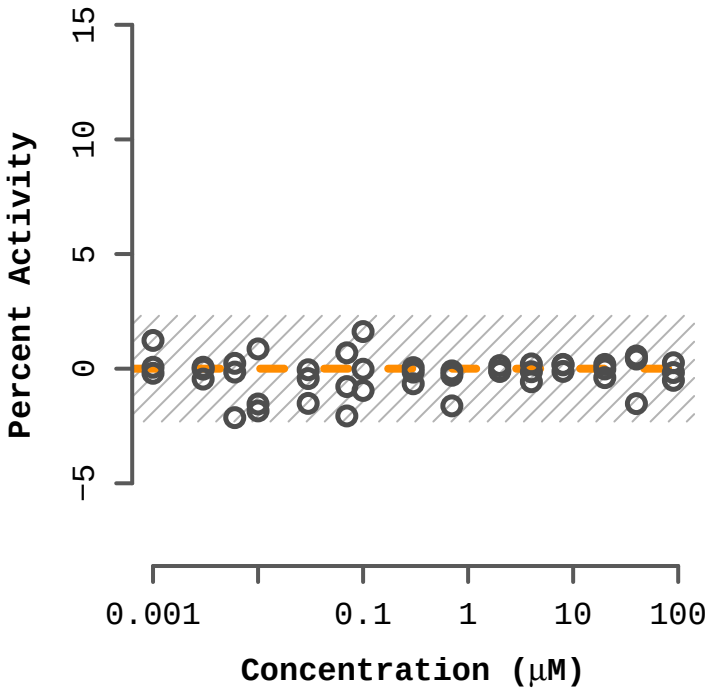
NAME: Trimethylolpropane trimethacrylate
CHID: 27530 **CASRN:** 3290-92-4
SPID(S): Tox21_201794
M4ID: 12480458

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.504 **MAX_MED:** 0.417 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

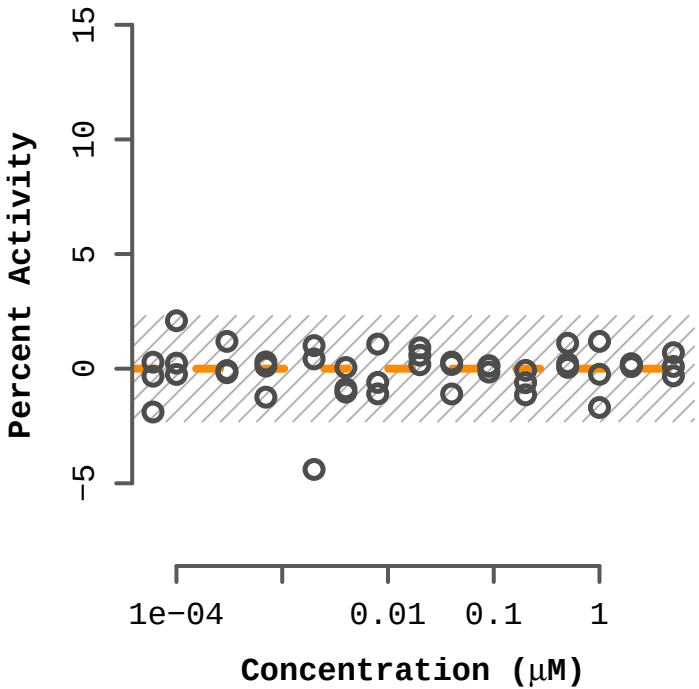
NAME: Dextrosil
CHID: 27534 CASRN: 3327-22-8
SPID(S): Tox21_202563
M4ID: 12479689

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.365 MAX_MED: 0.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

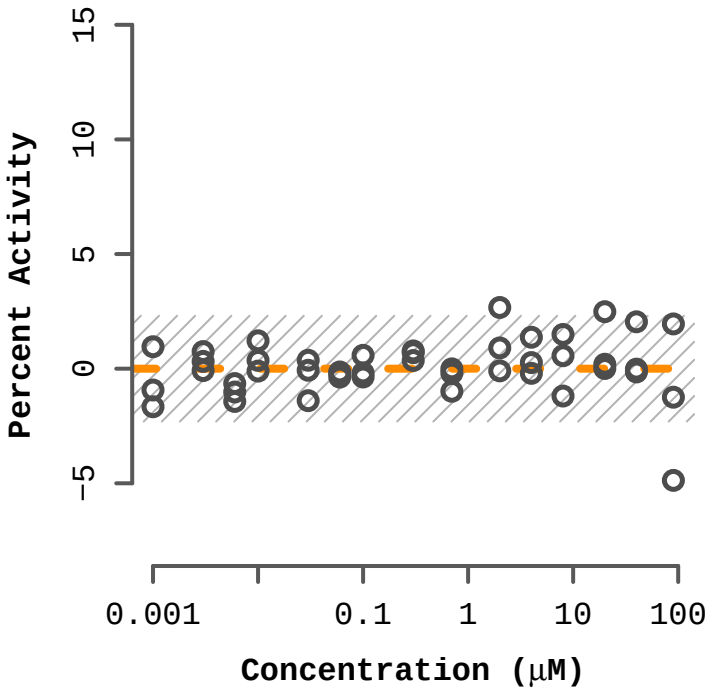
NAME: Octadecyl chloride
CHID: 27536 **CASRN:** 3386-33-2
SPID(S): Tox21_202998
M4ID: 12479254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.695 **MAX_MED:** 0.589 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

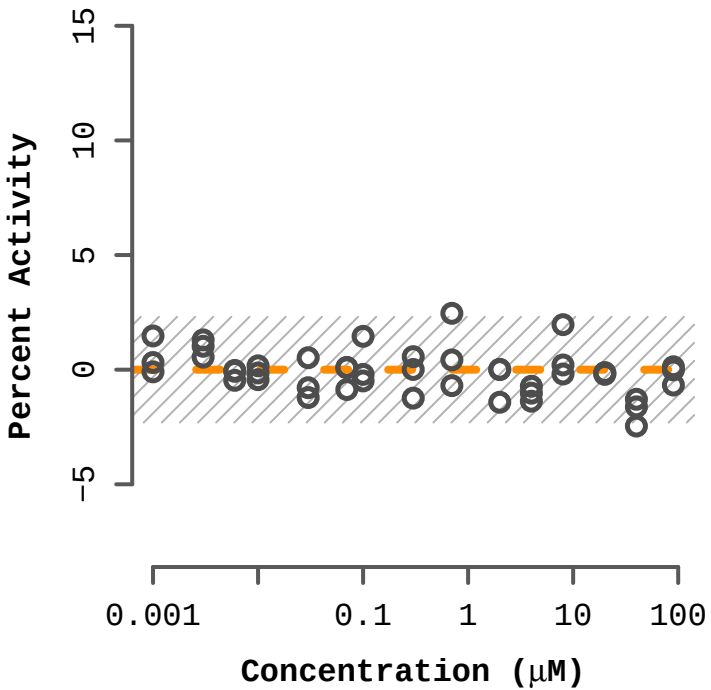
NAME: 1-Methyl-3-phenoxybenzene
CHID: 27537 **CASRN:** 3586-14-9
SPID(S): Tox21_200958
M4ID: 12481294

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

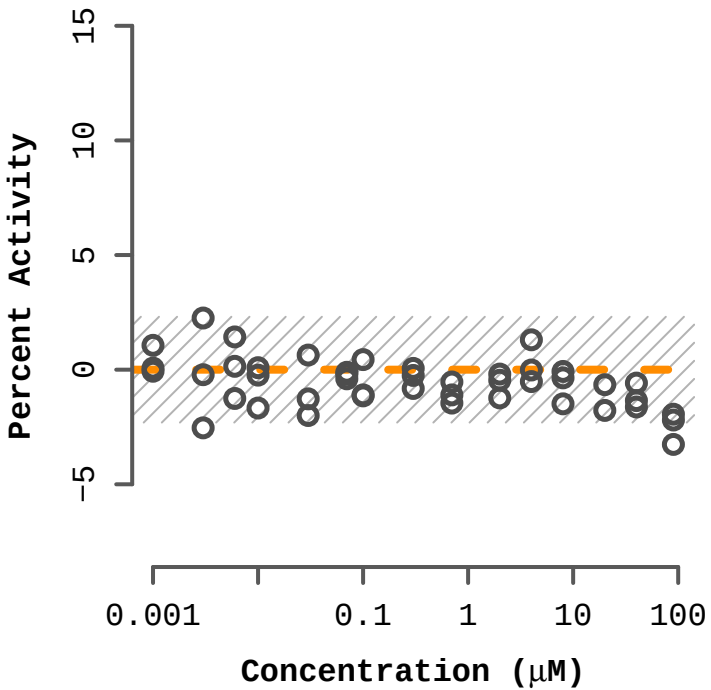
NAME: N-Butylbenzenesulfonamide
CHID: 27540 **CASRN:** 3622-84-2
SPID(S): Tox21_303184
M4ID: 12475949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

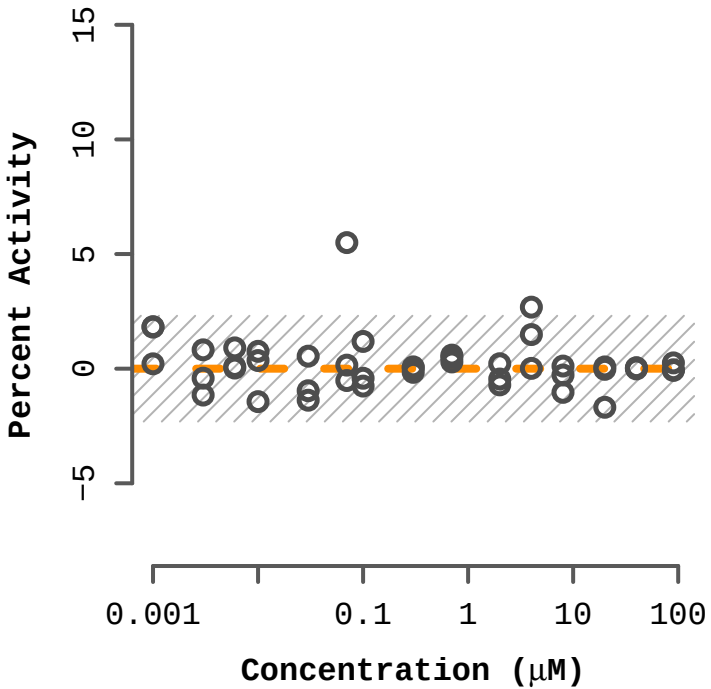
NAME: N-Butylbenzenesulfonamide
CHID: 27540 **CASRN:** 3622-84-2
SPID(S): Tox21_201692
M4ID: 12480560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.355 **MAX_MED:** 0.148 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

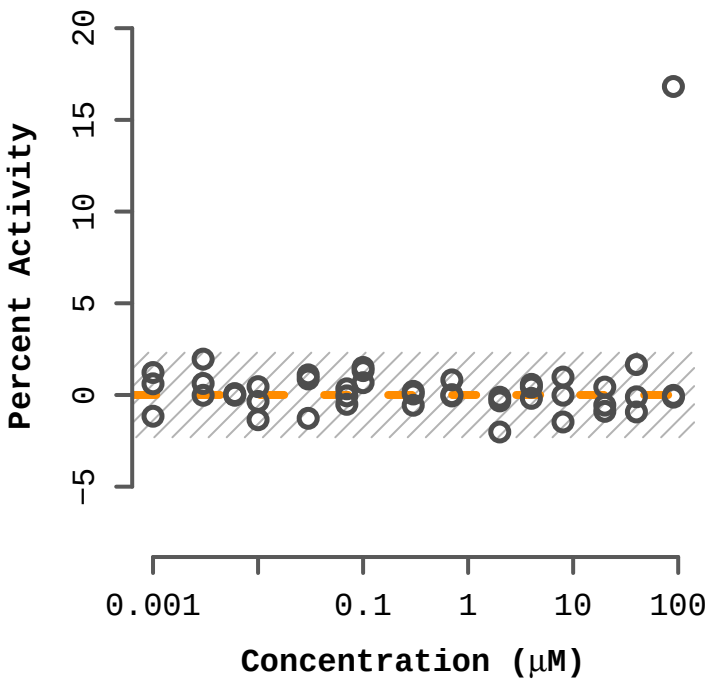
NAME: Disodium 4,4'−dinitro−2,2'−stilbenedisulfonate
CHID: 27542 CASRN: 3709−43−1
SPID(S): Tox21_303069
M4ID: 12476064

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.71 MAX_MED: 1.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

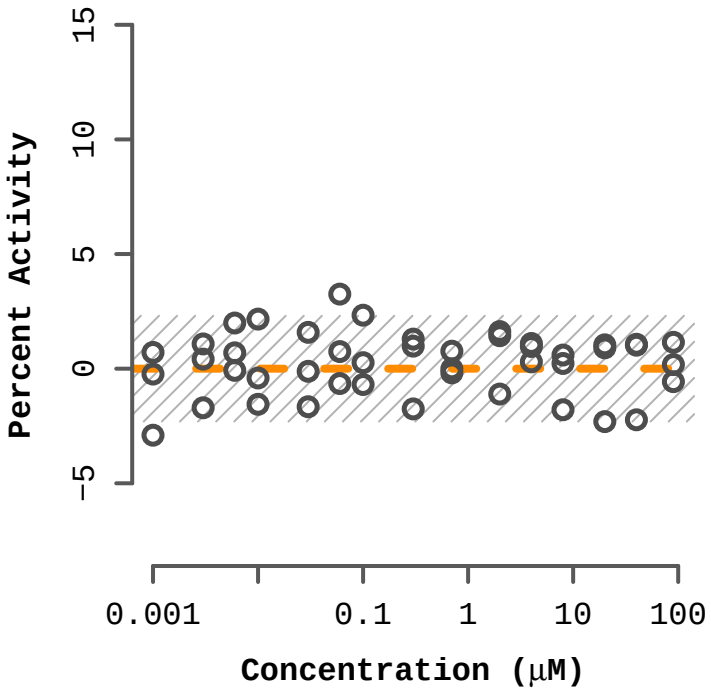
NAME: Disodium 4,4'−dinitro−2,2'−stilbenedisulfonate
CHID: 27542 CASRN: 3709−43−1
SPID(S): Tox21_201776
M4ID: 12480476

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 5.56 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

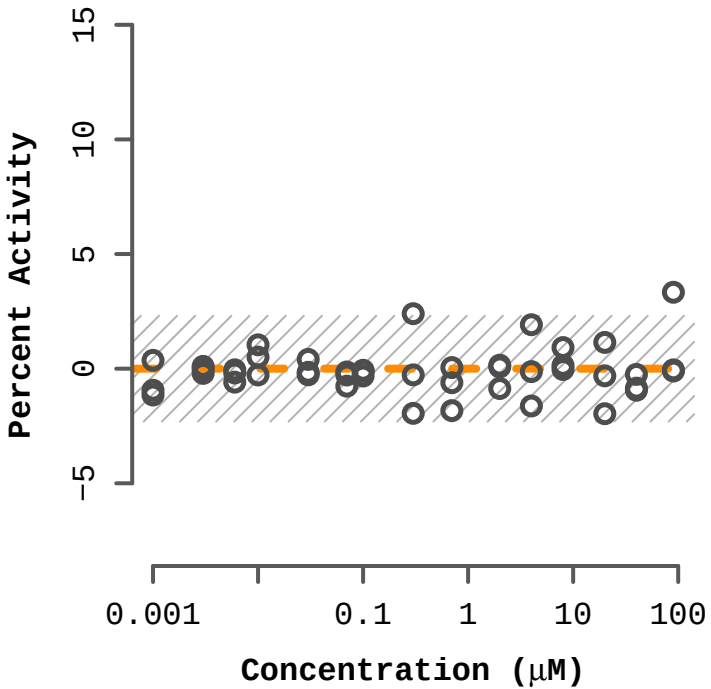
NAME: N,N−Diethylhydroxylamine
CHID: 27543 CASRN: 3710−84−7
SPID(S): Tox21_200264
M4ID: 12481988

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.12 MAX_MED: 1.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

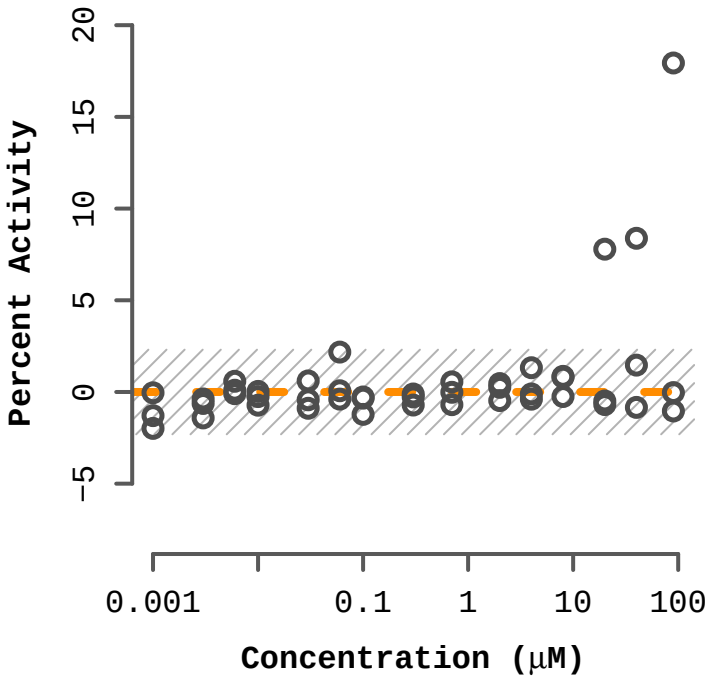
NAME: 2-Butenoic acid
CHID: 27544 **CASRN:** 3724-65-0
SPID(S): Tox21_303208
M4ID: 12475925

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.11	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.506 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

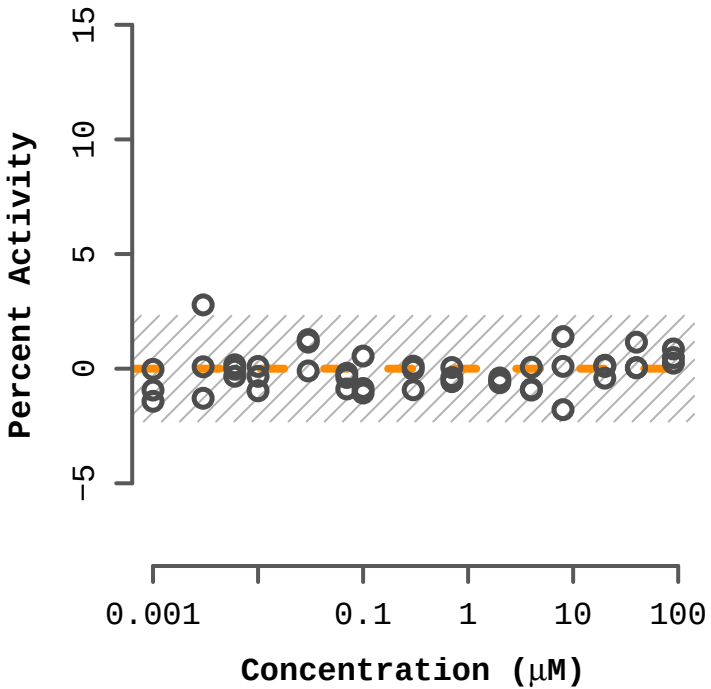
NAME: 2-Butenoic acid
CHID: 27544 CASRN: 3724-65-0
SPID(S): Tox21_201730
M4ID: 12480522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.55	NA	NA
PROB:	1	NA	NA
RMSE:	3.26	NA	NA

MAX_MEAN: 5.63 MAX_MED: 1.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

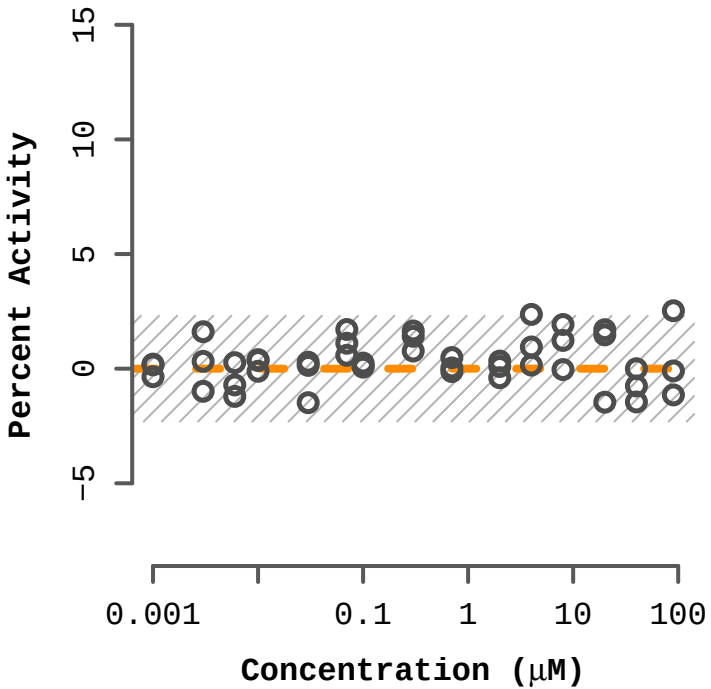
NAME: 1,3-Diisopropenylbenzene
CHID: 27546 **CASRN:** 3748-13-8
SPID(S): Tox21_200684
M4ID: 12481568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.778 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

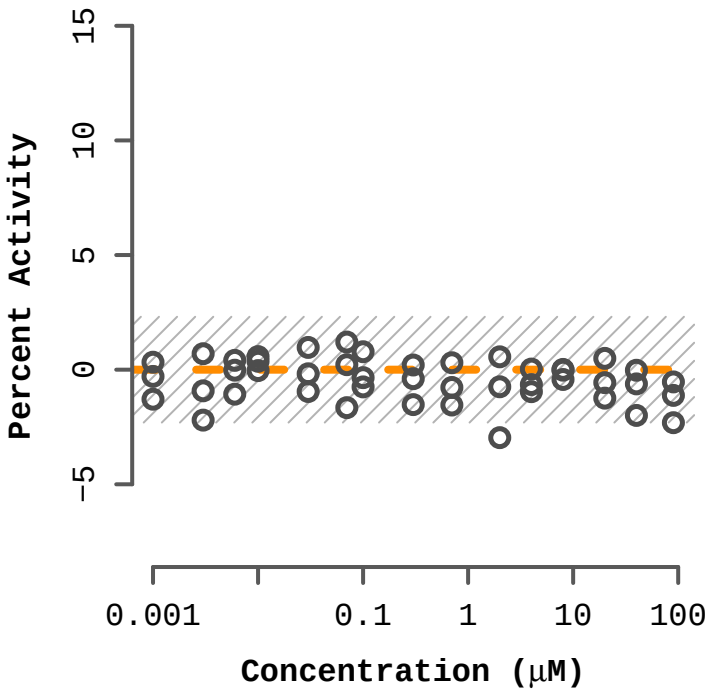
NAME: Sodium chloroacetate
CHID: 27550 CASRN: 3926-62-3
SPID(S): Tox21_303144
M4ID: 12475989

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

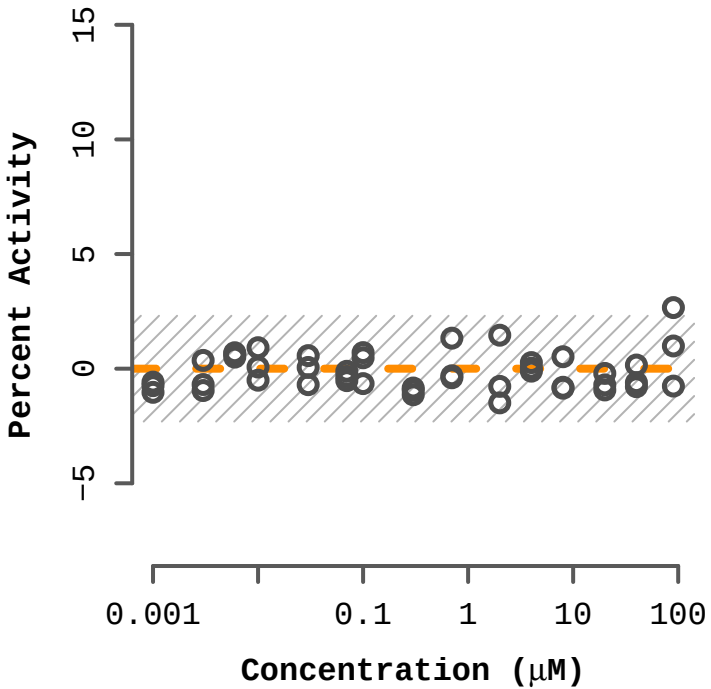
NAME: Sodium chloroacetate
CHID: 27550 **CASRN:** 3926-62-3
SPID(S): Tox21_202011
M4ID: 12480241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.301 **MAX_MED:** 0.368 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

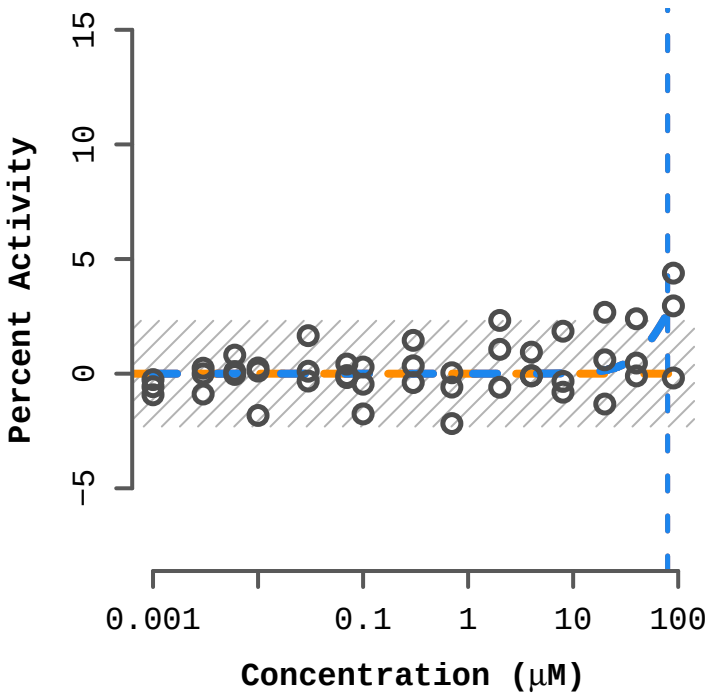
NAME: Sodium 3,5-bis(methoxycarbonyl)benzenesulfonat
CHID: 27551 CASRN: 3965-55-7
SPID(S): Tox21_200459
M4ID: 12481793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.966 MAX_MED: 0.991 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Calcium propionate
CHID: 27556 **CASRN:** 4075-81-4
SPID(S): Tox21_202432
M4ID: 12479820

HILL MODEL (in red):

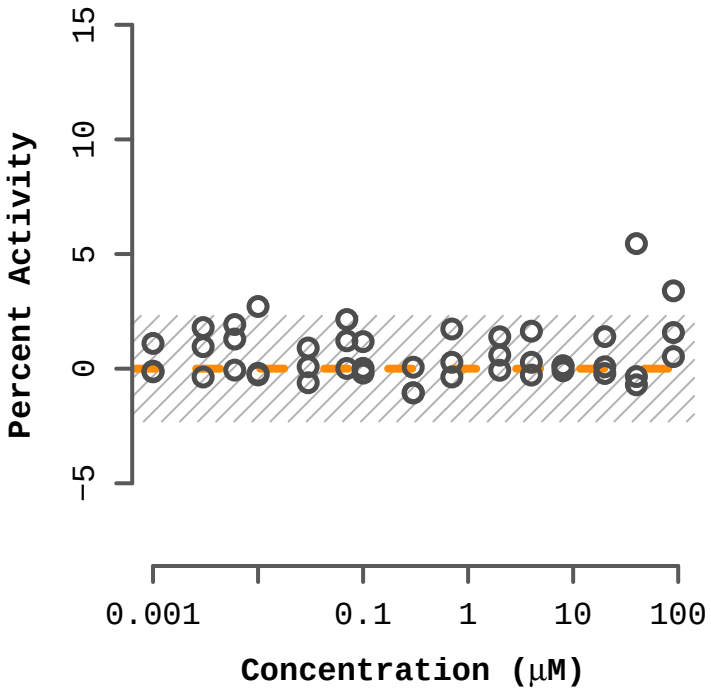
	tp	ga	gw
val:	5.26	1.9	2.56
sd:	10.6	0.745	3.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.26	1.9	2.56	2.69	14.3
sd:	10.6	0.744	3.51	25100	491000

	CNST	HILL	GNLS
AIC:	146.64	144.09	148.09
PROB:	0.2	0.71	0.1
RMSE:	1.29	1.12	1.12

MAX_MEAN: 2.39 **MAX_MED:** 2.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

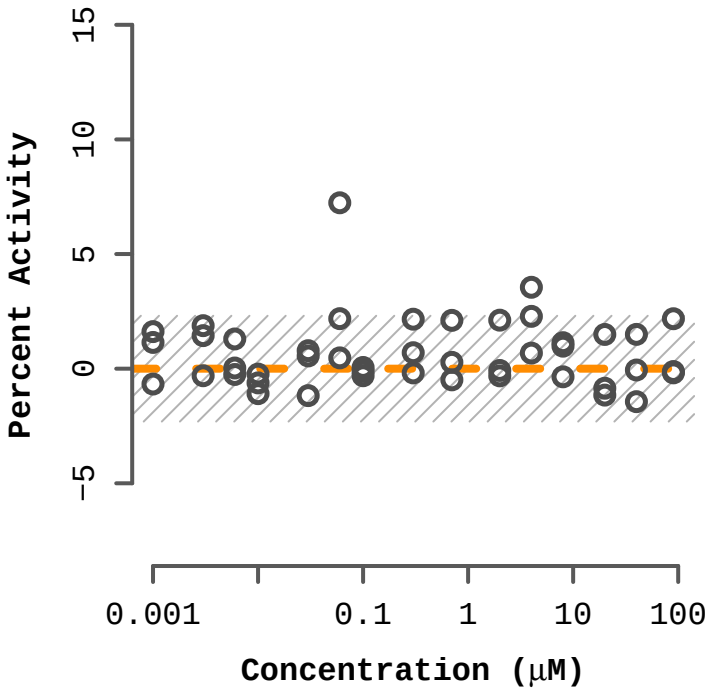
NAME: 4-Methylbenzenesulfonyl isocyanate
CHID: 27558 **CASRN:** 4083-64-1
SPID(S): Tox21_303136
M4ID: 12475997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

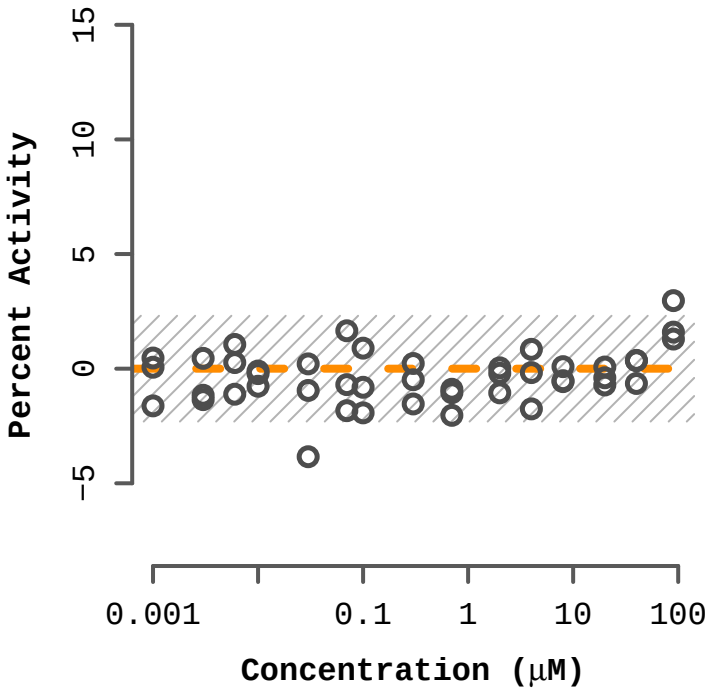
NAME: 4-Methylbenzenesulfonyl isocyanate
CHID: 27558 **CASRN:** 4083-64-1
SPID(S): Tox21_201698
M4ID: 12480554

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 3.3 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

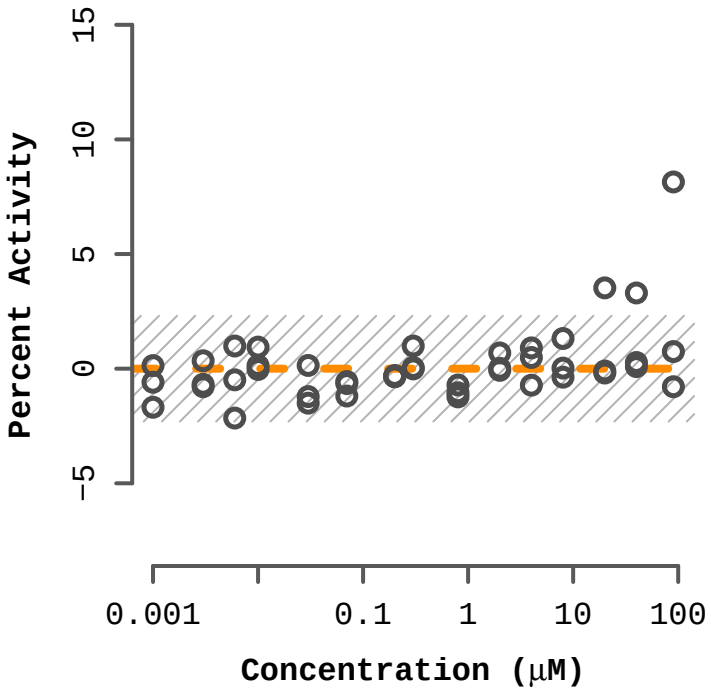
NAME: Dimethyl 3,3'−thiodipropionate
CHID: 27561 CASRN: 4131−74−2
SPID(S): Tox21_303275
M4ID: 12475858

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.95 MAX_MED: 1.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

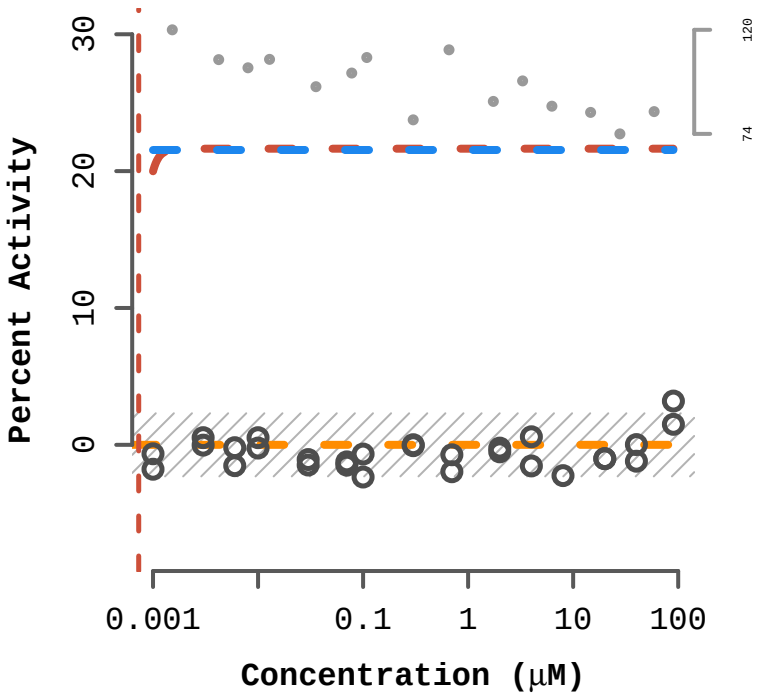
NAME: Methylsilanetriyl triacetate
CHID: 27565 **CASRN:** 4253-34-3
SPID(S): Tox21_200663
M4ID: 12481589

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 0.748 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Chloro-2,2-dimethylpropanoyl chloride
CHID: 27567 CASRN: 4300-97-4
SPID(S): Tox21_201227
M4ID: 12481025 BRK

HILL MODEL (in red):

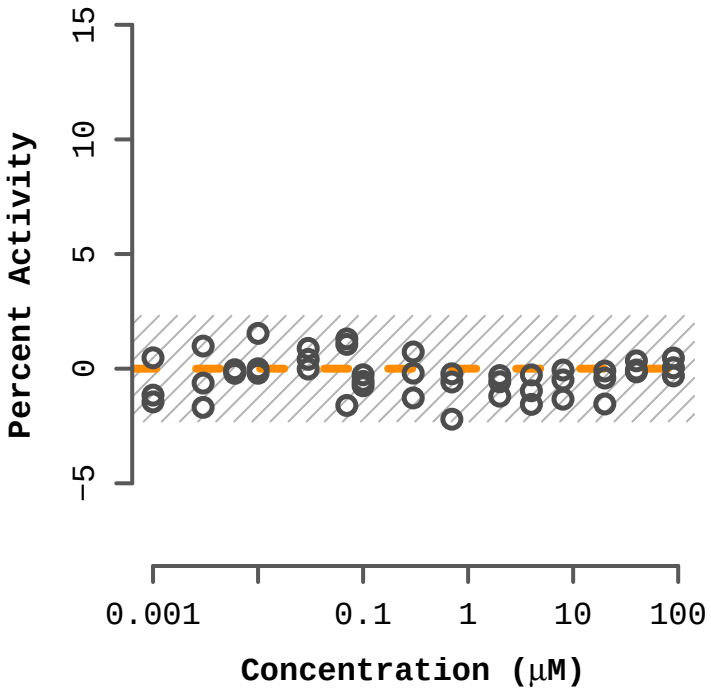
	tp	ga	gw
val:	21.6	-3.14	7.96
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.5	-4.94	7.8	2.81	16.6
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	503.1	476.77	480.77
PROB:	0	0.88	0.12
RMSE:	56.72	47.81	47.79

MAX_MEAN: 41.9 MAX_MED: 41.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

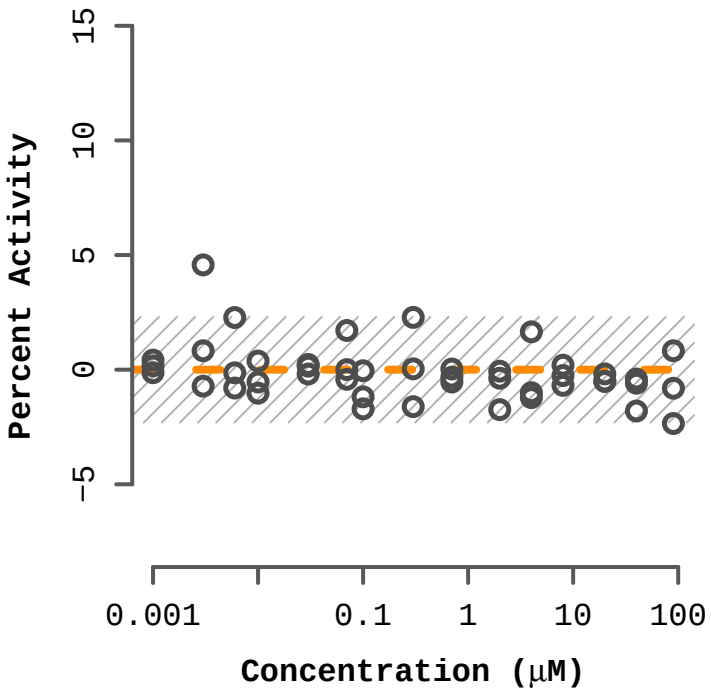
NAME: 2-Methoxy-3,4-dihydro-2H-pyran
CHID: 27570 **CASRN:** 4454-05-1
SPID(S): Tox21_200063
M4ID: 12482189

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.447 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

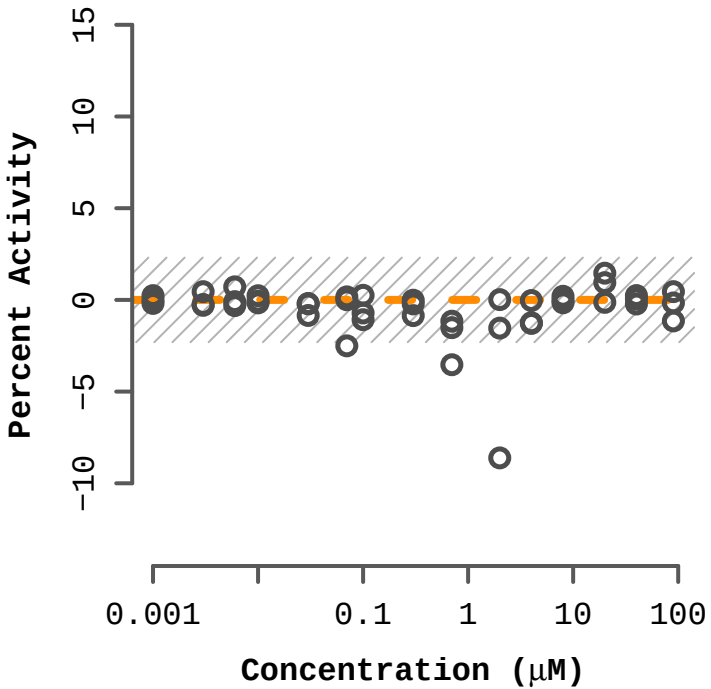
NAME: 3-Hydroxy-2-(hydroxymethyl)-2-methylpropanoic a
CHID: 27577 CASRN: 4767-03-7
SPID(S): Tox21_200460
M4ID: 12481792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.56 MAX_MED: 0.826 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

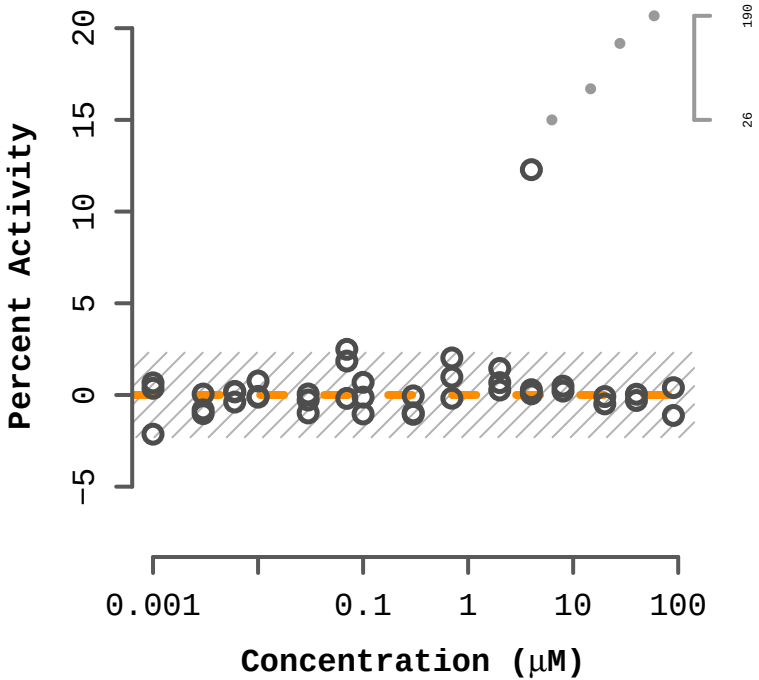
NAME: Pentaethylene glycol
CHID: 27579 **CASRN:** 4792-15-8
SPID(S): Tox21_303127
M4ID: 12476006

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 0.756 **MAX_MED:** 0.942 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

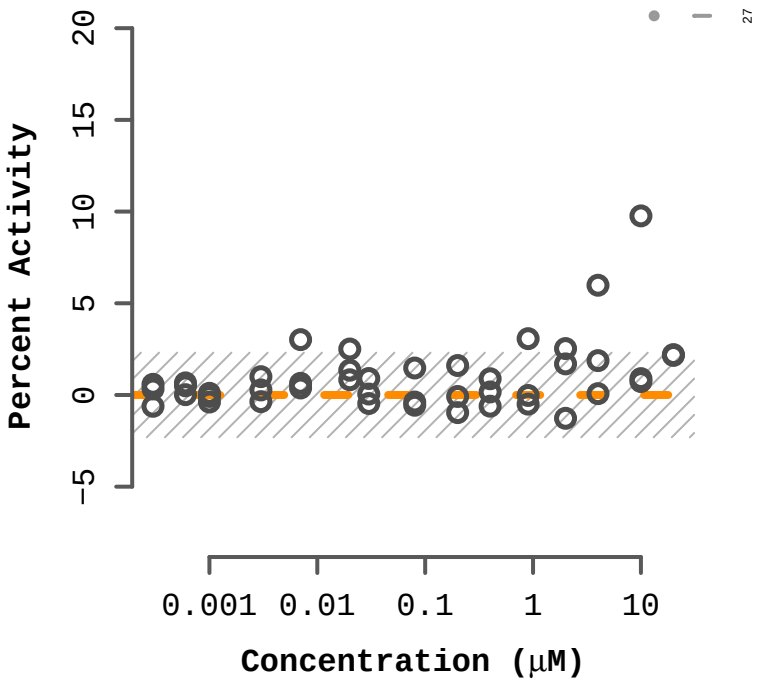
NAME: Pentaethylene glycol
CHID: 27579 **CASRN:** 4792-15-8
SPID(S): Tox21_201721
M4ID: 12480531 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	288.36	NA	NA
PROB:	1	NA	NA
RMSE:	37.38	NA	NA

MAX_MEAN: 62.5 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

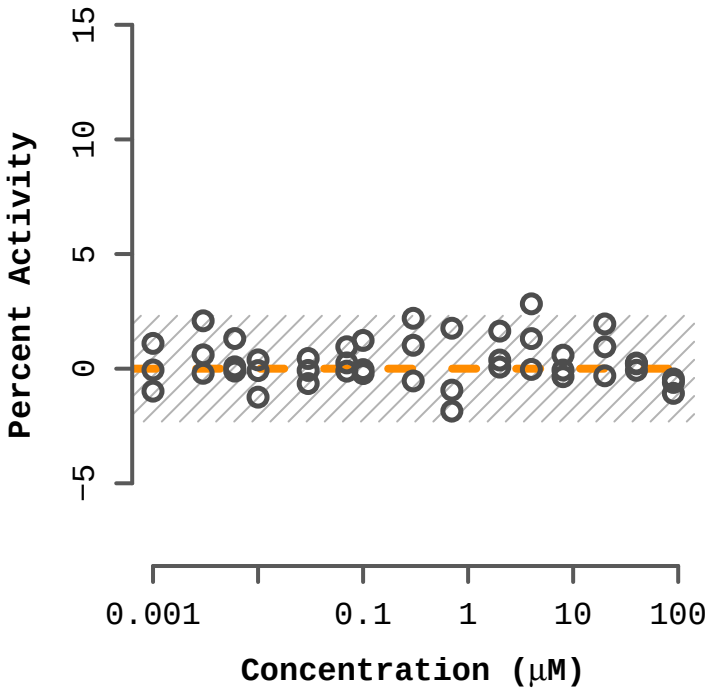
NAME: 1-Chlorohexadecane
CHID: 27580 **CASRN:** 4860-03-1
SPID(S): Tox21_202749
M4ID: 12479503 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.52	NA	NA
PROB:	1	NA	NA
RMSE:	4.6	NA	NA

MAX_MEAN: 10.6 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

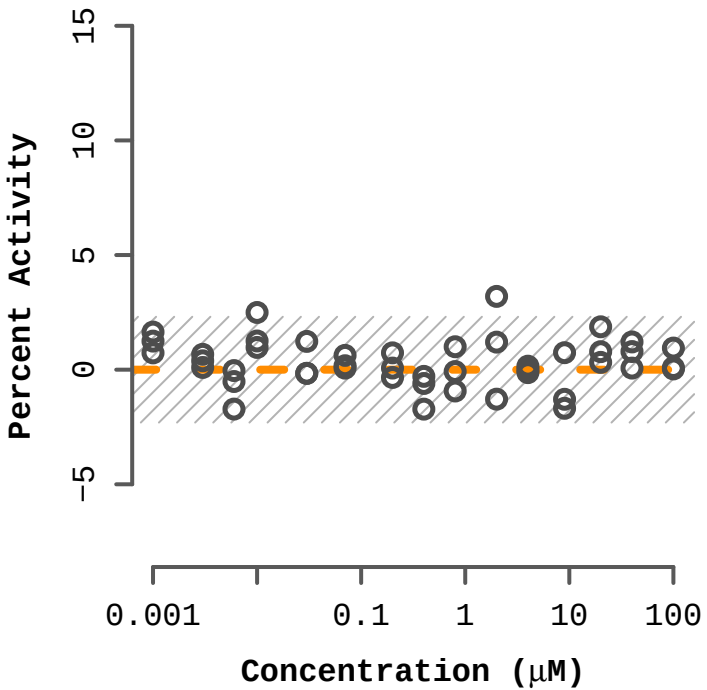
NAME: 1,5,9-Cyclododecatriene
CHID: 27581 CASRN: 4904-61-4
SPID(S): Tox21_300401
M4ID: 12478731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

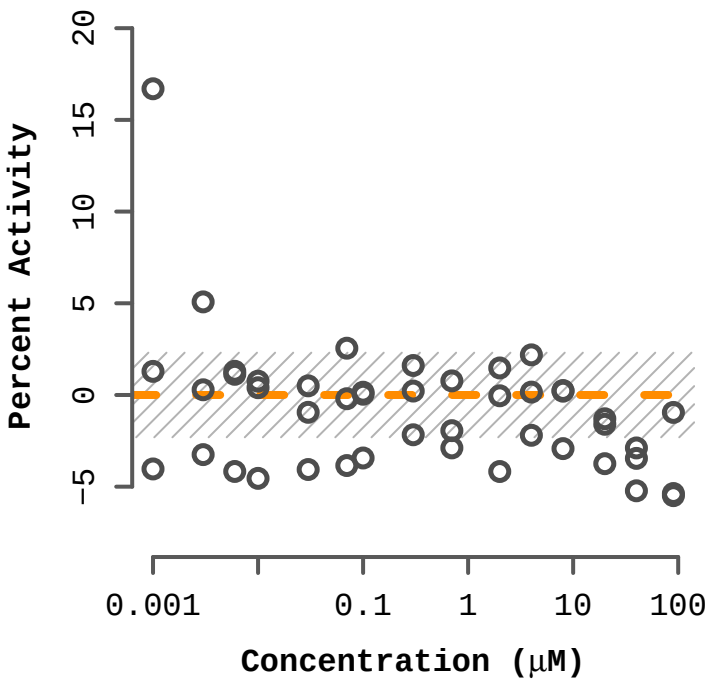
NAME: N,N−Dicyclohexyl−2−benzothiazolesulfenamide
CHID: 27584 **CASRN:** 4979−32−2
SPID(S): Tox21_301258
M4ID: 12477875

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

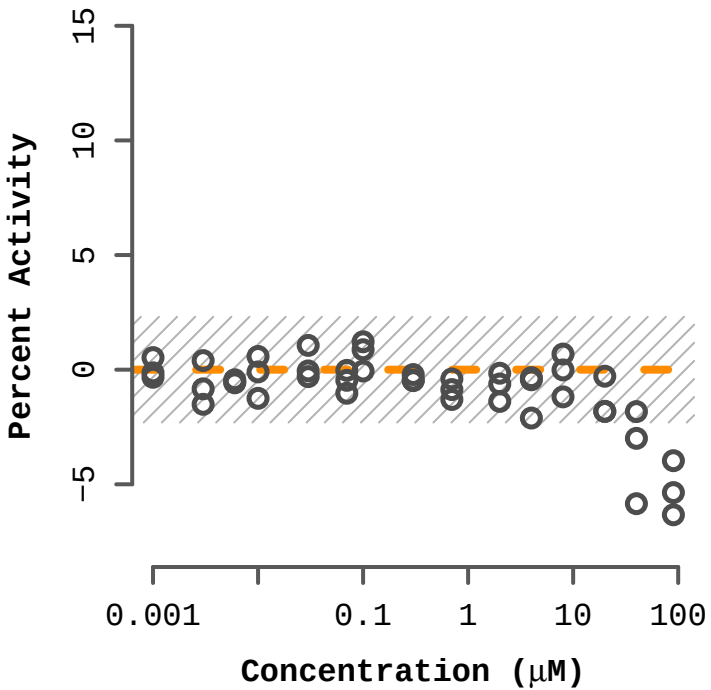
NAME: 4-(Diglycidylamino)phenyl glycidyl ether
CHID: 27585 CASRN: 5026-74-4
SPID(S): Tox21_302646
M4ID: 12476487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	235.94	NA	NA
PROB:	1	NA	NA
RMSE:	3.68	NA	NA

MAX_MEAN: 4.65 MAX_MED: 1.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

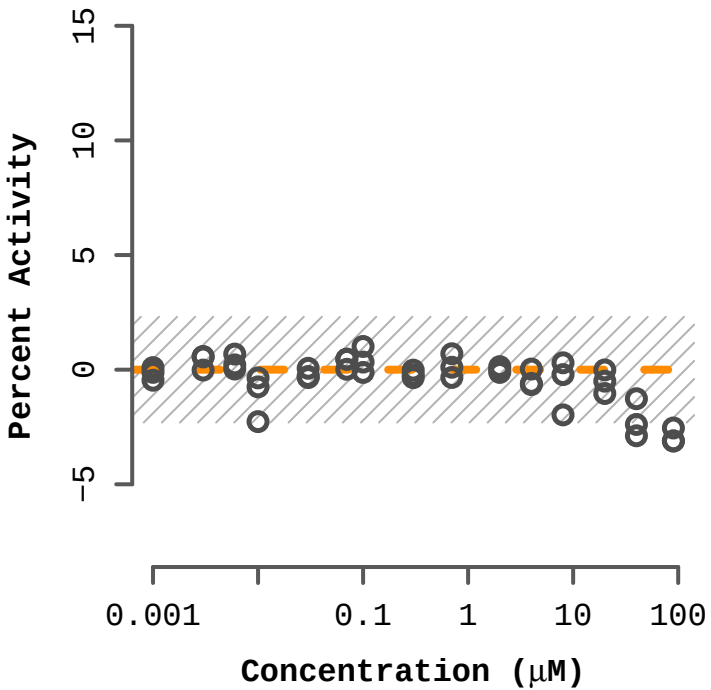
NAME: 4-(Diglycidylamino)phenyl glycidyl ether
CHID: 27585 CASRN: 5026-74-4
SPID(S): Tox21_201879
M4ID: 12480373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.677 MAX_MED: 0.871 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

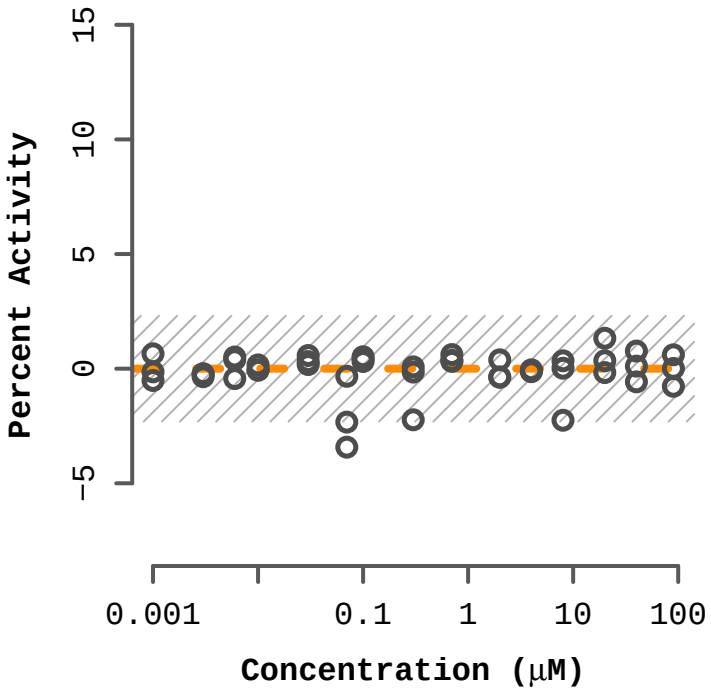
NAME: (2−(Methacryloyloxy)ethyl)trimethylammonium ch
CHID: 27586 **CASRN:** 5039−78−1
SPID(S): Tox21_202564
M4ID: 12479688

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.409 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

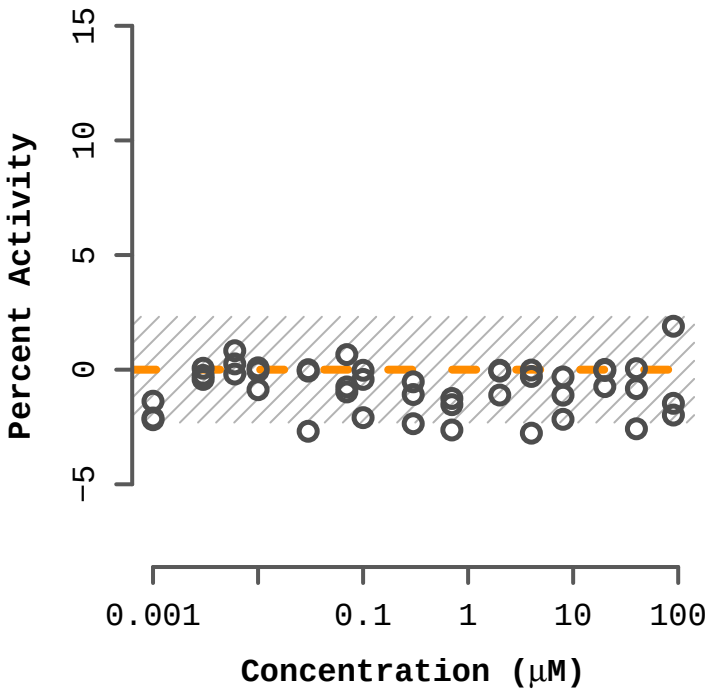
NAME: 1,1−Methylenebis(4−isocyanatocyclohexane)
CHID: 27588 **CASRN:** 5124−30−1
SPID(S): Tox21_301473
M4ID: 12477660

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.502 **MAX_MED:** 0.428 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

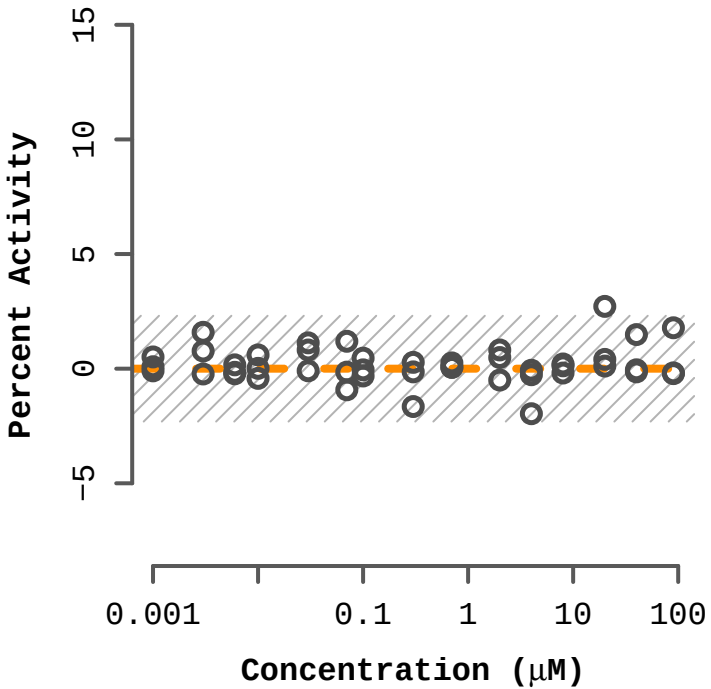
NAME: 1-Butoxy-2-propanol
CHID: 27589 CASRN: 5131-66-8
SPID(S): Tox21_200680
M4ID: 12481572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.298 MAX_MED: 0.254 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

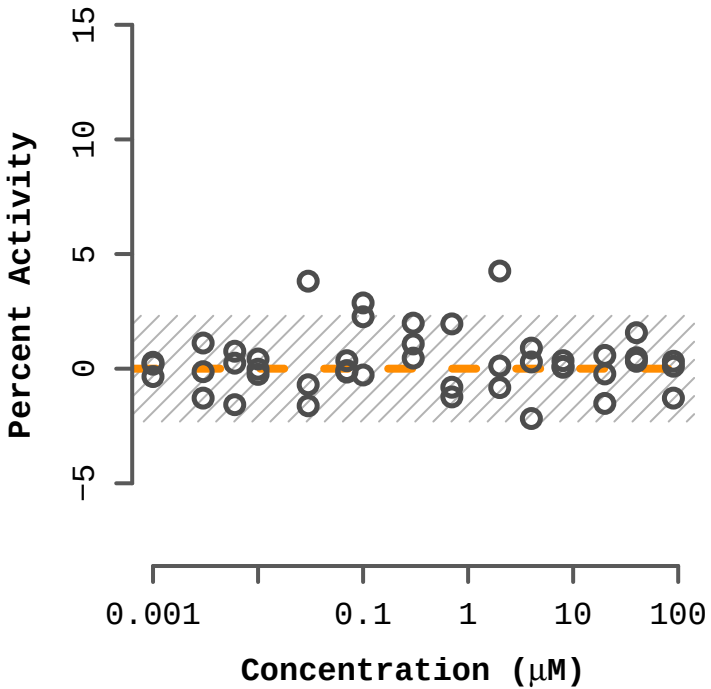
NAME: 2-Acrylamido-2-methylpropanesulphonate sodium s
CHID: 27591 **CASRN:** 5165-97-9
SPID(S): Tox21_202565
M4ID: 12479687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

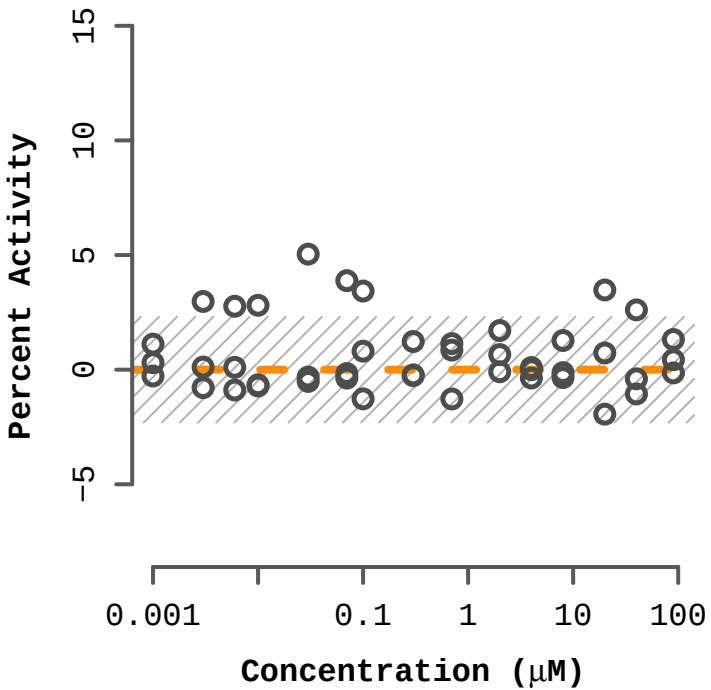
NAME: 4-Chlorobenzotrichloride
CHID: 27593 **CASRN:** 5216-25-1
SPID(S): Tox21_300560
M4ID: 12478573

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

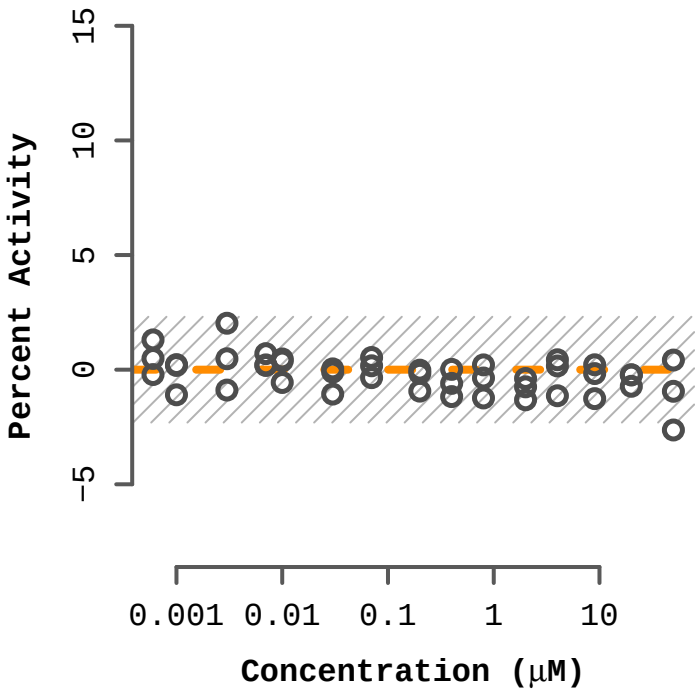
NAME: 4-Chlorobenzotrichloride
CHID: 27593 **CASRN:** 5216-25-1
SPID(S): Tox21_201845
M4ID: 12480407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

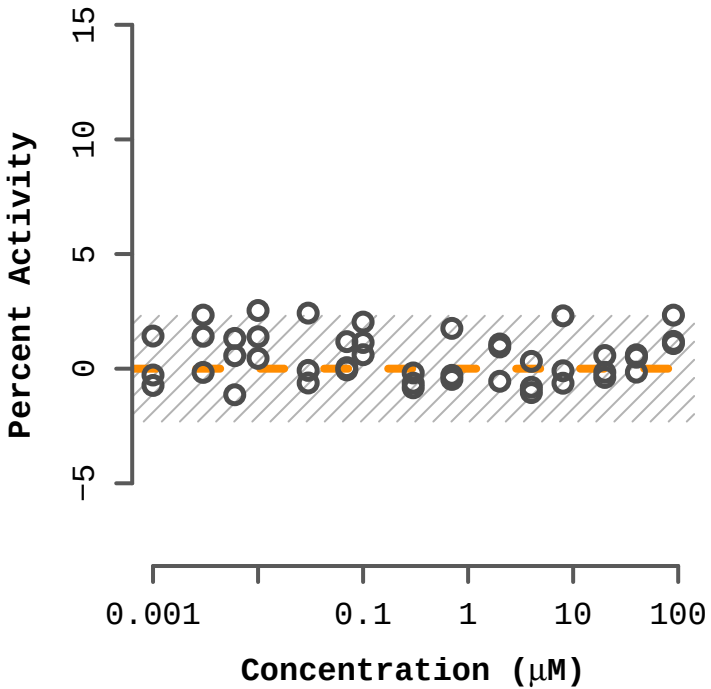
NAME: D&C Red No. 7
CHID: 27594 **CASRN:** 5281-04-9
SPID(S): Tox21_202750
M4ID: 12479502

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.539 **MAX_MED:** 0.491 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

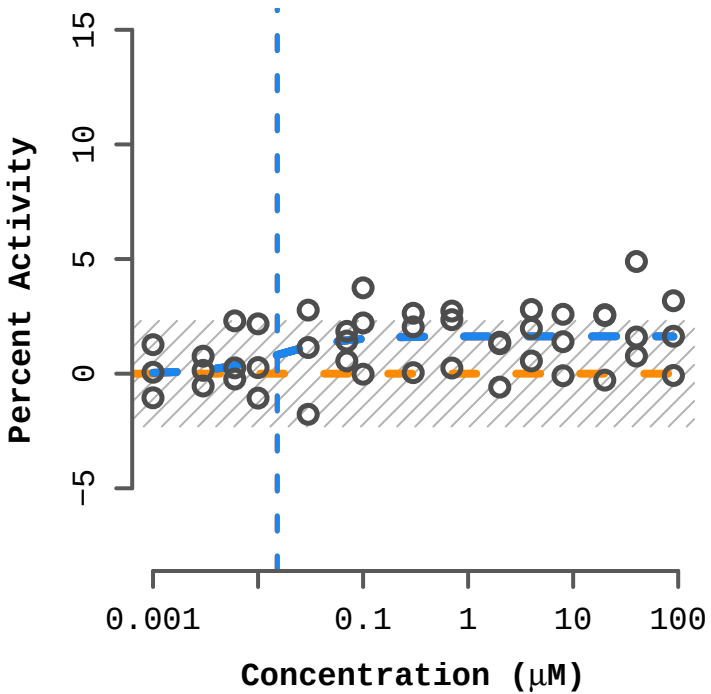
NAME: Sodium 1-octanesulfonate
CHID: 27595 **CASRN:** 5324-84-5
SPID(S): Tox21_201067
M4ID: 12481185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methoxypropylamine
CHID: 27596 CASRN: 5332-73-0
SPID(S): Tox21_303065
M4ID: 12476068

HILL MODEL (in red):

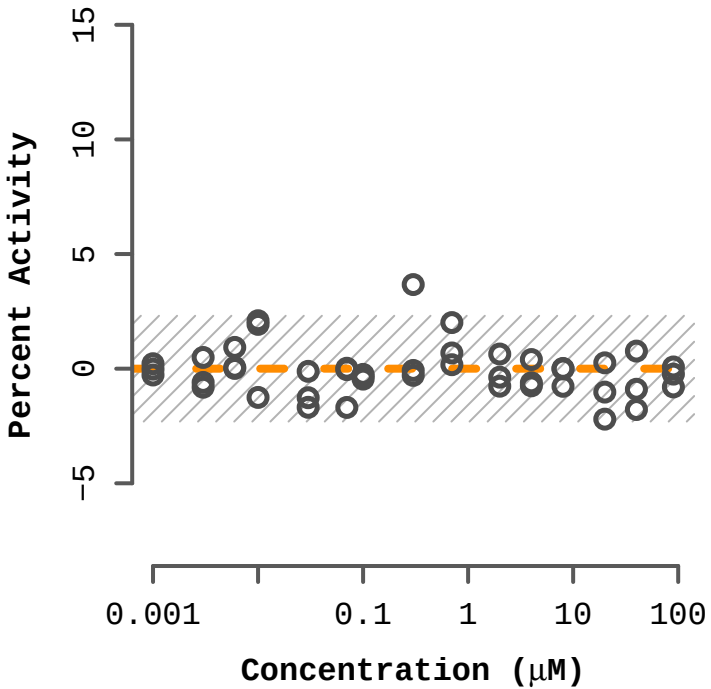
	tp	ga	gw
val:	1.63	-1.82	1.38
sd:	0.269	0.441	1.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.63	-1.82	1.38	2.17	8.95
sd:	0.285	0.444	1.26	19.4	782

	CNST	HILL	GNLS
AIC:	188.36	161.32	165.32
PROB:	0	0.88	0.12
RMSE:	1.85	1.28	1.28

MAX_MEAN: 2.42 MAX_MED: 2.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

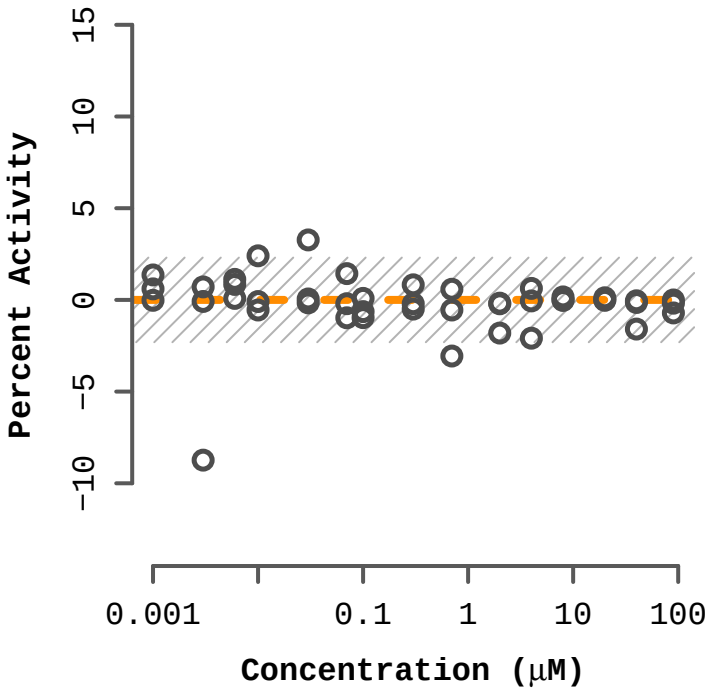
NAME: 3-Methoxypropylamine
CHID: 27596 **CASRN:** 5332-73-0
SPID(S): Tox21_201250
M4ID: 12481002

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

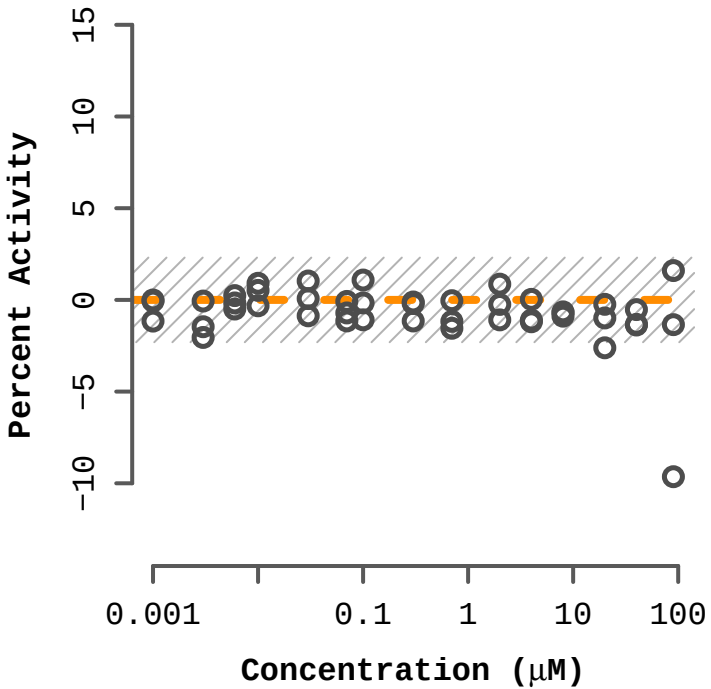
NAME: Triisopropyl orthoborate
CHID: 27598 **CASRN:** 5419-55-6
SPID(S): Tox21_303129
M4ID: 12476004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.845 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

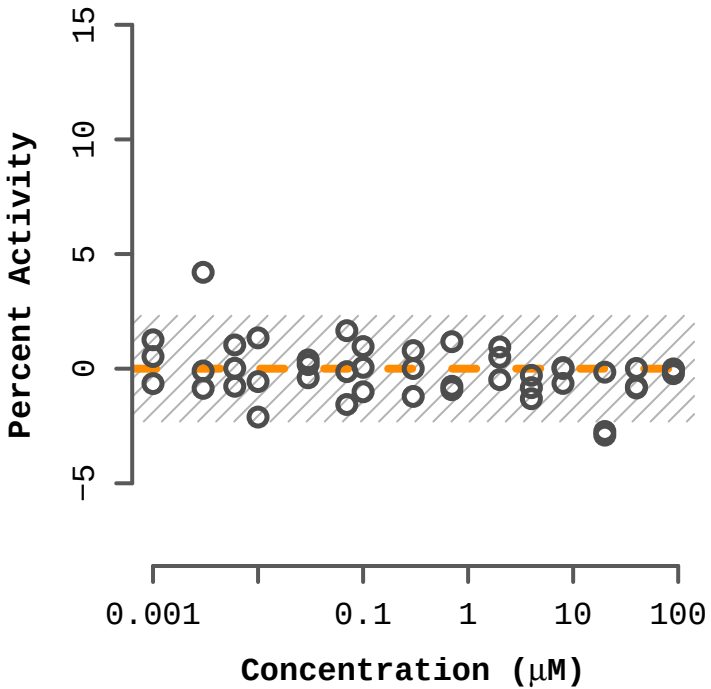
NAME: Triisopropyl orthoborate
CHID: 27598 **CASRN:** 5419-55-6
SPID(S): Tox21_201514
M4ID: 12480738

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 0.37 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

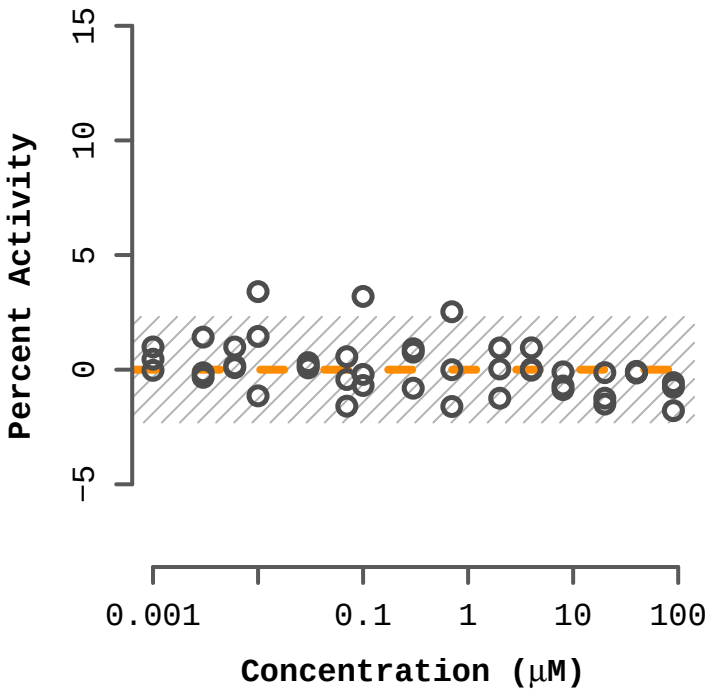
NAME: Ammonium thioglycolate
CHID: 27599 **CASRN:** 5421-46-5
SPID(S): Tox21_202751
M4ID: 12479501

HILL MODEL: Not applicable.

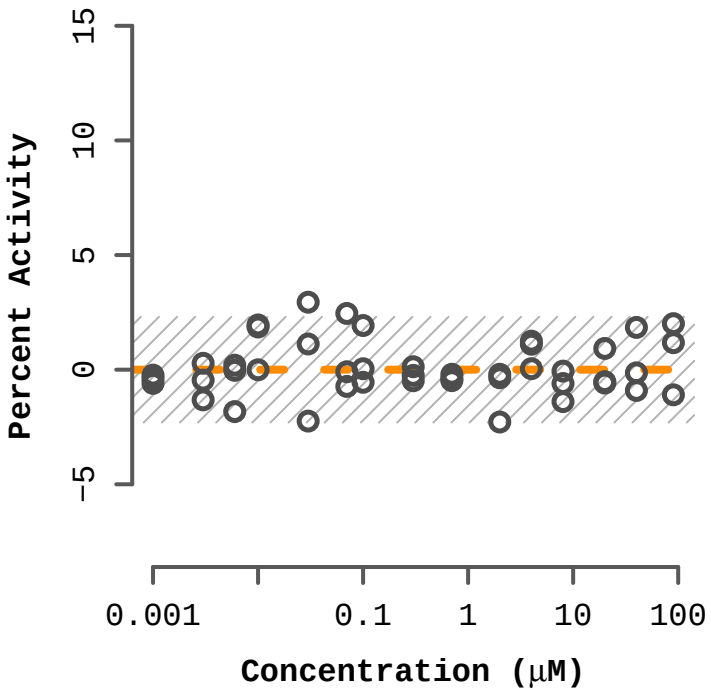
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.532 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Amino-5-hydroxy-2,7-naphthalenedisulfonic ac
CHID:    27600   CASRN: 5460-09-3
SPID(S): Tox21_202566
M4ID:    12479686

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

      CNST        HILL        GNLS
AIC:  136.45      NA          NA
PROB: 1           NA          NA
RMSE: 1.12        NA          NA

MAX_MEAN: 1.24      MAX_MED: 1.45      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

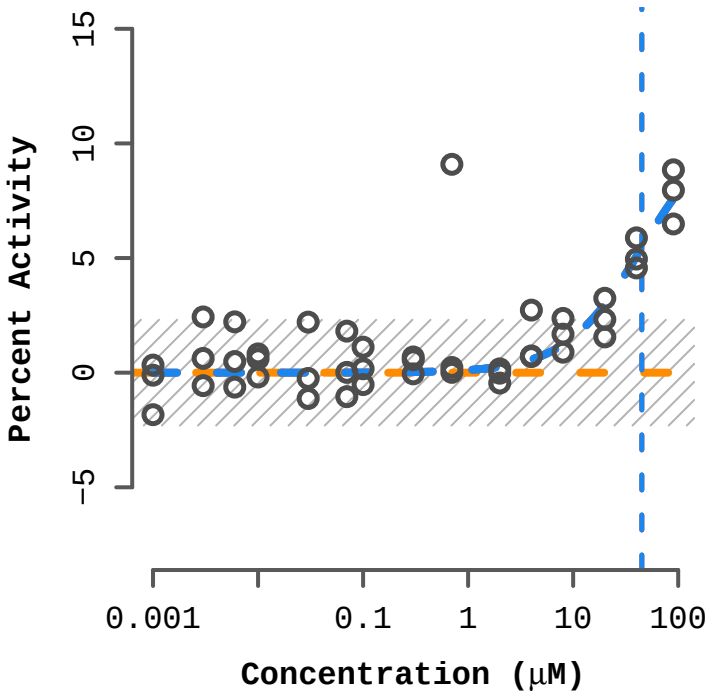
NAME: (Ethylenedinitrilo)tetraacetonitrile
CHID: 27603 **CASRN:** 5766-67-6
SPID(S): Tox21_301865
M4ID: 12477268

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-[4-(Diethylamino)-2-hydroxybenzoyl]benzoic a
CHID: 27604 CASRN: 5809-23-4
SPID(S): Tox21_303154
M4ID: 12475979

HILL MODEL (in red):

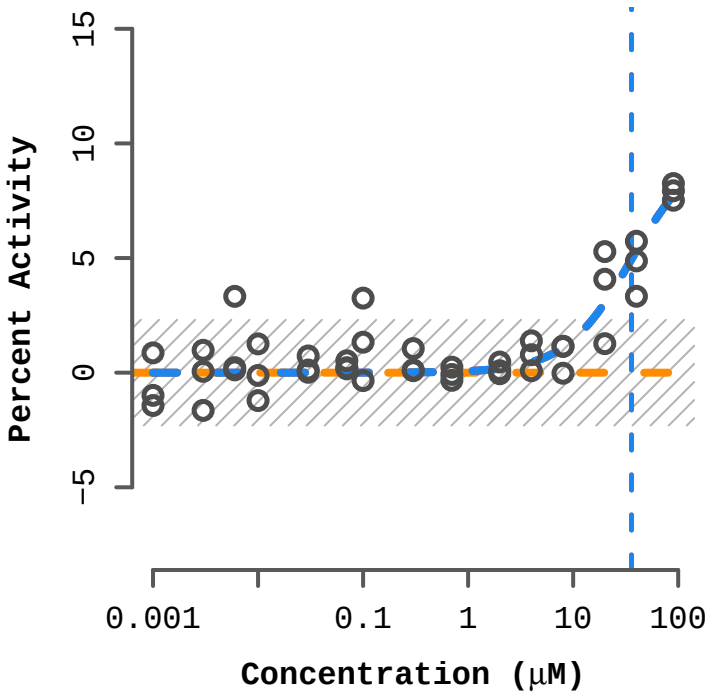
	tp	ga	gw
val:	10.9	1.65	1.2
sd:	2.78	0.204	0.281

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.9	1.65	1.2	3.57	4.72
sd:	2.78	0.204	0.281	751	2200

	CNST	HILL	GNLS
AIC:	217.18	150.13	154.13
PROB:	0	0.88	0.12
RMSE:	3.03	1.66	1.66

MAX_MEAN: 7.77 MAX_MED: 7.96 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-[4-(Diethylamino)-2-hydroxybenzoyl]benzoic a
CHID: 27604 CASRN: 5809-23-4
SPID(S): Tox21_201935
M4ID: 12480317

HILL MODEL (in red):

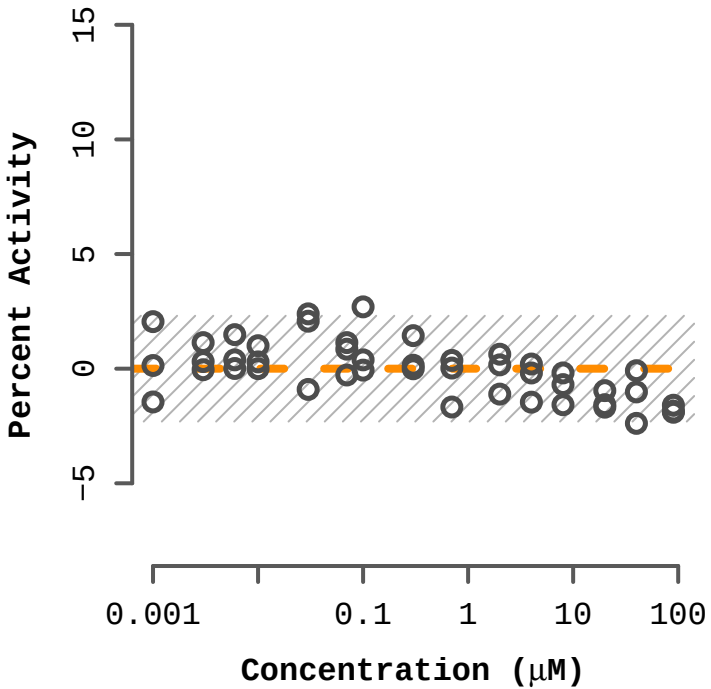
	tp	ga	gw
val:	9.9	1.56	1.38
sd:	1.88	0.167	0.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.9	1.56	1.38	3.4	6.28
sd:	1.89	0.167	0.31	2790	12100

	CNST	HILL	GNLS
AIC:	207.3	136.46	140.46
PROB:	0	0.88	0.12
RMSE:	2.76	1.08	1.08

MAX_MEAN: 7.9 MAX_MED: 7.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

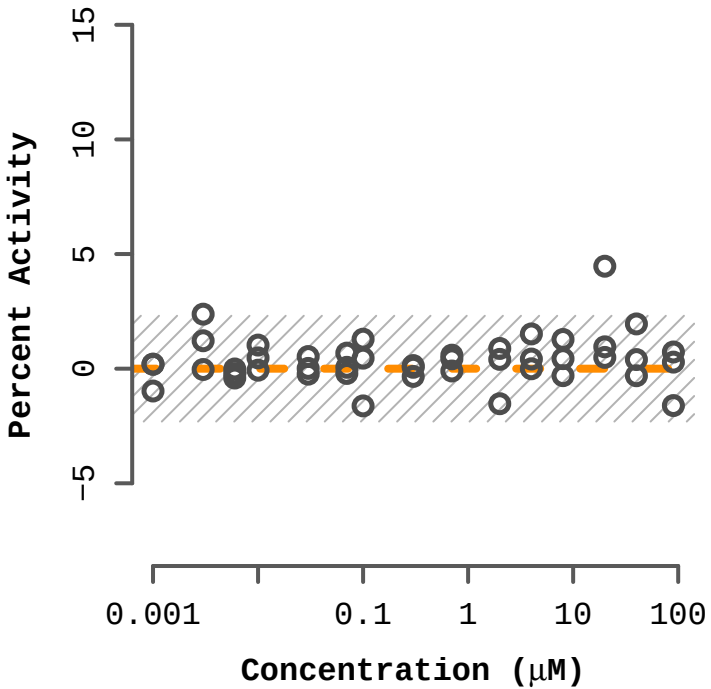
NAME: Terbuthylazine
CHID: 27608 CASRN: 5915-41-3
SPID(S): Tox21_300590
M4ID: 12478543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

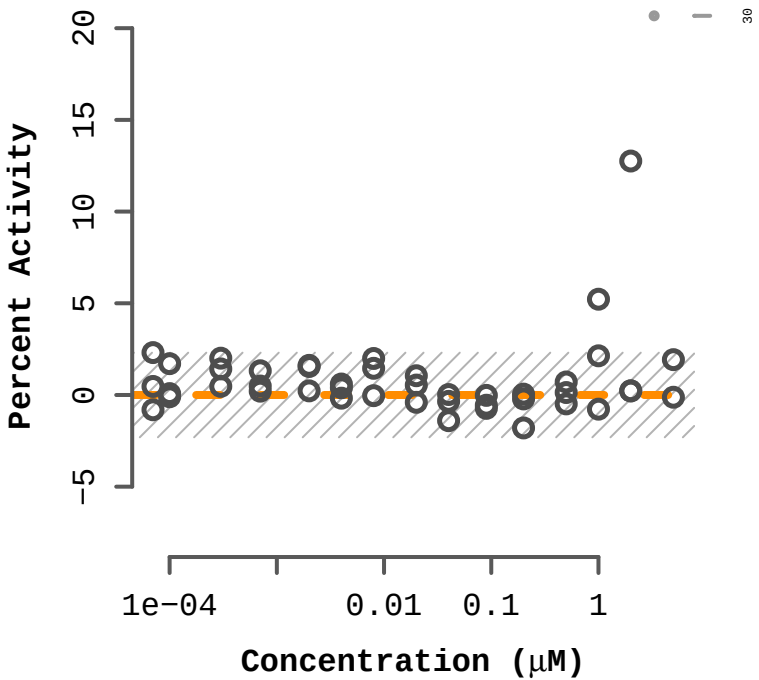
NAME: Tris(2-chloropropyl) phosphate
CHID: 27615 **CASRN:** 6145-73-9
SPID(S): Tox21_302421
M4ID: 12476712

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

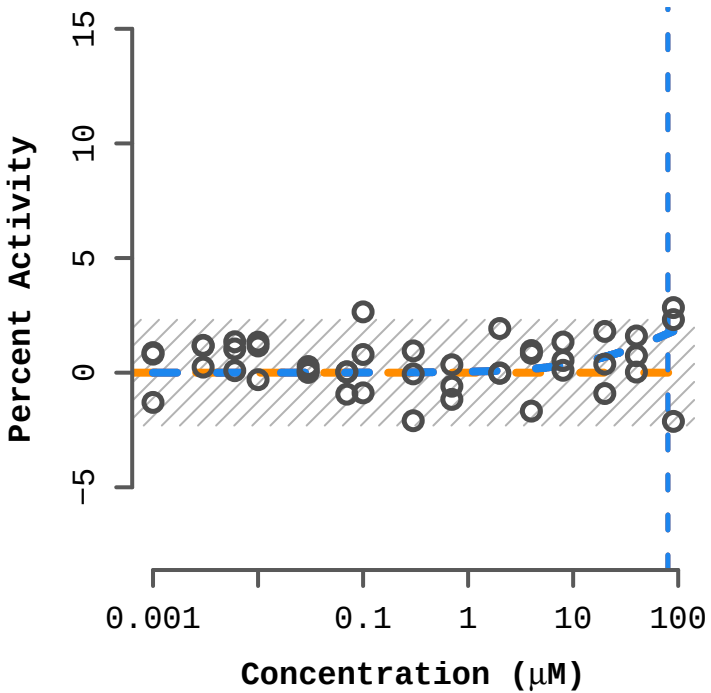
NAME: Dimethyl succinylsuccinate
CHID: 27617 **CASRN:** 6289-46-9
SPID(S): Tox21_202752
M4ID: 12479500 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.05	NA	NA
PROB:	1	NA	NA
RMSE:	5.07	NA	NA

MAX_MEAN: 10.7 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(3-Amino-4-methoxyphenyl)acetamide
CHID: 27620 CASRN: 6375-47-9
SPID(S): Tox21_303427
M4ID: 12475712

HILL MODEL (in red):

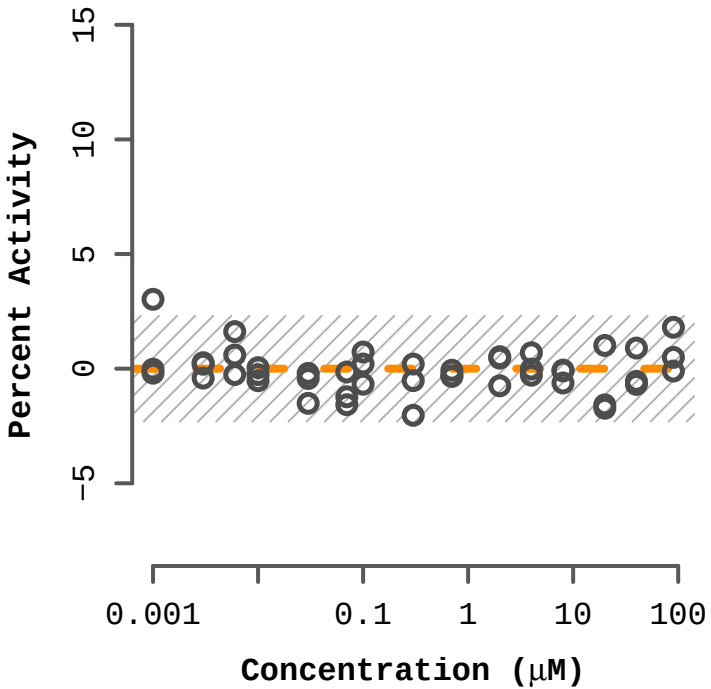
	tp	ga	gw
val:	3.41	1.9	0.992
sd:	3.74	0.819	0.946

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.41	1.9	0.992	3.55	7.63
sd:	3.74	0.819	0.946	131000	605000

	CNST	HILL	GNLS
AIC:	148.54	147.13	151.13
PROB:	0.3	0.61	0.08
RMSE:	1.19	1.16	1.16

MAX_MEAN: 1.01 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

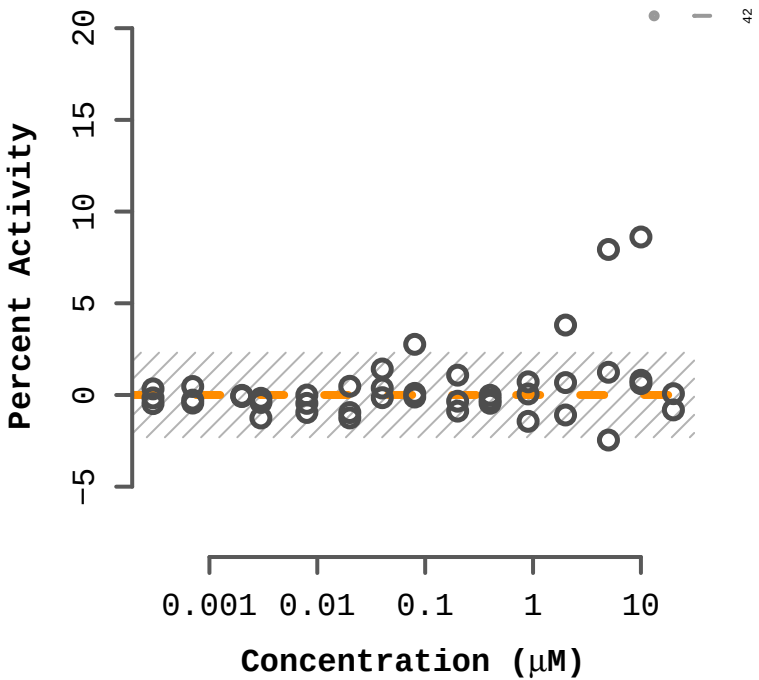
NAME: N-(3-Amino-4-methoxyphenyl)acetamide
CHID: 27620 CASRN: 6375-47-9
SPID(S): Tox21_201396
M4ID: 12480856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.937 MAX_MED: 0.599 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

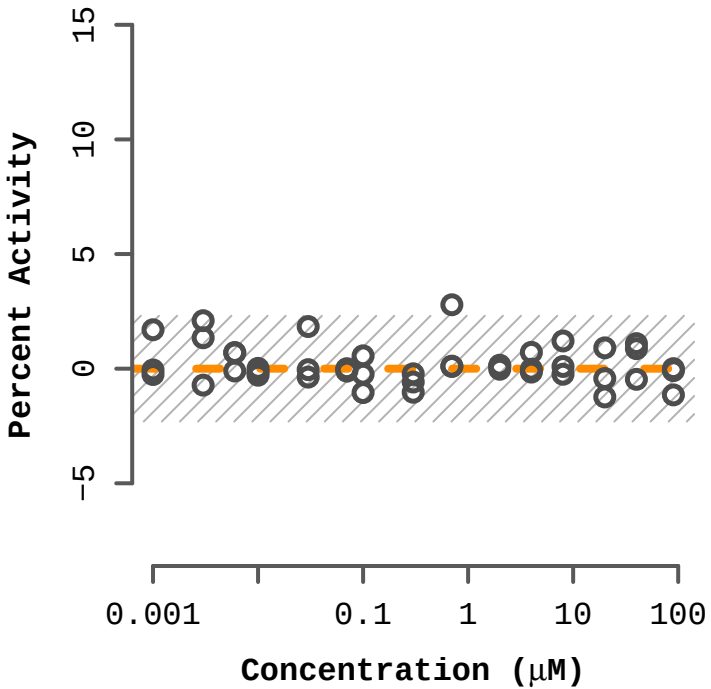
NAME: Aminotrimethylene phosphonic acid
CHID: 27624 **CASRN:** 6419-19-8
SPID(S): Tox21_202753
M4ID: 12479499 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.43	NA	NA
PROB:	1	NA	NA
RMSE:	6.62	NA	NA

MAX_MEAN: 13.9 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

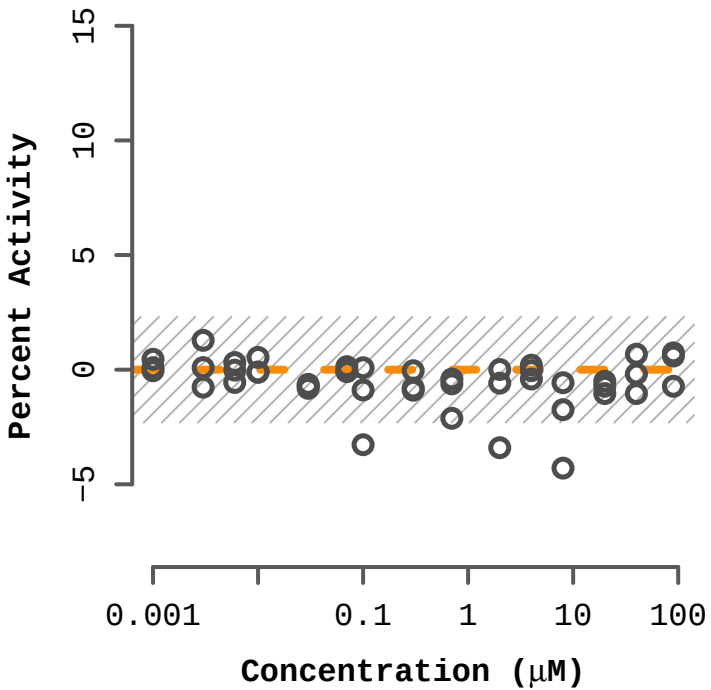
NAME: Bis(2-ethylhexyl) terephthalate
CHID: 27625 **CASRN:** 6422-86-2
SPID(S): Tox21_300322
M4ID: 12478809

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

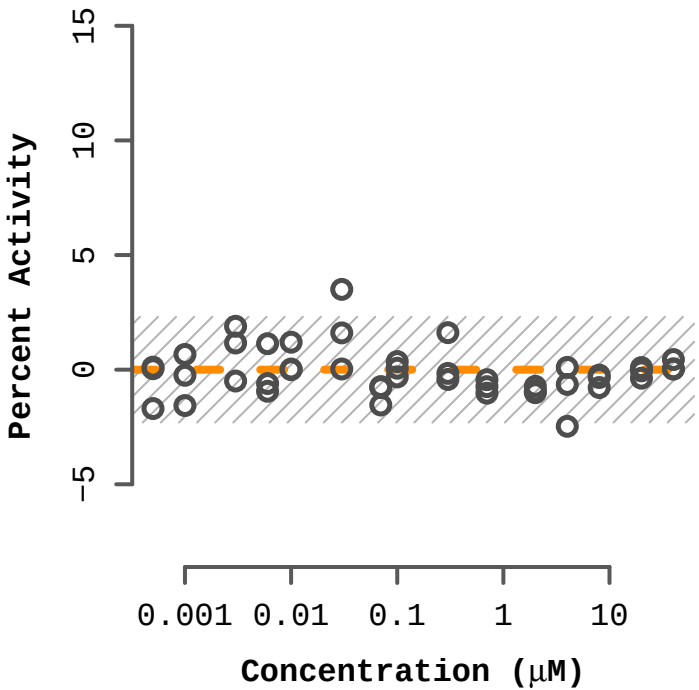
NAME: Bis(2-ethylhexyl) terephthalate
CHID: 27625 **CASRN:** 6422-86-2
SPID(S): Tox21_200461
M4ID: 12481791

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.204 **MAX_MED:** 0.596 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

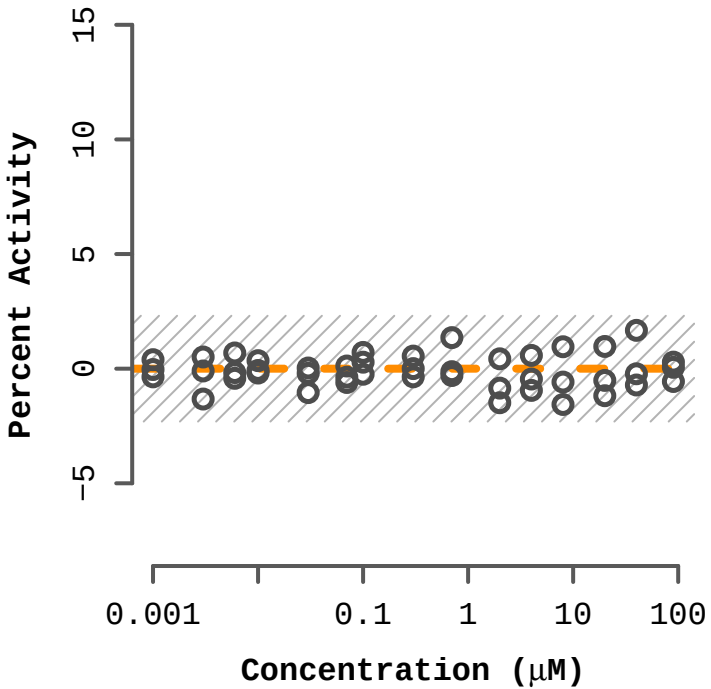
NAME: Irganox 1010
CHID: 27633 **CASRN:** 6683-19-8
SPID(S): Tox21_301970
M4ID: 12477163

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

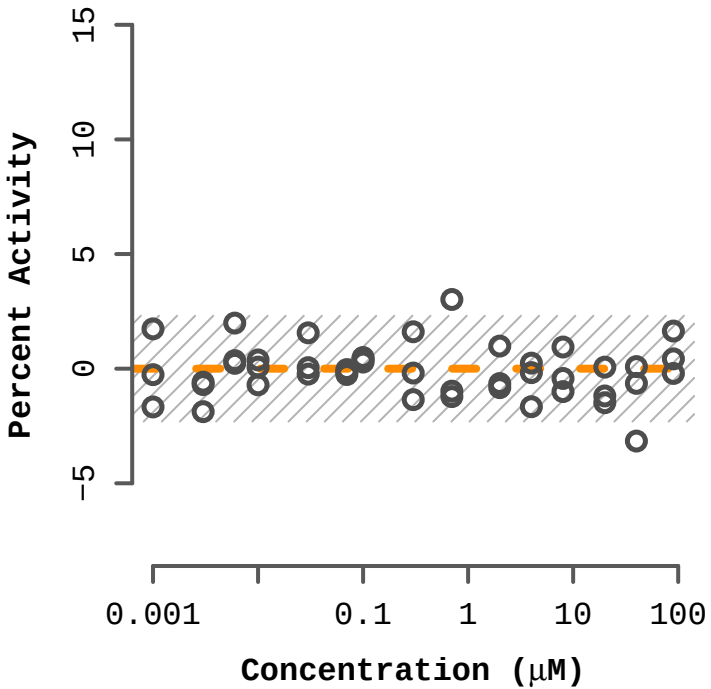
NAME: 1-Propene, tetramer
CHID: 27634 **CASRN:** 6842-15-5
SPID(S): Tox21_303865
M4ID: 12475323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.31 **MAX_MED:** 0.285 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

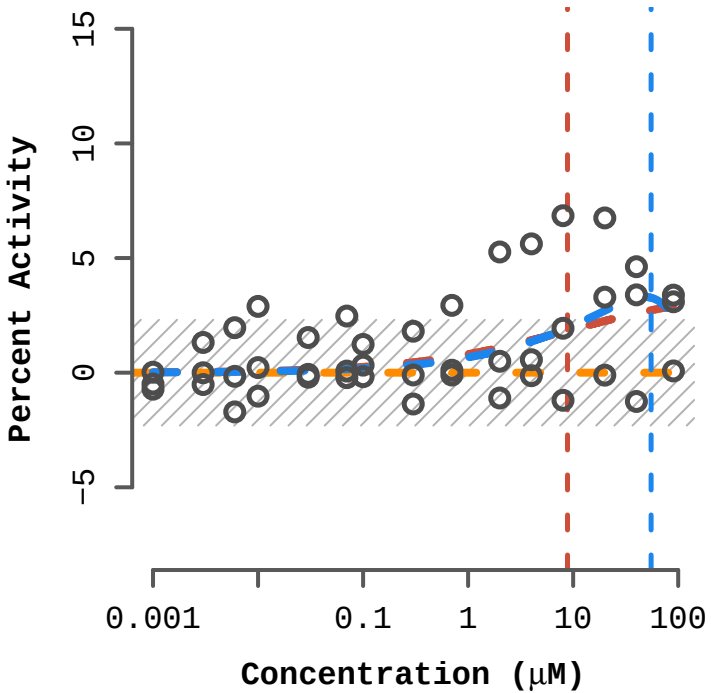
NAME: 2,2,4−Trimethyl−1,3−pentanediol diisobutyrate
CHID: 27635 **CASRN:** 6846−50−0
SPID(S): Tox21_300316
M4ID: 12478815

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 0.428 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2,4−Trimethyl−1,3−pentanediol diisobutyrate
CHID: 27635 CASRN: 6846−50−0
SPID(S): Tox21_202454
M4ID: 12479798

HILL MODEL (in red):

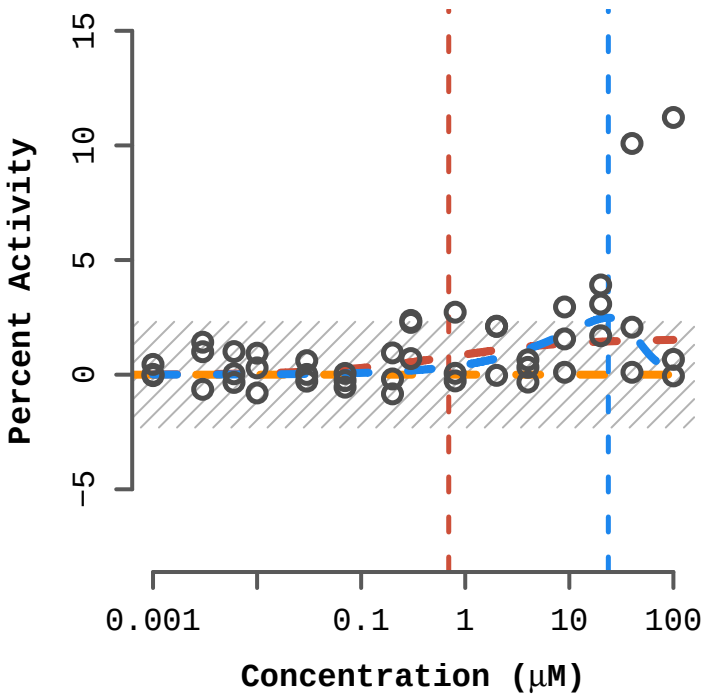
	tp	ga	gw
val:	3.66	0.946	0.582
sd:	3.29	1.71	0.739

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.65	1.74	0.584	1.99	3.08
sd:	17.3	2.81	0.555	0.253	10.1

	CNST	HILL	GNLS
AIC:	204.14	194.88	198.09
PROB:	0.01	0.83	0.17
RMSE:	2.44	1.95	1.95

MAX_MEAN: 3.31 MAX_MED: 3.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(2-butyl) ether
CHID: 27636 **CASRN:** 6863-58-7
SPID(S): Tox21_201188
M4ID: 12481064

HILL MODEL (in red):

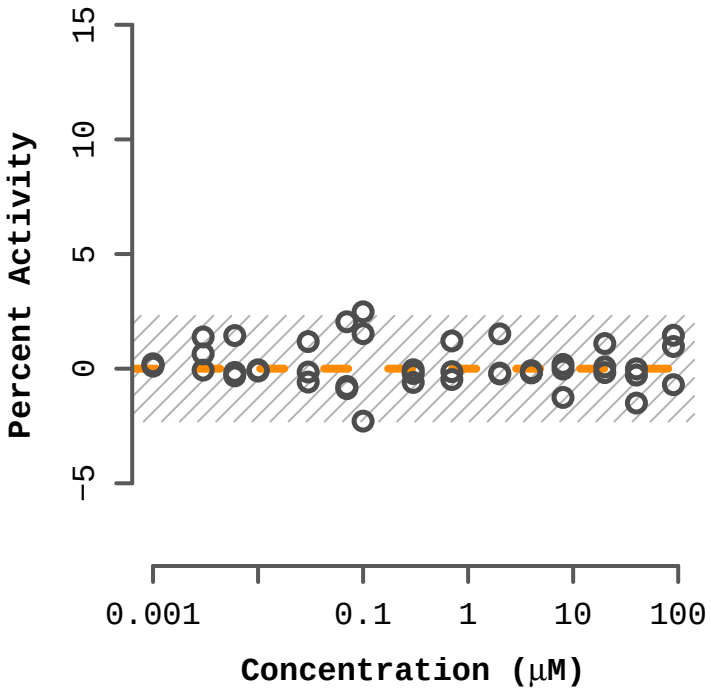
	tp	ga	gw
val:	1.55	−0.159	0.752
sd:	0.785	1.04	0.82

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.6	1.37	0.781	1.62	3.58
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	184.49	173.44	173.31
PROB:	0	0.48	0.52
RMSE:	2.62	2.19	2.27

MAX_MEAN: 4.09 **MAX_MED:** 3.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

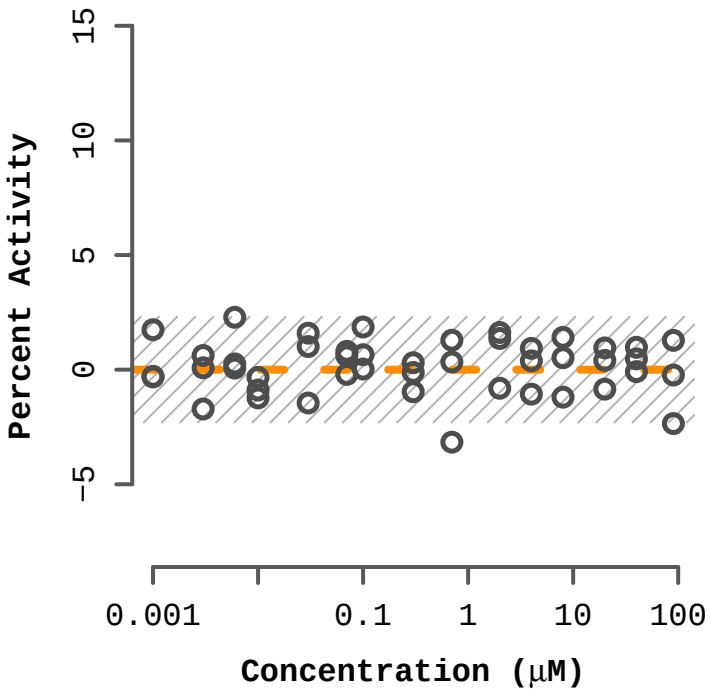
NAME: 2-(2-Propoxyethoxy)ethanol
CHID: 27639 **CASRN:** 6881-94-3
SPID(S): Tox21_200097
M4ID: 12482155

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.657 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

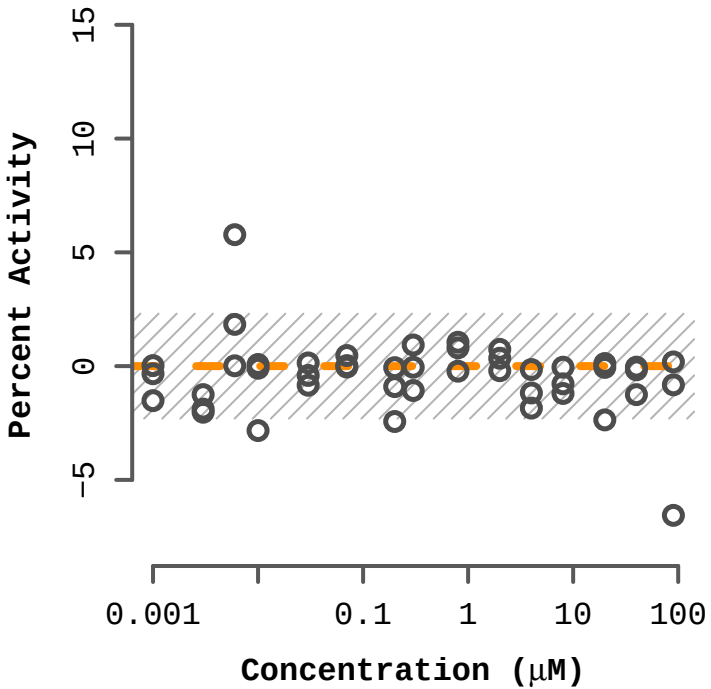
NAME: Malic acid
CHID: 27640 **CASRN:** 6915-15-7
SPID(S): Tox21_300372
M4ID: 12478760

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.87 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

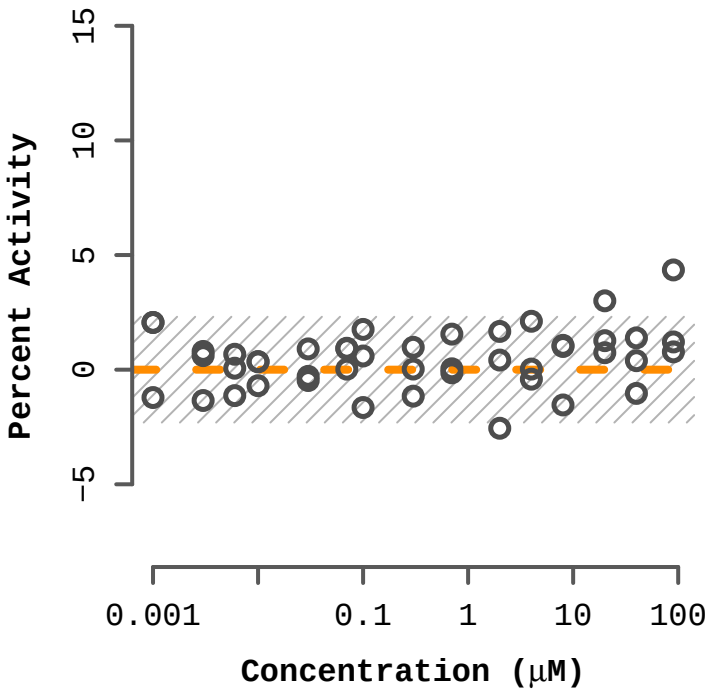
NAME: Malic acid
CHID: 27640 **CASRN:** 6915-15-7
SPID(S): Tox21_201536
M4ID: 12480716

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2.54 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

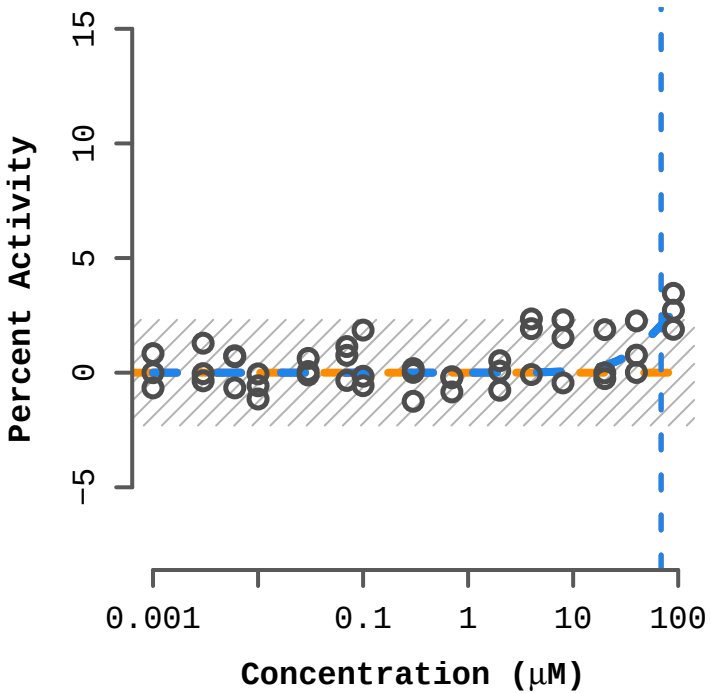
NAME: Diisopropyl adipate
CHID: 27641 **CASRN:** 6938-94-9
SPID(S): Tox21_200462
M4ID: 12481790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-(Trichlorosilyl)propyl methacrylate
CHID: 27647 **CASRN:** 7351-61-3
SPID(S): Tox21_202567
M4ID: 12479685

HILL MODEL (in red):

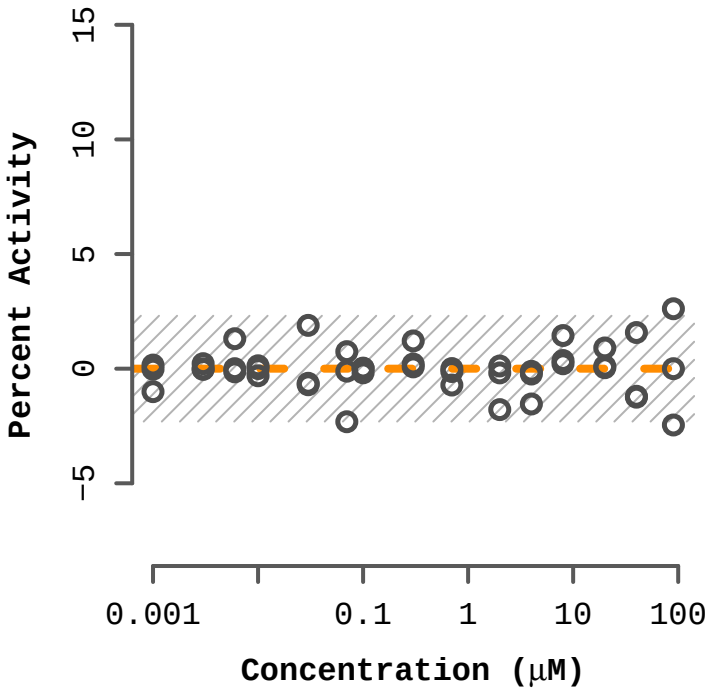
	tp	ga	gw
val:	4.15	1.84	2.03
sd:	5.79	0.658	3.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.15	1.84	2.03	2.92	8.15
sd:	5.79	0.658	3.54	1500	12700

	CNST	HILL	GNLS
AIC:	144.16	129.93	133.93
PROB:	0	0.88	0.12
RMSE:	1.2	0.93	0.93

MAX_MEAN: 2.69 **MAX_MED:** 2.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

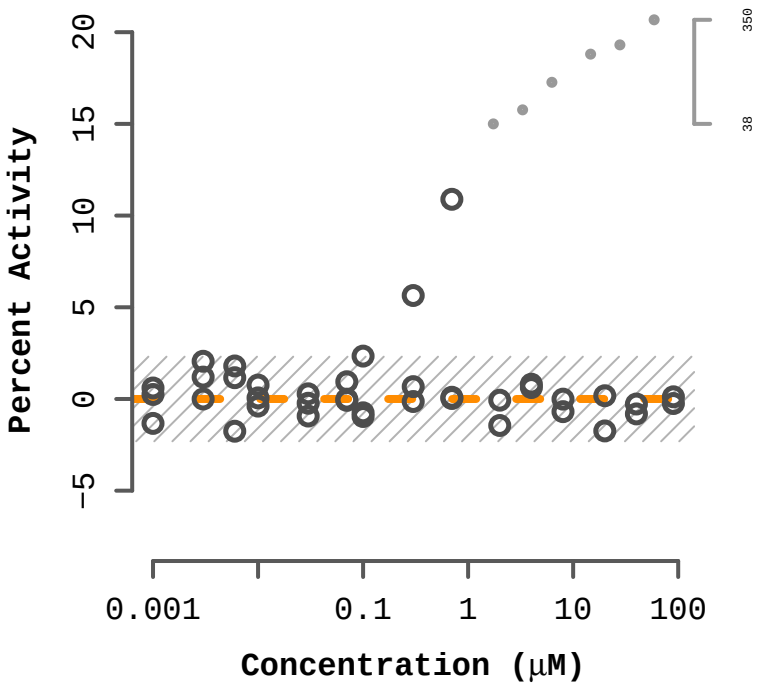
NAME: Dimethyldiallylammonium chloride
CHID: 27650 **CASRN:** 7398-69-8
SPID(S): Tox21_303355
M4ID: 12475778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.357 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

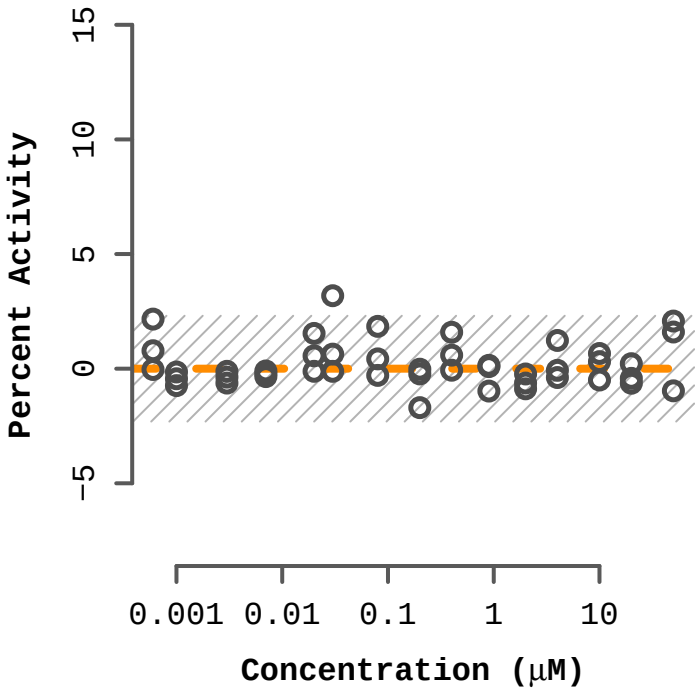
NAME: Dimethyldiallylammonium chloride
CHID: 27650 **CASRN:** 7398-69-8
SPID(S): Tox21_201695
M4ID: 12480557 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	395.9	NA	NA
PROB:	1	NA	NA
RMSE:	80.47	NA	NA

MAX_MEAN: 116 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

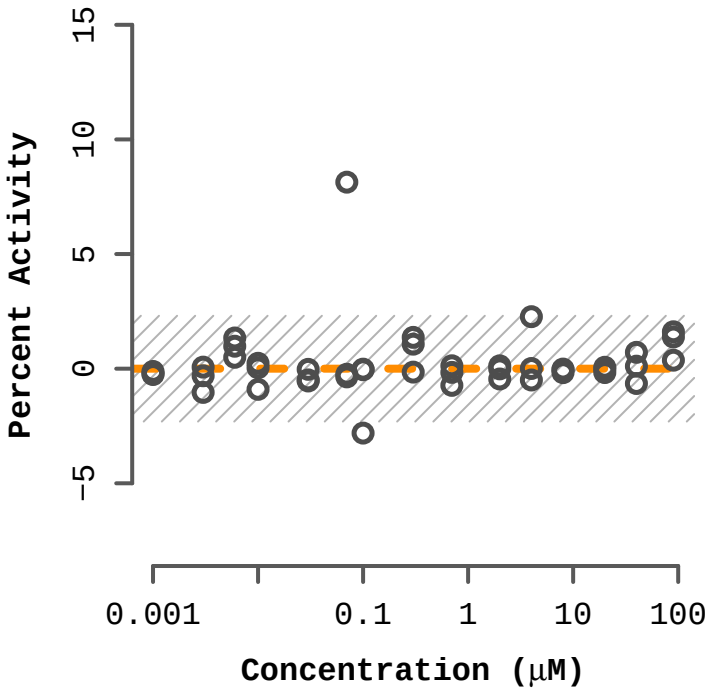
NAME: 2-Propenoic acid, sodium salt
CHID: 27652 **CASRN:** 7446-81-3
SPID(S): Tox21_202754
M4ID: 12479498

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

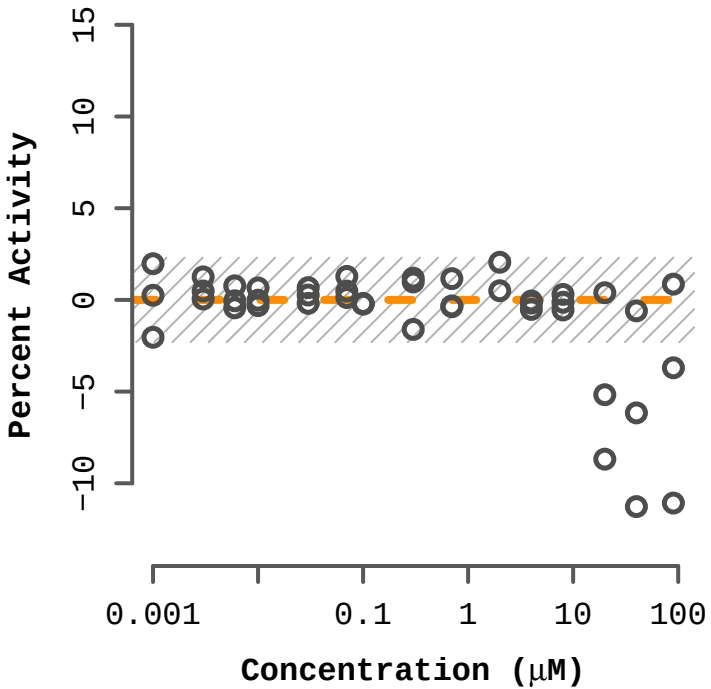
NAME: Isobornyl methacrylate
CHID: 27653 **CASRN:** 7534-94-3
SPID(S): Tox21_303579
M4ID: 12475566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.51 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

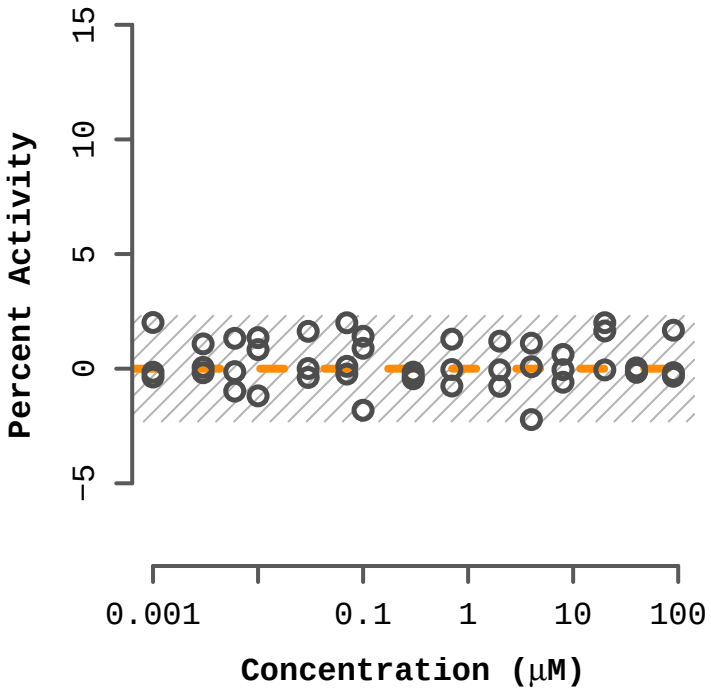
NAME: Isobornyl methacrylate
CHID: 27653 **CASRN:** 7534-94-3
SPID(S): Tox21_202201
M4ID: 12480051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.1	NA	NA
PROB:	1	NA	NA
RMSE:	3.13	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

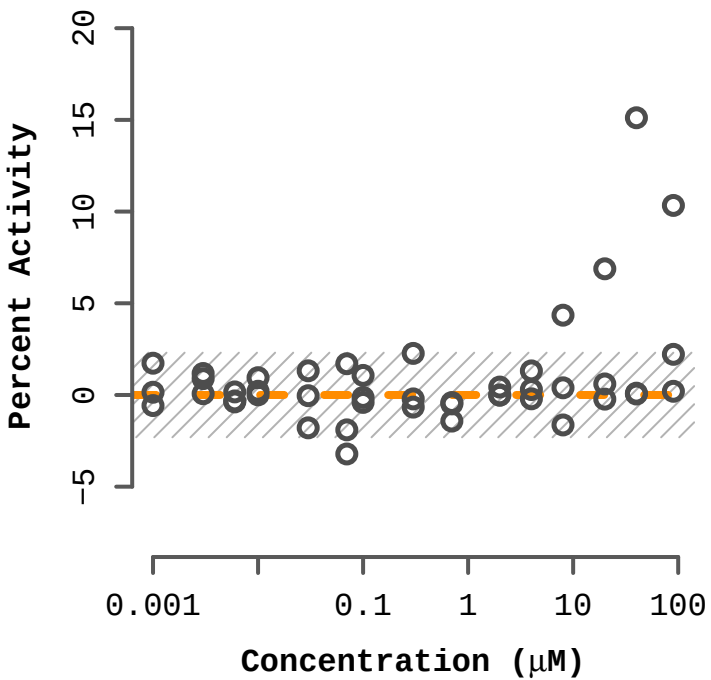
NAME: 2-Ethylhexyl sulfanylacetate
CHID: 27656 **CASRN:** 7659-86-1
SPID(S): Tox21_303486
M4ID: 12475655

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

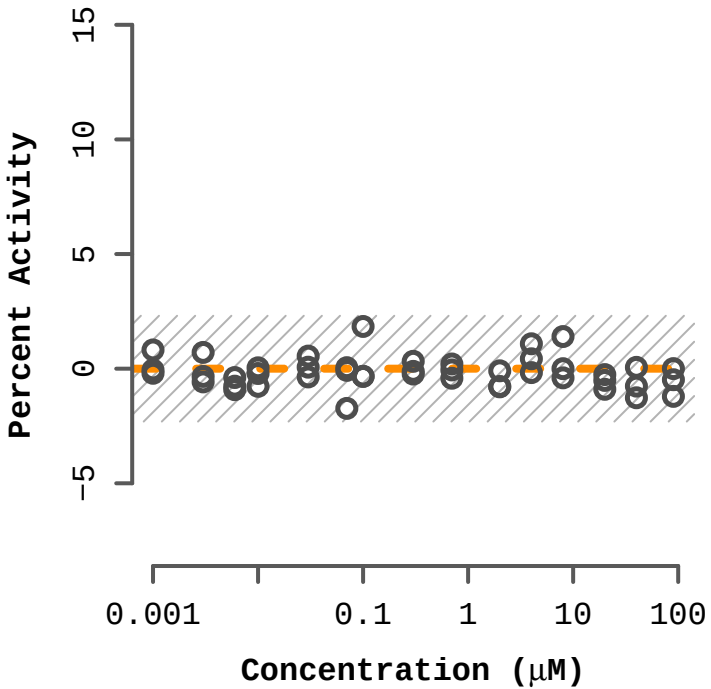
NAME: 2-Ethylhexyl sulfanylacetate
CHID: 27656 **CASRN:** 7659-86-1
SPID(S): Tox21_201541
M4ID: 12480711

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.27	NA	NA
PROB:	1	NA	NA
RMSE:	3.16	NA	NA

MAX_MEAN: 5.09 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

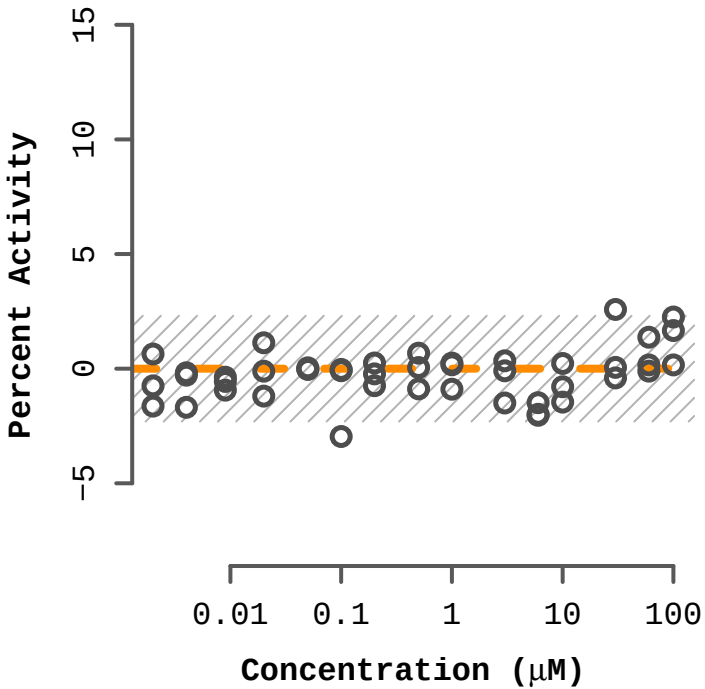
NAME: 1-Octanesulfonyl chloride
CHID: 27658 CASRN: 7795-95-1
SPID(S): Tox21_200714
M4ID: 12481538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.451 MAX_MED: 0.433 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

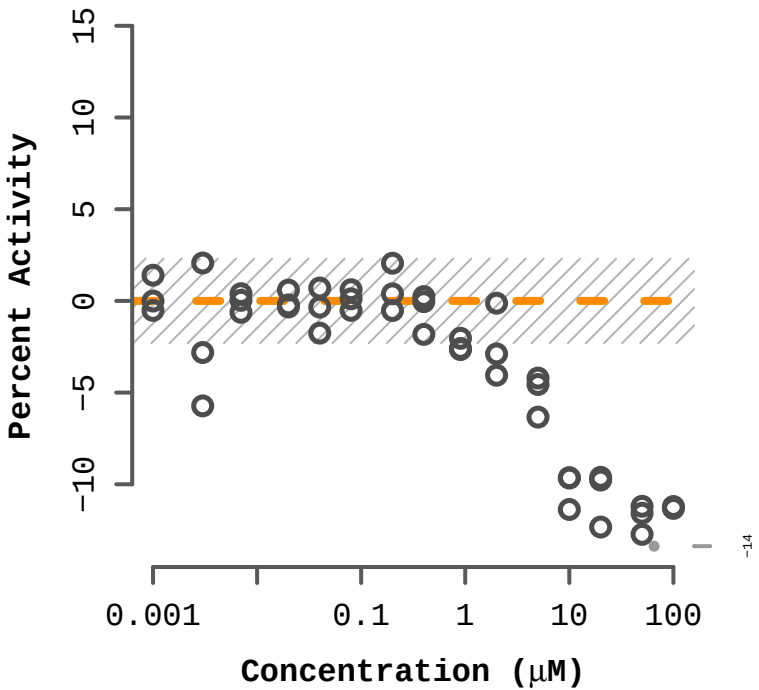
NAME: Polyoxyethylene monoleate
CHID: 27713 **CASRN:** 9004-96-0
SPID(S): Tox21_303475
M4ID: 12475665

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

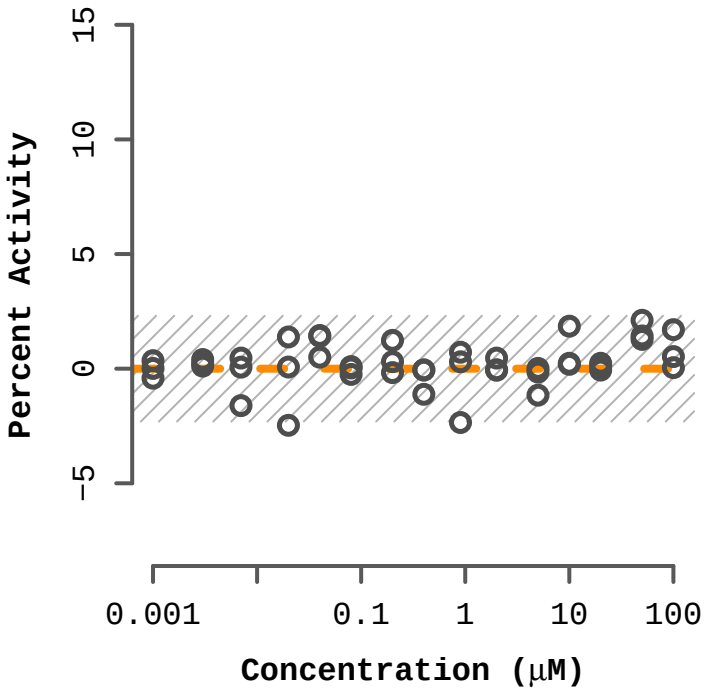
NAME: Polyoxyethylene (20) oleylether
CHID: 27714 **CASRN:** 9004-98-2
SPID(S): Tox21_200128
M4ID: 12482124 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	291.45	NA	NA
PROB:	1	NA	NA
RMSE:	6.14	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.387 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

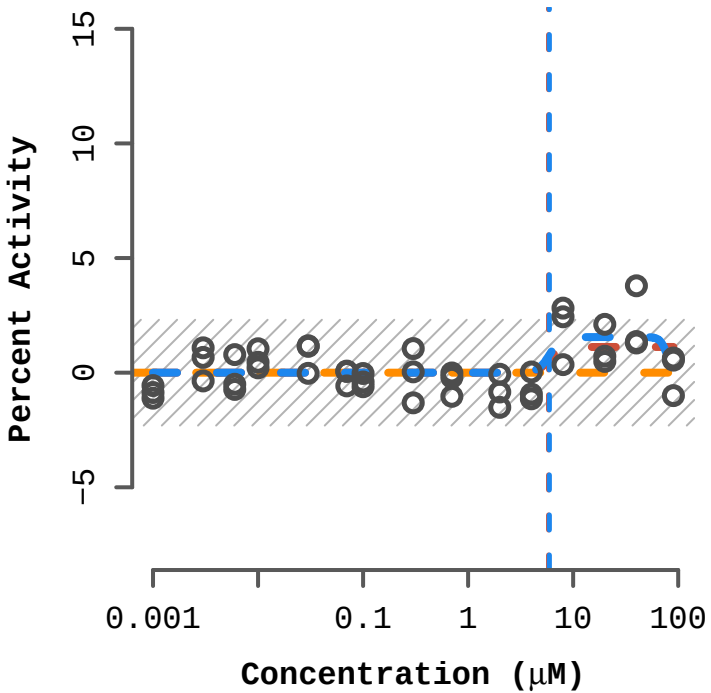
NAME: Polyethylene glycol dioleate
CHID: 27716 **CASRN:** 9005-07-6
SPID(S): Tox21_200224
M4ID: 12482028

HILL MODEL: Not applicable.

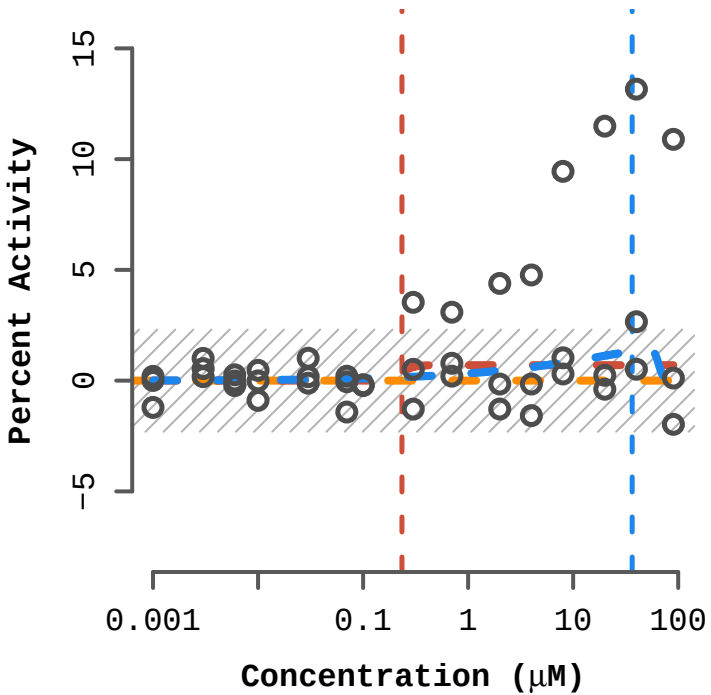
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.43 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-(2-Phenylpropan-2-yl)-N-[4-(2-phenylpropan-2-
CHID:    27721   CASRN: 10081-67-1
SPID(S): Tox21_303392
M4ID:    12475746

HILL MODEL (in red):
      tp       ga       gw
val:  1.12     0.766    8
sd:   0.304    0.102    5.39

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.55     0.773    8        1.89     13.5
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  138.69      131.22      130.21
PROB: 0.01        0.37        0.62
RMSE: 1.14        0.93        0.85

MAX_MEAN: 2.15      MAX_MED: 2.44      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(2-Phenylpropan-2-yl)-N-[4-(2-phenylpropan-2-
CHID: 27721 CASRN: 10081-67-1
SPID(S): Tox21_202099
M4ID: 12480153

HILL MODEL (in red):

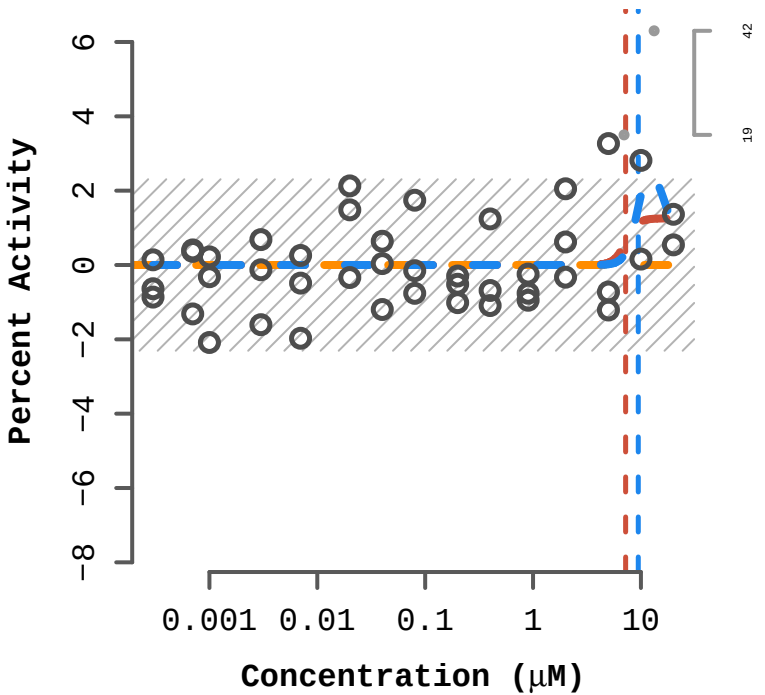
	tp	ga	gw
val:	0.699	-0.63	8
sd:	0.441	0.939	48.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.68	1.56	0.553	1.81	17.9
sd:	10.5	5.07	0.63	0.751	90.6

	CNST	HILL	GNLS
AIC:	213.29	216.1	219.38
PROB:	0.77	0.19	0.04
RMSE:	3.66	3.44	3.4

MAX_MEAN: 5.45 MAX_MED: 2.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Di(tridecyl) thiodipropionate
CHID: 27728 CASRN: 10595-72-9
SPID(S): Tox21_202755
M4ID: 12479497 BRK

HILL MODEL (in red):

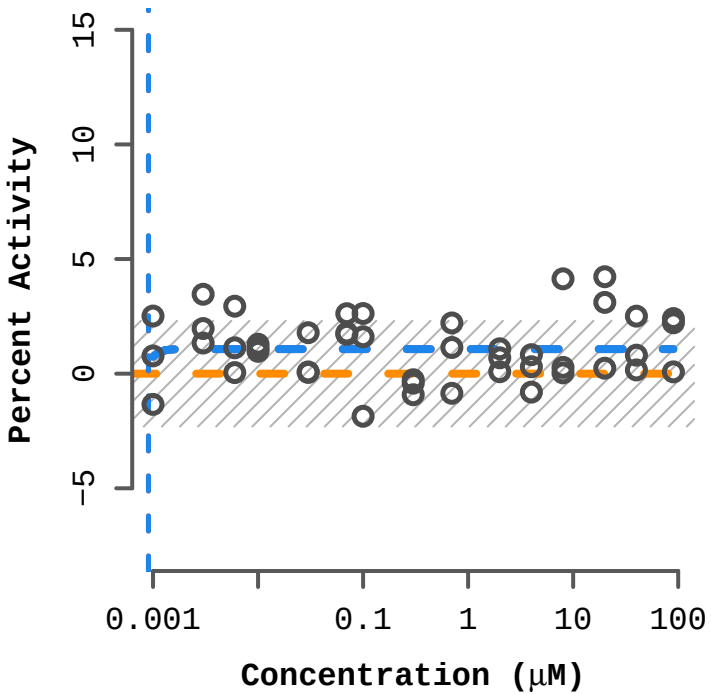
	tp	ga	gw
val:	1.25	0.858	8
sd:	0.647	0.195	10.4

GAIN-LOSS MODEL (in blue):

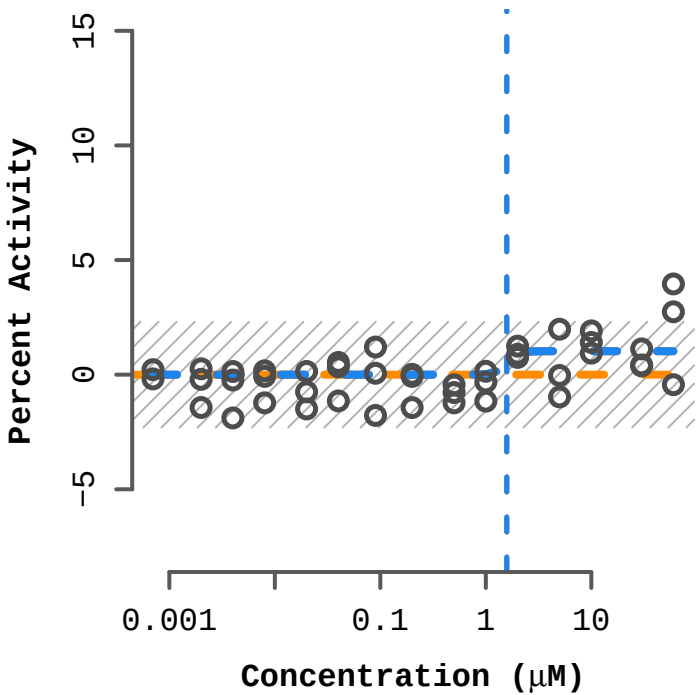
	tp	ga	gw	la	lw
val:	3.33	0.975	8	1.23	4.66
sd:	17.7	0.682	16.9	0.782	27.6

	CNST	HILL	GNLS
AIC:	195.85	197.89	201.36
PROB:	0.7	0.25	0.04
RMSE:	6.96	6.72	6.71

MAX_MEAN: 14.7 MAX_MED: 2.81 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Isomethyltetrahydrophthalic anhydride
CHID:    27729   CASRN: 11070-44-3
SPID(S): Tox21_301182
M4ID:    12477951

HILL MODEL (in red):
      tp       ga       gw
val:  1.07     -3.04    8
sd:   0.22     0.39     61.7

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.07     -3.04    8        3.05     7.2
sd:   0.22     0.39     61.8     1560     10200

      CNST        HILL        GNLS
AIC:  184.32      169.06      173.06
PROB: 0           0.88        0.12
RMSE: 1.78        1.39        1.39

MAX_MEAN: 2.53      MAX_MED: 3.11      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (Methylcyclopentadienyl)tricarbonylmanganese
CHID: 27738 CASRN: 12108-13-3
SPID(S): Tox21_302659
M4ID: 12476474

HILL MODEL (in red):

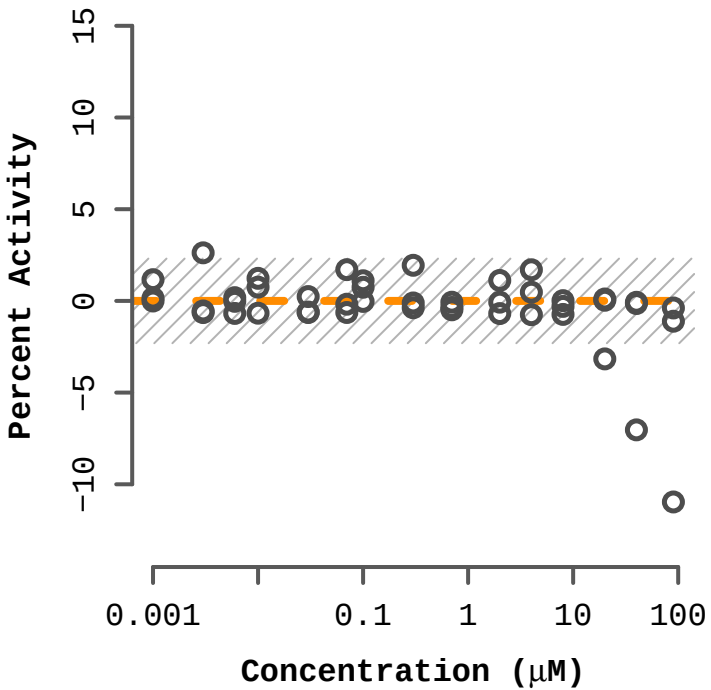
	tp	ga	gw
val:	1.02	0.199	8
sd:	0.294	0.145	7.88

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.02	0.199	8	2.69	10.4
sd:	0.294	0.145	7.88	6140	70700

	CNST	HILL	GNLS
AIC:	139.75	132.84	136.84
PROB:	0.03	0.86	0.12
RMSE:	1.18	1	1

MAX_MEAN: 2.09 MAX_MED: 2.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

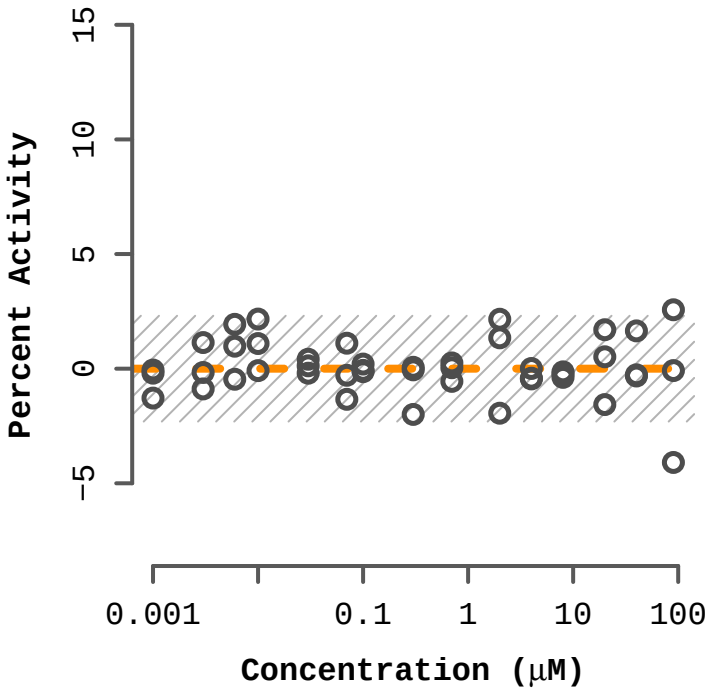
NAME: (Methylcyclopentadienyl)tricarbonylmanganese
CHID: 27738 **CASRN:** 12108-13-3
SPID(S): Tox21_201959
M4ID: 12480293

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.53	NA	NA
PROB:	1	NA	NA
RMSE:	2.16	NA	NA

MAX_MEAN: 0.606 **MAX_MED:** 0.752 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

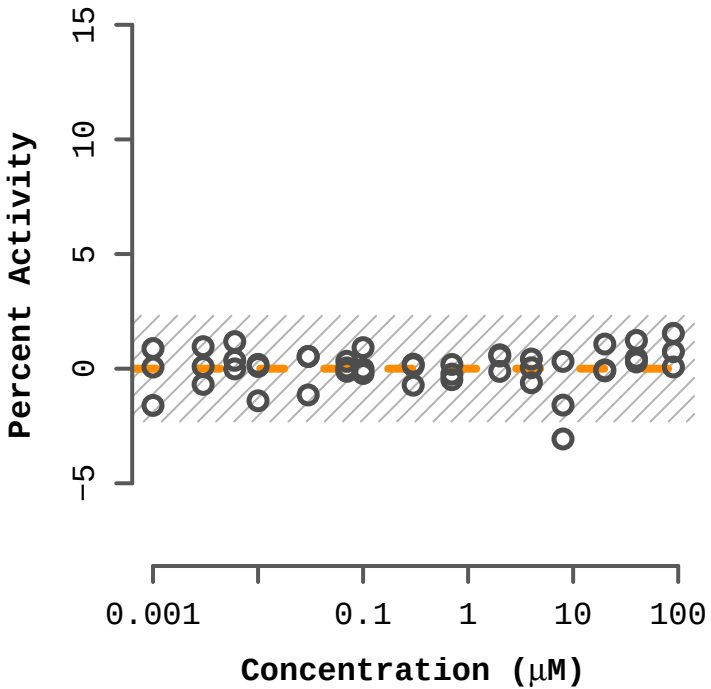
NAME: 2-Ethylhexyl phosphate
CHID: 27740 **CASRN:** 12645-31-7
SPID(S): Tox21_202126
M4ID: 12480126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

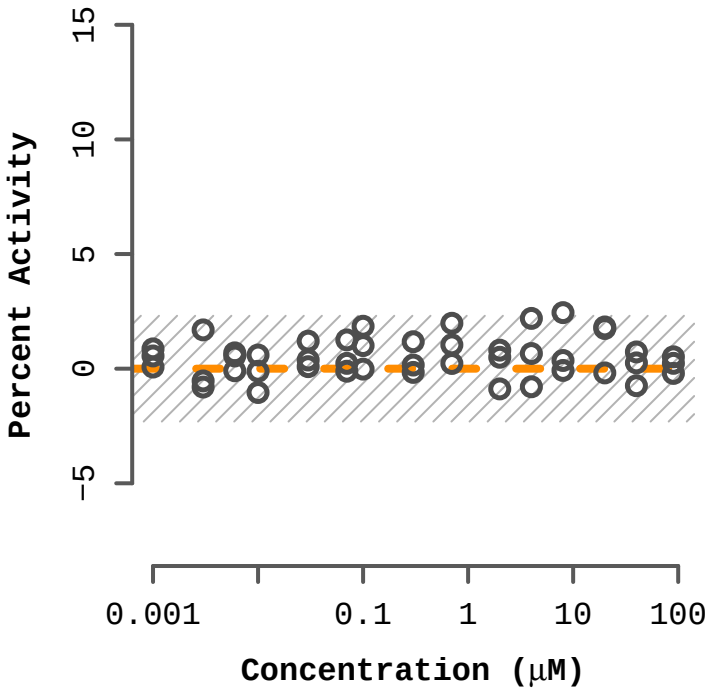
NAME: 2,2'−Azobis(2−methylbutanenitrile)
CHID: 27747 **CASRN:** 13472−08−7
SPID(S): Tox21_301414
M4ID: 12477719

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.787 **MAX_MED:** 0.744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

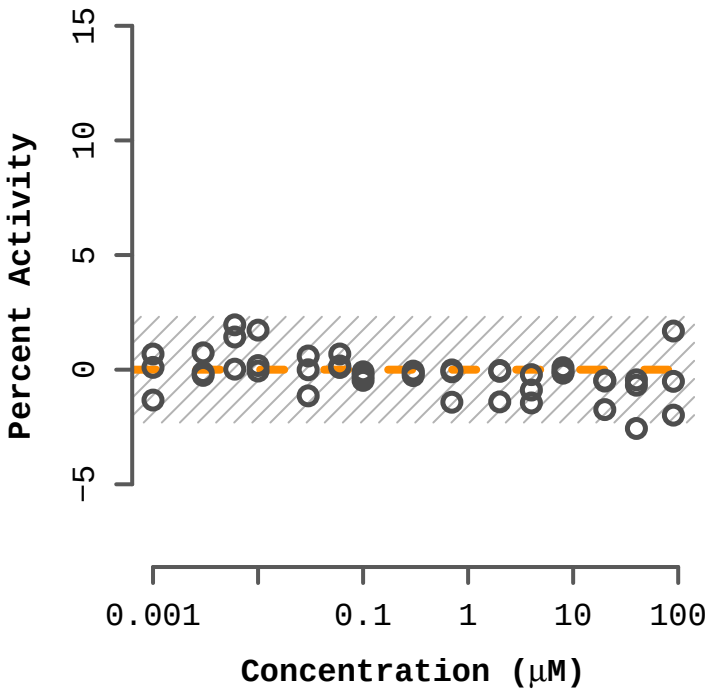
NAME: 1-Chloro-3,3-dimethyl-butan-2-one
CHID: 27749 **CASRN:** 13547-70-1
SPID(S): Tox21_303424
M4ID: 12475715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

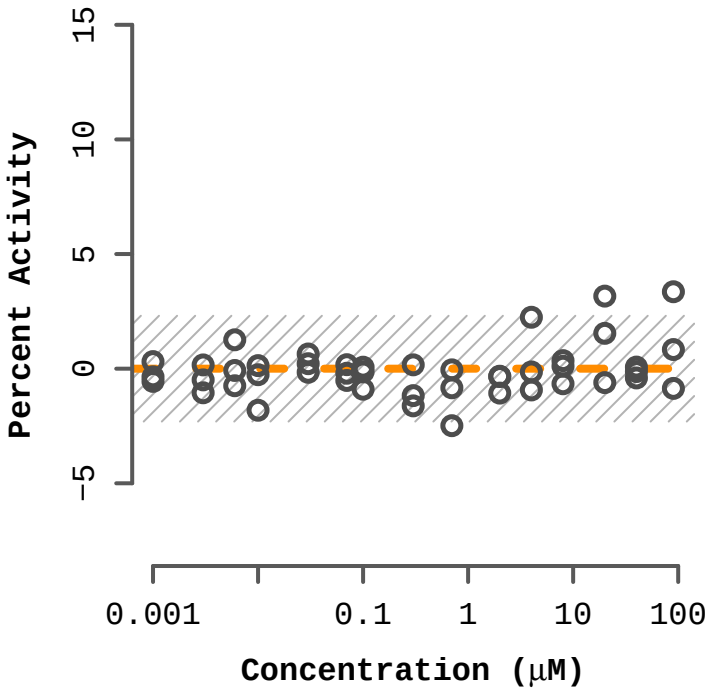
NAME: 1-Chloro-3,3-dimethyl-butan-2-one
CHID: 27749 **CASRN:** 13547-70-1
SPID(S): Tox21_202148
M4ID: 12480104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

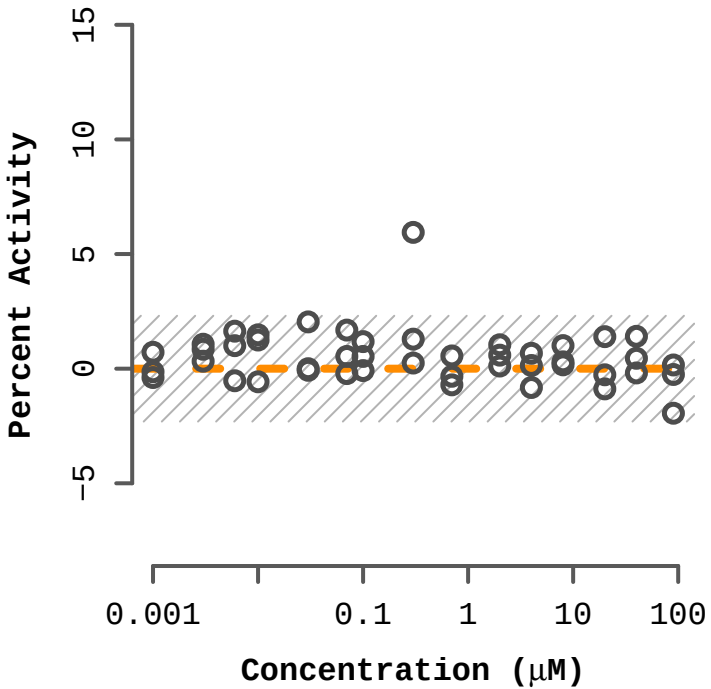
NAME: 3-Phenoxybenzenemethanol
CHID: 27756 CASRN: 13826-35-2
SPID(S): Tox21_303571
M4ID: 12475574

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

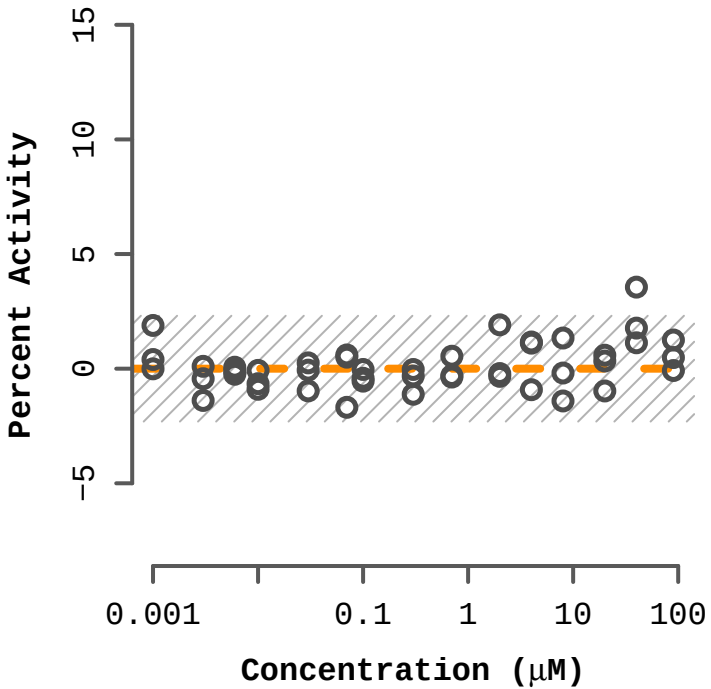
NAME: 3-Phenoxybenzenemethanol
CHID: 27756 **CASRN:** 13826-35-2
SPID(S): Tox21_201473
M4ID: 12480779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 2.49 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

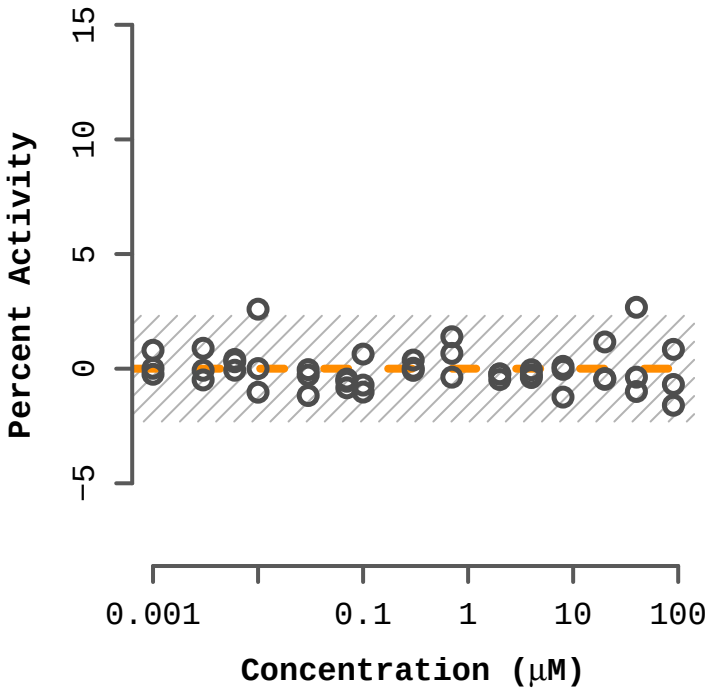
NAME: 2-Amino-2,3-dimethylbutanenitrile
CHID: 27759 **CASRN:** 13893-53-3
SPID(S): Tox21_302196
M4ID: 12476937

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.73	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

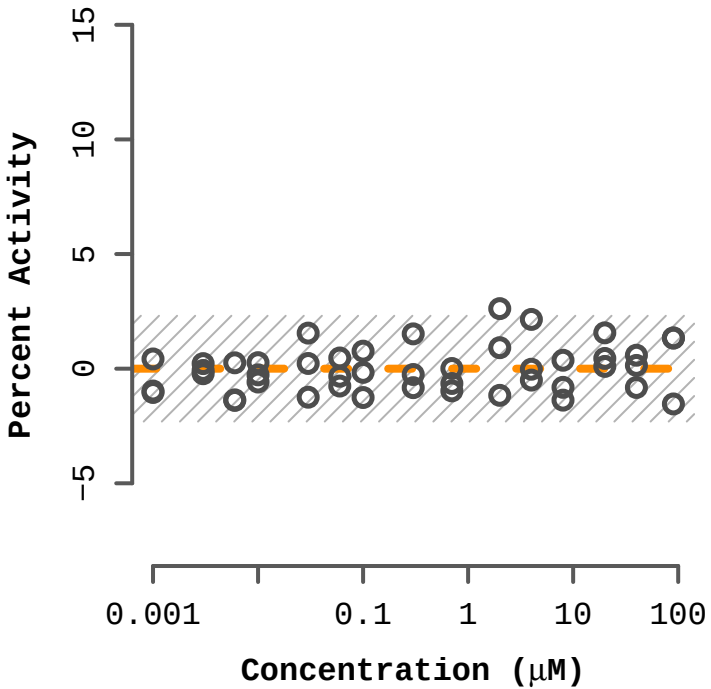
NAME: N,N−Dimethyldecanamide
CHID: 27764 **CASRN:** 14433−76−2
SPID(S): Tox21_200114
M4ID: 12482138

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.565 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

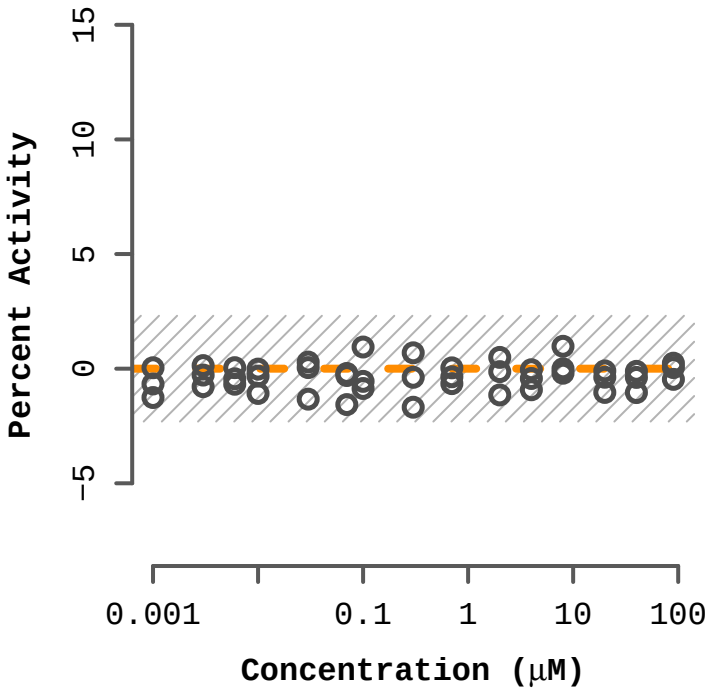
NAME: Zinc diacrylate
CHID: 27768 **CASRN:** 14643-87-9
SPID(S): Tox21_200463
M4ID: 12481789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

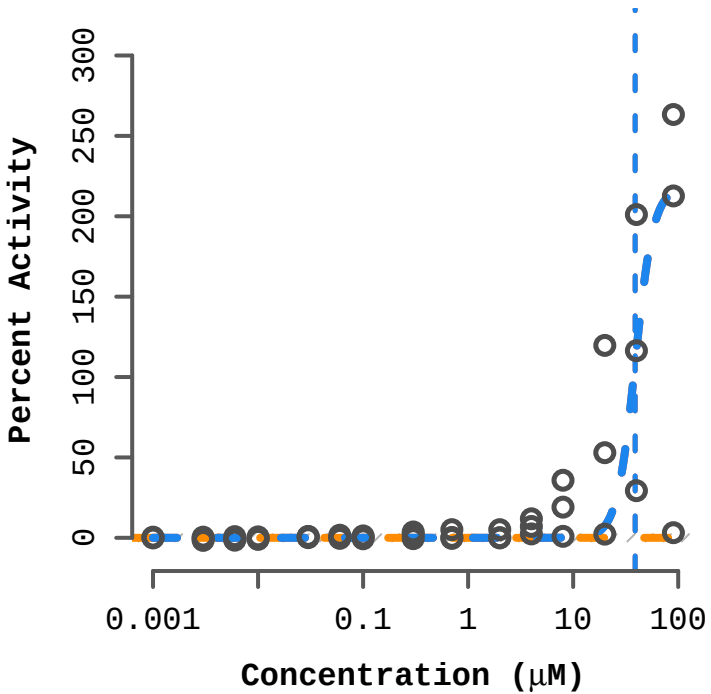
NAME: 2-Acrylamido-2-methyl-1-propanesulfonic acid
CHID: 27770 **CASRN:** 15214-89-8
SPID(S): Tox21_303523
M4ID: 12475620

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.259 **MAX_MED:** 0.0503 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Acrylamido-2-methyl-1-propanesulfonic acid
CHID: 27770 CASRN: 15214-89-8
SPID(S): Tox21_201781
M4ID: 12480471

HILL MODEL (in red):

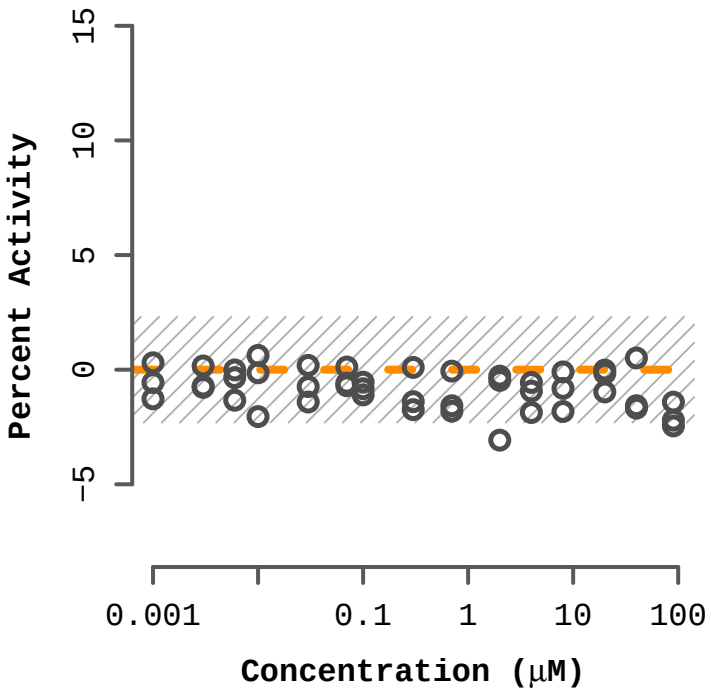
	tp	ga	gw
val:	218	1.59	5.01
sd:	8.1	0.0107	1.87

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	218	1.59	5.01	3.02	6.94
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	435.13	402.77	406.77
PROB:	0	0.88	0.12
RMSE:	64.72	41.76	41.76

MAX_MEAN: 160 MAX_MED: 213 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

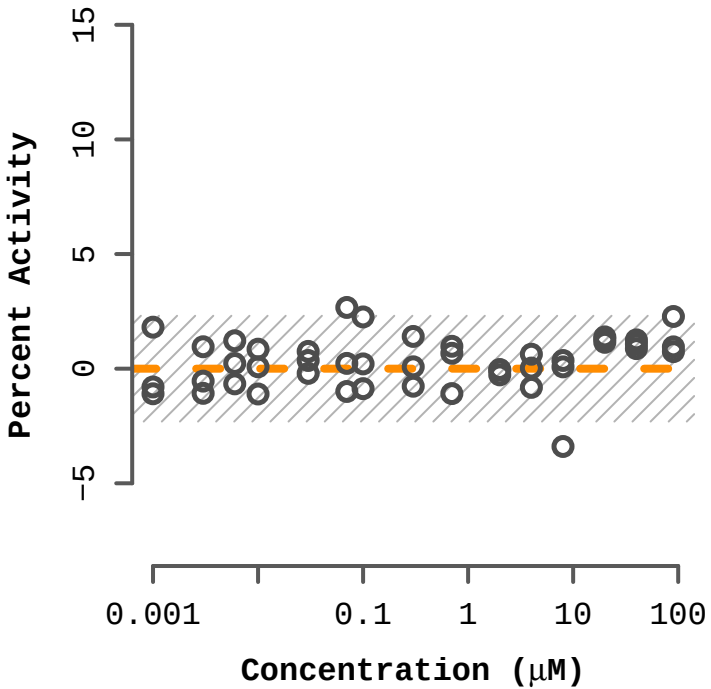
NAME: N−(1−Methylheptyl)−N'−phenyl−1,4−benzenediamine
CHID: 27771 **CASRN:** 15233−47−3
SPID(S): Tox21_301489
M4ID: 12477644

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: −0.382 **MAX_MED:** −0.134 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

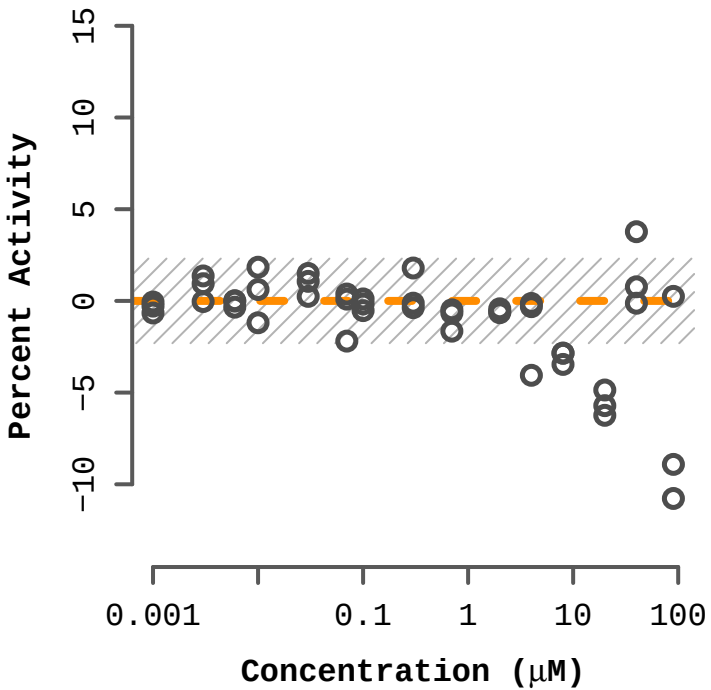
NAME: 2-Methylpentanediamine
CHID: 27772 **CASRN:** 15520-10-2
SPID(S): Tox21_301546
M4ID: 12477587

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

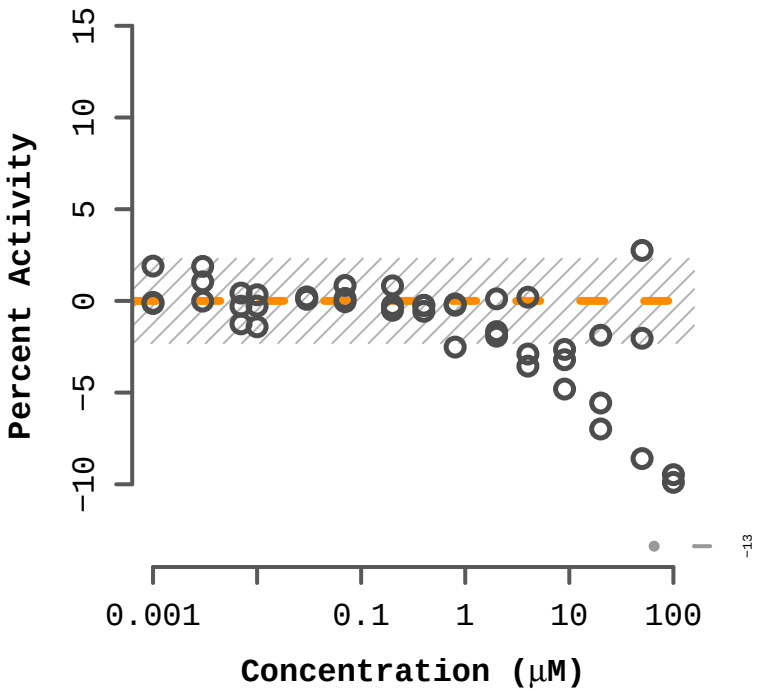
NAME: Trimethylolpropane triacrylate
CHID: 27773 **CASRN:** 15625-89-5
SPID(S): Tox21_303527
M4ID: 12475616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

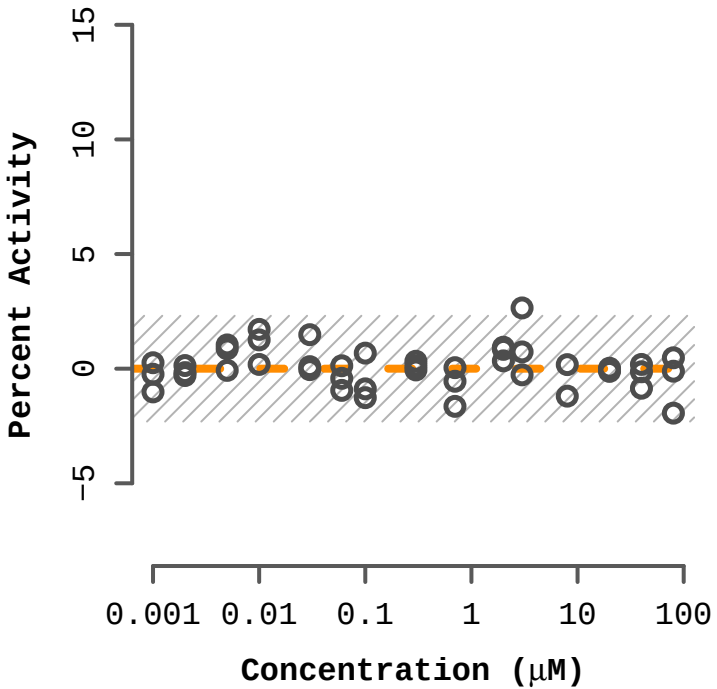
NAME: Trimethylolpropane triacrylate
CHID: 27773 **CASRN:** 15625-89-5
SPID(S): Tox21_202170
M4ID: 12480082 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.73	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

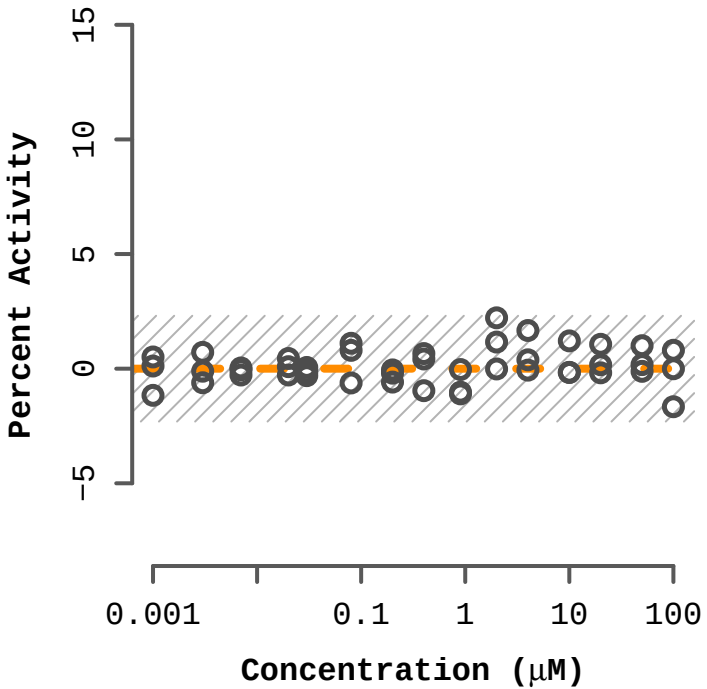
NAME: Ethylenediaminetetraacetic acid ferric sodium s
CHID: 27774 CASRN: 15708-41-5
SPID(S): Tox21_303443
M4ID: 12475697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

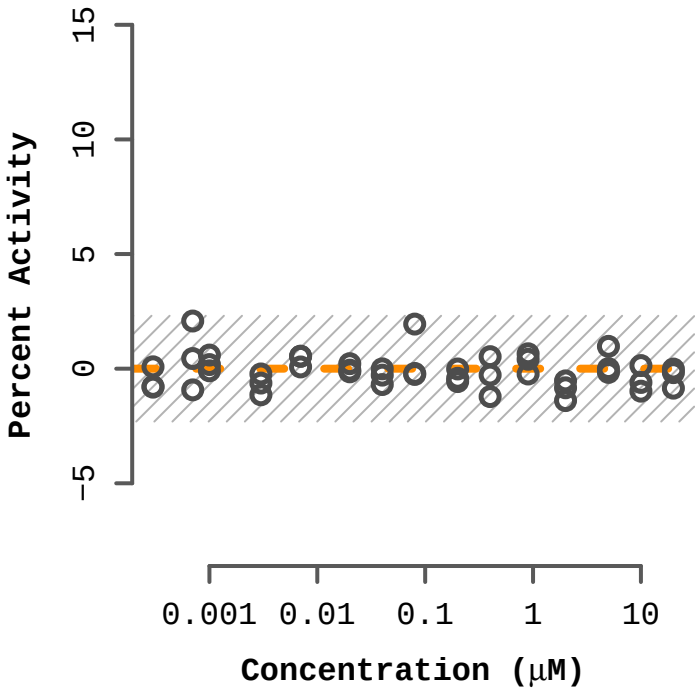
NAME: Ethylenediaminetetraacetic acid ferric sodium s
CHID: 27774 CASRN: 15708-41-5
SPID(S): Tox21_201923
M4ID: 12480329

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

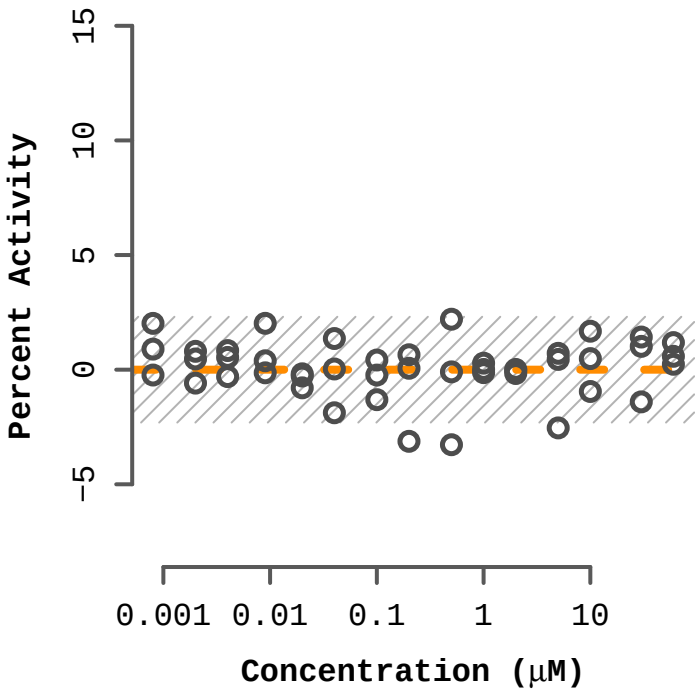
NAME: Ethylenediaminetetraacetic acid ferric sodium s
CHID: 27774 **CASRN:** 15708-41-5
SPID(S): Tox21_112117_1
M4ID: 12483308

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.533 **MAX_MED:** 0.543 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

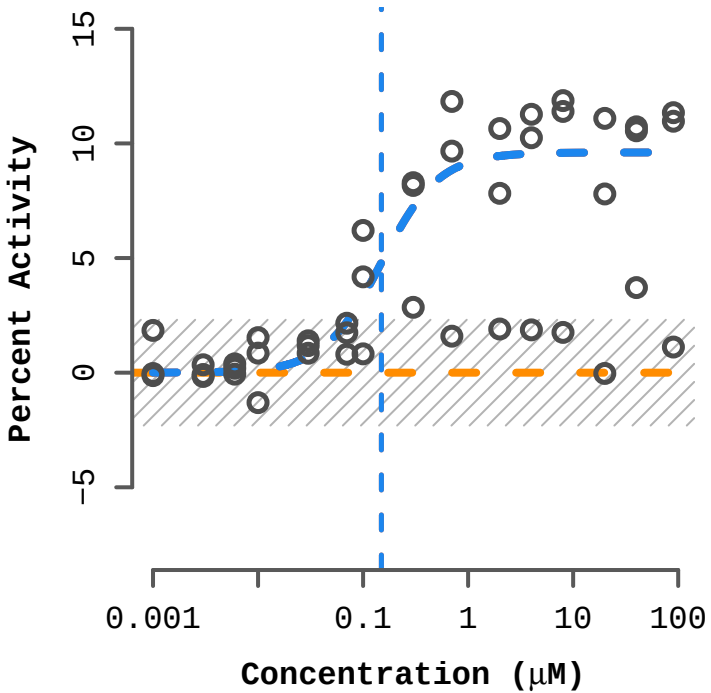
NAME: C.I. Fluorescent Brightener 220
CHID: 27781 **CASRN:** 16470-24-9
SPID(S): Tox21_301936
M4ID: 12477197

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: O,O−Dimethyl phosphoramidothioate
CHID: 27789 CASRN: 17321−47−0
SPID(S): Tox21_303881
M4ID: 12475307

HILL MODEL (in red):

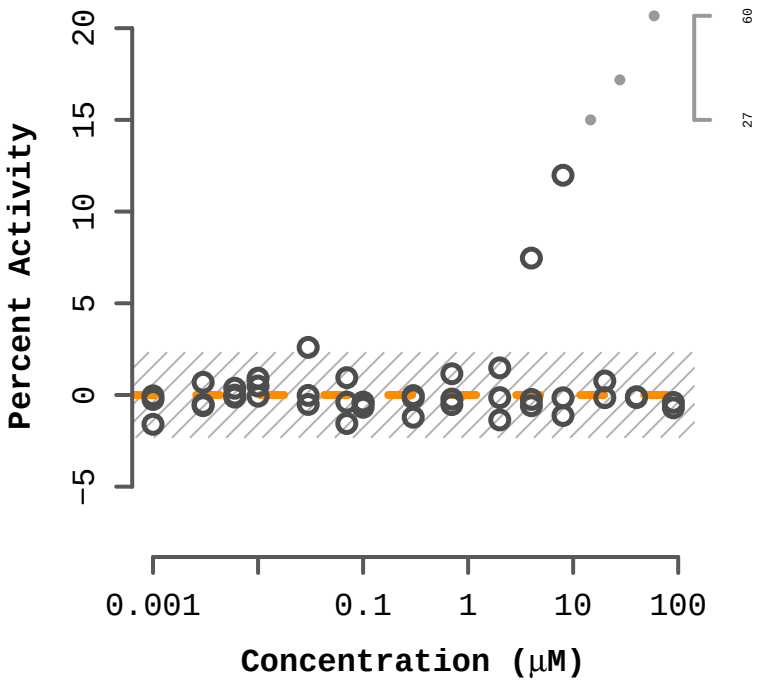
	tp	ga	gw
val:	9.61	−0.826	1.59
sd:	0.772	0.133	0.654

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.61	−0.826	1.59	3.86	4.26
sd:	0.772	0.133	0.654	2120	4730

	CNST	HILL	GNLS
AIC:	297.67	235.33	239.33
PROB:	0	0.88	0.12
RMSE:	6.36	3.38	3.38

MAX_MEAN: 8.34 MAX_MED: 11.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

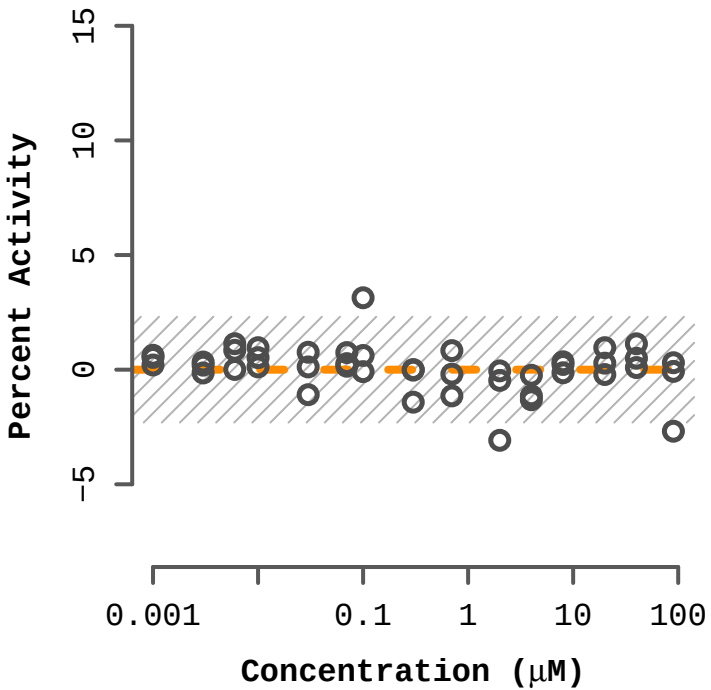
NAME: 2-(Chloromethyl)-1H-isoindole-1,3(2H)-dione
CHID: 27790 **CASRN:** 17564-64-6
SPID(S): Tox21_200731
M4ID: 12481521 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.47	NA	NA
PROB:	1	NA	NA
RMSE:	11.58	NA	NA

MAX_MEAN: 19.5 **MAX_MED:** 0.765 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

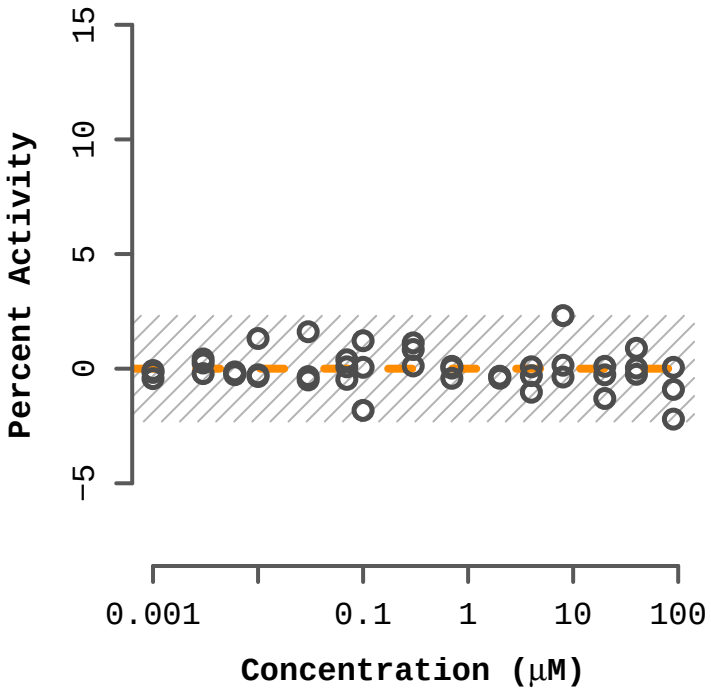
NAME: Ethyltriacetoxysilane
CHID: 27792 **CASRN:** 17689-77-9
SPID(S): Tox21_303413
M4ID: 12475726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.848 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

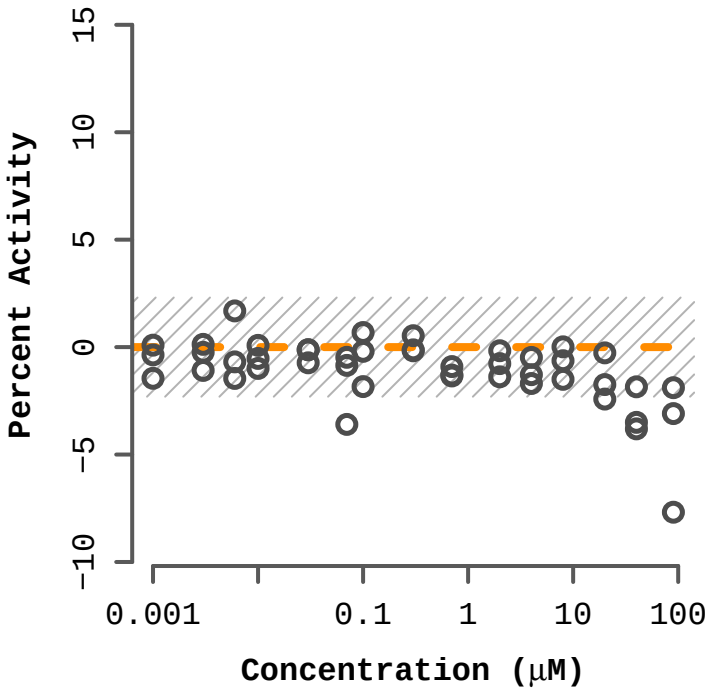
NAME: Ethyltriacetoxysilane
CHID: 27792 **CASRN:** 17689-77-9
SPID(S): Tox21_201643
M4ID: 12480609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.701 **MAX_MED:** 0.836 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

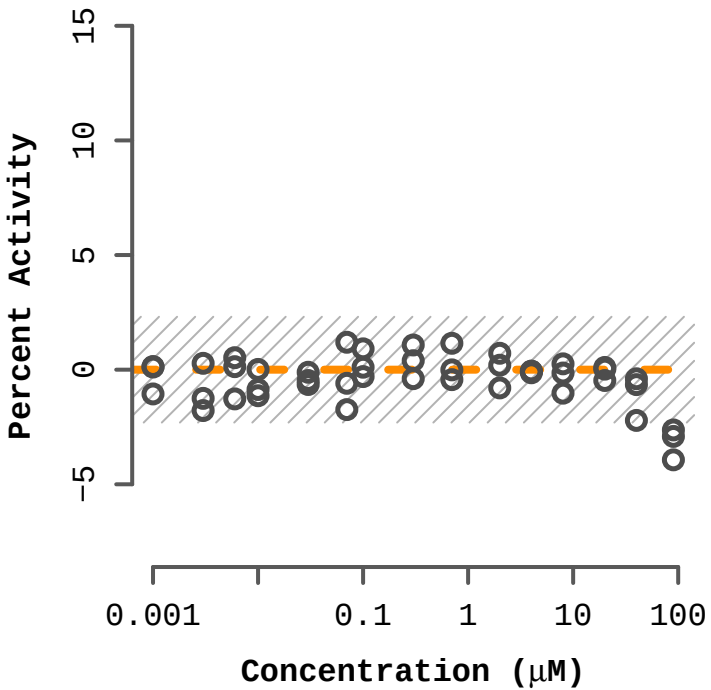
NAME: N-(Cyclohexylthio)phthalimide
CHID: 27793 **CASRN:** 17796-82-6
SPID(S): Tox21_303596
M4ID: 12475549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 0.0788 **MAX_MED:** −0.123 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

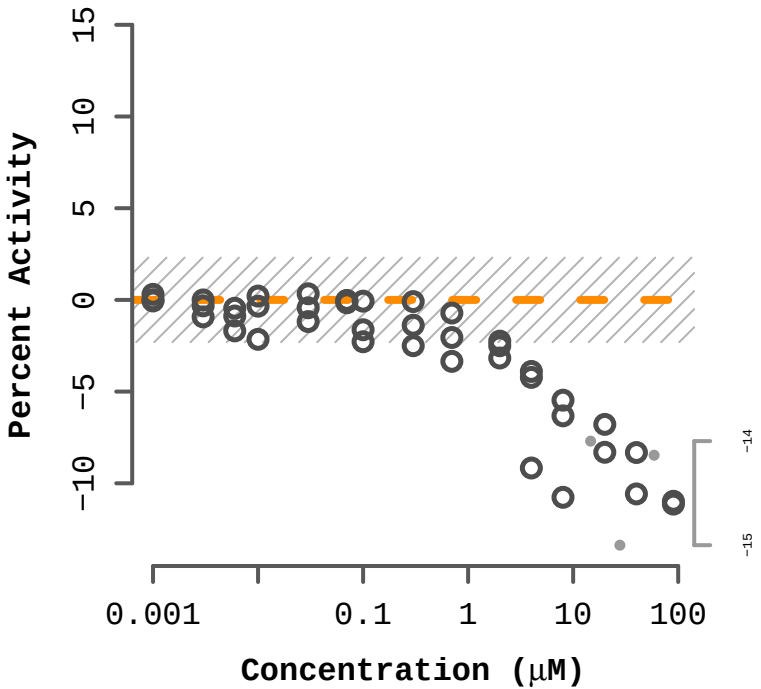
NAME: N-(Cyclohexylthio)phthalimide
CHID: 27793 **CASRN:** 17796-82-6
SPID(S): Tox21_201540
M4ID: 12480712

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.361 **MAX_MED:** 0.394 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

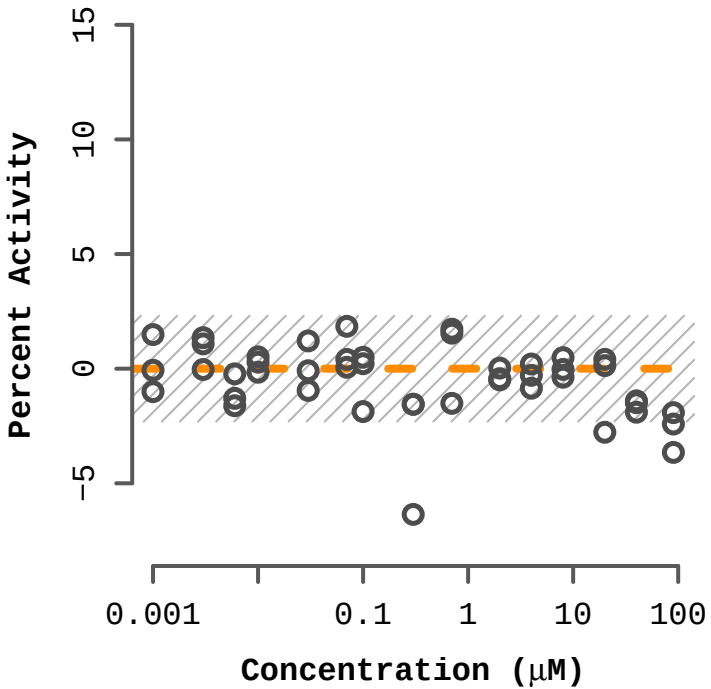
NAME: 3,4,5,6-Tetrachloro-2-pyridinecarbonitrile
CHID: 27795 **CASRN:** 17824-83-8
SPID(S): Tox21_301242
M4ID: 12477891 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	283.18	NA	NA
PROB:	1	NA	NA
RMSE:	5.82	NA	NA

MAX_MEAN: 0.0862 **MAX_MED:** 0.00893 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

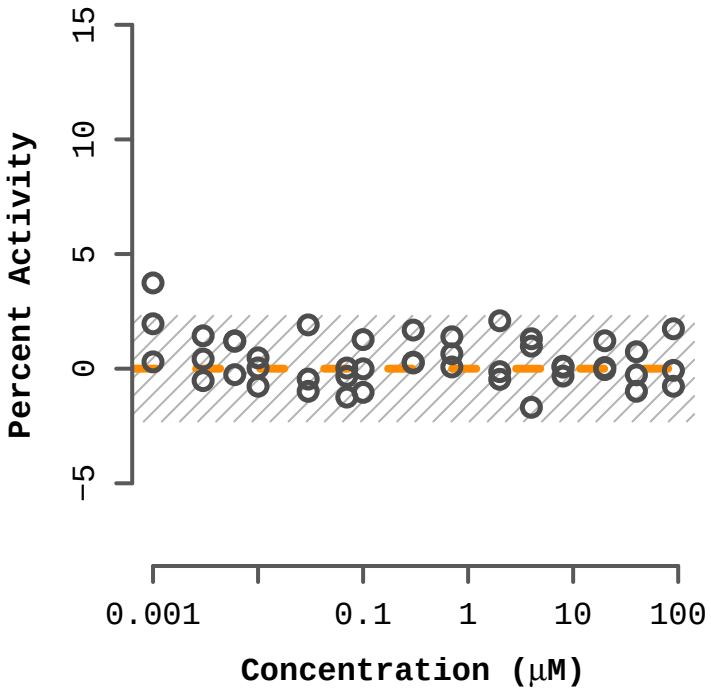
NAME: Tetraethylene glycol di(2-ethylhexanoate)
CHID: 27797 **CASRN:** 18268-70-7
SPID(S): Tox21_301106
M4ID: 12478027

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 0.8 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

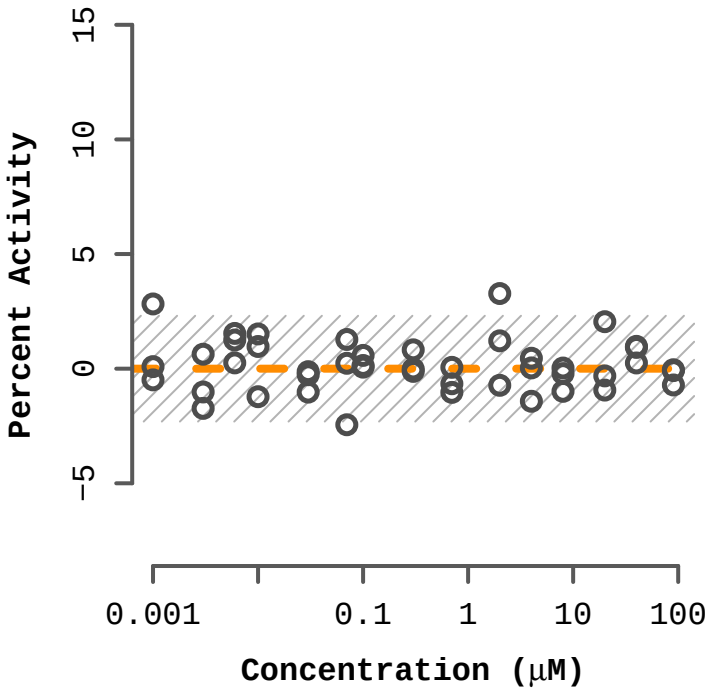
NAME: N-Ethyl-2-methyl-2-propen-1-amine
CHID: 27798 **CASRN:** 18328-90-0
SPID(S): Tox21_303447
M4ID: 12475693

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

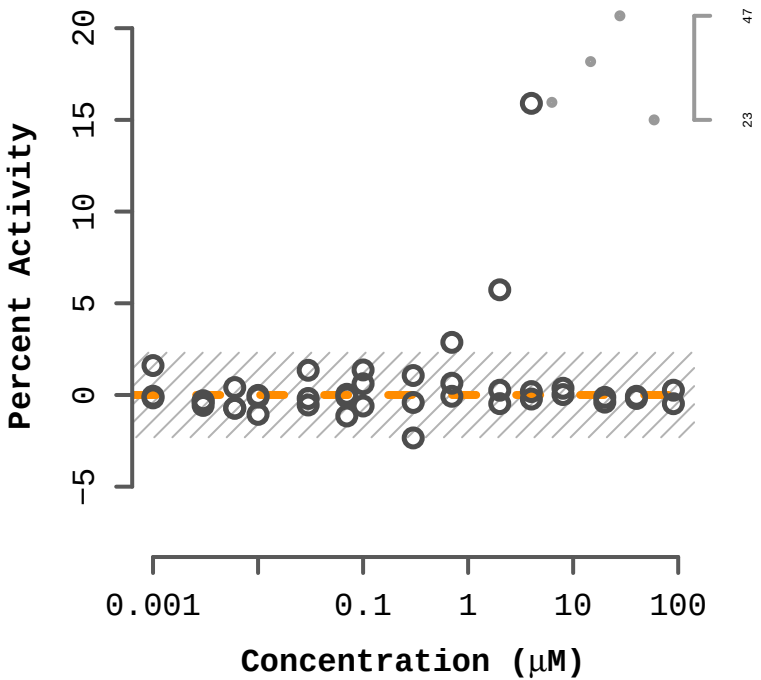
NAME: N-Ethyl-2-methyl-2-propen-1-amine
CHID: 27798 **CASRN:** 18328-90-0
SPID(S): Tox21_202086
M4ID: 12480166

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

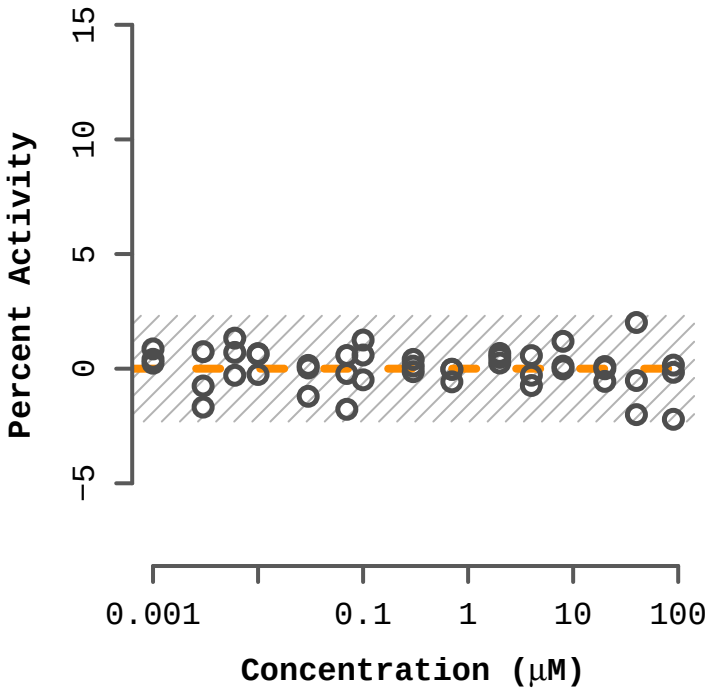
NAME: 1,2-Propanediol, dibenzoate
CHID: 27802 **CASRN:** 19224-26-1
SPID(S): Tox21_201183
M4ID: 12481069 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	257.76	NA	NA
PROB:	1	NA	NA
RMSE:	10.57	NA	NA

MAX_MEAN: 15.4 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

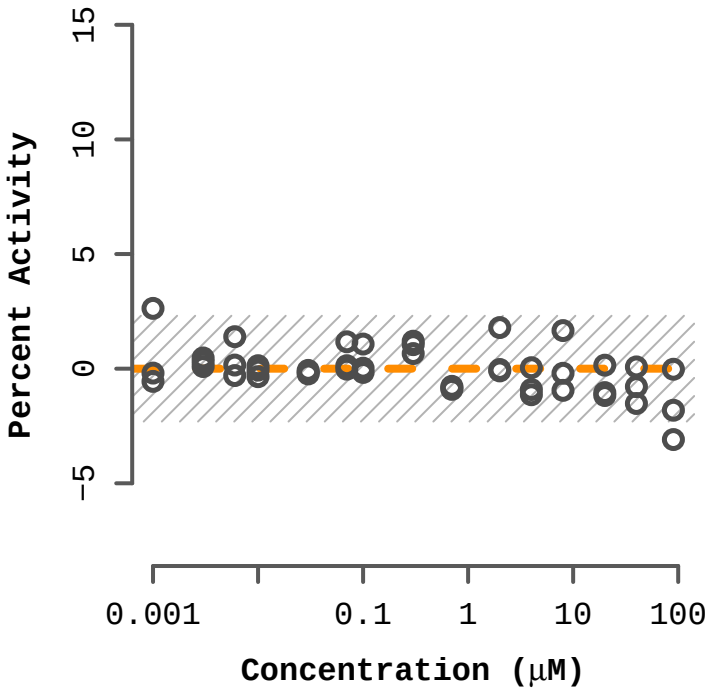
NAME: N-Ethyl-N-(3-methylphenyl)ethane-1,2-diamine
CHID: 27803 **CASRN:** 19248-13-6
SPID(S): Tox21_303371
M4ID: 12475764

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.711 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

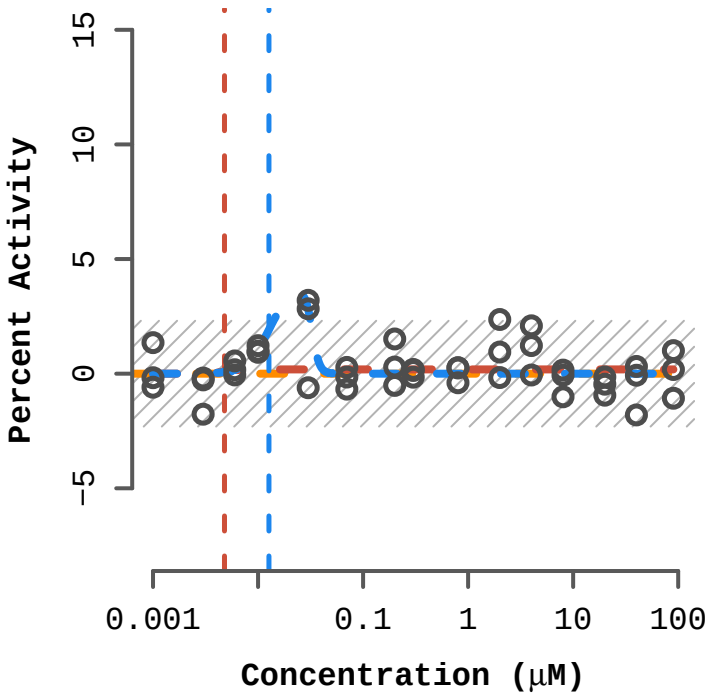
NAME: N-Ethyl-N-(3-methylphenyl)ethane-1,2-diamine
CHID: 27803 CASRN: 19248-13-6
SPID(S): Tox21_202192
M4ID: 12480060

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.6	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.97 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-2-methylpropionitrile
CHID: 27804 **CASRN:** 19355-69-2
SPID(S): Tox21_202756
M4ID: 12479496

HILL MODEL (in red):

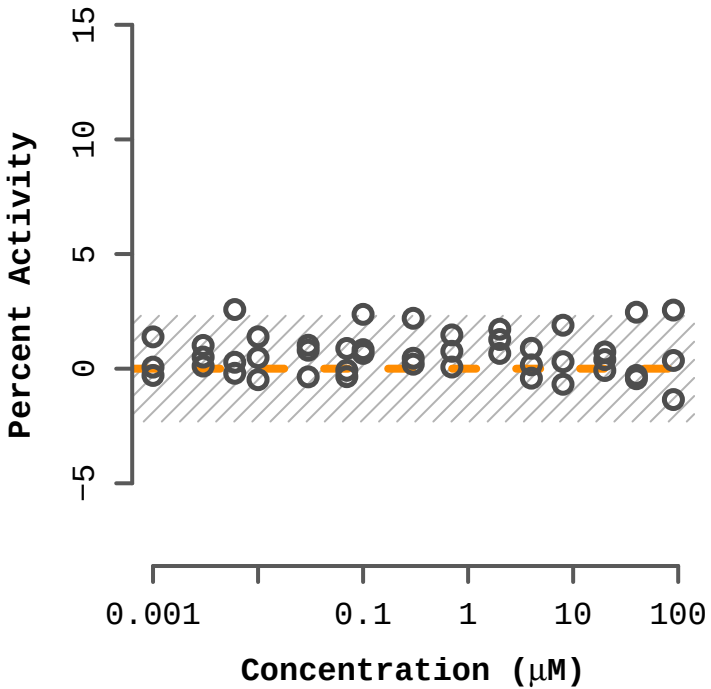
	tp	ga	gw
val:	0.186	−2.32	8
sd:	0.147	0.372	16.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.84	−1.9	4.1	−1.49	12.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	131.2	135.53	125.85
PROB:	0.06	0.01	0.93
RMSE:	1.07	1.03	0.96

MAX_MEAN: 1.81 **MAX_MED:** 2.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

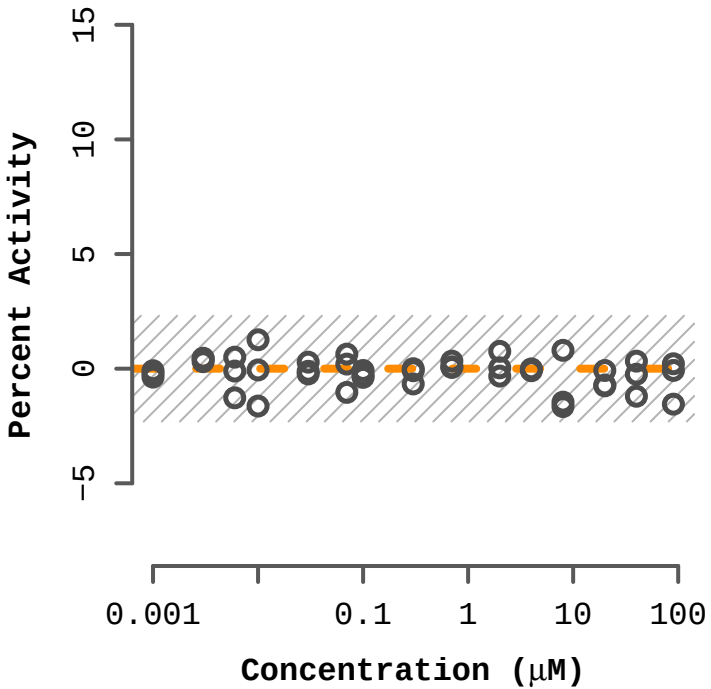
NAME: 4-Methylphthalic anhydride
CHID: 27805 **CASRN:** 19438-61-0
SPID(S): Tox21_303399
M4ID: 12475740

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

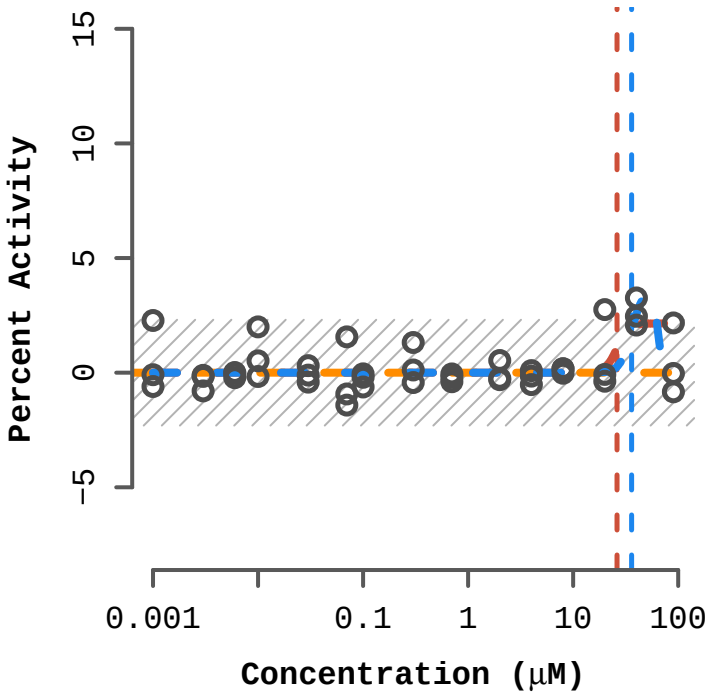
NAME: 4-Methylphthalic anhydride
CHID: 27805 **CASRN:** 19438-61-0
SPID(S): Tox21_202214
M4ID: 12480038

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.401 **MAX_MED:** 0.439 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Potassium anilinoacetate
CHID: 27806 **CASRN:** 19525-59-8
SPID(S): Tox21_303539
M4ID: 12475605

HILL MODEL (in red):

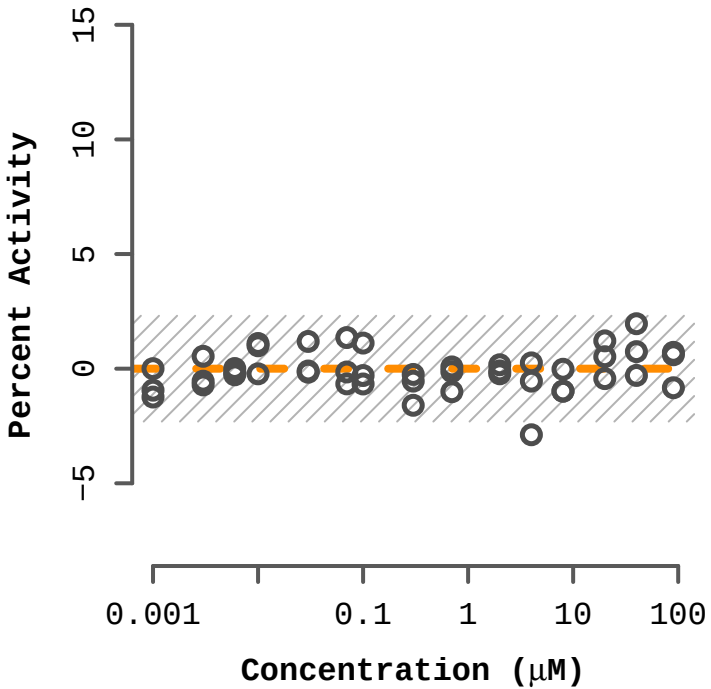
	tp	ga	gw
val:	2.15	1.42	8
sd:	0.353	0.0732	3.94

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.66	1.56	8	1.81	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	128.6	121.42	115.03
PROB:	0	0.04	0.96
RMSE:	1.09	0.96	0.86

MAX_MEAN: 2.6 **MAX_MED:** 2.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

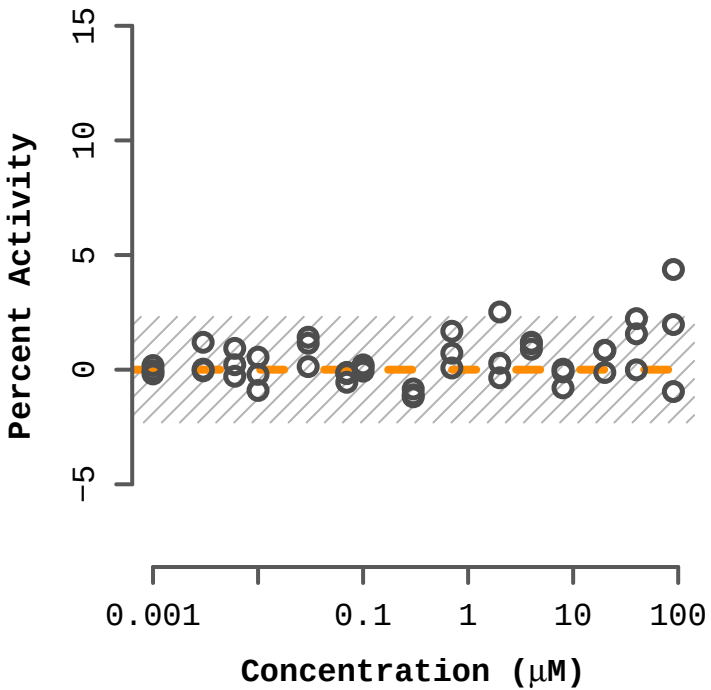
NAME: 1,1-Dichloro-3,3-dimethylbutan-2-one
CHID: 27822 **CASRN:** 22591-21-5
SPID(S): Tox21_200131
M4ID: 12482121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.804 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

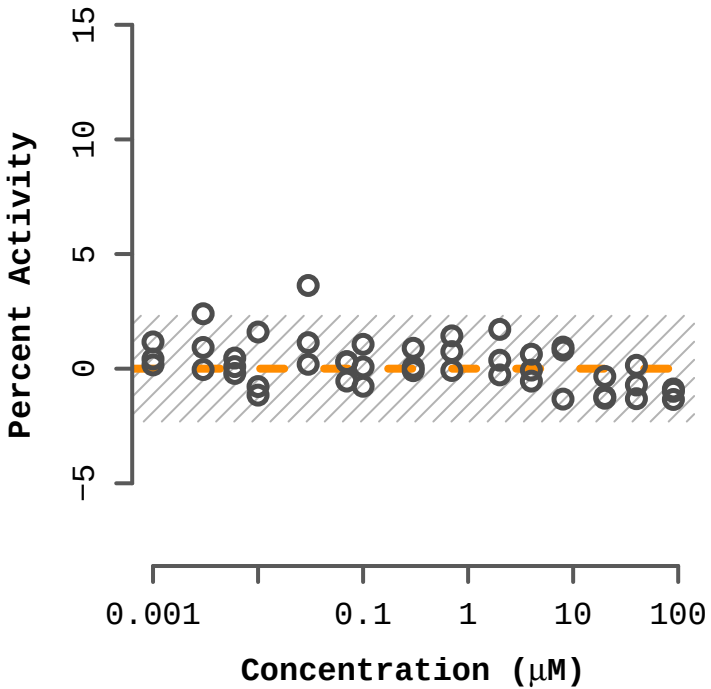
NAME: 2-Butanone, O,O',O''-(methylsilylidyne)trioxim
CHID: 27823 **CASRN:** 22984-54-9
SPID(S): Tox21_200464
M4ID: 12481788

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

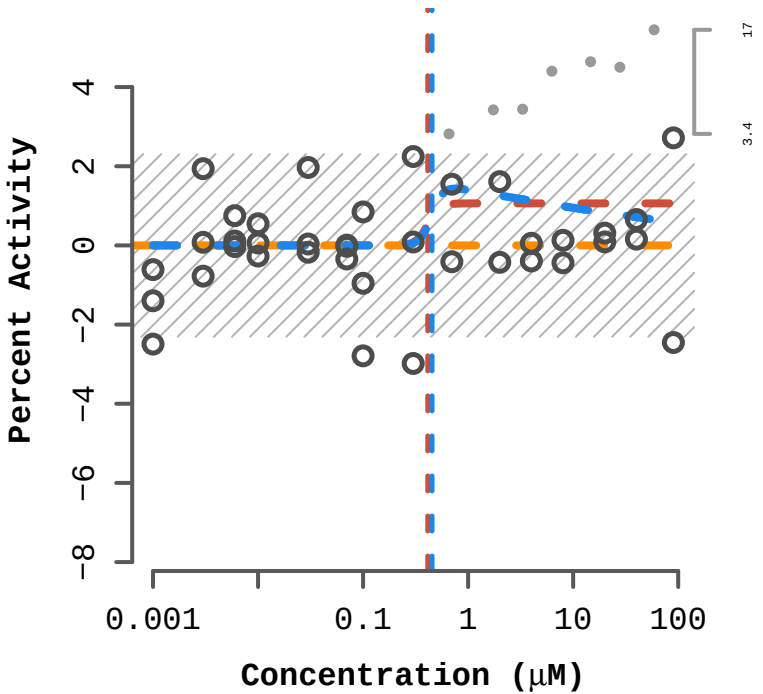
NAME: Dicyclohexyl sodium sulfosuccinate
CHID: 27826 **CASRN:** 23386-52-9
SPID(S): Tox21_303387
M4ID: 12475751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dicyclohexyl sodium sulfosuccinate
CHID: 27826 CASRN: 23386-52-9
SPID(S): Tox21_202103
M4ID: 12480149 BRK

HILL MODEL (in red):

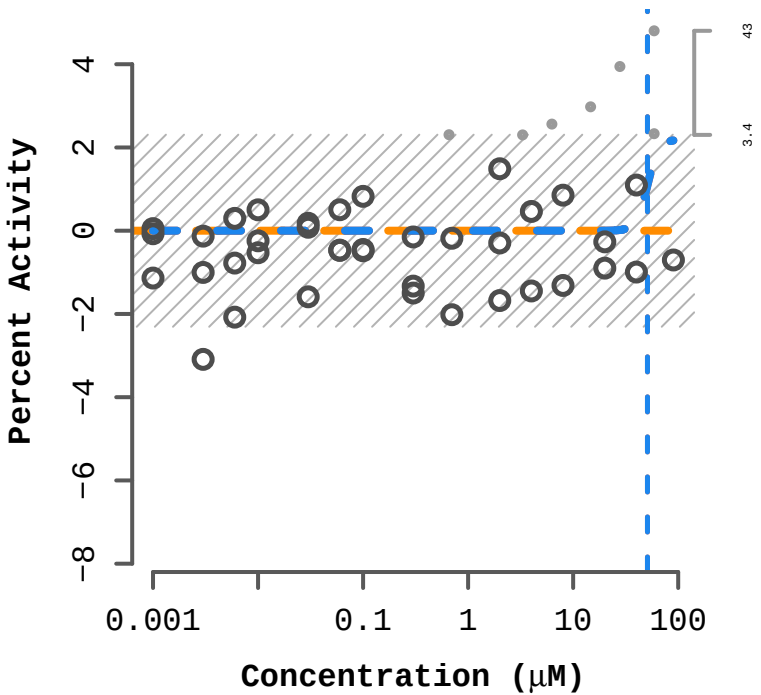
	tp	ga	gw
val:	1.06	−0.384	8
sd:	0.556	0.499	21.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.68	−0.344	8	0.131	0.3
sd:	20.2	0.715	28.8	20.4	1.06

	CNST	HILL	GNLS
AIC:	233.55	235.22	239.07
PROB:	0.67	0.29	0.04
RMSE:	4.41	4.07	4.13

MAX_MEAN: 5.69 **MAX_MED:** 2.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,5,8,11-Tetraoxatridecan-13-ol
CHID: 27829 CASRN: 23783-42-8
SPID(S): Tox21_200748
M4ID: 12481504 BRK

HILL MODEL (in red):

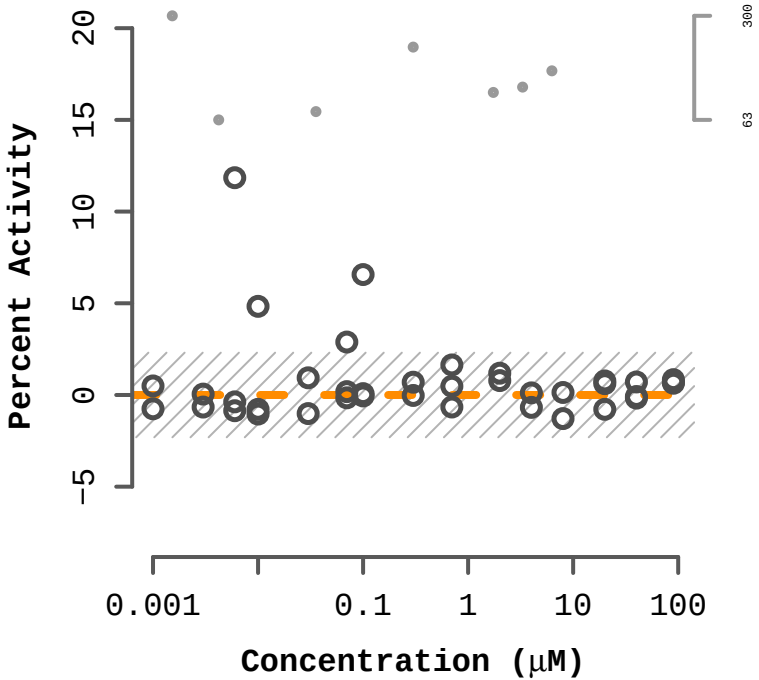
	tp	ga	gw
val:	2.19	1.71	8
sd:	2.7	1.24	86.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.19	1.71	8	2.18	16.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	235.89	240.8	244.8
PROB:	0.91	0.08	0.01
RMSE:	8.29	8.01	8.01

MAX_MEAN: 15.5 MAX_MED: 3.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

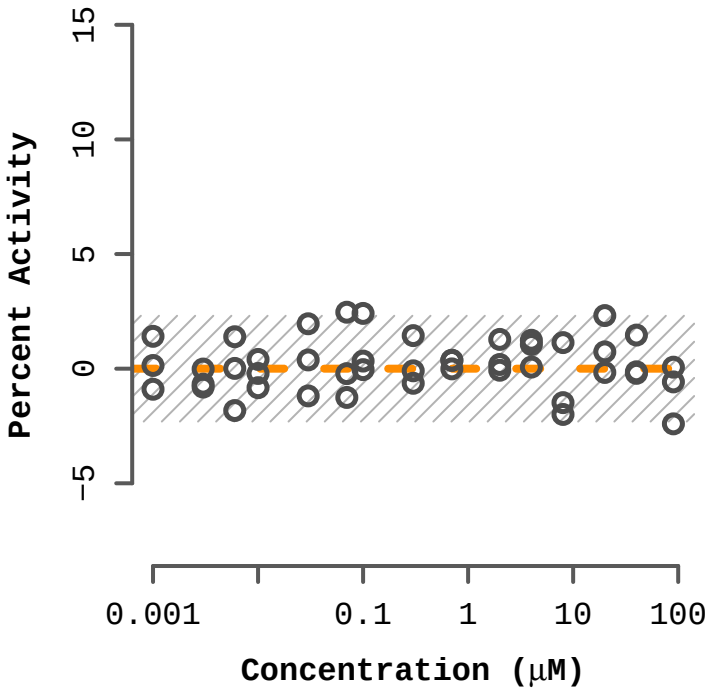
NAME: 3-(Chloromethyl)-1,2,3-benzotriazin-4(3H)-one
CHID: 27830 **CASRN:** 24310-41-6
SPID(S): Tox21_301065
M4ID: 12478068 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	428.31	NA	NA
PROB:	1	NA	NA
RMSE:	70.7	NA	NA

MAX_MEAN: 101 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

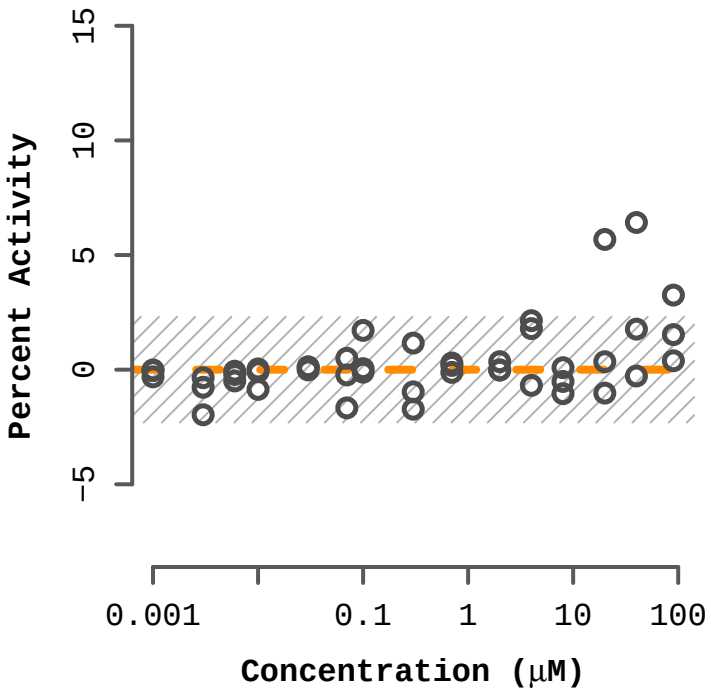
NAME: Carbonochloridic acid, 2-ethylhexyl ester
CHID: 27832 **CASRN:** 24468-13-1
SPID(S): Tox21_303512
M4ID: 12475630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

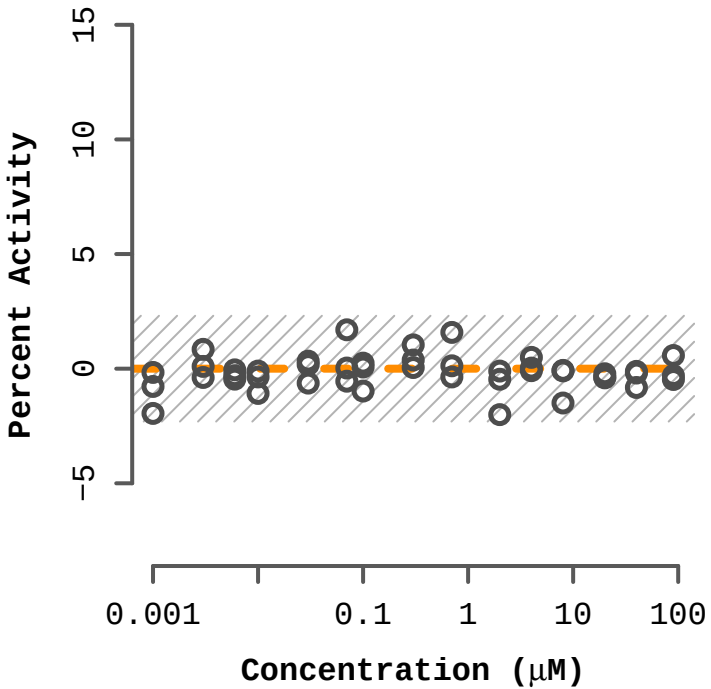
NAME: Carbonochloridic acid, 2-ethylhexyl ester
CHID: 27832 **CASRN:** 24468-13-1
SPID(S): Tox21_201491
M4ID: 12480761

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 2.64 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

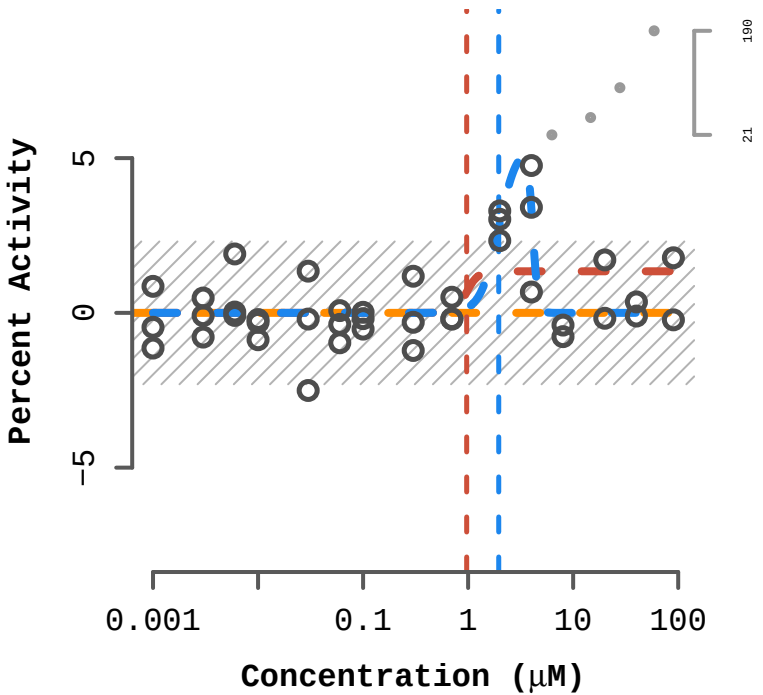
NAME: 2-Ethyl-6-methylaniline
CHID: 27833 **CASRN:** 24549-06-2
SPID(S): Tox21_303552
M4ID: 12475593

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.49 **MAX_MED:** 0.378 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethyl-6-methylaniline
CHID: 27833 **CASRN:** 24549-06-2
SPID(S): Tox21_201802
M4ID: 12480450 **BRK**

HILL MODEL (in red):

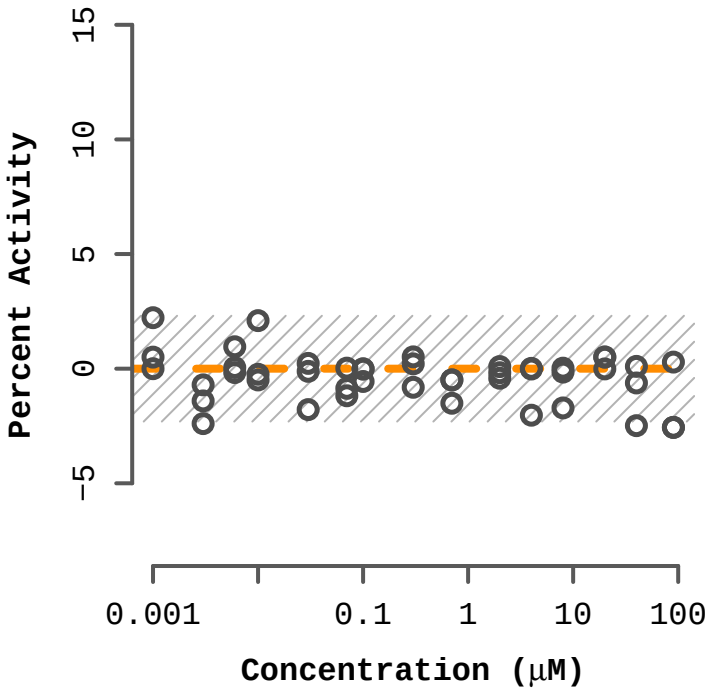
	tp	ga	gw
val:	1.34	−0.0139	8
sd:	0.496	0.316	12.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.48	0.291	5.03	0.615	17.8
sd:	43	1.42	18.5	0.325	288

	CNST	HILL	GNLS
AIC:	284.71	283.06	274.63
PROB:	0.01	0.01	0.98
RMSE:	33.41	33.07	33.39

MAX_MEAN: 65 **MAX_MED:** 3.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

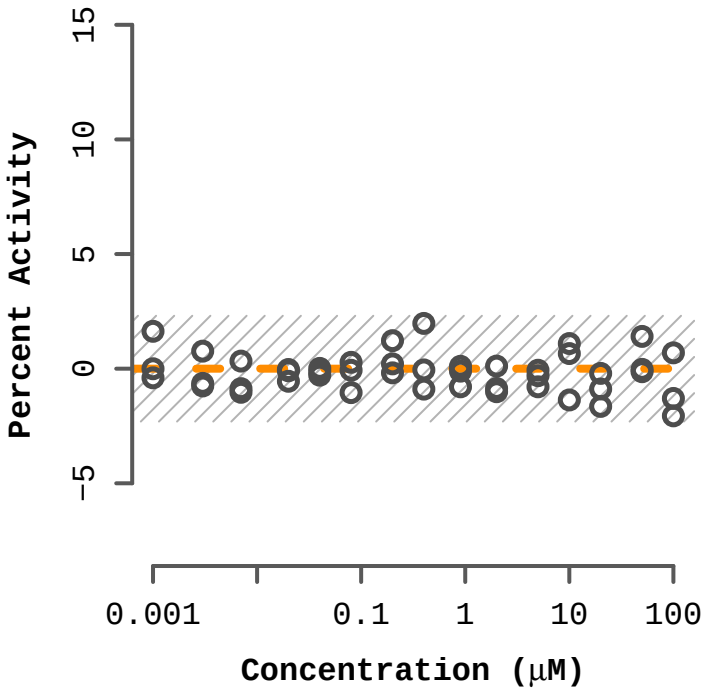
NAME: 2-Carboxyethyl acrylate
CHID: 27834 CASRN: 24615-84-7
SPID(S): Tox21_303489
M4ID: 12475652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.911 MAX_MED: 0.506 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

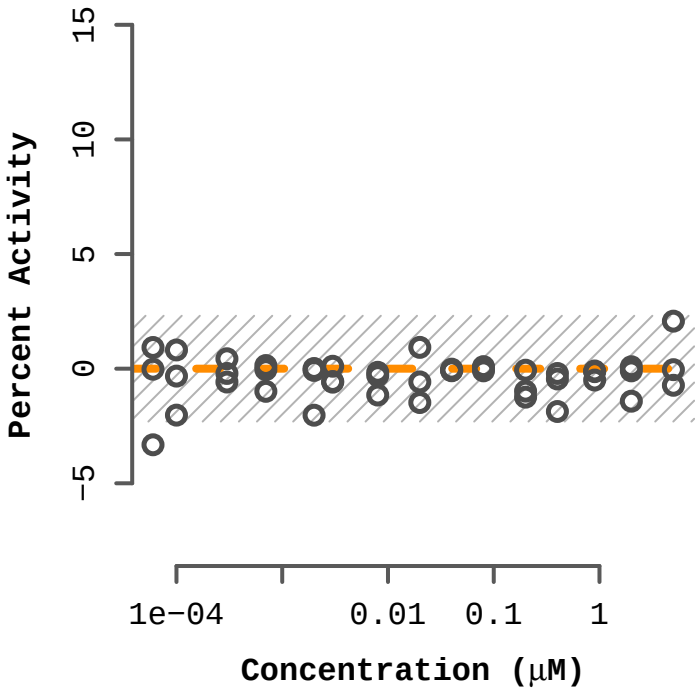
NAME: 2-Carboxyethyl acrylate
CHID: 27834 CASRN: 24615-84-7
SPID(S): Tox21_202236
M4ID: 12480016

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.418 MAX_MED: 0.661 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

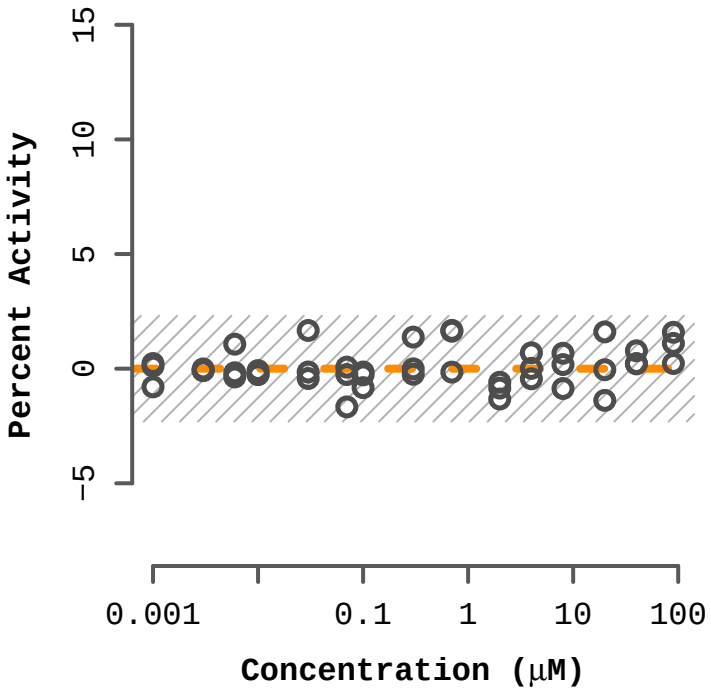
NAME: Potassium (2E,4E)-hexa-2,4-dienoate
CHID: 27835 **CASRN:** 24634-61-5
SPID(S): Tox21_202757
M4ID: 12479495

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.436 **MAX_MED:** 0.0422 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

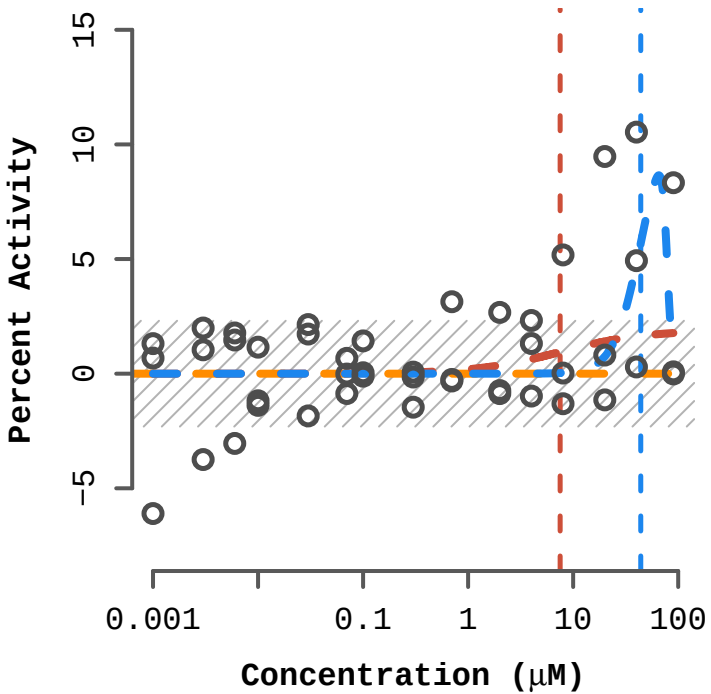
NAME: Tripropylene glycol
CHID: 27837 CASRN: 24800-44-0
SPID(S): Tox21_303535
M4ID: 12475609

HILL MODEL: Not applicable.

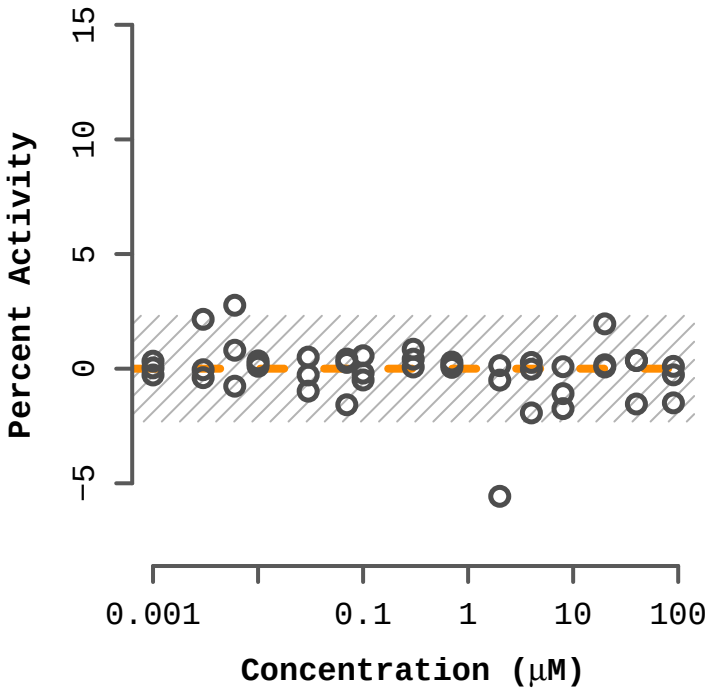
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.05 MAX_MED: 1.63 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tripropylene glycol
CHID:    27837   CASRN: 24800-44-0
SPID(S): Tox21_202104
M4ID:    12480148

HILL MODEL (in red):
      tp       ga       gw
val:  1.89     0.876    1.08
sd:   1.92     1.16     2.06

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  11.4     1.64     3.36     1.89     17.7
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  219.44      221.75      223.28
PROB: 0.68        0.22        0.1
RMSE: 3.15        2.81        2.75

MAX_MEAN: 5.25      MAX_MED: 4.93      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

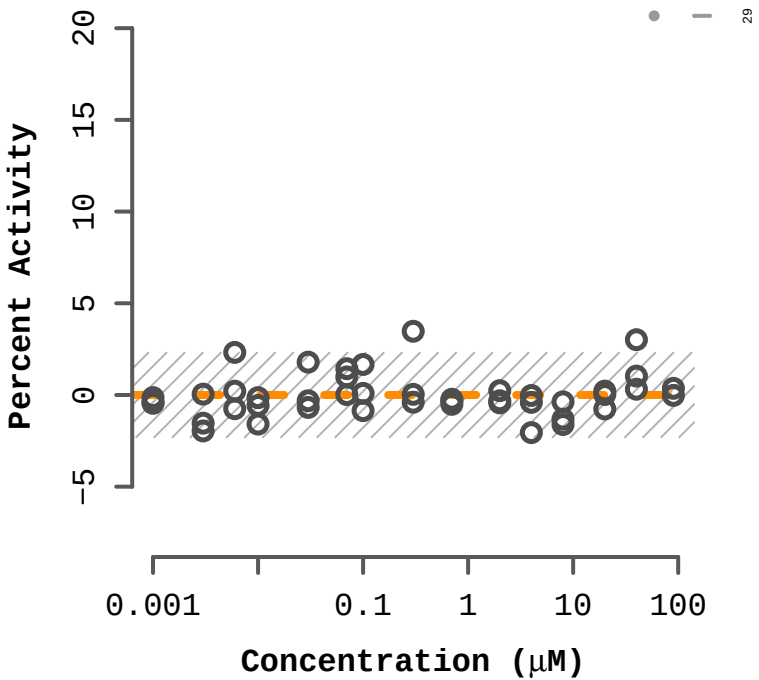
NAME: Isooctyl 2-mercaptoacetate
CHID: 27841 CASRN: 25103-09-7
SPID(S): Tox21_303417
M4ID: 12475722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.937 MAX_MED: 0.805 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

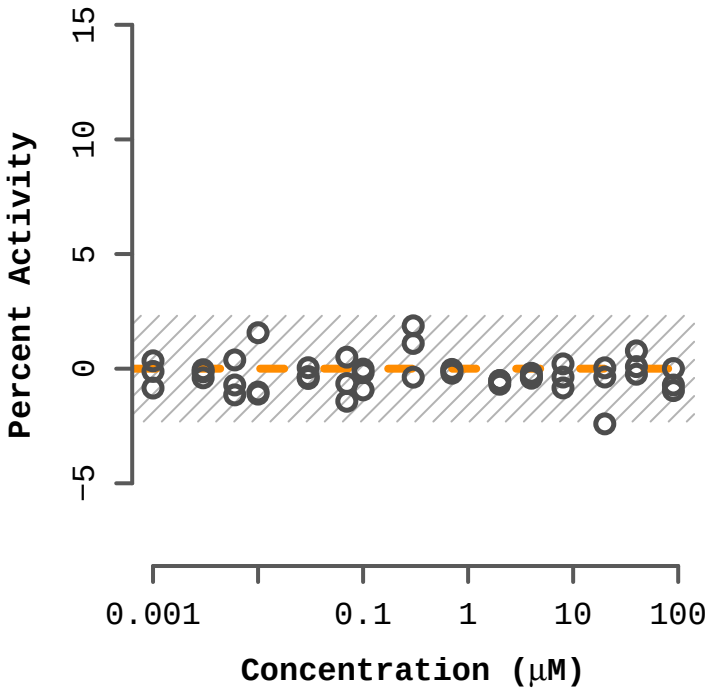
NAME: Methylnadic anhydride
CHID: 27844 CASRN: 25134-21-8
SPID(S): Tox21_201205
M4ID: 12481047 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.37	NA	NA
PROB:	1	NA	NA
RMSE:	4.5	NA	NA

MAX_MEAN: 9.86 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

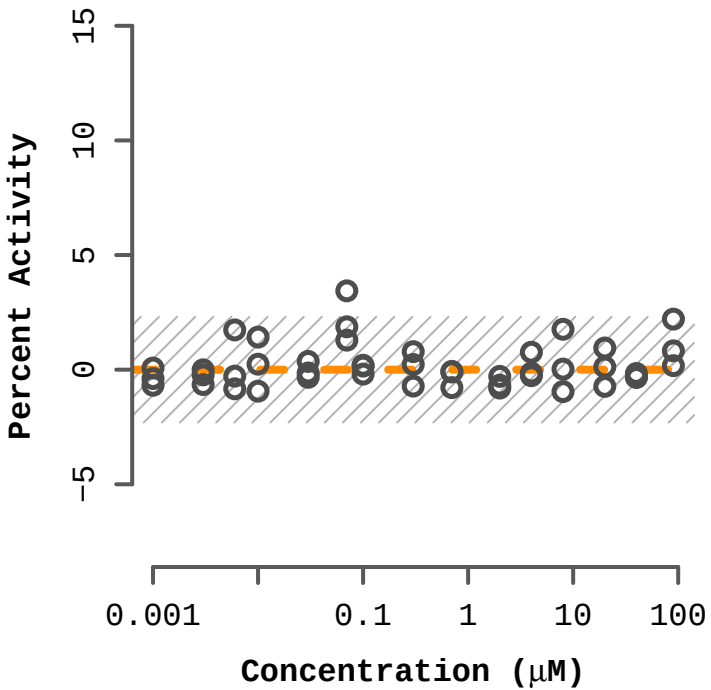
NAME: 2,4,4−Trimethylpentene
CHID: 27851 **CASRN:** 25167−70−8
SPID(S): Tox21_202554
M4ID: 12479698

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.868 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

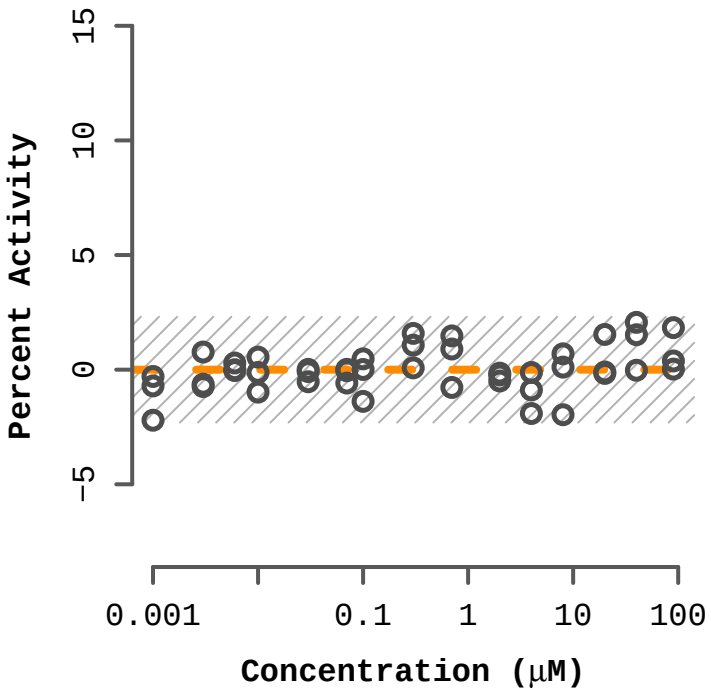
NAME: Chlorotoluene
CHID: 27852 CASRN: 25168-05-2
SPID(S): Tox21_300922
M4ID: 12478211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 2.2 MAX_MED: 1.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

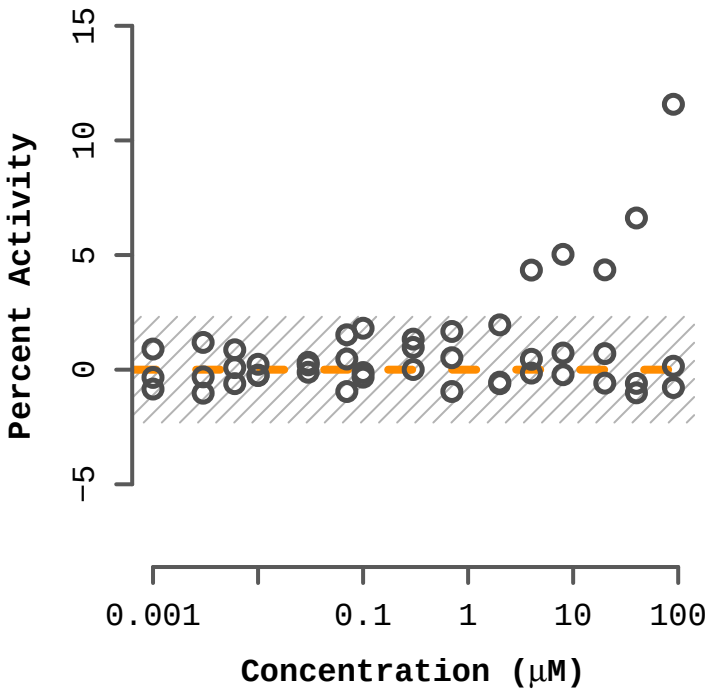
NAME: Dipropylene glycol
CHID: 27856 **CASRN:** 25265-71-8
SPID(S): Tox21_300565
M4ID: 12478568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

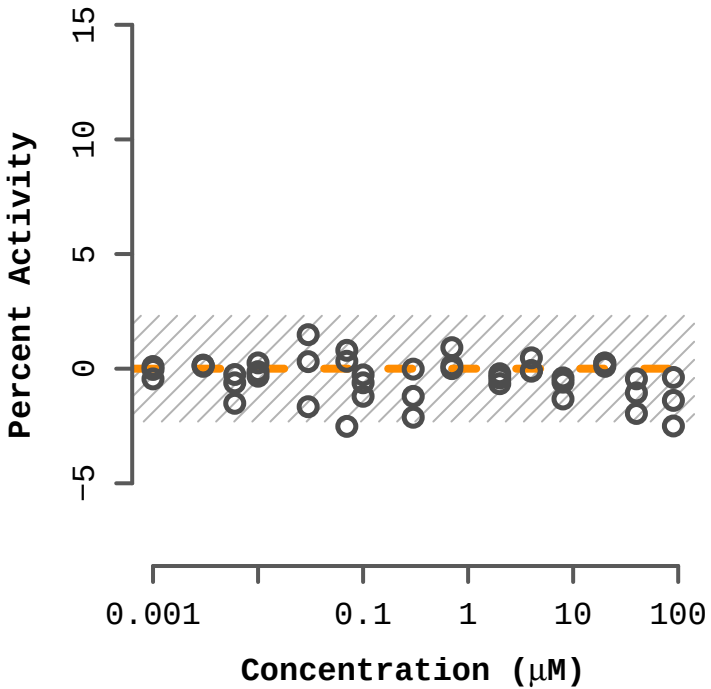
NAME: Dipropylene glycol
CHID: 27856 **CASRN:** 25265-71-8
SPID(S): Tox21_202321
M4ID: 12479931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.44	NA	NA

MAX_MEAN: 3.65 **MAX_MED:** 0.971 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2,4−Trimethyl−1,3−pentanediol monoisobutyrat

CHID: 27857 **CASRN:** 25265−77−4

SPID(S): Tox21_200148

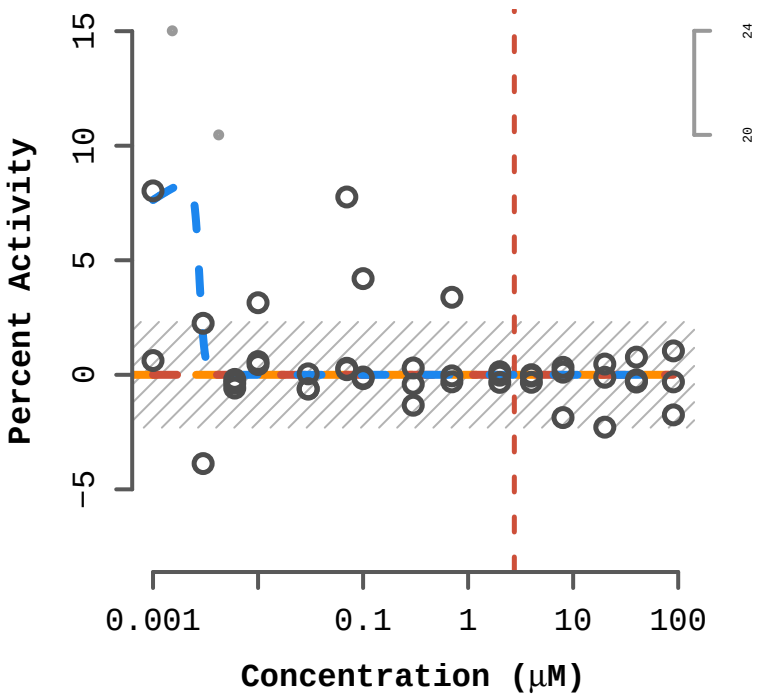
M4ID: 12482104

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.351 **MAX_MED:** 0.324 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diisopropylbenzene
CHID: 27858 CASRN: 25321-09-9
SPID(S): Tox21_202758
M4ID: 12479494 BRK

HILL MODEL (in red):

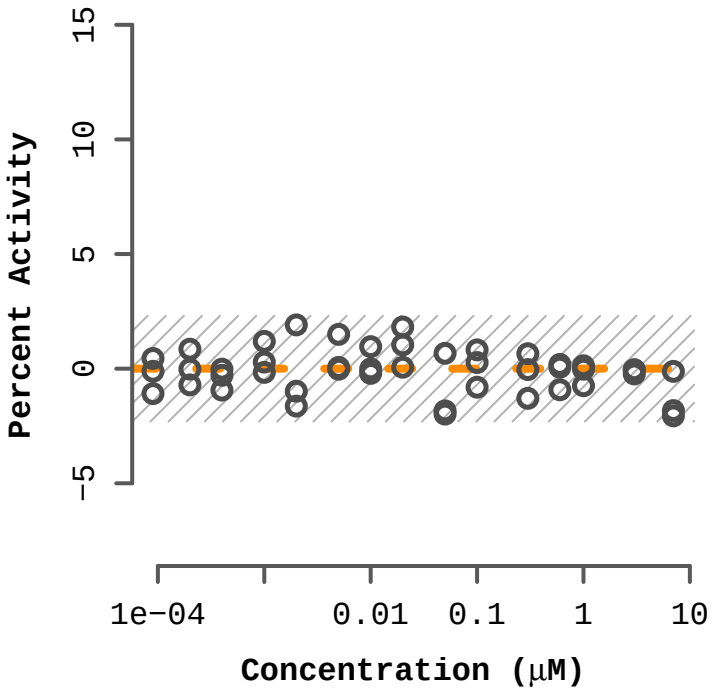
	tp	ga	gw
val:	5.71e-10	0.44	2.47
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.97	-3.69	0.738	-2.56	17.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	216.22	222.22	220.24
PROB:	0.84	0.04	0.11
RMSE:	5.14	5.14	4.24

MAX_MEAN: 10.9 MAX_MED: 8.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

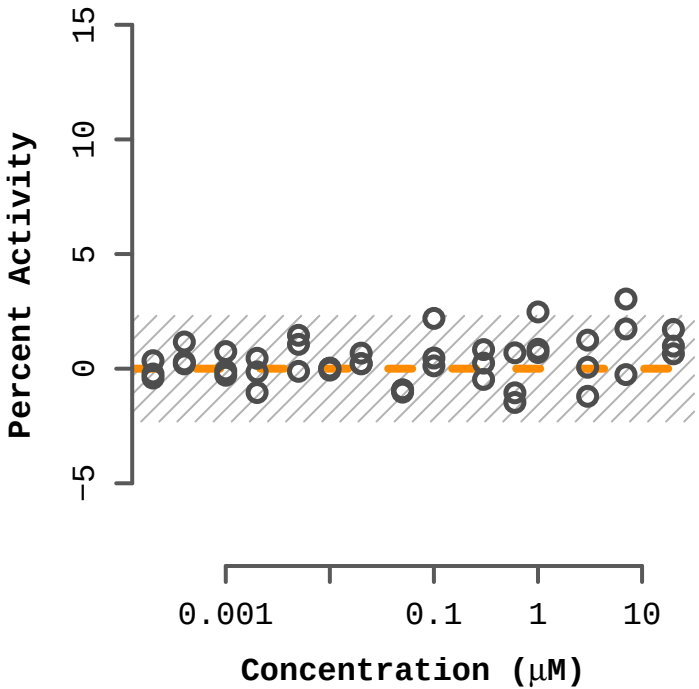
NAME: Polypropylene glycol
CHID: 27863 **CASRN:** 25322-69-4
SPID(S): Tox21_301441
M4ID: 12477692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.974 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

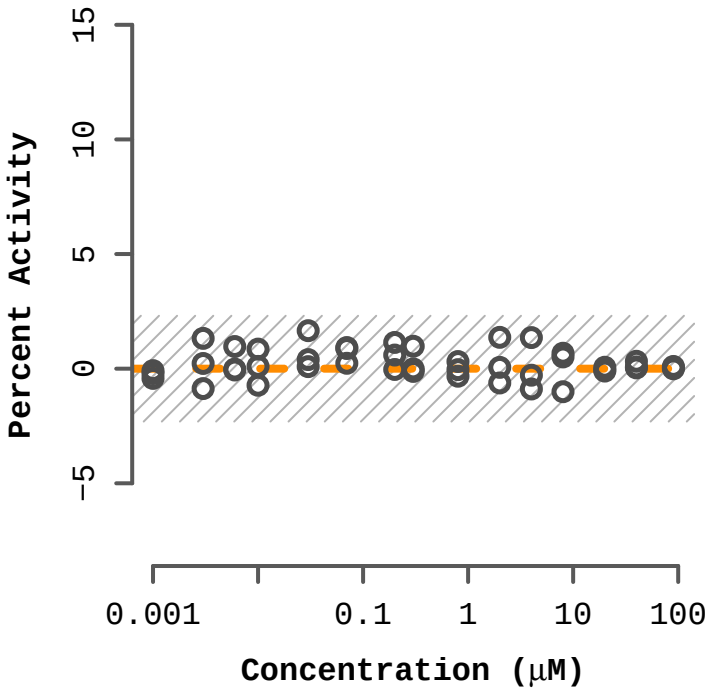
NAME: Diethylbenzene
CHID: 27866 **CASRN:** 25340-17-4
SPID(S): Tox21_303467
M4ID: 12475673

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

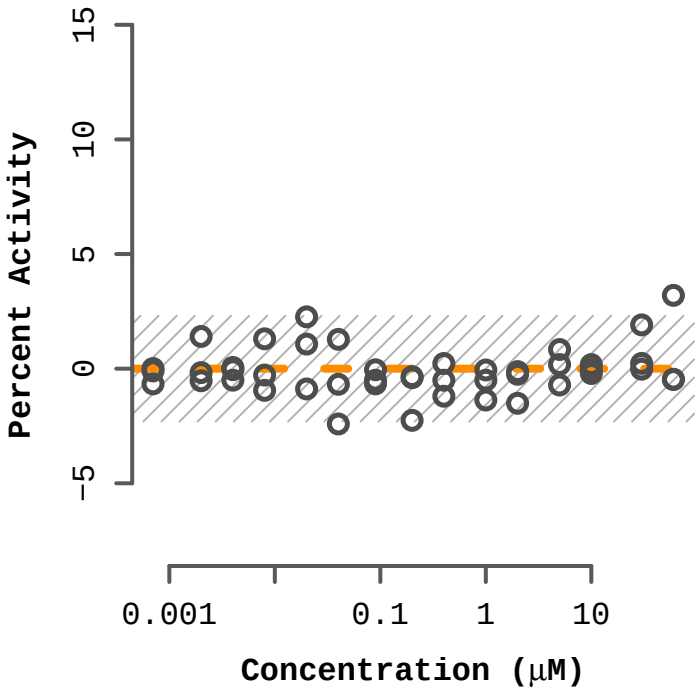
NAME: Diethylbenzene
CHID: 27866 **CASRN:** 25340-17-4
SPID(S): Tox21_202258
M4ID: 12479994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.716 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

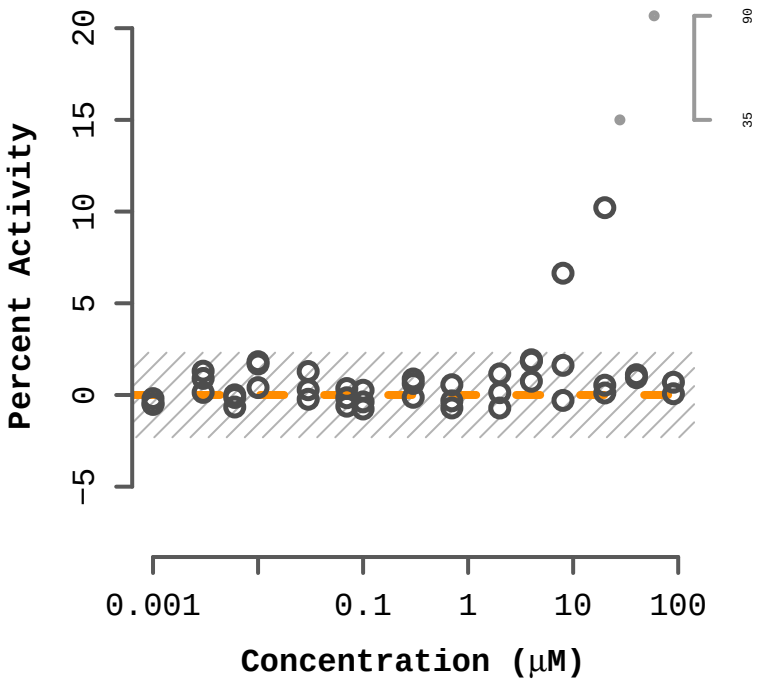
NAME: tert-Nonanethiol
CHID: 27868 **CASRN:** 25360-10-5
SPID(S): Tox21_303530
M4ID: 12475613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

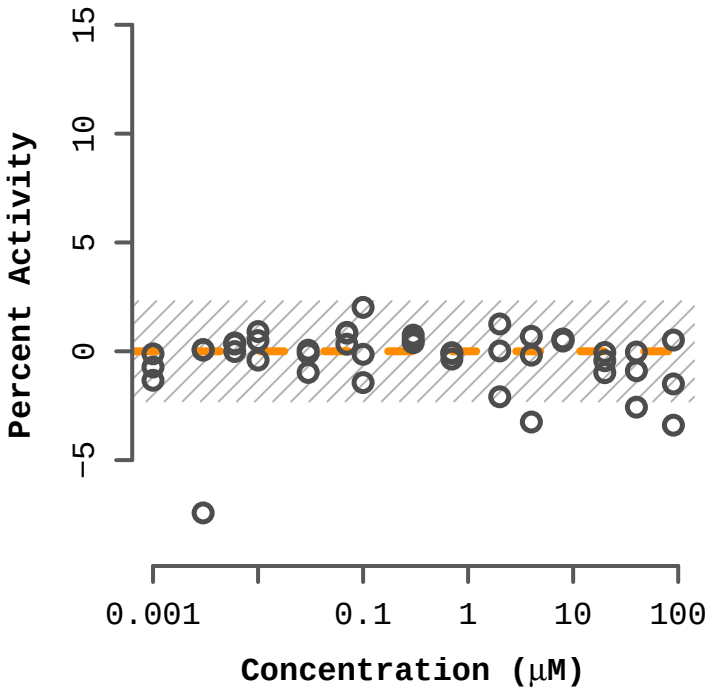
NAME: tert-Nonanethiol
CHID: 27868 **CASRN:** 25360-10-5
SPID(S): Tox21_201651
M4ID: 12480601 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.55	NA	NA
PROB:	1	NA	NA
RMSE:	14.59	NA	NA

MAX_MEAN: 30.4 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

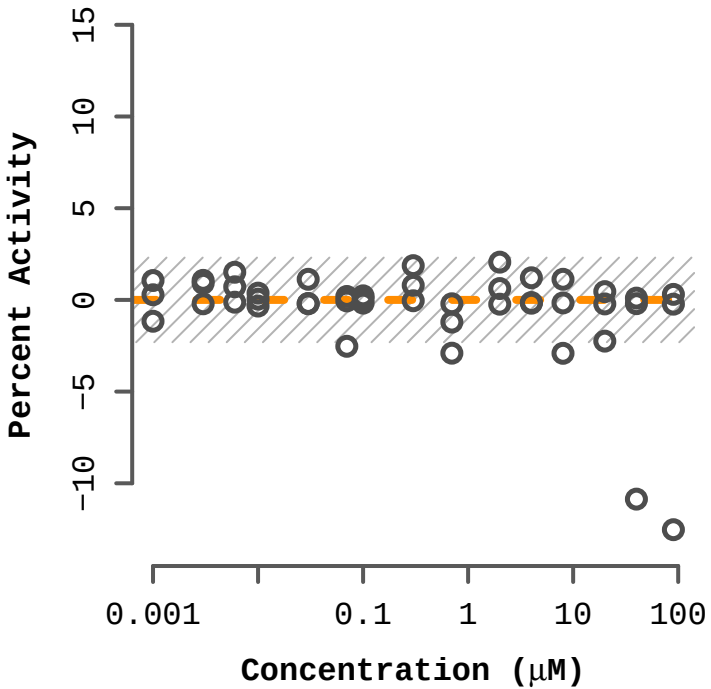
NAME: 3-(Dodecenyl)dihydro-2,5-furandione
CHID: 27870 **CASRN:** 25377-73-5
SPID(S): Tox21_303421
M4ID: 12475718

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 0.678 **MAX_MED:** 0.835 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

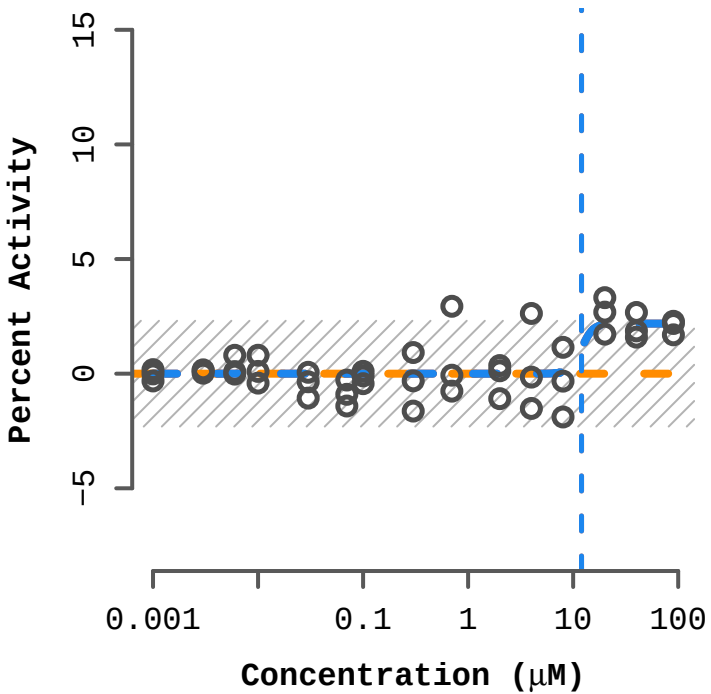
NAME: 3-(Dodecenyl)dihydro-2,5-furandione
CHID: 27870 **CASRN:** 25377-73-5
SPID(S): Tox21_201917
M4ID: 12480335

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.69	NA	NA

MAX_MEAN: 0.874 **MAX_MED:** 0.906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glyceryl monooleate
CHID: 27875 CASRN: 25496-72-4
SPID(S): Tox21_303545
M4ID: 12475599

HILL MODEL (in red):

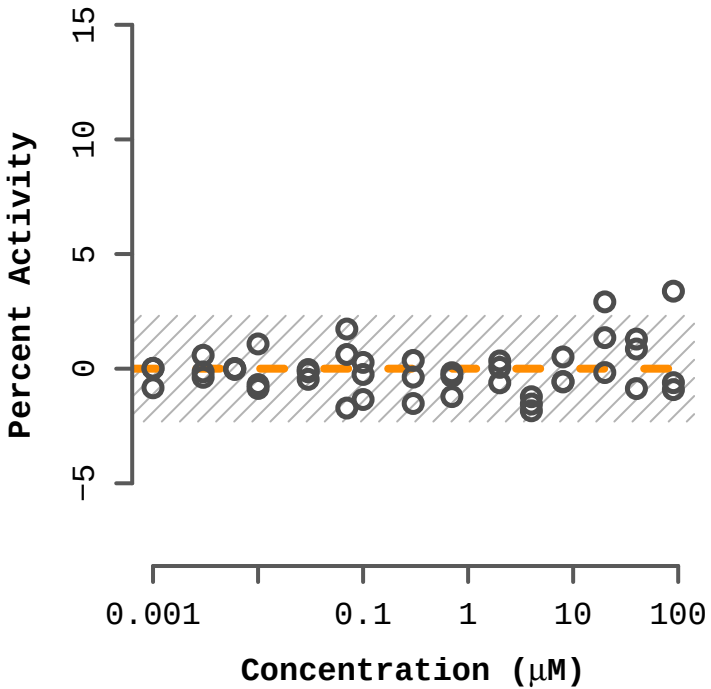
	tp	ga	gw
val:	2.18	1.08	8
sd:	0.231	0.132	5.29

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.18	1.08	8	3.94	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	156.52	120.27	124.27
PROB:	0	0.88	0.12
RMSE:	1.35	0.91	0.91

MAX_MEAN: 2.58 MAX_MED: 2.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

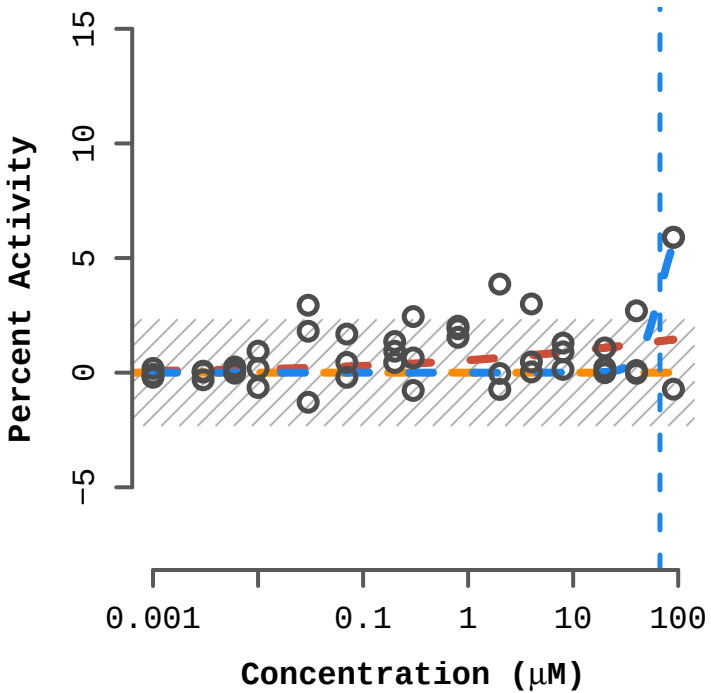
NAME: Diisodecylphenyl phosphite
CHID: 27877 **CASRN:** 25550-98-5
SPID(S): Tox21_303526
M4ID: 12475617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydroxypropyl acrylate
CHID: 27878 CASRN: 25584-83-2
SPID(S): Tox21_201177
M4ID: 12481075

HILL MODEL (in red):

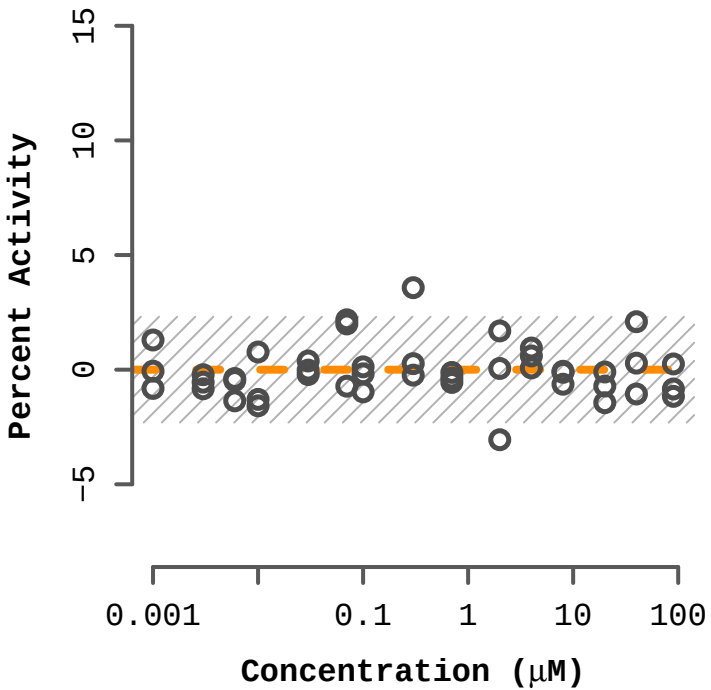
	tp	ga	gw
val:	3.46	2.43	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.09	1.83	4.5	3.32	8.9
sd:	13.8	0.62	9.87	371000	2520000

	CNST	HILL	GNLS
AIC:	170.35	166.08	168.89
PROB:	0.09	0.73	0.18
RMSE:	1.79	1.48	1.58

MAX_MEAN: 3.7 MAX_MED: 5.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

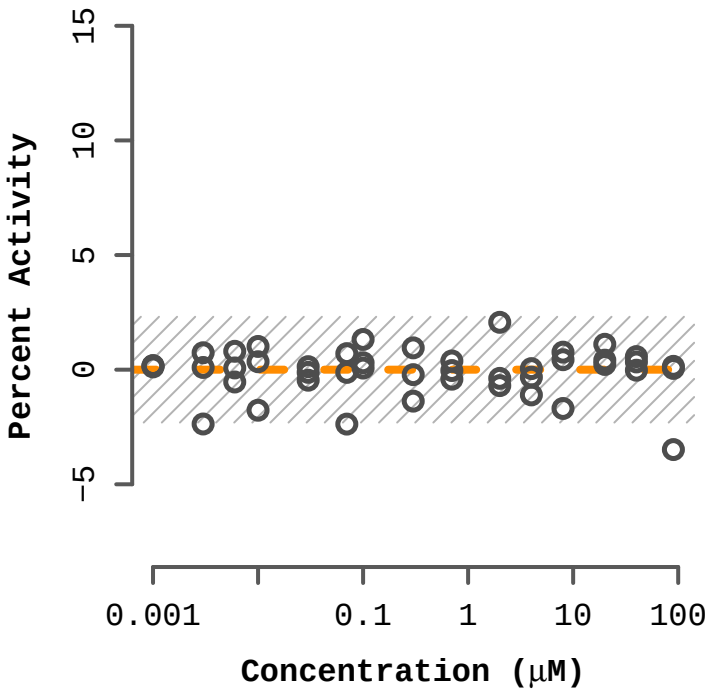
NAME: (2Z)-2-Pentenenitrile
CHID: 27884 **CASRN:** 25899-50-7
SPID(S): Tox21_301137
M4ID: 12477996

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1-dimethylp

CHID: 27886 **CASRN:** 25973-55-1

SPID(S): Tox21_200465

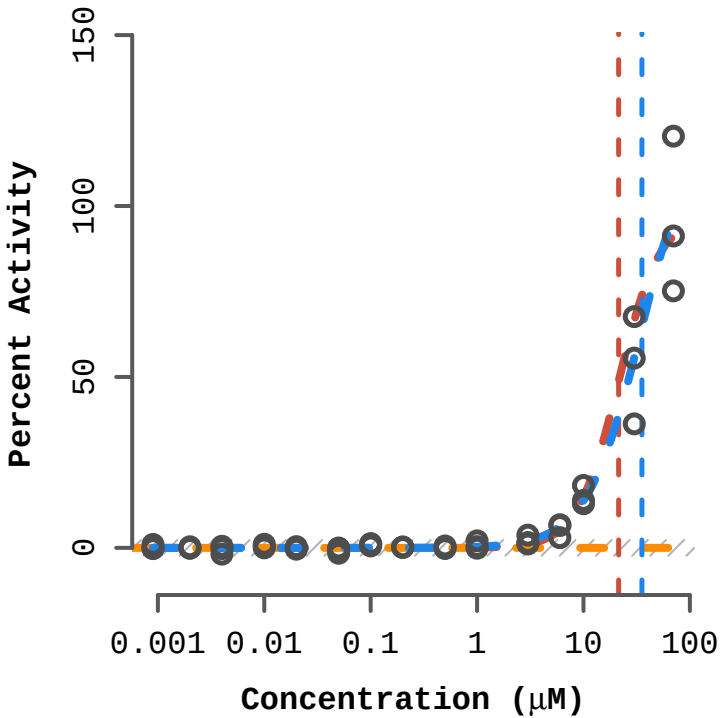
M4ID: 12481787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.585 **MAX_MED:** 0.436 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(2-ethylhexyl) tetrabromophthalate
CHID: 27887 CASRN: 26040-51-7
SPID(S): Tox21_302404
M4ID: 12476729

HILL MODEL (in red):

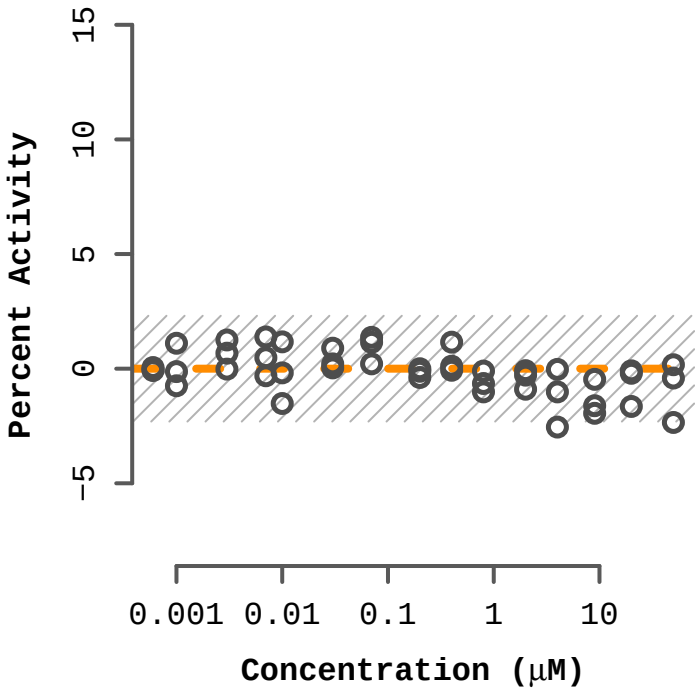
	tp	ga	gw
val:	97.5	1.33	2.25
sd:	1.95	0.0171	0.119

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	129	1.55	1.68	1.92	15.9
sd:	3.11	0.0155	0.0465	0.00906	1.69

	CNST	HILL	GNLS
AIC:	375.65	229.96	225.55
PROB:	0	0.1	0.9
RMSE:	29.17	6.98	6.12

MAX_MEAN: 95.6 MAX_MED: 91.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

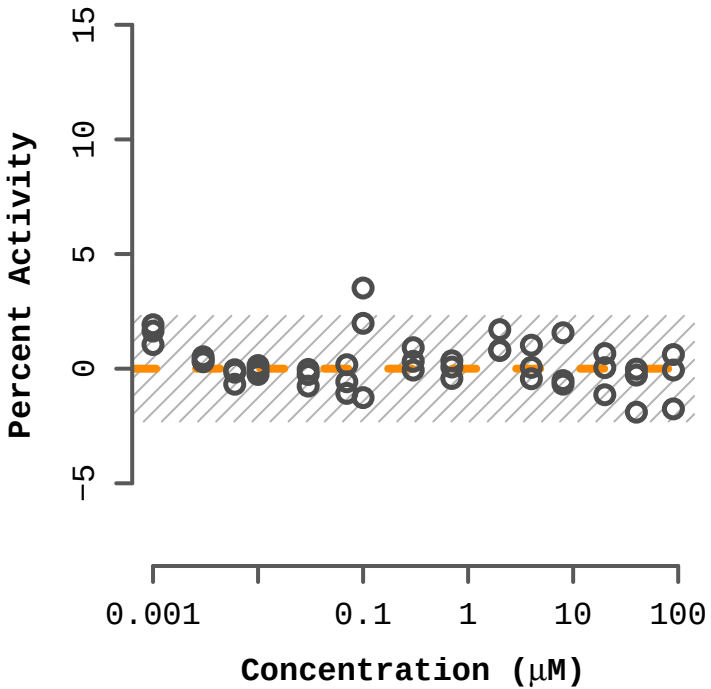
NAME: Calcium dodecylbenzene sulfonate
CHID: 27891 **CASRN:** 26264-06-2
SPID(S): Tox21_302388
M4ID: 12476745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

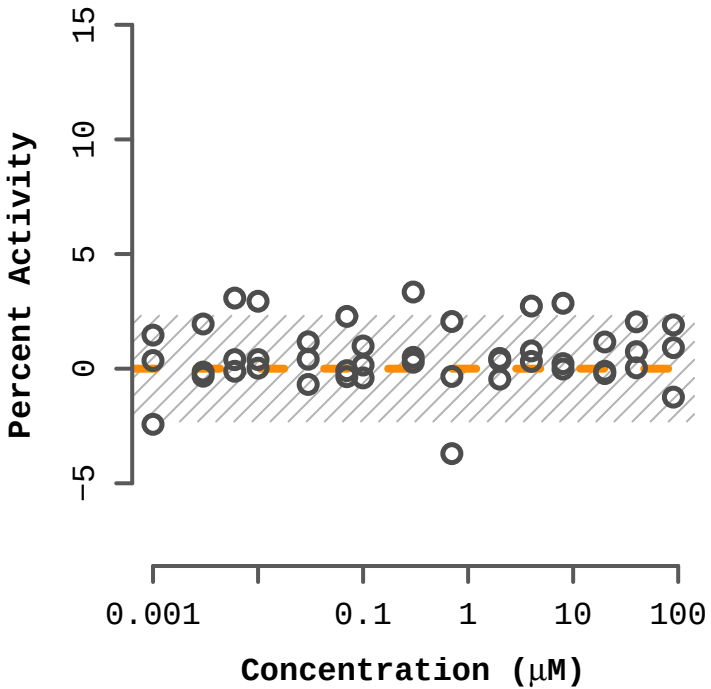
NAME: Ammonium xylene sulfonate
CHID: 27899 **CASRN:** 26447-10-9
SPID(S): Tox21_302389
M4ID: 12476744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

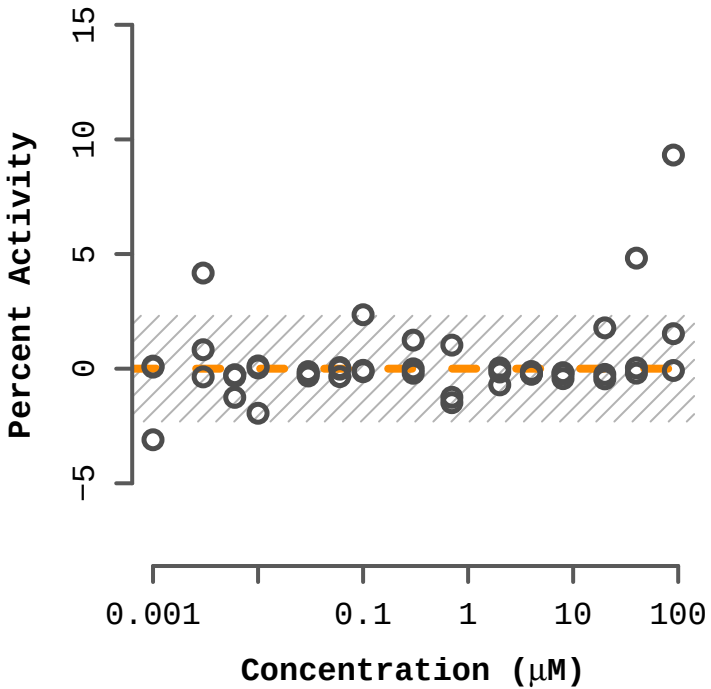
NAME: Methylcyclopentadiene dimer
CHID: 27902 **CASRN:** 26472-00-4
SPID(S): Tox21_303496
M4ID: 12475646

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

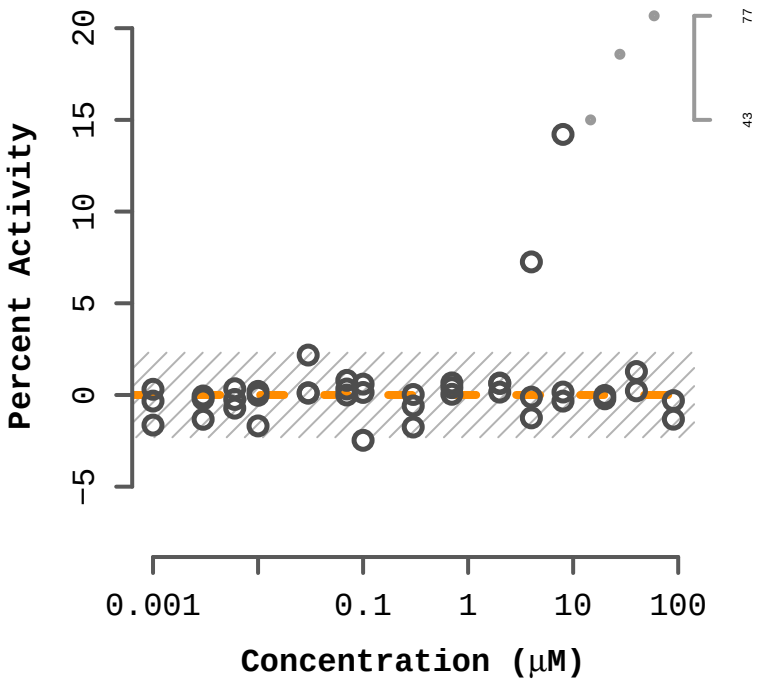
NAME: Methylcyclopentadiene dimer
CHID: 27902 **CASRN:** 26472-00-4
SPID(S): Tox21_201858
M4ID: 12480394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 3.59 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

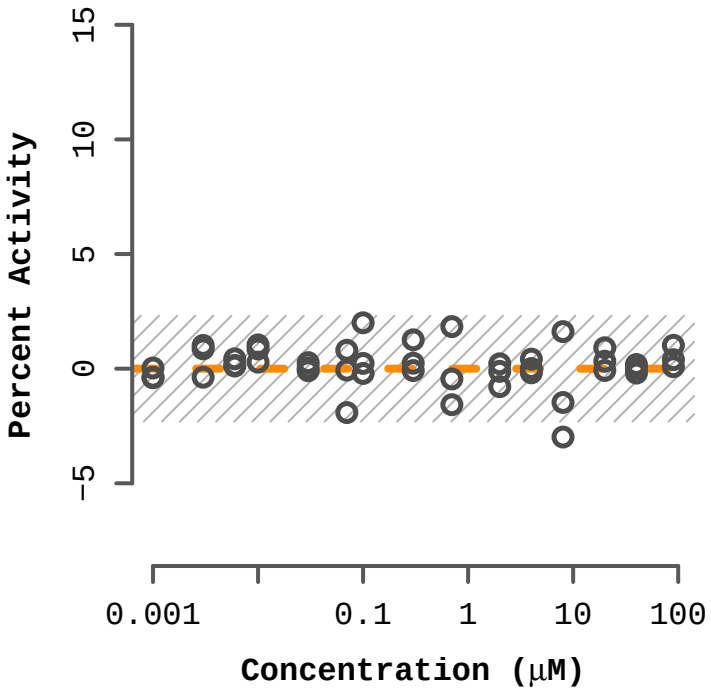
NAME: Dihydro-3-(tetrapropenyl)- 2,5-furandione
CHID: 27905 **CASRN:** 26544-38-7
SPID(S): Tox21_201216
M4ID: 12481036 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253.84	NA	NA
PROB:	1	NA	NA
RMSE:	16.54	NA	NA

MAX_MEAN: 25.2 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

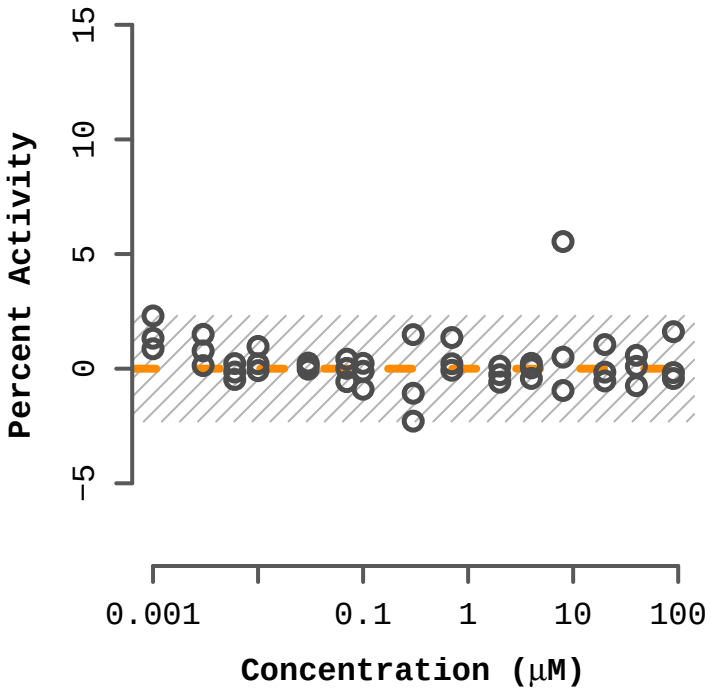
NAME: Neodecanoic acid
CHID: 27916 **CASRN:** 26896-20-8
SPID(S): Tox21_302244
M4ID: 12476889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.729 **MAX_MED:** 0.865 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

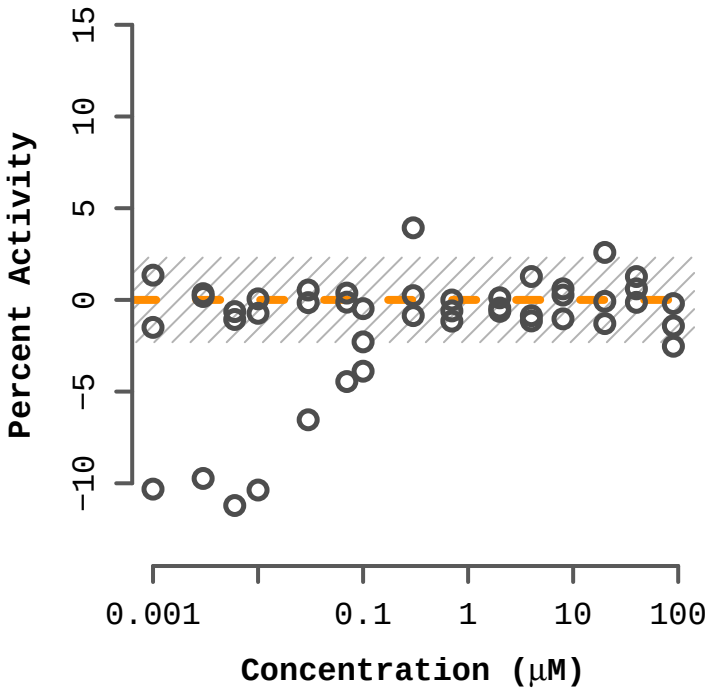
NAME: N,N,N',N'−Tetrabutyl−1,6−hexanediamine
CHID: 27920 **CASRN:** 27090−63−7
SPID(S): Tox21_303434
M4ID: 12475705

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

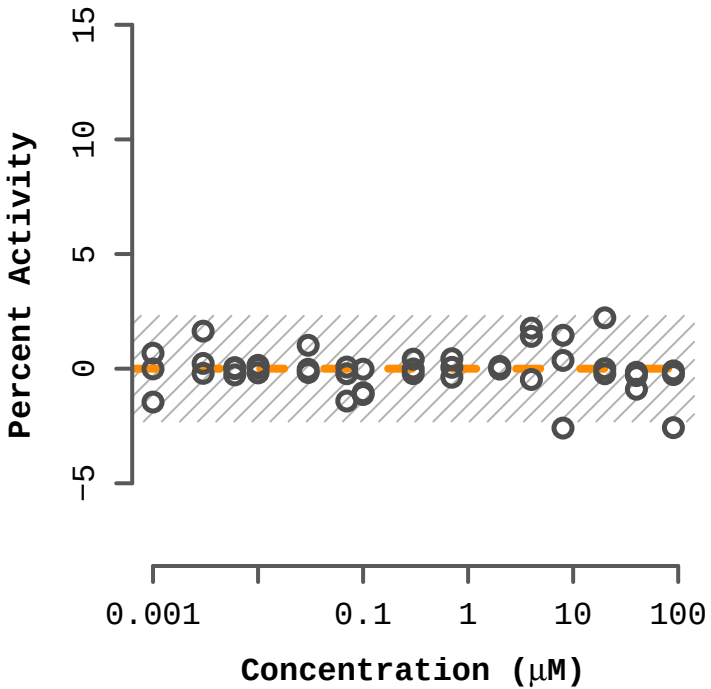
NAME: Di(propylene glycol) dibenzoate
CHID: 27921 **CASRN:** 27138-31-4
SPID(S): Tox21_300147
M4ID: 12478983

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.83	NA	NA
PROB:	1	NA	NA
RMSE:	3.55	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.605 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

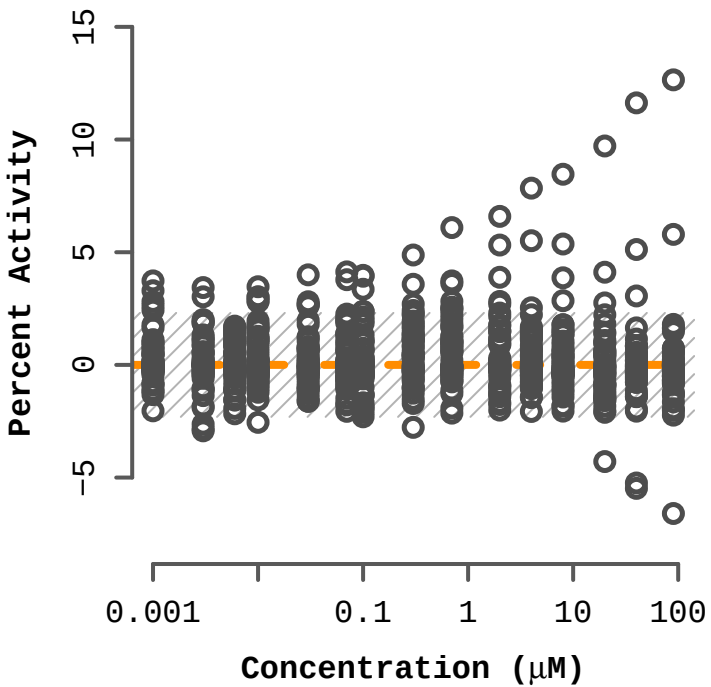
NAME: Di(propylene glycol) dibenzoate
CHID: 27921 **CASRN:** 27138-31-4
SPID(S): Tox21_202280
M4ID: 12479972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.903 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

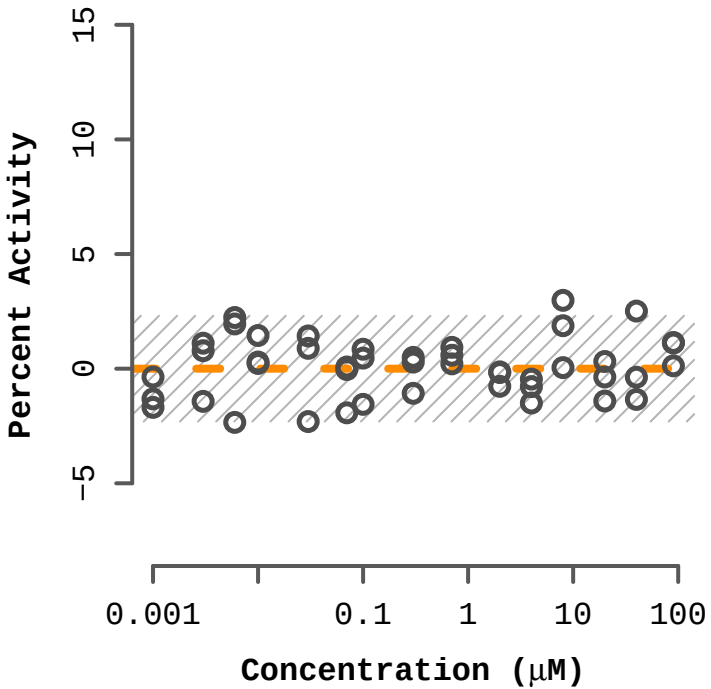
NAME: Dodecylbenzenesulfonic acid
CHID: 27923 **CASRN:** 27176-87-0
SPID(S): Tox21_400064
M4ID: 12475073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2492.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 0.689 **MAX_MED:** 0.568 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

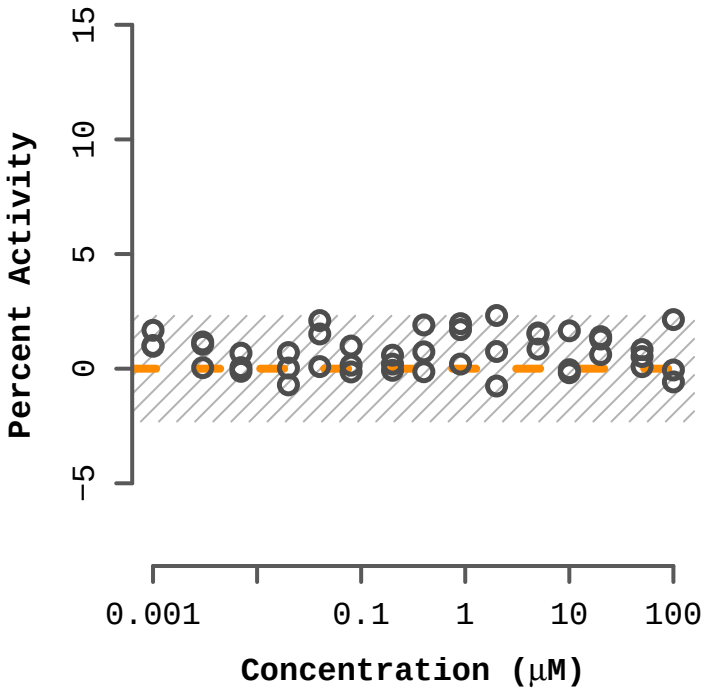
NAME: Diisodecyl hexanedioate
CHID: 27924 **CASRN:** 27178-16-1
SPID(S): Tox21_300310
M4ID: 12478820

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

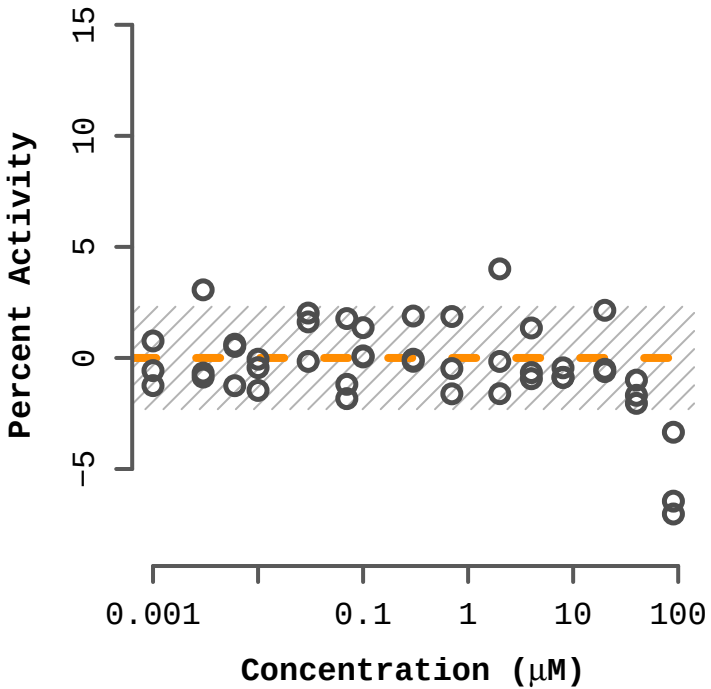
NAME: Diisodecyl hexanedioate
CHID: 27924 **CASRN:** 27178-16-1
SPID(S): Tox21_202302
M4ID: 12479950

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

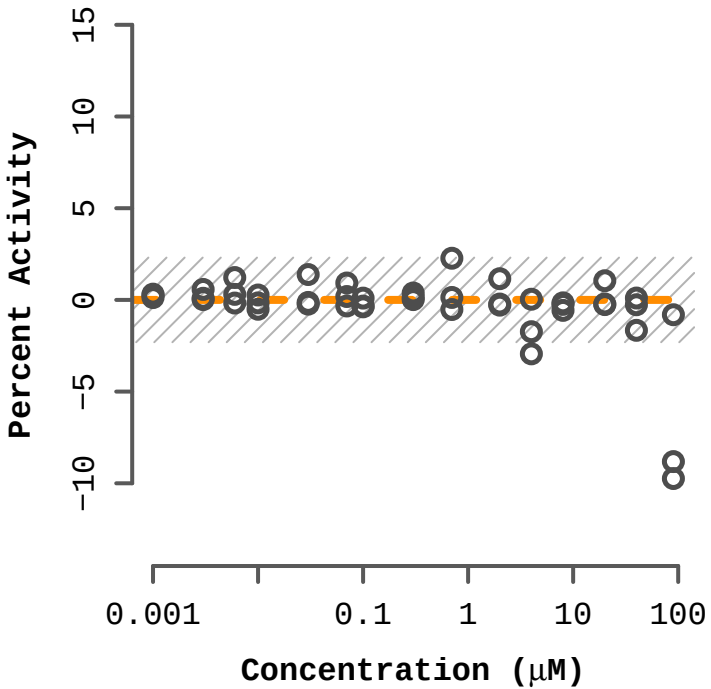
NAME: (1,1,3,3-Tetramethylbutyl)phenol
CHID: 27925 **CASRN:** 27193-28-8
SPID(S): Tox21_202324
M4ID: 12479928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

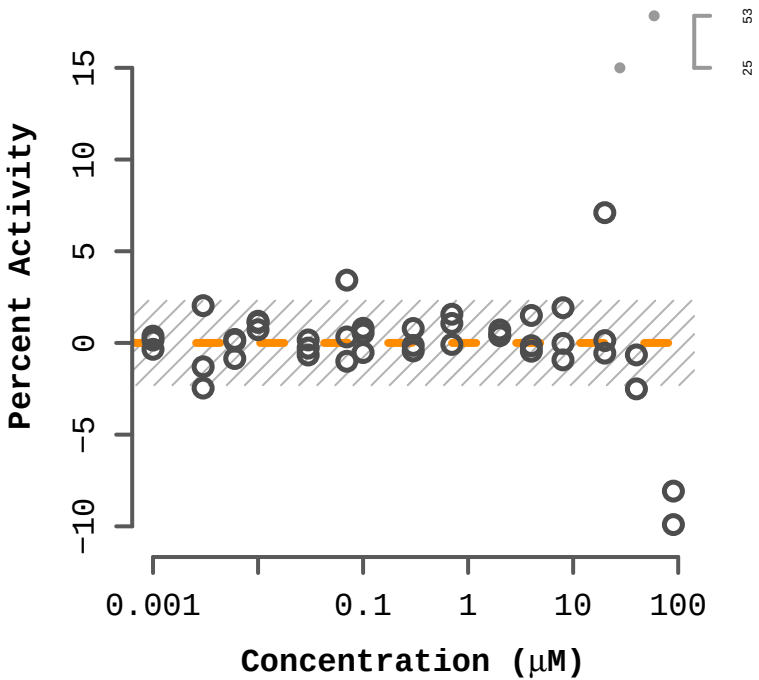
NAME: Dodecylphenol
CHID: 27926 **CASRN:** 27193-86-8
SPID(S): Tox21_303360
M4ID: 12475774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.12	NA	NA

MAX_MEAN: 0.629 **MAX_MED:** 0.302 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

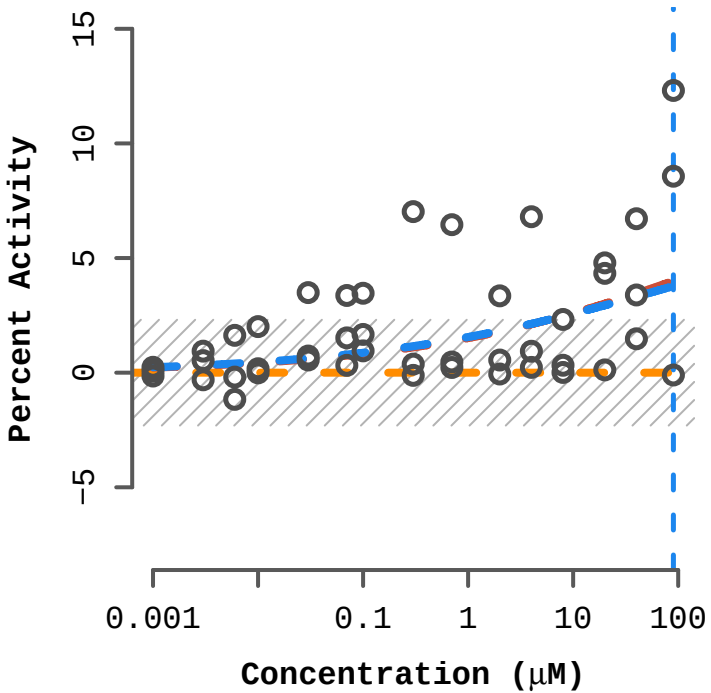
NAME: Dodecylphenol
CHID: 27926 **CASRN:** 27193-86-8
SPID(S): Tox21_200164
M4ID: 12482088 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.14	NA	NA
PROB:	1	NA	NA
RMSE:	9.02	NA	NA

MAX_MEAN: 11.6 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethylhexyl nitrate
CHID: 27928 CASRN: 27247-96-7
SPID(S): Tox21_303382
M4ID: 12475756

HILL MODEL (in red):

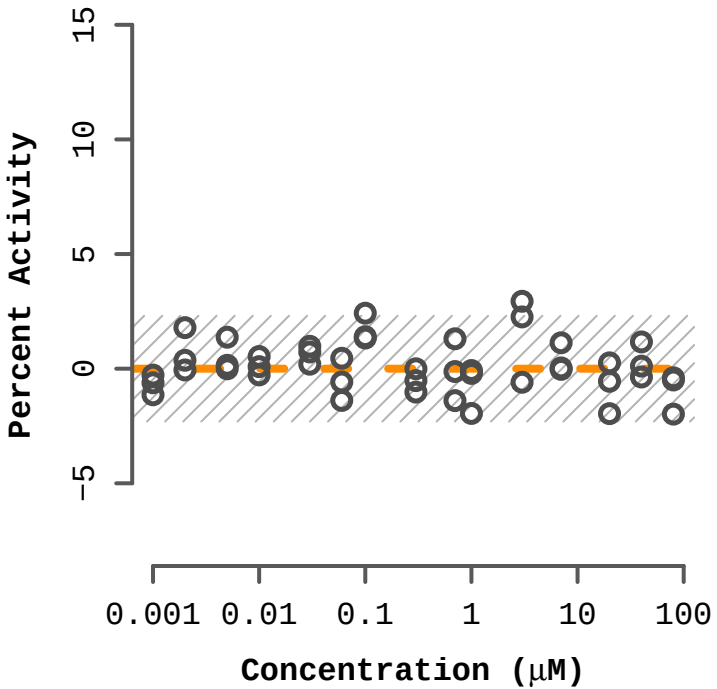
	tp	ga	gw
val:	9.5	2.41	0.3
sd:	131	24.9	0.337

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.55	1.95	0.3	3.59	6.28
sd:	55	15.1	0.149	23000	88100

	CNST	HILL	GNLS
AIC:	229.34	212.43	216.55
PROB:	0	0.89	0.11
RMSE:	3.44	2.48	2.49

MAX_MEAN: 6.93 MAX_MED: 8.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

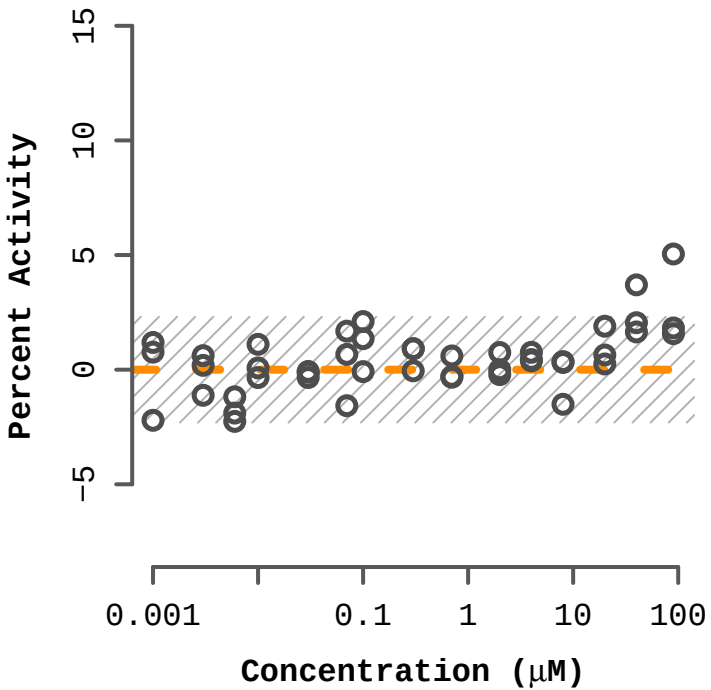
NAME: Dodecylbenzene sulfonate triethanolamine(1:1)
CHID: 27932 **CASRN:** 27323-41-7
SPID(S): Tox21_300593
M4ID: 12478540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

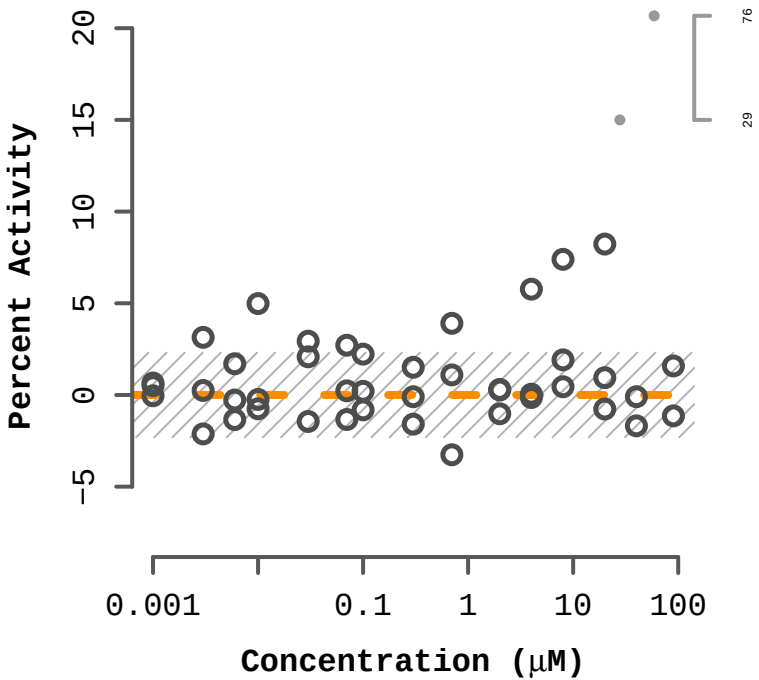
NAME: Diisooctyl phthalate
CHID: 27933 **CASRN:** 27554-26-3
SPID(S): Tox21_200466
M4ID: 12481786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.81 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

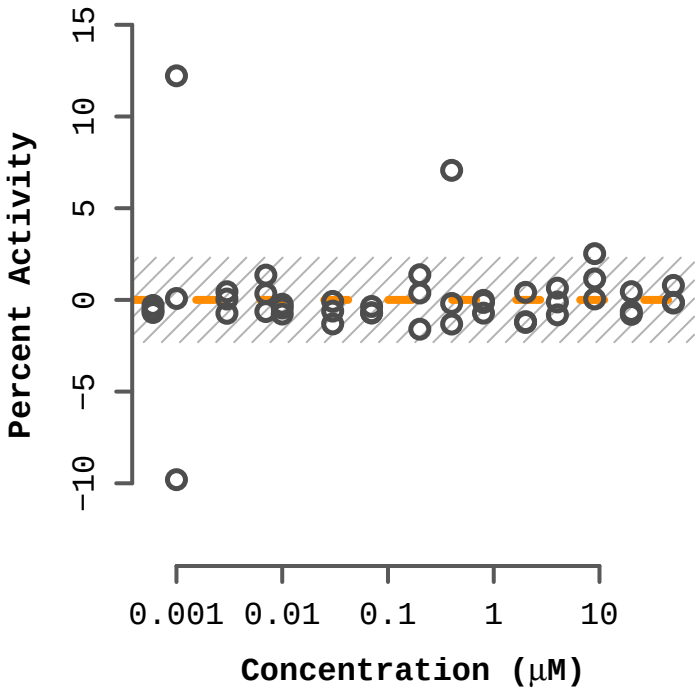
NAME: Hydroxypropyl methacrylate
CHID: 27936 **CASRN:** 27813-02-1
SPID(S): Tox21_201232
M4ID: 12481020 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253.1	NA	NA
PROB:	1	NA	NA
RMSE:	12.4	NA	NA

MAX_MEAN: 25.5 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

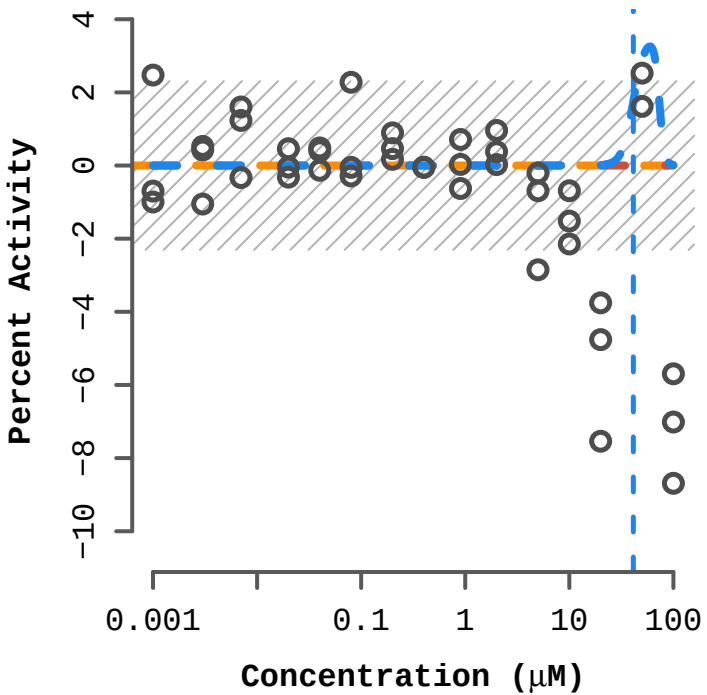
NAME: Dihydro-3-(octadecenyl)-2,5-furandione
CHID: 27948 **CASRN:** 28777-98-2
SPID(S): Tox21_202761
M4ID: 12479491

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trimethylolpropane ethoxylate triacrylate
CHID: 27950 **CASRN:** 28961-43-5
SPID(S): Tox21_200160
M4ID: 12482092

HILL MODEL (in red):

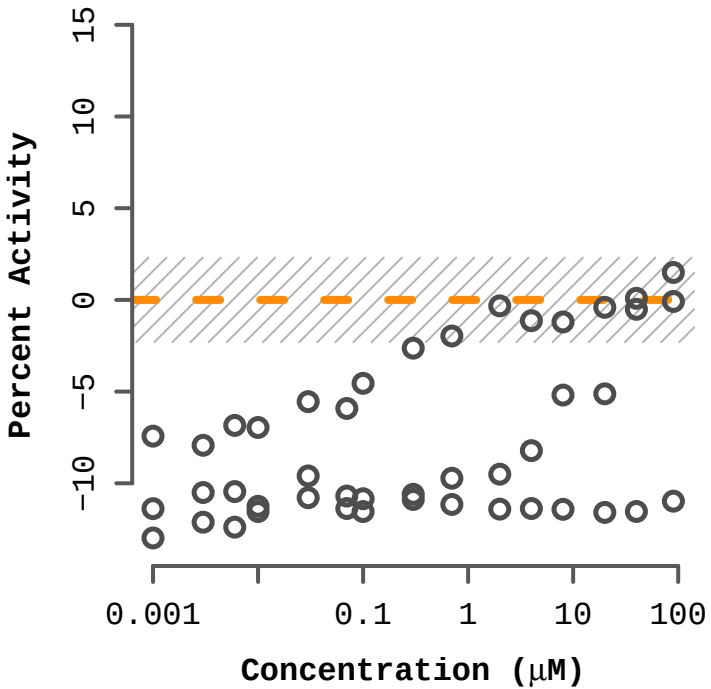
	tp	ga	gw
val:	1.05e-08	2.3	1.6
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.51	1.62	8	1.87	18
sd:	6.39	0.47	11.2	0.268	35.7

	CNST	HILL	GNLS
AIC:	209.98	215.98	212.82
PROB:	0.77	0.04	0.19
RMSE:	2.77	2.77	2.66

MAX_MEAN: 3.17 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

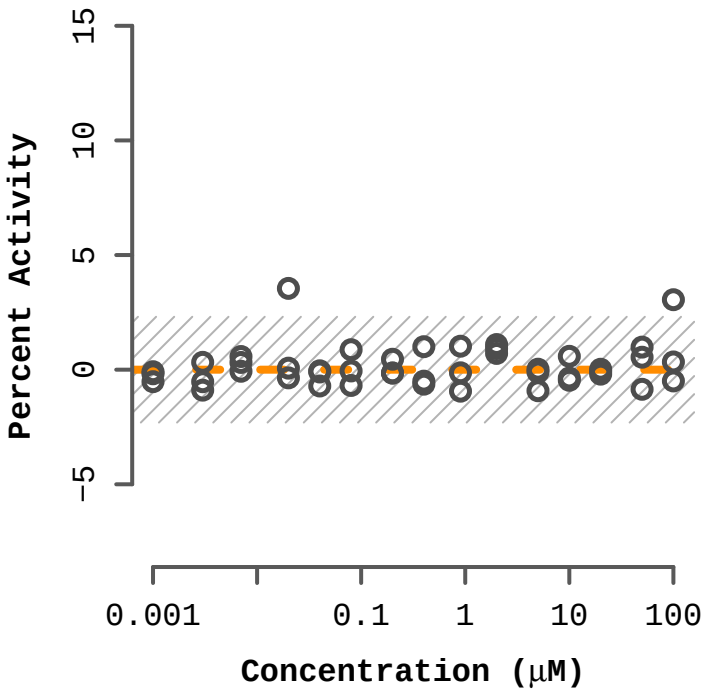
NAME: Isooctyl acrylate
CHID: 27955 **CASRN:** 29590-42-9
SPID(S): Tox21_300399
M4ID: 12478733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	334.36	NA	NA
PROB:	1	NA	NA
RMSE:	8.86	NA	NA

MAX_MEAN: −3.19 **MAX_MED:** −0.0819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

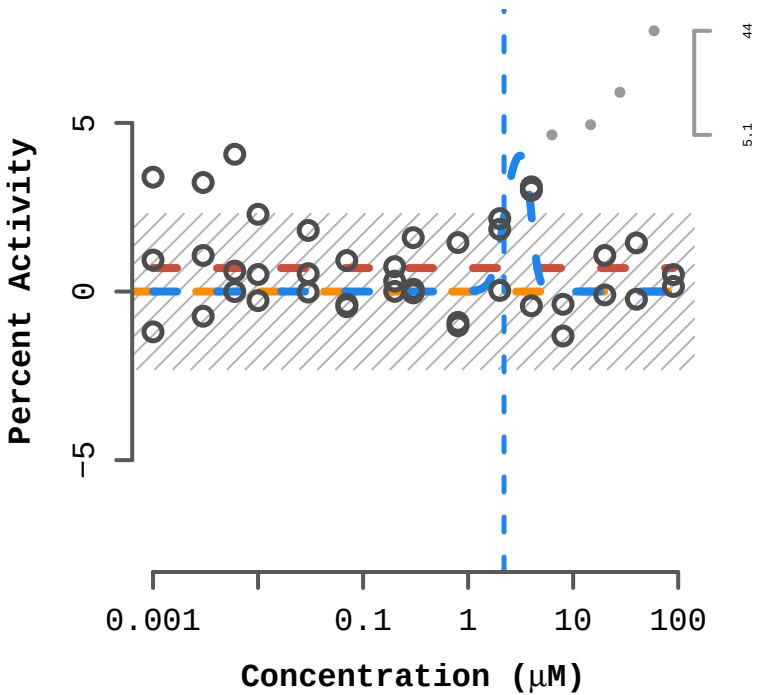
NAME: Isooctyl acrylate
CHID: 27955 CASRN: 29590-42-9
SPID(S): Tox21_202346
M4ID: 12479906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.09 MAX_MED: 0.923 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-(2-Butoxy-1-methylethoxy)propan-2-ol
CHID: 27959 CASRN: 29911-28-2
SPID(S): Tox21_200781
M4ID: 12481471 BRK

HILL MODEL (in red):

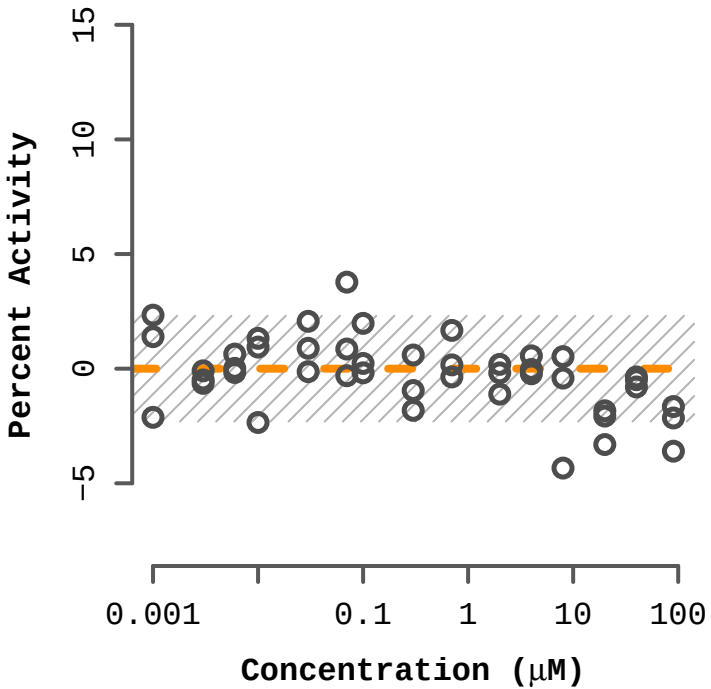
	tp	ga	gw
val:	0.696	-4.99	3.37
sd:	0.259	2110	3510

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.42	0.342	8	0.605	13.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	228.76	227.33	232.87
PROB:	0.32	0.64	0.04
RMSE:	7.53	7.34	7.51

MAX_MEAN: 14.8 MAX_MED: 3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

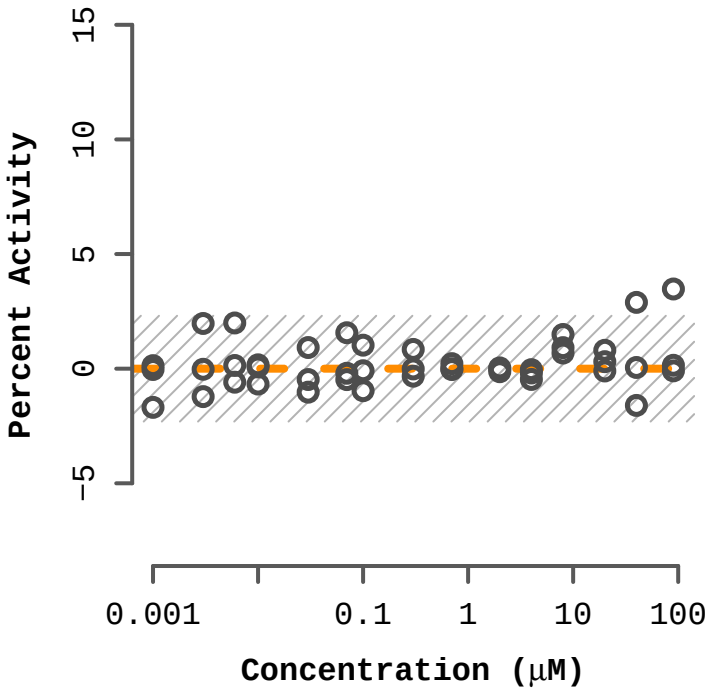
NAME: Isooctadecanoic acid
CHID: 27963 **CASRN:** 30399-84-9
SPID(S): Tox21_302276
M4ID: 12476857

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

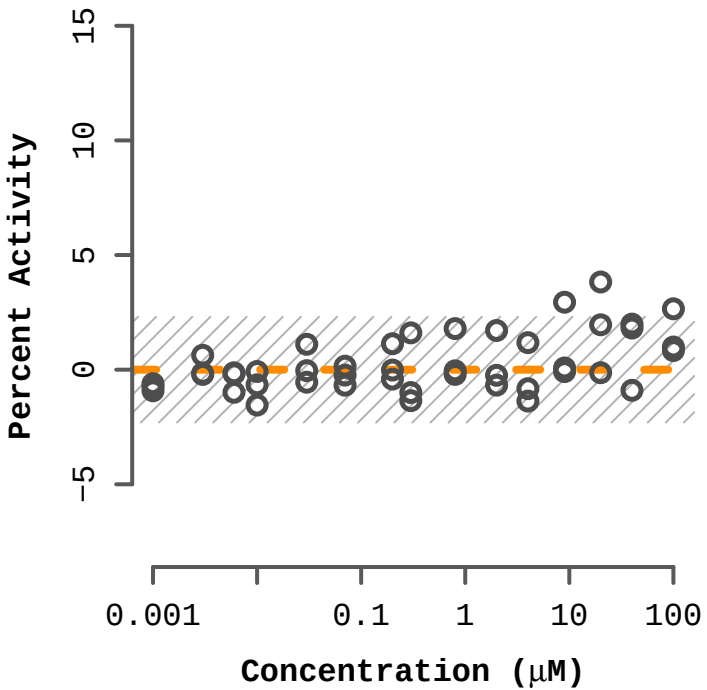
NAME: D-Gluco-heptonic acid, monosodium salt
CHID: 27966 **CASRN:** 31138-65-5
SPID(S): Tox21_200936
M4ID: 12481316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.919 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

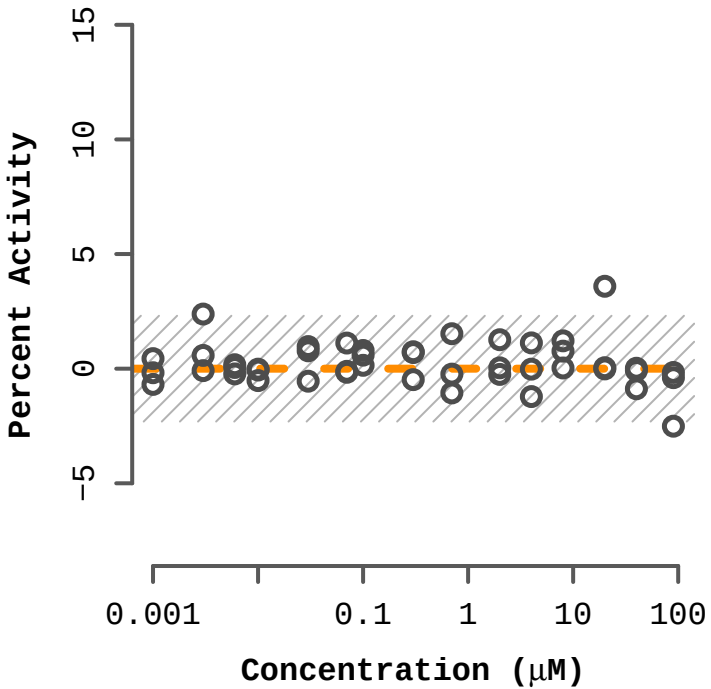
NAME: 4-(4-Hydroxy-4-methylpentyl)cyclohex-3-ene-1-ca
CHID: 27970 **CASRN:** 31906-04-4
SPID(S): Tox21_200394
M4ID: 12481858

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

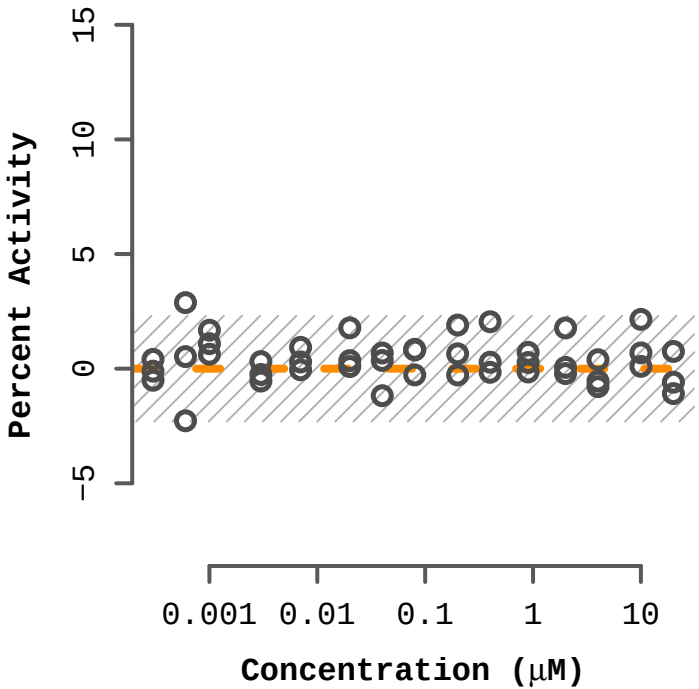
NAME: 4-tert-Butylcyclohexyl acetate
CHID: 27974 **CASRN:** 32210-23-4
SPID(S): Tox21_200180
M4ID: 12482072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.781 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

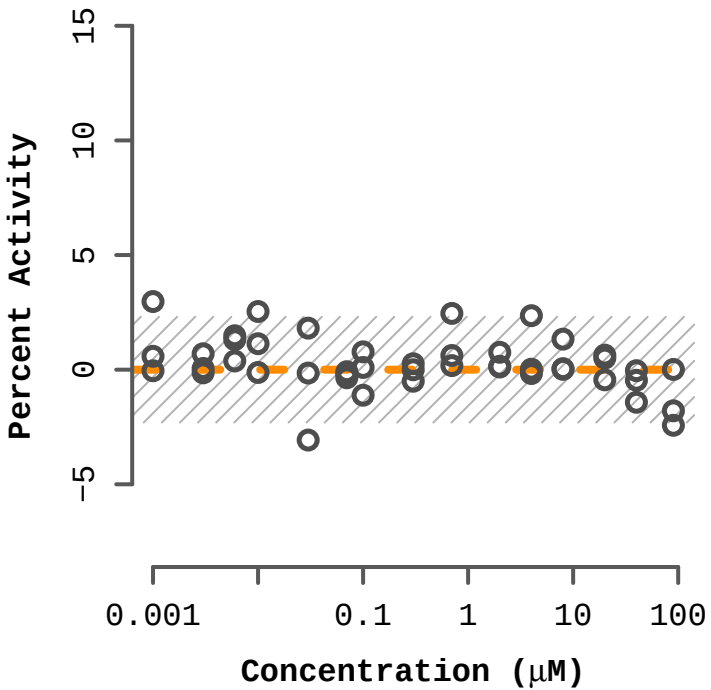
NAME: Stearyl methacrylate
CHID: 27975 **CASRN:** 32360-05-7
SPID(S): Tox21_202762
M4ID: 12479490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

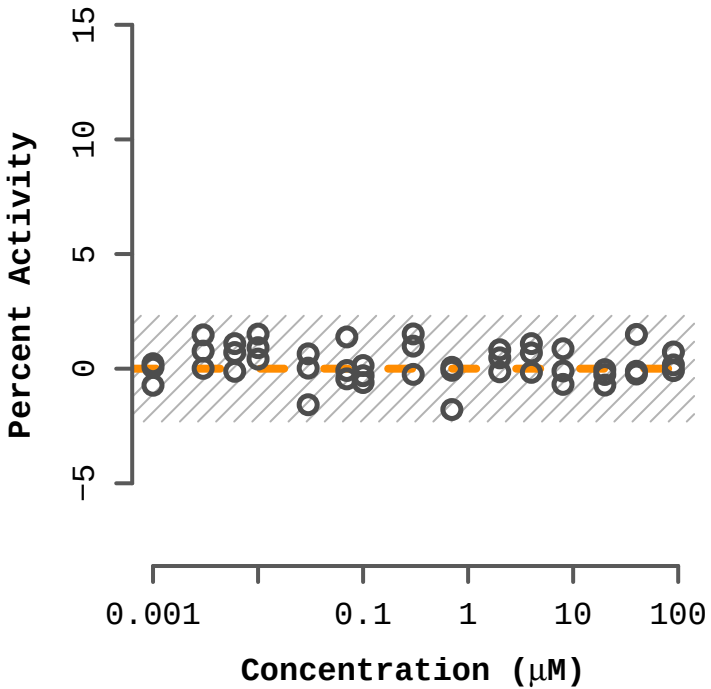
NAME: 3-[3,5-DI(tert-butyl)-4-hydroxyphenyl]propanoh
CHID: 27978 CASRN: 32687-77-7
SPID(S): Tox21_301238
M4ID: 12477895

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.18 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Amino-6-tert-butyl-3-thioxo-3,4-dihydro-1,2,4

CHID: 27981 **CASRN:** 33509-43-2

SPID(S): Tox21_301995

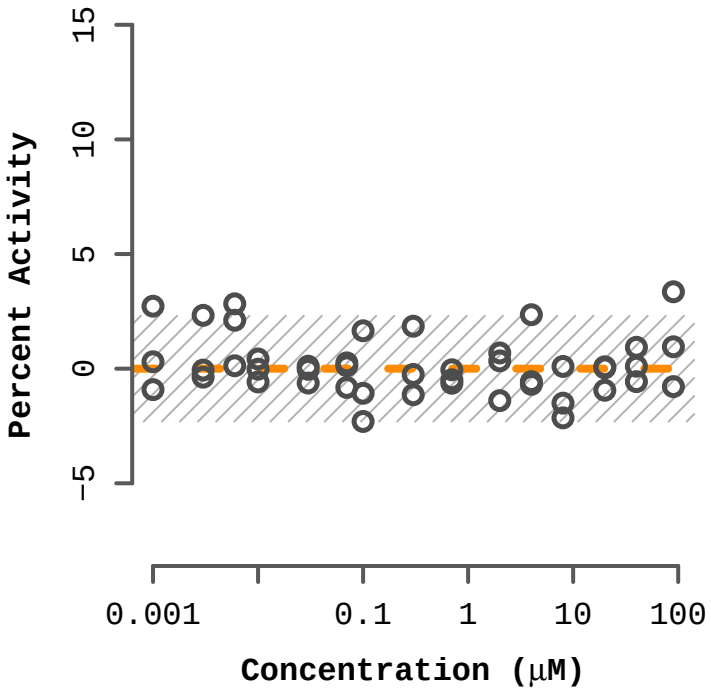
M4ID: 12477138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.949 **MAX_MED:** 0.984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

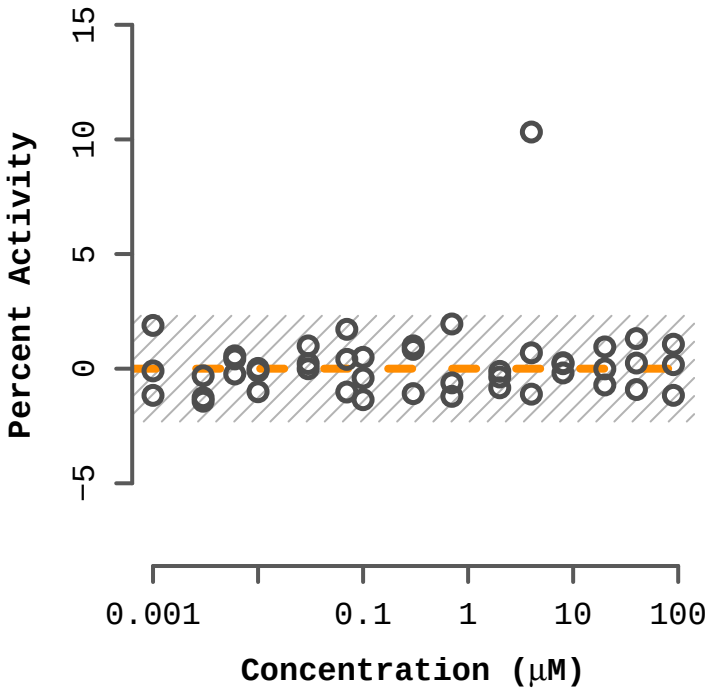
NAME: Hexanedioic acid, diisononyl ester
CHID: 27982 **CASRN:** 33703-08-1
SPID(S): Tox21_300291
M4ID: 12478839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

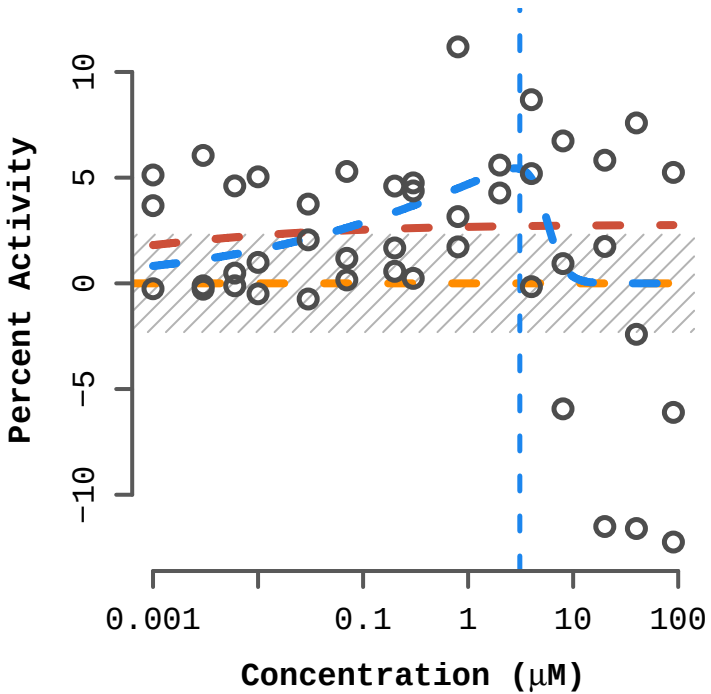
NAME: Dipropylene glycol monomethyl ether
CHID: 27983 **CASRN:** 34590-94-8
SPID(S): Tox21_300570
M4ID: 12478563

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.78	NA	NA

MAX_MEAN: 3.3 **MAX_MED:** 0.842 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dipropylene glycol monomethyl ether
CHID: 27983 CASRN: 34590-94-8
SPID(S): Tox21_201653
M4ID: 12480599

HILL MODEL (in red):

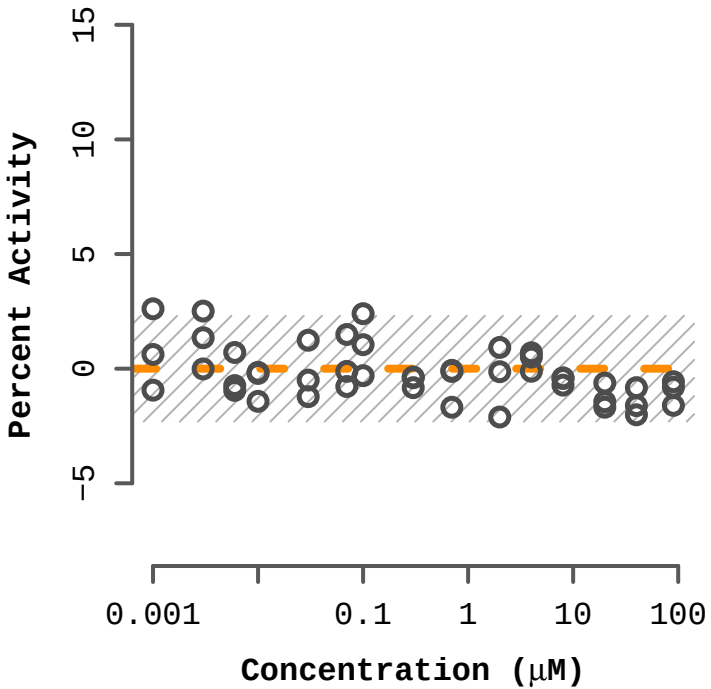
	tp	ga	gw
val:	2.78	−3.72	0.376
sd:	1.18	4.63	0.731

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.4	0.492	0.318	0.742	5.06
sd:	19.8	3.82	0.225	0.29	7.24

	CNST	HILL	GNLS
AIC:	283.95	277.71	275.17
PROB:	0.01	0.22	0.77
RMSE:	5.45	5.21	4.57

MAX_MEAN: 7.31 MAX_MED: 5.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

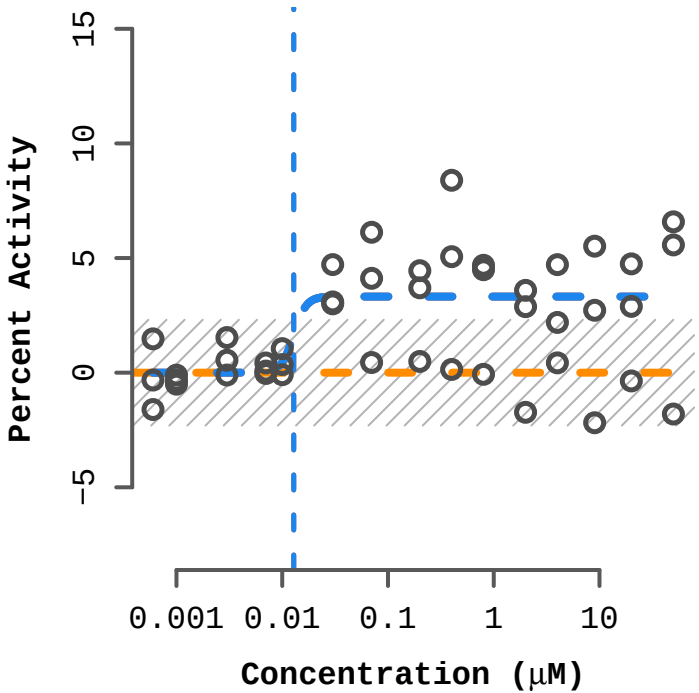
NAME: 1-Hexadecanol
CHID: 27991 CASRN: 36653-82-4
SPID(S): Tox21_300325
M4ID: 12478807

HILL MODEL: Not applicable.

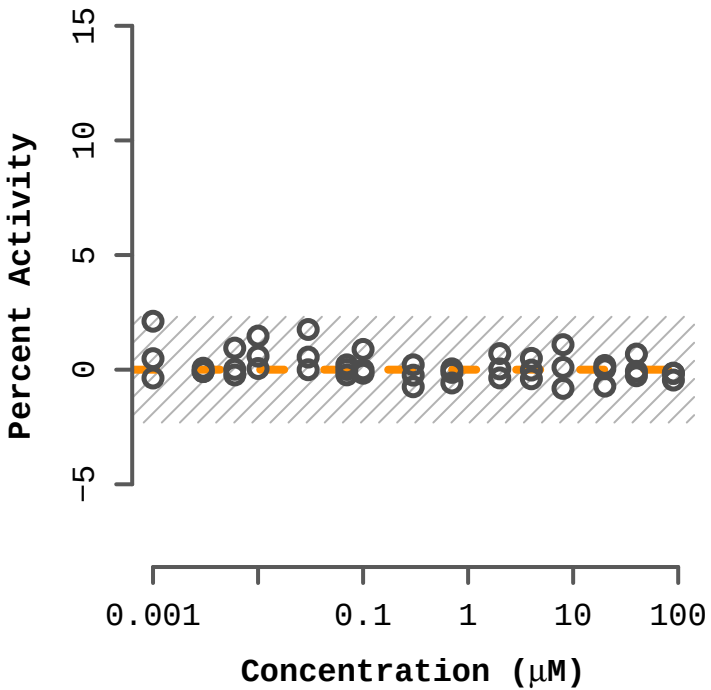
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.29 MAX_MED: 1.35 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Hexadecanol
CHID:    27991   CASRN: 36653-82-4
SPID(S): Tox21_111609_1
M4ID:    12483590

HILL MODEL (in red):
      tp       ga       gw
val:  3.32     -1.89    7.36
sd:   0.425    0.365    24.6

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.32     -1.89    7.36     2.78     12.6
sd:   0.425    0.365    24.6     170000   1770000

      CNST        HILL        GNLS
AIC:  238.07      206.12      210.12
PROB: 0           0.88        0.12
RMSE: 3.26        2.22        2.22

MAX_MEAN: 4.53      MAX_MED: 5.57      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

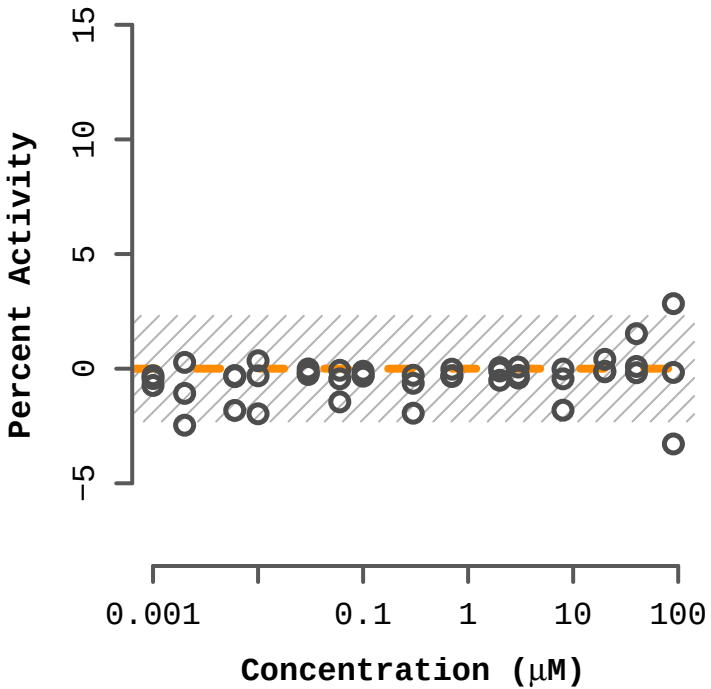
NAME: Dichlormid
CHID: 27997 **CASRN:** 37764-25-3
SPID(S): Tox21_303463
M4ID: 12475677

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	80.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 0.767 **MAX_MED:** 0.592 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

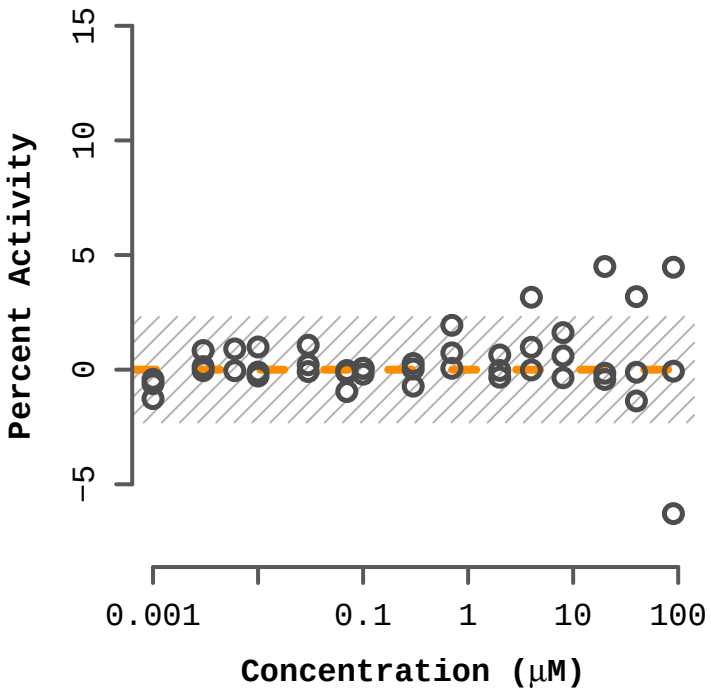
NAME: Dichlormid
CHID: 27997 **CASRN:** 37764-25-3
SPID(S): Tox21_202064
M4ID: 12480188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 0.0984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

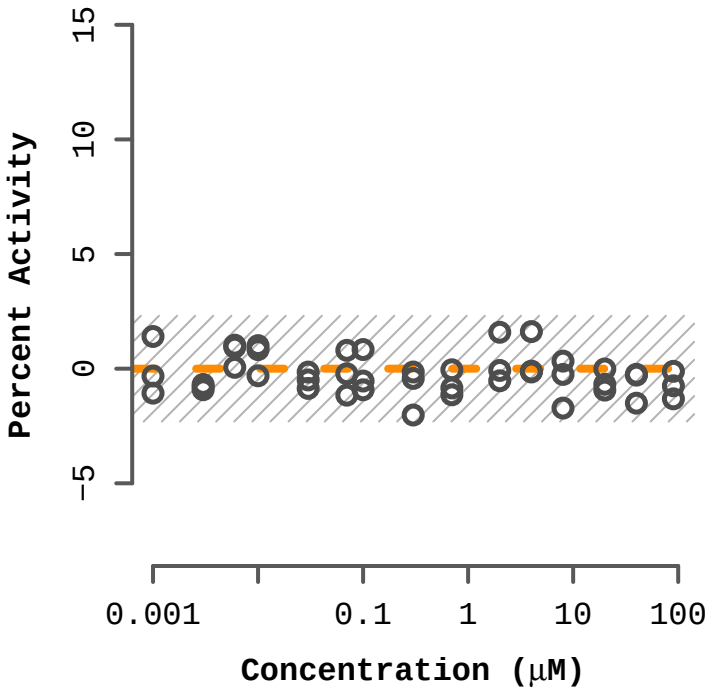
NAME: 5,5'-[Propane-2,2-diylbis(benzene-4,1-diyloxy)]
CHID: 28001 **CASRN:** 38103-06-9
SPID(S): Tox21_200467
M4ID: 12481785

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 0.977 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

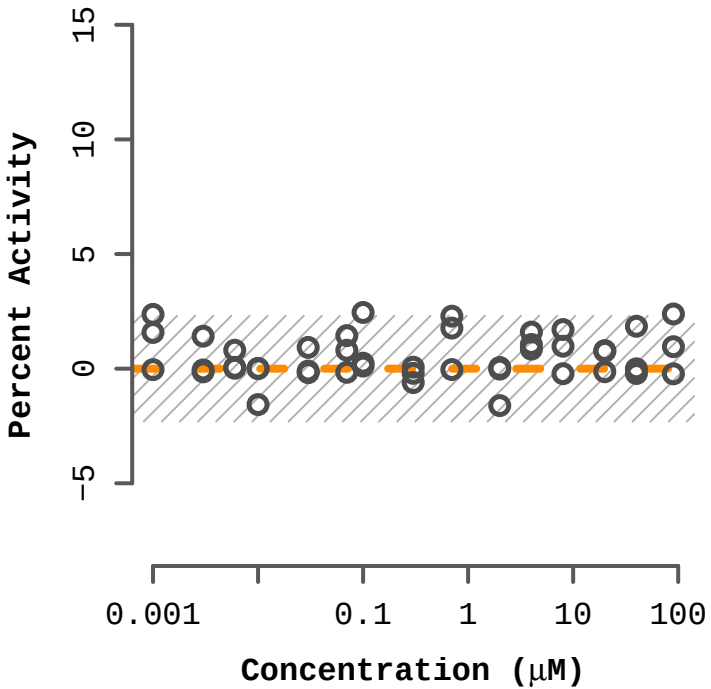
NAME: 3-Phenoxybenzaldehyde
CHID: 28005 **CASRN:** 39515-51-0
SPID(S): Tox21_303348
M4ID: 12475785

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.675 **MAX_MED:** 0.938 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

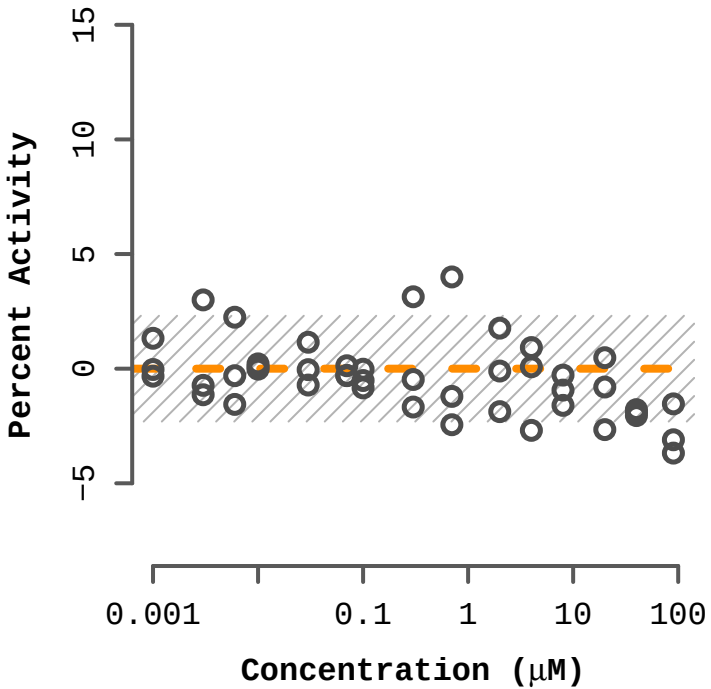
NAME: 3-Phenoxybenzaldehyde
CHID: 28005 **CASRN:** 39515-51-0
SPID(S): Tox21_202368
M4ID: 12479884

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

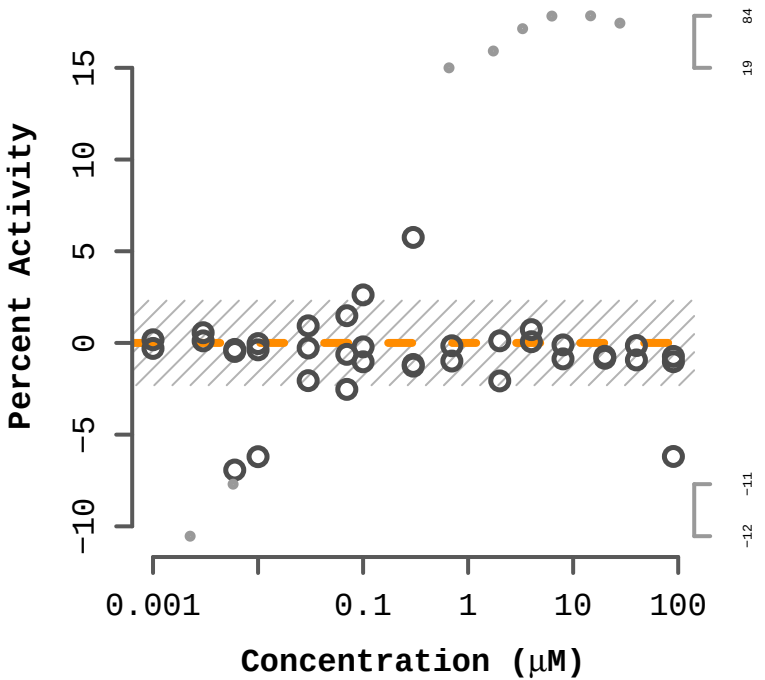
NAME: 1,3,5-Tris(4-tert-butyl-3-hydroxy-2,6-dimethyll
CHID: 28008 CASRN: 40601-76-1
SPID(S): Tox21_200797
M4ID: 12481455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 0.38 MAX_MED: 0.0834 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

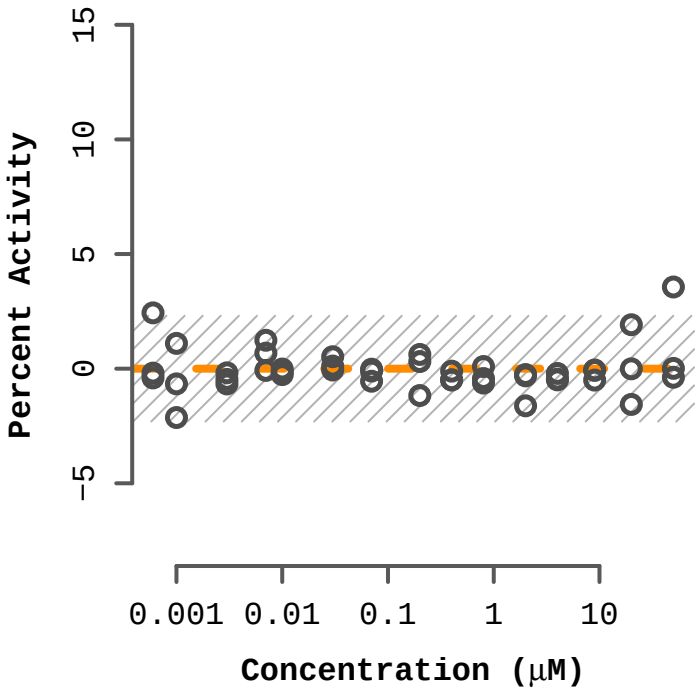
NAME: Sodium malate
CHID: 28010 **CASRN:** 40876-98-0
SPID(S): Tox21_201051
M4ID: 12481201 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	355.51	NA	NA
PROB:	1	NA	NA
RMSE:	24.45	NA	NA

MAX_MEAN: 27.6 **MAX_MED:** 0.728 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

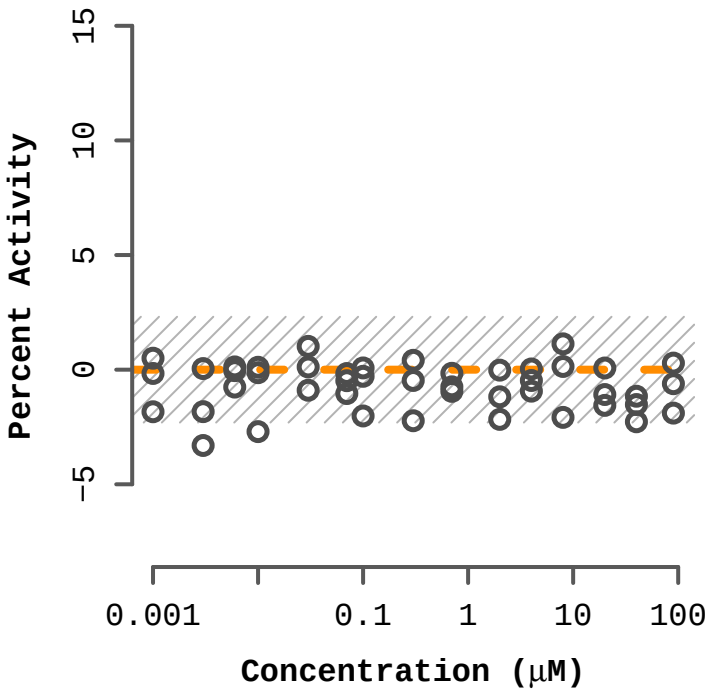
NAME: Thioethylene glycol bis(3,5-di-tert-butyl-4-hy
CHID: 28011 **CASRN:** 41484-35-9
SPID(S): Tox21_303739
M4ID: 12475449

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.679 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

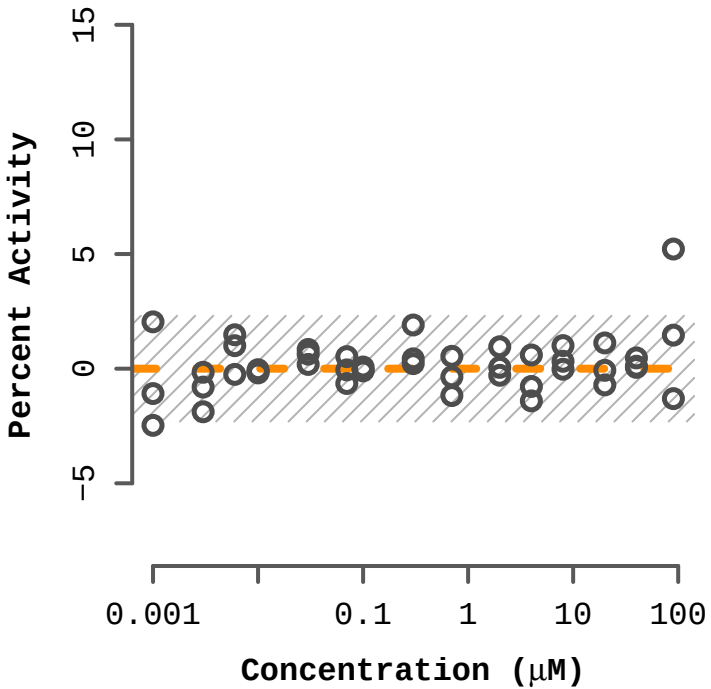
NAME: 2-Methyl-5-nitro-1H-isoindole-1,3(2H)-dione
CHID: 28013 **CASRN:** 41663-84-7
SPID(S): Tox21_200196
M4ID: 12482056

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.0798 **MAX_MED:** 0.141 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

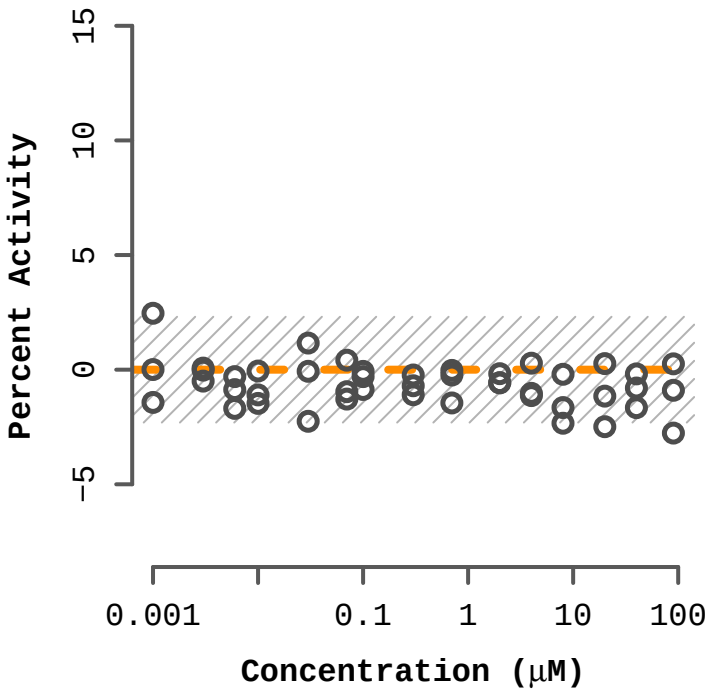
NAME: Tripropylene glycol diacrylate
CHID: 28015 **CASRN:** 42978-66-5
SPID(S): Tox21_301282
M4ID: 12477851

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

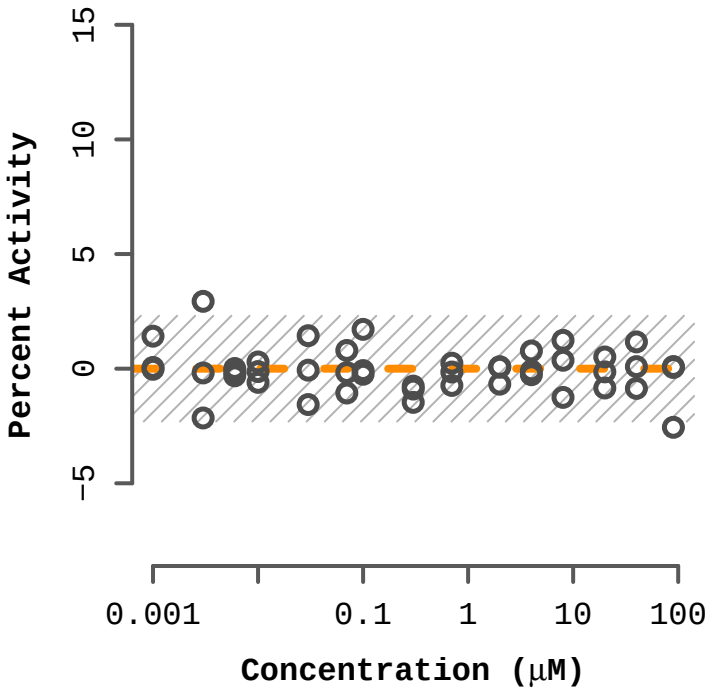
NAME: 2-(Dimethylamino)ethyl acrylate methochloride
CHID: 28016 **CASRN:** 44992-01-0
SPID(S): Tox21_202568
M4ID: 12479684

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.348 **MAX_MED:** 0.0074 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

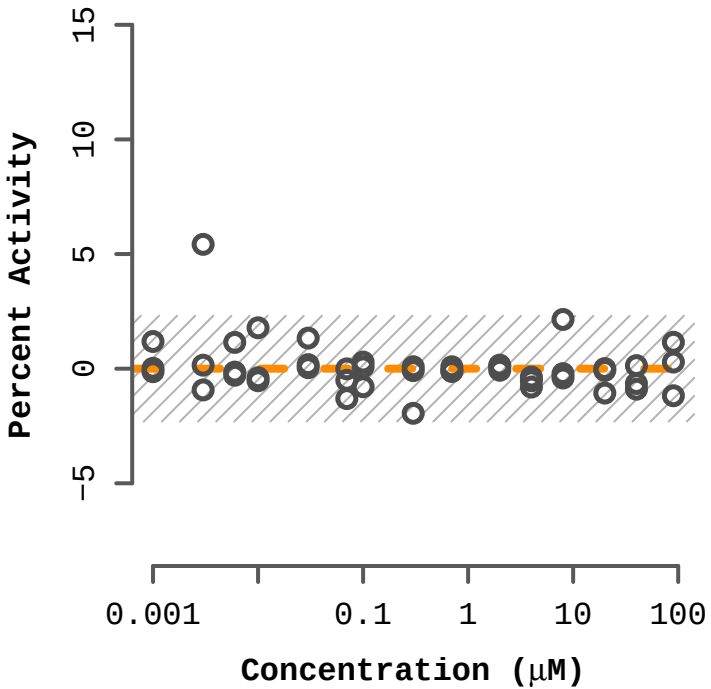
NAME: 1-(Bromomethyl)-3-phenoxybenzene
CHID: 28022 **CASRN:** 51632-16-7
SPID(S): Tox21_301643
M4ID: 12477490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.482 **MAX_MED:** 0.367 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

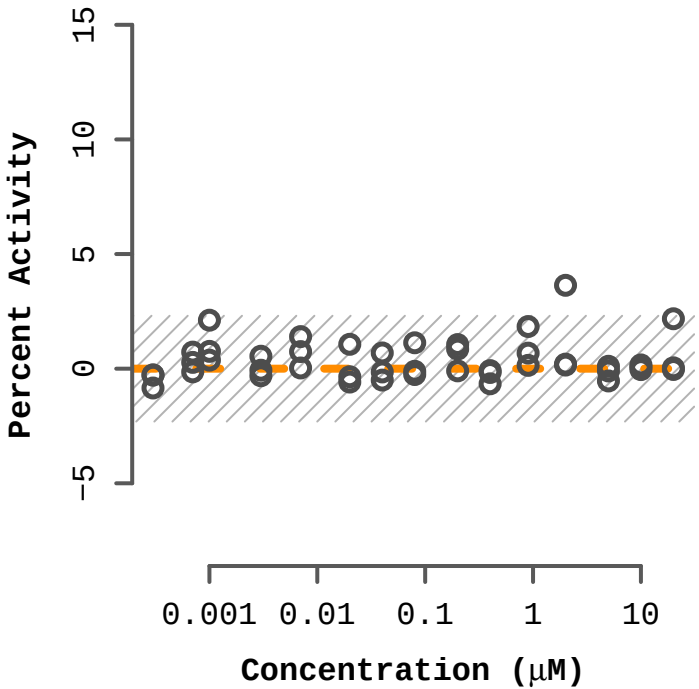
NAME: Sodium 3-(allyloxy)-2-hydroxypropanesulphonate
CHID: 28028 **CASRN:** 52556-42-0
SPID(S): Tox21_202569
M4ID: 12479683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 0.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

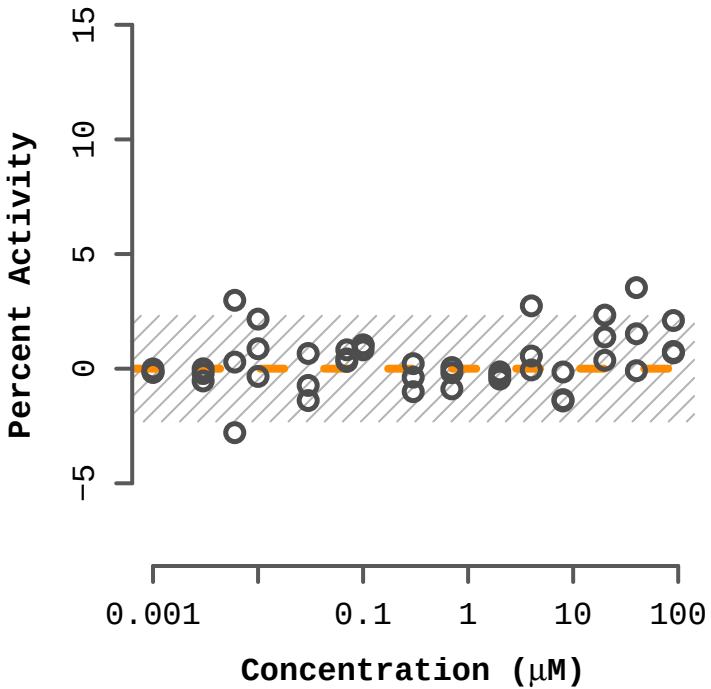
NAME: Bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate
CHID: 28030 **CASRN:** 52829-07-9
SPID(S): Tox21_202763
M4ID: 12479489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

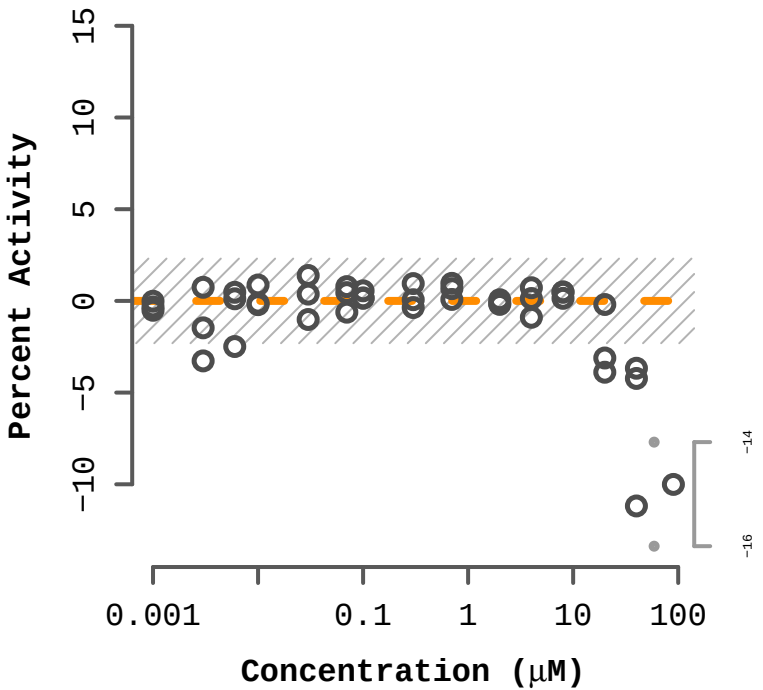
NAME: Triisononyl trimellitate
CHID: 28033 **CASRN:** 53894-23-8
SPID(S): Tox21_300639
M4ID: 12478494

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

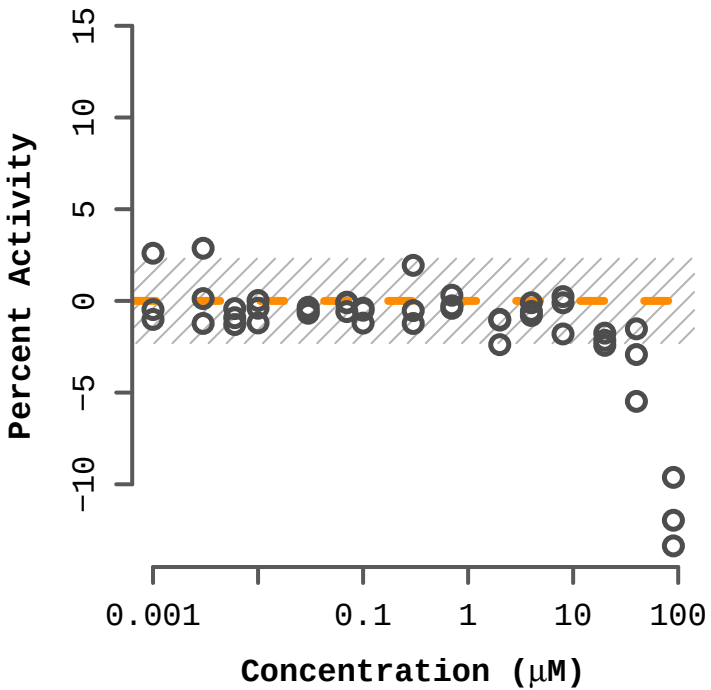
NAME: 3-Iodo-2-propynyl-N-butylcarbamate
CHID: 28038 **CASRN:** 55406-53-6
SPID(S): Tox21_301117
M4ID: 12478016 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.42	NA	NA
PROB:	1	NA	NA
RMSE:	4.17	NA	NA

MAX_MEAN: 0.57 **MAX_MED:** 0.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

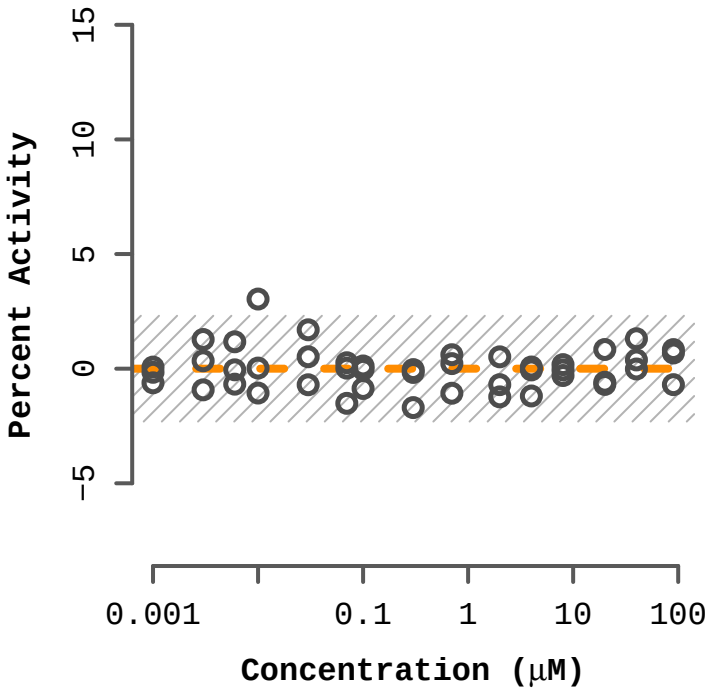
NAME: 3-Iodo-2-propynyl-N-butylcarbamate
CHID: 28038 **CASRN:** 55406-53-6
SPID(S): Tox21_201864
M4ID: 12480388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.84	NA	NA
PROB:	1	NA	NA
RMSE:	3.37	NA	NA

MAX_MEAN: 0.591 **MAX_MED:** 0.129 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

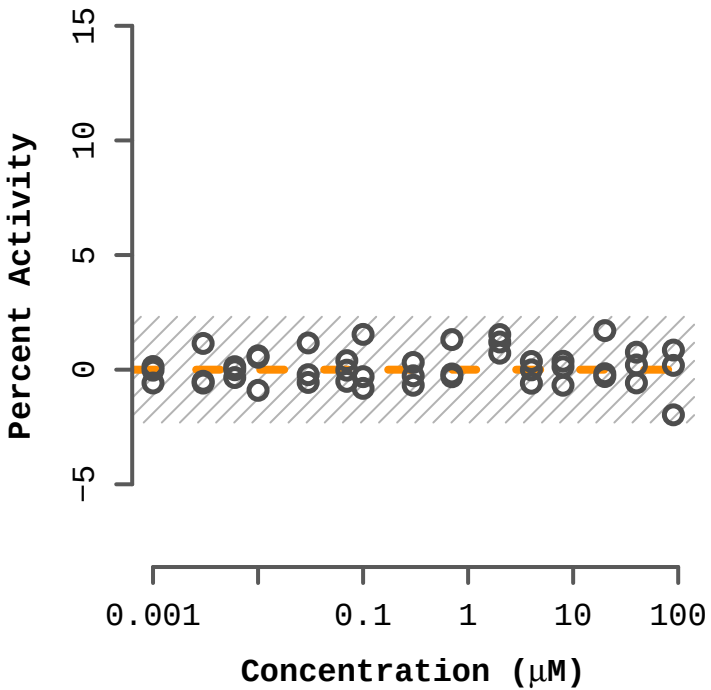
NAME: N-(1-Ethylpropyl)-3,4-xylidine
CHID: 28040 **CASRN:** 56038-89-2
SPID(S): Tox21_301810
M4ID: 12477323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.668 **MAX_MED:** 0.686 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

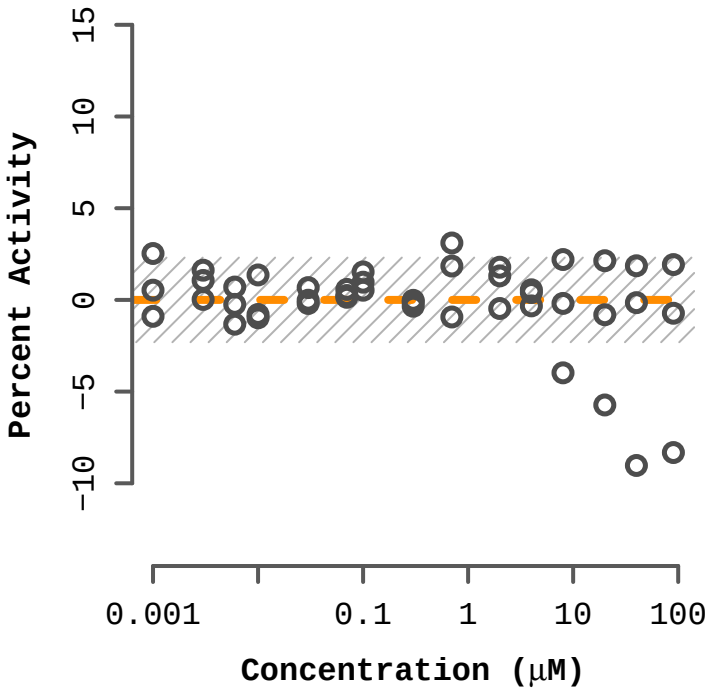
NAME: 2-(Ethyl(3-methylphenyl)amino)acetonitrile
CHID: 28114 **CASRN:** 63133-74-4
SPID(S): Tox21_301753
M4ID: 12477380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

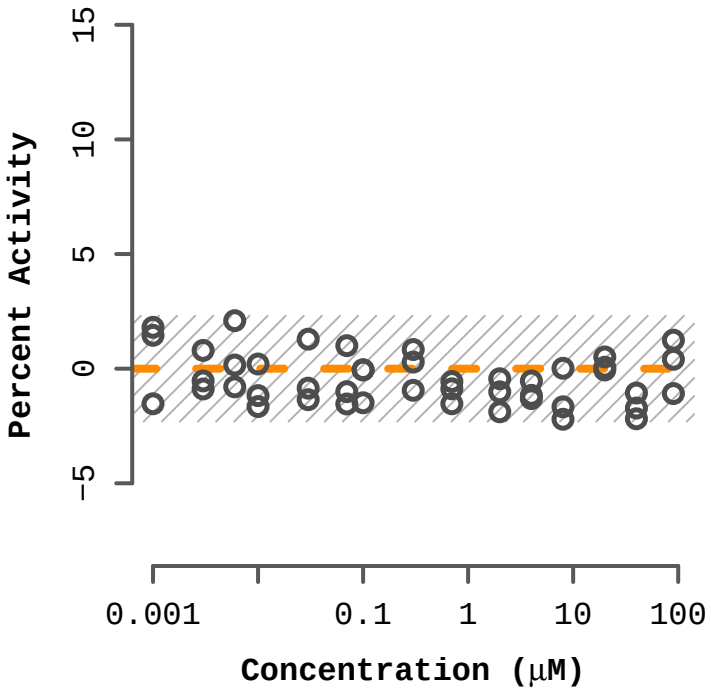
NAME: Methyl 3,3-dimethylpent-4-enoate
CHID: 28120 CASRN: 63721-05-1
SPID(S): Tox21_200468
M4ID: 12481784

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.29	NA	NA
PROB:	1	NA	NA
RMSE:	2.4	NA	NA

MAX_MEAN: 1.34 MAX_MED: 1.85 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

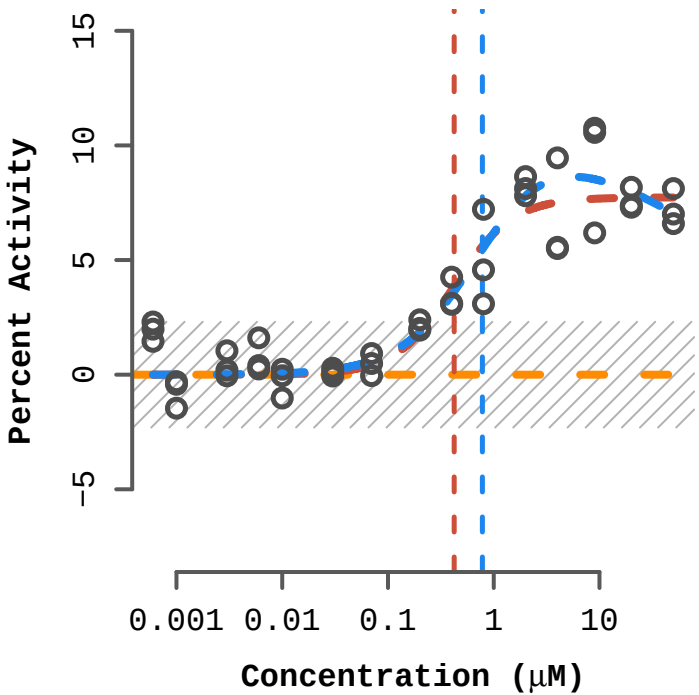
NAME: 1-(4-Chlorophenyl)-4,4-dimethyl-pentan-3-one
CHID: 28300 **CASRN:** 66346-01-8
SPID(S): Tox21_301988
M4ID: 12477145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fatty acids, C16-18
CHID: 28306 CASRN: 67701-03-5
SPID(S): Tox21_202550
M4ID: 12479702

HILL MODEL (in red):

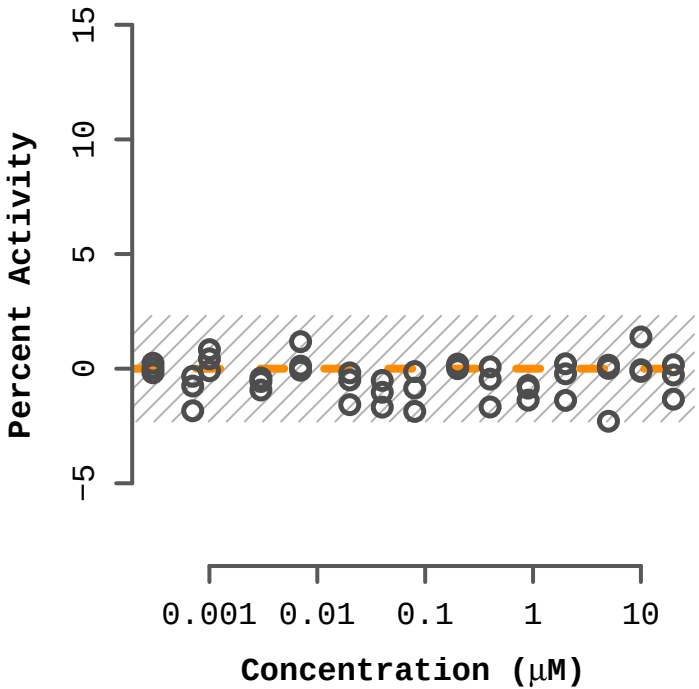
	tp	ga	gw
val:	7.73	−0.374	1.58
sd:	0.39	0.0711	0.342

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.9	−0.107	1.22	1.93	0.364
sd:	10.9	0.272	0.27	1.97	0.492

	CNST	HILL	GNLS
AIC:	275.57	155.48	155.96
PROB:	0	0.56	0.44
RMSE:	4.95	1.24	1.22

MAX_MEAN: 9.17 MAX_MED: 10.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

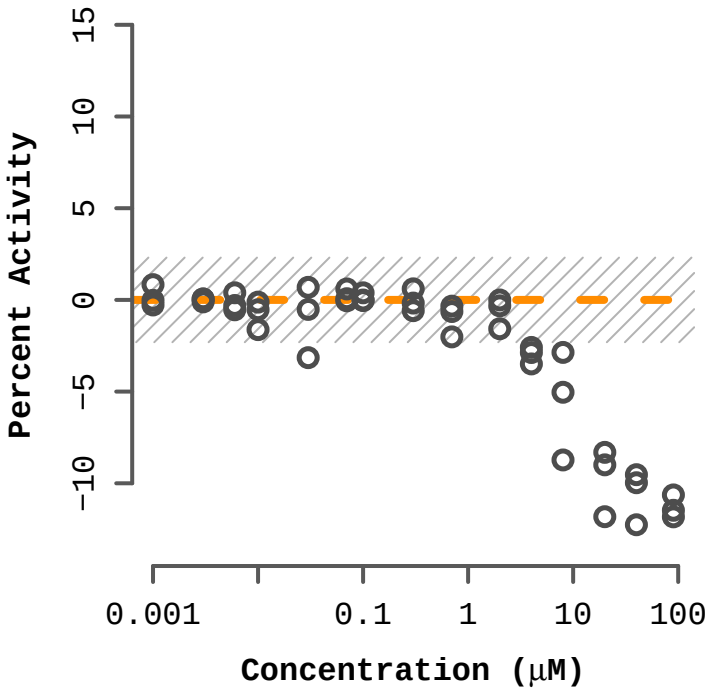
NAME: Alcohols, C16-18
CHID: 28323 **CASRN:** 67762-27-0
SPID(S): Tox21_303960
M4ID: 12475228

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.409 **MAX_MED:** 0.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

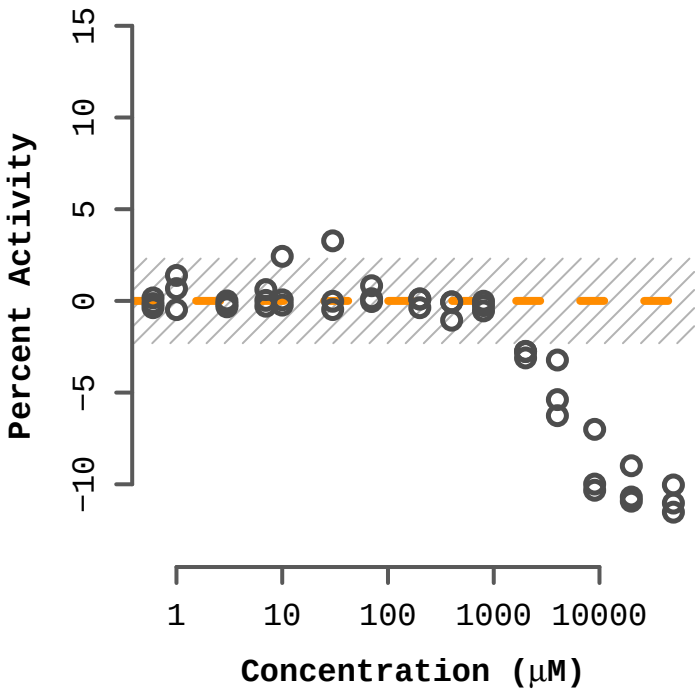
NAME: Quaternary ammonium compounds, benzyl-C12-18-a
CHID: 28460 CASRN: 68391-01-5
SPID(S): Tox21_202570
M4ID: 12479682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.88	NA	NA
PROB:	1	NA	NA
RMSE:	5.11	NA	NA

MAX_MEAN: 0.206 MAX_MED: 0.0669 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

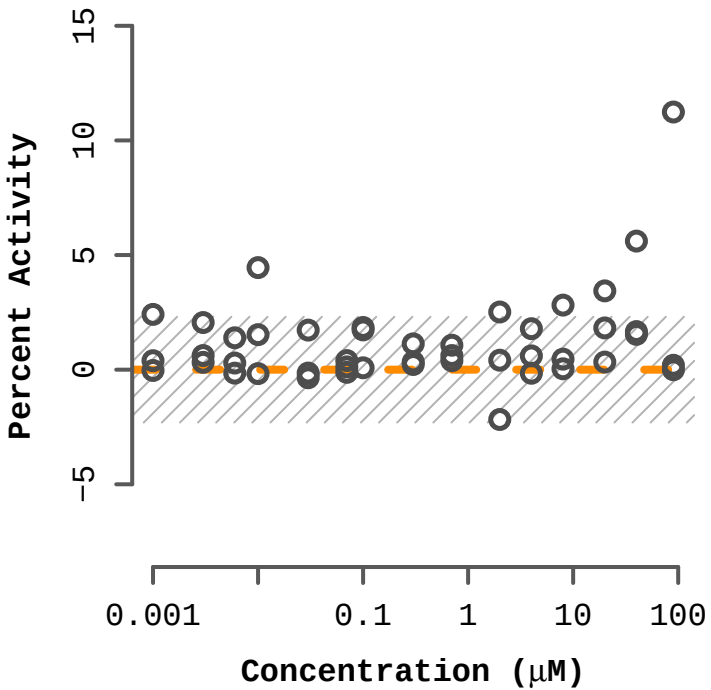
NAME: Quaternary ammonium compounds, benzyl-C12-16-a
CHID: 28492 CASRN: 68424-85-1
SPID(S): Tox21_303955
M4ID: 12475233

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	262.94	NA	NA
PROB:	1	NA	NA
RMSE:	4.83	NA	NA

MAX_MEAN: 0.929 **MAX_MED:** 0.672 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

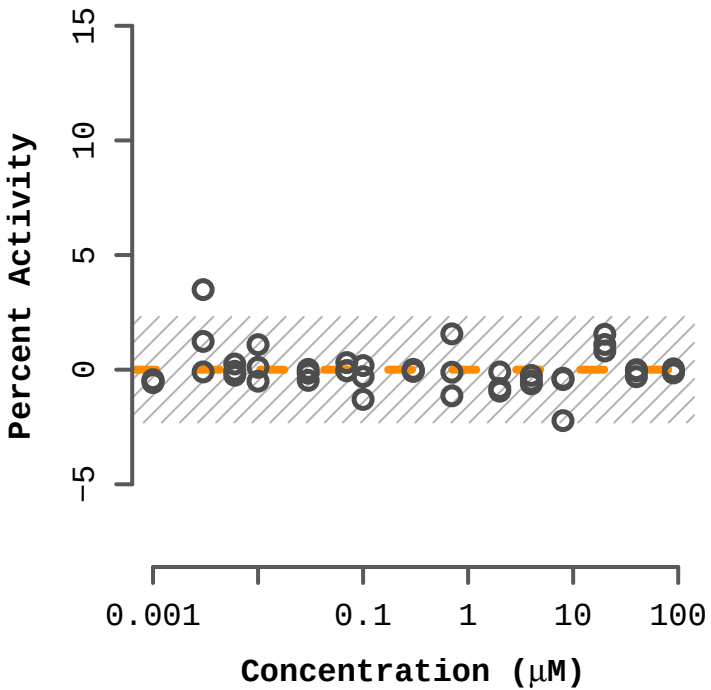
NAME: Diethylmethylbenzenediamine
CHID: 28618 **CASRN:** 75389-89-8
SPID(S): Tox21_303857
M4ID: 12475331

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.35	NA	NA

MAX_MEAN: 3.81 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

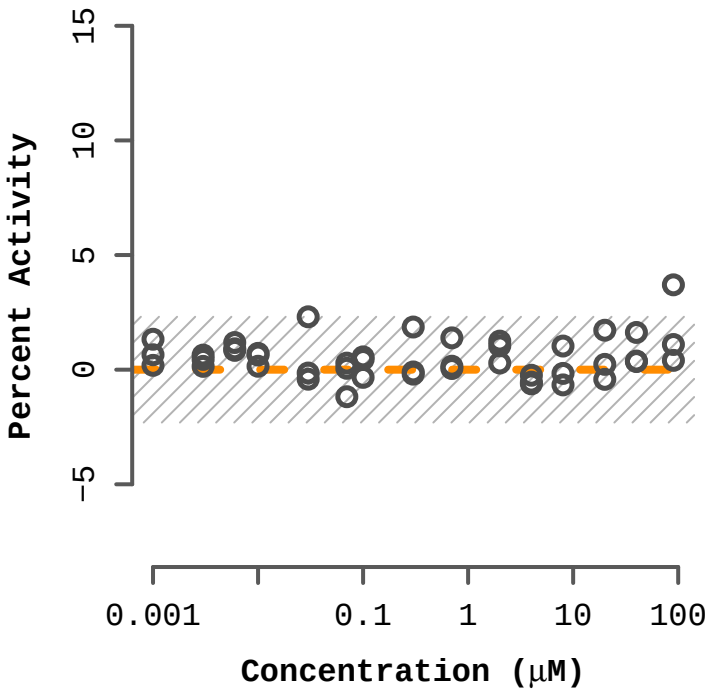
NAME: DINP branched
CHID: 28665 CASRN: 68515-48-0
SPID(S): Tox21_303462
M4ID: 12475678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.54 MAX_MED: 1.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

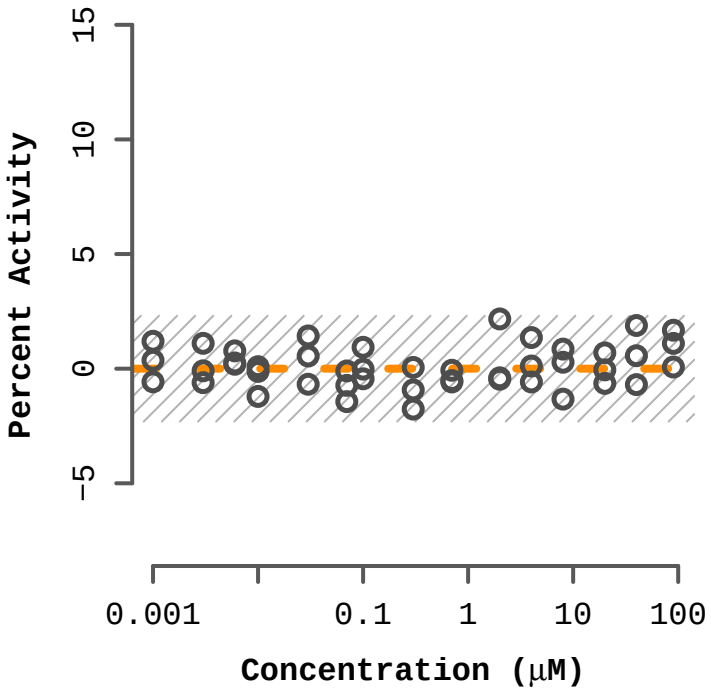
NAME: DINP branched
CHID: 28665 **CASRN:** 68515-48-0
SPID(S): Tox21_202296
M4ID: 12479956

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

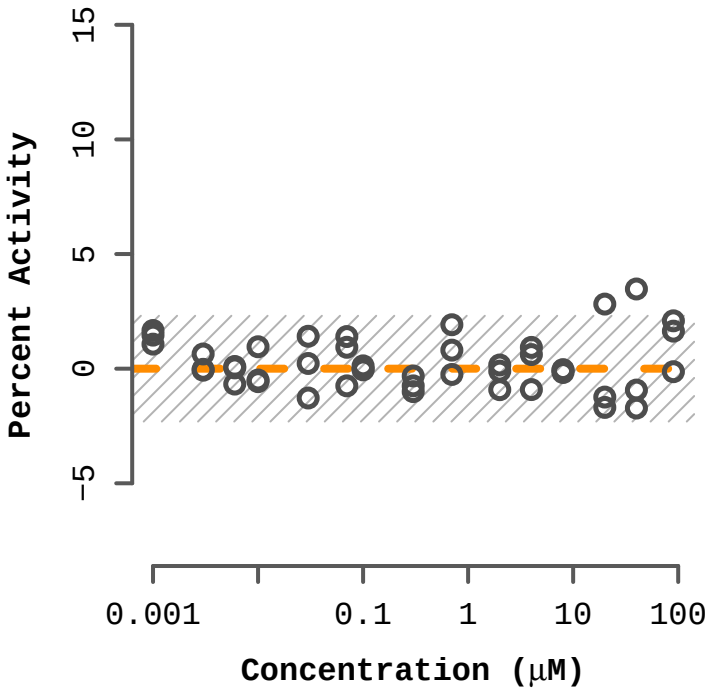
NAME: 1,2-Benzenedicarboxylic acid, di-C9-11-branche
CHID: 28666 **CASRN:** 68515-49-1
SPID(S): Tox21_300530
M4ID: 12478602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.952 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

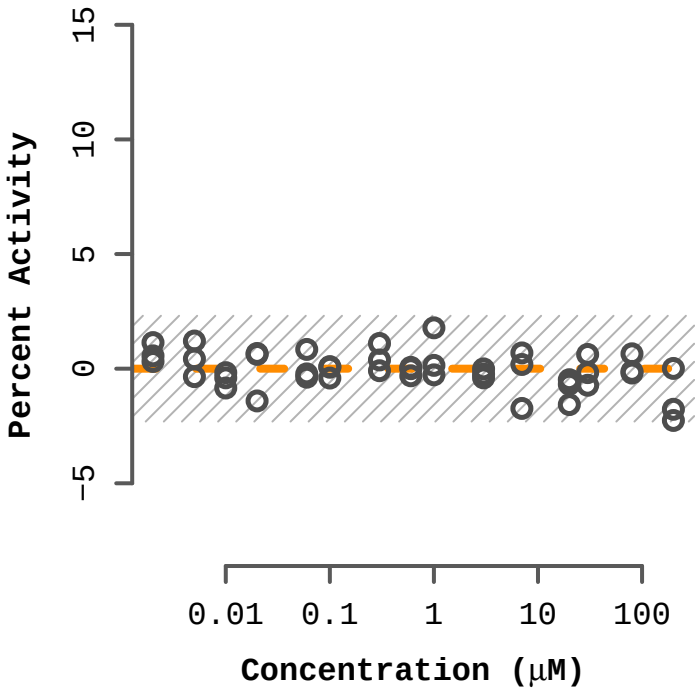
NAME: (C10−C16) Alkylbenzenesulfonic acid
CHID: 28723 **CASRN:** 68584−22−5
SPID(S): Tox21_202760
M4ID: 12479492

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

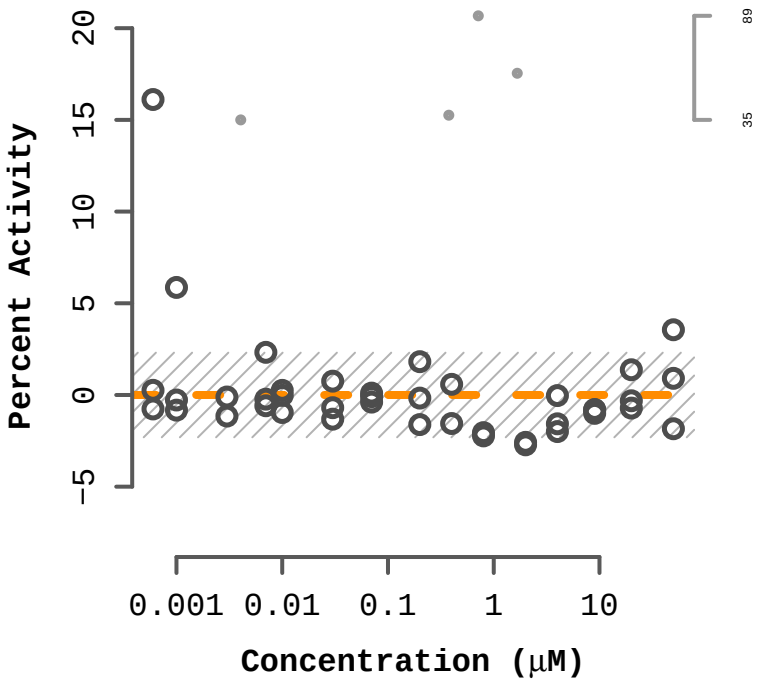
NAME: C12-14-Alkyl glycidyl ether
CHID: 28774 **CASRN:** 68609-97-2
SPID(S): Tox21_303452
M4ID: 12475688

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 0.624 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

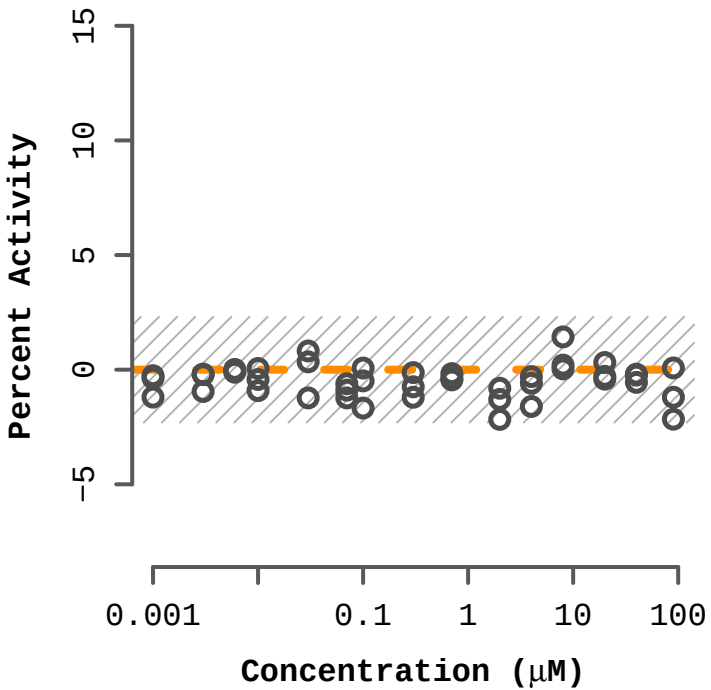
NAME: Poly(dicyclopentadiene-co-p-cresol)
CHID: 28776 **CASRN:** 68610-51-5
SPID(S): Tox21_302704
M4ID: 12476429 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	294.83	NA	NA
PROB:	1	NA	NA
RMSE:	18.01	NA	NA

MAX_MEAN: 28.3 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

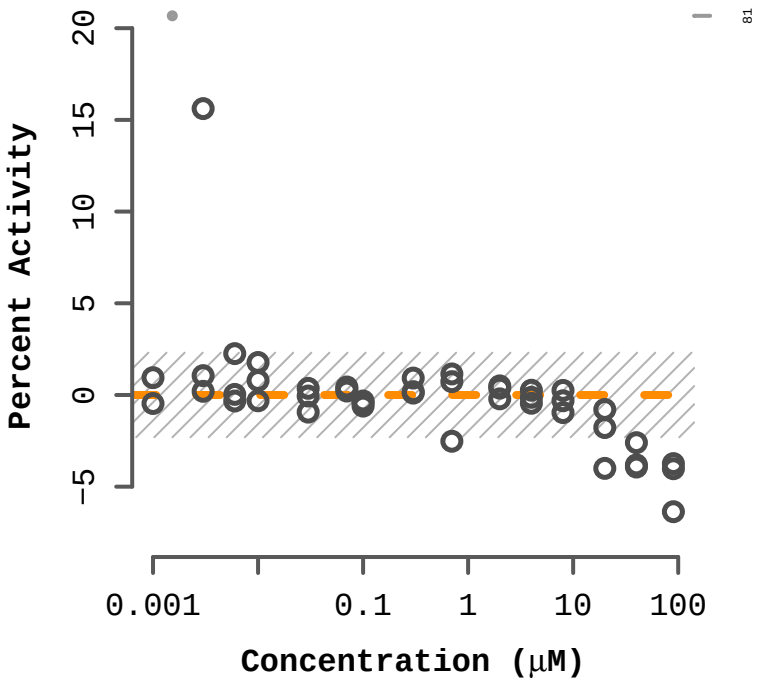
NAME: Sodium polyphosphate
CHID: 28842 CASRN: 68915-31-1
SPID(S): Tox21_200813
M4ID: 12481439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.556 **MAX_MED:** 0.342 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

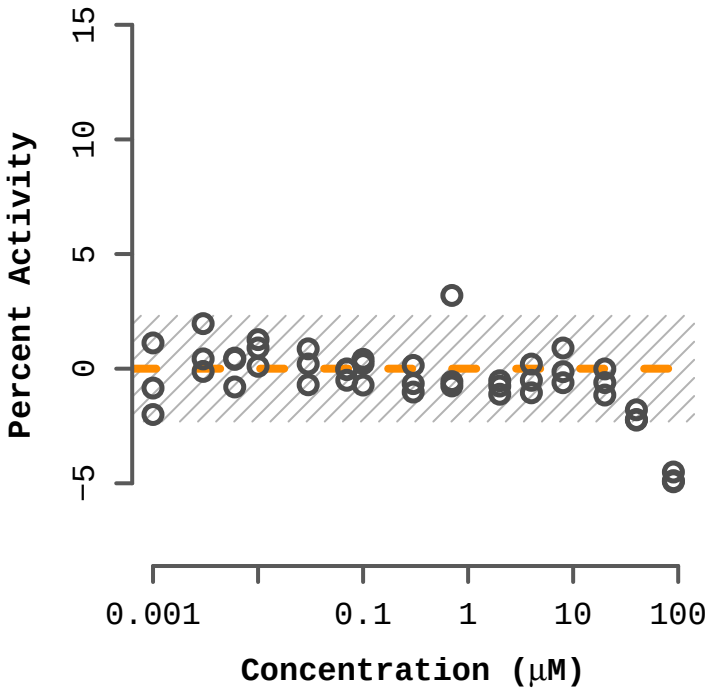
NAME: Triisopropylated phenyl phosphate
CHID: 28880 CASRN: 68937-41-7
SPID(S): Tox21_202766
M4ID: 12479486 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.76	NA	NA
PROB:	1	NA	NA
RMSE:	12.38	NA	NA

MAX_MEAN: 27 MAX_MED: 1.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

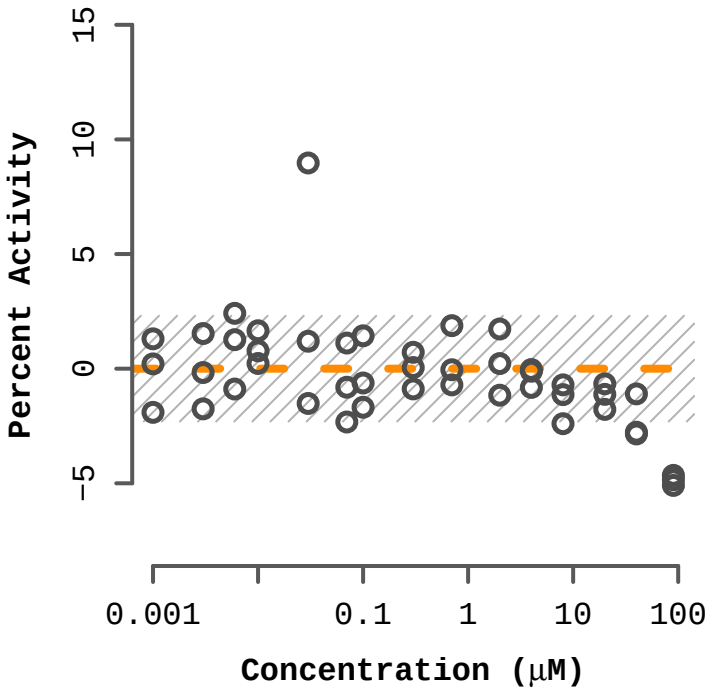
NAME: Triisopropylated phenyl phosphate
CHID: 28880 CASRN: 68937-41-7
SPID(S): Tox21_202765
M4ID: 12479487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 0.759 MAX_MED: 0.905 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

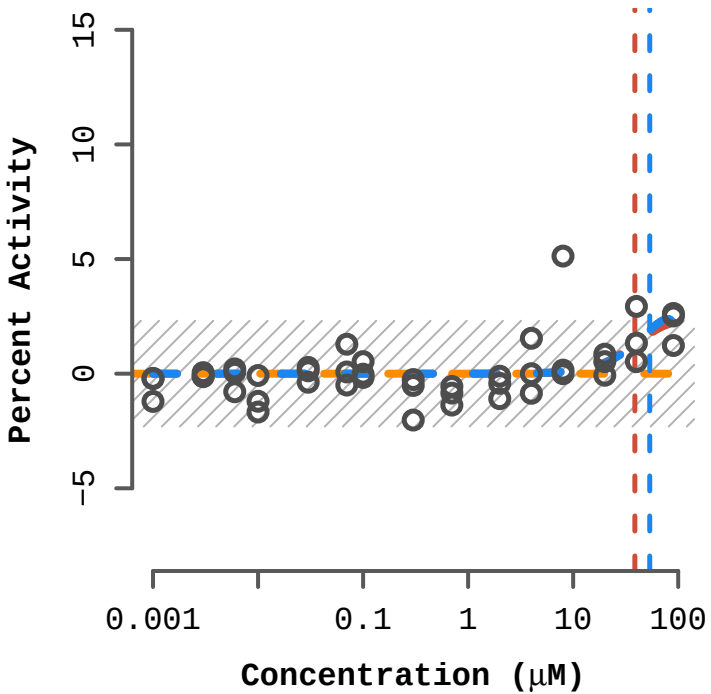
NAME: Triisopropylated phenyl phosphate
CHID: 28880 **CASRN:** 68937-41-7
SPID(S): Tox21_202764
M4ID: 12479488

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.88	NA	NA
PROB:	1	NA	NA
RMSE:	2.26	NA	NA

MAX_MEAN: 2.89 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-5-trichloromethylpyridine
CHID: 28967 CASRN: 69045-78-9
SPID(S): Tox21_301246
M4ID: 12477887

HILL MODEL (in red):

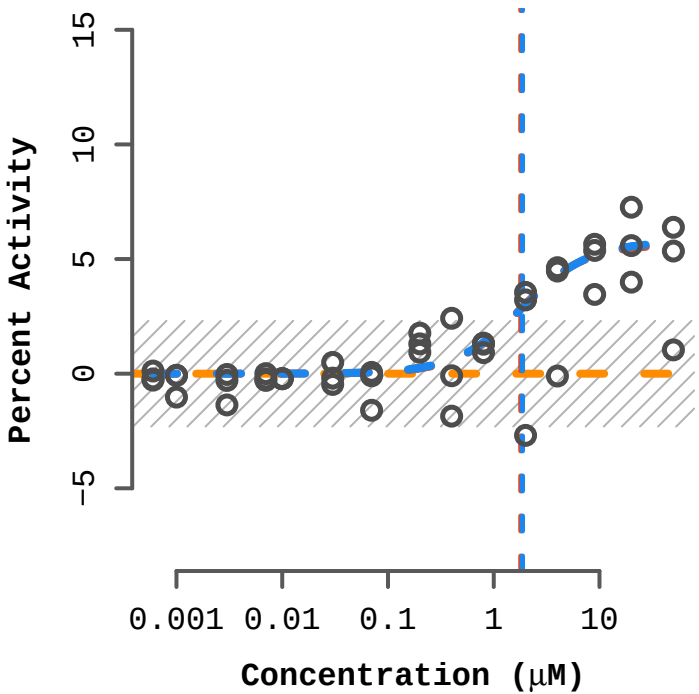
	tp	ga	gw
val:	2.59	1.59	2.23
sd:	1.27	0.301	1.97

GAIN-LOSS MODEL (in blue):

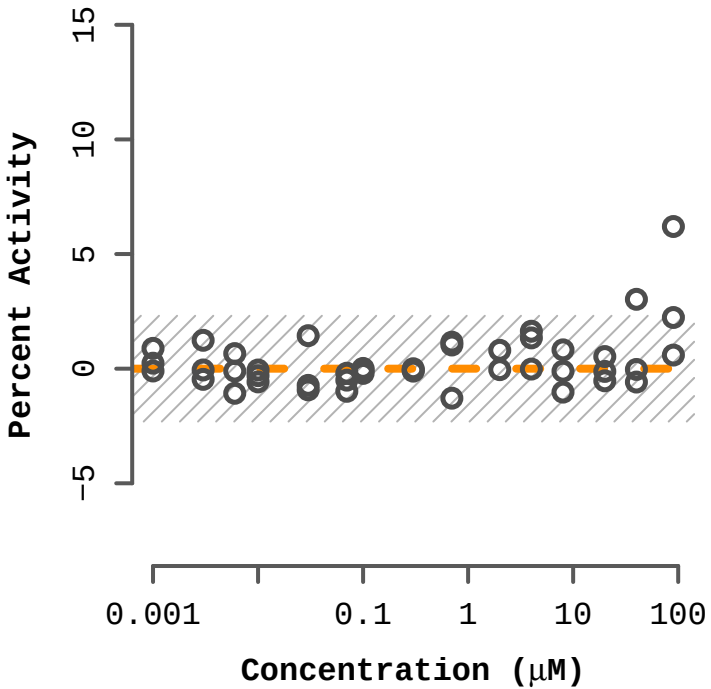
	tp	ga	gw	la	lw
val:	3.8	1.73	1.99	2.03	7.9
sd:	21	2.01	2.79	0.443	88.9

	CNST	HILL	GNLS
AIC:	140.05	123.4	127.39
PROB:	0	0.88	0.12
RMSE:	1.28	1.07	1.07

MAX_MEAN: 2.13 **MAX_MED:** 2.52 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-(2H-Benzotriazol-2-yl)-4,6-bis(1-methyl-1-ph
CHID:    28985   CASRN: 70321-86-7
SPID(S): Tox21_202571
M4ID:    12479681

HILL MODEL (in red):
      tp       ga       gw
val:  5.65     0.255    1.43
sd:   0.518    0.105    0.458

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.77     0.272    1.37     1.85     10.3
sd:   0.864    0.149    0.533    0.828    57.7

      CNST        HILL        GNLS
AIC:  216.96      151.98      155.94
PROB: 0           0.88        0.12
RMSE: 2.75        1.51        1.51

MAX_MEAN: 5.61      MAX_MED: 5.59      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

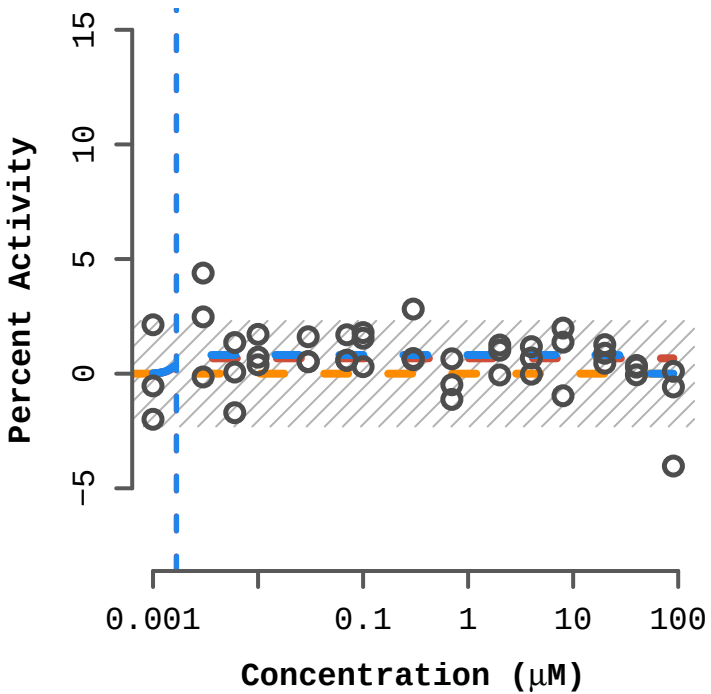
NAME: 1,2-Benzenedicarboxylic acid, di-C6-8-branched
CHID: 29017 CASRN: 71888-89-6
SPID(S): Tox21_200941
M4ID: 12481311

HILL MODEL: Not applicable.

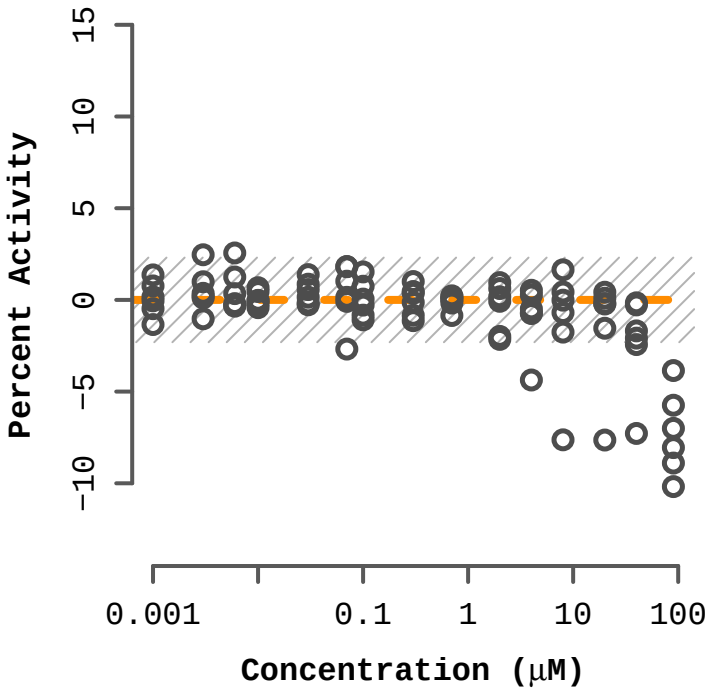
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 3.01 MAX_MED: 2.23 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Nonylphenol, branched
CHID:    29055   CASRN: 84852-15-3
SPID(S): Tox21_300576
M4ID:    12478557

HILL MODEL (in red):
      tp       ga       gw
val:  0.67     -2.78    8
sd:   0.163    0.426    14.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  0.816    -2.78    8        1.57     16.7
sd:   0.167    0.378    12.7     0.251    146

      CNST        HILL        GNLS
AIC:  162.37      154.23      153.24
PROB: 0.01        0.38        0.62
RMSE: 1.46        1.33        1.25

MAX_MEAN: 2.24      MAX_MED: 2.48      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

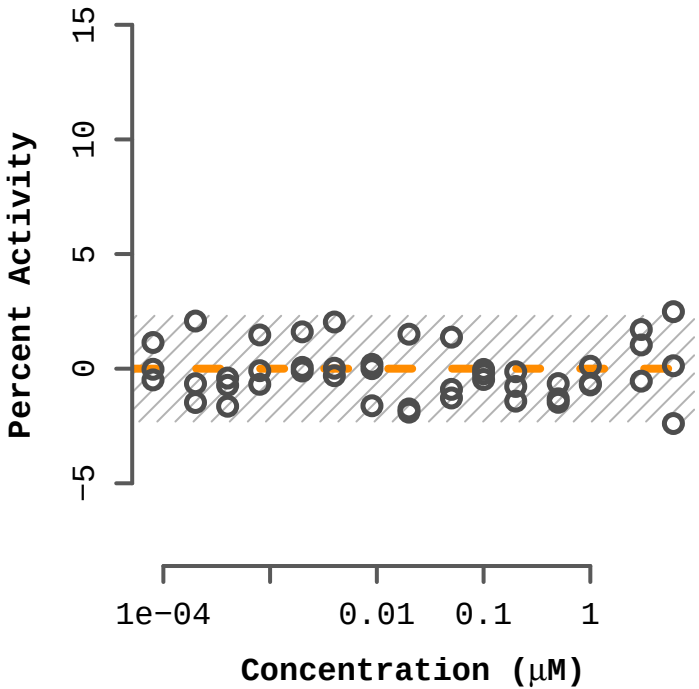
NAME: 4-Nonylphenol, branched
CHID: 29055 **CASRN:** 84852-15-3
SPID(S): Tox21_201528
M4ID: 12480724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	379.12	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 0.552 **MAX_MED:** 0.583 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

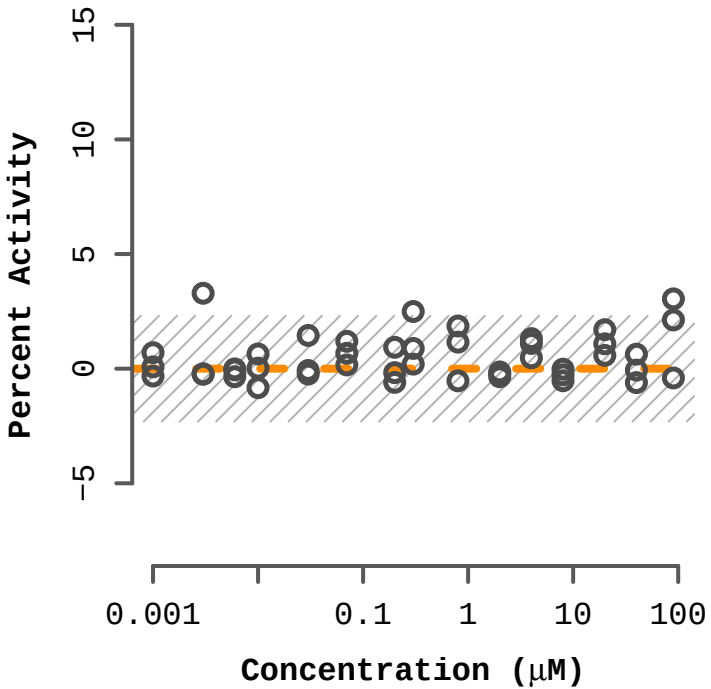
NAME: Perfluoro compounds, C5-18
CHID: 29059 **CASRN:** 86508-42-1
SPID(S): Tox21_202767
M4ID: 12479485

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.735 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

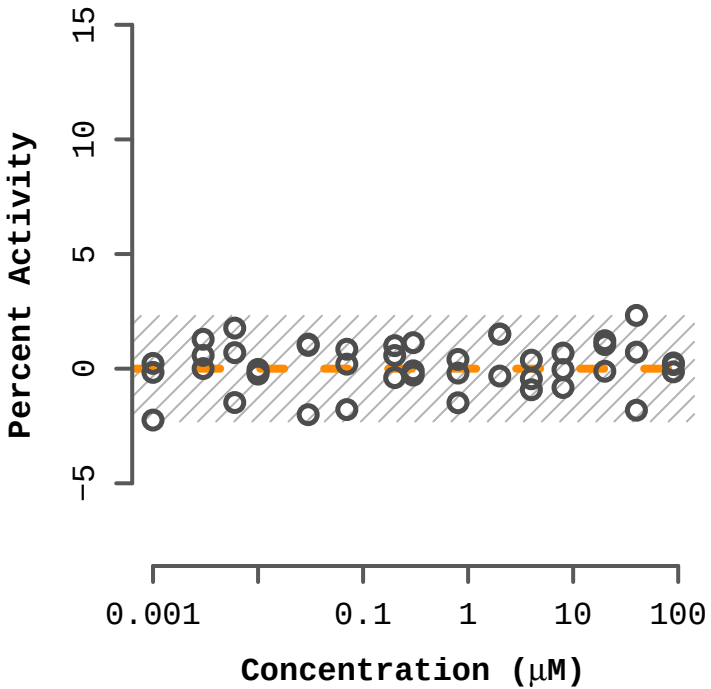
NAME: Hexanol, acetate, branched and linear
CHID: 29061 **CASRN:** 88230-35-7
SPID(S): Tox21_200711
M4ID: 12481541

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

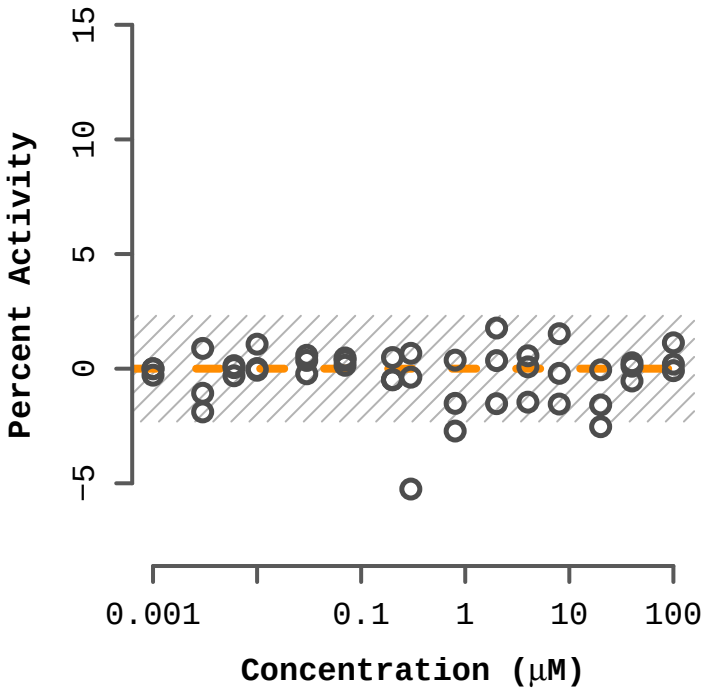
NAME: Dipropyleneglycol methyl ether acetate
CHID: 29062 CASRN: 88917-22-0
SPID(S): Tox21_200212
M4ID: 12482040

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.899 MAX_MED: 1.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

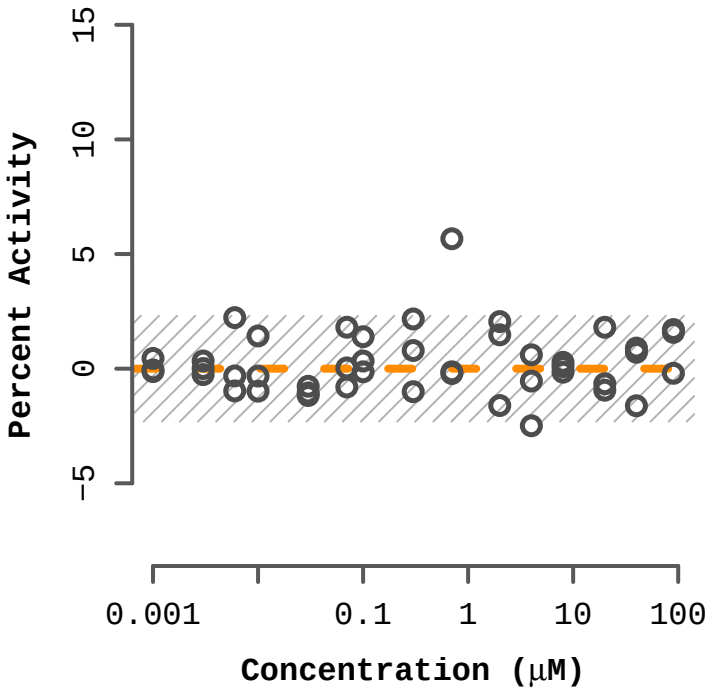
NAME: 5-Ethyl-2,3-pyridinedicarboxylic acid
CHID: 29072 **CASRN:** 102268-15-5
SPID(S): Tox21_300682
M4ID: 12478451

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.414 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

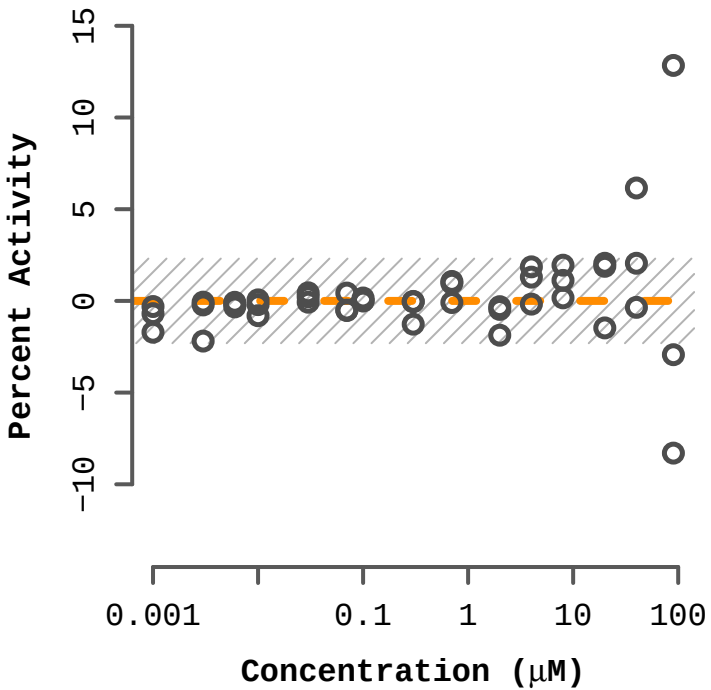
NAME: 4-Toluenesulfonamide
CHID: 29105 **CASRN:** 70-55-3
SPID(S): Tox21_303506
M4ID: 12475636

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

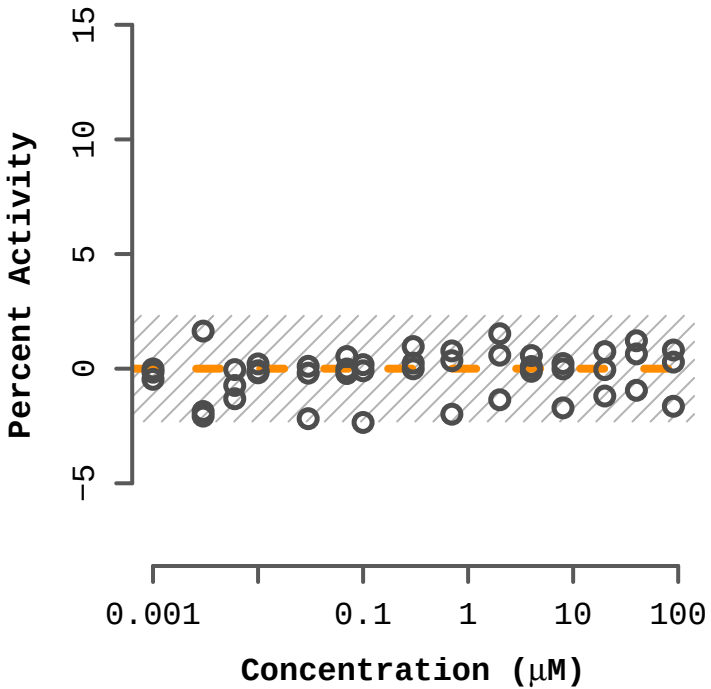
NAME: 4-Toluenesulfonamide
CHID: 29105 **CASRN:** 70-55-3
SPID(S): Tox21_201594
M4ID: 12480658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 2.62 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

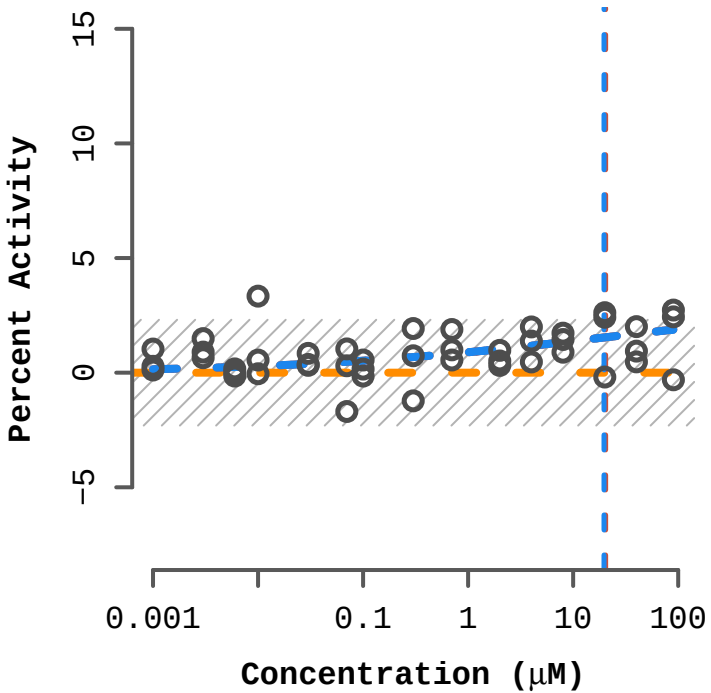
NAME: Tetramethylammonium hydroxide
CHID: 29108 **CASRN:** 75-59-2
SPID(S): Tox21_202572
M4ID: 12479680

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.23	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.402 **MAX_MED:** 0.646 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,7-Dimethyl-3-octanol
CHID: 29110 **CASRN:** 78-69-3
SPID(S): Tox21_303468
M4ID: 12475672

HILL MODEL (in red):

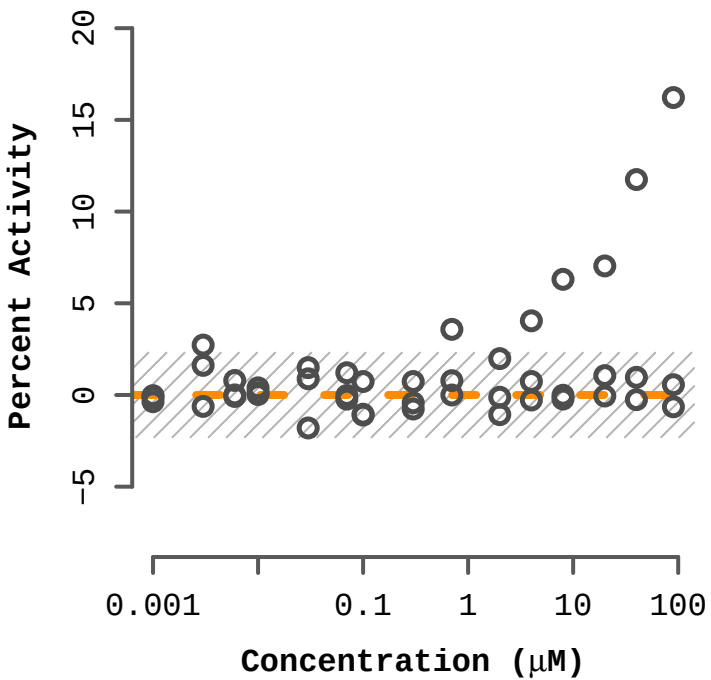
	tp	ga	gw
val:	3.09	1.31	0.3
sd:	7.9	7.39	0.442

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.07	1.29	0.3	3.54	4.95
sd:	7.11	6.69	0.4	1490	4710

	CNST	HILL	GNLS
AIC:	155.08	126.68	130.68
PROB:	0	0.88	0.12
RMSE:	1.31	0.95	0.95

MAX_MEAN: 1.62 **MAX_MED:** 2.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

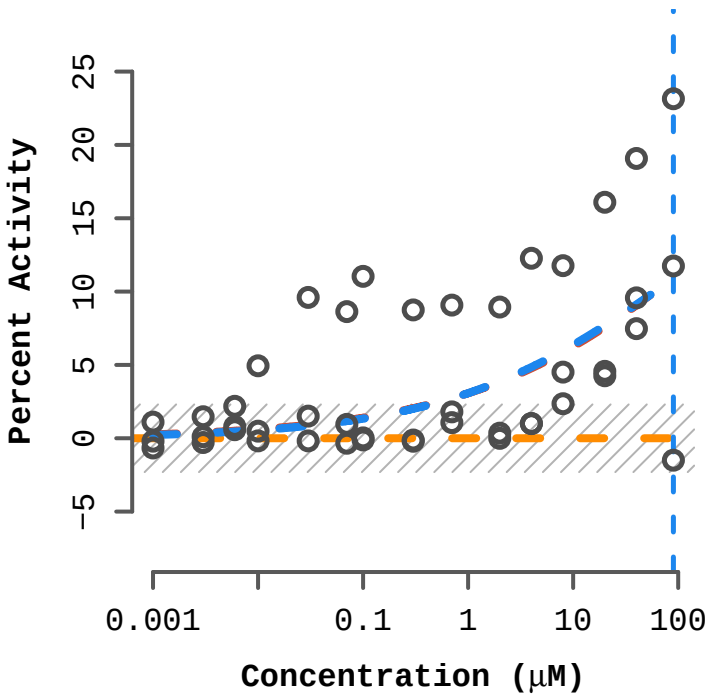
NAME: 3,7-Dimethyl-3-octanol
CHID: 29110 CASRN: 78-69-3
SPID(S): Tox21_202390
M4ID: 12479862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.28	NA	NA
PROB:	1	NA	NA
RMSE:	3.5	NA	NA

MAX_MEAN: 5.38 MAX_MED: 1.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1':3',1''-Terphenyl
CHID: 29117 CASRN: 92-06-8
SPID(S): Tox21_303528
M4ID: 12475615

HILL MODEL (in red):

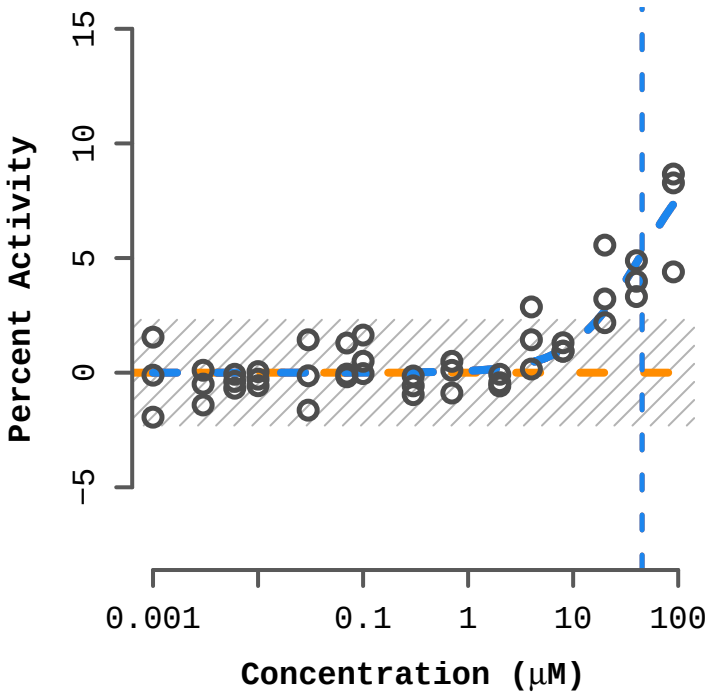
	tp	ga	gw
val:	27.8	2.45	0.369
sd:	30.5	2.09	0.157

GAIN-LOSS MODEL (in blue):

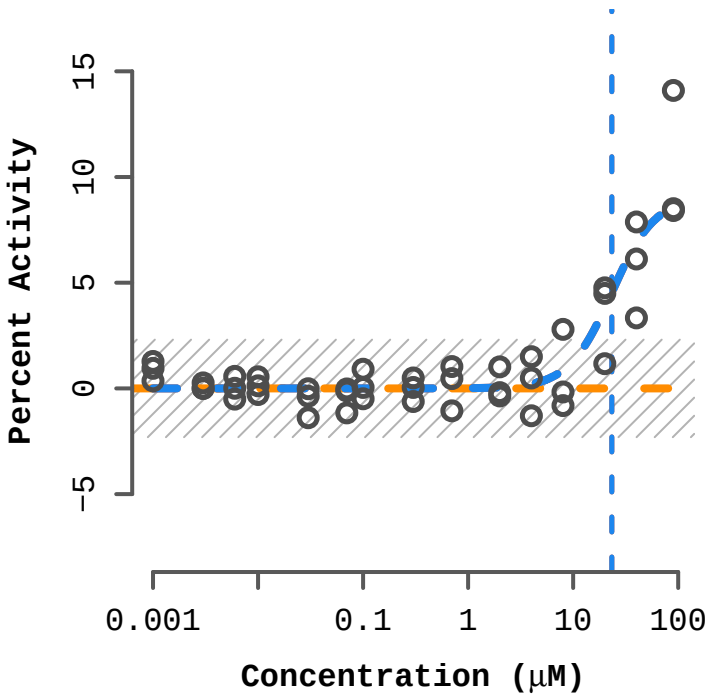
	tp	ga	gw	la	lw
val:	21.7	1.95	0.401	3.09	5.69
sd:	22.6	1.91	0.175	366	1830

	CNST	HILL	GNLS
AIC:	301.13	274.79	279.03
PROB:	0	0.89	0.11
RMSE:	7.26	4.81	4.82

MAX_MEAN: 12 MAX_MED: 11.7 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1,1':3',1''-Terphenyl
CHID:    29117   CASRN: 92-06-8
SPID(S): Tox21_201579
M4ID:    12480673

HILL MODEL (in red):
      tp       ga       gw
val:  10.4     1.66     1.28
sd:   3.52     0.226    0.259

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.4     1.66     1.28     3.6      4.87
sd:   3.53     0.227    0.258    808      2410

      CNST        HILL        GNLS
AIC:  200.32      140.15      144.15
PROB: 0           0.88        0.12
RMSE: 2.56        1.08        1.08

MAX_MEAN: 7.11      MAX_MED: 8.28      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Biphenyldiol
CHID: 29120 CASRN: 92−88−6
SPID(S): Tox21_200469
M4ID: 12481783

HILL MODEL (in red):

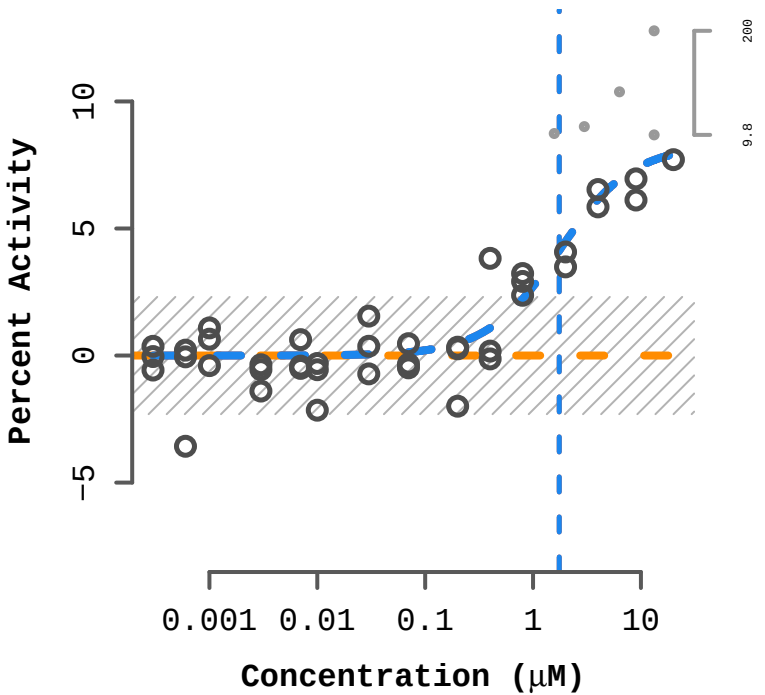
	tp	ga	gw
val:	9.07	1.37	2.11
sd:	1.17	0.107	0.892

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.07	1.37	2.11	3.37	5.53
sd:	1.17	0.107	0.892	1090	4260

	CNST	HILL	GNLS
AIC:	211.86	145.54	149.54
PROB:	0	0.88	0.12
RMSE:	3.41	1.31	1.31

MAX_MEAN: 10.3 MAX_MED: 8.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1':4',1''-Terphenyl
CHID: 29121 **CASRN:** 92-94-4
SPID(S): Tox21_202759
M4ID: 12479493 **BRK**

HILL MODEL (in red):

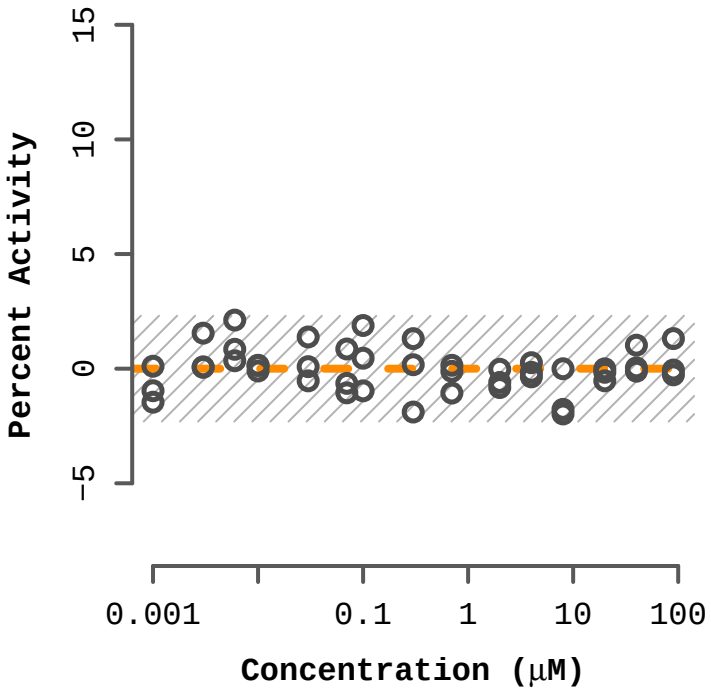
	tp	ga	gw
val:	8.27	0.243	1.28
sd:	1.31	0.184	0.39

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.27	0.243	1.28	2.71	6.67
sd:	1.31	0.184	0.39	4170	19800

	CNST	HILL	GNLS
AIC:	312.74	257.26	261.26
PROB:	0	0.88	0.12
RMSE:	33.44	31.69	31.69

MAX_MEAN: 73.4 **MAX_MED:** 9.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

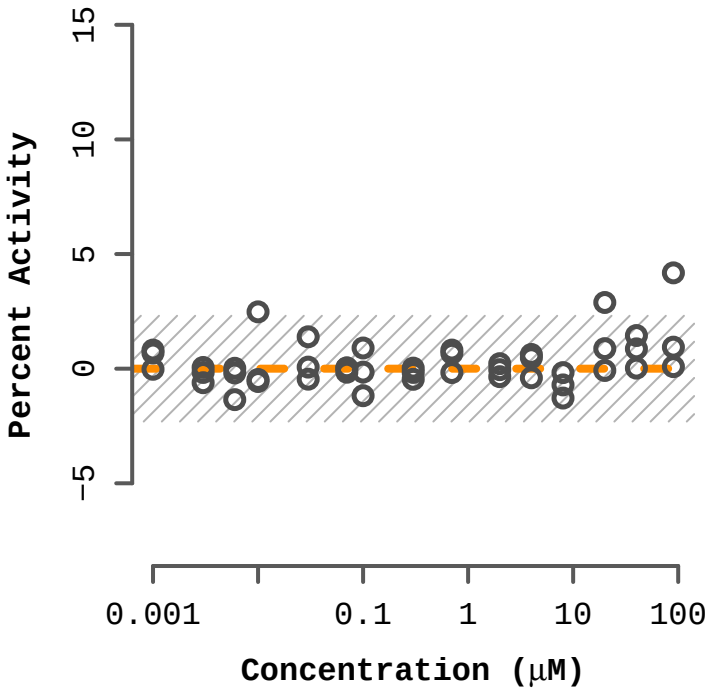
NAME: Benzoic anhydride
CHID: 29122 **CASRN:** 93-97-0
SPID(S): Tox21_200829
M4ID: 12481423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.847 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

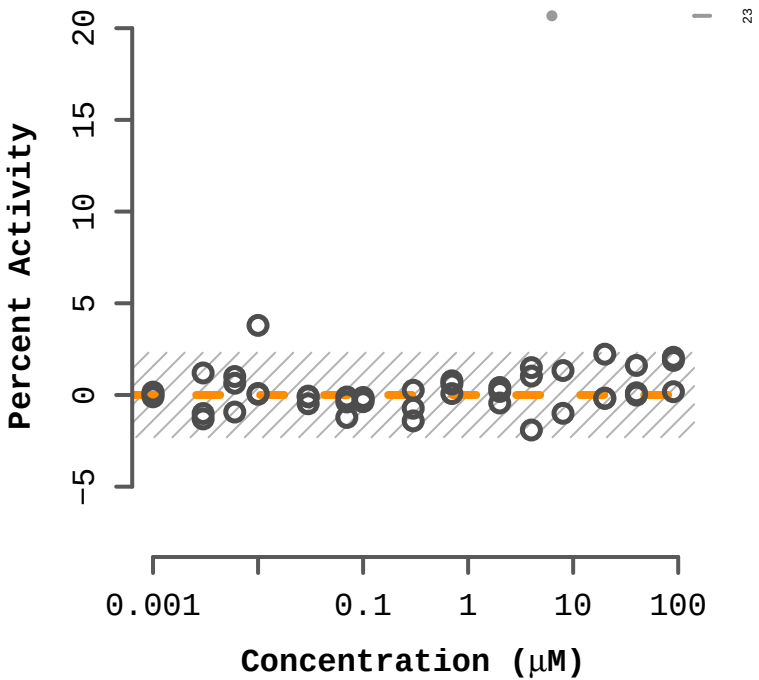
NAME: 1,2,4,5-Tetramethylbenzene
CHID: 29124 **CASRN:** 95-93-2
SPID(S): Tox21_303511
M4ID: 12475631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

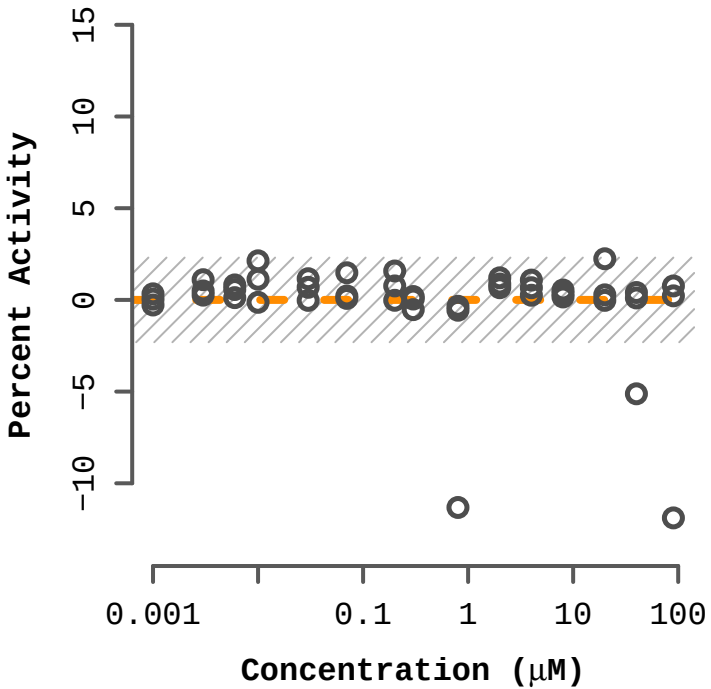
NAME: 1,2,4,5-Tetramethylbenzene
CHID: 29124 CASRN: 95-93-2
SPID(S): Tox21_201920
M4ID: 12480332 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.17	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 7.73 MAX_MED: 1.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

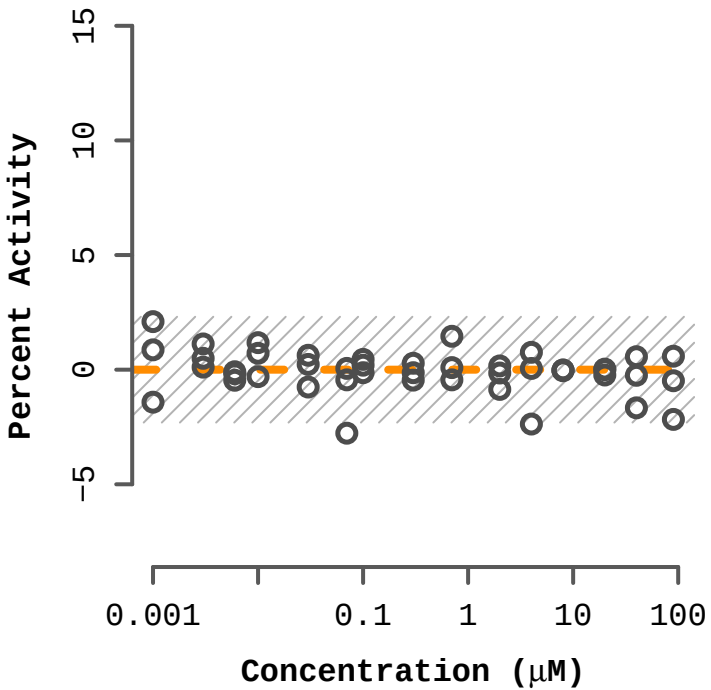
NAME: Ethyl lactate
CHID: 29127 CASRN: 97-64-3
SPID(S): Tox21_200889
M4ID: 12481363

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.9	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 1.04 MAX_MED: 1.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

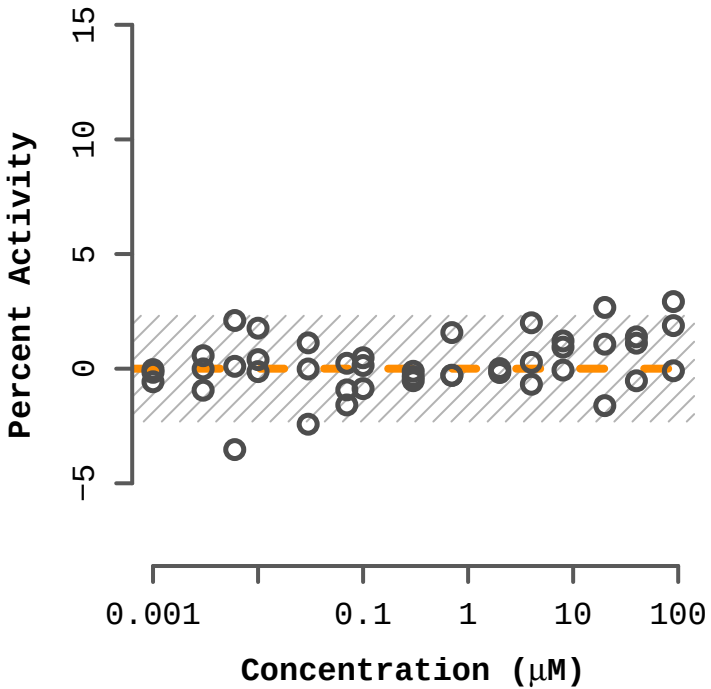
NAME: Tetrahydrofurfuryl alcohol
CHID: 29128 **CASRN:** 97-99-4
SPID(S): Tox21_303393
M4ID: 12475745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.578 **MAX_MED:** 0.866 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

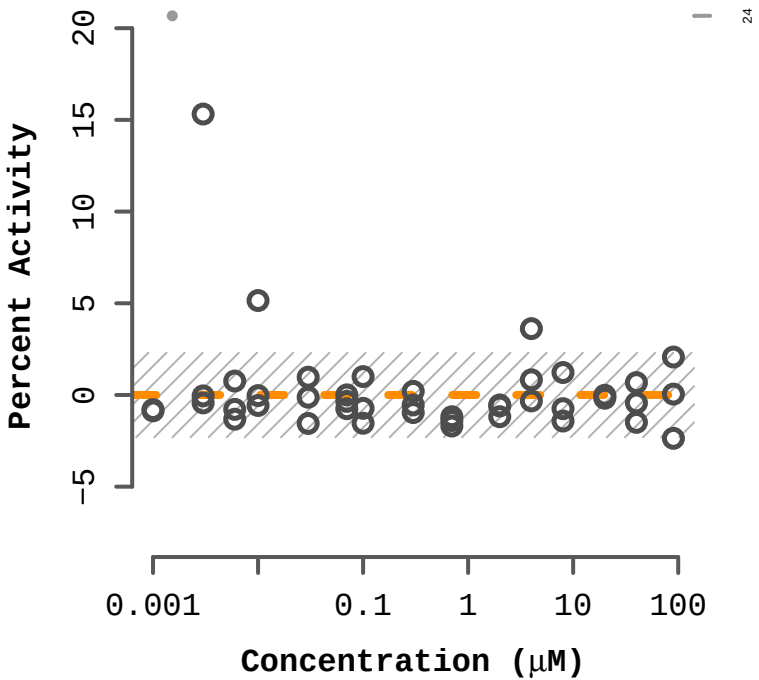
NAME: Tetrahydrofurfuryl alcohol
CHID: 29128 **CASRN:** 97-99-4
SPID(S): Tox21_201324
M4ID: 12480928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

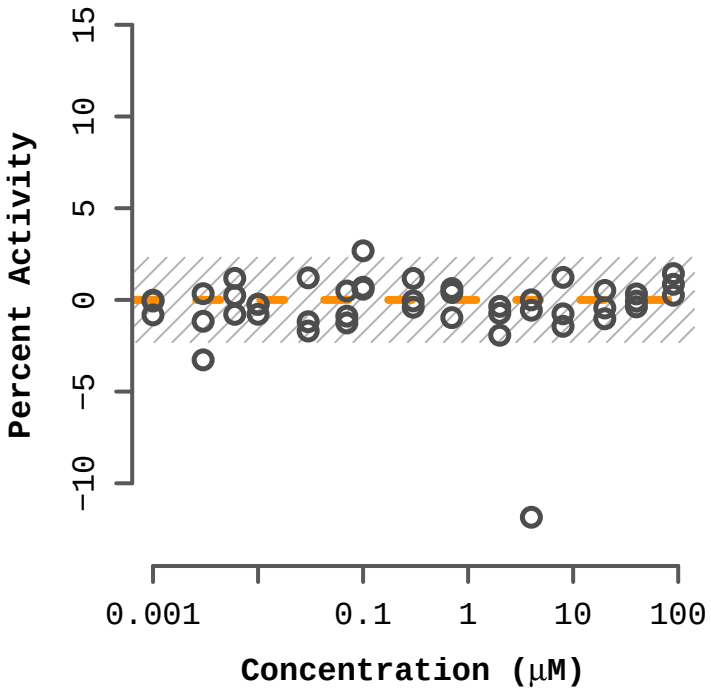
NAME: 4-Hydroxyacetophenone
CHID: 29133 CASRN: 99-93-4
SPID(S): Tox21_303602
M4ID: 12475543 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.95	NA	NA
PROB:	1	NA	NA
RMSE:	4.4	NA	NA

MAX_MEAN: 7.31 MAX_MED: 0.829 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

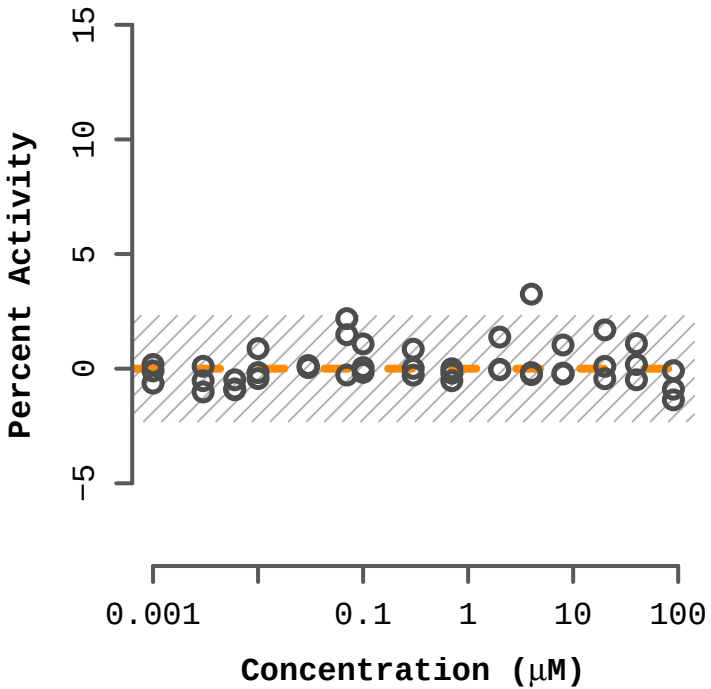
NAME: 4-Hydroxyacetophenone
CHID: 29133 **CASRN:** 99-93-4
SPID(S): Tox21_200228
M4ID: 12482024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

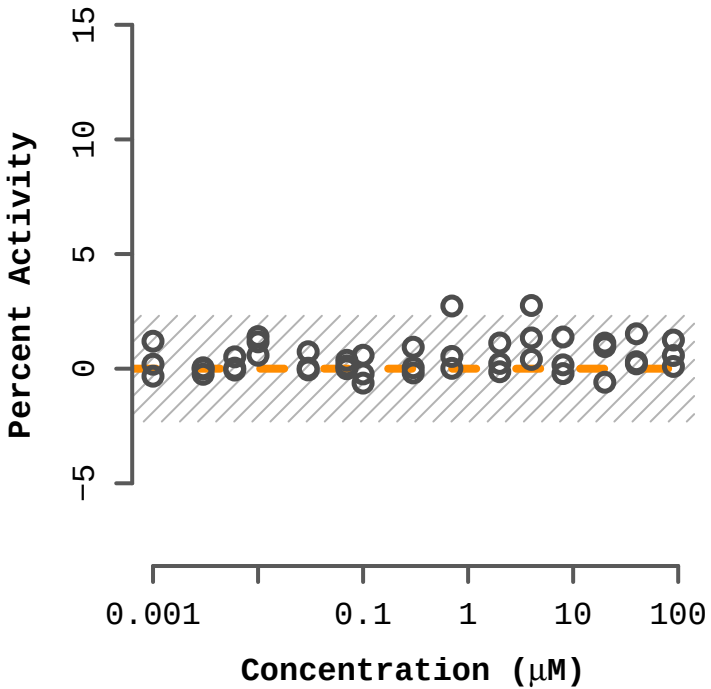
NAME: 3-((Ethylphenylamino)methyl)benzenesulfonic ac
CHID: 29136 **CASRN:** 101-11-1
SPID(S): Tox21_300921
M4ID: 12478212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

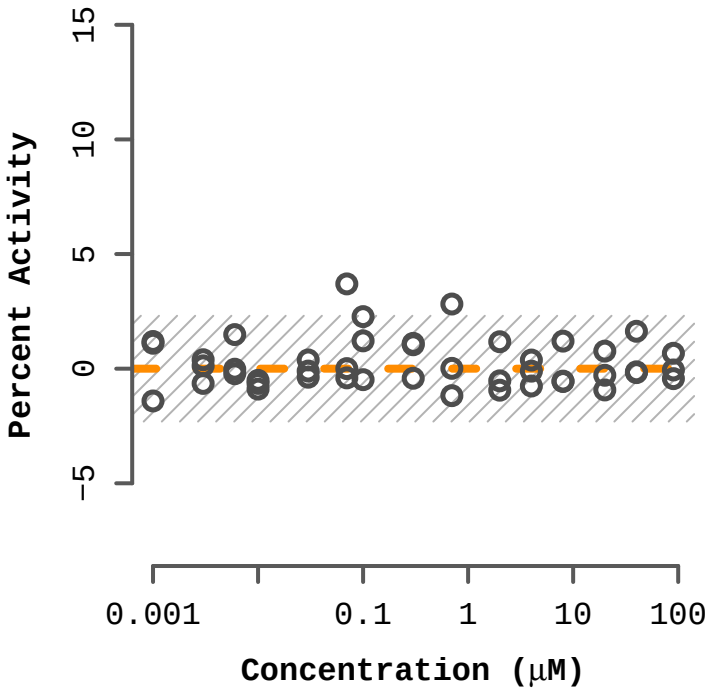
NAME: 2-Methylpentane
CHID: 29143 **CASRN:** 107-83-5
SPID(S): Tox21_200470
M4ID: 12481782

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

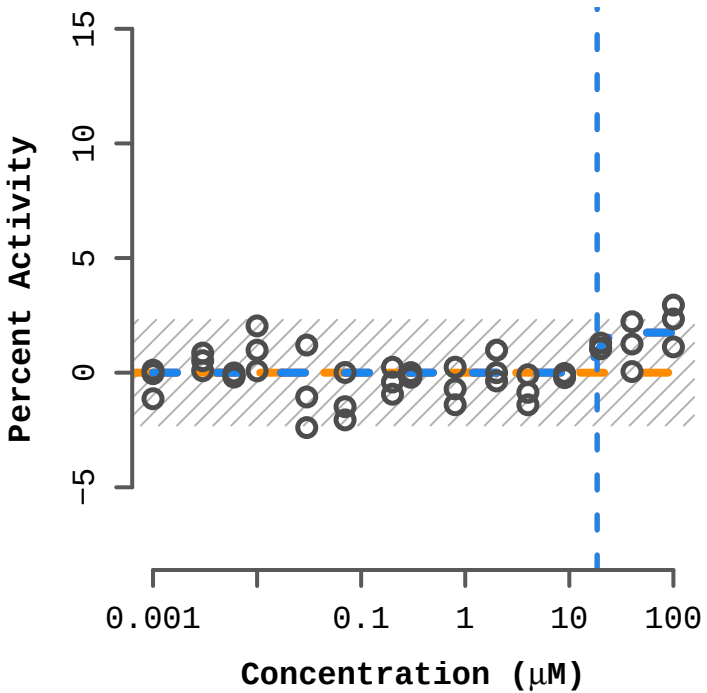
NAME: Dimethyl malonate
CHID: 29145 **CASRN:** 108-59-8
SPID(S): Tox21_300375
M4ID: 12478757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethyl malonate
CHID: 29145 CASRN: 108-59-8
SPID(S): Tox21_201608
M4ID: 12480644

HILL MODEL (in red):

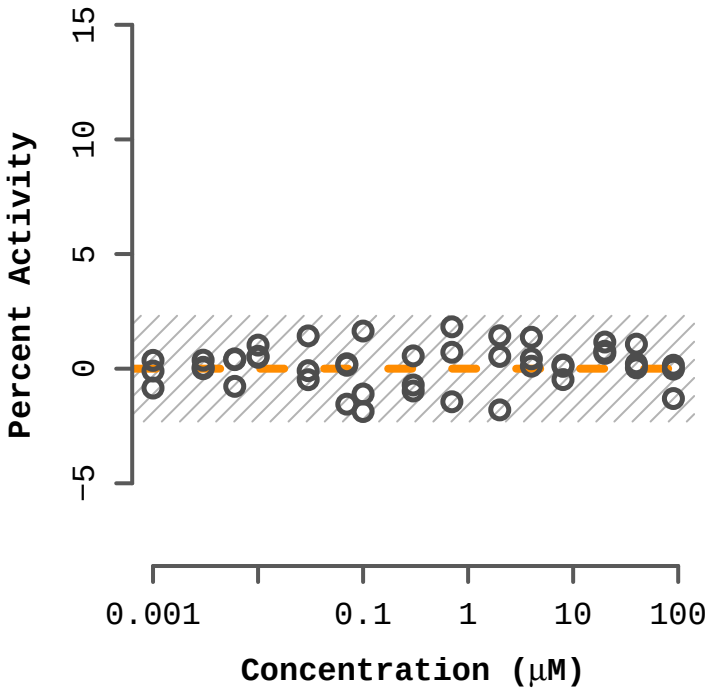
	tp	ga	gw
val:	1.75	1.27	7.76
sd:	0.421	0.144	38.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.75	1.27	7.71	3.78	4.59
sd:	0.421	0.141	36.9	2010	5220

	CNST	HILL	GNLS
AIC:	139.16	123.24	127.24
PROB:	0	0.88	0.12
RMSE:	1.11	0.89	0.89

MAX_MEAN: 2.14 MAX_MED: 2.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

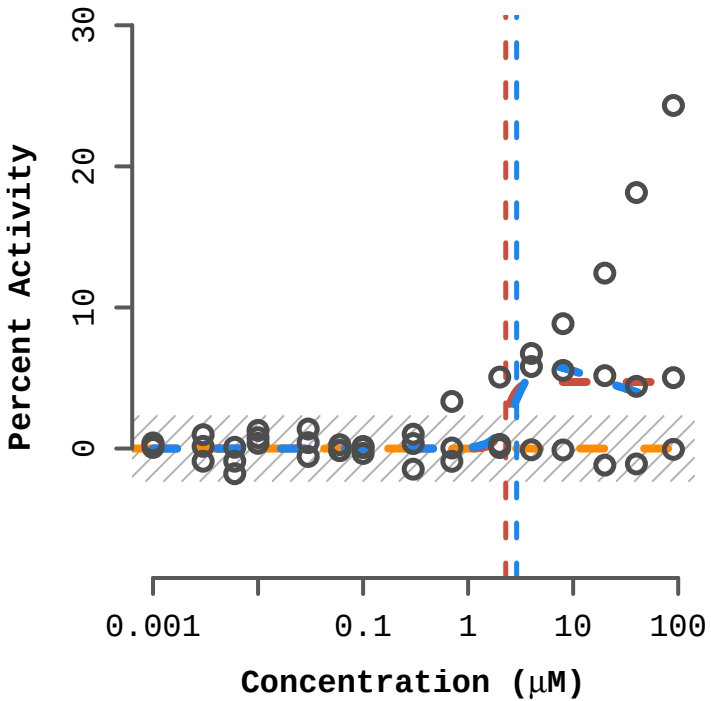
NAME: 4-Methylmorpholine
CHID: 29146 **CASRN:** 109-02-4
SPID(S): Tox21_303402
M4ID: 12475737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.865 **MAX_MED:** 0.761 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylmorpholine
CHID: 29146 CASRN: 109-02-4
SPID(S): Tox21_202412
M4ID: 12479840

HILL MODEL (in red):

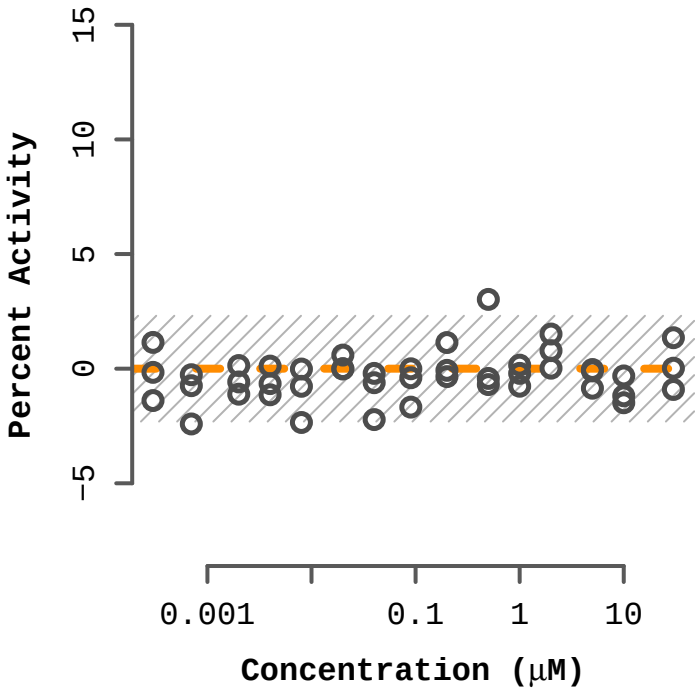
	tp	ga	gw
val:	4.72	0.358	8
sd:	0.836	0.106	11.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.6	0.462	4.51	0.712	0.372
sd:	72	0.217	4.18	12.7	1.22

	CNST	HILL	GNLS
AIC:	250.8	236.31	239.1
PROB:	0	0.8	0.2
RMSE:	5.56	4.29	4.47

MAX_MEAN: 9.76 MAX_MED: 5.82 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

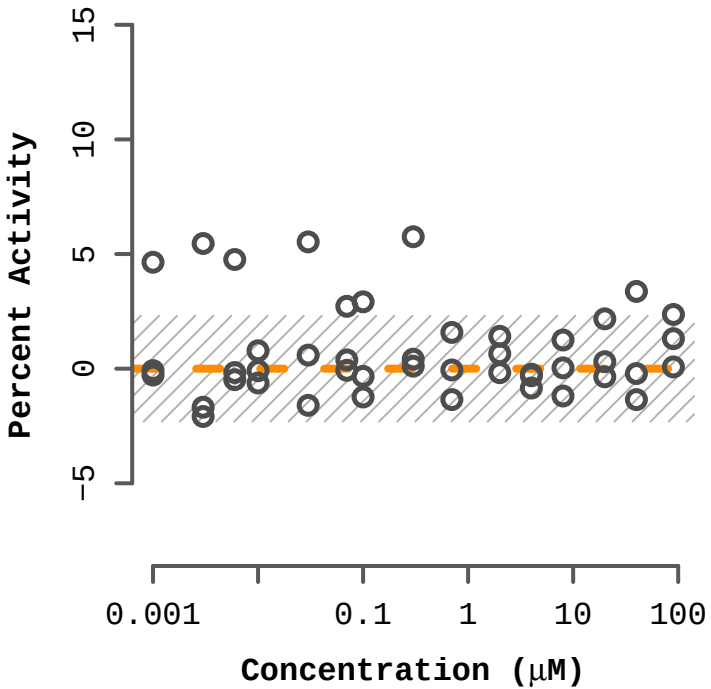
NAME: Methyl hexadecanoate
CHID: 29149 **CASRN:** 112-39-0
SPID(S): Tox21_202768
M4ID: 12479484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.774 **MAX_MED:** 0.788 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

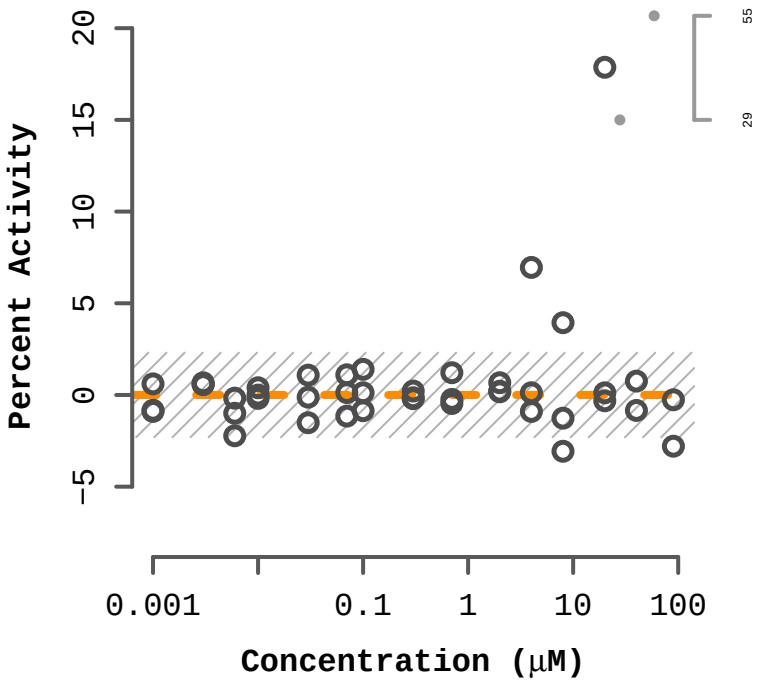
NAME: 2-Amino-2-ethyl-1,3-propanediol
CHID: 29150 **CASRN:** 115-70-8
SPID(S): Tox21_200845
M4ID: 12481407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.27	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

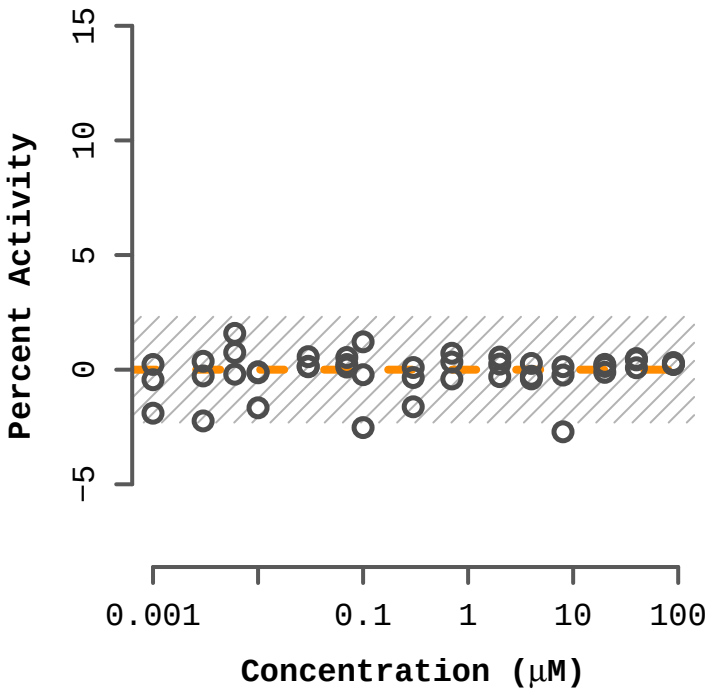
NAME: 1-Methoxy-4-methyl-2-nitrobenzene
CHID: 29152 **CASRN:** 119-10-8
SPID(S): Tox21_201221
M4ID: 12481031 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.19	NA	NA
PROB:	1	NA	NA
RMSE:	9.75	NA	NA

MAX_MEAN: 17.3 **MAX_MED:** 0.758 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

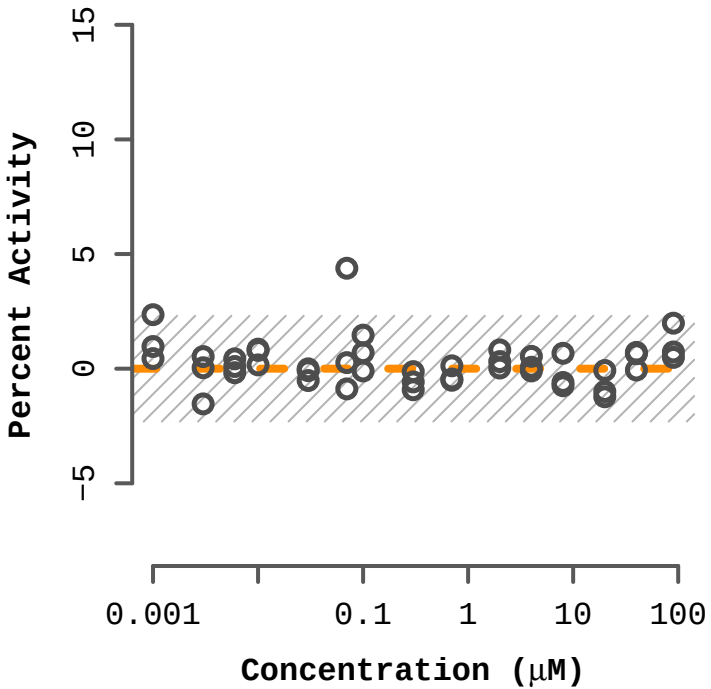
NAME: Benzyl benzoate
CHID: 29153 **CASRN:** 120-51-4
SPID(S): Tox21_303418
M4ID: 12475721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.713 **MAX_MED:** 0.751 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

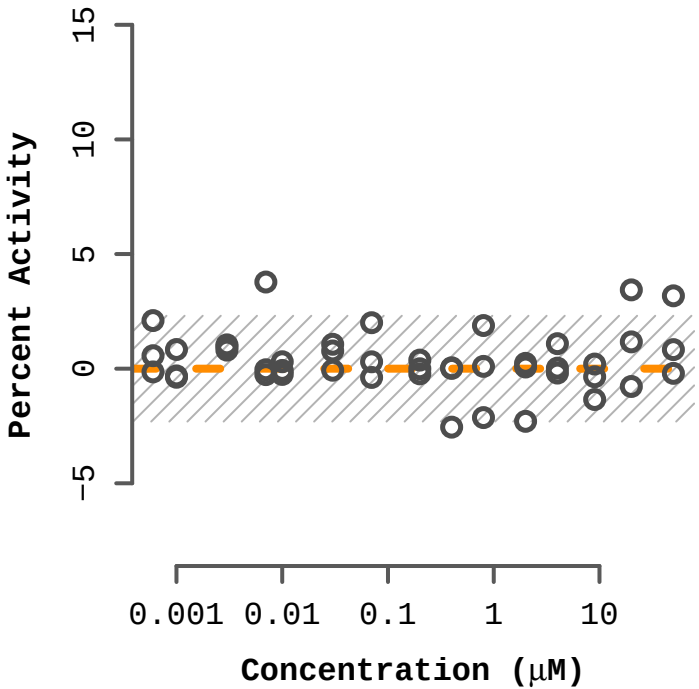
NAME: Benzyl benzoate
CHID: 29153 **CASRN:** 120-51-4
SPID(S): Tox21_201337
M4ID: 12480915

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.968 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

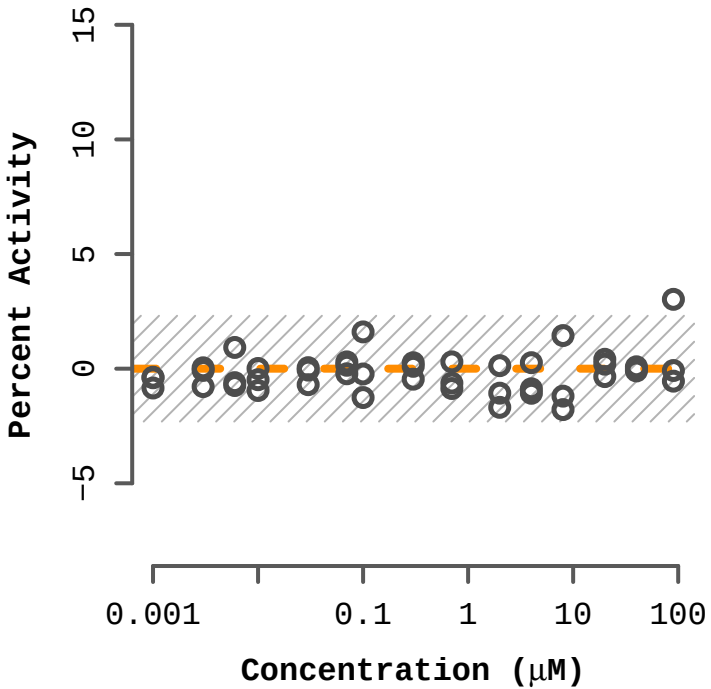
NAME: Benzyl benzoate
CHID: 29153 **CASRN:** 120-51-4
SPID(S): Tox21_111372_1
M4ID: 12483732

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

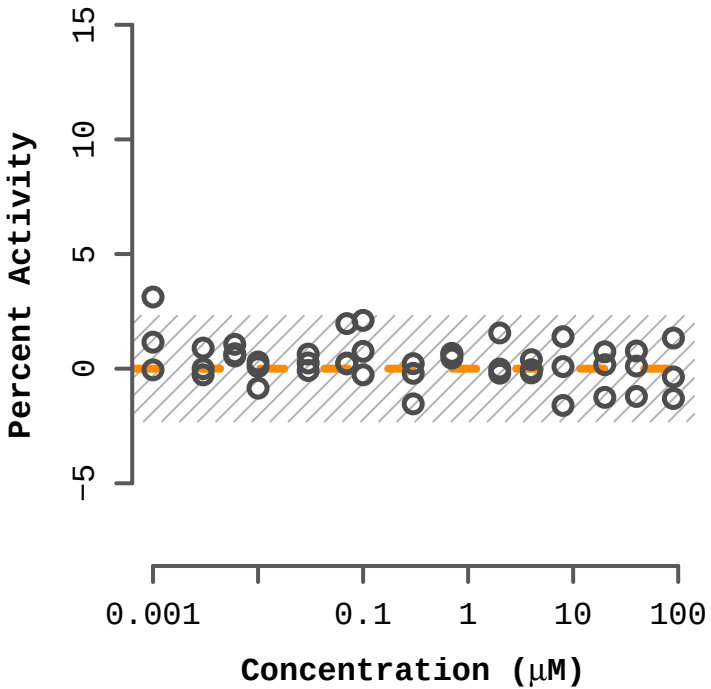
NAME: Cyclopentanone
CHID: 29154 **CASRN:** 120-92-3
SPID(S): Tox21_303562
M4ID: 12475583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.197 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

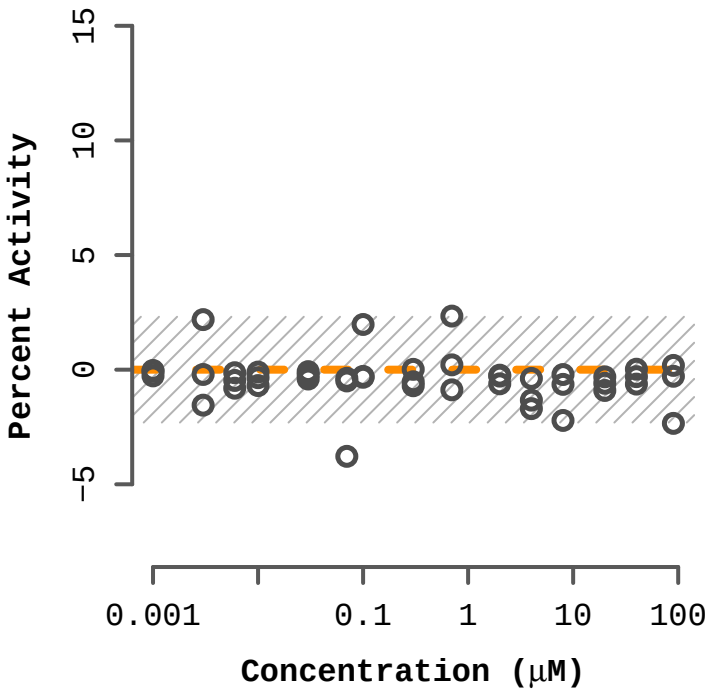
NAME: Cyclopentanone
CHID: 29154 CASRN: 120-92-3
SPID(S): Tox21_200244
M4ID: 12482008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.41 MAX_MED: 1.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

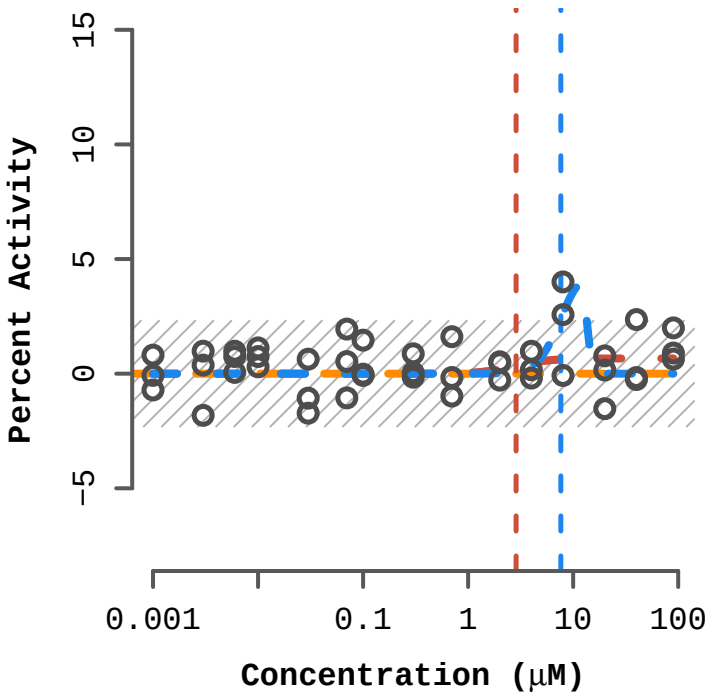
NAME: Pentylcinnamaldehyde
CHID: 29157 **CASRN:** 122-40-7
SPID(S): Tox21_303598
M4ID: 12475547

HILL MODEL: Not applicable.

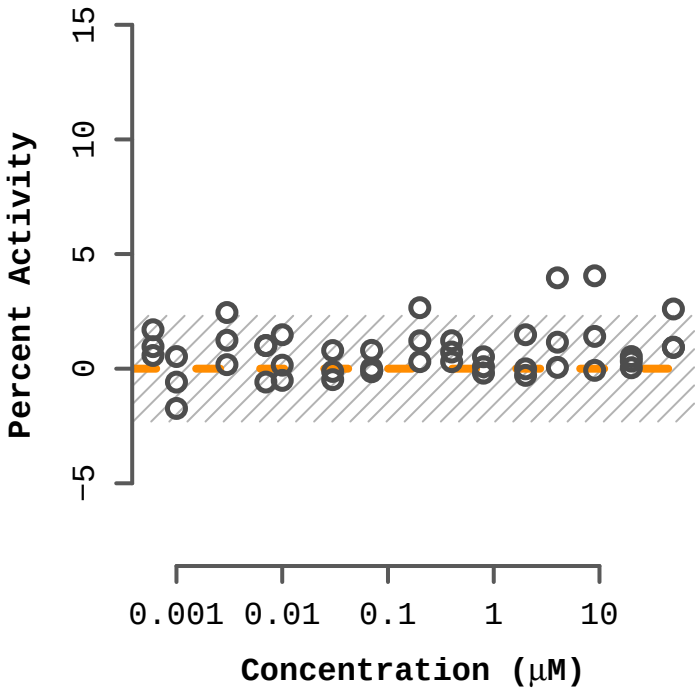
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.558 **MAX_MED:** 0.212 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pentylcinnamaldehyde
CHID:    29157   CASRN: 122-40-7
SPID(S): Tox21_202051
M4ID:    12480201

HILL MODEL (in red):
      tp       ga       gw
val:  0.665    0.457    2.69
sd:   0.346    0.541    6.07

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.81     0.882    3.99     1.13     17.9
sd:   21.5     1.04     8.42     2.13     225

      CNST        HILL        GNLS
AIC:  142.44      143.56      145.62
PROB: 0.56        0.32        0.11
RMSE: 1.19        1.09        1.05

MAX_MEAN: 2.17      MAX_MED: 2.58      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

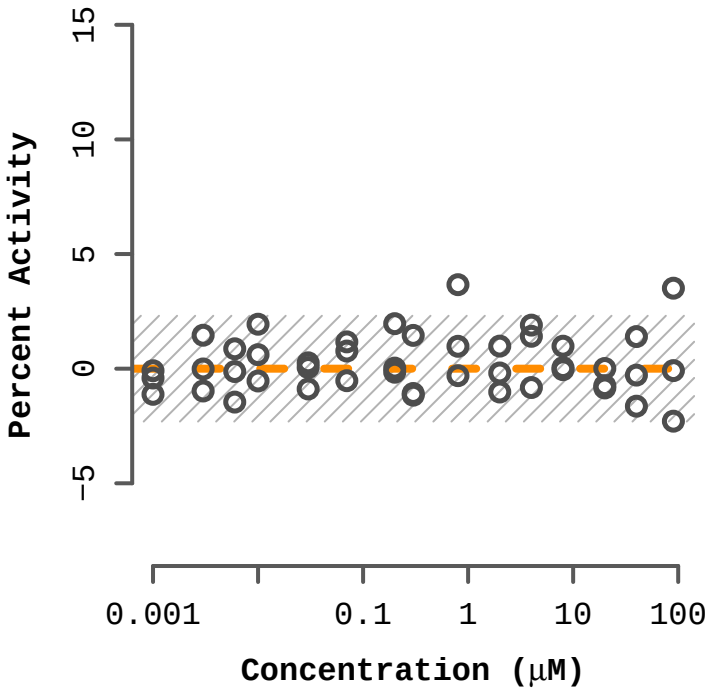
NAME: Pentylcinnamaldehyde
CHID: 29157 **CASRN:** 122-40-7
SPID(S): Tox21_112352_1
M4ID: 12483141

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

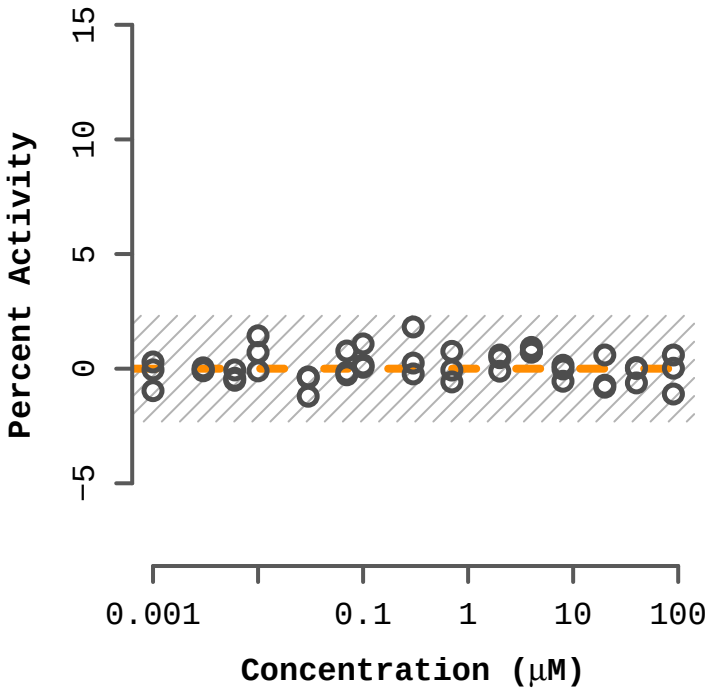
NAME: 1,4-Piperazinediethanol
CHID: 29158 **CASRN:** 122-96-3
SPID(S): Tox21_200471
M4ID: 12481781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

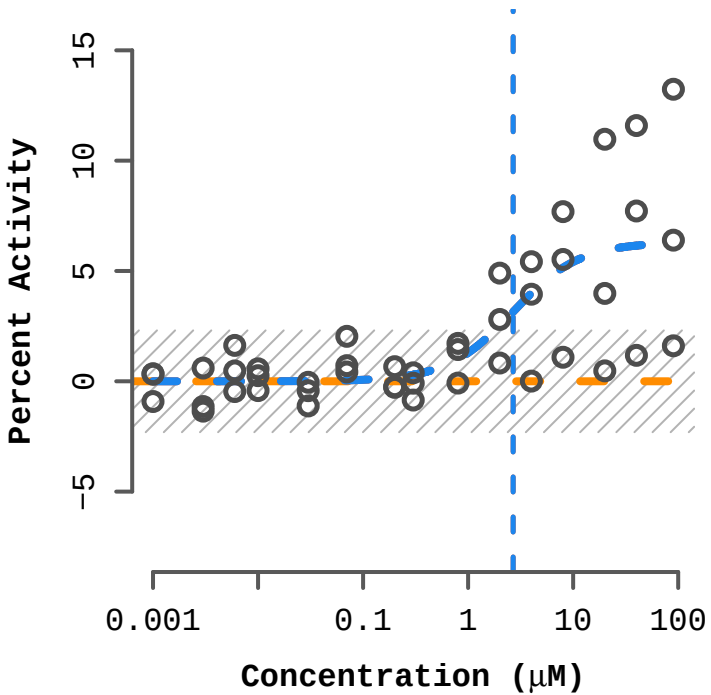
NAME: 2,6,8-Trimethyl-4-nonanol
CHID: 29159 **CASRN:** 123-17-1
SPID(S): Tox21_303455
M4ID: 12475685

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.757 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6,8-Trimethyl-4-nonanol
CHID: 29159 CASRN: 123-17-1
SPID(S): Tox21_202434
M4ID: 12479818

HILL MODEL (in red):

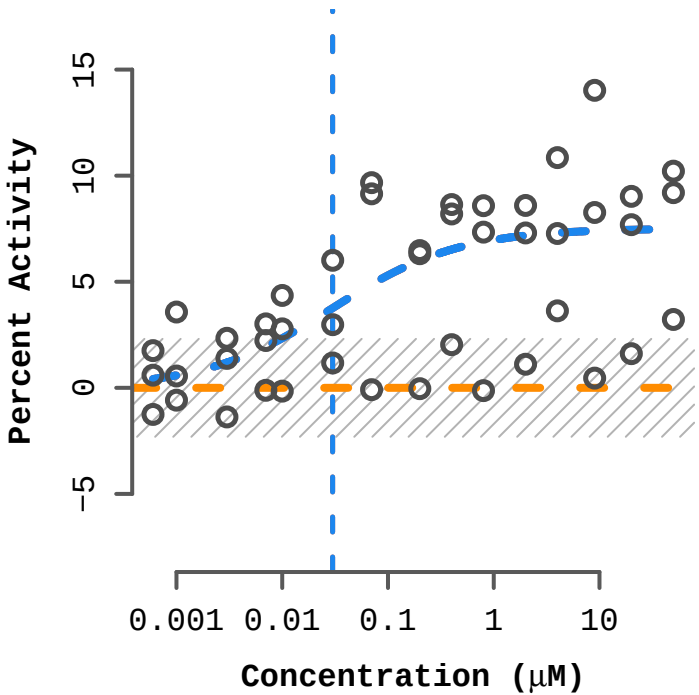
	tp	ga	gw
val:	6.3	0.429	1.37
sd:	1.53	0.26	0.705

GAIN-LOSS MODEL (in blue):

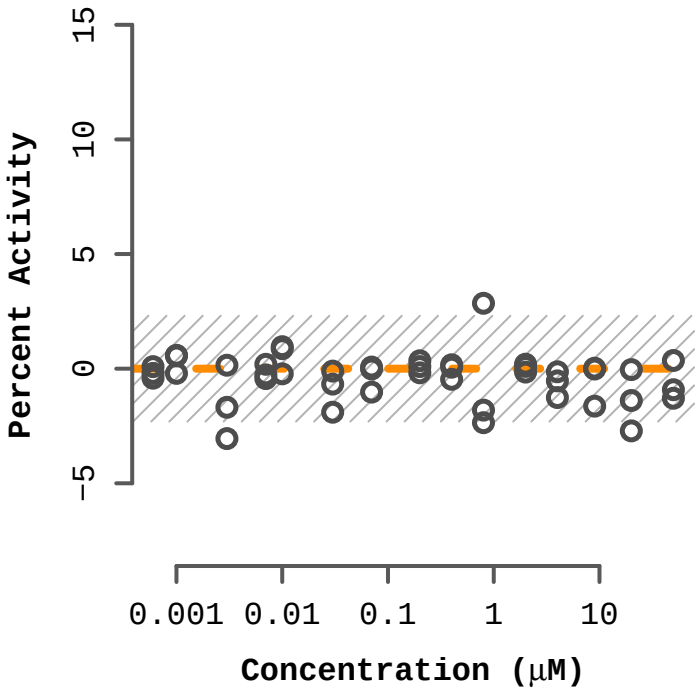
	tp	ga	gw	la	lw
val:	6.3	0.429	1.37	3.62	5.25
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	240.41	206.17	210.17
PROB:	0	0.88	0.12
RMSE:	4.06	2.38	2.38

MAX_MEAN: 7.08 MAX_MED: 7.72 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Stearoyl-rac-glycerol
CHID:    29160   CASRN: 123-94-4
SPID(S): Tox21_202573
M4ID:    12479679

HILL MODEL (in red):
      tp       ga       gw
val:  7.52     -1.52    0.726
sd:   1.16     0.433    0.422

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.52     -1.52    0.726    3.41     4.4
sd:   1.16     0.433    0.422    1380     3560

      CNST        HILL        GNLS
AIC:  292.88      241.37      245.37
PROB: 0           0.88        0.12
RMSE: 5.9         3.18        3.18

MAX_MEAN: 7.58      MAX_MED: 9.2       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

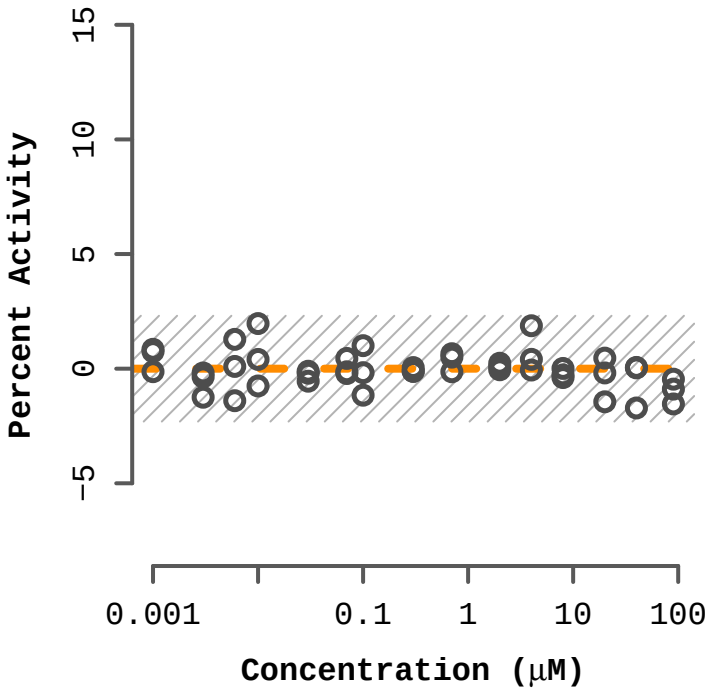
NAME: 1-Stearoyl-rac-glycerol
CHID: 29160 **CASRN:** 123-94-4
SPID(S): Tox21_112160_1
M4ID: 12483275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.537 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

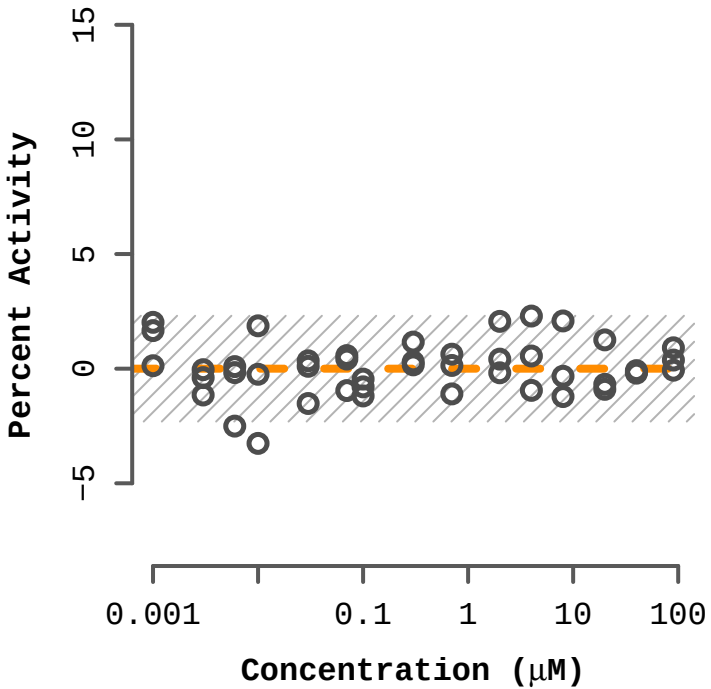
NAME: 3-Bromo-1-chloro-5,5-dimethylhydantoin
CHID: 29162 **CASRN:** 126-06-7
SPID(S): Tox21_301659
M4ID: 12477474

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.746 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

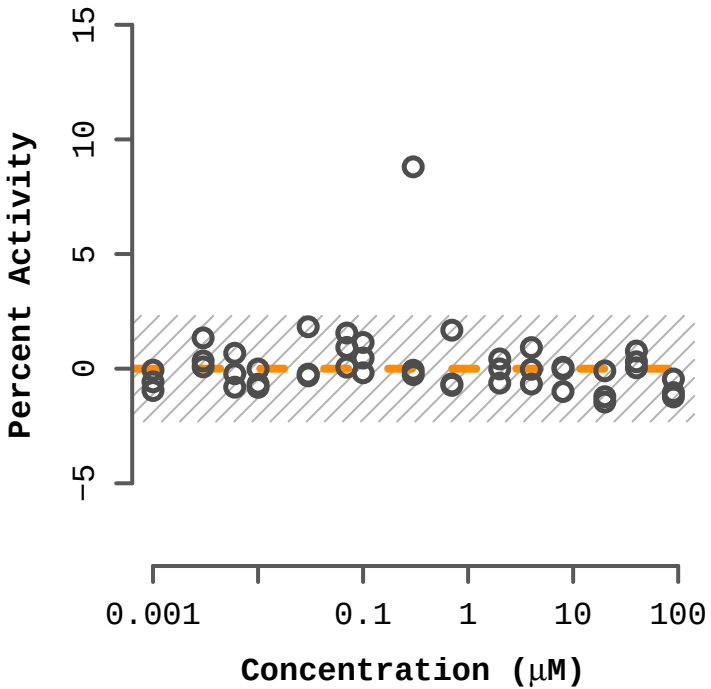
NAME: Sodium 1,4−diisobutyl sulfosuccinate
CHID: 29164 **CASRN:** 127−39−9
SPID(S): Tox21_302377
M4ID: 12476756

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

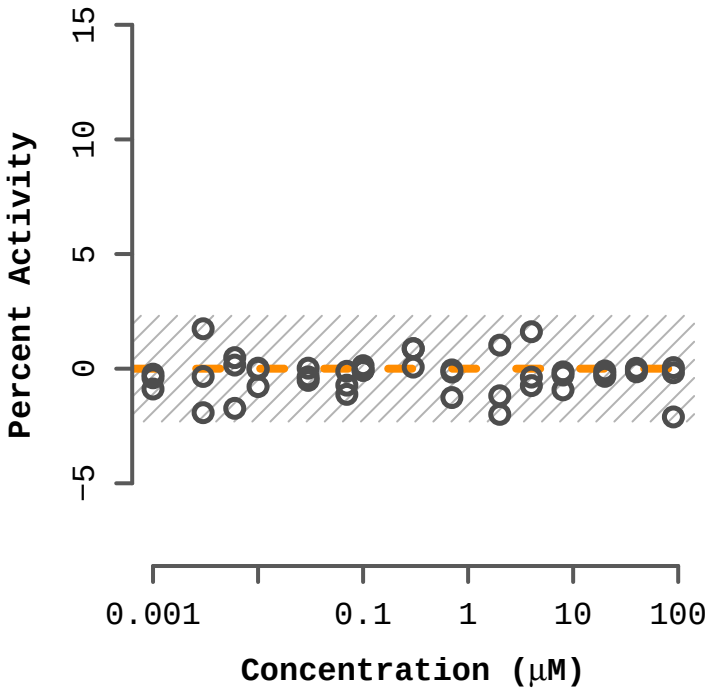
NAME: Sodium 6-hydroxynaphthalene-2-sulfonate
CHID: 29166 CASRN: 135-76-2
SPID(S): Tox21_303541
M4ID: 12475603

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 2.83 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

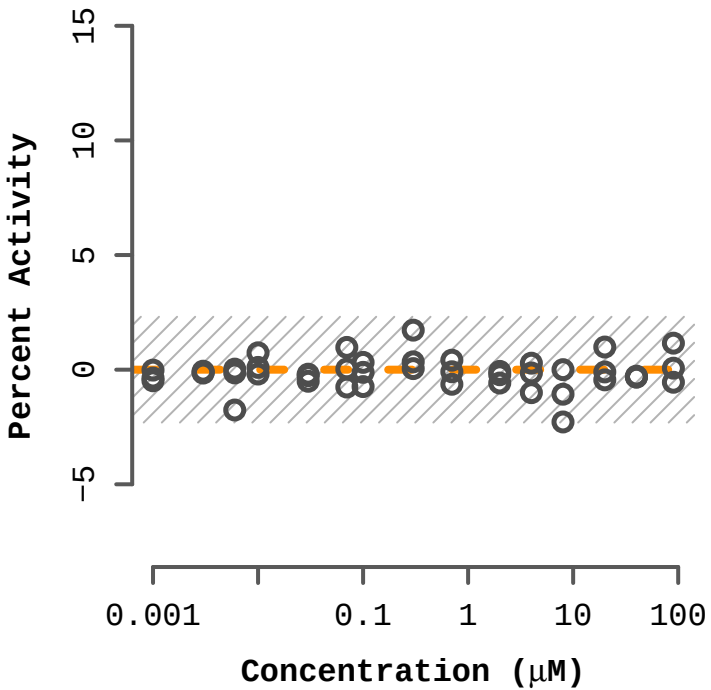
NAME: Sodium 6-hydroxynaphthalene-2-sulfonate
CHID: 29166 CASRN: 135-76-2
SPID(S): Tox21_201538
M4ID: 12480714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.606 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

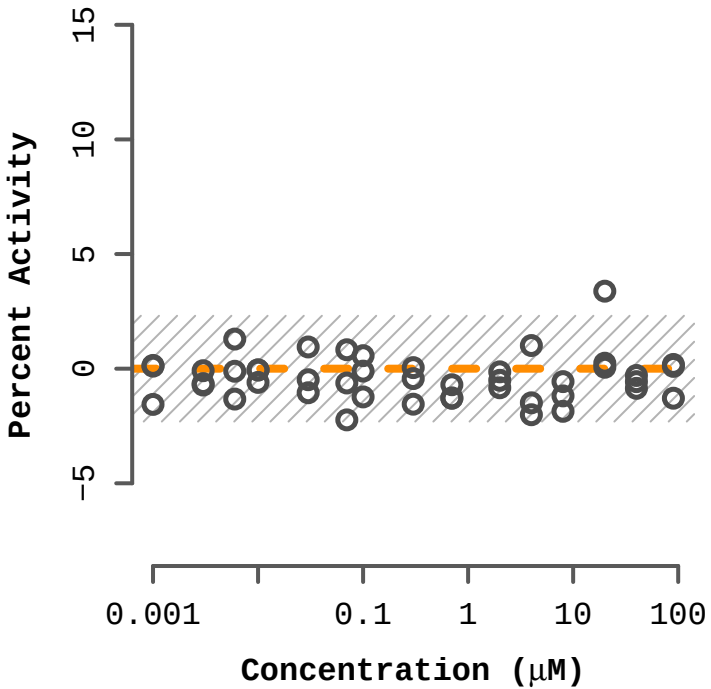
NAME: Metam−sodium
CHID: 29167 **CASRN:** 137−42−8
SPID(S): Tox21_302361
M4ID: 12476772

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.705 **MAX_MED:** 0.343 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

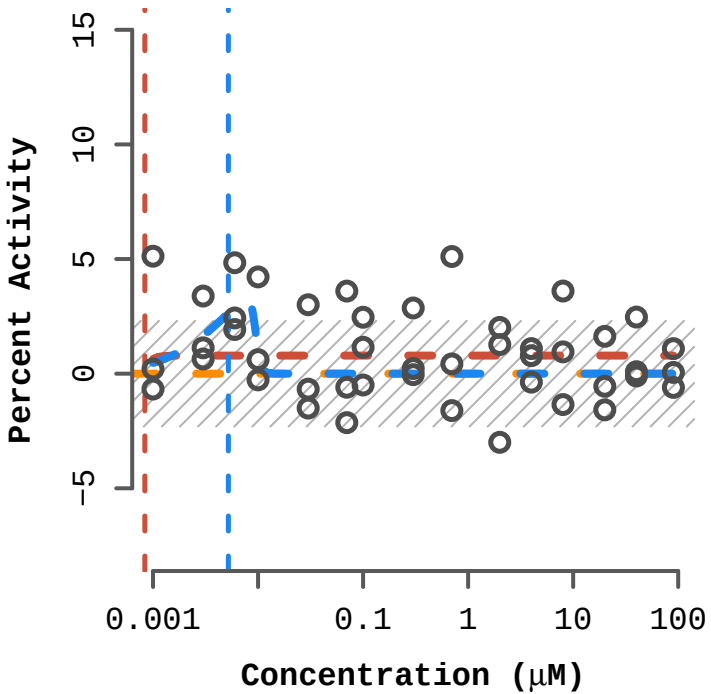
NAME: Methyl ricinoleate
CHID: 29169 **CASRN:** 141-24-2
SPID(S): Tox21_200861
M4ID: 12481391

HILL MODEL: Not applicable.

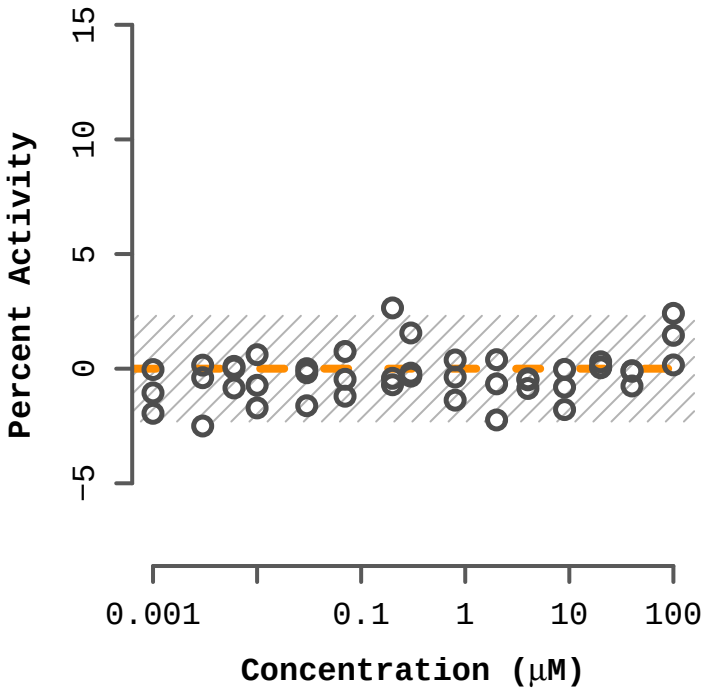
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.24 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Methylpent-3-en-2-one
CHID:    29170   CASRN: 141-79-7
SPID(S): Tox21_303606
M4ID:    12475539

HILL MODEL (in red):
      tp       ga       gw
val:  0.789    -3.08    7.99
sd:   0.301    3.21     312

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.26     -2.28    1.4      -2.02    17.6
sd:   15.5     1.85     2.64     0.0552   39.1

      CNST        HILL        GNLS
AIC:  199.8       198.7       198.37
PROB: 0.21        0.36        0.43
RMSE: 2.17        1.96        1.91

MAX_MEAN: 3.07      MAX_MED: 2.43      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

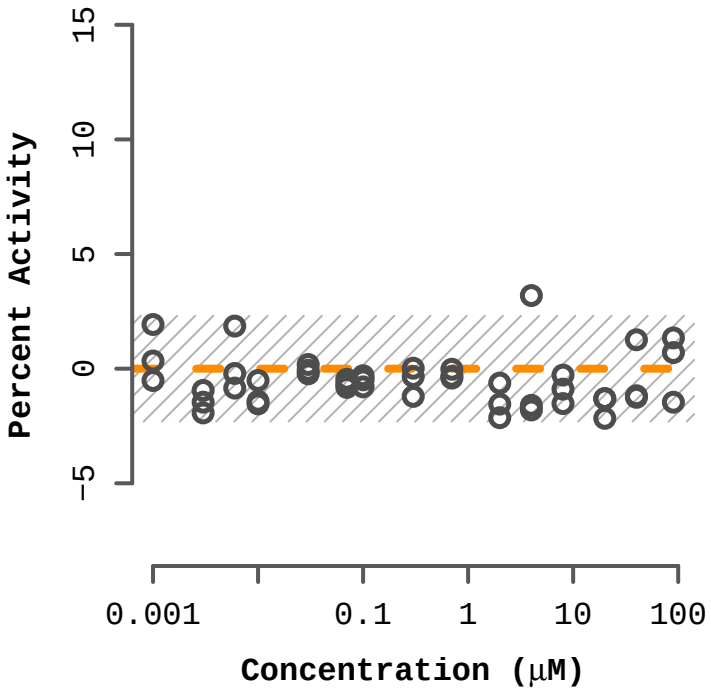
NAME: 4-Methylpent-3-en-2-one
CHID: 29170 **CASRN:** 141-79-7
SPID(S): Tox21_202080
M4ID: 12480172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

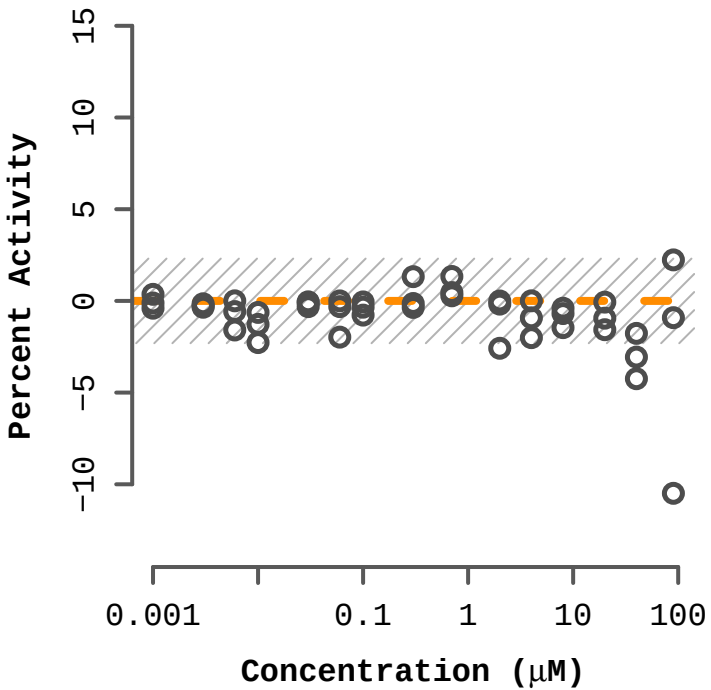
NAME: Cyclopentene
CHID: 29171 **CASRN:** 142-29-0
SPID(S): Tox21_303765
M4ID: 12475423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.584 **MAX_MED:** 0.705 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

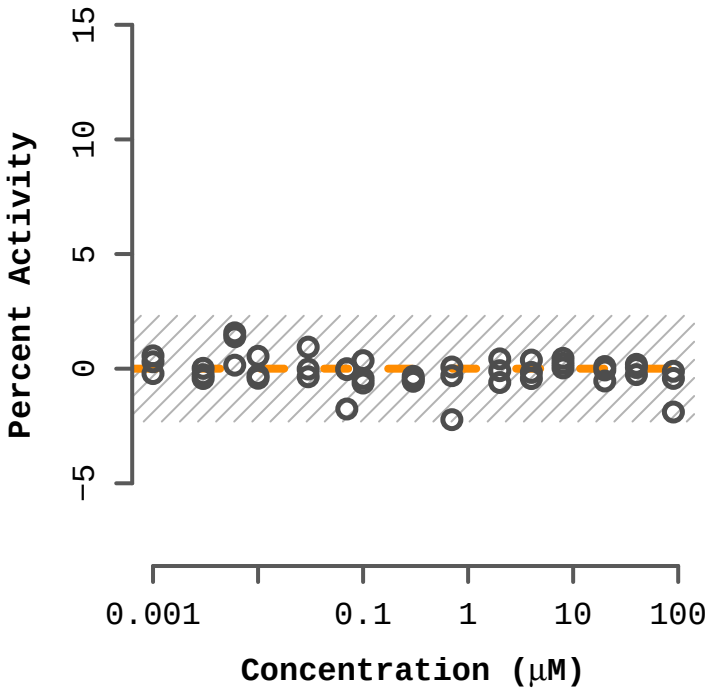
NAME: Isovaleric acid
CHID: 29182 **CASRN:** 503-74-2
SPID(S): Tox21_201604
M4ID: 12480648

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 0.69 **MAX_MED:** 0.457 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

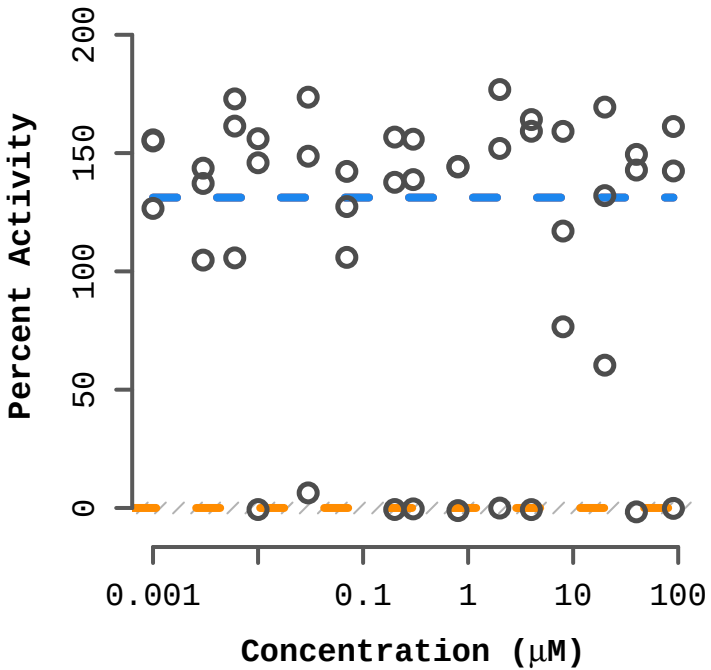
NAME: Sodium 4-aminobenzenesulfonate
CHID: 29184 CASRN: 515-74-2
SPID(S): Tox21_202574
M4ID: 12479678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	86.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 6-Methyl-1,3,5-triazine-2,4-diamine
CHID: 29186 CASRN: 542-02-9
SPID(S): Tox21_201166
M4ID: 12481086

HILL MODEL (in red):

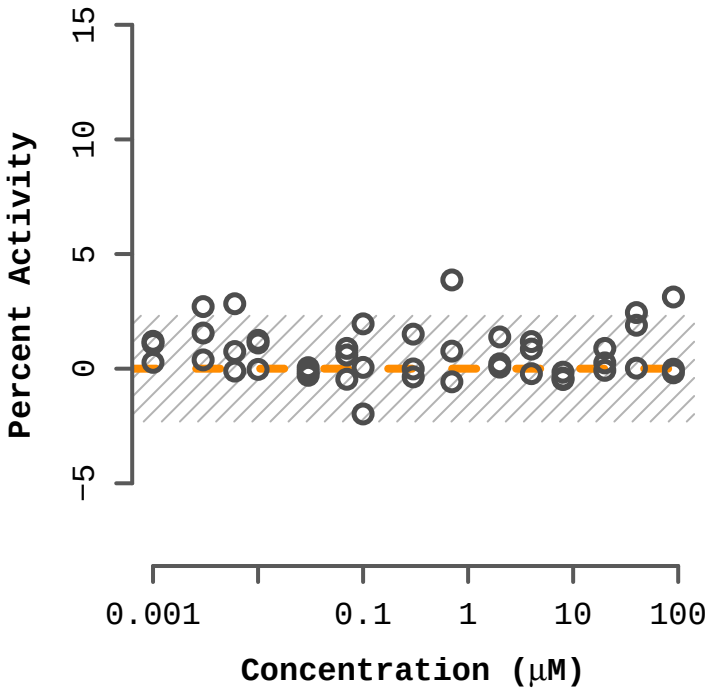
	tp	ga	gw
val:	131	-4.86	3.7
sd:	8.06	500	997

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	131	-4.65	4.48	2.46	16.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	575.84	505.16	509.16
PROB:	0	0.88	0.12
RMSE:	128.82	63.56	63.56

MAX_MEAN: 147 MAX_MED: 161 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

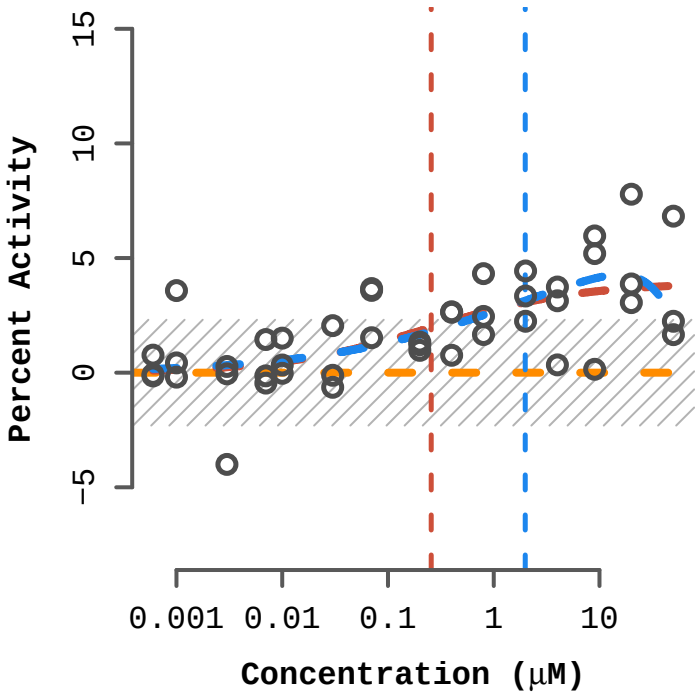
NAME: 2,6-Dimethylnaphthalene
CHID: 29187 **CASRN:** 581-42-0
SPID(S): Tox21_200260
M4ID: 12481992

HILL MODEL: Not applicable.

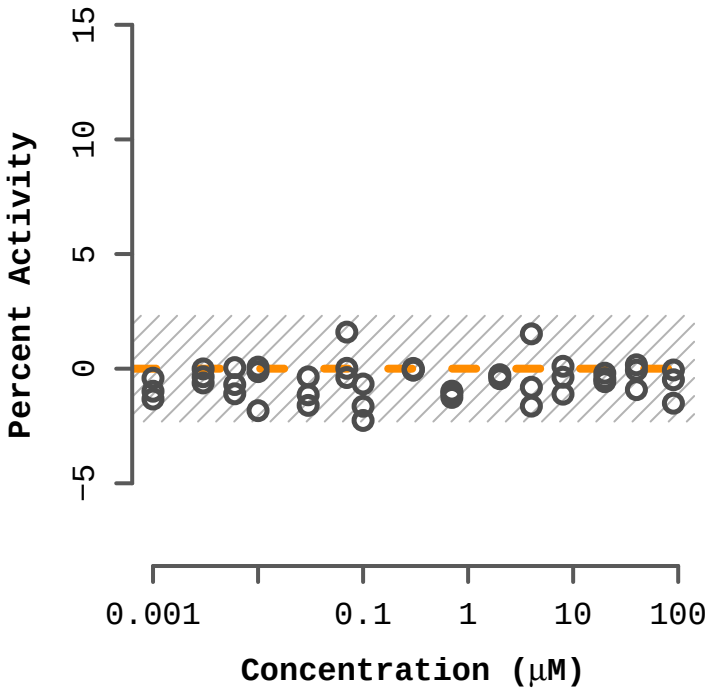
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.9 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Guanidine carbonate
CHID:    29189   CASRN: 593-85-1
SPID(S): Tox21_113187_1
M4ID:    12482778

HILL MODEL (in red):
      tp       ga       gw
val:  3.94     -0.591   0.615
sd:   0.986    0.527    0.277

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.28     0.298    0.446    1.69     2.6
sd:   6.97     2.21     0.282    0.222    3.8

      CNST       HILL       GNLS
AIC:  225.83     179.5      181.28
PROB: 0          0.71       0.29
RMSE: 2.89       1.66       1.68

MAX_MEAN: 4.91      MAX_MED: 5.2       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

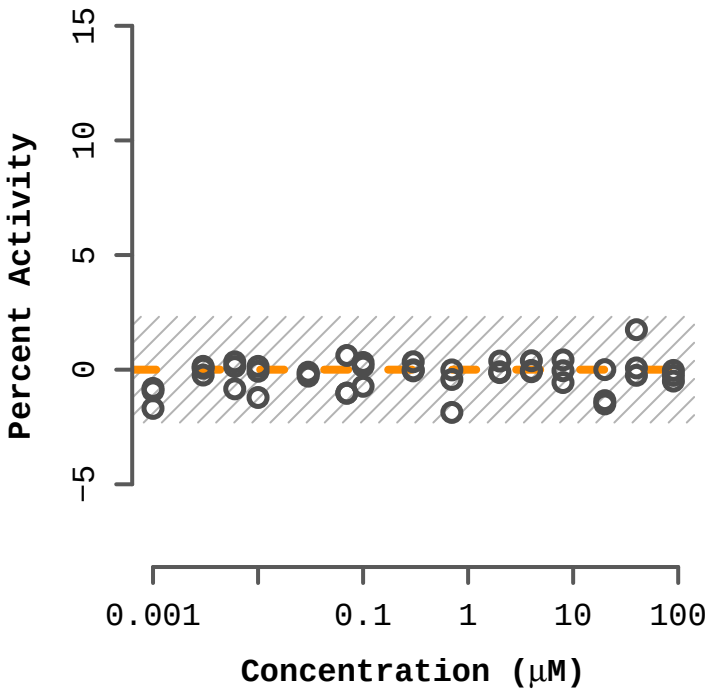
NAME: Dimethyl carbonate
CHID: 29192 **CASRN:** 616-38-6
SPID(S): Tox21_303590
M4ID: 12475555

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.409 **MAX_MED:** 0.017 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

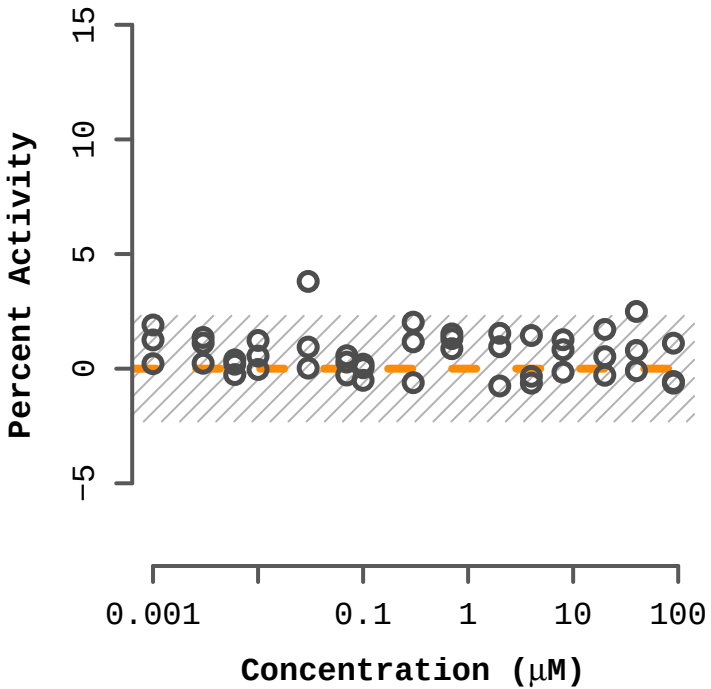
NAME: Dimethyl carbonate
CHID: 29192 **CASRN:** 616-38-6
SPID(S): Tox21_201940
M4ID: 12480312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.526 **MAX_MED:** 0.155 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

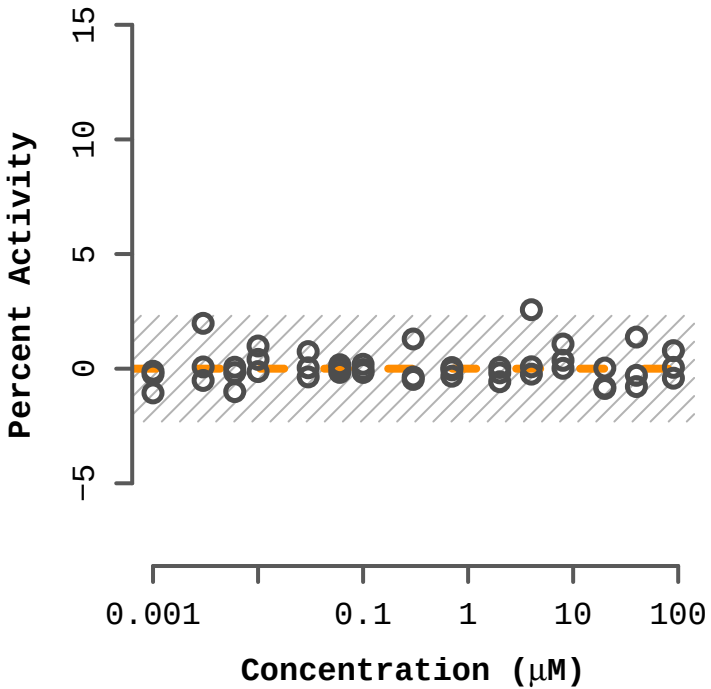
NAME: 4-Ethyltoluene
CHID: 29194 **CASRN:** 622-96-8
SPID(S): Tox21_200472
M4ID: 12481780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

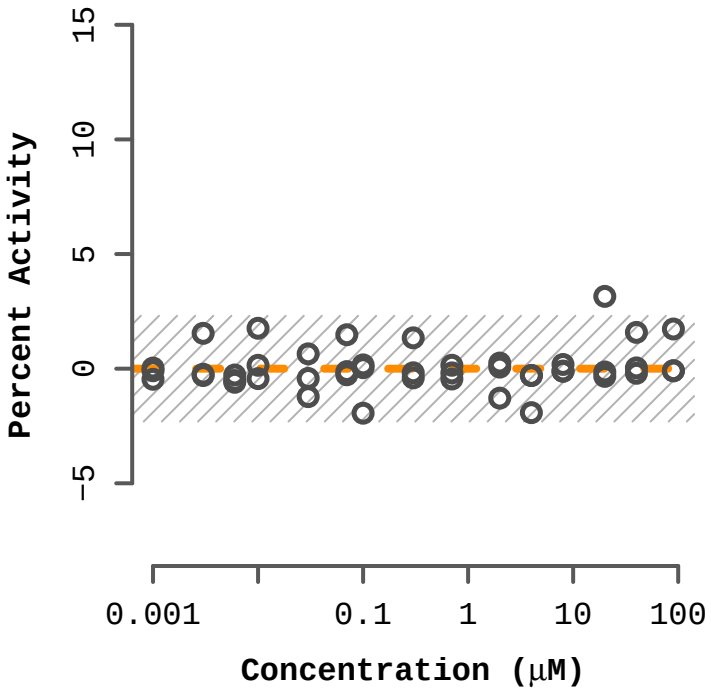
NAME: 3-Methylpiperidine
CHID: 29195 **CASRN:** 626-56-2
SPID(S): Tox21_200877
M4ID: 12481375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 0.408 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

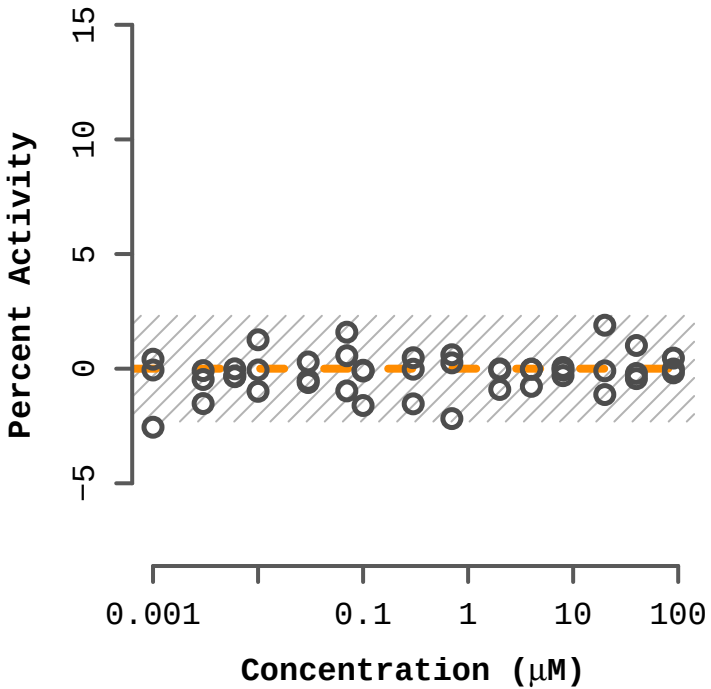
NAME: Potassium 6-hydroxynaphthalene-2-sulfonate
CHID: 29201 **CASRN:** 833-66-9
SPID(S): Tox21_303567
M4ID: 12475578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.893 **MAX_MED:** 0.149 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

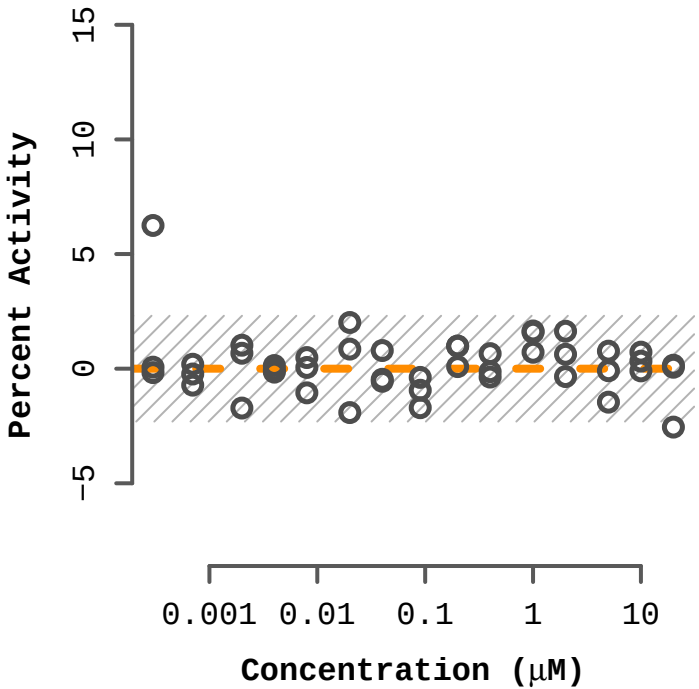
NAME: Potassium 6-hydroxynaphthalene-2-sulfonate
CHID: 29201 **CASRN:** 833-66-9
SPID(S): Tox21_201245
M4ID: 12481007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.396 **MAX_MED:** 0.565 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

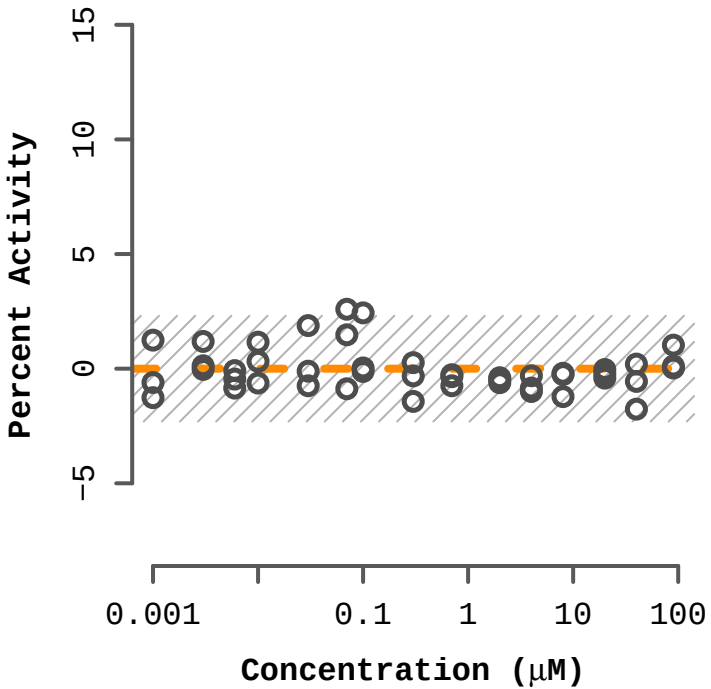
NAME: Dimethyl 2,6-naphthalenedicarboxylate
CHID: 29202 **CASRN:** 840-65-3
SPID(S): Tox21_202769
M4ID: 12479483

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

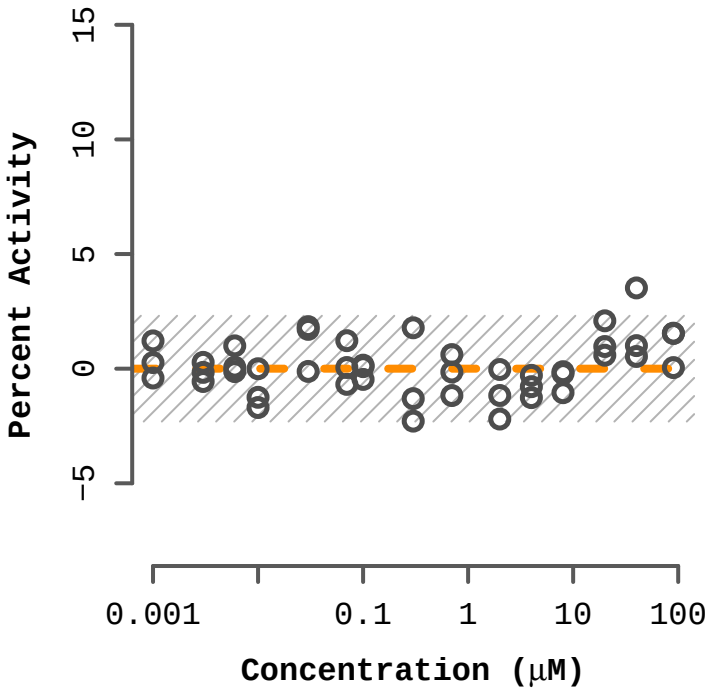
NAME: 1-Chloro-2-(diethylamine)ethane hydrochloride
CHID: 29203 **CASRN:** 869-24-9
SPID(S): Tox21_200014
M4ID: 12482238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

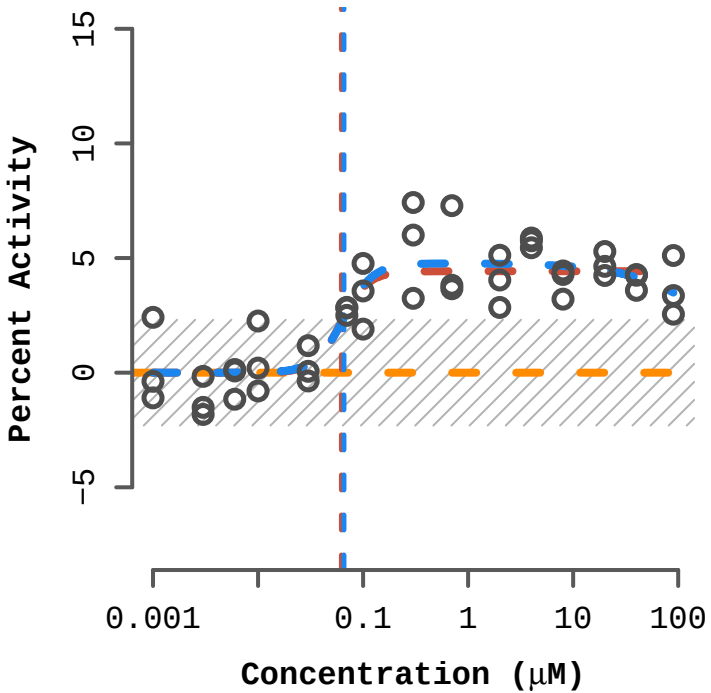
NAME: 2-Methylpyridine 1-oxide
CHID: 29207 **CASRN:** 931-19-1
SPID(S): Tox21_200473
M4ID: 12481779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyltin trichloride
CHID: 29210 CASRN: 1118-46-3
SPID(S): Tox21_303583
M4ID: 12475562

HILL MODEL (in red):

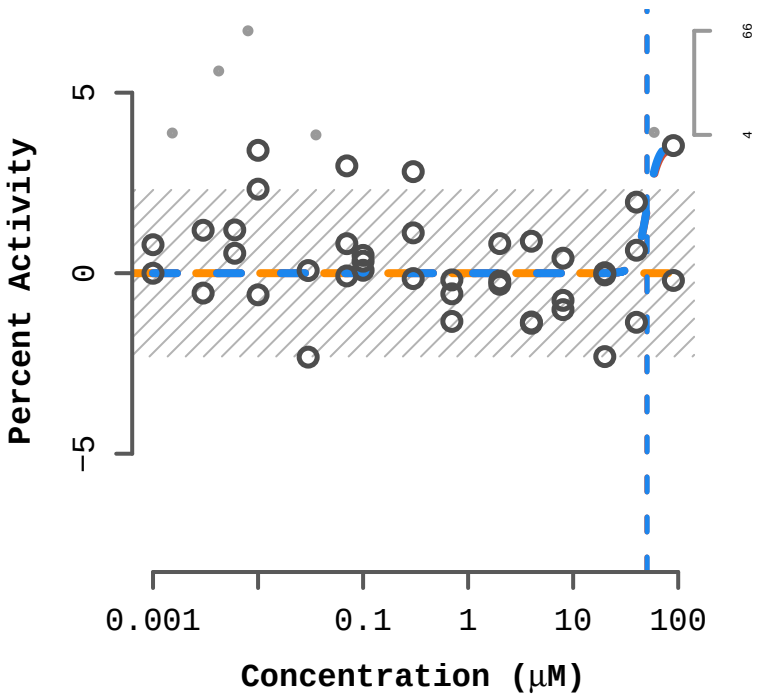
	tp	ga	gw
val:	4.43	−1.21	3.46
sd:	0.243	0.0614	1.72

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.77	−1.18	3.18	2.35	1.11
sd:	0.479	0.0617	1.44	0.597	1.35

	CNST	HILL	GNLS
AIC:	254.22	152.89	154.24
PROB:	0	0.66	0.34
RMSE:	3.72	1.19	1.15

MAX_MEAN: 5.69 MAX_MED: 6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyltin trichloride
CHID: 29210 CASRN: 1118-46-3
SPID(S): Tox21_202457
M4ID: 12479795 BRK

HILL MODEL (in red):

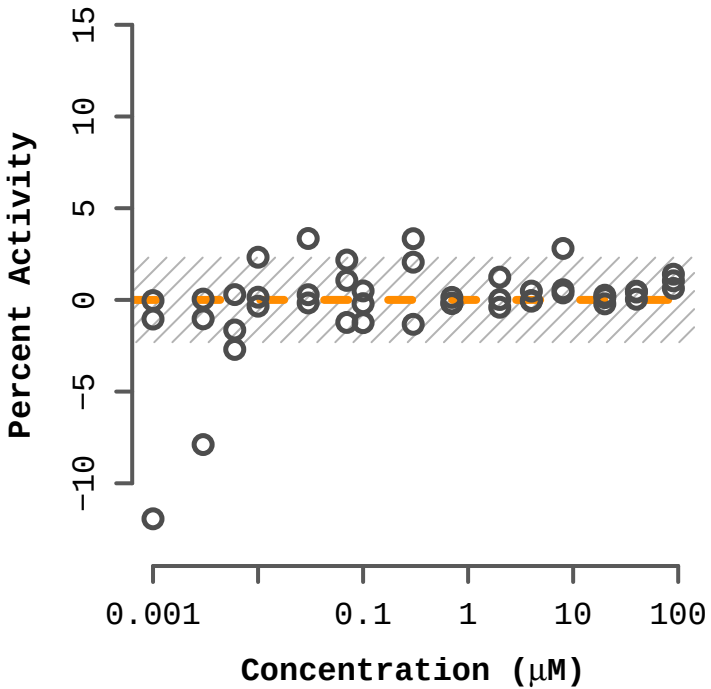
	tp	ga	gw
val:	3.49	1.7	8
sd:	1.59	0.484	35

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.65	1.7	8	2.14	7.17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	236.7	237.32	241.32
PROB:	0.55	0.4	0.05
RMSE:	11.89	11.86	11.86

MAX_MEAN: 22.7 MAX_MED: 3.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

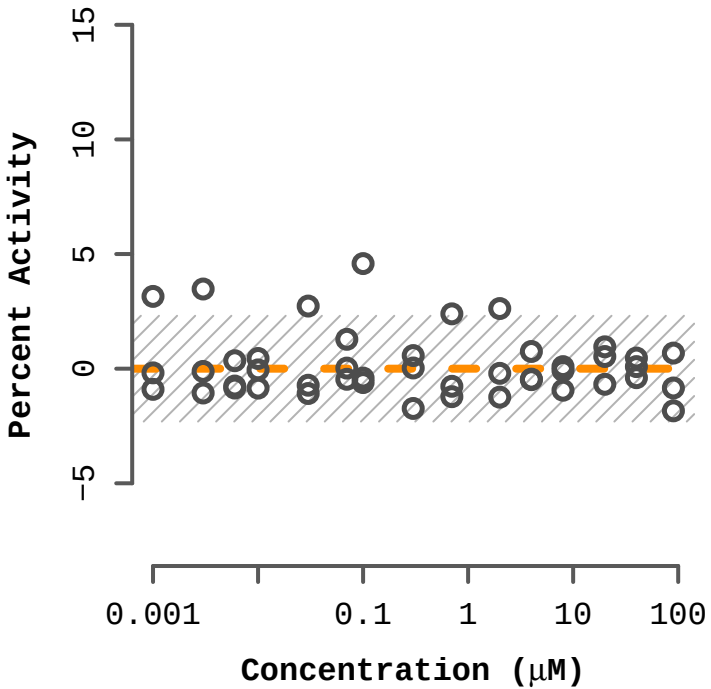
NAME: 2,6-Naphthalenedicarboxylic acid
CHID: 29211 **CASRN:** 1141-38-4
SPID(S): Tox21_201122
M4ID: 12481130

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.47	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

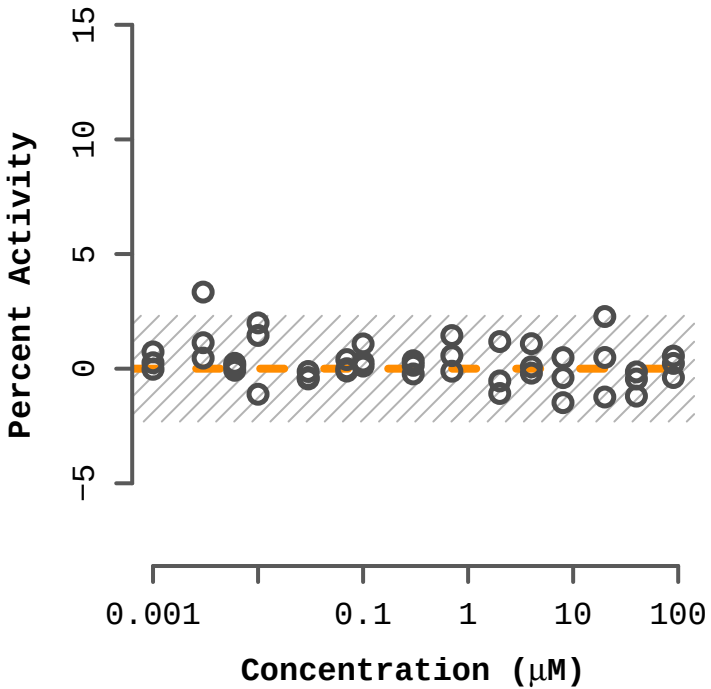
NAME: Methylionone
CHID: 29214 **CASRN:** 1335-46-2
SPID(S): Tox21_301465
M4ID: 12477668

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

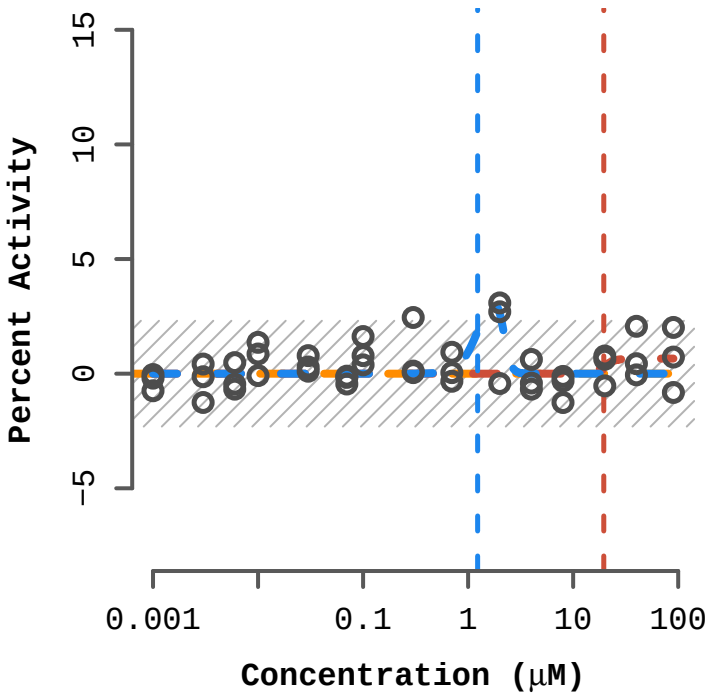
NAME: 1-Propoxy-2-propanol
CHID: 29217 **CASRN:** 1569-01-3
SPID(S): Tox21_303414
M4ID: 12475725

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Propoxy-2-propanol
CHID: 29217 CASRN: 1569-01-3
SPID(S): Tox21_201392
M4ID: 12480860

HILL MODEL (in red):

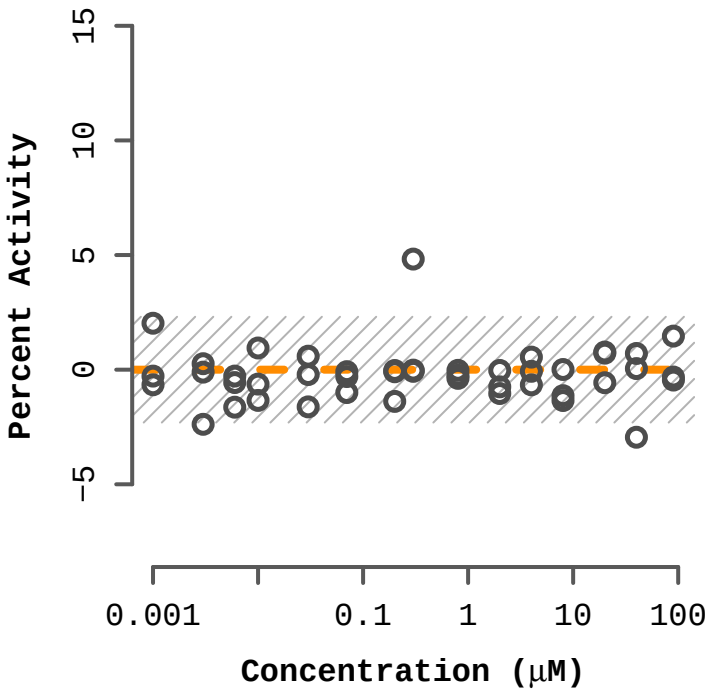
	tp	ga	gw
val:	0.658	1.29	8
sd:	0.414	0.167	31.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.71	0.0904	5.13	0.34	13.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	127.43	130.19	129.51
PROB:	0.62	0.16	0.22
RMSE:	1.03	1	0.95

MAX_MEAN: 1.79 MAX_MED: 2.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

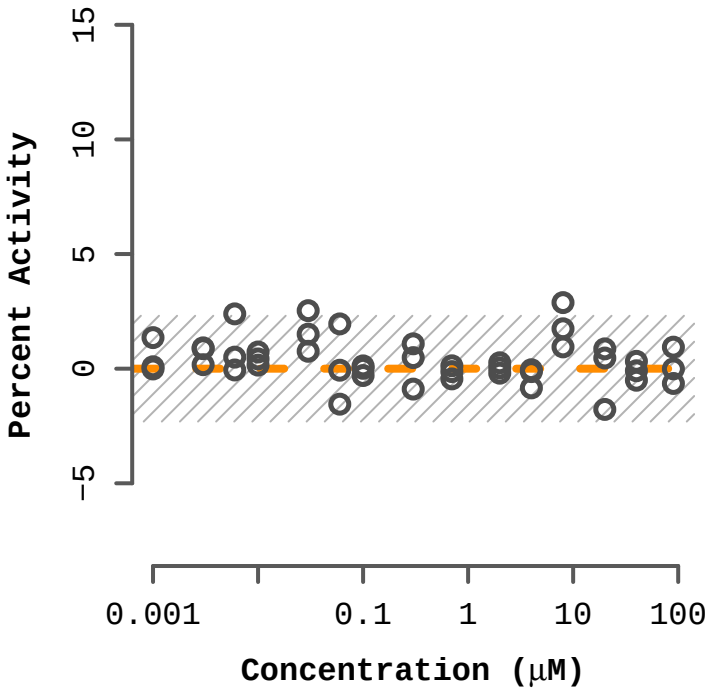
NAME: 1-Bromo-4-ethylbenzene
CHID: 29218 **CASRN:** 1585-07-5
SPID(S): Tox21_200031
M4ID: 12482221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.722 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

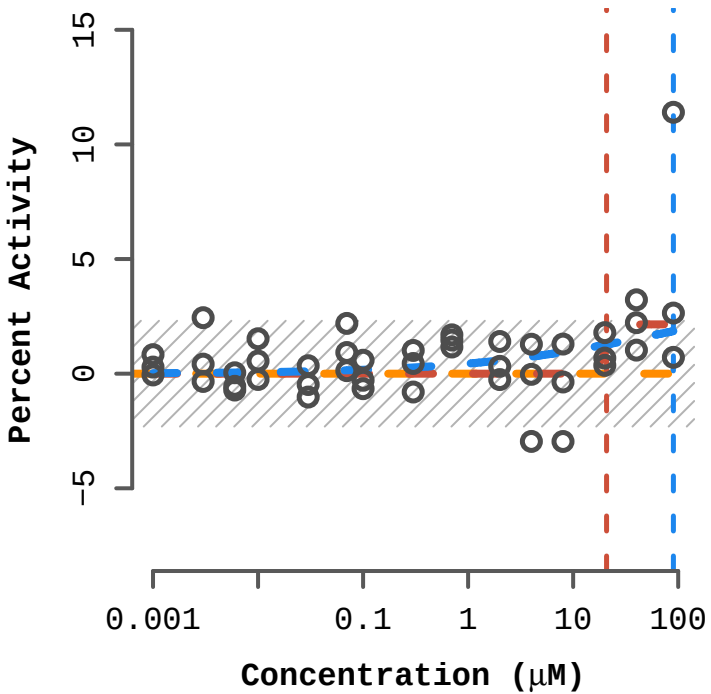
NAME: 5-Methylpyridin-2-amine
CHID: 29220 **CASRN:** 1603-41-4
SPID(S): Tox21_200474
M4ID: 12481778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clopyralid
CHID: 29221 CASRN: 1702-17-6
SPID(S): Tox21_300876
M4ID: 12478257

HILL MODEL (in red):

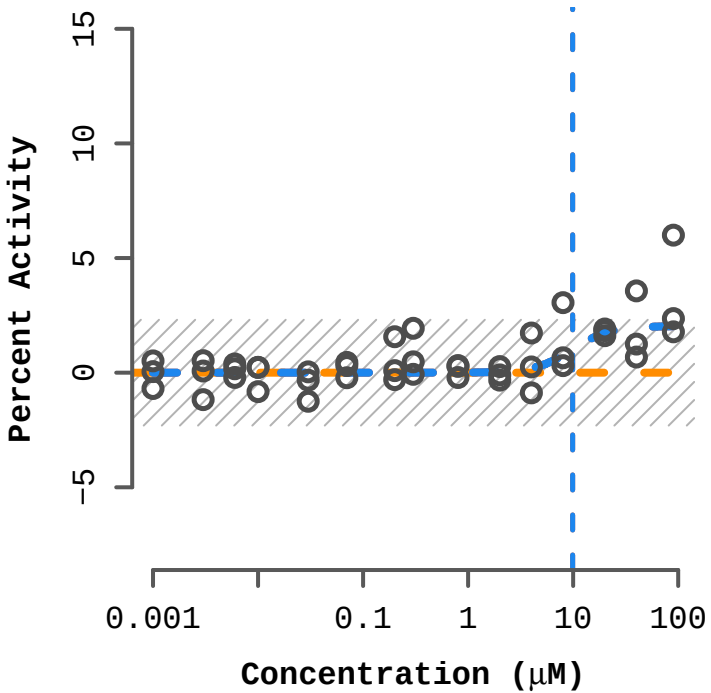
	tp	ga	gw
val:	2.15	1.32	8
sd:	0.545	0.0956	31.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.71	1.95	0.446	3.18	5.67
sd:	5.68	2.25	0.324	888	4050

	CNST	HILL	GNLS
AIC:	170.95	161	165.64
PROB:	0.01	0.9	0.09
RMSE:	2.15	1.77	1.85

MAX_MEAN: 4.92 **MAX_MED:** 2.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clopyralid
CHID: 29221 CASRN: 1702-17-6
SPID(S): Tox21_201435
M4ID: 12480817

HILL MODEL (in red):

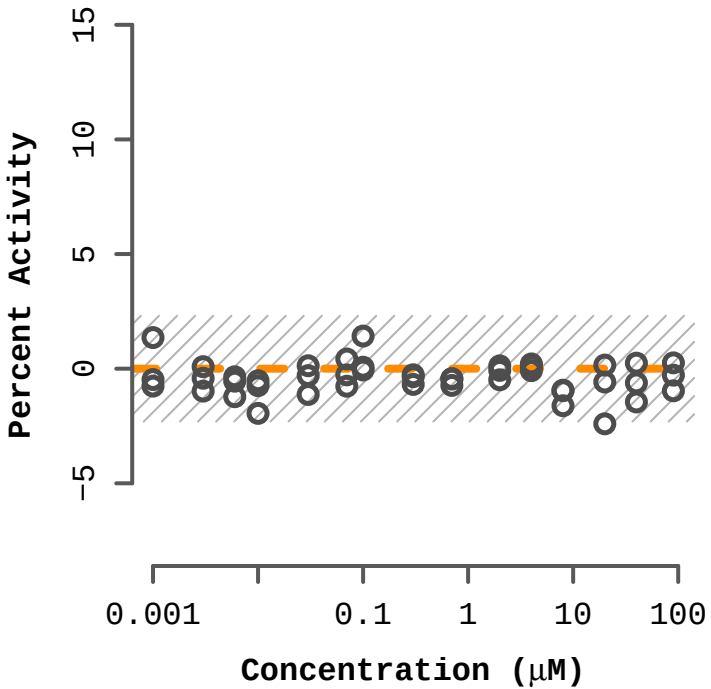
	tp	ga	gw
val:	2.03	0.995	2.46
sd:	0.474	0.178	2.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.03	0.995	2.46	2.93	8.84
sd:	0.474	0.178	2.13	1880	17000

	CNST	HILL	GNLS
AIC:	149.72	118.75	122.75
PROB:	0	0.88	0.12
RMSE:	1.45	0.97	0.97

MAX_MEAN: 3.38 **MAX_MED:** 2.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

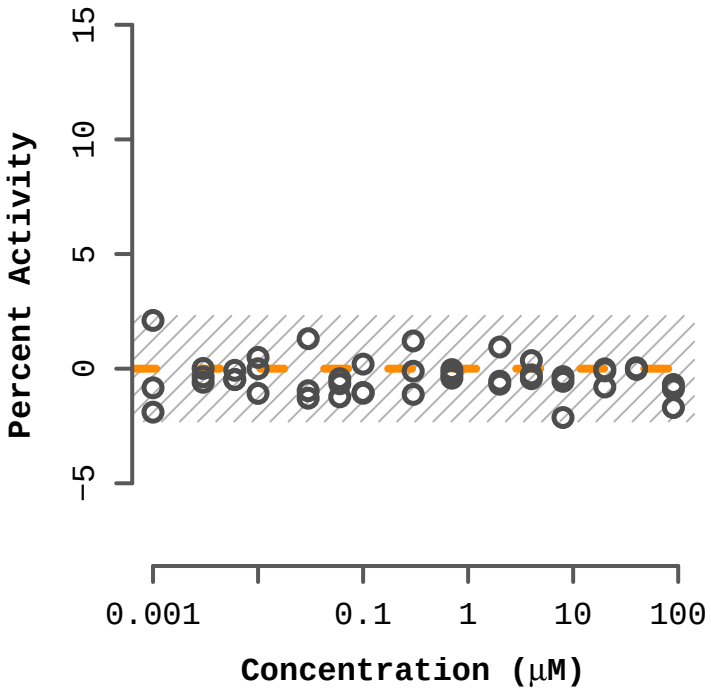
NAME: 1,1−Bis(3,4−dimethylphenyl)ethane
CHID: 29223 **CASRN:** 1742−14−9
SPID(S): Tox21_301768
M4ID: 12477365

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.478 **MAX_MED:** 0.129 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

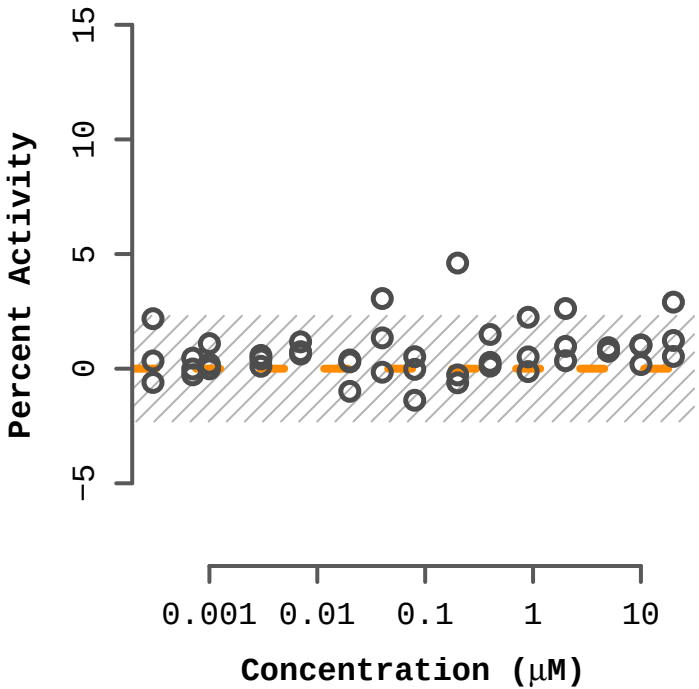
NAME: Amino(imino)methanesulfinic acid
CHID: 29224 **CASRN:** 1758-73-2
SPID(S): Tox21_200647
M4ID: 12481605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: −0.0025 **MAX_MED:** −0.00137 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

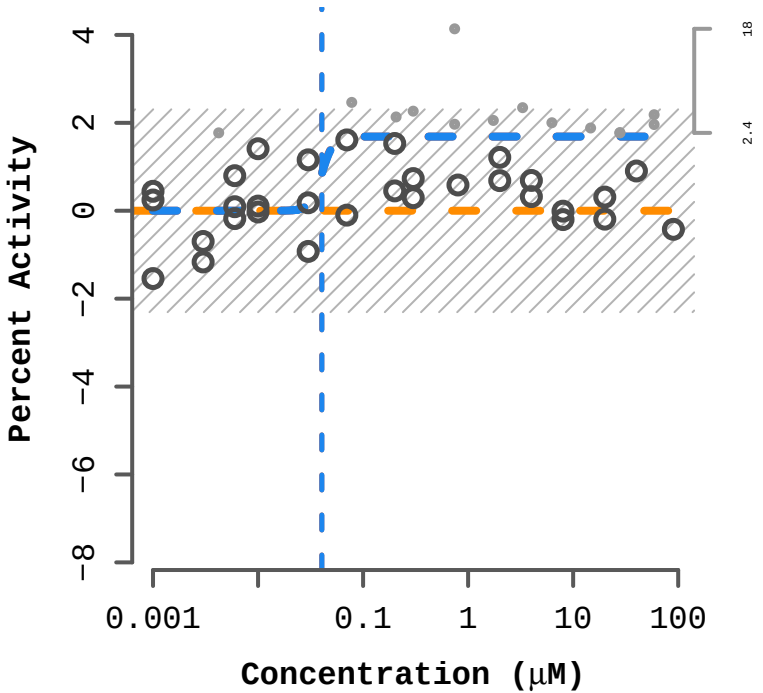
NAME: Trimethylenediaminetetraacetic acid
CHID: 29225 **CASRN:** 1939-36-2
SPID(S): Tox21_303722
M4ID: 12475466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'−(tert−Butylimino)diethanol
CHID: 29230 CASRN: 2160−93−2
SPID(S): Tox21_201065
M4ID: 12481187 BRK

HILL MODEL (in red):

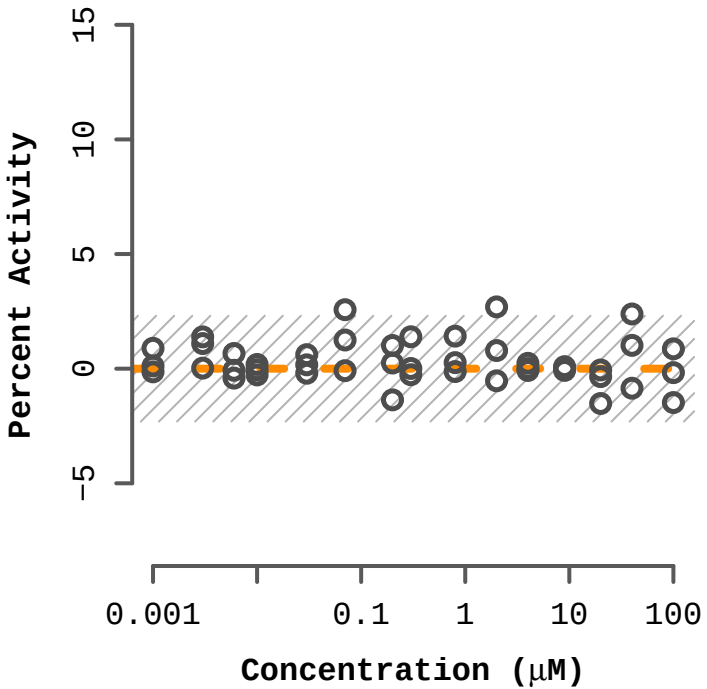
	tp	ga	gw
val:	1.69	−1.39	7.98
sd:	0.407	1.24	75.7

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.69	−1.39	7.88	3.95	2.53
sd:	0.406	1.13	67.6	126	159

	CNST	HILL	GNLS
AIC:	220.61	206.28	210.28
PROB:	0	0.88	0.12
RMSE:	3.6	3.01	3.01

MAX_MEAN: 7.34 **MAX_MED:** 3.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

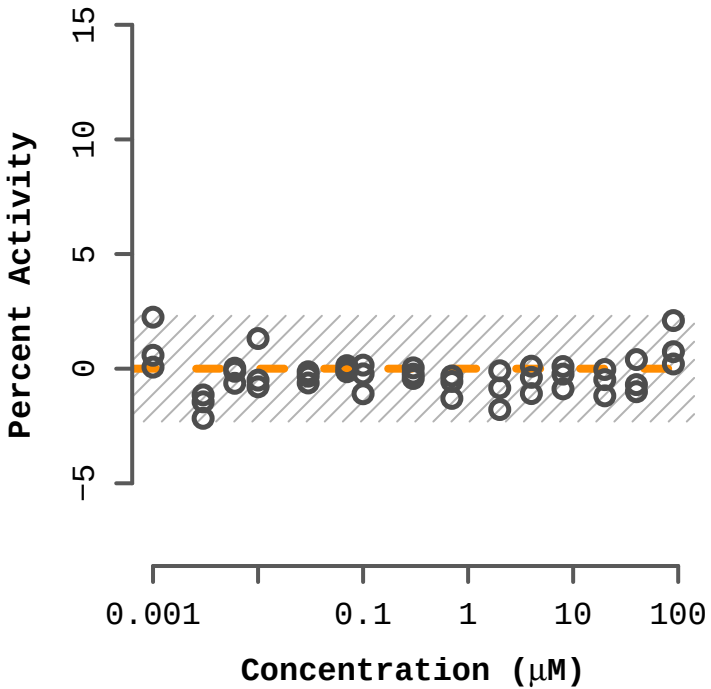
NAME: 2-Methylpropane-1,3-diol
CHID: 29231 CASRN: 2163-42-0
SPID(S): Tox21_200047
M4ID: 12482205

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.25 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

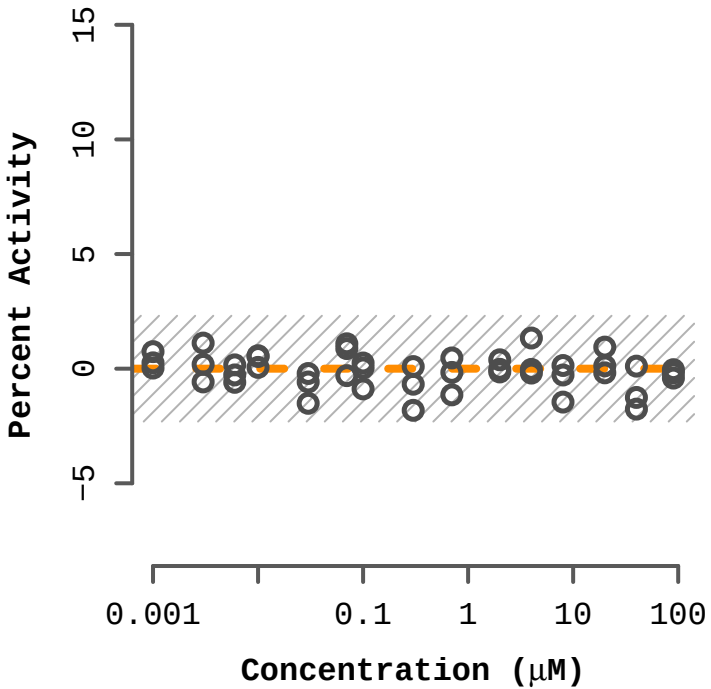
NAME: [Nitrilotris(methylene)]tris-phosphonic acid p
CHID: 29232 CASRN: 2235-43-0
SPID(S): Tox21_303716
M4ID: 12475472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.02 MAX_MED: 0.742 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

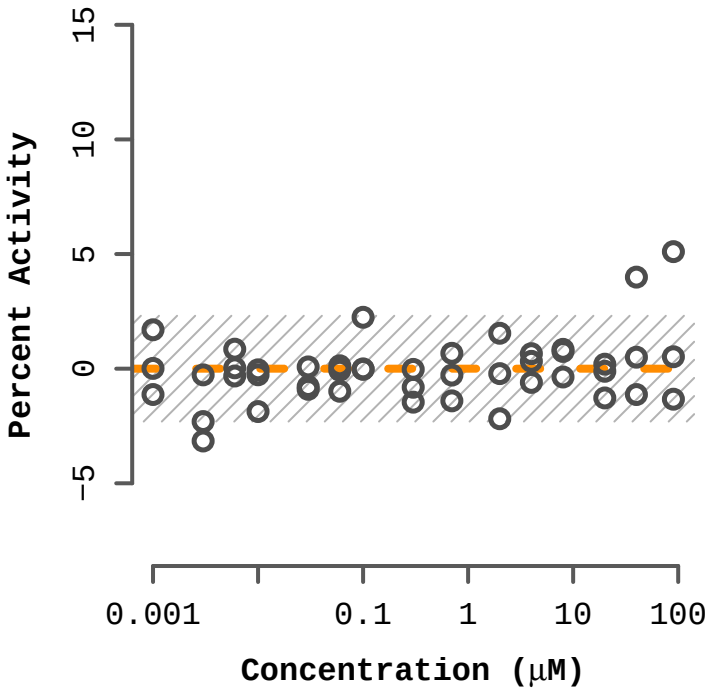
NAME: Benzophenonetetracarboxylic dianhydride
CHID: 29233 CASRN: 2421-28-5
SPID(S): Tox21_200475
M4ID: 12481777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.555 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

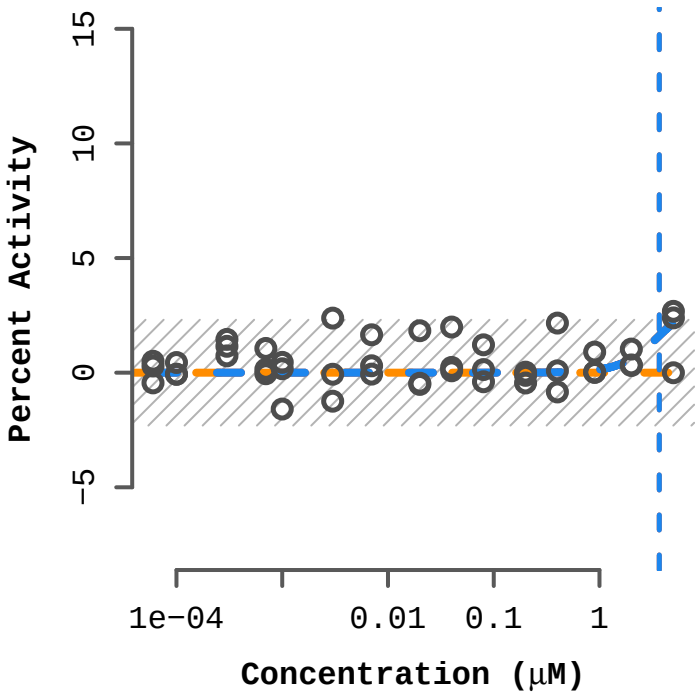
NAME: 3,7-Dimethylocta-1,6-diene
CHID: 29234 **CASRN:** 2436-90-0
SPID(S): Tox21_202044
M4ID: 12480208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Tridecene
CHID: 29235 **CASRN:** 2437-56-1
SPID(S): Tox21_202997
M4ID: 12479255

HILL MODEL (in red):

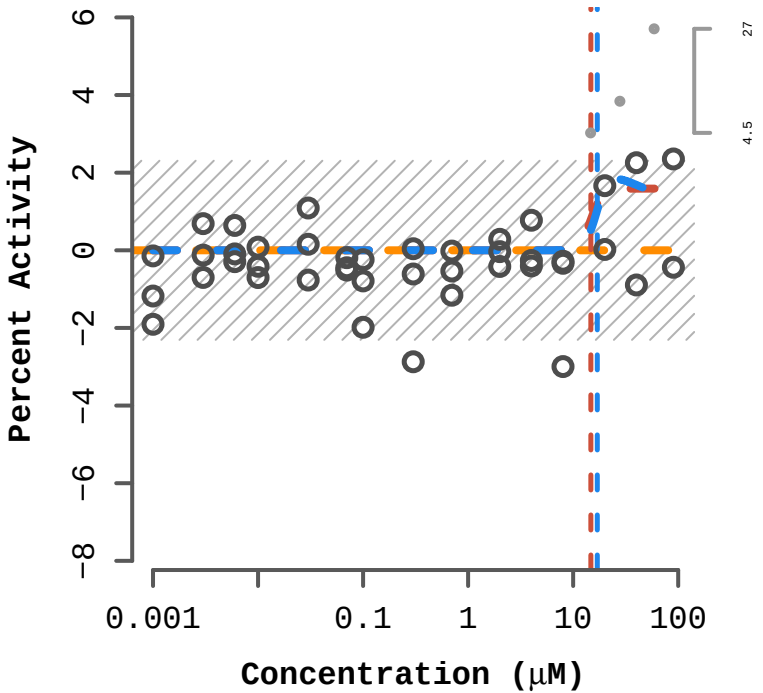
	tp	ga	gw
val:	3.21	0.565	2.38
sd:	3.96	0.547	2.64

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.21	0.566	2.38	2.51	2.84
sd:	3.96	0.548	2.66	268	426

	CNST	HILL	GNLS
AIC:	130.65	127.09	131.09
PROB:	0.13	0.77	0.1
RMSE:	1.04	0.94	0.94

MAX_MEAN: 1.69 **MAX_MED:** 2.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tridecyl methacrylate
CHID: 29236 **CASRN:** 2495-25-2
SPID(S): Tox21_200664
M4ID: 12481588 **BRK**

HILL MODEL (in red):

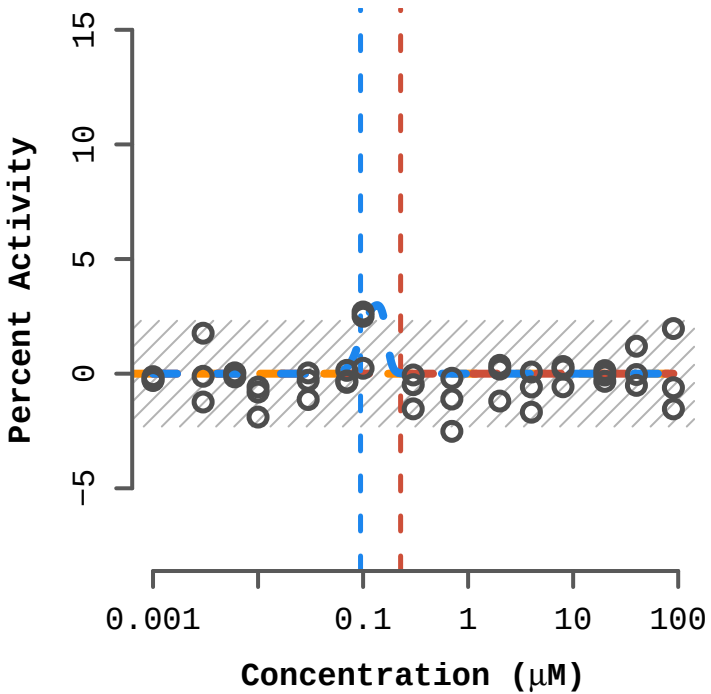
	tp	ga	gw
val:	1.59	1.17	8
sd:	0.666	0.237	9.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.88	1.23	8	1.81	0.721
sd:	43.8	0.489	11.7	18.9	11.4

	CNST	HILL	GNLS
AIC:	184.33	184.55	188.44
PROB:	0.49	0.44	0.06
RMSE:	4.5	4.18	4.21

MAX_MEAN: 9.56 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-(Trimethoxysilyl)propyl methacrylate
CHID: 29237 CASRN: 2530-85-0
SPID(S): Tox21_303351
M4ID: 12475782

HILL MODEL (in red):

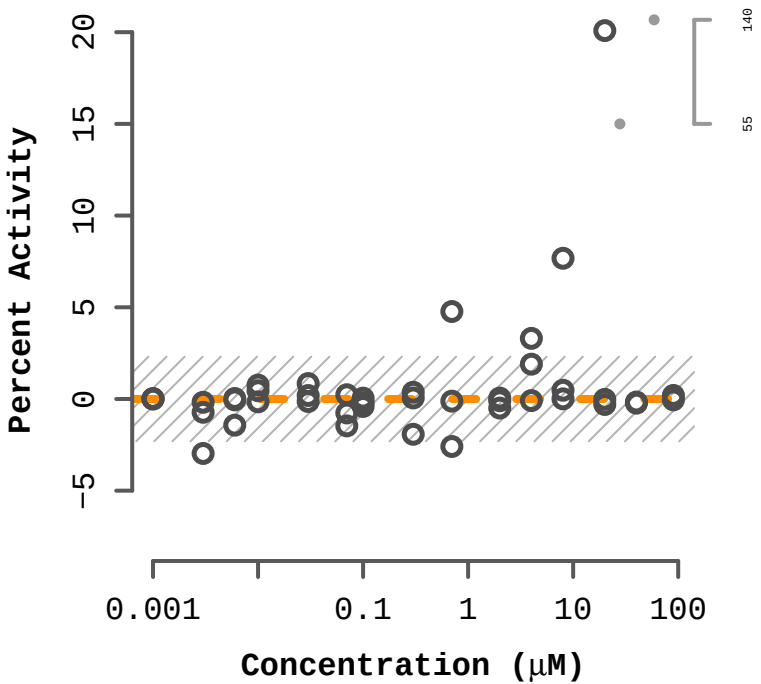
	tp	ga	gw
val:	2e-11	-0.643	1.69
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.23	-1.02	8	-0.774	17.4
sd:	1.92	0.0682	3.94	1.08	76.8

	CNST	HILL	GNLS
AIC:	129.7	135.7	132.48
PROB:	0.77	0.04	0.19
RMSE:	1.04	1.04	0.93

MAX_MEAN: 1.81 MAX_MED: 2.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

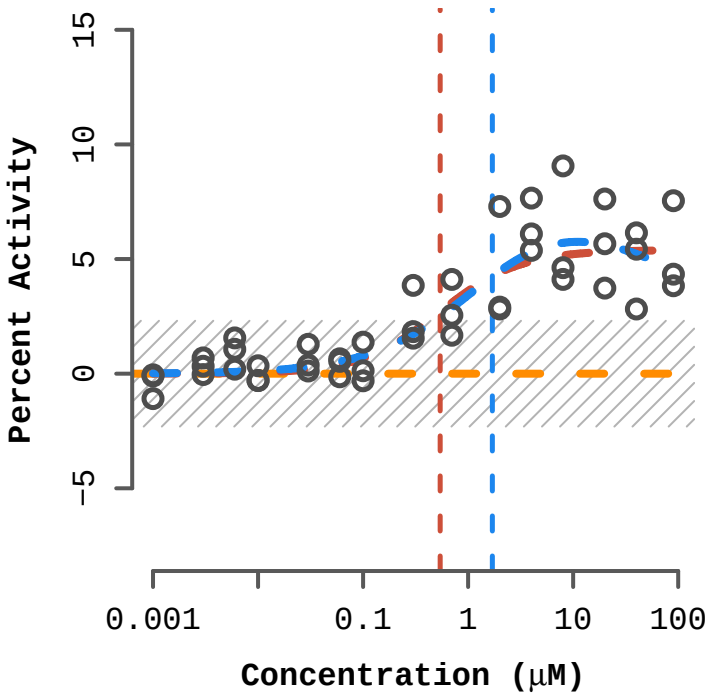
NAME: 3-(Trimethoxysilyl)propyl methacrylate
CHID: 29237 CASRN: 2530-85-0
SPID(S): Tox21_201739
M4ID: 12480513 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	244.83	NA	NA
PROB:	1	NA	NA
RMSE:	22.96	NA	NA

MAX_MEAN: 47.4 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vinyltrimethoxysilane
CHID: 29240 CASRN: 2768-02-7
SPID(S): Tox21_202575
M4ID: 12479677

HILL MODEL (in red):

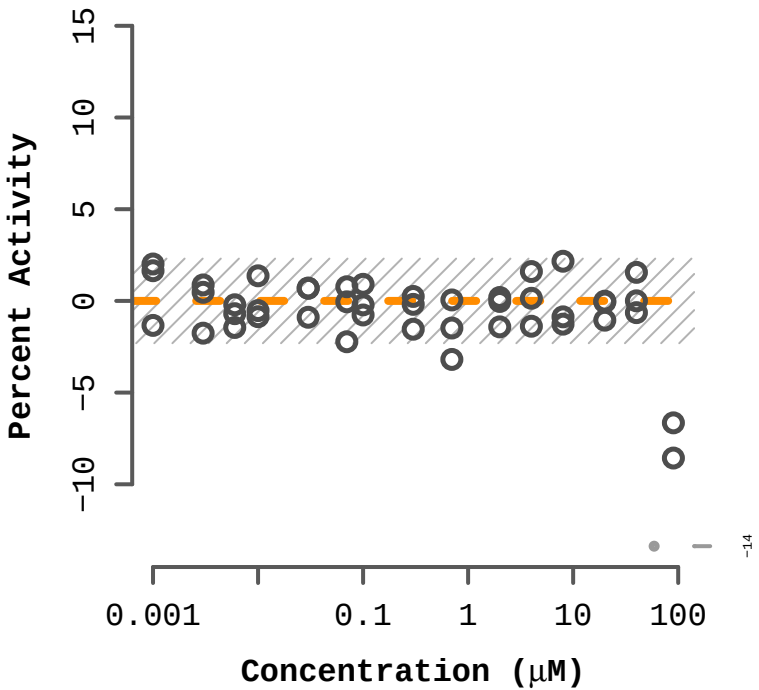
	tp	ga	gw
val:	5.39	−0.266	1.15
sd:	0.467	0.161	0.366

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.9	0.231	0.87	1.65	0.388
sd:	22.3	0.805	0.306	4.47	0.766

	CNST	HILL	GNLS
AIC:	250.06	159.78	161.73
PROB:	0	0.73	0.27
RMSE:	3.78	1.32	1.29

MAX_MEAN: 6.38 MAX_MED: 6.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

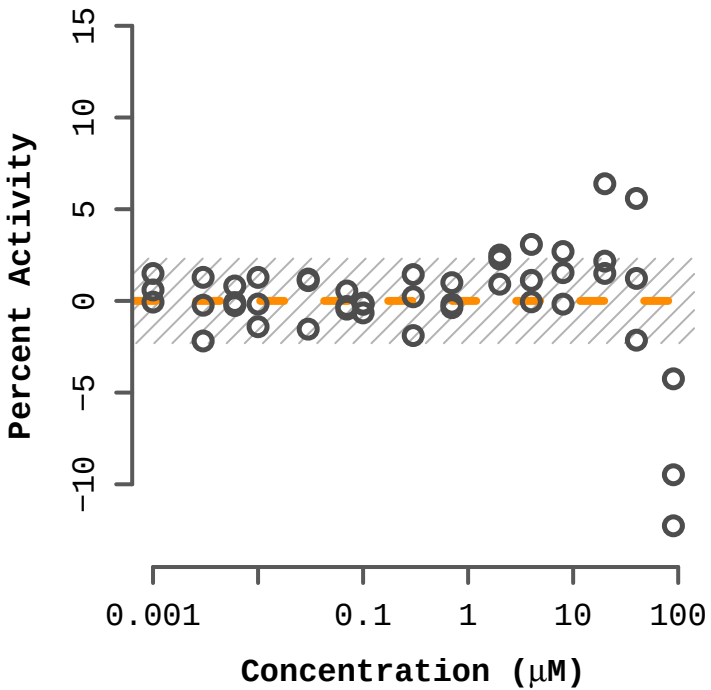
NAME: 2,4-Bis(1-methyl-1-phenylethyl)phenol
CHID: 29241 CASRN: 2772-45-4
SPID(S): Tox21_300317
M4ID: 12478814 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.84	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 0.776 MAX_MED: 1.65 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

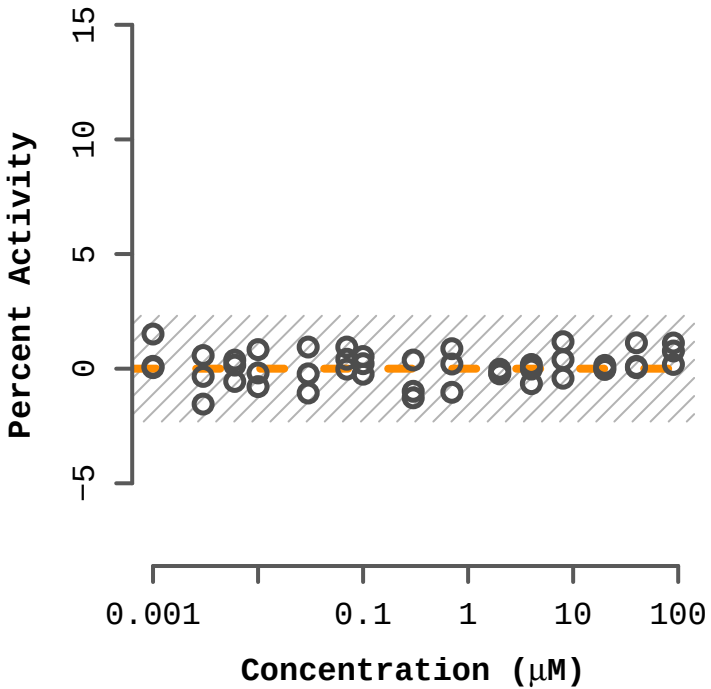
NAME: 2,4-Bis(1-methyl-1-phenylethyl)phenol
CHID: 29241 **CASRN:** 2772-45-4
SPID(S): Tox21_202456
M4ID: 12479796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.28	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 3.35 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

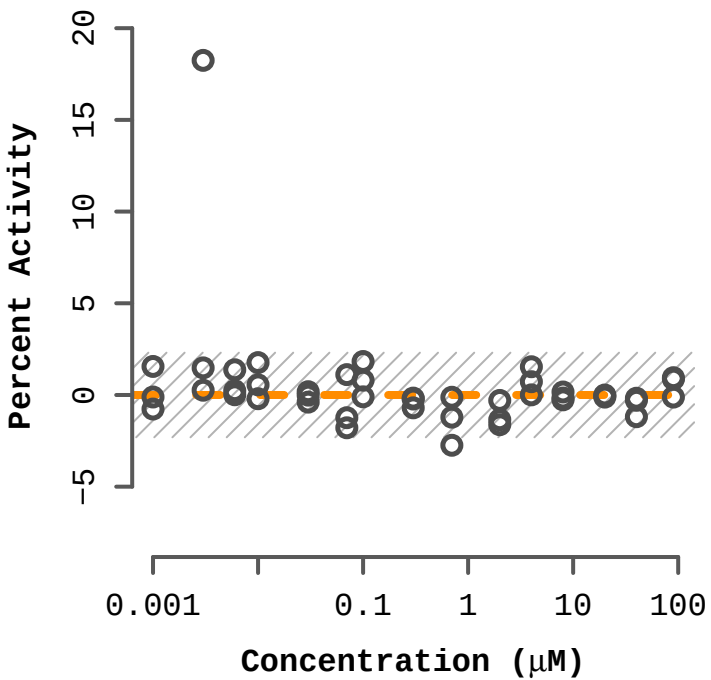
NAME: Diethyl((diethanolamino)methyl)phosphonate
CHID: 29242 **CASRN:** 2781-11-5
SPID(S): Tox21_301894
M4ID: 12477239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.693 **MAX_MED:** 0.771 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

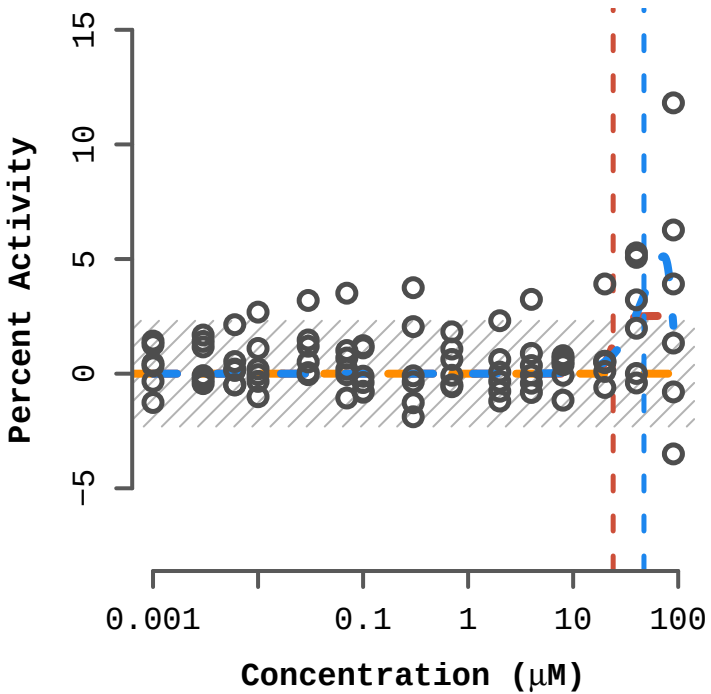
NAME: Octahydro-exo-4,7-methano-1H-indene
CHID: 29244 CASRN: 2825-82-3
SPID(S): Tox21_202770
M4ID: 12479482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 6.66 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triethoxyoctylsilane
CHID: 29246 CASRN: 2943-75-1
SPID(S): Tox21_303648
M4ID: 12475499

HILL MODEL (in red):

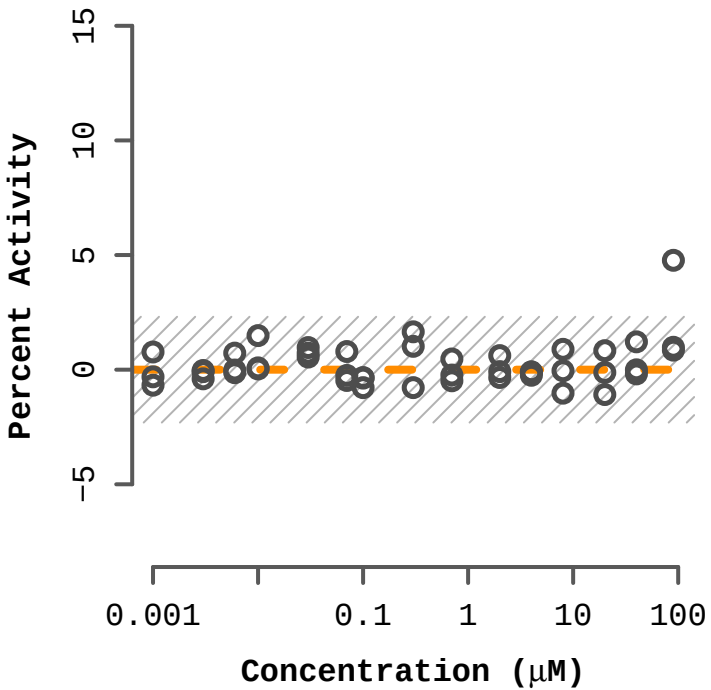
	tp	ga	gw
val:	2.52	1.38	8
sd:	0.856	0.181	16.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.83	1.67	2.92	1.94	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	353.29	347.39	351.2
PROB:	0.04	0.83	0.12
RMSE:	2.12	1.84	1.86

MAX_MEAN: 3.17 MAX_MED: 2.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

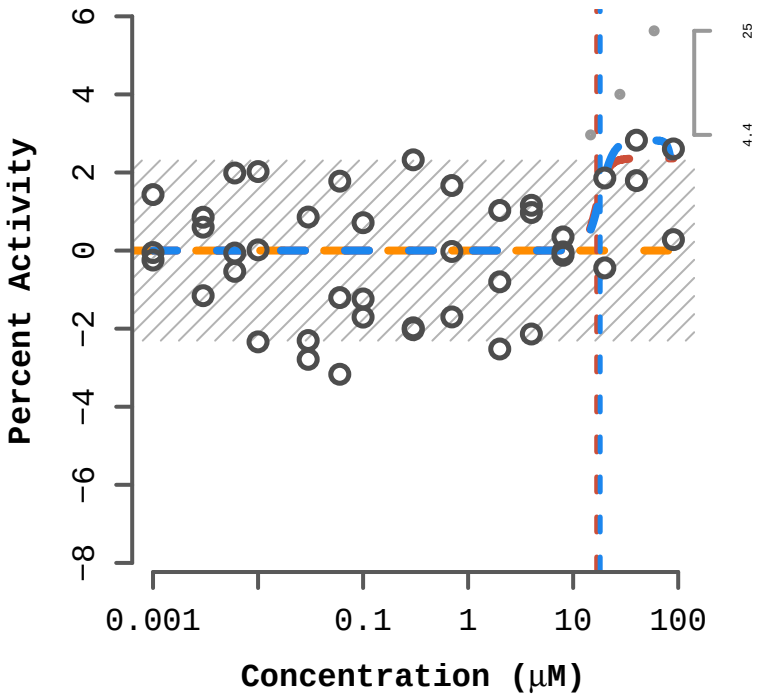
NAME: 1,4-Bis(2-hydroxy-2-propyl)benzene
CHID: 29247 **CASRN:** 2948-46-1
SPID(S): Tox21_200476
M4ID: 12481776

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 2.2 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1,4,7,7-Pentamethyldiethylenetriamine
CHID: 29249 CASRN: 3030-47-5
SPID(S): Tox21_200681
M4ID: 12481571 BRK

HILL MODEL (in red):

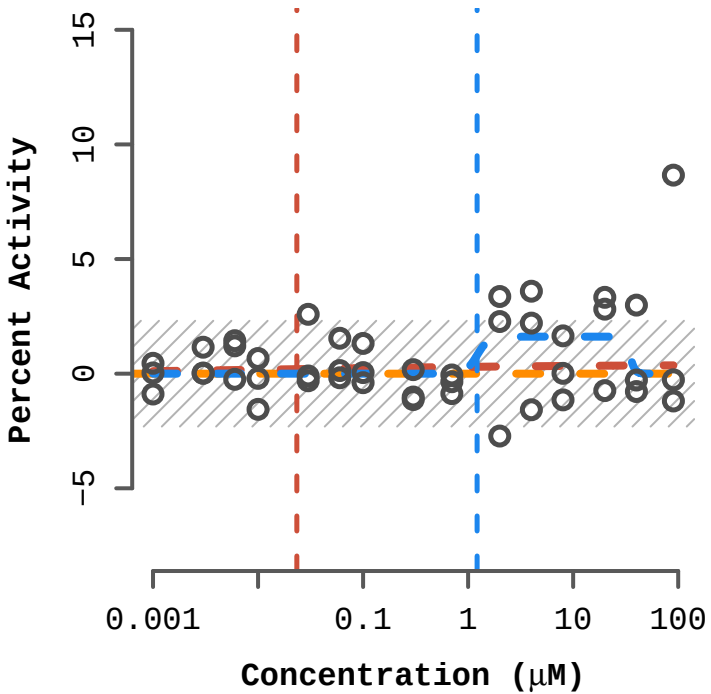
	tp	ga	gw
val:	2.36	1.22	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.82	1.26	7.01	1.97	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	215.49	211.76	215.33
PROB:	0.12	0.76	0.13
RMSE:	4.56	4.06	4.11

MAX_MEAN: 9.45 MAX_MED: 2.83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Vinyl-2-norbornene
CHID: 29250 **CASRN:** 3048-64-4
SPID(S): Tox21_201144
M4ID: 12481108

HILL MODEL (in red):

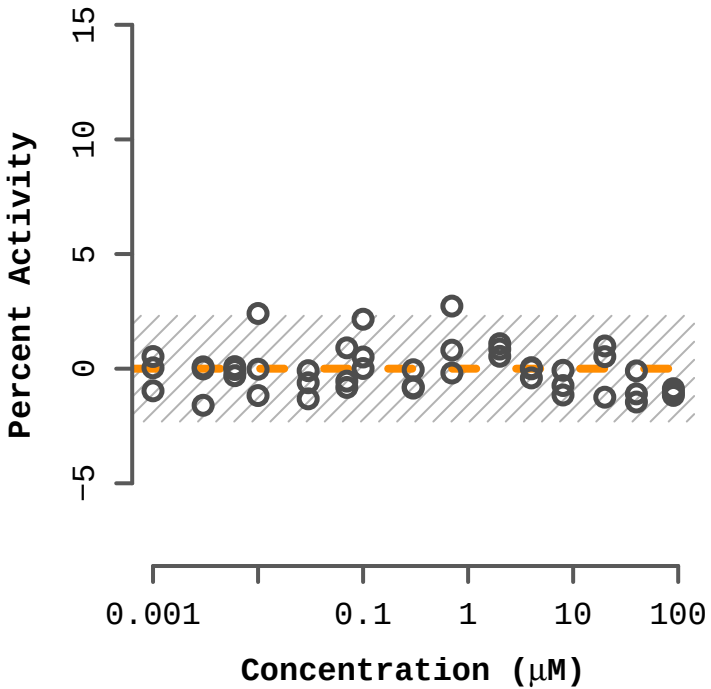
	tp	ga	gw
val:	0.393	-1.63	0.3
sd:	2.76	29.4	1.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.61	0.0856	8	1.54	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	179.23	184.11	183.19
PROB:	0.82	0.07	0.11
RMSE:	1.98	1.91	1.92

MAX_MEAN: 2.4 **MAX_MED:** 2.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

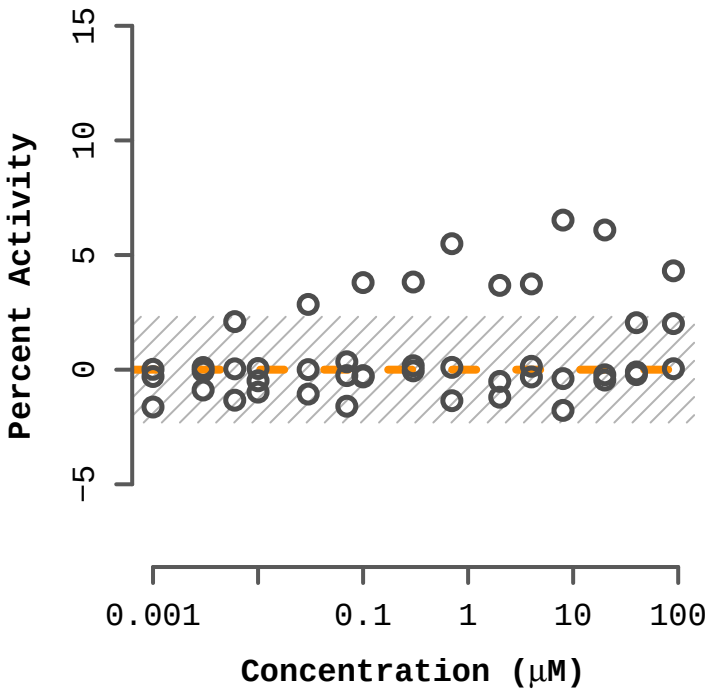
NAME: 2-Butenedioic acid (2Z)-, monomethyl ester
CHID: 29251 **CASRN:** 3052-50-4
SPID(S): Tox21_301490
M4ID: 12477643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

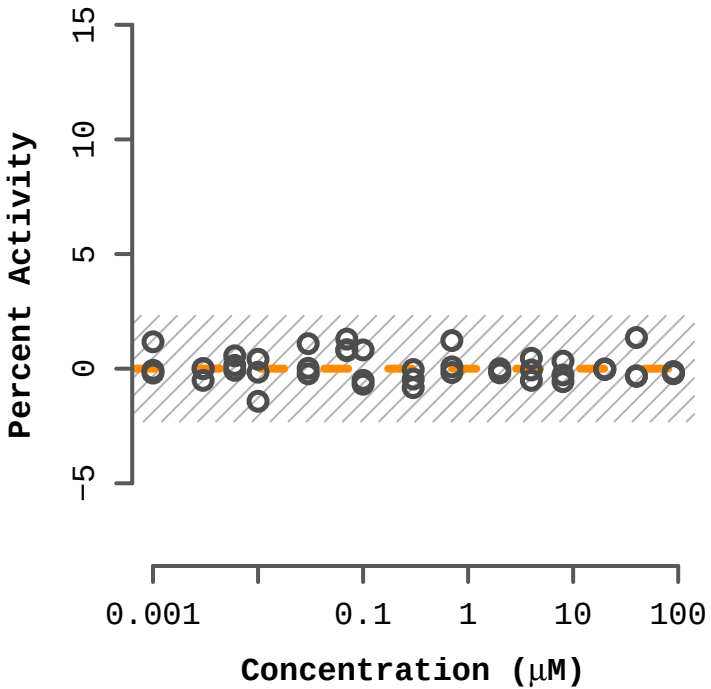
NAME: 3,5,5−Trimethylhexanoic acid
CHID: 29254 **CASRN:** 3302−10−1
SPID(S): Tox21_200081
M4ID: 12482171

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 2.12 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

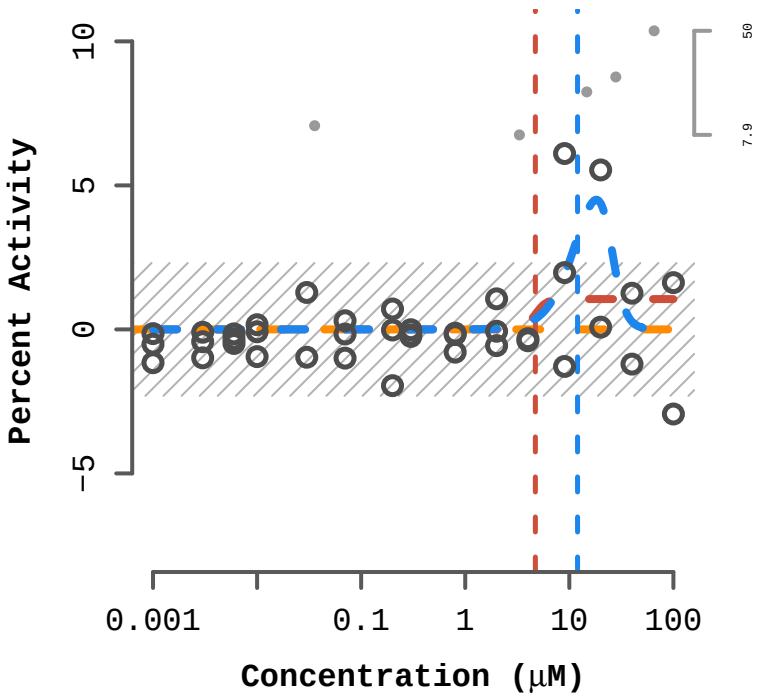
NAME: Dimethyl trans-cyclohexane-1,4-dicarboxylate
CHID: 29255 **CASRN:** 3399-22-2
SPID(S): Tox21_200477
M4ID: 12481775

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	80.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.59	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 0.832 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-(2-Hydroxyethyl)-2-imidazolidinone
CHID: 29260 CASRN: 3699-54-5
SPID(S): Tox21_200698
M4ID: 12481554 BRK

HILL MODEL (in red):

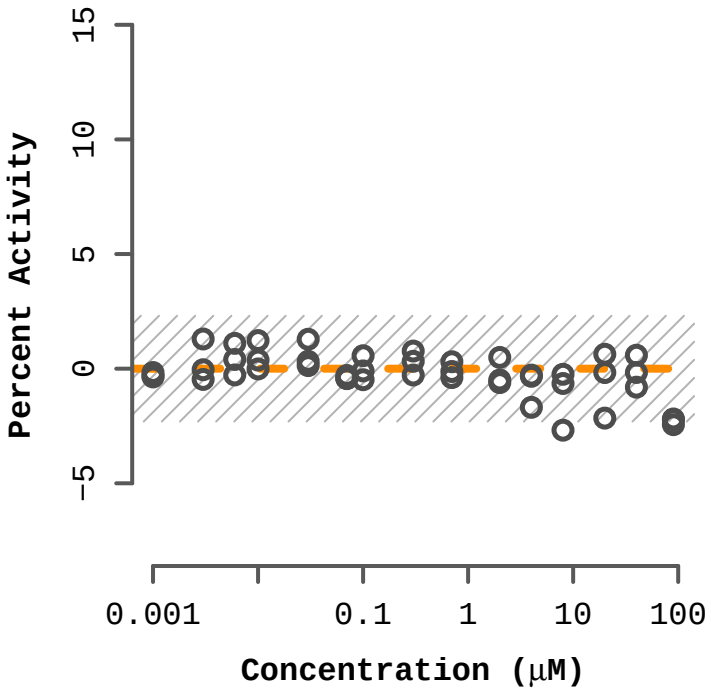
	tp	ga	gw
val:	1.05	0.674	8
sd:	0.763	0.352	28

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.43	1.08	3.01	1.4	6.72
sd:	119	4.09	9.75	3.57	80.6

	CNST	HILL	GNLS
AIC:	255.62	259.61	260.9
PROB:	0.83	0.11	0.06
RMSE:	9.83	9.56	9.54

MAX_MEAN: 16.1 MAX_MED: 5.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

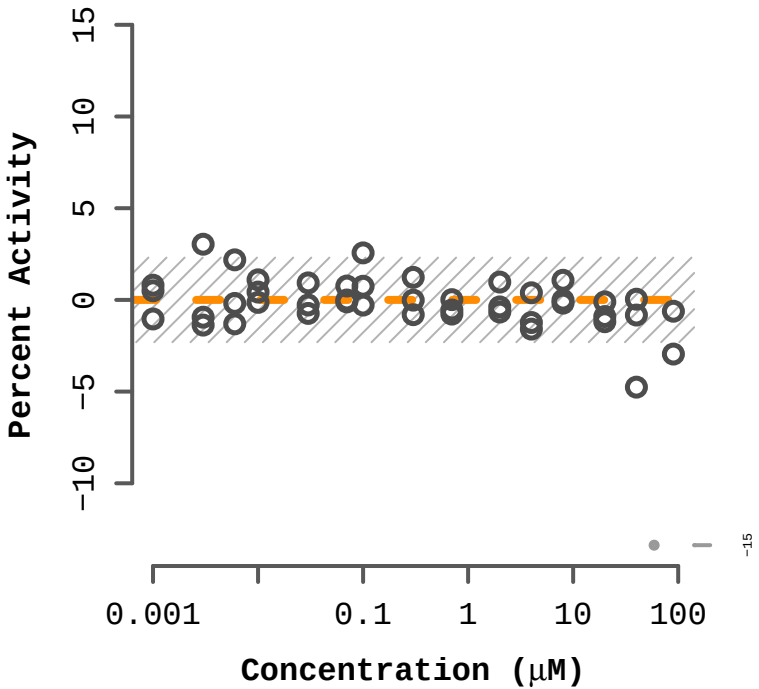
NAME: 2,6-Di-tert-butyl-4-ethylphenol
CHID: 29262 CASRN: 4130-42-1
SPID(S): Tox21_303397
M4ID: 12475741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.58 MAX_MED: 0.403 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

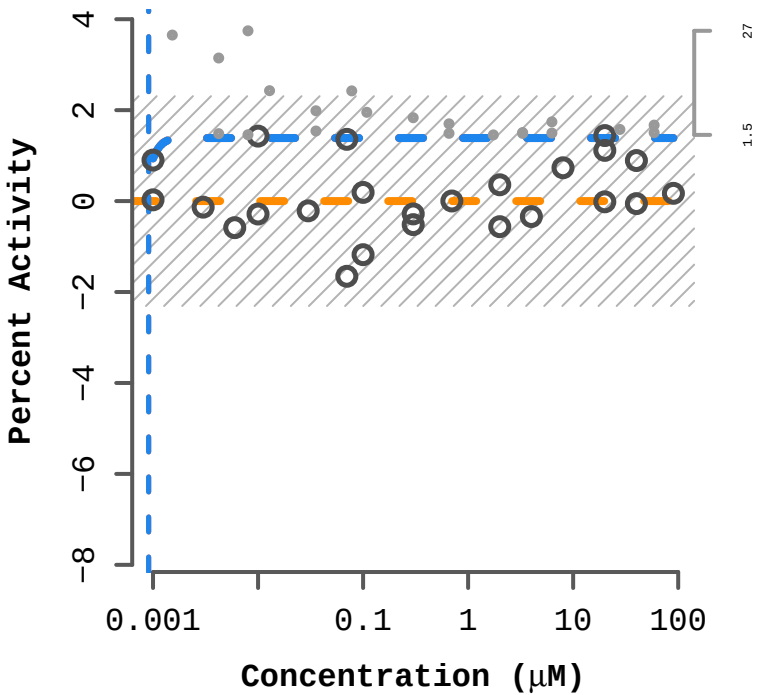
NAME: 2,6-Di-tert-butyl-4-ethylphenol
CHID: 29262 **CASRN:** 4130-42-1
SPID(S): Tox21_201584
M4ID: 12480668 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.56	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.746 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium 2-(methylamino)ethanesulfonate
CHID: 29263 **CASRN:** 4316-74-9
SPID(S): Tox21_200996
M4ID: 12481256 **BRK**

HILL MODEL (in red):

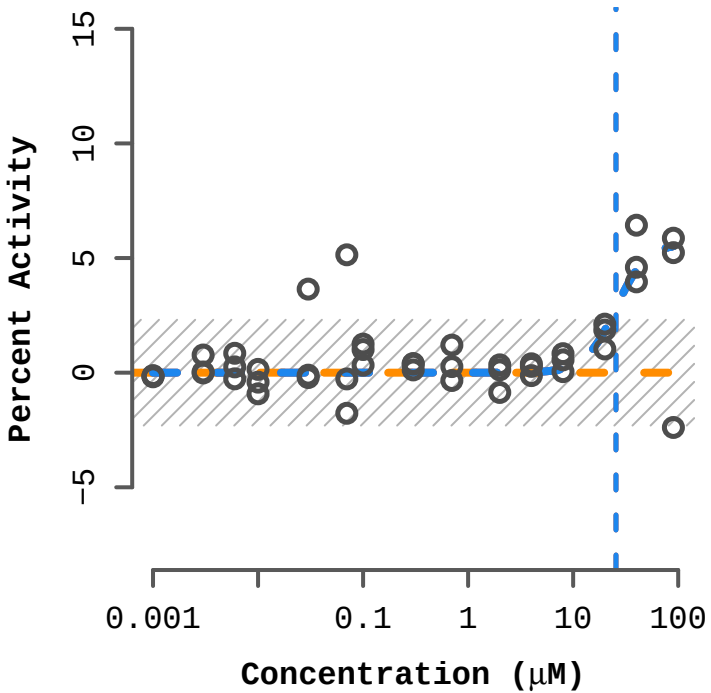
	tp	ga	gw
val:	1.39	−3.04	7.87
sd:	0.43	0.717	138

GAIN-LOSS MODEL (in blue):

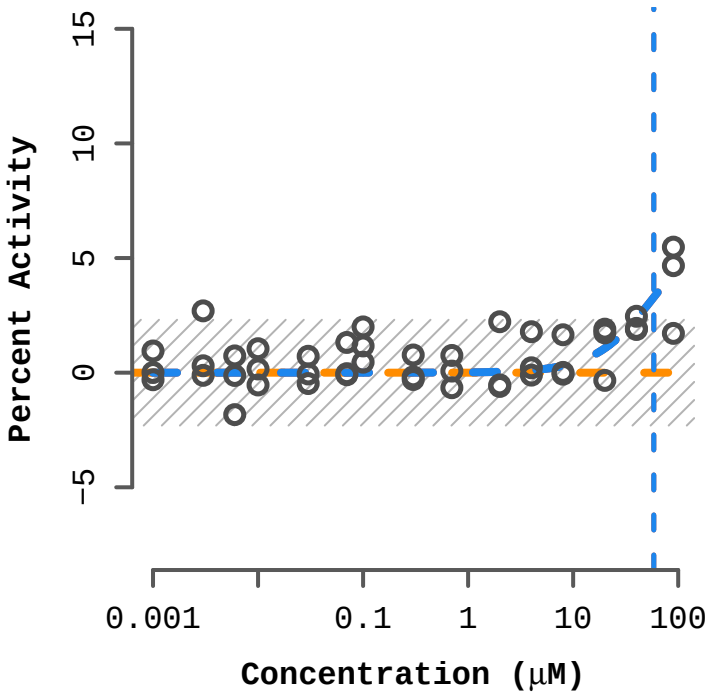
	tp	ga	gw	la	lw
val:	1.39	−3.04	7.67	3.87	17
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	273.92	268.98	272.98
PROB:	0.07	0.82	0.11
RMSE:	7.25	6.74	6.74

MAX_MEAN: 9.31 **MAX_MED:** 2.45 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-(4-Chloro-2,5-dimethoxyphenyl)-3-oxobutanami
CHID:    29265   CASRN: 4433-79-8
SPID(S): Tox21_303485
M4ID:    12475656

HILL MODEL (in red):
      tp       ga       gw
val:  5.65     1.41     2.96
sd:   0.569    0.0546   1.18

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.65     1.41     2.96     3.64     6.52
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  183.87      136.52      140.52
PROB: 0           0.88        0.12
RMSE: 2.15        1.63        1.63

MAX_MEAN: 5         MAX_MED: 5.24      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N−(4−Chloro−2,5−dimethoxyphenyl)−3−oxobutanami
CHID: 29265 CASRN: 4433−79−8
SPID(S): Tox21_201666
M4ID: 12480586

HILL MODEL (in red):

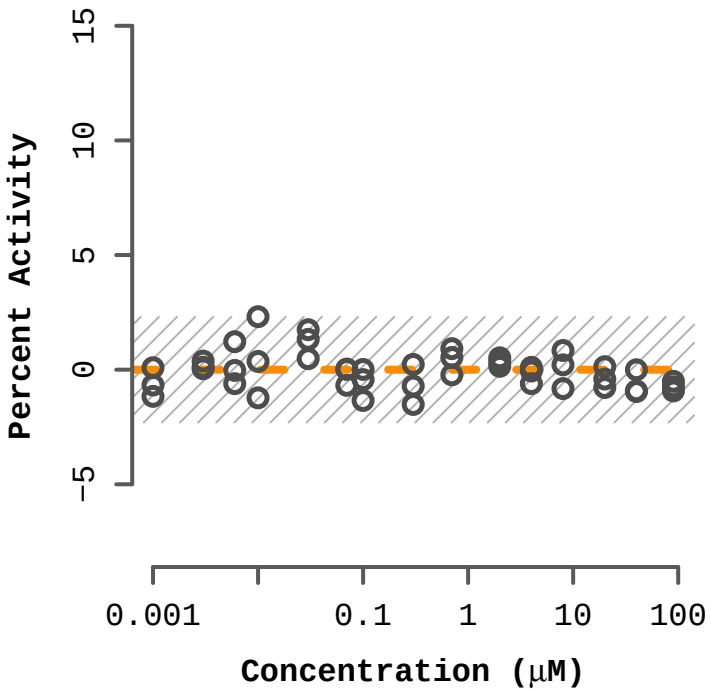
	tp	ga	gw
val:	6.57	1.77	1.53
sd:	2.92	0.263	0.662

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.57	1.77	1.53	3.92	7.15
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	162.15	134.4	138.4
PROB:	0	0.88	0.12
RMSE:	1.56	1.01	1.01

MAX_MEAN: 3.95 MAX_MED: 4.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

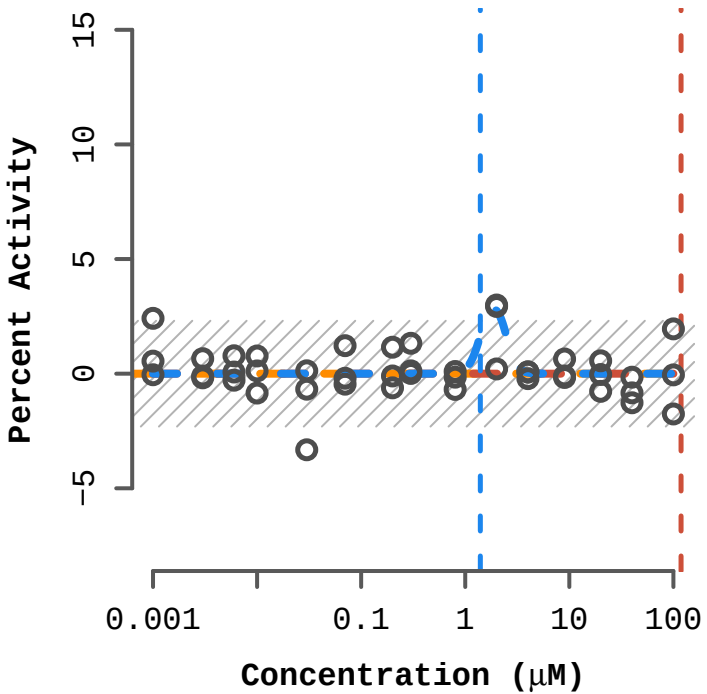
NAME: (3-Chloropropyl)(triethoxy)silane
CHID: 29267 **CASRN:** 5089-70-3
SPID(S): Tox21_200098
M4ID: 12482154

HILL MODEL: Not applicable.

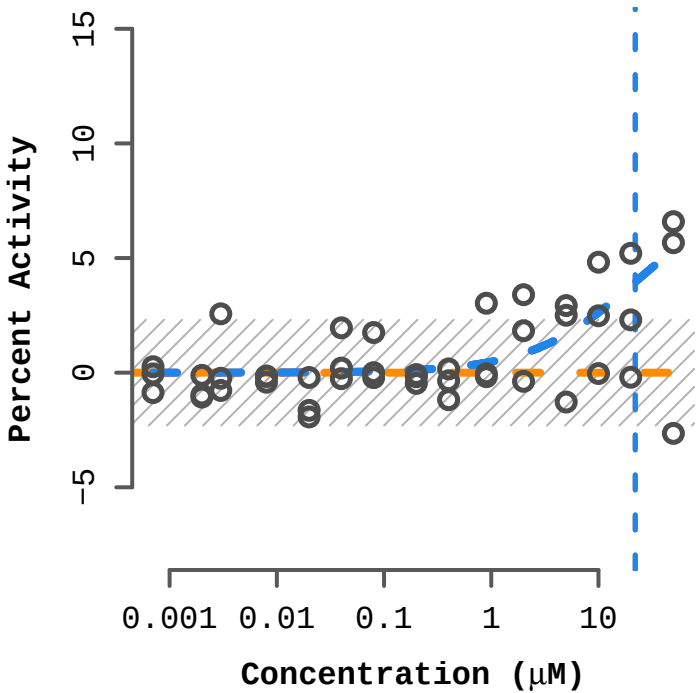
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

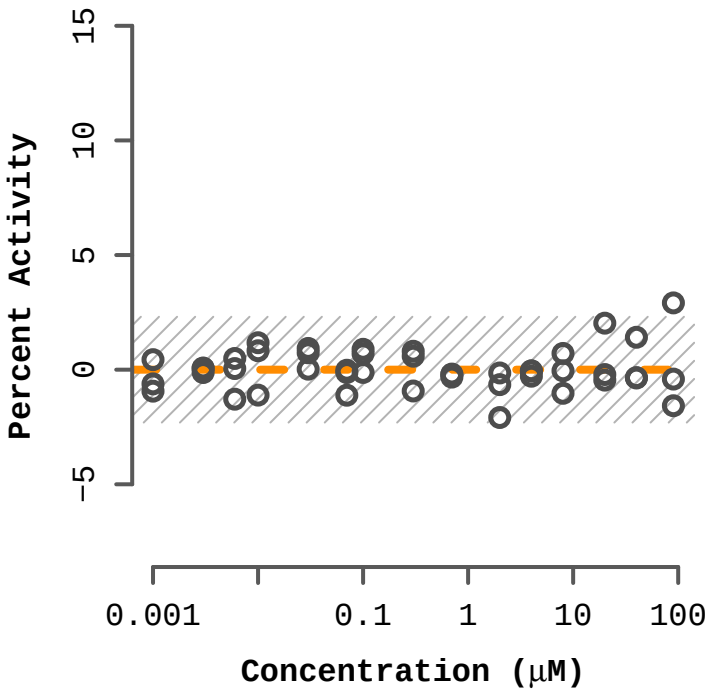
MAX_MEAN: 1.18 **MAX_MED:** 1.32 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (2R)-2-Aminobutan-1-ol
CHID:    29275   CASRN: 5856-63-3
SPID(S): Tox21_200478
M4ID:    12481774

HILL MODEL (in red):
      tp       ga       gw
val:  4.3e-10  2.07     2.03
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.35     0.145    8        0.395    8.64
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  128.39      134.39      128.55
PROB: 0.51        0.03        0.47
RMSE: 1.1         1.1         0.98

MAX_MEAN: 2.05      MAX_MED: 2.93      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Bromamine acid sodium salt
CHID:    29277   CASRN: 6258-06-6
SPID(S): Tox21_202576
M4ID:    12479676

HILL MODEL (in red):
      tp       ga       gw
val:  7.91     1.34     0.888
sd:   4.61     0.644    0.343

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.91     1.34     0.888    2.26     15.3
sd:   4.61     0.644    0.343    796      21700

      CNST        HILL        GNLS
AIC:  192.56      177.97      181.97
PROB: 0           0.88        0.12
RMSE: 2.16        1.83        1.83

MAX_MEAN: 3.2       MAX_MED: 5.67      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

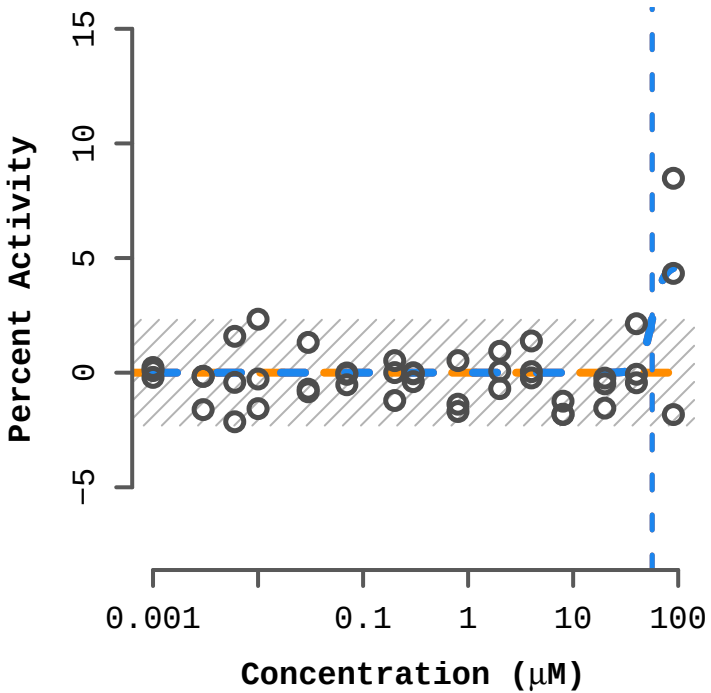
NAME: Sodium 5-sulfoisophthalate
CHID: 29279 **CASRN:** 6362-79-4
SPID(S): Tox21_200715
M4ID: 12481537

HILL MODEL: Not applicable.

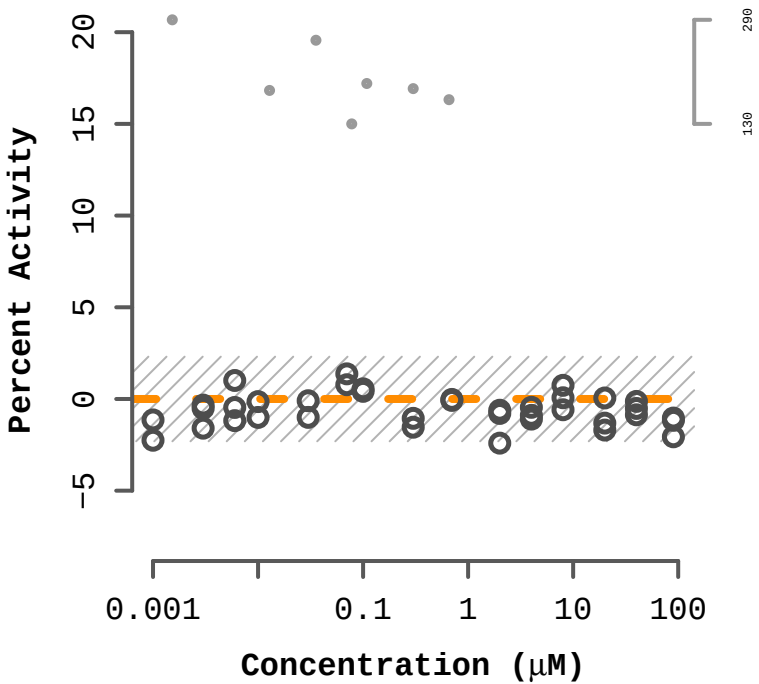
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.564 **MAX_MED:** 0.827 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    6-Amino-1,3-dimethyl-5-nitroso- 2,4(1H,3H)-pyr
CHID:    29280   CASRN: 6632-68-4
SPID(S): Tox21_200968
M4ID:    12481284

HILL MODEL (in red):
      tp       ga       gw
val:  4.68     1.75     8
sd:   2.86     0.602    28.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.69     1.75     8        2.81     3.15
sd:   30.8     0.72     29.4     939      2170

      CNST        HILL        GNLS
AIC:  161.23      160.63      164.63
PROB: 0.39        0.53        0.07
RMSE: 1.77        1.51        1.51

MAX_MEAN: 3.66      MAX_MED: 4.33      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

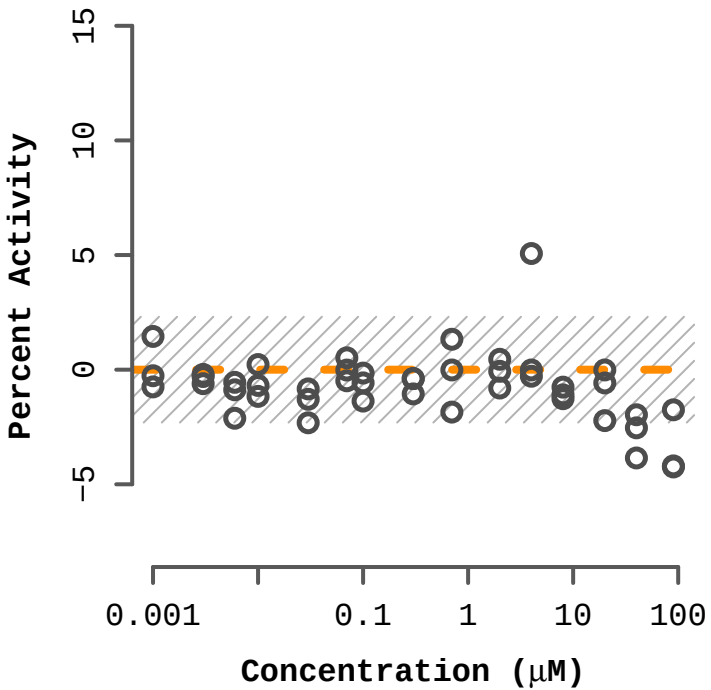
NAME: 1-Phenylundecane
CHID: 29281 CASRN: 6742-54-7
SPID(S): Tox21_200115
M4ID: 12482137 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	436.12	NA	NA
PROB:	1	NA	NA
RMSE:	81.01	NA	NA

MAX_MEAN: 95.1 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

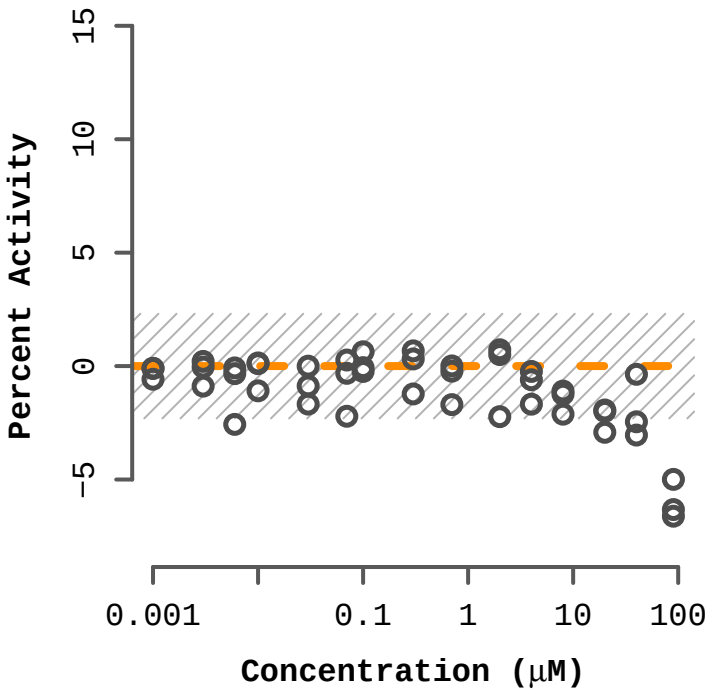
NAME: 4,4'-(4-Methylpentane-2,2-diyl)diphenol
CHID: 29282 **CASRN:** 6807-17-6
SPID(S): Tox21_303608
M4ID: 12475537

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** −0.0114 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

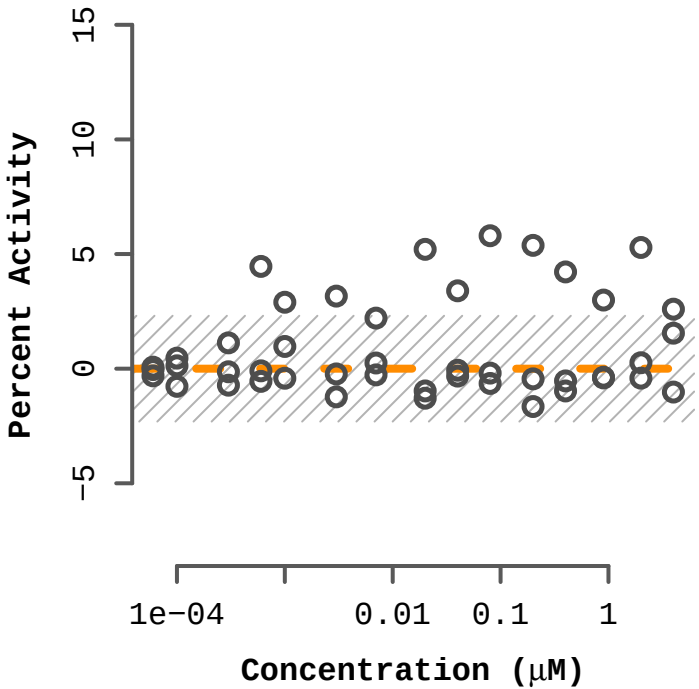
NAME: 4,4'-(4-Methylpentane-2,2-diyl)diphenol
CHID: 29282 **CASRN:** 6807-17-6
SPID(S): Tox21_202128
M4ID: 12480124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.05	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 0.111 **MAX_MED:** 0.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

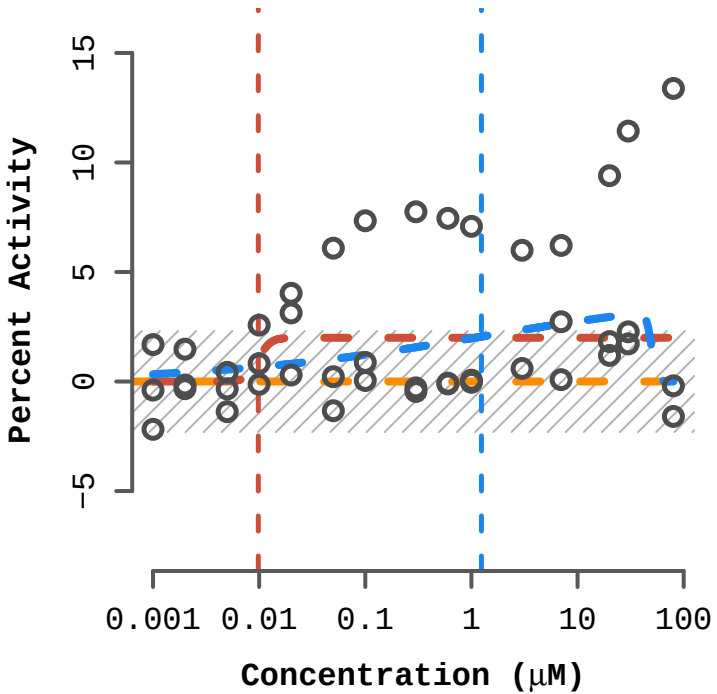
NAME: Acetic acid, antimony(3+) salt
CHID: 29283 **CASRN:** 6923-52-0
SPID(S): Tox21_202771
M4ID: 12479481

HILL MODEL: Not applicable.

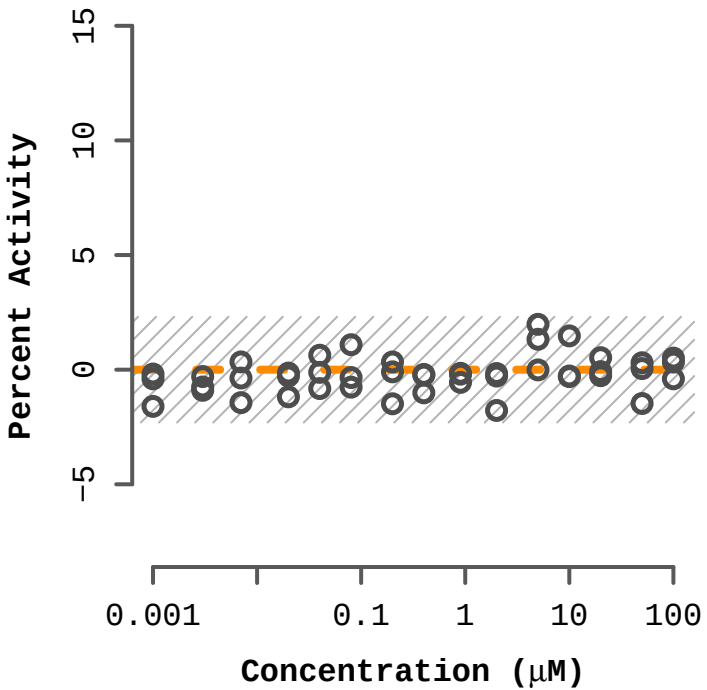
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.55 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,2',2'',2'''-[Ethane-1,1,2,2-tetrayltetrakis(4
CHID:    29286   CASRN: 7328-97-4
SPID(S): Tox21_303396
M4ID:    12475742

HILL MODEL (in red):
      tp       ga       gw
val:  2        -2.01    8
sd:   0.605    0.155    23

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.1      0.0942   0.34     1.7      17.9
sd:   6.73     5.01     0.463    5.95     494

      CNST        HILL        GNLS
AIC:  245.52      238.03      241.14
PROB: 0.02        0.81        0.17
RMSE: 4.27        3.49        3.57

MAX_MEAN: 5.14      MAX_MED: 3.3       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

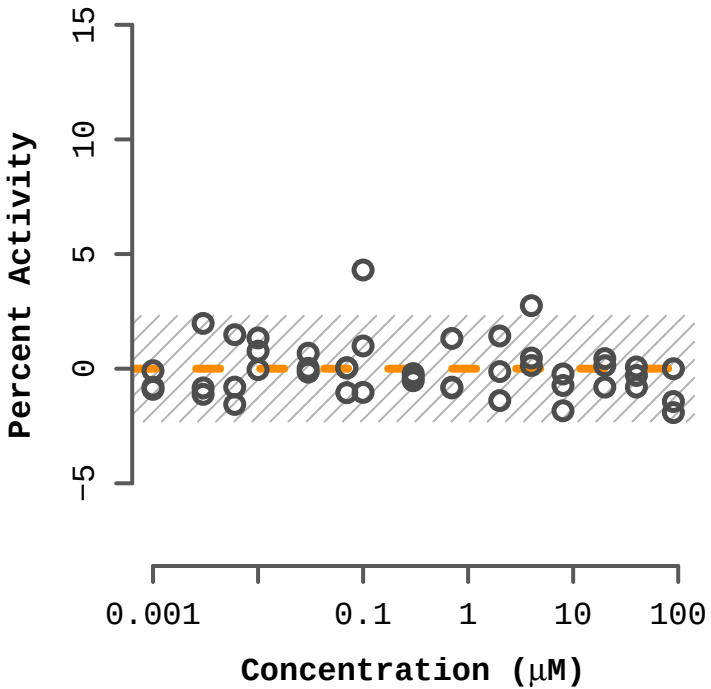
NAME: 2,2',2'',2'''-[Ethane-1,1,2,2-tetrayltetrakis(4
CHID: 29286 CASRN: 7328-97-4
SPID(S): Tox21_202150
M4ID: 12480102

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

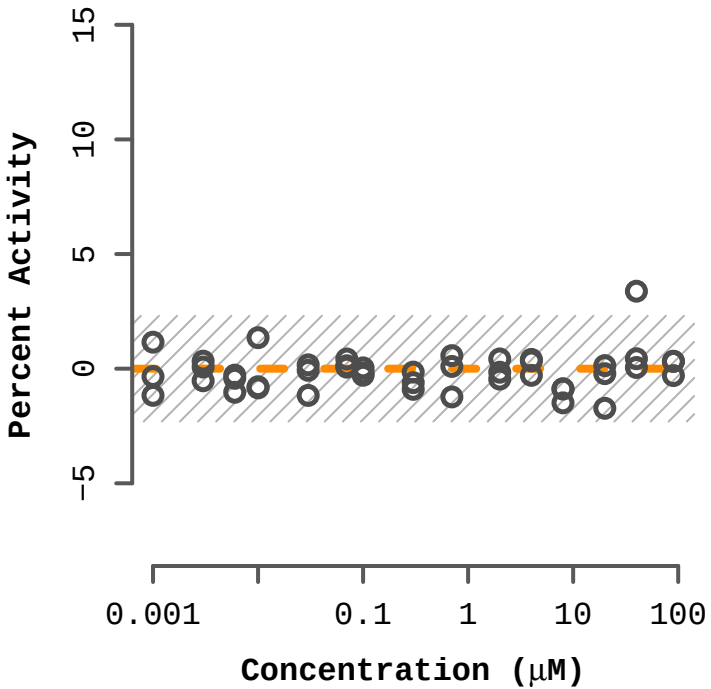
NAME: 4-Methylmorpholine 4-oxide
CHID: 29287 **CASRN:** 7529-22-8
SPID(S): Tox21_200479
M4ID: 12481773

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 0.991 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

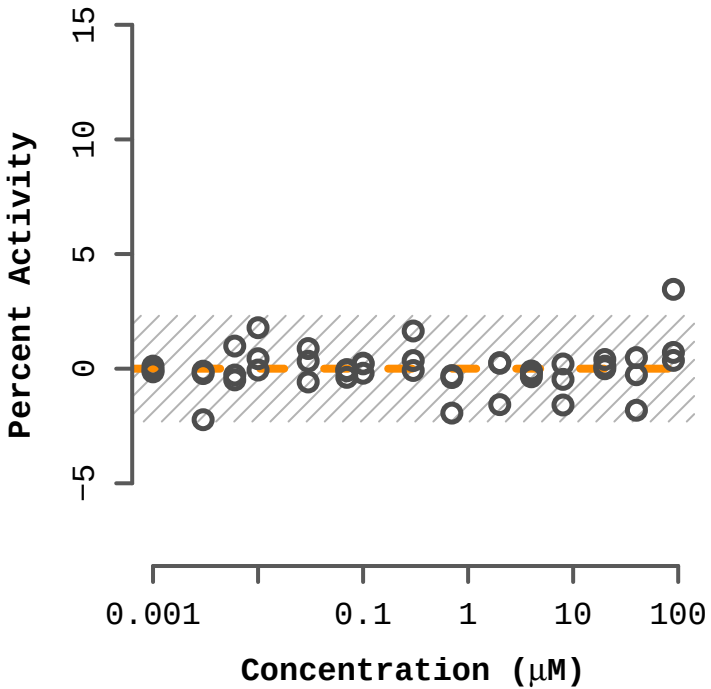
NAME: 5-Ethyl-1-aza-3,7-dioxabicyclo[3.3.0]octane
CHID: 29289 **CASRN:** 7747-35-5
SPID(S): Tox21_300546
M4ID: 12478586

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.435 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

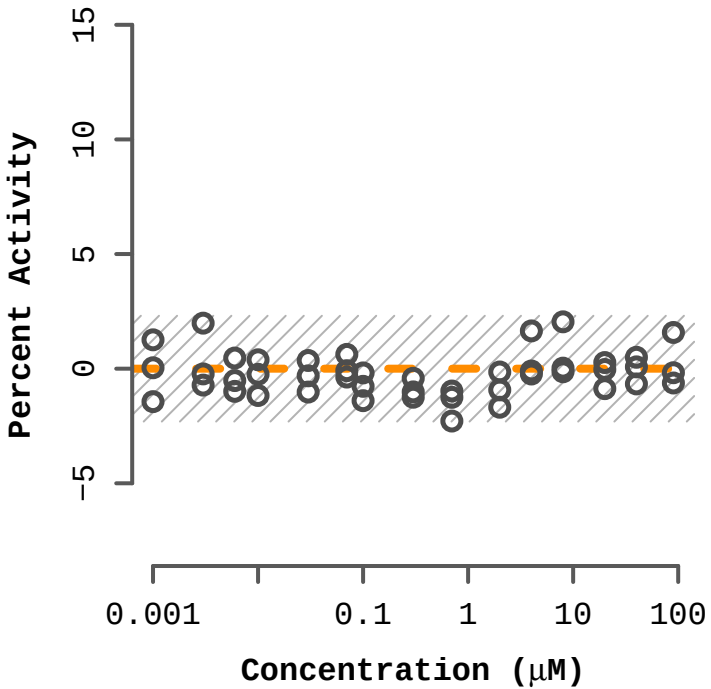
NAME: 5-Ethyl-1-aza-3,7-dioxabicyclo[3.3.0]octane
CHID: 29289 **CASRN:** 7747-35-5
SPID(S): Tox21_201455
M4ID: 12480797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 0.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

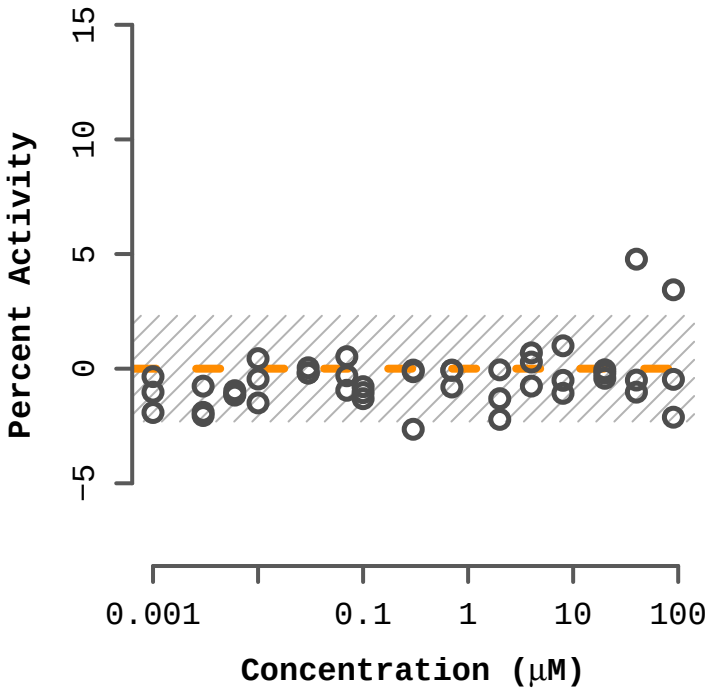
NAME: (−)−alpha−Pinene
CHID: 29290 **CASRN:** 7785−26−4
SPID(S): Tox21_303591
M4ID: 12475554

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.645 **MAX_MED:** 0.081 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

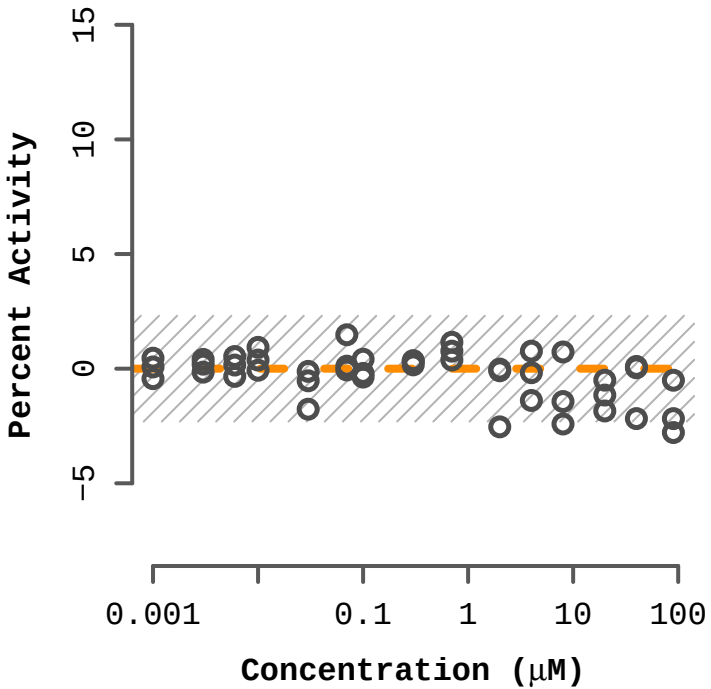
NAME: (−)−alpha−Pinene
CHID: 29290 **CASRN:** 7785−26−4
SPID(S): Tox21_201760
M4ID: 12480492

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

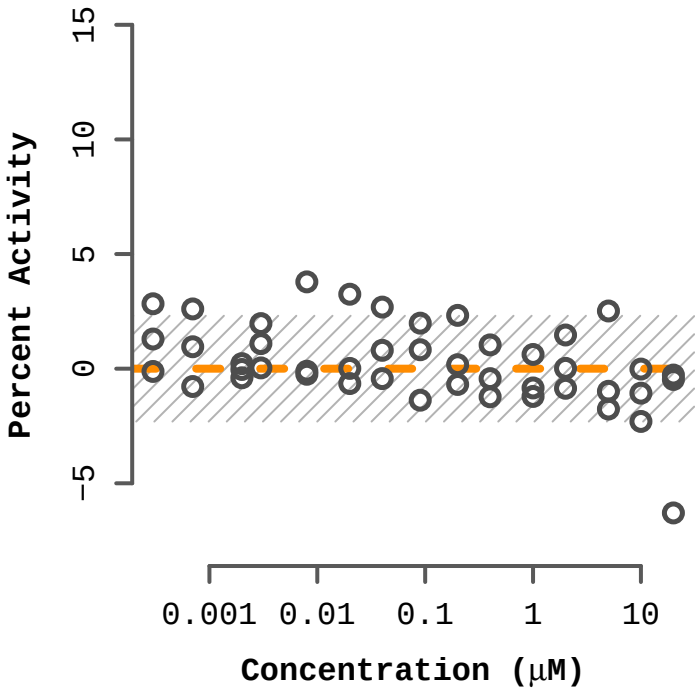
NAME: Sodium lauryl polyoxyethylene ether sulfate
CHID: 29298 CASRN: 9004-82-4
SPID(S): Tox21_302374
M4ID: 12476759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.765 **MAX_MED:** 0.765 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

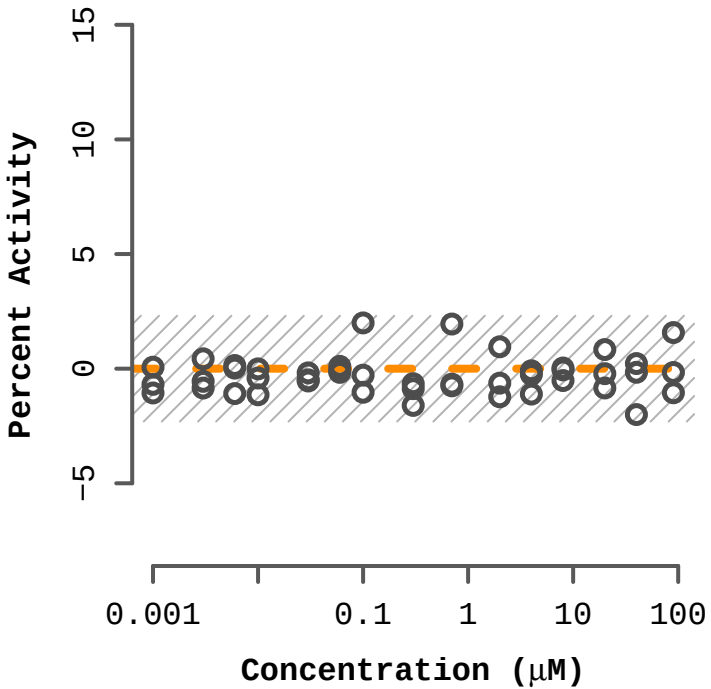
NAME: Polyethylene glycol stearyl ether
CHID: 29299 **CASRN:** 9005-00-9
SPID(S): Tox21_202772
M4ID: 12479480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

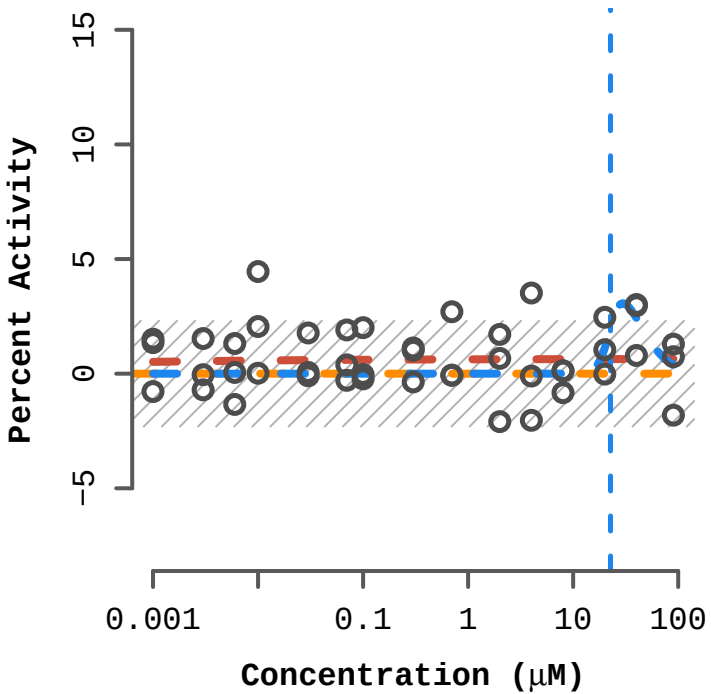
NAME: Polysorbate 60
CHID: 29300 CASRN: 9005-67-8
SPID(S): Tox21_200064
M4ID: 12482188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.23 MAX_MED: 0.0264 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Propyl-1-heptanol
CHID: 29302 CASRN: 10042-59-8
SPID(S): Tox21_300903
M4ID: 12478230

HILL MODEL (in red):

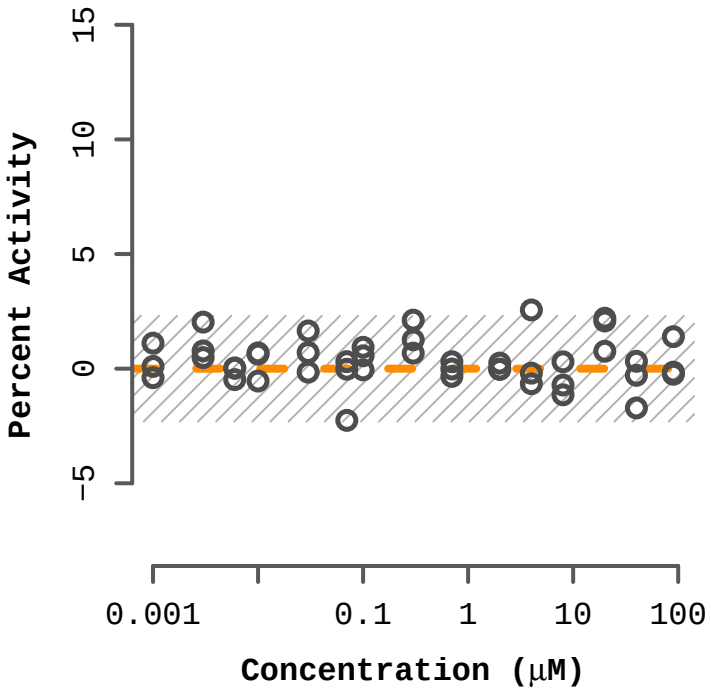
	tp	ga	gw
val:	0.644	-5	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.65	1.36	8	1.62	3.08
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	171.36	169.3	171.5
PROB:	0.21	0.59	0.2
RMSE:	1.58	1.43	1.44

MAX_MEAN: 2.26 MAX_MED: 2.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

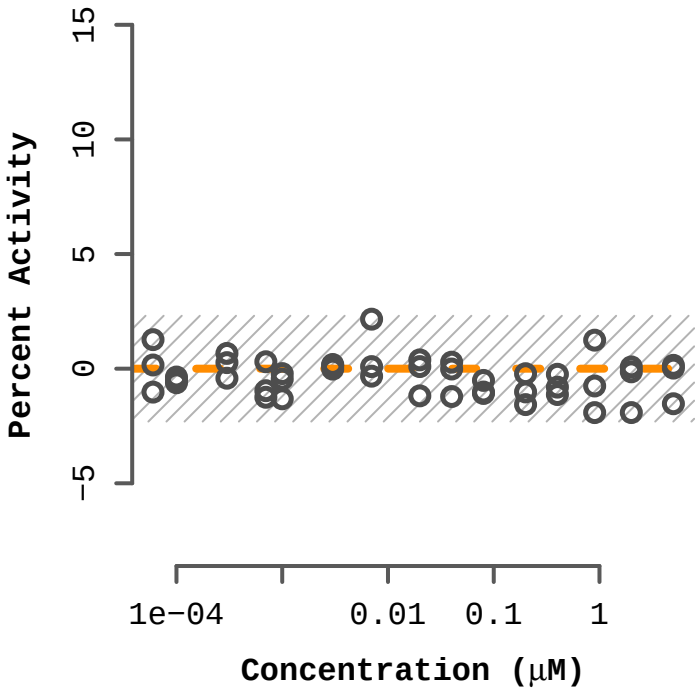
NAME: Glyceryl stearates
CHID: 29304 **CASRN:** 11099-07-3
SPID(S): Tox21_301104
M4ID: 12478029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

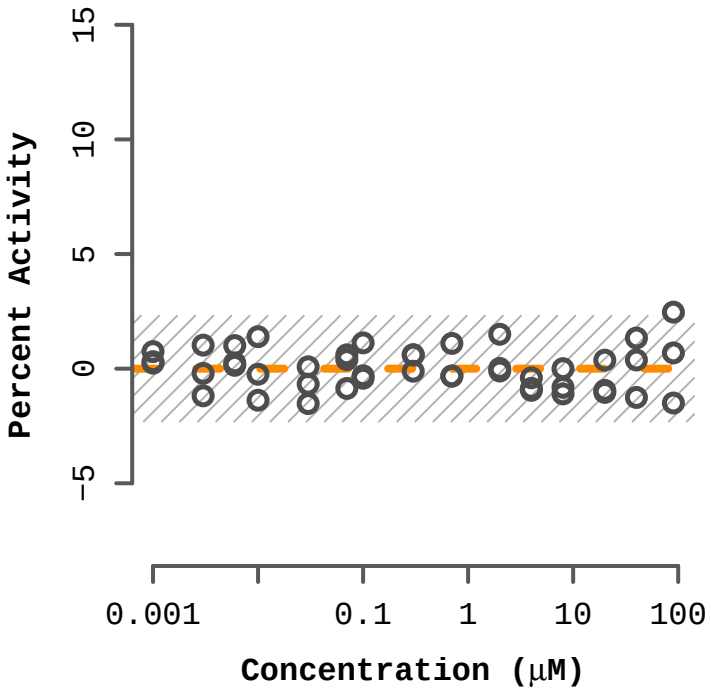
NAME: 4,4'−bis(1,1,3,3−Tetramethylbutyl)diphenylamine
CHID: 29310 **CASRN:** 15721−78−5
SPID(S): Tox21_202773
M4ID: 12479479

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.643 **MAX_MED:** 0.266 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

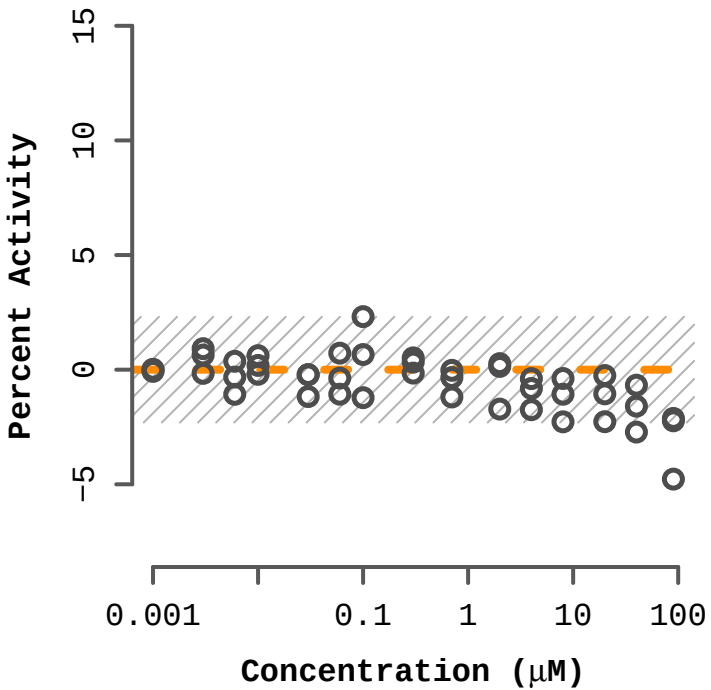
NAME: 6-Hydroxy-2-naphthoic acid
CHID: 29312 **CASRN:** 16712-64-4
SPID(S): Tox21_200732
M4ID: 12481520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.554 **MAX_MED:** 0.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

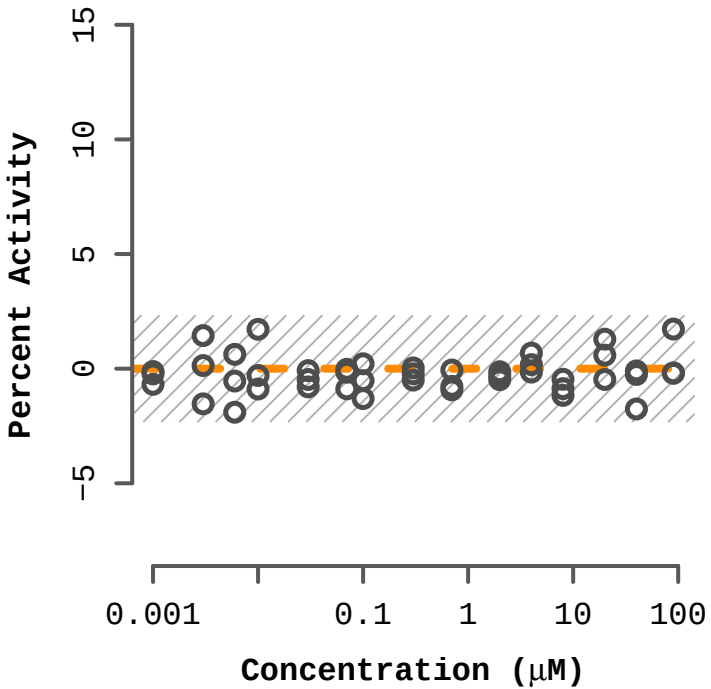
NAME: 4-(Butan-2-yl)-2,6-di-tert-butylphenol
CHID: 29315 **CASRN:** 17540-75-9
SPID(S): Tox21_201062
M4ID: 12481190

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.663 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

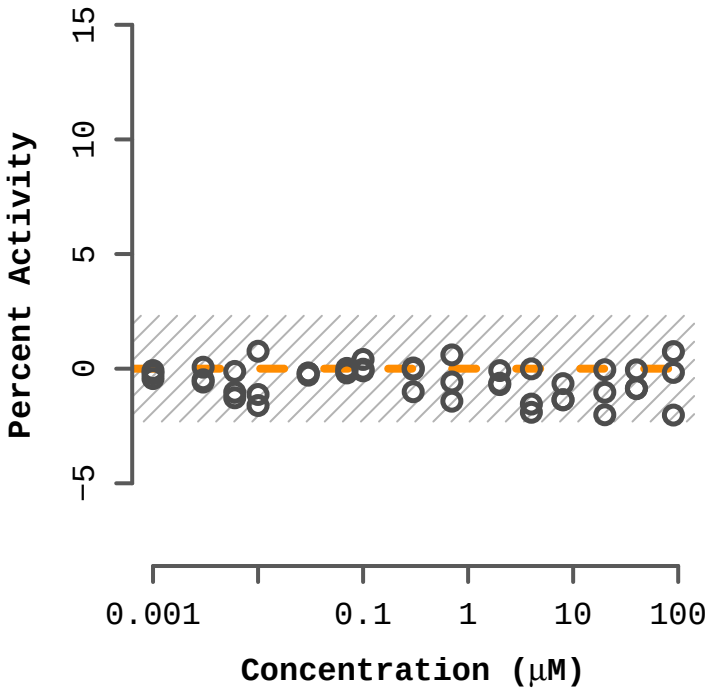
NAME: 1,1,5-Trimethyl-6-heptenol
CHID: 29317 **CASRN:** 18479-58-8
SPID(S): Tox21_200132
M4ID: 12482120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.469 **MAX_MED:** 0.588 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

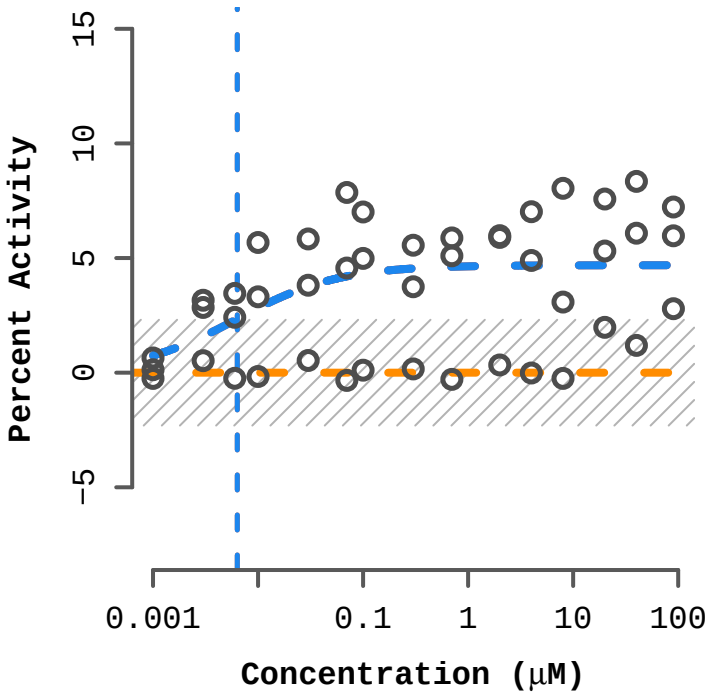
NAME: 2-Ethylhexyl 4-(dimethylamino)benzoate
CHID: 29320 CASRN: 21245-02-3
SPID(S): Tox21_303574
M4ID: 12475571

HILL MODEL: Not applicable.

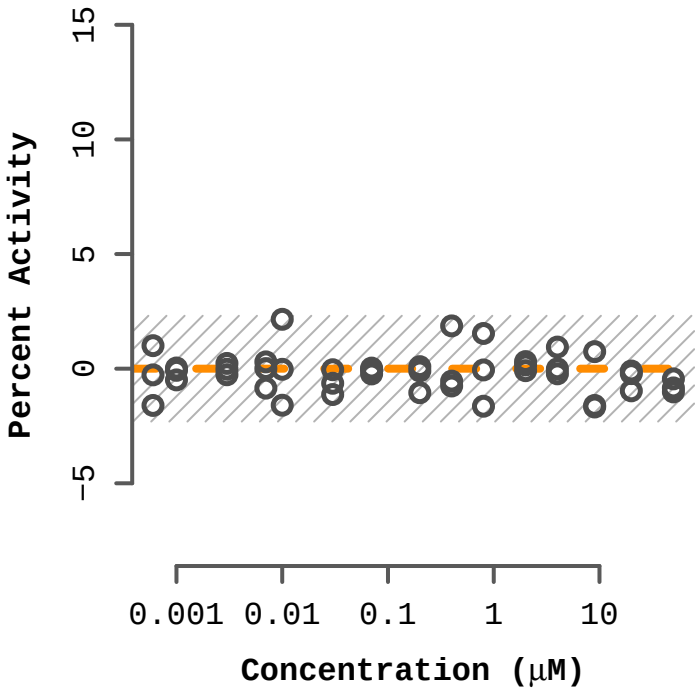
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.0959 MAX_MED: -0.0221 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Ethylhexyl 4-(dimethylamino)benzoate
CHID:    29320   CASRN: 21245-02-3
SPID(S): Tox21_202421
M4ID:    12479831

HILL MODEL (in red):
      tp       ga       gw
val:  4.69     -2.2     0.898
sd:   0.7      0.401    0.835

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.69     -2.2     0.898    3.72     8.09
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  270.05      225.1       229.1
PROB: 0           0.88        0.12
RMSE: 4.48        2.56        2.56

MAX_MEAN: 5.33      MAX_MED: 6.09      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

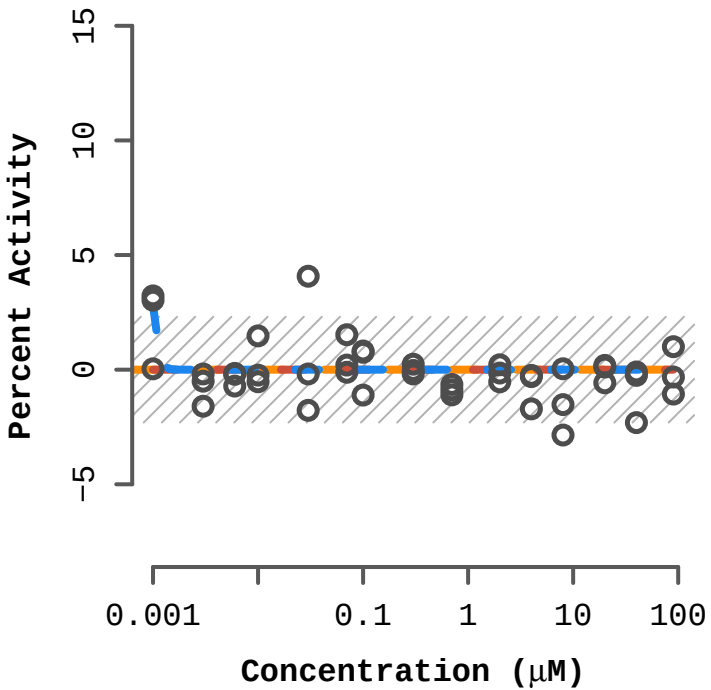
NAME: 2-Ethylhexyl 4-(dimethylamino)benzoate
CHID: 29320 **CASRN:** 21245-02-3
SPID(S): Tox21_111013_1
M4ID: 12483949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.239 **MAX_MED:** 0.162 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl dihydrojasmonate
CHID: 29325 CASRN: 24851-98-7
SPID(S): Tox21_303588
M4ID: 12475557

HILL MODEL (in red):

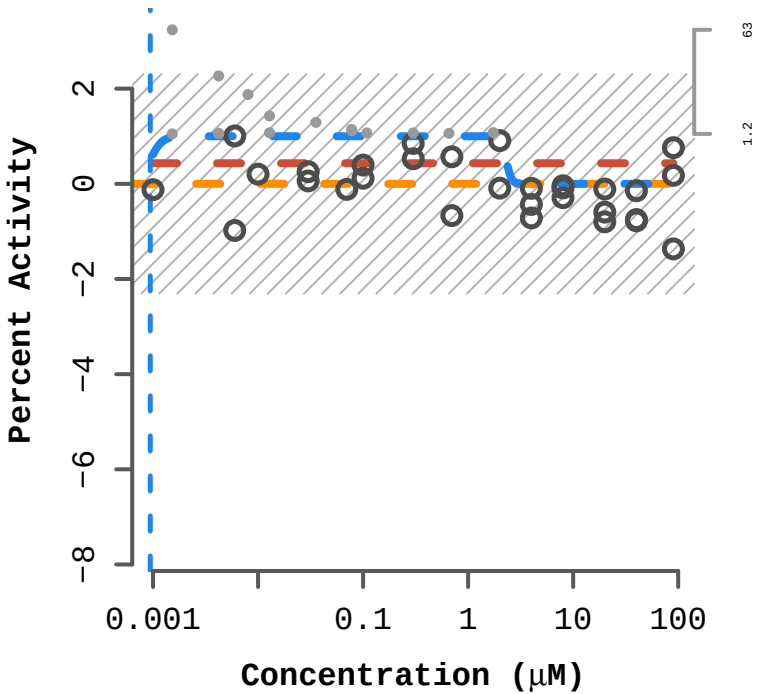
	tp	ga	gw
val:	1.94e-10	-4.01	1.32
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	-3.44	1.59	-2.98	15.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	145.35	151.35	147.27
PROB:	0.7	0.03	0.27
RMSE:	1.29	1.29	1.18

MAX_MEAN: 2.1 **MAX_MED:** 3.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl dihydrojasmonate
CHID: 29325 CASRN: 24851-98-7
SPID(S): Tox21_202172
M4ID: 12480080 BRK

HILL MODEL (in red):

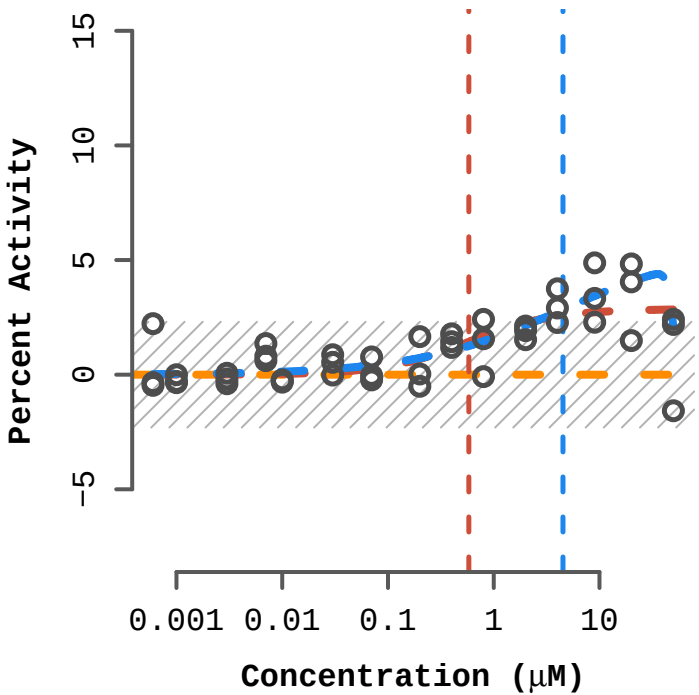
	tp	ga	gw
val:	0.432	−4.48	4.24
sd:	0.239	1250	3490

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1	−3.03	7.94	0.363	17.9
sd:	0.306	0.305	75.6	0.729	199

	CNST	HILL	GNLS
AIC:	252.51	255.15	250.66
PROB:	0.26	0.07	0.66
RMSE:	11.62	11.5	11.38

MAX_MEAN: 21.3 **MAX_MED:** 3.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetrabromobisphenol A diallyl ether
CHID: 29327 **CASRN:** 25327-89-3
SPID(S): Tox21_202577
M4ID: 12479675

HILL MODEL (in red):

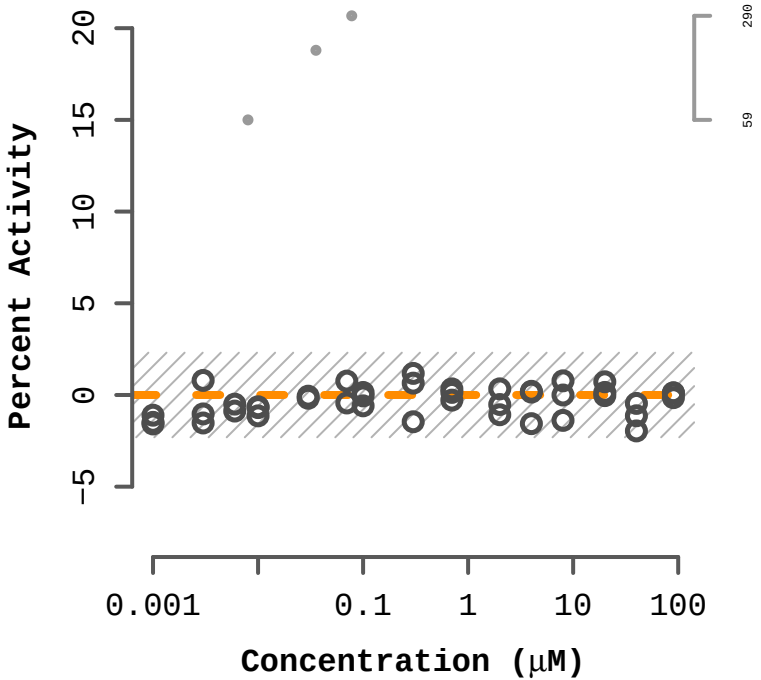
	tp	ga	gw
val:	2.87	−0.235	1.08
sd:	0.432	0.225	0.431

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.68	0.655	0.616	1.69	14
sd:	3.62	0.963	0.261	0.0187	42.5

	CNST	HILL	GNLS
AIC:	186.85	131.87	127.89
PROB:	0	0.12	0.88
RMSE:	1.9	1.08	0.97

MAX_MEAN: 3.5 **MAX_MED:** 4.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

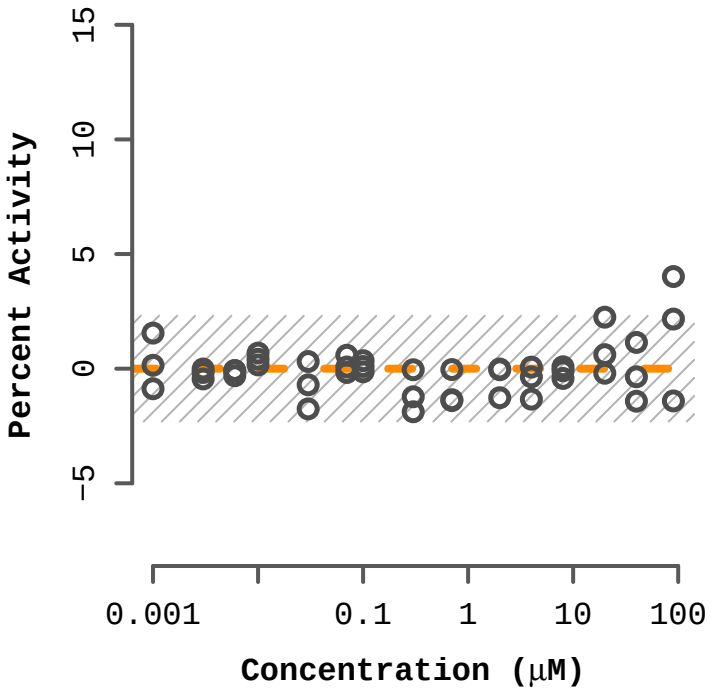
NAME: Tripropylene glycol monomethyl ether
CHID: 29329 **CASRN:** 25498-49-1
SPID(S): Tox21_300370
M4ID: 12478762 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	252.6	NA	NA
PROB:	1	NA	NA
RMSE:	54.91	NA	NA

MAX_MEAN: 97.8 **MAX_MED:** 0.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

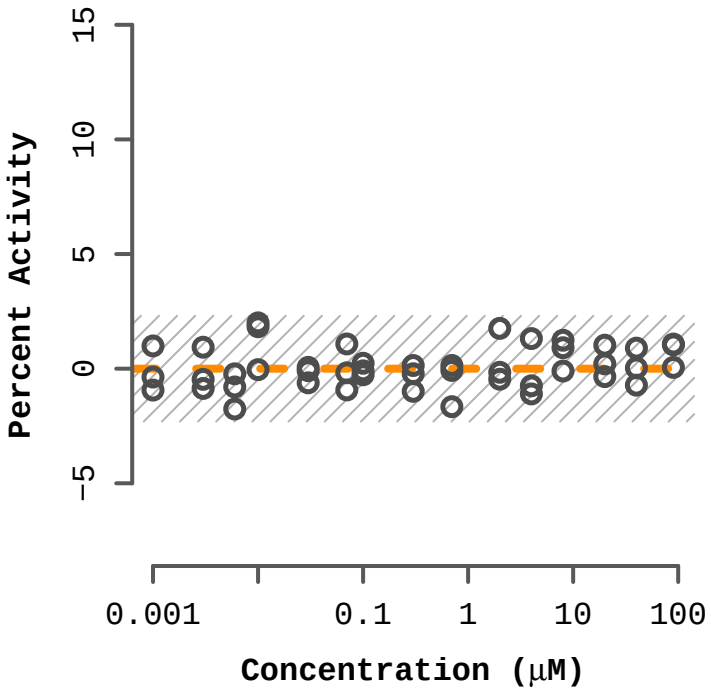
NAME: Tripropylene glycol monomethyl ether
CHID: 29329 **CASRN:** 25498-49-1
SPID(S): Tox21_201437
M4ID: 12480815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

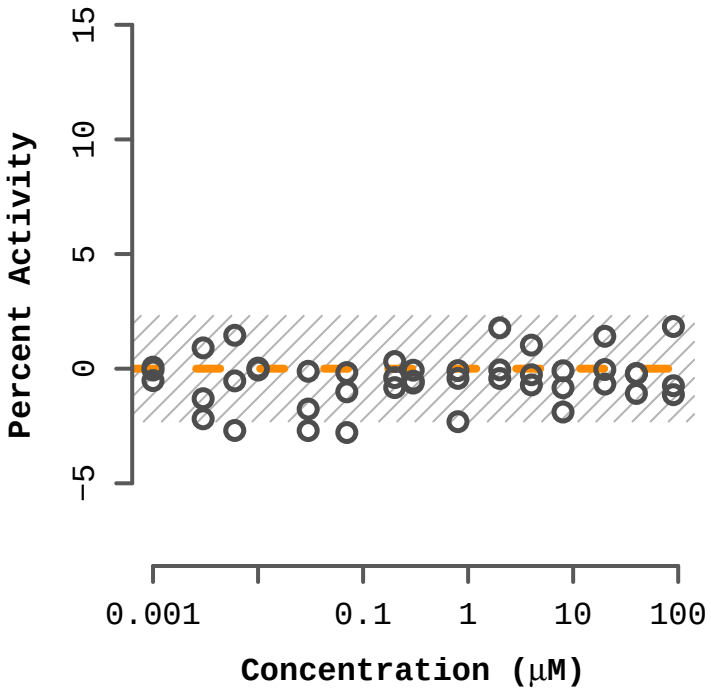
NAME: 2-Pentyl-2-cyclopenten-1-one
CHID: 29331 **CASRN:** 25564-22-1
SPID(S): Tox21_303448
M4ID: 12475692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

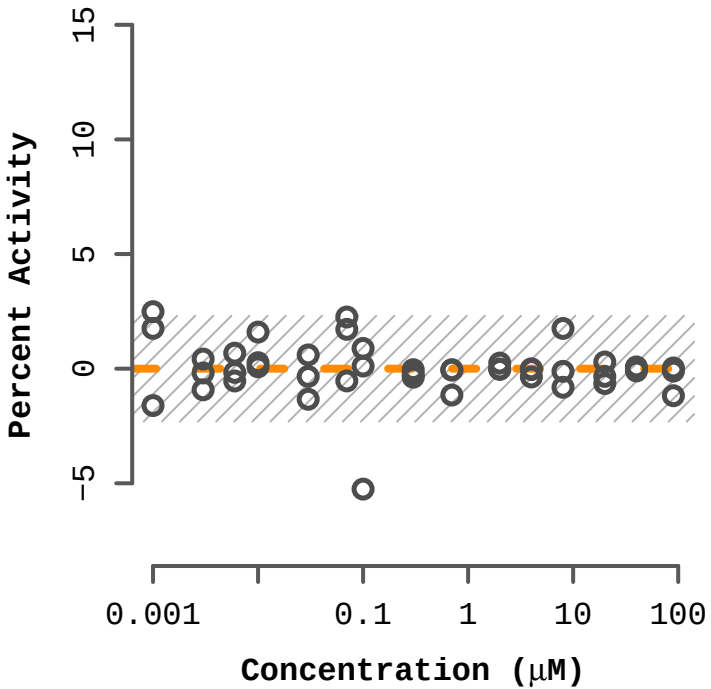
NAME: 2-Pentyl-2-cyclopenten-1-one
CHID: 29331 **CASRN:** 25564-22-1
SPID(S): Tox21_201738
M4ID: 12480514

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.435 **MAX_MED:** 0.00952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

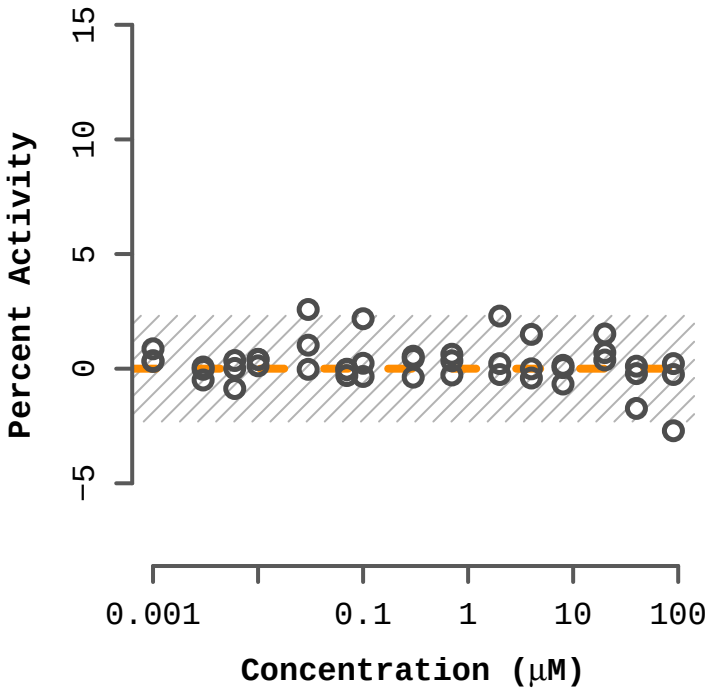
NAME: 1-Bromo-4-methoxy-2-methylbenzene
CHID: 29338 **CASRN:** 27060-75-9
SPID(S): Tox21_200480
M4ID: 12481772

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

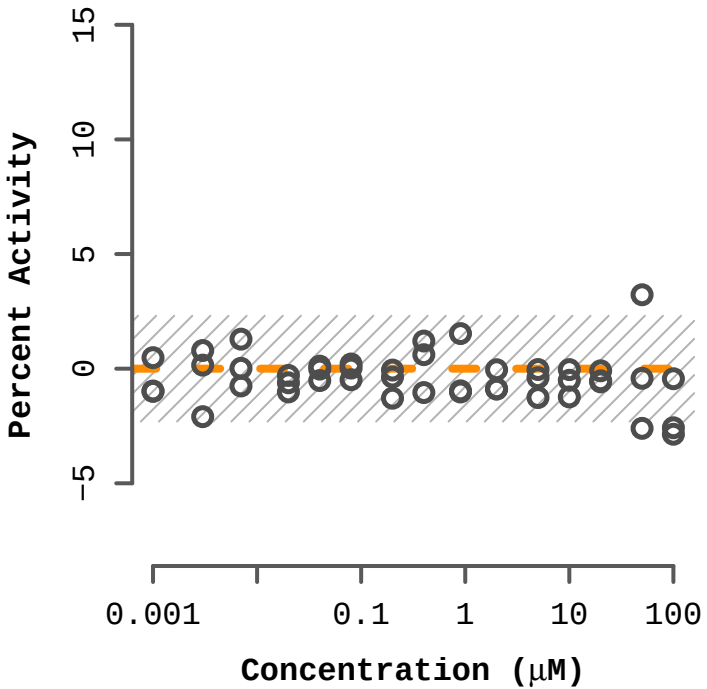
NAME: 1-Cedr-8-en-9-ylethanone
CHID: 29353 **CASRN:** 32388-55-9
SPID(S): Tox21_303481
M4ID: 12475660

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

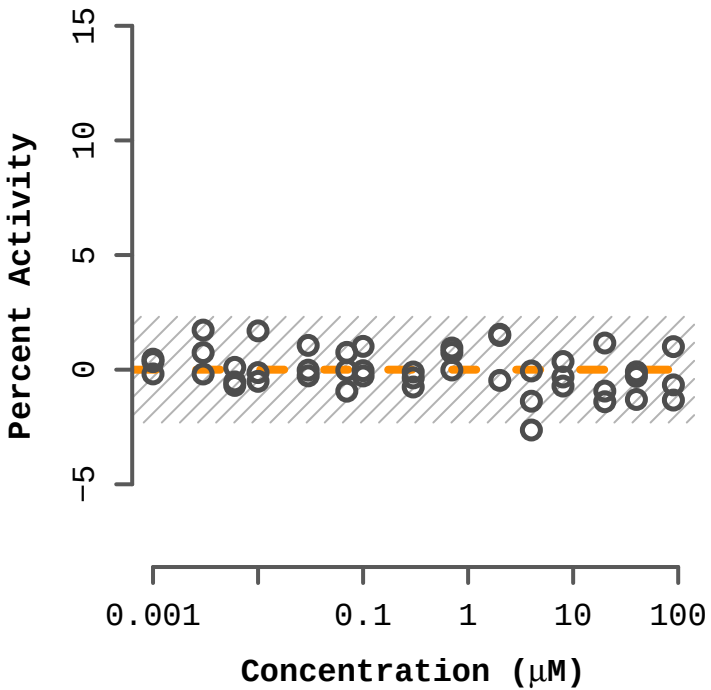
NAME: 1-Cedr-8-en-9-ylethanone
CHID: 29353 **CASRN:** 32388-55-9
SPID(S): Tox21_202194
M4ID: 12480058

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.26 **MAX_MED:** 0.612 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

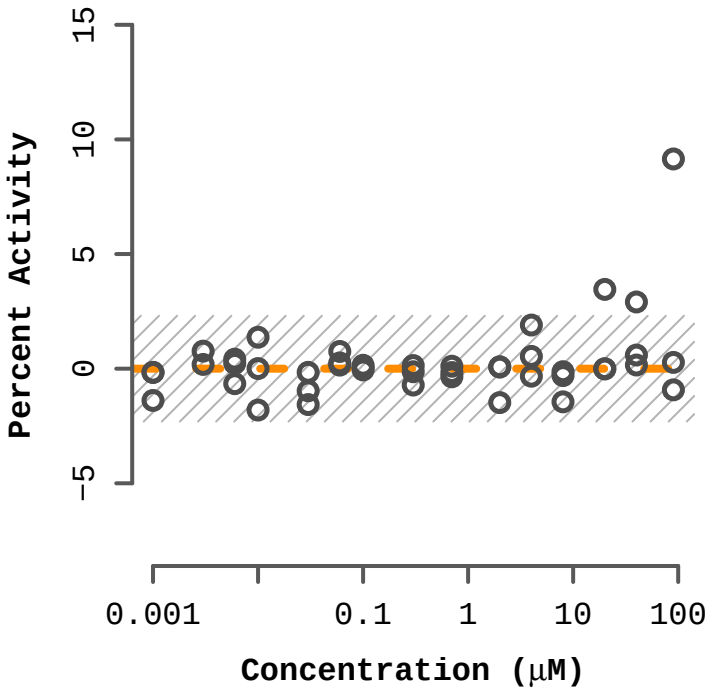
NAME: 1-Methoxy-2-propylamine
CHID: 29359 **CASRN:** 37143-54-7
SPID(S): Tox21_303553
M4ID: 12475592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

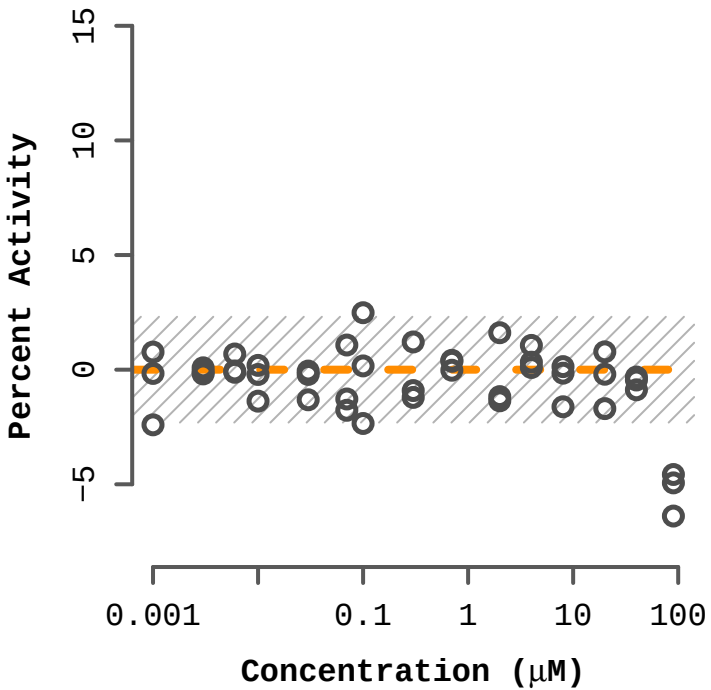
NAME: 1-Methoxy-2-propylamine
CHID: 29359 **CASRN:** 37143-54-7
SPID(S): Tox21_202050
M4ID: 12480202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 2.83 **MAX_MED:** 0.596 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4,15,15−Tetraethoxy−3,16−dioxa−8,9,10,11−tet

CHID: 29362 **CASRN:** 40372−72−3

SPID(S): Tox21_202578

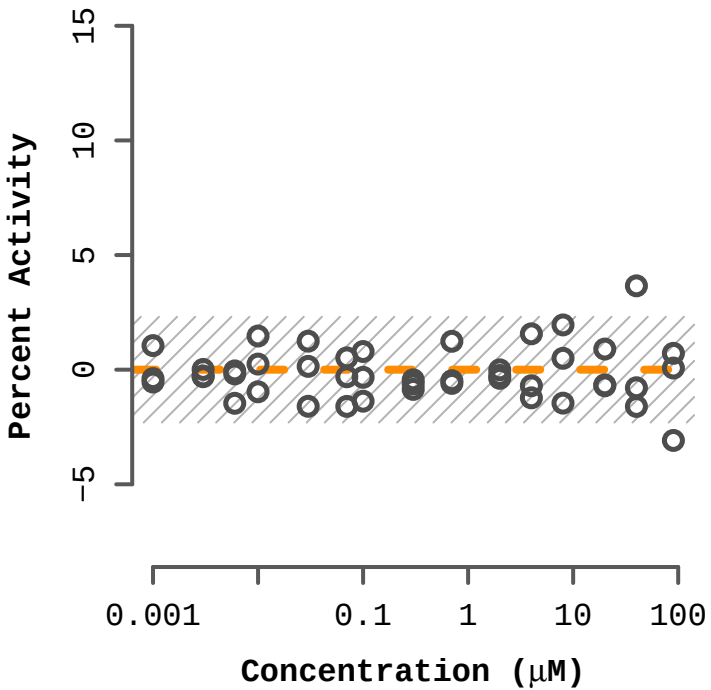
M4ID: 12479674

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 0.495 **MAX_MED:** 0.366 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

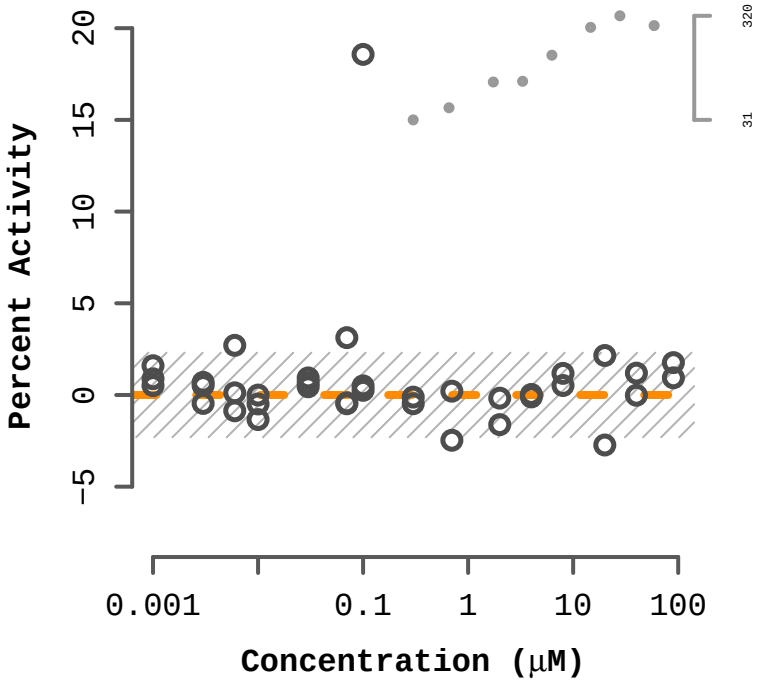
NAME: 4-Methoxy-2-methyl-N-phenylaniline
CHID: 29364 **CASRN:** 41317-15-1
SPID(S): Tox21_303502
M4ID: 12475640

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.423 **MAX_MED:** 0.496 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

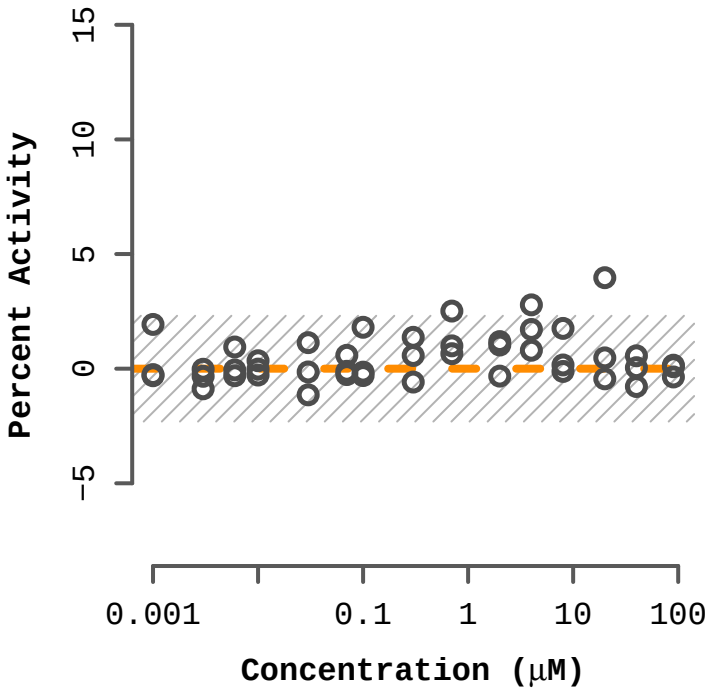
NAME: 4-Methoxy-2-methyl-N-phenylaniline
CHID: 29364 **CASRN:** 41317-15-1
SPID(S): Tox21_201840
M4ID: 12480412 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	460	NA	NA
PROB:	1	NA	NA
RMSE:	88.02	NA	NA

MAX_MEAN: 105 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

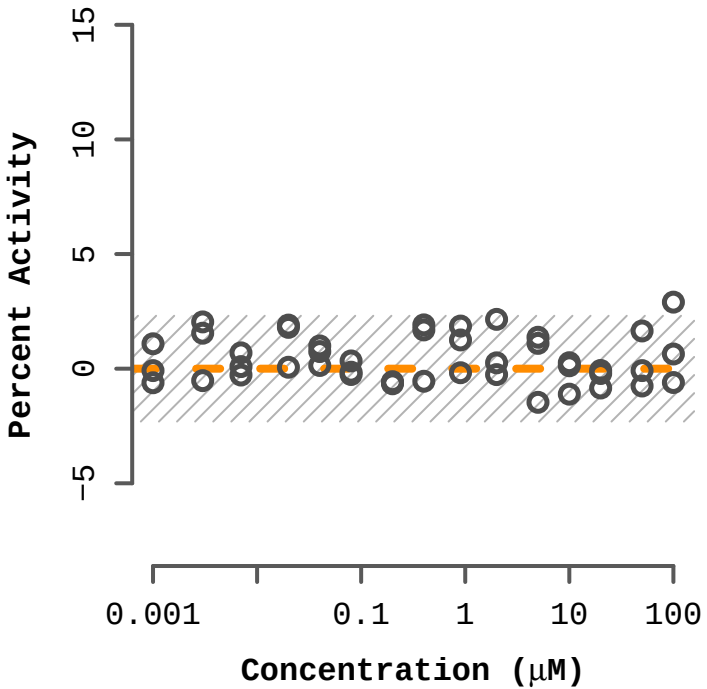
NAME: Vinyl neodecanoate
CHID: 29369 **CASRN:** 51000-52-3
SPID(S): Tox21_301396
M4ID: 12477737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

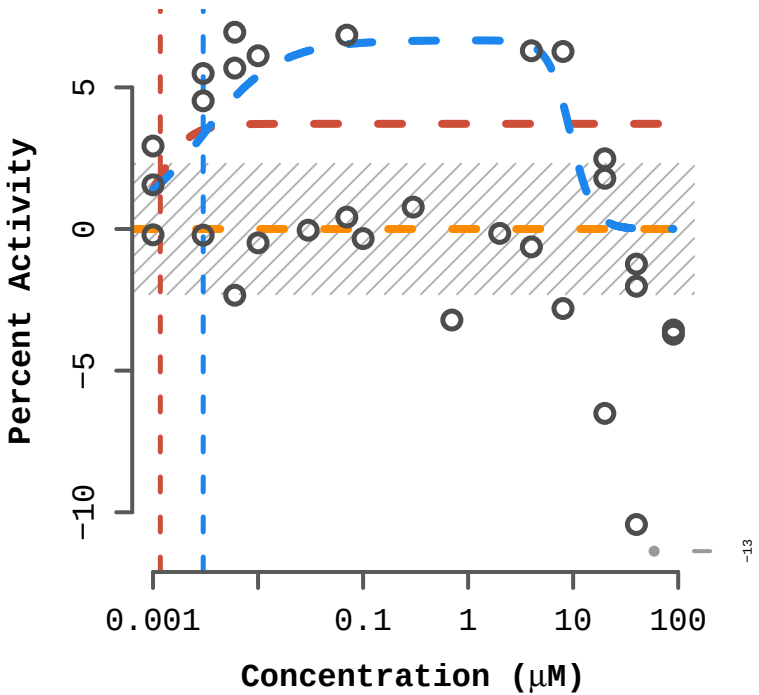
NAME: Alkyl (C8,C10) glycidyl ether
CHID: 29474 **CASRN:** 68609-96-1
SPID(S): Tox21_200176
M4ID: 12482076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dichloro-5-(trichloromethyl)pyridine
CHID: 29534 CASRN: 69045-83-6
SPID(S): Tox21_301744
M4ID: 12477389 BRK

HILL MODEL (in red):

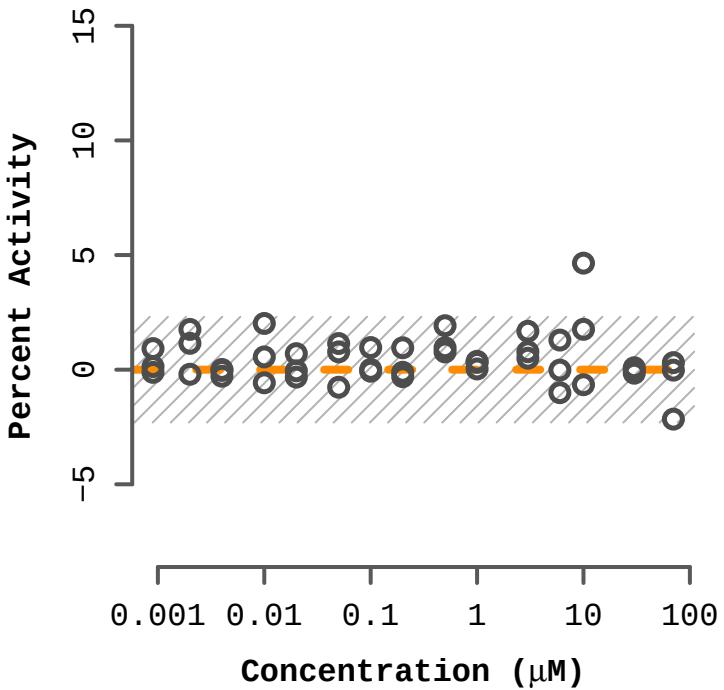
	tp	ga	gw
val:	3.71	-2.93	3
sd:	1.01	0.469	10.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.66	-2.52	1.22	0.977	4.05
sd:	1.36	0.378	1.19	0.222	7.49

	CNST	HILL	GNLS
AIC:	303.74	296.36	282.84
PROB:	0	0	1
RMSE:	6.53	5.8	4.81

MAX_MEAN: 7.06 MAX_MED: 9.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

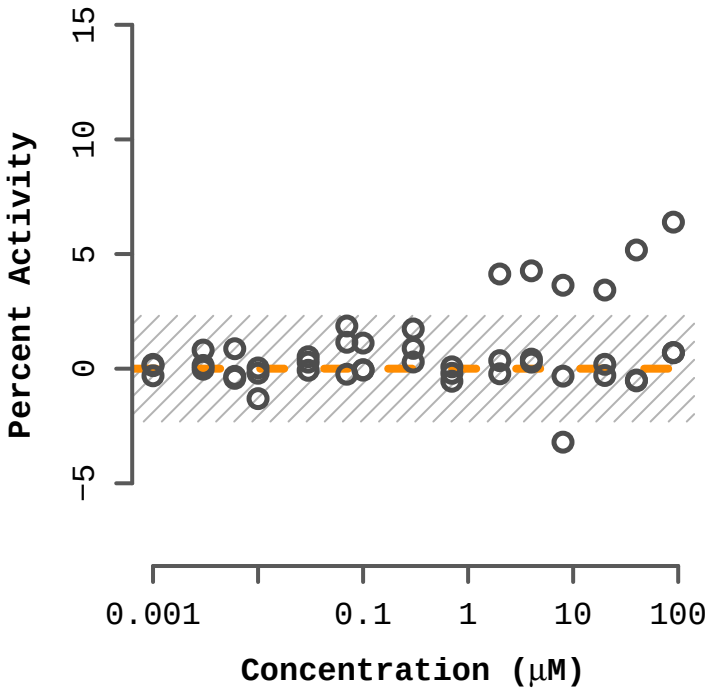
NAME: Diazolidinyl urea
CHID: 29559 **CASRN:** 78491-02-8
SPID(S): Tox21_303365
M4ID: 12475770

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

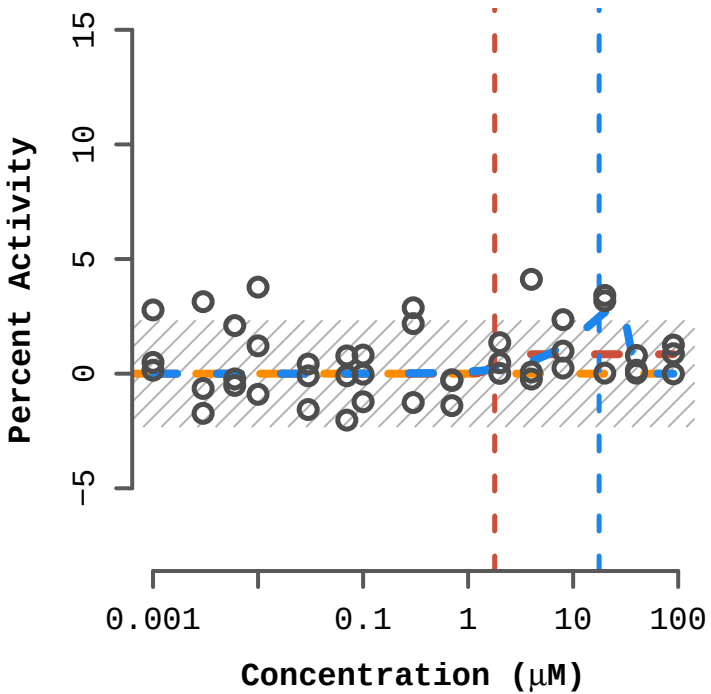
NAME: Diazolidinyl urea
CHID: 29559 **CASRN:** 78491-02-8
SPID(S): Tox21_202068
M4ID: 12480184

HILL MODEL: Not applicable.

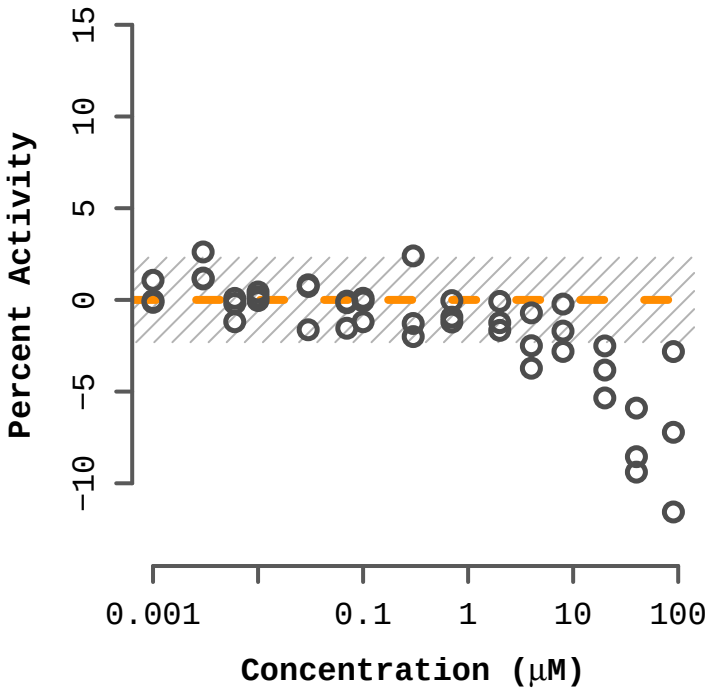
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 2.6 **MAX_MED:** 1.15 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phthalic acid, diundecyl ester, branched and l
CHID:    29565   CASRN: 85507-79-5
SPID(S): Tox21_302418
M4ID:    12476715

HILL MODEL (in red):
      tp       ga       gw
val:  0.848    0.253    8
sd:   0.355    0.324    47.7

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.94     1.25     1.4      1.52     12.8
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  172.45      171.61      172.93
PROB: 0.3         0.46        0.24
RMSE: 1.63        1.49        1.47

MAX_MEAN: 2.21      MAX_MED: 3.18      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

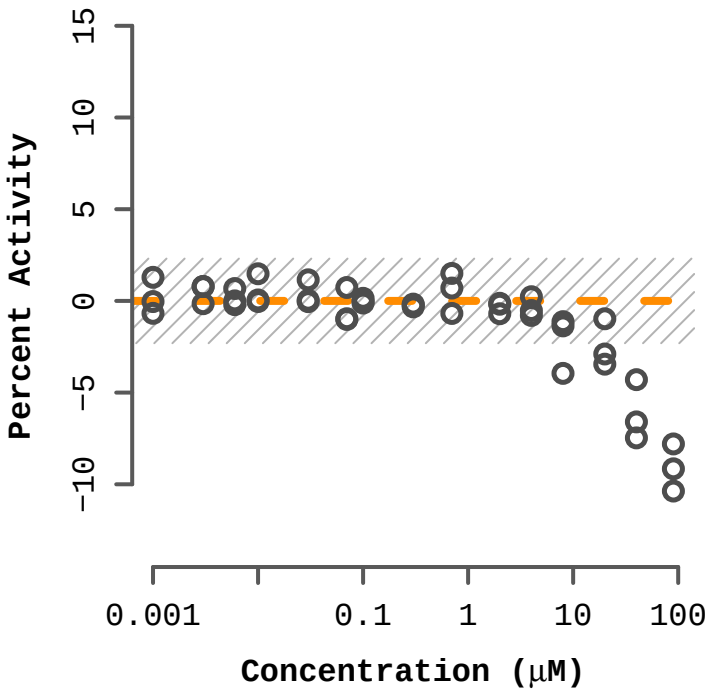
NAME: Benoxacor
CHID: 29572 **CASRN:** 98730-04-2
SPID(S): Tox21_303359
M4ID: 12475775

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.44	NA	NA
PROB:	1	NA	NA
RMSE:	3.36	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

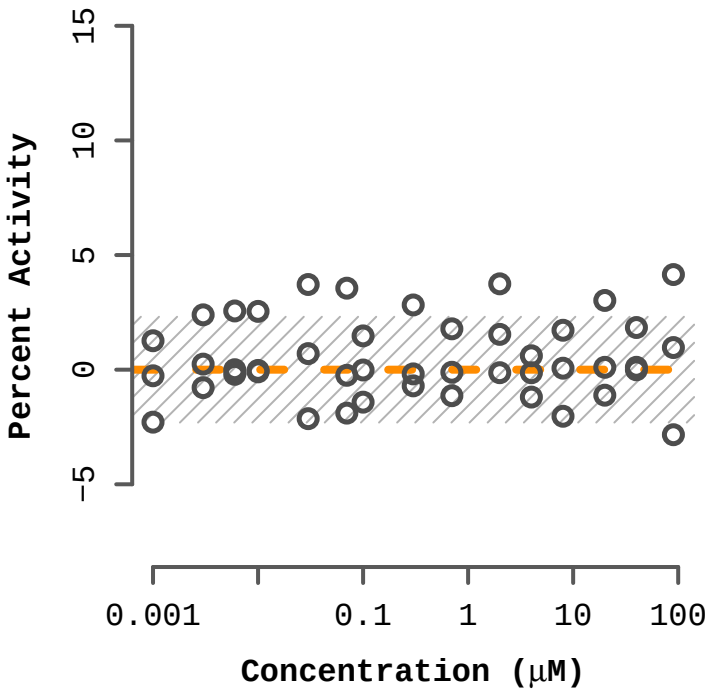
NAME: Benoxacor
CHID: 29572 **CASRN:** 98730-04-2
SPID(S): Tox21_202216
M4ID: 12480036

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.93	NA	NA
PROB:	1	NA	NA
RMSE:	3.07	NA	NA

MAX_MEAN: 0.506 **MAX_MED:** 0.782 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

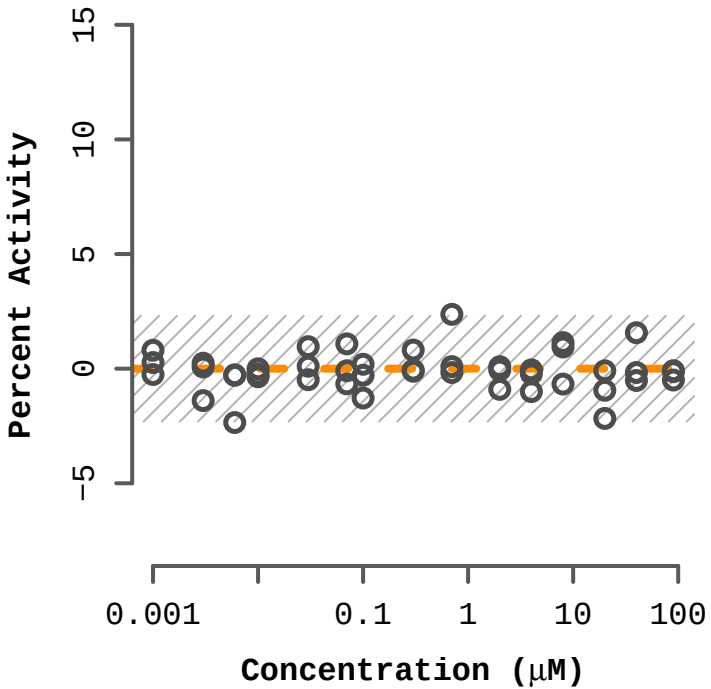
NAME: {4-[(Ethenyloxy)methyl]cyclohexyl}methanol
CHID: 29575 **CASRN:** 114651-37-5
SPID(S): Tox21_303607
M4ID: 12475538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

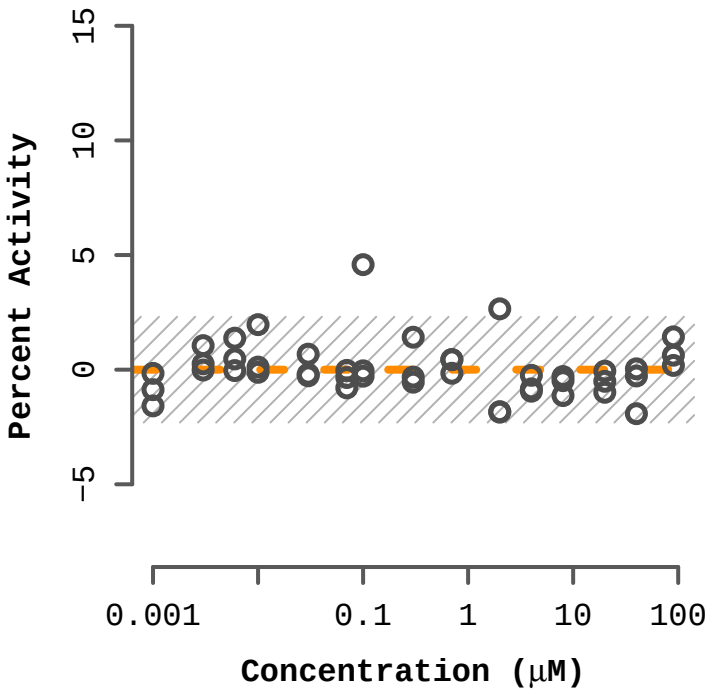
NAME: Methacrylamide
CHID: 29600 **CASRN:** 79-39-0
SPID(S): Tox21_300001
M4ID: 12479129

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.766 **MAX_MED:** 0.947 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

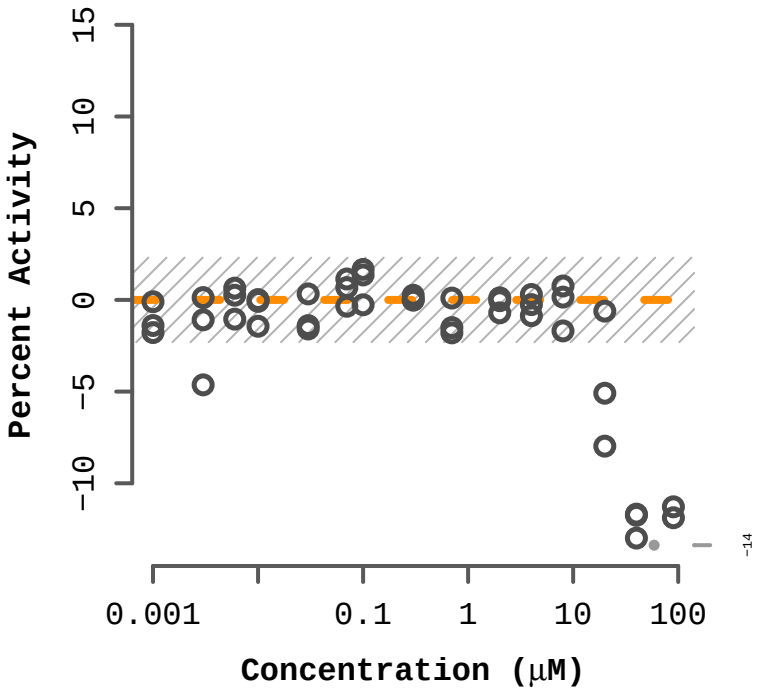
NAME: Methacrylamide
CHID: 29600 CASRN: 79-39-0
SPID(S): Tox21_202281
M4ID: 12479971

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.42 MAX_MED: 0.632 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

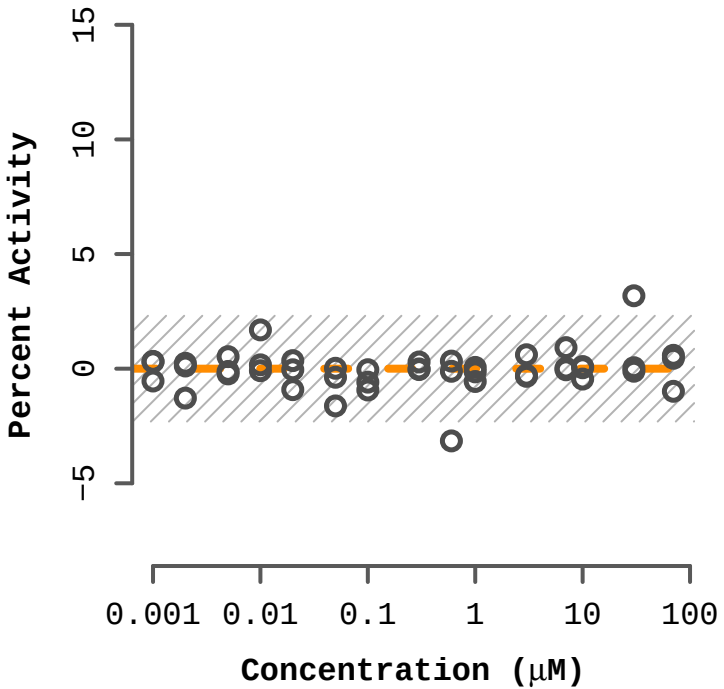
NAME: 4,4'-Butane-1,1-diylbis(2-tert-butyl-5-methylpl
CHID: 29602 **CASRN:** 85-60-9
SPID(S): Tox21_200749
M4ID: 12481503 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.87	NA	NA
PROB:	1	NA	NA
RMSE:	4.8	NA	NA

MAX_MEAN: 0.921 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

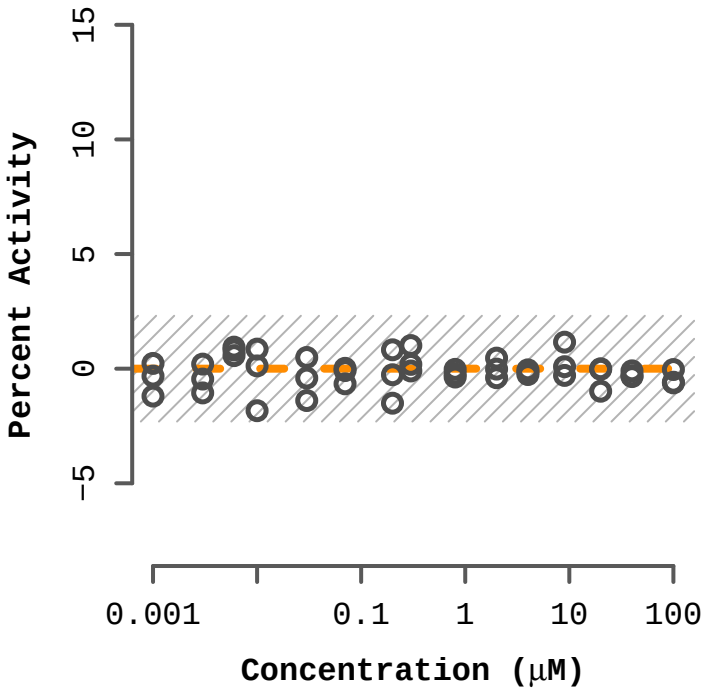
NAME: 1,2−Benzenedicarbonitrile
CHID: 29604 **CASRN:** 91−15−6
SPID(S): Tox21_200999
M4ID: 12481253

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

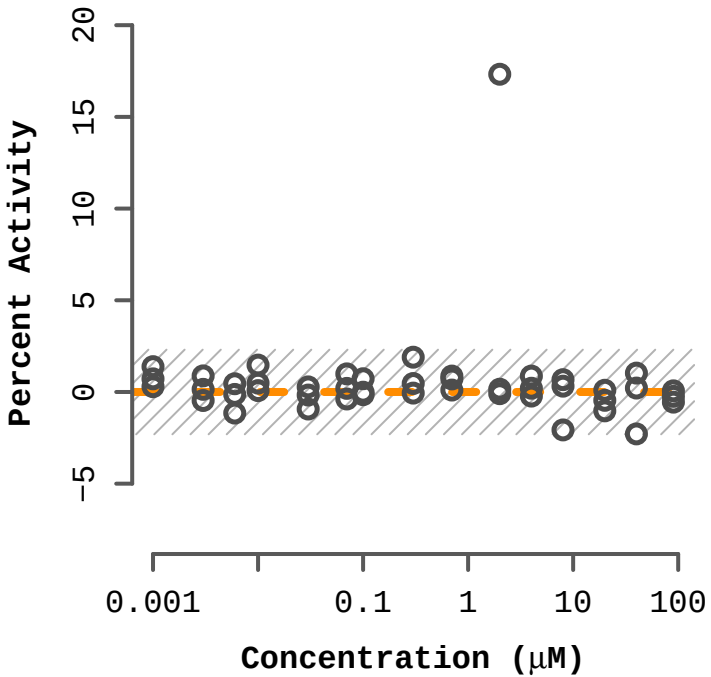
NAME: 3-Methylbut-2-enal
CHID: 29606 **CASRN:** 107-86-8
SPID(S): Tox21_200149
M4ID: 12482103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.776 **MAX_MED:** 0.815 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

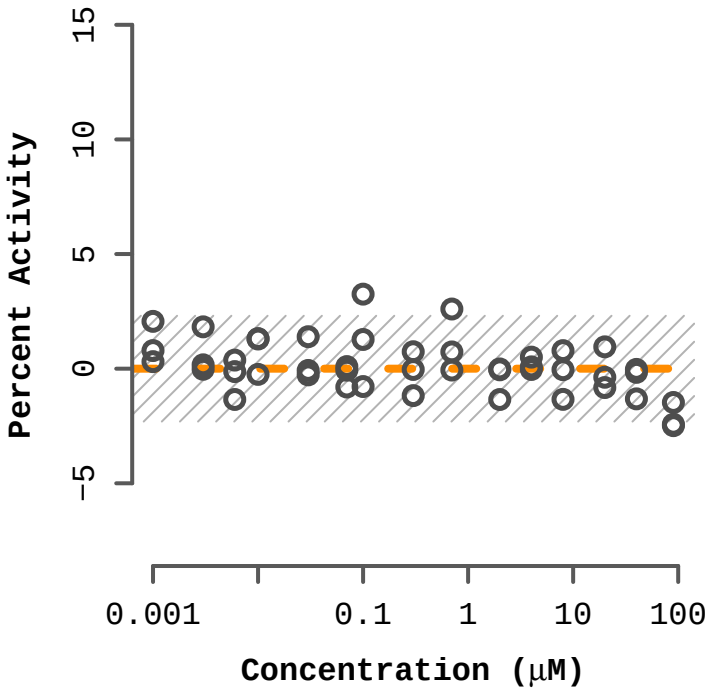
NAME: Triethylene glycol dimethacrylate
CHID: 29607 **CASRN:** 109-16-0
SPID(S): Tox21_303364
M4ID: 12475771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.35	NA	NA
PROB:	1	NA	NA
RMSE:	2.7	NA	NA

MAX_MEAN: 5.8 **MAX_MED:** 0.718 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

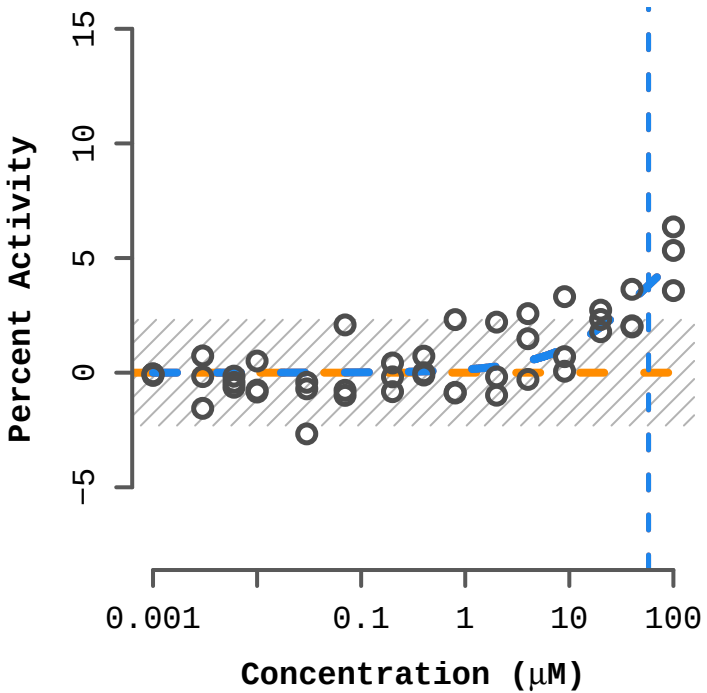
NAME: Triethylene glycol dimethacrylate
CHID: 29607 **CASRN:** 109-16-0
SPID(S): Tox21_202238
M4ID: 12480014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Vinyl isobutyl ether
CHID: 29608 CASRN: 109-53-5
SPID(S): Tox21_202579
M4ID: 12479673

HILL MODEL (in red):

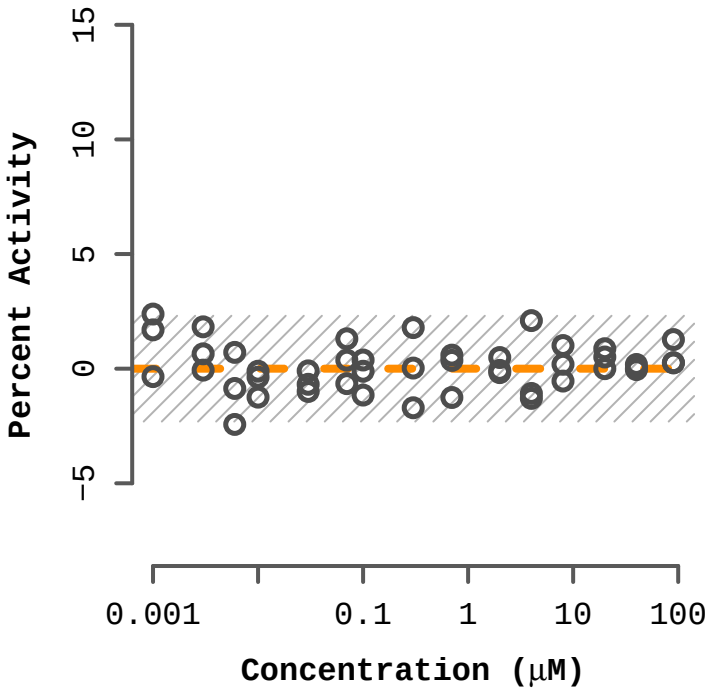
	tp	ga	gw
val:	7.63	1.76	0.984
sd:	3.98	0.472	0.349

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.63	1.76	0.984	3.66	11.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	185.28	144.39	148.39
PROB:	0	0.88	0.12
RMSE:	1.96	1.08	1.08

MAX_MEAN: 5.09 MAX_MED: 5.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

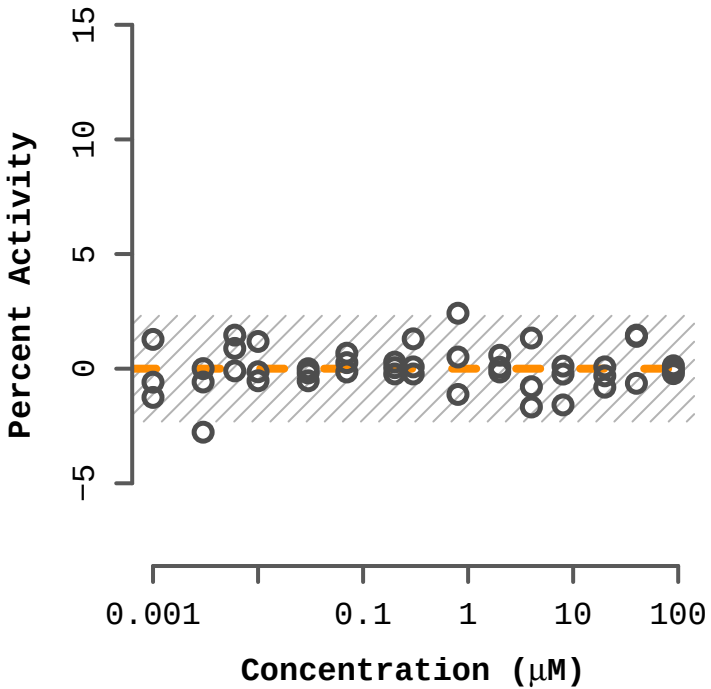
NAME: Triethylene glycol dibenzoate
CHID: 29611 **CASRN:** 120-56-9
SPID(S): Tox21_301896
M4ID: 12477237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

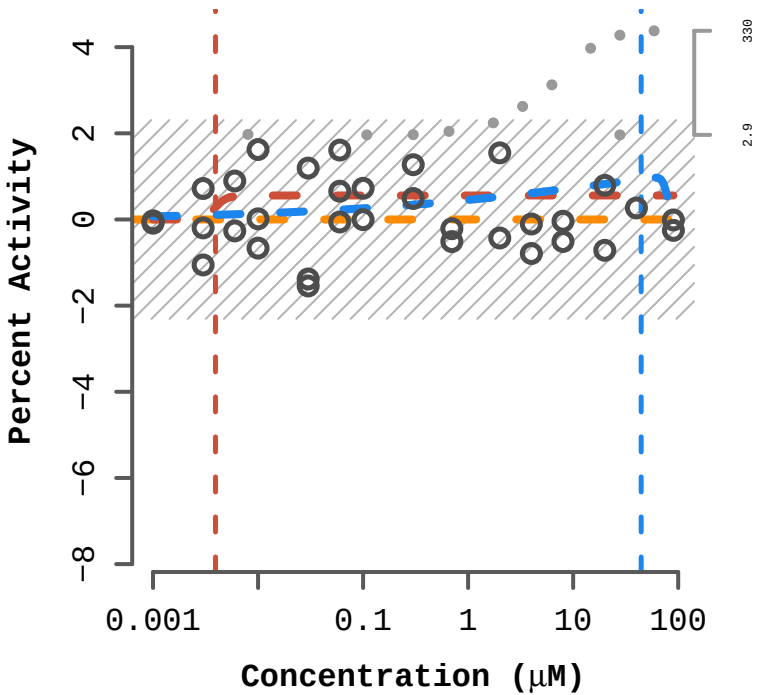
NAME: Limonene
CHID: 29612 **CASRN:** 138-86-3
SPID(S): Tox21_303409
M4ID: 12475730

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.752 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Limonene
CHID: 29612 CASRN: 138-86-3
SPID(S): Tox21_201818
M4ID: 12480434 BRK

HILL MODEL (in red):

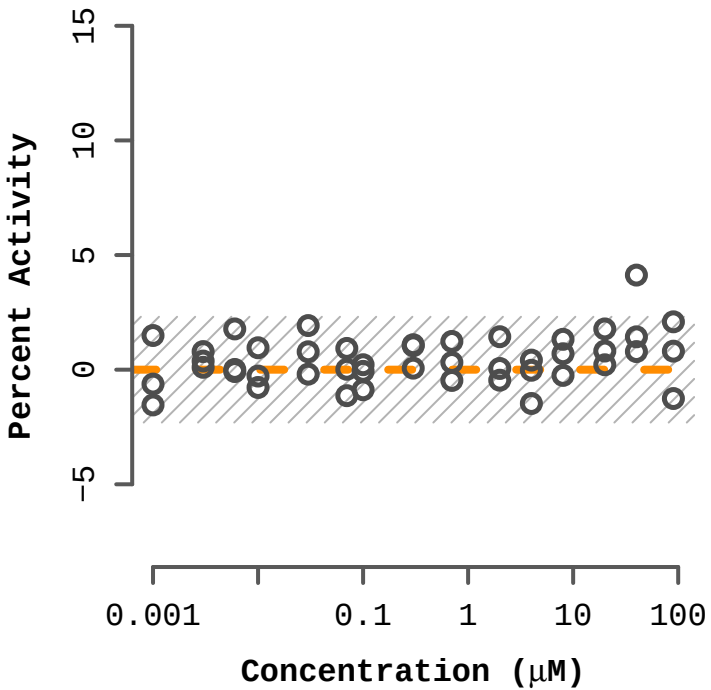
	tp	ga	gw
val:	0.557	−2.41	8
sd:	0.427	0.462	24.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.87	1.65	0.3	1.9	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	403.52	407.77	412.35
PROB:	0.88	0.11	0.01
RMSE:	83.5	83.31	83.3

MAX_MEAN: 109 MAX_MED: 2.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

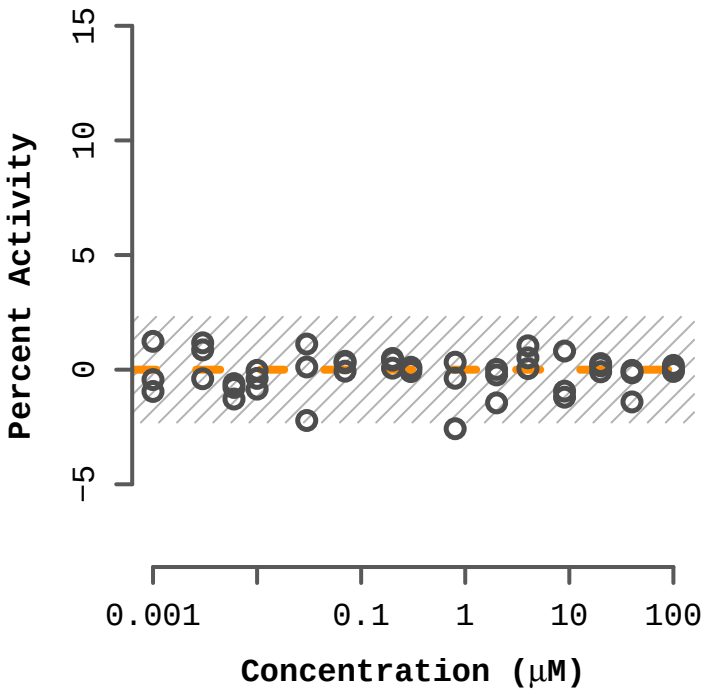
NAME: Imidazole
CHID: 29616 **CASRN:** 288-32-4
SPID(S): Tox21_303345
M4ID: 12475788

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 2.12 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

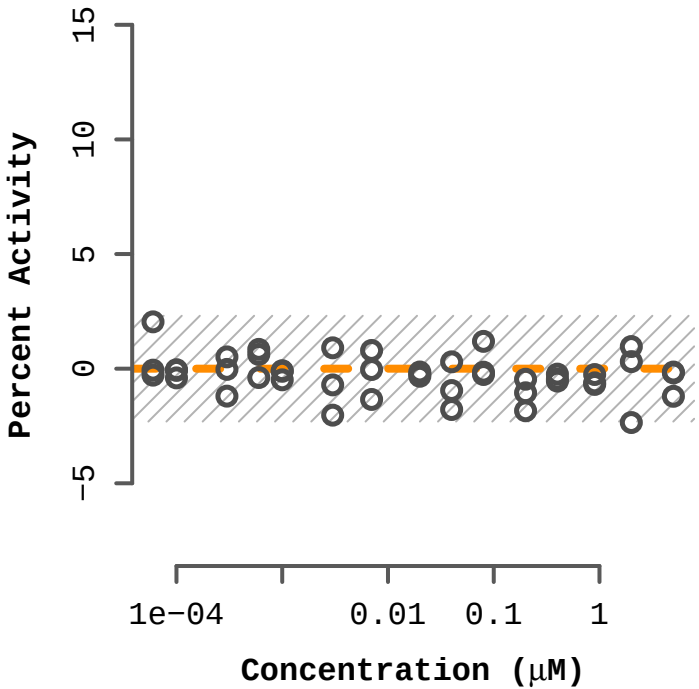
NAME: Imidazole
CHID: 29616 **CASRN:** 288-32-4
SPID(S): Tox21_201504
M4ID: 12480748

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.864 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

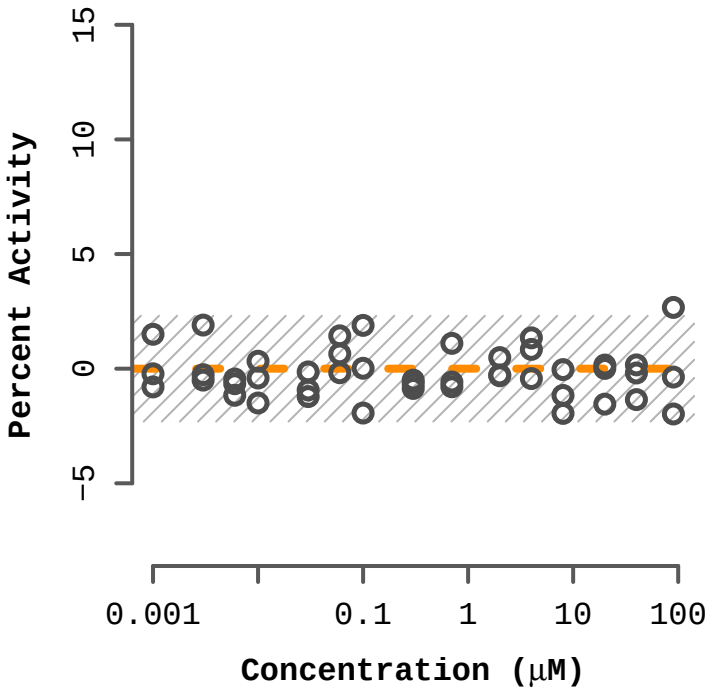
NAME: Potassium D−gluconate
CHID: 29617 **CASRN:** 299−27−4
SPID(S): Tox21_202774
M4ID: 12479478

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.567 **MAX_MED:** 0.623 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

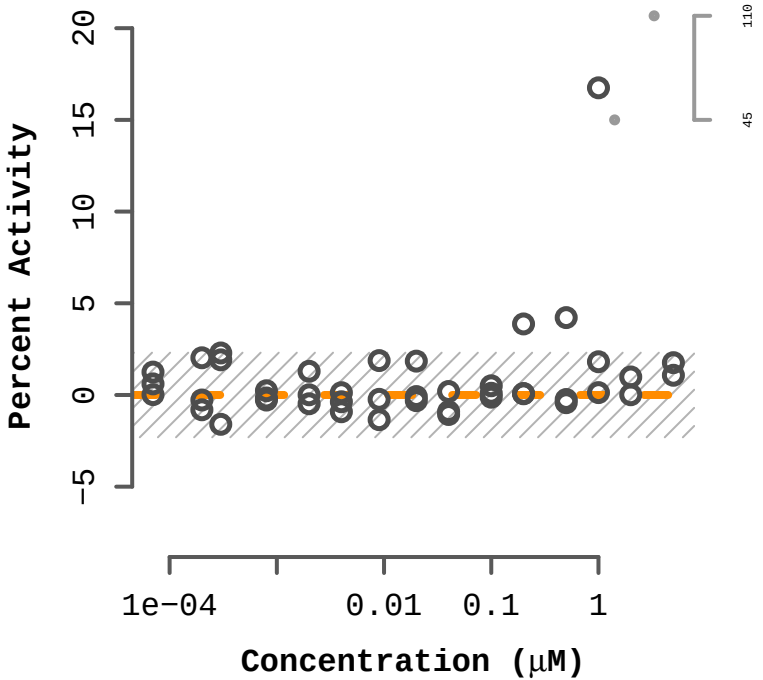
NAME: Potassium thiocyanate
CHID: 29619 CASRN: 333-20-0
SPID(S): Tox21_200481
M4ID: 12481771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.636 MAX_MED: 0.842 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

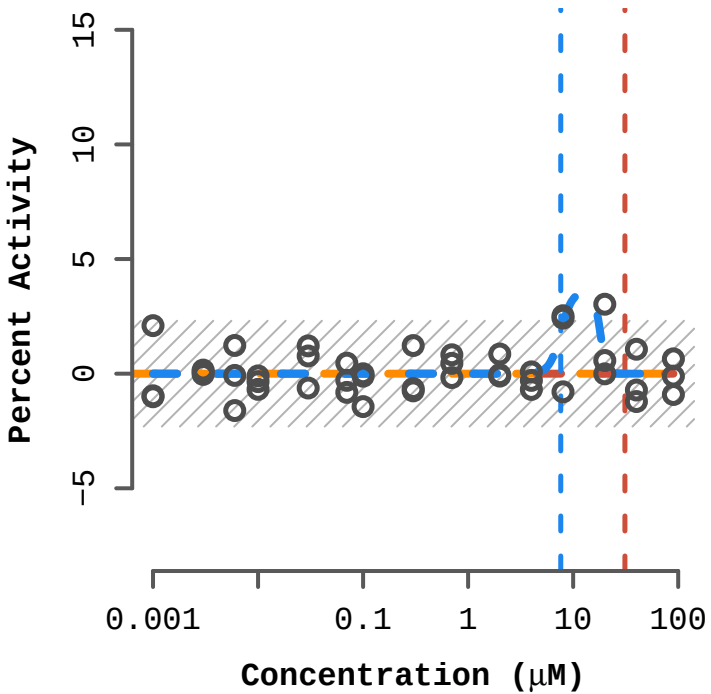
NAME: Formic acid, potassium salt
CHID: 29626 CASRN: 590-29-4
SPID(S): Tox21_202775
M4ID: 12479477 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	236.41	NA	NA
PROB:	1	NA	NA
RMSE:	18.08	NA	NA

MAX_MEAN: 38 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxypropyl 2-methylacrylate
CHID: 29629 CASRN: 923-26-2
SPID(S): Tox21_200694
M4ID: 12481558

HILL MODEL (in red):

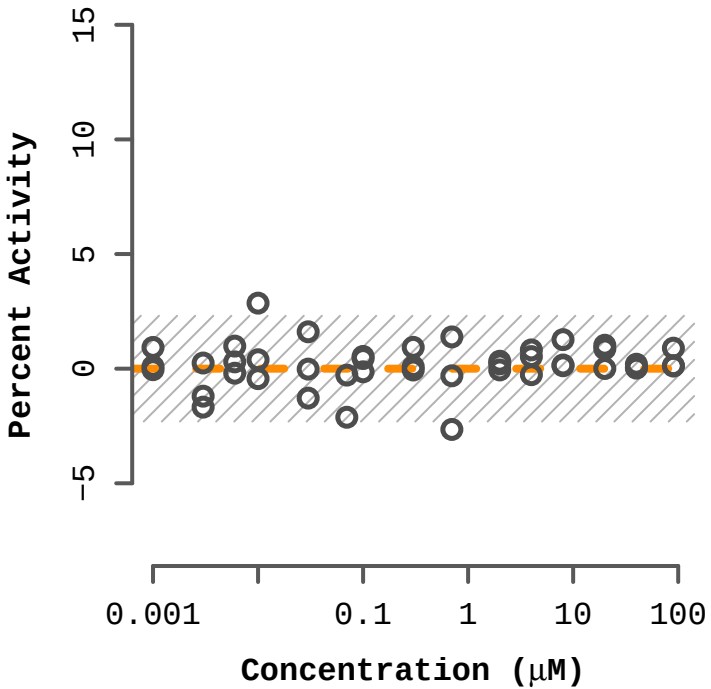
	tp	ga	gw
val:	7.92e-09	1.49	1.49
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.62	0.882	8	1.26	14.6
sd:	9.77	0.347	9.15	0.21	57.3

	CNST	HILL	GNLS
AIC:	130.81	136.81	133.32
PROB:	0.75	0.04	0.21
RMSE:	1.03	1.03	0.95

MAX_MEAN: 1.39 MAX_MED: 2.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

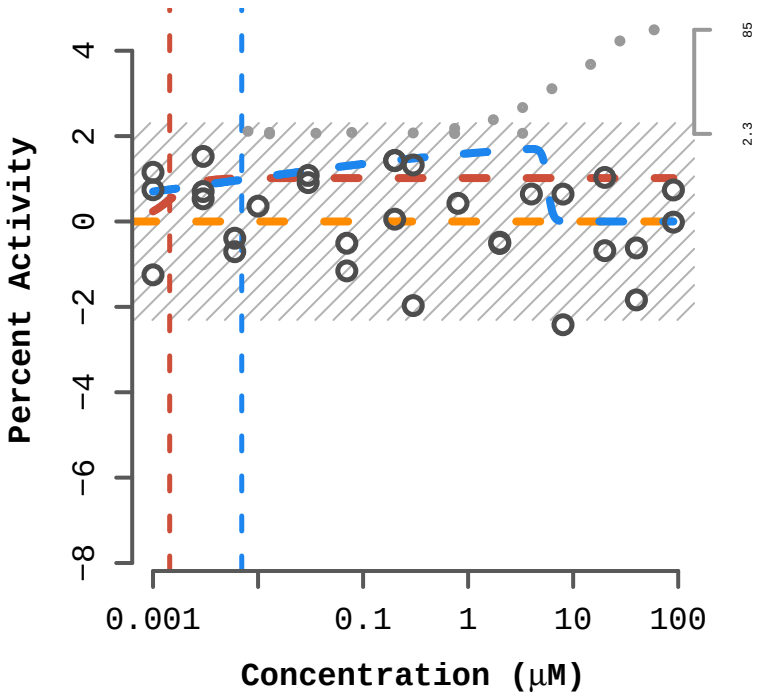
NAME: 1,3−Benzenedimethanamine
CHID: 29649 **CASRN:** 1477−55−0
SPID(S): Tox21_303362
M4ID: 12475773

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.94 **MAX_MED:** 0.866 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3−Benzenedimethanamine
CHID: 29649 CASRN: 1477−55−0
SPID(S): Tox21_200766
M4ID: 12481486 BRK

HILL MODEL (in red):

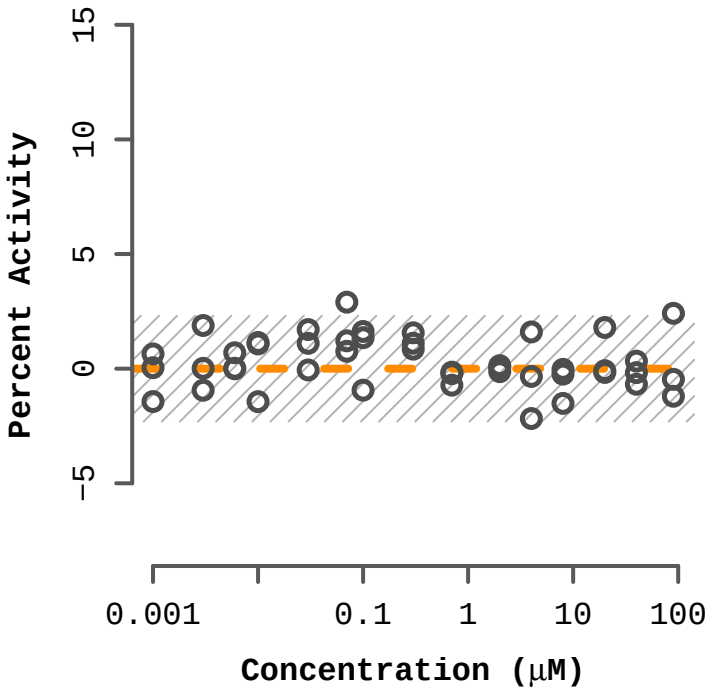
	tp	ga	gw
val:	1.02	−2.84	3.27
sd:	0.494	1.1	15.2

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.95	−2.16	0.3	0.757	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	323.19	324.49	326.61
PROB:	0.59	0.31	0.11
RMSE:	20.27	19.93	20.18

MAX_MEAN: 28.4 MAX_MED: 2.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

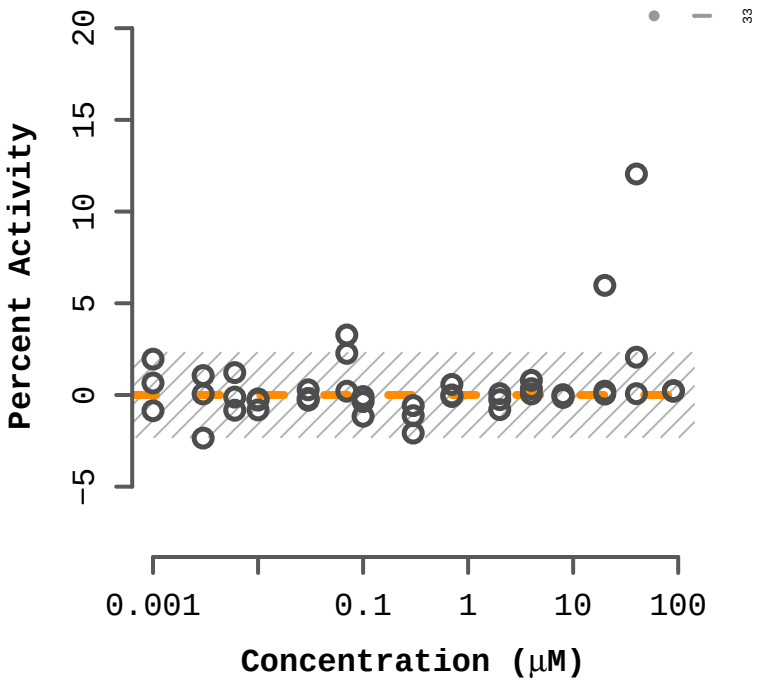
NAME: Menthol
CHID: 29650 **CASRN:** 1490-04-6
SPID(S): Tox21_303464
M4ID: 12475676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

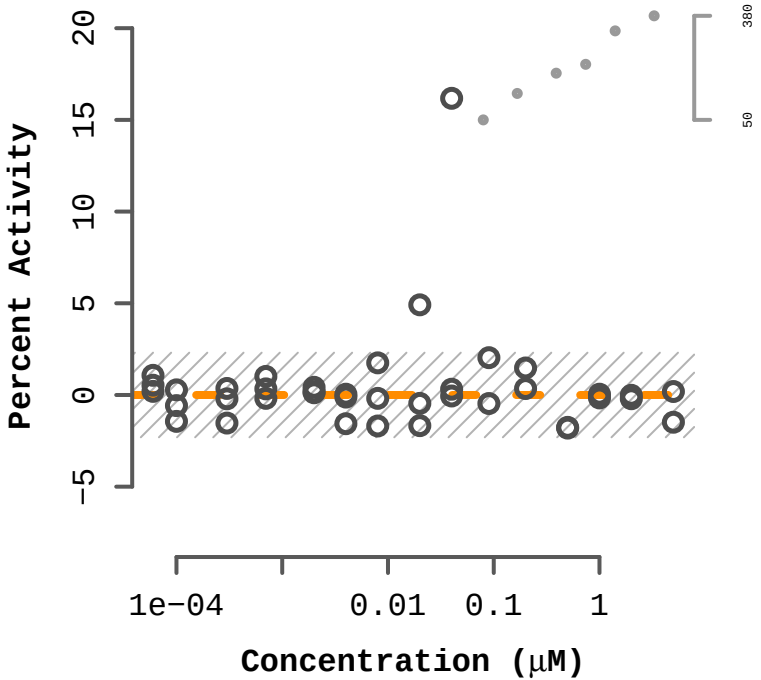
NAME: Menthol
CHID: 29650 CASRN: 1490-04-6
SPID(S): Tox21_200010
M4ID: 12482242 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.14	NA	NA
PROB:	1	NA	NA
RMSE:	5.38	NA	NA

MAX_MEAN: 11.1 MAX_MED: 2.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

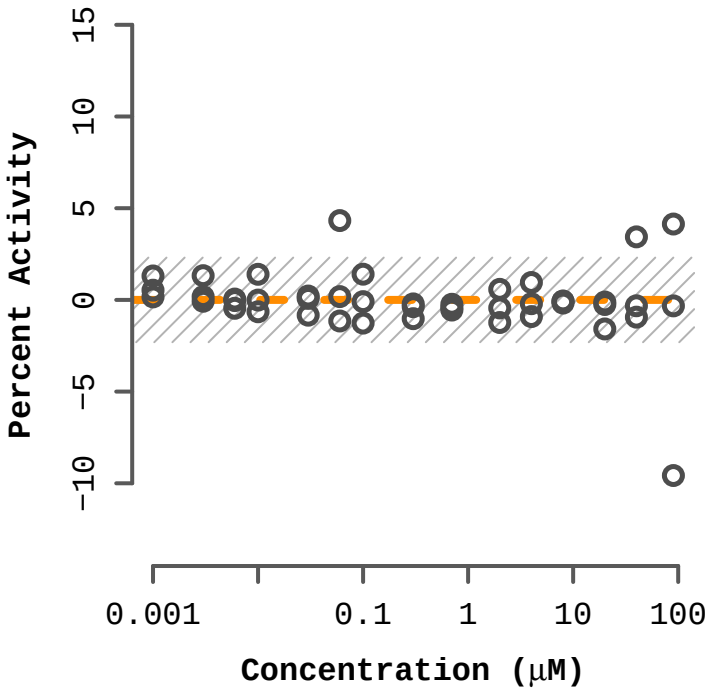
NAME: Carbonic acid, strontium salt (1:1)
CHID: 29651 **CASRN:** 1633-05-2
SPID(S): Tox21_202776
M4ID: 12479476 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	410.91	NA	NA
PROB:	1	NA	NA
RMSE:	90.12	NA	NA

MAX_MEAN: 126 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

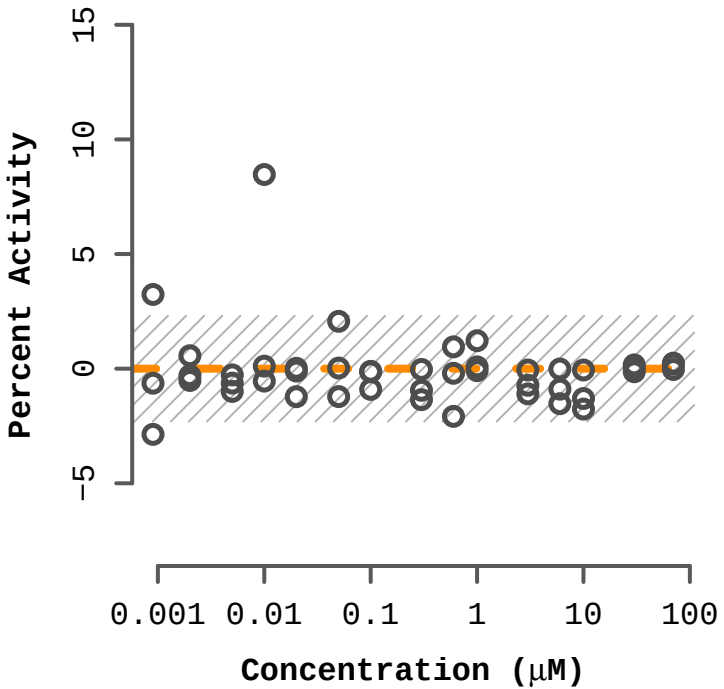
NAME: tert-Butyl acrylate
CHID: 29652 **CASRN:** 1663-39-4
SPID(S): Tox21_201117
M4ID: 12481135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.531 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

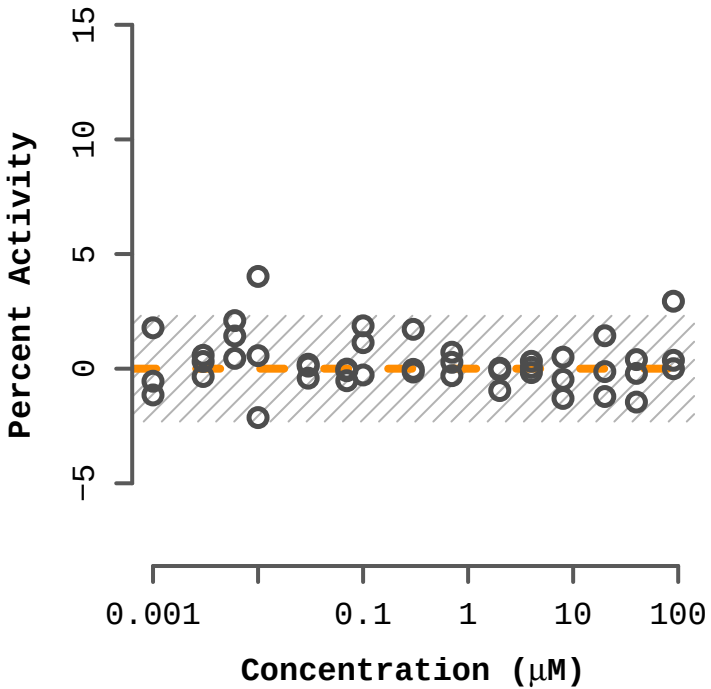
NAME: Thiocyanic acid, ammonium salt
CHID: 29653 **CASRN:** 1762-95-4
SPID(S): Tox21_301967
M4ID: 12477166

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 2.68 **MAX_MED:** 0.192 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

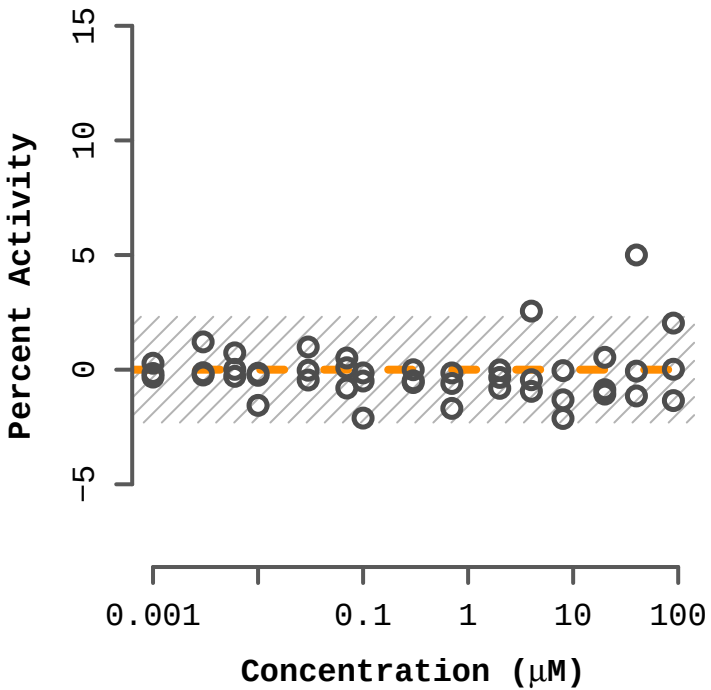
NAME: 2,2,6,6−Tetramethyl− 4−piperidinol
CHID: 29655 CASRN: 2403−88−5
SPID(S): Tox21_200165
M4ID: 12482087

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

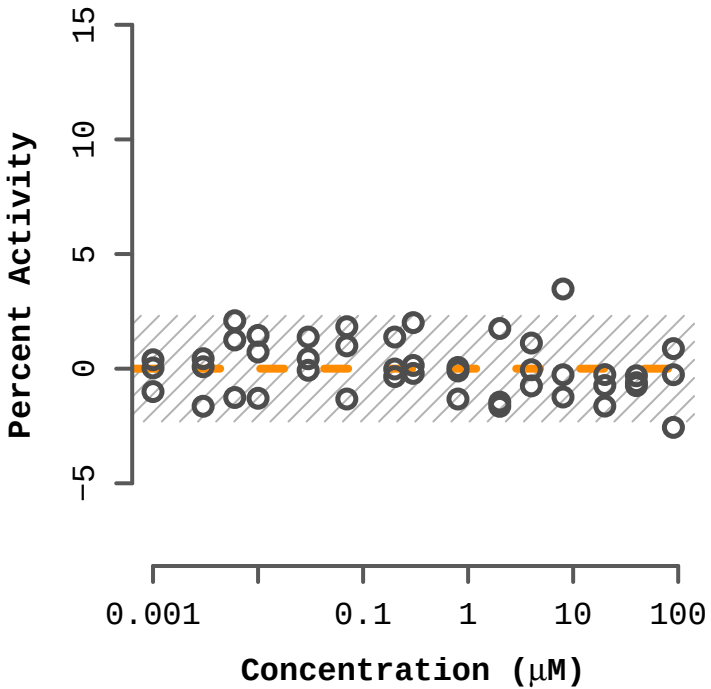
NAME: 3,5,5-Trimethyl-1-hexanol
CHID: 29661 **CASRN:** 3452-97-9
SPID(S): Tox21_303600
M4ID: 12475545

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.0867 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

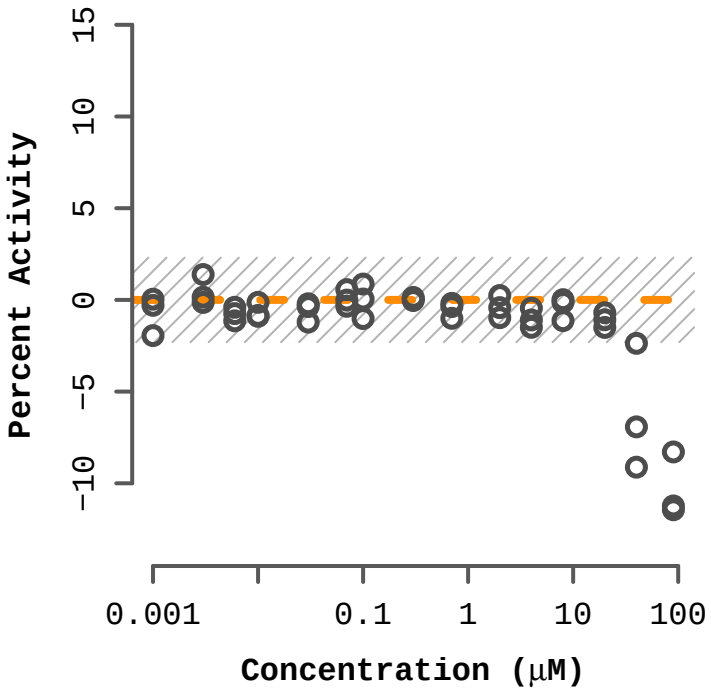
NAME: 3,5,5-Trimethyl-1-hexanol
CHID: 29661 **CASRN:** 3452-97-9
SPID(S): Tox21_202260
M4ID: 12479992

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.697 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

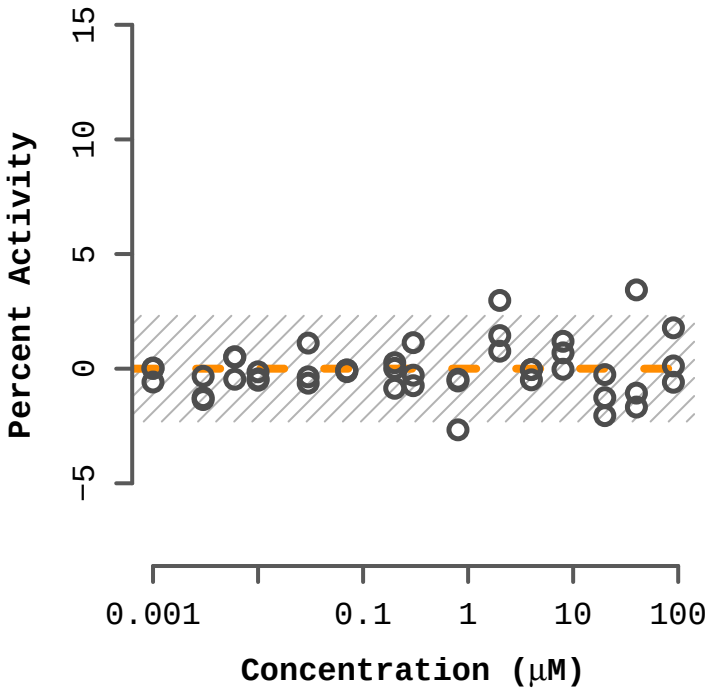
NAME: Dichloro(dioctyl)stannane
CHID: 29662 **CASRN:** 3542-36-7
SPID(S): Tox21_200482
M4ID: 12481770

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.7	NA	NA
PROB:	1	NA	NA
RMSE:	3.29	NA	NA

MAX_MEAN: 0.468 **MAX_MED:** 0.152 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

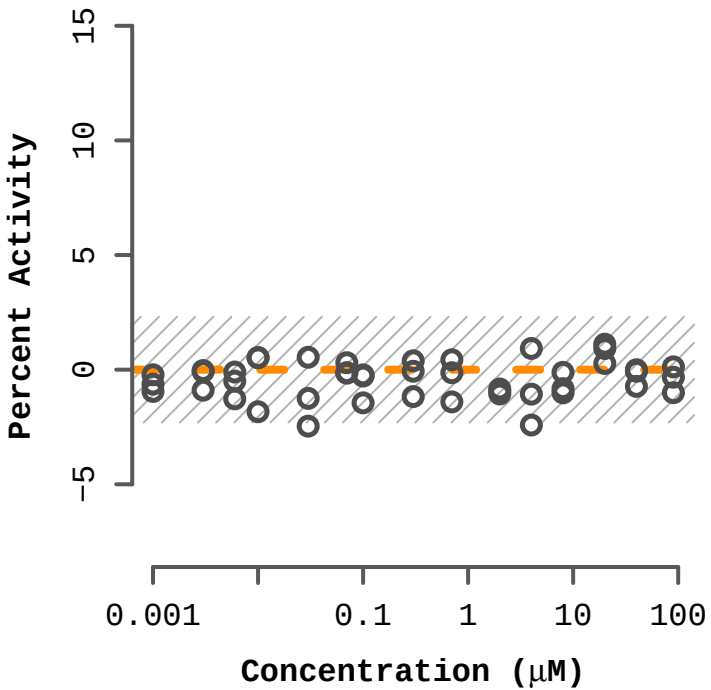
NAME: 2-Phenoxy-1-propanol
CHID: 29665 **CASRN:** 4169-04-4
SPID(S): Tox21_200782
M4ID: 12481470

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

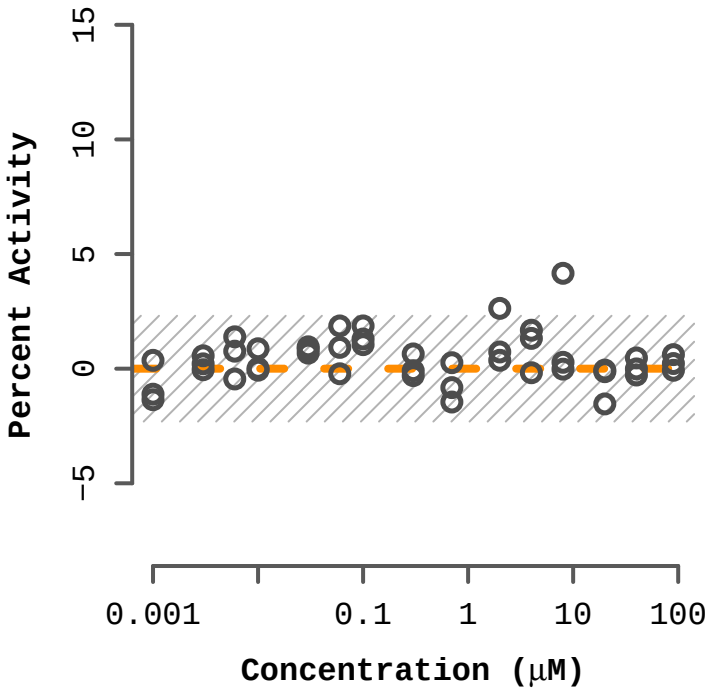
NAME: Ammonium nitrate
CHID: 29668 **CASRN:** 6484-52-2
SPID(S): Tox21_303522
M4ID: 12475621

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.769 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

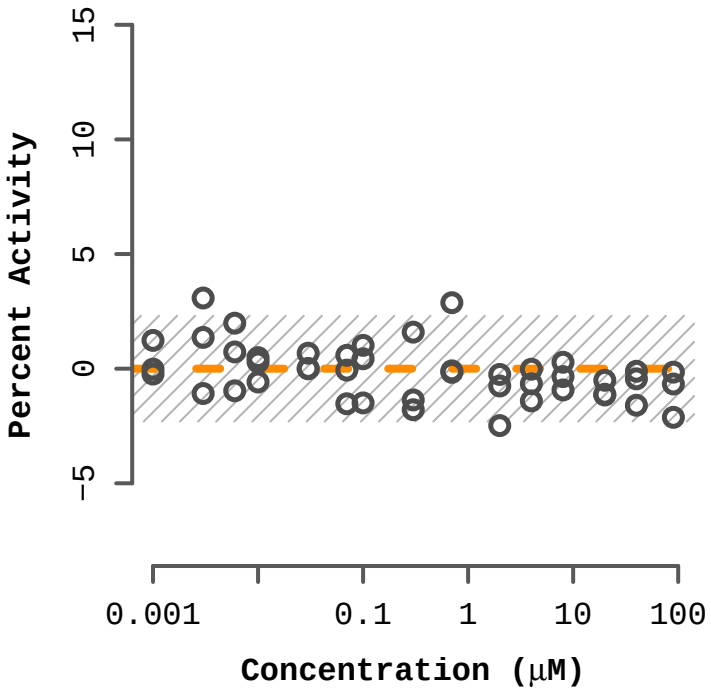
NAME: Ammonium nitrate
CHID: 29668 **CASRN:** 6484-52-2
SPID(S): Tox21_202271
M4ID: 12479981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

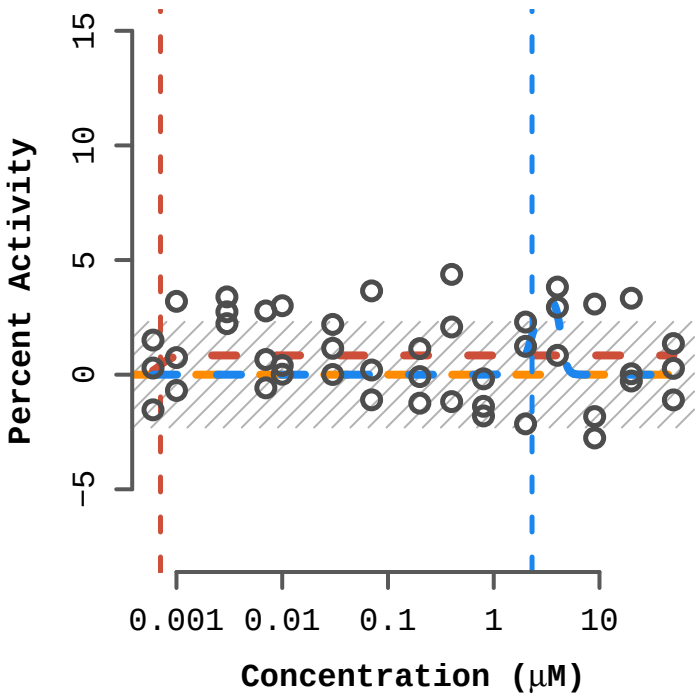
NAME: 4,4'−Methylenebis(2−methylcyclohexanamine)
CHID: 29670 **CASRN:** 6864−37−5
SPID(S): Tox21_201139
M4ID: 12481113

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Etidronate disodium
CHID: 29671 CASRN: 7414-83-7
SPID(S): Tox21_111596_1
M4ID: 12483597

HILL MODEL (in red):

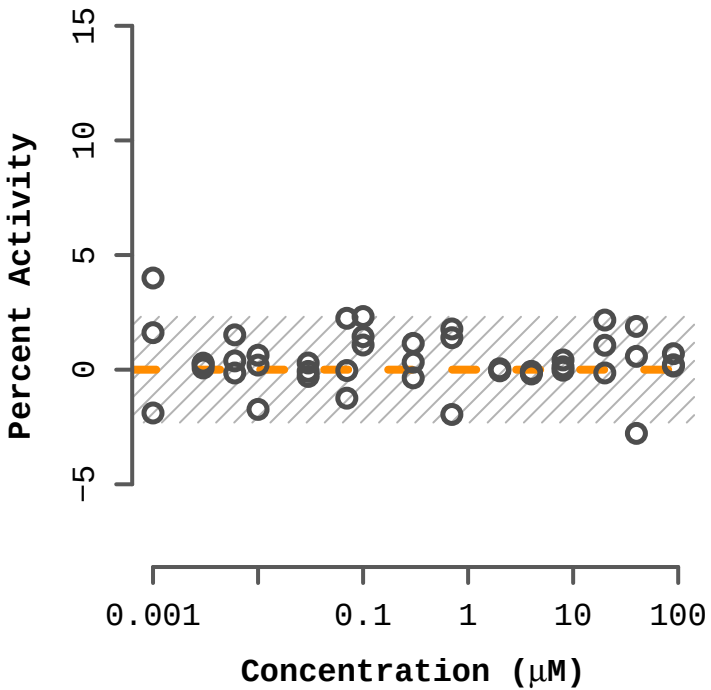
	tp	ga	gw
val:	0.839	−3.15	8
sd:	0.317	0.32	26.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.43	0.362	8	0.636	15.8
sd:	147	3.21	38.2	4.94	302

	CNST	HILL	GNLS
AIC:	196.76	195.74	200.85
PROB:	0.36	0.6	0.05
RMSE:	2.01	1.82	1.9

MAX_MEAN: 2.79 **MAX_MED:** 2.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

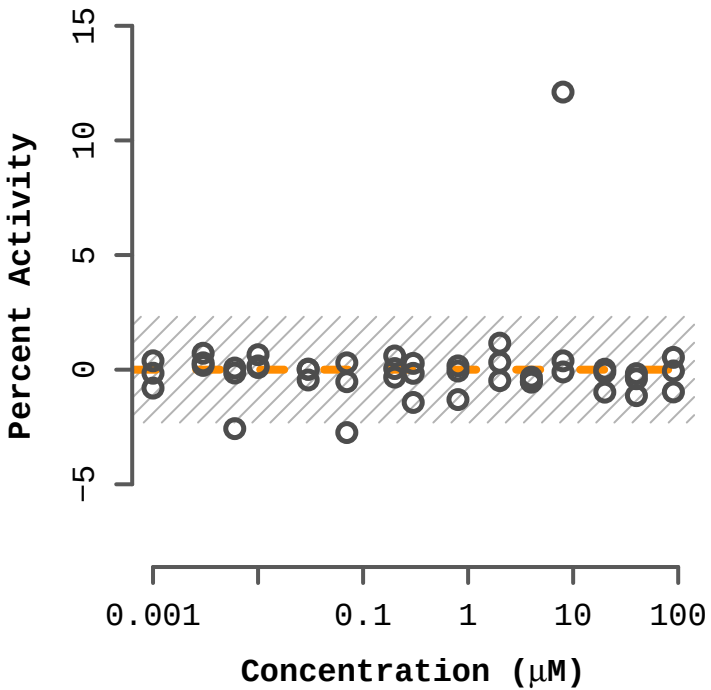
NAME: Silica
CHID: 29677 **CASRN:** 7631-86-9
SPID(S): Tox21_301288
M4ID: 12477845

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

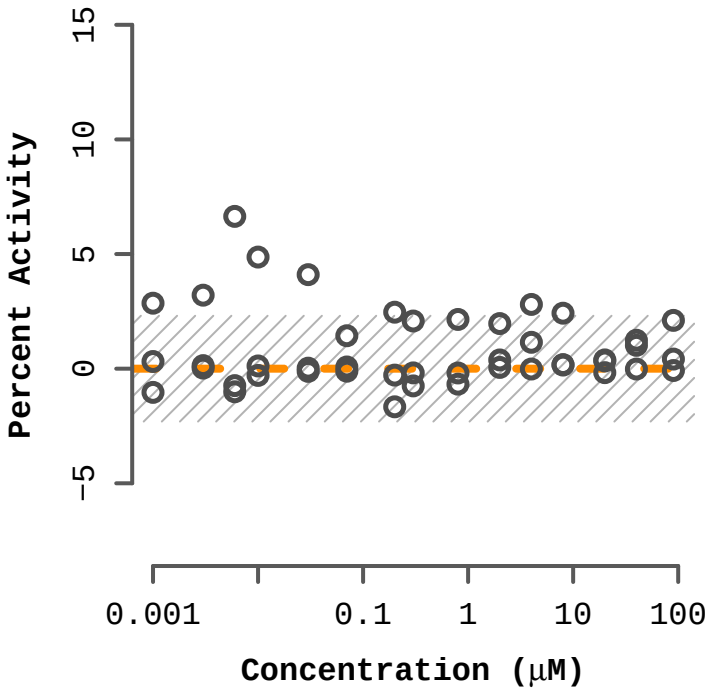
NAME: Tetrachlorostannane
CHID: 29679 **CASRN:** 7646-78-8
SPID(S): Tox21_200181
M4ID: 12482071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 4.13 **MAX_MED:** 0.388 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

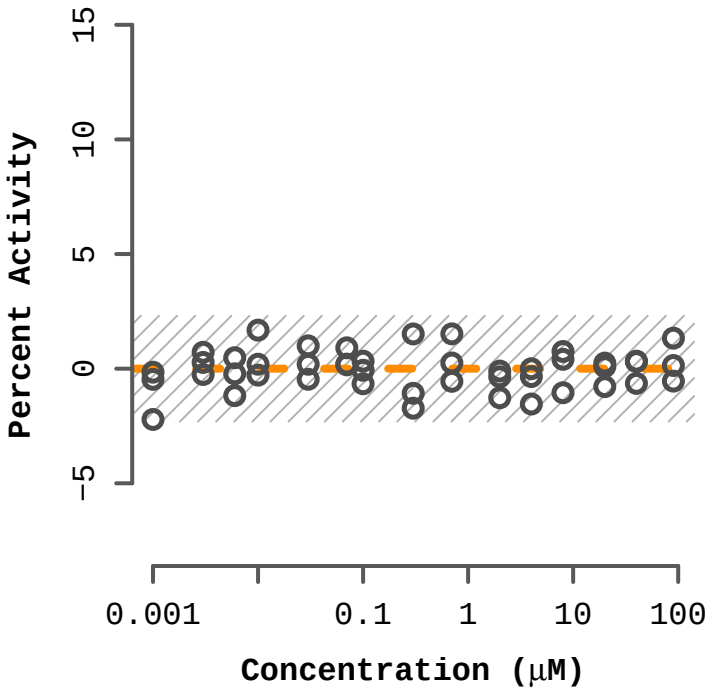
NAME: Sulfuric acid
CHID: 29683 **CASRN:** 7664-93-9
SPID(S): Tox21_200483
M4ID: 12481769

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

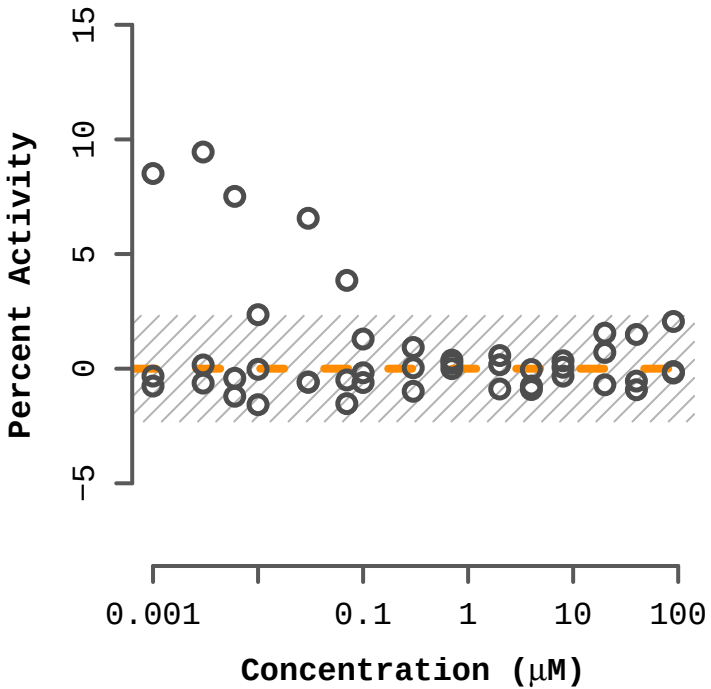
NAME: Iron(II) sulfate
CHID: 29688 **CASRN:** 7720-78-7
SPID(S): Tox21_202580
M4ID: 12479672

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.533 **MAX_MED:** 0.409 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

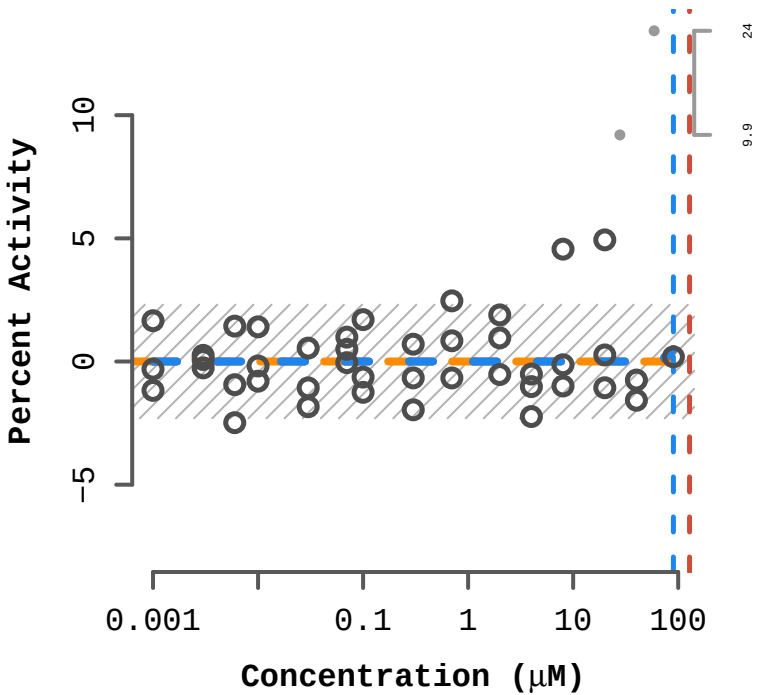
NAME: Potassium persulfate
CHID: 29690 **CASRN:** 7727-21-1
SPID(S): Tox21_200798
M4ID: 12481454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.74	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 3 **MAX_MED:** 0.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diammonium peroxydisulfate
CHID: 29691 CASRN: 7727-54-0
SPID(S): Tox21_201161
M4ID: 12481091 BRK

HILL MODEL (in red):

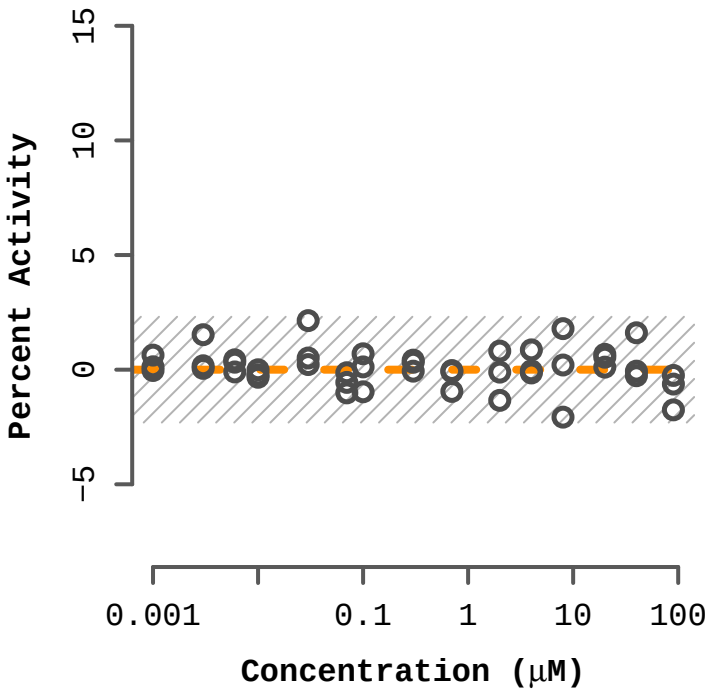
	tp	ga	gw
val:	8.76	2.11	7.89
sd:	153	1.54	68.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.77	1.95	8	2.37	0.301
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	195.66	201.49	205.49
PROB:	0.94	0.05	0.01
RMSE:	4.16	4.1	4.1

MAX_MEAN: 12 MAX_MED: 12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

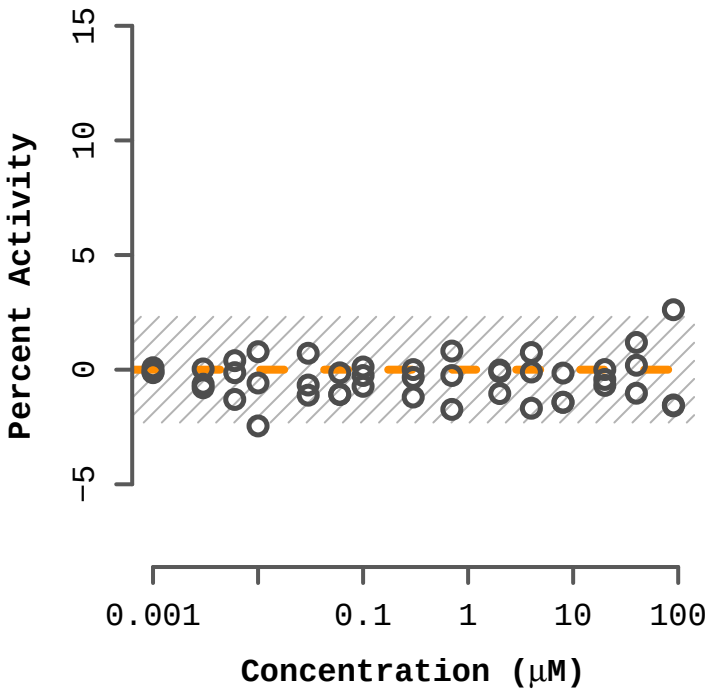
NAME: Potassium nitrate
CHID: 29692 **CASRN:** 7757-79-1
SPID(S): Tox21_303394
M4ID: 12475744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.959 **MAX_MED:** 0.545 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

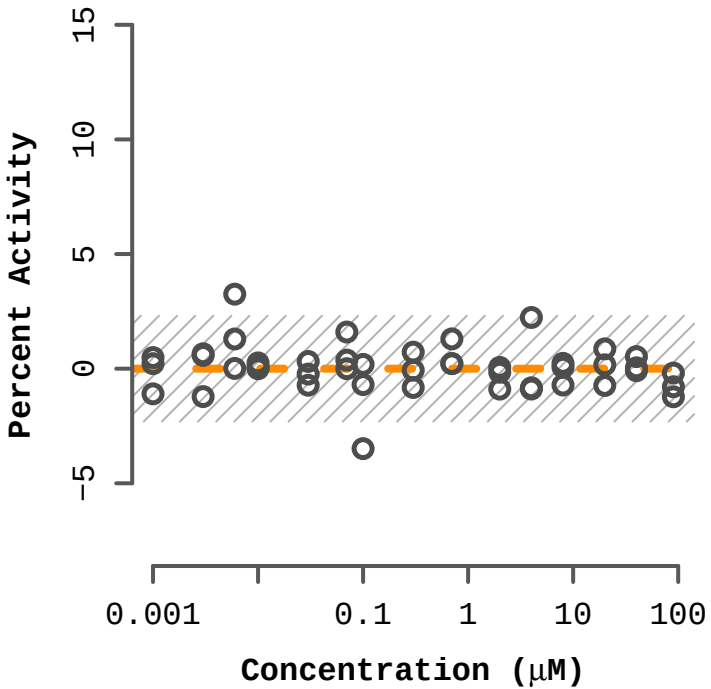
NAME: Potassium nitrate
CHID: 29692 **CASRN:** 7757-79-1
SPID(S): Tox21_201581
M4ID: 12480671

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.12 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

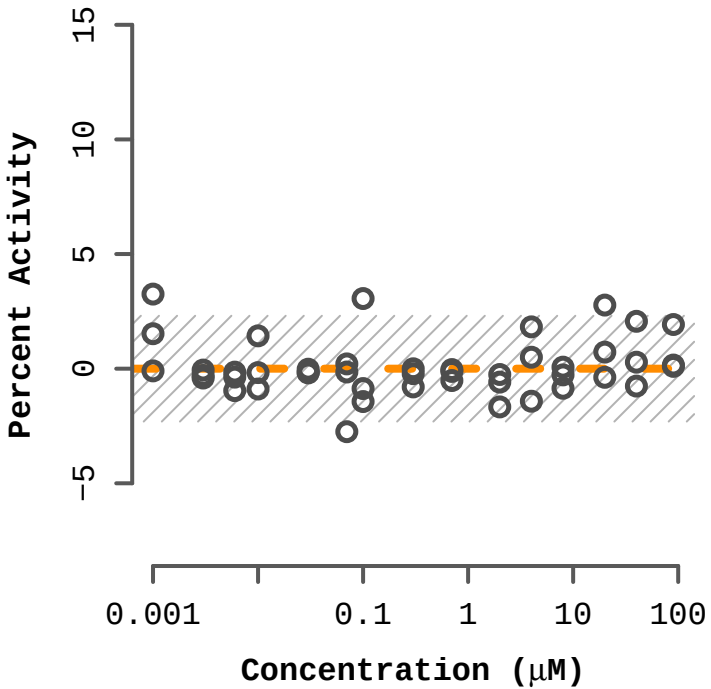
NAME: Iron(II) chloride
CHID: 29695 CASRN: 7758-94-3
SPID(S): Tox21_200197
M4ID: 12482055

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

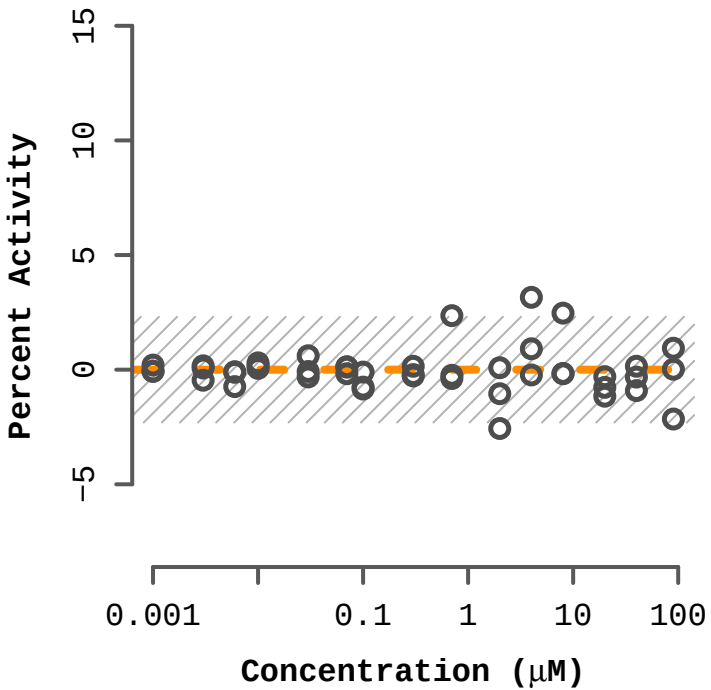
NAME: Sodium persulfate
CHID: 29698 CASRN: 7775-27-1
SPID(S): Tox21_303592
M4ID: 12475553

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

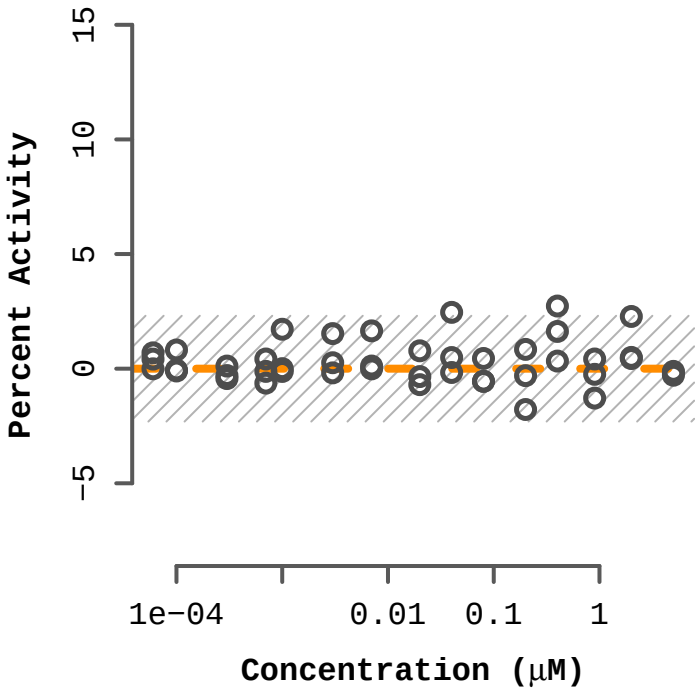
NAME: Sodium persulfate
CHID: 29698 **CASRN:** 7775-27-1
SPID(S): Tox21_201326
M4ID: 12480926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

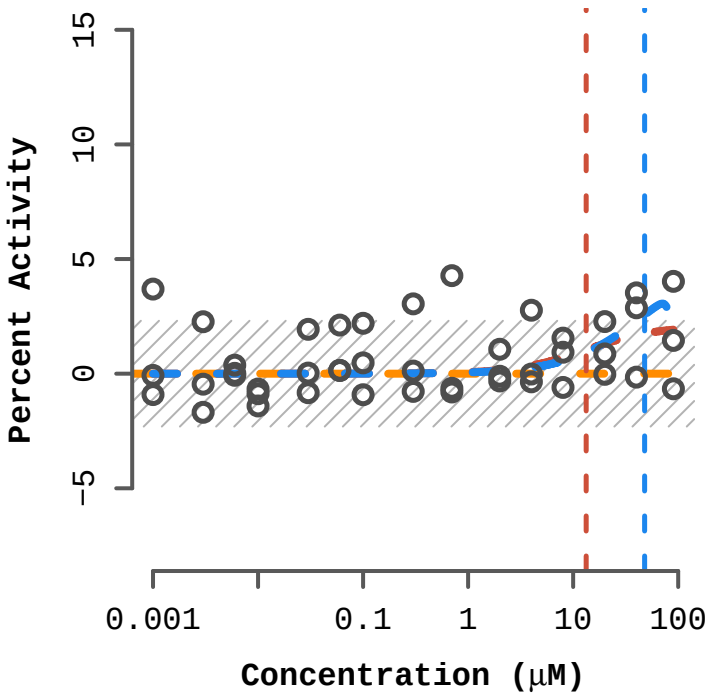
NAME: Ammonium thiosulfate
CHID: 29703 **CASRN:** 7783-18-8
SPID(S): Tox21_202777
M4ID: 12479475

HILL MODEL: Not applicable.

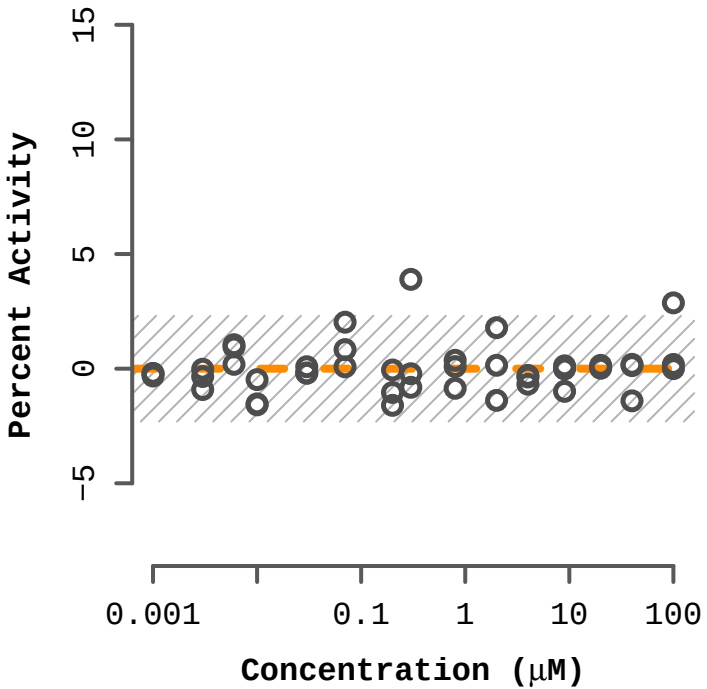
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.63 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Sulfuryl chloride
CHID:    29707   CASRN: 7791-25-5
SPID(S): Tox21_200484
M4ID:    12481768

HILL MODEL (in red):
      tp       ga       gw
val:  2.07     1.12     1.33
sd:   1.43     0.627    1.74

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.13     1.68     1.18     1.95     16
sd:   9.37     1.15     1.11     0.0529   91.4

      CNST        HILL        GNLS
AIC:  175.21      172.36      175.54
PROB: 0.17        0.69        0.14
RMSE: 1.69        1.51        1.51

MAX_MEAN: 2.08      MAX_MED: 2.87      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

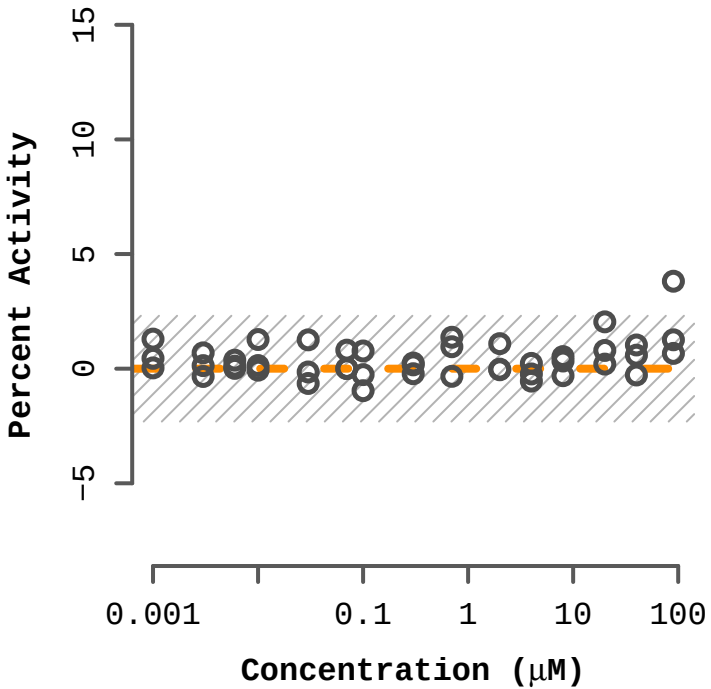
NAME: Phosphoric trichloride
CHID: 29710 **CASRN:** 10025-87-3
SPID(S): Tox21_200814
M4ID: 12481438

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

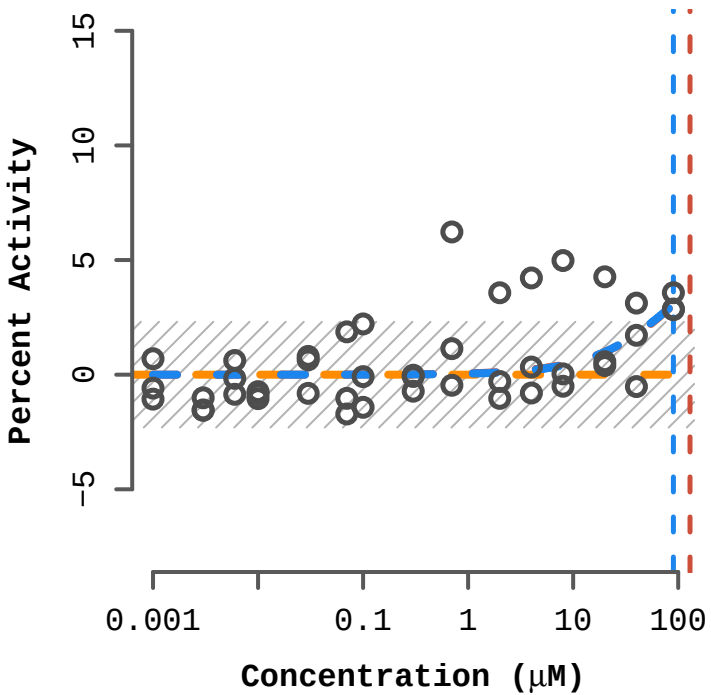
NAME: (1S,2R,5S)−(+)−Menthol
CHID: 29733 **CASRN:** 15356−60−2
SPID(S): Tox21_201043
M4ID: 12481209

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Borate(1−), tetrafluoro−, hydrogen
CHID: 29739 CASRN: 16872−11−0
SPID(S): Tox21_202581
M4ID: 12479671

HILL MODEL (in red):

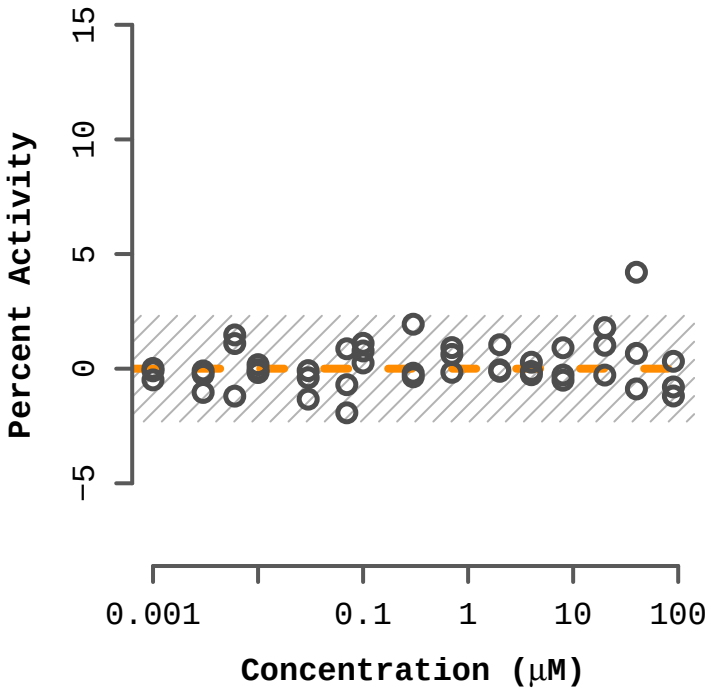
	tp	ga	gw
val:	7.47	2.11	1.01
sd:	19.7	2.05	1.01

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.11	1.95	1.09	2.73	17.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	189.18	177.82	181.84
PROB:	0	0.88	0.12
RMSE:	2.04	1.76	1.76

MAX_MEAN: 3.09 MAX_MED: 2.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

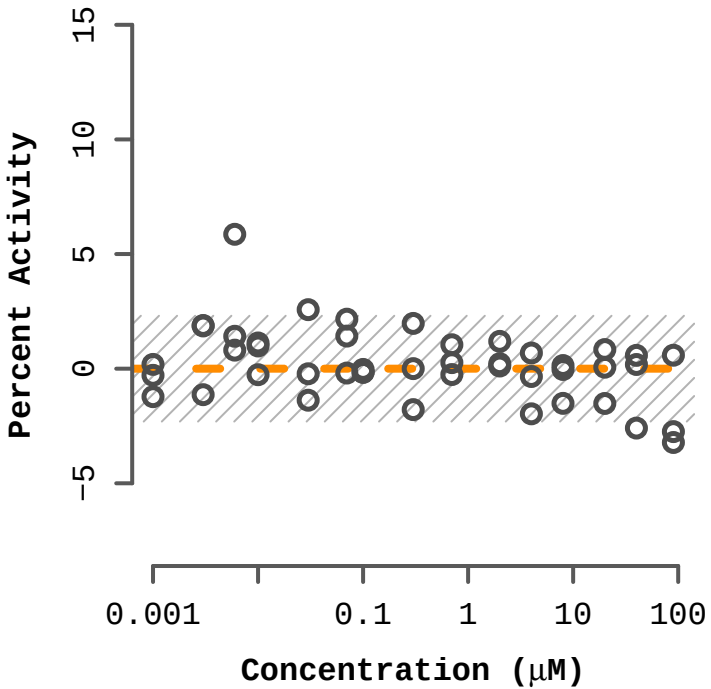
NAME: Propylene glycol monobutyl ether
CHID: 29755 **CASRN:** 29387-86-8
SPID(S): Tox21_301305
M4ID: 12477828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

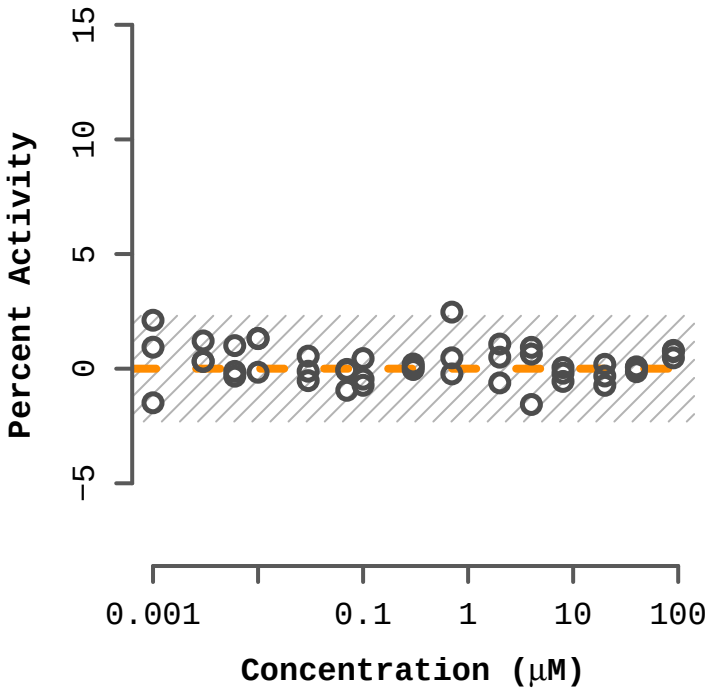
NAME: Sodium dichloro-s-triazinetrione dihydrate
CHID: 29761 **CASRN:** 51580-86-0
SPID(S): Tox21_303426
M4ID: 12475713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

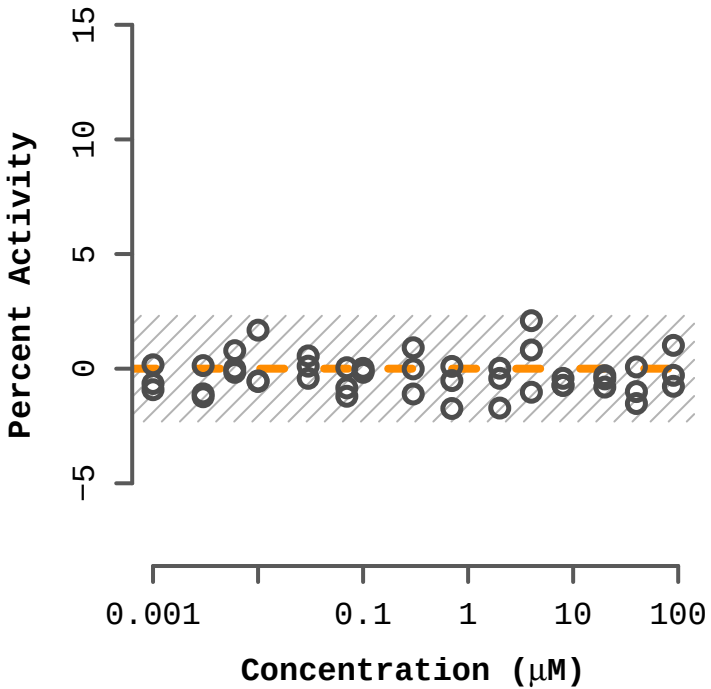
NAME: Sodium dichloro-s-triazinetrione dihydrate
CHID: 29761 **CASRN:** 51580-86-0
SPID(S): Tox21_201922
M4ID: 12480330

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

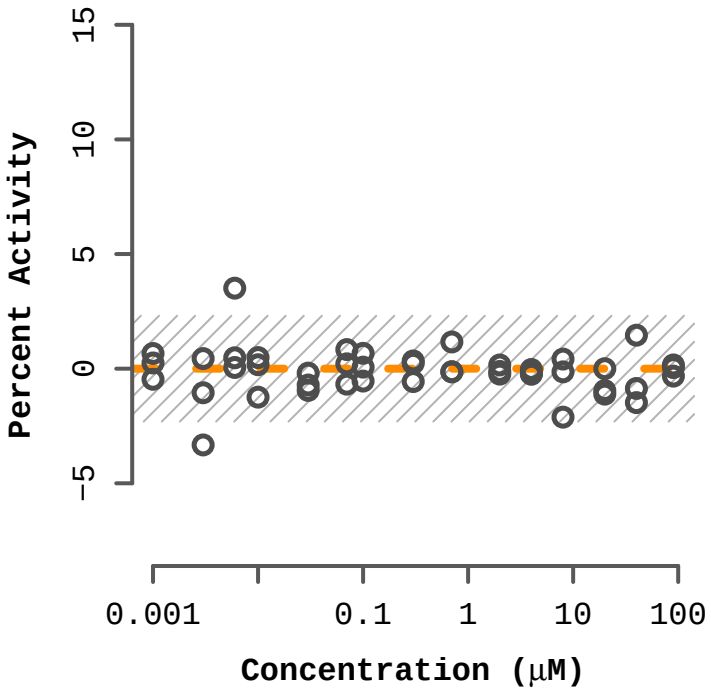
NAME: 2-[4-(Dibutylamino)-2-hydroxybenzoyl]benzoic a
CHID: 29762 CASRN: 54574-82-2
SPID(S): Tox21_200213
M4ID: 12482039

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.628 MAX_MED: 0.817 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

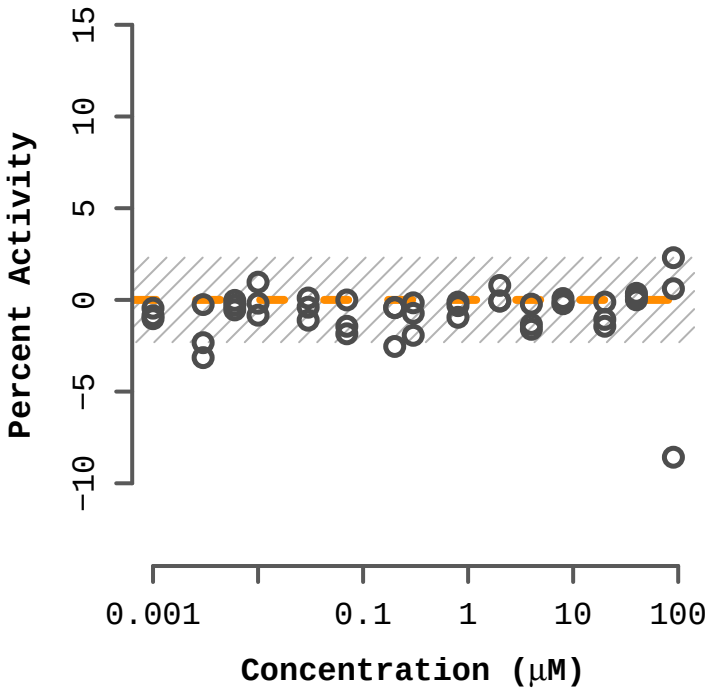
NAME: Benzenesulfonic acid, C10-14-alkyl derivs., so
CHID: 29806 CASRN: 69669-44-9
SPID(S): Tox21_200193
M4ID: 12482059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.69	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.35 MAX_MED: 0.476 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

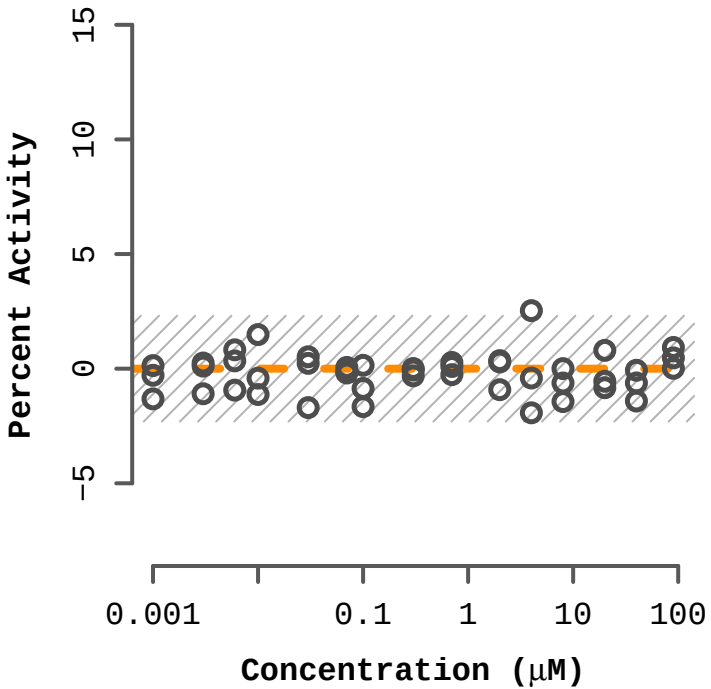
NAME: Tridecylamine, branched and linear
CHID: 29815 **CASRN:** 86089-17-0
SPID(S): Tox21_200485
M4ID: 12481767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.225 **MAX_MED:** 0.611 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

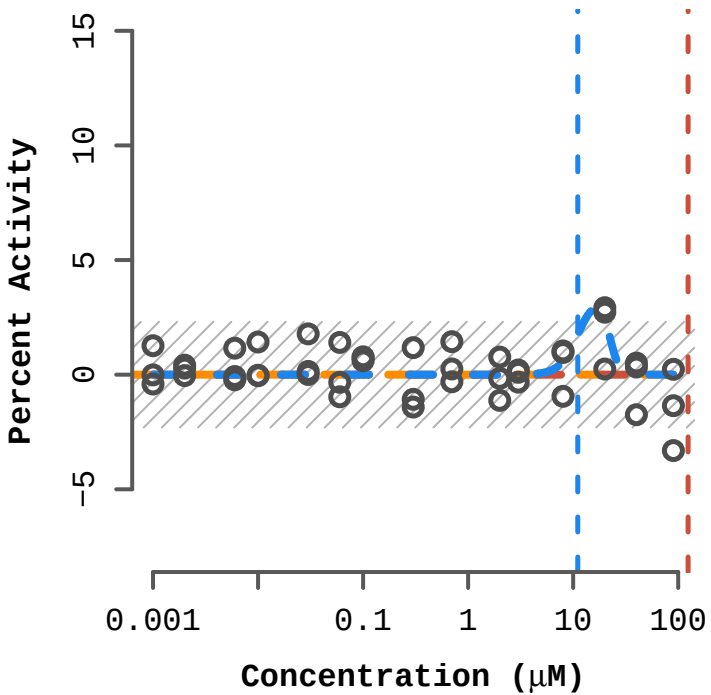
NAME: Acetic acid, C8-10-branched alkyl esters, C9-r
CHID: 29848 CASRN: 108419-33-6
SPID(S): Tox21_300939
M4ID: 12478194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.472 MAX_MED: 0.472 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Atorvastatin
CHID: 29868 CASRN: 134523-00-5
SPID(S): Tox21_302417
M4ID: 12476716

HILL MODEL (in red):

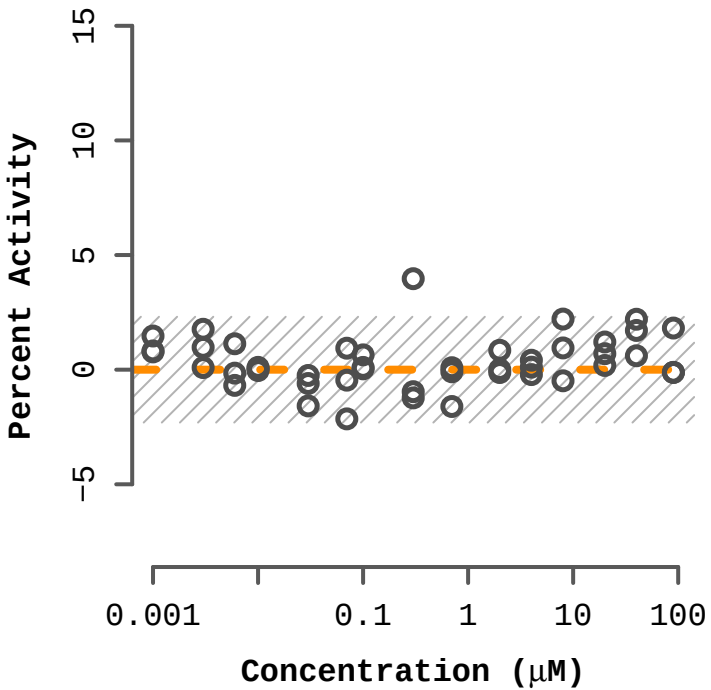
	tp	ga	gw
val:	1.6e-09	2.09	1.8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.51	1.04	4.94	1.35	9.67
sd:	36.2	1.81	38.4	1.02	123

	CNST	HILL	GNLS
AIC:	138.16	144.16	139
PROB:	0.59	0.03	0.38
RMSE:	1.13	1.13	1.01

MAX_MEAN: 1.97 MAX_MED: 2.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

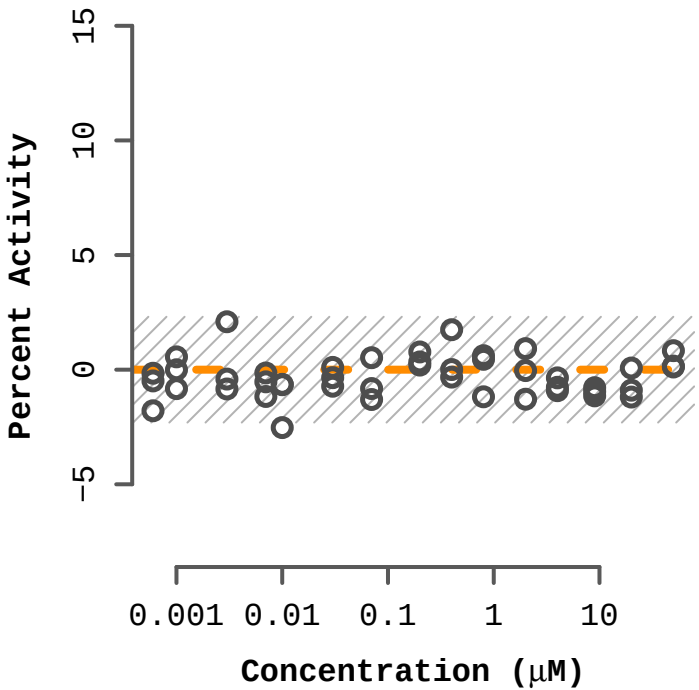
NAME: Bezafibrate
CHID: 29869 **CASRN:** 41859-67-0
SPID(S): Tox21_301845
M4ID: 12477288

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

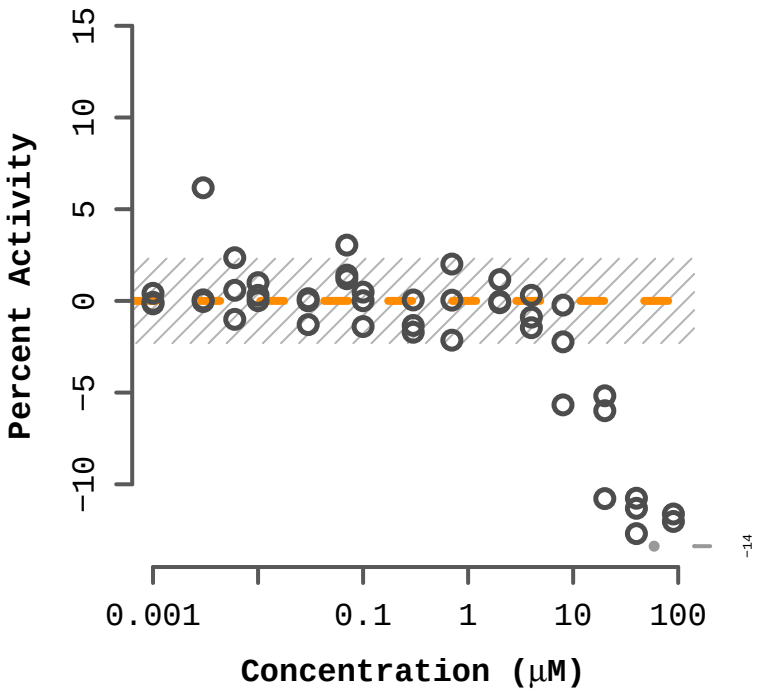
NAME: Bezafibrate
CHID: 29869 **CASRN:** 41859-67-0
SPID(S): Tox21_110645_1
M4ID: 12484210

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.476 **MAX_MED:** 0.453 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

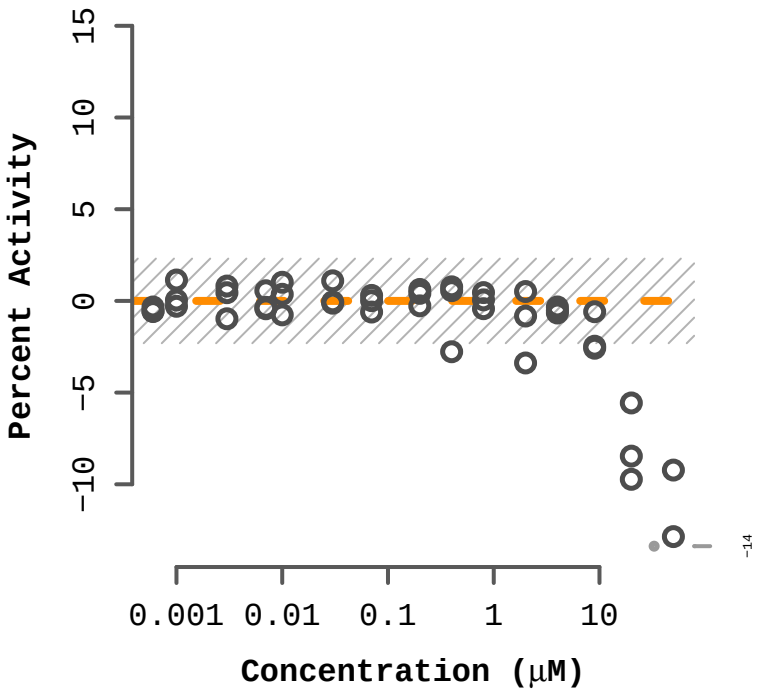
NAME: Clotrimazole
CHID: 29871 CASRN: 23593-75-1
SPID(S): Tox21_300415
M4ID: 12478717 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.16	NA	NA
PROB:	1	NA	NA
RMSE:	5.13	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

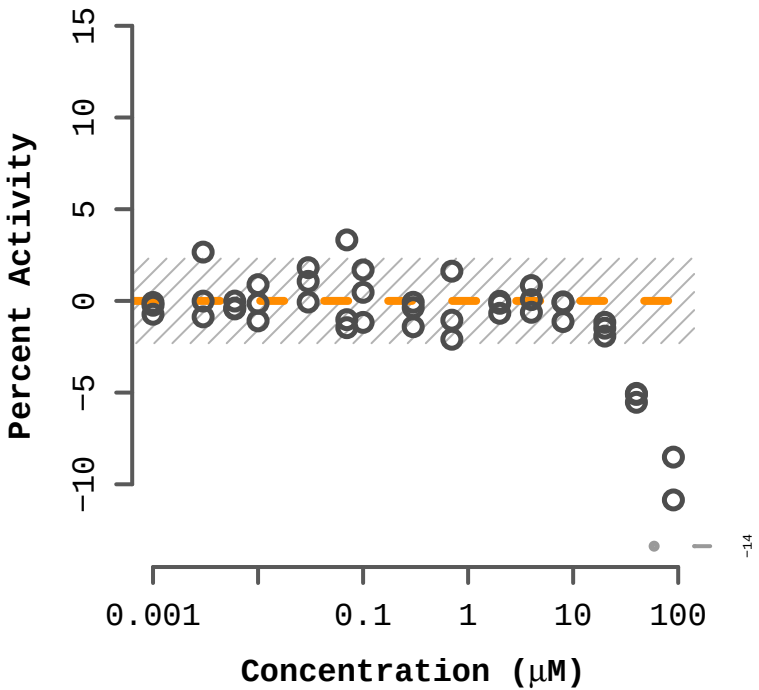
NAME: Clotrimazole
CHID: 29871 CASRN: 23593-75-1
SPID(S): Tox21_110111_1
M4ID: 12484642 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.22	NA	NA
PROB:	1	NA	NA
RMSE:	3.9	NA	NA

MAX_MEAN: 0.309 **MAX_MED:** 0.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

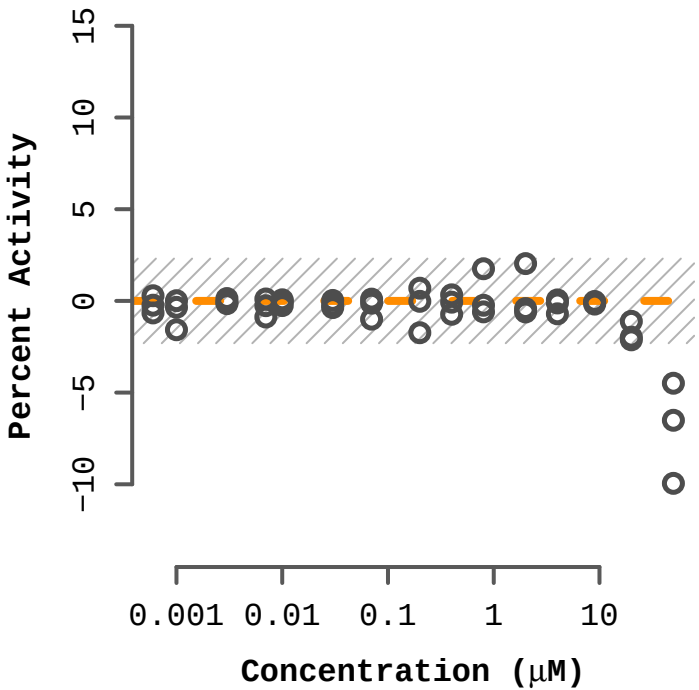
NAME: Fenofibrate
CHID: 29874 CASRN: 49562-28-9
SPID(S): Tox21_300151
M4ID: 12478979 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.23	NA	NA
PROB:	1	NA	NA
RMSE:	3.4	NA	NA

MAX_MEAN: 0.94 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

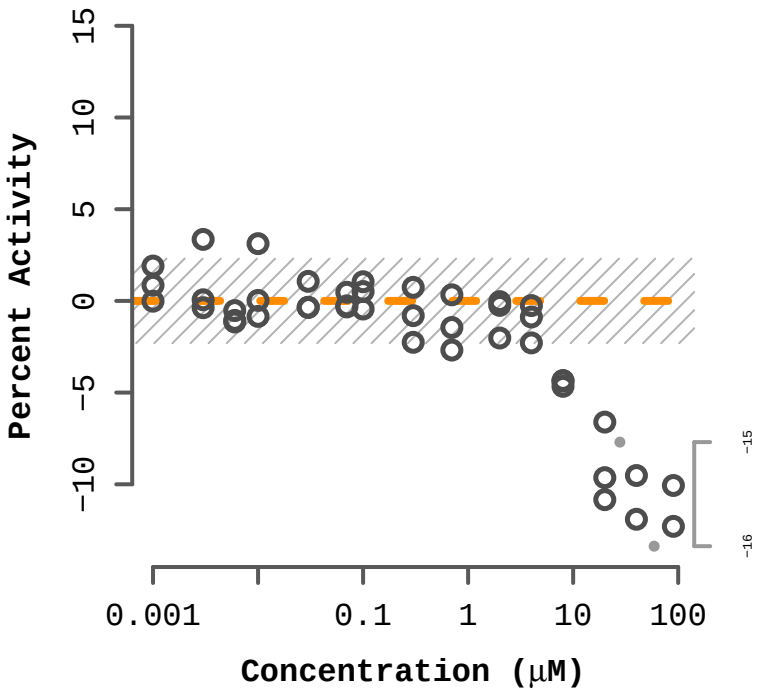
NAME: Fenofibrate
CHID: 29874 **CASRN:** 49562-28-9
SPID(S): Tox21_110147_1
M4ID: 12484609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 0.339 **MAX_MED:** −0.0208 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

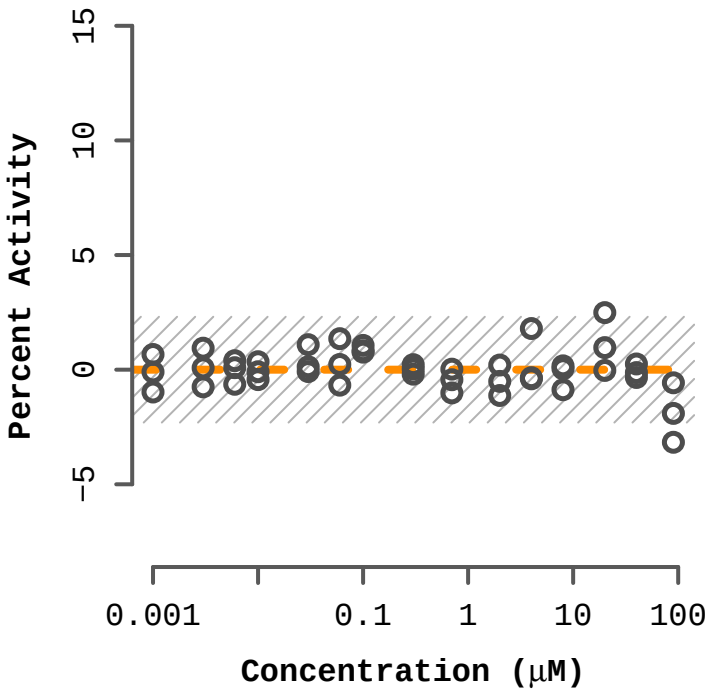
NAME: Ketoconazole
CHID: 29879 **CASRN:** 65277-42-1
SPID(S): Tox21_300267
M4ID: 12478863 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.34	NA	NA
PROB:	1	NA	NA
RMSE:	5.46	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

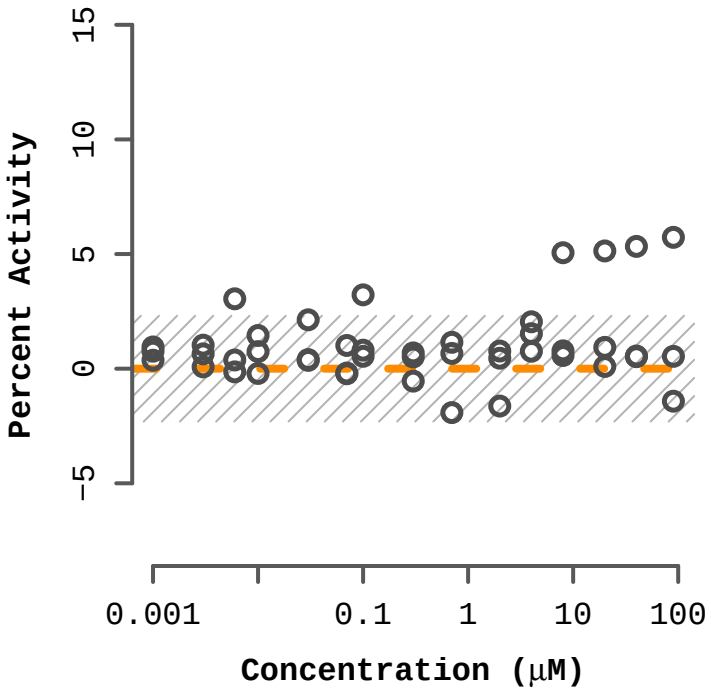
NAME: (−)−Epigallocatechin gallate
CHID: 29889 **CASRN:** 989−51−5
SPID(S): Tox21_303457
M4ID: 12475683

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.964 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

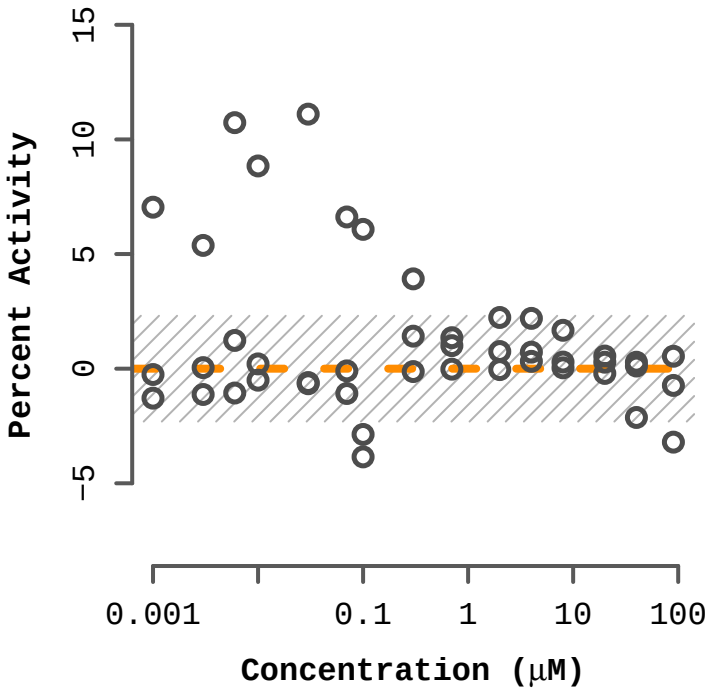
NAME: (−)−Epigallocatechin gallate
CHID: 29889 **CASRN:** 989−51−5
SPID(S): Tox21_201468
M4ID: 12480784

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

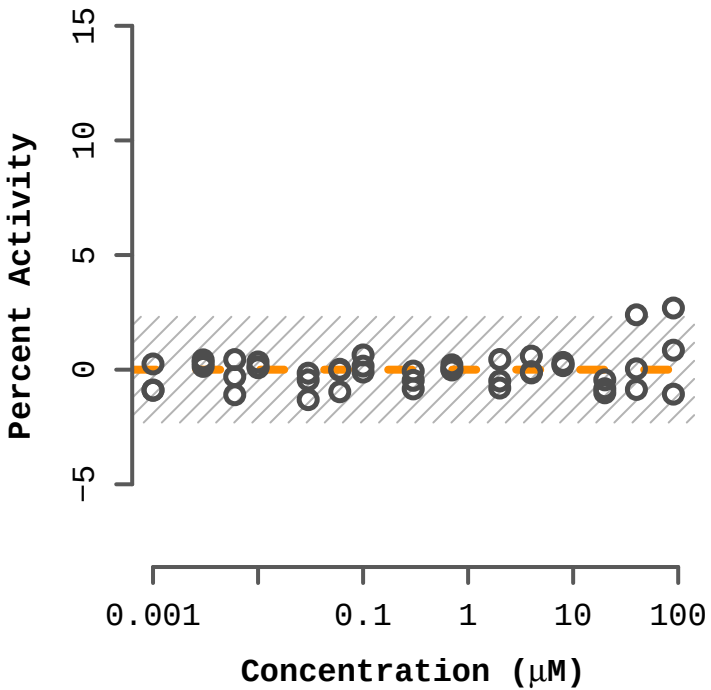
NAME: 1,1,2,2-Tetrahydroperfluoro-1-decanol
CHID: 29904 CASRN: 678-39-7
SPID(S): Tox21_300397
M4ID: 12478735

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.2	NA	NA
PROB:	1	NA	NA
RMSE:	3.52	NA	NA

MAX_MEAN: 3.64 MAX_MED: 1.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

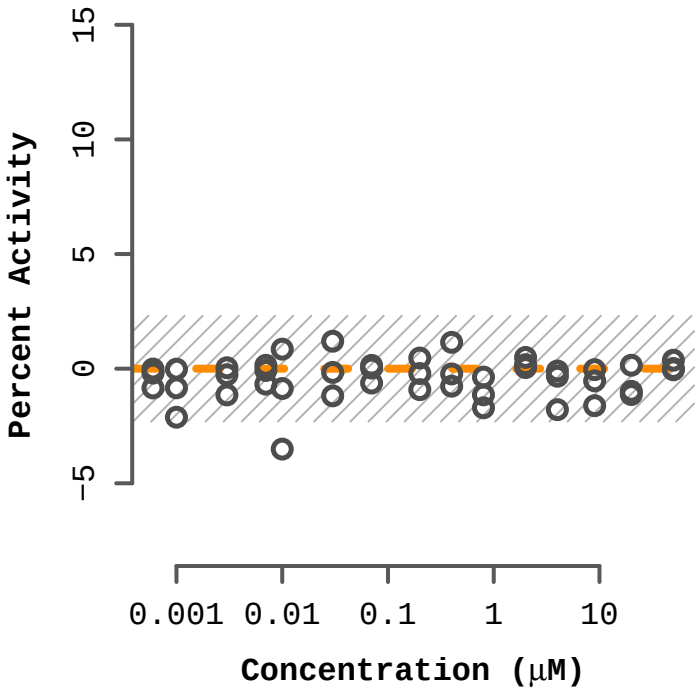
NAME: 1,1−Dichloropropene
CHID: 29910 **CASRN:** 563−58−6
SPID(S): Tox21_200331
M4ID: 12481921

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

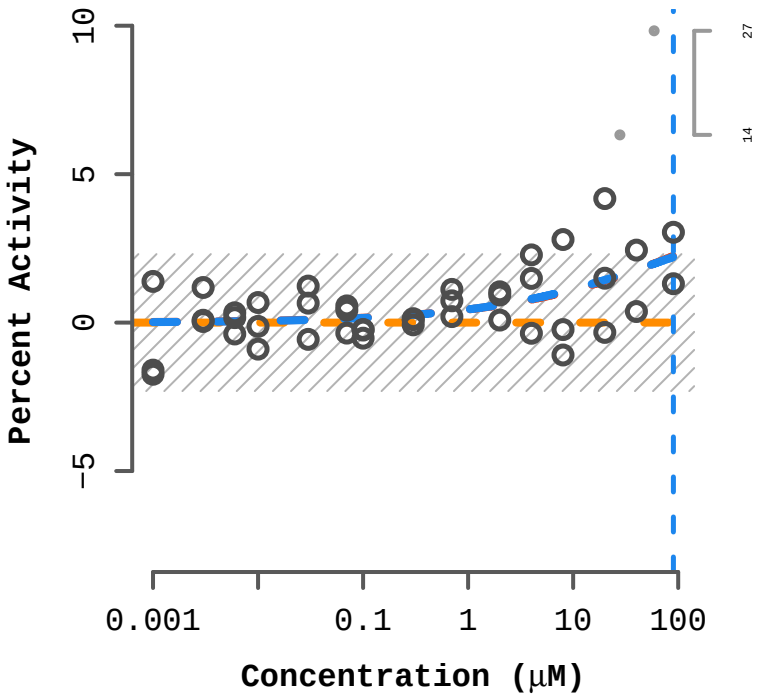
NAME: 2,2',4,4',5,5'−Hexabromodiphenyl ether
CHID: 30047 **CASRN:** 68631−49−2
SPID(S): Tox21_202469
M4ID: 12479783

HILL MODEL: Not applicable.

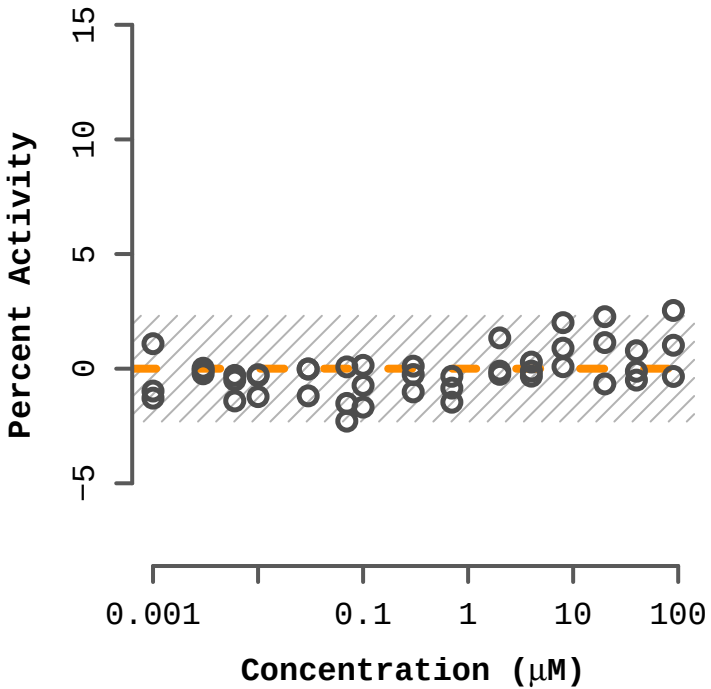
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.24 **MAX_MED:** 0.177 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,2',4,4',5-Pentabromodiphenyl ether
CHID:    30048   CASRN: 60348-60-9
SPID(S): Tox21_200156
M4ID:    12482096  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  6.02     2.45     0.449
sd:   28       7.33     0.467

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.42     1.95     0.487    2.92     7.44
sd:   11.5     4.26     0.433    1200     9220

      CNST        HILL        GNLS
AIC:  191.08      181.24      185.25
PROB: 0.01        0.88        0.12
RMSE: 4.79        4.32        4.32

MAX_MEAN: 10.6      MAX_MED: 3.04      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

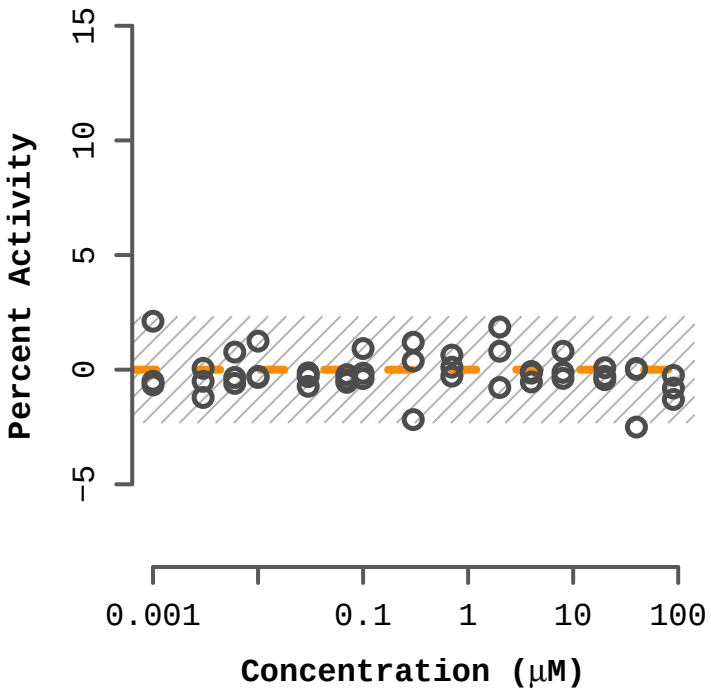
NAME: 2,2'4,4'−Tetrabromodiphenyl ether
CHID: 30056 CASRN: 5436−43−1
SPID(S): Tox21_200327
M4ID: 12481925

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.07 MAX_MED: 1.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

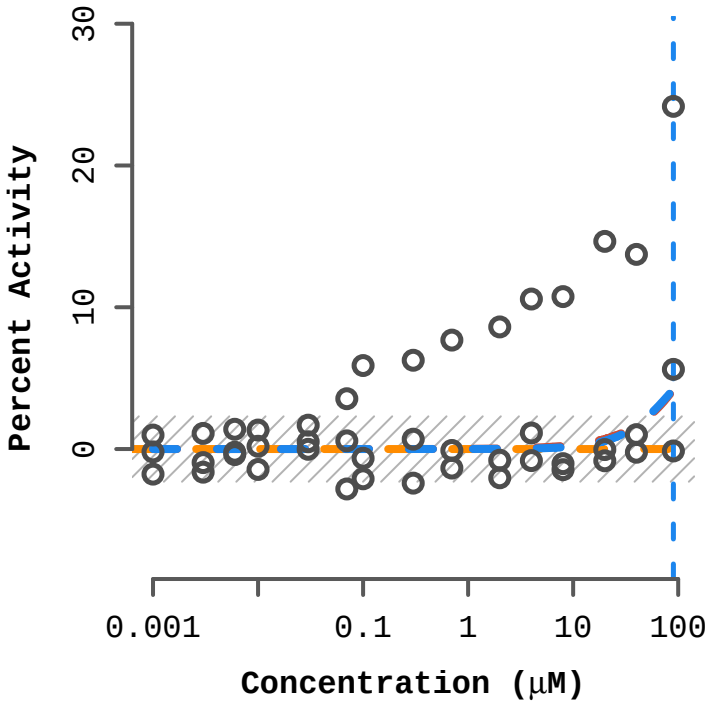
NAME: 2,2−Dichloropropane
CHID: 30060 **CASRN:** 594−20−7
SPID(S): Tox21_303540
M4ID: 12475604

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.63 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2-Dichloropropane
CHID: 30060 CASRN: 594-20-7
SPID(S): Tox21_202311
M4ID: 12479941

HILL MODEL (in red):

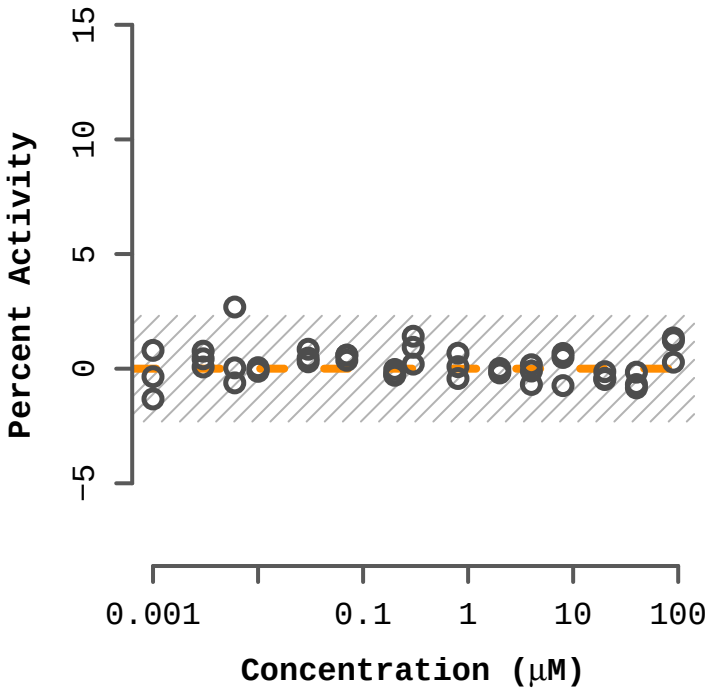
	tp	ga	gw
val:	22.8	2.45	1.3
sd:	267	5.72	2.85

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.43	1.95	1.75	3.53	3.59
sd:	51.9	3.06	6.01	1060	2450

	CNST	HILL	GNLS
AIC:	265.19	267.77	271.8
PROB:	0.76	0.21	0.03
RMSE:	5.81	5.29	5.3

MAX_MEAN: 9.89 MAX_MED: 5.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

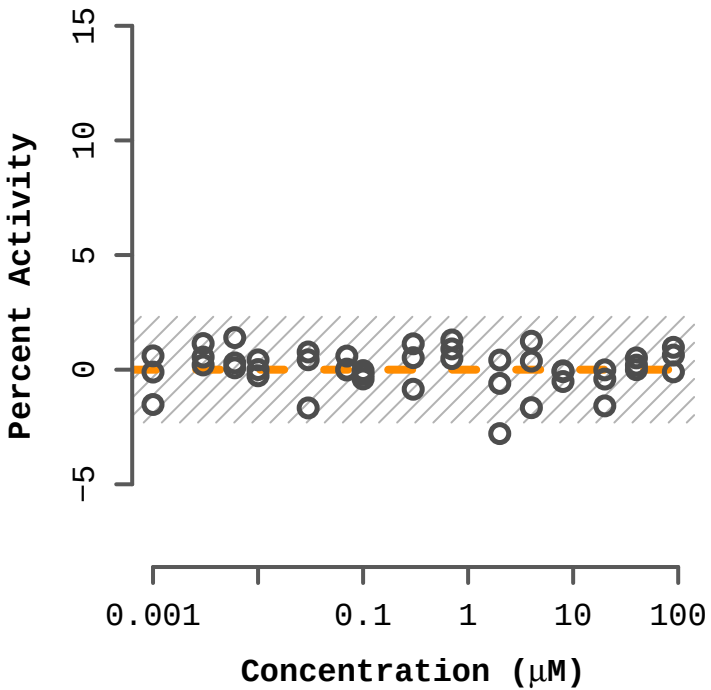
NAME: 2,5-Hexanedione
CHID: 30138 **CASRN:** 110-13-4
SPID(S): Tox21_200618
M4ID: 12481634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.949 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

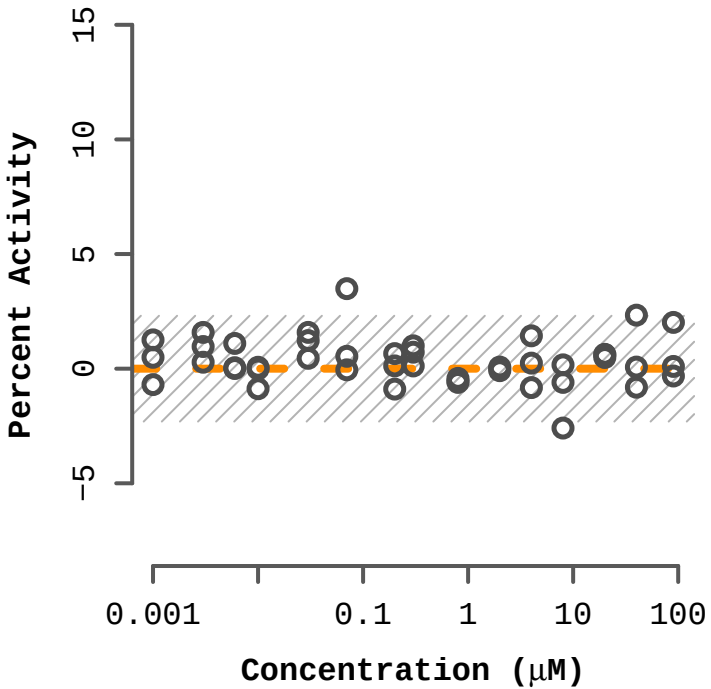
NAME: 2-Acetylthiazole
CHID: 30162 **CASRN:** 24295-03-2
SPID(S): Tox21_303515
M4ID: 12475627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

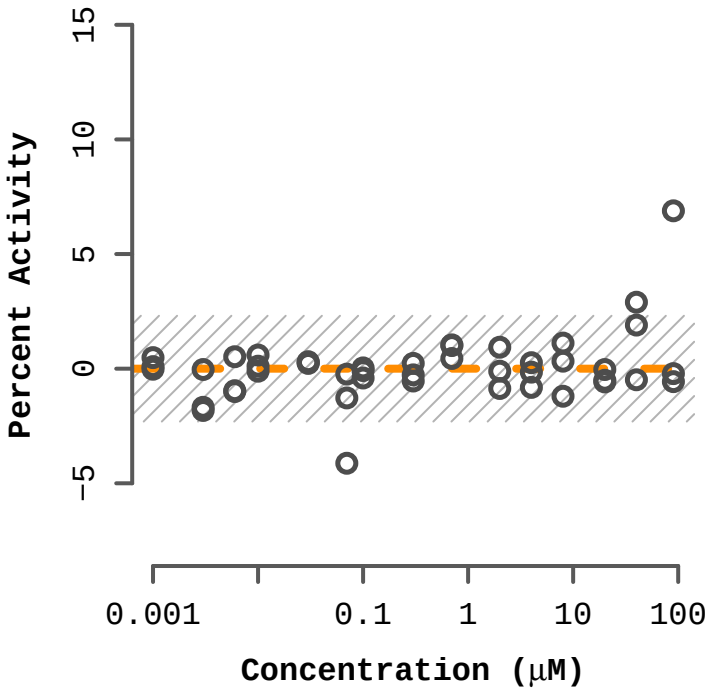
NAME: 2-Acetylthiazole
CHID: 30162 **CASRN:** 24295-03-2
SPID(S): Tox21_202054
M4ID: 12480198

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

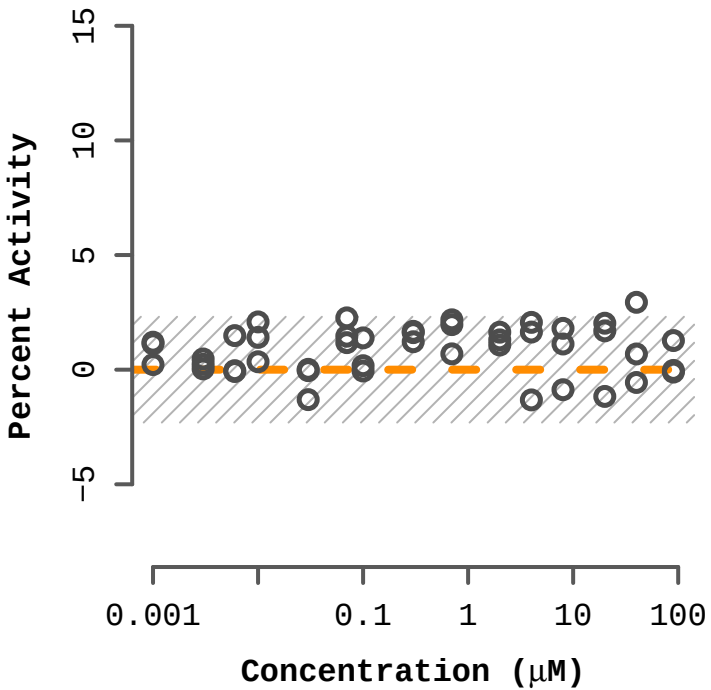
NAME: 2-Biphenylamine
CHID: 30189 **CASRN:** 90-41-5
SPID(S): Tox21_200959
M4ID: 12481293

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

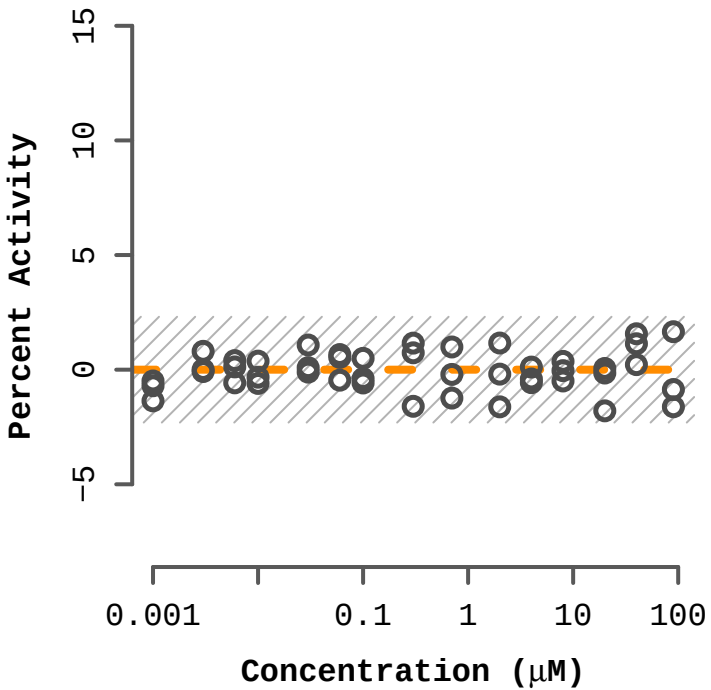
NAME: 2-Bromopropane
CHID: 30197 **CASRN:** 75-26-3
SPID(S): Tox21_200356
M4ID: 12481896

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

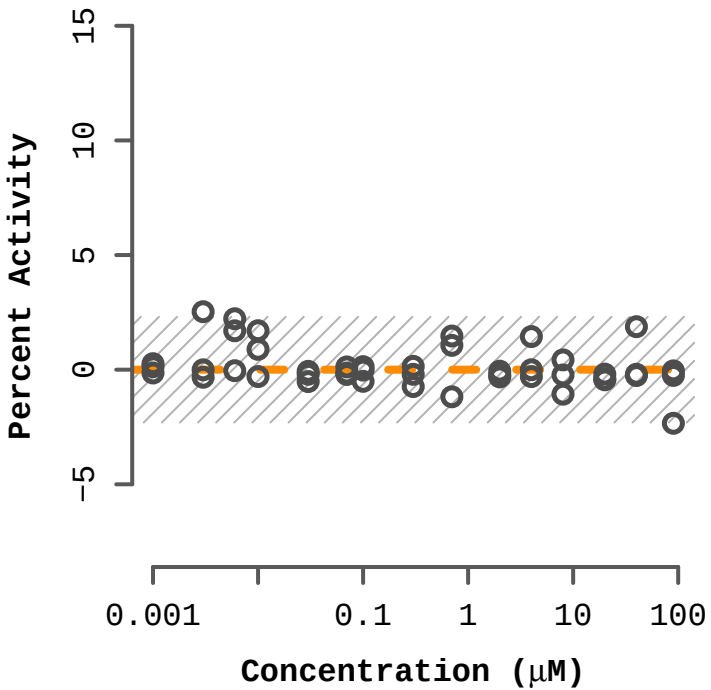
NAME: 2-Methyltetrahydrofuran
CHID: 30258 **CASRN:** 96-47-9
SPID(S): Tox21_200383
M4ID: 12481869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.975 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

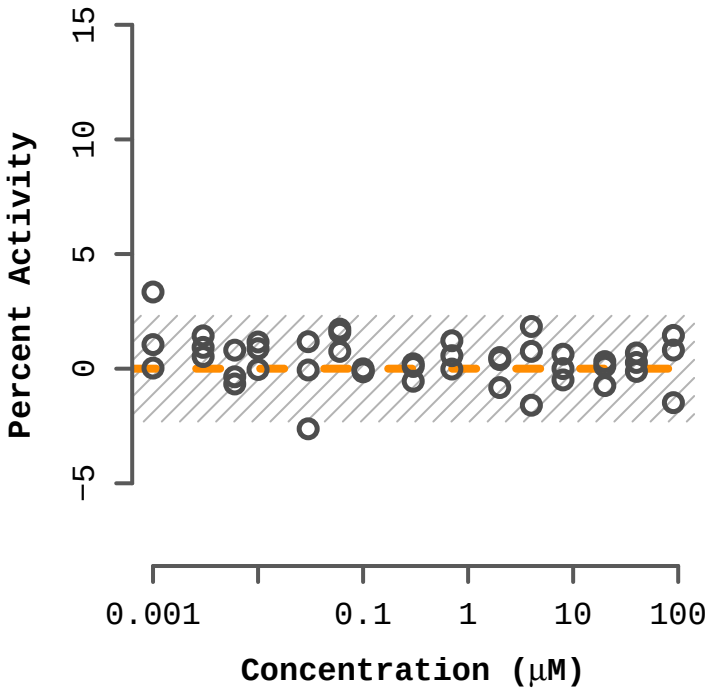
NAME: 3,5-Dichloroaniline
CHID: 30307 **CASRN:** 626-43-7
SPID(S): Tox21_303569
M4ID: 12475576

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

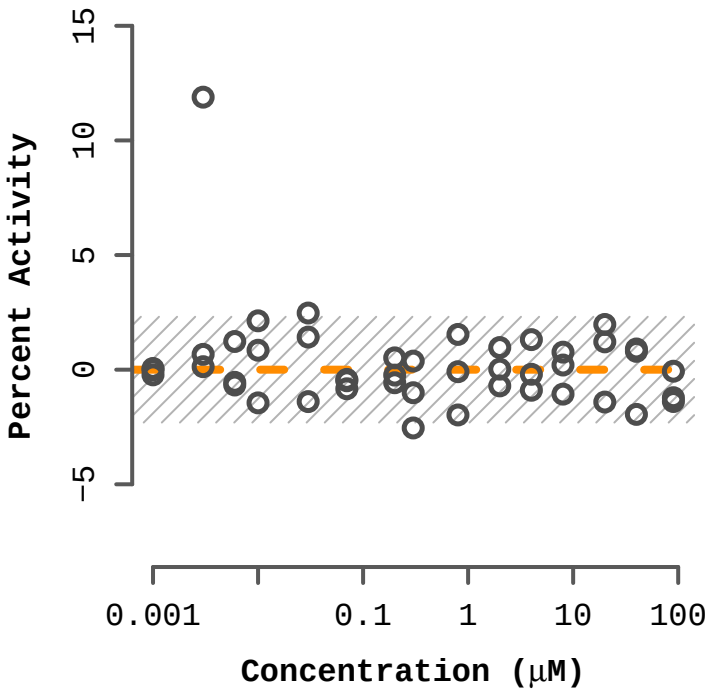
NAME: 3,5−Dichloroaniline
CHID: 30307 **CASRN:** 626−43−7
SPID(S): Tox21_200023
M4ID: 12482229

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

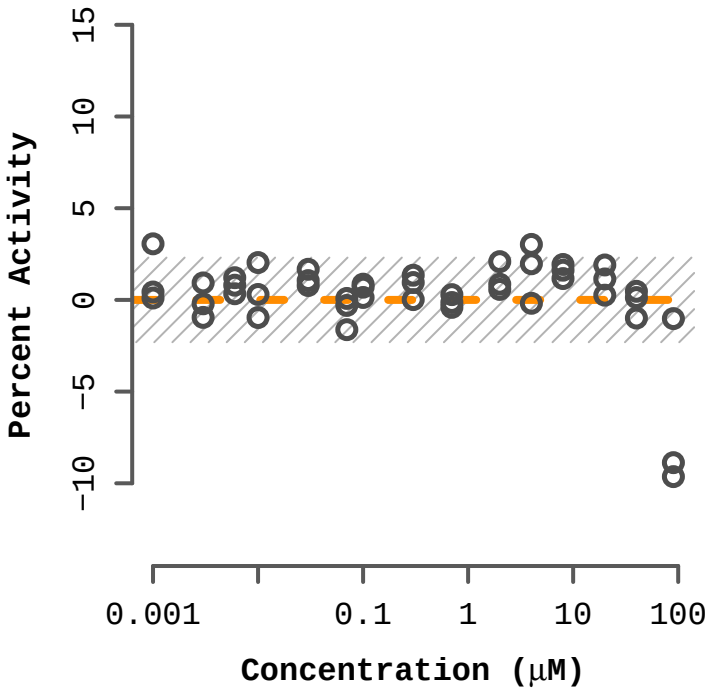
NAME: 3-Acetyl-2,5-dimethylfuran
CHID: 30317 **CASRN:** 10599-70-9
SPID(S): Tox21_200275
M4ID: 12481977

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.1	NA	NA

MAX_MEAN: 4.23 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

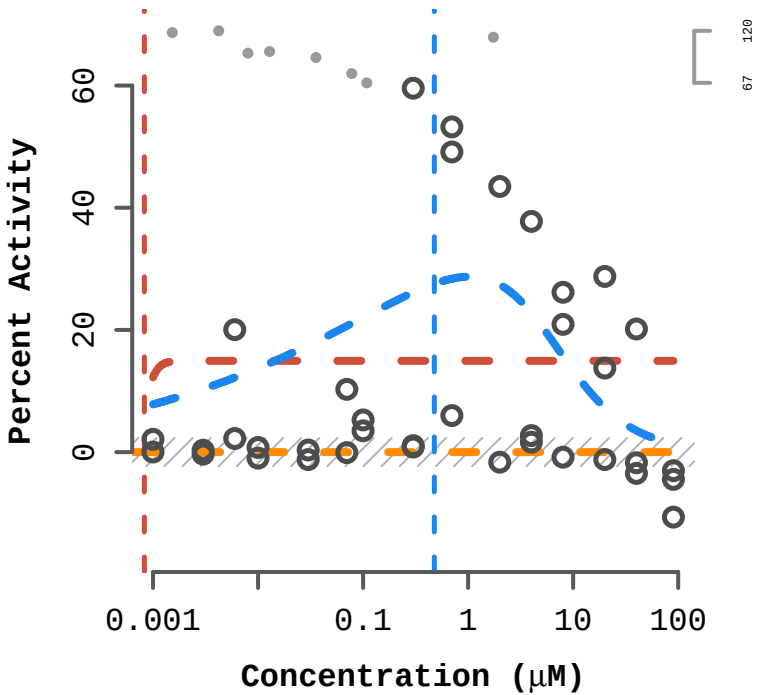
NAME: 3-Amino-9-ethylcarbazole
CHID: 30319 **CASRN:** 132-32-1
SPID(S): Tox21_303548
M4ID: 12475597

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Amino-9-ethylcarbazole
CHID: 30319 CASRN: 132-32-1
SPID(S): Tox21_202398
M4ID: 12479854 BRK

HILL MODEL (in red):

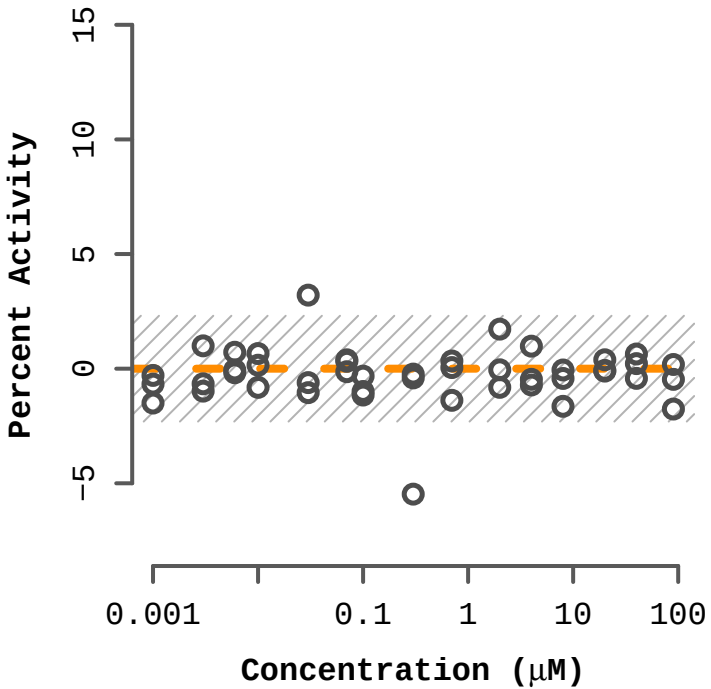
	tp	ga	gw
val:	14.9	-3.08	7.98
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	57.6	-0.322	0.3	0.749	1.26
sd:	387	17.8	0.783	1.68	1.02

	CNST	HILL	GNLS
AIC:	462.97	457.78	457.88
PROB:	0.04	0.49	0.47
RMSE:	44.69	38.37	37.4

MAX_MEAN: 50.4 MAX_MED: 49.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

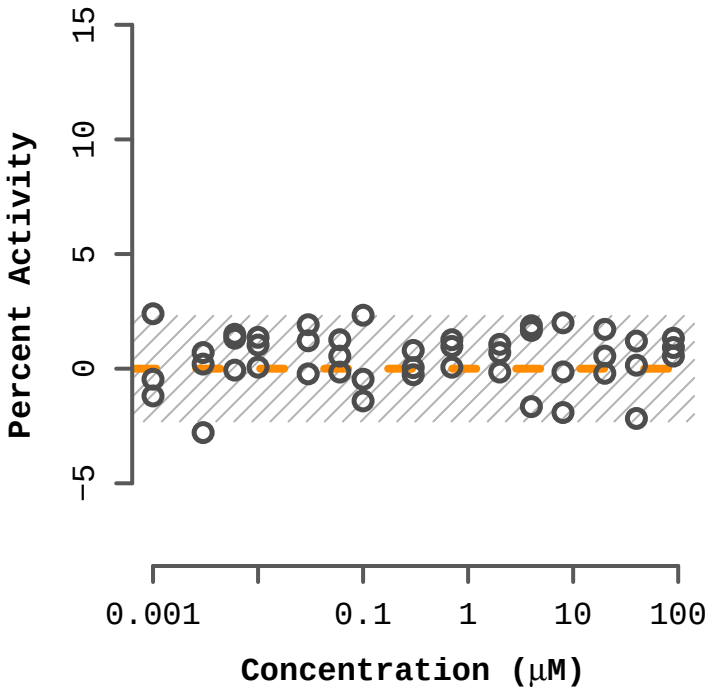
NAME: 3-Chloropropionitrile
CHID: 30336 **CASRN:** 542-76-7
SPID(S): Tox21_303460
M4ID: 12475680

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.52 **MAX_MED:** 0.322 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

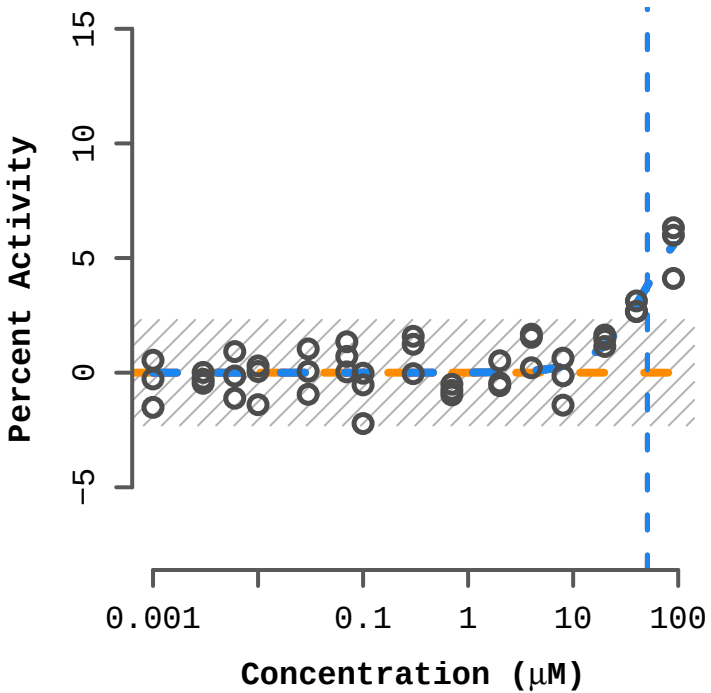
NAME: 3-Chloropropionitrile
CHID: 30336 **CASRN:** 542-76-7
SPID(S): Tox21_202225
M4ID: 12480027

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chloro-2-nitroaniline
CHID: 30384 CASRN: 89-63-4
SPID(S): Tox21_200807
M4ID: 12481445

HILL MODEL (in red):

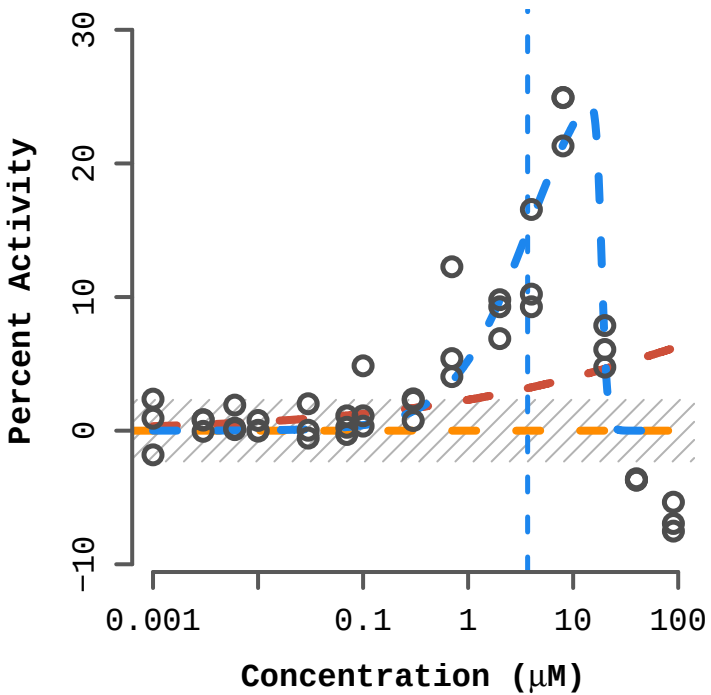
	tp	ga	gw
val:	7.59	1.71	1.78
sd:	2.37	0.177	0.572

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.59	1.71	1.78	3.94	4.04
sd:	2.37	0.177	0.572	1790	3680

	CNST	HILL	GNLS
AIC:	174.24	125.67	129.67
PROB:	0	0.88	0.12
RMSE:	1.85	0.88	0.88

MAX_MEAN: 5.48 MAX_MED: 6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5,6-Benzoflavone
CHID: 30423 CASRN: 6051-87-2
SPID(S): Tox21_302024
M4ID: 12477109

HILL MODEL (in red):

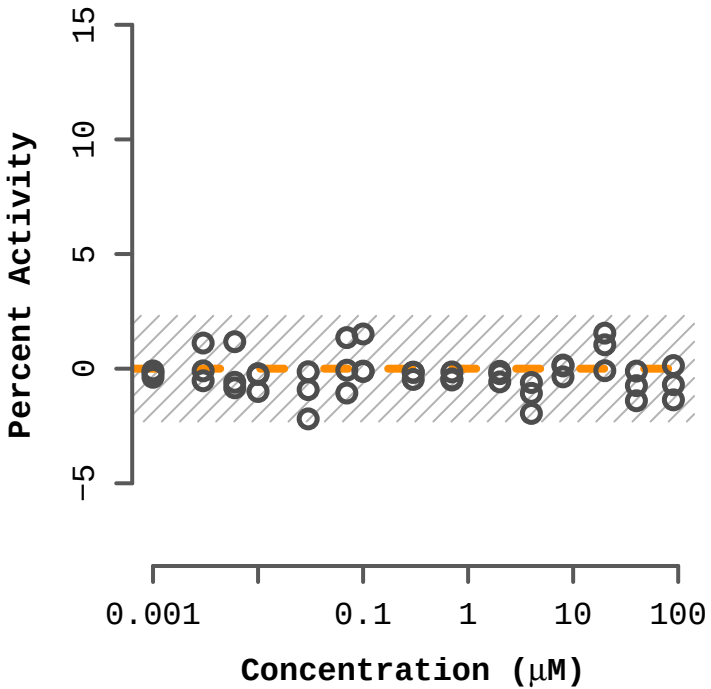
	tp	ga	gw
val:	14.9	2.45	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29.9	0.567	1.18	1.27	16.3
sd:	5.42	0.145	0.219	0.0127	6.5

	CNST	HILL	GNLS
AIC:	306.84	308.23	232.72
PROB:	0	0	1
RMSE:	8.08	7.41	2.99

MAX_MEAN: 23.7 MAX_MED: 24.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

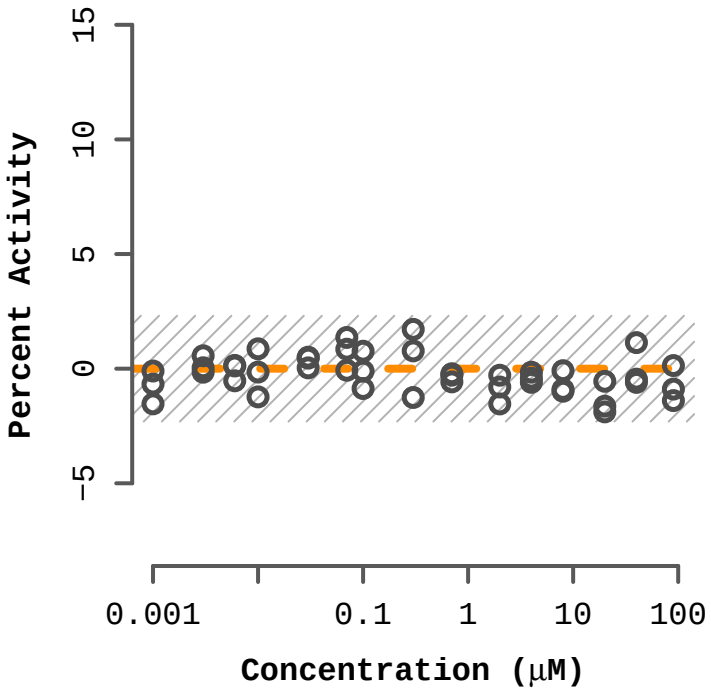
NAME: 5-(Hydroxymethyl)-2-furfural
CHID: 30428 **CASRN:** 67-47-0
SPID(S): Tox21_303551
M4ID: 12475594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.836 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

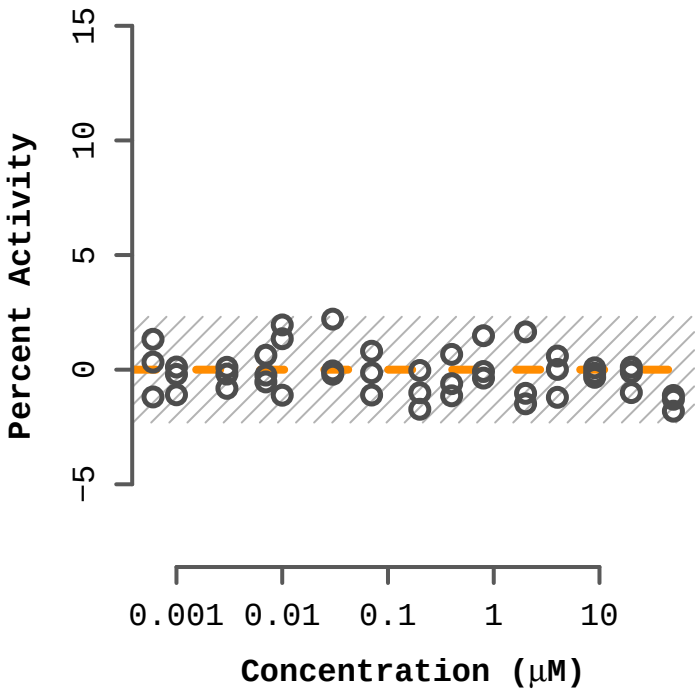
NAME: 5-(Hydroxymethyl)-2-furfural
CHID: 30428 CASRN: 67-47-0
SPID(S): Tox21_201892
M4ID: 12480360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.715 MAX_MED: 0.851 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

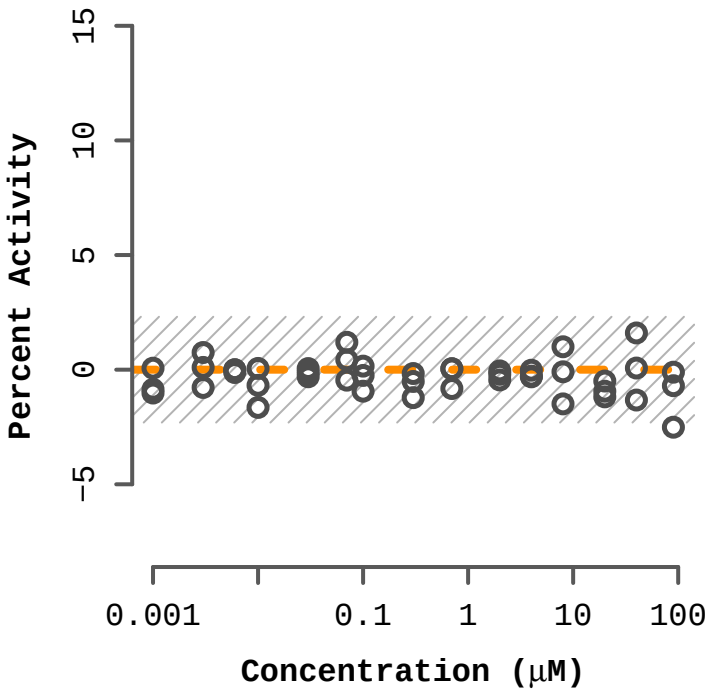
NAME: Decitabine
CHID: 30432 CASRN: 2353-33-5
SPID(S): Tox21_112311_1
M4ID: 12483169

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.73 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

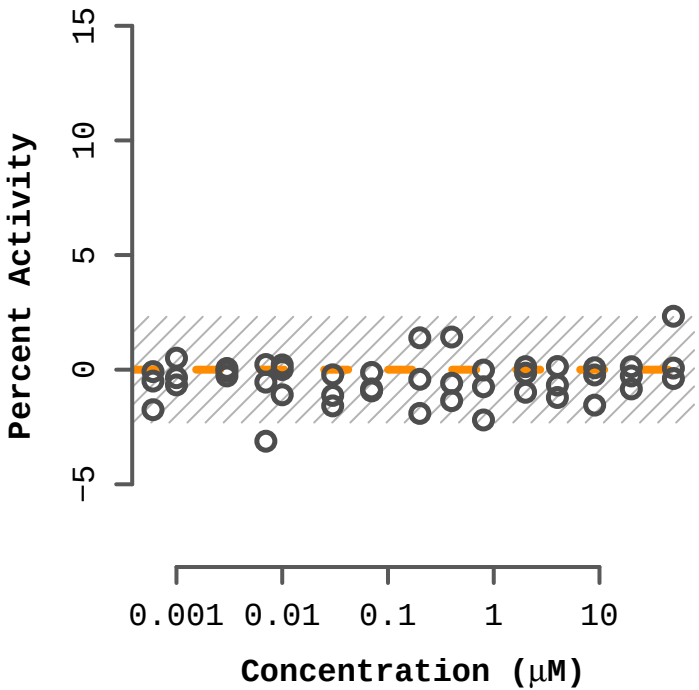
NAME: p-Synephrine
CHID: 30588 **CASRN:** 94-07-5
SPID(S): Tox21_200962
M4ID: 12481290

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.392 **MAX_MED:** 0.434 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

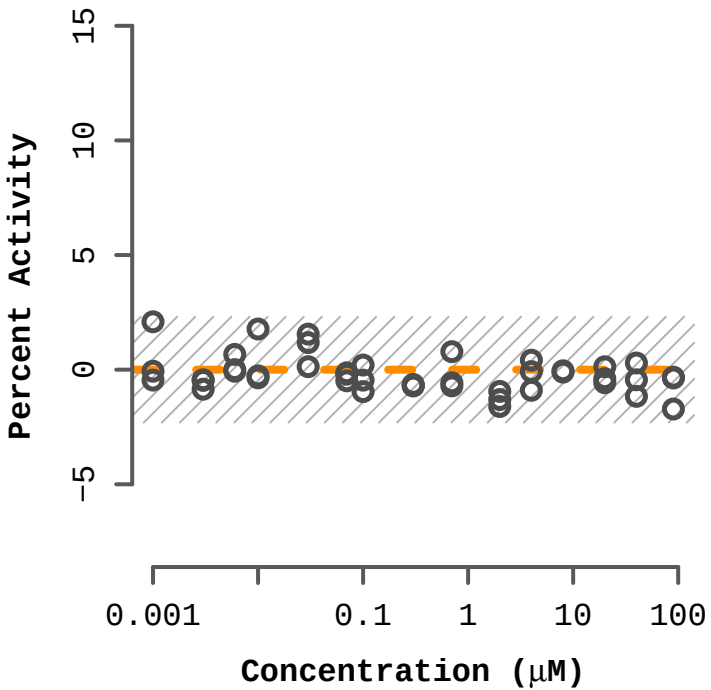
NAME: p-Synephrine
CHID: 30588 **CASRN:** 94-07-5
SPID(S): Tox21_110390_1
M4ID: 12484401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.0713 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

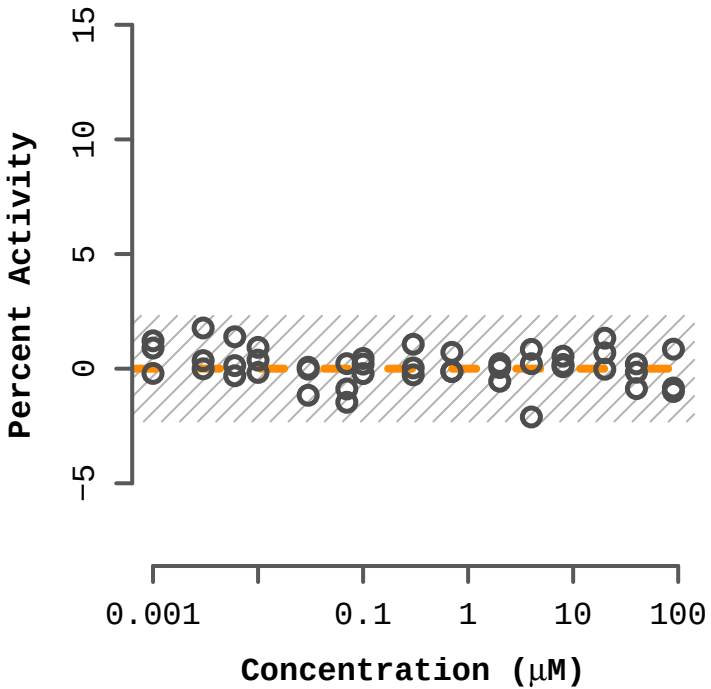
NAME: Abscisic acid
CHID: 30604 **CASRN:** 14375-45-2
SPID(S): Tox21_201137
M4ID: 12481115

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

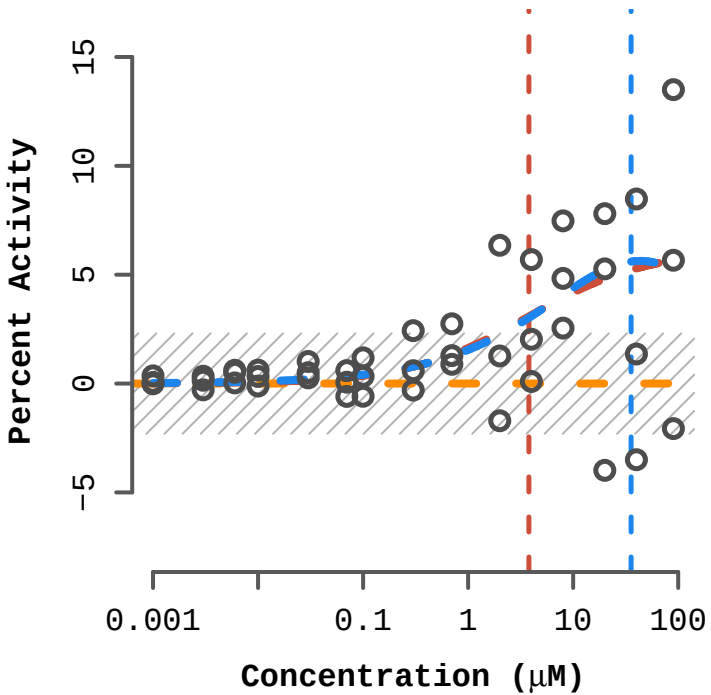
NAME: Acesulfame potassium
CHID: 30606 CASRN: 55589-62-3
SPID(S): Tox21_303370
M4ID: 12475765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.709 **MAX_MED:** 0.902 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acesulfame potassium
CHID: 30606 CASRN: 55589-62-3
SPID(S): Tox21_202423
M4ID: 12479829

HILL MODEL (in red):

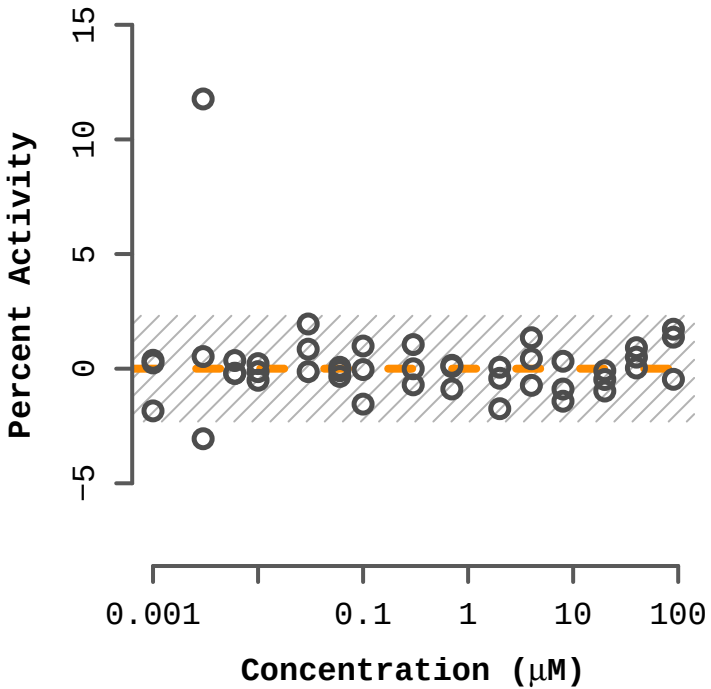
	tp	ga	gw
val:	6.16	0.578	0.766
sd:	2.35	0.586	0.441

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.2	1.55	0.622	1.97	0.843
sd:	59.8	3.68	0.455	2.01	1.5

	CNST	HILL	GNLS
AIC:	233.92	217.12	220.83
PROB:	0	0.87	0.13
RMSE:	3.65	2.93	2.98

MAX_MEAN: 5.7 **MAX_MED:** 5.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

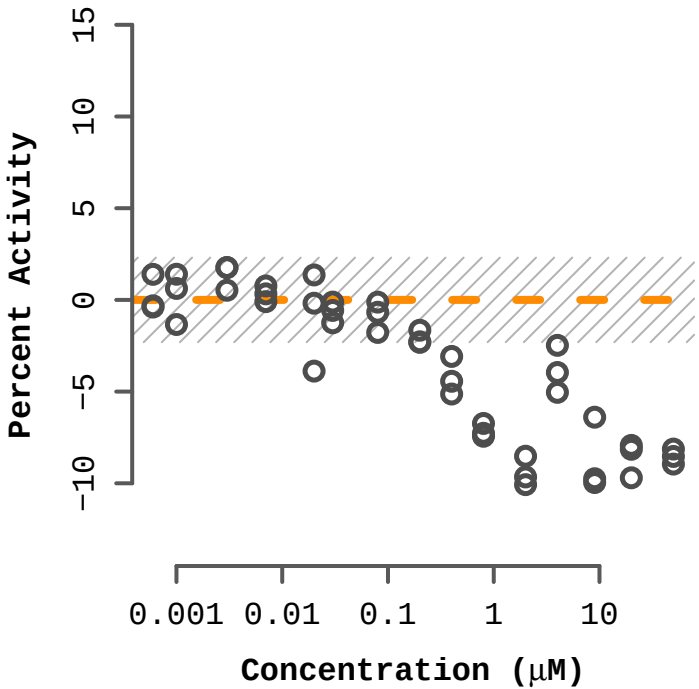
NAME: Acetal
CHID: 30607 **CASRN:** 105-57-7
SPID(S): Tox21_200274
M4ID: 12481978

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 3.08 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

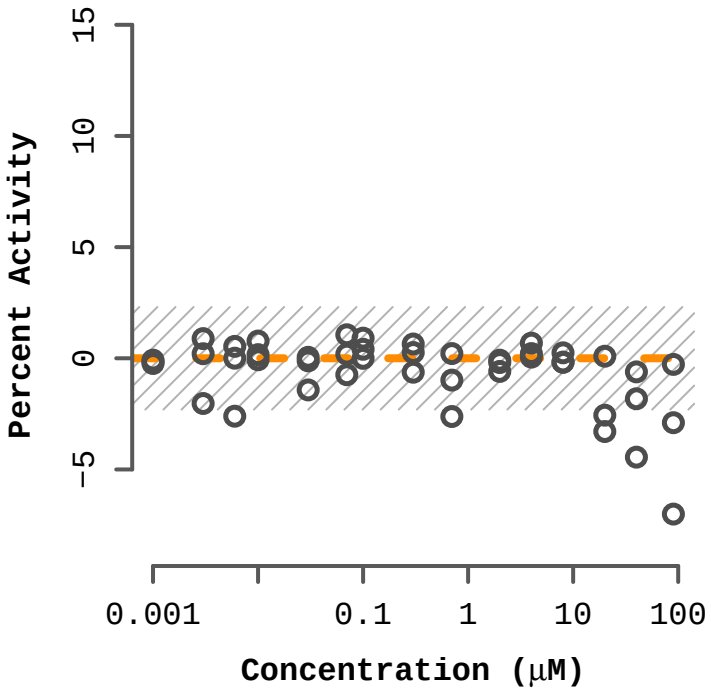
NAME: Adriamycin hydrochloride
CHID: 30636 **CASRN:** 25316-40-9
SPID(S): Tox21_202483
M4ID: 12479769

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	281.83	NA	NA
PROB:	1	NA	NA
RMSE:	5.27	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

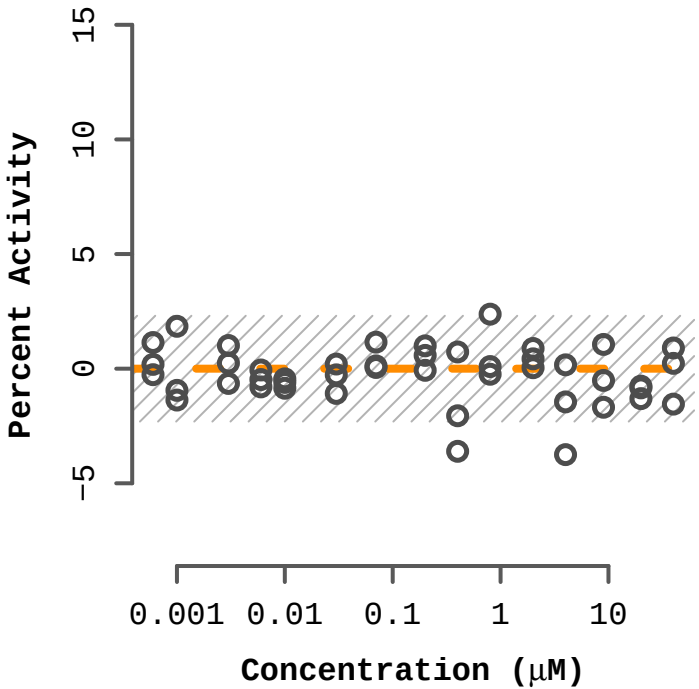
NAME: Aloe−emodin
CHID: 30695 **CASRN:** 481−72−1
SPID(S): Tox21_302400
M4ID: 12476733

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.437 **MAX_MED:** 0.406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

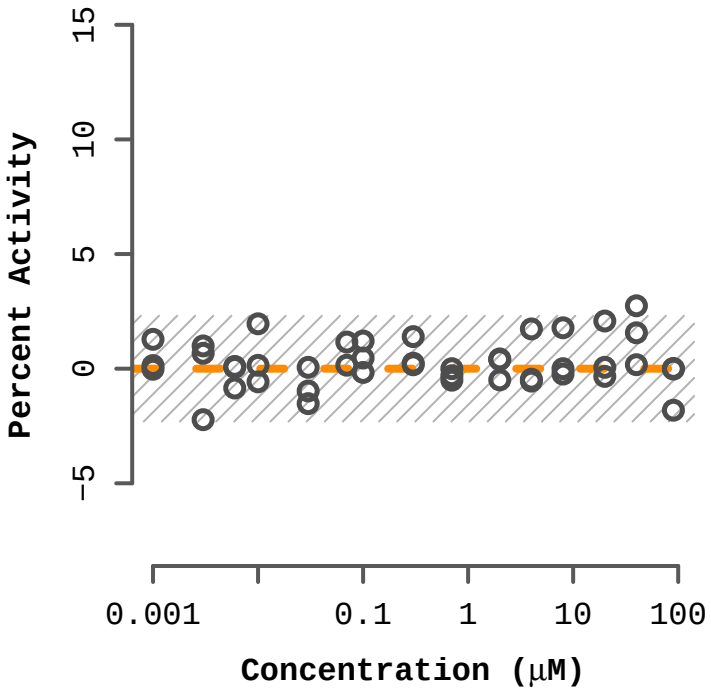
NAME: alpha-Cyclodextrin
CHID: 30698 CASRN: 10016-20-3
SPID(S): Tox21_300302
M4ID: 12478828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.744 **MAX_MED:** 0.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

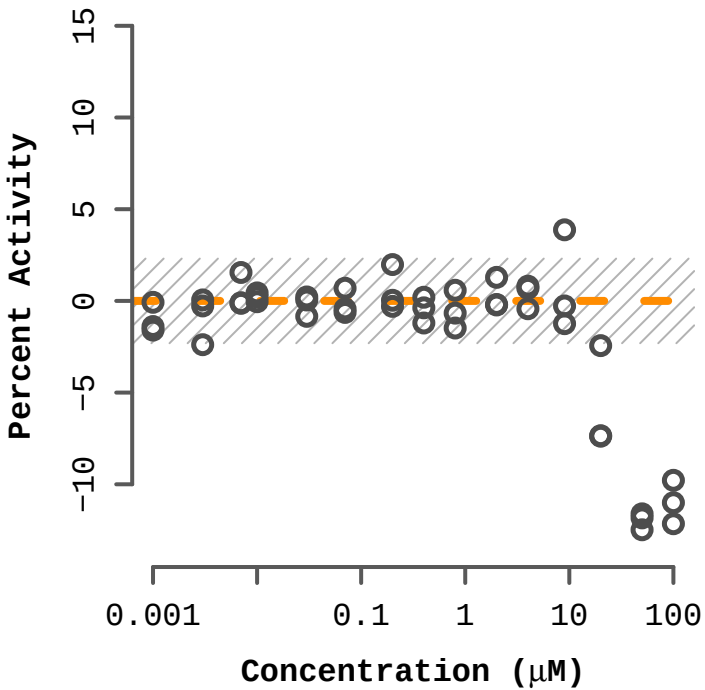
NAME: alpha-Cyclodextrin
CHID: 30698 **CASRN:** 10016-20-3
SPID(S): Tox21_201252
M4ID: 12481000

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

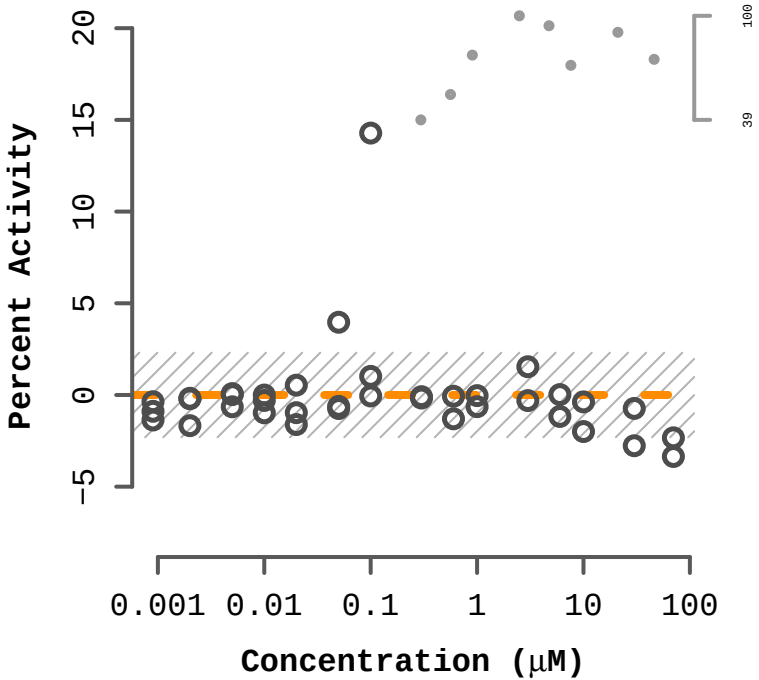
NAME: alpha-Solanine
CHID: 30707 **CASRN:** 20562-02-1
SPID(S): Tox21_200104
M4ID: 12482148

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.96	NA	NA
PROB:	1	NA	NA
RMSE:	4.6	NA	NA

MAX_MEAN: 0.788 **MAX_MED:** 0.687 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

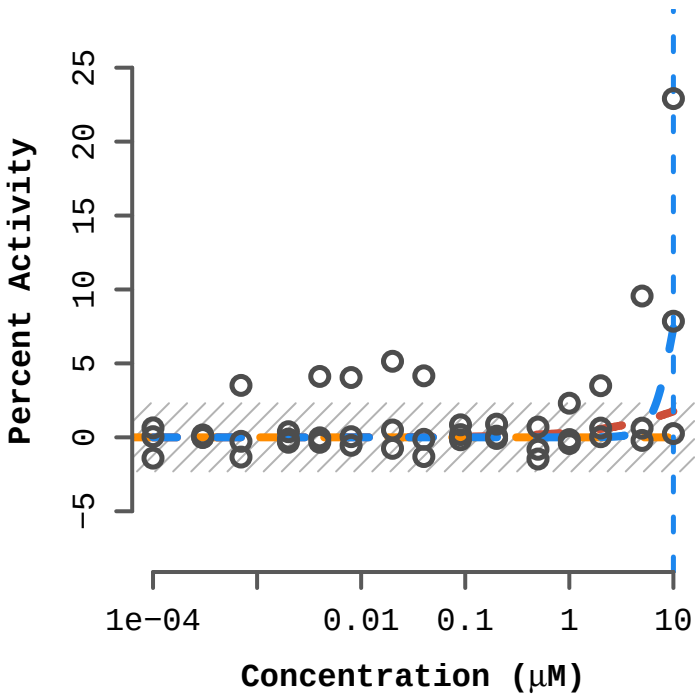
NAME: Azithromycin
CHID: 30760 **CASRN:** 83905-01-5
SPID(S): Tox21_201011
M4ID: 12481241 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	405.2	NA	NA
PROB:	1	NA	NA
RMSE:	34.06	NA	NA

MAX_MEAN: 35.4 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Black cohosh
CHID: 30857 CASRN: 84776-26-1
SPID(S): Tox21_202729
M4ID: 12479523

HILL MODEL (in red):

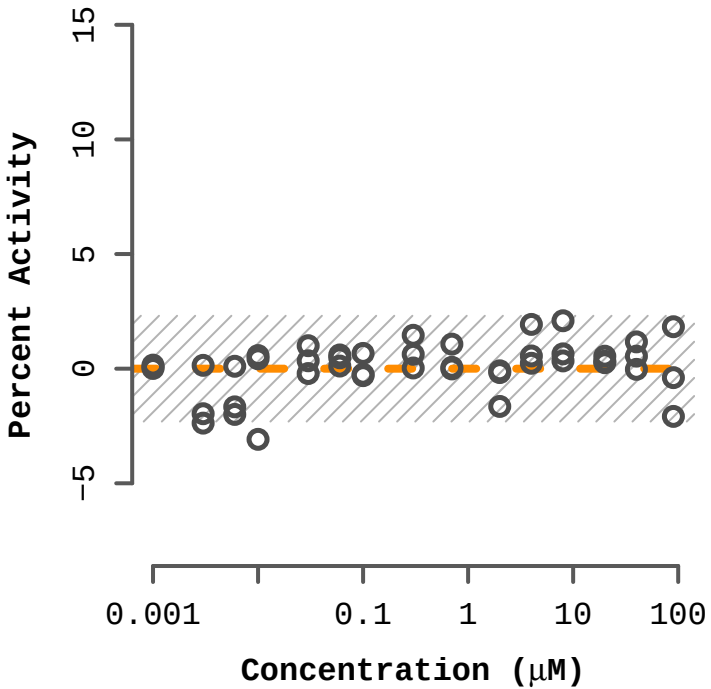
	tp	ga	gw
val:	6.37	1.5	0.841
sd:	60.1	6.6	1.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.8	1	4.42	2.8	3.55
sd:	116	1.55	12	3650	7440

	CNST	HILL	GNLS
AIC:	209.76	212.75	214.71
PROB:	0.76	0.17	0.06
RMSE:	4.21	3.88	3.3

MAX_MEAN: 10.3 **MAX_MED:** 7.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

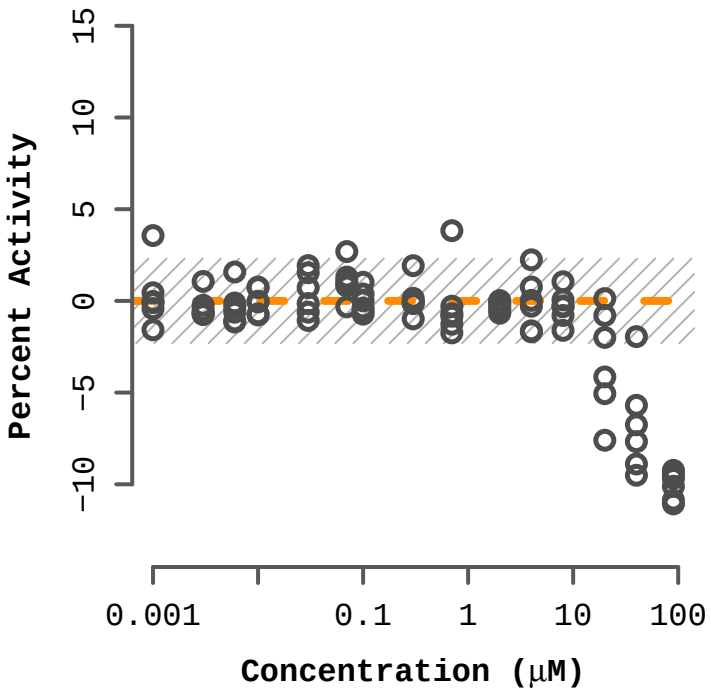
NAME: Camphor
CHID: 30955 **CASRN:** 76-22-2
SPID(S): Tox21_200237
M4ID: 12482015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.648 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

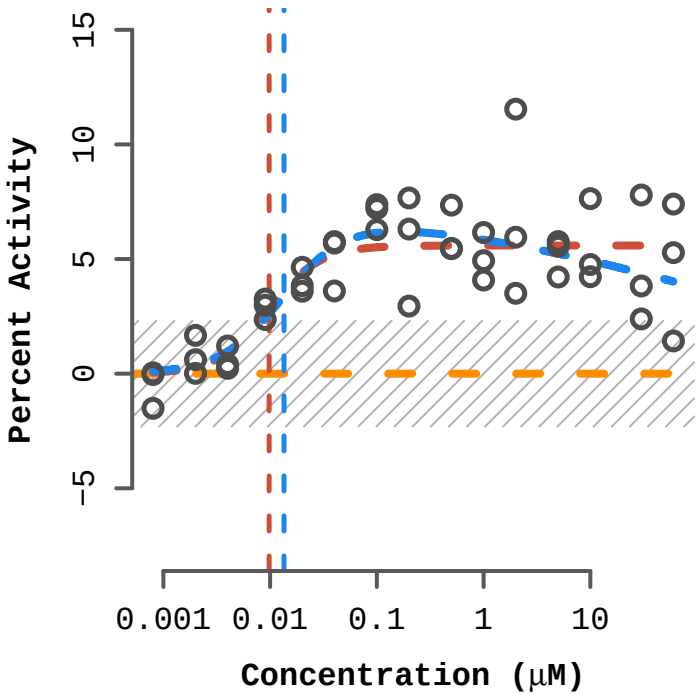
NAME: Curcumin
CHID: 31077 **CASRN:** 458-37-7
SPID(S): Tox21_201116
M4ID: 12481136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	441.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.52	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.994 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D&C Red 27
CHID: 31089 CASRN: 13473-26-2
SPID(S): Tox21_303604
M4ID: 12475541

HILL MODEL (in red):

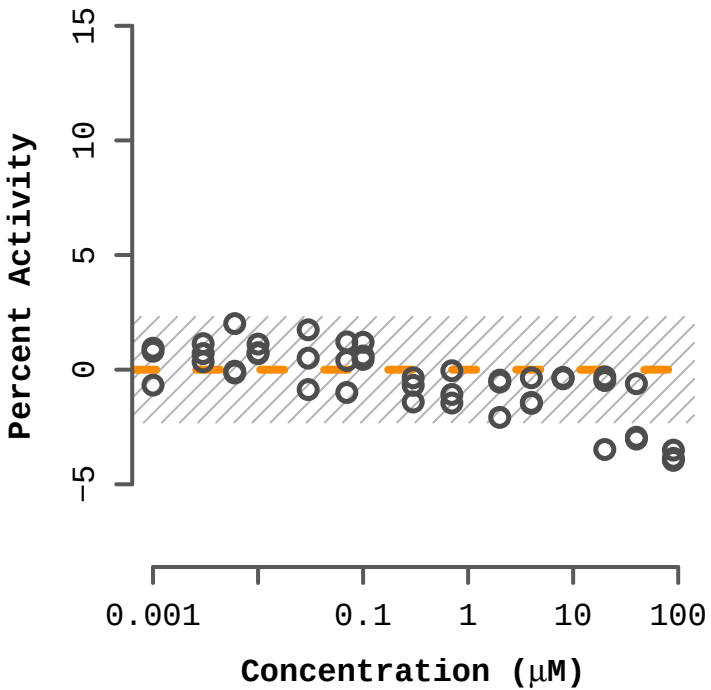
	tp	ga	gw
val:	5.59	−2.01	1.84
sd:	0.307	0.0916	0.524

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.2	−1.87	1.49	2.12	0.3
sd:	6.74	0.311	0.557	1.74	0.842

	CNST	HILL	GNLS
AIC:	281.38	175.48	175.67
PROB:	0	0.52	0.48
RMSE:	5.02	1.65	1.62

MAX_MEAN: 7 MAX_MED: 7.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

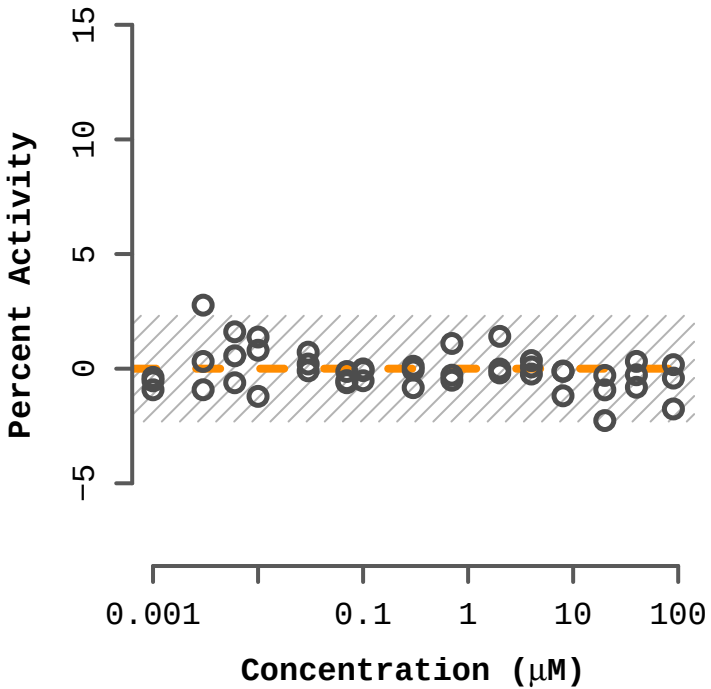
NAME: D&C Red 27
CHID: 31089 **CASRN:** 13473-26-2
SPID(S): Tox21_202165
M4ID: 12480087

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 0.853 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

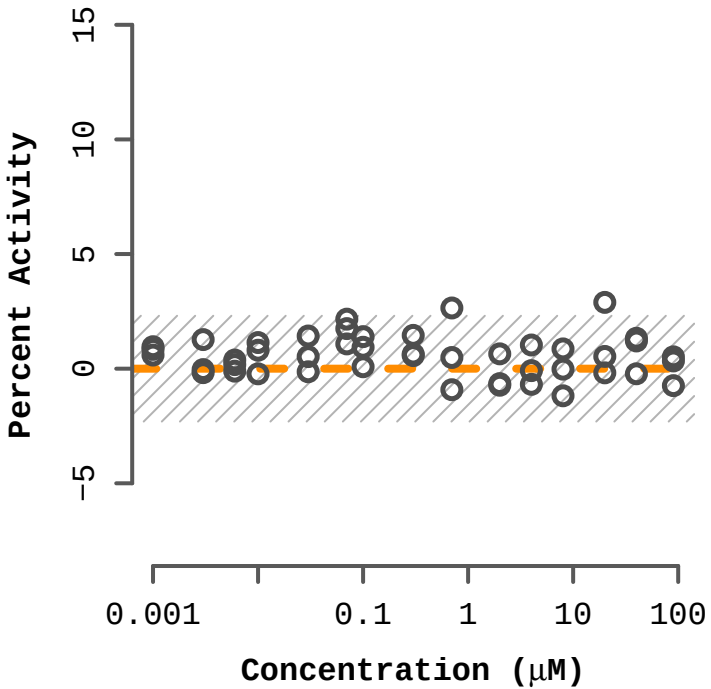
NAME: Dipentyl phthalate
CHID: 31131 CASRN: 131-18-0
SPID(S): Tox21_300304
M4ID: 12478826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.724 **MAX_MED:** 0.805 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

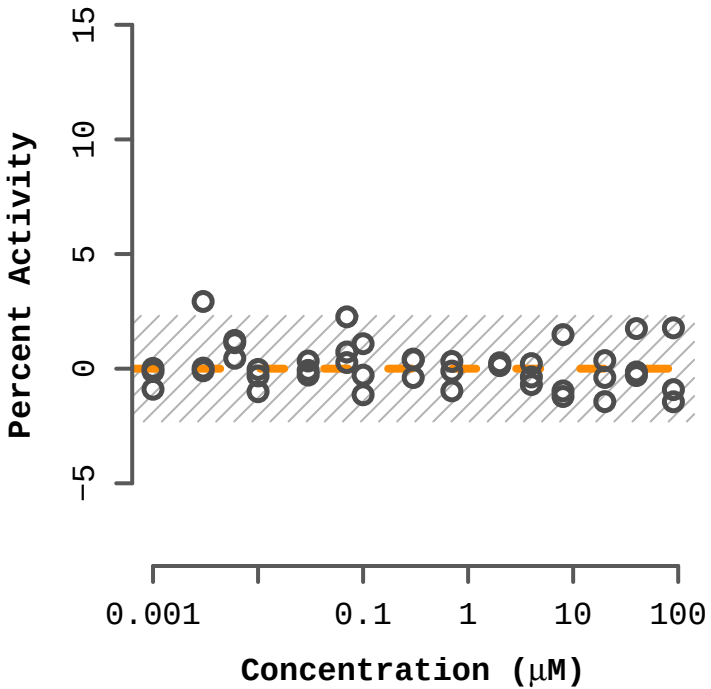
NAME: Dipentyl phthalate
CHID: 31131 CASRN: 131-18-0
SPID(S): Tox21_201519
M4ID: 12480733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

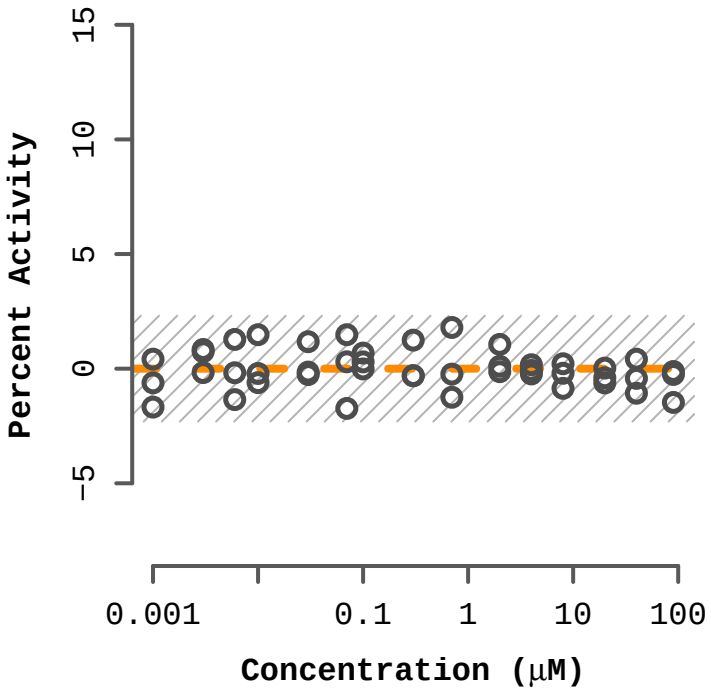
NAME: Dipropyl phthalate
CHID: 31133 **CASRN:** 131-16-8
SPID(S): Tox21_303379
M4ID: 12475758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

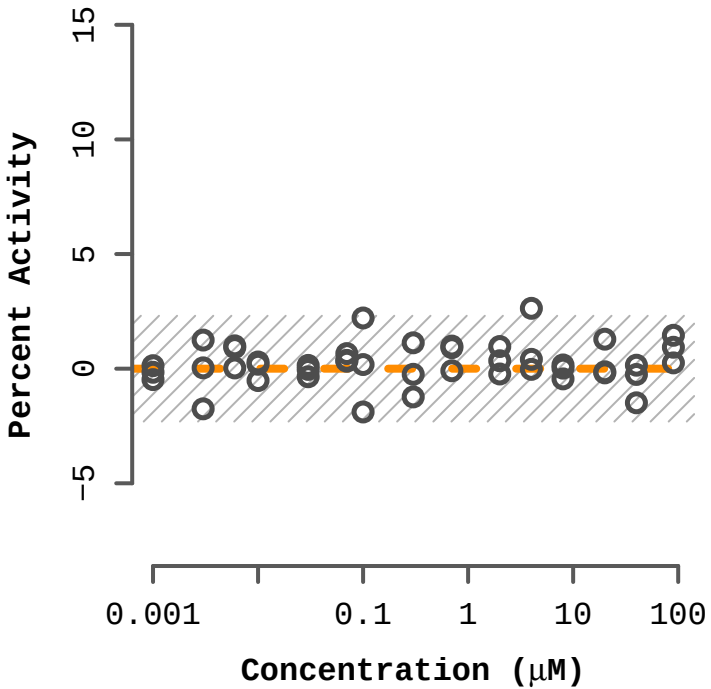
NAME: Dipropyl phthalate
CHID: 31133 **CASRN:** 131-16-8
SPID(S): Tox21_201662
M4ID: 12480590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.471 **MAX_MED:** 0.743 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

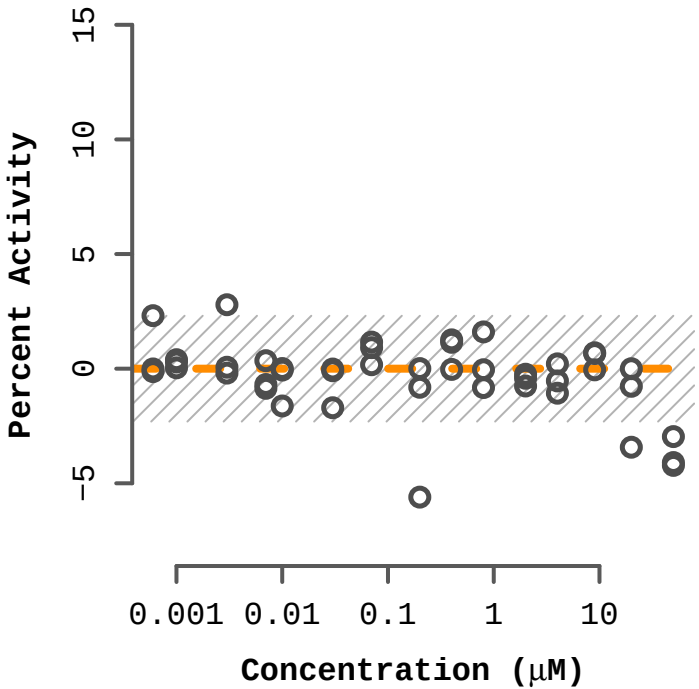
NAME: tert−Butyl hydroperoxide (70% Solution in Wate
CHID: 31209 CASRN: NOCAS_31209
SPID(S): Tox21_200838
M4ID: 12481414

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1 MAX_MED: 0.936 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

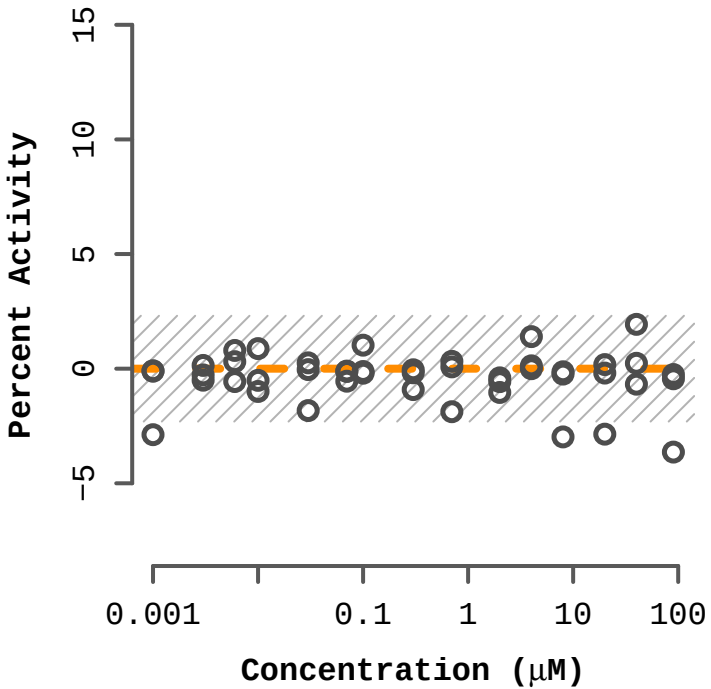
NAME: Diquat dibromide monohydrate
CHID: 31248 CASRN: 6385-62-2
SPID(S): Tox21_301145
M4ID: 12477988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 0.888 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

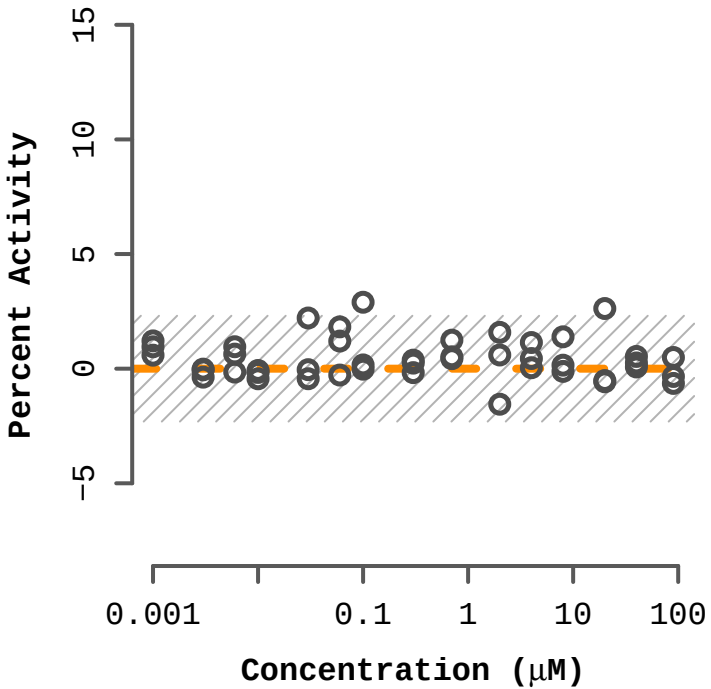
NAME: 1-(2,3,8,8-Tetramethyl-1,2,3,4,5,6,7,8-octahydr
CHID: 31290 **CASRN:** 54464-57-2
SPID(S): Tox21_303483
M4ID: 12475658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.509 **MAX_MED:** 0.307 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

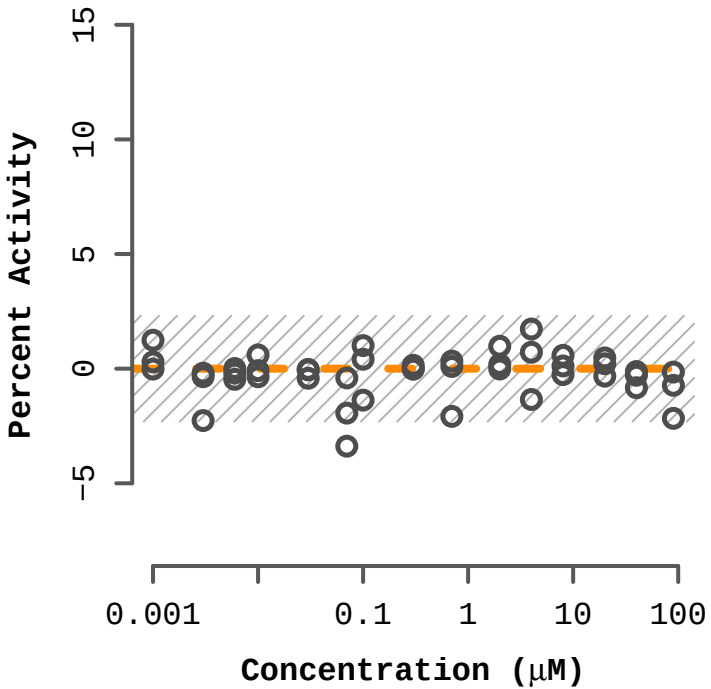
NAME: 1-(2,3,8,8-Tetramethyl-1,2,3,4,5,6,7,8-octahydr
CHID: 31290 **CASRN:** 54464-57-2
SPID(S): Tox21_201355
M4ID: 12480897

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

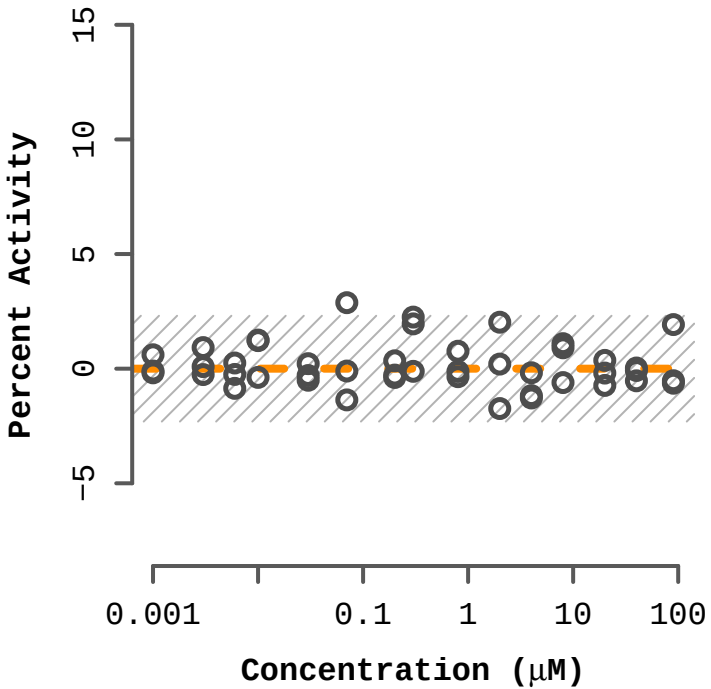
NAME: Ethoxyacetic acid
CHID: 31294 **CASRN:** 627-03-2
SPID(S): Tox21_303384
M4ID: 12475754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.507 **MAX_MED:** 0.716 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

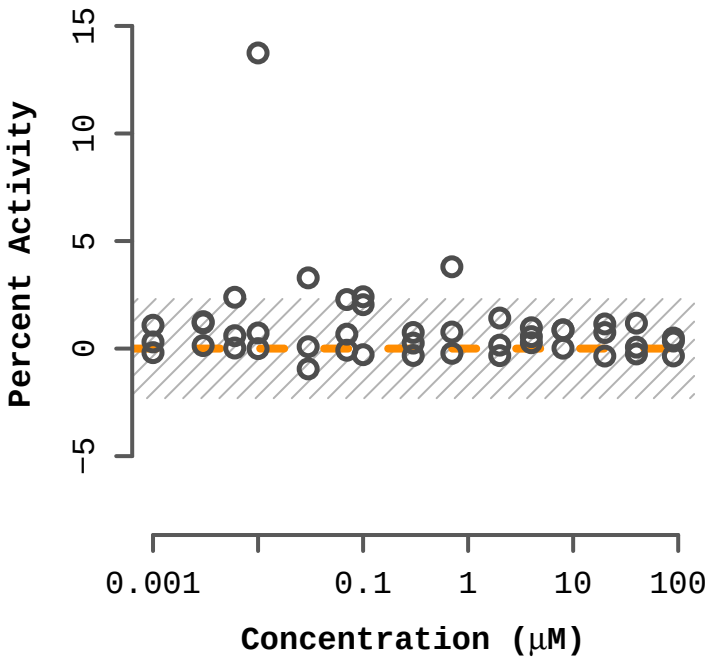
NAME: Ethoxyacetic acid
CHID: 31294 CASRN: 627-03-2
SPID(S): Tox21_202431
M4ID: 12479821

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.36 MAX_MED: 1.96 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

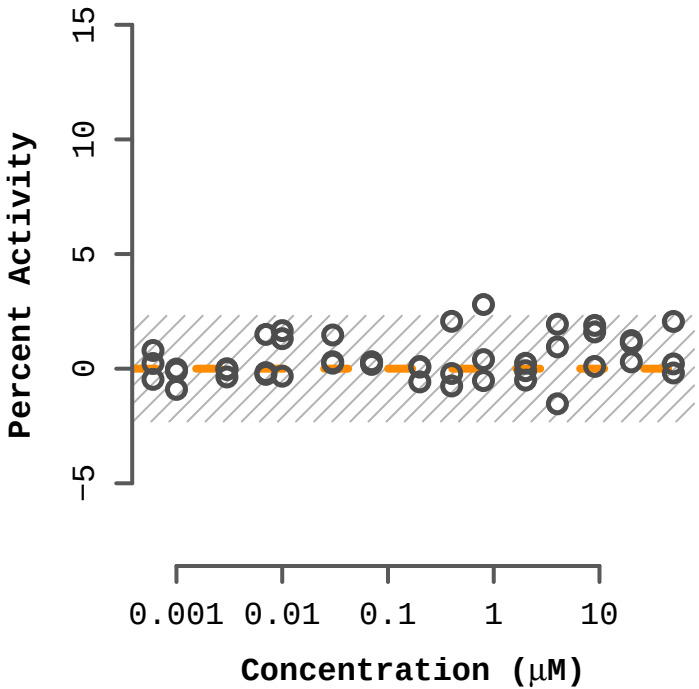
NAME: Galactosamine hydrochloride
CHID: 31356 CASRN: 1772-03-8
SPID(S): Tox21_302002
M4ID: 12477131

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.89	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 4.82 MAX_MED: 2.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

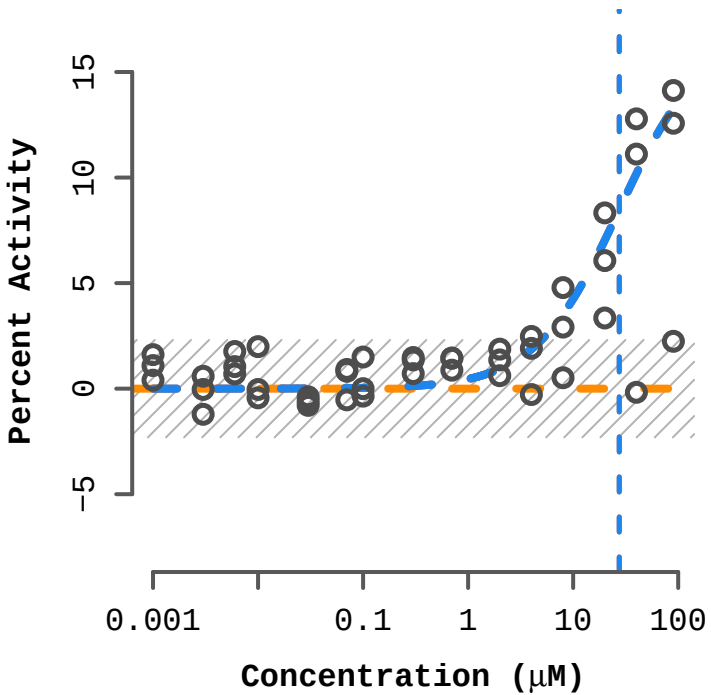
NAME: Ginkgo biloba extract
CHID: 31366 CASRN: 90045-36-6
SPID(S): Tox21_202516
M4ID: 12479736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.2 MAX_MED: 1.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glycidamide
CHID: 31374 CASRN: 5694-00-8
SPID(S): Tox21_303874
M4ID: 12475314

HILL MODEL (in red):

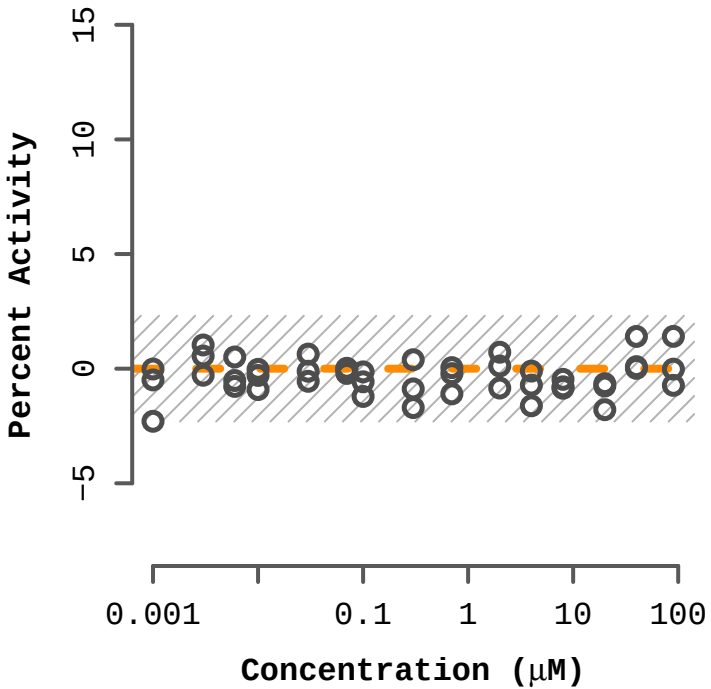
	tp	ga	gw
val:	17	1.44	1.08
sd:	3.95	0.244	0.331

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17	1.44	1.08	3.38	5.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	238.52	187.01	191.01
PROB:	0	0.88	0.12
RMSE:	4.33	2.57	2.57

MAX_MEAN: 9.65 MAX_MED: 12.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

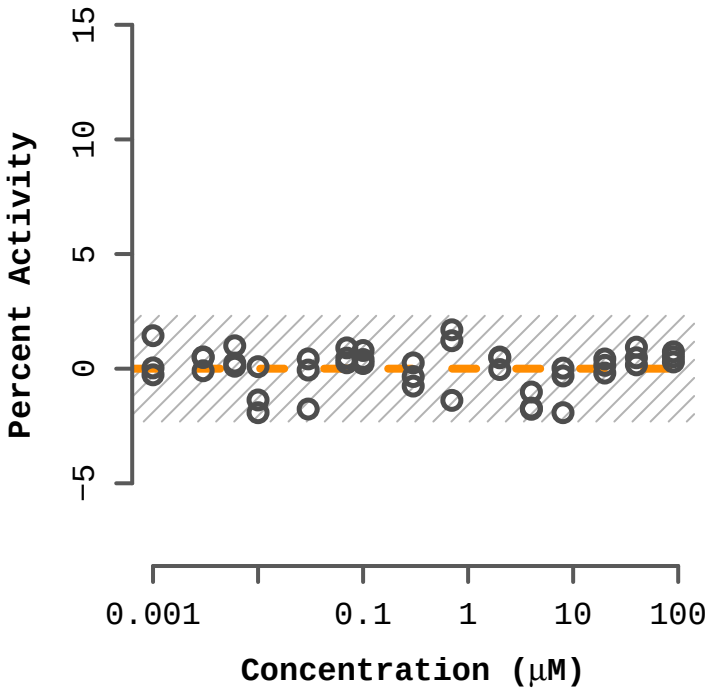
NAME: Glycoluril
CHID: 31380 CASRN: 496-46-8
SPID(S): Tox21_301392
M4ID: 12477741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.504 MAX_MED: 0.553 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

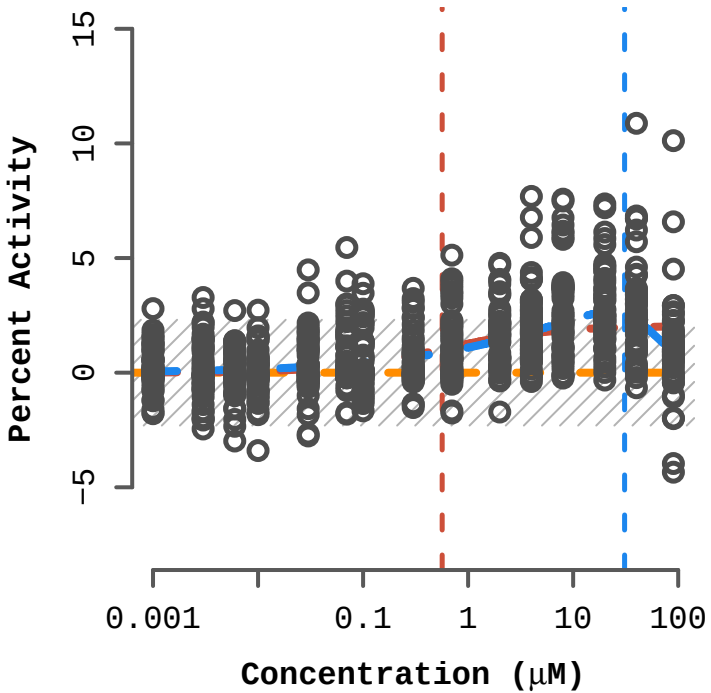
NAME: Indium(III) phosphide
CHID: 31444 CASRN: 22398-80-7
SPID(S): Tox21_302280
M4ID: 12476853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.544 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indole-3-carbinol
CHID: 31458 CASRN: 700-06-1
SPID(S): Tox21_400055
M4ID: 12475082

HILL MODEL (in red):

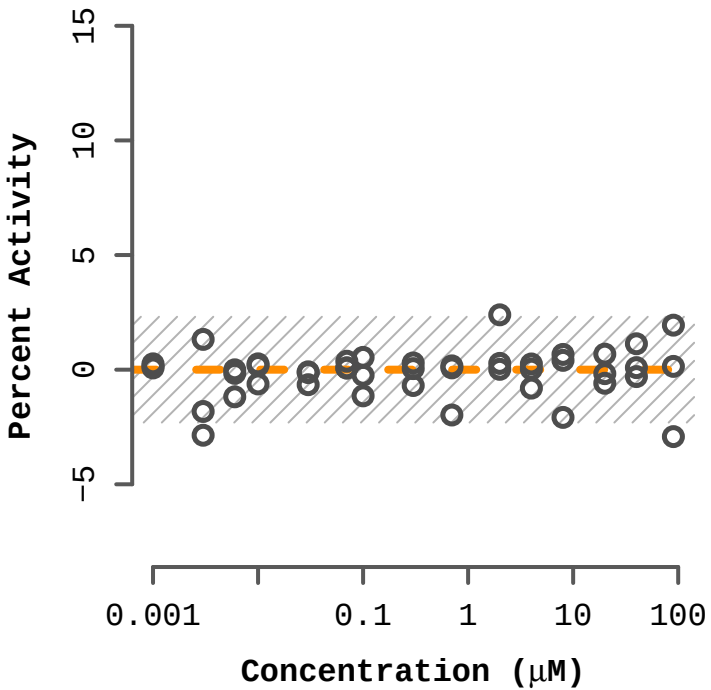
	tp	ga	gw
val:	2.04	−0.247	0.847
sd:	0.133	0.138	0.169

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.34	1.49	0.457	1.74	2.43
sd:	6.51	1.61	0.126	0.126	0.723

	CNST	HILL	GNLS
AIC:	3047.18	2656.35	2612.03
PROB:	0	0	1
RMSE:	2.15	1.62	1.57

MAX_MEAN: 2.83 MAX_MED: 2.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

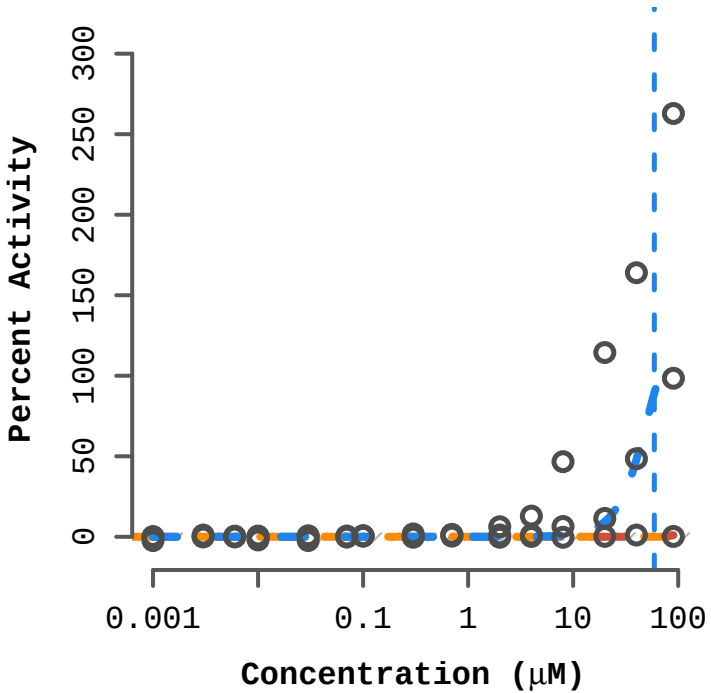
NAME: 1-Butyl-1-methylpyrrolidinium chloride
CHID: 31460 **CASRN:** 479500-35-1
SPID(S): Tox21_303389
M4ID: 12475749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 0.407 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-1-methylpyrrolidinium chloride
CHID: 31460 CASRN: 479500-35-1
SPID(S): Tox21_201819
M4ID: 12480433

HILL MODEL (in red):

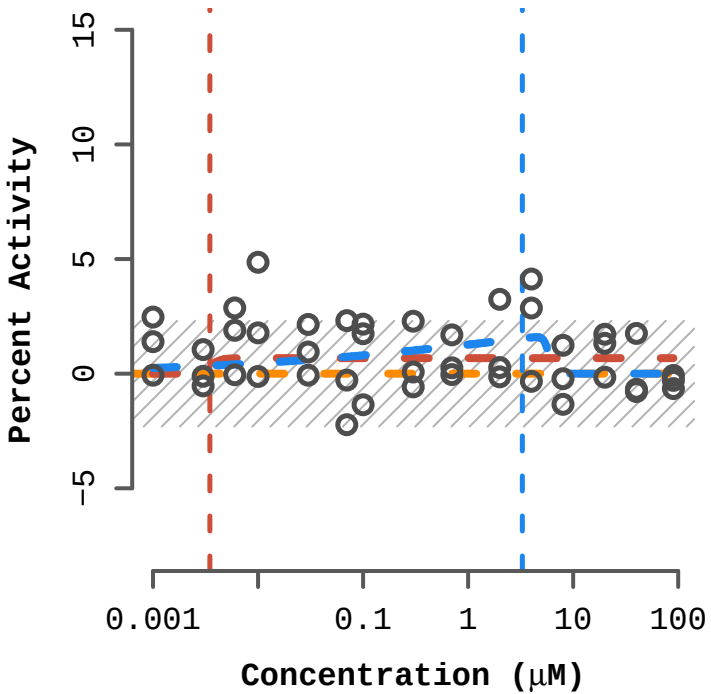
	tp	ga	gw
val:	89.6	2.45	3.89
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	188	1.77	2.71	2.02	5.14
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	386.61	392.5	385.2
PROB:	0.33	0.02	0.66
RMSE:	52.44	52.28	38.26

MAX_MEAN: 121 MAX_MED: 98.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylimidazolium chloride
CHID: 31461 **CASRN:** 79917-90-1
SPID(S): Tox21_303611
M4ID: 12475534

HILL MODEL (in red):

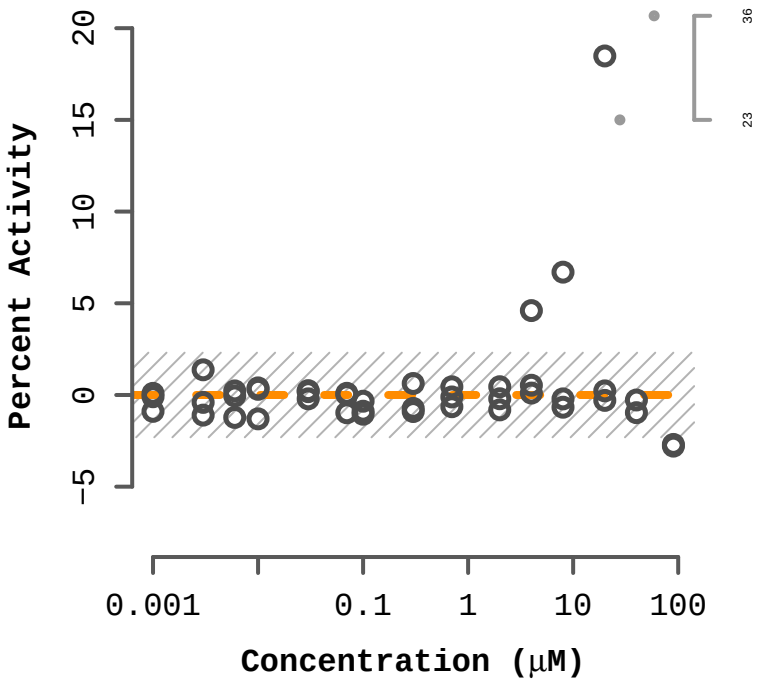
	tp	ga	gw
val:	0.677	−2.46	8
sd:	0.258	0.263	16.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.07	0.516	0.3	0.768	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	177.76	176.65	178.68
PROB:	0.3	0.52	0.19
RMSE:	1.71	1.53	1.49

MAX_MEAN: 2.22 **MAX_MED:** 2.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

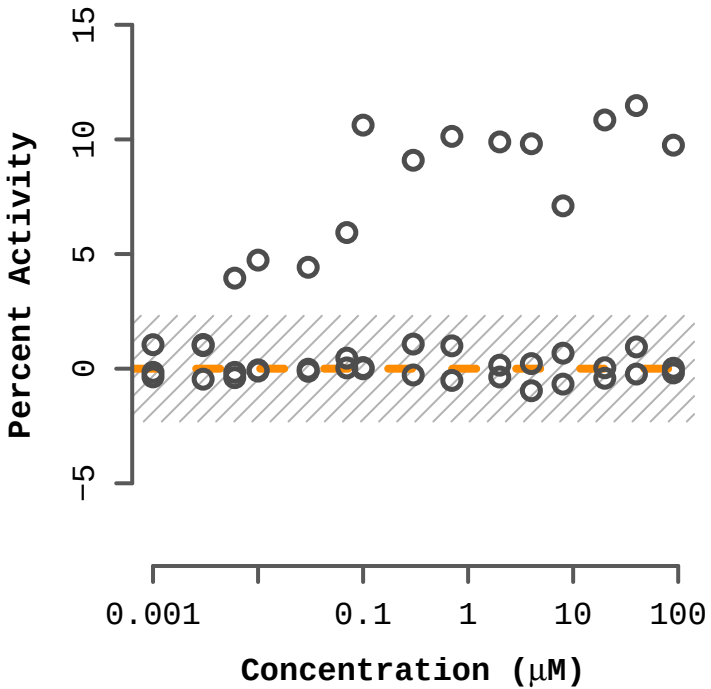
NAME: 1-Butyl-3-methylimidazolium chloride
CHID: 31461 **CASRN:** 79917-90-1
SPID(S): Tox21_201690
M4ID: 12480562 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.84	NA	NA
PROB:	1	NA	NA
RMSE:	7.1	NA	NA

MAX_MEAN: 10.2 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

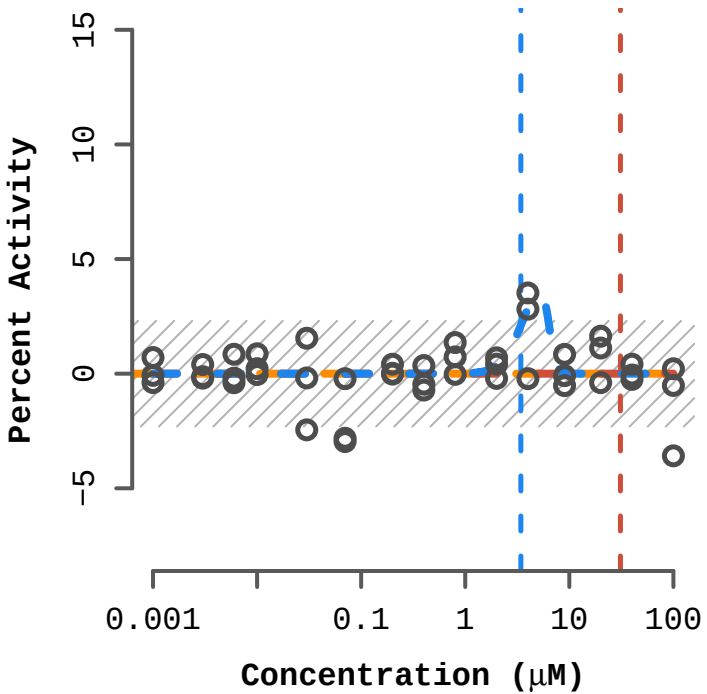
NAME: N-Butylpyridinium chloride
CHID: 31462 **CASRN:** 1124-64-7
SPID(S): Tox21_303503
M4ID: 12475639

HILL MODEL: Not applicable.

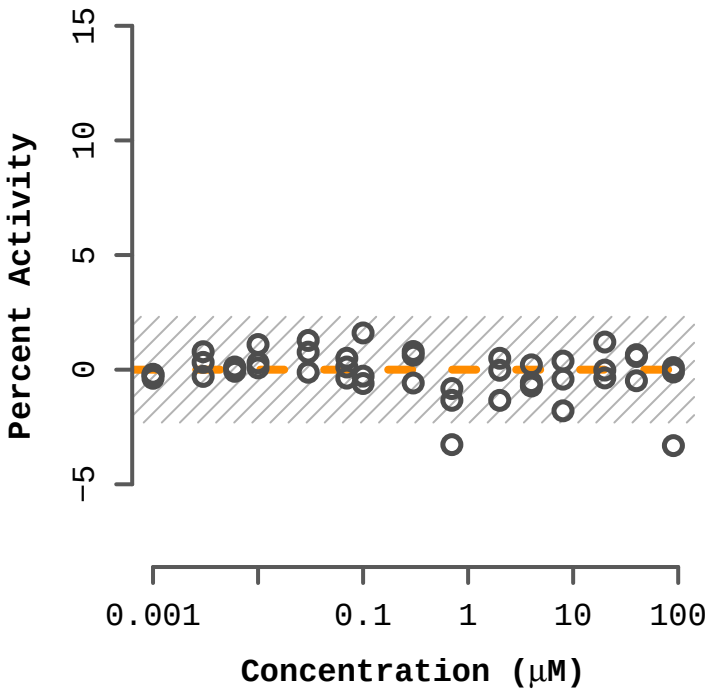
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.56	NA	NA
PROB:	1	NA	NA
RMSE:	4.69	NA	NA

MAX_MEAN: 4.06 **MAX_MED:** 1.07 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Butylpyridinium chloride
CHID:    31462   CASRN: 1124-64-7
SPID(S): Tox21_201416
M4ID:    12480836

HILL MODEL (in red):
      tp       ga       gw
val:  3.31e-09 1.49     1.55
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.23     0.534    4.58     0.808    14
sd:   13.3     0.768    9.98     1.35     129

      CNST        HILL        GNLS
AIC:  139.06      145.06      140.37
PROB: 0.64        0.03        0.33
RMSE: 1.25        1.25        1.15

MAX_MEAN: 2.04      MAX_MED: 2.82      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

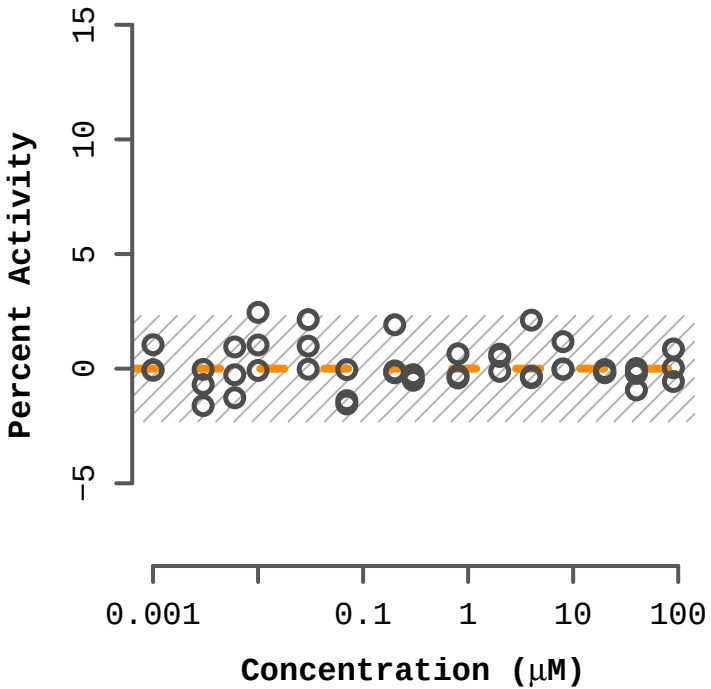
NAME: Isopropenyl acetate
CHID: 31492 **CASRN:** 108-22-5
SPID(S): Tox21_303350
M4ID: 12475783

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.644 **MAX_MED:** 0.767 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

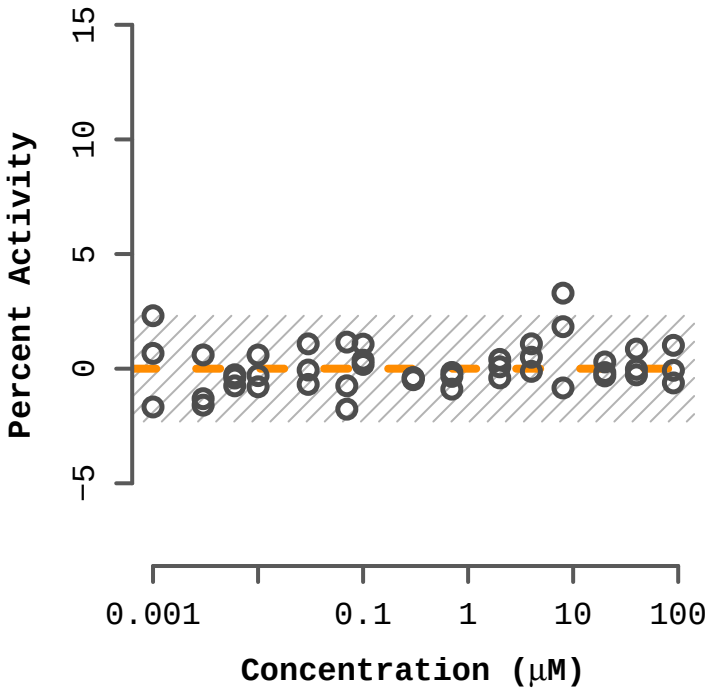
NAME: Isopropenyl acetate
CHID: 31492 **CASRN:** 108-22-5
SPID(S): Tox21_201748
M4ID: 12480504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

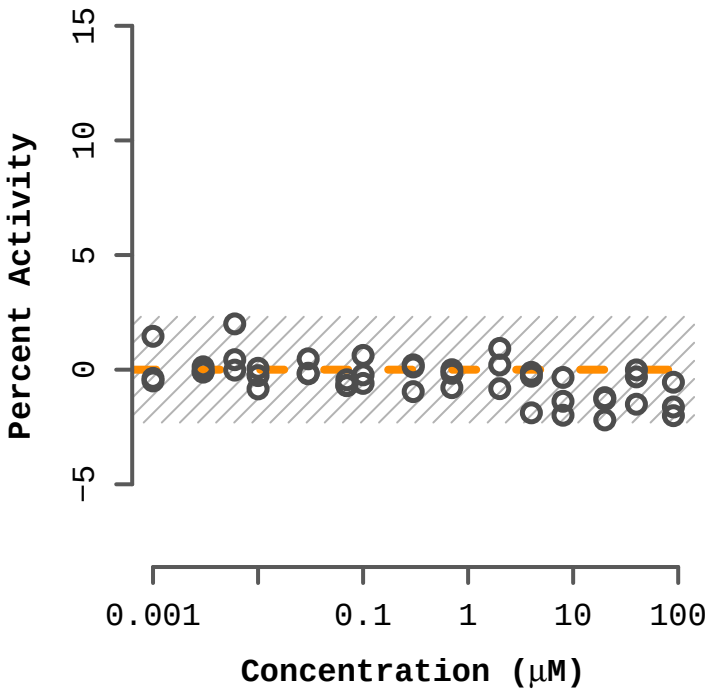
NAME: Isopropyl methanesulfonate
CHID: 31497 **CASRN:** 926-06-7
SPID(S): Tox21_200855
M4ID: 12481397

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

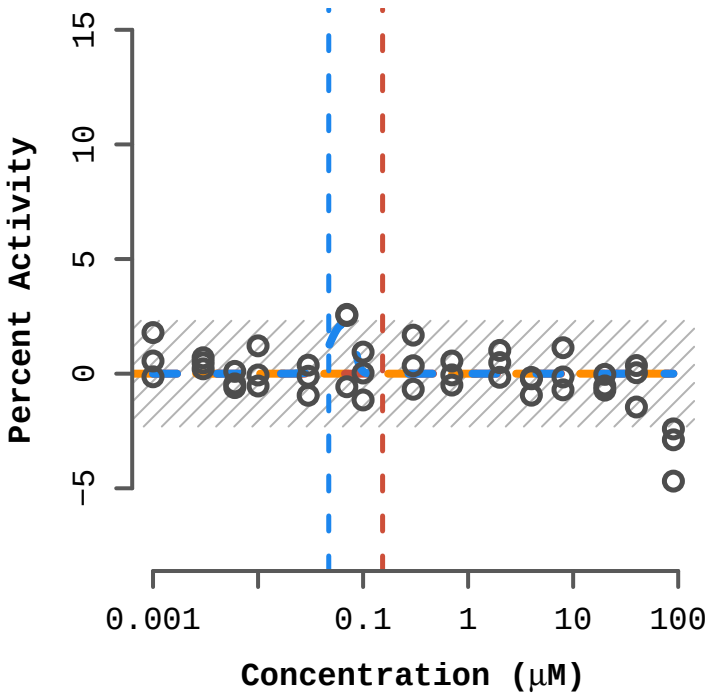
NAME: Lead(II) acetate trihydrate
CHID: 31521 **CASRN:** 6080-56-4
SPID(S): Tox21_303505
M4ID: 12475637

HILL MODEL: Not applicable.

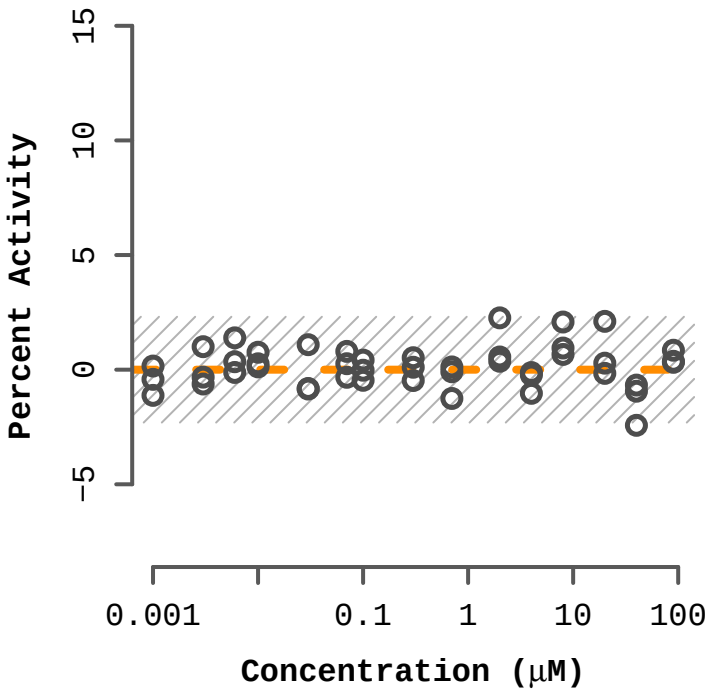
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.806 **MAX_MED:** 0.437 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Leucomalachite green
CHID:    31531   CASRN: 129-73-7
SPID(S): Tox21_302103
M4ID:    12477030

HILL MODEL (in red):
      tp        ga        gw
val:  1.92e-10 -0.814    2.19
sd:   6.4e-06  2660      209000

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  2.4       -1.33     8         -1.08     18
sd:   1.41      0.263     9.99      0.147     31.8

      CNST         HILL         GNLS
AIC:  140.45       146.45       144.68
PROB: 0.85         0.04         0.1
RMSE: 1.25         1.25         1.2

MAX_MEAN: 1.52      MAX_MED: 2.54      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

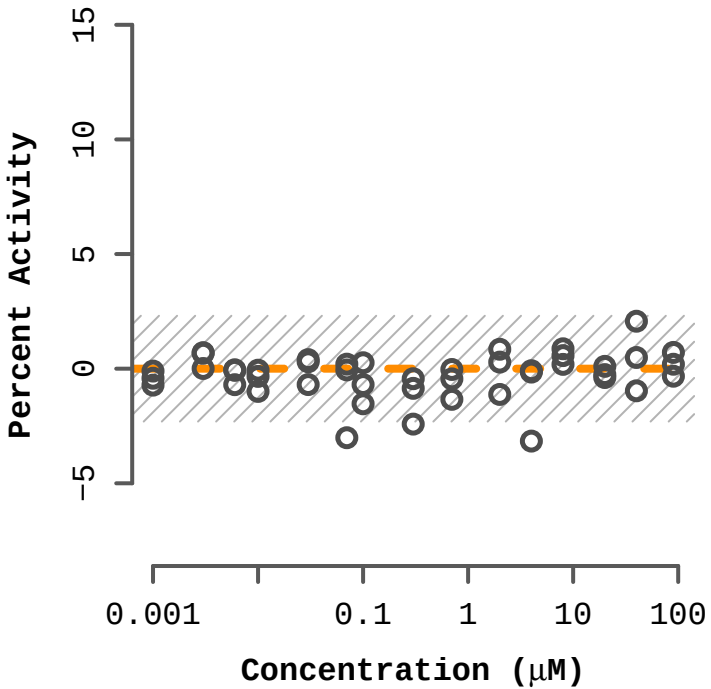
NAME: Lime oil
CHID: 31532 **CASRN:** 8008-26-2
SPID(S): Tox21_200691
M4ID: 12481561

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.944 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

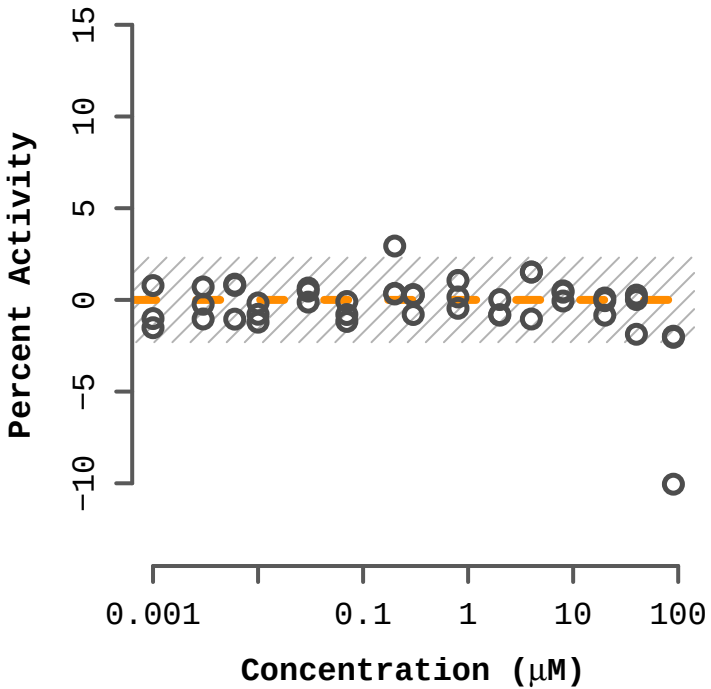
NAME: Methoxyacetic acid
CHID: 31591 **CASRN:** 625-45-6
SPID(S): Tox21_303516
M4ID: 12475626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.543 **MAX_MED:** 0.675 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

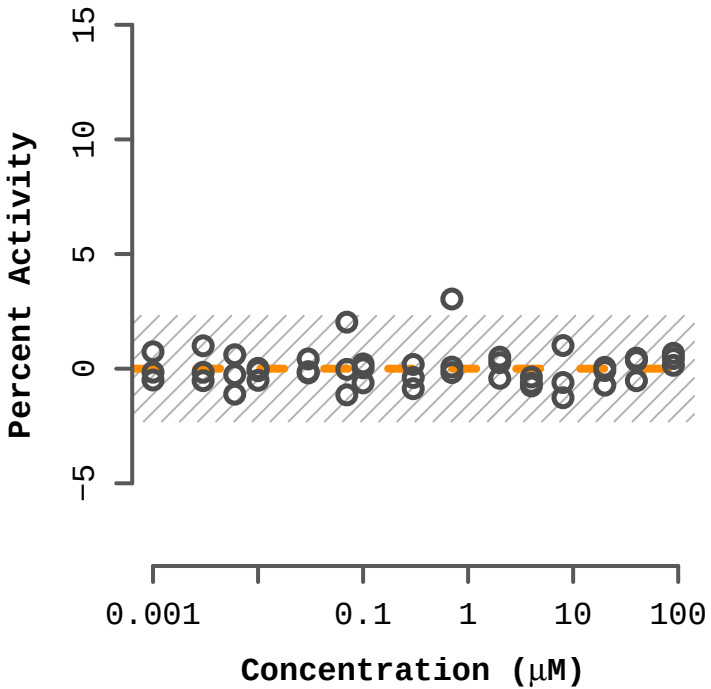
NAME: Methoxyacetic acid
CHID: 31591 **CASRN:** 625-45-6
SPID(S): Tox21_201571
M4ID: 12480681

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

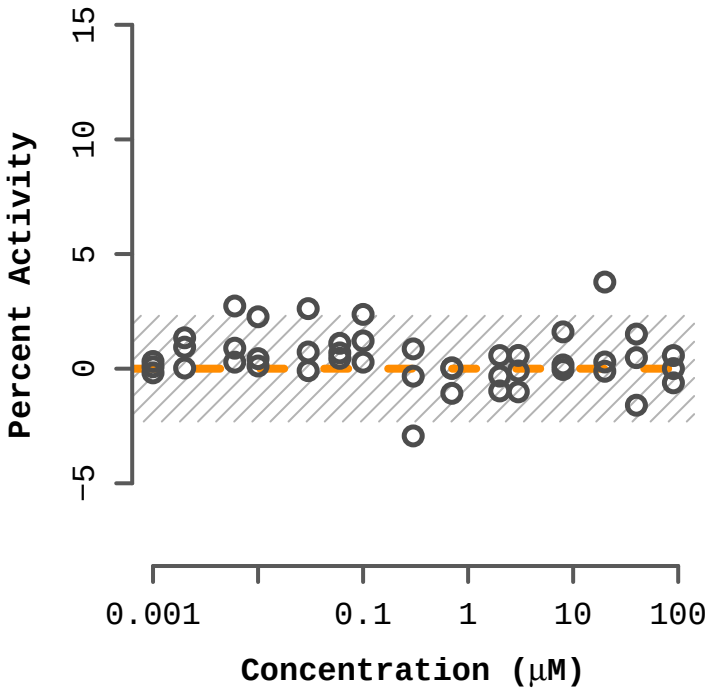
NAME: Methyl trans-styryl ketone
CHID: 31626 **CASRN:** 1896-62-4
SPID(S): Tox21_301598
M4ID: 12477535

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 0.443 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

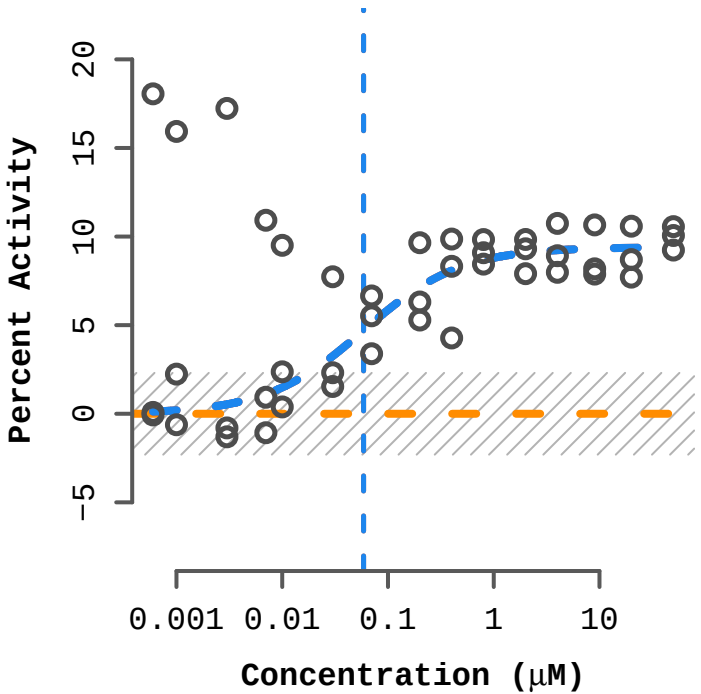
NAME: Nevirapine
CHID: 31797 CASRN: 129618-40-2
SPID(S): Tox21_200770
M4ID: 12481482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.32 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nevirapine
CHID: 31797 CASRN: 129618-40-2
SPID(S): Tox21_110982_1
M4ID: 12483968

HILL MODEL (in red):

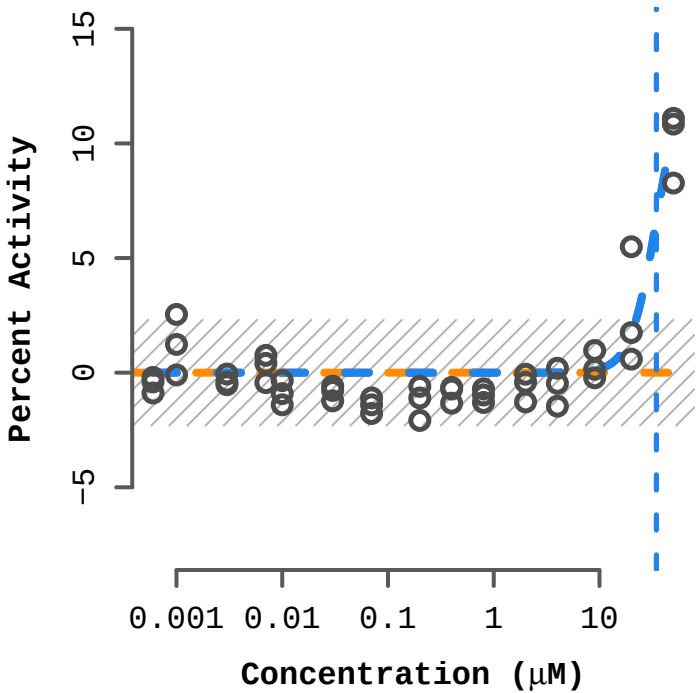
	tp	ga	gw
val:	9.4	−1.23	0.946
sd:	0.564	0.168	0.305

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.4	−1.23	0.946	3.13	5.84
sd:	0.564	0.168	0.305	1550	6340

	CNST	HILL	GNLS
AIC:	326.92	244.45	248.45
PROB:	0	0.88	0.12
RMSE:	8.36	4.95	4.95

MAX_MEAN: 9.95 MAX_MED: 10.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nocodazole
CHID: 31800 CASRN: 31430-18-9
SPID(S): Tox21_110189_1
M4ID: 12484570

HILL MODEL (in red):

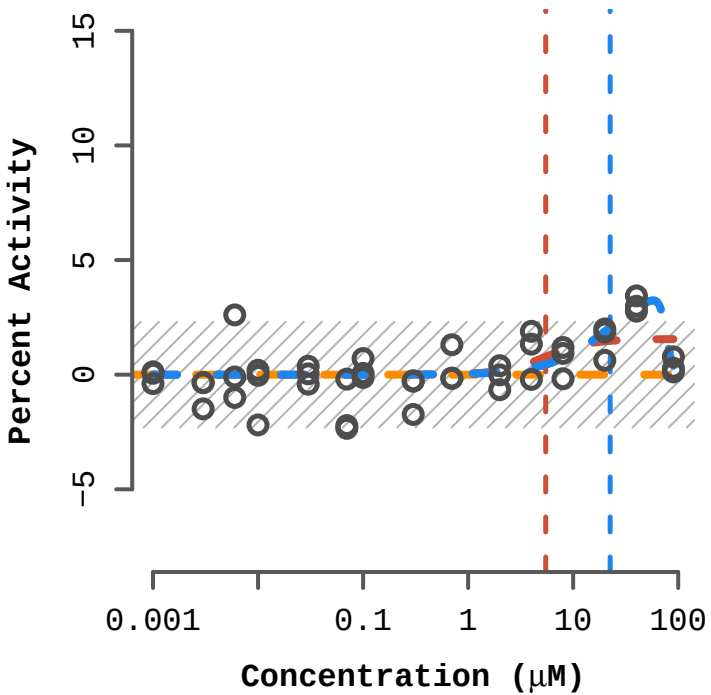
	tp	ga	gw
val:	13.3	1.54	3.53
sd:	12.8	0.387	3.72

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.3	1.54	3.53	2.91	5.65
sd:	12.8	0.389	3.74	1370	6410

	CNST	HILL	GNLS
AIC:	190.24	147.72	151.72
PROB:	0	0.88	0.12
RMSE:	2.91	1.15	1.15

MAX_MEAN: 10.1 MAX_MED: 10.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PFDA
CHID: 31860 CASRN: 335-76-2
SPID(S): Tox21_300608
M4ID: 12478525

HILL MODEL (in red):

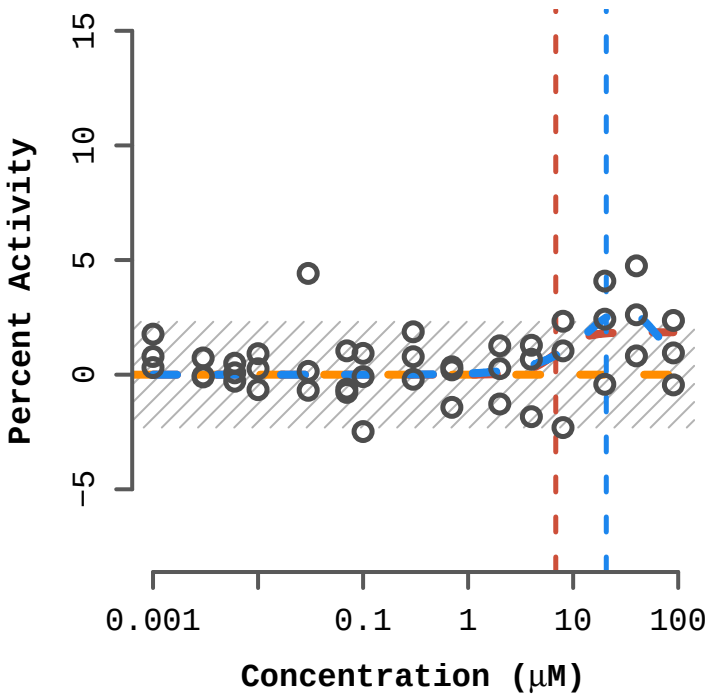
	tp	ga	gw
val:	1.56	0.739	2.1
sd:	0.545	0.345	1.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.12	1.35	1.5	1.88	13.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	151.46	139.86	126.67
PROB:	0	0	1
RMSE:	1.31	1.05	0.93

MAX_MEAN: 3.06 MAX_MED: 2.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PFHxA
CHID: 31862 CASRN: 307-24-4
SPID(S): Tox21_300394
M4ID: 12478738

HILL MODEL (in red):

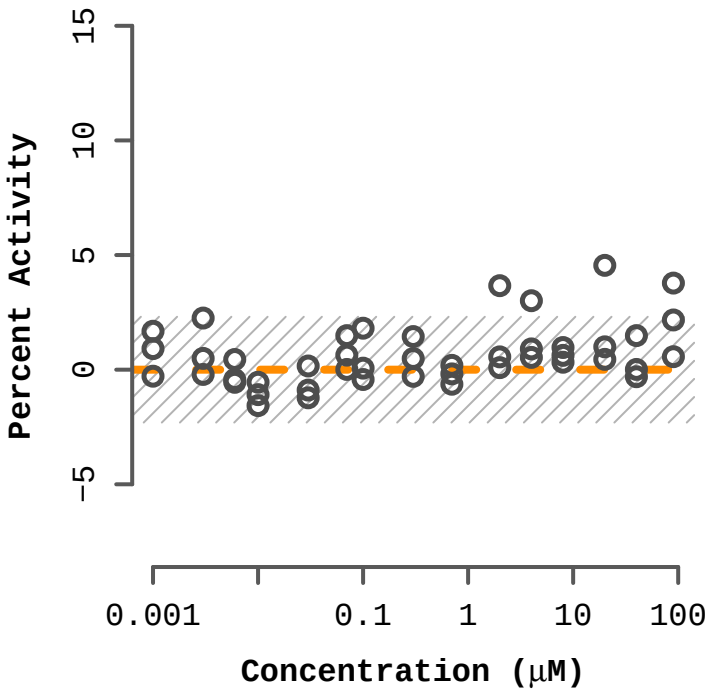
	tp	ga	gw
val:	1.85	0.834	3.31
sd:	0.545	0.272	4.27

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.5	1.32	1.53	1.71	2.54
sd:	68.3	5.84	5.17	2.72	7.13

	CNST	HILL	GNLS
AIC:	170.78	164.6	165.96
PROB:	0.03	0.64	0.33
RMSE:	1.64	1.42	1.38

MAX_MEAN: 2.73 MAX_MED: 2.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

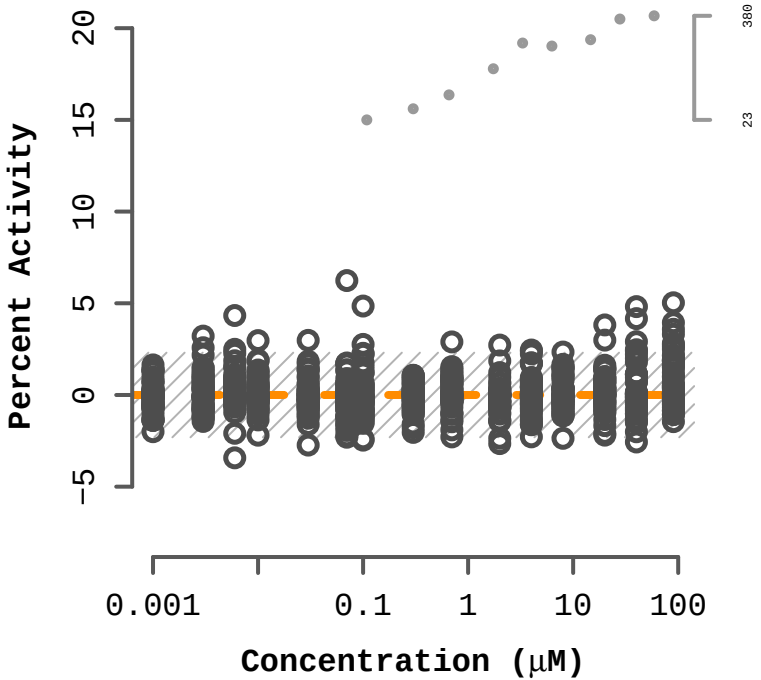
NAME: PFNA
CHID: 31863 CASRN: 375-95-1
SPID(S): Tox21_300380
M4ID: 12478752

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.17 MAX_MED: 2.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

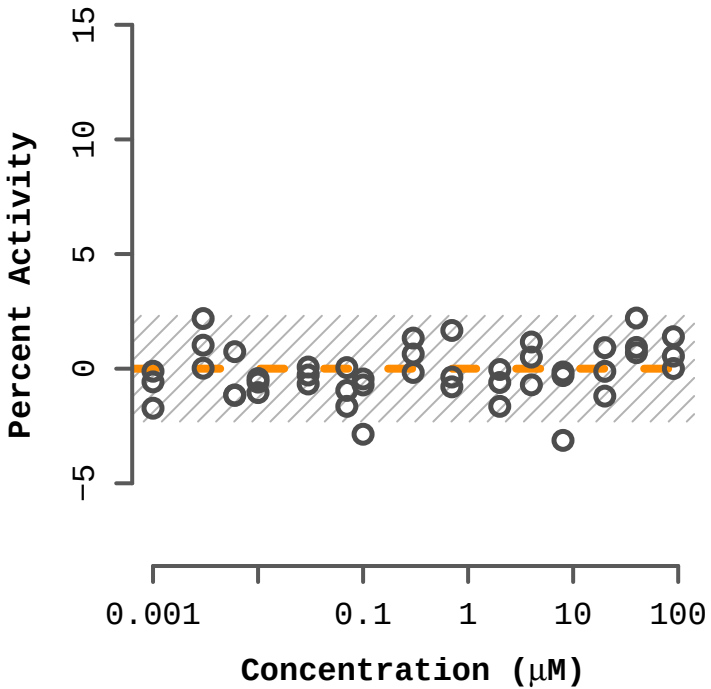
NAME: PFOS
CHID: 31864 **CASRN:** 1763-23-1
SPID(S): Tox21_400083
M4ID: 12475054 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2497.5	NA	NA
PROB:	1	NA	NA
RMSE:	28.53	NA	NA

MAX_MEAN: 8.9 **MAX_MED:** 0.601 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

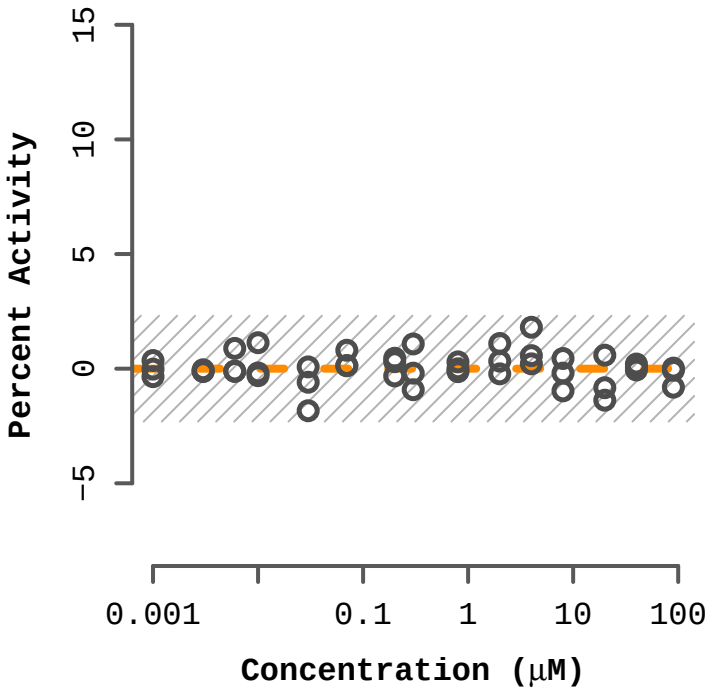
NAME: PFOA
CHID: 31865 **CASRN:** 335-67-1
SPID(S): Tox21_300688
M4ID: 12478445

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

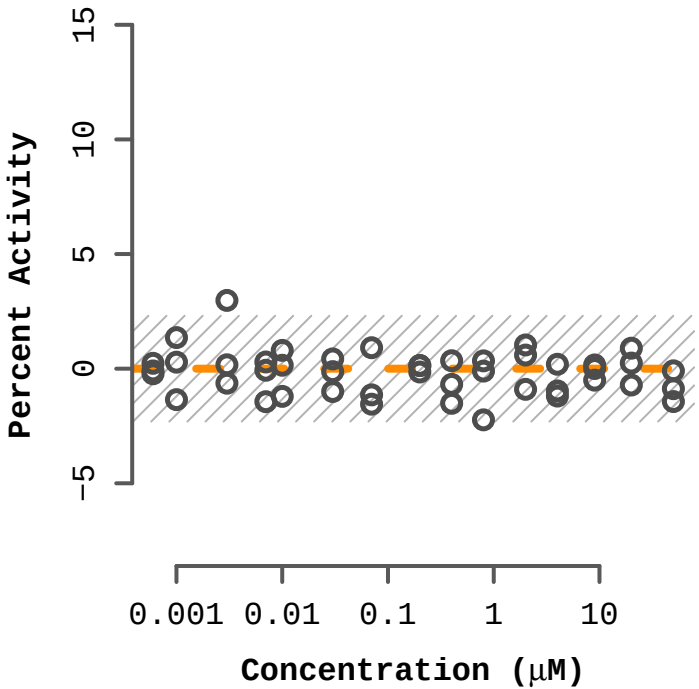
NAME: Picolinic acid
CHID: 31903 **CASRN:** 98-98-6
SPID(S): Tox21_202953
M4ID: 12479299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.863 **MAX_MED:** 0.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

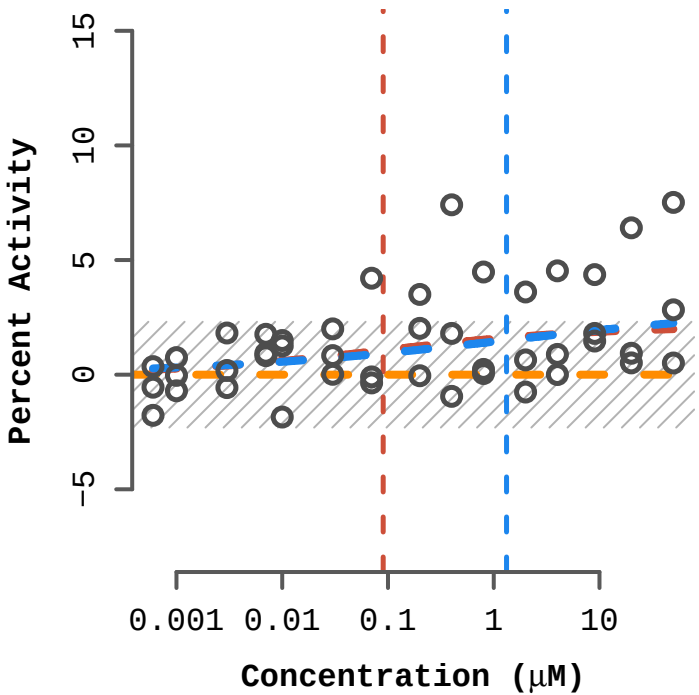
NAME: Picolinic acid
CHID: 31903 **CASRN:** 98-98-6
SPID(S): Tox21_112282_1
M4ID: 12483183

HILL MODEL: Not applicable.

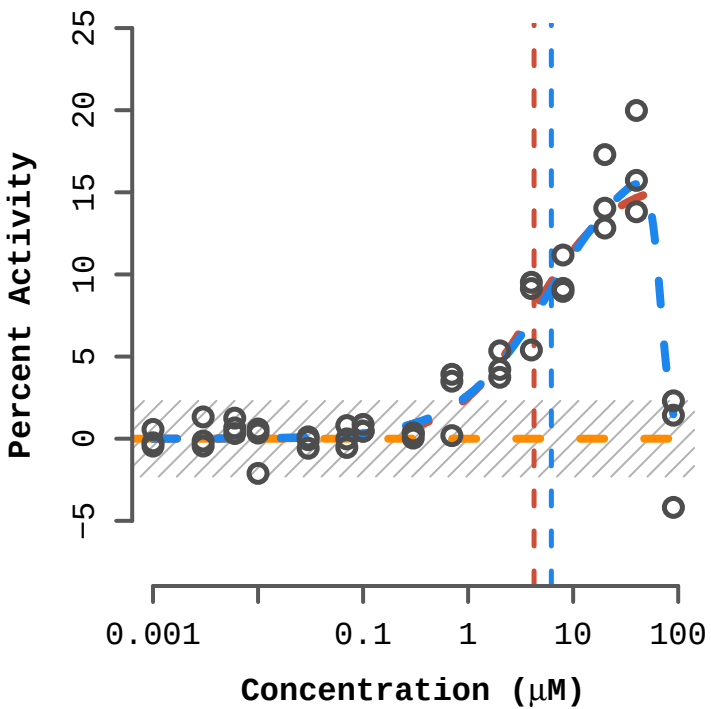
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.839 **MAX_MED:** 0.596 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Prilocaine hydrochloride
CHID:    31956   CASRN: 1786-81-8
SPID(S): Tox21_110513_1
M4ID:    12484304

HILL MODEL (in red):
      tp       ga       gw
val:  2.12     -1.05    0.429
sd:   2.89     4.5      0.957

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3        0.121    0.3      3.69     16.3
sd:   NA       NA       NA       NA       NA

      CNST       HILL       GNLS
AIC:  209.14     195.73     199.76
PROB: 0          0.88       0.12
RMSE: 2.6        2          2

MAX_MEAN: 3.62      MAX_MED: 2.83      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Resveratrol
CHID: 31980 CASRN: 501-36-0
SPID(S): Tox21_303376
M4ID: 12475760

HILL MODEL (in red):

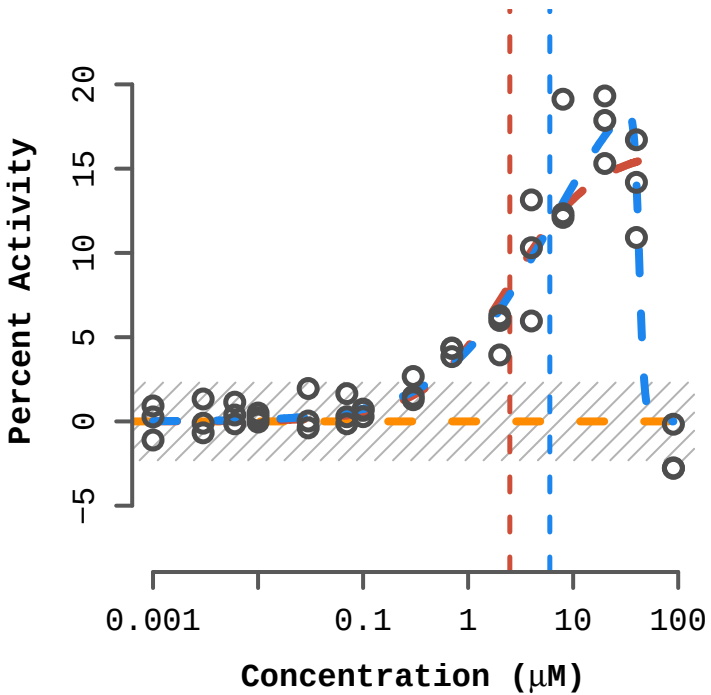
	tp	ga	gw
val:	15.8	0.628	1.14
sd:	1.57	0.118	0.224

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.3	0.792	0.971	1.83	8.32
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	294.52	213.85	169.77
PROB:	0	0	1
RMSE:	6.86	4.29	1.55

MAX_MEAN: 16.5 MAX_MED: 15.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Resveratrol
CHID: 31980 CASRN: 501-36-0
SPID(S): Tox21_201374
M4ID: 12480878

HILL MODEL (in red):

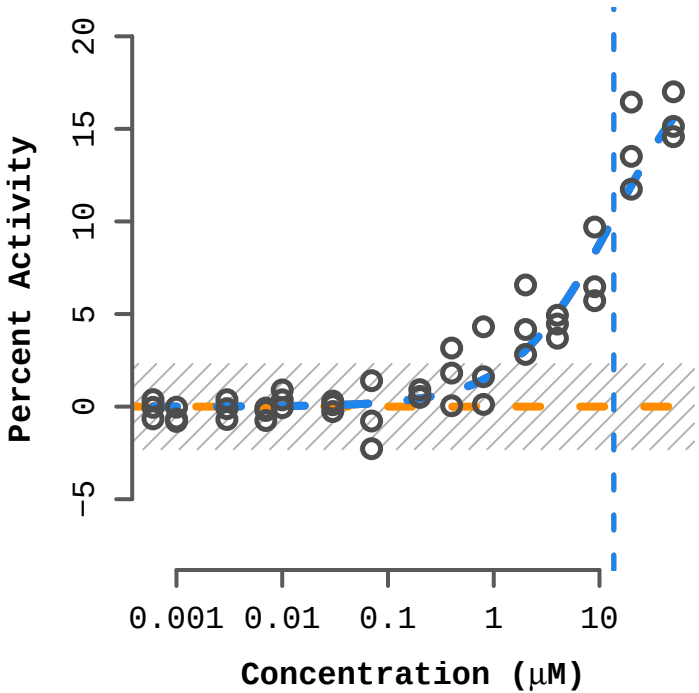
	tp	ga	gw
val:	16.2	0.397	1.06
sd:	1.49	0.118	0.192

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.2	0.778	0.831	1.63	17.7
sd:	4.17	0.211	0.115	0.0136	8.6

	CNST	HILL	GNLS
AIC:	307.49	234.77	179.14
PROB:	0	0	1
RMSE:	7.73	4.96	1.69

MAX_MEAN: 17.5 MAX_MED: 17.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Resveratrol
CHID: 31980 CASRN: 501-36-0
SPID(S): Tox21_110257_1
M4ID: 12484507

HILL MODEL (in red):

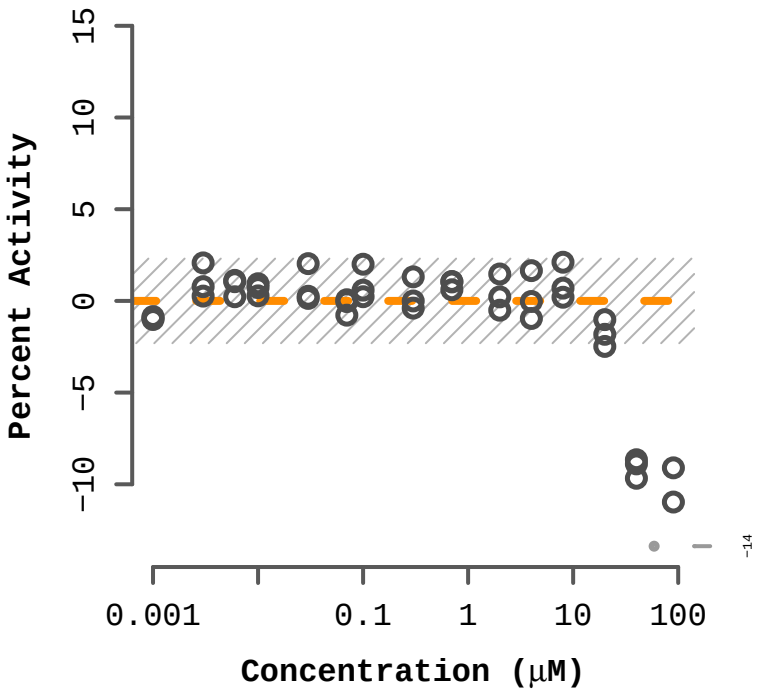
	tp	ga	gw
val:	20.4	1.14	0.902
sd:	3.12	0.188	0.153

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	20.4	1.14	0.902	3.7	5.48
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	279.39	157.58	161.58
PROB:	0	0.88	0.12
RMSE:	6.08	1.36	1.36

MAX_MEAN: 15.6 MAX_MED: 15.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

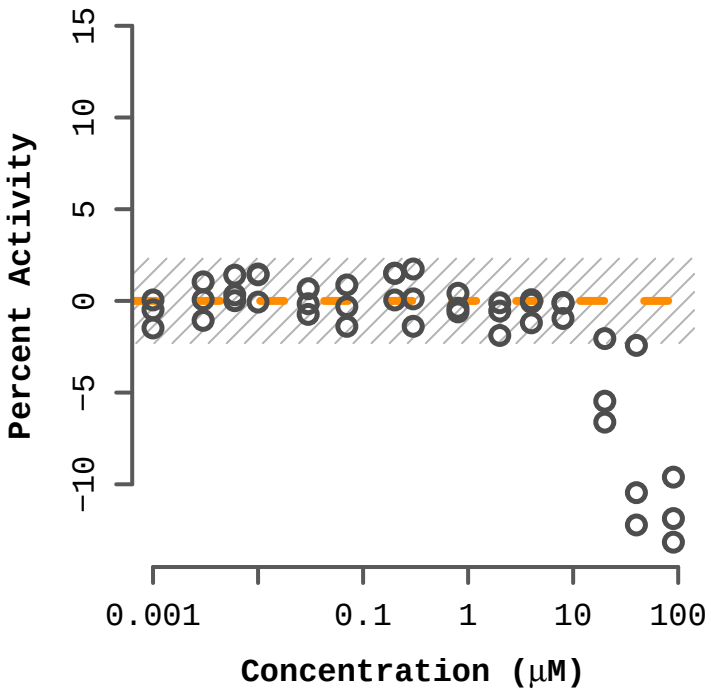
NAME: Flutamide
CHID: 32004 CASRN: 13311-84-7
SPID(S): Tox21_300536
M4ID: 12478596 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.27	NA	NA
PROB:	1	NA	NA
RMSE:	3.91	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

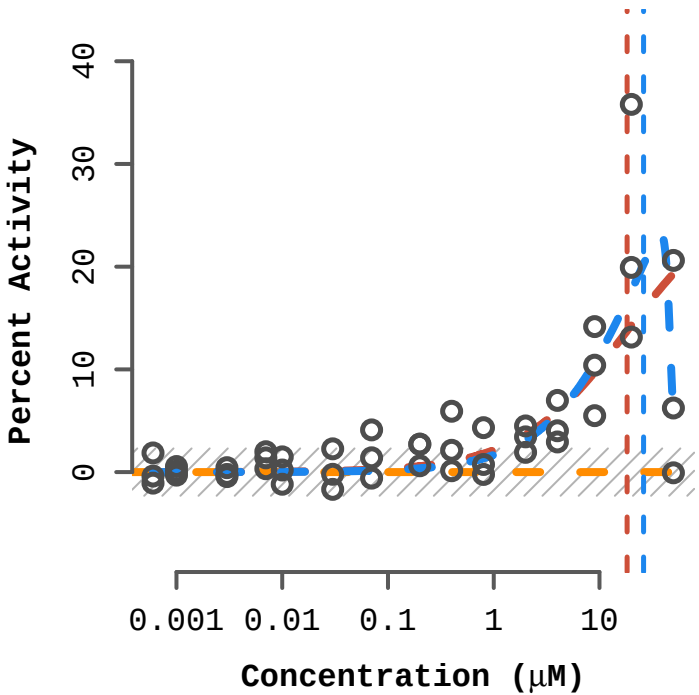
NAME: Flutamide
CHID: 32004 **CASRN:** 13311-84-7
SPID(S): Tox21_202169
M4ID: 12480083

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.88	NA	NA
PROB:	1	NA	NA
RMSE:	4.16	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flutamide
CHID: 32004 CASRN: 13311-84-7
SPID(S): Tox21_110154_1
M4ID: 12484603

HILL MODEL (in red):

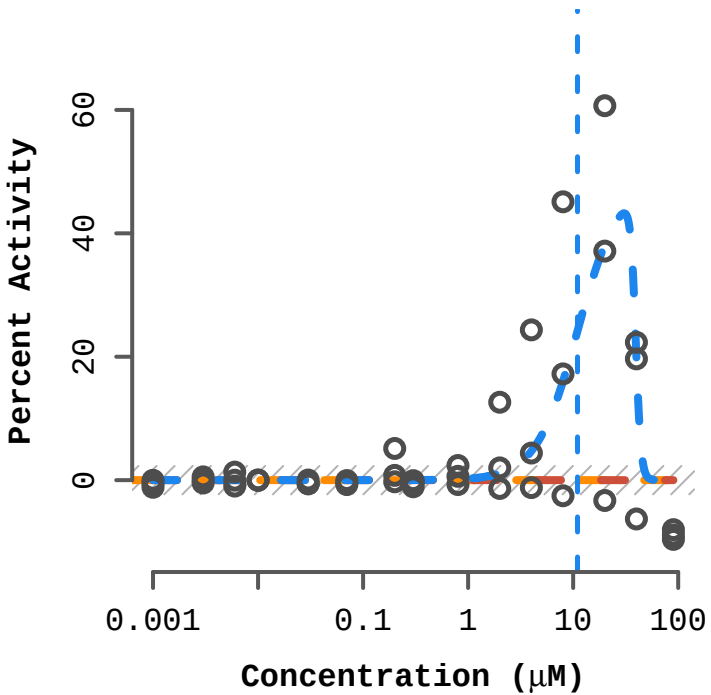
	tp	ga	gw
val:	27.5	1.26	0.853
sd:	15.8	0.683	0.423

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	40.5	1.42	0.965	1.67	18
sd:	42.8	0.759	0.3	0.016	8.98

	CNST	HILL	GNLS
AIC:	287.93	244.21	237.11
PROB:	0	0.03	0.97
RMSE:	8	5.14	4.11

MAX_MEAN: 23 MAX_MED: 19.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydroxyphenyl retinamide
CHID: 32005 CASRN: 65646-68-6
SPID(S): Tox21_200989
M4ID: 12481263

HILL MODEL (in red):

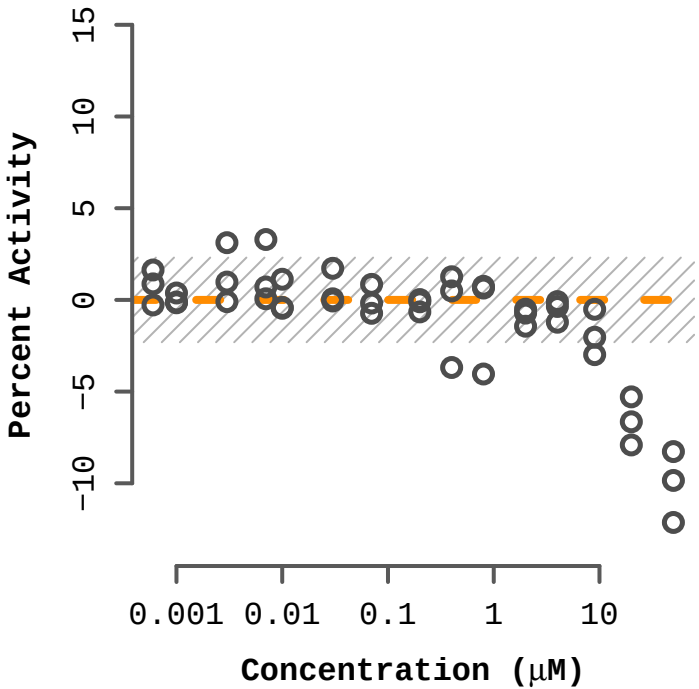
	tp	ga	gw
val:	0.163	2.45	7.98
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	48.4	1.04	2.2	1.6	17.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	334.53	340.53	320.87
PROB:	0	0	1
RMSE:	14.45	14.45	10.48

MAX_MEAN: 31.5 MAX_MED: 37.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

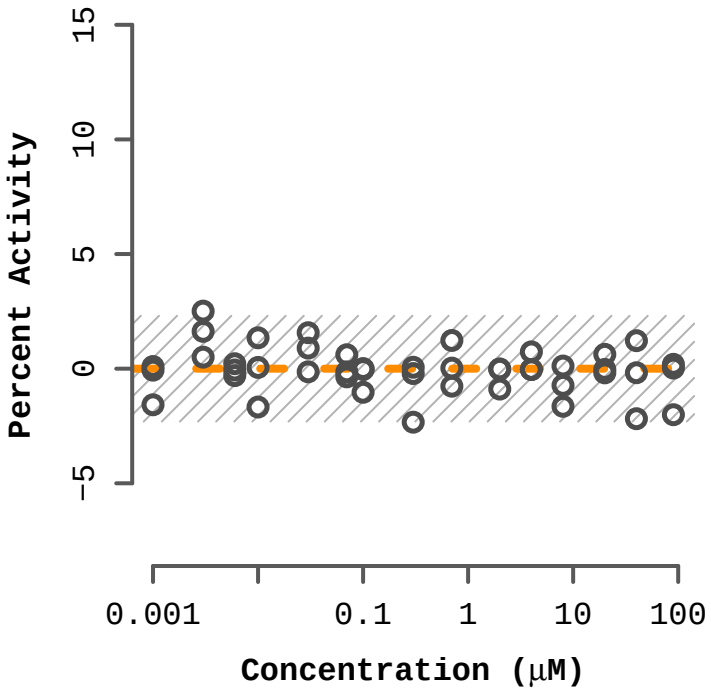
NAME: 4-Hydroxyphenyl retinamide
CHID: 32005 **CASRN:** 65646-68-6
SPID(S): Tox21_111007_1
M4ID: 12483952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.975 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

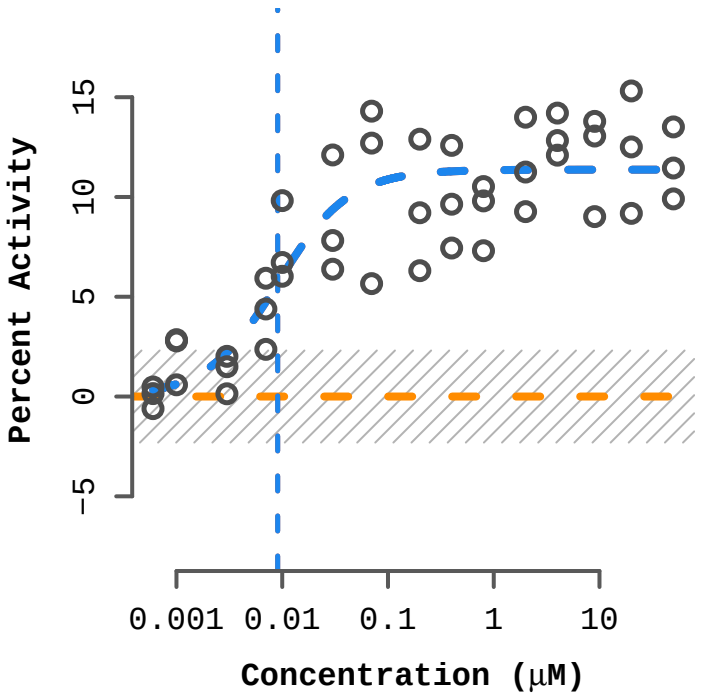
NAME: Scopolamine hydrobromide
CHID: 32029 **CASRN:** 114-49-8
SPID(S): Tox21_302019
M4ID: 12477114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Scopolamine hydrobromide
CHID: 32029 CASRN: 114-49-8
SPID(S): Tox21_110035_1
M4ID: 12484700

HILL MODEL (in red):

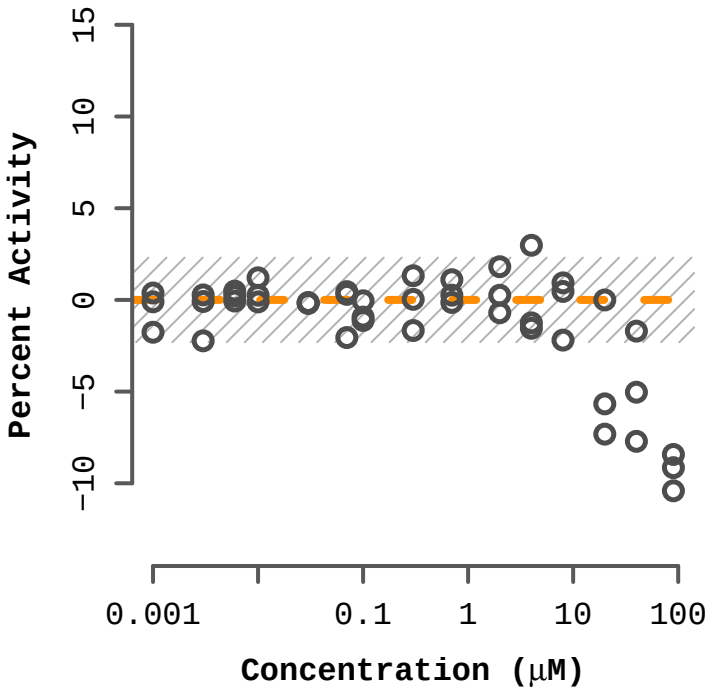
	tp	ga	gw
val:	11.4	−2.04	1.29
sd:	0.555	0.118	0.657

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.4	−2.04	1.29	3.24	6.83
sd:	0.555	0.118	0.657	30600	136000

	CNST	HILL	GNLS
AIC:	339.55	214.07	218.07
PROB:	0	0.88	0.12
RMSE:	9.45	2.27	2.27

MAX_MEAN: 13 MAX_MED: 13.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

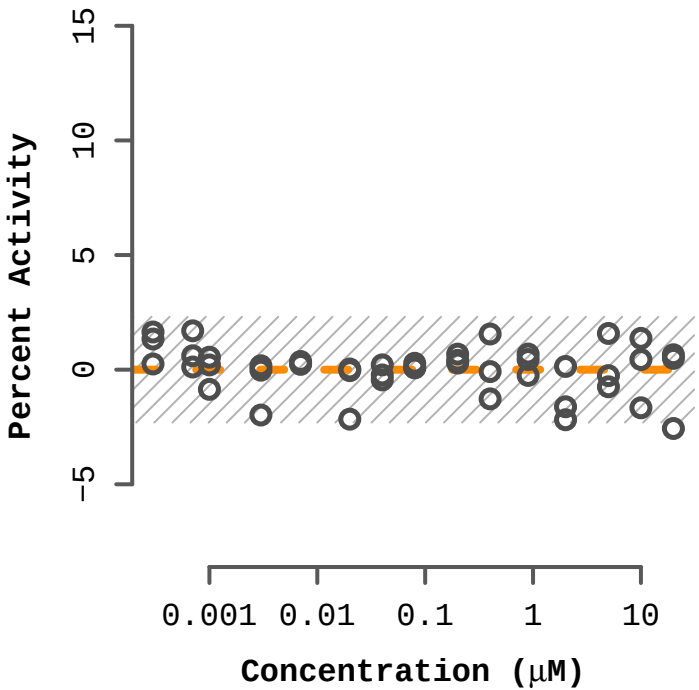
NAME: Sodium dichromate(VI) dihydrate
CHID: 32061 **CASRN:** 7789-12-0
SPID(S): Tox21_202536
M4ID: 12479716

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.21	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 0.455 **MAX_MED:** 0.462 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

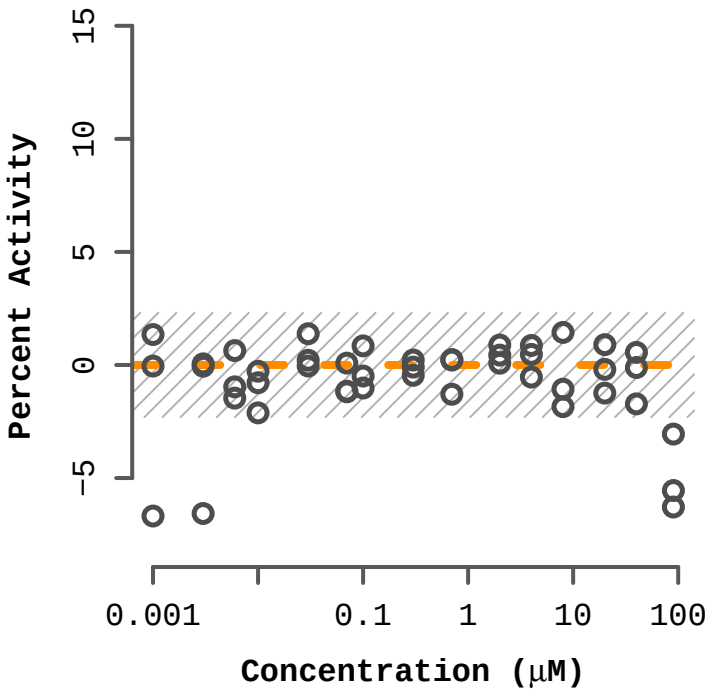
NAME: Sodium selenite
CHID: 32077 CASRN: 10102-18-8
SPID(S): Tox21_202977
M4ID: 12479275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

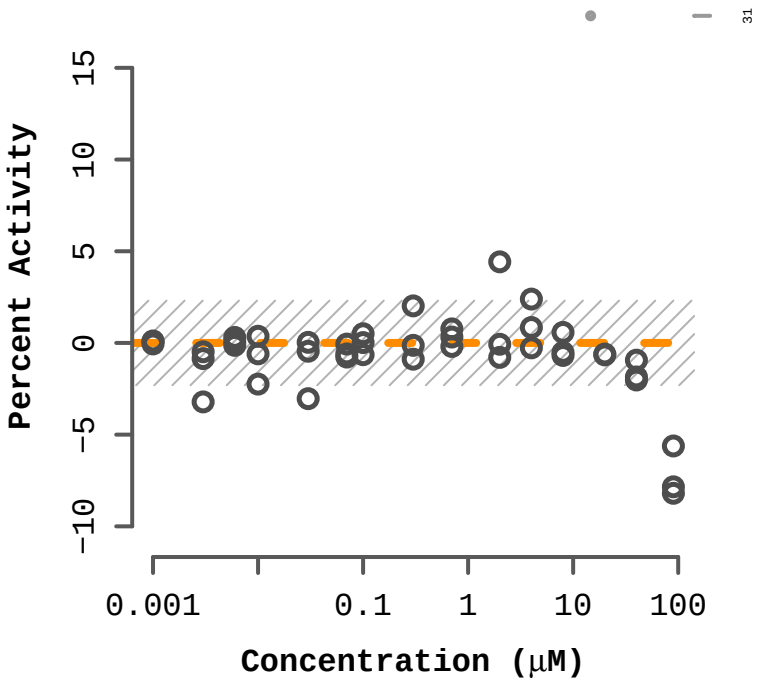
NAME: Tebuconazole
CHID: 32113 **CASRN:** 107534-96-3
SPID(S): Tox21_300487
M4ID: 12478645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.56	NA	NA
PROB:	1	NA	NA
RMSE:	2.11	NA	NA

MAX_MEAN: 0.518 **MAX_MED:** 0.471 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

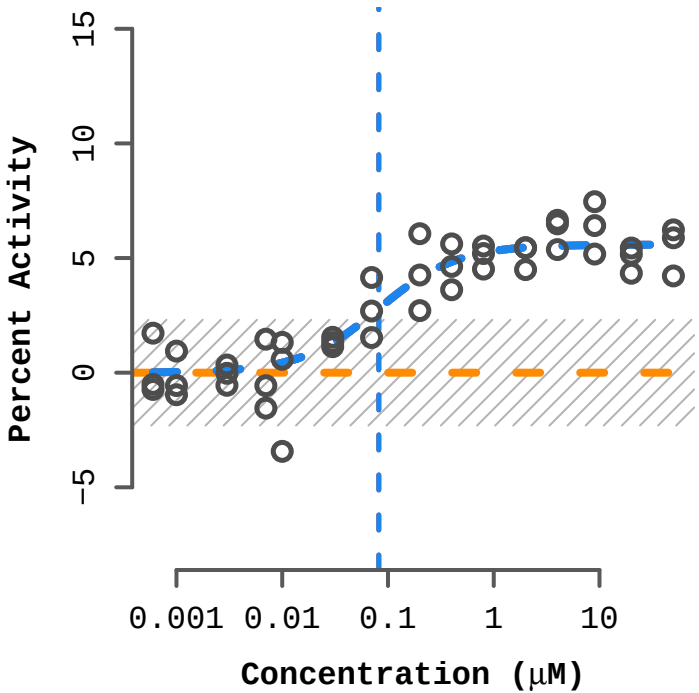
NAME: Tebuconazole
CHID: 32113 **CASRN:** 107534-96-3
SPID(S): Tox21_202331
M4ID: 12479921 **BRK**

HILL MODEL: Not applicable.

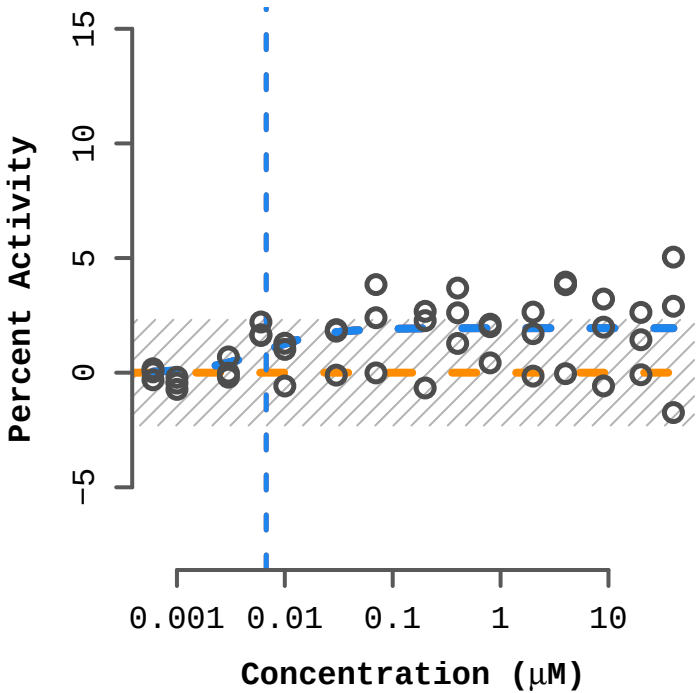
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.73	NA	NA
PROB:	1	NA	NA
RMSE:	5.17	NA	NA

MAX_MEAN: 9.97 **MAX_MED:** 0.843 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tetrabromobisphenol A-bis(2,3-dibromopropyl etl
CHID:    32129   CASRN: 21850-44-2
SPID(S): Tox21_202540
M4ID:    12479712

HILL MODEL (in red):
      tp       ga       gw
val:  5.59     -1.09    1.18
sd:   0.273    0.123    0.281

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.59     -1.09    1.18     3.7      3.79
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  262.61      139.42      143.42
PROB: 0           0.88        0.12
RMSE: 4.08        1.07        1.07

MAX_MEAN: 6.35      MAX_MED: 6.49      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2',4,4',5,5'−Hexachlorobiphenyl
CHID: 32180 **CASRN:** 35065−27−1
SPID(S): Tox21_202470
M4ID: 12479782

HILL MODEL (in red):

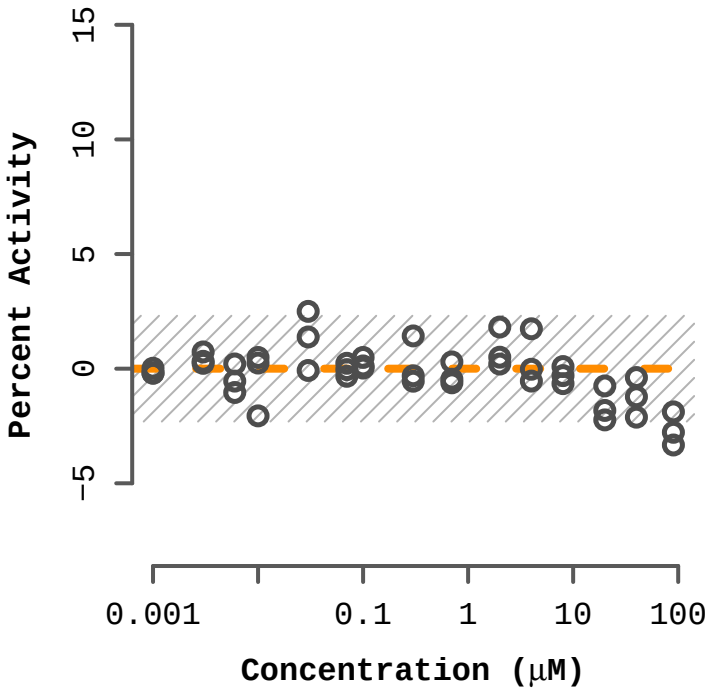
	tp	ga	gw
val:	1.94	−2.17	1.53
sd:	0.345	0.444	1.55

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.94	−2.17	1.53	3.48	3.82
sd:	0.345	0.444	1.55	1020	2110

	CNST	HILL	GNLS
AIC:	196.53	166.1	170.1
PROB:	0	0.88	0.12
RMSE:	2.03	1.39	1.39

MAX_MEAN: 2.58 **MAX_MED:** 3.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

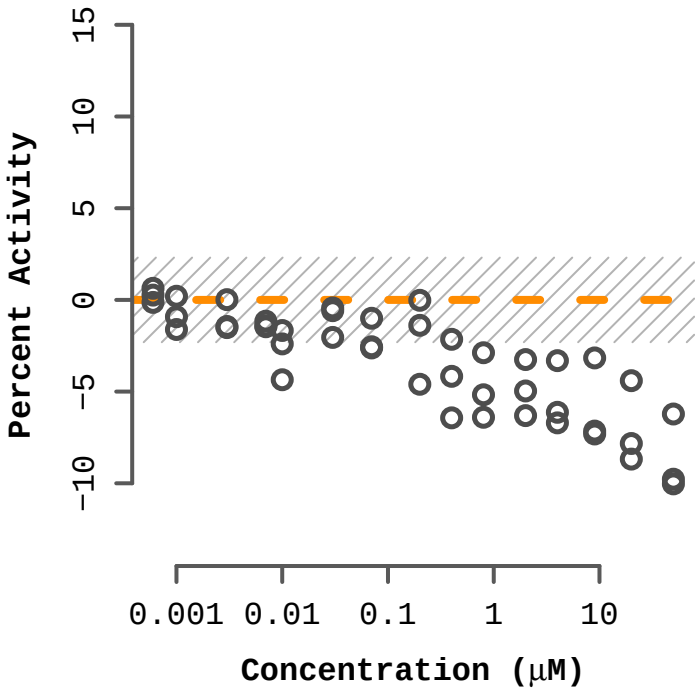
NAME: Tri-o-cresyl phosphate
CHID: 32192 **CASRN:** 78-30-8
SPID(S): Tox21_202983
M4ID: 12479269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

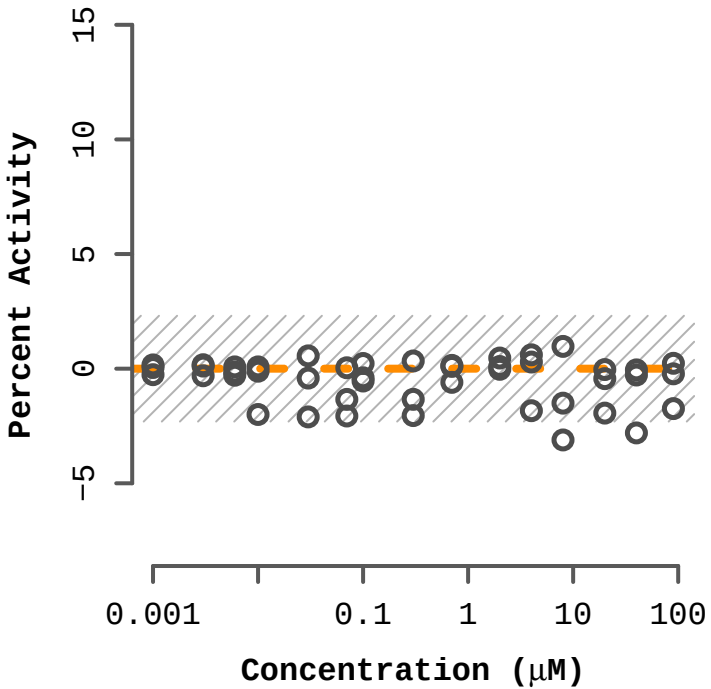
NAME: Vincristine
CHID: 32278 **CASRN:** 57-22-7
SPID(S): Tox21_112067_1
M4ID: 12483340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.09	NA	NA
PROB:	1	NA	NA
RMSE:	4.46	NA	NA

MAX_MEAN: 0.254 **MAX_MED:** 0.264 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

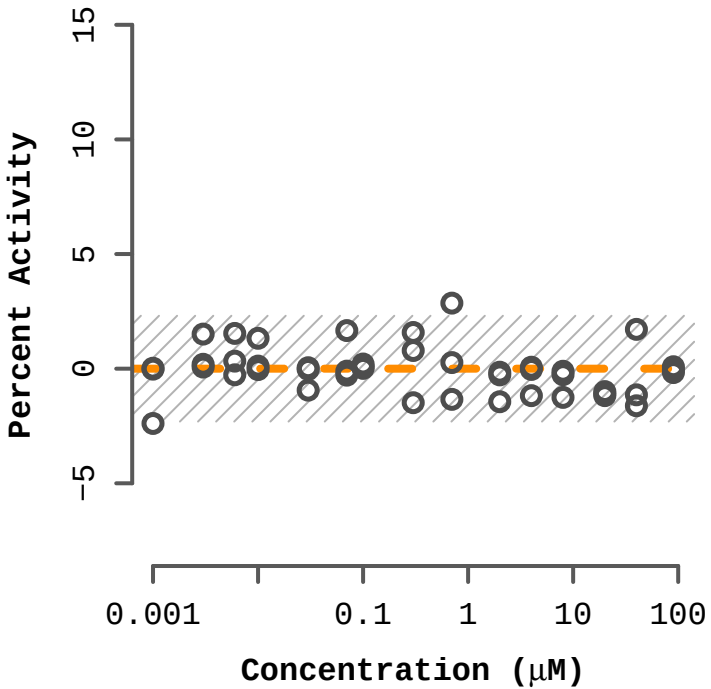
NAME: (Z)-11-Hexadecenal
CHID: 32303 **CASRN:** 53939-28-9
SPID(S): Tox21_301824
M4ID: 12477309

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.178 **MAX_MED:** 0.291 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

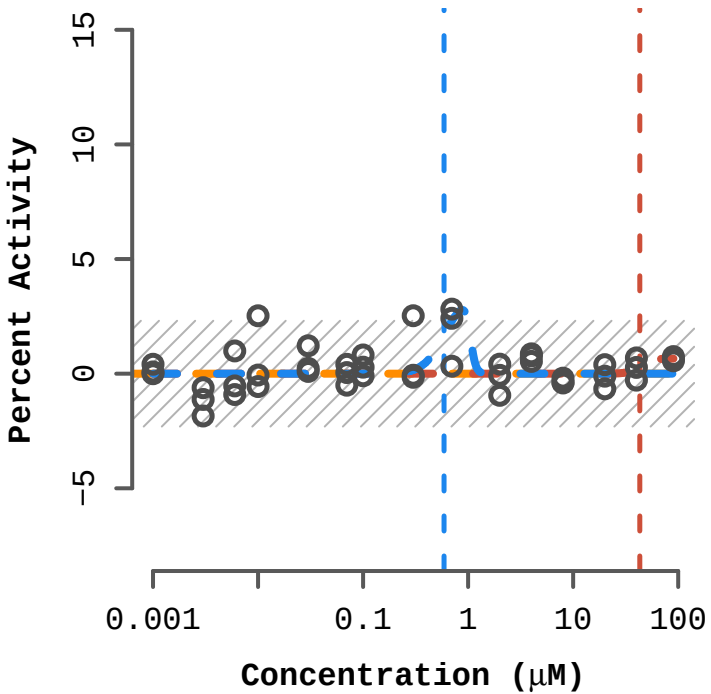
NAME: (Z)−Dichloropropene
CHID: 32305 CASRN: 10061−01−5
SPID(S): Tox21_303973
M4ID: 12475215

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.597 MAX_MED: 0.793 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-D-Butotyl
CHID: 32309 CASRN: 1929-73-3
SPID(S): Tox21_301559
M4ID: 12477574

HILL MODEL (in red):

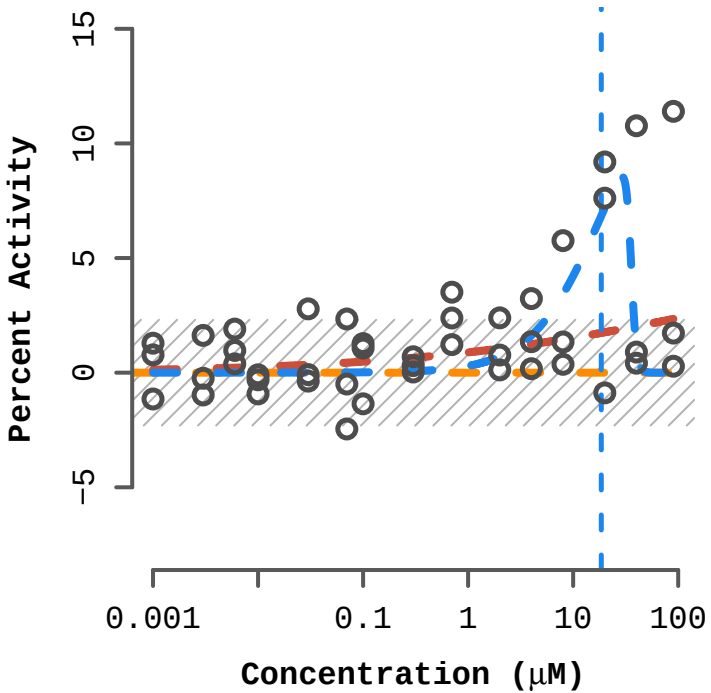
	tp	ga	gw
val:	0.658	1.63	8
sd:	0.33	0.23	40.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.38	−0.229	4.42	0.023	18
sd:	57.5	4.49	45.4	5.53	377

	CNST	HILL	GNLS
AIC:	120.32	122.5	120.33
PROB:	0.43	0.14	0.43
RMSE:	0.97	0.96	0.85

MAX_MEAN: 1.85 MAX_MED: 2.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4-Dimethyloxazolidine
CHID: 32314 **CASRN:** 51200-87-4
SPID(S): Tox21_303770
M4ID: 12475418

HILL MODEL (in red):

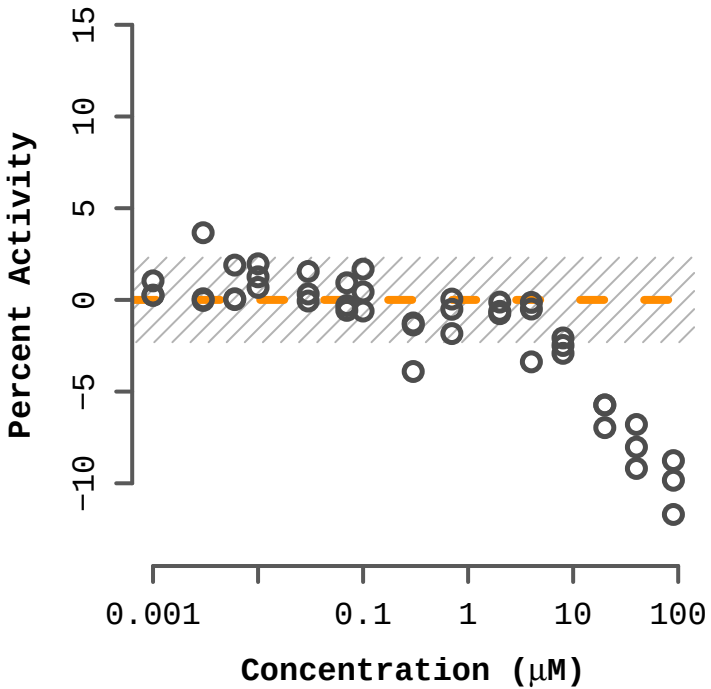
	tp	ga	gw
val:	5.55	2.41	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.7	1.27	1.31	1.55	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	218.07	211.3	212.69
PROB:	0.02	0.65	0.33
RMSE:	3.35	2.74	2.9

MAX_MEAN: 5.31 **MAX_MED:** 7.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

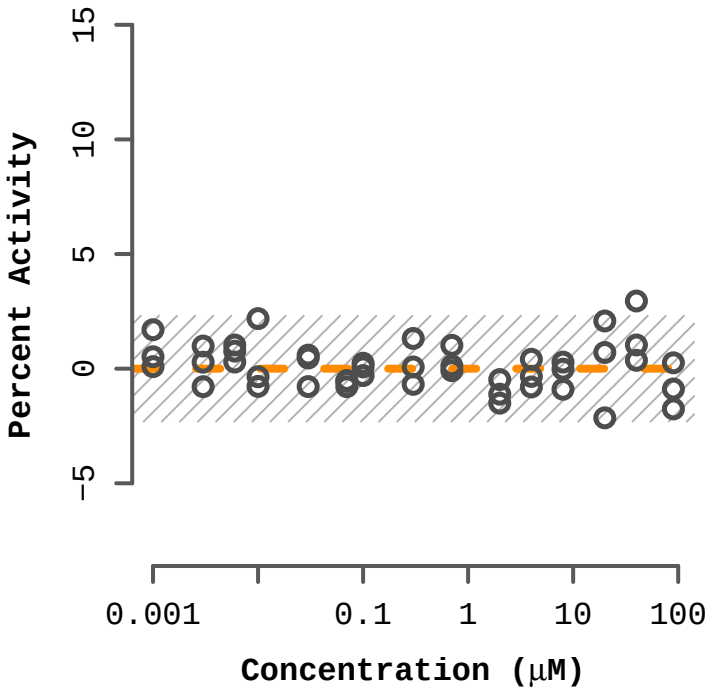
NAME: 4,5-Dichloro-2-octyl-3(2H)-isothiazolone
CHID: 32315 **CASRN:** 64359-81-5
SPID(S): Tox21_302409
M4ID: 12476724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	244.53	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

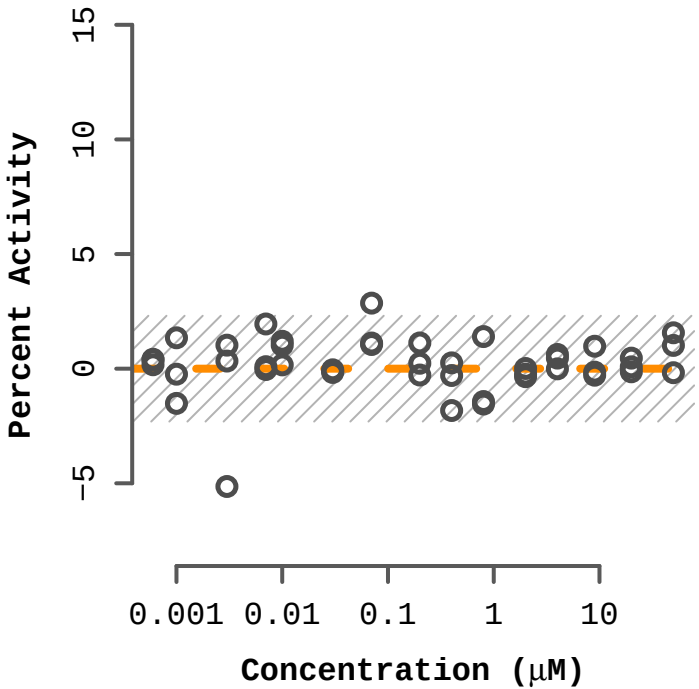
NAME: 4-Chloro-3,5-dimethylphenol
CHID: 32316 **CASRN:** 88-04-0
SPID(S): Tox21_302047
M4ID: 12477086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

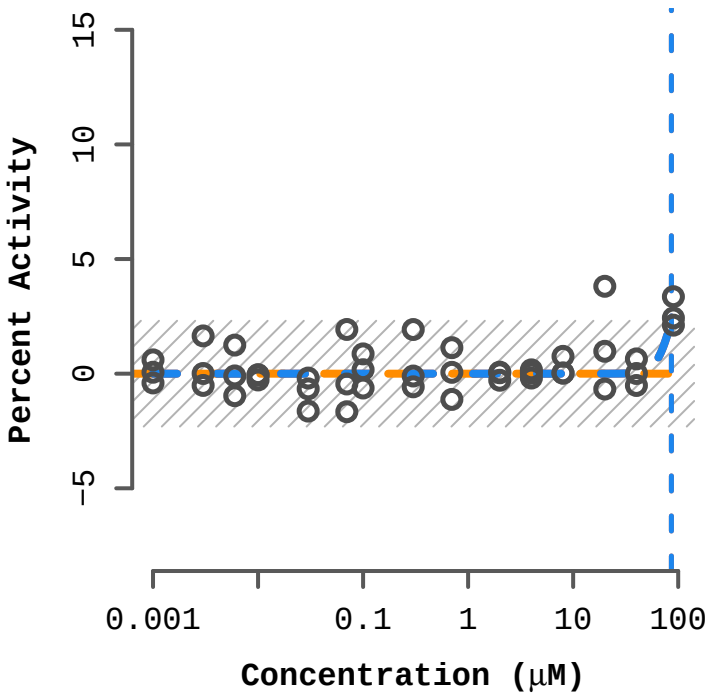
NAME: 4-Chloro-3,5-dimethylphenol
CHID: 32316 **CASRN:** 88-04-0
SPID(S): Tox21_111305_1
M4ID: 12483778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bendiocarb
CHID: 32327 CASRN: 22781-23-3
SPID(S): Tox21_300777
M4ID: 12478356

HILL MODEL (in red):

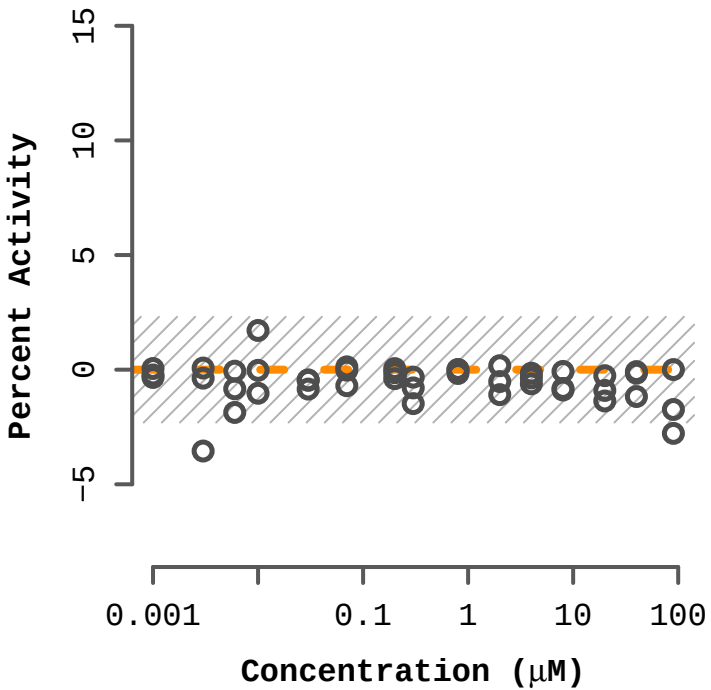
	tp	ga	gw
val:	4.58	1.94	5.98
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.58	1.94	5.98	3.14	4.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	137.43	123.33	127.33
PROB:	0	0.88	0.12
RMSE:	1.18	0.96	0.96

MAX_MEAN: 2.64 MAX_MED: 2.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

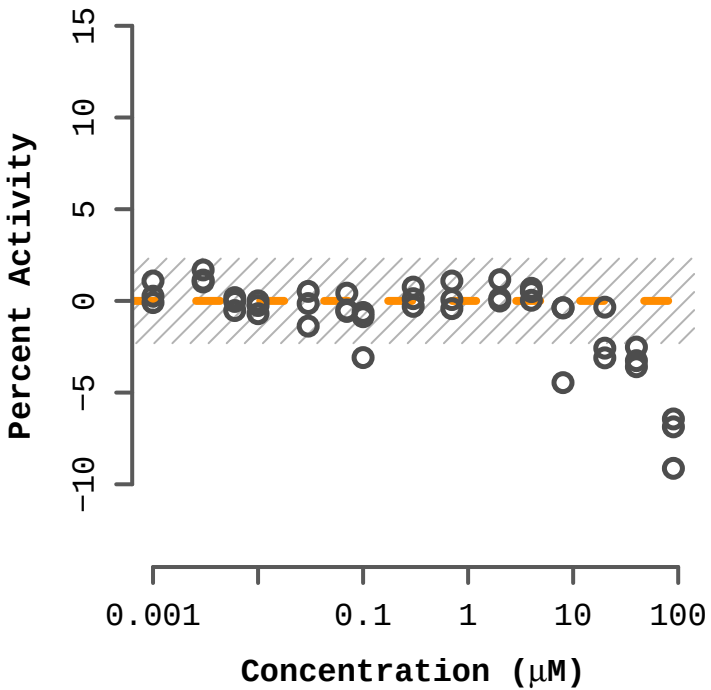
NAME: Bendiocarb
CHID: 32327 **CASRN:** 22781-23-3
SPID(S): Tox21_201562
M4ID: 12480690

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.219 **MAX_MED:** 0 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

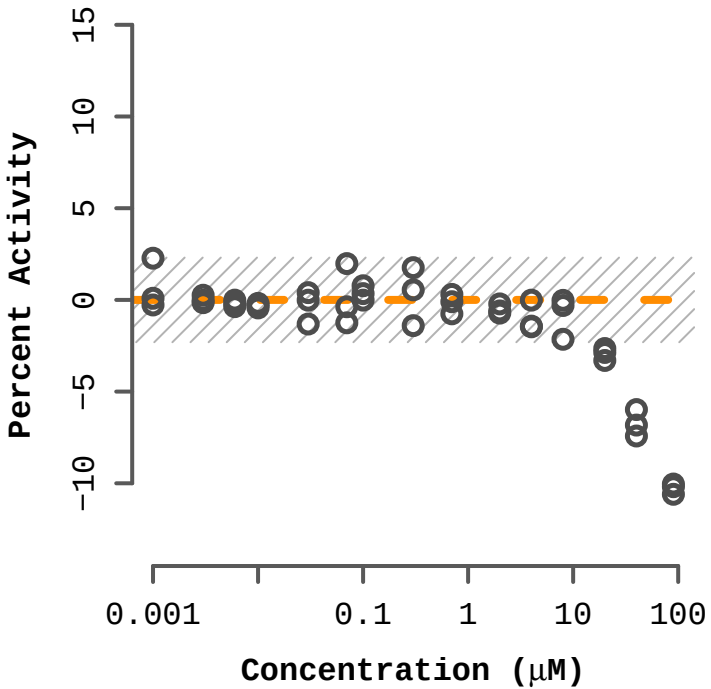
NAME: Bensulide
CHID: 32329 **CASRN:** 741-58-2
SPID(S): Tox21_300733
M4ID: 12478400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.27	NA	NA
PROB:	1	NA	NA
RMSE:	2.42	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

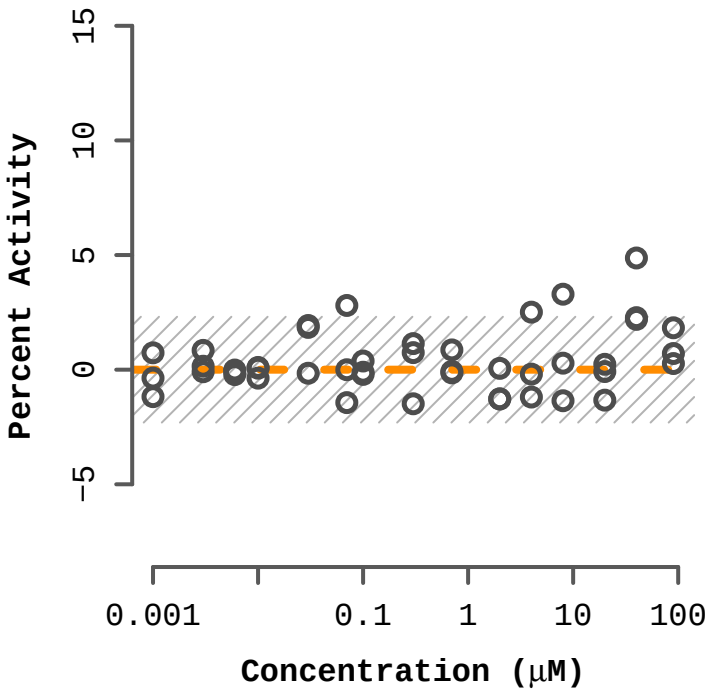
NAME: Bis(trichloromethyl)sulfone
CHID: 32331 **CASRN:** 3064-70-8
SPID(S): Tox21_303827
M4ID: 12475361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.26	NA	NA
PROB:	1	NA	NA
RMSE:	3.37	NA	NA

MAX_MEAN: 0.696 **MAX_MED:** 0.548 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

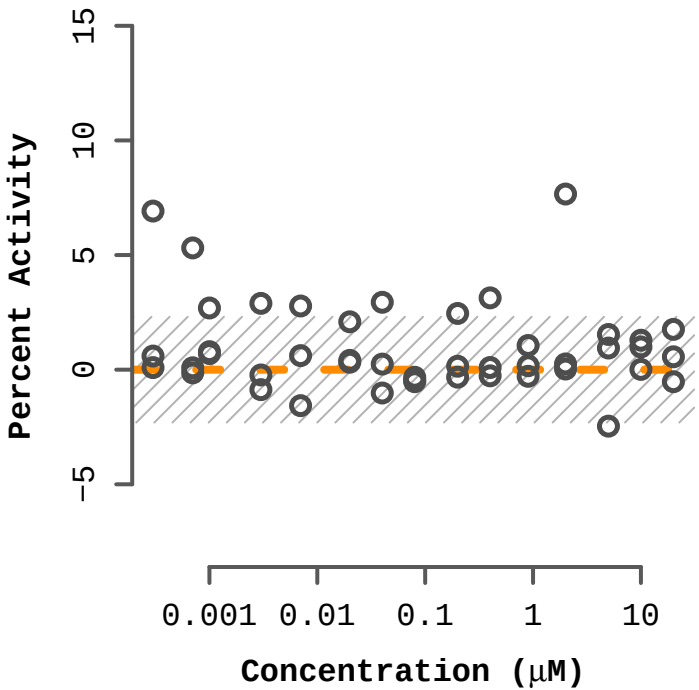
NAME: Butralin
CHID: 32337 CASRN: 33629-47-9
SPID(S): Tox21_301120
M4ID: 12478013

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 3.11 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

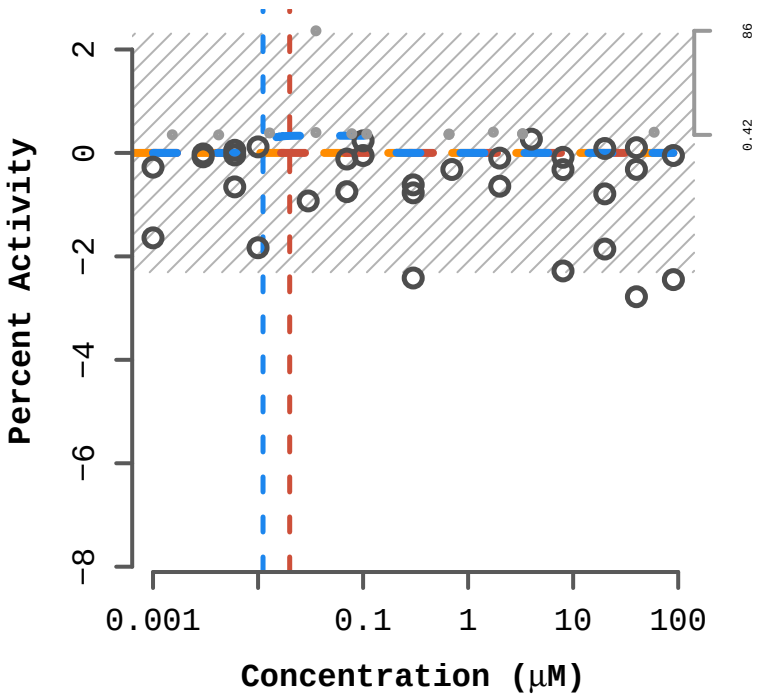
NAME: Chinomethionate
CHID: 32342 **CASRN:** 2439-01-2
SPID(S): Tox21_303968
M4ID: 12475220

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.97	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 2.65 **MAX_MED:** 0.994 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorethoxyfos
CHID: 32344 CASRN: 54593-83-8
SPID(S): Tox21_300896
M4ID: 12478237 BRK

HILL MODEL (in red):

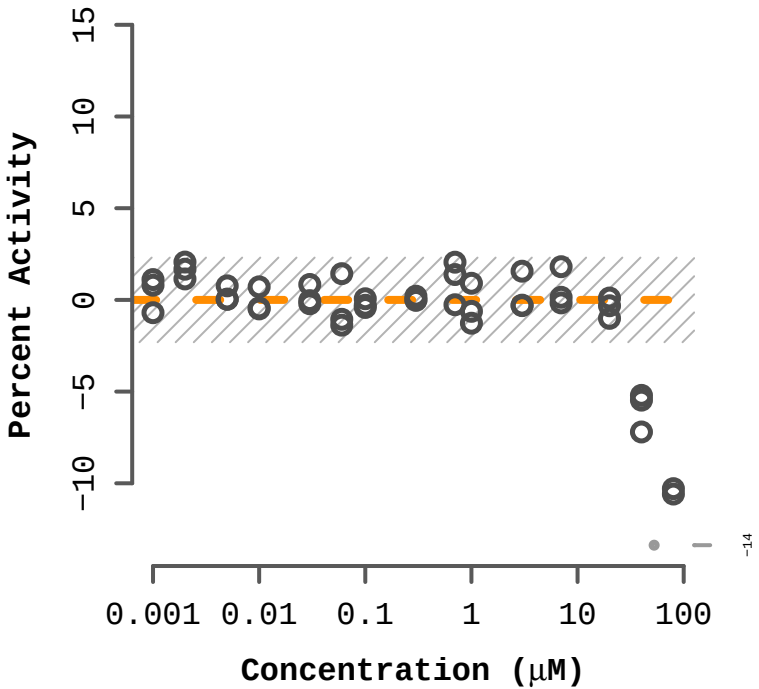
	tp	ga	gw
val:	1.07e-10	-1.7	1.9
sd:	1.18e-05	63100	216000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.332	-1.95	8	-0.79	17.5
sd:	0.441	0.93	54.9	4.19	307

	CNST	HILL	GNLS
AIC:	187.89	193.89	197.31
PROB:	0.94	0.05	0.01
RMSE:	12.93	12.93	12.88

MAX_MEAN: 29.3 MAX_MED: 2.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

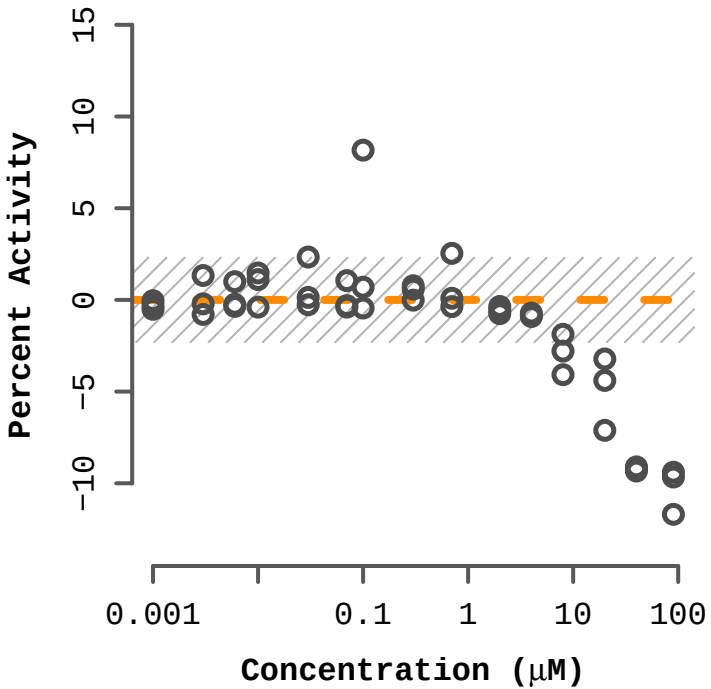
NAME: Chlorhexidine diacetate
CHID: 32345 **CASRN:** 56-95-1
SPID(S): Tox21_302363
M4ID: 12476770 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.27	NA	NA
PROB:	1	NA	NA
RMSE:	3.48	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

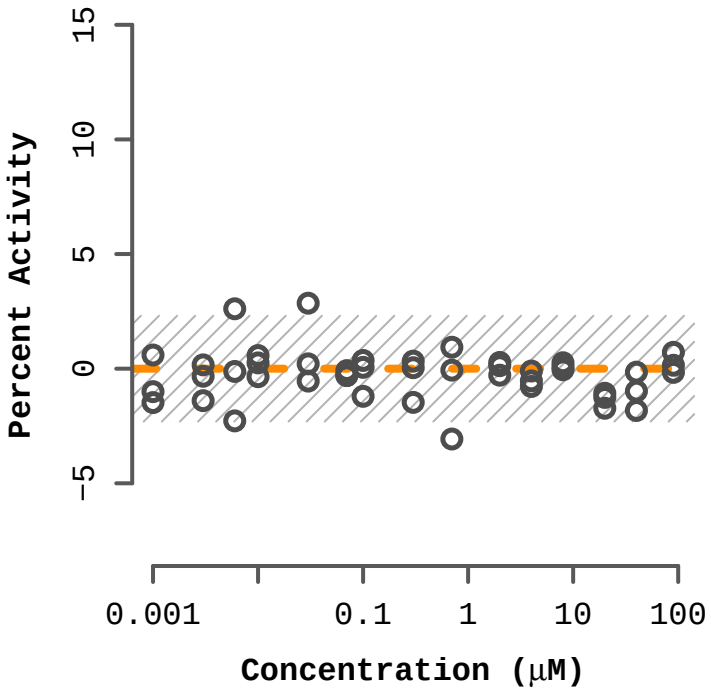
NAME: Chlorophacinone
CHID: 32348 **CASRN:** 3691-35-8
SPID(S): Tox21_301565
M4ID: 12477568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.42	NA	NA
PROB:	1	NA	NA
RMSE:	4.14	NA	NA

MAX_MEAN: 2.81 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

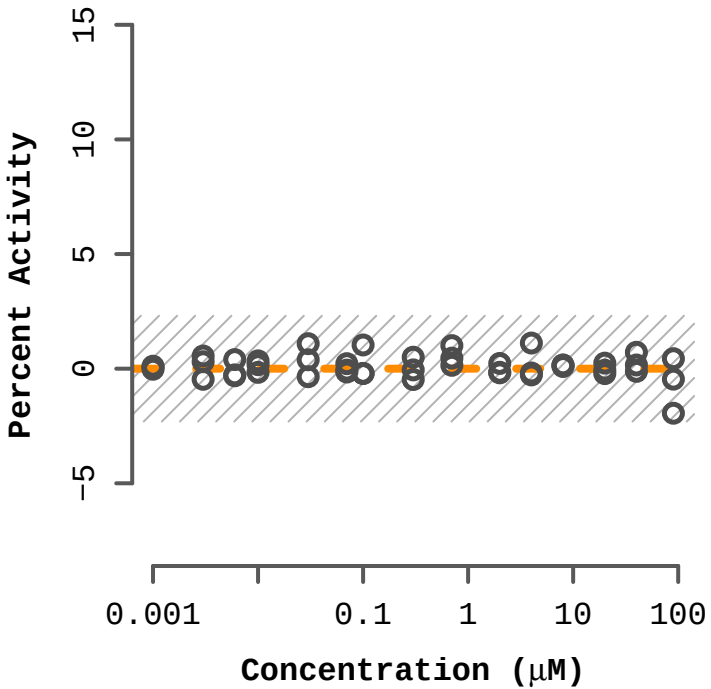
NAME: Chlorpyrifos-methyl
CHID: 32352 CASRN: 5598-13-0
SPID(S): Tox21_300700
M4ID: 12478433

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.843 MAX_MED: 0.254 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

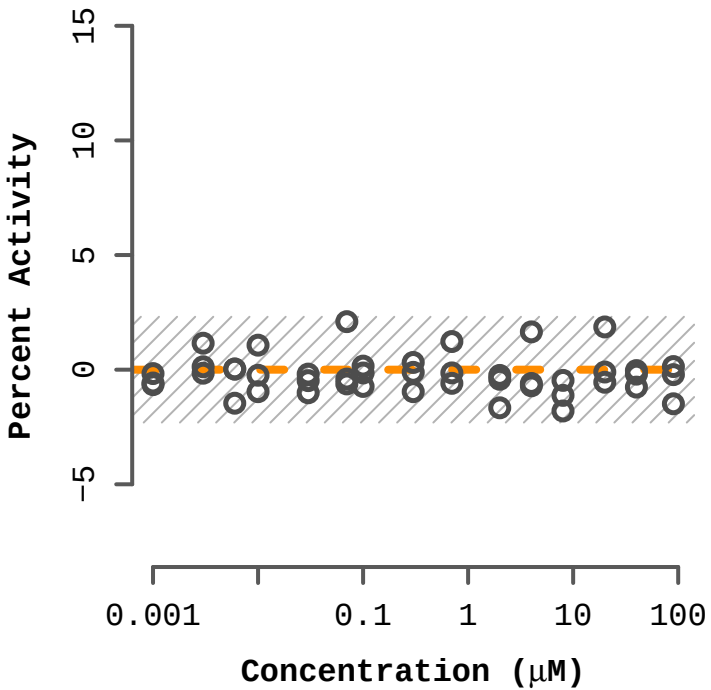
NAME: Clodinafop-propargyl
CHID: 32354 **CASRN:** 105512-06-9
SPID(S): Tox21_300724
M4ID: 12478409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	61.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.51	NA	NA

MAX_MEAN: 0.539 **MAX_MED:** 0.461 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

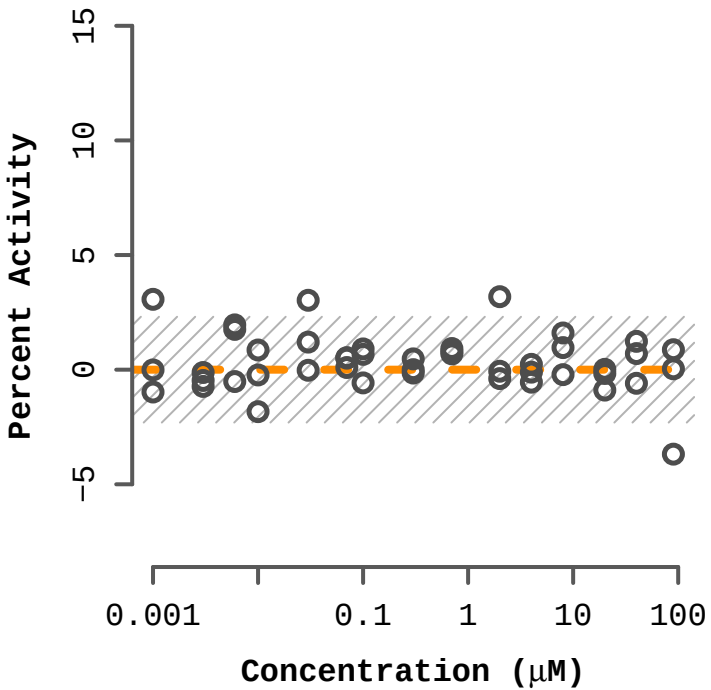
NAME: Clomazone
CHID: 32355 **CASRN:** 81777-89-1
SPID(S): Tox21_300958
M4ID: 12478175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.406 **MAX_MED:** 0.128 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

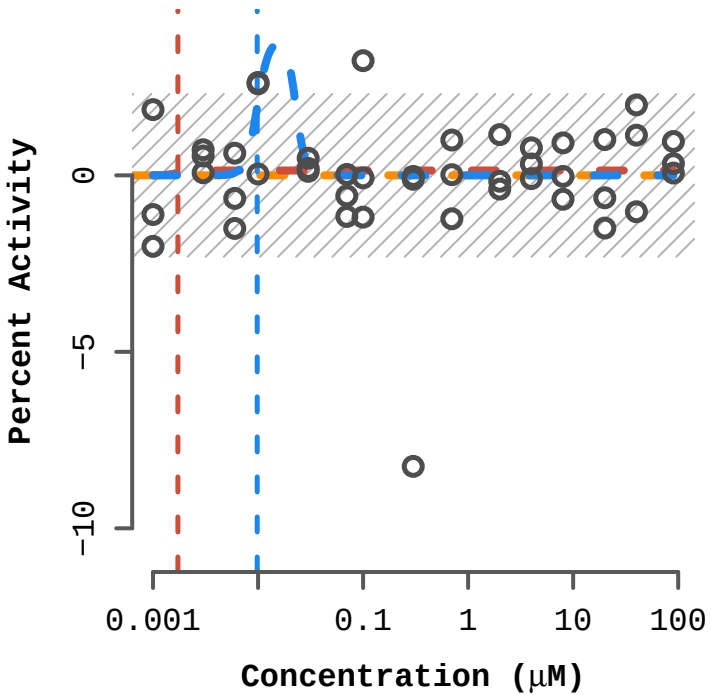
NAME: Cycloate
CHID: 32356 CASRN: 1134-23-2
SPID(S): Tox21_300884
M4ID: 12478249

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.4 MAX_MED: 1.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cymoxanil
CHID: 32358 CASRN: 57966-95-7
SPID(S): Tox21_300680
M4ID: 12478453

HILL MODEL (in red):

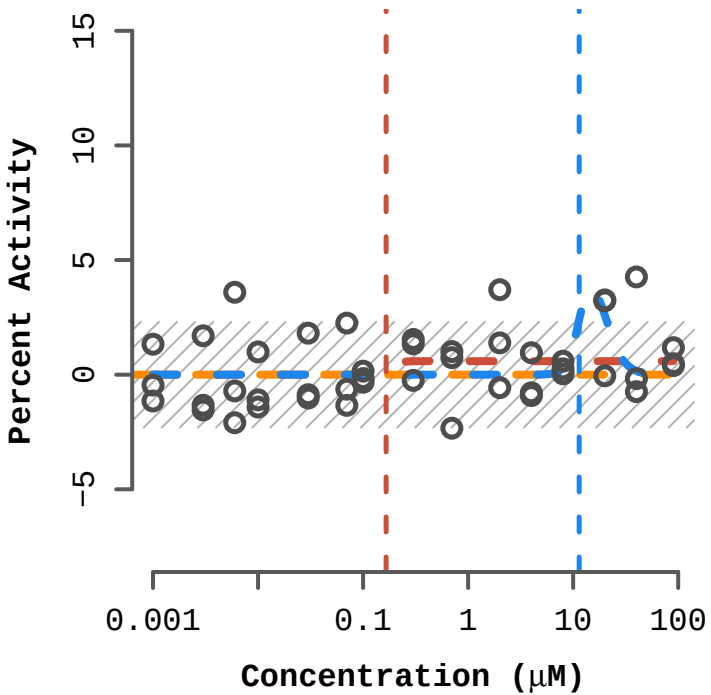
	tp	ga	gw
val:	0.137	−2.76	8
sd:	0.167	0.881	29.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.9	−2.01	8	−1.64	9.77
sd:	6.56	0.192	6.54	0.787	65.8

	CNST	HILL	GNLS
AIC:	154.74	160.07	158.44
PROB:	0.82	0.06	0.13
RMSE:	1.67	1.67	1.61

MAX_MEAN: 1.76 MAX_MED: 2.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyprodinil
CHID: 32359 CASRN: 121552-61-2
SPID(S): Tox21_300944
M4ID: 12478189

HILL MODEL (in red):

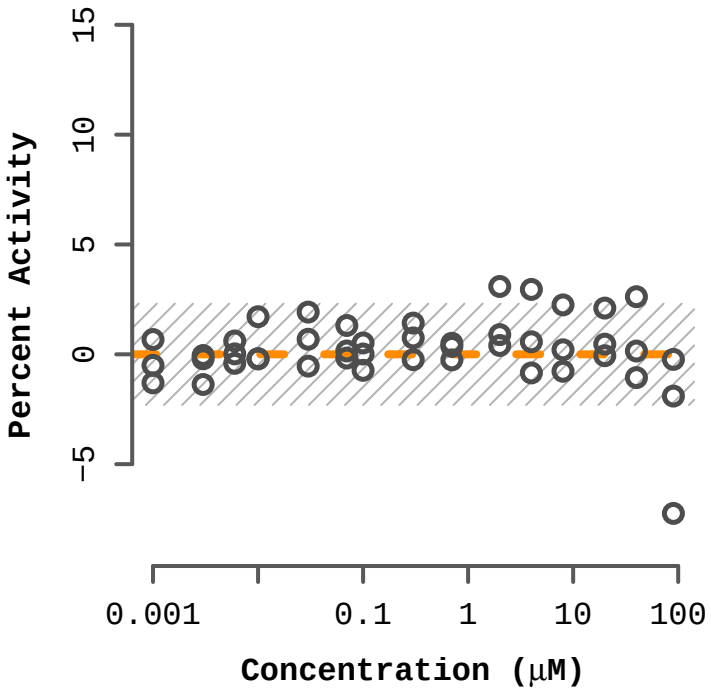
	tp	ga	gw
val:	0.589	−0.781	8
sd:	0.294	0.67	21.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.08	1.06	7.84	1.31	5.01
sd:	93.1	1.23	46.5	3.24	43.4

	CNST	HILL	GNLS
AIC:	172.42	174.4	176.65
PROB:	0.67	0.25	0.08
RMSE:	1.61	1.51	1.51

MAX_MEAN: 2.15 MAX_MED: 3.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

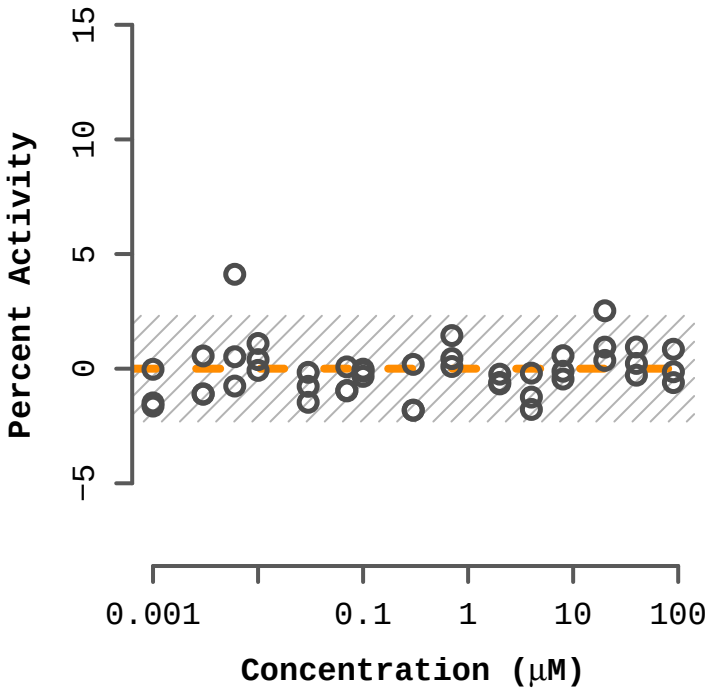
NAME: 2,2-Dibromo-3-nitrilopropionamide
CHID: 32361 **CASRN:** 10222-01-2
SPID(S): Tox21_300089
M4ID: 12479041

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 0.898 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

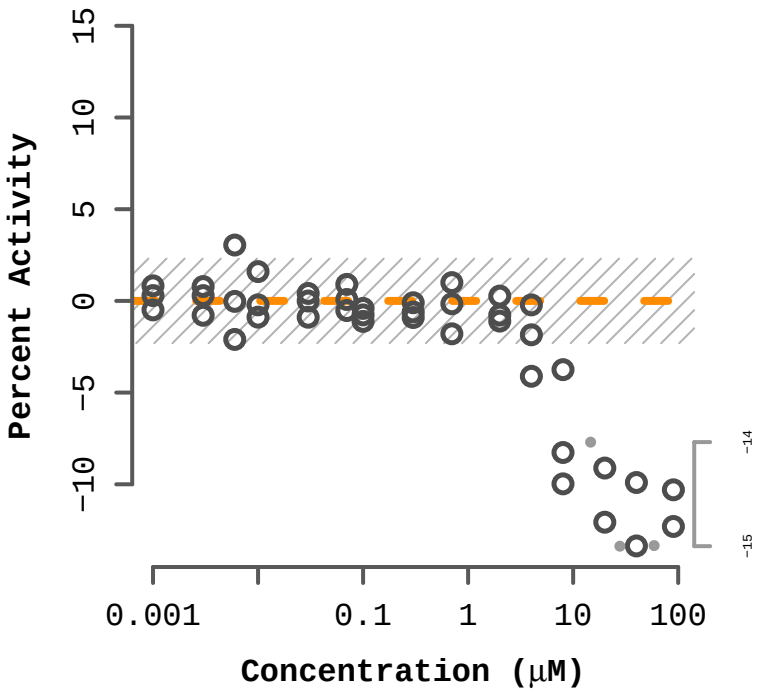
NAME: Dichlobenil
CHID: 32365 **CASRN:** 1194-65-6
SPID(S): Tox21_300791
M4ID: 12478342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

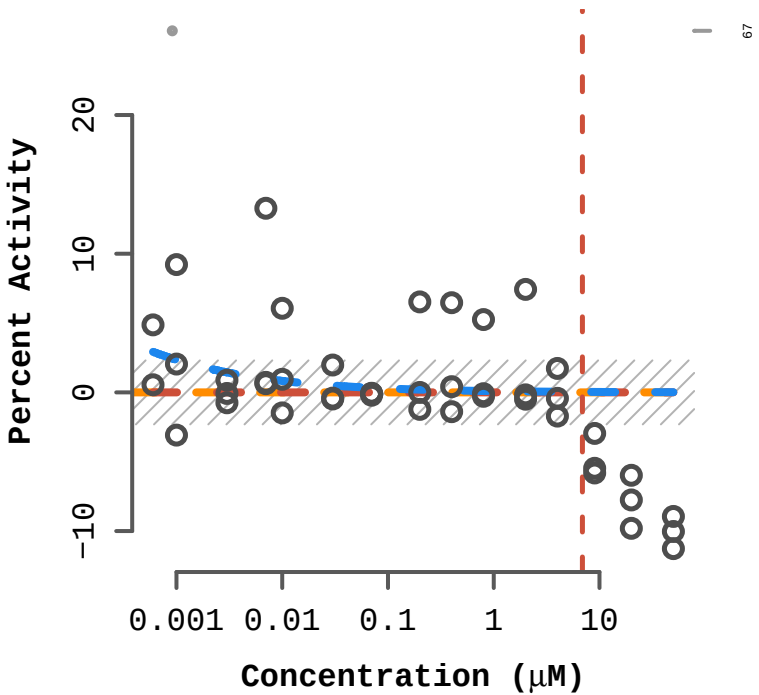
NAME: Difenoconazole
CHID: 32372 **CASRN:** 119446-68-3
SPID(S): Tox21_301110
M4ID: 12478023 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.12	NA	NA
PROB:	1	NA	NA
RMSE:	6.04	NA	NA

MAX_MEAN: 0.308 **MAX_MED:** 0.292 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Difethialone
CHID: 32374 CASRN: 104653-34-1
SPID(S): Tox21_113950
M4ID: 12482281 BRK

HILL MODEL (in red):

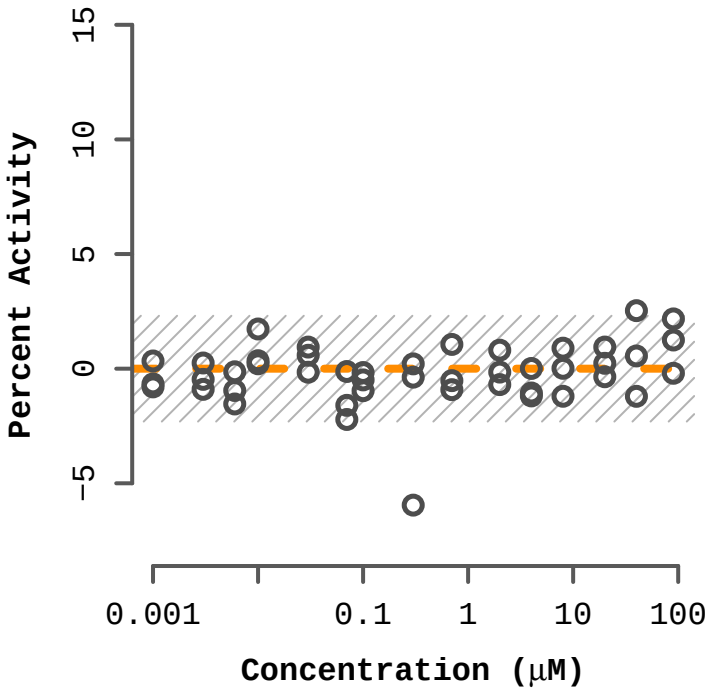
	tp	ga	gw
val:	1.42e-10	0.839	0.683
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.3	-5.11	7.54	-4.86	0.486
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	292.57	298.57	300.11
PROB:	0.93	0.05	0.02
RMSE:	11.12	11.12	10.66

MAX_MEAN: 24.1 **MAX_MED:** 4.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

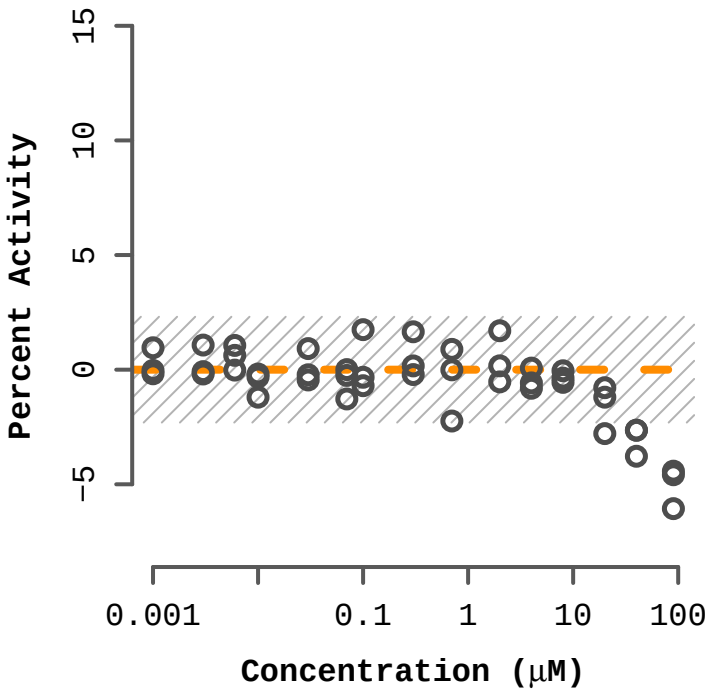
NAME: Diflufenzopyr-sodium
CHID: 32375 **CASRN:** 109293-98-3
SPID(S): Tox21_300997
M4ID: 12478136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

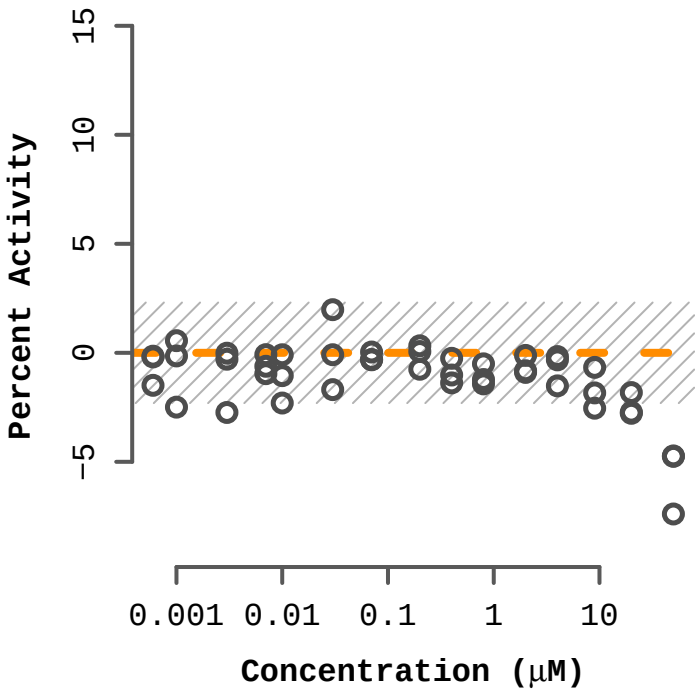
NAME: Dimethenamid
CHID: 32376 **CASRN:** 87674-68-8
SPID(S): Tox21_300705
M4ID: 12478428

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 0.556 **MAX_MED:** 0.626 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

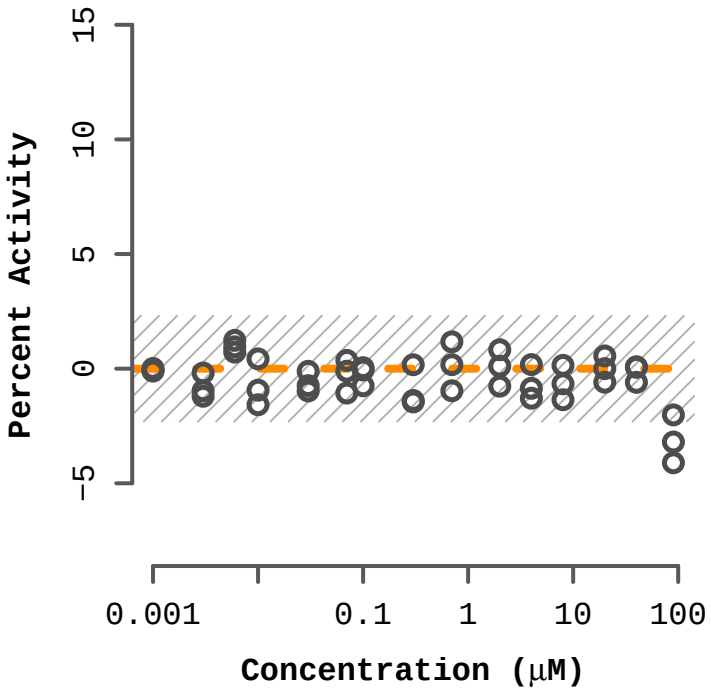
NAME: Diphacinone
CHID: 32378 **CASRN:** 82-66-6
SPID(S): Tox21_111893_1
M4ID: 12483431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 0.0693 **MAX_MED:** 0.0616 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

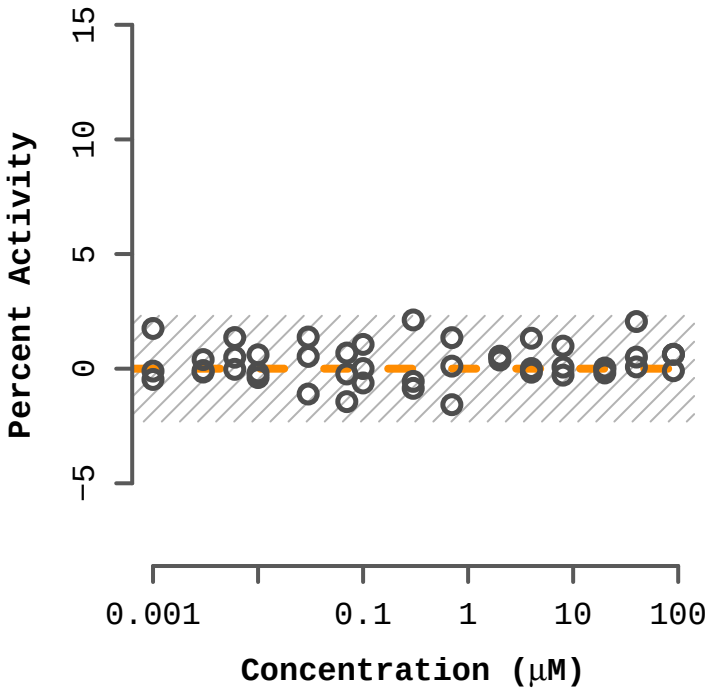
NAME: Dithiopyr
CHID: 32379 CASRN: 97886-45-8
SPID(S): Tox21_301150
M4ID: 12477983

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.972 MAX_MED: 0.955 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

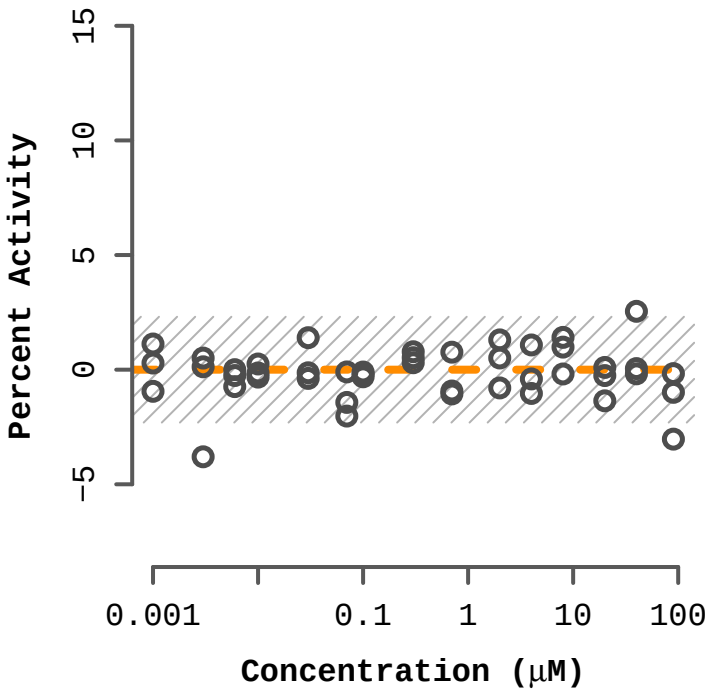
NAME: Ethalfluralin
CHID: 32386 **CASRN:** 55283-68-6
SPID(S): Tox21_301082
M4ID: 12478051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 0.626 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

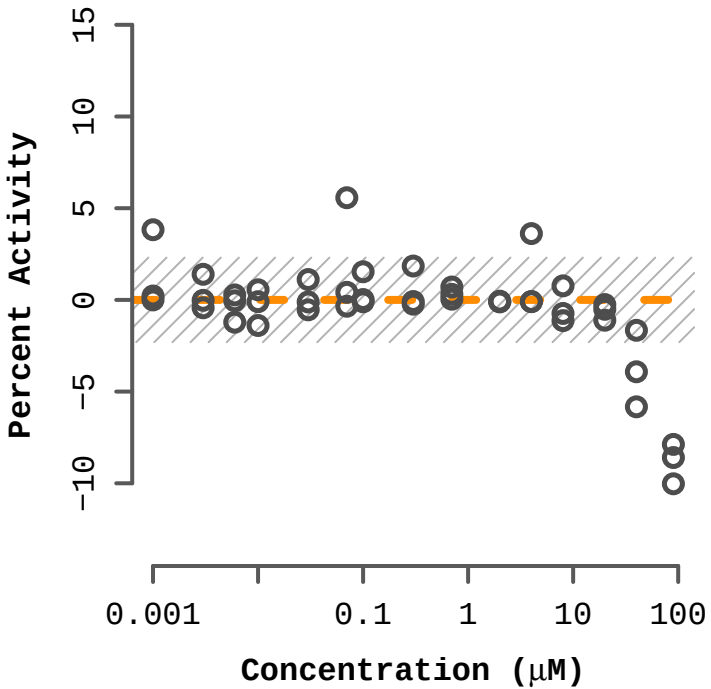
NAME: Farnesol
CHID: 32389 **CASRN:** 4602-84-0
SPID(S): Tox21_302034
M4ID: 12477099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 0.986 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

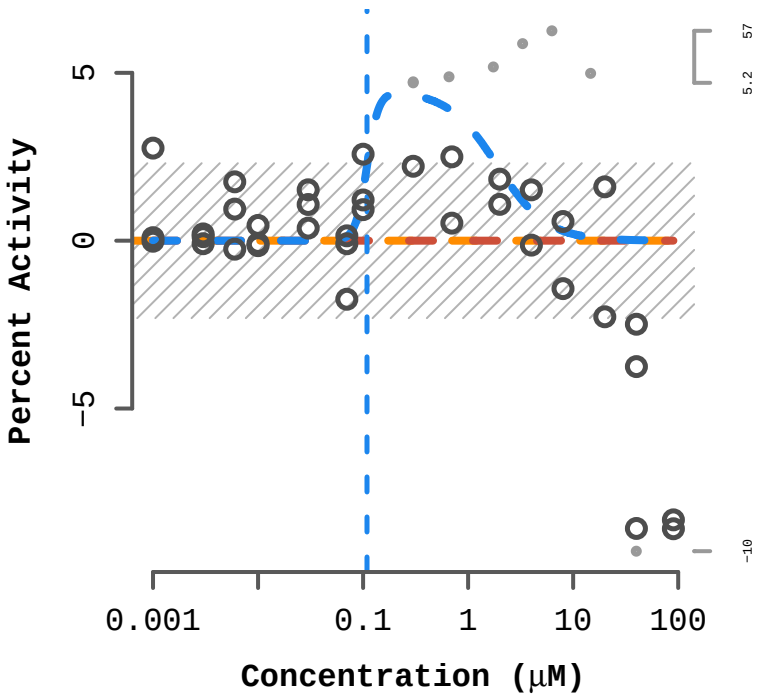
NAME: Fenarimol
CHID: 32390 **CASRN:** 60168-88-9
SPID(S): Tox21_300650
M4ID: 12478483

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.09	NA	NA
PROB:	1	NA	NA
RMSE:	2.85	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 0.415 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenarimol
CHID: 32390 CASRN: 60168-88-9
SPID(S): Tox21_201631
M4ID: 12480621 BRK

HILL MODEL (in red):

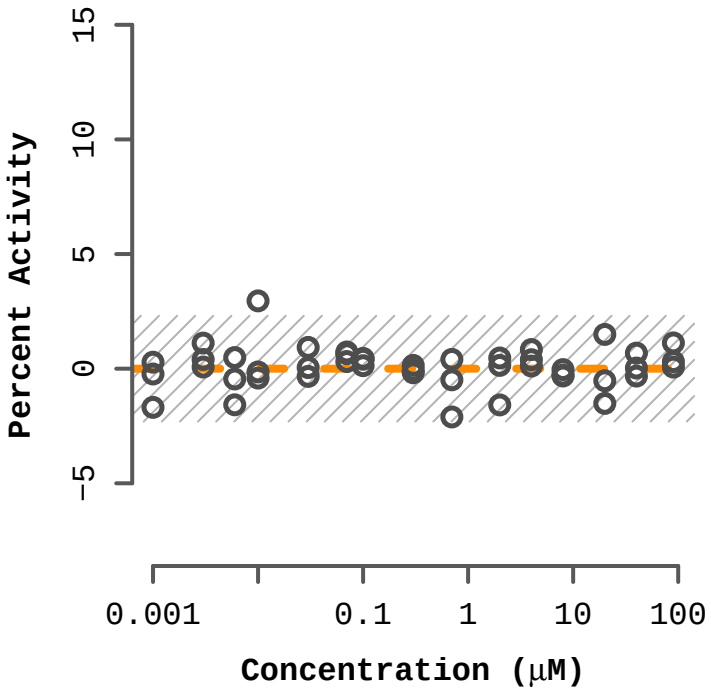
	tp	ga	gw
val:	2.01e-09	2.44	0.634
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.48	−0.963	8	0.277	1.84
sd:	2.46	0.131	14.9	0.63	2.55

	CNST	HILL	GNLS
AIC:	300.97	306.97	301.17
PROB:	0.51	0.03	0.46
RMSE:	12.06	12.06	11.74

MAX_MEAN: 18.9 MAX_MED: 5.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

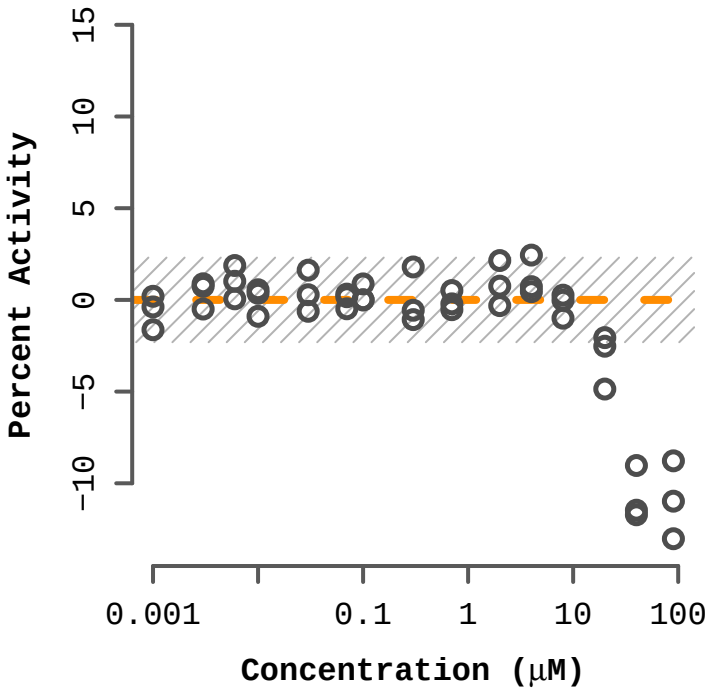
NAME: Fenoxaprop-ethyl
CHID: 32392 **CASRN:** 66441-23-4
SPID(S): Tox21_301166
M4ID: 12477967

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 0.654 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

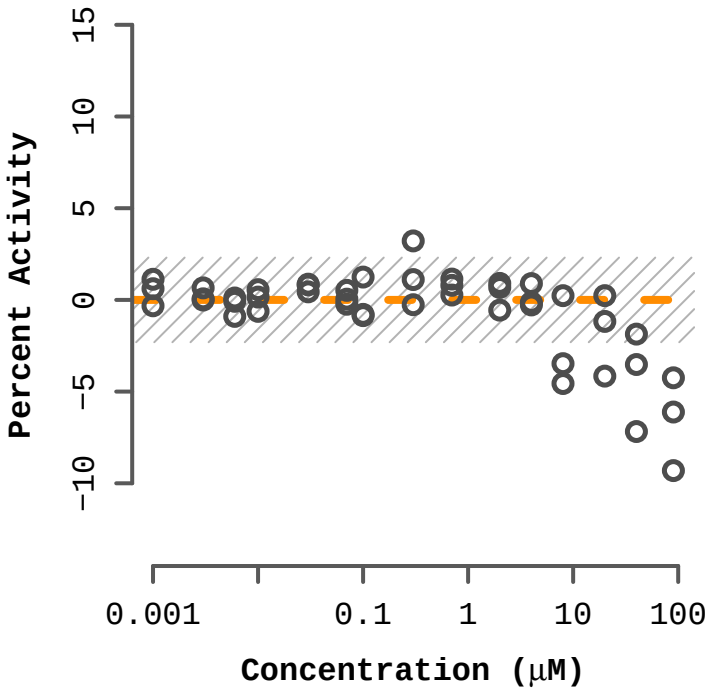
NAME: Fenoxycarb
CHID: 32393 CASRN: 72490-01-8
SPID(S): Tox21_301209
M4ID: 12477924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.89	NA	NA
PROB:	1	NA	NA
RMSE:	4.17	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

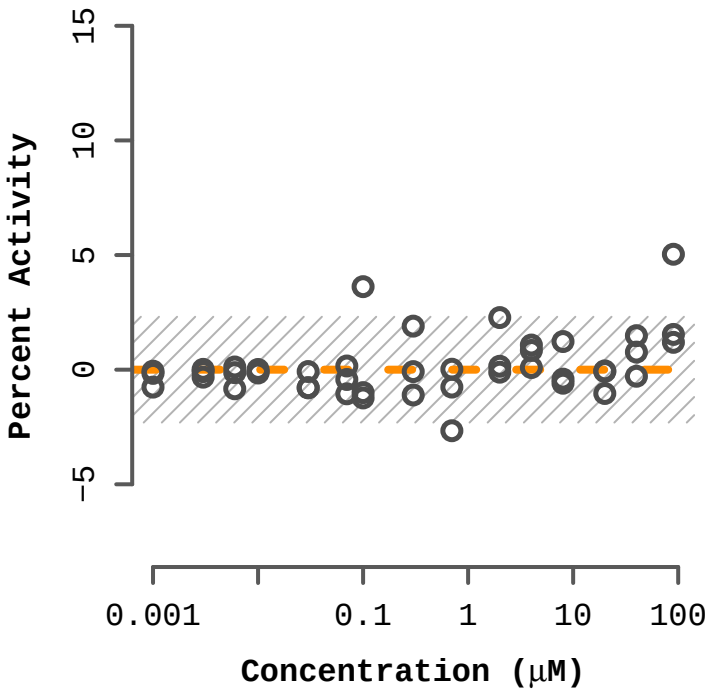
NAME: Fludioxonil
CHID: 32398 **CASRN:** 131341-86-1
SPID(S): Tox21_301049
M4ID: 12478084

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.05	NA	NA
PROB:	1	NA	NA
RMSE:	2.52	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

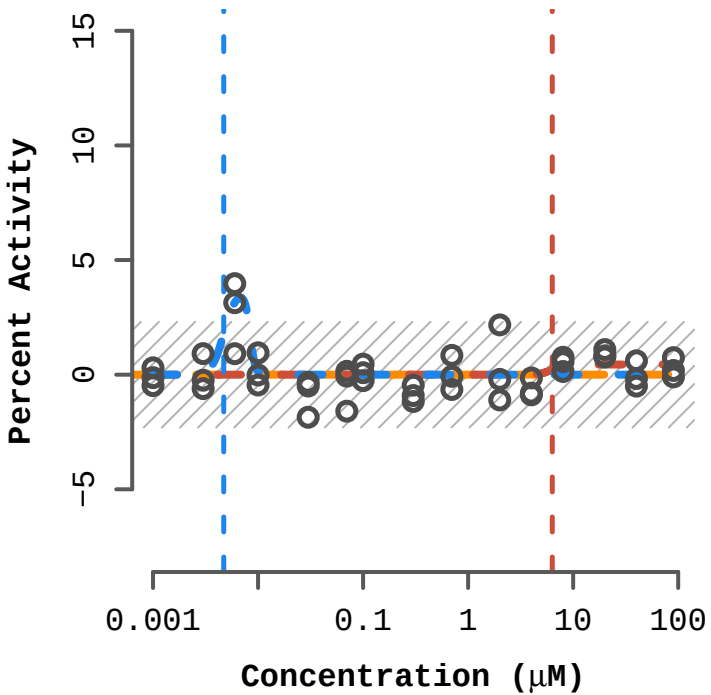
NAME: Formetanate hydrochloride
CHID: 32405 **CASRN:** 23422-53-9
SPID(S): Tox21_300778
M4ID: 12478355

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 2.59 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fosamine ammonium
CHID: 32406 CASRN: 25954-13-6
SPID(S): Tox21_301917
M4ID: 12477216

HILL MODEL (in red):

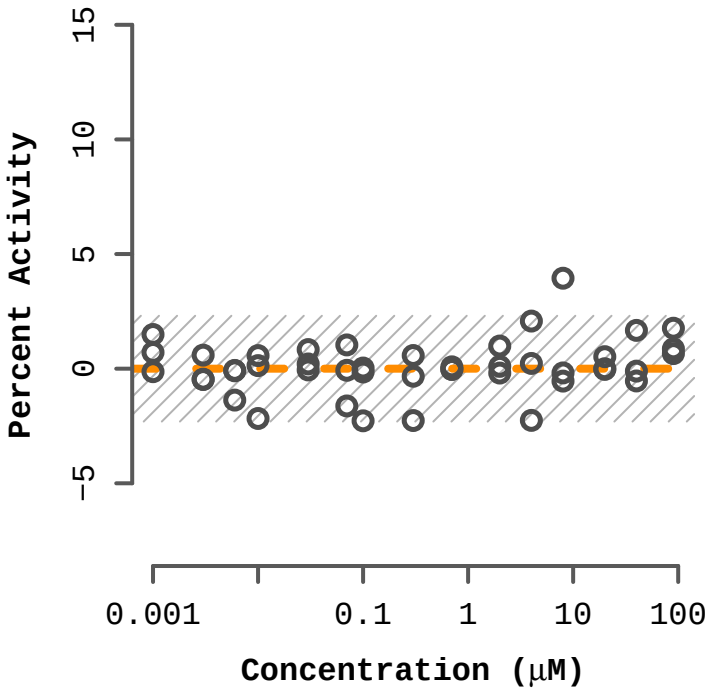
	tp	ga	gw
val:	0.443	0.801	8
sd:	0.216	0.191	9.69

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.62	−2.33	7.95	−2.08	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	126.2	128.11	122.01
PROB:	0.11	0.04	0.85
RMSE:	1.07	1.05	0.82

MAX_MEAN: 2.68 MAX_MED: 3.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

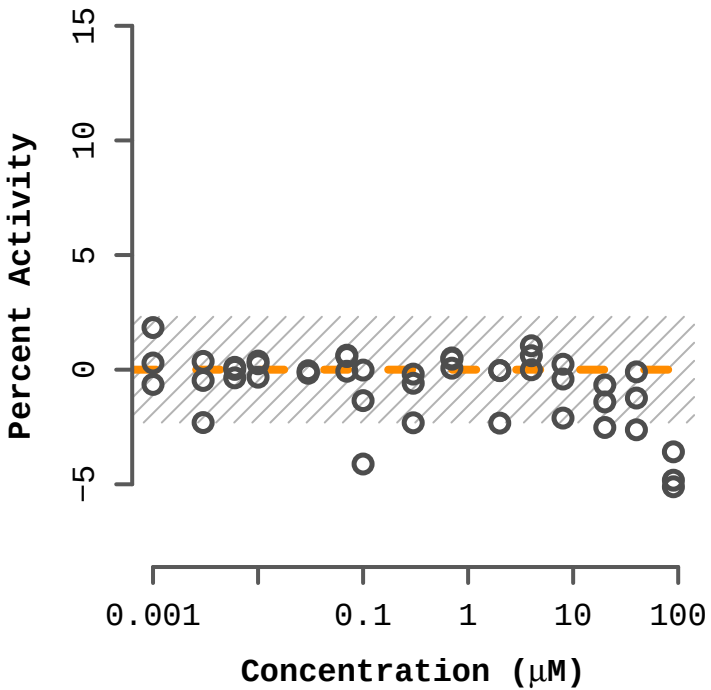
NAME: Imazamethabenz
CHID: 32412 **CASRN:** 81405-85-8
SPID(S): Tox21_302218
M4ID: 12476915

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.867 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

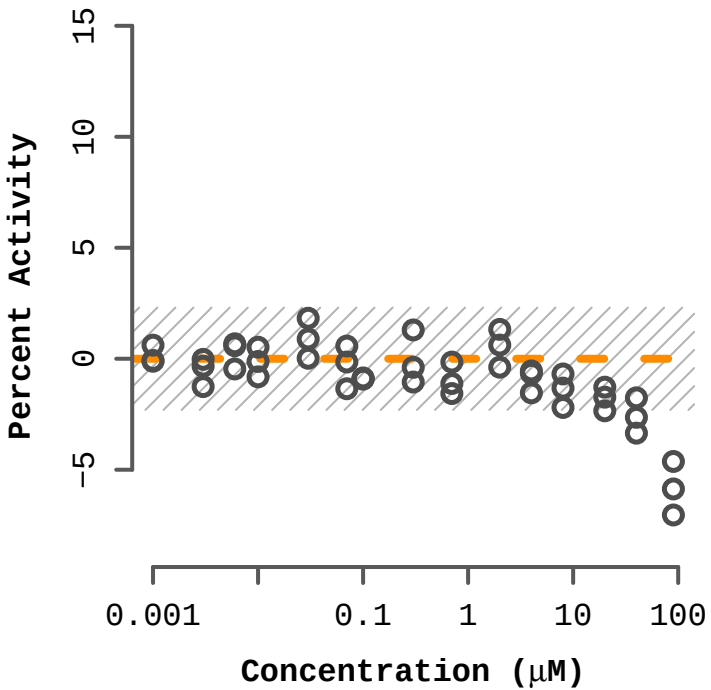
NAME: Cybutryne
CHID: 32416 CASRN: 28159-98-0
SPID(S): Tox21_302267
M4ID: 12476866

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 0.551 MAX_MED: 0.611 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

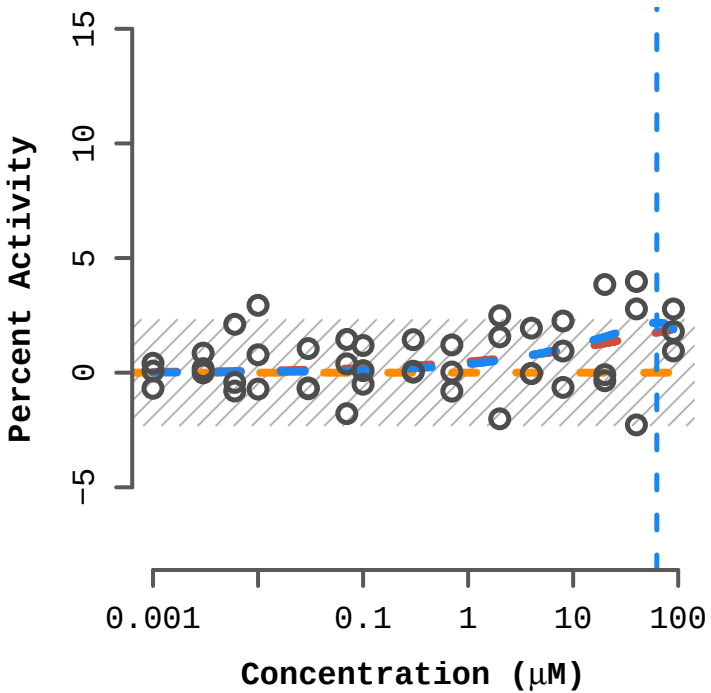
NAME: Isofenphos
CHID: 32417 CASRN: 25311-71-1
SPID(S): Tox21_302219
M4ID: 12476914

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 0.914 **MAX_MED:** 0.892 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lithium perfluorooctane sulfonate
CHID: 32421 CASRN: 29457-72-5
SPID(S): Tox21_302319
M4ID: 12476814

HILL MODEL (in red):

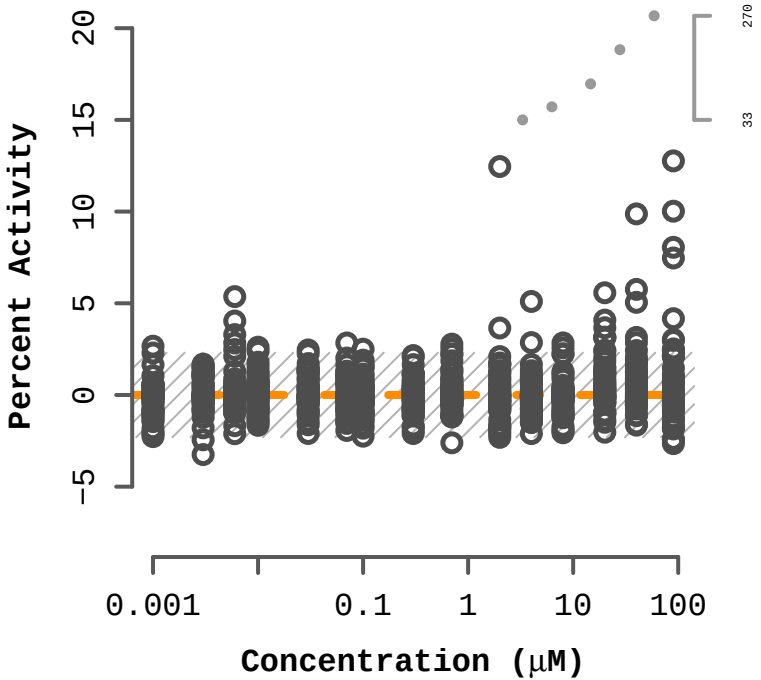
	tp	ga	gw
val:	4.77	2.4	0.399
sd:	10.6	4.24	0.34

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.62	1.8	0.589	2.05	4.88
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	169.54	163.77	167.74
PROB:	0.05	0.84	0.12
RMSE:	1.55	1.35	1.36

MAX_MEAN: 1.84 MAX_MED: 2.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

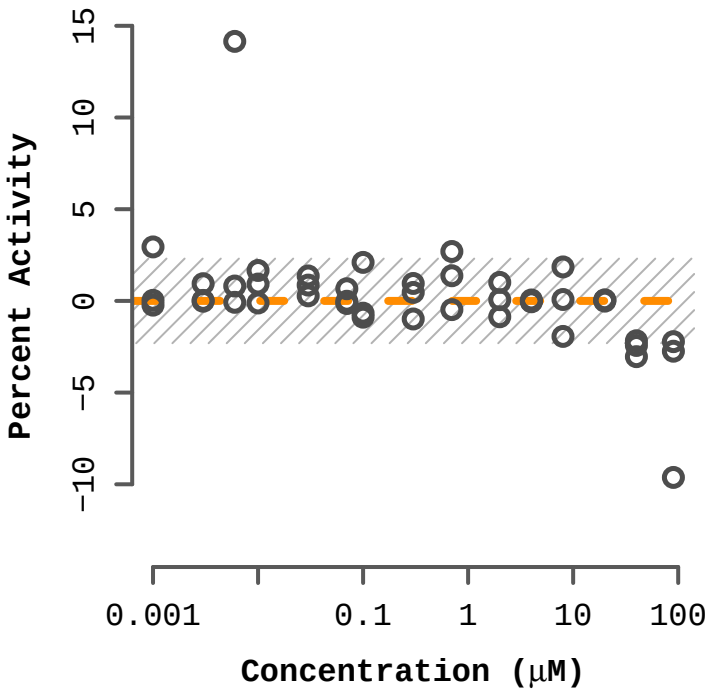
NAME: Mesotrione
CHID: 32424 **CASRN:** 104206-82-8
SPID(S): Tox21_400050
M4ID: 12475087 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2509.69	NA	NA
PROB:	1	NA	NA
RMSE:	13.44	NA	NA

MAX_MEAN: 6.69 **MAX_MED:** 0.413 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

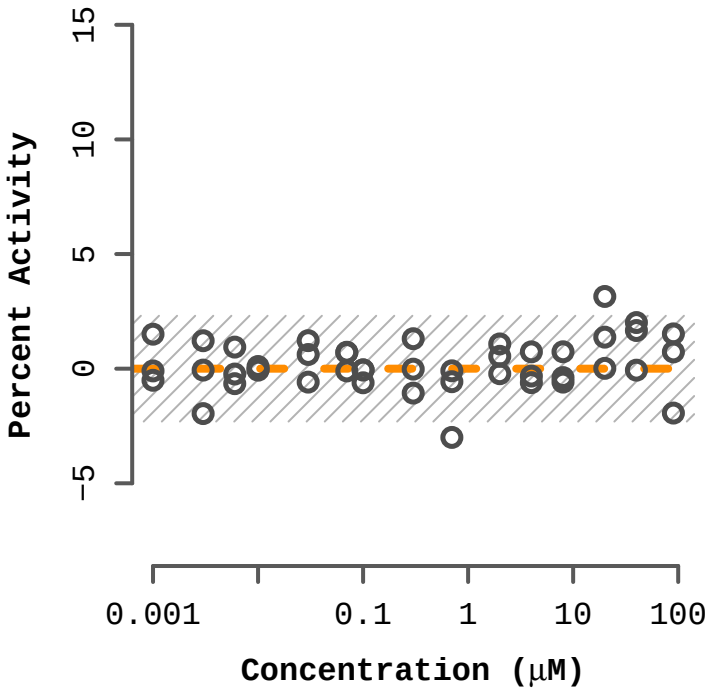
NAME: S-Metolachlor
CHID: 32431 **CASRN:** 87392-12-9
SPID(S): Tox21_301577
M4ID: 12477556

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.86	NA	NA
PROB:	1	NA	NA
RMSE:	2.86	NA	NA

MAX_MEAN: 4.96 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

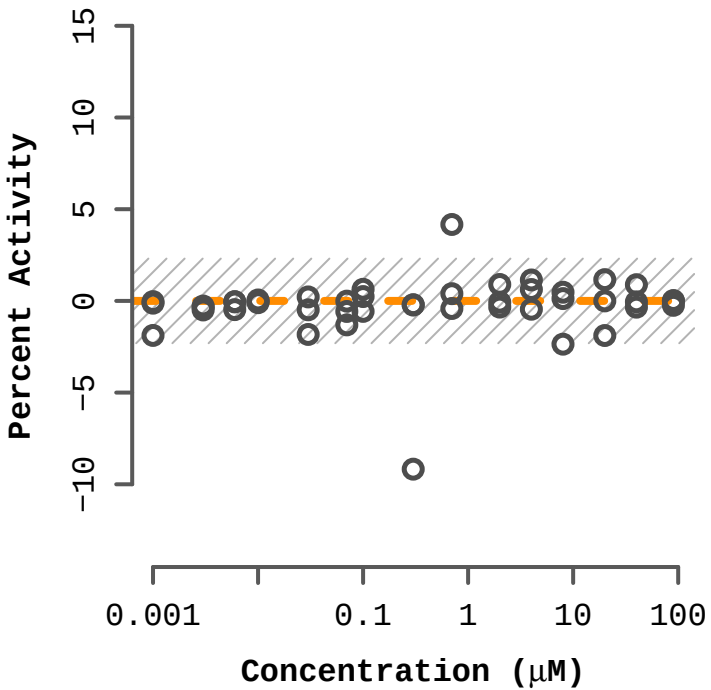
NAME: Naptalam
CHID: 32437 **CASRN:** 132-66-1
SPID(S): Tox21_302279
M4ID: 12476854

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

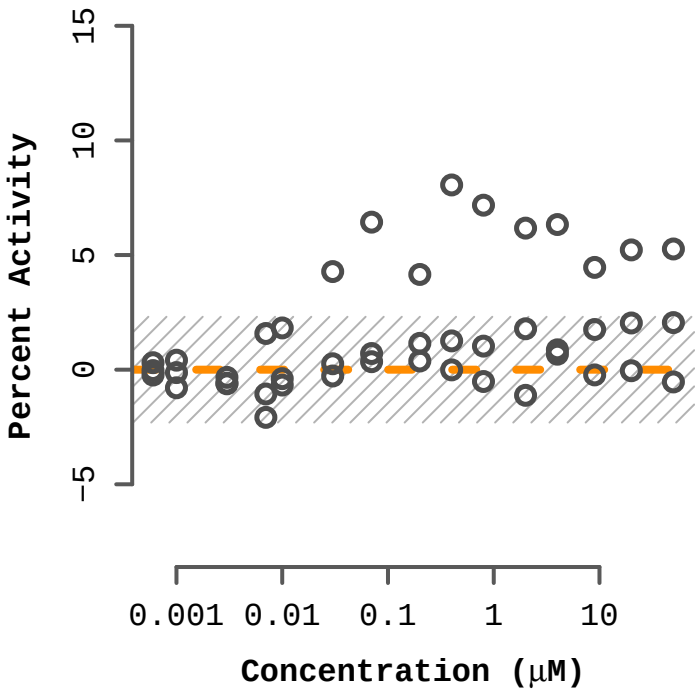
NAME: Imidacloprid
CHID: 32442 **CASRN:** 138261-41-3
SPID(S): Tox21_301028
M4ID: 12478105

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 0.623 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

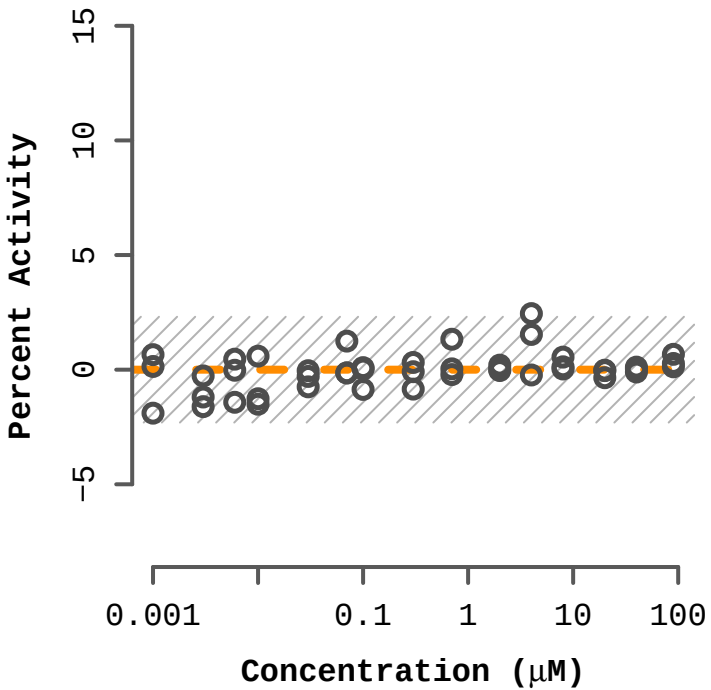
NAME: Imidacloprid
CHID: 32442 **CASRN:** 138261-41-3
SPID(S): Tox21_111298_1
M4ID: 12483783

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.92	NA	NA

MAX_MEAN: 3.1 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

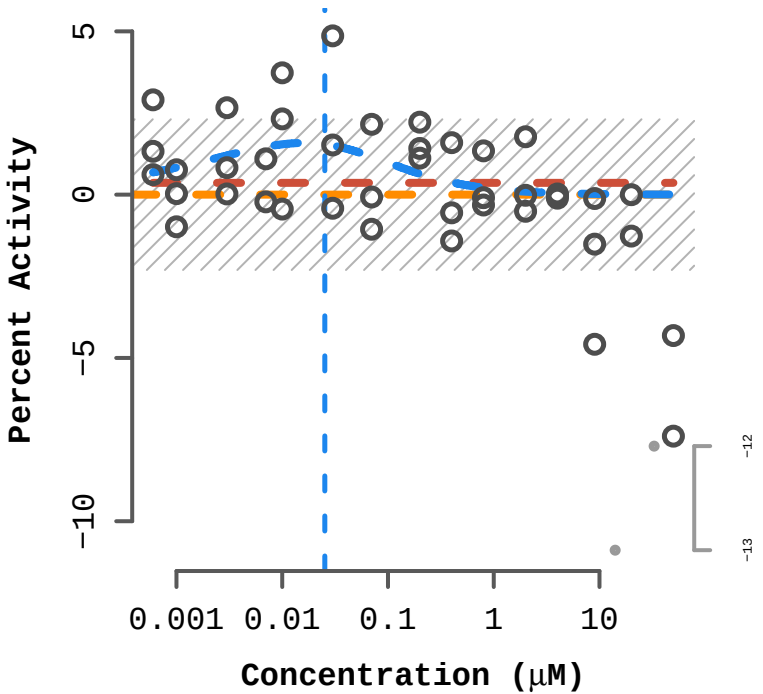
NAME: Phorate
CHID: 32459 **CASRN:** 298-02-2
SPID(S): Tox21_300398
M4ID: 12478734

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Profenofos
CHID: 32464 CASRN: 41198-08-7
SPID(S): Tox21_300752
M4ID: 12478381 BRK

HILL MODEL (in red):

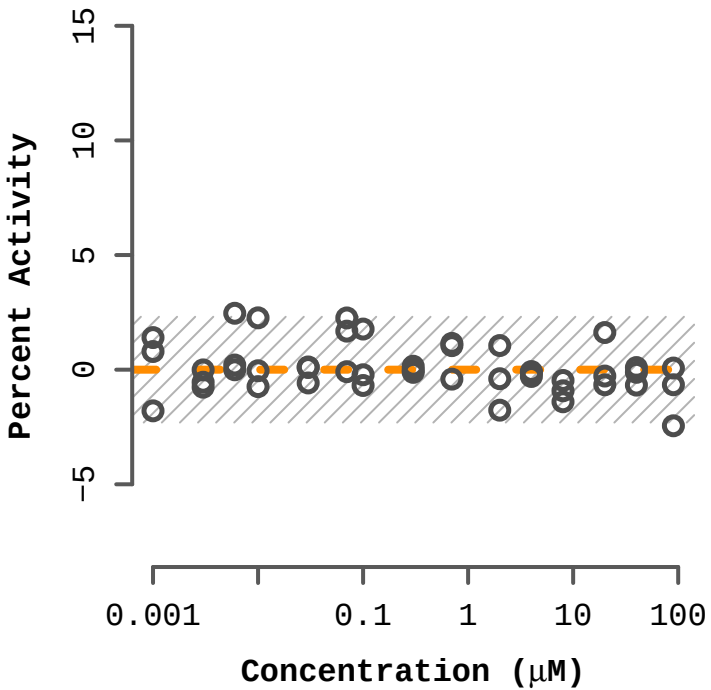
	tp	ga	gw
val:	0.361	−5.13	3.87
sd:	0.3	2650	5420

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.81	−1.6	0.477	−1.35	1.01
sd:	133	34	1.26	10.1	0.874

	CNST	HILL	GNLS
AIC:	219.9	224.49	221.52
PROB:	0.65	0.07	0.29
RMSE:	3.39	3.43	3.25

MAX_MEAN: 2.08 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

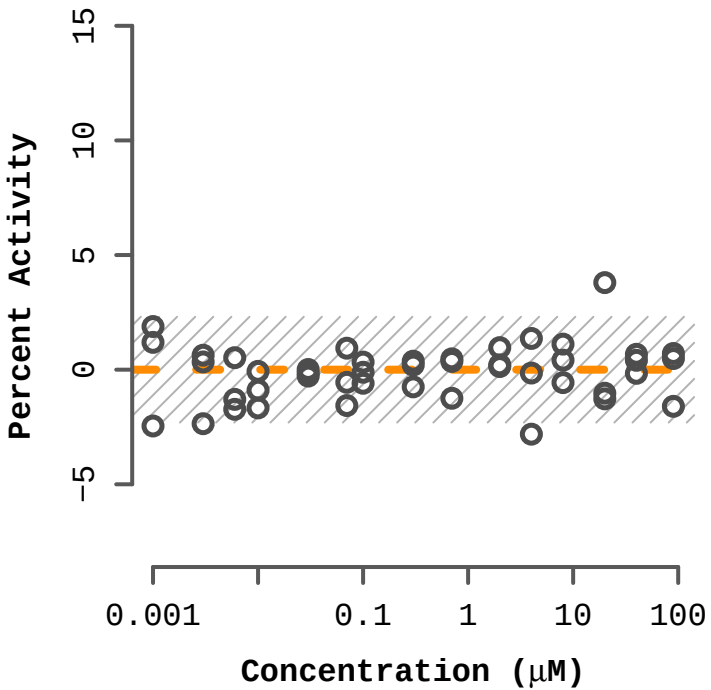
NAME: Propetamphos
CHID: 32470 **CASRN:** 31218-83-4
SPID(S): Tox21_300863
M4ID: 12478270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

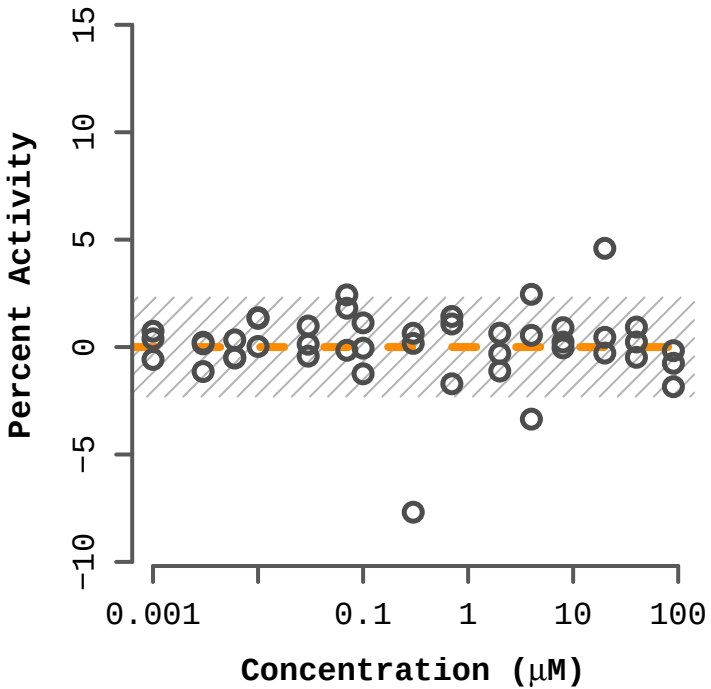
NAME: Siduron
CHID: 32474 CASRN: 1982-49-6
SPID(S): Tox21_301425
M4ID: 12477708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.501 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

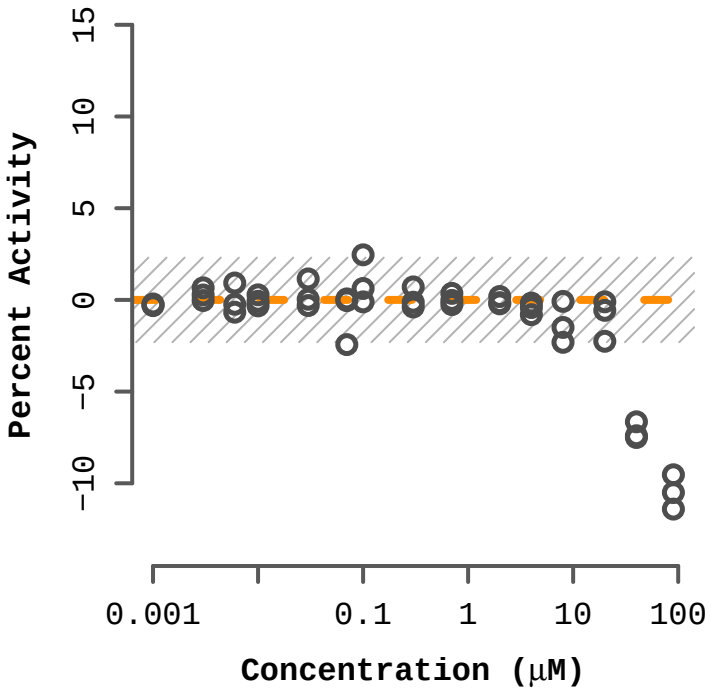
NAME: Tebupirimfos
CHID: 32482 CASRN: 96182-53-5
SPID(S): Tox21_300965
M4ID: 12478168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 1.59 MAX_MED: 1.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

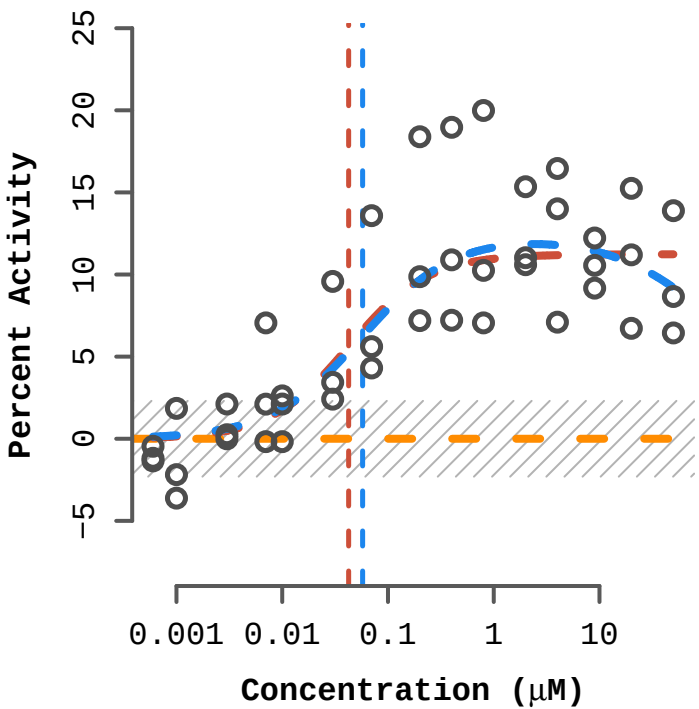
NAME: Temephos
CHID: 32484 **CASRN:** 3383-96-8
SPID(S): Tox21_301778
M4ID: 12477355

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.37	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 0.992 **MAX_MED:** 0.624 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Temephos
CHID: 32484 **CASRN:** 3383-96-8
SPID(S): Tox21_112075_1
M4ID: 12483335

HILL MODEL (in red):

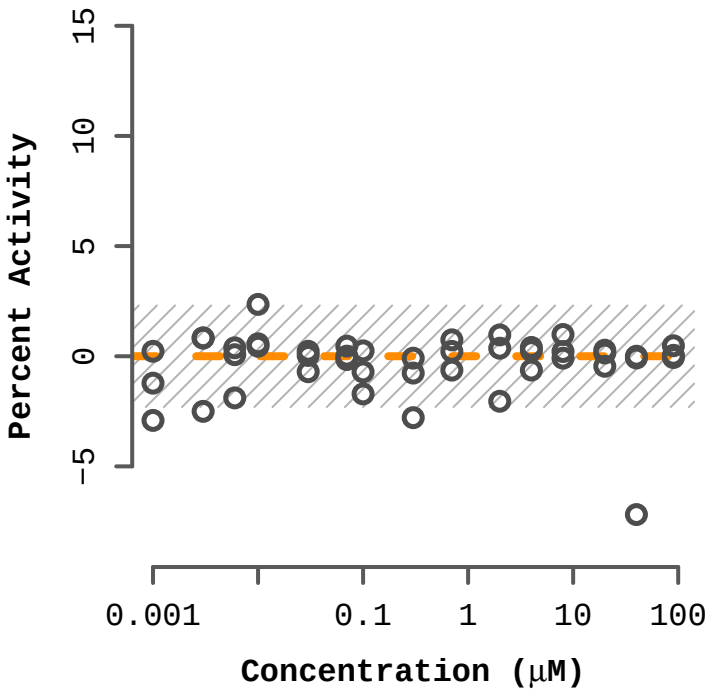
	tp	ga	gw
val:	11.2	−1.37	1.16
sd:	0.846	0.192	0.388

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.5	−1.24	1	2.25	0.821
sd:	3.17	0.338	0.4	0.994	1.64

	CNST	HILL	GNLS
AIC:	336.73	249.3	251.89
PROB:	0	0.78	0.22
RMSE:	9.49	3.55	3.49

MAX_MEAN: 12.5 **MAX_MED:** 14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

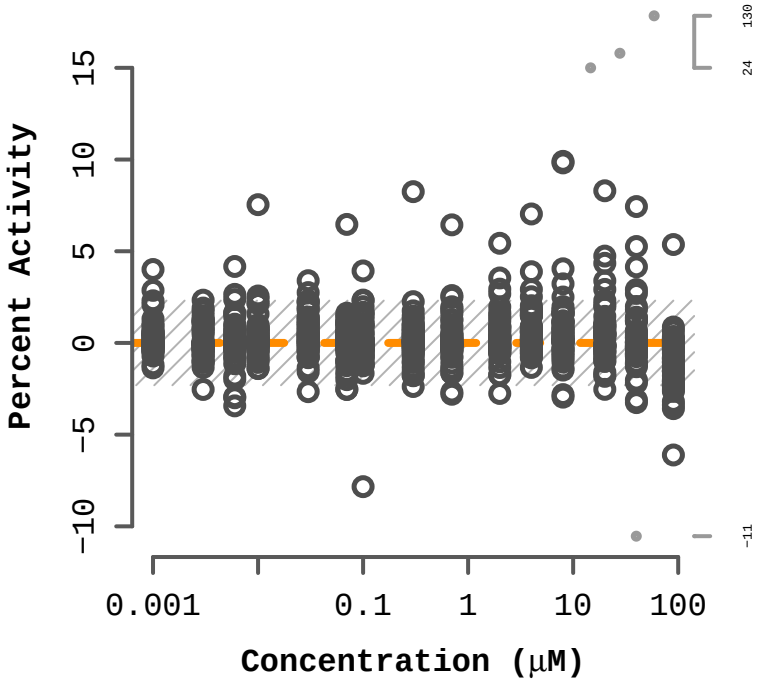
NAME: Thiazopyr
CHID: 32488 **CASRN:** 117718-60-2
SPID(S): Tox21_300822
M4ID: 12478311

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.828 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

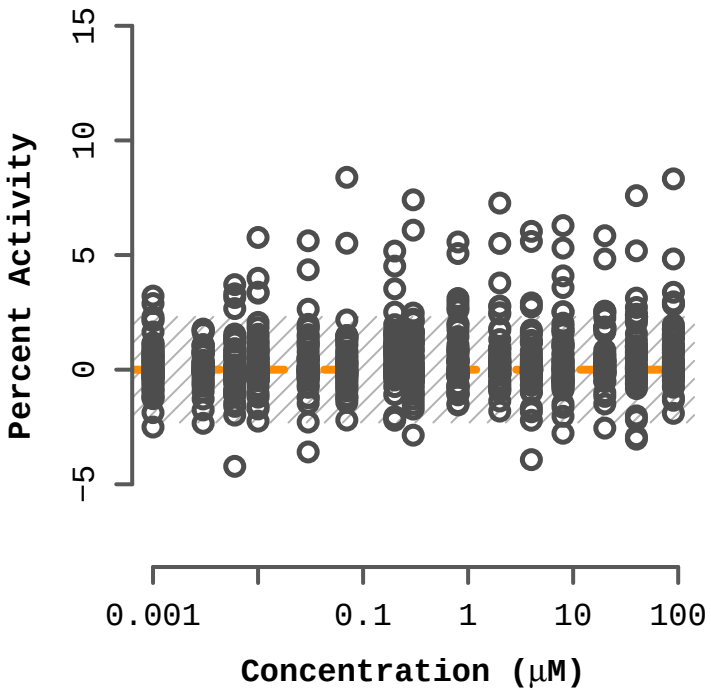
NAME: Triadimenol
CHID: 32493 **CASRN:** 55219-65-3
SPID(S): Tox21_400077
M4ID: 12475060 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2512.12	NA	NA
PROB:	1	NA	NA
RMSE:	5.53	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 0.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

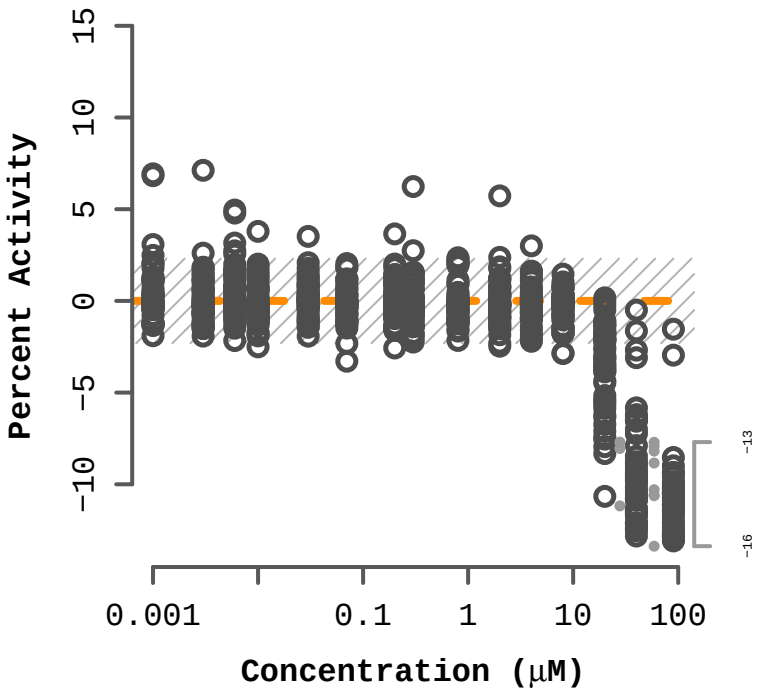
NAME: Triclopyr
CHID: 32497 **CASRN:** 55335-06-3
SPID(S): Tox21_400073
M4ID: 12475064

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2468.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 0.912 **MAX_MED:** 0.736 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

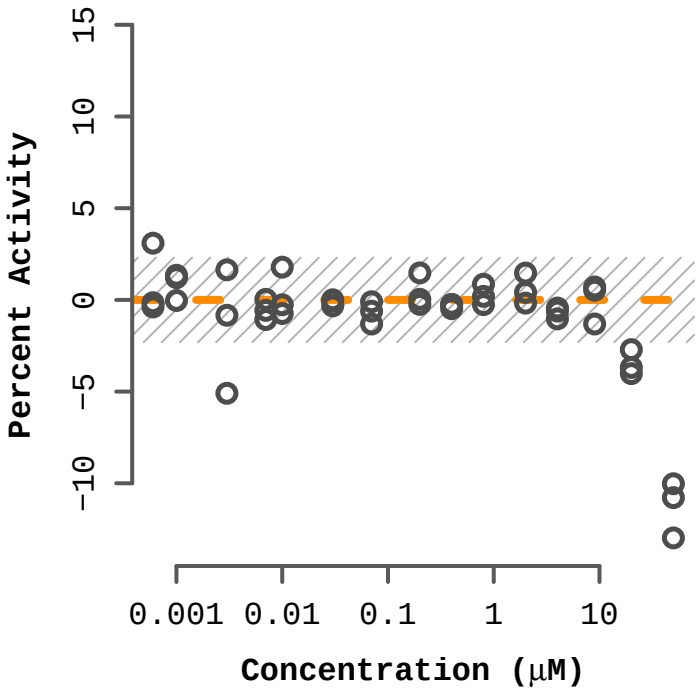
NAME: Triclosan
CHID: 32498 **CASRN:** 3380-34-5
SPID(S): Tox21_400079
M4ID: 12475058 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3737.93	NA	NA
PROB:	1	NA	NA
RMSE:	4.26	NA	NA

MAX_MEAN: 0.537 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

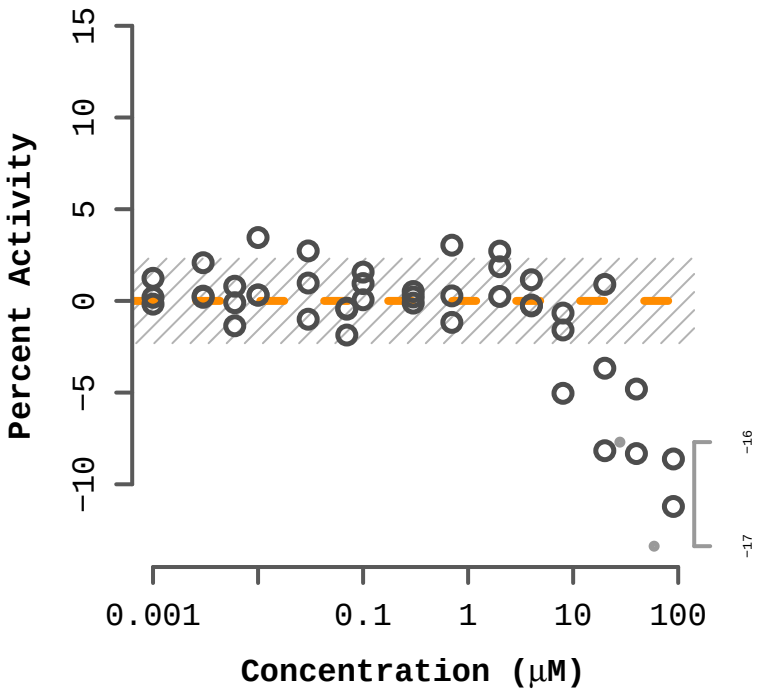
NAME: Triclosan
CHID: 32498 **CASRN:** 3380-34-5
SPID(S): Tox21_111648_1
M4ID: 12483560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.06	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 0.853 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

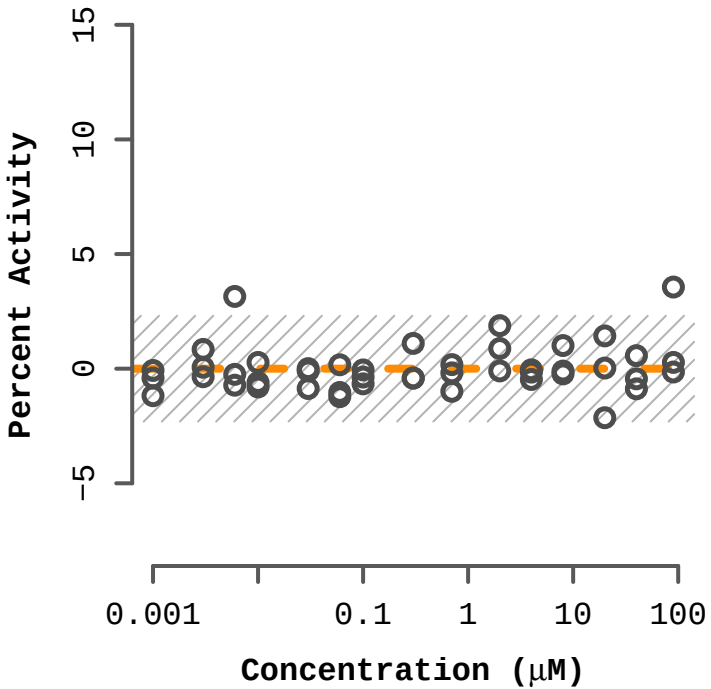
NAME: Triflumizole
CHID: 32500 **CASRN:** 68694-11-1
SPID(S): Tox21_300866
M4ID: 12478267 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.65	NA	NA
PROB:	1	NA	NA
RMSE:	4.74	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

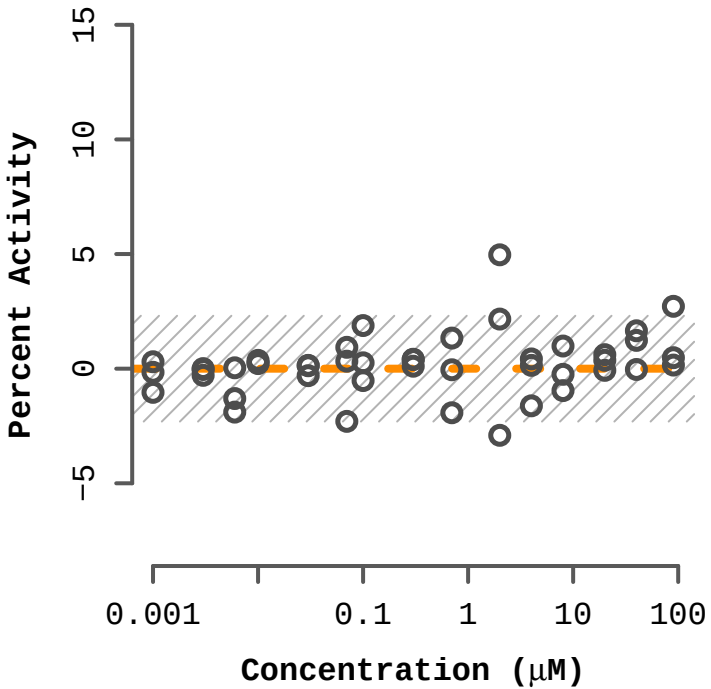
NAME: 1,3,5-Triethylhexahydro-s-triazine
CHID: 32511 **CASRN:** 7779-27-3
SPID(S): Tox21_301622
M4ID: 12477511

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

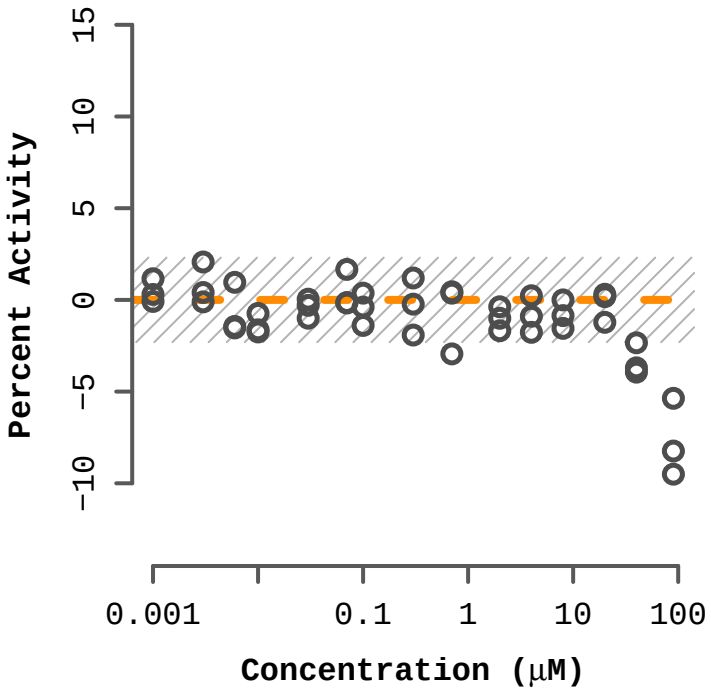
NAME: (3,5-Dimethyl-1H-pyrazol-1-yl)methanol
CHID: 32513 **CASRN:** 85264-33-1
SPID(S): Tox21_301192
M4ID: 12477941

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

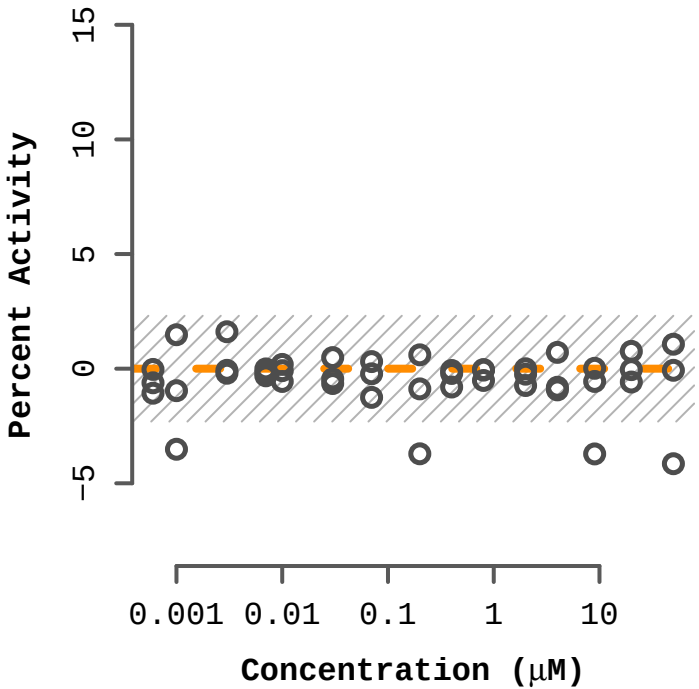
NAME: 1,2-Benzenedicarboxaldehyde
CHID: 32514 **CASRN:** 643-79-8
SPID(S): Tox21_300404
M4ID: 12478728

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.36	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.407 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

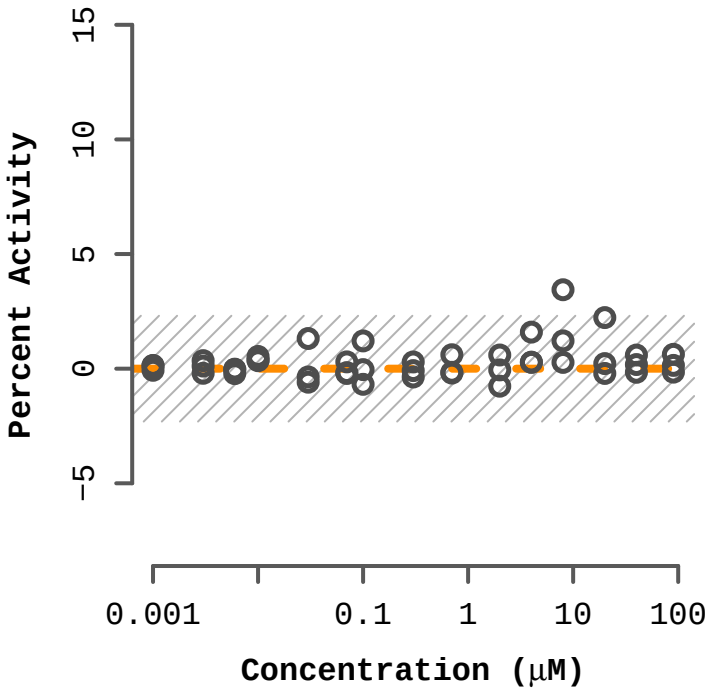
NAME: 1,2−Benzenedicarboxaldehyde
CHID: 32514 **CASRN:** 643−79−8
SPID(S): Tox21_112347_1
M4ID: 12483145

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.448 **MAX_MED:** −0.0408 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

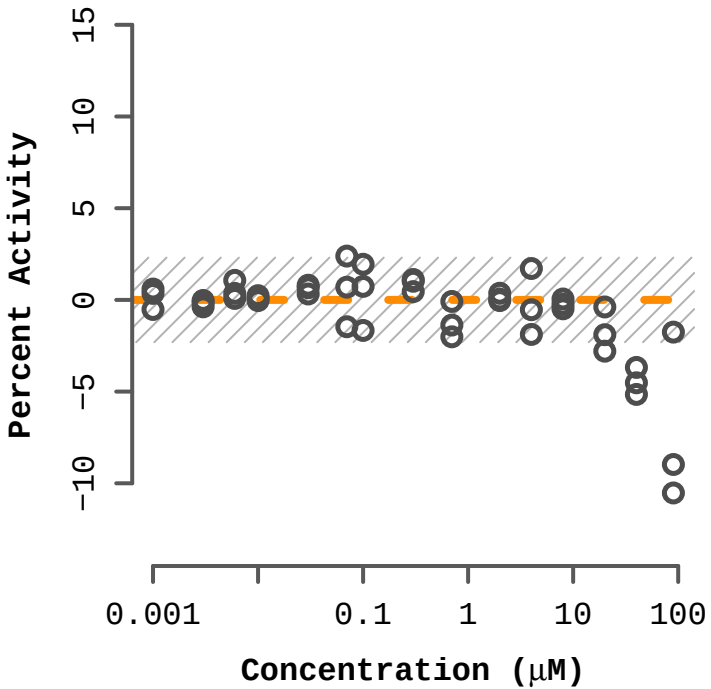
NAME: 2-Hydroxyethyl octyl sulfide
CHID: 32516 **CASRN:** 3547-33-9
SPID(S): Tox21_301965
M4ID: 12477168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

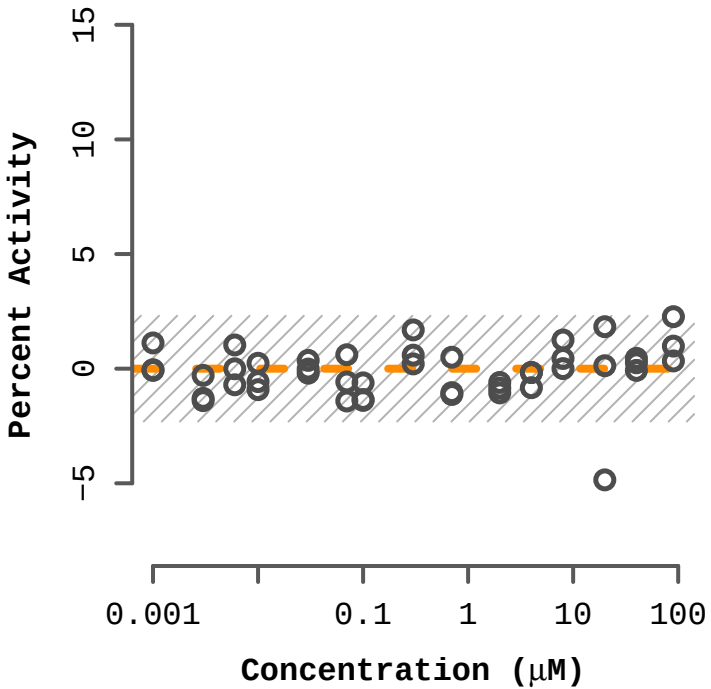
NAME: 4,5-Dichloro-3H-1,2-dithiol-3-one
CHID: 32518 **CASRN:** 1192-52-5
SPID(S): Tox21_303406
M4ID: 12475733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.59	NA	NA

MAX_MEAN: 0.863 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

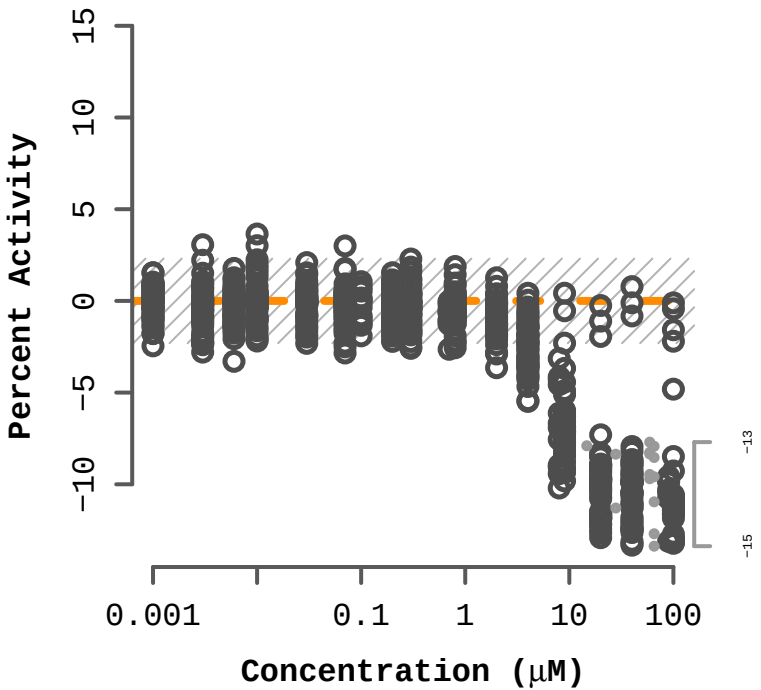
NAME: Acibenzolar-S-methyl
CHID: 32519 **CASRN:** 135158-54-2
SPID(S): Tox21_300864
M4ID: 12478269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.985 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

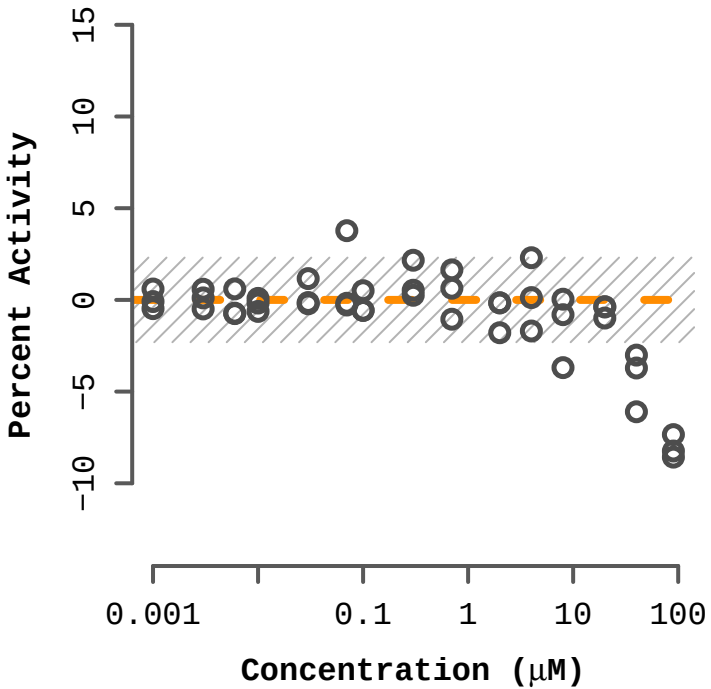
NAME: Azoxystrobin
CHID: 32520 **CASRN:** 131860-33-8
SPID(S): Tox21_400087
M4ID: 12475050 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	4287.93	NA	NA
PROB:	1	NA	NA
RMSE:	5.25	NA	NA

MAX_MEAN: 0.0421 **MAX_MED:** 0.0347 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

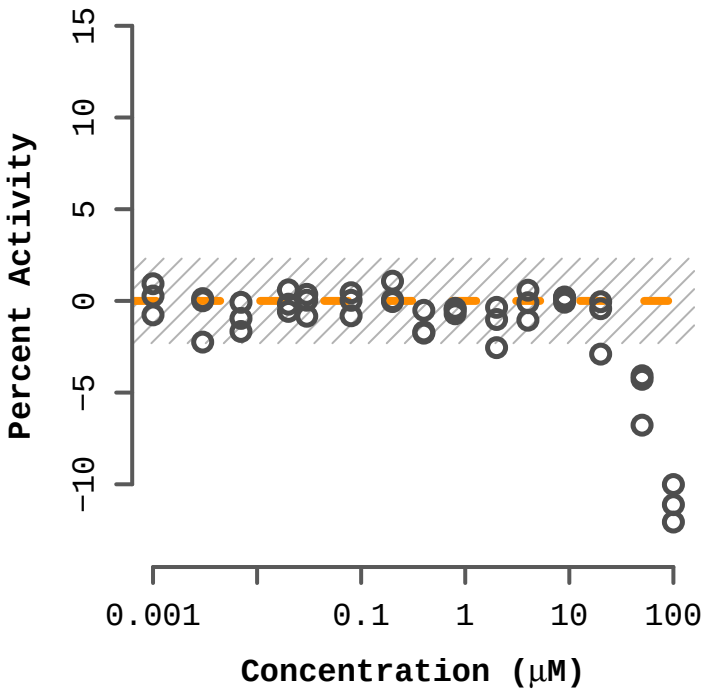
NAME: 1,2-Benzisothiazolin-3-one
CHID: 32523 **CASRN:** 2634-33-5
SPID(S): Tox21_300489
M4ID: 12478643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.06	NA	NA
PROB:	1	NA	NA
RMSE:	2.63	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.638 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

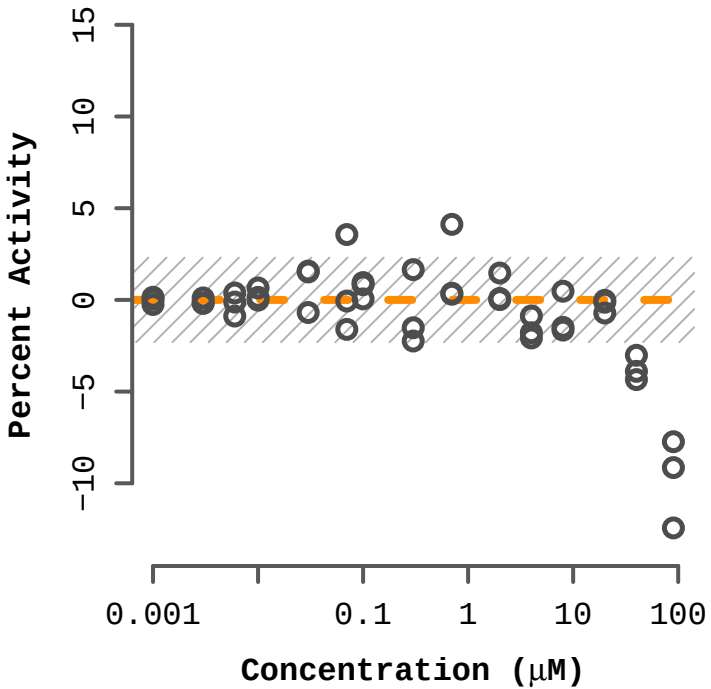
NAME: Bifenazate
CHID: 32525 **CASRN:** 149877-41-8
SPID(S): Tox21_300871
M4ID: 12478262

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.67	NA	NA
PROB:	1	NA	NA
RMSE:	3.29	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.268 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

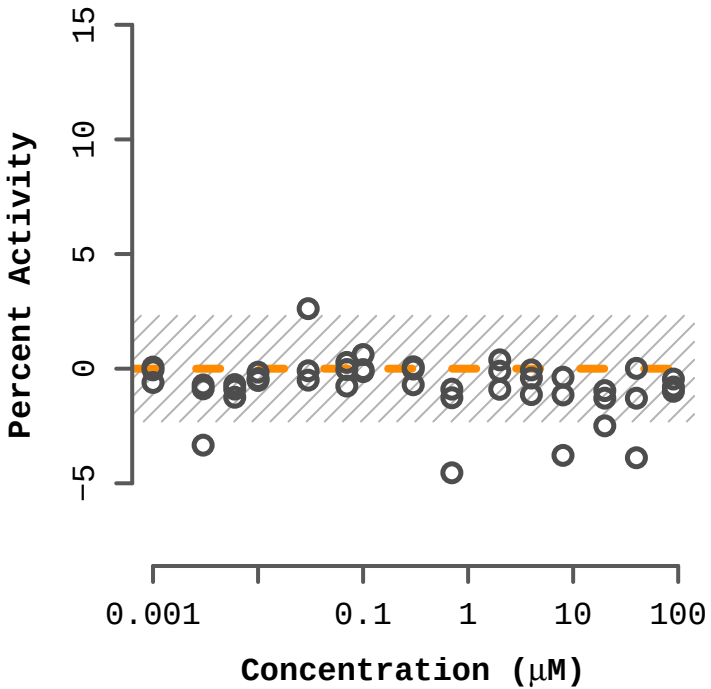
NAME: Bromuconazole
CHID: 32531 **CASRN:** 116255-48-2
SPID(S): Tox21_302434
M4ID: 12476699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.01	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

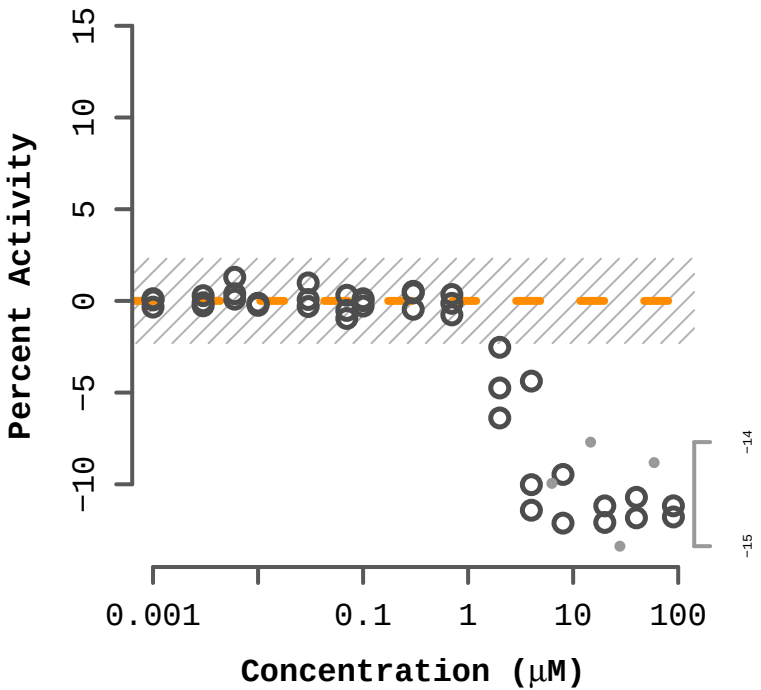
NAME: Carfentrazone-ethyl
CHID: 32532 **CASRN:** 128639-02-1
SPID(S): Tox21_300994
M4ID: 12478139

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.677 **MAX_MED:** −0.0175 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

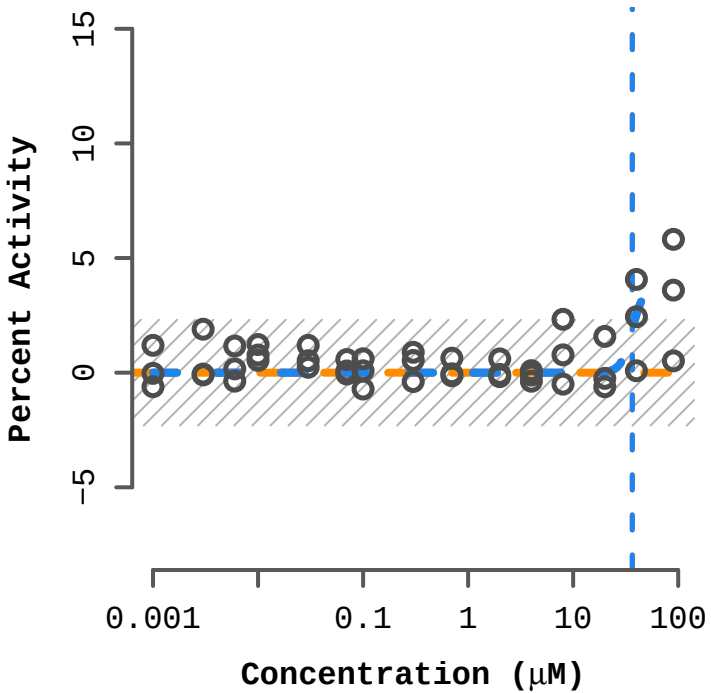
NAME: Chlorfenapyr
CHID: 32533 **CASRN:** 122453-73-0
SPID(S): Tox21_301579
M4ID: 12477554 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	302.04	NA	NA
PROB:	1	NA	NA
RMSE:	6.94	NA	NA

MAX_MEAN: 0.594 **MAX_MED:** 0.441 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trinexapac-ethyl
CHID: 32535 CASRN: 95266-40-3
SPID(S): Tox21_301906
M4ID: 12477227

HILL MODEL (in red):

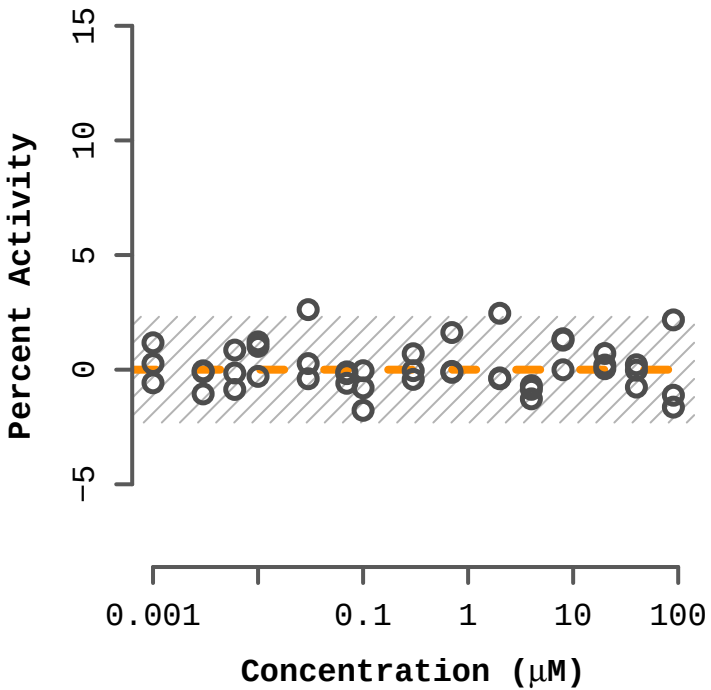
	tp	ga	gw
val:	3.75	1.56	8
sd:	0.745	0.0858	14.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.77	1.56	8	3.92	1.08
sd:	14.8	0.272	15.9	51.8	182

	CNST	HILL	GNLS
AIC:	143.12	132.12	136.12
PROB:	0	0.88	0.12
RMSE:	1.44	1.02	1.02

MAX_MEAN: 3.31 MAX_MED: 3.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

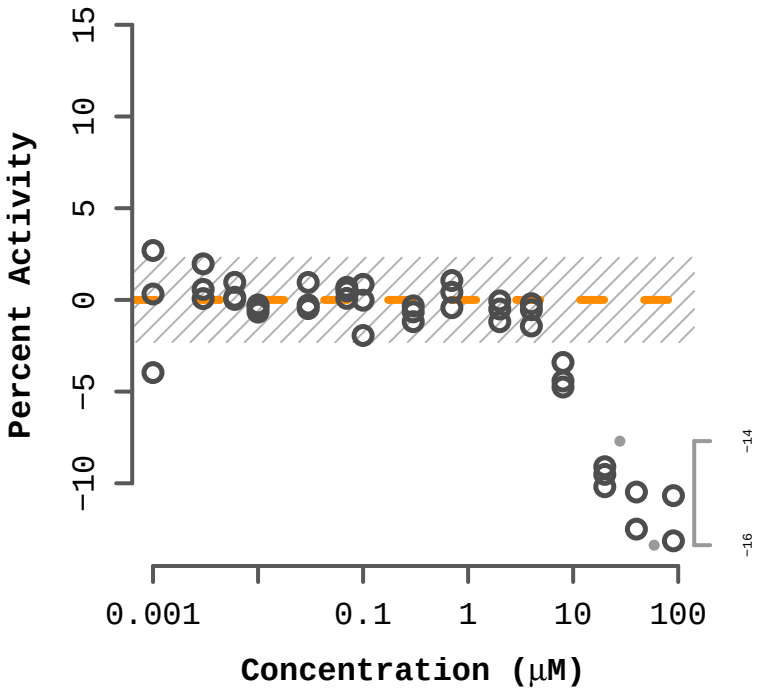
NAME: Cyphenothrin
CHID: 32536 **CASRN:** 39515-40-7
SPID(S): Tox21_301919
M4ID: 12477214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.879 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

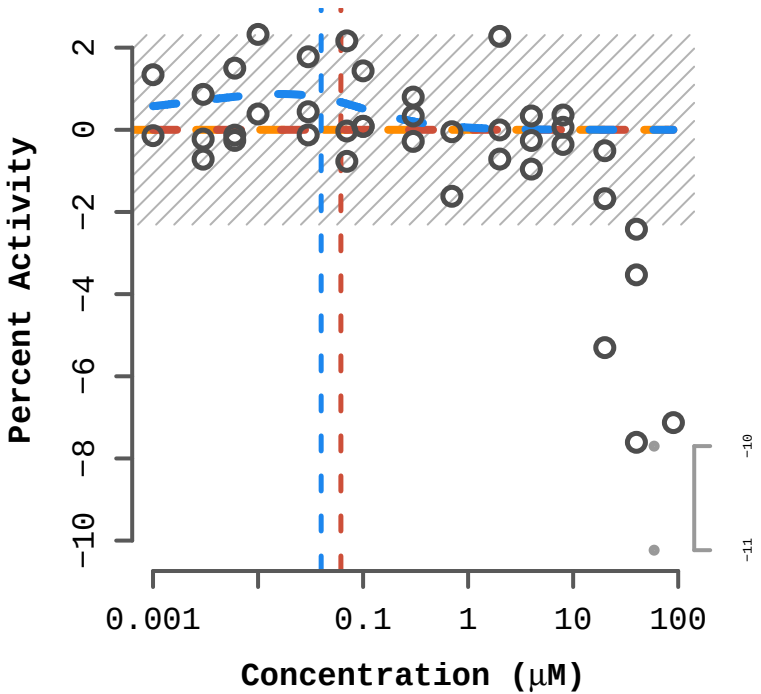
NAME: Didecyldimethylammonium chloride
CHID: 32537 **CASRN:** 7173-51-5
SPID(S): Tox21_300598
M4ID: 12478535 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.31	NA	NA
PROB:	1	NA	NA
RMSE:	5.5	NA	NA

MAX_MEAN: 0.873 **MAX_MED:** 0.575 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diiodomethyl 4-methylphenyl sulfone
CHID: 32541 CASRN: 20018-09-1
SPID(S): Tox21_303744
M4ID: 12475444 BRK

HILL MODEL (in red):

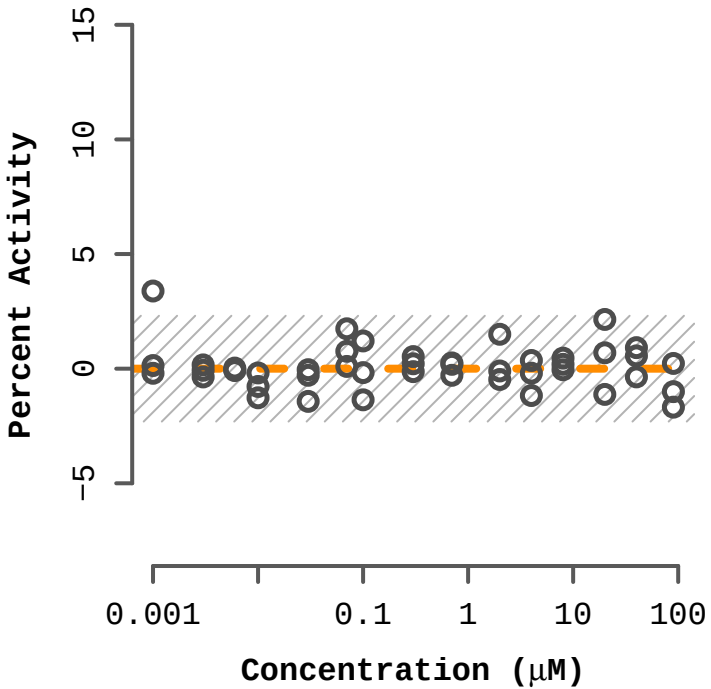
	tp	ga	gw
val:	6.64e-10	-1.21	1.61
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.32	-1.4	0.3	-1.15	1.28
sd:	16	7	1.58	3.64	2.28

	CNST	HILL	GNLS
AIC:	215.95	221.95	222.26
PROB:	0.92	0.05	0.04
RMSE:	3.21	3.21	3.16

MAX_MEAN: 2 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

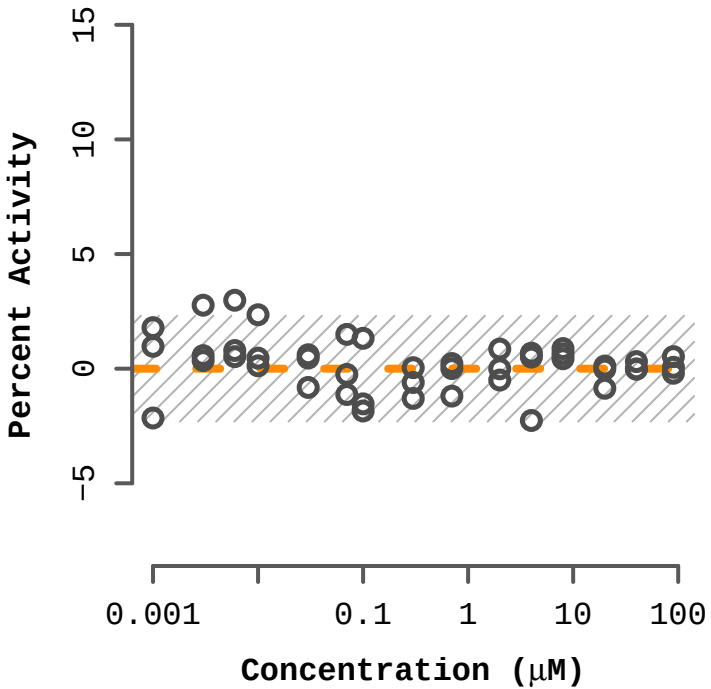
NAME: Dipropyl 2,5-pyridinedicarboxylate
CHID: 32544 **CASRN:** 136-45-8
SPID(S): Tox21_300729
M4ID: 12478404

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

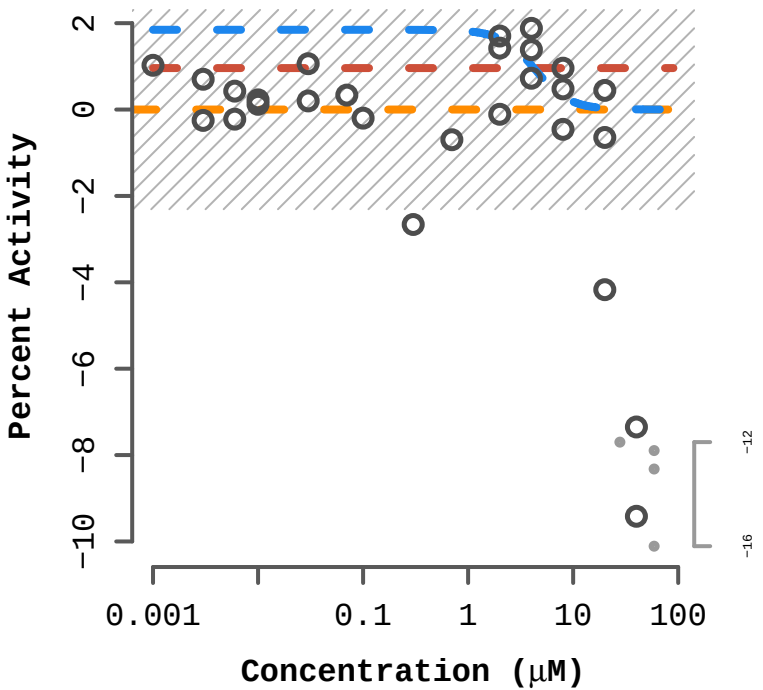
NAME: Etridiazole
CHID: 32547 **CASRN:** 2593-15-9
SPID(S): Tox21_300924
M4ID: 12478209

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.974 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenbuconazole
CHID: 32548 CASRN: 114369-43-6
SPID(S): Tox21_300795
M4ID: 12478338 BRK

HILL MODEL (in red):

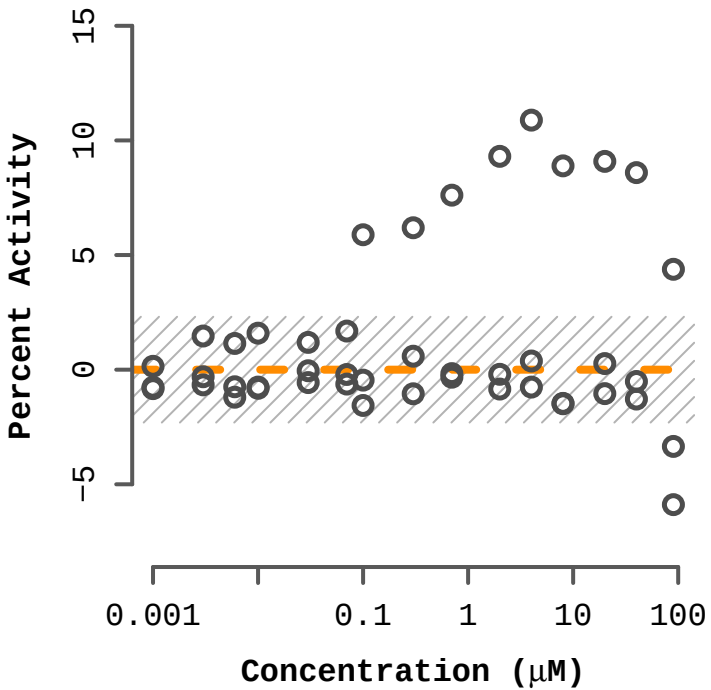
	tp	ga	gw
val:	0.96	−4.75	4.15
sd:	0.474	1610	3800

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.85	−3.95	7.94	0.639	2.67
sd:	0.598	1010	8360	0.658	5.6

	CNST	HILL	GNLS
AIC:	262.5	264.96	260.68
PROB:	0.27	0.08	0.66
RMSE:	4.86	5.01	4.62

MAX_MEAN: 3.18 MAX_MED: 2.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

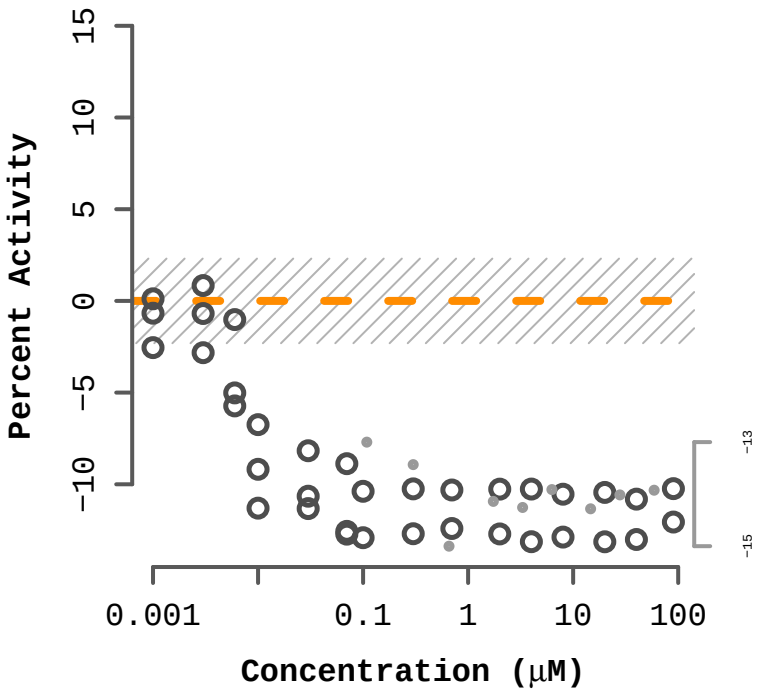
NAME: Fenhexamid
CHID: 32549 CASRN: 126833-17-8
SPID(S): Tox21_301042
M4ID: 12478091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	239.45	NA	NA
PROB:	1	NA	NA
RMSE:	3.85	NA	NA

MAX_MEAN: 3.5 MAX_MED: 0.589 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

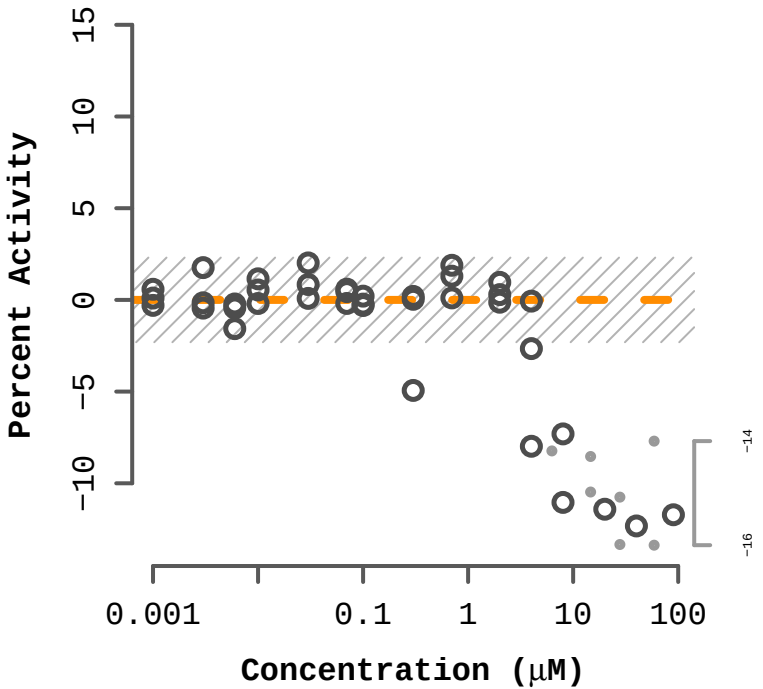
NAME: Fenpyroximate (Z,E)
CHID: 32550 **CASRN:** 111812-58-9
SPID(S): Tox21_300898
M4ID: 12478235 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	353.59	NA	NA
PROB:	1	NA	NA
RMSE:	10.88	NA	NA

MAX_MEAN: −0.89 **MAX_MED:** −0.669 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

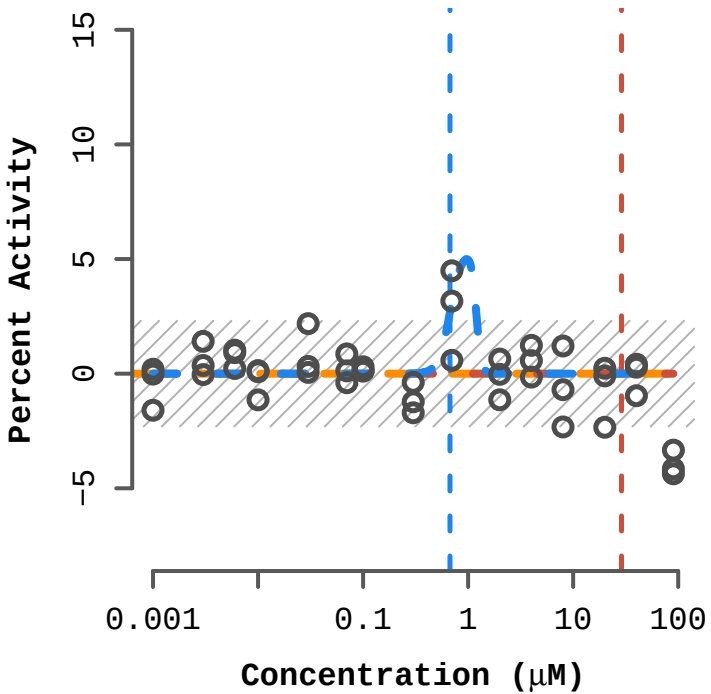
NAME: Fluazinam
CHID: 32551 **CASRN:** 79622-59-6
SPID(S): Tox21_301177
M4ID: 12477956 **BRK**

HILL MODEL: Not applicable.

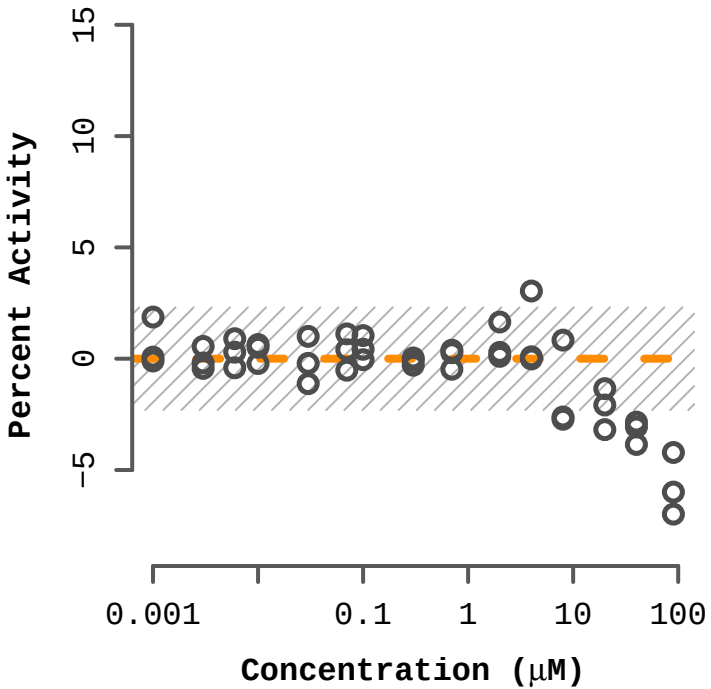
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	298.6	NA	NA
PROB:	1	NA	NA
RMSE:	6.99	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.3 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Flufenacet
CHID:    32552   CASRN: 142459-58-3
SPID(S): Tox21_301073
M4ID:    12478060

HILL MODEL (in red):
      tp       ga       gw
val:  4e-10    1.46     1.95
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.39     -0.173   7.97     0.0773   18
sd:   16.2     0.379    8.83     3.27     262

      CNST        HILL        GNLS
AIC:  163.73      169.73      164.9
PROB: 0.62        0.03        0.35
RMSE: 1.59        1.59        1.43

MAX_MEAN: 2.75      MAX_MED: 3.17      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

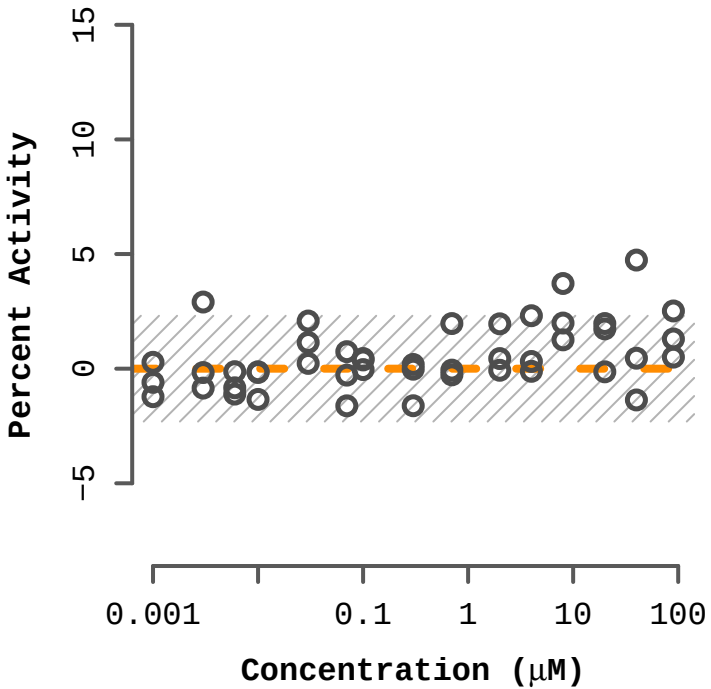
NAME: Flumetralin
CHID: 32553 **CASRN:** 62924-70-3
SPID(S): Tox21_300955
M4ID: 12478178

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.513 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

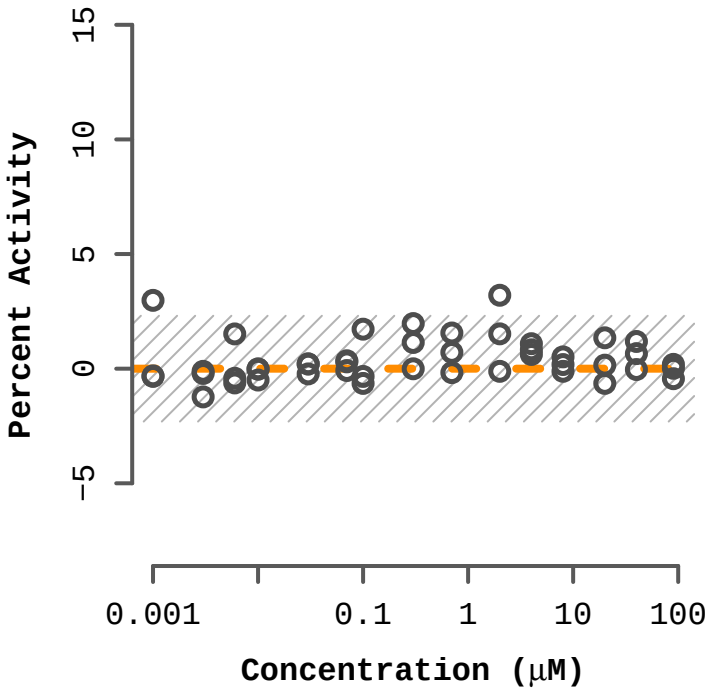
NAME: Flumiclorac-pentyl
CHID: 32554 **CASRN:** 87546-18-7
SPID(S): Tox21_300821
M4ID: 12478312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

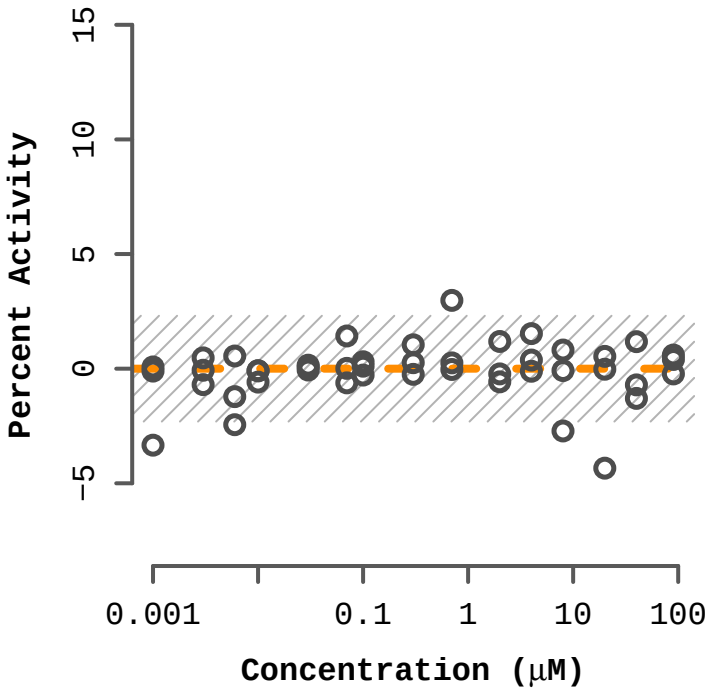
NAME: Flumioxazin
CHID: 32555 **CASRN:** 103361-09-7
SPID(S): Tox21_301061
M4ID: 12478072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.2	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

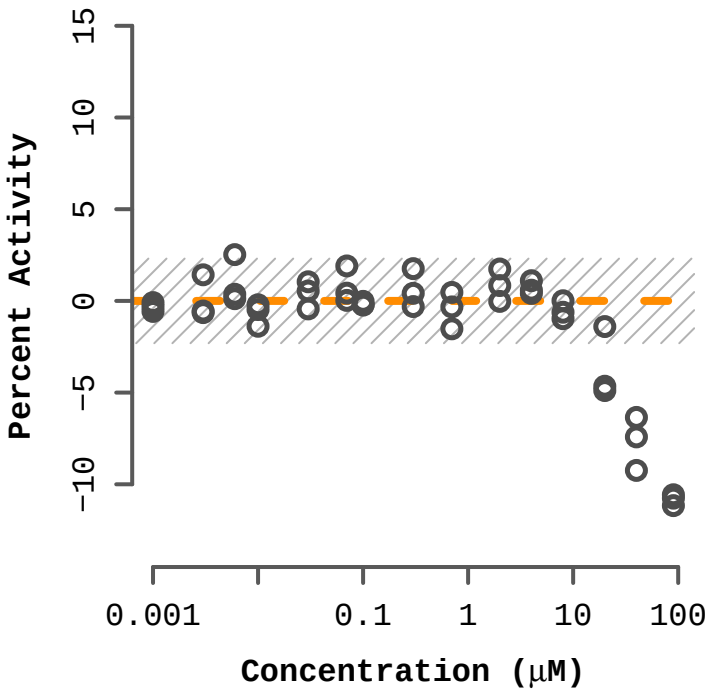
NAME: Fluthiacet-methyl
CHID: 32556 **CASRN:** 117337-19-6
SPID(S): Tox21_300834
M4ID: 12478299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.402 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

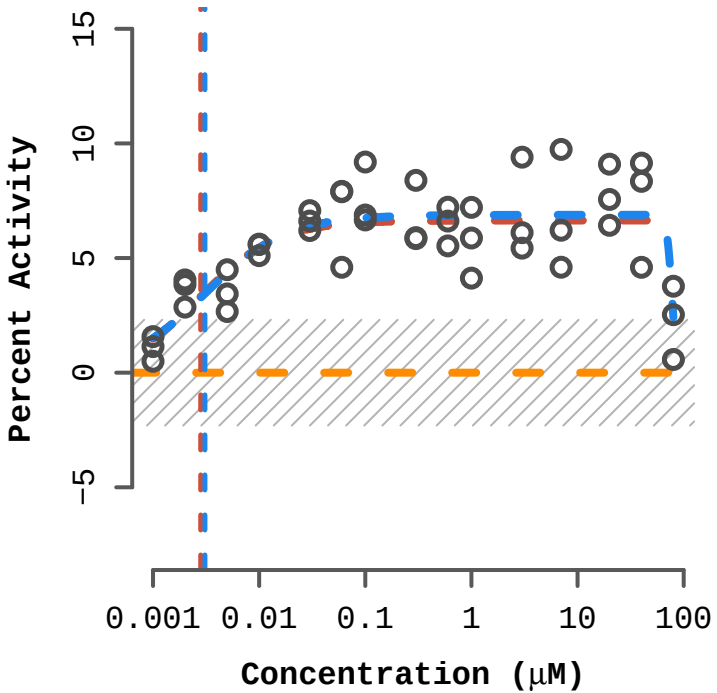
NAME: Kresoxim-methyl
CHID: 32558 **CASRN:** 143390-89-0
SPID(S): Tox21_302251
M4ID: 12476882

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.68	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: lambda-Cyhalothrin
CHID: 32559 **CASRN:** 91465-08-6
SPID(S): Tox21_303423
M4ID: 12475716

HILL MODEL (in red):

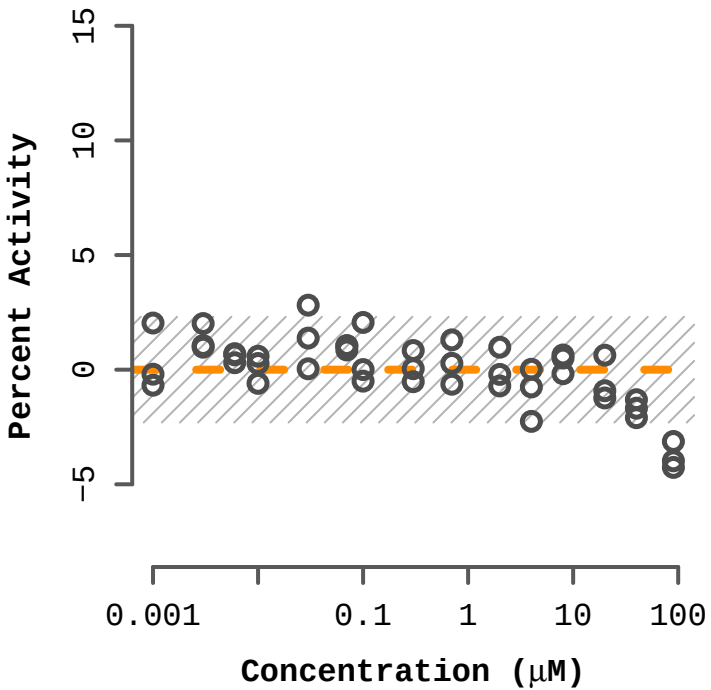
	tp	ga	gw
val:	6.64	−2.55	1.21
sd:	0.325	0.123	0.311

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.89	−2.51	1.13	1.89	18
sd:	0.313	0.111	0.262	0.0145	17.5

	CNST	HILL	GNLS
AIC:	301.24	184.89	171.24
PROB:	0	0	1
RMSE:	6.11	1.78	1.36

MAX_MEAN: 7.69 **MAX_MED:** 8.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

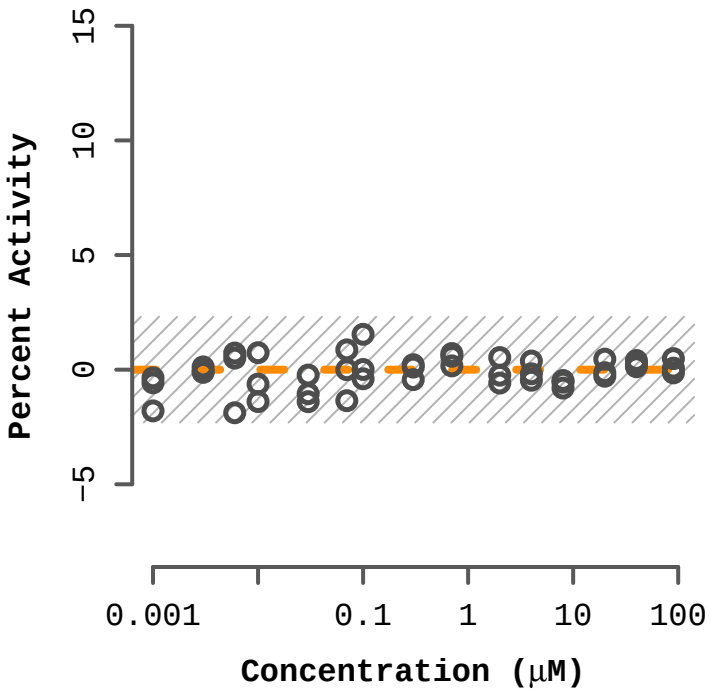
NAME: MGK−264
CHID: 32562 **CASRN:** 113−48−4
SPID(S): Tox21_300786
M4ID: 12478347

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

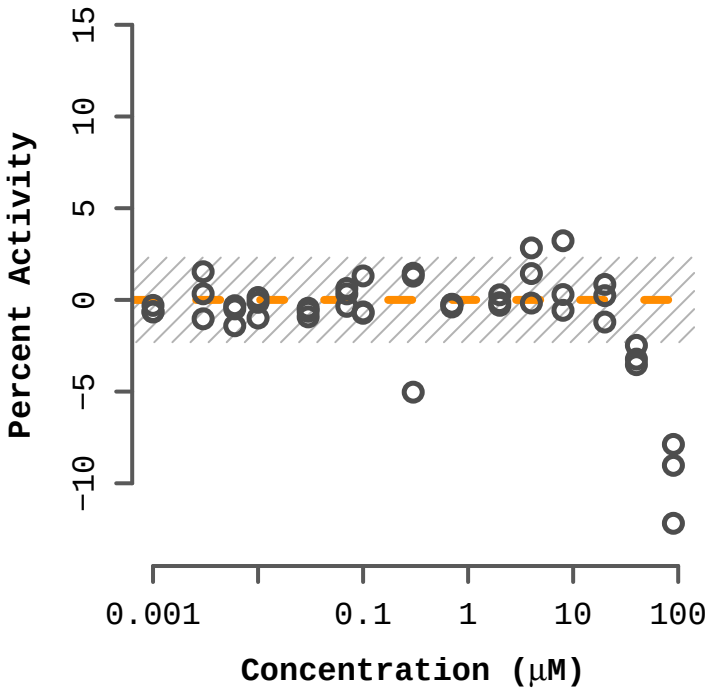
NAME: Pirimicarb
CHID: 32569 **CASRN:** 23103-98-2
SPID(S): Tox21_301003
M4ID: 12478130

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.485 **MAX_MED:** 0.586 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

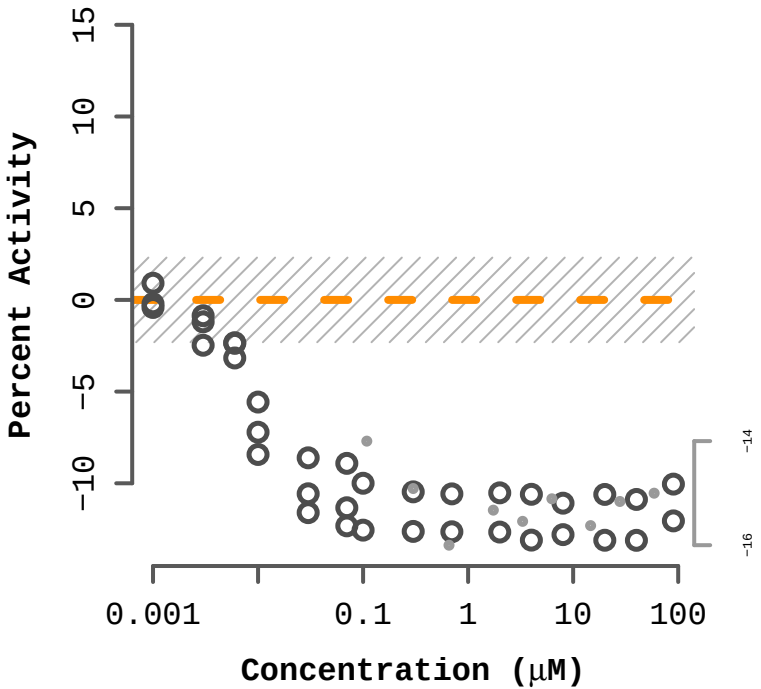
NAME: Prallethrin
CHID: 32572 **CASRN:** 23031-36-9
SPID(S): Tox21_300644
M4ID: 12478489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

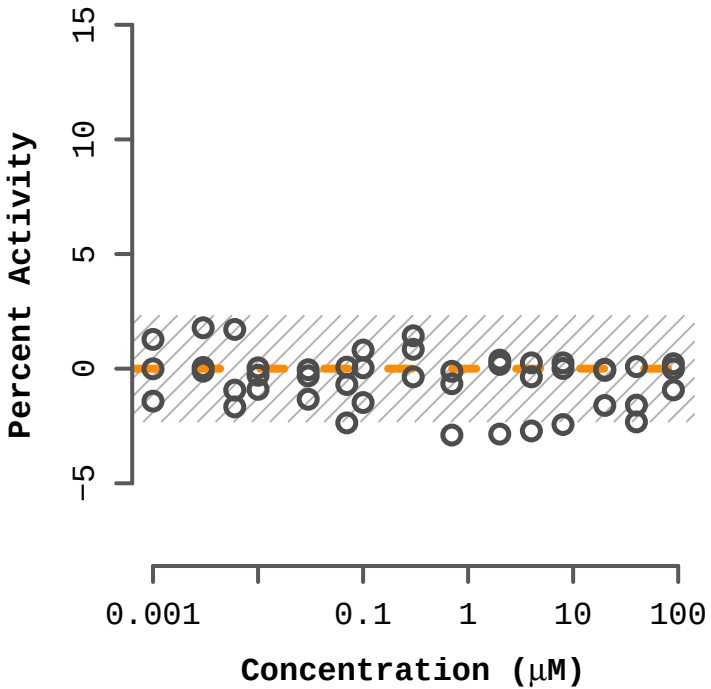
NAME: Pyridaben
CHID: 32573 **CASRN:** 96489-71-3
SPID(S): Tox21_301090
M4ID: 12478043 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	353.69	NA	NA
PROB:	1	NA	NA
RMSE:	10.94	NA	NA

MAX_MEAN: 0.0962 **MAX_MED:** −0.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

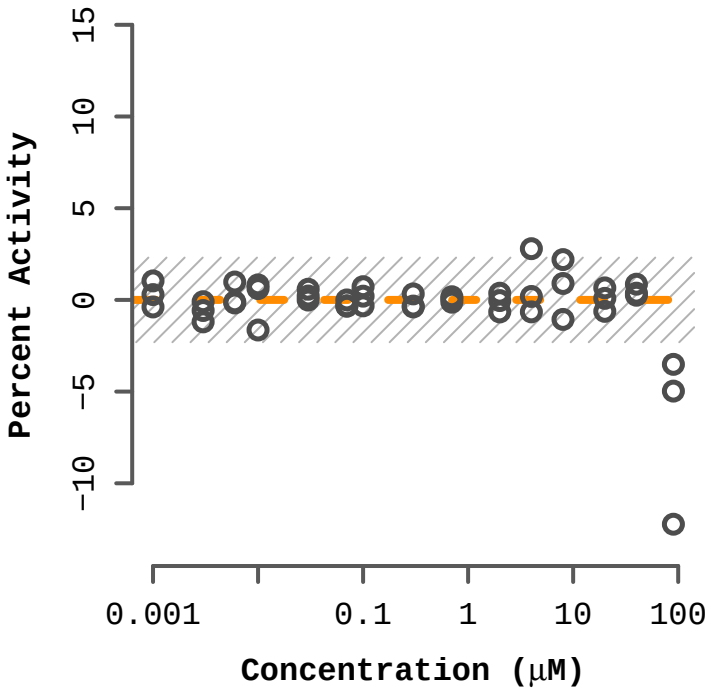
NAME: Tefluthrin
CHID: 32577 **CASRN:** 79538-32-2
SPID(S): Tox21_300900
M4ID: 12478233

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.642 **MAX_MED:** 0.847 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

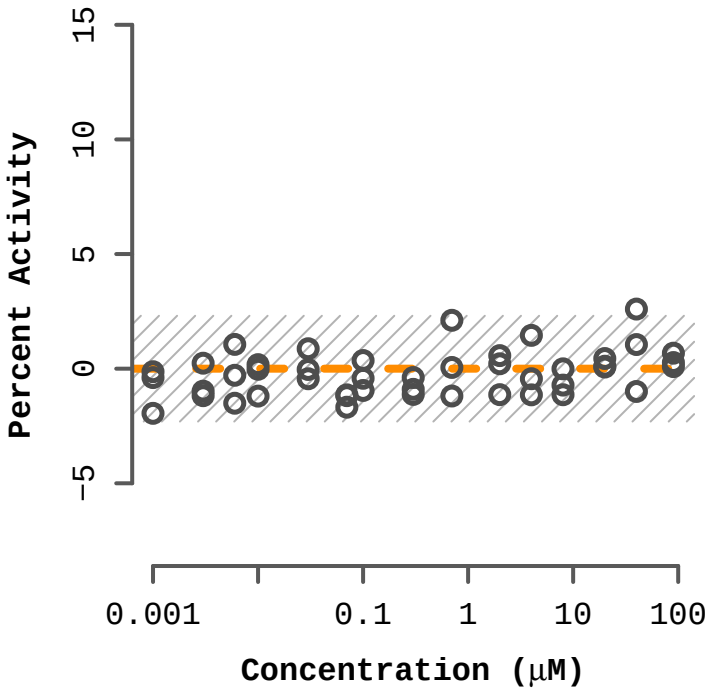
NAME: Thiodicarb
CHID: 32578 **CASRN:** 59669-26-0
SPID(S): Tox21_300855
M4ID: 12478278

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 0.778 **MAX_MED:** 0.897 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

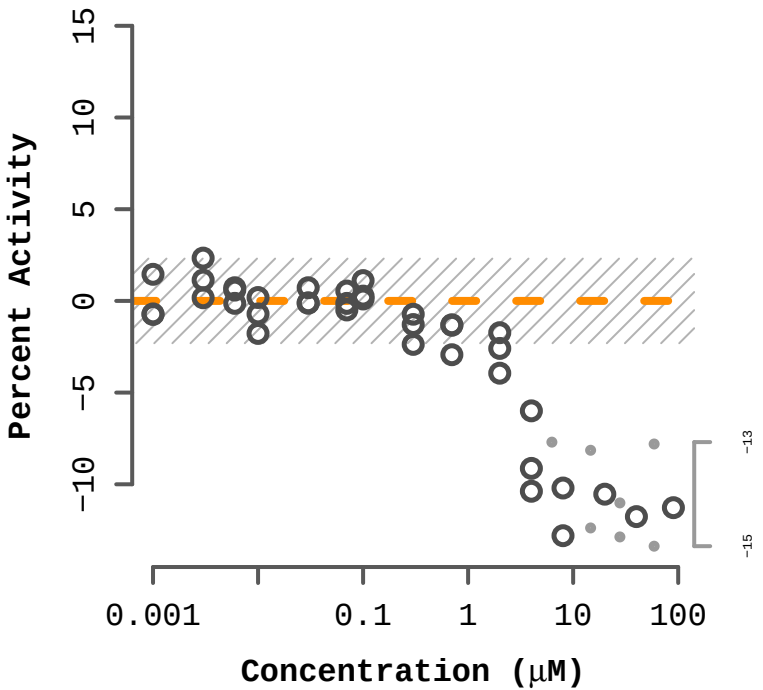
NAME: Triclopyr-butotyl
CHID: 32579 **CASRN:** 64700-56-7
SPID(S): Tox21_301913
M4ID: 12477220

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.888 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

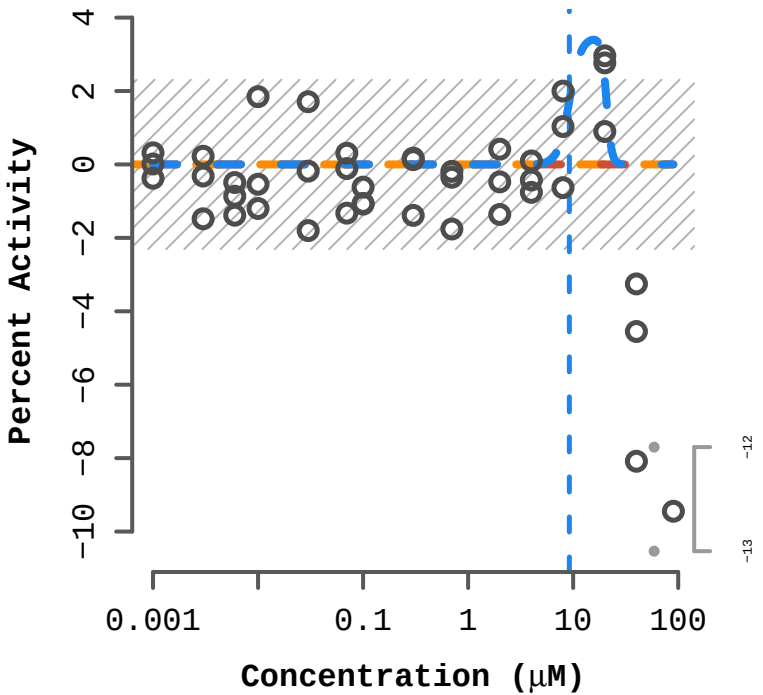
NAME: Trifloxystrobin
CHID: 32580 **CASRN:** 141517-21-7
SPID(S): Tox21_301047
M4ID: 12478086 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	305.84	NA	NA
PROB:	1	NA	NA
RMSE:	7.26	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zoxamide
CHID: 32581 CASRN: 156052-68-5
SPID(S): Tox21_300943
M4ID: 12478190 BRK

HILL MODEL (in red):

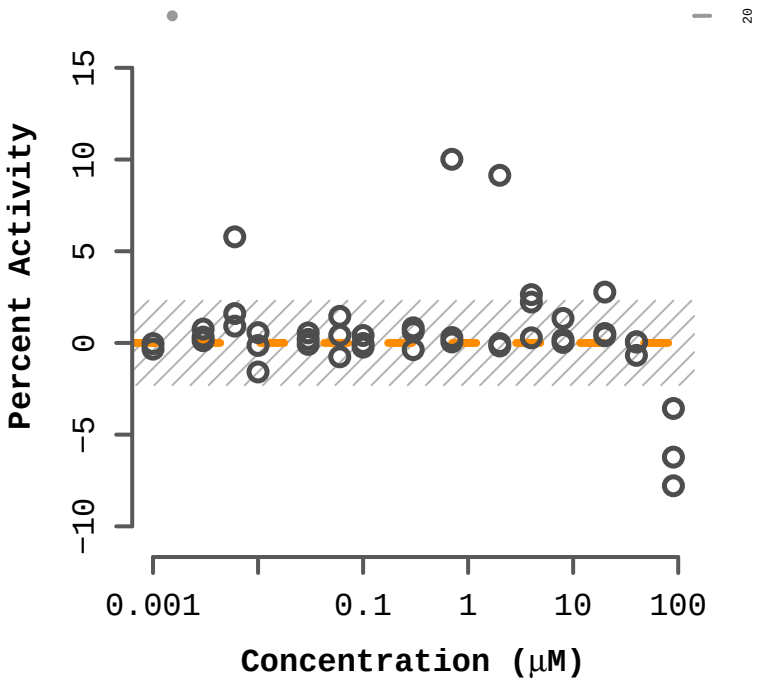
	tp	ga	gw
val:	7.54e-09	2.35	1.92
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.47	0.964	8	1.32	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	212.61	218.61	215.73
PROB:	0.79	0.04	0.17
RMSE:	3.52	3.52	3.46

MAX_MEAN: 2.21 **MAX_MED:** 2.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

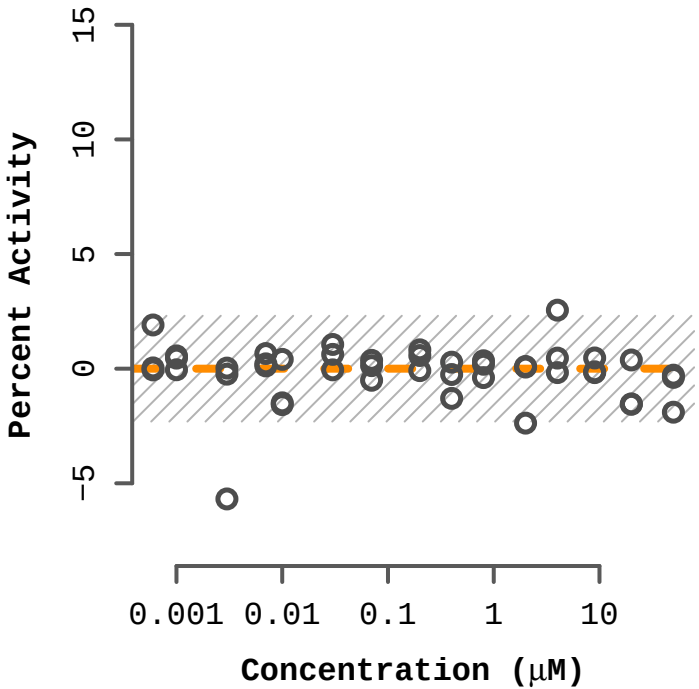
NAME: Bromadiolone
CHID: 32589 **CASRN:** 28772-56-7
SPID(S): Tox21_301920
M4ID: 12477213 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.92	NA	NA
PROB:	1	NA	NA
RMSE:	4.07	NA	NA

MAX_MEAN: 6.38 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

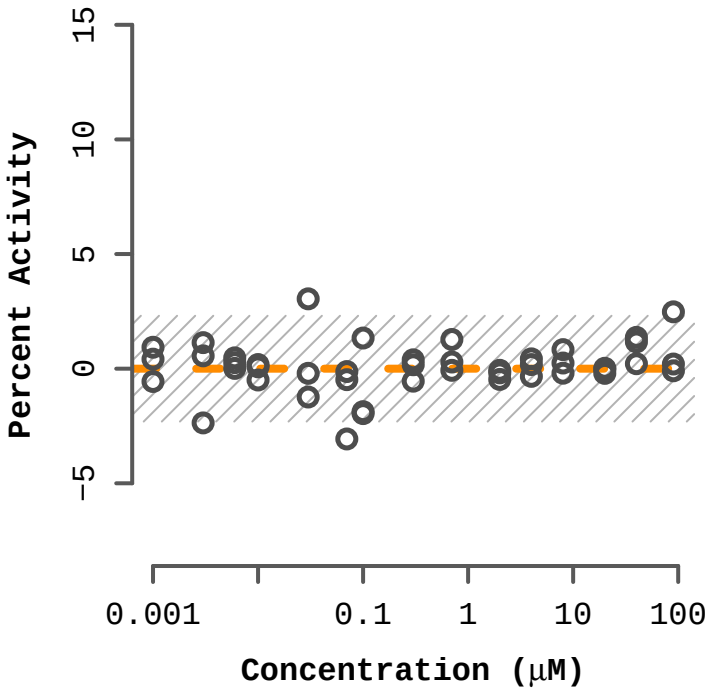
NAME: Bromadiolone
CHID: 32589 **CASRN:** 28772-56-7
SPID(S): Tox21_112561_1
M4ID: 12483032

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.949 **MAX_MED:** 0.624 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

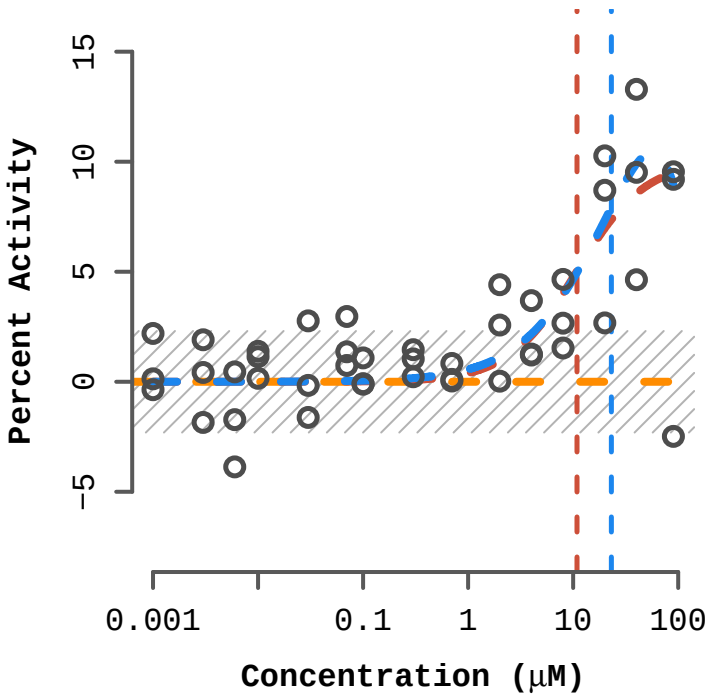
NAME: Bromo-3-chloro-5,5-dimethylhydantoin
CHID: 32591 **CASRN:** 16079-88-2
SPID(S): Tox21_302375
M4ID: 12476758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclanilide
CHID: 32600 CASRN: 113136-77-9
SPID(S): Tox21_301076
M4ID: 12478057

HILL MODEL (in red):

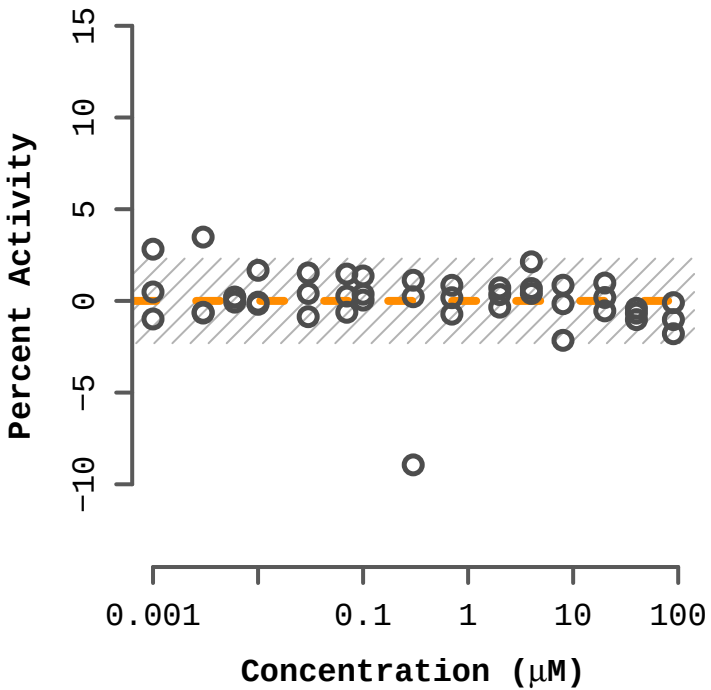
	tp	ga	gw
val:	10.1	1.04	1.34
sd:	1.91	0.219	0.993

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.9	1.36	1.05	2.07	3.2
sd:	10.5	0.56	0.558	0.218	7.69

	CNST	HILL	GNLS
AIC:	248.79	206.14	208.2
PROB:	0	0.74	0.26
RMSE:	4.2	2.59	2.53

MAX_MEAN: 9.15 MAX_MED: 9.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

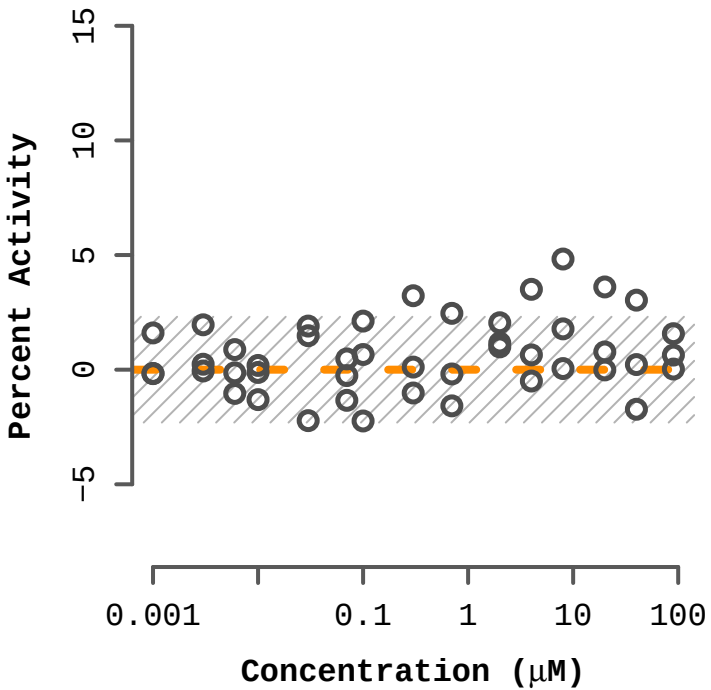
NAME: Cyproconazole
CHID: 32601 **CASRN:** 94361-06-5
SPID(S): Tox21_301185
M4ID: 12477948

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.677 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

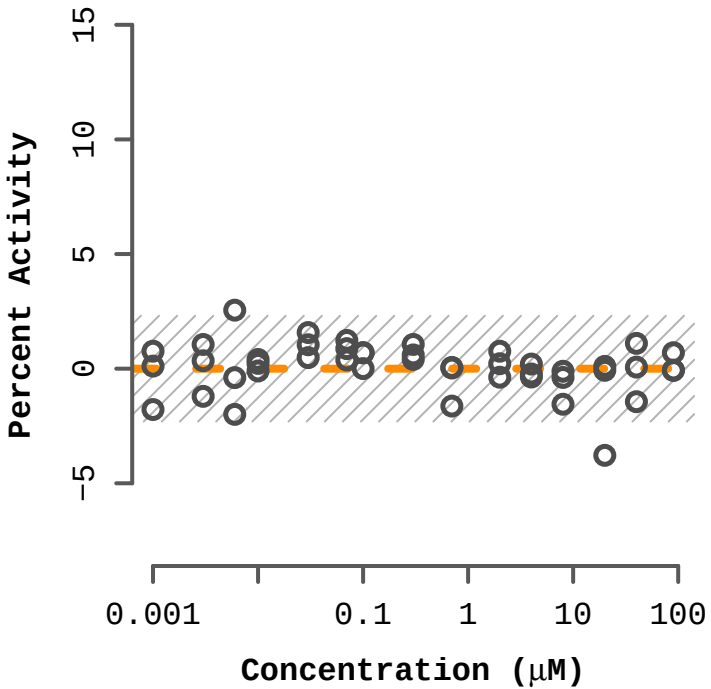
NAME: Diclofop-methyl
CHID: 32605 **CASRN:** 51338-27-3
SPID(S): Tox21_300779
M4ID: 12478354

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

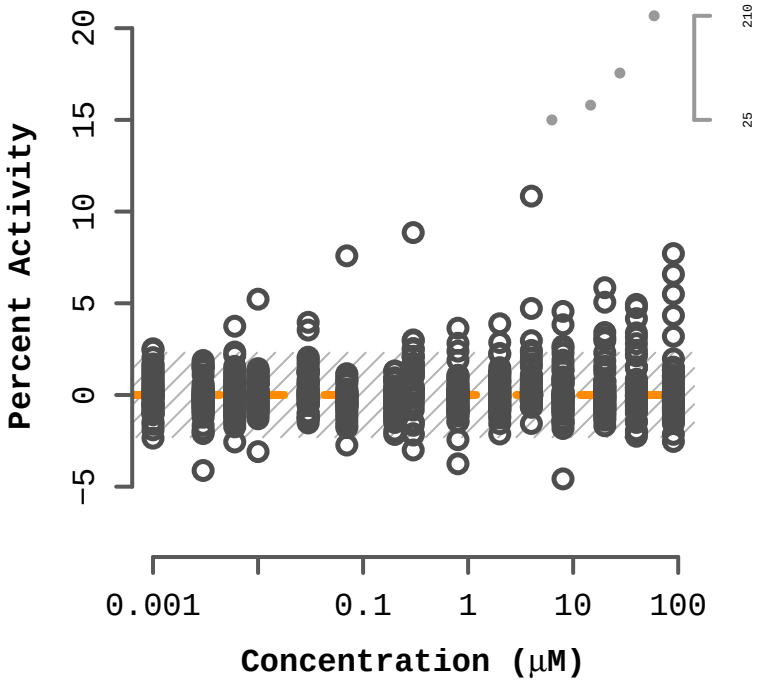
NAME: Etofenprox
CHID: 32610 **CASRN:** 80844-07-1
SPID(S): Tox21_300378
M4ID: 12478754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

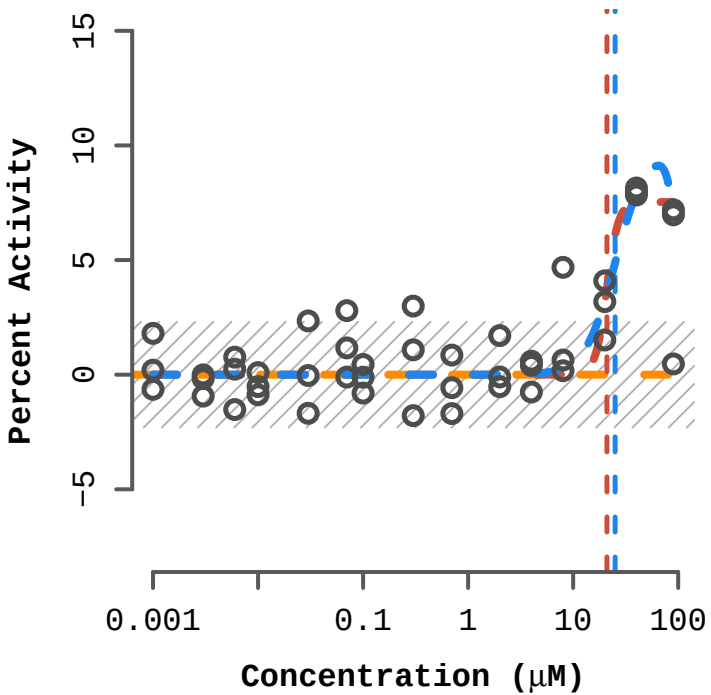
NAME: Ethoprop
CHID: 32611 **CASRN:** 13194-48-4
SPID(S): Tox21_400082
M4ID: 12475055 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2455.75	NA	NA
PROB:	1	NA	NA
RMSE:	9.05	NA	NA

MAX_MEAN: 4.81 **MAX_MED:** 0.249 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenitrothion
CHID: 32613 CASRN: 122-14-5
SPID(S): Tox21_300906
M4ID: 12478227

HILL MODEL (in red):

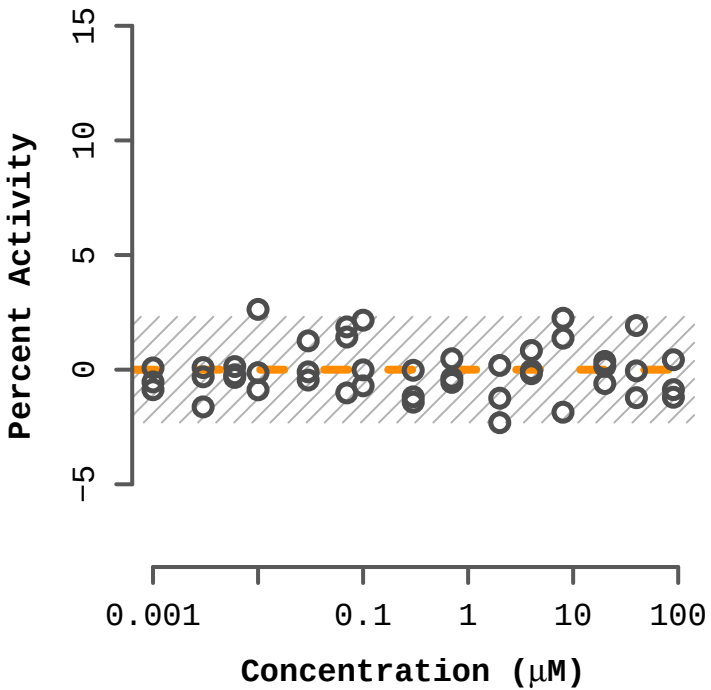
	tp	ga	gw
val:	7.53	1.32	8
sd:	0.454	0.0252	5.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.77	1.4	3.09	1.99	9.59
sd:	3.56	0.136	2.09	0.0291	11.4

	CNST	HILL	GNLS
AIC:	214.82	166.21	167.22
PROB:	0	0.62	0.38
RMSE:	2.95	1.67	1.58

MAX_MEAN: 7.99 MAX_MED: 7.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

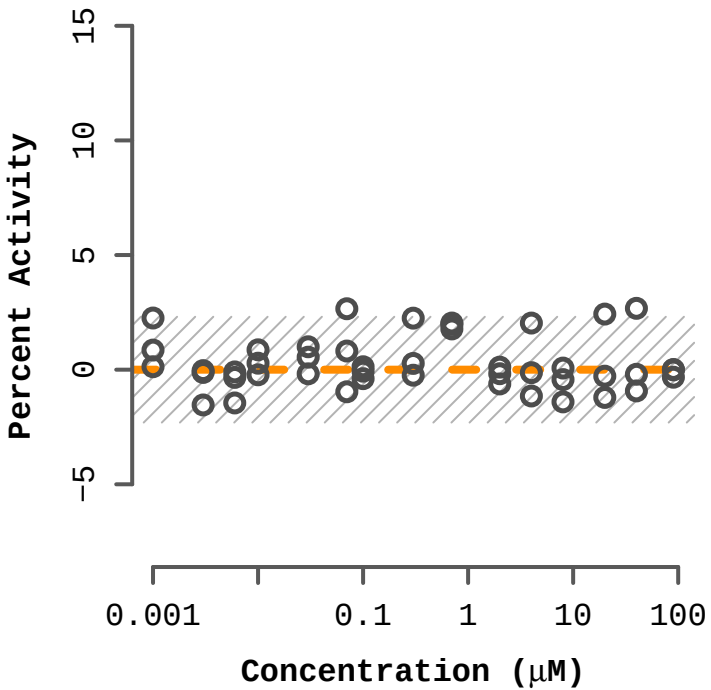
NAME: Fluchloralin
CHID: 32614 **CASRN:** 33245-39-5
SPID(S): Tox21_301333
M4ID: 12477800

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.76 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

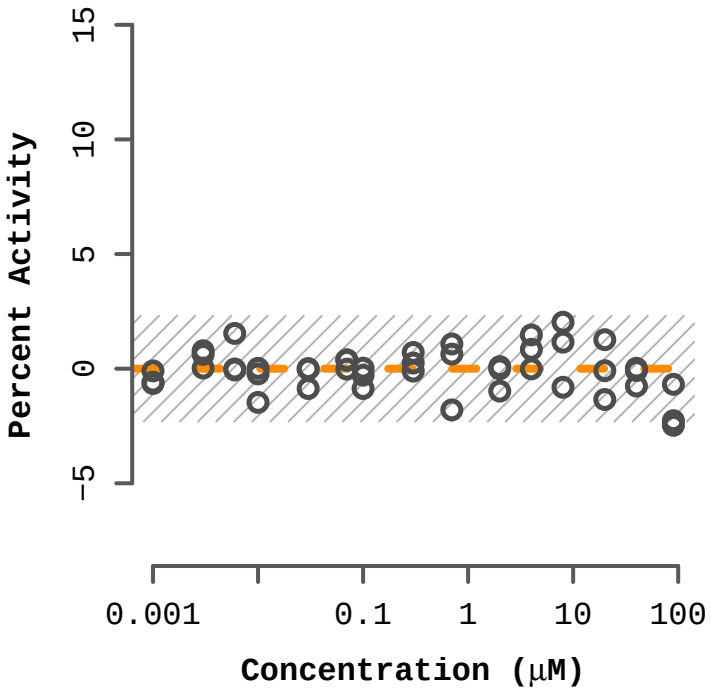
NAME: Flumetsulam
CHID: 32615 **CASRN:** 98967-40-9
SPID(S): Tox21_300828
M4ID: 12478305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

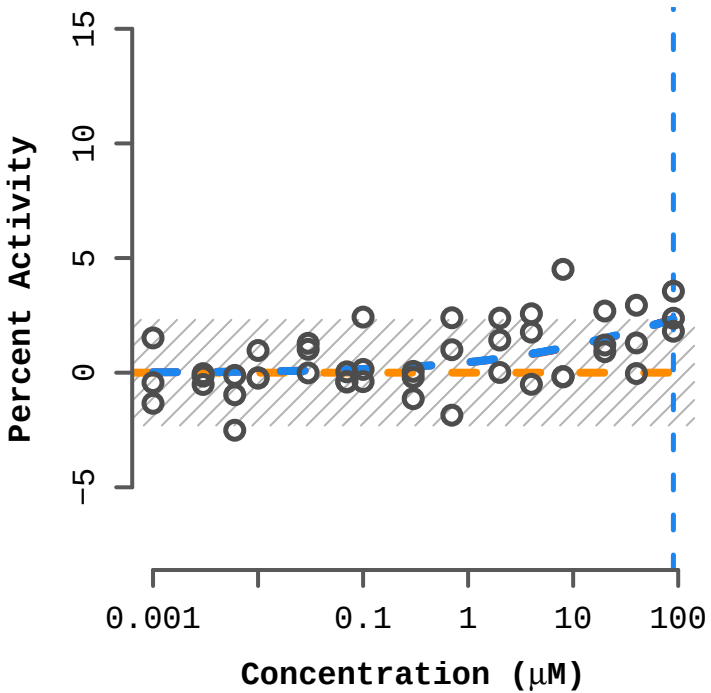
NAME: Halofenozide
CHID: 32619 **CASRN:** 112226-61-6
SPID(S): Tox21_302655
M4ID: 12476478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexaflumuron
CHID: 32620 CASRN: 86479-06-3
SPID(S): Tox21_300411
M4ID: 12478721

HILL MODEL (in red):

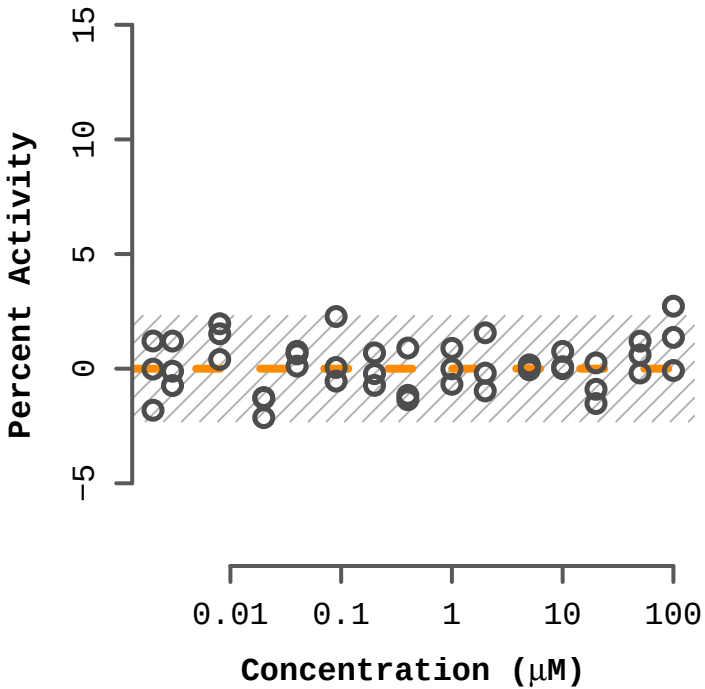
	tp	ga	gw
val:	5.41	2.2	0.474
sd:	16.5	4.81	0.382

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.65	1.95	0.493	3.76	3.93
sd:	11.1	3.86	0.379	1000	2200

	CNST	HILL	GNLS
AIC:	171	154.92	158.93
PROB:	0	0.88	0.12
RMSE:	1.58	1.22	1.22

MAX_MEAN: 2.58 MAX_MED: 2.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

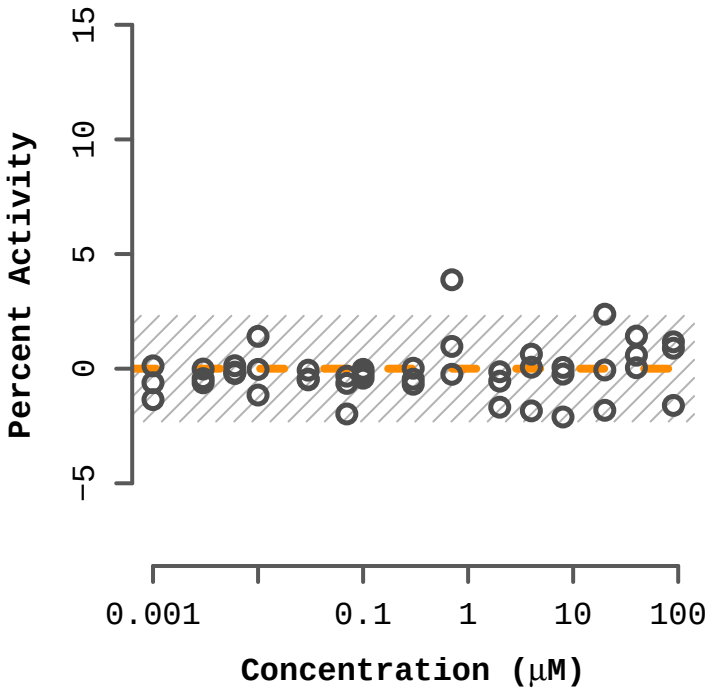
NAME: Hymexazol
CHID: 32622 **CASRN:** 10004-44-1
SPID(S): Tox21_300856
M4ID: 12478277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

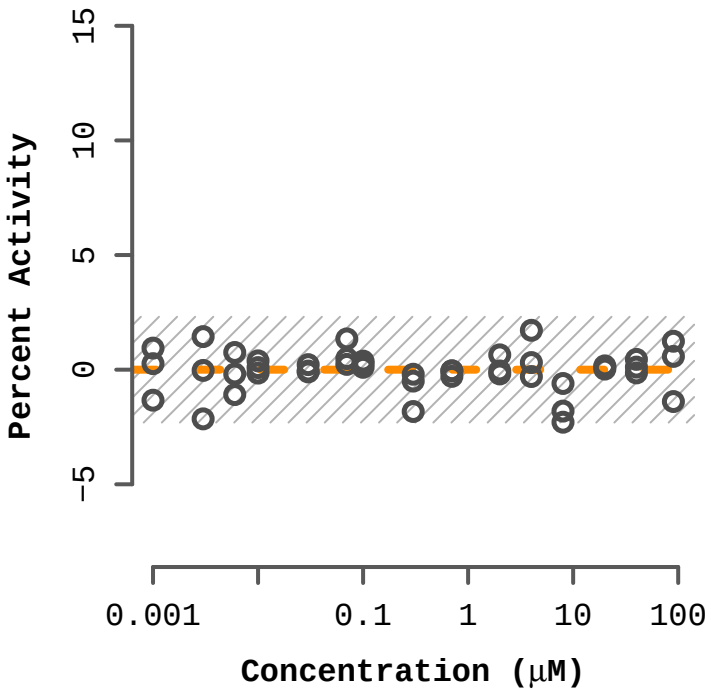
NAME: Indole-3-butyric acid
CHID: 32623 **CASRN:** 133-32-4
SPID(S): Tox21_301287
M4ID: 12477846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.971 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

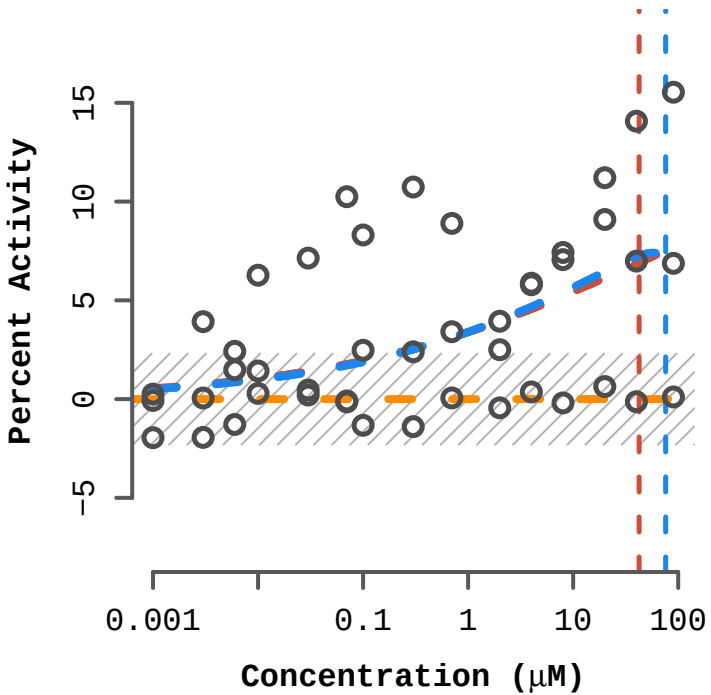
NAME: Kinoprene
CHID: 32624 **CASRN:** 42588-37-4
SPID(S): Tox21_302008
M4ID: 12477125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.687 **MAX_MED:** 0.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methiocarb
CHID: 32626 CASRN: 2032-65-7
SPID(S): Tox21_303856
M4ID: 12475332

HILL MODEL (in red):

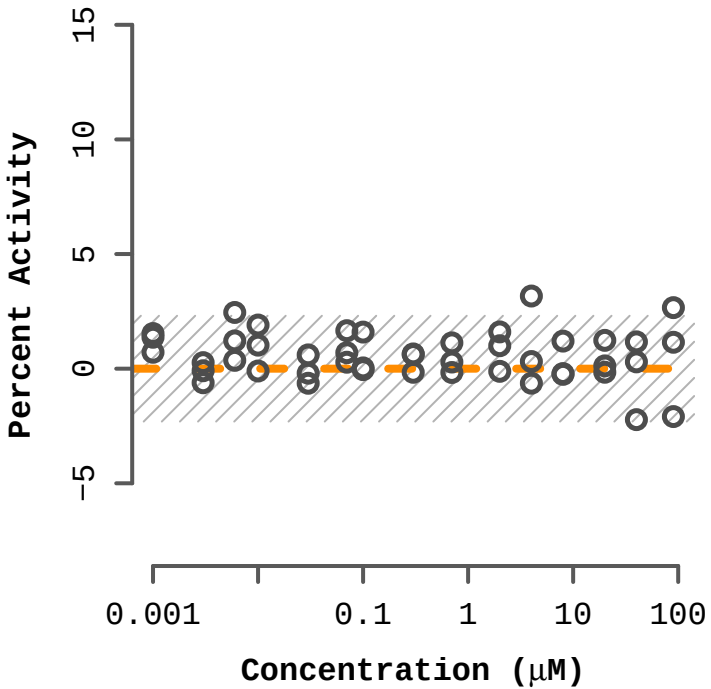
	tp	ga	gw
val:	13.8	1.63	0.3
sd:	24.8	4.87	0.239

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.2	1.88	0.306	2.13	3.6
sd:	31.6	4.51	0.174	1.05	21.1

	CNST	HILL	GNLS
AIC:	284.38	262.66	266.5
PROB:	0	0.87	0.13
RMSE:	5.7	3.99	4

MAX_MEAN: 7.51 MAX_MED: 9.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

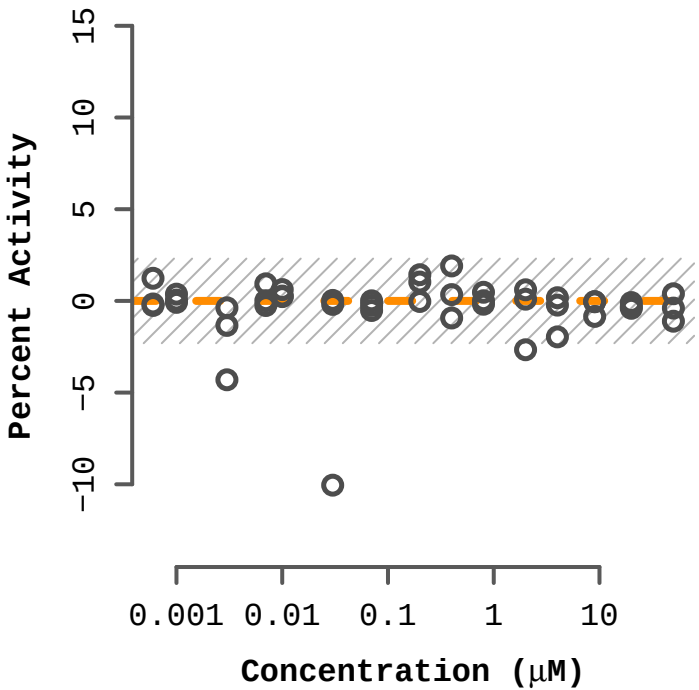
NAME: Methoprene
CHID: 32627 **CASRN:** 40596-69-8
SPID(S): Tox21_200654
M4ID: 12481598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

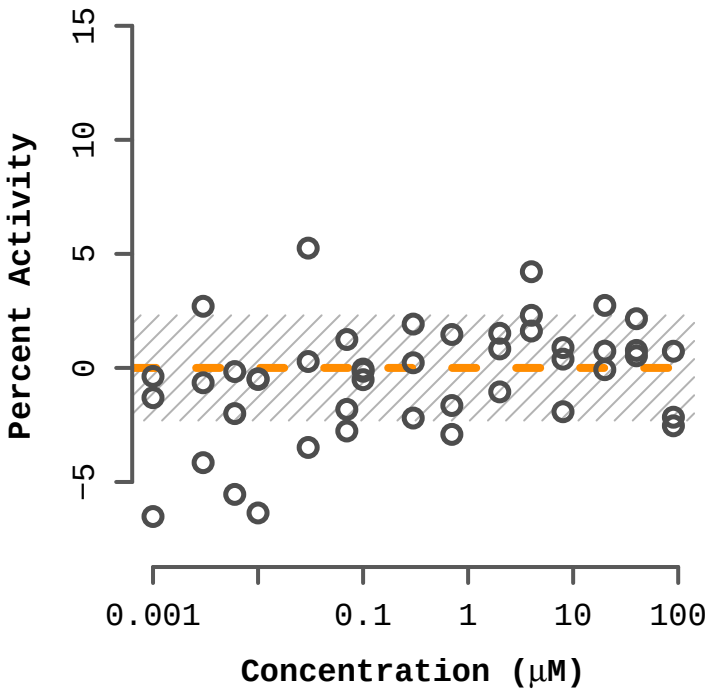
NAME: Methoprene
CHID: 32627 **CASRN:** 40596-69-8
SPID(S): Tox21_111019_1
M4ID: 12483944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 0.811 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

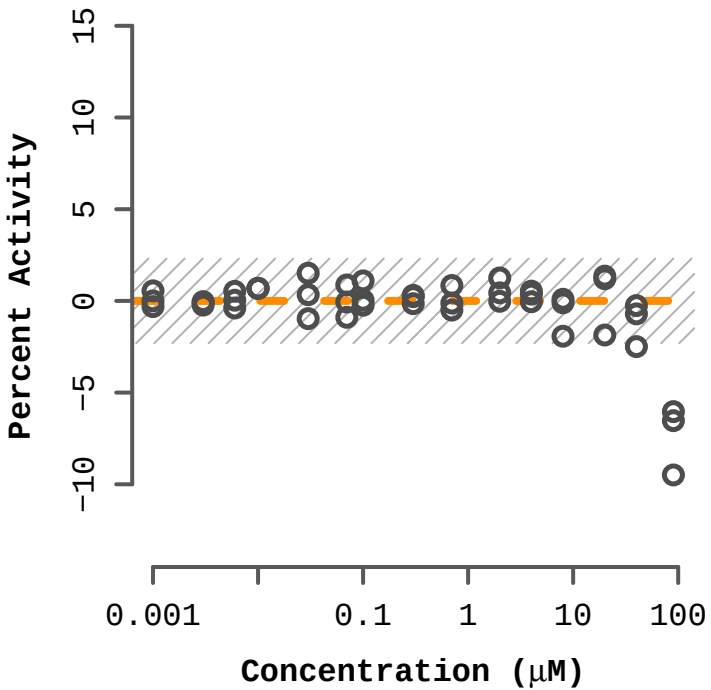
NAME: Methoxyfenozide
CHID: 32628 **CASRN:** 161050-58-4
SPID(S): Tox21_301100
M4ID: 12478033

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 2.72 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

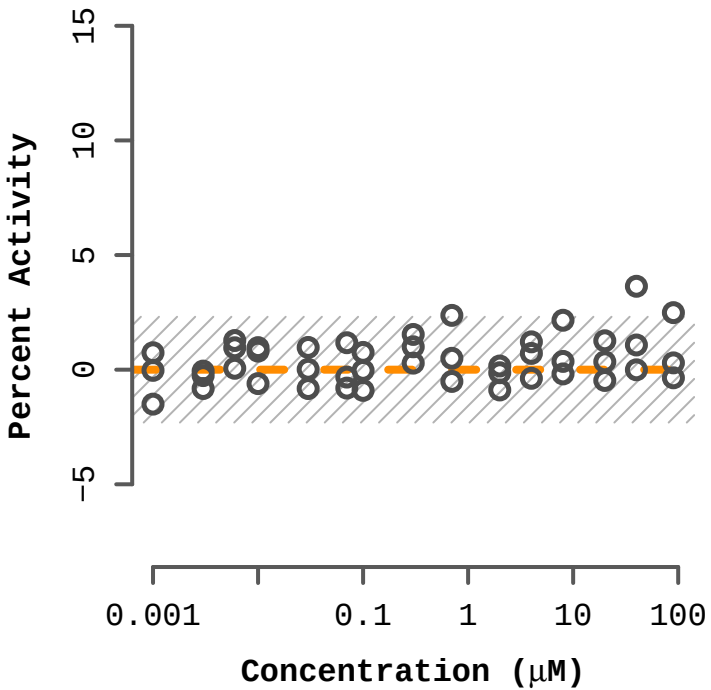
NAME: N-Benzyladenine
CHID: 32630 **CASRN:** 1214-39-7
SPID(S): Tox21_301307
M4ID: 12477826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.1	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

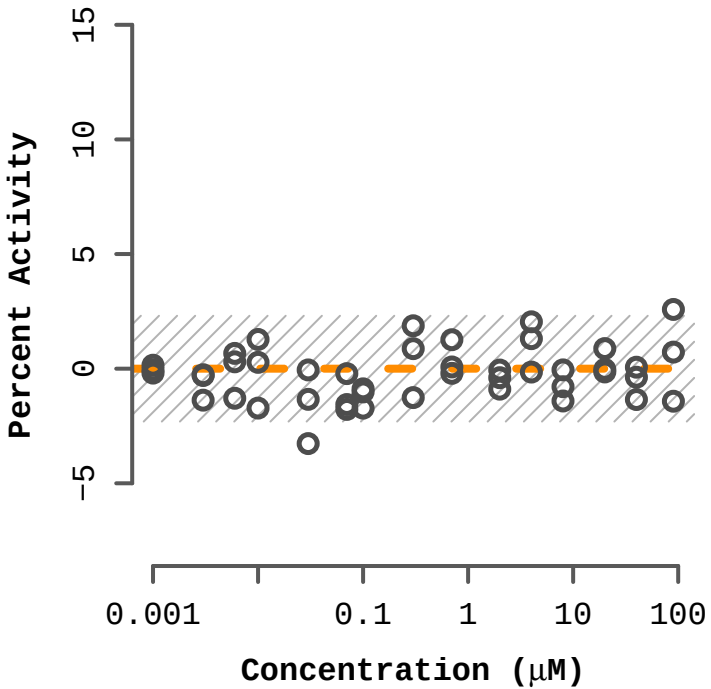
NAME: Oxadixyl
CHID: 32631 **CASRN:** 77732-09-3
SPID(S): Tox21_301853
M4ID: 12477280

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

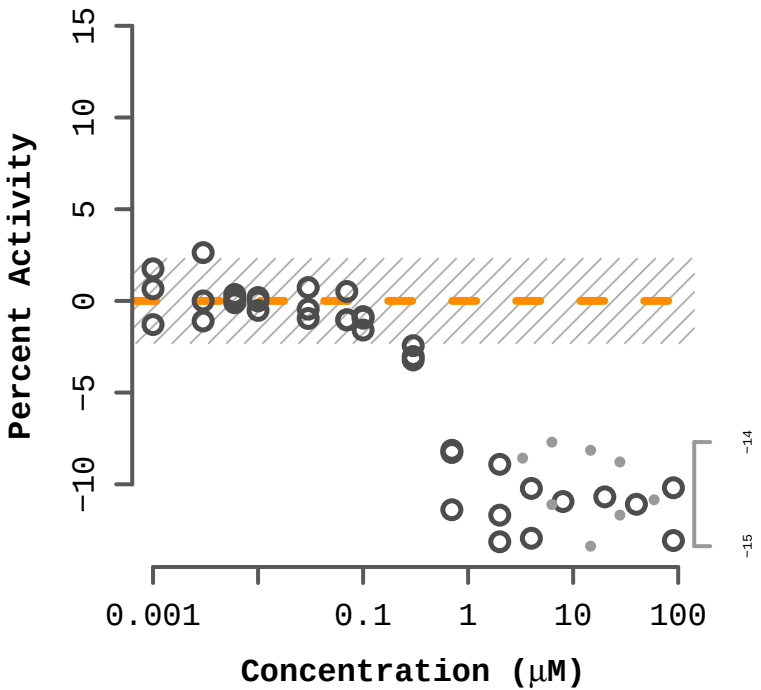
NAME: Pymetrozine
CHID: 32637 **CASRN:** 123312-89-0
SPID(S): Tox21_300879
M4ID: 12478254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

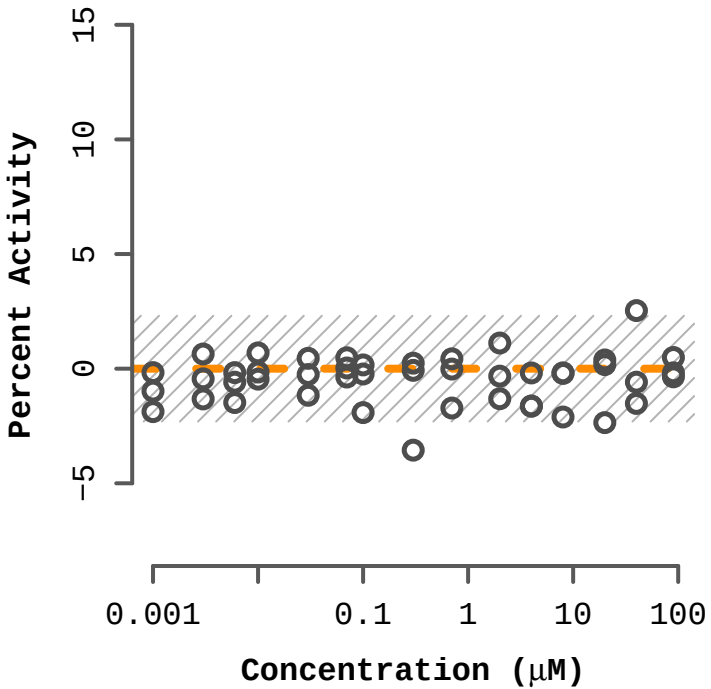
NAME: Pyraclostrobin
CHID: 32638 **CASRN:** 175013-18-0
SPID(S): Tox21_301130
M4ID: 12478003 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	325.88	NA	NA
PROB:	1	NA	NA
RMSE:	8.5	NA	NA

MAX_MEAN: 0.514 **MAX_MED:** 0.659 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

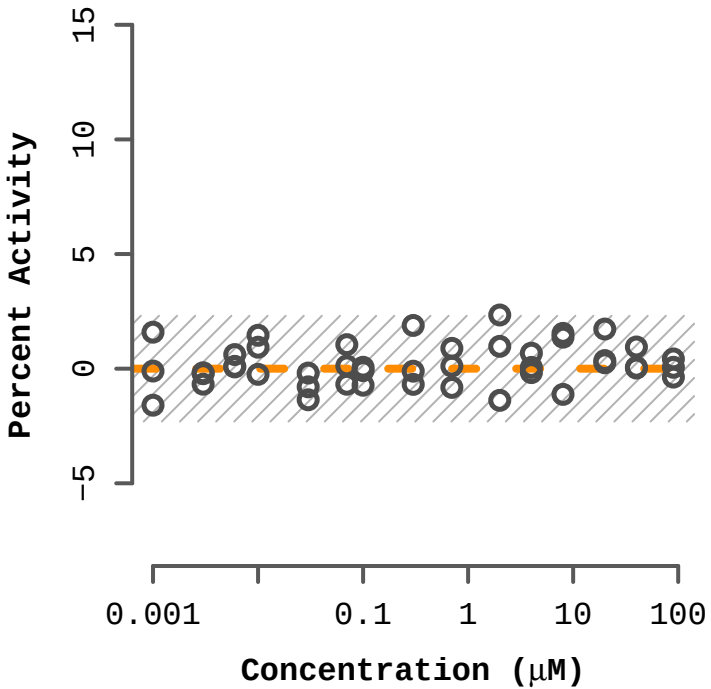
NAME: Pyridate
CHID: 32639 **CASRN:** 55512-33-9
SPID(S): Tox21_301247
M4ID: 12477886

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.145 **MAX_MED:** 0.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

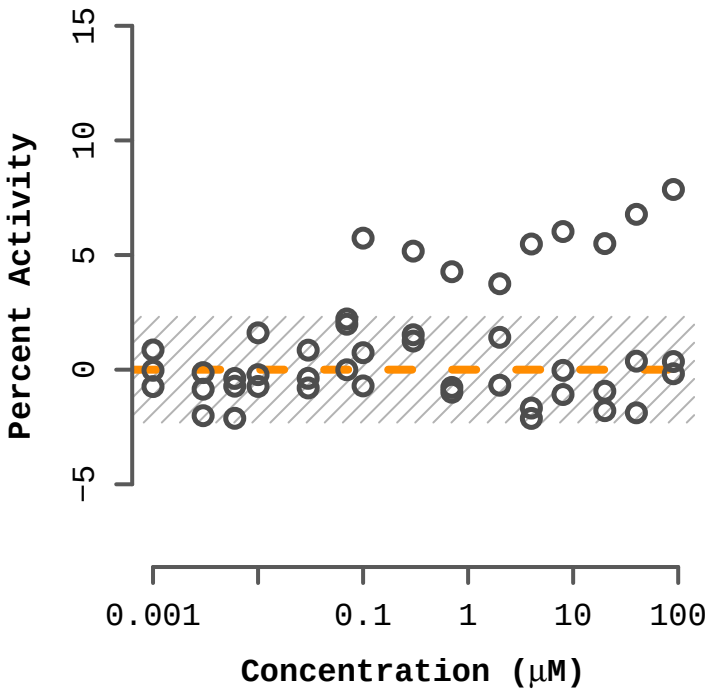
NAME: Pyriproxyfen
CHID: 32640 **CASRN:** 95737-68-1
SPID(S): Tox21_300716
M4ID: 12478417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

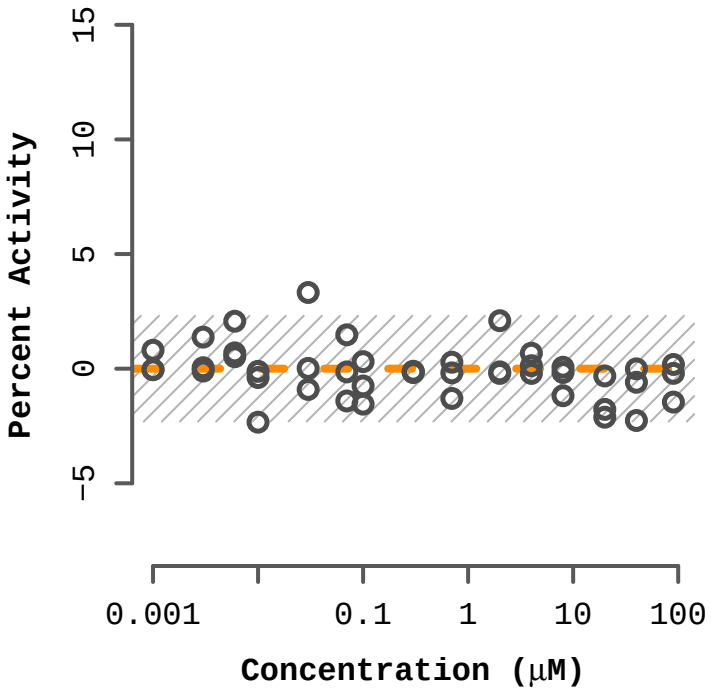
NAME: Quinclorac
CHID: 32641 **CASRN:** 84087-01-4
SPID(S): Tox21_300738
M4ID: 12478395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.77	NA	NA

MAX_MEAN: 2.68 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

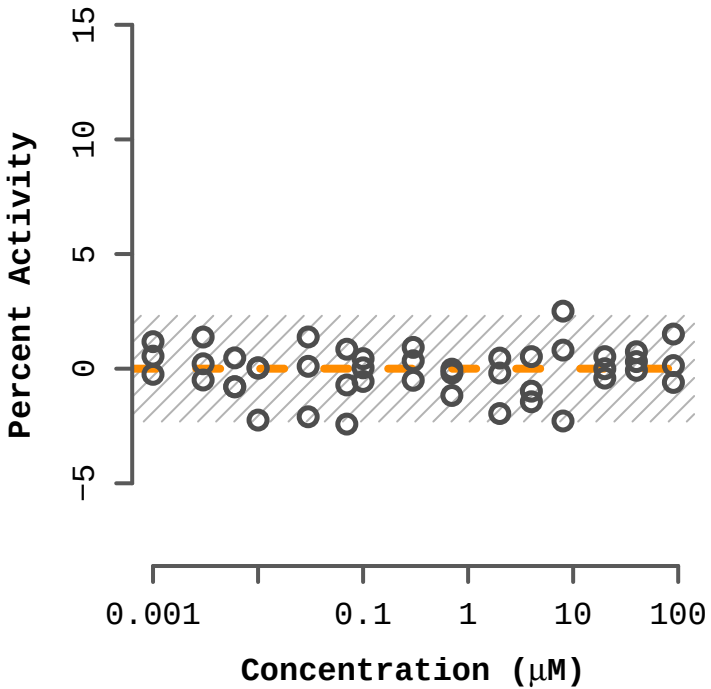
NAME: Rimsulfuron
CHID: 32642 **CASRN:** 122931-48-0
SPID(S): Tox21_304014
M4ID: 12475174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

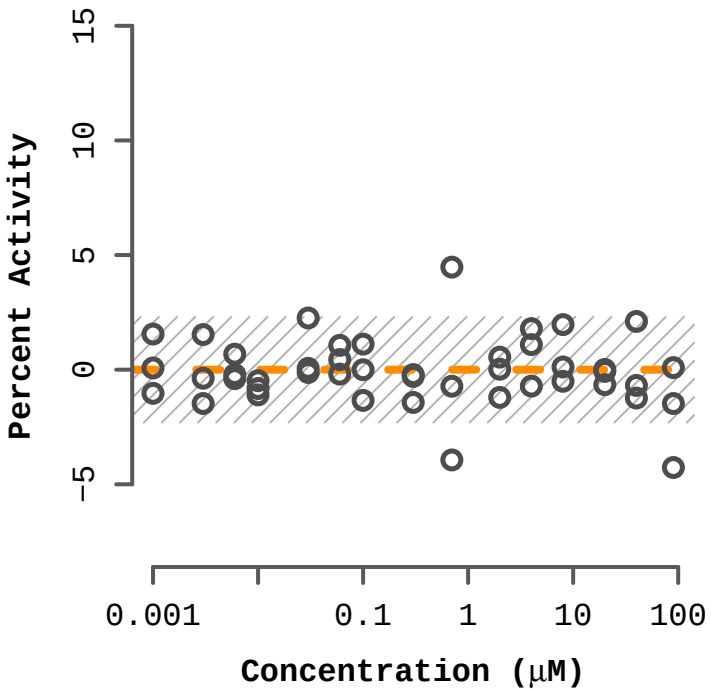
NAME: Sulfentrazone
CHID: 32645 **CASRN:** 122836-35-5
SPID(S): Tox21_301091
M4ID: 12478042

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.494 **MAX_MED:** 0.811 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

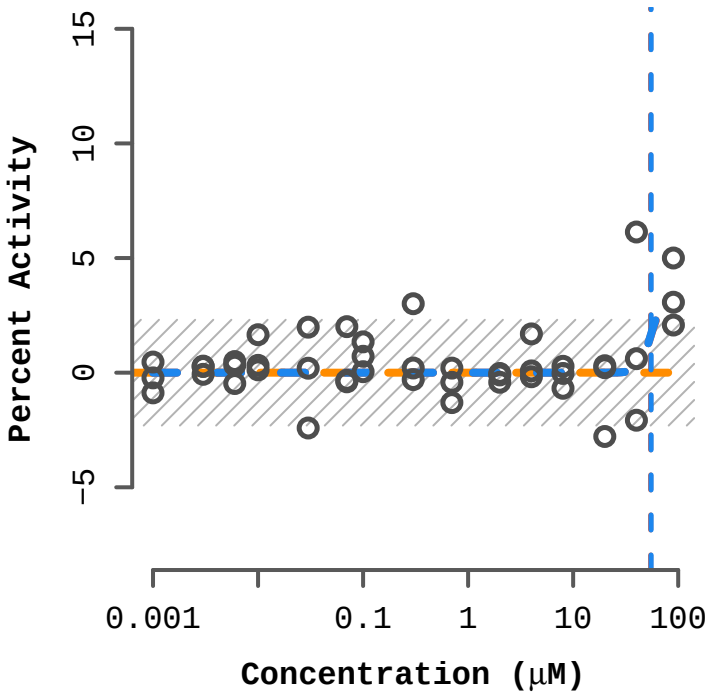
NAME: Sulfluramid
CHID: 32646 **CASRN:** 4151-50-2
SPID(S): Tox21_300377
M4ID: 12478755

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.732 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Thiocyanomethylthio)benzothiazole
CHID: 32647 **CASRN:** 21564-17-0
SPID(S): Tox21_301072
M4ID: 12478061

HILL MODEL (in red):

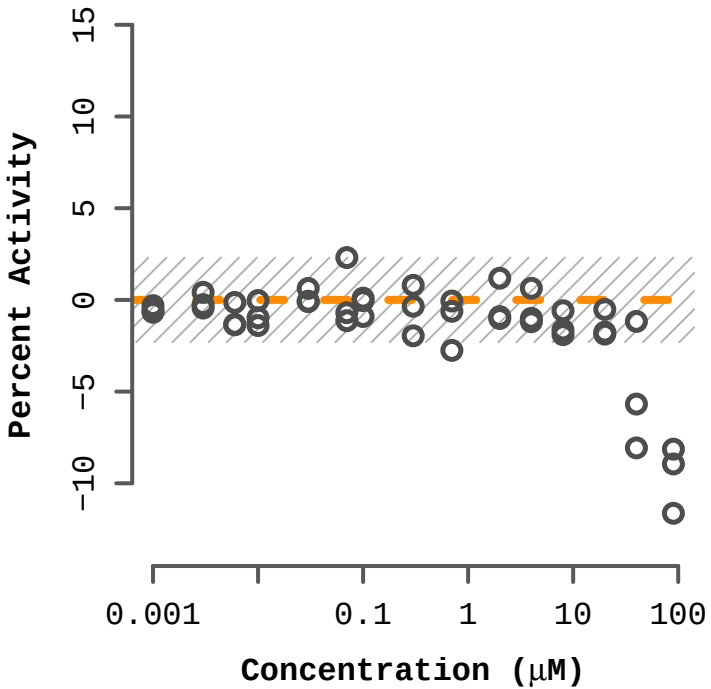
	tp	ga	gw
val:	3.2	1.74	8
sd:	3.15	1.16	63.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.55	1.74	8	2.58	1.55
sd:	39.9	1.21	62.4	35.1	85.2

	CNST	HILL	GNLS
AIC:	162.13	151.32	155.32
PROB:	0	0.88	0.12
RMSE:	1.67	1.4	1.4

MAX_MEAN: 3.39 **MAX_MED:** 3.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

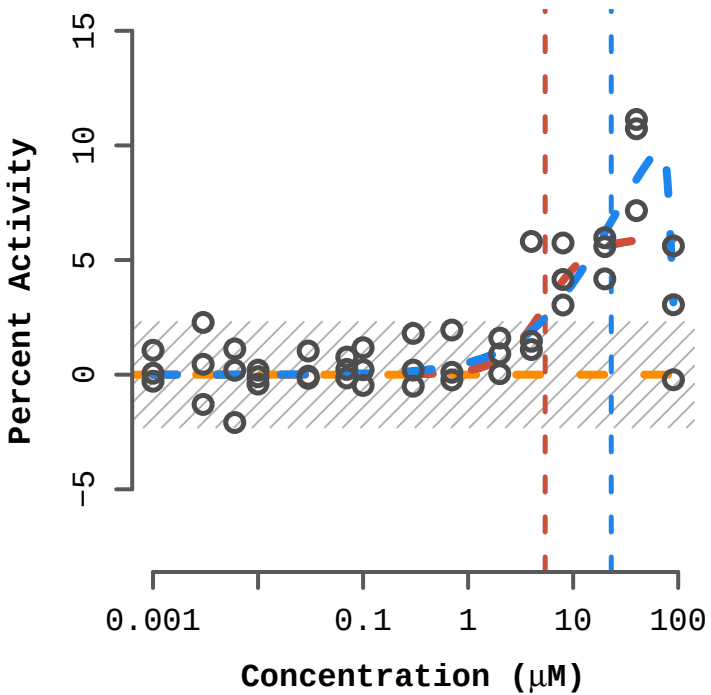
NAME: Z-Tetrachlorvinphos
CHID: 32648 **CASRN:** 22248-79-9
SPID(S): Tox21_301751
M4ID: 12477382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.44	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 0.161 **MAX_MED:** −0.0366 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetramethrin
CHID: 32649 **CASRN:** 7696-12-0
SPID(S): Tox21_301017
M4ID: 12478116

HILL MODEL (in red):

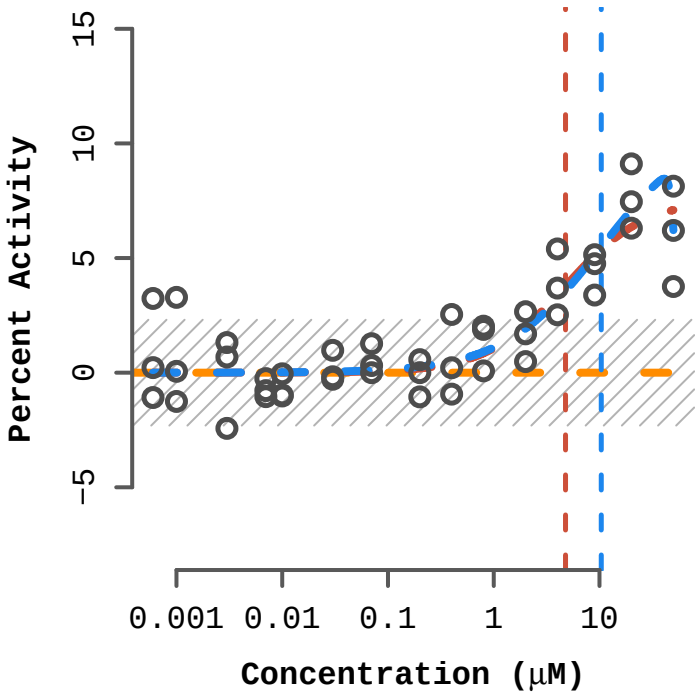
	tp	ga	gw
val:	5.95	0.733	2.04
sd:	0.746	0.11	0.849

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.4	1.36	1.02	1.93	18
sd:	10	0.57	0.272	0.0199	13.2

	CNST	HILL	GNLS
AIC:	230.16	175.12	164.65
PROB:	0	0.01	0.99
RMSE:	3.47	1.81	1.36

MAX_MEAN: 9.67 **MAX_MED:** 10.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetramethrin
CHID: 32649 **CASRN:** 7696-12-0
SPID(S): Tox21_112623_1
M4ID: 12483005

HILL MODEL (in red):

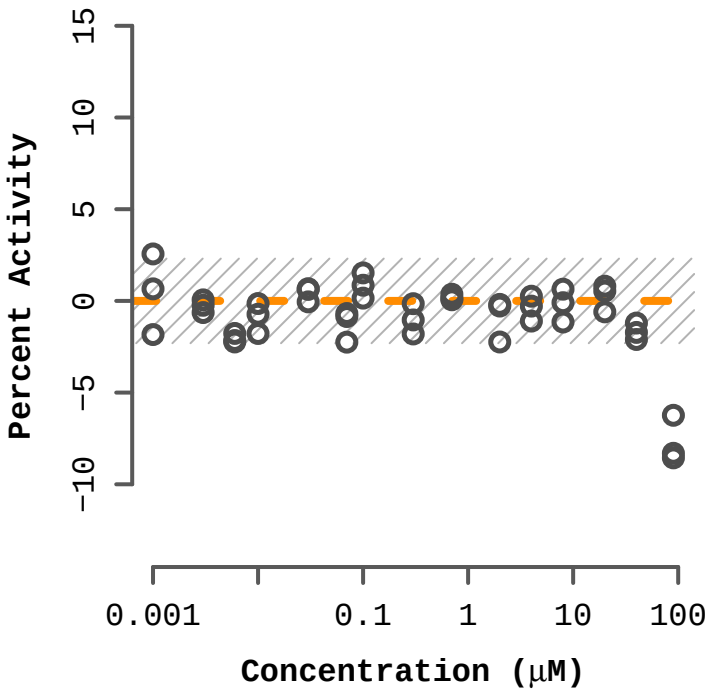
	tp	ga	gw
val:	7.56	0.679	1.16
sd:	1.22	0.175	0.352

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.9	1.02	0.937	1.72	17.8
sd:	4.68	0.423	0.274	0.0214	20

	CNST	HILL	GNLS
AIC:	231.39	162.68	163.85
PROB:	0	0.64	0.36
RMSE:	3.24	1.35	1.3

MAX_MEAN: 7.62 **MAX_MED:** 7.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

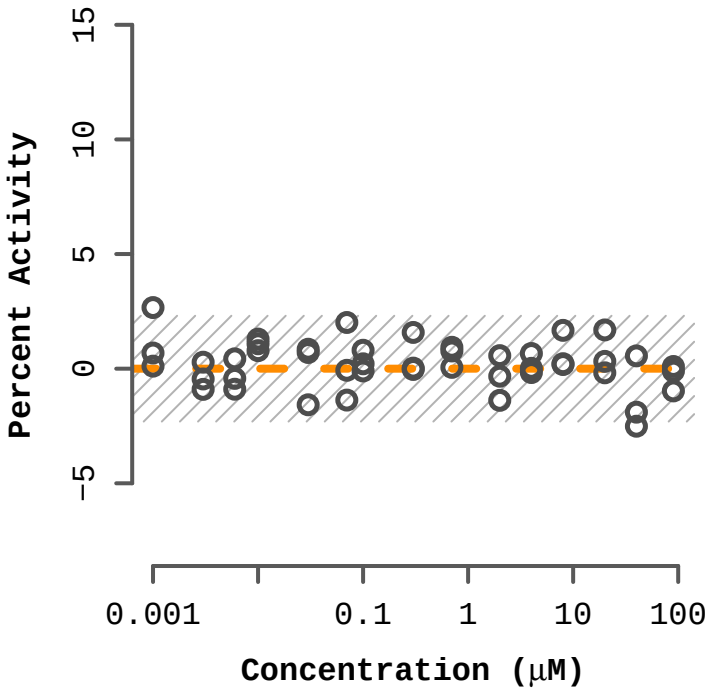
NAME: Thidiazuron
CHID: 32651 **CASRN:** 51707-55-2
SPID(S): Tox21_300651
M4ID: 12478482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.74	NA	NA
PROB:	1	NA	NA
RMSE:	2.32	NA	NA

MAX_MEAN: 0.846 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

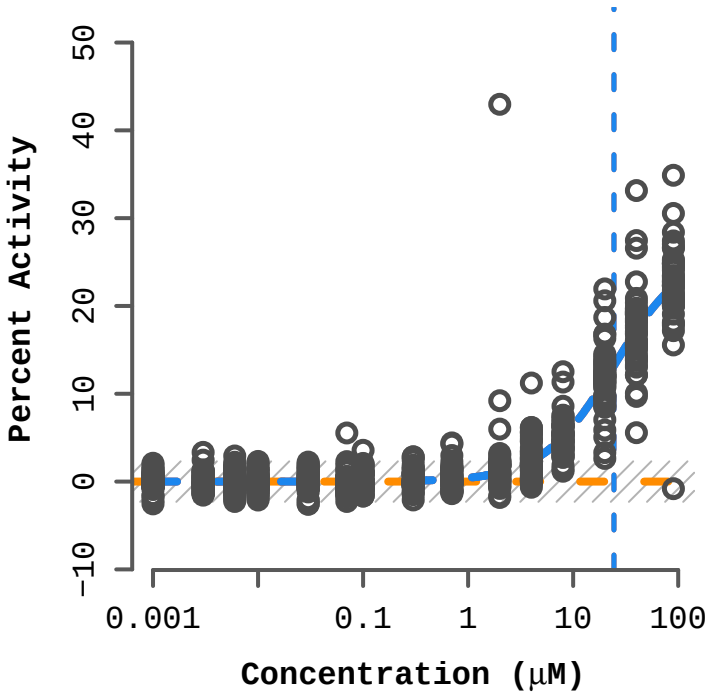
NAME: Triforine
CHID: 32654 **CASRN:** 26644-46-2
SPID(S): Tox21_302268
M4ID: 12476865

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triticonazole
CHID: 32655 CASRN: 131983-72-7
SPID(S): Tox21_400047
M4ID: 12475090

HILL MODEL (in red):

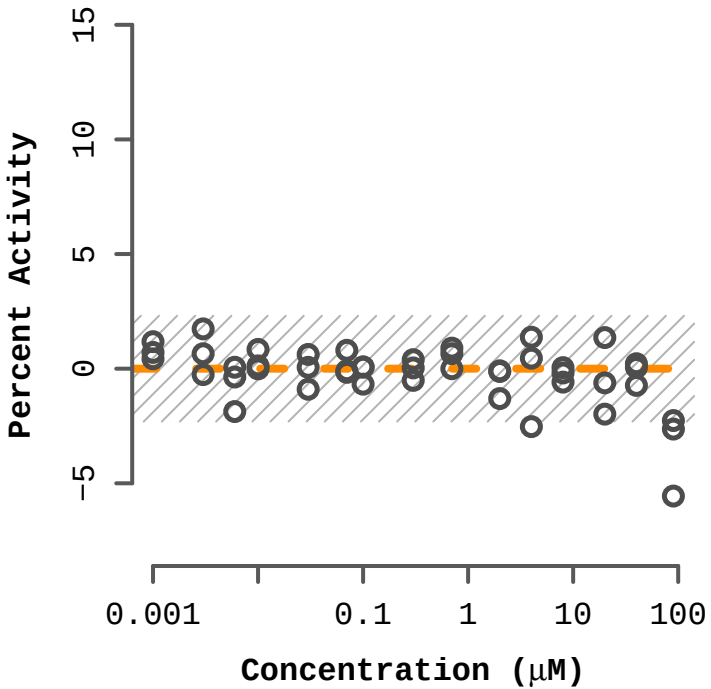
	tp	ga	gw
val:	26.4	1.39	1.29
sd:	0.903	0.0315	0.0566

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	26.4	1.39	1.29	2.99	8.11
sd:	0.903	0.0315	0.0566	585	4570

	CNST	HILL	GNLS
AIC:	4793.73	2893.85	2897.85
PROB:	0	0.88	0.12
RMSE:	8.49	2.79	2.79

MAX_MEAN: 22.3 MAX_MED: 22.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

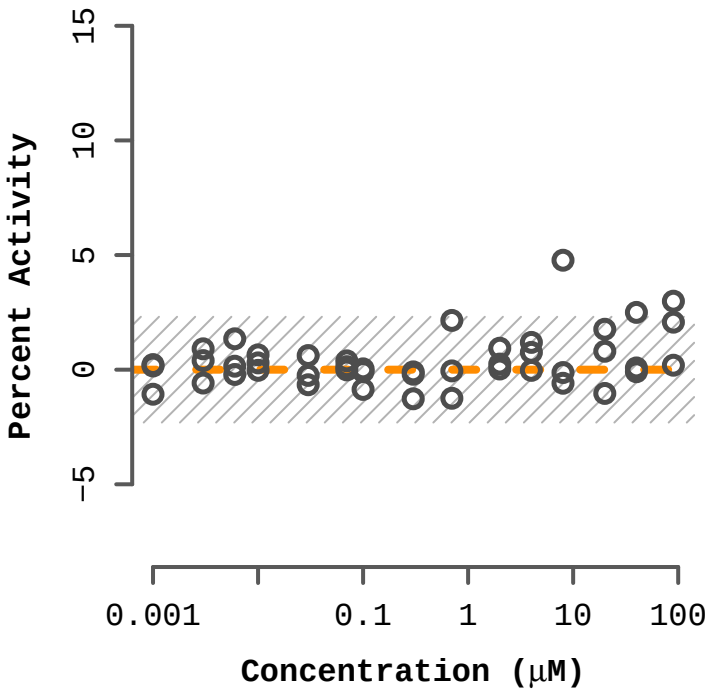
NAME: Esfenvalerate
CHID: 32667 CASRN: 66230-04-4
SPID(S): Tox21_300785
M4ID: 12478348

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.774 MAX_MED: 0.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

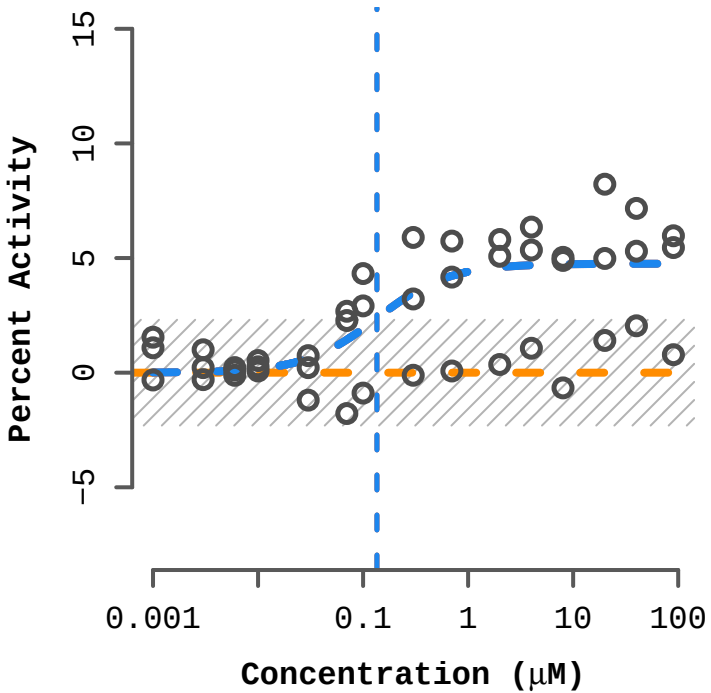
NAME: Mecoprop-P
CHID: 32670 **CASRN:** 16484-77-8
SPID(S): Tox21_303709
M4ID: 12475479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Metalaxyl-M
CHID: 32671 CASRN: 70630-17-0
SPID(S): Tox21_303887
M4ID: 12475301

HILL MODEL (in red):

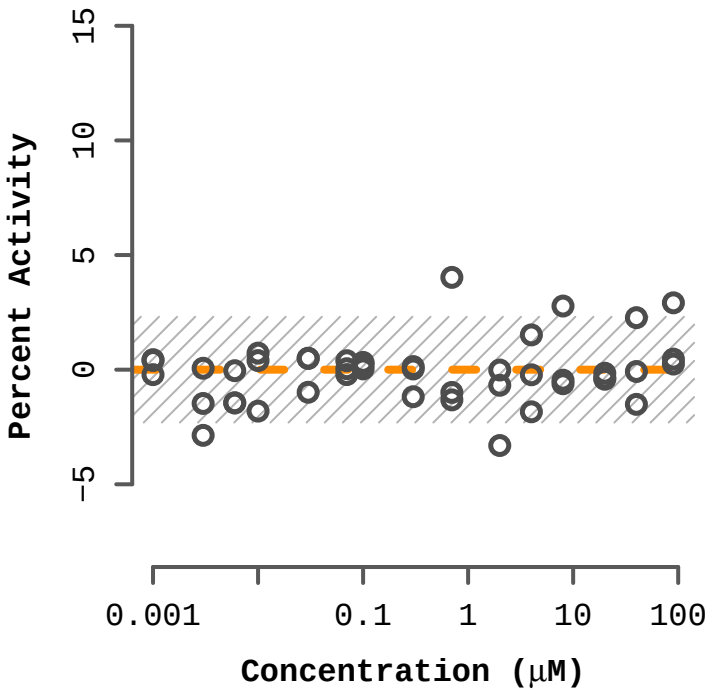
	tp	ga	gw
val:	4.75	−0.868	1.26
sd:	0.611	0.319	0.906

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.75	−0.868	1.26	3.18	6.48
sd:	0.611	0.319	0.907	3020	15900

	CNST	HILL	GNLS
AIC:	245.92	201.12	205.12
PROB:	0	0.88	0.12
RMSE:	3.56	2.07	2.07

MAX_MEAN: 4.87 MAX_MED: 5.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

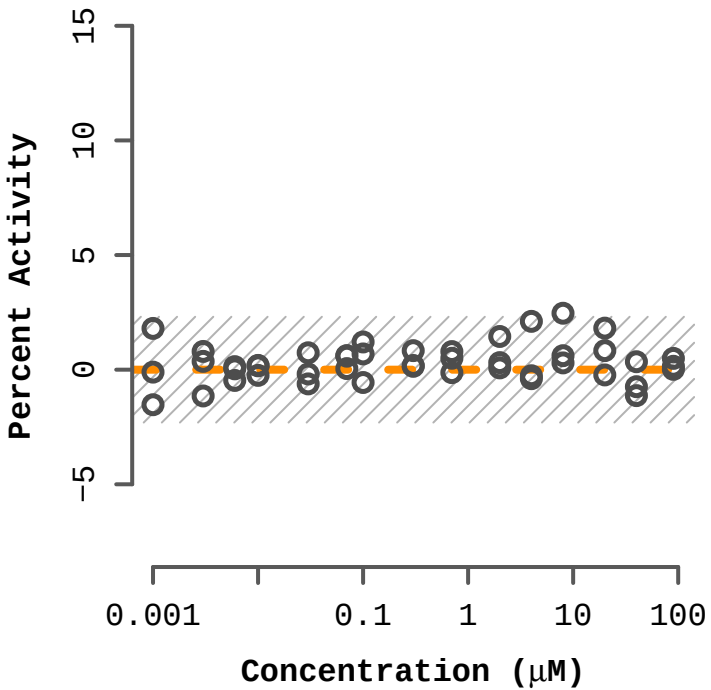
NAME: Pyrithiobac−sodium
CHID: 32673 **CASRN:** 123343−16−8
SPID(S): Tox21_300849
M4ID: 12478284

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.491 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

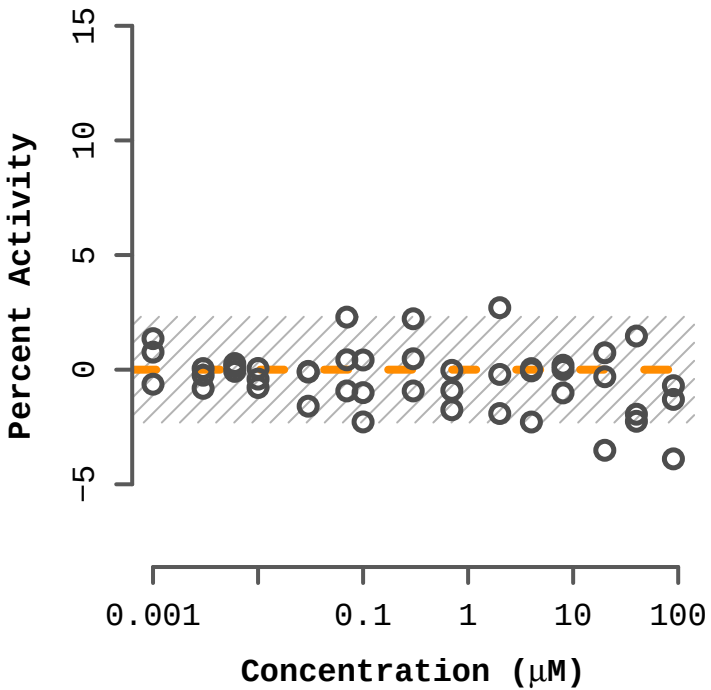
NAME: Sulprofos
CHID: 32675 **CASRN:** 35400-43-2
SPID(S): Tox21_301358
M4ID: 12477775

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.832 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

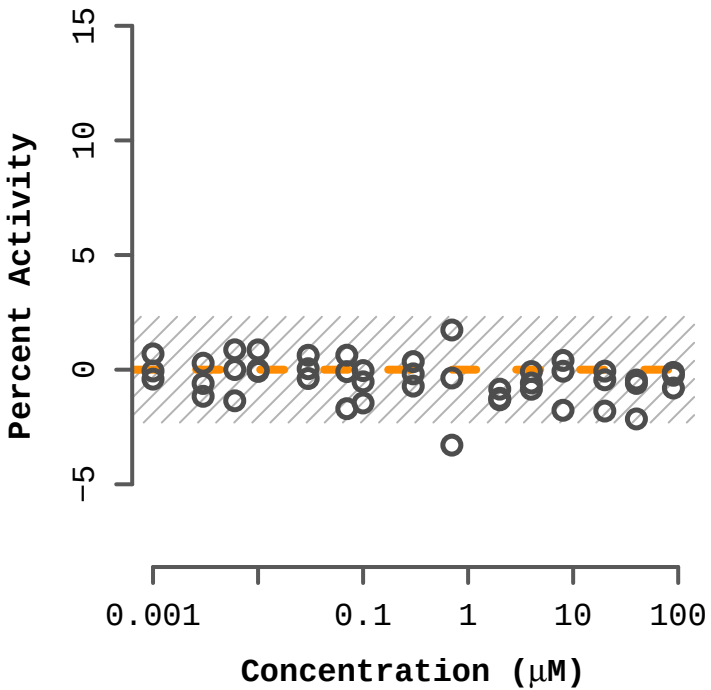
NAME: Mevinphos
CHID: 32683 **CASRN:** 7786-34-7
SPID(S): Tox21_301153
M4ID: 12477980

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.6 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

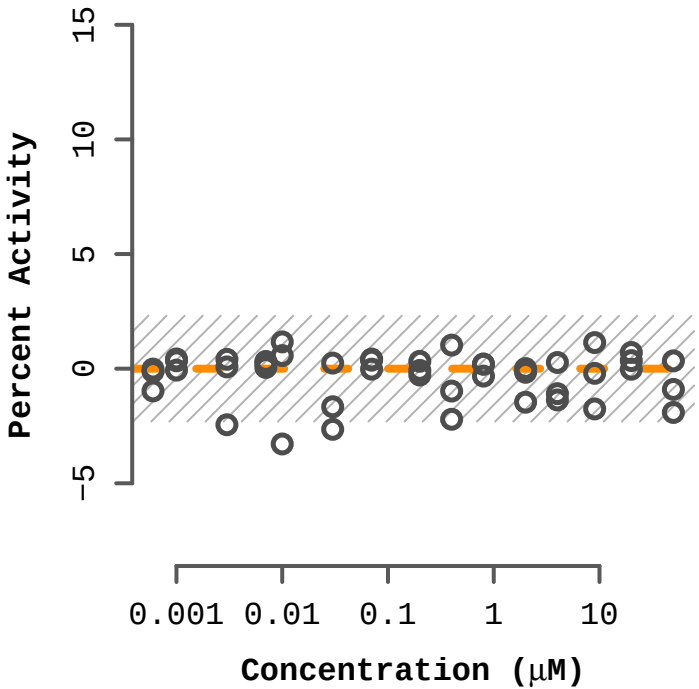
NAME: Phenothrin
CHID: 32688 **CASRN:** 26002-80-2
SPID(S): Tox21_301570
M4ID: 12477563

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.265 **MAX_MED:** 0.0433 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

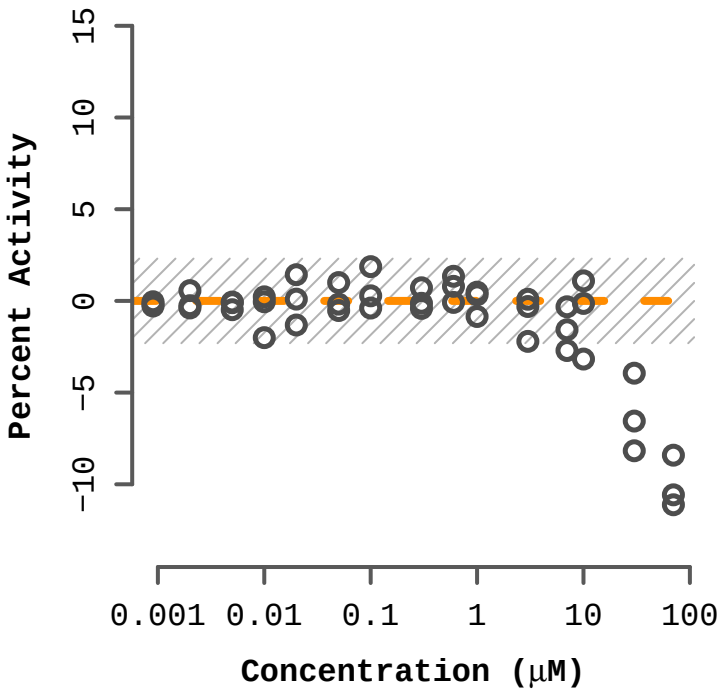
NAME: Phenothrin
CHID: 32688 **CASRN:** 26002-80-2
SPID(S): Tox21_111297_1
M4ID: 12483784

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.346 **MAX_MED:** 0.573 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

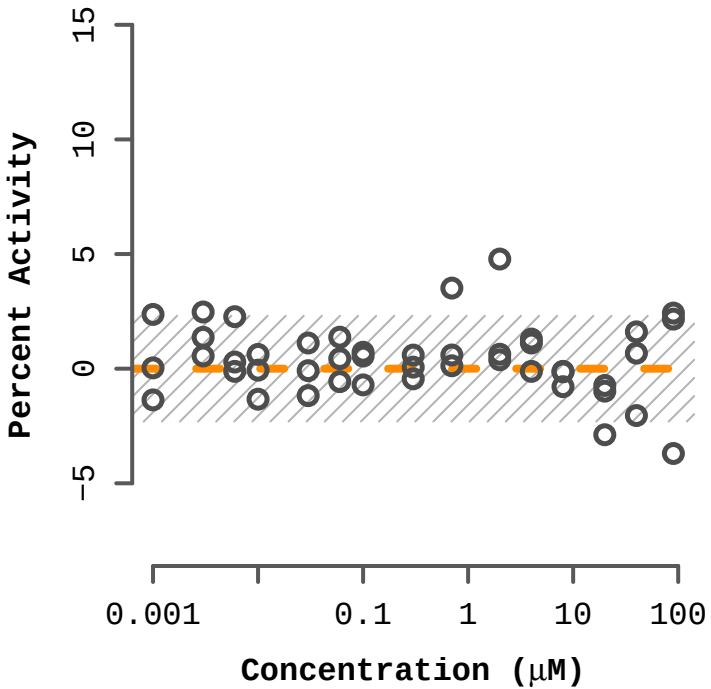
NAME: Indoxacarb
CHID: 32690 **CASRN:** 173584-44-6
SPID(S): Tox21_300723
M4ID: 12478410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208	NA	NA
PROB:	1	NA	NA
RMSE:	3.25	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 0.795 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

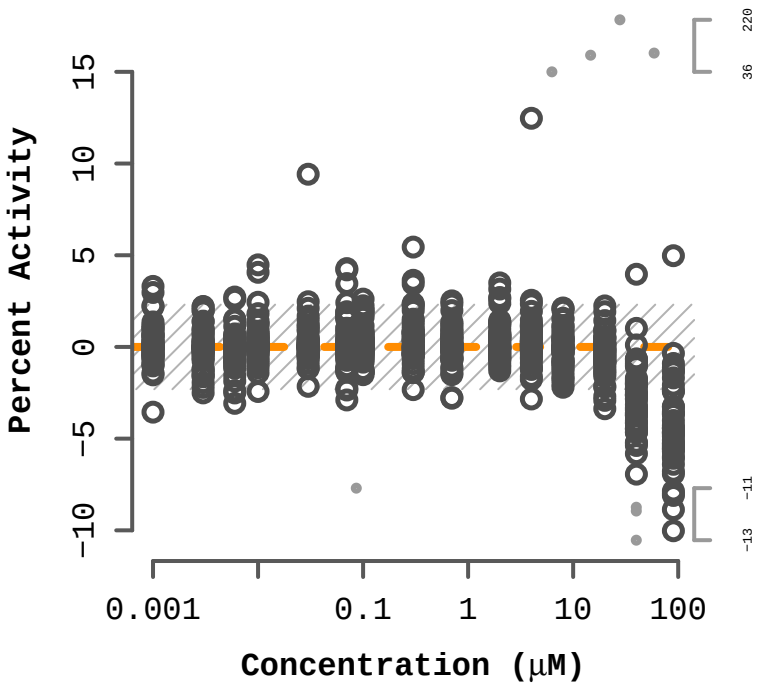
NAME: 1,2,4−Triazole, sodium salt
CHID: 32722 CASRN: 41253−21−8
SPID(S): Tox21_200054
M4ID: 12482198

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

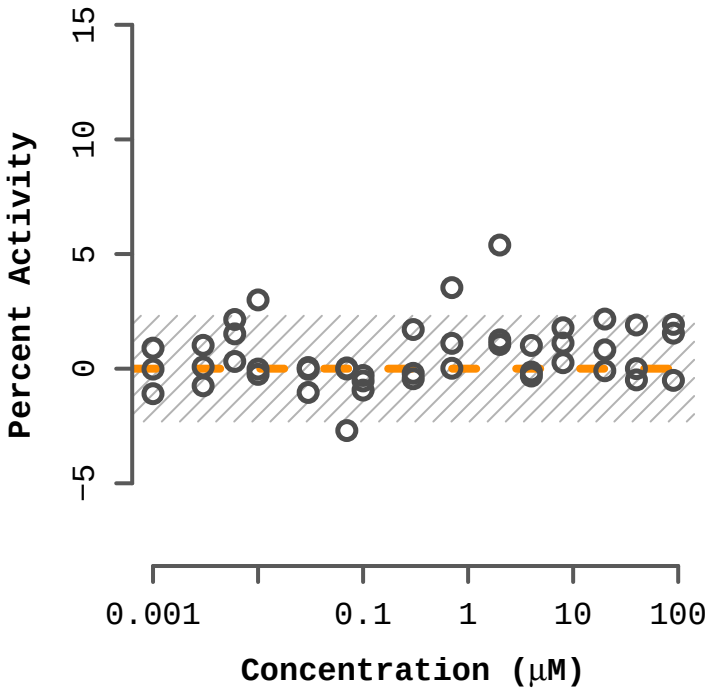
NAME: 1,3-Diiminobenz(f)isoindoline
CHID: 32751 **CASRN:** 65558-69-2
SPID(S): Tox21_400043
M4ID: 12475094 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2958.47	NA	NA
PROB:	1	NA	NA
RMSE:	10.09	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 0.198 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

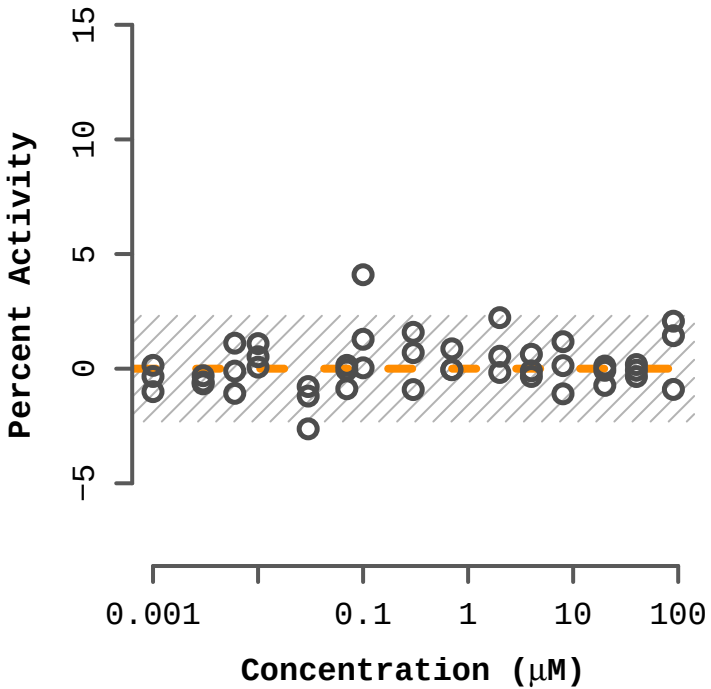
NAME: 1,4,5−Trihydroxynaphthalene
CHID: 32759 **CASRN:** 481−40−3
SPID(S): Tox21_201120
M4ID: 12481132

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.57 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

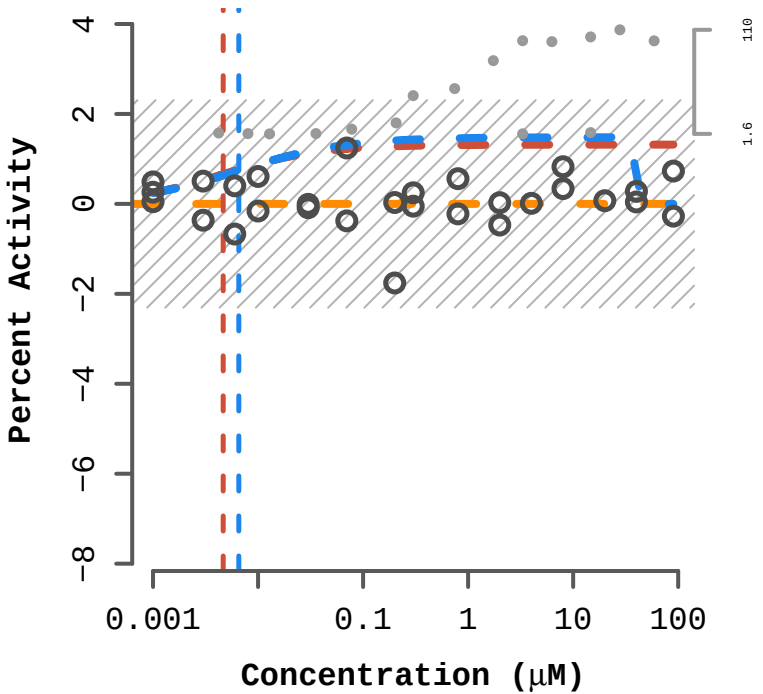
NAME: 2,2−Dimethylbutanoic acid
CHID: 32811 **CASRN:** 595−37−9
SPID(S): Tox21_200740
M4ID: 12481512

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2-Dimethyl-3-pentanol
CHID: 32813 **CASRN:** 3970-62-5
SPID(S): Tox21_201174
M4ID: 12481078 **BRK**

HILL MODEL (in red):

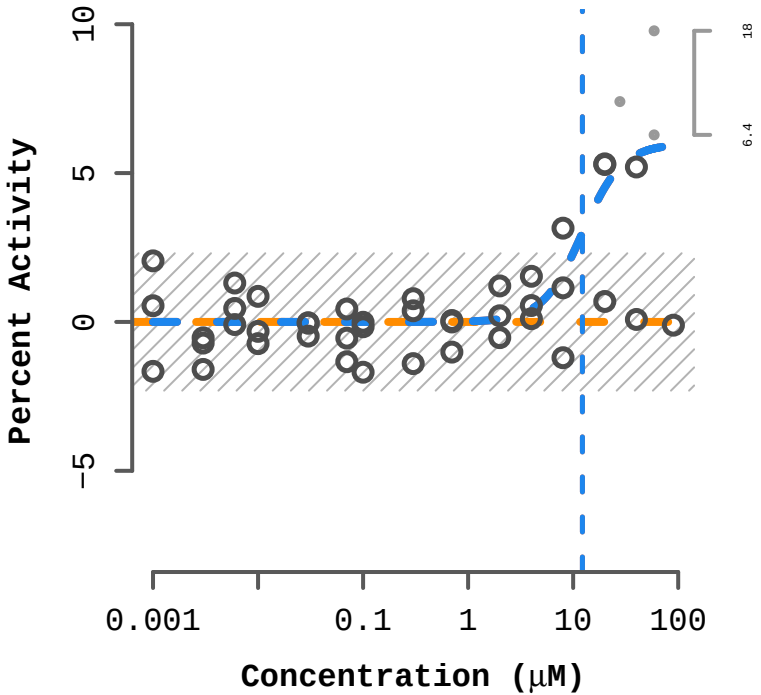
	tp	ga	gw
val:	1.32	−2.33	0.95
sd:	1.26	2.67	3.43

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.48	−2.18	0.862	1.6	14.3
sd:	1.49	2.48	3.24	0.375	674

	CNST	HILL	GNLS
AIC:	413.1	417.3	421.28
PROB:	0.88	0.11	0.01
RMSE:	38.14	37.6	37.68

MAX_MEAN: 37.8 **MAX_MED:** 2.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dibromopropionic acid
CHID: 32832 CASRN: 600-05-5
SPID(S): Tox21_200140
M4ID: 12482112 BRK

HILL MODEL (in red):

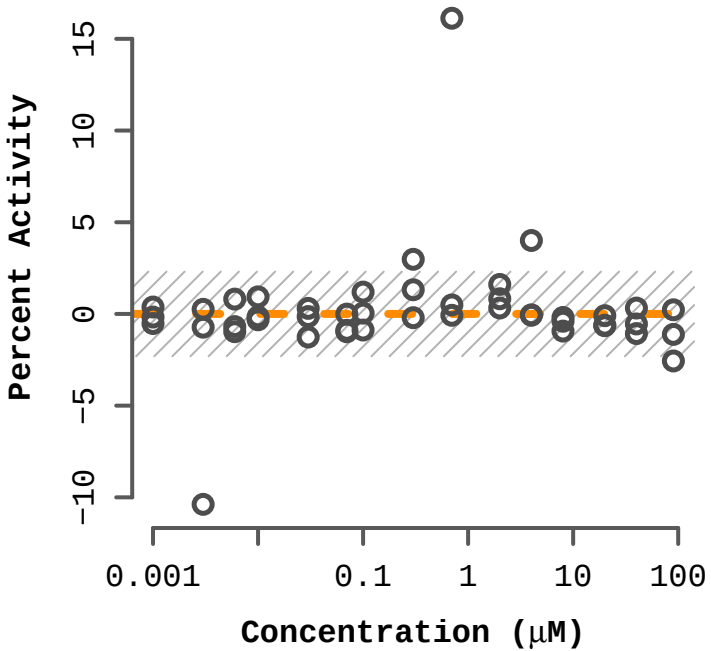
	tp	ga	gw
val:	5.98	1.09	2.29
sd:	1.1	0.142	1.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.98	1.09	2.29	3	7.24
sd:	1.1	0.142	1.31	1760	12200

	CNST	HILL	GNLS
AIC:	206.04	189.33	193.33
PROB:	0	0.88	0.12
RMSE:	3.67	2.56	2.56

MAX_MEAN: 8.2 MAX_MED: 6.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

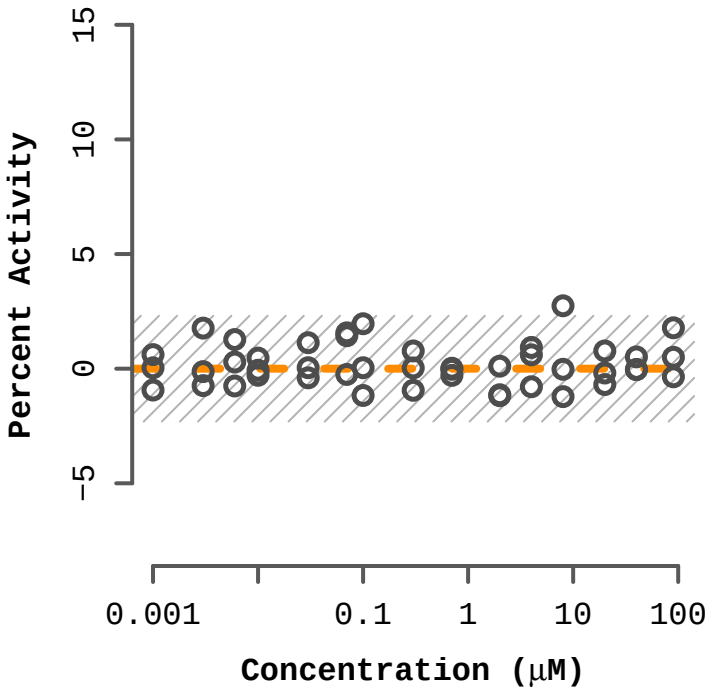
NAME: 2,4-Difluoronitrobenzene
CHID: 32869 CASRN: 446-35-5
SPID(S): Tox21_200688
M4ID: 12481564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.75	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 5.52 MAX_MED: 1.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

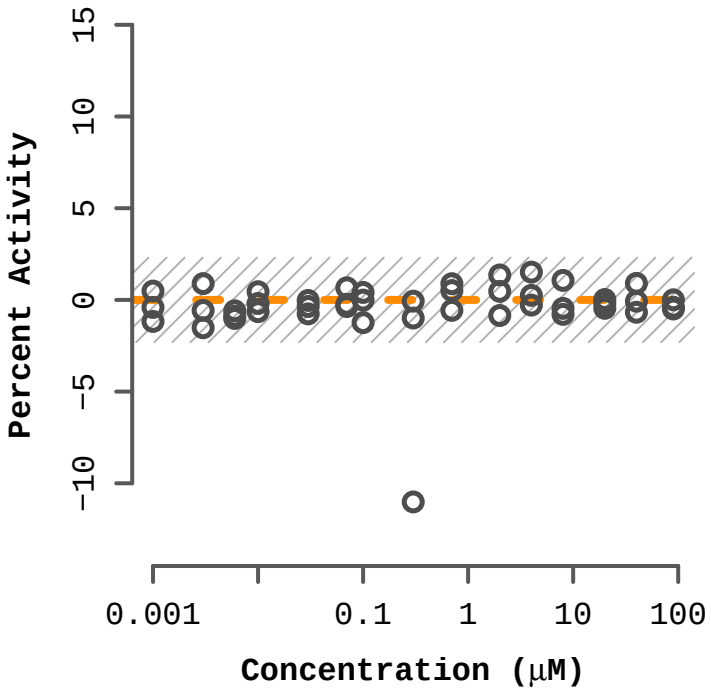
NAME: 2,4-Pentanediol
CHID: 32878 **CASRN:** 625-69-4
SPID(S): Tox21_200916
M4ID: 12481336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

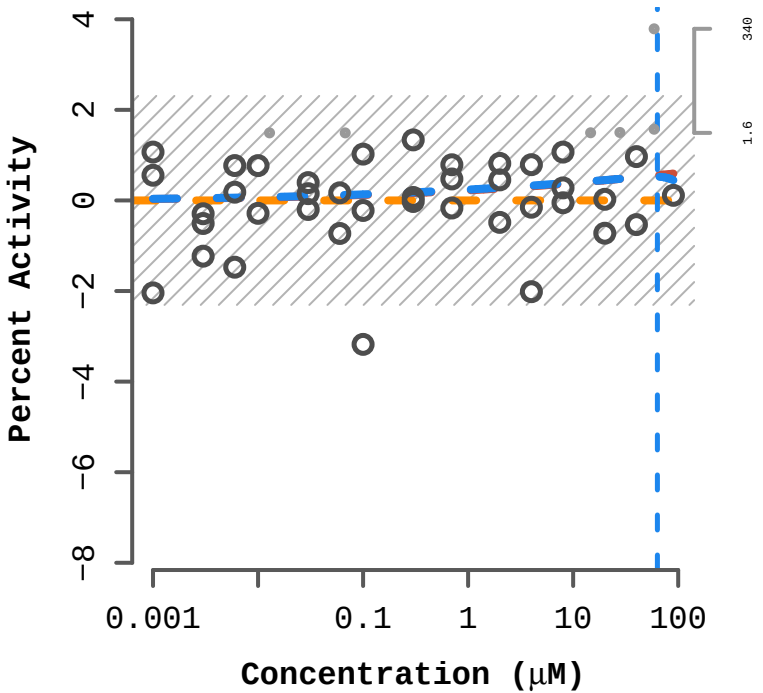
NAME: 2,6-Dichlorobenzoyl chloride
CHID: 32891 **CASRN:** 4659-45-4
SPID(S): Tox21_200318
M4ID: 12481934

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 0.495 **MAX_MED:** 0.508 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxyisobutyric acid
CHID: 32954 **CASRN:** 594-61-6
SPID(S): Tox21_200123
M4ID: 12482129 **BRK**

HILL MODEL (in red):

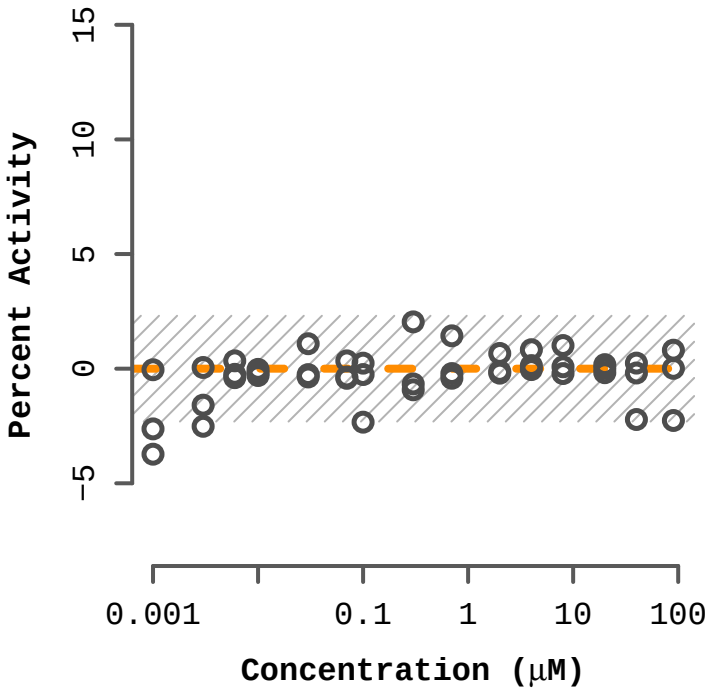
	tp	ga	gw
val:	1.42	2.44	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.09	1.8	0.305	2.05	5.66
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	206.73	210.34	214.31
PROB:	0.84	0.14	0.02
RMSE:	51.21	51.12	51.14

MAX_MEAN: 119 **MAX_MED:** 13.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

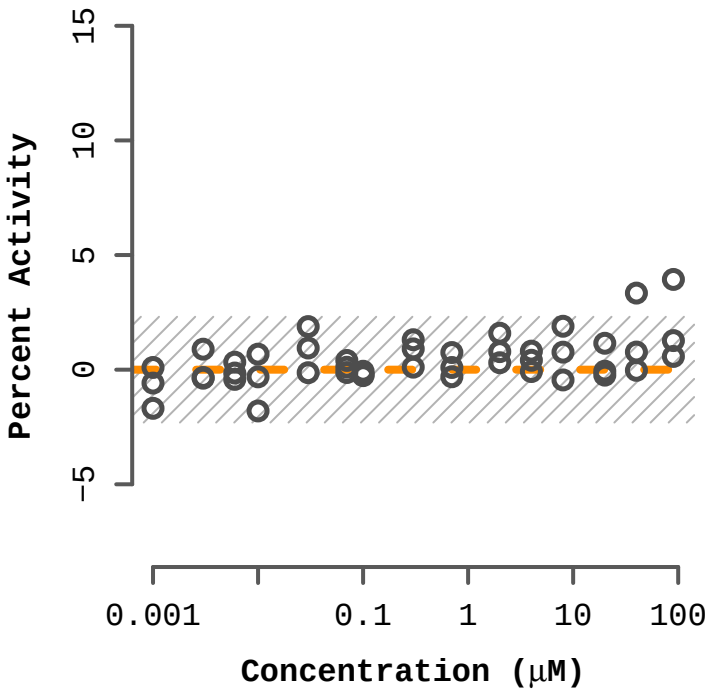
NAME: 3,3'−Dithiodipropionic acid
CHID: 32998 **CASRN:** 1119−62−6
SPID(S): Tox21_200951
M4ID: 12481301

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.31 **MAX_MED:** 0.137 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

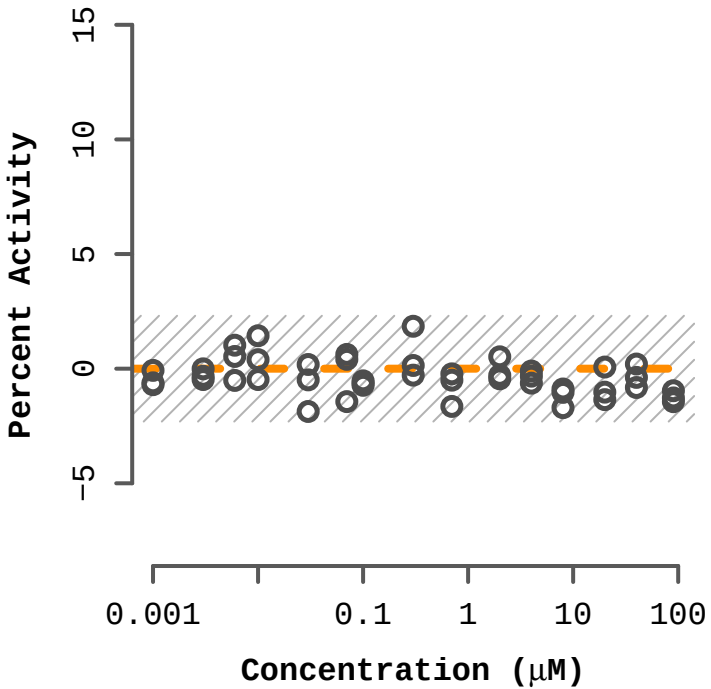
NAME: 3,4−Dichlorophenyl isocyanate
CHID: 33008 **CASRN:** 102−36−3
SPID(S): Tox21_200085
M4ID: 12482167

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

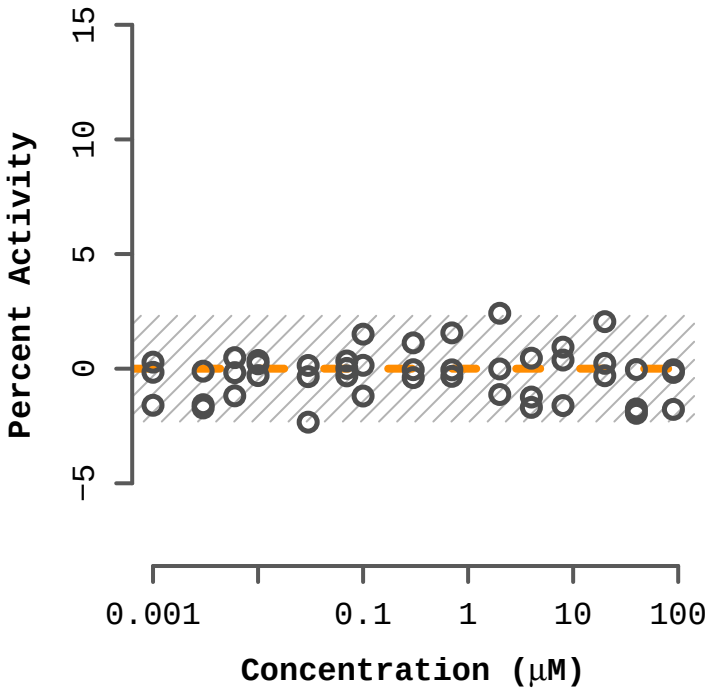
NAME: 4-(Methylthio)benzaldehyde
CHID: 33047 CASRN: 3446-89-7
SPID(S): Tox21_200004
M4ID: 12482248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.57 MAX_MED: 0.534 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

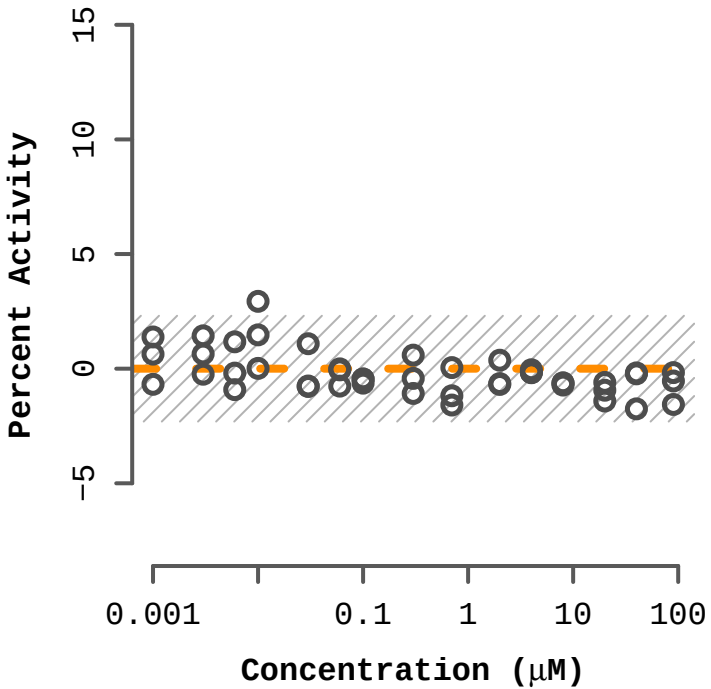
NAME: 4-Amino-1,2,4-triazole
CHID: 33058 **CASRN:** 584-13-4
SPID(S): Tox21_300197
M4ID: 12478933

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.66 **MAX_MED:** 0.377 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

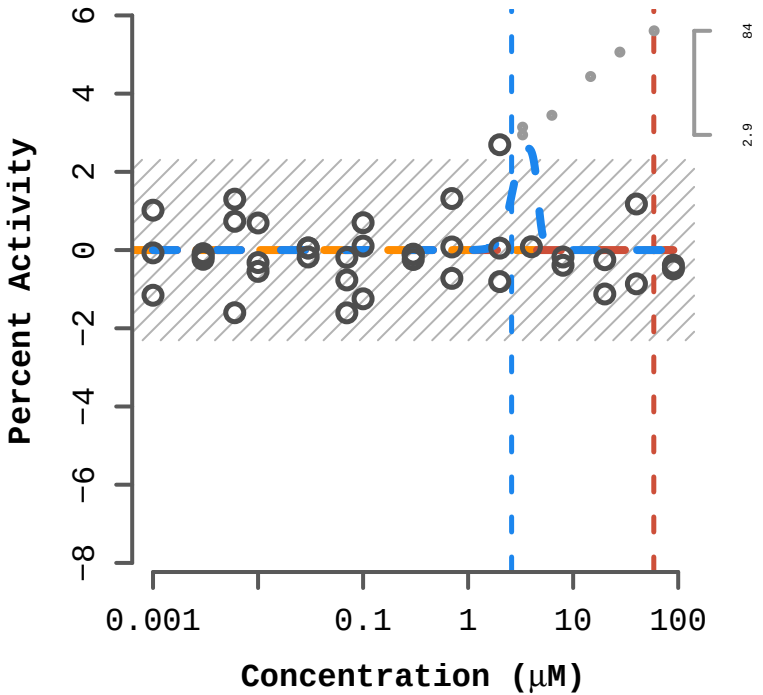
NAME: 4-Amino-1,2,4-triazole
CHID: 33058 CASRN: 584-13-4
SPID(S): Tox21_201893
M4ID: 12480359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.48 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-(Hydroxymethyl-2-furoyl)glycine
CHID: 33096 CASRN: 38716-68-6
SPID(S): Tox21_200944
M4ID: 12481308 BRK

HILL MODEL (in red):

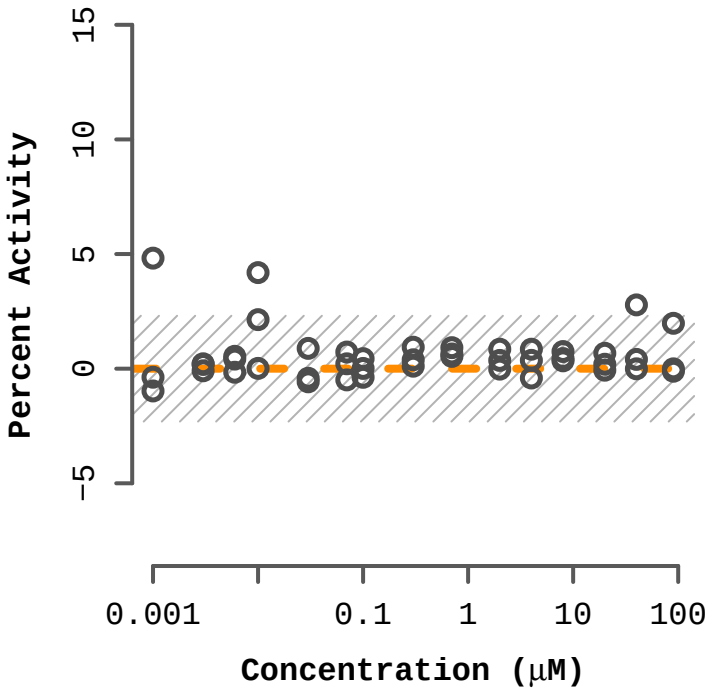
	tp	ga	gw
val:	1.39e-09	1.77	1.52
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.8	0.414	7.99	0.664	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	263.89	269.89	269.81
PROB:	0.91	0.05	0.05
RMSE:	17.82	17.82	17.79

MAX_MEAN: 27.6 MAX_MED: 2.95 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

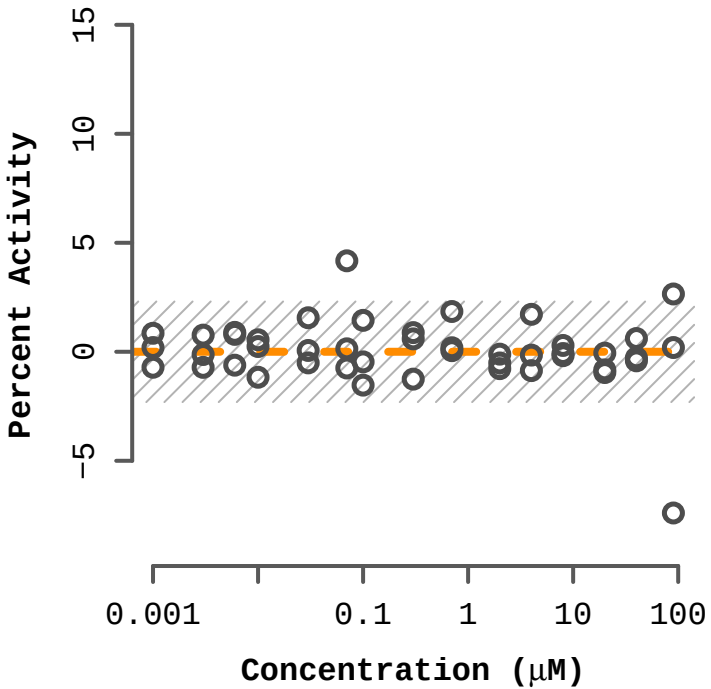
NAME: 5-(Hydroxymethyl)-2-furoic acid
CHID: 33098 CASRN: 6338-41-6
SPID(S): Tox21_201082
M4ID: 12481170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 2.12 MAX_MED: 2.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

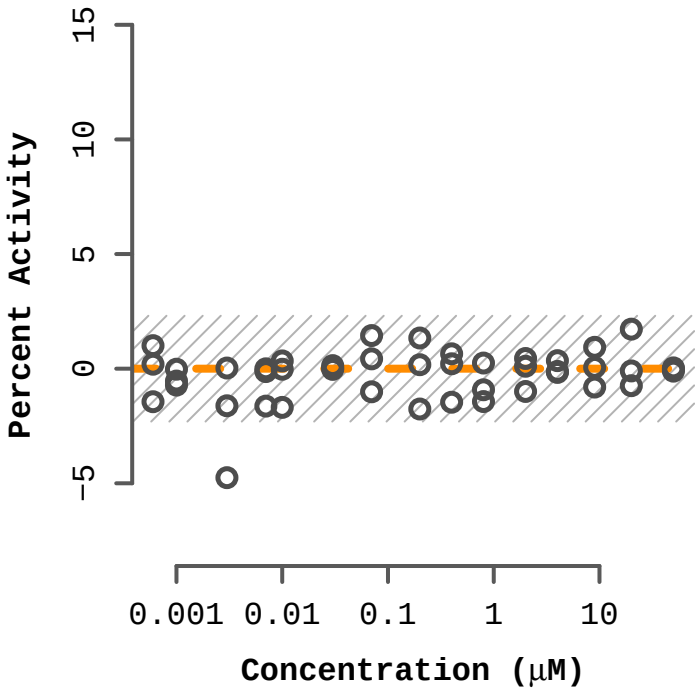
NAME: 5-Bromo-2'-deoxyuridine
CHID: 33105 CASRN: 59-14-3
SPID(S): Tox21_200106
M4ID: 12482146

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.19 MAX_MED: 0.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

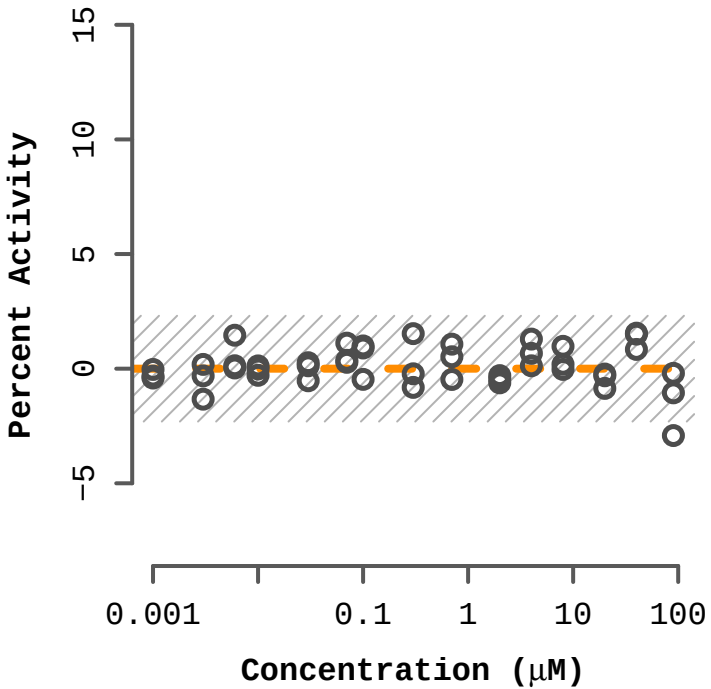
NAME: 5−Bromo−2'−deoxyuridine
CHID: 33105 **CASRN:** 59−14−3
SPID(S): Tox21_111016_1
M4ID: 12483947

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.296 **MAX_MED:** 0.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

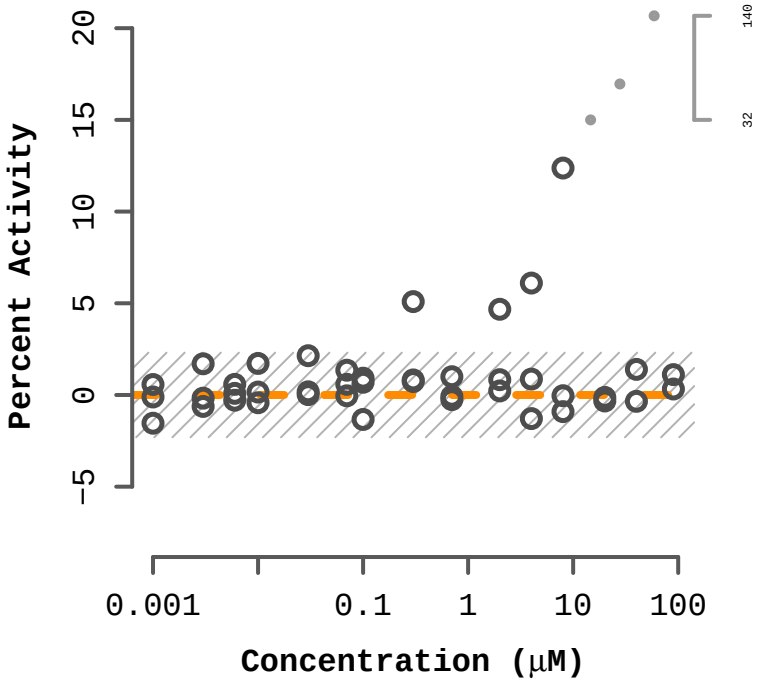
NAME: Aldicarb sulfoxide
CHID: 33161 **CASRN:** 1646-87-3
SPID(S): Tox21_303449
M4ID: 12475691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

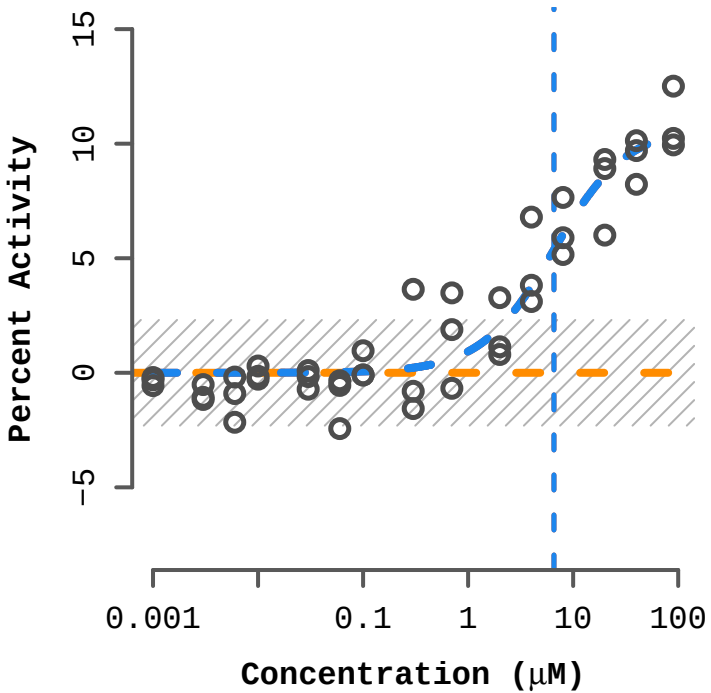
NAME: Aldicarb sulfoxide
CHID: 33161 CASRN: 1646-87-3
SPID(S): Tox21_201744
M4ID: 12480508 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.05	NA	NA
PROB:	1	NA	NA
RMSE:	23.34	NA	NA

MAX_MEAN: 46 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Alizarin Yellow R
CHID: 33163 CASRN: 2243-76-7
SPID(S): Tox21_200305
M4ID: 12481947

HILL MODEL (in red):

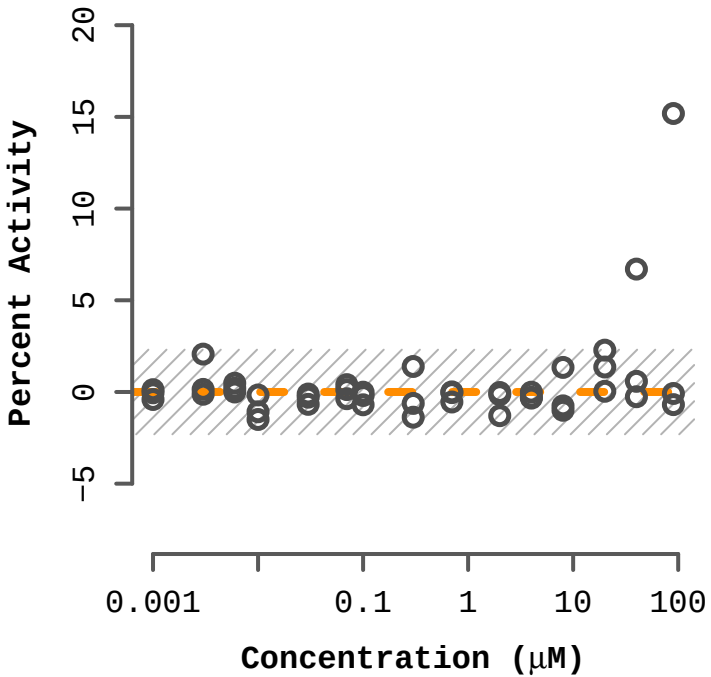
	tp	ga	gw
val:	10.7	0.817	1.25
sd:	0.875	0.0984	0.305

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.7	0.817	1.25	3.4	5.35
sd:	0.875	0.0984	0.305	721	2680

	CNST	HILL	GNLS
AIC:	269.62	157.9	161.9
PROB:	0	0.88	0.12
RMSE:	4.9	1.3	1.3

MAX_MEAN: 10.9 MAX_MED: 10.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

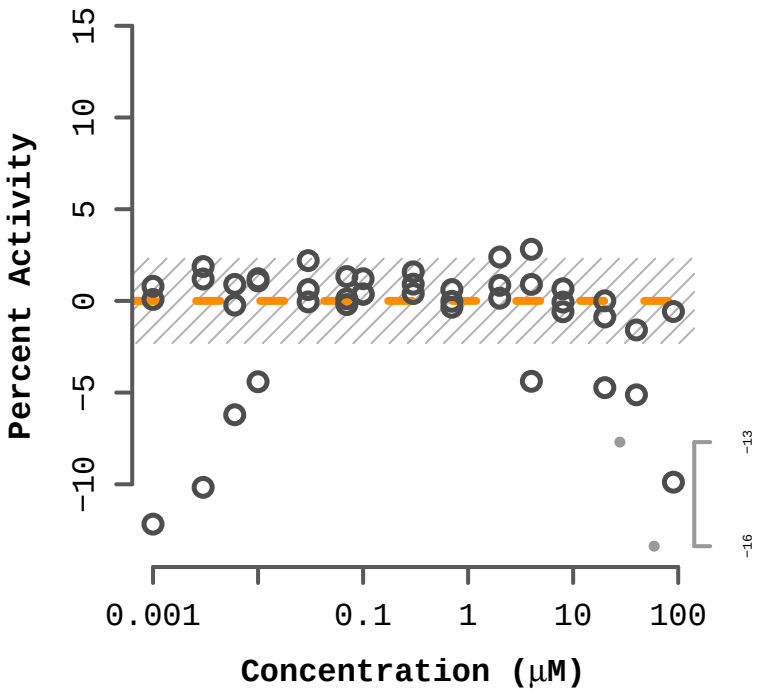
NAME: alpha-Ketoglutaric acid
CHID: 33179 **CASRN:** 328-50-7
SPID(S): Tox21_200918
M4ID: 12481334

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.84	NA	NA
PROB:	1	NA	NA
RMSE:	2.59	NA	NA

MAX_MEAN: 4.81 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

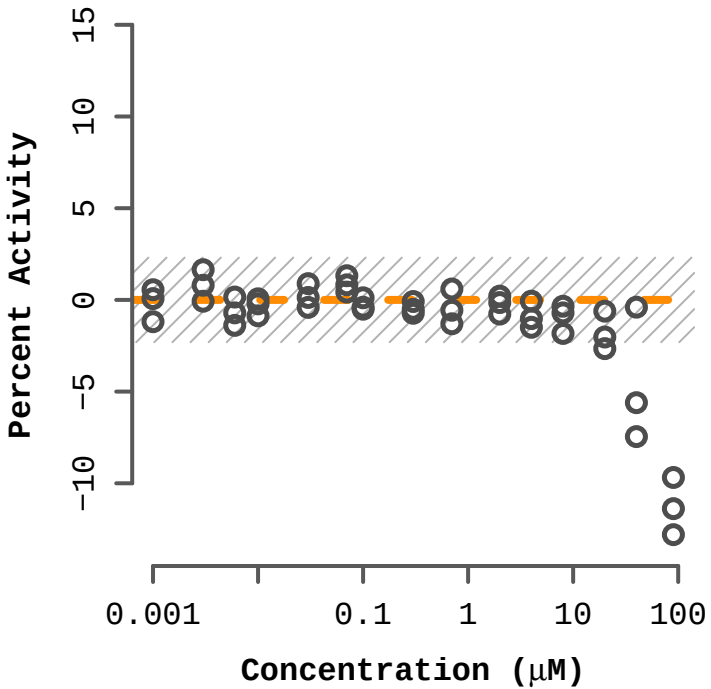
NAME: Amitriptyline hydrochloride
CHID: 33187 CASRN: 549-18-8
SPID(S): Tox21_303612
M4ID: 12475533 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.22	NA	NA
PROB:	1	NA	NA
RMSE:	4.56	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

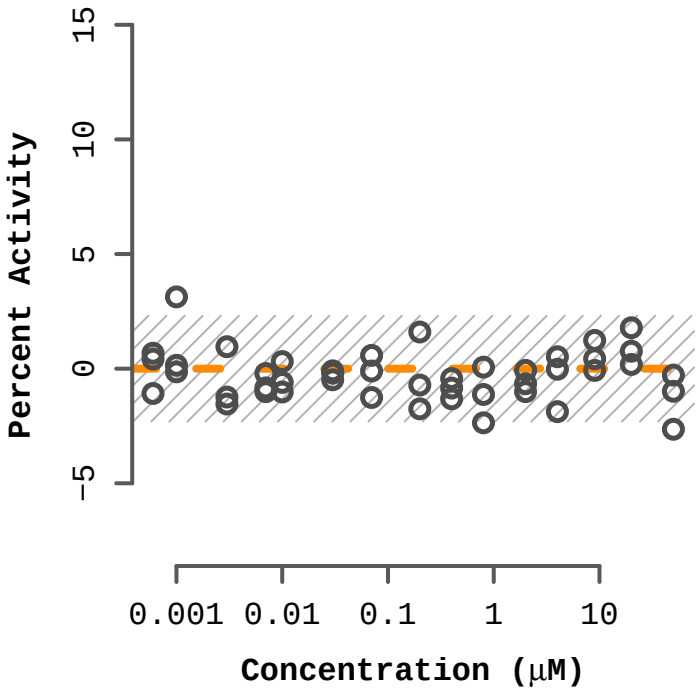
NAME: Amitriptyline hydrochloride
CHID: 33187 **CASRN:** 549-18-8
SPID(S): Tox21_201278
M4ID: 12480974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.78	NA	NA
PROB:	1	NA	NA
RMSE:	3.36	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 0.825 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

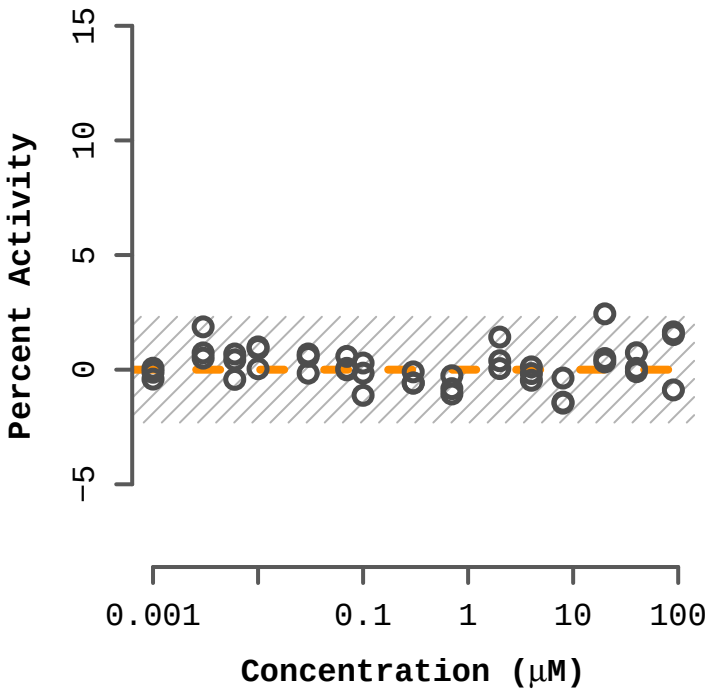
NAME: Amitriptyline hydrochloride
CHID: 33187 CASRN: 549-18-8
SPID(S): Tox21_113122_1
M4ID: 12482800

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.764 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

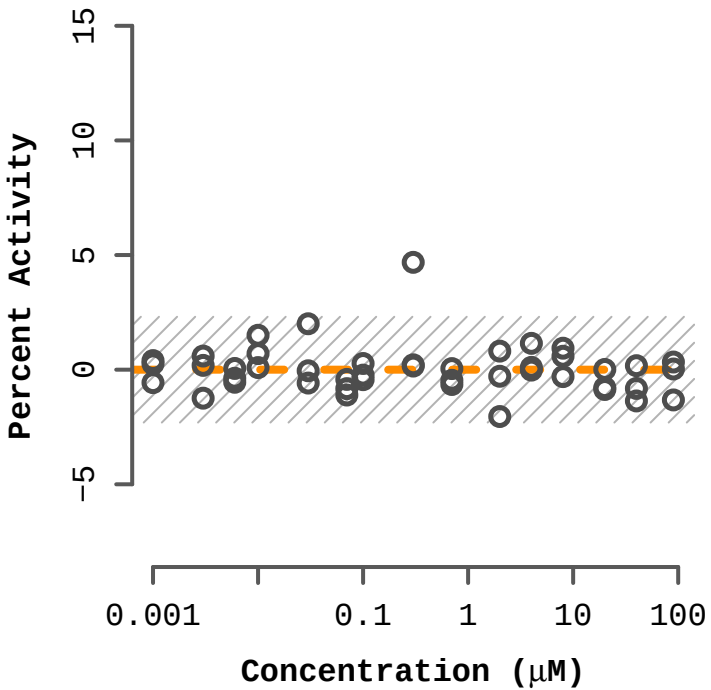
NAME: Benzylacetone
CHID: 33241 **CASRN:** 2550-26-7
SPID(S): Tox21_303341
M4ID: 12475792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

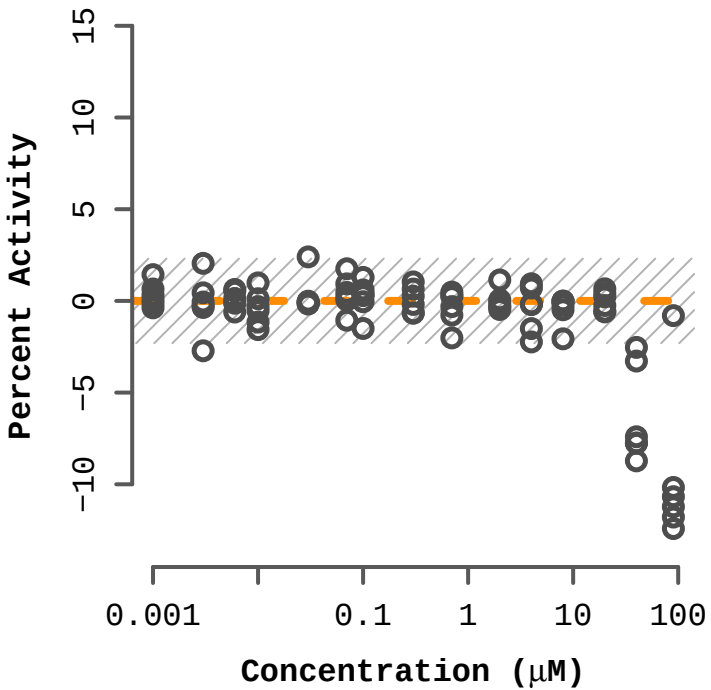
NAME: Benzylacetone
CHID: 33241 **CASRN:** 2550-26-7
SPID(S): Tox21_201240
M4ID: 12481012

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 0.702 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

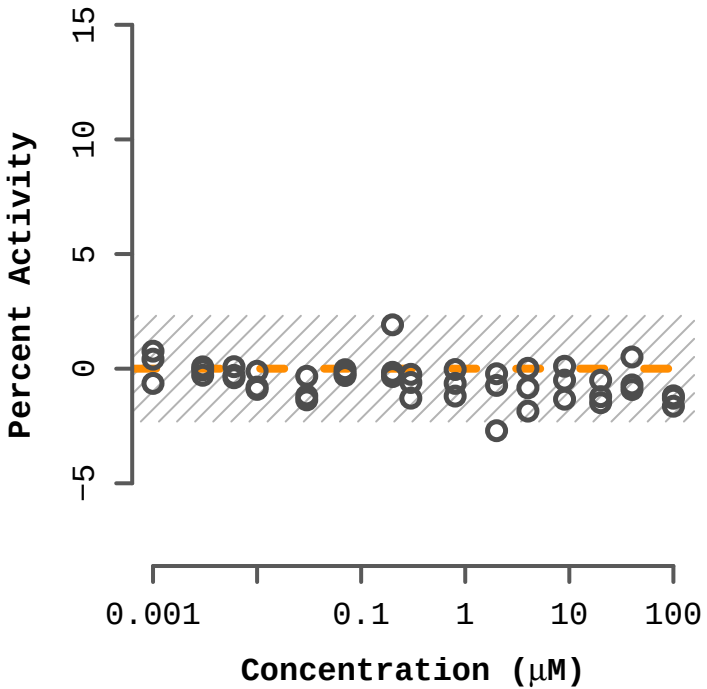
NAME: (E)-beta-Nitrostyrene
CHID: 33247 CASRN: 5153-67-3
SPID(S): Tox21_200772
M4ID: 12481480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	390.04	NA	NA
PROB:	1	NA	NA
RMSE:	3.28	NA	NA

MAX_MEAN: 0.391 MAX_MED: 0.331 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

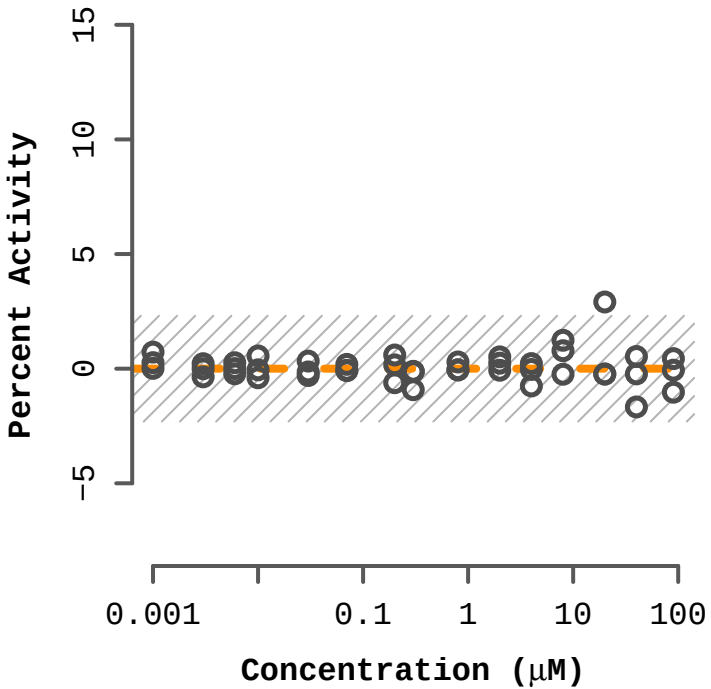
NAME: Boron trifluoride dihydrate
CHID: 33264 CASRN: 13319-75-0
SPID(S): Tox21_202490
M4ID: 12479762

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.472 **MAX_MED:** 0.416 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

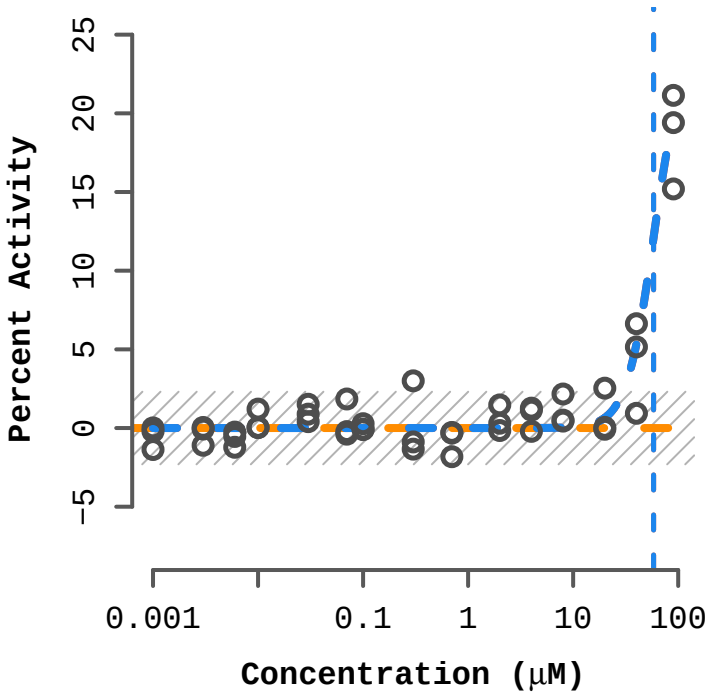
NAME: Butyl dipropasol solvent
CHID: 33276 CASRN: 29911-27-1
SPID(S): Tox21_200819
M4ID: 12481433

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	74.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.815 **MAX_MED:** 0.785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cadmium acetate dihydrate
CHID: 33281 CASRN: 5743-04-4
SPID(S): Tox21_200055
M4ID: 12482197

HILL MODEL (in red):

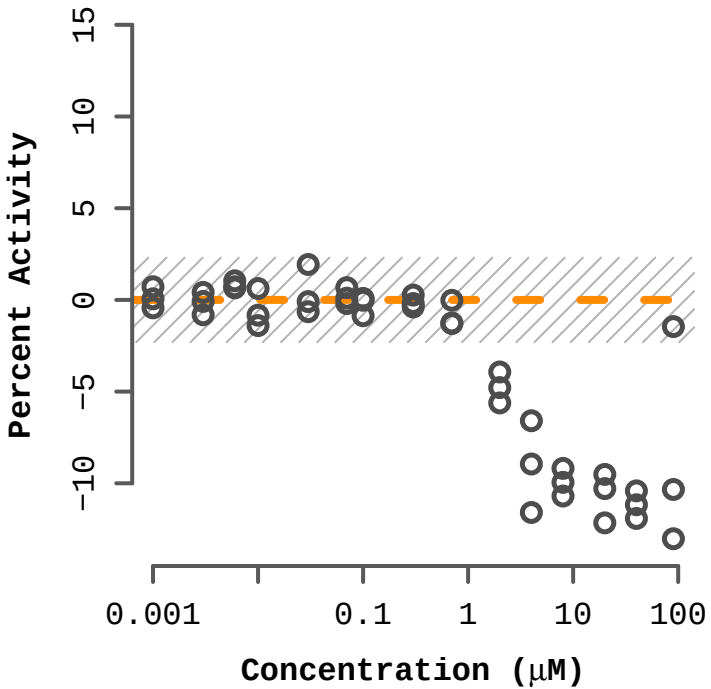
	tp	ga	gw
val:	24.3	1.77	3.35
sd:	8.49	0.145	1.67

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.3	1.77	3.36	3.35	1.96
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	218.11	157.46	161.46
PROB:	0	0.88	0.12
RMSE:	5.1	1.38	1.38

MAX_MEAN: 18.6 MAX_MED: 19.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

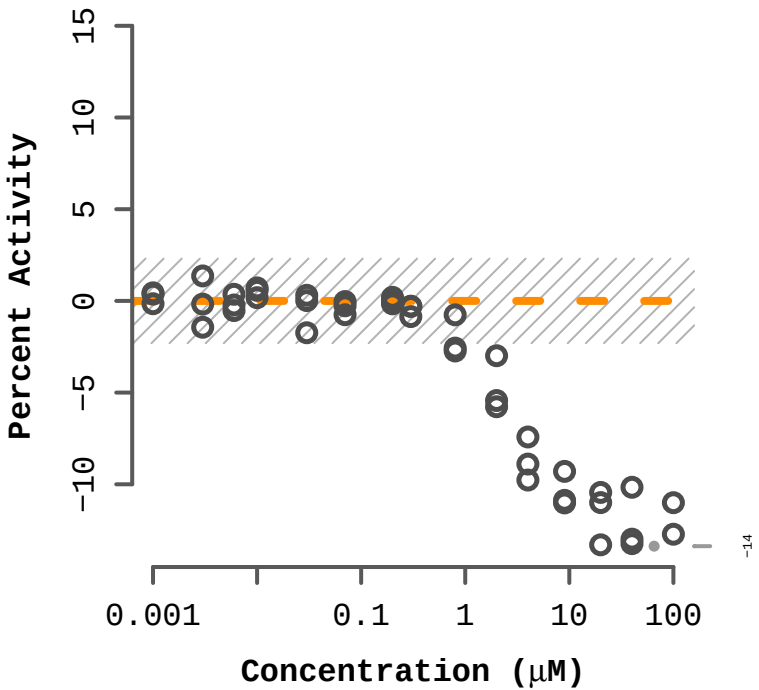
NAME: Cetylpyridinium bromide
CHID: 33307 **CASRN:** 140-72-7
SPID(S): Tox21_303438
M4ID: 12475702

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.82	NA	NA
PROB:	1	NA	NA
RMSE:	6.03	NA	NA

MAX_MEAN: 0.806 **MAX_MED:** 0.719 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

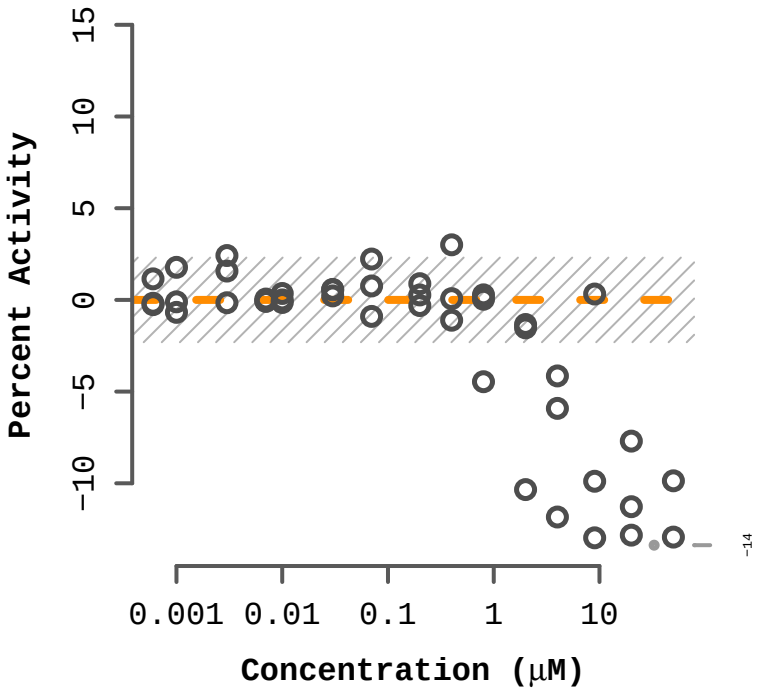
NAME: Cetylpyridinium bromide
CHID: 33307 CASRN: 140-72-7
SPID(S): Tox21_201549
M4ID: 12480703 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	299.22	NA	NA
PROB:	1	NA	NA
RMSE:	6.62	NA	NA

MAX_MEAN: 0.488 **MAX_MED:** 0.578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

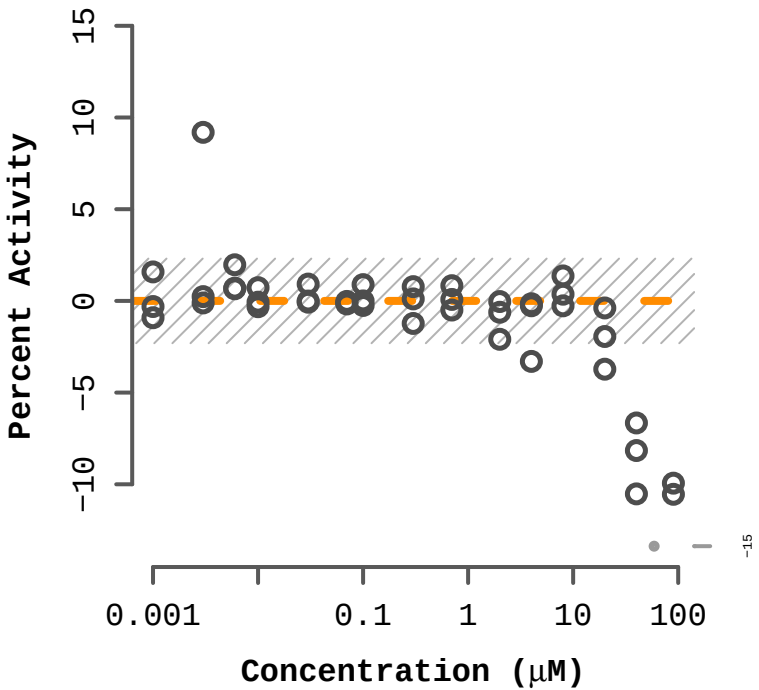
NAME: Cetylpyridinium bromide
CHID: 33307 **CASRN:** 140-72-7
SPID(S): Tox21_111061_1
M4ID: 12483927 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.62	NA	NA
PROB:	1	NA	NA
RMSE:	5.65	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

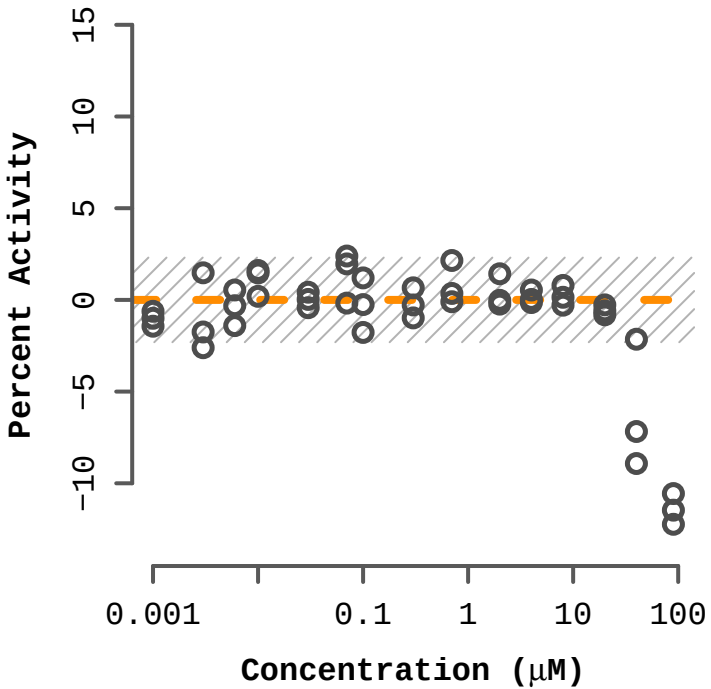
NAME: Chlorhexidine
CHID: 33314 **CASRN:** 55-56-1
SPID(S): Tox21_303445
M4ID: 12475695 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233	NA	NA
PROB:	1	NA	NA
RMSE:	4.2	NA	NA

MAX_MEAN: 3.11 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

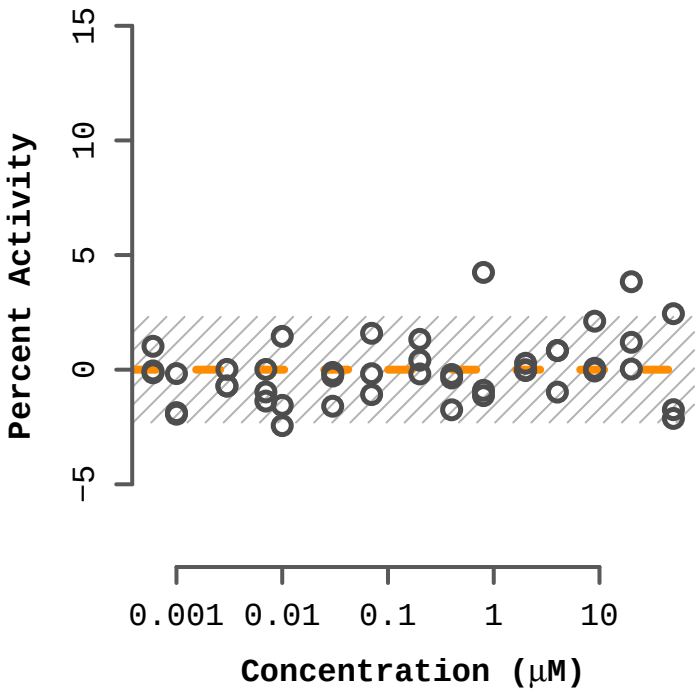
NAME: Chlorhexidine
CHID: 33314 **CASRN:** 55-56-1
SPID(S): Tox21_201404
M4ID: 12480848

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.58	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

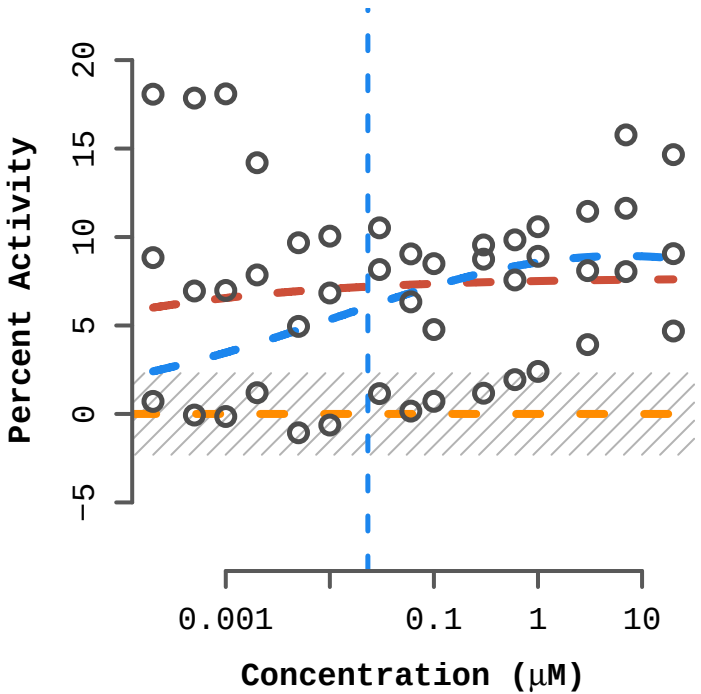
NAME: Chlorhexidine
CHID: 33314 **CASRN:** 55-56-1
SPID(S): Tox21_110325_1
M4ID: 12484454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorowax 500C
CHID: 33326 CASRN: NOCAS_33326
SPID(S): Tox21_202497
M4ID: 12479755

HILL MODEL (in red):

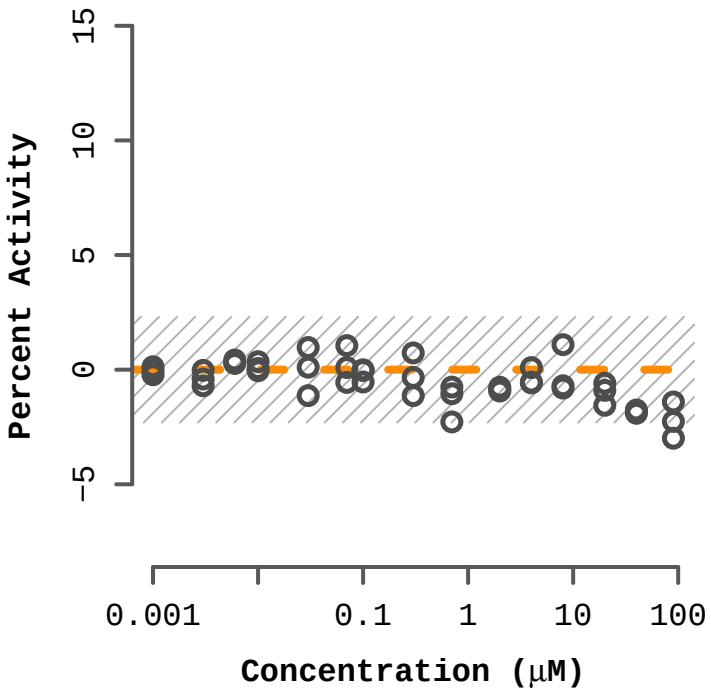
	tp	ga	gw
val:	7.67	−5.56	0.3
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.5	−1.63	0.3	3.26	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	331.92	286.67	294.65
PROB:	0	0.98	0.02
RMSE:	8.92	5.19	5.66

MAX_MEAN: 11.8 MAX_MED: 11.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

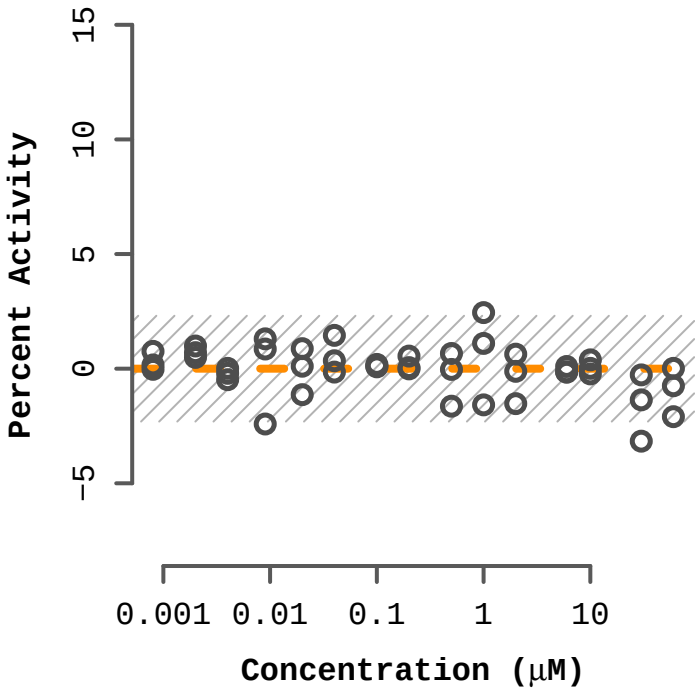
NAME: L-Cichoric acid
CHID: 33332 CASRN: 70831-56-0
SPID(S): Tox21_201055
M4ID: 12481197

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.341 MAX_MED: 0.329 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

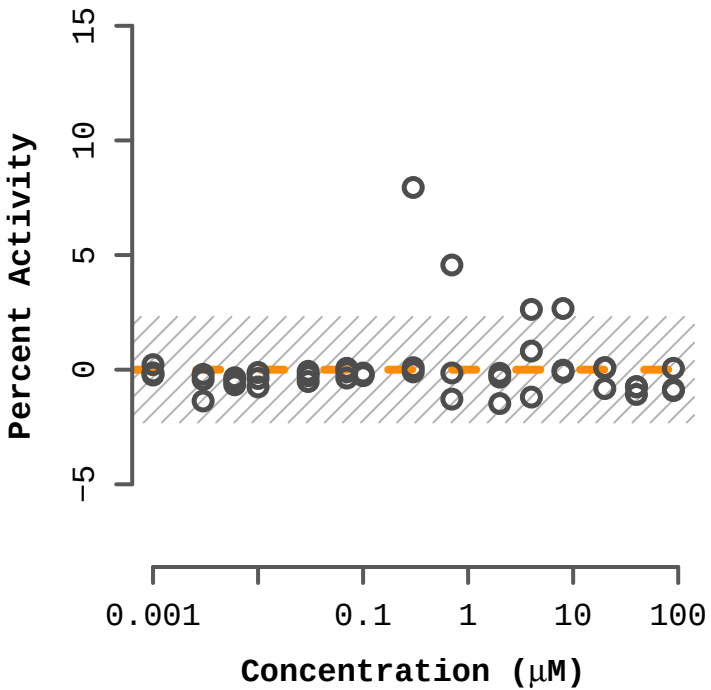
NAME: Cimicifugoside
CHID: 33334 **CASRN:** 27994-11-2
SPID(S): Tox21_200929
M4ID: 12481323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.727 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

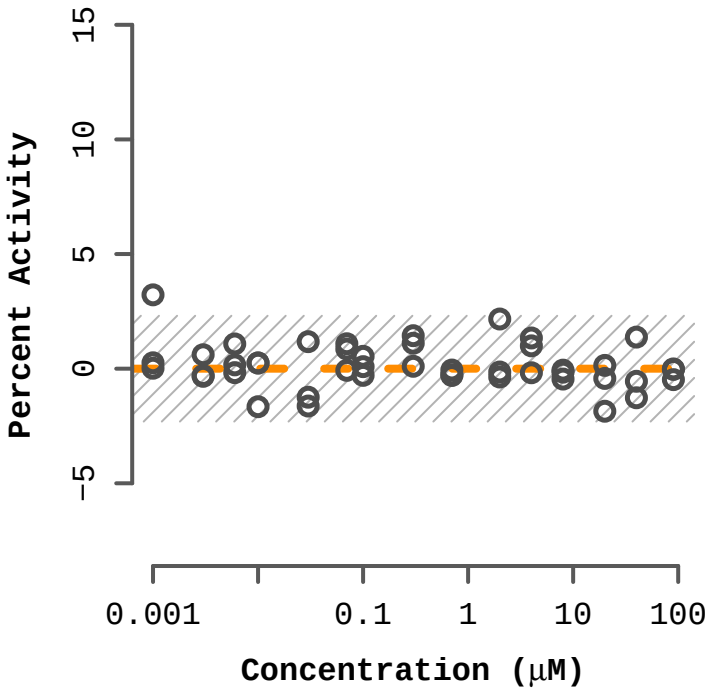
NAME: Cyclopentanol
CHID: 33371 CASRN: 96-41-3
SPID(S): Tox21_303563
M4ID: 12475582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 2.65 MAX_MED: 0.813 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

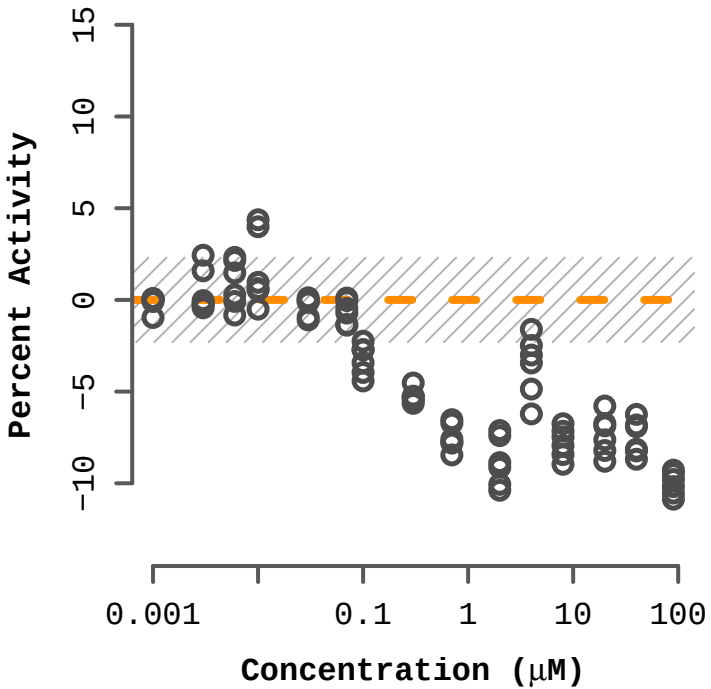
NAME: Cyclopentanol
CHID: 33371 **CASRN:** 96-41-3
SPID(S): Tox21_200109
M4ID: 12482143

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

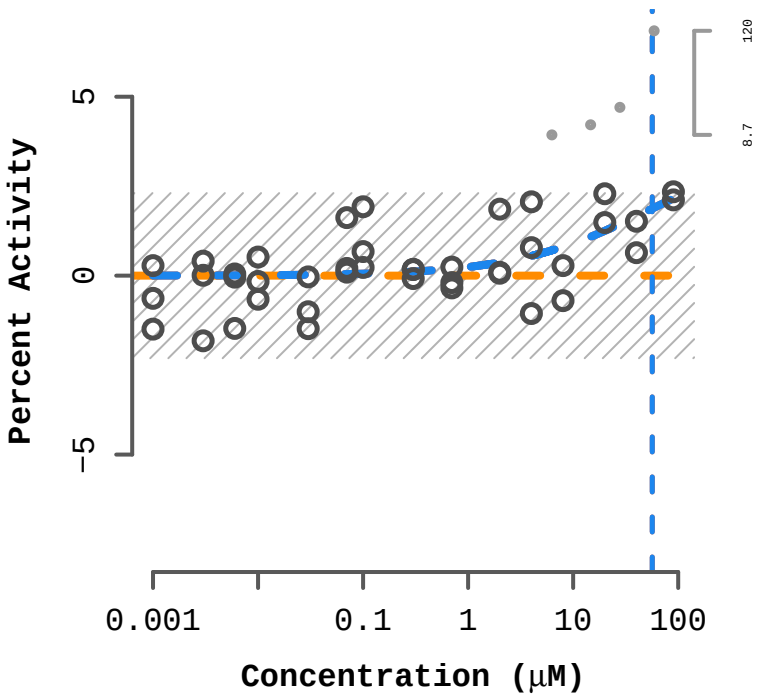
NAME: Daunomycin hydrochloride
CHID: 33382 CASRN: 23541-50-6
SPID(S): Tox21_201159
M4ID: 12481093

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	578.07	NA	NA
PROB:	1	NA	NA
RMSE:	5.63	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 0.875 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium deoxycholate
CHID: 33389 CASRN: 302-95-4
SPID(S): Tox21_200896
M4ID: 12481356 BRK

HILL MODEL (in red):

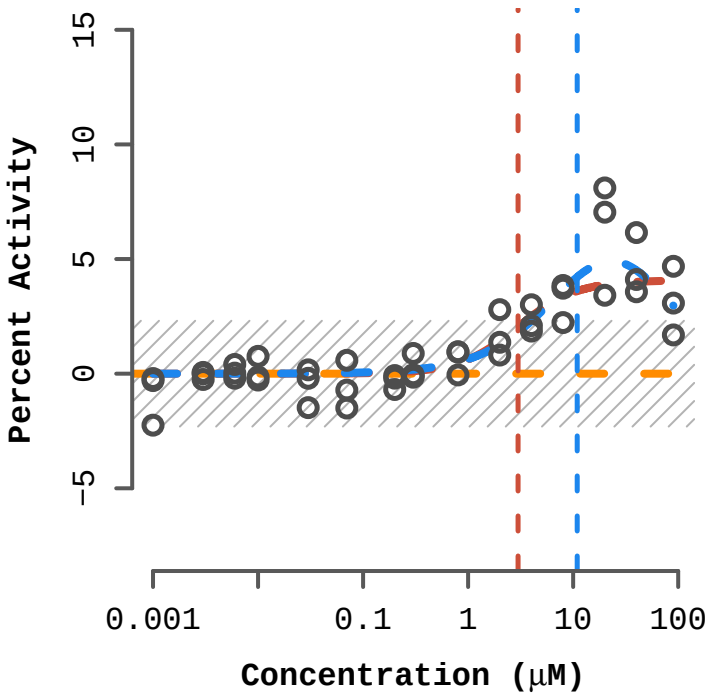
	tp	ga	gw
val:	3.75	1.75	0.663
sd:	8.28	2.95	0.755

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.75	1.75	0.663	3.68	3.72
sd:	8.28	2.95	0.755	835	1880

	CNST	HILL	GNLS
AIC:	241.63	233.54	237.54
PROB:	0.02	0.87	0.12
RMSE:	18.92	18.5	18.5

MAX_MEAN: 41.2 **MAX_MED:** 2.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Desmethoxyyangonin
CHID: 33390 CASRN: 15345-89-8
SPID(S): Tox21_200296
M4ID: 12481956

HILL MODEL (in red):

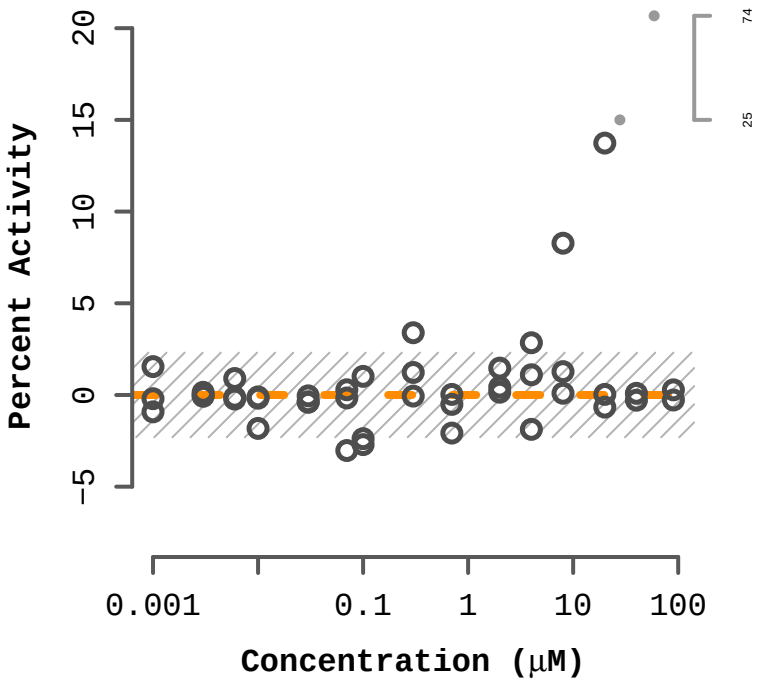
	tp	ga	gw
val:	4.07	0.475	1.57
sd:	0.406	0.112	0.445

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.72	1.04	1.11	1.71	1.21
sd:	20.2	1.11	0.37	1.14	1.08

	CNST	HILL	GNLS
AIC:	209.22	134.56	134.98
PROB:	0	0.55	0.45
RMSE:	2.6	1.14	1

MAX_MEAN: 6.19 MAX_MED: 7.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

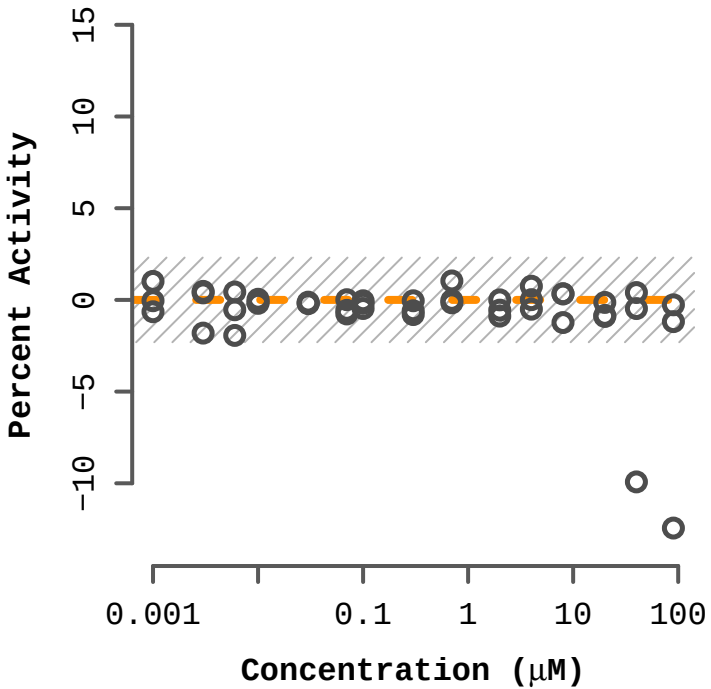
NAME: Dibenzoyl−L−tartaric acid
CHID: 33401 **CASRN:** 2743−38−6
SPID(S): Tox21_201220
M4ID: 12481032 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.48	NA	NA
PROB:	1	NA	NA
RMSE:	12	NA	NA

MAX_MEAN: 24.8 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

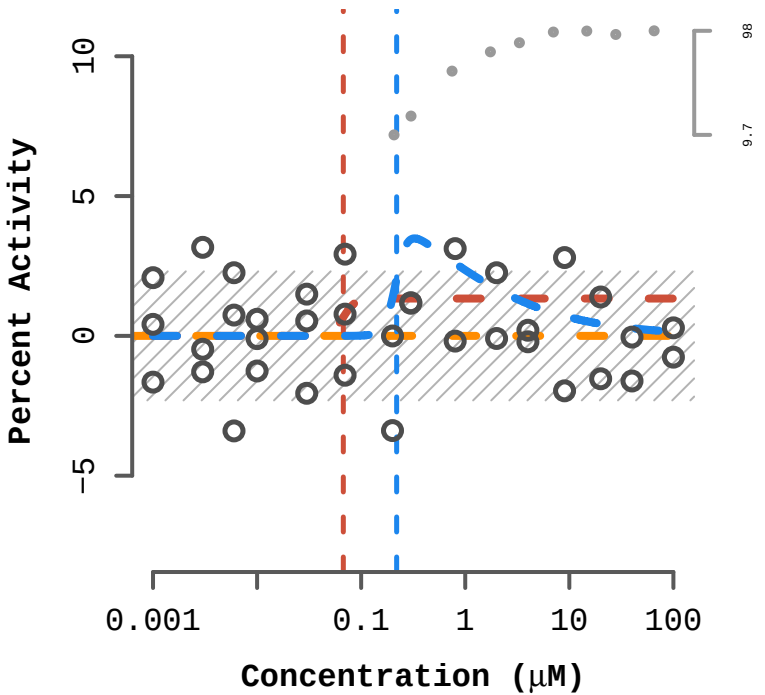
NAME: Dibenzyl phosphate
CHID: 33402 **CASRN:** 1623-08-1
SPID(S): Tox21_201050
M4ID: 12481202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.81	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 0.284 **MAX_MED:** 0.384 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dihydrokavain
CHID: 33433 **CASRN:** 587-63-3
SPID(S): Tox21_201033
M4ID: 12481219 **BRK**

HILL MODEL (in red):

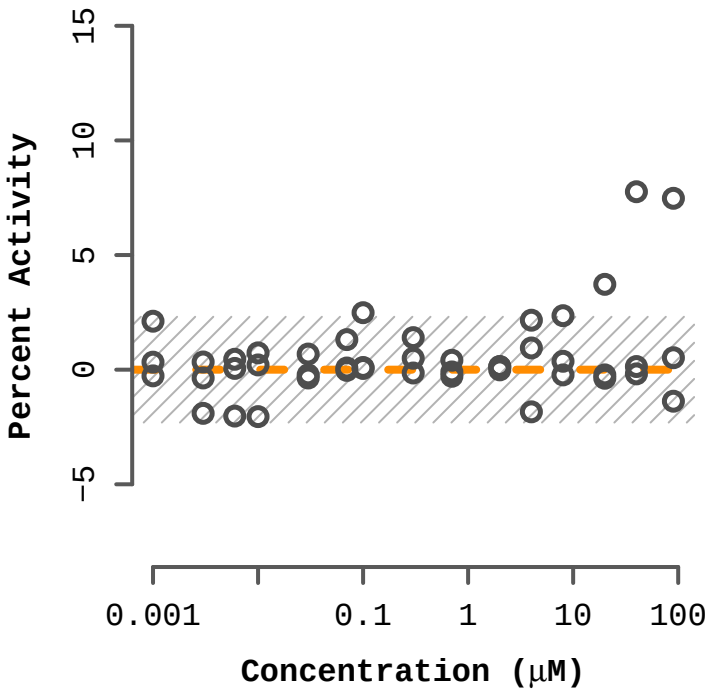
	tp	ga	gw
val:	1.33	−1.17	7.79
sd:	1.34	1.14	470

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.85	−0.659	7.99	−0.409	0.687
sd:	86.1	0.669	77	13.9	2.99

	CNST	HILL	GNLS
AIC:	405.72	410.49	413.84
PROB:	0.9	0.08	0.02
RMSE:	35.37	34.84	34.98

MAX_MEAN: 32.5 **MAX_MED:** 3.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

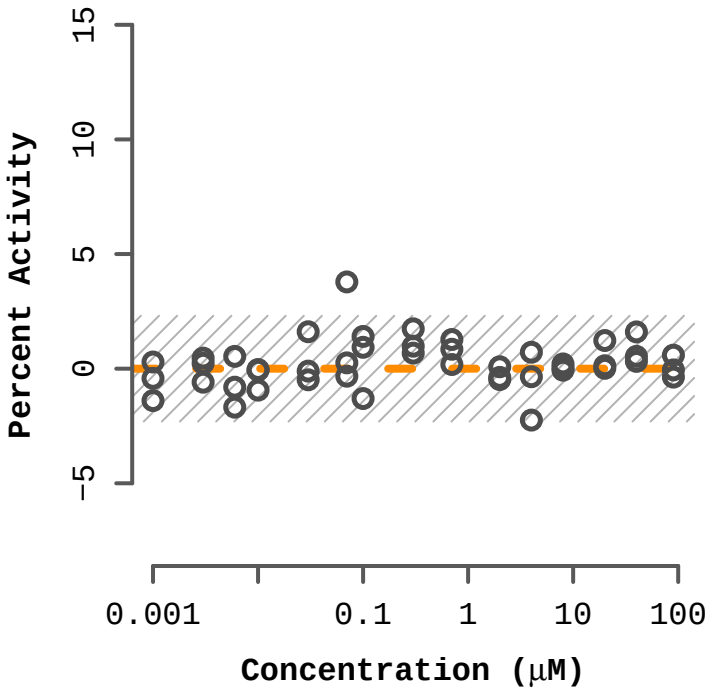
NAME: Dimethyldipropylenetriamine
CHID: 33445 **CASRN:** 10563-29-8
SPID(S): Tox21_201176
M4ID: 12481076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 2.57 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

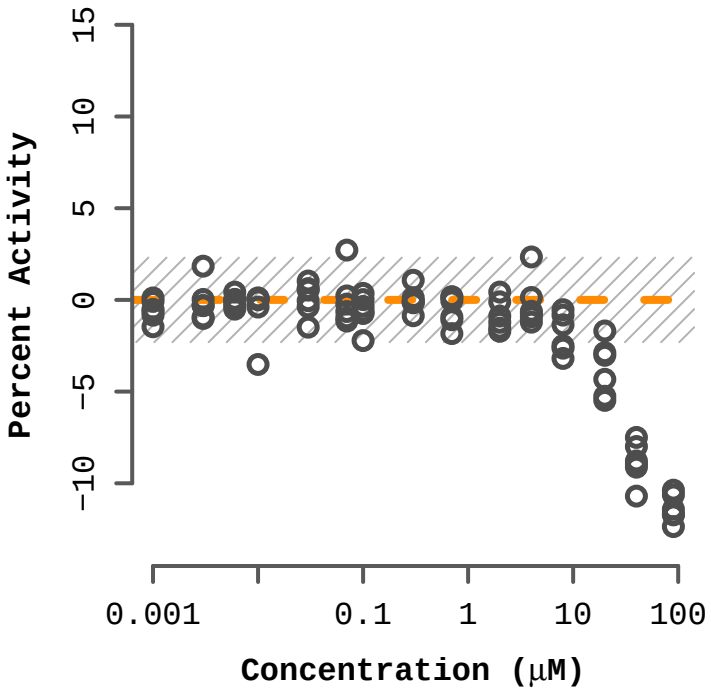
NAME: Dimethylisopropylamine
CHID: 33447 **CASRN:** 996-35-0
SPID(S): Tox21_200792
M4ID: 12481460

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

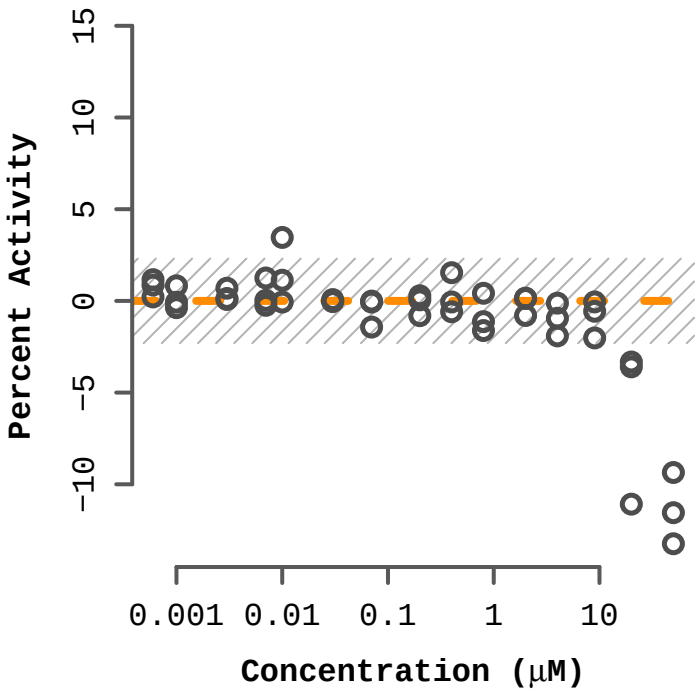
NAME: Domiphen bromide
CHID: 33468 **CASRN:** 538-71-6
SPID(S): Tox21_200219
M4ID: 12482033

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	466.58	NA	NA
PROB:	1	NA	NA
RMSE:	4	NA	NA

MAX_MEAN: 0.0459 **MAX_MED:** 0.246 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

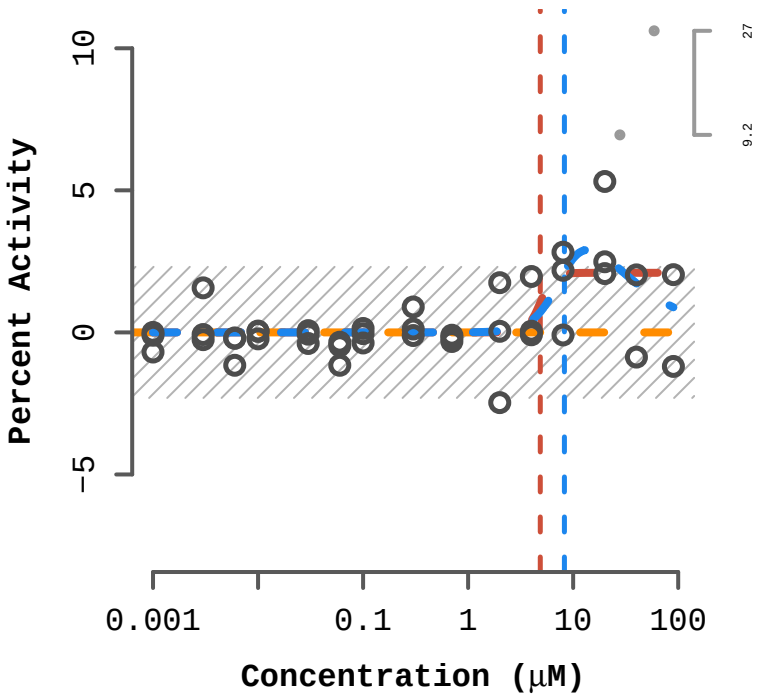
NAME: Domiphen bromide
CHID: 33468 **CASRN:** 538-71-6
SPID(S): Tox21_111054_1
M4ID: 12483929

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.07	NA	NA
PROB:	1	NA	NA
RMSE:	3.59	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Echinacoside
CHID: 33469 CASRN: 82854-37-3
SPID(S): Tox21_200945
M4ID: 12481307 BRK

HILL MODEL (in red):

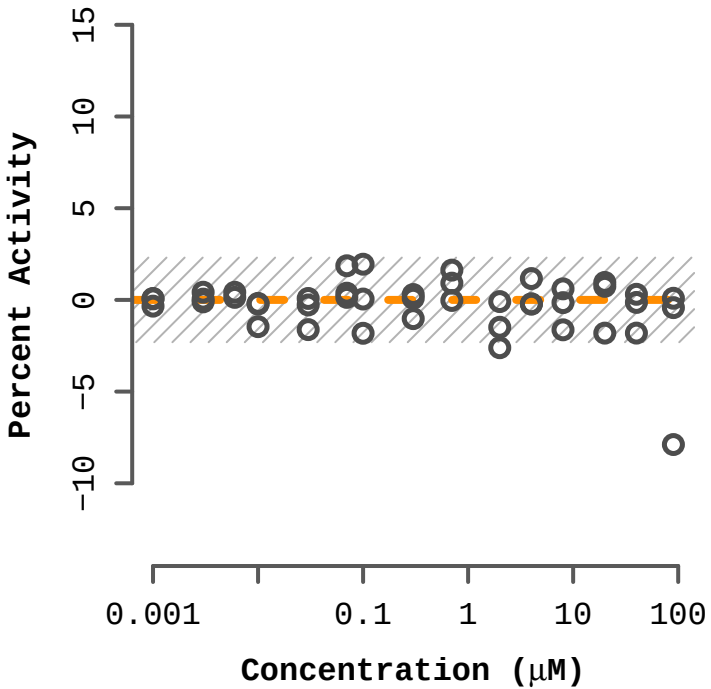
	tp	ga	gw
val:	2.1	0.687	7.15
sd:	0.387	0.228	18.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.62	0.917	3.39	1.17	1.03
sd:	34.7	0.405	2.56	3.99	2.49

	CNST	HILL	GNLS
AIC:	187.97	174.75	176.51
PROB:	0	0.71	0.29
RMSE:	4.4	3.95	4.1

MAX_MEAN: 9.12 **MAX_MED:** 2.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

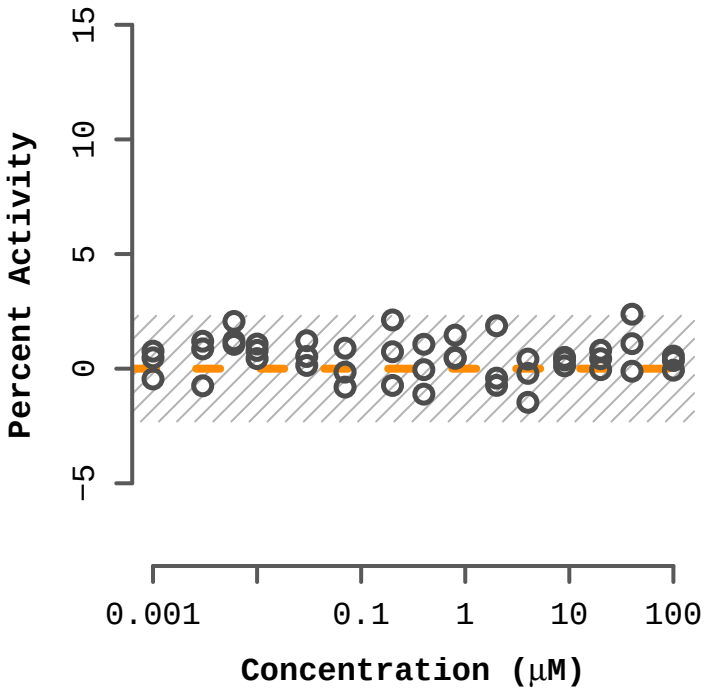
NAME: Ethyl−2−methyl acetoacetate
CHID: 33493 **CASRN:** 609−14−3
SPID(S): Tox21_201138
M4ID: 12481114

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 0.837 **MAX_MED:** 0.915 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

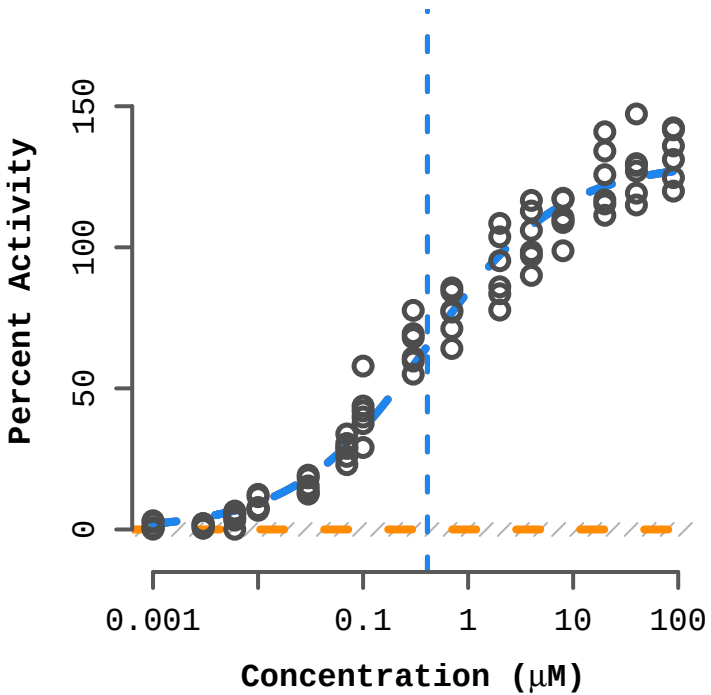
NAME: Fluorosulfonic acid
CHID: 33511 **CASRN:** 7789-21-1
SPID(S): Tox21_202147
M4ID: 12480105

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluoxymestrone
CHID: 33512 CASRN: 76-43-7
SPID(S): Tox21_200854
M4ID: 12481398

HILL MODEL (in red):

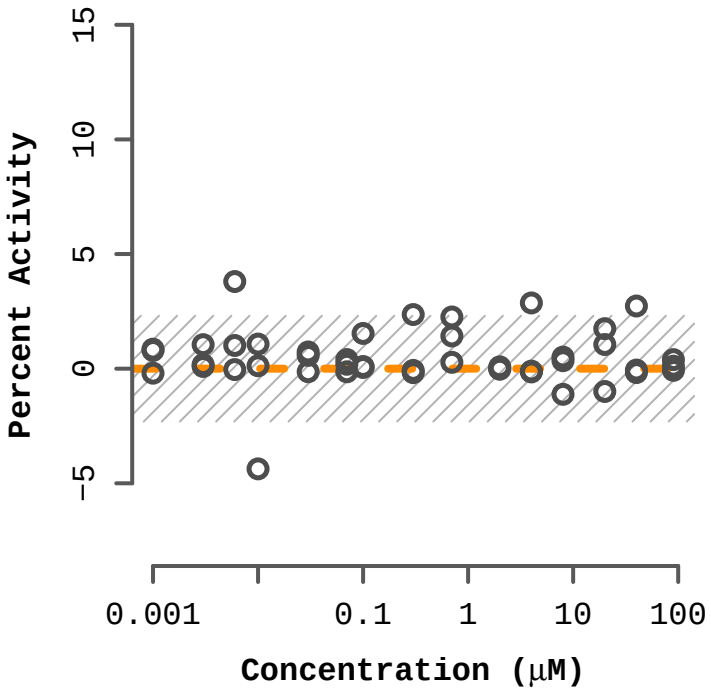
	tp	ga	gw
val:	130	-0.388	0.688
sd:	3.06	0.0582	0.0388

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	130	-0.388	0.688	3.95	17.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	1054.85	634.76	638.76
PROB:	0	0.88	0.12
RMSE:	79.39	8.04	8.04

MAX_MEAN: 133 MAX_MED: 134 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

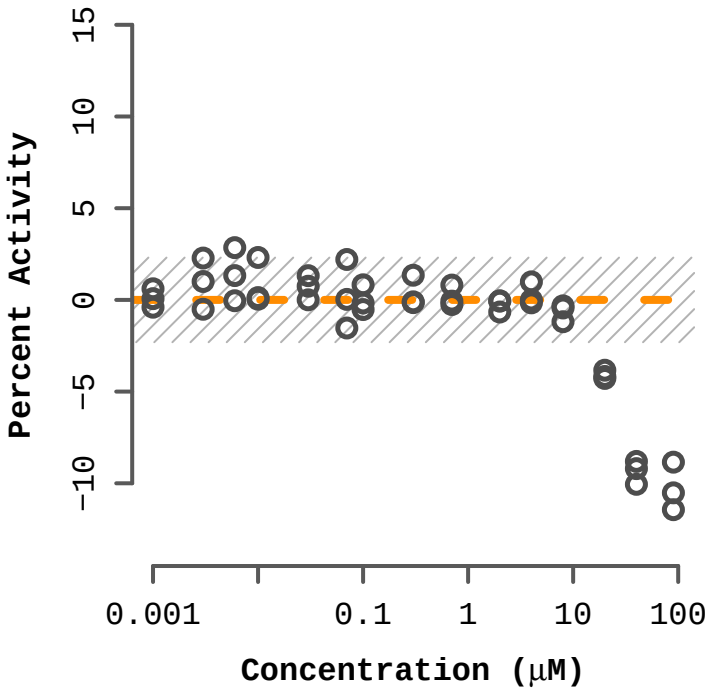
NAME: Fumaryl chloride
CHID: 33519 **CASRN:** 627-63-4
SPID(S): Tox21_200639
M4ID: 12481613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

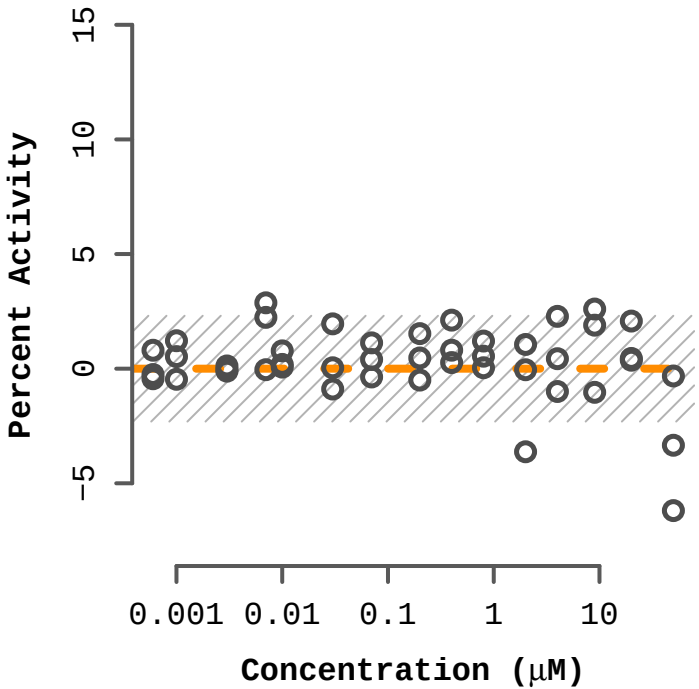
NAME: Guggulsterone E
CHID: 33538 CASRN: 39025-24-6
SPID(S): Tox21_200314
M4ID: 12481938

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.26	NA	NA
PROB:	1	NA	NA
RMSE:	3.86	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

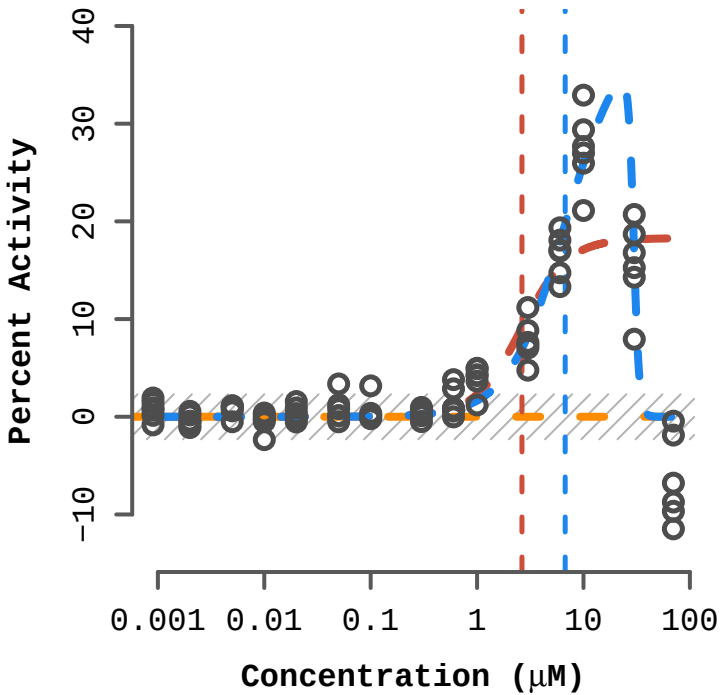
NAME: Guggulsterone Z
CHID: 33539 **CASRN:** 39025-23-5
SPID(S): Tox21_202518
M4ID: 12479734

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydroxyflutamide
CHID: 33562 **CASRN:** 52806-53-8
SPID(S): Tox21_303659
M4ID: 12475489

HILL MODEL (in red):

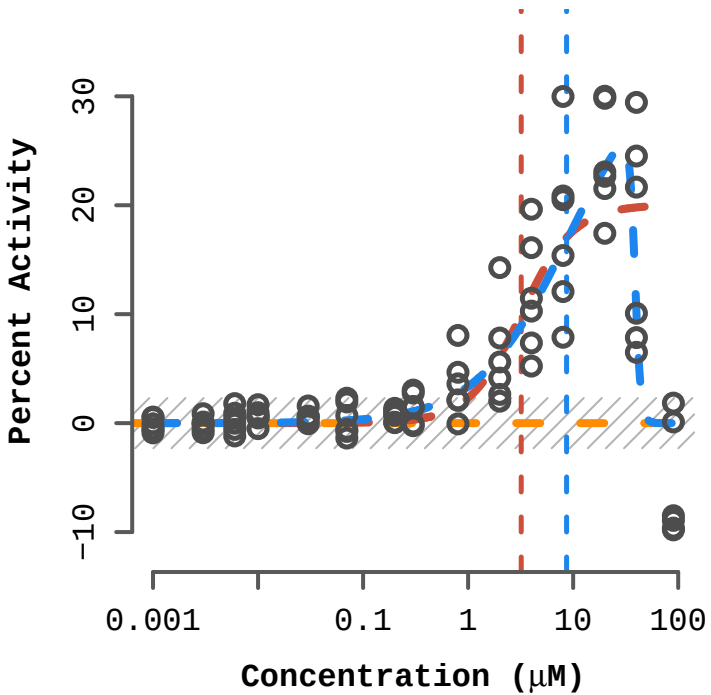
	tp	ga	gw
val:	18.3	0.422	2.01
sd:	1.27	0.0777	0.447

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	39.5	0.828	1.64	1.47	17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	642.5	538.01	417.57
PROB:	0	0	1
RMSE:	9.84	7.3	2.79

MAX_MEAN: 27.3 **MAX_MED:** 27.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydroxyflutamide
CHID: 33562 CASRN: 52806-53-8
SPID(S): Tox21_201204
M4ID: 12481048

HILL MODEL (in red):

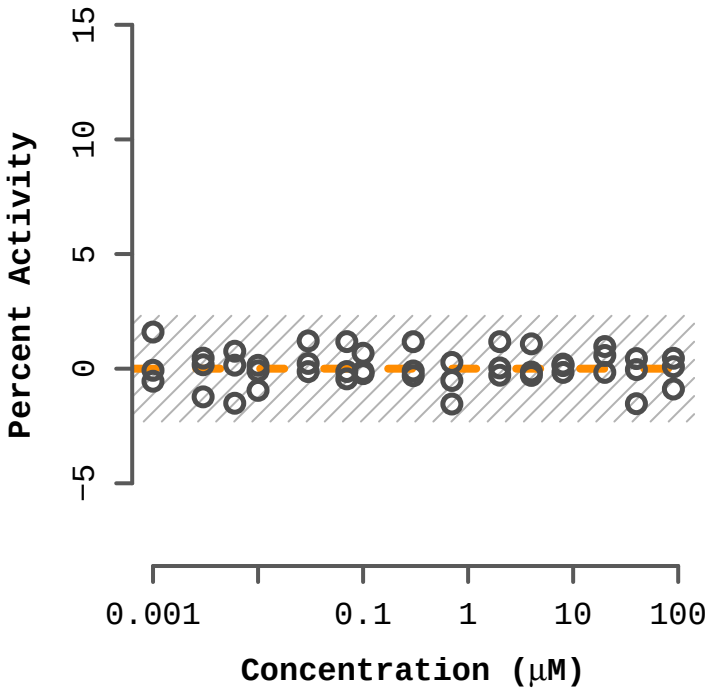
	tp	ga	gw
val:	20	0.505	1.75
sd:	2.3	0.0929	0.501

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	33.5	0.938	1.01	1.59	15.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	656.64	577.11	505.49
PROB:	0	0	1
RMSE:	10.4	7.88	4.53

MAX_MEAN: 24.1 MAX_MED: 22.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

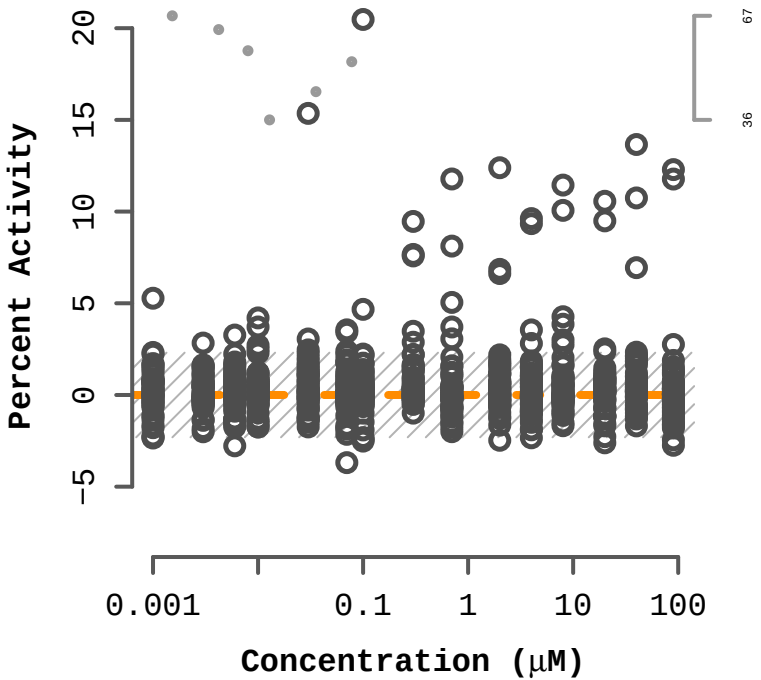
NAME: Hydroxyvalerenic acid
CHID: 33564 **CASRN:** 1619-16-5
SPID(S): Tox21_200020
M4ID: 12482232

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.461 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

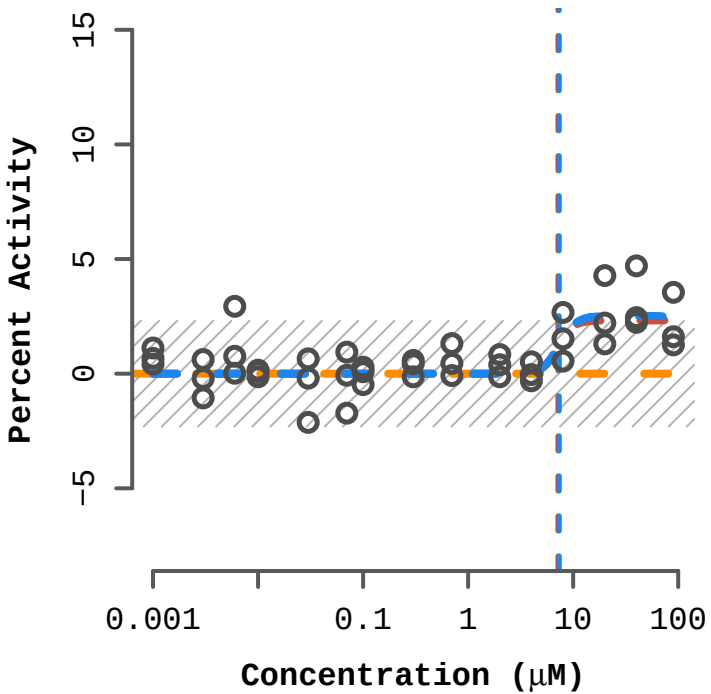
NAME: Indium trichloride
CHID: 33566 **CASRN:** 10025-82-8
SPID(S): Tox21_400067
M4ID: 12475070 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2737.93	NA	NA
PROB:	1	NA	NA
RMSE:	5.43	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 0.329 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Kavain
CHID: 33595 CASRN: 500-64-1
SPID(S): Tox21_200907
M4ID: 12481345

HILL MODEL (in red):

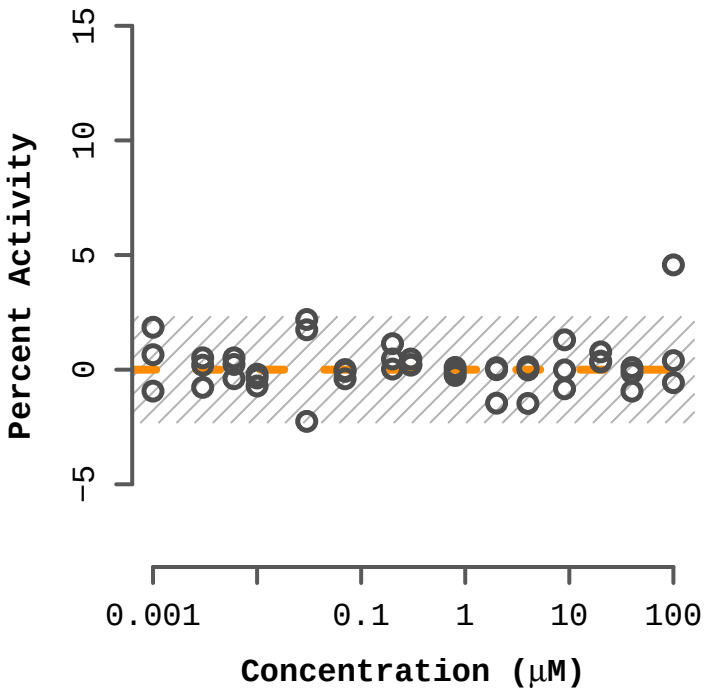
	tp	ga	gw
val:	2.32	0.855	6.15
sd:	0.335	0.102	10.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.52	0.868	5.49	1.98	16.6
sd:	0.403	0.0807	8.7	0.0349	24.8

	CNST	HILL	GNLS
AIC:	164.38	128.56	131.5
PROB:	0	0.81	0.19
RMSE:	1.56	0.96	0.95

MAX_MEAN: 3.13 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

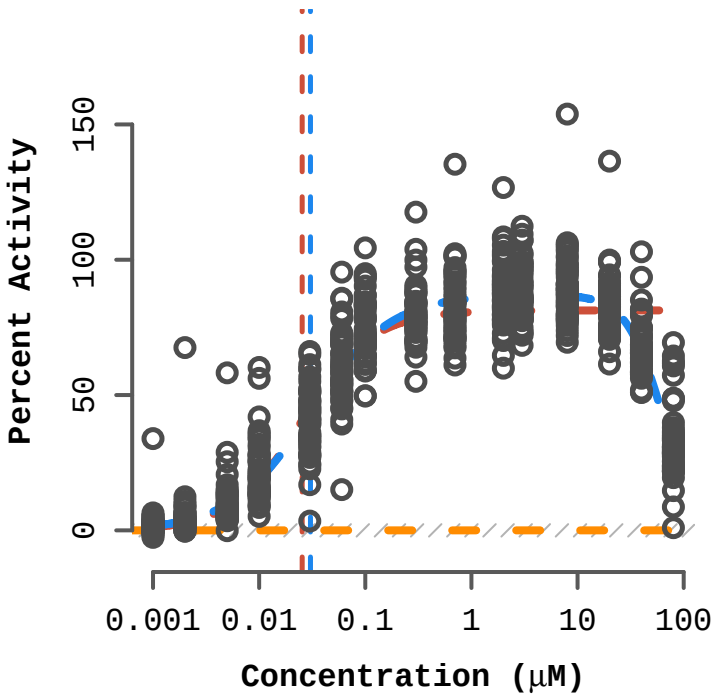
NAME: Methyl cyanoacetate
CHID: 33649 **CASRN:** 105-34-0
SPID(S): Tox21_200938
M4ID: 12481314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17-Methyltestosterone
CHID: 33664 CASRN: 58-18-4
SPID(S): Tox21_400058
M4ID: 12475079

HILL MODEL (in red):

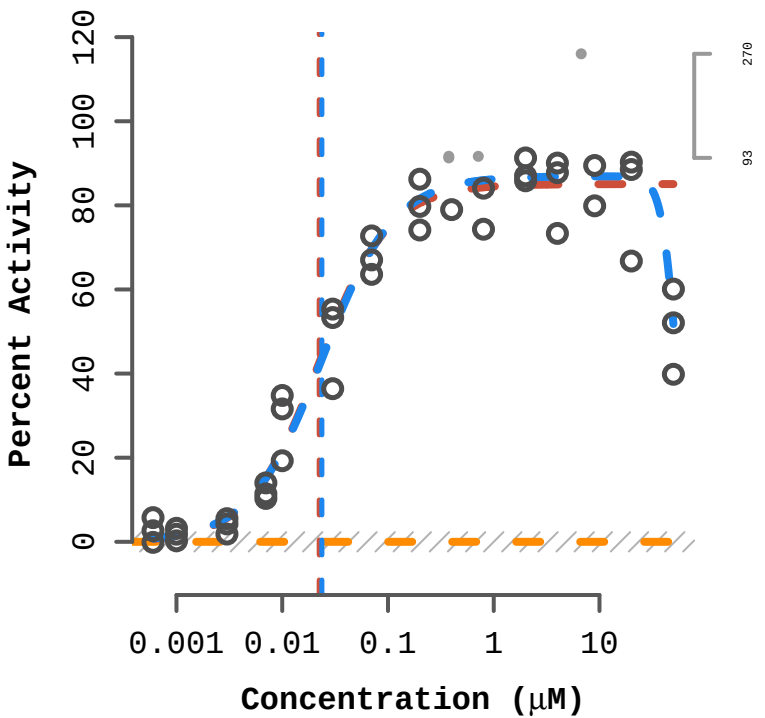
	tp	ga	gw
val:	81.3	-1.59	1.31
sd:	0.752	0.0212	0.0603

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	87.2	-1.52	1.16	1.79	2.56
sd:	0.752	0.018	0.0431	0.00994	0.145

	CNST	HILL	GNLS
AIC:	8168.11	5987.25	5450.2
PROB:	0	0	1
RMSE:	64.79	17.77	11.63

MAX_MEAN: 89.9 MAX_MED: 88.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17-Methyltestosterone
CHID: 33664 CASRN: 58-18-4
SPID(S): Tox21_113162_1
M4ID: 12482785 BRK

HILL MODEL (in red):

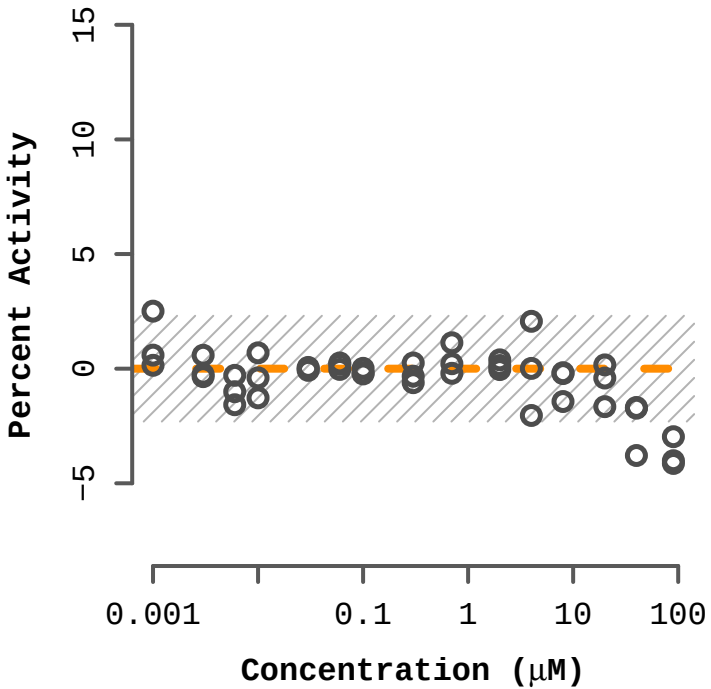
	tp	ga	gw
val:	85.1	-1.65	1.31
sd:	2.17	0.0568	0.155

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	86.9	-1.62	1.28	1.73	6.19
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	518.28	361.9	339.08
PROB:	0	0	1
RMSE:	74.66	30.15	28.55

MAX_MEAN: 147 MAX_MED: 92.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

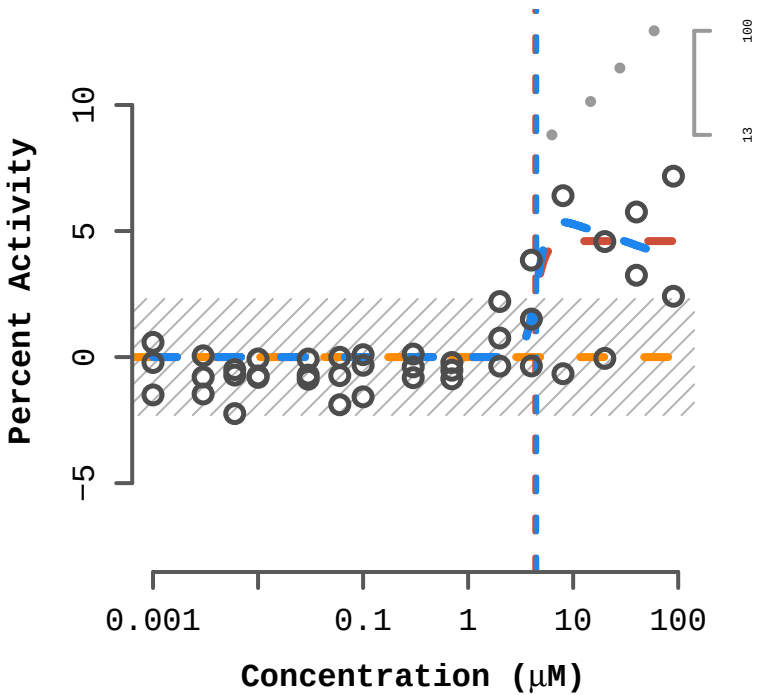
NAME: Methyl thioglycolate
CHID: 33673 CASRN: 2365-48-2
SPID(S): Tox21_201130
M4ID: 12481122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.592 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methysticin
CHID: 33674 **CASRN:** 495-85-2
SPID(S): Tox21_200901
M4ID: 12481351 **BRK**

HILL MODEL (in red):

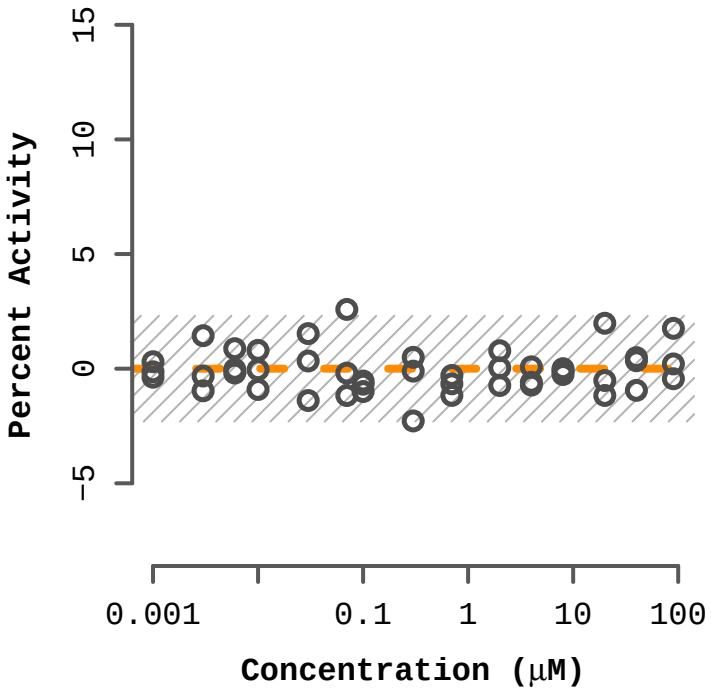
	tp	ga	gw
val:	4.6	0.635	8
sd:	0.889	0.0801	17.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.39	0.653	8	1.77	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	288.83	272.67	276.54
PROB:	0	0.87	0.13
RMSE:	19.97	18.75	18.83

MAX_MEAN: 37.8 **MAX_MED:** 7.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

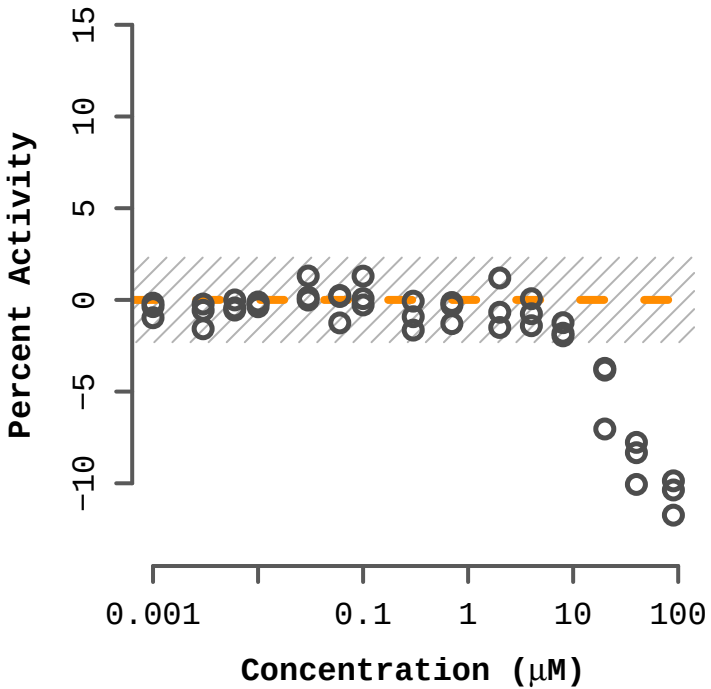
NAME: N,N,N',N`−Tetramethylhexanediamine
CHID: 33701 CASRN: 111−18−2
SPID(S): Tox21_200982
M4ID: 12481270

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.51 **MAX_MED:** 0.348 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

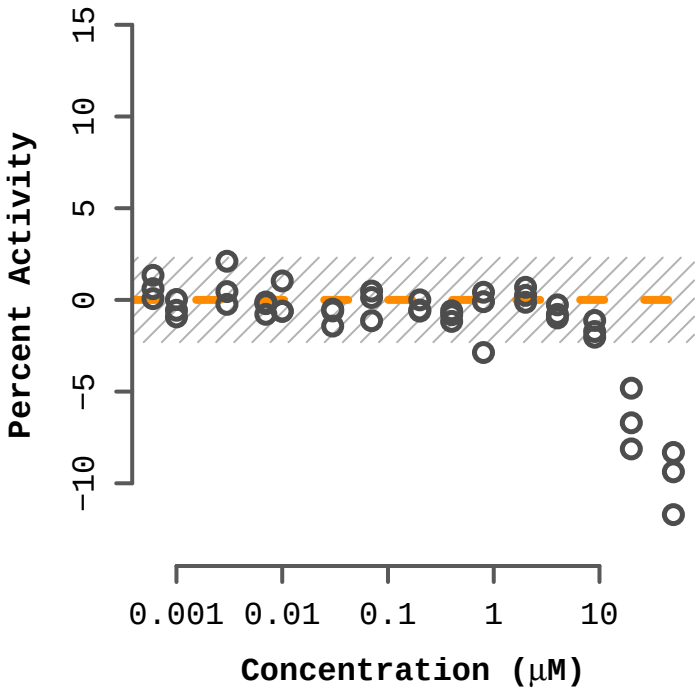
NAME: Nelfinavir mesylate
CHID: 33736 **CASRN:** 159989-65-8
SPID(S): Tox21_200921
M4ID: 12481331

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.24	NA	NA
PROB:	1	NA	NA
RMSE:	3.89	NA	NA

MAX_MEAN: 0.482 **MAX_MED:** 0.186 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

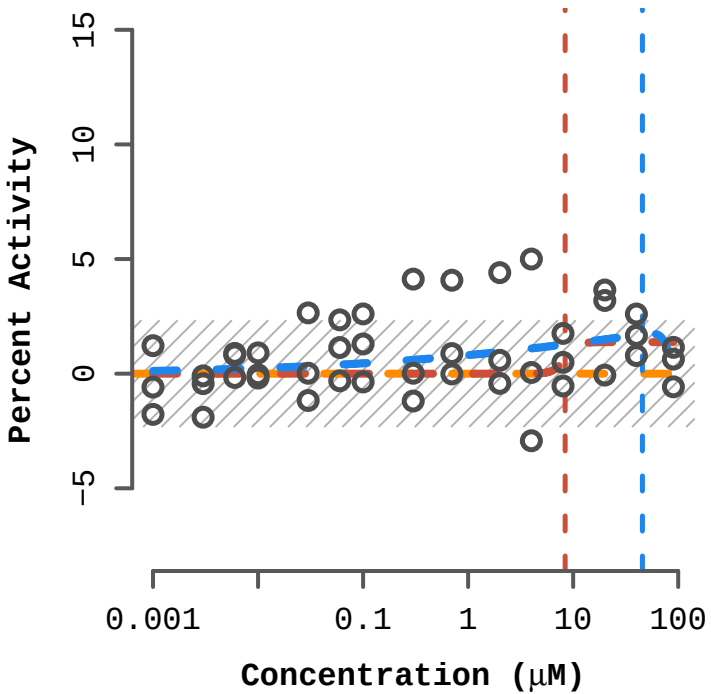
NAME: Nelfinavir mesylate
CHID: 33736 **CASRN:** 159989-65-8
SPID(S): Tox21_111021_1
M4ID: 12483943

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.34	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 0.774 **MAX_MED:** 0.613 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Isopropylacrylamide
CHID: 33754 **CASRN:** 2210-25-5
SPID(S): Tox21_200738
M4ID: 12481514

HILL MODEL (in red):

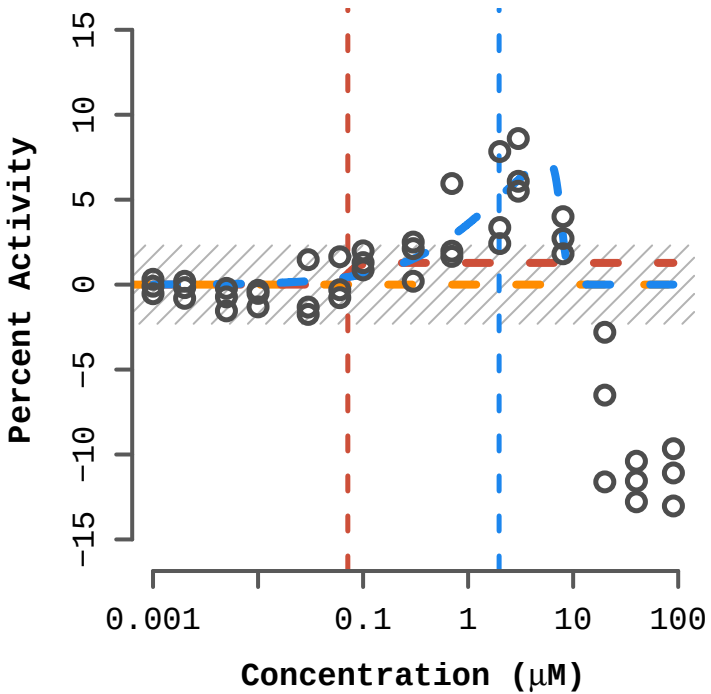
	tp	ga	gw
val:	1.38	0.924	8
sd:	0.525	0.149	27.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.42	1.66	0.307	1.91	11.8
sd:	11.9	8.85	0.333	1.19	312

	CNST	HILL	GNLS
AIC:	186.01	184.97	184.78
PROB:	0.22	0.37	0.41
RMSE:	1.91	1.79	1.64

MAX_MEAN: 2.26 **MAX_MED:** 3.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nitazoxanide
CHID: 33757 **CASRN:** 55981-09-4
SPID(S): Tox21_201226
M4ID: 12481026

HILL MODEL (in red):

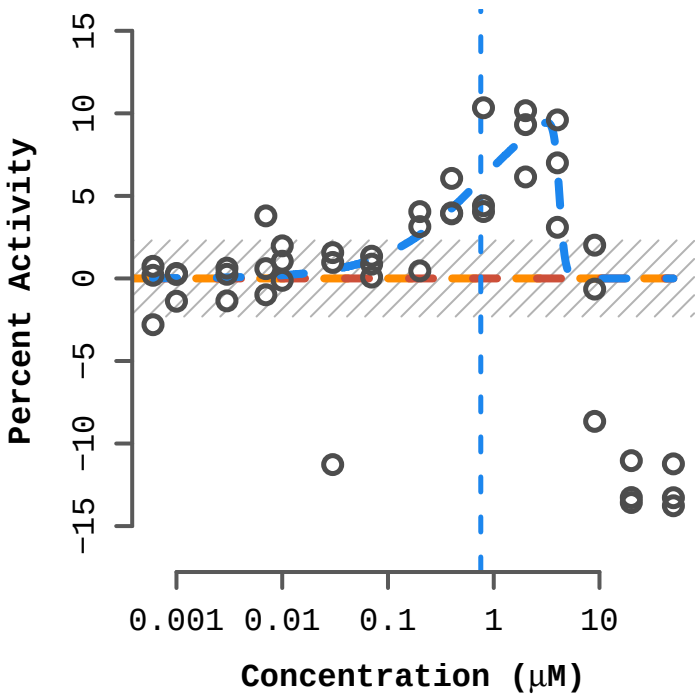
	tp	ga	gw
val:	1.28	−1.15	8
sd:	0.975	0.387	28.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.3	0.295	0.933	0.882	12.7
sd:	12.9	1.23	0.611	0.17	100

	CNST	HILL	GNLS
AIC:	276.75	281.23	264.32
PROB:	0	0	1
RMSE:	5.37	5.61	4.8

MAX_MEAN: 6.73 **MAX_MED:** 6.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nitazoxanide
CHID: 33757 CASRN: 55981-09-4
SPID(S): Tox21_111018_1
M4ID: 12483945

HILL MODEL (in red):

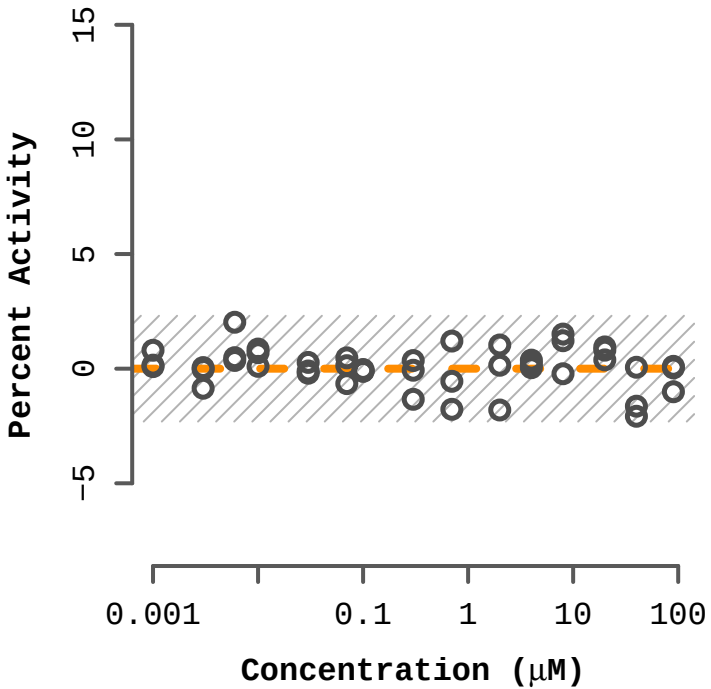
	tp	ga	gw
val:	2.53e-09	2.17	0.713
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12	−0.122	0.949	0.622	16.4
sd:	12.2	1.09	0.911	0.346	291

	CNST	HILL	GNLS
AIC:	296.42	302.42	276.57
PROB:	0	0	1
RMSE:	6.39	6.39	5.36

MAX_MEAN: 8.55 **MAX_MED:** 9.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

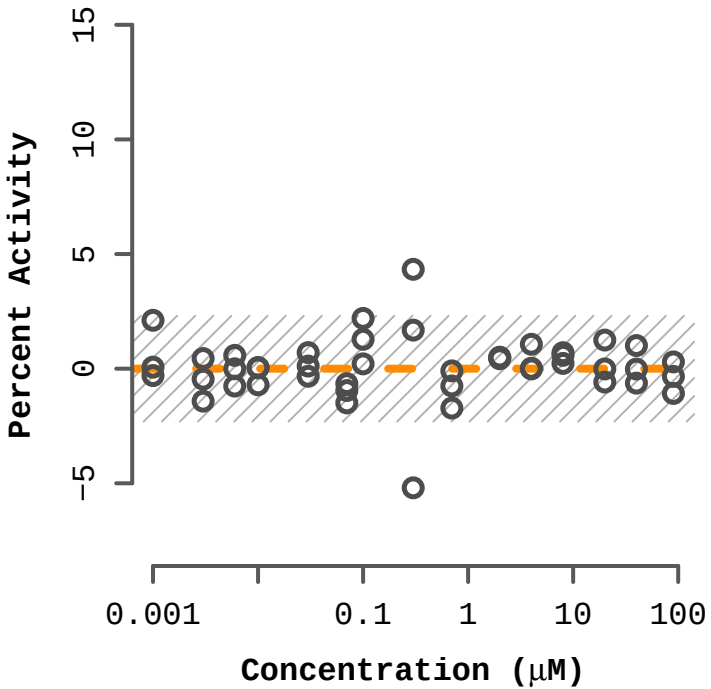
NAME: Octopamine hydrochloride
CHID: 33803 CASRN: 770-05-8
SPID(S): Tox21_200870
M4ID: 12481382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

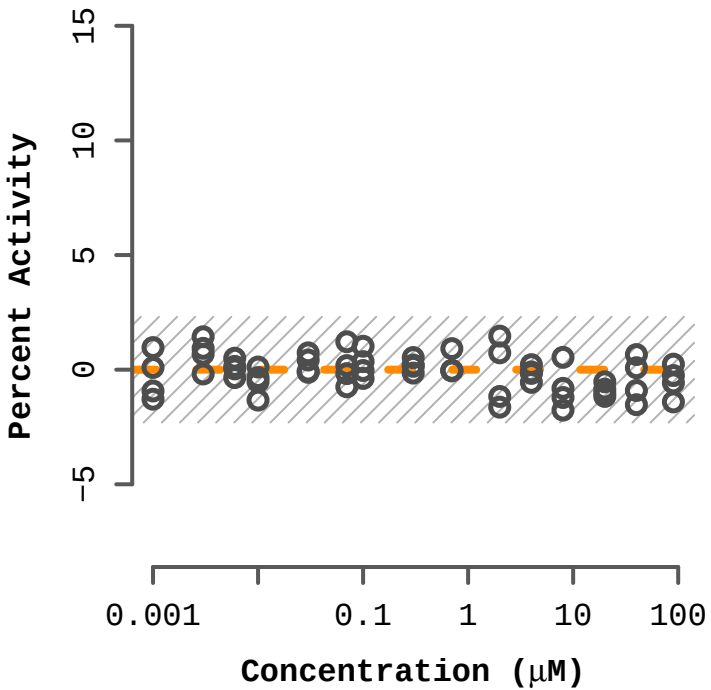
NAME: 3-(Trimethoxysilyl)-N-[3-(trimethoxysilyl)propy
CHID: 33825 **CASRN:** 82985-35-1
SPID(S): Tox21_200368
M4ID: 12481884

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

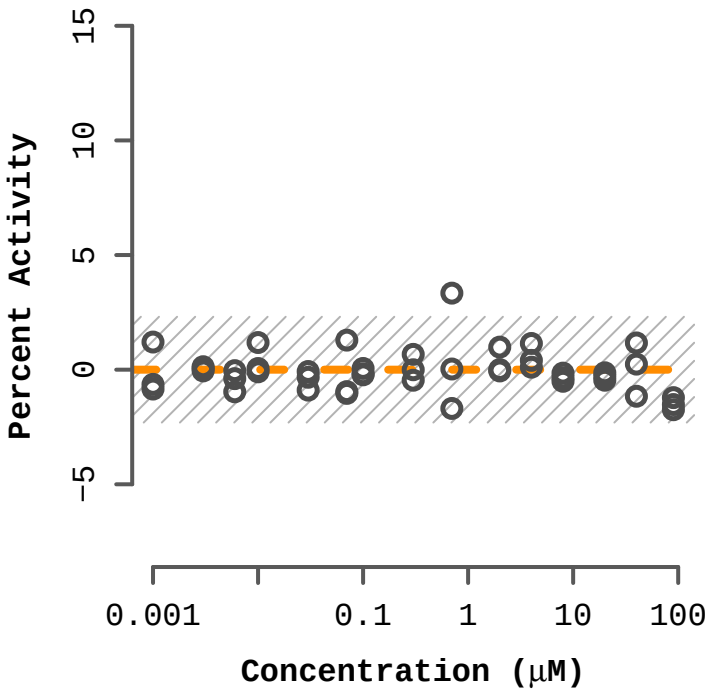
NAME: 4-Nonylphenol
CHID: 33836 **CASRN:** 104-40-5
SPID(S): Tox21_303647
M4ID: 12475500

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.715 **MAX_MED:** 0.806 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

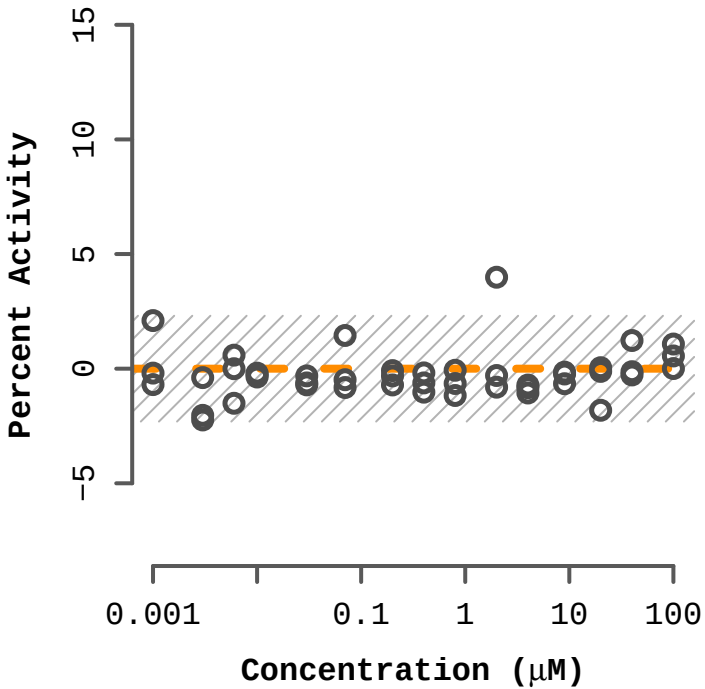
NAME: 4-Nonylphenol
CHID: 33836 **CASRN:** 104-40-5
SPID(S): Tox21_201241
M4ID: 12481011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.56 **MAX_MED:** 0.408 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

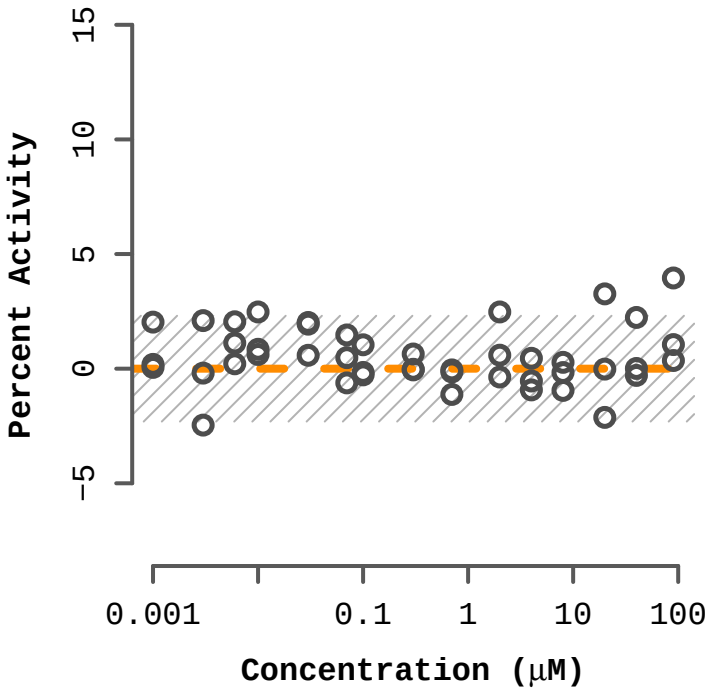
NAME: 1,4-Divinylbenzene
CHID: 33863 CASRN: 105-06-6
SPID(S): Tox21_202529
M4ID: 12479723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.963 MAX_MED: 0.556 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

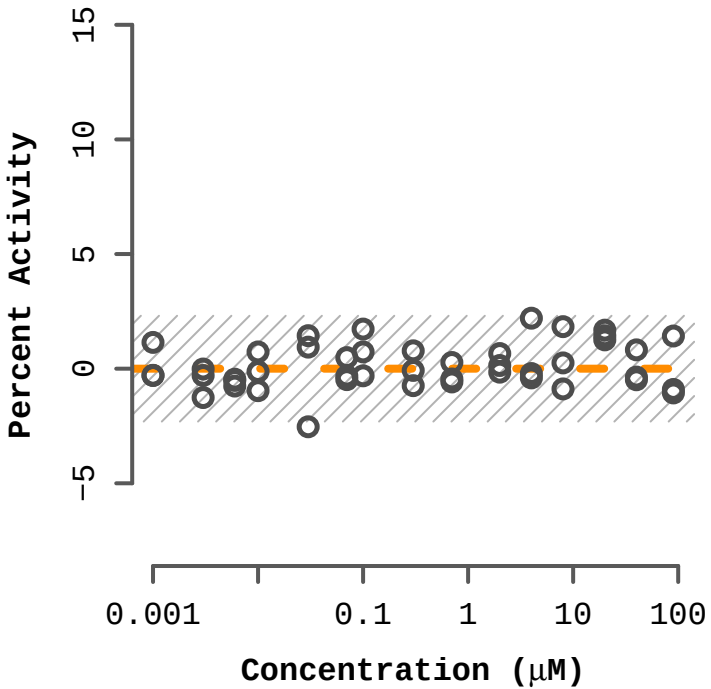
NAME: Phenethyl bromide
CHID: 33876 CASRN: 103-63-9
SPID(S): Tox21_200102
M4ID: 12482150

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.79 MAX_MED: 1.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

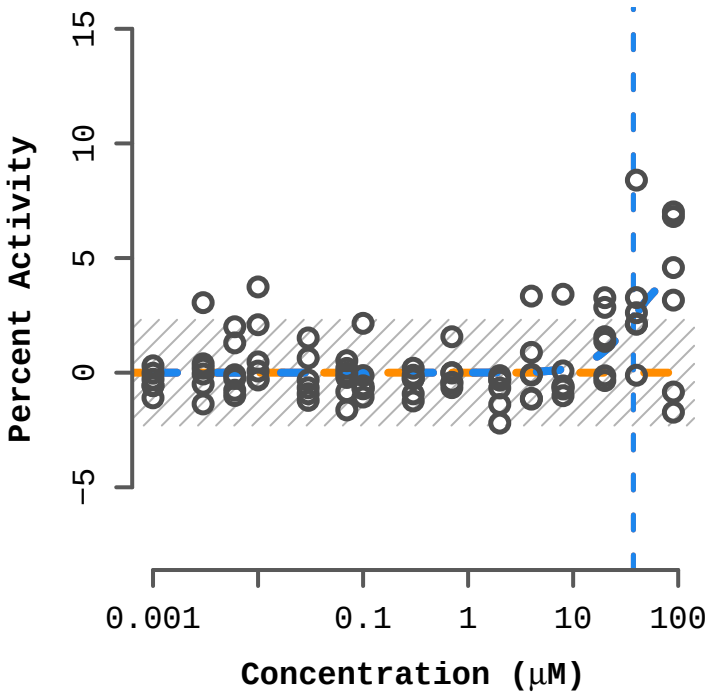
NAME: Phosphorus pentachloride
CHID: 33896 **CASRN:** 10026-13-8
SPID(S): Tox21_202530
M4ID: 12479722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Procymidone
CHID: 33923 **CASRN:** 32809-16-8
SPID(S): Tox21_303640
M4ID: 12475505

HILL MODEL (in red):

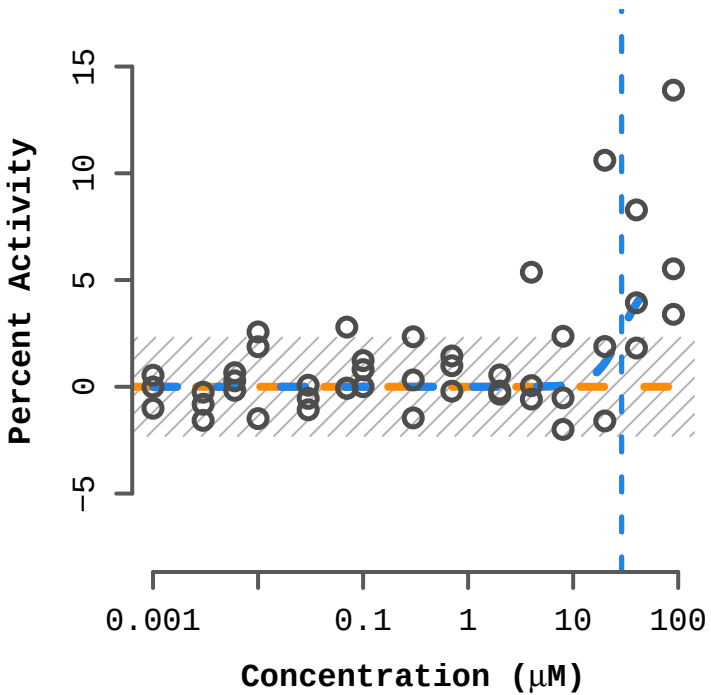
	tp	ga	gw
val:	4.81	1.57	2.23
sd:	1.93	0.204	0.957

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.81	1.57	2.23	3.27	5.79
sd:	1.93	0.204	0.957	1640	7280

	CNST	HILL	GNLS
AIC:	349.63	325.69	329.69
PROB:	0	0.88	0.12
RMSE:	1.97	1.59	1.59

MAX_MEAN: 3.17 **MAX_MED:** 3.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Procymidone
CHID: 33923 CASRN: 32809-16-8
SPID(S): Tox21_201913
M4ID: 12480339

HILL MODEL (in red):

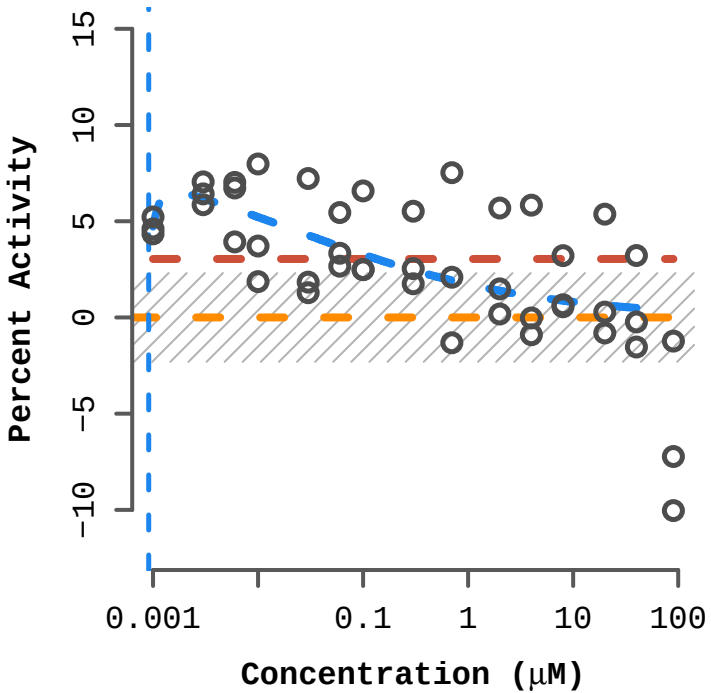
	tp	ga	gw
val:	5.16	1.46	3.46
sd:	1.39	0.164	3.04

GAIN-LOSS MODEL (in blue):

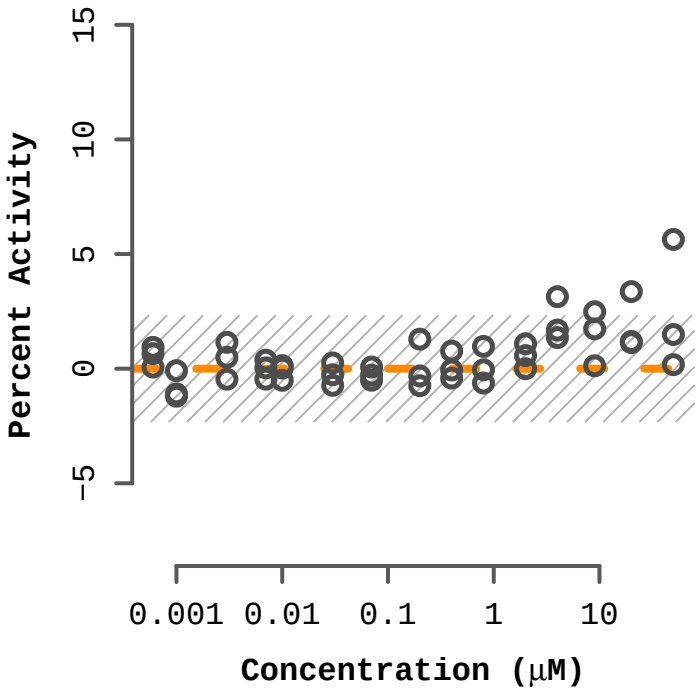
	tp	ga	gw	la	lw
val:	5.16	1.46	3.46	3.56	3.9
sd:	1.39	0.164	3.04	1700	4180

	CNST	HILL	GNLS
AIC:	216.58	198.47	202.47
PROB:	0	0.88	0.12
RMSE:	3.4	2.5	2.5

MAX_MEAN: 7.61 MAX_MED: 5.53 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Rifabutin
CHID:    33960   CASRN: 72559-06-9
SPID(S): Tox21_200758
M4ID:    12481494

HILL MODEL (in red):
      tp       ga       gw
val:  3.04     -4.99    3.7
sd:   0.506    1100     2020

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.08     -3.04    7.99     -1.66    0.381
sd:   8.14     0.0773   15.5     2.29     0.238

      CNST       HILL       GNLS
AIC:  270.63     249.44     229.22
PROB: 0          0          1
RMSE: 4.53       3.67       2.9

MAX_MEAN: 6.44      MAX_MED: 6.73      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

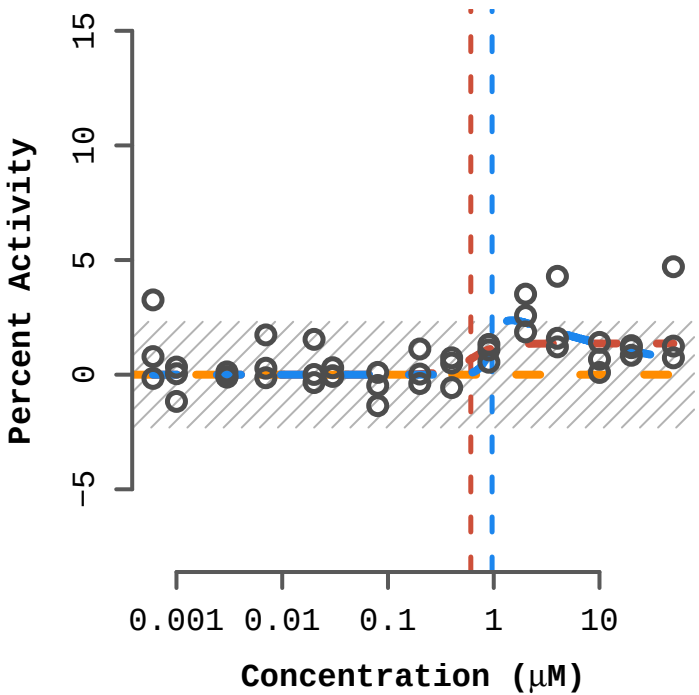
NAME: Sodium cholate
CHID: 33979 **CASRN:** 361-09-1
SPID(S): Tox21_202535
M4ID: 12479717

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 2.43 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium hydrogen sulfate
CHID: 33983 CASRN: 7681-38-1
SPID(S): Tox21_202537
M4ID: 12479715

HILL MODEL (in red):

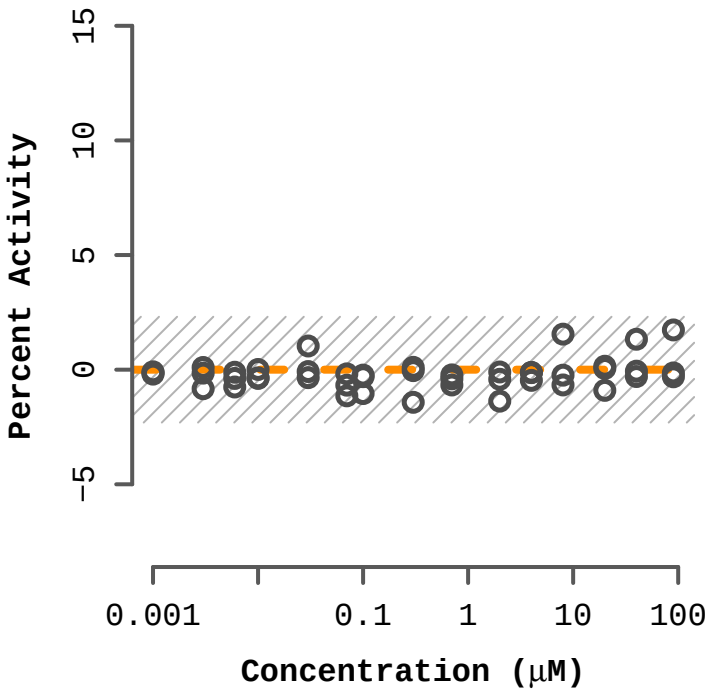
	tp	ga	gw
val:	1.36	−0.217	3.64
sd:	0.212	0.206	2.59

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.72	−0.0154	8	0.235	0.515
sd:	4.8	0.0646	14.1	1.51	0.247

	CNST	HILL	GNLS
AIC:	159.1	130.37	128.27
PROB:	0	0.26	0.74
RMSE:	1.5	1.08	1.06

MAX_MEAN: 2.65 **MAX_MED:** 2.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

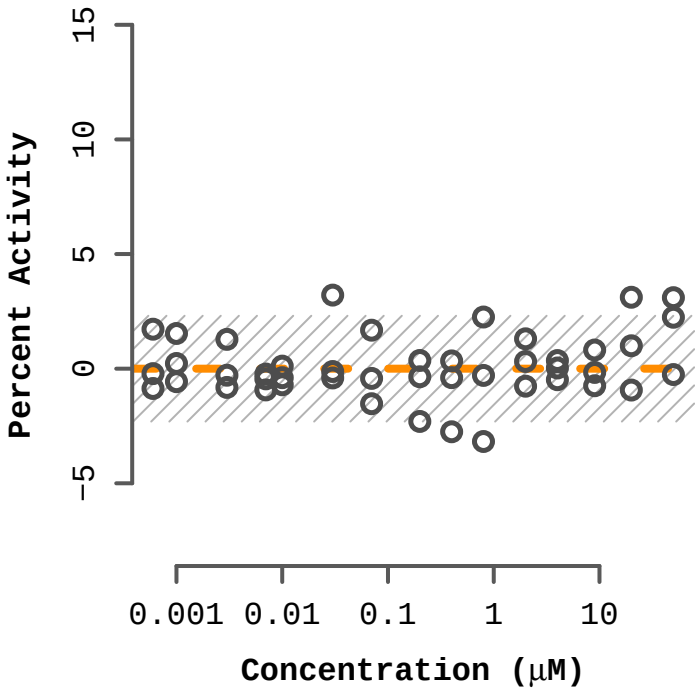
NAME: Sodium zomepirac
CHID: 33989 CASRN: 64092-48-4
SPID(S): Tox21_202177
M4ID: 12480075

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.428 **MAX_MED:** 0.0549 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

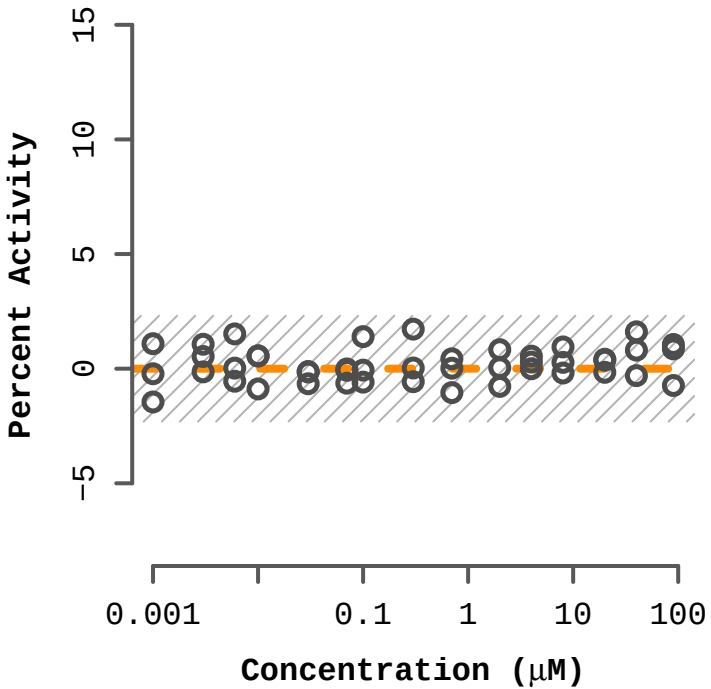
NAME: Sodium zomepirac
CHID: 33989 **CASRN:** 64092-48-4
SPID(S): Tox21_111006_1
M4ID: 12483953

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

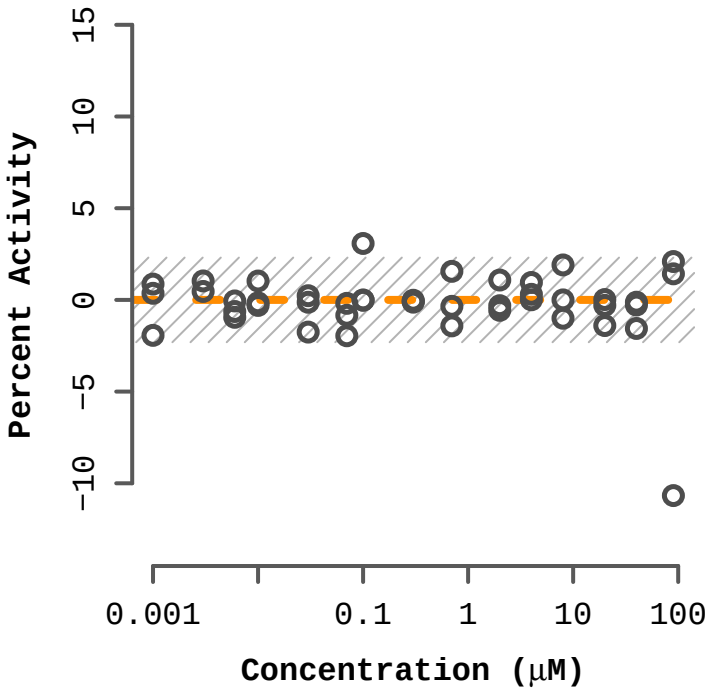
NAME: Sulfamic acid
CHID: 34005 **CASRN:** 5329-14-6
SPID(S): Tox21_303482
M4ID: 12475659

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.706 **MAX_MED:** 0.864 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

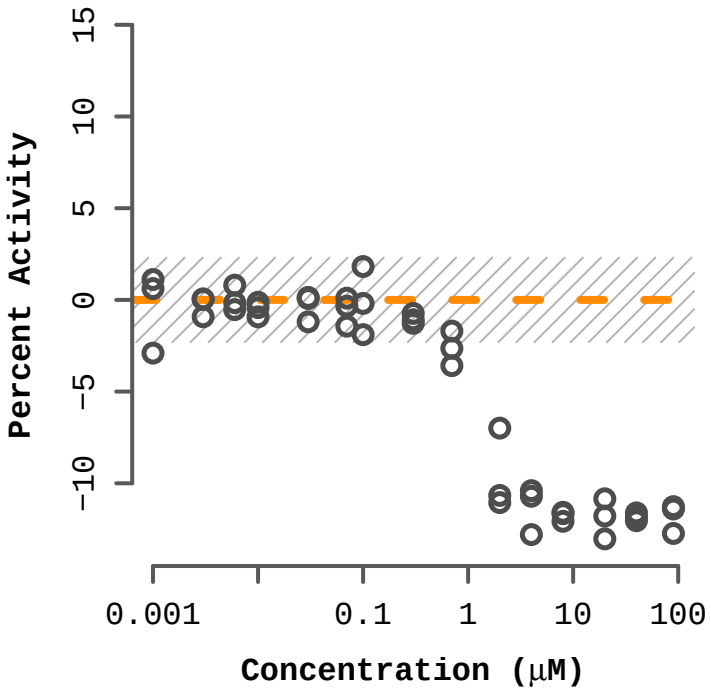
NAME: Sulfamic acid
CHID: 34005 **CASRN:** 5329-14-6
SPID(S): Tox21_201905
M4ID: 12480347

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

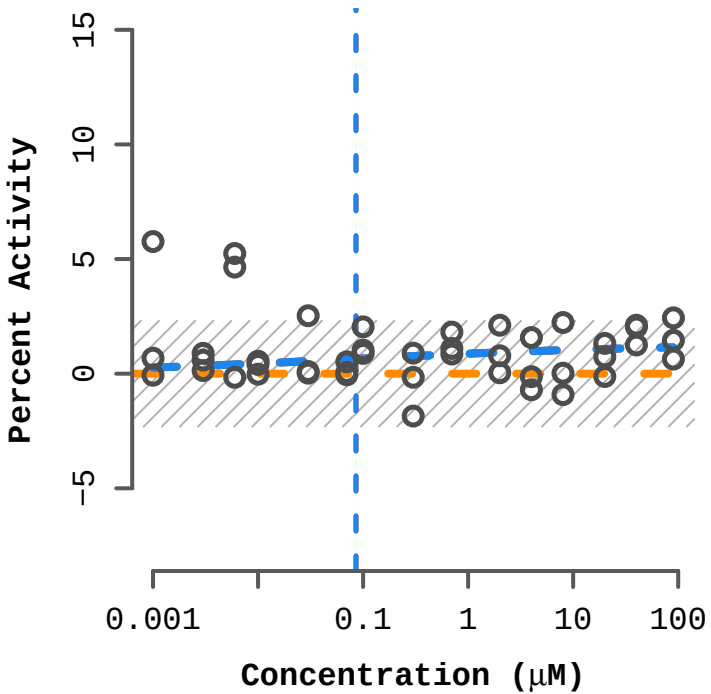
NAME: Tetra-N-octylammonium bromide
CHID: 34042 **CASRN:** 14866-33-2
SPID(S): Tox21_201028
M4ID: 12481224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	310.85	NA	NA
PROB:	1	NA	NA
RMSE:	7.31	NA	NA

MAX_MEAN: 0.0444 **MAX_MED:** 0.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trichloroacetyl chloride
CHID: 34070 CASRN: 76-02-8
SPID(S): Tox21_201070
M4ID: 12481182

HILL MODEL (in red):

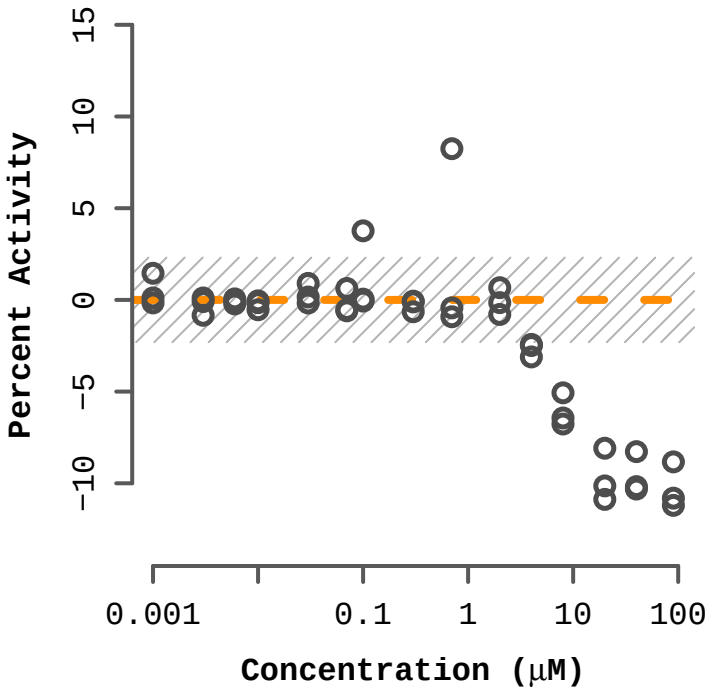
	tp	ga	gw
val:	1.29	−1.07	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.29	−1.07	0.3	3.95	17
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	172.98	159.42	163.42
PROB:	0	0.88	0.12
RMSE:	1.77	1.54	1.54

MAX_MEAN: 3.25 **MAX_MED:** 4.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

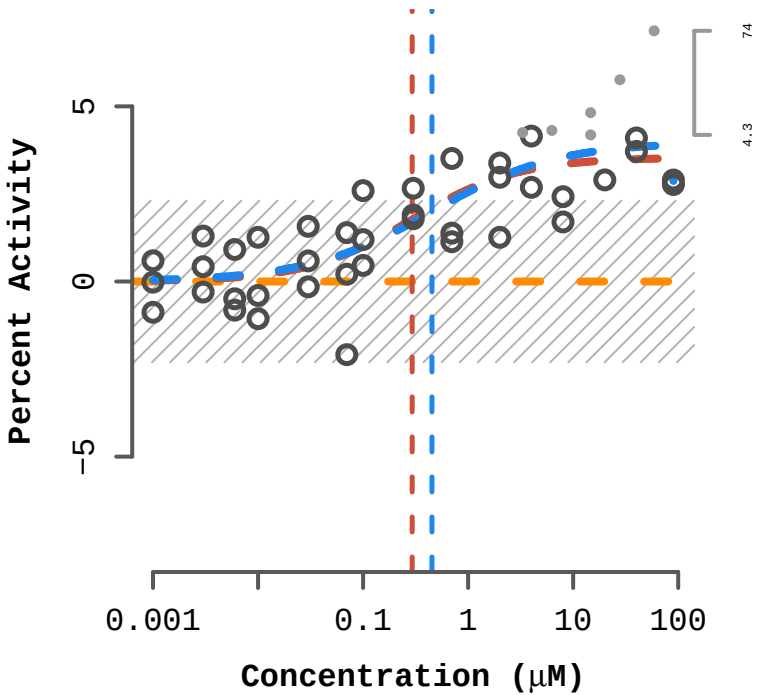
NAME: Triton X-100
CHID: 34085 **CASRN:** 9002-93-1
SPID(S): Tox21_202544
M4ID: 12479708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	268.88	NA	NA
PROB:	1	NA	NA
RMSE:	4.97	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 0.159 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tyramine hydrochloride
CHID: 34087 CASRN: 60-19-5
SPID(S): Tox21_201198
M4ID: 12481054 BRK

HILL MODEL (in red):

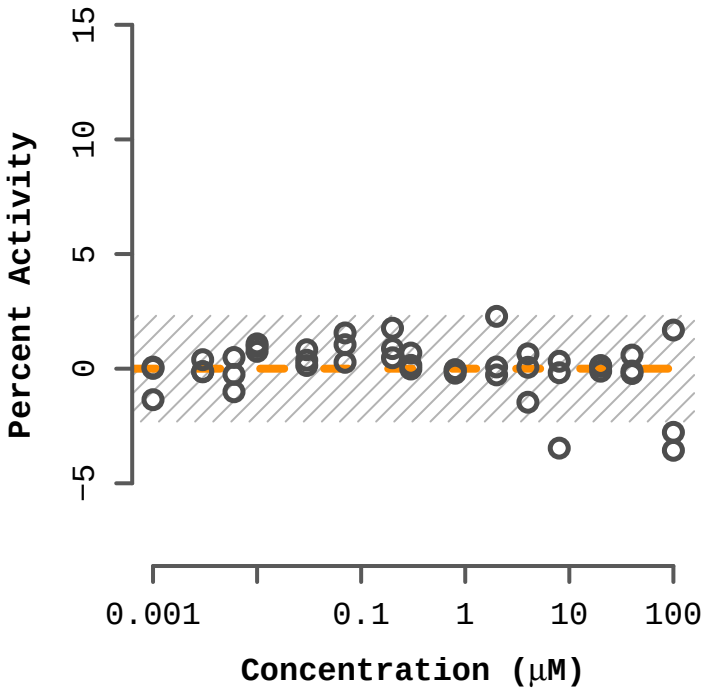
	tp	ga	gw
val:	3.54	−0.533	0.865
sd:	0.509	0.314	0.384

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.99	−0.344	0.727	1.98	15.5
sd:	0.826	0.429	0.329	0.0412	23

	CNST	HILL	GNLS
AIC:	275.5	229.74	232.59
PROB:	0	0.81	0.19
RMSE:	13.21	12.24	12.28

MAX_MEAN: 26.6 MAX_MED: 4.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

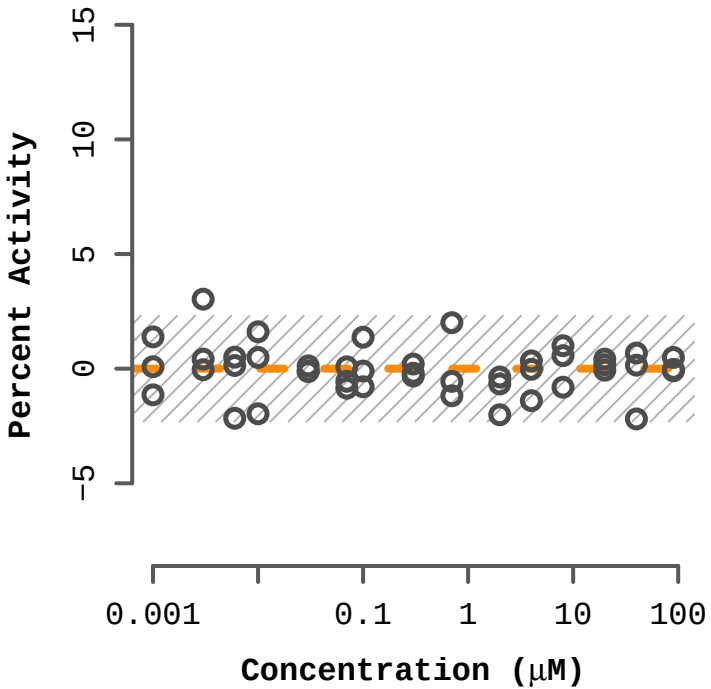
NAME: Valerenic acid
CHID: 34089 **CASRN:** 3569-10-6
SPID(S): Tox21_200313
M4ID: 12481939

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

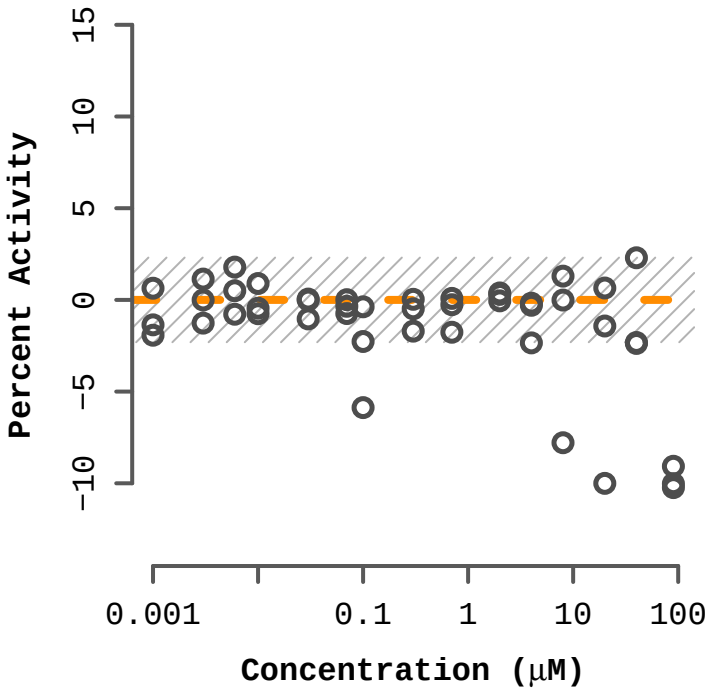
NAME: Valeryl chloride
CHID: 34091 **CASRN:** 638-29-9
SPID(S): Tox21_200690
M4ID: 12481562

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.569 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

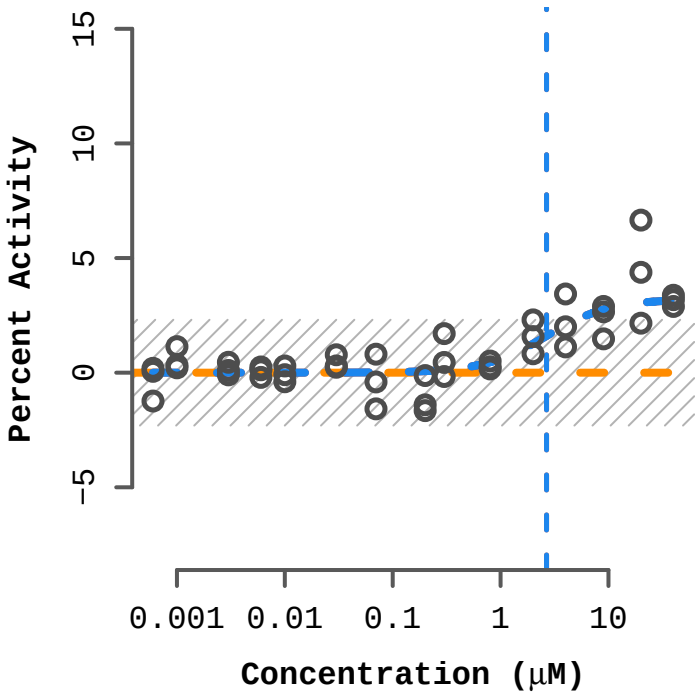
NAME: Verapamil hydrochloride
CHID: 34095 **CASRN:** 152-11-4
SPID(S): Tox21_201180
M4ID: 12481072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.09	NA	NA
PROB:	1	NA	NA
RMSE:	3.45	NA	NA

MAX_MEAN: 0.503 **MAX_MED:** 0.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Yangonin
CHID: 34102 **CASRN:** 500-62-9
SPID(S): Tox21_202547
M4ID: 12479705

HILL MODEL (in red):

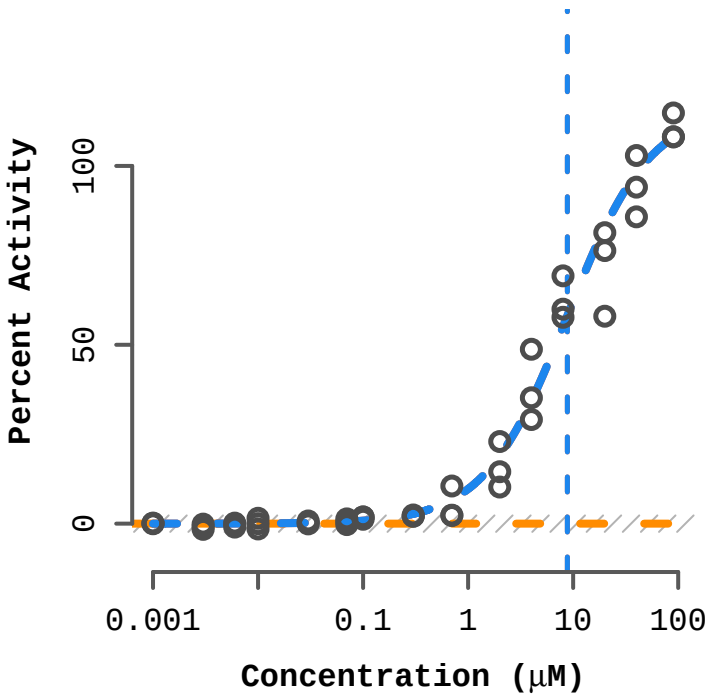
	tp	ga	gw
val:	3.2	0.426	1.48
sd:	0.404	0.17	0.554

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.2	0.426	1.48	2.65	6.89
sd:	0.404	0.17	0.554	1700	10600

	CNST	HILL	GNLS
AIC:	179.43	118.2	122.2
PROB:	0	0.88	0.12
RMSE:	1.87	0.91	0.91

MAX_MEAN: 4.4 **MAX_MED:** 4.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydroxyandrostenedione
CHID: 34113 CASRN: 566-48-3
SPID(S): Tox21_302286
M4ID: 12476847

HILL MODEL (in red):

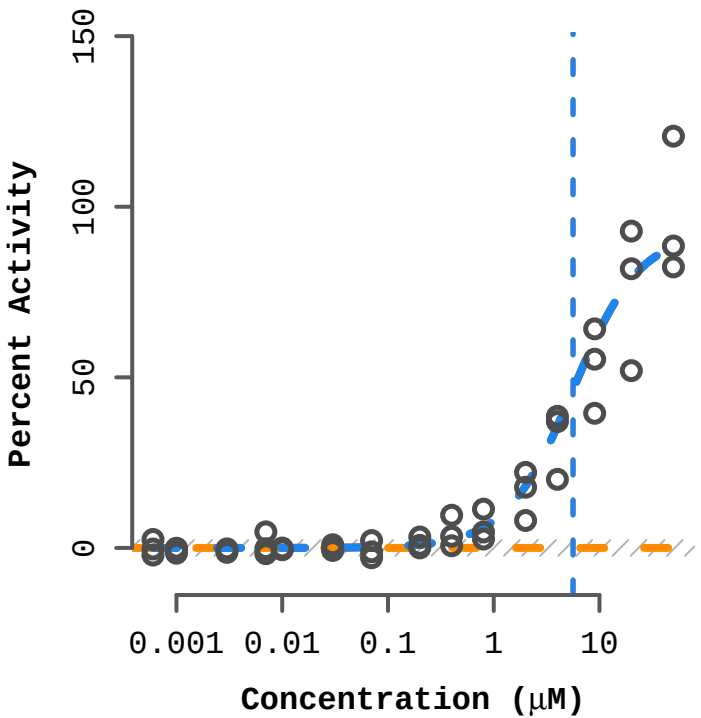
	tp	ga	gw
val:	116	0.945	1.1
sd:	4.13	0.052	0.0966

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	116	0.945	1.1	3.89	11.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	467.86	273.26	277.26
PROB:	0	0.88	0.12
RMSE:	46.28	5.85	5.85

MAX_MEAN: 110 MAX_MED: 108 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydroxyandrostenedione
CHID: 34113 CASRN: 566-48-3
SPID(S): Tox21_112111_1
M4ID: 12483313

HILL MODEL (in red):

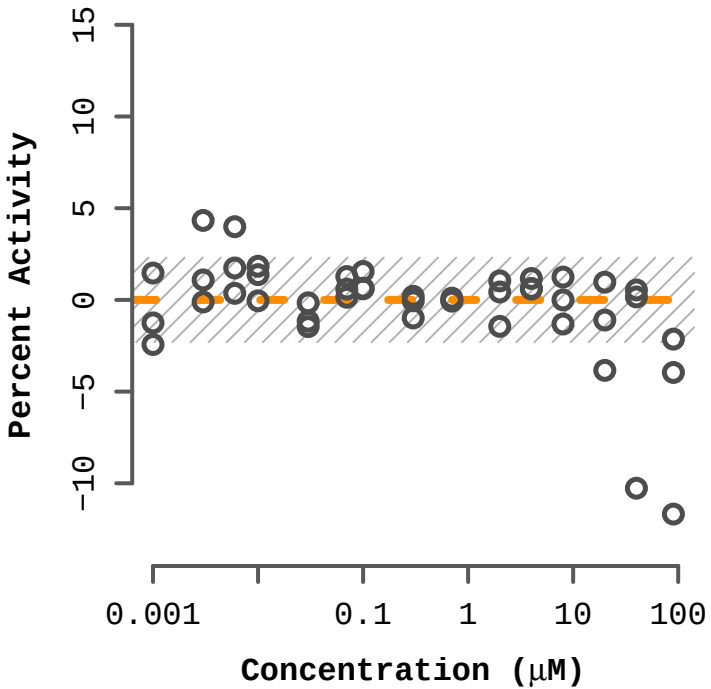
	tp	ga	gw
val:	92.7	0.75	1.37
sd:	4.29	0.0534	0.155

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	92.7	0.75	1.37	3.22	14
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	436.88	295.42	299.42
PROB:	0	0.88	0.12
RMSE:	36.64	8.22	8.22

MAX_MEAN: 97.2 MAX_MED: 88.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

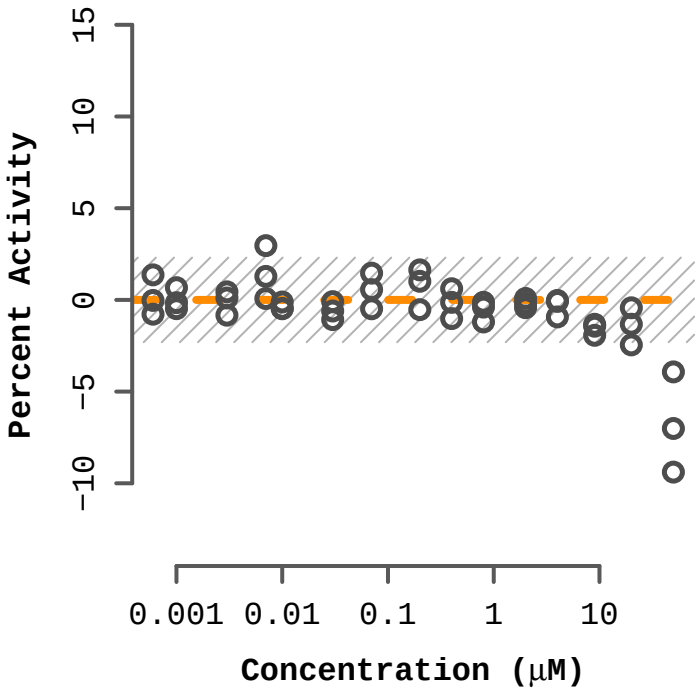
NAME: Haloperidol
CHID: 34150 **CASRN:** 52-86-8
SPID(S): Tox21_300475
M4ID: 12478657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.8	NA	NA

MAX_MEAN: 2.03 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

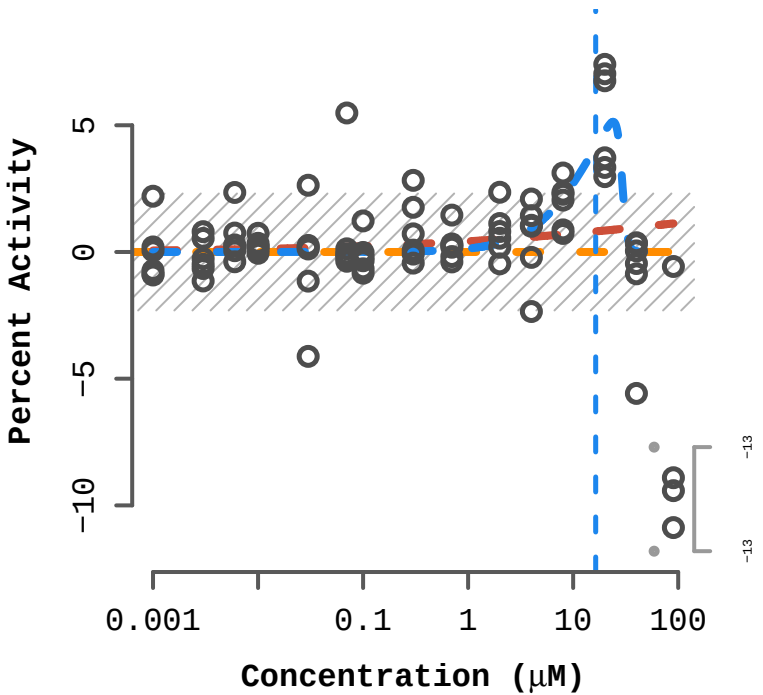
NAME: Haloperidol
CHID: 34150 **CASRN:** 52-86-8
SPID(S): Tox21_110162_1
M4ID: 12484595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nilutamide
CHID: 34165 **CASRN:** 63612-50-0
SPID(S): Tox21_301589
M4ID: 12477544 **BRK**

HILL MODEL (in red):

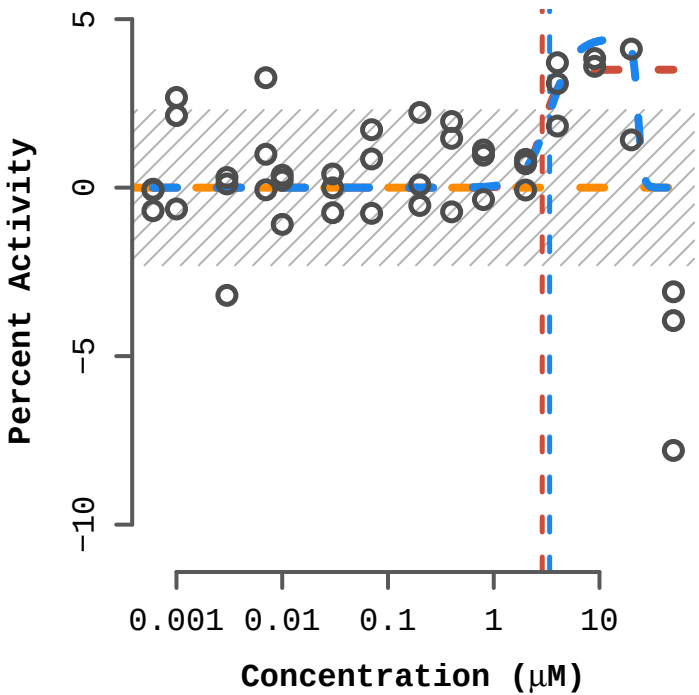
	tp	ga	gw
val:	2.71	2.44	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.31	1.21	1.47	1.46	18
sd:	6.31	0.429	0.668	0.193	24.9

	CNST	HILL	GNLS
AIC:	419.36	419.7	381.05
PROB:	0	0	1
RMSE:	3.26	3.39	2.92

MAX_MEAN: 5.2 **MAX_MED:** 5.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nilutamide
CHID: 34165 CASRN: 63612-50-0
SPID(S): Tox21_110213_1
M4ID: 12484547

HILL MODEL (in red):

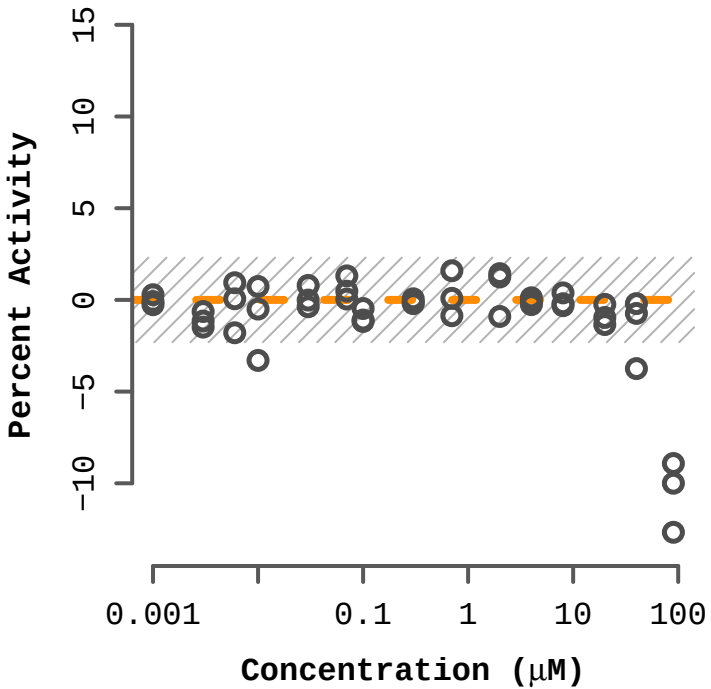
	tp	ga	gw
val:	3.5	0.458	4.97
sd:	0.731	0.122	3.49

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.43	0.529	3.69	1.36	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	209.85	197.23	185.46
PROB:	0	0	1
RMSE:	2.54	2.59	1.88

MAX_MEAN: 4.43 MAX_MED: 4.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

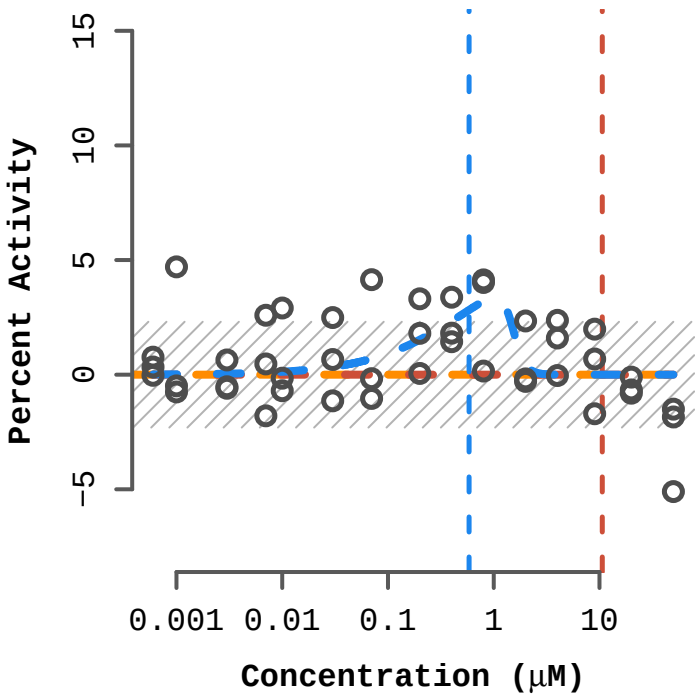
NAME: Raloxifene hydrochloride
CHID: 34181 **CASRN:** 82640-04-8
SPID(S): Tox21_302369
M4ID: 12476764

HILL MODEL: Not applicable.

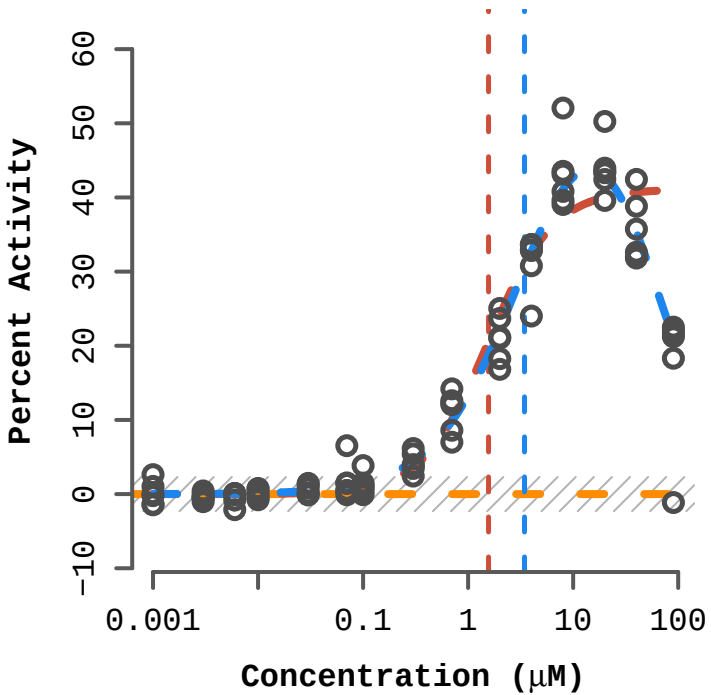
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.95	NA	NA

MAX_MEAN: 0.612 **MAX_MED:** 1.25 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Raloxifene hydrochloride
CHID:    34181   CASRN: 82640-04-8
SPID(S): Tox21_110255_1
M4ID:    12484509

HILL MODEL (in red):
      tp        ga        gw
val:  3.86e-10  1.03      2.02
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  5.65      -0.233    0.926     0.181     7.7
sd:   8.96      1.47      1         0.558     38

      CNST          HILL          GNLS
AIC:  194.05        200.05        188.57
PROB: 0.06          0             0.94
RMSE: 2.05          2.05          1.74

MAX_MEAN: 2.77      MAX_MED: 4.02      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Spironolactone
CHID: 34186 CASRN: 52-01-7
SPID(S): Tox21_302154
M4ID: 12476979

HILL MODEL (in red):

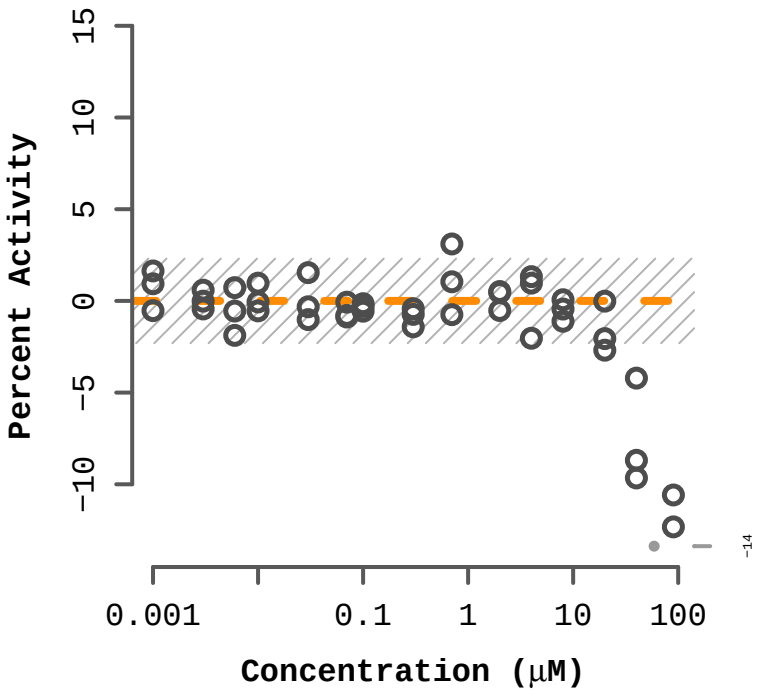
	tp	ga	gw
val:	41.1	0.194	1.41
sd:	1.49	0.0419	0.118

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	62.5	0.537	1.05	1.75	1.32
sd:	6.74	0.0834	0.0655	0.0697	0.154

	CNST	HILL	GNLS
AIC:	808.94	546.49	424.79
PROB:	0	0	1
RMSE:	21.7	7.28	3.43

MAX_MEAN: 43.8 MAX_MED: 43.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

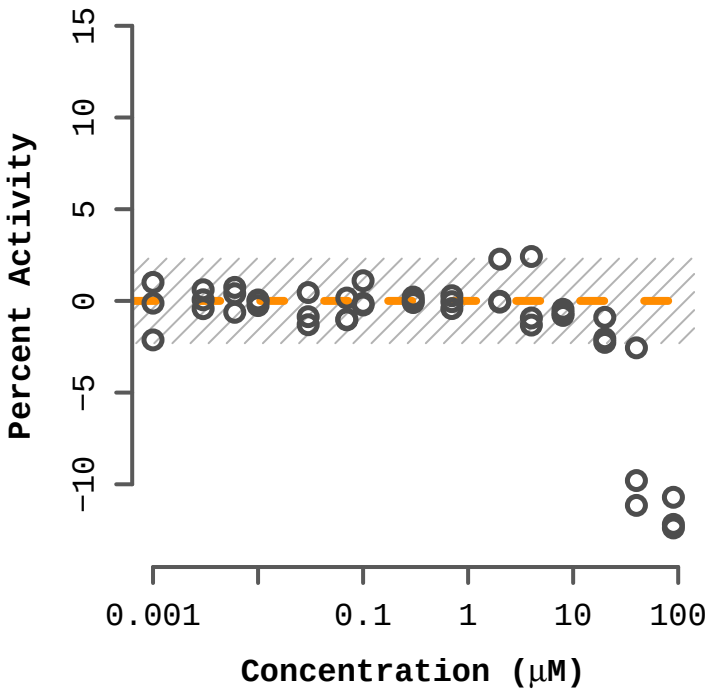
NAME: Tamoxifen
CHID: 34187 CASRN: 10540-29-1
SPID(S): Tox21_300539
M4ID: 12478593 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.74	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

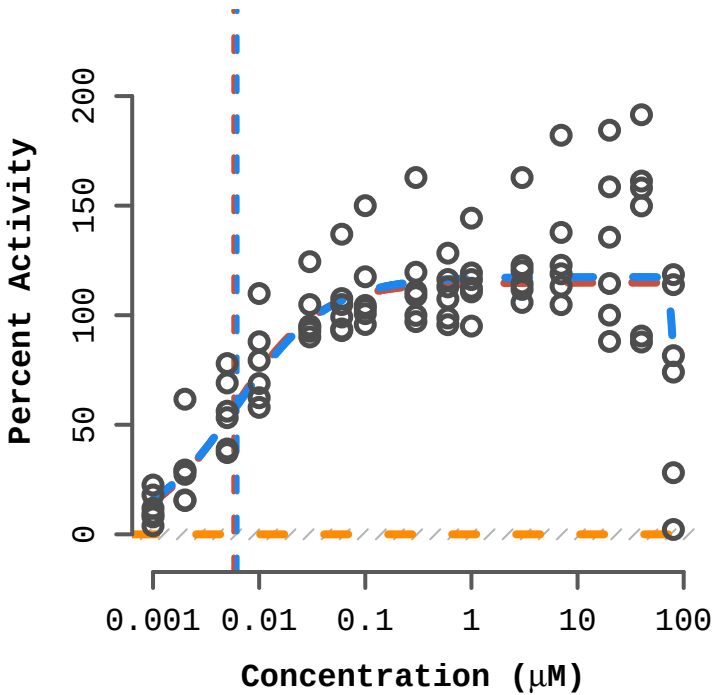
NAME: Tamoxifen
CHID: 34187 **CASRN:** 10540-29-1
SPID(S): Tox21_201243
M4ID: 12481009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.89	NA	NA

MAX_MEAN: 0.732 **MAX_MED:** 0.391 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17beta-Trenbolone
CHID: 34192 CASRN: 10161-33-8
SPID(S): Tox21_303654
M4ID: 12475494

HILL MODEL (in red):

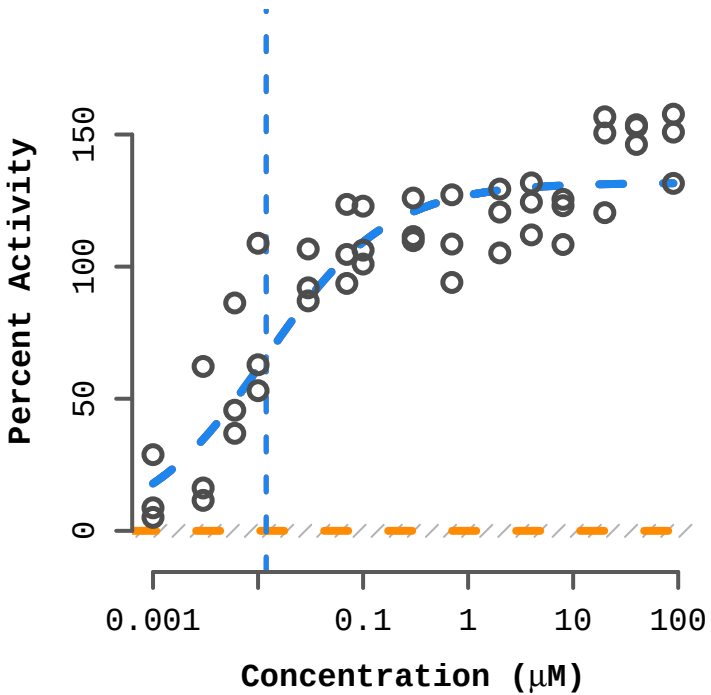
	tp	ga	gw
val:	115	-2.24	1.09
sd:	3.18	0.0714	0.176

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	117	-2.21	1.01	1.92	17.3
sd:	3.61	0.0756	0.168	0.0153	12.6

	CNST	HILL	GNLS
AIC:	1111.13	833.22	829.17
PROB:	0	0.12	0.88
RMSE:	104.63	27	24.16

MAX_MEAN: 140 **MAX_MED:** 154 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17beta-Trenbolone
CHID: 34192 CASRN: 10161-33-8
SPID(S): Tox21_200539
M4ID: 12481713

HILL MODEL (in red):

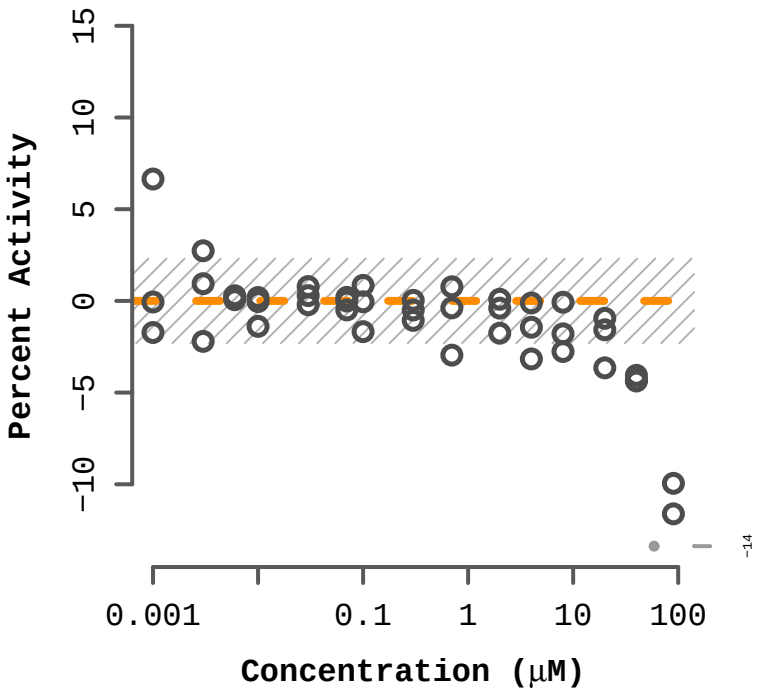
	tp	ga	gw
val:	132	-1.92	0.745
sd:	5.55	0.108	0.172

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	132	-1.92	0.745	3.9	15.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	561.1	395.06	399.06
PROB:	0	0.88	0.12
RMSE:	109.17	17.31	17.31

MAX_MEAN: 151 MAX_MED: 153 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

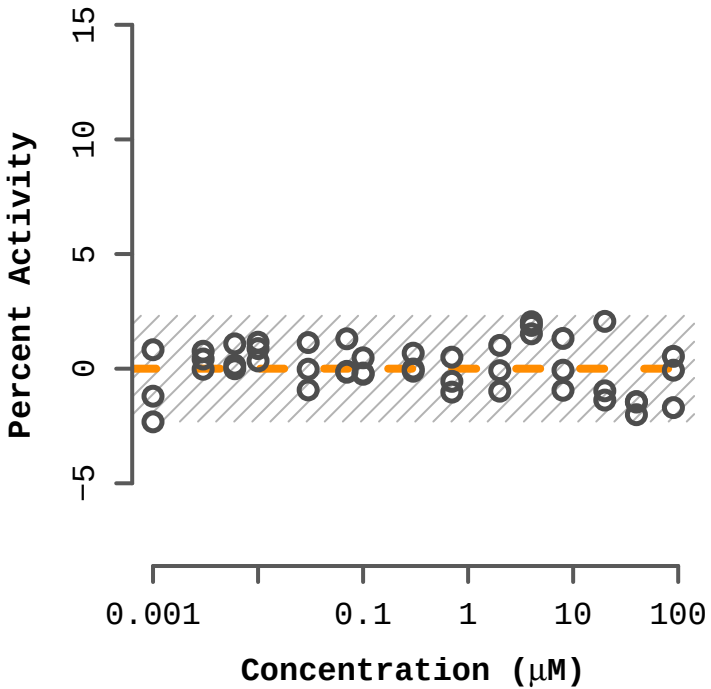
NAME: Prodiamine
CHID: 34210 **CASRN:** 29091-21-2
SPID(S): Tox21_300694
M4ID: 12478439 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.16	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

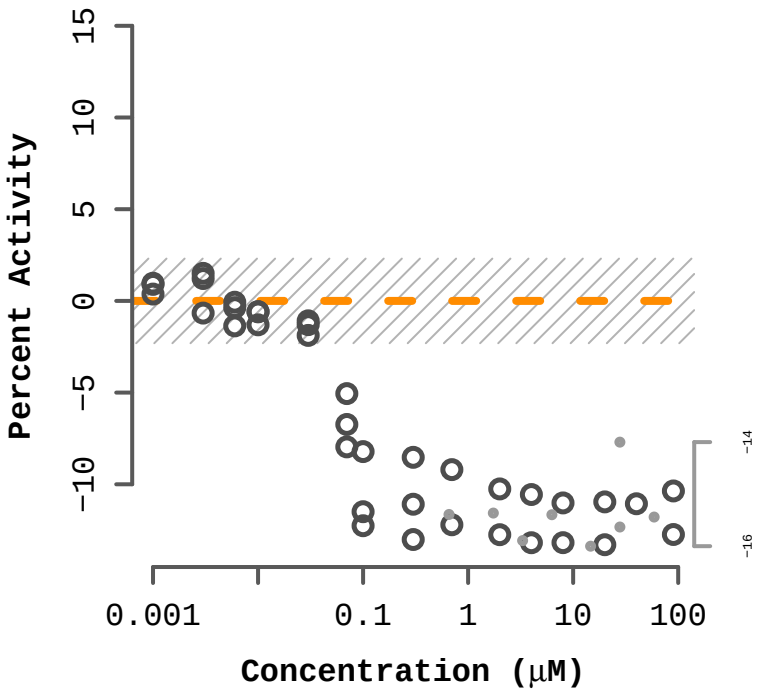
NAME: Spiroxamine
CHID: 34212 **CASRN:** 118134-30-8
SPID(S): Tox21_301163
M4ID: 12477970

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

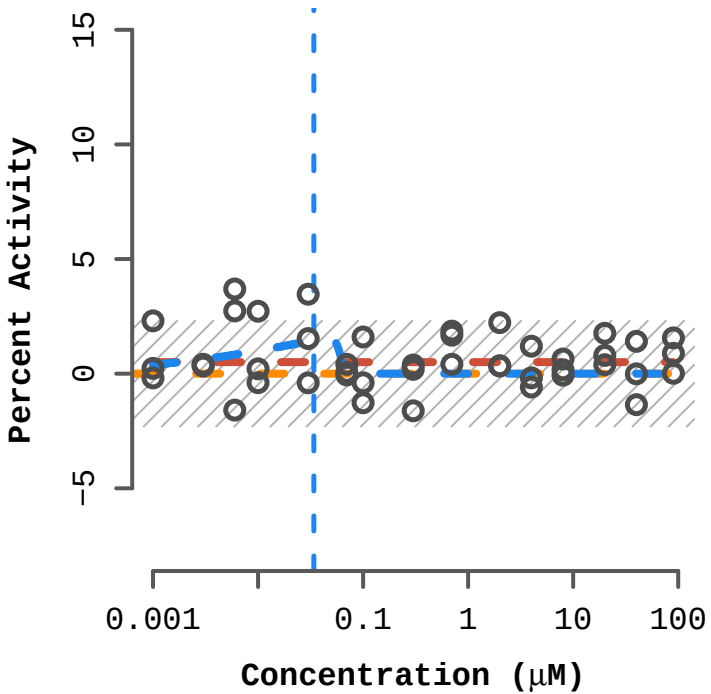
NAME: Tebufenpyrad
CHID: 34223 **CASRN:** 119168-77-3
SPID(S): Tox21_301038
M4ID: 12478095 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	343.39	NA	NA
PROB:	1	NA	NA
RMSE:	9.95	NA	NA

MAX_MEAN: 0.747 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Icaridin
CHID: 34227 CASRN: 119515-38-7
SPID(S): Tox21_301141
M4ID: 12477992

HILL MODEL (in red):

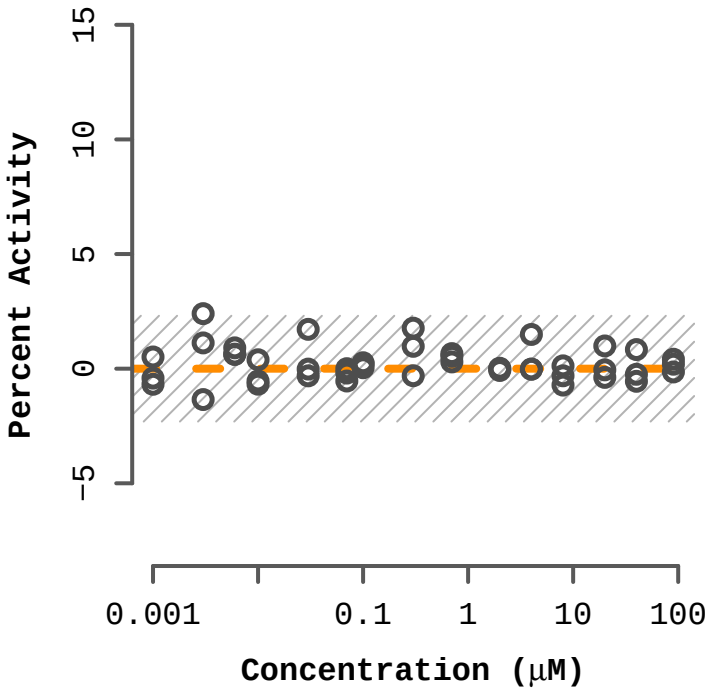
	tp	ga	gw
val:	0.503	−4.62	3.74
sd:	0.17	1470	3450

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.92	−1.47	0.532	−1.22	16.7
sd:	11.4	6.07	1.1	1.08	276

	CNST	HILL	GNLS
AIC:	156.28	153.61	160.65
PROB:	0.2	0.77	0.02
RMSE:	1.36	1.22	1.22

MAX_MEAN: 1.62 **MAX_MED:** 2.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

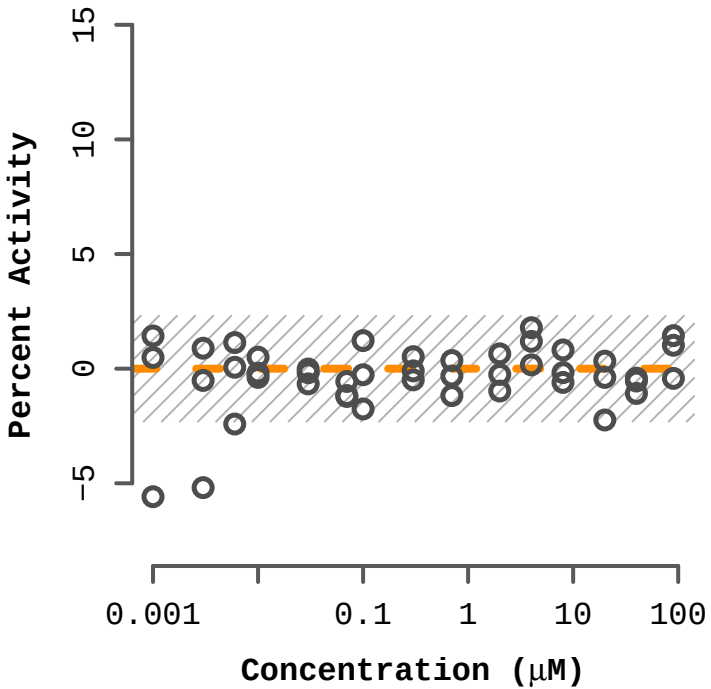
NAME: gamma−Nonanolactone
CHID: 34229 **CASRN:** 104−61−0
SPID(S): Tox21_301039
M4ID: 12478094

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.813 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

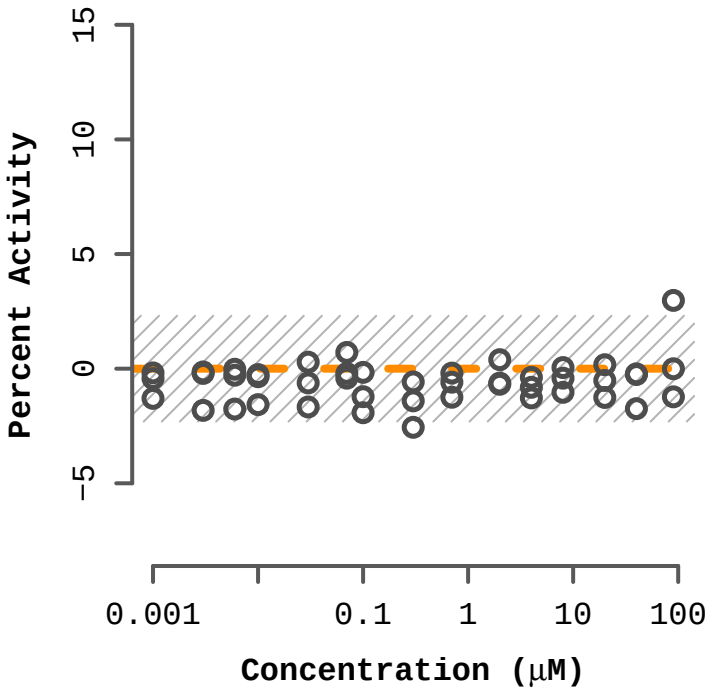
NAME: Cloprop
CHID: 34232 **CASRN:** 101-10-0
SPID(S): Tox21_300676
M4ID: 12478457

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

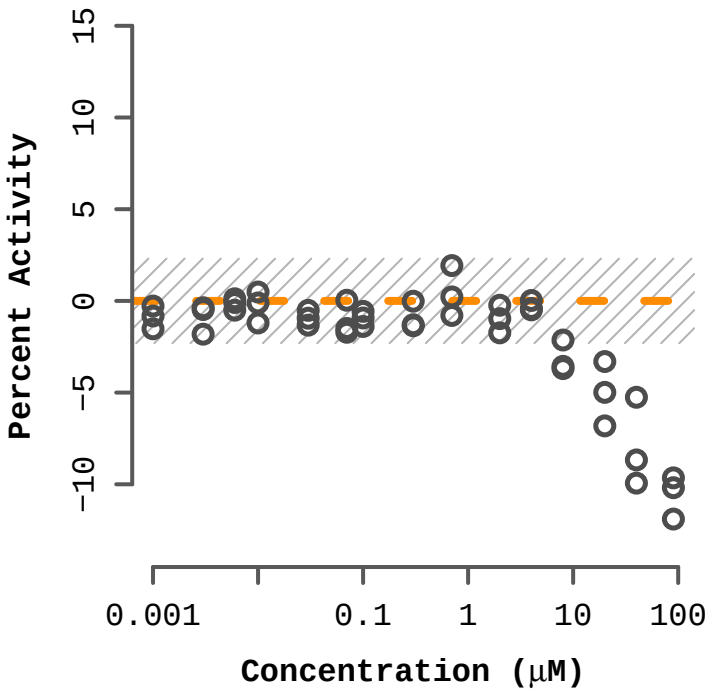
NAME: 2,4−D, isopropylamine salt
CHID: 34241 CASRN: 5742−17−6
SPID(S): Tox21_303714
M4ID: 12475474

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.583 **MAX_MED:** −0.00179 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

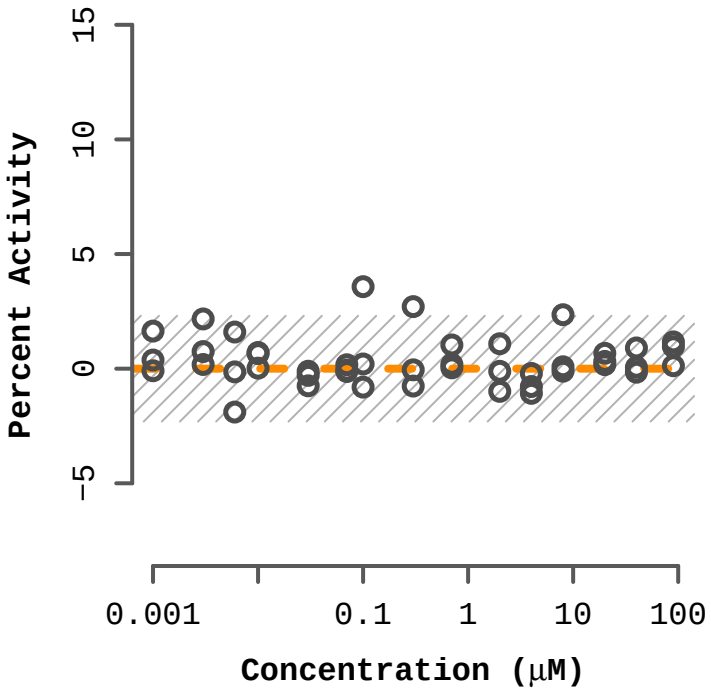
NAME: Chlorfenvinphos
CHID: 34250 **CASRN:** 470-90-6
SPID(S): Tox21_301573
M4ID: 12477560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.86	NA	NA
PROB:	1	NA	NA
RMSE:	3.9	NA	NA

MAX_MEAN: 0.452 **MAX_MED:** 0.219 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

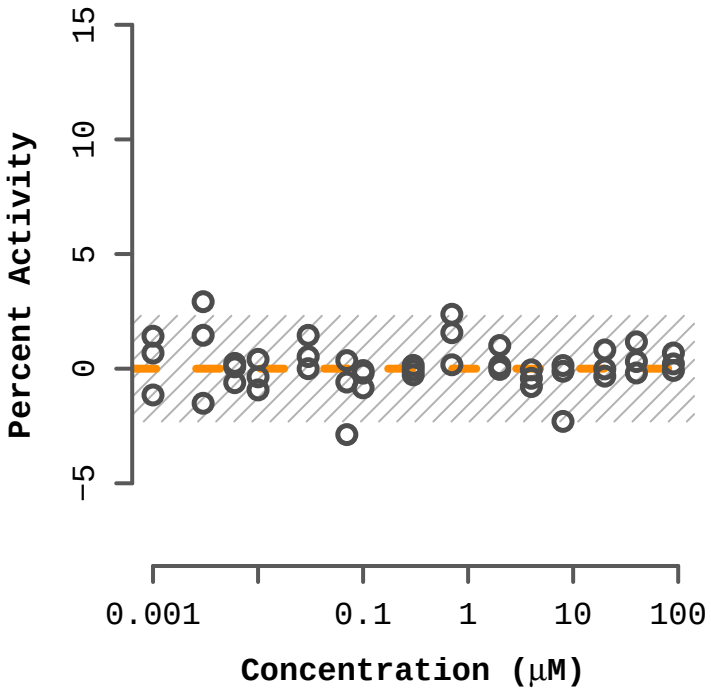
NAME: Tepraloxydim
CHID: 34252 **CASRN:** 149979-41-9
SPID(S): Tox21_301109
M4ID: 12478024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.959 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

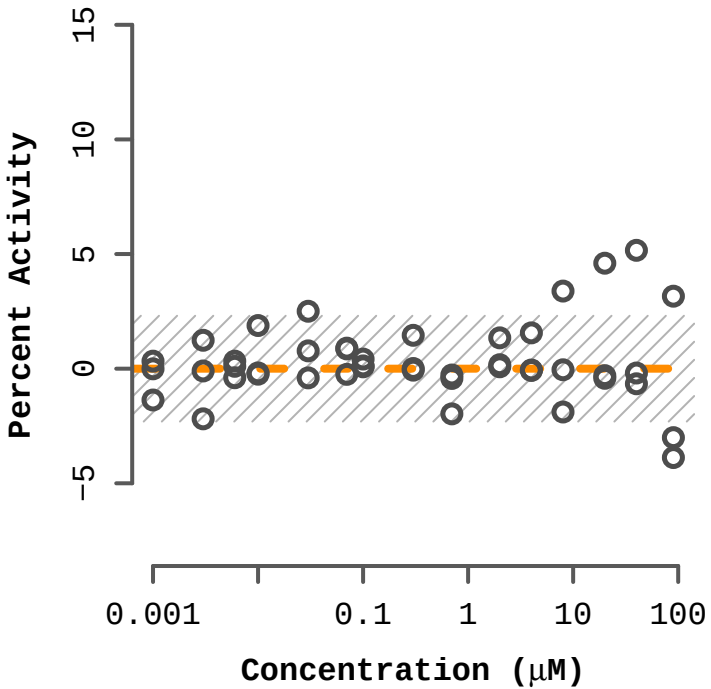
NAME: 2-Fluoroacetamide
CHID: 34255 **CASRN:** 640-19-7
SPID(S): Tox21_301297
M4ID: 12477836

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

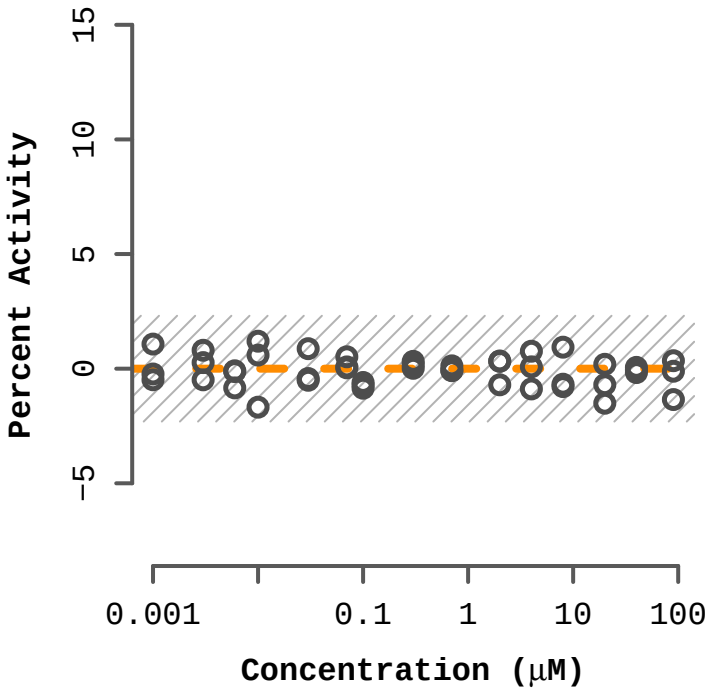
NAME: 2-Methyl-3(2H)-isothiazolone
CHID: 34259 **CASRN:** 2682-20-4
SPID(S): Tox21_303814
M4ID: 12475374

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.863 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

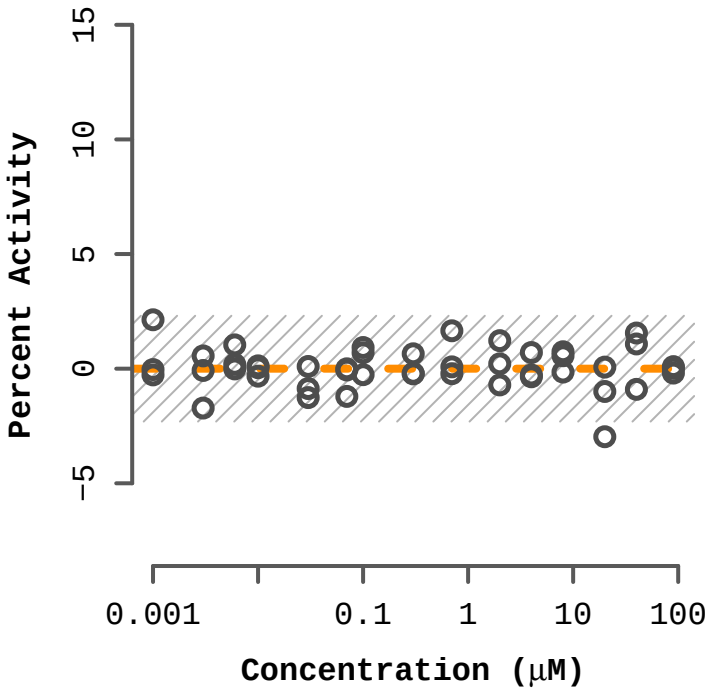
NAME: Oxytetracycline
CHID: 34260 CASRN: 79-57-2
SPID(S): Tox21_302380
M4ID: 12476753

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.212 **MAX_MED:** 0.595 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

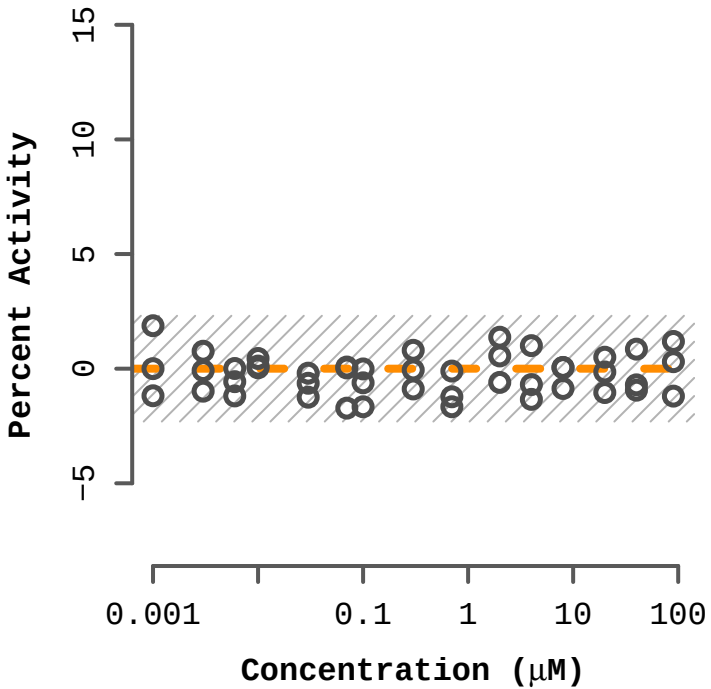
NAME: Clopyralid-olamine
CHID: 34265 **CASRN:** 57754-85-5
SPID(S): Tox21_300763
M4ID: 12478370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.609 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

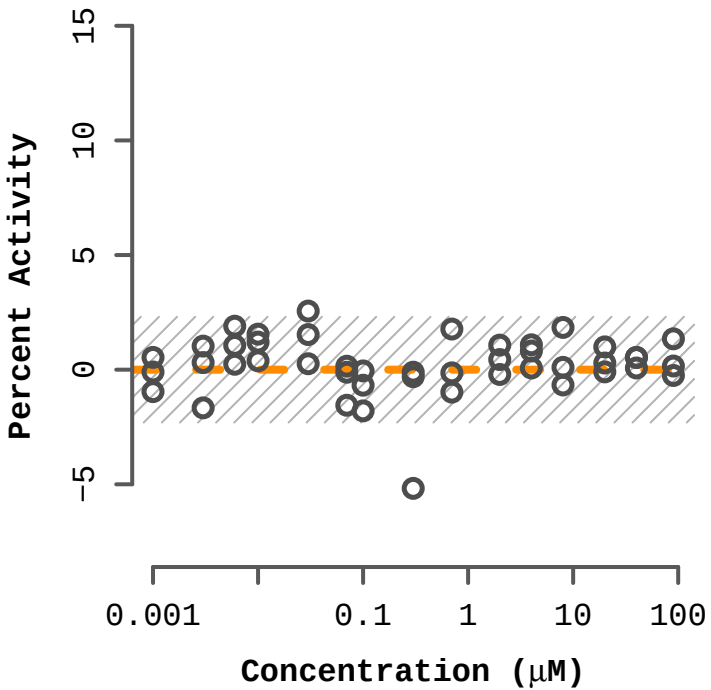
NAME: Imazapic
CHID: 34270 CASRN: 104098-48-8
SPID(S): Tox21_300901
M4ID: 12478232

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.444 MAX_MED: 0.556 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

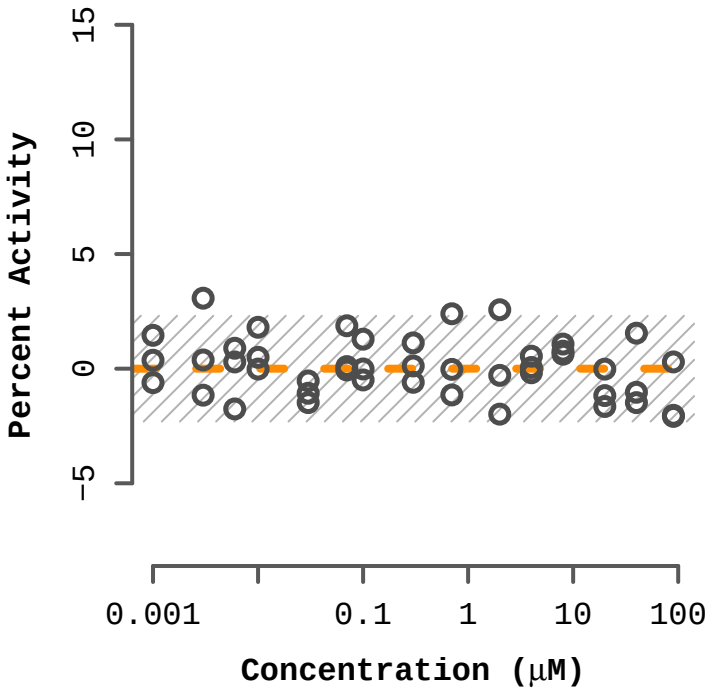
NAME: 4-Chlorophenoxyacetic acid
CHID: 34282 **CASRN:** 122-88-3
SPID(S): Tox21_300744
M4ID: 12478389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

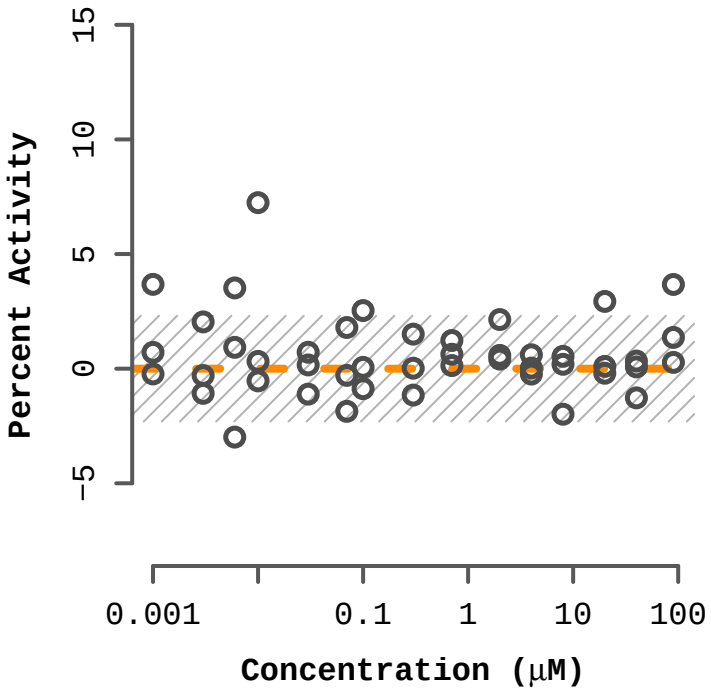
NAME: 5-Chloro-2-methyl-3(2H)-isothiazolone
CHID: 34286 **CASRN:** 26172-55-4
SPID(S): Tox21_300199
M4ID: 12478931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

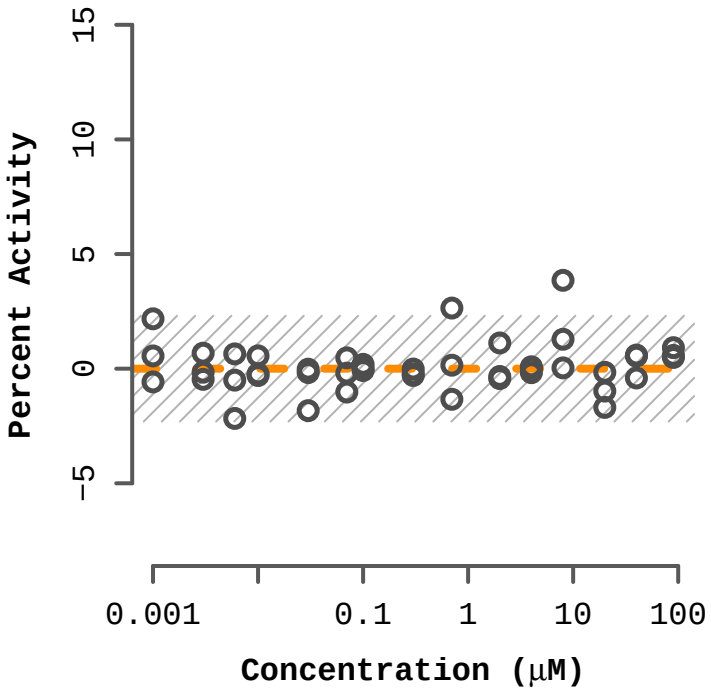
NAME: 5-Heptyldihydro-2(3H)-furanone
CHID: 34287 CASRN: 104-67-6
SPID(S): Tox21_300063
M4ID: 12479067

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

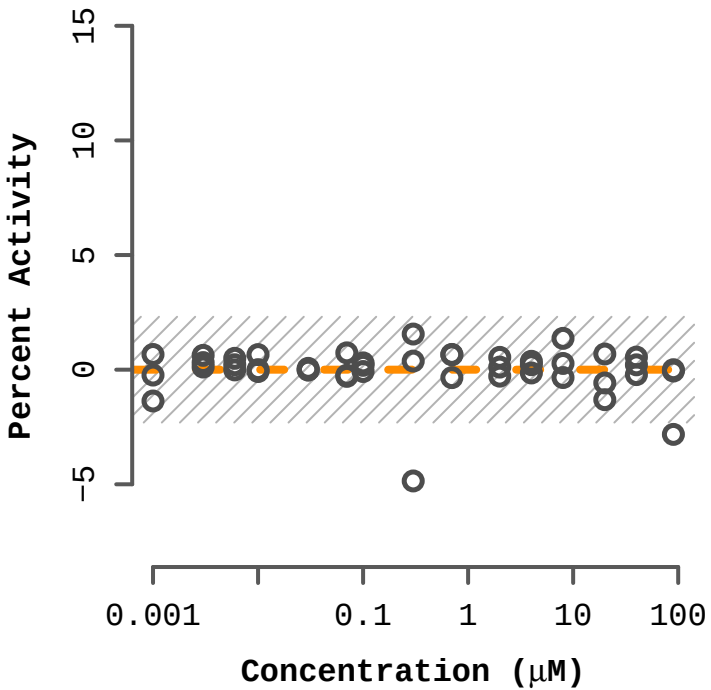
NAME: Acetamiprid
CHID: 34300 CASRN: 135410-20-7
SPID(S): Tox21_301046
M4ID: 12478087

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

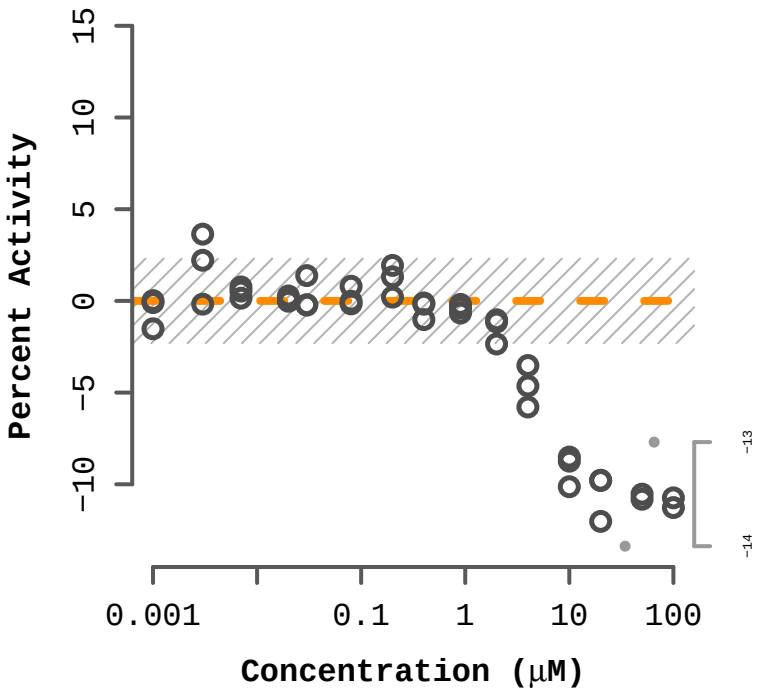
NAME: Fluroxypyr-meptyl
CHID: 34303 **CASRN:** 81406-37-3
SPID(S): Tox21_300897
M4ID: 12478236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.02	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.433 **MAX_MED:** 0.651 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

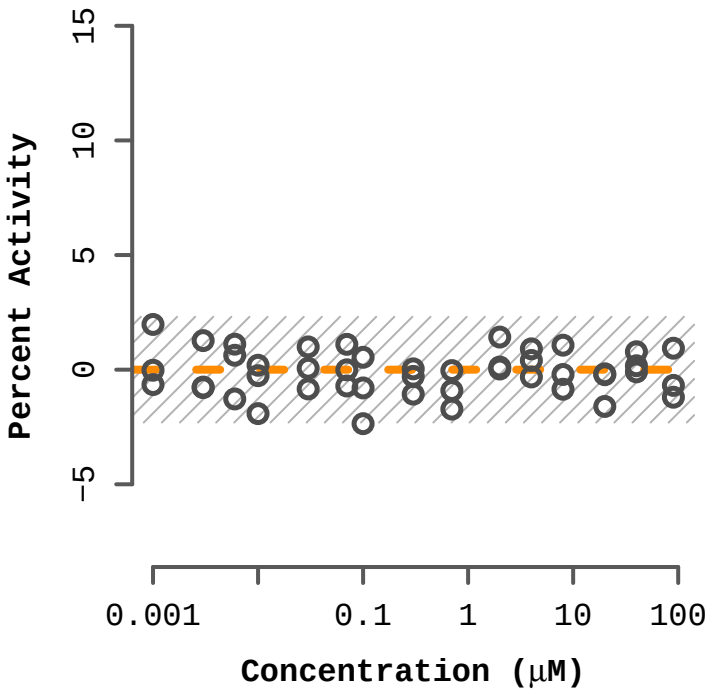
NAME: Benzalkonium chloride
CHID: 34317 **CASRN:** 8001-54-5
SPID(S): Tox21_302065
M4ID: 12477068 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	284.65	NA	NA
PROB:	1	NA	NA
RMSE:	5.87	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

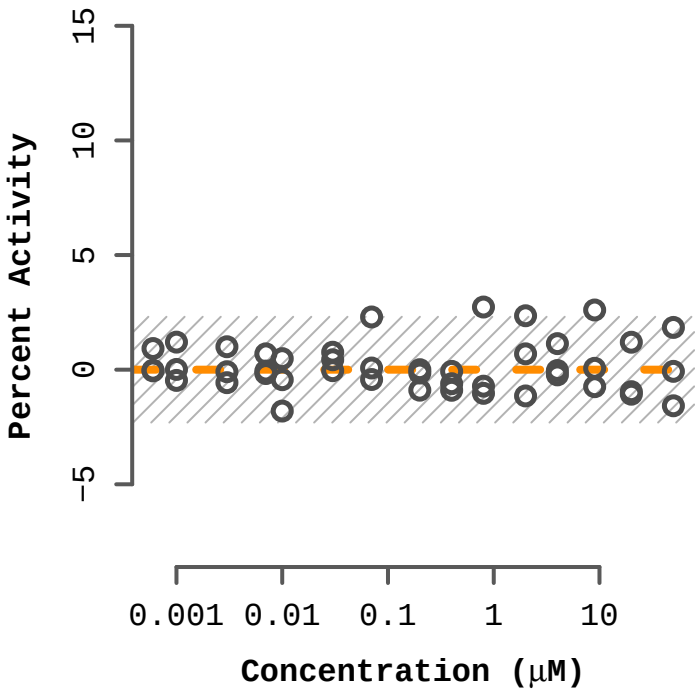
NAME: Phoxim
CHID: 34324 CASRN: 14816-18-3
SPID(S): Tox21_301580
M4ID: 12477553

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.524 MAX_MED: 0.629 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

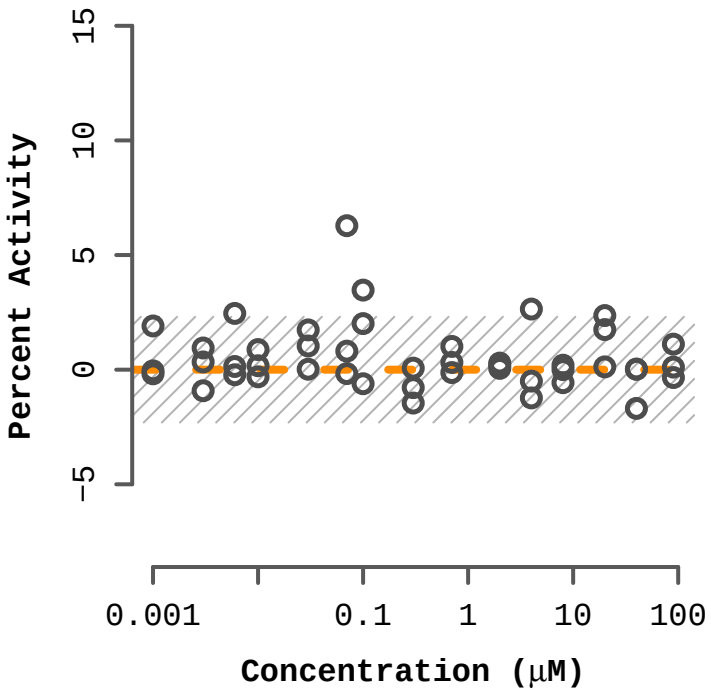
NAME: Phoxim
CHID: 34324 **CASRN:** 14816-18-3
SPID(S): Tox21_113357_1
M4ID: 12482676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.648 **MAX_MED:** 0.692 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

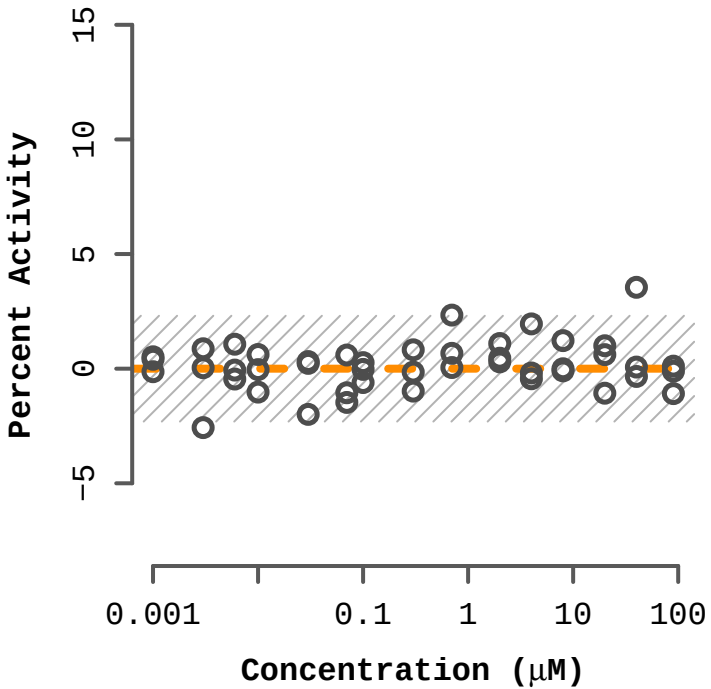
NAME: Ancymidol
CHID: 34338 **CASRN:** 12771-68-5
SPID(S): Tox21_301025
M4ID: 12478108

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.31 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

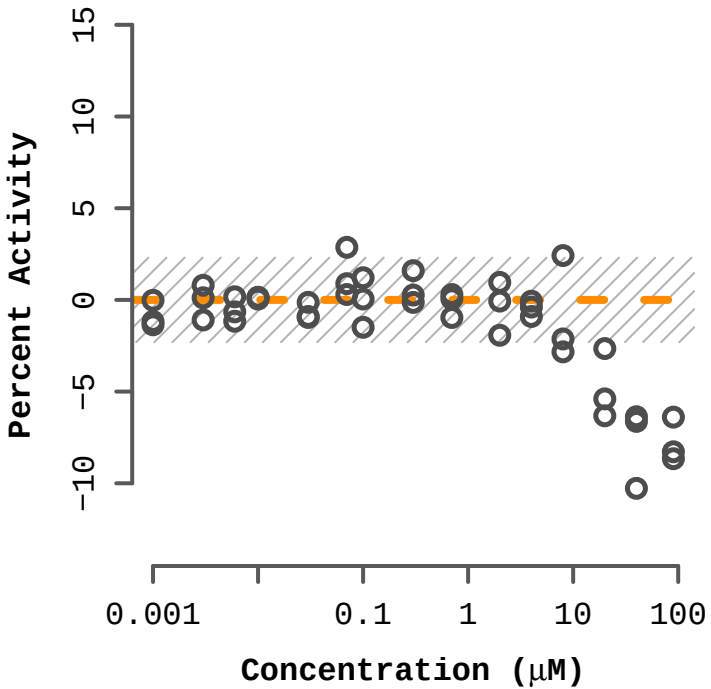
NAME: Triflumuron
CHID: 34355 CASRN: 64628-44-0
SPID(S): Tox21_301874
M4ID: 12477259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

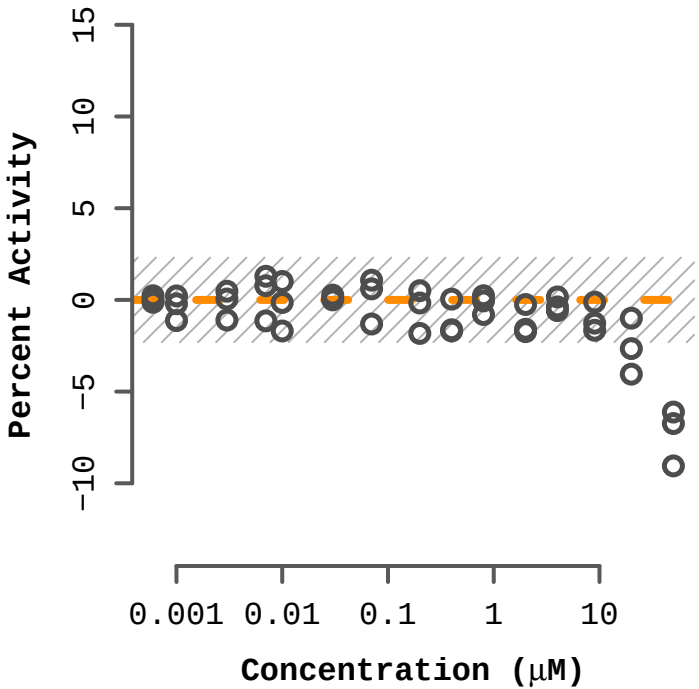
NAME: Lufenuron
CHID: 34357 CASRN: 103055-07-8
SPID(S): Tox21_300907
M4ID: 12478226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.85	NA	NA
PROB:	1	NA	NA
RMSE:	3.33	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.889 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

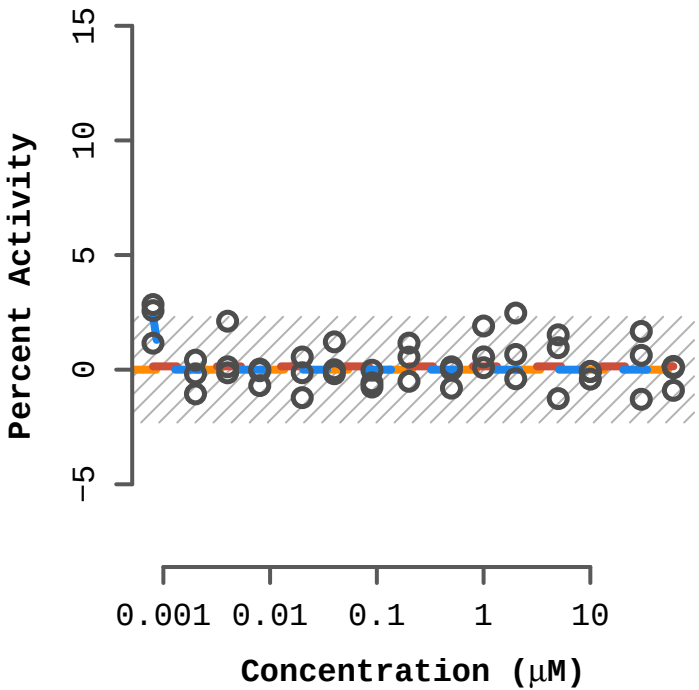
NAME: Lufenuron
CHID: 34357 **CASRN:** 103055-07-8
SPID(S): Tox21_111542_1
M4ID: 12483626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 0.307 **MAX_MED:** 0.775 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Denatonium saccharide
CHID: 34361 CASRN: 90823-38-4
SPID(S): Tox21_302351
M4ID: 12476782

HILL MODEL (in red):

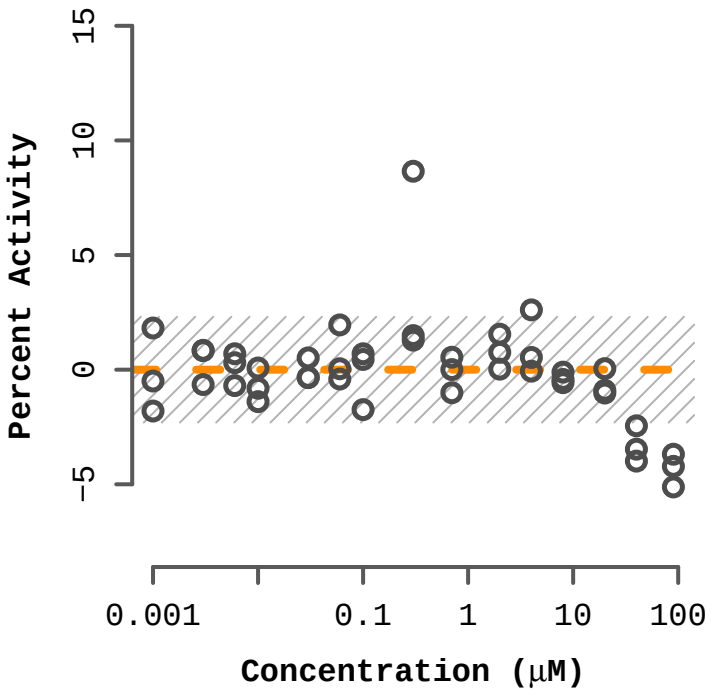
	tp	ga	gw
val:	0.144	−5.09	3.84
sd:	0.143	2980	5740

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.32	−4.66	1.13	−3.07	17.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	133.19	138.16	129.39
PROB:	0.13	0.01	0.86
RMSE:	1.06	1.03	0.9

MAX_MEAN: 2.19 **MAX_MED:** 2.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

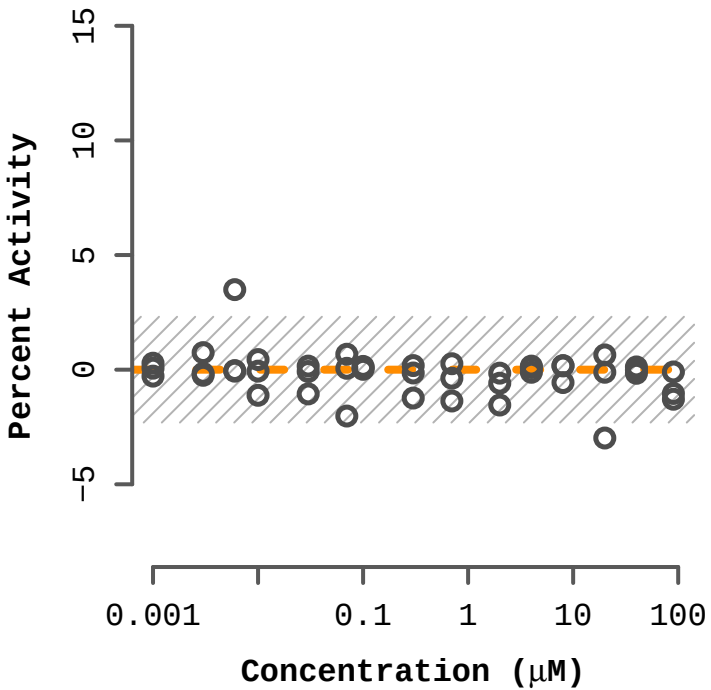
NAME: Butafenacil
CHID: 34365 CASRN: 134605-64-4
SPID(S): Tox21_301146
M4ID: 12477987

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.22	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 3.81 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

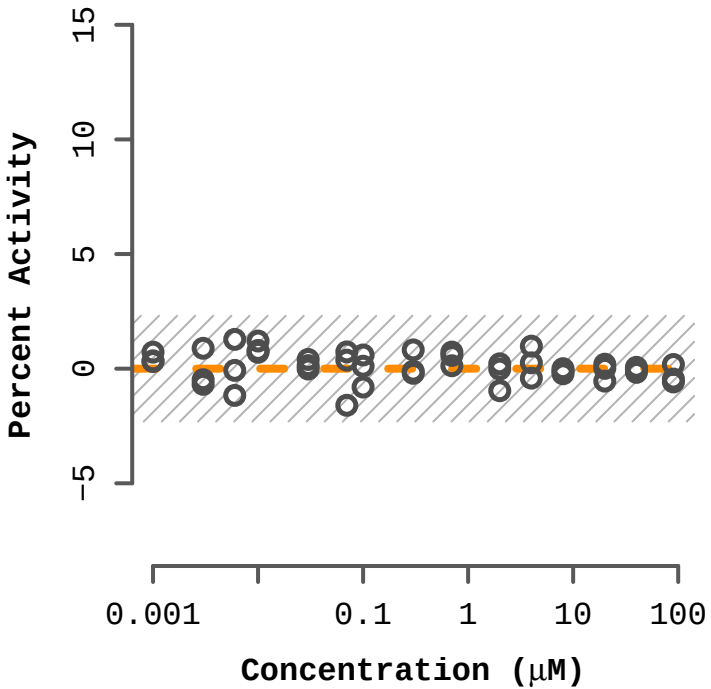
NAME: Cloransulam-methyl
CHID: 34372 **CASRN:** 147150-35-4
SPID(S): Tox21_304004
M4ID: 12475184

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.165 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

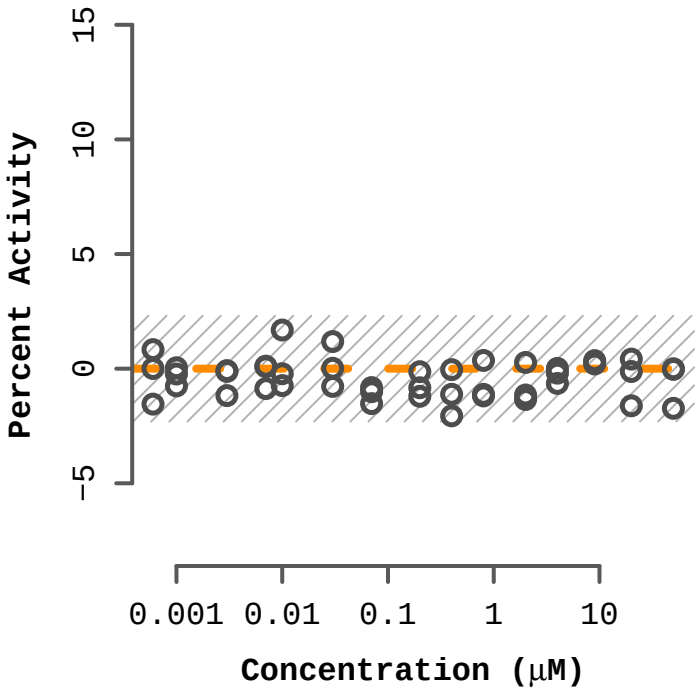
NAME: Denatonium benzoate
CHID: 34376 **CASRN:** 3734-33-6
SPID(S): Tox21_301587
M4ID: 12477546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 0.796 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

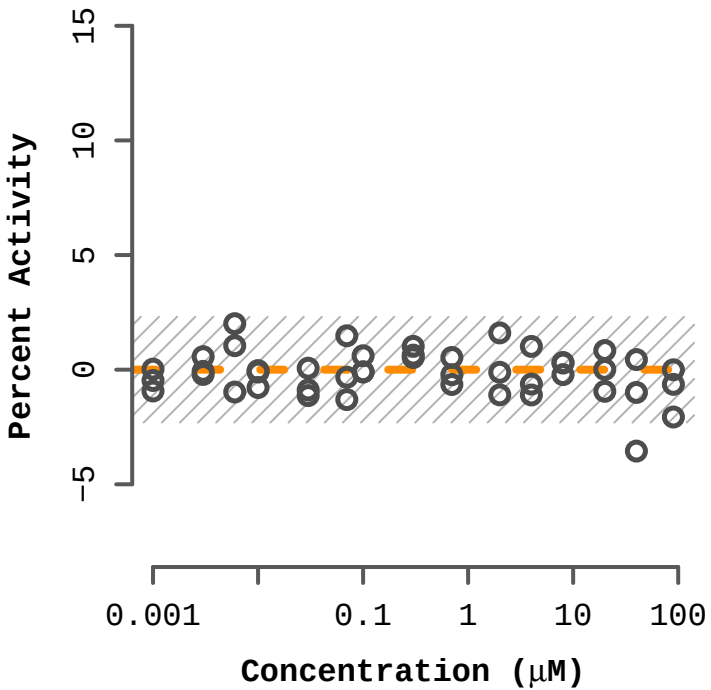
NAME: Denatonium benzoate
CHID: 34376 **CASRN:** 3734-33-6
SPID(S): Tox21_110754_1
M4ID: 12484133

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.277 **MAX_MED:** 0.273 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

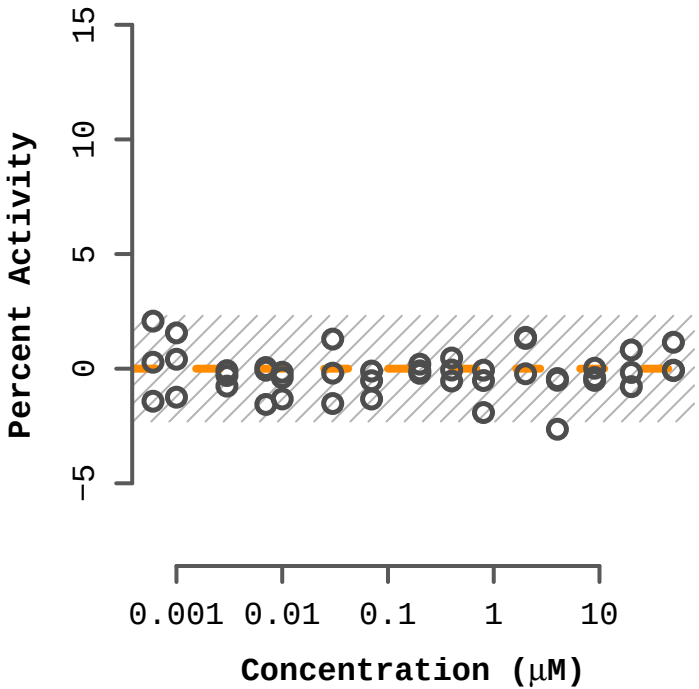
NAME: Bioresmethrin
CHID: 34382 **CASRN:** 28434-01-7
SPID(S): Tox21_302393
M4ID: 12476740

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

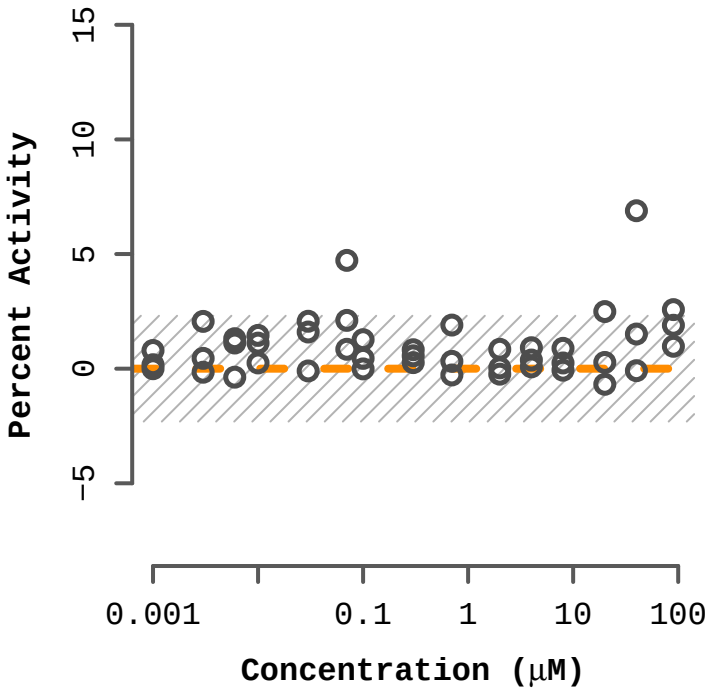
NAME: Bioresmethrin
CHID: 34382 **CASRN:** 28434-01-7
SPID(S): Tox21_112072_1
M4ID: 12483337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.823 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

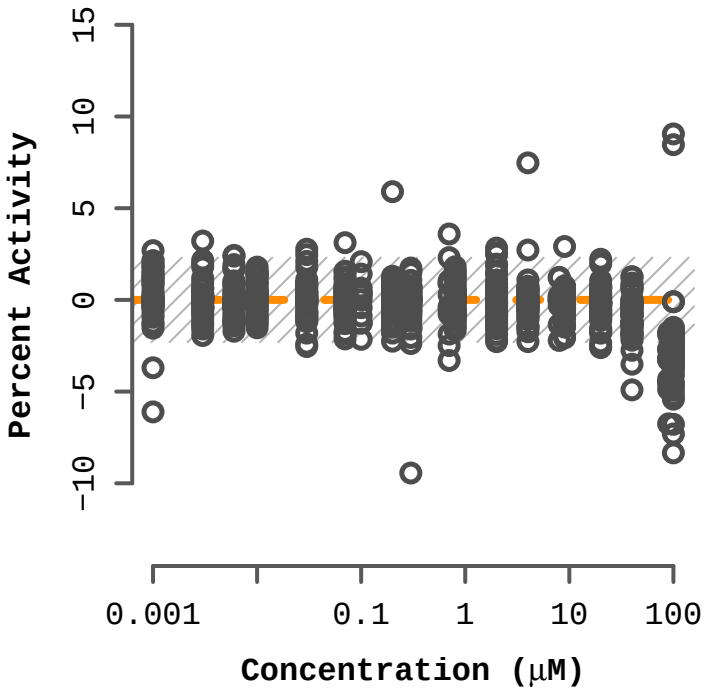
NAME: Bispyribac−sodium
CHID: 34383 **CASRN:** 125401−92−5
SPID(S): Tox21_302435
M4ID: 12476698

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 2.77 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

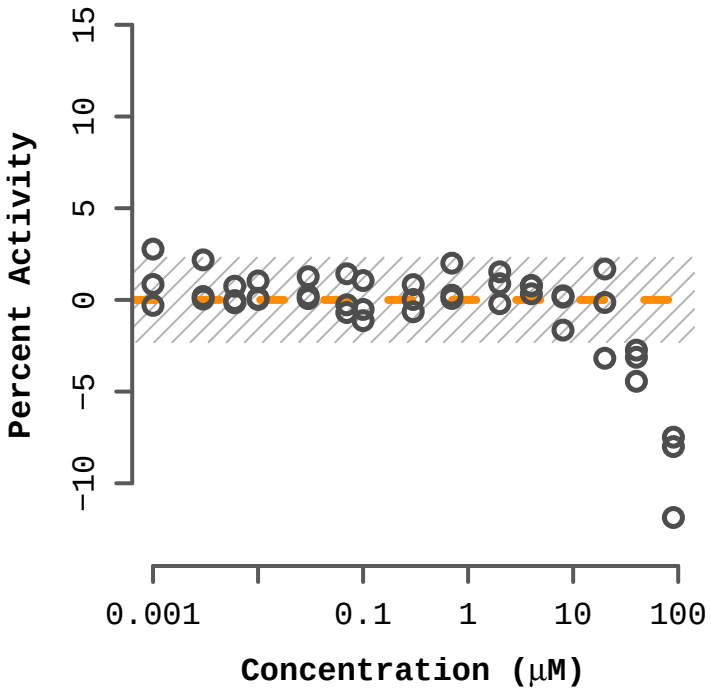
NAME: Boscalid
CHID: 34392 **CASRN:** 188425-85-6
SPID(S): Tox21_400045
M4ID: 12475092

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2442.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 0.182 **MAX_MED:** 0.171 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

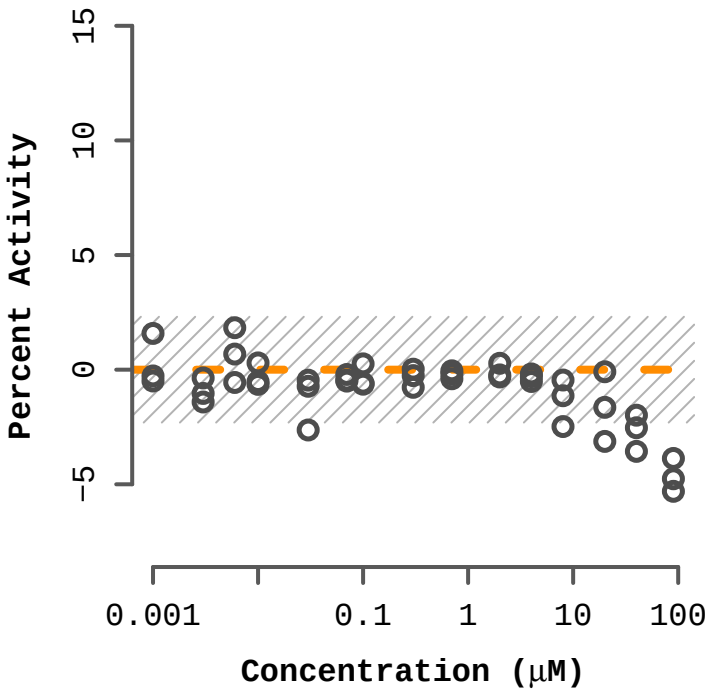
NAME: Buprofezin
CHID: 34401 CASRN: 69327-76-0
SPID(S): Tox21_301088
M4ID: 12478045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.33	NA	NA
PROB:	1	NA	NA
RMSE:	2.77	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.886 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

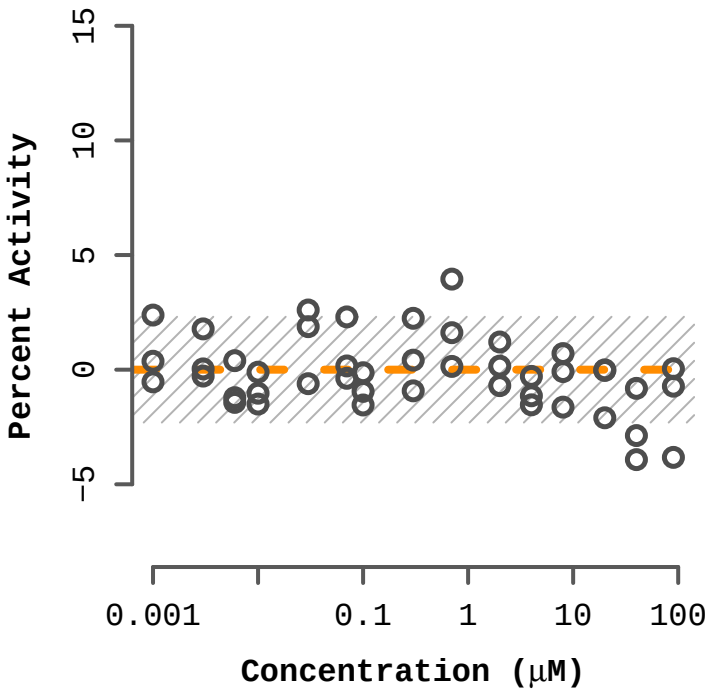
NAME: Butachlor
CHID: 34402 CASRN: 23184-66-9
SPID(S): Tox21_300940
M4ID: 12478193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 0.652 MAX_MED: 0.682 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

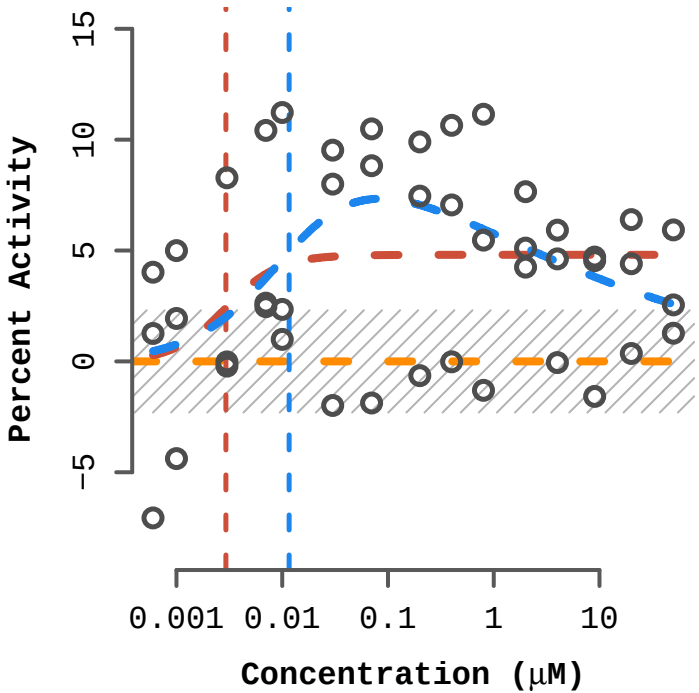
NAME: Cinmethylin
CHID: 34456 **CASRN:** 87818-31-3
SPID(S): Tox21_301127
M4ID: 12478006

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clethodim
CHID: 34458 CASRN: 99129-21-2
SPID(S): Tox21_304029
M4ID: 12475159

HILL MODEL (in red):

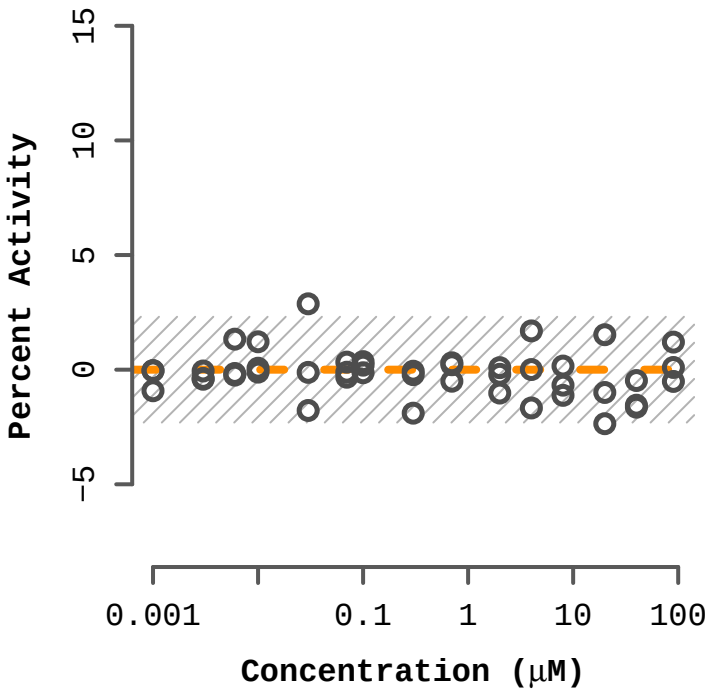
	tp	ga	gw
val:	4.81	−2.53	1.75
sd:	0.802	0.507	2.29

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.2	−1.93	1.07	−0.345	0.3
sd:	52.8	1.3	1	11.3	0.703

	CNST	HILL	GNLS
AIC:	294.31	269.13	269.31
PROB:	0	0.52	0.48
RMSE:	5.91	4.11	4.1

MAX_MEAN: 5.9 MAX_MED: 8.83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

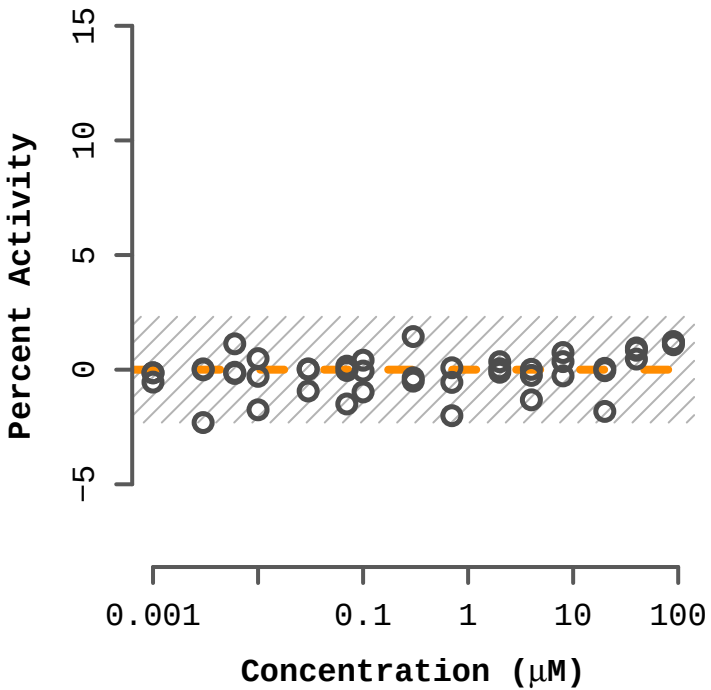
NAME: Clofencet-potassium
CHID: 34460 **CASRN:** 82697-71-0
SPID(S): Tox21_303919
M4ID: 12475269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.02	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.393 **MAX_MED:** 0.216 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

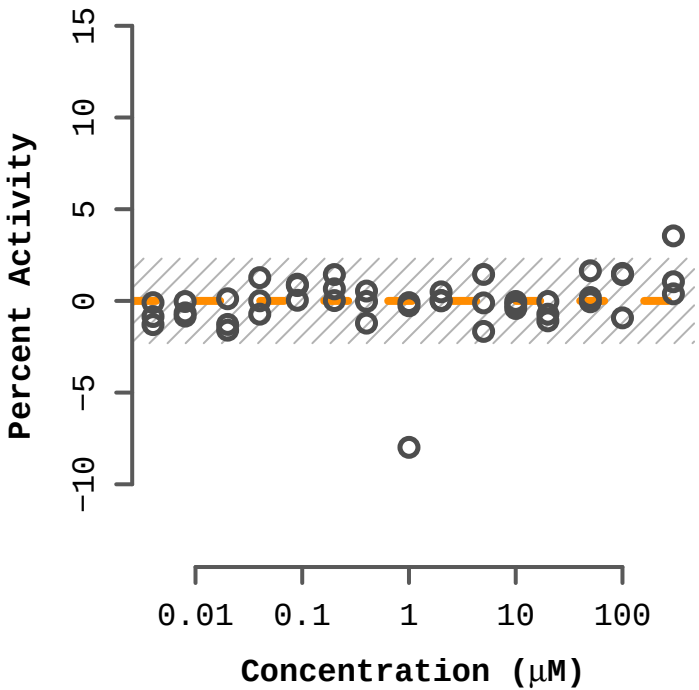
NAME: Clothianidin
CHID: 34465 **CASRN:** 210880-92-5
SPID(S): Tox21_301191
M4ID: 12477942

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

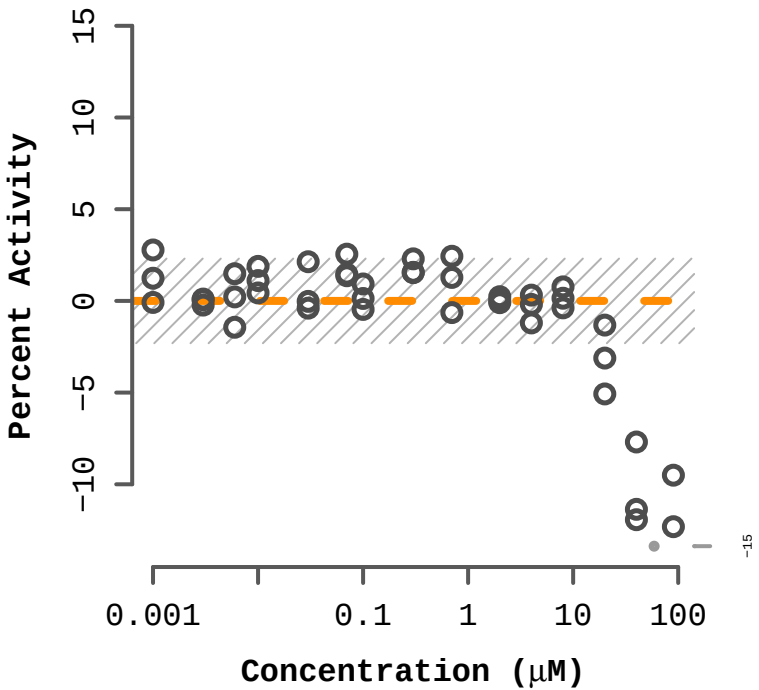
NAME: Cyanamide
CHID: 34490 **CASRN:** 420-04-2
SPID(S): Tox21_300678
M4ID: 12478455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

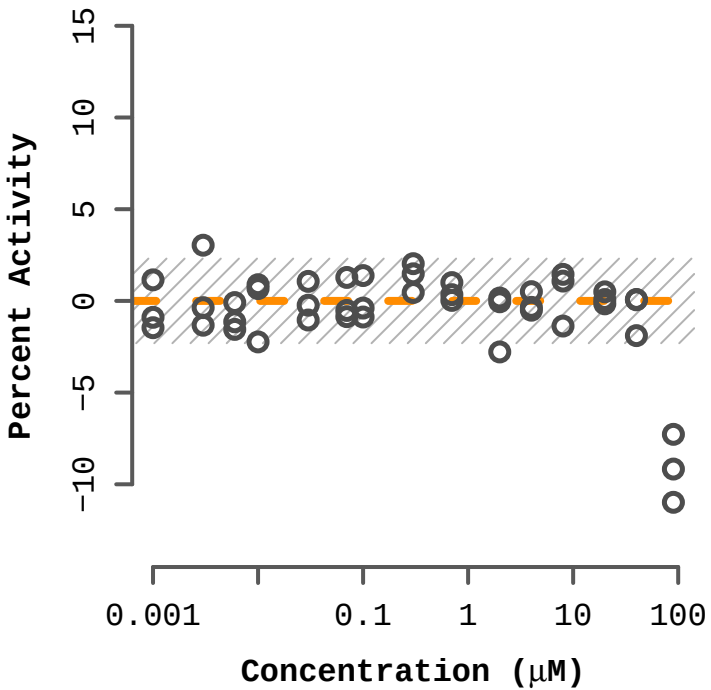
NAME: Cyazofamid
CHID: 34492 **CASRN:** 120116-88-3
SPID(S): Tox21_300788
M4ID: 12478345 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	240.77	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

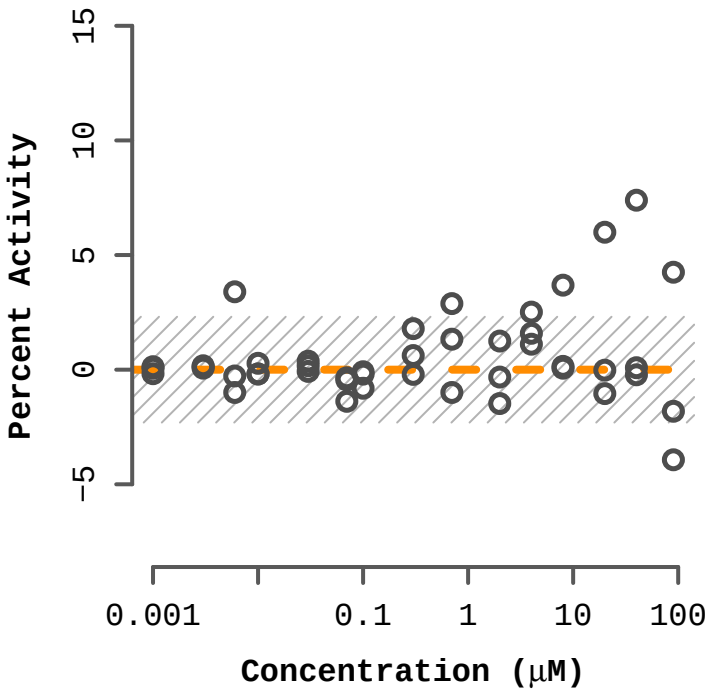
NAME: Metconazole
CHID: 34497 **CASRN:** 125116-23-6
SPID(S): Tox21_302273
M4ID: 12476860

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

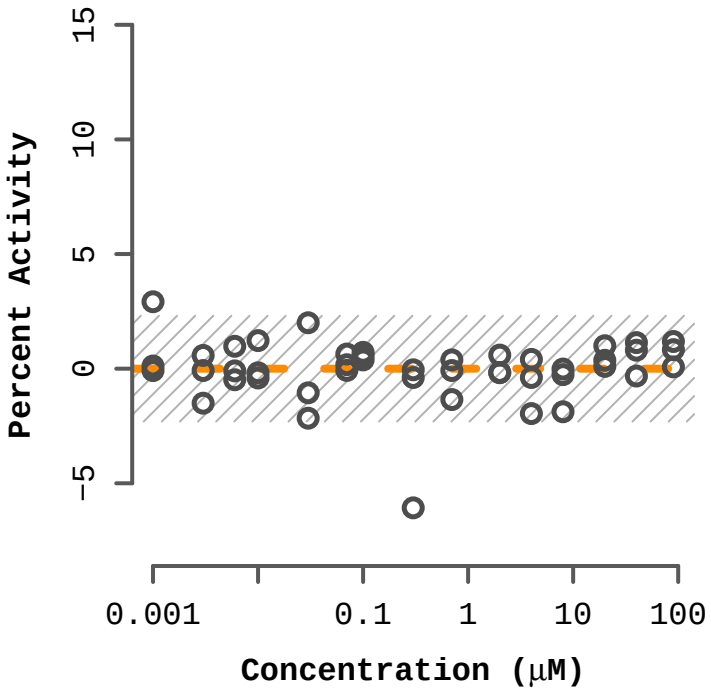
NAME: gamma-Cyhalothrin
CHID: 34501 **CASRN:** 76703-62-3
SPID(S): Tox21_303815
M4ID: 12475373

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 2.42 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

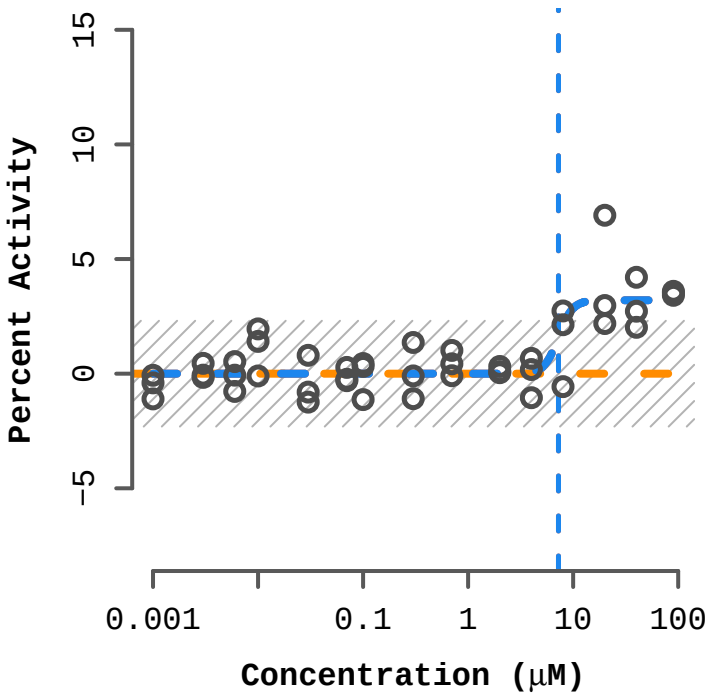
NAME: Cyhalofop-butyl
CHID: 34503 CASRN: 122008-85-9
SPID(S): Tox21_301029
M4ID: 12478104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.986 MAX_MED: 0.831 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Desmedipham
CHID: 34518 CASRN: 13684-56-5
SPID(S): Tox21_301854
M4ID: 12477279

HILL MODEL (in red):

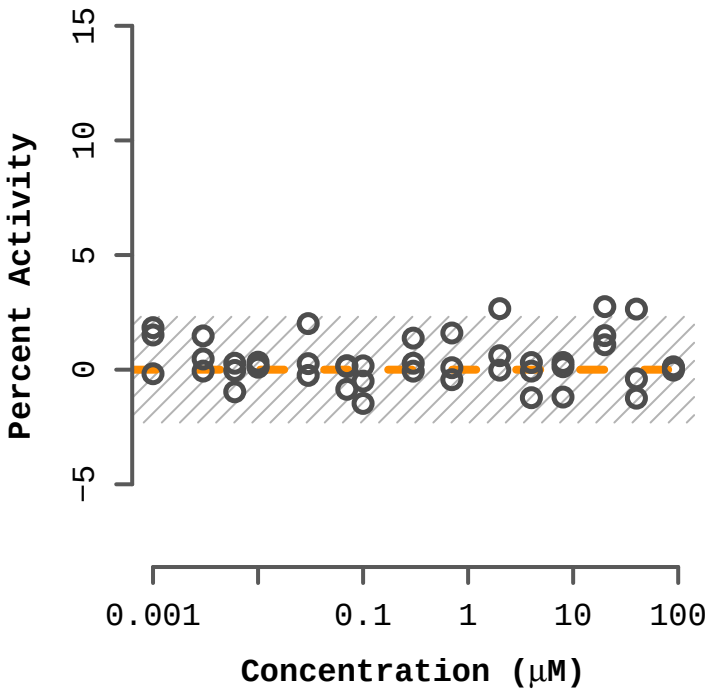
	tp	ga	gw
val:	3.2	0.86	6.49
sd:	0.288	0.0875	12.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.2	0.86	6.49	3.34	6.31
sd:	0.288	0.0875	12.3	1850	8460

	CNST	HILL	GNLS
AIC:	178.25	127.2	131.2
PROB:	0	0.88	0.12
RMSE:	1.88	0.99	0.99

MAX_MEAN: 4.02 MAX_MED: 3.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

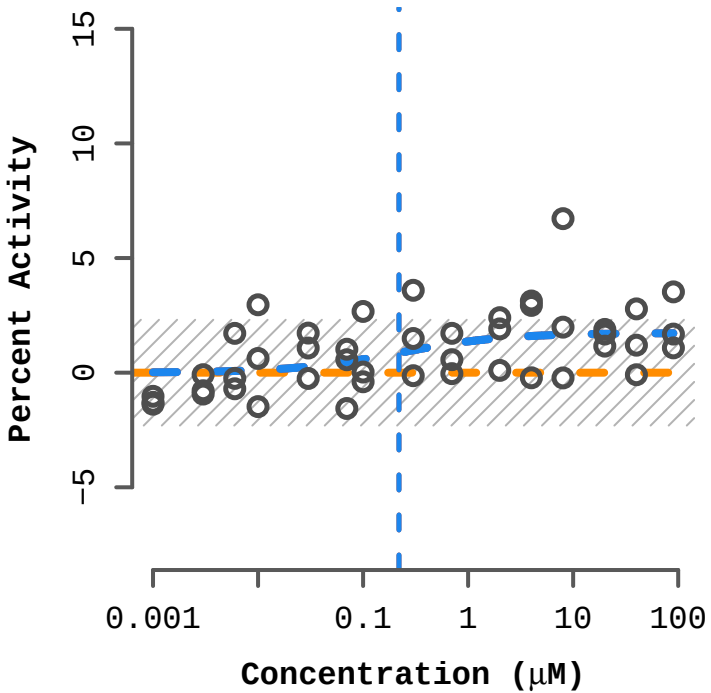
NAME: Diclosulam
CHID: 34528 **CASRN:** 145701-21-9
SPID(S): Tox21_300765
M4ID: 12478368

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiophanate
CHID: 34531 CASRN: 23564-06-9
SPID(S): Tox21_301909
M4ID: 12477224

HILL MODEL (in red):

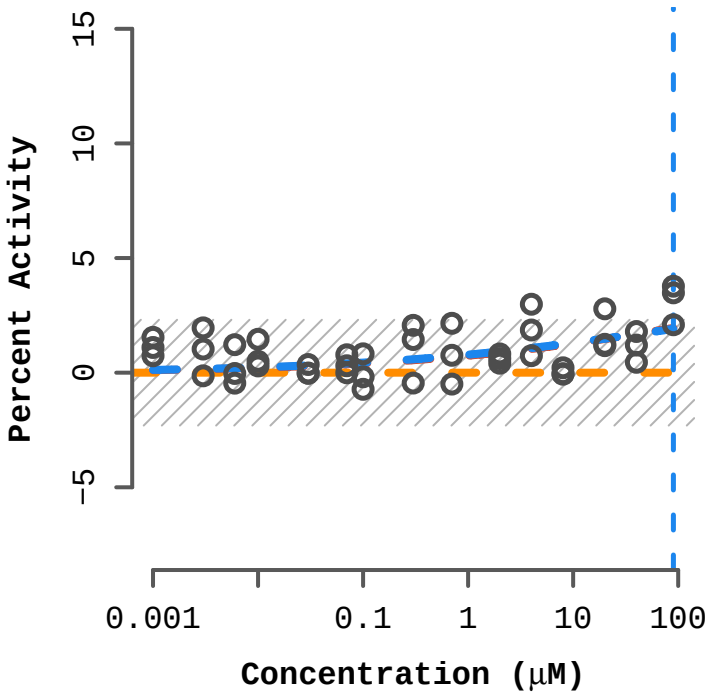
	tp	ga	gw
val:	1.73	−0.658	0.863
sd:	0.412	0.639	0.594

GAIN-LOSS MODEL (in blue):

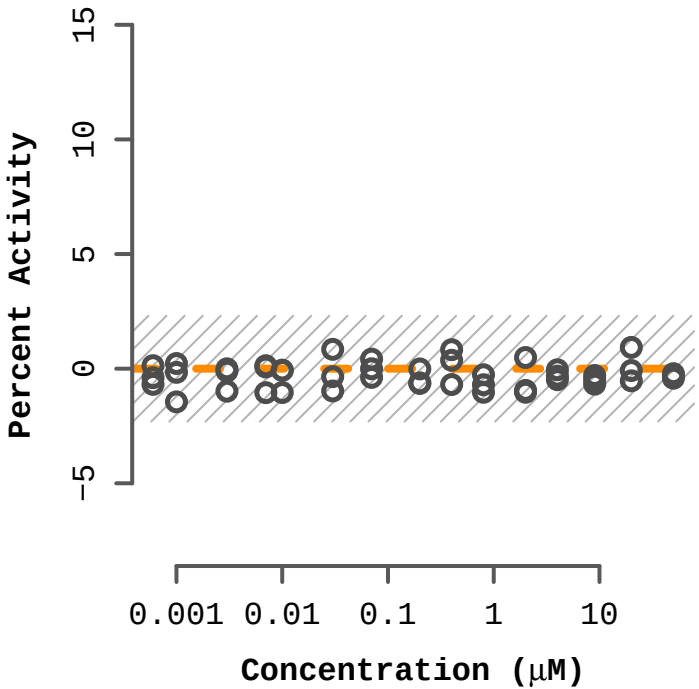
	tp	ga	gw	la	lw
val:	1.73	−0.658	0.863	3.77	3.46
sd:	0.412	0.639	0.594	565	1100

	CNST	HILL	GNLS
AIC:	186.48	167.37	171.37
PROB:	0	0.88	0.12
RMSE:	1.92	1.44	1.44

MAX_MEAN: 2.83 MAX_MED: 2.94 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diflufenzopyr
CHID:    34538   CASRN: 109293-97-2
SPID(S): Tox21_303700
M4ID:    12475488

HILL MODEL (in red):
      tp       ga       gw
val:  4.53     2.36     0.3
sd:   3.81     1.95     0.171

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.82     1.95     0.3      3.76     4.43
sd:   4.74     2.68     0.15     1220     3000

      CNST        HILL        GNLS
AIC:  159.07      133.69      137.97
PROB: 0           0.89        0.11
RMSE: 1.4         0.93        0.93

MAX_MEAN: 3.12      MAX_MED: 3.48      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

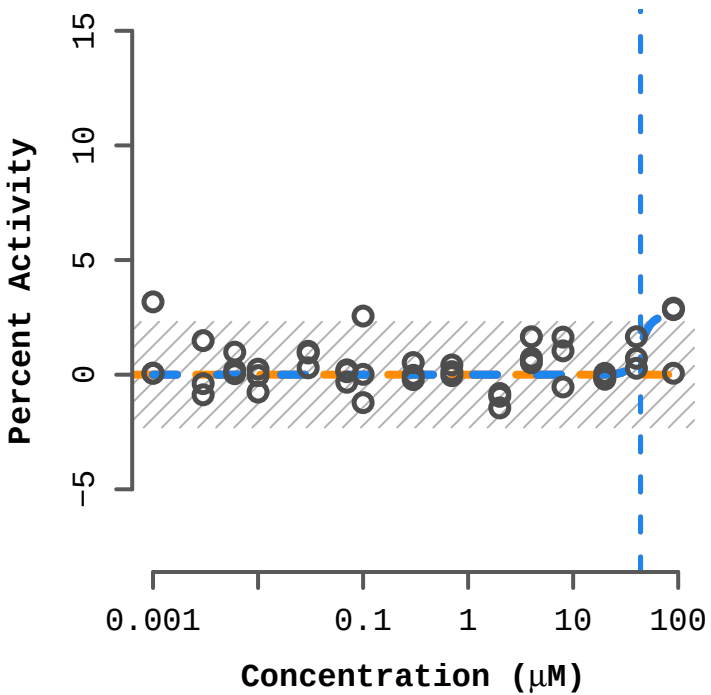
NAME: Dikegulac sodium
CHID: 34540 **CASRN:** 52508-35-7
SPID(S): Tox21_112391_1
M4ID: 12483119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.169 **MAX_MED:** 0.367 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethenamid-P
CHID: 34542 CASRN: 163515-14-8
SPID(S): Tox21_303923
M4ID: 12475265

HILL MODEL (in red):

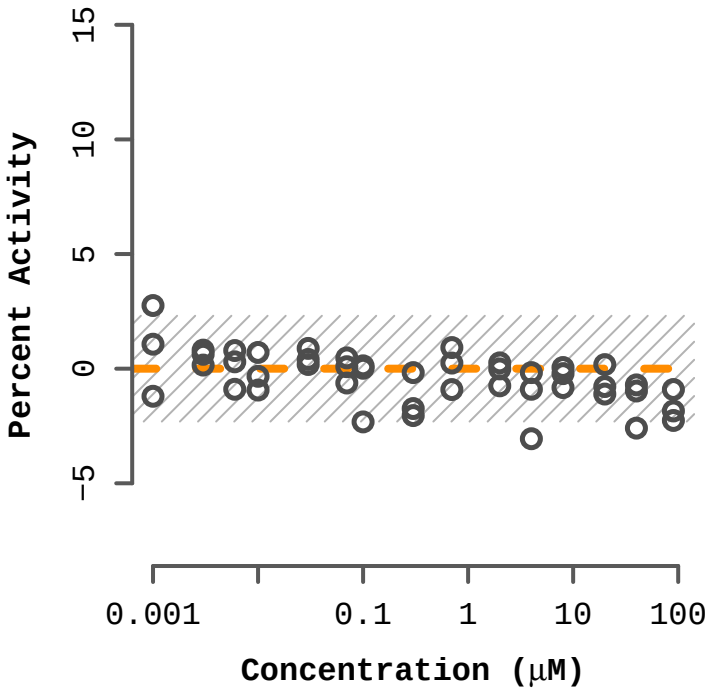
	tp	ga	gw
val:	2.57	1.64	8
sd:	0.522	0.127	22.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.57	1.64	8	3.93	9.84
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	134.86	129.16	133.16
PROB:	0.05	0.84	0.11
RMSE:	1.12	0.99	0.99

MAX_MEAN: 1.93 MAX_MED: 2.84 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

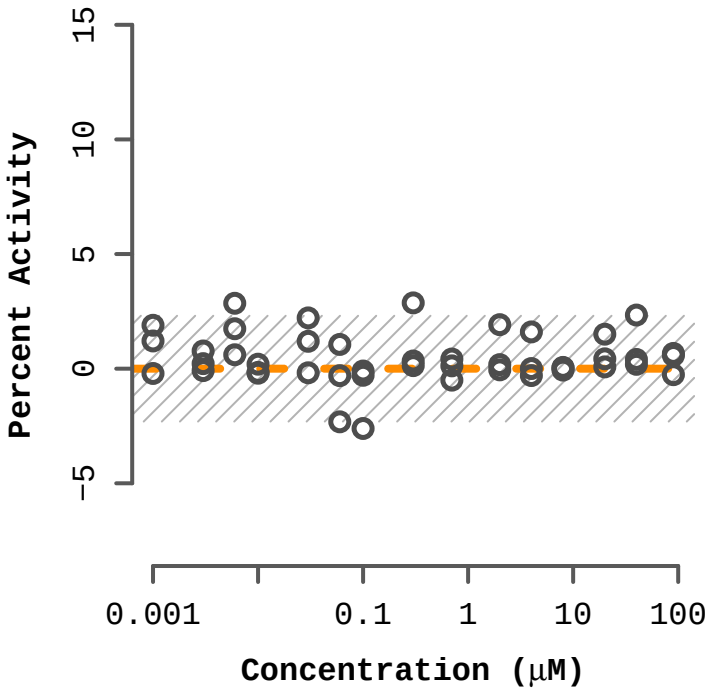
NAME: Dimethomorph
CHID: 34545 CASRN: 110488-70-5
SPID(S): Tox21_300911
M4ID: 12478222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.874 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

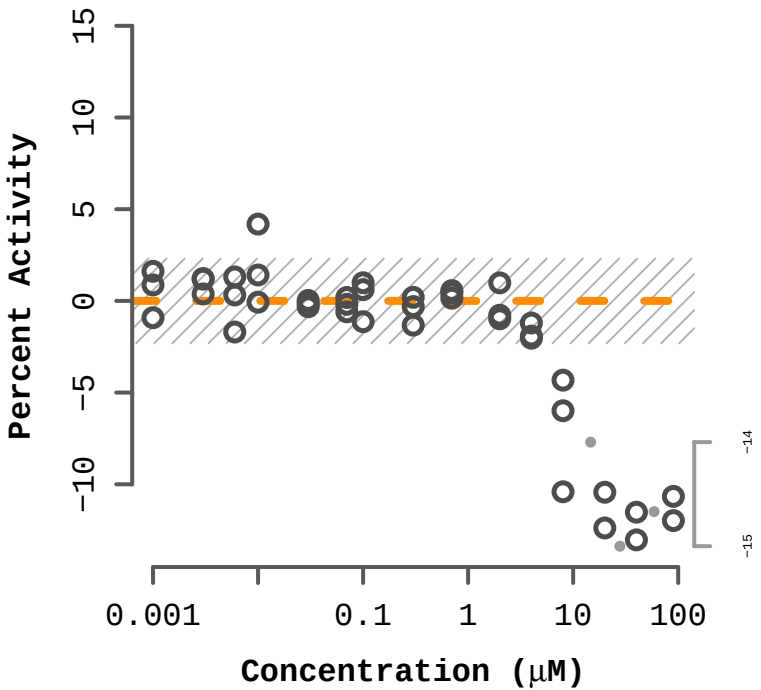
NAME: Dinotefuran
CHID: 34549 **CASRN:** 165252-70-0
SPID(S): Tox21_302442
M4ID: 12476691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

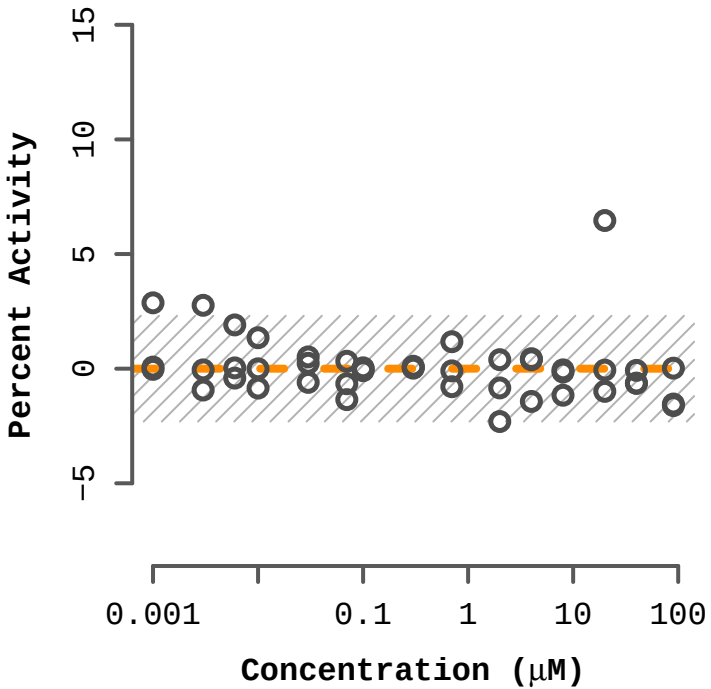
NAME: Emamectin benzoate
CHID: 34566 **CASRN:** 155569-91-8
SPID(S): Tox21_300787
M4ID: 12478346 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.84	NA	NA
PROB:	1	NA	NA
RMSE:	6.1	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

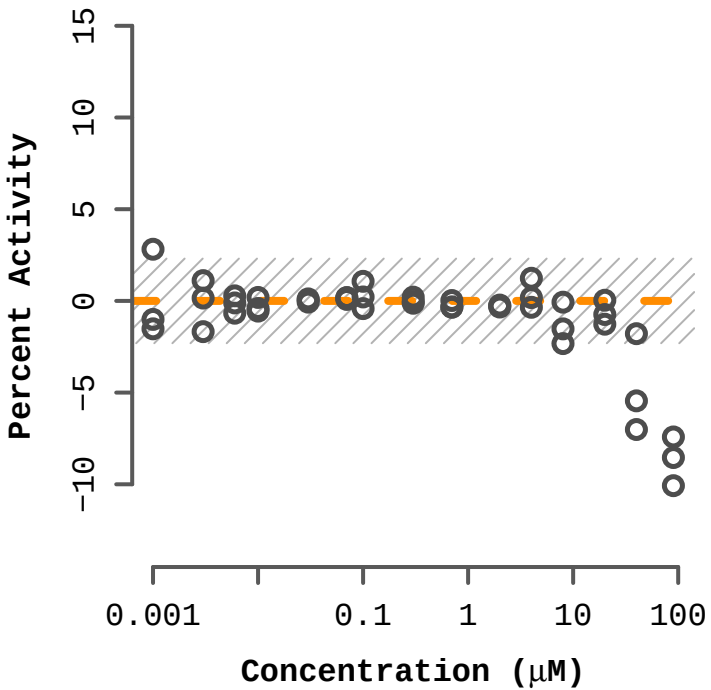
NAME: 2-Bromo-4-hydroxyacetophenone
CHID: 34576 **CASRN:** 2491-38-5
SPID(S): Tox21_301941
M4ID: 12477192

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 0.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

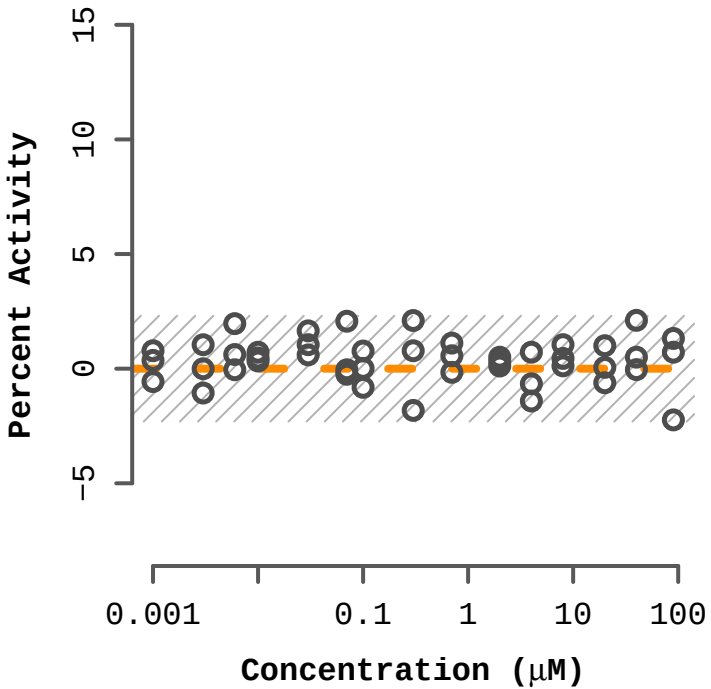
NAME: Ethofumesate
CHID: 34580 **CASRN:** 26225-79-6
SPID(S): Tox21_301112
M4ID: 12478021

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 0.357 **MAX_MED:** 0.218 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

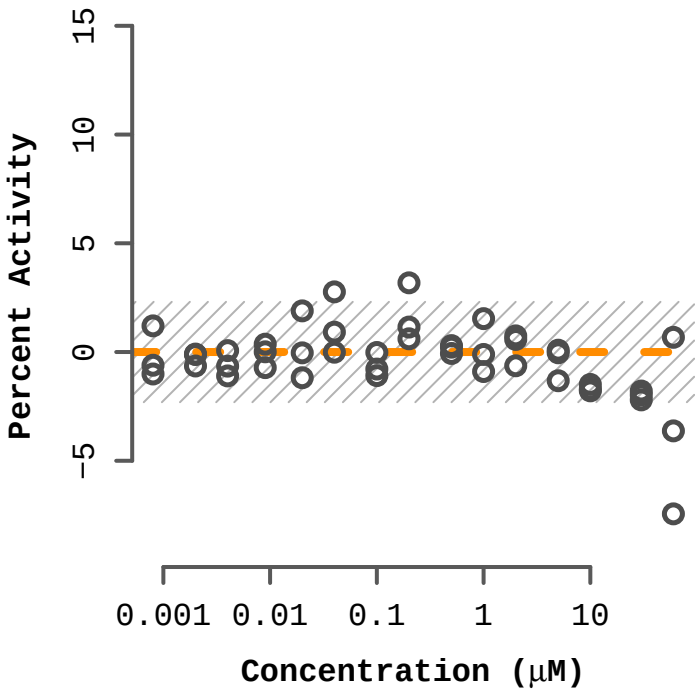
NAME: Ethyl 1-naphthaleneacetate
CHID: 34583 **CASRN:** 2122-70-5
SPID(S): Tox21_301469
M4ID: 12477664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

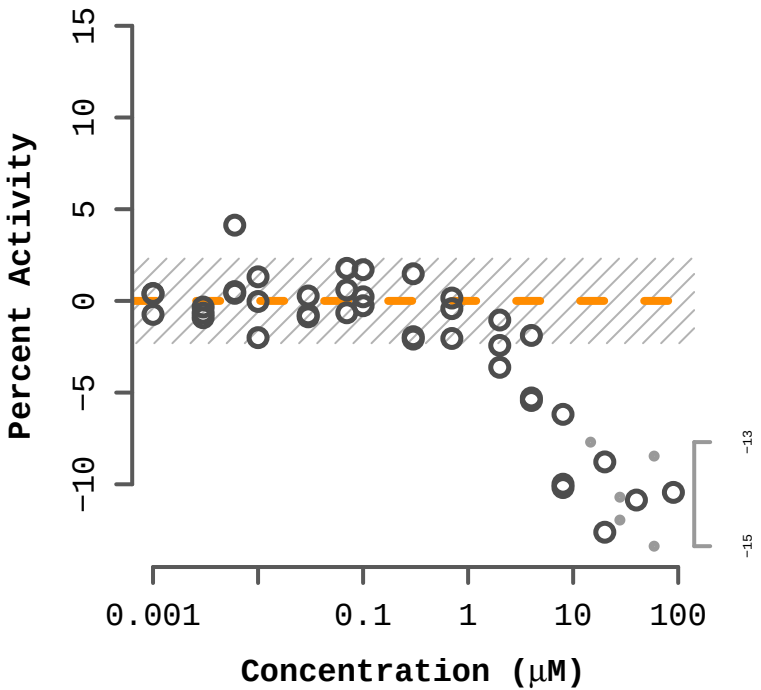
NAME: Etoxazole
CHID: 34586 CASRN: 153233-91-1
SPID(S): Tox21_301024
M4ID: 12478109

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 1.65 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

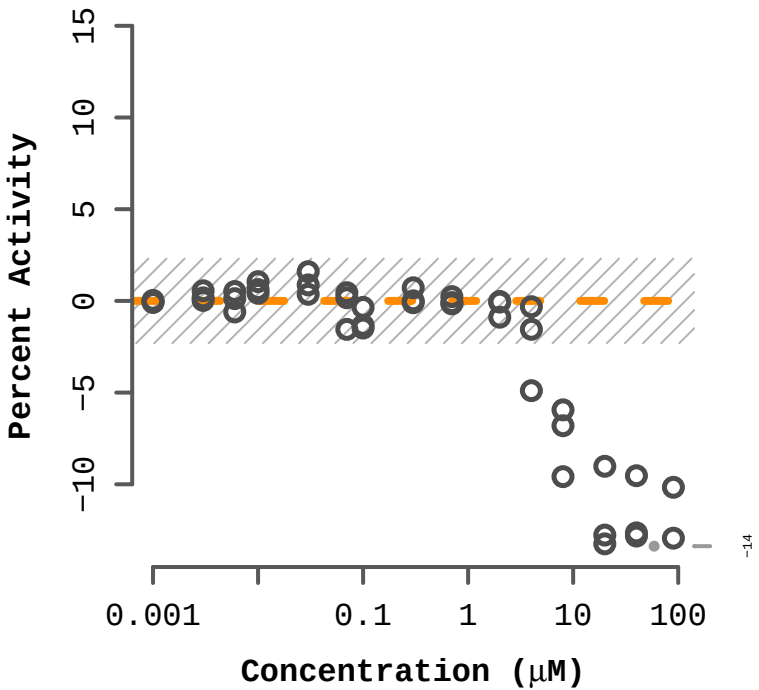
NAME: Famoxadone
CHID: 34588 **CASRN:** 131807-57-3
SPID(S): Tox21_301144
M4ID: 12477989 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	291.38	NA	NA
PROB:	1	NA	NA
RMSE:	6.37	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 0.601 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

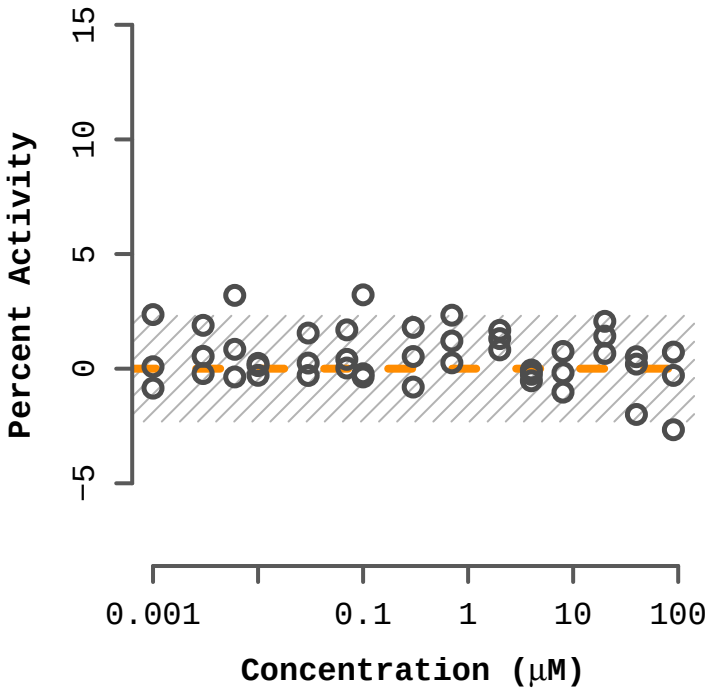
NAME: Fenamidone
CHID: 34590 **CASRN:** 161326-34-7
SPID(S): Tox21_301093
M4ID: 12478040 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	279.03	NA	NA
PROB:	1	NA	NA
RMSE:	5.83	NA	NA

MAX_MEAN: 0.945 **MAX_MED:** 0.876 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

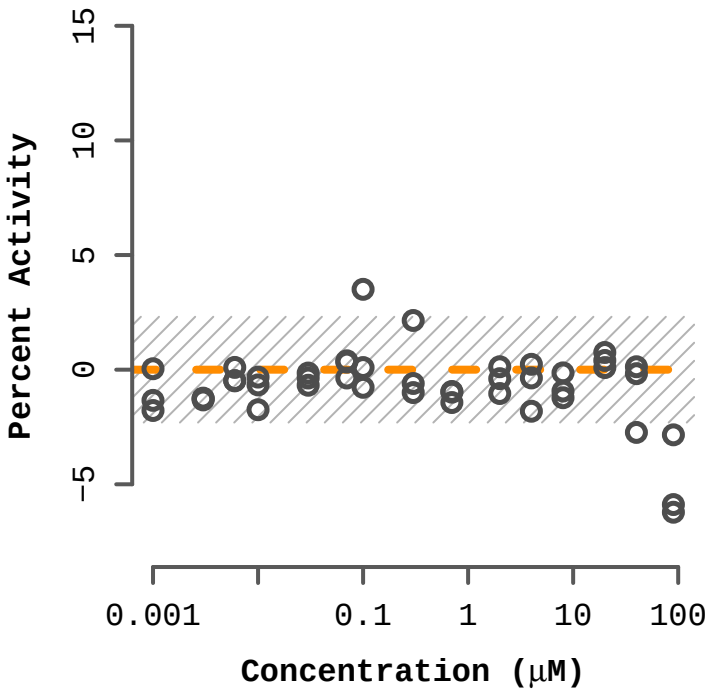
NAME: Fenoxaprop-P-ethyl
CHID: 34598 **CASRN:** 71283-80-2
SPID(S): Tox21_301569
M4ID: 12477564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

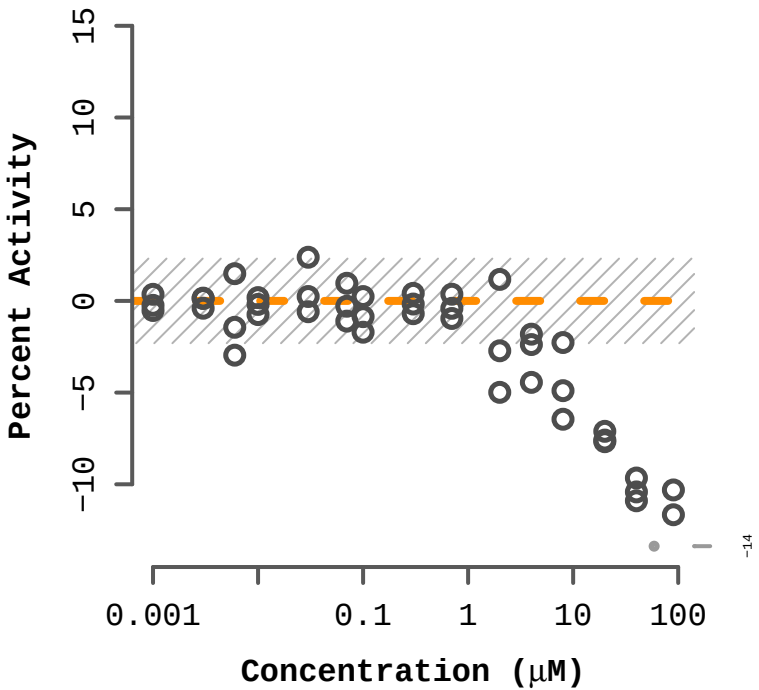
NAME: (2R,6S)-Fenpropimorph
CHID: 34601 **CASRN:** 67564-91-4
SPID(S): Tox21_301571
M4ID: 12477562

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 0.403 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

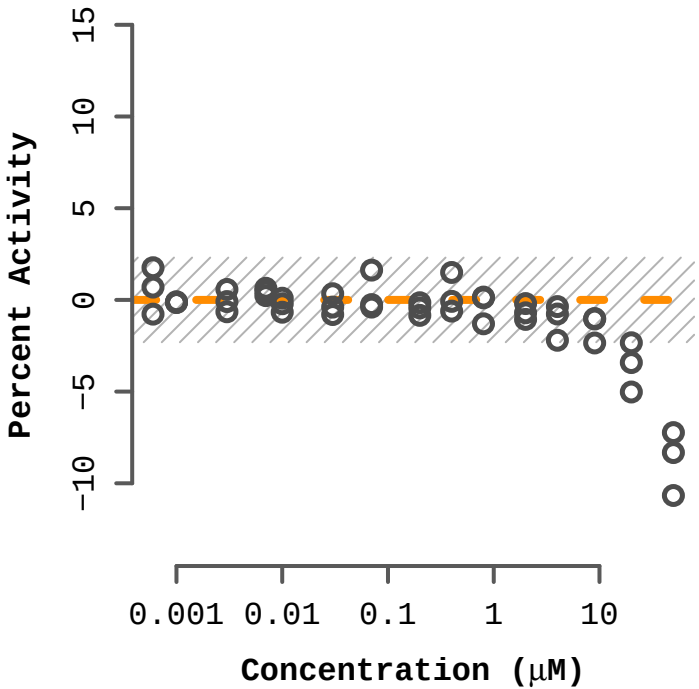
NAME: Fipronil
CHID: 34609 CASRN: 120068-37-3
SPID(S): Tox21_301114
M4ID: 12478019 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.83	NA	NA
PROB:	1	NA	NA
RMSE:	4.95	NA	NA

MAX_MEAN: 0.678 MAX_MED: 0.241 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

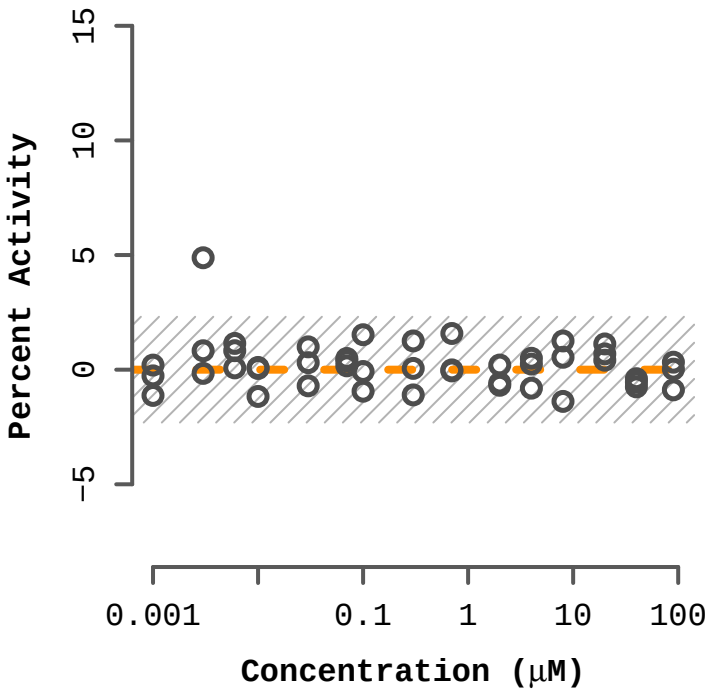
NAME: Fipronil
CHID: 34609 **CASRN:** 120068-37-3
SPID(S): Tox21_111300_1
M4ID: 12483781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.9	NA	NA
PROB:	1	NA	NA
RMSE:	2.61	NA	NA

MAX_MEAN: 0.56 **MAX_MED:** 0.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

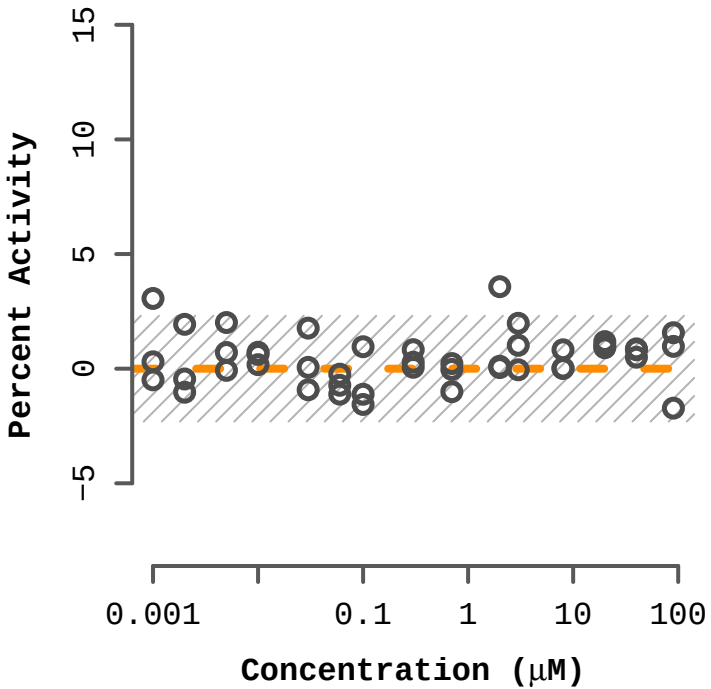
NAME: Fluazifop-butyl
CHID: 34612 **CASRN:** 69806-50-4
SPID(S): Tox21_301085
M4ID: 12478048

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 0.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

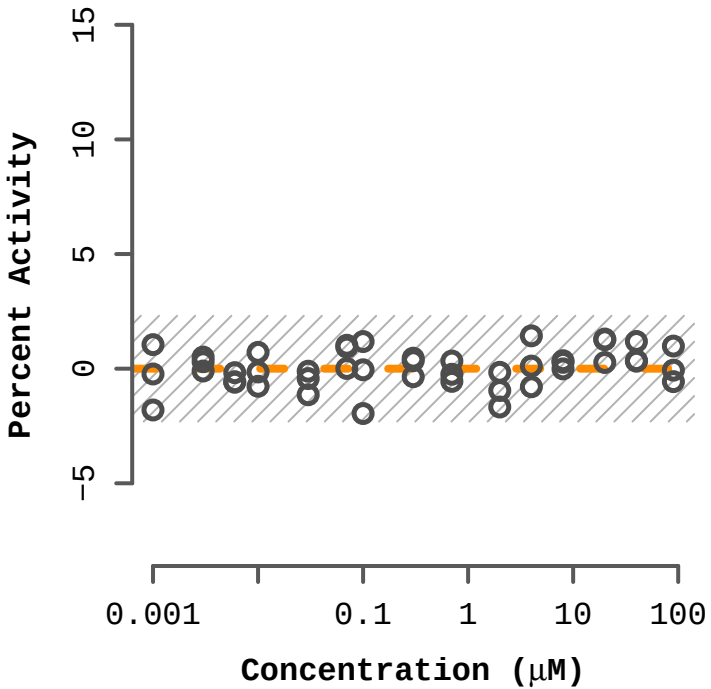
NAME: Flucarbazone−sodium
CHID: 34614 **CASRN:** 181274−17−9
SPID(S): Tox21_303495
M4ID: 12475647

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

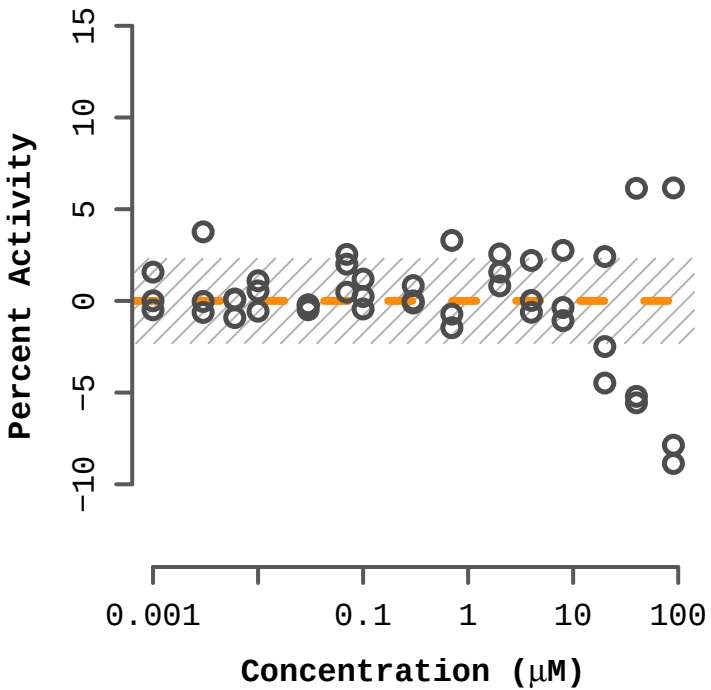
NAME: Flufenpyr-ethyl
CHID: 34618 **CASRN:** 188489-07-8
SPID(S): Tox21_300852
M4ID: 12478281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.943 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

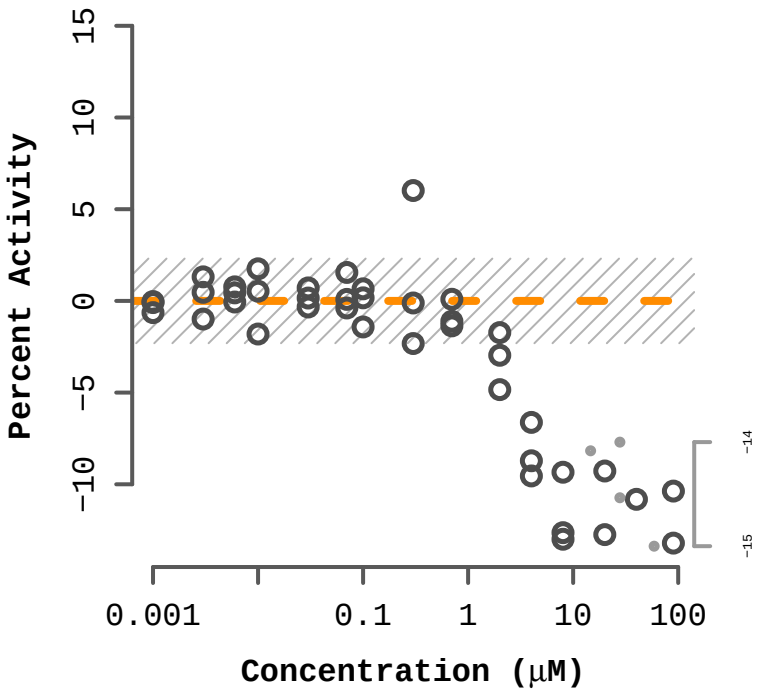
NAME: Fluopicolide
CHID: 34624 **CASRN:** 239110-15-7
SPID(S): Tox21_303793
M4ID: 12475395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

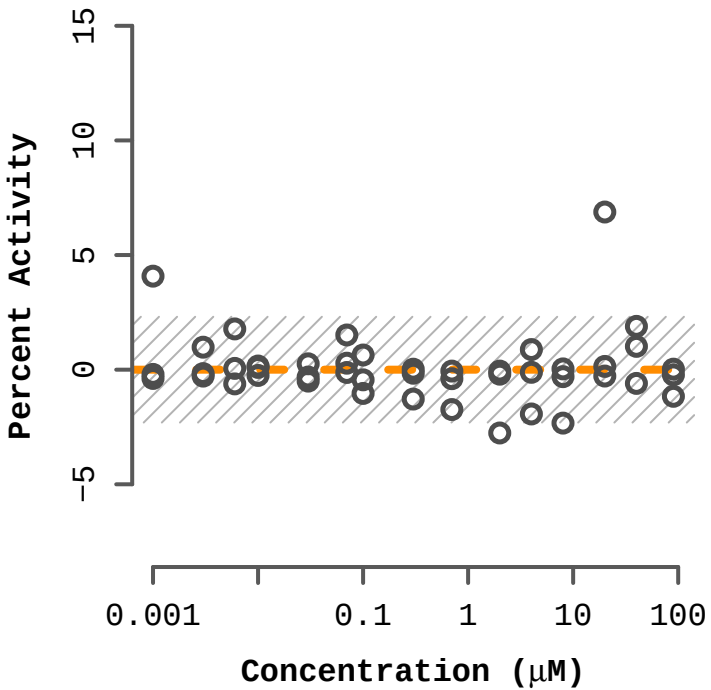
NAME: Fluoxastrobin
CHID: 34625 **CASRN:** 361377-29-9
SPID(S): Tox21_300824
M4ID: 12478309 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.23	NA	NA
PROB:	1	NA	NA
RMSE:	7	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

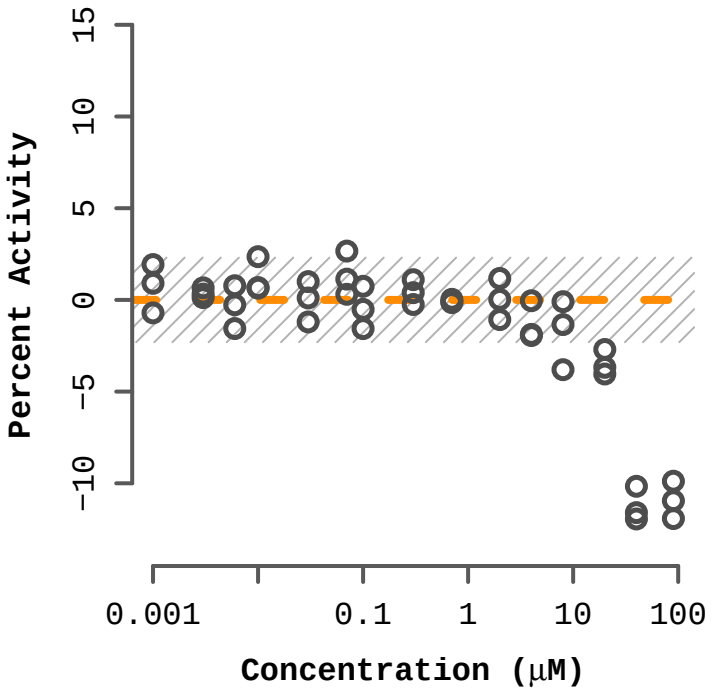
NAME: Fluroxypyr
CHID: 34627 **CASRN:** 69377-81-7
SPID(S): Tox21_301096
M4ID: 12478037

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

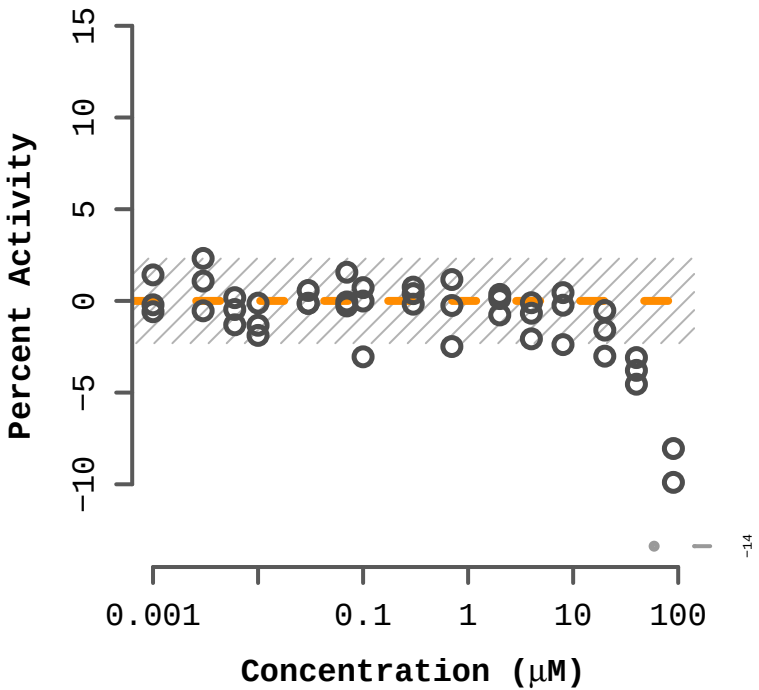
NAME: Forchlorfenuron
CHID: 34634 **CASRN:** 68157-60-8
SPID(S): Tox21_301094
M4ID: 12478039

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.01	NA	NA
PROB:	1	NA	NA
RMSE:	4.31	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

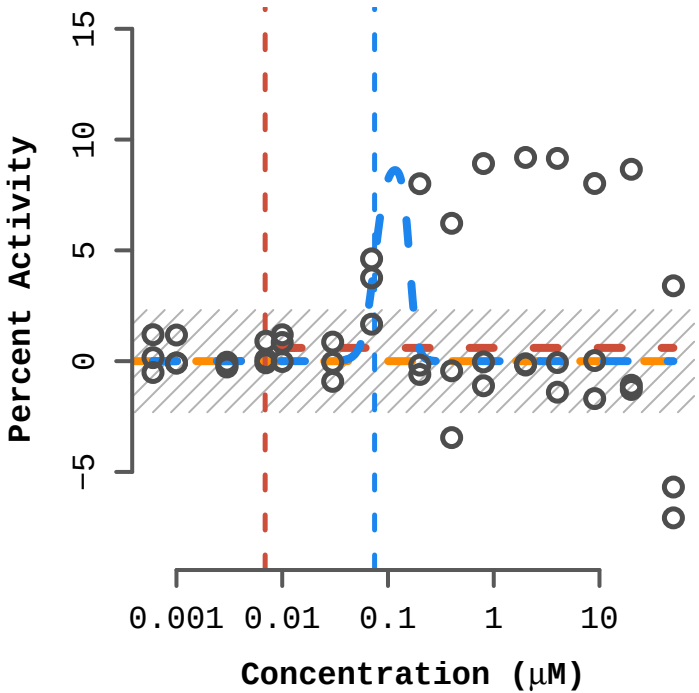
NAME: Hexaconazole
CHID: 34653 **CASRN:** 79983-71-4
SPID(S): Tox21_300684
M4ID: 12478449 **BRK**

HILL MODEL: Not applicable.

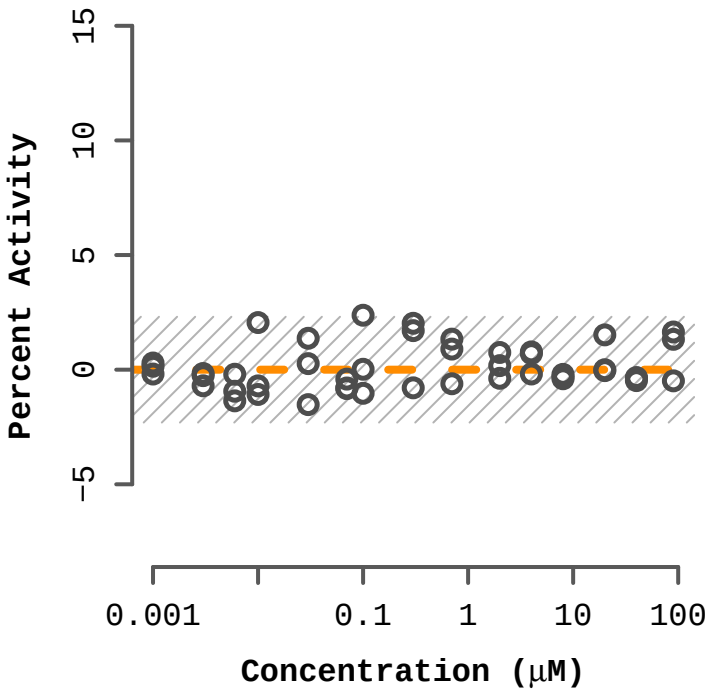
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.74	NA	NA
PROB:	1	NA	NA
RMSE:	3.23	NA	NA

MAX_MEAN: 0.953 **MAX_MED:** 1.08 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Imazalil sulfate
CHID:    34662   CASRN: 58594-72-2
SPID(S): Tox21_112071_1
M4ID:    12483338

HILL MODEL (in red):
      tp       ga       gw
val:  0.599    -2.16    8
sd:   0.559    0.474    57.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.06     -1.13    7.8      -0.795   12.5
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  241.51      246.15      245.35
PROB: 0.8         0.08        0.12
RMSE: 3.8         3.66        3.68

MAX_MEAN: 3.35      MAX_MED: 3.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

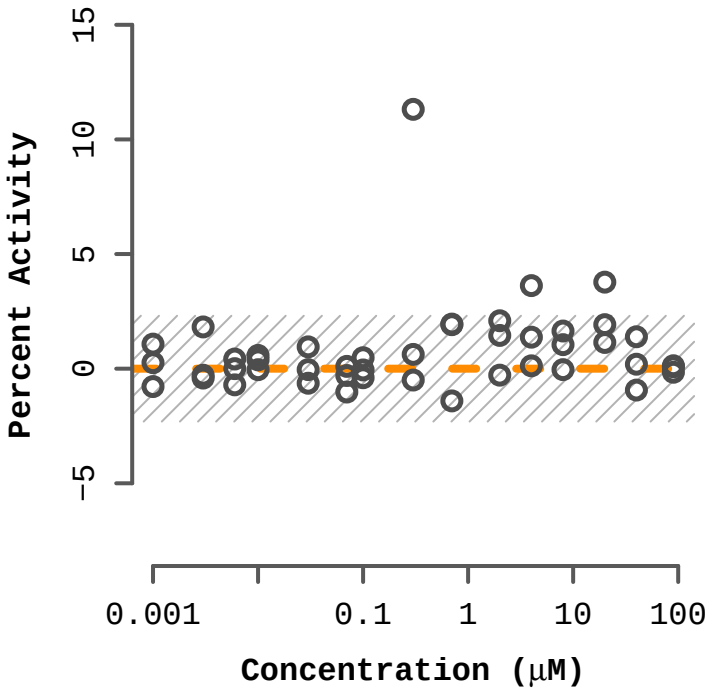
NAME: Imazamox
CHID: 34664 **CASRN:** 114311-32-9
SPID(S): Tox21_301007
M4ID: 12478126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

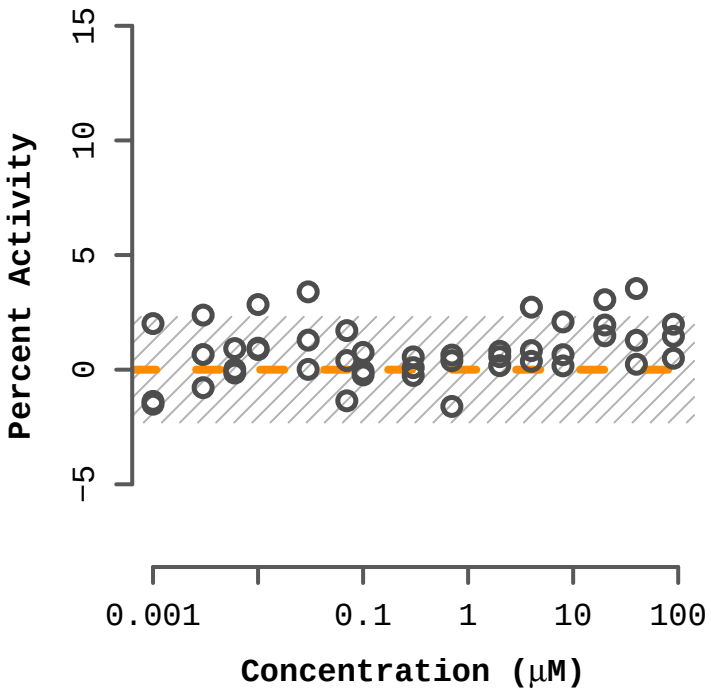
NAME: Imazapyr
CHID: 34665 CASRN: 81334-34-1
SPID(S): Tox21_301001
M4ID: 12478132

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.41	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 3.81 MAX_MED: 1.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

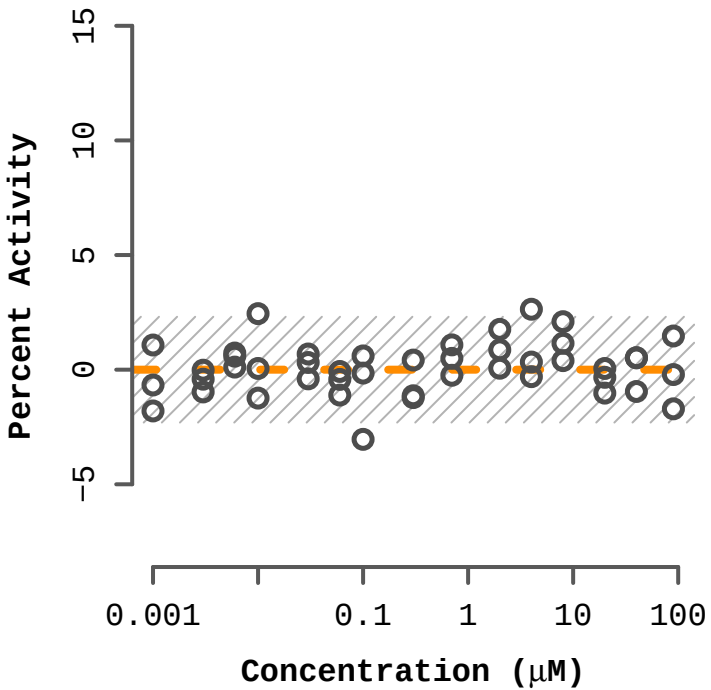
NAME: Iodine
CHID: 34672 **CASRN:** 7553-56-2
SPID(S): Tox21_301294
M4ID: 12477839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

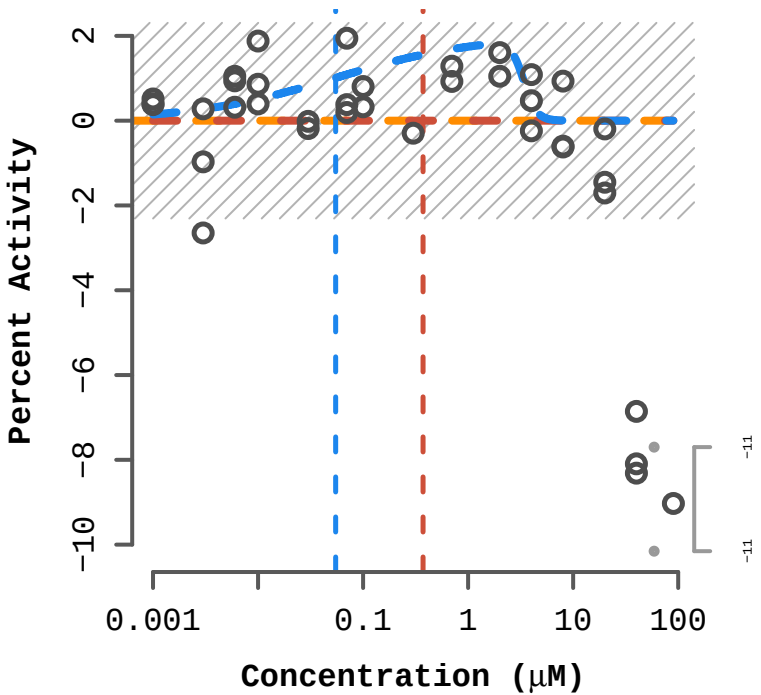
NAME: Iodosulfuron-methyl-sodium
CHID: 34673 **CASRN:** 144550-36-7
SPID(S): Tox21_300726
M4ID: 12478407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ipconazole
CHID: 34674 CASRN: 125225-28-7
SPID(S): Tox21_302497
M4ID: 12476636 BRK

HILL MODEL (in red):

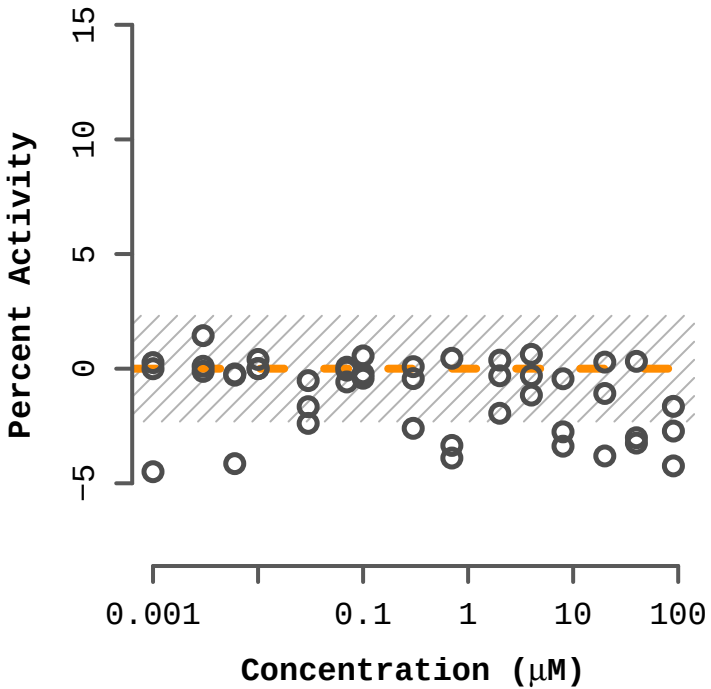
	tp	ga	gw
val:	6.09e-09	-0.429	1.83
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.02	-1.26	0.638	0.529	7.12
sd:	2.22	1.91	0.895	0.566	47.4

	CNST	HILL	GNLS
AIC:	227.5	233.5	225.24
PROB:	0.24	0.01	0.75
RMSE:	3.56	3.56	3.44

MAX_MEAN: 2.11 MAX_MED: 2.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

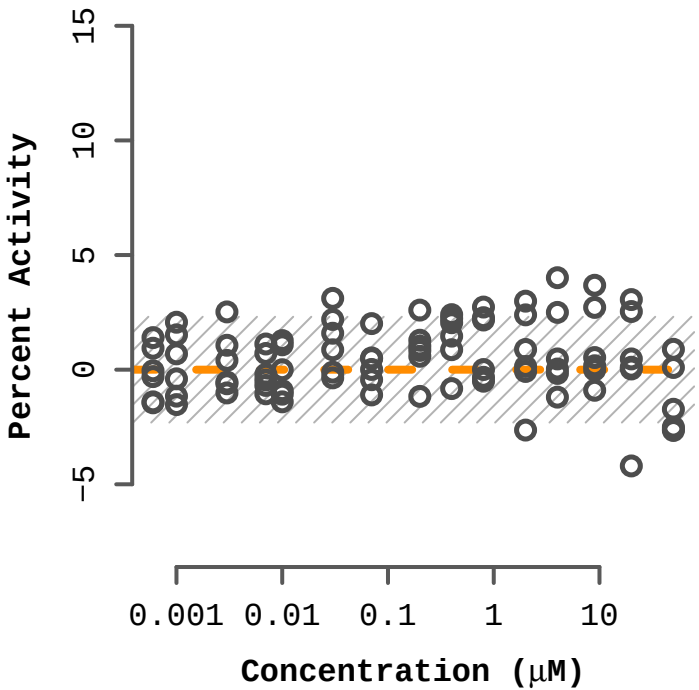
NAME: Isazofos
CHID: 34676 CASRN: 42509-80-8
SPID(S): Tox21_300833
M4ID: 12478300

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 0.477 MAX_MED: 0.106 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

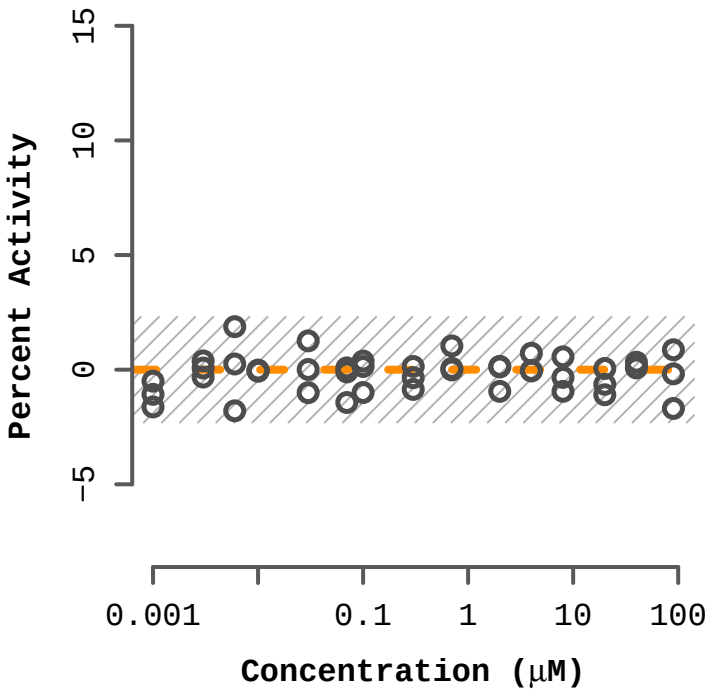
NAME: Mancozeb
CHID: 34695 **CASRN:** 8018-01-7
SPID(S): Tox21_300314
M4ID: 12478817

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	348.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

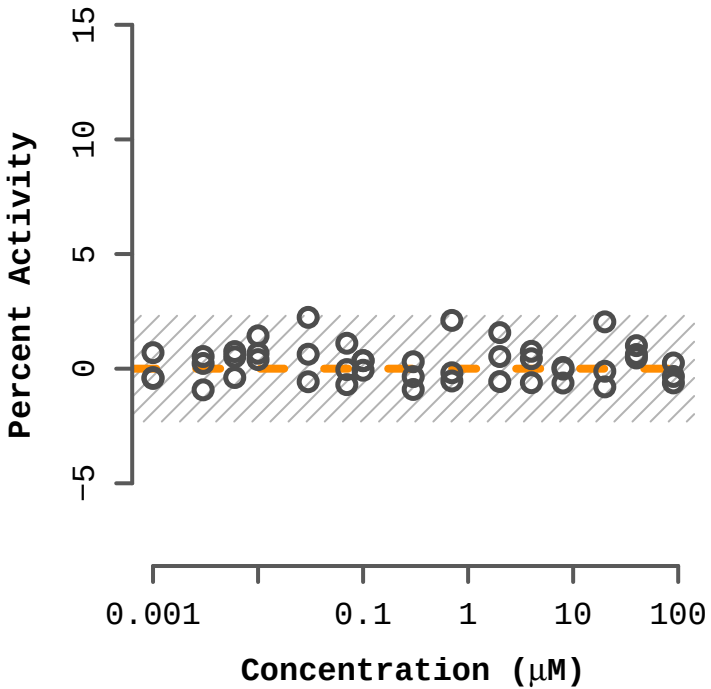
NAME: MCPA-2-ethylhexyl
CHID: 34698 **CASRN:** 29450-45-1
SPID(S): Tox21_302260
M4ID: 12476873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.362 **MAX_MED:** 0.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

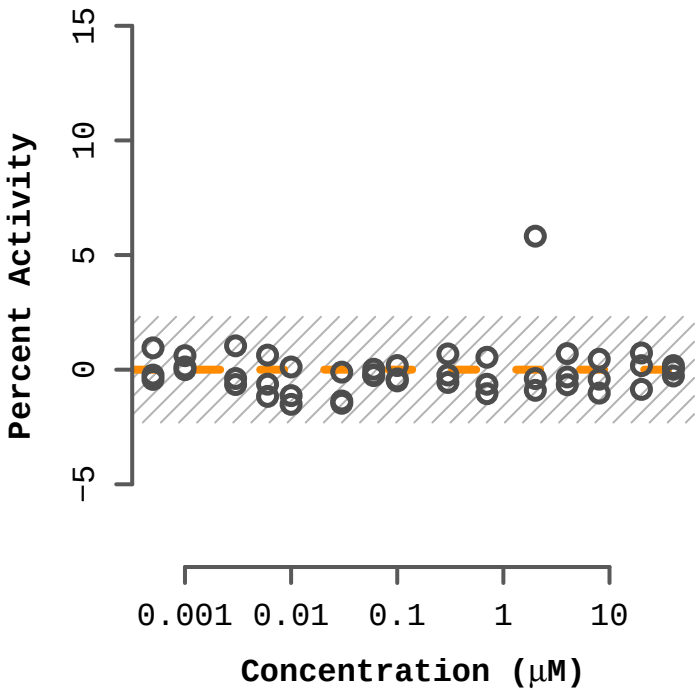
NAME: MCPA-sodium
CHID: 34700 **CASRN:** 3653-48-3
SPID(S): Tox21_302386
M4ID: 12476747

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.835 **MAX_MED:** 0.674 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

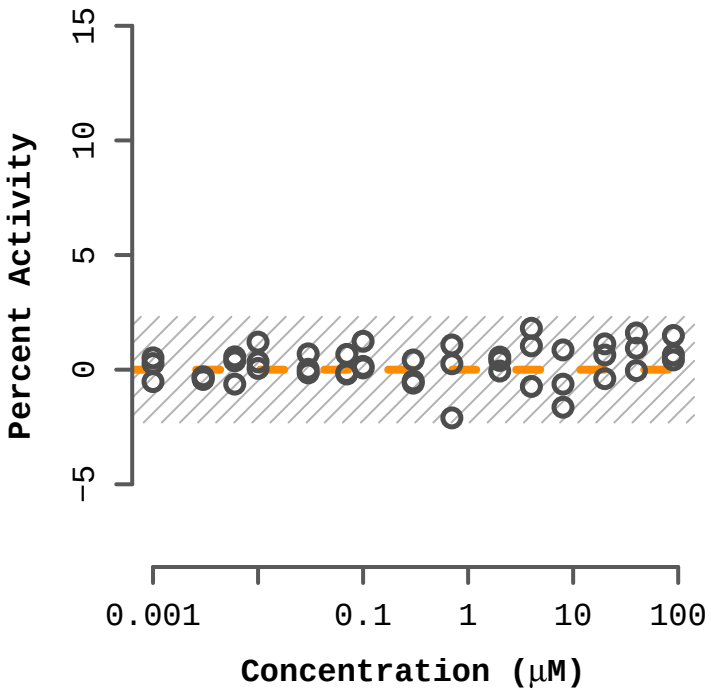
NAME: Topramezone
CHID: 34722 **CASRN:** 210631-68-8
SPID(S): Tox21_302441
M4ID: 12476692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 0.178 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

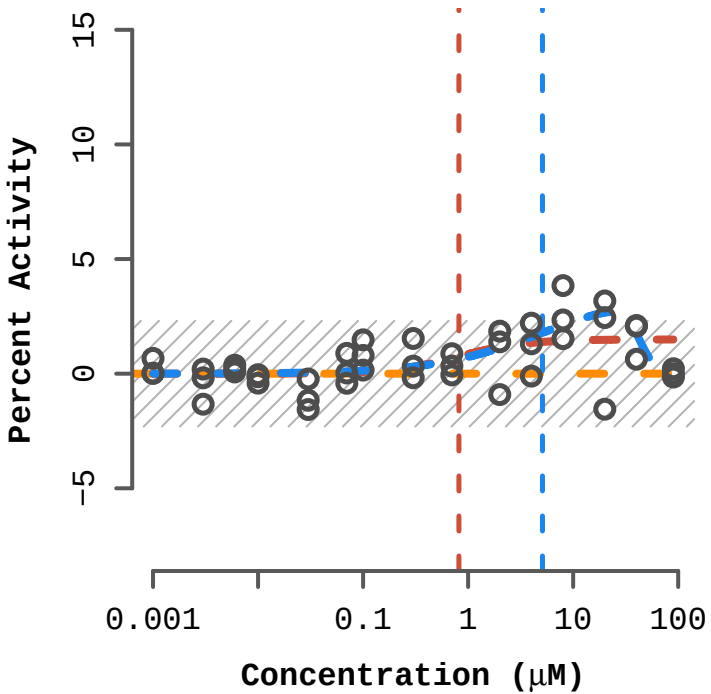
NAME: Isoxaflutole
CHID: 34723 **CASRN:** 141112-29-0
SPID(S): Tox21_300923
M4ID: 12478210

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.856 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flurenol-methyl
CHID: 34729 CASRN: 1216-44-0
SPID(S): Tox21_301428
M4ID: 12477705

HILL MODEL (in red):

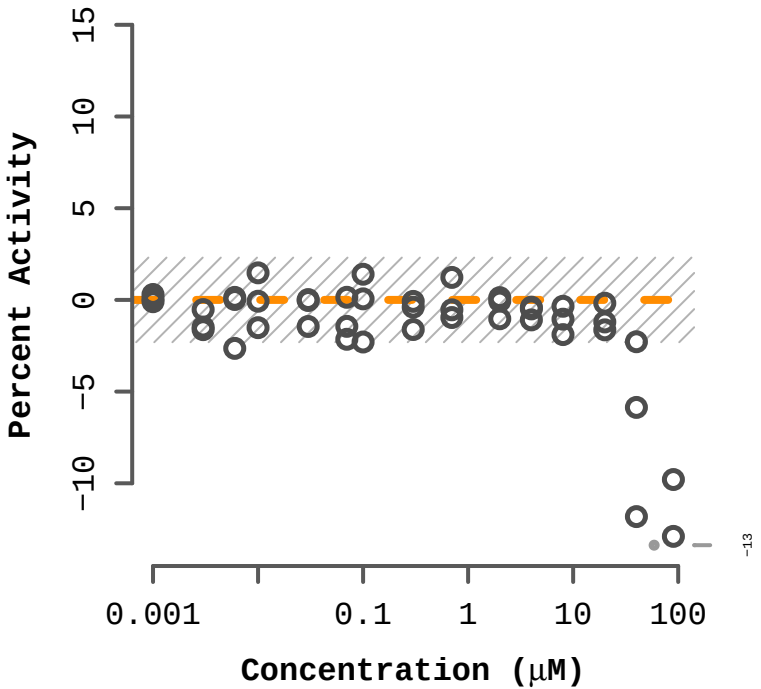
	tp	ga	gw
val:	1.49	−0.0877	1.39
sd:	0.368	0.429	1.15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.57	0.708	0.834	1.63	5.62
sd:	2.17	0.738	0.452	0.0669	8.71

	CNST	HILL	GNLS
AIC:	151.92	137.72	124.69
PROB:	0	0	1
RMSE:	1.31	1.03	0.98

MAX_MEAN: 2.57 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

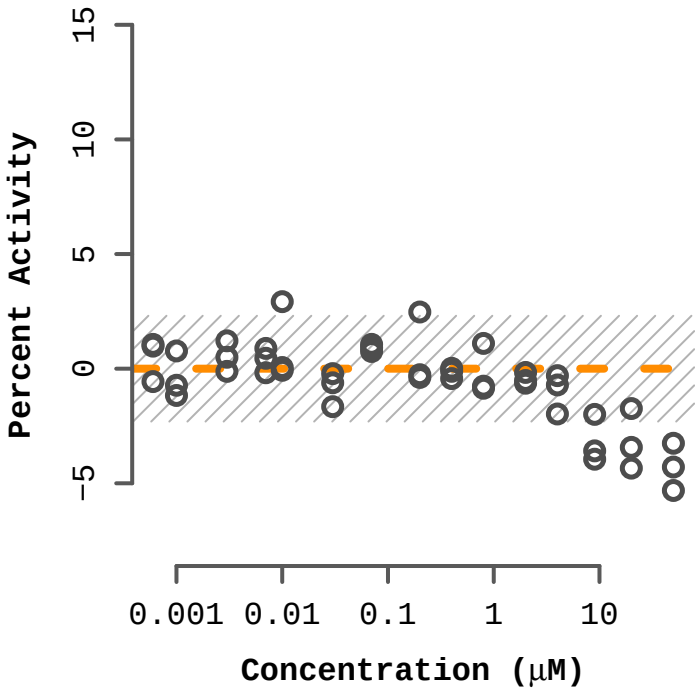
NAME: Milbemectin (mixture of 70% Milbemcin A4, 30% I
CHID: 34742 CASRN: NOCAS_34742
SPID(S): Tox21_300945
M4ID: 12478188 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.95	NA	NA
PROB:	1	NA	NA
RMSE:	3.86	NA	NA

MAX_MEAN: 0.0906 MAX_MED: 0.0708 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

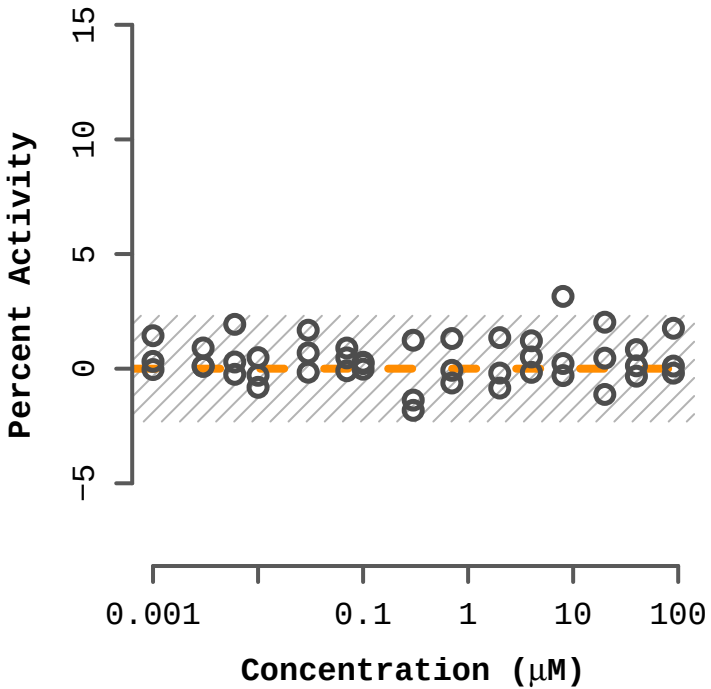
NAME: Nicarbazin
CHID: 34762 **CASRN:** 330-95-0
SPID(S): Tox21_304000
M4ID: 12475188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 0.969 **MAX_MED:** 0.984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

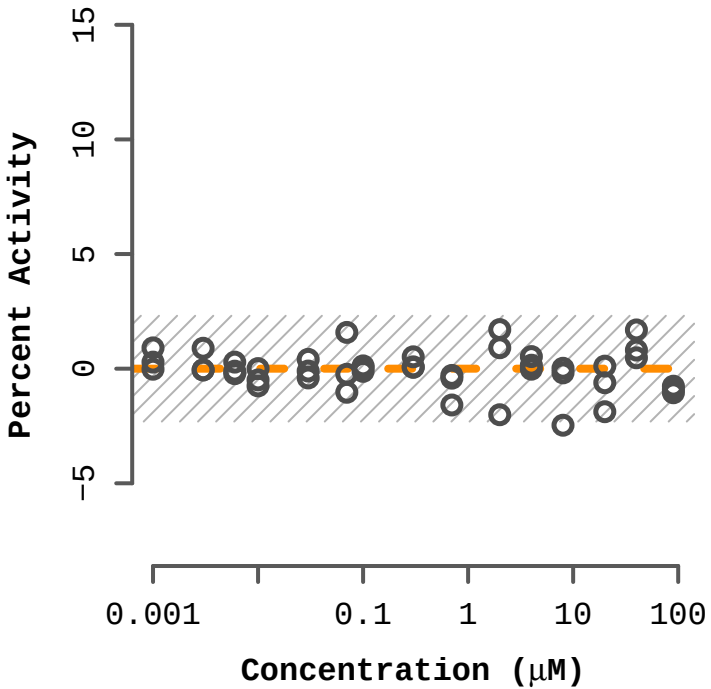
NAME: Nicosulfuron
CHID: 34764 **CASRN:** 111991-09-4
SPID(S): Tox21_301842
M4ID: 12477291

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.14	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.691 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

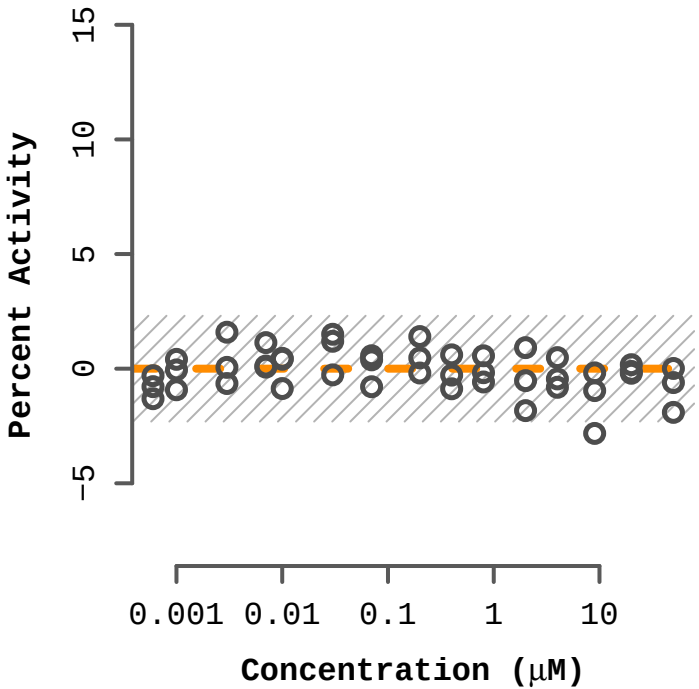
NAME: Nonivamide
CHID: 34769 **CASRN:** 2444-46-4
SPID(S): Tox21_301218
M4ID: 12477915

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

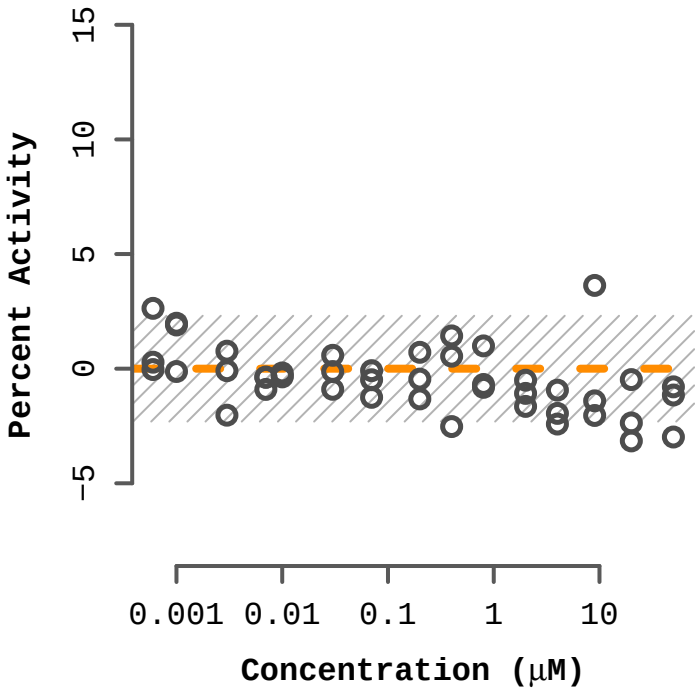
NAME: Nonivamide
CHID: 34769 **CASRN:** 2444-46-4
SPID(S): Tox21_110302_1
M4ID: 12484470

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.81 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

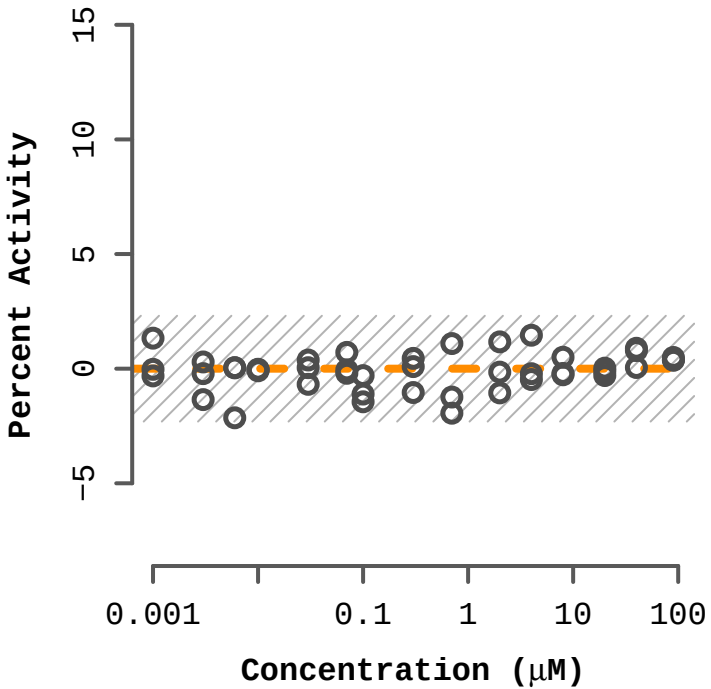
NAME: Novaluron
CHID: 34773 **CASRN:** 116714-46-6
SPID(S): Tox21_300959
M4ID: 12478174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

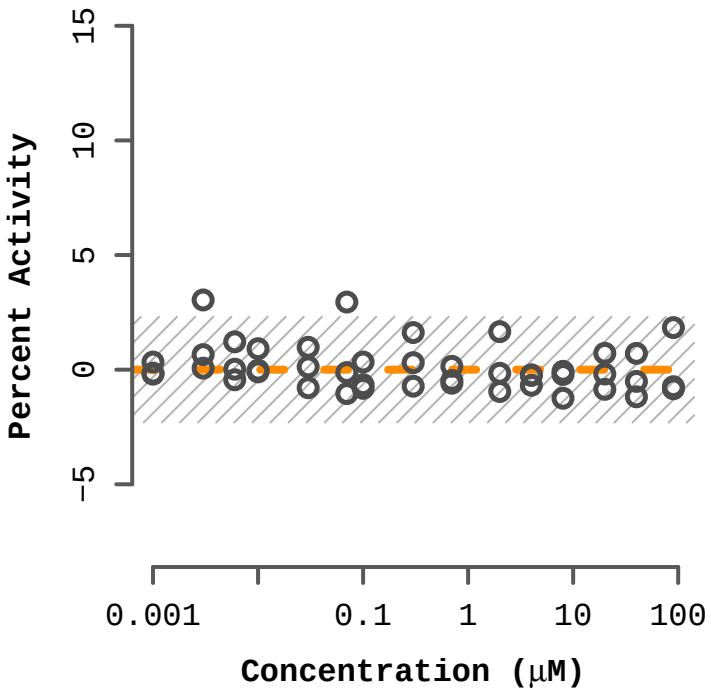
NAME: Tolclofos-methyl
CHID: 34776 **CASRN:** 57018-04-9
SPID(S): Tox21_301347
M4ID: 12477786

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.579 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

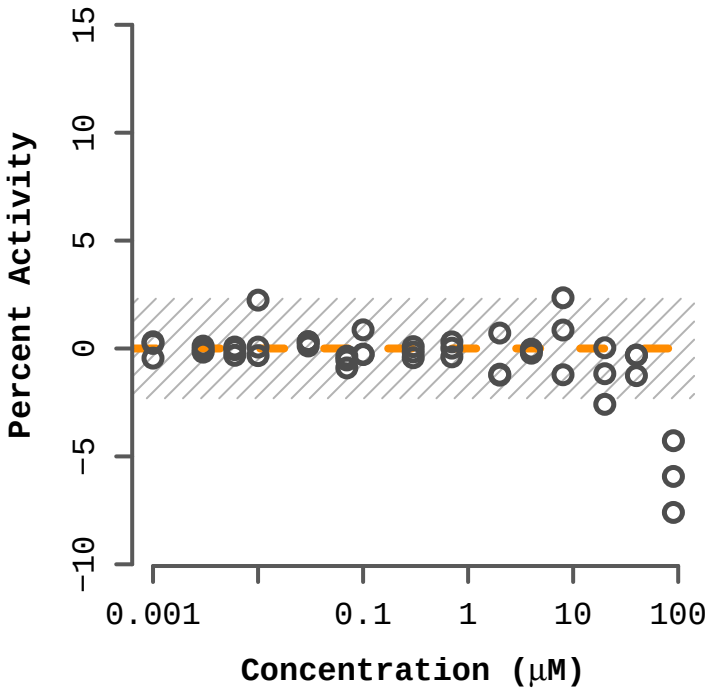
NAME: Orthosulfamuron
CHID: 34788 **CASRN:** 213464-77-8
SPID(S): Tox21_304028
M4ID: 12475160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.659 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

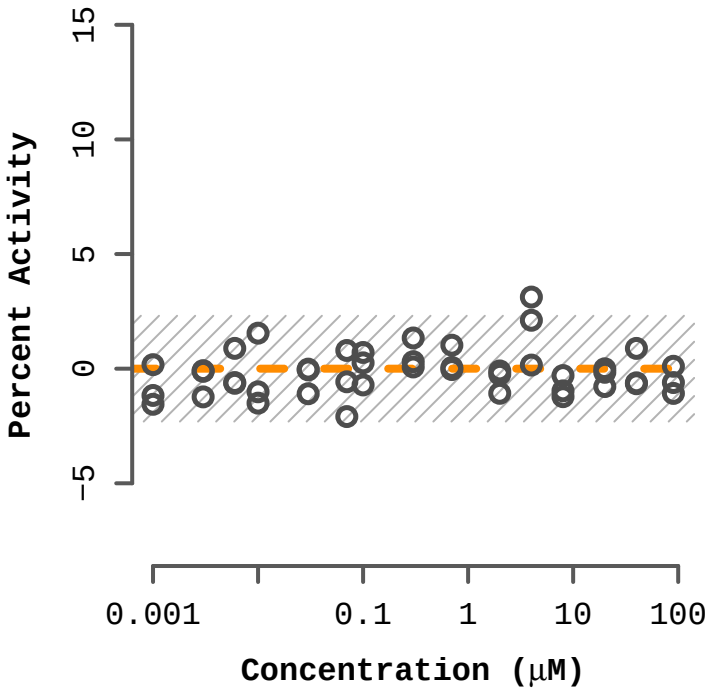
NAME: Oxycarboxin
CHID: 34792 CASRN: 5259-88-1
SPID(S): Tox21_301331
M4ID: 12477802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 0.665 MAX_MED: 0.857 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

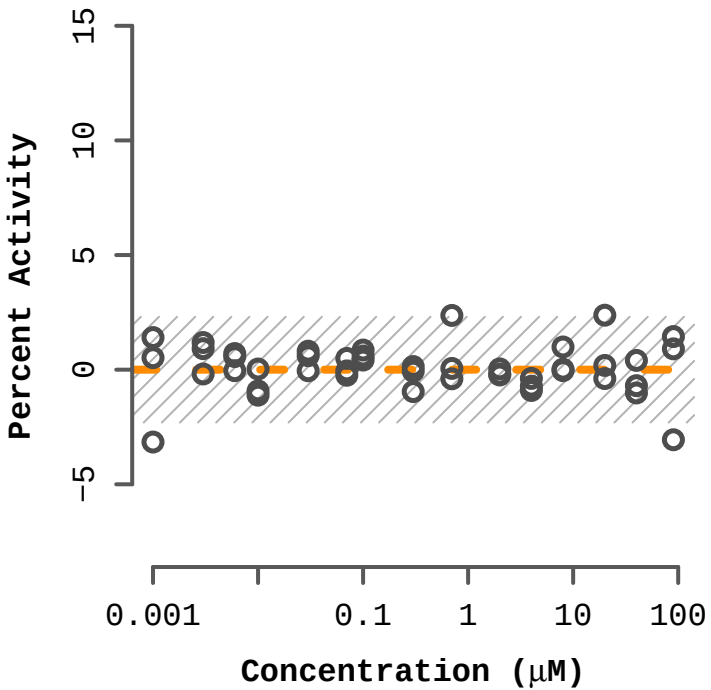
NAME: Penoxsulam
CHID: 34803 **CASRN:** 219714-96-2
SPID(S): Tox21_301010
M4ID: 12478123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.46	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

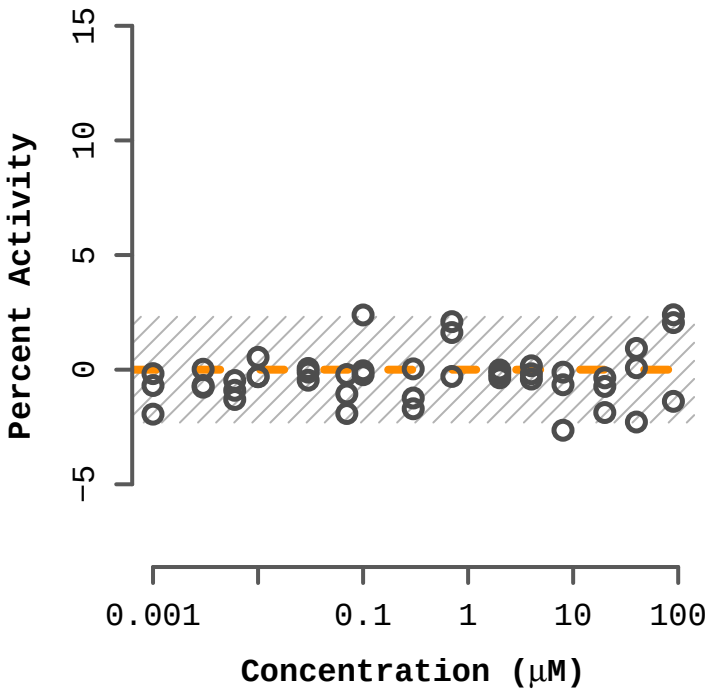
NAME: Monocrotophos
CHID: 34816 **CASRN:** 6923-22-4
SPID(S): Tox21_300806
M4ID: 12478327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.726 **MAX_MED:** 0.919 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

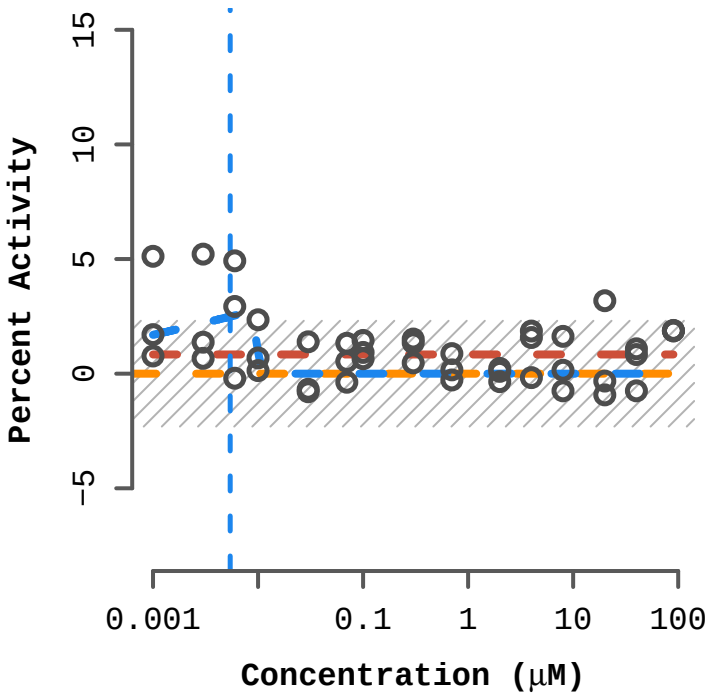
NAME: Azamethiphos
CHID: 34818 **CASRN:** 35575-96-3
SPID(S): Tox21_301009
M4ID: 12478124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pinoxaden
CHID: 34823 CASRN: 243973-20-8
SPID(S): Tox21_304033
M4ID: 12475155

HILL MODEL (in red):

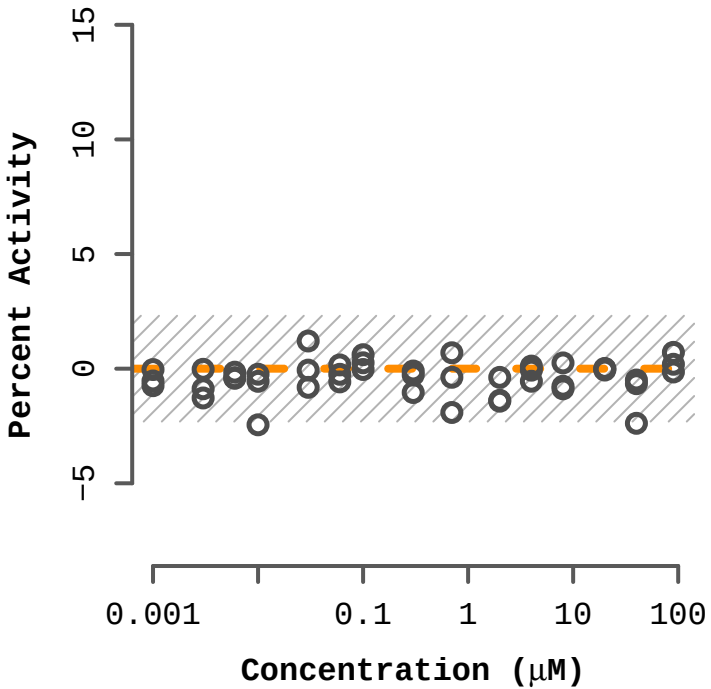
	tp	ga	gw
val:	0.837	−4.76	4.23
sd:	0.188	1360	3250

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.98	−2.27	0.392	−2.02	17.9
sd:	20.6	8.57	0.901	0.0405	43.1

	CNST	HILL	GNLS
AIC:	177.01	165.22	171.94
PROB:	0	0.96	0.03
RMSE:	1.8	1.47	1.4

MAX_MEAN: 2.55 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

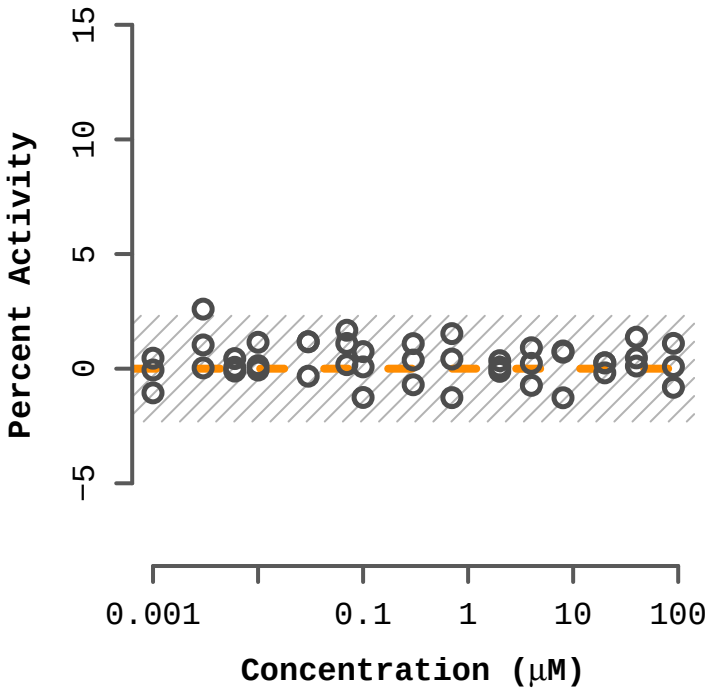
NAME: Potassium 1-naphthaleneacetate
CHID: 34833 CASRN: 15165-79-4
SPID(S): Tox21_301346
M4ID: 12477787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.279 MAX_MED: 0.259 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

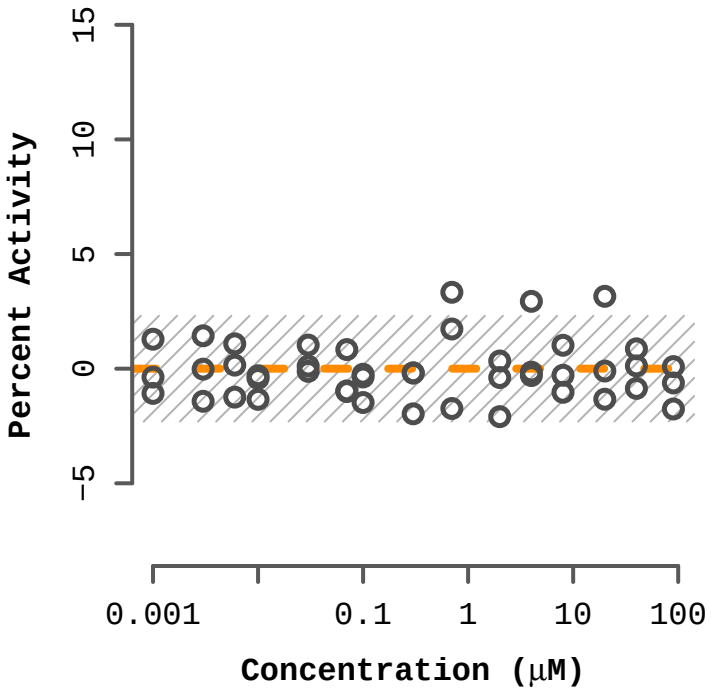
NAME: Potassium iodide
CHID: 34836 **CASRN:** 7681-11-0
SPID(S): Tox21_301293
M4ID: 12477840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

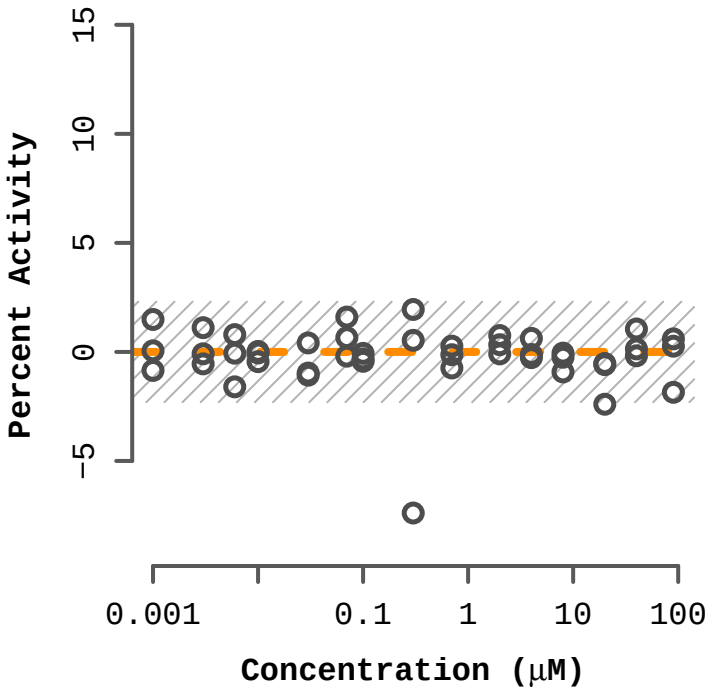
NAME: Procyazine
CHID: 34844 CASRN: 32889-48-8
SPID(S): Tox21_301904
M4ID: 12477229

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.11 MAX_MED: 1.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

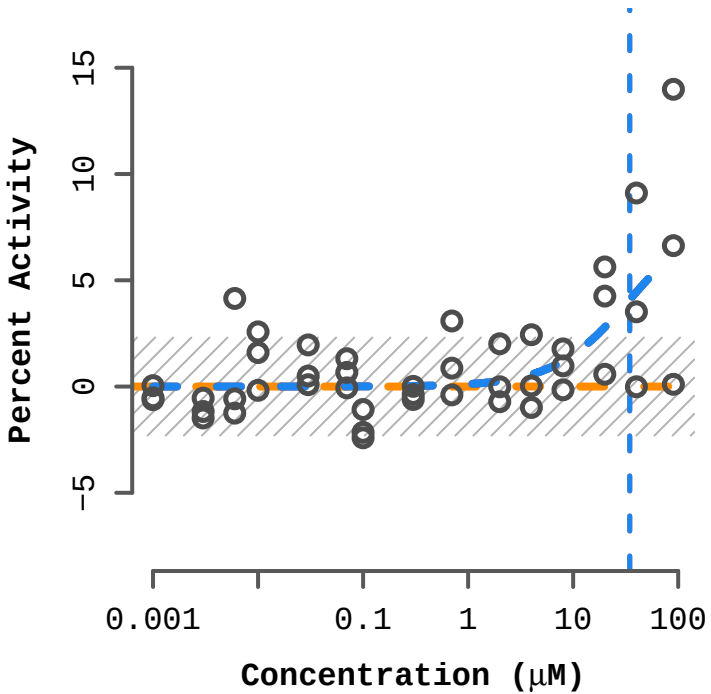
NAME: Propamocarb hydrochloride
CHID: 34849 CASRN: 25606-41-1
SPID(S): Tox21_300681
M4ID: 12478452

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.656 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dichlorprop-P
CHID: 34851 CASRN: 15165-67-0
SPID(S): Tox21_303875
M4ID: 12475313

HILL MODEL (in red):

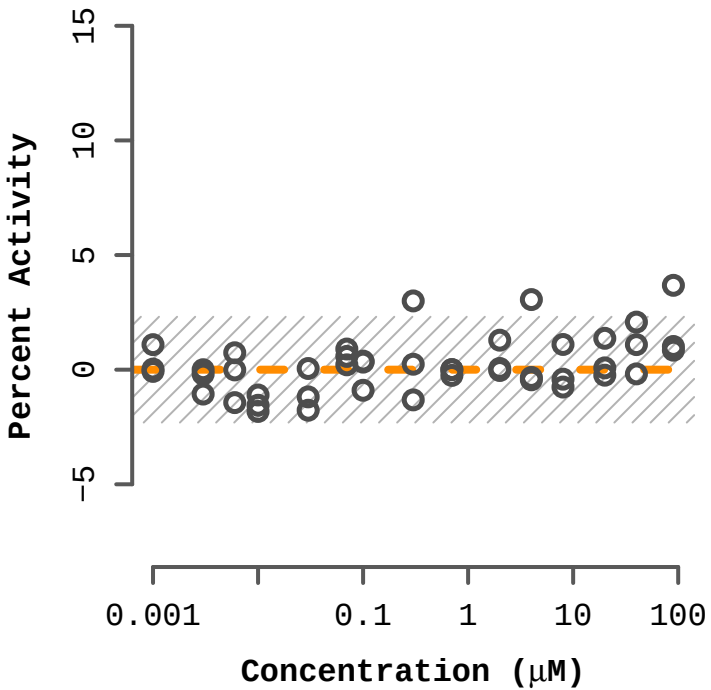
	tp	ga	gw
val:	8.18	1.54	1.2
sd:	10.4	1.18	1.33

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.18	1.54	1.2	3.13	7.08
sd:	10.4	1.18	1.33	3370	20200

	CNST	HILL	GNLS
AIC:	212.39	201.38	205.38
PROB:	0	0.88	0.12
RMSE:	3.21	2.26	2.26

MAX_MEAN: 6.91 MAX_MED: 6.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

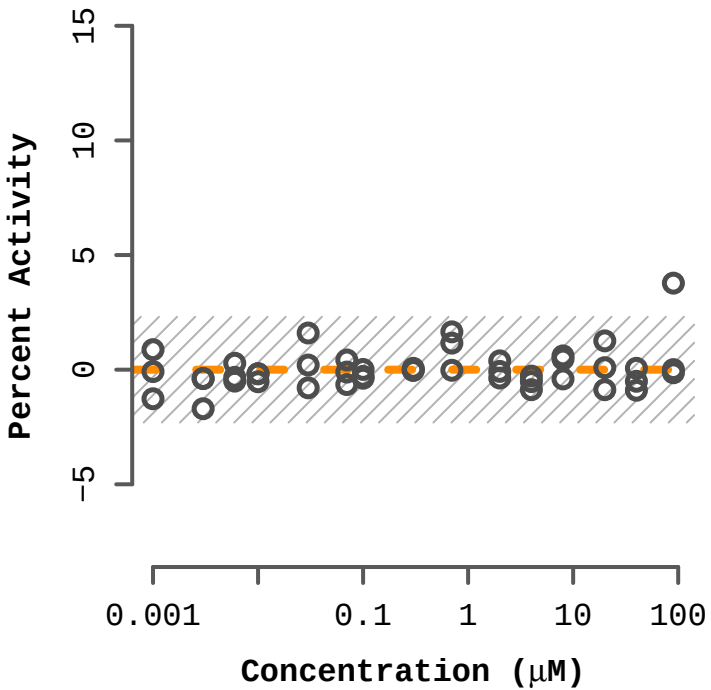
NAME: Fluazifop-P-butyl
CHID: 34855 **CASRN:** 79241-46-6
SPID(S): Tox21_301193
M4ID: 12477940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

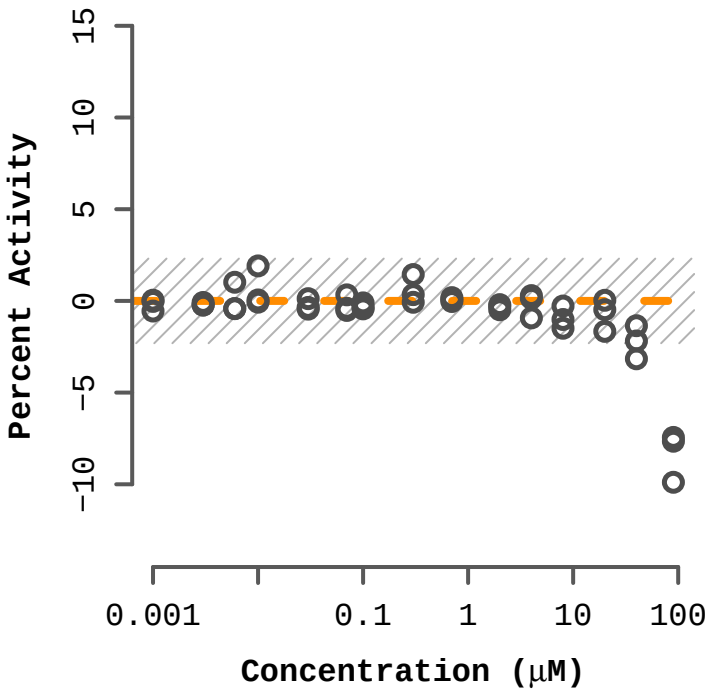
NAME: Propoxycarbazone-sodium
CHID: 34864 **CASRN:** 181274-15-7
SPID(S): Tox21_301132
M4ID: 12478001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

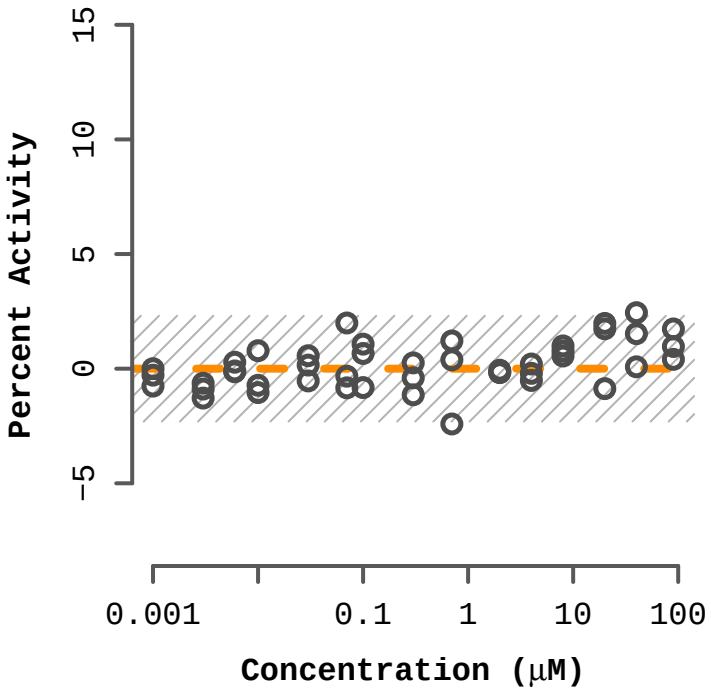
NAME: Prothioconazole
CHID: 34869 **CASRN:** 178928-70-6
SPID(S): Tox21_303849
M4ID: 12475339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.29	NA	NA
PROB:	1	NA	NA
RMSE:	2.33	NA	NA

MAX_MEAN: 0.632 **MAX_MED:** 0.344 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

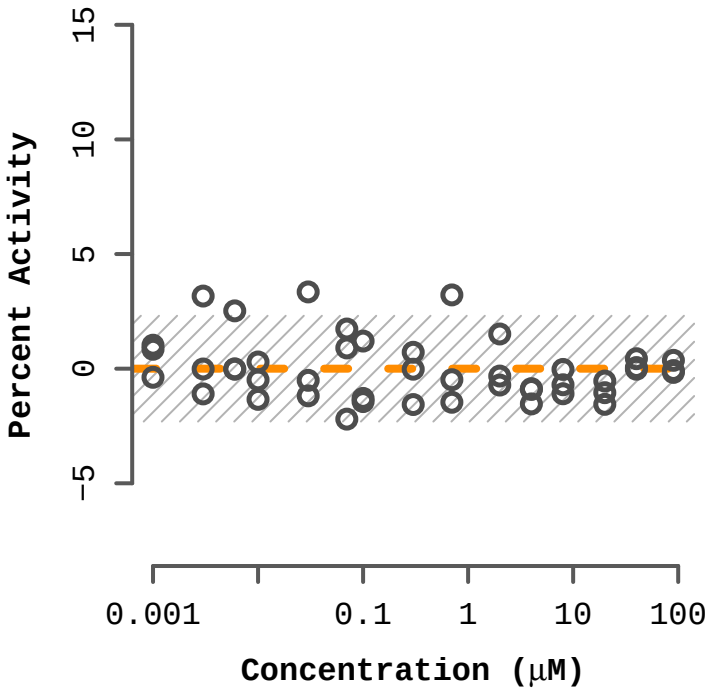
NAME: Pyraflufen-ethyl
CHID: 34871 **CASRN:** 129630-19-9
SPID(S): Tox21_300698
M4ID: 12478435

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.78	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

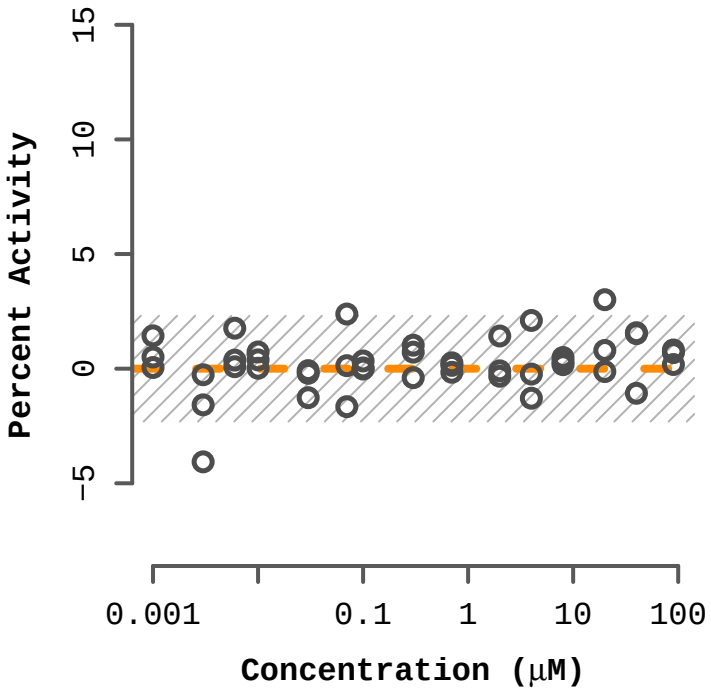
NAME: Chloridazon
CHID: 34872 **CASRN:** 1698-60-8
SPID(S): Tox21_300721
M4ID: 12478412

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.832 **MAX_MED:** 0.906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

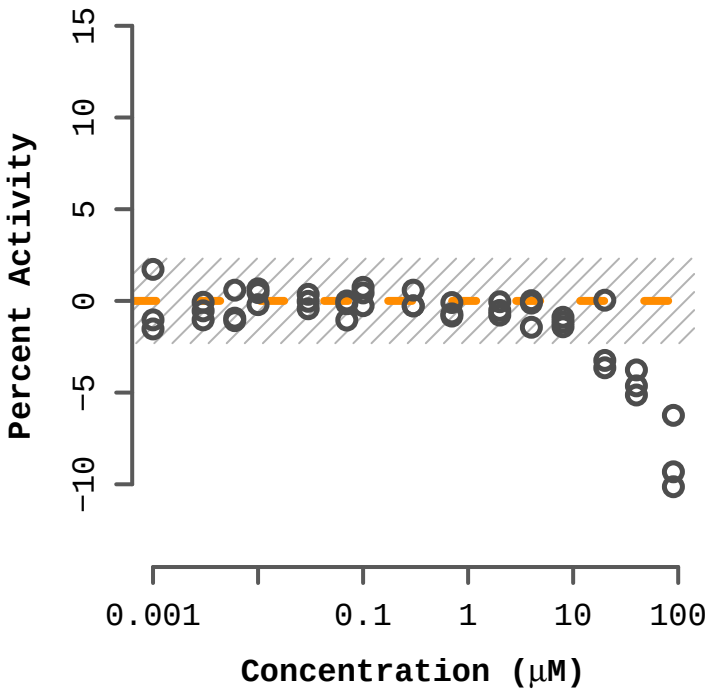
NAME: Pyrimethanil
CHID: 34877 CASRN: 53112-28-0
SPID(S): Tox21_300808
M4ID: 12478325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.23 MAX_MED: 1.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

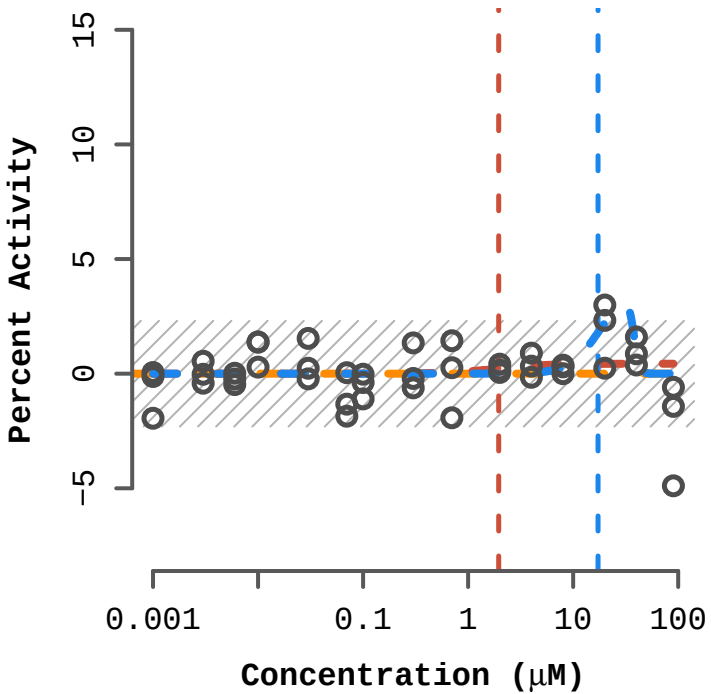
NAME: Quinoxyfen
CHID: 34881 **CASRN:** 124495-18-7
SPID(S): Tox21_300844
M4ID: 12478289

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 0.306 **MAX_MED:** 0.457 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenchlorphos
CHID: 34885 CASRN: 299-84-3
SPID(S): Tox21_301334
M4ID: 12477799

HILL MODEL (in red):

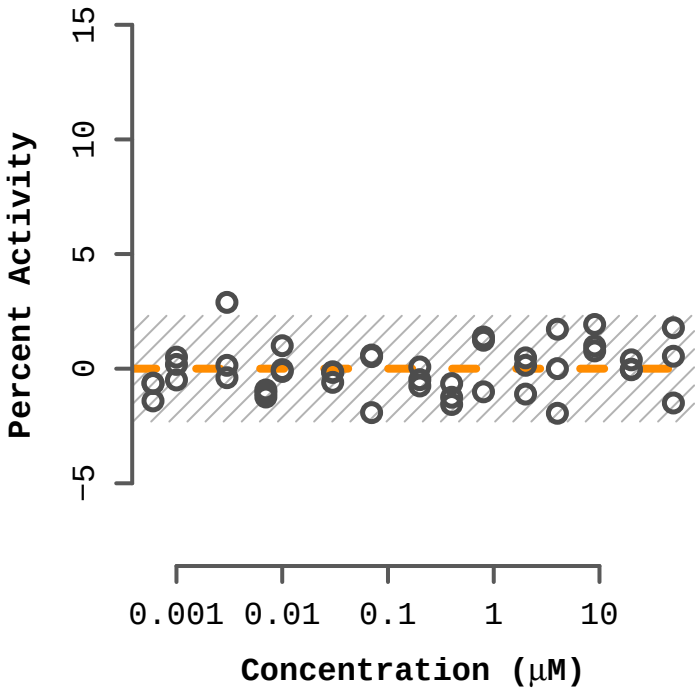
	tp	ga	gw
val:	0.435	0.291	1.85
sd:	0.36	1.08	3.21

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.6	1.24	3.17	1.58	17.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	141.42	144.72	139.49
PROB:	0.26	0.05	0.69
RMSE:	1.26	1.26	1.14

MAX_MEAN: 1.85 MAX_MED: 2.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

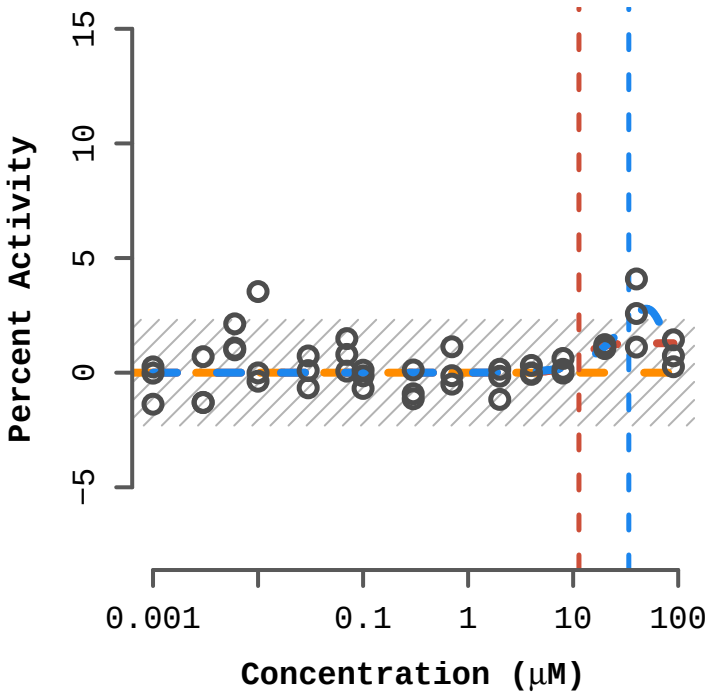
NAME: Fenchlorphos
CHID: 34885 **CASRN:** 299-84-3
SPID(S): Tox21_113416_1
M4ID: 12482657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium bromide
CHID: 34903 CASRN: 7647-15-6
SPID(S): Tox21_301343
M4ID: 12477790

HILL MODEL (in red):

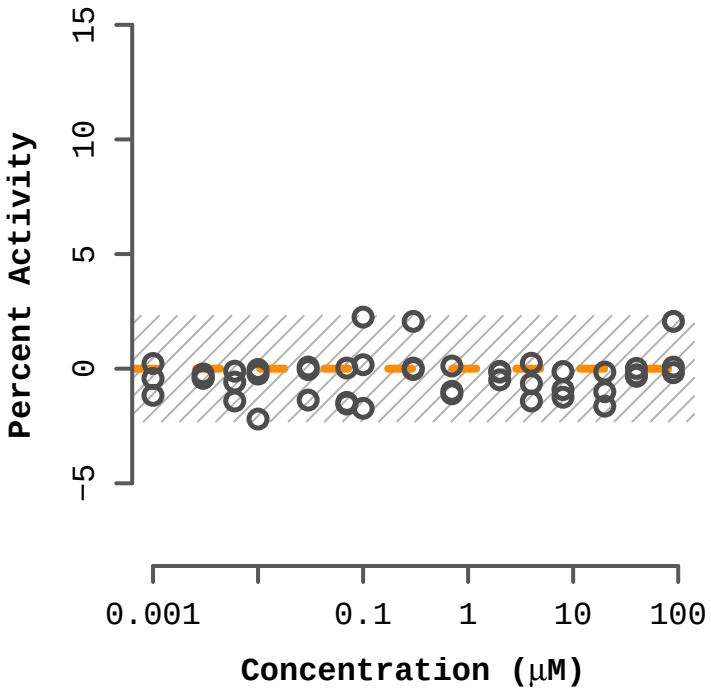
	tp	ga	gw
val:	1.29	1.06	4.17
sd:	0.357	0.228	4.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.57	1.53	2.08	1.85	5.81
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	141.2	129.59	128.5
PROB:	0	0.37	0.63
RMSE:	1.21	1.01	0.94

MAX_MEAN: 2.6 MAX_MED: 2.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

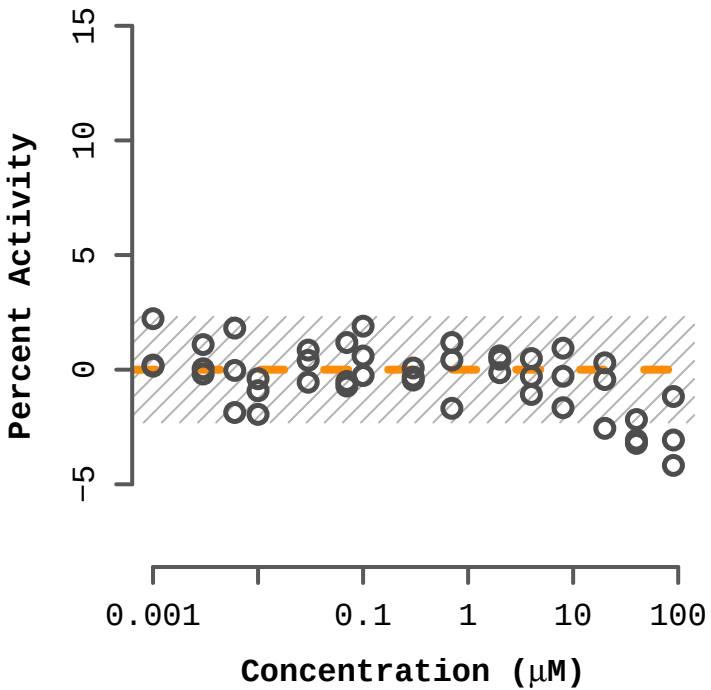
NAME: Sodium trichloroacetate
CHID: 34924 **CASRN:** 650-51-1
SPID(S): Tox21_301313
M4ID: 12477820

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.685 **MAX_MED:** 0.173 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

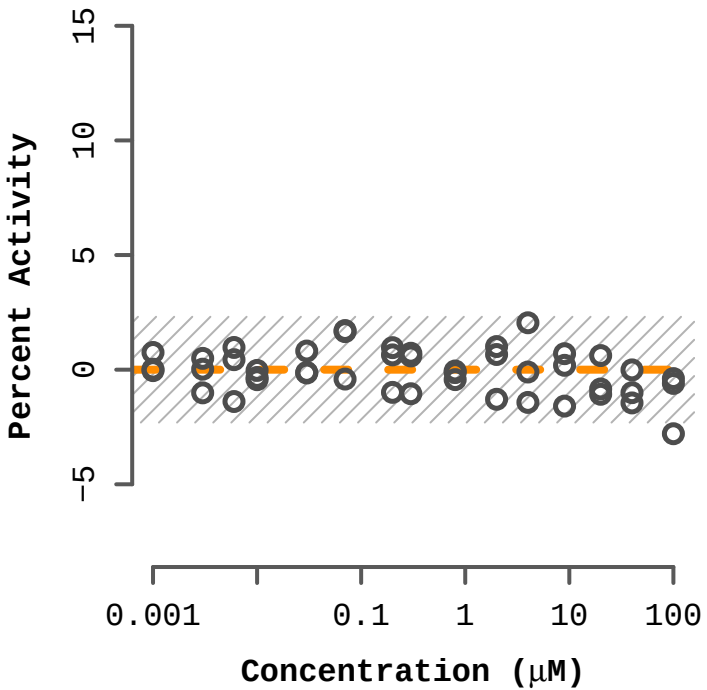
NAME: Spirodiclofen
CHID: 34928 **CASRN:** 148477-71-8
SPID(S): Tox21_301133
M4ID: 12478000

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 0.597 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

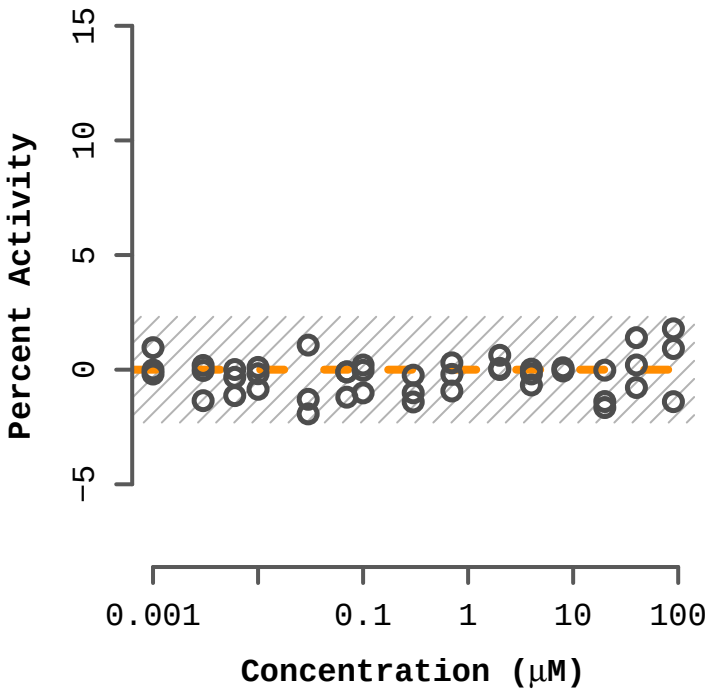
NAME: Spiromesifen
CHID: 34929 **CASRN:** 283594-90-1
SPID(S): Tox21_301233
M4ID: 12477900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.987 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

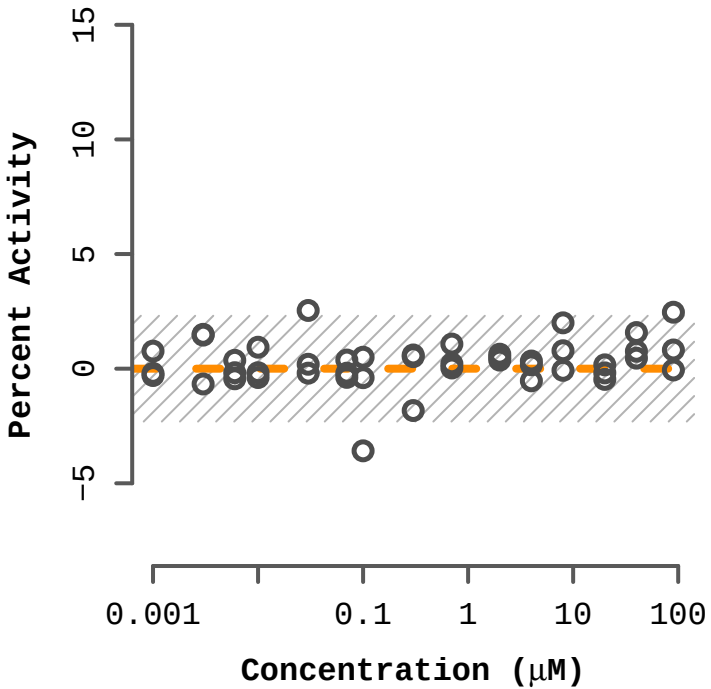
NAME: Fosthiazate
CHID: 34930 **CASRN:** 98886-44-3
SPID(S): Tox21_301059
M4ID: 12478074

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.438 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

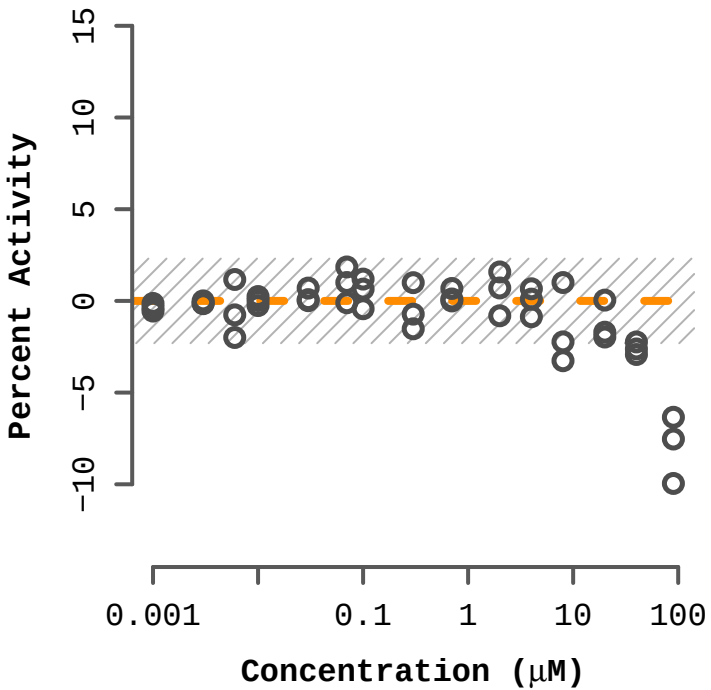
NAME: Sulfometuron-methyl
CHID: 34936 **CASRN:** 74222-97-2
SPID(S): Tox21_301843
M4ID: 12477290

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

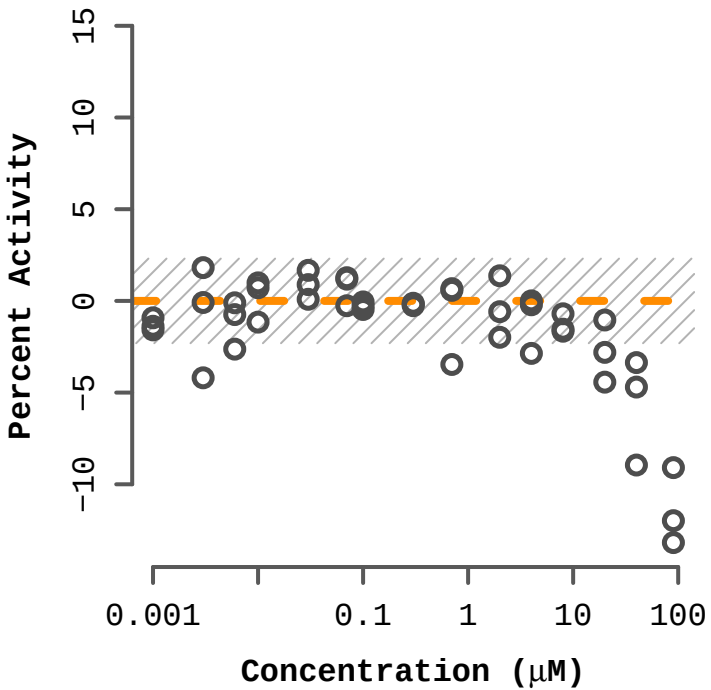
NAME: Tebufenozide
CHID: 34948 CASRN: 112410-23-8
SPID(S): Tox21_300685
M4ID: 12478448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.72	NA	NA
PROB:	1	NA	NA
RMSE:	2.41	NA	NA

MAX_MEAN: 0.92 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

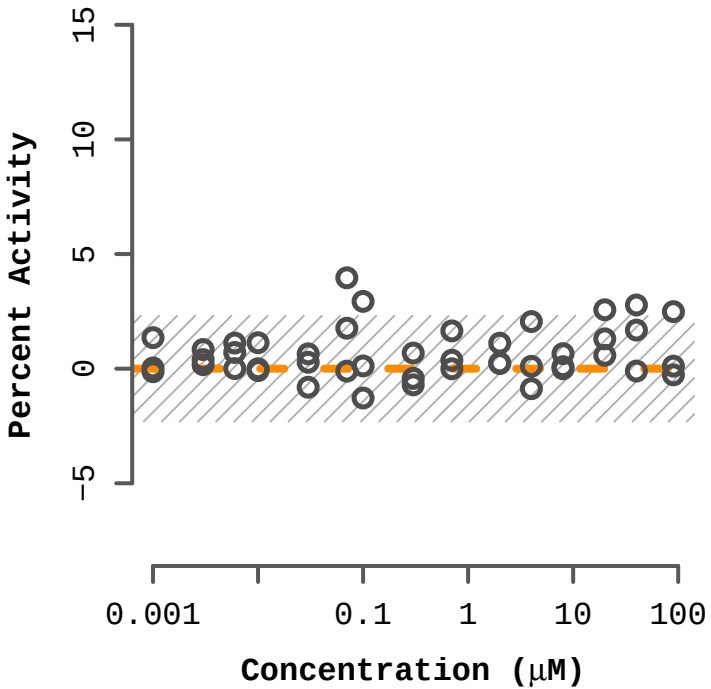
NAME: Tetraconazole
CHID: 34956 CASRN: 112281-77-3
SPID(S): Tox21_300995
M4ID: 12478138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.48	NA	NA
PROB:	1	NA	NA
RMSE:	3.71	NA	NA

MAX_MEAN: 0.883 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

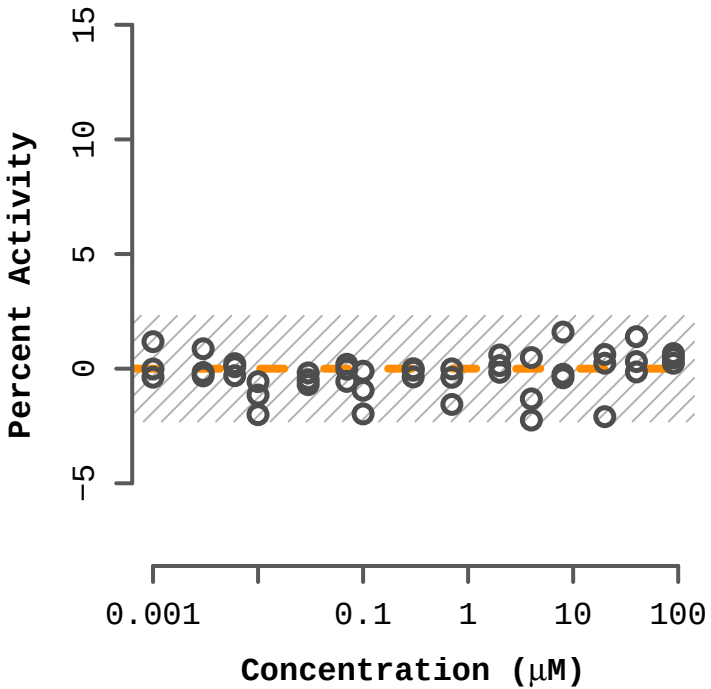
NAME: Tetraethyl pyrophosphate
CHID: 34957 **CASRN:** 107-49-3
SPID(S): Tox21_301172
M4ID: 12477961

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

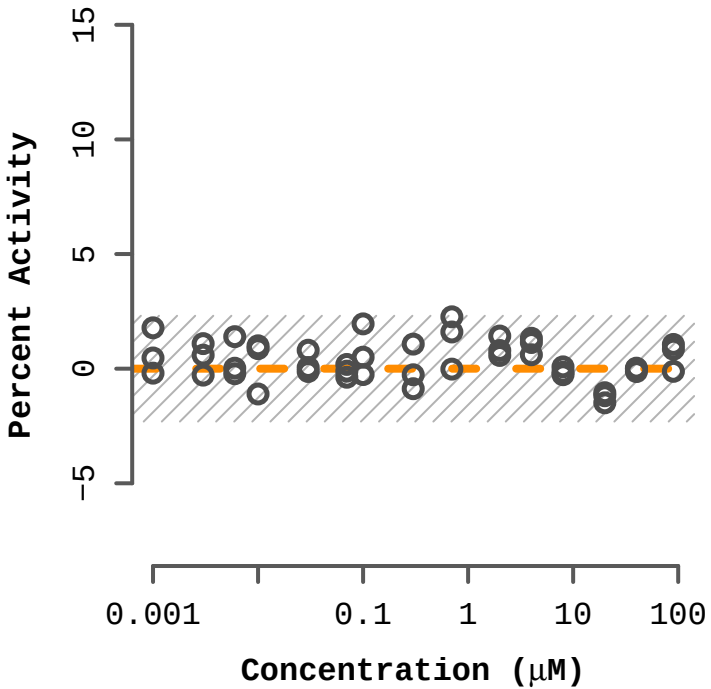
NAME: Thiacloprid
CHID: 34961 **CASRN:** 111988-49-9
SPID(S): Tox21_300697
M4ID: 12478436

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.522 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

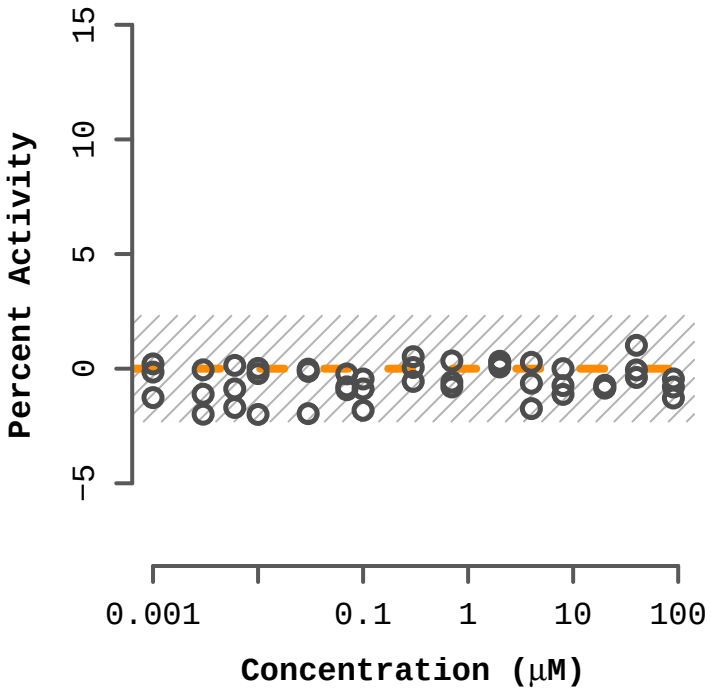
NAME: Thiamethoxam
CHID: 34962 **CASRN:** 153719-23-4
SPID(S): Tox21_301154
M4ID: 12477979

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

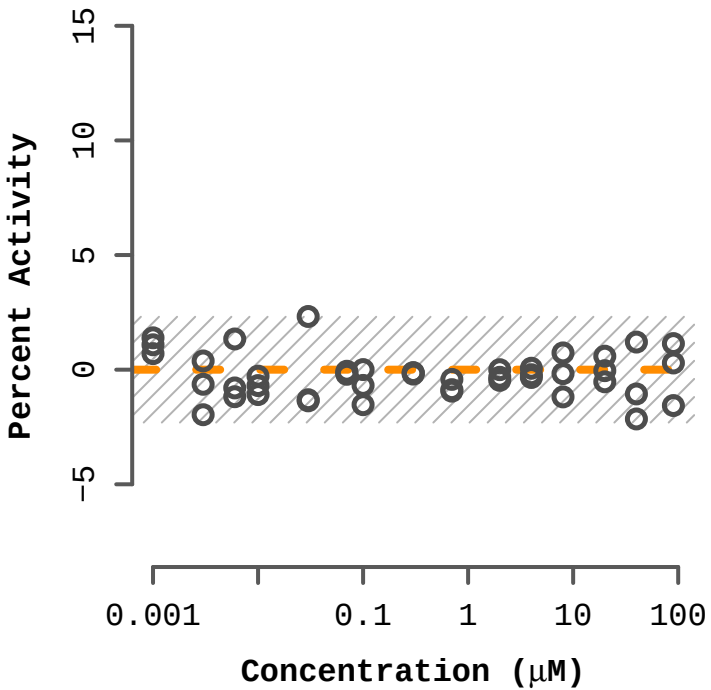
NAME: 2,4-Dithiobiuret
CHID: 34968 **CASRN:** 541-53-7
SPID(S): Tox21_301949
M4ID: 12477184

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.224 **MAX_MED:** 0.272 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

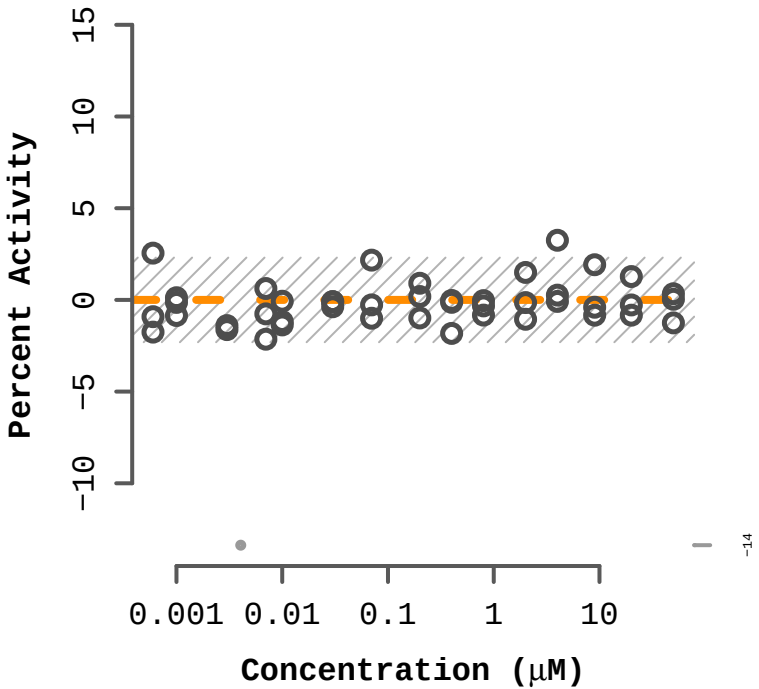
NAME: Thymol
CHID: 34972 **CASRN:** 89-83-8
SPID(S): Tox21_300358
M4ID: 12478774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

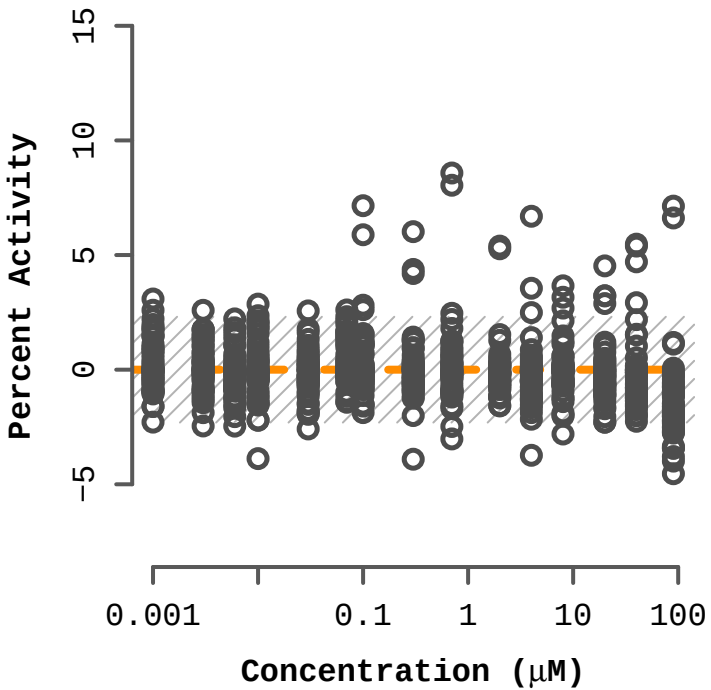
NAME: Thymol
CHID: 34972 **CASRN:** 89-83-8
SPID(S): Tox21_111613_1
M4ID: 12483587 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.33	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.262 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

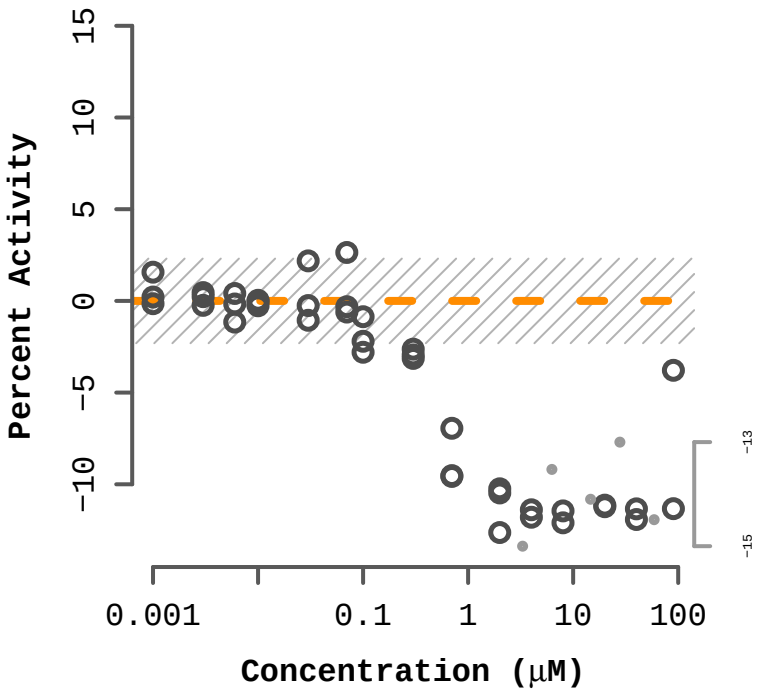
NAME: Tralkoxydim
CHID: 34973 CASRN: 87820-88-0
SPID(S): Tox21_400001
M4ID: 12475136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2392.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.317 **MAX_MED:** 0.0301 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

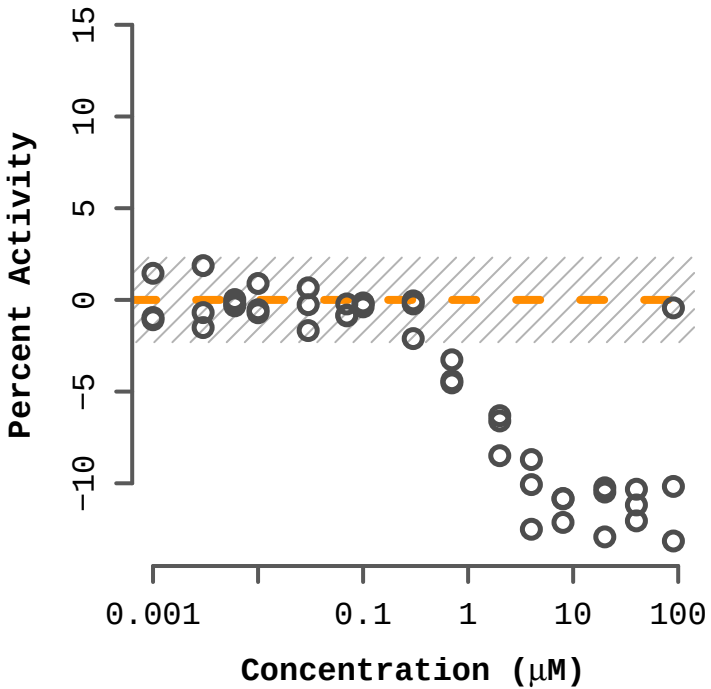
NAME: Tributyltin benzoate
CHID: 34981 **CASRN:** 4342-36-3
SPID(S): Tox21_303395
M4ID: 12475743 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	320.64	NA	NA
PROB:	1	NA	NA
RMSE:	8.04	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 0.233 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

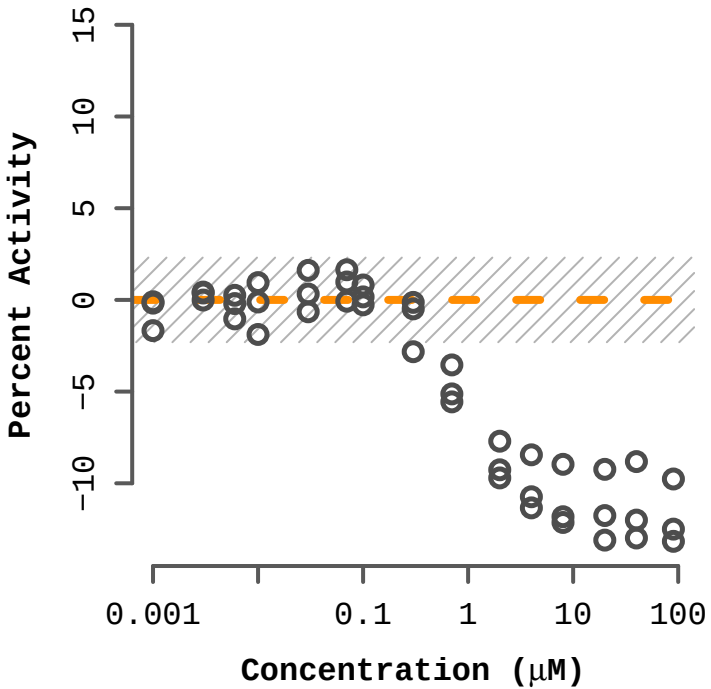
NAME: Tributyltetradecylphosphonium chloride
CHID: 34997 **CASRN:** 81741-28-8
SPID(S): Tox21_303556
M4ID: 12475589

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.92	NA	NA
PROB:	1	NA	NA
RMSE:	6.63	NA	NA

MAX_MEAN: −0.109 **MAX_MED:** −0.196 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

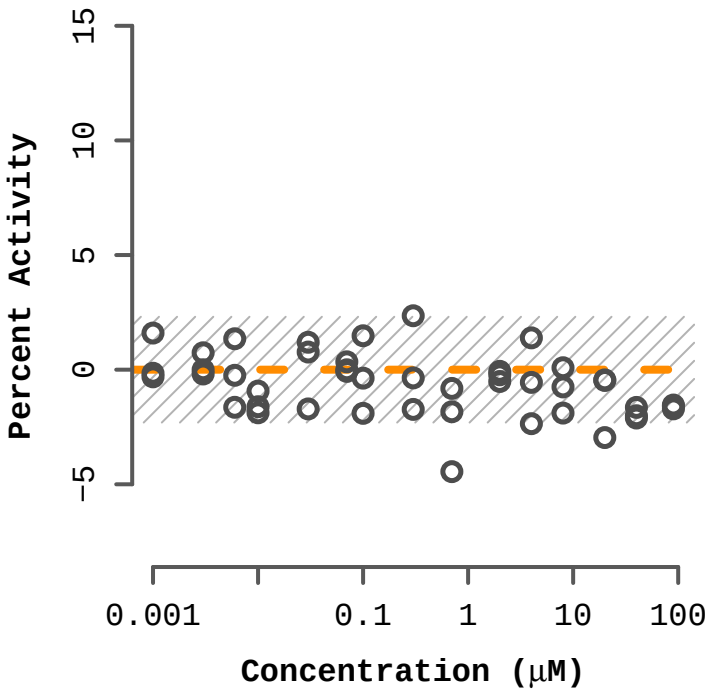
NAME: Tributyltetradecylphosphonium chloride
CHID: 34997 **CASRN:** 81741-28-8
SPID(S): Tox21_202009
M4ID: 12480243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	307.6	NA	NA
PROB:	1	NA	NA
RMSE:	7.03	NA	NA

MAX_MEAN: 0.851 **MAX_MED:** 0.979 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

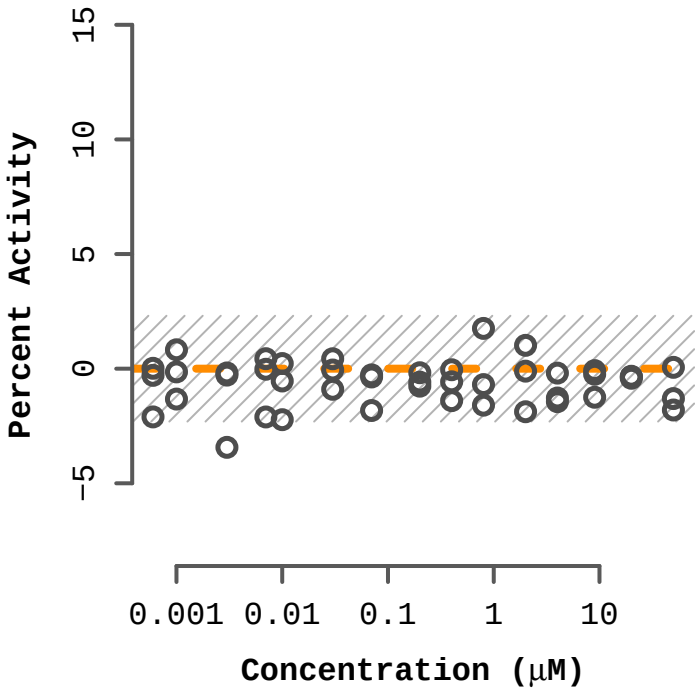
NAME: 10-Undecenoic acid
CHID: 35001 **CASRN:** 112-38-9
SPID(S): Tox21_300383
M4ID: 12478749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.377 **MAX_MED:** 0.771 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

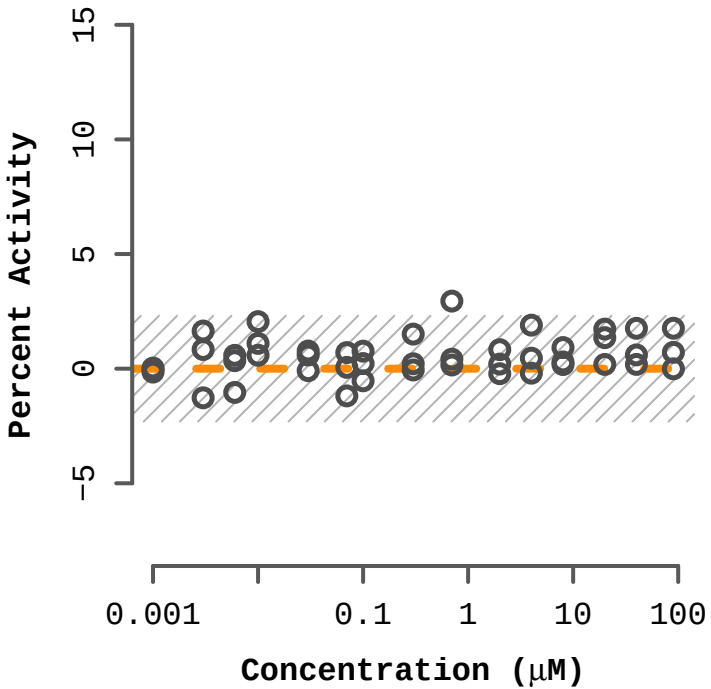
NAME: 10-Undecenoic acid
CHID: 35001 **CASRN:** 112-38-9
SPID(S): Tox21_111657_1
M4ID: 12483552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: −0.174 **MAX_MED:** −0.0247 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

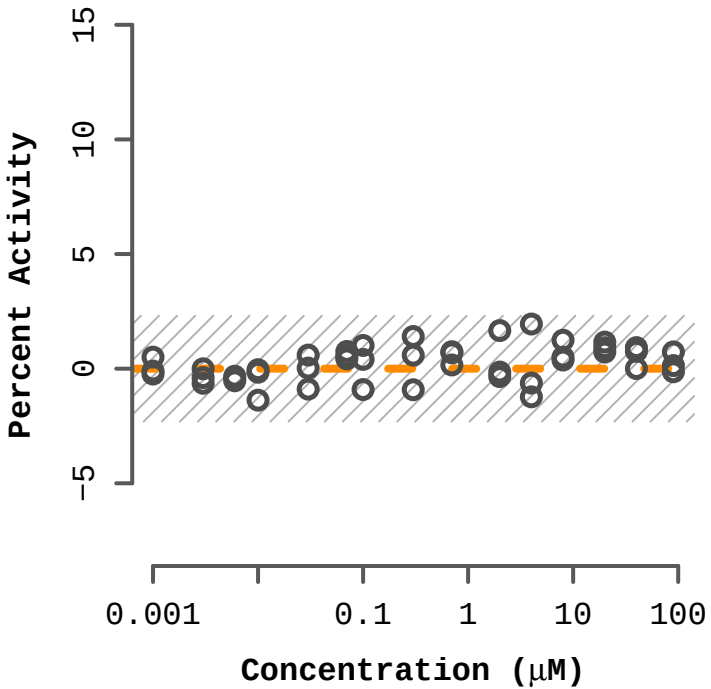
NAME: Sodium warfarin
CHID: 35010 **CASRN:** 129-06-6
SPID(S): Tox21_301545
M4ID: 12477588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.12	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

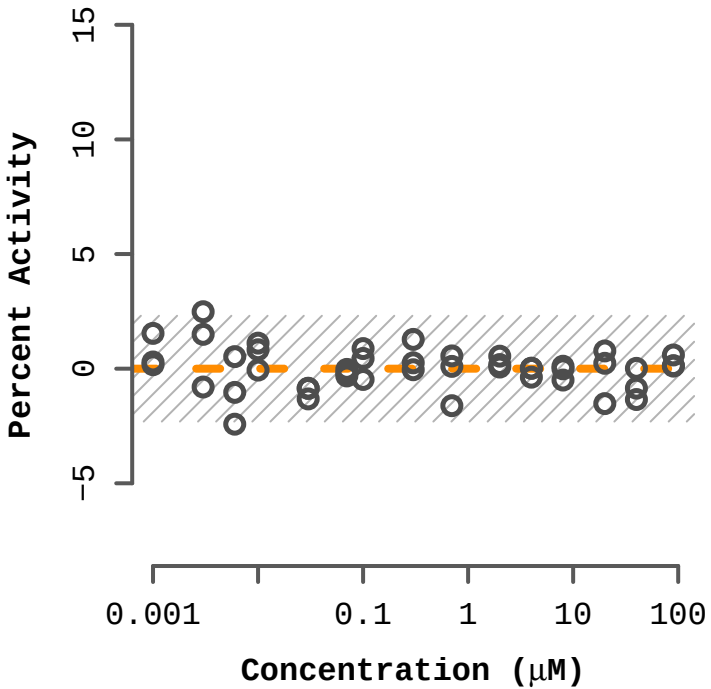
NAME: Zinc chloride
CHID: 35013 **CASRN:** 7646-85-7
SPID(S): Tox21_301492
M4ID: 12477641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.917 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

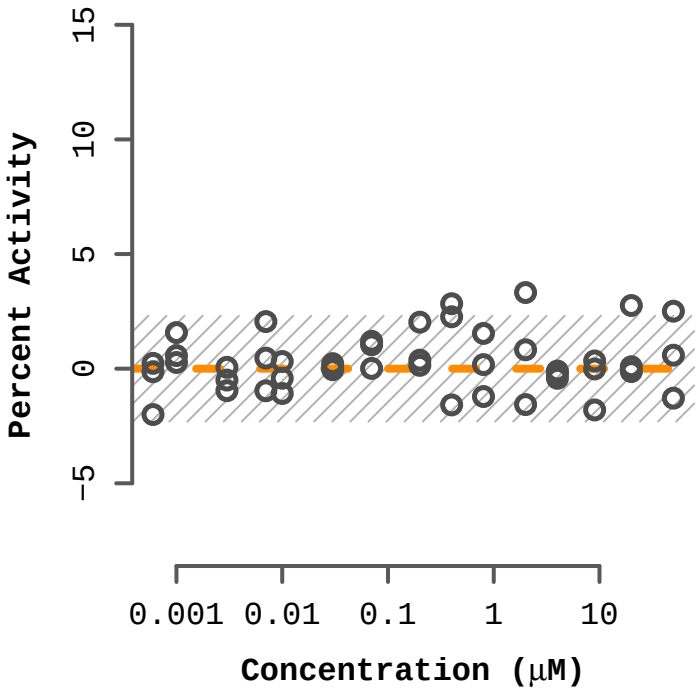
NAME: (4-Aminophenyl)arsonic acid
CHID: 35138 **CASRN:** 98-50-0
SPID(S): Tox21_301443
M4ID: 12477690

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

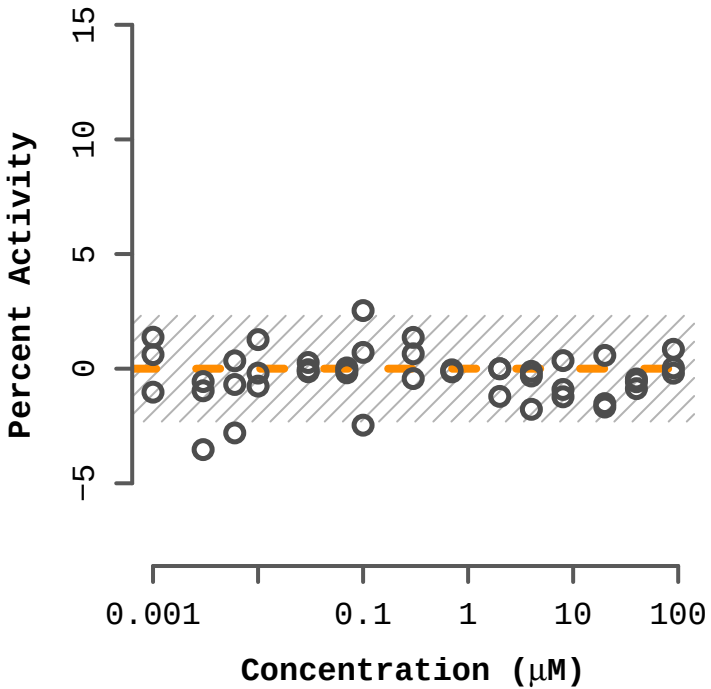
NAME: (4-Aminophenyl)arsonic acid
CHID: 35138 **CASRN:** 98-50-0
SPID(S): Tox21_111204_1
M4ID: 12483843

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

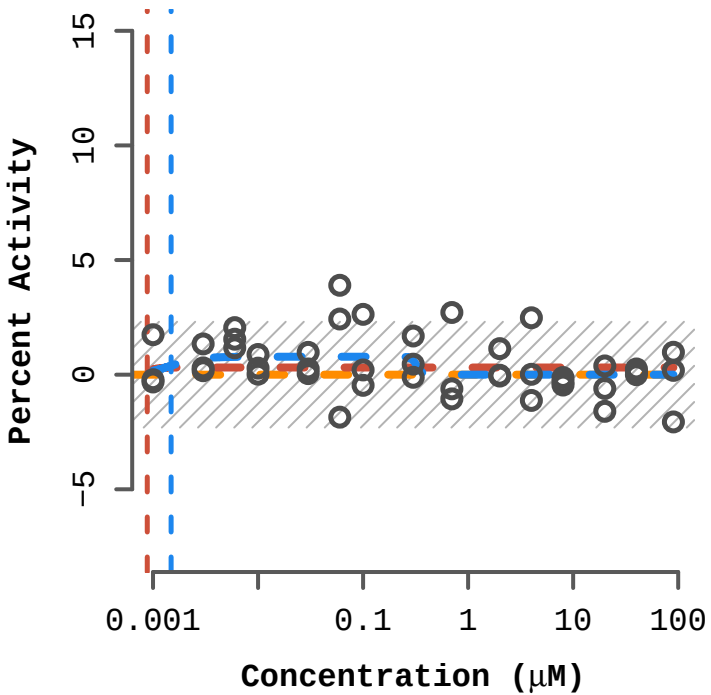
NAME: 1-(Hydroxymethyl)-5,5-dimethylhydantoin
CHID: 35152 **CASRN:** 116-25-6
SPID(S): Tox21_300102
M4ID: 12479028

HILL MODEL: Not applicable.

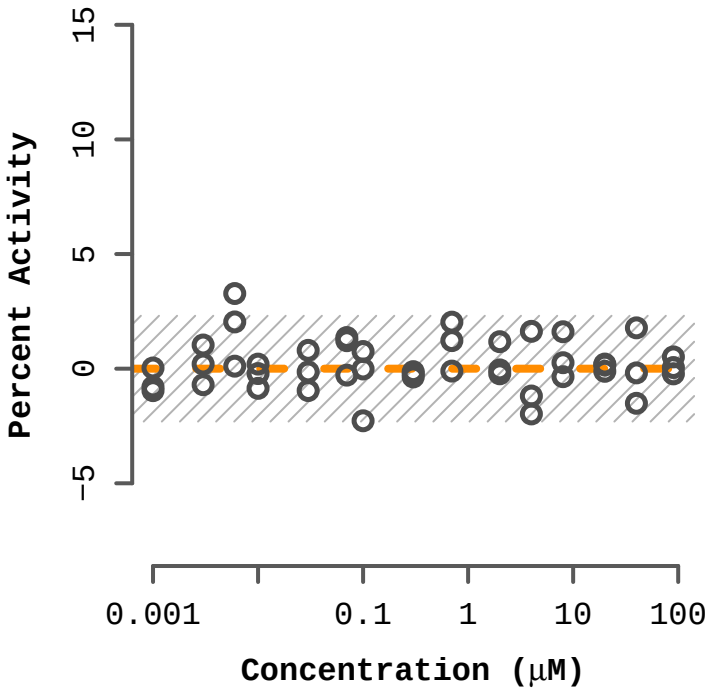
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.711 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Phenylethyl propionate
CHID:    35156   CASRN: 122-70-3
SPID(S): Tox21_300974
M4ID:    12478159

HILL MODEL (in red):
      tp       ga       gw
val:  0.313    -3.05    7.99
sd:   0.174    1.33     181

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  0.782    -2.83    3.27     -0.488   16.6
sd:   0.292    0.64     5.32     1.86     891

      CNST       HILL       GNLS
AIC:  151.25     153.83     151.51
PROB: 0.46       0.13       0.41
RMSE: 1.3        1.23       1.16

MAX_MEAN: 1.59      MAX_MED: 2.43      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

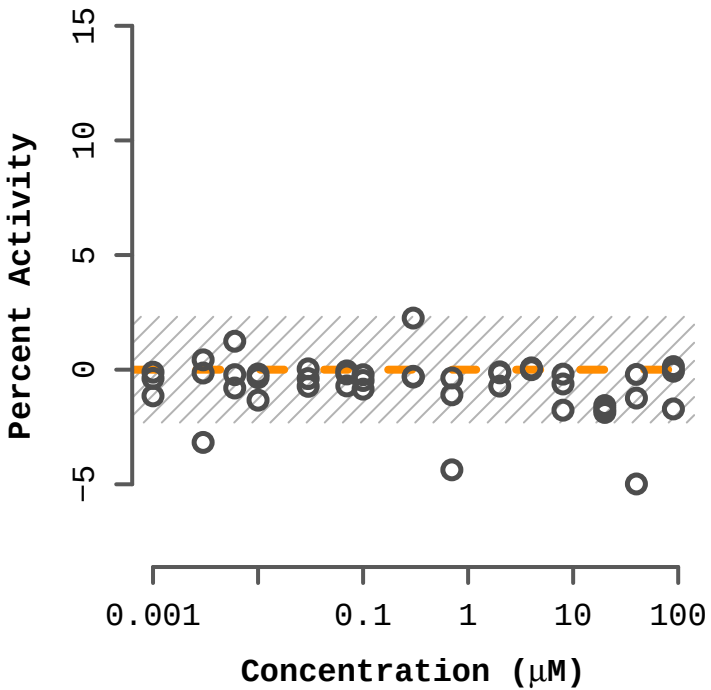
NAME: alpha−Ionone
CHID: 35160 **CASRN:** 127−41−3
SPID(S): Tox21_301173
M4ID: 12477960

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

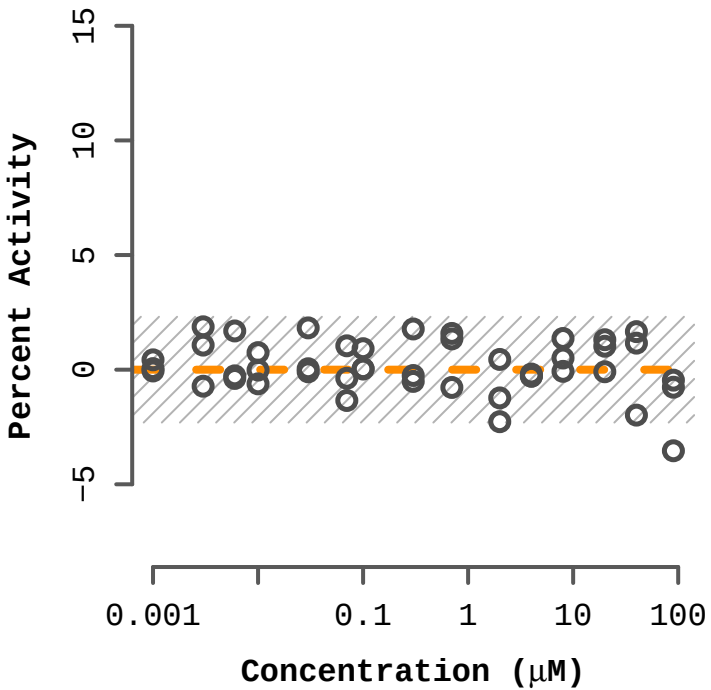
NAME: 1,2,4−Trimethoxybenzene
CHID: 35163 **CASRN:** 135−77−3
SPID(S): Tox21_300993
M4ID: 12478140

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.0533 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

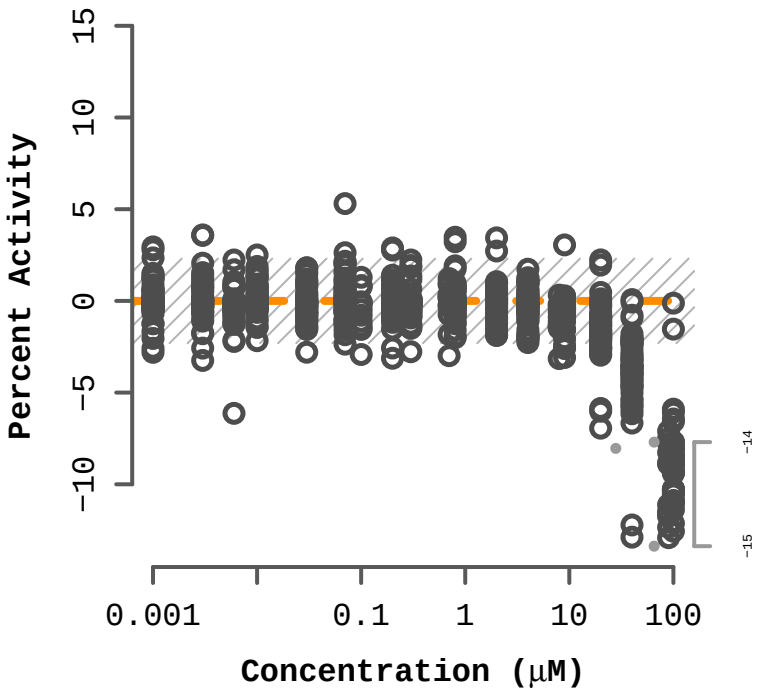
NAME: Kinetin
CHID: 35175 CASRN: 525-79-1
SPID(S): Tox21_301214
M4ID: 12477919

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.748 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

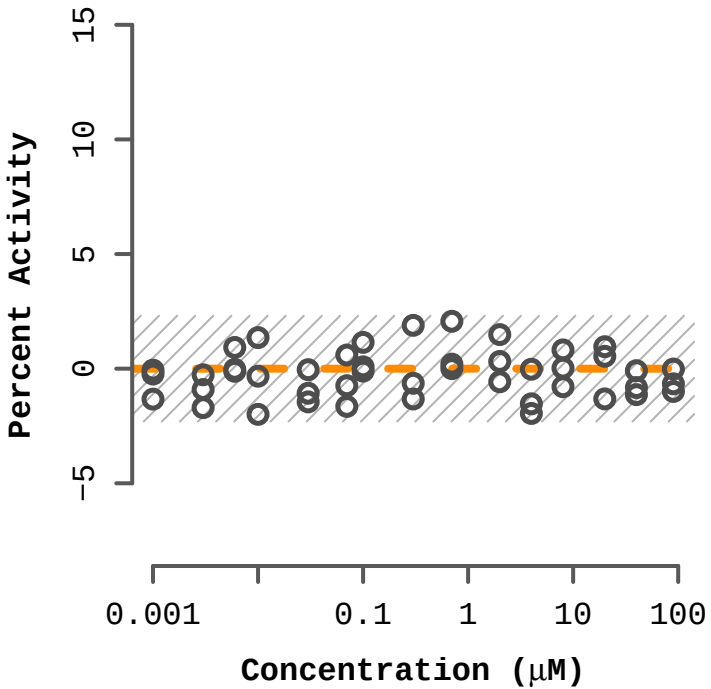
NAME: Allethrin
CHID: 35180 **CASRN:** 584-79-2
SPID(S): Tox21_400074
M4ID: 12475063 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3168.59	NA	NA
PROB:	1	NA	NA
RMSE:	3.02	NA	NA

MAX_MEAN: 0.245 **MAX_MED:** 0.163 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

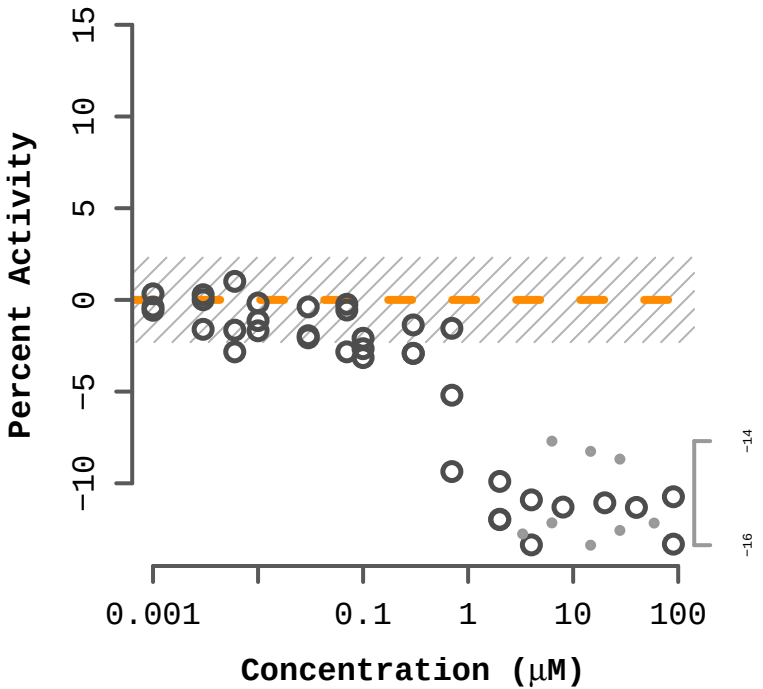
NAME: 3-Methyl-2-cyclohexen-1-one
CHID: 35186 **CASRN:** 1193-18-6
SPID(S): Tox21_302036
M4ID: 12477097

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.757 **MAX_MED:** 0.541 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

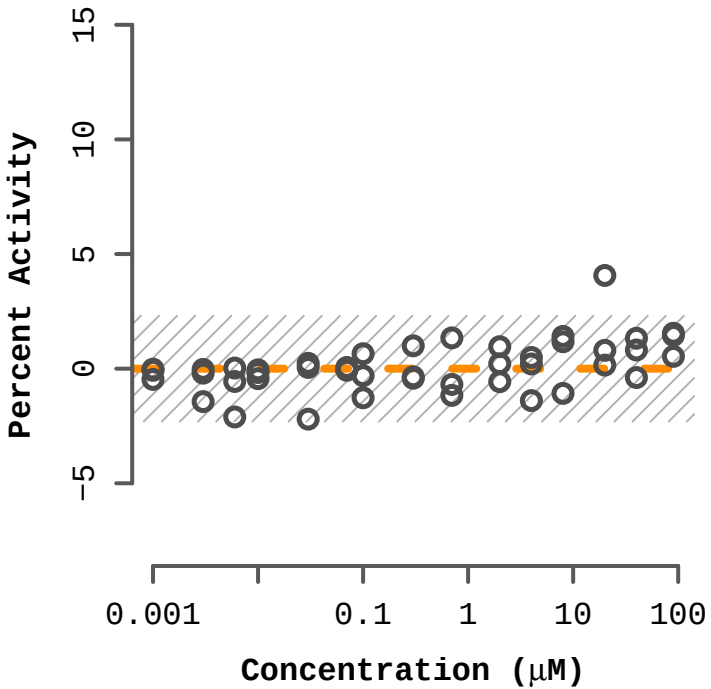
NAME: Tributyltin methacrylate
CHID: 35204 **CASRN:** 2155-70-6
SPID(S): Tox21_300409
M4ID: 12478723 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	326.81	NA	NA
PROB:	1	NA	NA
RMSE:	8.66	NA	NA

MAX_MEAN: −0.206 **MAX_MED:** 0.011 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

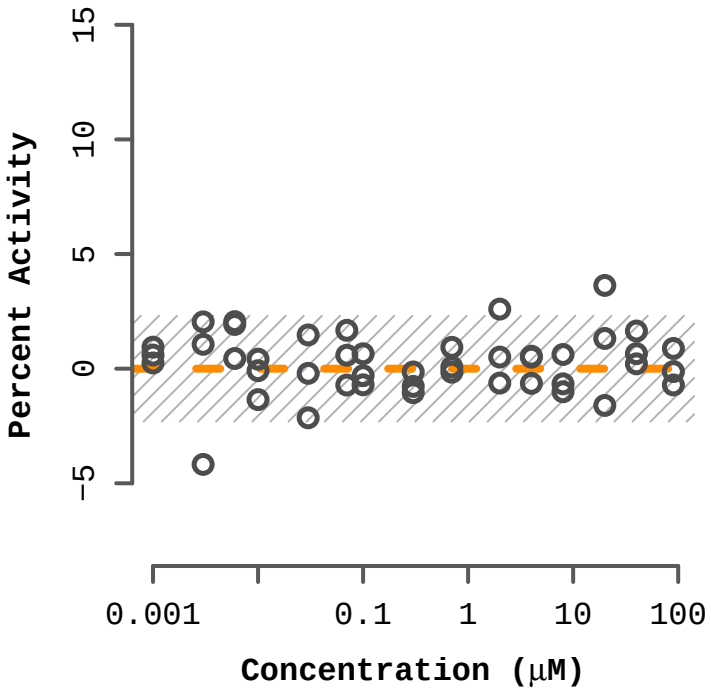
NAME: Diallyl disulfide
CHID: 35206 **CASRN:** 2179-57-9
SPID(S): Tox21_302178
M4ID: 12476955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

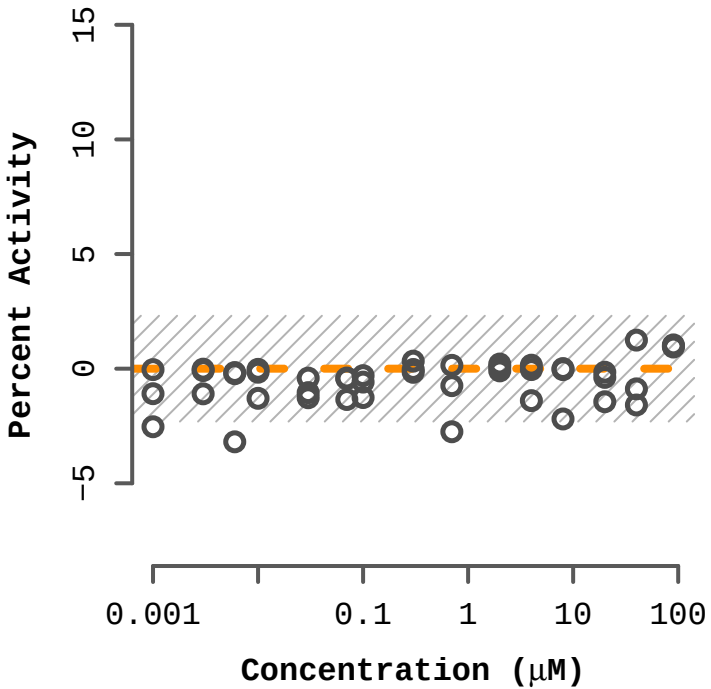
NAME: Oxypurinol
CHID: 35209 **CASRN:** 2465-59-0
SPID(S): Tox21_301220
M4ID: 12477913

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

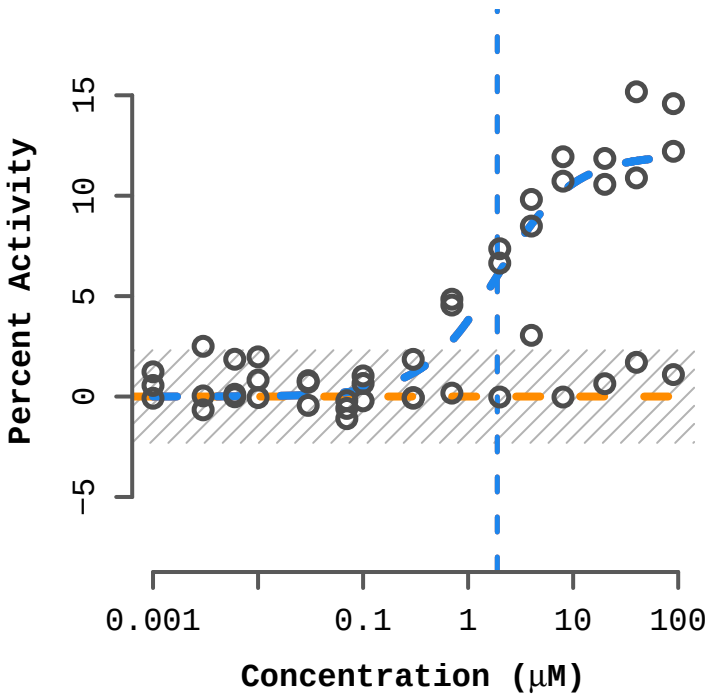
NAME: 1-Octen-3-ol
CHID: 35214 **CASRN:** 3391-86-4
SPID(S): Tox21_302039
M4ID: 12477094

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.99 **MAX_MED:** 0.985 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3-Dimethylol-5,5-dimethylhydantoin
CHID: 35217 CASRN: 6440-58-0
SPID(S): Tox21_303842
M4ID: 12475346

HILL MODEL (in red):

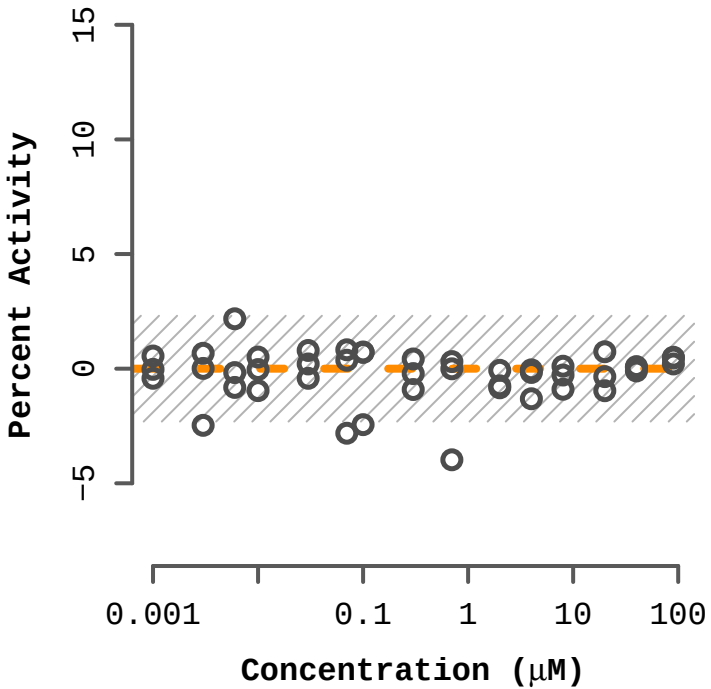
	tp	ga	gw
val:	12	0.278	1.21
sd:	1.11	0.139	0.334

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12	0.278	1.21	3.22	6.32
sd:	1.11	0.139	0.334	972	4860

	CNST	HILL	GNLS
AIC:	282.93	228.46	232.46
PROB:	0	0.88	0.12
RMSE:	5.91	3.57	3.57

MAX_MEAN: 9.3 MAX_MED: 12.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

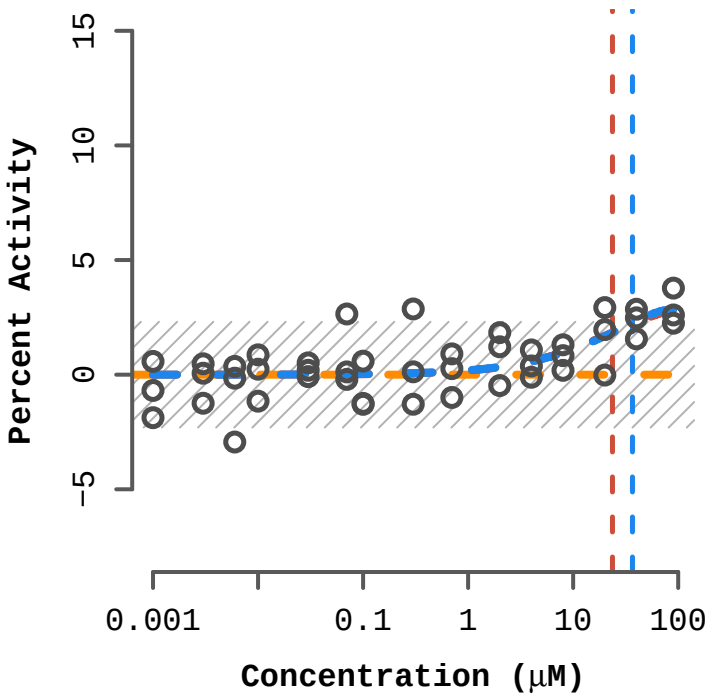
NAME: (Z)-11-Tetradecenyl acetate
CHID: 35266 **CASRN:** 20711-10-8
SPID(S): Tox21_302204
M4ID: 12476929

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.398 **MAX_MED:** 0.712 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6-Diisopropylnaphthalene
CHID: 35272 **CASRN:** 24157-81-1
SPID(S): Tox21_301083
M4ID: 12478050

HILL MODEL (in red):

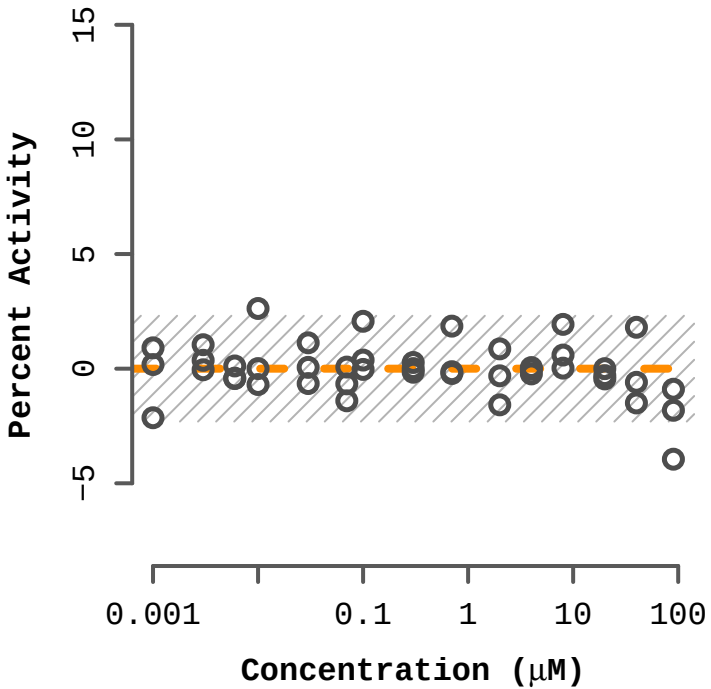
	tp	ga	gw
val:	3.68	1.37	0.94
sd:	2.42	0.754	0.716

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.53	1.56	0.867	2.19	4.1
sd:	7.86	1.64	0.726	4.12	76.7

	CNST	HILL	GNLS
AIC:	168.65	140.1	144.04
PROB:	0	0.88	0.12
RMSE:	1.52	1.07	1.07

MAX_MEAN: 2.88 **MAX_MED:** 2.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

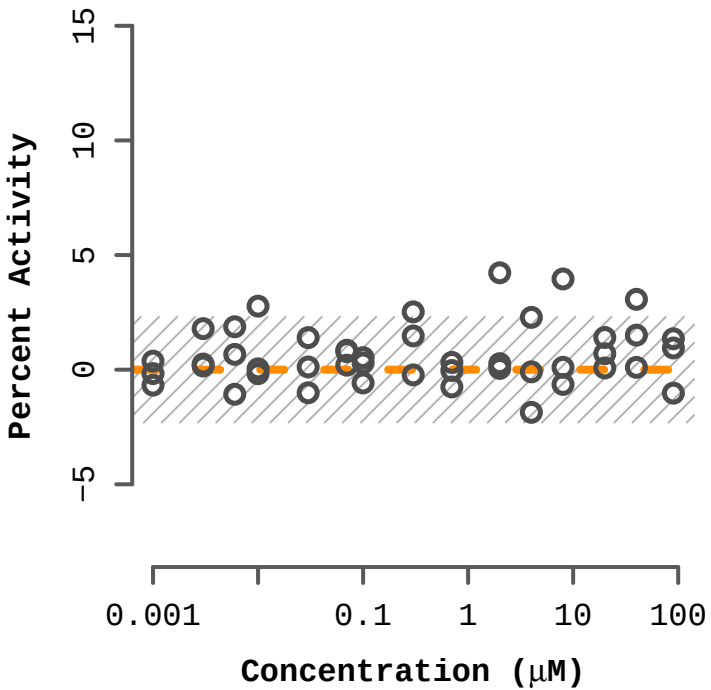
NAME: (9E,12Z)-9,12-Tetradecadien-1-ol acetate
CHID: 35285 CASRN: 31654-77-0
SPID(S): Tox21_302010
M4ID: 12477123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.851 MAX_MED: 0.596 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

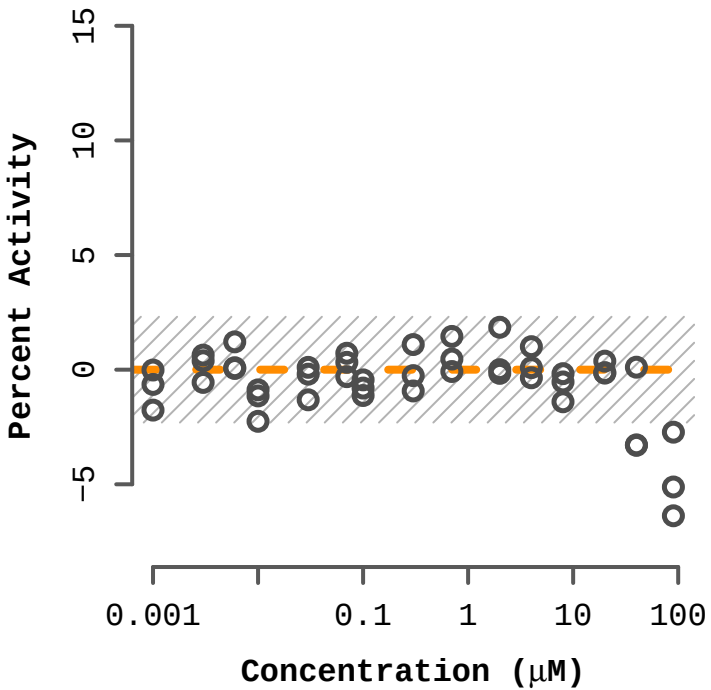
NAME: (E)−11−Tetradecen−1−ol acetate
CHID: 35286 CASRN: 33189−72−9
SPID(S): Tox21_301051
M4ID: 12478082

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.56 MAX_MED: 1.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

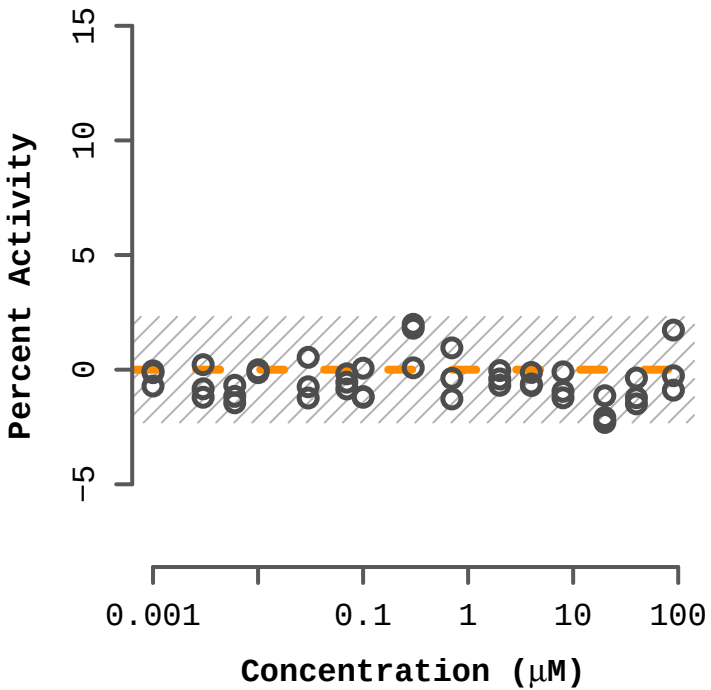
NAME: Codlelure
CHID: 35288 CASRN: 33956-49-9
SPID(S): Tox21_300836
M4ID: 12478297

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.613 **MAX_MED:** 0.465 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

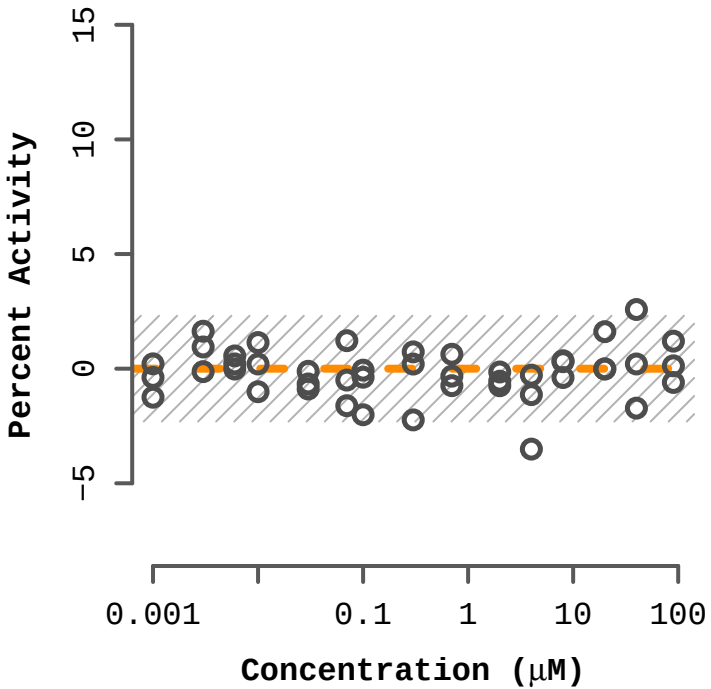
NAME: (E)−5−Decen−1−ol
CHID: 35305 **CASRN:** 56578−18−8
SPID(S): Tox21_300978
M4ID: 12478155

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.69	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

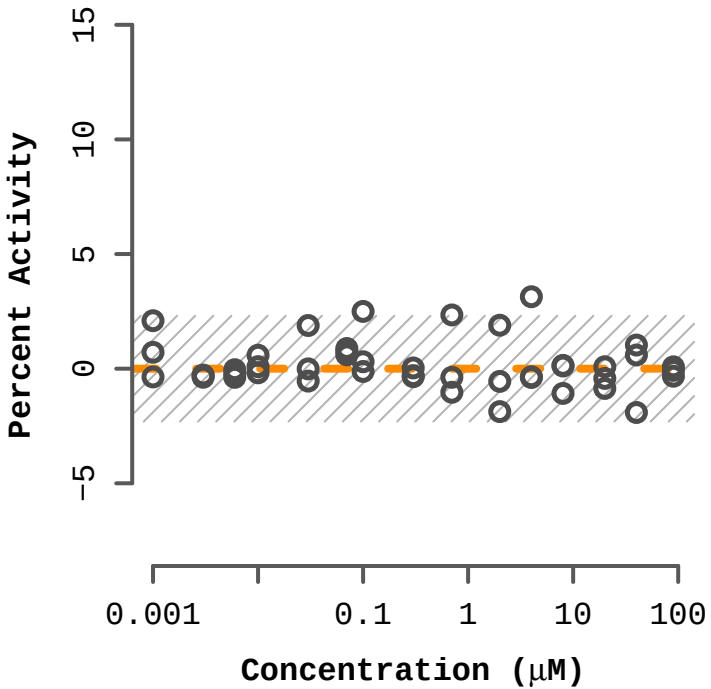
NAME: 1,3-Dibromo-5,5-dimethylhydantoin
CHID: 35341 CASRN: 77-48-5
SPID(S): Tox21_300158
M4ID: 12478972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

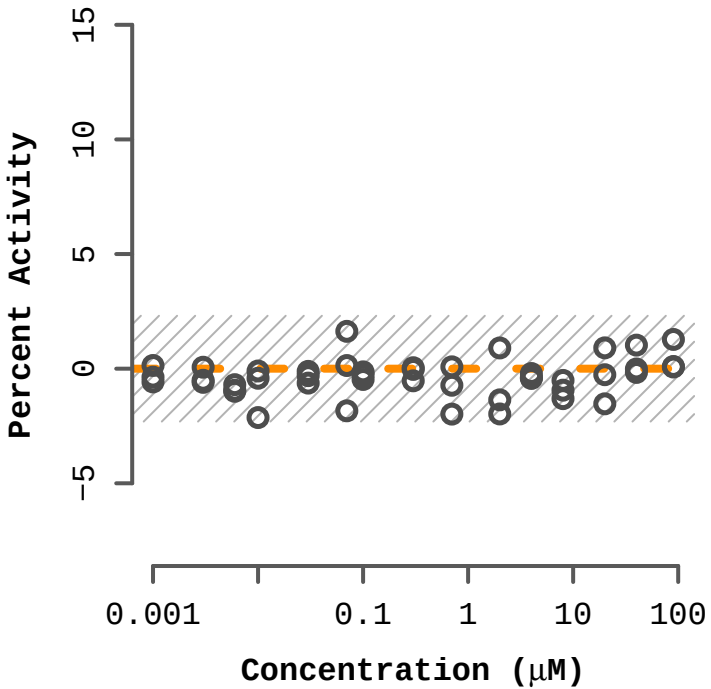
NAME: 1,4-Dimethylnaphthalene
CHID: 35423 **CASRN:** 571-58-4
SPID(S): Tox21_300881
M4ID: 12478252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 0.756 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

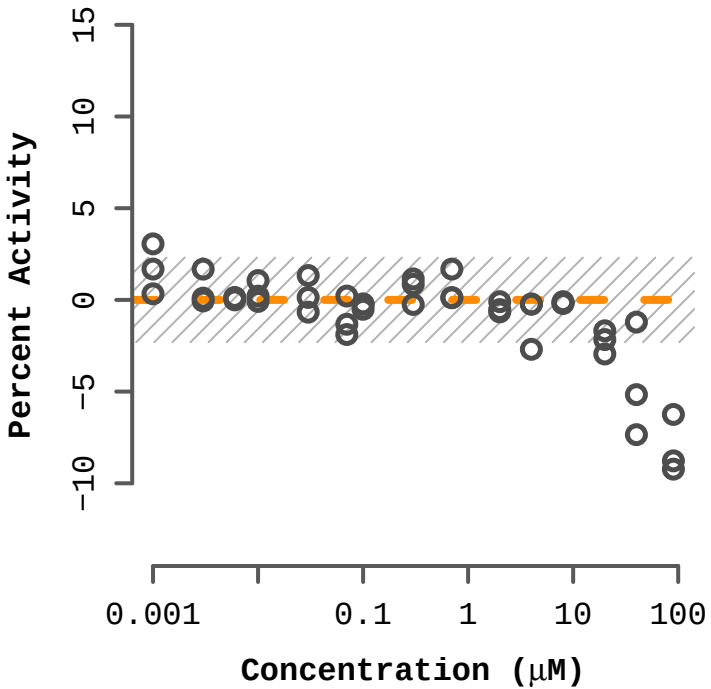
NAME: 4-(4-(Acetyloxy)phenyl)-2-butanone
CHID: 35481 **CASRN:** 3572-06-3
SPID(S): Tox21_301631
M4ID: 12477502

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.482 **MAX_MED:** 0.139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

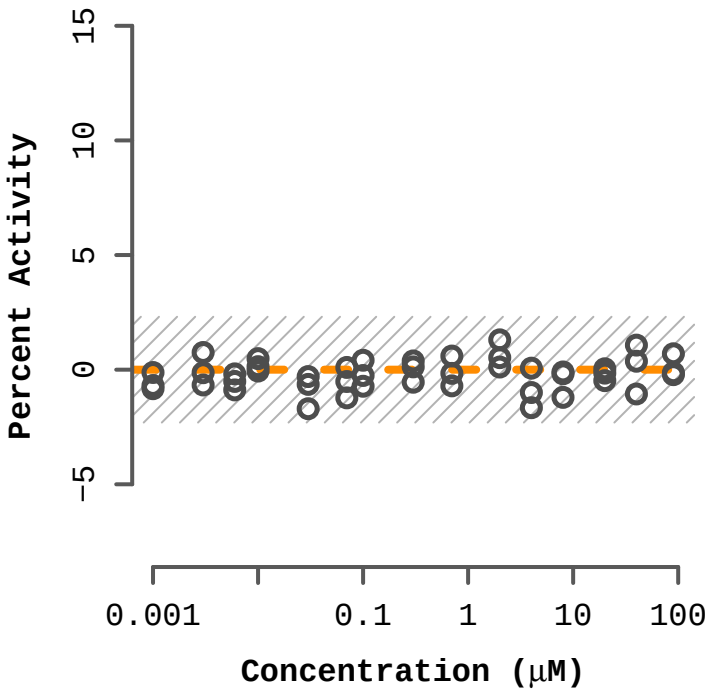
NAME: Disiquonium chloride
CHID: 35589 CASRN: 68959-20-6
SPID(S): Tox21_302379
M4ID: 12476754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.8	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

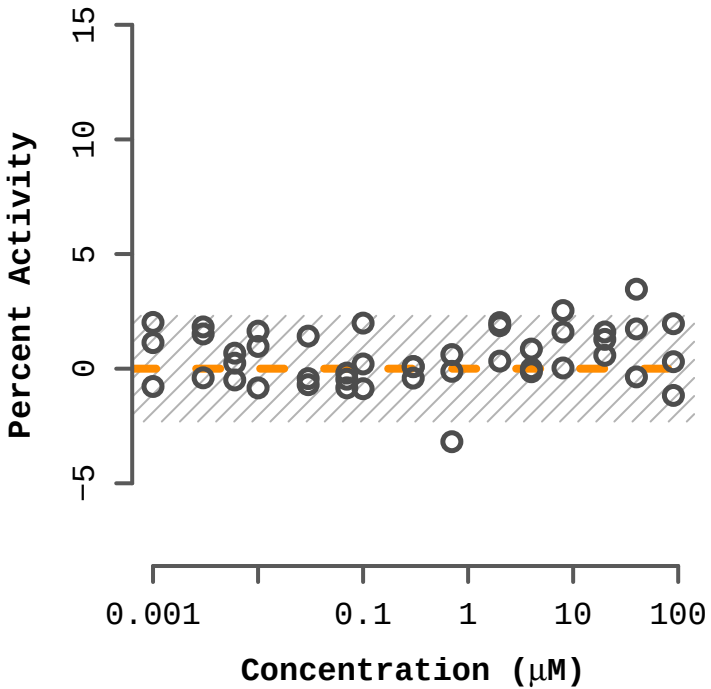
NAME: (E)-4-Tridecen-l-yl acetate
CHID: 35592 **CASRN:** 72269-48-8
SPID(S): Tox21_301764
M4ID: 12477369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.649 **MAX_MED:** 0.526 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

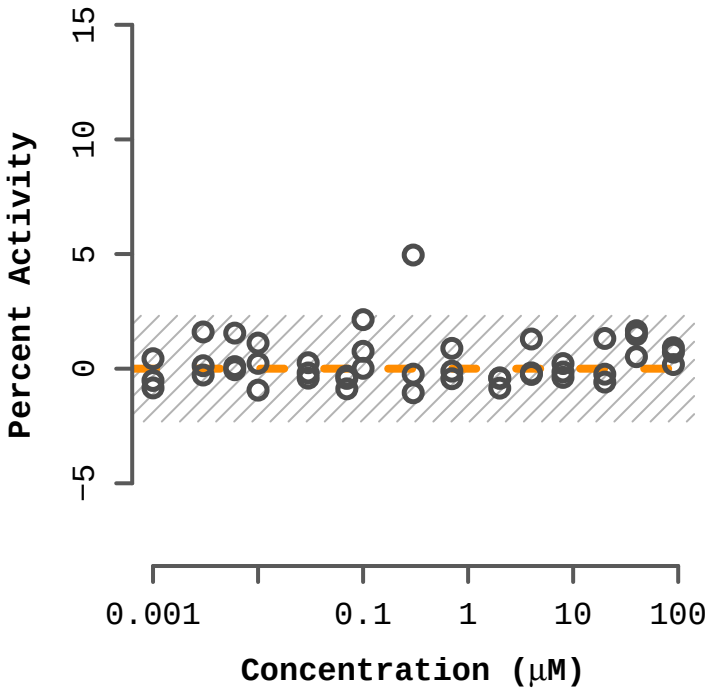
NAME: Sodium 2-nitrophenolate
CHID: 35616 **CASRN:** 824-39-5
SPID(S): Tox21_301461
M4ID: 12477672

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

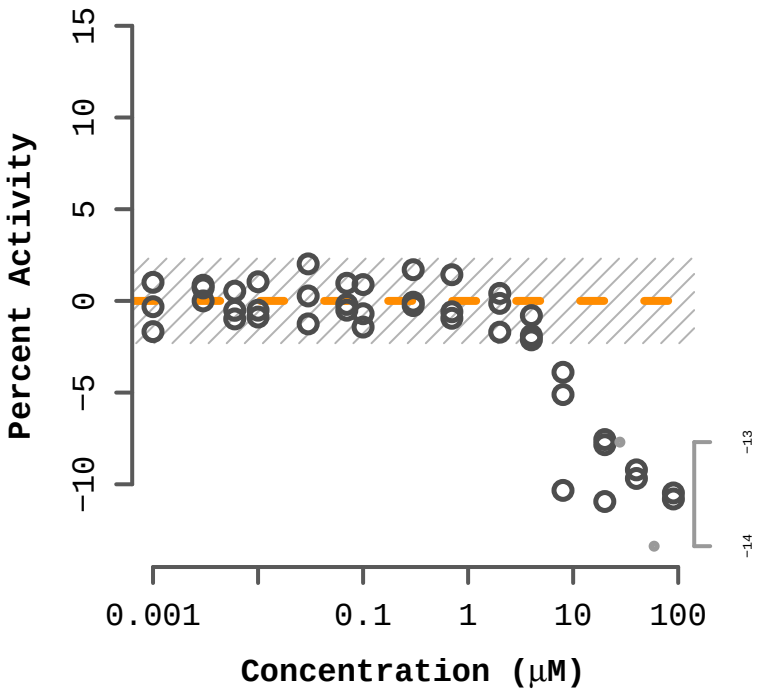
NAME: L−Verbenone
CHID: 35620 **CASRN:** 1196−01−6
SPID(S): Tox21_301431
M4ID: 12477702

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

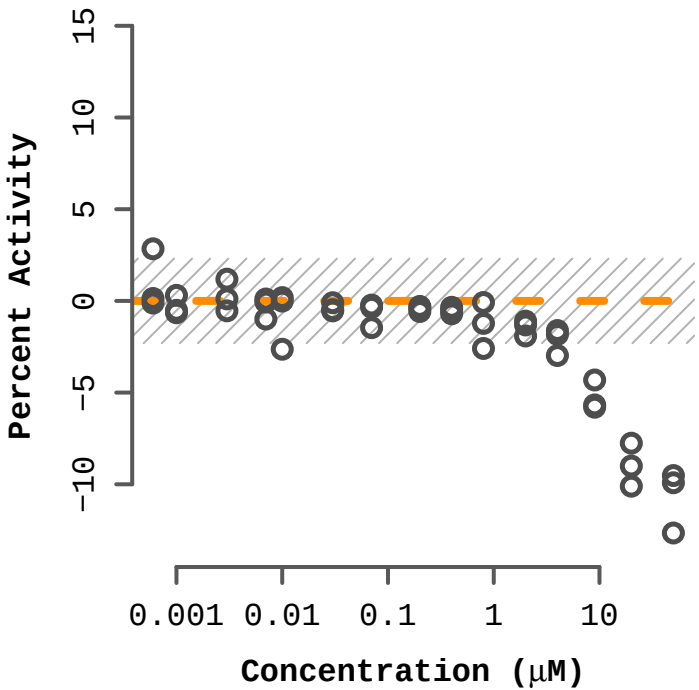
NAME: Methylbenzethonium chloride
CHID: 35708 **CASRN:** 25155-18-4
SPID(S): Tox21_301446
M4ID: 12477687 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.32	NA	NA
PROB:	1	NA	NA
RMSE:	5.16	NA	NA

MAX_MEAN: 0.523 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

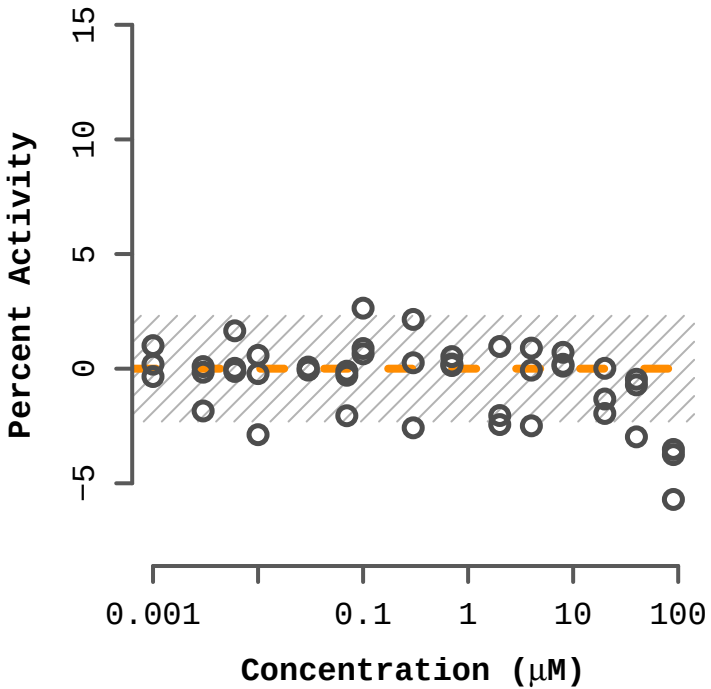
NAME: Methylbenzethonium chloride
CHID: 35708 **CASRN:** 25155-18-4
SPID(S): Tox21_113530_1
M4ID: 12482619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	239.83	NA	NA
PROB:	1	NA	NA
RMSE:	4.03	NA	NA

MAX_MEAN: 0.953 **MAX_MED:** 0.134 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

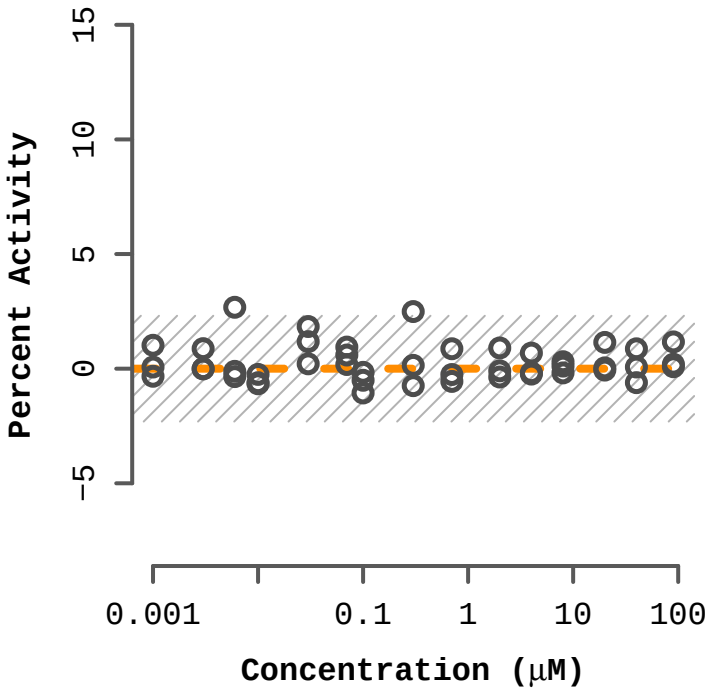
NAME: Chloroallyl methenamine chloride
CHID: 35748 **CASRN:** 51229-78-8
SPID(S): Tox21_301946
M4ID: 12477187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

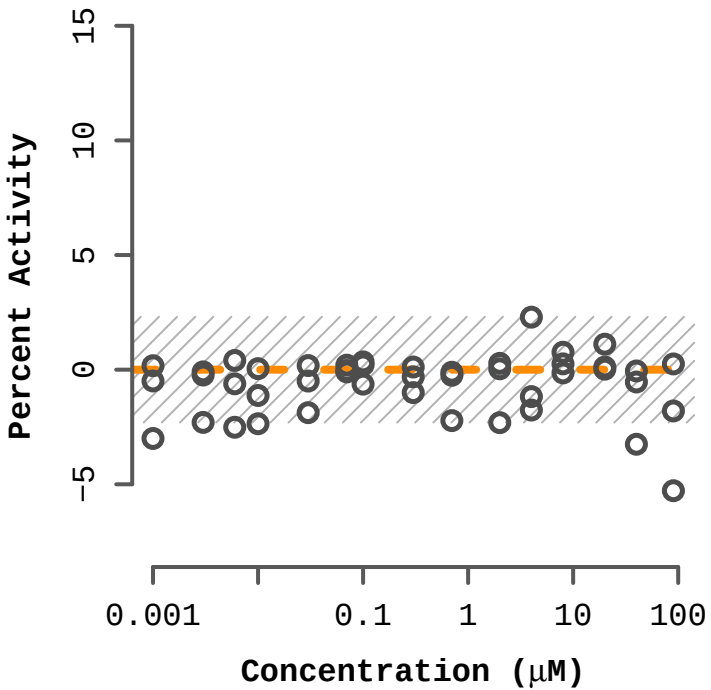
NAME: Ethyl 3-(N-butylacetamido)propionate
CHID: 35753 **CASRN:** 52304-36-6
SPID(S): Tox21_301772
M4ID: 12477361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

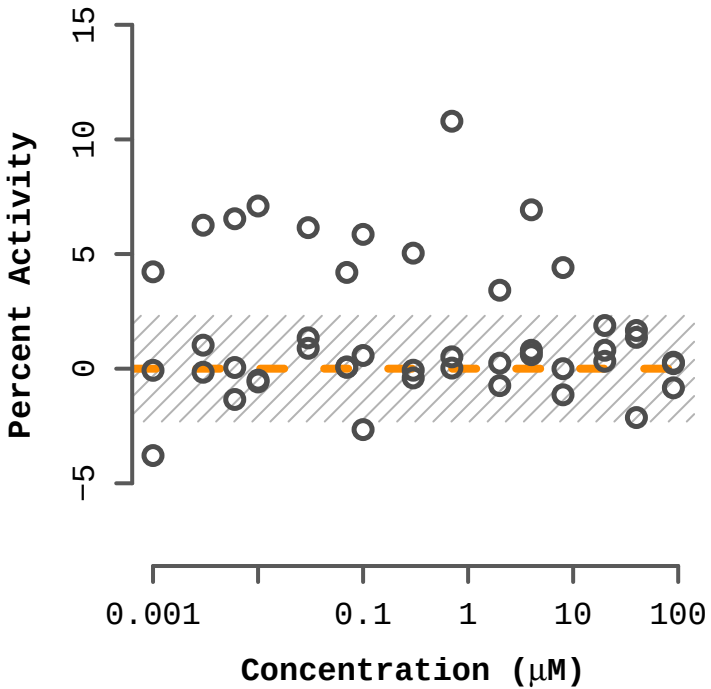
NAME: S-Methoprene
CHID: 35783 **CASRN:** 65733-16-6
SPID(S): Tox21_301409
M4ID: 12477724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.418 **MAX_MED:** 0.255 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

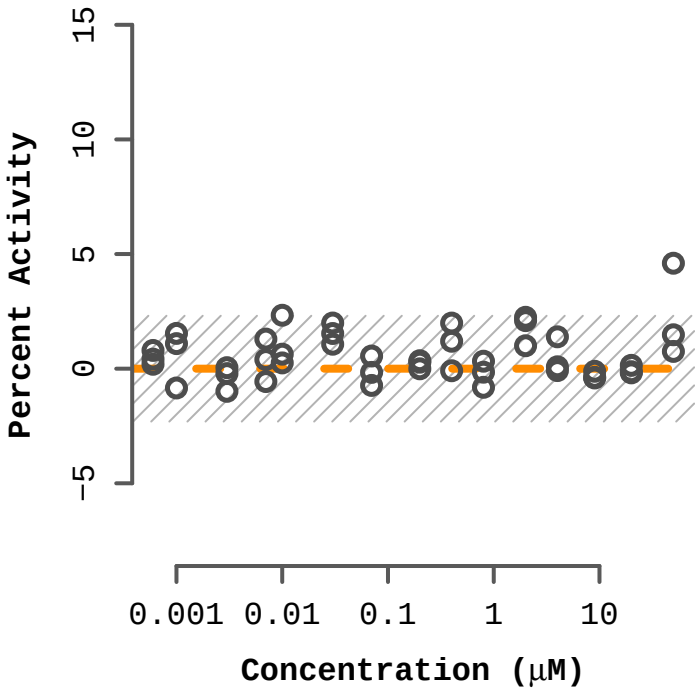
NAME: (7S)-Hydroprene
CHID: 35784 CASRN: 65733-18-8
SPID(S): Tox21_301066
M4ID: 12478067

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.24	NA	NA
PROB:	1	NA	NA
RMSE:	3.36	NA	NA

MAX_MEAN: 3.78 MAX_MED: 1.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

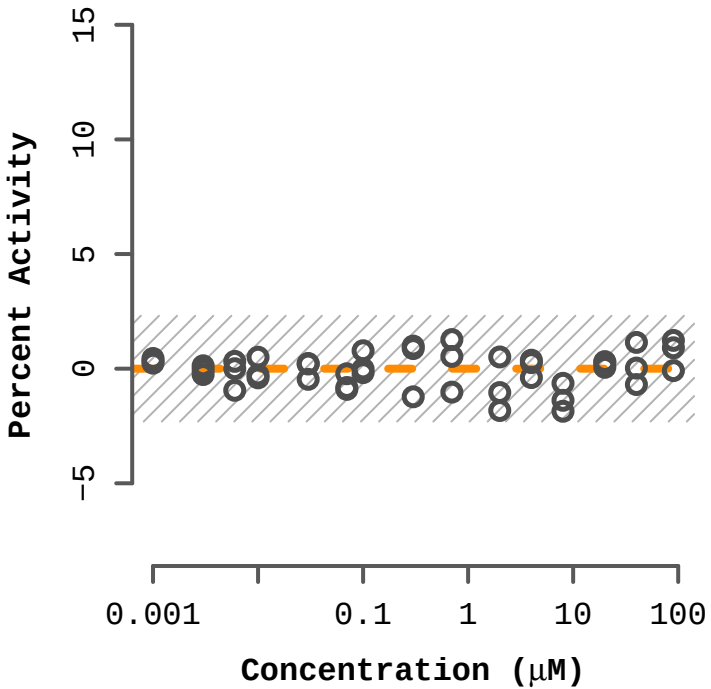
NAME: Sodium 2-methoxy-5-nitrophenolate
CHID: 35790 **CASRN:** 67233-85-6
SPID(S): Tox21_303810
M4ID: 12475378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

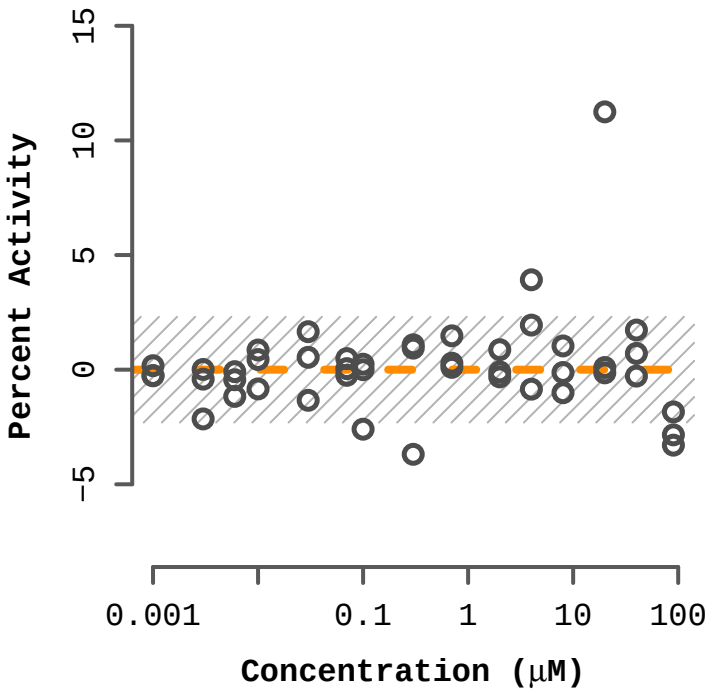
NAME: 1,3-Dichloro-5-ethyl-5-methylhydantoin
CHID: 35839 **CASRN:** 89415-87-2
SPID(S): Tox21_303928
M4ID: 12475260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

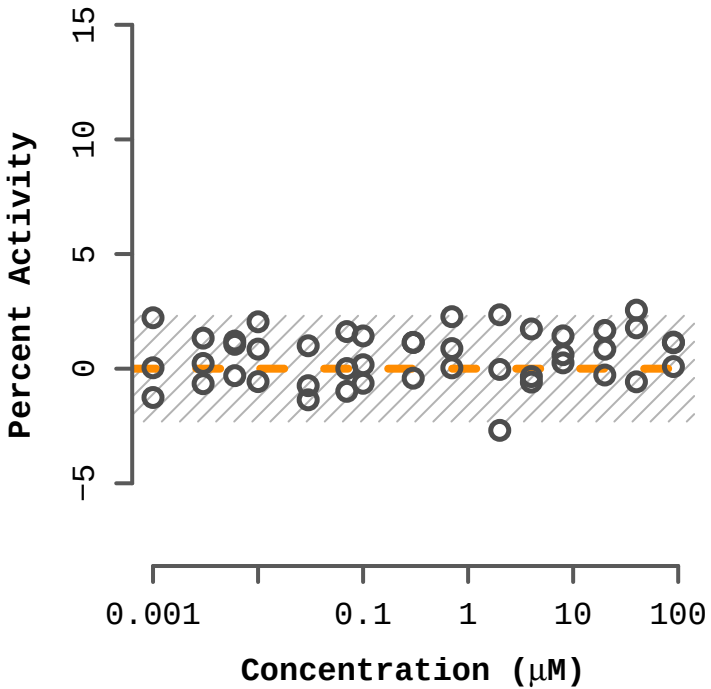
NAME: Cyfluthrin
CHID: 35957 **CASRN:** 68359-37-5
SPID(S): Tox21_300645
M4ID: 12478488

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 3.74 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

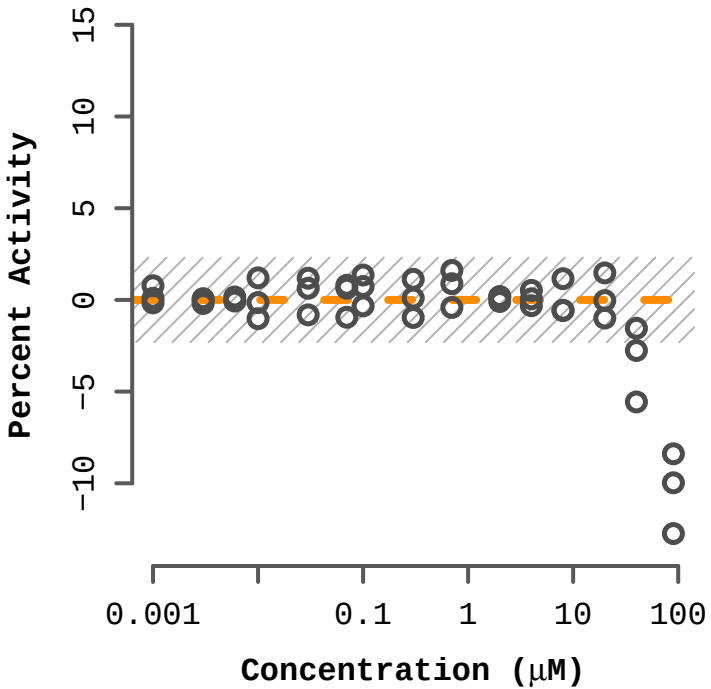
NAME: 2-tert-Butylcyclohexyl acetate
CHID: 36105 **CASRN:** 88-41-5
SPID(S): Tox21_301404
M4ID: 12477729

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

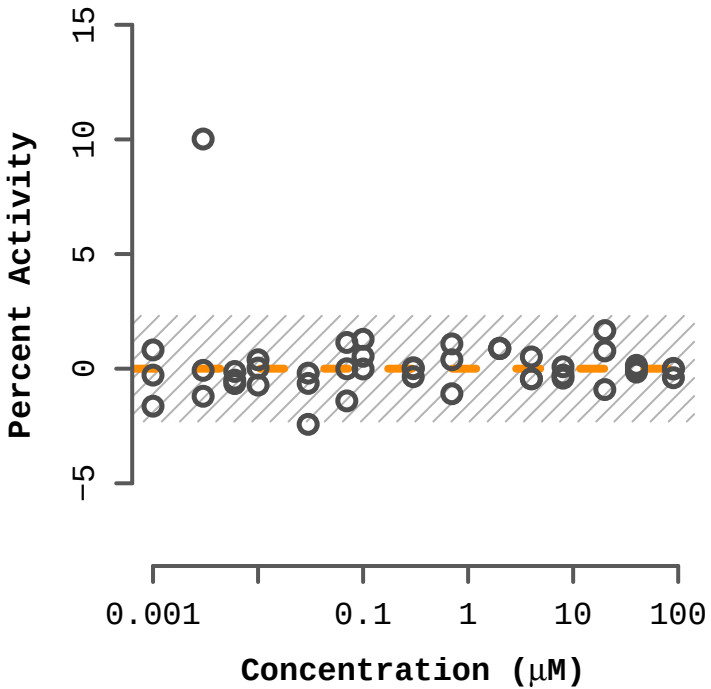
NAME: 2-(8-Heptadecenyl)-2-imidazoline-1-ethanol
CHID: 36112 **CASRN:** 95-38-5
SPID(S): Tox21_303368
M4ID: 12475767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.53	NA	NA
PROB:	1	NA	NA
RMSE:	2.96	NA	NA

MAX_MEAN: 0.695 **MAX_MED:** 0.885 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

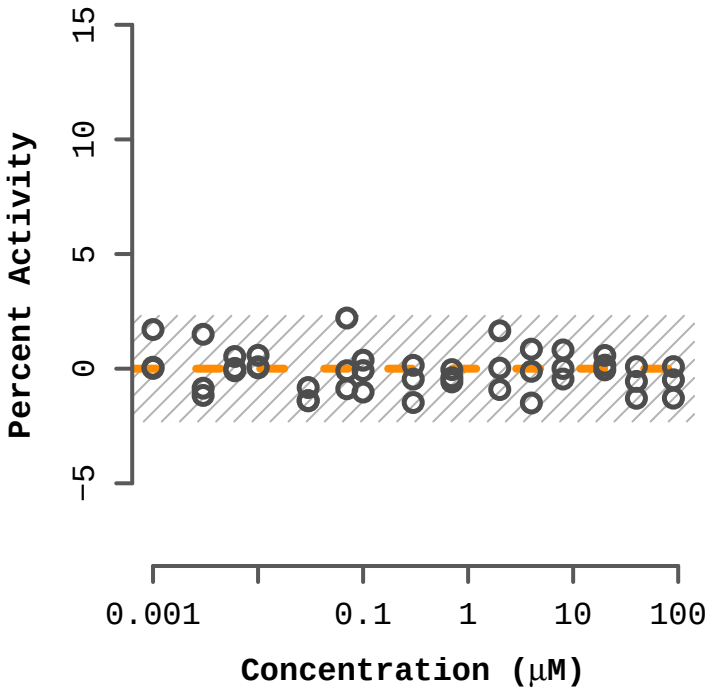
NAME: Sodium octyl sulfate
CHID: 36226 **CASRN:** 142-31-4
SPID(S): Tox21_301327
M4ID: 12477806

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 2.92 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

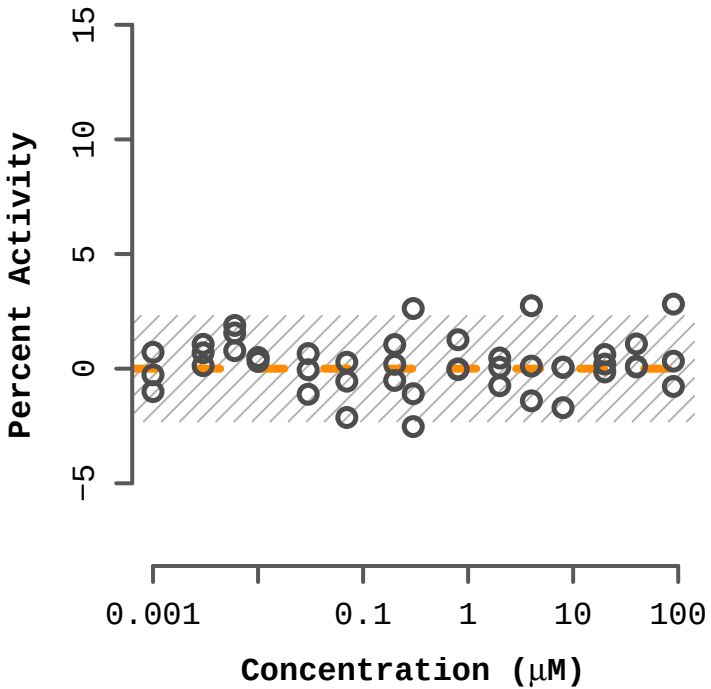
NAME: Sodium decyl sulfate
CHID: 36229 **CASRN:** 142-87-0
SPID(S): Tox21_302082
M4ID: 12477051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.154 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

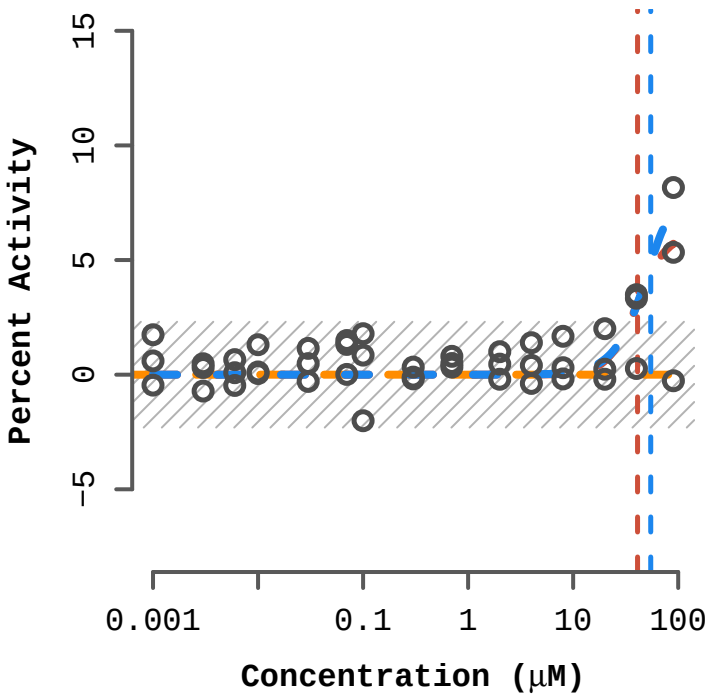
NAME: 3,7-Dimethyl-2,6-octadienenitrile
CHID: 36286 **CASRN:** 5146-66-7
SPID(S): Tox21_302113
M4ID: 12477020

HILL MODEL: Not applicable.

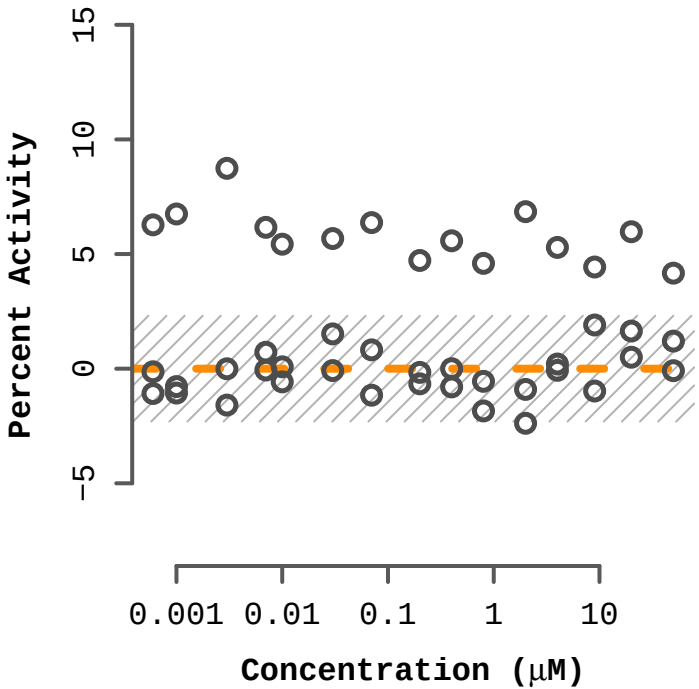
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.56 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Octyl-1-dodecanol
CHID:    36288   CASRN: 5333-42-6
SPID(S): Tox21_302294
M4ID:    12476839

HILL MODEL (in red):
      tp       ga       gw
val:  6.22     1.61     3.08
sd:   1.95     0.129    2.6

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.69     1.74     2.58     1.99     12.4
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  160.58      147.79      151.73
PROB: 0           0.88        0.12
RMSE: 1.83        1.34        1.33

MAX_MEAN: 4.41      MAX_MED: 5.34      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

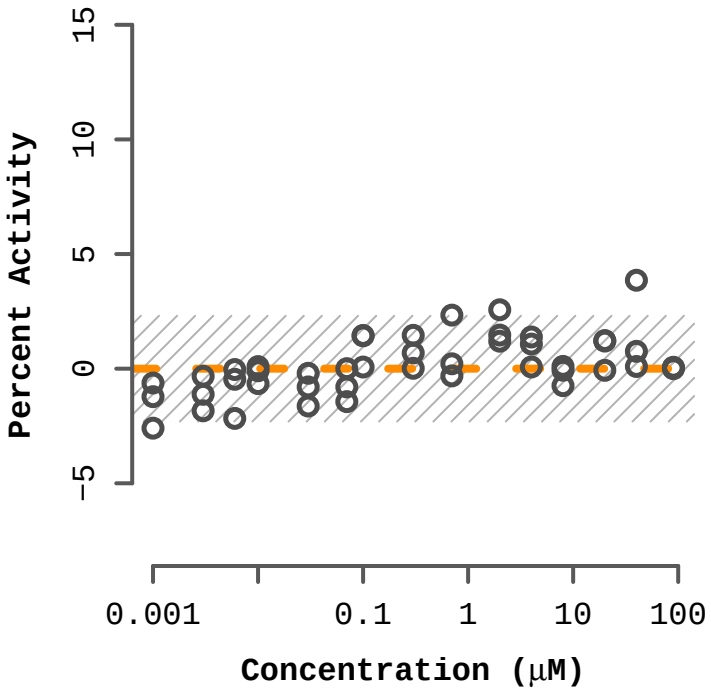
NAME: 2-Octyl-1-dodecanol
CHID: 36288 **CASRN:** 5333-42-6
SPID(S): Tox21_112351_1
M4ID: 12483142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	242.16	NA	NA
PROB:	1	NA	NA
RMSE:	3.51	NA	NA

MAX_MEAN: 2.71 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

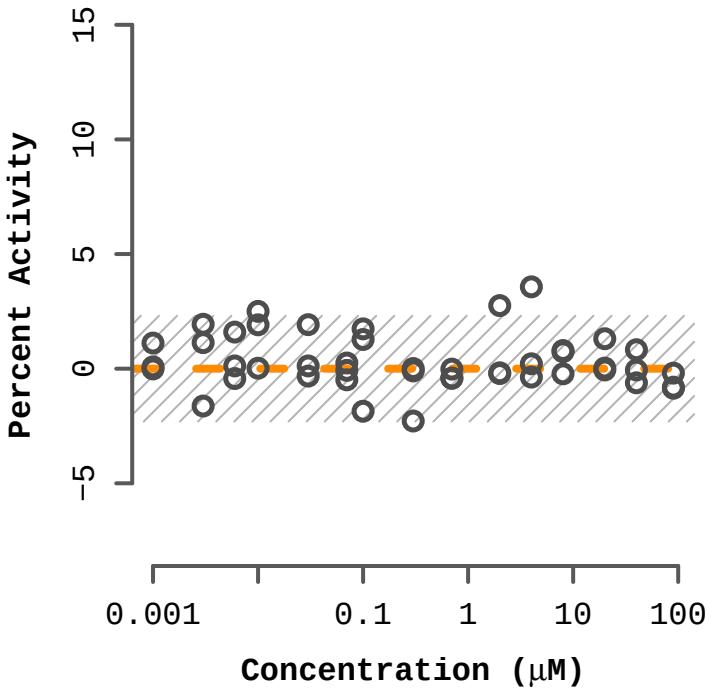
NAME: N,N−Dimethyloctylamine
CHID: 36299 **CASRN:** 7378−99−6
SPID(S): Tox21_300349
M4ID: 12478783

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

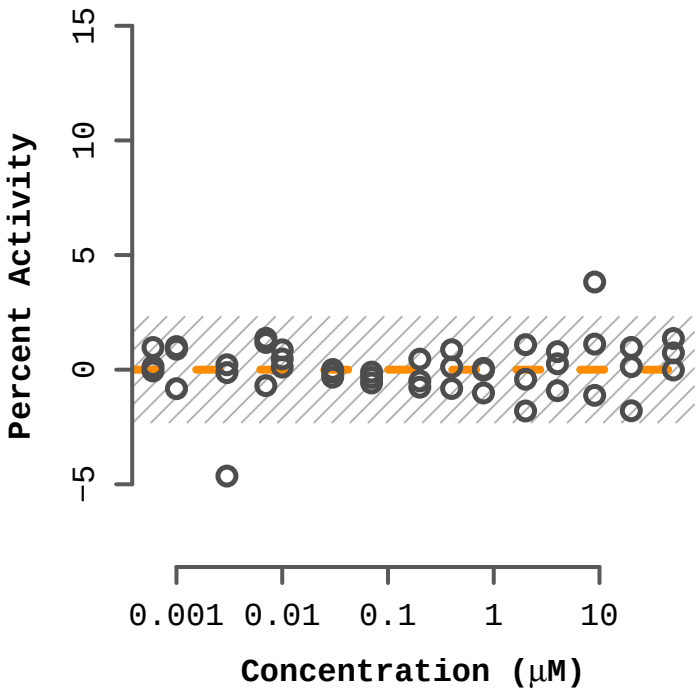
NAME: N-Octyl-2-pyrrolidone
CHID: 36435 **CASRN:** 2687-94-7
SPID(S): Tox21_301550
M4ID: 12477583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

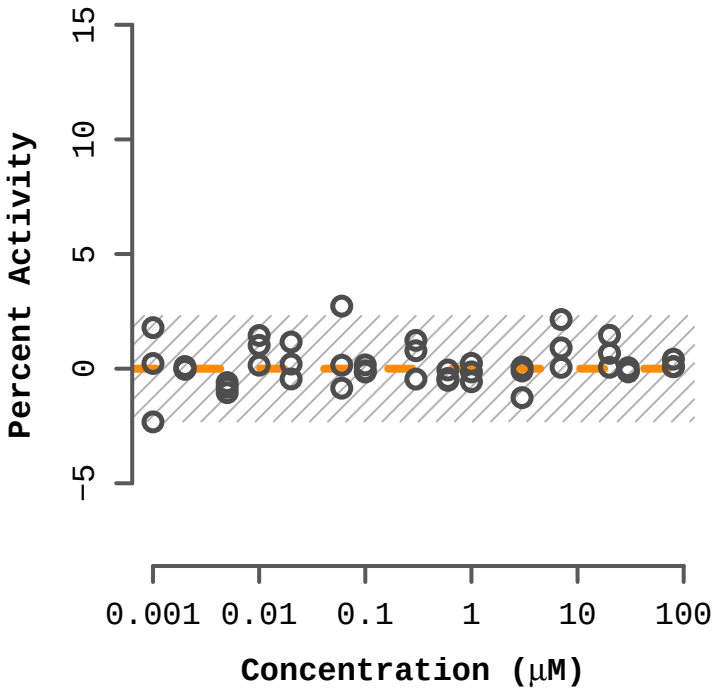
NAME: Bumetrizole
CHID: 36438 **CASRN:** 3896-11-5
SPID(S): Tox21_112379_1
M4ID: 12483125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

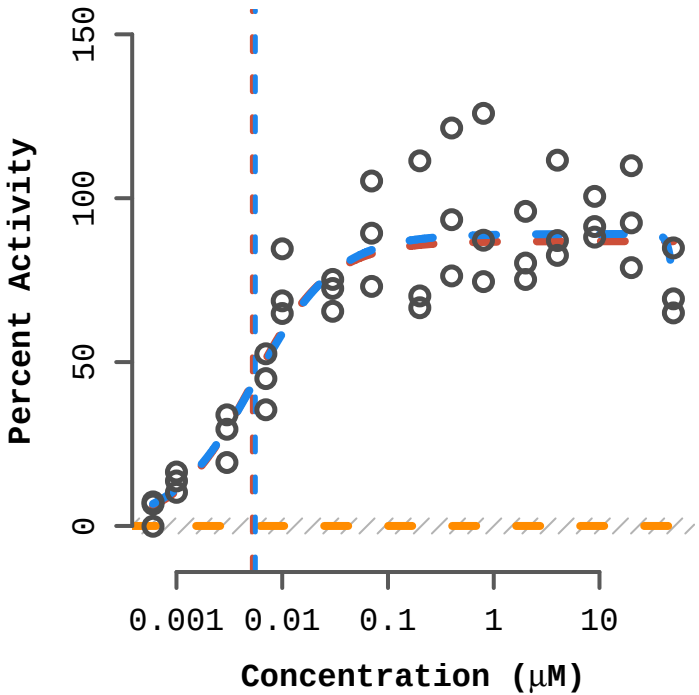
NAME: Disodium 4,4'−bis(2−sulfostyryl)biphenyl
CHID: 36467 **CASRN:** 27344−41−8
SPID(S): Tox21_301540
M4ID: 12477593

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mibolerone
CHID: 36489 CASRN: 3704-09-4
SPID(S): Tox21_113738
M4ID: 12482476

HILL MODEL (in red):

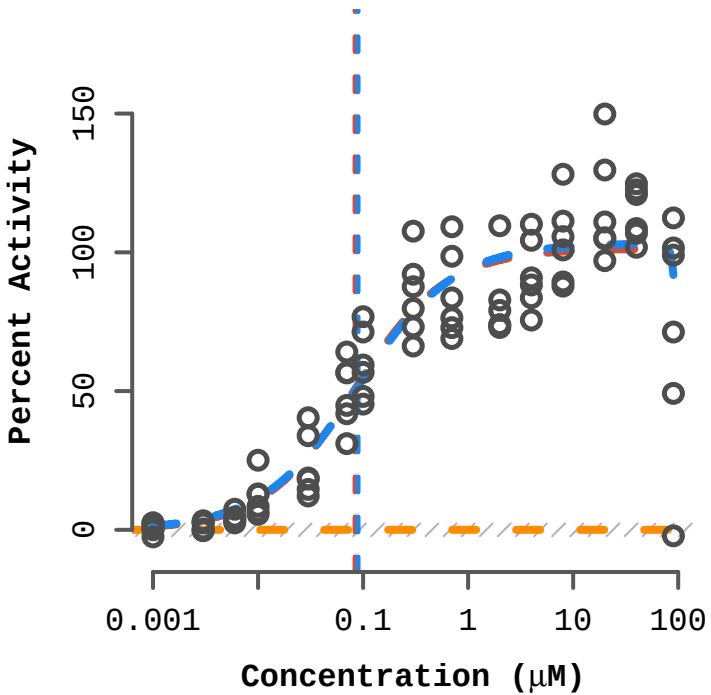
	tp	ga	gw
val:	86.9	-2.28	1.19
sd:	2.88	0.0751	0.226

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	89.1	-2.25	1.12	1.75	13.1
sd:	3.06	0.0762	0.205	0.0577	16.2

	CNST	HILL	GNLS
AIC:	528.34	372.68	371.99
PROB:	0	0.42	0.58
RMSE:	76.35	14.05	13.3

MAX_MEAN: 97.1 MAX_MED: 93.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norgestrel
CHID: 36496 CASRN: 797-63-7
SPID(S): Tox21_303658
M4ID: 12475490

HILL MODEL (in red):

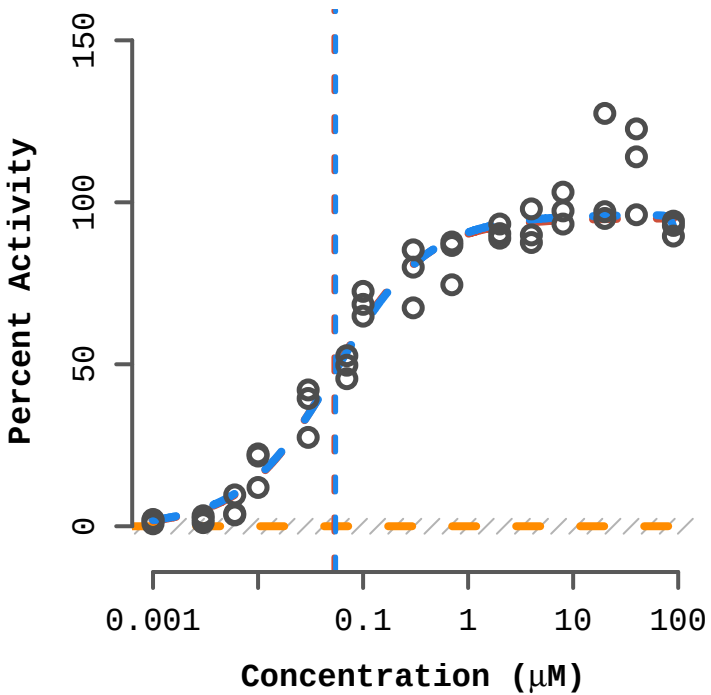
	tp	ga	gw
val:	101	-1.08	0.995
sd:	3.06	0.0699	0.142

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	103	-1.05	0.949	2.01	17.6
sd:	3.56	0.0788	0.141	0.0828	27.1

	CNST	HILL	GNLS
AIC:	1044.3	753.32	755.6
PROB:	0	0.76	0.24
RMSE:	73.93	18.1	17.17

MAX_MEAN: 116 MAX_MED: 115 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norgestrel
CHID: 36496 CASRN: 797-63-7
SPID(S): Tox21_202872
M4ID: 12479380

HILL MODEL (in red):

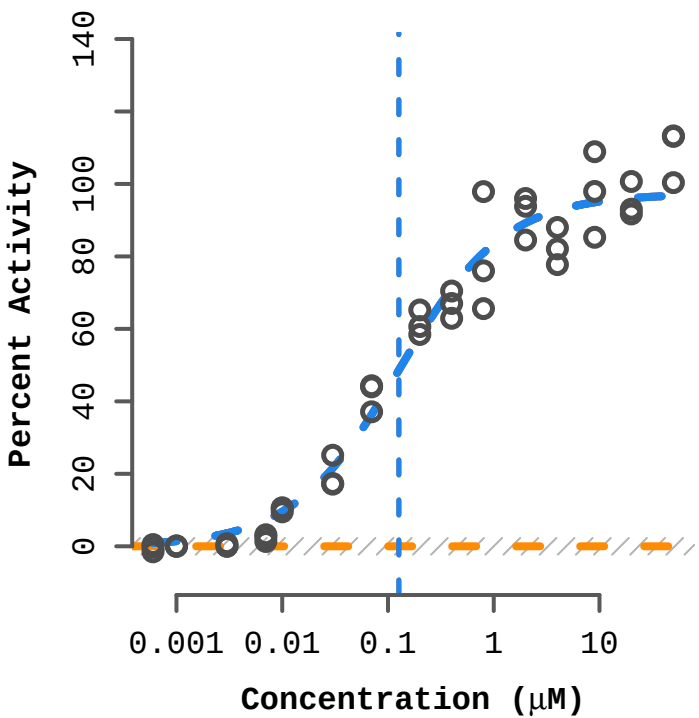
	tp	ga	gw
val:	95.1	-1.28	0.999
sd:	1.6	0.0466	0.0891

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	96.1	-1.26	0.972	2.05	14.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	523.68	316.14	318.91
PROB:	0	0.8	0.2
RMSE:	73.38	8.69	8.48

MAX_MEAN: 111 MAX_MED: 114 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norgestrel
CHID: 36496 CASRN: 797-63-7
SPID(S): Tox21_111593_1
M4ID: 12483599

HILL MODEL (in red):

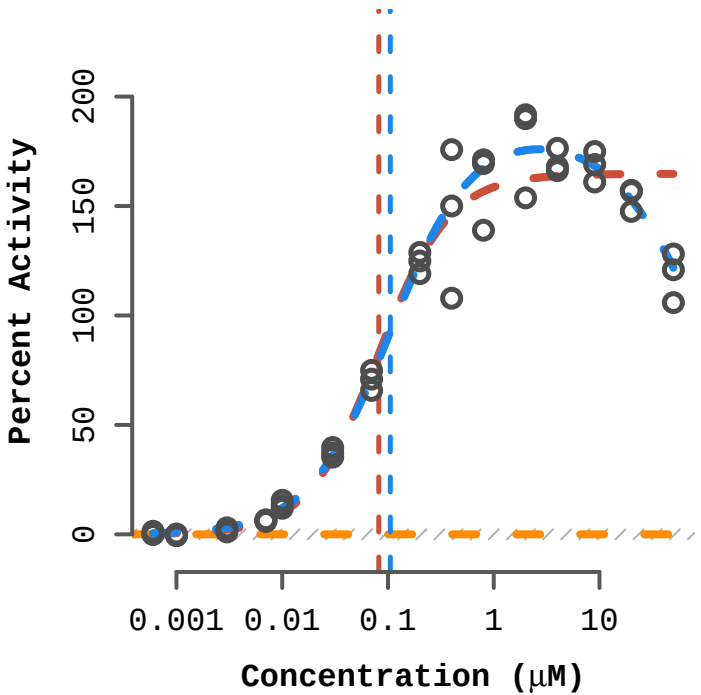
	tp	ga	gw
val:	97.3	-0.897	0.872
sd:	2.94	0.0629	0.0761

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	97.3	-0.897	0.872	2.78	8.23
sd:	2.94	0.0629	0.0761	625	4770

	CNST	HILL	GNLS
AIC:	510.62	312.44	316.44
PROB:	0	0.88	0.12
RMSE:	64.74	7.2	7.2

MAX_MEAN: 109 MAX_MED: 113 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Medroxyprogesterone
CHID: 36508 CASRN: 520-85-4
SPID(S): Tox21_113401_1
M4ID: 12482660

HILL MODEL (in red):

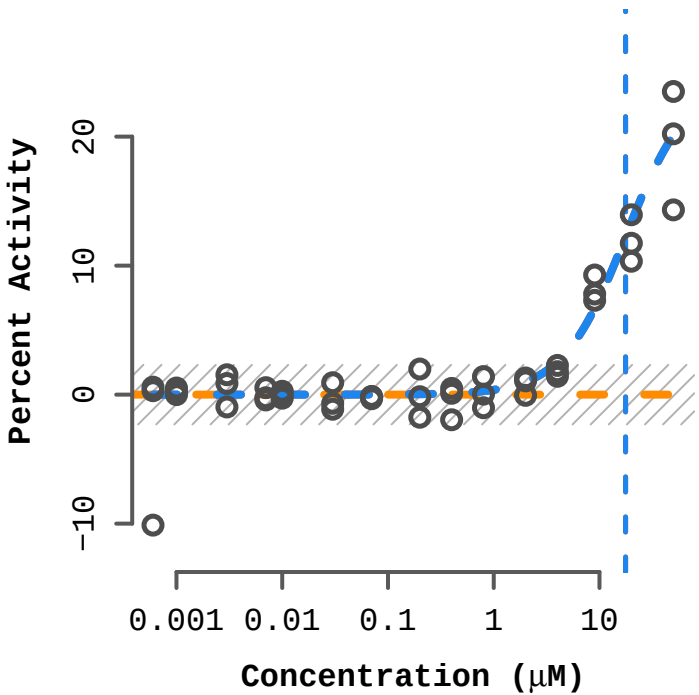
	tp	ga	gw
val:	165	-1.09	1.3
sd:	3.51	0.0343	0.104

GAIN-LOSS MODEL (in blue):

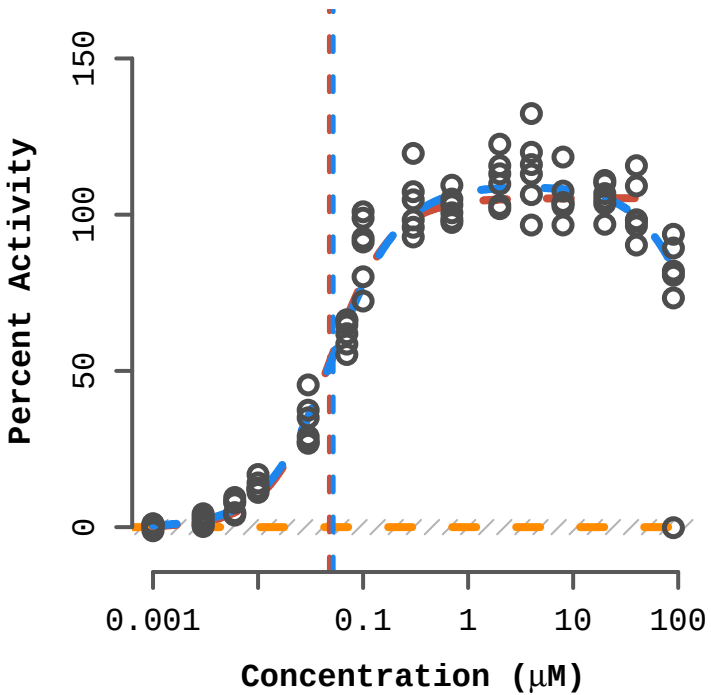
	tp	ga	gw	la	lw
val:	186	-0.978	1.14	1.98	0.987
sd:	8.29	0.0459	0.0689	0.0741	0.259

	CNST	HILL	GNLS
AIC:	562.26	373.23	329.12
PROB:	0	0	1
RMSE:	114.54	16.61	10.54

MAX_MEAN: 178 MAX_MED: 190 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    5alpha-Androstan-3beta-ol
CHID:    36514   CASRN: 1224-92-6
SPID(S): Tox21_113391
M4ID:    12482665

HILL MODEL (in red):
      tp       ga       gw
val:  24.5     1.25     1.45
sd:   3.55     0.12     0.225

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  24.5     1.25     1.45     2.25     16.3
sd:   3.55     0.12     0.225    669      19600

      CNST        HILL        GNLS
AIC:  276.22      172.02      176.02
PROB: 0           0.88        0.12
RMSE: 6.57        2.07        2.07

MAX_MEAN: 19.3      MAX_MED: 20.2      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Testosterone propionate
CHID: 36515 CASRN: 57-85-2
SPID(S): Tox21_302270
M4ID: 12476863

HILL MODEL (in red):

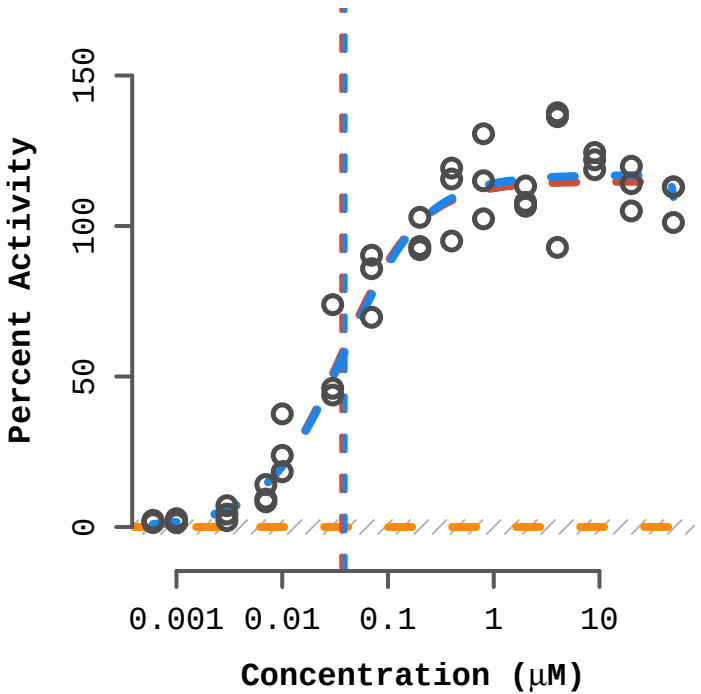
	tp	ga	gw
val:	105	-1.32	1.47
sd:	1.4	0.0271	0.121

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	109	-1.29	1.35	2.31	1.41
sd:	1.97	0.027	0.0969	0.128	0.438

	CNST	HILL	GNLS
AIC:	1063.67	675.7	643.48
PROB:	0	0	1
RMSE:	81.11	14.54	11.59

MAX_MEAN: 114 MAX_MED: 115 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Testosterone propionate
CHID: 36515 CASRN: 57-85-2
SPID(S): Tox21_110330_1
M4ID: 12484450

HILL MODEL (in red):

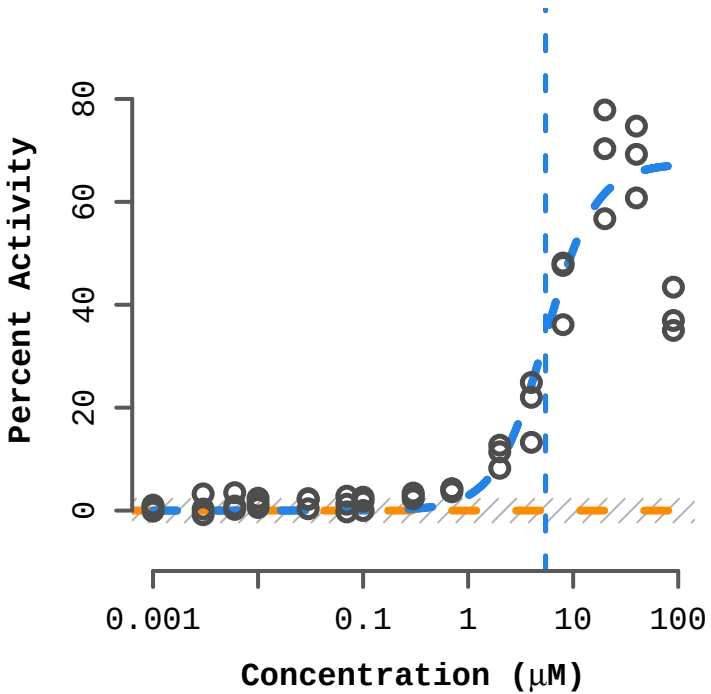
	tp	ga	gw
val:	115	-1.44	1.19
sd:	2.39	0.0557	0.125

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	117	-1.4	1.14	1.76	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	538.58	339.8	342.12
PROB:	0	0.76	0.24
RMSE:	86.73	9.75	9.61

MAX_MEAN: 122 MAX_MED: 136 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Androsterone
CHID: 36525 CASRN: 53-41-8
SPID(S): Tox21_303701
M4ID: 12475487

HILL MODEL (in red):

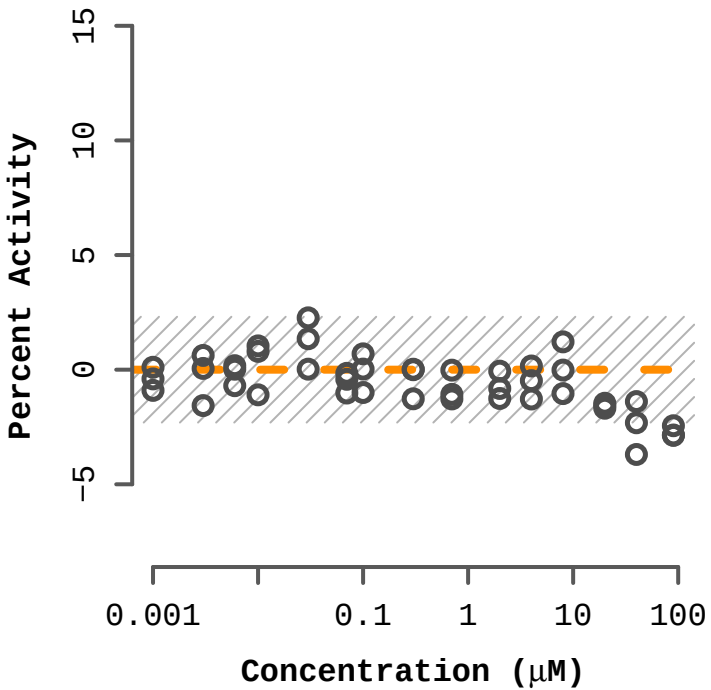
	tp	ga	gw
val:	67.5	0.737	1.82
sd:	4.91	0.0485	0.28

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	67.5	0.737	1.82	2.81	10.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	427.13	300.22	304.22
PROB:	0	0.88	0.12
RMSE:	29.98	8.58	8.58

MAX_MEAN: 68.3 MAX_MED: 70.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

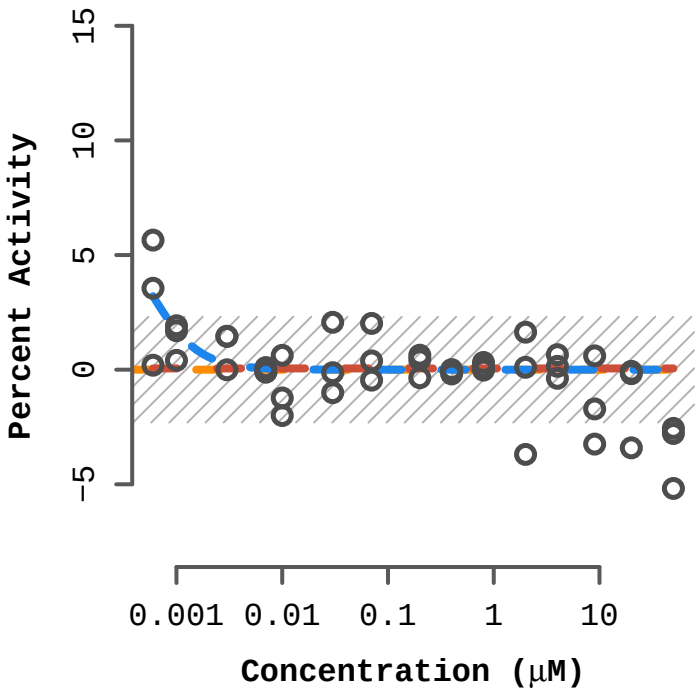
NAME: Pregnenolone
CHID: 36541 CASRN: 145-13-1
SPID(S): Tox21_302141
M4ID: 12476992

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.21 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pregnenolone
CHID: 36541 CASRN: 145-13-1
SPID(S): Tox21_112011_1
M4ID: 12483373

HILL MODEL (in red):

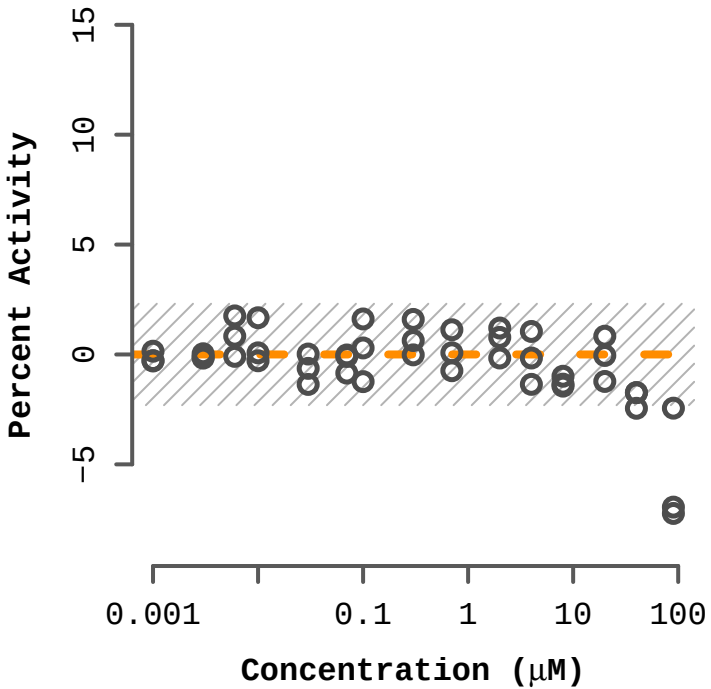
	tp	ga	gw
val:	0.0546	−5	3.73
sd:	0.216	2040	4200

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.78	−5.17	3.9	−3.25	1.91
sd:	7.98	2070	4220	0.468	1.84

	CNST	HILL	GNLS
AIC:	179.35	185.29	178.36
PROB:	0.37	0.02	0.61
RMSE:	1.86	1.86	1.63

MAX_MEAN: 3.13 **MAX_MED:** 3.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

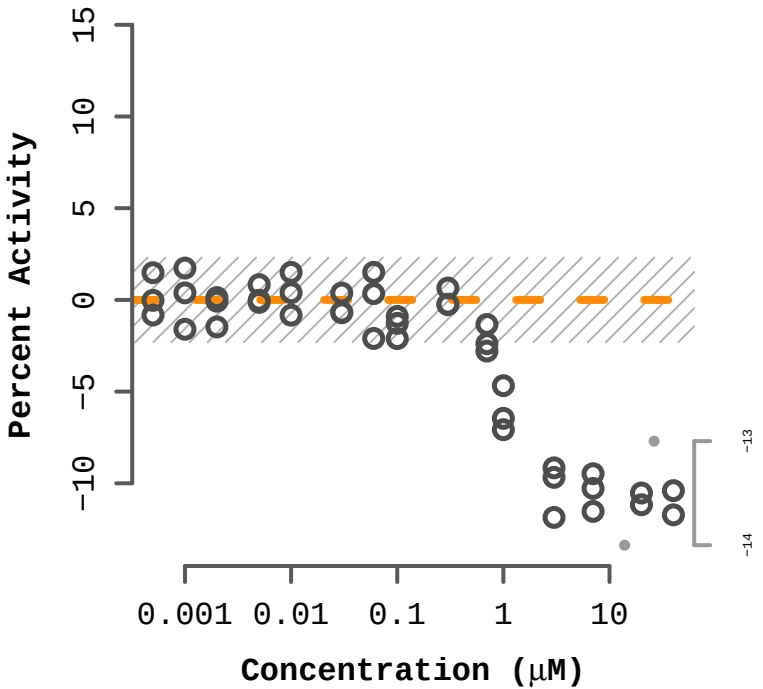
NAME: Triphenylsilanol
CHID: 36545 **CASRN:** 791-31-1
SPID(S): Tox21_304018
M4ID: 12475170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 0.834 **MAX_MED:** 0.832 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

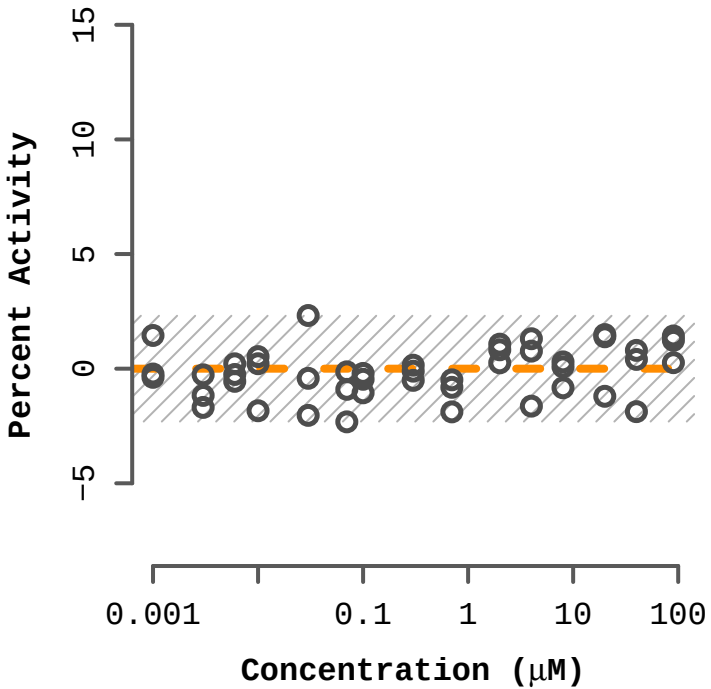
NAME: Polyoxyethylene(10)nonylphenyl ether
CHID: 36588 **CASRN:** 26027-38-3
SPID(S): Tox21_302133
M4ID: 12477000 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.34	NA	NA
PROB:	1	NA	NA
RMSE:	6.08	NA	NA

MAX_MEAN: 0.355 **MAX_MED:** 0.394 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

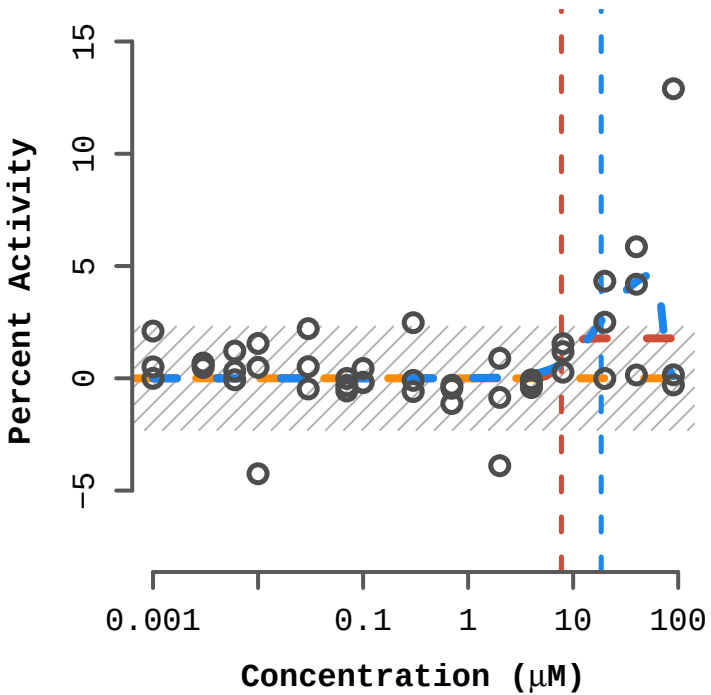
NAME: 1,2-Octanediol
CHID: 36646 **CASRN:** 1117-86-8
SPID(S): Tox21_301019
M4ID: 12478114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydroxybenzophenone
CHID: 36684 CASRN: 1137-42-4
SPID(S): Tox21_201229
M4ID: 12481023

HILL MODEL (in red):

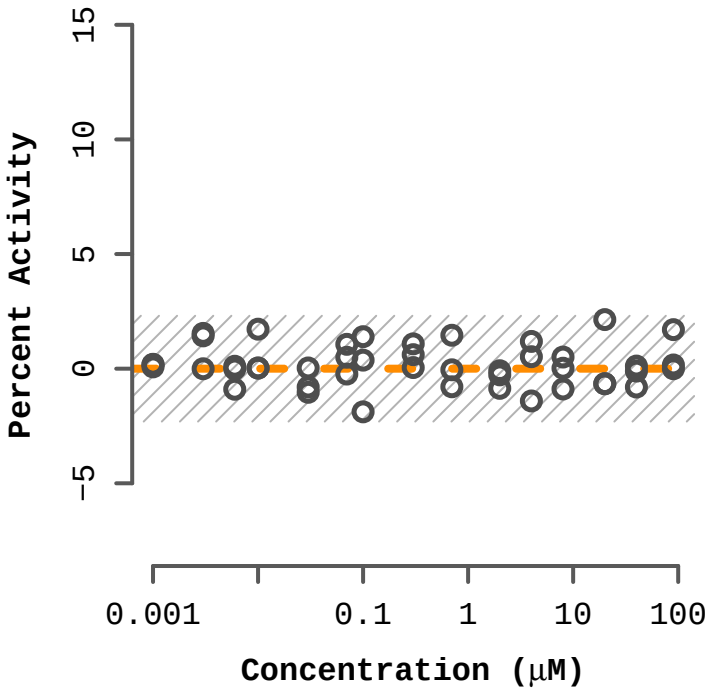
	tp	ga	gw
val:	1.78	0.888	8
sd:	0.959	0.106	16.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.09	1.27	2.21	1.85	17.2
sd:	2.51	0.3	1.2	0.306	49.3

	CNST	HILL	GNLS
AIC:	185.68	183.63	179.91
PROB:	0.05	0.13	0.83
RMSE:	2.61	2.24	2.38

MAX_MEAN: 4.25 MAX_MED: 4.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

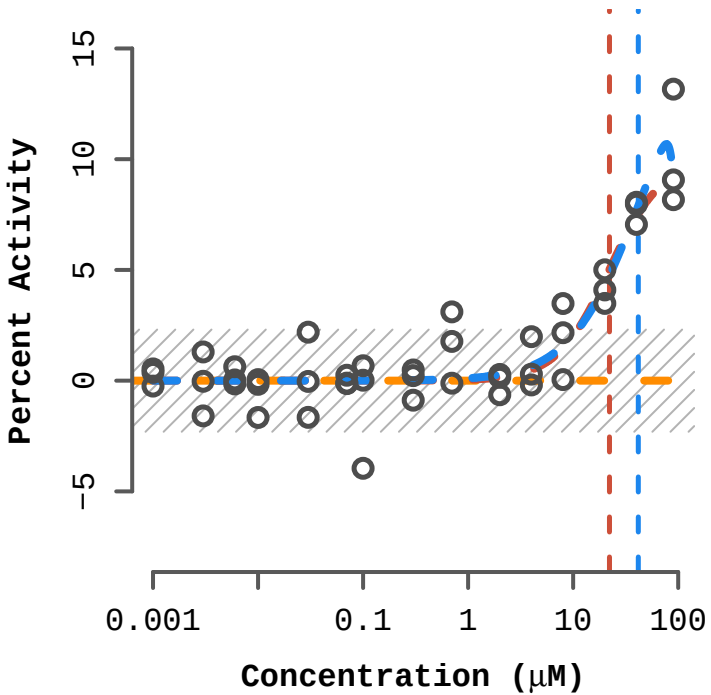
NAME: Diisobutyl adipate
CHID: 36690 CASRN: 141-04-8
SPID(S): Tox21_300353
M4ID: 12478779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.99 MAX_MED: 1.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−Diaminobenzidine
CHID: 36827 CASRN: 91−95−2
SPID(S): Tox21_302170
M4ID: 12476963

HILL MODEL (in red):

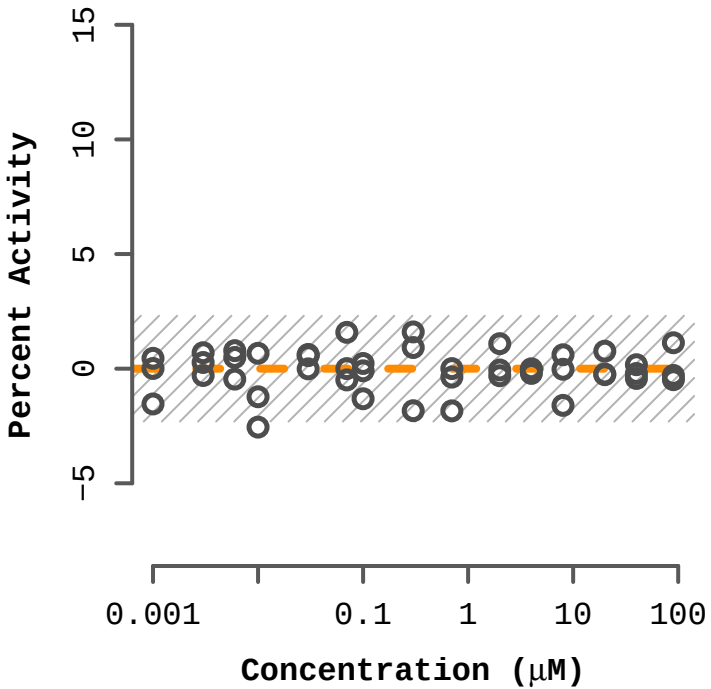
	tp	ga	gw
val:	10	1.35	1.74
sd:	1.26	0.0848	0.493

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.8	1.62	1.33	1.99	15.6
sd:	12.4	0.49	0.497	0.0106	17

	CNST	HILL	GNLS
AIC:	233.56	150.27	153.1
PROB:	0	0.8	0.2
RMSE:	3.72	1.29	1.29

MAX_MEAN: 10.1 **MAX_MED:** 9.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

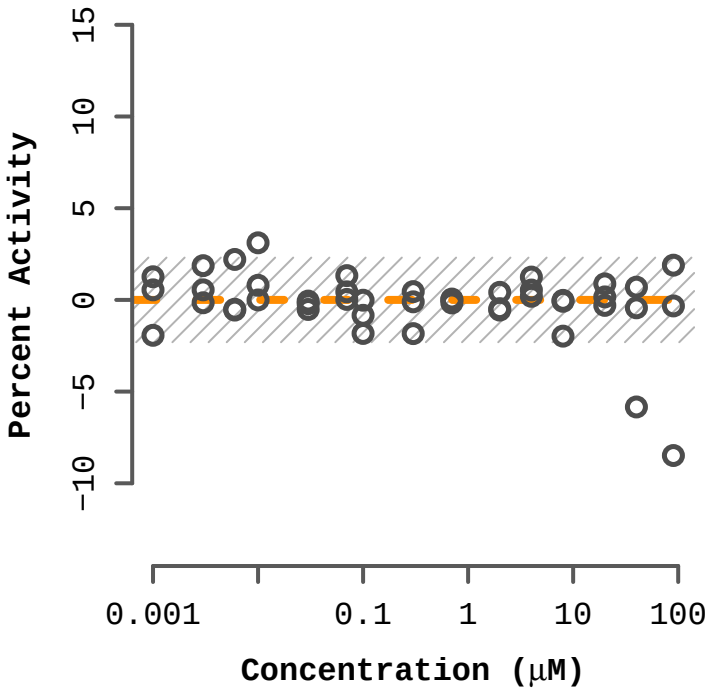
NAME: Sodium hexafluorosilicate
CHID: 36933 **CASRN:** 16893-85-9
SPID(S): Tox21_302311
M4ID: 12476822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.395 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

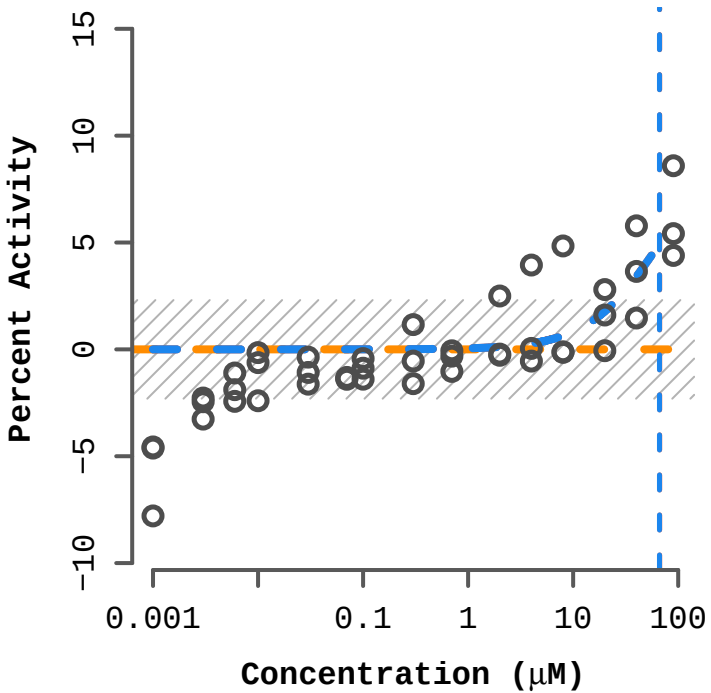
NAME: Potassium tetrafluoroborate
CHID: 37015 **CASRN:** 14075-53-7
SPID(S): Tox21_202804
M4ID: 12479448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.799 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: tetra-Aminopyrimidine sulfate
CHID: 37023 CASRN: 5392-28-9
SPID(S): Tox21_202843
M4ID: 12479409

HILL MODEL (in red):

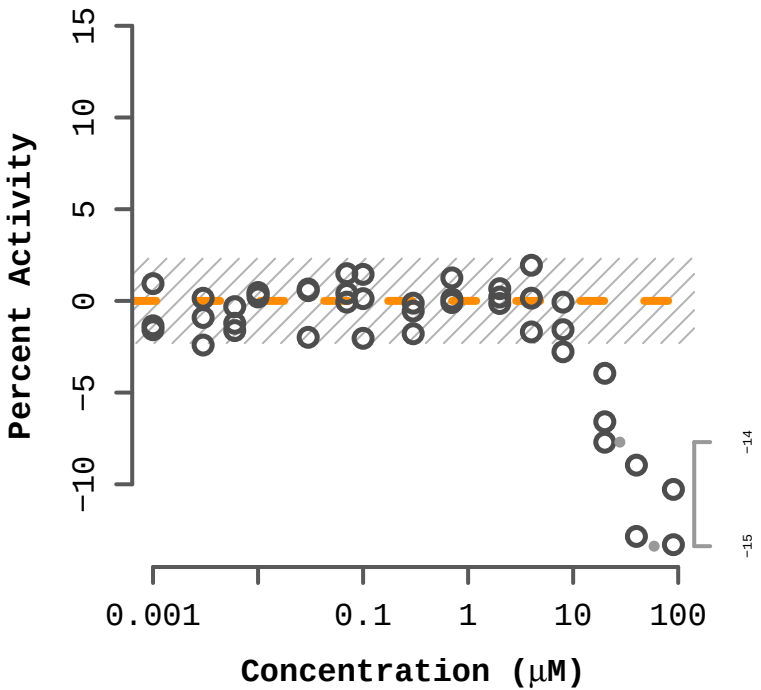
	tp	ga	gw
val:	9.9	1.82	1.26
sd:	14.4	1.07	1.18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.88	1.82	1.27	3.66	1.54
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	223.53	204.02	208.02
PROB:	0	0.88	0.12
RMSE:	2.93	2.22	2.22

MAX_MEAN: 6.14 MAX_MED: 5.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

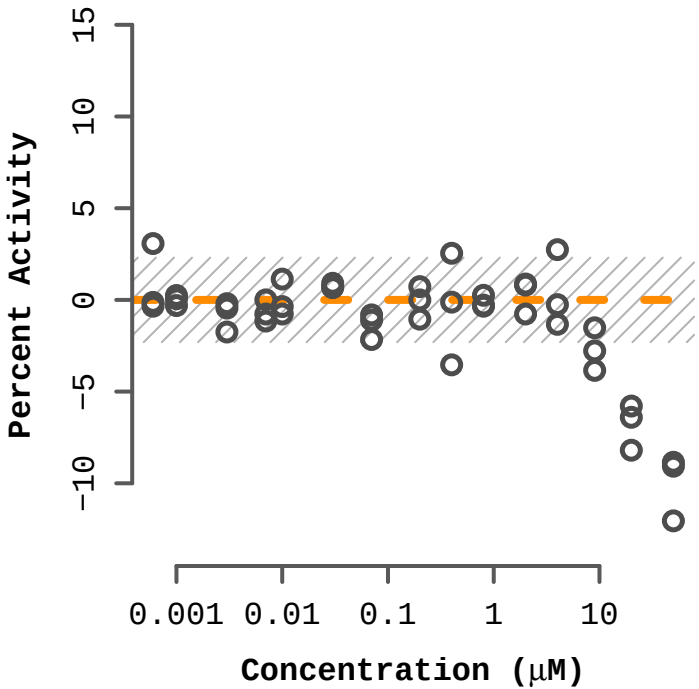
NAME: Hexadecyltrimethylammonium bromide
CHID: 37028 **CASRN:** 57-09-0
SPID(S): Tox21_300853
M4ID: 12478280 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.11	NA	NA
PROB:	1	NA	NA
RMSE:	4.96	NA	NA

MAX_MEAN: 0.61 **MAX_MED:** 0.562 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

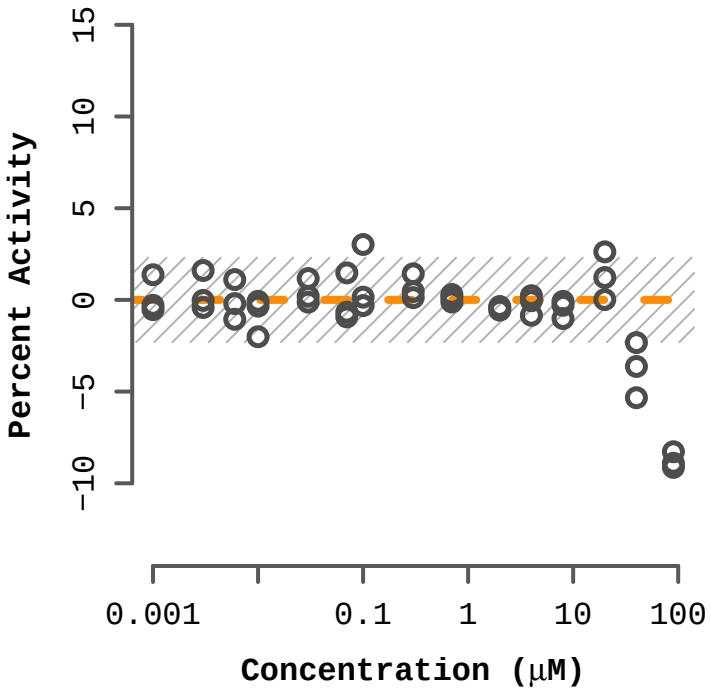
NAME: Hexadecyltrimethylammonium bromide
CHID: 37028 **CASRN:** 57-09-0
SPID(S): Tox21_112096_1
M4ID: 12483323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	223.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 0.866 **MAX_MED:** 0.807 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

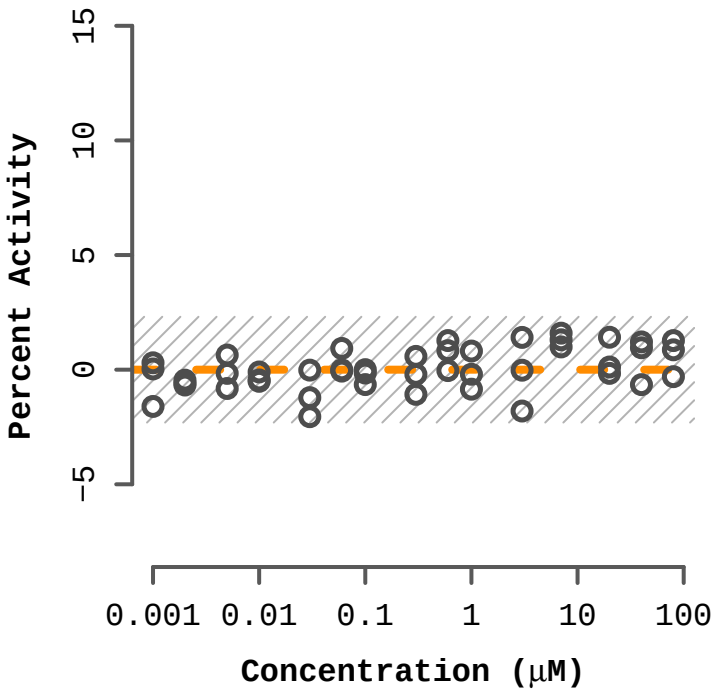
NAME: 2-Nitro-4-thiocyanoaniline
CHID: 37038 **CASRN:** 54029-45-7
SPID(S): Tox21_202844
M4ID: 12479408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

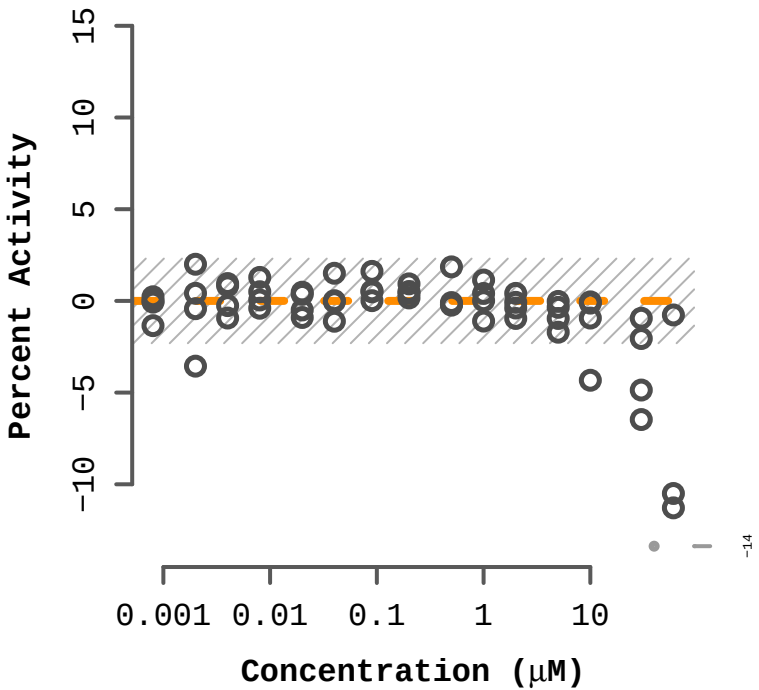
NAME: Sodium valproate
CHID: 37072 **CASRN:** 1069-66-5
SPID(S): Tox21_302623
M4ID: 12476510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

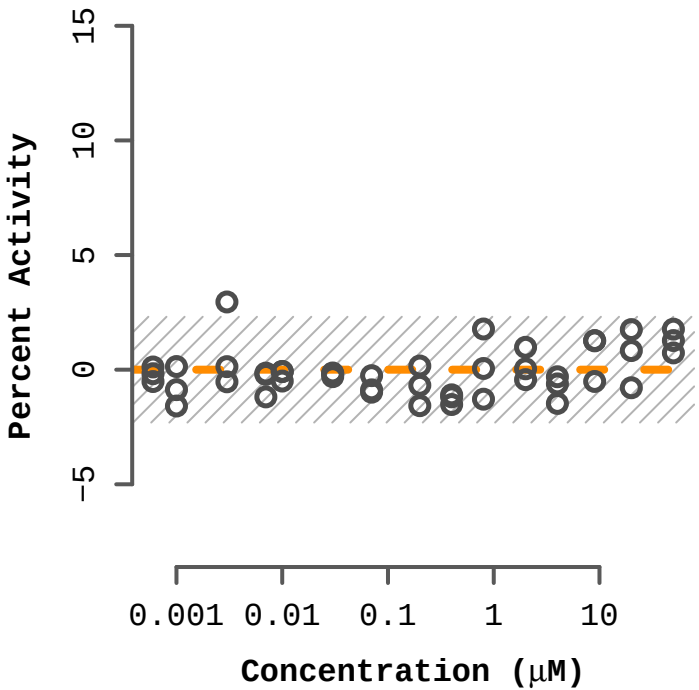
NAME: 4-Hydroxytamoxifen
CHID: 37094 **CASRN:** 68392-35-8
SPID(S): Tox21_303657
M4ID: 12475491 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.8	NA	NA
PROB:	1	NA	NA
RMSE:	3.1	NA	NA

MAX_MEAN: 0.668 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

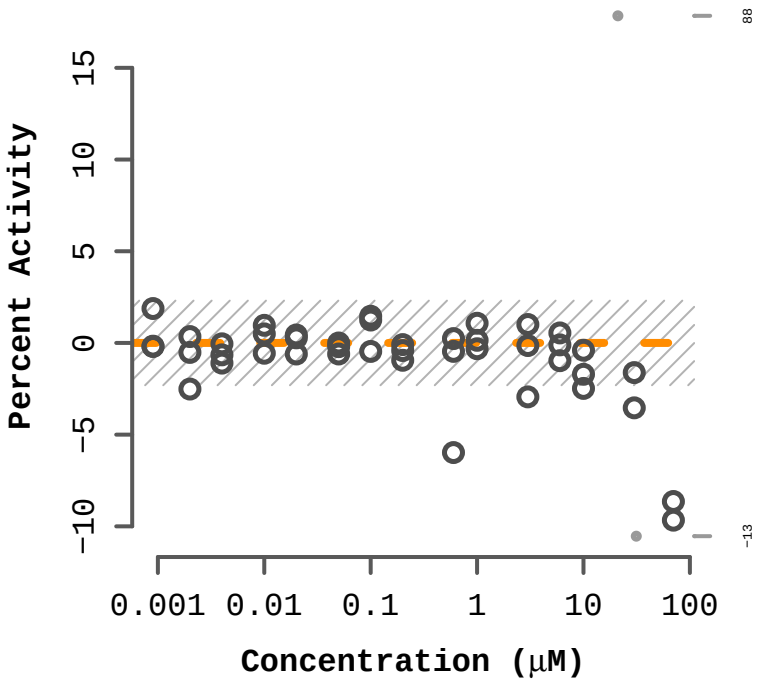
NAME: Rosiglitazone
CHID: 37131 **CASRN:** 122320-73-4
SPID(S): Tox21_111434_1
M4ID: 12483691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

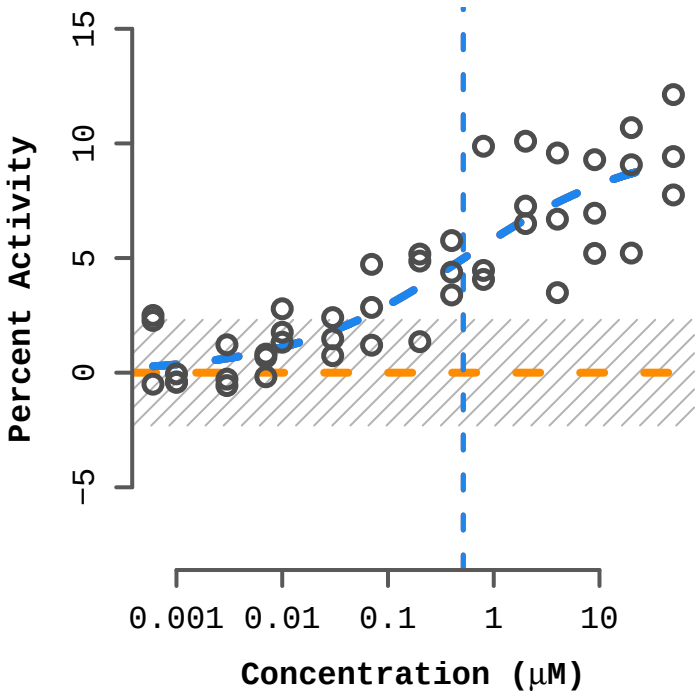
NAME: Amiodarone hydrochloride
CHID: 37185 **CASRN:** 19774-82-4
SPID(S): Tox21_300395
M4ID: 12478737 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.27	NA	NA
PROB:	1	NA	NA
RMSE:	13.42	NA	NA

MAX_MEAN: 27.5 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Captopril
CHID: 37197 **CASRN:** 62571-86-2
SPID(S): Tox21_110890_1
M4ID: 12484037

HILL MODEL (in red):

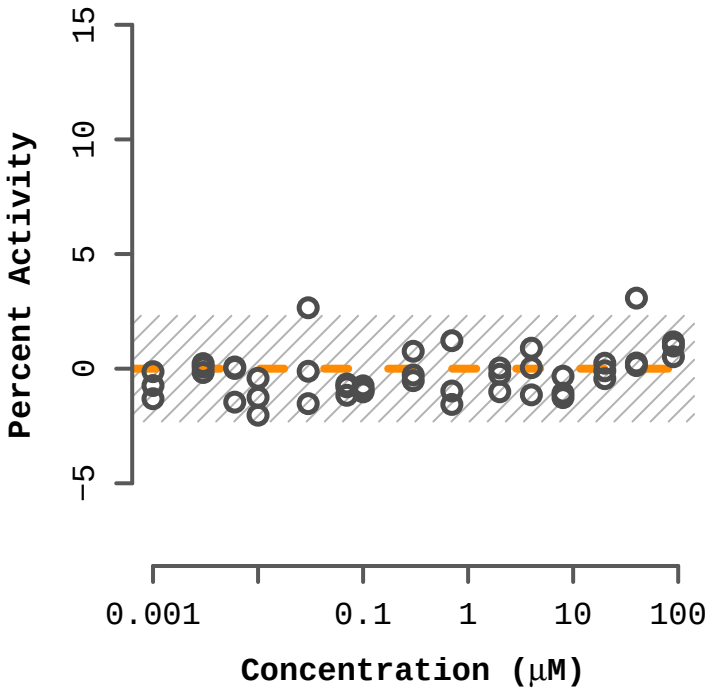
	tp	ga	gw
val:	9.96	−0.288	0.526
sd:	1.56	0.379	0.129

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.96	−0.288	0.526	2.92	6.47
sd:	1.56	0.379	0.129	1010	5360

	CNST	HILL	GNLS
AIC:	285.64	185.2	189.2
PROB:	0	0.88	0.12
RMSE:	5.47	1.71	1.71

MAX_MEAN: 9.77 **MAX_MED:** 9.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

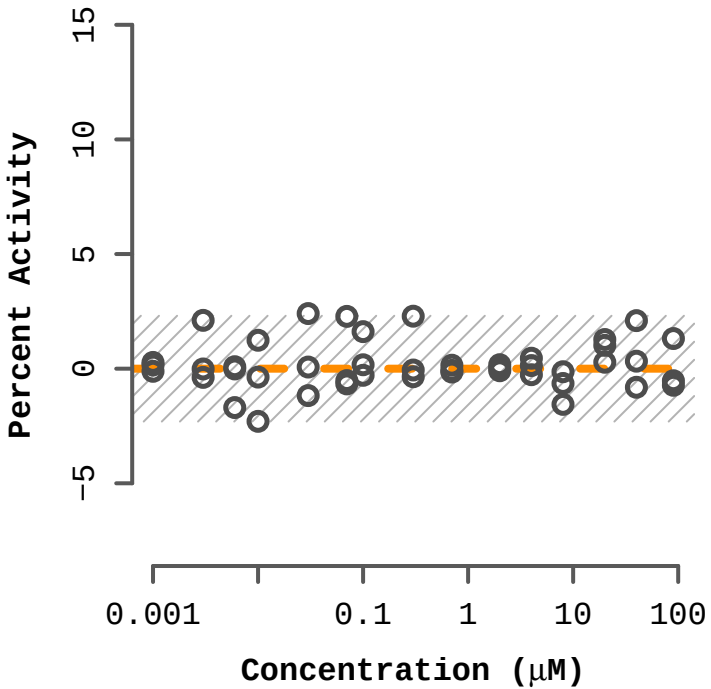
NAME: Sodium dichloroacetate
CHID: 37207 CASRN: 2156-56-1
SPID(S): Tox21_301394
M4ID: 12477739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.987 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

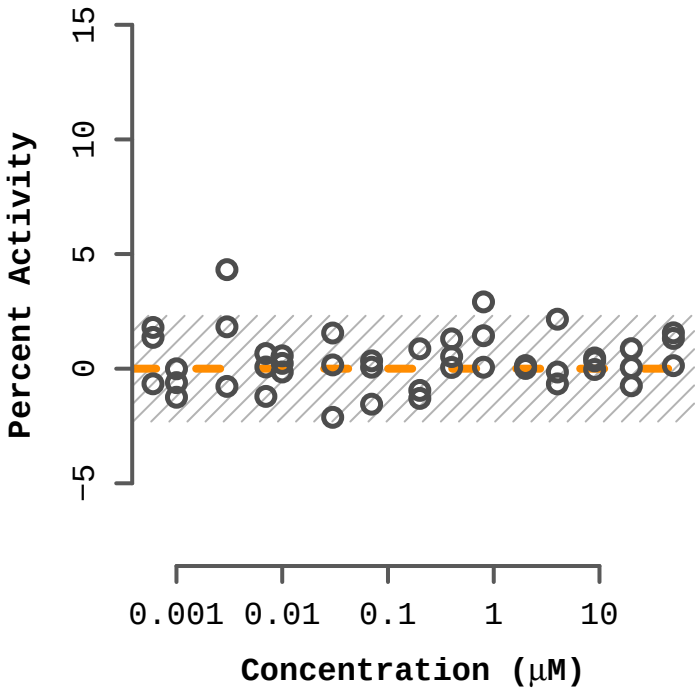
NAME: Diclofenac sodium
CHID: 37208 CASRN: 15307-79-6
SPID(S): Tox21_300265
M4ID: 12478865

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

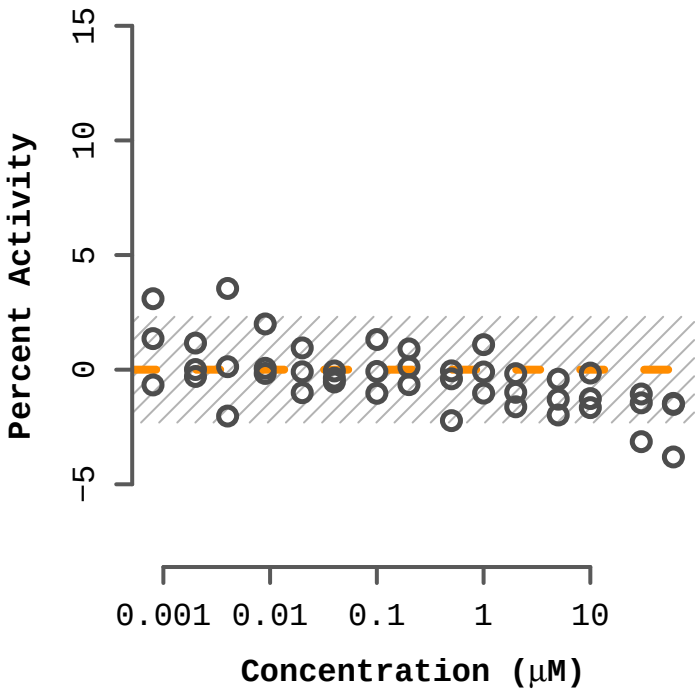
NAME: Diclofenac sodium
CHID: 37208 **CASRN:** 15307-79-6
SPID(S): Tox21_110770_1
M4ID: 12484124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

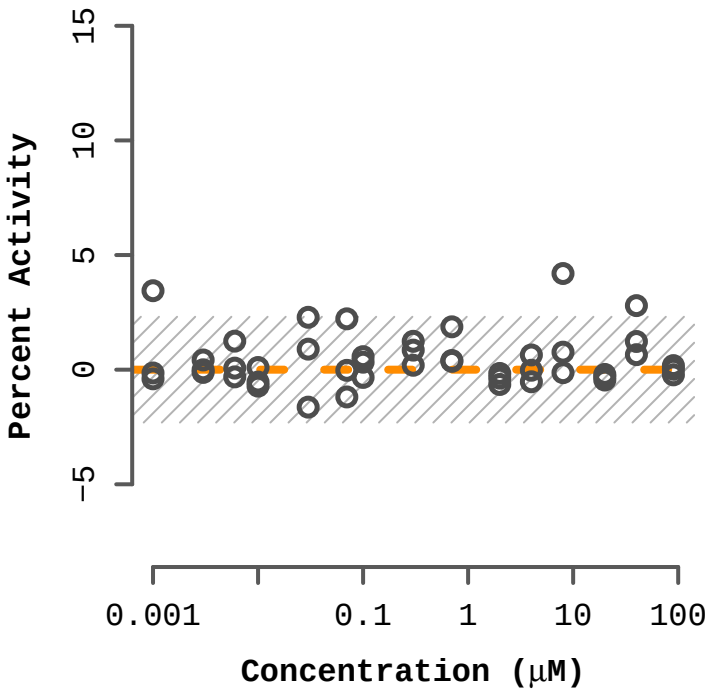
NAME: Erythromycin estolate
CHID: 37224 **CASRN:** 3521-62-8
SPID(S): Tox21_302229
M4ID: 12476904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

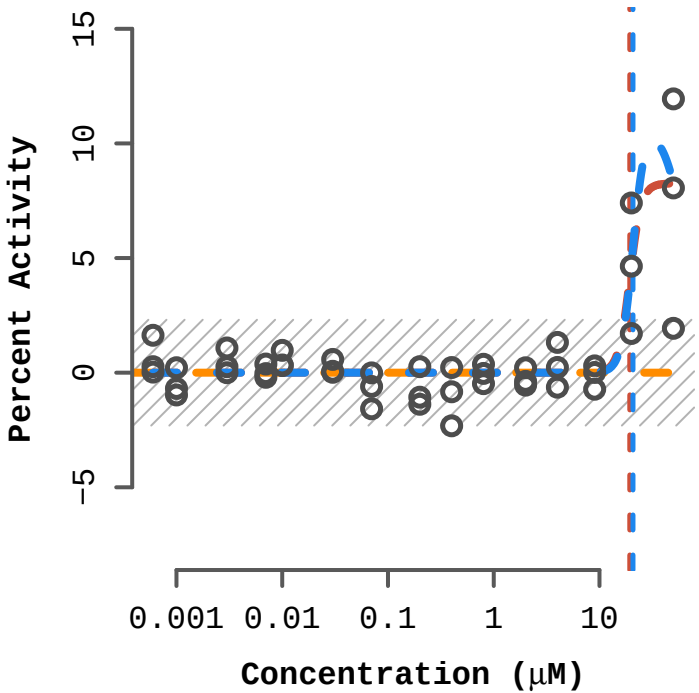
NAME: Flurbiprofen
CHID: 37231 CASRN: 5104-49-4
SPID(S): Tox21_302353
M4ID: 12476780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.61 MAX_MED: 1.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glucosamine hydrochloride
CHID: 37236 **CASRN:** 66-84-2
SPID(S): Tox21_111314_1
M4ID: 12483775

HILL MODEL (in red):

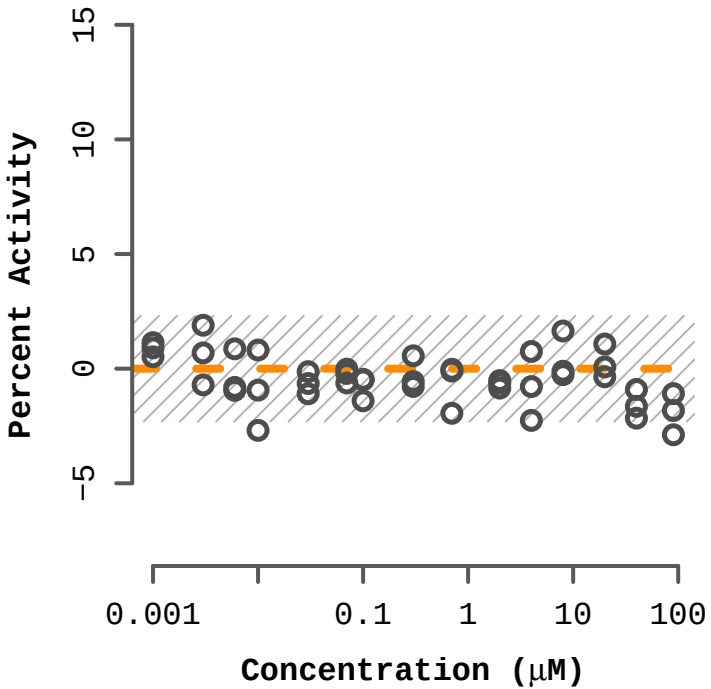
	tp	ga	gw
val:	8.26	1.29	8
sd:	0.753	0.0274	9.74

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11	1.32	7.95	1.82	3.96
sd:	6.64	0.0401	11.8	0.282	14.1

	CNST	HILL	GNLS
AIC:	174.07	146.72	150.71
PROB:	0	0.88	0.12
RMSE:	2.64	1.43	1.43

MAX_MEAN: 7.31 **MAX_MED:** 8.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

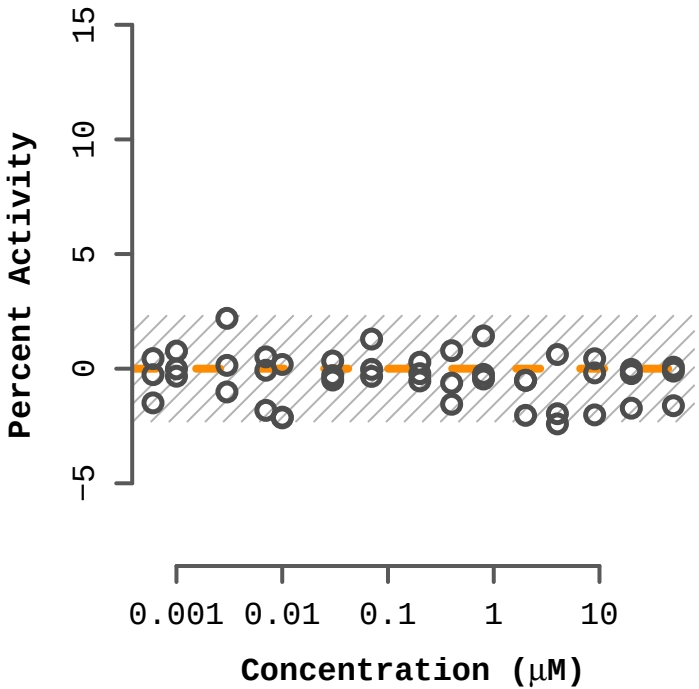
NAME: Glybenclamide
CHID: 37237 **CASRN:** 10238-21-8
SPID(S): Tox21_300758
M4ID: 12478375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.856 **MAX_MED:** 0.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

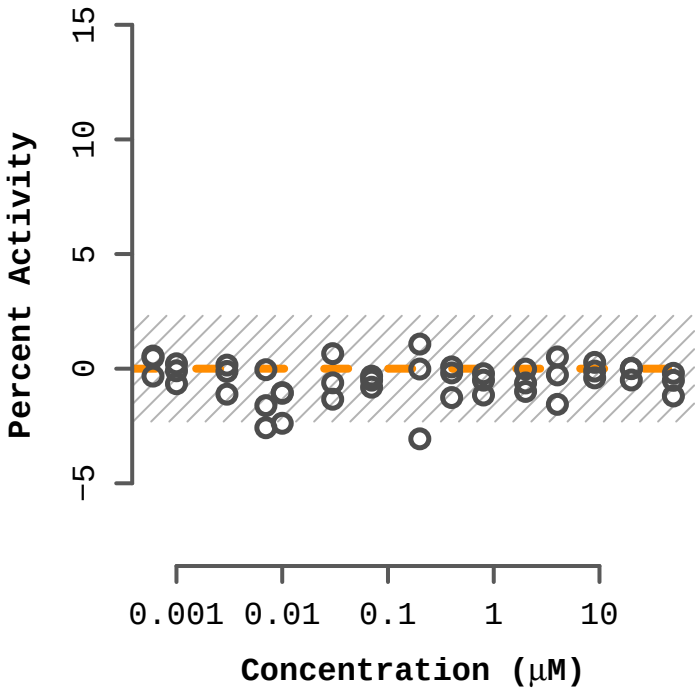
NAME: Glybenclamide
CHID: 37237 **CASRN:** 10238-21-8
SPID(S): Tox21_110158_1
M4ID: 12484599

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.442 **MAX_MED:** 0.145 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

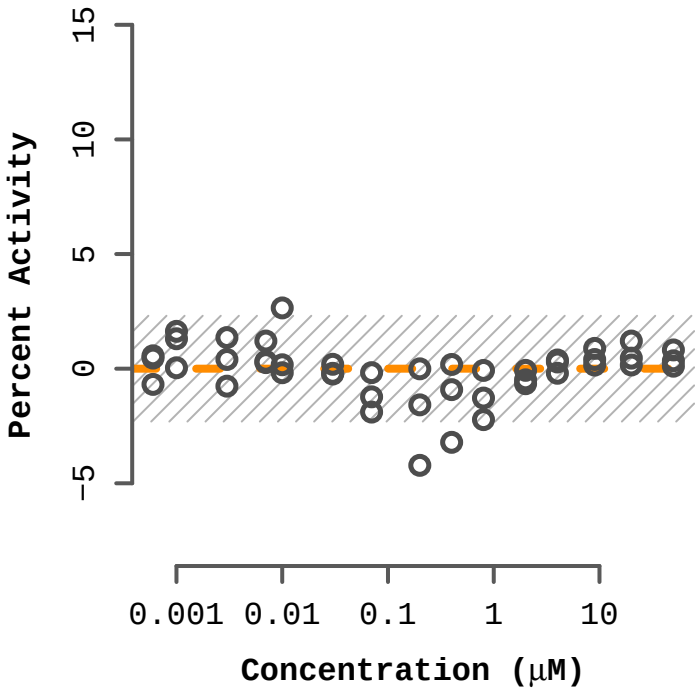
NAME: Metformin hydrochloride
CHID: 37246 **CASRN:** 1115-70-4
SPID(S): Tox21_110498_1
M4ID: 12484311

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.237 **MAX_MED:** 0.482 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

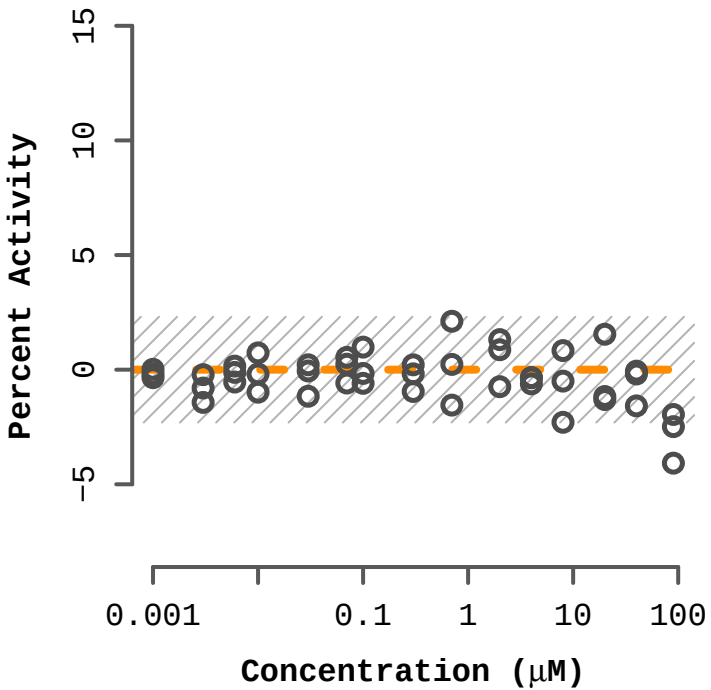
NAME: Metoprolol tartrate
CHID: 37248 **CASRN:** 56392-17-7
SPID(S): Tox21_110787_1
M4ID: 12484113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

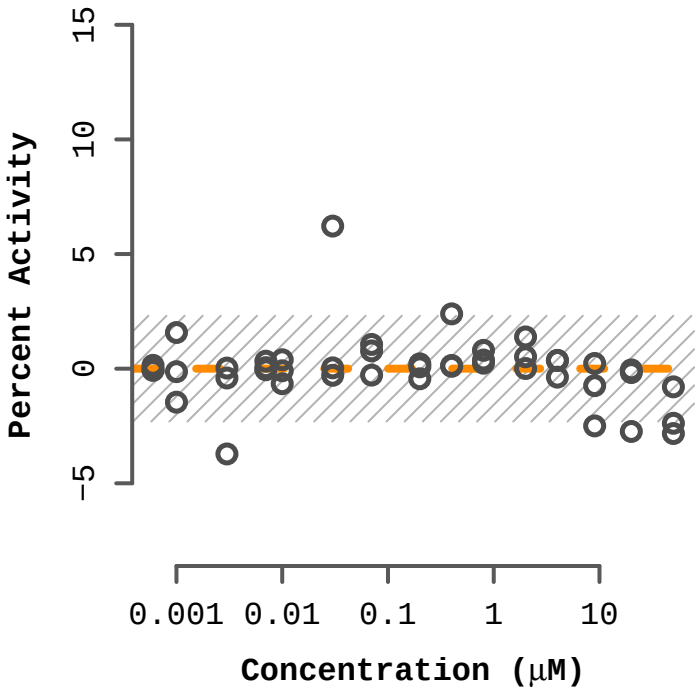
NAME: Nimesulide
CHID: 37250 **CASRN:** 51803-78-2
SPID(S): Tox21_301850
M4ID: 12477283

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

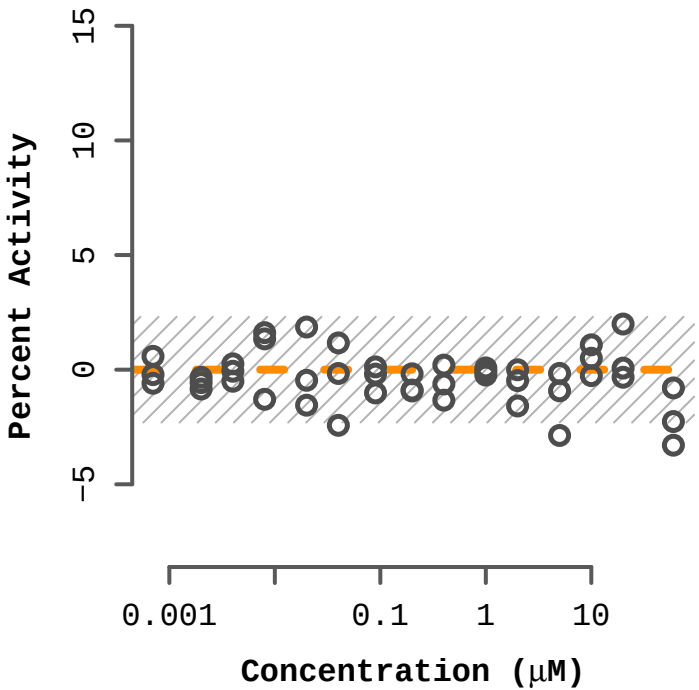
NAME: Nimesulide
CHID: 37250 CASRN: 51803-78-2
SPID(S): Tox21_110207_1
M4ID: 12484552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 0.778 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

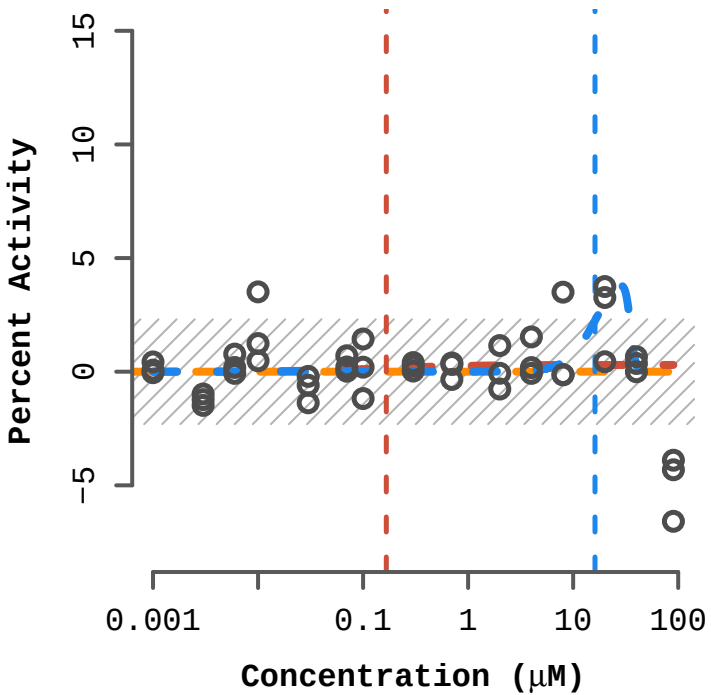
NAME: Pregnenolone carbonitrile
CHID: 37262 **CASRN:** 1434-54-4
SPID(S): Tox21_303525
M4ID: 12475618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.578 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tacrine
CHID: 37272 CASRN: 321-64-2
SPID(S): Tox21_302277
M4ID: 12476856

HILL MODEL (in red):

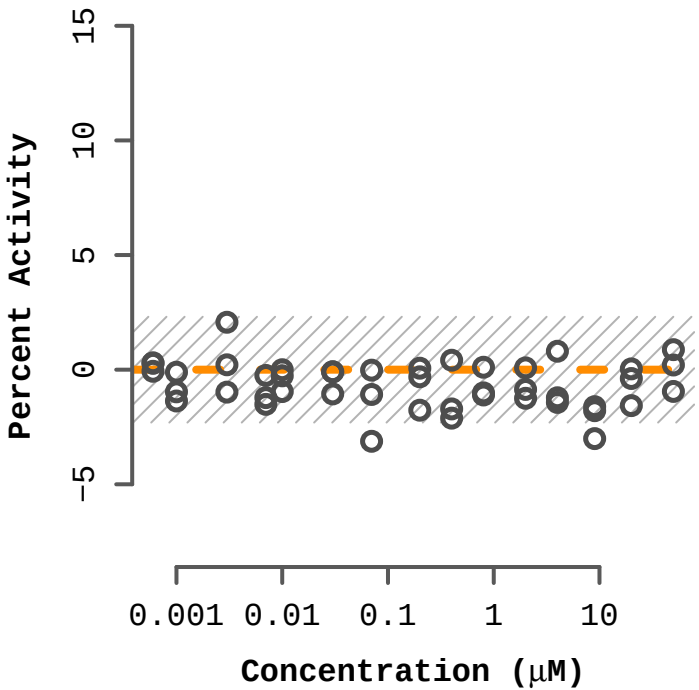
	tp	ga	gw
val:	0.297	-0.779	1.04
sd:	0.362	2.54	3.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.5	1.21	3.24	1.54	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	167.78	172.43	168.02
PROB:	0.5	0.05	0.45
RMSE:	1.8	1.81	1.67

MAX_MEAN: 2.49 MAX_MED: 3.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

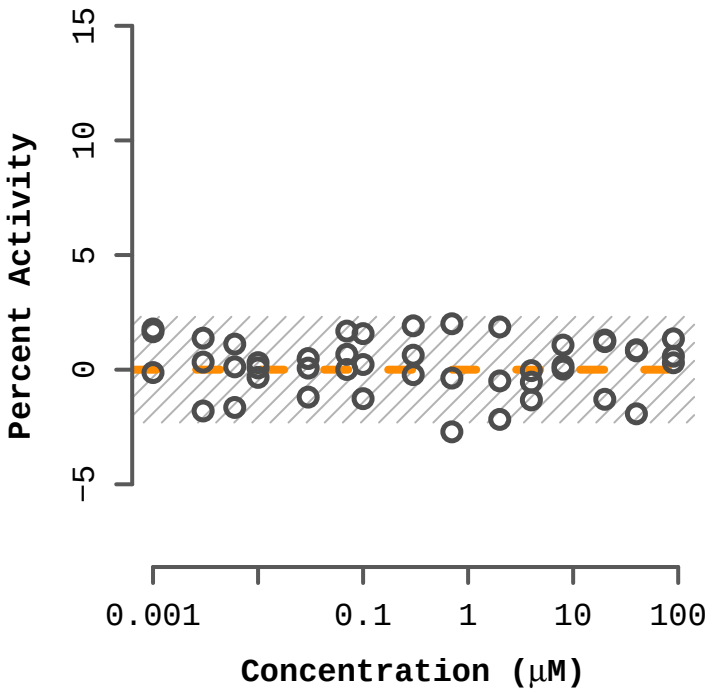
NAME: Tacrine
CHID: 37272 **CASRN:** 321-64-2
SPID(S): Tox21_110073_1
M4ID: 12484679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.435 **MAX_MED:** 0.278 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

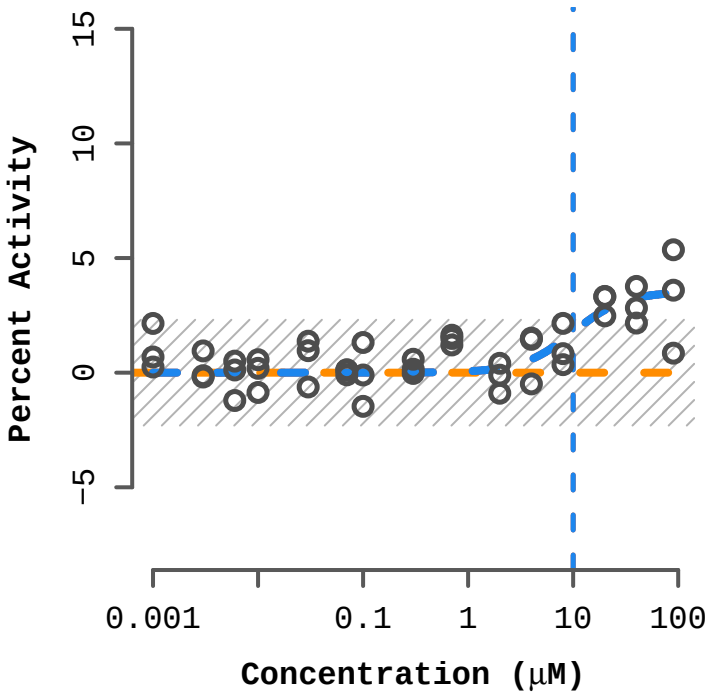
NAME: Perfluoroheptanoic acid
CHID: 37303 CASRN: 375-85-9
SPID(S): Tox21_300616
M4ID: 12478517

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,7,8,9−Tricyclazole
CHID: 37478 **CASRN:** 41814−78−2
SPID(S): Tox21_302419
M4ID: 12476714

HILL MODEL (in red):

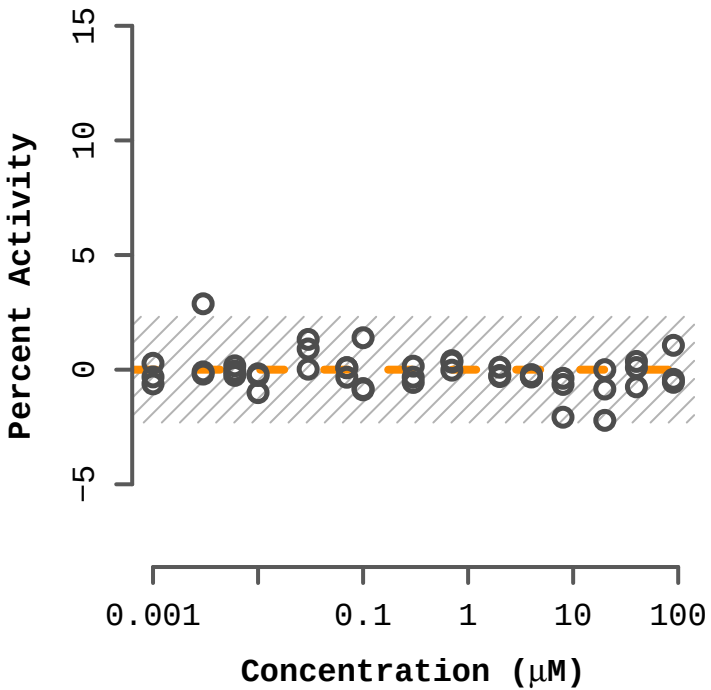
	tp	ga	gw
val:	3.54	1	1.77
sd:	0.969	0.192	1.8

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.54	1	1.77	3.69	4.08
sd:	0.969	0.192	1.8	947	2290

	CNST	HILL	GNLS
AIC:	174.61	133.96	137.96
PROB:	0	0.88	0.12
RMSE:	1.71	0.96	0.96

MAX_MEAN: 3.27 **MAX_MED:** 3.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

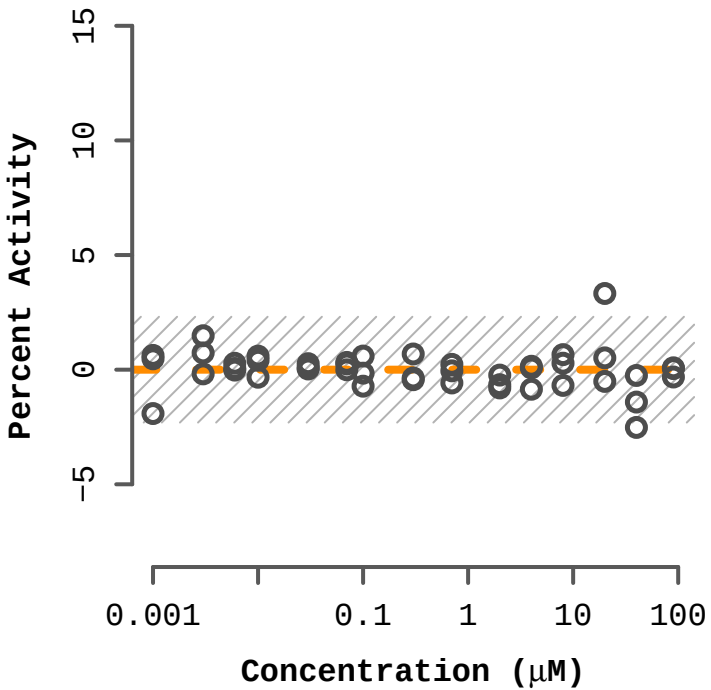
NAME: Acetochlor ESA
CHID: 37483 **CASRN:** 187022-11-3
SPID(S): Tox21_303784
M4ID: 12475404

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.863 **MAX_MED:** 0.905 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

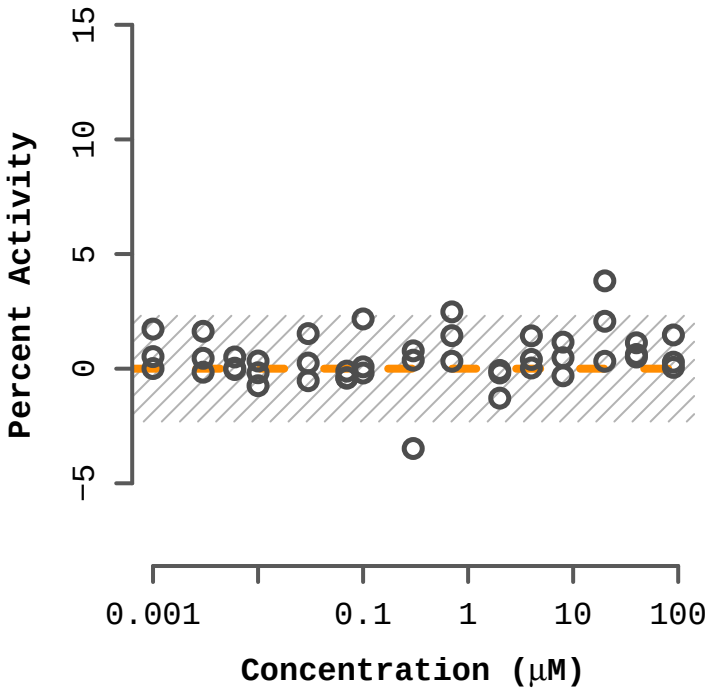
NAME: Atraton
CHID: 37493 **CASRN:** 1610-17-9
SPID(S): Tox21_301814
M4ID: 12477319

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.733 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

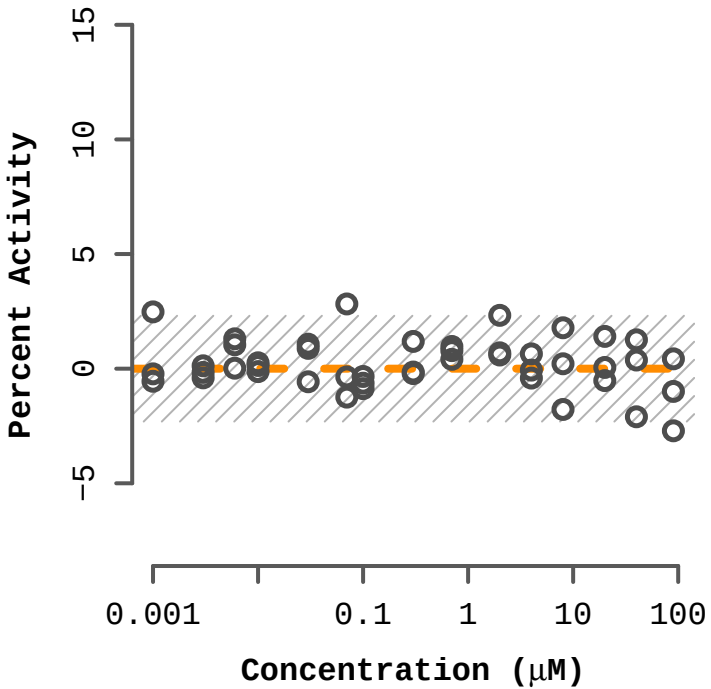
NAME: Deethylatrazine
CHID: 37494 **CASRN:** 6190-65-4
SPID(S): Tox21_301071
M4ID: 12478062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

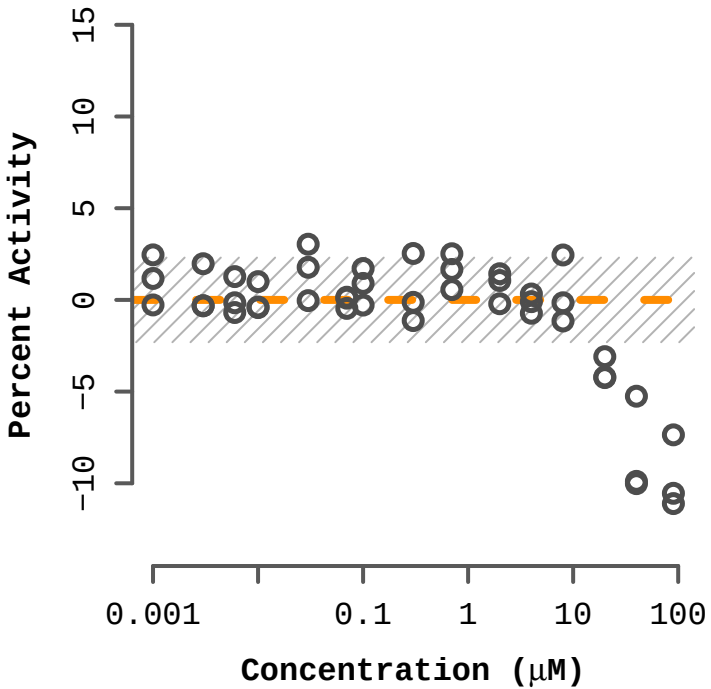
NAME: Deisopropylatrazine
CHID: 37495 **CASRN:** 1007-28-9
SPID(S): Tox21_300753
M4ID: 12478380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

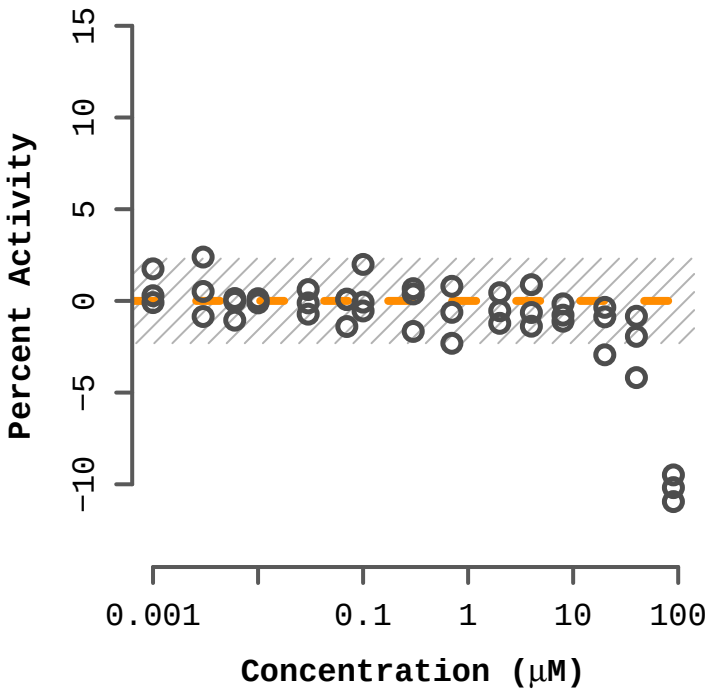
NAME: Azinphos-ethyl
CHID: 37498 **CASRN:** 2642-71-9
SPID(S): Tox21_301421
M4ID: 12477712

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.14	NA	NA
PROB:	1	NA	NA
RMSE:	3.71	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

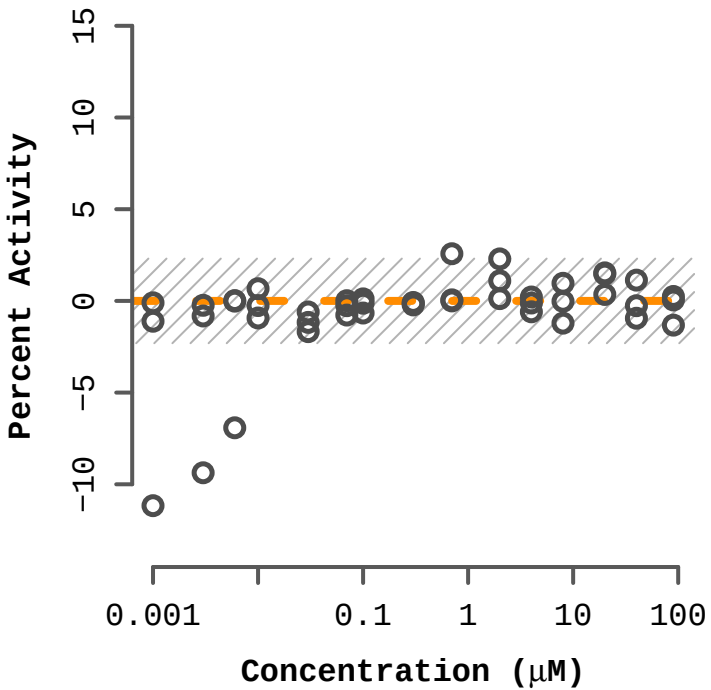
NAME: Bitertanol
CHID: 37502 **CASRN:** 55179-31-2
SPID(S): Tox21_303756
M4ID: 12475432

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.9	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

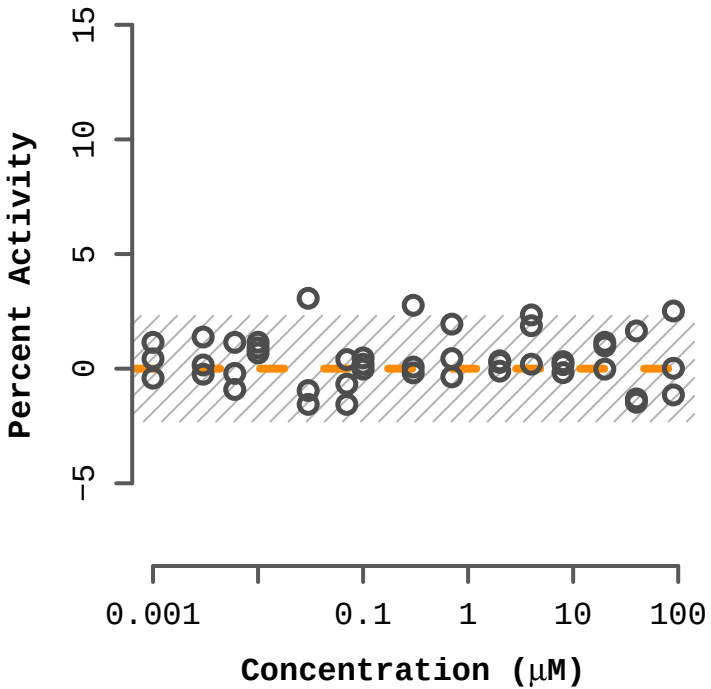
NAME: Chlordimeform
CHID: 37508 **CASRN:** 6164-98-3
SPID(S): Tox21_301576
M4ID: 12477557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.75	NA	NA
PROB:	1	NA	NA
RMSE:	2.56	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

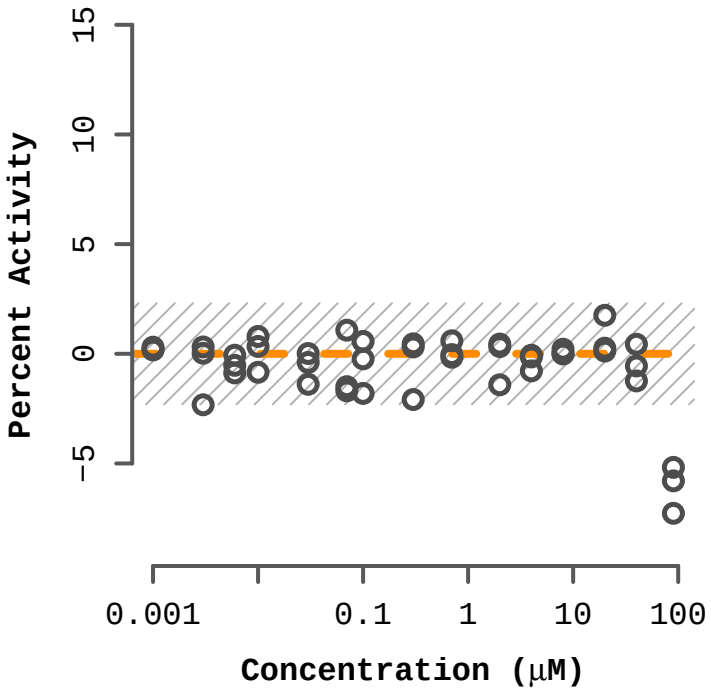
NAME: Chlormephos
CHID: 37511 **CASRN:** 24934-91-6
SPID(S): Tox21_300825
M4ID: 12478308

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

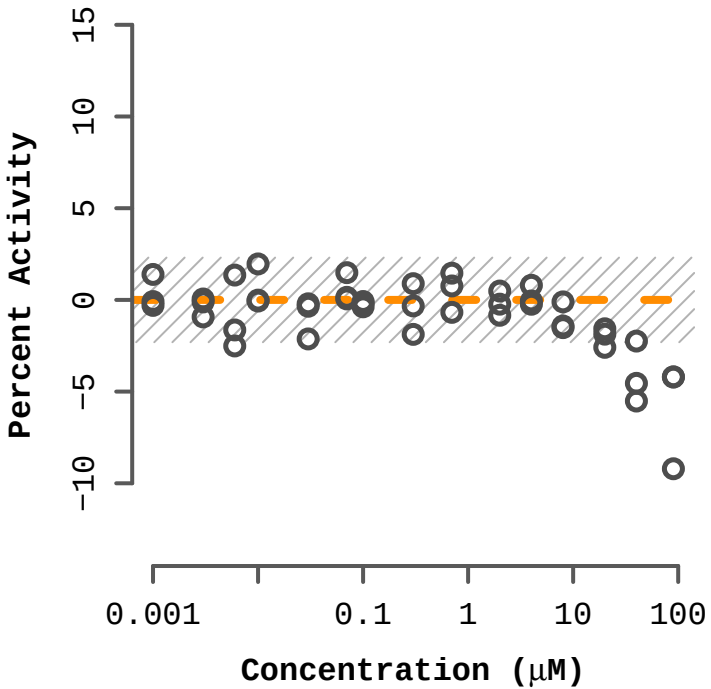
NAME: Crufomate
CHID: 37515 **CASRN:** 299-86-5
SPID(S): Tox21_302262
M4ID: 12476871

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 0.713 **MAX_MED:** 0.337 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

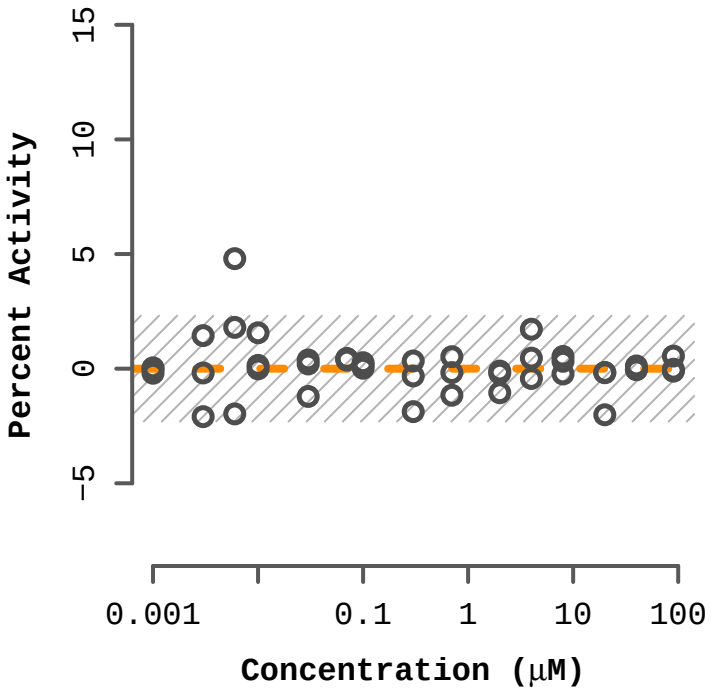
NAME: Dialifor
CHID: 37522 **CASRN:** 10311-84-9
SPID(S): Tox21_300794
M4ID: 12478339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.44	NA	NA
PROB:	1	NA	NA
RMSE:	2.25	NA	NA

MAX_MEAN: 0.631 **MAX_MED:** 0.763 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

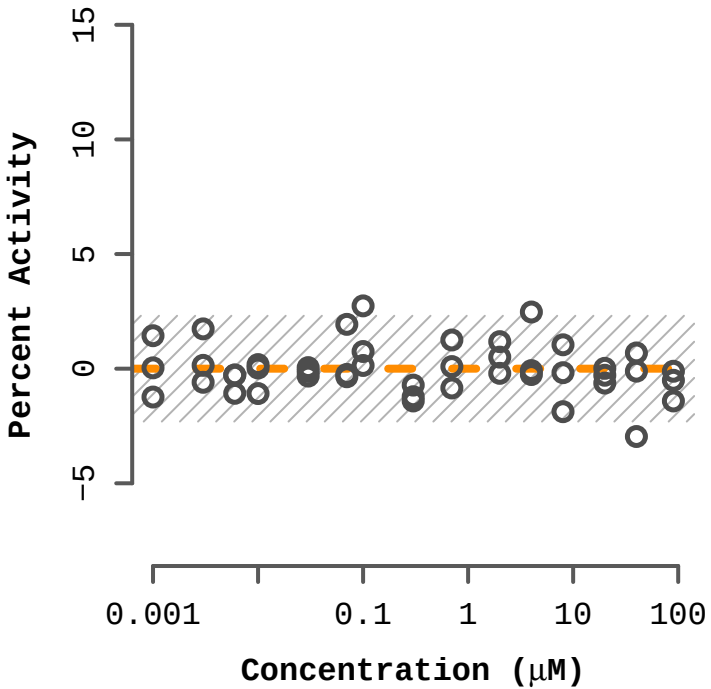
NAME: Diazoxon
CHID: 37523 **CASRN:** 962-58-3
SPID(S): Tox21_301125
M4ID: 12478008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

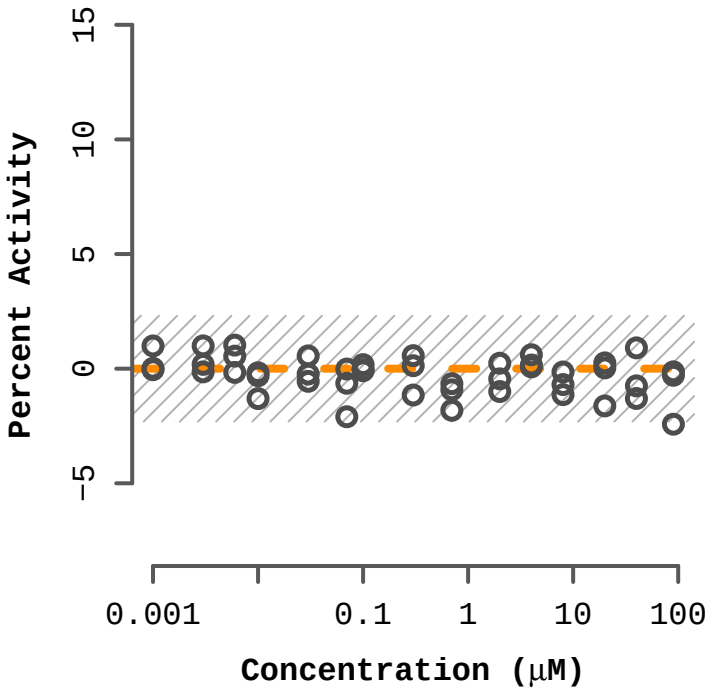
NAME: Diethofencarb
CHID: 37527 **CASRN:** 87130-20-9
SPID(S): Tox21_301915
M4ID: 12477218

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.751 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

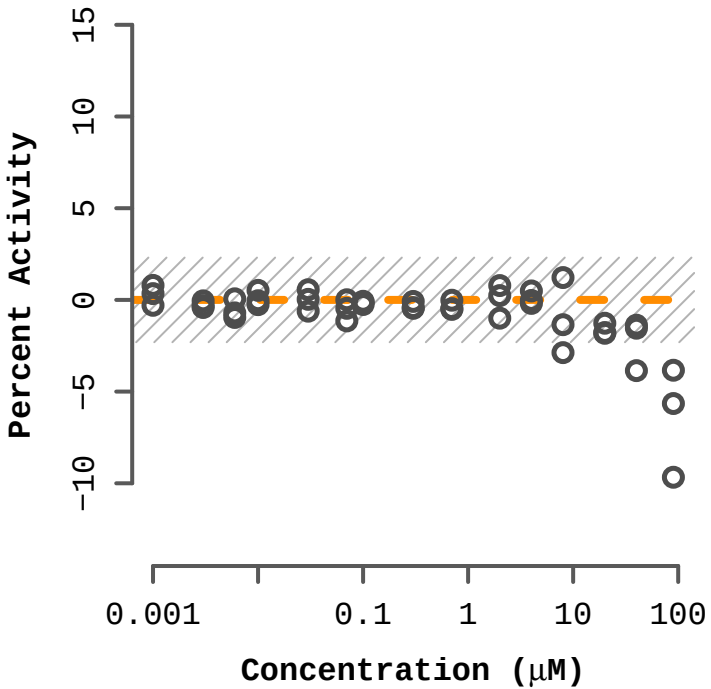
NAME: Demeton-S
CHID: 37535 **CASRN:** 126-75-0
SPID(S): Tox21_303989
M4ID: 12475199

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.472 **MAX_MED:** 0.548 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

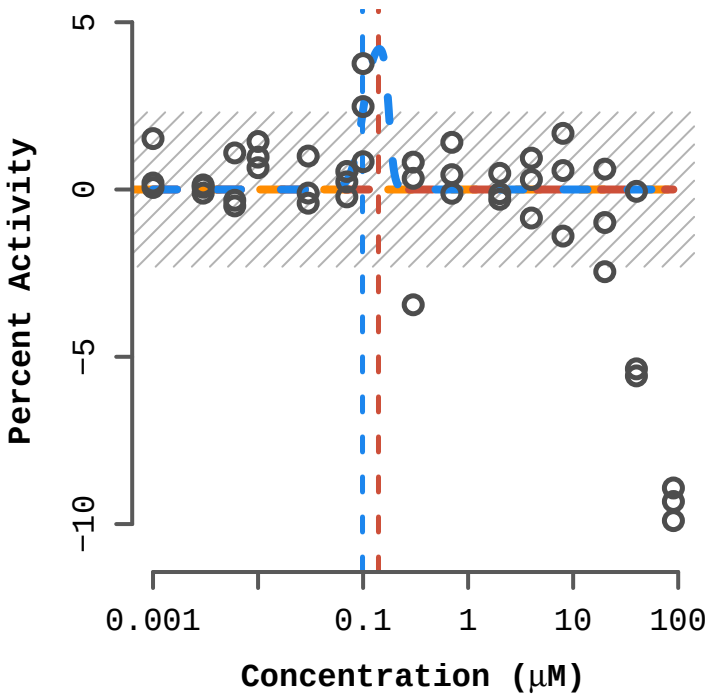
NAME: Endosulfan I
CHID: 37539 **CASRN:** 959-98-8
SPID(S): Tox21_301581
M4ID: 12477552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 0.282 **MAX_MED:** 0.345 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Endosulfan sulfate
CHID: 37541 CASRN: 1031-07-8
SPID(S): Tox21_300782
M4ID: 12478351

HILL MODEL (in red):

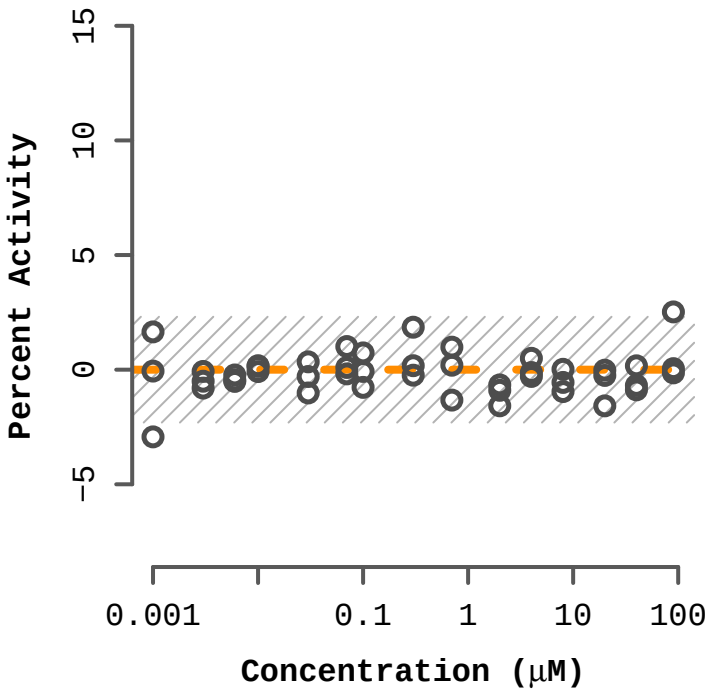
	tp	ga	gw
val:	3.41e-11	-0.853	1.88
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.52	-1.01	8	-0.753	17.8
sd:	10.7	0.266	9.33	5.83	447

	CNST	HILL	GNLS
AIC:	201.55	207.55	204.73
PROB:	0.8	0.04	0.16
RMSE:	2.92	2.92	2.85

MAX_MEAN: 2.36 MAX_MED: 2.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

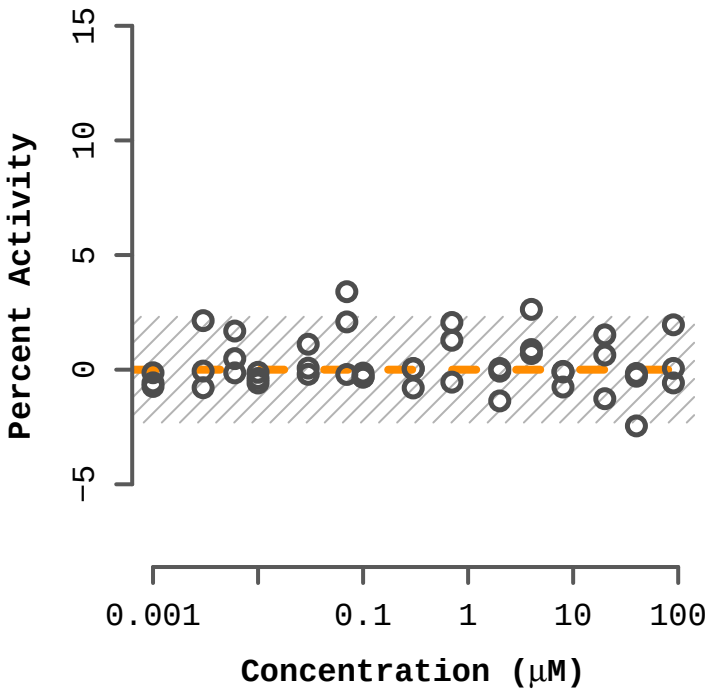
NAME: Ethiofencarb
CHID: 37545 **CASRN:** 29973-13-5
SPID(S): Tox21_301356
M4ID: 12477777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.81 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

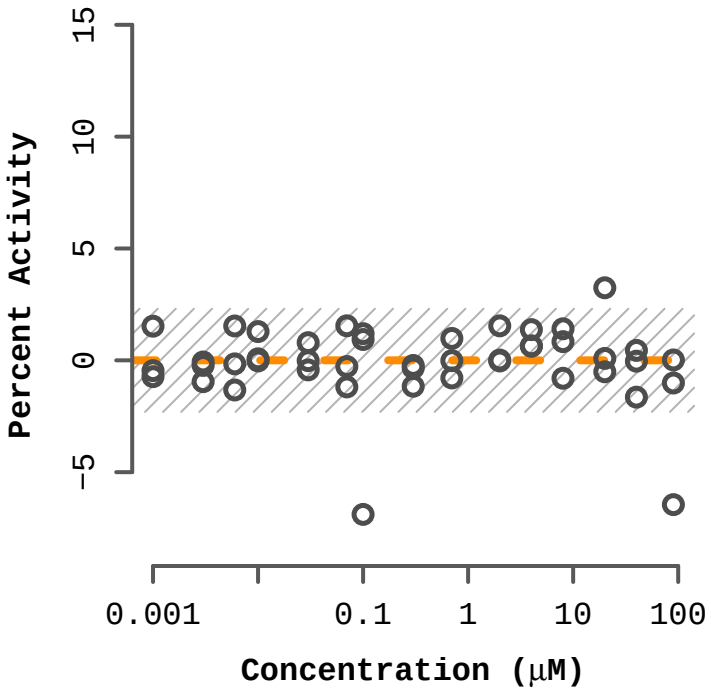
NAME: Fenuron
CHID: 37551 **CASRN:** 101-42-8
SPID(S): Tox21_300902
M4ID: 12478231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

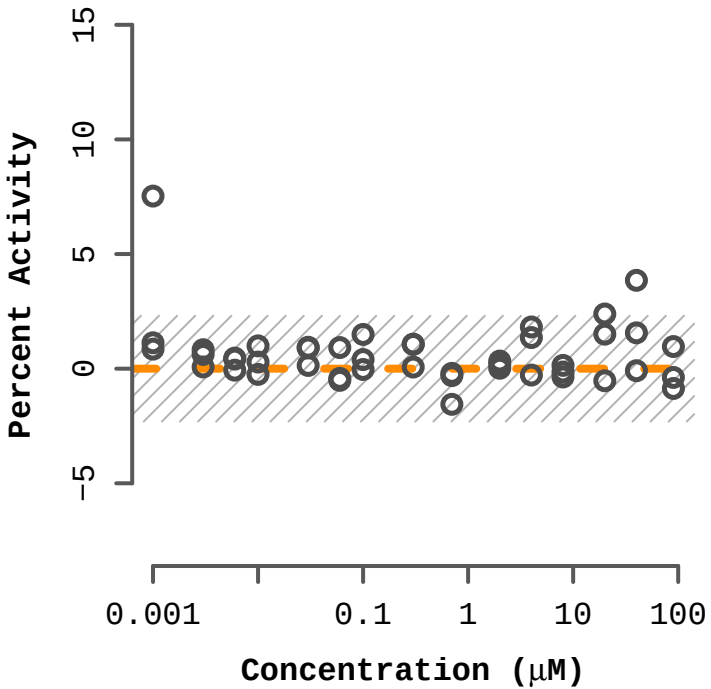
NAME: Fluorodifen
CHID: 37553 **CASRN:** 15457-05-3
SPID(S): Tox21_301354
M4ID: 12477779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 0.94 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

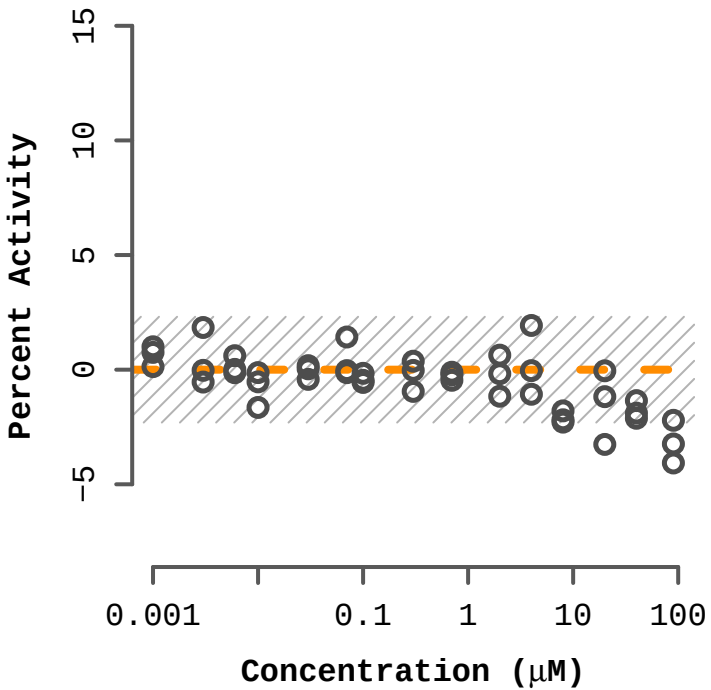
NAME: tau-Fluvalinate
CHID: 37555 **CASRN:** 102851-06-9
SPID(S): Tox21_300722
M4ID: 12478411

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 3.17 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

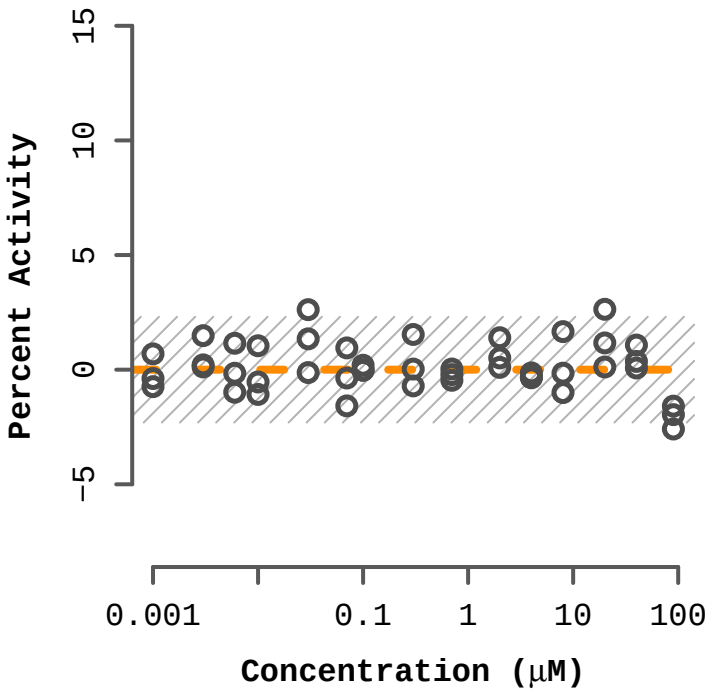
NAME: Mefenpyr-diethyl
CHID: 37564 **CASRN:** 135590-91-9
SPID(S): Tox21_304023
M4ID: 12475165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.63 **MAX_MED:** 0.755 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

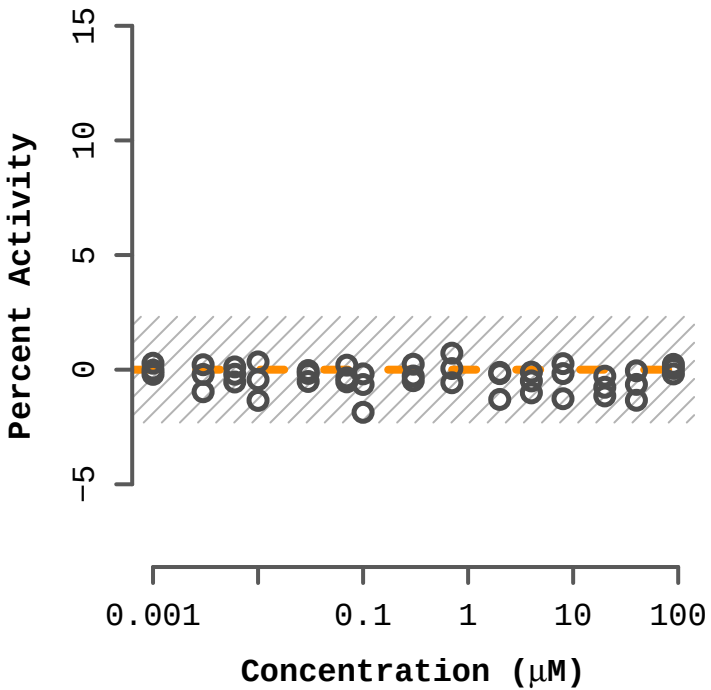
NAME: Mepronil
CHID: 37565 CASRN: 55814-41-0
SPID(S): Tox21_302431
M4ID: 12476702

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.31 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

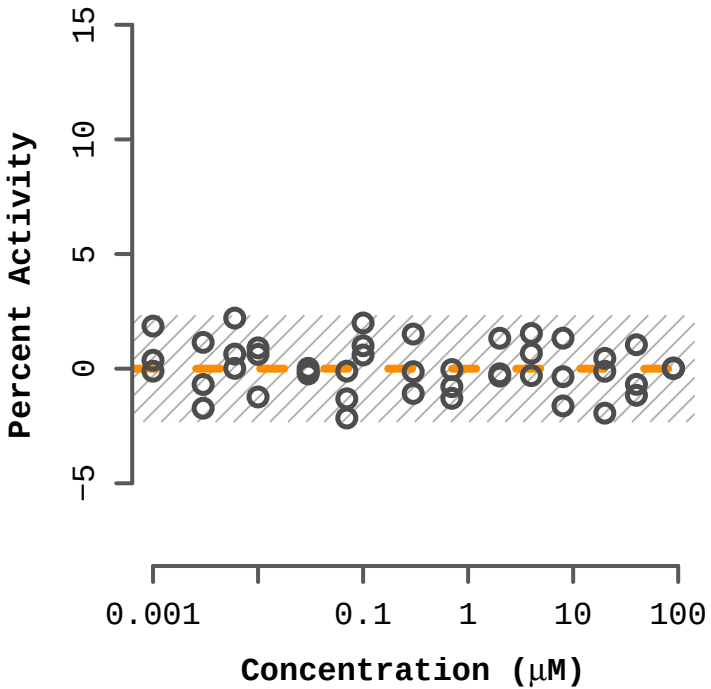
NAME: Metolachlor ESA
CHID: 37567 CASRN: 171118-09-5
SPID(S): Tox21_303740
M4ID: 12475448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.0676 MAX_MED: 0.0556 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

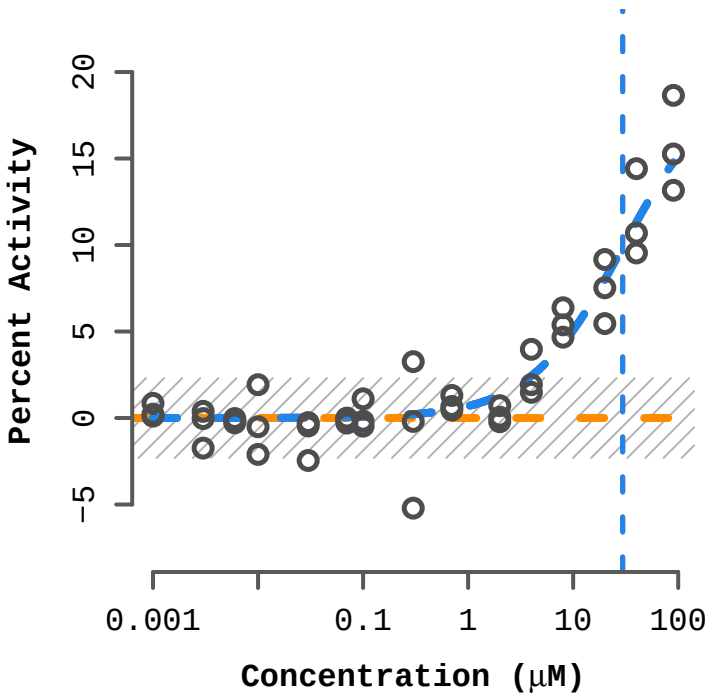
NAME: Metolachlor OA
CHID: 37568 CASRN: 152019-73-3
SPID(S): Tox21_304002
M4ID: 12475186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.2 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methabenzthiazuron
CHID: 37570 **CASRN:** 18691-97-9
SPID(S): Tox21_300966
M4ID: 12478167

HILL MODEL (in red):

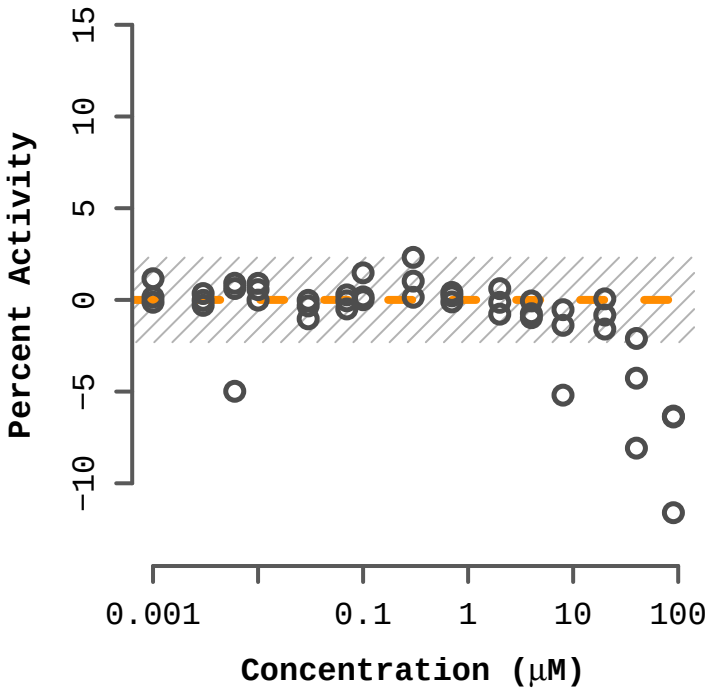
	tp	ga	gw
val:	19.7	1.47	0.979
sd:	4.95	0.266	0.204

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.7	1.47	0.979	3.91	3.97
sd:	4.95	0.266	0.204	1130	2330

	CNST	HILL	GNLS
AIC:	275.13	171.39	175.39
PROB:	0	0.88	0.12
RMSE:	5.8	1.58	1.58

MAX_MEAN: 15.7 **MAX_MED:** 15.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

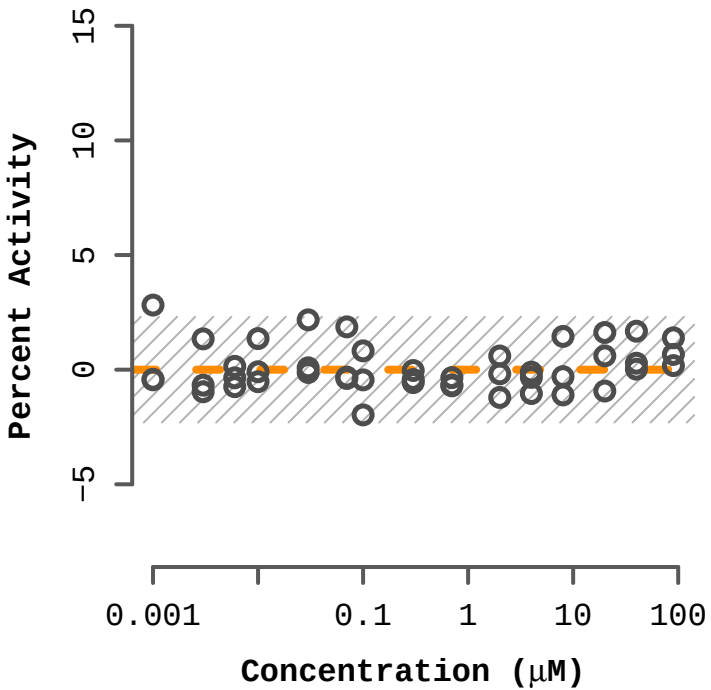
NAME: Methylparaoxon
CHID: 37571 **CASRN:** 950-35-6
SPID(S): Tox21_302009
M4ID: 12477124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.9	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

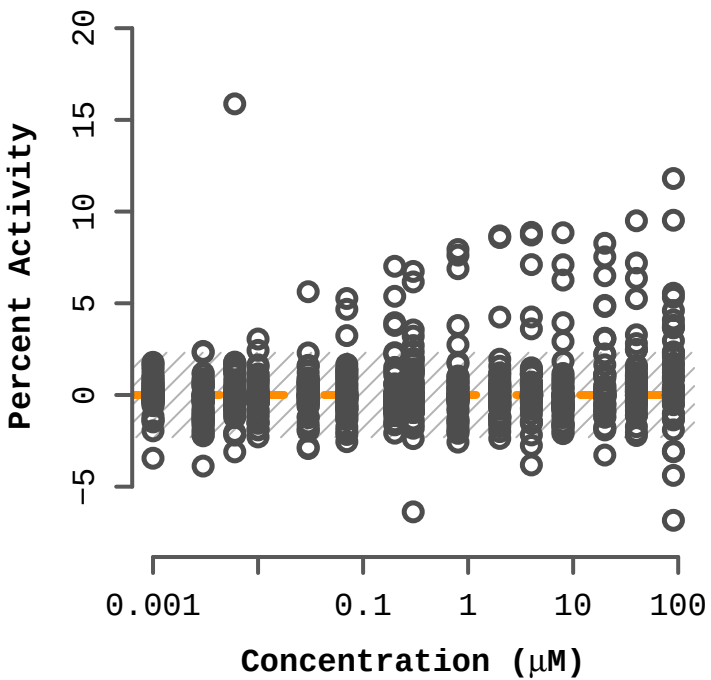
NAME: Monolinuron
CHID: 37576 **CASRN:** 1746-81-2
SPID(S): Tox21_301360
M4ID: 12477773

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.82	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.746 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

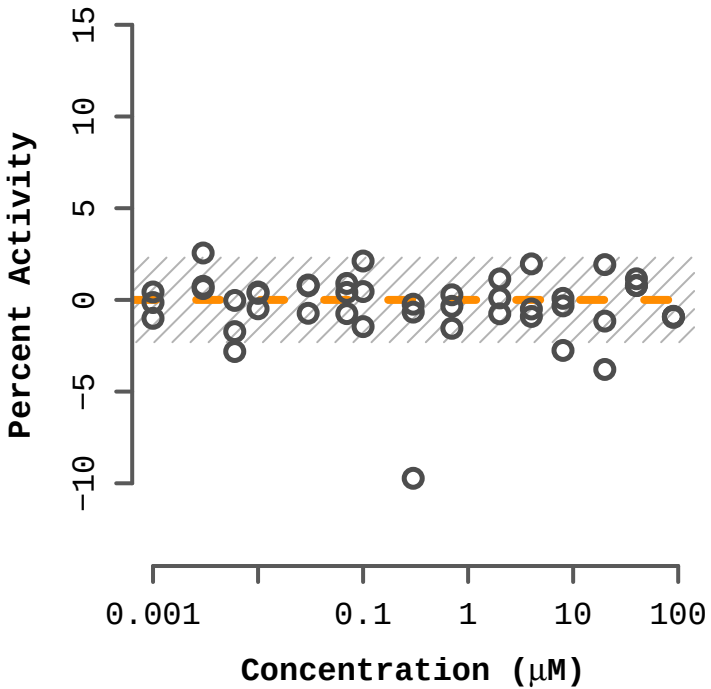
NAME: Nitrothal-isopropyl
CHID: 37579 **CASRN:** 10552-74-6
SPID(S): Tox21_400066
M4ID: 12475071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2680.13	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.366 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

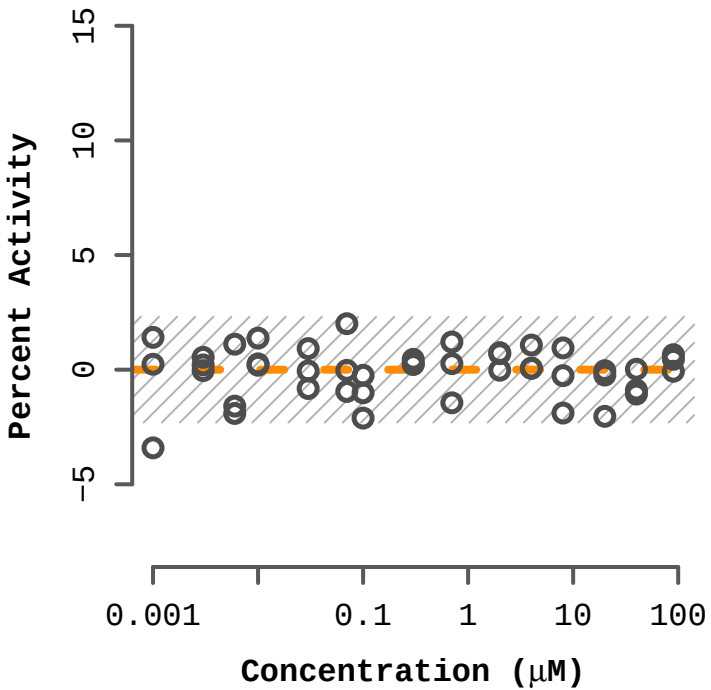
NAME: Omethoate
CHID: 37580 **CASRN:** 1113-02-6
SPID(S): Tox21_300968
M4ID: 12478165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

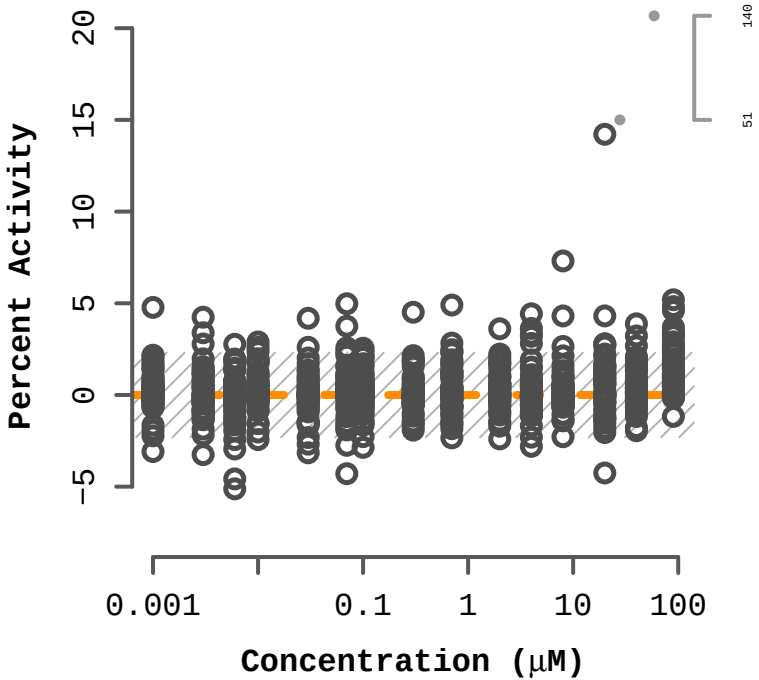
NAME: Demeton-S-methylsulphon
CHID: 37582 **CASRN:** 17040-19-6
SPID(S): Tox21_301575
M4ID: 12477558

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.609 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

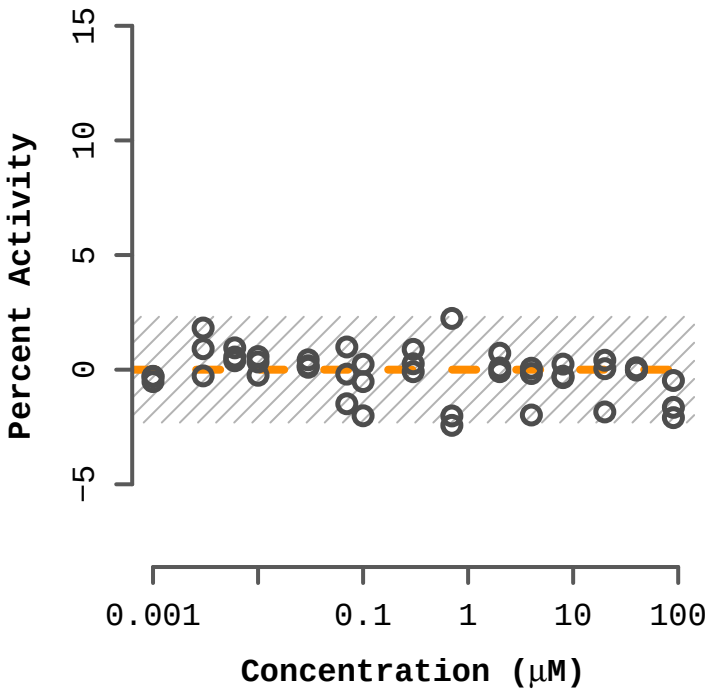
NAME: Pentachloroaniline
CHID: 37584 **CASRN:** 527-20-8
SPID(S): Tox21_400021
M4ID: 12475116 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2481.03	NA	NA
PROB:	1	NA	NA
RMSE:	5.82	NA	NA

MAX_MEAN: 4.38 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

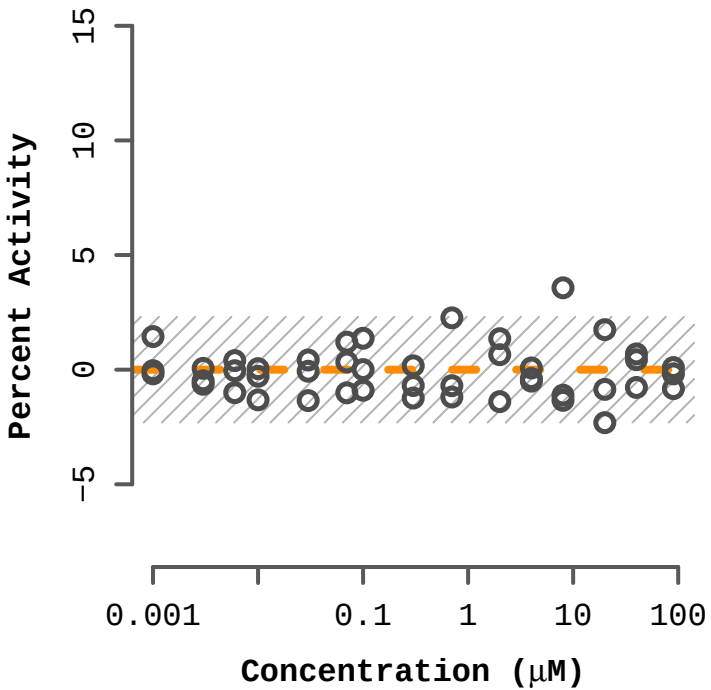
NAME: Secbumeton
CHID: 37594 **CASRN:** 26259-45-0
SPID(S): Tox21_301419
M4ID: 12477714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.822 **MAX_MED:** 0.915 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

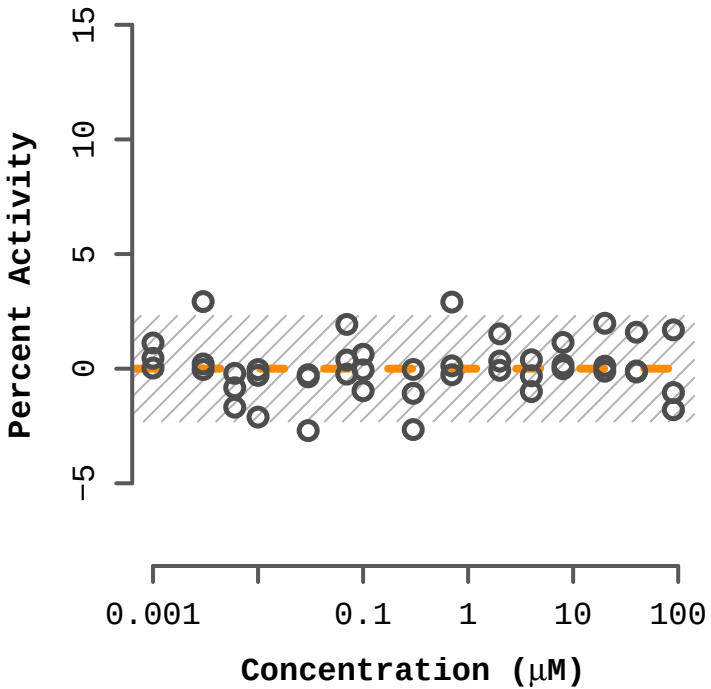
NAME: Simetryn
CHID: 37596 **CASRN:** 1014-70-6
SPID(S): Tox21_300702
M4ID: 12478431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.408 **MAX_MED:** 0.655 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

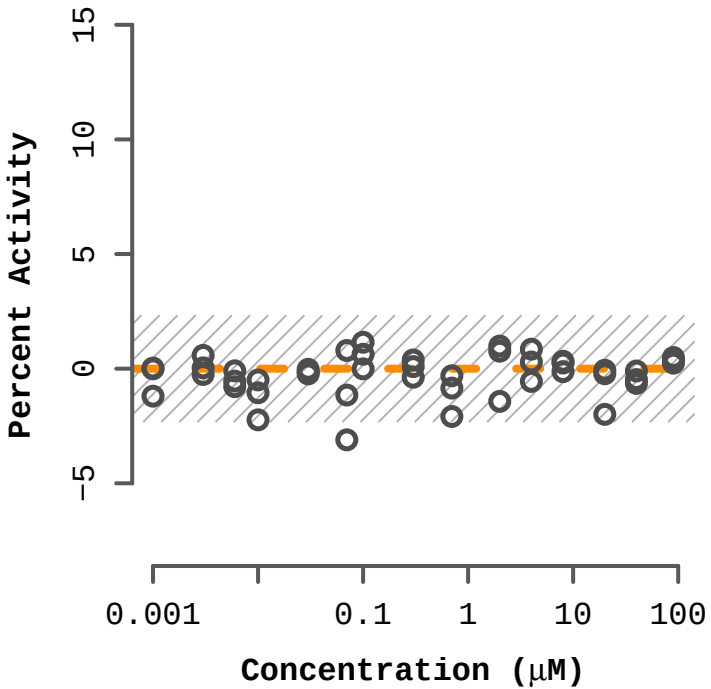
NAME: Triazophos
CHID: 37612 **CASRN:** 24017-47-8
SPID(S): Tox21_301578
M4ID: 12477555

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

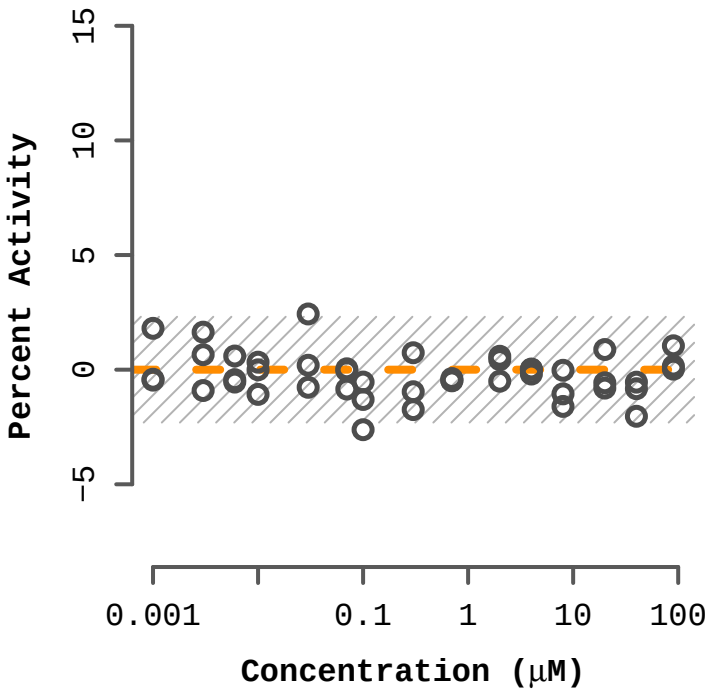
NAME: Diketometribuzin
CHID: 37616 CASRN: 56507-37-0
SPID(S): Tox21_303948
M4ID: 12475240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.593 **MAX_MED:** 0.763 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

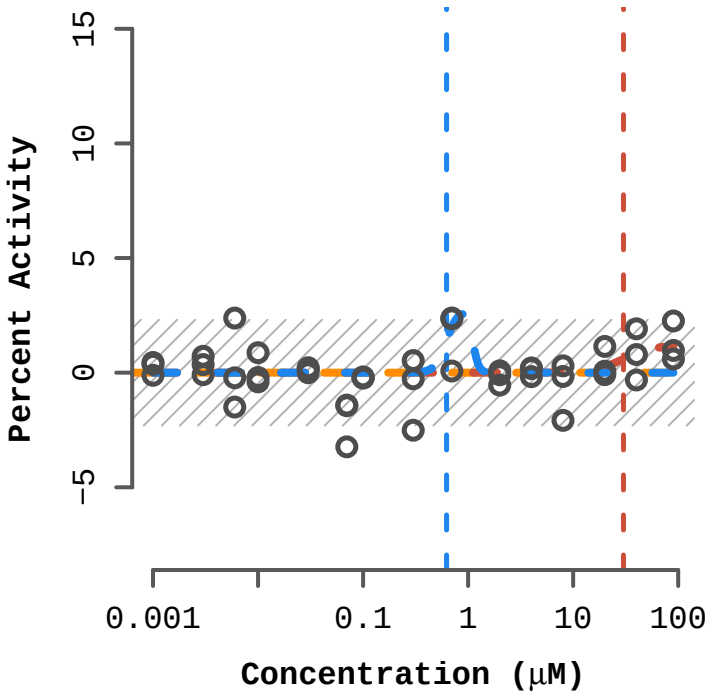
NAME: Promecarb
CHID: 37617 **CASRN:** 2631-37-0
SPID(S): Tox21_301424
M4ID: 12477709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.62 **MAX_MED:** 0.655 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Dichlorobenzophenone
CHID: 37626 CASRN: 90−98−2
SPID(S): Tox21_302130
M4ID: 12477003

HILL MODEL (in red):

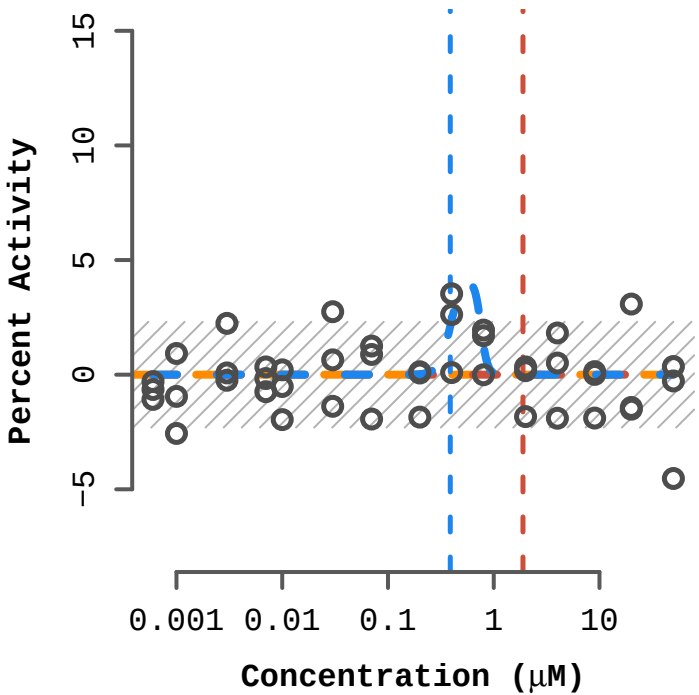
	tp	ga	gw
val:	1.19	1.48	3.1
sd:	0.656	0.348	4.07

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.79	−0.205	8	0.0448	15.7
sd:	9.61	0.601	16.4	2.65	164

	CNST	HILL	GNLS
AIC:	137.13	135.25	140.13
PROB:	0.26	0.68	0.06
RMSE:	1.15	1.08	1.08

MAX_MEAN: 1.6 MAX_MED: 2.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Deferoxamine mesylate
CHID: 37649 **CASRN:** 138-14-7
SPID(S): Tox21_110741_1
M4ID: 12484140

HILL MODEL (in red):

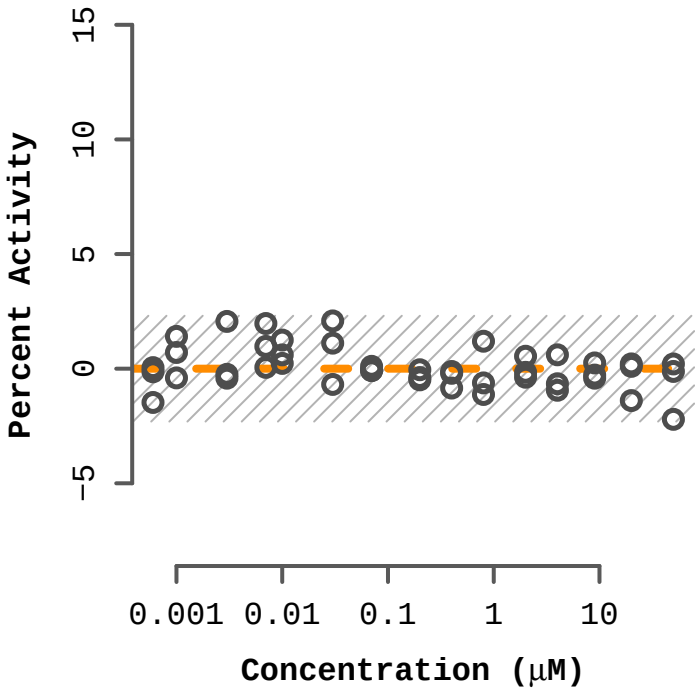
	tp	ga	gw
val:	1.7e-10	0.277	1.74
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.24	−0.411	8	−0.121	14.3
sd:	15.3	0.434	12.2	1.24	710

	CNST	HILL	GNLS
AIC:	172.16	178.16	174.12
PROB:	0.7	0.03	0.26
RMSE:	1.59	1.59	1.47

MAX_MEAN: 2.08 **MAX_MED:** 2.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

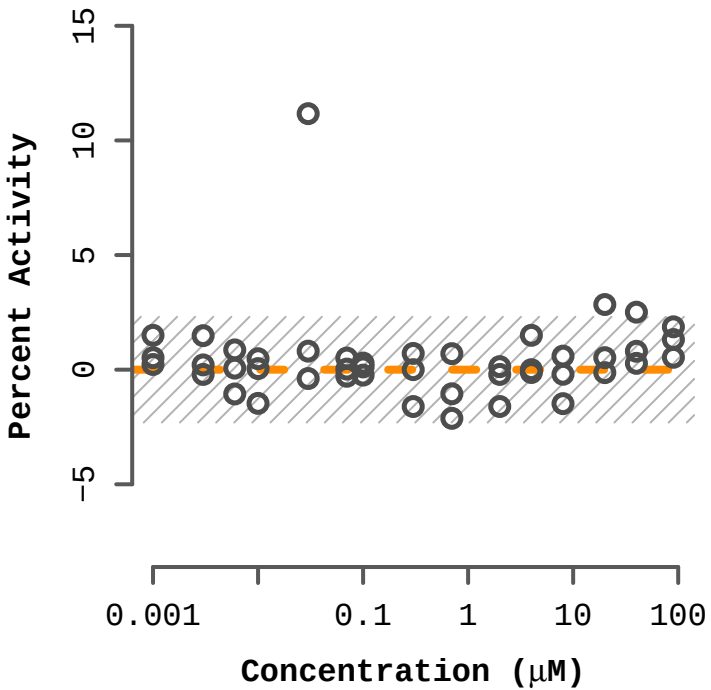
NAME: Norfloxacin
CHID: 37680 **CASRN:** 70458-96-7
SPID(S): Tox21_110682_1
M4ID: 12484182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

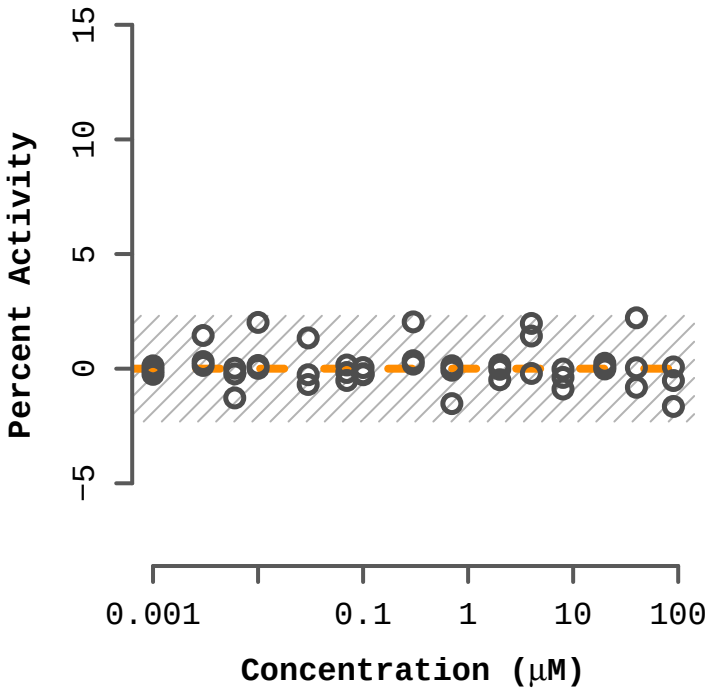
NAME: N'-(2,4-Dimethylphenyl)-N-methylformamidine
CHID: 37696 **CASRN:** 33089-74-6
SPID(S): Tox21_301746
M4ID: 12477387

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 3.87 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

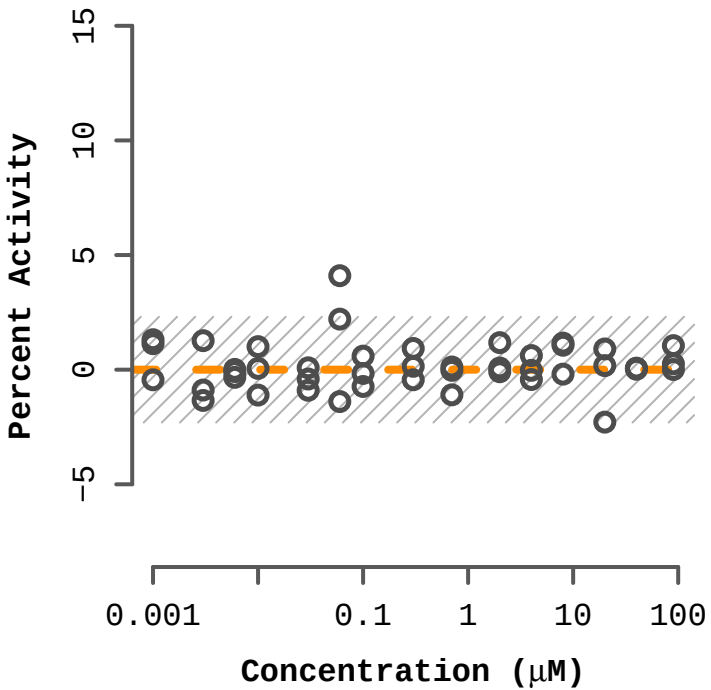
NAME: N-(2,4-Dimethylphenyl)formamide
CHID: 37697 **CASRN:** 60397-77-5
SPID(S): Tox21_301442
M4ID: 12477691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

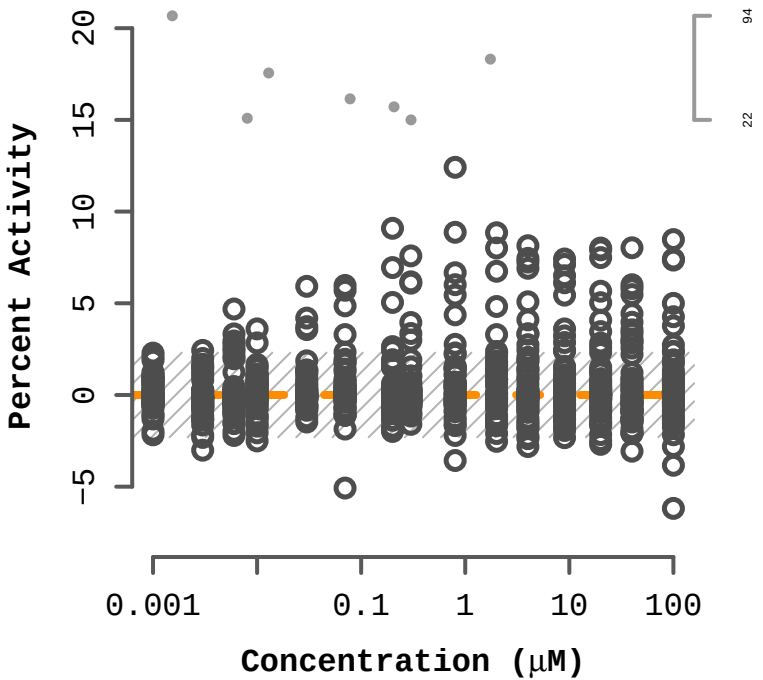
NAME: PFOS-K
CHID: 37706 CASRN: 2795-39-3
SPID(S): Tox21_300544
M4ID: 12478588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

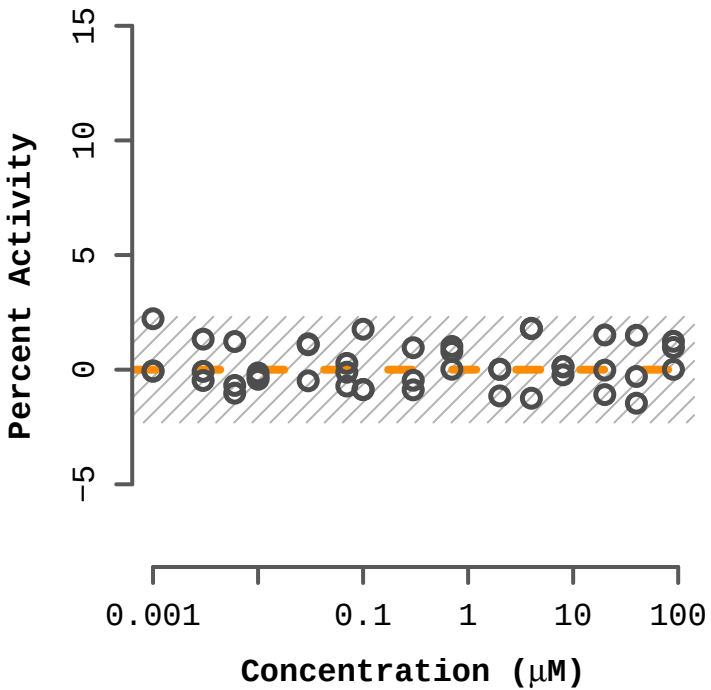
NAME: PFBS-K
CHID: 37707 **CASRN:** 29420-49-3
SPID(S): Tox21_400051
M4ID: 12475086 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3143.93	NA	NA
PROB:	1	NA	NA
RMSE:	5.43	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 0.688 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

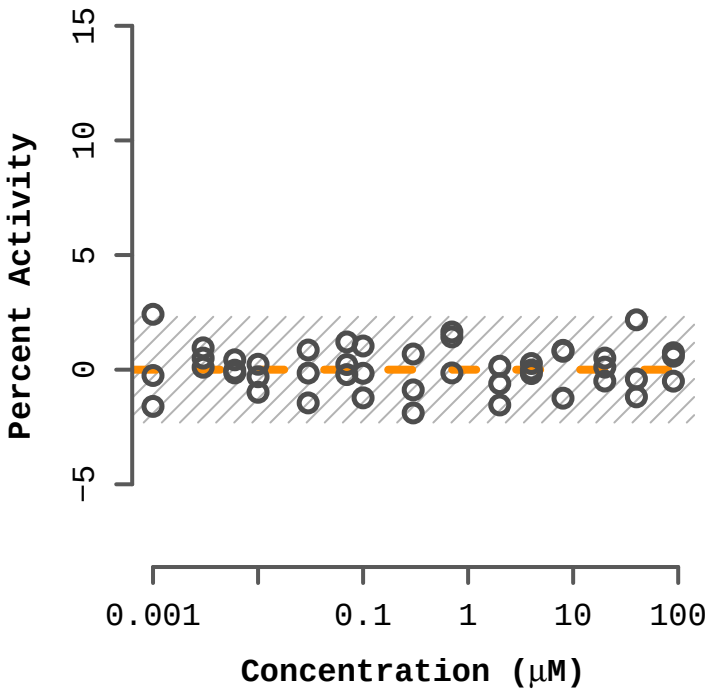
NAME: PFOA, ammonium salt
CHID: 37708 **CASRN:** 3825-26-1
SPID(S): Tox21_300595
M4ID: 12478538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.784 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

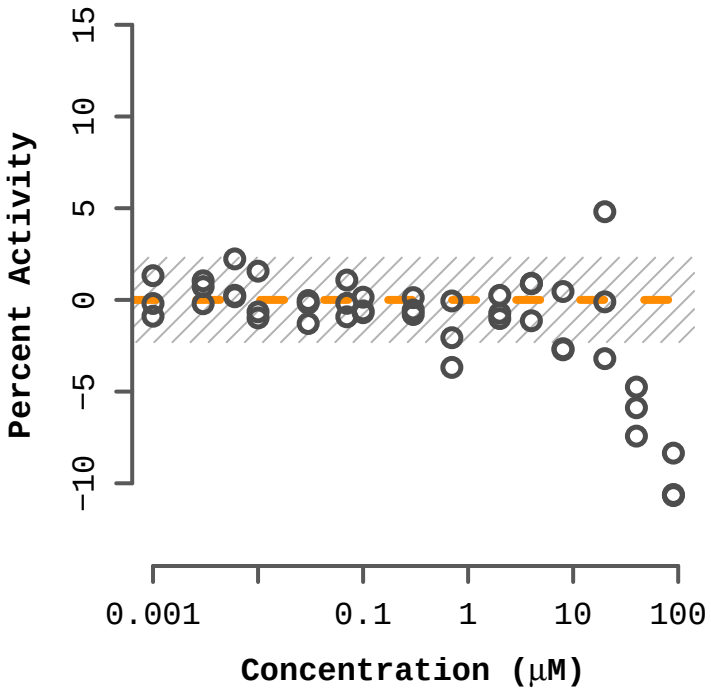
NAME: PFHS-K
CHID: 37709 **CASRN:** 3871-99-6
SPID(S): Tox21_300396
M4ID: 12478736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

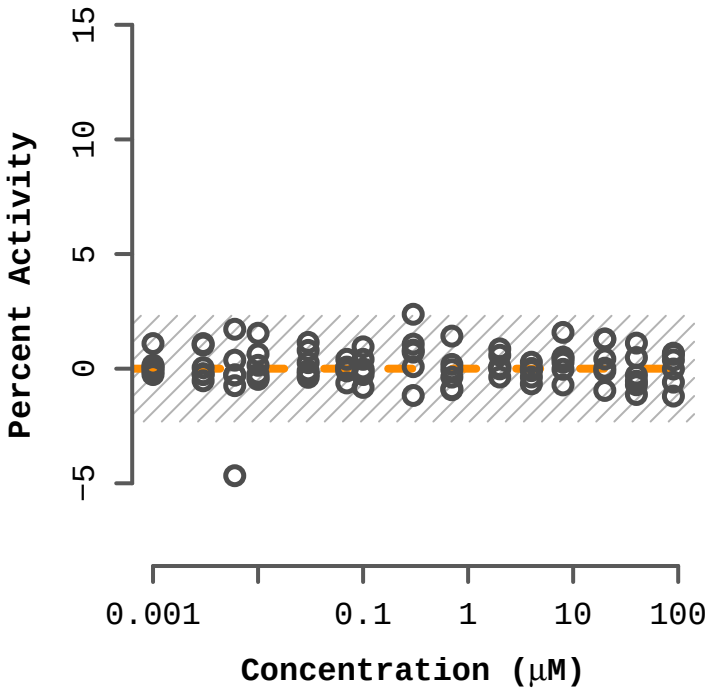
NAME: 4,4',4"-Ethane-1,1,1-triyltriphenol
CHID: 37712 **CASRN:** 27955-94-8
SPID(S): Tox21_300402
M4ID: 12478730

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.95	NA	NA
PROB:	1	NA	NA
RMSE:	3.33	NA	NA

MAX_MEAN: 0.887 **MAX_MED:** 0.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

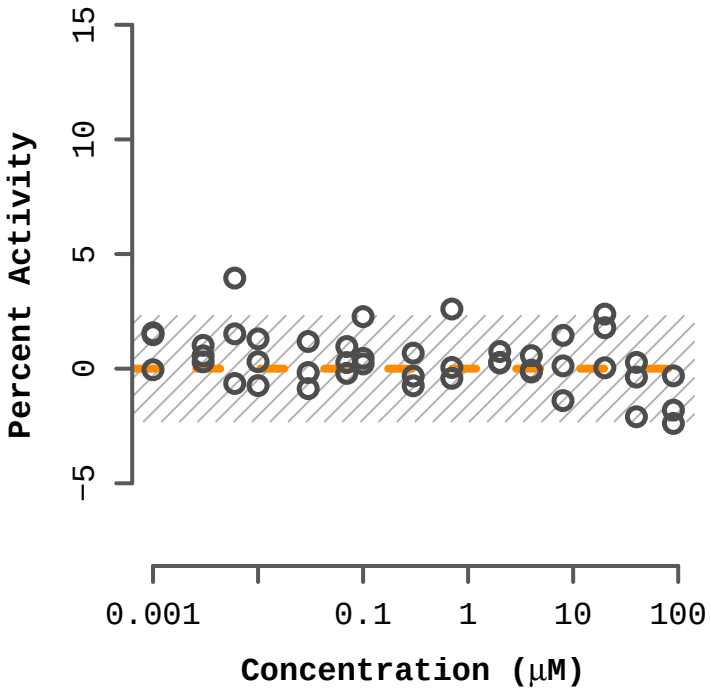
NAME: 4-Heptylphenol
CHID: 37714 **CASRN:** 1987-50-4
SPID(S): Tox21_301548
M4ID: 12477585

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.65 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

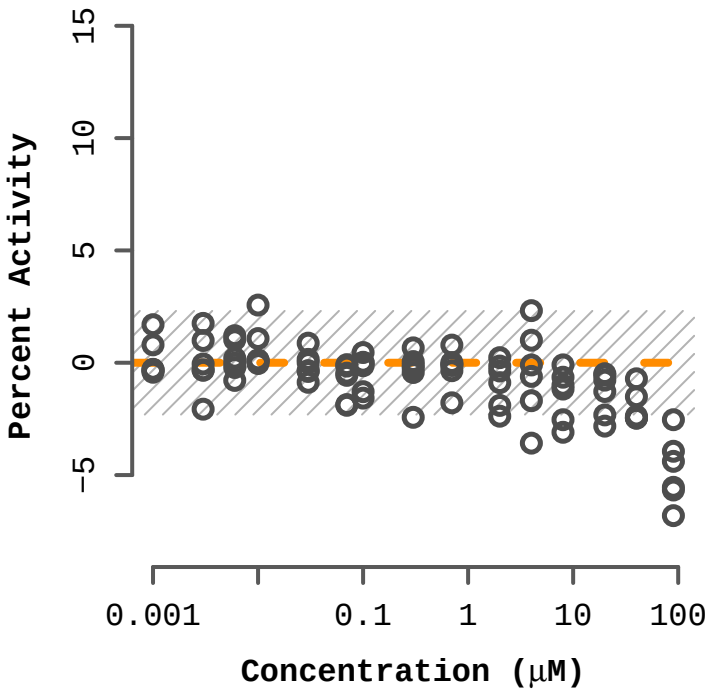
NAME: 2,2−Dimethoxy−1,2−diphenylethanone
CHID: 37715 **CASRN:** 24650−42−8
SPID(S): Tox21_302150
M4ID: 12476983

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

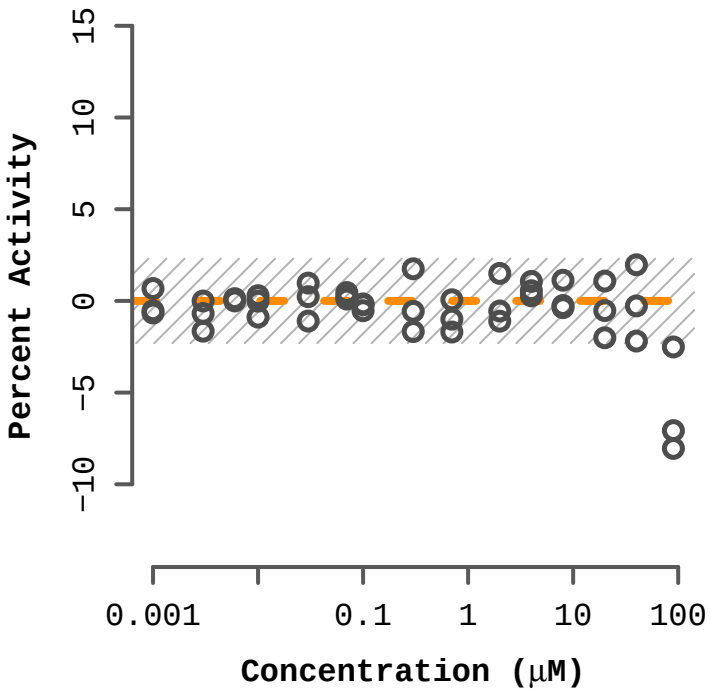
NAME: Bisphenol AF
CHID: 37717 **CASRN:** 1478-61-1
SPID(S): Tox21_303641
M4ID: 12475504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	347.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 0.653 **MAX_MED:** 0.114 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

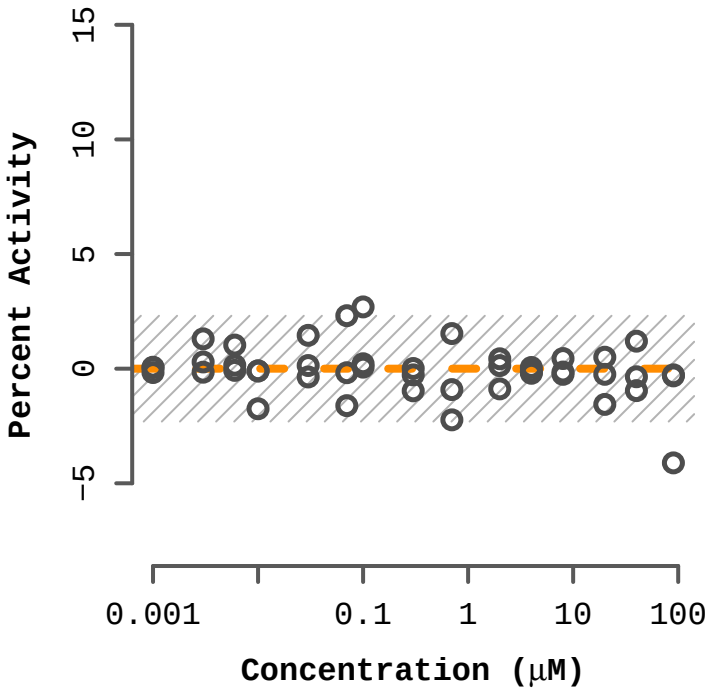
NAME: Bisphenol AF
CHID: 37717 **CASRN:** 1478-61-1
SPID(S): Tox21_201467
M4ID: 12480785

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 0.634 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

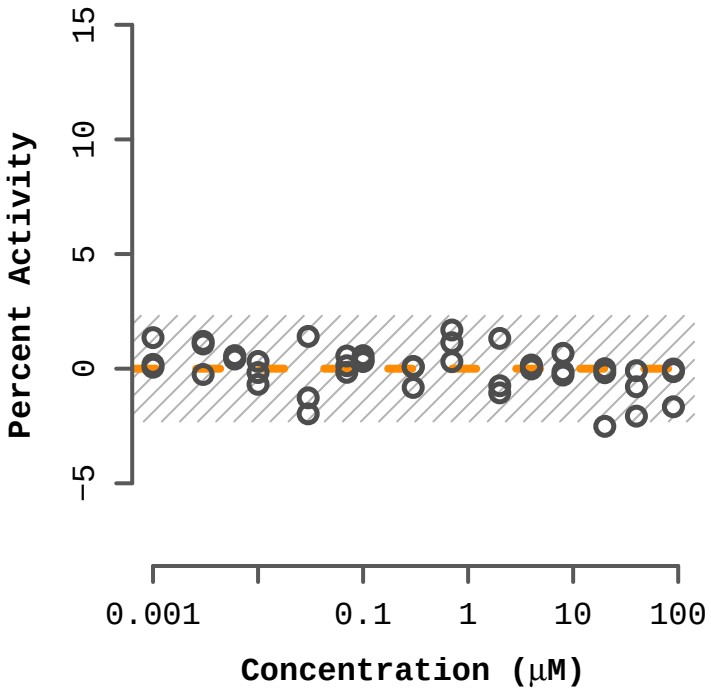
NAME: 2,3,4−Trihydroxbenzophenone
CHID: 37728 **CASRN:** 1143−72−2
SPID(S): Tox21_303374
M4ID: 12475762

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 0.294 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

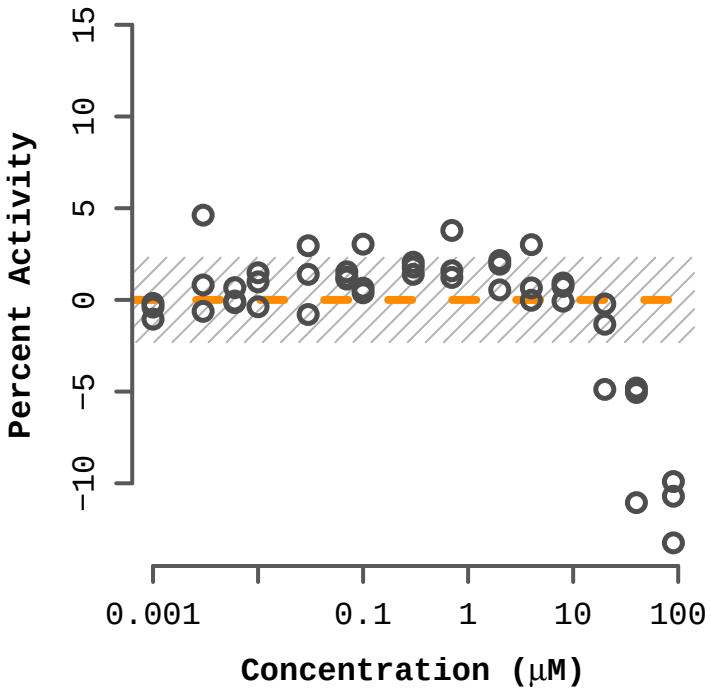
NAME: 2,3,4−Trihydroxbenzophenone
CHID: 37728 **CASRN:** 1143−72−2
SPID(S): Tox21_201936
M4ID: 12480316

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

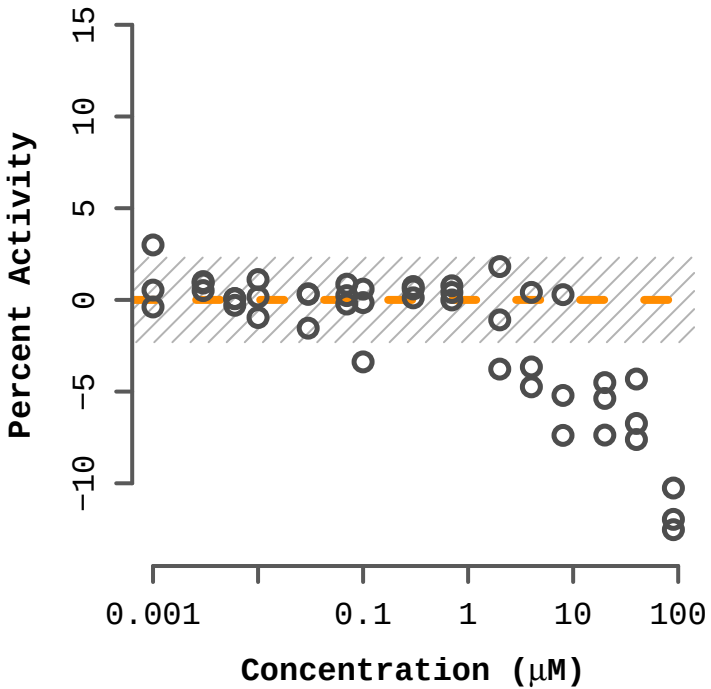
NAME: 1,4-Dihydroxy-2-naphthoic acid
CHID: 37730 **CASRN:** 31519-22-9
SPID(S): Tox21_301655
M4ID: 12477478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	235.53	NA	NA
PROB:	1	NA	NA
RMSE:	3.9	NA	NA

MAX_MEAN: 2.2 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

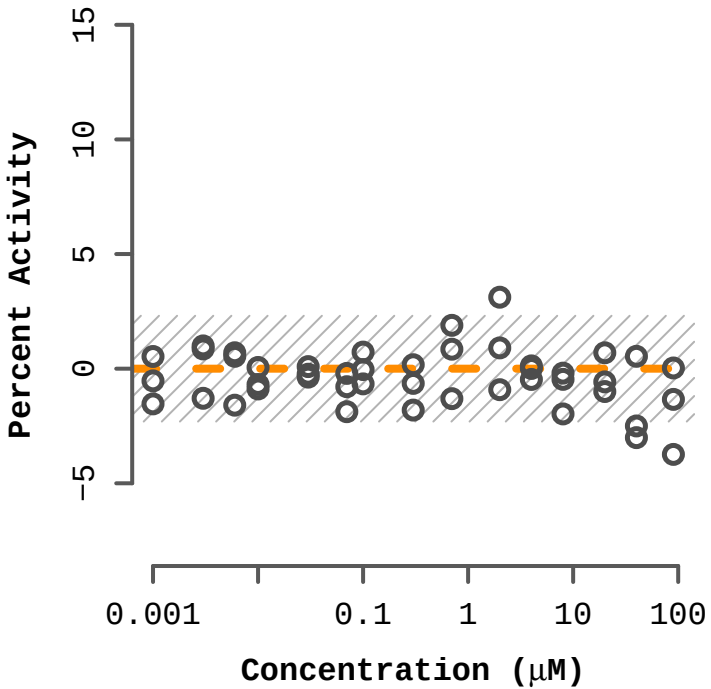
NAME: 4,4'-(9H-Fluorene-9,9-diyl)diphenol
CHID: 37731 **CASRN:** 3236-71-3
SPID(S): Tox21_301584
M4ID: 12477549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	250.21	NA	NA
PROB:	1	NA	NA
RMSE:	4.21	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.921 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

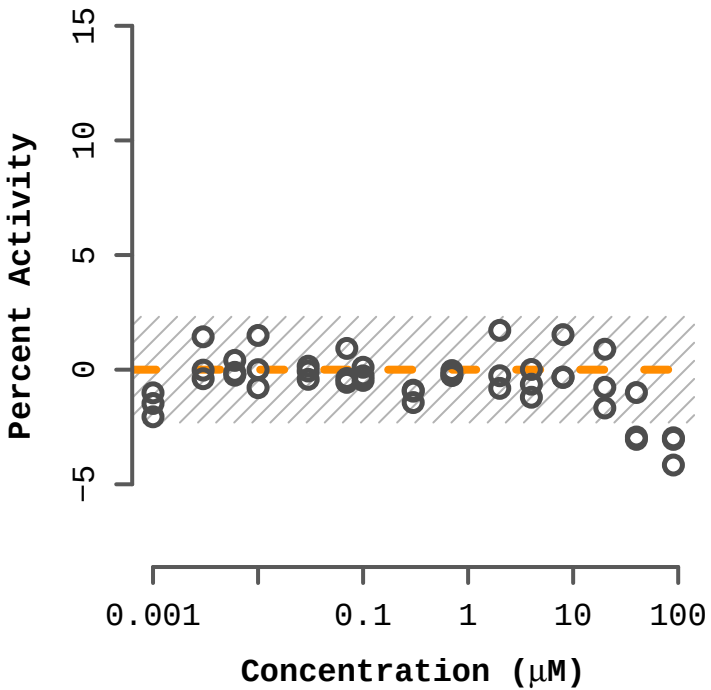
NAME: 2-Bromohexadecanoic acid
CHID: 37734 **CASRN:** 18263-25-7
SPID(S): Tox21_301033
M4ID: 12478100

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

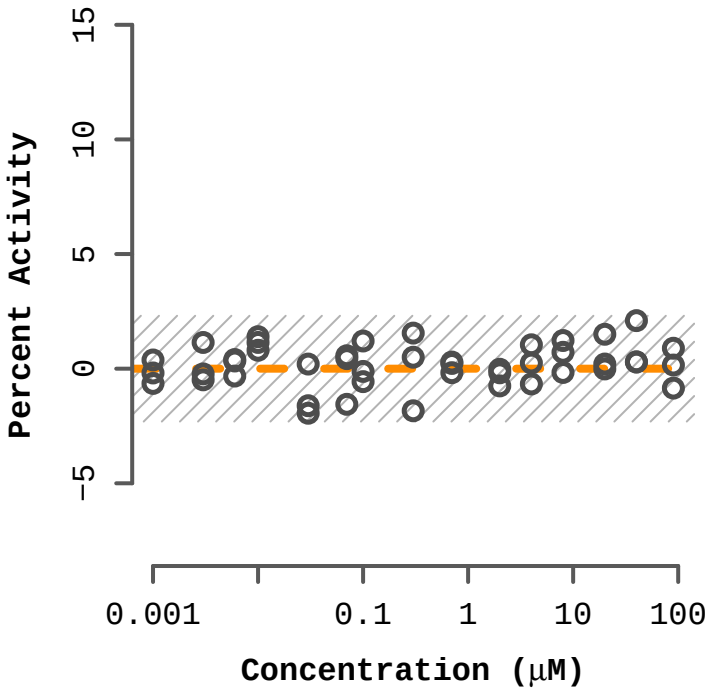
NAME: 4-Anilinophenol
CHID: 37739 **CASRN:** 122-37-2
SPID(S): Tox21_301986
M4ID: 12477147

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.341 **MAX_MED:** 0.00203 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

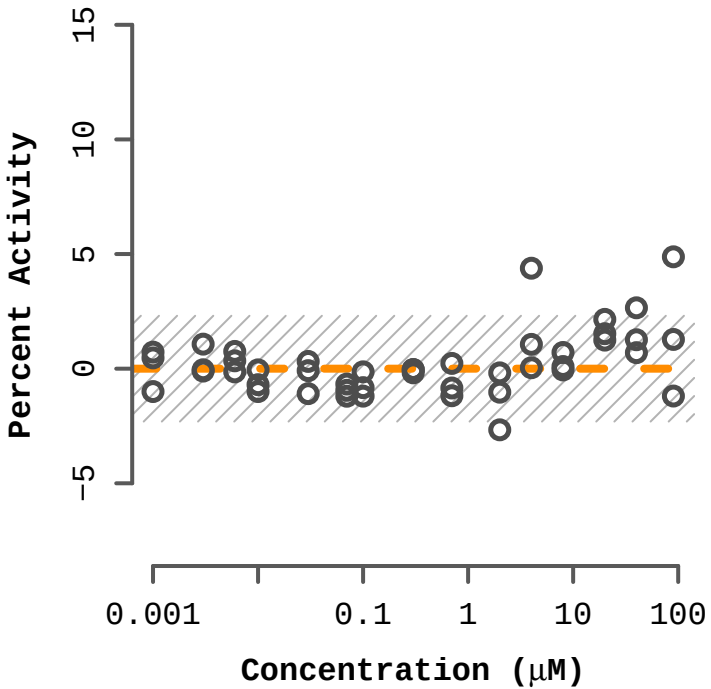
NAME: 4-Methylbenzophenone
CHID: 37741 **CASRN:** 134-84-9
SPID(S): Tox21_301629
M4ID: 12477504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

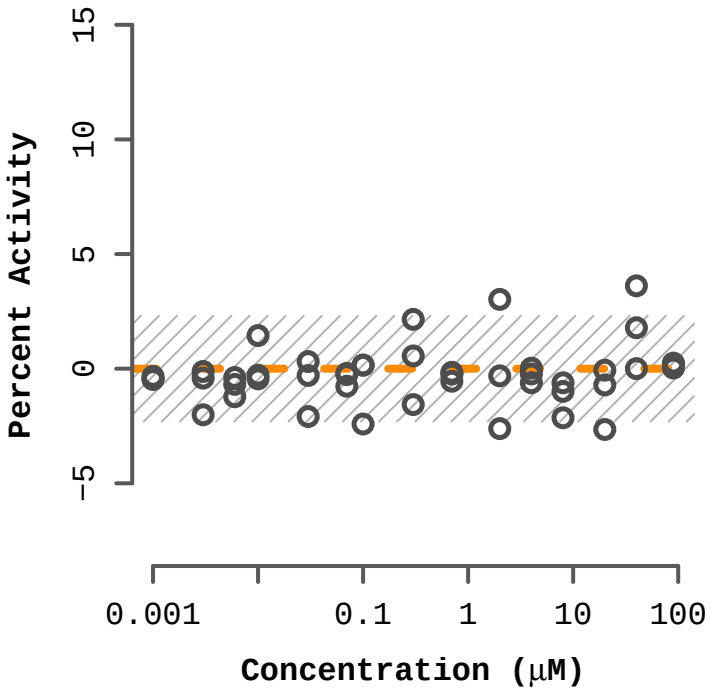
NAME: 4-tert-Butylphenyl salicylate
CHID: 37745 **CASRN:** 87-18-3
SPID(S): Tox21_303577
M4ID: 12475568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2,4,4,6,6−Hexamethyl−1,3,5,2,4,6−triazatrisi

CHID: 37748 **CASRN:** 1009−93−4

SPID(S): Tox21_300757

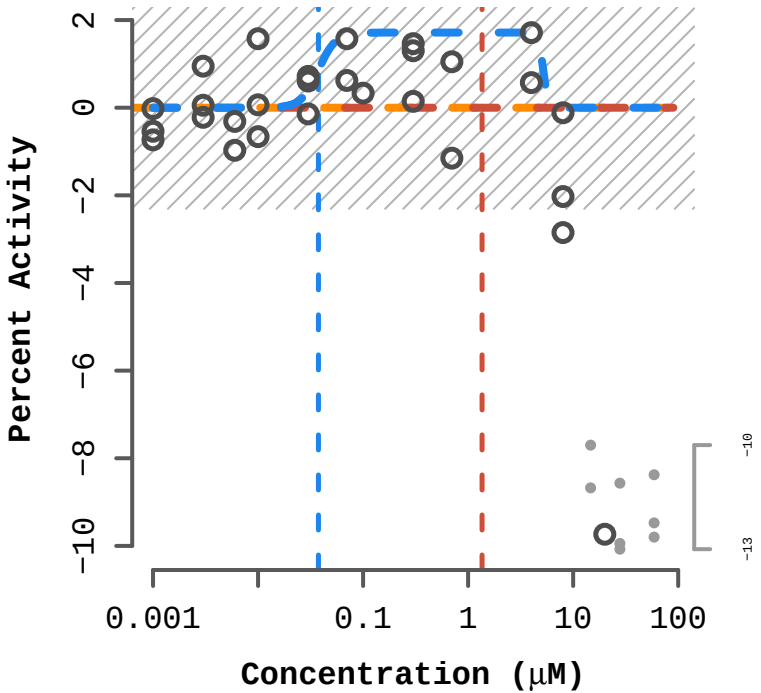
M4ID: 12478376

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Chlorosalicylanilide
CHID: 37749 **CASRN:** 4638-48-6
SPID(S): Tox21_301637
M4ID: 12477496 **BRK**

HILL MODEL (in red):

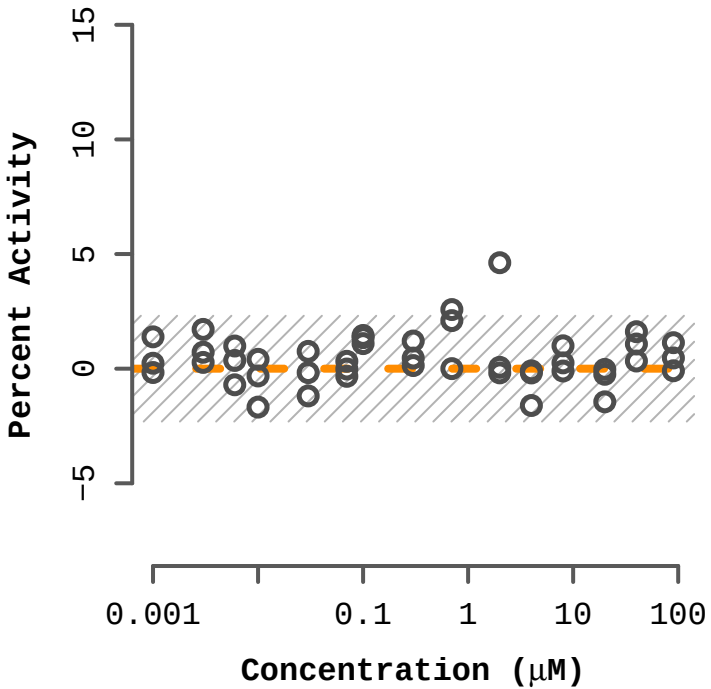
	tp	ga	gw
val:	5.34e-11	0.133	1.48
sd:	5.04e-05	7740	69500

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.71	-1.43	5.34	0.715	18
sd:	0.691	0.57	26.6	0.74	87.6

	CNST	HILL	GNLS
AIC:	272.8	278.8	276.52
PROB:	0.83	0.04	0.13
RMSE:	5.47	5.47	5.36

MAX_MEAN: 2.6 **MAX_MED:** 2.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

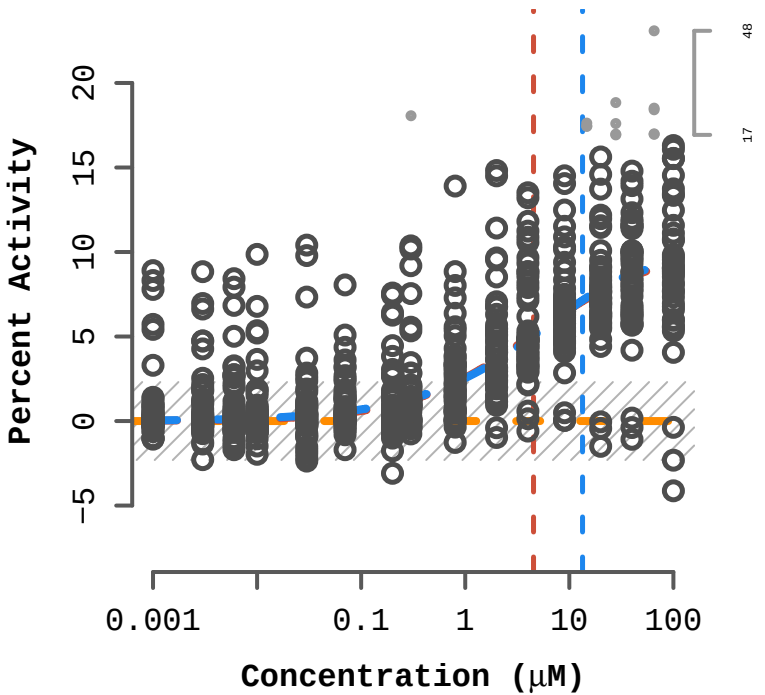
NAME: (3Z)-Hex-3-en-1-yl salicylate
CHID: 37750 CASRN: 65405-77-8
SPID(S): Tox21_301692
M4ID: 12477441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diphenyl isophthalate
CHID: 37752 CASRN: 744-45-6
SPID(S): Tox21_400023
M4ID: 12475114 BRK

HILL MODEL (in red):

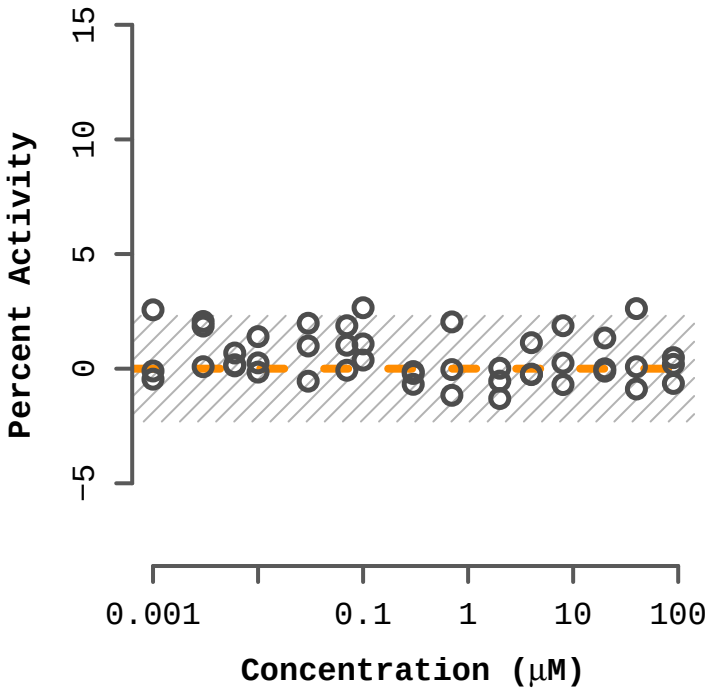
	tp	ga	gw
val:	10.3	0.656	0.73
sd:	0.685	0.109	0.0757

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.1	1.13	0.633	2.76	0.547
sd:	21.9	1.08	0.12	1.87	1

	CNST	HILL	GNLS
AIC:	4533.69	3528.66	3531.69
PROB:	0	0.82	0.18
RMSE:	6.2	3.65	3.65

MAX_MEAN: 10.6 **MAX_MED:** 9.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

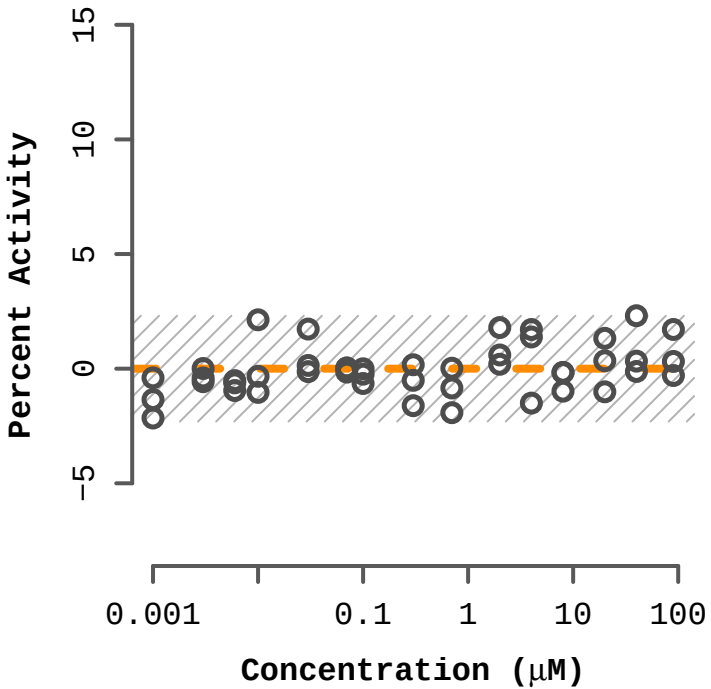
NAME: 2,4,6-Tris(allyloxy)-1,3,5-triazine
CHID: 37754 **CASRN:** 101-37-1
SPID(S): Tox21_300737
M4ID: 12478396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

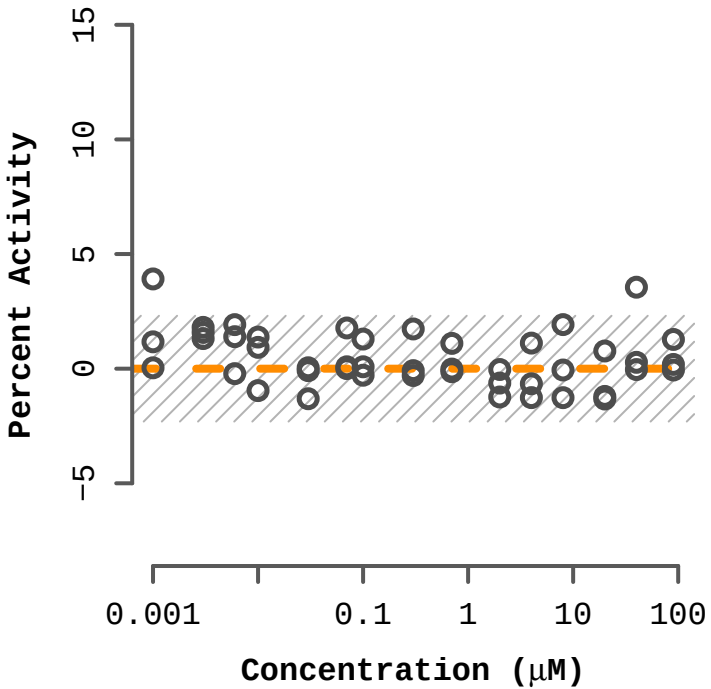
NAME: 2-Phenylpropan-1-ol
CHID: 37756 CASRN: 1123-85-9
SPID(S): Tox21_302341
M4ID: 12476792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.863 MAX_MED: 1.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

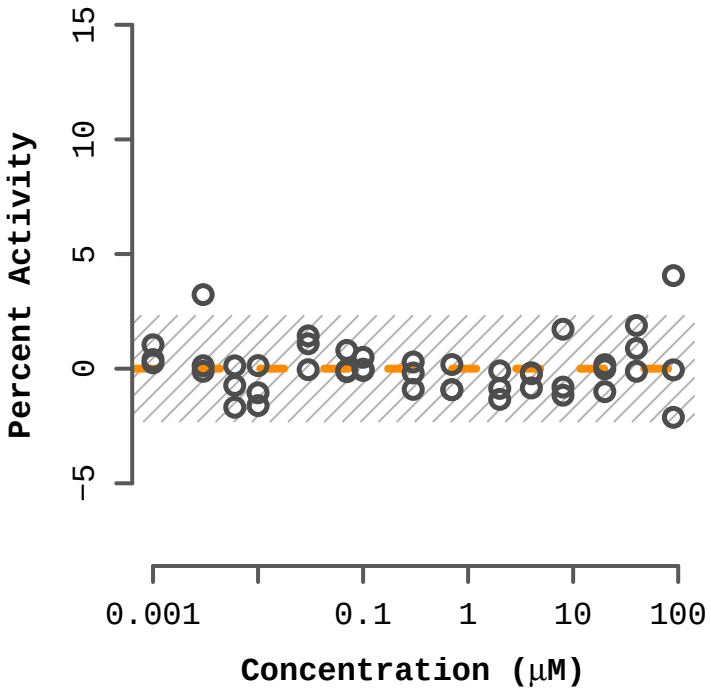
NAME: Undec-10-enal
CHID: 37757 **CASRN:** 112-45-8
SPID(S): Tox21_302293
M4ID: 12476840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

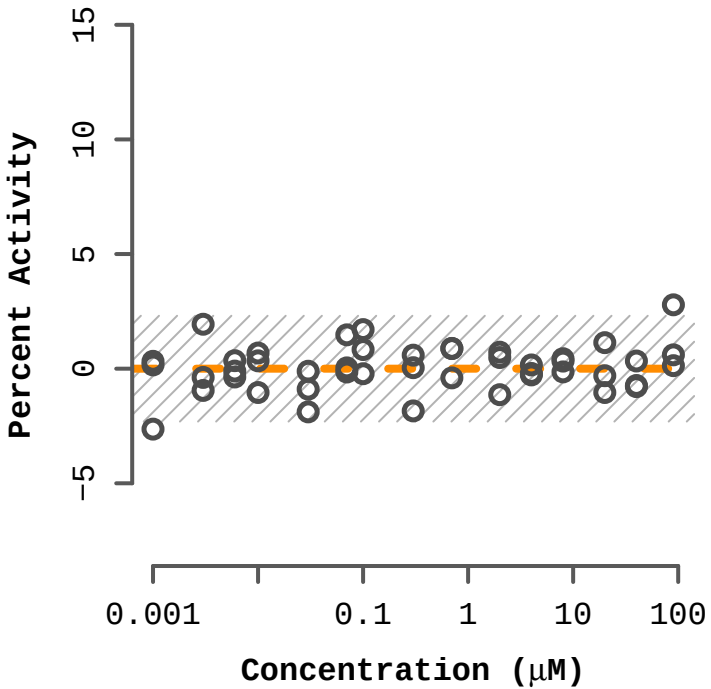
NAME: 2-Chloro-4,6-diamino-1,3,5-triazine
CHID: 37806 **CASRN:** 3397-62-4
SPID(S): Tox21_301105
M4ID: 12478028

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

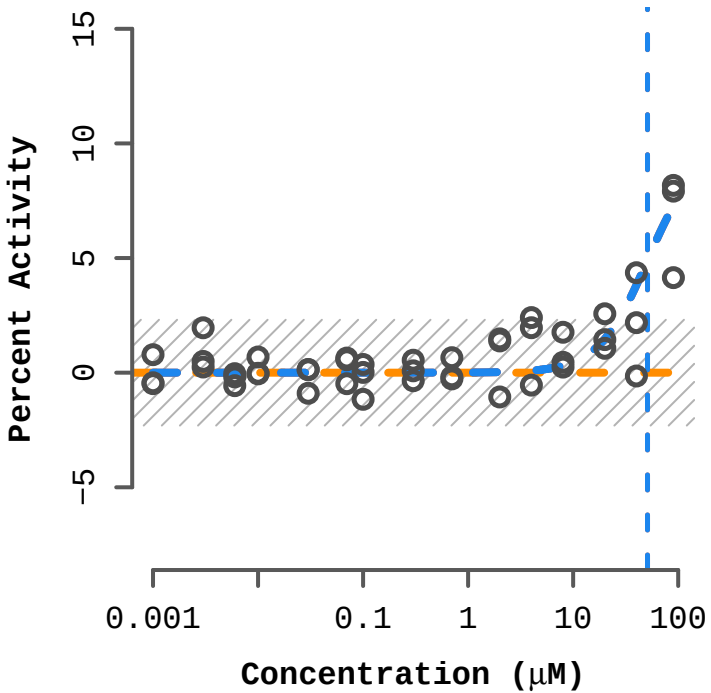
NAME: 1-Hydroxypyrene
CHID: 38298 **CASRN:** 5315-79-7
SPID(S): Tox21_300617
M4ID: 12478516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,5,6-Trichloro-2-pyridinol
CHID: 38317 CASRN: 6515-38-4
SPID(S): Tox21_301556
M4ID: 12477577

HILL MODEL (in red):

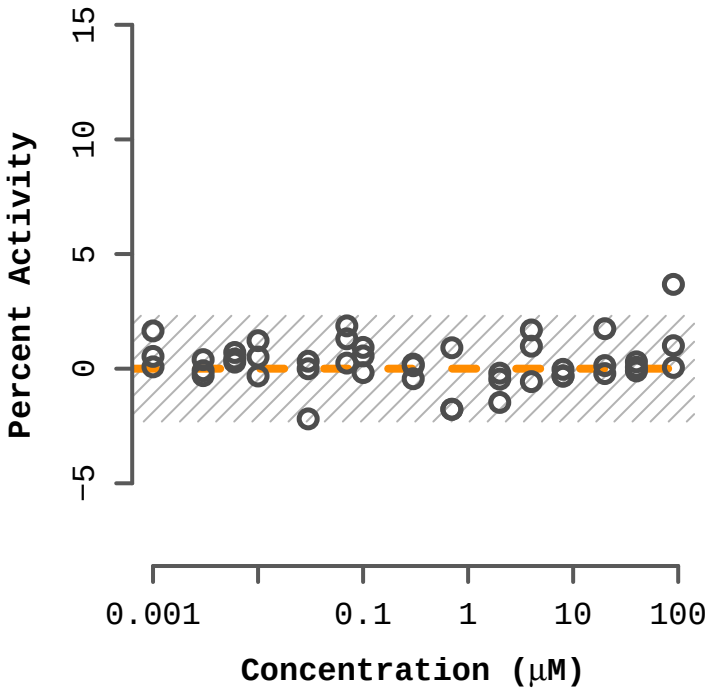
	tp	ga	gw
val:	9.81	1.71	1.85
sd:	2.35	0.135	0.525

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.81	1.71	1.85	3.95	3.17
sd:	2.35	0.135	0.525	188	300

	CNST	HILL	GNLS
AIC:	175.28	139.56	143.56
PROB:	0	0.88	0.12
RMSE:	2.16	1.13	1.13

MAX_MEAN: 6.75 MAX_MED: 7.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

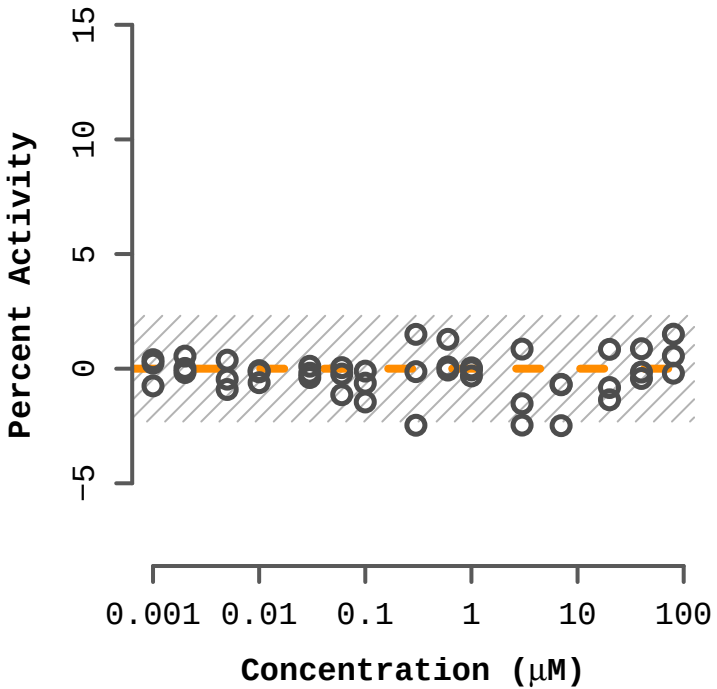
NAME: 3-Phenoxybenzoic acid
CHID: 38321 **CASRN:** 3739-38-6
SPID(S): Tox21_300610
M4ID: 12478523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

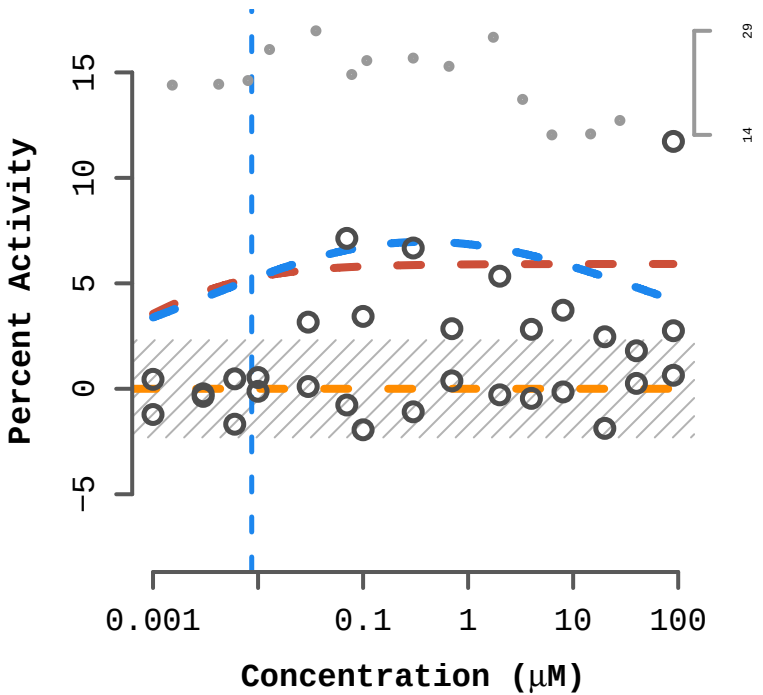
NAME: cis-Chlordane
CHID: 38326 **CASRN:** 5103-71-9
SPID(S): Tox21_303821
M4ID: 12475367

HILL MODEL: Not applicable.

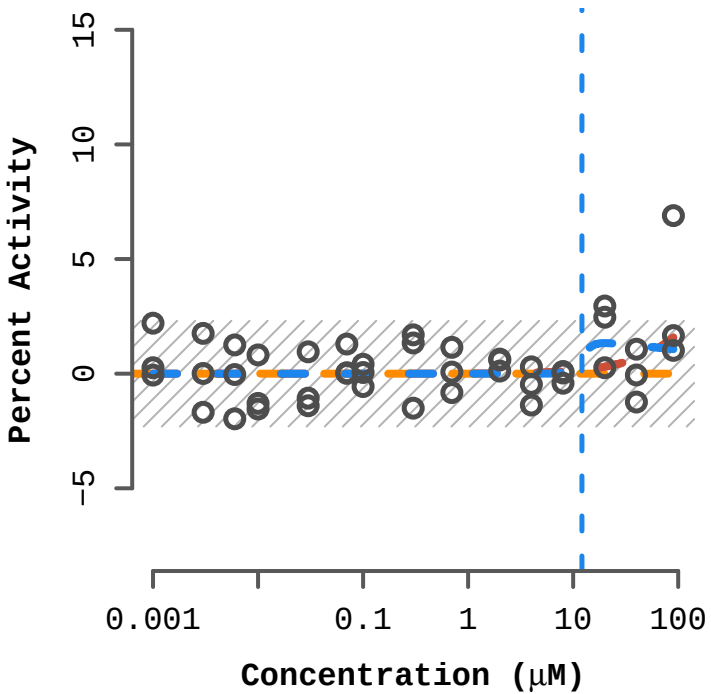
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.623 **MAX_MED:** 0.559 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    trans-Chlordane
CHID:    38346   CASRN: 5103-74-2
SPID(S): Tox21_303985
M4ID:    12475203  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  5.92     -3.23    0.755
sd:   1.87     2.51     1.95

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  11.5     -2.06    0.368    1.24     0.3
sd:   101      15.8     1.8      22       1.57

      CNST        HILL        GNLS
AIC:  356.6       348.03      351.74
PROB: 0.01        0.85        0.13
RMSE: 12.82       10.38       10.27

MAX_MEAN: 10.9      MAX_MED: 7.13      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorpyrifos oxon
CHID: 38666 CASRN: 5598-15-2
SPID(S): Tox21_301063
M4ID: 12478070

HILL MODEL (in red):

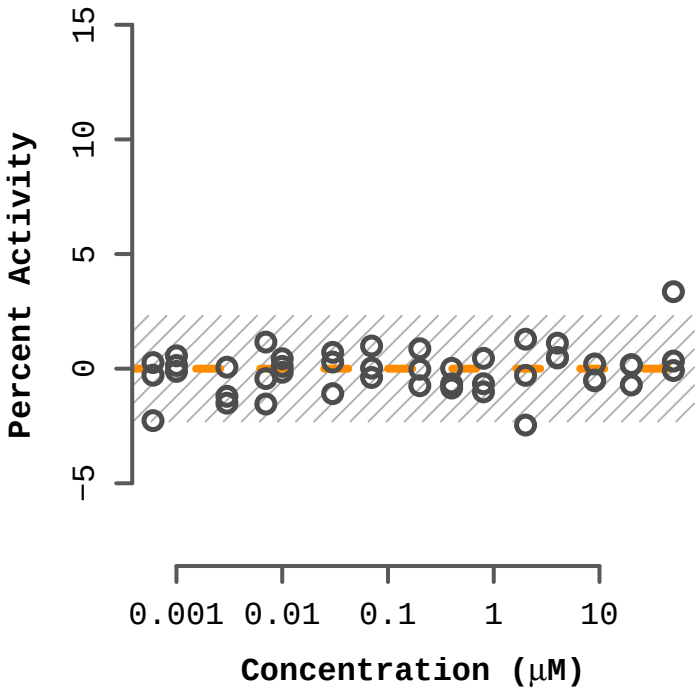
	tp	ga	gw
val:	8.04	2.45	1.22
sd:	43.9	2.52	1.51

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.57	1.08	8	1.46	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	158.61	158.83	162.09
PROB:	0.48	0.43	0.08
RMSE:	1.55	1.37	1.39

MAX_MEAN: 3.19 MAX_MED: 2.46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

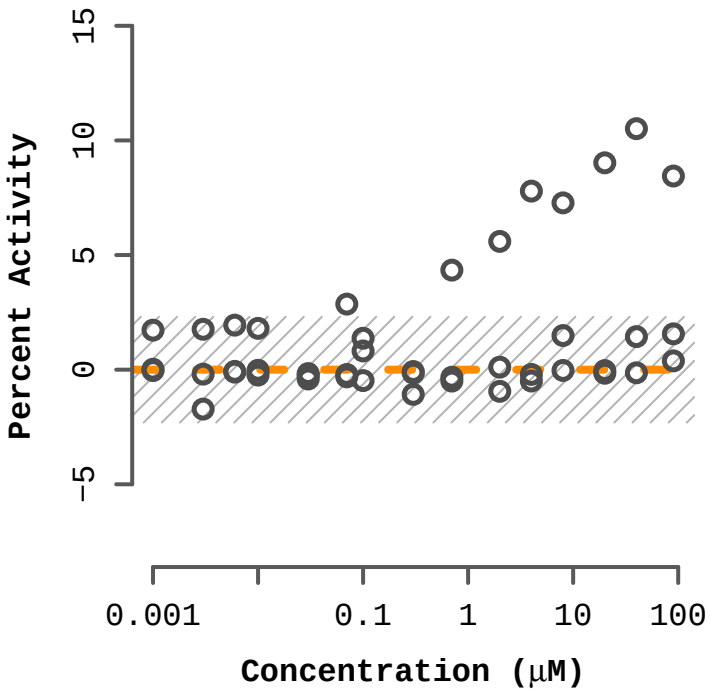
NAME: 2-Hydroxy-3-methylbenzoic acid
CHID: 38686 **CASRN:** 83-40-9
SPID(S): Tox21_111523_1
M4ID: 12483636

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.492 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

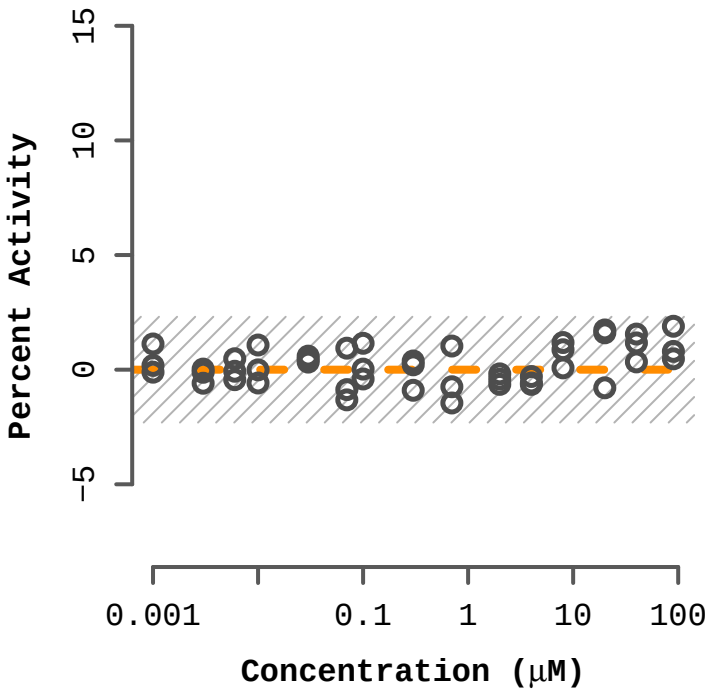
NAME: Isatin
CHID: 38694 CASRN: 91-56-5
SPID(S): Tox21_202876
M4ID: 12479376

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.69	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 3.94 MAX_MED: 1.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

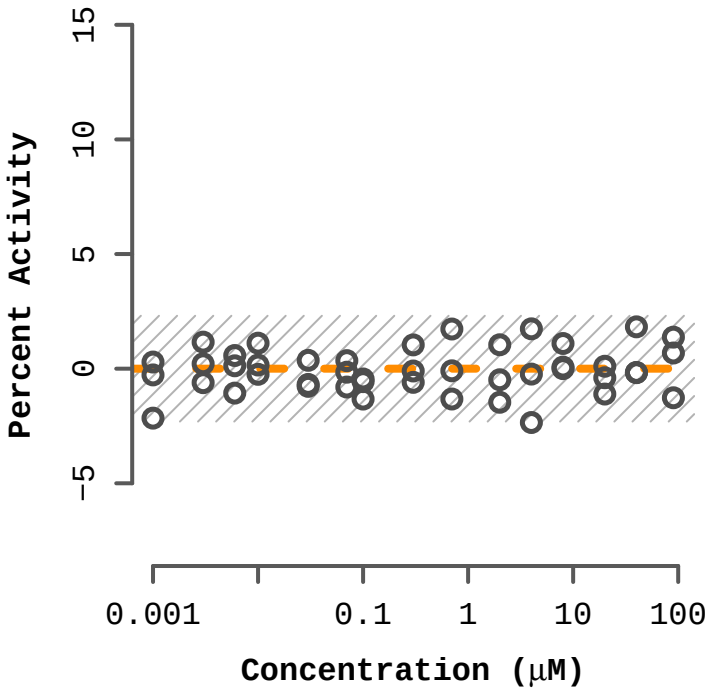
NAME: Ethyl benzoate
CHID: 38696 **CASRN:** 93-89-0
SPID(S): Tox21_302021
M4ID: 12477112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

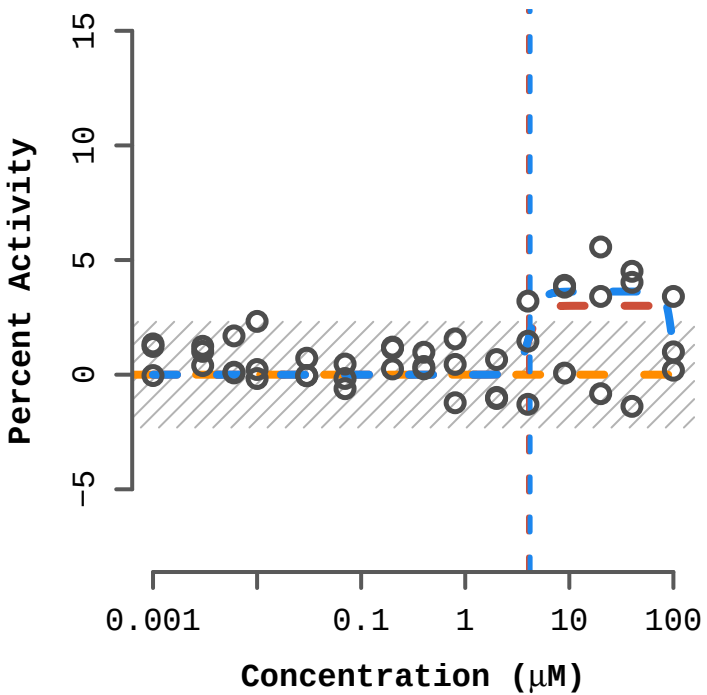
NAME: 2-Methoxy-4-nitroaniline
CHID: 38700 **CASRN:** 97-52-9
SPID(S): Tox21_302128
M4ID: 12477005

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.497 **MAX_MED:** 0.685 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Bromotetradecane
CHID: 38725 **CASRN:** 112-71-0
SPID(S): Tox21_202721
M4ID: 12479531

HILL MODEL (in red):

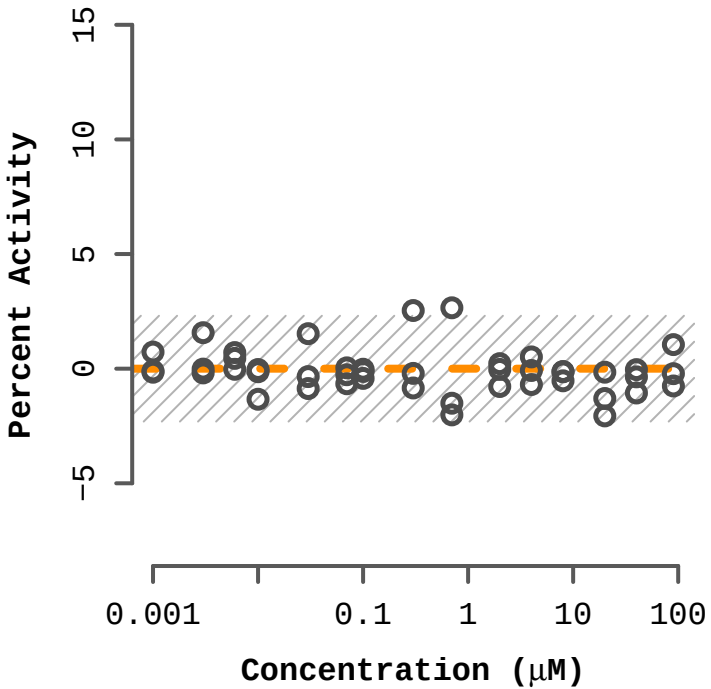
	tp	ga	gw
val:	3	0.608	8
sd:	0.569	0.075	12.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.63	0.623	8	1.98	15.4
sd:	0.48	0.0863	18.6	0.0461	36.6

	CNST	HILL	GNLS
AIC:	183.48	171.25	170.41
PROB:	0	0.4	0.6
RMSE:	1.91	1.51	1.53

MAX_MEAN: 2.72 **MAX_MED:** 4.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

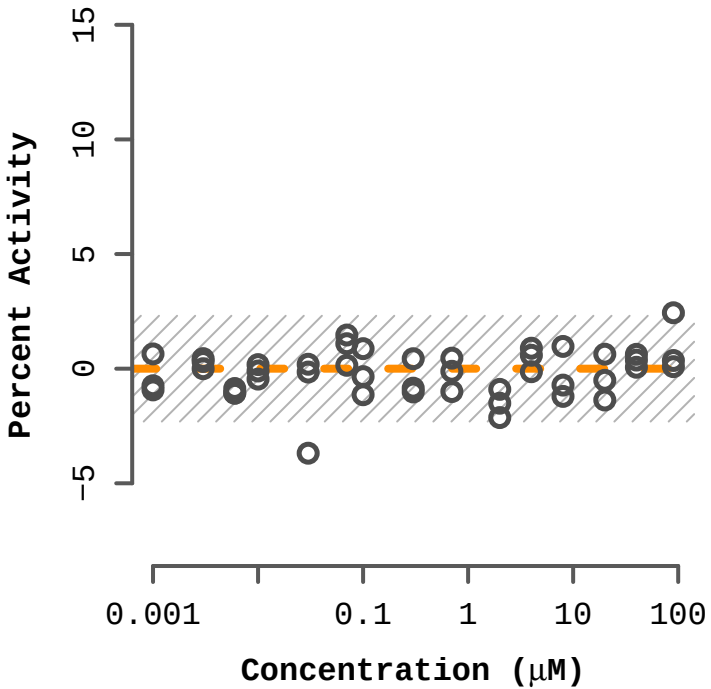
NAME: Diethyl butanedioate
CHID: 38732 CASRN: 123-25-1
SPID(S): Tox21_300286
M4ID: 12478844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.498 MAX_MED: 0.451 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

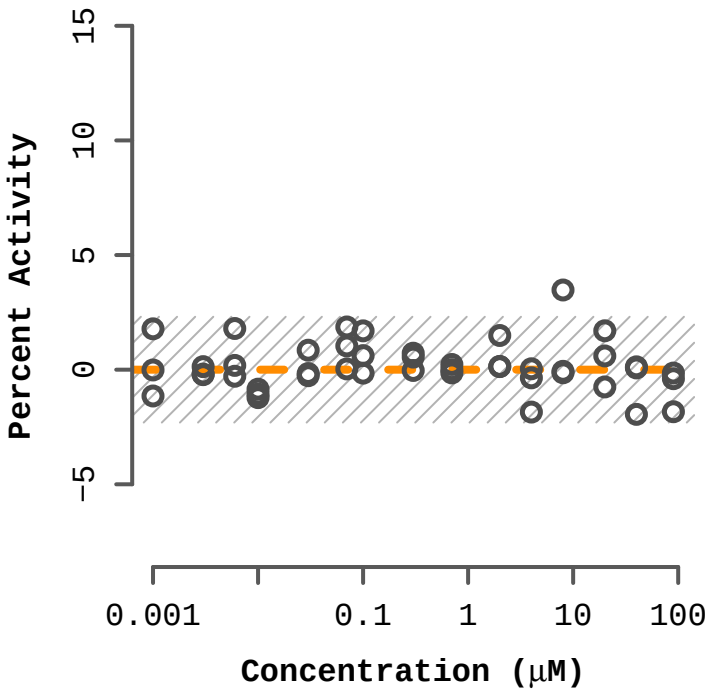
NAME: 5-Methyl-1H-benzotriazole
CHID: 38743 **CASRN:** 136-85-6
SPID(S): Tox21_303925
M4ID: 12475263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

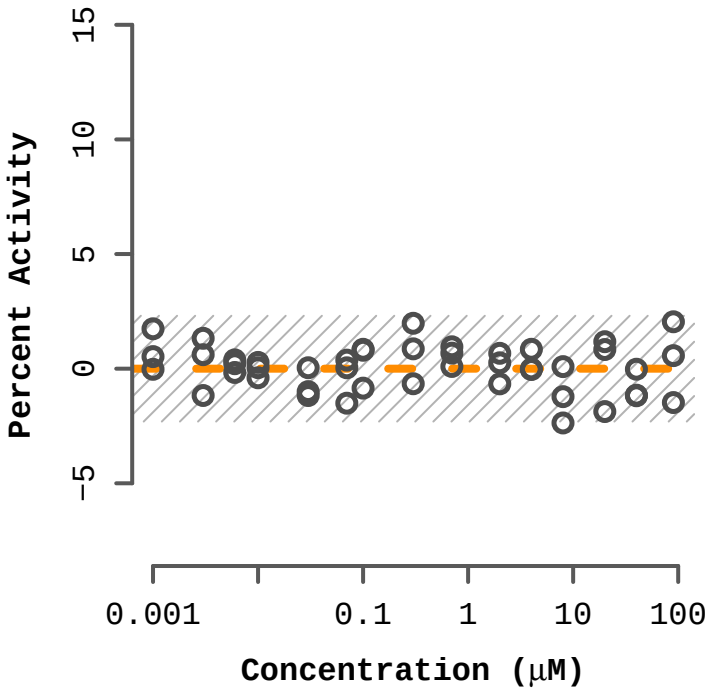
NAME: 4-Fluorobenzaldehyde
CHID: 38756 **CASRN:** 459-57-4
SPID(S): Tox21_302122
M4ID: 12477011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

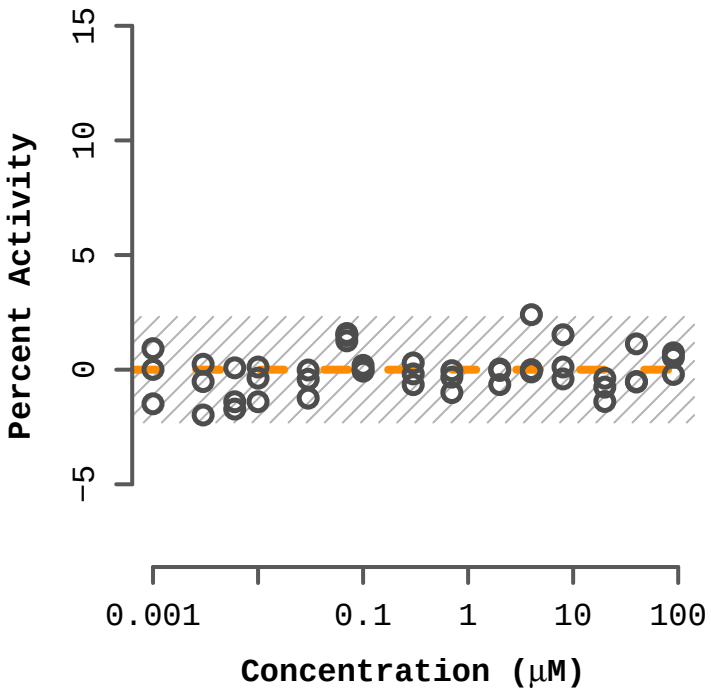
NAME: Thiamine nitrate
CHID: 38762 **CASRN:** 532-43-4
SPID(S): Tox21_302321
M4ID: 12476812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.748 **MAX_MED:** 0.867 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

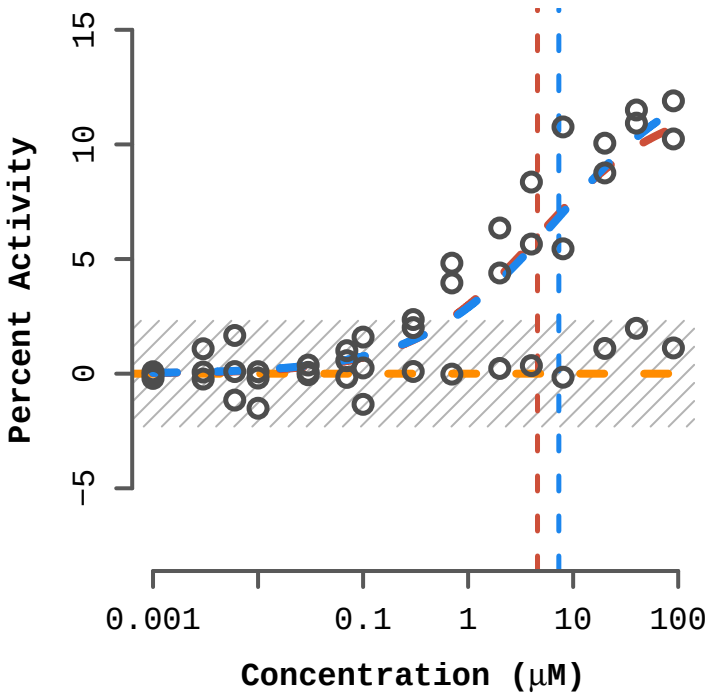
NAME: Zinc acetate
CHID: 38770 CASRN: 557-34-6
SPID(S): Tox21_302016
M4ID: 12477117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.44 MAX_MED: 1.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-Dimethylpentan-3-one
CHID: 38771 **CASRN:** 565-80-0
SPID(S): Tox21_303876
M4ID: 12475312

HILL MODEL (in red):

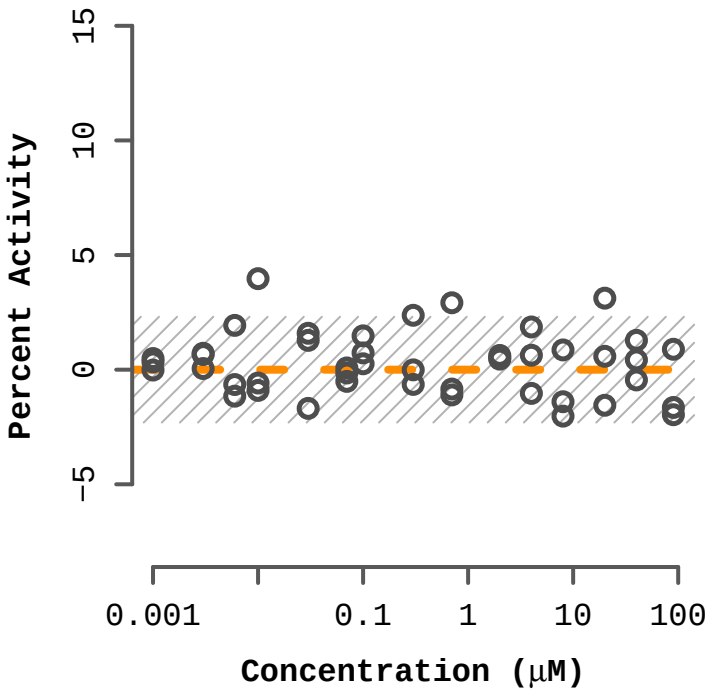
	tp	ga	gw
val:	12	0.66	0.723
sd:	2.23	0.356	0.199

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.6	0.864	0.661	2.01	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	264.31	216.01	219.81
PROB:	0	0.87	0.13
RMSE:	4.84	2.9	2.9

MAX_MEAN: 8.14 **MAX_MED:** 10.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

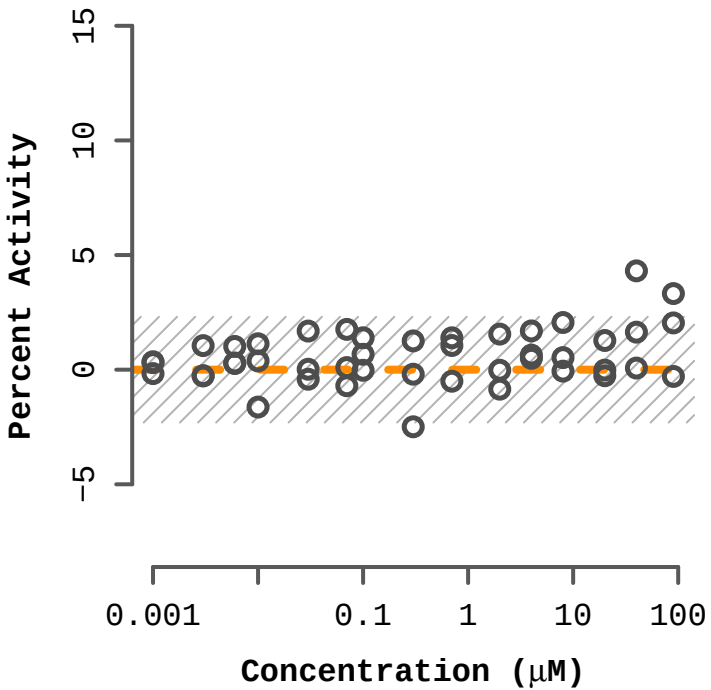
NAME: 1,4-Cyclohexanedicarboxylic acid
CHID: 38788 **CASRN:** 1076-97-7
SPID(S): Tox21_300649
M4ID: 12478484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.829 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

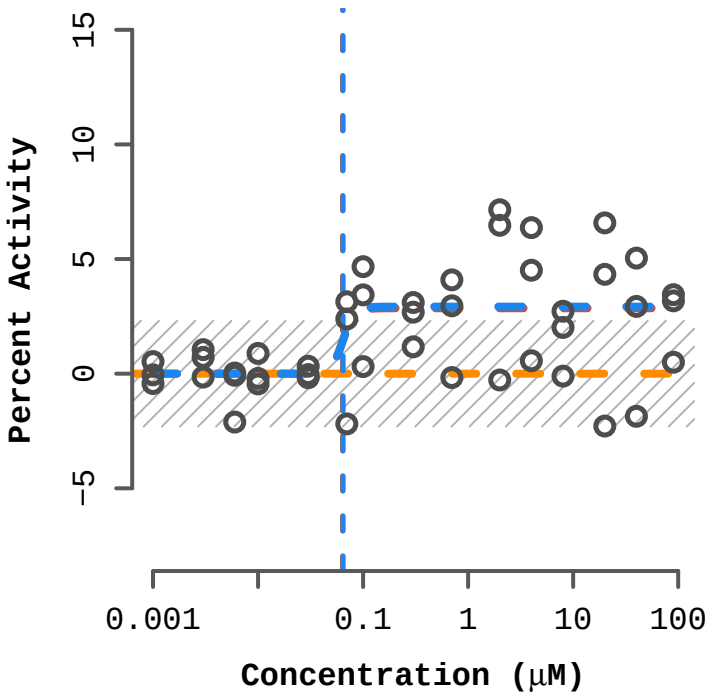
NAME: 1,1,1,3,5,5,5-Heptamethyltrisiloxane
CHID: 38795 **CASRN:** 1873-88-7
SPID(S): Tox21_301069
M4ID: 12478064

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2−Diethoxybenzene
CHID: 38798 CASRN: 2050−46−6
SPID(S): Tox21_302095
M4ID: 12477038

HILL MODEL (in red):

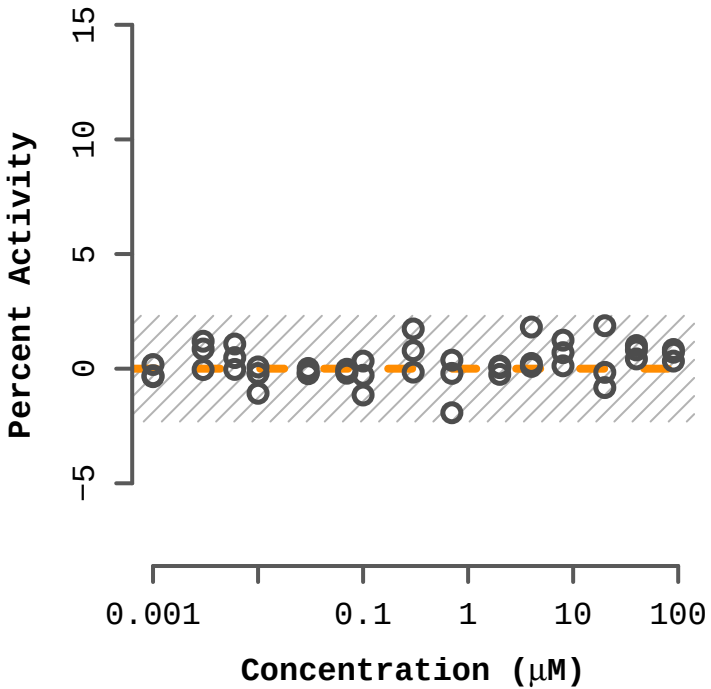
	tp	ga	gw
val:	2.85	−1.2	8
sd:	0.433	0.17	21.3

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.92	−1.19	8	2.02	12.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	228.46	201.75	205.63
PROB:	0	0.87	0.13
RMSE:	2.98	2.09	2.09

MAX_MEAN: 4.45 MAX_MED: 6.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

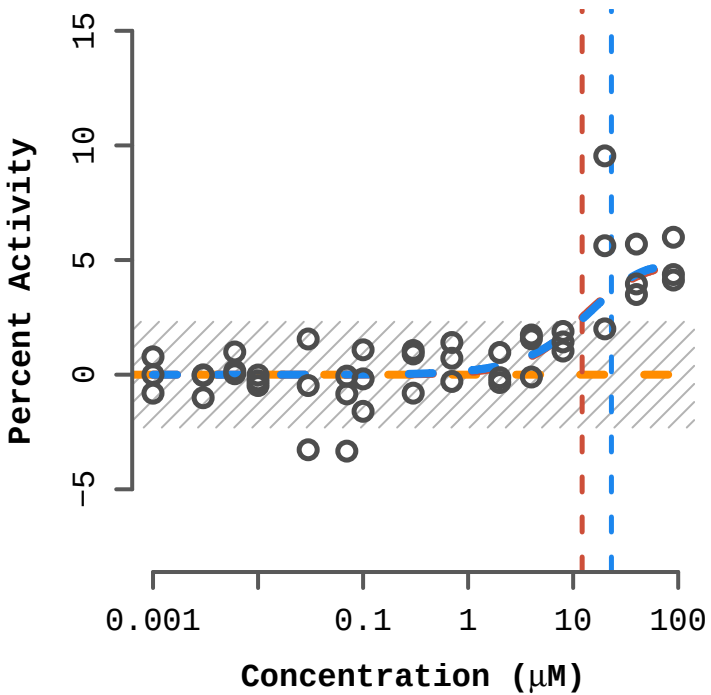
NAME: Butyl 4-oxopentanoate
CHID: 38800 CASRN: 2052-15-5
SPID(S): Tox21_301714
M4ID: 12477419

HILL MODEL: Not applicable.

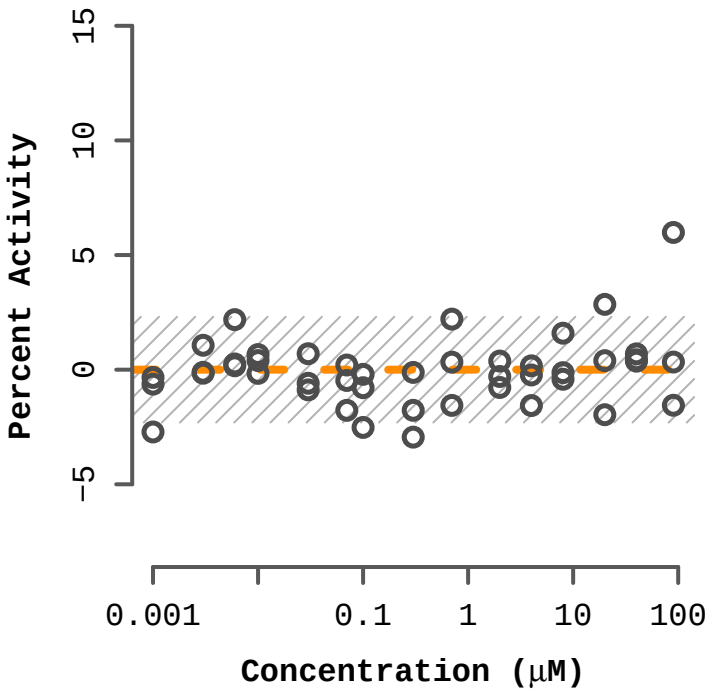
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.791 **MAX_MED:** 0.857 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Benzyl-9-(tetrahydro-2H-pyran-2-yl)adenine
CHID:    38801   CASRN: 2312-73-4
SPID(S): Tox21_301613
M4ID:    12477520

HILL MODEL (in red):
      tp       ga       gw
val:  5        1.09     1.5
sd:   1.03     0.237    0.961

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.1     1.36     1.26     2.11     0.533
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  206.34      153.08      156.95
PROB: 0           0.87        0.13
RMSE: 2.63        1.42        1.43

MAX_MEAN: 5.72      MAX_MED: 5.63      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

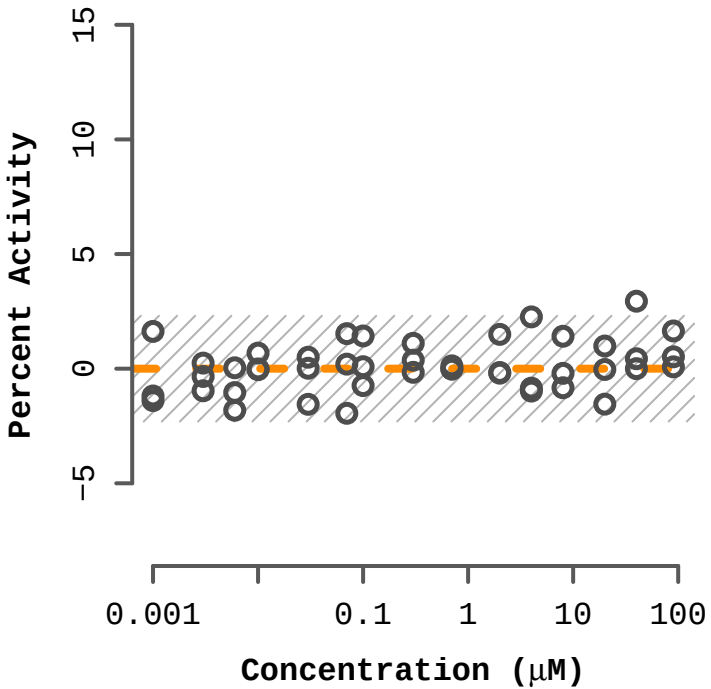
NAME: 1,3,5,7-Tetramethyl-1,3,5,7-tetravinylcyclotet
CHID: 38808 CASRN: 2554-06-5
SPID(S): Tox21_301527
M4ID: 12477606

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.59 MAX_MED: 0.433 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

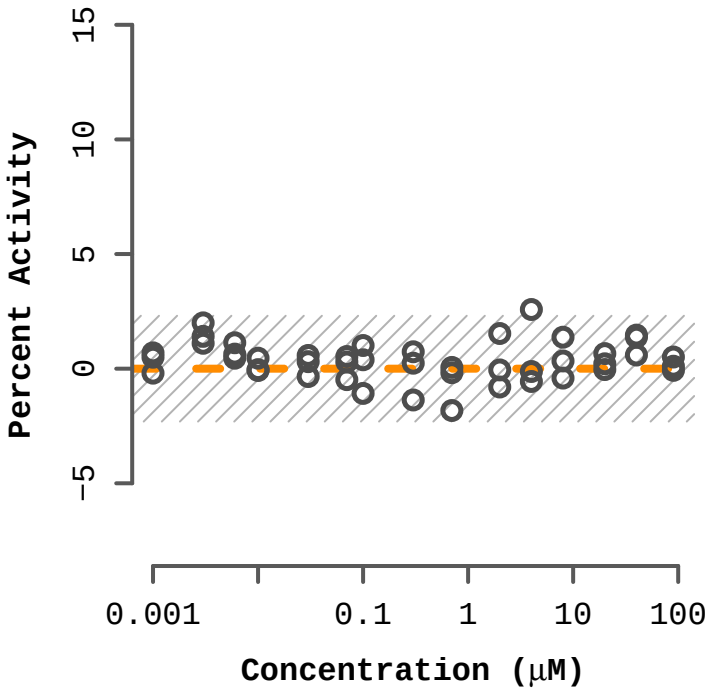
NAME: 1,3-Divinyl-1,1,3,3-tetramethyl disiloxane
CHID: 38810 **CASRN:** 2627-95-4
SPID(S): Tox21_301726
M4ID: 12477407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.519 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

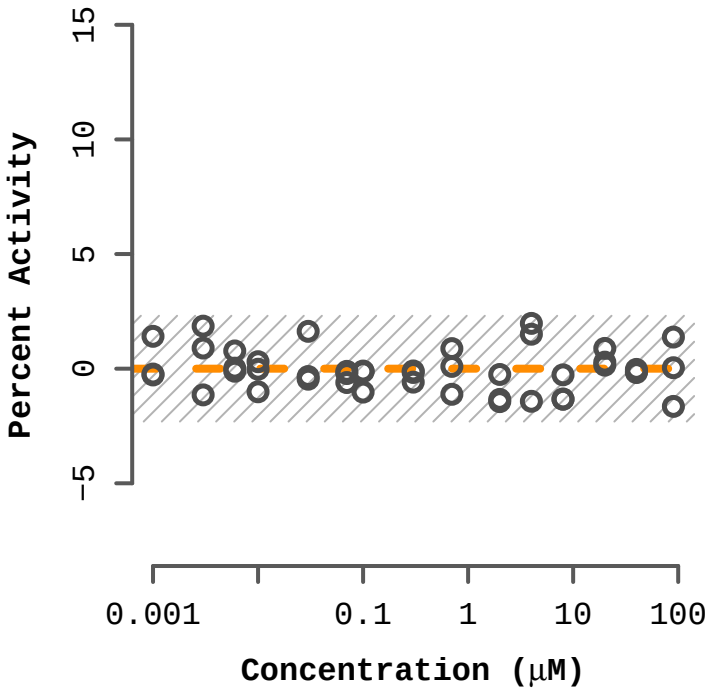
NAME: 1,3−Benzenedicarboxylic acid, dihydrazide
CHID: 38813 CASRN: 2760−98−7
SPID(S): Tox21_301460
M4ID: 12477673

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.51 MAX_MED: 1.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

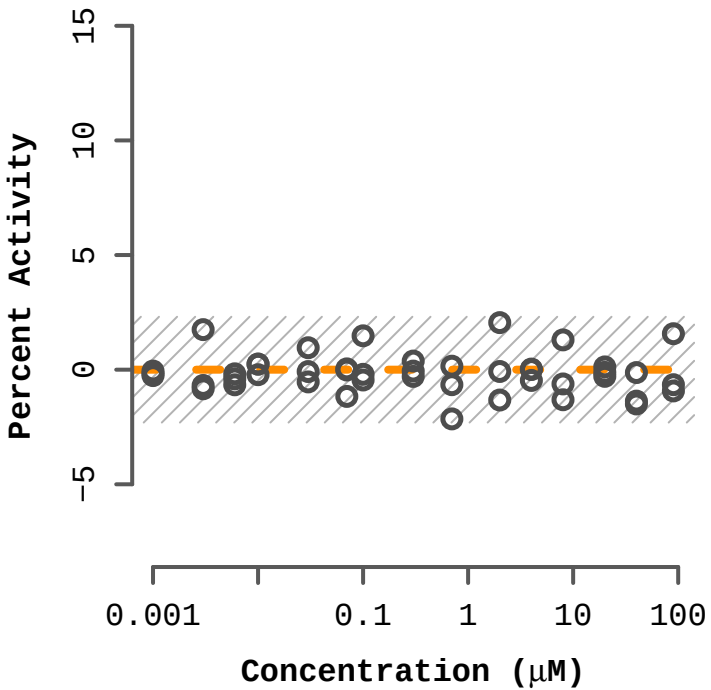
NAME: 4-Aminobenzamide
CHID: 38814 **CASRN:** 2835-68-9
SPID(S): Tox21_301656
M4ID: 12477477

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

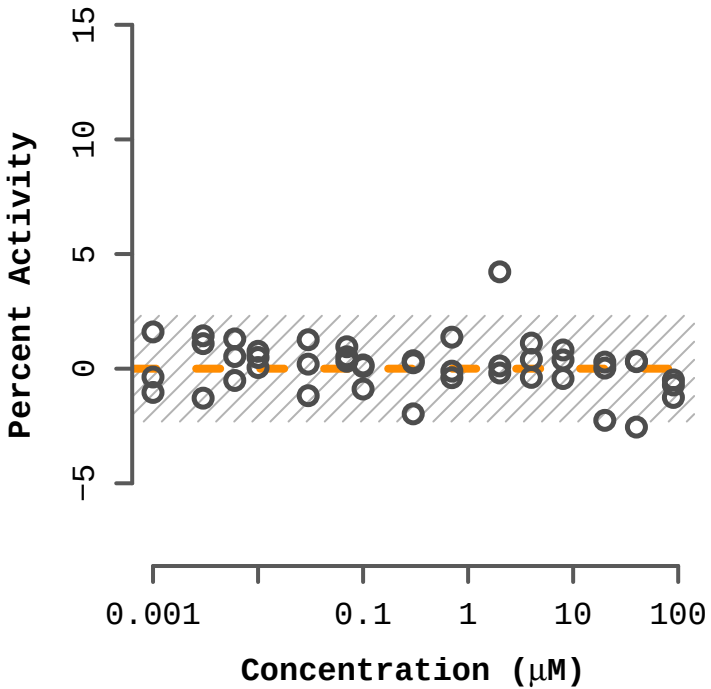
NAME: 7-Methoxy-3,7-dimethyloctanal
CHID: 38818 **CASRN:** 3613-30-7
SPID(S): Tox21_301955
M4ID: 12477178

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.277 **MAX_MED:** 0.244 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

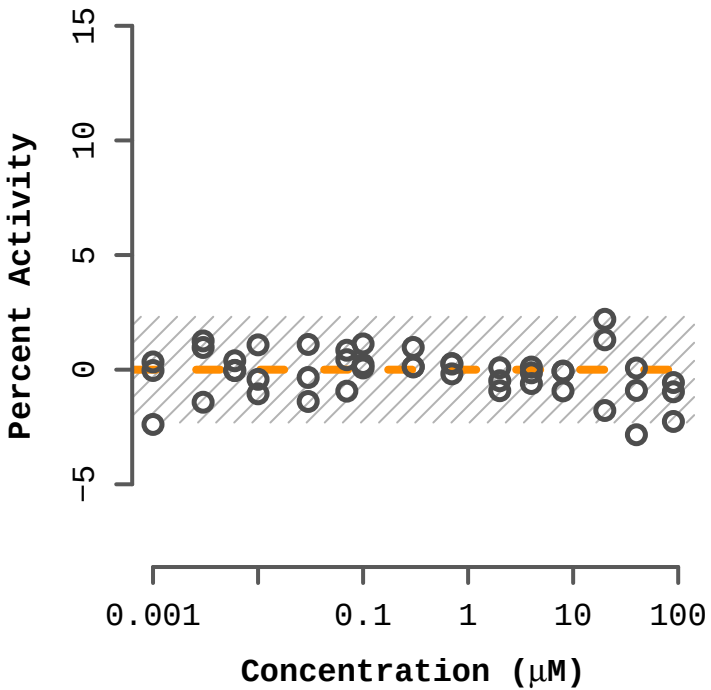
NAME: Neopentyl glycol dibenzoate
CHID: 38822 **CASRN:** 4196-89-8
SPID(S): Tox21_301517
M4ID: 12477616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

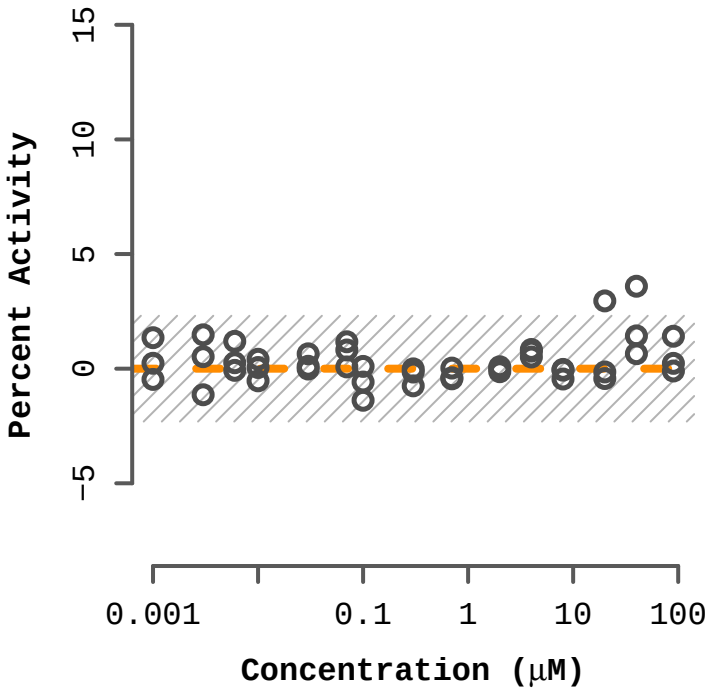
NAME: 1,4-Dioxane-2,3-diol
CHID: 38824 **CASRN:** 4845-50-5
SPID(S): Tox21_301406
M4ID: 12477727

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

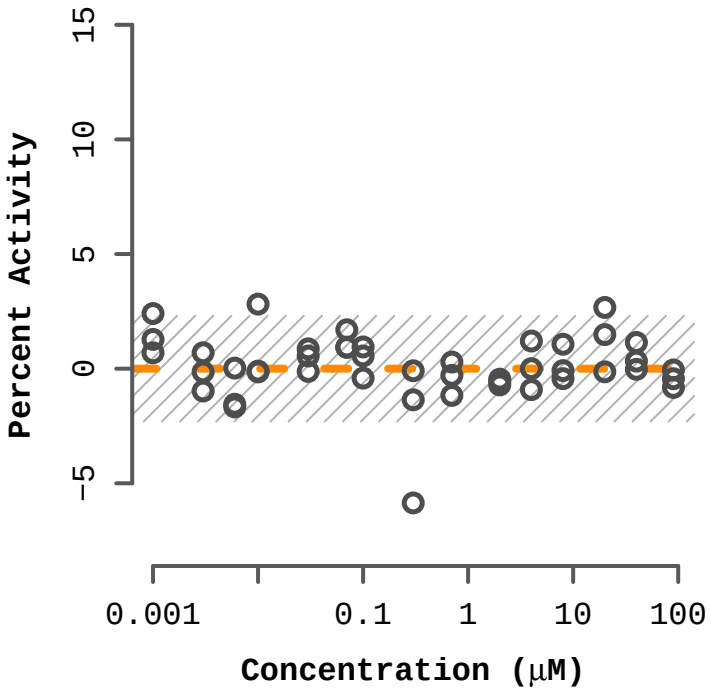
NAME: 2-Chloro-5-nitroaniline
CHID: 38827 **CASRN:** 6283-25-6
SPID(S): Tox21_303861
M4ID: 12475327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

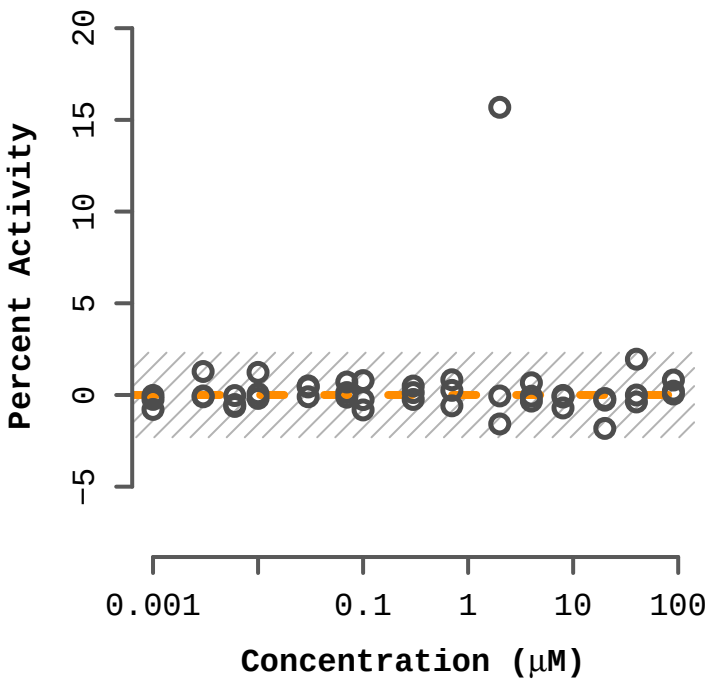
NAME: 1,1-Dimethyl-2-phenylethyl butanoate
CHID: 38830 **CASRN:** 10094-34-5
SPID(S): Tox21_300643
M4ID: 12478490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

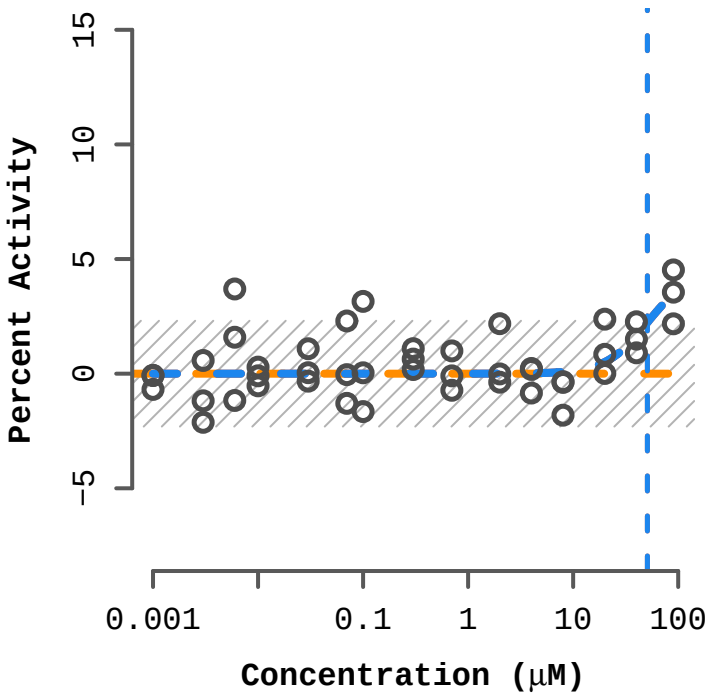
NAME: 2-Methoxyethyl cyanoacetate
CHID: 38831 CASRN: 10258-54-5
SPID(S): Tox21_300797
M4ID: 12478336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.89	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 4.69 MAX_MED: 0.439 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-5-nitrobenzonitrile
CHID: 38839 **CASRN:** 17420-30-3
SPID(S): Tox21_304032
M4ID: 12475156

HILL MODEL (in red):

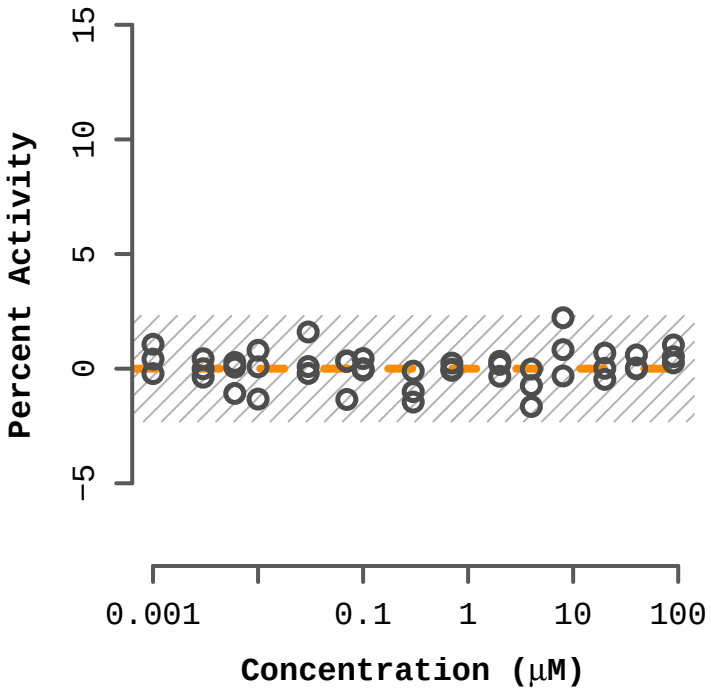
	tp	ga	gw
val:	4.45	1.71	2.19
sd:	2.68	0.312	1.49

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.45	1.71	2.19	3.18	5.84
sd:	2.68	0.312	1.49	1840	8830

	CNST	HILL	GNLS
AIC:	167.84	149.89	153.89
PROB:	0	0.88	0.12
RMSE:	1.57	1.21	1.21

MAX_MEAN: 3.42 **MAX_MED:** 3.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

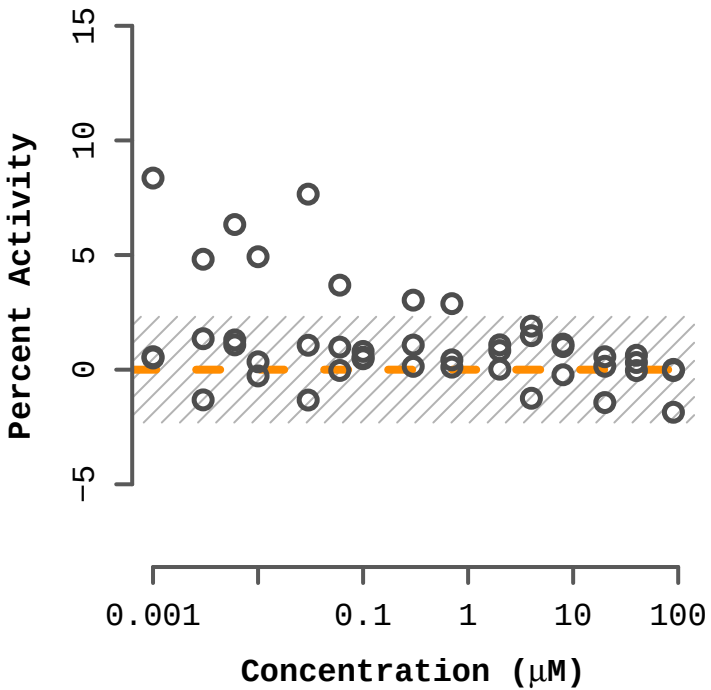
NAME: 3-Isocyanatopropyltriethoxysilane
CHID: 38847 CASRN: 24801-88-5
SPID(S): Tox21_302179
M4ID: 12476954

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.913 MAX_MED: 0.831 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

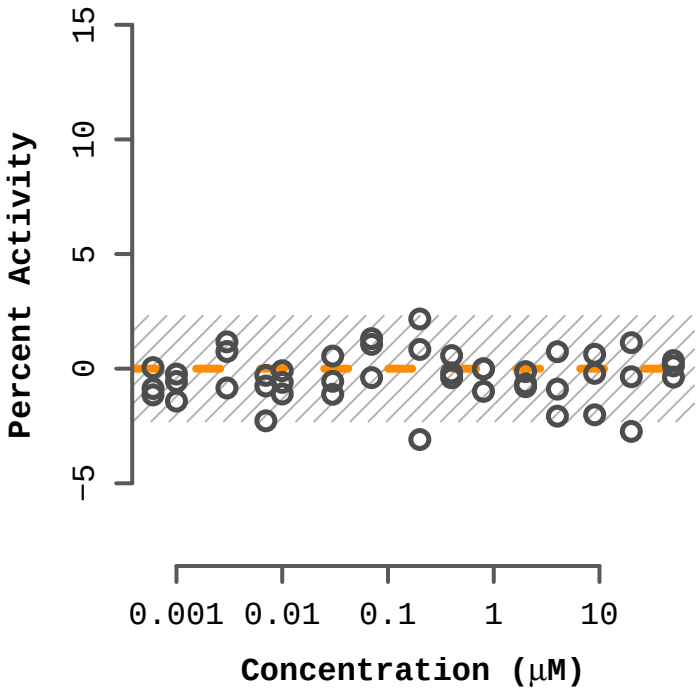
NAME: Ensulizole
CHID: 38852 **CASRN:** 27503-81-7
SPID(S): Tox21_200995
M4ID: 12481257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 3.15 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

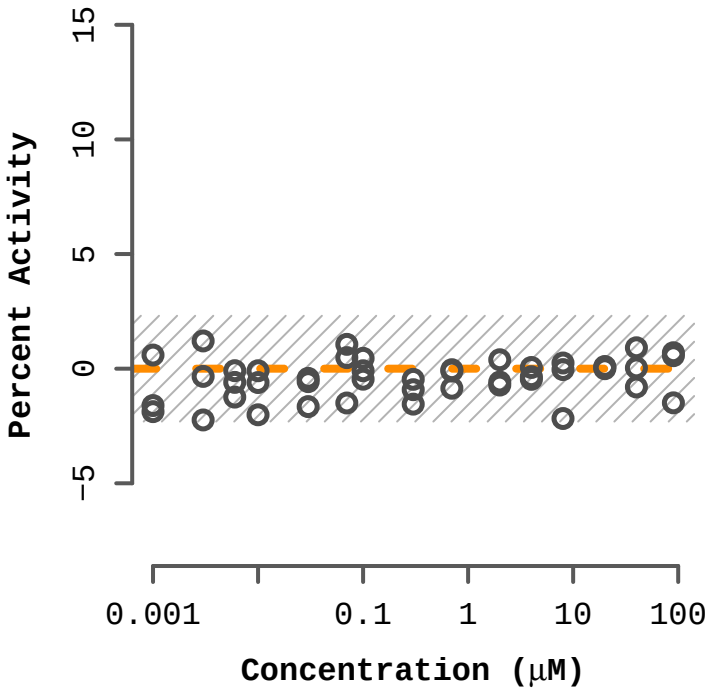
NAME: Ensulizole
CHID: 38852 **CASRN:** 27503-81-7
SPID(S): Tox21_112381_1
M4ID: 12483124

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.662 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

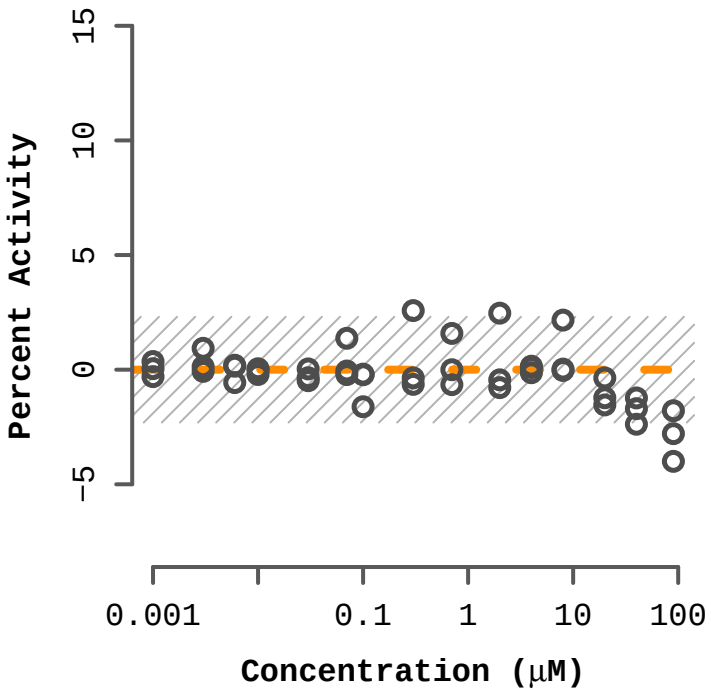
NAME: 1-Chloro-2-(chloromethyl)-3-fluorobenzene
CHID: 38855 **CASRN:** 55117-15-2
SPID(S): Tox21_301630
M4ID: 12477503

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.0528 **MAX_MED:** 0.568 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

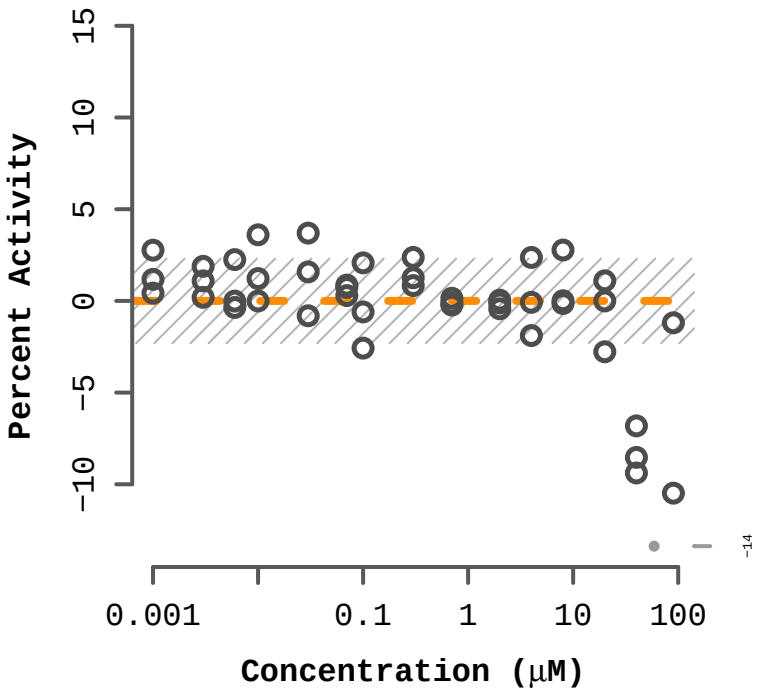
NAME: 2-Methyl-4'-(methylthio)-2-morpholinopropiophe
CHID: 38857 **CASRN:** 71868-10-5
SPID(S): Tox21_301664
M4ID: 12477469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.719 **MAX_MED:** 0.153 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

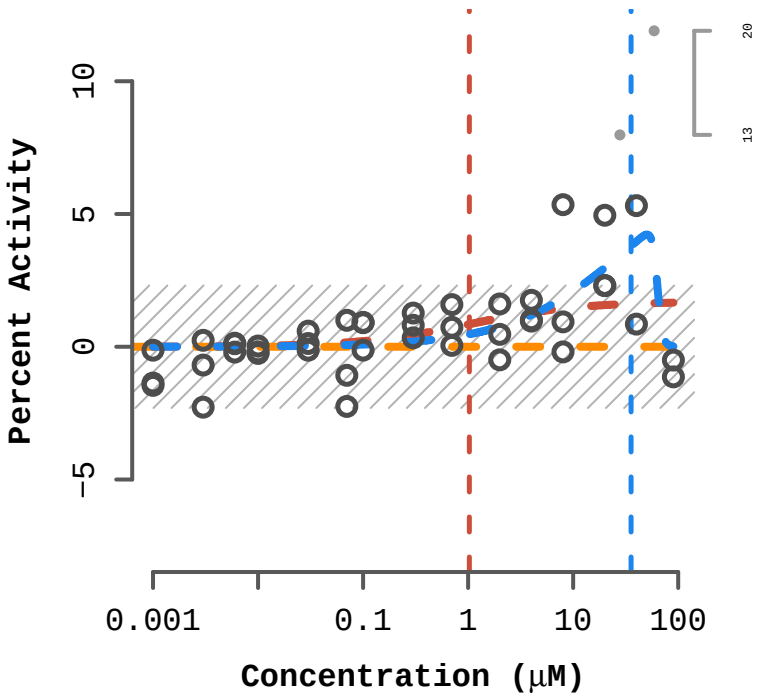
NAME: 2,2'-Methylenebis(ethyl-6-tert-butylphenol)
CHID: 38864 **CASRN:** 88-24-4
SPID(S): Tox21_303358
M4ID: 12475776 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.08	NA	NA
PROB:	1	NA	NA
RMSE:	3.68	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'−Dihydroxy−4,4'−dimethoxybenzophenone
CHID: 38875 CASRN: 131−54−4
SPID(S): Tox21_200543
M4ID: 12481709 BRK

HILL MODEL (in red):

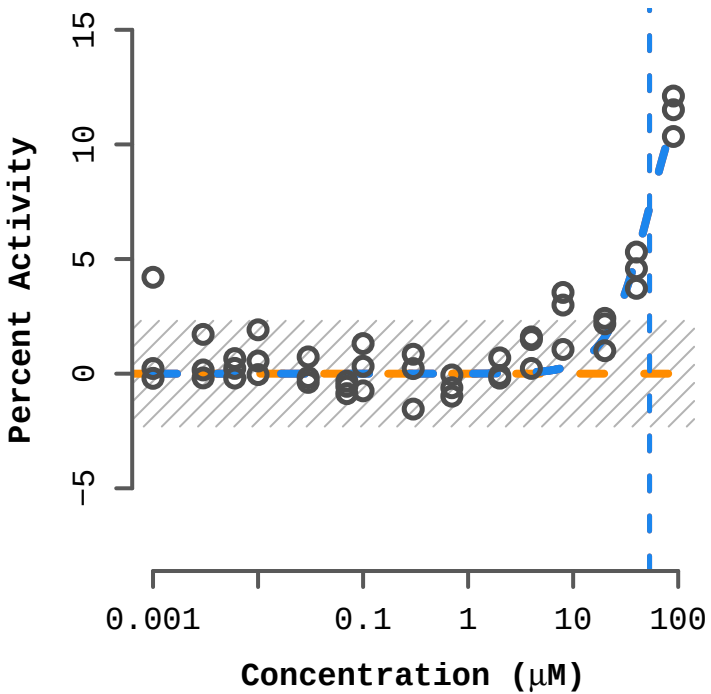
	tp	ga	gw
val:	1.7	0.0114	0.838
sd:	0.945	0.927	0.534

GAIN−LOSS MODEL (in blue):

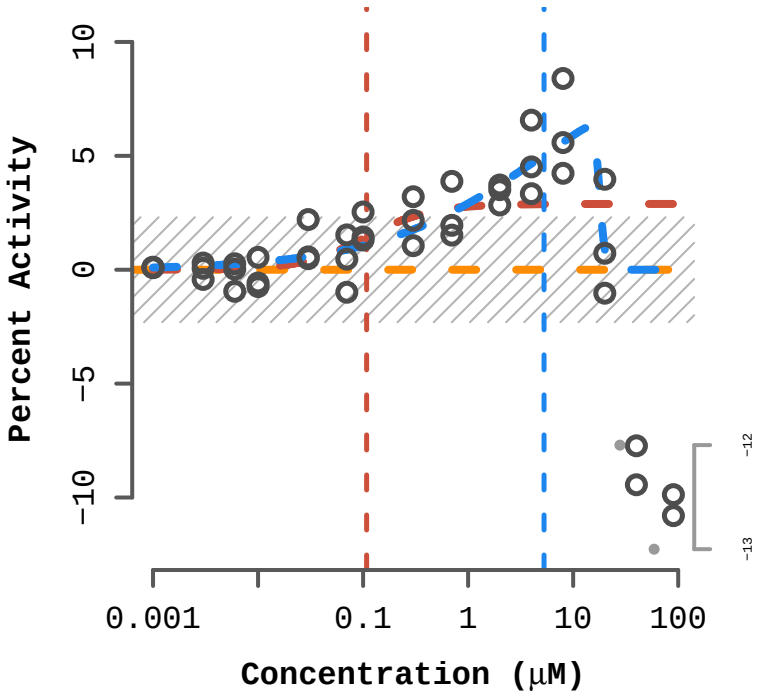
	tp	ga	gw	la	lw
val:	7.6	1.55	0.766	1.8	17.5
sd:	9.85	1.14	0.345	0.303	34.2

	CNST	HILL	GNLS
AIC:	203.74	195.73	189.4
PROB:	0	0.04	0.96
RMSE:	4.02	3.57	3.55

MAX_MEAN: 6.5 MAX_MED: 5.32 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenyl 1-hydroxy-2-naphthoate
CHID:    38876   CASRN: 132-54-7
SPID(S): Tox21_301650
M4ID:    12477483

HILL MODEL (in red):
      tp       ga       gw
val:  14.5     1.73     2.13
sd:   2.42     0.0838   0.515

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  14.5     1.73     2.13     3.65     5.17
sd:   2.42     0.0838   0.515    1630     5000

      CNST        HILL        GNLS
AIC:  215.03      143.3       147.3
PROB: 0           0.88        0.12
RMSE: 3.41        1.19        1.19

MAX_MEAN: 11.3      MAX_MED: 11.5      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Hydroxy-2-naphthoic o-anisidide
CHID: 38877 CASRN: 135-62-6
SPID(S): Tox21_301992
M4ID: 12477141 BRK

HILL MODEL (in red):

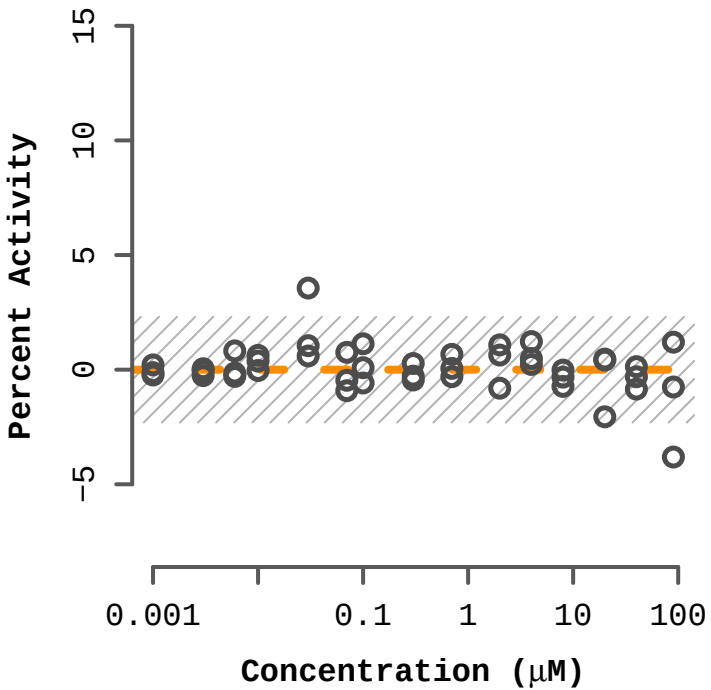
	tp	ga	gw
val:	2.89	-0.966	1.42
sd:	0.735	0.373	1.11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.1	0.723	0.541	1.25	16.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	262.54	255.66	235.7
PROB:	0	0	1
RMSE:	4.69	5.15	4.03

MAX_MEAN: 6.07 MAX_MED: 5.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

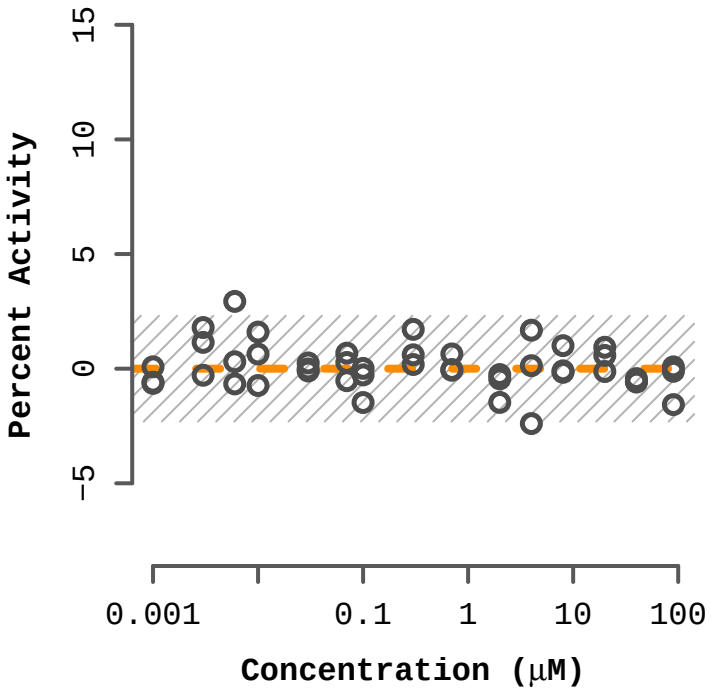
NAME: C.I. Acid Orange 7
CHID: 38881 CASRN: 633-96-5
SPID(S): Tox21_302088
M4ID: 12477045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

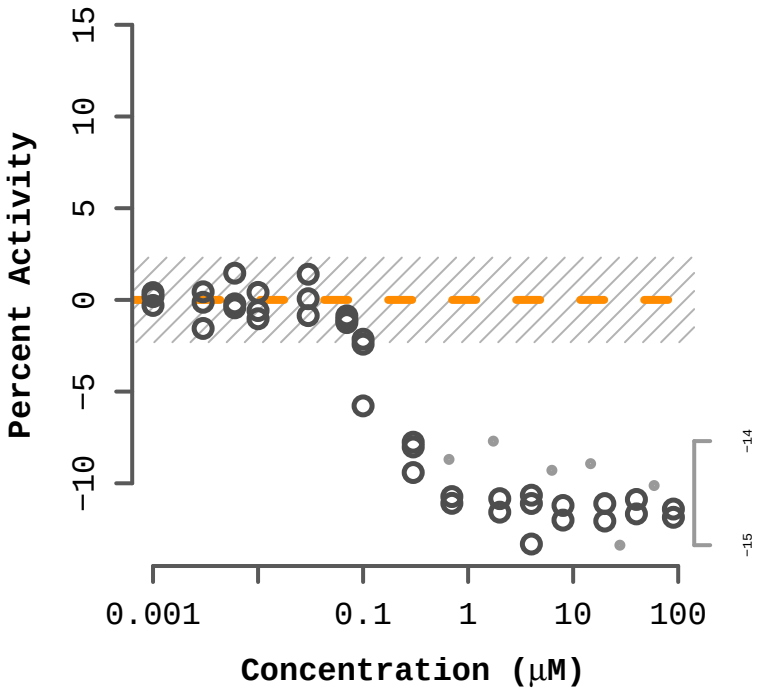
NAME: Fluorescein
CHID: 38887 **CASRN:** 2321-07-5
SPID(S): Tox21_303508
M4ID: 12475634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.886 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

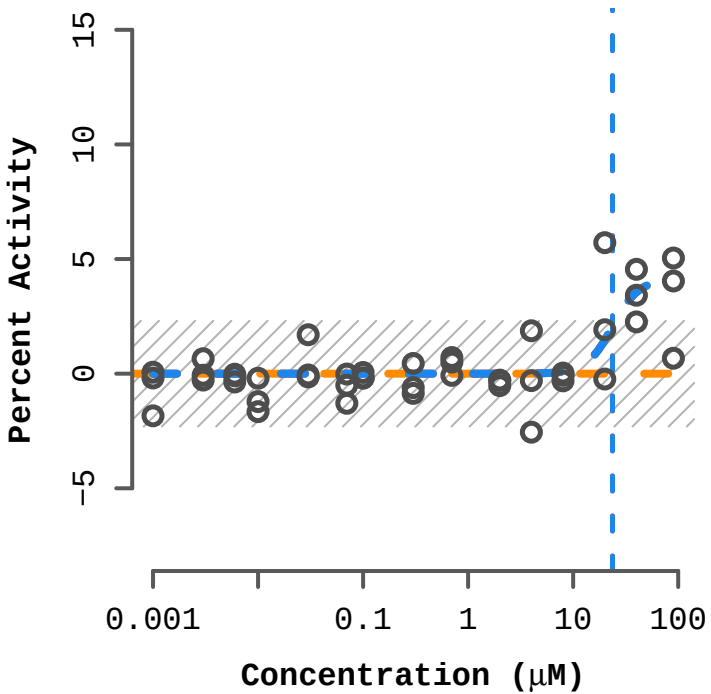
NAME: Basic Blue 7
CHID: 38888 CASRN: 2390-60-5
SPID(S): Tox21_301536
M4ID: 12477597 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	330.33	NA	NA
PROB:	1	NA	NA
RMSE:	8.74	NA	NA

MAX_MEAN: 0.272 **MAX_MED:** 0.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetrabutyl ethylidenebisphenol
CHID: 38899 CASRN: 35958-30-6
SPID(S): Tox21_303979
M4ID: 12475209

HILL MODEL (in red):

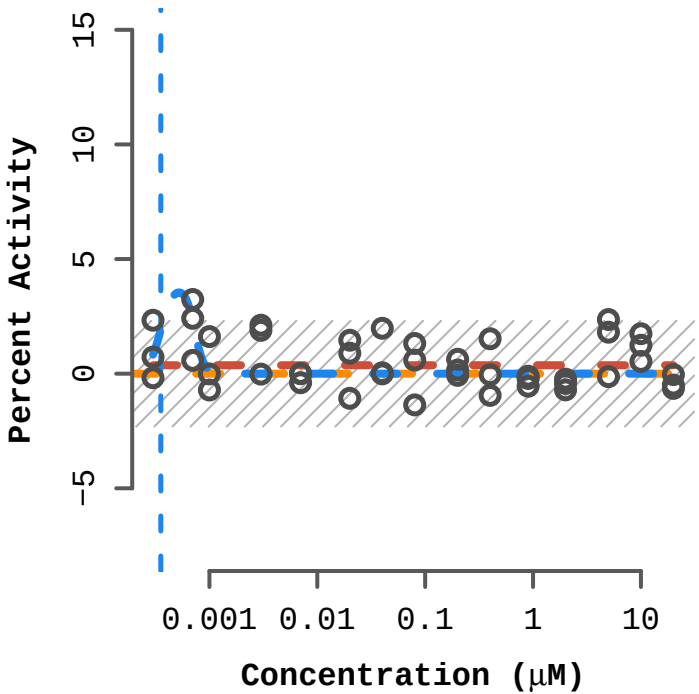
	tp	ga	gw
val:	4.11	1.37	3.51
sd:	0.725	0.128	2.01

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.11	1.37	3.51	3.17	8.74
sd:	0.725	0.128	2.01	32900	236000

	CNST	HILL	GNLS
AIC:	167.58	138.84	142.84
PROB:	0	0.88	0.12
RMSE:	1.78	1.18	1.18

MAX_MEAN: 3.41 **MAX_MED:** 4.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3-Bis(isocyanatomethyl)benzene
CHID: 38919 **CASRN:** 3634-83-1
SPID(S): Tox21_303869
M4ID: 12475319

HILL MODEL (in red):

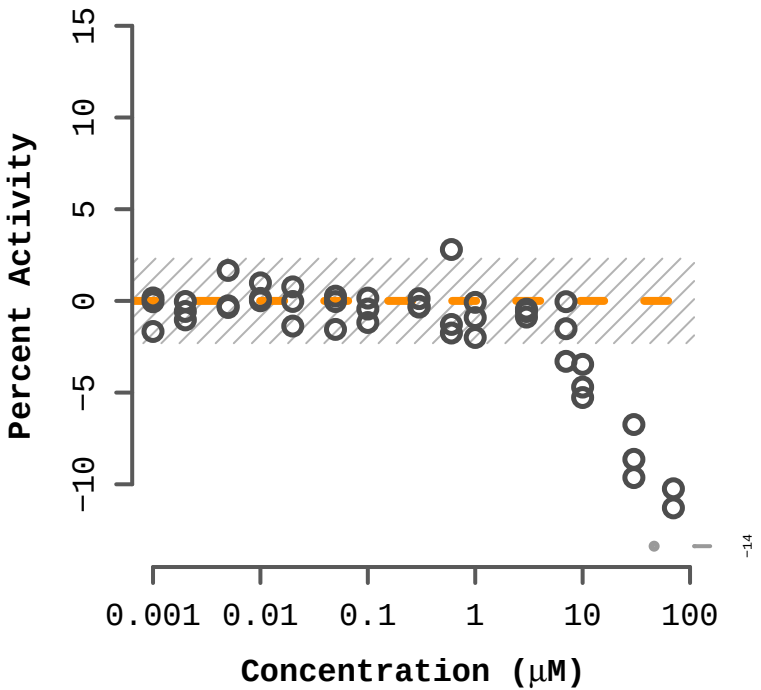
	tp	ga	gw
val:	0.369	−5.42	3.64
sd:	0.171	1450	2730

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.85	−3.45	7.77	−3.14	10
sd:	32.8	0.316	41.8	0.861	58

	CNST	HILL	GNLS
AIC:	146.61	147.74	146.47
PROB:	0.38	0.22	0.41
RMSE:	1.2	1.1	1.05

MAX_MEAN: 2.08 **MAX_MED:** 2.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

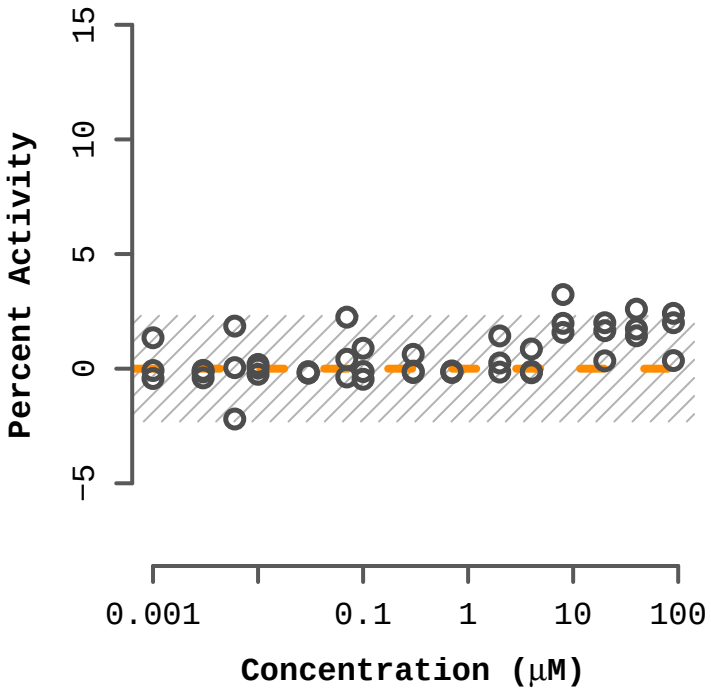
NAME: Tetrabromobisphenol A bis(2-hydroxyethyl) ether
CHID: 38922 **CASRN:** 4162-45-2
SPID(S): Tox21_301731
M4ID: 12477402 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	236.44	NA	NA
PROB:	1	NA	NA
RMSE:	4.07	NA	NA

MAX_MEAN: 0.378 **MAX_MED:** 0.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

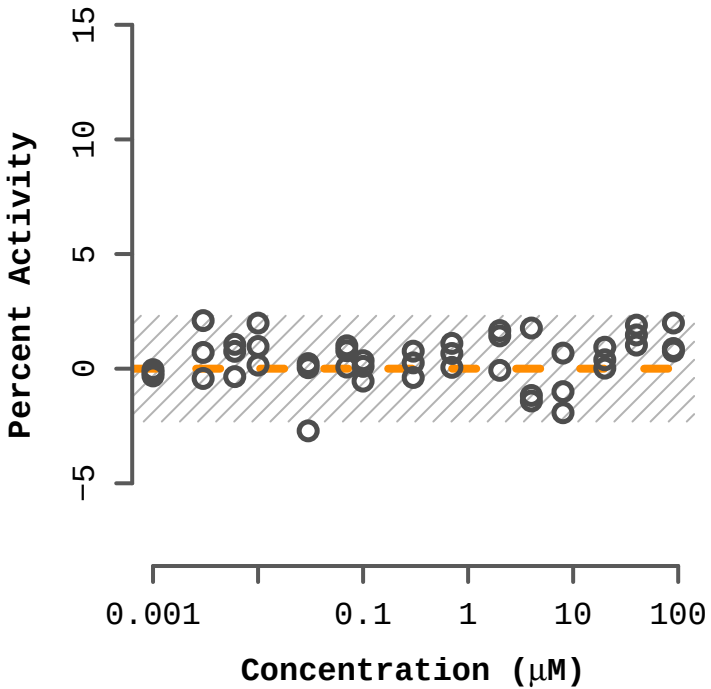
NAME: Hexyl salicylate
CHID: 38924 **CASRN:** 6259-76-3
SPID(S): Tox21_301381
M4ID: 12477752

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.27 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

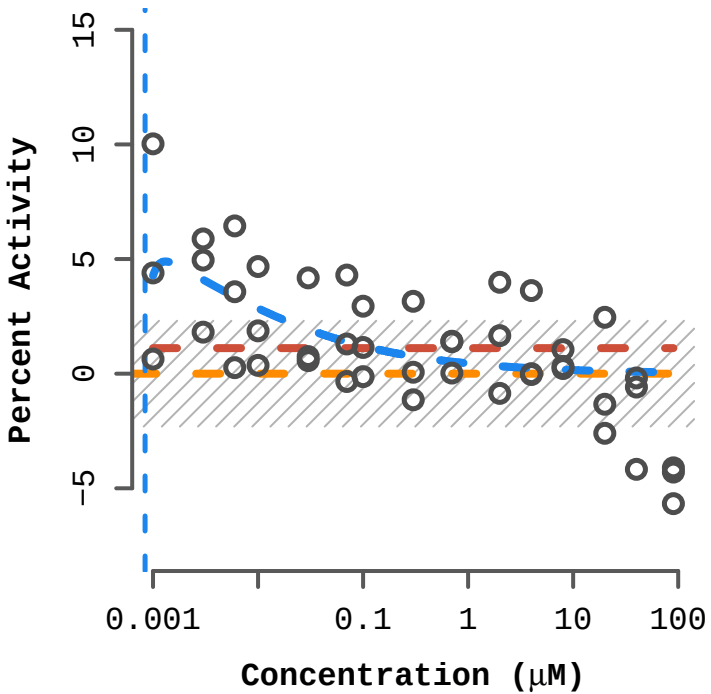
NAME: Dibenzyl oxalate
CHID: 38926 **CASRN:** 7579-36-4
SPID(S): Tox21_301279
M4ID: 12477854

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PFOSA
CHID: 38939 CASRN: 754-91-6
SPID(S): Tox21_300412
M4ID: 12478720

HILL MODEL (in red):

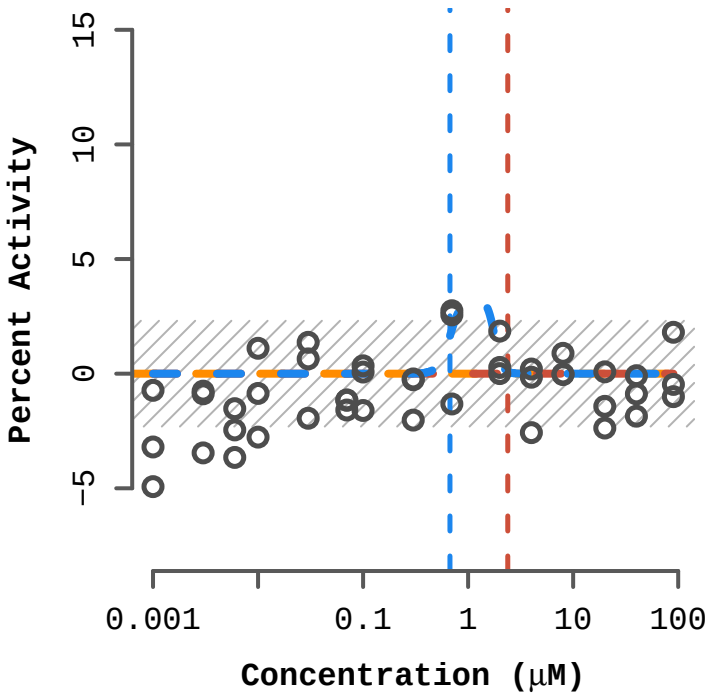
	tp	ga	gw
val:	1.11	−4.71	4.26
sd:	0.402	1310	3250

GAIN-LOSS MODEL (in blue):

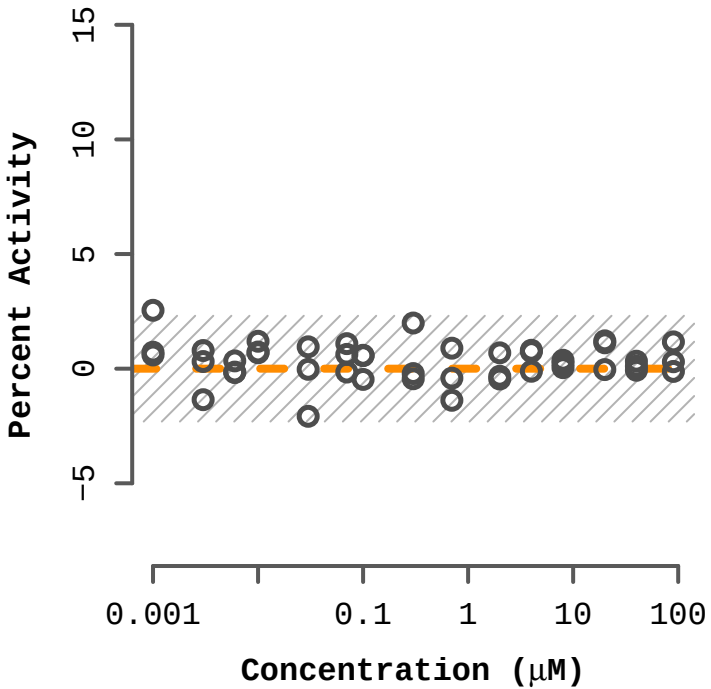
	tp	ga	gw	la	lw
val:	9.78	−3.08	7.94	−2.83	0.467
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	233.62	232.29	219.37
PROB:	0	0	1
RMSE:	3.2	2.96	2.37

MAX_MEAN: 5.02 MAX_MED: 4.96 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Aldicarb
CHID:    39223   CASRN: 116-06-3
SPID(S): Tox21_300846
M4ID:    12478287

HILL MODEL (in red):
      tp        ga        gw
val:  1.02e-10  0.377     1.72
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.3       -0.173    8         0.252     12.1
sd:   18.2      0.697     17.6      0.497     105

      CNST         HILL         GNLS
AIC:  182.62       188.62       189.5
PROB: 0.92         0.05         0.03
RMSE: 1.77         1.77         1.73

MAX_MEAN: 1.33      MAX_MED: 2.57      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

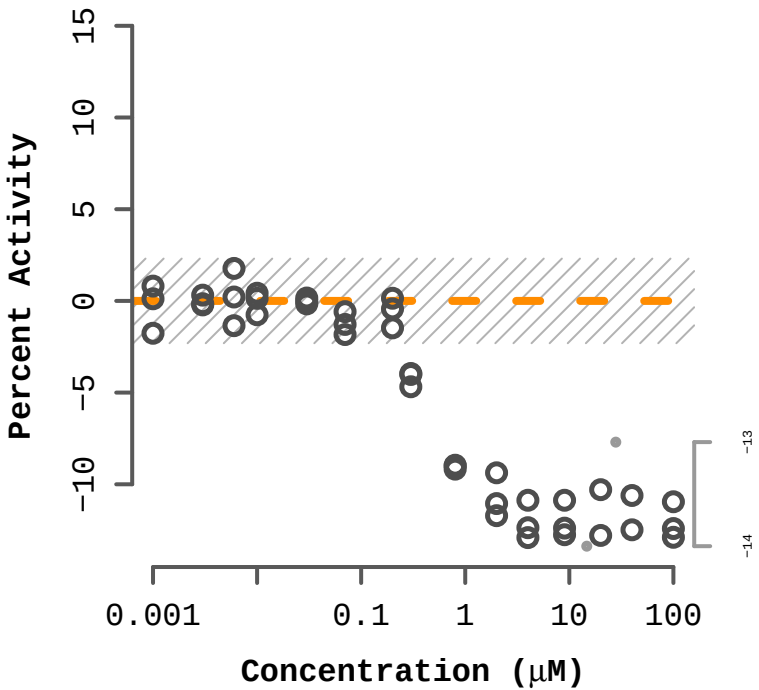
NAME: Aldicarb
CHID: 39223 **CASRN:** 116-06-3
SPID(S): Tox21_202227
M4ID: 12480025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

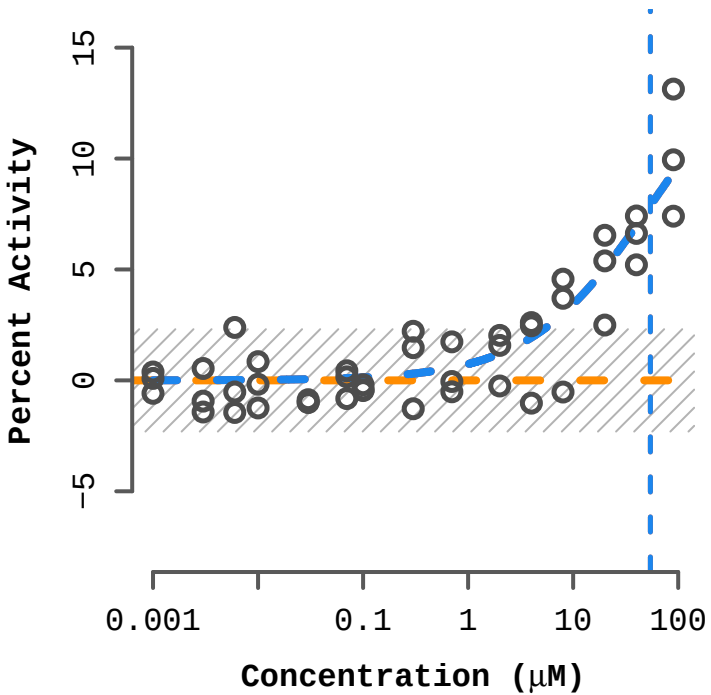
NAME: Acetaldehyde
CHID: 39224 **CASRN:** 75-07-0
SPID(S): Tox21_202479
M4ID: 12479773 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	321.34	NA	NA
PROB:	1	NA	NA
RMSE:	8.01	NA	NA

MAX_MEAN: 0.213 **MAX_MED:** 0.214 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Acetylaminofluorene
CHID: 39227 CASRN: 53-96-3
SPID(S): Tox21_200830
M4ID: 12481422

HILL MODEL (in red):

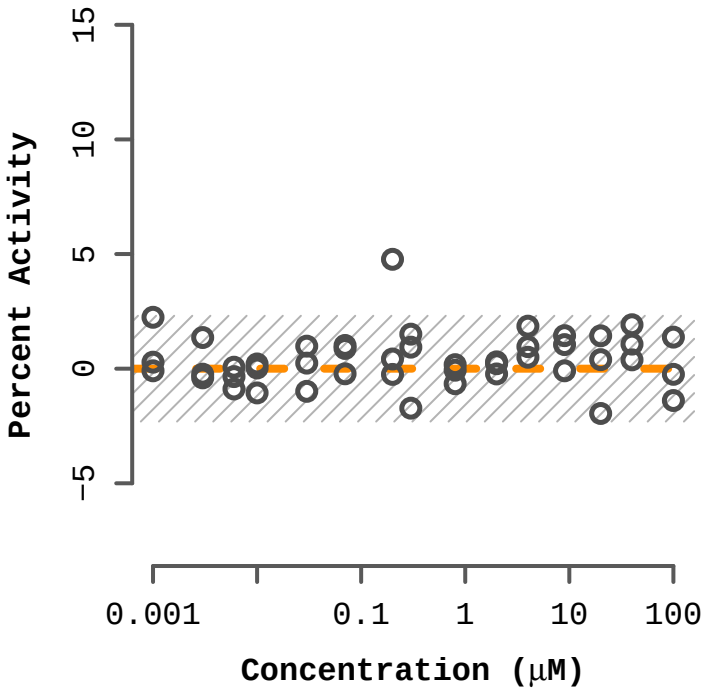
	tp	ga	gw
val:	15.8	1.74	0.755
sd:	10.3	0.741	0.225

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.8	1.74	0.755	3.85	4.35
sd:	10.3	0.741	0.225	2090	4860

	CNST	HILL	GNLS
AIC:	235.64	166.28	170.28
PROB:	0	0.88	0.12
RMSE:	3.7	1.4	1.4

MAX_MEAN: 10.2 MAX_MED: 9.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

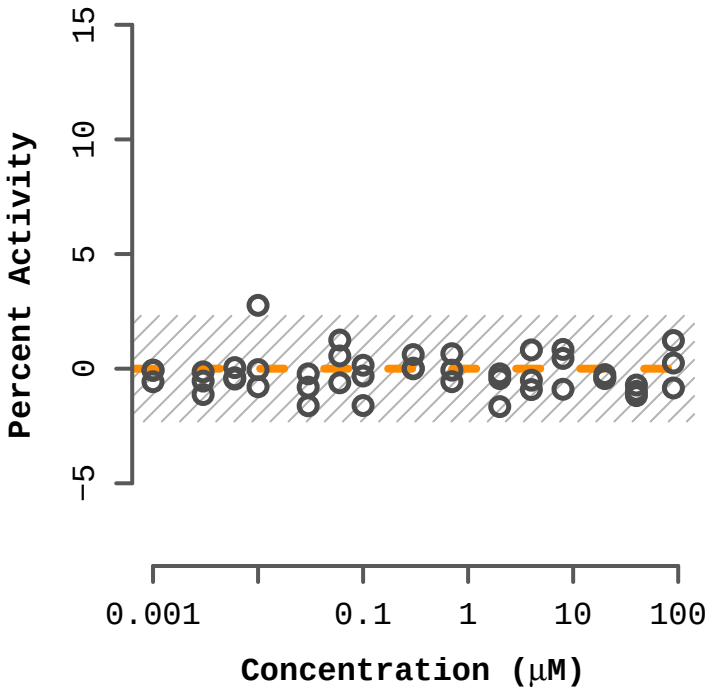
NAME: Allyl chloride
CHID: 39231 **CASRN:** 107-05-1
SPID(S): Tox21_200824
M4ID: 12481428

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

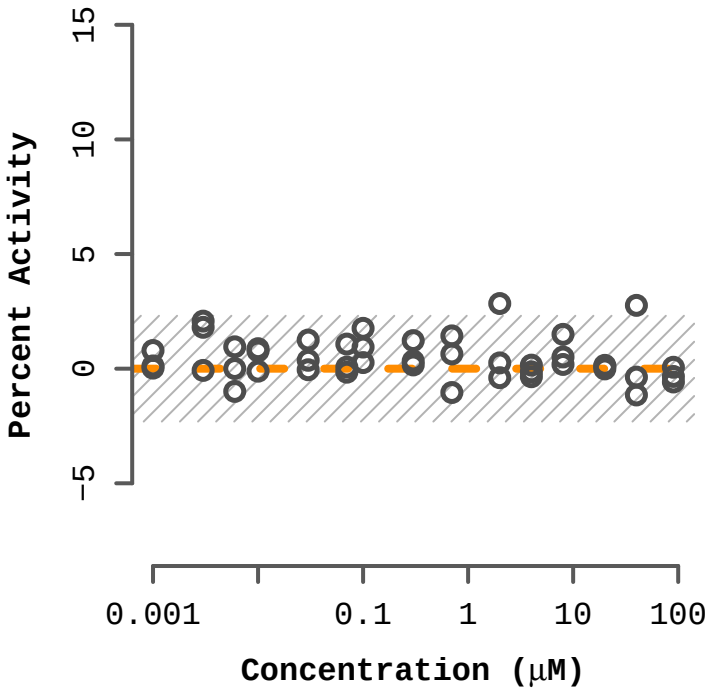
NAME: Allyl glycidyl ether
CHID: 39232 **CASRN:** 106-92-3
SPID(S): Tox21_200389
M4ID: 12481863

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.647 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

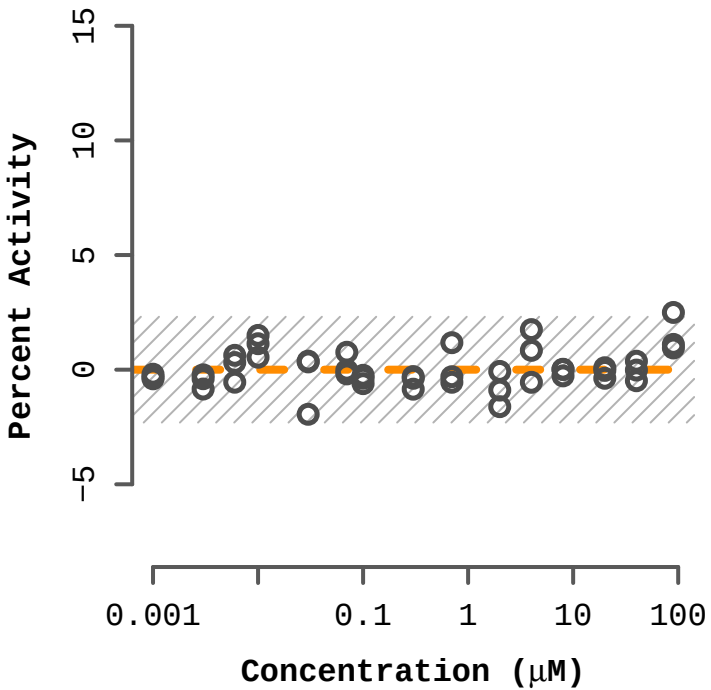
NAME: Allyl isovalerate
CHID: 39233 **CASRN:** 2835-39-4
SPID(S): Tox21_303369
M4ID: 12475766

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

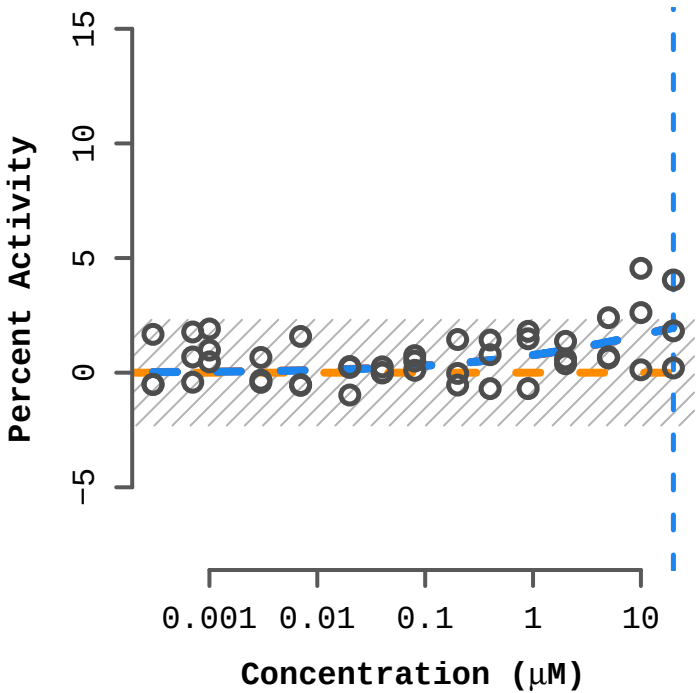
NAME: Allyl isovalerate
CHID: 39233 **CASRN:** 2835-39-4
SPID(S): Tox21_201307
M4ID: 12480945

HILL MODEL: Not applicable.

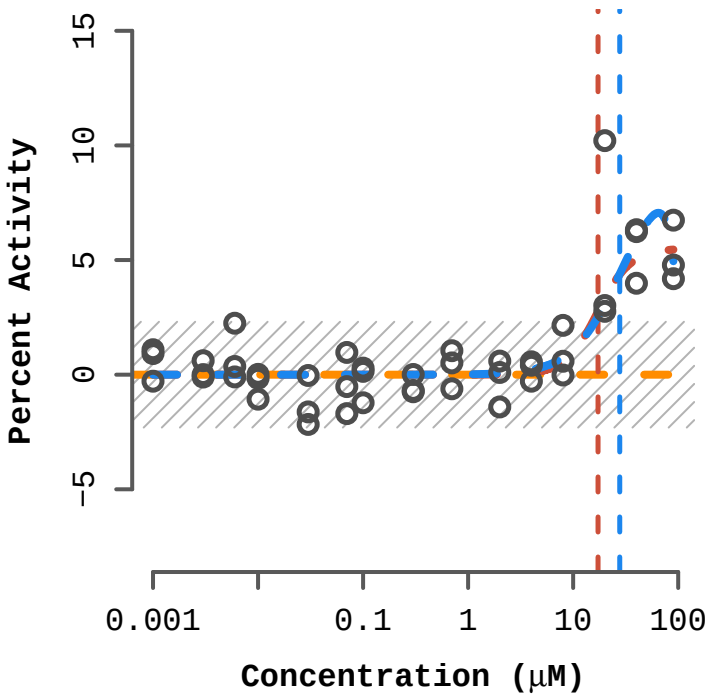
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.13 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Amino-2,4-dibromoanthraquinone
CHID:    39235   CASRN: 81-49-2
SPID(S): Tox21_202582
M4ID:    12479670

HILL MODEL (in red):
      tp       ga       gw
val:  5.25     1.8      0.427
sd:   16.5     5.34     0.391

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.92     1.3      0.469    3.23     4.15
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  153.03      139.51      143.55
PROB: 0           0.88        0.12
RMSE: 1.38        1.02        1.02

MAX_MEAN: 2.43      MAX_MED: 2.62      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-4-(p-nitrophenyl)thiazole
CHID: 39238 CASRN: 2104-09-8
SPID(S): Tox21_200846
M4ID: 12481406

HILL MODEL (in red):

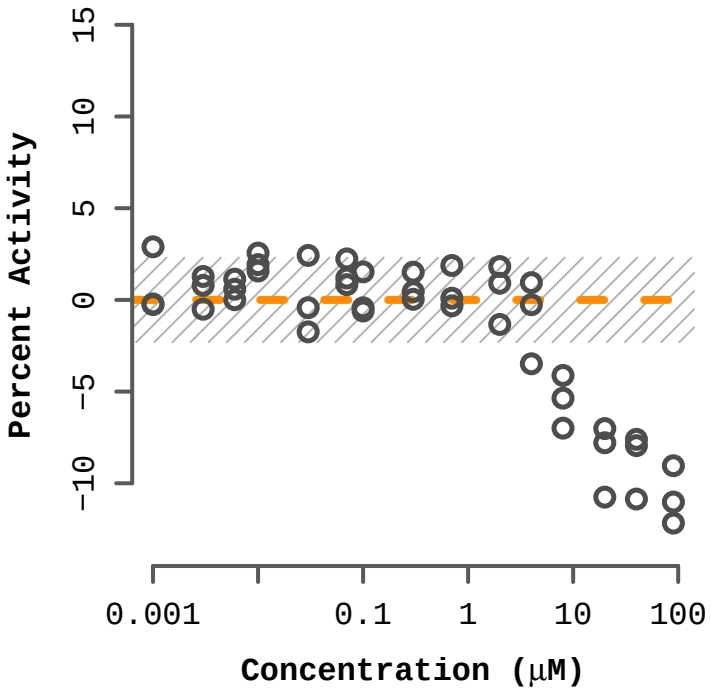
	tp	ga	gw
val:	5.51	1.24	2.82
sd:	0.686	0.083	1.26

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.79	1.44	1.91	1.98	8.3
sd:	11.1	0.64	1.77	0.0503	26.2

	CNST	HILL	GNLS
AIC:	204.37	146.08	147.63
PROB:	0	0.68	0.32
RMSE:	2.73	1.38	1.41

MAX_MEAN: 5.52 MAX_MED: 6.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

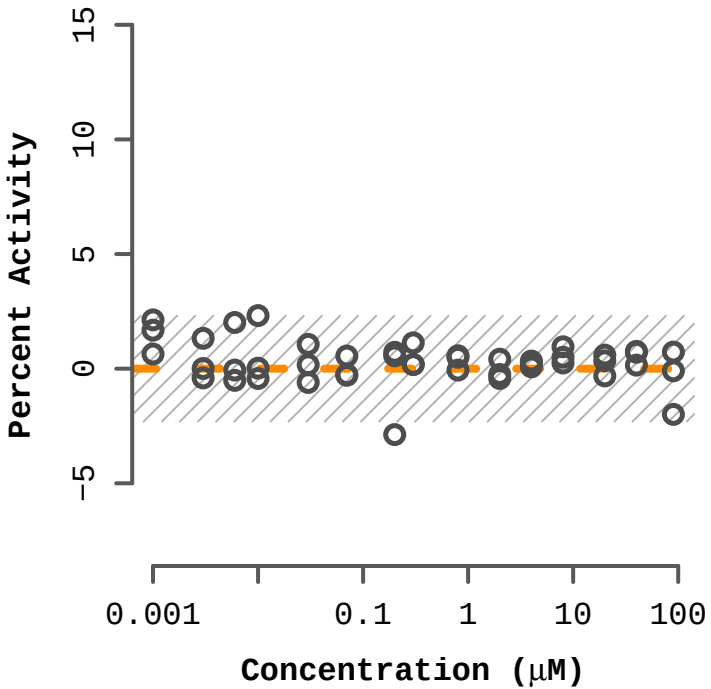
NAME: Antimony potassium tartrate trihydrate
CHID: 39240 **CASRN:** 28300-74-5
SPID(S): Tox21_202583
M4ID: 12479669

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	262.26	NA	NA
PROB:	1	NA	NA
RMSE:	4.67	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

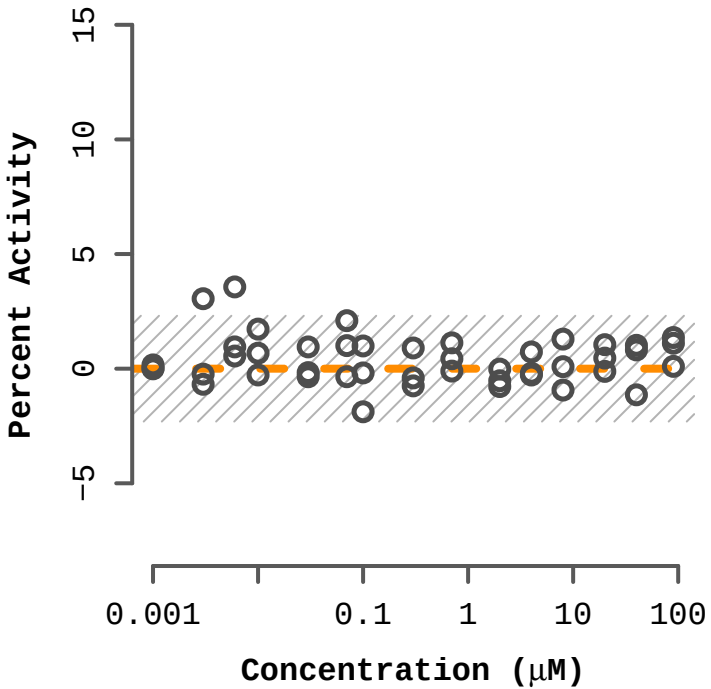
NAME: Benzaldehyde
CHID: 39241 **CASRN:** 100-52-7
SPID(S): Tox21_200634
M4ID: 12481618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

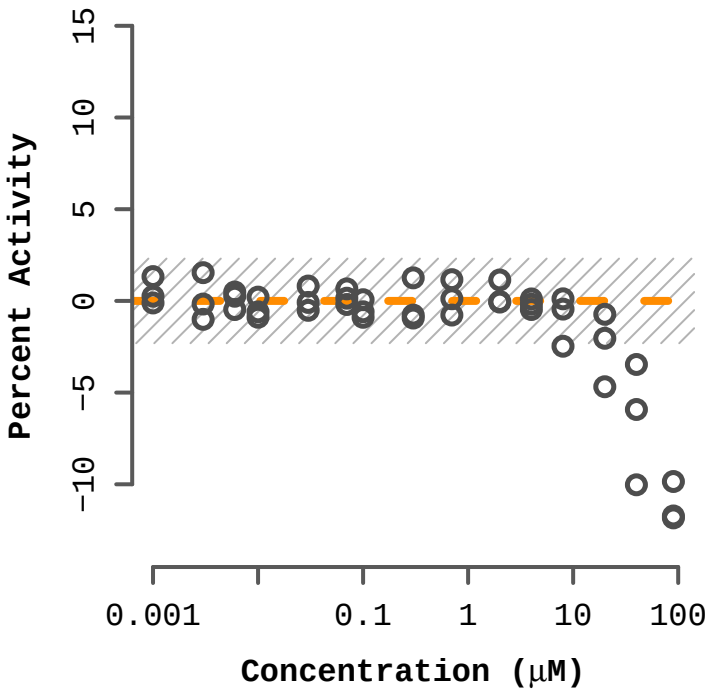
NAME: Benzene
CHID: 39242 **CASRN:** 71-43-2
SPID(S): Tox21_202487
M4ID: 12479765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

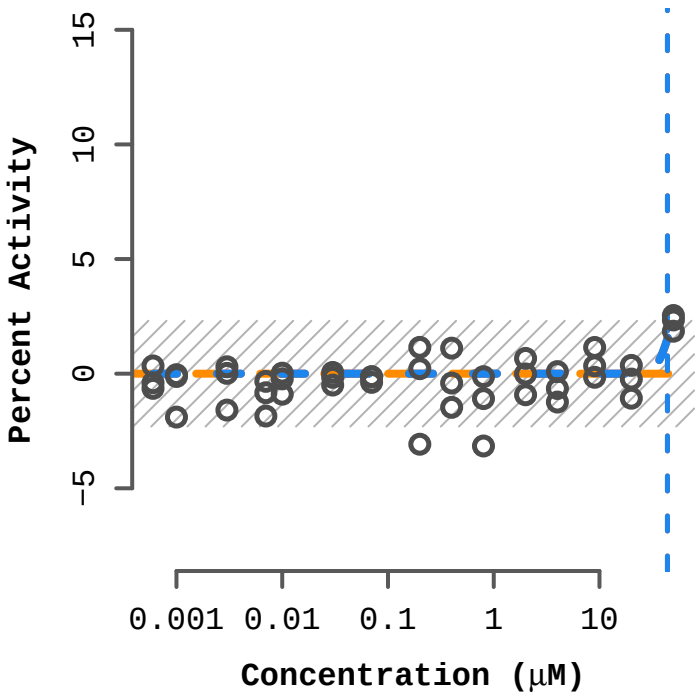
NAME: S-Bioallethrin
CHID: 39336 **CASRN:** 28434-00-6
SPID(S): Tox21_301044
M4ID: 12478089

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.62	NA	NA
PROB:	1	NA	NA
RMSE:	3.56	NA	NA

MAX_MEAN: 0.491 **MAX_MED:** 0.257 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fludarabine
CHID: 39657 **CASRN:** 21679-14-1
SPID(S): Tox21_113419_1
M4ID: 12482656

HILL MODEL (in red):

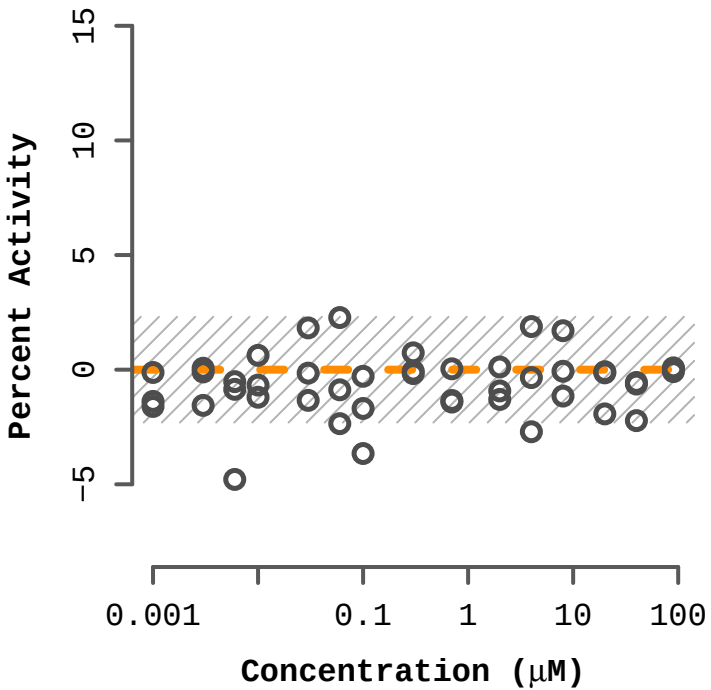
	tp	ga	gw
val:	3.05	1.64	8
sd:	8.47	0.514	15.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.05	1.64	8	3.69	4.38
sd:	8.23	0.499	15	42300	93000

	CNST	HILL	GNLS
AIC:	138.61	127.58	131.58
PROB:	0	0.88	0.12
RMSE:	1.15	0.99	0.99

MAX_MEAN: 2.25 **MAX_MED:** 2.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

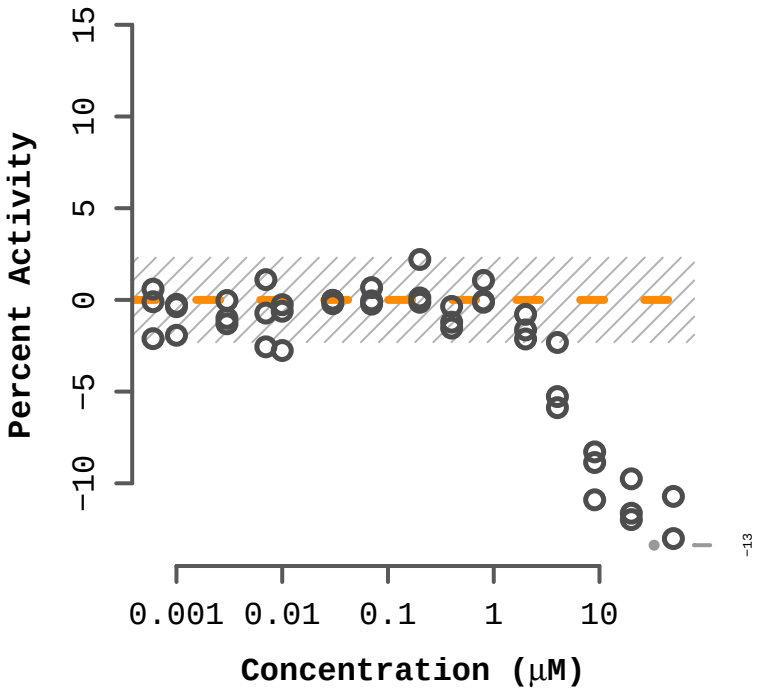
NAME: Calcium nitrate
CHID: 39719 **CASRN:** 10124-37-5
SPID(S): Tox21_300814
M4ID: 12478319

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.168 **MAX_MED:** 0.0463 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

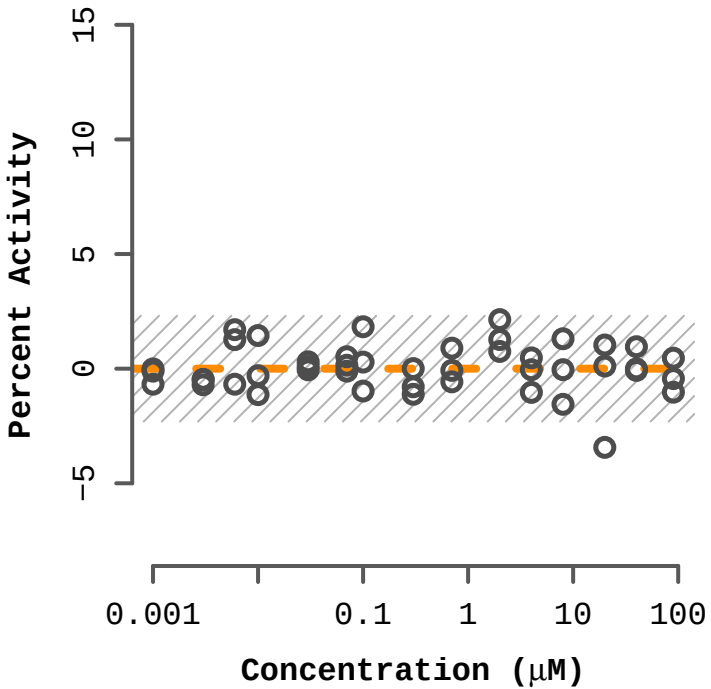
NAME: Polyoxyethylene (9) lauryl ether
CHID: 39721 **CASRN:** 3055-99-0
SPID(S): Tox21_112394_1
M4ID: 12483117 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.68	NA	NA
PROB:	1	NA	NA
RMSE:	5.2	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 0.109 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

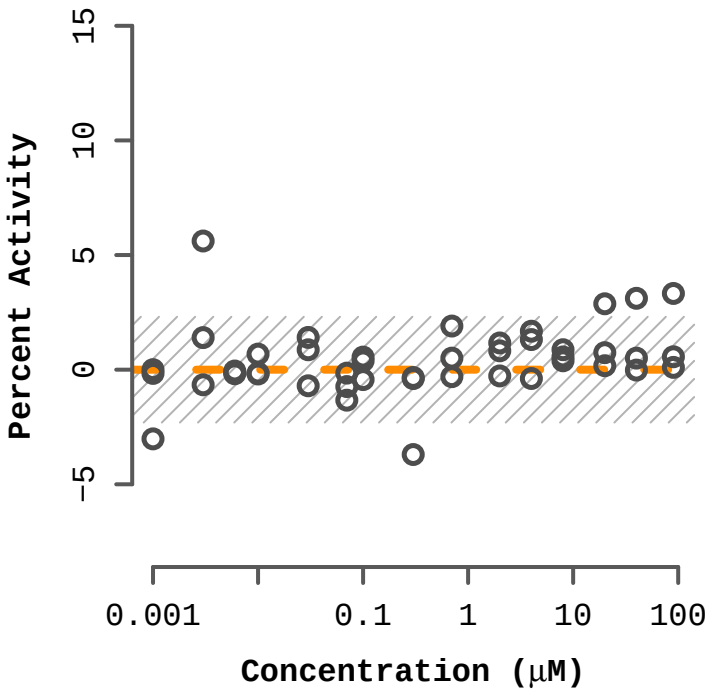
NAME: Monomethyl phthalate
CHID: 40001 CASRN: 4376-18-5
SPID(S): Tox21_300735
M4ID: 12478398

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.66	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

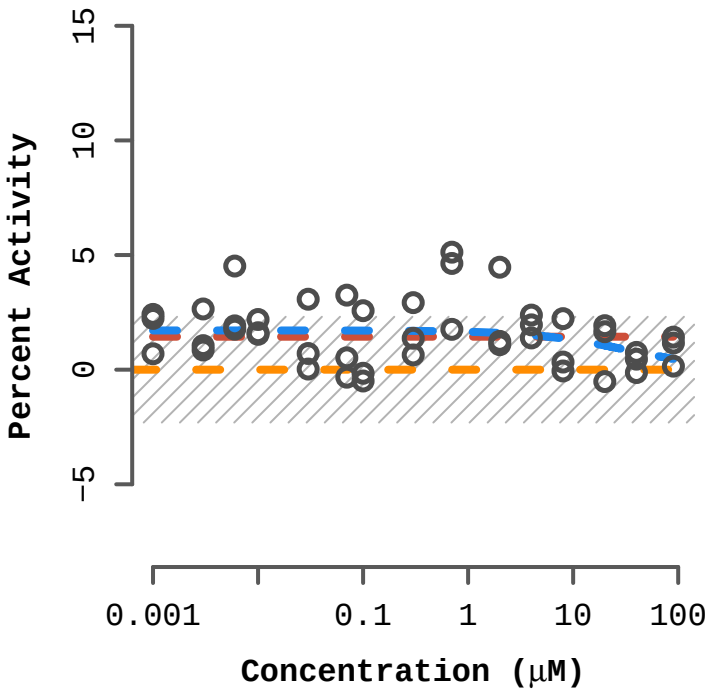
NAME: Monobutyl phthalate
CHID: 40002 **CASRN:** 131-70-4
SPID(S): Tox21_300888
M4ID: 12478245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 2.12 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl propionate
CHID: 40110 CASRN: 105-37-3
SPID(S): Tox21_301081
M4ID: 12478052

HILL MODEL (in red):

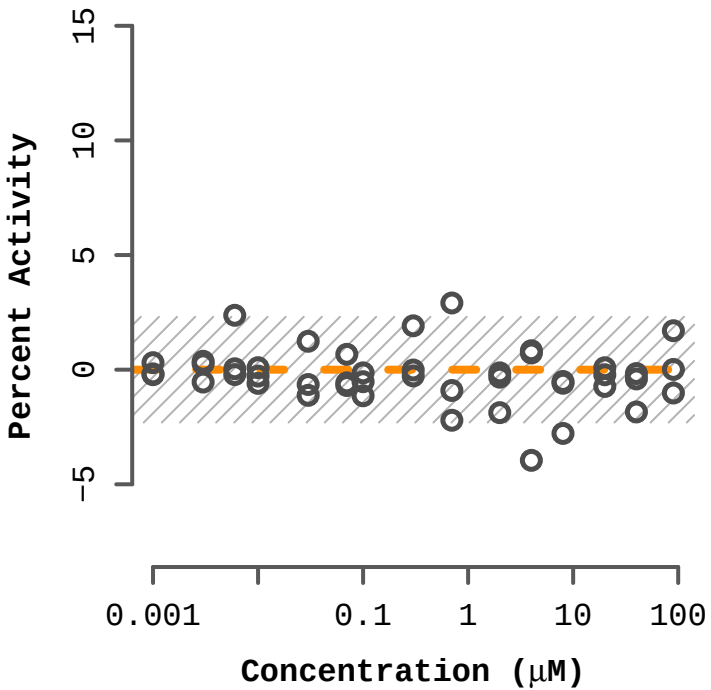
	tp	ga	gw
val:	1.44	−4.21	6.06
sd:	0.196	881	4400

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.71	−4.48	7.94	1.52	0.957
sd:	0.245	176000	922000	0.477	0.774

	CNST	HILL	GNLS
AIC:	198.05	164.92	164.83
PROB:	0	0.49	0.51
RMSE:	2.09	1.38	1.31

MAX_MEAN: 3.84 **MAX_MED:** 4.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

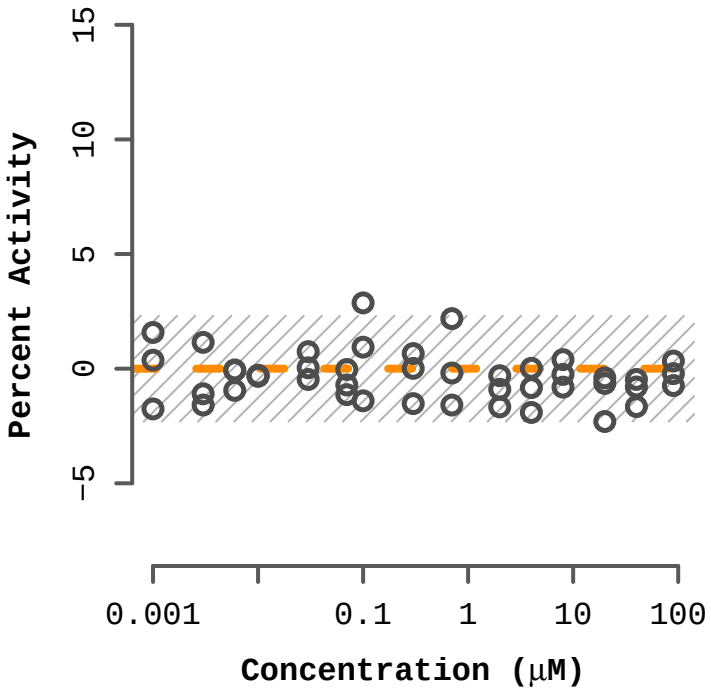
NAME: Ethyl butyrate
CHID: 40111 CASRN: 105-54-4
SPID(S): Tox21_300065
M4ID: 12479065

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.734 **MAX_MED:** 0.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

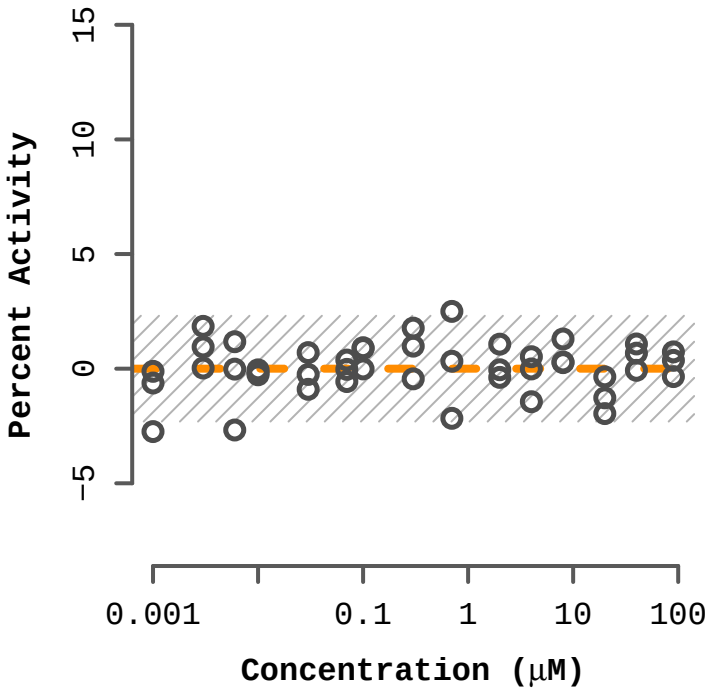
NAME: Ethyl heptanoate
CHID: 40112 **CASRN:** 106-30-9
SPID(S): Tox21_300382
M4ID: 12478750

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.803 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

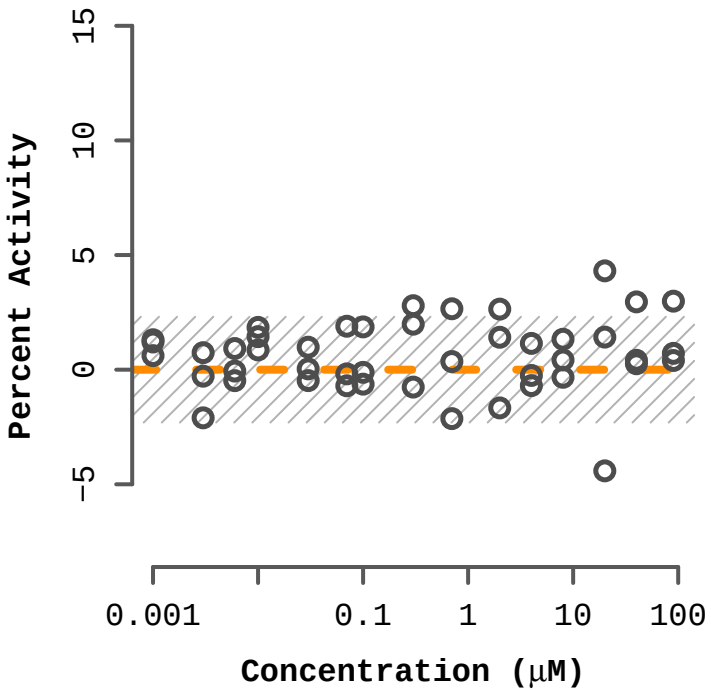
NAME: tert-Butylacrylamide
CHID: 40114 **CASRN:** 107-58-4
SPID(S): Tox21_301092
M4ID: 12478041

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 0.985 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

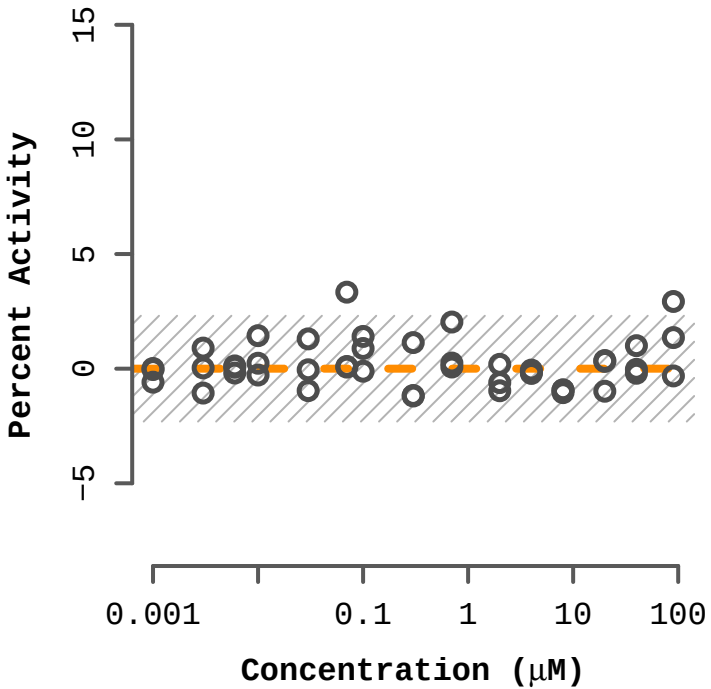
NAME: 2,5−Dimercapto−1,3,4−thiadiazole
CHID: 40115 **CASRN:** 1072−71−5
SPID(S): Tox21_301157
M4ID: 12477976

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

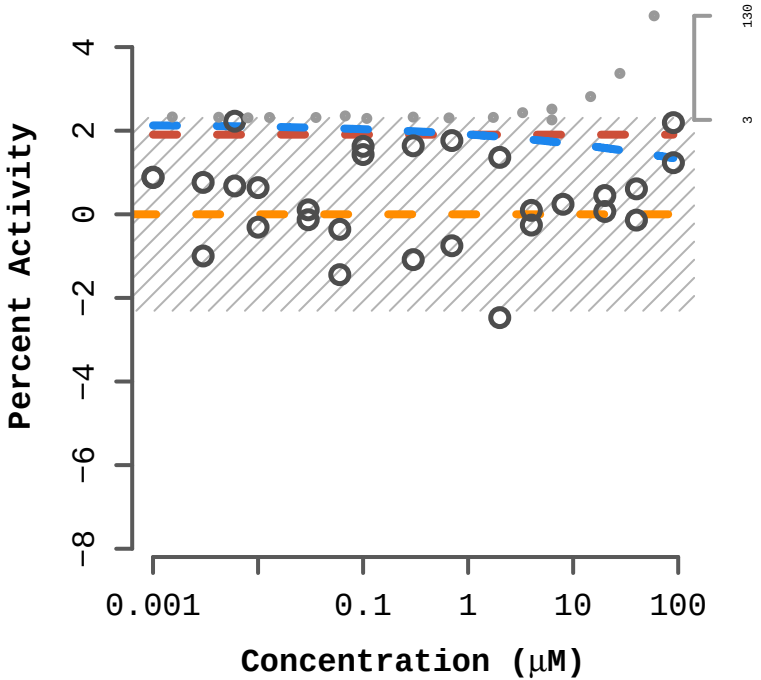
NAME: 2,6-Diaminopyridine
CHID: 40127 **CASRN:** 141-86-6
SPID(S): Tox21_303403
M4ID: 12475736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6-Diaminopyridine
CHID: 40127 **CASRN:** 141-86-6
SPID(S): Tox21_201654
M4ID: 12480598 **BRK**

HILL MODEL (in red):

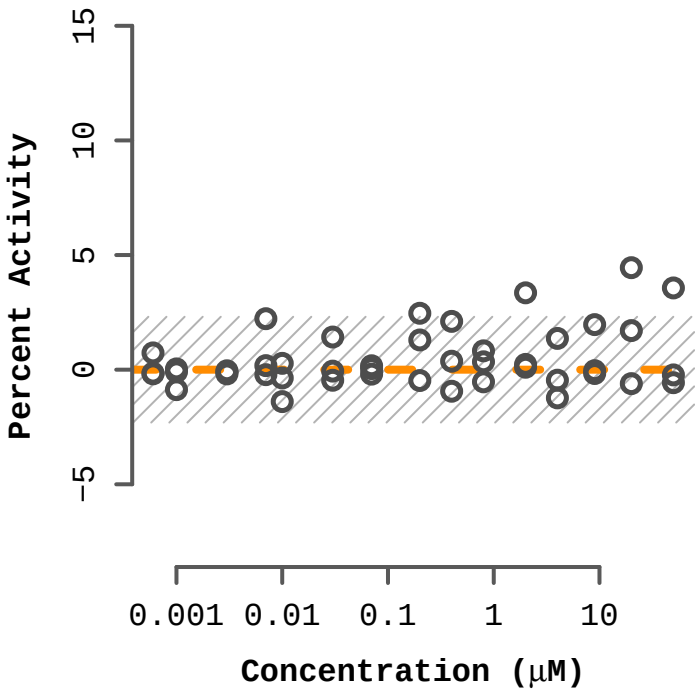
	tp	ga	gw
val:	1.91	−4.61	4.06
sd:	0.593	1110	2810

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.15	−4.78	3.5	2.6	0.347
sd:	1.82	1120	2210	7.23	2.64

	CNST	HILL	GNLS
AIC:	317.64	313.02	316.84
PROB:	0.08	0.8	0.12
RMSE:	22.45	21.91	22.02

MAX_MEAN: 44.9 **MAX_MED:** 2.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

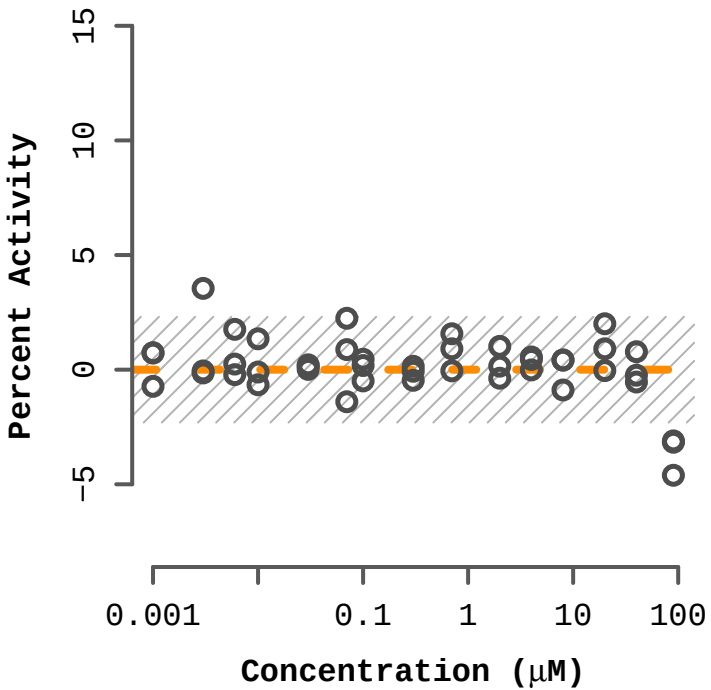
NAME: Yohimbine
CHID: 40130 **CASRN:** 146-48-5
SPID(S): Tox21_110019_1
M4ID: 12484708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

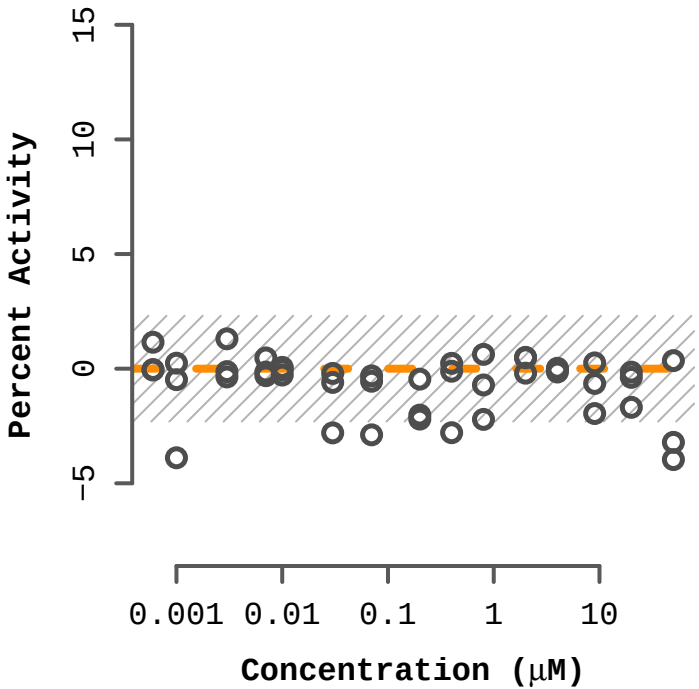
NAME: Vincamine
CHID: 40134 **CASRN:** 1617-90-9
SPID(S): Tox21_301968
M4ID: 12477165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

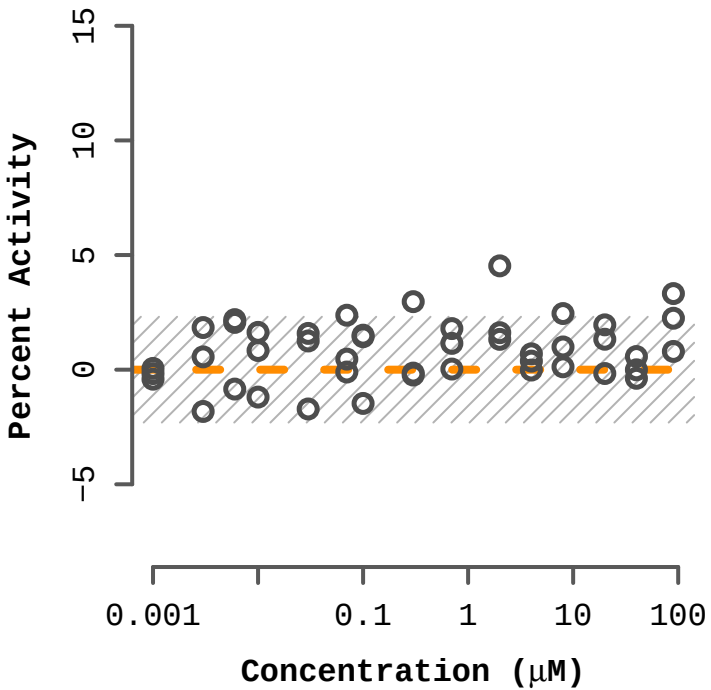
NAME: Vincamine
CHID: 40134 **CASRN:** 1617-90-9
SPID(S): Tox21_111342_1
M4ID: 12483752

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.353 **MAX_MED:** 0.477 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

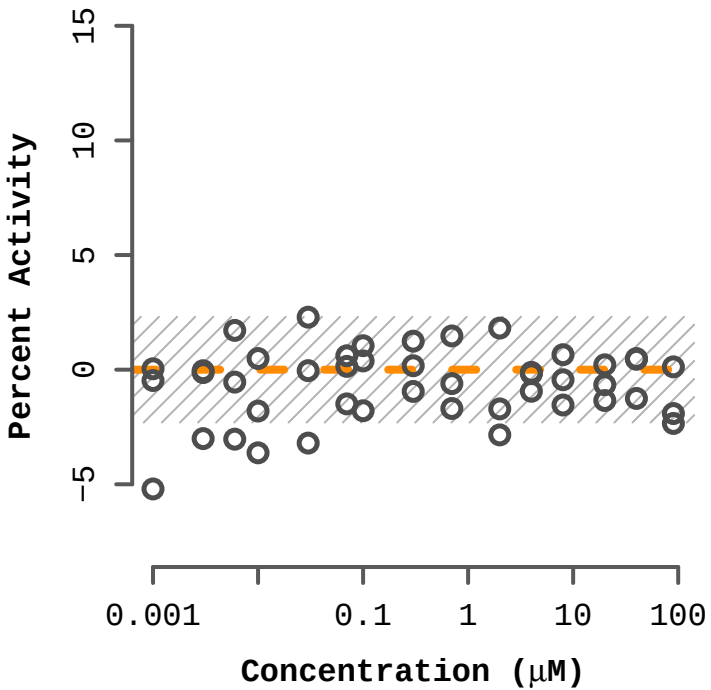
NAME: Imidazolidinyl urea
CHID: 40151 **CASRN:** 39236-46-9
SPID(S): Tox21_302325
M4ID: 12476808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.49 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

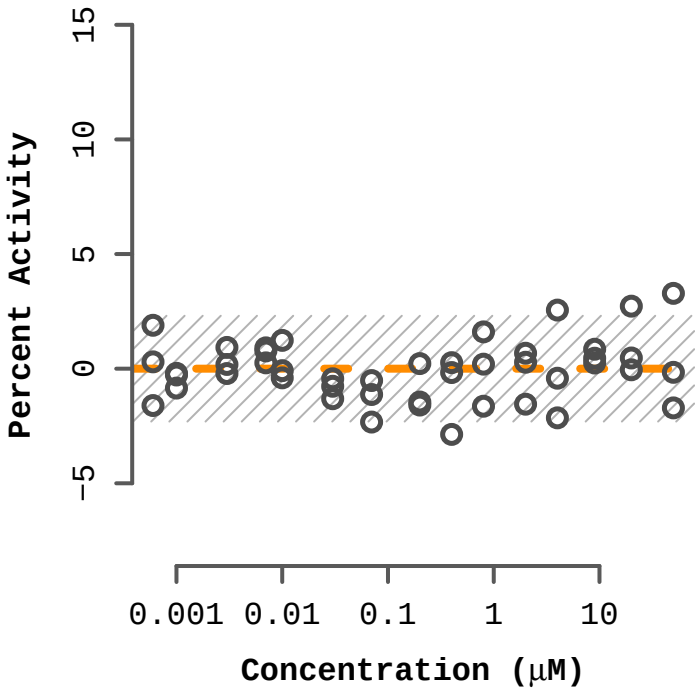
NAME: Arbutin
CHID: 40152 **CASRN:** 497-76-7
SPID(S): Tox21_302428
M4ID: 12476705

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 0.157 **MAX_MED:** 0.454 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

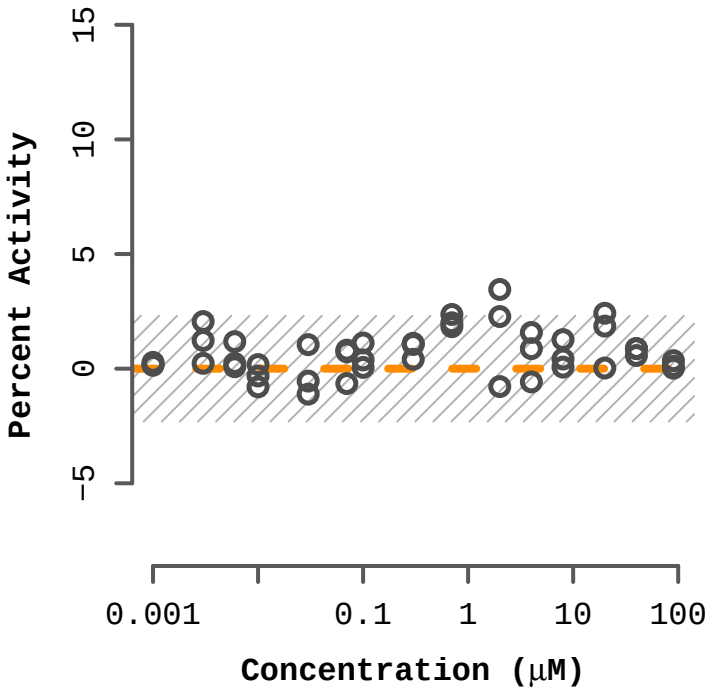
NAME: Arbutin
CHID: 40152 CASRN: 497-76-7
SPID(S): Tox21_111509_1
M4ID: 12483645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.774 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

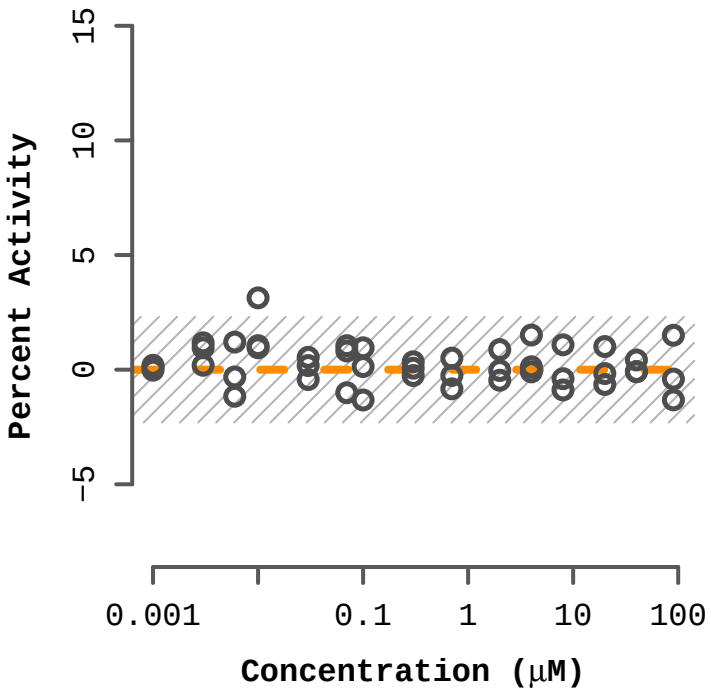
NAME: N−[3−(Dimethylamino)propyl]methacrylamide
CHID: 40154 **CASRN:** 5205−93−6
SPID(S): Tox21_301671
M4ID: 12477462

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

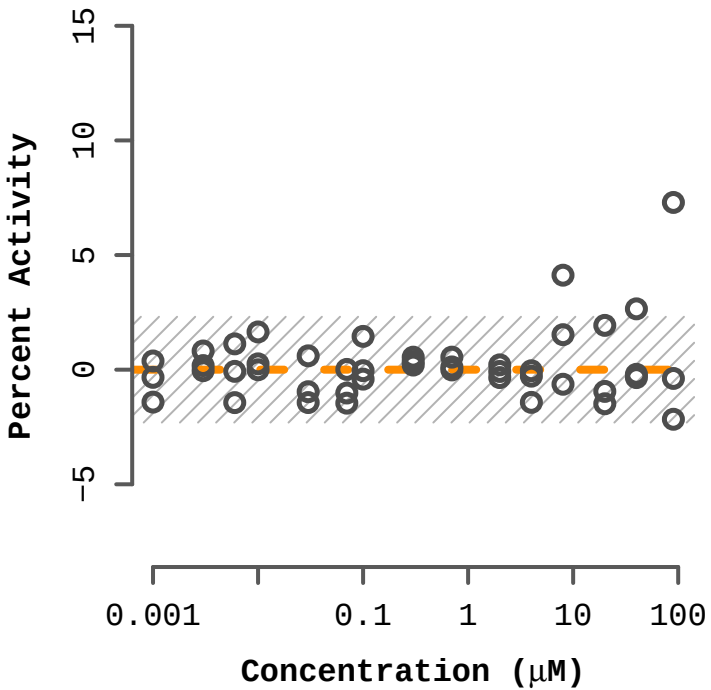
NAME: 3-Oxobutanamide
CHID: 40164 **CASRN:** 5977-14-0
SPID(S): Tox21_303947
M4ID: 12475241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

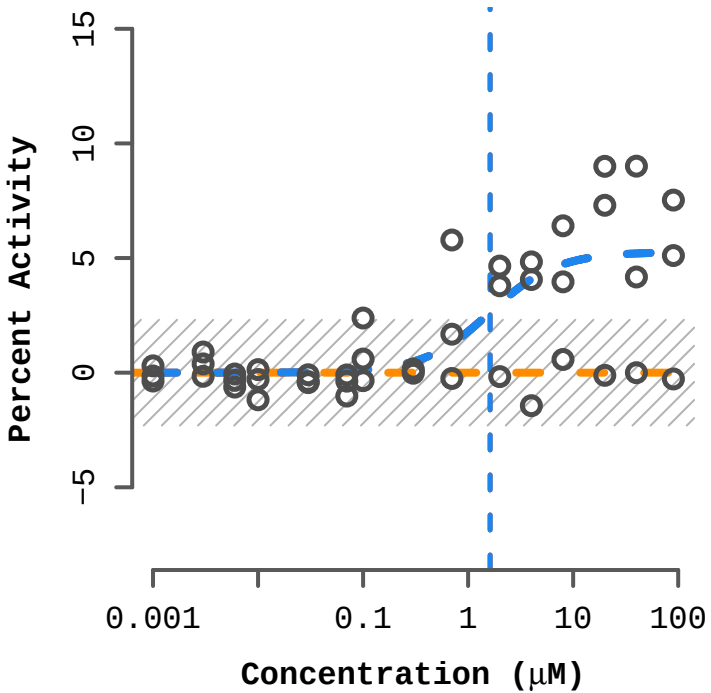
NAME: Rifamycin SV sodium salt
CHID: 40208 CASRN: 14897-39-3
SPID(S): Tox21_202806
M4ID: 12479446

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethyl N-methylolphosphonopropionamide
CHID: 40215 CASRN: 20120-33-6
SPID(S): Tox21_303831
M4ID: 12475357

HILL MODEL (in red):

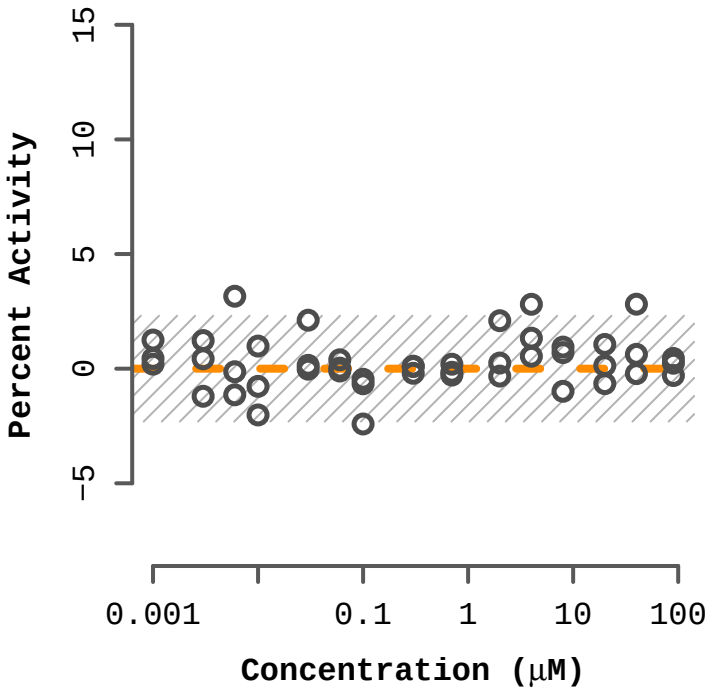
	tp	ga	gw
val:	5.27	0.209	1.37
sd:	1.15	0.293	0.688

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.27	0.209	1.37	3.62	3.65
sd:	1.15	0.293	0.688	1230	3290

	CNST	HILL	GNLS
AIC:	229.73	201.57	205.57
PROB:	0	0.88	0.12
RMSE:	3.33	2.23	2.23

MAX_MEAN: 5.4 **MAX_MED:** 7.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

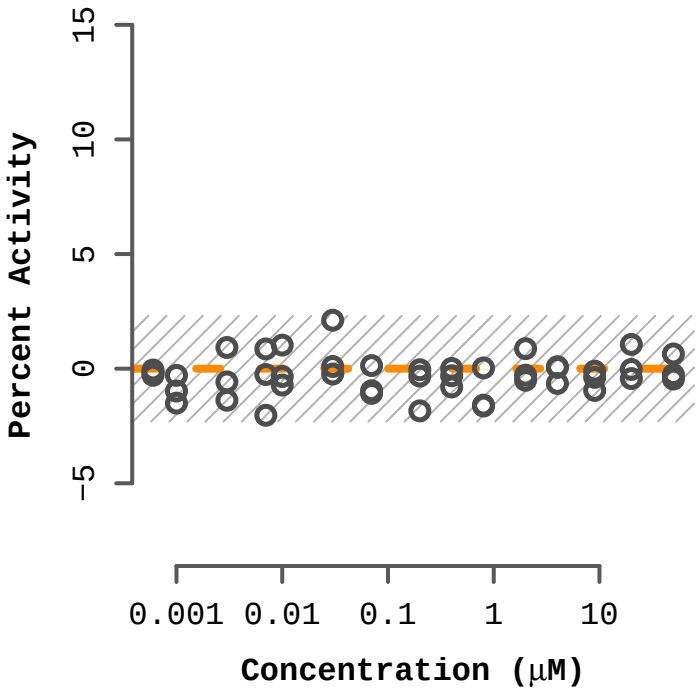
NAME: Trifloxysulfuron-sodium
CHID: 40222 **CASRN:** 199119-58-9
SPID(S): Tox21_301184
M4ID: 12477949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

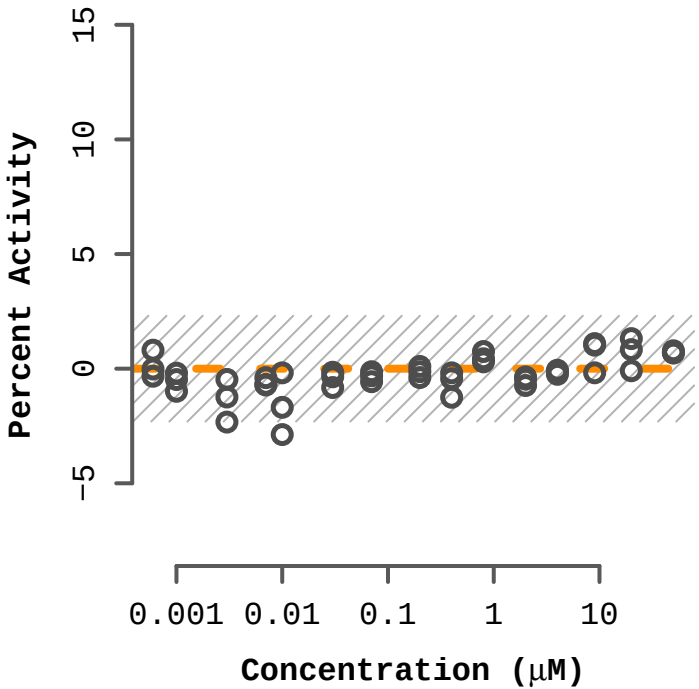
NAME: Irsogladine maleate
CHID: 40234 CASRN: 84504-69-8
SPID(S): Tox21_111786_1
M4ID: 12483482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.661 **MAX_MED:** 0.0983 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

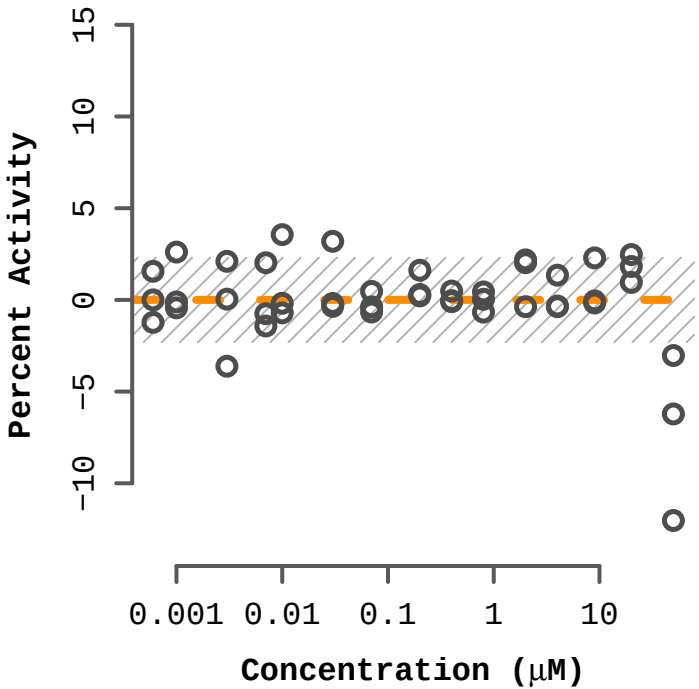
NAME: Kojic acid
CHID: 40236 **CASRN:** 501-30-4
SPID(S): Tox21_110814_1
M4ID: 12484099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

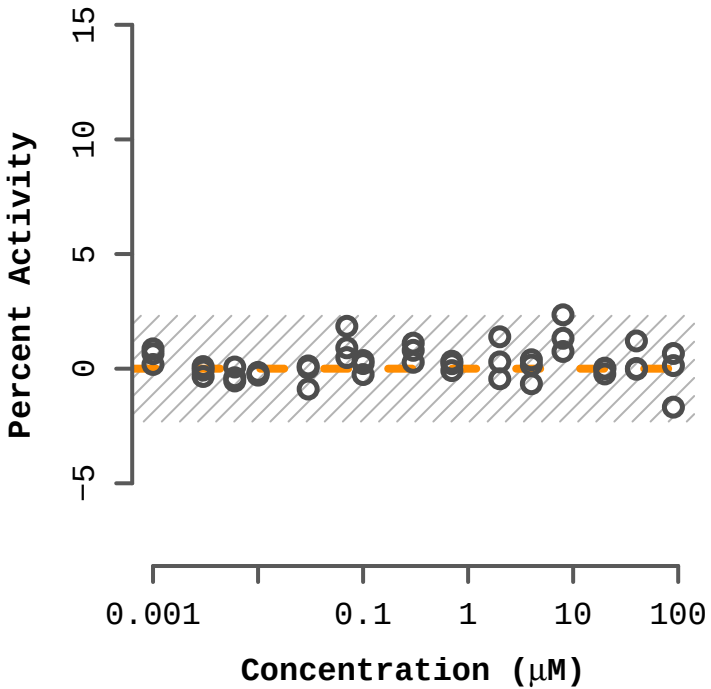
NAME: Sertraline hydrochloride
CHID: 40243 **CASRN:** 79559-97-0
SPID(S): Tox21_111199_1
M4ID: 12483847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.51	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

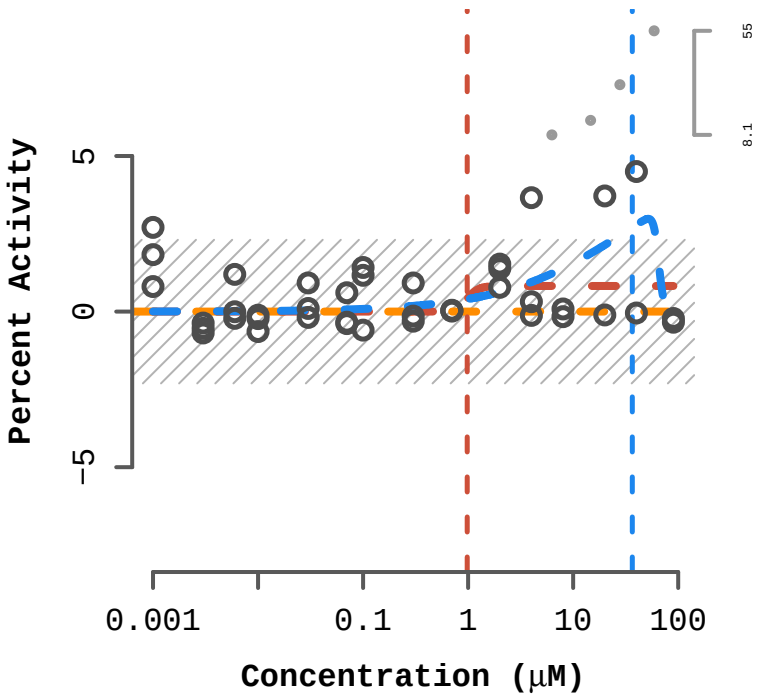
NAME: Sucralose
CHID: 40245 CASRN: 56038-13-2
SPID(S): Tox21_303425
M4ID: 12475714

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.48 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sucralose
CHID: 40245 CASRN: 56038-13-2
SPID(S): Tox21_201752
M4ID: 12480500 BRK

HILL MODEL (in red):

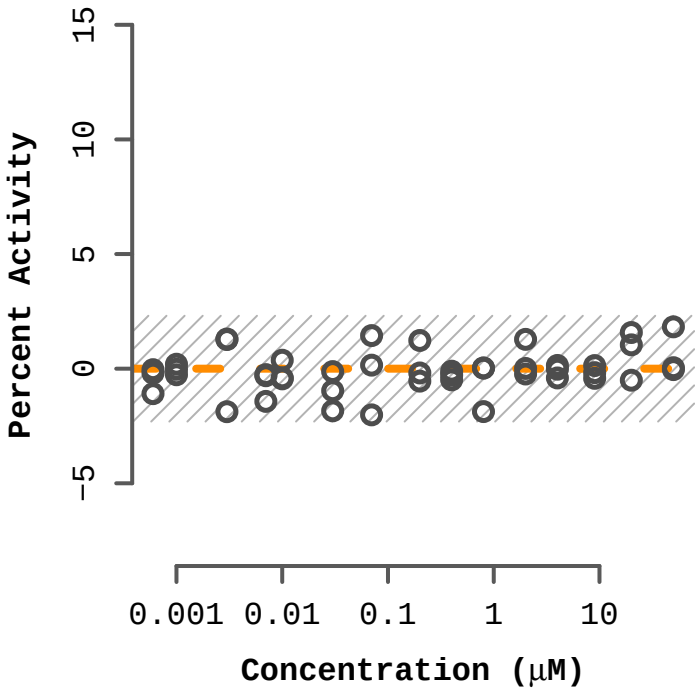
	tp	ga	gw
val:	0.823	−0.00877	8
sd:	0.424	0.538	21.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.41	1.56	0.699	1.81	17.9
sd:	13.3	2.32	0.54	0.658	83.7

	CNST	HILL	GNLS
AIC:	232	233.41	235.12
PROB:	0.59	0.29	0.12
RMSE:	9.79	9.57	9.49

MAX_MEAN: 18.1 **MAX_MED:** 4.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

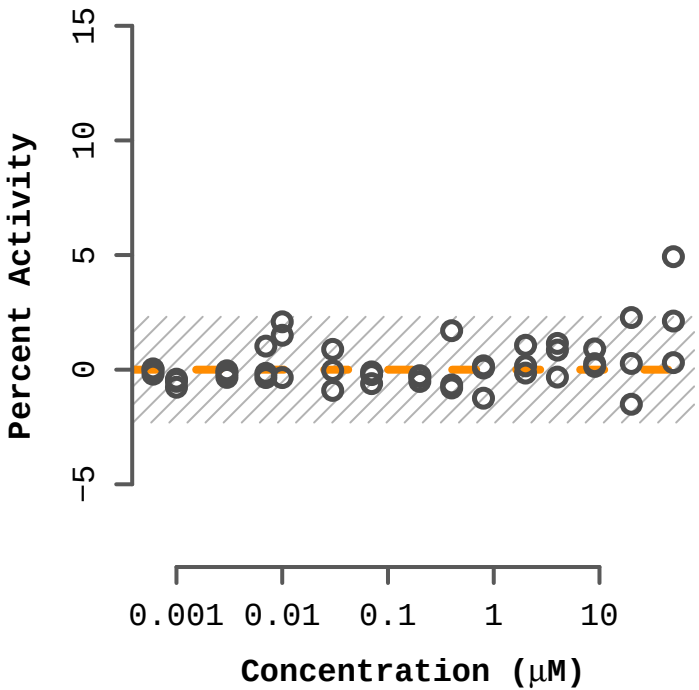
NAME: Sucralose
CHID: 40245 **CASRN:** 56038-13-2
SPID(S): Tox21_113658
M4ID: 12482555

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.706 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

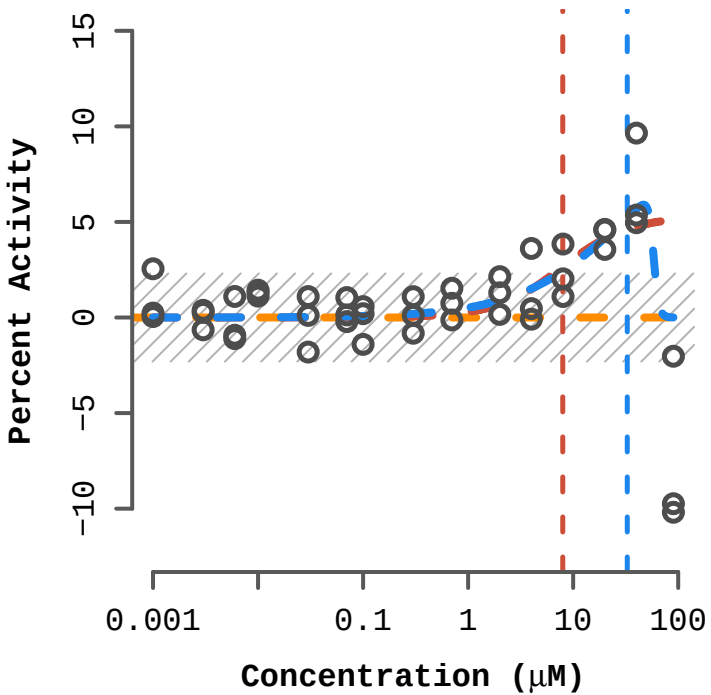
NAME: Sulindac sulfone
CHID: 40246 CASRN: 59973-80-7
SPID(S): Tox21_113524_1
M4ID: 12482620

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 2.45 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium pentachlorophenate
CHID: 40264 CASRN: 131-52-2
SPID(S): Tox21_303795
M4ID: 12475393

HILL MODEL (in red):

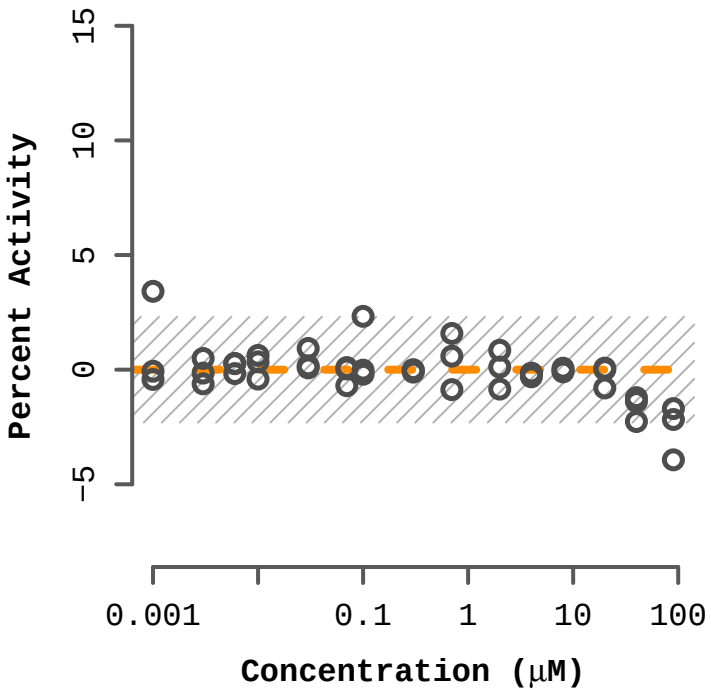
	tp	ga	gw
val:	5.29	0.901	1.37
sd:	1.35	0.229	0.861

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.52	0.849	1.77	17.7
sd:	9.75	0.927	0.427	0.57	53

	CNST	HILL	GNLS
AIC:	222	200.96	185.69
PROB:	0	0	1
RMSE:	3.24	3.57	2.41

MAX_MEAN: 6.66 **MAX_MED:** 5.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

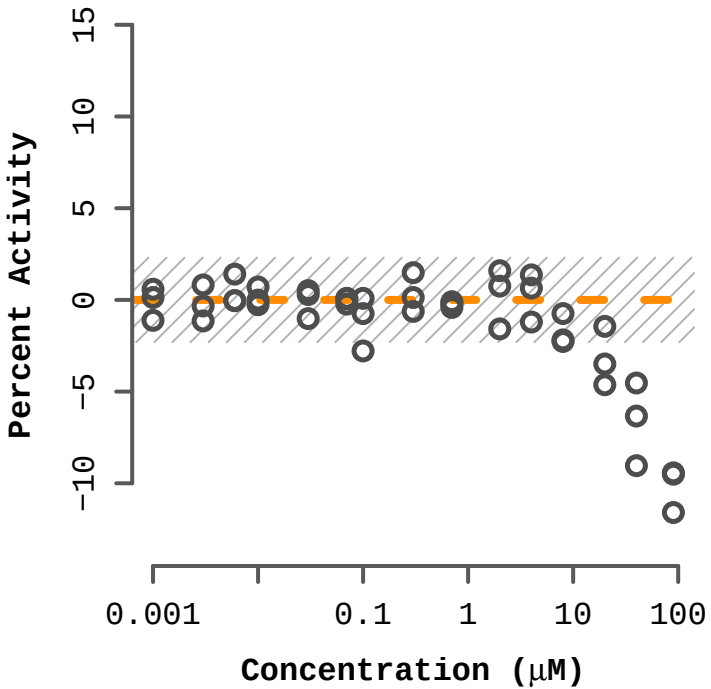
NAME: Dinitramine
CHID: 40265 **CASRN:** 29091-05-2
SPID(S): Tox21_302221
M4ID: 12476912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.975 **MAX_MED:** 0.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

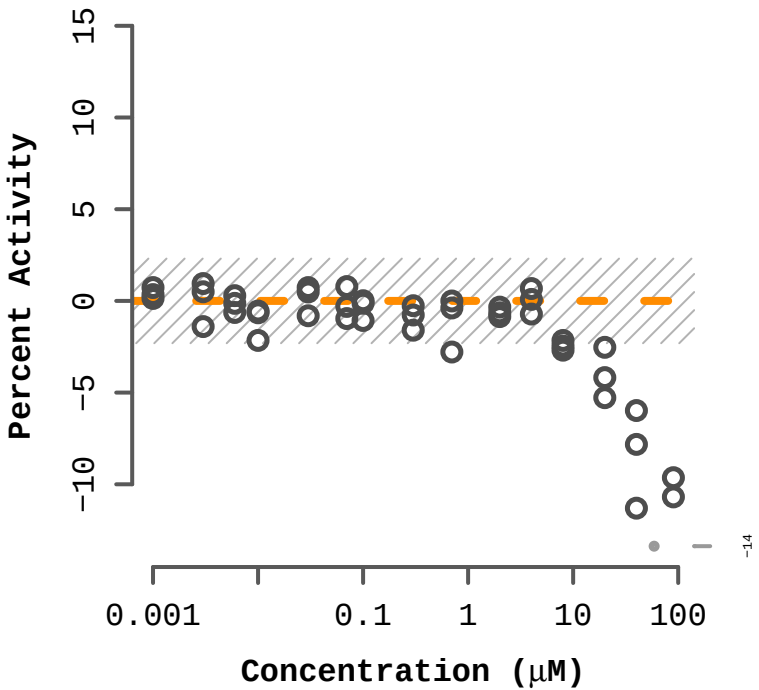
NAME: Dinobuton
CHID: 40268 **CASRN:** 973-21-7
SPID(S): Tox21_302224
M4ID: 12476909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.71	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 0.443 **MAX_MED:** 0.753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

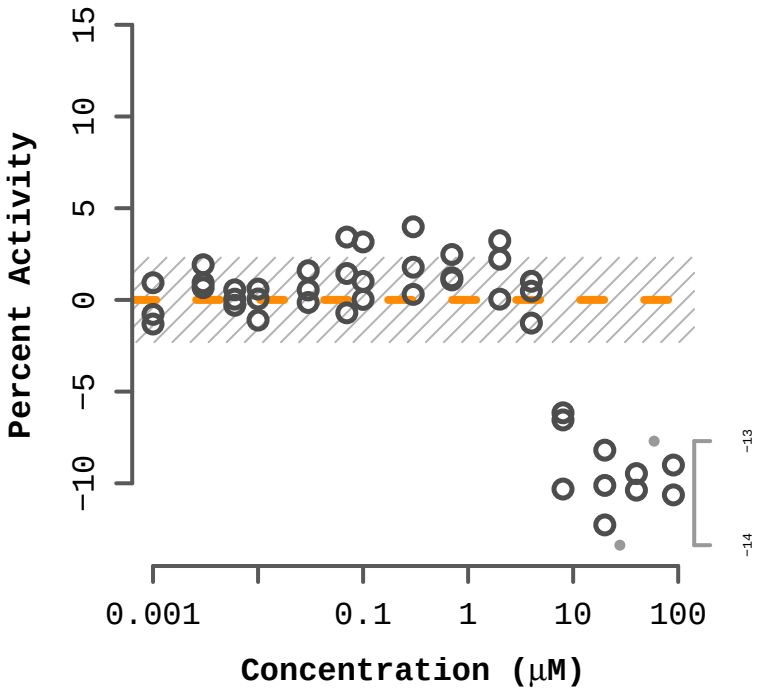
NAME: Binapacryl
CHID: 40269 **CASRN:** 485-31-4
SPID(S): Tox21_301554
M4ID: 12477579 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233.19	NA	NA
PROB:	1	NA	NA
RMSE:	4.02	NA	NA

MAX_MEAN: 0.404 **MAX_MED:** 0.501 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

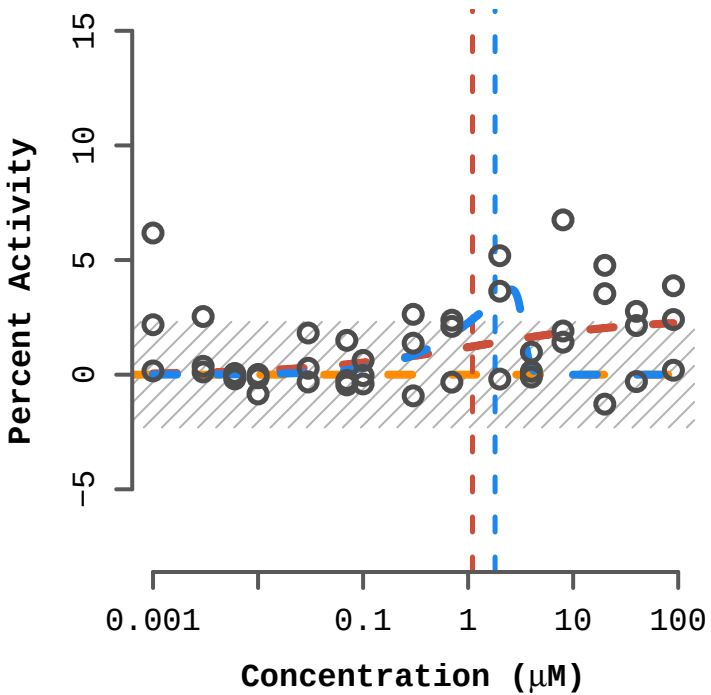
NAME: Dithianon
CHID: 40270 CASRN: 3347-22-6
SPID(S): Tox21_302405
M4ID: 12476728 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	277.08	NA	NA
PROB:	1	NA	NA
RMSE:	5.47	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Quinaldine
CHID: 40271 **CASRN:** 91-63-4
SPID(S): Tox21_302026
M4ID: 12477107

HILL MODEL (in red):

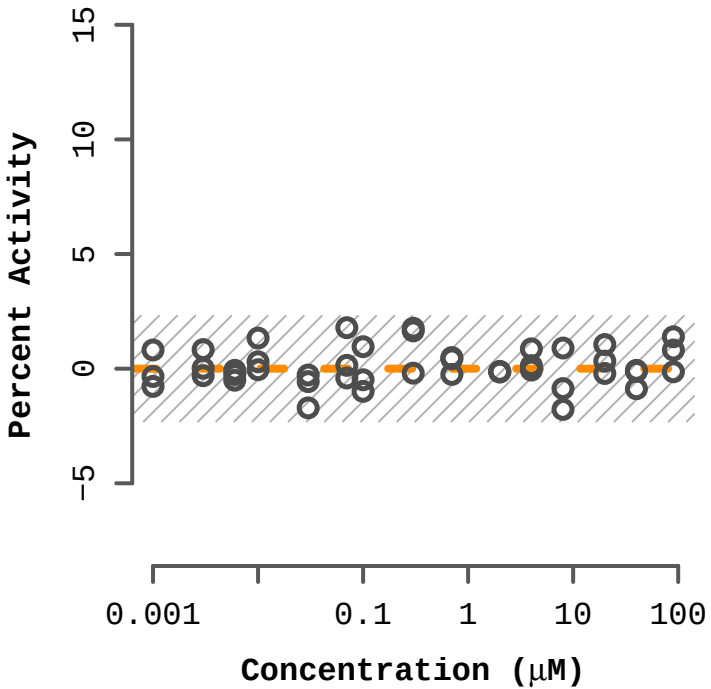
	tp	ga	gw
val:	2.46	0.0415	0.54
sd:	2.13	2.14	0.874

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.47	0.257	1.05	0.521	13.5
sd:	14.3	1.77	1.14	0.765	127

	CNST	HILL	GNLS
AIC:	199.92	186.26	201.04
PROB:	0	1	0
RMSE:	2.31	1.84	2.14

MAX_MEAN: 3.36 **MAX_MED:** 3.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

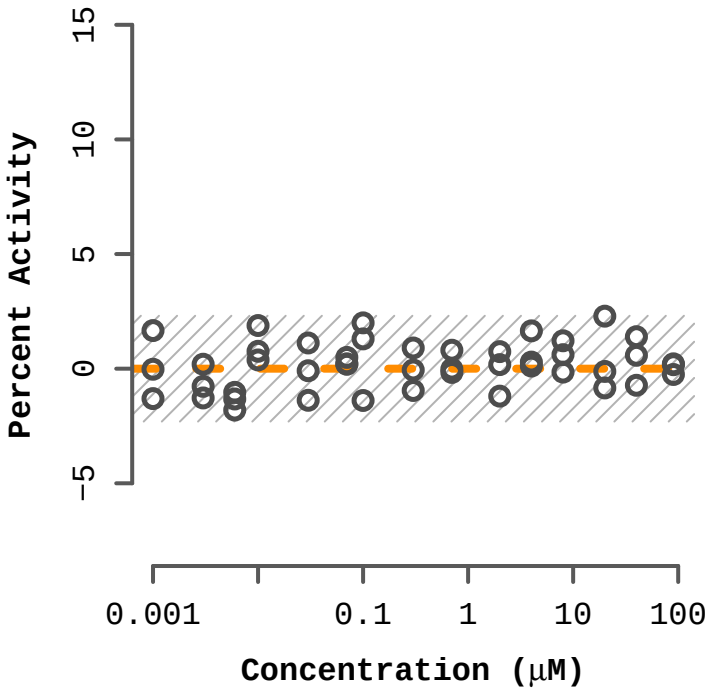
NAME: Dichlofenthion
CHID: 40274 CASRN: 97-17-6
SPID(S): Tox21_301160
M4ID: 12477973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.07 MAX_MED: 1.65 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

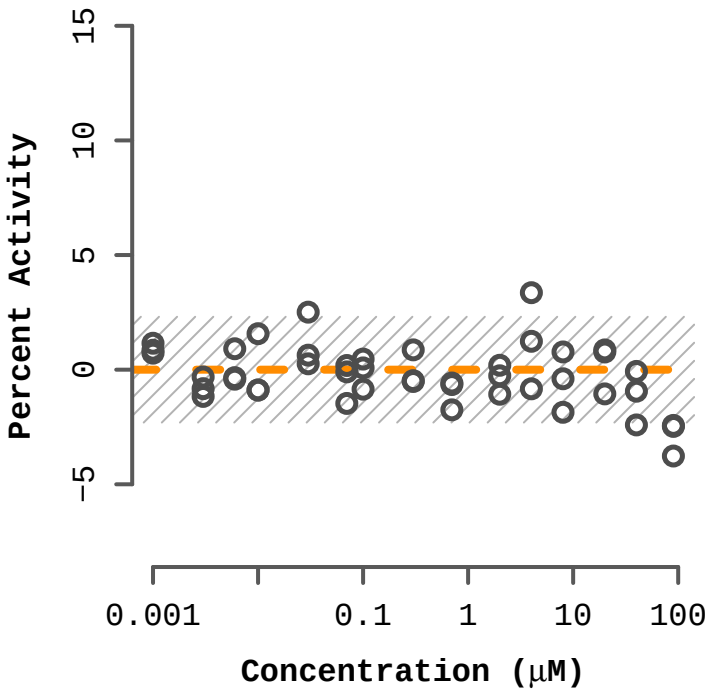
NAME: Iodenphos
CHID: 40278 **CASRN:** 18181-70-9
SPID(S): Tox21_300910
M4ID: 12478223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

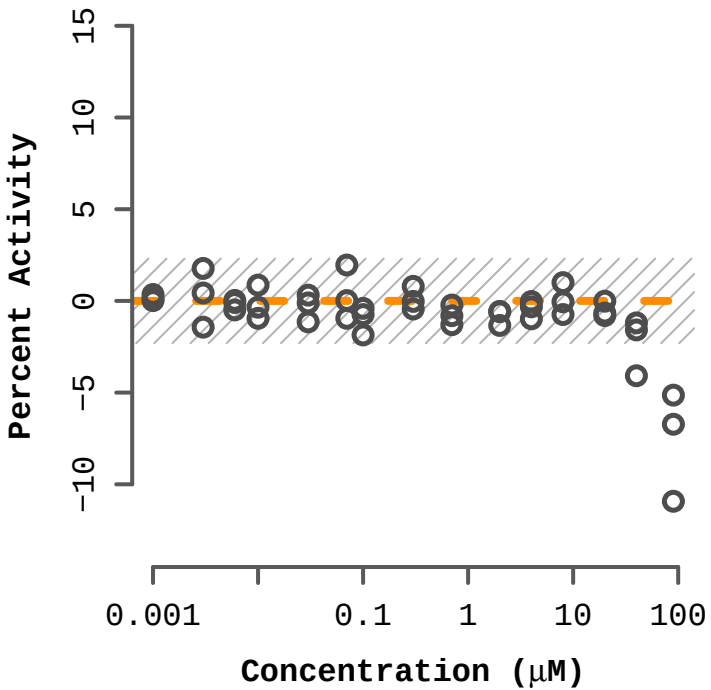
NAME: Leptophos
CHID: 40279 **CASRN:** 21609-90-5
SPID(S): Tox21_301903
M4ID: 12477230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

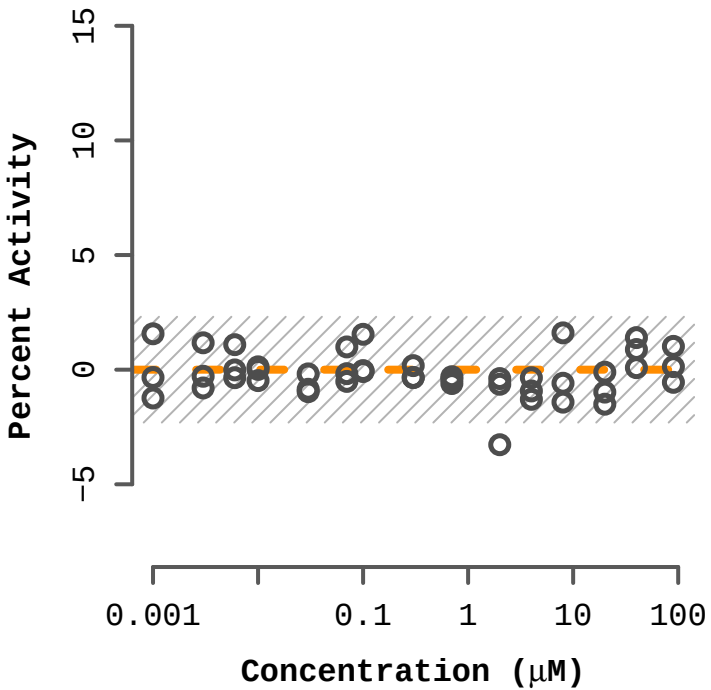
NAME: Chlorfenethol
CHID: 40283 CASRN: 80-06-8
SPID(S): Tox21_301458
M4ID: 12477675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.21	NA	NA
PROB:	1	NA	NA
RMSE:	2.3	NA	NA

MAX_MEAN: 0.344 MAX_MED: 0.434 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

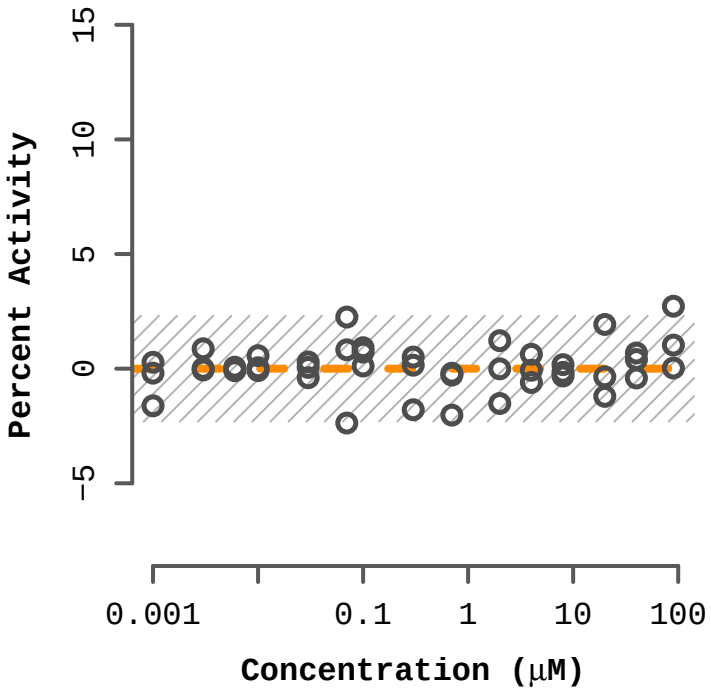
NAME: Chlorfenac
CHID: 40284 **CASRN:** 85-34-7
SPID(S): Tox21_301910
M4ID: 12477223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

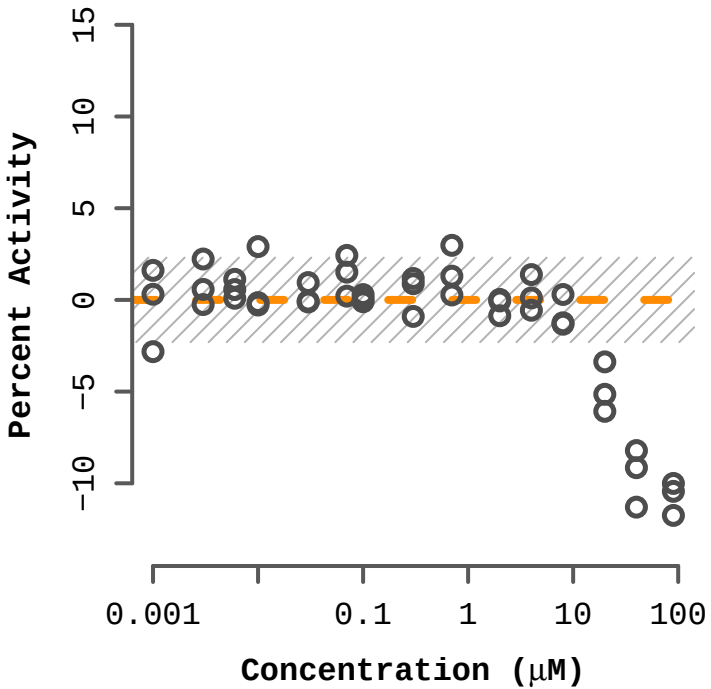
NAME: 2-Hydroxyacetophenone
CHID: 40285 **CASRN:** 118-93-4
SPID(S): Tox21_301119
M4ID: 12478014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

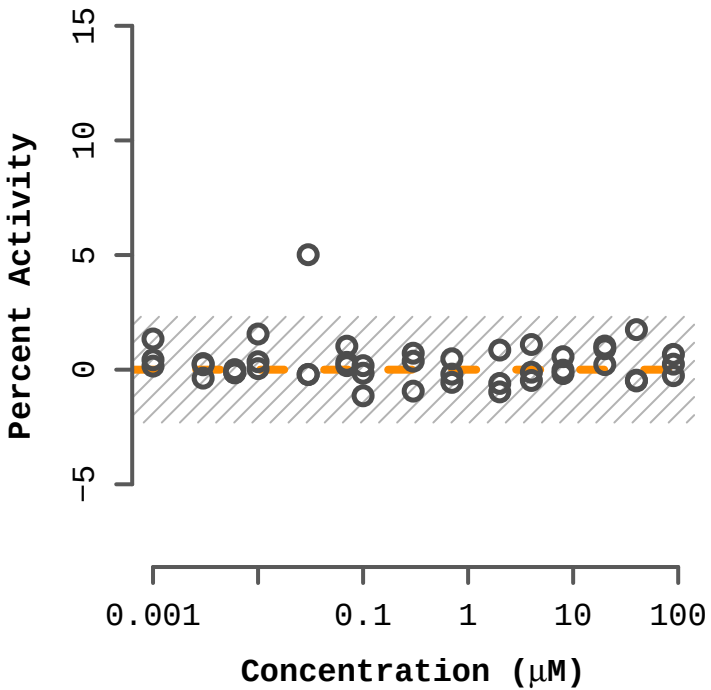
NAME: Chloroxuron
CHID: 40287 **CASRN:** 1982-47-4
SPID(S): Tox21_301902
M4ID: 12477231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	240.89	NA	NA
PROB:	1	NA	NA
RMSE:	4.1	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

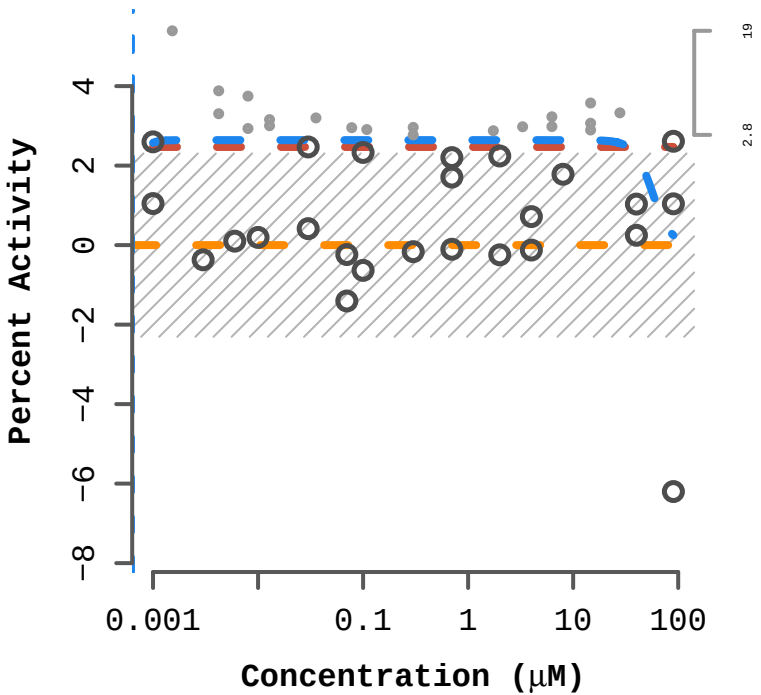
NAME: 6-Chloro-2-picolinic acid
CHID: 40289 **CASRN:** 4684-94-0
SPID(S): Tox21_301603
M4ID: 12477530

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.64	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorbromuron
CHID: 40290 CASRN: 13360-45-7
SPID(S): Tox21_300793
M4ID: 12478340 BRK

HILL MODEL (in red):

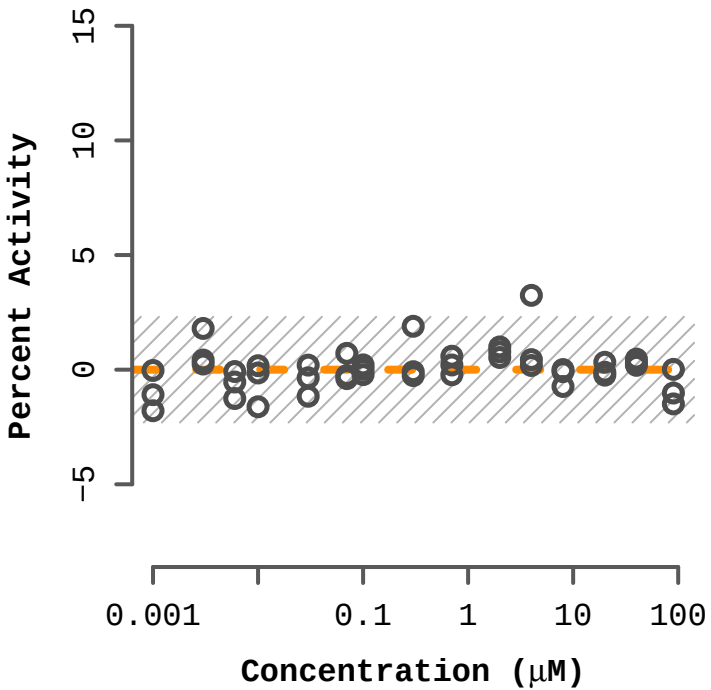
	tp	ga	gw
val:	2.47	−4.6	4.05
sd:	0.44	1600	3850

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.64	−3.2	8	1.75	4.94
sd:	0.501	3.34	134	0.839	12.2

	CNST	HILL	GNLS
AIC:	263.28	243.43	245.95
PROB:	0	0.78	0.22
RMSE:	4.77	3.82	3.71

MAX_MEAN: 7.61 MAX_MED: 6.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

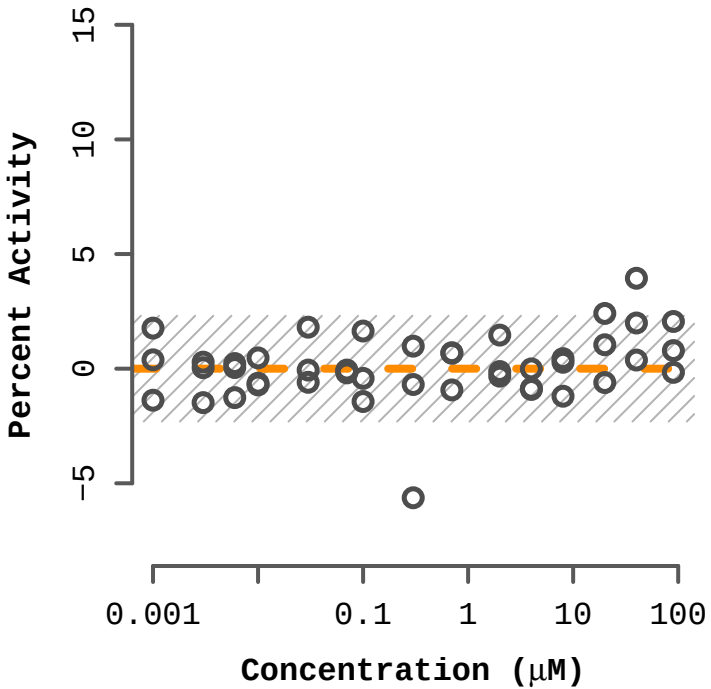
NAME: Propamocarb
CHID: 40295 CASRN: 24579-73-5
SPID(S): Tox21_301213
M4ID: 12477920

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.29 MAX_MED: 0.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

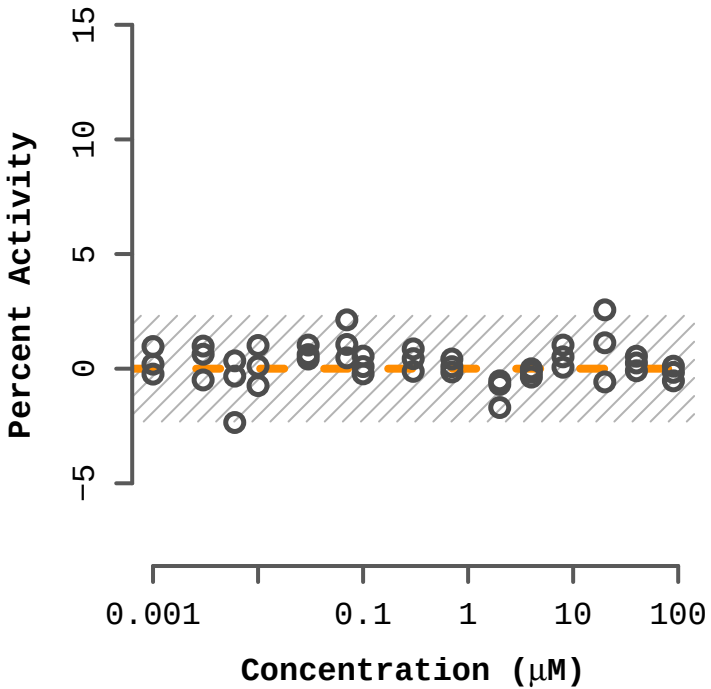
NAME: 2,3,6-Trichlorobenzoic acid
CHID: 40296 CASRN: 50-31-7
SPID(S): Tox21_300747
M4ID: 12478386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

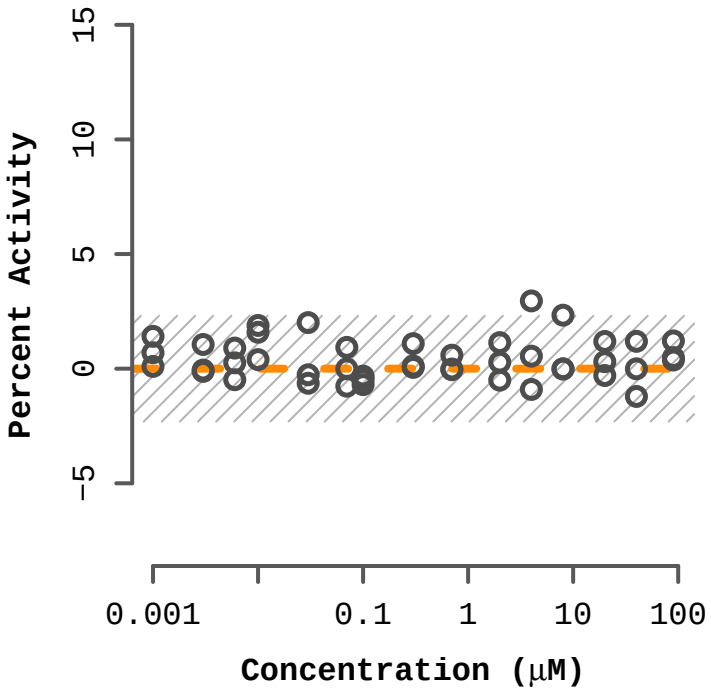
NAME: 4-Chlorobiphenyl
CHID: 40300 **CASRN:** 2051-62-9
SPID(S): Tox21_303788
M4ID: 12475400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

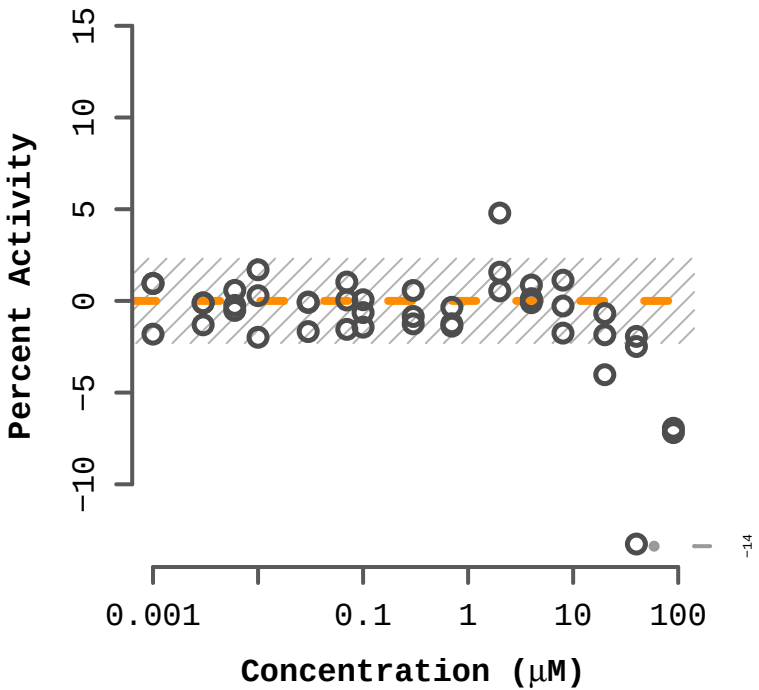
NAME: Nickel(II) chloride
CHID: 40316 CASRN: 7718-54-9
SPID(S): Tox21_302175
M4ID: 12476958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

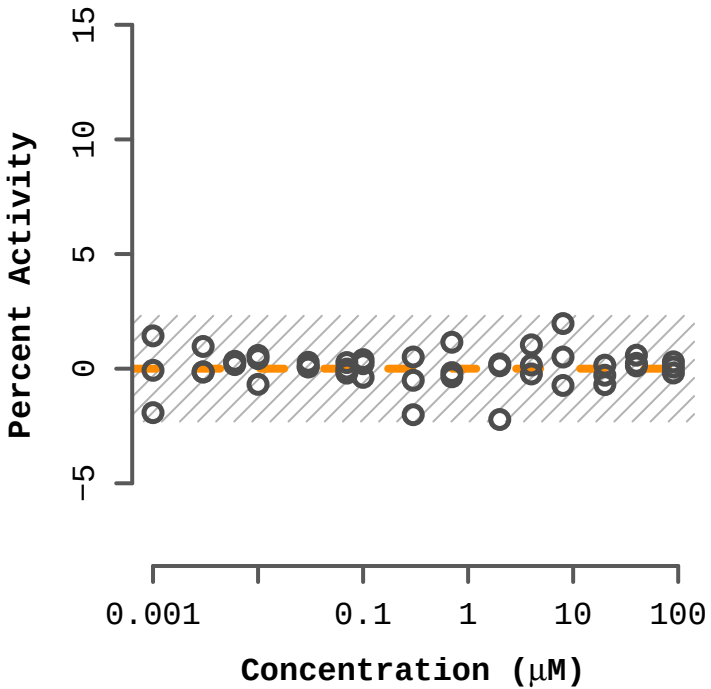
NAME: Bifenox
CHID: 40320 **CASRN:** 42576-02-3
SPID(S): Tox21_301616
M4ID: 12477517 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.64	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

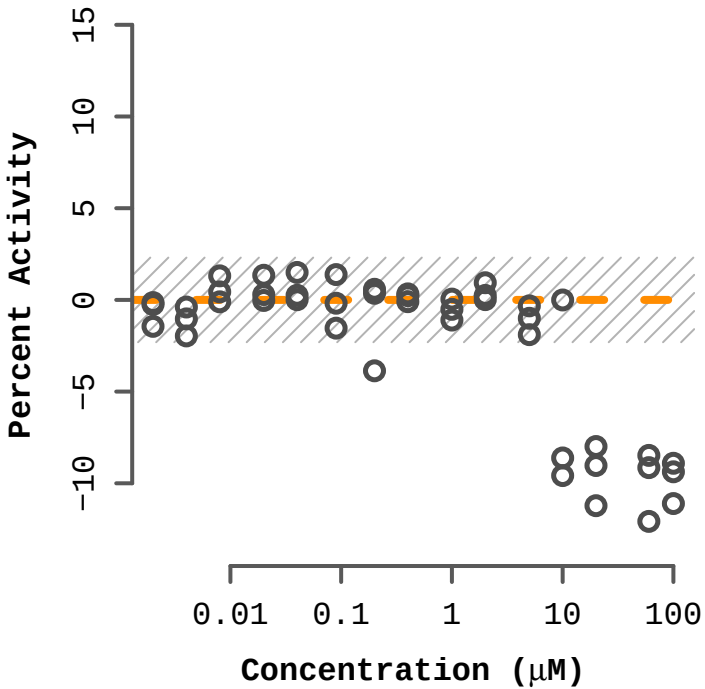
NAME: m-Cumenyl methylcarbamate
CHID: 40324 **CASRN:** 64-00-6
SPID(S): Tox21_302006
M4ID: 12477127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.582 **MAX_MED:** 0.508 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

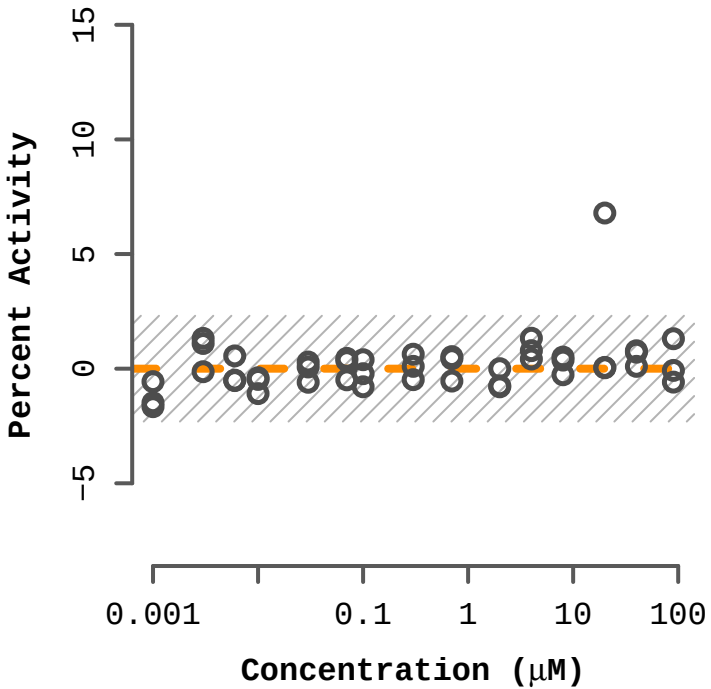
NAME: 8-Hydroxyquinoline citrate
CHID: 40326 **CASRN:** 134-30-5
SPID(S): Tox21_302376
M4ID: 12476757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	263.76	NA	NA
PROB:	1	NA	NA
RMSE:	4.87	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 0.439 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

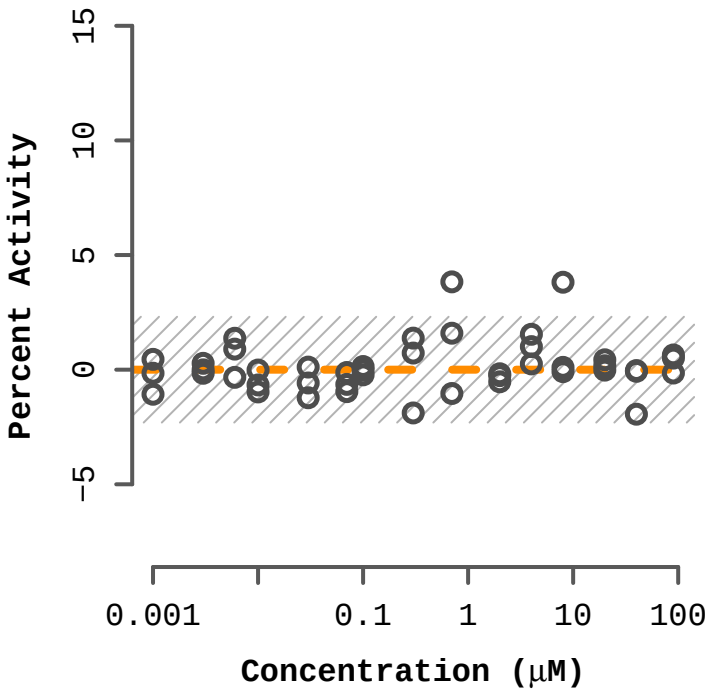
NAME: Butylene carbonate
CHID: 40342 **CASRN:** 4437-85-8
SPID(S): Tox21_301471
M4ID: 12477662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

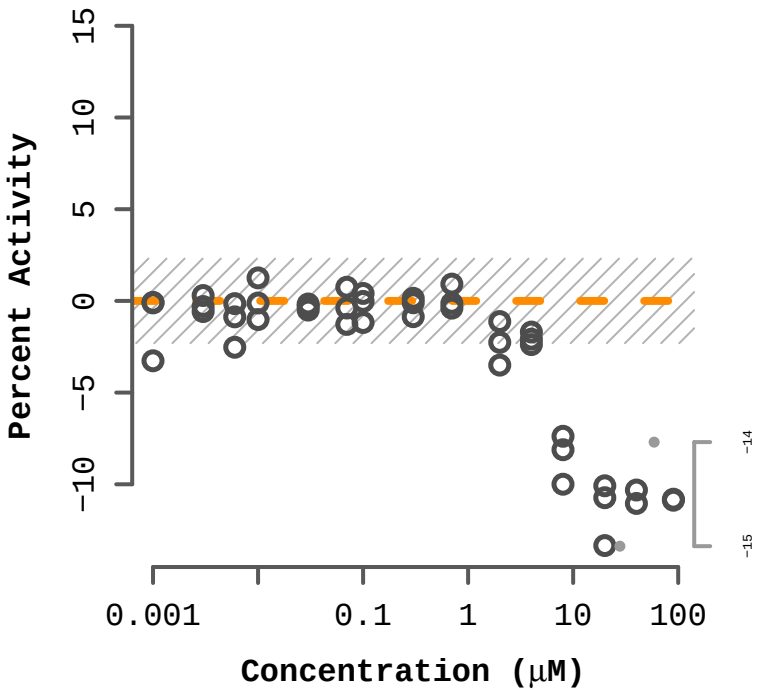
NAME: Benzyl bromoacetate
CHID: 40343 CASRN: 5437-45-6
SPID(S): Tox21_302092
M4ID: 12477041

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

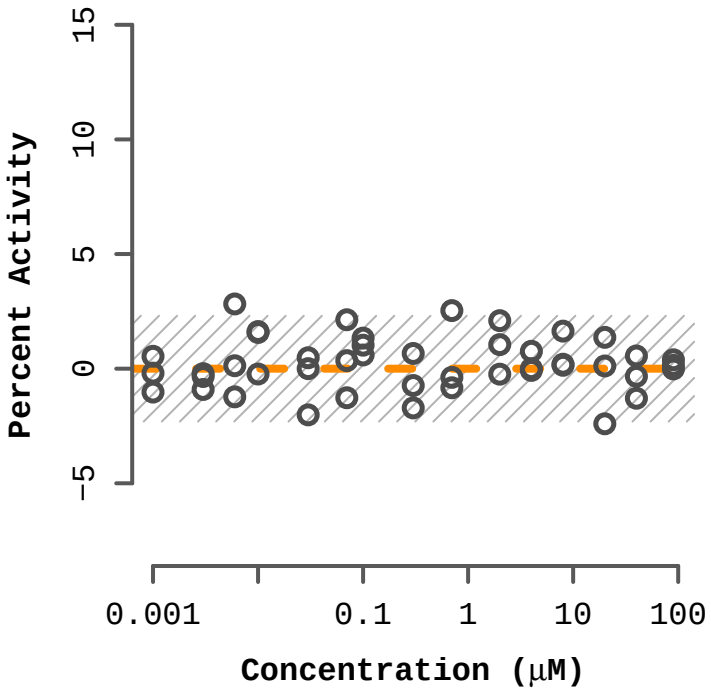
NAME: Dinocap
CHID: 40352 CASRN: 39300-45-3
SPID(S): Tox21_302217
M4ID: 12476916 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.17	NA	NA
PROB:	1	NA	NA
RMSE:	5.87	NA	NA

MAX_MEAN: 0.131 **MAX_MED:** −0.0254 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

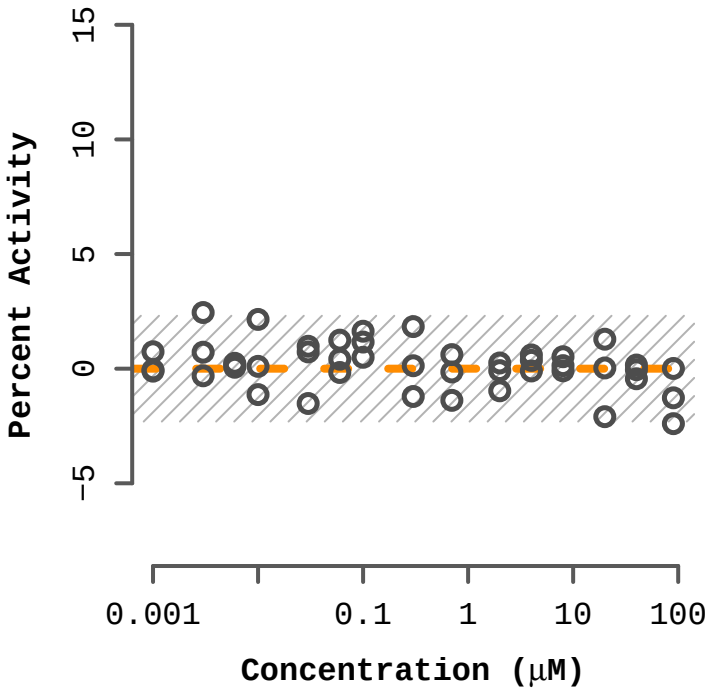
NAME: Isoxadifen-ethyl
CHID: 40360 **CASRN:** 163520-33-0
SPID(S): Tox21_301253
M4ID: 12477880

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.99 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

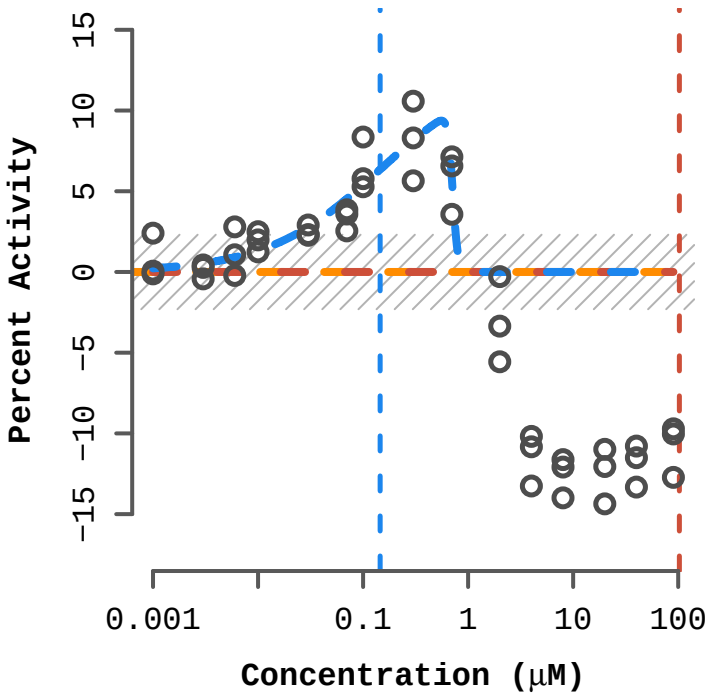
NAME: Metam−sodium hydrate
CHID: 40361 CASRN: 6734−80−1
SPID(S): Tox21_300736
M4ID: 12478397

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Niclosamide
CHID: 40362 CASRN: 50-65-7
SPID(S): Tox21_300749
M4ID: 12478384

HILL MODEL (in red):

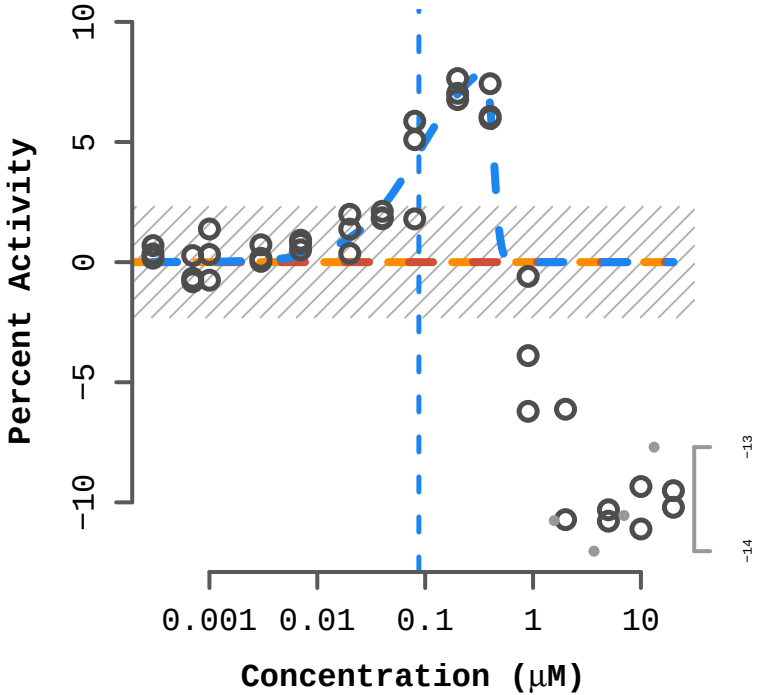
	tp	ga	gw
val:	1.7e-09	2.01	1.14
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.7	−0.838	0.805	−0.147	18
sd:	18.1	1.63	0.881	0.76	1680

	CNST	HILL	GNLS
AIC:	318.77	324.77	314.7
PROB:	0.11	0.01	0.88
RMSE:	7.75	7.75	7.02

MAX_MEAN: 8.18 MAX_MED: 8.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Niclosamide
CHID: 40362 CASRN: 50-65-7
SPID(S): Tox21_110209_1
M4ID: 12484550 BRK

HILL MODEL (in red):

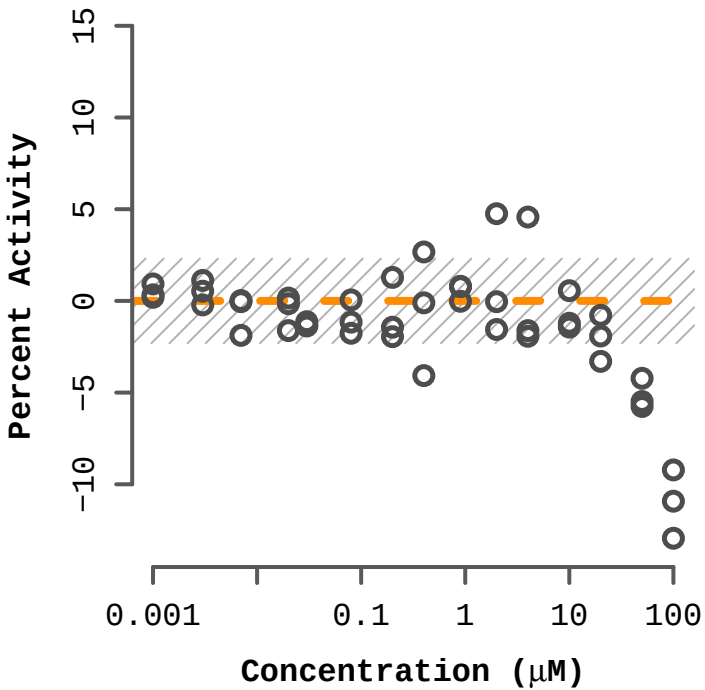
	tp	ga	gw
val:	3.02e-09	1.69	0.971
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.17	−1.06	1.41	−0.361	15.6
sd:	8.39	0.701	1.66	0.435	179

	CNST	HILL	GNLS
AIC:	300.35	306.35	293.05
PROB:	0.03	0	0.97
RMSE:	6.55	6.55	5.92

MAX_MEAN: 7.15 MAX_MED: 7.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

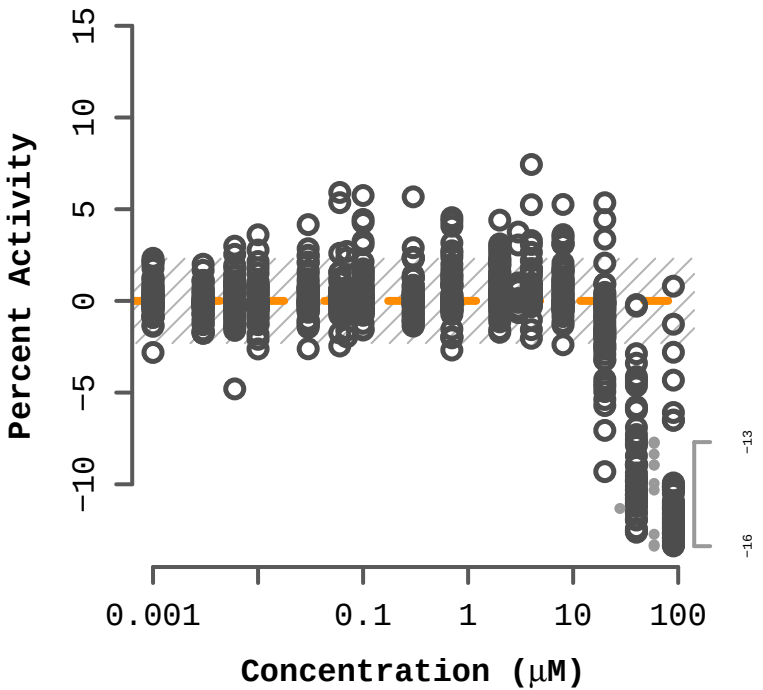
NAME: Diniconazole
CHID: 40363 **CASRN:** 83657-24-3
SPID(S): Tox21_300887
M4ID: 12478246

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.63	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

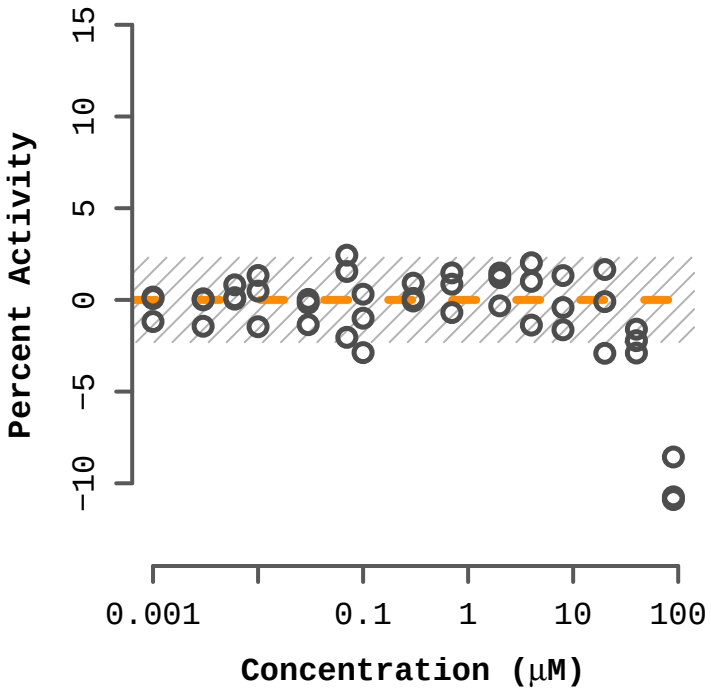
NAME: Fenaminosulf
CHID: 40371 **CASRN:** 140-56-7
SPID(S): Tox21_400002
M4ID: 12475135 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	3890.17	NA	NA
PROB:	1	NA	NA
RMSE:	4.11	NA	NA

MAX_MEAN: 0.934 **MAX_MED:** 0.649 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

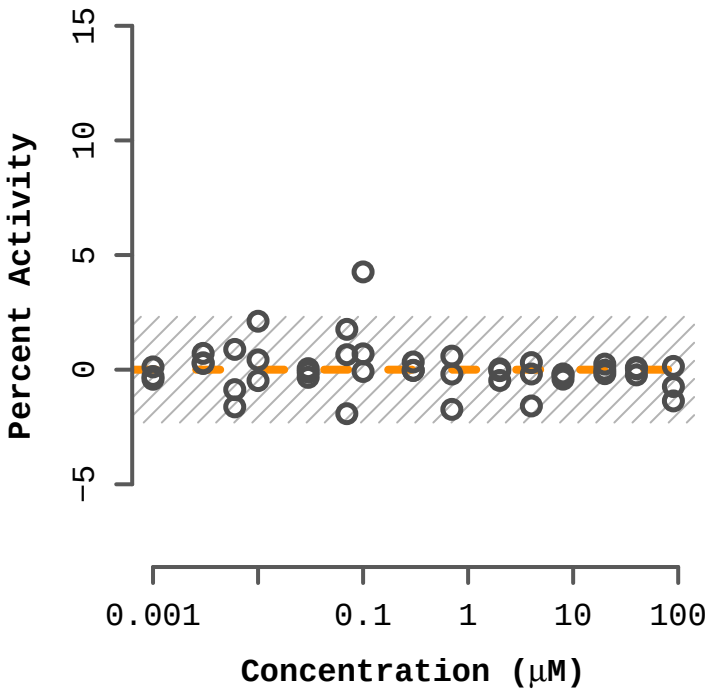
NAME: Epoxiconazole
CHID: 40372 **CASRN:** 133855-98-8
SPID(S): Tox21_300947
M4ID: 12478186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 0.789 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

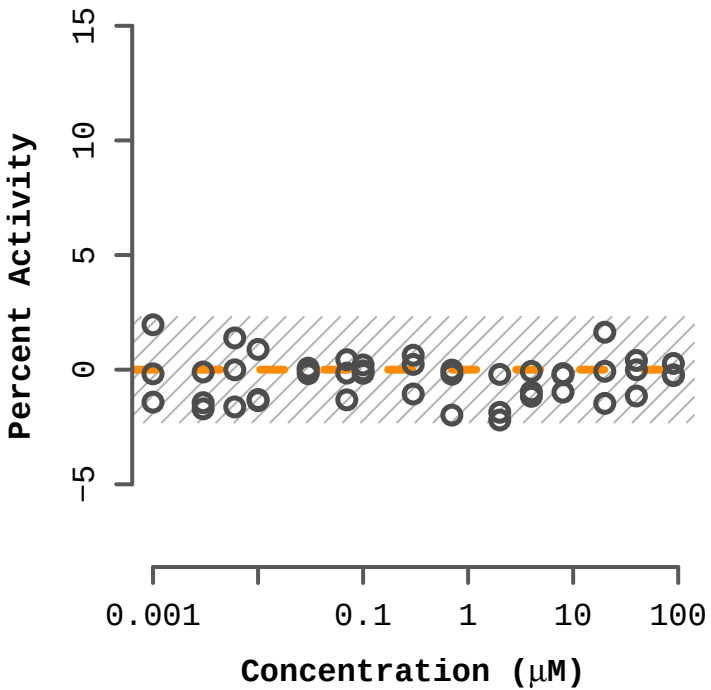
NAME: Metaflumizone
CHID: 40373 **CASRN:** 139968-49-3
SPID(S): Tox21_303944
M4ID: 12475244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.04	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 0.693 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

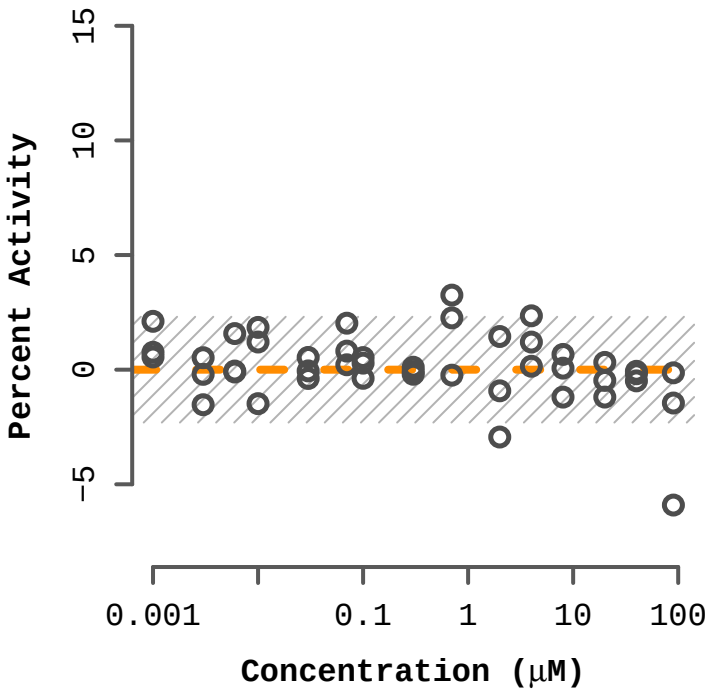
NAME: 1,2-Butanediol
CHID: 40375 **CASRN:** 584-03-2
SPID(S): Tox21_303800
M4ID: 12475388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.123 **MAX_MED:** 0.232 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

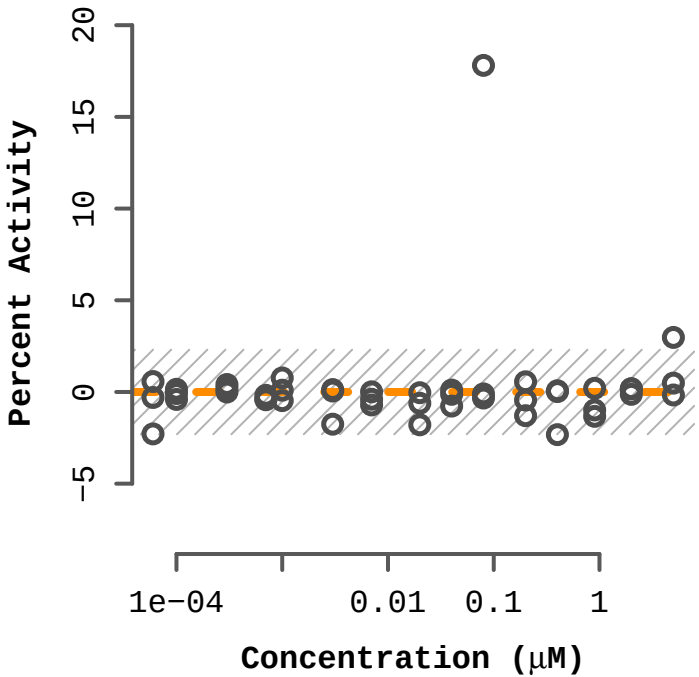
NAME: 9-cis Retinoic acid
CHID: 40404 **CASRN:** 5300-03-8
SPID(S): Tox21_302195
M4ID: 12476938

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

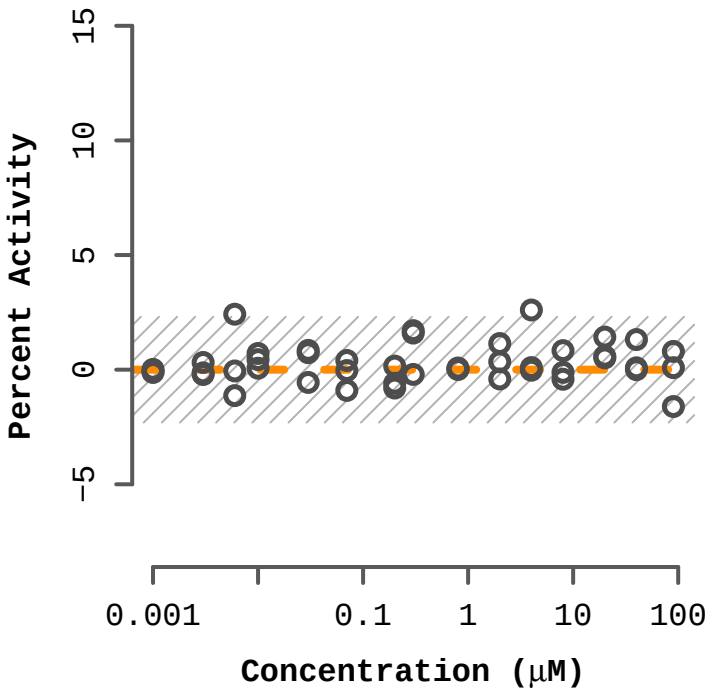
NAME: cAMP
CHID: 40436 **CASRN:** 60-92-4
SPID(S): Tox21_113510_1
M4ID: 12482624

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.8	NA	NA

MAX_MEAN: 5.79 **MAX_MED:** 0.485 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

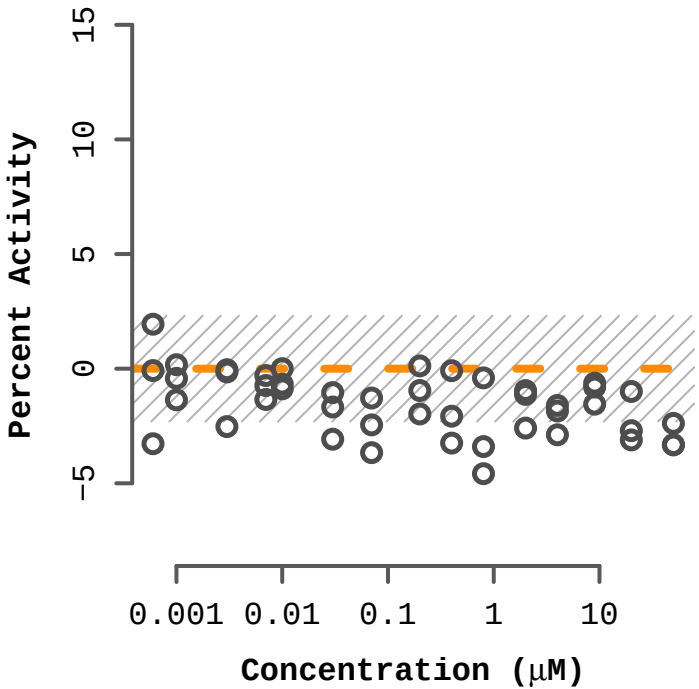
NAME: Copper(II) chloride
CHID: 40449 CASRN: 7447-39-4
SPID(S): Tox21_202868
M4ID: 12479384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

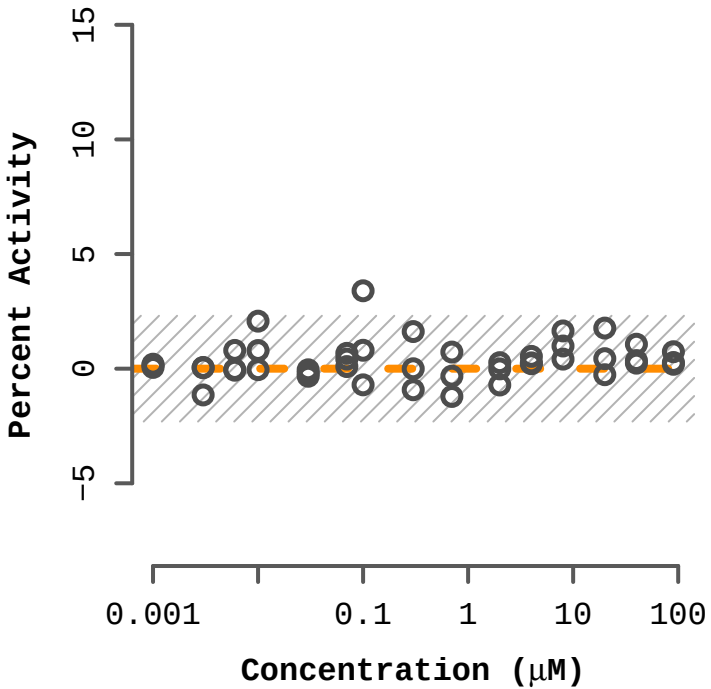
NAME: Docetaxel
CHID: 40464 **CASRN:** 114977-28-5
SPID(S): Tox21_112781_1
M4ID: 12482954

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.84	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: −0.471 **MAX_MED:** −0.0801 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

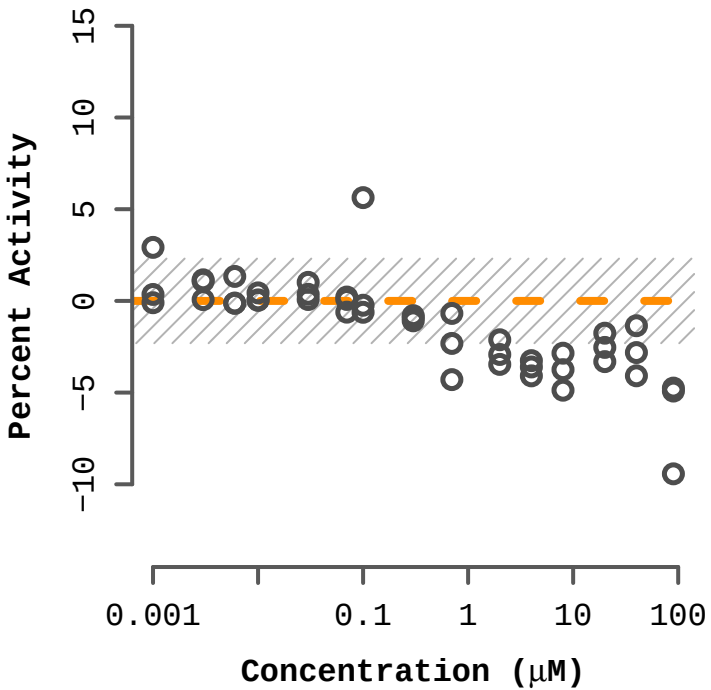
NAME: Fenazaquin
CHID: 40476 **CASRN:** 120928-09-8
SPID(S): Tox21_301223
M4ID: 12477910

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

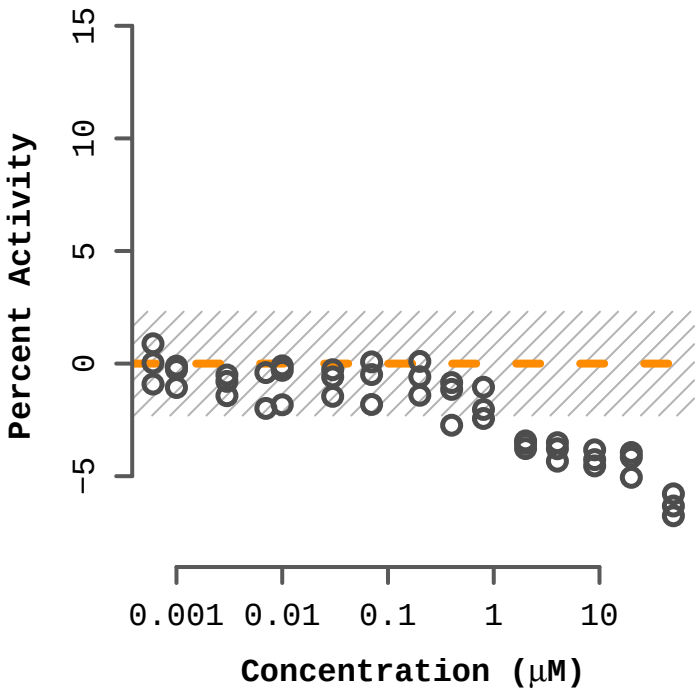
NAME: Forskolin
CHID: 40484 **CASRN:** 66575-29-9
SPID(S): Tox21_302399
M4ID: 12476734

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.75	NA	NA
PROB:	1	NA	NA
RMSE:	2.86	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

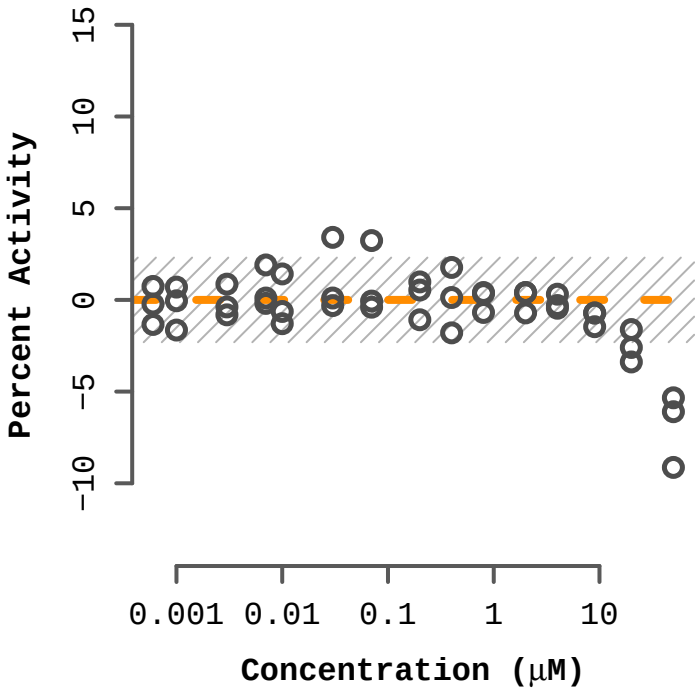
NAME: Forskolin
CHID: 40484 **CASRN:** 66575-29-9
SPID(S): Tox21_110940_1
M4ID: 12483998

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.85	NA	NA

MAX_MEAN: 0.00191 **MAX_MED:** 0.0315 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

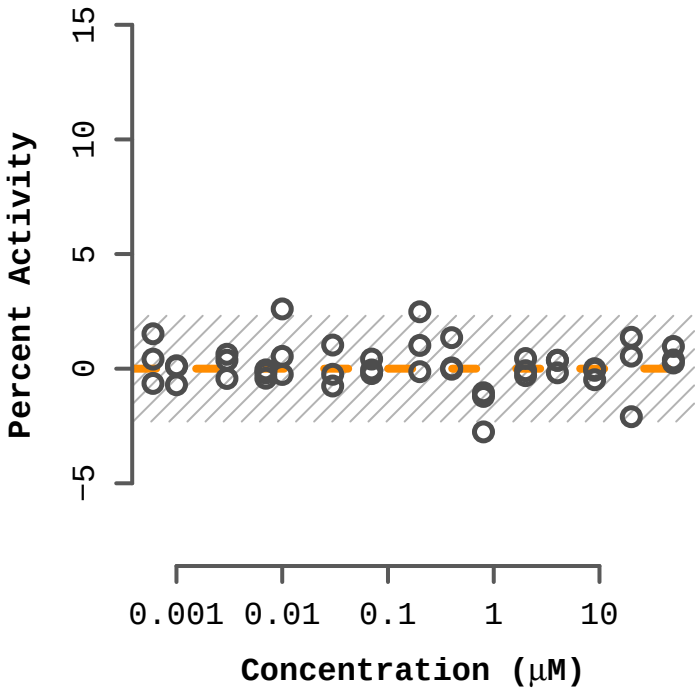
NAME: Imatinib mesylate
CHID: 40502 **CASRN:** 220127-57-1
SPID(S): Tox21_111684_1
M4ID: 12483537

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.539 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

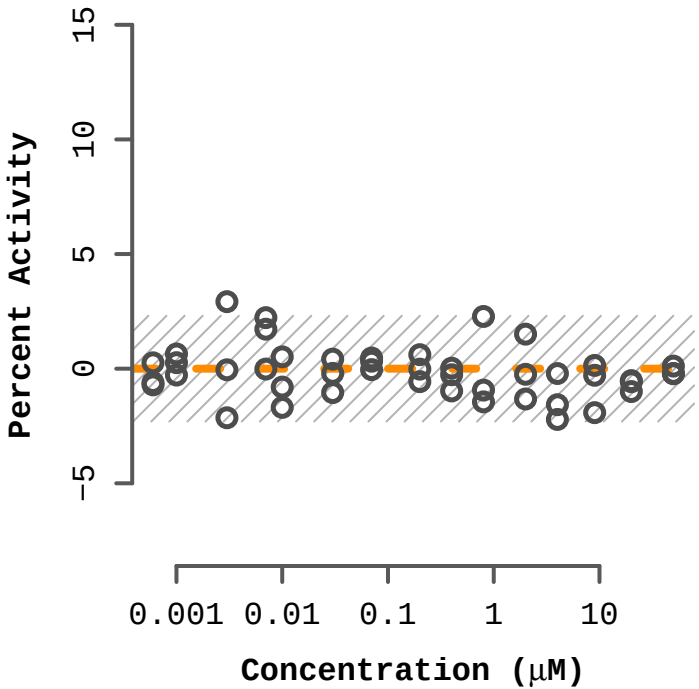
NAME: Kainic acid
CHID: 40526 **CASRN:** 487-79-6
SPID(S): Tox21_110905_1
M4ID: 12484026

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

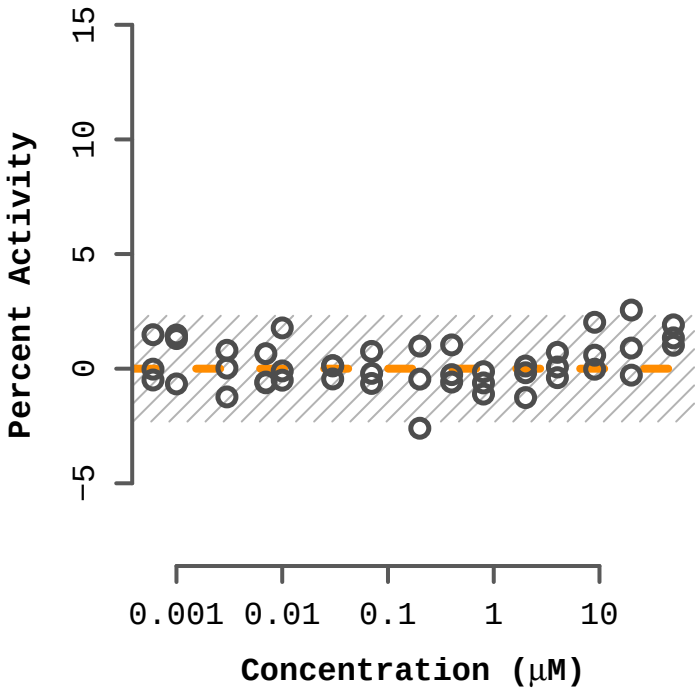
NAME: L−Nitroarginine methyl ester
CHID: 40540 **CASRN:** 50903−99−6
SPID(S): Tox21_110920_1
M4ID: 12484014

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

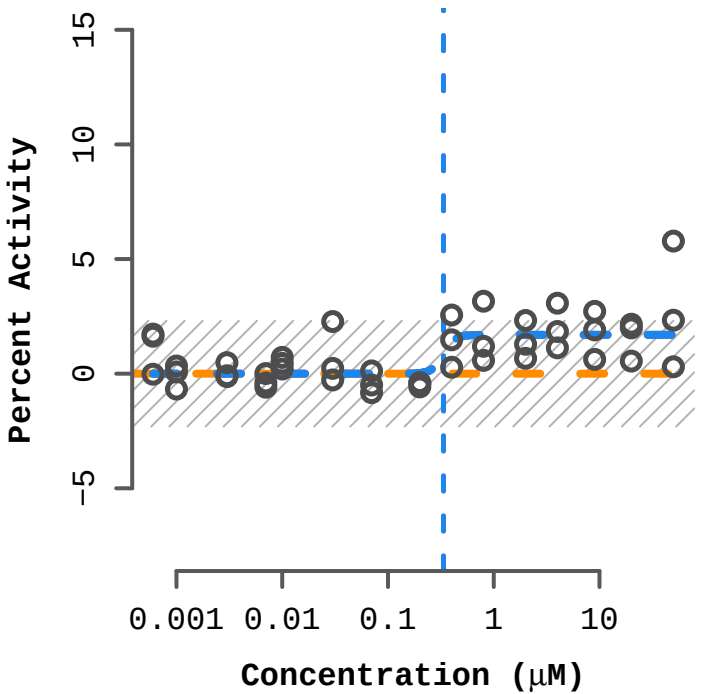
NAME: Moclobemide
CHID: 40554 **CASRN:** 71320-77-9
SPID(S): Tox21_110971_1
M4ID: 12483976

HILL MODEL: Not applicable.

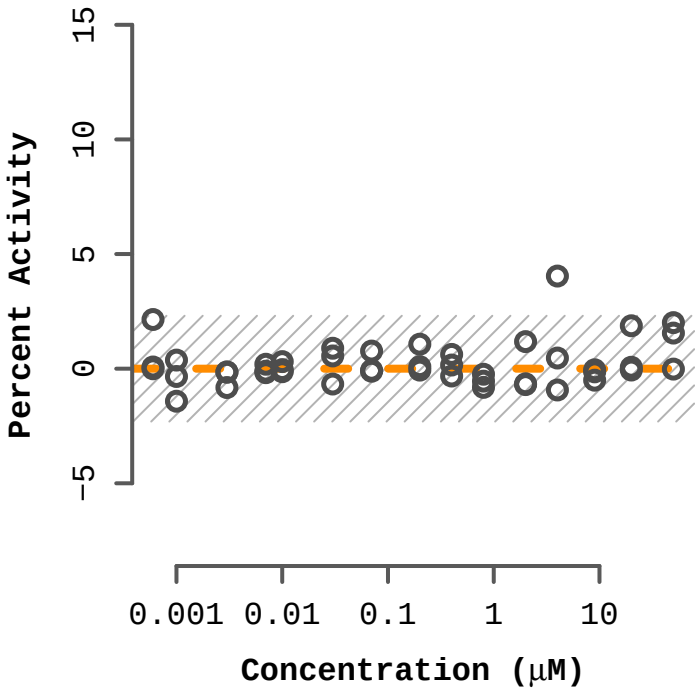
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.35 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pergolide methanesulfonate
CHID:    40583   CASRN: 66104-23-2
SPID(S): Tox21_110820_1
M4ID:    12484096

HILL MODEL (in red):
      tp       ga       gw
val:  1.69     -0.475   8
sd:   0.232    0.0959   5.96

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.69     -0.475   8        3.67     5.67
sd:   0.232    0.0959   5.96     110000   315000

      CNST        HILL        GNLS
AIC:  167.81      131.64      135.64
PROB: 0           0.88        0.12
RMSE: 1.61        1.03        1.03

MAX_MEAN: 2.81      MAX_MED: 2.33      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

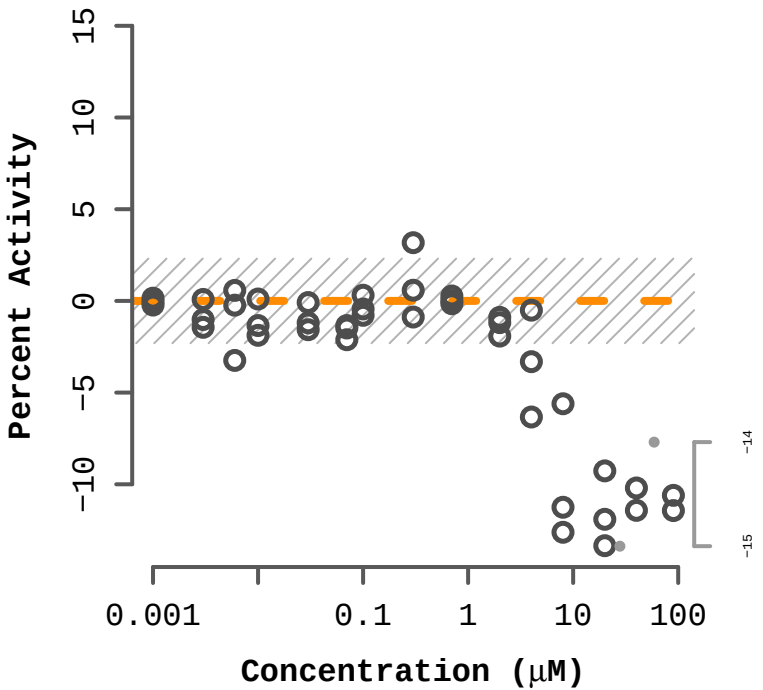
NAME: Scopolamine methylbromide
CHID: 40608 **CASRN:** 155-41-9
SPID(S): Tox21_110037_1
M4ID: 12484699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

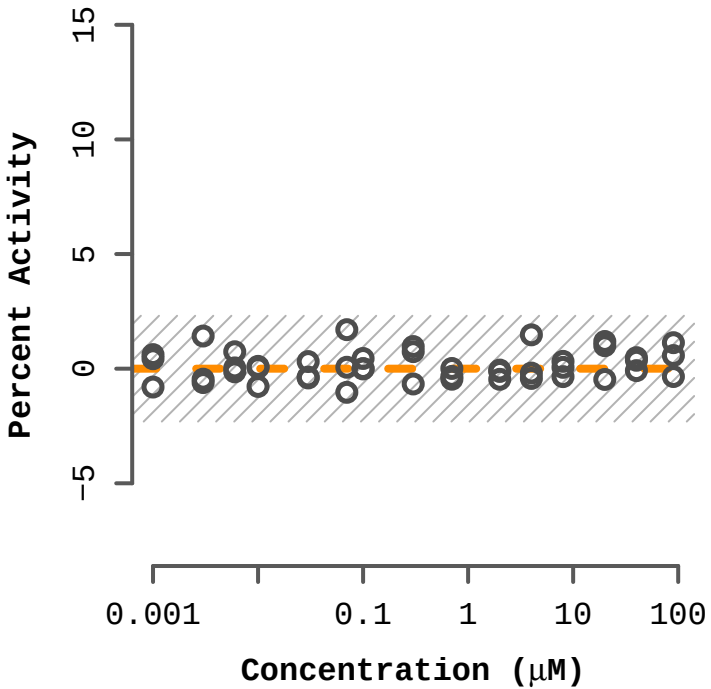
NAME: Silwet L77
CHID: 40611 **CASRN:** 27306-78-1
SPID(S): Tox21_301769
M4ID: 12477364 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	287.71	NA	NA
PROB:	1	NA	NA
RMSE:	6.16	NA	NA

MAX_MEAN: 0.961 **MAX_MED:** 0.583 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

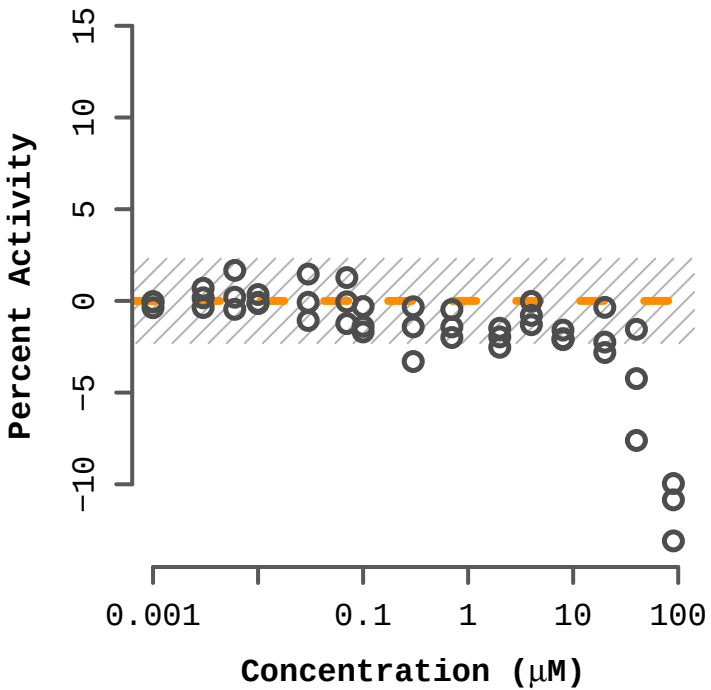
NAME: Sodium pyruvate
CHID: 40614 **CASRN:** 113-24-6
SPID(S): Tox21_301486
M4ID: 12477647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

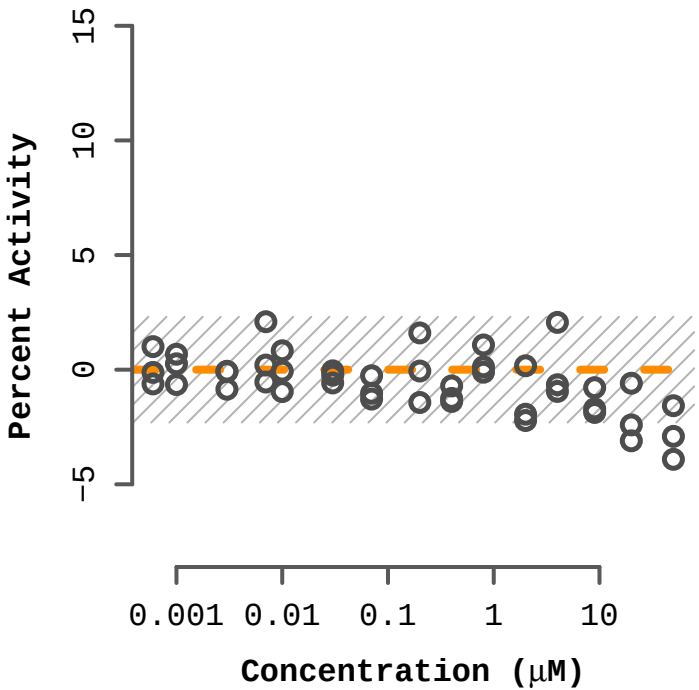
NAME: Bexarotene
CHID: 40619 **CASRN:** 153559-49-0
SPID(S): Tox21_302407
M4ID: 12476726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.46	NA	NA

MAX_MEAN: 0.47 **MAX_MED:** 0.203 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

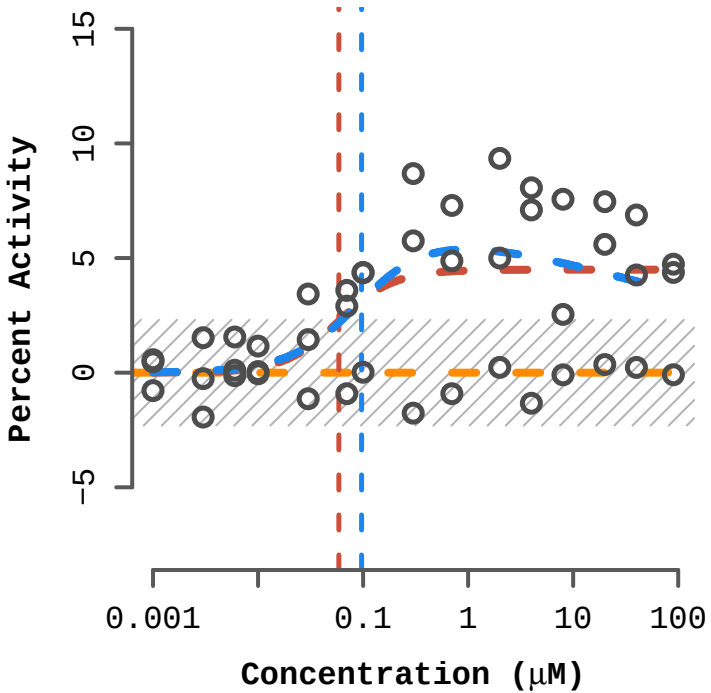
NAME: Bexarotene
CHID: 40619 **CASRN:** 153559-49-0
SPID(S): Tox21_112666_1
M4ID: 12482989

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.259 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'−Dipyridyl
CHID: 40635 CASRN: 366−18−7
SPID(S): Tox21_301430
M4ID: 12477703

HILL MODEL (in red):

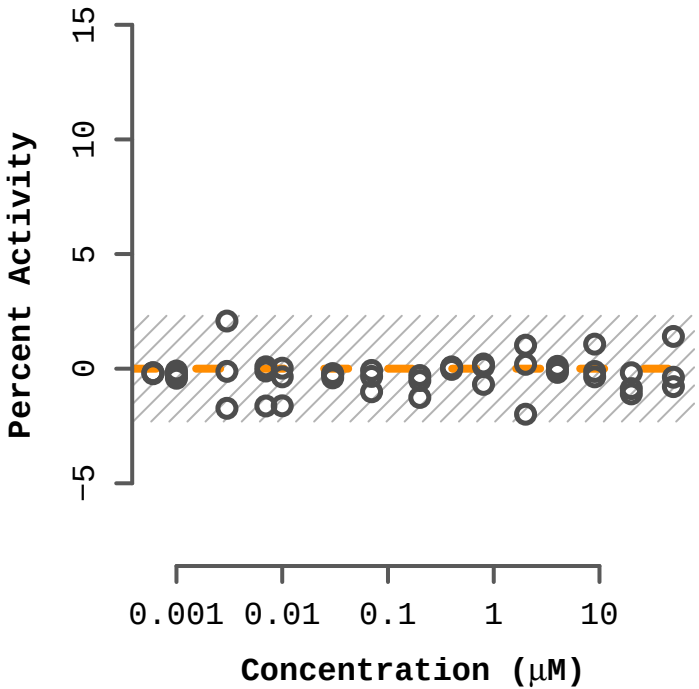
	tp	ga	gw
val:	4.49	−1.23	1.67
sd:	0.713	0.262	1.45

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.01	−1.01	1.31	1.99	0.306
sd:	23.9	0.878	1.26	8.89	2.11

	CNST	HILL	GNLS
AIC:	258.36	230.01	232.85
PROB:	0	0.81	0.19
RMSE:	4.12	2.77	2.78

MAX_MEAN: 4.86 MAX_MED: 7.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

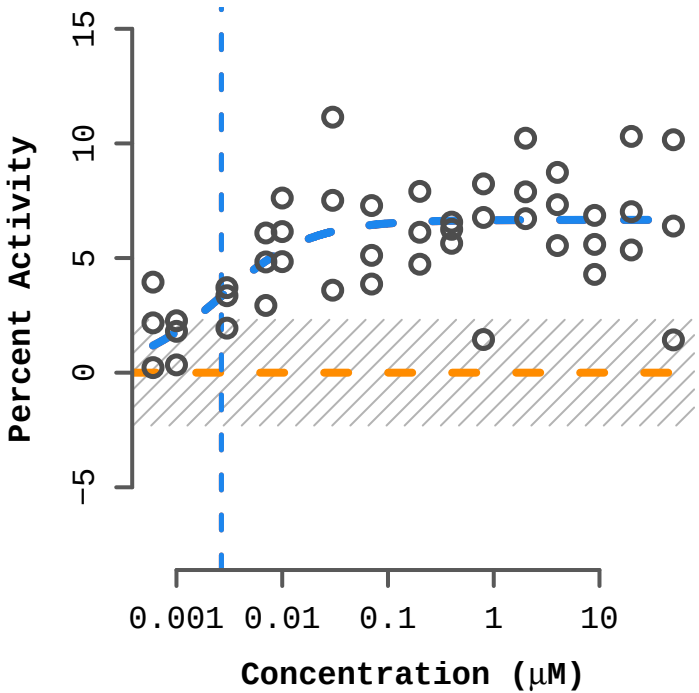
NAME: Xylazine
CHID: 40643 **CASRN:** 7361-61-7
SPID(S): Tox21_110303_1
M4ID: 12484469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.198 **MAX_MED:** 0.191 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexrazone
CHID: 40647 CASRN: 24584-09-6
SPID(S): Tox21_112256_1
M4ID: 12483198

HILL MODEL (in red):

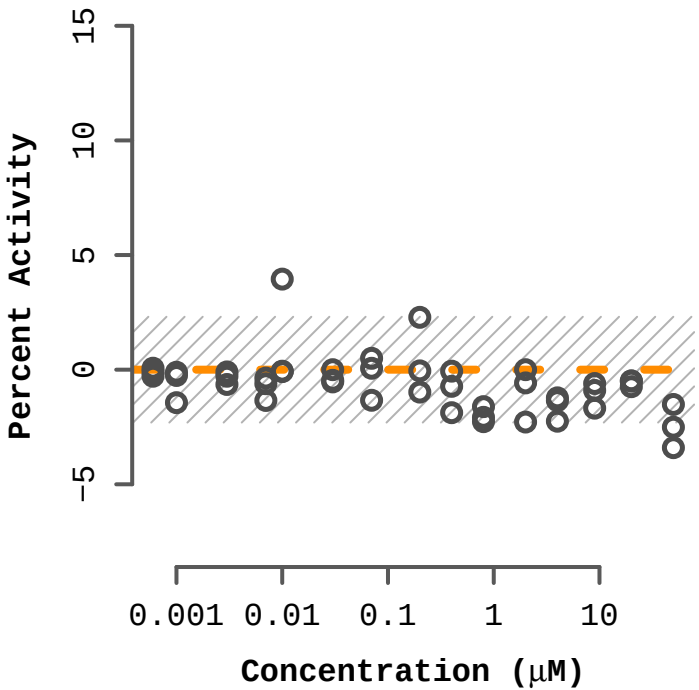
	tp	ga	gw
val:	6.66	−2.58	1.03
sd:	0.378	0.15	0.413

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.67	−2.57	1.03	1.86	11.2
sd:	0.391	0.151	0.414	2.3	163

	CNST	HILL	GNLS
AIC:	300.54	198.18	202.18
PROB:	0	0.88	0.12
RMSE:	6.12	2.04	2.03

MAX_MEAN: 8.28 **MAX_MED:** 7.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

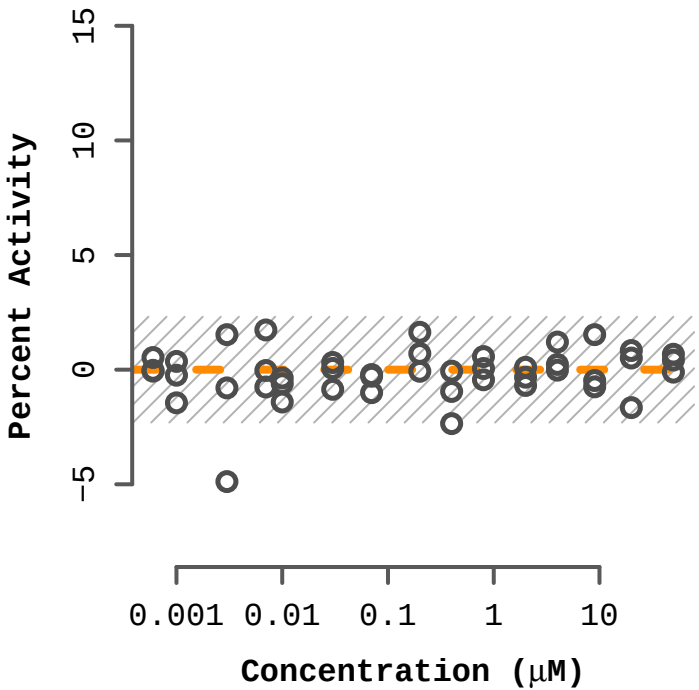
NAME: Artemisinin
CHID: 40652 **CASRN:** 63968-64-9
SPID(S): Tox21_111750_1
M4ID: 12483500

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.0615 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

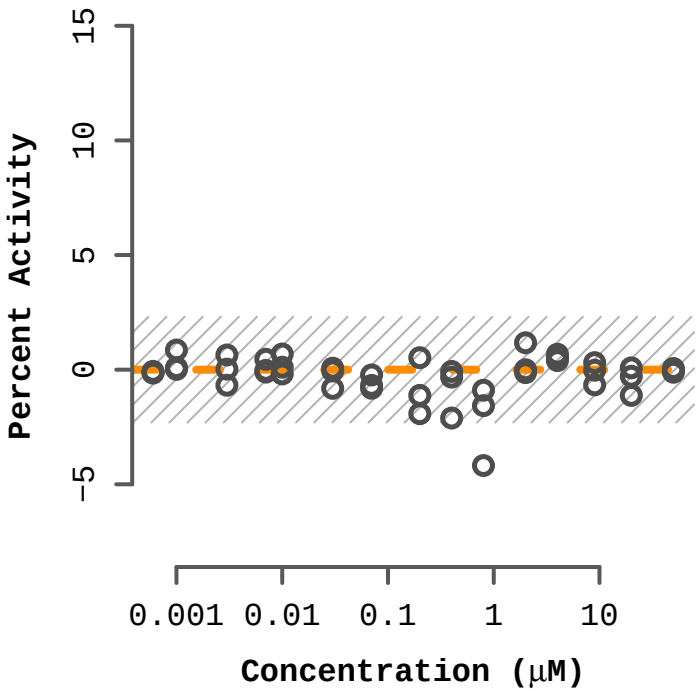
NAME: Balsalazide
CHID: 40653 **CASRN:** 80573-04-2
SPID(S): Tox21_112252_1
M4ID: 12483200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.757 **MAX_MED:** 0.707 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

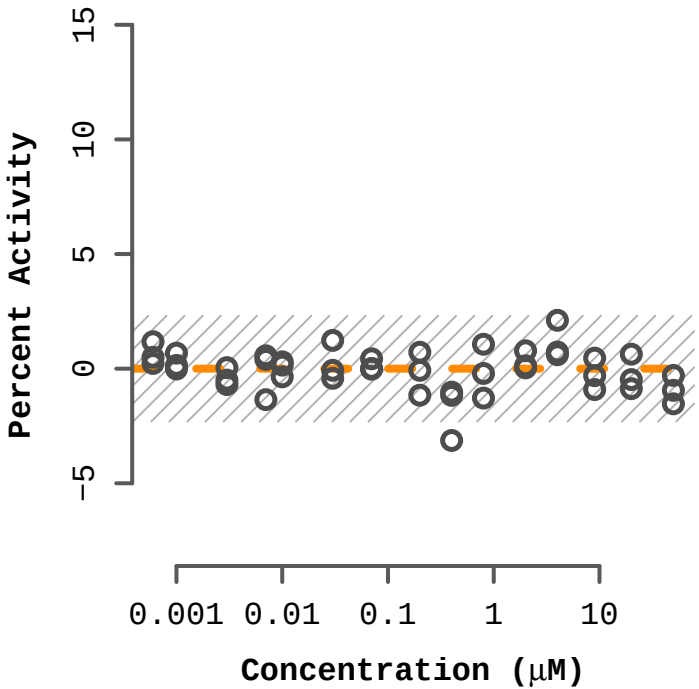
NAME: Bromisovalum
CHID: 40656 **CASRN:** 496-67-3
SPID(S): Tox21_111815_1
M4ID: 12483461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.54 **MAX_MED:** 0.549 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

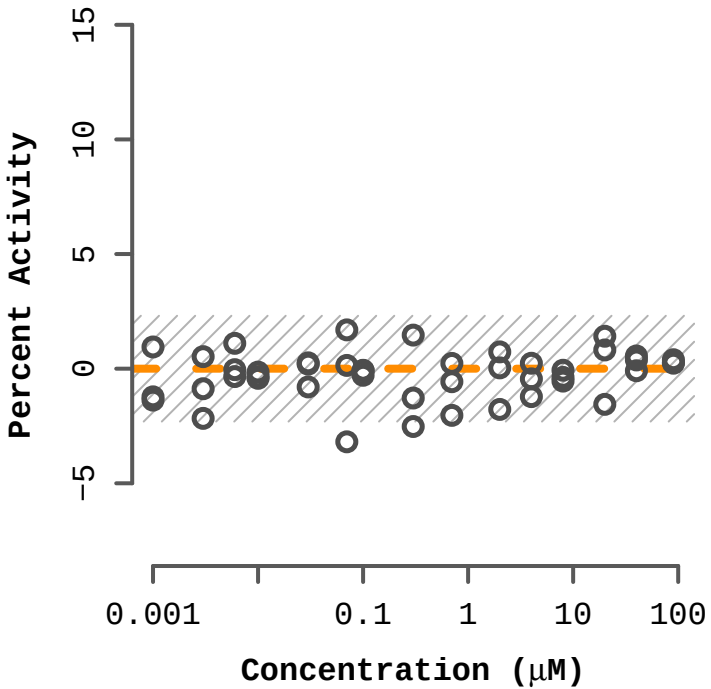
NAME: Butenafine
CHID: 40657 **CASRN:** 101828-21-1
SPID(S): Tox21_111729_1
M4ID: 12483517

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.729 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

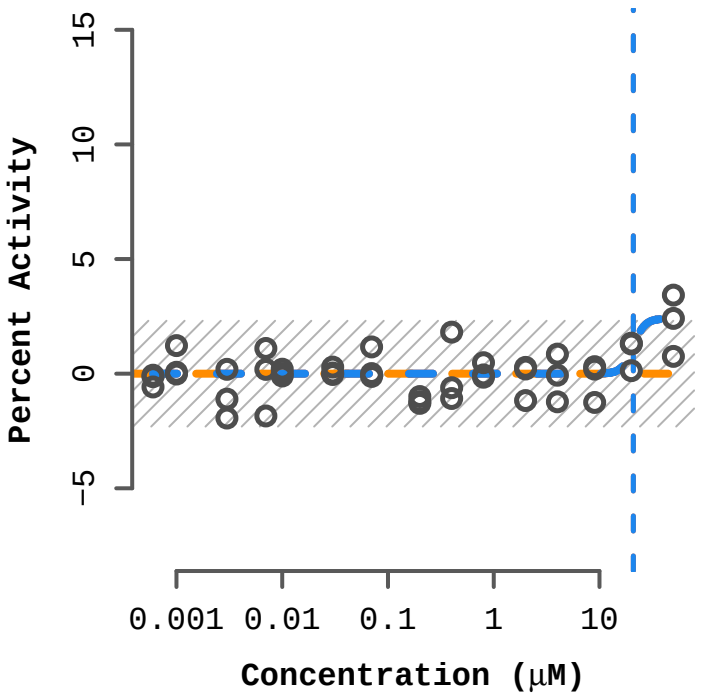
NAME: Clofibric acid
CHID: 40661 **CASRN:** 882-09-7
SPID(S): Tox21_301680
M4ID: 12477453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.301 **MAX_MED:** 0.818 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clofibric acid
CHID: 40661 **CASRN:** 882-09-7
SPID(S): Tox21_110486_1
M4ID: 12484320

HILL MODEL (in red):

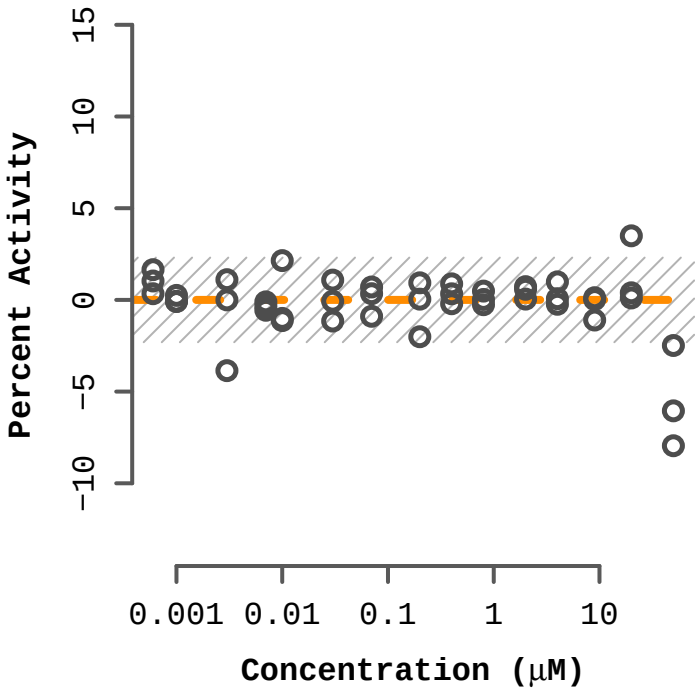
	tp	ga	gw
val:	2.4	1.32	8
sd:	0.586	0.0913	31.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.4	1.32	8	2.61	10.4
sd:	0.586	0.0914	31.4	95000	1550000

	CNST	HILL	GNLS
AIC:	131.27	122.21	126.21
PROB:	0.01	0.87	0.12
RMSE:	1.05	0.85	0.85

MAX_MEAN: 2.2 **MAX_MED:** 2.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

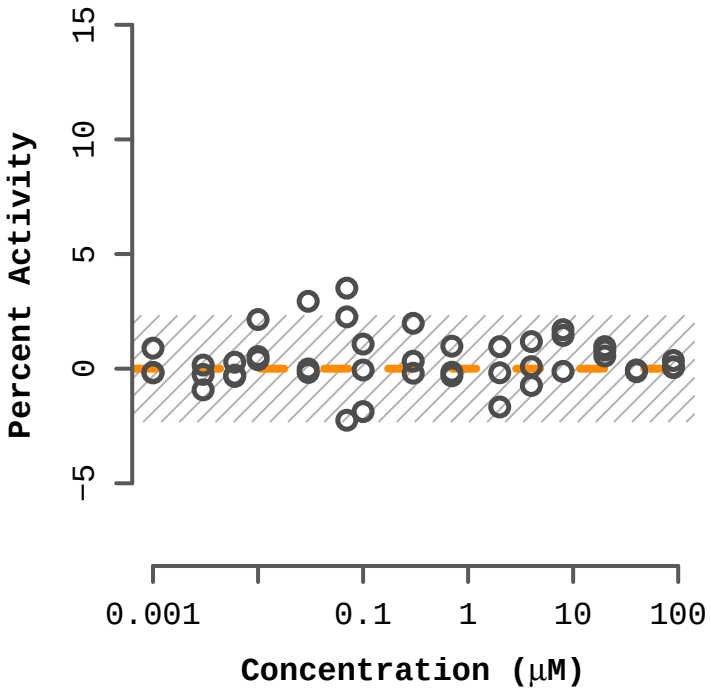
NAME: Closantel
CHID: 40662 **CASRN:** 57808-65-8
SPID(S): Tox21_112408_1
M4ID: 12483112

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

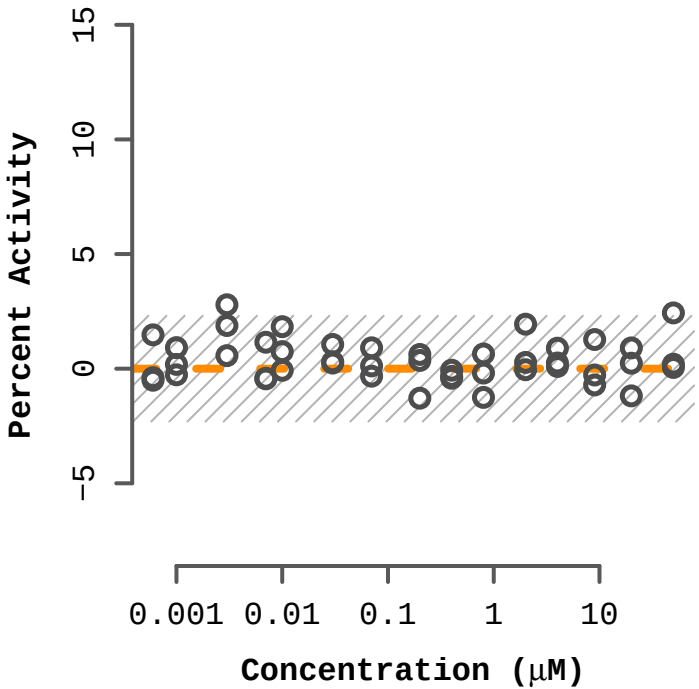
NAME: Crotamiton
CHID: 40664 **CASRN:** 483-63-6
SPID(S): Tox21_300804
M4ID: 12478329

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

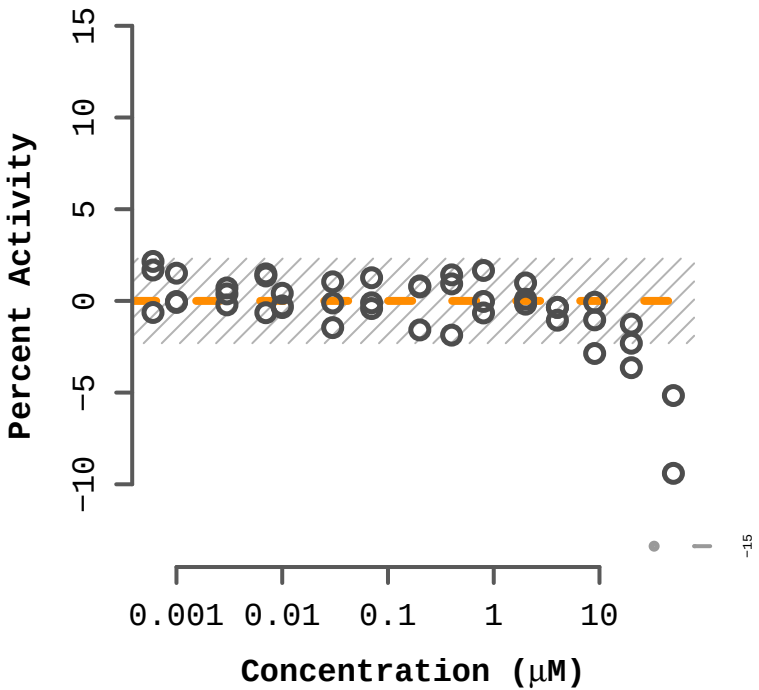
NAME: Crotamiton
CHID: 40664 **CASRN:** 483-63-6
SPID(S): Tox21_110446_1
M4ID: 12484349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

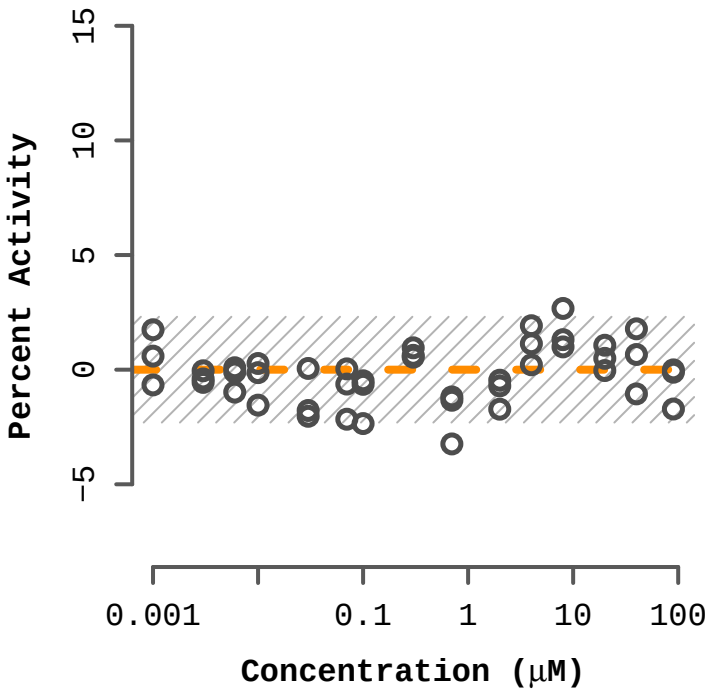
NAME: Dipyridamole
CHID: 40668 **CASRN:** 58-32-2
SPID(S): Tox21_110133_1
M4ID: 12484621 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.02	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

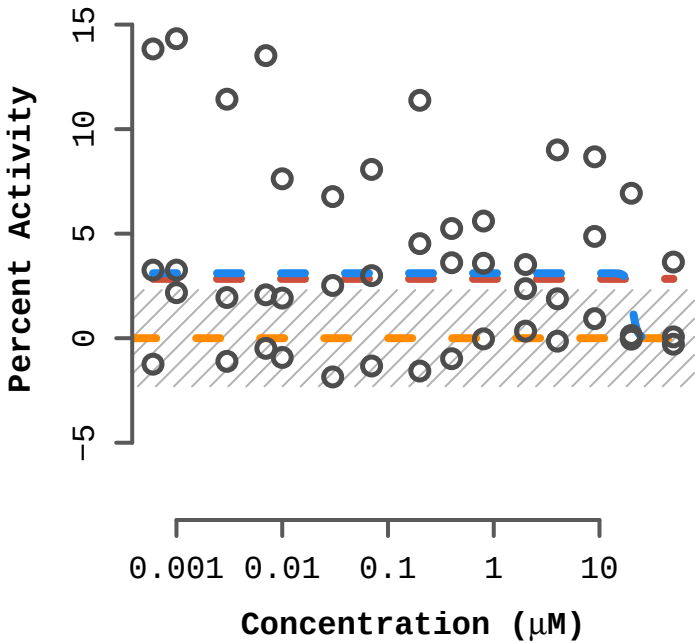
NAME: Fenbendazole
CHID: 40672 **CASRN:** 43210-67-9
SPID(S): Tox21_301828
M4ID: 12477305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenbendazole
CHID: 40672 **CASRN:** 43210-67-9
SPID(S): Tox21_110649_1
M4ID: 12484206

HILL MODEL (in red):

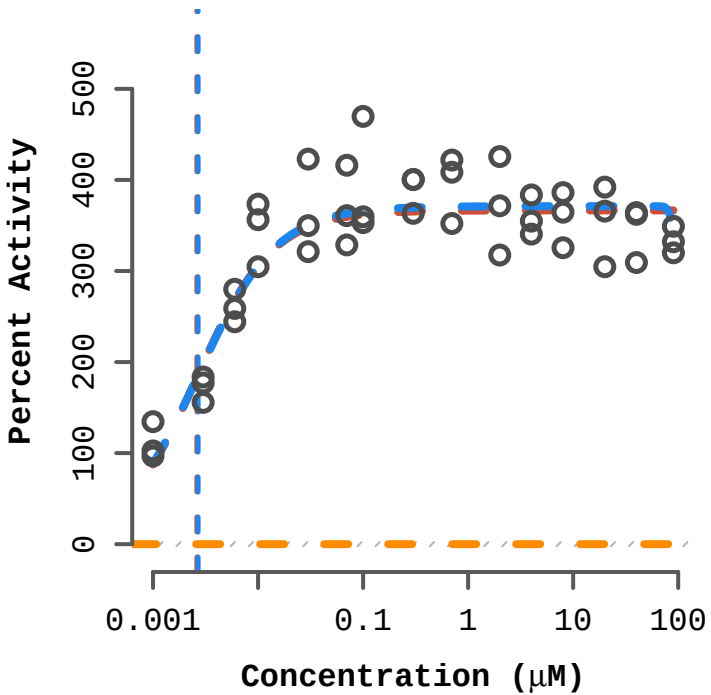
	tp	ga	gw
val:	2.84	−4.74	4.42
sd:	0.625	1250	3460

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.11	−4.88	4.1	1.31	17.9
sd:	0.676	1990	4540	0.149	346

	CNST	HILL	GNLS
AIC:	283.21	269.22	272.35
PROB:	0	0.83	0.17
RMSE:	5.66	4.44	4.38

MAX_MEAN: 6.59 **MAX_MED:** 4.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluocinolone acetonide
CHID: 40674 CASRN: 67-73-2
SPID(S): Tox21_302364
M4ID: 12476769

HILL MODEL (in red):

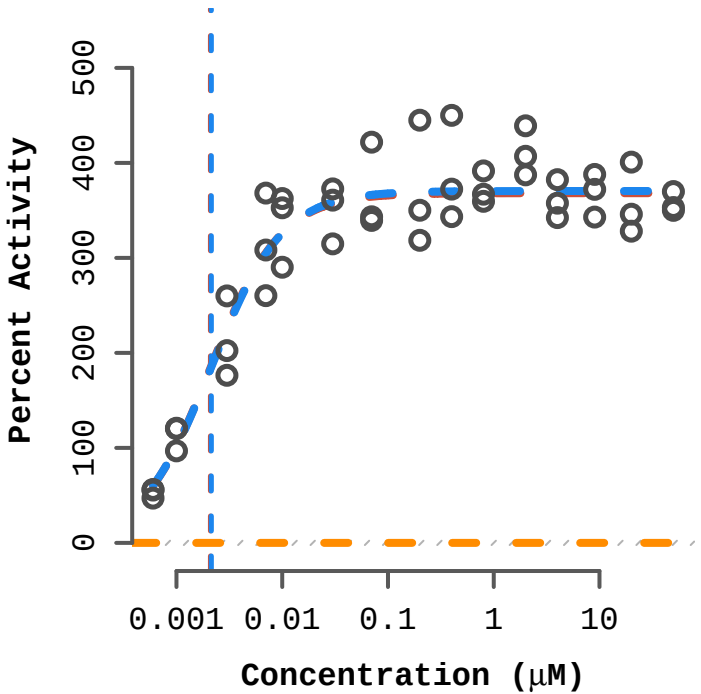
	tp	ga	gw
val:	367	-2.58	1.2
sd:	6.72	0.057	0.175

GAIN-LOSS MODEL (in blue):

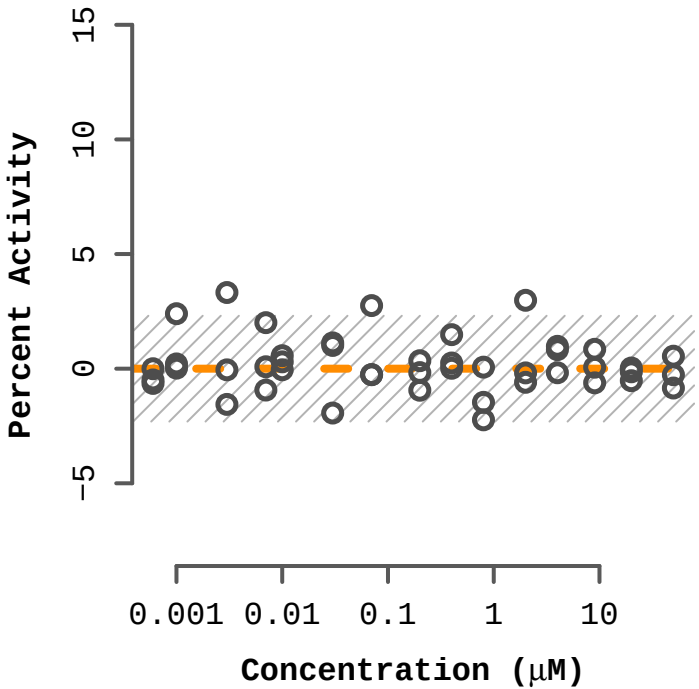
	tp	ga	gw	la	lw
val:	371	-2.57	1.17	2.01	18
sd:	6.84	0.0539	0.164	0.0191	7.16

	CNST	HILL	GNLS
AIC:	664.02	463.32	463.17
PROB:	0	0.48	0.52
RMSE:	339.14	37.48	36.19

MAX_MEAN: 394 MAX_MED: 408 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Fluocinolone acetonide
CHID:    40674   CASRN: 67-73-2
SPID(S): Tox21_110869_1
M4ID:    12484056

HILL MODEL (in red):
      tp       ga       gw
val:  368      -2.68    1.31
sd:   6.28     0.0519   0.157

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  370      -2.67    1.29     1.78     18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  662.01      453.46      456.84
PROB: 0           0.84        0.16
RMSE: 332.73      33.43       33.11

MAX_MEAN: 411       MAX_MED: 407       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

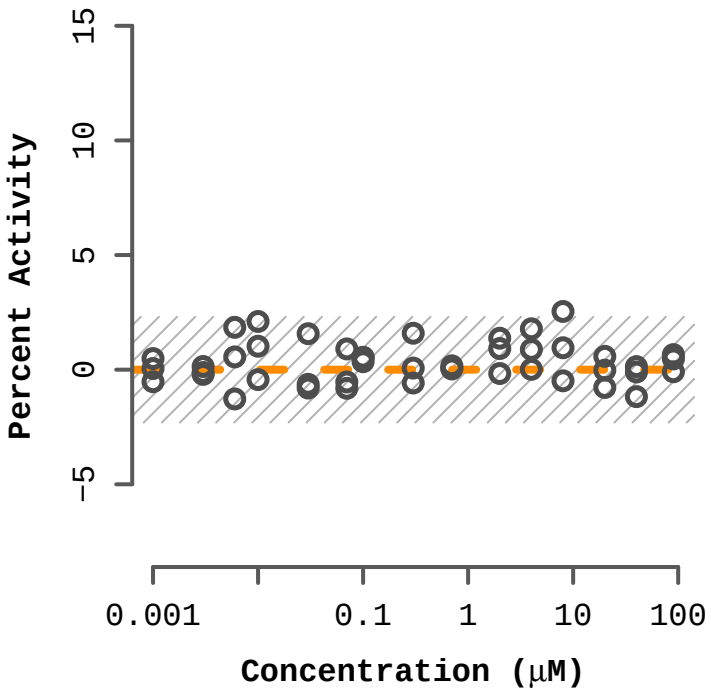
NAME: Glimepiride
CHID: 40675 **CASRN:** 93479-97-1
SPID(S): Tox21_110713_1
M4ID: 12484155

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

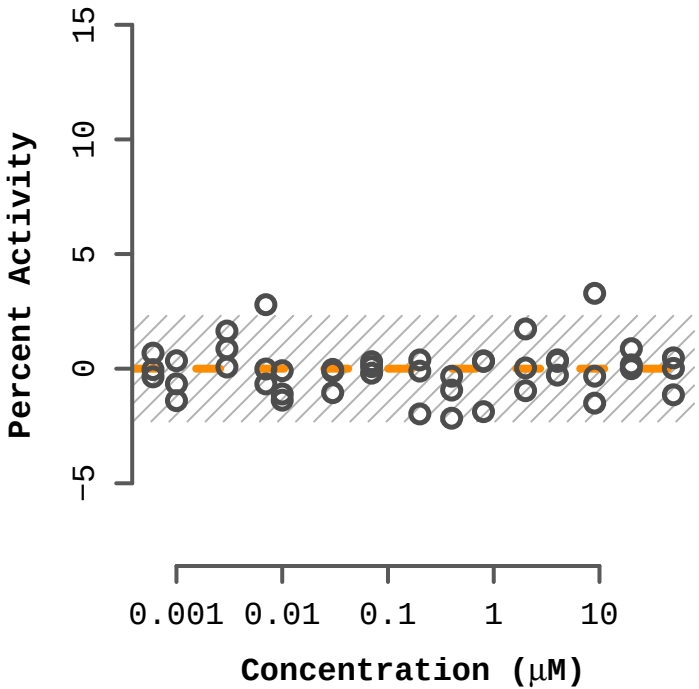
NAME: Glipizide
CHID: 40676 **CASRN:** 29094-61-9
SPID(S): Tox21_301834
M4ID: 12477299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

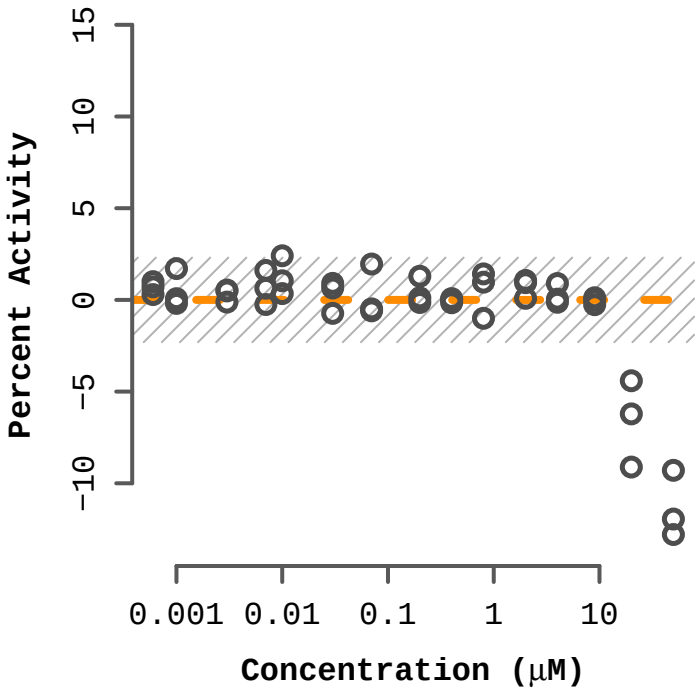
NAME: Glipizide
CHID: 40676 **CASRN:** 29094-61-9
SPID(S): Tox21_110156_1
M4ID: 12484601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 0.865 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

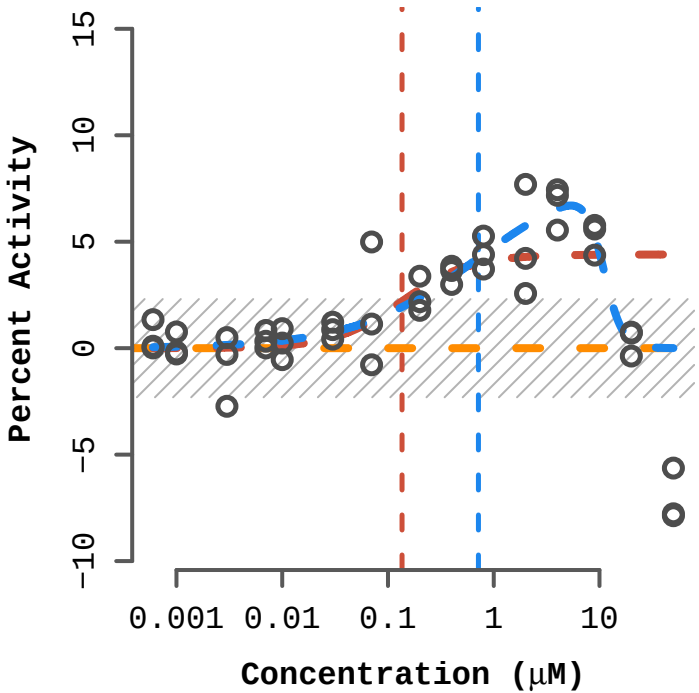
NAME: Idebenone
CHID: 40678 **CASRN:** 58186-27-9
SPID(S): Tox21_111864_1
M4ID: 12483442

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.74	NA	NA
PROB:	1	NA	NA
RMSE:	3.54	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ipriflavone
CHID: 40679 CASRN: 35212-22-7
SPID(S): Tox21_113172_1
M4ID: 12482783

HILL MODEL (in red):

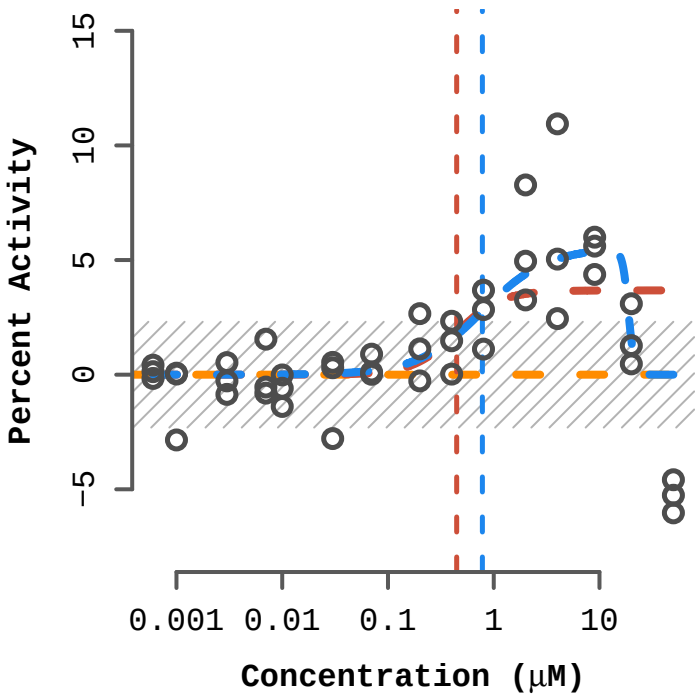
	tp	ga	gw
val:	4.4	−0.867	1.36
sd:	0.67	0.261	0.639

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.47	−0.145	0.732	1.04	5.03
sd:	2.72	0.449	0.239	0.0605	2.13

	CNST	HILL	GNLS
AIC:	249.12	218.54	181.3
PROB:	0	0	1
RMSE:	3.71	3.4	2.15

MAX_MEAN: 6.72 MAX_MED: 7.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ipriflavone
CHID: 40679 **CASRN:** 35212-22-7
SPID(S): Tox21_111532_1
M4ID: 12483632

HILL MODEL (in red):

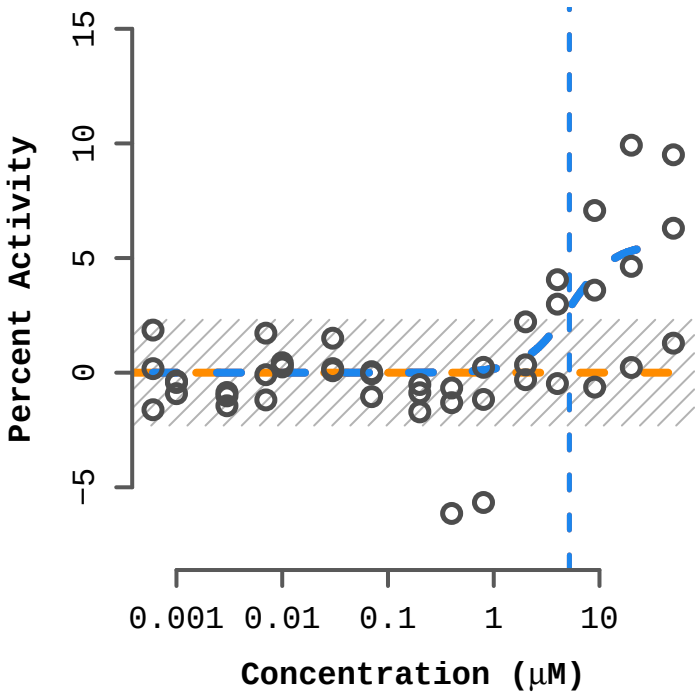
	tp	ga	gw
val:	3.68	−0.35	2.1
sd:	0.662	0.202	1.28

GAIN-LOSS MODEL (in blue):

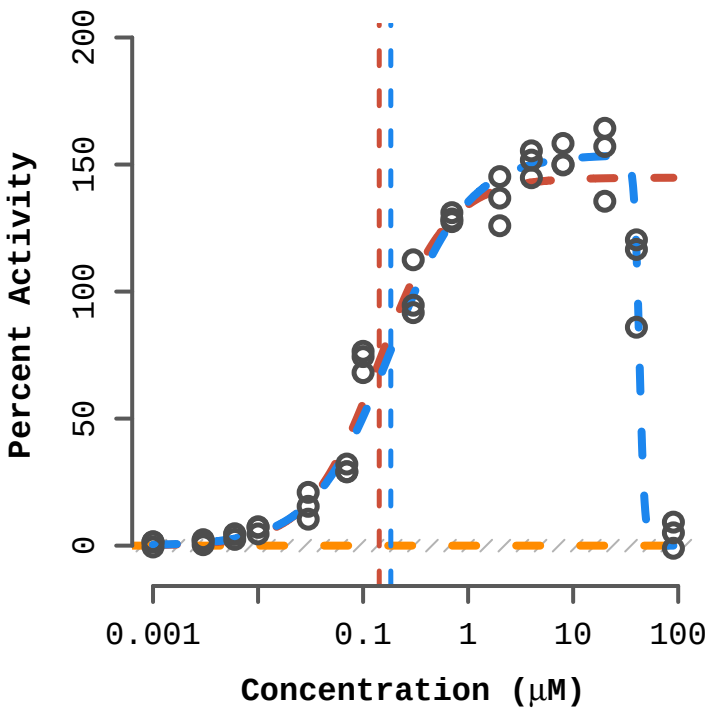
	tp	ga	gw	la	lw
val:	5.54	−0.107	1.42	1.27	15.5
sd:	0.847	0.175	0.69	0.092	52.2

	CNST	HILL	GNLS
AIC:	233.43	213.03	191.5
PROB:	0	0	1
RMSE:	3.34	2.93	2.02

MAX_MEAN: 6.14 **MAX_MED:** 5.61 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Mebendazole
CHID:    40682   CASRN: 31431-39-7
SPID(S): Tox21_110620_1
M4ID:    12484226

HILL MODEL (in red):
      tp       ga       gw
val:  5.63     0.715    2.09
sd:   2.09     0.384    1.68

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.63     0.716    2.09     2.59     9.21
sd:   2.09     0.384    1.68     1250     13000

      CNST        HILL        GNLS
AIC:  219.47      202.82      206.82
PROB: 0           0.88        0.12
RMSE: 3.14        2.25        2.25

MAX_MEAN: 5.7       MAX_MED: 6.3       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Megestrol acetate
CHID: 40683 CASRN: 595-33-5
SPID(S): Tox21_302360
M4ID: 12476773

HILL MODEL (in red):

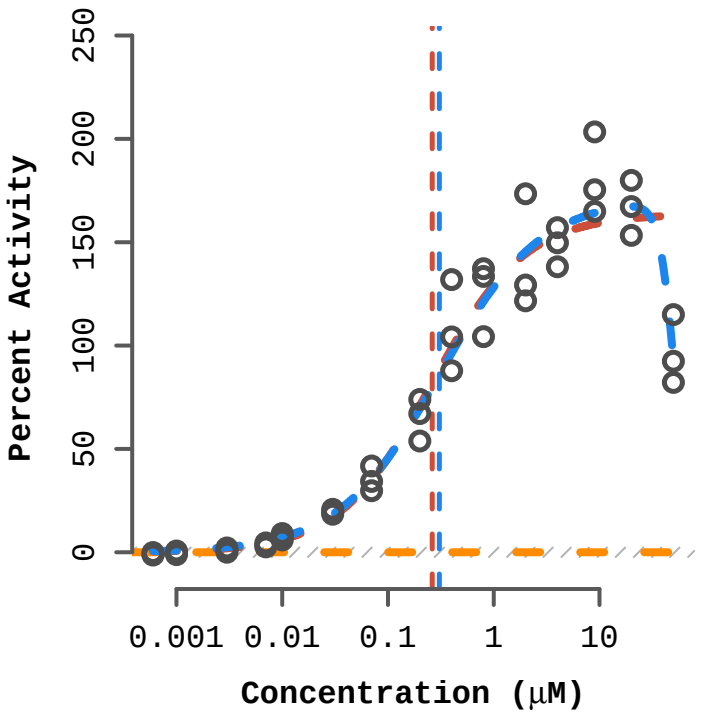
	tp	ga	gw
val:	145	-0.846	1.3
sd:	4.77	0.0648	0.167

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	154	-0.736	1.17	1.63	17.8
sd:	2.85	0.0434	0.0849	0.00618	2.91

	CNST	HILL	GNLS
AIC:	543.4	413.72	332.91
PROB:	0	0	1
RMSE:	94.2	38.61	9.54

MAX_MEAN: 153 MAX_MED: 157 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Megestrol acetate
CHID: 40683 CASRN: 595-33-5
SPID(S): Tox21_110469_1
M4ID: 12484331

HILL MODEL (in red):

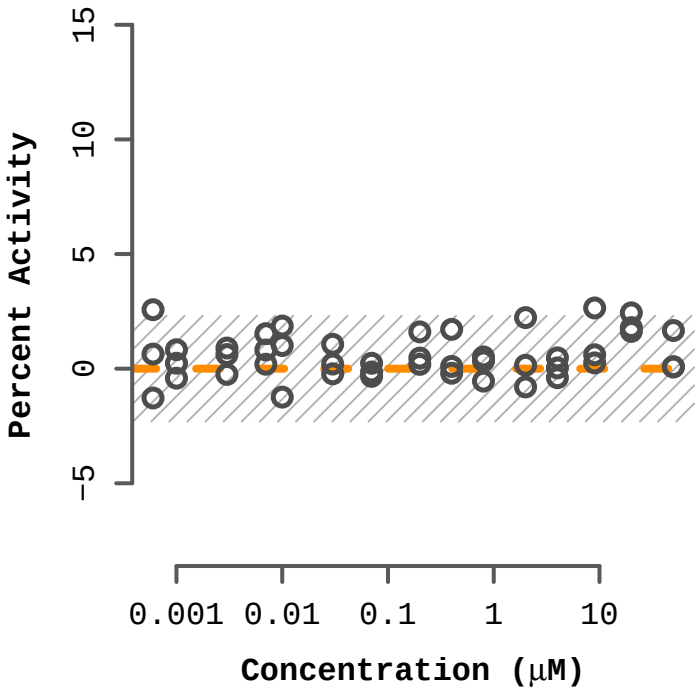
	tp	ga	gw
val:	164	-0.582	0.989
sd:	6.48	0.0699	0.114

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	172	-0.514	0.912	1.71	5.86
sd:	6.85	0.0789	0.0981	0.0136	6.01

	CNST	HILL	GNLS
AIC:	546.83	390.08	359.8
PROB:	0	0	1
RMSE:	99.01	21.43	12.57

MAX_MEAN: 181 MAX_MED: 175 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

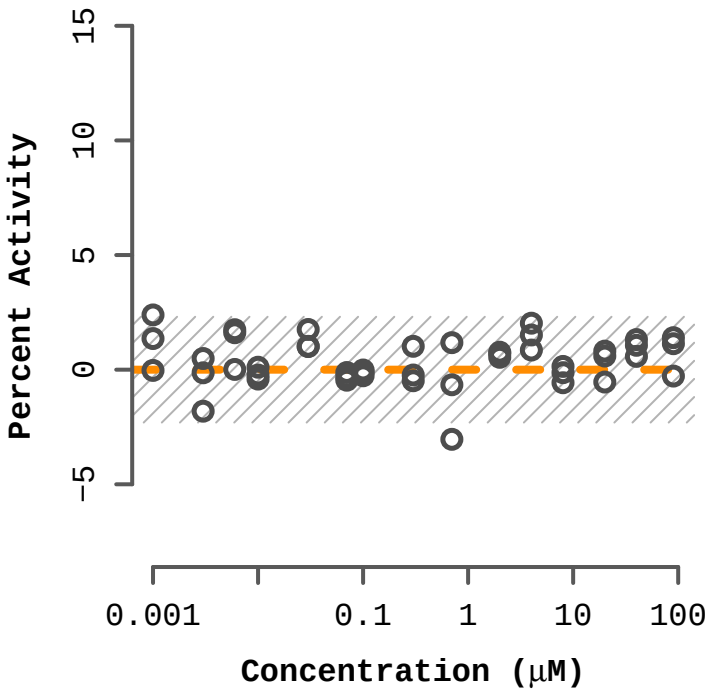
NAME: Minoxidil
CHID: 40685 **CASRN:** 38304-91-5
SPID(S): Tox21_110193_1
M4ID: 12484566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

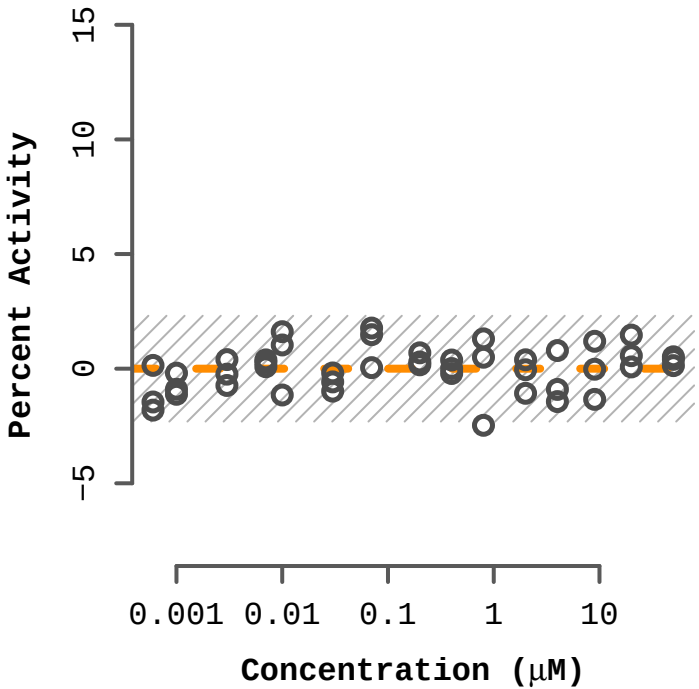
NAME: Naproxen
CHID: 40686 CASRN: 22204-53-1
SPID(S): Tox21_301953
M4ID: 12477180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.47 MAX_MED: 1.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

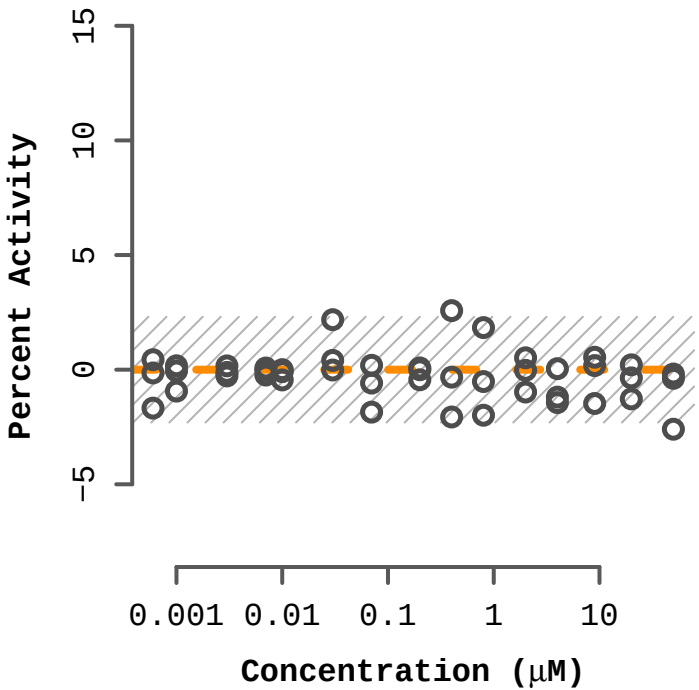
NAME: Nateglinide
CHID: 40687 **CASRN:** 105816-04-4
SPID(S): Tox21_111432_1
M4ID: 12483693

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

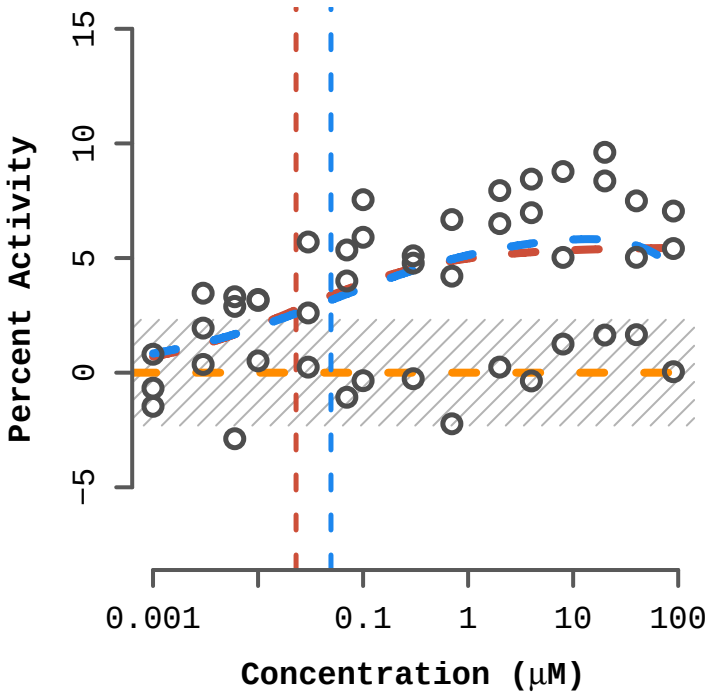
NAME: Oxymetazoline
CHID: 40691 **CASRN:** 1491-59-4
SPID(S): Tox21_110217_1
M4ID: 12484543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 0.405 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acetyl−L−carnitine hydrochloride
CHID: 40693 CASRN: 5080−50−2
SPID(S): Tox21_302340
M4ID: 12476793

HILL MODEL (in red):

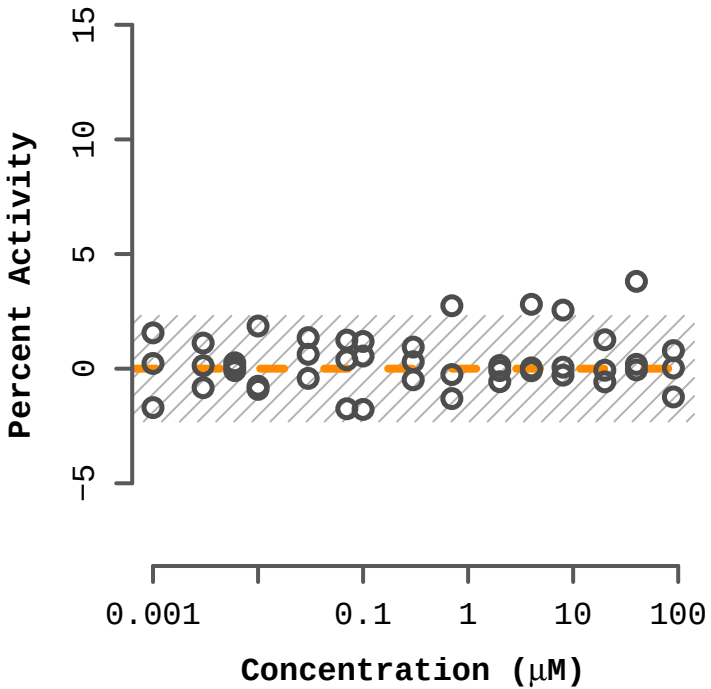
	tp	ga	gw
val:	5.48	−1.64	0.612
sd:	1.04	0.564	0.382

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.33	−1.31	0.483	2.27	1.51
sd:	3.05	1.27	0.408	0.879	3.42

	CNST	HILL	GNLS
AIC:	274.8	237.25	240.93
PROB:	0	0.86	0.14
RMSE:	4.76	2.96	2.95

MAX_MEAN: 6.54 MAX_MED: 8.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

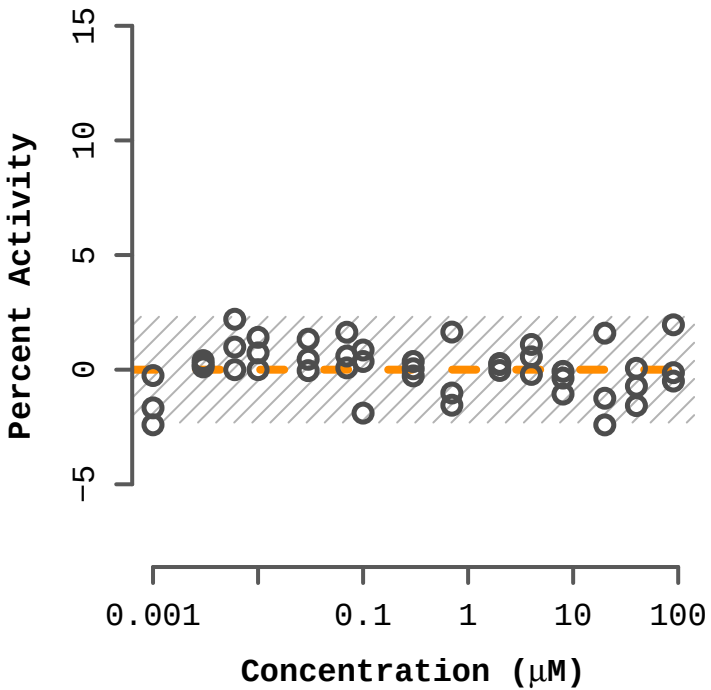
NAME: Butyl benzoate
CHID: 40694 **CASRN:** 136-60-7
SPID(S): Tox21_300510
M4ID: 12478622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

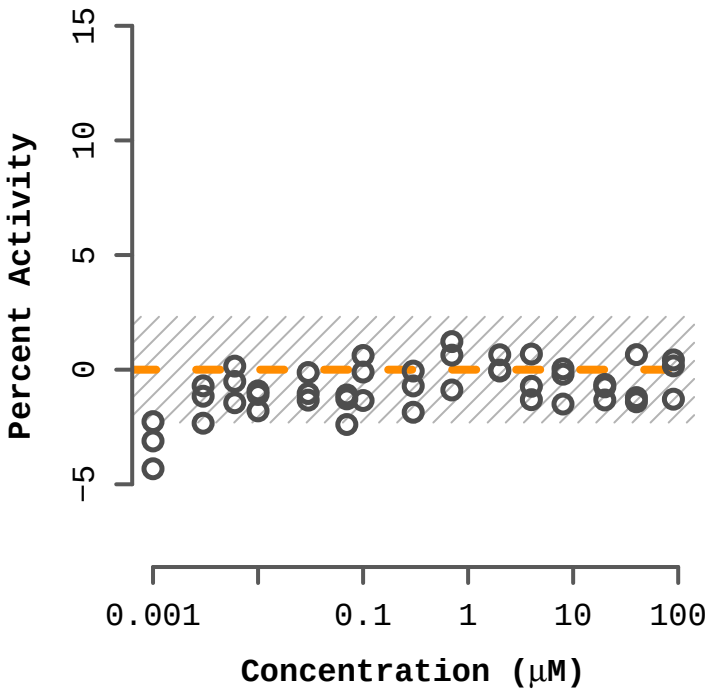
NAME: 2,6-Dichlorotoluene
CHID: 40697 **CASRN:** 118-69-4
SPID(S): Tox21_302049
M4ID: 12477084

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.987 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

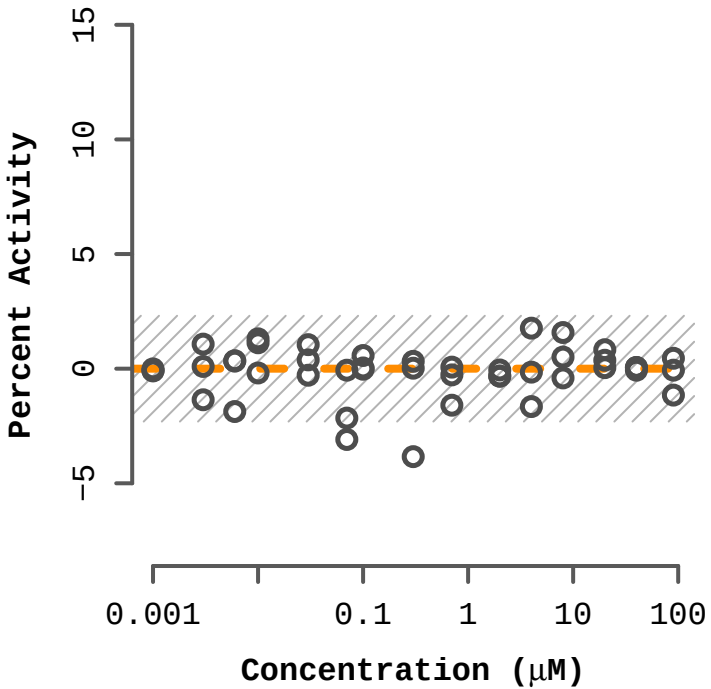
NAME: Triisobutyl phosphate
CHID: 40698 CASRN: 126-71-6
SPID(S): Tox21_301244
M4ID: 12477889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.325 **MAX_MED:** 0.635 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

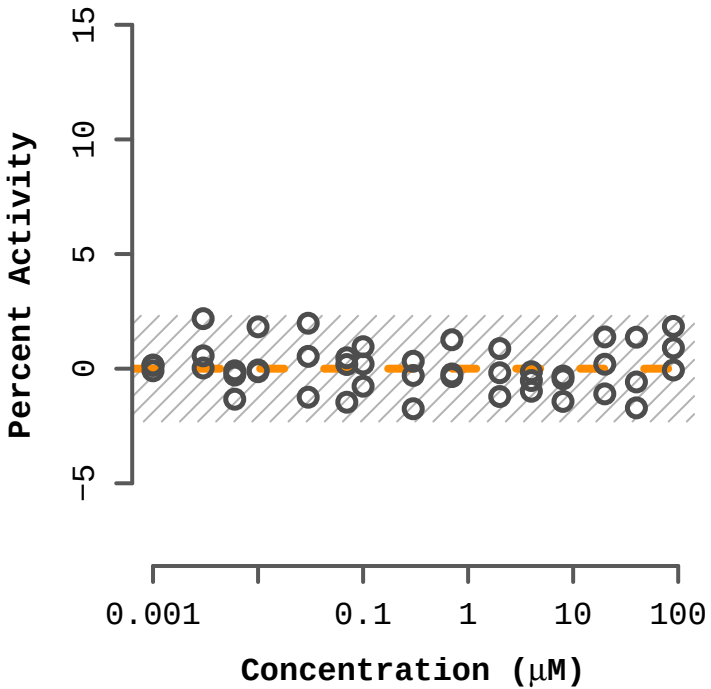
NAME: p,p'−DDA
CHID: 40699 **CASRN:** 83−05−6
SPID(S): Tox21_301432
M4ID: 12477701

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.749 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

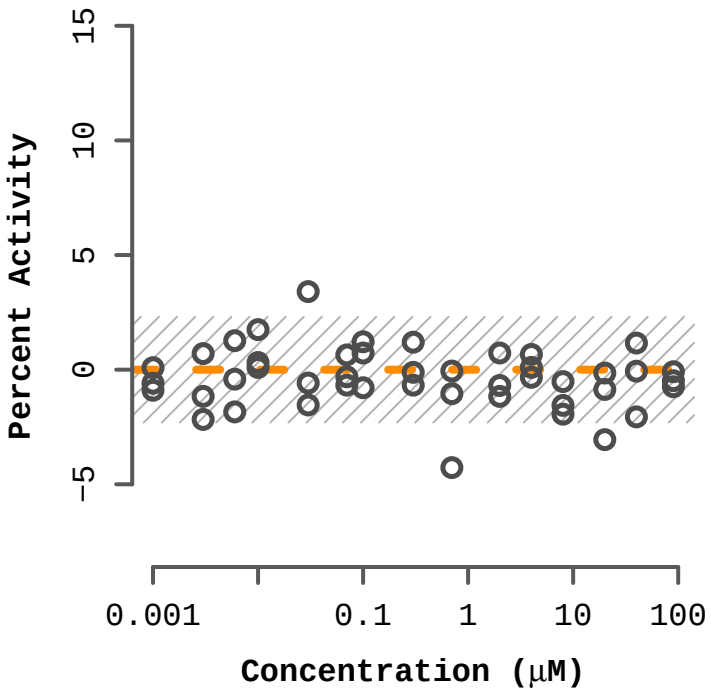
NAME: Trimethoxyphenylsilane
CHID: 40700 **CASRN:** 2996-92-1
SPID(S): Tox21_301311
M4ID: 12477822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.926 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

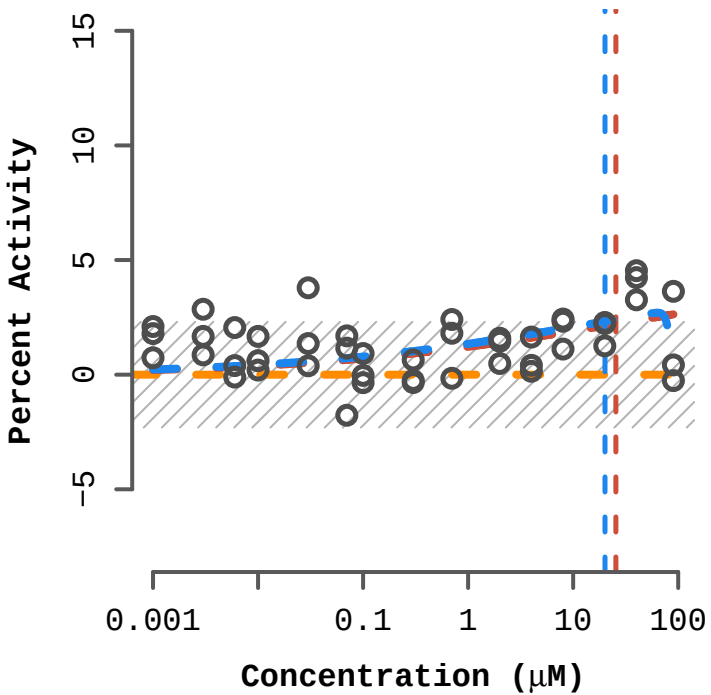
NAME: Triethyl citrate
CHID: 40701 CASRN: 77-93-0
SPID(S): Tox21_300004
M4ID: 12479126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 0.728 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-Dichlorotoluene
CHID: 40702 CASRN: 95-73-8
SPID(S): Tox21_302123
M4ID: 12477010

HILL MODEL (in red):

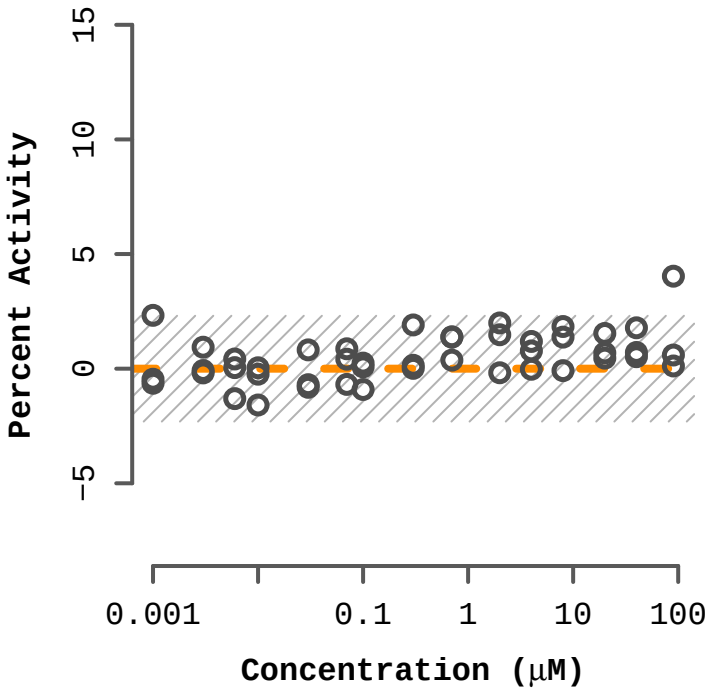
	tp	ga	gw
val:	4.43	1.41	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.65	1.3	0.3	1.92	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	188.05	162.29	162.53
PROB:	0	0.53	0.47
RMSE:	1.87	1.31	1.27

MAX_MEAN: 4.01 MAX_MED: 4.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

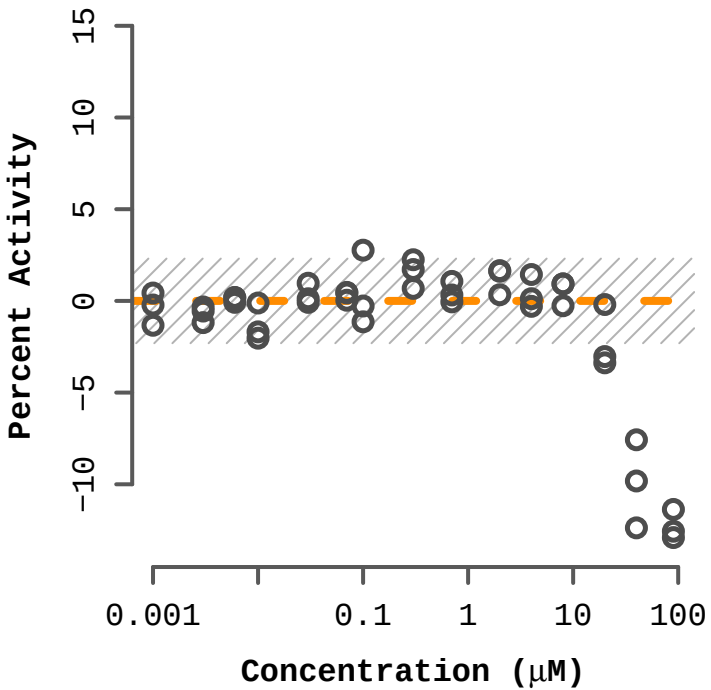
NAME: 4-tert-Butylbenzoic acid
CHID: 40703 **CASRN:** 98-73-7
SPID(S): Tox21_301337
M4ID: 12477796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

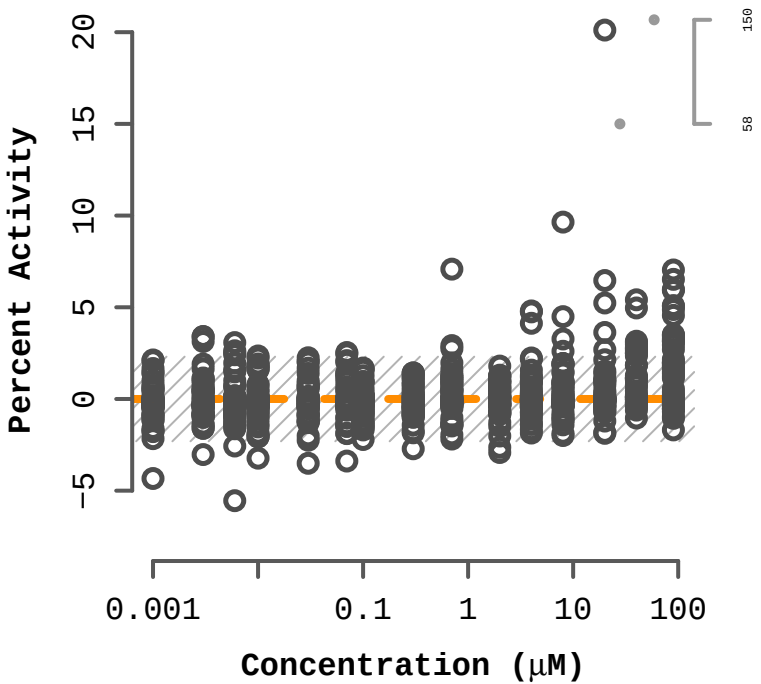
NAME: 1,4-Naphthoquinone
CHID: 40704 **CASRN:** 130-15-4
SPID(S): Tox21_303967
M4ID: 12475221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.66	NA	NA
PROB:	1	NA	NA
RMSE:	4.27	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

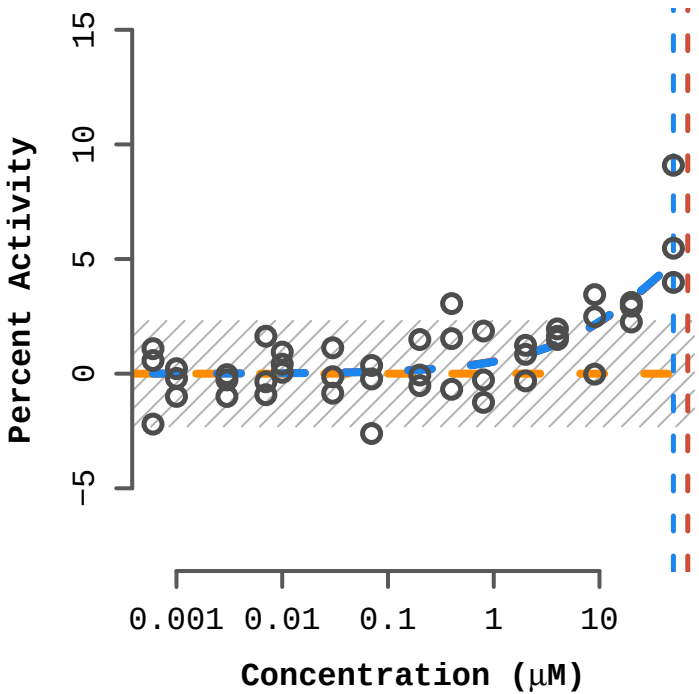
NAME: Cinchophen
CHID: 40705 **CASRN:** 132-60-5
SPID(S): Tox21_400022
M4ID: 12475115 **BRK**

HILL MODEL: Not applicable.

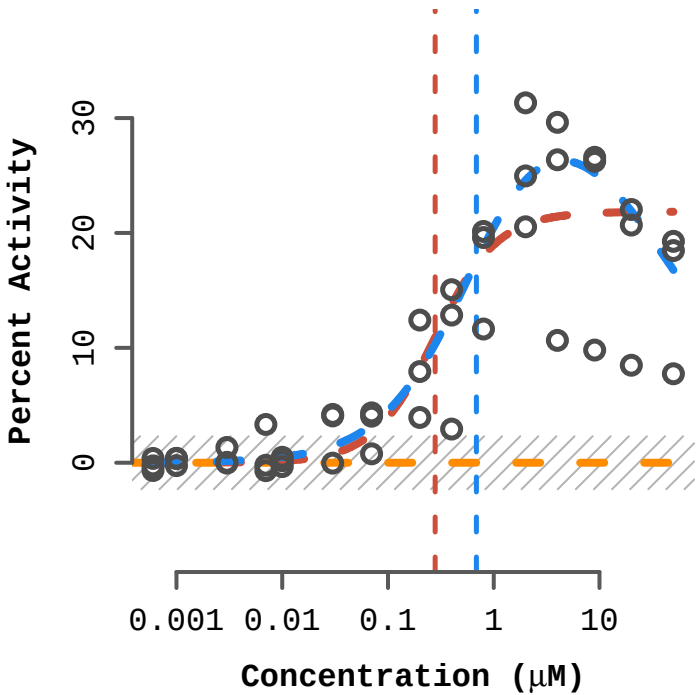
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	2493.54	NA	NA
PROB:	1	NA	NA
RMSE:	6.1	NA	NA

MAX_MEAN: 4.95 **MAX_MED:** 1.82 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cinchophen
CHID:    40705   CASRN: 132-60-5
SPID(S): Tox21_110841_1
M4ID:    12484078

HILL MODEL (in red):
      tp       ga       gw
val:  10.9     1.83     0.701
sd:   10.1     0.997    0.236

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.69     1.7      0.734    2.87     7.04
sd:   9.09     1        0.265    1310     7900

      CNST        HILL        GNLS
AIC:  191.38      151.5       155.6
PROB: 0           0.89        0.11
RMSE: 2.23        1.24        1.24

MAX_MEAN: 6.18      MAX_MED: 5.47      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Solvent Orange 7
CHID: 40706 CASRN: 3118-97-6
SPID(S): Tox21_303836
M4ID: 12475352

HILL MODEL (in red):

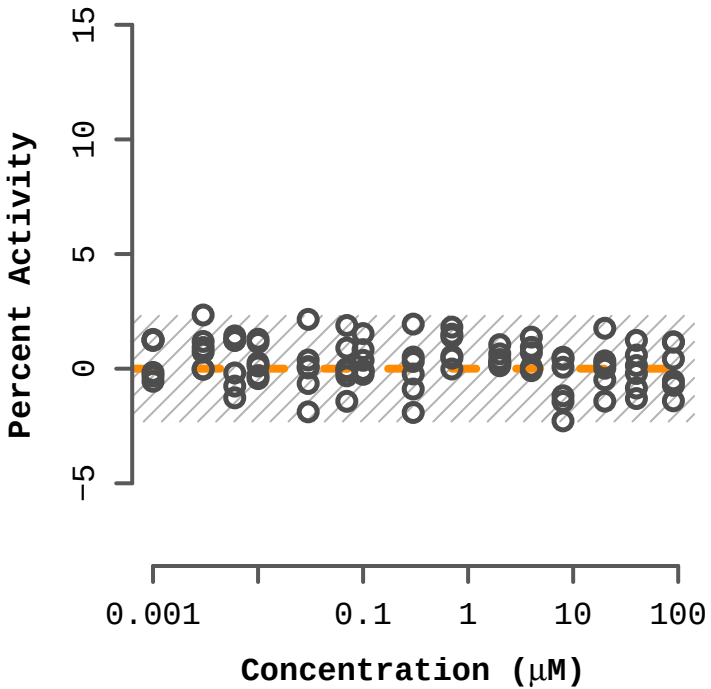
	tp	ga	gw
val:	21.9	-0.554	1.47
sd:	1.48	0.0983	0.375

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	37.6	-0.164	1.02	1.57	0.66
sd:	13.4	0.229	0.198	0.471	0.332

	CNST	HILL	GNLS
AIC:	366.52	274.49	263.48
PROB:	0	0	1
RMSE:	13.83	5.1	4.86

MAX_MEAN: 25.6 MAX_MED: 26.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

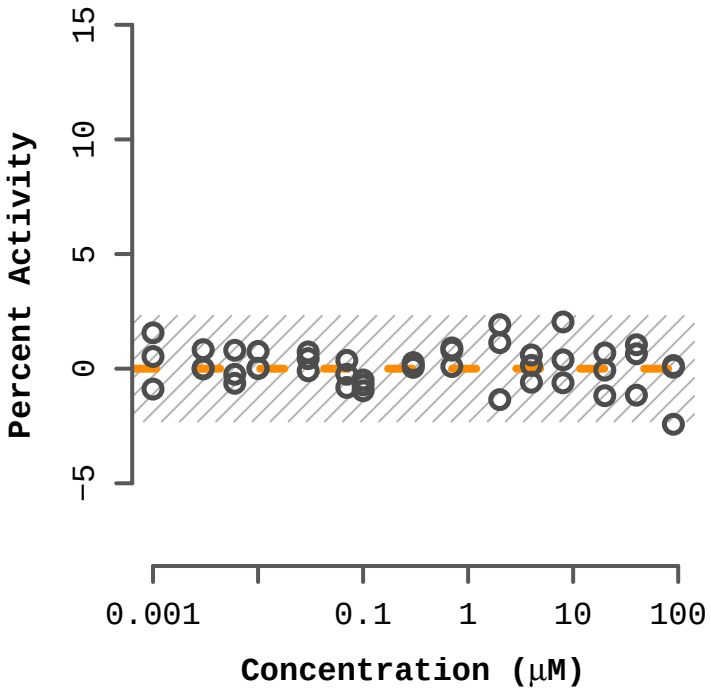
NAME: 4-Pentylaniline
CHID: 40707 **CASRN:** 33228-44-3
SPID(S): Tox21_301699
M4ID: 12477434

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	262.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.953 **MAX_MED:** 0.974 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

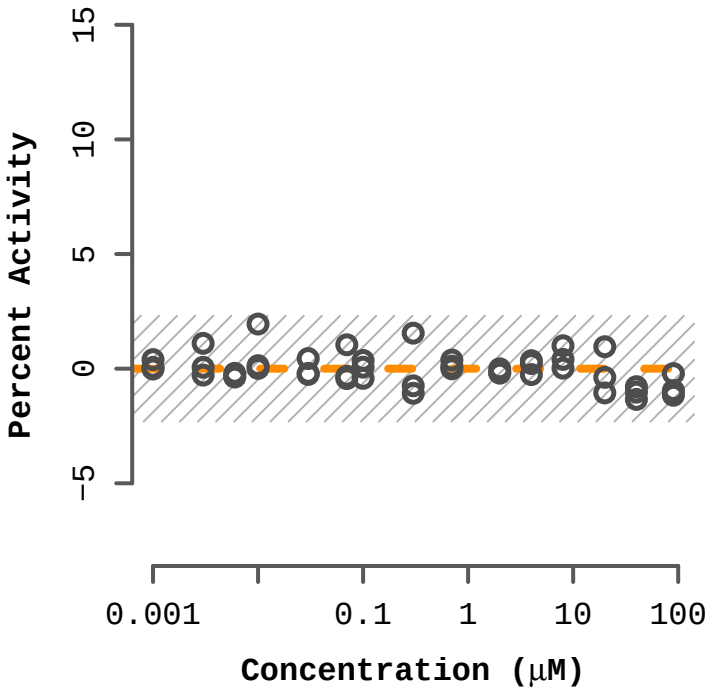
NAME: 4-Hexylaniline
CHID: 40708 CASRN: 33228-45-4
SPID(S): Tox21_302012
M4ID: 12477121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.604 MAX_MED: 1.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

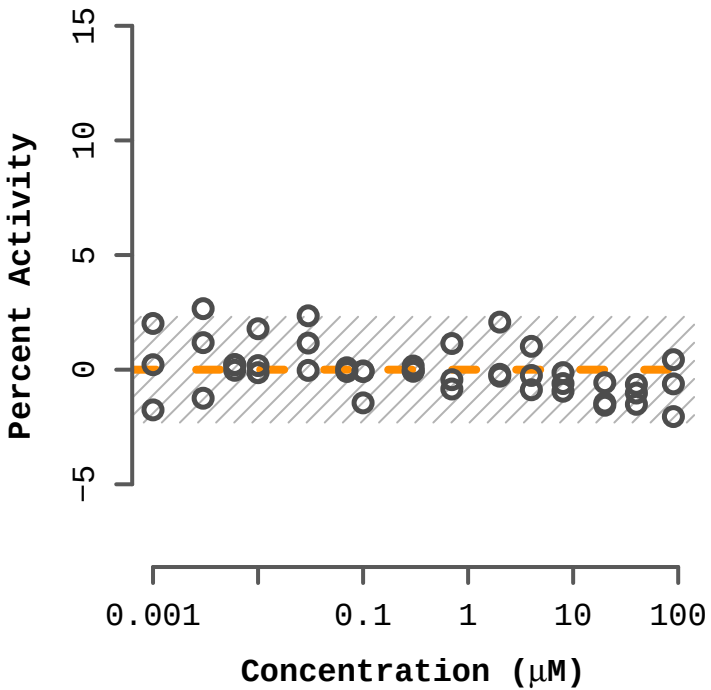
NAME: Octamethyltrisiloxane
CHID: 40710 CASRN: 107-51-7
SPID(S): Tox21_301002
M4ID: 12478131

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.698 MAX_MED: 0.406 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

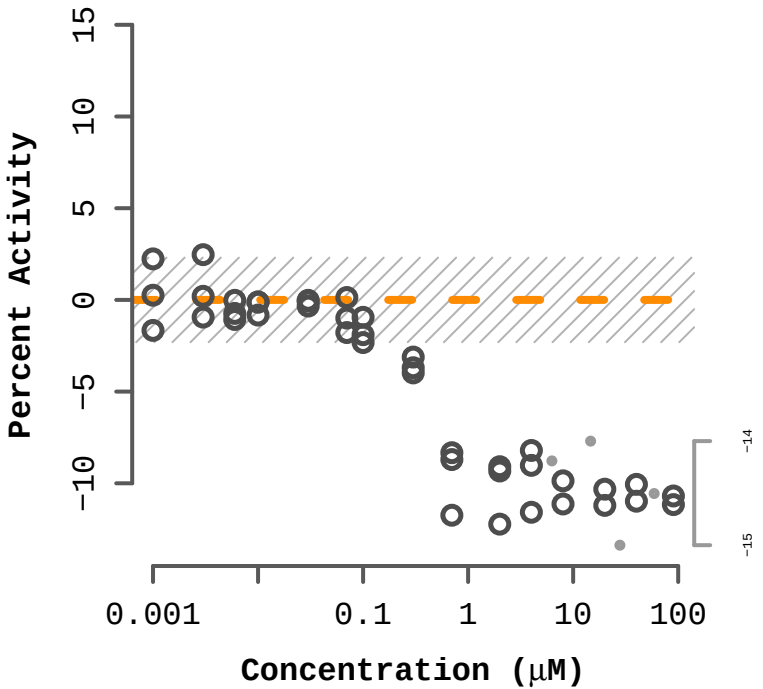
NAME: Ethyl 2-methylbenzoate
CHID: 40711 **CASRN:** 87-24-1
SPID(S): Tox21_302249
M4ID: 12476884

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

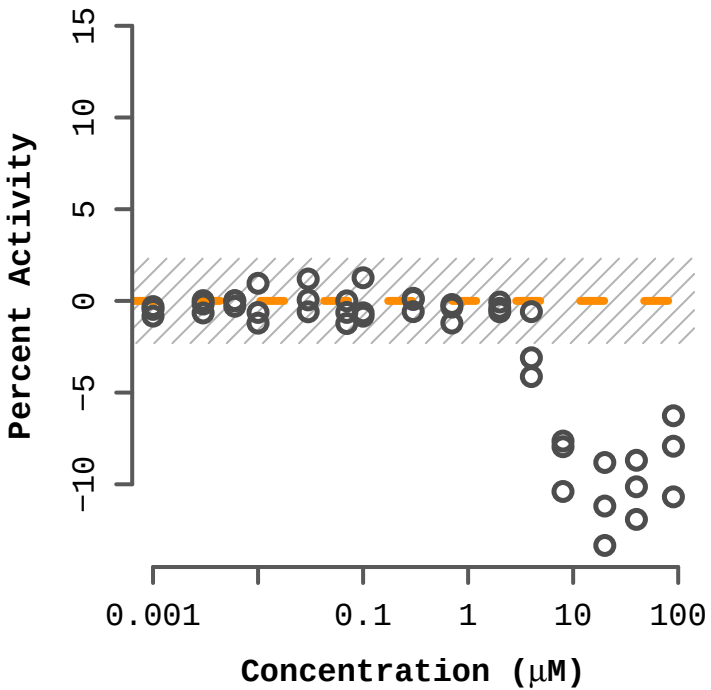
NAME: Triethyltin bromide
CHID: 40712 **CASRN:** 2767-54-6
SPID(S): Tox21_301405
M4ID: 12477728 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	317.67	NA	NA
PROB:	1	NA	NA
RMSE:	7.74	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** 0.256 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

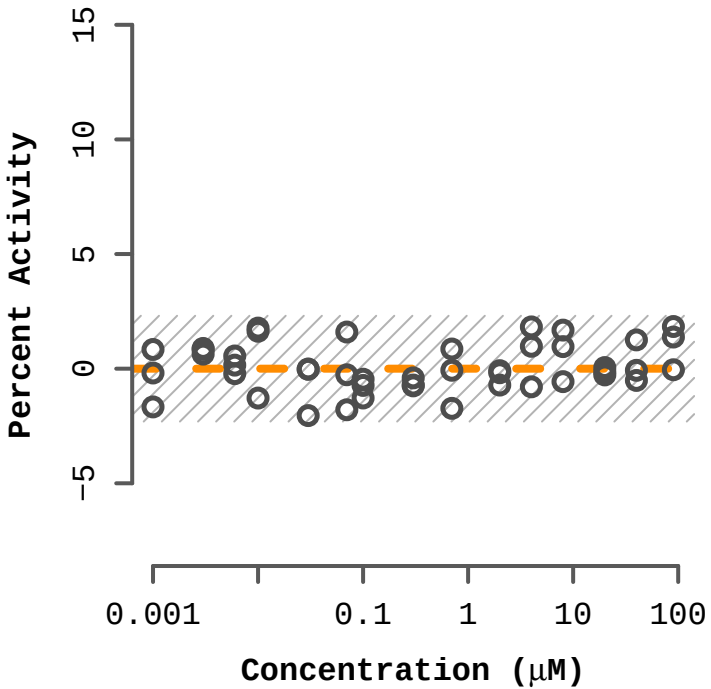
NAME: Octyl gallate
CHID: 40713 CASRN: 1034-01-1
SPID(S): Tox21_300272
M4ID: 12478858

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	269.26	NA	NA
PROB:	1	NA	NA
RMSE:	5.13	NA	NA

MAX_MEAN: 0.22 MAX_MED: 0.0771 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

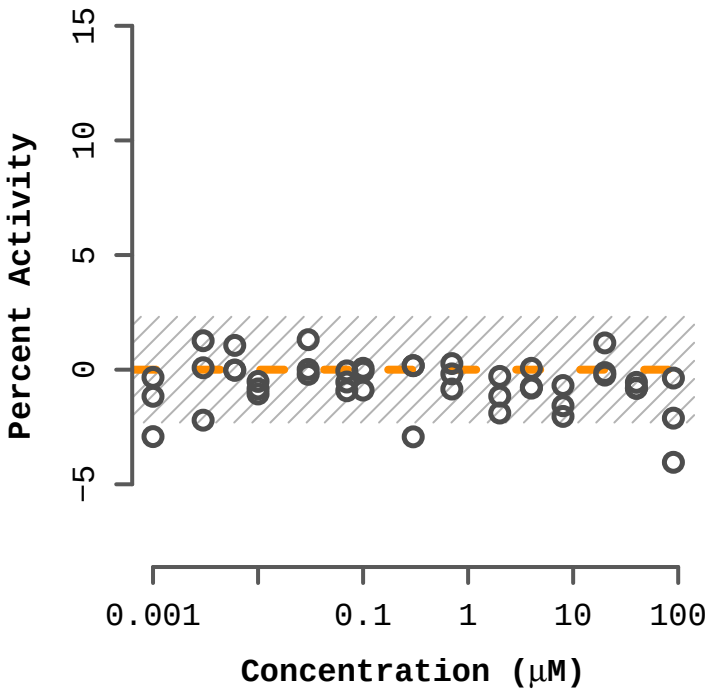
NAME: 2-Chloro-4,6-dimethylaniline
CHID: 40714 **CASRN:** 63133-82-4
SPID(S): Tox21_301996
M4ID: 12477137

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

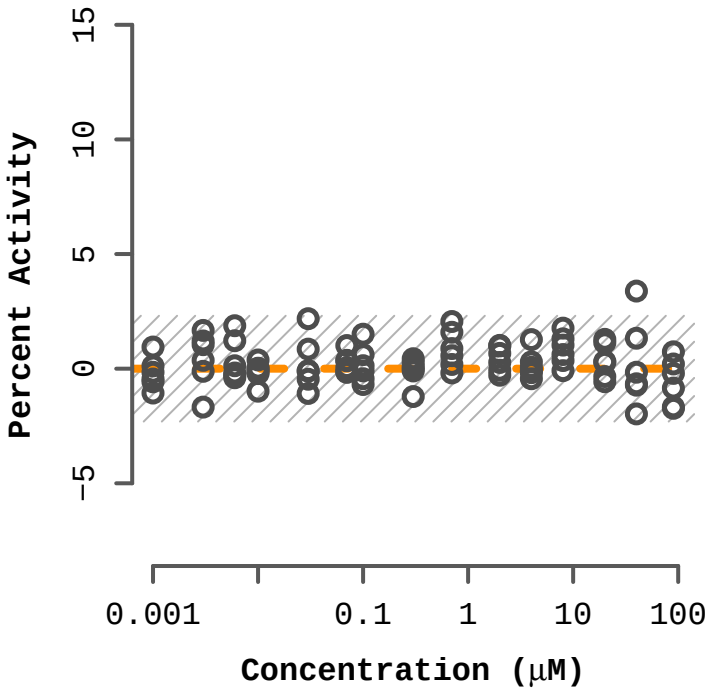
NAME: 2-Phenoxyethyl acrylate
CHID: 40715 **CASRN:** 48145-04-6
SPID(S): Tox21_301723
M4ID: 12477410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.173 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

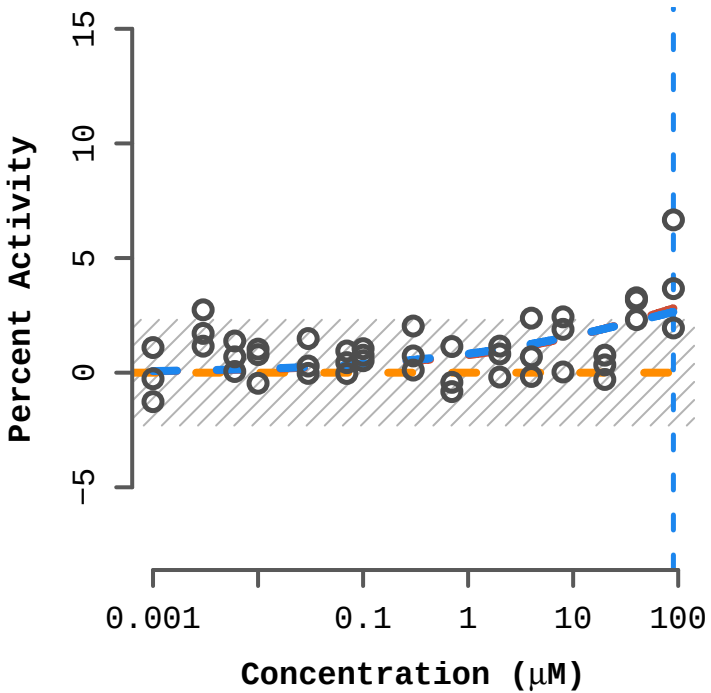
NAME: 4-(2-Methylbutan-2-yl)cyclohexanol
CHID: 40716 CASRN: 5349-51-9
SPID(S): Tox21_301635
M4ID: 12477498

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.849 MAX_MED: 0.825 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,5-Dimethoxy-4-chloroaniline
CHID: 40718 **CASRN:** 6358-64-1
SPID(S): Tox21_301725
M4ID: 12477408

HILL MODEL (in red):

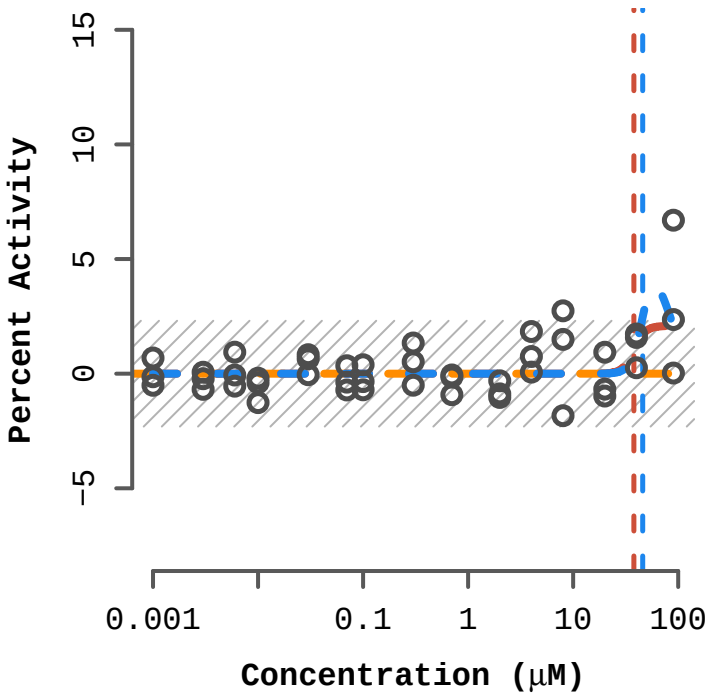
	tp	ga	gw
val:	7.13	2.45	0.375
sd:	8.04	1.76	0.209

GAIN-LOSS MODEL (in blue):

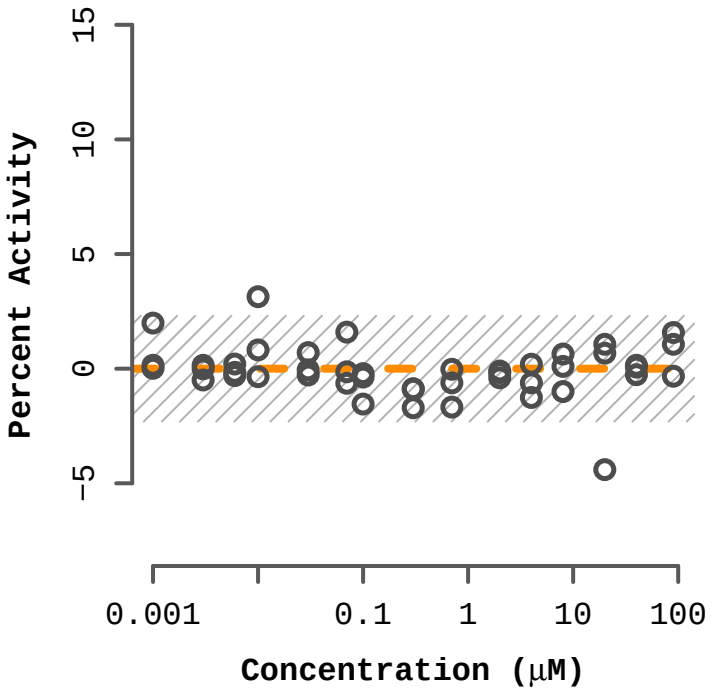
	tp	ga	gw	la	lw
val:	5.3	1.95	0.376	3.59	4.62
sd:	5.64	1.69	0.23	892	2510

	CNST	HILL	GNLS
AIC:	173.67	149.29	153.84
PROB:	0	0.91	0.09
RMSE:	1.75	1.17	1.18

MAX_MEAN: 4.1 **MAX_MED:** 3.67 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-(2,4-Dimethylphenyl)-3-oxobutanamide
CHID:    40719   CASRN: 97-36-9
SPID(S): Tox21_302083
M4ID:    12477050

HILL MODEL (in red):
      tp       ga       gw
val:  2.08     1.58     8
sd:   0.814    0.0792   11.7

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.32     1.66     8        1.91     4.52
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  141.36      138.08      142.07
PROB: 0.15        0.75        0.1
RMSE: 1.39        1.14        1.14

MAX_MEAN: 3.03      MAX_MED: 2.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

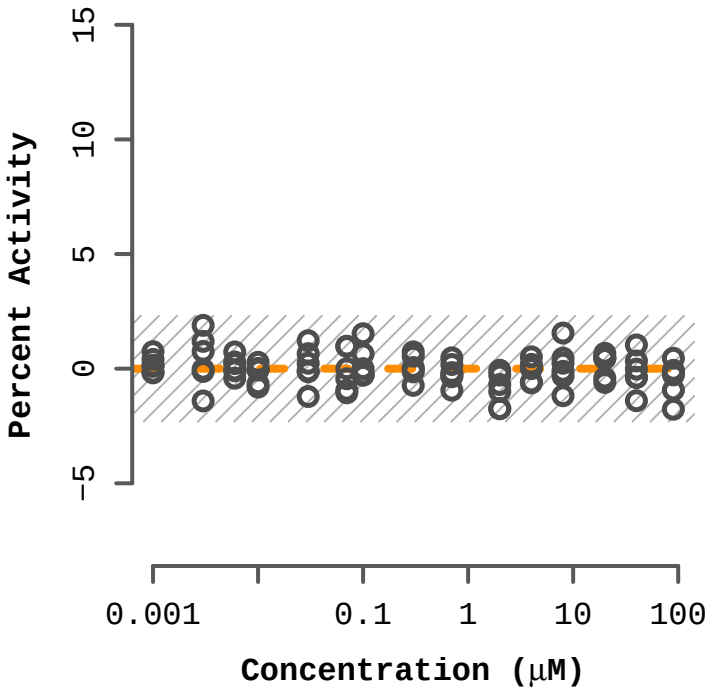
NAME: 4-Amino-2,6-dichlorophenol
CHID: 40720 **CASRN:** 5930-28-9
SPID(S): Tox21_301640
M4ID: 12477493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

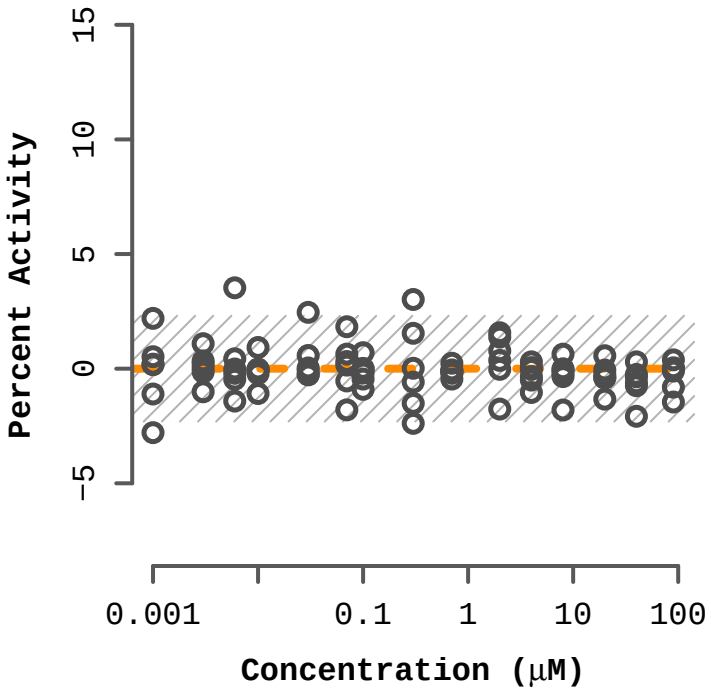
NAME: 4-Cyclohexylcyclohexanone
CHID: 40721 **CASRN:** 92-68-2
SPID(S): Tox21_301879
M4ID: 12477254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.382 **MAX_MED:** 0.449 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

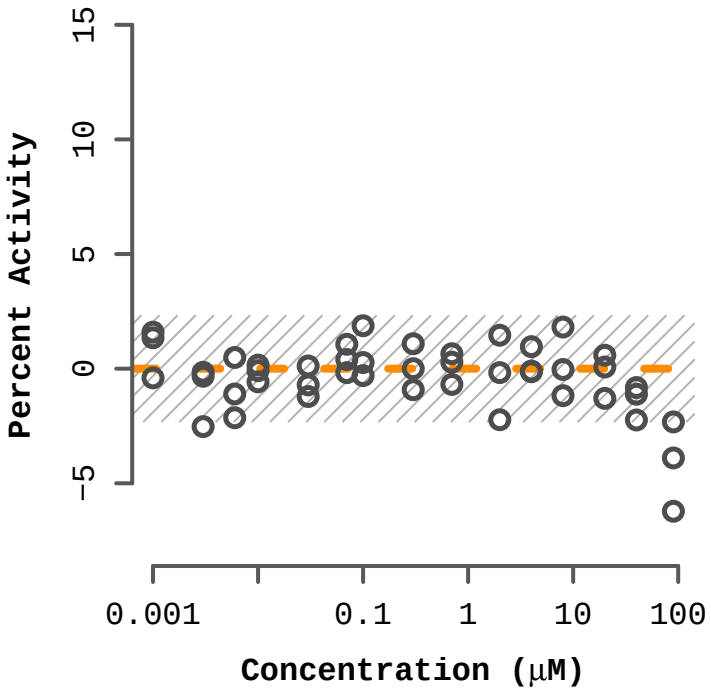
NAME: 4-Cyclohexylcyclohexanol
CHID: 40722 CASRN: 2433-14-9
SPID(S): Tox21_301763
M4ID: 12477370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.414 MAX_MED: 0.572 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

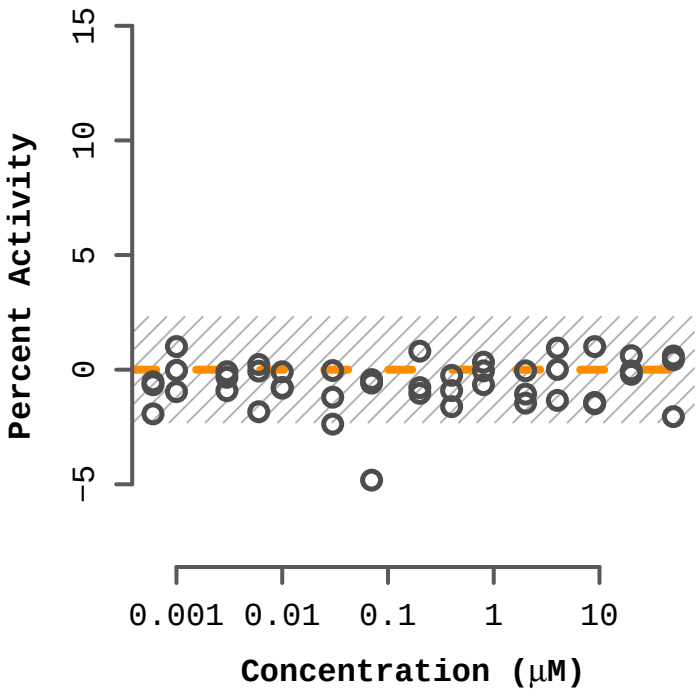
NAME: 2-Chloro-5-nitro-N-phenylbenzamide
CHID: 40723 **CASRN:** 22978-25-2
SPID(S): Tox21_301993
M4ID: 12477140

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 0.847 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

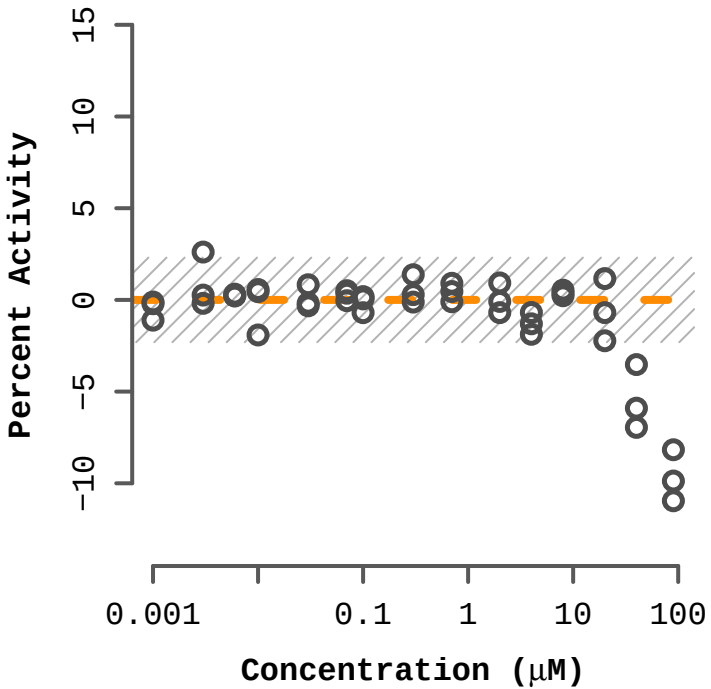
NAME: Atropine sulfate monohydrate
CHID: 40724 **CASRN:** 5908-99-6
SPID(S): Tox21_302173
M4ID: 12476960

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.119 **MAX_MED:** 0.432 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

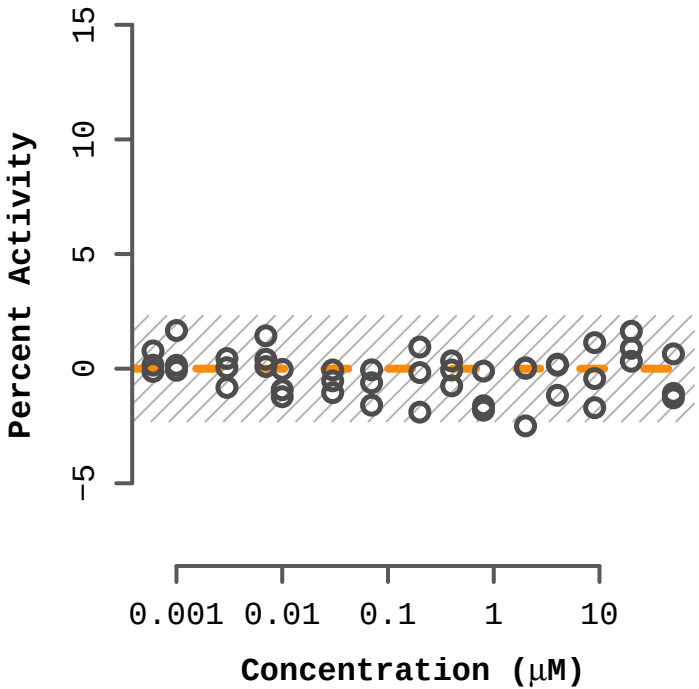
NAME: 4-Chloromercuribenzoic acid
CHID: 40725 **CASRN:** 59-85-8
SPID(S): Tox21_301861
M4ID: 12477272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.02	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 0.458 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

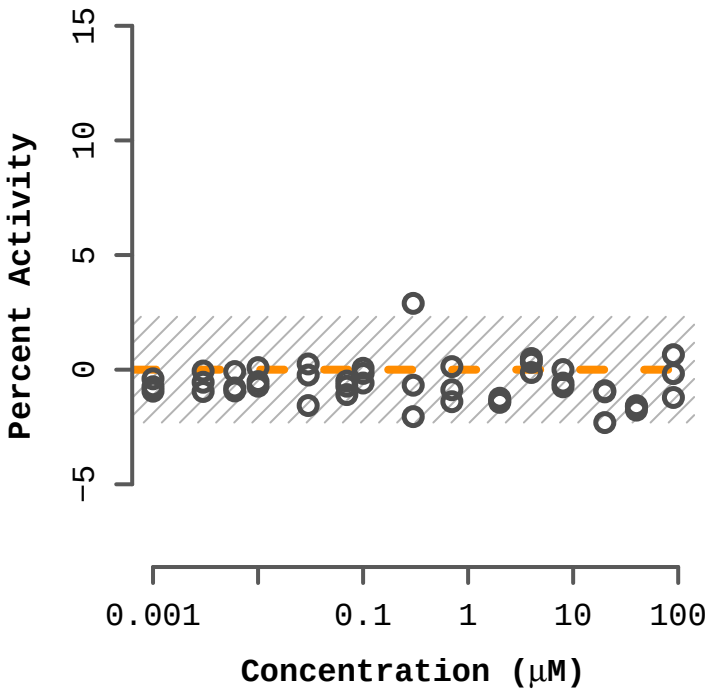
NAME: Olaquindox
CHID: 40726 **CASRN:** 23696-28-8
SPID(S): Tox21_112095_1
M4ID: 12483324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.948 **MAX_MED:** 0.888 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

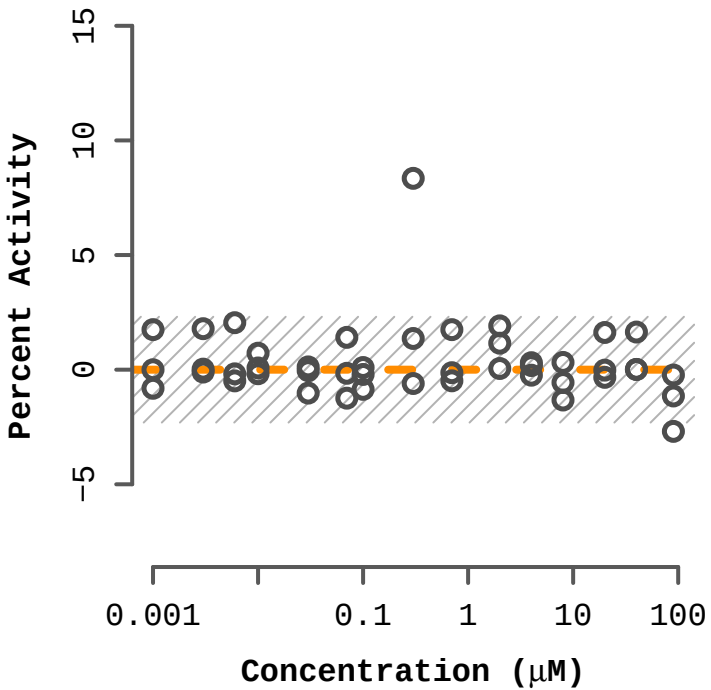
NAME: Flutriafol
CHID: 40727 **CASRN:** 76674-21-0
SPID(S): Tox21_301338
M4ID: 12477795

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.23 **MAX_MED:** 0.324 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

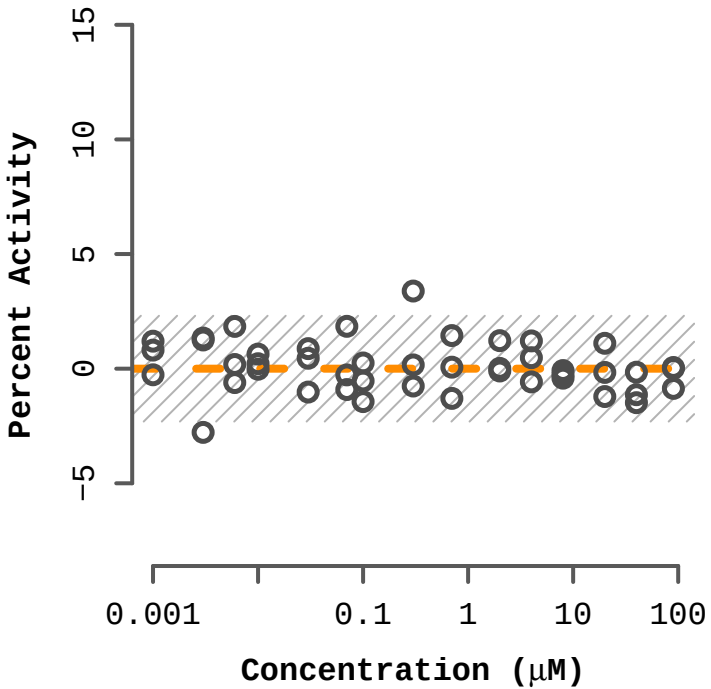
NAME: Phosphoric acid, dibutyl ester
CHID: 40728 CASRN: 107-66-4
SPID(S): Tox21_301186
M4ID: 12477947

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 3.04 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

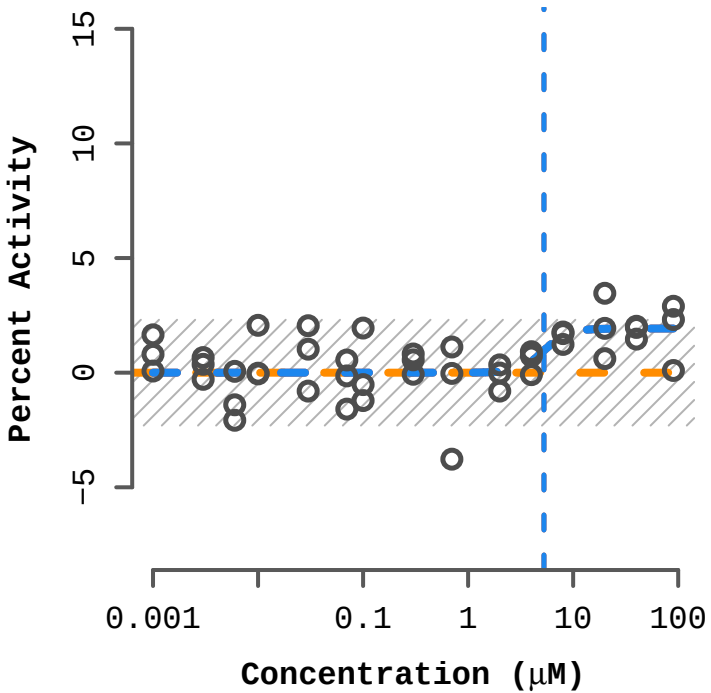
NAME: Diisopropyl phthalate
CHID: 40731 CASRN: 605-45-8
SPID(S): Tox21_301512
M4ID: 12477621

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chlorophenyl isocyanate
CHID: 40732 **CASRN:** 104-12-1
SPID(S): Tox21_300991
M4ID: 12478142

HILL MODEL (in red):

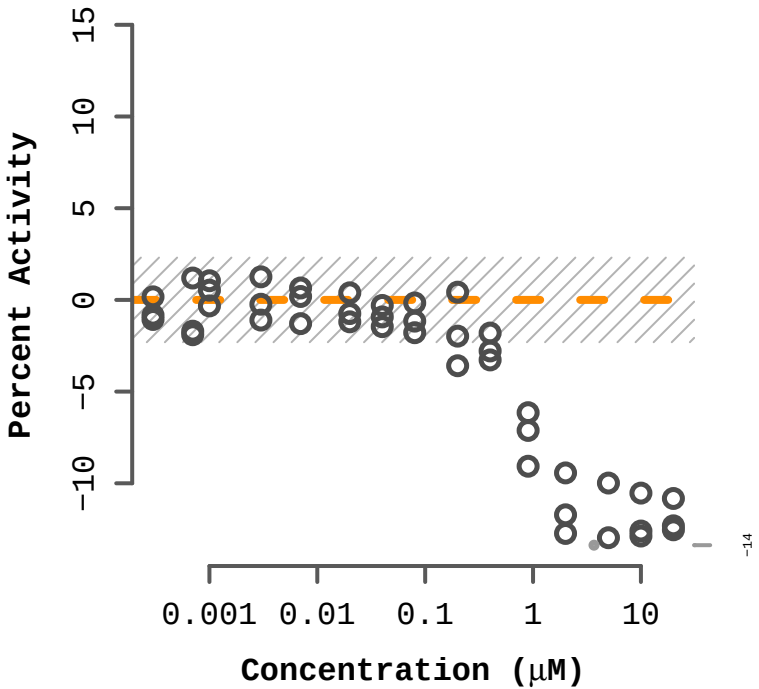
	tp	ga	gw
val:	1.92	0.722	3.83
sd:	0.336	0.136	2.89

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.92	0.722	3.83	3	7.39
sd:	0.336	0.136	2.89	1290	9150

	CNST	HILL	GNLS
AIC:	165.14	142.13	146.13
PROB:	0	0.88	0.12
RMSE:	1.45	1.11	1.11

MAX_MEAN: 2 **MAX_MED:** 2.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

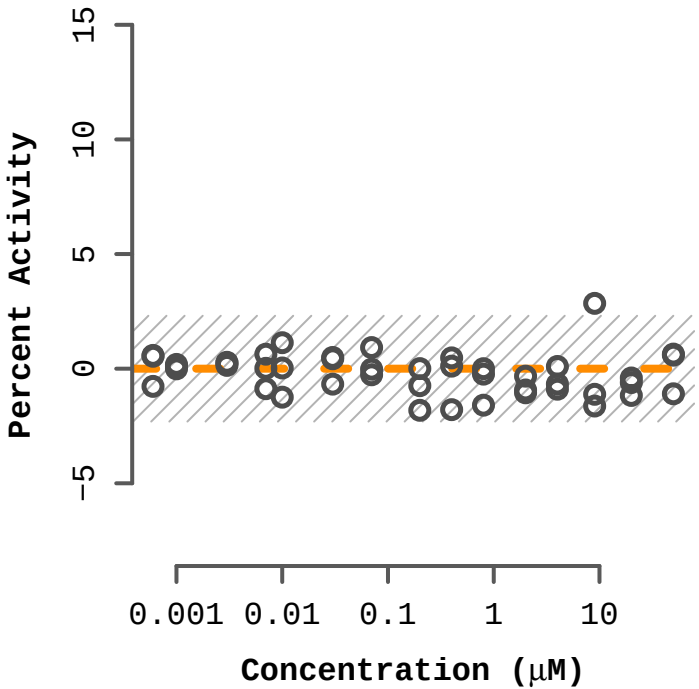
NAME: Triphenyltin chloride
CHID: 40733 CASRN: 639-58-7
SPID(S): Tox21_303984
M4ID: 12475204 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	297.33	NA	NA
PROB:	1	NA	NA
RMSE:	6.56	NA	NA

MAX_MEAN: 0.418 **MAX_MED:** 0.533 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

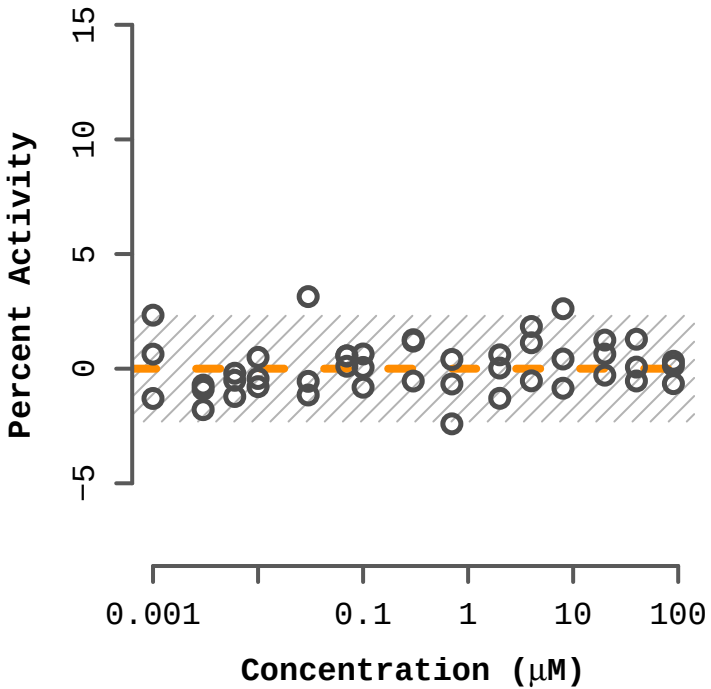
NAME: 2-Ethylhexyl salicylate
CHID: 40734 **CASRN:** 118-60-5
SPID(S): Tox21_111573_1
M4ID: 12483611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.224 **MAX_MED:** 0.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

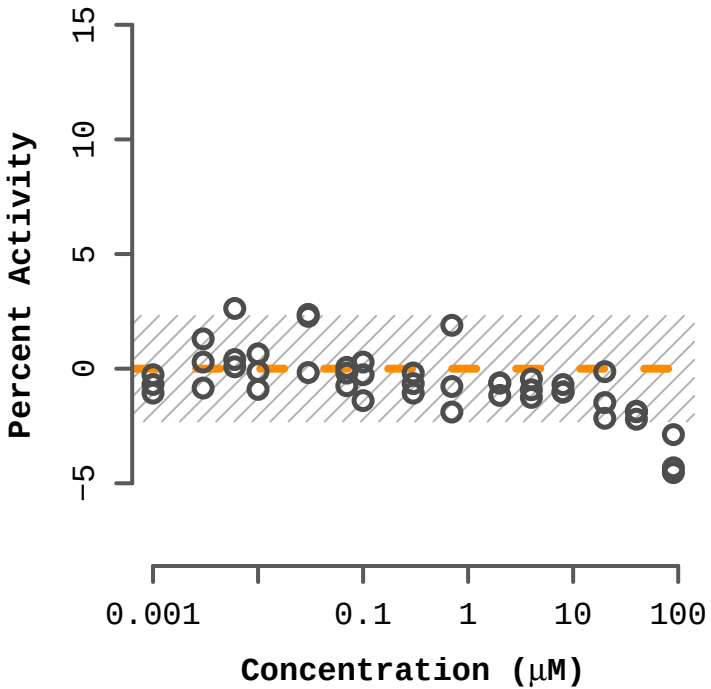
NAME: 1,7-Dioxaspiro[5.5]undecane
CHID: 40735 **CASRN:** 180-84-7
SPID(S): Tox21_300659
M4ID: 12478474

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.815 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

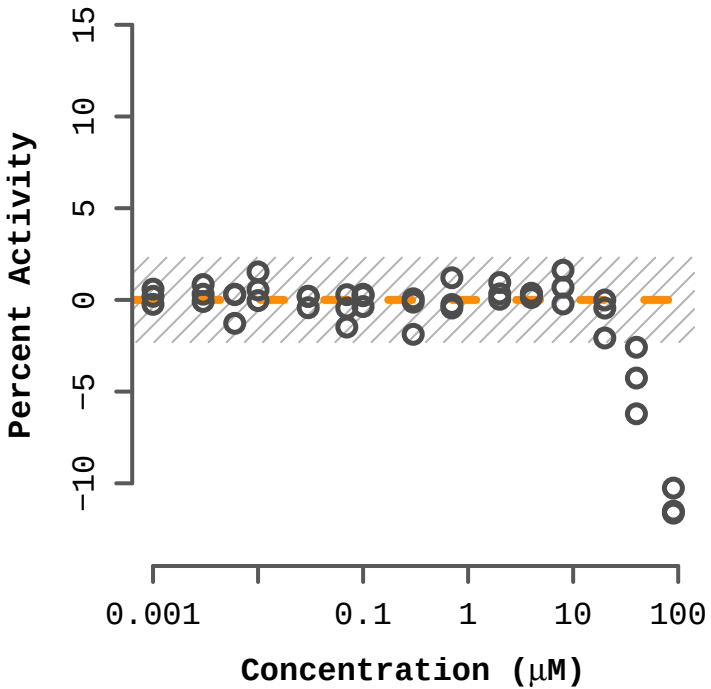
NAME: Fumagillin
CHID: 40736 **CASRN:** 23110-15-8
SPID(S): Tox21_302410
M4ID: 12476723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

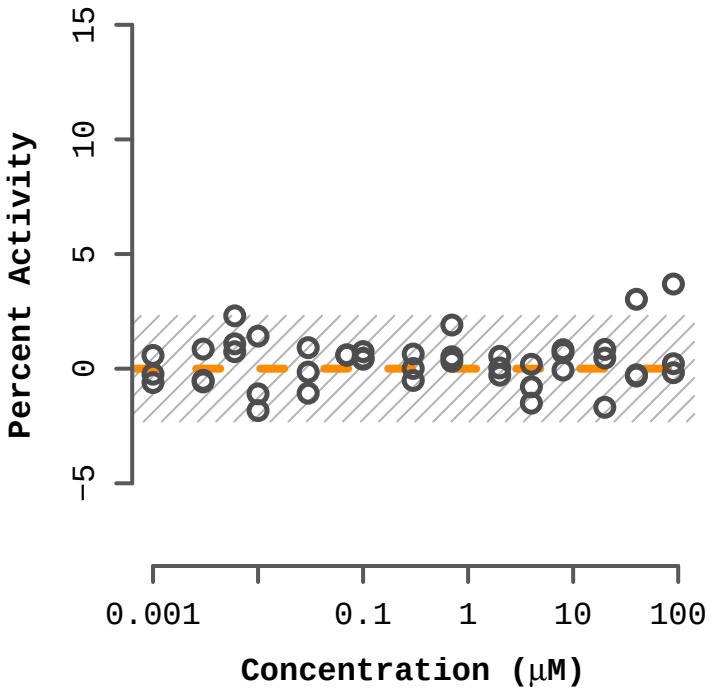
NAME: Imipramine hydrochloride
CHID: 40738 **CASRN:** 113-52-0
SPID(S): Tox21_301417
M4ID: 12477716

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.3	NA	NA
PROB:	1	NA	NA
RMSE:	3.19	NA	NA

MAX_MEAN: 0.697 **MAX_MED:** 0.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

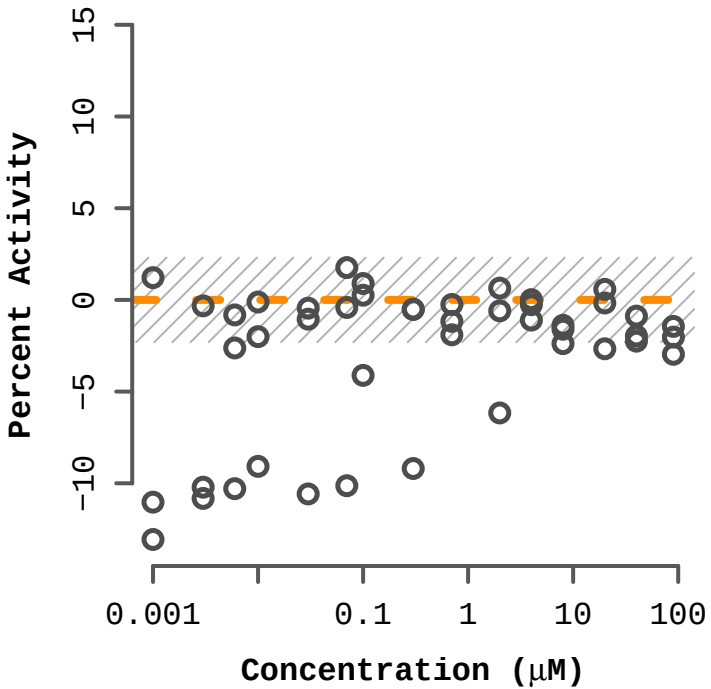
NAME: Kasugamycin hydrochloride
CHID: 40739 **CASRN:** 19408-46-9
SPID(S): Tox21_302236
M4ID: 12476897

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

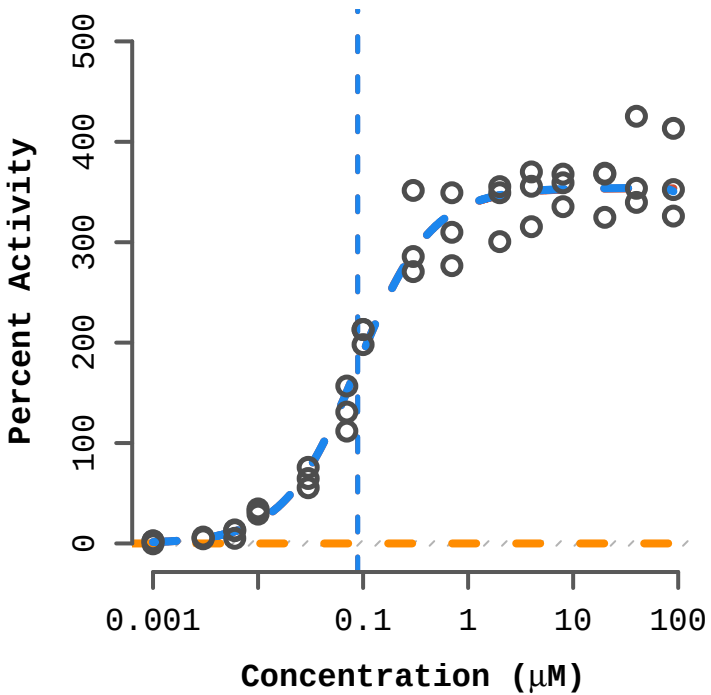
NAME: 2-Methyl-4-isothiazolin-3-one hydrochloride
CHID: 40740 **CASRN:** 26172-54-3
SPID(S): Tox21_301935
M4ID: 12477198

HILL MODEL: Not applicable.

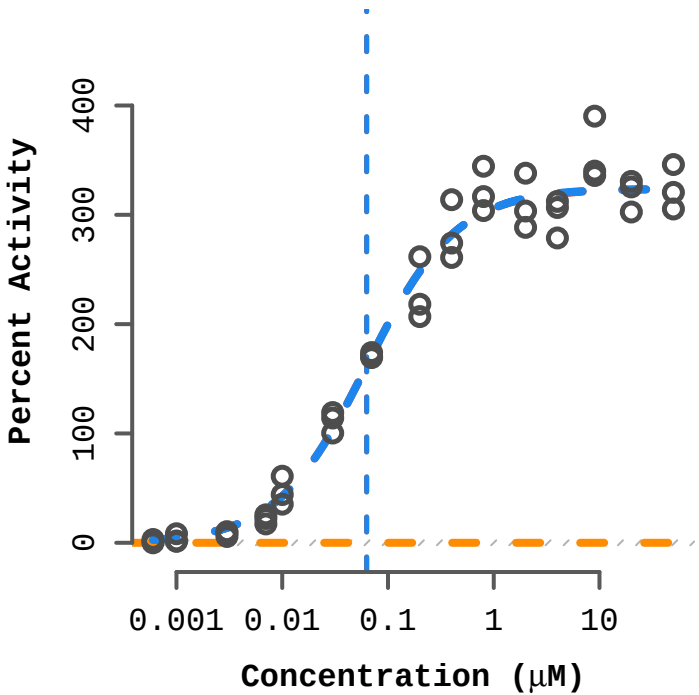
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	266.38	NA	NA
PROB:	1	NA	NA
RMSE:	5	NA	NA

MAX_MEAN: −0.447 **MAX_MED:** 0.256 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Triamcinolone
CHID:    40742   CASRN: 124-94-7
SPID(S): Tox21_300178
M4ID:    12478952

HILL MODEL (in red):
      tp       ga       gw
val:  354      -1.05    1.24
sd:   5.55     0.0354   0.116

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  354      -1.05    1.24     2.22     7.54
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  637.19      418.11      422.07
PROB: 0           0.88        0.12
RMSE: 260.45      24.44       24.54

MAX_MEAN: 373       MAX_MED: 368       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamcinolone
CHID: 40742 CASRN: 124-94-7
SPID(S): Tox21_111332_1
M4ID: 12483760

HILL MODEL (in red):

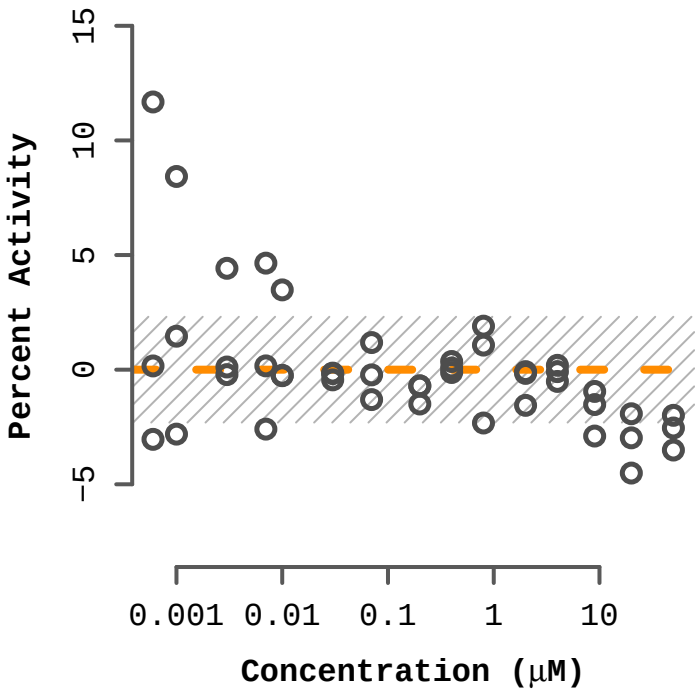
	tp	ga	gw
val:	324	-1.2	1.03
sd:	5.25	0.0354	0.0701

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	324	-1.2	1.03	2.39	3.23
sd:	6.24	0.0377	0.0723	4.94	23.1

	CNST	HILL	GNLS
AIC:	626.23	398.2	402.17
PROB:	0	0.88	0.12
RMSE:	231.35	19.62	19.6

MAX_MEAN: 355 MAX_MED: 340 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

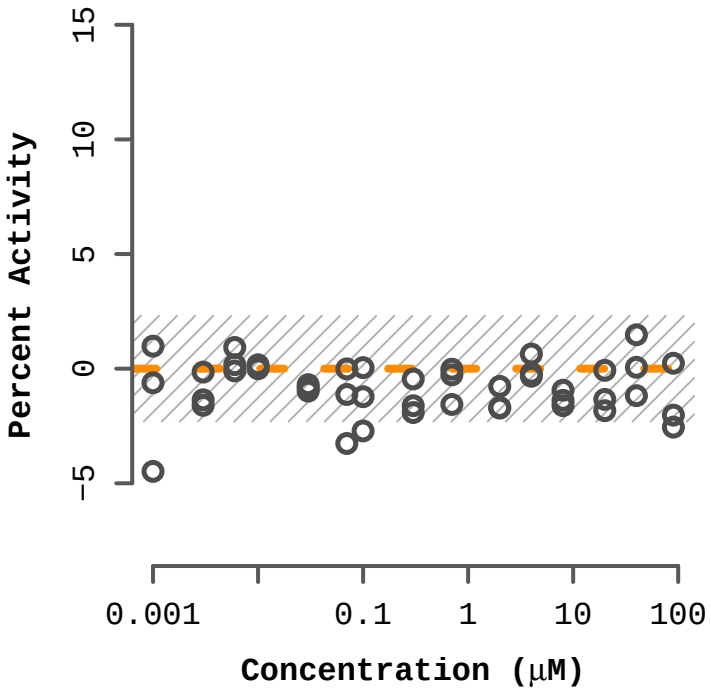
NAME: Arotinoid acid
CHID: 40743 **CASRN:** 71441-28-6
SPID(S): Tox21_304044
M4ID: 12475144

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 2.94 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

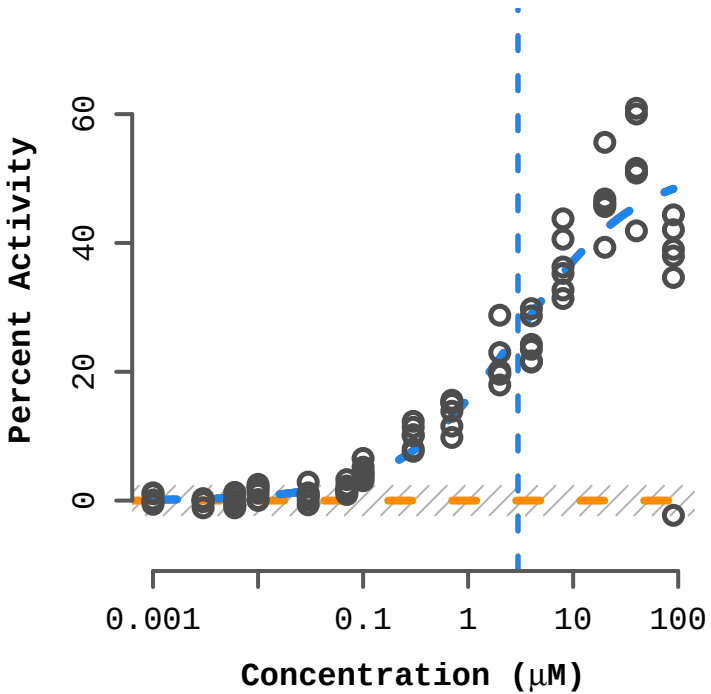
NAME: 4-[3-(4-Acetyl-3-hydroxy-2-propylphenoxy)propo
CHID: 40745 CASRN: 79558-09-1
SPID(S): Tox21_302413
M4ID: 12476720

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 0.335 MAX_MED: 0.177 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Hydroxyprogesterone
CHID: 40747 CASRN: 68-96-2
SPID(S): Tox21_301530
M4ID: 12477603

HILL MODEL (in red):

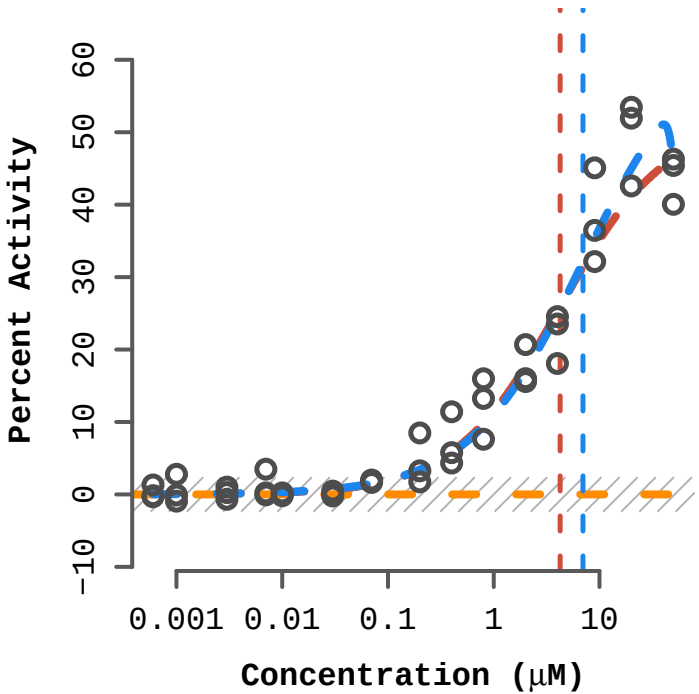
	tp	ga	gw
val:	52.1	0.475	0.758
sd:	4.71	0.123	0.0618

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	52.1	0.475	0.758	3.47	9.55
sd:	4.71	0.123	0.0618	194000	1090000

	CNST	HILL	GNLS
AIC:	831.79	528.88	532.88
PROB:	0	0.88	0.12
RMSE:	24.67	6.91	6.91

MAX_MEAN: 52.7 MAX_MED: 51.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 17alpha-Hydroxyprogesterone
CHID: 40747 **CASRN:** 68-96-2
SPID(S): Tox21_111233_1
M4ID: 12483824

HILL MODEL (in red):

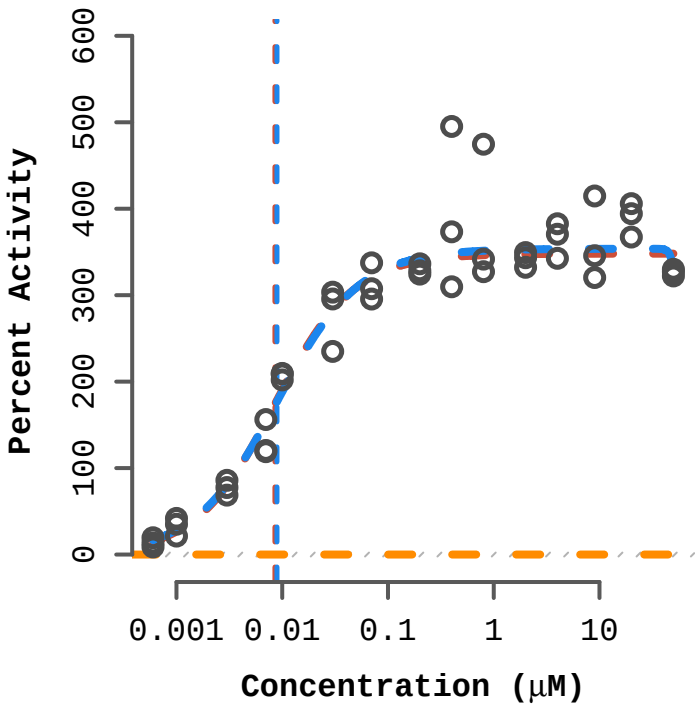
	tp	ga	gw
val:	51.8	0.628	0.869
sd:	2.92	0.0825	0.0918

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	64.1	0.844	0.811	1.75	13
sd:	10.9	0.178	0.0826	0.014	5.75

	CNST	HILL	GNLS
AIC:	399.88	241.86	237.53
PROB:	0	0.1	0.9
RMSE:	21.49	3.82	3.23

MAX_MEAN: 49.3 **MAX_MED:** 51.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Beclomethasone
CHID: 40750 CASRN: 4419-39-0
SPID(S): Tox21_112116_1
M4ID: 12483309

HILL MODEL (in red):

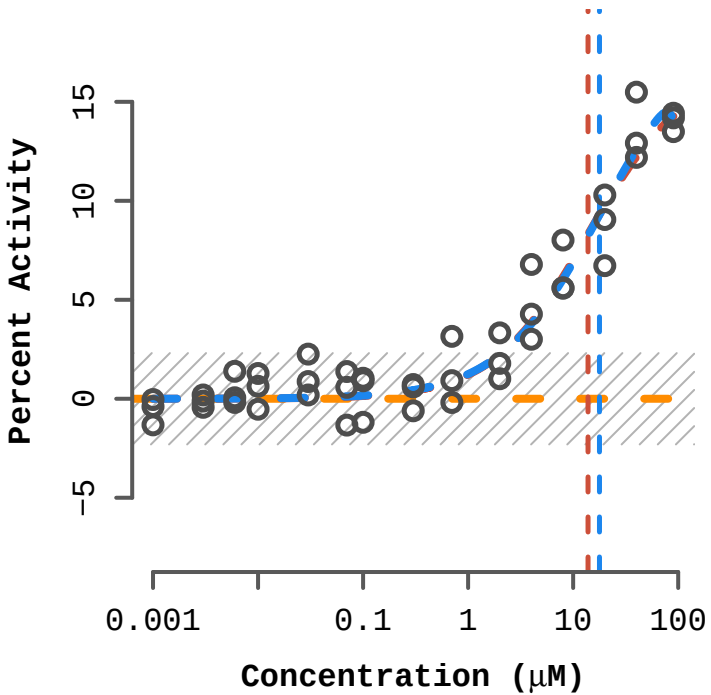
	tp	ga	gw
val:	348	-2.07	1.16
sd:	6.36	0.0437	0.126

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	354	-2.05	1.12	1.76	18
sd:	7.15	0.0469	0.121	0.0305	10

	CNST	HILL	GNLS
AIC:	649.79	445.38	445.39
PROB:	0	0.5	0.5
RMSE:	294.8	37.82	36.27

MAX_MEAN: 393 MAX_MED: 394 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(9-Fluorenylmethoxycarbonyl)-L-leucine
CHID: 40751 CASRN: 35661-60-0
SPID(S): Tox21_301495
M4ID: 12477638

HILL MODEL (in red):

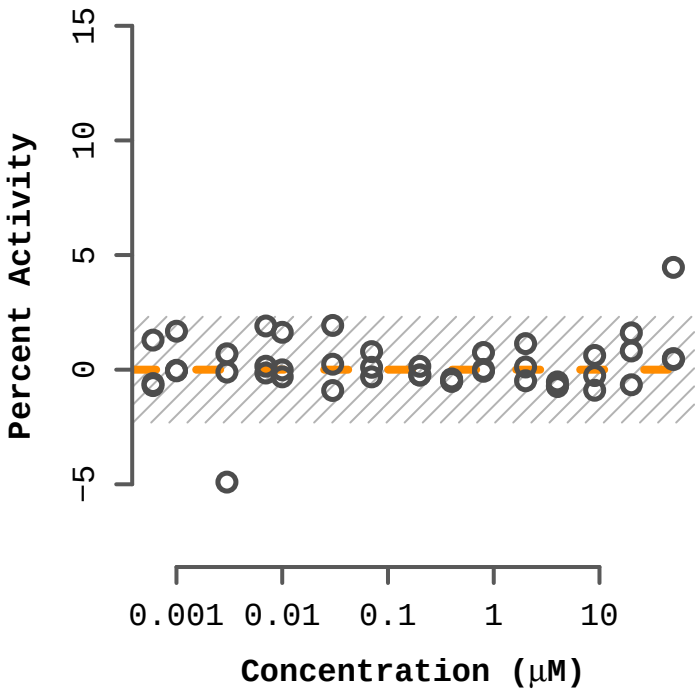
	tp	ga	gw
val:	16.6	1.14	0.965
sd:	1.6	0.123	0.157

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.6	1.25	0.914	2.07	9.76
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	283.55	150.11	152.81
PROB:	0	0.79	0.21
RMSE:	6.01	1.2	1.18

MAX_MEAN: 14 MAX_MED: 14.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

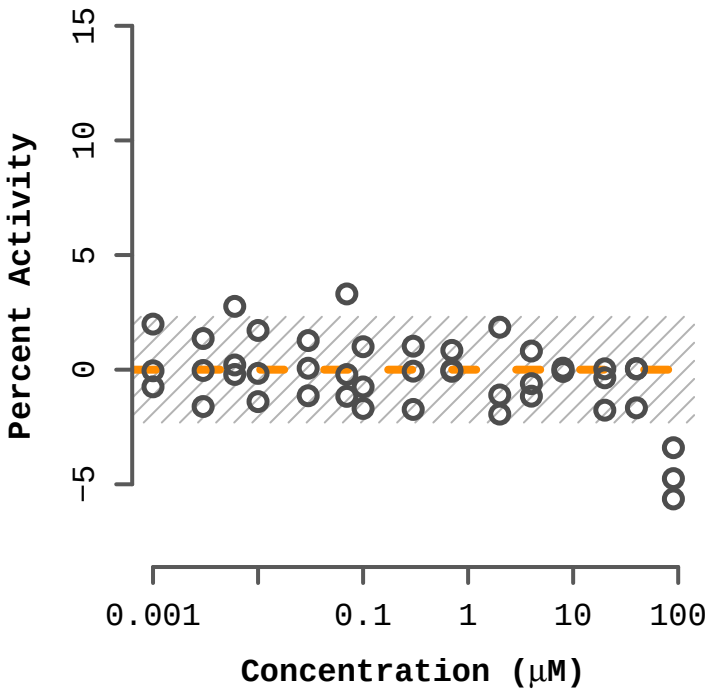
NAME: Ciglitizone
CHID: 40757 **CASRN:** 74772-77-3
SPID(S): Tox21_112120_1
M4ID: 12483306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

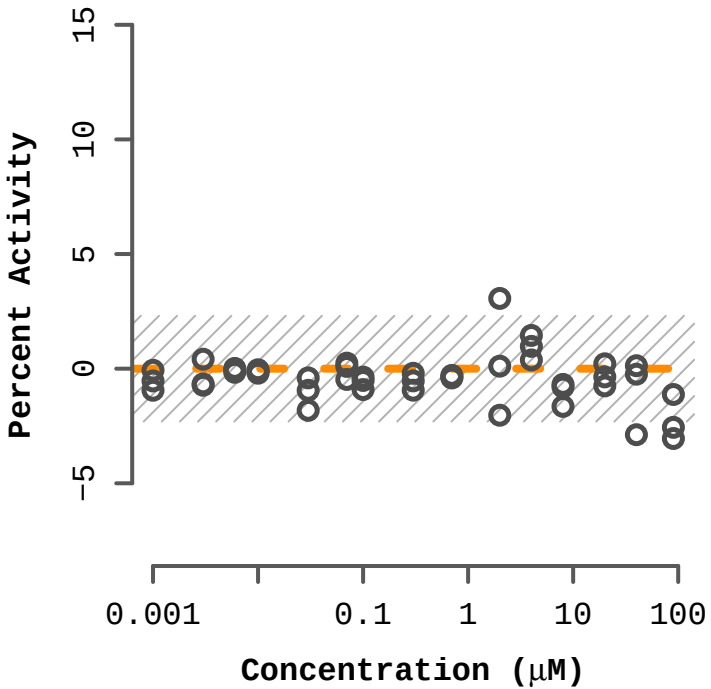
NAME: AM580
CHID: 40758 **CASRN:** 102121-60-8
SPID(S): Tox21_300780
M4ID: 12478353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 0.921 **MAX_MED:** 0.207 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: {4-[({2-[3-Fluoro-4-(trifluoromethyl)phenyl]-4·

CHID: 40760 **CASRN:** 317318-84-6

SPID(S): Tox21_302411

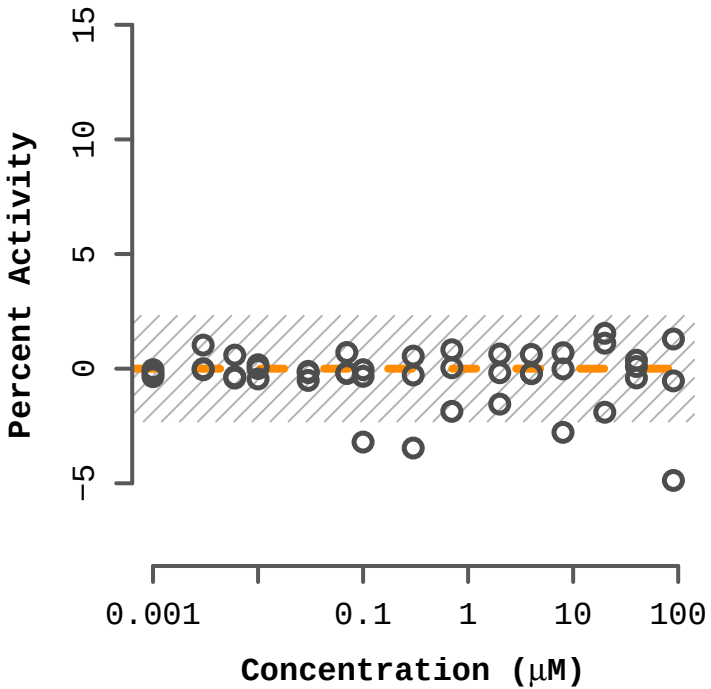
M4ID: 12476722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.936 **MAX_MED:** 0.974 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

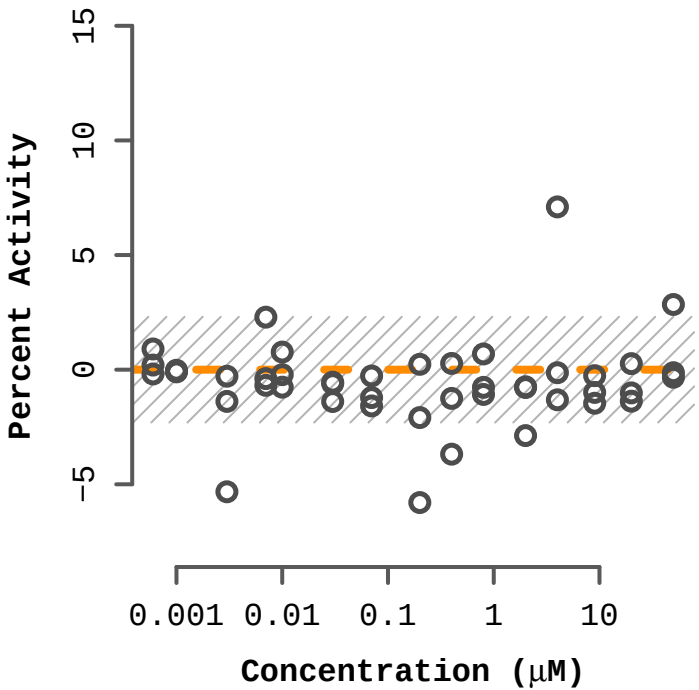
NAME: Dimethyl maleate
CHID: 40765 **CASRN:** 624-48-6
SPID(S): Tox21_300996
M4ID: 12478137

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.328 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

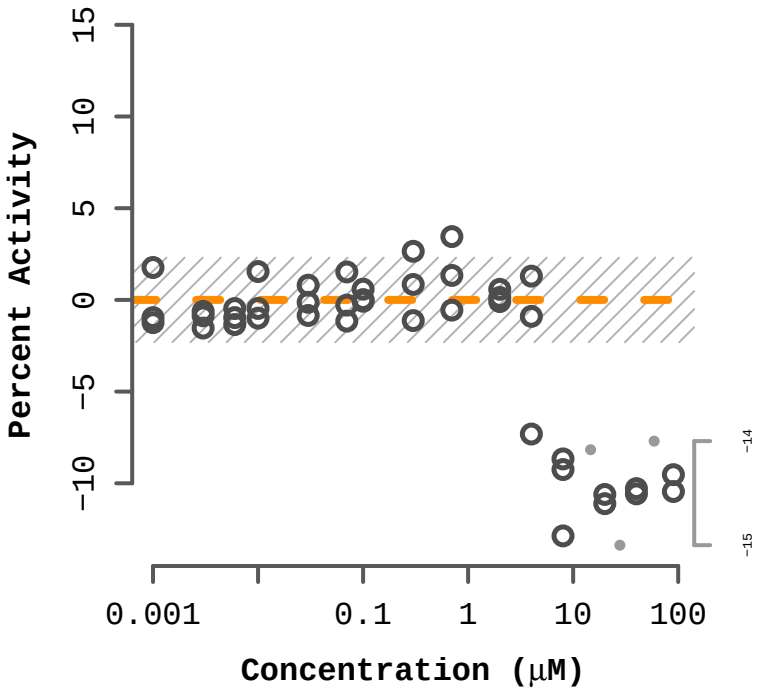
NAME: Dimethyl maleate
CHID: 40765 **CASRN:** 624-48-6
SPID(S): Tox21_113653
M4ID: 12482559

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 0.203 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

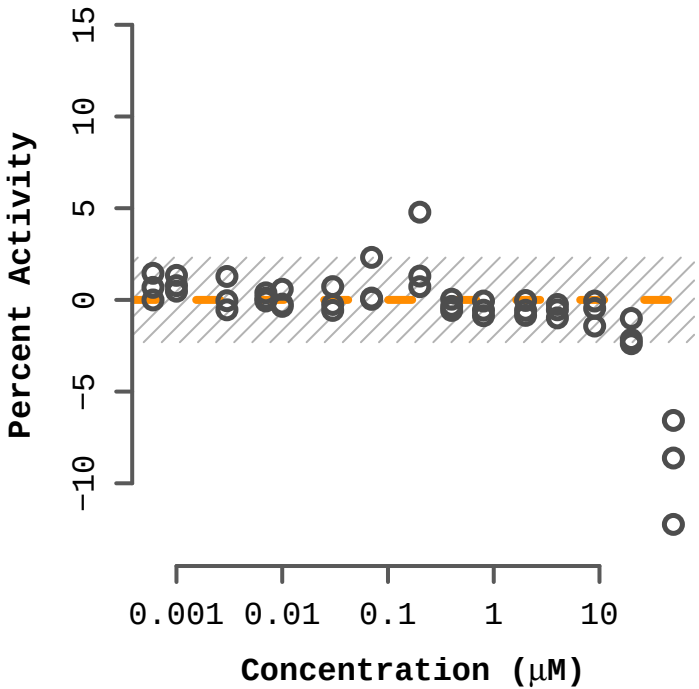
NAME: 3,5-Dichlorosalicyl-3,4-dichloroanilide
CHID: 40767 **CASRN:** 1154-59-2
SPID(S): Tox21_302073
M4ID: 12477060 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.75	NA	NA
PROB:	1	NA	NA
RMSE:	6.07	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

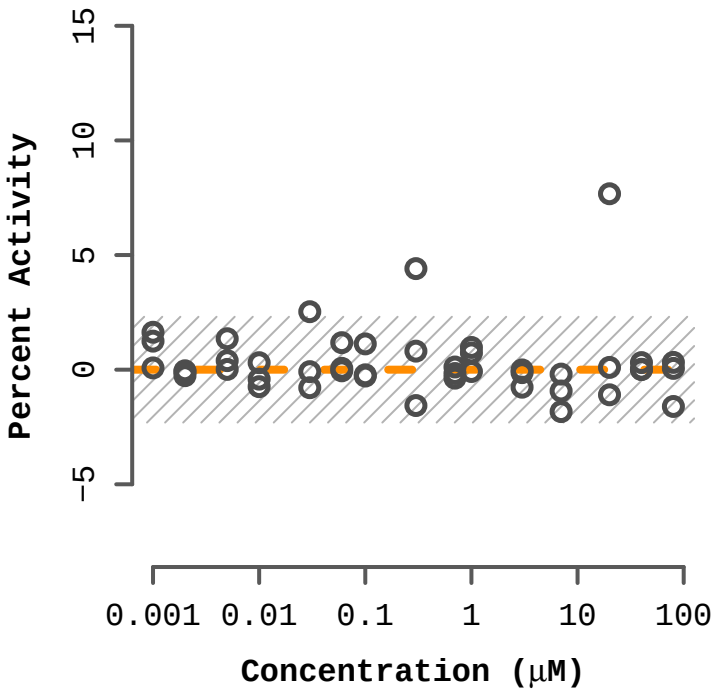
NAME: (Z,E)-Diethylstilbestrol
CHID: 40770 **CASRN:** 6898-97-1
SPID(S): Tox21_111005_1
M4ID: 12483954

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.63	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 2.27 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

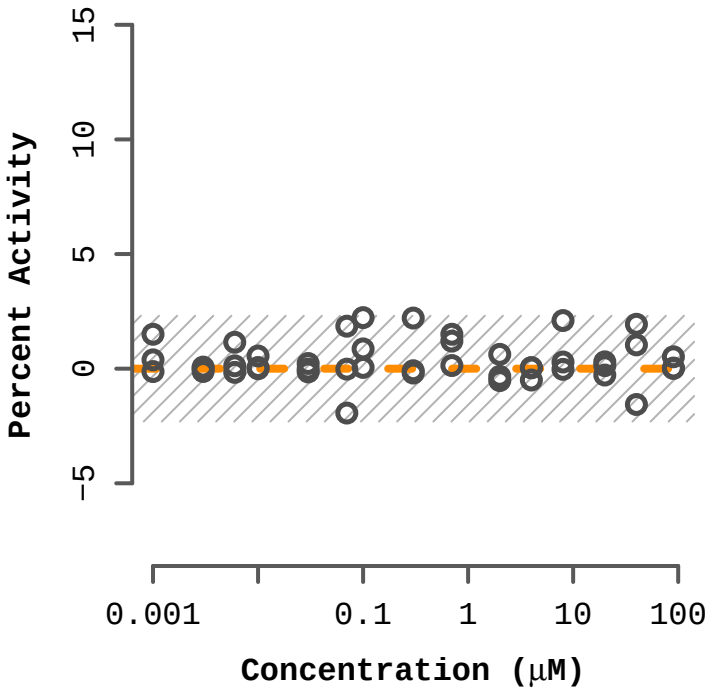
NAME: (−)−alpha,beta−Thujone
CHID: 40774 **CASRN:** 76231−76−0
SPID(S): Tox21_301840
M4ID: 12477293

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

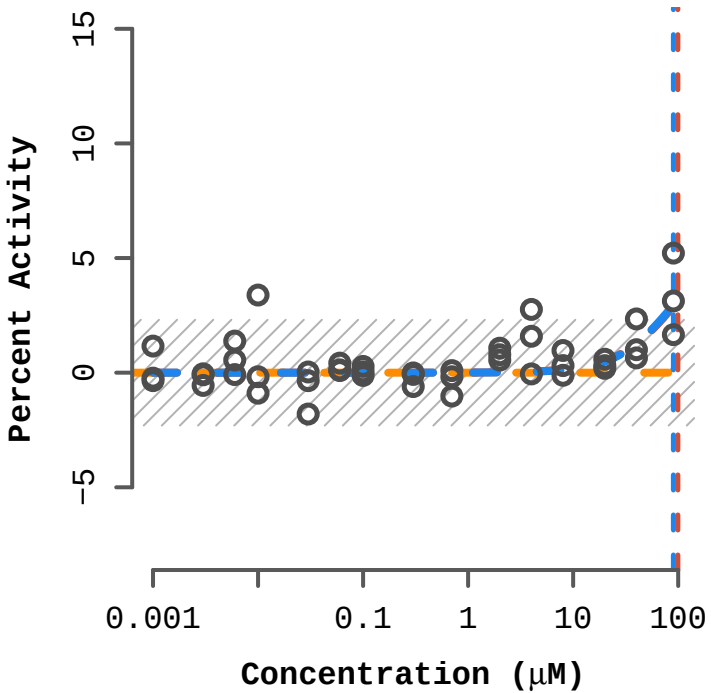
NAME: Terpineol
CHID: 40775 CASRN: 8000-41-7
SPID(S): Tox21_302298
M4ID: 12476835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.05 MAX_MED: 1.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Morin hydrate
CHID: 40776 CASRN: 654055-01-3
SPID(S): Tox21_301216
M4ID: 12477917

HILL MODEL (in red):

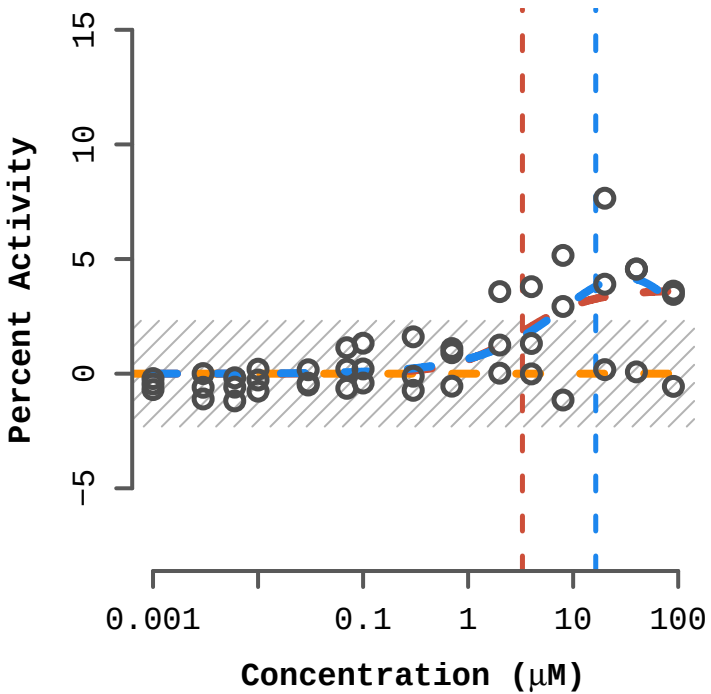
	tp	ga	gw
val:	6.26	2	1.51
sd:	6.96	0.631	1.04

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.91	1.95	1.6	3.9	3.75
sd:	8.28	0.752	1.27	1840	3580

	CNST	HILL	GNLS
AIC:	142.28	123.1	127.15
PROB:	0	0.88	0.12
RMSE:	1.35	0.97	0.97

MAX_MEAN: 3.34 **MAX_MED:** 3.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diheptyl phthalate
CHID: 40779 CASRN: 3648-21-3
SPID(S): Tox21_303892
M4ID: 12475296

HILL MODEL (in red):

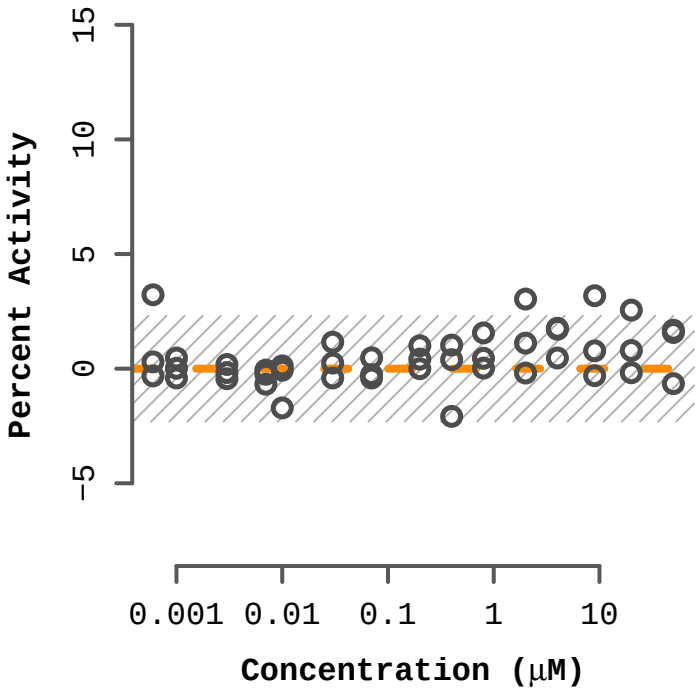
	tp	ga	gw
val:	3.65	0.517	1.35
sd:	0.605	0.244	0.792

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.69	1.21	0.9	1.86	1.32
sd:	43.9	3.33	0.672	2.36	3.57

	CNST	HILL	GNLS
AIC:	191.7	169.26	171.57
PROB:	0	0.76	0.24
RMSE:	2.22	1.56	1.55

MAX_MEAN: 3.91 MAX_MED: 4.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

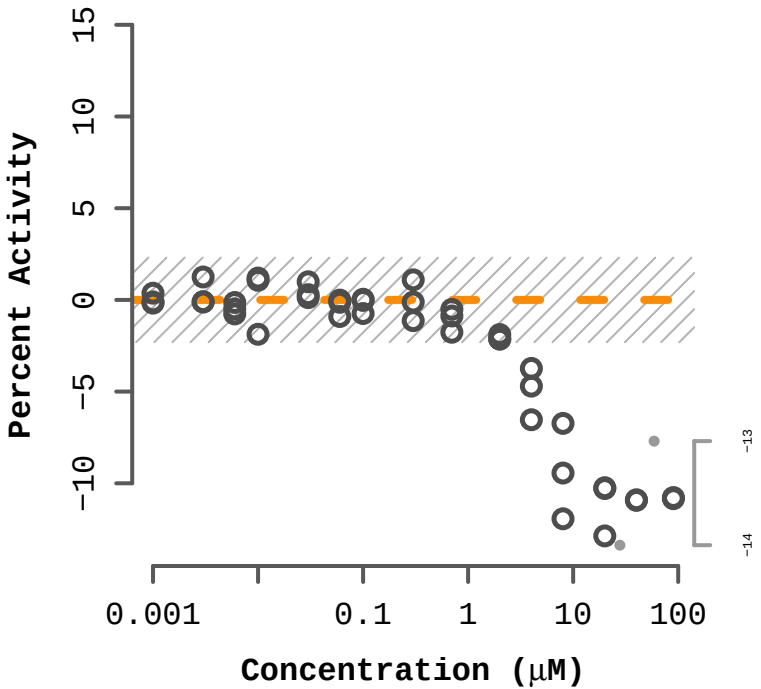
NAME: 1-Phenyltridecane
CHID: 40784 **CASRN:** 123-02-4
SPID(S): Tox21_303706
M4ID: 12475482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

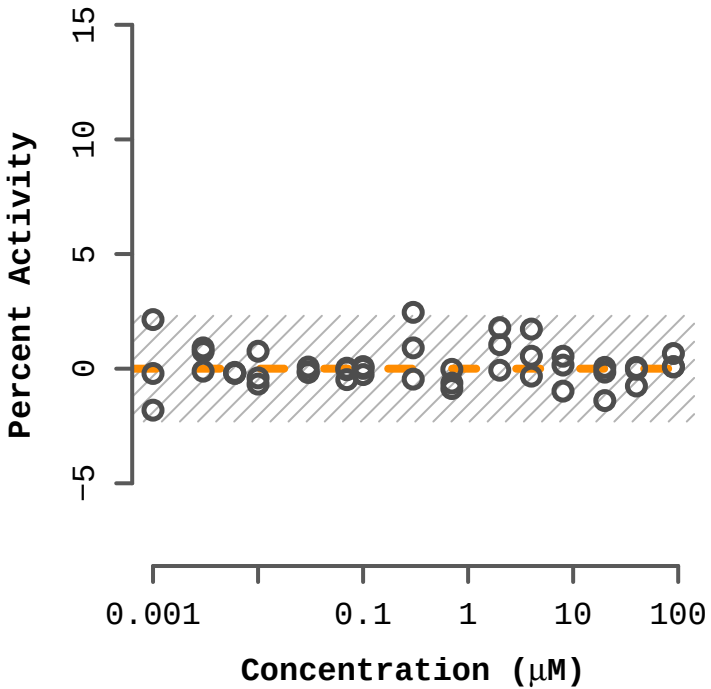
NAME: Benzyldimethyldodecylammonium chloride
CHID: 40787 CASRN: 139-07-1
SPID(S): Tox21_301369
M4ID: 12477764 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.06	NA	NA
PROB:	1	NA	NA
RMSE:	5.99	NA	NA

MAX_MEAN: 0.469 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

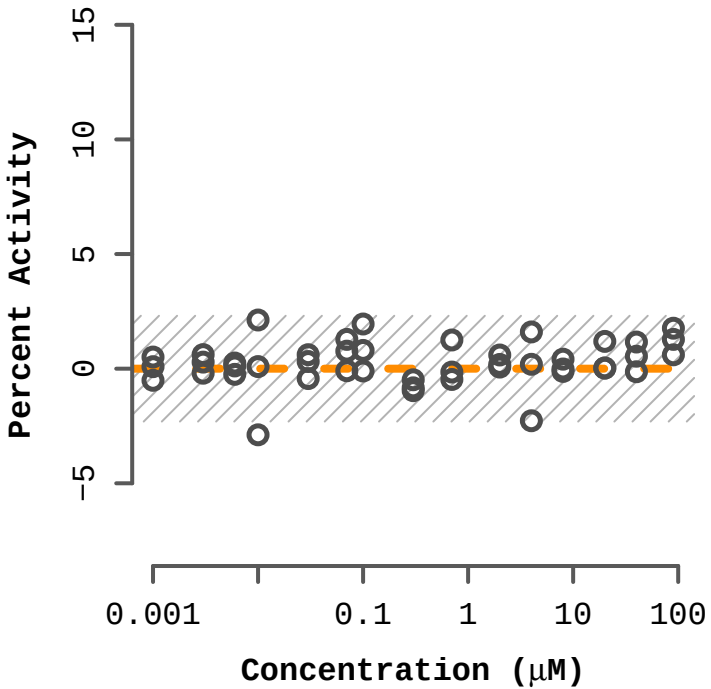
NAME: 2-tert-Butyl-4-methoxyphenol
CHID: 40788 **CASRN:** 121-00-6
SPID(S): Tox21_300082
M4ID: 12479048

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

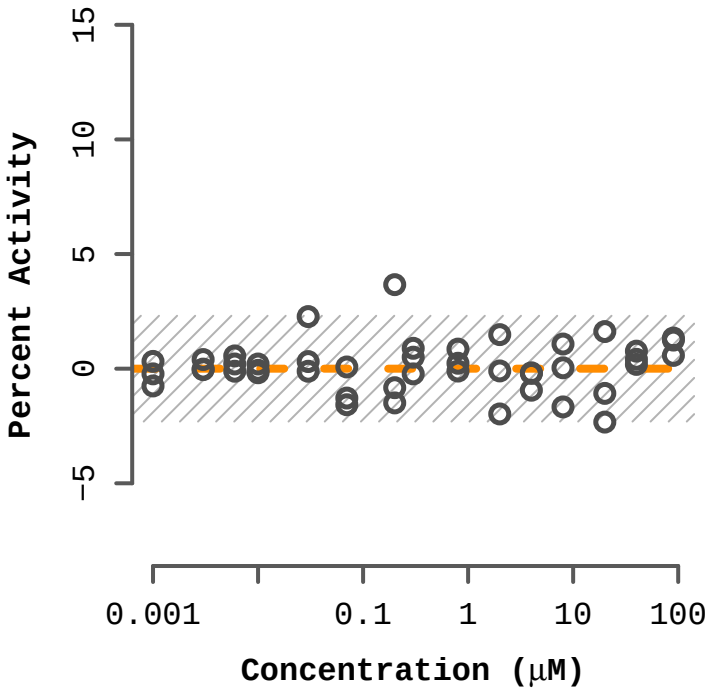
NAME: Pyridoxine hydrochloride
CHID: 40792 CASRN: 58-56-0
SPID(S): Tox21_302476
M4ID: 12476657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

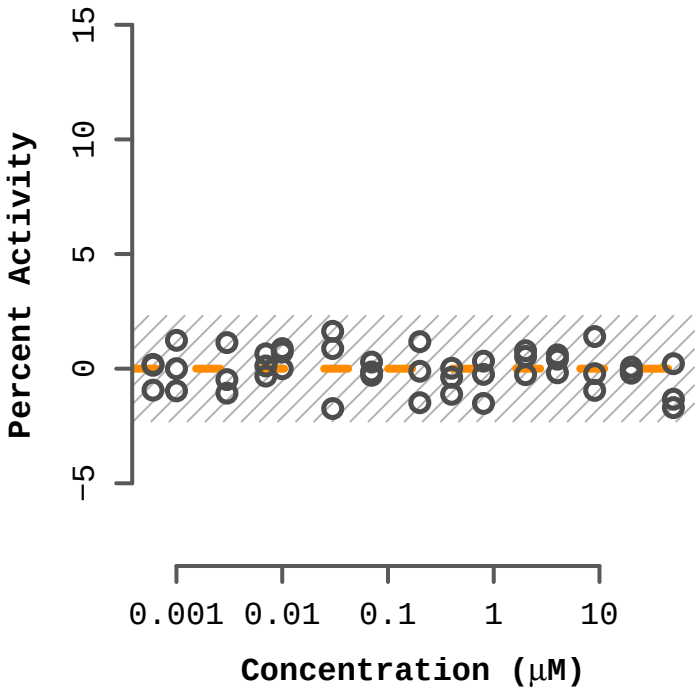
NAME: Sodium 2-phenylphenate tetrahydrate
CHID: 40794 **CASRN:** 6152-33-6
SPID(S): Tox21_301387
M4ID: 12477746

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

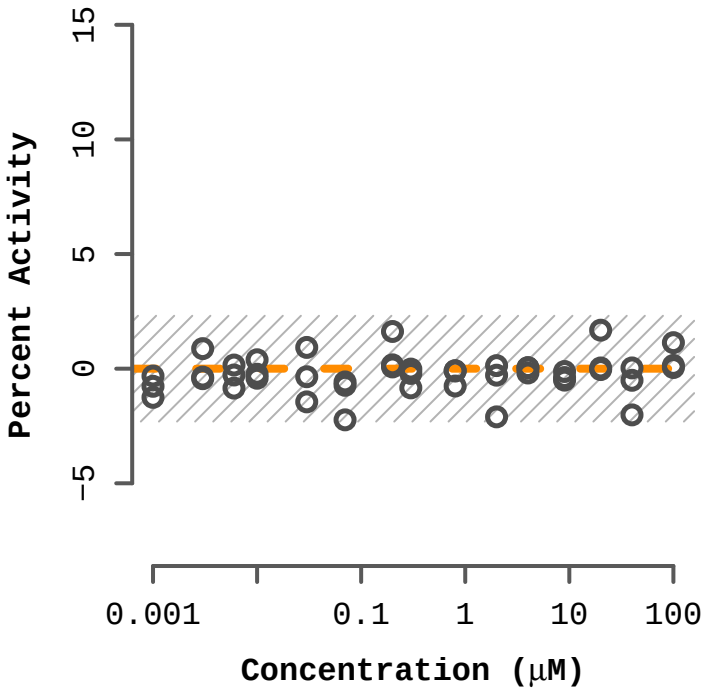
NAME: Sodium 2-phenylphenate tetrahydrate
CHID: 40794 **CASRN:** 6152-33-6
SPID(S): Tox21_112097_1
M4ID: 12483322

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.536 **MAX_MED:** 0.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

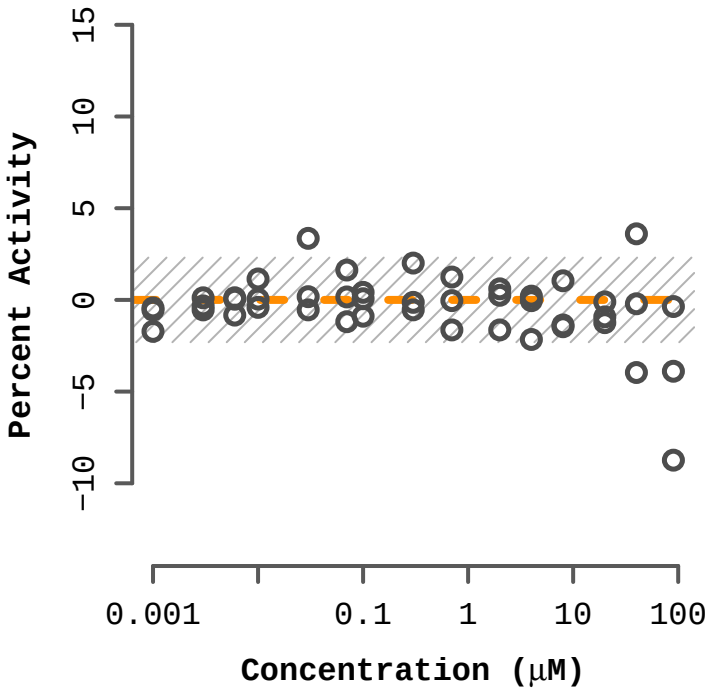
NAME: Chloramine-T trihydrate
CHID: 40795 **CASRN:** 7080-50-4
SPID(S): Tox21_302436
M4ID: 12476697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.623 **MAX_MED:** 0.169 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

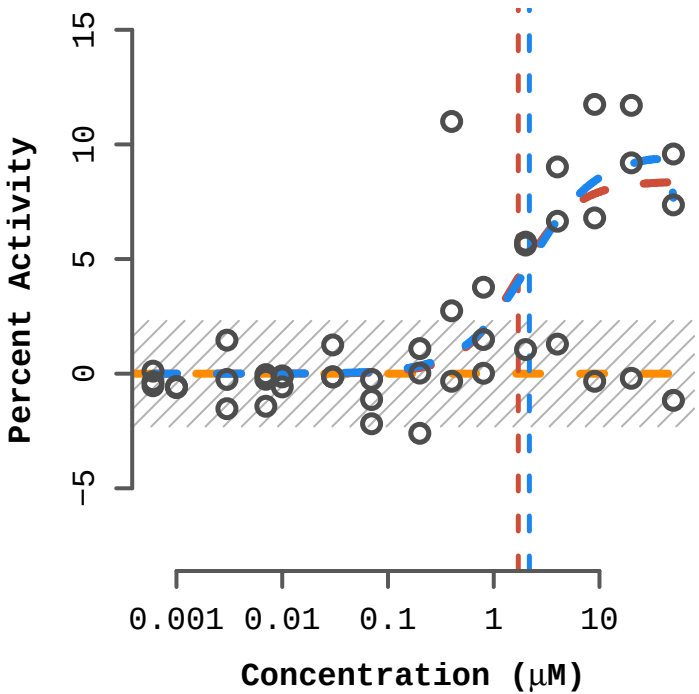
NAME: Etidronic acid monohydrate
CHID: 40800 **CASRN:** 25211-86-3
SPID(S): Tox21_301371
M4ID: 12477762

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 0.998 **MAX_MED:** 0.253 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (+−)−Indoxacarb
CHID: 40801 **CASRN:** 144171−61−9
SPID(S): Tox21_303872
M4ID: 12475316

HILL MODEL (in red):

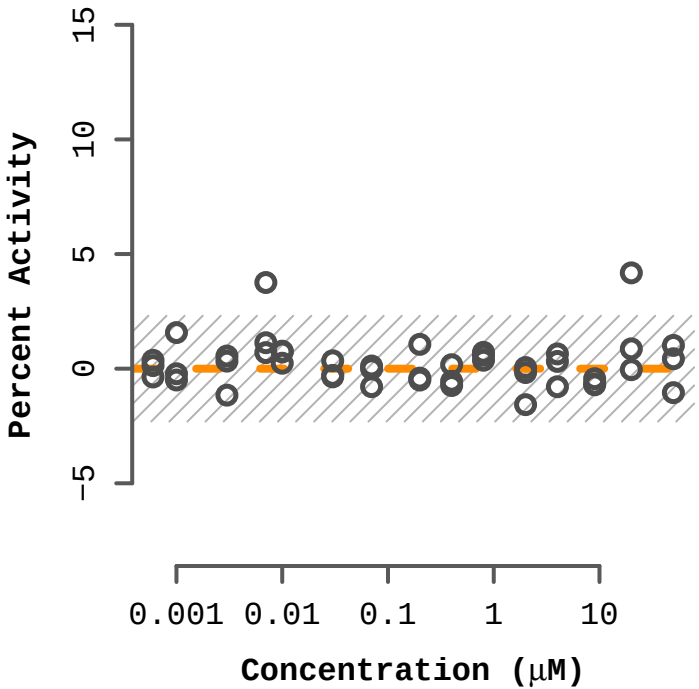
	tp	ga	gw
val:	8.39	0.232	1.61
sd:	1.08	0.149	0.638

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.59	0.337	1.38	1.75	12.2
sd:	2.01	0.222	0.581	0.136	32.9

	CNST	HILL	GNLS
AIC:	256.06	222.5	225.81
PROB:	0	0.84	0.16
RMSE:	4.51	3.17	3.19

MAX_MEAN: 6.9 **MAX_MED:** 9.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

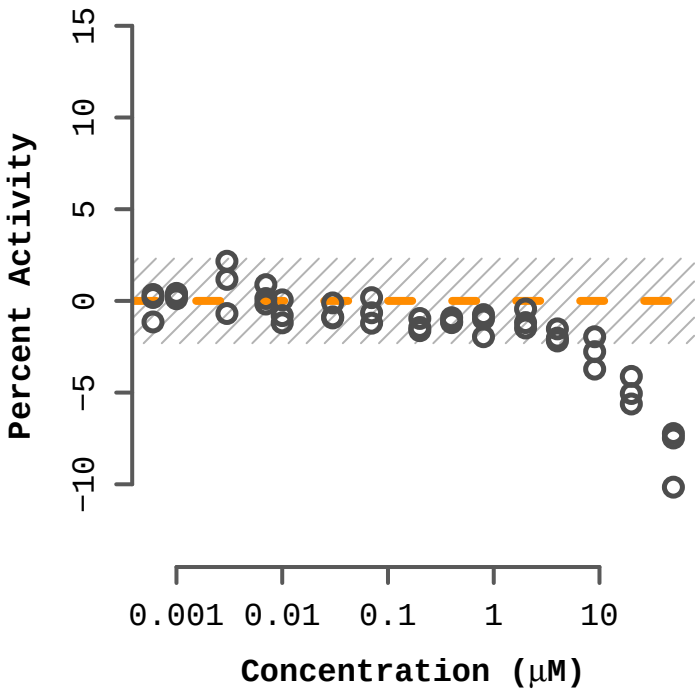
NAME: Sodium 4-phenylbutyrate
CHID: 40948 **CASRN:** 1716-12-7
SPID(S): Tox21_110826_1
M4ID: 12484090

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

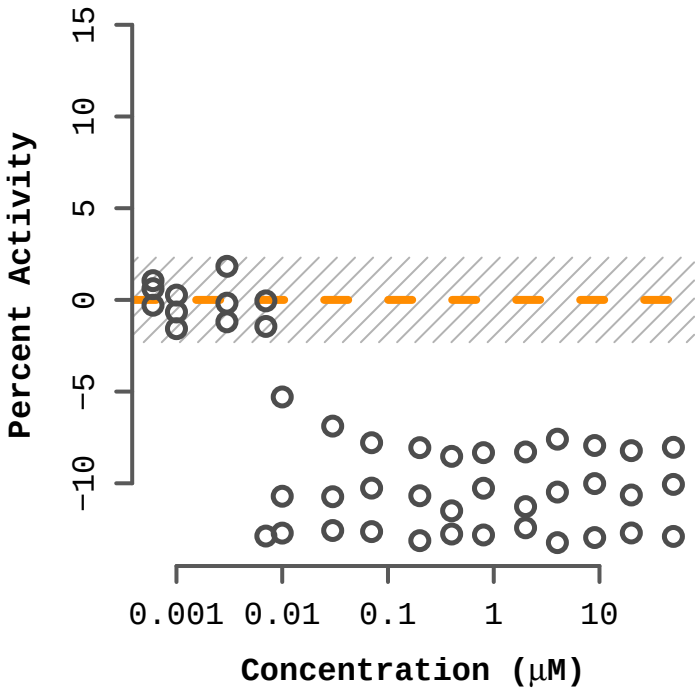
NAME: Dasatinib
CHID: 40979 **CASRN:** 302962-49-8
SPID(S): Tox21_112736_1
M4ID: 12482971

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.81	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

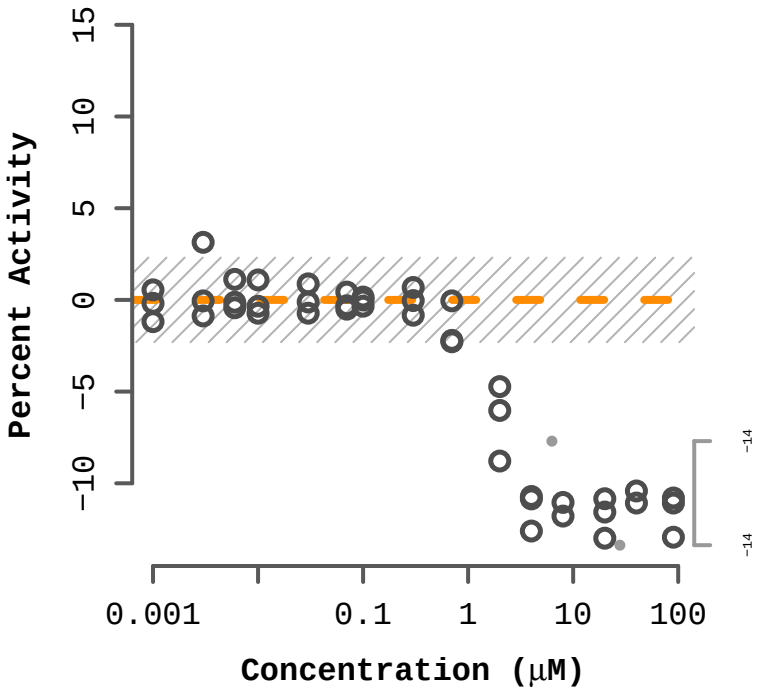
NAME: Bortezomib
CHID: 40980 CASRN: 179324-69-7
SPID(S): Tox21_112672_1
M4ID: 12482987

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	338.49	NA	NA
PROB:	1	NA	NA
RMSE:	9.29	NA	NA

MAX_MEAN: 0.458 **MAX_MED:** 0.613 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

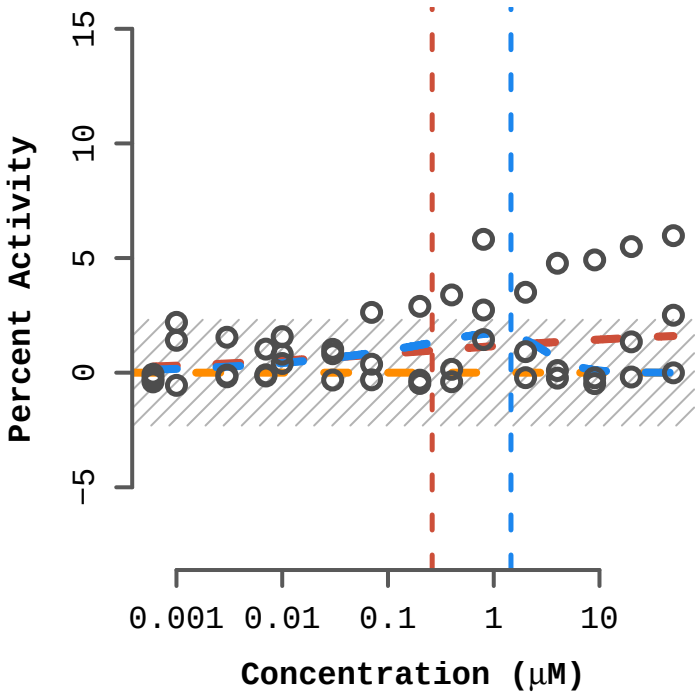
NAME: Carbonyl cyanide chlorophenylhydrazone
CHID: 40990 **CASRN:** 555-60-2
SPID(S): Tox21_302066
M4ID: 12477067 **BRK**

HILL MODEL: Not applicable.

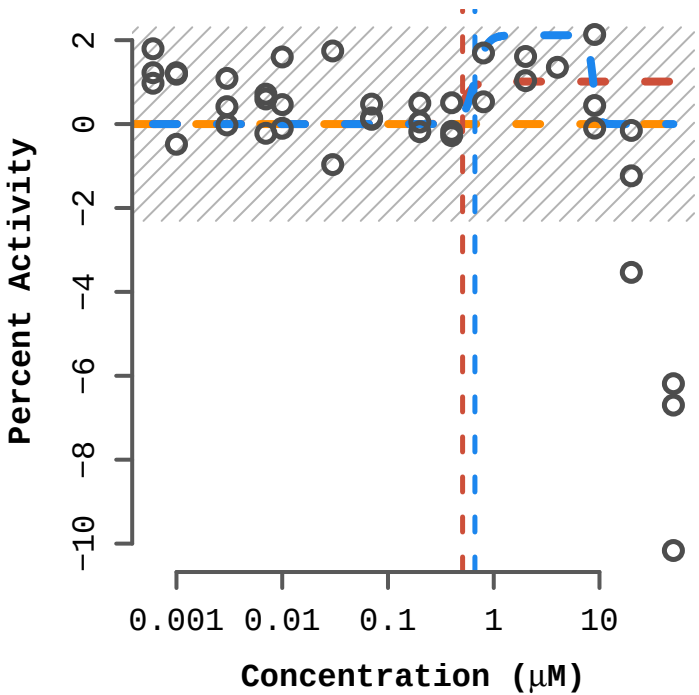
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	306.53	NA	NA
PROB:	1	NA	NA
RMSE:	7.07	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** −0.00409 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ganciclovir
CHID:    41032   CASRN: 82410-32-0
SPID(S): Tox21_110160_1
M4ID:    12484597

HILL MODEL (in red):
      tp       ga       gw
val:  1.93     -0.582   0.3
sd:   4.83     8.84     0.842

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.08     0.163    0.434    0.413    2.51
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  193.86      186.42      193.52
PROB: 0.02        0.95        0.03
RMSE: 2.22        1.76        1.97

MAX_MEAN: 3.33      MAX_MED: 2.73      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Gefitinib
CHID: 41034 **CASRN:** 184475-35-2
SPID(S): Tox21_111683_1
M4ID: 12483538

HILL MODEL (in red):

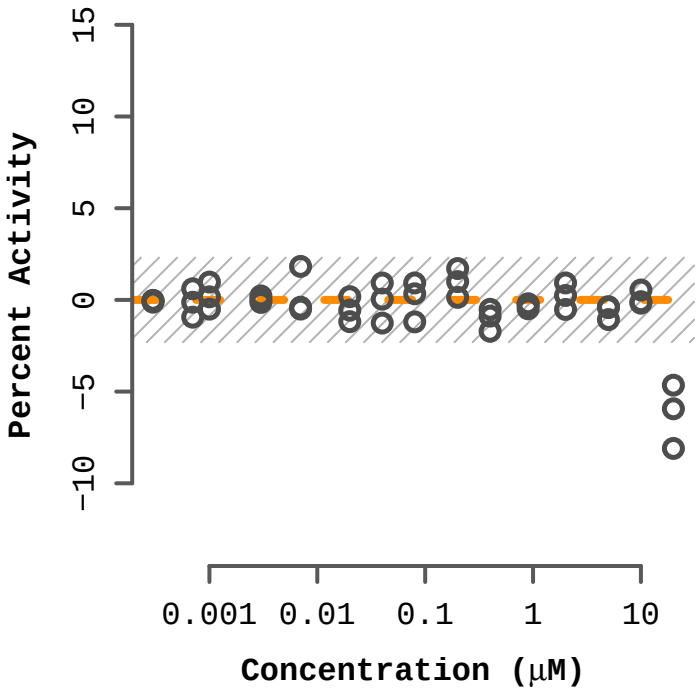
	tp	ga	gw
val:	1.01	−0.294	8
sd:	0.422	0.194	10.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.12	−0.178	8	0.938	18
sd:	0.483	0.223	20.3	0.187	210

	CNST	HILL	GNLS
AIC:	193.78	194.91	184.62
PROB:	0.01	0.01	0.98
RMSE:	2.47	2.62	2.29

MAX_MEAN: 2.52 **MAX_MED:** 2.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

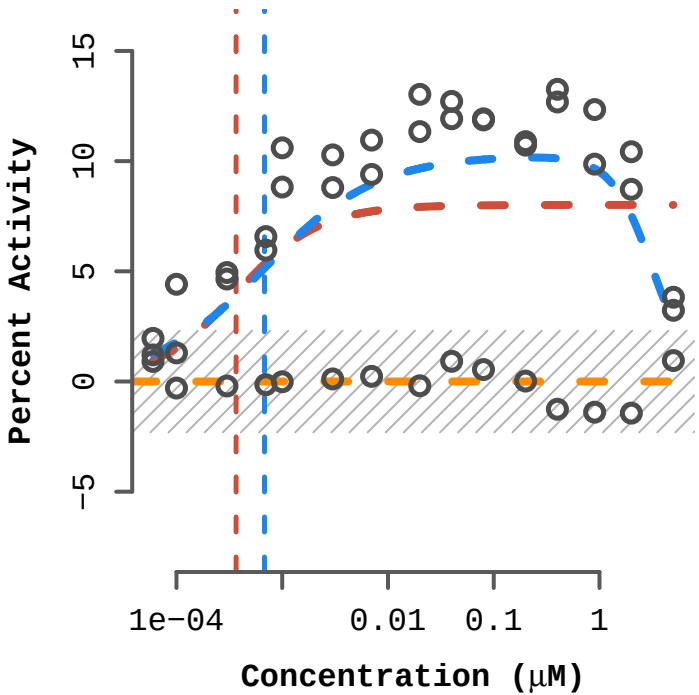
NAME: Imiquimod
CHID: 41047 **CASRN:** 99011-02-6
SPID(S): Tox21_110985_1
M4ID: 12483965

HILL MODEL: Not applicable.

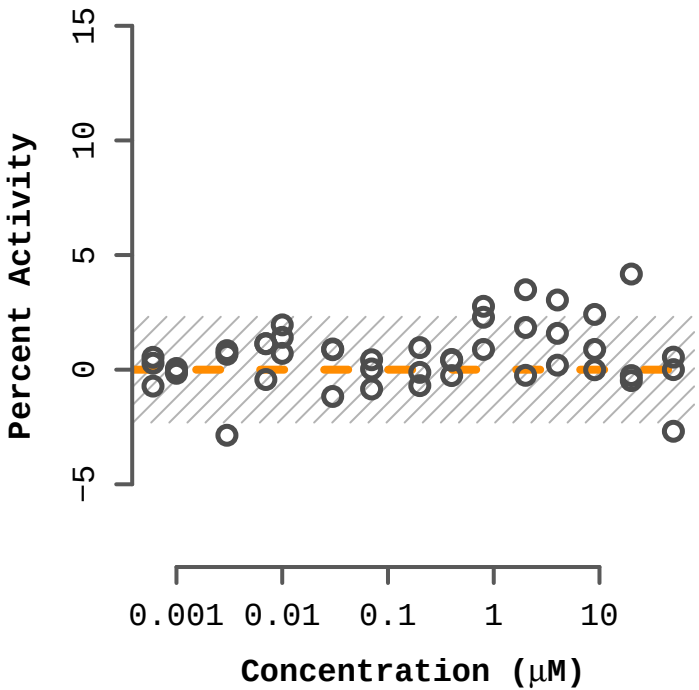
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.8	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 0.998 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    L-Arginine
CHID:    41056   CASRN: 74-79-3
SPID(S): Tox21_113046_1
M4ID:    12482830

HILL MODEL (in red):
      tp       ga       gw
val:  8.01     -3.44    1.11
sd:   1.19     0.328    0.716

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.3     -3.17    0.815    0.499    2.22
sd:   1.55     0.337    0.438    0.177    1.75

      CNST        HILL        GNLS
AIC:  318.14      282.54      279.03
PROB: 0           0.15        0.85
RMSE: 7.68        4.83        4.83

MAX_MEAN: 8.52      MAX_MED: 12.7      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

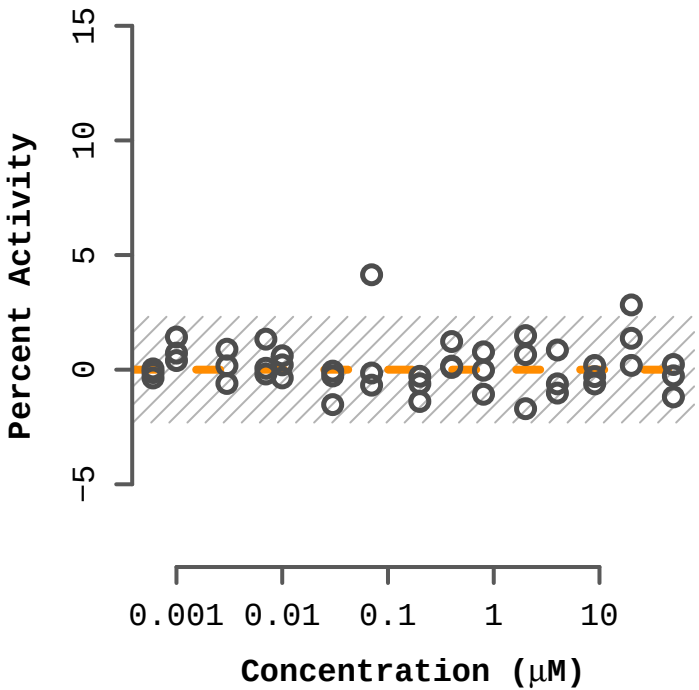
NAME: Mycophenolic acid
CHID: 41070 **CASRN:** 24280-93-1
SPID(S): Tox21_110610_1
M4ID: 12484233

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.98 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

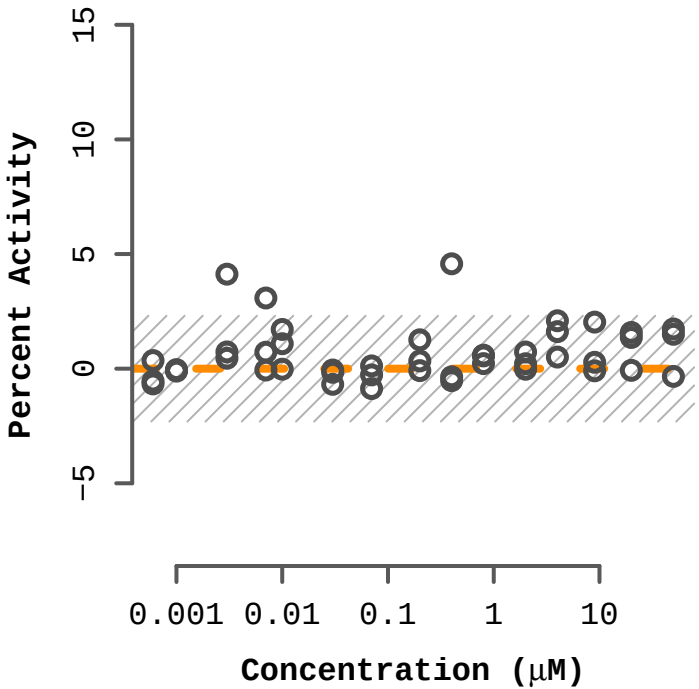
NAME: Neostigmine bromide
CHID: 41075 **CASRN:** 114-80-7
SPID(S): Tox21_112037_1
M4ID: 12483356

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

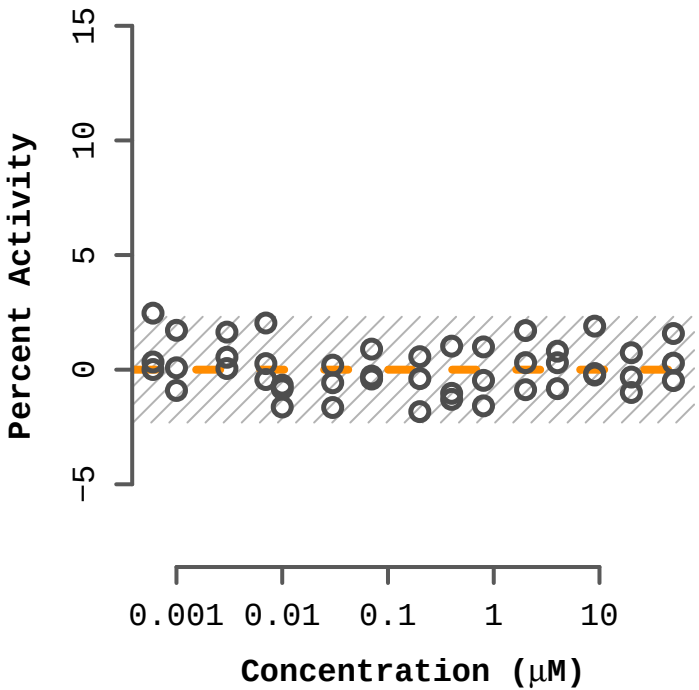
NAME: (E)−Nitenpyram
CHID: 41080 **CASRN:** 150824−47−8
SPID(S): Tox21_112342_1
M4ID: 12483149

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

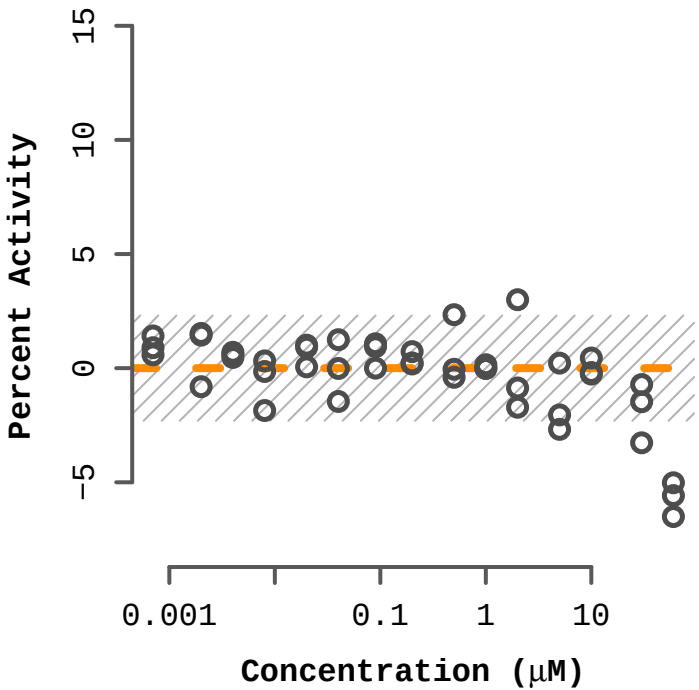
NAME: Ofloxacin
CHID: 41085 **CASRN:** 82419-36-1
SPID(S): Tox21_110703_1
M4ID: 12484165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.937 **MAX_MED:** 0.542 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

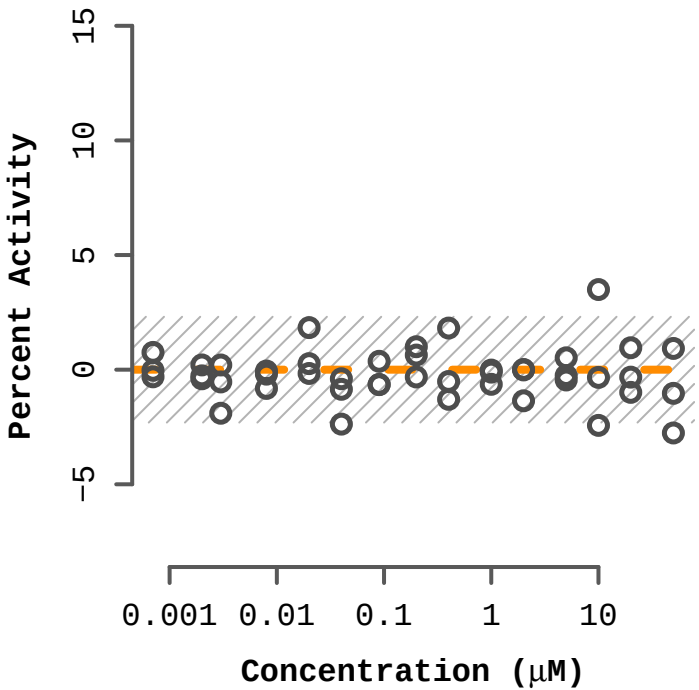
NAME: PK 11195
CHID: 41097 CASRN: 85532-75-8
SPID(S): Tox21_300620
M4ID: 12478513

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 0.965 MAX_MED: 1.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

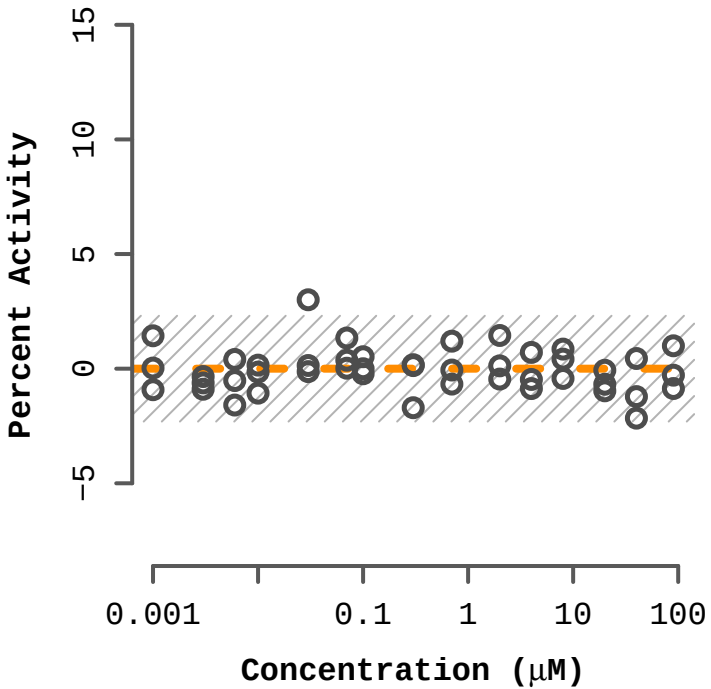
NAME: Roxithromycin
CHID: 41117 **CASRN:** 80214-83-1
SPID(S): Tox21_301835
M4ID: 12477298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.646 **MAX_MED:** 0.639 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

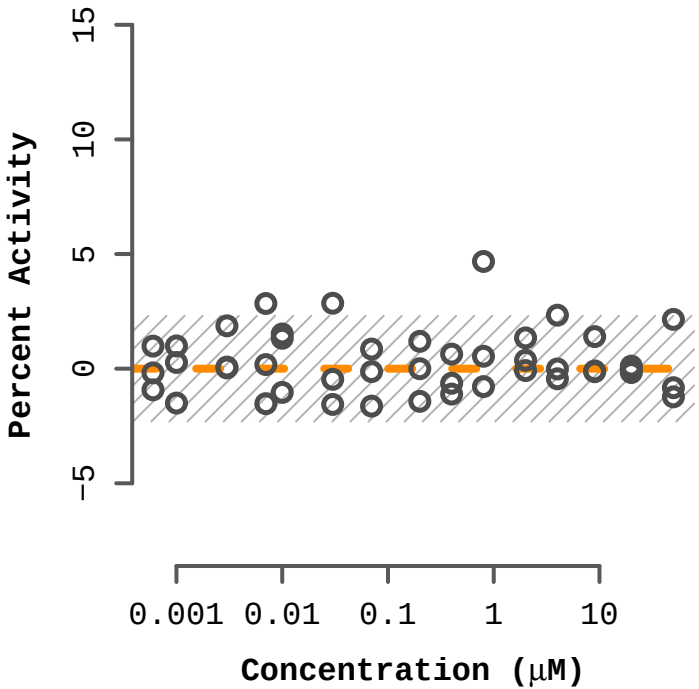
NAME: Sodium iodide
CHID: 41125 **CASRN:** 7681-82-5
SPID(S): Tox21_301379
M4ID: 12477754

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.418 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

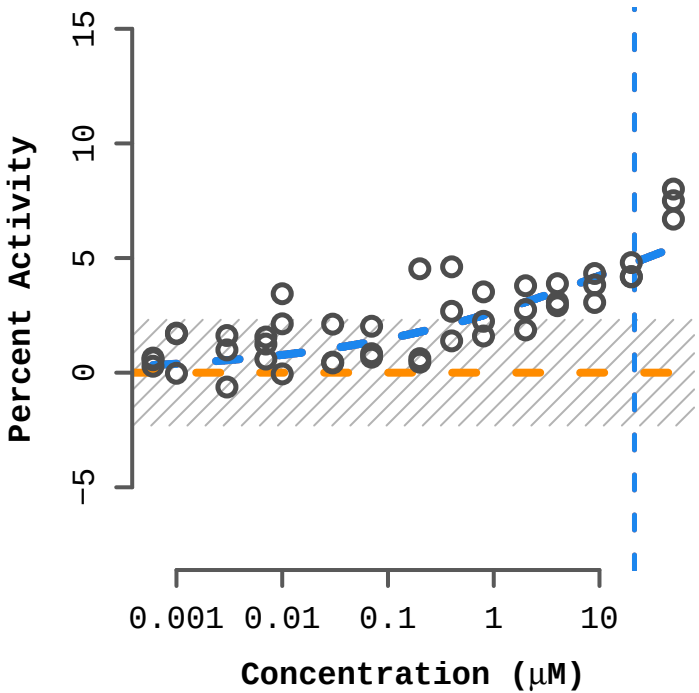
NAME: Sodium nitroprusside dihydrate
CHID: 41126 **CASRN:** 13755-38-9
SPID(S): Tox21_110314_1
M4ID: 12484462

HILL MODEL: Not applicable.

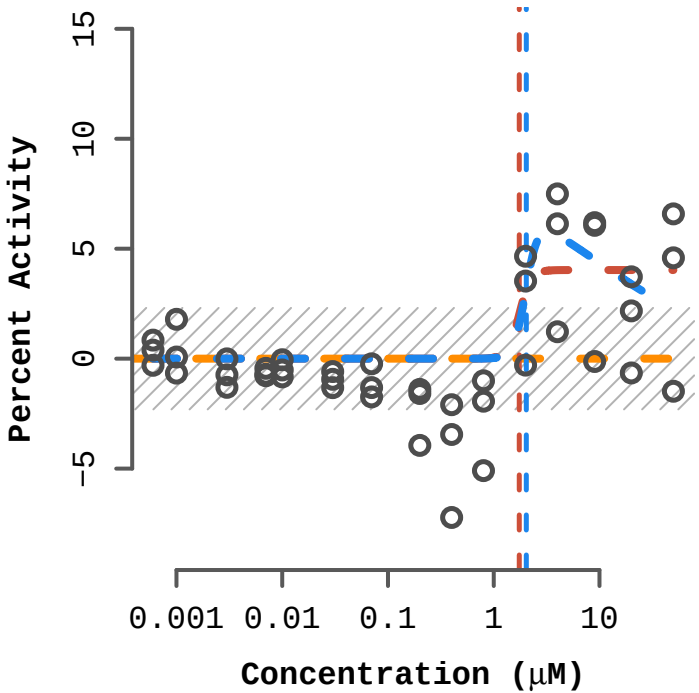
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.33 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    SU-5416
CHID:    41132   CASRN: 204005-46-9
SPID(S): Tox21_111271_1
M4ID:    12483803

HILL MODEL (in red):
      tp       ga       gw
val:  9.61     1.33     0.317
sd:   3.19     0.812    0.0619

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.61     1.33     0.317    3.54     4.58
sd:   3.19     0.812    0.0619   1070     2670

      CNST        HILL        GNLS
AIC:  233.86      147.41      151.41
PROB: 0           0.88        0.12
RMSE: 3.12        1.13        1.13

MAX_MEAN: 7.4       MAX_MED: 7.5       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Suberoylanilide hydroxamic acid
CHID: 41133 CASRN: 149647-78-9
SPID(S): Tox21_112605_1
M4ID: 12483009

HILL MODEL (in red):

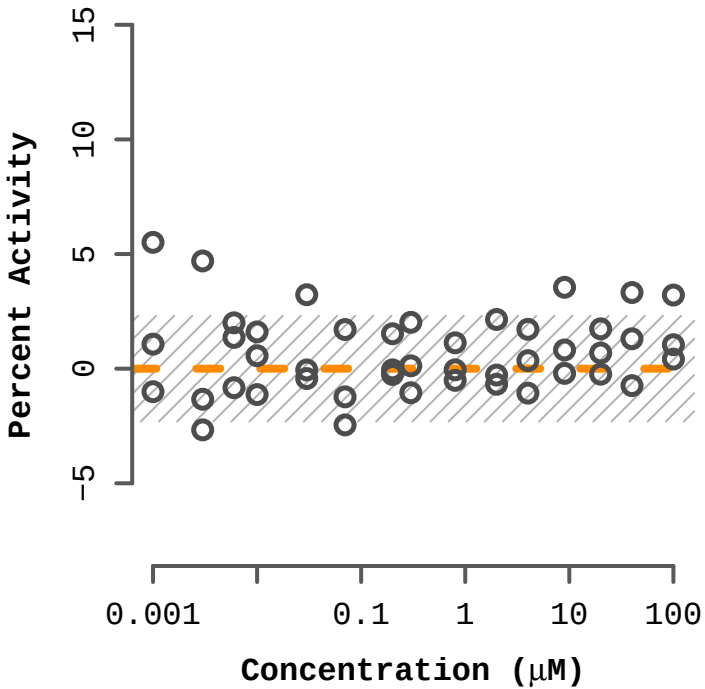
	tp	ga	gw
val:	4.03	0.241	8
sd:	0.859	0.115	9.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.99	0.308	7.71	0.957	0.634
sd:	8.72	0.0621	10.6	1.37	0.764

	CNST	HILL	GNLS
AIC:	228.35	213.44	215.93
PROB:	0	0.78	0.22
RMSE:	3.08	2.42	2.38

MAX_MEAN: 4.95 MAX_MED: 6.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

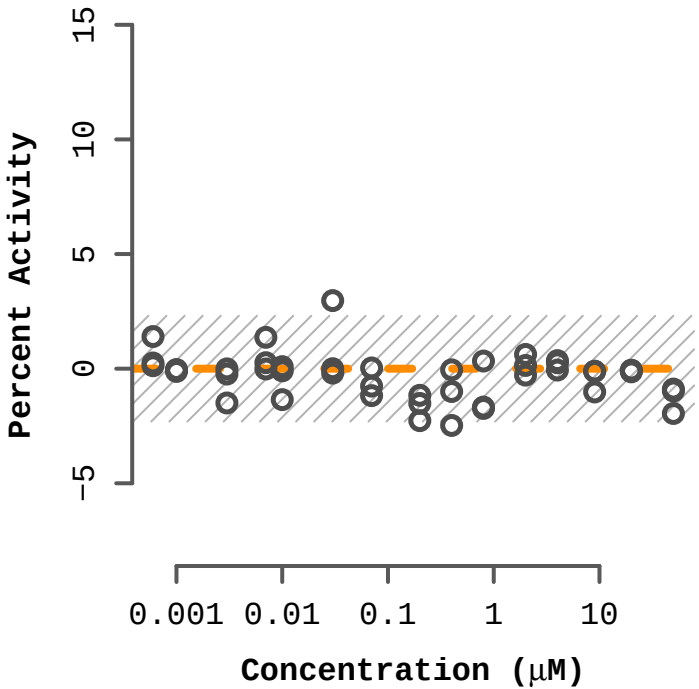
NAME: Tetraethylammonium chloride
CHID: 41137 **CASRN:** 56-34-8
SPID(S): Tox21_302129
M4ID: 12477004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 1.86 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

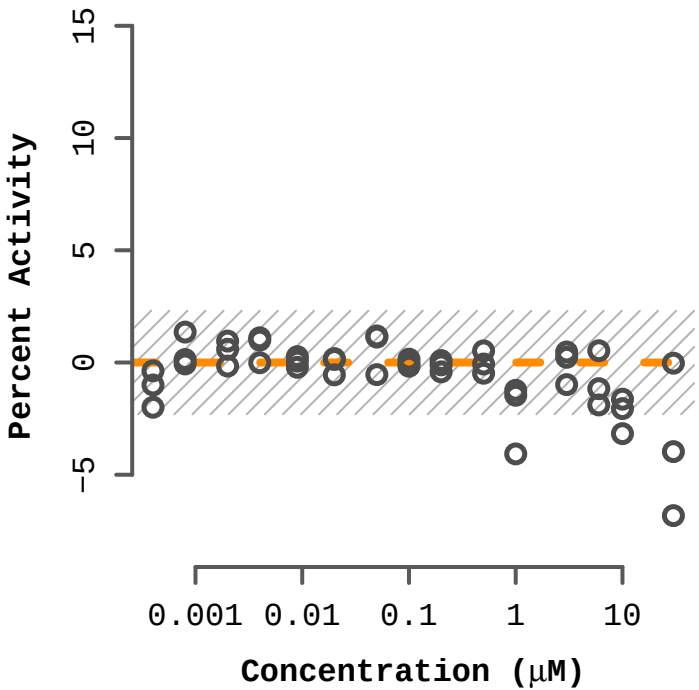
NAME: Tetraethylammonium chloride
CHID: 41137 **CASRN:** 56-34-8
SPID(S): Tox21_111281_1
M4ID: 12483795

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.927 **MAX_MED:** 0.262 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

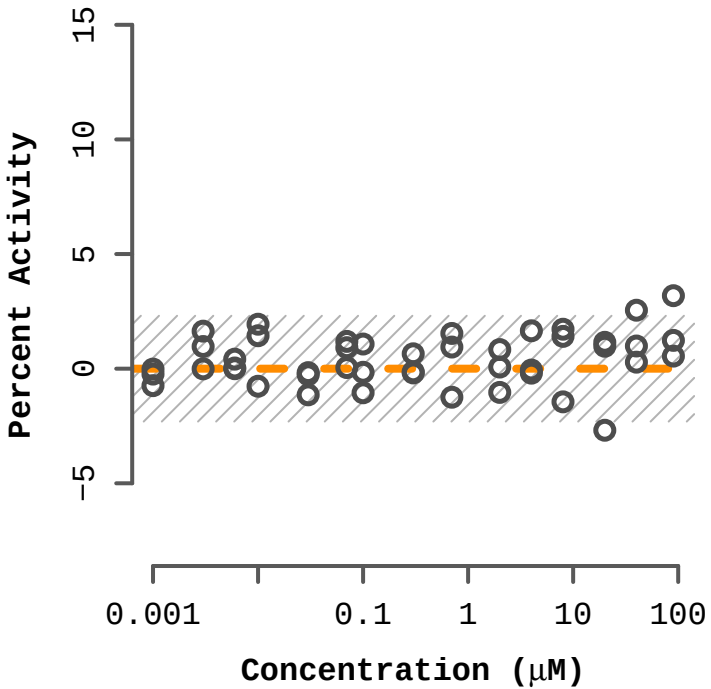
NAME: TNP-470
CHID: 41141 **CASRN:** 129298-91-5
SPID(S): Tox21_303433
M4ID: 12475706

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 0.697 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

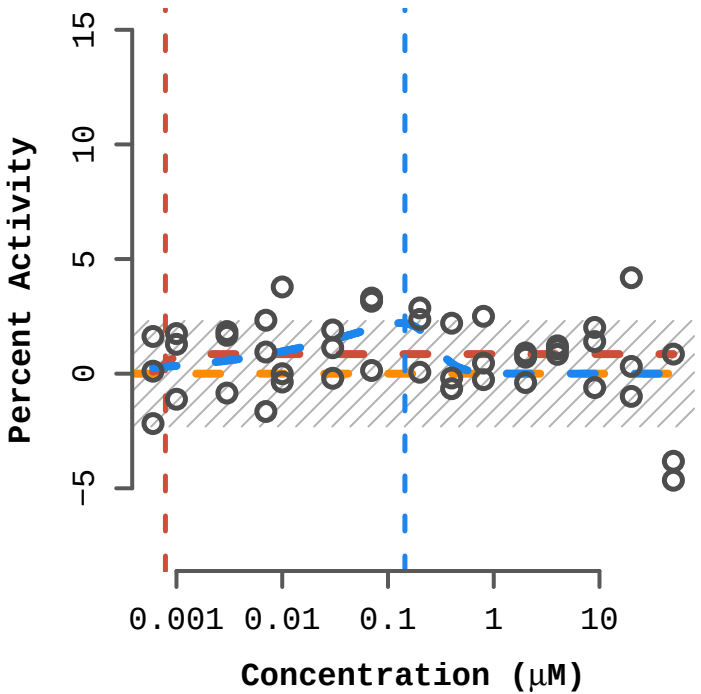
NAME: Urocanic acid
CHID: 41148 **CASRN:** 104-98-3
SPID(S): Tox21_202978
M4ID: 12479274

HILL MODEL: Not applicable.

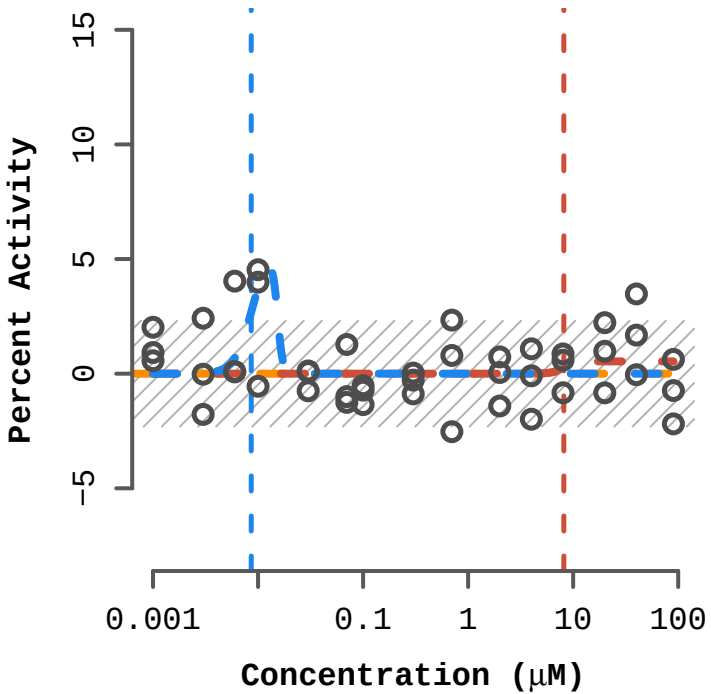
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

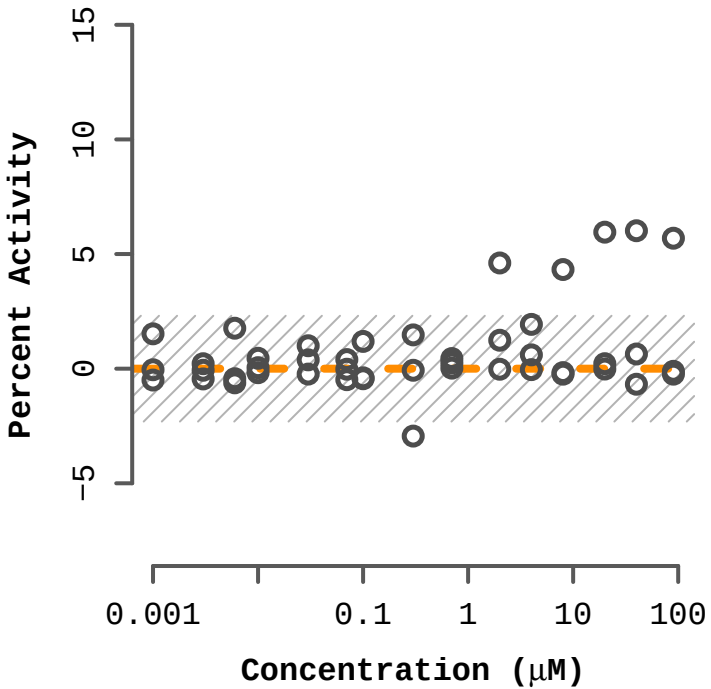
MAX_MEAN: 1.66 **MAX_MED:** 1.44 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Verapamil
CHID:    41152   CASRN: 52-53-9
SPID(S): Tox21_110300_1
M4ID:    12484471

HILL MODEL (in red):
      tp       ga       gw
val:  0.854    -3.1     8
sd:   0.258    0.32     22.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.86     -0.84    0.521    -0.59    3.91
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  189.25      185.03      188.05
PROB: 0.09        0.75        0.16
RMSE: 1.9         1.76        1.69

MAX_MEAN: 2.2       MAX_MED: 3.16      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Naphthalenesulfonic acid, 6-diazo-5,6-dihydr
CHID:    41178   CASRN: 2657-00-3
SPID(S): Tox21_302203
M4ID:    12476930

HILL MODEL (in red):
      tp       ga       gw
val:  0.537    0.911    8
sd:   0.538    0.317    48.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.38     -2.07    5.34     -1.81    17.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  173.99      178.89      176.69
PROB: 0.74        0.06        0.19
RMSE: 1.67        1.65        1.51

MAX_MEAN: 2.66      MAX_MED: 3.99      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

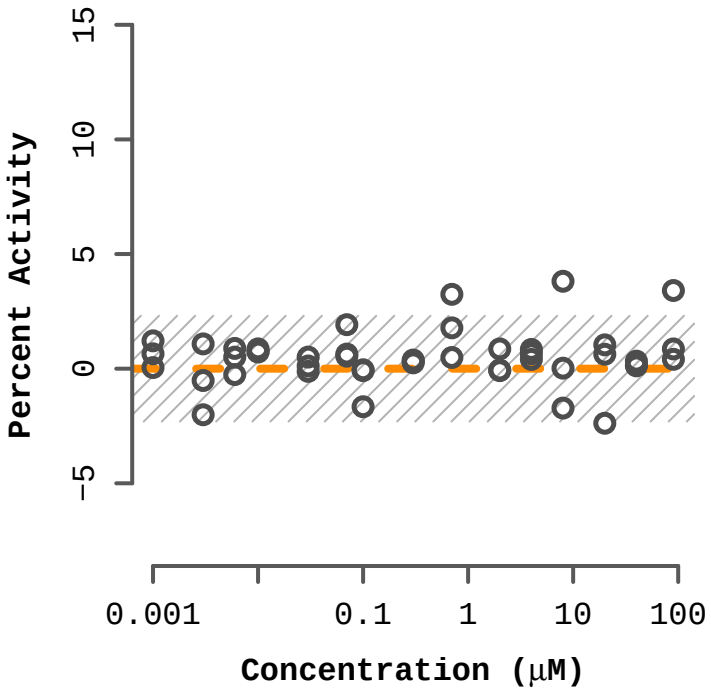
NAME: 1-Ethyl-3-methylimidazolium chloride
CHID: 41180 **CASRN:** 65039-09-0
SPID(S): Tox21_200577
M4ID: 12481675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

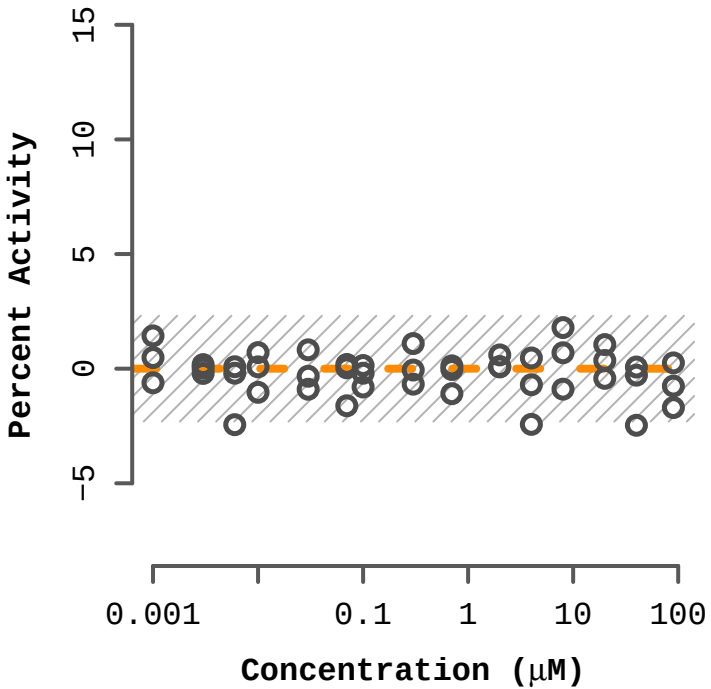
NAME: (−)−beta−Pinene
CHID: 41184 **CASRN:** 18172−67−3
SPID(S): Tox21_301162
M4ID: 12477971

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

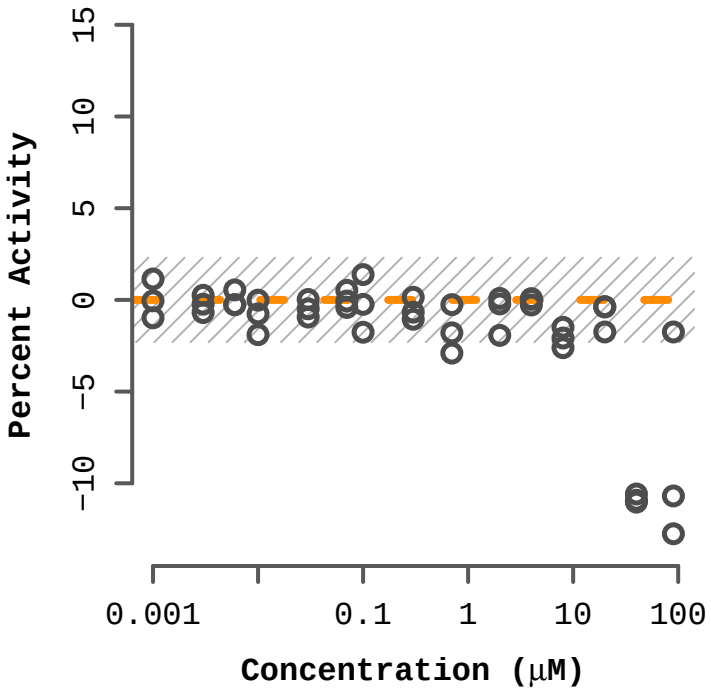
NAME: (2,4−Dichlorophenyl)acetonitrile
CHID: 41185 **CASRN:** 6306−60−1
SPID(S): Tox21_301022
M4ID: 12478111

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.533 **MAX_MED:** 0.696 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

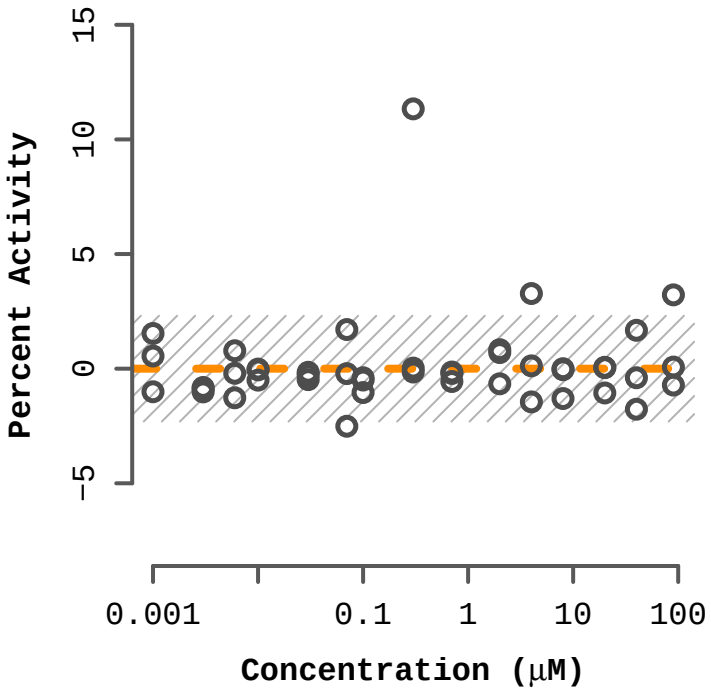
NAME: (2-Nitro-1-propenyl)benzene
CHID: 41188 **CASRN:** 705-60-2
SPID(S): Tox21_303610
M4ID: 12475535

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.64	NA	NA
PROB:	1	NA	NA
RMSE:	3.89	NA	NA

MAX_MEAN: 0.0391 **MAX_MED:** 0.0336 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

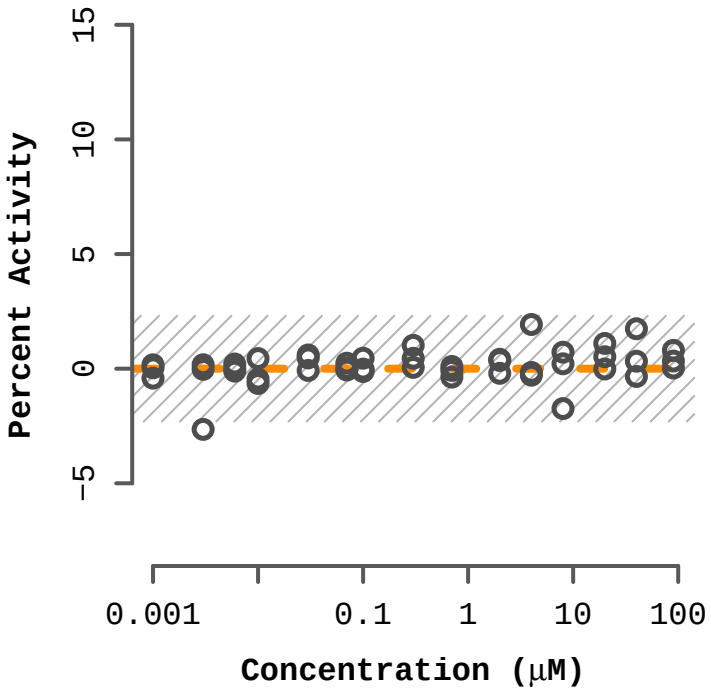
NAME: (S)−4−Isopropenyl−1−cyclohexene−1−carboxaldehyd
CHID: 41190 **CASRN:** 18031−40−8
SPID(S): Tox21_300969
M4ID: 12478164

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 3.74 **MAX_MED:** 0.703 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

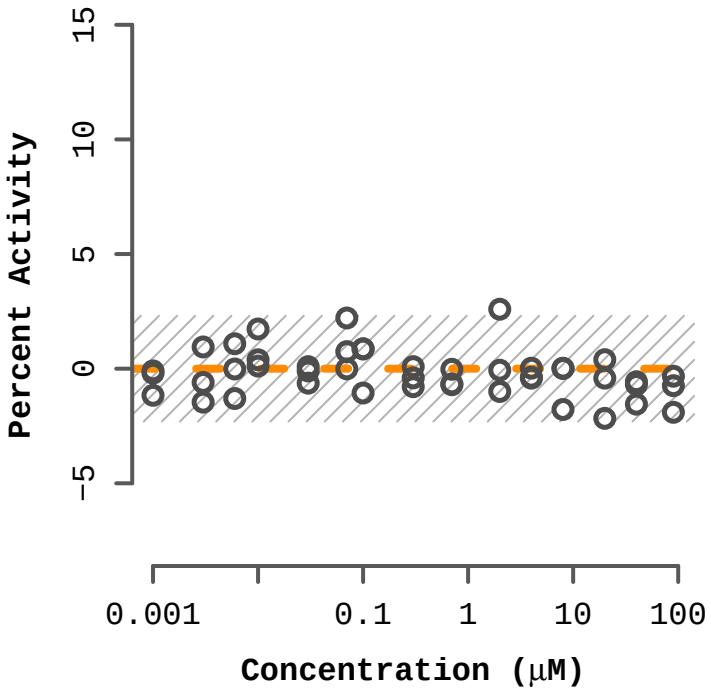
NAME: (Z)-Hexadec-9-enoic acid
CHID: 41197 **CASRN:** 373-49-9
SPID(S): Tox21_300950
M4ID: 12478183

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	86.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** 0.522 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

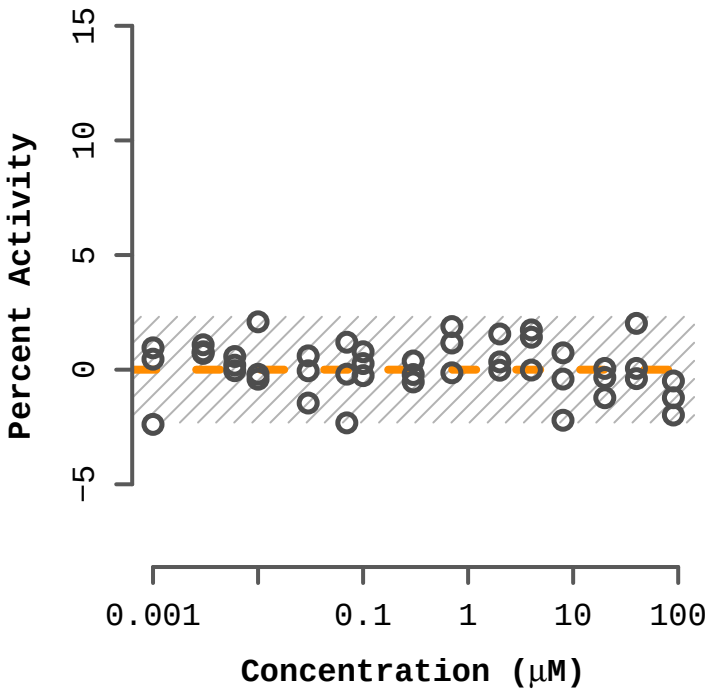
NAME: N,N'−Disalicylidene−1,2−diaminopropane
CHID: 41200 **CASRN:** 94−91−7
SPID(S): Tox21_301950
M4ID: 12477183

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.56	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

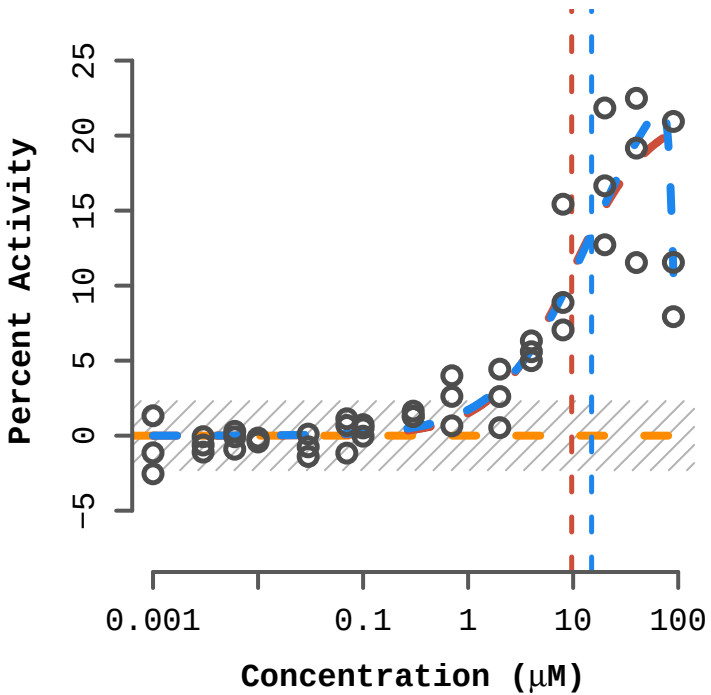
NAME: alpha-Cypermethrin
CHID: 41201 **CASRN:** 67375-30-8
SPID(S): Tox21_302007
M4ID: 12477126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: alpha−Terthiophene
CHID: 41206 CASRN: 1081−34−1
SPID(S): Tox21_300648
M4ID: 12478485

HILL MODEL (in red):

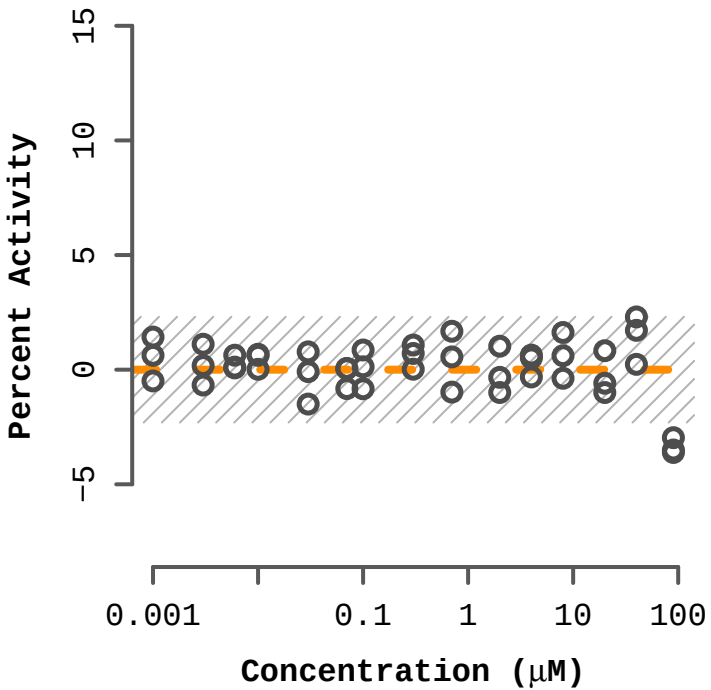
	tp	ga	gw
val:	21.8	0.986	1.15
sd:	2.71	0.144	0.286

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27	1.18	0.992	1.95	17.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	310.12	216.45	208.54
PROB:	0	0.02	0.98
RMSE:	8.29	3.08	2.66

MAX_MEAN: 17.7 MAX_MED: 19.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

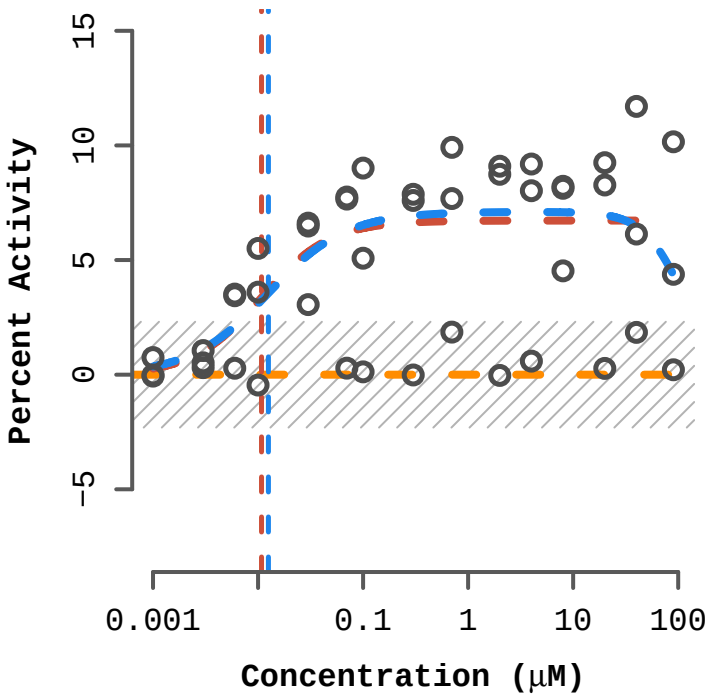
NAME: Decyl beta-D-glucopyranoside
CHID: 41208 CASRN: 58846-77-8
SPID(S): Tox21_301937
M4ID: 12477196

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: beta-Terpineol
CHID: 41209 CASRN: 138-87-4
SPID(S): Tox21_302378
M4ID: 12476755

HILL MODEL (in red):

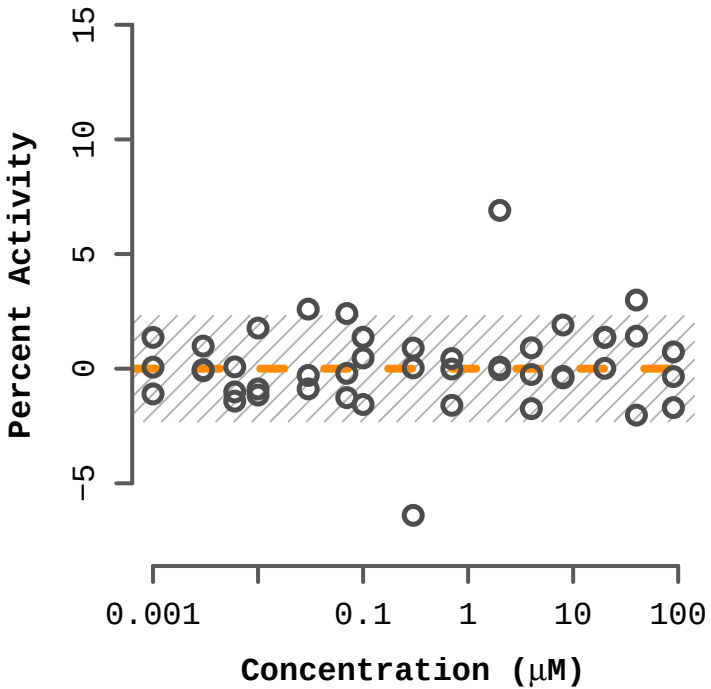
	tp	ga	gw
val:	6.72	−1.97	1.33
sd:	0.768	0.243	0.854

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.11	−1.9	1.17	2.04	2.28
sd:	0.916	0.27	0.706	0.317	3.93

	CNST	HILL	GNLS
AIC:	295.31	243.07	245.91
PROB:	0	0.8	0.2
RMSE:	5.94	3.24	3.25

MAX_MEAN: 6.96 MAX_MED: 8.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

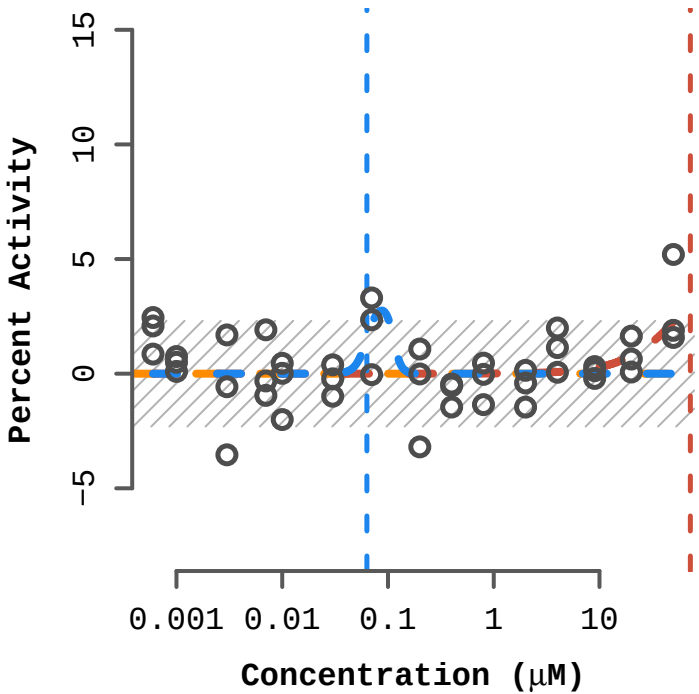
NAME: gamma−Terpinene
CHID: 41210 **CASRN:** 99−85−4
SPID(S): Tox21_300963
M4ID: 12478170

HILL MODEL: Not applicable.

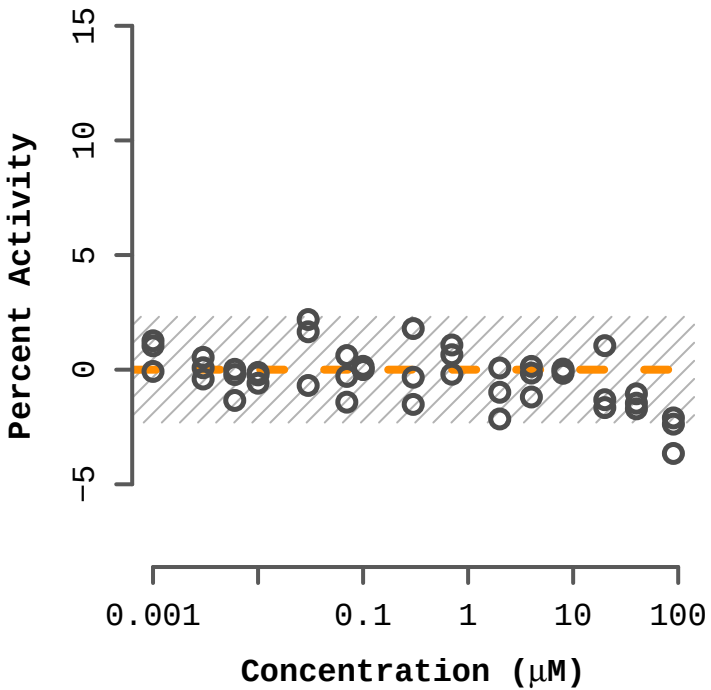
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 2.31 **MAX_MED:** 1.42 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1,1,1-Trichloro-2-methyl-2-propanol
CHID:    41217   CASRN: 57-15-8
SPID(S): Tox21_111629_1
M4ID:    12483575

HILL MODEL (in red):
      tp       ga       gw
val:  6.24     1.86     1.53
sd:   27.8     2.16     1.96

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.1      -1.2     8        -0.949   11.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  168.33      164.36      173.54
PROB: 0.12        0.87        0.01
RMSE: 1.59        1.4         1.52

MAX_MEAN: 2.89      MAX_MED: 2.35      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

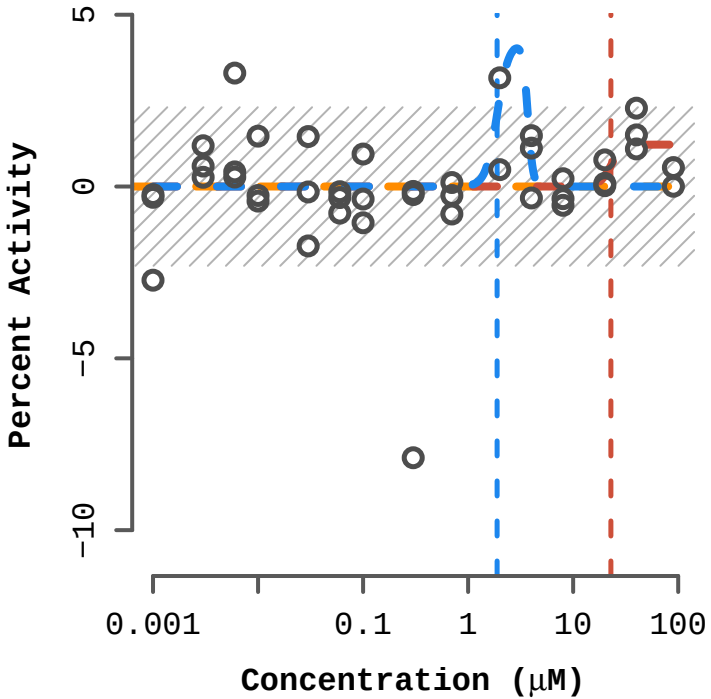
NAME: cis−1,2,3,6−Tetrahydrophthalimide
CHID: 41220 **CASRN:** 1469−48−3
SPID(S): Tox21_302043
M4ID: 12477090

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2,6-Hexanetriol
CHID: 41224 CASRN: 106-69-4
SPID(S): Tox21_300999
M4ID: 12478134

HILL MODEL (in red):

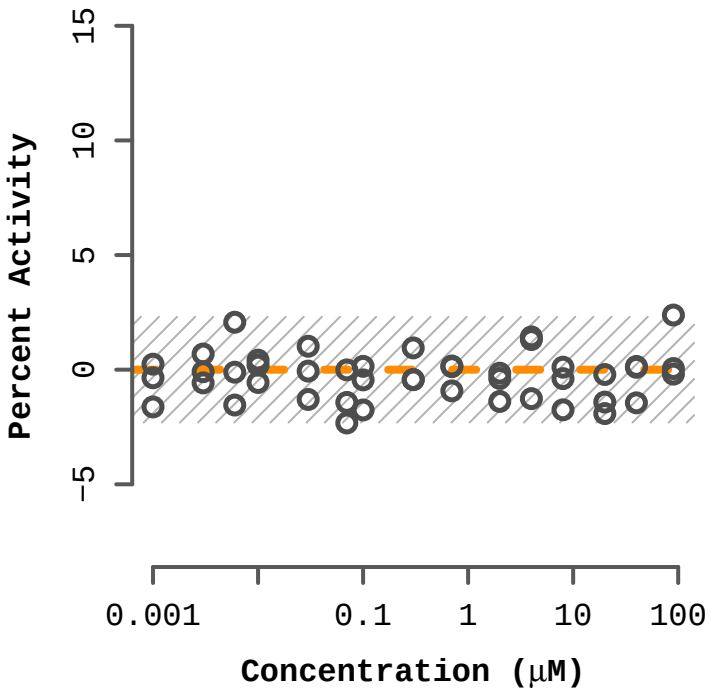
	tp	ga	gw
val:	1.22	1.36	8
sd:	0.49	0.129	11.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.21	0.276	8	0.568	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	181.39	181.19	184.84
PROB:	0.44	0.48	0.08
RMSE:	2.6	2.49	2.35

MAX_MEAN: 4.8 MAX_MED: 3.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

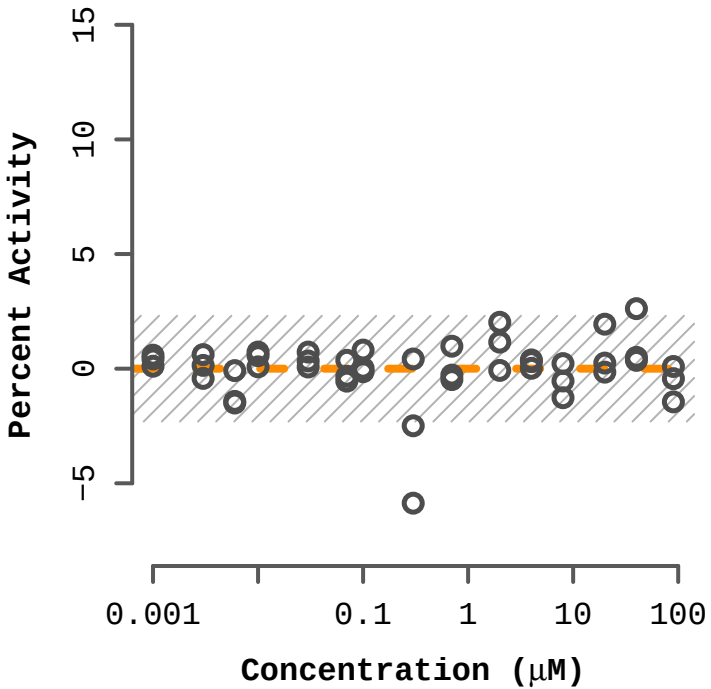
NAME: 2-Methyl-4-amino-6-methoxy-s-triazine
CHID: 41230 **CASRN:** 1668-54-8
SPID(S): Tox21_302097
M4ID: 12477036

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.748 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

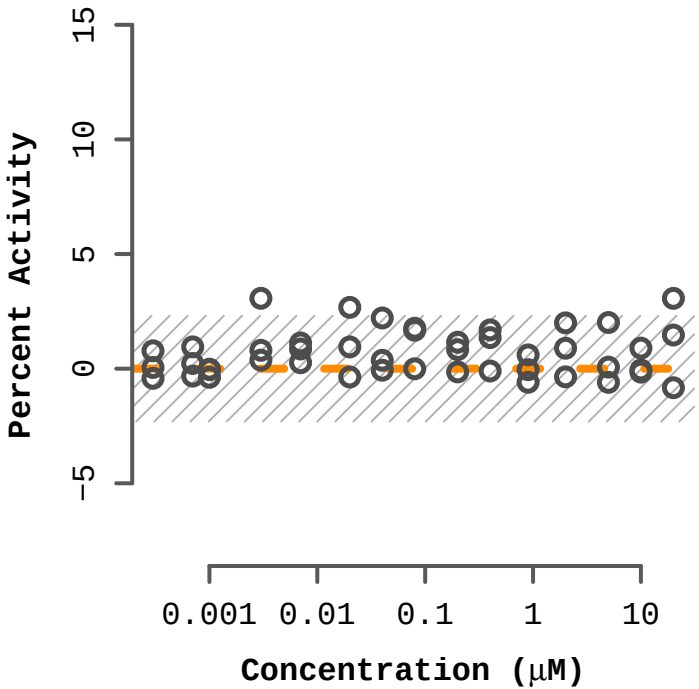
NAME: 1,3,5-Triisopropylbenzene
CHID: 41232 **CASRN:** 717-74-8
SPID(S): Tox21_301030
M4ID: 12478103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

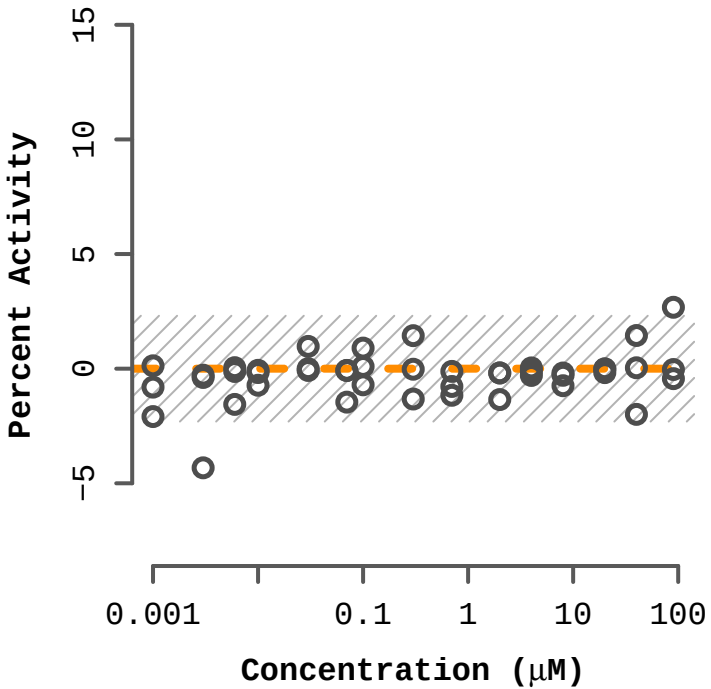
NAME: 1,3,6,8−Pyrenetetrasulfonic acid, tetrasodium s
CHID: 41233 CASRN: 59572−10−0
SPID(S): Tox21_303858
M4ID: 12475330

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

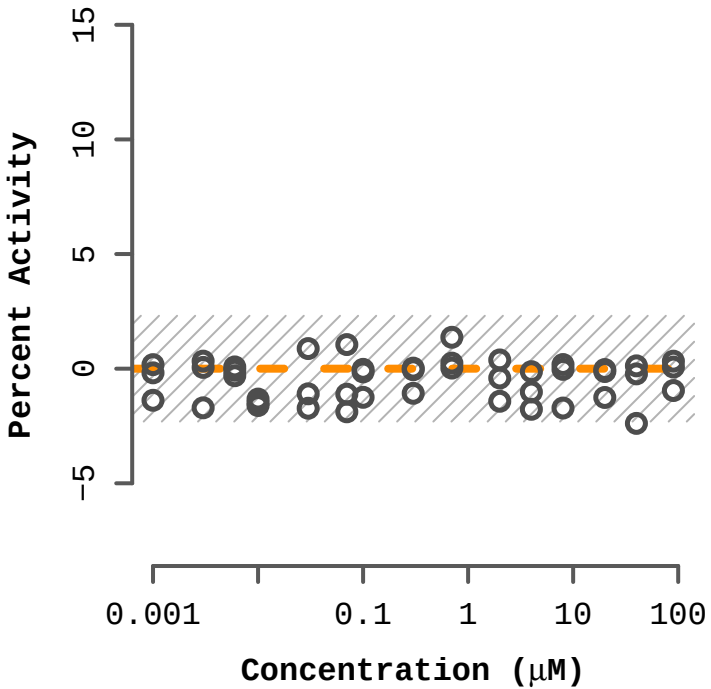
NAME: 1,3,6-Hexanetricarbonitrile
CHID: 41234 **CASRN:** 1772-25-4
SPID(S): Tox21_300976
M4ID: 12478157

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.737 **MAX_MED:** 0.0982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

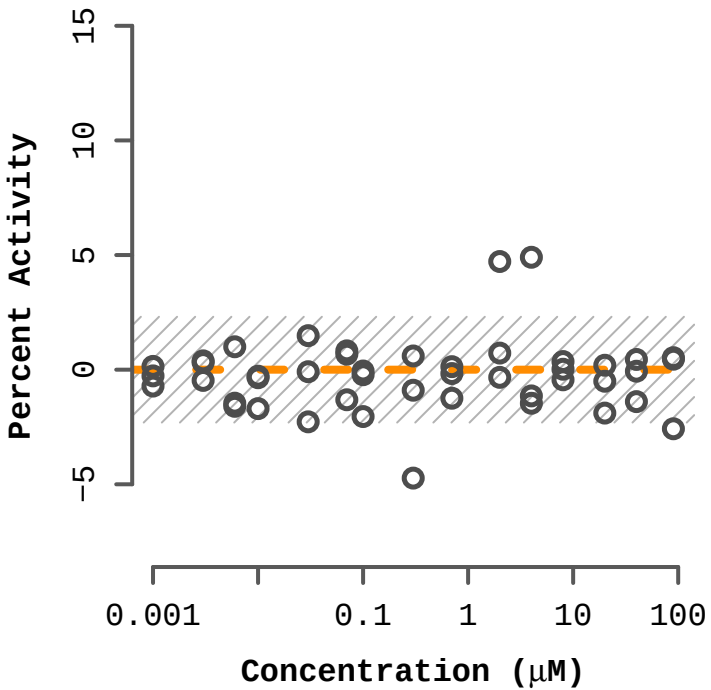
NAME: alpha-Terpinene
CHID: 41237 **CASRN:** 99-86-5
SPID(S): Tox21_301126
M4ID: 12478007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.09	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.547 **MAX_MED:** 0.243 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

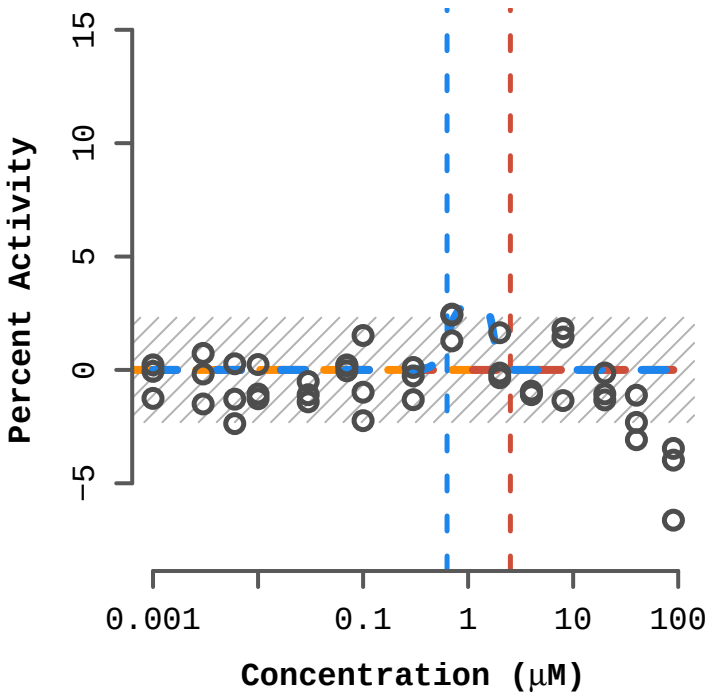
NAME: 1,3-Cyclohexanedimethanamine
CHID: 41238 **CASRN:** 2579-20-6
SPID(S): Tox21_301175
M4ID: 12477958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 0.725 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2,4−Trimethylpentane−1,3−diyl dibenzoate
CHID: 41242 CASRN: 68052−23−3
SPID(S): Tox21_300835
M4ID: 12478298

HILL MODEL (in red):

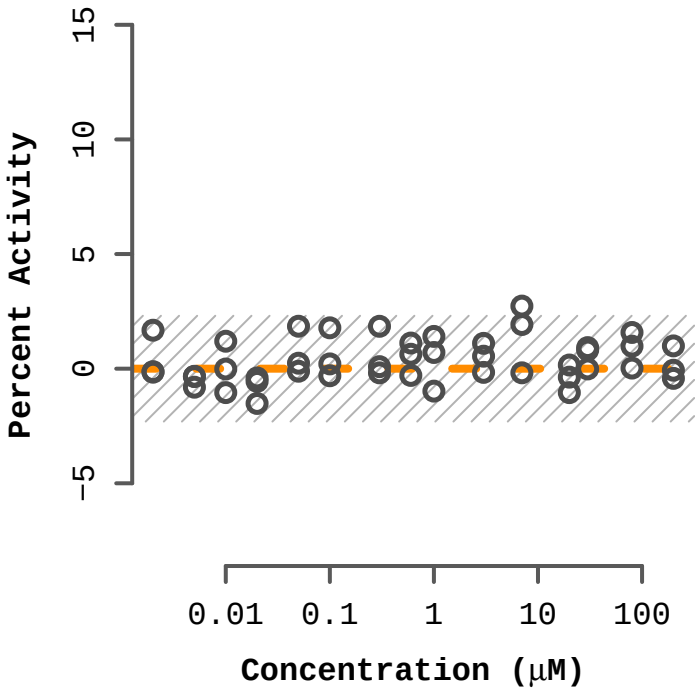
	tp	ga	gw
val:	2.86e−10	0.402	1.78
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.96	−0.201	8	0.244	16.7
sd:	10.4	0.585	16.4	1.92	563

	CNST	HILL	GNLS
AIC:	178.36	184.36	181.26
PROB:	0.78	0.04	0.18
RMSE:	1.8	1.8	1.72

MAX_MEAN: 2.05 MAX_MED: 2.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

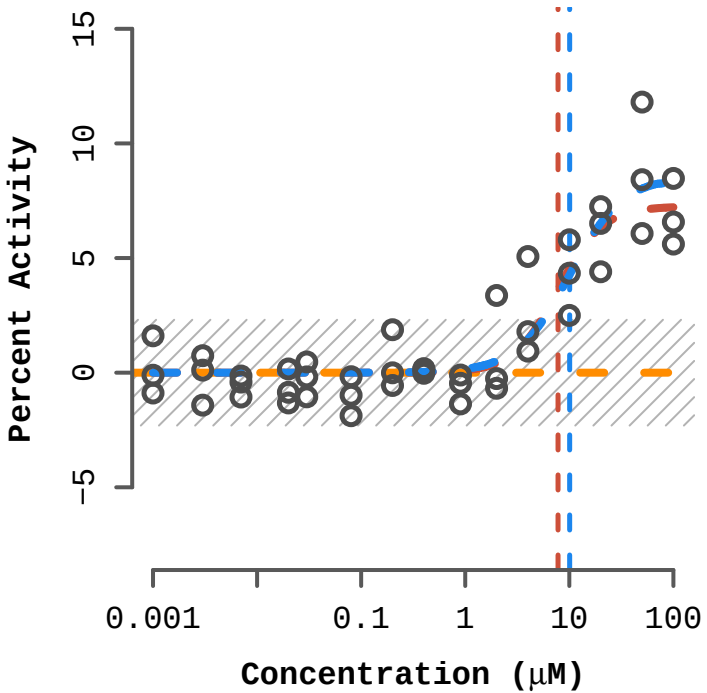
NAME: 1,3-Propanediol
CHID: 41246 **CASRN:** 504-63-2
SPID(S): Tox21_300750
M4ID: 12478383

HILL MODEL: Not applicable.

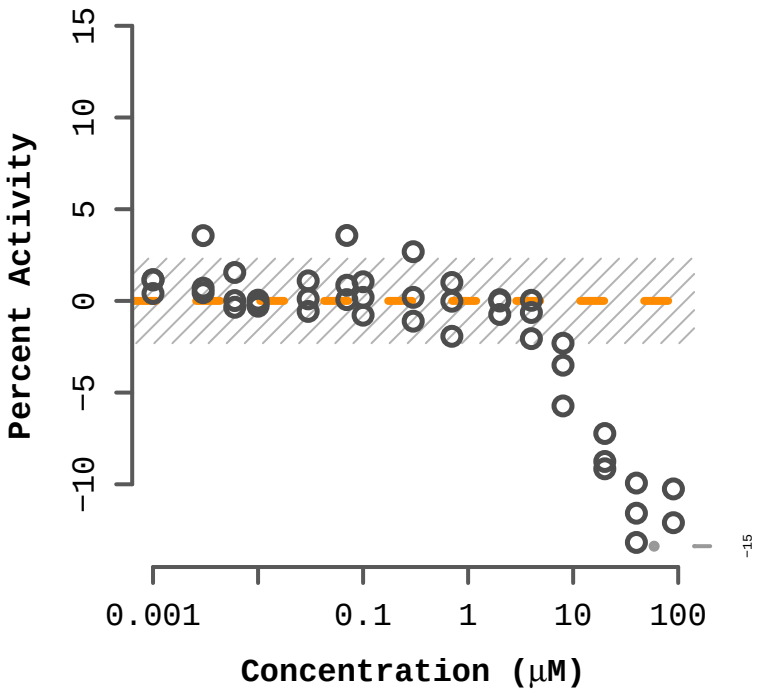
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.42	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.93 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1,3-Diphenyl-1,3-propanedione
CHID:    41247   CASRN: 120-46-7
SPID(S): Tox21_300686
M4ID:    12478447

HILL MODEL (in red):
      tp       ga       gw
val:  7.25     0.892    2.06
sd:   0.691    0.0966   0.566

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.55     1        1.71     2.04     15.8
sd:   1.69     0.157    0.534    0.025    12.4

      CNST        HILL        GNLS
AIC:  241.36      160.3       163.03
PROB: 0           0.8         0.2
RMSE: 3.74        1.38        1.32

MAX_MEAN: 8.77      MAX_MED: 8.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

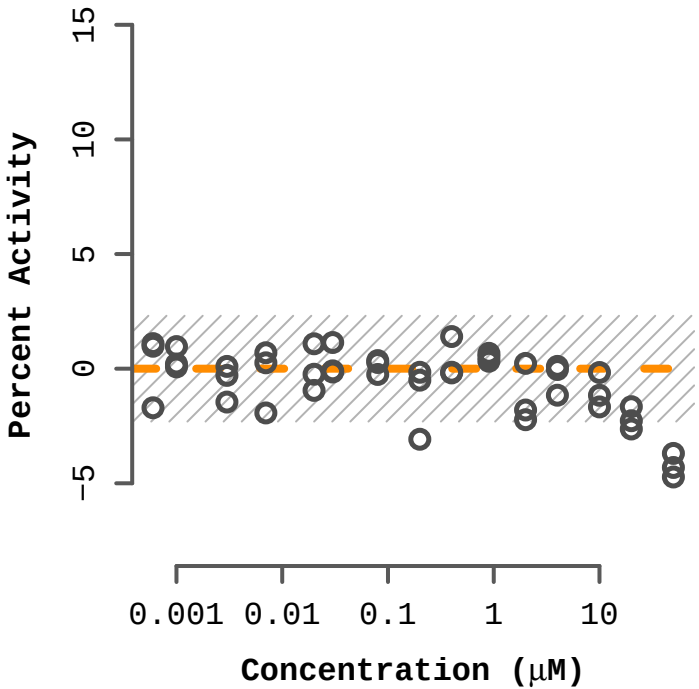
NAME: 2,5-Di-tert-butylbenzene-1,4-diol
CHID: 41248 **CASRN:** 88-58-4
SPID(S): Tox21_300385
M4ID: 12478747 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.32	NA	NA
PROB:	1	NA	NA
RMSE:	5.14	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

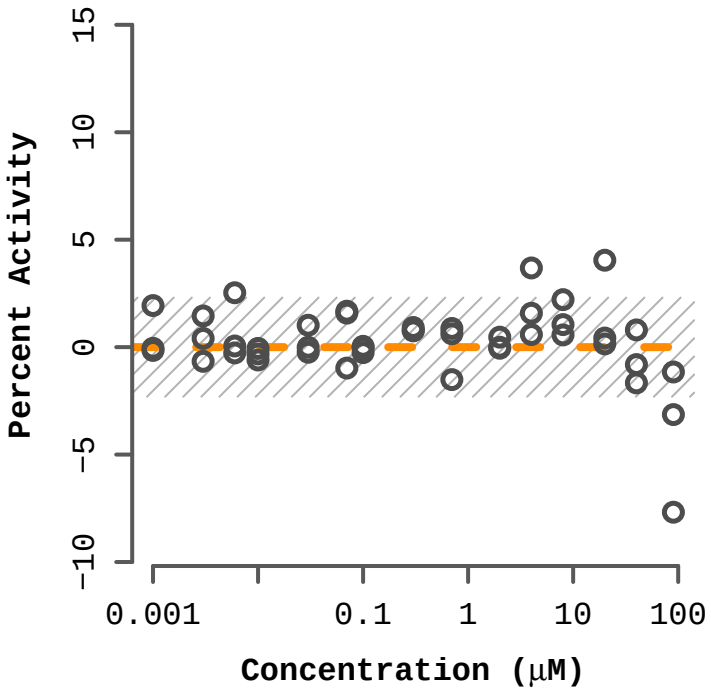
NAME: 1,4-Bis(N-isopropylamino)anthraquinone
CHID: 41250 **CASRN:** 14233-37-5
SPID(S): Tox21_300781
M4ID: 12478352

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 0.503 **MAX_MED:** 0.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

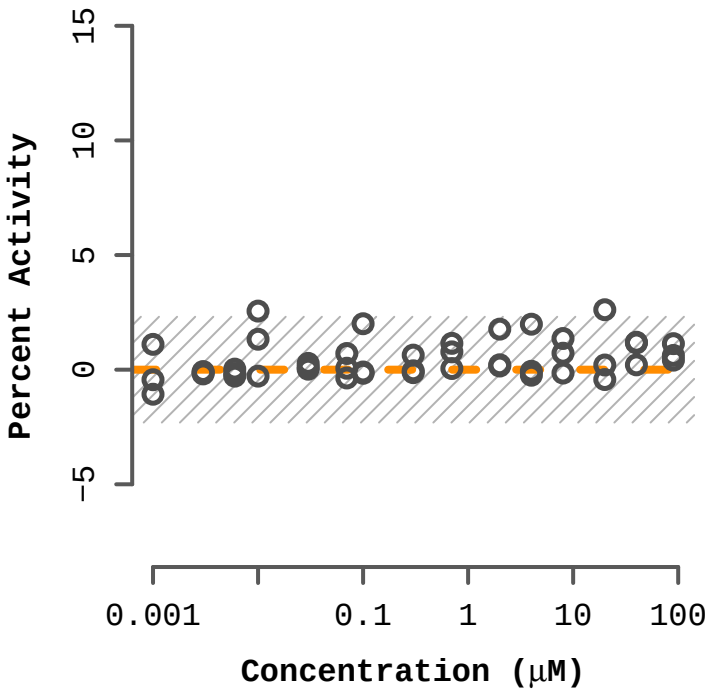
NAME: 1,4-Diaminoanthraquinone
CHID: 41252 **CASRN:** 128-95-0
SPID(S): Tox21_300683
M4ID: 12478450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

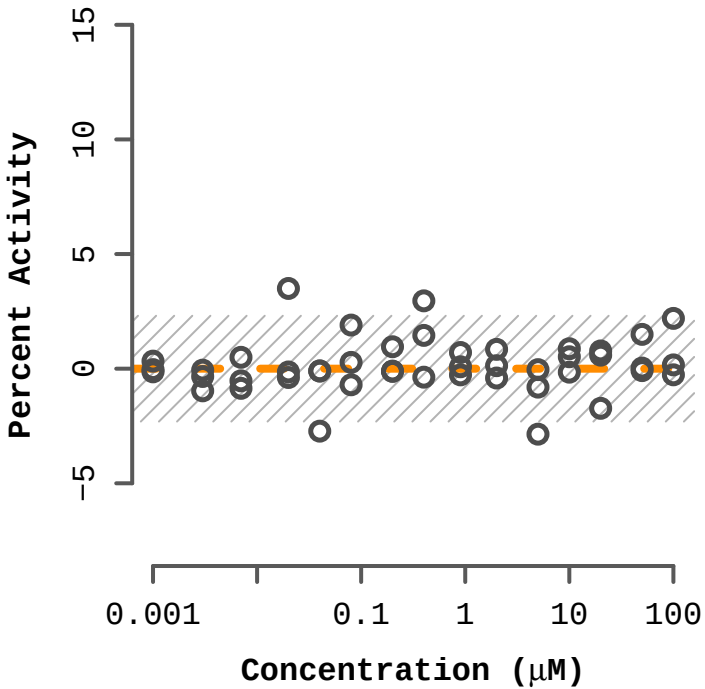
NAME: 3,6-Dimethyl-2,5-dioxo-1,4-dioxane
CHID: 41253 **CASRN:** 95-96-5
SPID(S): Tox21_302164
M4ID: 12476969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

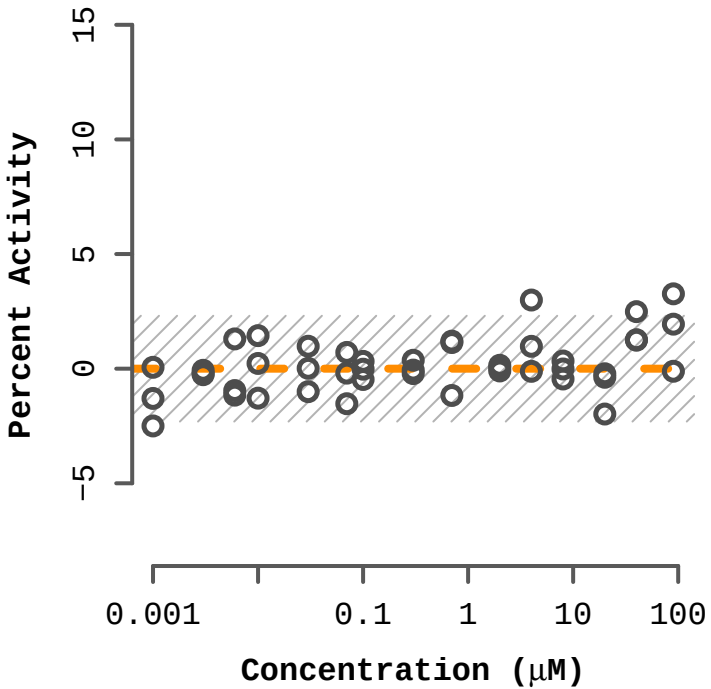
NAME: 1,5-Pentanediol
CHID: 41256 **CASRN:** 111-29-5
SPID(S): Tox21_300880
M4ID: 12478253

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

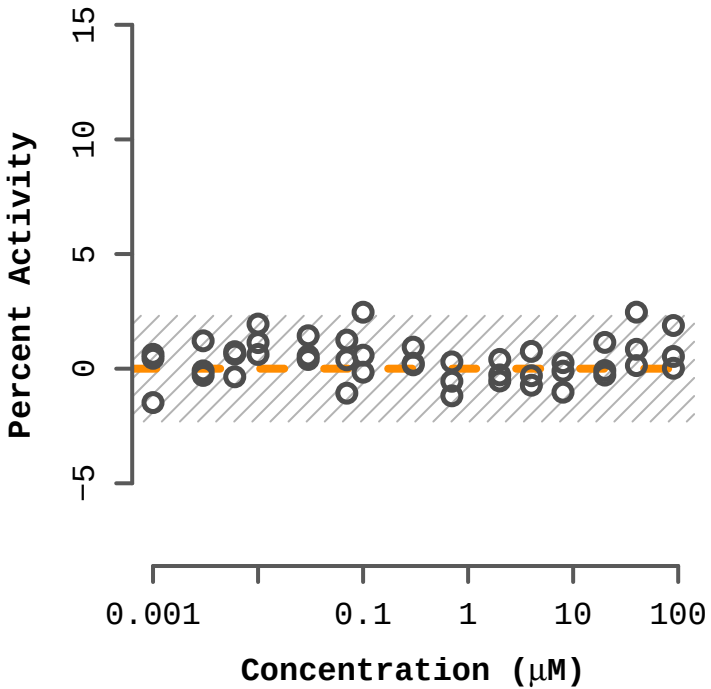
NAME: 1-Allyloxy-3-chloro-2-propanol
CHID: 41261 **CASRN:** 4638-03-3
SPID(S): Tox21_302238
M4ID: 12476895

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

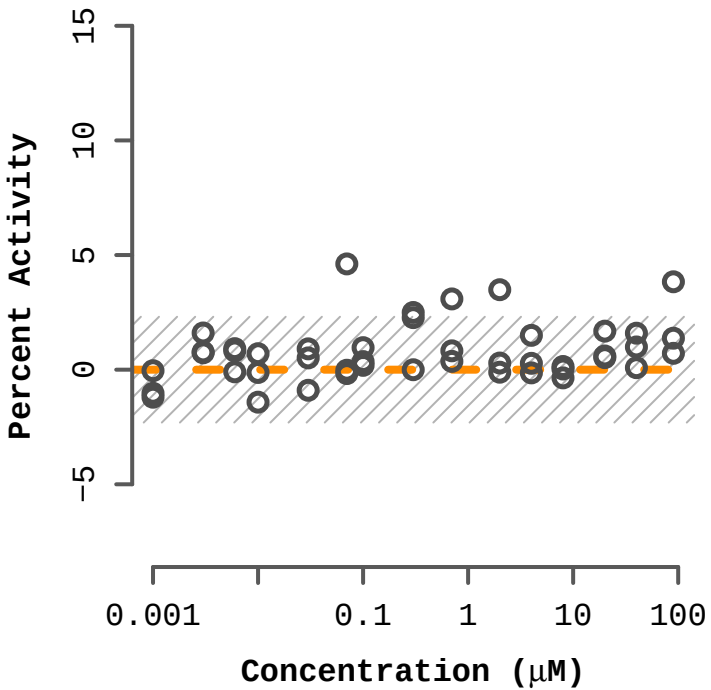
NAME: 1-Chloro-2-methyl-3-nitrobenzene
CHID: 41263 **CASRN:** 83-42-1
SPID(S): Tox21_300660
M4ID: 12478473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

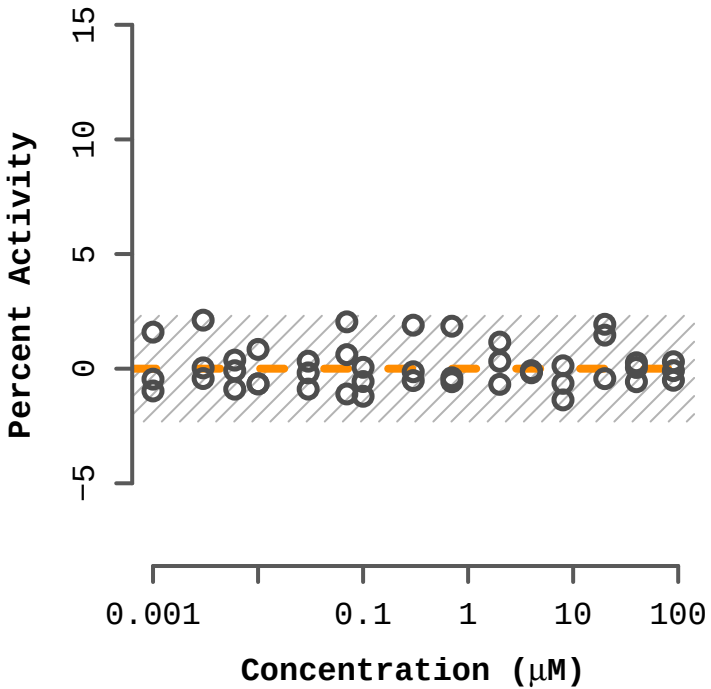
NAME: 2-Hexyl-1-decanol
CHID: 41265 **CASRN:** 2425-77-6
SPID(S): Tox21_300799
M4ID: 12478334

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

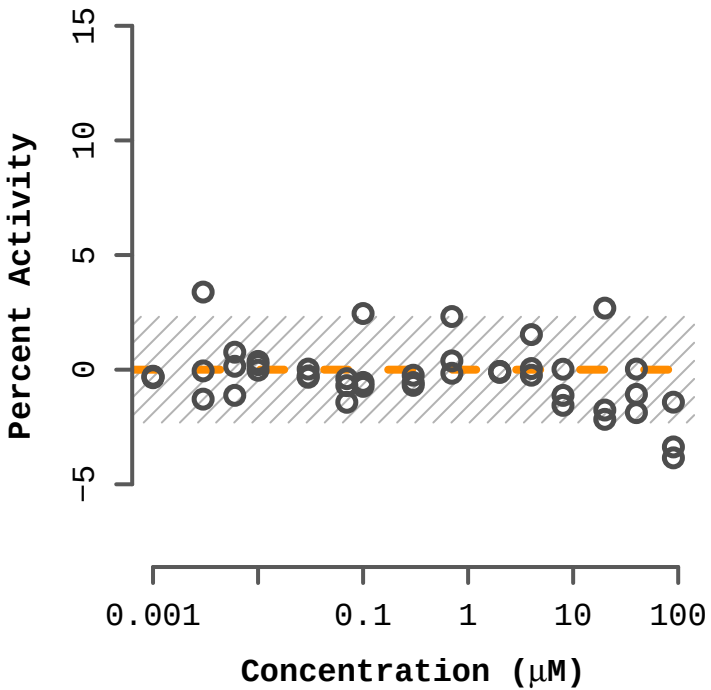
NAME: 1-Ethoxy-2-propanol
CHID: 41267 **CASRN:** 1569-02-4
SPID(S): Tox21_301831
M4ID: 12477302

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.989 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

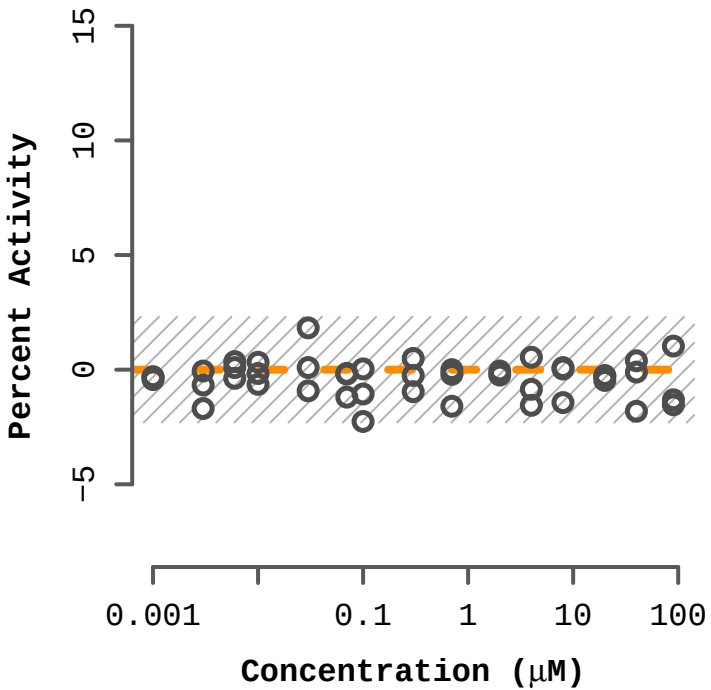
NAME: Fenchlorazole-ethyl
CHID: 41268 **CASRN:** 103112-35-2
SPID(S): Tox21_300653
M4ID: 12478480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 0.385 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

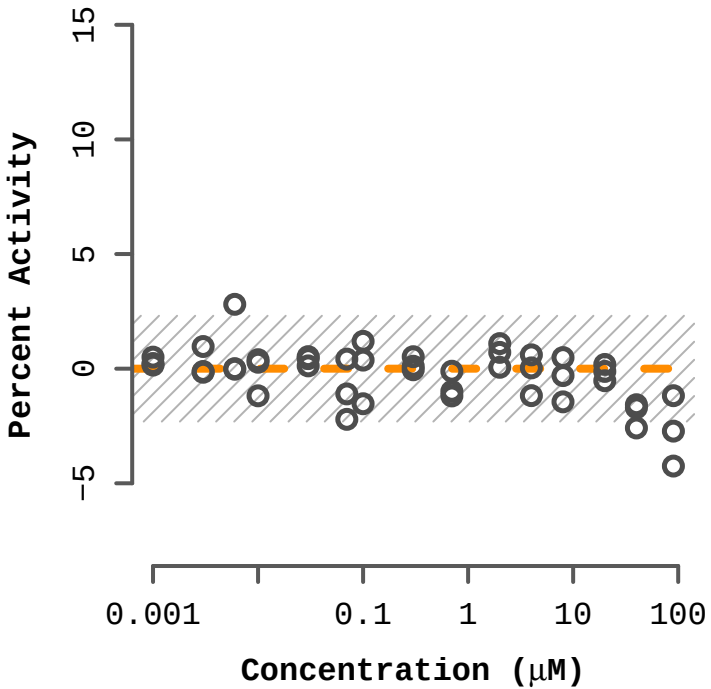
NAME: (+)−Cedrol
CHID: 41269 CASRN: 77−53−2
SPID(S): Tox21_202945
M4ID: 12479307

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.333 MAX_MED: 0.0946 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

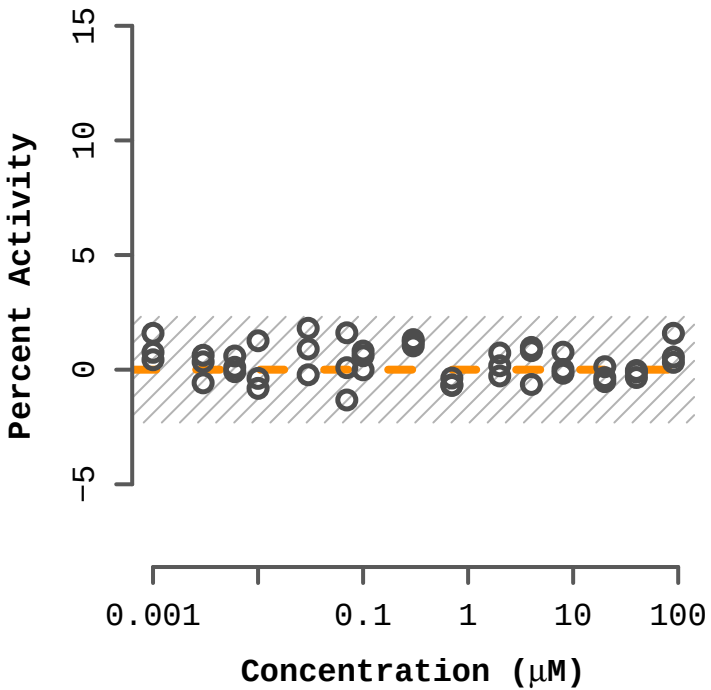
NAME: 3,5,5-Trimethylhexyl acetate
CHID: 41270 **CASRN:** 58430-94-7
SPID(S): Tox21_301881
M4ID: 12477252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.929 **MAX_MED:** 0.712 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

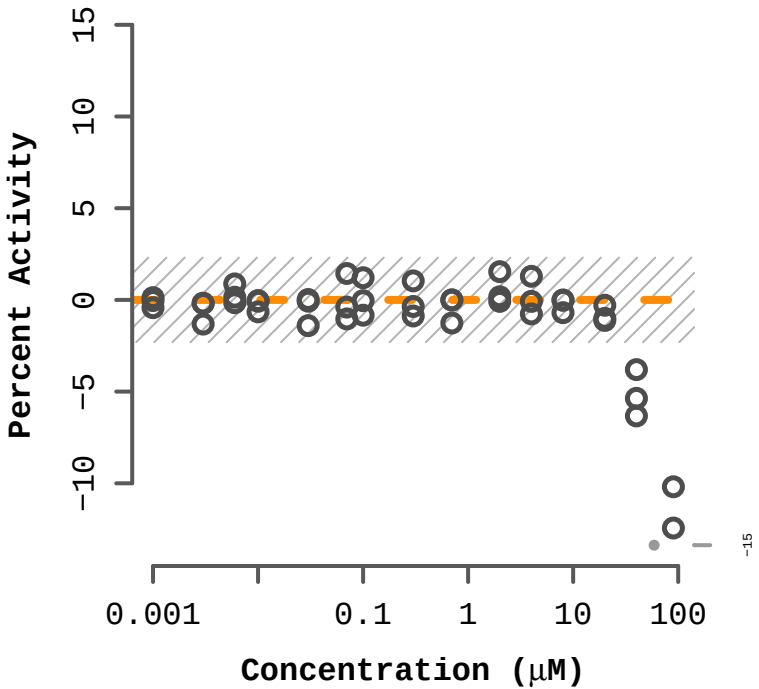
NAME: Pyrazolone T
CHID: 41273 **CASRN:** 118-47-8
SPID(S): Tox21_302220
M4ID: 12476913

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

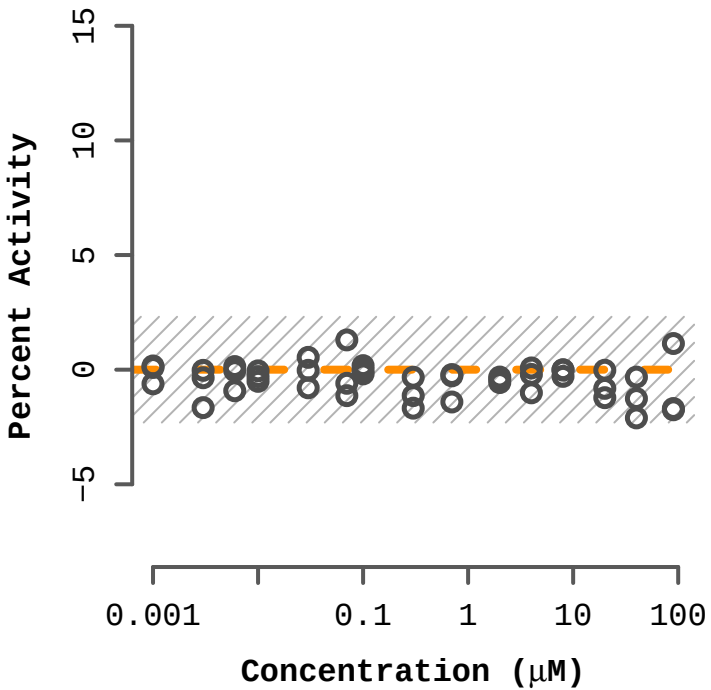
NAME: 1-Phenyl-1H-pyrrole-2,5-dione
CHID: 41274 **CASRN:** 941-69-5
SPID(S): Tox21_300672
M4ID: 12478461 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.38	NA	NA
PROB:	1	NA	NA
RMSE:	3.59	NA	NA

MAX_MEAN: 0.545 **MAX_MED:** 0.172 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

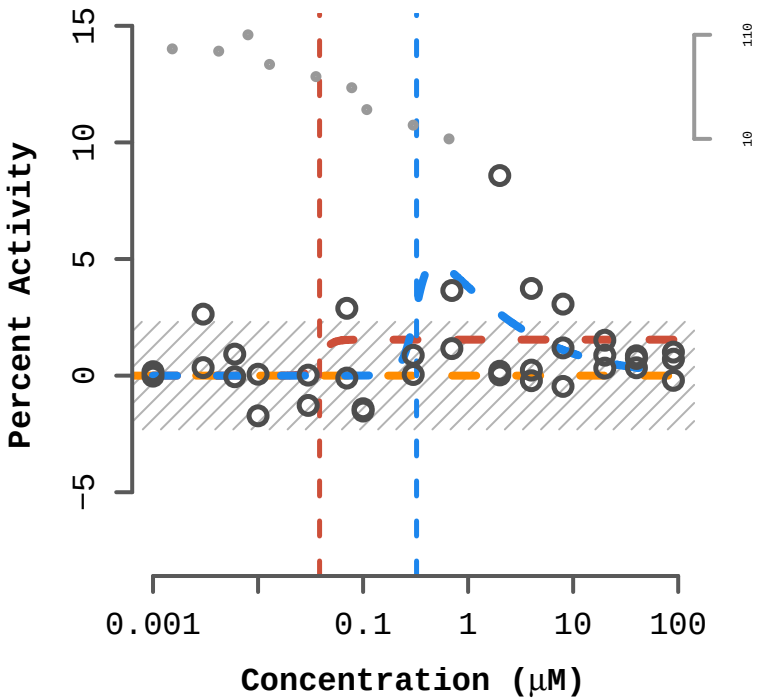
NAME: 1−Monolaurin
CHID: 41275 **CASRN:** 142−18−7
SPID(S): Tox21_300759
M4ID: 12478374

HILL MODEL: Not applicable.

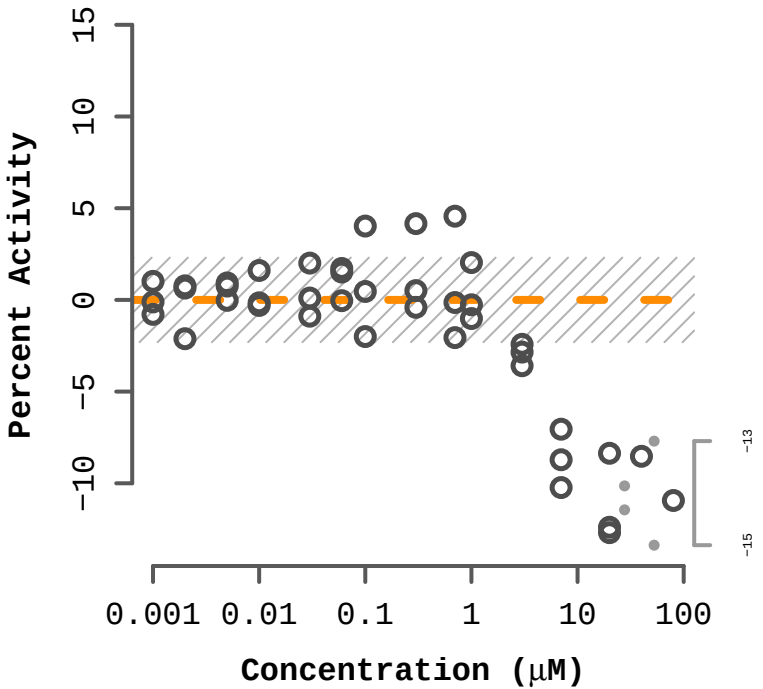
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: −0.00781 **MAX_MED:** 0.0966 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Hydroxy-2,2,6,6-tetramethylpiperidin-1-yl)ox
CHID:    41280   CASRN: 2226-96-2
SPID(S): Tox21_300872
M4ID:    12478261  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  1.54     -1.41    8
sd:   0.994    0.922    50.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.67     -0.491   6.84     -0.241   0.779
sd:   33.9     0.411    64.1     3.48     1.23

      CNST        HILL        GNLS
AIC:  398.1       401.57      404.24
PROB: 0.82        0.14        0.04
RMSE: 33.68       33.53       33.61

MAX_MEAN: 38.3      MAX_MED: 3.65      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

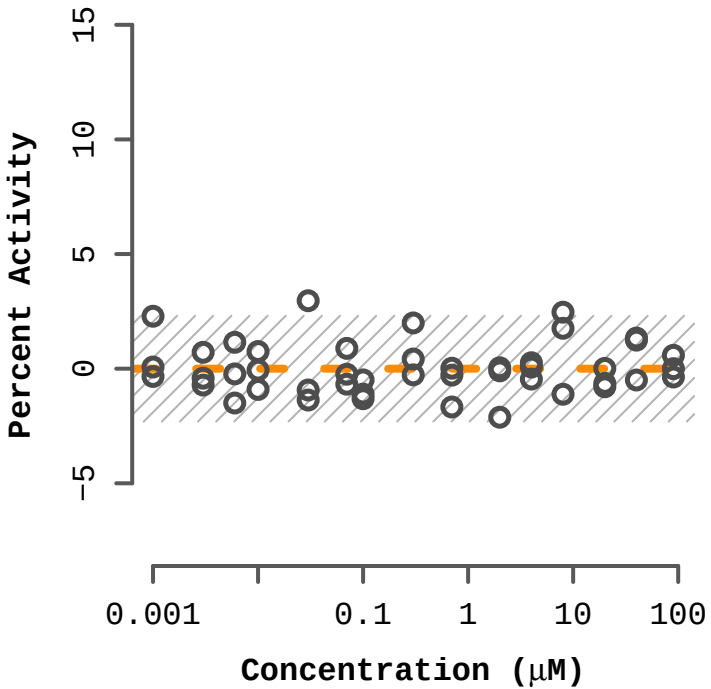
NAME: Myristyltrimethylammonium chlorideN,N,N−Trimetl
CHID: 41289 **CASRN:** 4574−04−3
SPID(S): Tox21_300908
M4ID: 12478225 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	288.72	NA	NA
PROB:	1	NA	NA
RMSE:	6.21	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

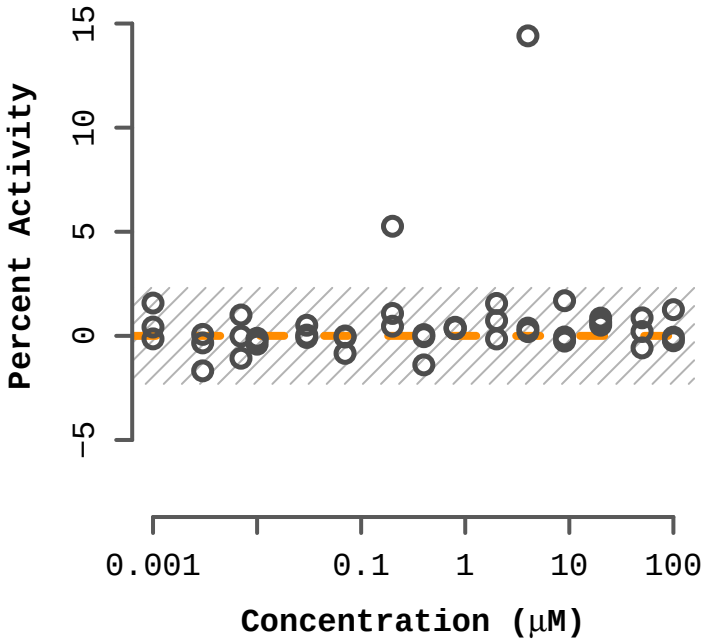
NAME: 2-((Dimethylamino)methyl)phenol
CHID: 41293 **CASRN:** 120-65-0
SPID(S): Tox21_301544
M4ID: 12477589

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

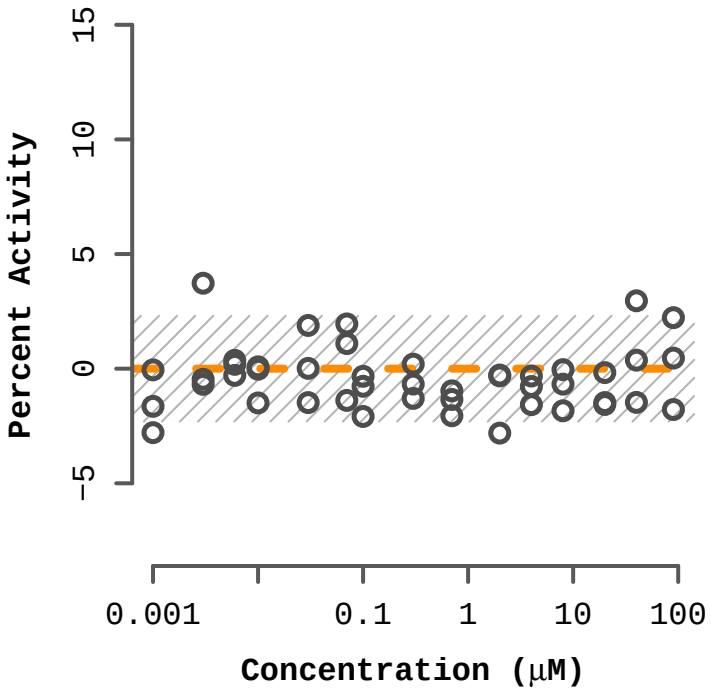
NAME: gamma-Caprolactone
CHID: 41298 **CASRN:** 695-06-7
SPID(S): Tox21_300875
M4ID: 12478258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.03	NA	NA
PROB:	1	NA	NA
RMSE:	2.4	NA	NA

MAX_MEAN: 5 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

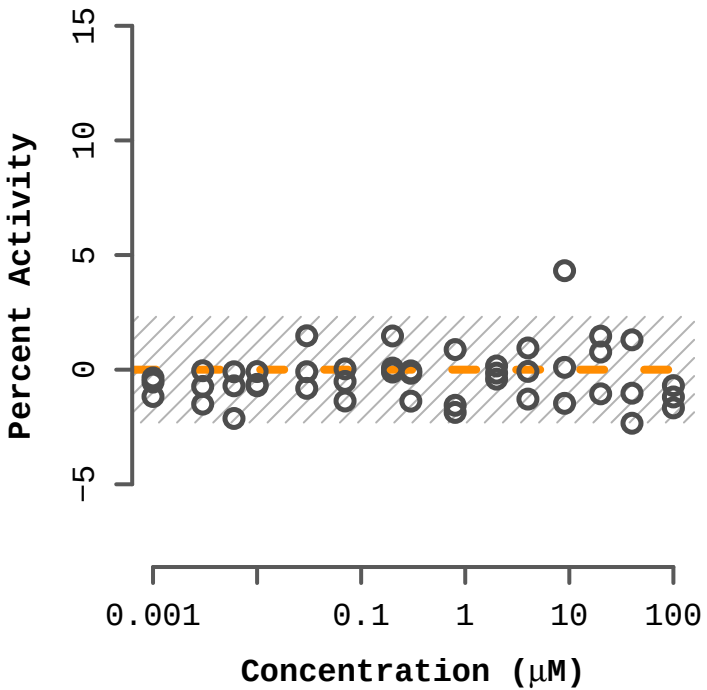
NAME: Dihydrojasmone lactone
CHID: 41299 **CASRN:** 7011-83-8
SPID(S): Tox21_302312
M4ID: 12476821

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

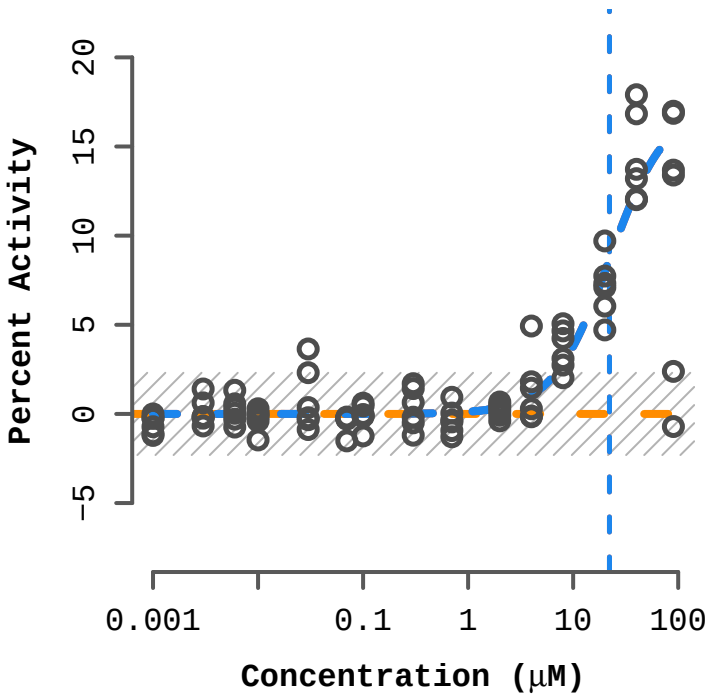
NAME: (Dicyclopentadienyloxy)ethyl methacrylate
CHID: 41302 **CASRN:** 68169-03-9
SPID(S): Tox21_300832
M4ID: 12478301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.985 **MAX_MED:** 0.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2',4,4'−Tetrahydroxybenzophenone
CHID: 41306 CASRN: 131−55−5
SPID(S): Tox21_303639
M4ID: 12475506

HILL MODEL (in red):

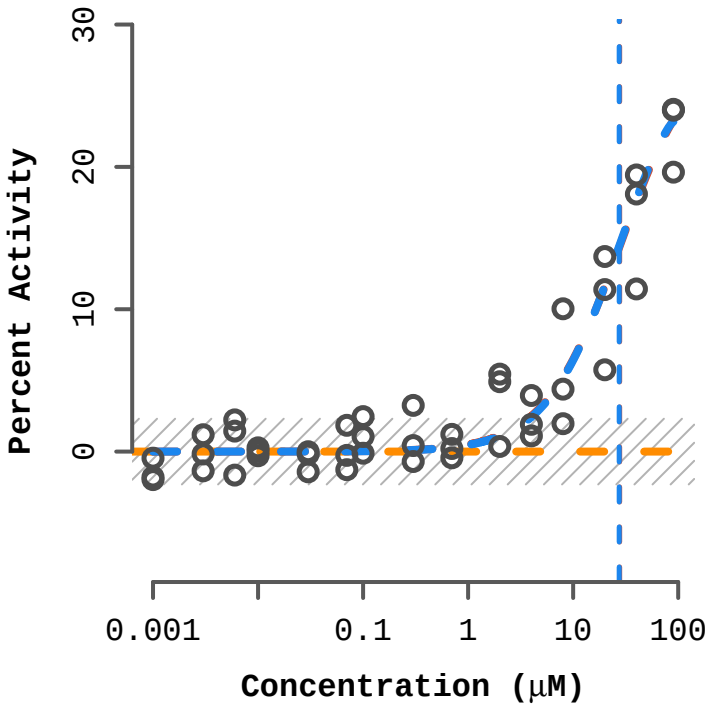
	tp	ga	gw
val:	17.4	1.35	1.6
sd:	1.75	0.0718	0.196

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.4	1.35	1.6	3.61	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	515.89	336.32	340.32
PROB:	0	0.88	0.12
RMSE:	5.46	2.59	2.59

MAX_MEAN: 14.3 **MAX_MED:** 13.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2',4,4'-Tetrahydroxybenzophenone
CHID: 41306 CASRN: 131-55-5
SPID(S): Tox21_202288
M4ID: 12479964

HILL MODEL (in red):

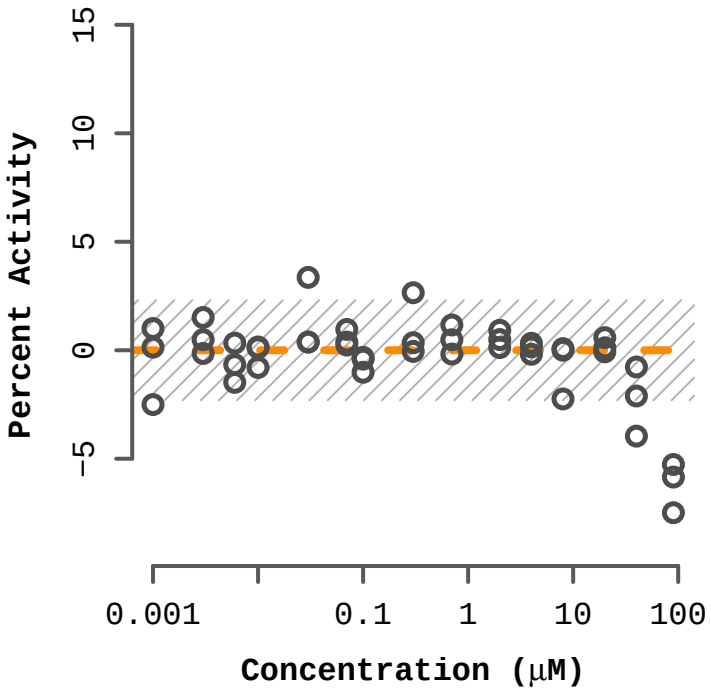
	tp	ga	gw
val:	28.9	1.44	1.22
sd:	4.77	0.155	0.285

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	28.9	1.44	1.24	2.15	9.82
sd:	14.6	0.376	0.409	2.09	84.4

	CNST	HILL	GNLS
AIC:	301.42	202.27	206.24
PROB:	0	0.88	0.12
RMSE:	8.13	2.18	2.19

MAX_MEAN: 22.6 MAX_MED: 24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

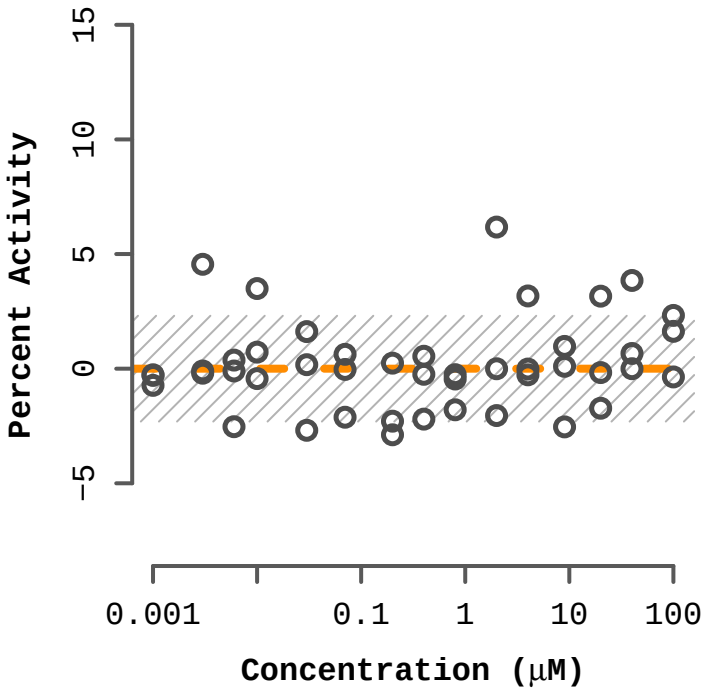
NAME: 2,2-Bis(4-chlorophenyl)ethanol
CHID: 41308 **CASRN:** 2642-82-2
SPID(S): Tox21_300725
M4ID: 12478408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.495 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

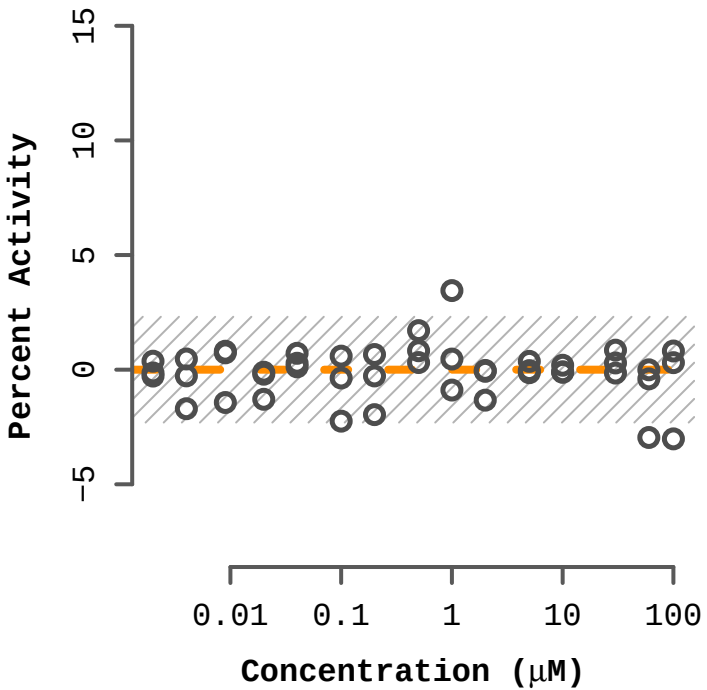
NAME: 2,3,5-Triiodobenzoic acid
CHID: 41317 CASRN: 88-82-4
SPID(S): Tox21_300914
M4ID: 12478219

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 1.5 MAX_MED: 1.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

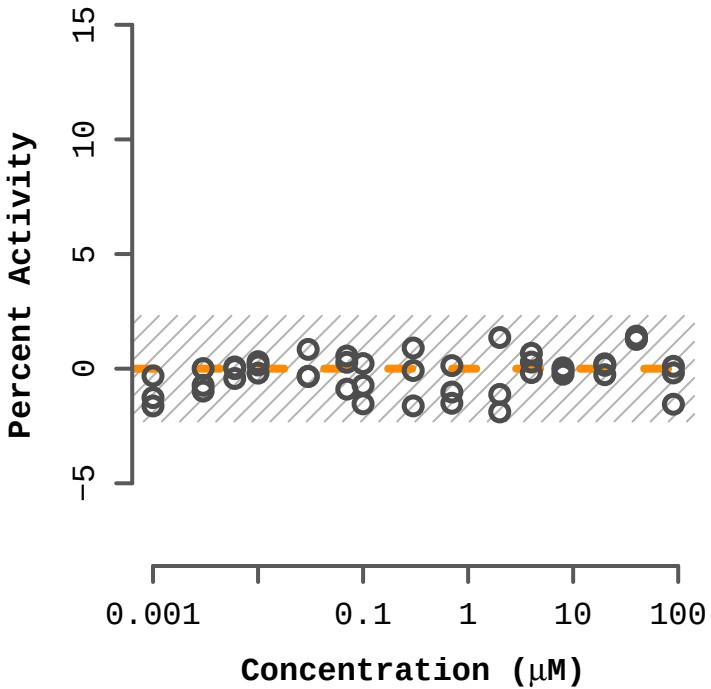
NAME: 2,3-Butanediol
CHID: 41321 **CASRN:** 513-85-9
SPID(S): Tox21_300789
M4ID: 12478344

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

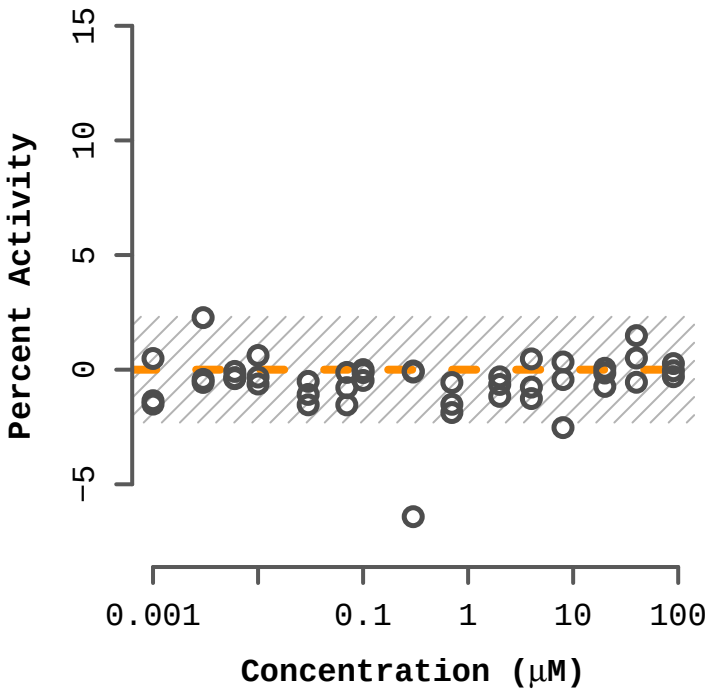
NAME: 2,3-Pyridinedicarboxylic acid
CHID: 41327 **CASRN:** 89-00-9
SPID(S): Tox21_302051
M4ID: 12477082

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

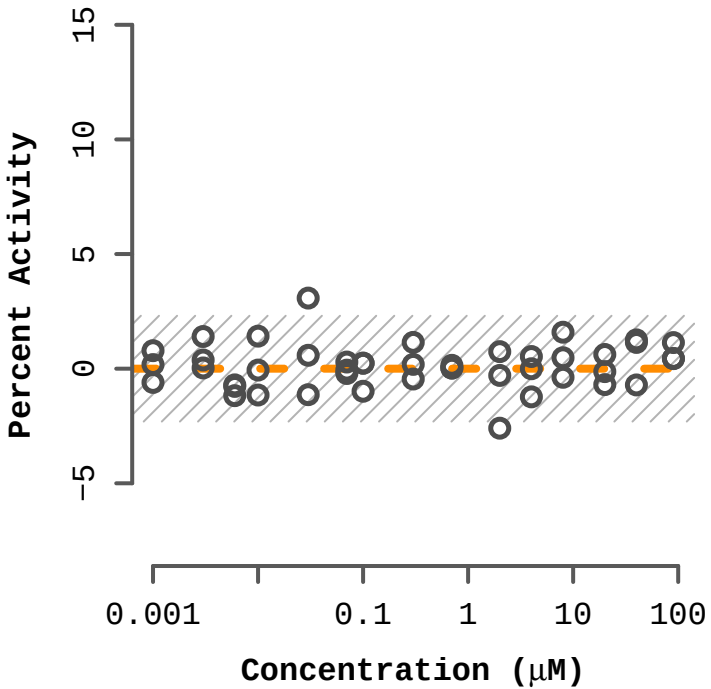
NAME: 2,4,5-T-butotyl
CHID: 41328 **CASRN:** 2545-59-7
SPID(S): Tox21_301916
M4ID: 12477217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.483 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

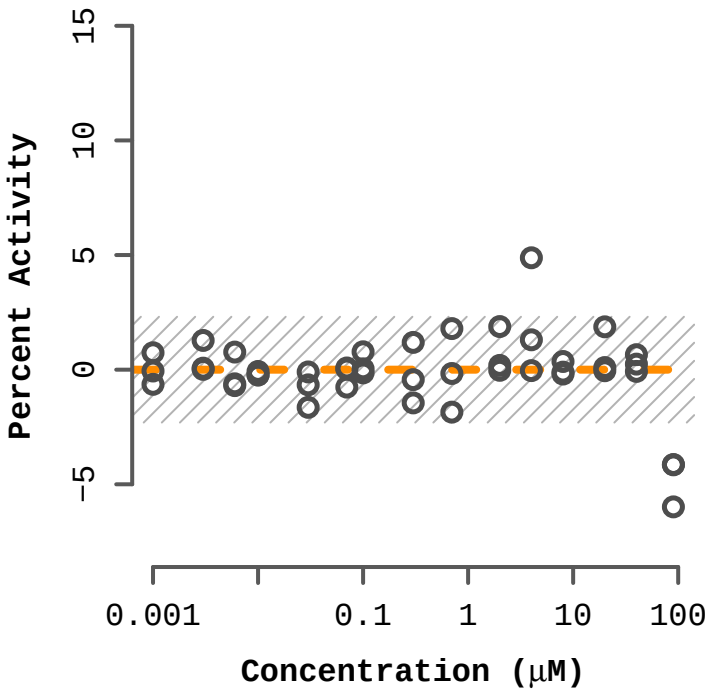
NAME: 2,4,5-T-2-ethylhexyl
CHID: 41329 **CASRN:** 1928-47-8
SPID(S): Tox21_301912
M4ID: 12477221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.844 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

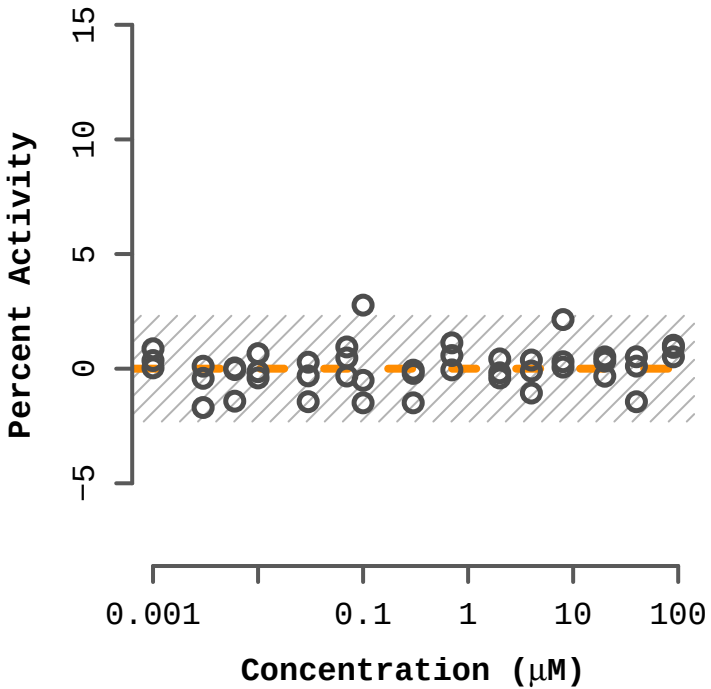
NAME: 2,4,5-Trichlorophenol sodium salt
CHID: 41336 **CASRN:** 136-32-3
SPID(S): Tox21_300704
M4ID: 12478429

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

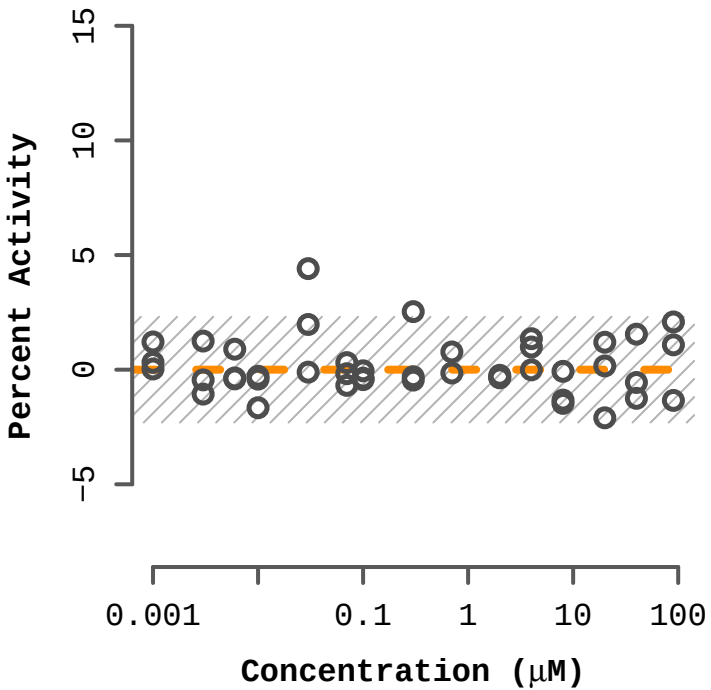
NAME: 2,4−D−ethyl ester
CHID: 41346 CASRN: 533−23−3
SPID(S): Tox21_302216
M4ID: 12476917

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.839 MAX_MED: 0.93 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

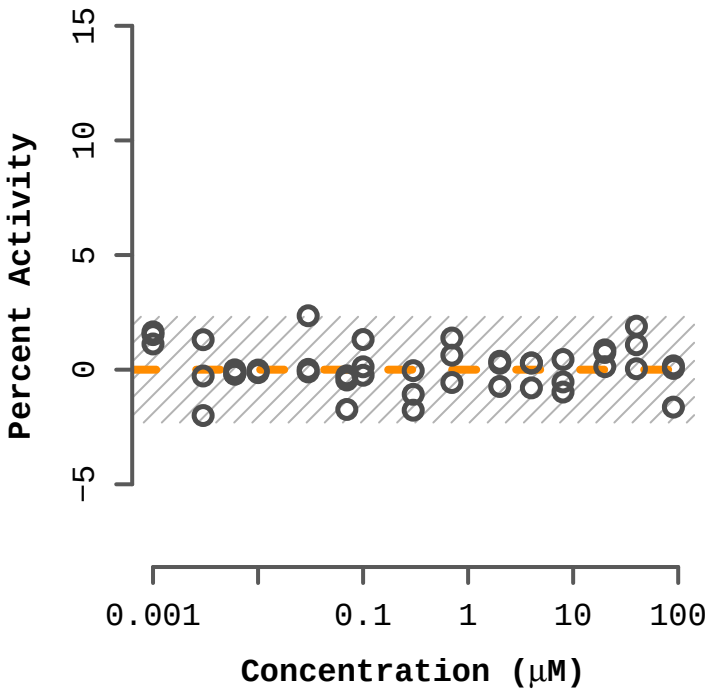
NAME: 2,4-D-isobutyl
CHID: 41347 **CASRN:** 1713-15-1
SPID(S): Tox21_302403
M4ID: 12476730

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

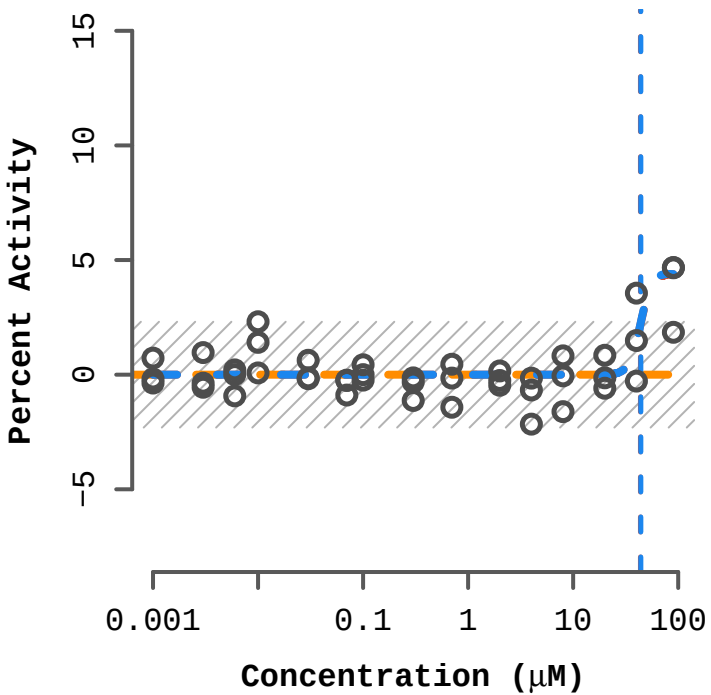
NAME: 2,4-D-methyl
CHID: 41349 **CASRN:** 1928-38-7
SPID(S): Tox21_301422
M4ID: 12477711

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-DB-sodium
CHID: 41356 CASRN: 10433-59-7
SPID(S): Tox21_301097
M4ID: 12478036

HILL MODEL (in red):

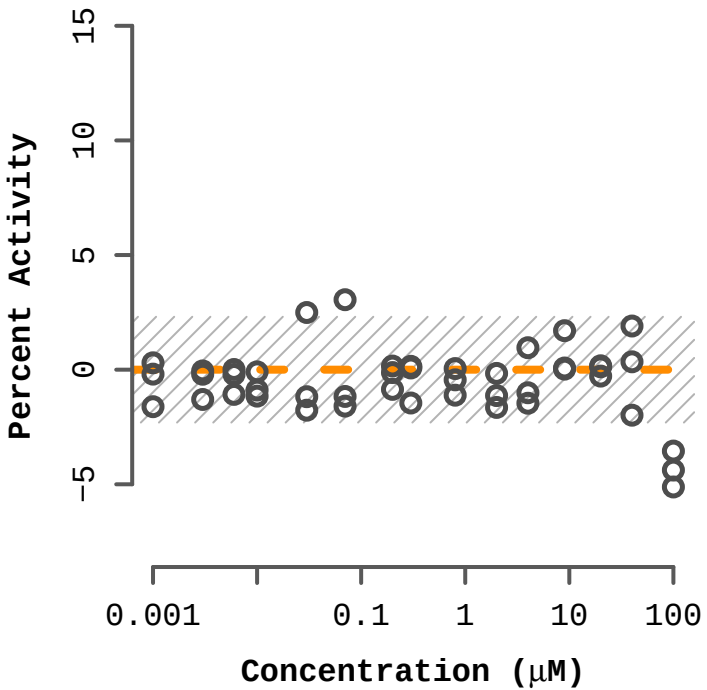
	tp	ga	gw
val:	4.4	1.64	8
sd:	0.529	0.112	21.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.51	1.64	8	3.95	0.3
sd:	94.2	0.176	25.5	114	14.4

	CNST	HILL	GNLS
AIC:	144.42	125.45	129.45
PROB:	0	0.88	0.12
RMSE:	1.39	0.93	0.93

MAX_MEAN: 3.73 MAX_MED: 4.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

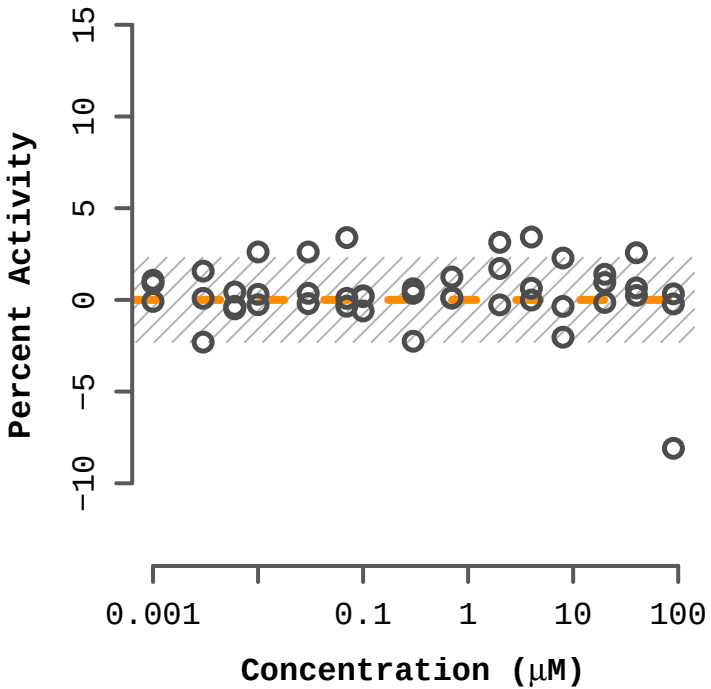
NAME: Ethyl (2E,4Z)-deca-2,4-dienoate
CHID: 41357 **CASRN:** 3025-30-7
SPID(S): Tox21_300673
M4ID: 12478460

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 0.601 **MAX_MED:** 0.344 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

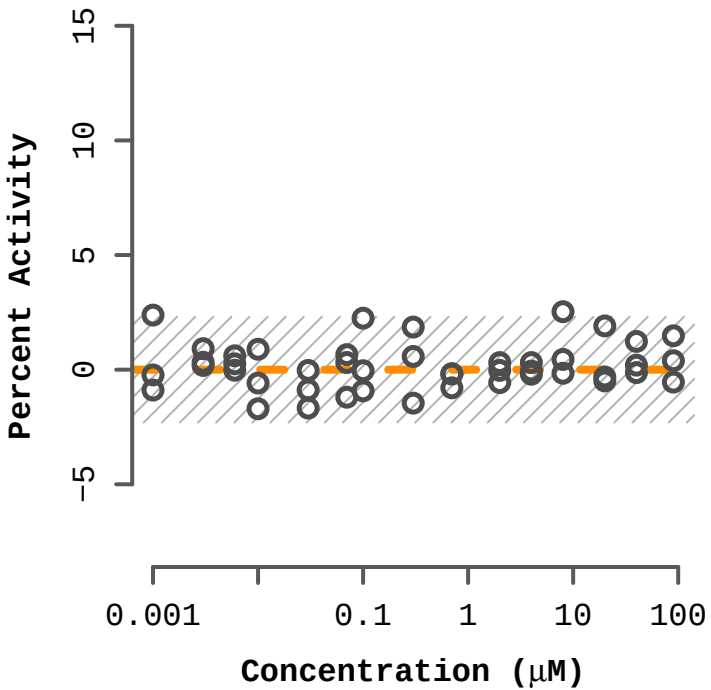
NAME: 2,4-Dichloro-3,5-dimethylphenol
CHID: 41359 **CASRN:** 133-53-9
SPID(S): Tox21_301201
M4ID: 12477932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

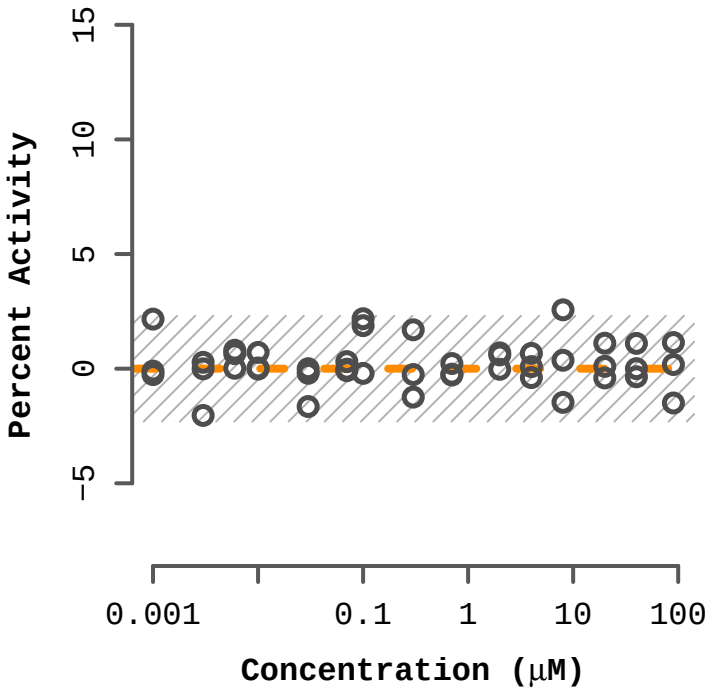
NAME: 2,4-Dichloro-6-nitroaniline
CHID: 41361 **CASRN:** 2683-43-4
SPID(S): Tox21_300652
M4ID: 12478481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.04	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.941 **MAX_MED:** 0.579 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

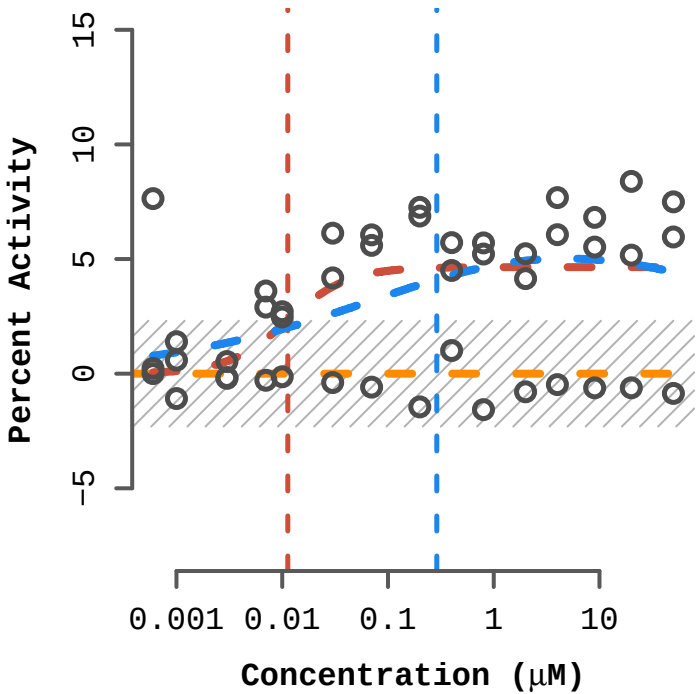
NAME: 2,4-Dichlorobenzyl alcohol
CHID: 41362 **CASRN:** 1777-82-8
SPID(S): Tox21_300895
M4ID: 12478238

HILL MODEL: Not applicable.

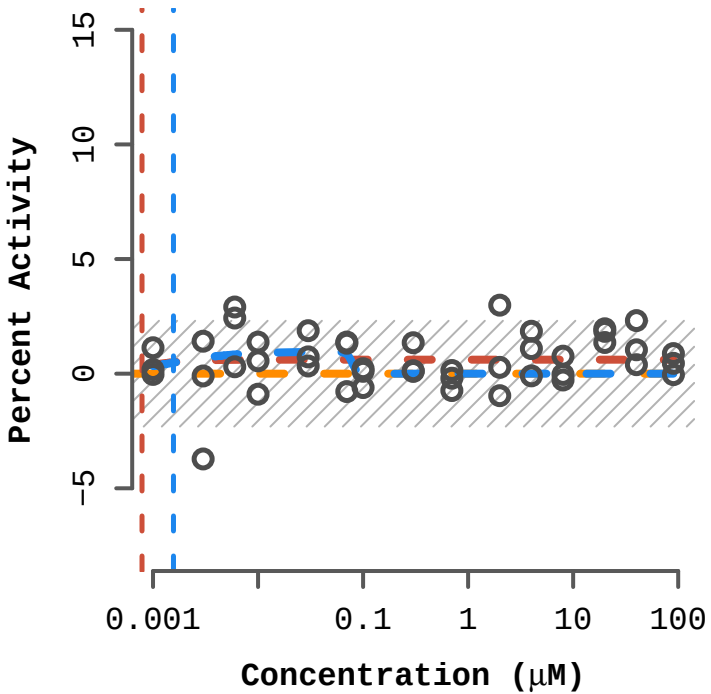
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.88 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,4-Dichlorobenzyl alcohol
CHID:    41362   CASRN: 1777-82-8
SPID(S): Tox21_112796_1
M4ID:    12482951

HILL MODEL (in red):
      tp       ga       gw
val:  4.65     -1.95    1.52
sd:   0.666    0.268    1.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.94     -0.539   0.392    1.73     0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  266.34      236.22      242.06
PROB: 0           0.95        0.05
RMSE: 4.34        3.04        3.03

MAX_MEAN: 4.42      MAX_MED: 6.88      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4−Dichlorophenylacetic acid
CHID: 41363 CASRN: 19719−28−9
SPID(S): Tox21_301932
M4ID: 12477201

HILL MODEL (in red):

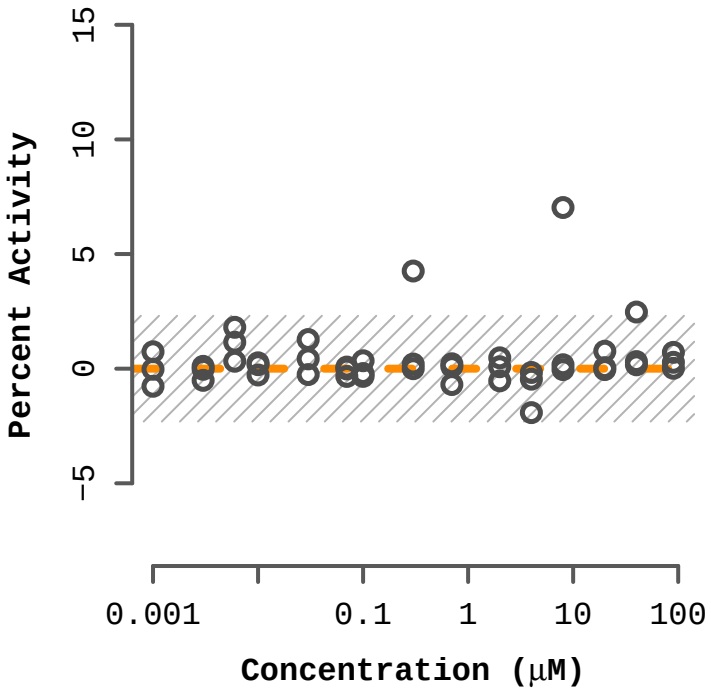
	tp	ga	gw
val:	0.611	−3.1	2.18
sd:	0.17	0.844	6.68

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.959	−2.81	1.43	−1.1	18
sd:	0.488	0.741	2.95	0.163	44.1

	CNST	HILL	GNLS
AIC:	153.65	146.68	155.94
PROB:	0.03	0.96	0.01
RMSE:	1.32	1.17	1.26

MAX_MEAN: 1.88 **MAX_MED:** 2.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

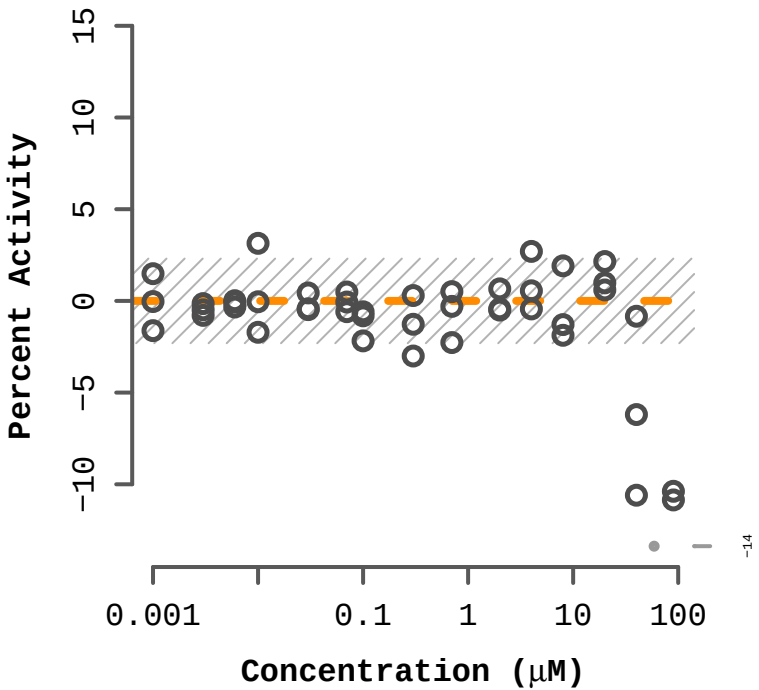
NAME: 2,4−Dinitroanisole
CHID: 41366 **CASRN:** 119−27−7
SPID(S): Tox21_302199
M4ID: 12476934

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.39 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

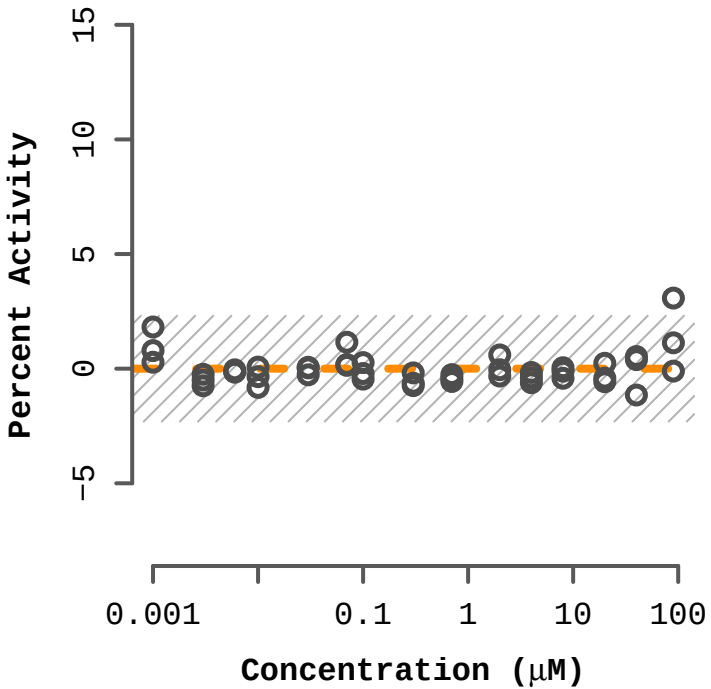
NAME: 2,4-Dinitrophenyl thiocyanate
CHID: 41367 **CASRN:** 1594-56-5
SPID(S): Tox21_301463
M4ID: 12477670 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.11	NA	NA
PROB:	1	NA	NA
RMSE:	3.8	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.985 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

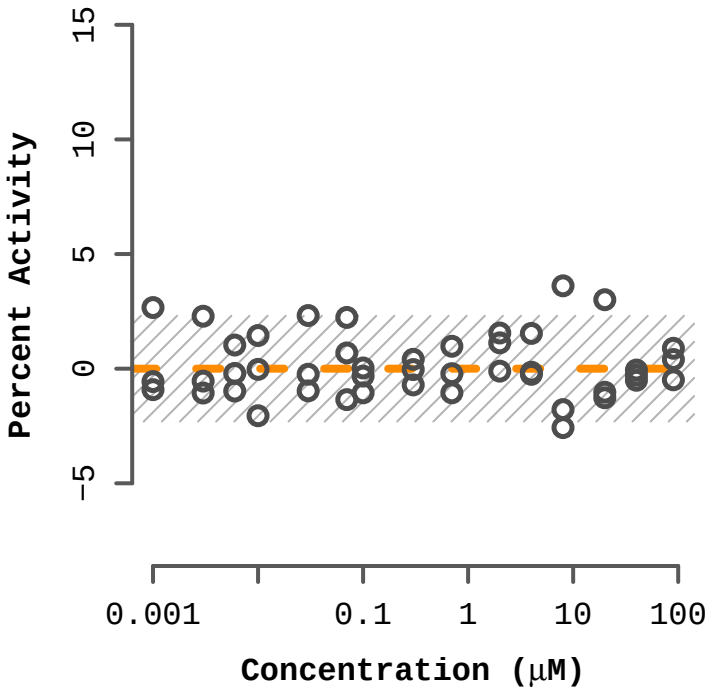
NAME: 5-Ethyl-5-methylhydantoin
CHID: 41368 **CASRN:** 5394-36-5
SPID(S): Tox21_301987
M4ID: 12477146

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

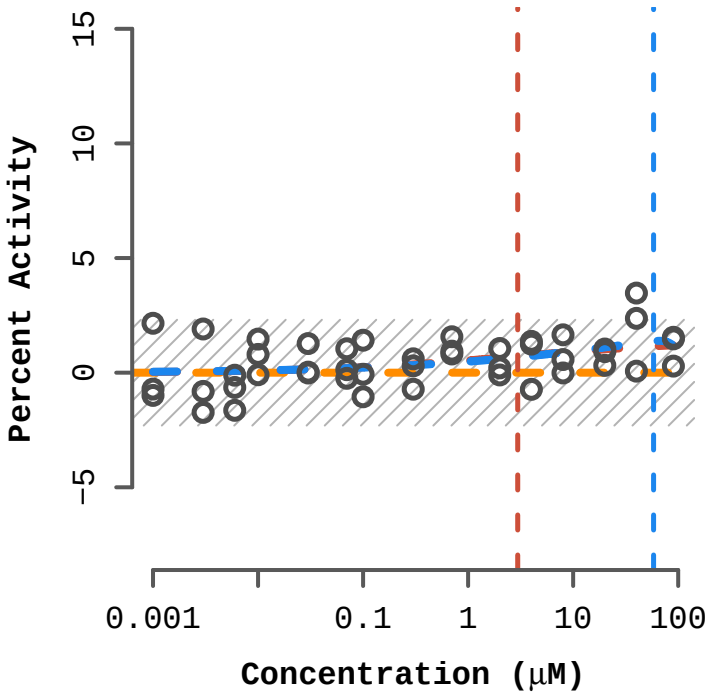
NAME: 3-(Hydroxymethyl)pentane-2,4-diol
CHID: 41370 **CASRN:** 921-20-0
SPID(S): Tox21_301877
M4ID: 12477256

HILL MODEL: Not applicable.

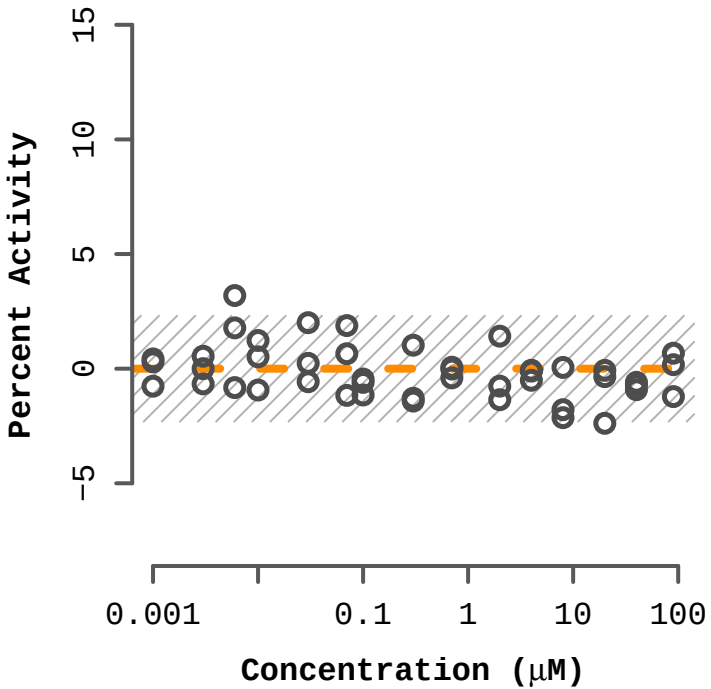
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.86 **MAX_MED:** 1.13 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,5,8,11,14-Pentaoxahexadecan-16-ol
CHID:    41371   CASRN: 23778-52-1
SPID(S): Tox21_301472
M4ID:    12477661

HILL MODEL (in red):
      tp       ga       gw
val:  1.43     0.472    0.476
sd:   1.46     2.43     0.473

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.77     1.77     0.383    2.02     8.66
sd:   16.8     11.3     0.476    0.652    67.1

      CNST        HILL        GNLS
AIC:  146.87      136.21      140.11
PROB: 0           0.87        0.12
RMSE: 1.18        0.97        0.96

MAX_MEAN: 1.97      MAX_MED: 2.37      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

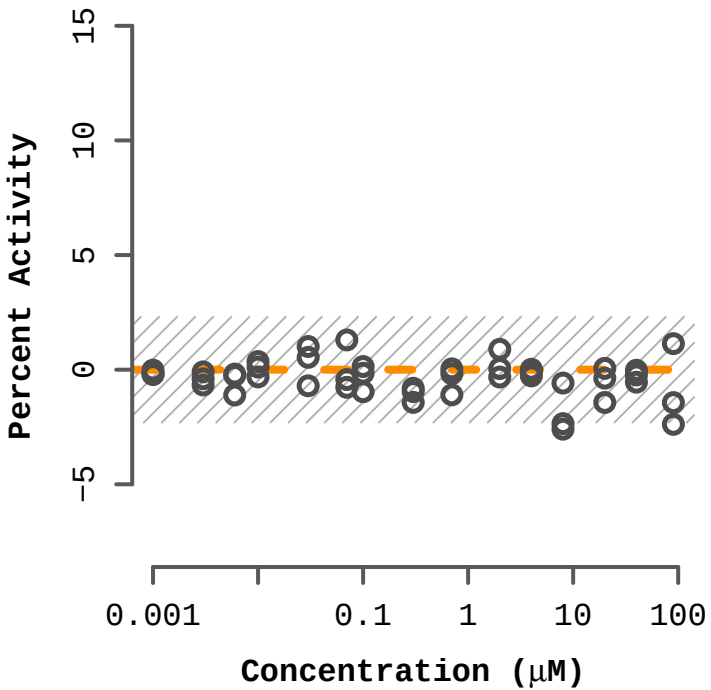
NAME: 2,5-Dichloro-3-nitrobenzoic acid
CHID: 41372 **CASRN:** 88-86-8
SPID(S): Tox21_300775
M4ID: 12478358

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

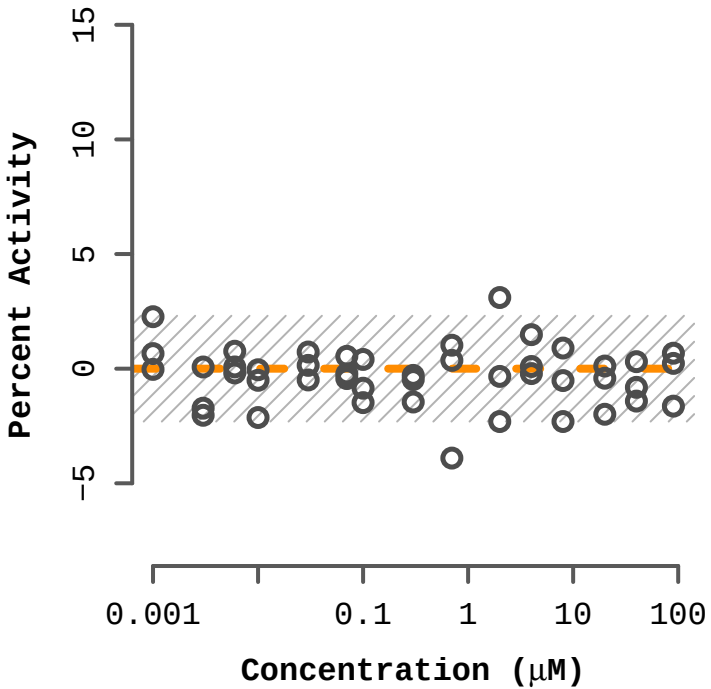
NAME: 2-Octen-1-ylsuccinic anhydride
CHID: 41373 **CASRN:** 42482-06-4
SPID(S): Tox21_301521
M4ID: 12477612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.283 **MAX_MED:** 0.539 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

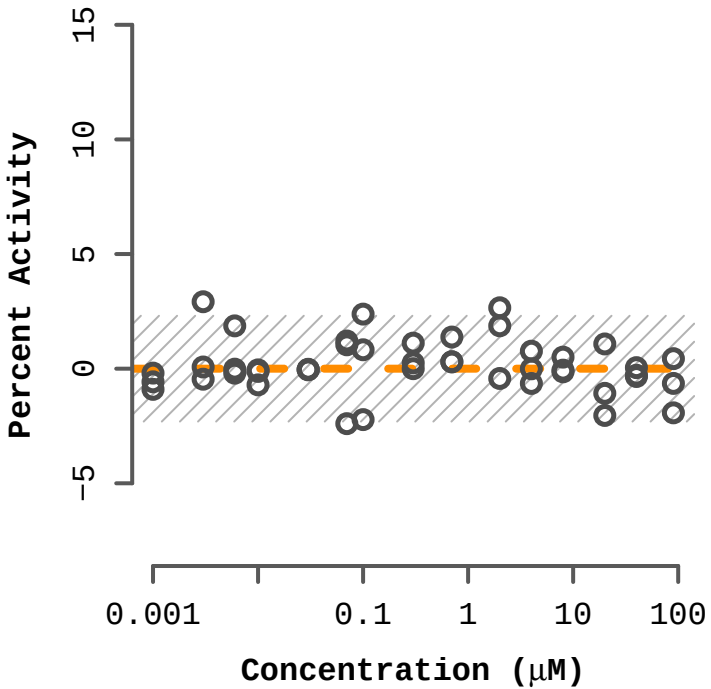
NAME: Tridemorph
CHID: 41376 **CASRN:** 24602-86-6
SPID(S): Tox21_300591
M4ID: 12478542

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

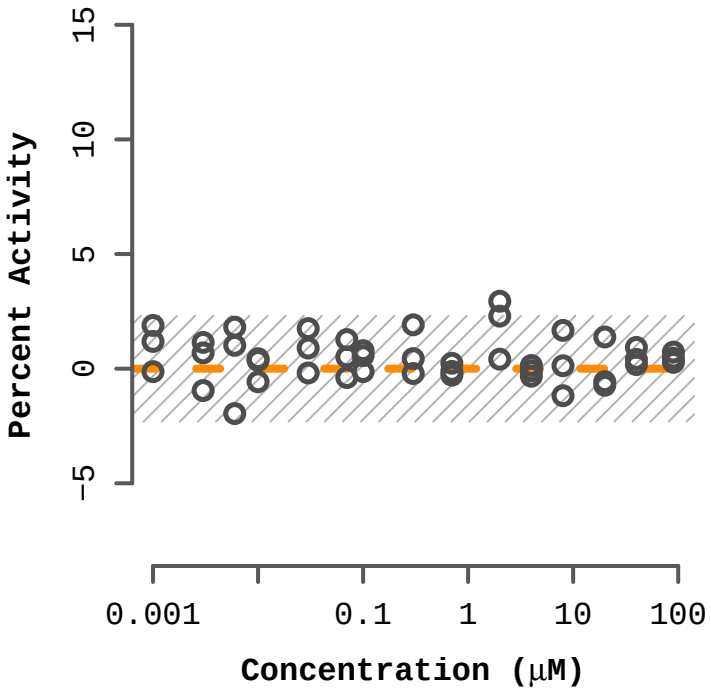
NAME: 2,6-Di-tert-butyl-4-methoxyphenol
CHID: 41379 **CASRN:** 489-01-0
SPID(S): Tox21_301055
M4ID: 12478078

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

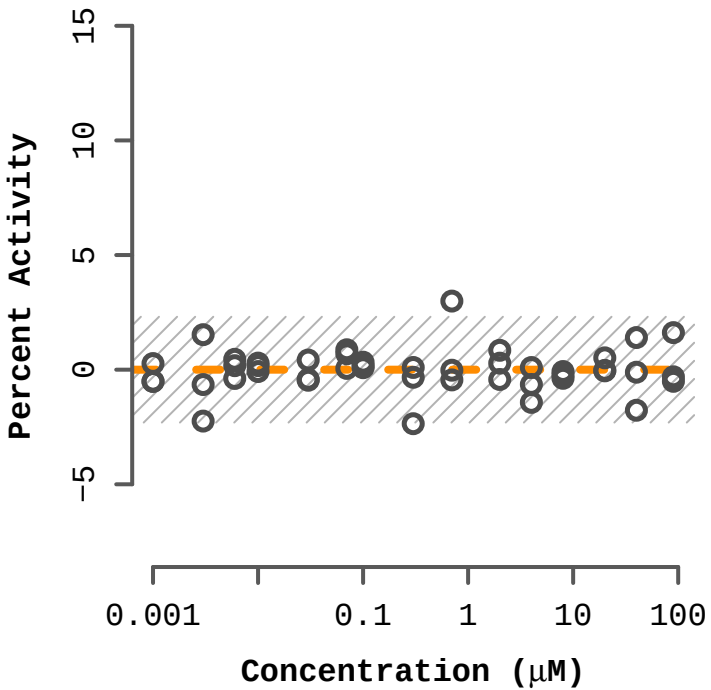
NAME: 2-[Methacryloyloxy]ethyl acetoacetate
CHID: 41388 **CASRN:** 21282-97-3
SPID(S): Tox21_301183
M4ID: 12477950

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

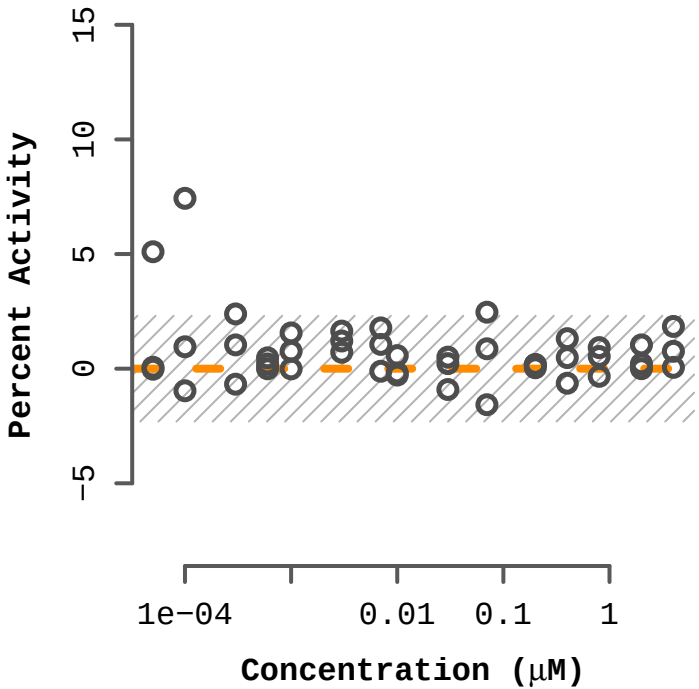
NAME: 2'−Acetonaphthone
CHID: 41389 **CASRN:** 93−08−3
SPID(S): Tox21_302186
M4ID: 12476947

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 0.696 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

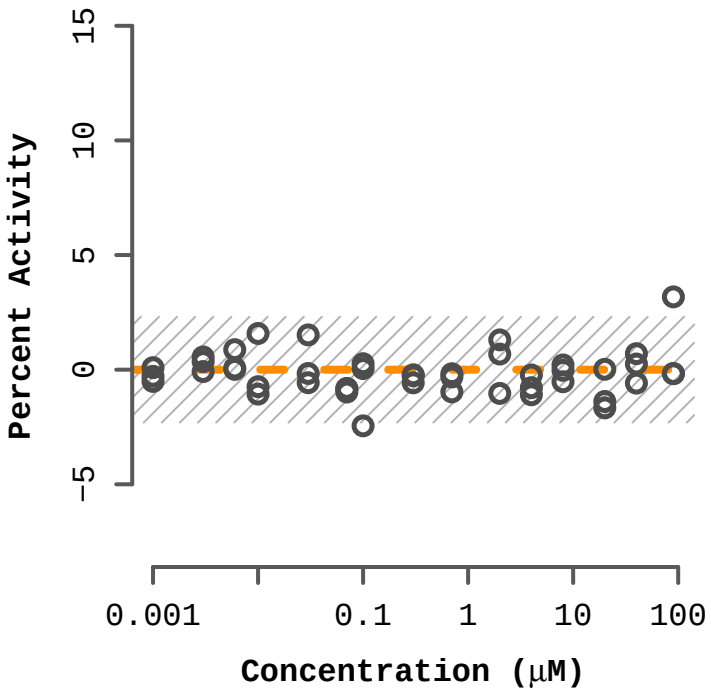
NAME: 2-Butanethiol
CHID: 41396 **CASRN:** 513-53-1
SPID(S): Tox21_301086
M4ID: 12478047

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 2.48 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

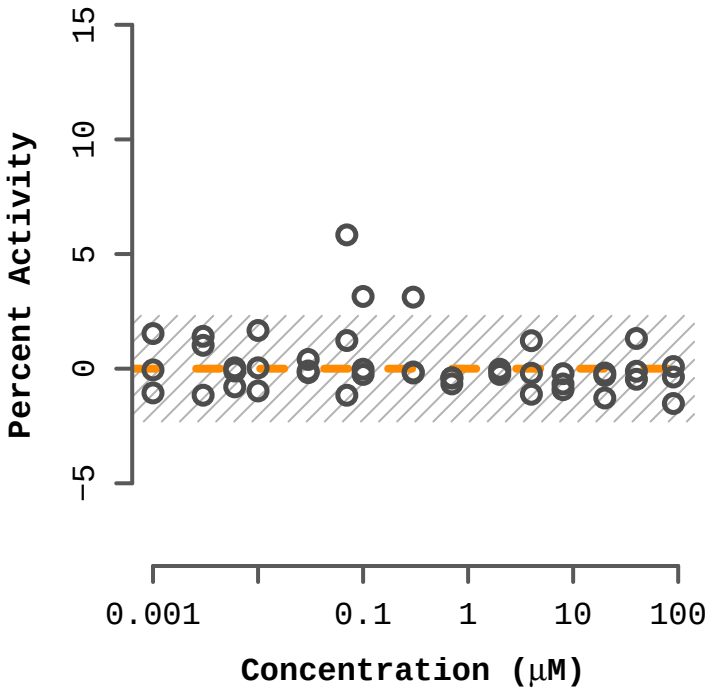
NAME: Damascenone
CHID: 41397 **CASRN:** 23696-85-7
SPID(S): Tox21_304001
M4ID: 12475187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.946 **MAX_MED:** 0.682 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

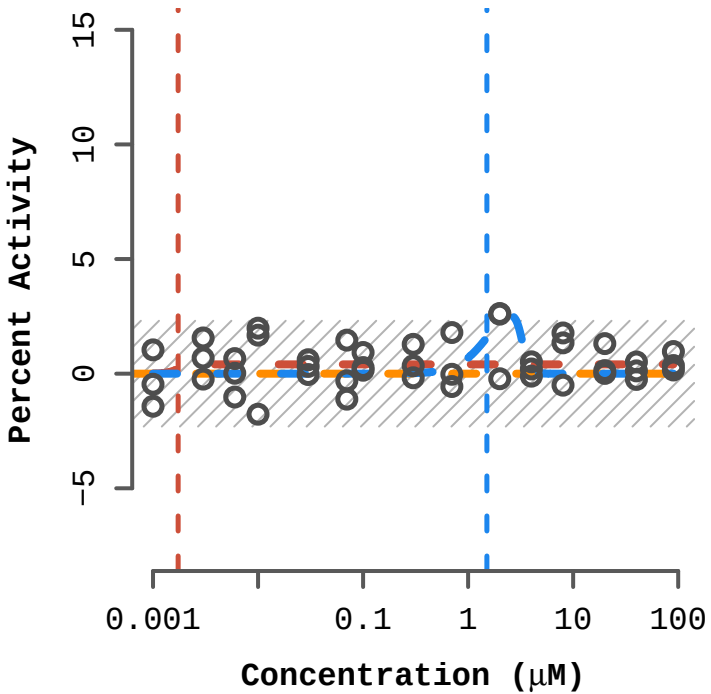
NAME: 2-Butyl-2-ethyl-1,3-propanediol
CHID: 41400 **CASRN:** 115-84-4
SPID(S): Tox21_301187
M4ID: 12477946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-1,4-dimethoxybenzene
CHID: 41403 **CASRN:** 2100-42-7
SPID(S): Tox21_302090
M4ID: 12477043

HILL MODEL (in red):

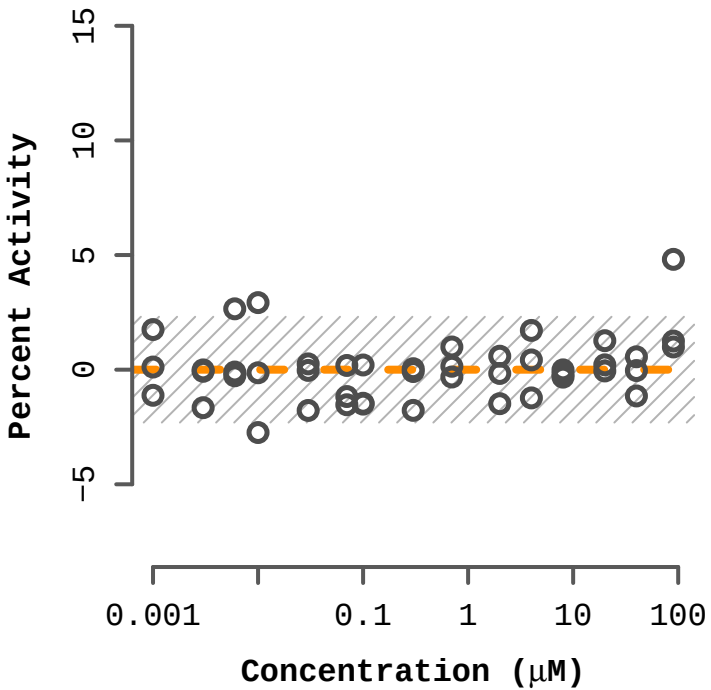
	tp	ga	gw
val:	0.406	−2.76	8
sd:	0.144	0.558	18.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.15	0.179	3.09	0.513	12.7
sd:	17.6	1.94	20.1	0.951	140

	CNST	HILL	GNLS
AIC:	135.37	133.44	138.61
PROB:	0.26	0.69	0.05
RMSE:	1.06	0.95	0.97

MAX_MEAN: 1.67 **MAX_MED:** 2.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

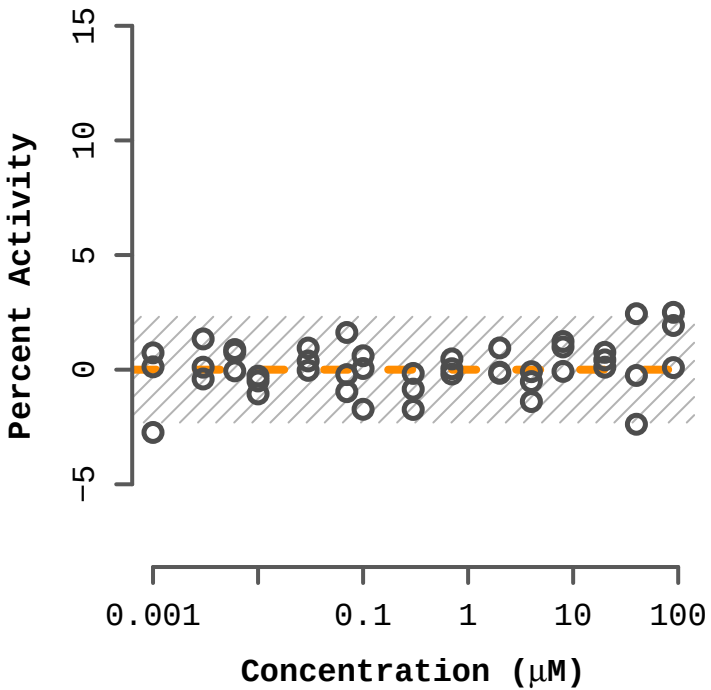
NAME: 2-Chloro-4,5-dimethylphenol
CHID: 41404 **CASRN:** 1124-04-5
SPID(S): Tox21_301925
M4ID: 12477208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 2.35 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

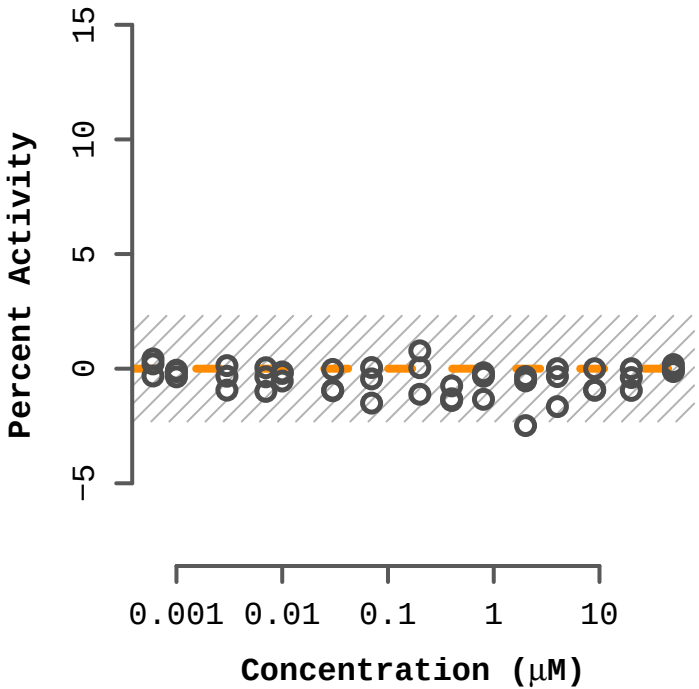
NAME: 2-Chloro-4-nitrobenzamide
CHID: 41405 **CASRN:** 3011-89-0
SPID(S): Tox21_301142
M4ID: 12477991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

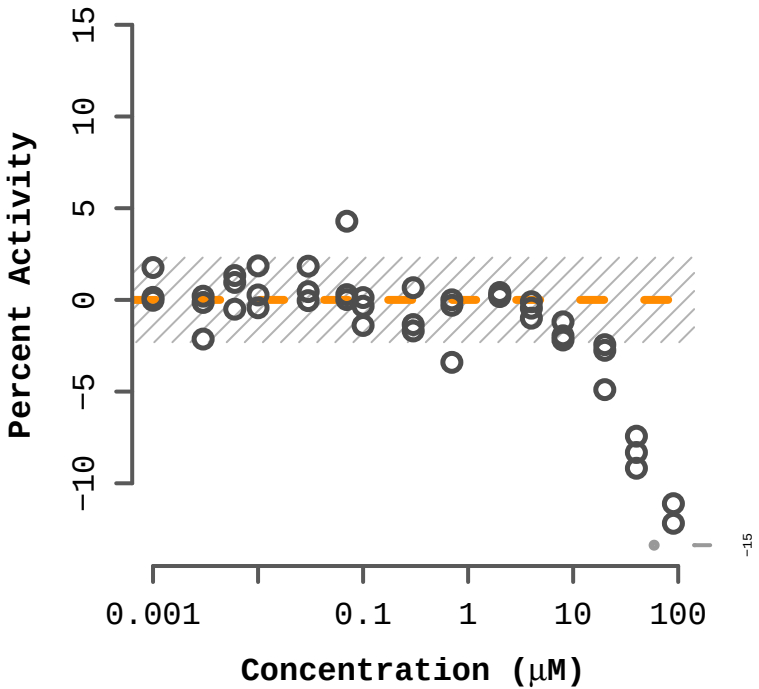
NAME: 2-Chloro-4-nitrobenzamide
CHID: 41405 **CASRN:** 3011-89-0
SPID(S): Tox21_111296_1
M4ID: 12483785

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.106 **MAX_MED:** 0.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

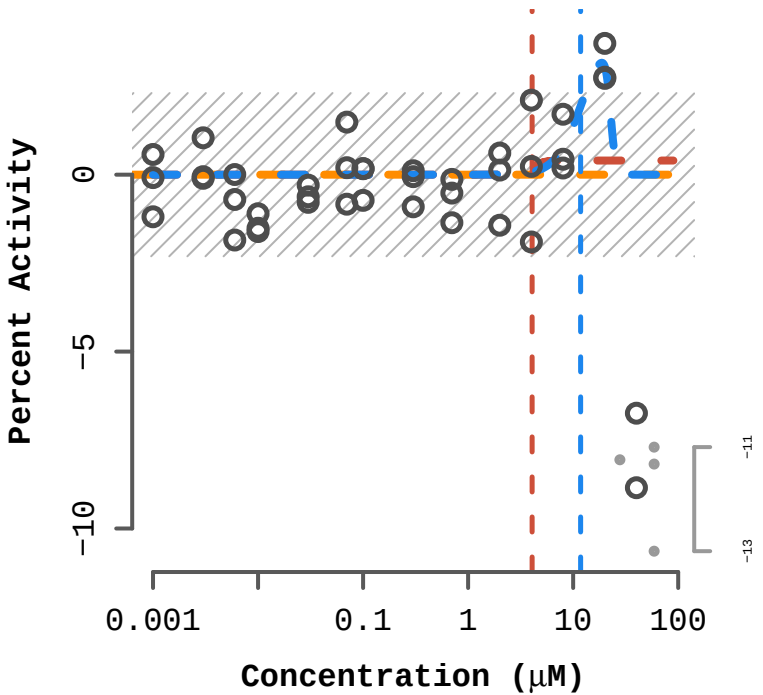
NAME: 2-Chloro-N-phenylacetamide
CHID: 41409 CASRN: 587-65-5
SPID(S): Tox21_300983
M4ID: 12478150 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	238.98	NA	NA
PROB:	1	NA	NA
RMSE:	4.26	NA	NA

MAX_MEAN: 1.53 MAX_MED: 0.955 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-N-(2-methyl-4-bromophenyl)acetamide
CHID: 41411 CASRN: 96686-51-0
SPID(S): Tox21_301981
M4ID: 12477152 BRK

HILL MODEL (in red):

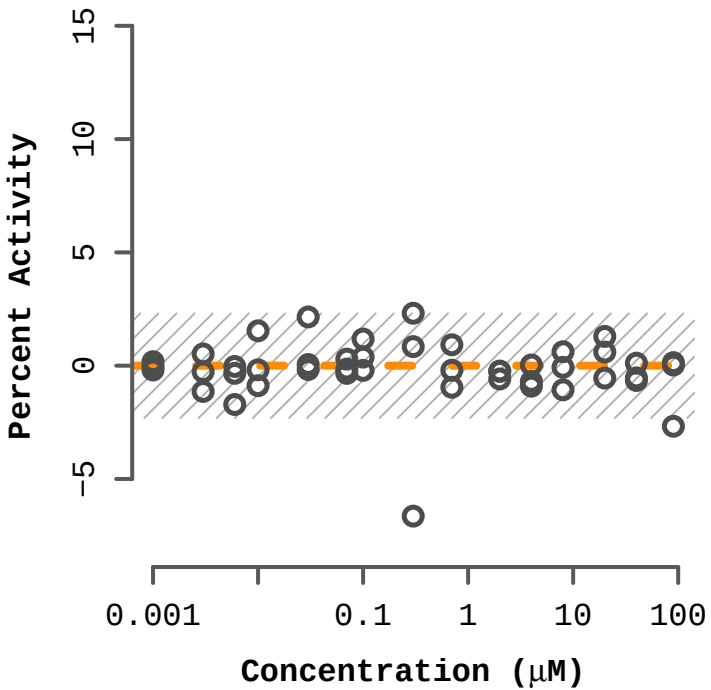
	tp	ga	gw
val:	0.399	0.609	8
sd:	1.04	0.639	44.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.87	1.07	3.63	1.36	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	229.9	235.75	229.15
PROB:	0.4	0.02	0.58
RMSE:	4.08	4.2	4

MAX_MEAN: 3.06 MAX_MED: 2.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

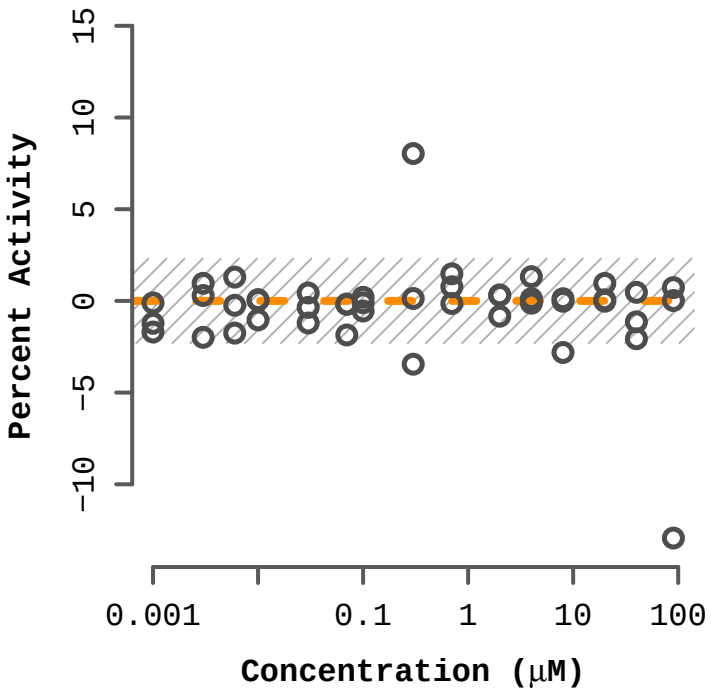
NAME: 2-Chloro-N-(hydroxymethyl)acetamide
CHID: 41412 CASRN: 2832-19-1
SPID(S): Tox21_300964
M4ID: 12478169

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.679 MAX_MED: 0.842 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

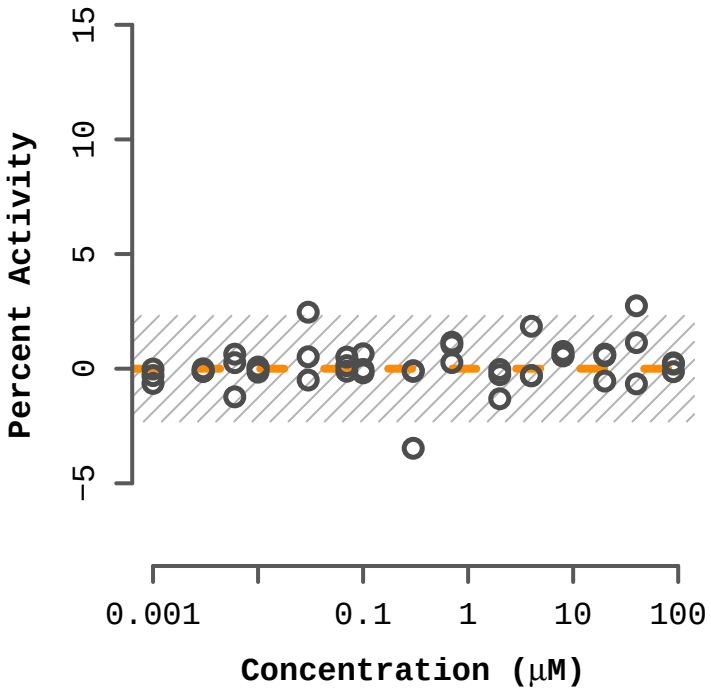
NAME: R-(−)-Carvone
CHID: 41413 **CASRN:** 6485-40-1
SPID(S): Tox21_300931
M4ID: 12478202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.52	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 0.774 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

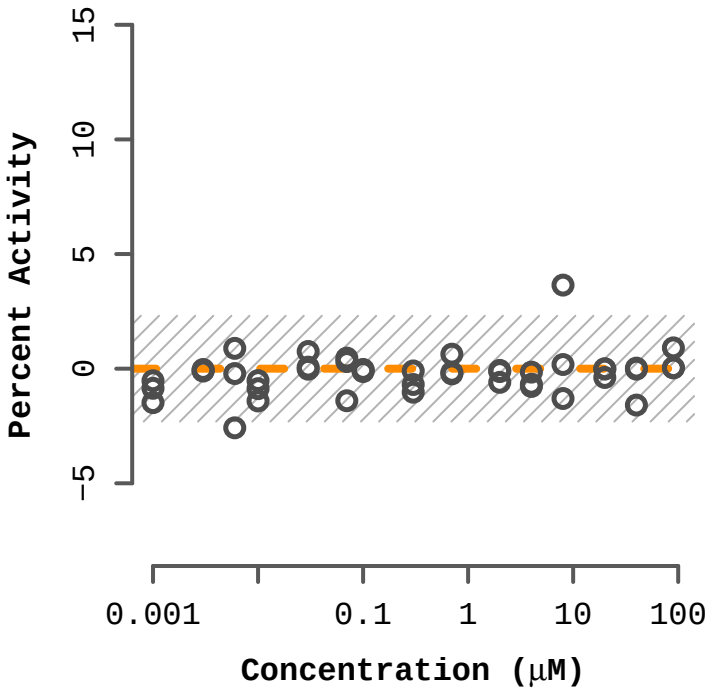
NAME: 2-Ethyl-1-butanol
CHID: 41416 **CASRN:** 97-95-0
SPID(S): Tox21_300926
M4ID: 12478207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

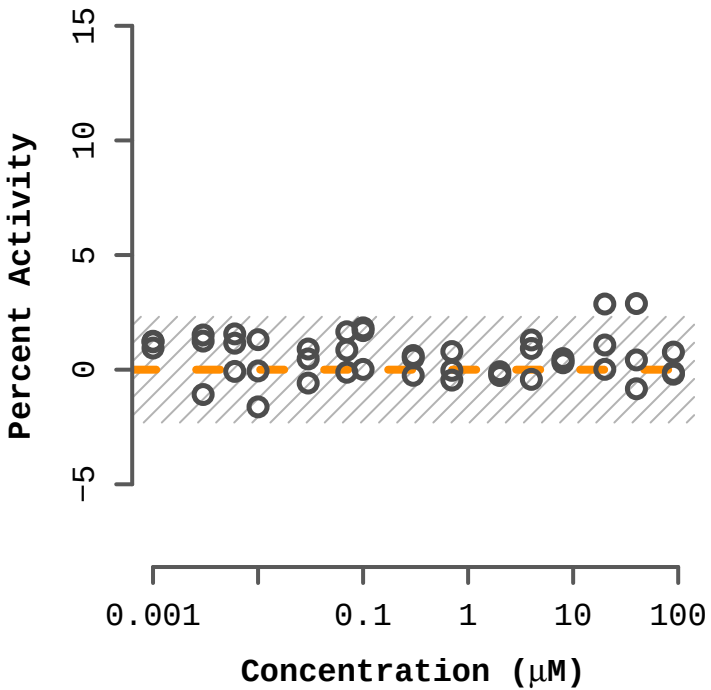
NAME: 2-Ethyl-2-nitro-1,3-propanediol
CHID: 41417 CASRN: 597-09-1
SPID(S): Tox21_301742
M4ID: 12477391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.843 MAX_MED: 0.313 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

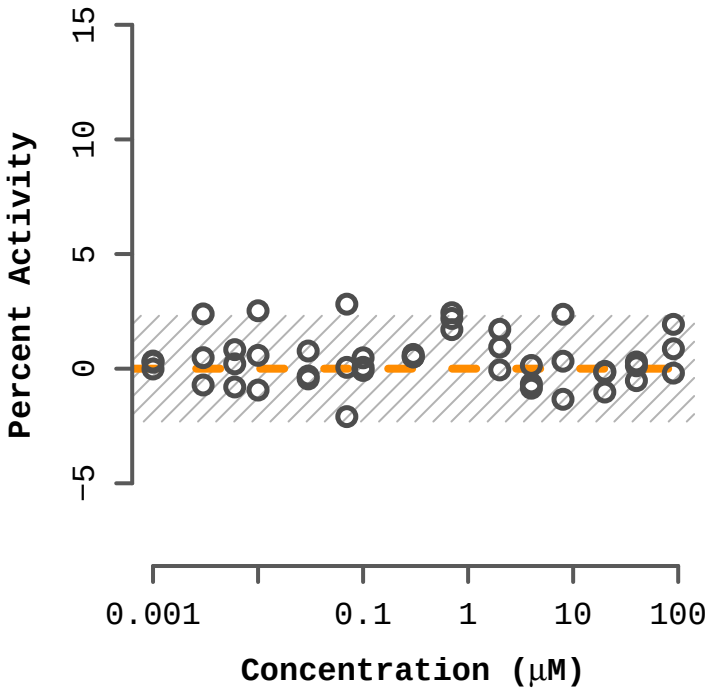
NAME: 2-Ethylbutyric acid
CHID: 41418 **CASRN:** 88-09-5
SPID(S): Tox21_301054
M4ID: 12478079

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

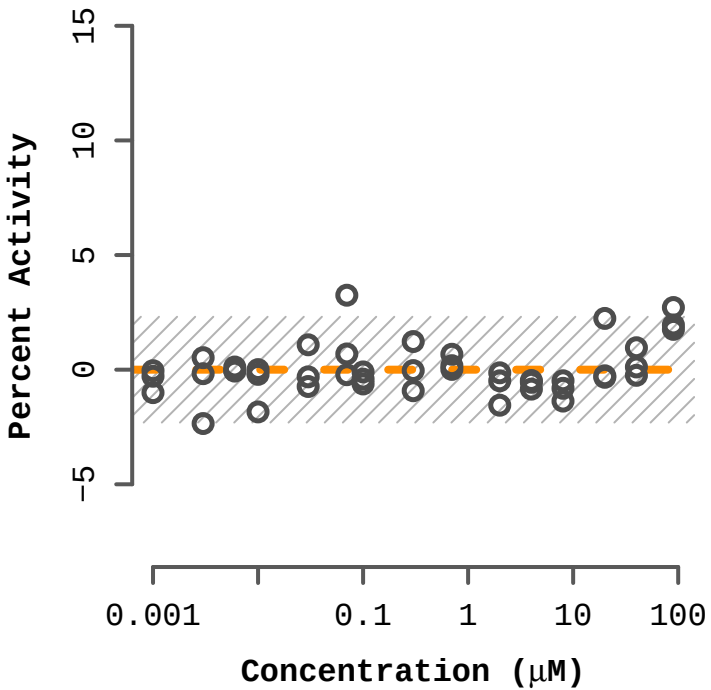
NAME: 2-Furancarboxylic acid
CHID: 41420 **CASRN:** 88-14-2
SPID(S): Tox21_301128
M4ID: 12478005

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

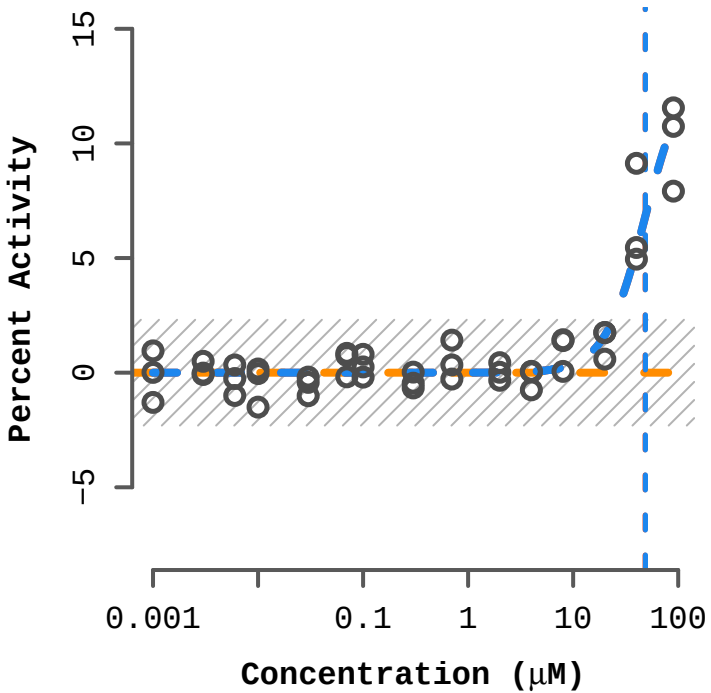
NAME: 5,7-Dimethoxy-2H-chromen-2-one
CHID: 41421 **CASRN:** 487-06-9
SPID(S): Tox21_300942
M4ID: 12478191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 7-(Dimethylamino)-4-methylcoumarin
CHID: 41422 **CASRN:** 87-01-4
SPID(S): Tox21_301534
M4ID: 12477599

HILL MODEL (in red):

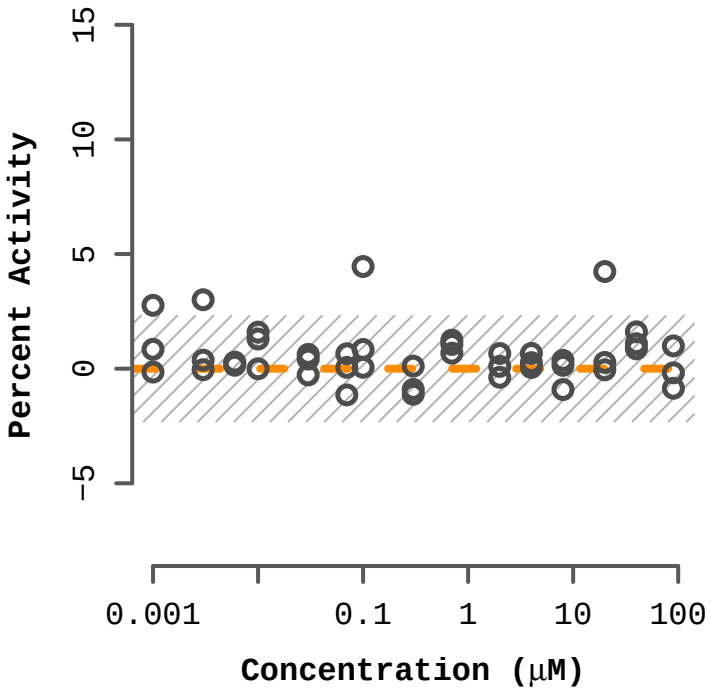
	tp	ga	gw
val:	13.5	1.68	2.25
sd:	2.37	0.0921	0.561

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.9	1.69	2.26	3.66	0.989
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	199.24	118.22	122.21
PROB:	0	0.88	0.12
RMSE:	3.24	0.95	0.95

MAX_MEAN: 10.1 **MAX_MED:** 10.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

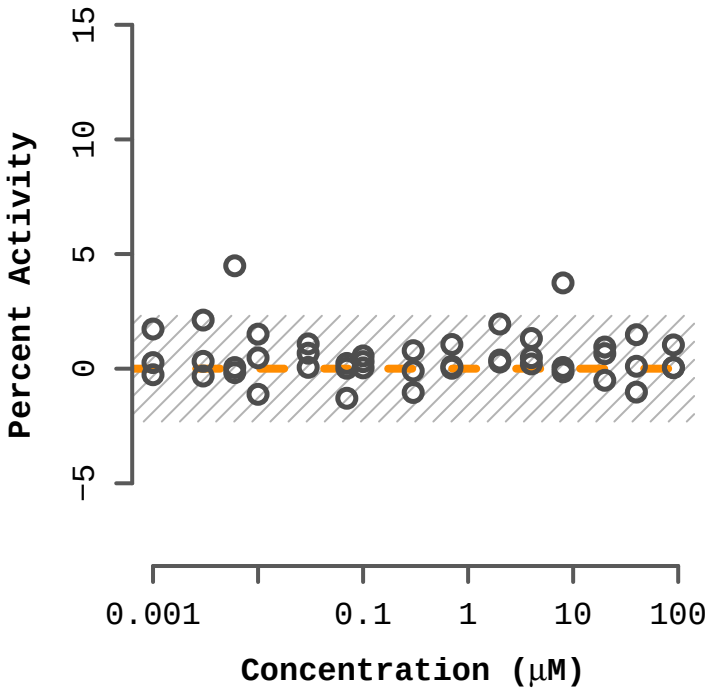
NAME: 1-Ethenylazepan-2-one
CHID: 41423 **CASRN:** 2235-00-9
SPID(S): Tox21_301124
M4ID: 12478009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

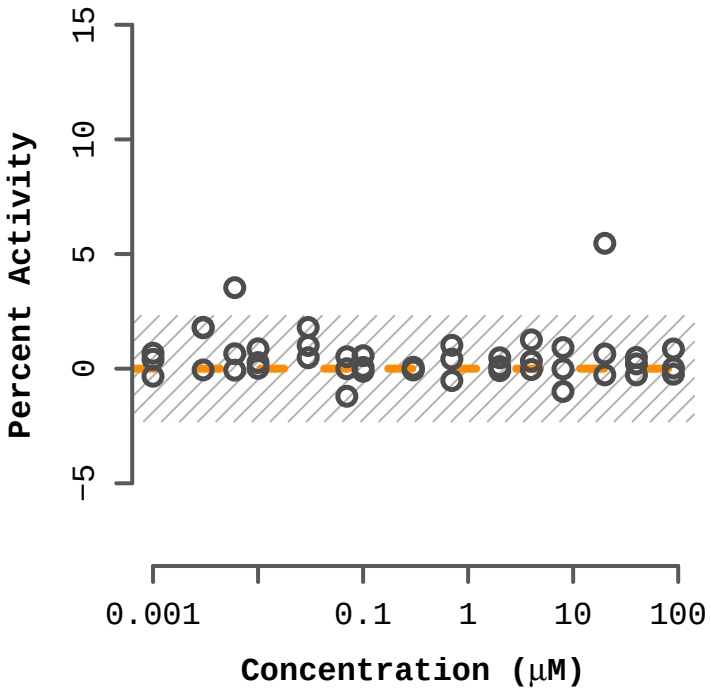
NAME: 2,6-Dimethyl-2-heptanol
CHID: 41424 **CASRN:** 13254-34-7
SPID(S): Tox21_301948
M4ID: 12477185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 0.676 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

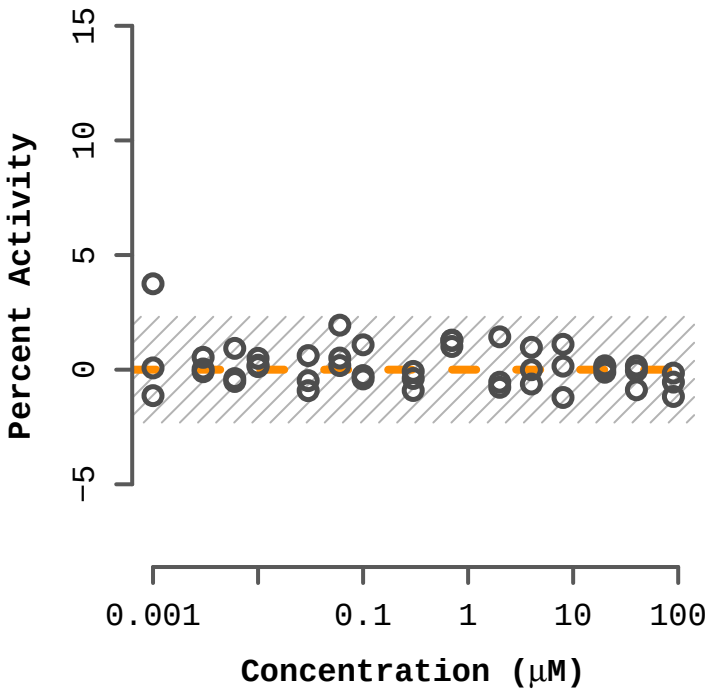
NAME: (2E)-2-Hexenal
CHID: 41425 **CASRN:** 6728-26-3
SPID(S): Tox21_303390
M4ID: 12475748

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

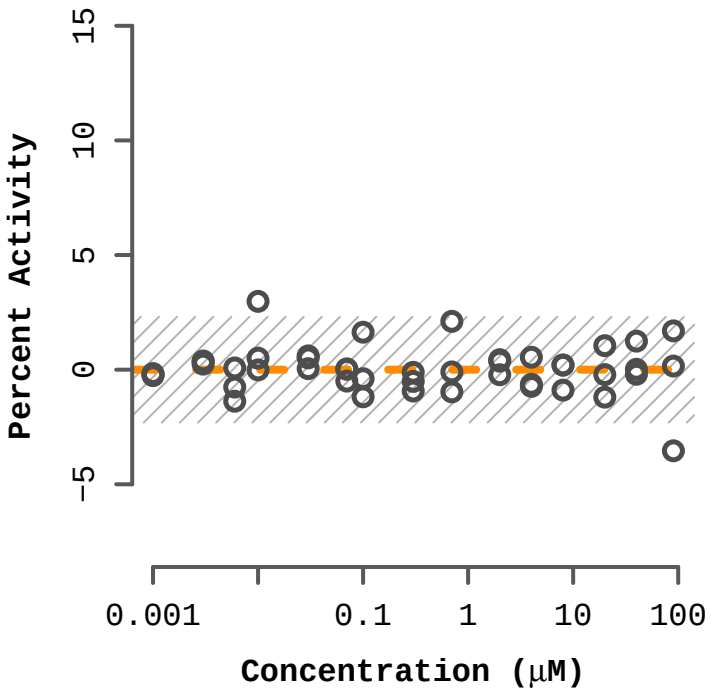
NAME: (2E)-2-Hexenal
CHID: 41425 **CASRN:** 6728-26-3
SPID(S): Tox21_201286
M4ID: 12480966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

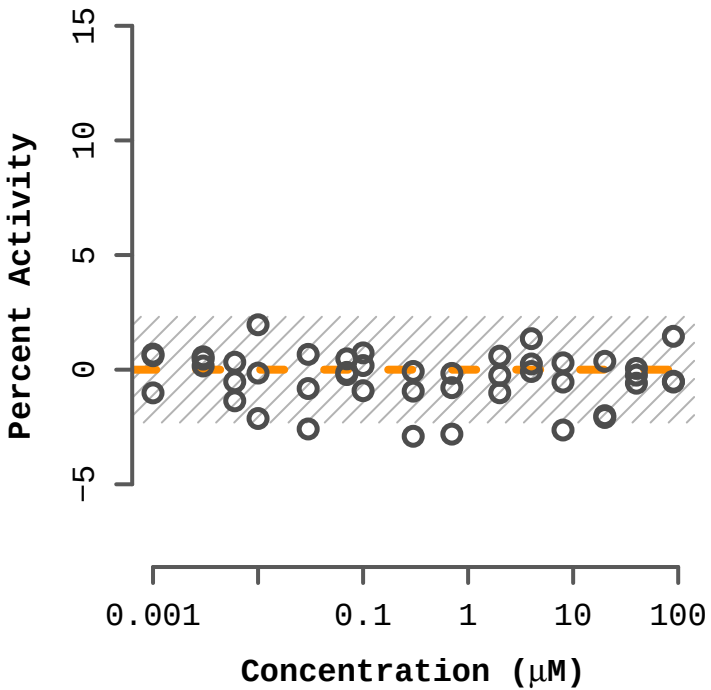
NAME: 3,4-Dihydro-2H-pyran
CHID: 41426 **CASRN:** 110-87-2
SPID(S): Tox21_301188
M4ID: 12477945

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

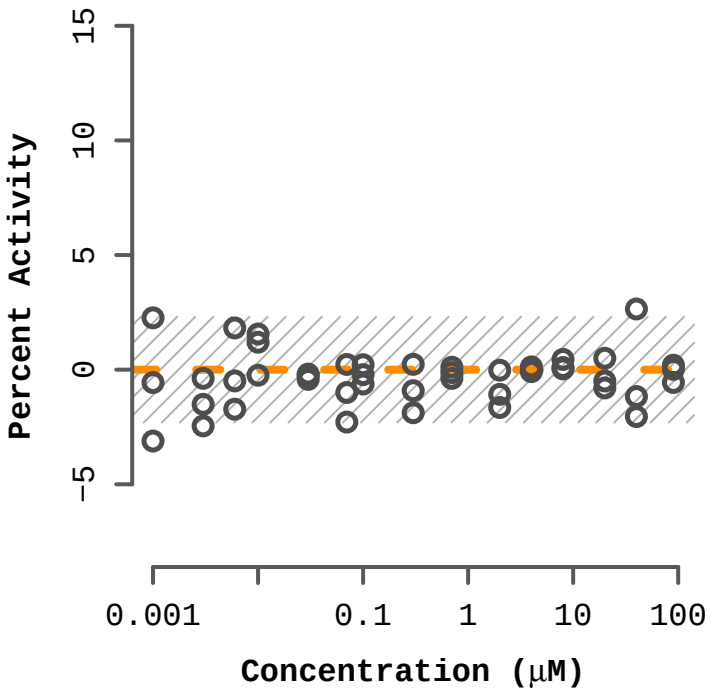
NAME: 2-Isopropoxyphenol
CHID: 41431 **CASRN:** 4812-20-8
SPID(S): Tox21_301189
M4ID: 12477944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.509 **MAX_MED:** 0.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

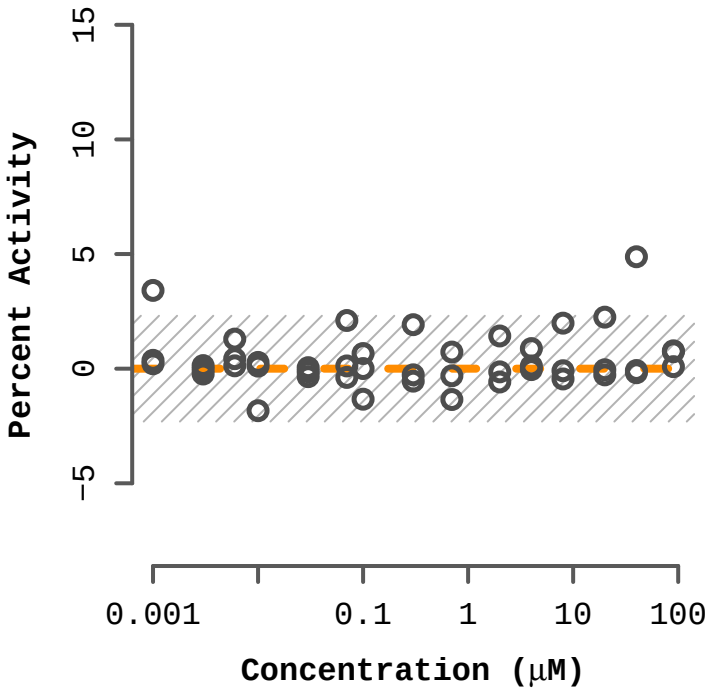
NAME: 2-Methyl-2-butanol
CHID: 41436 **CASRN:** 75-85-4
SPID(S): Tox21_302356
M4ID: 12476777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.838 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

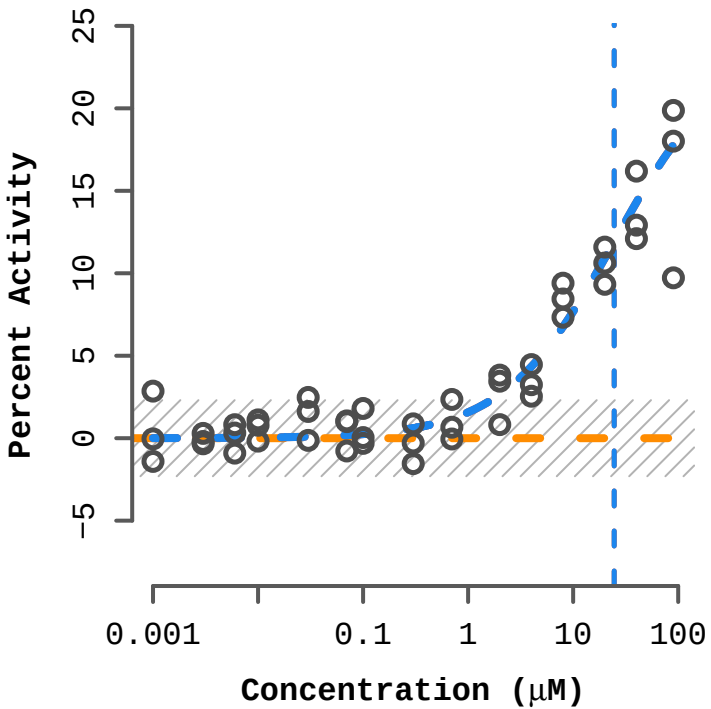
NAME: 2-Methyl-2-nitro-1,3-propanediol
CHID: 41437 **CASRN:** 77-49-6
SPID(S): Tox21_302028
M4ID: 12477105

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methylanthraquinone
CHID: 41439 CASRN: 84-54-8
SPID(S): Tox21_302044
M4ID: 12477089

HILL MODEL (in red):

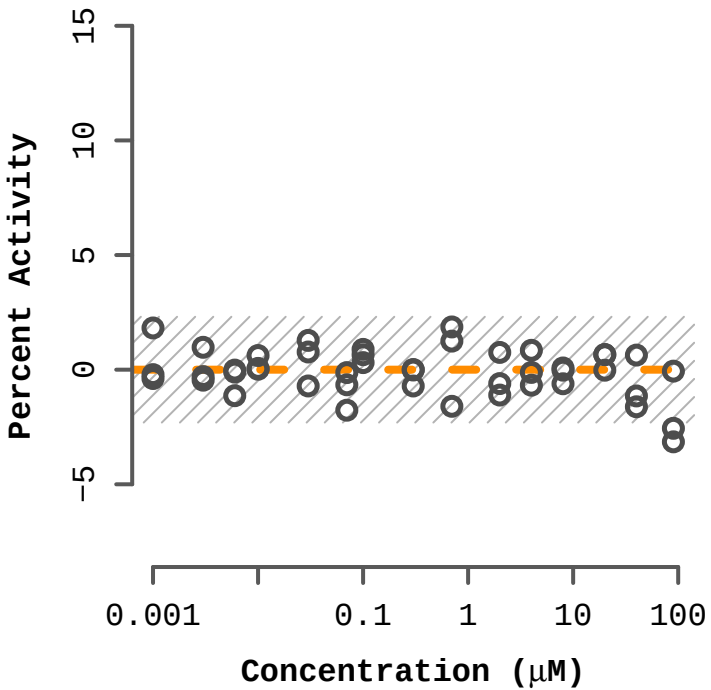
	tp	ga	gw
val:	23.9	1.39	0.828
sd:	4.93	0.251	0.147

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.9	1.39	0.828	3.23	6.85
sd:	4.92	0.251	0.147	1400	7500

	CNST	HILL	GNLS
AIC:	292.44	174.66	178.66
PROB:	0	0.88	0.12
RMSE:	6.73	1.75	1.75

MAX_MEAN: 15.9 MAX_MED: 18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

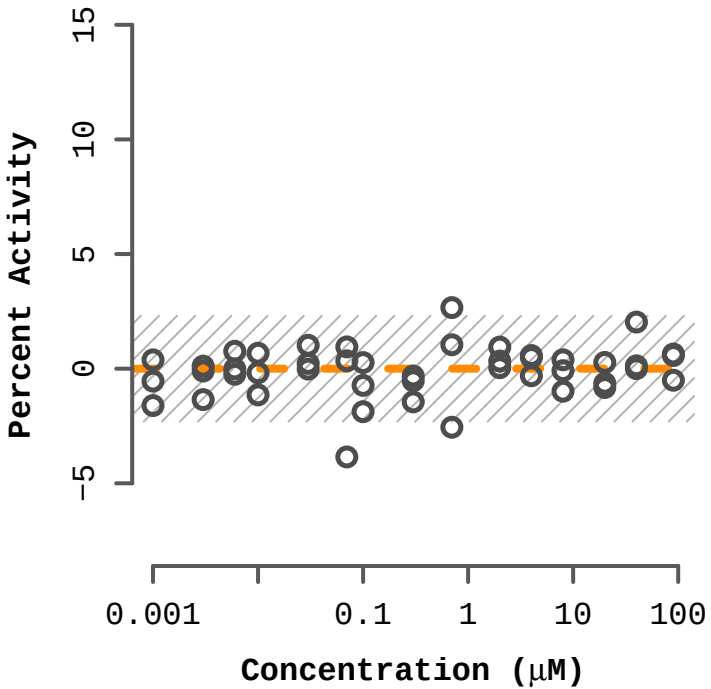
NAME: 2-Methylbutyl isovalerate
CHID: 41440 CASRN: 2445-77-4
SPID(S): Tox21_301592
M4ID: 12477541

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.617 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

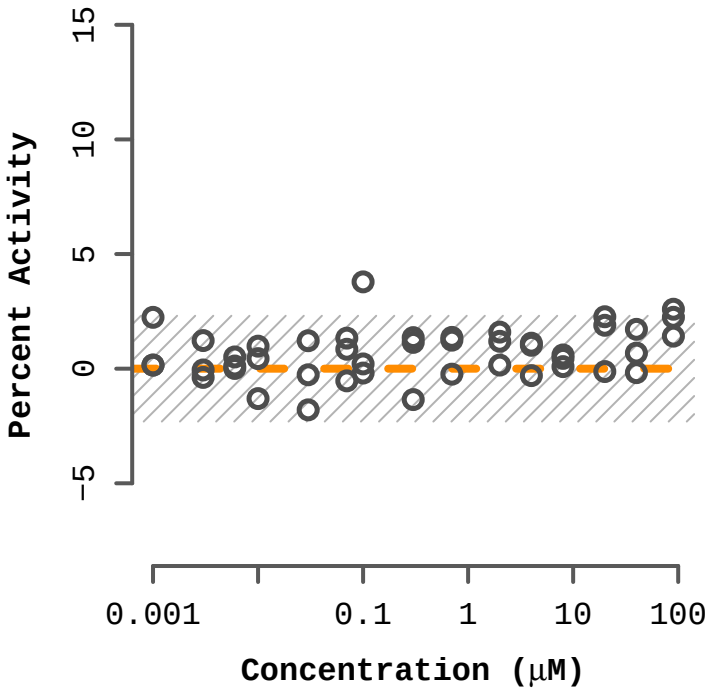
NAME: (2-Methylphenoxy)acetic acid
CHID: 41441 CASRN: 1878-49-5
SPID(S): Tox21_301121
M4ID: 12478012

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.722 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

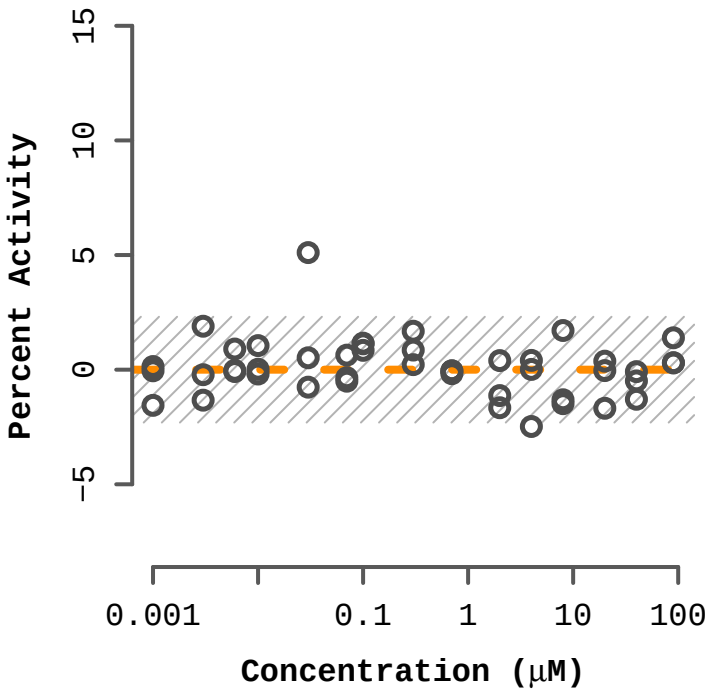
NAME: Sodium 2-naphthalenesulfonate
CHID: 41442 **CASRN:** 532-02-5
SPID(S): Tox21_301018
M4ID: 12478115

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

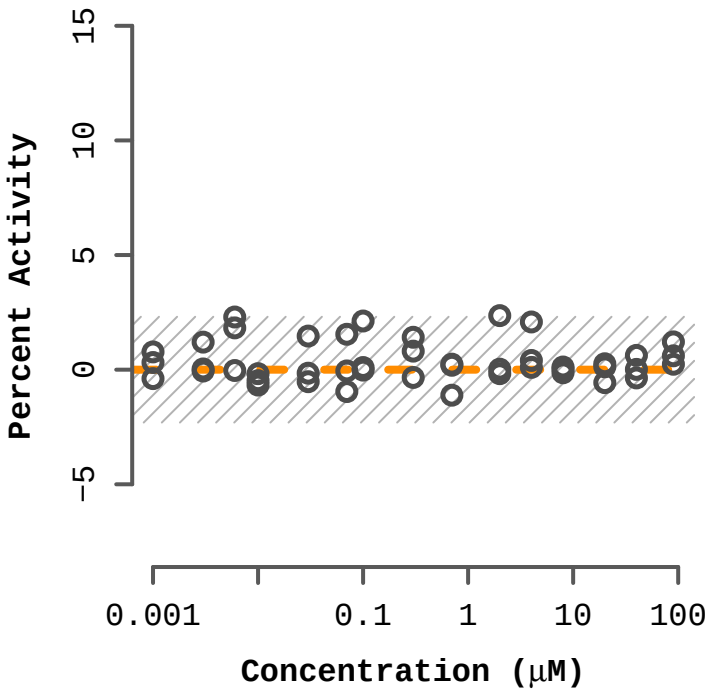
NAME: 5-Methyl-2-octanone
CHID: 41444 **CASRN:** 58654-67-4
SPID(S): Tox21_303922
M4ID: 12475266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

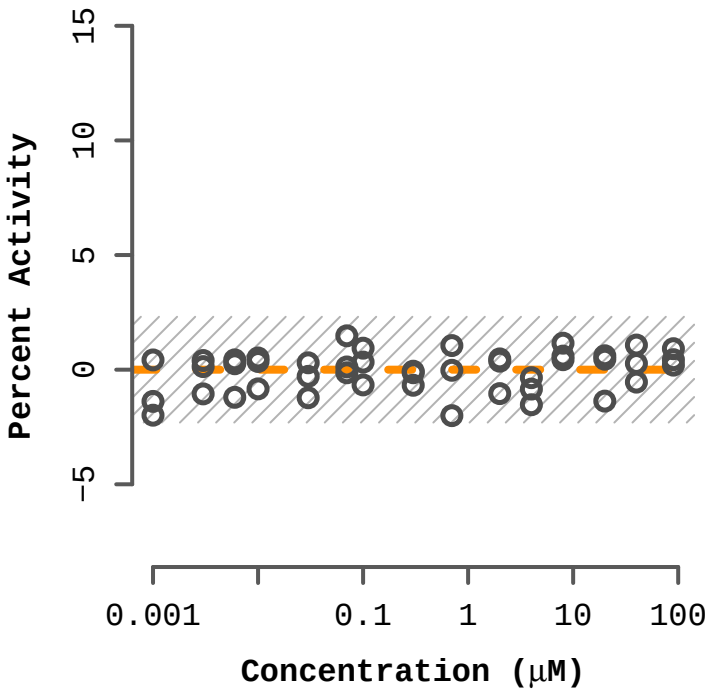
NAME: 2-Phenylcyclohexanol
CHID: 41446 **CASRN:** 1444-64-0
SPID(S): Tox21_301942
M4ID: 12477191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

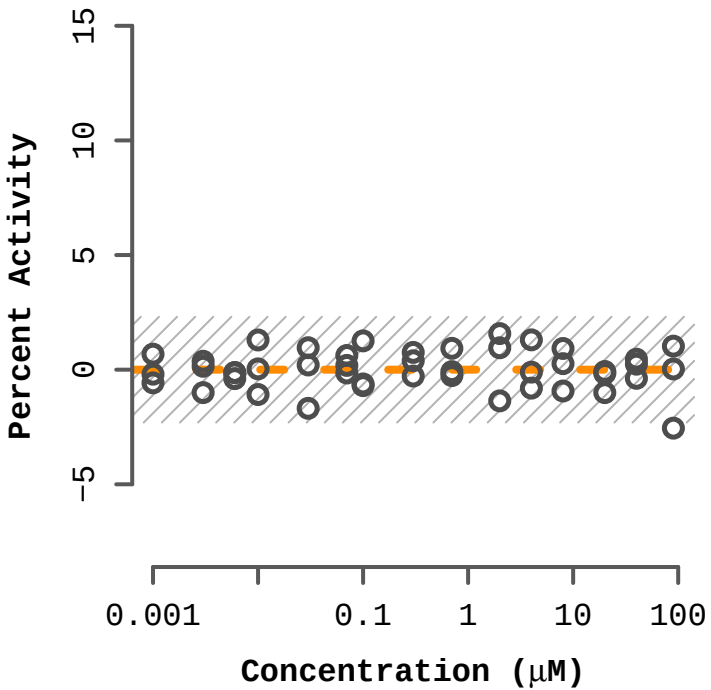
NAME: 2-Propene-1-sulfonic acid, sodium salt
CHID: 41451 **CASRN:** 2495-39-8
SPID(S): Tox21_301805
M4ID: 12477328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.729 **MAX_MED:** 0.593 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

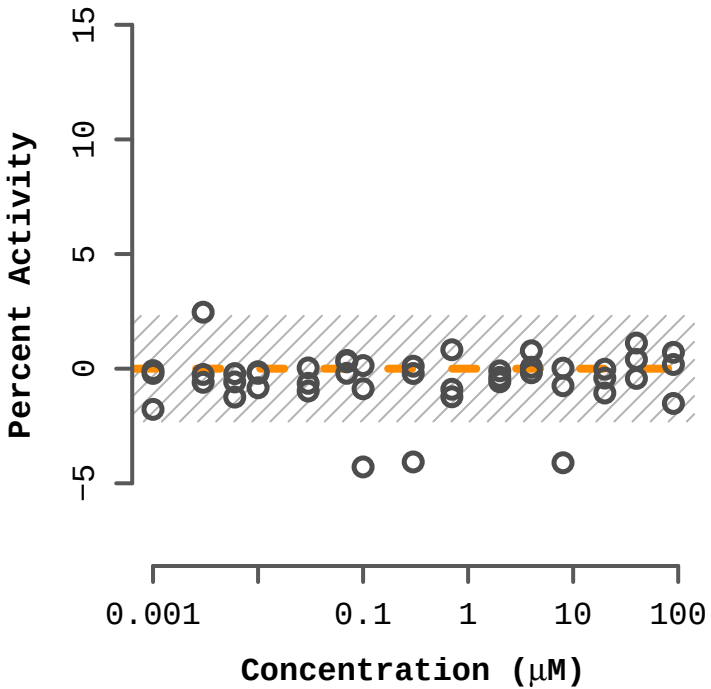
NAME: 2-(1-Methylbutyl)phenol
CHID: 41452 **CASRN:** 87-26-3
SPID(S): Tox21_301939
M4ID: 12477194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.391 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

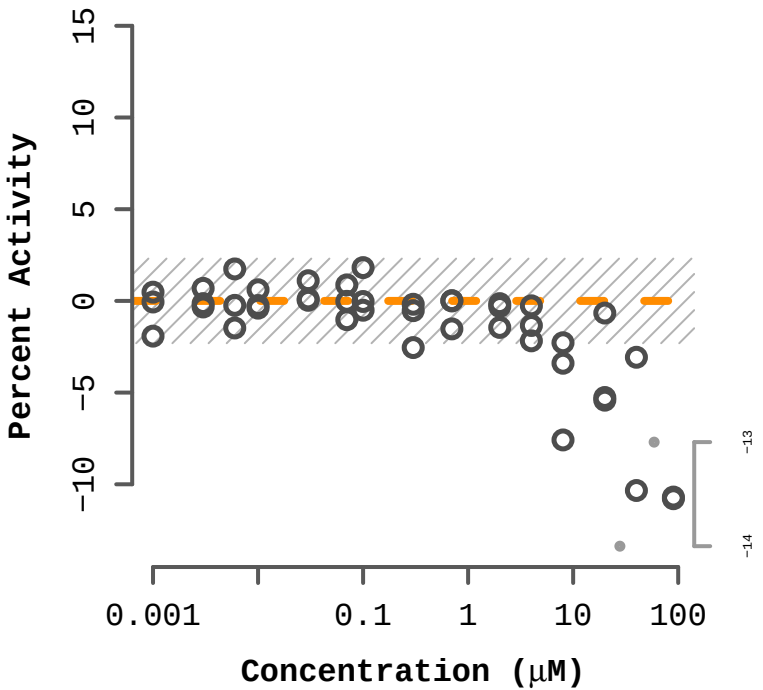
NAME: 3-(Trifluoromethyl)benzoic acid
CHID: 41460 **CASRN:** 454-92-2
SPID(S): Tox21_300654
M4ID: 12478479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.541 **MAX_MED:** 0.404 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

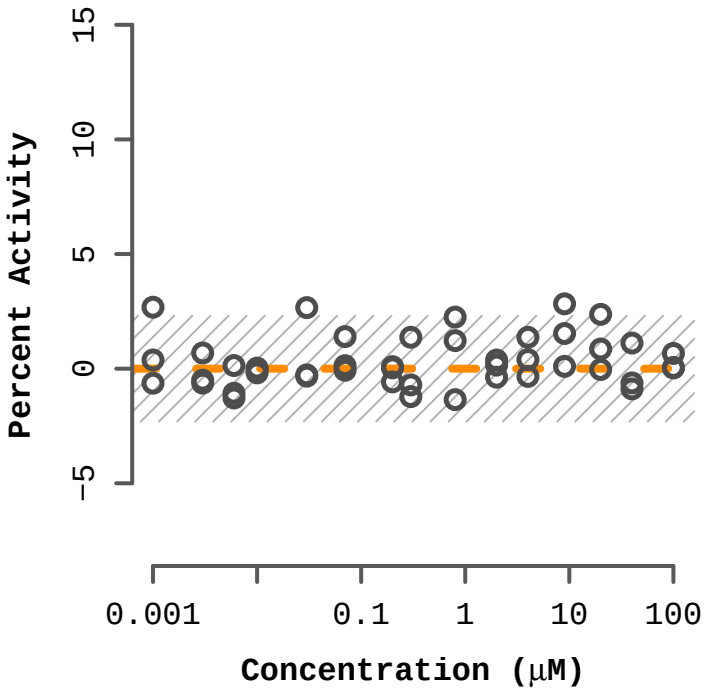
NAME: 3,3,4,4−Tetrachlorotetrahydrothiophene 1,1−dio
CHID: 41461 CASRN: 3737−41−5
SPID(S): Tox21_302200
M4ID: 12476933 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	243.76	NA	NA
PROB:	1	NA	NA
RMSE:	4.47	NA	NA

MAX_MEAN: 0.427 MAX_MED: 0.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

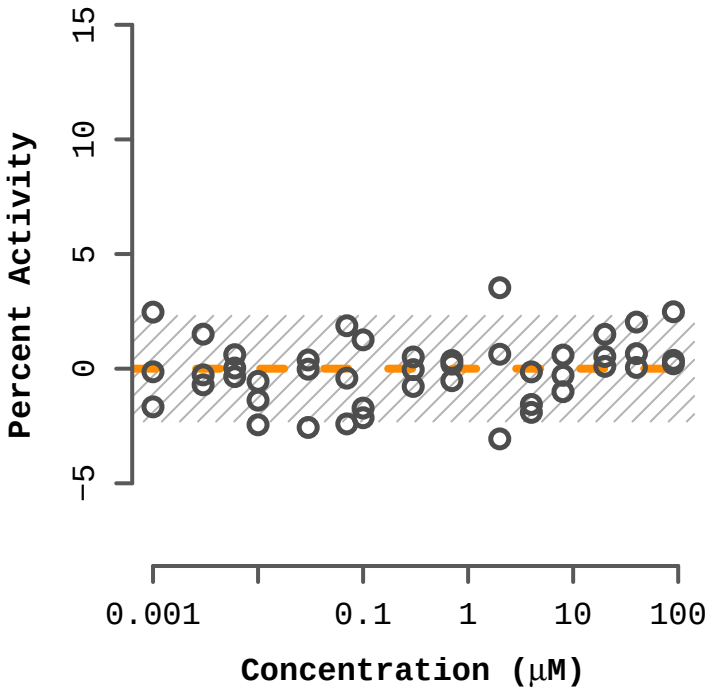
NAME: 3,3'−Iminobispropanenitrile
CHID: 41464 **CASRN:** 111−94−4
SPID(S): Tox21_300770
M4ID: 12478363

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

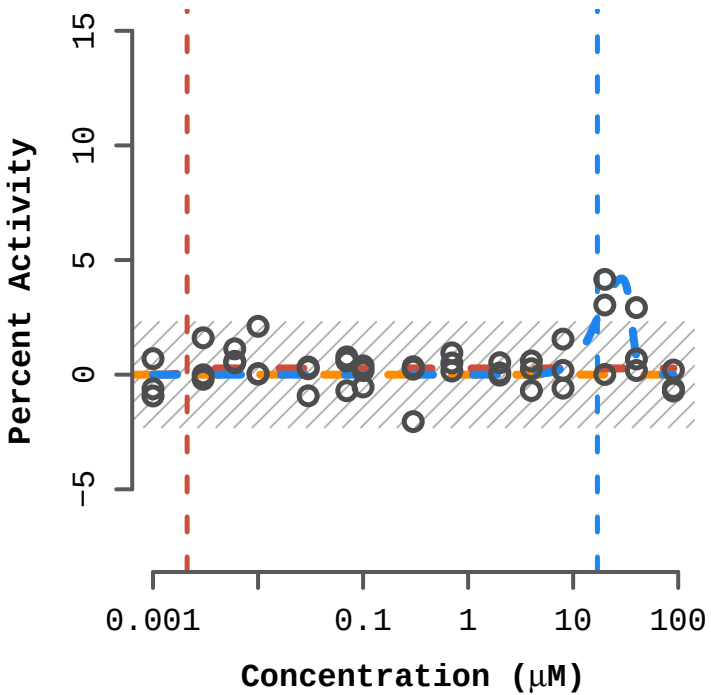
NAME: 3,4-Dichloro-5-isothiazolecarboxylic acid
CHID: 41467 **CASRN:** 18480-53-0
SPID(S): Tox21_300870
M4ID: 12478263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,4−Dichlorophenylurea
CHID: 41468 CASRN: 2327−02−8
SPID(S): Tox21_302258
M4ID: 12476875

HILL MODEL (in red):

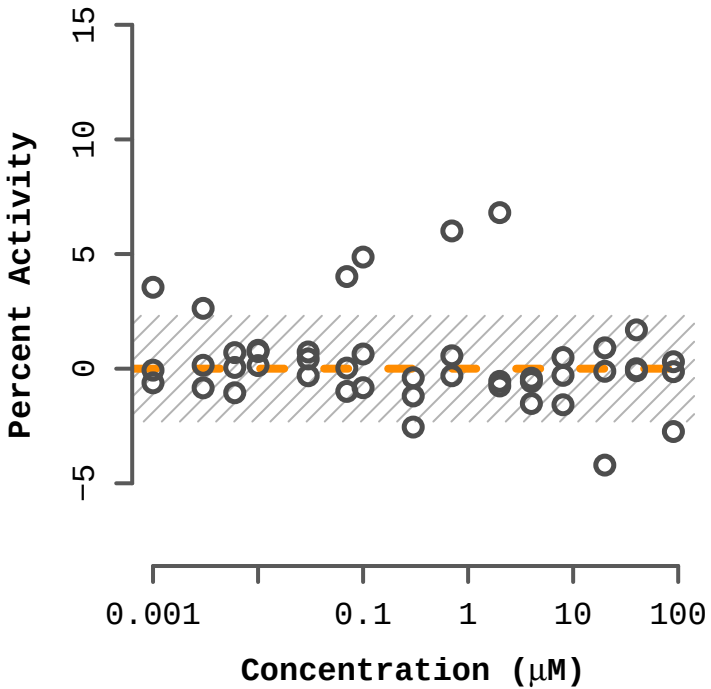
	tp	ga	gw
val:	0.273	−2.68	8
sd:	0.123	1	31.3

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.94	1.23	3.71	1.56	15.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	131.04	132.18	129.1
PROB:	0.24	0.13	0.63
RMSE:	1.15	1.08	0.94

MAX_MEAN: 2.4 MAX_MED: 3.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

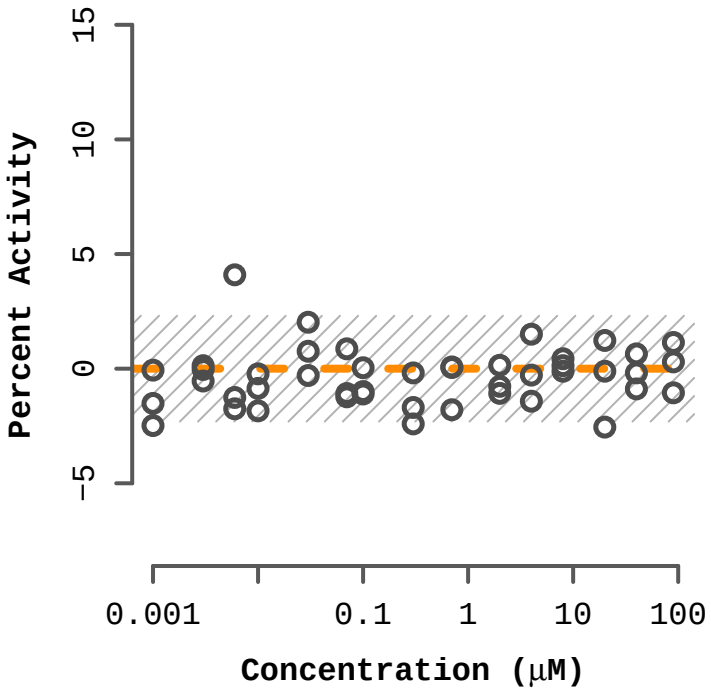
NAME: 3,5-Dimethyl-1-hexyn-3-ol
CHID: 41472 **CASRN:** 107-54-0
SPID(S): Tox21_301138
M4ID: 12477995

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 0.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

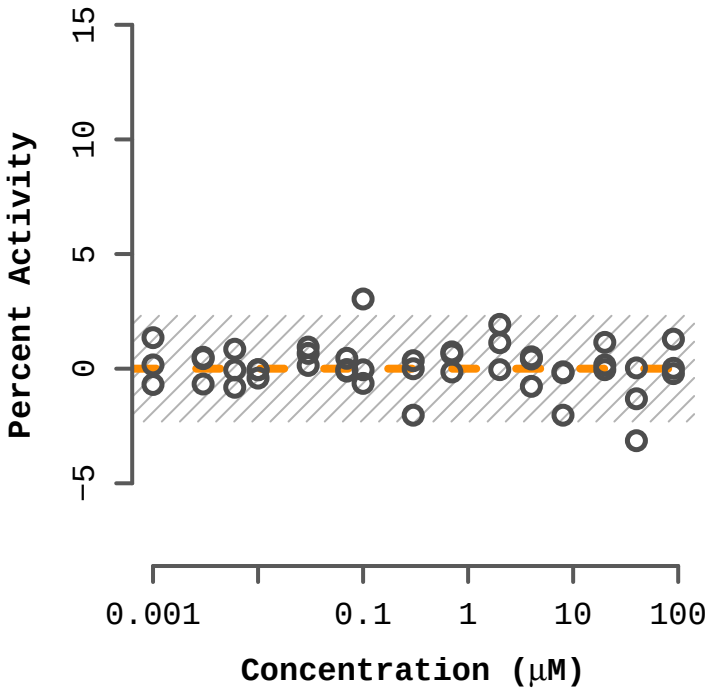
NAME: (3Z)-3-Hexenyl acetate
CHID: 41484 **CASRN:** 3681-71-8
SPID(S): Tox21_302290
M4ID: 12476843

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.831 **MAX_MED:** 0.761 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

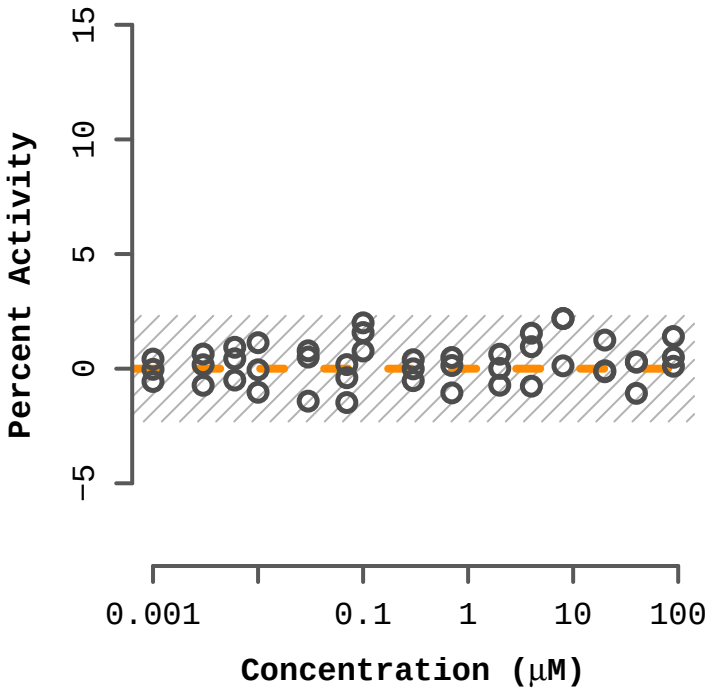
NAME: 3,7-Dimethyloctan-3-yl acetate
CHID: 41487 **CASRN:** 20780-48-7
SPID(S): Tox21_301933
M4ID: 12477200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

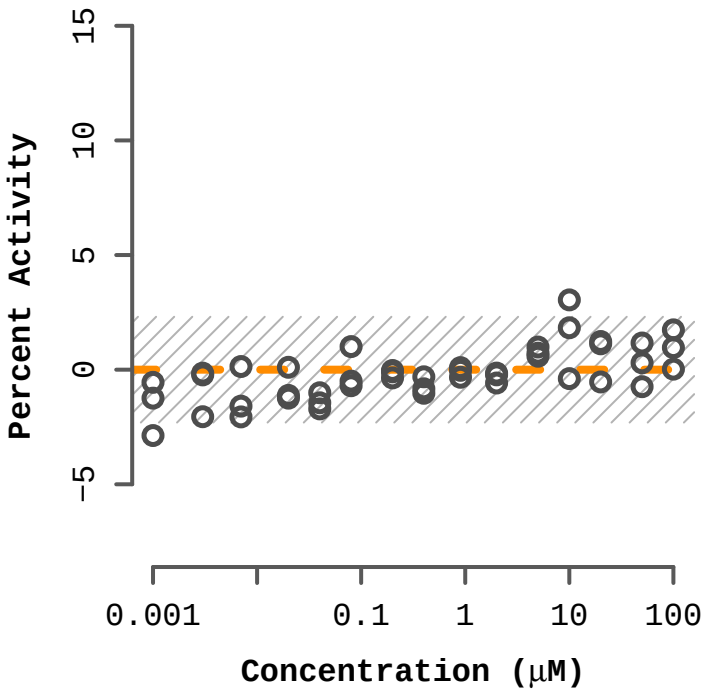
NAME: 3-Methyl-3-penten-2-one
CHID: 41490 **CASRN:** 565-62-8
SPID(S): Tox21_302357
M4ID: 12476776

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

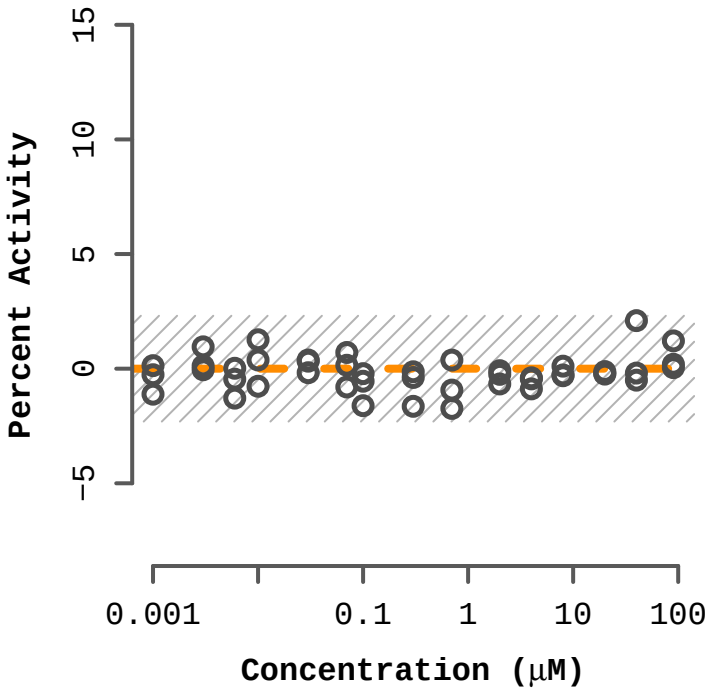
NAME: 3-Phenyl-2-propen-1-ol
CHID: 41491 **CASRN:** 104-54-1
SPID(S): Tox21_300847
M4ID: 12478286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

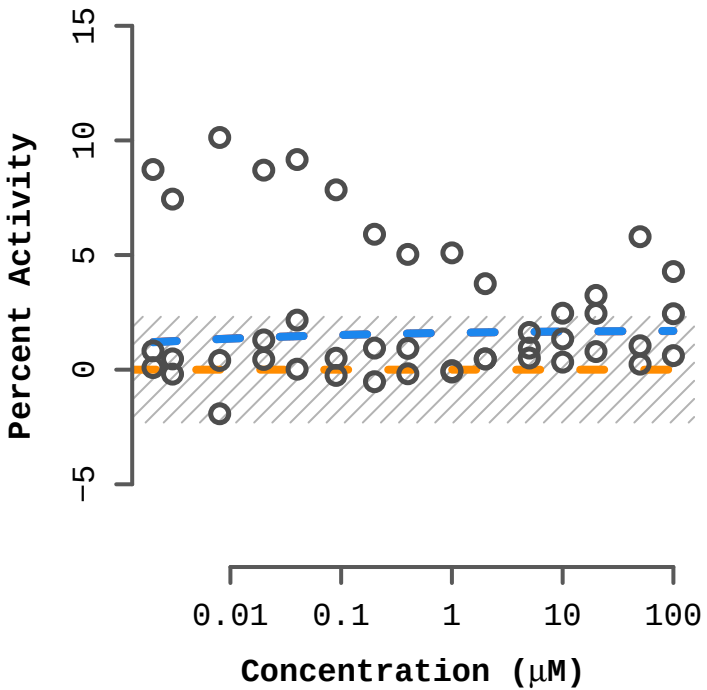
NAME: 3-Phenylhexane
CHID: 41492 **CASRN:** 4468-42-2
SPID(S): Tox21_301226
M4ID: 12477907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.485 **MAX_MED:** 0.381 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diflufenican
CHID: 41494 CASRN: 83164-33-4
SPID(S): Tox21_300818
M4ID: 12478315

HILL MODEL (in red):

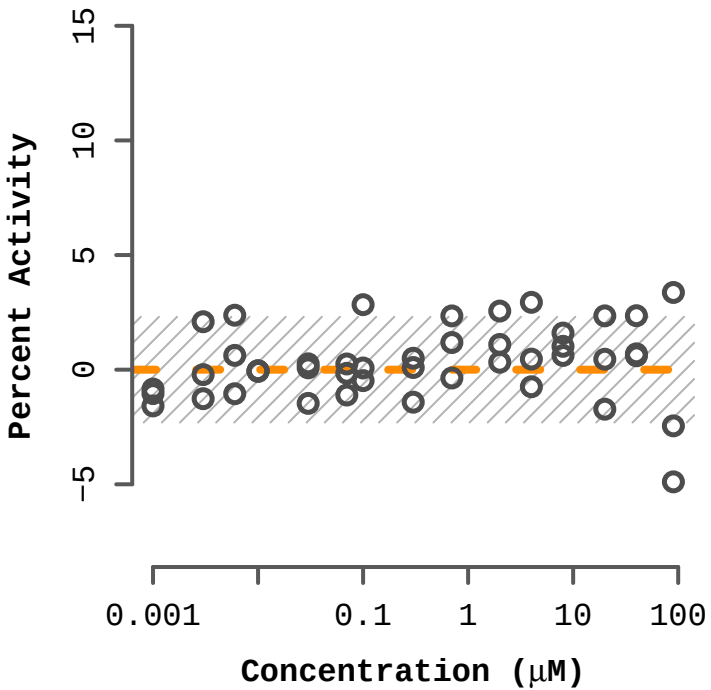
	tp	ga	gw
val:	1.71	−3.95	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.72	−3.89	0.3	3.04	7.76
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	244.14	233.07	237.07
PROB:	0	0.88	0.12
RMSE:	3.83	3.16	3.16

MAX_MEAN: 3.78 **MAX_MED:** 2.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

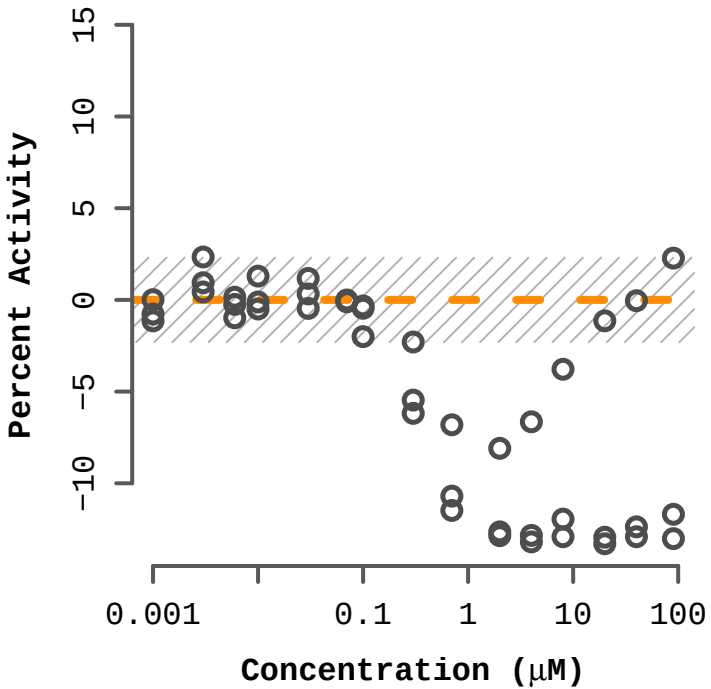
NAME: 4,6-Di-tert-butyl-m-cresol
CHID: 41502 **CASRN:** 497-39-2
SPID(S): Tox21_301524
M4ID: 12477609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

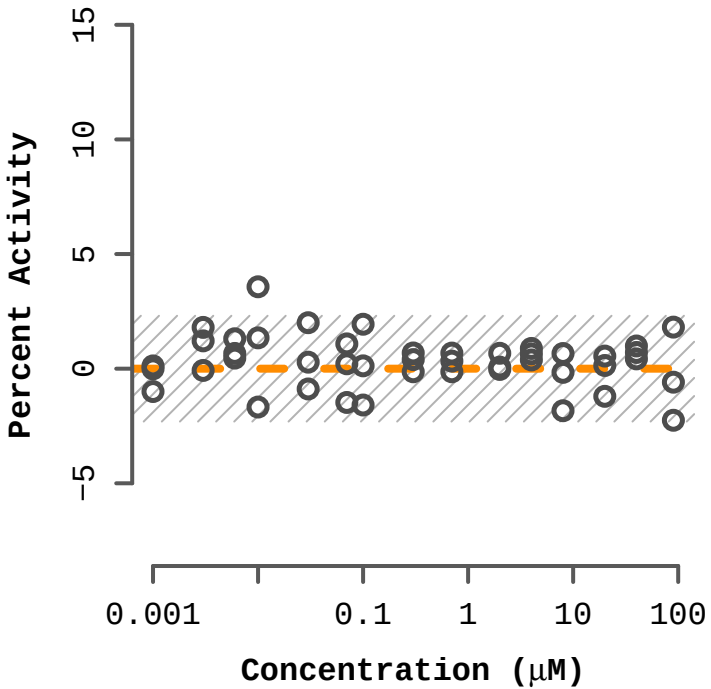
NAME: Tralopyril
CHID: 41503 **CASRN:** 122454-29-9
SPID(S): Tox21_303769
M4ID: 12475419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	311.04	NA	NA
PROB:	1	NA	NA
RMSE:	7.39	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

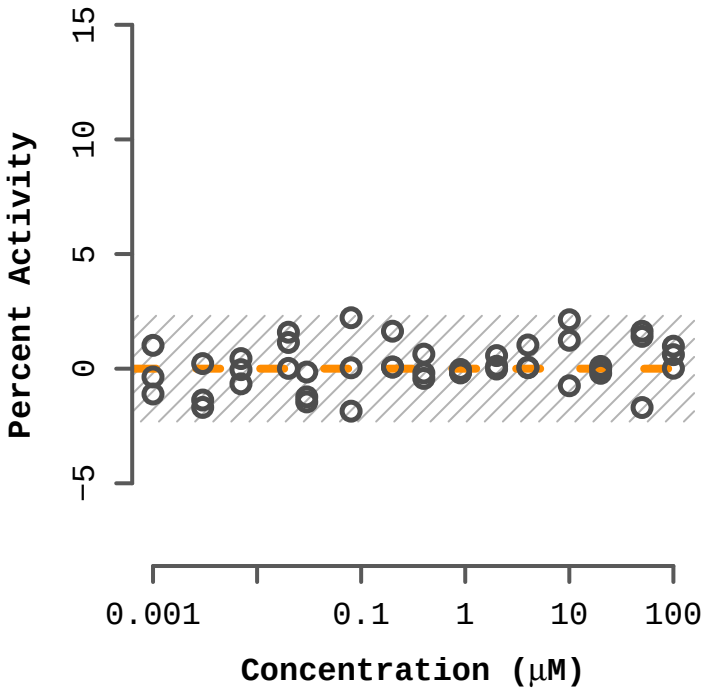
NAME: 4-Chloro-2-cyclopentylphenol
CHID: 41506 **CASRN:** 13347-42-7
SPID(S): Tox21_301228
M4ID: 12477905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

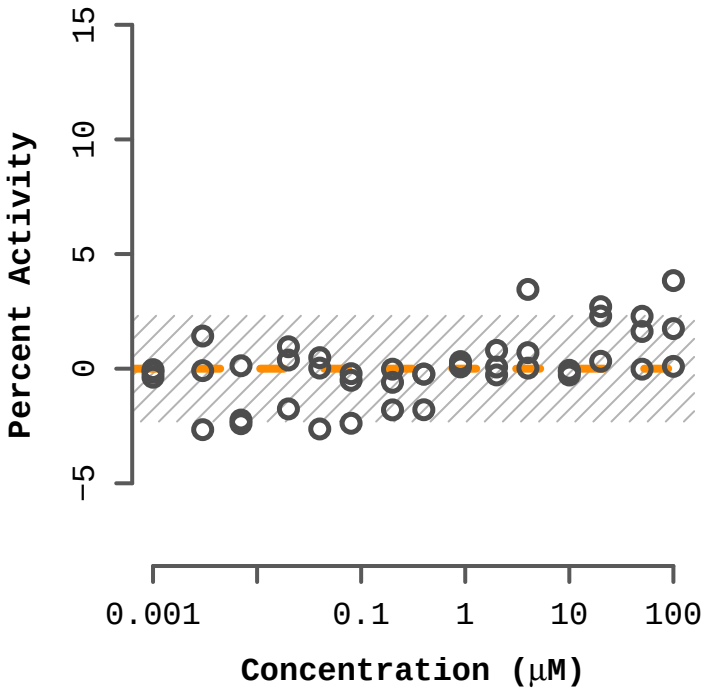
NAME: 4-Chloro-2-methylanisole
CHID: 41507 **CASRN:** 3260-85-3
SPID(S): Tox21_300717
M4ID: 12478416

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.917 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

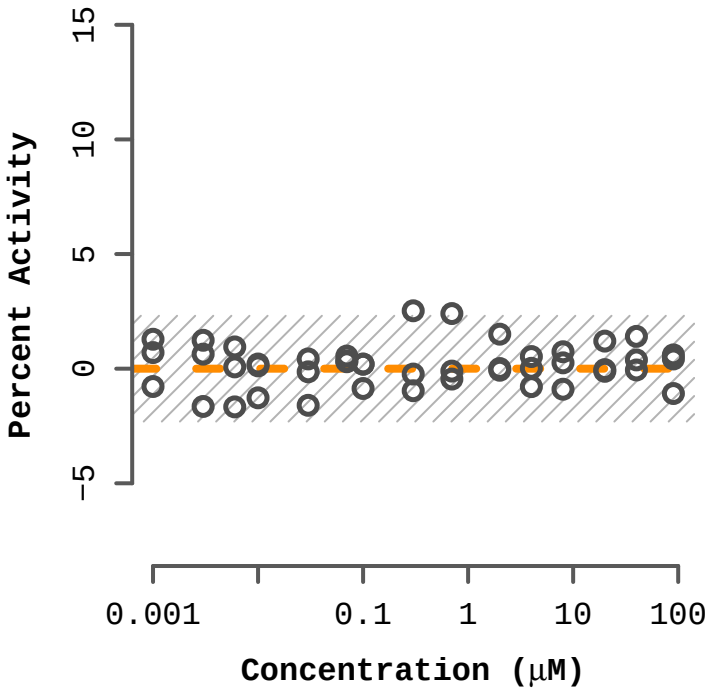
NAME: 4-Chloro-2-methylaniline
CHID: 41508 **CASRN:** 95-69-2
SPID(S): Tox21_300857
M4ID: 12478276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

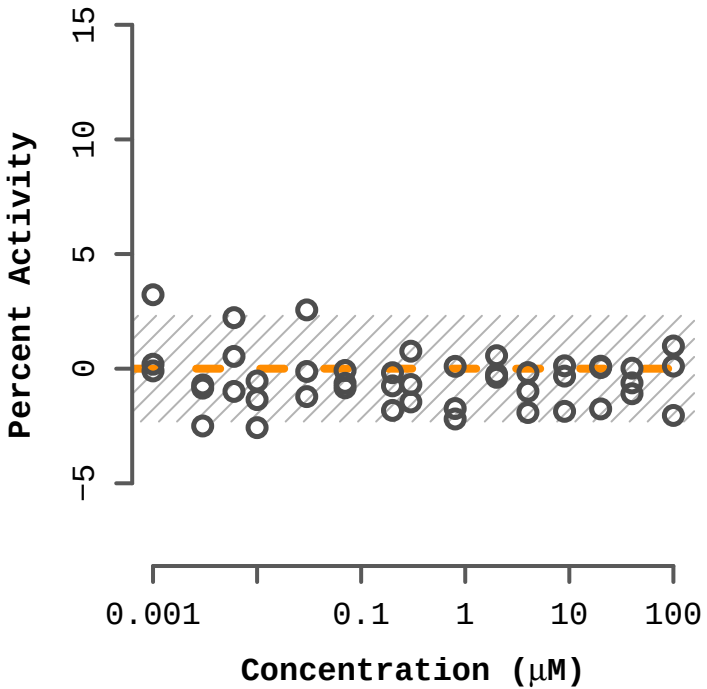
NAME: 4-Chlorophenylurea
CHID: 41512 CASRN: 140-38-5
SPID(S): Tox21_300837
M4ID: 12478296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.616 MAX_MED: 0.705 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

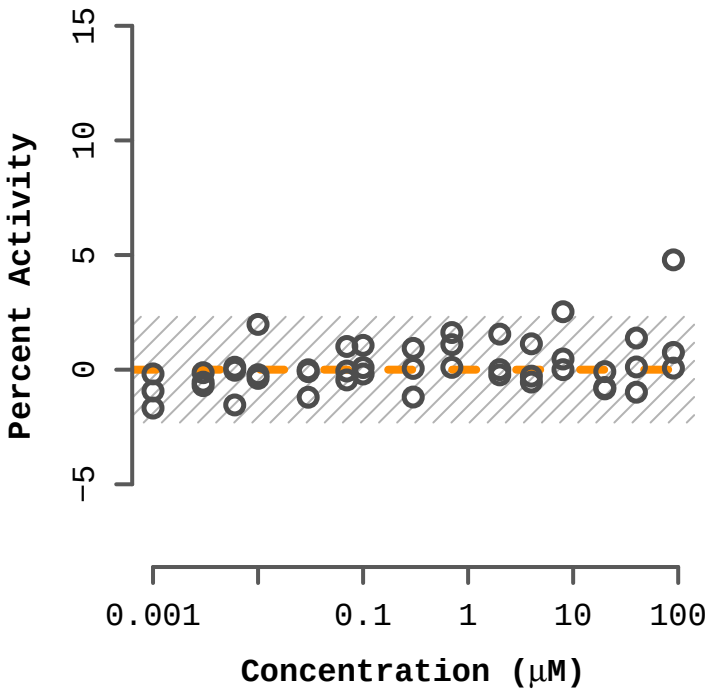
NAME: 4-Chloropyridine 1-oxide
CHID: 41513 **CASRN:** 1121-76-2
SPID(S): Tox21_300883
M4ID: 12478250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.537 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

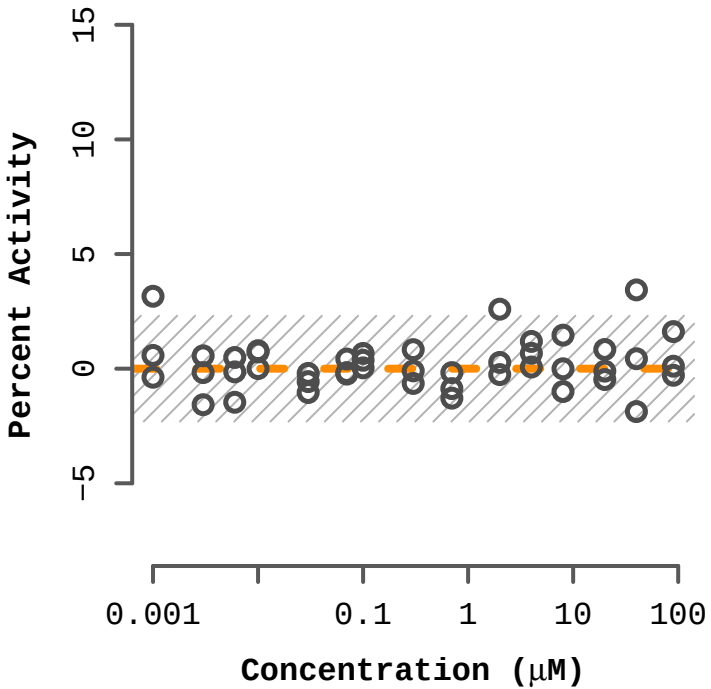
NAME: (4Z)-4-Decenal
CHID: 41514 CASRN: 21662-09-9
SPID(S): Tox21_300829
M4ID: 12478304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.87 MAX_MED: 1.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

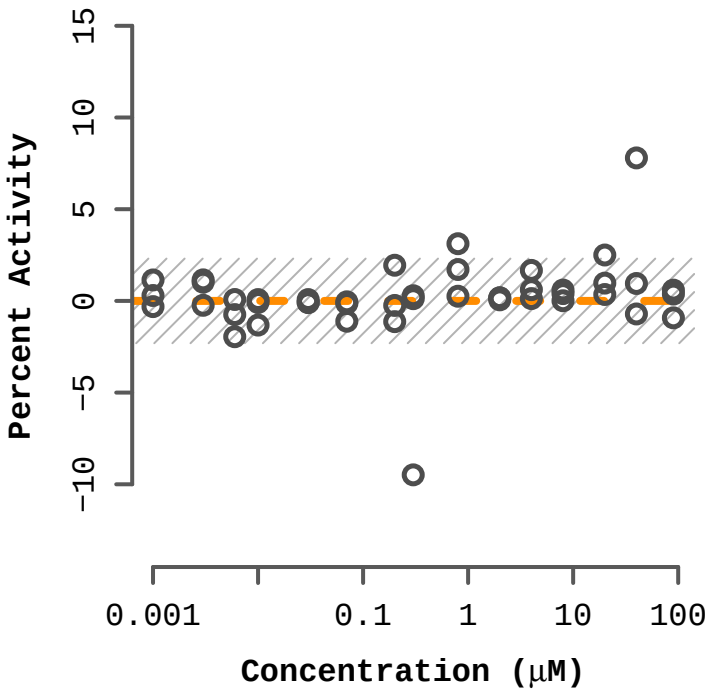
NAME: 2-Ethyl-3-hydroxy-4H-pyran-4-one
CHID: 41516 **CASRN:** 4940-11-8
SPID(S): Tox21_300800
M4ID: 12478333

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

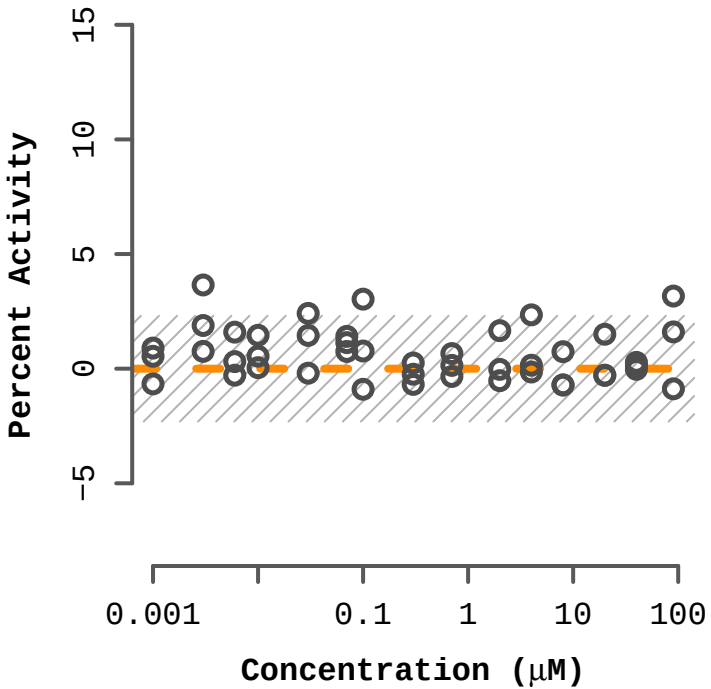
NAME: 4-Hydroxy-2,5-dimethyl-3(2H)furanone
CHID: 41517 CASRN: 3658-77-3
SPID(S): Tox21_300823
M4ID: 12478310

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 2.68 MAX_MED: 1.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

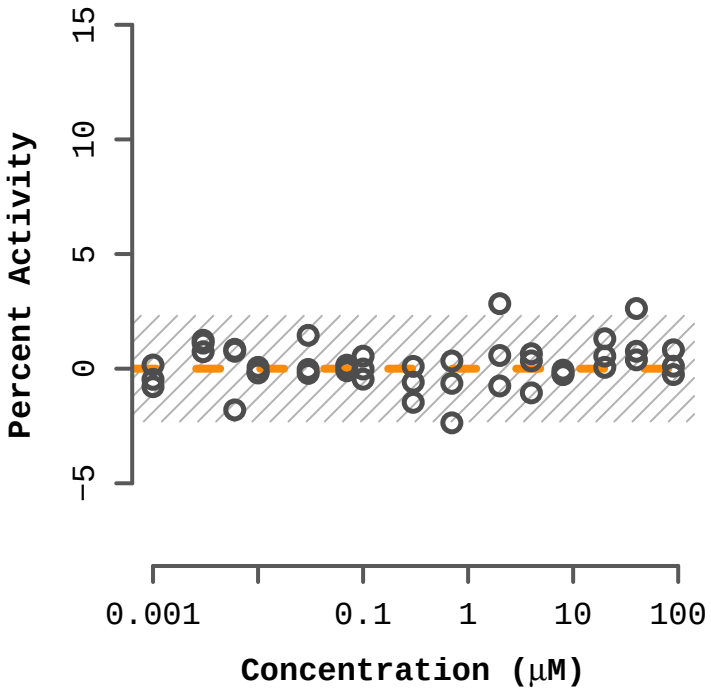
NAME: 4-Methoxybenzeneethanol
CHID: 41518 **CASRN:** 702-23-8
SPID(S): Tox21_300755
M4ID: 12478378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

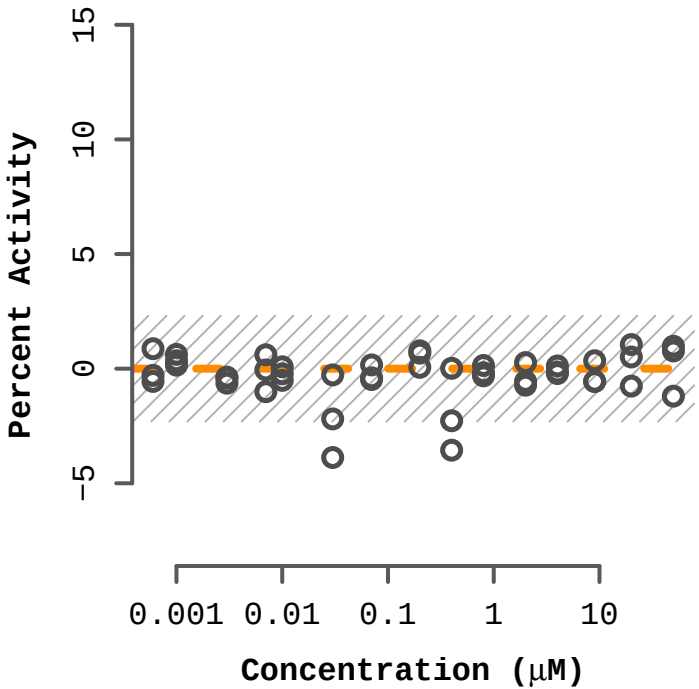
NAME: 4-Methyl-3-heptanol
CHID: 41519 **CASRN:** 14979-39-6
SPID(S): Tox21_300692
M4ID: 12478441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

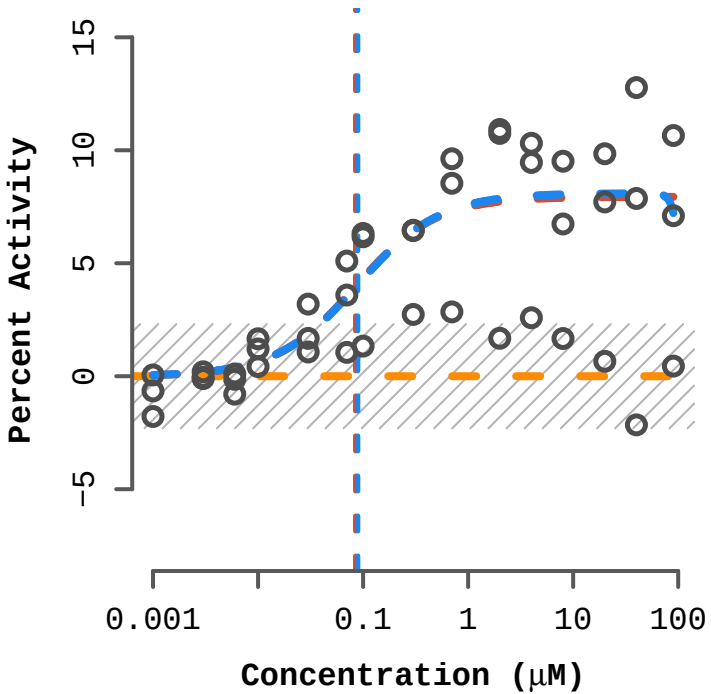
NAME: 4-Methylbenzaldehyde
CHID: 41520 **CASRN:** 104-87-0
SPID(S): Tox21_304012
M4ID: 12475176

HILL MODEL: Not applicable.

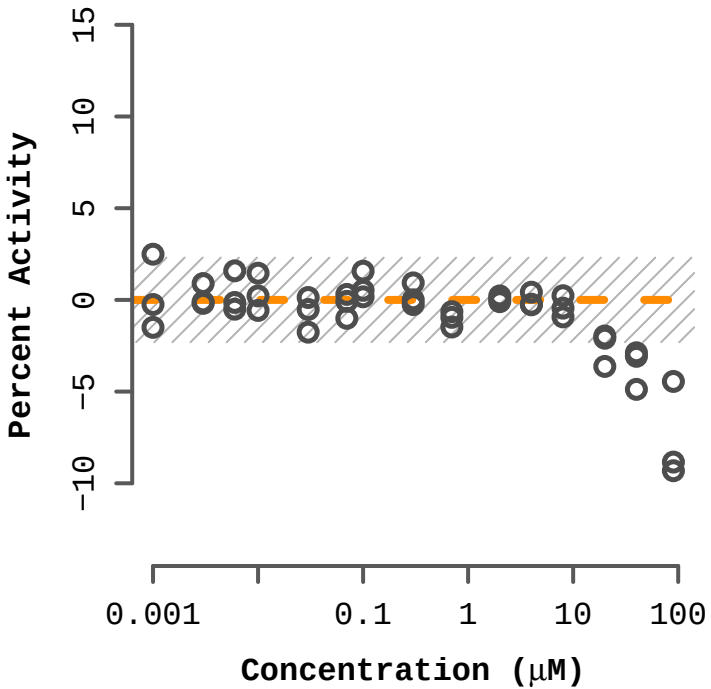
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.507 **MAX_MED:** 0.774 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Morpholinepropanamine
CHID:    41521   CASRN: 123-00-2
SPID(S): Tox21_302076
M4ID:    12477057

HILL MODEL (in red):
      tp       ga       gw
val:  7.94     -1.07    1.14
sd:   0.833    0.195    0.411

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.1      -1.05    1.11     2.04     10.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  290.92      234.42      238.25
PROB: 0           0.87        0.13
RMSE: 5.84        3.18        3.18

MAX_MEAN: 7.78      MAX_MED: 10.7      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

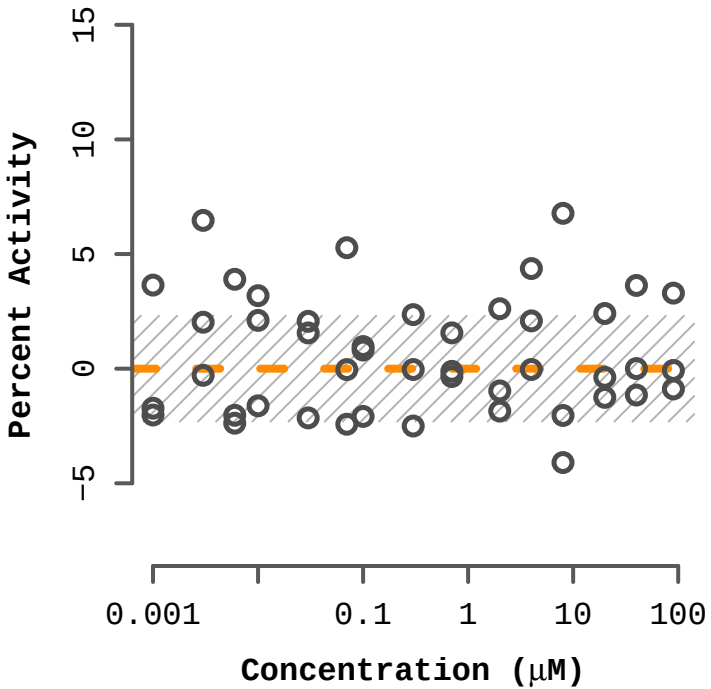
NAME: 4-Nitropyridine-1-oxide
CHID: 41524 **CASRN:** 1124-33-0
SPID(S): Tox21_300690
M4ID: 12478443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.96	NA	NA
PROB:	1	NA	NA
RMSE:	2.47	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

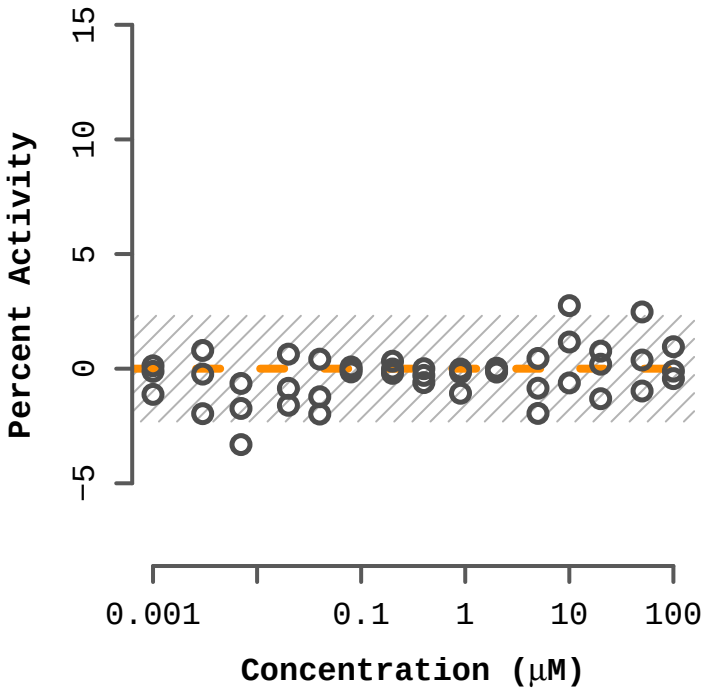
NAME: 2,2,6,6-Tetramethyl-4-piperidone
CHID: 41527 **CASRN:** 826-36-8
SPID(S): Tox21_300816
M4ID: 12478317

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 2.74 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

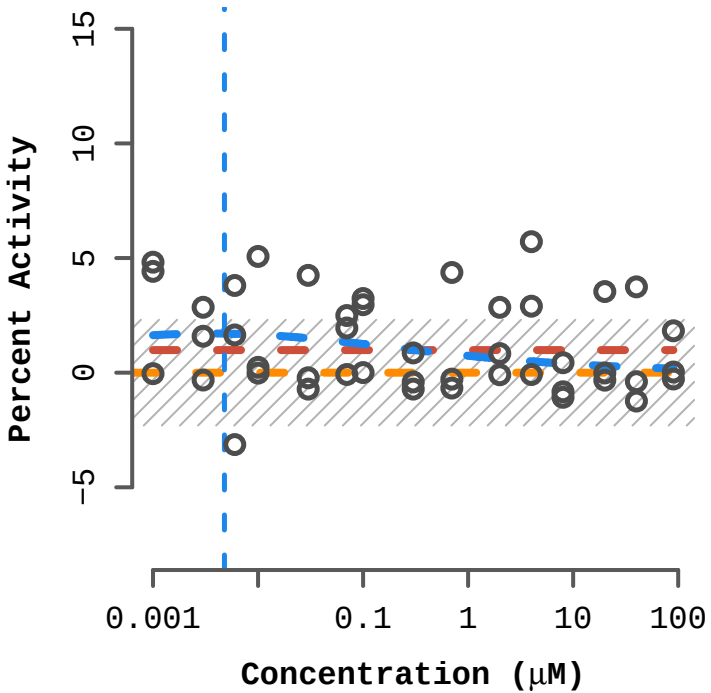
NAME: 4-Pyridinecarbonitrile
CHID: 41528 **CASRN:** 100-48-1
SPID(S): Tox21_300741
M4ID: 12478392

HILL MODEL: Not applicable.

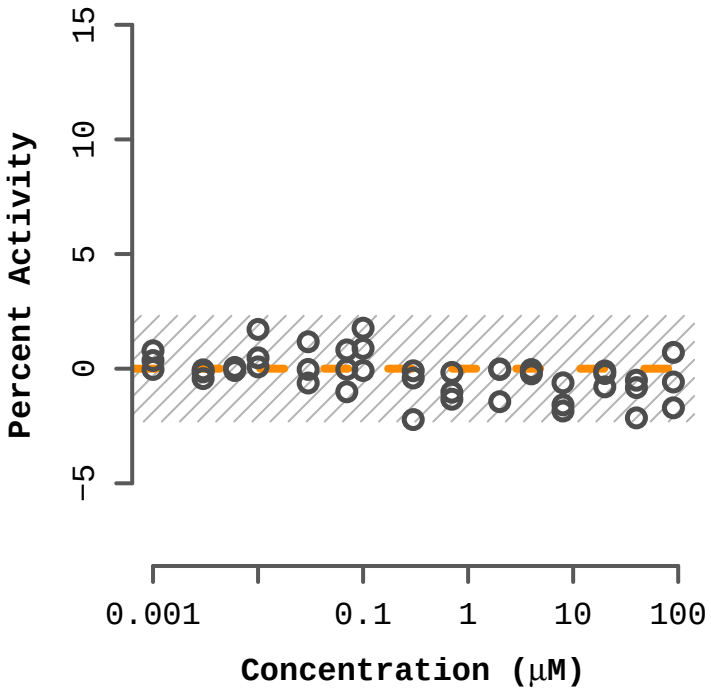
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.16 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4'-Sulfamylacetanilide
CHID:    41529   CASRN: 121-61-9
SPID(S): Tox21_300850
M4ID:    12478283

HILL MODEL (in red):
      tp       ga       gw
val:  0.985    -4.14    6.68
sd:   0.332    1220     7170

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.15     -2.32    0.3      -2.07    0.374
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  208.98      205.66      207.55
PROB: 0.12        0.63        0.25
RMSE: 2.4         2.07        2.06

MAX_MEAN: 3.07      MAX_MED: 4.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

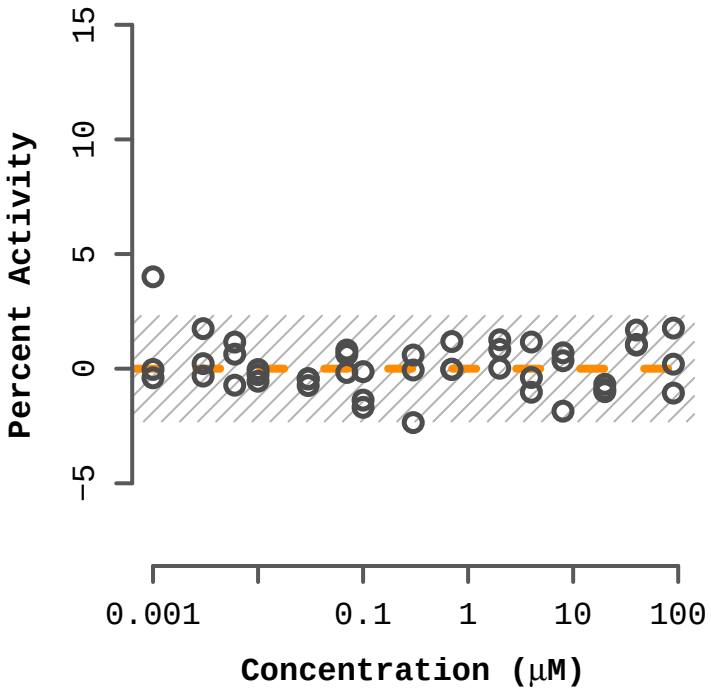
NAME: 7-Ethyl-2-methyl-4-undecanolsulfate, sodium sa
CHID: 41530 **CASRN:** 139-88-8
SPID(S): Tox21_301555
M4ID: 12477578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 0.885 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

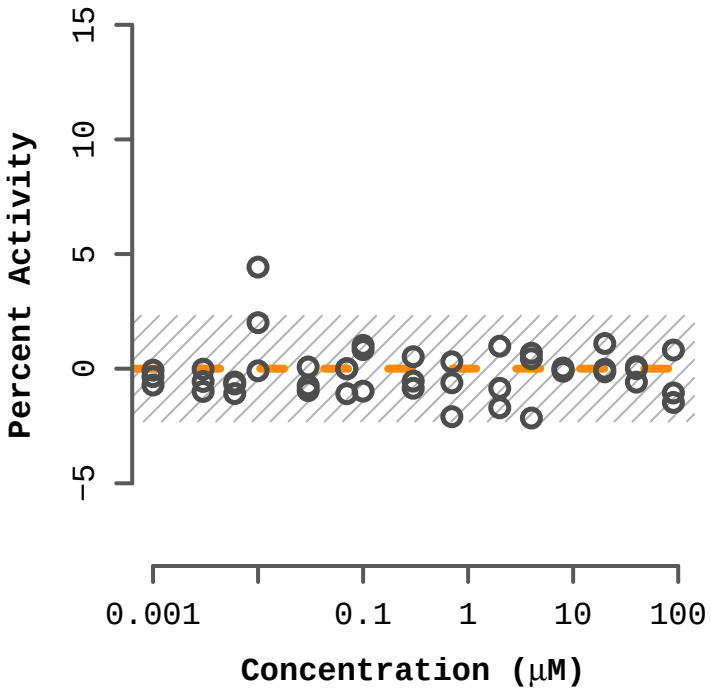
NAME: 5-Nitroisophthalic acid
CHID: 41540 **CASRN:** 618-88-2
SPID(S): Tox21_300768
M4ID: 12478365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

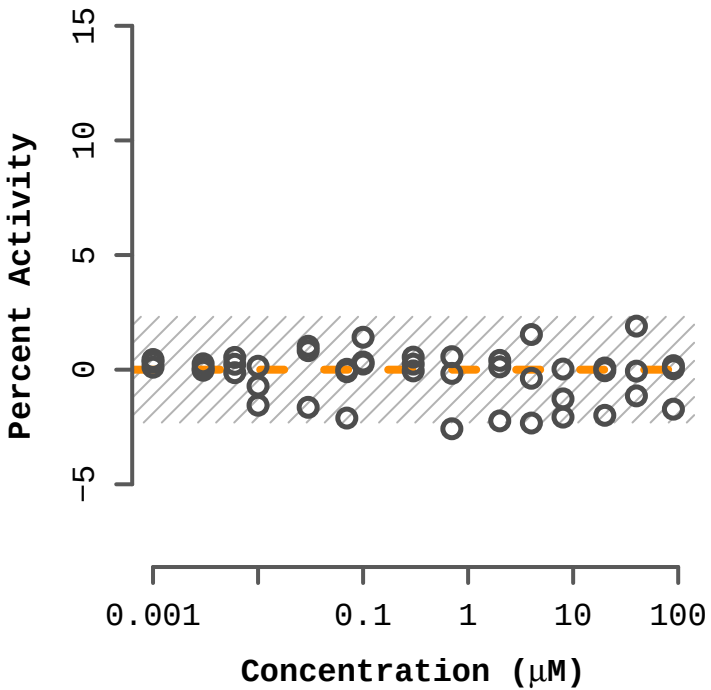
NAME: 2,8-Dimethylnonan-5-one
CHID: 41541 **CASRN:** 2050-99-9
SPID(S): Tox21_302232
M4ID: 12476901

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 2.12 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

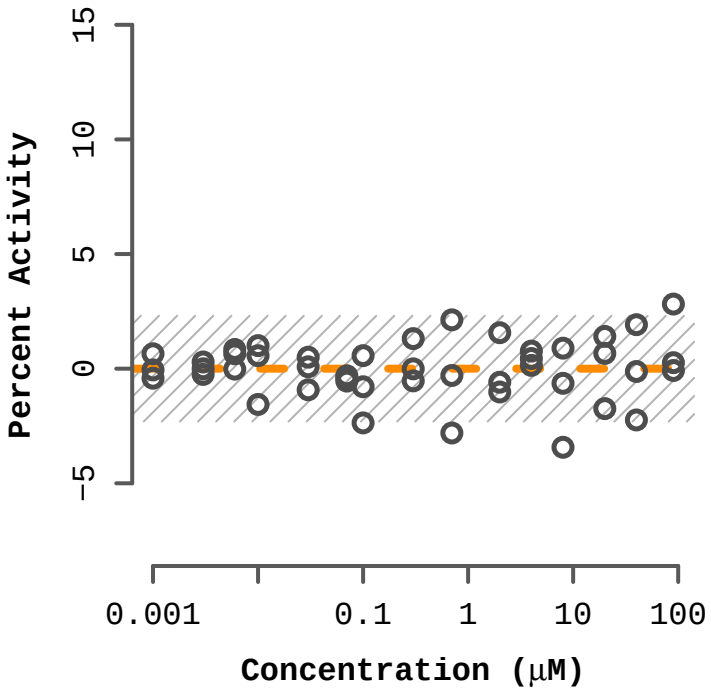
NAME: 6-Acetyl-1,1,2,4,4,7-hexamethyltetralin
CHID: 41544 **CASRN:** 21145-77-7
SPID(S): Tox21_301256
M4ID: 12477877

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.666 **MAX_MED:** 0.831 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

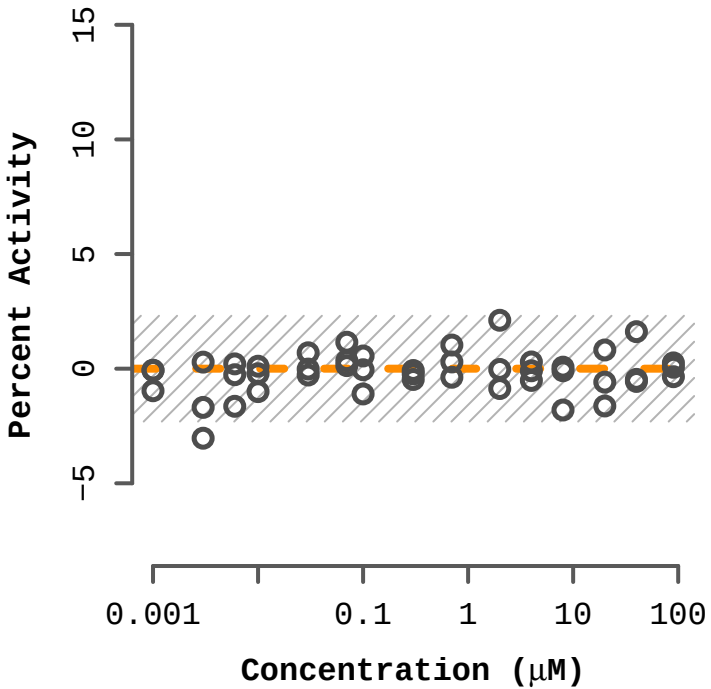
NAME: 6-Chloro-2,3-dihydrobenzoxazol-2-one
CHID: 41545 **CASRN:** 19932-84-4
SPID(S): Tox21_301408
M4ID: 12477725

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.665 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

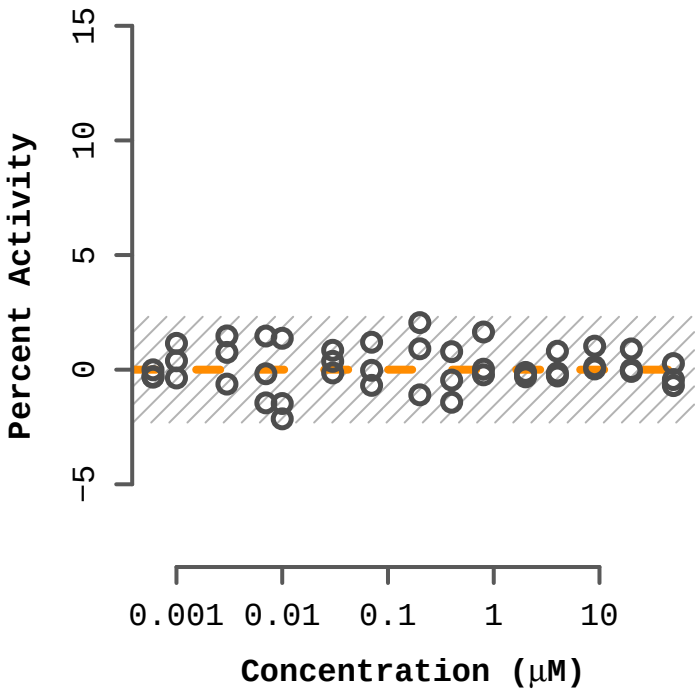
NAME: 6-Chlorothymol
CHID: 41547 **CASRN:** 89-68-9
SPID(S): Tox21_300909
M4ID: 12478224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.352 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

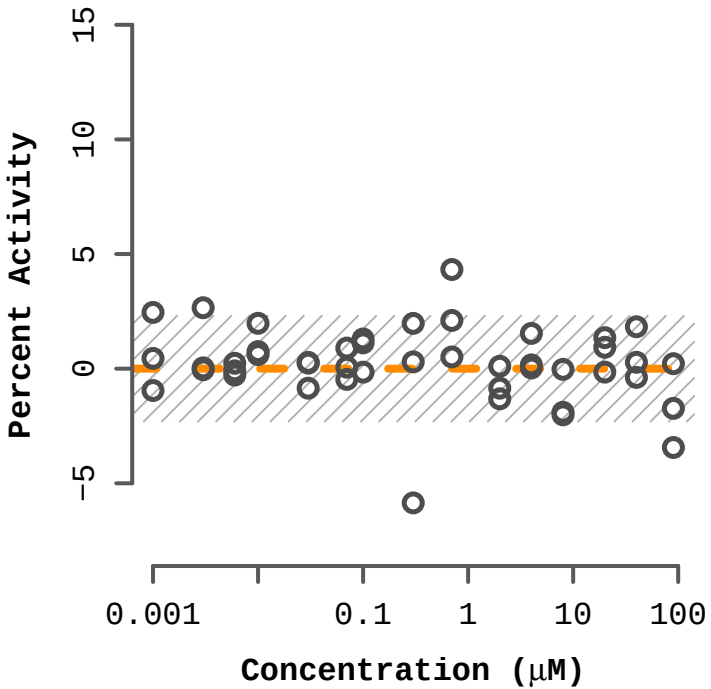
NAME: 6-Chlorothymol
CHID: 41547 **CASRN:** 89-68-9
SPID(S): Tox21_111622_1
M4ID: 12483579

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.624 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

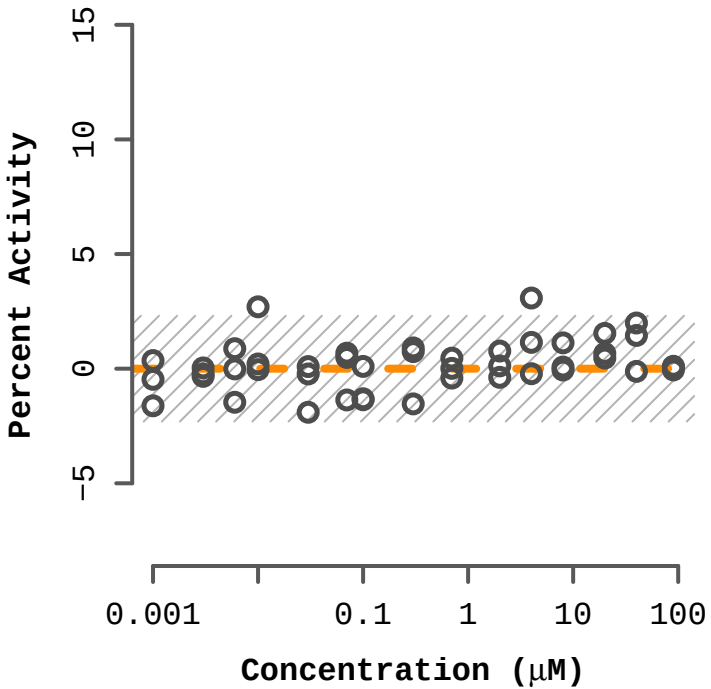
NAME: (S)-(-)-beta-Citronellol
CHID: 41550 **CASRN:** 7540-51-4
SPID(S): Tox21_300711
M4ID: 12478422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

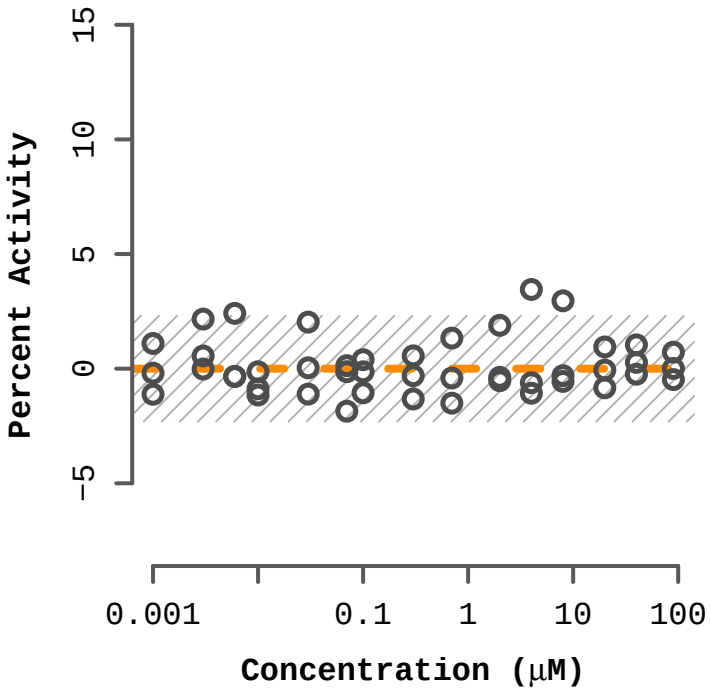
NAME: 6-tert-Butyl-2,4-dimethylphenol
CHID: 41551 **CASRN:** 1879-09-0
SPID(S): Tox21_303705
M4ID: 12475483

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

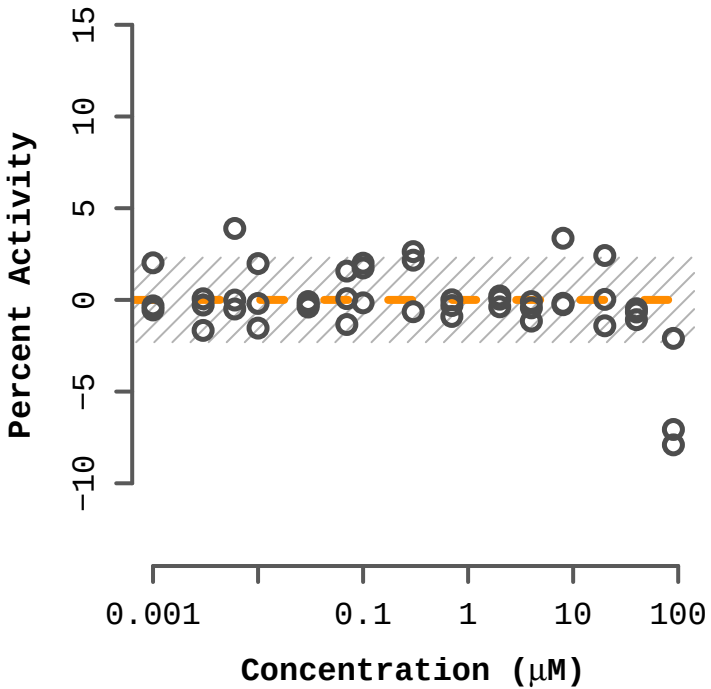
NAME: Dihydromyrcenol
CHID: 41557 **CASRN:** 53219-21-9
SPID(S): Tox21_302391
M4ID: 12476742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

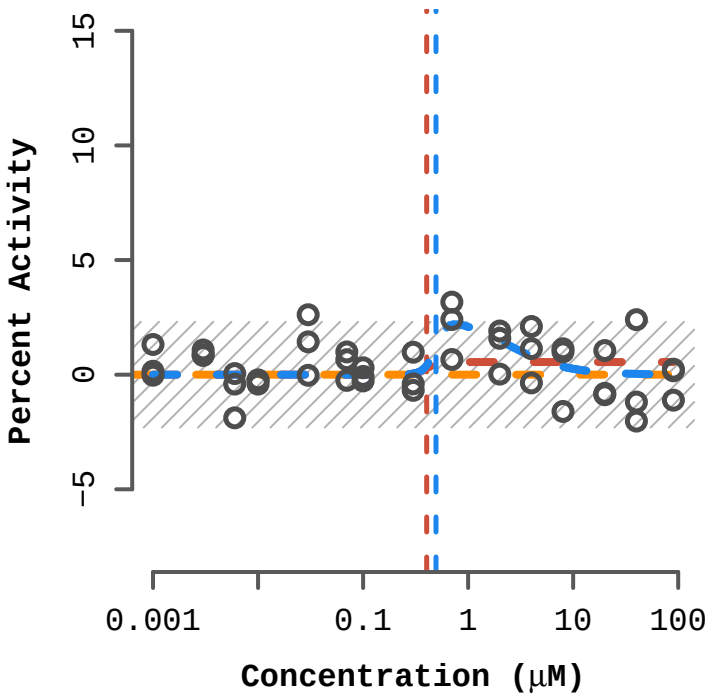
NAME: Methyl linolenate
CHID: 41560 **CASRN:** 301-00-8
SPID(S): Tox21_303764
M4ID: 12475424

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.8	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (9Z,12R)-12-Hydroxyoctadec-9-enoic acid
CHID: 41567 CASRN: 141-22-0
SPID(S): Tox21_301098
M4ID: 12478035

HILL MODEL (in red):

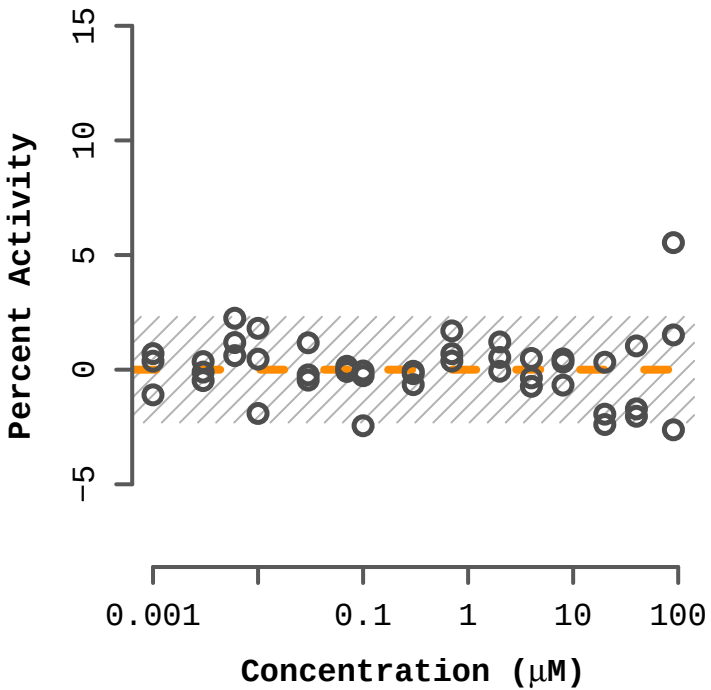
	tp	ga	gw
val:	0.551	−0.395	8
sd:	0.301	0.294	12.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.68	−0.306	8	0.364	1.53
sd:	2.64	0.273	10.3	0.692	1.27

	CNST	HILL	GNLS
AIC:	150.6	153.33	146.31
PROB:	0.1	0.03	0.87
RMSE:	1.24	1.18	1.05

MAX_MEAN: 2.08 MAX_MED: 2.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

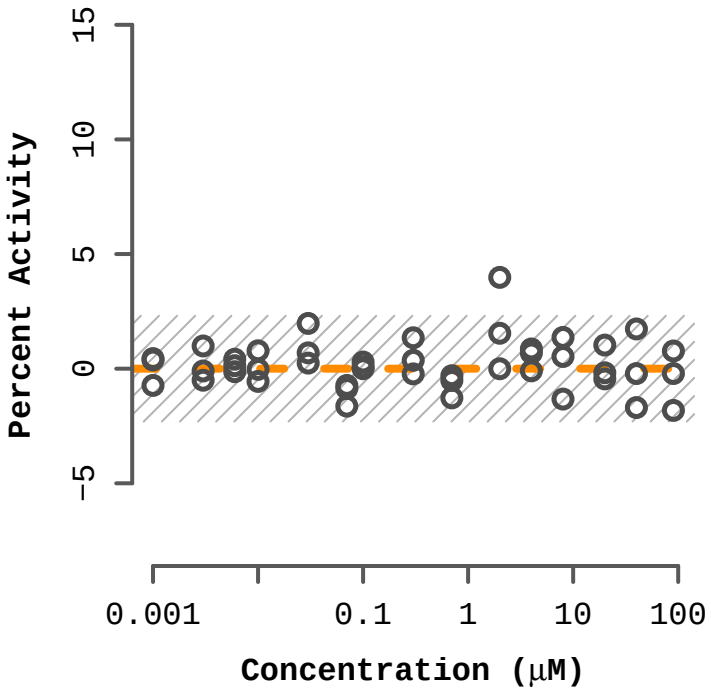
NAME: Chloroacetamide
CHID: 41570 **CASRN:** 79-07-2
SPID(S): Tox21_304037
M4ID: 12475151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

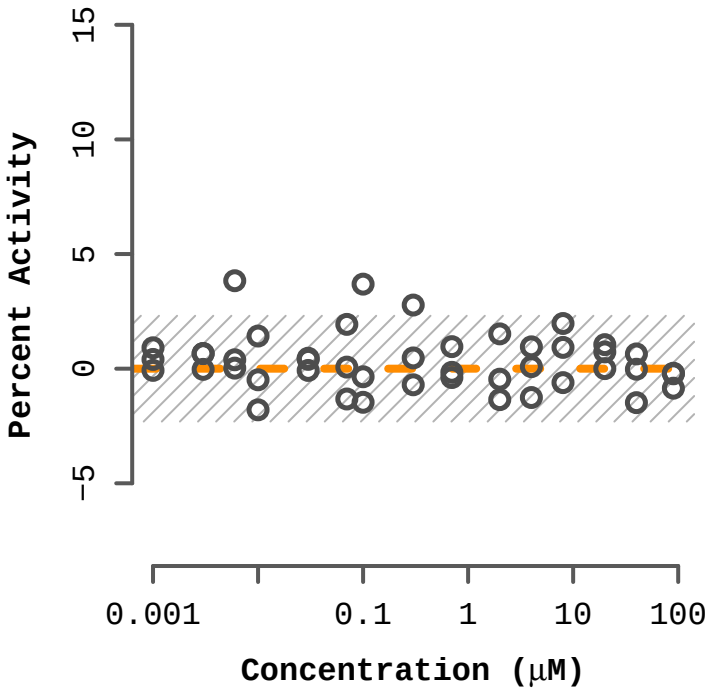
NAME: Triethyl phosphonoacetate
CHID: 41573 **CASRN:** 867-13-0
SPID(S): Tox21_302053
M4ID: 12477080

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

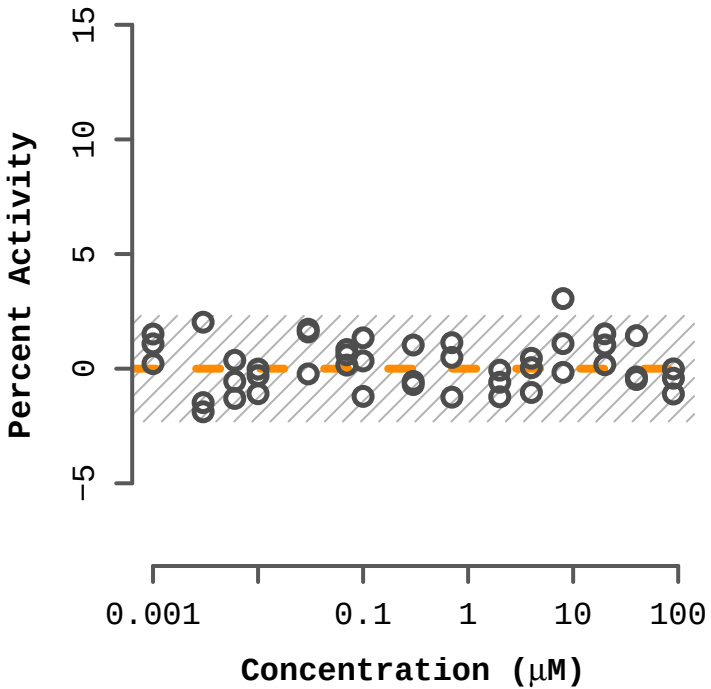
NAME: Diglycolic acid
CHID: 41575 **CASRN:** 110-99-6
SPID(S): Tox21_301036
M4ID: 12478097

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

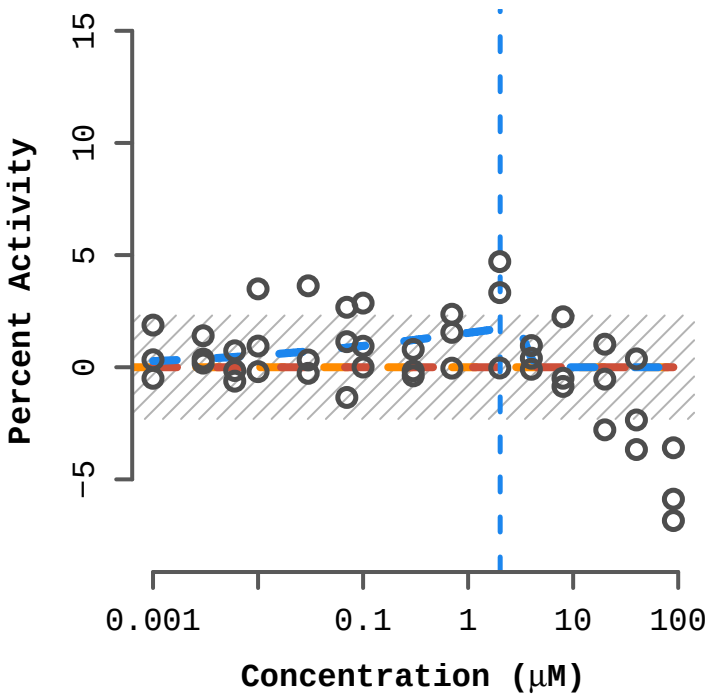
NAME: Iminodiacetonitrile
CHID: 41580 **CASRN:** 628-87-5
SPID(S): Tox21_301075
M4ID: 12478058

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amiprofos-methyl
CHID: 41600 CASRN: 36001-88-4
SPID(S): Tox21_301206
M4ID: 12477927

HILL MODEL (in red):

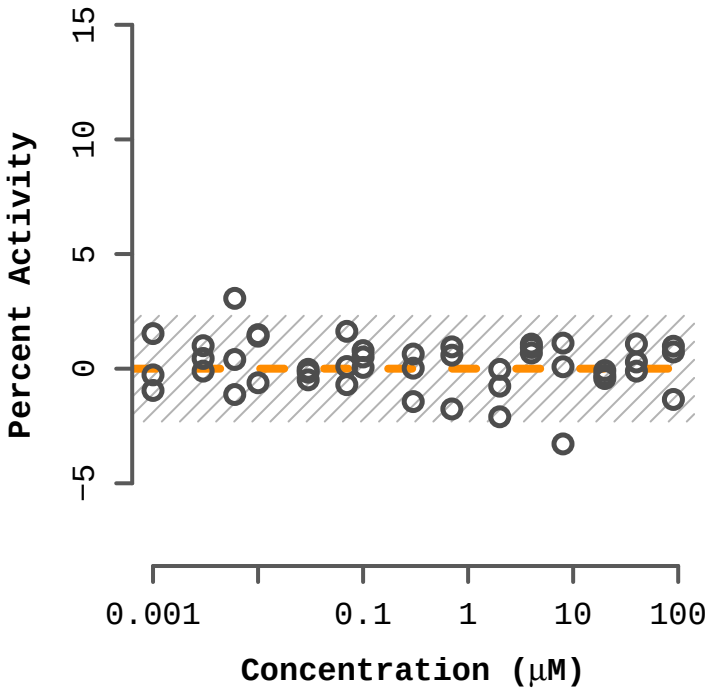
	tp	ga	gw
val:	2.28e-09	2.34	1.83
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.45	0.305	0.321	0.555	11.9
sd:	12.1	7.14	0.274	0.205	45.3

	CNST	HILL	GNLS
AIC:	197.59	203.59	198.77
PROB:	0.62	0.03	0.35
RMSE:	2.23	2.23	2.05

MAX_MEAN: 2.67 **MAX_MED:** 3.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

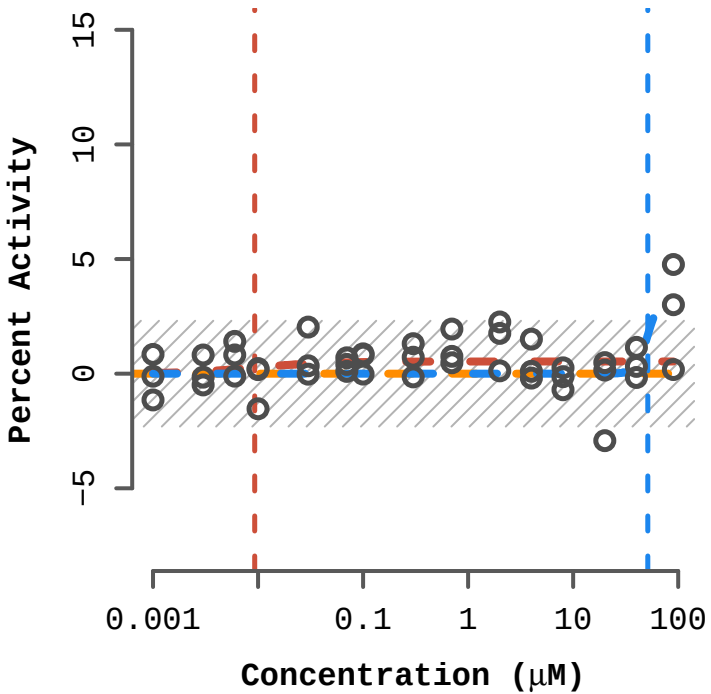
NAME: Pentyl butyrate
CHID: 41604 **CASRN:** 540-18-1
SPID(S): Tox21_302013
M4ID: 12477120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.896 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: L−3−(2'−Piperidyl)pyridine
CHID: 41607 CASRN: 494−52−0
SPID(S): Tox21_301952
M4ID: 12477181

HILL MODEL (in red):

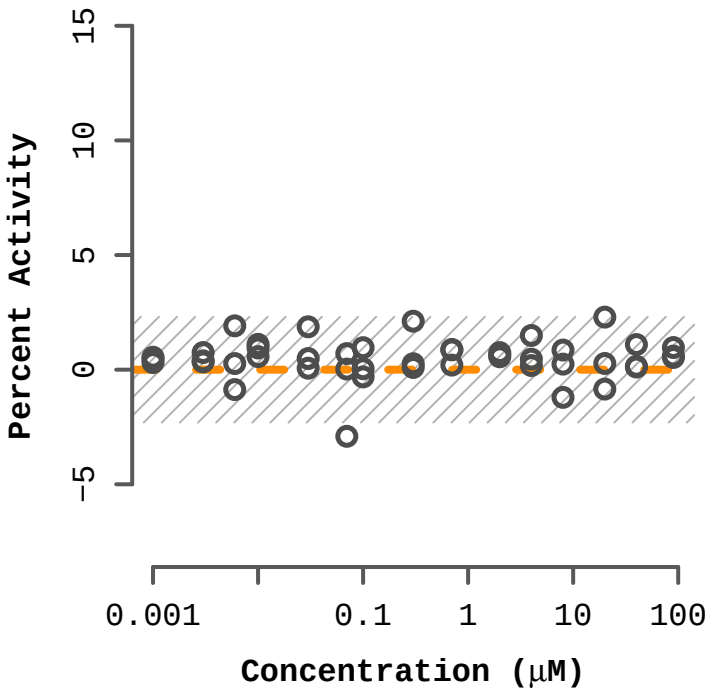
	tp	ga	gw
val:	0.531	−2.03	1.27
sd:	0.178	0.913	1.69

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.06	1.71	8	2.68	0.314
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	143.56	138.41	144.95
PROB:	0.07	0.9	0.03
RMSE:	1.29	1.16	1.09

MAX_MEAN: 2.65 MAX_MED: 3.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

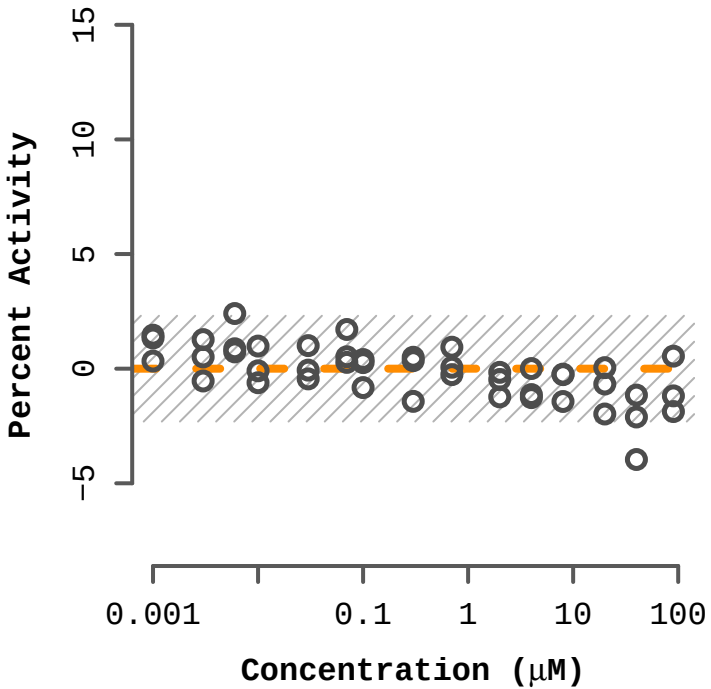
NAME: Arabinose
CHID: 41610 **CASRN:** 147-81-9
SPID(S): Tox21_301533
M4ID: 12477600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

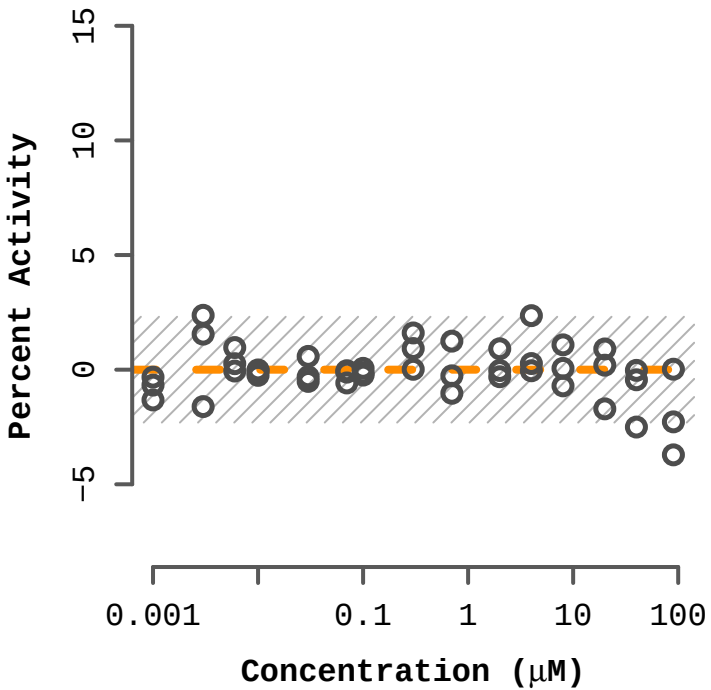
NAME: Ascorbyl palmitate
CHID: 41611 **CASRN:** 137-66-6
SPID(S): Tox21_301926
M4ID: 12477207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

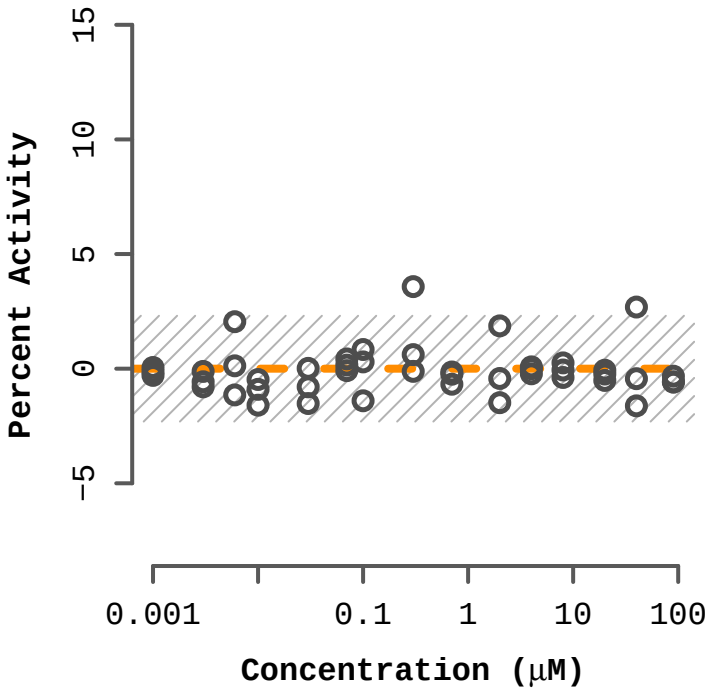
NAME: Azaconazole
CHID: 41613 CASRN: 60207-31-0
SPID(S): Tox21_301852
M4ID: 12477281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.86 MAX_MED: 1.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

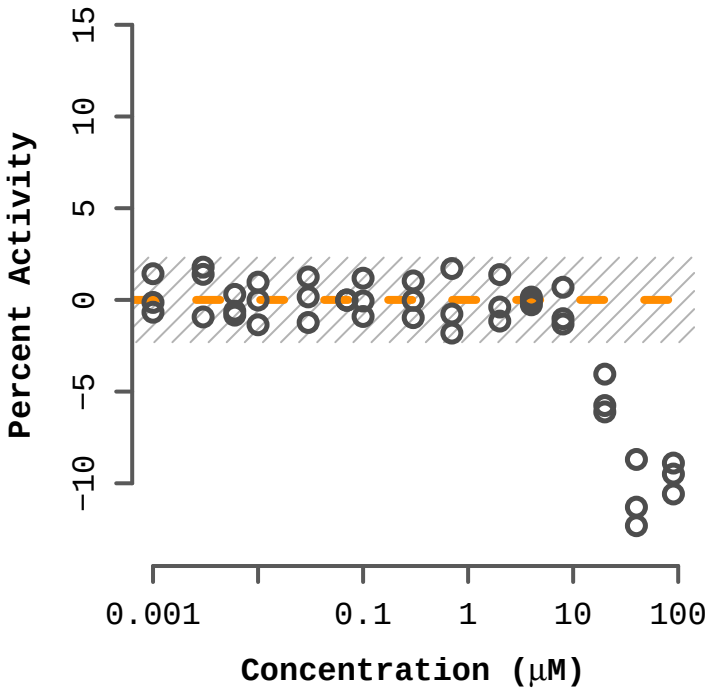
NAME: Aziprotryne
CHID: 41615 **CASRN:** 4658-28-0
SPID(S): Tox21_301004
M4ID: 12478129

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.616 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

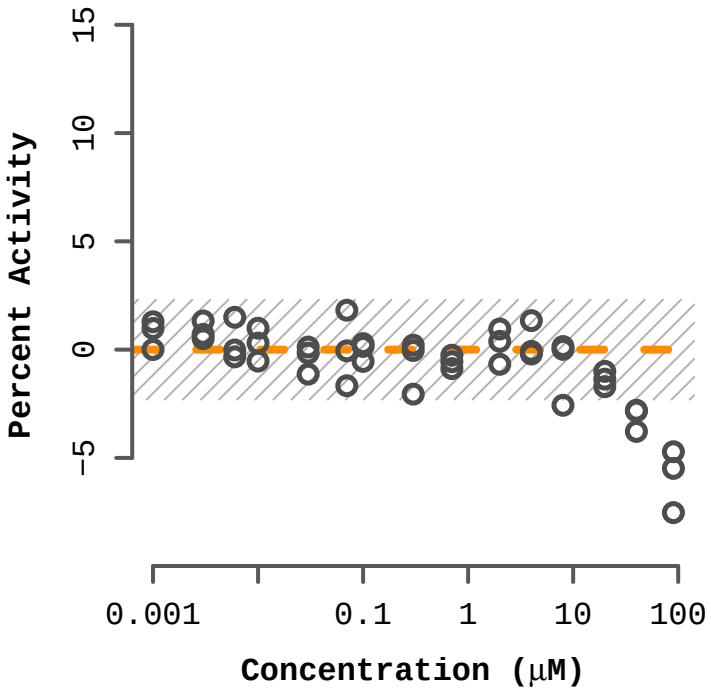
NAME: Barban
CHID: 41617 **CASRN:** 101-27-9
SPID(S): Tox21_300669
M4ID: 12478464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.87	NA	NA
PROB:	1	NA	NA
RMSE:	4.1	NA	NA

MAX_MEAN: 0.751 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

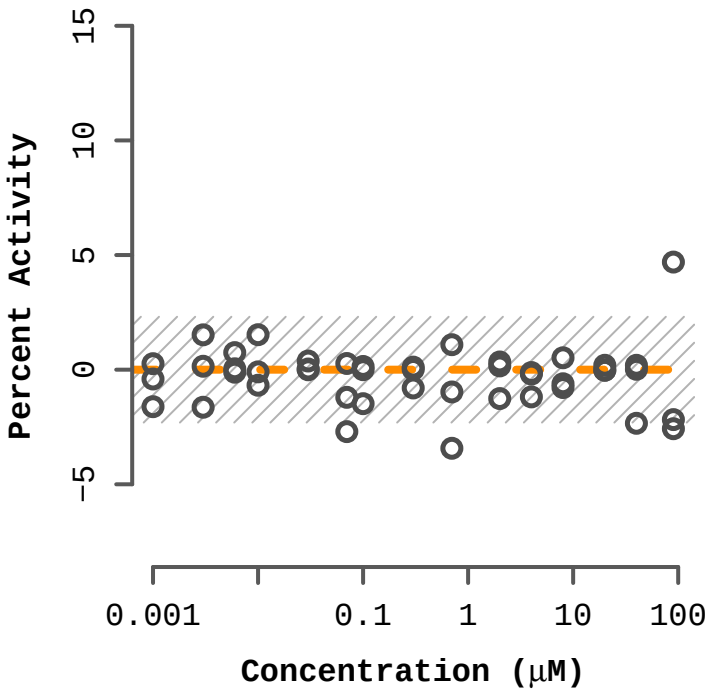
NAME: Benalaxyl
CHID: 41619 CASRN: 71626-11-4
SPID(S): Tox21_301557
M4ID: 12477576

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 0.847 MAX_MED: 0.979 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

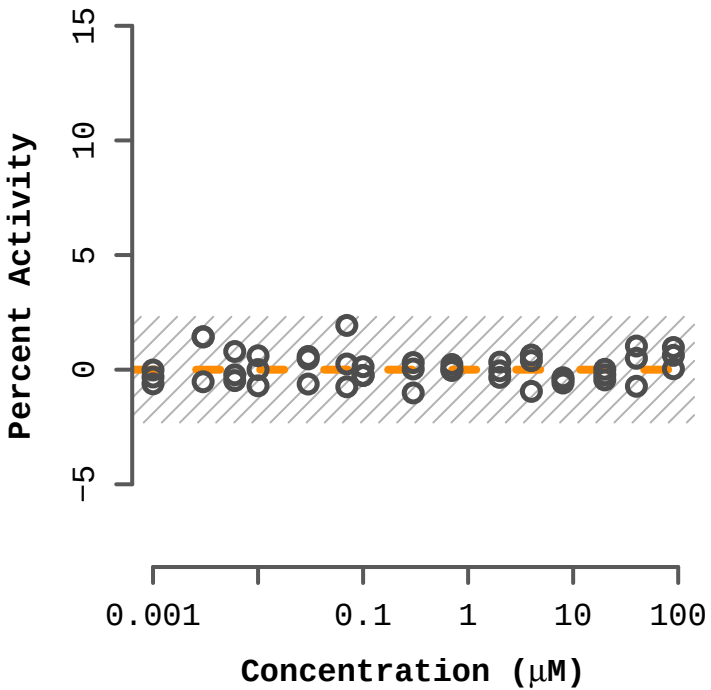
NAME: Benazolin-ethyl
CHID: 41621 **CASRN:** 25059-80-7
SPID(S): Tox21_301963
M4ID: 12477170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.252 **MAX_MED:** 0.166 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

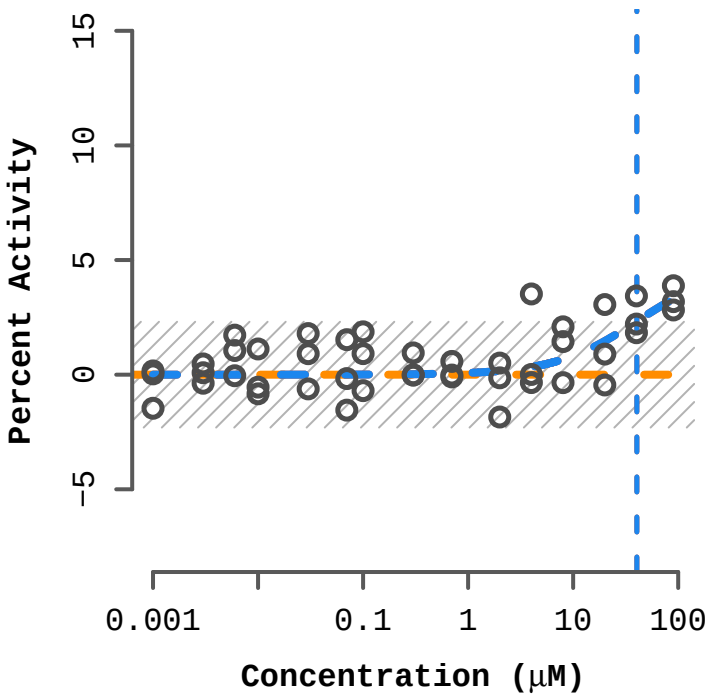
NAME: Benfuracarb
CHID: 41622 **CASRN:** 82560-54-1
SPID(S): Tox21_301582
M4ID: 12477551

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.78 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benodanil
CHID: 41623 CASRN: 15310-01-7
SPID(S): Tox21_300420
M4ID: 12478712

HILL MODEL (in red):

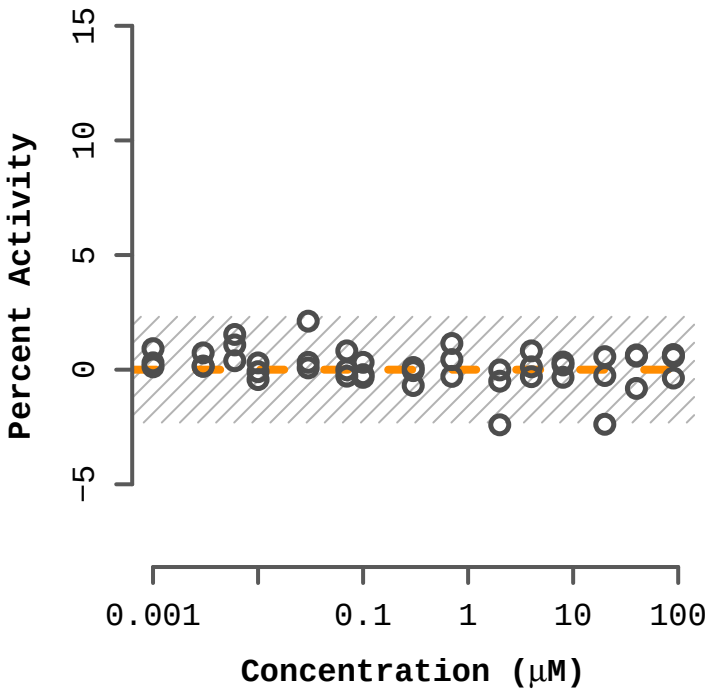
	tp	ga	gw
val:	4.66	1.61	1.1
sd:	3.62	0.72	0.844

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.66	1.61	1.1	3.51	6.07
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	169.87	142.38	146.38
PROB:	0	0.88	0.12
RMSE:	1.57	1.07	1.07

MAX_MEAN: 3.3 MAX_MED: 3.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

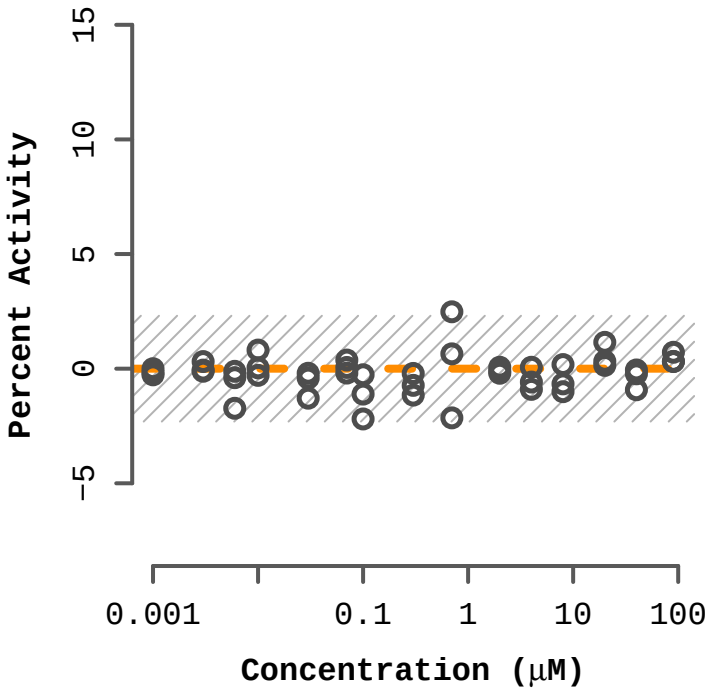
NAME: Benzadox
CHID: 41625 **CASRN:** 5251-93-4
SPID(S): Tox21_301883
M4ID: 12477250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

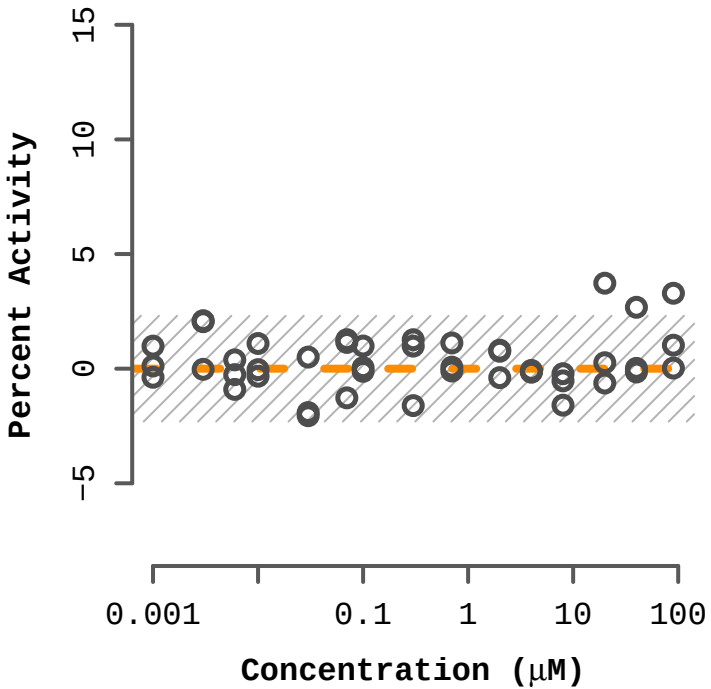
NAME: 3,4−Dimethylbenzaldehyde
CHID: 41626 **CASRN:** 5973−71−7
SPID(S): Tox21_301638
M4ID: 12477495

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.54 **MAX_MED:** 0.648 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

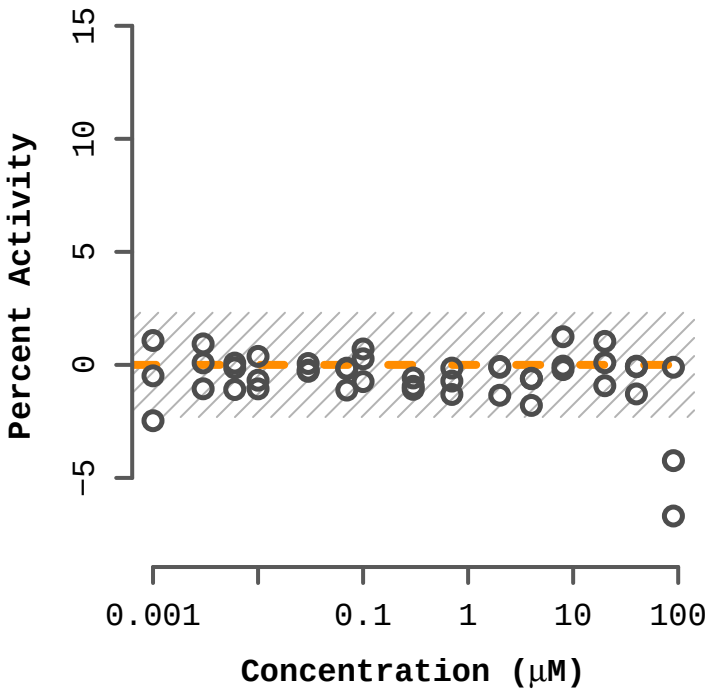
NAME: 2-Amino-N-(1-methylethyl)benzamide
CHID: 41627 **CASRN:** 30391-89-0
SPID(S): Tox21_301979
M4ID: 12477154

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

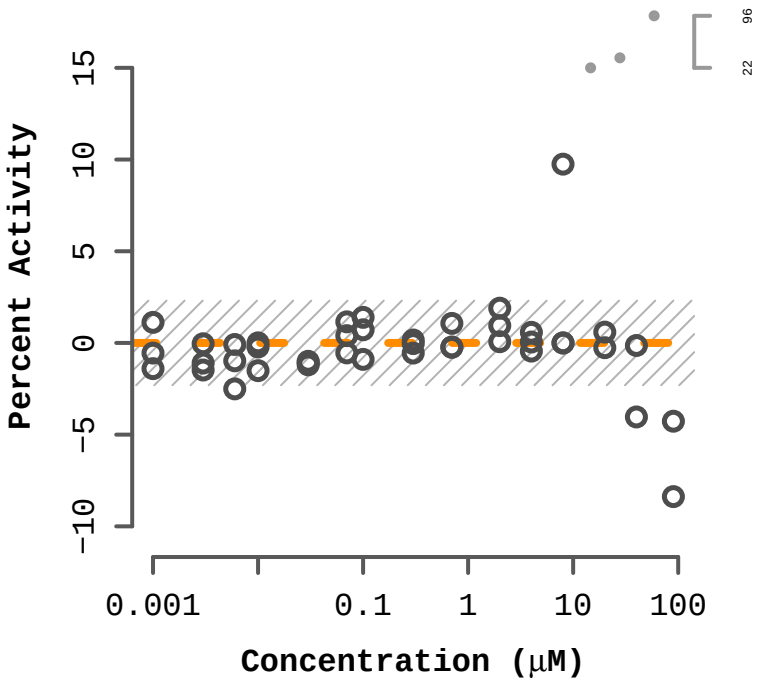
NAME: 2,2'−Dibenzoylaminodiphenyl disulfide
CHID: 41629 **CASRN:** 135−57−9
SPID(S): Tox21_303466
M4ID: 12475674

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.33 **MAX_MED:** 0.271 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

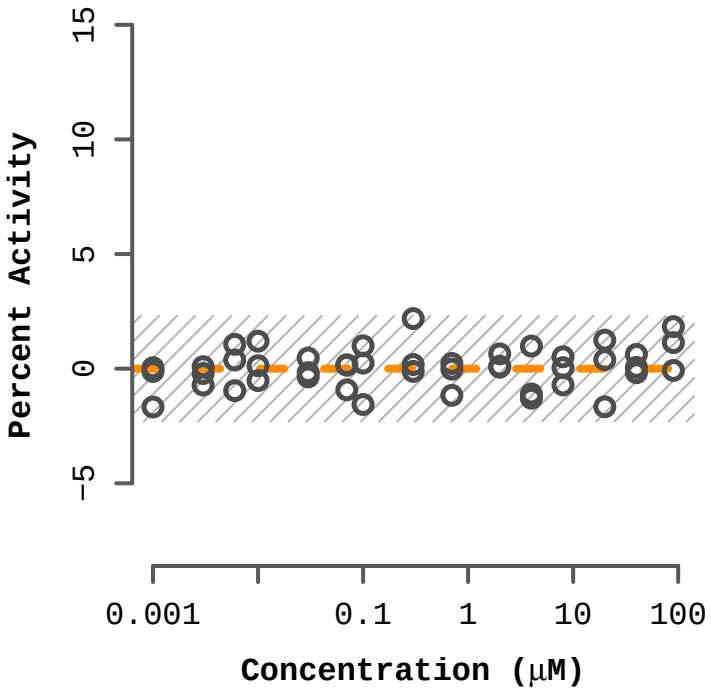
NAME: 2,2'−Dibenzoylaminodiphenyl disulfide
CHID: 41629 **CASRN:** 135−57−9
SPID(S): Tox21_201711
M4ID: 12480541 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	255.83	NA	NA
PROB:	1	NA	NA
RMSE:	15.82	NA	NA

MAX_MEAN: 27.9 **MAX_MED:** 0.946 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

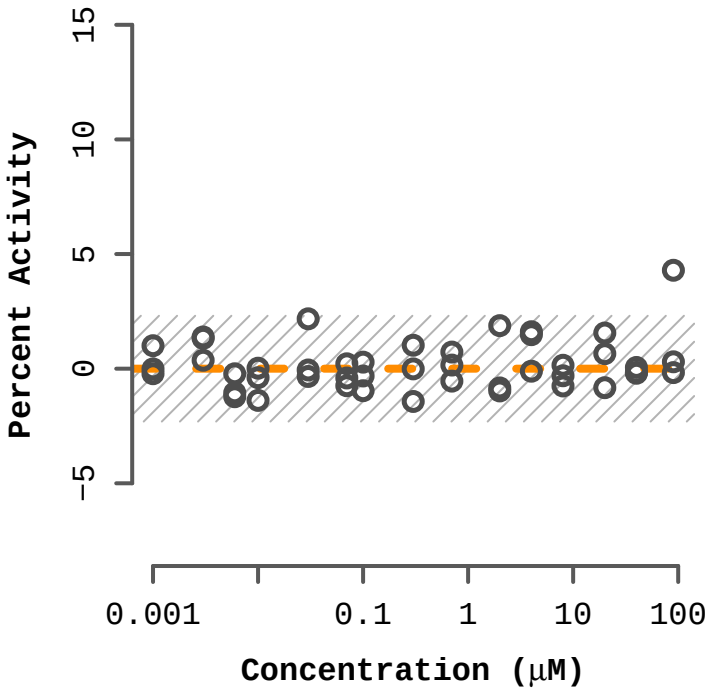
NAME: (+/−)-alpha-Methylbenzyl acetate
CHID: 41636 **CASRN:** 93-92-5
SPID(S): Tox21_300948
M4ID: 12478185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.967 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

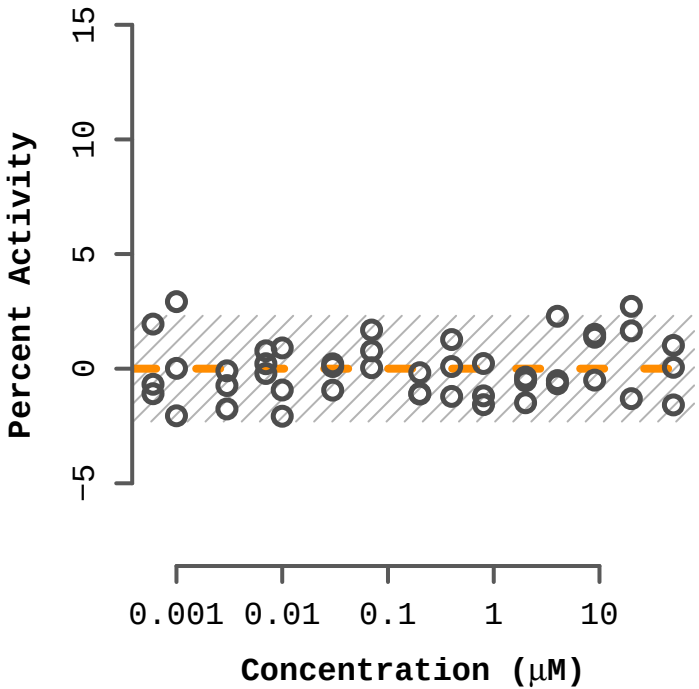
NAME: 3-Phenyl-1-propanol
CHID: 41638 **CASRN:** 122-97-4
SPID(S): Tox21_301674
M4ID: 12477459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

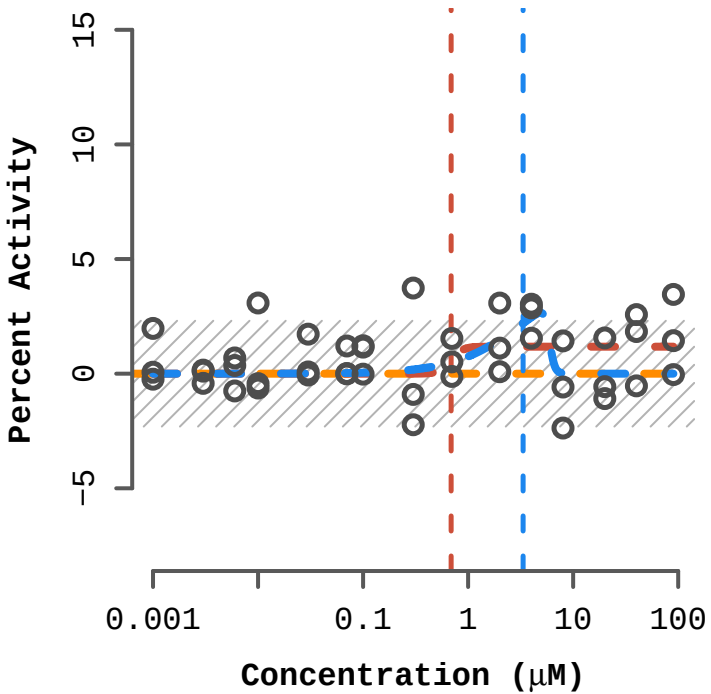
NAME: 3-Phenyl-1-propanol
CHID: 41638 **CASRN:** 122-97-4
SPID(S): Tox21_113458_1
M4ID: 12482647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium m-xylene-4-sulfonate
CHID: 41639 CASRN: 827-21-4
SPID(S): Tox21_301766
M4ID: 12477367

HILL MODEL (in red):

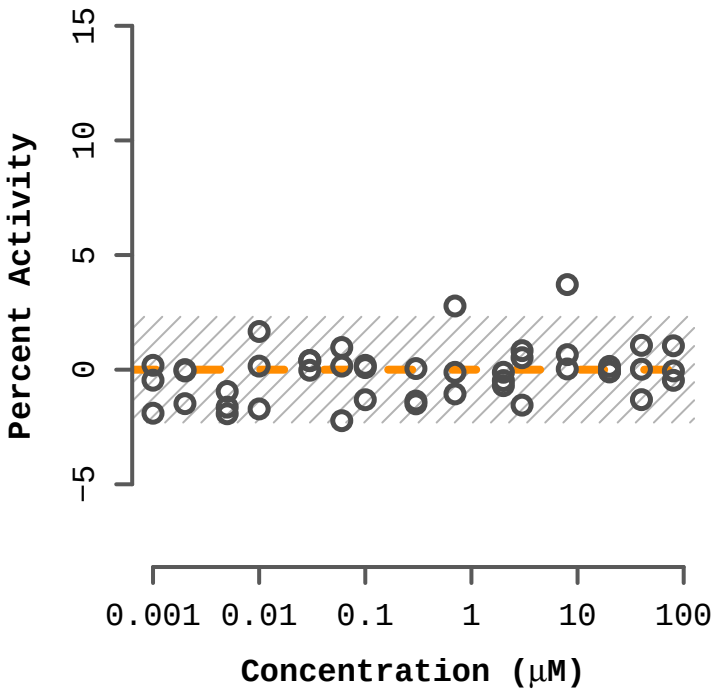
	tp	ga	gw
val:	1.18	-0.162	8
sd:	0.368	0.128	31.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.4	0.523	1.31	0.773	18
sd:	9.61	1.5	2.3	0.343	46.9

	CNST	HILL	GNLS
AIC:	171.57	167.69	168.03
PROB:	0.07	0.5	0.43
RMSE:	1.58	1.42	1.38

MAX_MEAN: 2.48 MAX_MED: 2.87 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

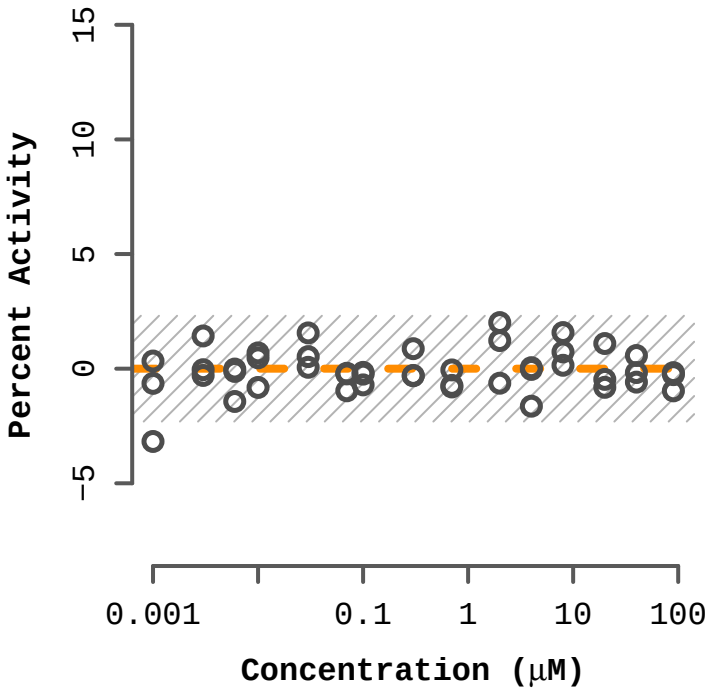
NAME: 2,5-Dimethylbenzenesulfonic acid
CHID: 41641 **CASRN:** 609-54-1
SPID(S): Tox21_301014
M4ID: 12478119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

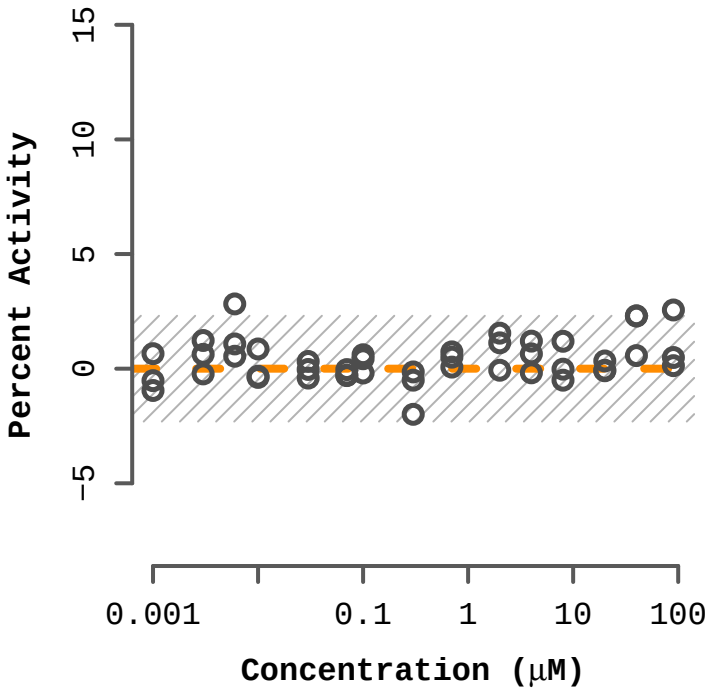
NAME: Sodium 2-formylbenzenesulfonate
CHID: 41643 **CASRN:** 1008-72-6
SPID(S): Tox21_301057
M4ID: 12478076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.869 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

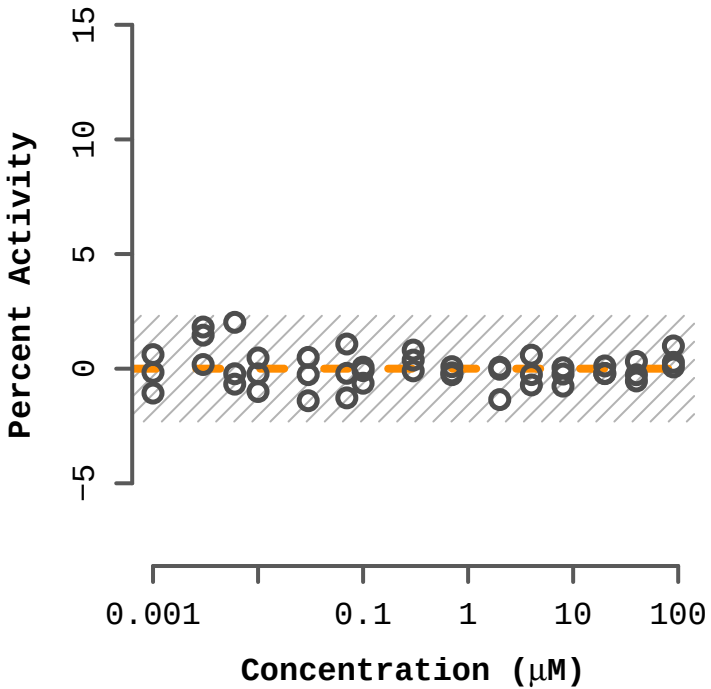
NAME: C.I. Acid Yellow 34, monosodium salt
CHID: 41646 **CASRN:** 6359-90-6
SPID(S): Tox21_301934
M4ID: 12477199

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.33	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

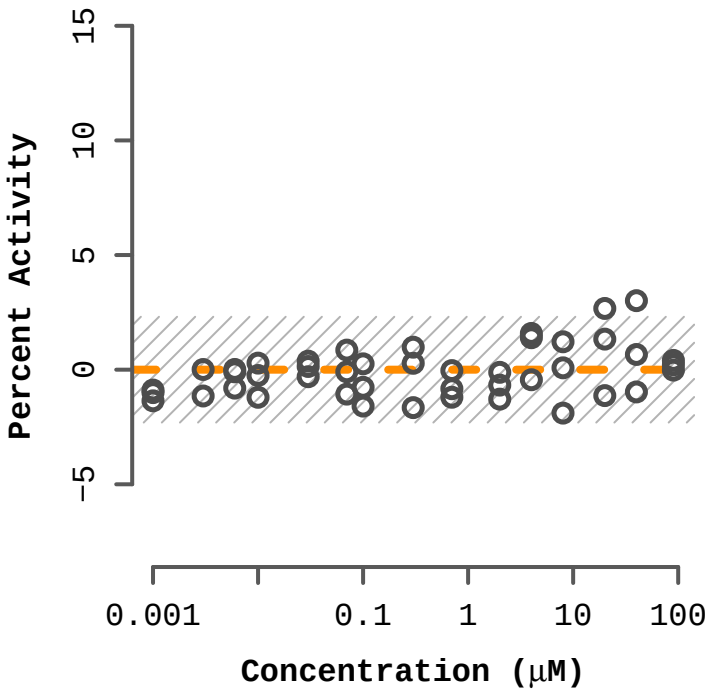
NAME: Methyl 2,4-dihydroxy-3,6-dimethylbenzoate
CHID: 41653 **CASRN:** 4707-47-5
SPID(S): Tox21_301667
M4ID: 12477466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

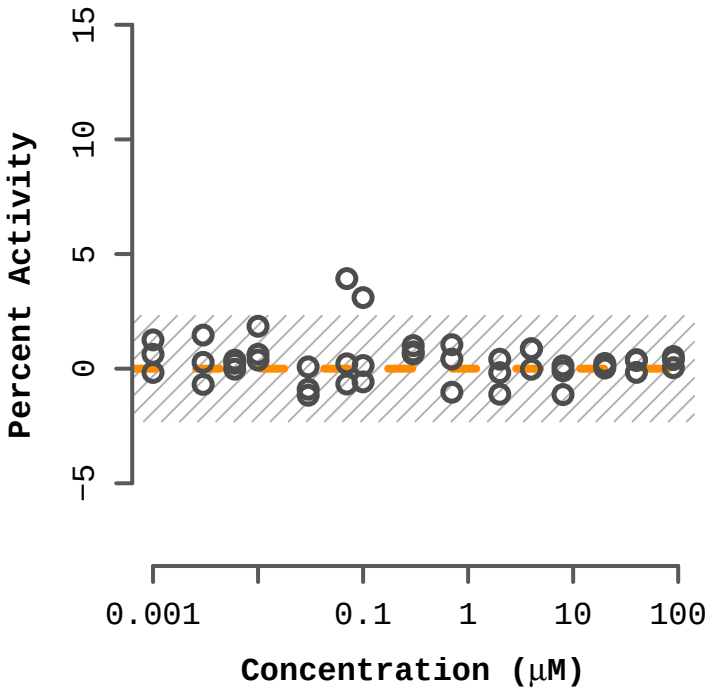
NAME: 2-Ethylhexyl benzoate
CHID: 41654 **CASRN:** 5444-75-7
SPID(S): Tox21_301476
M4ID: 12477657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.959 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

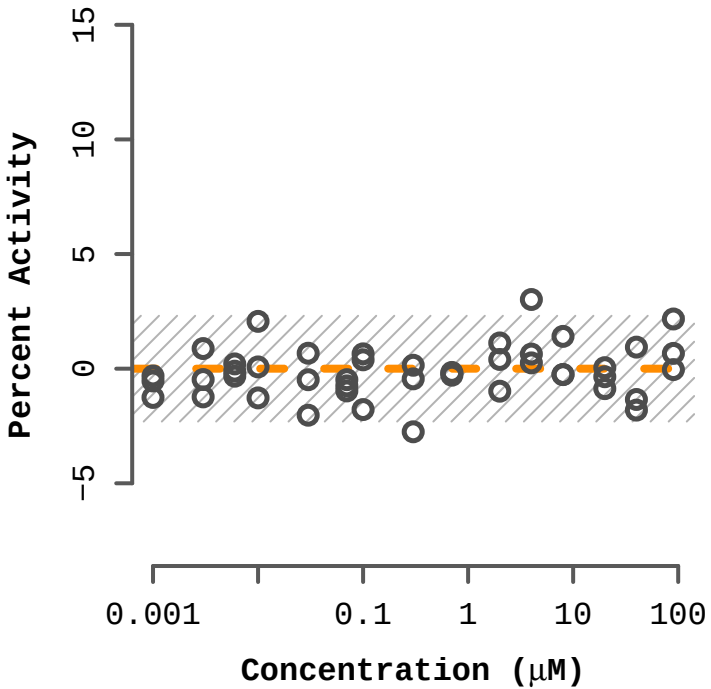
NAME: 3,5-Dibromo-4-hydroxybenzoic acid
CHID: 41656 **CASRN:** 3337-62-0
SPID(S): Tox21_301956
M4ID: 12477177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.868 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

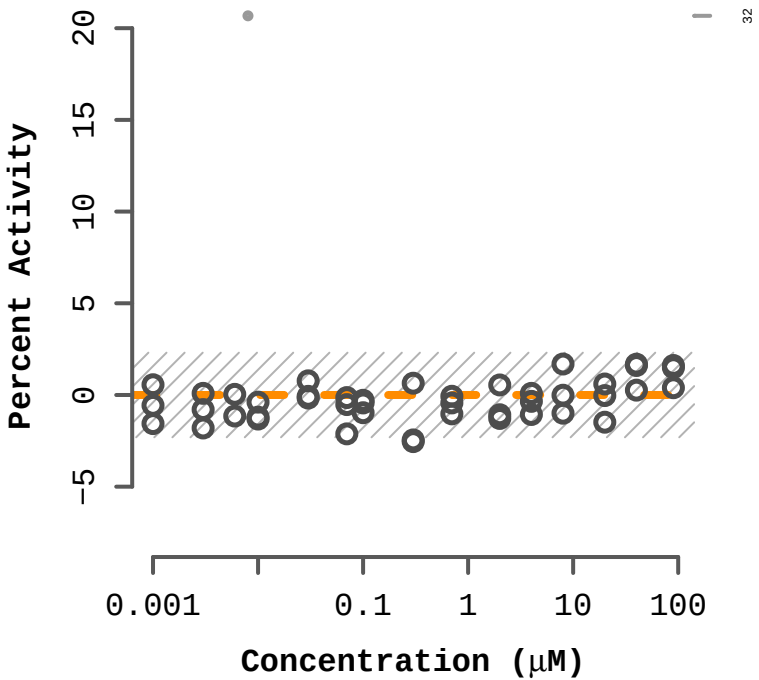
NAME: 4-Cyanobenzoic acid
CHID: 41659 **CASRN:** 619-65-8
SPID(S): Tox21_302120
M4ID: 12477013

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.669 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

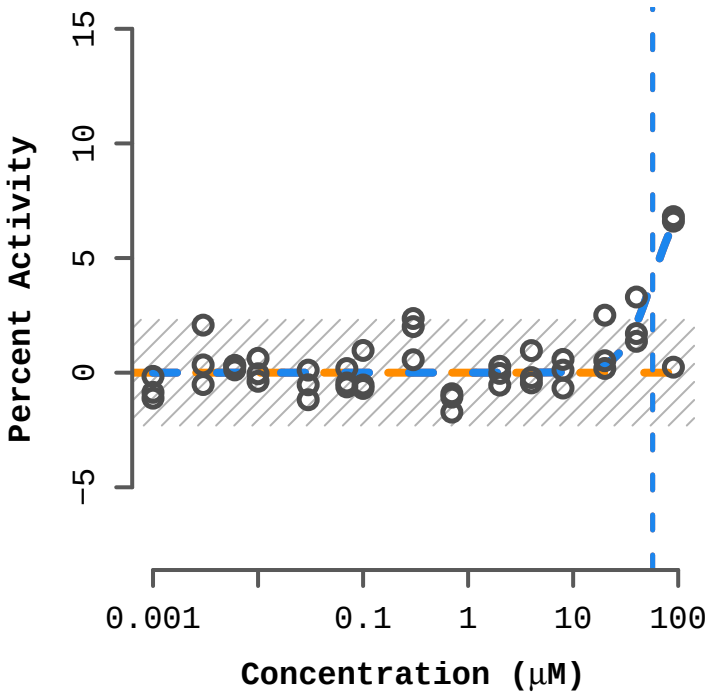
NAME: 2-Hydroxybenzonitrile
CHID: 41661 **CASRN:** 611-20-1
SPID(S): Tox21_302110
M4ID: 12477023 **BRK**

HILL MODEL: Not applicable.

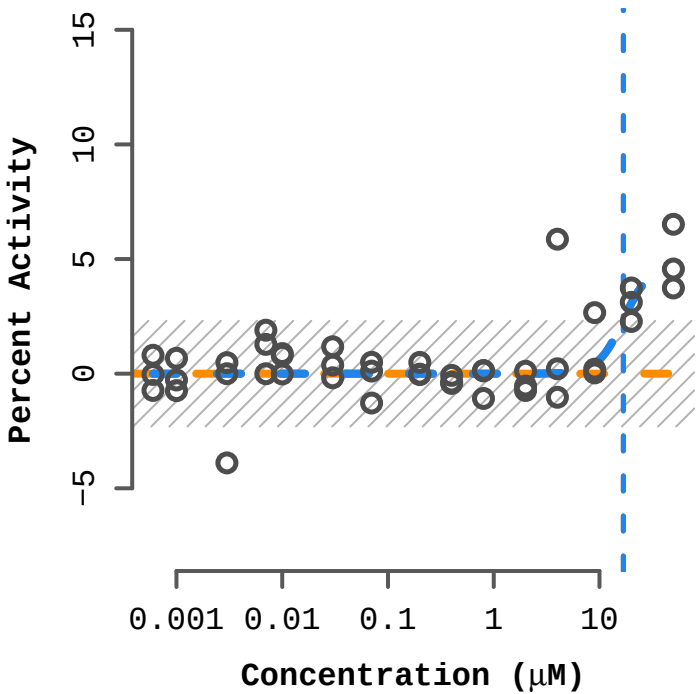
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.62	NA	NA
PROB:	1	NA	NA
RMSE:	4.89	NA	NA

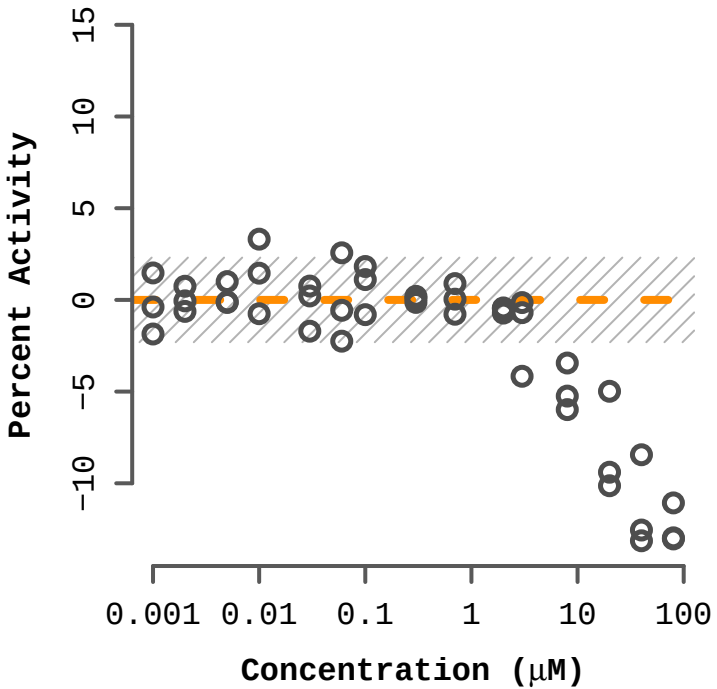
MAX_MEAN: 10.3 **MAX_MED:** 1.61 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzyl cinnamate
CHID:    41663   CASRN: 103-41-3
SPID(S): Tox21_300699
M4ID:    12478434

HILL MODEL (in red):
      tp       ga       gw
val:  8.17     1.76     2.92
sd:   2.75     0.144    1.44

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.17     1.76     2.92     3.95     4.78
sd:   2.75     0.144    1.44     11900    28500

      CNST        HILL        GNLS
AIC:  159.36      138.32      142.32
PROB: 0           0.88        0.12
RMSE: 1.77        1.28        1.28

MAX_MEAN: 4.55      MAX_MED: 6.61      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzyl cinnamate
CHID:    41663   CASRN: 103-41-3
SPID(S): Tox21_112329_1
M4ID:    12483158

HILL MODEL (in red):
      tp       ga       gw
val:  4.7      1.23     3.64
sd:   0.667    0.066    1.71

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.7      1.23     3.64     3.35     2.95
sd:   0.675    0.0663   1.71     543      997

      CNST        HILL        GNLS
AIC:  178.15      137.54      141.54
PROB: 0           0.88        0.12
RMSE: 2           1.3         1.3

MAX_MEAN: 4.94      MAX_MED: 4.57      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

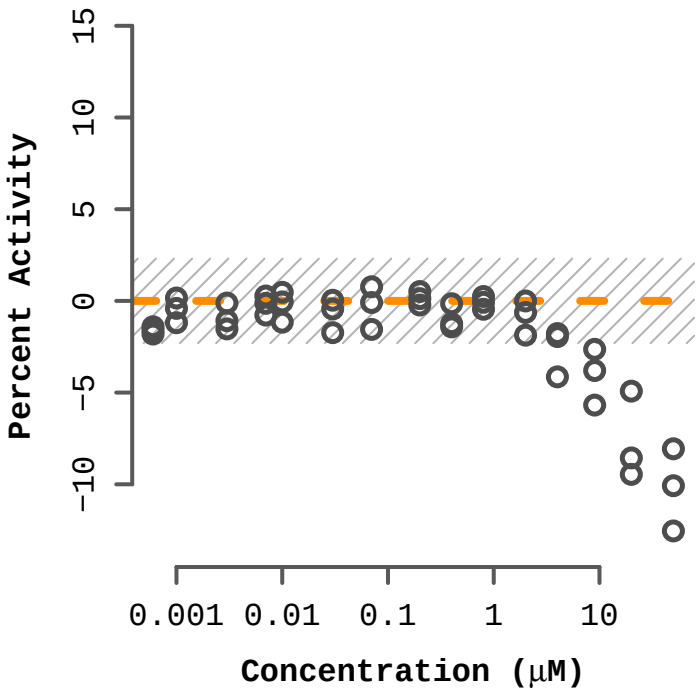
NAME: Benzylhexadecyldimethylammonium chloride
CHID: 41665 **CASRN:** 122-18-9
SPID(S): Tox21_302079
M4ID: 12477054

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.66	NA	NA
PROB:	1	NA	NA
RMSE:	5.2	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

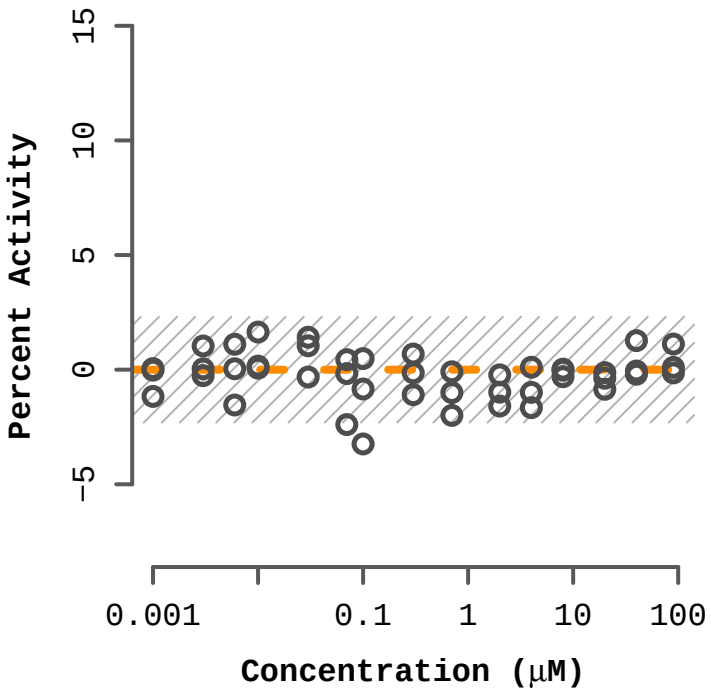
NAME: Benzylhexadecyldimethylammonium chloride
CHID: 41665 **CASRN:** 122-18-9
SPID(S): Tox21_112574_1
M4ID: 12483026

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.71	NA	NA

MAX_MEAN: 0.139 **MAX_MED:** 0.125 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

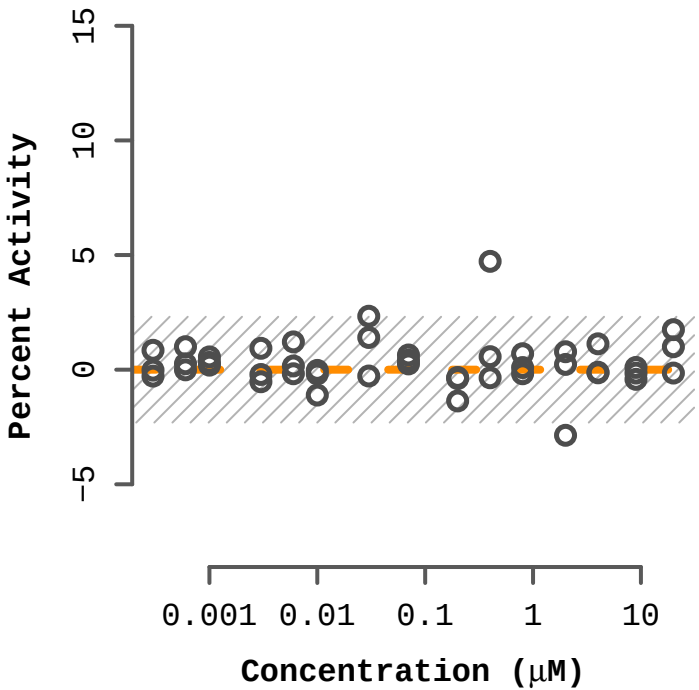
NAME: Bibenzyl
CHID: 41668 **CASRN:** 103-29-7
SPID(S): Tox21_300820
M4ID: 12478313

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.713 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

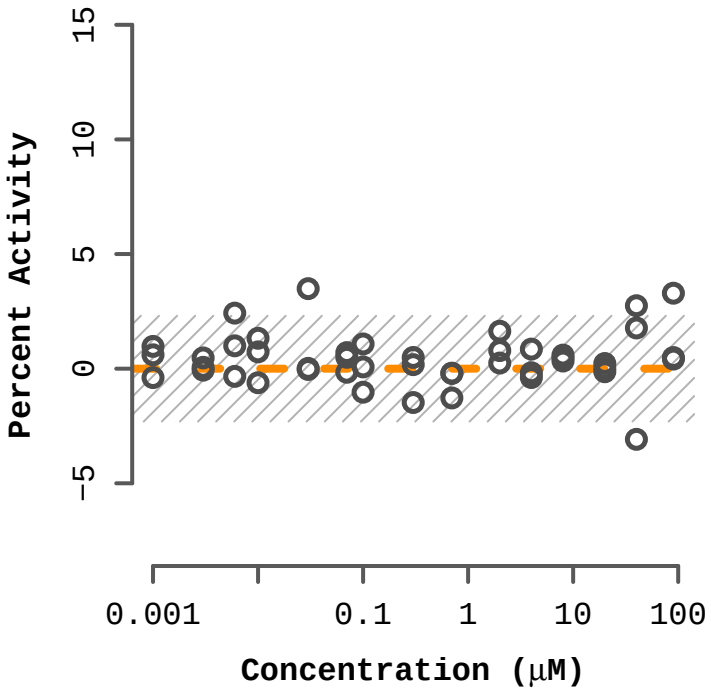
NAME: (+)−alpha−Pinene
CHID: 41671 **CASRN:** 7785−70−8
SPID(S): Tox21_303429
M4ID: 12475710

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

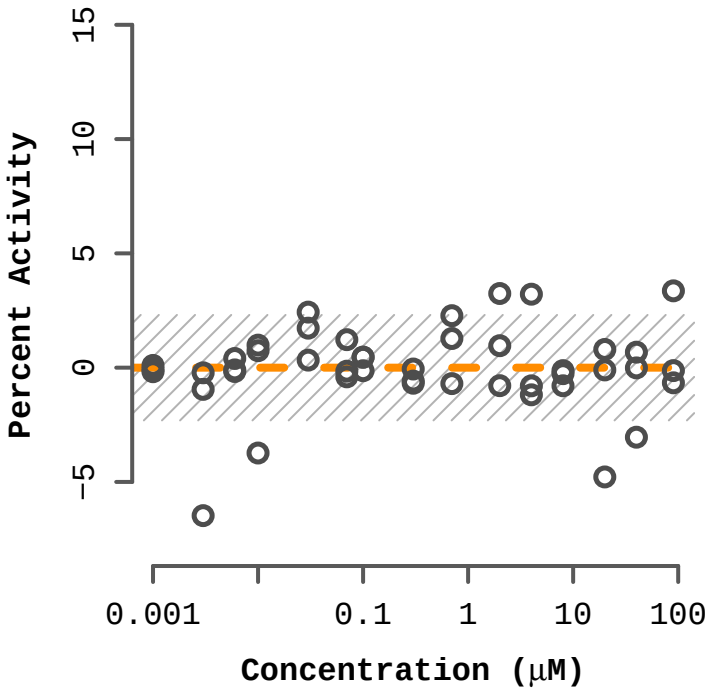
NAME: Bis(ethylxanthogen)
CHID: 41672 **CASRN:** 502-55-6
SPID(S): Tox21_302227
M4ID: 12476906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

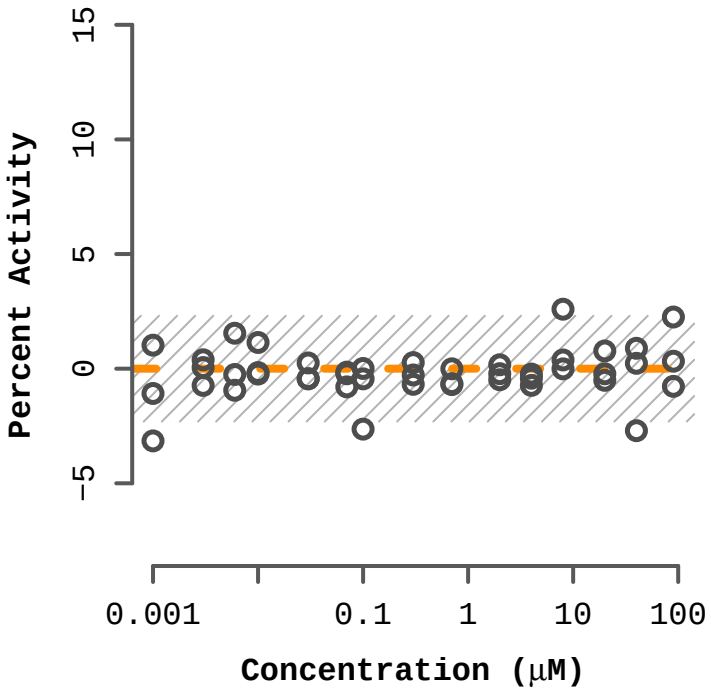
NAME: Triethyl borate
CHID: 41674 **CASRN:** 150-46-9
SPID(S): Tox21_303940
M4ID: 12475248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

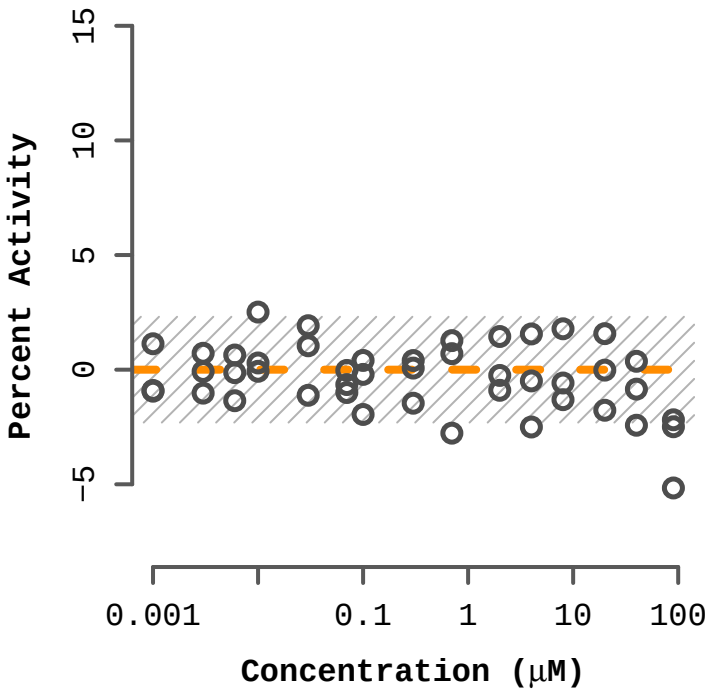
NAME: Bornyl acetate
CHID: 41675 CASRN: 76-49-3
SPID(S): Tox21_301733
M4ID: 12477400

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.99 **MAX_MED:** 0.381 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

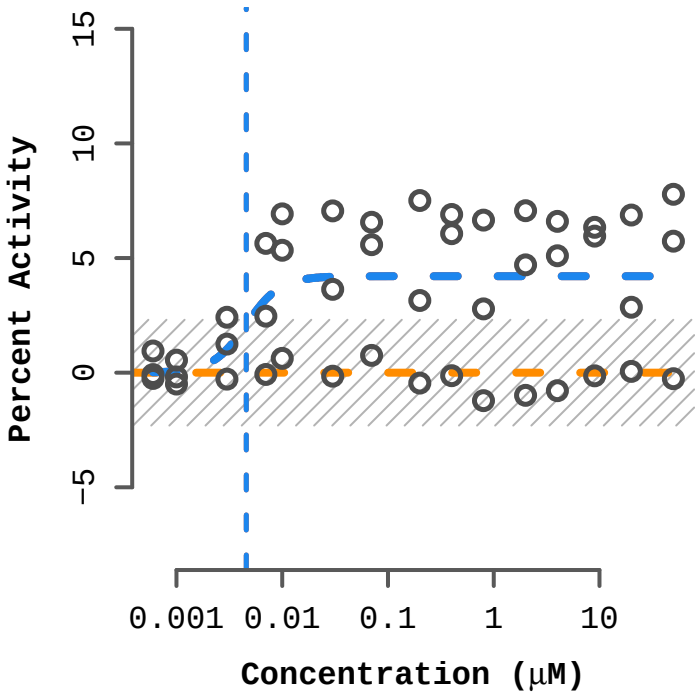
NAME: Bromociclen
CHID: 41680 **CASRN:** 1715-40-8
SPID(S): Tox21_301856
M4ID: 12477277

HILL MODEL: Not applicable.

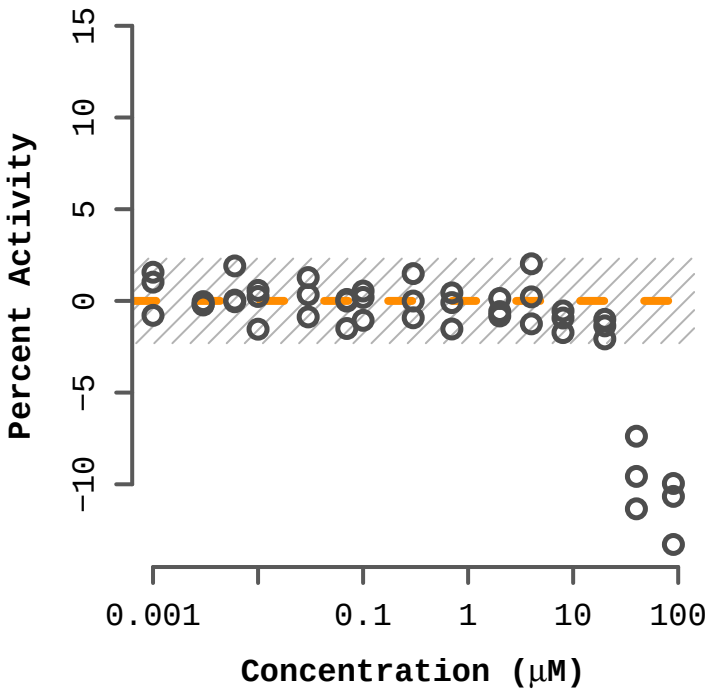
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 1.04 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Bromociclen
CHID:    41680   CASRN: 1715-40-8
SPID(S): Tox21_112345_1
M4ID:    12483146

HILL MODEL (in red):
      tp       ga       gw
val:  4.21     -2.34    2.71
sd:   0.619    0.227    2.57

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.21     -2.34    2.71     2.82     8.18
sd:   0.619    0.227    2.57     5960     43700

      CNST        HILL        GNLS
AIC:  265.39      233.05      237.05
PROB: 0           0.88        0.12
RMSE: 4.31        2.78        2.78

MAX_MEAN: 4.42      MAX_MED: 6.06      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

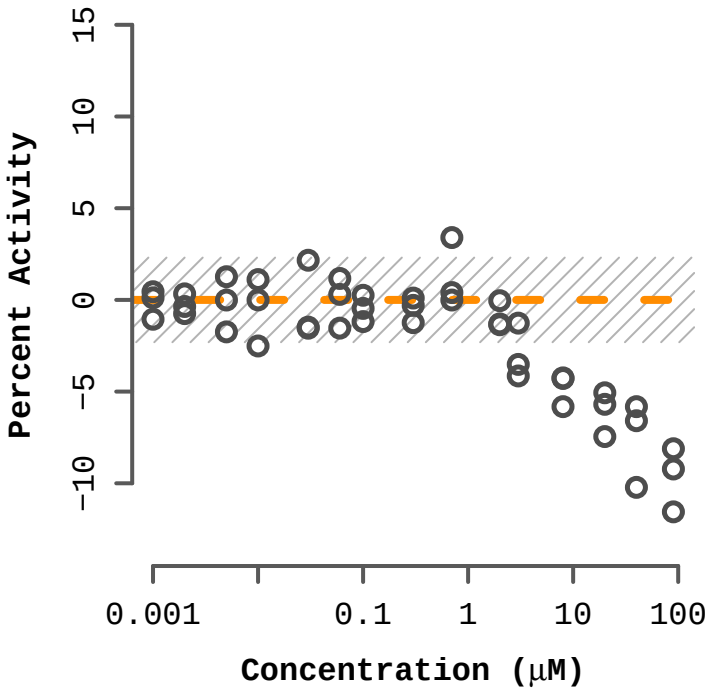
NAME: Bromofenoxim
CHID: 41681 **CASRN:** 13181-17-4
SPID(S): Tox21_300946
M4ID: 12478187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.79	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

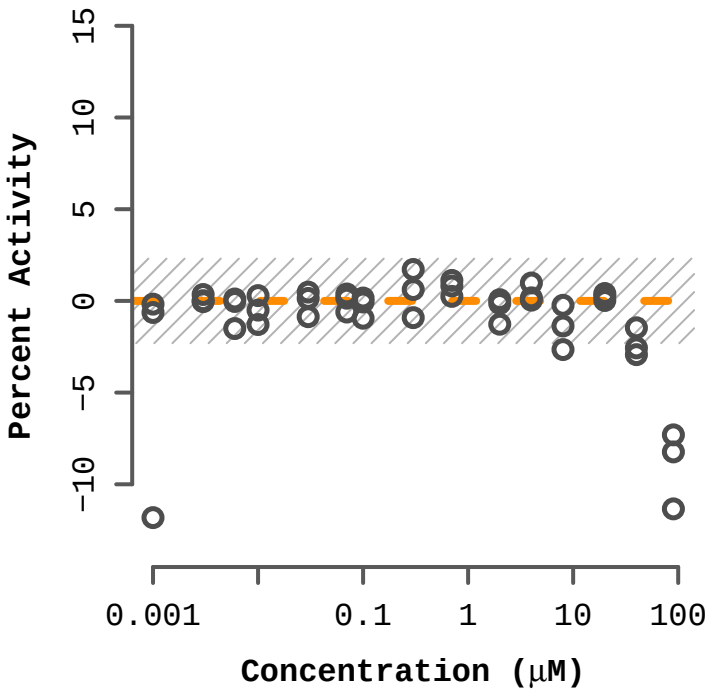
NAME: Bromophenol blue
CHID: 41682 CASRN: 115-39-9
SPID(S): Tox21_302080
M4ID: 12477053

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.54	NA	NA
PROB:	1	NA	NA
RMSE:	4.02	NA	NA

MAX_MEAN: 1.27 MAX_MED: 0.402 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

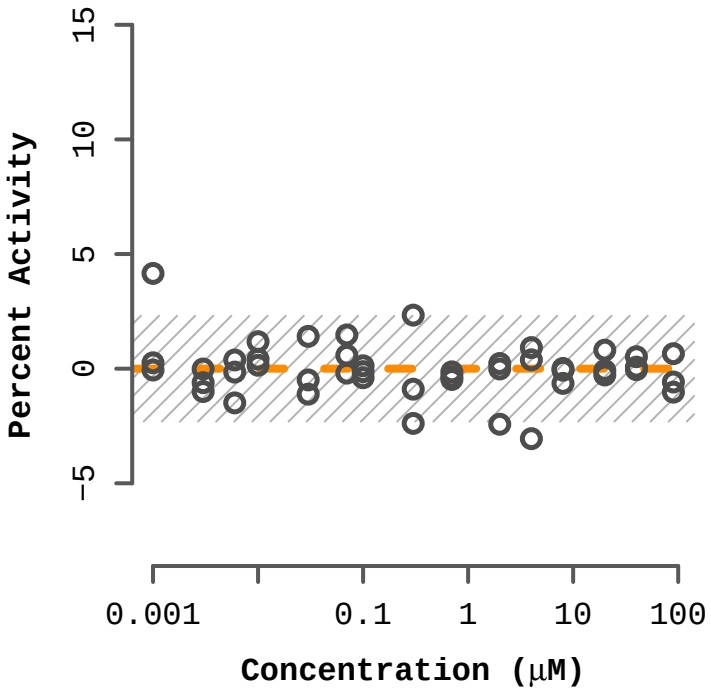
NAME: Bromofos
CHID: 41683 **CASRN:** 2104-96-3
SPID(S): Tox21_301918
M4ID: 12477215

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.45	NA	NA
PROB:	1	NA	NA
RMSE:	3.1	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 0.818 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

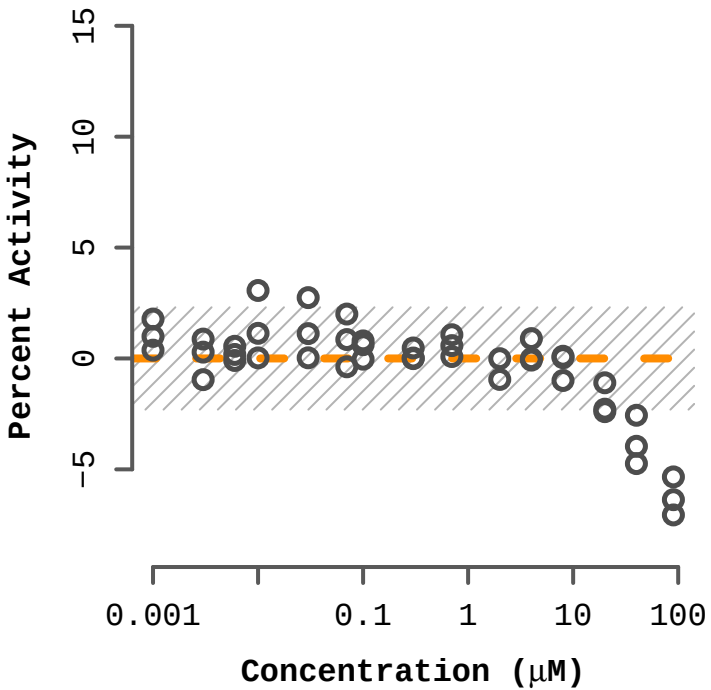
NAME: Bromophos-ethyl
CHID: 41684 **CASRN:** 4824-78-6
SPID(S): Tox21_301099
M4ID: 12478034

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 0.583 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

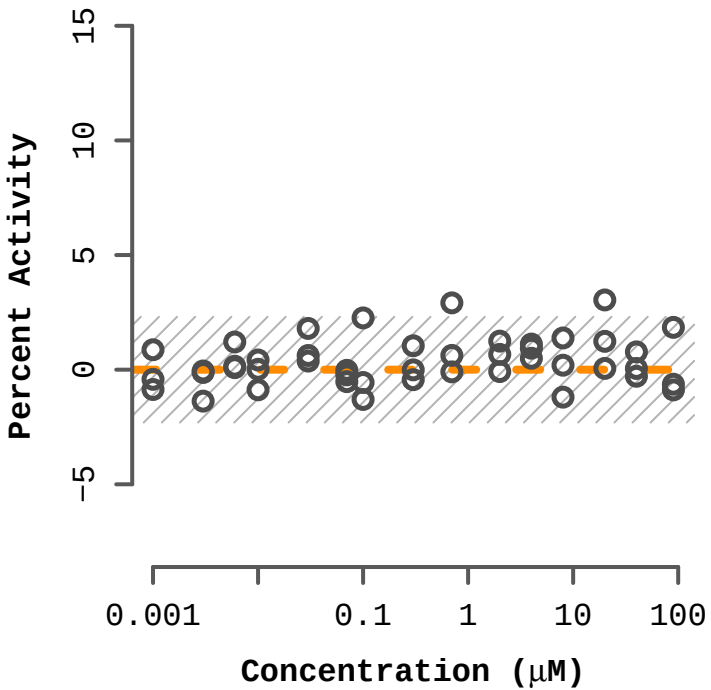
NAME: Bupirimate
CHID: 41688 CASRN: 41483-43-6
SPID(S): Tox21_301427
M4ID: 12477706

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.22	NA	NA
PROB:	1	NA	NA
RMSE:	2.19	NA	NA

MAX_MEAN: 1.41 MAX_MED: 1.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

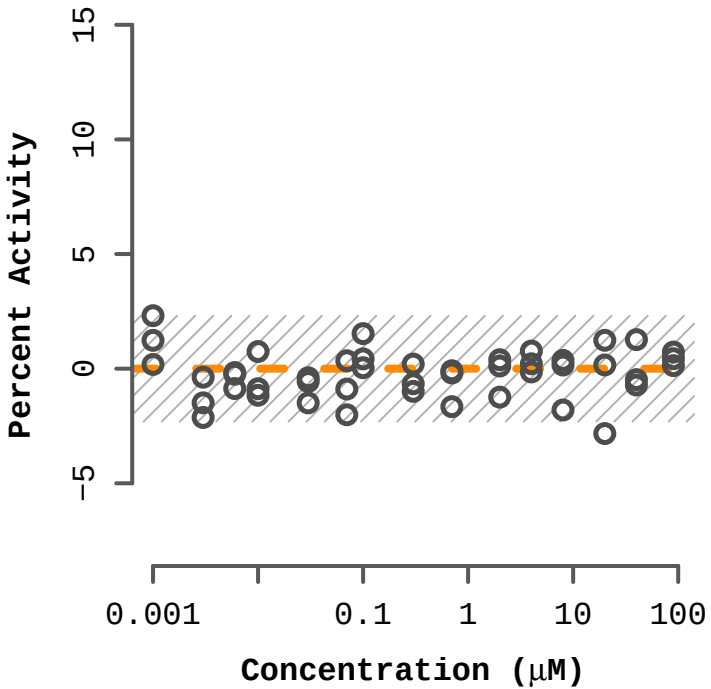
NAME: Butam
CHID: 41691 **CASRN:** 35256-85-0
SPID(S): Tox21_300476
M4ID: 12478656

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

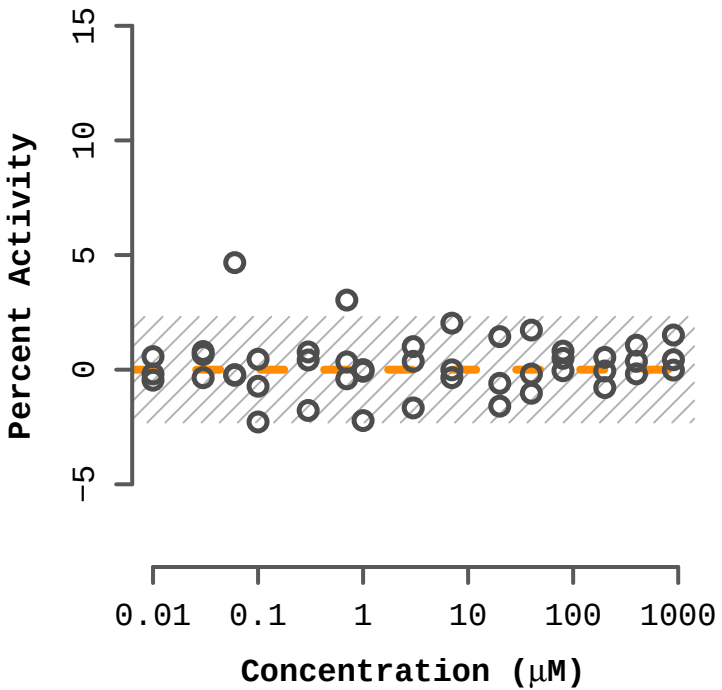
NAME: Dimethyl acetylsuccinate
CHID: 41692 **CASRN:** 10420-33-4
SPID(S): Tox21_300972
M4ID: 12478161

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

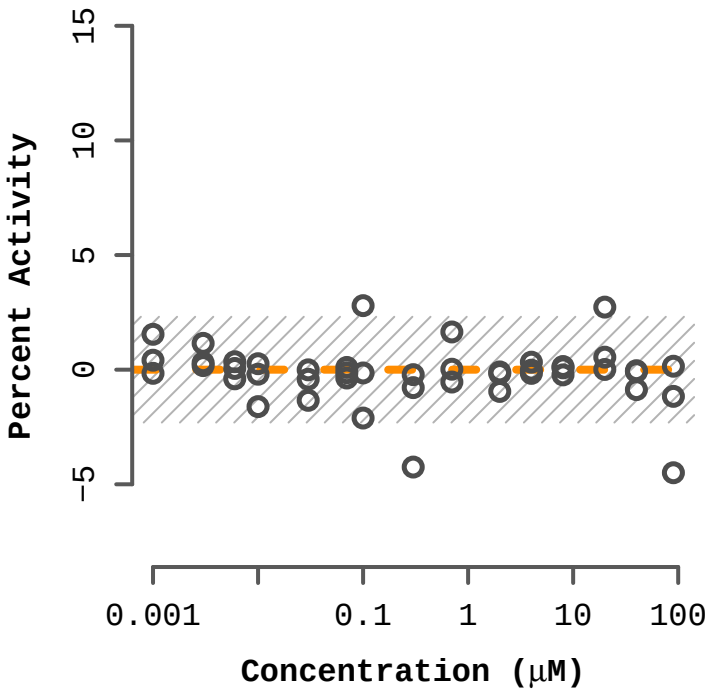
NAME: Butoxycarboxim
CHID: 41698 **CASRN:** 34681-23-7
SPID(S): Tox21_302272
M4ID: 12476861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.662 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

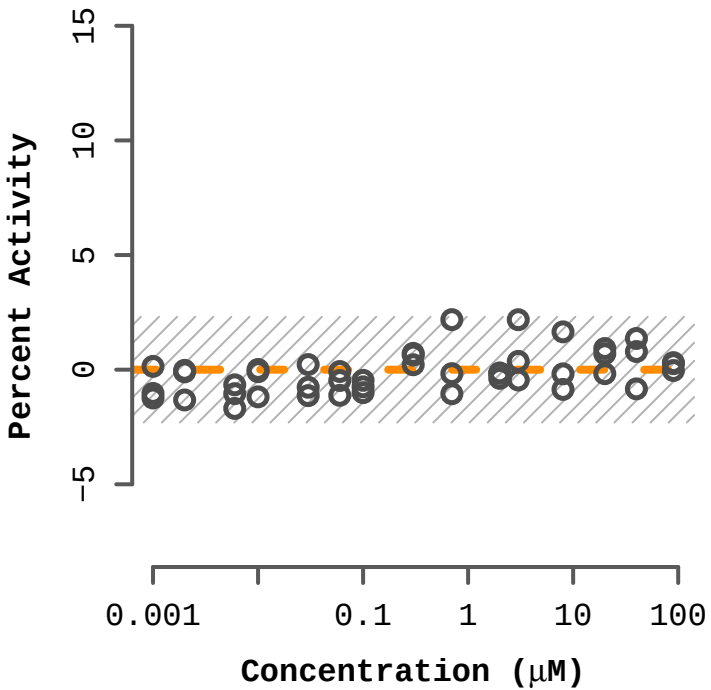
NAME: Buturon
CHID: 41699 CASRN: 3766-60-7
SPID(S): Tox21_301176
M4ID: 12477957

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.547 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

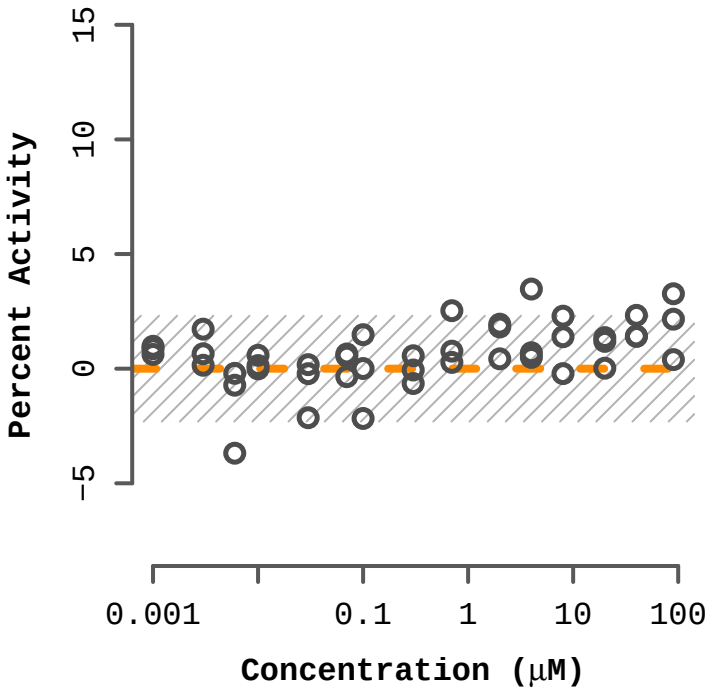
NAME: Butylnaphthalenesulfonic acid sodium salt
CHID: 41703 **CASRN:** 25638-17-9
SPID(S): Tox21_301770
M4ID: 12477363

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.698 **MAX_MED:** 0.794 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

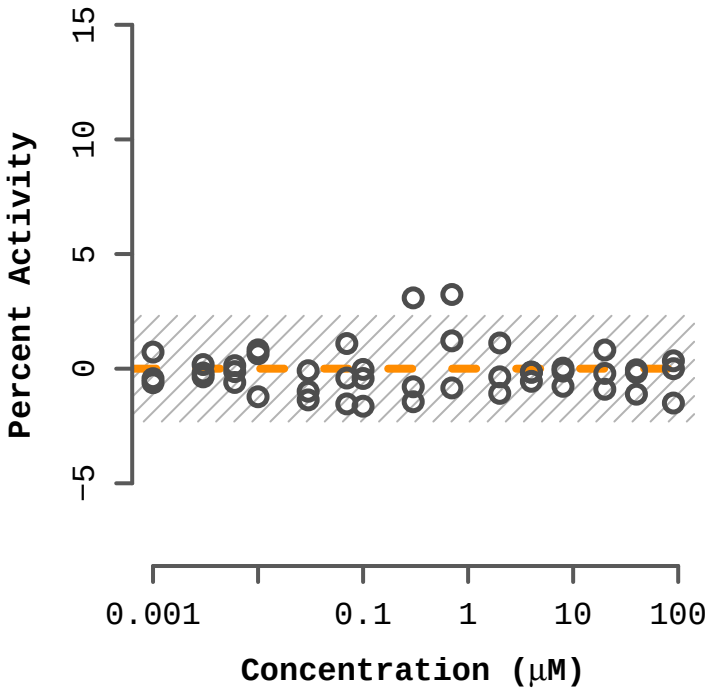
NAME: C.I. Acid Orange 24, monosodium salt
CHID: 41708 **CASRN:** 1320-07-6
SPID(S): Tox21_301862
M4ID: 12477271

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

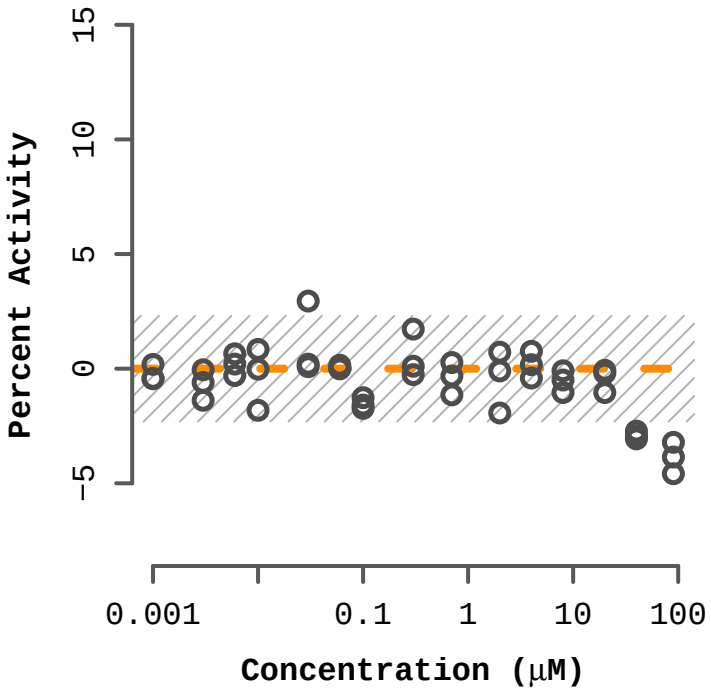
NAME: C.I. Acid Orange 8, monosodium salt
CHID: 41709 CASRN: 5850-86-2
SPID(S): Tox21_301654
M4ID: 12477479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.2 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

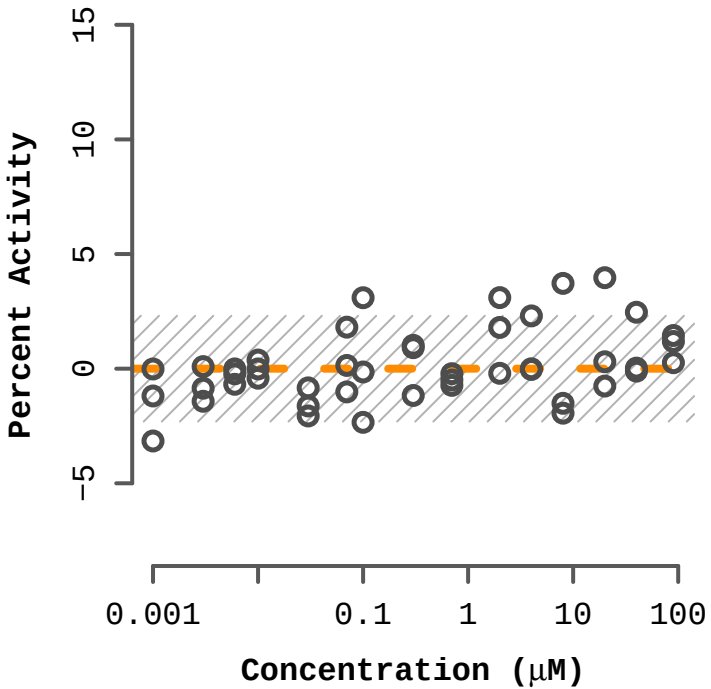
NAME: C.I. Acid Violet 12, disodium salt
CHID: 41715 CASRN: 6625-46-3
SPID(S): Tox21_301771
M4ID: 12477362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.08 MAX_MED: 0.201 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

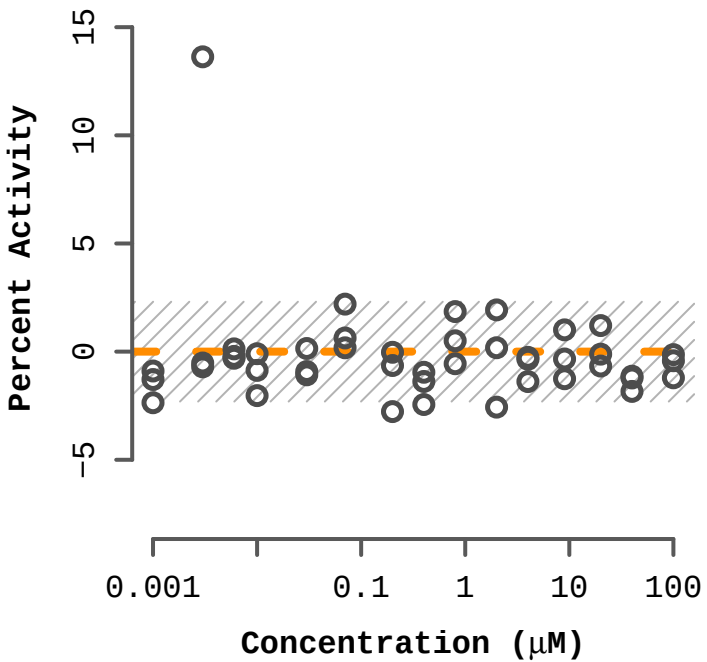
NAME: C.I. Acid Yellow 17, disodium salt
CHID: 41719 **CASRN:** 6359-98-4
SPID(S): Tox21_302264
M4ID: 12476869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

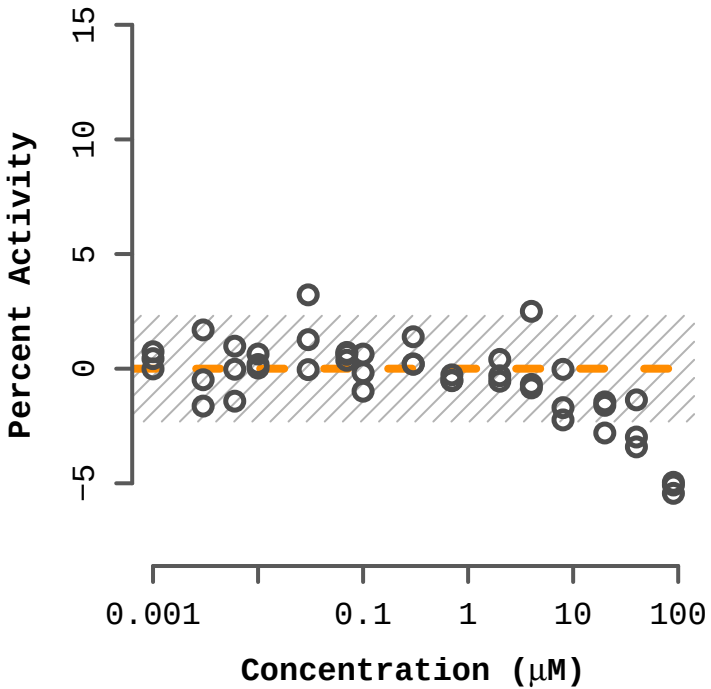
NAME: C.I. Acid Yellow 3 disodium salt
CHID: 41721 CASRN: 8004-92-0
SPID(S): Tox21_302091
M4ID: 12477042

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 4.14 MAX_MED: 0.633 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

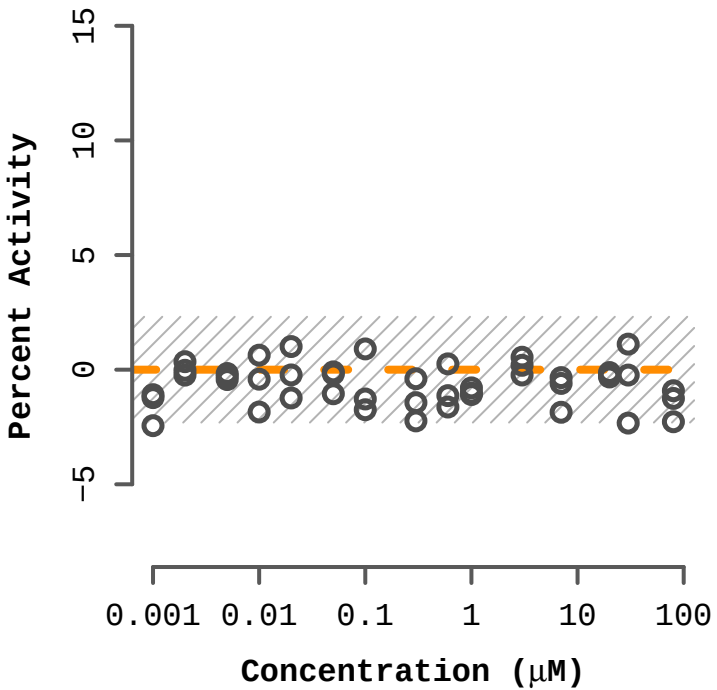
NAME: C.I. Direct Red 81 disodium salt
CHID: 41726 **CASRN:** 2610-11-9
SPID(S): Tox21_301538
M4ID: 12477595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.87	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

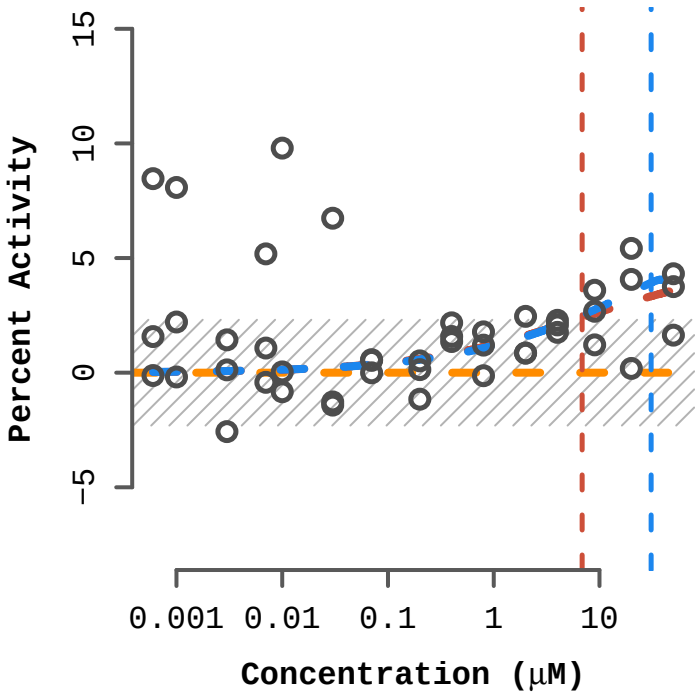
NAME: C.I. Direct Yellow 12
CHID: 41728 **CASRN:** 2870-32-8
SPID(S): Tox21_301479
M4ID: 12477654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.169 **MAX_MED:** 0.192 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Solvent Red 24
CHID: 41743 CASRN: 85-83-6
SPID(S): Tox21_112307_1
M4ID: 12483173

HILL MODEL (in red):

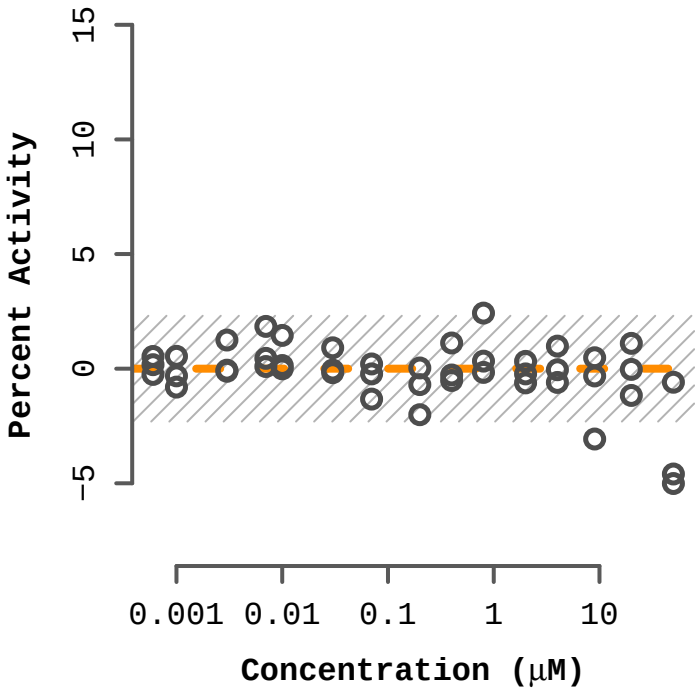
	tp	ga	gw
val:	4.79	0.836	0.55
sd:	4.61	1.77	0.554

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.87	1.49	0.507	1.75	9.96
sd:	15.5	2.91	0.358	0.369	73.9

	CNST	HILL	GNLS
AIC:	228.29	207.4	211.03
PROB:	0	0.86	0.14
RMSE:	3.22	2.8	2.8

MAX_MEAN: 3.37 **MAX_MED:** 4.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

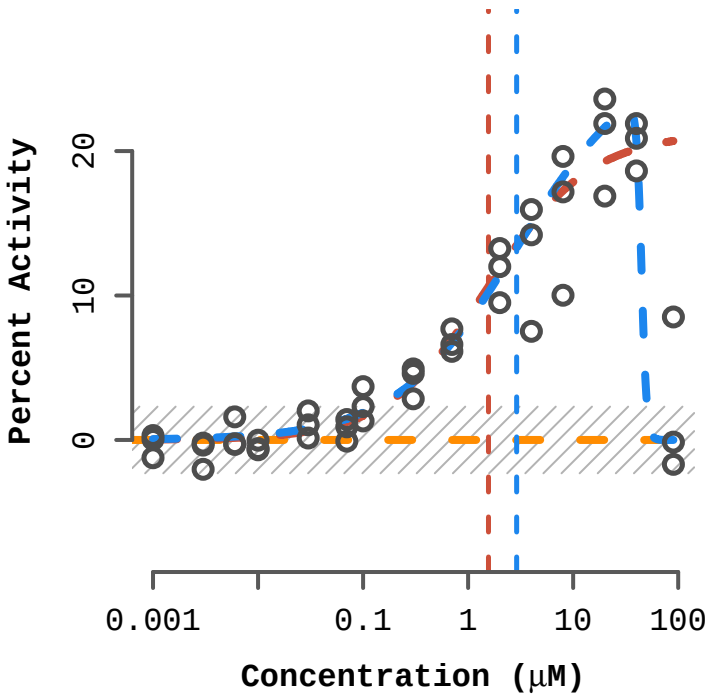
NAME: C.I. Solvent Red 49
CHID: 41744 **CASRN:** 509-34-2
SPID(S): Tox21_303794
M4ID: 12475394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.865 **MAX_MED:** 0.452 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Solvent Yellow 56
CHID: 41745 CASRN: 2481-94-9
SPID(S): Tox21_303805
M4ID: 12475383

HILL MODEL (in red):

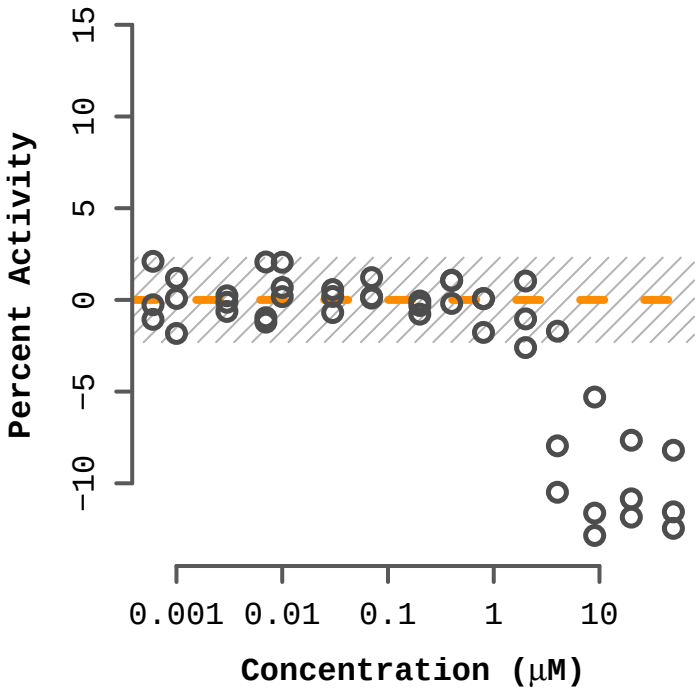
	tp	ga	gw
val:	21.2	0.194	0.895
sd:	1.5	0.105	0.118

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	26.6	0.462	0.763	1.65	18
sd:	3.34	0.178	0.0944	0.0232	10.5

	CNST	HILL	GNLS
AIC:	335.85	237.69	196.79
PROB:	0	0	1
RMSE:	10.11	5.3	2.43

MAX_MEAN: 20.8 MAX_MED: 21.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

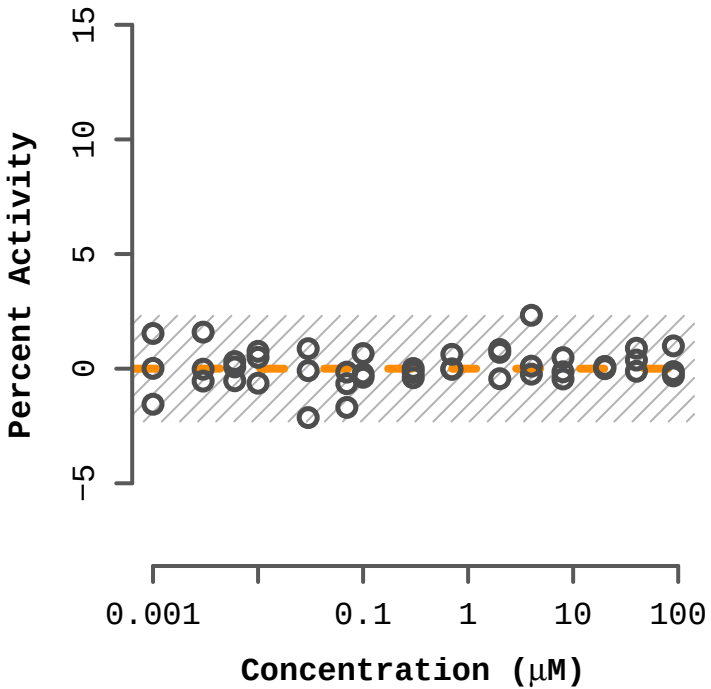
NAME: Cantharidin
CHID: 41752 **CASRN:** 56-25-7
SPID(S): Tox21_110326_1
M4ID: 12484453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.52	NA	NA
PROB:	1	NA	NA
RMSE:	5.2	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

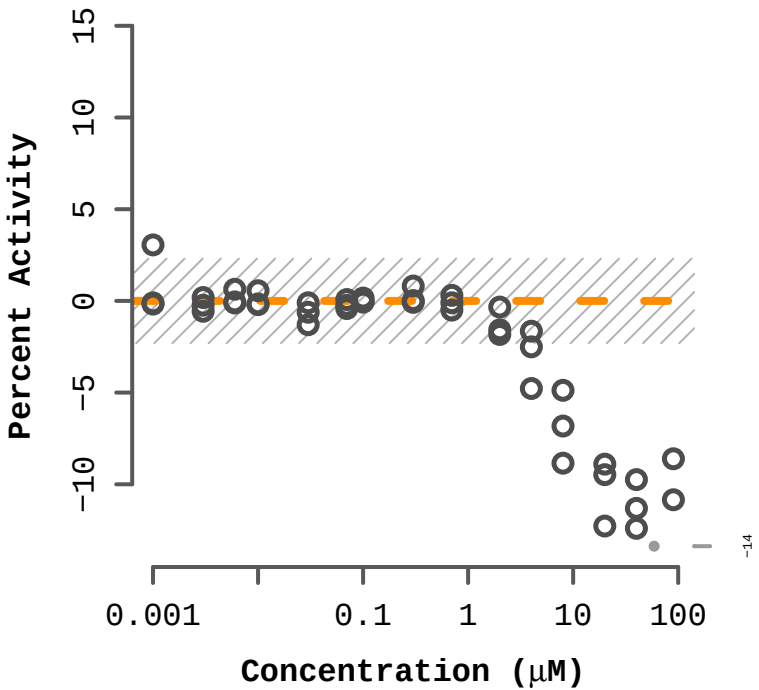
NAME: Carbetamide
CHID: 41756 CASRN: 16118-49-3
SPID(S): Tox21_301562
M4ID: 12477571

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.734 MAX_MED: 0.713 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

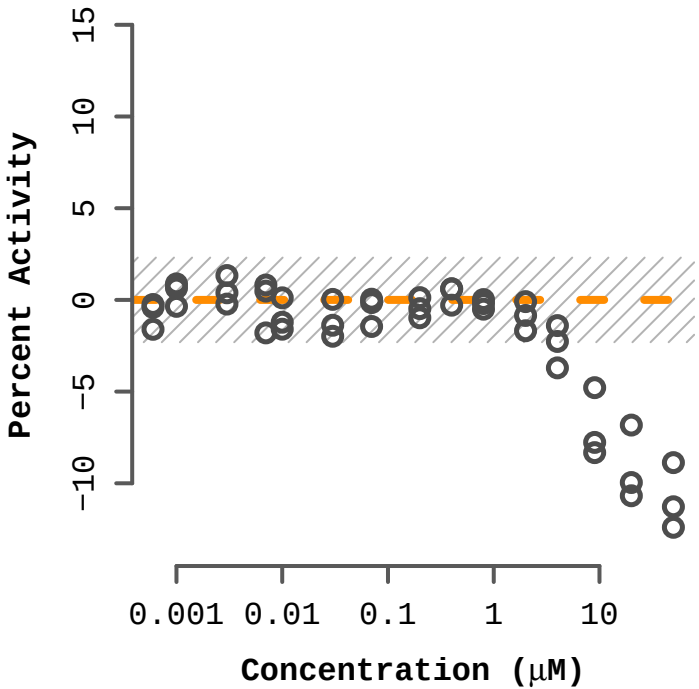
NAME: Ethylhexadecyldimethylammonium bromide
CHID: 41759 **CASRN:** 124-03-8
SPID(S): Tox21_302614
M4ID: 12476519 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	272.45	NA	NA
PROB:	1	NA	NA
RMSE:	5.35	NA	NA

MAX_MEAN: 0.927 **MAX_MED:** 0.0212 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

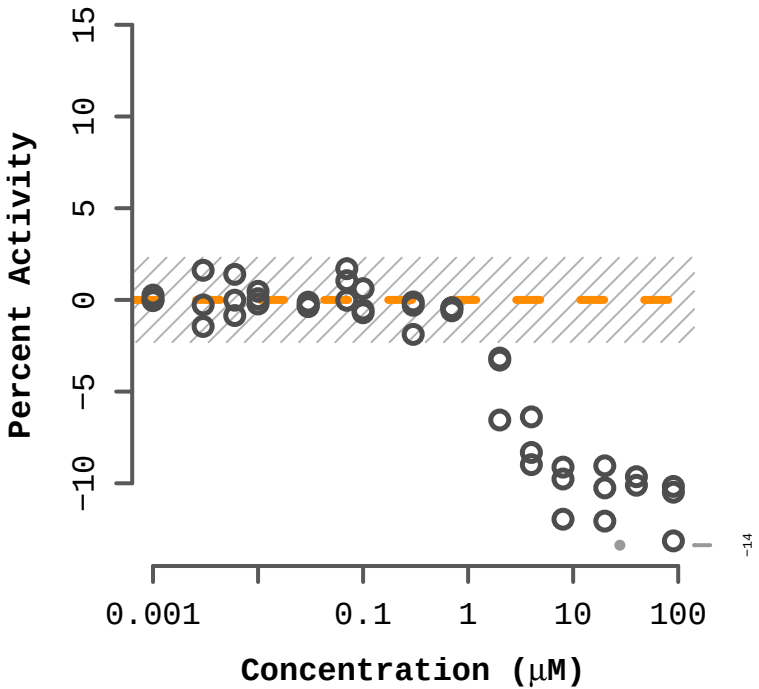
NAME: Ethylhexadecyldimethylammonium bromide
CHID: 41759 **CASRN:** 124-03-8
SPID(S): Tox21_112326_1
M4ID: 12483160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.03	NA	NA
PROB:	1	NA	NA
RMSE:	4.27	NA	NA

MAX_MEAN: 0.498 **MAX_MED:** 0.648 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

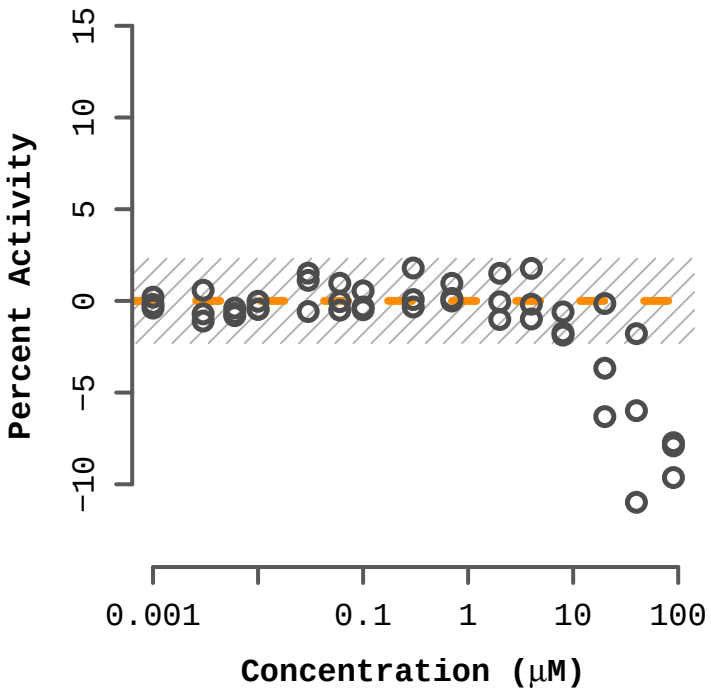
NAME: Cetylpyridinium chloride
CHID: 41761 CASRN: 123-03-5
SPID(S): Tox21_301296
M4ID: 12477837 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.09	NA	NA
PROB:	1	NA	NA
RMSE:	6.15	NA	NA

MAX_MEAN: 0.91 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

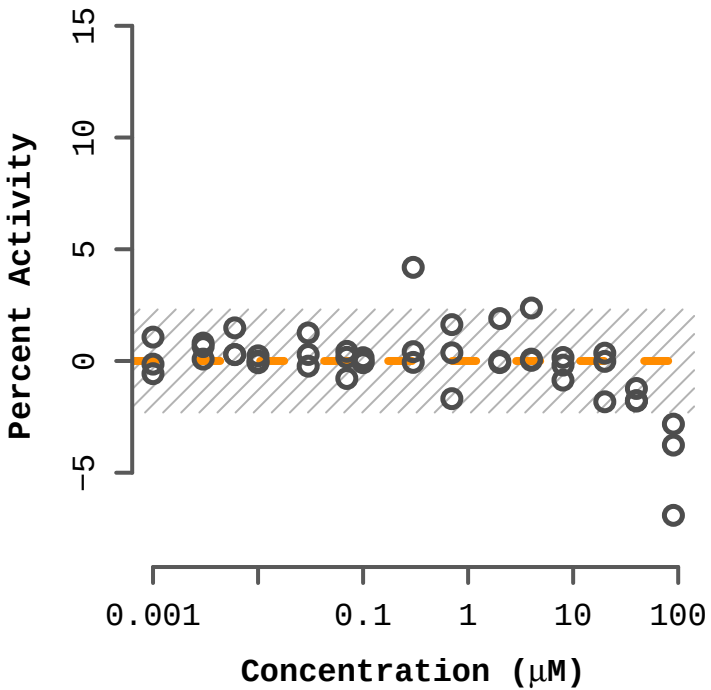
NAME: Chlorfluazuron
CHID: 41772 **CASRN:** 71422-67-8
SPID(S): Tox21_301567
M4ID: 12477566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.35	NA	NA
PROB:	1	NA	NA
RMSE:	3.18	NA	NA

MAX_MEAN: 0.686 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

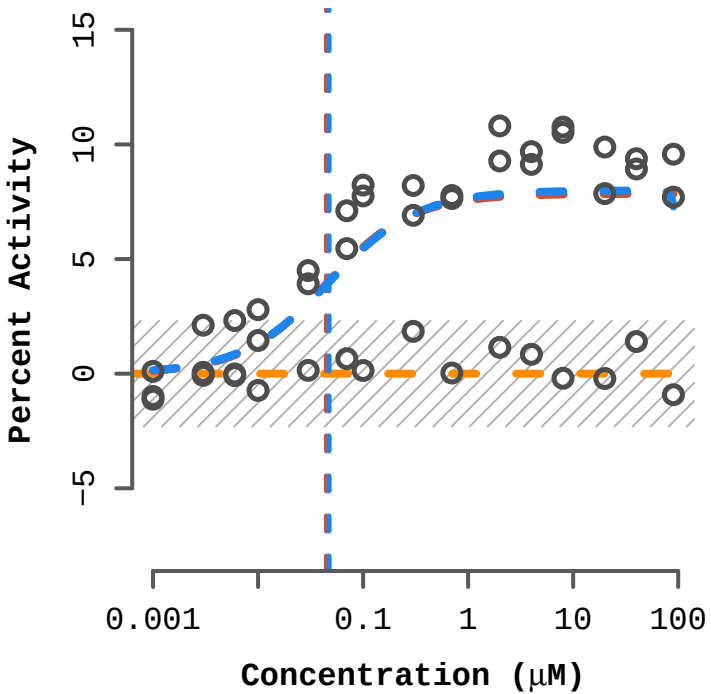
NAME: Chloropropylate
CHID: 41778 CASRN: 5836-10-2
SPID(S): Tox21_301914
M4ID: 12477219

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 1.52 MAX_MED: 0.645 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chlorthiamid
CHID: 41783 CASRN: 1918-13-4
SPID(S): Tox21_302207
M4ID: 12476926

HILL MODEL (in red):

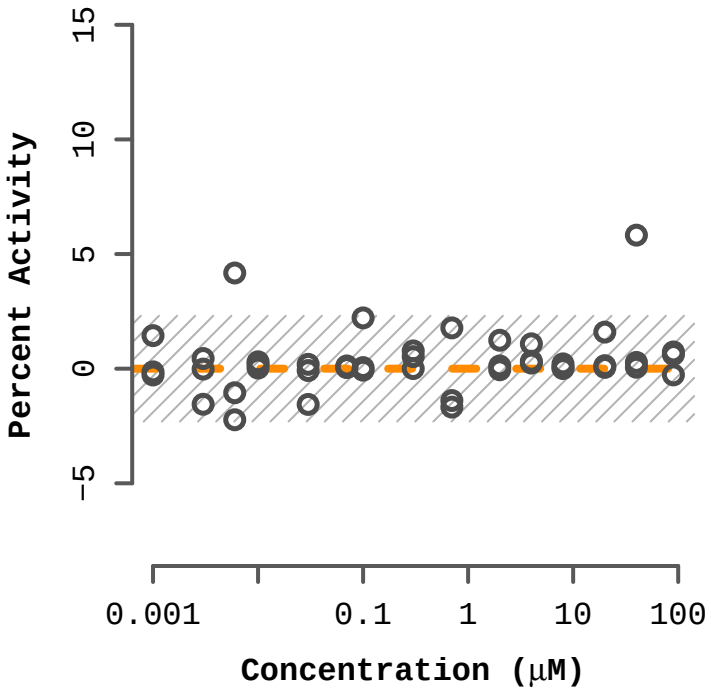
	tp	ga	gw
val:	7.85	−1.35	1.07
sd:	0.891	0.253	0.534

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8	−1.32	1.03	2.01	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	294.15	246.19	250.08
PROB:	0	0.88	0.12
RMSE:	5.95	3.52	3.52

MAX_MEAN: 7.08 MAX_MED: 10.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

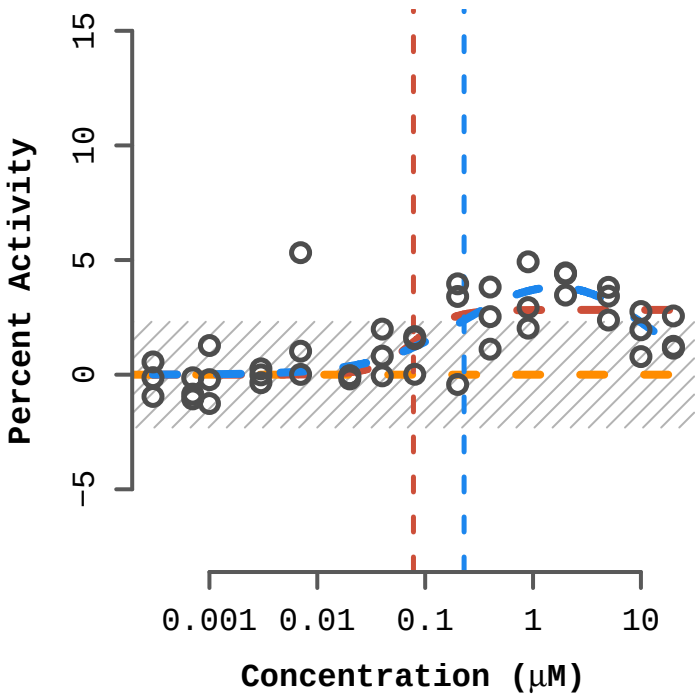
NAME: Citronellal
CHID: 41790 **CASRN:** 106-23-0
SPID(S): Tox21_301195
M4ID: 12477938

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 0.619 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clopidol
CHID: 41793 **CASRN:** 2971-90-6
SPID(S): Tox21_111465_1
M4ID: 12483669

HILL MODEL (in red):

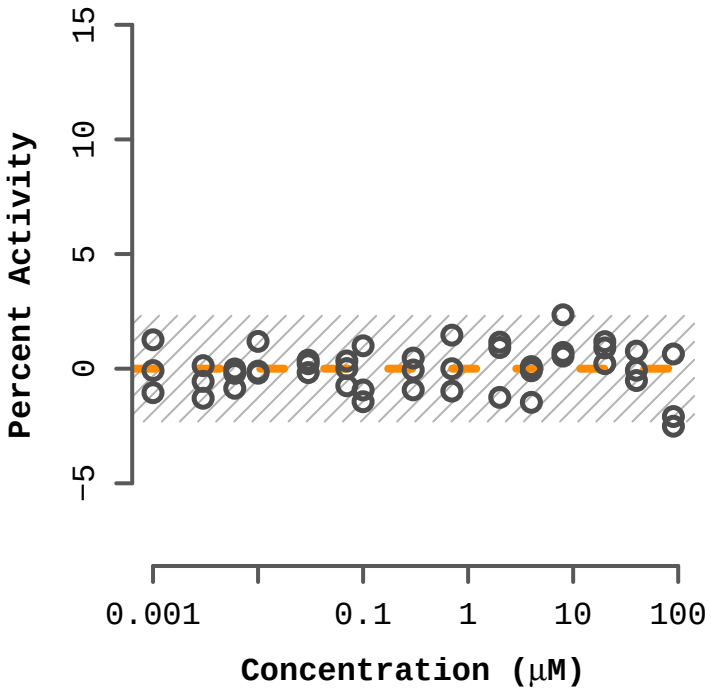
	tp	ga	gw
val:	2.83	−1.11	2.4
sd:	0.287	0.136	1.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.79	−0.639	1.02	0.984	1.27
sd:	3.44	0.831	0.709	0.479	0.87

	CNST	HILL	GNLS
AIC:	206.05	153.68	147.23
PROB:	0	0.04	0.96
RMSE:	2.3	1.32	1.21

MAX_MEAN: 4.1 **MAX_MED:** 4.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

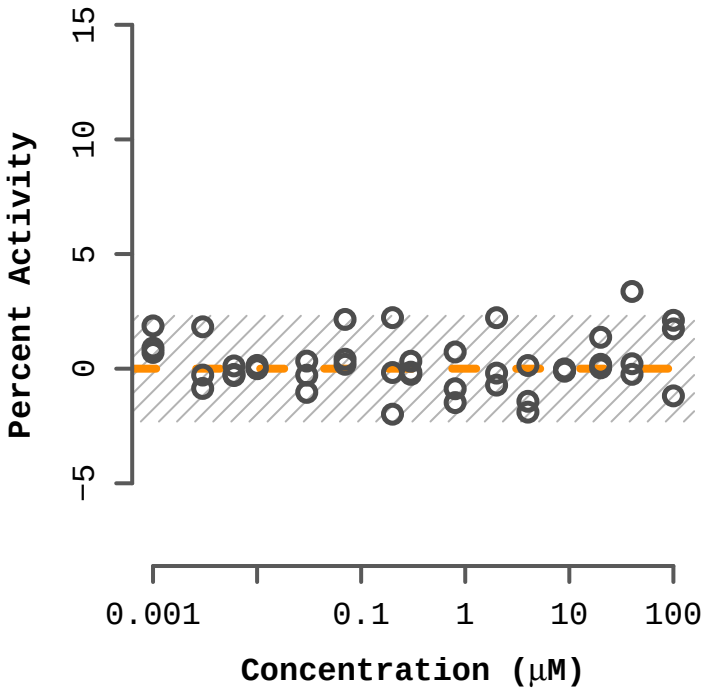
NAME: Cloquintocet-mexyl
CHID: 41794 **CASRN:** 99607-70-2
SPID(S): Tox21_301561
M4ID: 12477572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.925 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

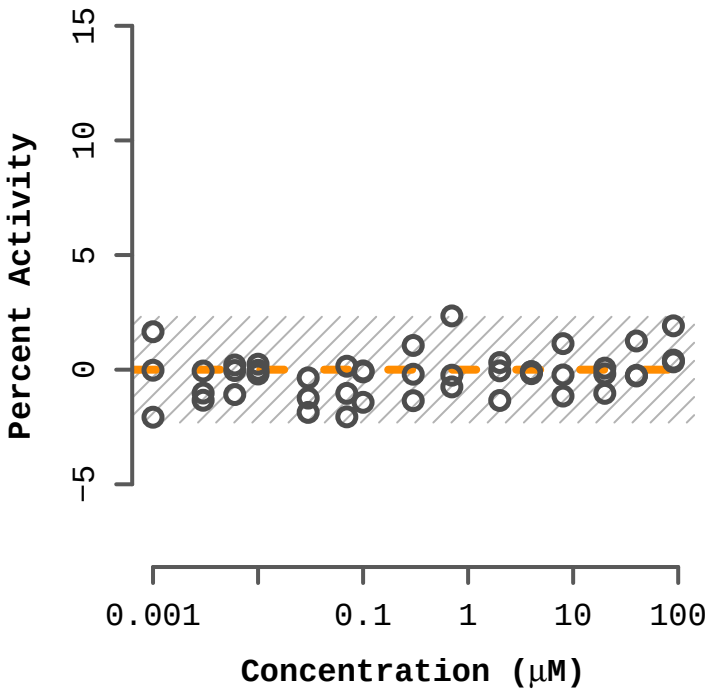
NAME: Coumachlor
CHID: 41797 CASRN: 81-82-3
SPID(S): Tox21_301860
M4ID: 12477273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.16 MAX_MED: 1.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

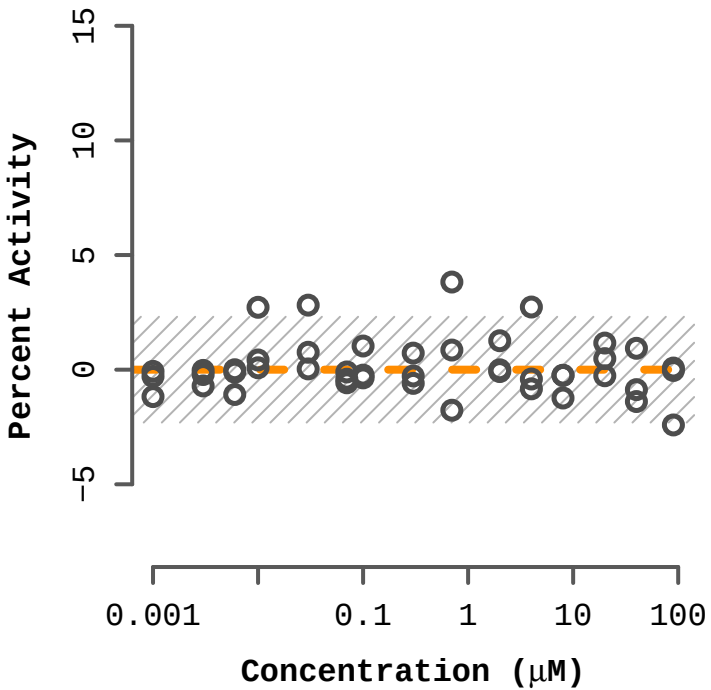
NAME: Coumatetralyl
CHID: 41799 **CASRN:** 5836-29-3
SPID(S): Tox21_301252
M4ID: 12477881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 0.421 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

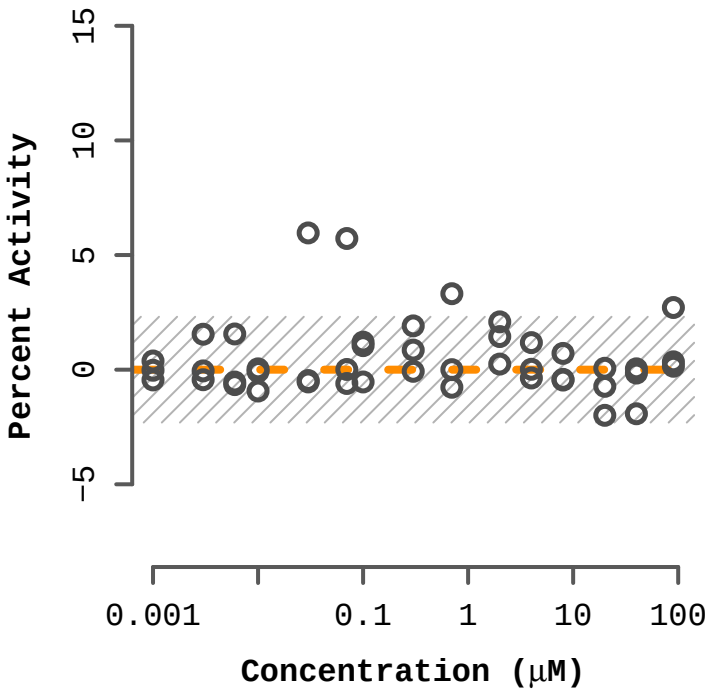
NAME: Copper(I) iodide
CHID: 41803 **CASRN:** 7681-65-4
SPID(S): Tox21_300719
M4ID: 12478414

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.858 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

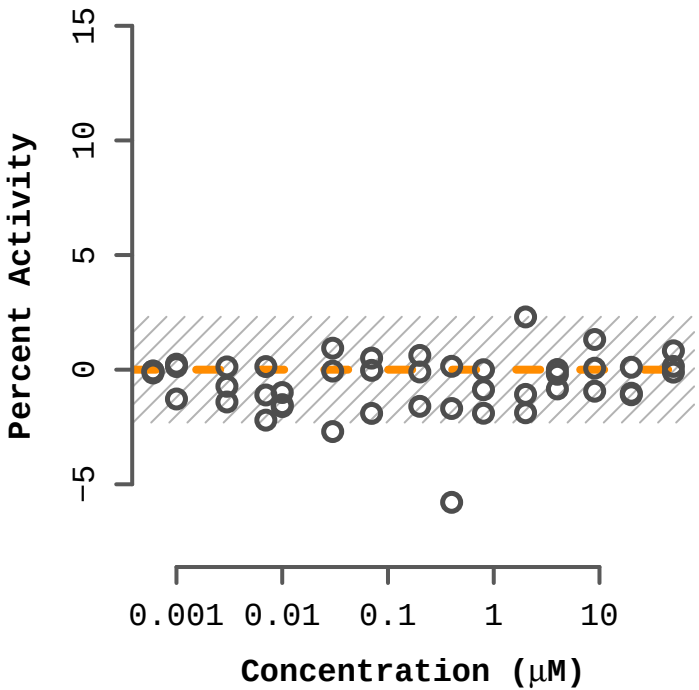
NAME: Cyclamic acid
CHID: 41809 **CASRN:** 100-88-9
SPID(S): Tox21_301008
M4ID: 12478125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

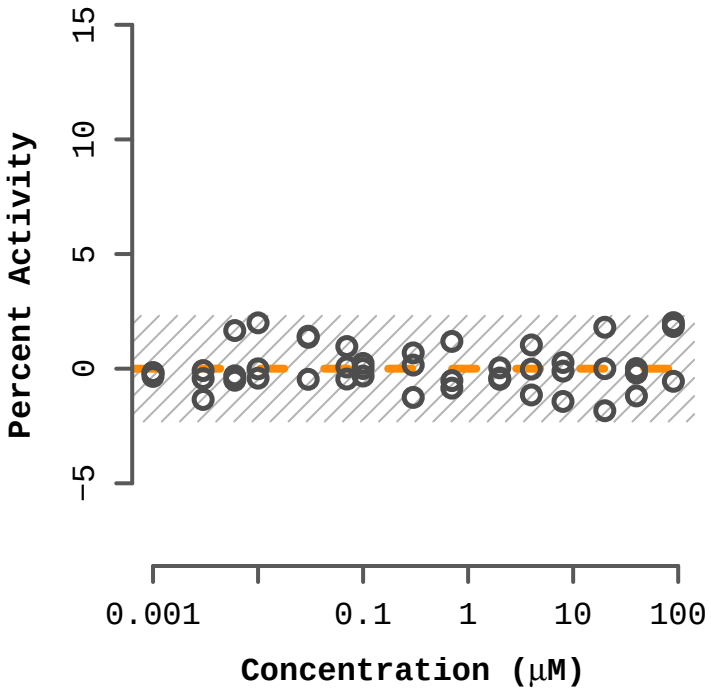
NAME: Cyclamic acid
CHID: 41809 **CASRN:** 100-88-9
SPID(S): Tox21_112285_1
M4ID: 12483182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.287 **MAX_MED:** 0.143 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

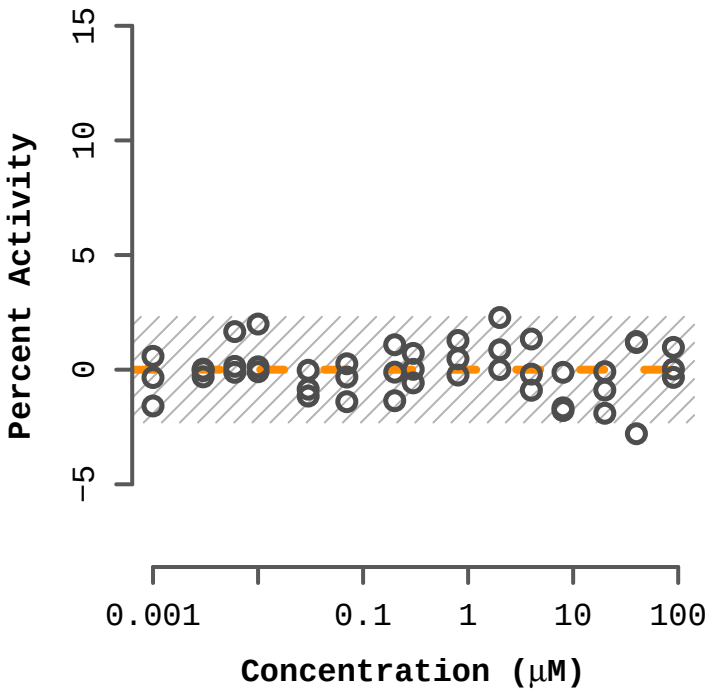
NAME: Dihydro-alpha-terpineol
CHID: 41812 **CASRN:** 498-81-7
SPID(S): Tox21_303808
M4ID: 12475380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

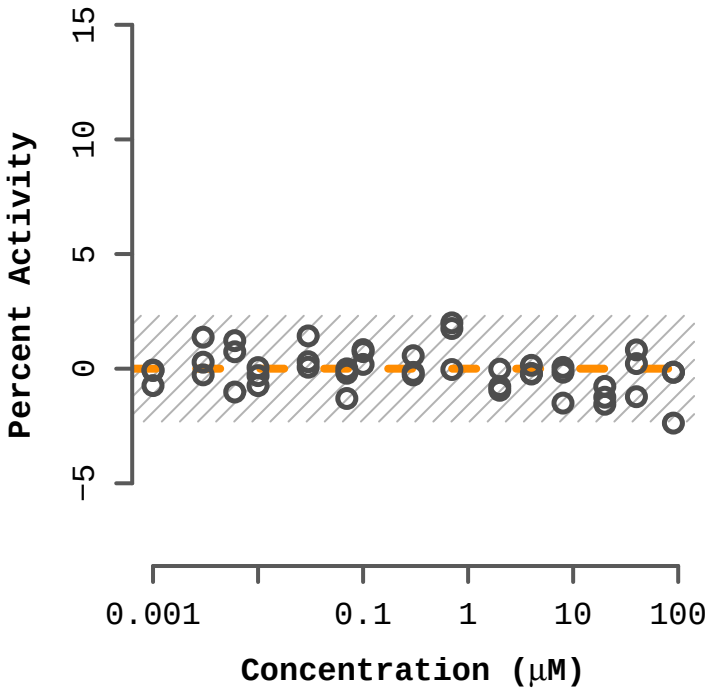
NAME: 4-Methylcyclohexanemethanol
CHID: 41813 **CASRN:** 34885-03-5
SPID(S): Tox21_301528
M4ID: 12477605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

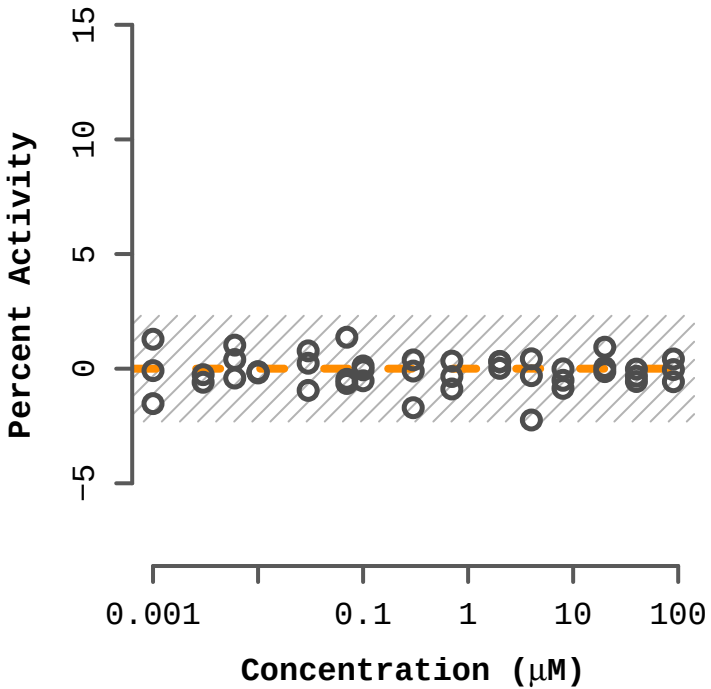
NAME: 3,3,5-Trimethylcyclohexanol
CHID: 41815 **CASRN:** 116-02-9
SPID(S): Tox21_301500
M4ID: 12477633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

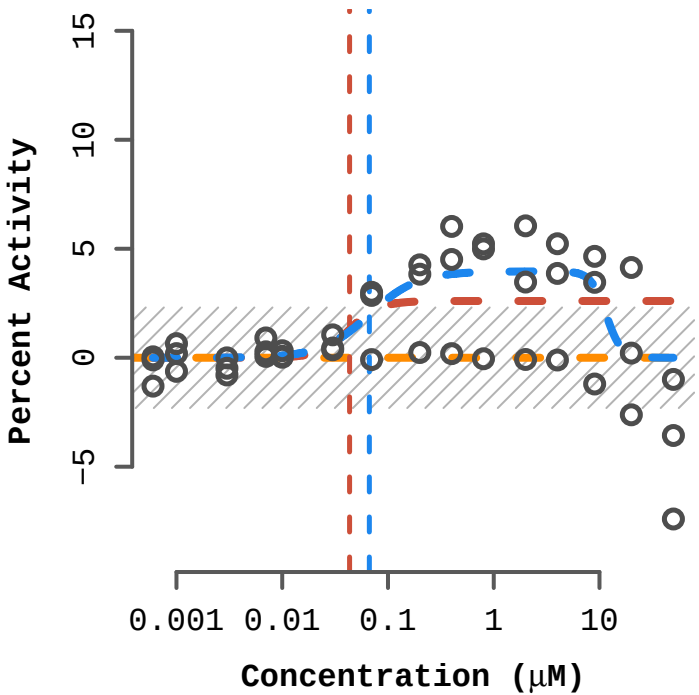
NAME: 2-sec-Butylcyclohexanone
CHID: 41818 CASRN: 14765-30-1
SPID(S): Tox21_301774
M4ID: 12477359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.34 MAX_MED: 0.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cypromid
CHID: 41827 CASRN: 2759-71-9
SPID(S): Tox21_111954_1
M4ID: 12483411

HILL MODEL (in red):

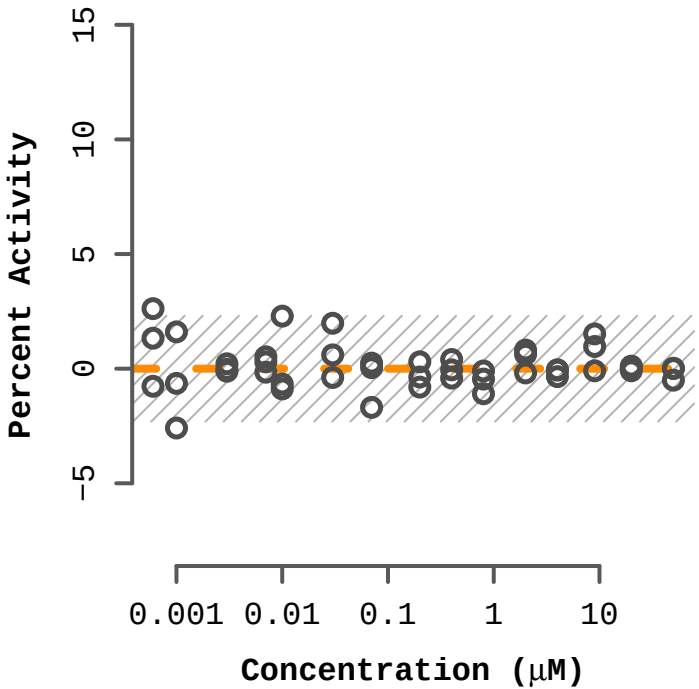
	tp	ga	gw
val:	2.6	−1.36	3.11
sd:	0.64	0.251	3.89

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.96	−1.18	1.92	1.06	6.07
sd:	0.664	0.211	1.39	0.228	11.7

	CNST	HILL	GNLS
AIC:	225.67	214.36	202.8
PROB:	0	0	1
RMSE:	2.92	2.59	2.17

MAX_MEAN: 3.58 MAX_MED: 5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

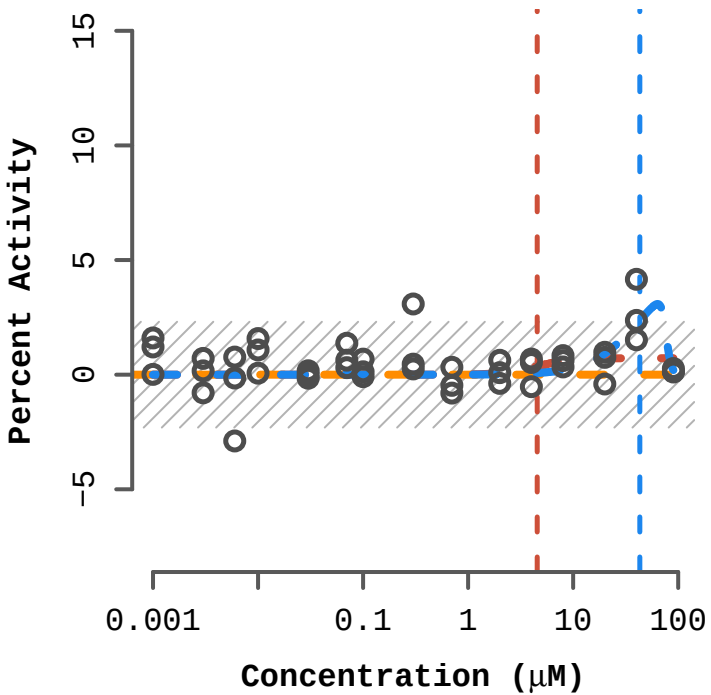
NAME: Cythioate
CHID: 41828 **CASRN:** 115-93-5
SPID(S): Tox21_113080
M4ID: 12482816

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D-Glucuronolactone
CHID: 41844 CASRN: 32449-92-6
SPID(S): Tox21_300949
M4ID: 12478184

HILL MODEL (in red):

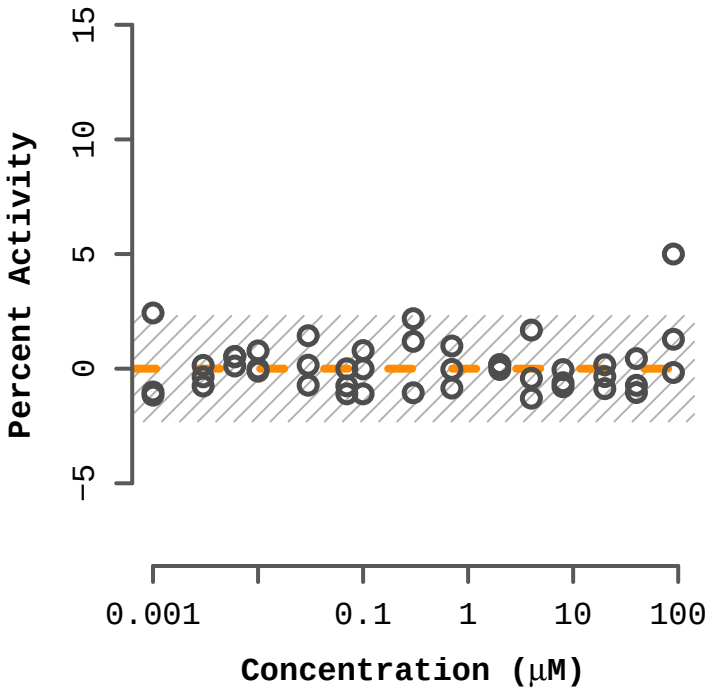
	tp	ga	gw
val:	0.719	0.658	2.74
sd:	0.321	0.376	4.34

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.74	1.63	1.86	1.88	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	133.49	131.23	125.62
PROB:	0.02	0.06	0.93
RMSE:	1.17	1.06	0.94

MAX_MEAN: 2.68 MAX_MED: 2.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

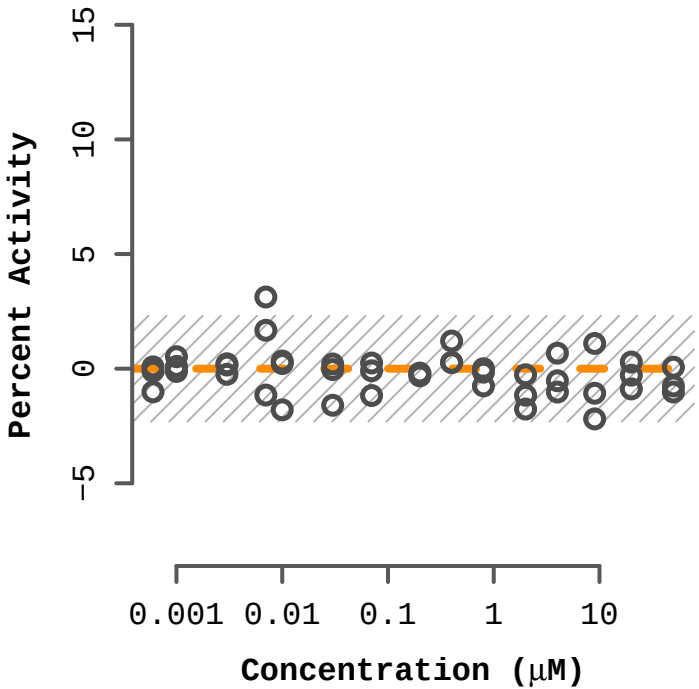
NAME: Dibutyl decanedioate
CHID: 41847 **CASRN:** 109-43-3
SPID(S): Tox21_300154
M4ID: 12478976

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

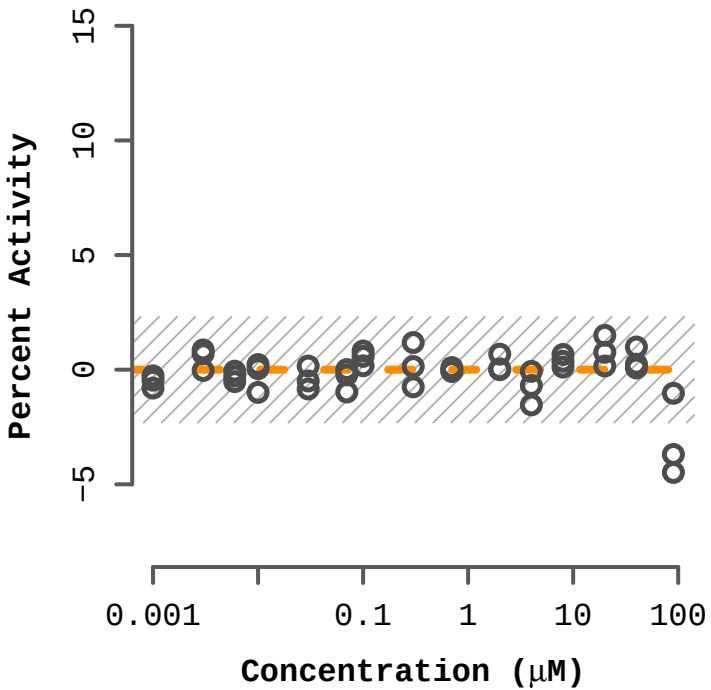
NAME: Dibutyl decanedioate
CHID: 41847 **CASRN:** 109-43-3
SPID(S): Tox21_113651
M4ID: 12482561

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

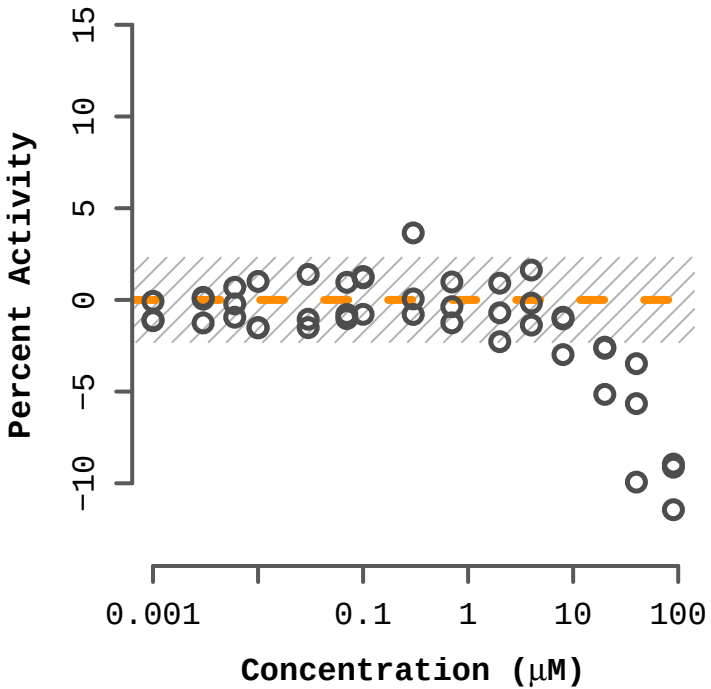
NAME: Dicapthon
CHID: 41850 **CASRN:** 2463-84-5
SPID(S): Tox21_301908
M4ID: 12477225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 0.759 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

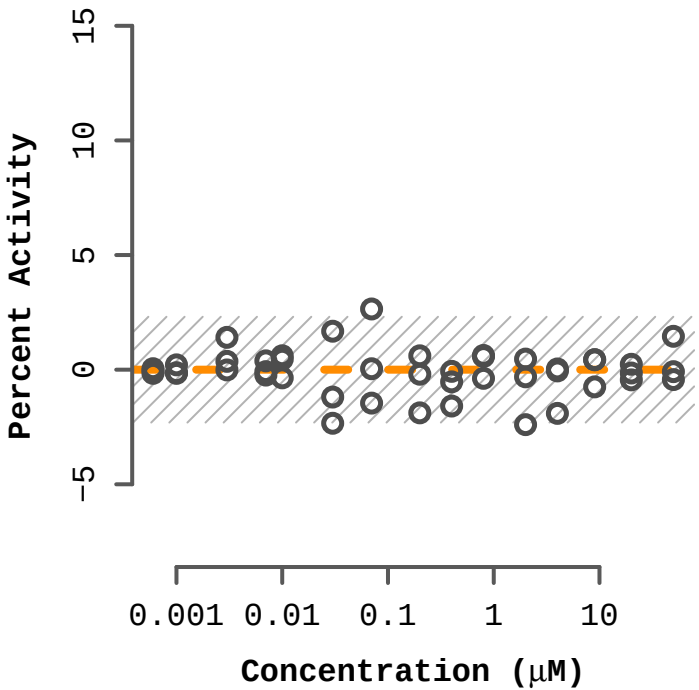
NAME: Dichlofluanid
CHID: 41851 **CASRN:** 1085-98-9
SPID(S): Tox21_300960
M4ID: 12478173

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.09	NA	NA
PROB:	1	NA	NA
RMSE:	3.46	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

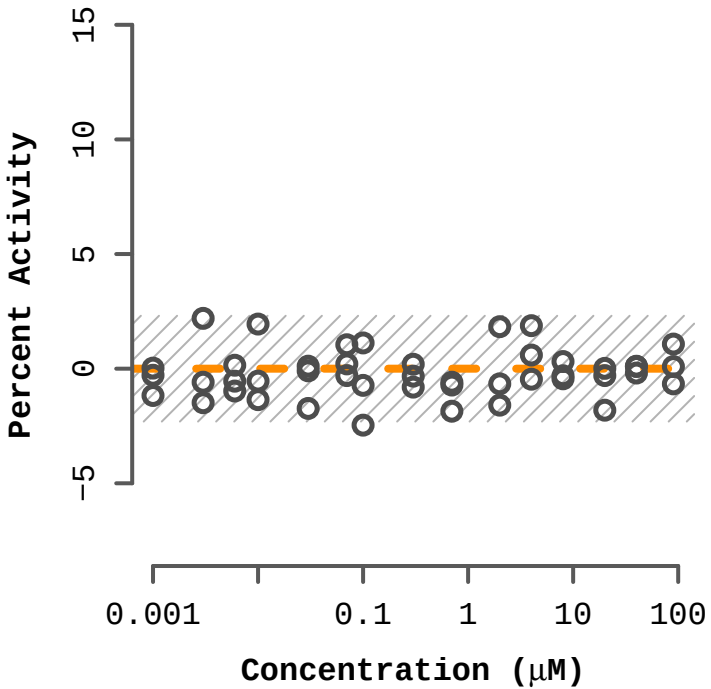
NAME: Dichloralurea
CHID: 41852 **CASRN:** 116-52-9
SPID(S): Tox21_112344_1
M4ID: 12483147

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 0.573 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

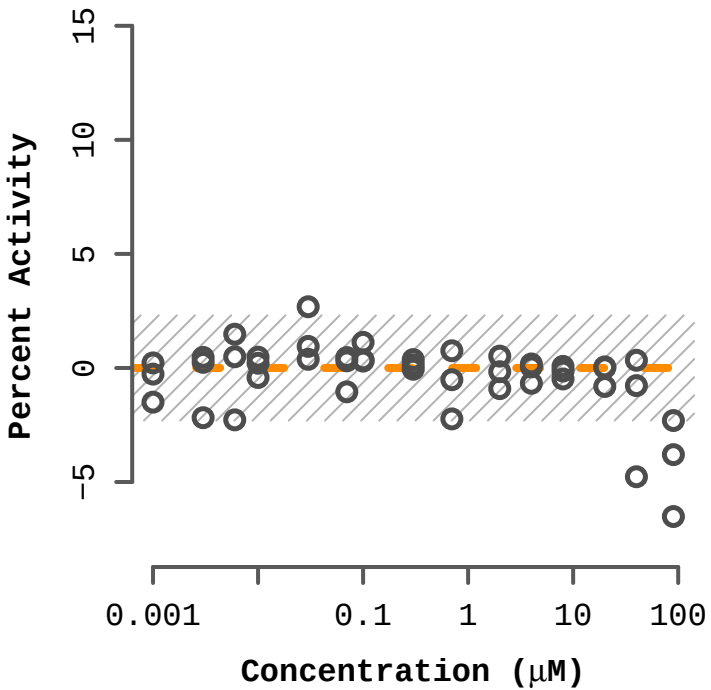
NAME: Diethyl phosphite
CHID: 41861 **CASRN:** 762-04-9
SPID(S): Tox21_302033
M4ID: 12477100

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 0.595 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

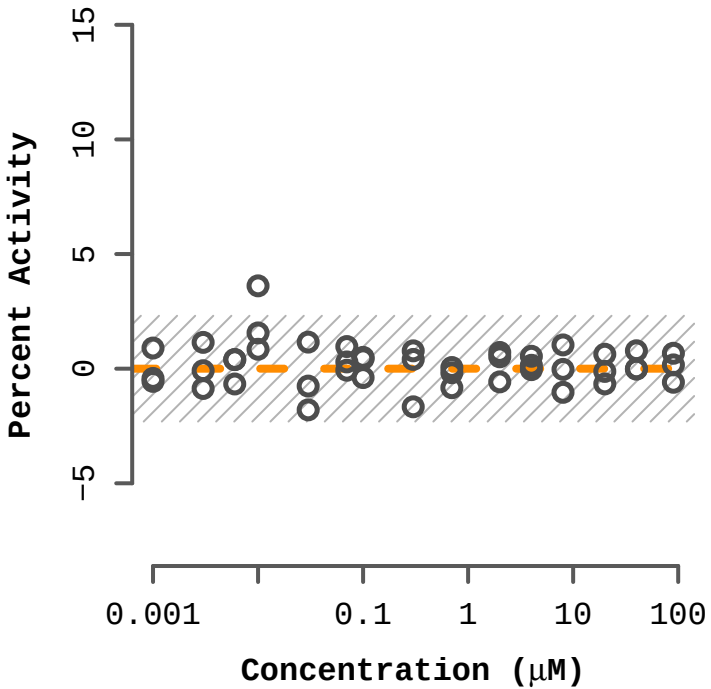
NAME: Dimethametryn
CHID: 41873 **CASRN:** 22936-75-0
SPID(S): Tox21_302223
M4ID: 12476910

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 0.947 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

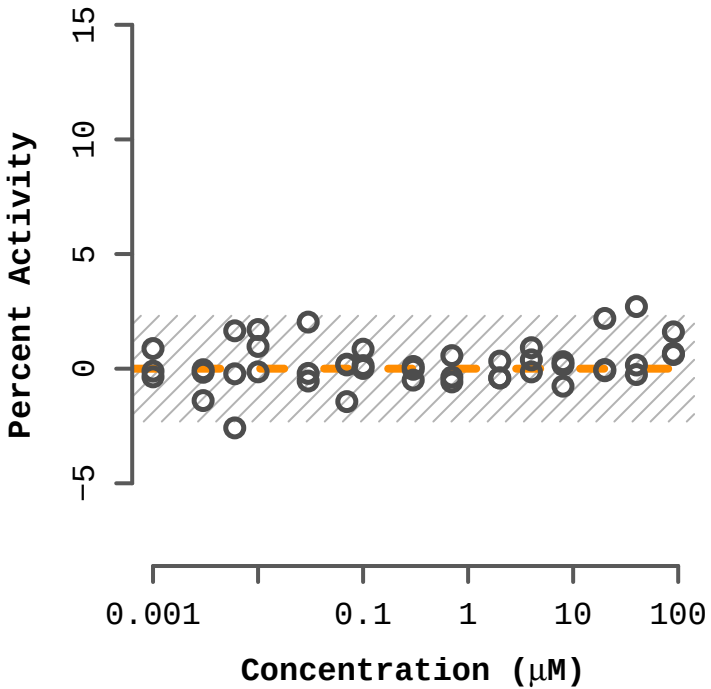
NAME: Dimethylbenzylcarbinyl acetate
CHID: 41877 **CASRN:** 151-05-3
SPID(S): Tox21_301781
M4ID: 12477352

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

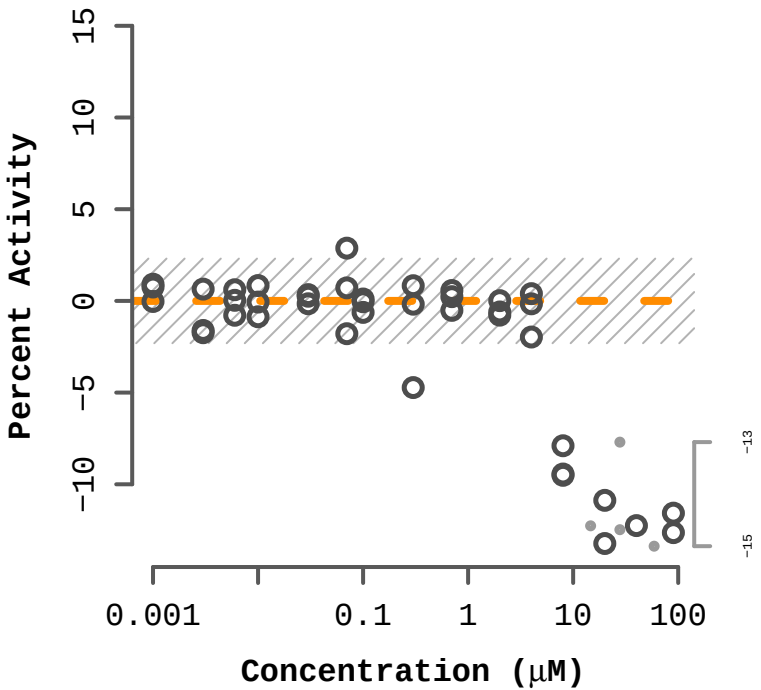
NAME: Dimetilan
CHID: 41880 CASRN: 644-64-4
SPID(S): Tox21_301855
M4ID: 12477278

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.968 **MAX_MED:** 0.972 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

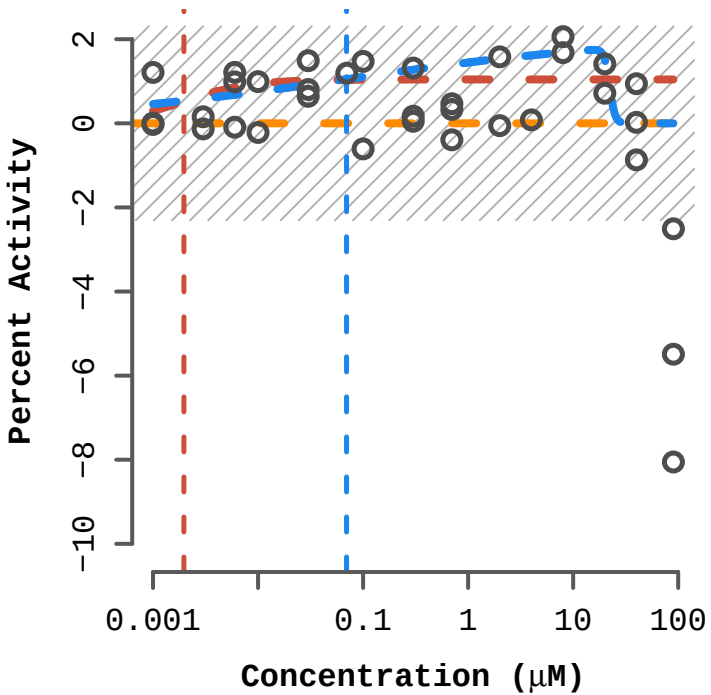
NAME: Dinoterb
CHID: 41883 CASRN: 1420-07-1
SPID(S): Tox21_300743
M4ID: 12478390 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.03	NA	NA
PROB:	1	NA	NA
RMSE:	6.48	NA	NA

MAX_MEAN: 0.601 **MAX_MED:** 0.758 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diofenolan
CHID: 41884 CASRN: 63837-33-2
SPID(S): Tox21_301560
M4ID: 12477573

HILL MODEL (in red):

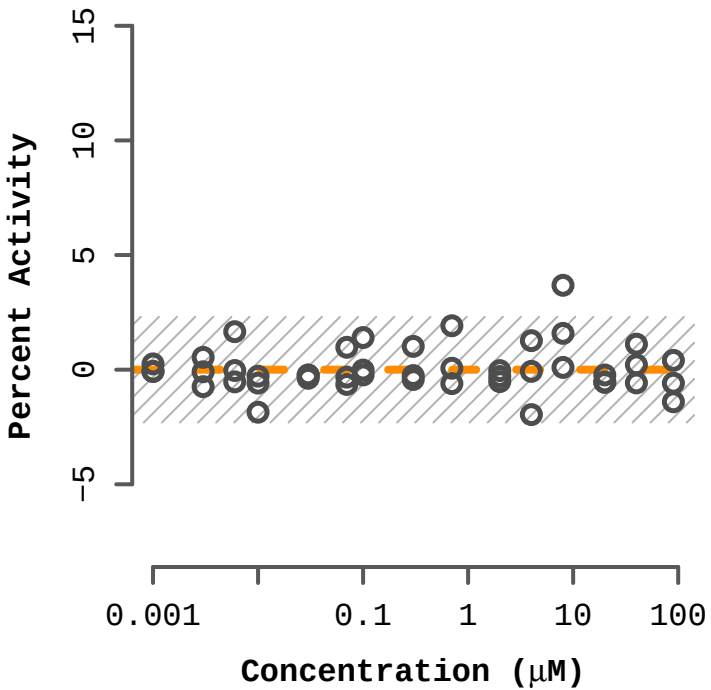
	tp	ga	gw
val:	1.04	−2.71	1.34
sd:	0.249	0.725	1.82

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.1	−1.16	0.3	1.35	16.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	190.43	178.91	173.89
PROB:	0	0.08	0.92
RMSE:	2.12	2.05	1.8

MAX_MEAN: 2.54 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

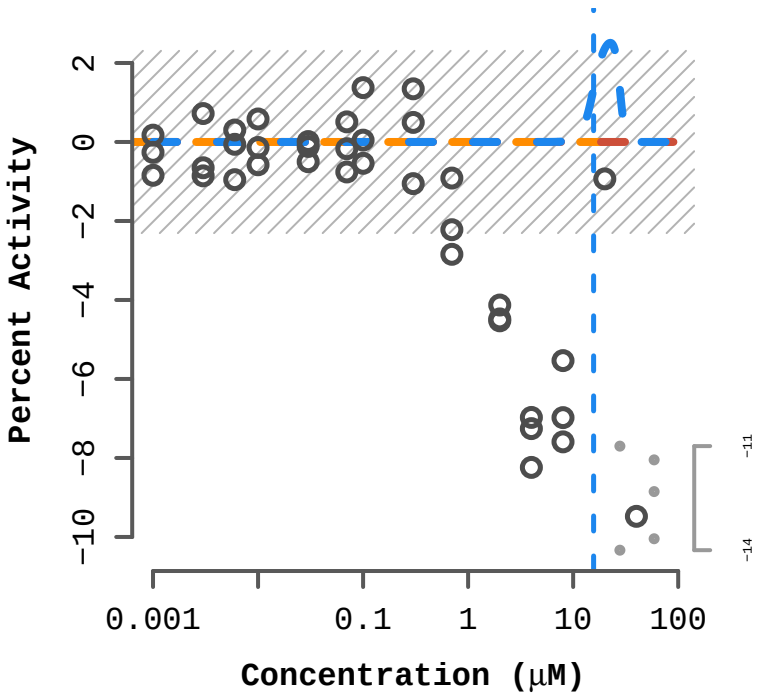
NAME: Dioxacarb
CHID: 41886 CASRN: 6988-21-2
SPID(S): Tox21_302420
M4ID: 12476713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.79 MAX_MED: 1.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dipentaerythritol pentaacrylate
CHID: 41887 CASRN: 60506-81-2
SPID(S): Tox21_301722
M4ID: 12477411 BRK

HILL MODEL (in red):

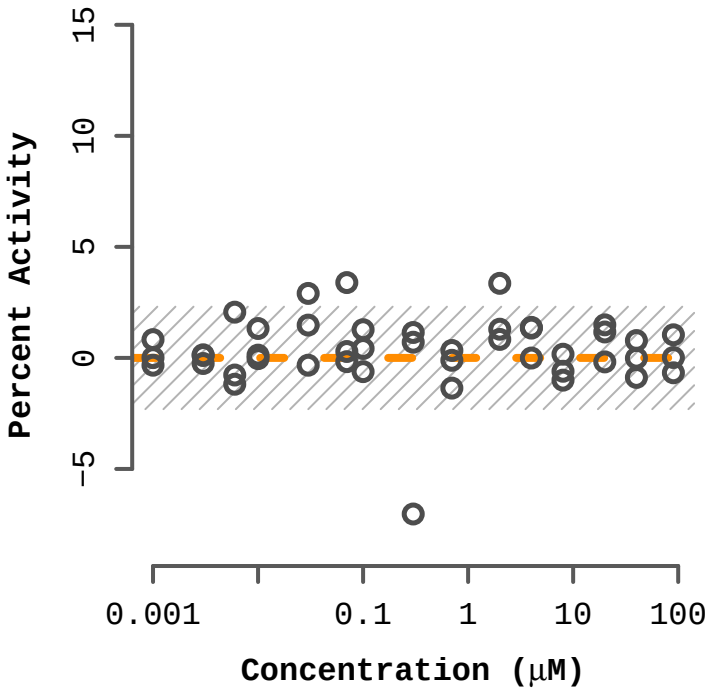
	tp	ga	gw
val:	2.79e-08	2.36	3.43
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.7	1.19	8	1.44	18
sd:	5.97	0.703	17.3	0.702	80

	CNST	HILL	GNLS
AIC:	274.91	280.91	283.72
PROB:	0.94	0.05	0.01
RMSE:	5.35	5.35	5.32

MAX_MEAN: 2.24 MAX_MED: 3.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

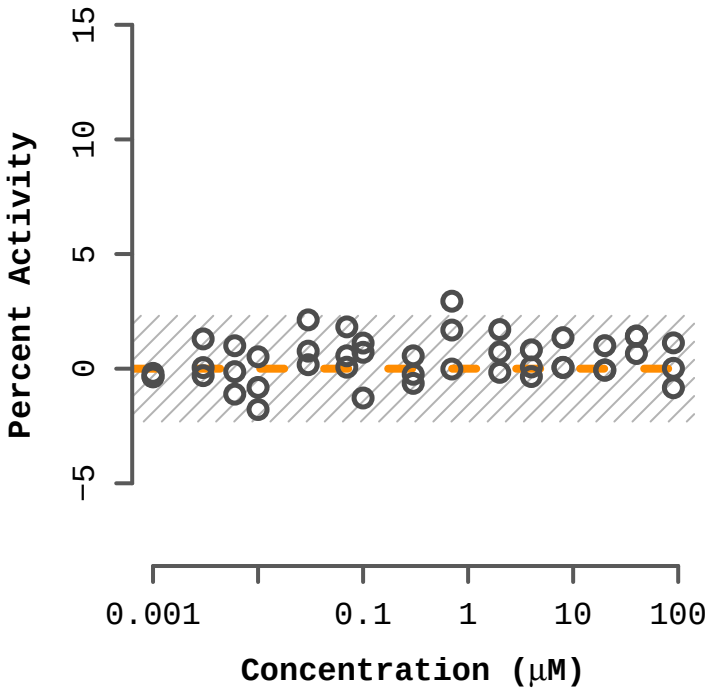
NAME: Diphenyl phosphite
CHID: 41889 **CASRN:** 4712-55-4
SPID(S): Tox21_301210
M4ID: 12477923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

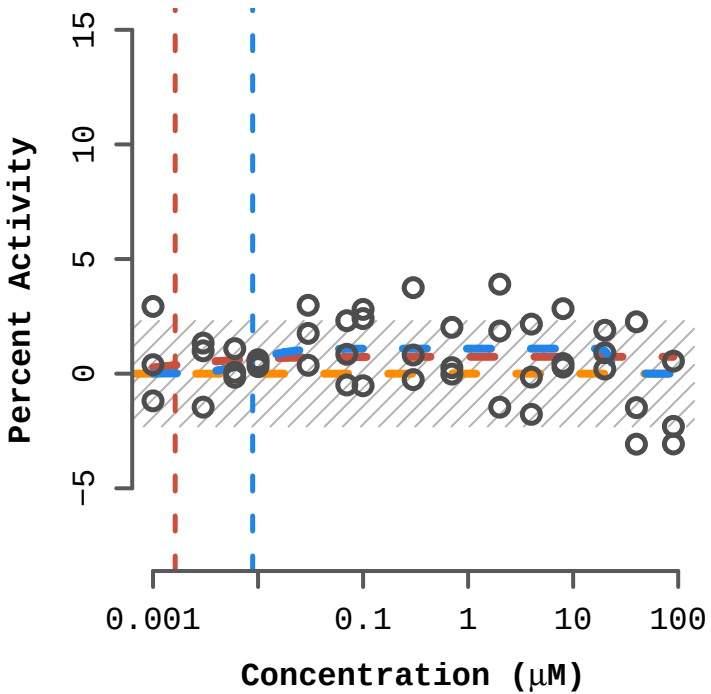
NAME: Diphenylmethane
CHID: 41891 **CASRN:** 101-81-5
SPID(S): Tox21_301147
M4ID: 12477986

HILL MODEL: Not applicable.

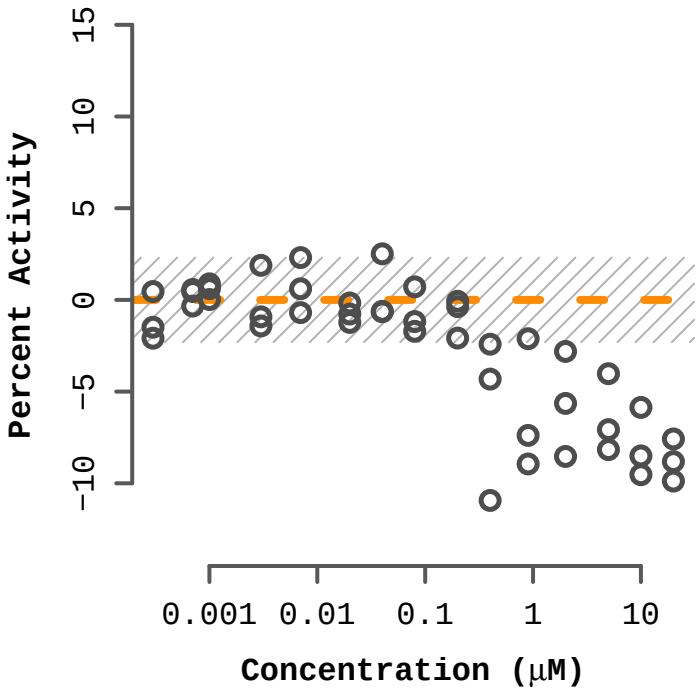
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.69 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diphenylsulfone
CHID:    41892   CASRN: 127-63-9
SPID(S): Tox21_301190
M4ID:    12477943

HILL MODEL (in red):
      tp       ga       gw
val:  0.736    -2.79    1.11
sd:   0.32     2.26     2.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.09     -2.05    2.52     1.36     17.6
sd:   0.37     0.501    6.46     4.41     1310

      CNST        HILL        GNLS
AIC:  184.8       183.73      182.89
PROB: 0.19        0.32        0.49
RMSE: 1.77        1.66        1.54

MAX_MEAN: 1.7       MAX_MED: 2.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

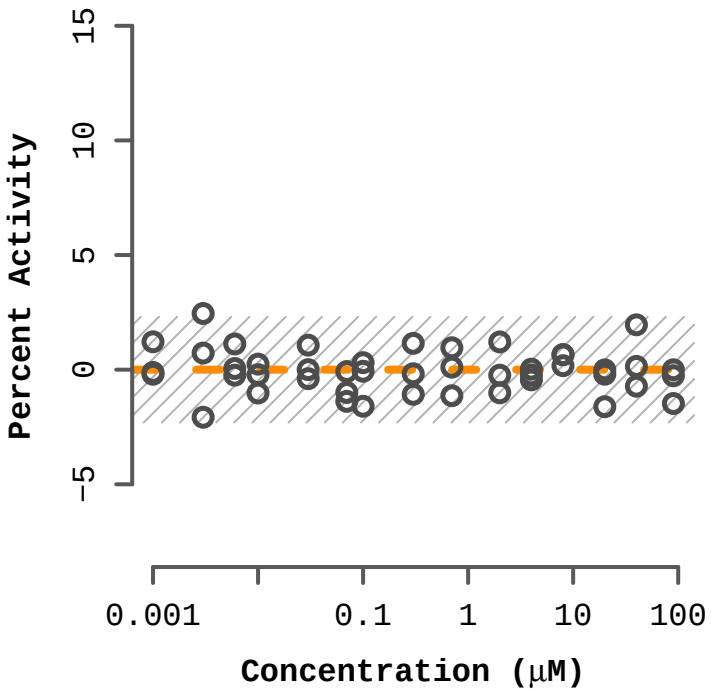
NAME: Dipyrithione
CHID: 41897 **CASRN:** 3696-28-4
SPID(S): Tox21_112131_1
M4ID: 12483296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.89	NA	NA
PROB:	1	NA	NA
RMSE:	4.71	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

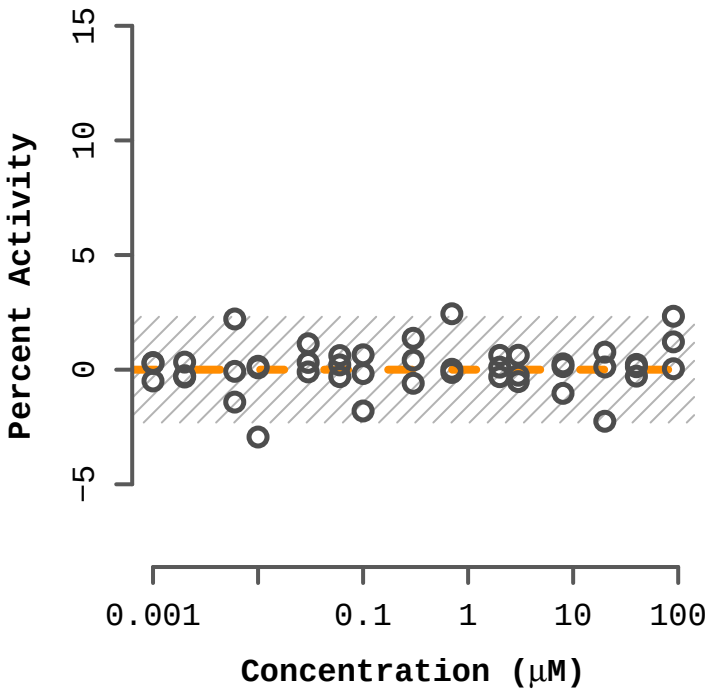
NAME: Disulfoton sulfone
CHID: 41901 CASRN: 2497-06-5
SPID(S): Tox21_304043
M4ID: 12475145

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.495 MAX_MED: 0.726 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

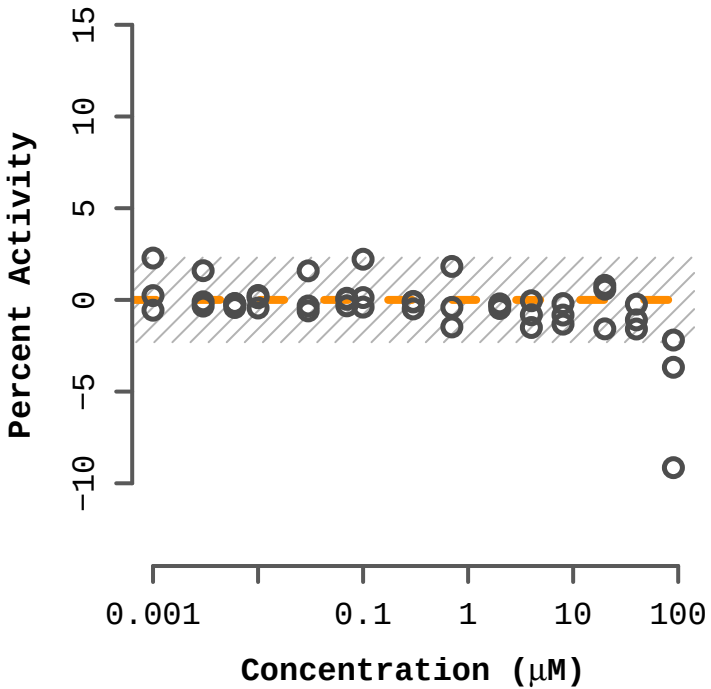
NAME: Dysprosium(III) chloride
CHID: 41909 **CASRN:** 10025-74-8
SPID(S): Tox21_300819
M4ID: 12478314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.43	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

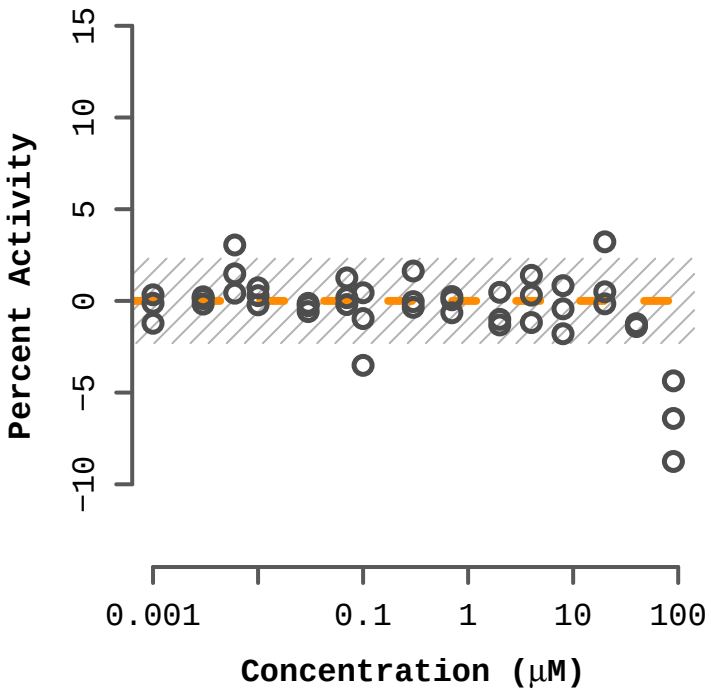
NAME: Edifenphos
CHID: 41910 **CASRN:** 17109-49-8
SPID(S): Tox21_301355
M4ID: 12477778

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 0.653 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

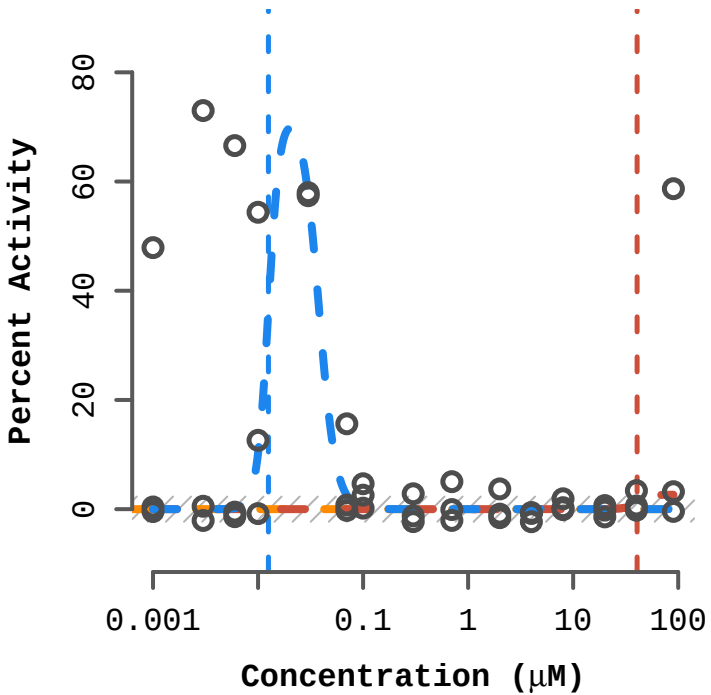
NAME: Etaconazole
CHID: 41913 **CASRN:** 60207-93-4
SPID(S): Tox21_301568
M4ID: 12477565

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.09	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'-Oxybis(ethylamine)
CHID: 41914 CASRN: 2752-17-2
SPID(S): Tox21_301395
M4ID: 12477738

HILL MODEL (in red):

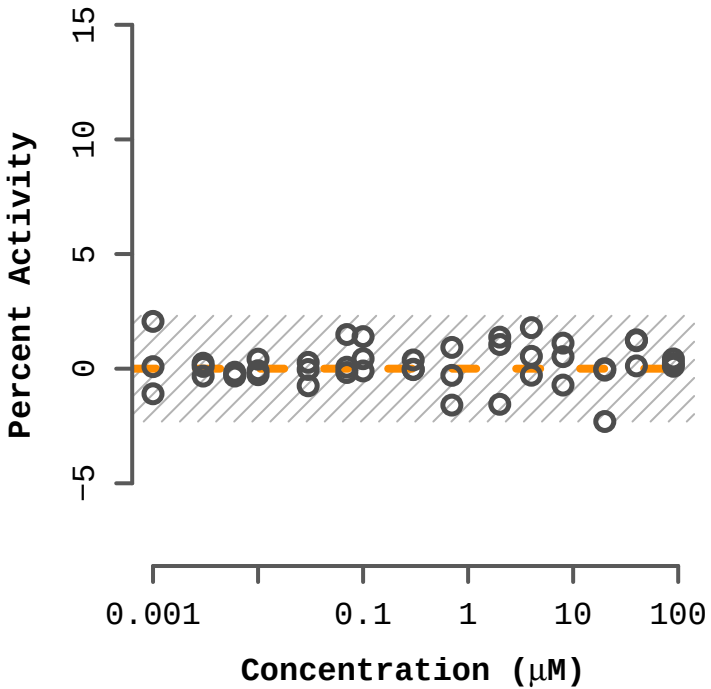
	tp	ga	gw
val:	2.64	1.61	8
sd:	3.96	0.311	81.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	73.6	-1.9	8	-1.42	5.46
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	371.96	377.33	340.8
PROB:	0	0	1
RMSE:	24.15	24	20.15

MAX_MEAN: 57.7 MAX_MED: 57.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

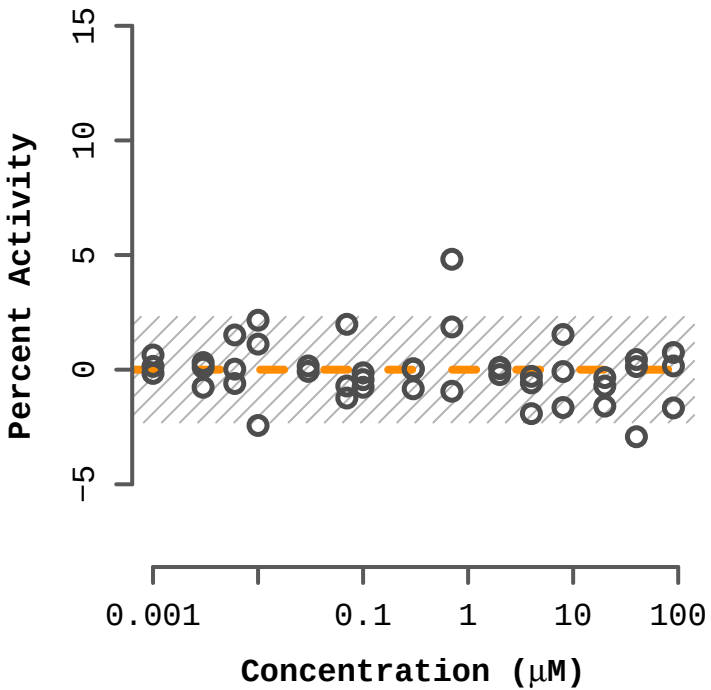
NAME: Dibutyl ethanedioate
CHID: 41916 **CASRN:** 2050-60-4
SPID(S): Tox21_301389
M4ID: 12477744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.868 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2',2'',2'''-(1,2-Ethanediyldinitrilo)tetrakis

CHID: 41917 **CASRN:** 140-07-8

SPID(S): Tox21_302089

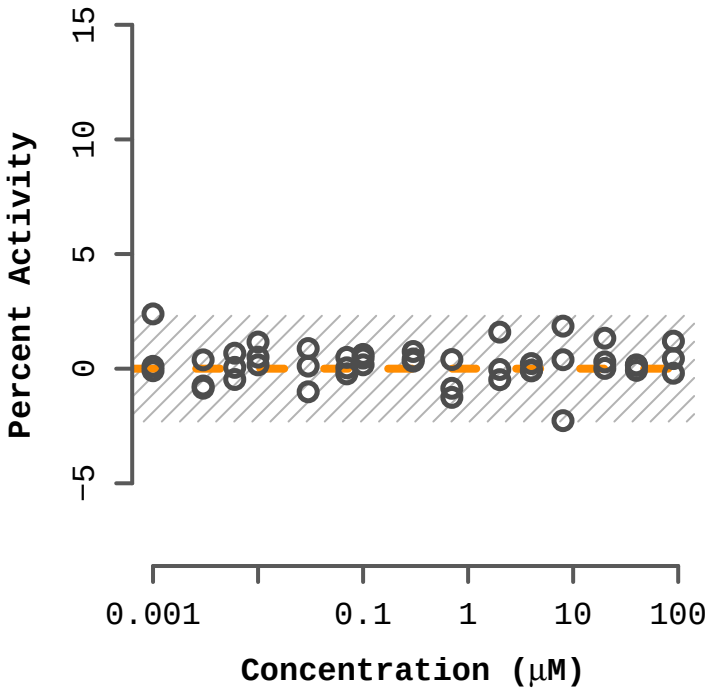
M4ID: 12477044

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

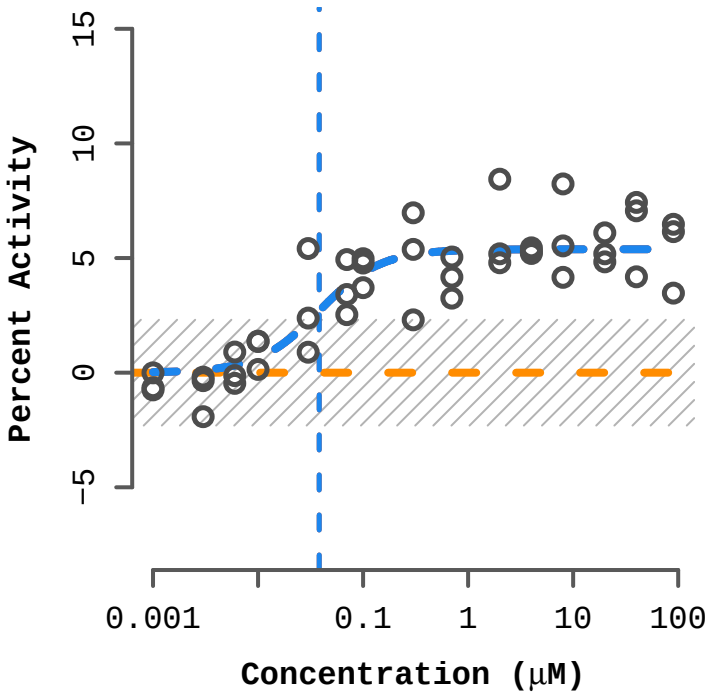
NAME: 1,4-Bis(2-hydroxyethoxy)-2-butyne
CHID: 41918 **CASRN:** 1606-85-5
SPID(S): Tox21_301678
M4ID: 12477455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 0.505 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(2-Ethylhexyloxy)ethanol
CHID: 41920 CASRN: 1559-35-9
SPID(S): Tox21_301871
M4ID: 12477262

HILL MODEL (in red):

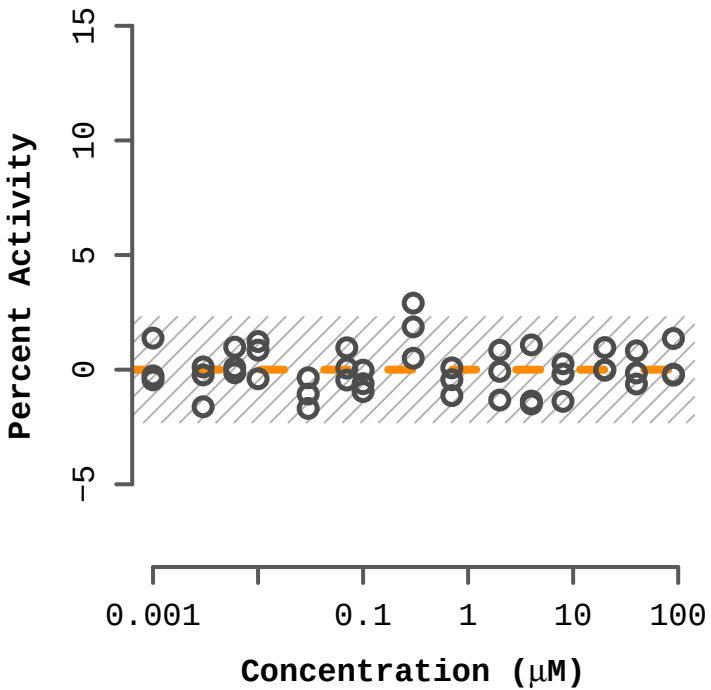
	tp	ga	gw
val:	5.38	-1.42	1.49
sd:	0.273	0.114	0.405

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.38	-1.42	1.49	3.89	3.97
sd:	0.273	0.114	0.405	1230	2470

	CNST	HILL	GNLS
AIC:	271.7	158.55	162.55
PROB:	0	0.88	0.12
RMSE:	4.49	1.29	1.29

MAX_MEAN: 6.22 MAX_MED: 7.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

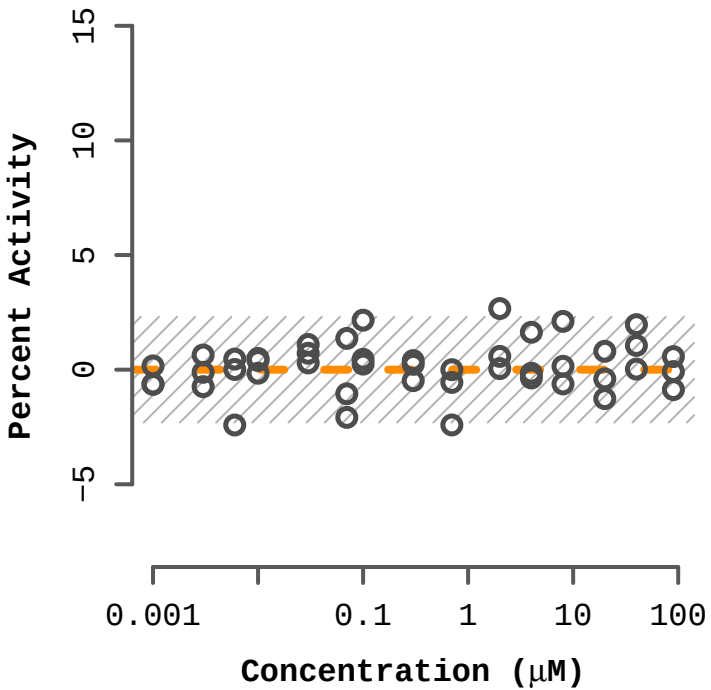
NAME: Ethiolate
CHID: 41925 **CASRN:** 2941-55-1
SPID(S): Tox21_301357
M4ID: 12477776

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

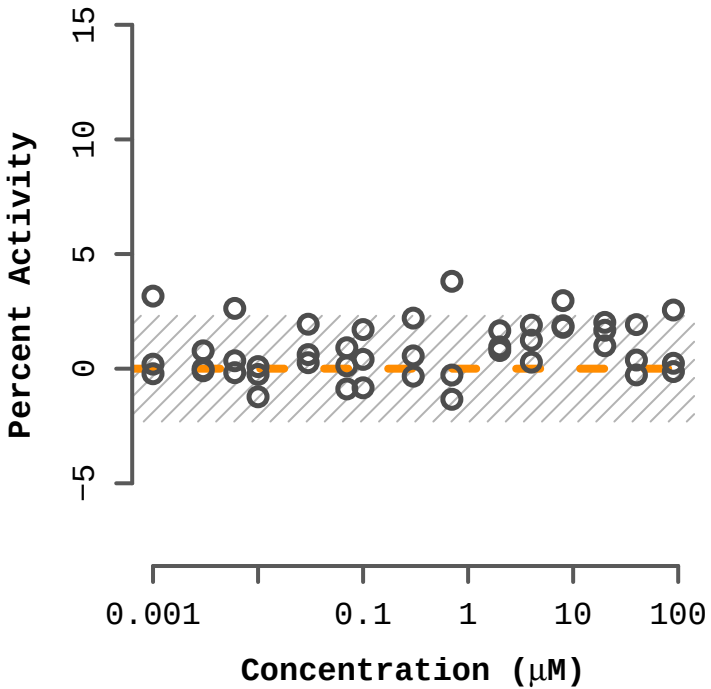
NAME: Ethirimol
CHID: 41927 **CASRN:** 23947-60-6
SPID(S): Tox21_301780
M4ID: 12477353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

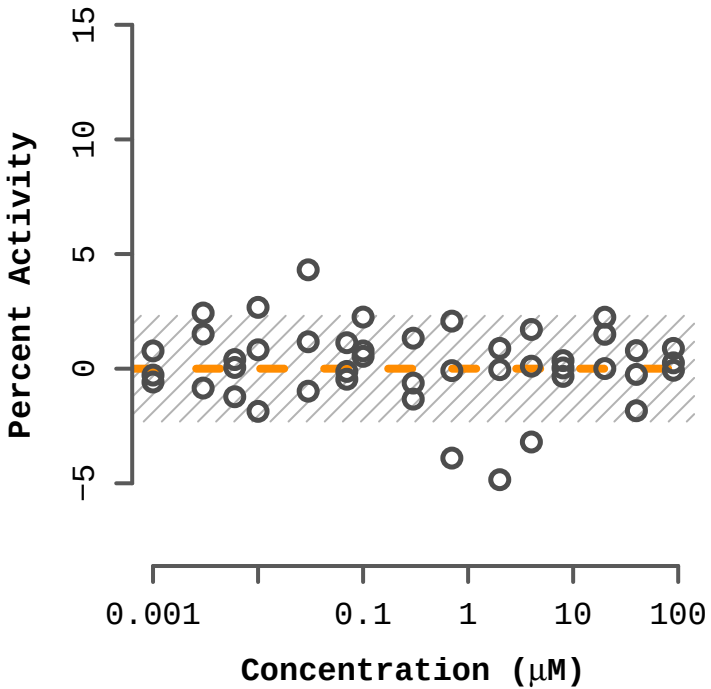
NAME: Ethyl bromophenylacetate
CHID: 41951 CASRN: 2882-19-1
SPID(S): Tox21_301444
M4ID: 12477689

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

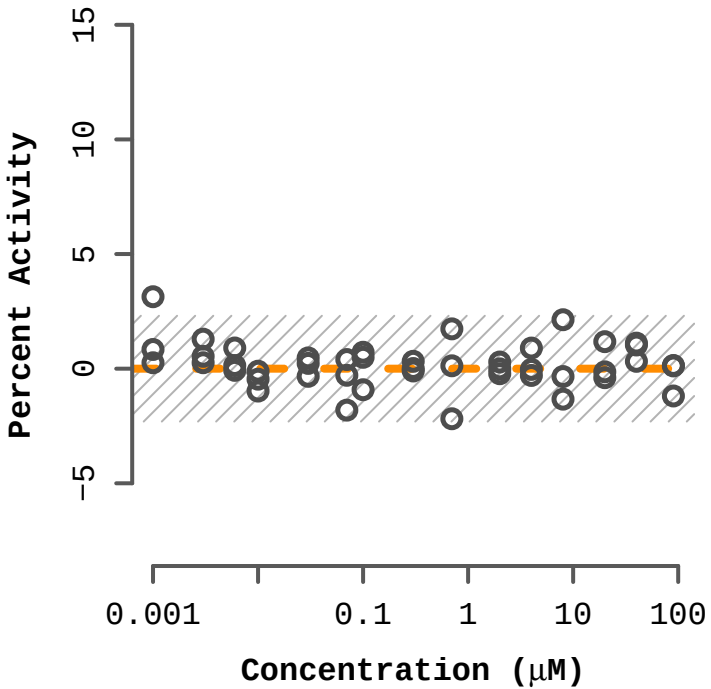
NAME: 3-Octanone
CHID: 41954 **CASRN:** 106-68-3
SPID(S): Tox21_301208
M4ID: 12477925

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

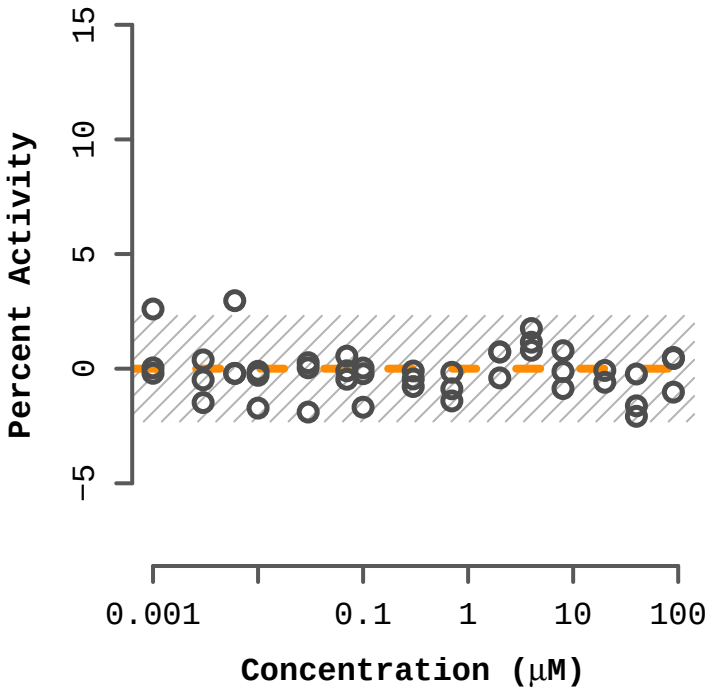
NAME: Ethyl diethanolamine
CHID: 41955 **CASRN:** 139-87-7
SPID(S): Tox21_301350
M4ID: 12477783

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

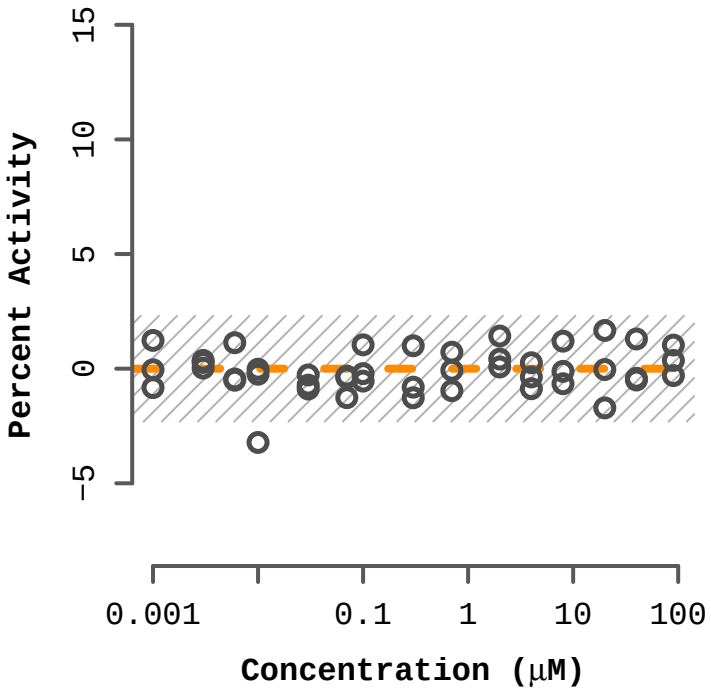
NAME: Ethyl orthoformate
CHID: 41957 CASRN: 122-51-0
SPID(S): Tox21_301314
M4ID: 12477819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.24 MAX_MED: 1.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

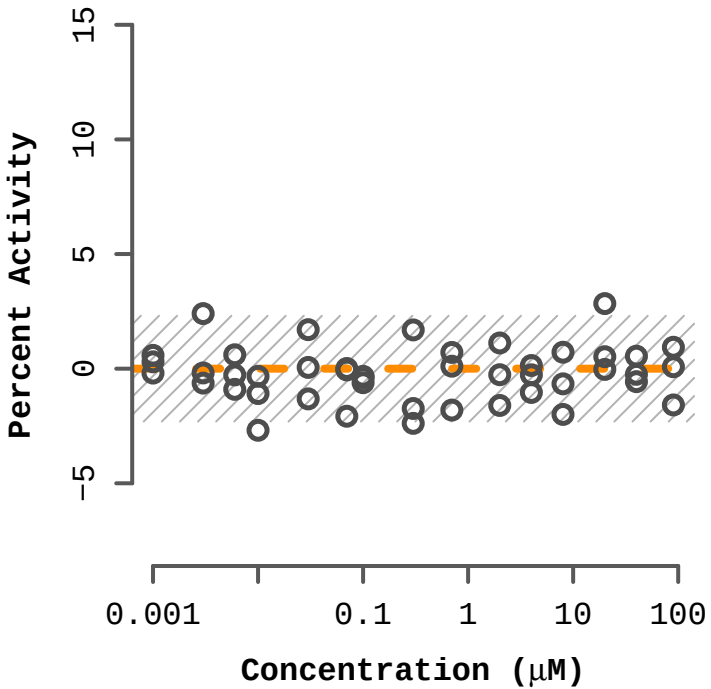
NAME: Ethyl trifluoroacetate
CHID: 41959 CASRN: 383-63-1
SPID(S): Tox21_301309
M4ID: 12477824

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.641 MAX_MED: 0.421 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

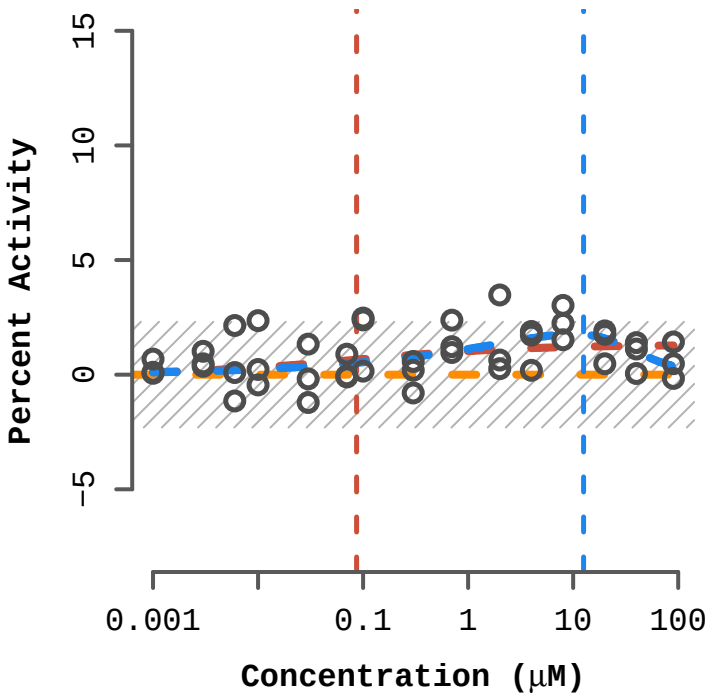
NAME: Ethyltriethoxysilane
CHID: 41962 **CASRN:** 78-07-9
SPID(S): Tox21_301374
M4ID: 12477759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Etrimfos
CHID: 41964 CASRN: 38260-54-7
SPID(S): Tox21_301572
M4ID: 12477561

HILL MODEL (in red):

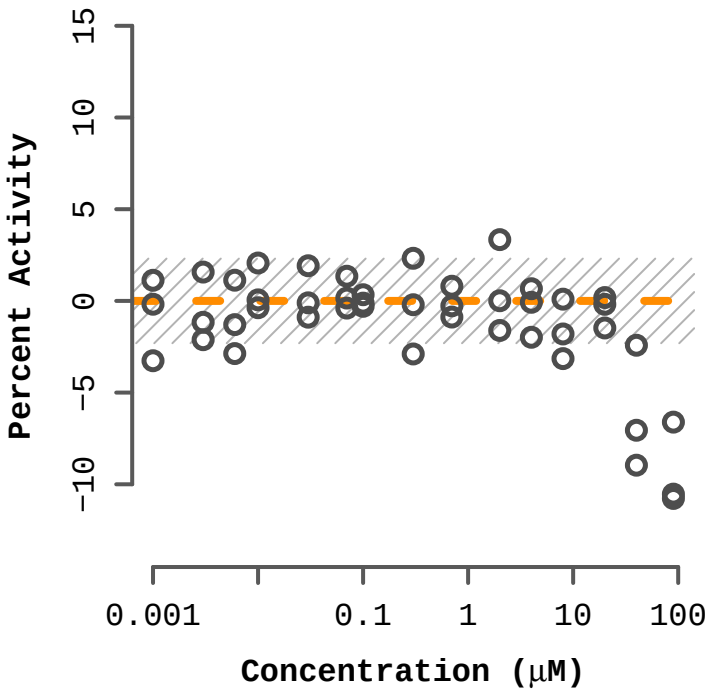
	tp	ga	gw
val:	1.31	−1.06	0.538
sd:	0.321	0.862	0.523

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.17	1.1	0.395	1.5	1.81
sd:	4.85	2.27	0.246	0.262	1.14

	CNST	HILL	GNLS
AIC:	161.21	140.17	138.75
PROB:	0	0.33	0.67
RMSE:	1.39	1.02	0.97

MAX_MEAN: 2.26 **MAX_MED:** 2.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

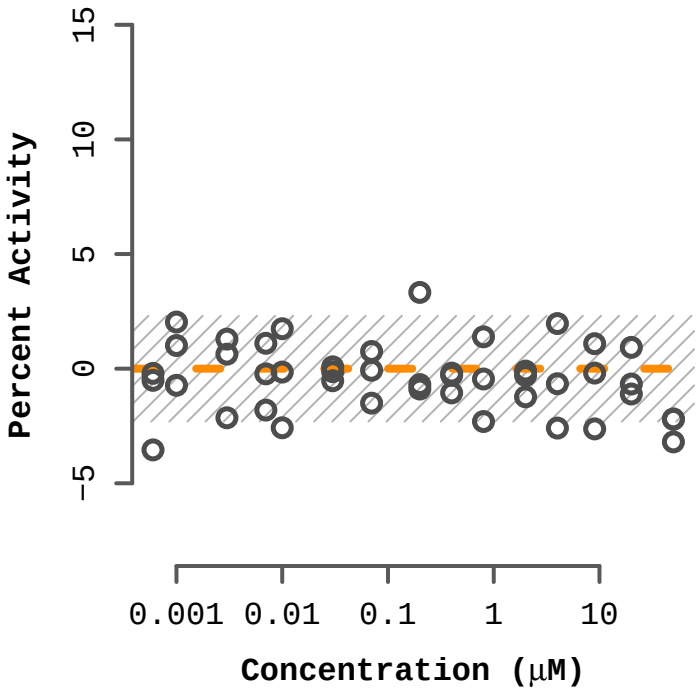
NAME: Famphur
CHID: 41966 **CASRN:** 52-85-7
SPID(S): Tox21_301907
M4ID: 12477226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.63	NA	NA
PROB:	1	NA	NA
RMSE:	3.33	NA	NA

MAX_MEAN: 0.585 **MAX_MED:** 0.157 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

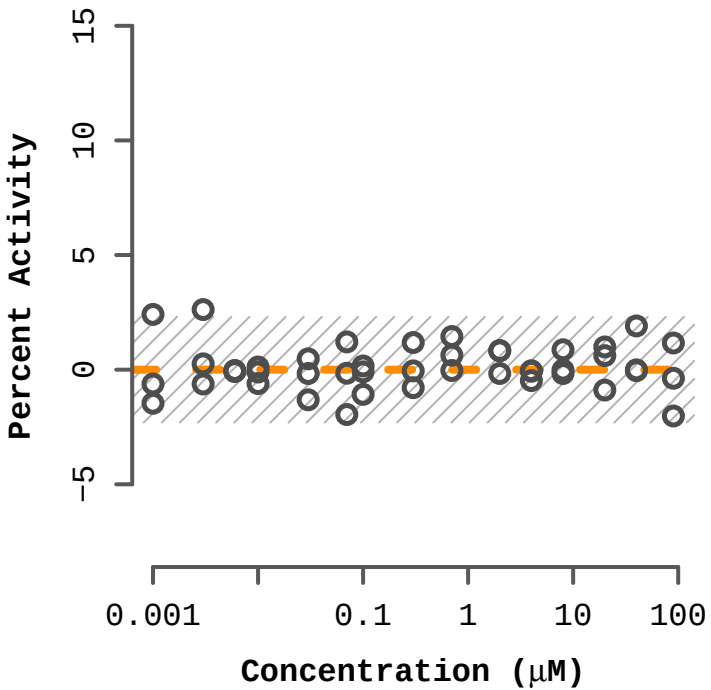
NAME: Famphur
CHID: 41966 **CASRN:** 52-85-7
SPID(S): Tox21_111946_1
M4ID: 12483416

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 0.774 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

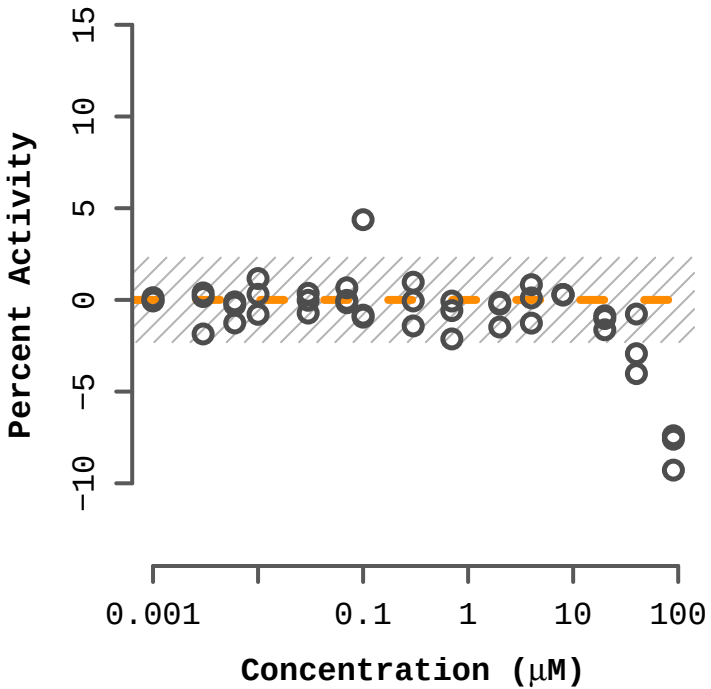
NAME: Fenchol
CHID: 41970 **CASRN:** 1632-73-1
SPID(S): Tox21_303498
M4ID: 12475644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.752 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

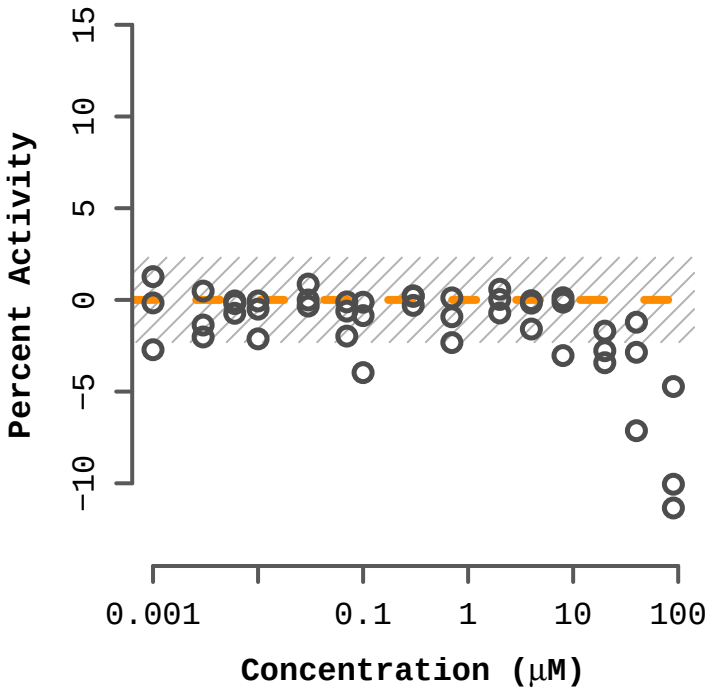
NAME: Fenson
CHID: 41973 **CASRN:** 80-38-6
SPID(S): Tox21_301324
M4ID: 12477809

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.45	NA	NA

MAX_MEAN: 0.87 **MAX_MED:** 0.308 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

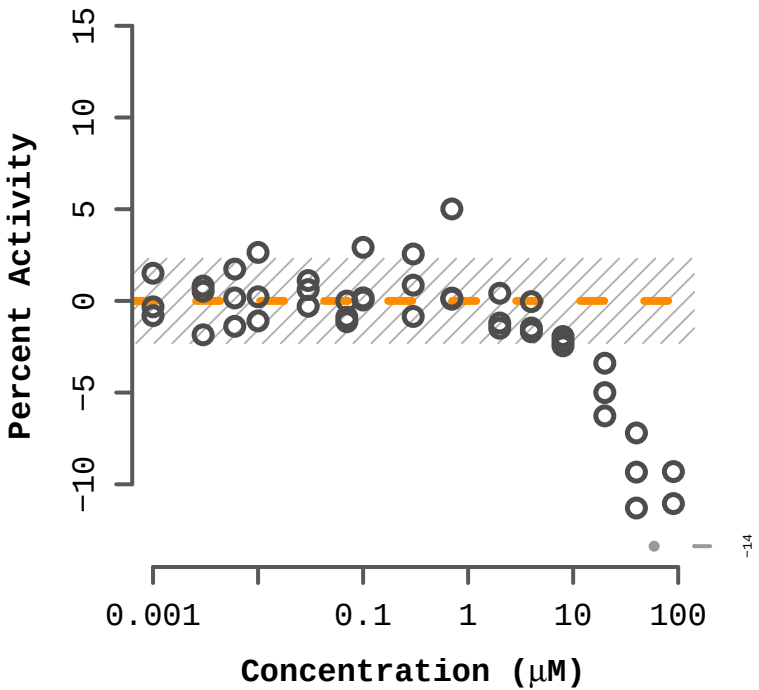
NAME: Flamprop-isopropyl
CHID: 41977 **CASRN:** 52756-22-6
SPID(S): Tox21_301563
M4ID: 12477570

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.53	NA	NA
PROB:	1	NA	NA
RMSE:	2.97	NA	NA

MAX_MEAN: 0.176 **MAX_MED:** 0.194 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

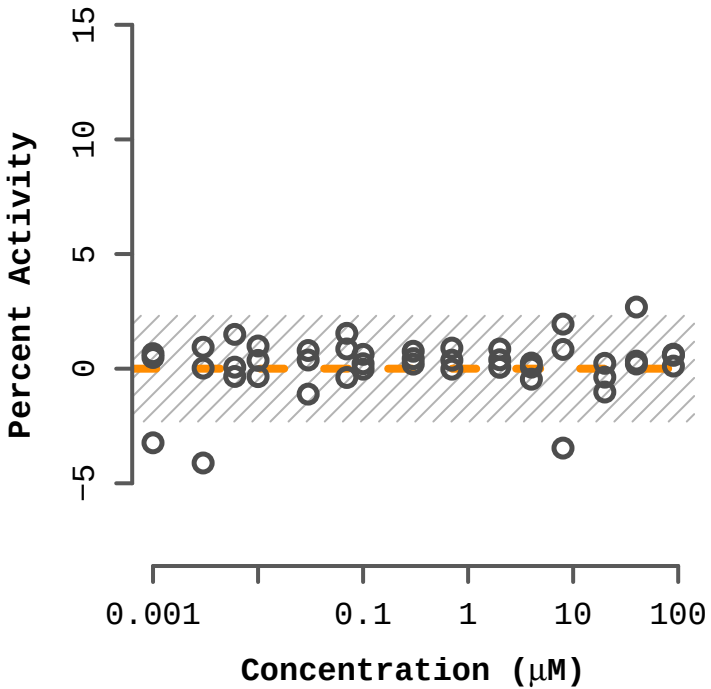
NAME: Flufenoxuron
CHID: 41978 **CASRN:** 101463-69-8
SPID(S): Tox21_300764
M4ID: 12478369 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	247.78	NA	NA
PROB:	1	NA	NA
RMSE:	4.34	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 0.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

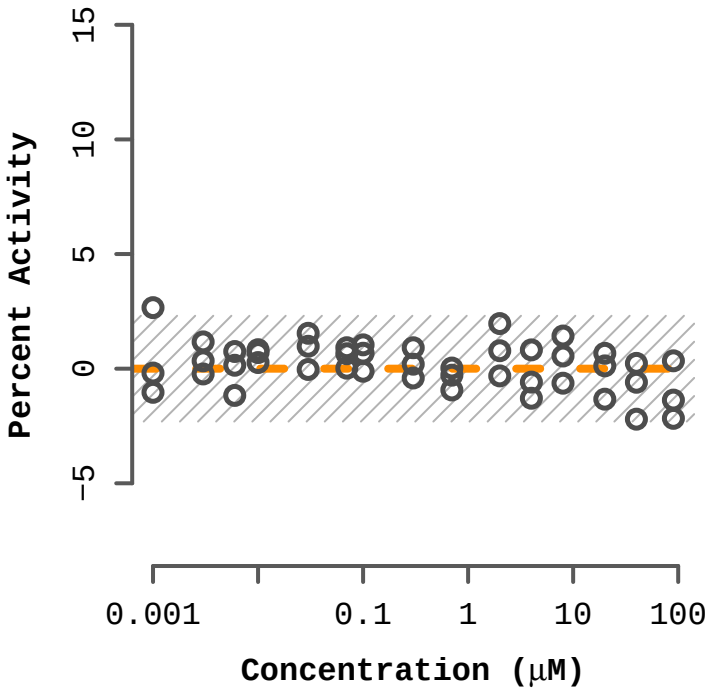
NAME: Fluoroacetic acid
CHID: 41981 **CASRN:** 144-49-0
SPID(S): Tox21_302429
M4ID: 12476704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

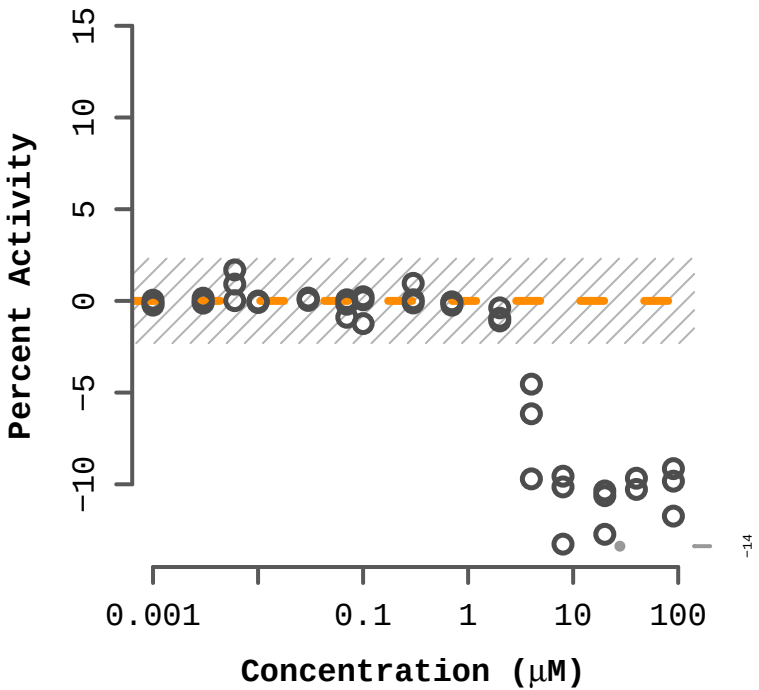
NAME: Fluoroglycofen-ethyl
CHID: 41983 **CASRN:** 77501-90-7
SPID(S): Tox21_301254
M4ID: 12477879

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.63	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.83 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

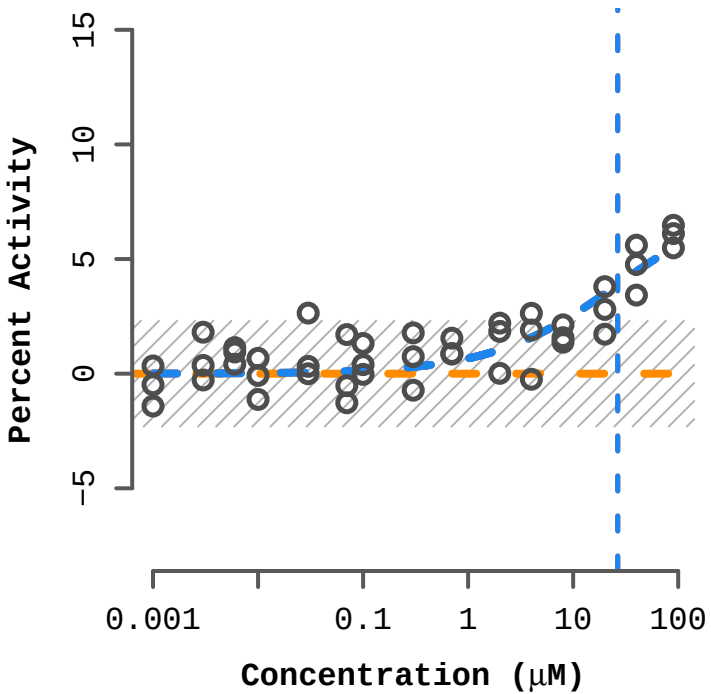
NAME: Fluorosalan
CHID: 41985 **CASRN:** 4776-06-1
SPID(S): Tox21_302424
M4ID: 12476709 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	286.89	NA	NA
PROB:	1	NA	NA
RMSE:	6	NA	NA

MAX_MEAN: 0.875 **MAX_MED:** 0.918 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flurochloridone
CHID: 41987 CASRN: 61213-25-0
SPID(S): Tox21_302259
M4ID: 12476874

HILL MODEL (in red):

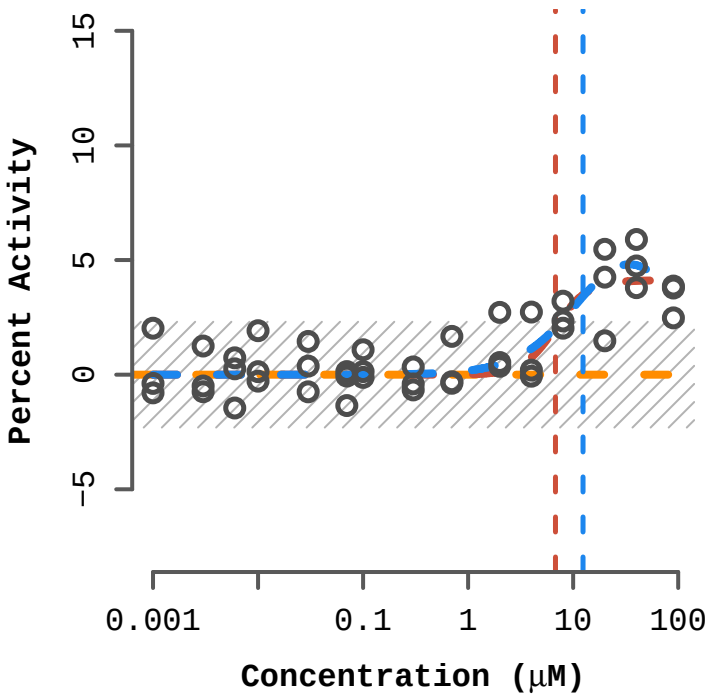
	tp	ga	gw
val:	7.77	1.42	0.722
sd:	1.72	0.292	0.197

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.77	1.42	0.722	3.68	4.86
sd:	1.72	0.292	0.197	1230	3460

	CNST	HILL	GNLS
AIC:	205.02	138.7	142.7
PROB:	0	0.88	0.12
RMSE:	2.4	0.99	0.99

MAX_MEAN: 6.03 MAX_MED: 6.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fuberidazole
CHID: 41995 CASRN: 3878-19-1
SPID(S): Tox21_301574
M4ID: 12477559

HILL MODEL (in red):

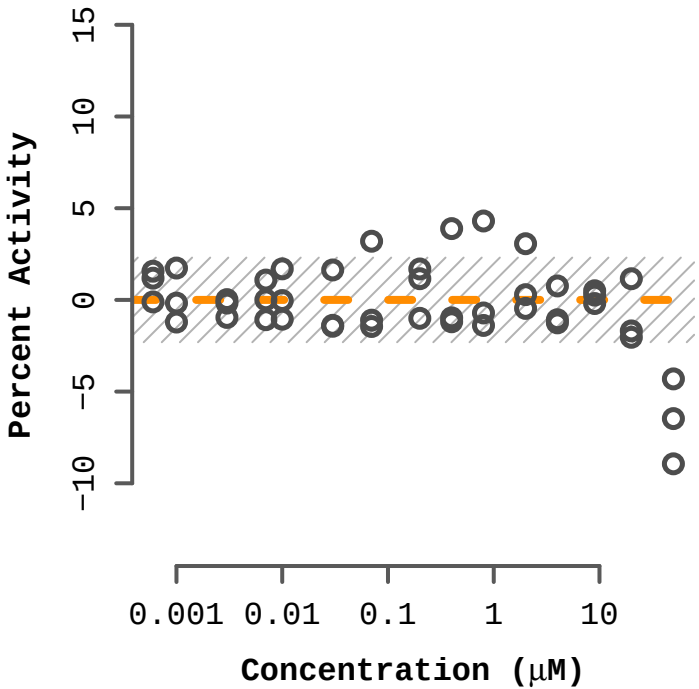
	tp	ga	gw
val:	4.12	0.832	2.83
sd:	0.391	0.087	2.15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.08	1.09	1.46	1.97	1.62
sd:	15	1.01	1.14	0.982	4.46

	CNST	HILL	GNLS
AIC:	197.57	142.19	142.29
PROB:	0	0.51	0.49
RMSE:	2.19	1.06	1.02

MAX_MEAN: 4.81 MAX_MED: 4.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

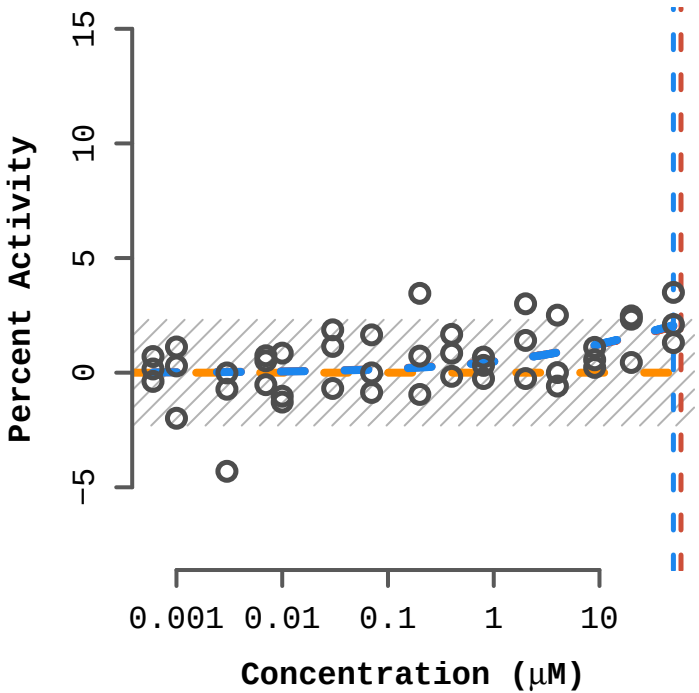
NAME: Furazolidone
CHID: 41997 **CASRN:** 67-45-8
SPID(S): Tox21_111502_1
M4ID: 12483647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.29	NA	NA
PROB:	1	NA	NA
RMSE:	2.32	NA	NA

MAX_MEAN: 0.964 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glycerol 1-(p-aminobenzoate)
CHID: 42002 CASRN: 136-44-7
SPID(S): Tox21_113940
M4ID: 12482291

HILL MODEL (in red):

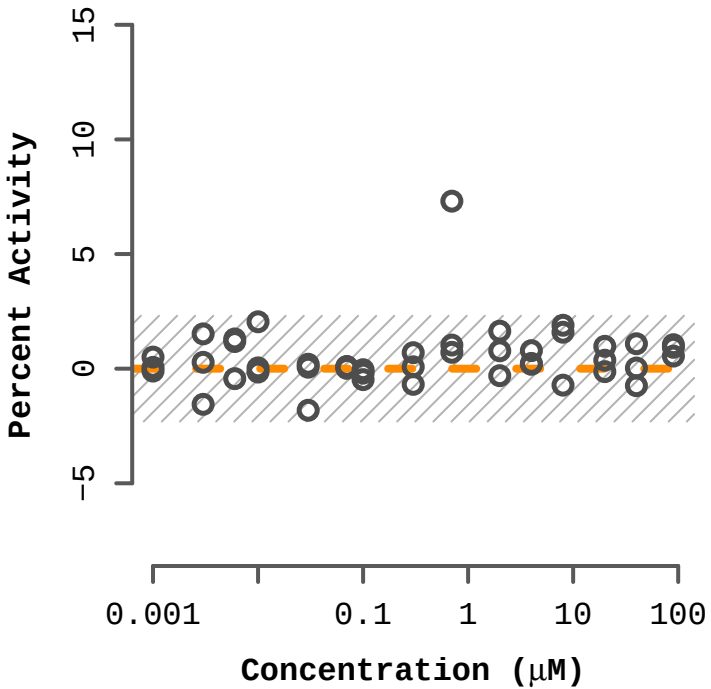
	tp	ga	gw
val:	4.2	1.77	0.494
sd:	4.54	1.68	0.302

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.12	1.7	0.517	2.42	10.2
sd:	5.64	1.99	0.309	614	8640

	CNST	HILL	GNLS
AIC:	166.88	154.79	158.81
PROB:	0	0.88	0.12
RMSE:	1.53	1.27	1.27

MAX_MEAN: 2.31 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

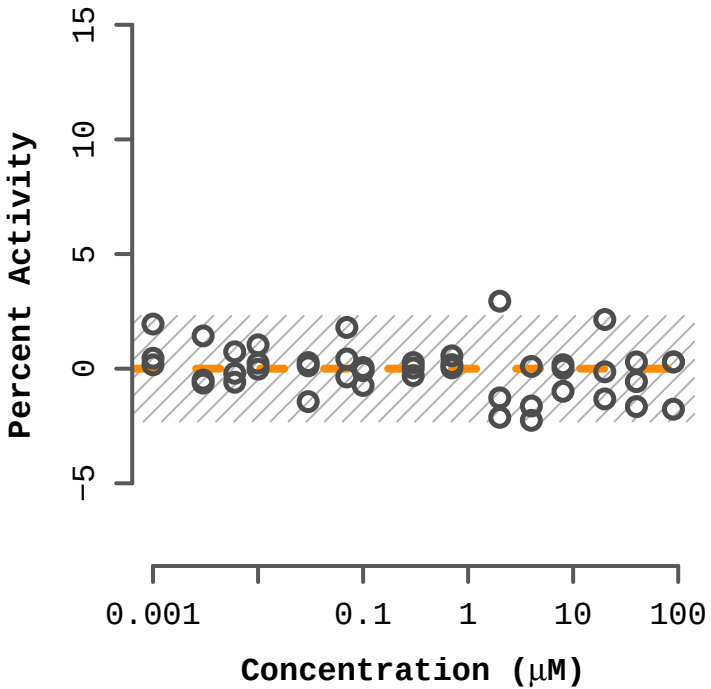
NAME: Glyceryl monooctanoate
CHID: 42006 **CASRN:** 26402-26-6
SPID(S): Tox21_301535
M4ID: 12477598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 3.02 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

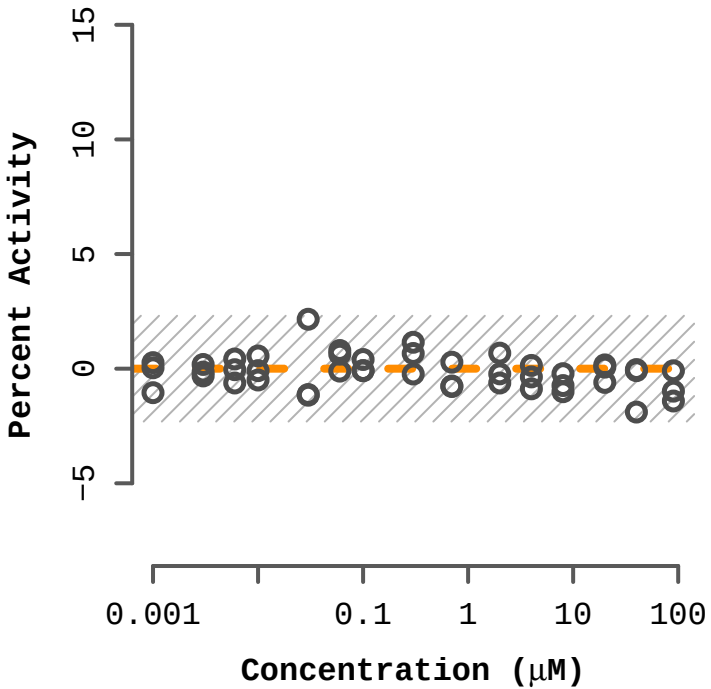
NAME: Glyceryl monoricinoleate
CHID: 42007 CASRN: 1323-38-2
SPID(S): Tox21_301962
M4ID: 12477171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.859 **MAX_MED:** 0.456 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

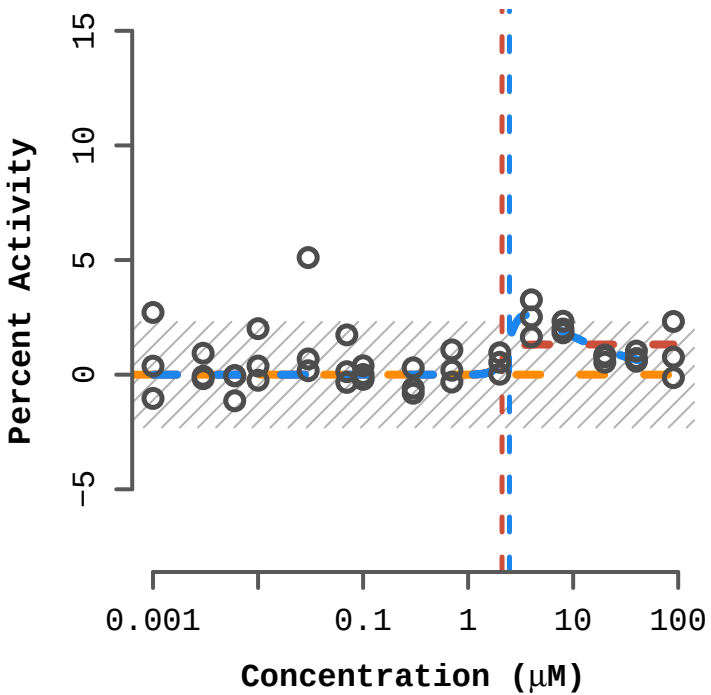
NAME: N-Dodecanoyl-N-methylglycine
CHID: 42011 **CASRN:** 97-78-9
SPID(S): Tox21_301352
M4ID: 12477781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.665 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Glyoxime
CHID: 42014 **CASRN:** 557-30-2
SPID(S): Tox21_302390
M4ID: 12476743

HILL MODEL (in red):

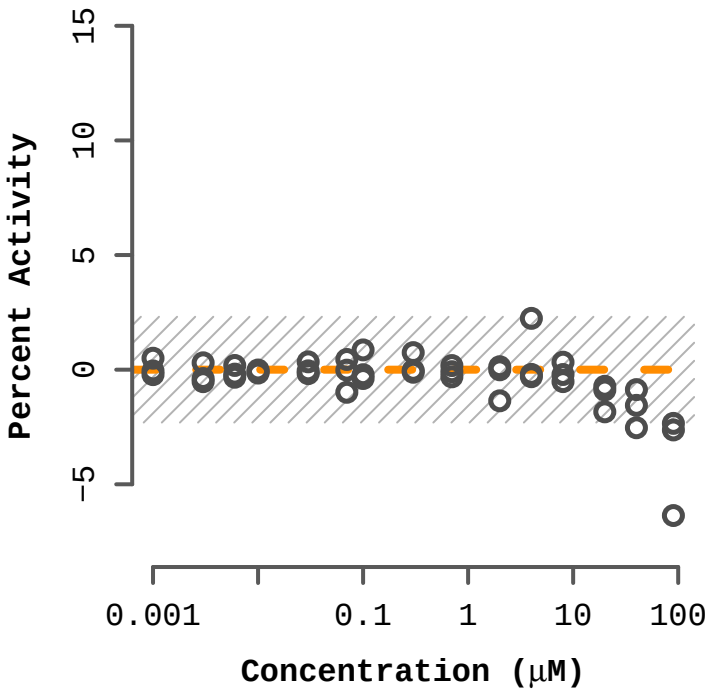
	tp	ga	gw
val:	1.32	0.323	8
sd:	0.247	0.0709	8.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.03	0.394	8	0.644	0.86
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	154.74	134.71	124.94
PROB:	0	0.01	0.99
RMSE:	1.42	1.16	1.1

MAX_MEAN: 2.48 **MAX_MED:** 2.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

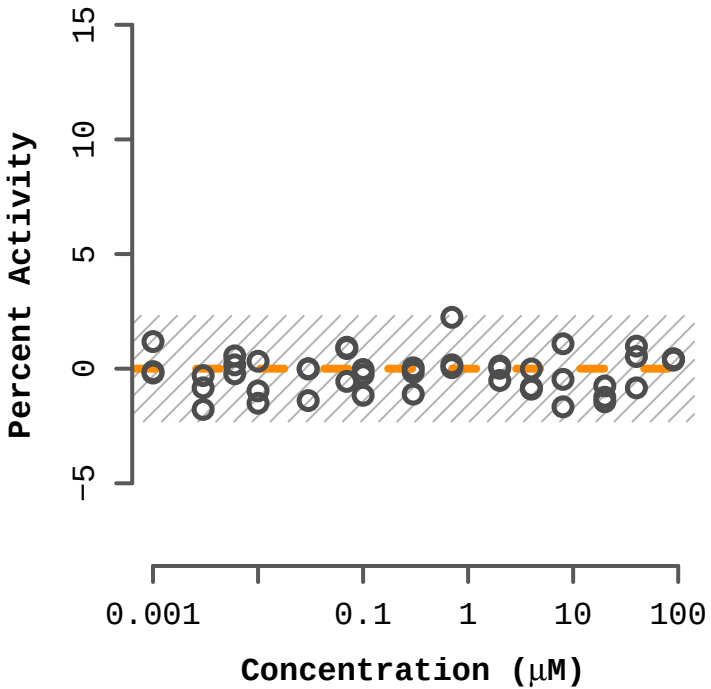
NAME: Haloxyfop
CHID: 42019 **CASRN:** 69806-34-4
SPID(S): Tox21_301857
M4ID: 12477276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** −0.00455 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

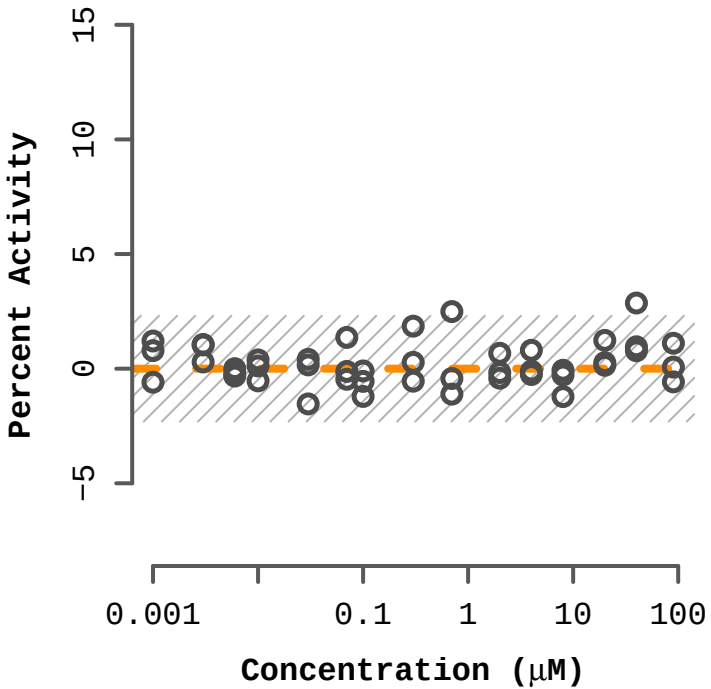
NAME: Heptyl butanoate
CHID: 42038 CASRN: 5870-93-9
SPID(S): Tox21_301377
M4ID: 12477756

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.82 MAX_MED: 0.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

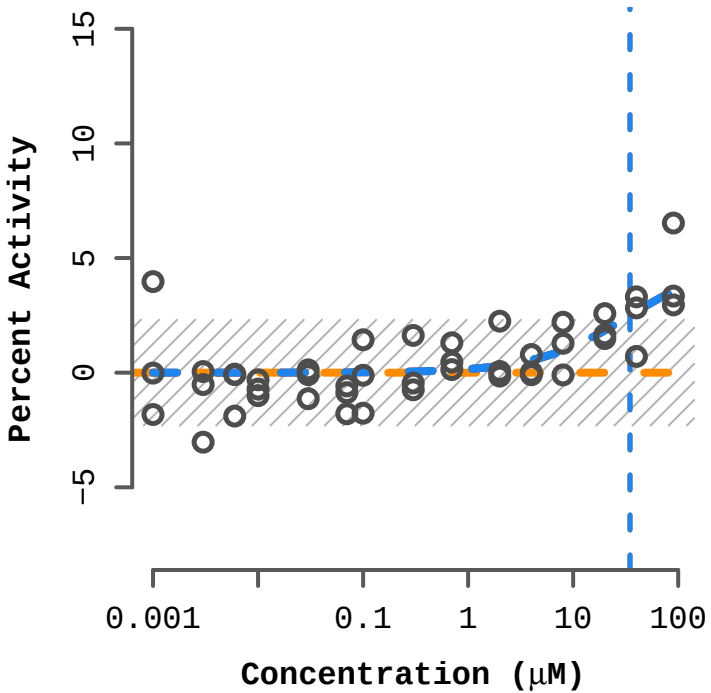
NAME: 1-(o-Tolyl)biguanide
CHID: 42051 **CASRN:** 93-69-6
SPID(S): Tox21_301315
M4ID: 12477818

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indene
CHID: 42052 **CASRN:** 95-13-6
SPID(S): Tox21_301215
M4ID: 12477918

HILL MODEL (in red):

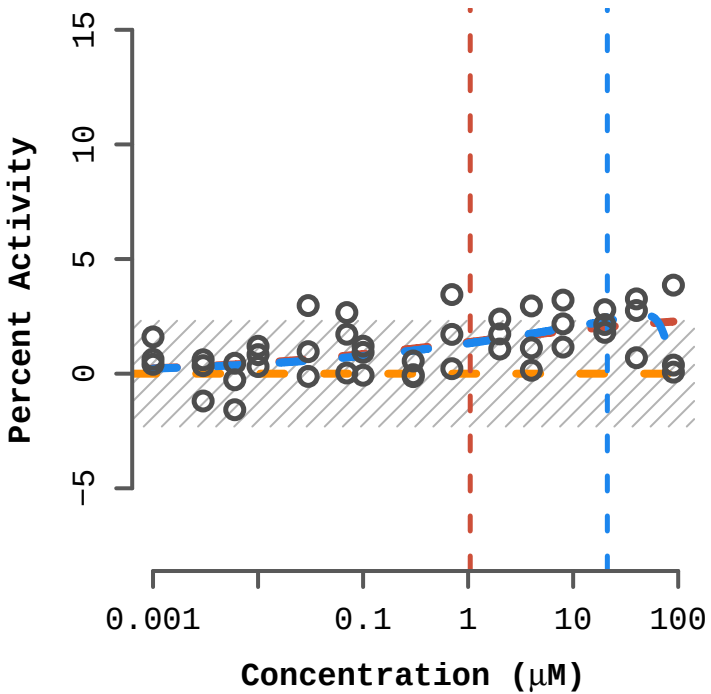
	tp	ga	gw
val:	4.98	1.54	0.967
sd:	3.59	0.737	0.571

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.98	1.54	0.967	3.4	4.77
sd:	3.59	0.737	0.572	1300	4340

	CNST	HILL	GNLS
AIC:	181.53	152.68	156.68
PROB:	0	0.88	0.12
RMSE:	1.86	1.26	1.26

MAX_MEAN: 4.28 **MAX_MED:** 3.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indole-3-pyruvic acid
CHID: 42053 CASRN: 392-12-1
SPID(S): Tox21_301365
M4ID: 12477768

HILL MODEL (in red):

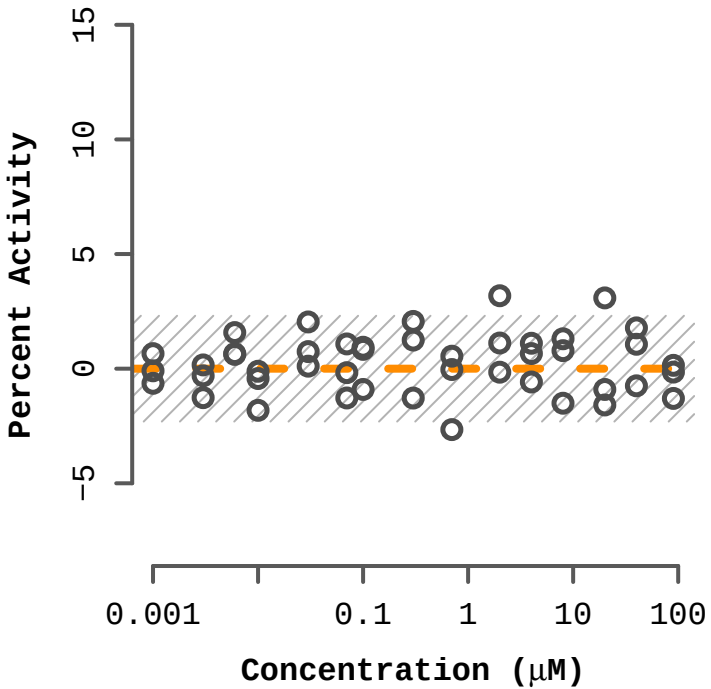
	tp	ga	gw
val:	2.77	0.0199	0.343
sd:	1.78	1.93	0.247

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.62	1.33	0.3	1.89	8.67
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	181.13	147.44	147.29
PROB:	0	0.48	0.52
RMSE:	1.72	1.09	1.09

MAX_MEAN: 2.25 **MAX_MED:** 2.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

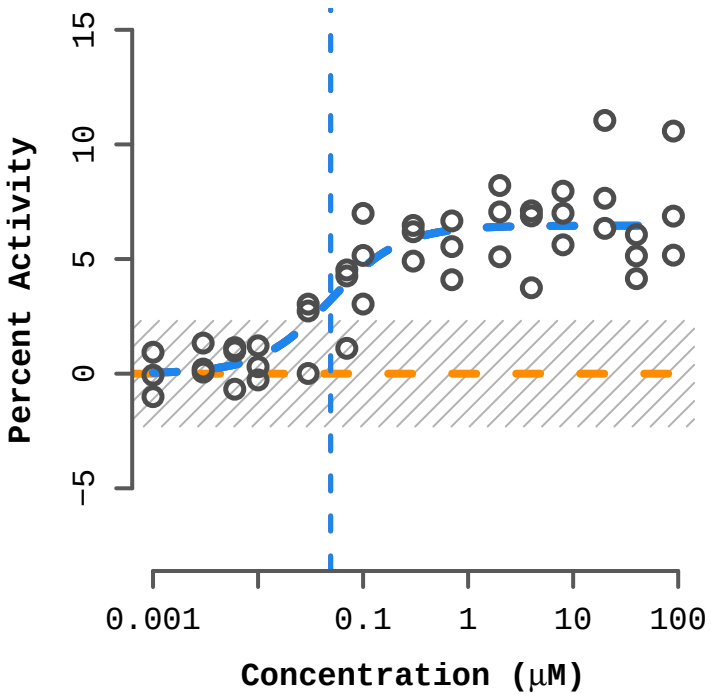
NAME: Isopentyl butyrate
CHID: 42059 **CASRN:** 106-27-4
SPID(S): Tox21_300384
M4ID: 12478748

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoborneol
CHID: 42060 CASRN: 124-76-5
SPID(S): Tox21_301645
M4ID: 12477488

HILL MODEL (in red):

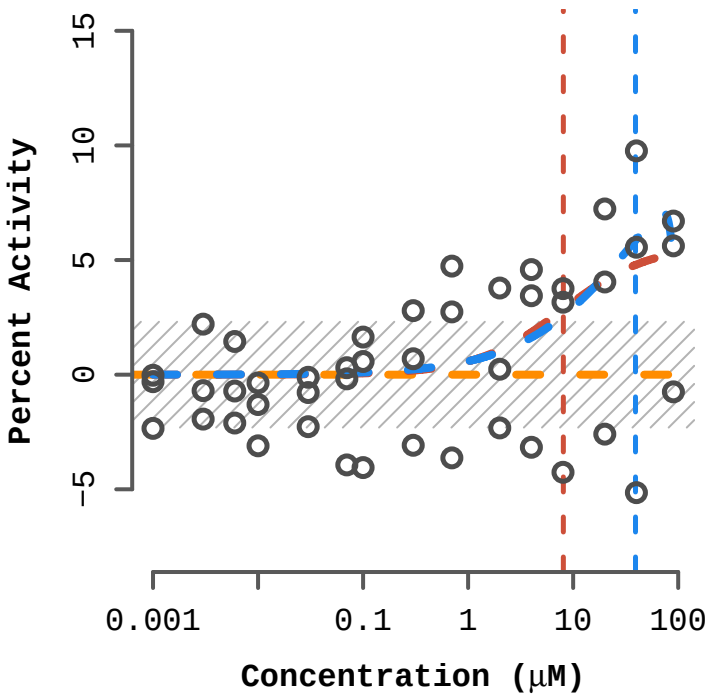
	tp	ga	gw
val:	6.46	−1.31	1.3
sd:	0.337	0.115	0.401

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.46	−1.31	1.3	3.42	5.36
sd:	0.337	0.115	0.401	1410	5280

	CNST	HILL	GNLS
AIC:	284.51	169.45	173.45
PROB:	0	0.88	0.12
RMSE:	5.23	1.5	1.5

MAX_MEAN: 8.35 MAX_MED: 7.65 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isobornyl acetate
CHID: 42061 CASRN: 125-12-2
SPID(S): Tox21_303558
M4ID: 12475587

HILL MODEL (in red):

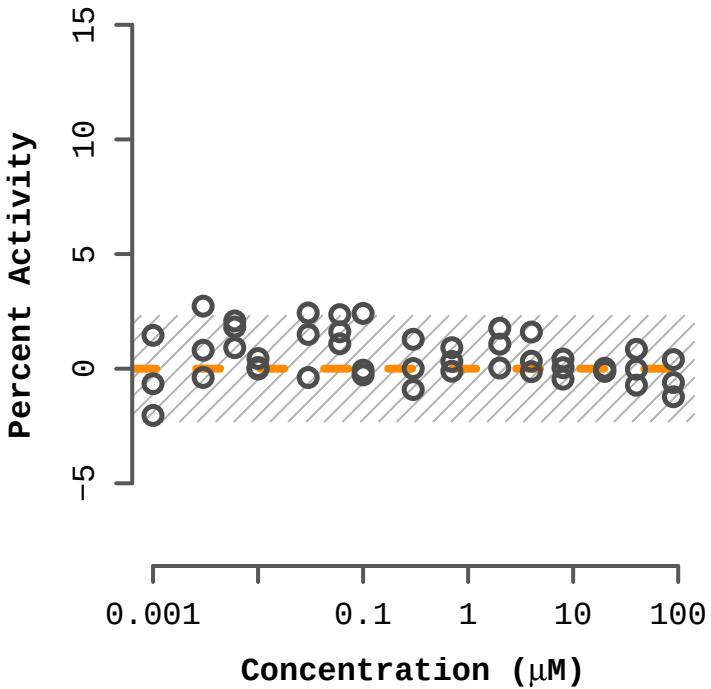
	tp	ga	gw
val:	5.7	0.907	1.04
sd:	2.43	0.554	0.872

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.7	1.59	0.802	1.97	14.6
sd:	32.4	2.71	0.74	0.0708	70.7

	CNST	HILL	GNLS
AIC:	244.43	238.22	241.86
PROB:	0.04	0.83	0.13
RMSE:	3.48	3.18	3.21

MAX_MEAN: 3.86 **MAX_MED:** 5.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

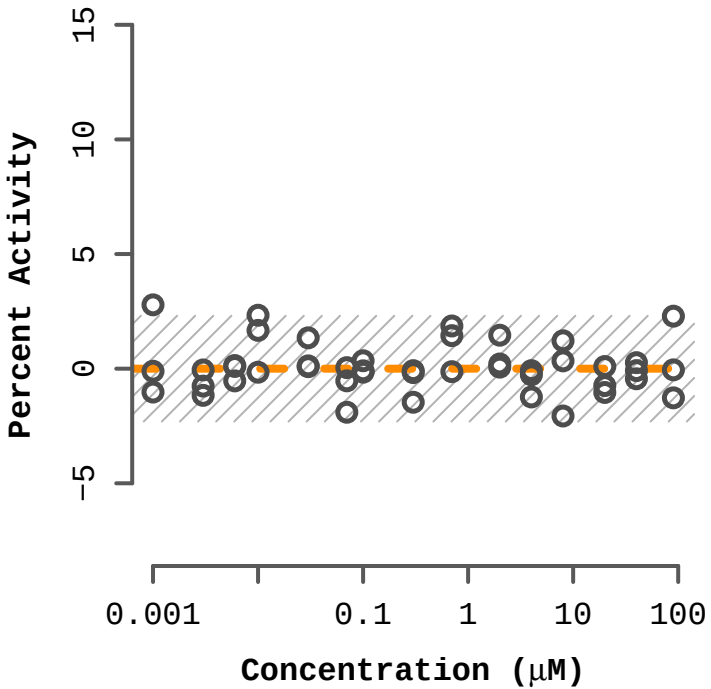
NAME: Isobornyl propanoate
CHID: 42062 **CASRN:** 2756-56-1
SPID(S): Tox21_301344
M4ID: 12477789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

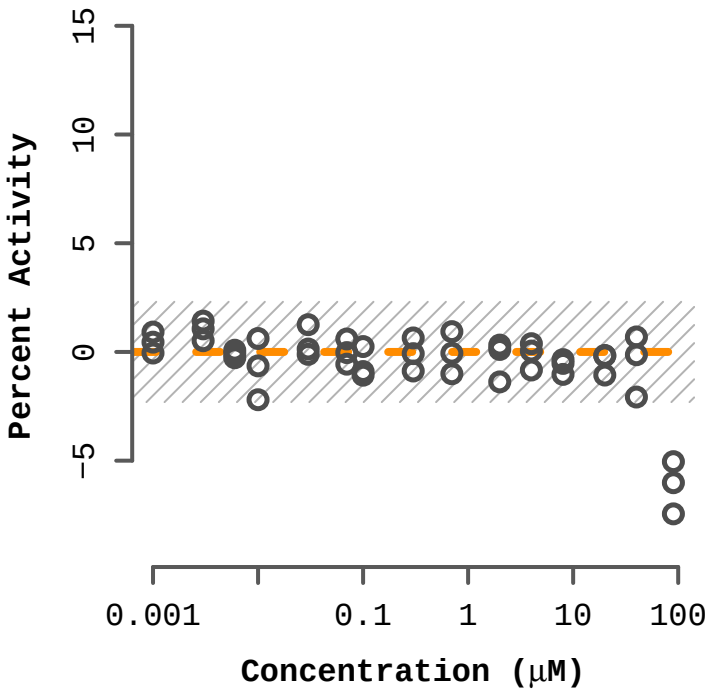
NAME: Isocarbophos
CHID: 42063 **CASRN:** 24353-61-5
SPID(S): Tox21_301328
M4ID: 12477805

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

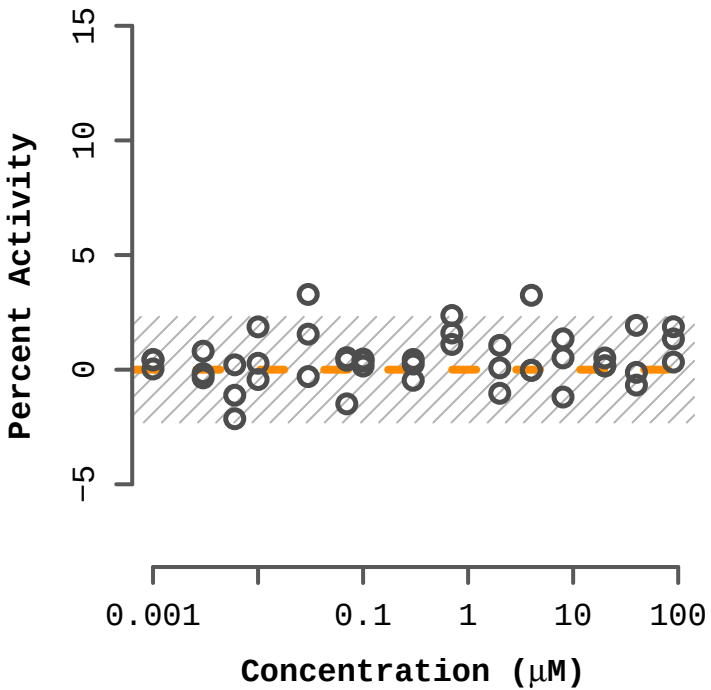
NAME: Isodrin
CHID: 42065 CASRN: 465-73-6
SPID(S): Tox21_301429
M4ID: 12477704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1 MAX_MED: 1.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

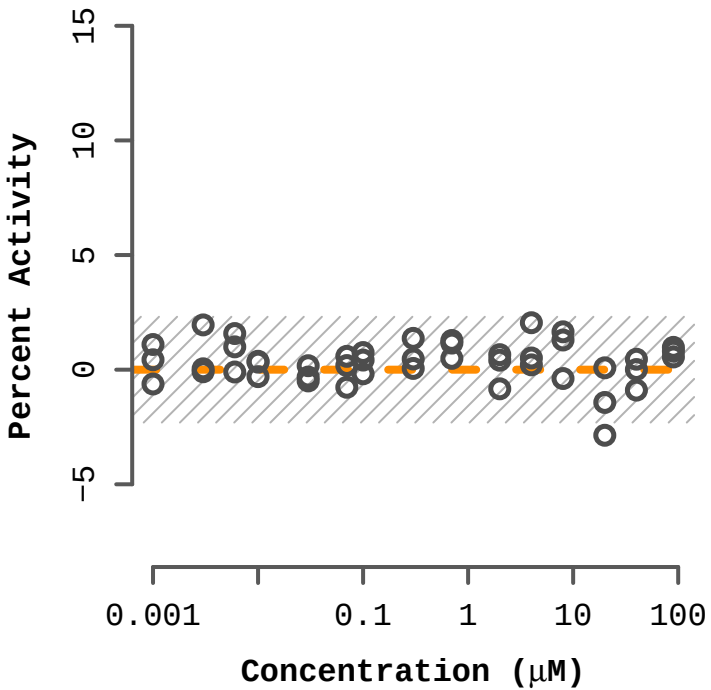
NAME: Isoprocarb
CHID: 42072 **CASRN:** 2631-40-5
SPID(S): Tox21_301361
M4ID: 12477772

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

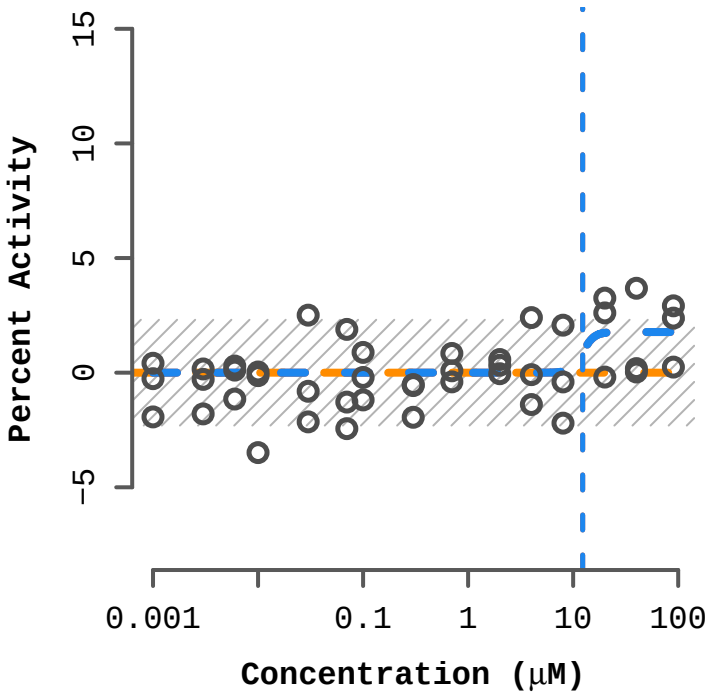
NAME: Isopropyl-o-cresol
CHID: 42074 **CASRN:** 499-75-2
SPID(S): Tox21_301378
M4ID: 12477755

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.977 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoproturon
CHID: 42077 CASRN: 34123-59-6
SPID(S): Tox21_301329
M4ID: 12477804

HILL MODEL (in red):

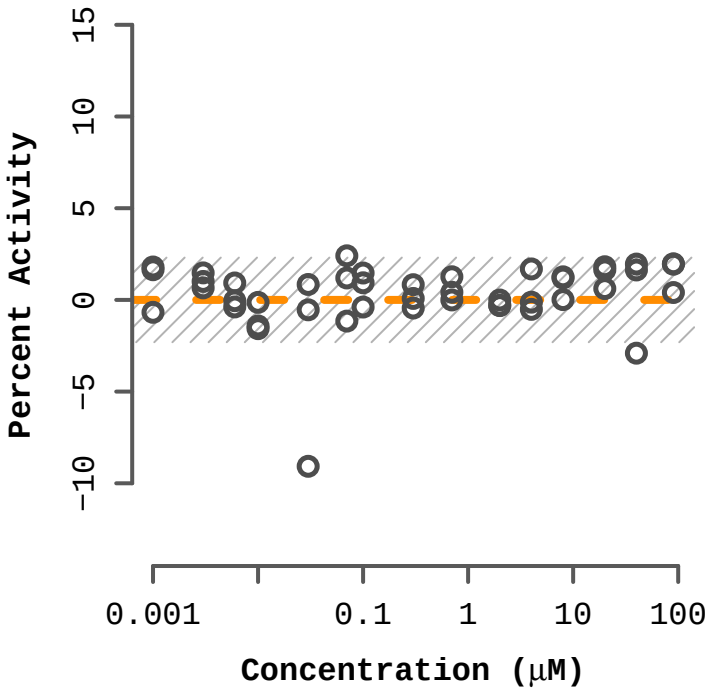
	tp	ga	gw
val:	1.77	1.09	8
sd:	0.593	0.262	10.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.77	1.09	8	3.81	3.8
sd:	0.593	0.261	10.6	1460	3070

	CNST	HILL	GNLS
AIC:	172.74	169.93	173.93
PROB:	0.18	0.72	0.1
RMSE:	1.59	1.4	1.4

MAX_MEAN: 1.89 MAX_MED: 2.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

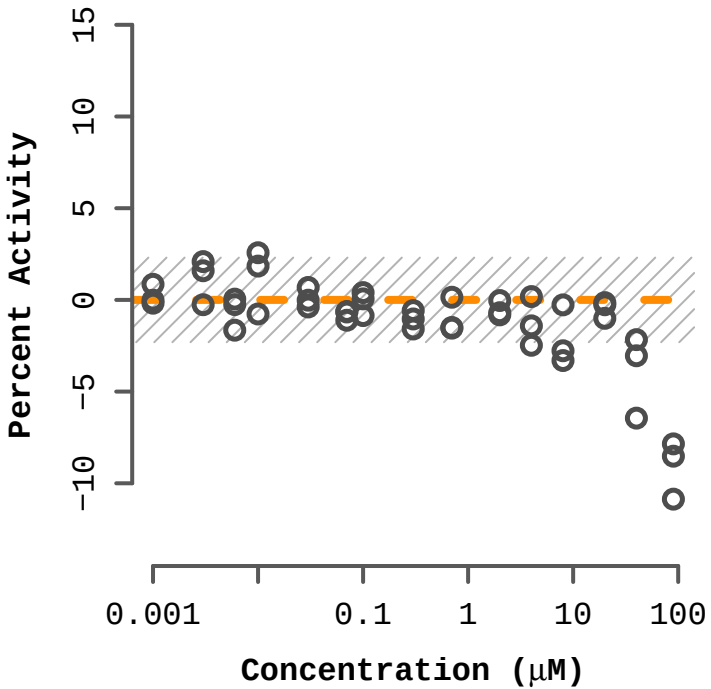
NAME: Isoxathion
CHID: 42080 CASRN: 18854-01-8
SPID(S): Tox21_302209
M4ID: 12476924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

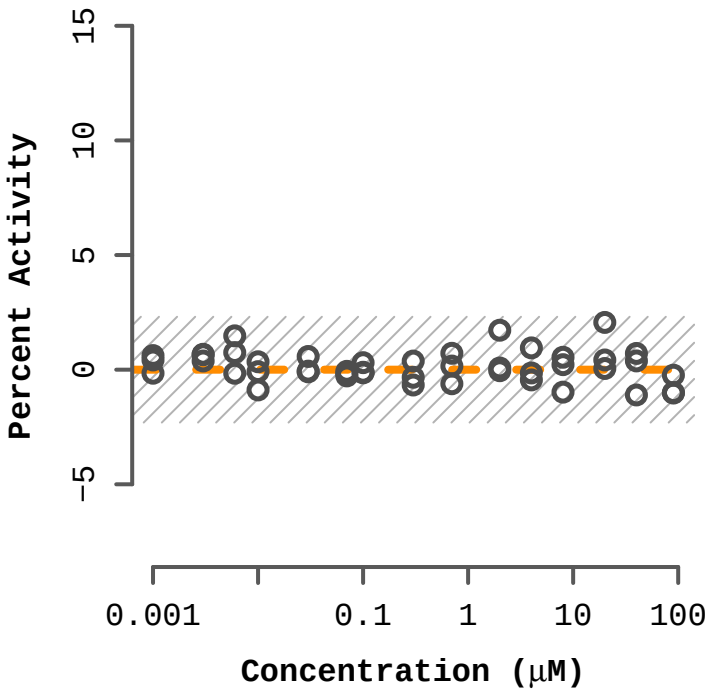
NAME: Kadethrin
CHID: 42083 **CASRN:** 58769-20-3
SPID(S): Tox21_302222
M4ID: 12476911

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.87	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

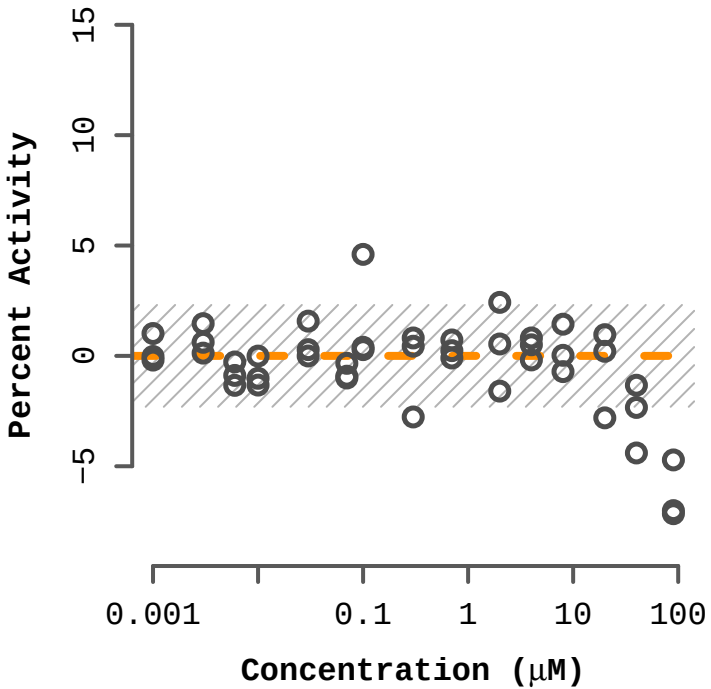
NAME: Karbutilate
CHID: 42084 CASRN: 4849-32-5
SPID(S): Tox21_301748
M4ID: 12477385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.847 MAX_MED: 0.748 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

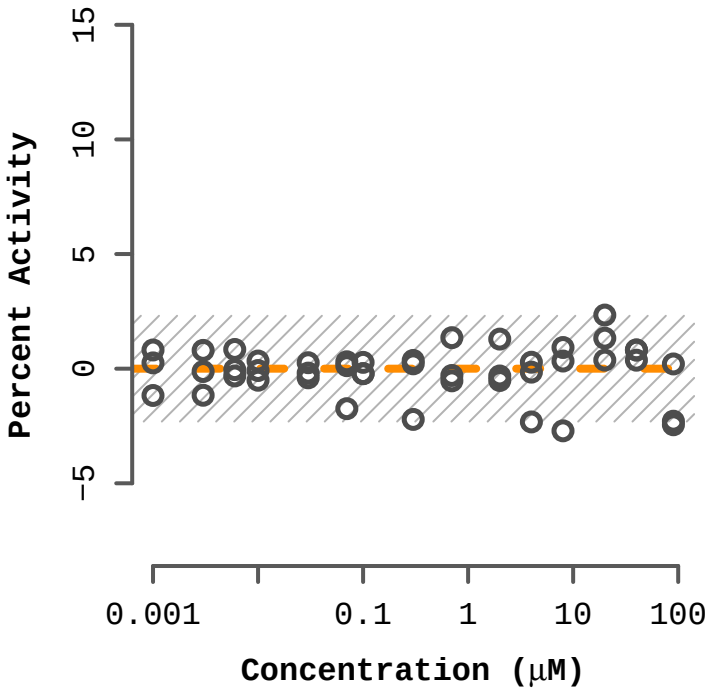
NAME: Laurocapram
CHID: 42086 **CASRN:** 59227-89-3
SPID(S): Tox21_301757
M4ID: 12477376

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 0.617 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

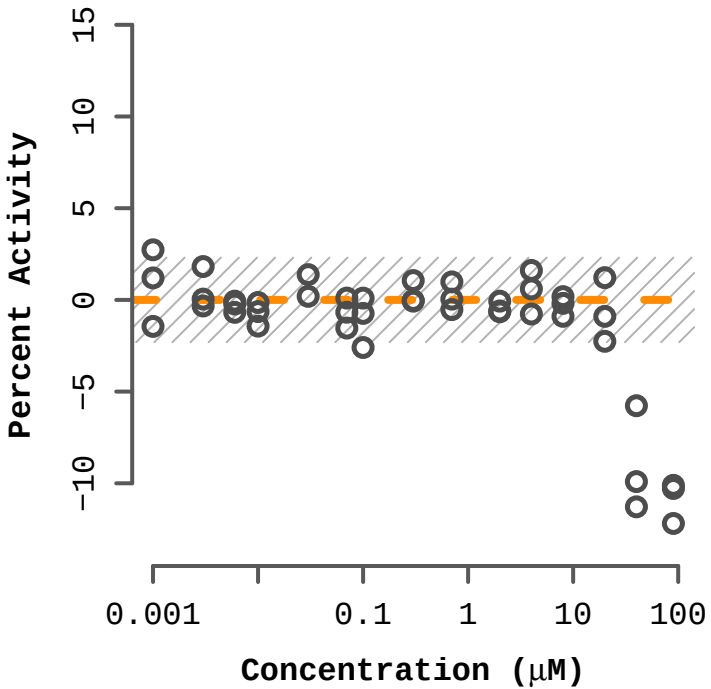
NAME: Lauryl thiocyanate
CHID: 42089 **CASRN:** 765-15-1
SPID(S): Tox21_301924
M4ID: 12477209

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

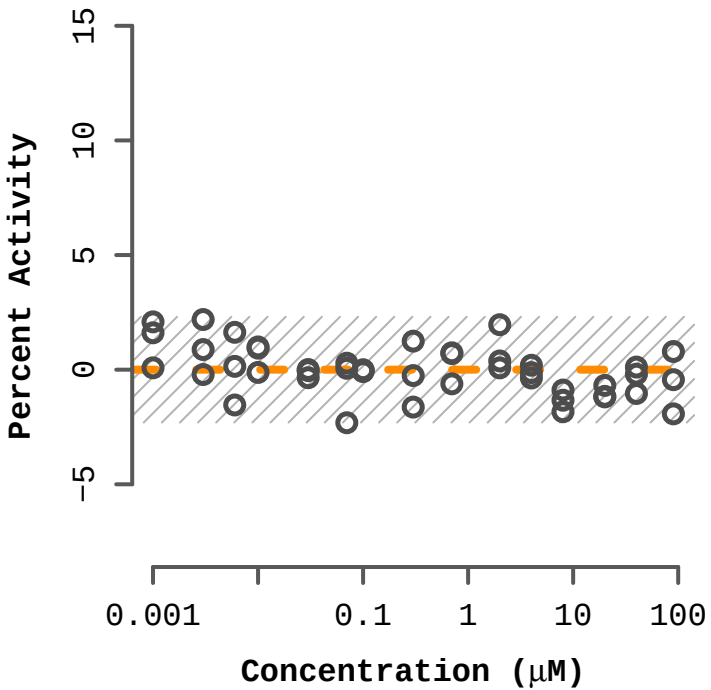
NAME: Lauryldiethanolamine
CHID: 42090 **CASRN:** 1541-67-9
SPID(S): Tox21_301529
M4ID: 12477604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.06	NA	NA
PROB:	1	NA	NA
RMSE:	3.87	NA	NA

MAX_MEAN: 0.83 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

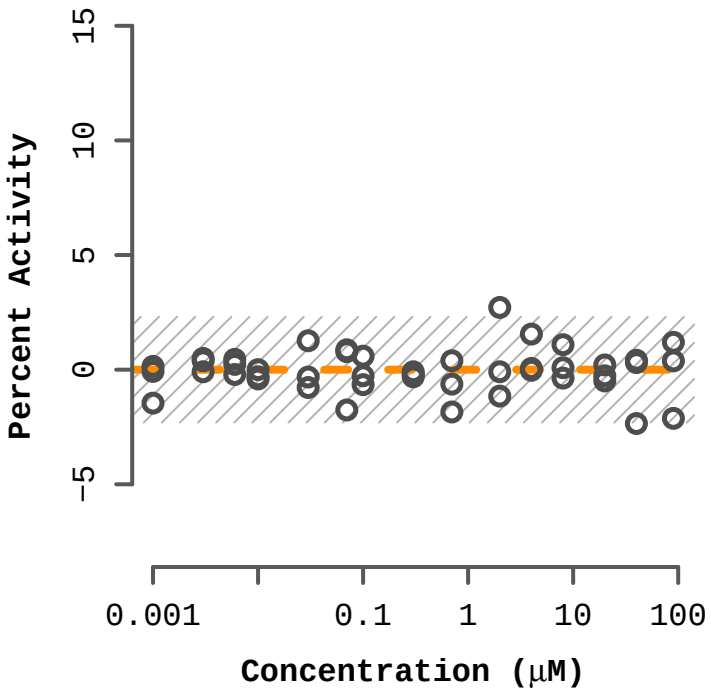
NAME: Levomenol
CHID: 42094 CASRN: 23089-26-1
SPID(S): Tox21_301375
M4ID: 12477758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.26 MAX_MED: 1.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

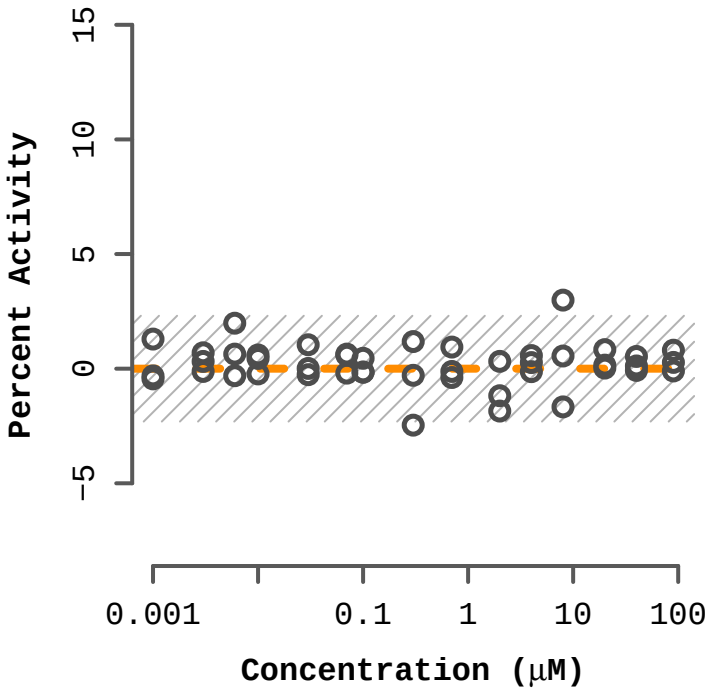
NAME: L-Glucitol
CHID: 42096 **CASRN:** 6706-59-8
SPID(S): Tox21_301754
M4ID: 12477379

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** 0.789 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

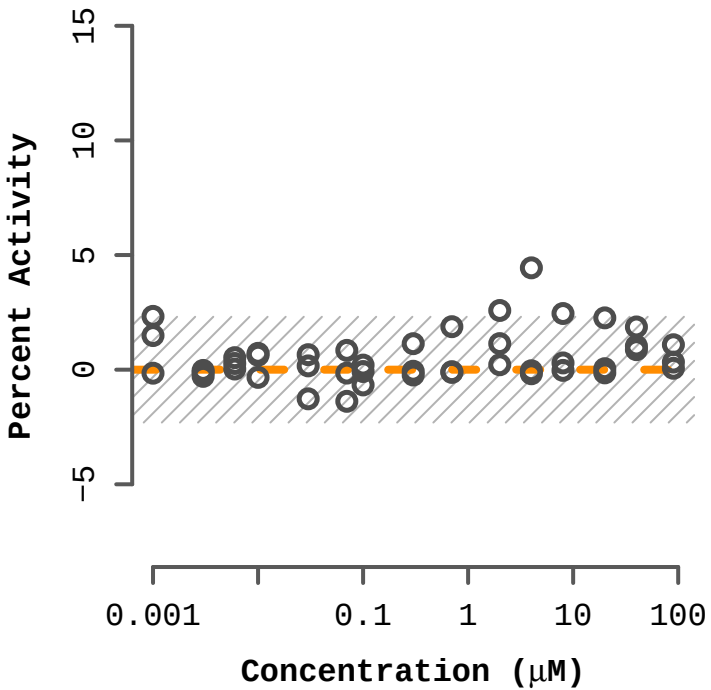
NAME: Limonene dioxide
CHID: 42097 **CASRN:** 96-08-2
SPID(S): Tox21_302214
M4ID: 12476919

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.772 **MAX_MED:** 0.637 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

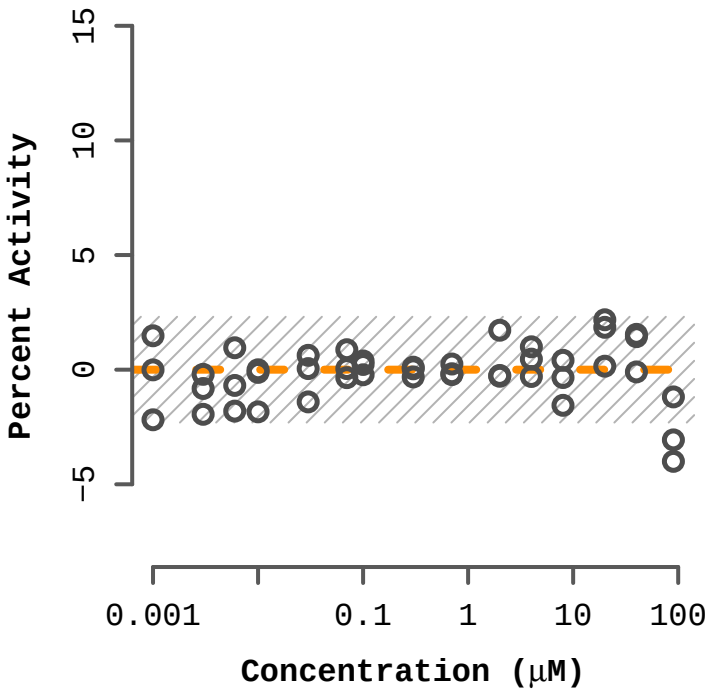
NAME: Mecarbam
CHID: 42117 CASRN: 2595-54-2
SPID(S): Tox21_302005
M4ID: 12477128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

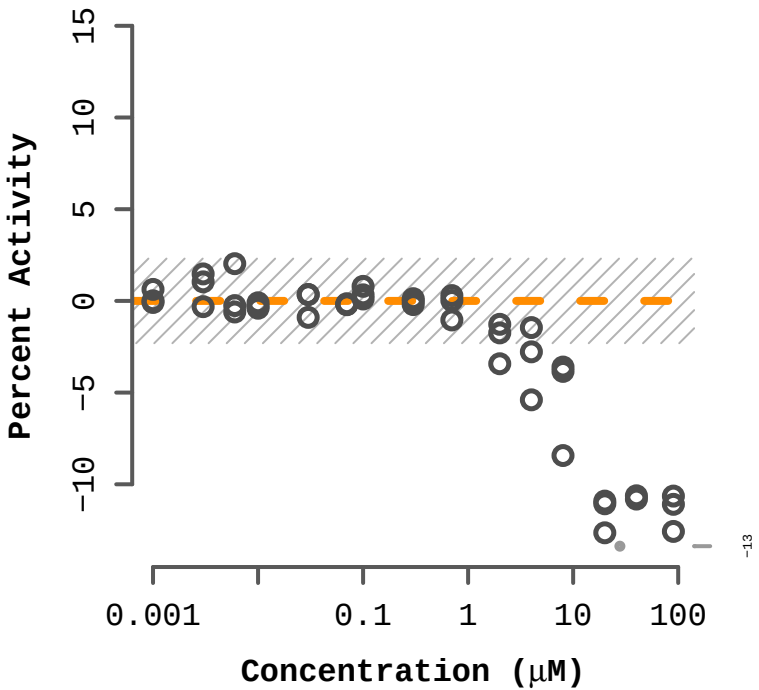
NAME: Mepanipyrim
CHID: 42121 **CASRN:** 110235-47-7
SPID(S): Tox21_300635
M4ID: 12478498

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

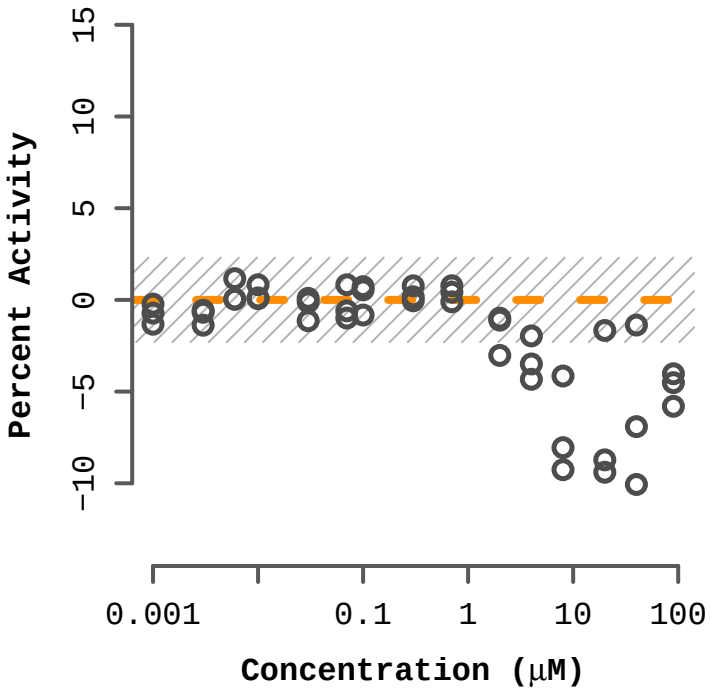
NAME: Mercury(II) acetate
CHID: 42123 **CASRN:** 1600-27-7
SPID(S): Tox21_302000
M4ID: 12477133 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	274.8	NA	NA
PROB:	1	NA	NA
RMSE:	5.52	NA	NA

MAX_MEAN: 0.734 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

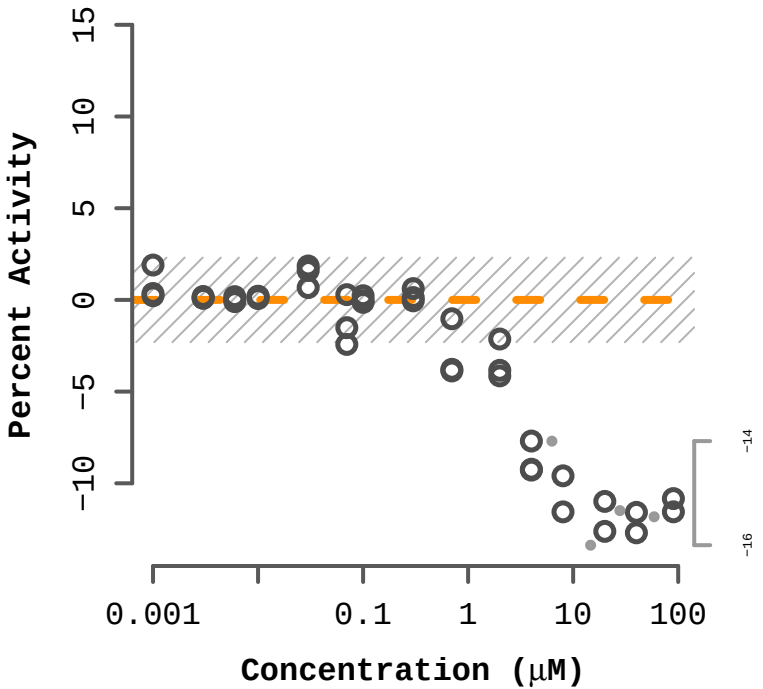
NAME: Mercury(II) iodide
CHID: 42124 **CASRN:** 7774-29-0
SPID(S): Tox21_301595
M4ID: 12477538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.48	NA	NA
PROB:	1	NA	NA
RMSE:	3.7	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.549 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

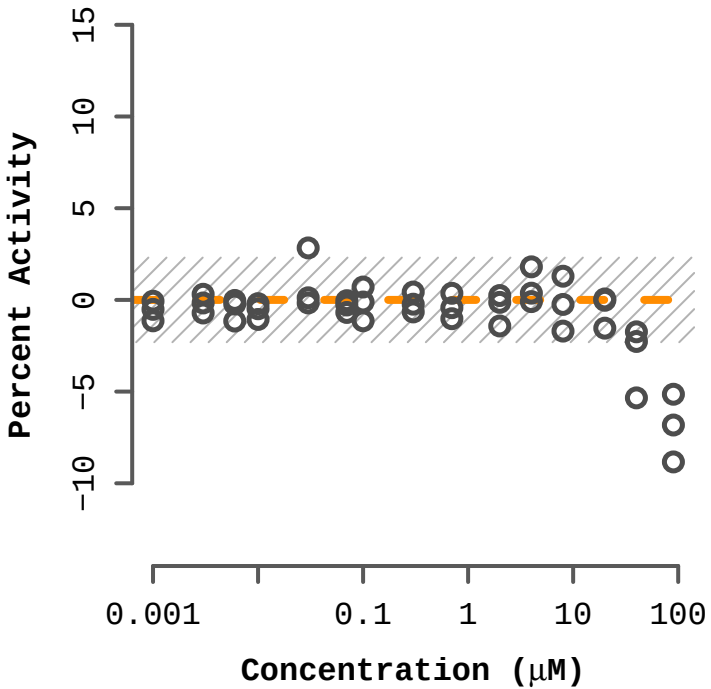
NAME: Phenylmercuric chloride
CHID: 42129 **CASRN:** 100-56-1
SPID(S): Tox21_300878
M4ID: 12478255 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	305.14	NA	NA
PROB:	1	NA	NA
RMSE:	7.16	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

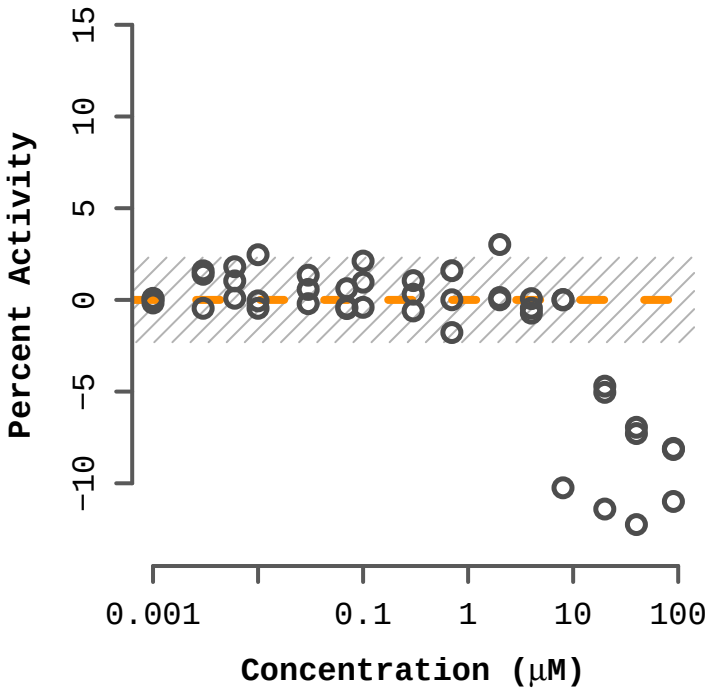
NAME: Diphenylmercury(II)
CHID: 42130 **CASRN:** 587-85-9
SPID(S): Tox21_301326
M4ID: 12477807

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.89	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 0.369 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

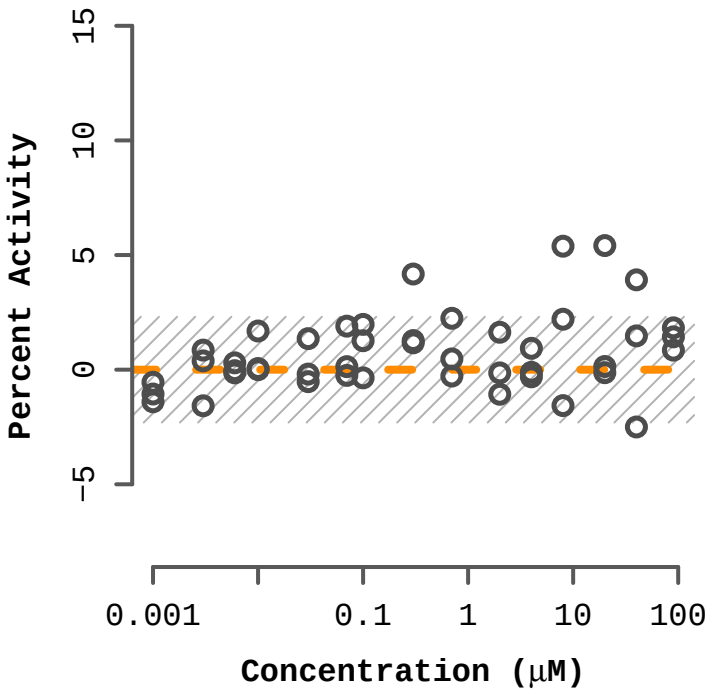
NAME: Methfuroxam
CHID: 42137 CASRN: 28730-17-8
SPID(S): Tox21_301332
M4ID: 12477801

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.69	NA	NA
PROB:	1	NA	NA
RMSE:	4.29	NA	NA

MAX_MEAN: 1.05 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

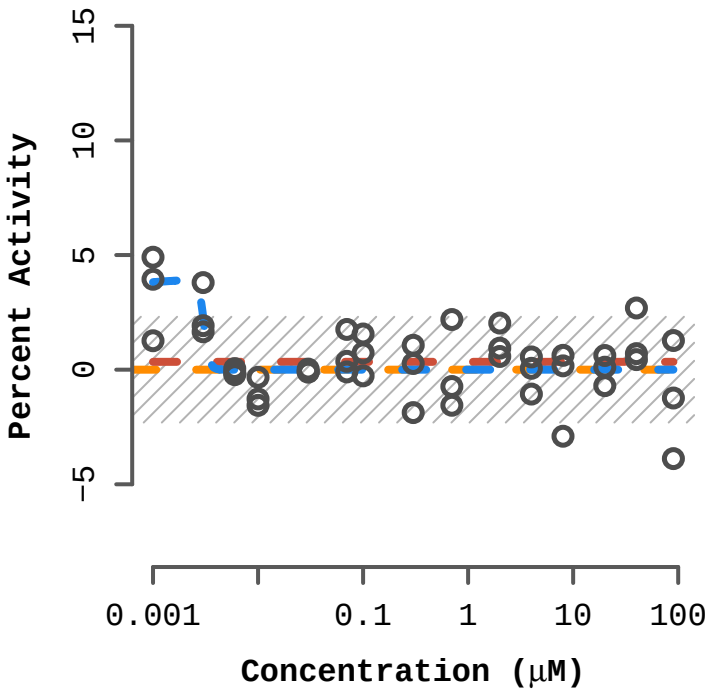
NAME: Methiuron
CHID: 42140 **CASRN:** 21540-35-2
SPID(S): Tox21_301890
M4ID: 12477243

HILL MODEL: Not applicable.

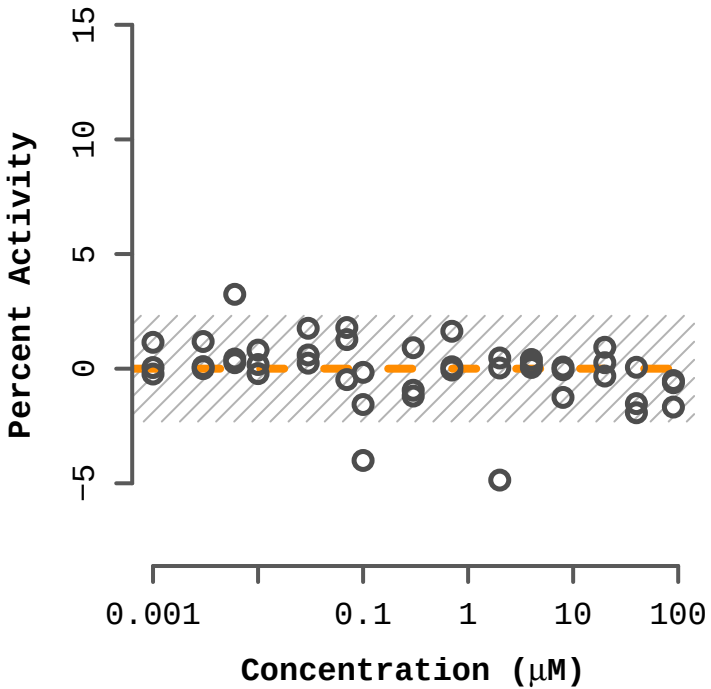
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.2 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Methyl 1-naphthaleneacetate
CHID:    42143   CASRN: 2876-78-0
SPID(S): Tox21_300665
M4ID:    12478468

HILL MODEL (in red):
      tp       ga       gw
val:  0.342    -4.78    4.16
sd:   0.21     1680     3930

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.09     -4.96    0.587    -2.51    17
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  173.52      176.92      162.08
PROB: 0           0           1
RMSE: 1.68        1.64        1.3

MAX_MEAN: 3.37      MAX_MED: 3.95      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

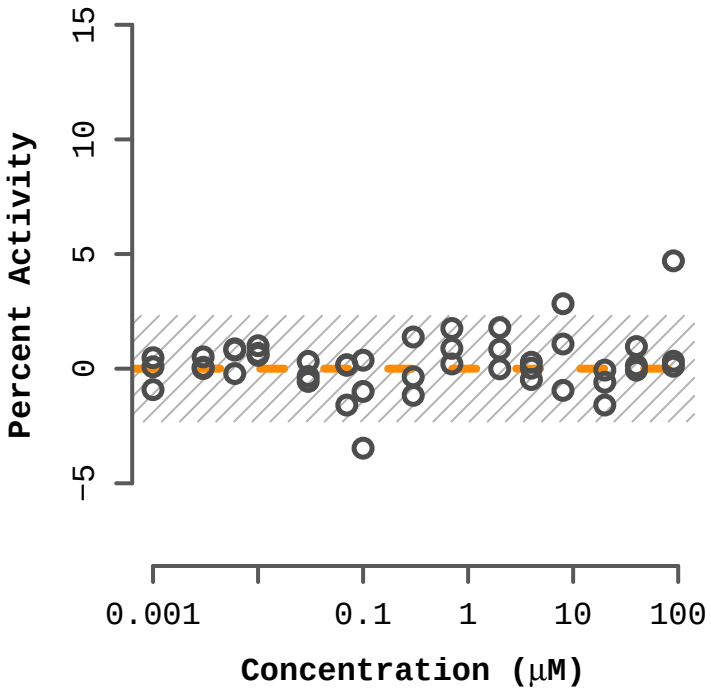
NAME: Methyl 2,3-dibromopropionate
CHID: 42145 **CASRN:** 1729-67-5
SPID(S): Tox21_301977
M4ID: 12477156

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

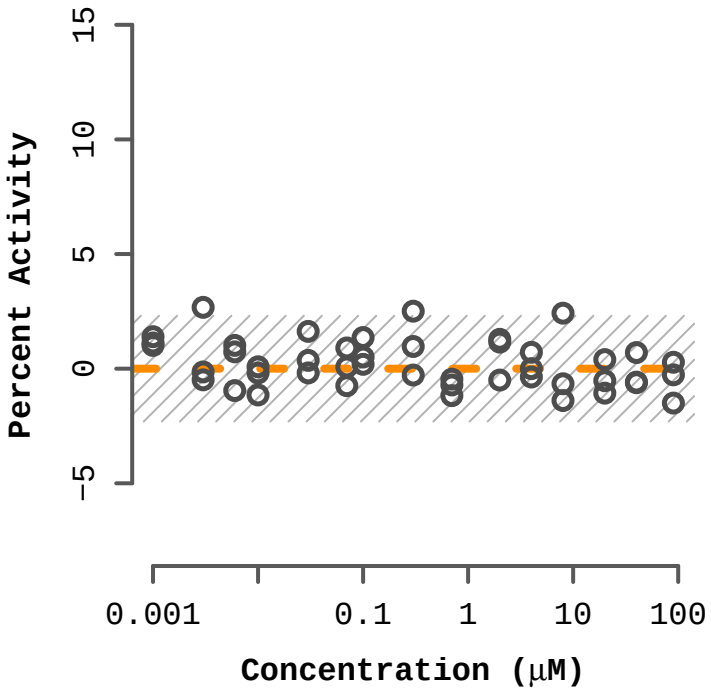
NAME: Methyl 3,5-dichlorobenzoate
CHID: 42146 **CASRN:** 2905-67-1
SPID(S): Tox21_302235
M4ID: 12476898

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

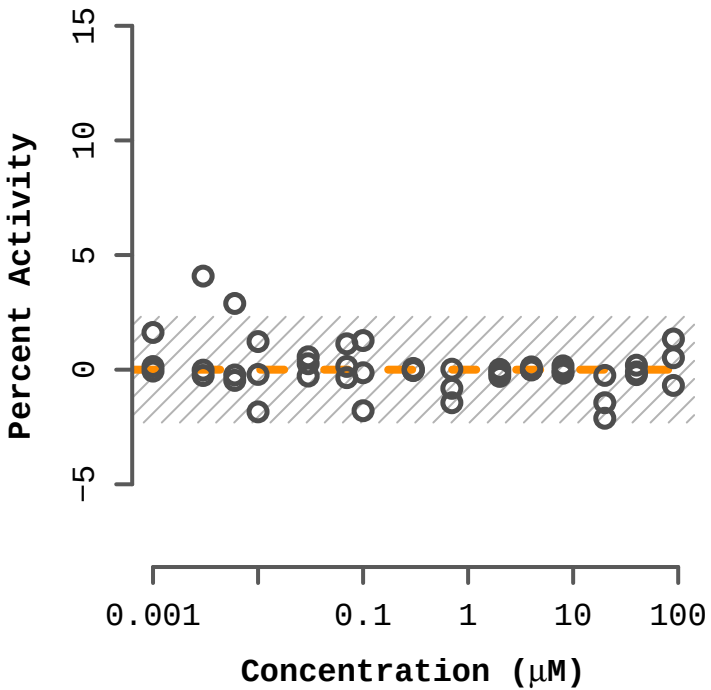
NAME: Methyl 4,4,4−trimethylacetoacetate
CHID: 42149 **CASRN:** 55107−14−7
SPID(S): Tox21_301364
M4ID: 12477769

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

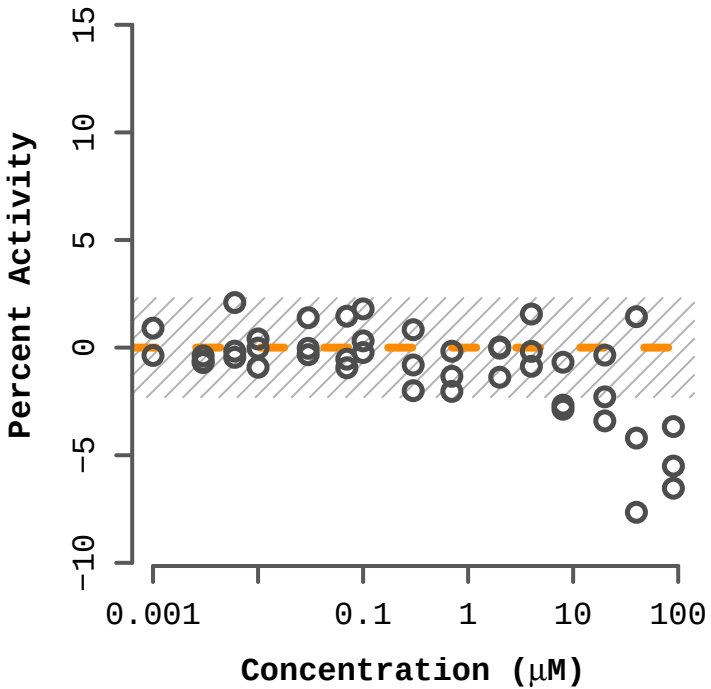
NAME: Methyl cinnamate
CHID: 42151 CASRN: 103-26-4
SPID(S): Tox21_304025
M4ID: 12475163

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.27 MAX_MED: 0.521 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

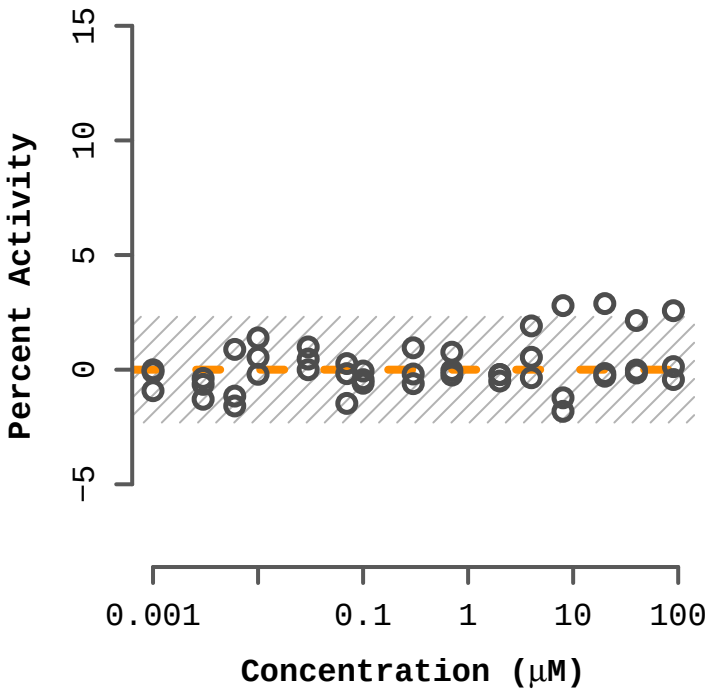
NAME: Methyl red
CHID: 42154 **CASRN:** 493-52-7
SPID(S): Tox21_301336
M4ID: 12477797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 0.629 **MAX_MED:** 0.314 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

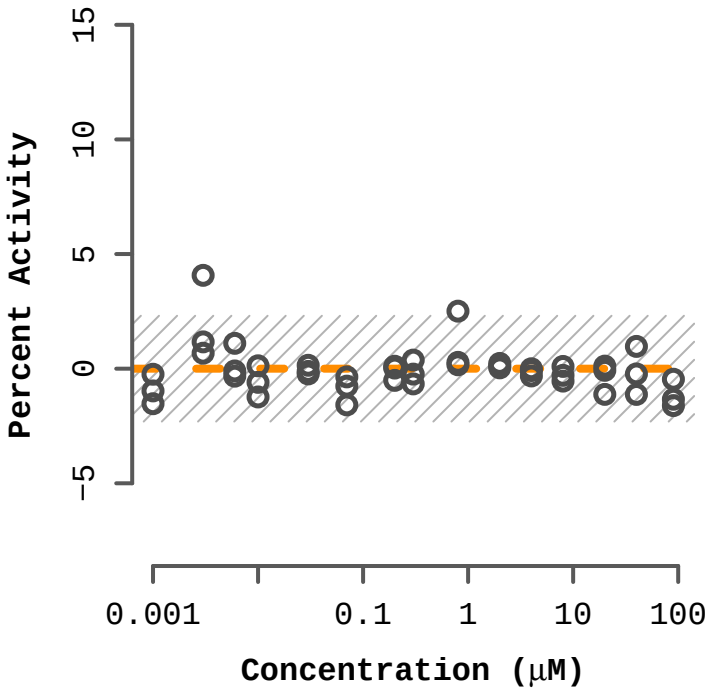
NAME: Metobromuron
CHID: 42157 CASRN: 3060-89-7
SPID(S): Tox21_301964
M4ID: 12477169

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.811 **MAX_MED:** 0.542 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

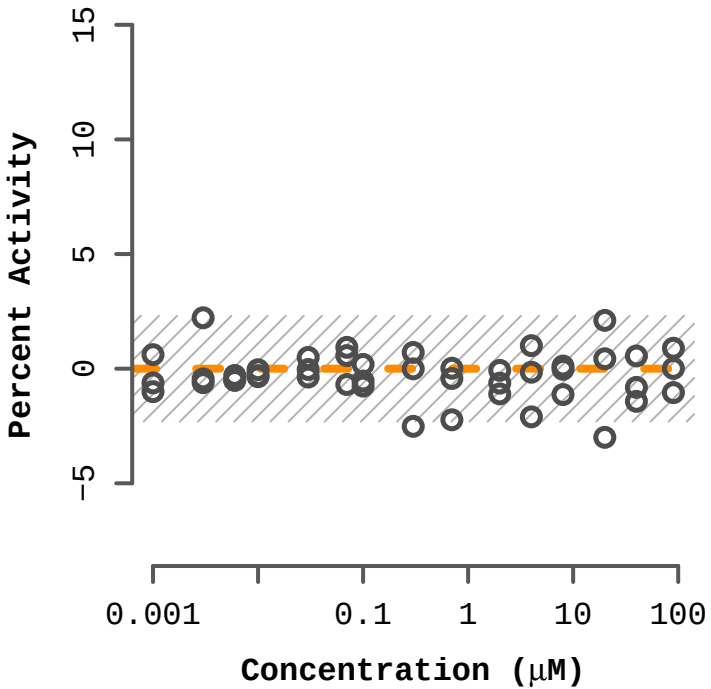
NAME: Monopotassium phthalate
CHID: 42167 **CASRN:** 877-24-7
SPID(S): Tox21_301351
M4ID: 12477782

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

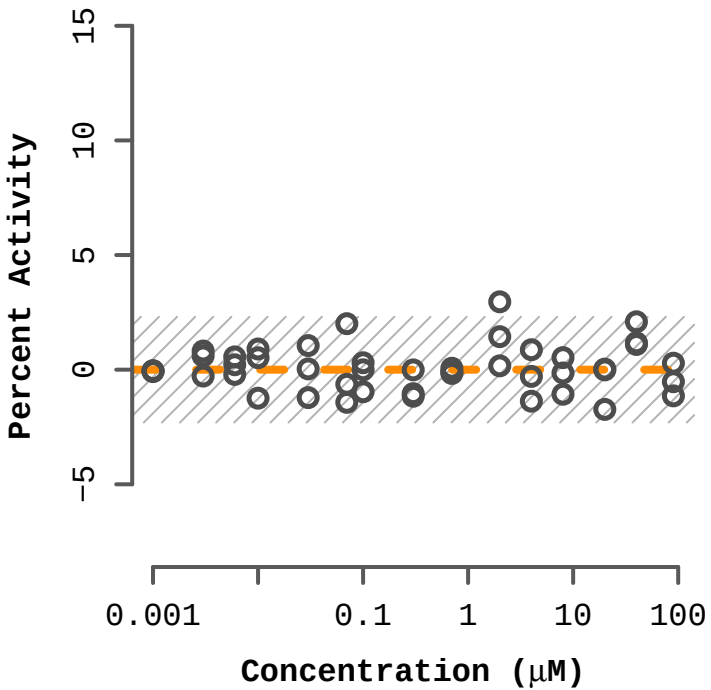
NAME: Monotridecyl phosphate
CHID: 42169 **CASRN:** 5116-94-9
SPID(S): Tox21_301966
M4ID: 12477167

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.39 **MAX_MED:** 0.572 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

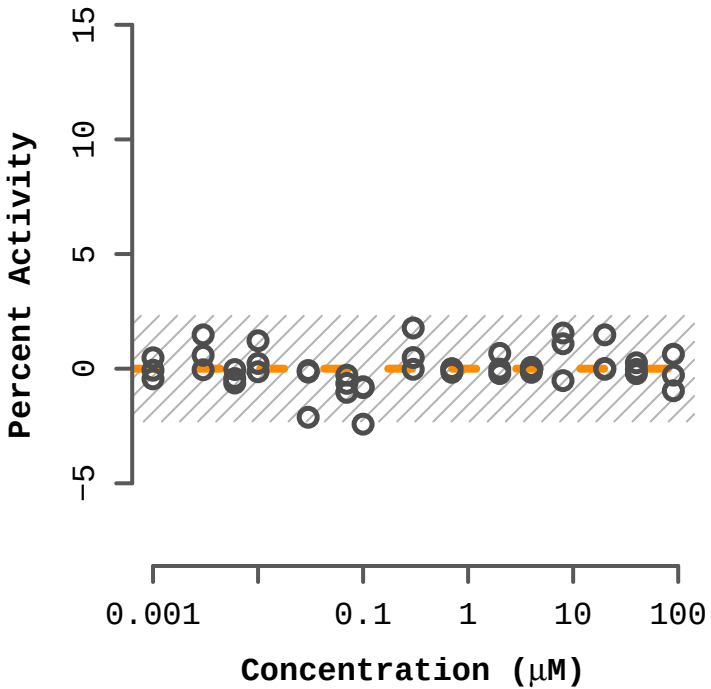
NAME: 4,4'−(Oxydiethylene)bis(morpholine)
CHID: 42170 CASRN: 6425−39−4
SPID(S): Tox21_301312
M4ID: 12477821

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

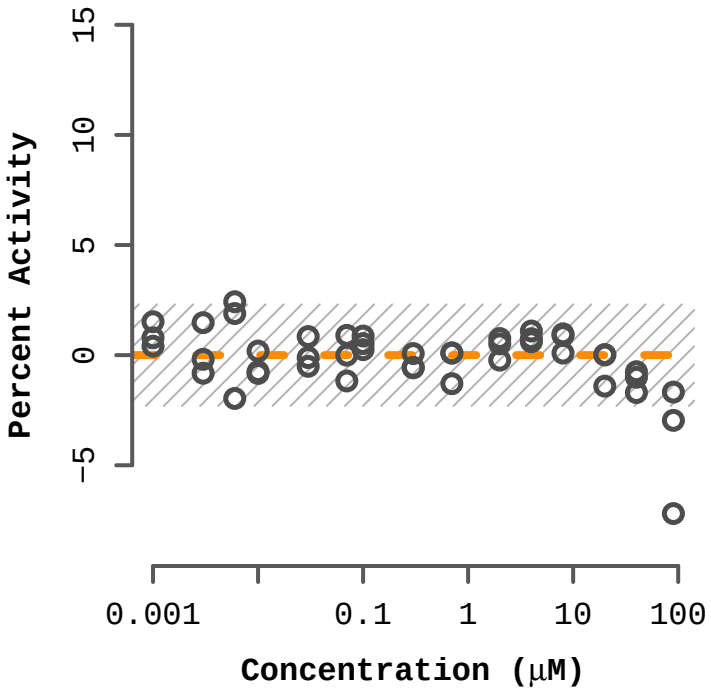
NAME: 4-Dodecylmorpholine
CHID: 42171 **CASRN:** 1541-81-7
SPID(S): Tox21_301236
M4ID: 12477897

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.746 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

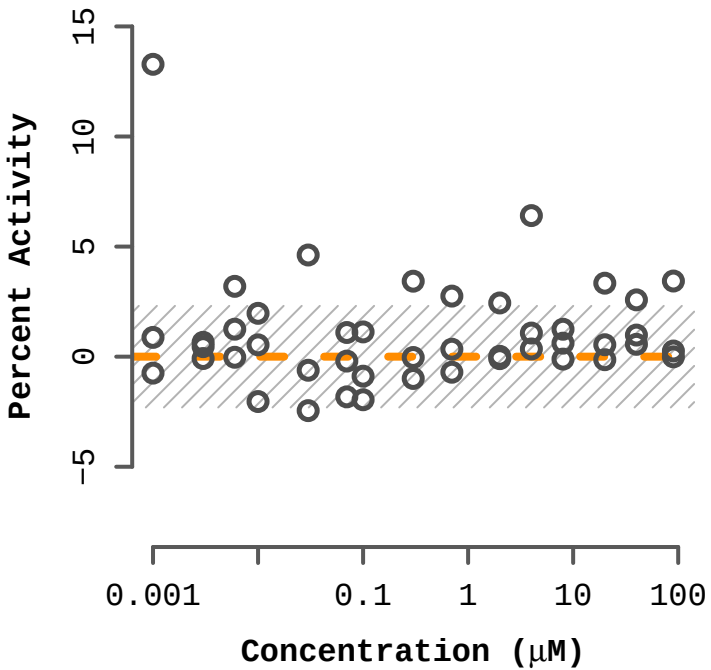
NAME: N-(3,4-Dichlorophenyl)-N'-methylurea
CHID: 42180 **CASRN:** 3567-62-2
SPID(S): Tox21_301892
M4ID: 12477241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

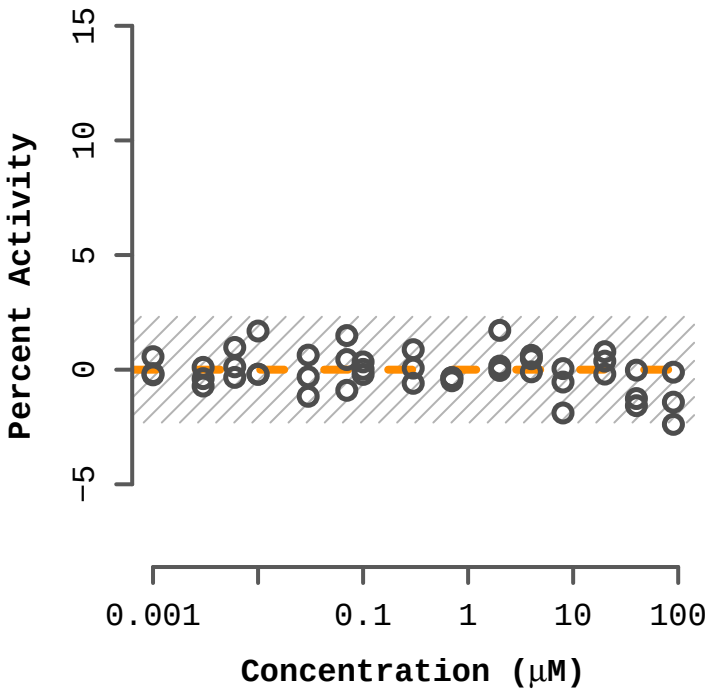
NAME: N-(3-Chloro-4-methylphenyl)acetamide
CHID: 42181 CASRN: 7149-79-3
SPID(S): Tox21_302189
M4ID: 12476944

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.07	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 4.47 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

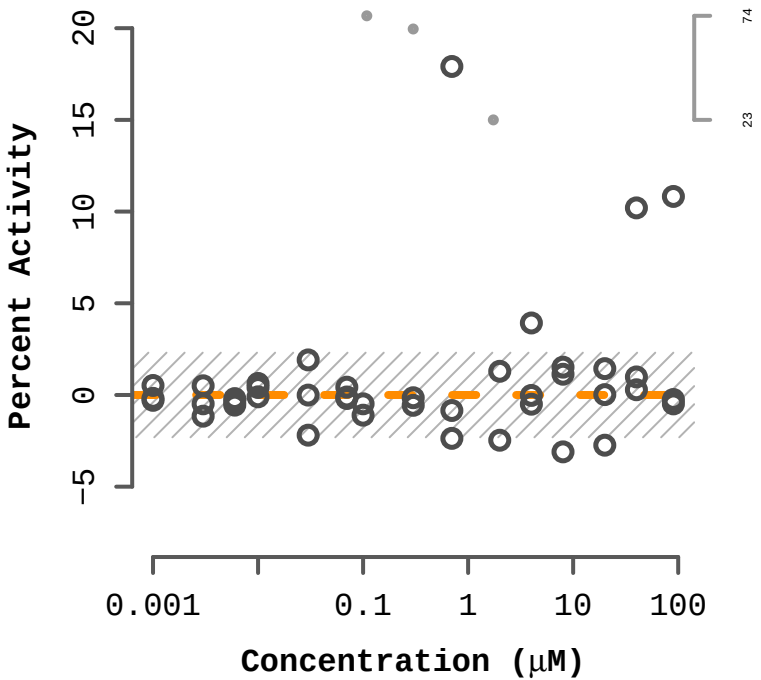
NAME: N,N'−Dibutylthiourea
CHID: 42187 CASRN: 109−46−6
SPID(S): Tox21_300986
M4ID: 12478147

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.614 **MAX_MED:** 0.479 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

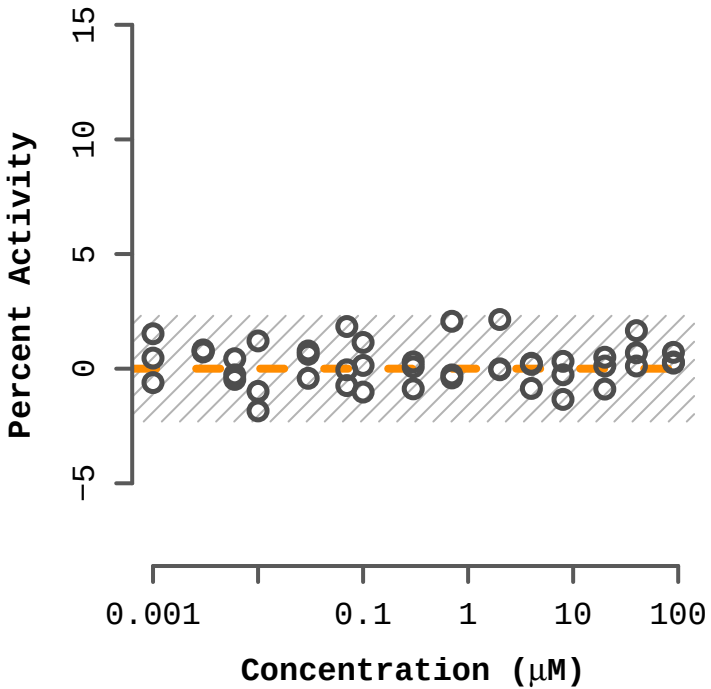
NAME: N,N'−Dibutylurea
CHID: 42188 **CASRN:** 1792−17−2
SPID(S): Tox21_301353
M4ID: 12477780 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	281.29	NA	NA
PROB:	1	NA	NA
RMSE:	15.79	NA	NA

MAX_MEAN: 24.2 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

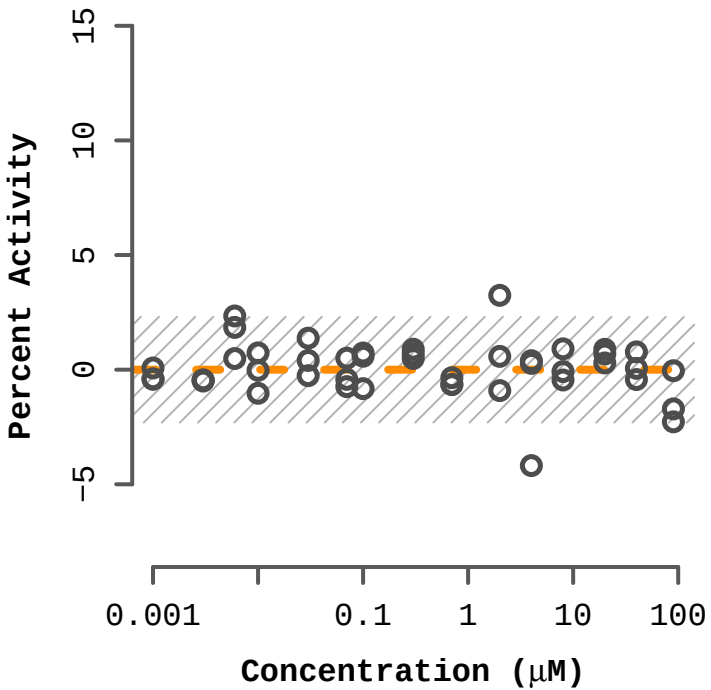
NAME: N,N−Diisopropylaniline
CHID: 42189 **CASRN:** 4107−98−6
SPID(S): Tox21_301373
M4ID: 12477760

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.824 **MAX_MED:** 0.779 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

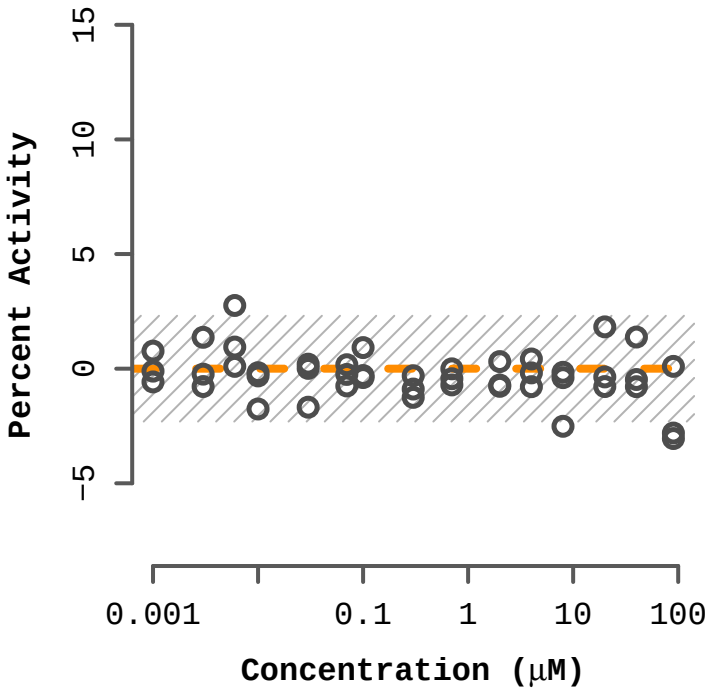
NAME: N,N−Dimethyldecylamine oxide
CHID: 42190 **CASRN:** 2605−79−0
SPID(S): Tox21_302233
M4ID: 12476900

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

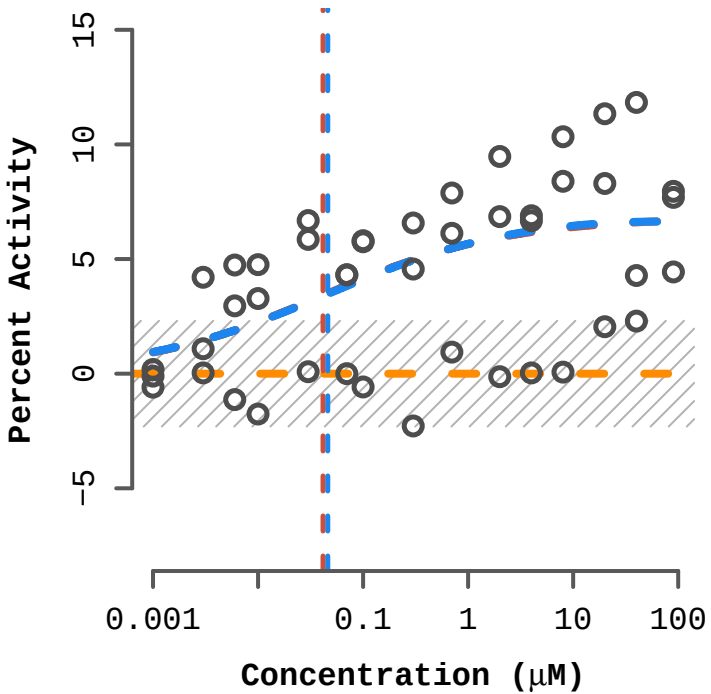
NAME: N,N'−Dimethylthiourea
CHID: 42191 **CASRN:** 534−13−4
SPID(S): Tox21_301391
M4ID: 12477742

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.945 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Naphthoxyacetic acid
CHID: 42195 CASRN: 120-23-0
SPID(S): Tox21_301390
M4ID: 12477743

HILL MODEL (in red):

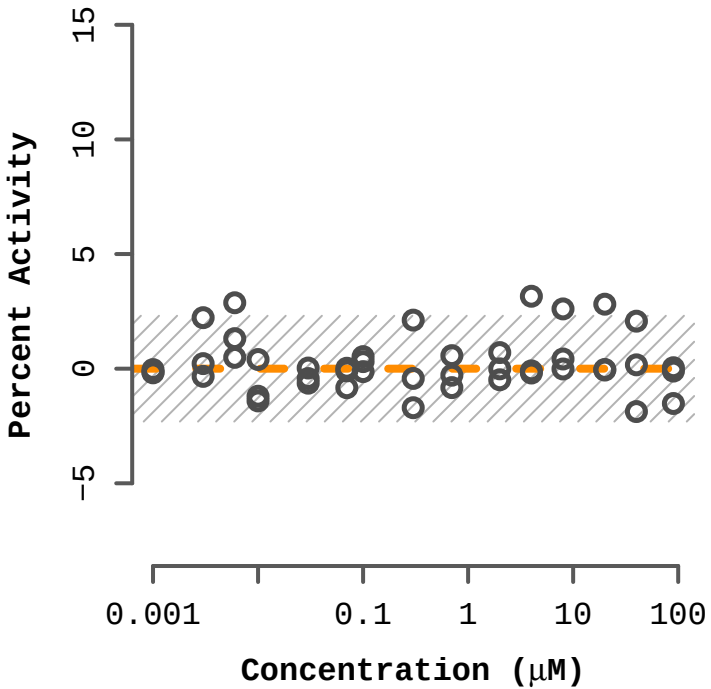
	tp	ga	gw
val:	6.82	−1.38	0.495
sd:	1.47	0.676	0.282

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.95	−1.34	0.482	3.57	1
sd:	3.08	1.16	0.372	15.7	9.04

	CNST	HILL	GNLS
AIC:	287.34	244.66	248.66
PROB:	0	0.88	0.12
RMSE:	5.49	3.21	3.21

MAX_MEAN: 7.23 MAX_MED: 8.39 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

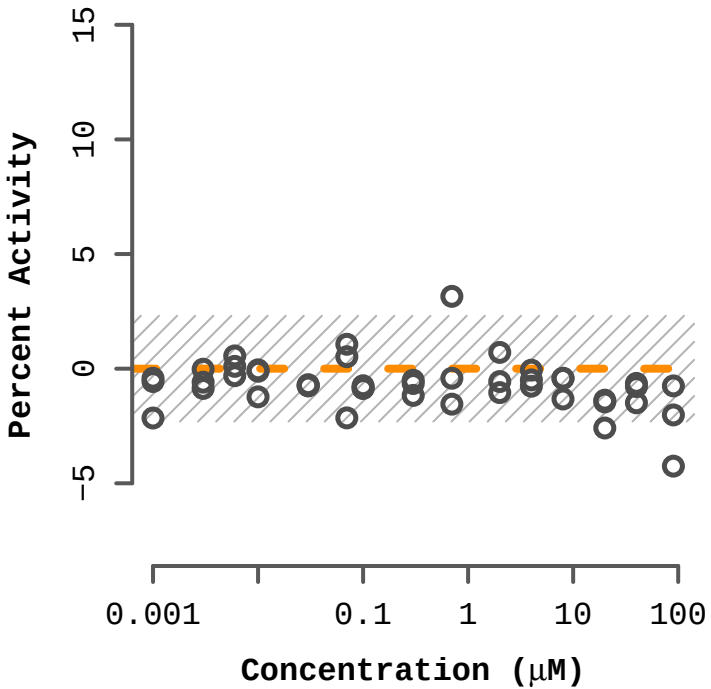
NAME: Butyl lactate
CHID: 42196 CASRN: 138-22-7
SPID(S): Tox21_301349
M4ID: 12477784

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.56 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

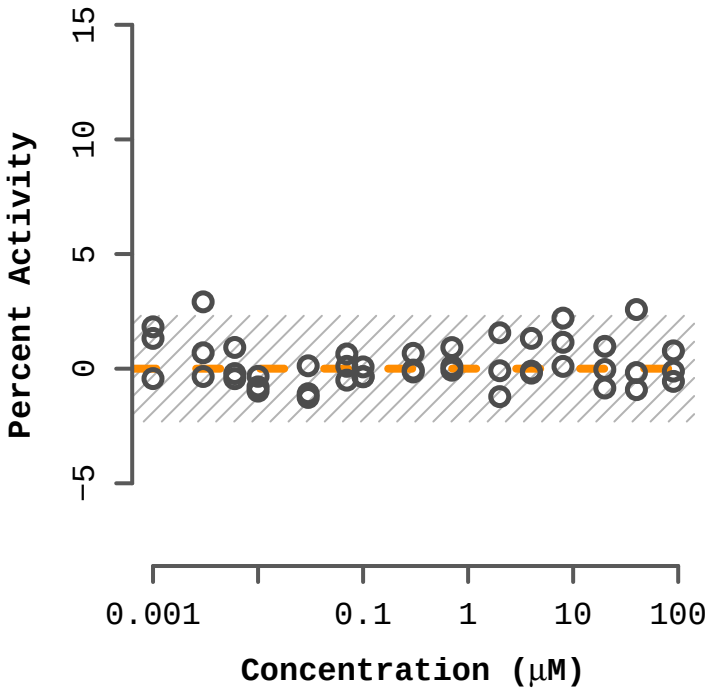
NAME: N-Butyl-p-toluenesulfonamide
CHID: 42198 **CASRN:** 1907-65-9
SPID(S): Tox21_301798
M4ID: 12477335

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.398 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

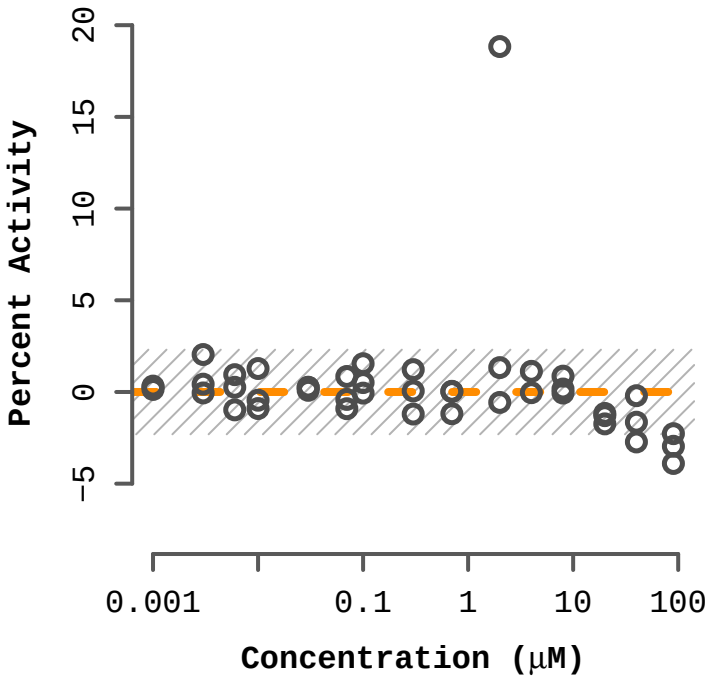
NAME: N-Chlorosuccinimide
CHID: 42199 **CASRN:** 128-09-6
SPID(S): Tox21_301368
M4ID: 12477765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

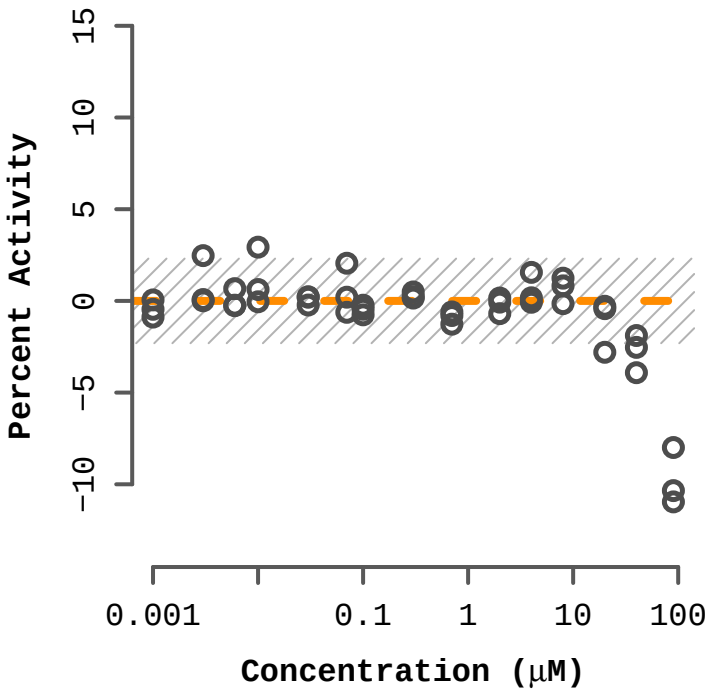
NAME: Nitralin
CHID: 42203 CASRN: 4726-14-1
SPID(S): Tox21_301901
M4ID: 12477232

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.48	NA	NA
PROB:	1	NA	NA
RMSE:	3.1	NA	NA

MAX_MEAN: 6.53 MAX_MED: 1.33 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

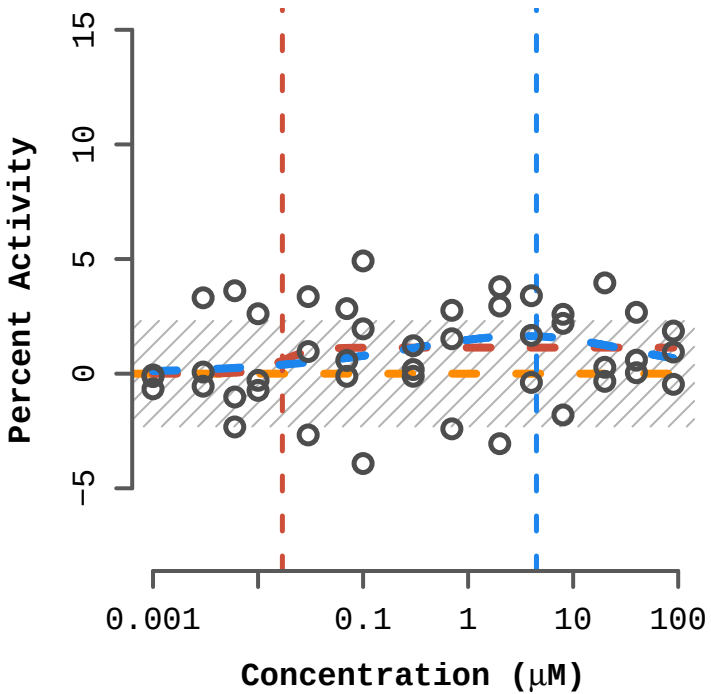
NAME: 1-Dodecyl-2-pyrrolidinone
CHID: 42206 **CASRN:** 2687-96-9
SPID(S): Tox21_300374
M4ID: 12478758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.81	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.821 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-methyl-alpha-phenylbenzeneacetamide
CHID: 42208 **CASRN:** 954-21-2
SPID(S): Tox21_301994
M4ID: 12477139

HILL MODEL (in red):

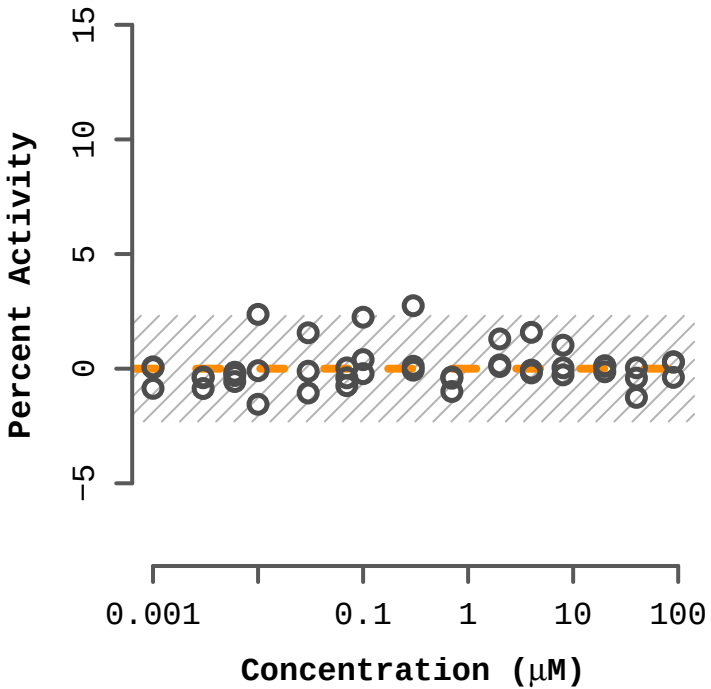
	tp	ga	gw
val:	1.14	−1.77	3.05
sd:	0.388	1.03	9.56

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.44	0.651	0.457	0.901	0.698
sd:	58.5	14.3	0.797	5.34	1.24

	CNST	HILL	GNLS
AIC:	204.64	201.79	205.5
PROB:	0.17	0.72	0.11
RMSE:	2.2	2.03	2.03

MAX_MEAN: 1.56 **MAX_MED:** 2.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

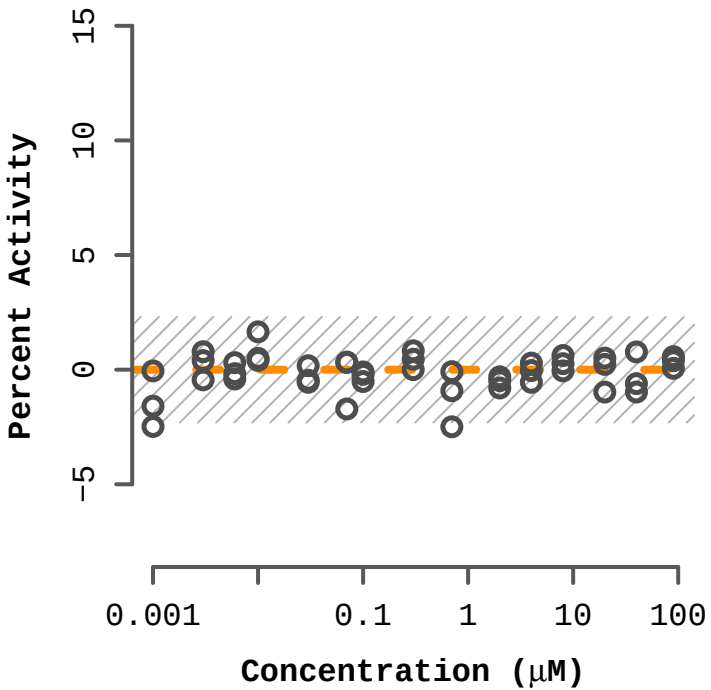
NAME: N-Methyldioctylamine
CHID: 42209 **CASRN:** 4455-26-9
SPID(S): Tox21_300368
M4ID: 12478764

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.929 **MAX_MED:** 0.395 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

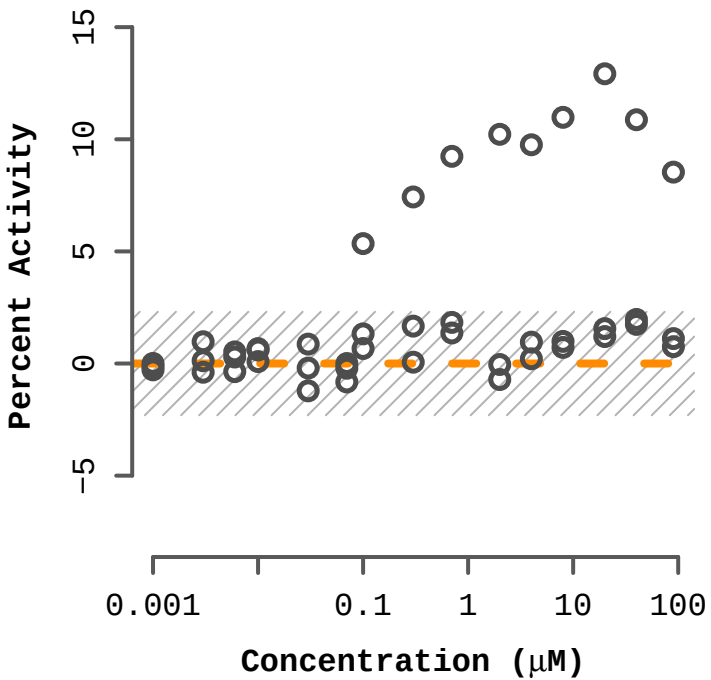
NAME: N-Methylpyrrolidine
CHID: 42210 **CASRN:** 120-94-5
SPID(S): Tox21_301212
M4ID: 12477921

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.851 **MAX_MED:** 0.495 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

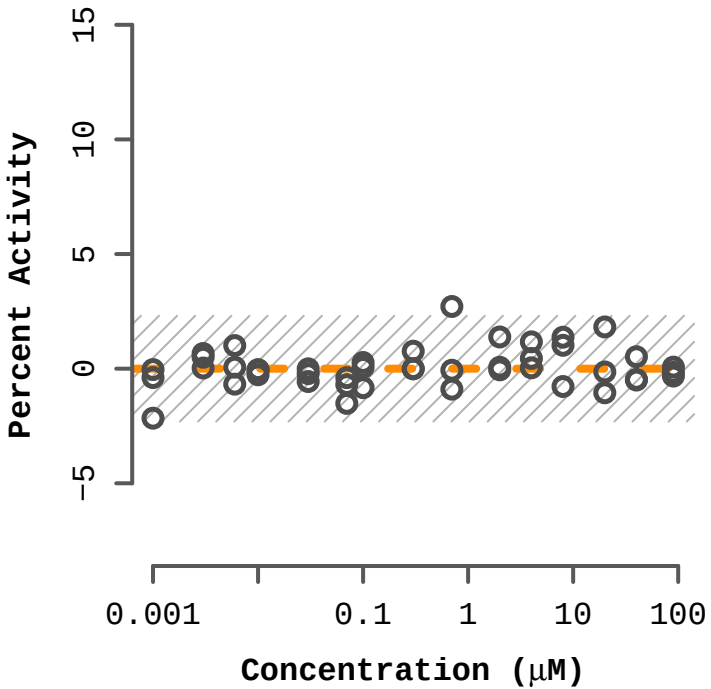
NAME: Nonanoyl chloride
CHID: 42215 **CASRN:** 764-85-2
SPID(S): Tox21_202869
M4ID: 12479383

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.53	NA	NA
PROB:	1	NA	NA
RMSE:	4.42	NA	NA

MAX_MEAN: 5.23 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

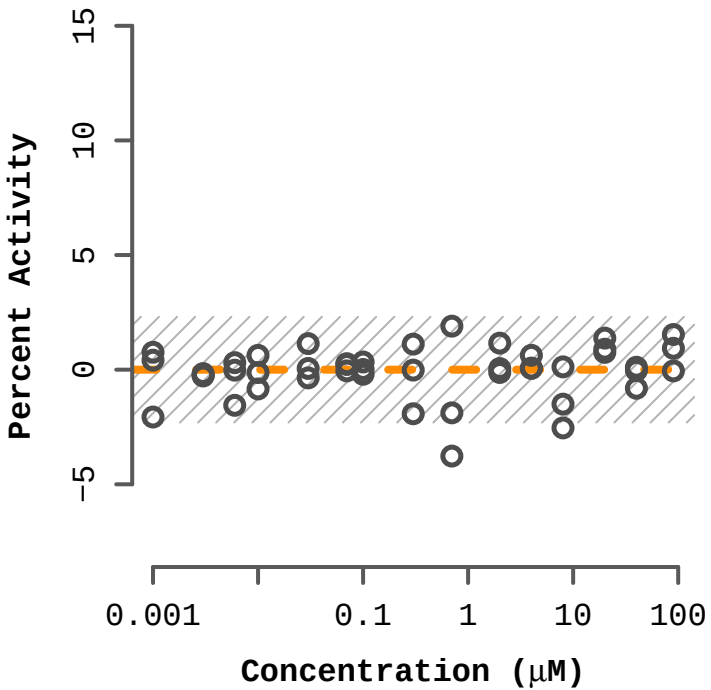
NAME: Pentyl valerate
CHID: 42218 CASRN: 2173-56-0
SPID(S): Tox21_302212
M4ID: 12476921

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.585 MAX_MED: 1.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

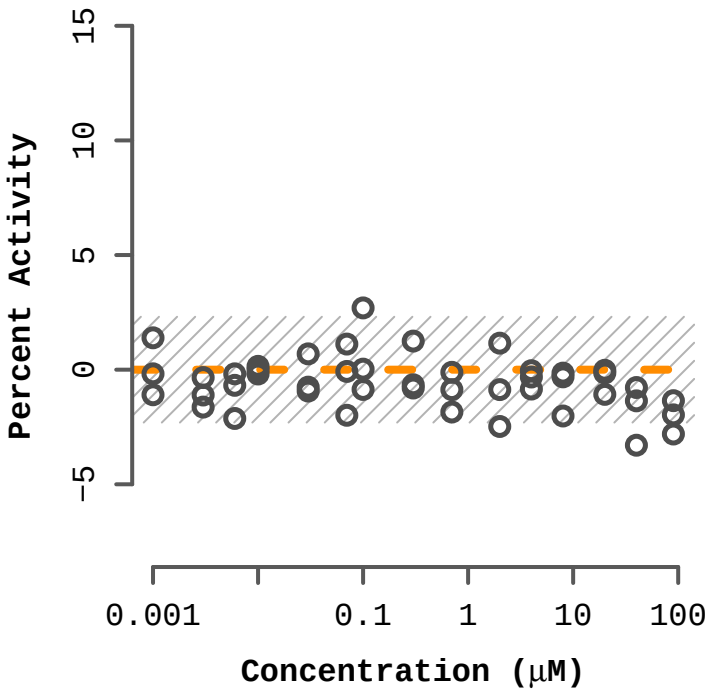
NAME: Propylbenzene
CHID: 42219 **CASRN:** 103-65-1
SPID(S): Tox21_300567
M4ID: 12478566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.934 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

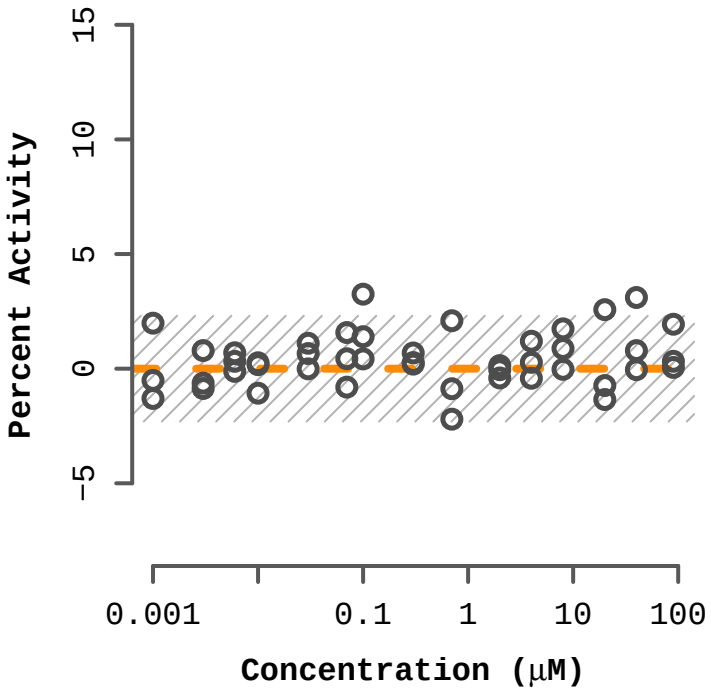
NAME: Nuarimol
CHID: 42220 CASRN: 63284-71-9
SPID(S): Tox21_301251
M4ID: 12477882

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.62 MAX_MED: 0.0242 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

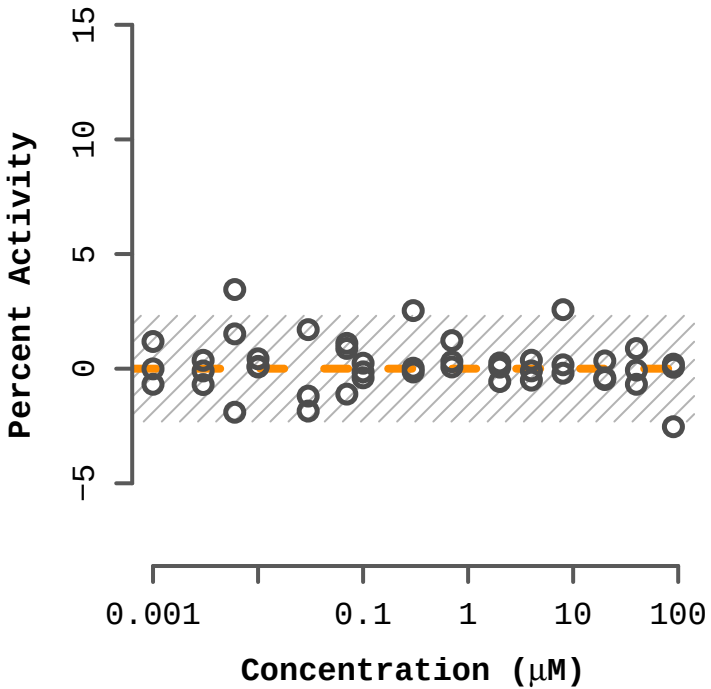
NAME: 7-Hydroxy-3,7-dimethyloctanal
CHID: 42232 **CASRN:** 107-75-5
SPID(S): Tox21_301174
M4ID: 12477959

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

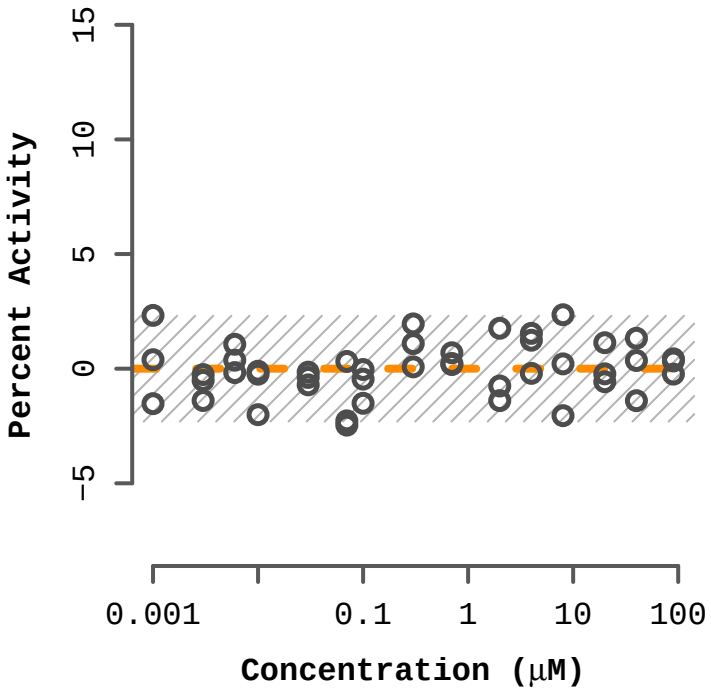
NAME: Octyl beta-D-glucopyranoside
CHID: 42234 CASRN: 29836-26-8
SPID(S): Tox21_302162
M4ID: 12476971

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.02 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

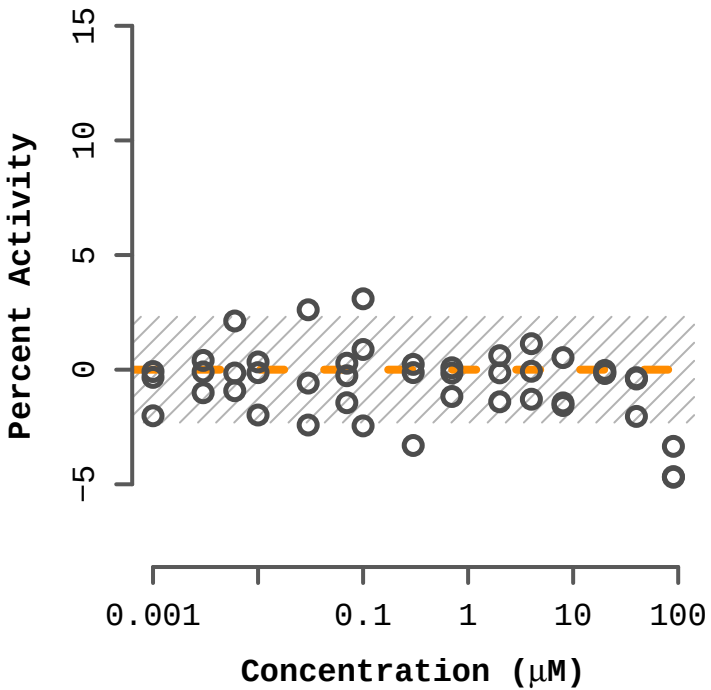
NAME: 2-Ethylaniline
CHID: 42242 **CASRN:** 578-54-1
SPID(S): Tox21_301376
M4ID: 12477757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

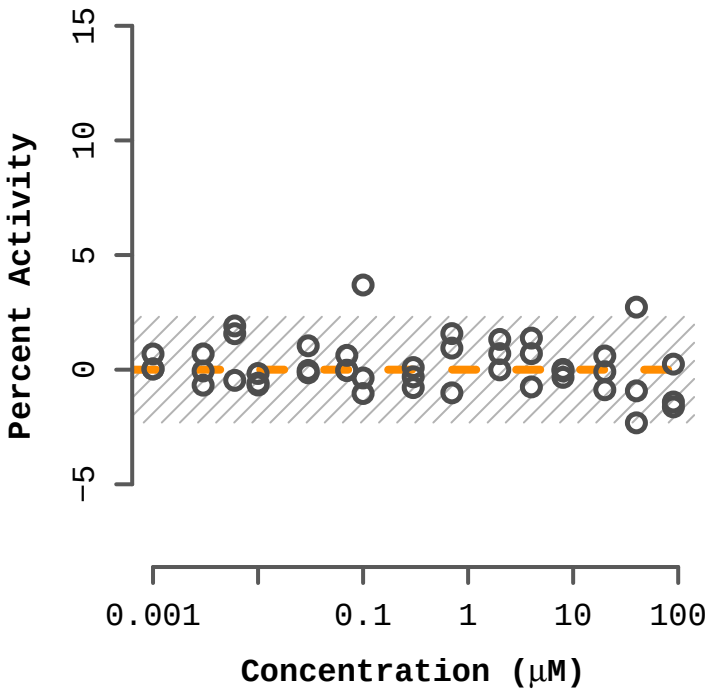
NAME: Oleyl sarcosine
CHID: 42243 **CASRN:** 110-25-8
SPID(S): Tox21_300927
M4ID: 12478206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 0.508 **MAX_MED:** 0.882 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

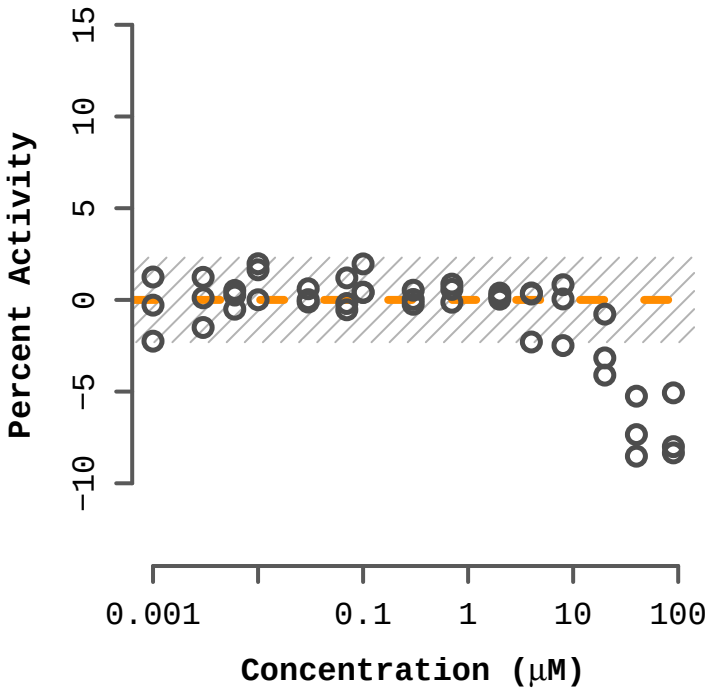
NAME: 2-(2-(4-Chlorophenyl)ethyl)-2-(1,1-dimethyleth
CHID: 42247 **CASRN:** 80443-63-6
SPID(S): Tox21_301539
M4ID: 12477594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

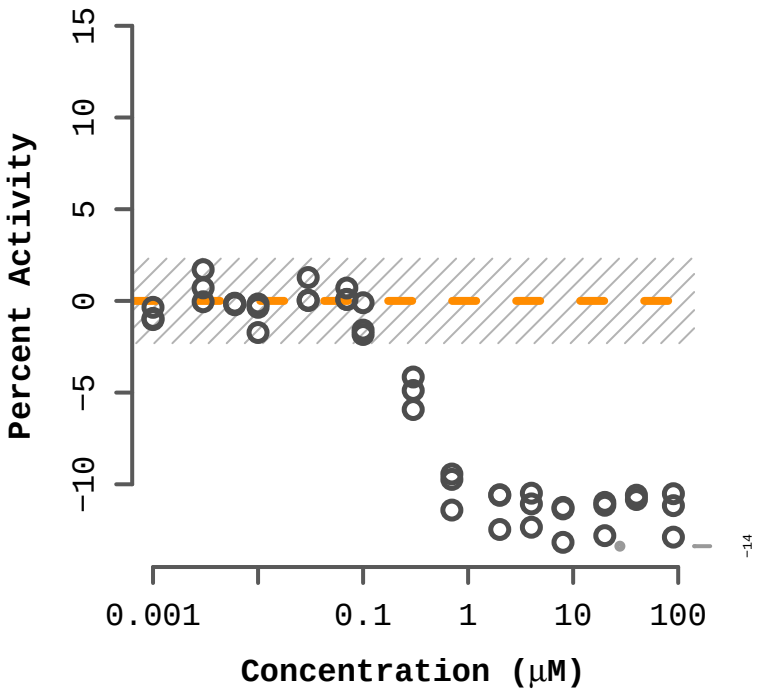
NAME: 4,4'-Methylenebis(N,N-diglycidylaniline)
CHID: 42248 **CASRN:** 28768-32-3
SPID(S): Tox21_301386
M4ID: 12477747

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	209.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.9	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

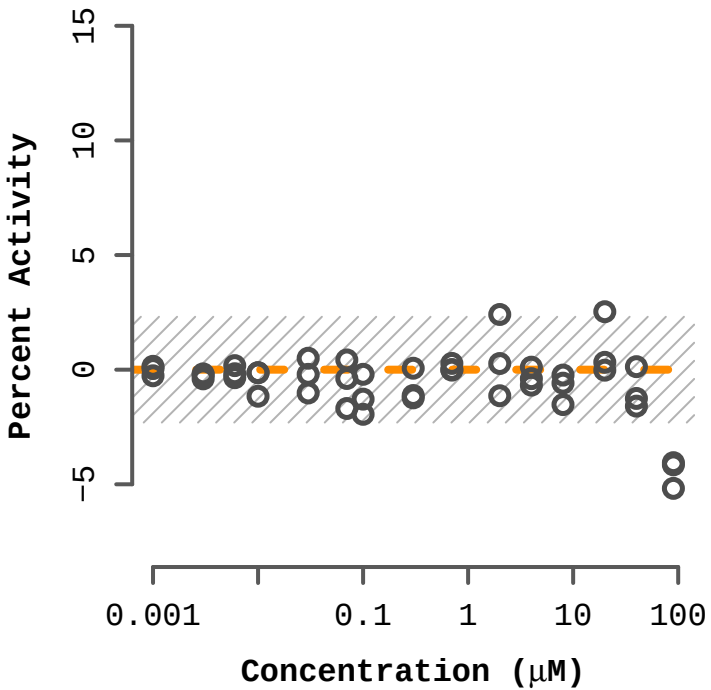
NAME: Phenylarsine oxide
CHID: 42249 **CASRN:** 637-03-6
SPID(S): Tox21_301319
M4ID: 12477814 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	320.81	NA	NA
PROB:	1	NA	NA
RMSE:	7.93	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 0.712 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

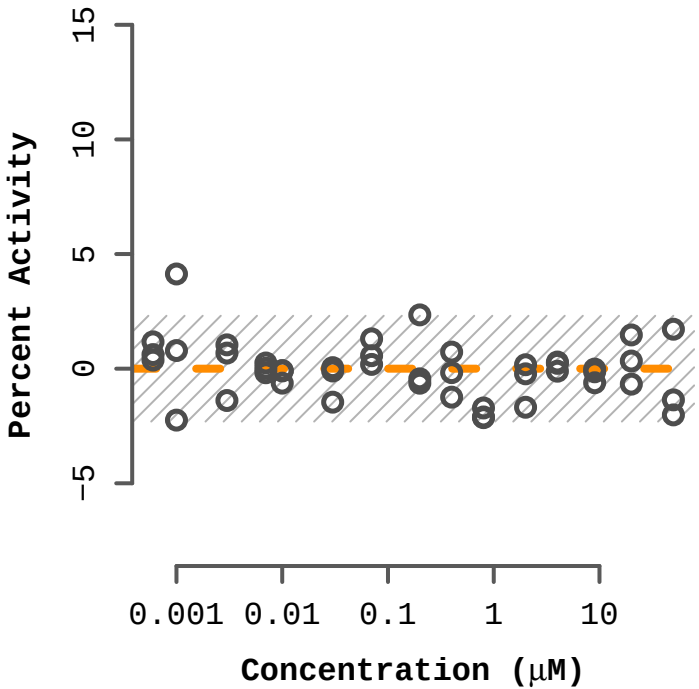
NAME: 4−(Dimethylamino)phenylthiocyanate
CHID: 42252 **CASRN:** 7152−80−9
SPID(S): Tox21_302191
M4ID: 12476942

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 0.323 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

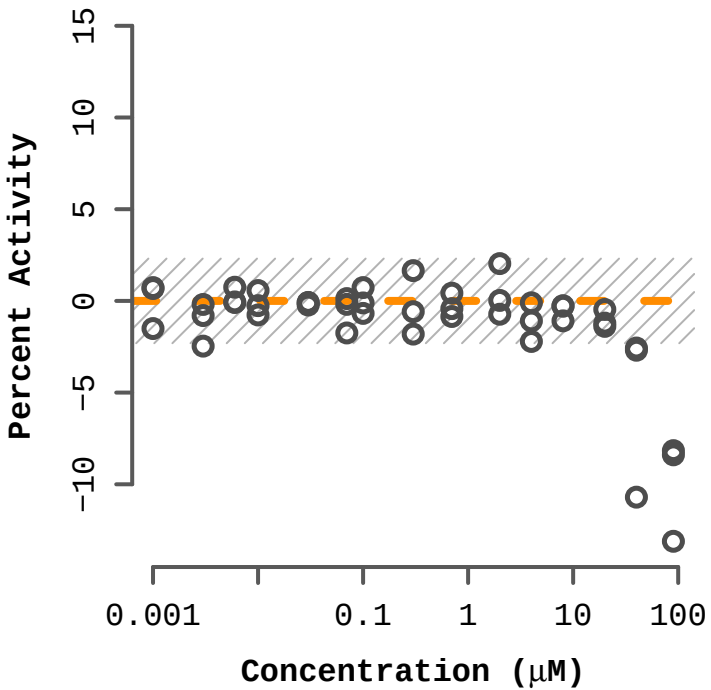
NAME: Palmitoylethanolamide
CHID: 42254 **CASRN:** 544-31-0
SPID(S): Tox21_110222_1
M4ID: 12484539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 0.793 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

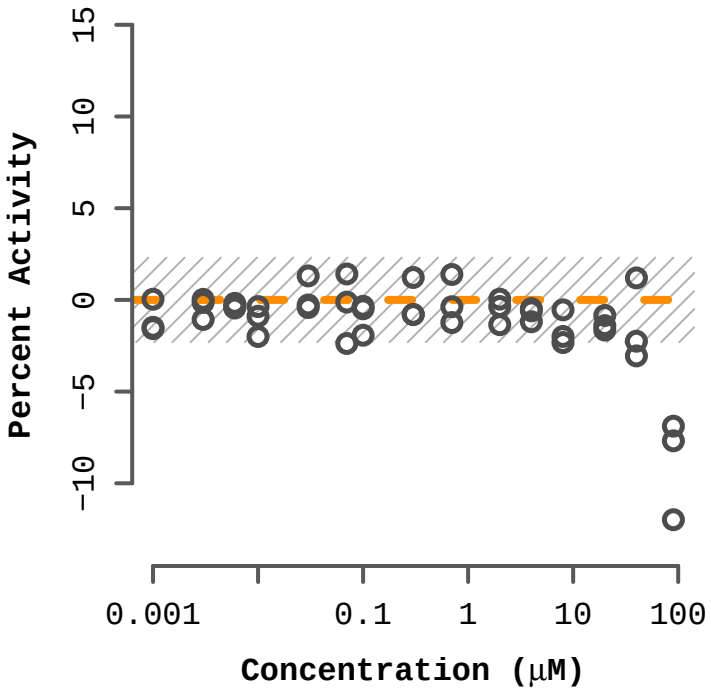
NAME: Parinol
CHID: 42256 **CASRN:** 17781-31-6
SPID(S): Tox21_301259
M4ID: 12477874

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.69	NA	NA
PROB:	1	NA	NA
RMSE:	3.25	NA	NA

MAX_MEAN: 0.446 **MAX_MED:** 0.677 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

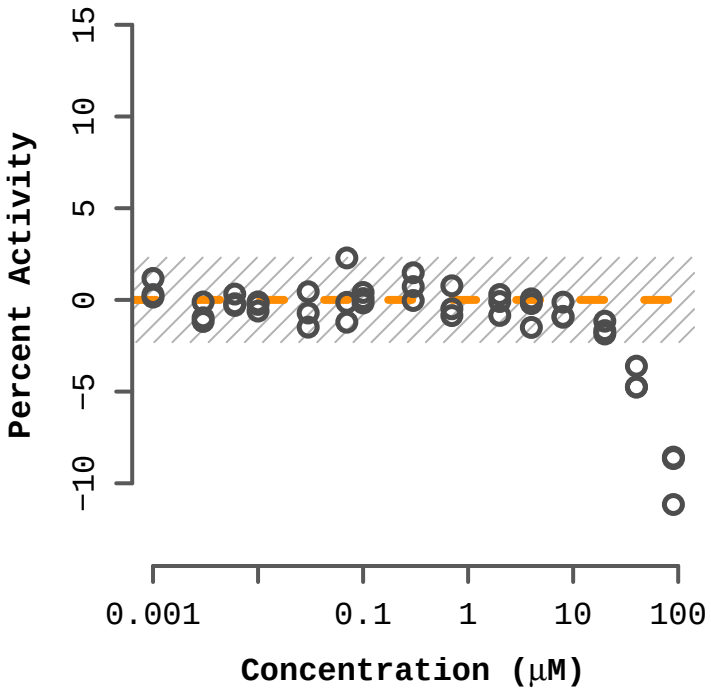
NAME: 4-Chlorophenyl phenyl sulfone
CHID: 42259 **CASRN:** 80-00-2
SPID(S): Tox21_301666
M4ID: 12477467

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 0.206 **MAX_MED:** −0.118 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

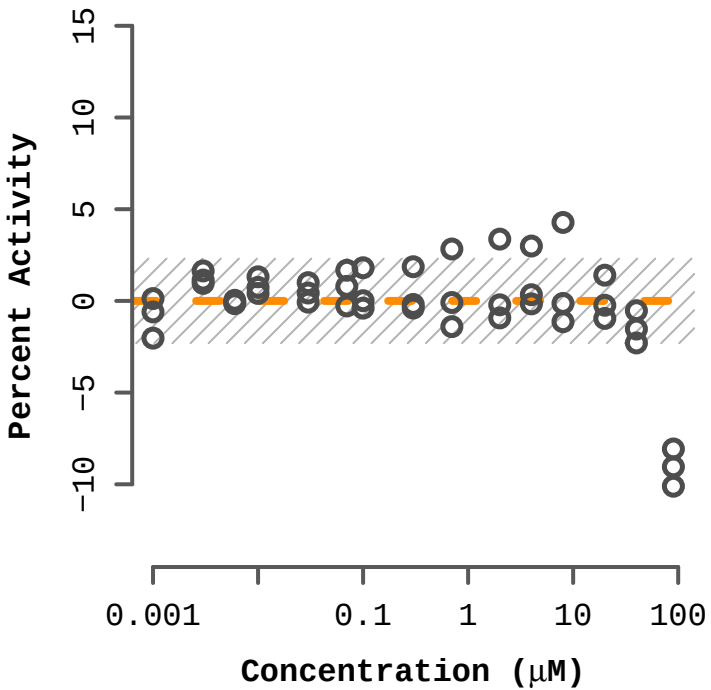
NAME: Penconazole
CHID: 42260 **CASRN:** 66246-88-6
SPID(S): Tox21_301318
M4ID: 12477815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.21	NA	NA
PROB:	1	NA	NA
RMSE:	2.84	NA	NA

MAX_MEAN: 0.727 **MAX_MED:** 0.728 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

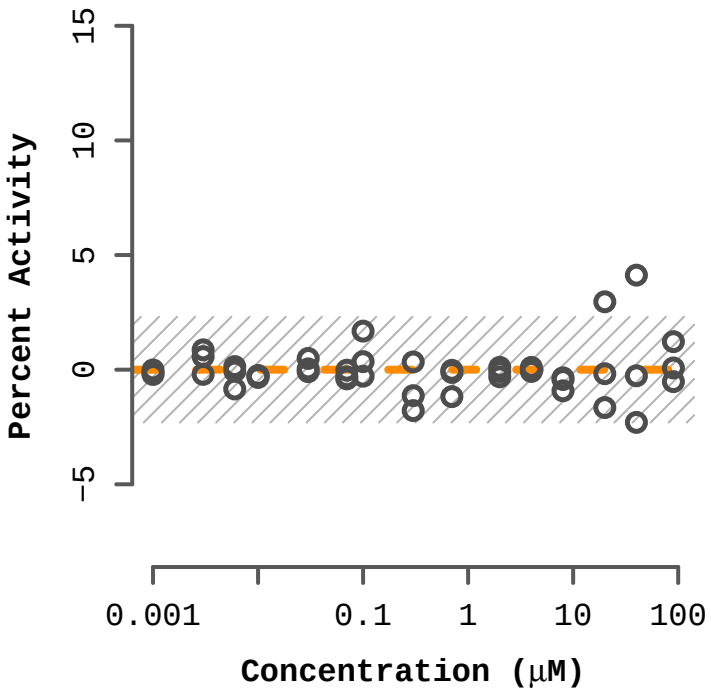
NAME: Pencycuron
CHID: 42261 **CASRN:** 66063-05-6
SPID(S): Tox21_301255
M4ID: 12477878

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

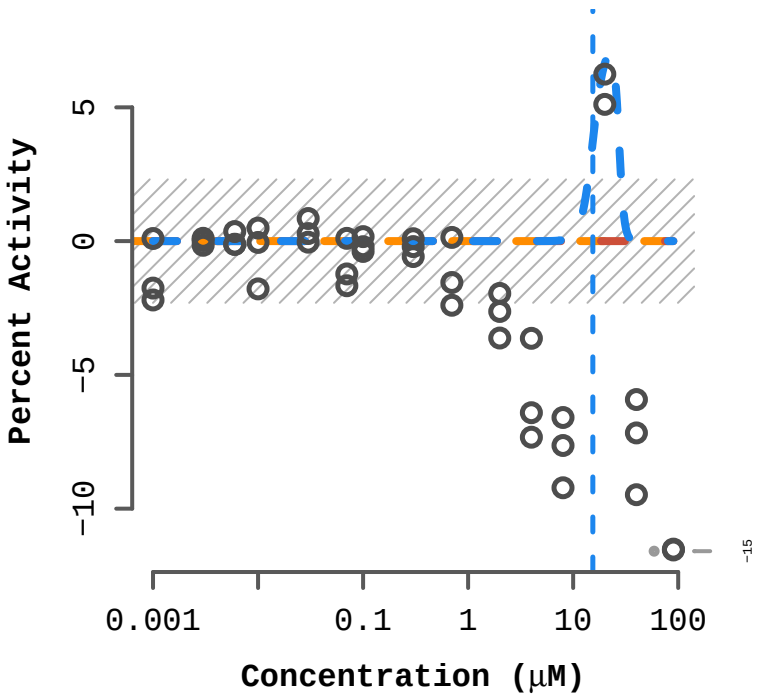
NAME: Pentachlorothioanisole
CHID: 42263 **CASRN:** 1825-19-0
SPID(S): Tox21_300809
M4ID: 12478324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.584 **MAX_MED:** 0.571 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentaerythritol tetraacrylate
CHID: 42264 CASRN: 4986-89-4
SPID(S): Tox21_301685
M4ID: 12477448 BRK

HILL MODEL (in red):

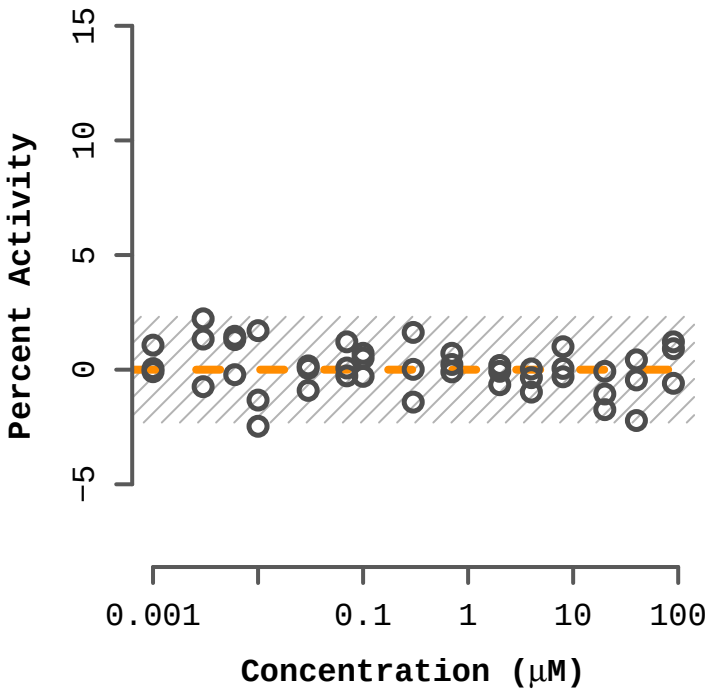
	tp	ga	gw
val:	0.00455	2.45	7.93
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.49	1.19	8	1.44	18
sd:	7.5	0.372	9.4	0.424	46.2

	CNST	HILL	GNLS
AIC:	270.65	276.65	270.53
PROB:	0.47	0.02	0.5
RMSE:	5.04	5.04	4.74

MAX_MEAN: 6.71 **MAX_MED:** 6.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

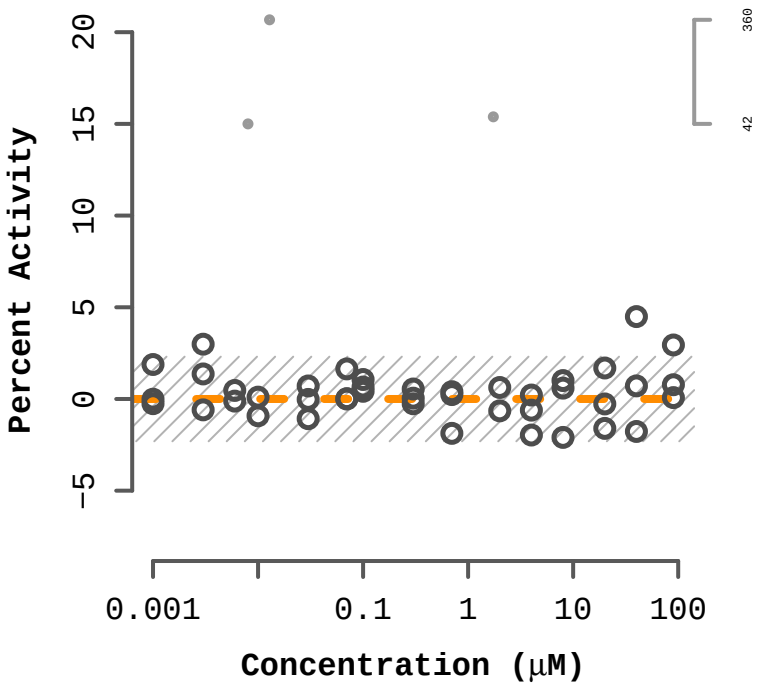
NAME: Pentyl sulfide
CHID: 42266 **CASRN:** 872-10-6
SPID(S): Tox21_301954
M4ID: 12477179

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

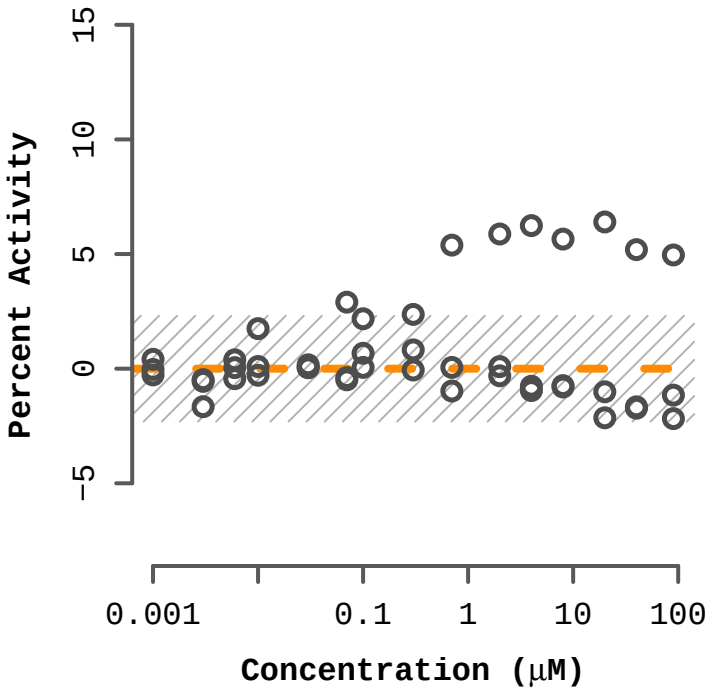
NAME: Phenkapton
CHID: 42269 **CASRN:** 2275-14-1
SPID(S): Tox21_301741
M4ID: 12477392 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	261.93	NA	NA
PROB:	1	NA	NA
RMSE:	54.67	NA	NA

MAX_MEAN: 119 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

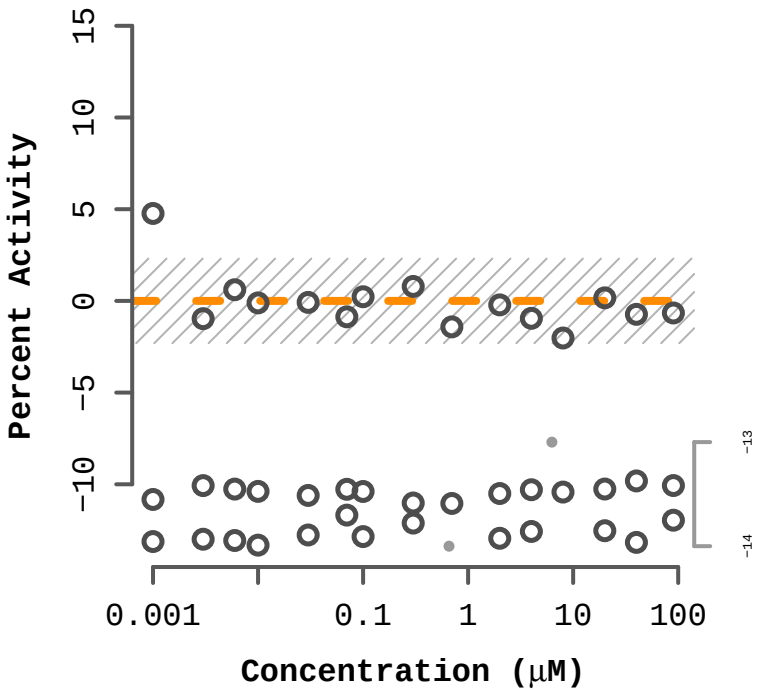
NAME: 2,4-Diisopropylphenol
CHID: 42273 **CASRN:** 2934-05-6
SPID(S): Tox21_301372
M4ID: 12477761

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.47	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

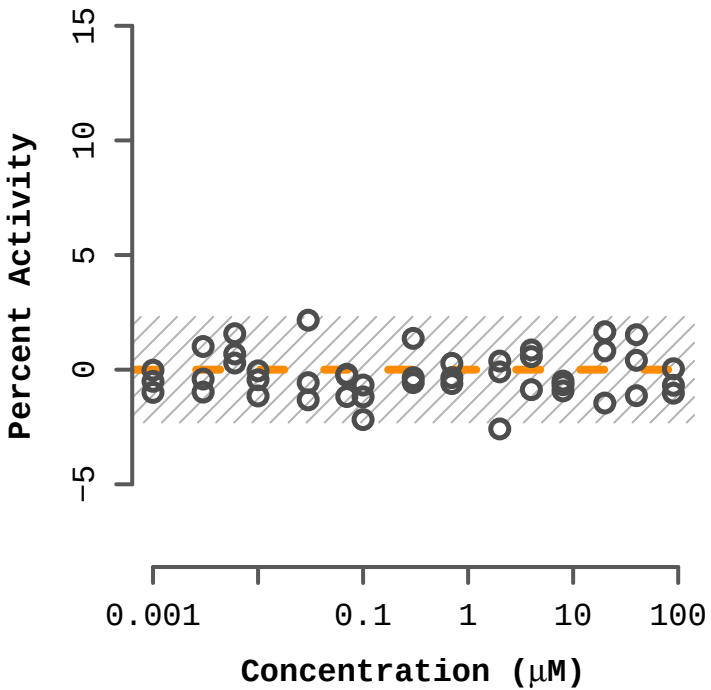
NAME: 2-Ethoxyphenol
CHID: 42276 **CASRN:** 94-71-3
SPID(S): Tox21_301383
M4ID: 12477750 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	340.93	NA	NA
PROB:	1	NA	NA
RMSE:	9.58	NA	NA

MAX_MEAN: −6.39 **MAX_MED:** −9.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

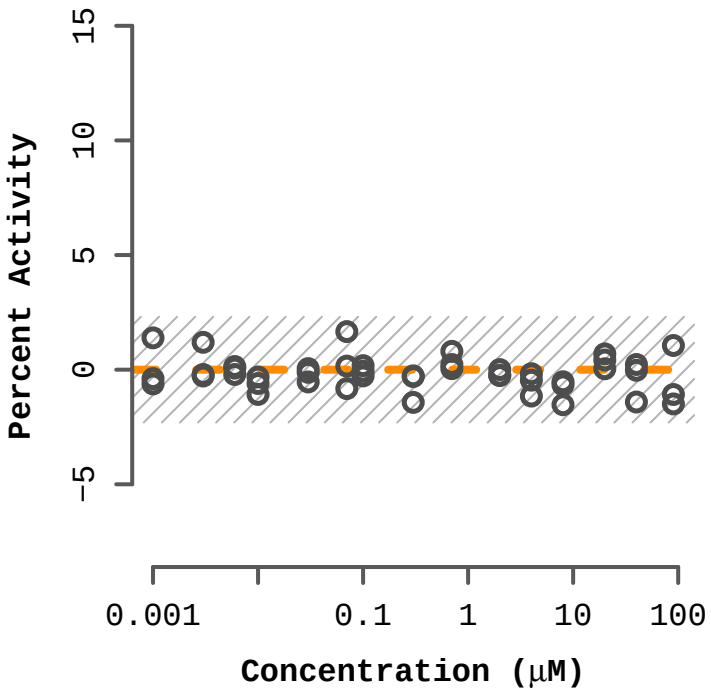
NAME: Phenoxyethyl isobutyrate
CHID: 42279 **CASRN:** 103-60-6
SPID(S): Tox21_301056
M4ID: 12478077

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

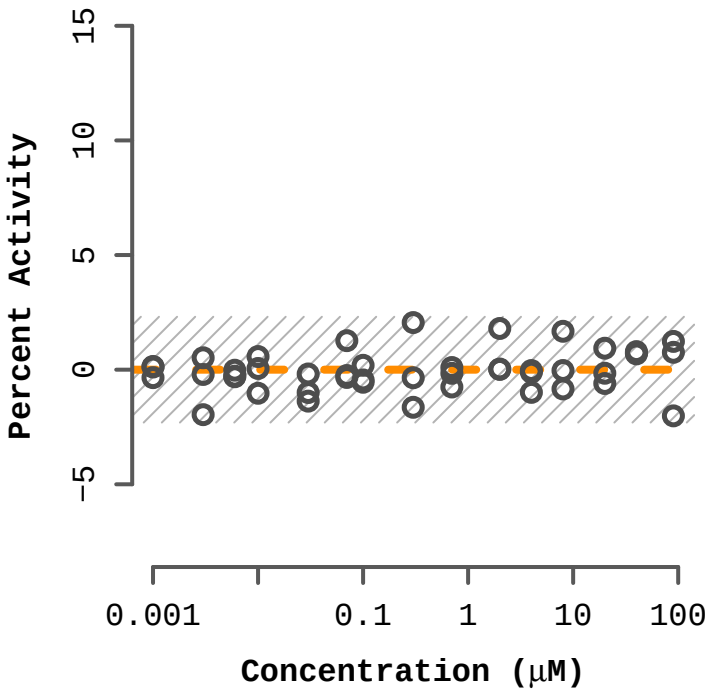
NAME: Phenthoate
CHID: 42280 **CASRN:** 2597-03-7
SPID(S): Tox21_301564
M4ID: 12477569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.385 **MAX_MED:** 0.424 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

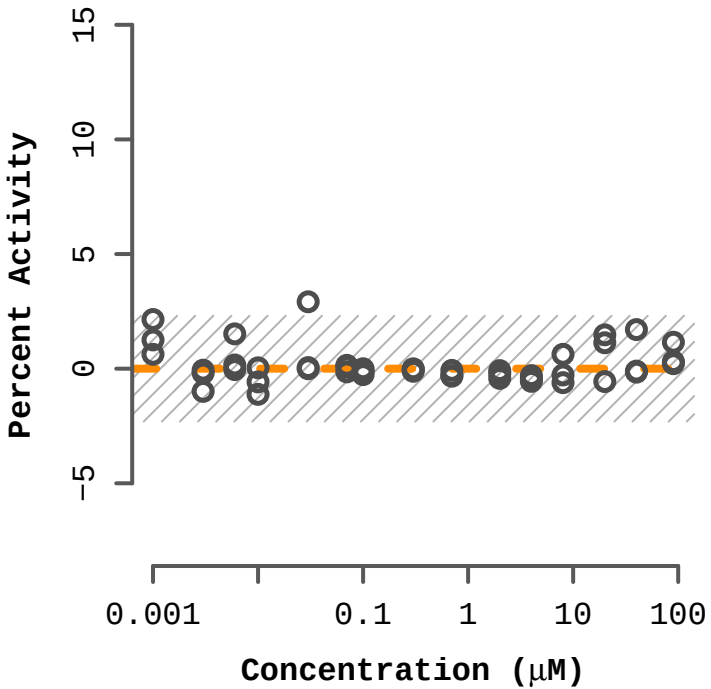
NAME: Phenylpyruvic acid
CHID: 42281 **CASRN:** 156-06-9
SPID(S): Tox21_301362
M4ID: 12477771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.738 **MAX_MED:** 0.759 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

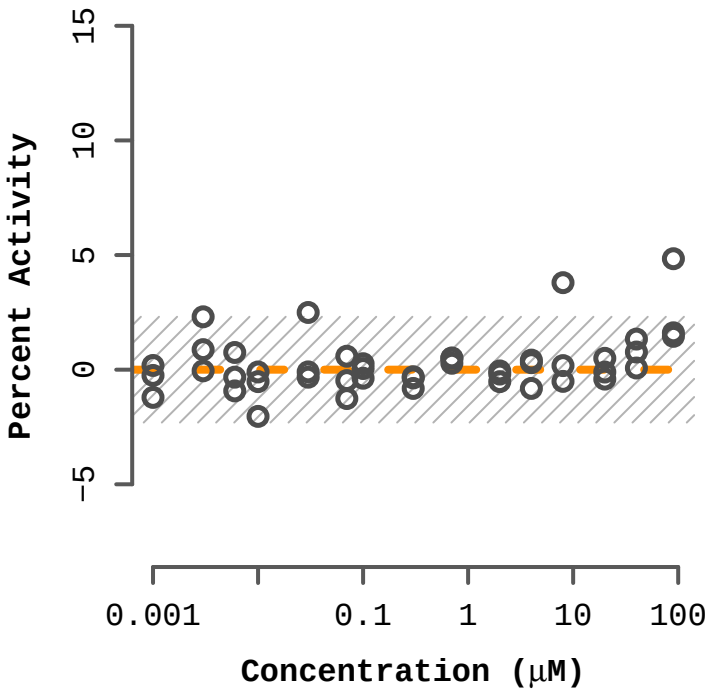
NAME: Phorate sulfone
CHID: 42282 CASRN: 2588-04-7
SPID(S): Tox21_303939
M4ID: 12475249

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.34 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

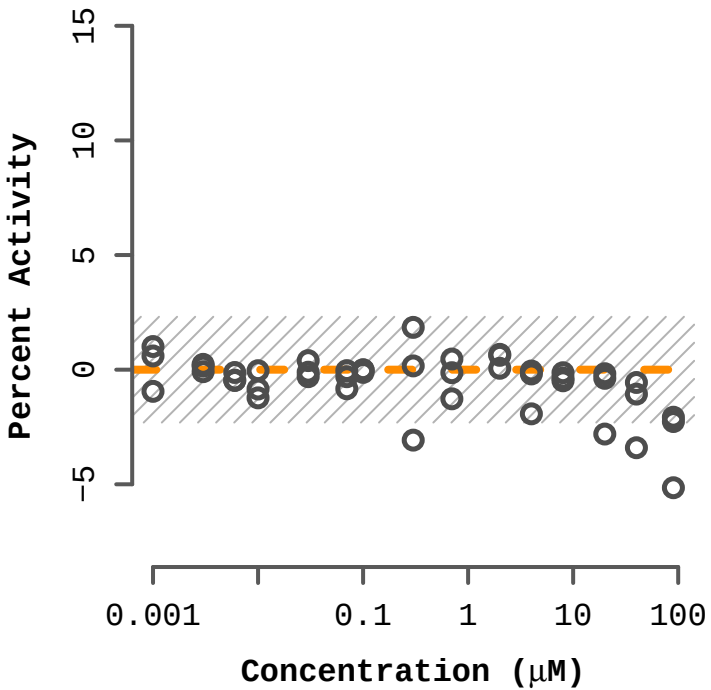
NAME: Phosfolan
CHID: 42285 **CASRN:** 947-02-4
SPID(S): Tox21_301905
M4ID: 12477228

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 2.64 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

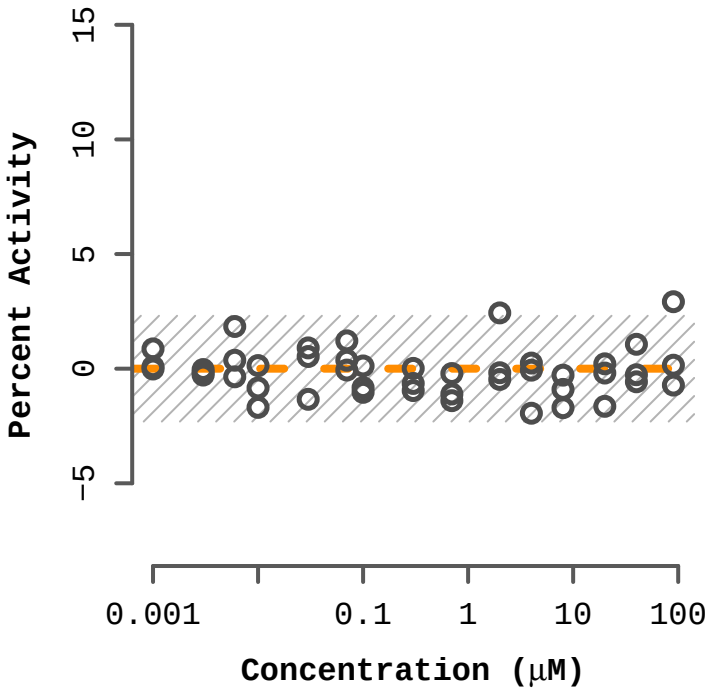
NAME: Pirimiphos-ethyl
CHID: 42297 CASRN: 23505-41-1
SPID(S): Tox21_301447
M4ID: 12477686

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.453 MAX_MED: 0.627 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

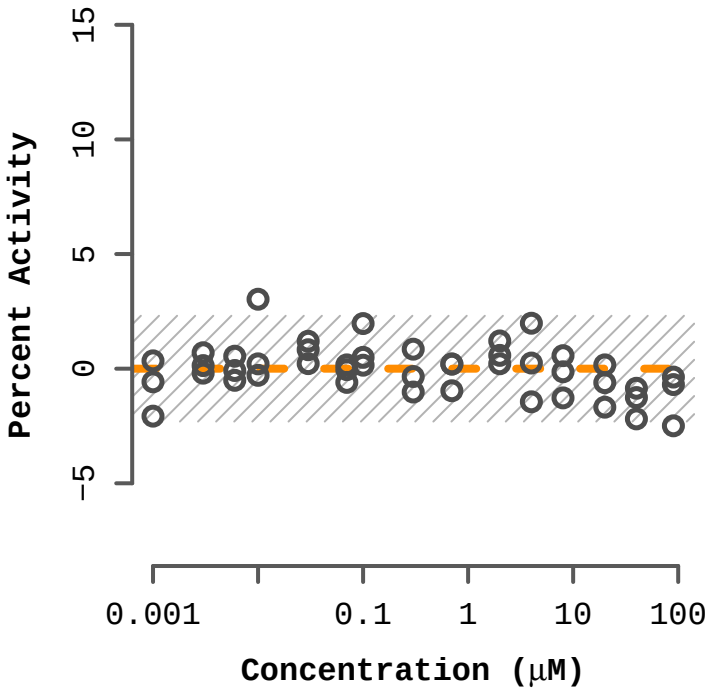
NAME: 4-Isopropylphenol
CHID: 42299 **CASRN:** 99-89-8
SPID(S): Tox21_301323
M4ID: 12477810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.787 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

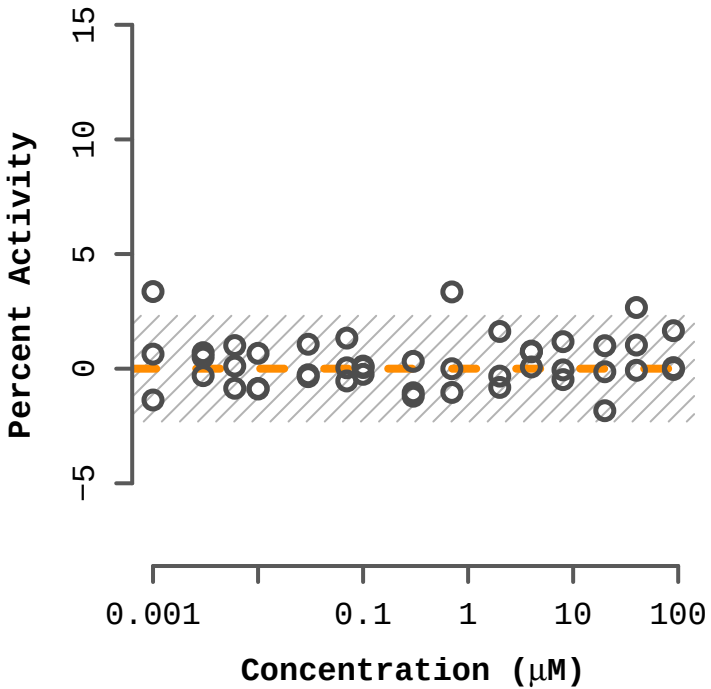
NAME: Potassium ethyl xanthate
CHID: 42315 **CASRN:** 140-89-6
SPID(S): Tox21_301211
M4ID: 12477922

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.984 **MAX_MED:** 0.829 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

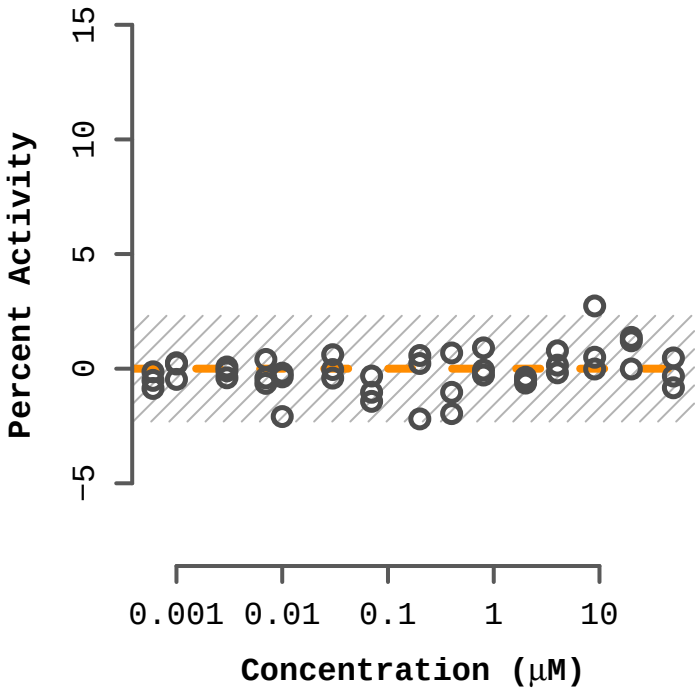
NAME: Potassium nitrite
CHID: 42320 **CASRN:** 7758-09-0
SPID(S): Tox21_301322
M4ID: 12477811

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

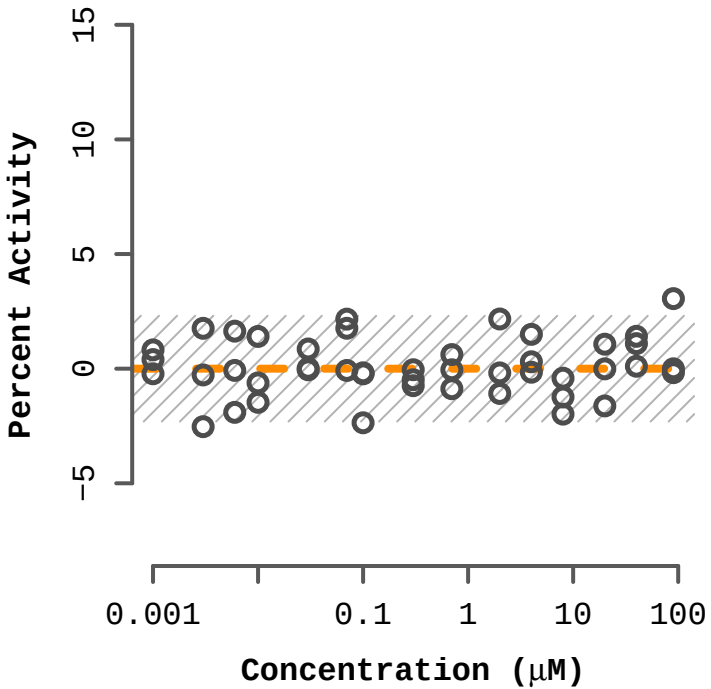
NAME: Potassium warfarin
CHID: 42324 CASRN: 2610-86-8
SPID(S): Tox21_111637_1
M4ID: 12483570

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

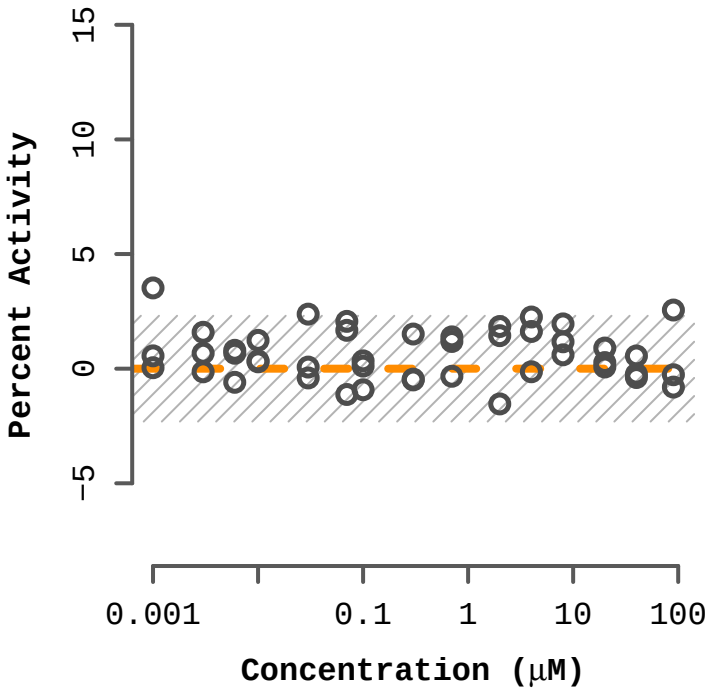
NAME: 4-Propylanisole
CHID: 42325 **CASRN:** 104-45-0
SPID(S): Tox21_301169
M4ID: 12477964

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

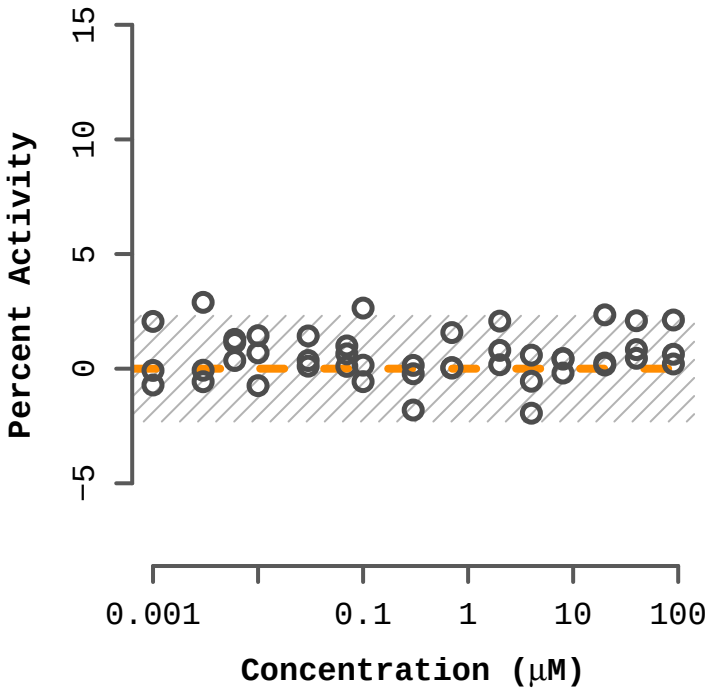
NAME: Dipropylene glycol dimethyl ether
CHID: 42327 **CASRN:** 111109-77-4
SPID(S): Tox21_301158
M4ID: 12477975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

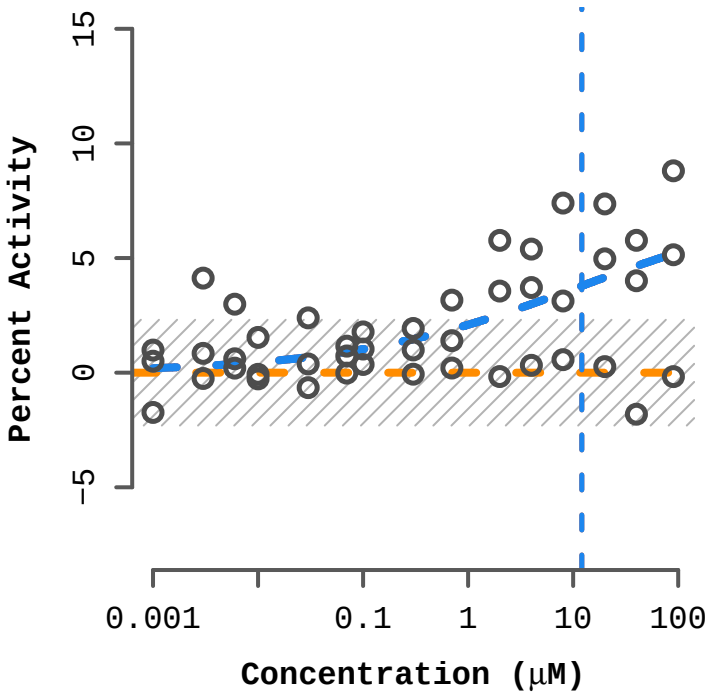
NAME: Butyl (2S)−2−hydroxypropanoate
CHID: 42335 CASRN: 34451−19−9
SPID(S): Tox21_301317
M4ID: 12477816

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (L)-(-)-Ethyl lactate
CHID: 42336 CASRN: 687-47-8
SPID(S): Tox21_303905
M4ID: 12475283

HILL MODEL (in red):

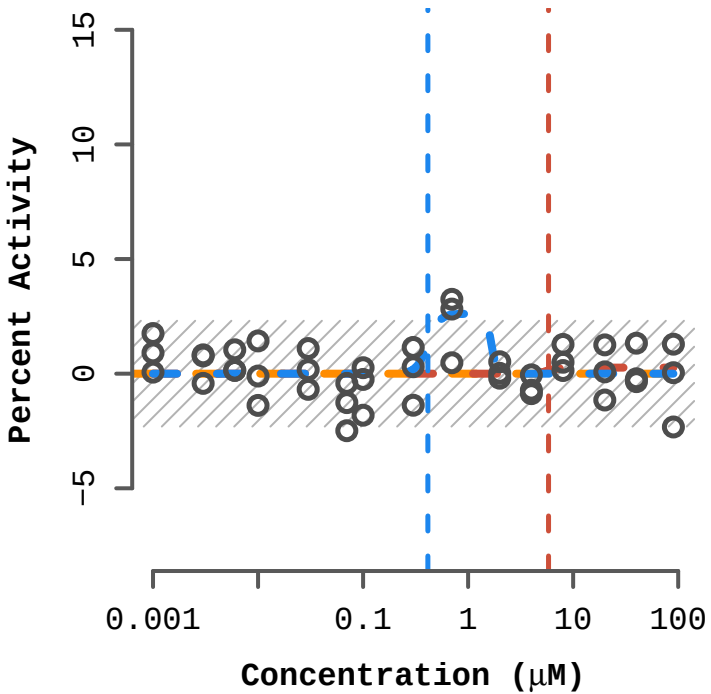
	tp	ga	gw
val:	7.57	1.08	0.387
sd:	8.21	2.68	0.294

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.57	1.08	0.387	3.33	5.27
sd:	8.21	2.68	0.294	1820	7160

	CNST	HILL	GNLS
AIC:	230.47	202.6	206.6
PROB:	0	0.88	0.12
RMSE:	3.17	2.16	2.16

MAX_MEAN: 4.59 MAX_MED: 5.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propyl propionate
CHID: 42337 CASRN: 106-36-5
SPID(S): Tox21_301107
M4ID: 12478026

HILL MODEL (in red):

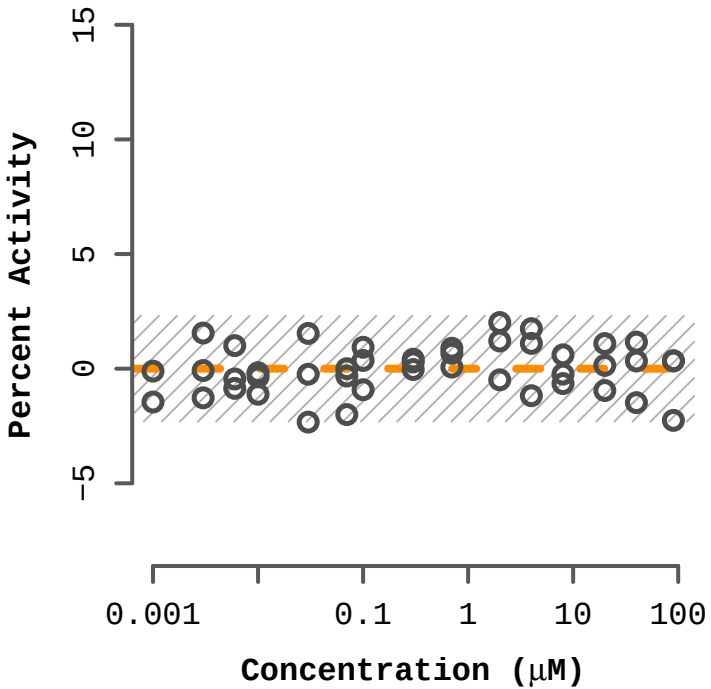
	tp	ga	gw
val:	0.264	0.765	8
sd:	0.321	0.254	13.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.61	−0.383	7.94	0.221	17
sd:	3.99	2.13	115	5.32	1130

	CNST	HILL	GNLS
AIC:	142.95	148.25	143.84
PROB:	0.58	0.04	0.37
RMSE:	1.16	1.16	1.02

MAX_MEAN: 2.18 **MAX_MED:** 2.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

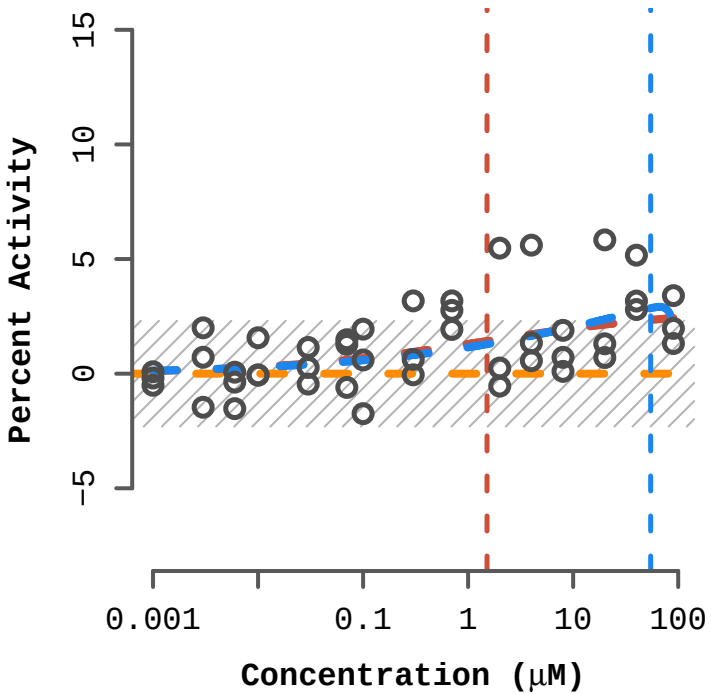
NAME: Di(propylene glycol) tert-butyl ether
CHID: 42338 **CASRN:** 132739-31-2
SPID(S): Tox21_301345
M4ID: 12477788

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propyl ether
CHID: 42343 CASRN: 111-43-3
SPID(S): Tox21_301041
M4ID: 12478092

HILL MODEL (in red):

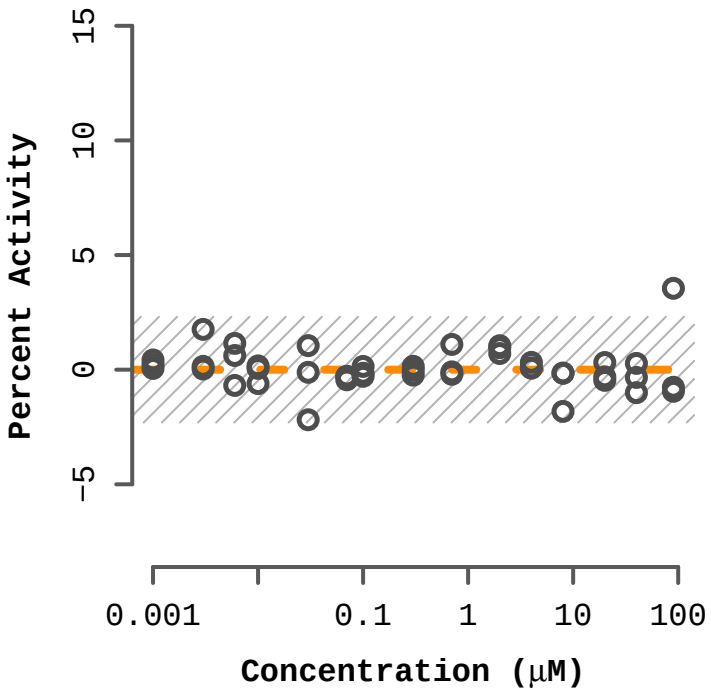
	tp	ga	gw
val:	2.85	0.18	0.431
sd:	3.2	3.3	0.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.72	1.74	0.345	1.99	11.2
sd:	12.1	4.58	0.188	0.132	42.6

	CNST	HILL	GNLS
AIC:	198.69	175.18	178.58
PROB:	0	0.85	0.15
RMSE:	2.23	1.55	1.54

MAX_MEAN: 3.71 MAX_MED: 3.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

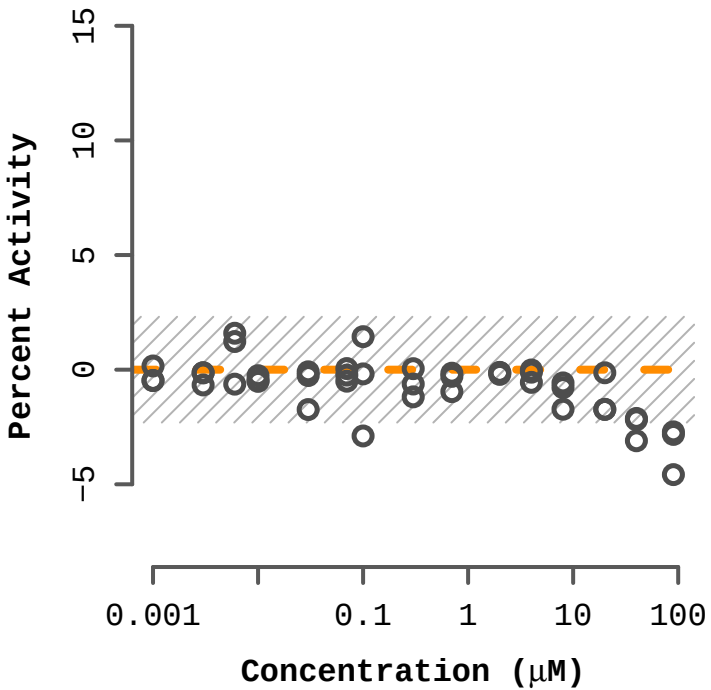
NAME: Prothiofos
CHID: 42349 **CASRN:** 34643-46-4
SPID(S): Tox21_301219
M4ID: 12477914

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.905 **MAX_MED:** 0.962 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

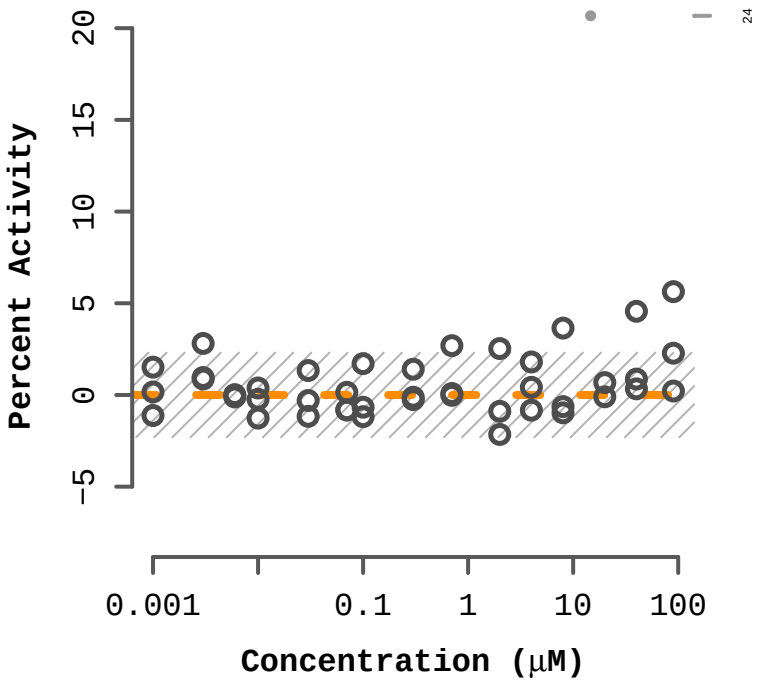
NAME: Pyrazophos
CHID: 42352 **CASRN:** 13457-18-6
SPID(S): Tox21_301359
M4ID: 12477774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.73 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

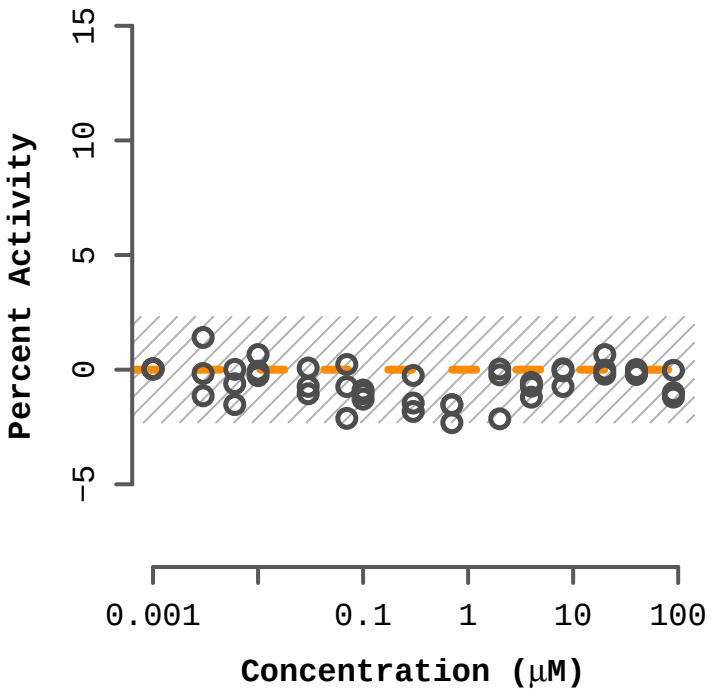
NAME: 2-(3-Phenylpropyl)pyridine
CHID: 42356 **CASRN:** 2110-18-1
SPID(S): Tox21_301773
M4ID: 12477360 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.74	NA	NA
PROB:	1	NA	NA
RMSE:	3.9	NA	NA

MAX_MEAN: 8.09 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

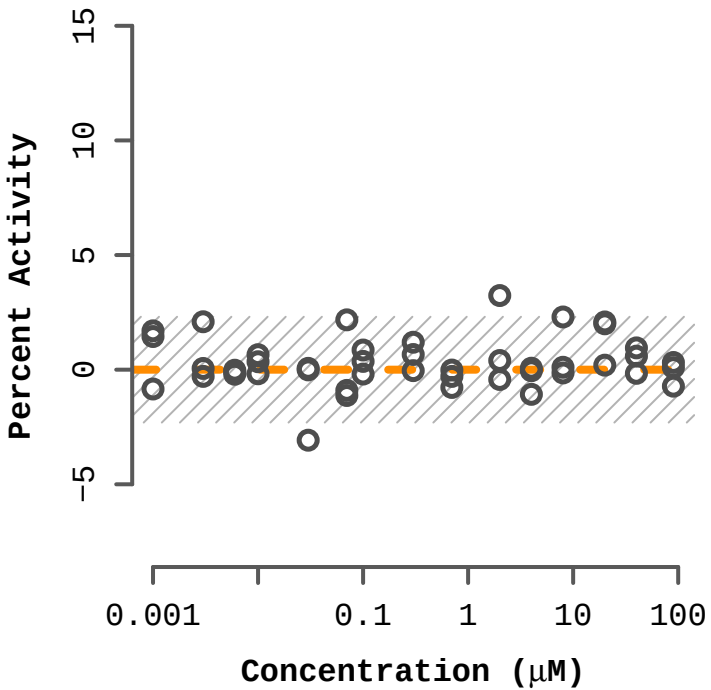
NAME: Pyrinuron
CHID: 42360 CASRN: 53558-25-1
SPID(S): Tox21_302252
M4ID: 12476881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.15 MAX_MED: 0.0407 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

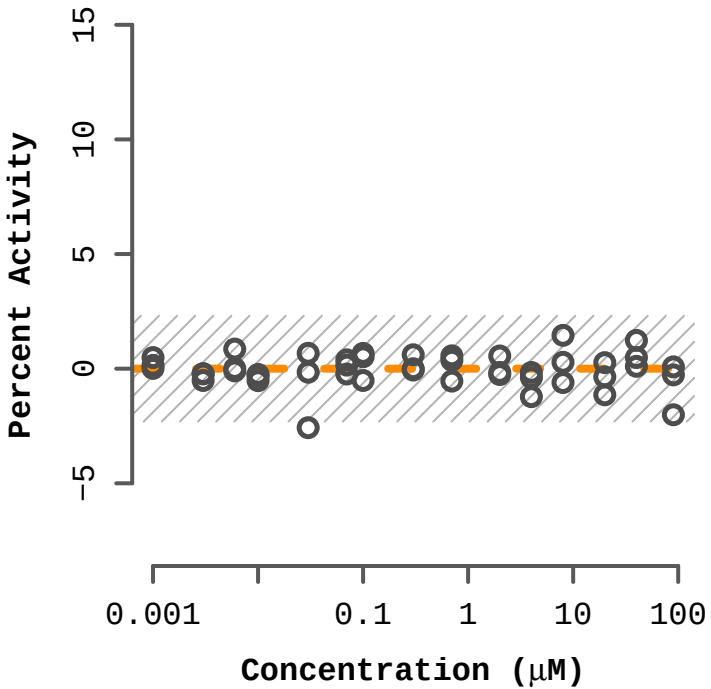
NAME: Quinmerac
CHID: 42364 **CASRN:** 90717-03-6
SPID(S): Tox21_301872
M4ID: 12477261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

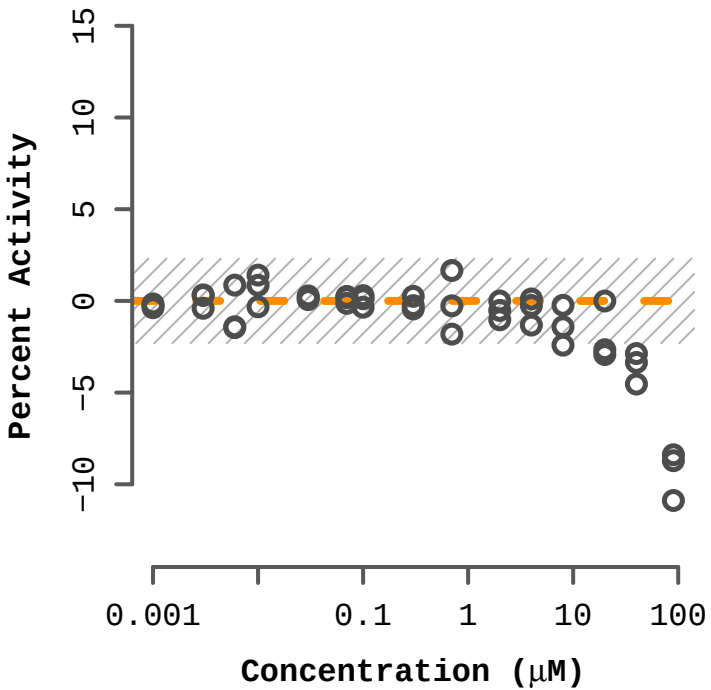
NAME: 6-Ethoxy-2,3,4-trimethyl-1,2,3,4-tetrahydroqui
CHID: 42365 **CASRN:** 16489-90-0
SPID(S): Tox21_301229
M4ID: 12477904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

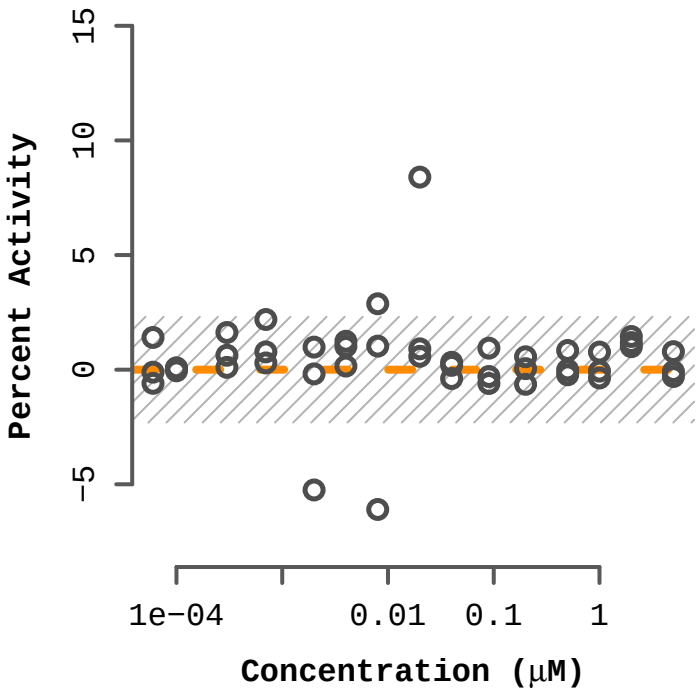
NAME: Rhodamine B
CHID: 42369 **CASRN:** 81-88-9
SPID(S): Tox21_301450
M4ID: 12477683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.88	NA	NA
PROB:	1	NA	NA
RMSE:	2.77	NA	NA

MAX_MEAN: 0.647 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

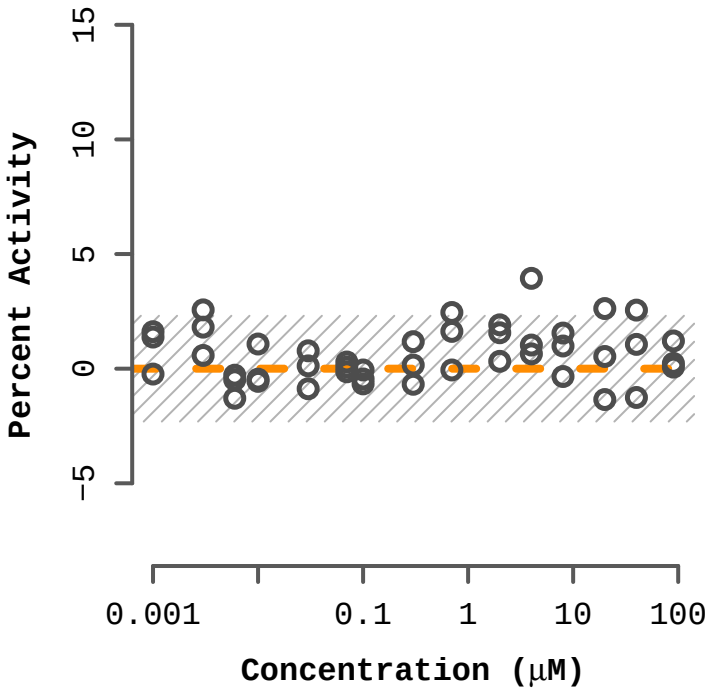
NAME: Chloro(dimethyl)vinylsilane
CHID: 42378 **CASRN:** 1719-58-0
SPID(S): Tox21_303724
M4ID: 12475464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.94	NA	NA

MAX_MEAN: 3.3 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

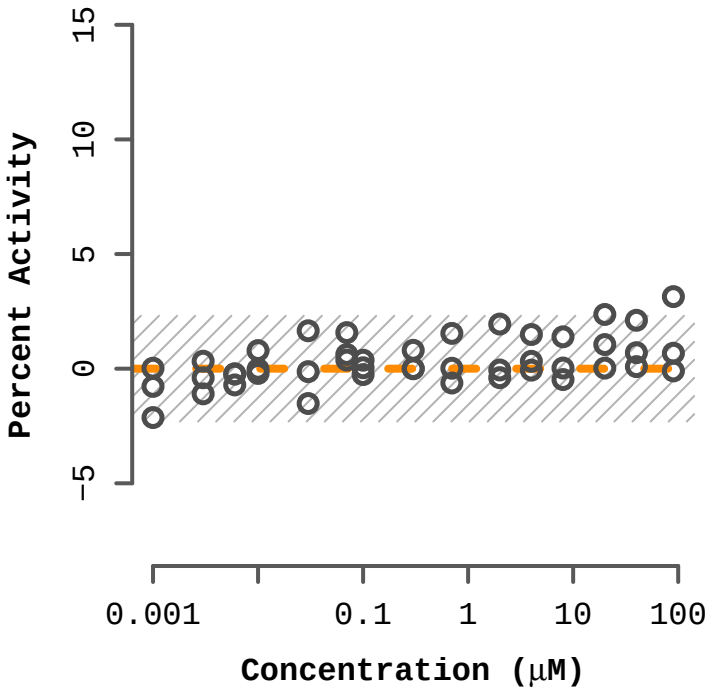
NAME: Dimethoxydimethylsilane
CHID: 42379 **CASRN:** 1112-39-6
SPID(S): Tox21_301035
M4ID: 12478098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

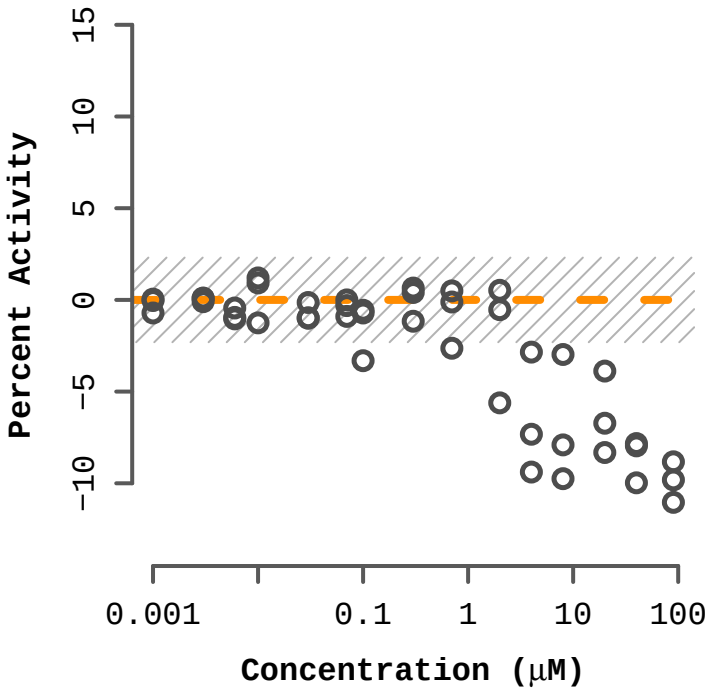
NAME: Tetrapropyl orthosilicate
CHID: 42382 **CASRN:** 682-01-9
SPID(S): Tox21_301445
M4ID: 12477688

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

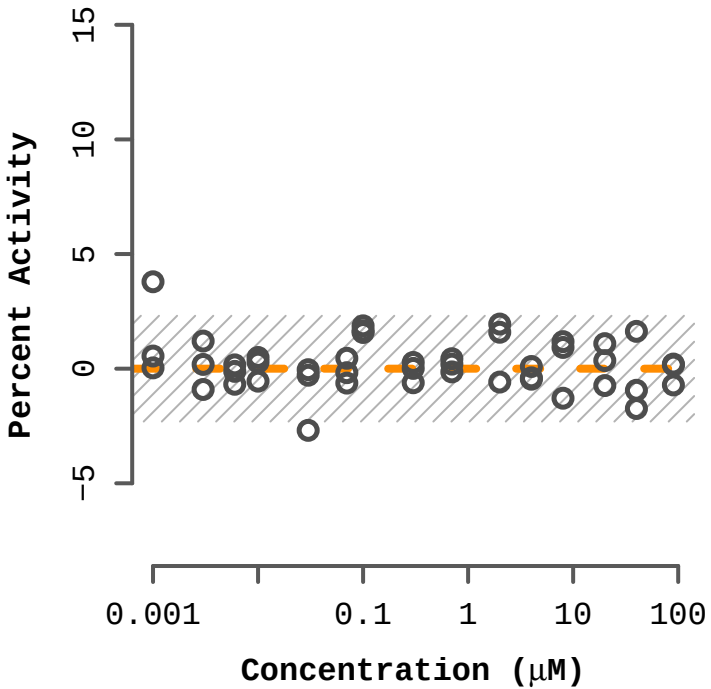
NAME: Sodium (2-pyridylthio)-N-oxide
CHID: 42390 **CASRN:** 3811-73-2
SPID(S): Tox21_300128
M4ID: 12479002

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	267.57	NA	NA
PROB:	1	NA	NA
RMSE:	4.78	NA	NA

MAX_MEAN: 0.292 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

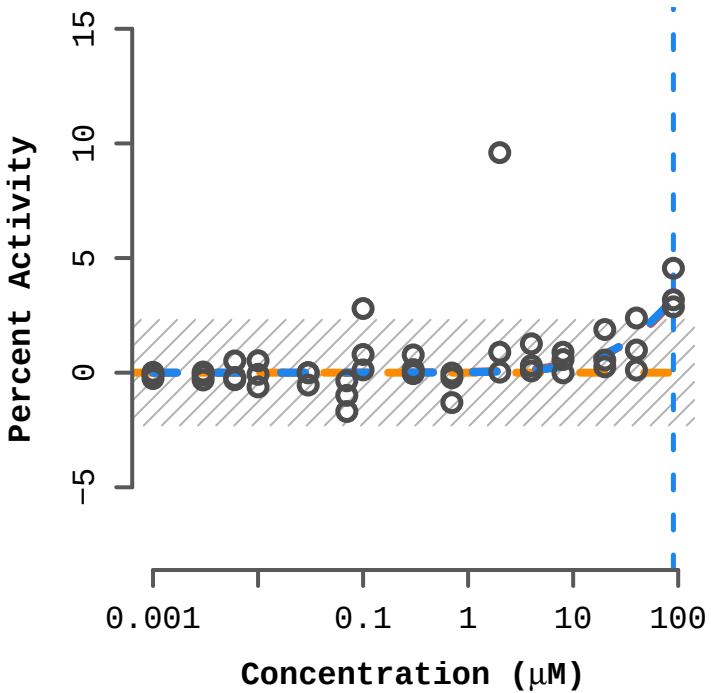
NAME: Sodium 1-naphthalenesulfonate
CHID: 42394 CASRN: 130-14-3
SPID(S): Tox21_301522
M4ID: 12477611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium abietate
CHID: 42399 CASRN: 14351-66-7
SPID(S): Tox21_301864
M4ID: 12477269

HILL MODEL (in red):

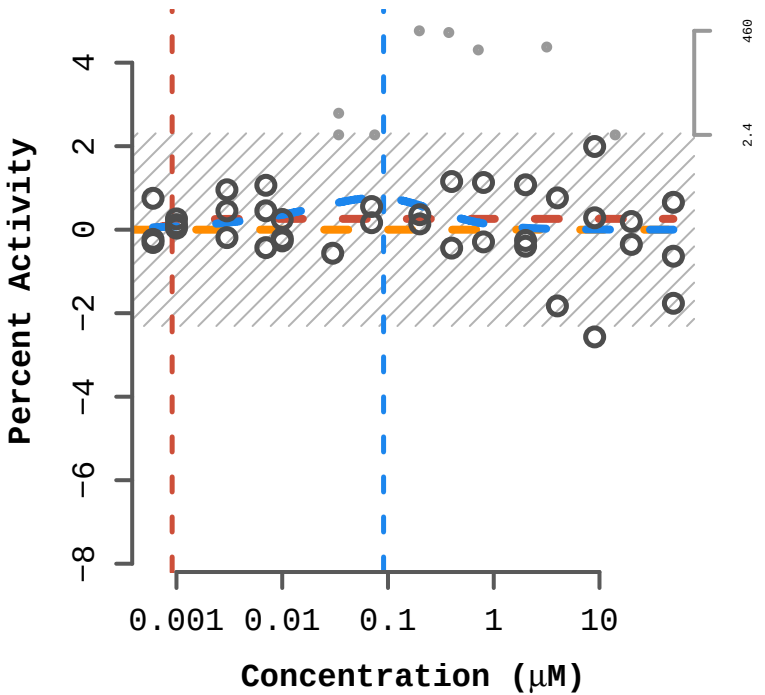
	tp	ga	gw
val:	11.5	2.34	1.07
sd:	12.2	0.678	0.393

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.42	1.95	1.3	3.95	3.59
sd:	4.71	0.473	0.559	860	1570

	CNST	HILL	GNLS
AIC:	153.31	124.46	129.17
PROB:	0	0.91	0.09
RMSE:	1.9	1.61	1.61

MAX_MEAN: 3.54 **MAX_MED:** 3.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium hexyldecyl sulfate
CHID: 42400 CASRN: 1120-01-0
SPID(S): Tox21_300381
M4ID: 12478751 BRK

HILL MODEL (in red):

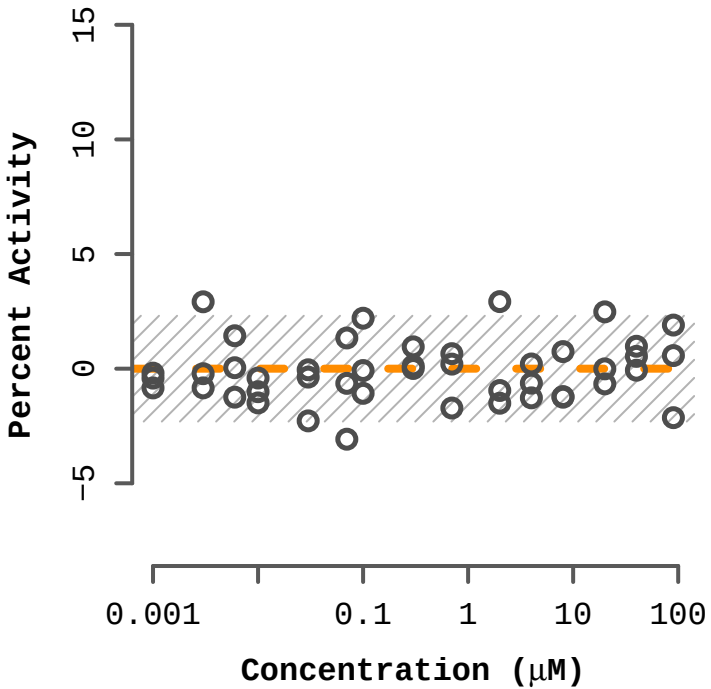
	tp	ga	gw
val:	0.259	−3.04	4.04
sd:	0.24	1.14	30.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.16	−1.04	0.725	−0.792	1.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	379.78	384.58	387.62
PROB:	0.9	0.08	0.02
RMSE:	126.69	126.6	126.59

MAX_MEAN: 154 MAX_MED: 2.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

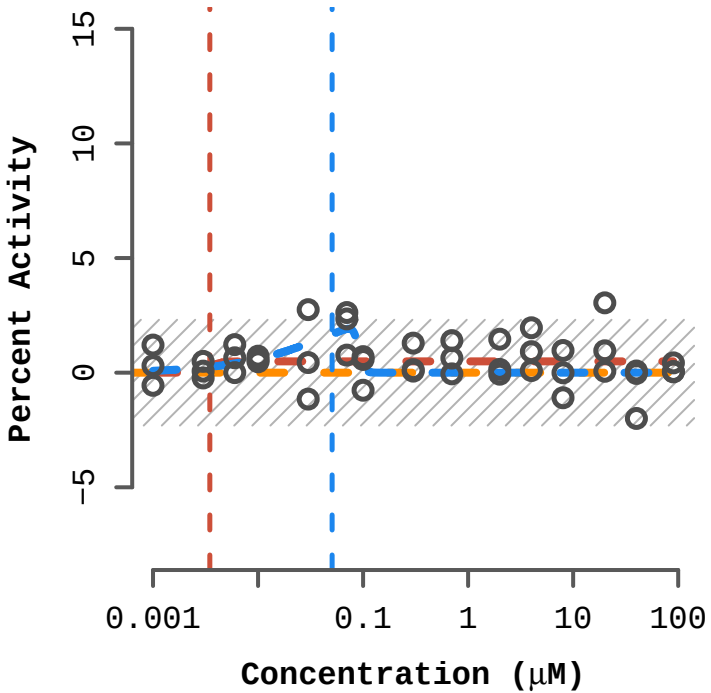
NAME: Sodium methyl sulfate
CHID: 42406 **CASRN:** 512-42-5
SPID(S): Tox21_301316
M4ID: 12477817

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.622 **MAX_MED:** 0.573 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sodium 4-methylbenzenesulfonate
CHID: 42415 CASRN: 657-84-1
SPID(S): Tox21_301380
M4ID: 12477753

HILL MODEL (in red):

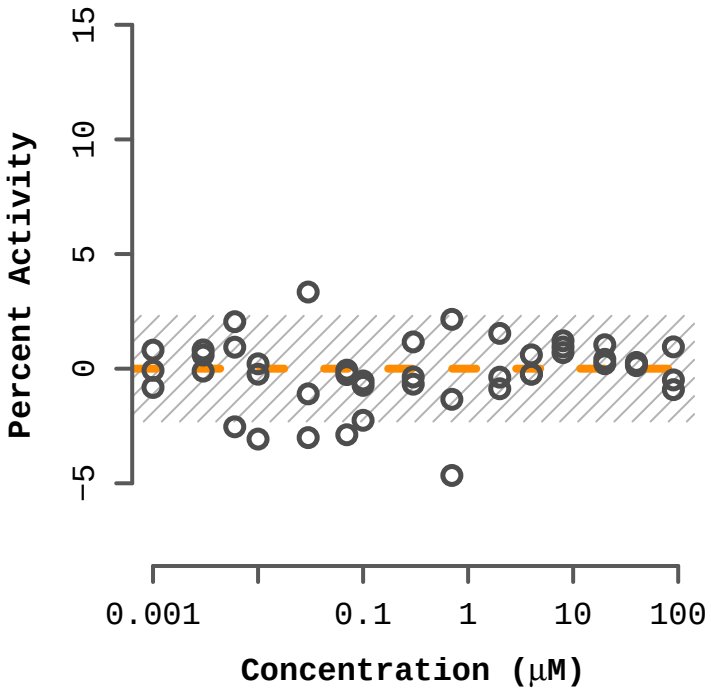
	tp	ga	gw
val:	0.493	−2.46	8
sd:	0.136	0.247	21.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.35	−1.29	0.939	−1.04	17.9
sd:	4.23	1.16	0.586	0.0696	24.1

	CNST	HILL	GNLS
AIC:	136.86	130.61	133.37
PROB:	0.03	0.77	0.19
RMSE:	1.12	0.98	0.97

MAX_MEAN: 1.91 MAX_MED: 2.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

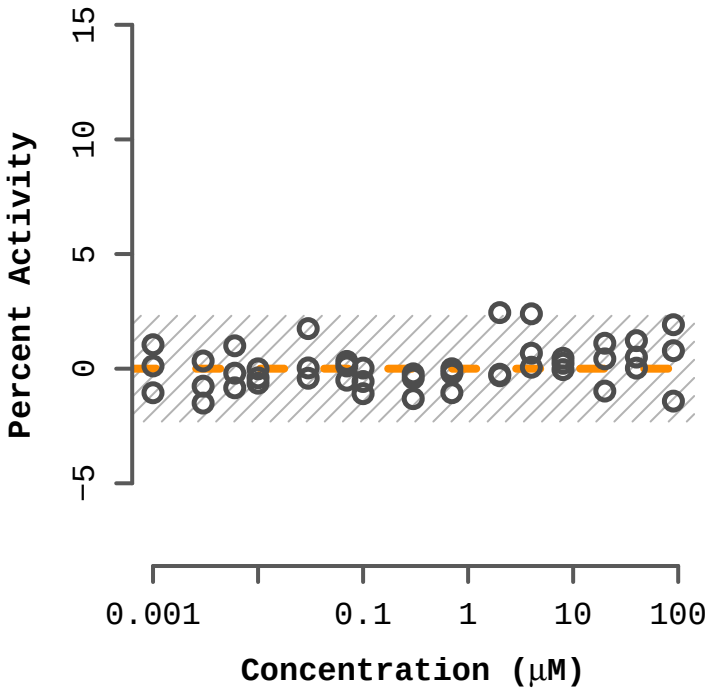
NAME: Sodium myristyl sulfate
CHID: 42416 **CASRN:** 1191-50-0
SPID(S): Tox21_300376
M4ID: 12478756

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 0.948 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

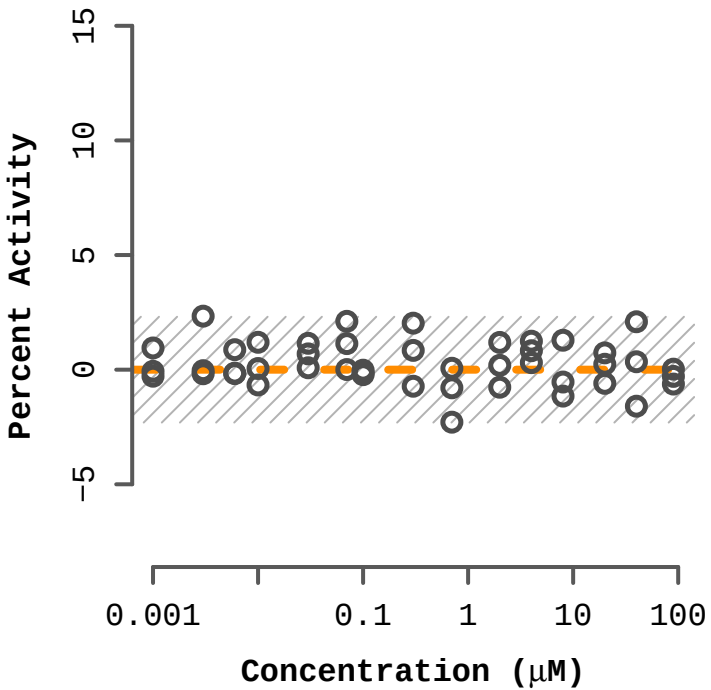
NAME: Sodium tridecyl sulfate
CHID: 42418 CASRN: 3026-63-9
SPID(S): Tox21_302101
M4ID: 12477032

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.787 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

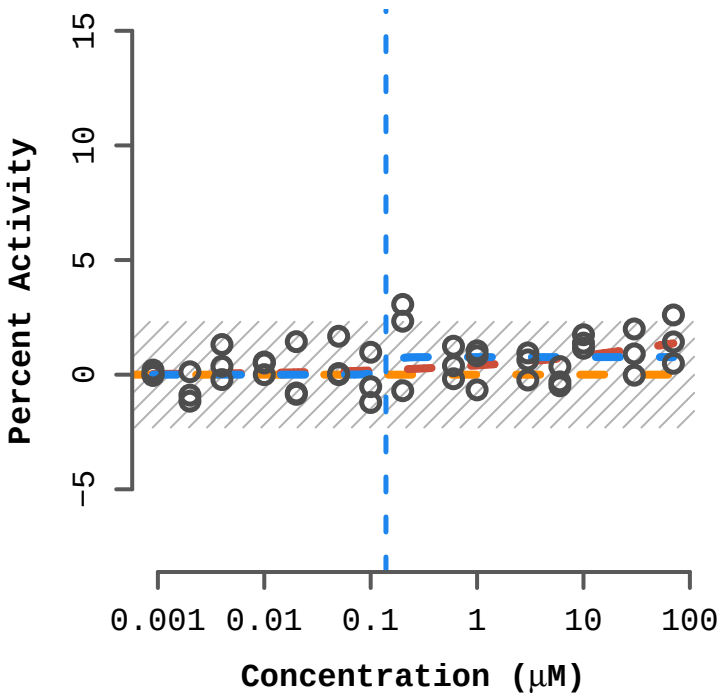
NAME: Styrene glycol
CHID: 42422 **CASRN:** 93-56-1
SPID(S): Tox21_302040
M4ID: 12477093

HILL MODEL: Not applicable.

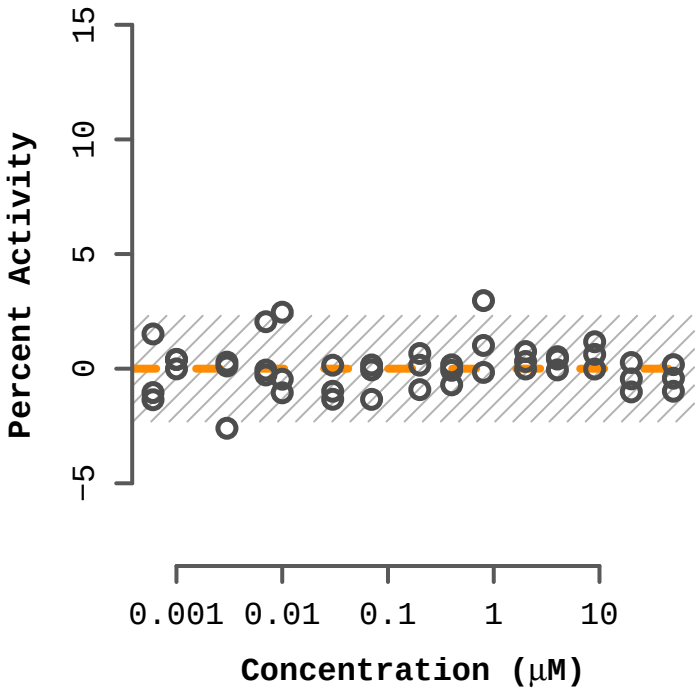
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.14 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Sucrose octaacetate
CHID:    42423   CASRN: 126-14-7
SPID(S): Tox21_300386
M4ID:    12478746

HILL MODEL (in red):
      tp       ga       gw
val:  3.47     2.35     0.375
sd:   8.95     4.92     0.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  0.767    -0.856   8        3.83     4.01
sd:   0.202    0.168    9.13     2420     4890

      CNST        HILL        GNLS
AIC:  139.29      130.29      136.08
PROB: 0.01        0.94        0.05
RMSE: 1.1         0.93        0.93

MAX_MEAN: 1.57      MAX_MED: 2.33      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

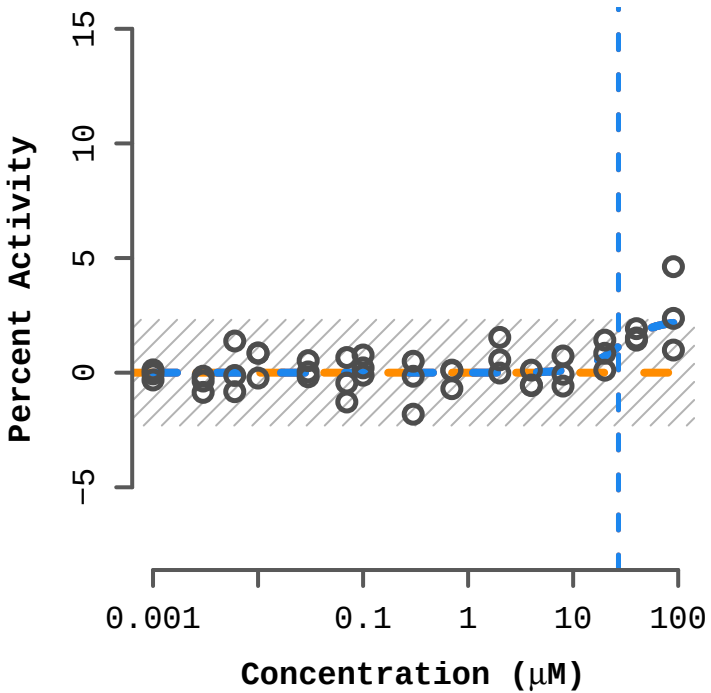
NAME: Sucrose octaacetate
CHID: 42423 **CASRN:** 126-14-7
SPID(S): Tox21_111938_1
M4ID: 12483421

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfaquinoxaline
CHID: 42424 **CASRN:** 59-40-5
SPID(S): Tox21_300894
M4ID: 12478239

HILL MODEL (in red):

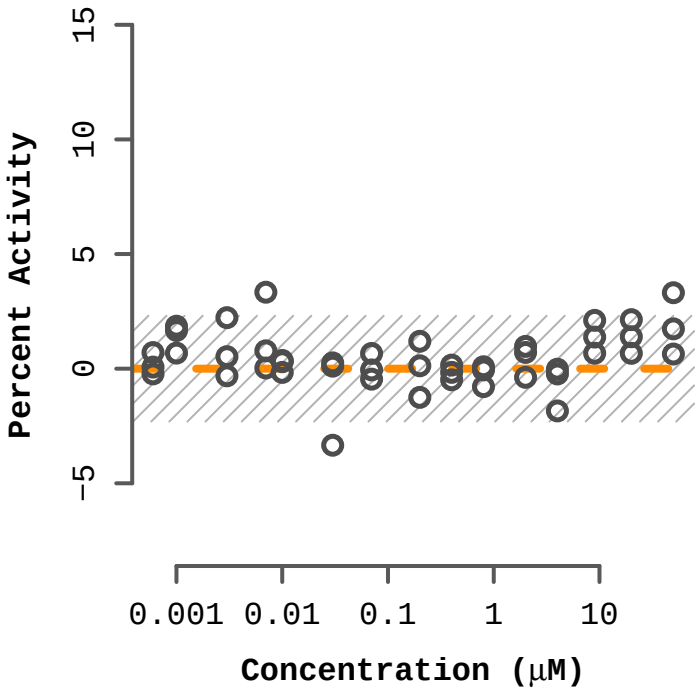
	tp	ga	gw
val:	2.27	1.43	2.56
sd:	0.846	0.197	1.61

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.27	1.43	2.56	3.15	6.37
sd:	0.846	0.197	1.61	1840	9890

	CNST	HILL	GNLS
AIC:	129.2	106.05	110.05
PROB:	0	0.88	0.12
RMSE:	1.11	0.75	0.75

MAX_MEAN: 2.66 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

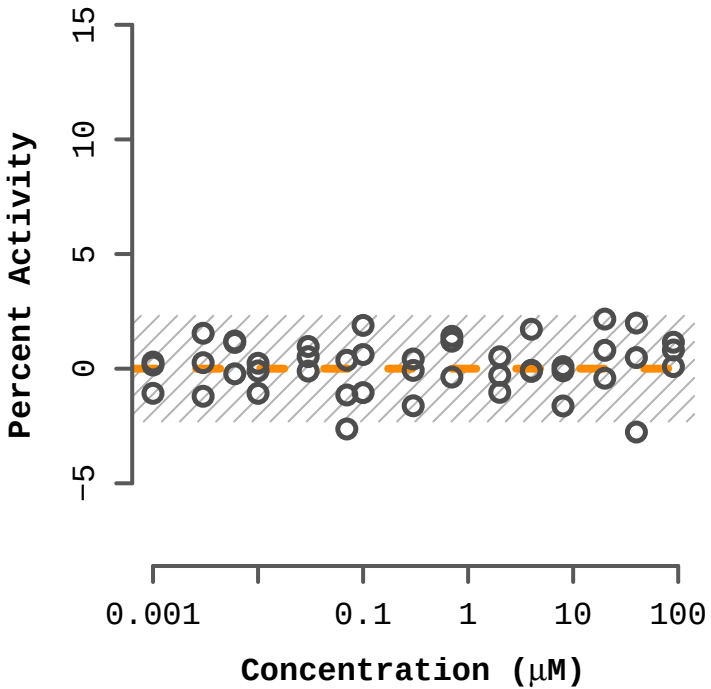
NAME: Sulfaquinoxaline
CHID: 42424 **CASRN:** 59-40-5
SPID(S): Tox21_110027_1
M4ID: 12484703

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

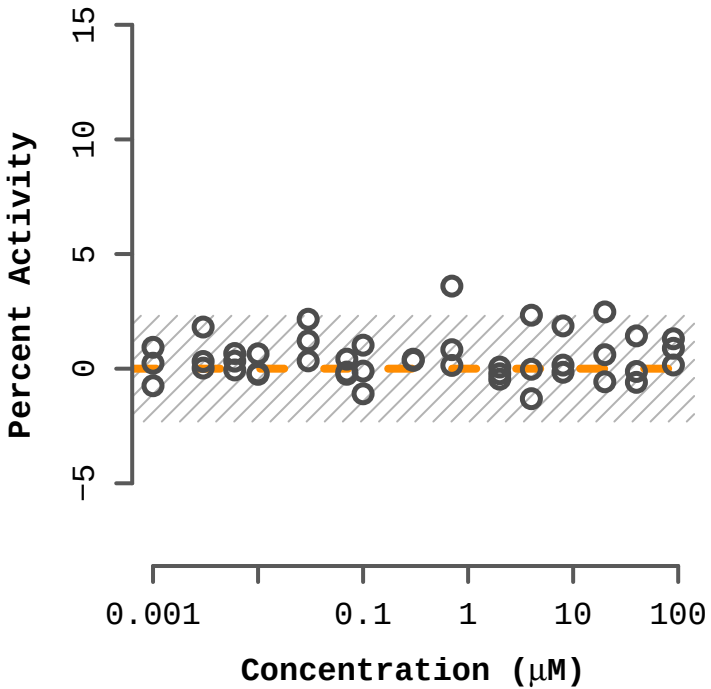
NAME: Sulfosuccinic acid
CHID: 42426 **CASRN:** 5138-18-1
SPID(S): Tox21_301599
M4ID: 12477534

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.851 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

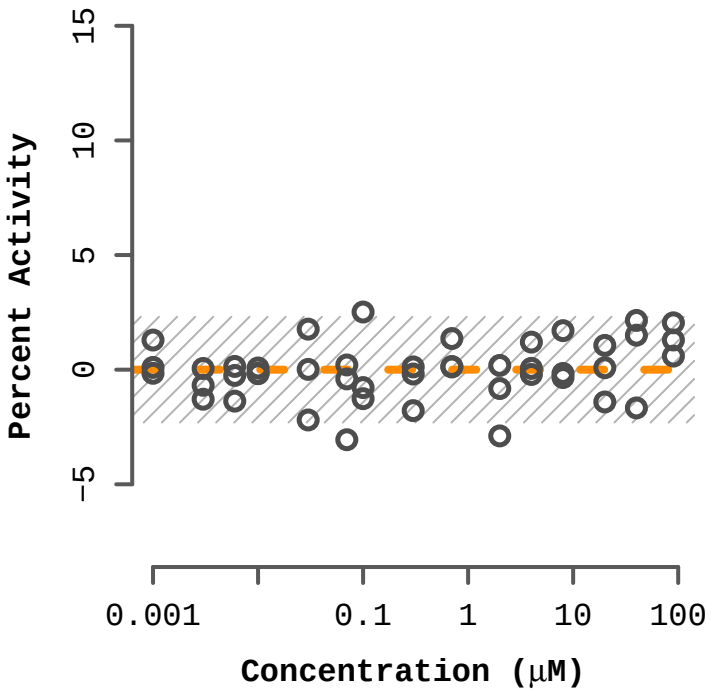
NAME: Sulisobenzone
CHID: 42436 **CASRN:** 4065-45-6
SPID(S): Tox21_303469
M4ID: 12475671

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

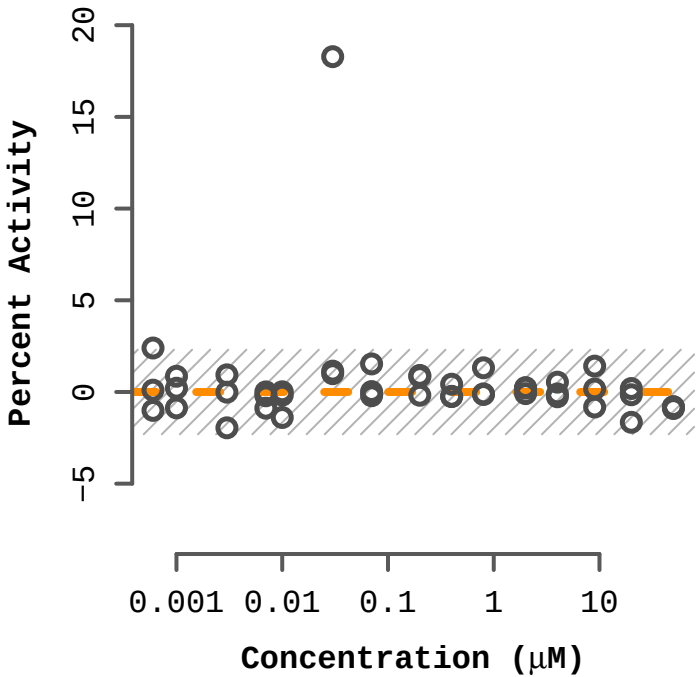
NAME: Sulisobenzone
CHID: 42436 **CASRN:** 4065-45-6
SPID(S): Tox21_202332
M4ID: 12479920

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

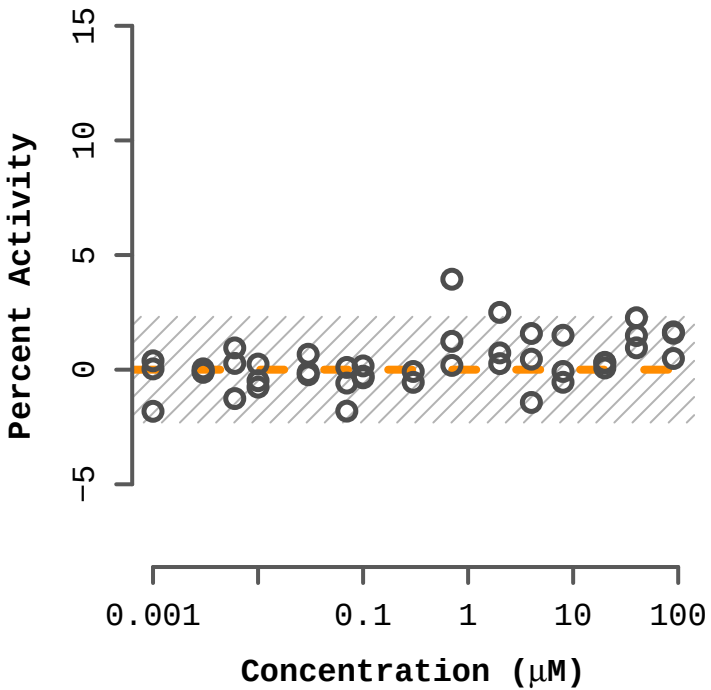
NAME: Sulisobenzone
CHID: 42436 CASRN: 4065-45-6
SPID(S): Tox21_111639_1
M4ID: 12483568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.85	NA	NA

MAX_MEAN: 6.81 MAX_MED: 1.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

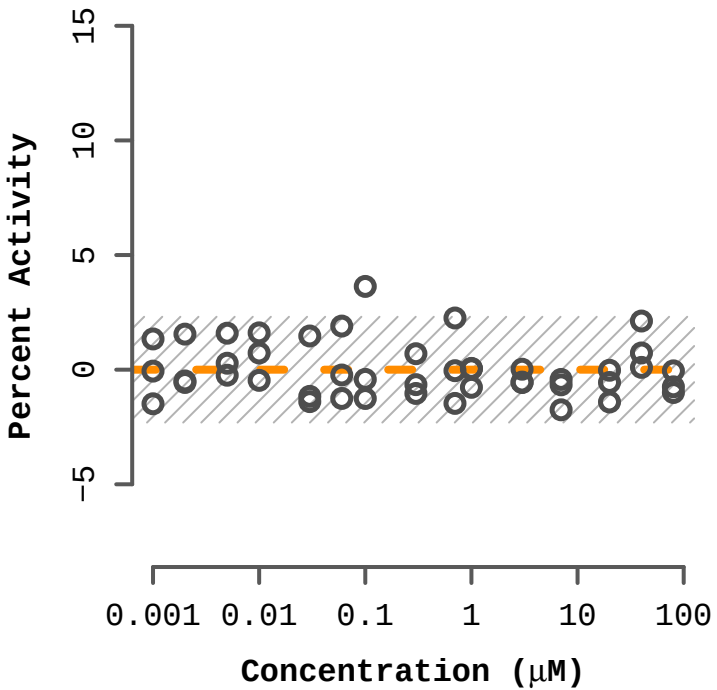
NAME: Swep
CHID: 42437 **CASRN:** 1918-18-9
SPID(S): Tox21_301335
M4ID: 12477798

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

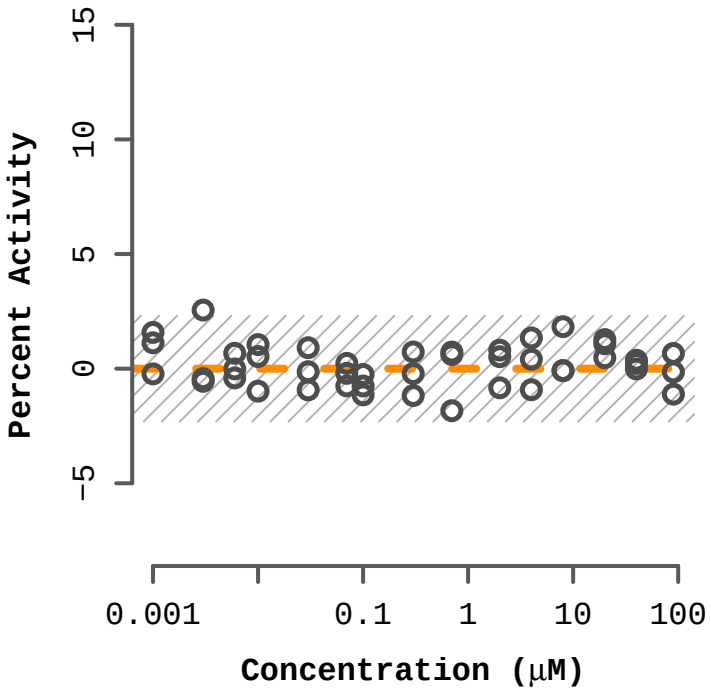
NAME: Teflubenzuron
CHID: 42440 **CASRN:** 83121-18-0
SPID(S): Tox21_301448
M4ID: 12477685

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.985 **MAX_MED:** 0.731 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

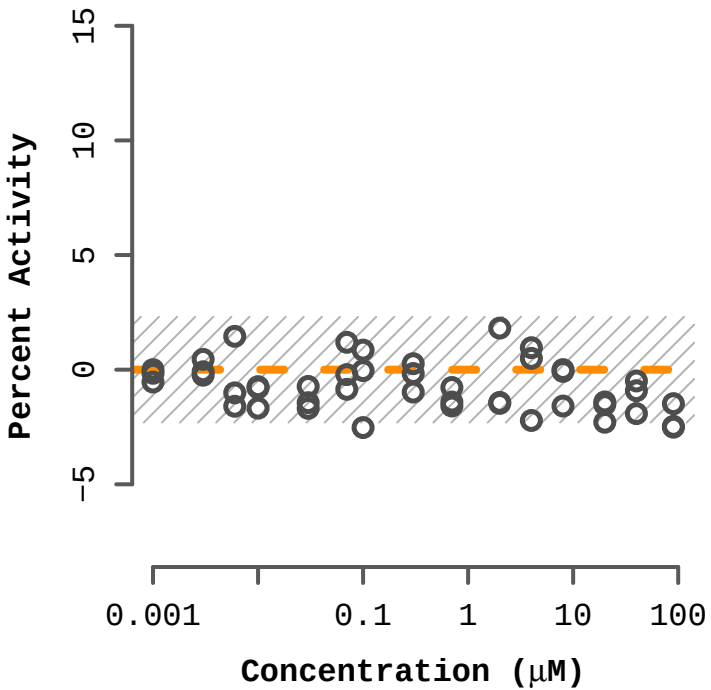
NAME: Terbucarb
CHID: 42441 **CASRN:** 1918-11-2
SPID(S): Tox21_302210
M4ID: 12476923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.946 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

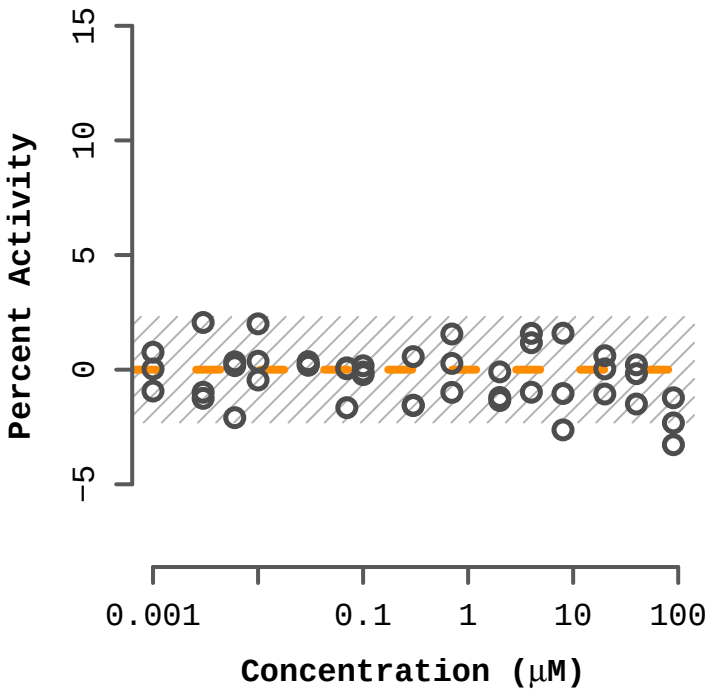
NAME: Terbufos sulfone
CHID: 42443 CASRN: 56070-16-7
SPID(S): Tox21_304046
M4ID: 12475142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.0423 MAX_MED: 0.493 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

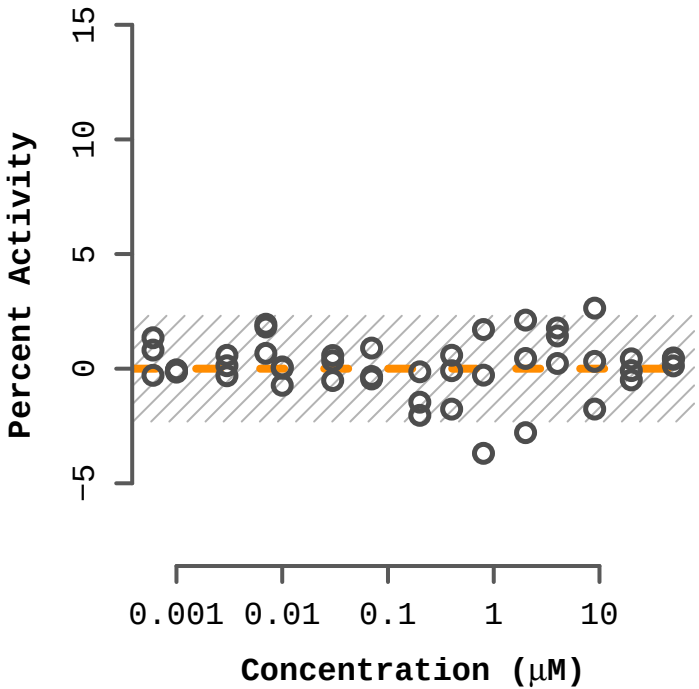
NAME: Terbumeton
CHID: 42445 **CASRN:** 33693-04-8
SPID(S): Tox21_303900
M4ID: 12475288

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

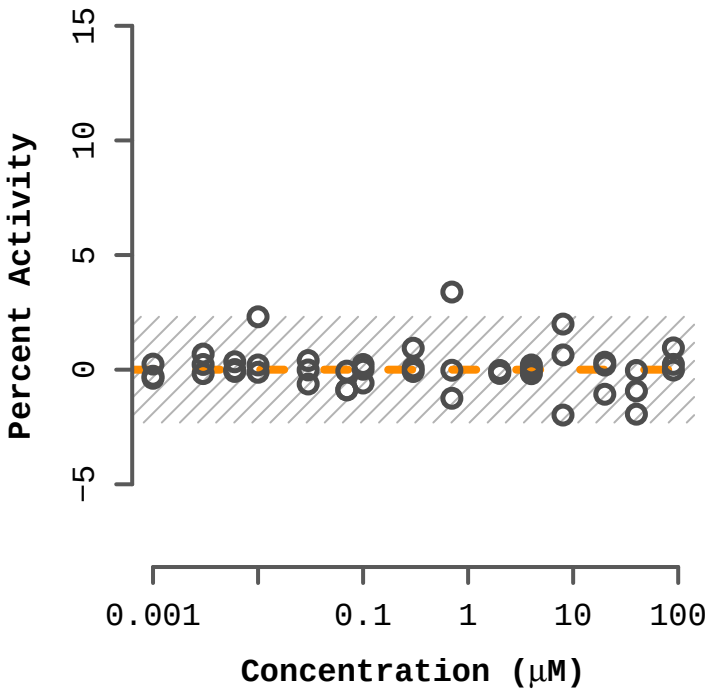
NAME: Tetracaine hydrochloride
CHID: 42448 **CASRN:** 136-47-0
SPID(S): Tox21_110290_1
M4ID: 12484479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

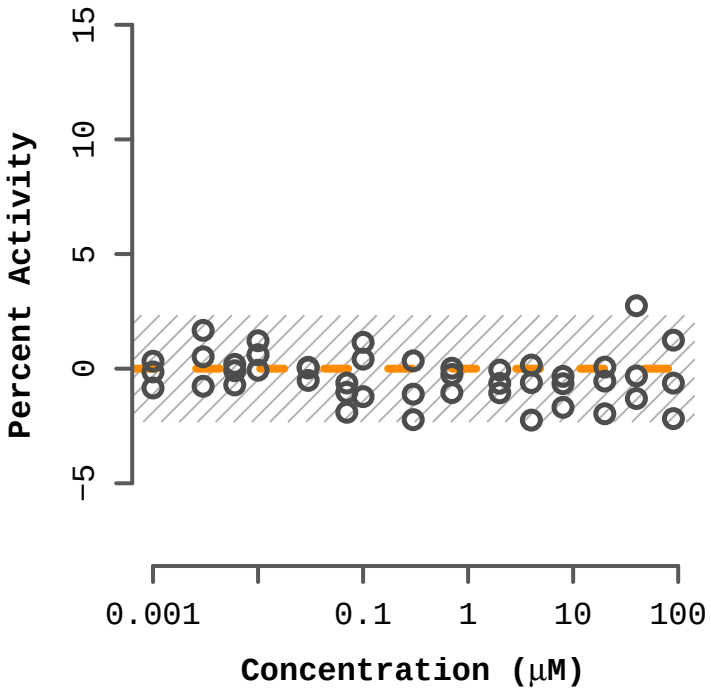
NAME: Tetrachlorothiophene
CHID: 42451 CASRN: 6012-97-1
SPID(S): Tox21_301370
M4ID: 12477763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.801 MAX_MED: 0.645 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

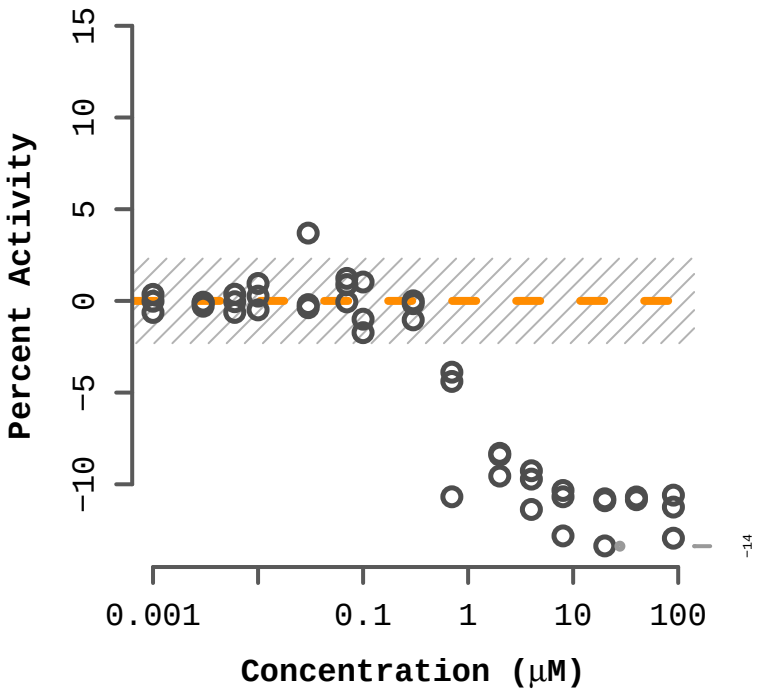
NAME: Tetradecanoic acid, 2,3-dihydroxypropyl ester
CHID: 42454 **CASRN:** 589-68-4
SPID(S): Tox21_301507
M4ID: 12477626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 0.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

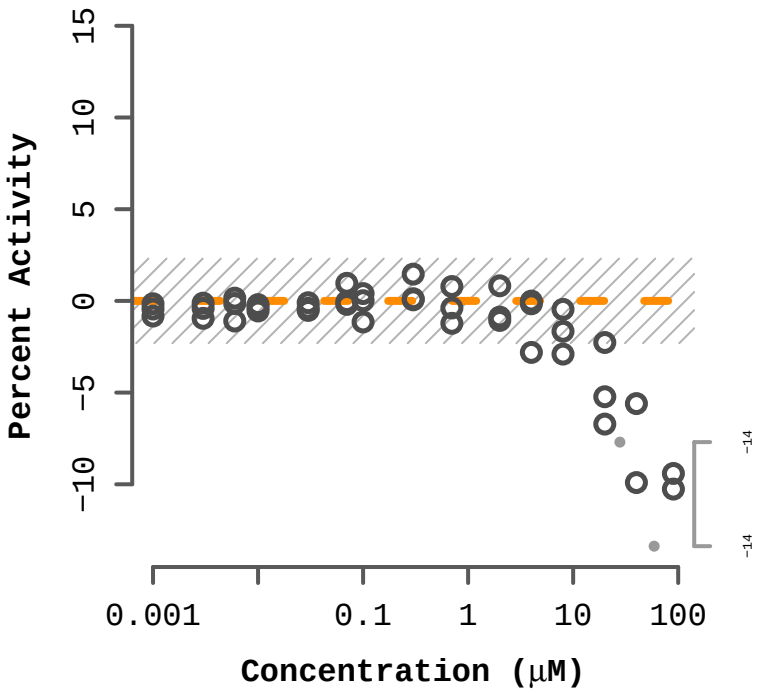
NAME: Tetradecylpyridinium bromide
CHID: 42459 **CASRN:** 1155-74-4
SPID(S): Tox21_301239
M4ID: 12477894 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	310.42	NA	NA
PROB:	1	NA	NA
RMSE:	7.22	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.893 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

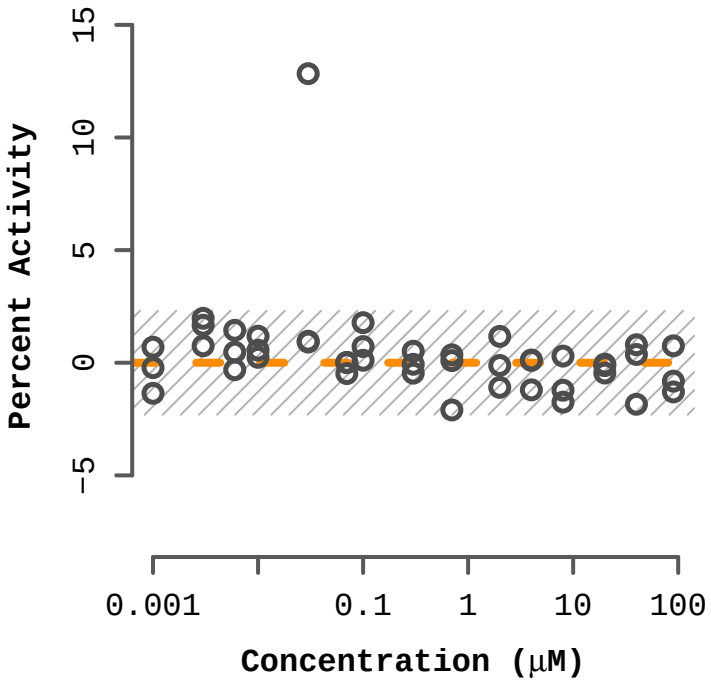
NAME: Tetraiodoethene
CHID: 42462 **CASRN:** 513-92-8
SPID(S): Tox21_301628
M4ID: 12477505 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	235.23	NA	NA
PROB:	1	NA	NA
RMSE:	4.31	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.121 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

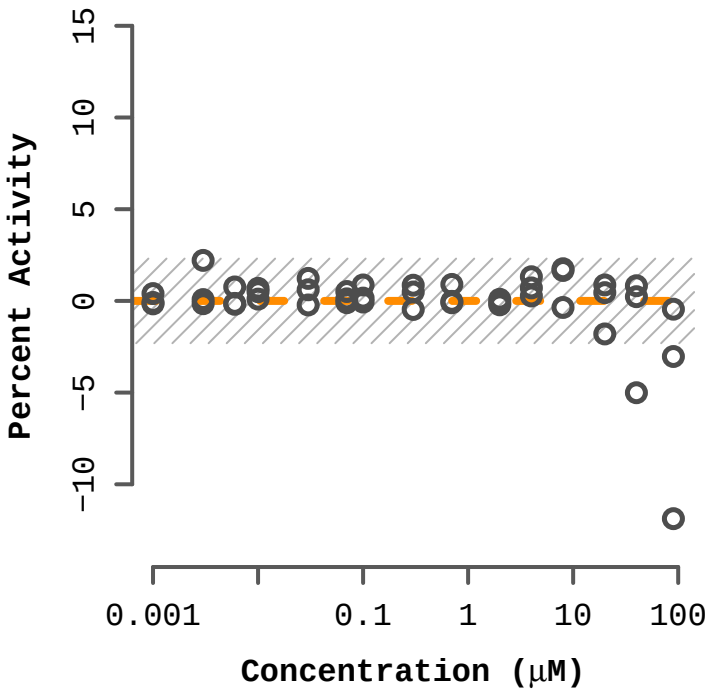
NAME: Thiofanox
CHID: 42468 CASRN: 39196-18-4
SPID(S): Tox21_301851
M4ID: 12477282

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 4.9 MAX_MED: 1.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

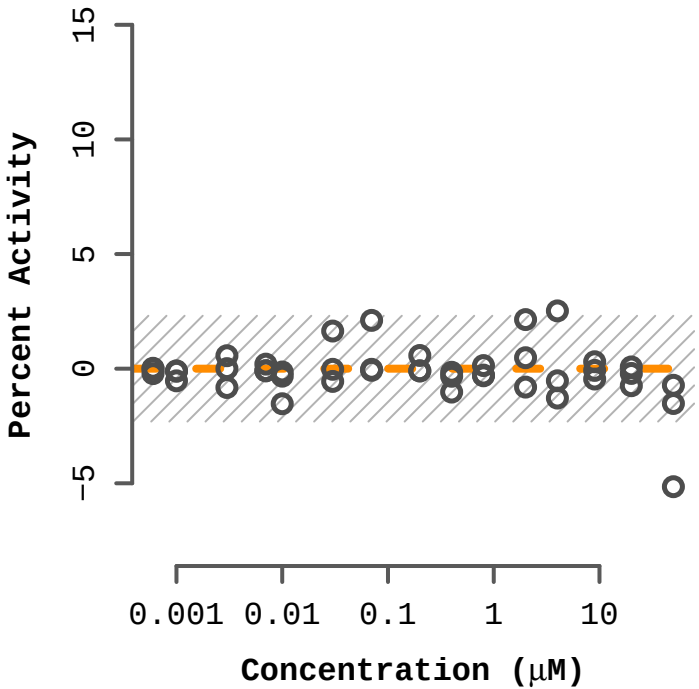
NAME: Tolnaftate
CHID: 42477 **CASRN:** 2398-96-1
SPID(S): Tox21_301363
M4ID: 12477770

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.24	NA	NA
PROB:	1	NA	NA
RMSE:	2.11	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

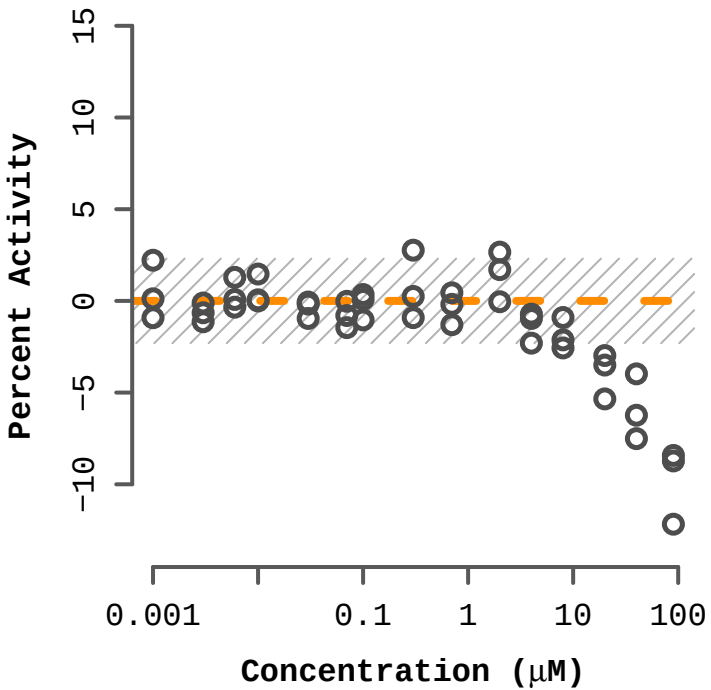
NAME: Tolnaftate
CHID: 42477 CASRN: 2398-96-1
SPID(S): Tox21_110521_1
M4ID: 12484298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.67 **MAX_MED:** 0.479 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

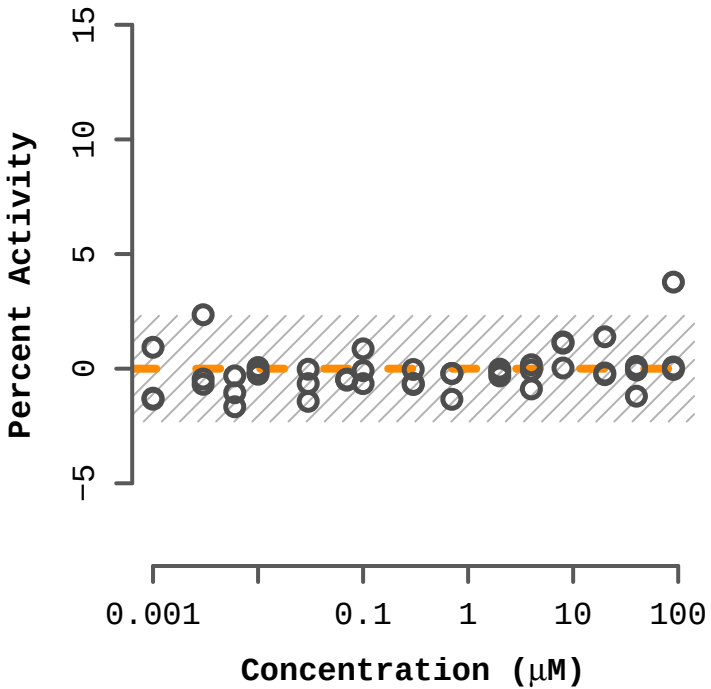
NAME: Tolylfluanid
CHID: 42478 **CASRN:** 731-27-1
SPID(S): Tox21_301224
M4ID: 12477909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.06	NA	NA
PROB:	1	NA	NA
RMSE:	3.37	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

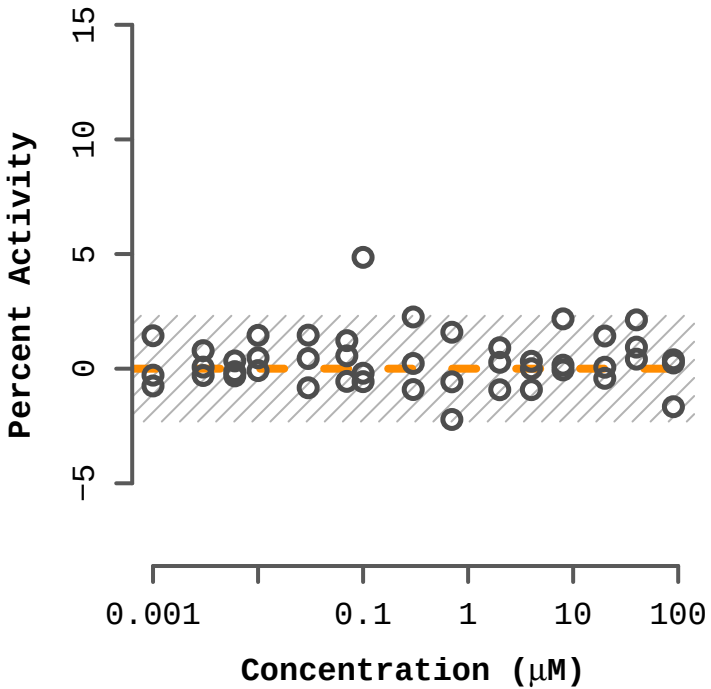
NAME: Triethoxymethylsilane
CHID: 42490 **CASRN:** 2031-67-6
SPID(S): Tox21_301310
M4ID: 12477823

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

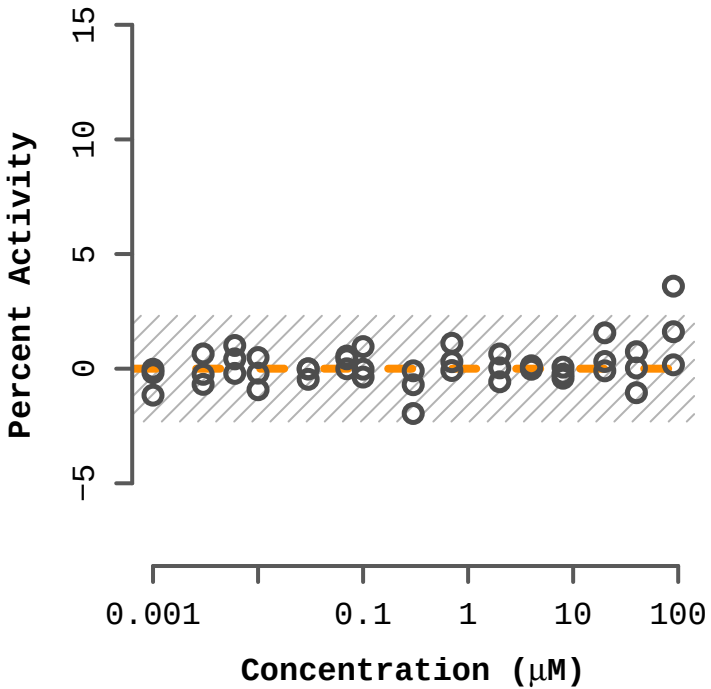
NAME: Triethoxypentylsilane
CHID: 42491 **CASRN:** 2761-24-2
SPID(S): Tox21_301870
M4ID: 12477263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.942 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

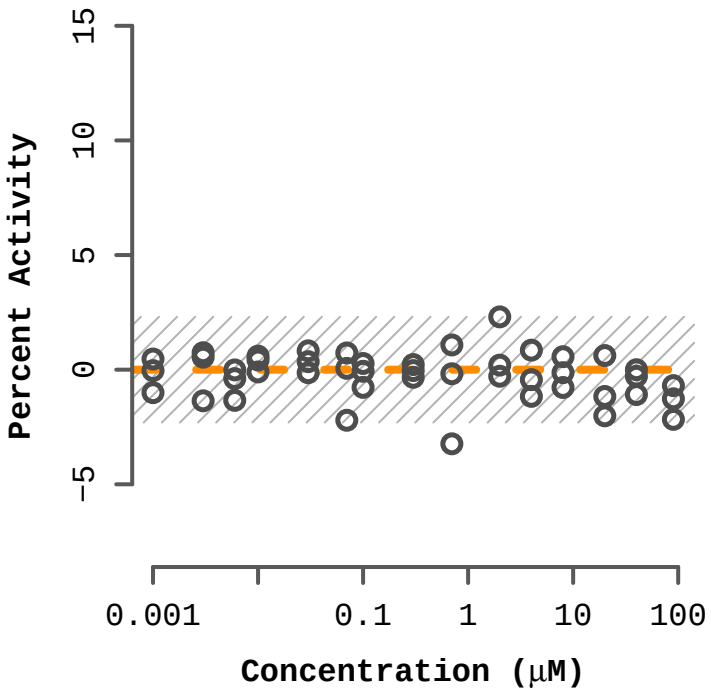
NAME: Trimethoxypropylsilane
CHID: 42494 CASRN: 1067-25-0
SPID(S): Tox21_300951
M4ID: 12478182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.79 MAX_MED: 1.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

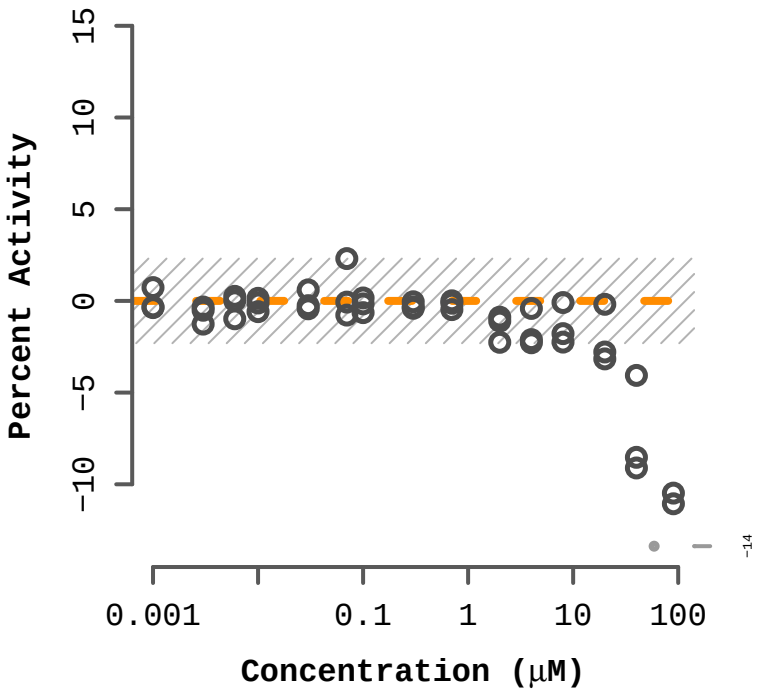
NAME: Triphenylbismuth
CHID: 42498 **CASRN:** 603-33-8
SPID(S): Tox21_302240
M4ID: 12476893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.74 **MAX_MED:** 0.546 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

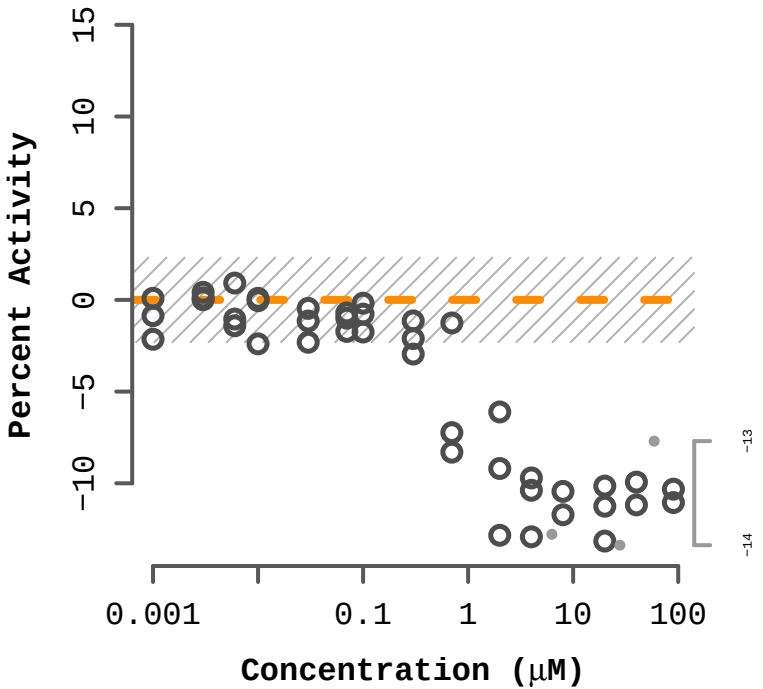
NAME: Triphenylbismuthine dichloride
CHID: 42499 CASRN: 594-30-9
SPID(S): Tox21_302322
M4ID: 12476811 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.23	NA	NA
PROB:	1	NA	NA
RMSE:	3.78	NA	NA

MAX_MEAN: 0.491 **MAX_MED:** 0.00906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

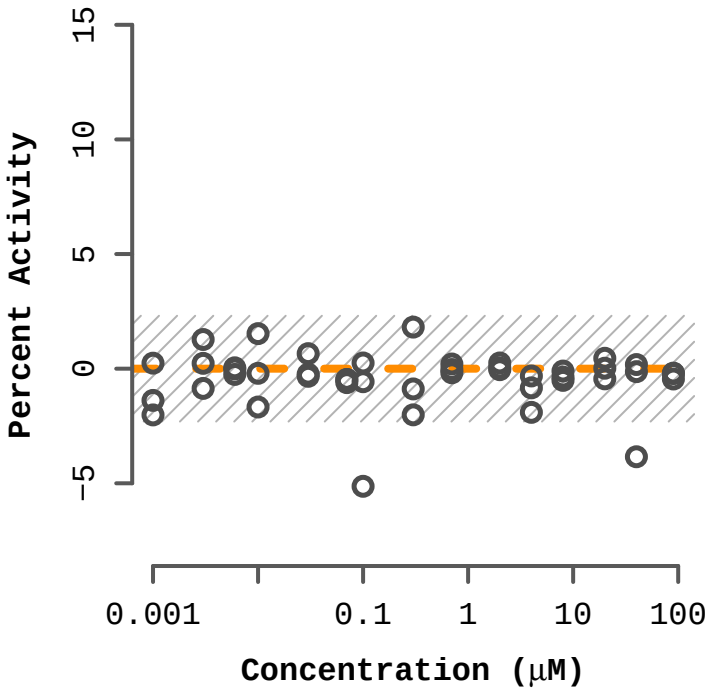
NAME: Triphenyltin fluoride
CHID: 42500 **CASRN:** 379-52-2
SPID(S): Tox21_302241
M4ID: 12476892 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	313.16	NA	NA
PROB:	1	NA	NA
RMSE:	7.44	NA	NA

MAX_MEAN: 0.18 **MAX_MED:** 0.115 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

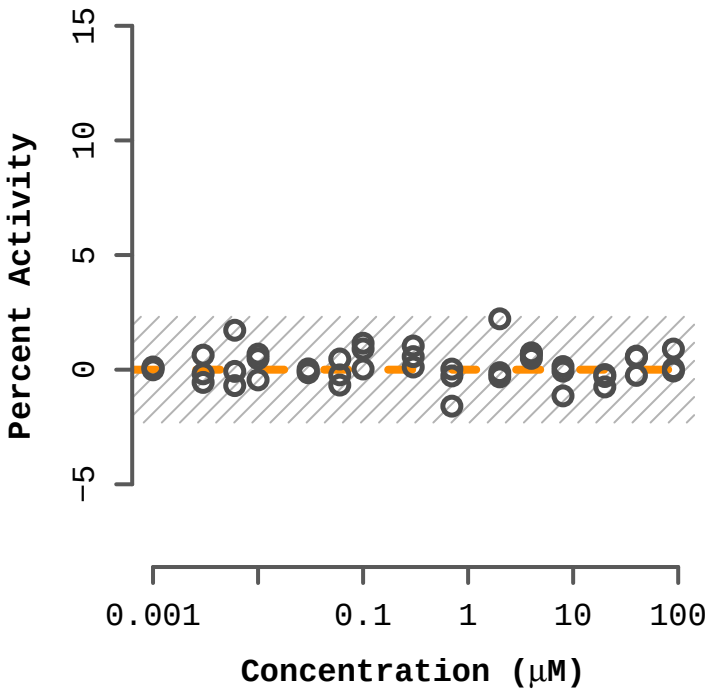
NAME: Tripropylene glycol butyl ether
CHID: 42503 **CASRN:** 55934-93-5
SPID(S): Tox21_301304
M4ID: 12477829

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.216 **MAX_MED:** 0.234 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

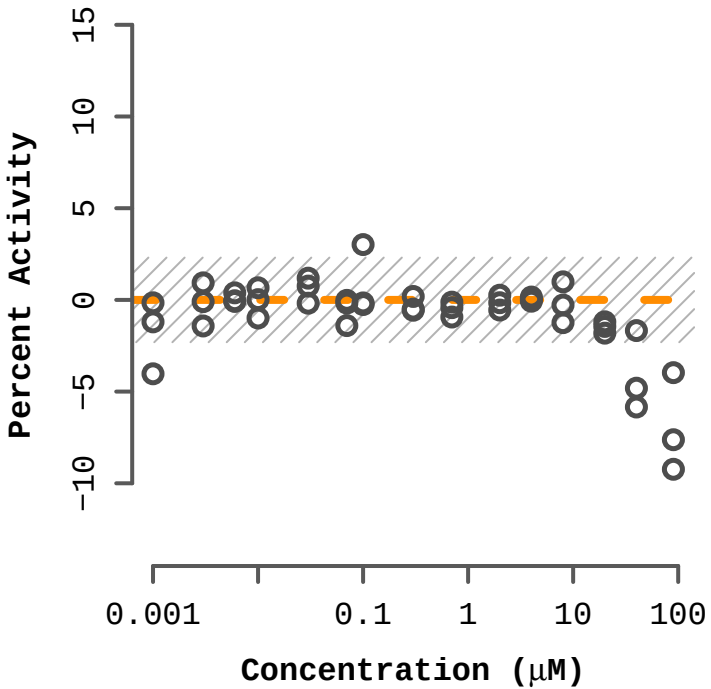
NAME: 1-Phenylurea
CHID: 42507 **CASRN:** 64-10-8
SPID(S): Tox21_301449
M4ID: 12477684

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.697 **MAX_MED:** 0.906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

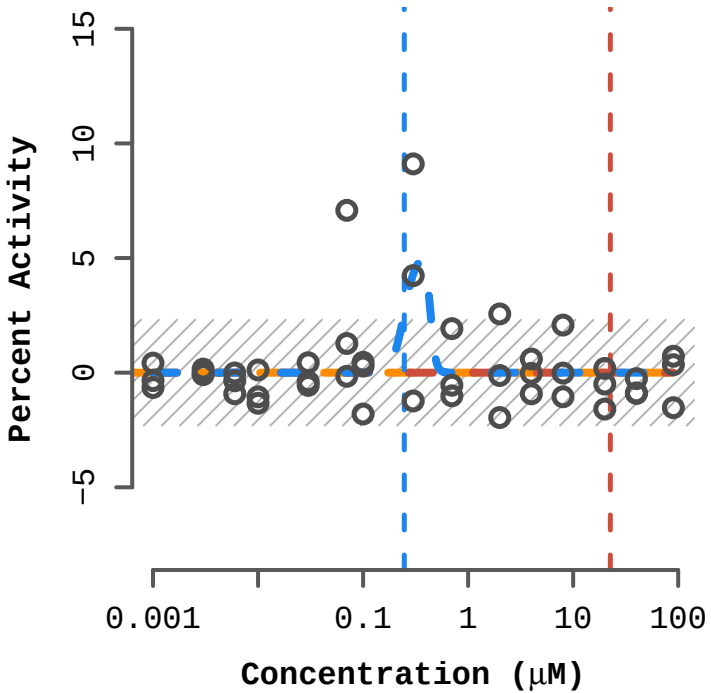
NAME: 2-Isovaleryl-1,3-indanedione
CHID: 42509 **CASRN:** 83-28-3
SPID(S): Tox21_301261
M4ID: 12477872

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 0.868 **MAX_MED:** 0.755 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Xylitol
CHID: 42514 CASRN: 87-99-0
SPID(S): Tox21_201056
M4ID: 12481196

HILL MODEL (in red):

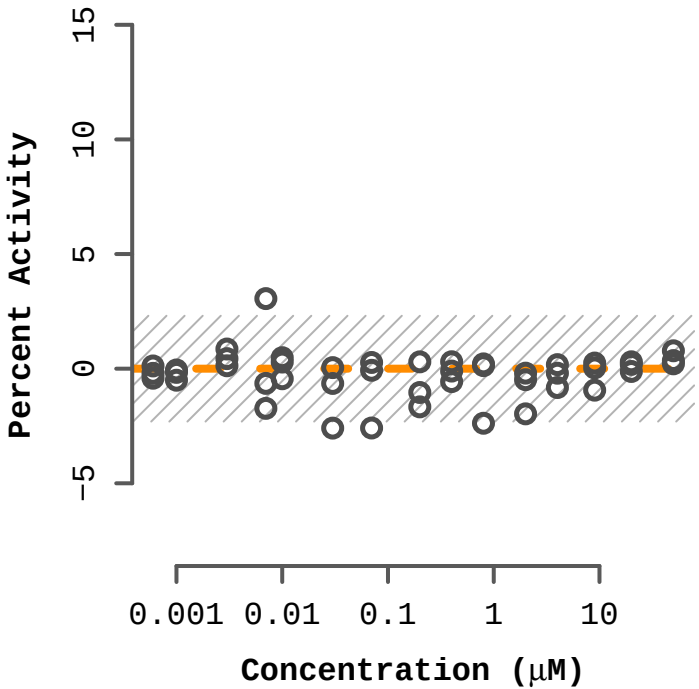
	tp	ga	gw
val:	2.47e-10	1.35	2.35
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.25	−0.608	7.72	−0.358	18
sd:	22.1	1.1	38.4	1.96	174

	CNST	HILL	GNLS
AIC:	166.75	172.75	171.55
PROB:	0.88	0.04	0.08
RMSE:	2.07	2.07	1.79

MAX_MEAN: 4.04 MAX_MED: 4.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

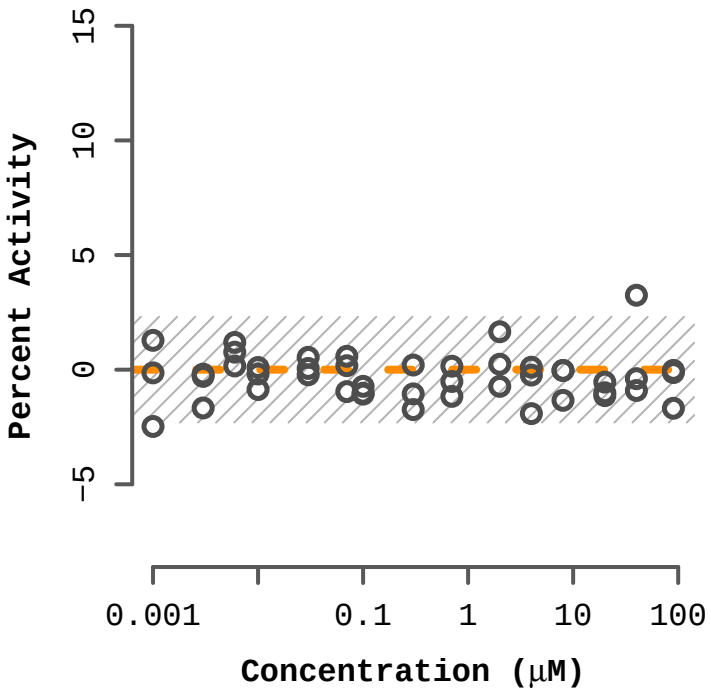
NAME: Zinc octanoate
CHID: 42517 **CASRN:** 557-09-5
SPID(S): Tox21_113995
M4ID: 12482252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.476 **MAX_MED:** 0.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

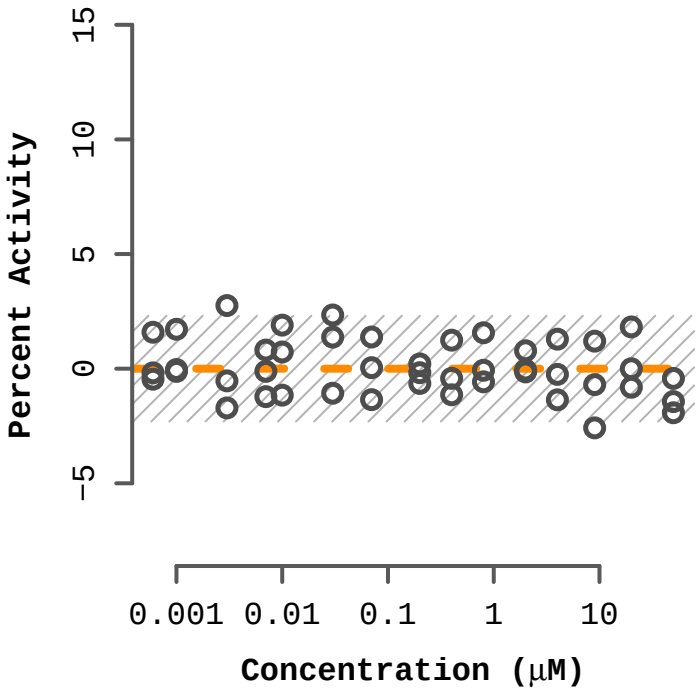
NAME: Zoalene
CHID: 42521 **CASRN:** 148-01-6
SPID(S): Tox21_301320
M4ID: 12477813

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.706 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

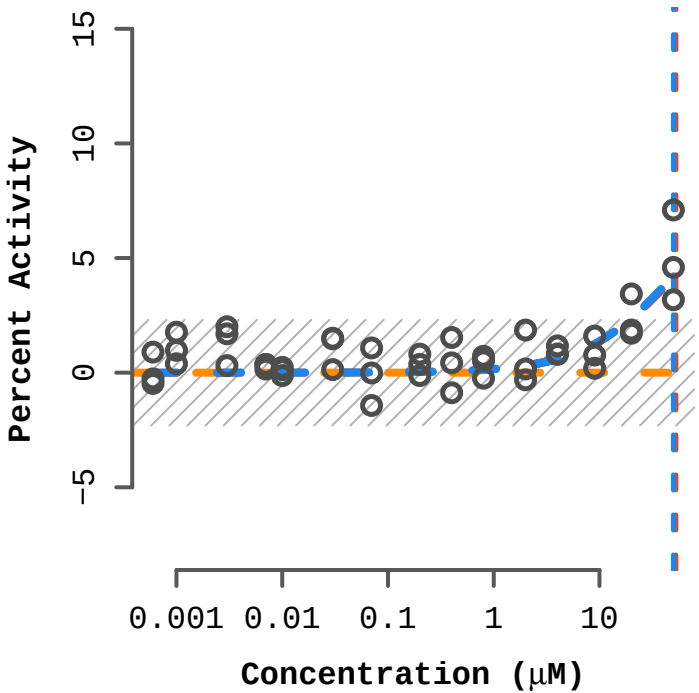
NAME: Zoalene
CHID: 42521 **CASRN:** 148-01-6
SPID(S): Tox21_111374_1
M4ID: 12483730

HILL MODEL: Not applicable.

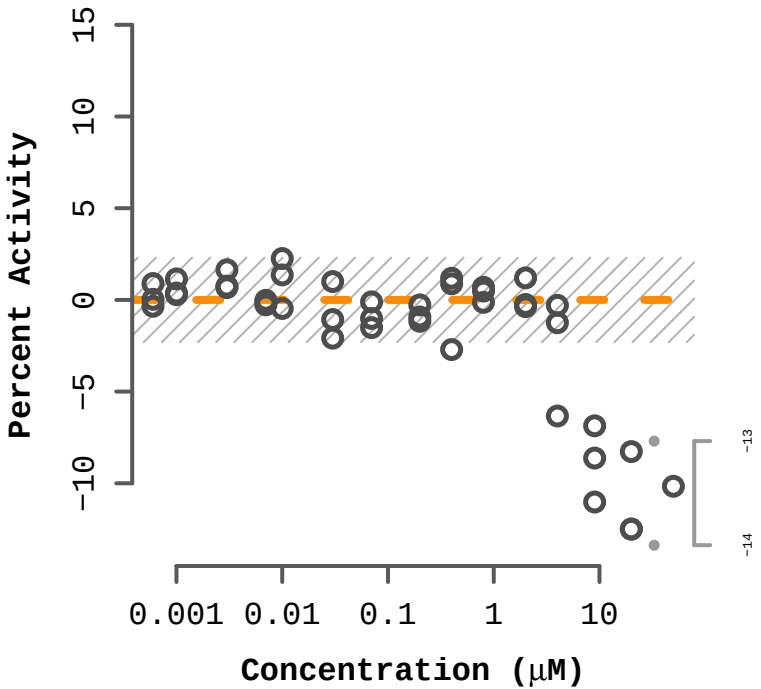
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 1.38 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Zardaverine
CHID:    42559   CASRN: 101975-10-4
SPID(S): Tox21_110307_1
M4ID:    12484466

HILL MODEL (in red):
      tp       ga       gw
val:  8.52     1.72     0.99
sd:   5.44     0.532    0.38

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.47     1.7      1.02     3.39     6.23
sd:   6.58     0.613    0.404    30200    111000

      CNST        HILL        GNLS
AIC:  166.01      131.11      135.14
PROB: 0           0.88        0.12
RMSE: 1.73        0.96        0.95

MAX_MEAN: 4.96      MAX_MED: 4.59      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

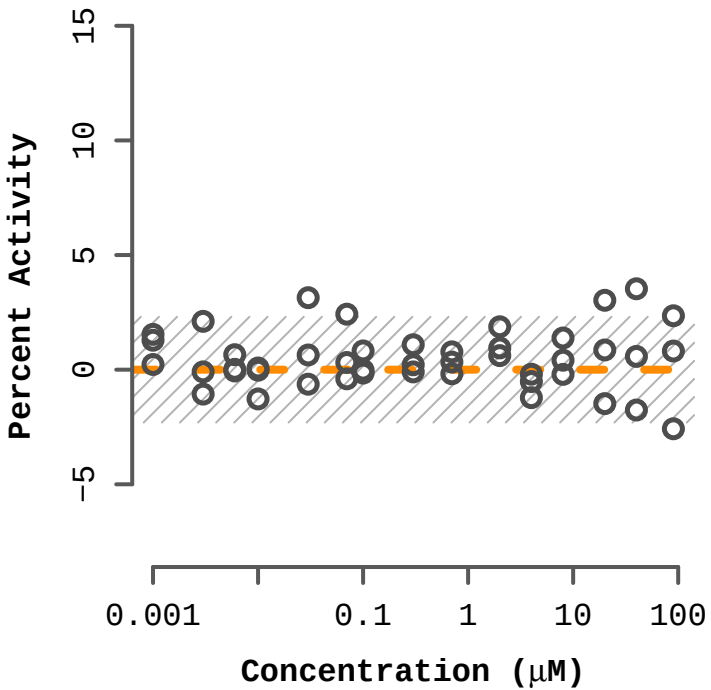
NAME: GBR 12909 dihydrochloride
CHID: 42570 **CASRN:** 67469-78-7
SPID(S): Tox21_110125_1
M4ID: 12484628 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	261.92	NA	NA
PROB:	1	NA	NA
RMSE:	5.13	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

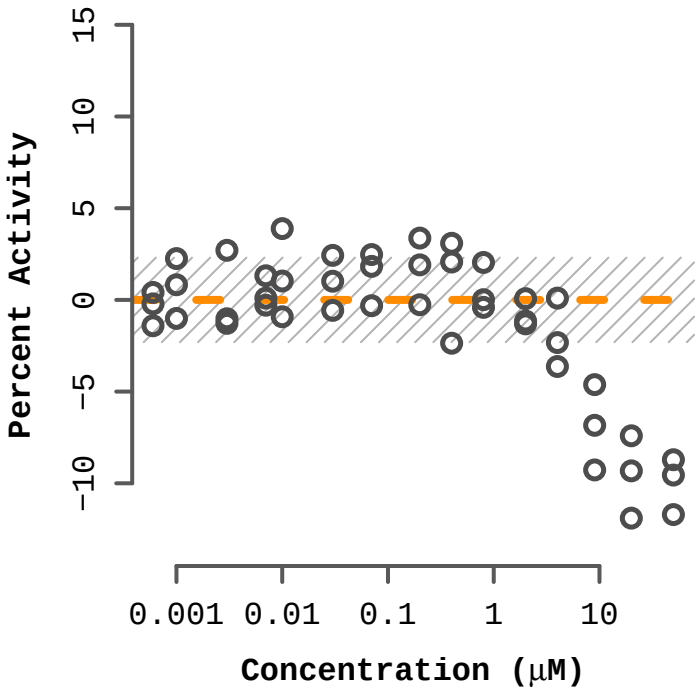
NAME: (RS)−(+/−)−sulpiride
CHID: 42574 **CASRN:** 15676−16−1
SPID(S): Tox21_302205
M4ID: 12476928

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

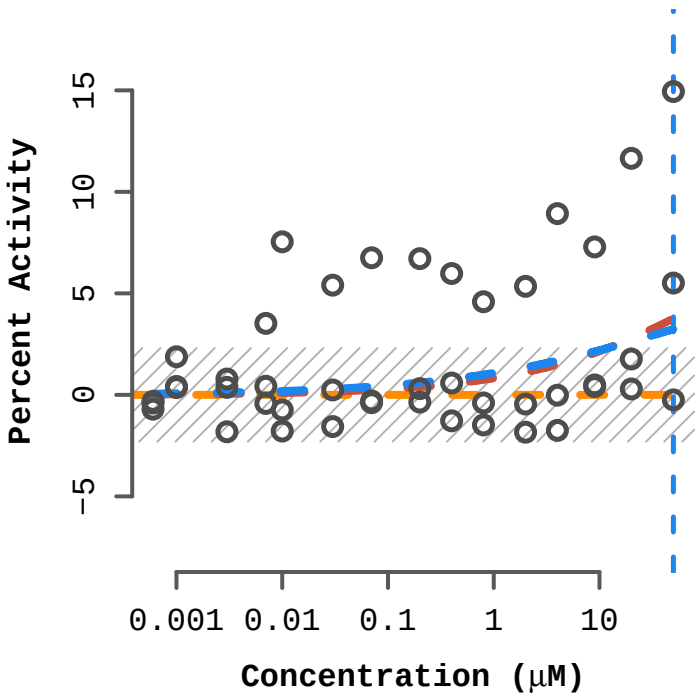
NAME: AMI-193
CHID: 42579 **CASRN:** 510-74-7
SPID(S): Tox21_110914_1
M4ID: 12484019

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.71	NA	NA
PROB:	1	NA	NA
RMSE:	4.36	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Levosulpiride
CHID: 42583 CASRN: 23672-07-3
SPID(S): Tox21_110933_1
M4ID: 12484004

HILL MODEL (in red):

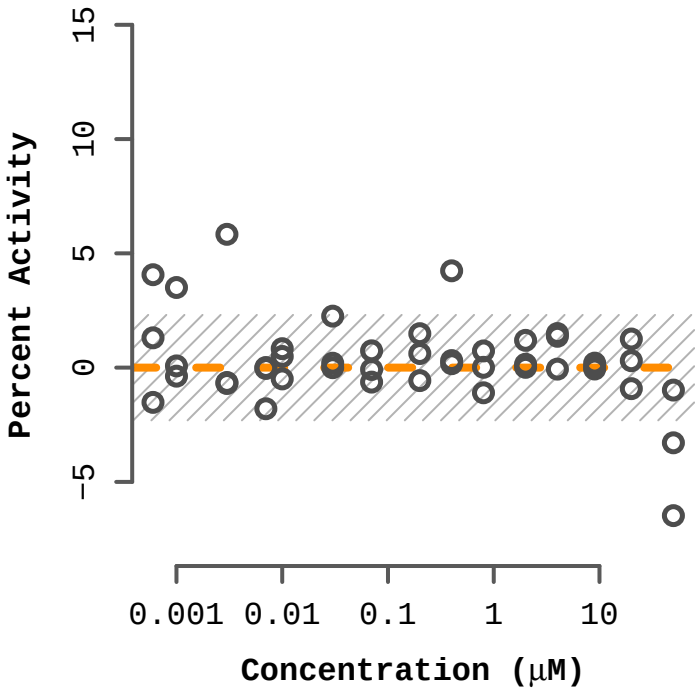
	tp	ga	gw
val:	10.3	2.2	0.482
sd:	45	3.72	1.39

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.47	1.7	0.413	3.02	5.43
sd:	31.7	6.5	0.89	956	3940

	CNST	HILL	GNLS
AIC:	249.56	248.95	253.05
PROB:	0.39	0.54	0.07
RMSE:	4.29	3.68	3.69

MAX_MEAN: 6.74 MAX_MED: 5.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

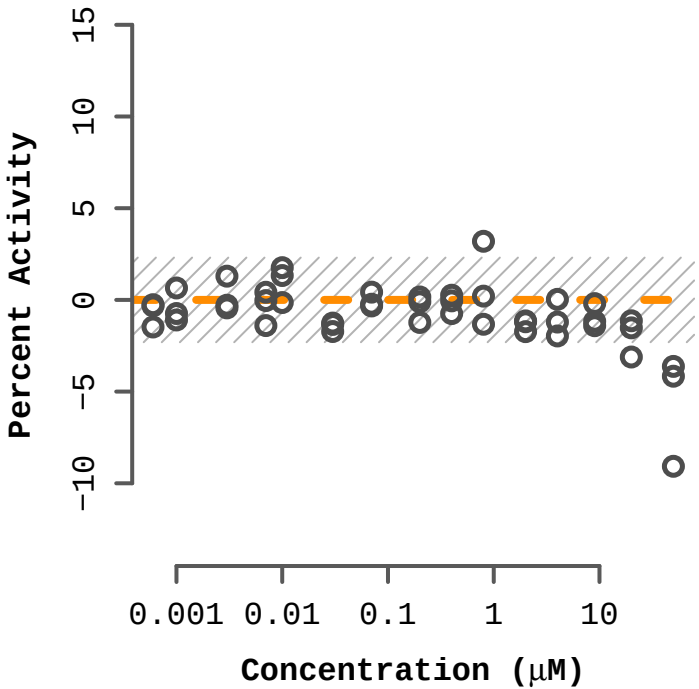
NAME: Metergoline
CHID: 42584 **CASRN:** 17692-51-2
SPID(S): Tox21_110808_1
M4ID: 12484103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

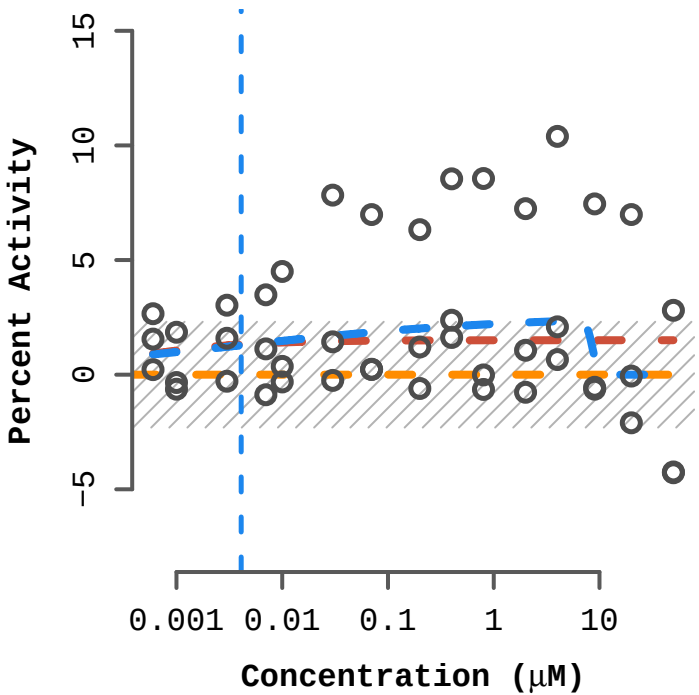
NAME: Altanserin hydrochloride
CHID: 42592 **CASRN:** 1135280-78-2
SPID(S): Tox21_110960_1
M4ID: 12483982

HILL MODEL: Not applicable.

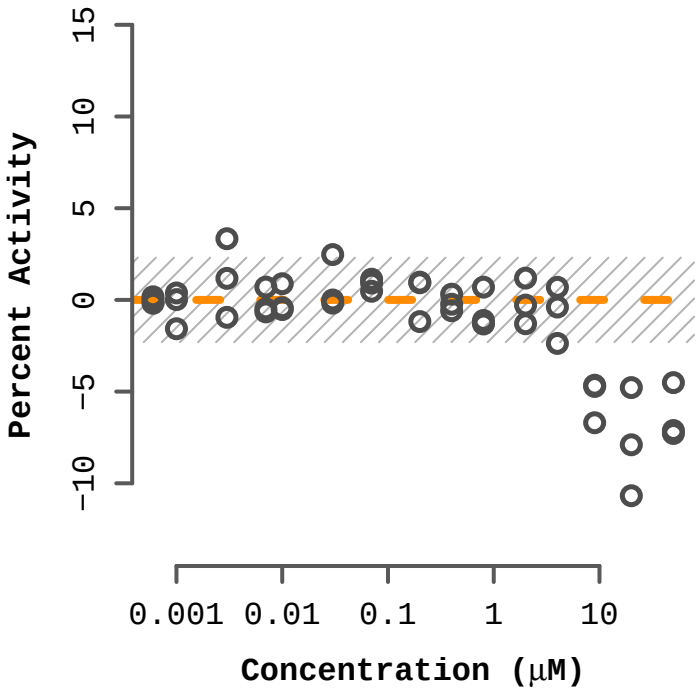
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.97	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 1.33 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ritanserin
CHID:    42594   CASRN: 87051-43-2
SPID(S): Tox21_110251_1
M4ID:    12484513

HILL MODEL (in red):
      tp       ga       gw
val:  1.5      -3.46    0.789
sd:   0.63     2.3      1.89

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.56     -2.39    0.333    0.932    15.6
sd:   3.25     3.82     0.999    0.8      569

      CNST        HILL        GNLS
AIC:  248.91      245.9       246.87
PROB: 0.12        0.54        0.33
RMSE: 3.92        3.42        3.27

MAX_MEAN: 4.38      MAX_MED: 2.38      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

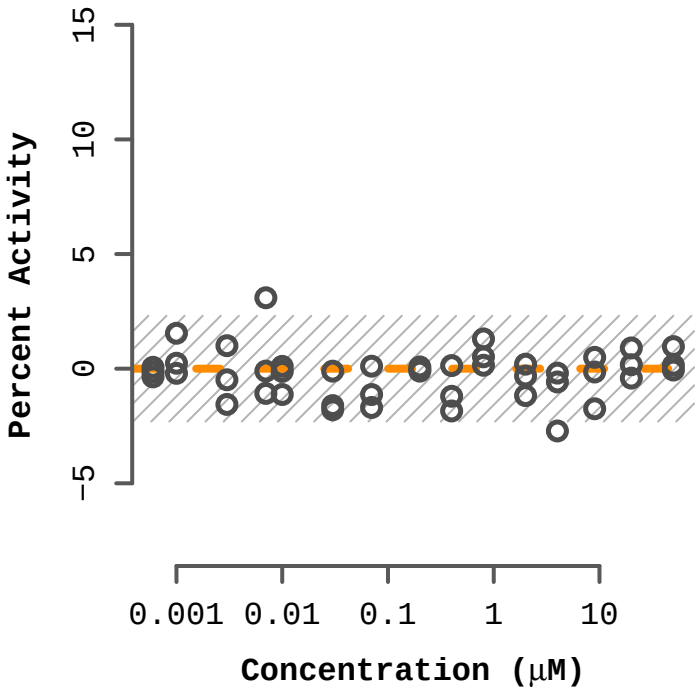
NAME: GR 103691
CHID: 42602 **CASRN:** 162408-66-4
SPID(S): Tox21_110943_1
M4ID: 12483995

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.11	NA	NA
PROB:	1	NA	NA
RMSE:	3.18	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

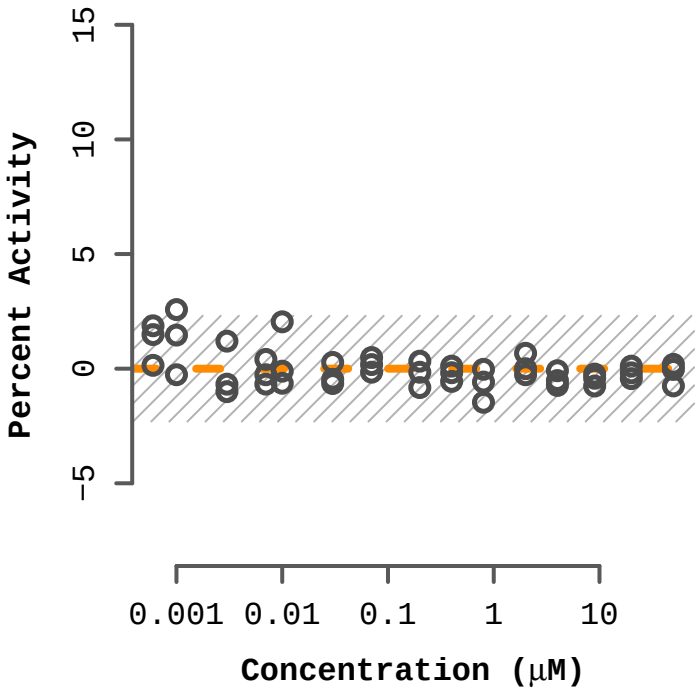
NAME: Amisulpride
CHID: 42613 **CASRN:** 71675-85-9
SPID(S): Tox21_113392_1
M4ID: 12482664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 0.519 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

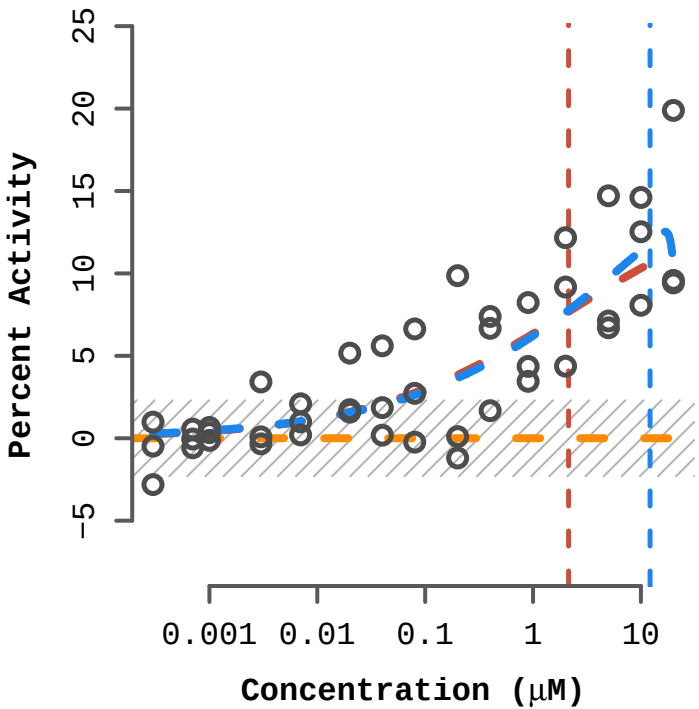
NAME: Tetrabenazine
CHID: 42614 **CASRN:** 58-46-8
SPID(S): Tox21_111803_1
M4ID: 12483471

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SB 206553 hydrochloride
CHID: 42622 CASRN: 1197334-04-5
SPID(S): Tox21_111278_1
M4ID: 12483798

HILL MODEL (in red):

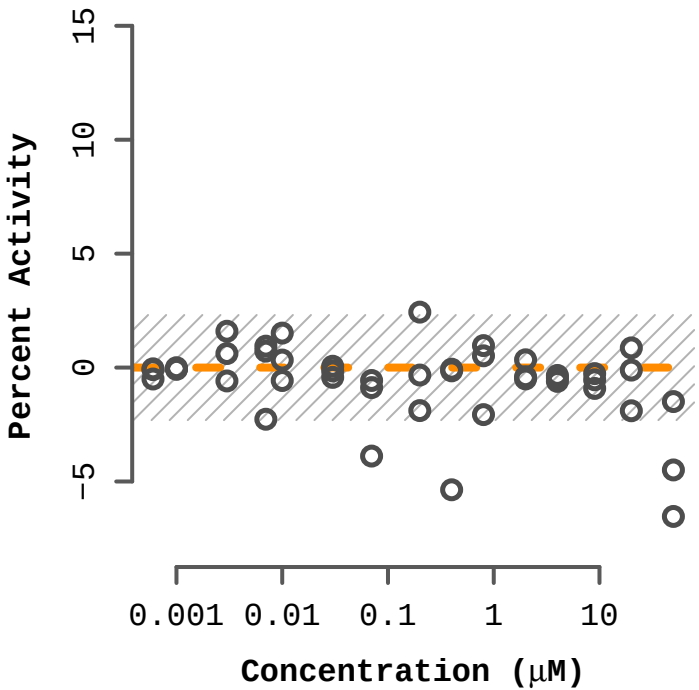
	tp	ga	gw
val:	15.4	0.33	0.463
sd:	7.12	1.01	0.17

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.8	1.08	0.415	1.33	17.6
sd:	26	2.06	0.157	0.0983	55.4

	CNST	HILL	GNLS
AIC:	298.79	231.31	234.47
PROB:	0	0.83	0.17
RMSE:	6.7	2.86	2.88

MAX_MEAN: 13 MAX_MED: 12.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

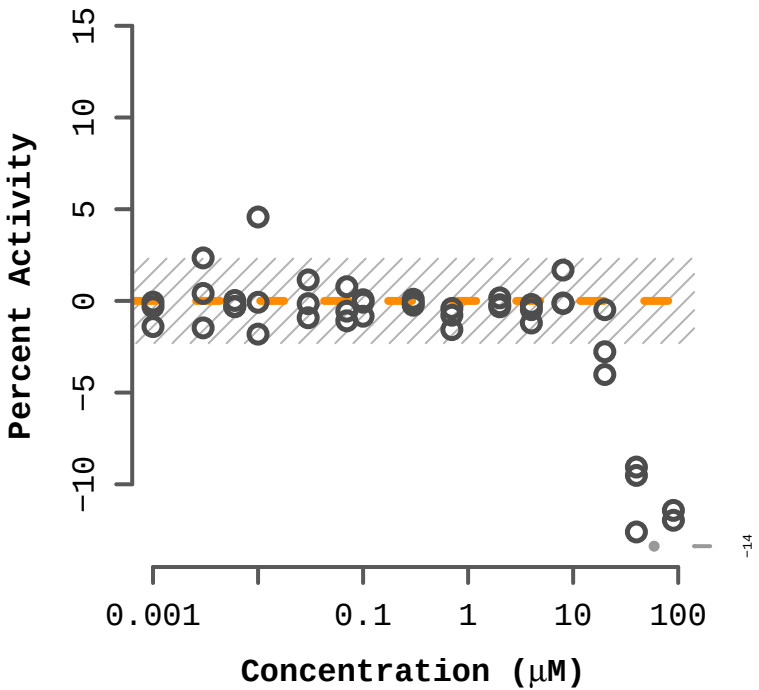
NAME: MDL 72222
CHID: 42632 **CASRN:** 40796-97-2
SPID(S): Tox21_110293_1
M4ID: 12484476

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 0.542 **MAX_MED:** 0.722 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

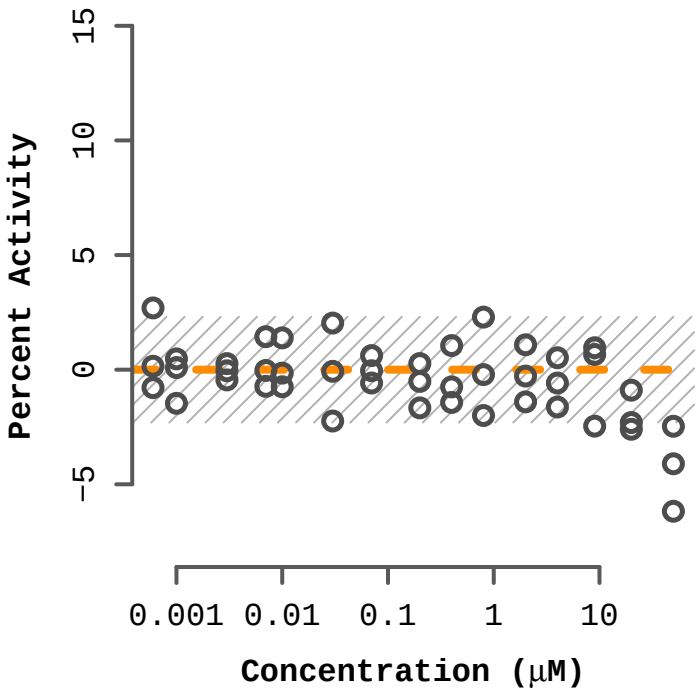
NAME: Clomipramine hydrochloride
CHID: 42633 **CASRN:** 17321-77-6
SPID(S): Tox21_301819
M4ID: 12477314 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.99	NA	NA
PROB:	1	NA	NA
RMSE:	4.38	NA	NA

MAX_MEAN: 0.897 **MAX_MED:** 0.409 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

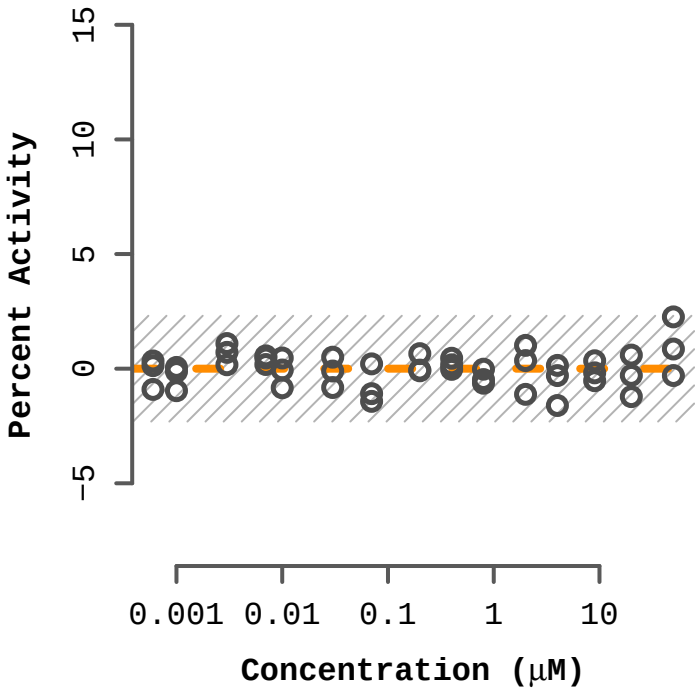
NAME: Cyclopamine
CHID: 43709 **CASRN:** 4449-51-8
SPID(S): Tox21_300632
M4ID: 12478501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 0.687 **MAX_MED:** 0.664 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

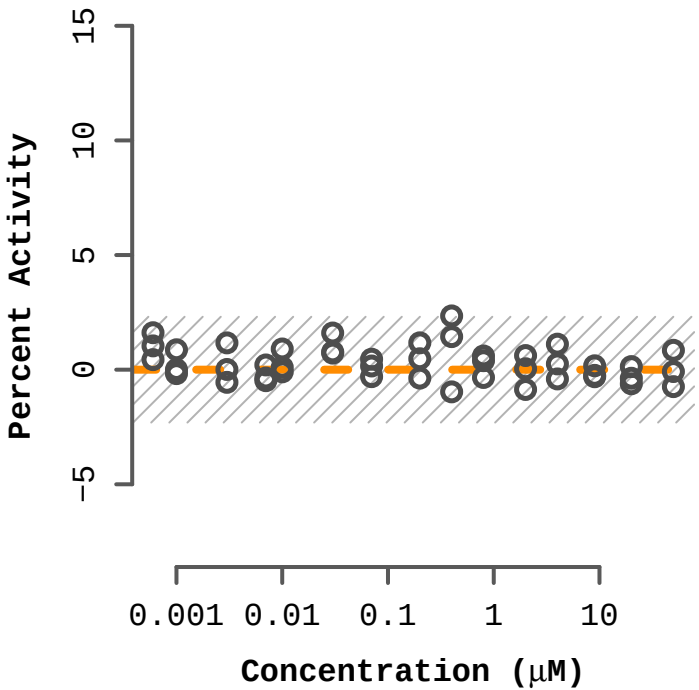
NAME: Temozolomide
CHID: 43714 **CASRN:** 85622-93-1
SPID(S): Tox21_112433_1
M4ID: 12483105

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.941 **MAX_MED:** 0.859 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

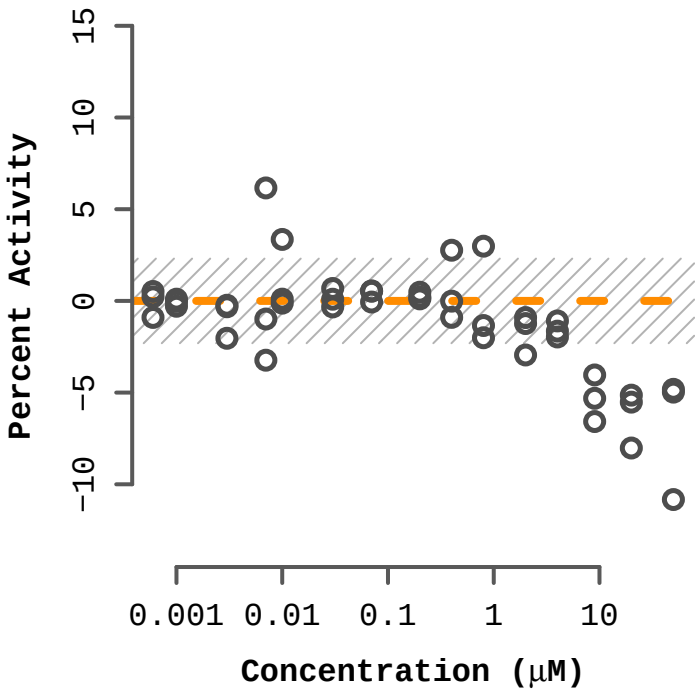
NAME: Watanidipine
CHID: 43747 **CASRN:** 116308-55-5
SPID(S): Tox21_113741
M4ID: 12482473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

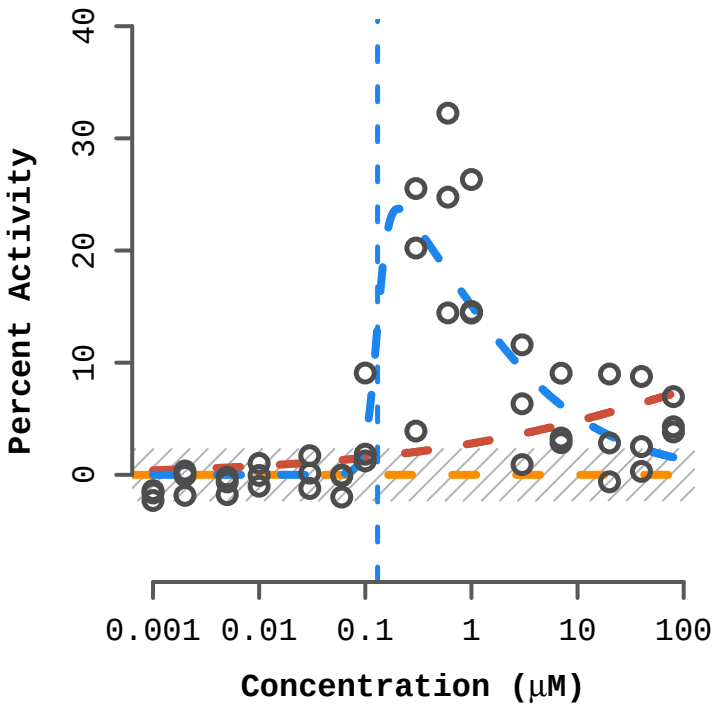
NAME: 4,4'−Dinitrodiphenylurea
CHID: 43761 **CASRN:** 587−90−6
SPID(S): Tox21_112354_1
M4ID: 12483139

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.09	NA	NA
PROB:	1	NA	NA
RMSE:	3.28	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ouabain
CHID: 43765 CASRN: 630-60-4
SPID(S): Tox21_301547
M4ID: 12477586

HILL MODEL (in red):

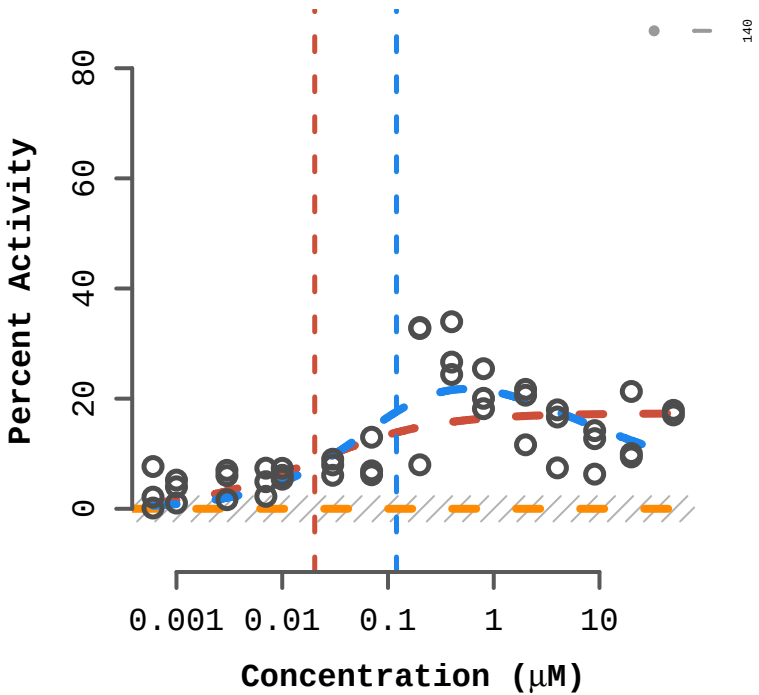
	tp	ga	gw
val:	17.5	2.4	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	38.7	-0.884	7.84	-0.313	0.62
sd:	21.7	1.08	70.1	0.767	0.225

	CNST	HILL	GNLS
AIC:	326.66	316.28	267.8
PROB:	0	0	1
RMSE:	10.22	8.93	4.84

MAX_MEAN: 23.8 MAX_MED: 24.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ouabain
CHID: 43765 CASRN: 630-60-4
SPID(S): Tox21_112057_1
M4ID: 12483343 BRK

HILL MODEL (in red):

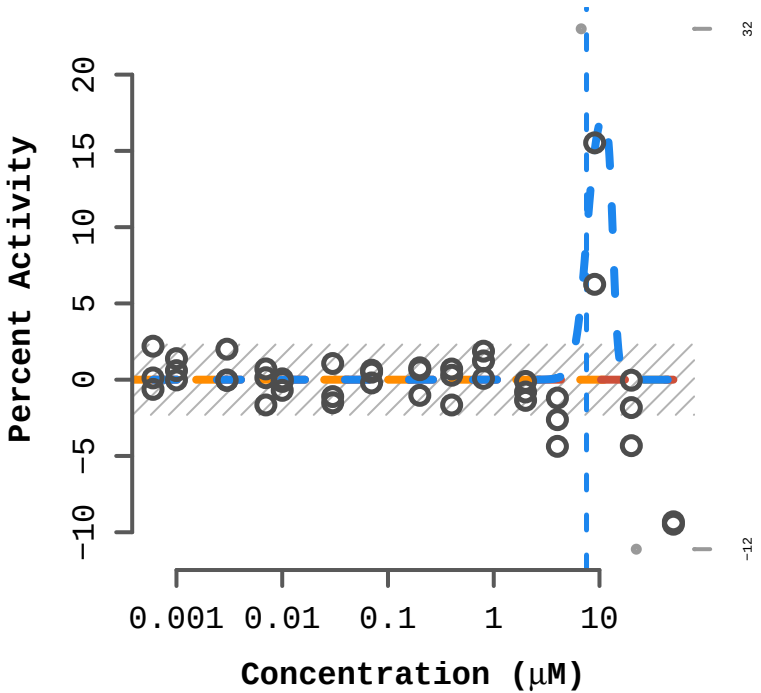
	tp	ga	gw
val:	17.3	-1.69	0.778
sd:	1.58	0.231	0.27

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	64.7	-0.919	0.867	-0.669	0.314
sd:	93.5	0.435	0.301	3.22	0.159

	CNST	HILL	GNLS
AIC:	393.46	325.72	322.58
PROB:	0	0.17	0.83
RMSE:	25.58	19.24	20.01

MAX_MEAN: 57.8 MAX_MED: 32.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Proflavin hemisulfate
CHID: 43777 **CASRN:** 1811-28-5
SPID(S): Tox21_112371_1
M4ID: 12483130 **BRK**

HILL MODEL (in red):

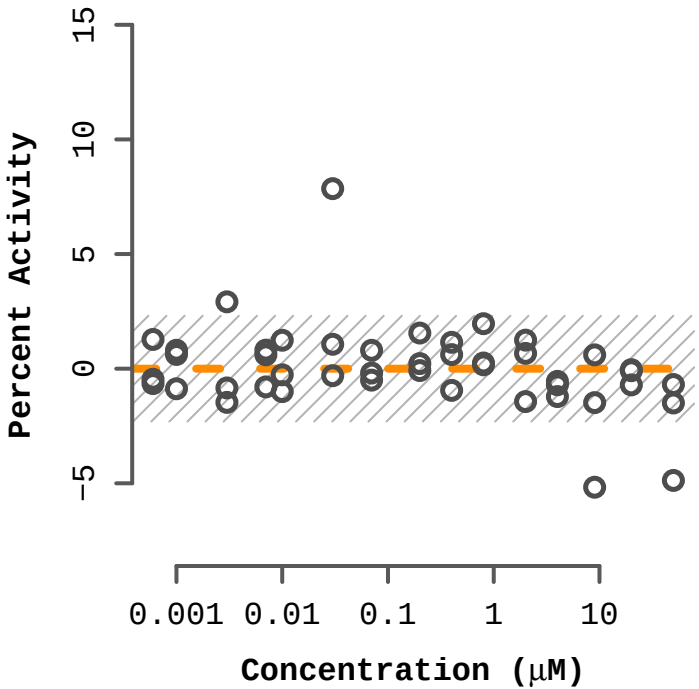
	tp	ga	gw
val:	8.51e-05	2.18	7.26
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.7	0.877	8	1.13	18
sd:	13.6	0.171	4.23	0.326	33.7

	CNST	HILL	GNLS
AIC:	244.45	250.45	236.54
PROB:	0.02	0	0.98
RMSE:	6.13	6.13	4.12

MAX_MEAN: 17.8 **MAX_MED:** 15.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

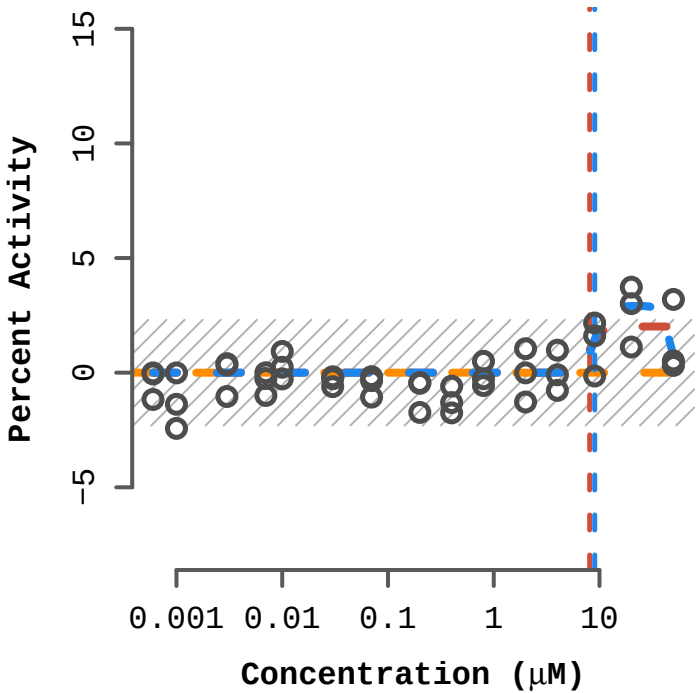
NAME: Pranlukast
CHID: 43782 **CASRN:** 103177-37-3
SPID(S): Tox21_112952
M4ID: 12482866

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 2.87 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ecopipam
CHID: 43814 CASRN: 112108-01-7
SPID(S): Tox21_111197_1
M4ID: 12483849

HILL MODEL (in red):

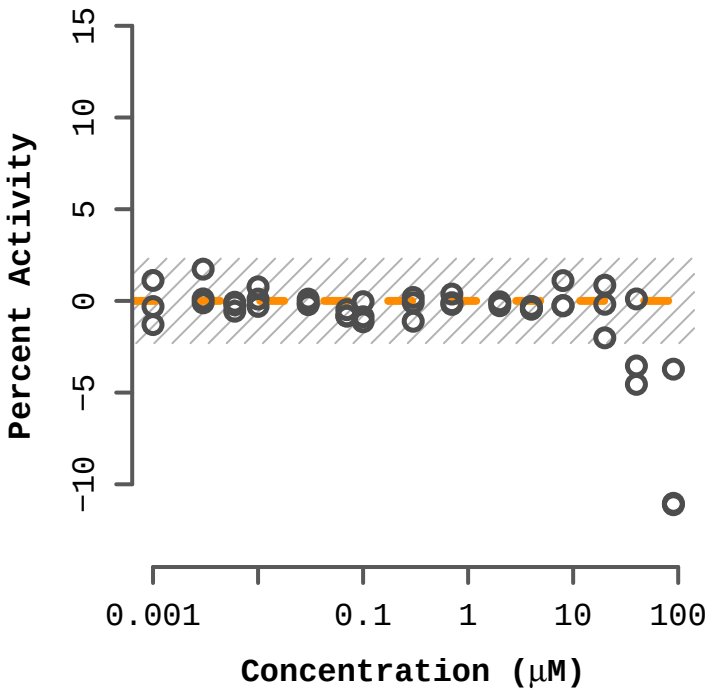
	tp	ga	gw
val:	2.01	0.907	8
sd:	0.75	0.18	24.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.91	0.955	8	1.66	10.7
sd:	0.66	0.051	73.9	0.16	41.6

	CNST	HILL	GNLS
AIC:	145.3	135.96	135.57
PROB:	0	0.45	0.55
RMSE:	1.25	0.97	0.95

MAX_MEAN: 2.62 **MAX_MED:** 3.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

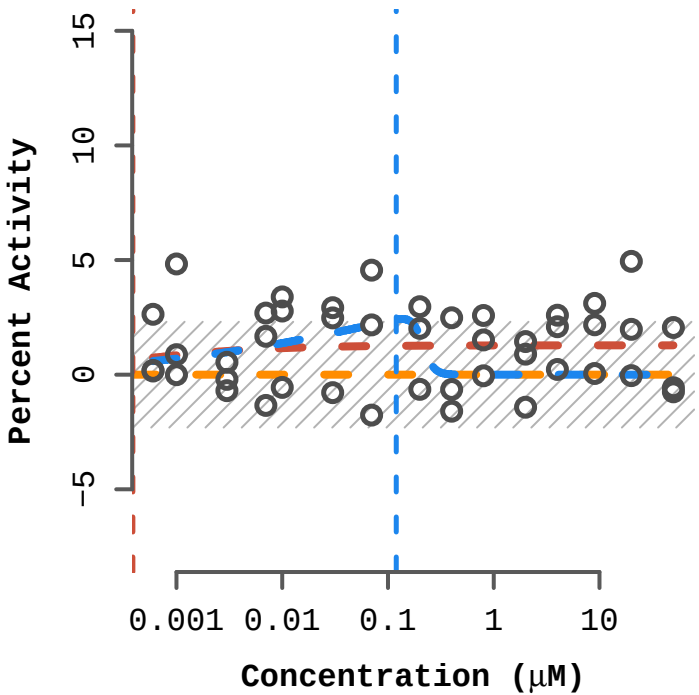
NAME: 2,4-Dimethoxyaniline
CHID: 43829 **CASRN:** 2735-04-8
SPID(S): Tox21_202957
M4ID: 12479295

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.63	NA	NA

MAX_MEAN: 0.579 **MAX_MED:** 0.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pirmenol
CHID: 43839 CASRN: 68252-19-7
SPID(S): Tox21_113702
M4ID: 12482512

HILL MODEL (in red):

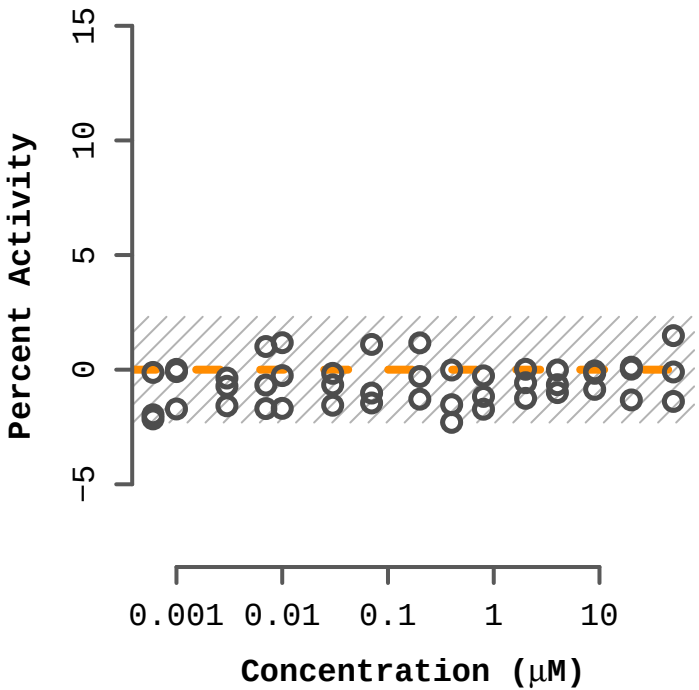
	tp	ga	gw
val:	1.28	−3.41	0.69
sd:	0.362	1.91	1.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.84	−0.922	0.373	−0.672	8.63
sd:	24.1	10.5	0.798	0.222	39.6

	CNST	HILL	GNLS
AIC:	200.75	191.44	201.06
PROB:	0.01	0.98	0.01
RMSE:	2.12	1.76	1.91

MAX_MEAN: 2.29 MAX_MED: 2.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

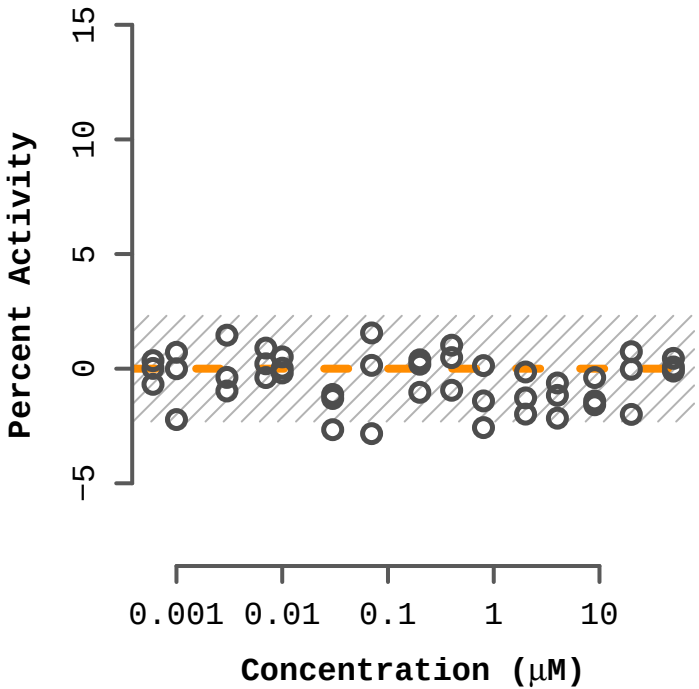
NAME: Xibenolol
CHID: 43848 **CASRN:** 30187-90-7
SPID(S): Tox21_113884
M4ID: 12482341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.00112 **MAX_MED:** 0.0235 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

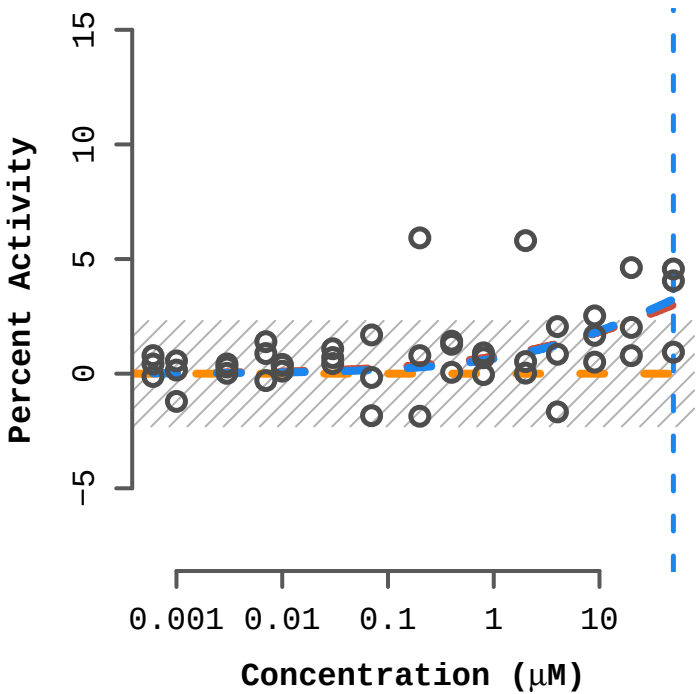
NAME: 1-(2-Chloroethyl)pyrrolidine
CHID: 43850 **CASRN:** 5050-41-9
SPID(S): Tox21_113851
M4ID: 12482371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.242 **MAX_MED:** 0.484 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amiloride
CHID: 43853 CASRN: 2609-46-3
SPID(S): Tox21_110080_1
M4ID: 12484672

HILL MODEL (in red):

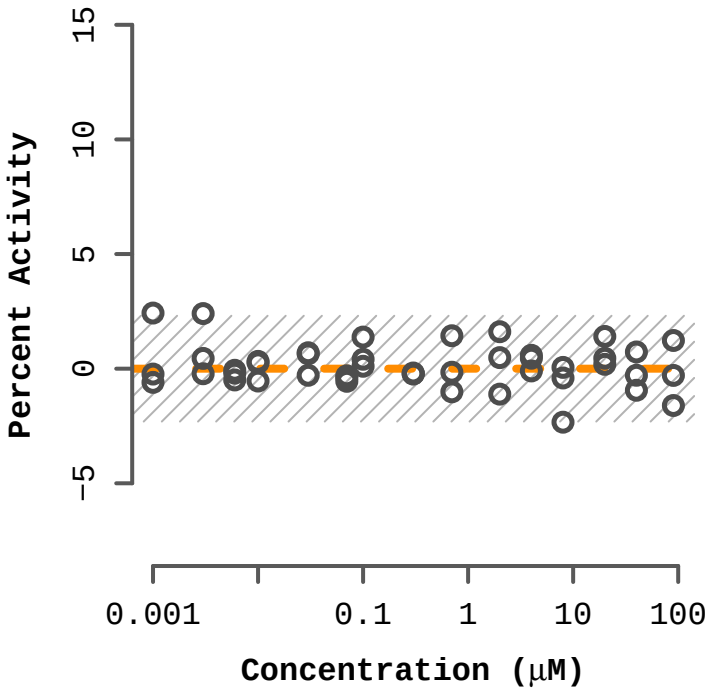
	tp	ga	gw
val:	7.11	1.99	0.468
sd:	6.03	1.33	0.316

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.48	1.7	0.562	3.02	5.84
sd:	6.55	1.27	0.313	959	4250

	CNST	HILL	GNLS
AIC:	180.78	161.1	165.3
PROB:	0	0.89	0.11
RMSE:	1.96	1.51	1.52

MAX_MEAN: 3.19 **MAX_MED:** 4.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

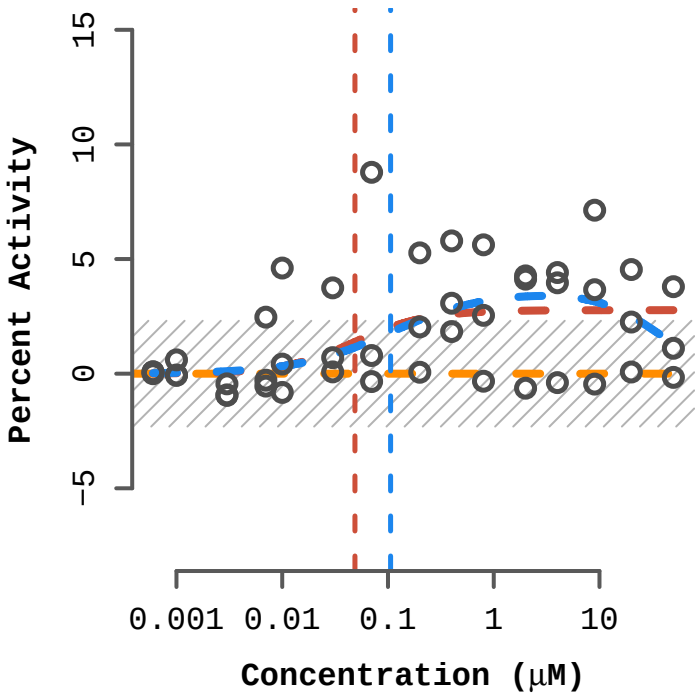
NAME: 2-Amino-6-chloro-4-nitrophenol
CHID: 43855 **CASRN:** 6358-09-4
SPID(S): Tox21_303798
M4ID: 12475390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 0.649 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Octopamine
CHID: 43873 **CASRN:** 104-14-3
SPID(S): Tox21_110215_1
M4ID: 12484545

HILL MODEL (in red):

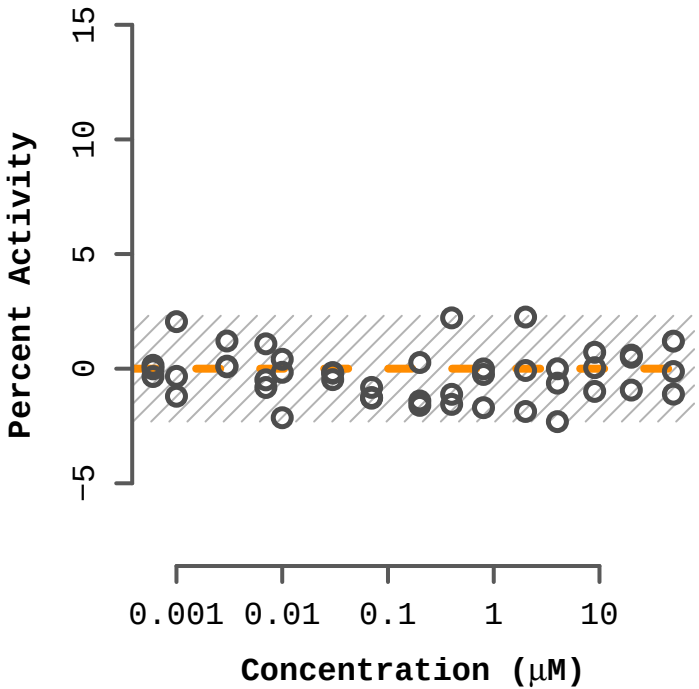
	tp	ga	gw
val:	2.77	−1.31	1.29
sd:	0.548	0.49	0.903

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.61	−0.975	0.978	1.54	1.51
sd:	1.36	0.609	0.744	0.386	2.07

	CNST	HILL	GNLS
AIC:	227.88	205.96	207.8
PROB:	0	0.72	0.28
RMSE:	3.04	2.2	2.2

MAX_MEAN: 3.57 **MAX_MED:** 4.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

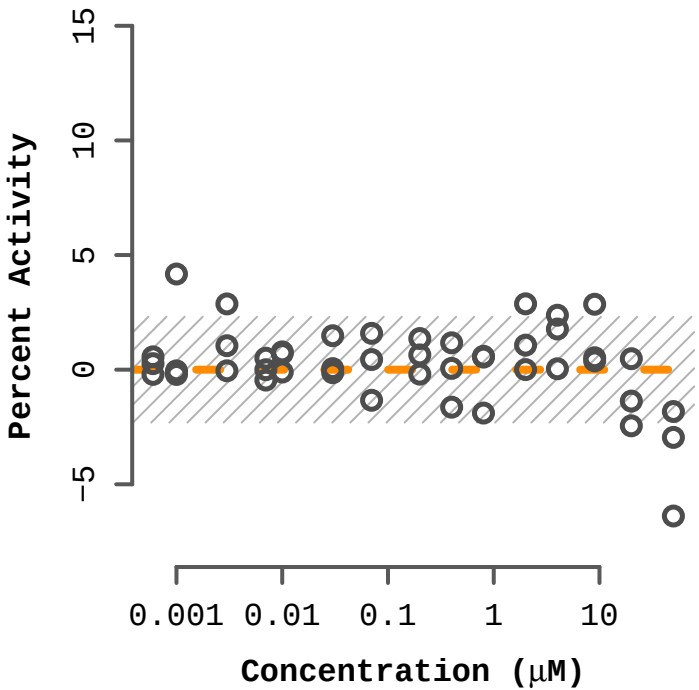
NAME: Tyramine
CHID: 43874 **CASRN:** 51-67-2
SPID(S): Tox21_110282_1
M4ID: 12484486

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.468 **MAX_MED:** 0.499 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

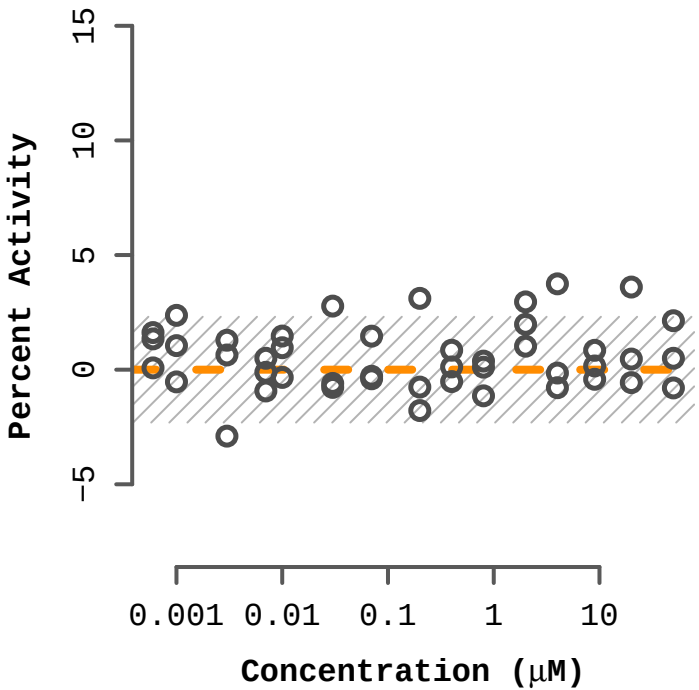
NAME: Imipramine
CHID: 43881 **CASRN:** 50-49-7
SPID(S): Tox21_110174_1
M4ID: 12484584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

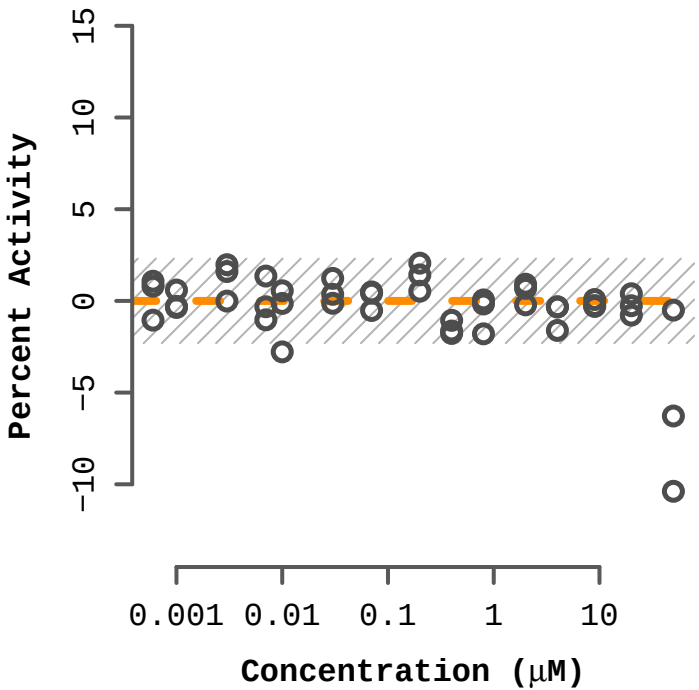
NAME: Carmoxirole
CHID: 43892 **CASRN:** 98323-83-2
SPID(S): Tox21_111193_1
M4ID: 12483853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

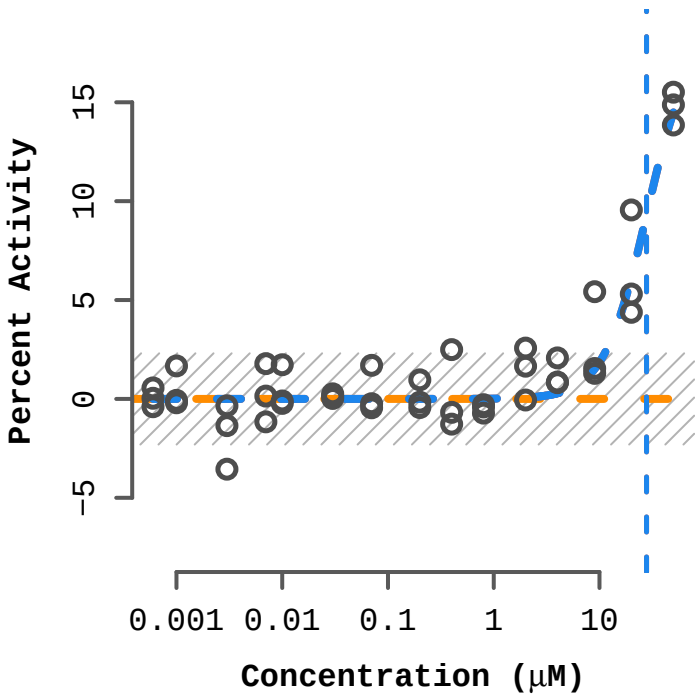
NAME: Roxindole
CHID: 43895 **CASRN:** 112192-04-8
SPID(S): Tox21_110955_1
M4ID: 12483986

HILL MODEL: Not applicable.

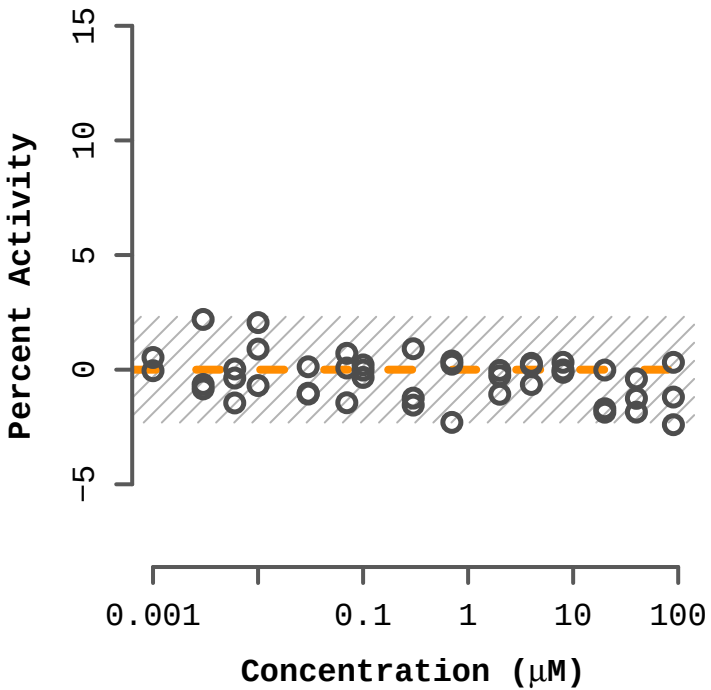
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.6 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Fenoldopam
CHID:    43896   CASRN: 67227-56-9
SPID(S): Tox21_110152_1
M4ID:    12484605

HILL MODEL (in red):
      tp       ga       gw
val:  18.6     1.44     2.15
sd:   3.07     0.0969   0.517

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  18.6     1.44     2.15     2.34     18
sd:   3.06     0.0966   0.515    5840     161000

      CNST        HILL        GNLS
AIC:  231.94      159.37      163.37
PROB: 0           0.88        0.12
RMSE: 4.42        1.37        1.37

MAX_MEAN: 14.7      MAX_MED: 14.9      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

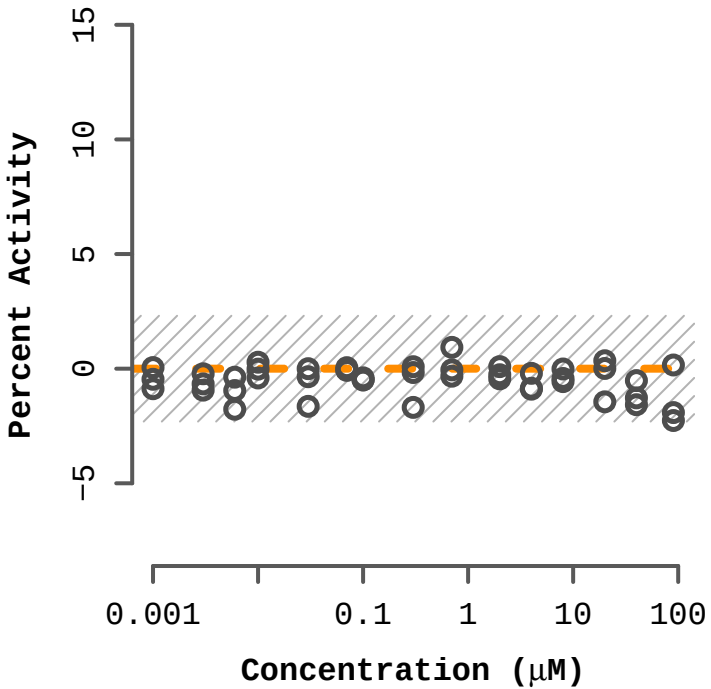
NAME: 1,1,3,3-Tetrabutylurea
CHID: 43902 **CASRN:** 4559-86-8
SPID(S): Tox21_301515
M4ID: 12477618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 0.898 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

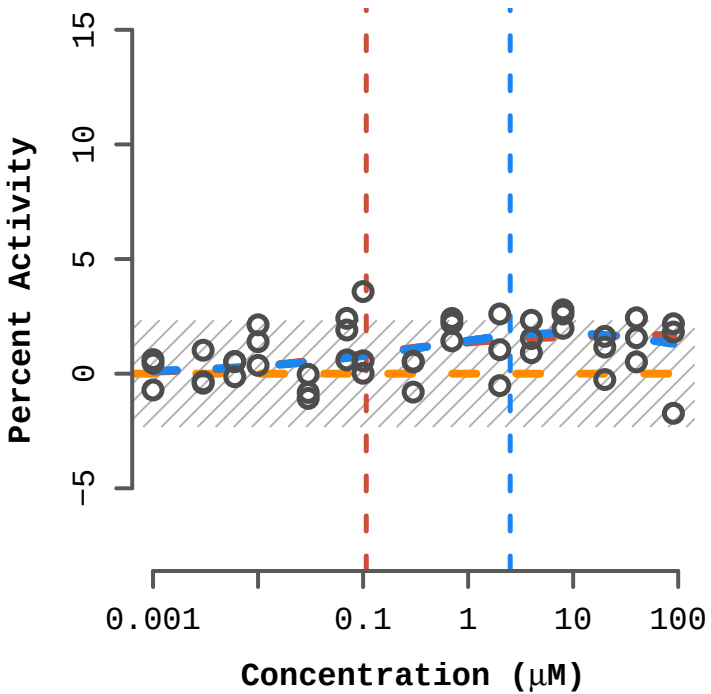
NAME: 2,3-Dihydroxynaphthalene
CHID: 43903 CASRN: 92-44-4
SPID(S): Tox21_303850
M4ID: 12475338

HILL MODEL: Not applicable.

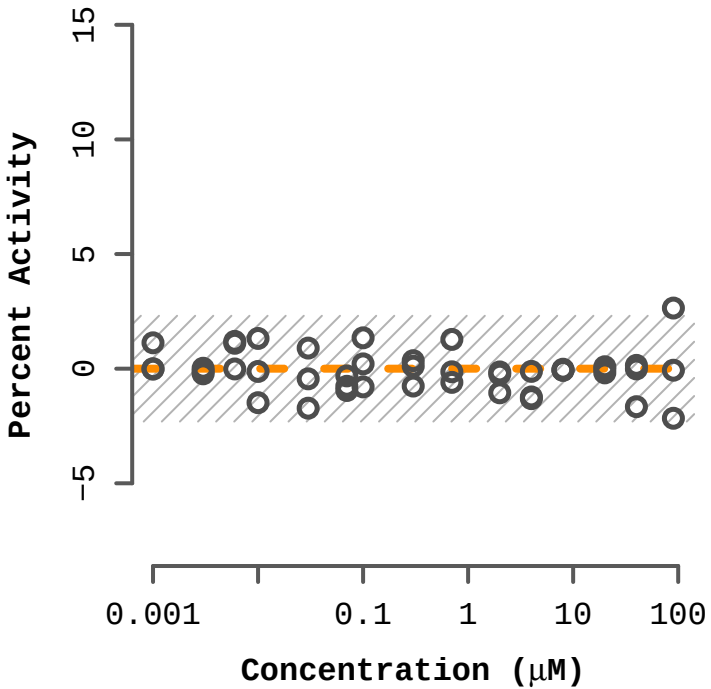
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.185 MAX_MED: 0.0112 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    alpha-Methyl-3,4-methylene-dioxyhydrocinnamic a
CHID:    43908   CASRN: 1205-17-0
SPID(S): Tox21_301642
M4ID:    12477491

HILL MODEL (in red):
      tp       ga       gw
val:  1.71     -0.97    0.612
sd:   0.353    0.621    0.418

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.3      0.401    0.448    1.47     0.495
sd:   10.9     3.68     0.398    2.99     0.809

      CNST        HILL        GNLS
AIC:  173.3       146.34      149.64
PROB: 0           0.84        0.16
RMSE: 1.55        1.13        1.11

MAX_MEAN: 2.46      MAX_MED: 2.6       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: beta-(3,4-Epoxycyclohexyl)ethyltrimethoxysilan

CHID: 43910 **CASRN:** 3388-04-3

SPID(S): Tox21_303998

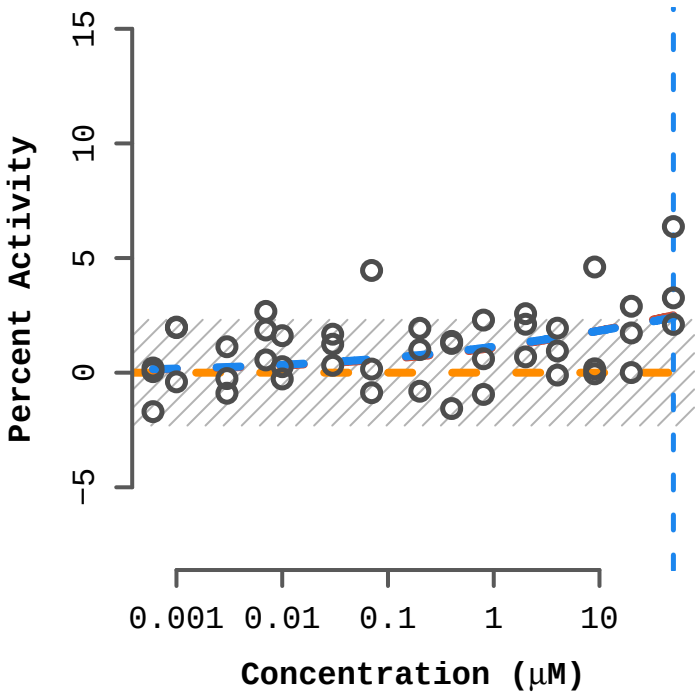
M4ID: 12475190

HILL MODEL: Not applicable.

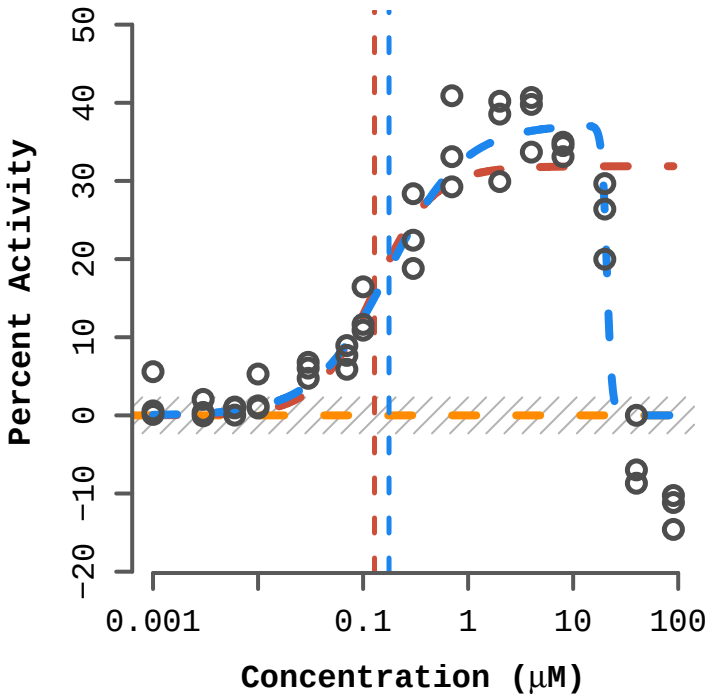
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.763 **MAX_MED:** 1.11 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Carbadox
CHID:    43913   CASRN: 6804-07-5
SPID(S): Tox21_111456_1
M4ID:    12483676

HILL MODEL (in red):
      tp       ga       gw
val:  6.04     2.2      0.3
sd:   22       8.71     0.31

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.8      1.7      0.3      3.66     18
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  188.67      172.62      176.66
PROB: 0           0.88        0.12
RMSE: 1.97        1.49        1.49

MAX_MEAN: 3.91      MAX_MED: 3.26      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydroxyprogesterone caproate
CHID: 43915 CASRN: 630-56-8
SPID(S): Tox21_302333
M4ID: 12476800

HILL MODEL (in red):

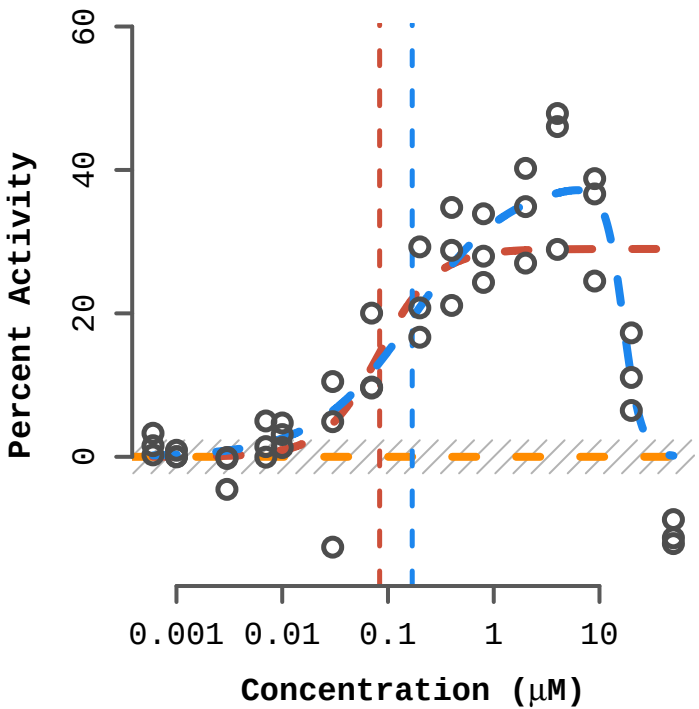
	tp	ga	gw
val:	31.9	−0.891	1.56
sd:	2.17	0.0952	0.426

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	37.2	−0.753	1.21	1.32	18
sd:	1.74	0.0731	0.196	0.0168	14.7

	CNST	HILL	GNLS
AIC:	408.15	354.86	275.14
PROB:	0	0	1
RMSE:	21.39	15.45	4.68

MAX_MEAN: 38.1 **MAX_MED:** 39.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydroxyprogesterone caproate
CHID: 43915 CASRN: 630-56-8
SPID(S): Tox21_113502_1
M4ID: 12482627

HILL MODEL (in red):

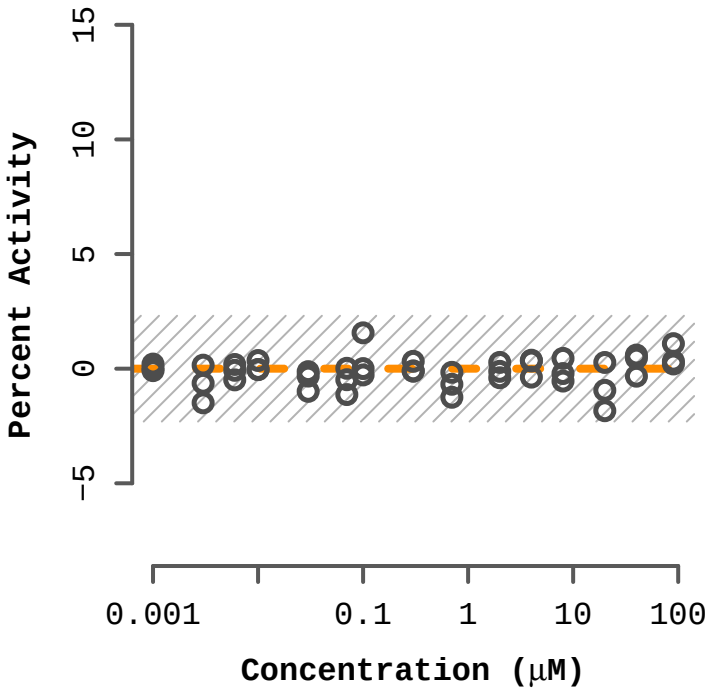
	tp	ga	gw
val:	29	-1.08	1.62
sd:	2.77	0.147	0.691

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	38.7	-0.771	0.936	1.22	5.06
sd:	6.73	0.245	0.267	0.0998	4.36

	CNST	HILL	GNLS
AIC:	407.75	349.7	302.04
PROB:	0	0	1
RMSE:	21.41	12.83	6.15

MAX_MEAN: 40.9 MAX_MED: 46 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

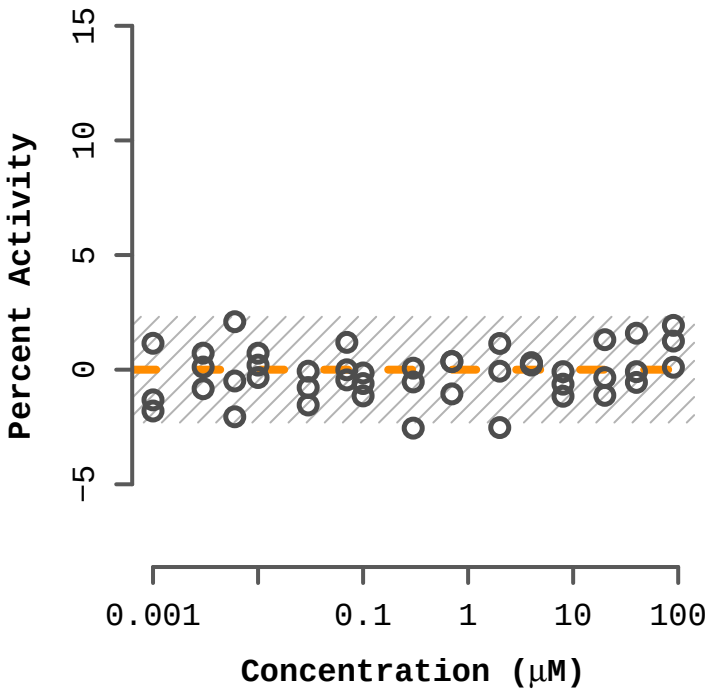
NAME: D−Ribose
CHID: 43917 CASRN: 50−69−1
SPID(S): Tox21_303971
M4ID: 12475217

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	84.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.63	NA	NA

MAX_MEAN: 0.542 **MAX_MED:** 0.462 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

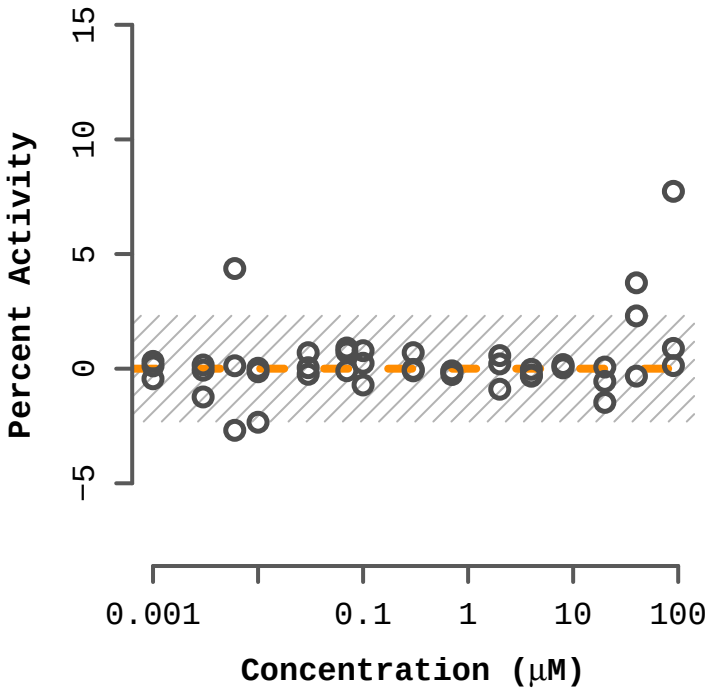
NAME: Erythritol
CHID: 43919 **CASRN:** 149-32-6
SPID(S): Tox21_200564
M4ID: 12481688

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

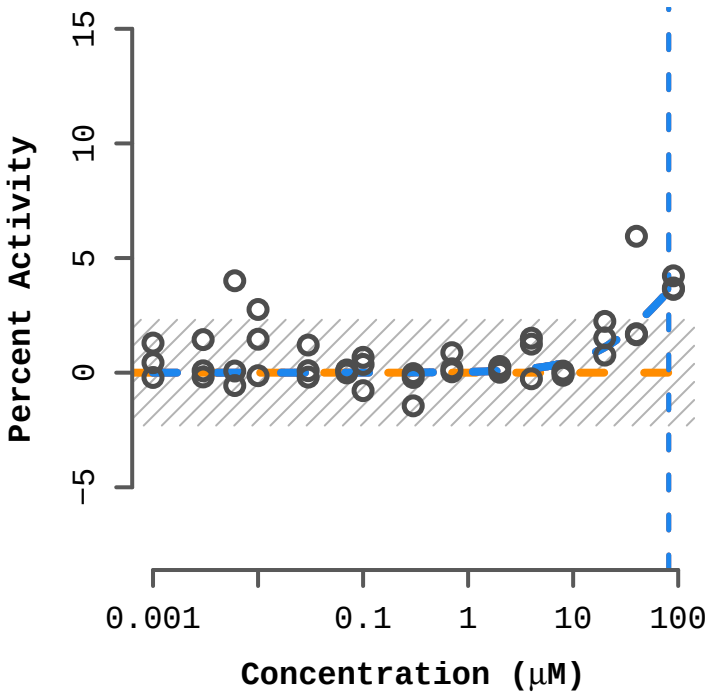
NAME: Dimethyl sulfone
CHID: 43937 CASRN: 67-71-0
SPID(S): Tox21_303712
M4ID: 12475476

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 2.92 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Monobenzyl phthalate
CHID: 43938 CASRN: 2528-16-7
SPID(S): Tox21_300626
M4ID: 12478507

HILL MODEL (in red):

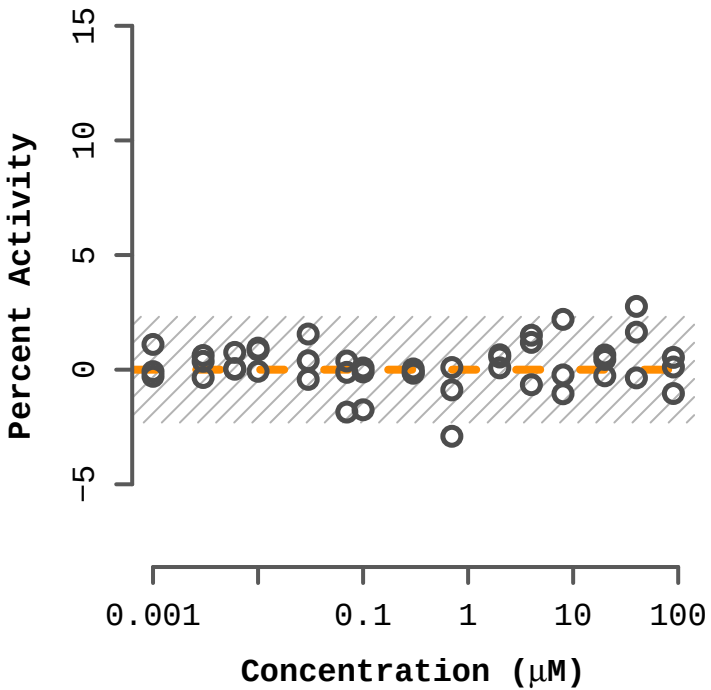
	tp	ga	gw
val:	7.14	1.91	1.21
sd:	6.01	0.614	0.56

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.14	1.91	1.21	3.9	3.72
sd:	5.97	0.61	0.558	1140	2230

	CNST	HILL	GNLS
AIC:	167.51	128.5	132.5
PROB:	0	0.88	0.12
RMSE:	1.72	1.12	1.12

MAX_MEAN: 3.85 **MAX_MED:** 3.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

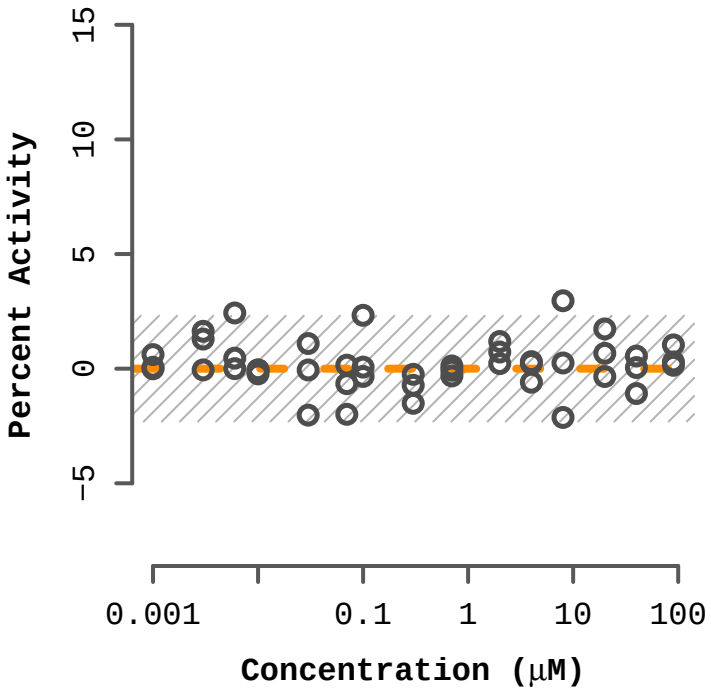
NAME: N-Formylpiperidine
CHID: 43941 **CASRN:** 2591-86-8
SPID(S): Tox21_302107
M4ID: 12477026

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

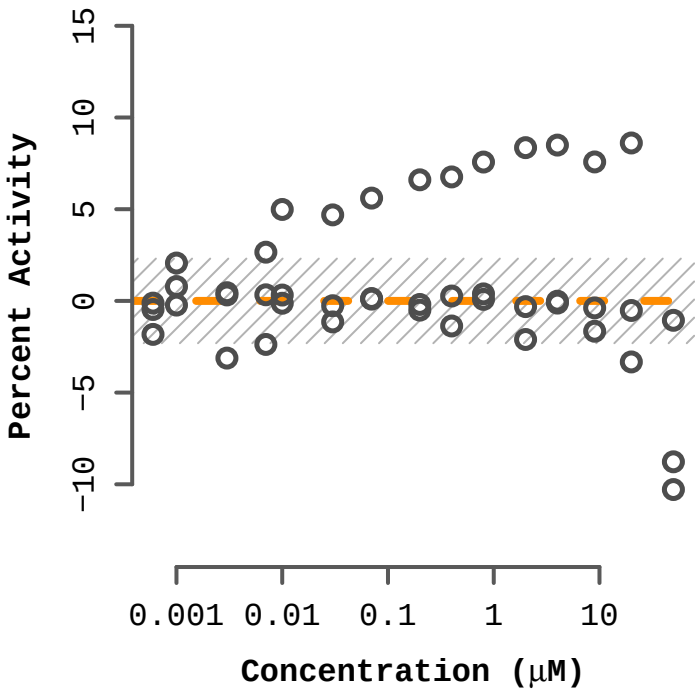
NAME: Tiron
CHID: 43950 **CASRN:** 149-45-1
SPID(S): Tox21_302148
M4ID: 12476985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.965 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

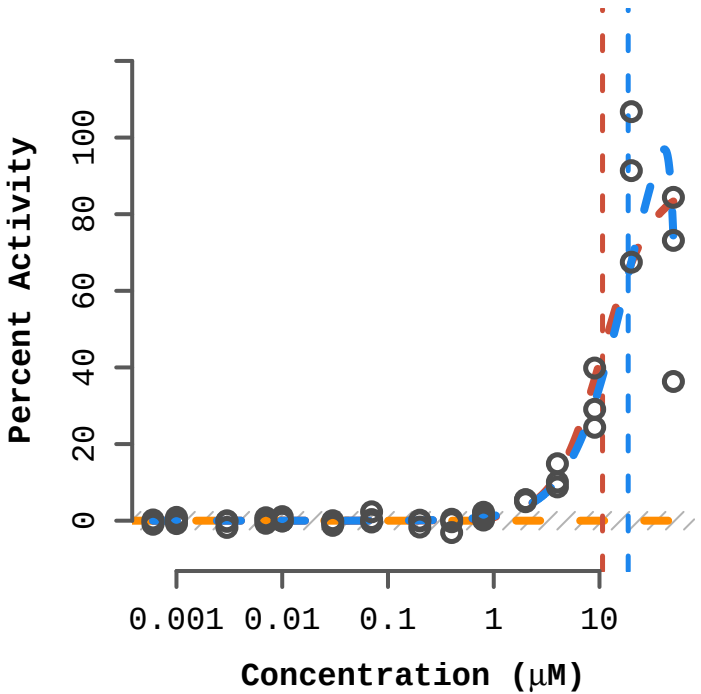
NAME: Metitepine
CHID: 44000 **CASRN:** 20229-30-5
SPID(S): Tox21_110916_1
M4ID: 12484017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	250.71	NA	NA
PROB:	1	NA	NA
RMSE:	4.05	NA	NA

MAX_MEAN: 2.79 **MAX_MED:** 0.784 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluvoxamine
CHID: 44002 **CASRN:** 54739-18-3
SPID(S): Tox21_110837_1
M4ID: 12484081

HILL MODEL (in red):

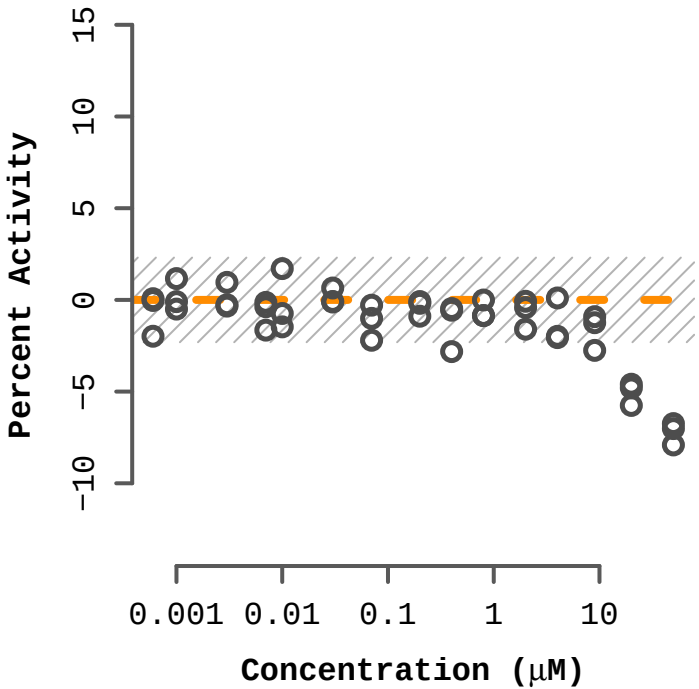
	tp	ga	gw
val:	87.8	1.03	1.89
sd:	3.31	0.0361	0.157

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	128	1.27	1.57	1.72	14.5
sd:	15.9	0.0724	0.119	0.00613	4.3

	CNST	HILL	GNLS
AIC:	401.4	273.33	267.96
PROB:	0	0.06	0.94
RMSE:	30.42	10.27	9.22

MAX_MEAN: 88.5 **MAX_MED:** 91.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

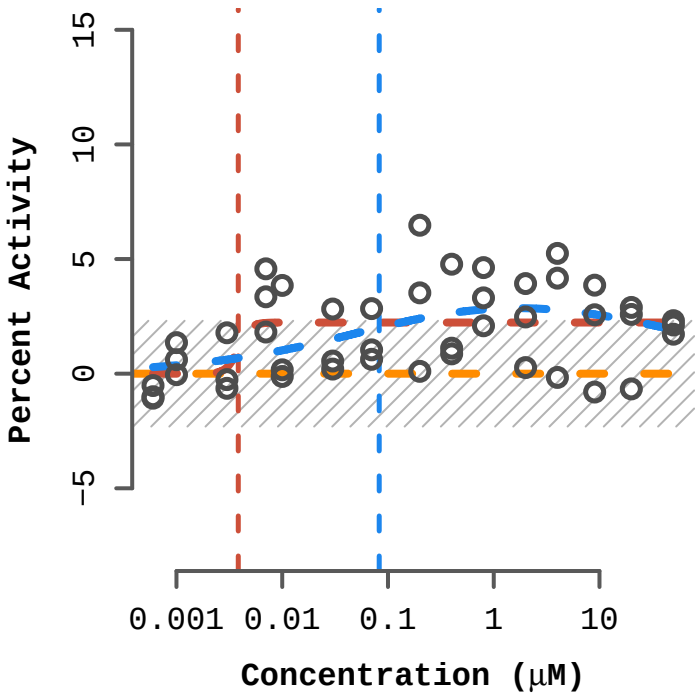
NAME: Enzastaurin
CHID: 44029 **CASRN:** 170364-57-5
SPID(S): Tox21_113367_1
M4ID: 12482671

HILL MODEL: Not applicable.

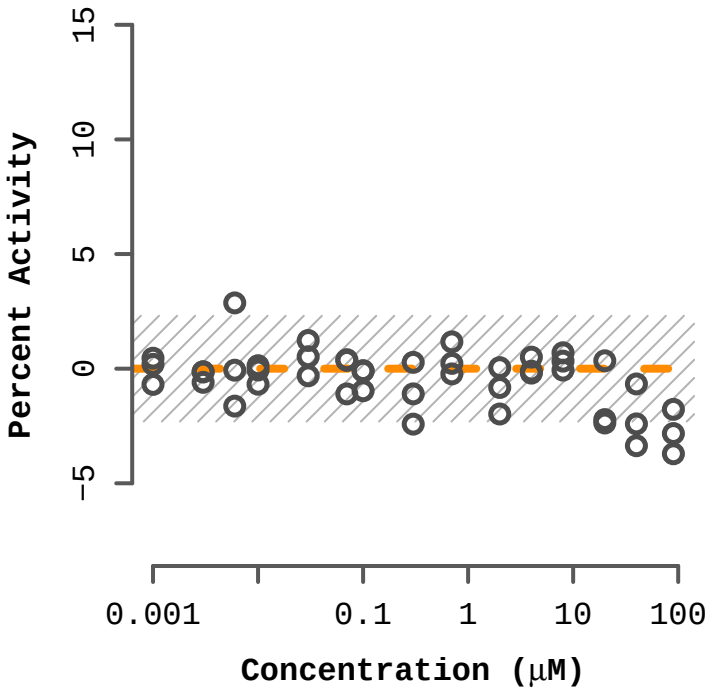
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200	NA	NA
PROB:	1	NA	NA
RMSE:	2.53	NA	NA

MAX_MEAN: 0.191 **MAX_MED:** −0.0305 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ibufenac
CHID:    44107   CASRN: 1553-60-2
SPID(S): Tox21_111821_1
M4ID:    12483458

HILL MODEL (in red):
      tp       ga       gw
val:  2.23     -2.42    8
sd:   0.311    0.172    9.44

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.26     -1.08    0.534    1.57     0.46
sd:   14.9     4.44     0.555    6.08     1.79

      CNST        HILL        GNLS
AIC:  219.24      186.57      191.22
PROB: 0           0.91        0.09
RMSE: 2.62        1.68        1.71

MAX_MEAN: 3.37      MAX_MED: 4.17      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

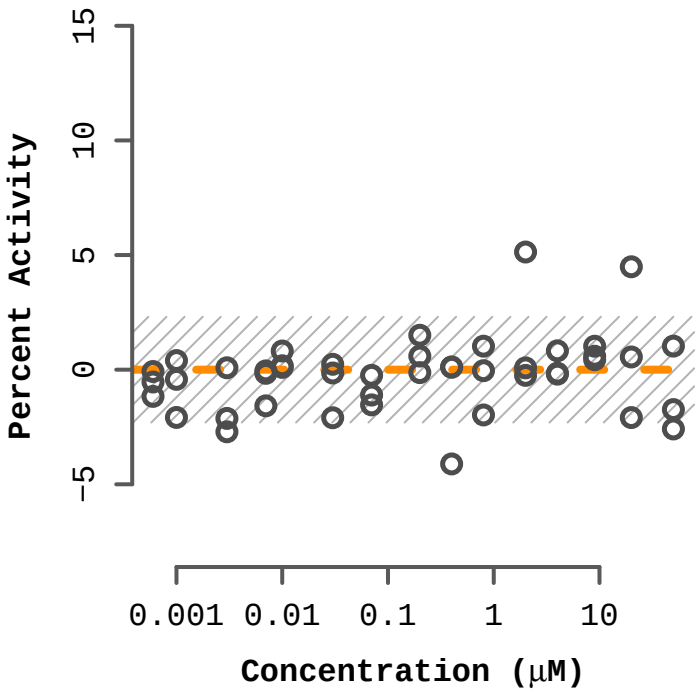
NAME: Oxfendazole
CHID: 44112 **CASRN:** 53716-50-0
SPID(S): Tox21_302383
M4ID: 12476750

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

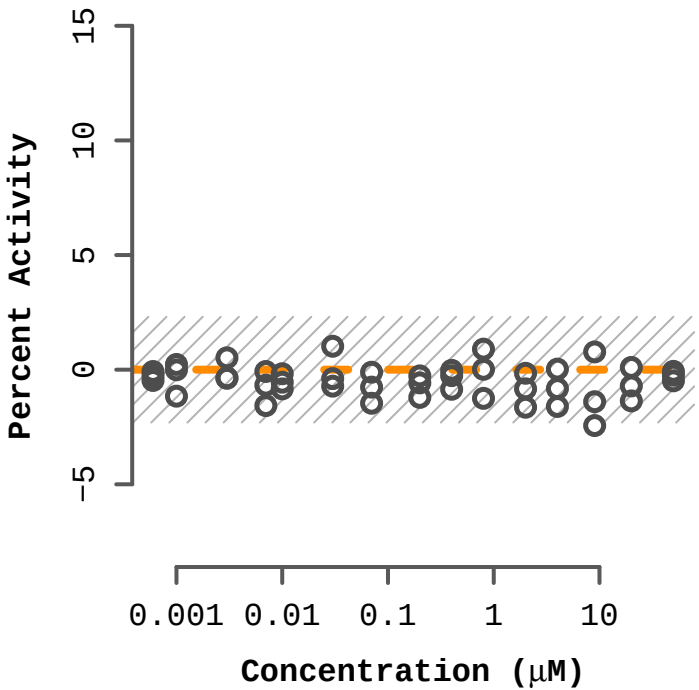
NAME: Oxfendazole
CHID: 44112 **CASRN:** 53716-50-0
SPID(S): Tox21_113444_1
M4ID: 12482651

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 0.595 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

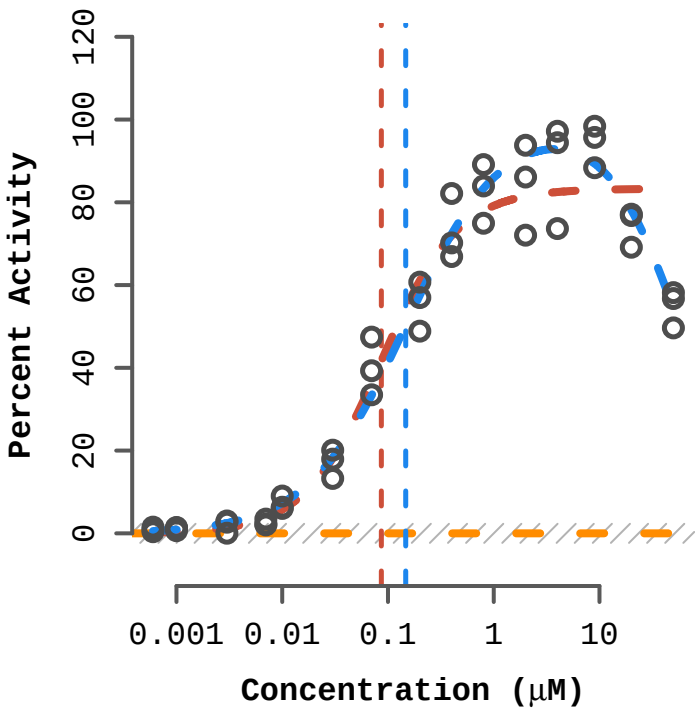
NAME: Rolipram
CHID: 44124 CASRN: 61413-54-5
SPID(S): Tox21_110672_1
M4ID: 12484188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: −0.028 **MAX_MED:** 0.0163 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Stanozolol
CHID: 44128 **CASRN:** 10418-03-8
SPID(S): Tox21_113993
M4ID: 12482253

HILL MODEL (in red):

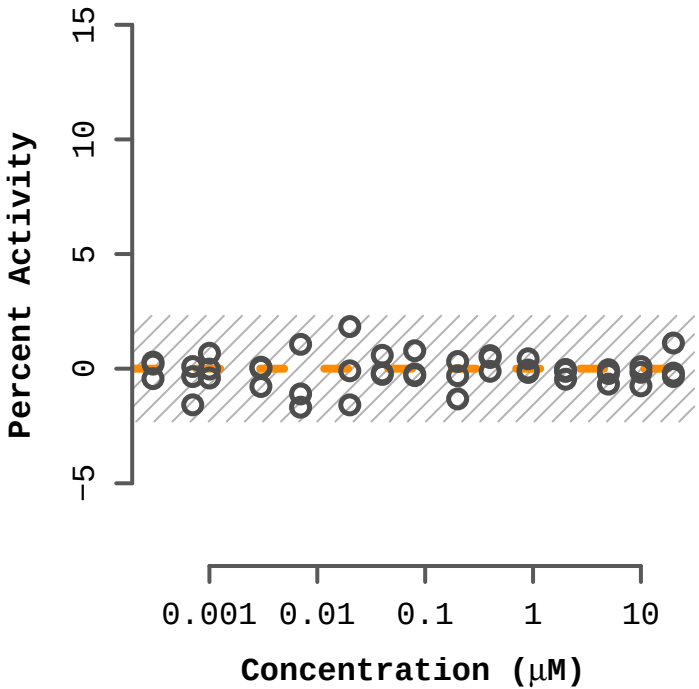
	tp	ga	gw
val:	83.3	-1.06	1.21
sd:	3.5	0.0664	0.142

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	101	-0.832	0.946	1.76	1.22
sd:	5.39	0.0746	0.0773	0.0513	0.242

	CNST	HILL	GNLS
AIC:	500.23	335.81	293.01
PROB:	0	0	1
RMSE:	57.67	10.02	6.08

MAX_MEAN: 94.2 **MAX_MED:** 95.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

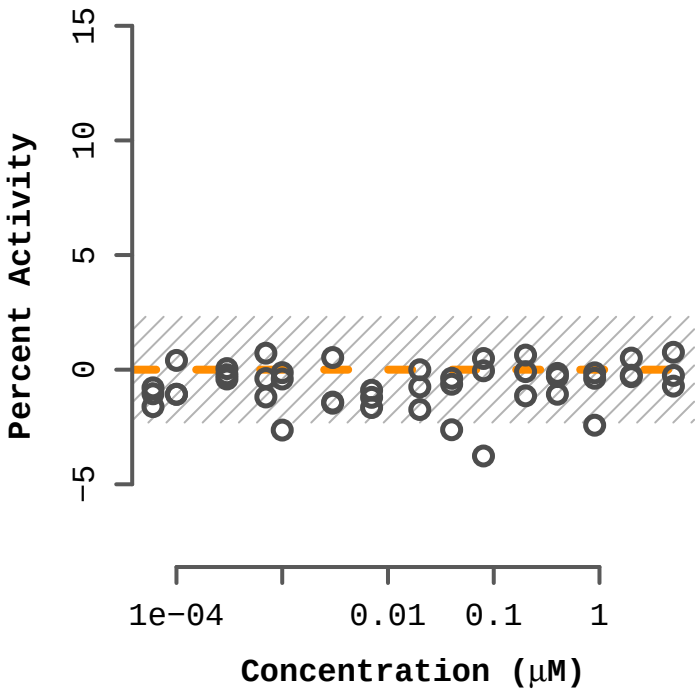
NAME: Sulfaphenazole
CHID: 44131 **CASRN:** 526-08-9
SPID(S): Tox21_110262_1
M4ID: 12484503

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.316 **MAX_MED:** 0.489 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

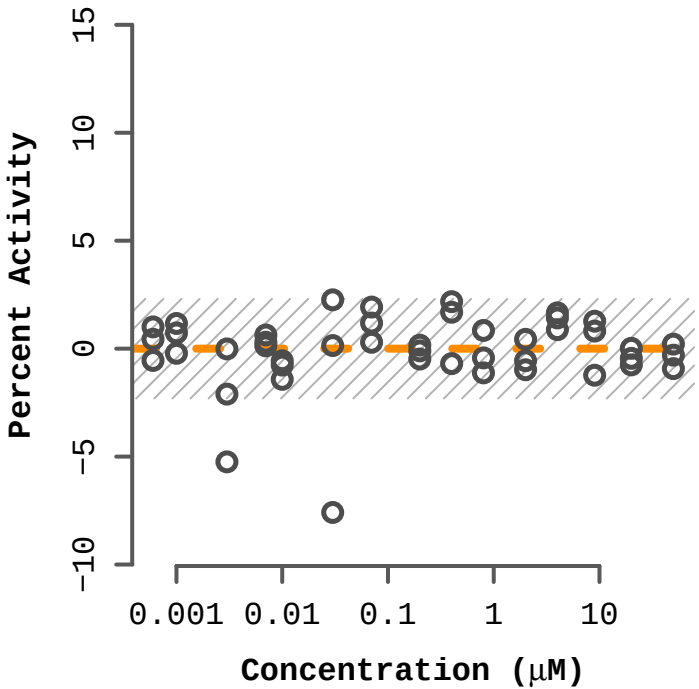
NAME: Temafloxacin
CHID: 44132 **CASRN:** 108319-06-8
SPID(S): Tox21_113306
M4ID: 12482720

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: −0.0129 **MAX_MED:** −0.0475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

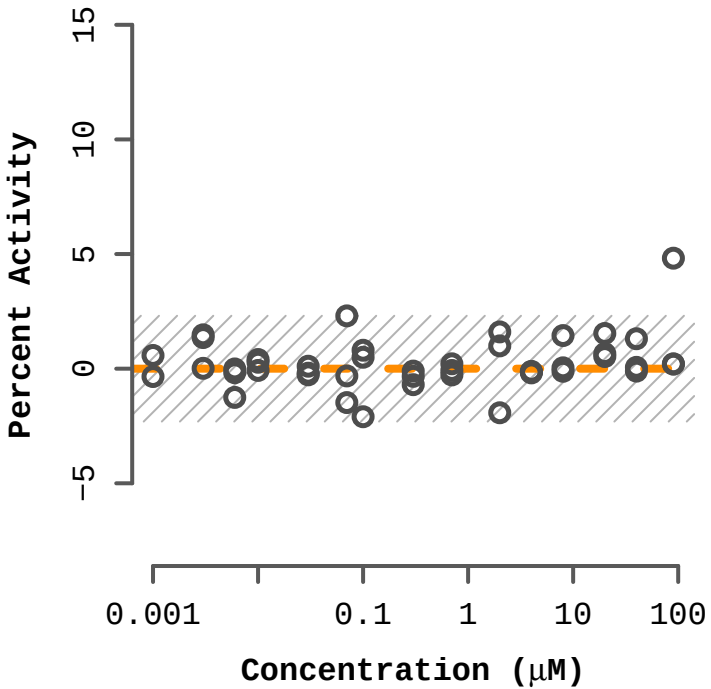
NAME: Tropisetron
CHID: 44137 **CASRN:** 89565-68-4
SPID(S): Tox21_110272_1
M4ID: 12484495

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

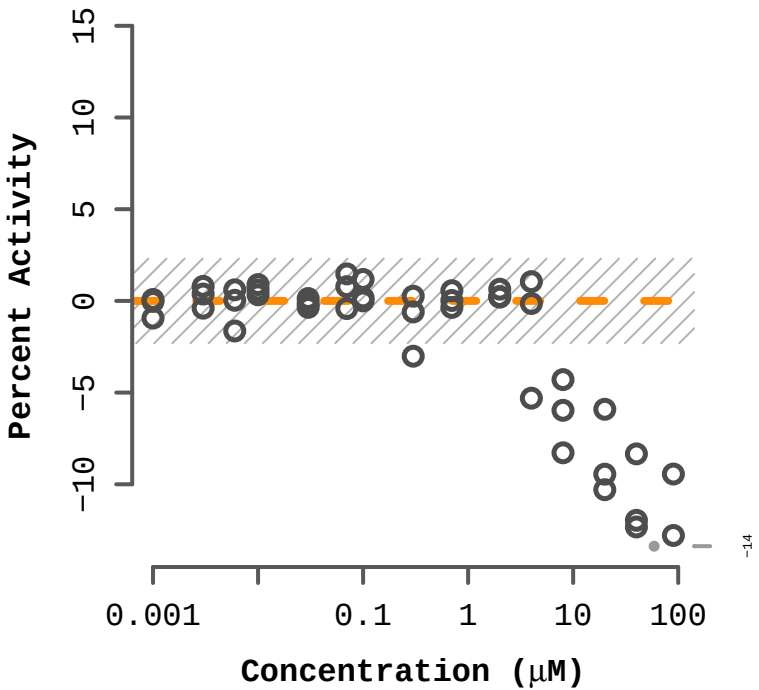
NAME: 3,3'−Oxydipropionitrile
CHID: 44154 **CASRN:** 1656−48−0
SPID(S): Tox21_303726
M4ID: 12475462

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

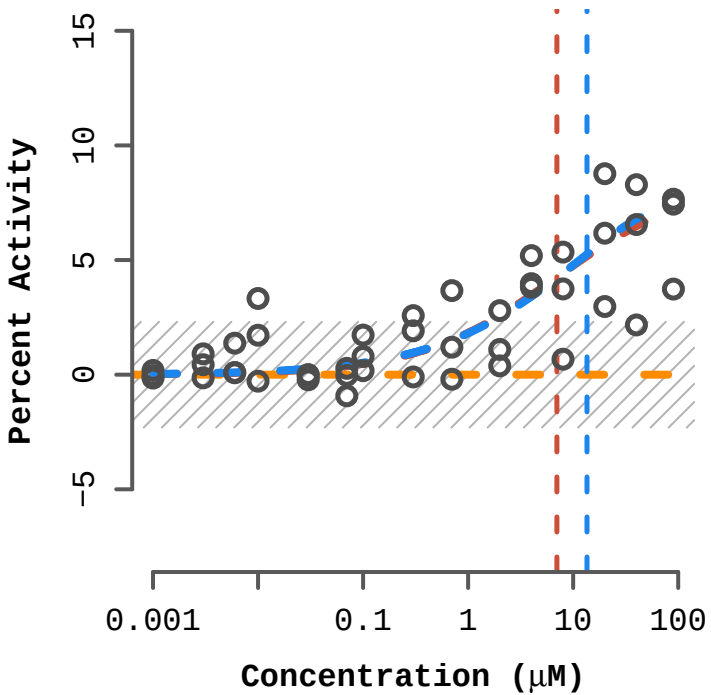
NAME: Antimony trichloride
CHID: 44161 CASRN: 10025-91-9
SPID(S): Tox21_300641
M4ID: 12478492 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	268.03	NA	NA
PROB:	1	NA	NA
RMSE:	5.2	NA	NA

MAX_MEAN: 0.612 MAX_MED: 0.778 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Pentylphenol
CHID: 44164 CASRN: 14938-35-3
SPID(S): Tox21_303837
M4ID: 12475351

HILL MODEL (in red):

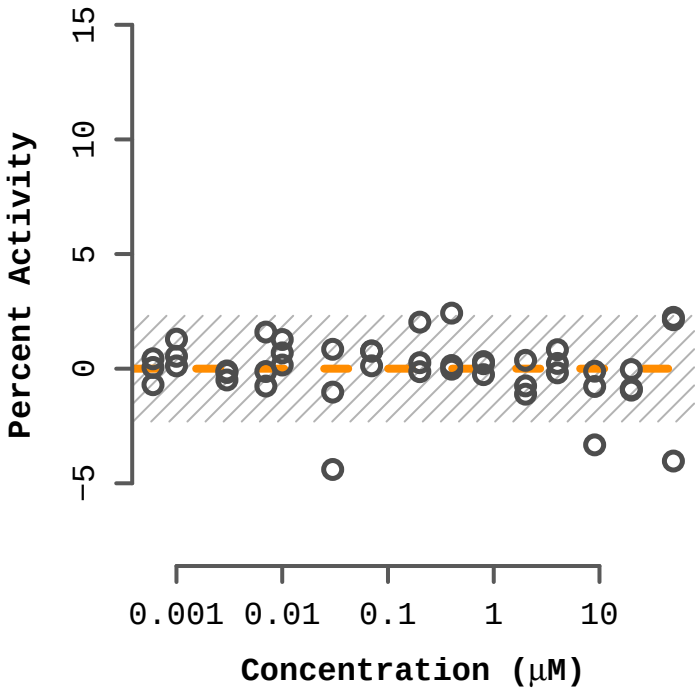
	tp	ga	gw
val:	8.5	0.845	0.666
sd:	2.15	0.437	0.254

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.13	0.603	2.31	2.4
sd:	8.49	1.11	0.259	1.49	12.5

	CNST	HILL	GNLS
AIC:	236.79	172.33	175.99
PROB:	0	0.86	0.14
RMSE:	3.41	1.56	1.56

MAX_MEAN: 6.28 MAX_MED: 7.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

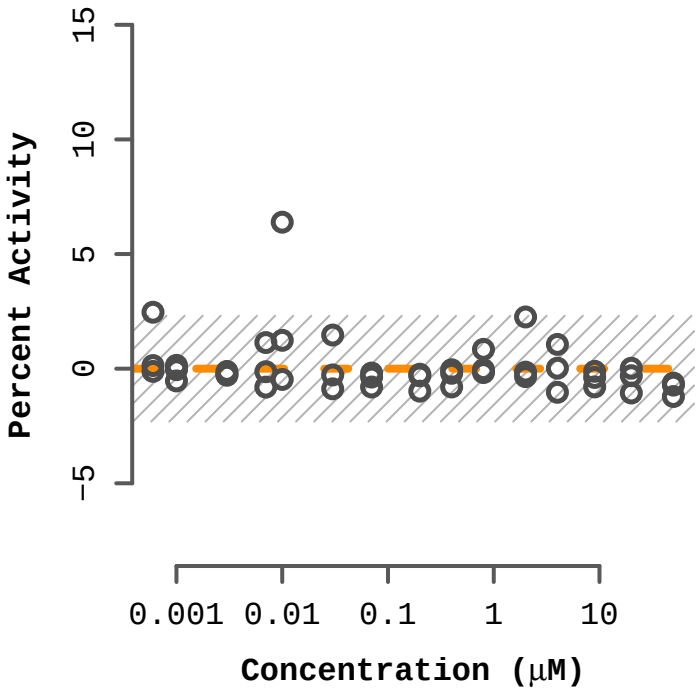
NAME: Clove leaf oil
CHID: 44175 CASRN: 8000-34-8
SPID(S): Tox21_302538
M4ID: 12476595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.847 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

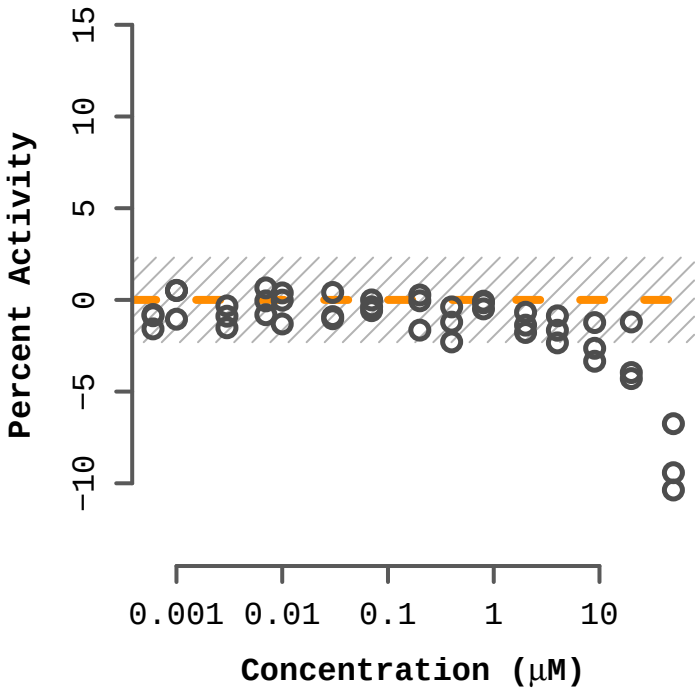
NAME: Nutmeg oil
CHID: 44177 **CASRN:** 8008-45-5
SPID(S): Tox21_302654
M4ID: 12476479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 2.39 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

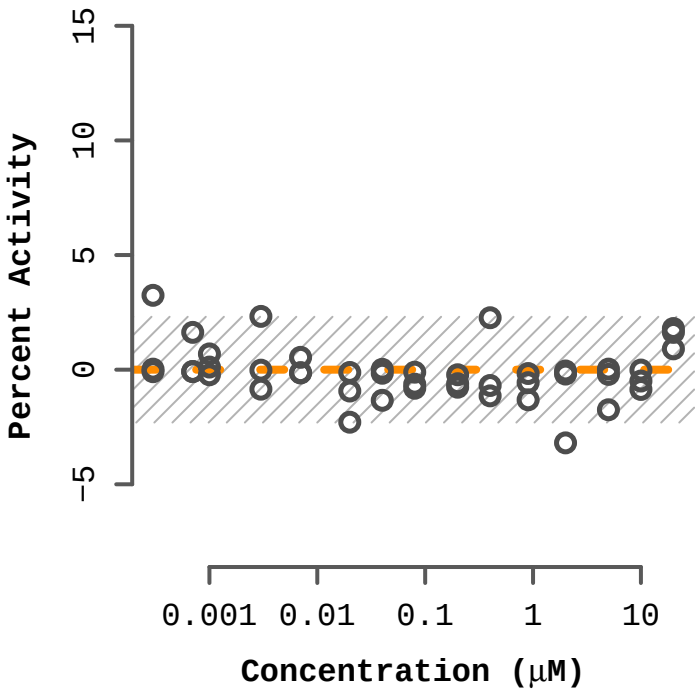
NAME: Desloratadine
CHID: 44196 **CASRN:** 100643-71-8
SPID(S): Tox21_111574_1
M4ID: 12483610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.21	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: −0.0054 **MAX_MED:** 0.511 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

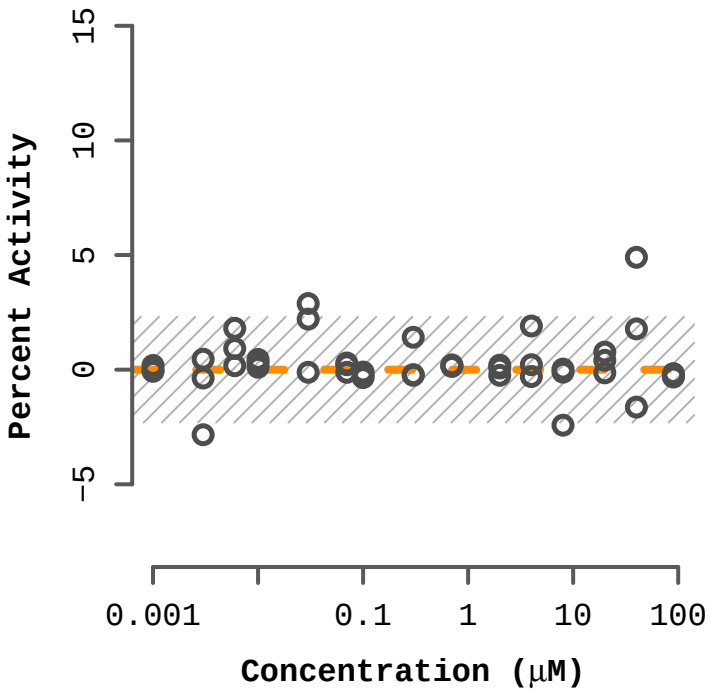
NAME: Perindopril erbumine
CHID: 44198 CASRN: 107133-36-8
SPID(S): Tox21_303915
M4ID: 12475273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

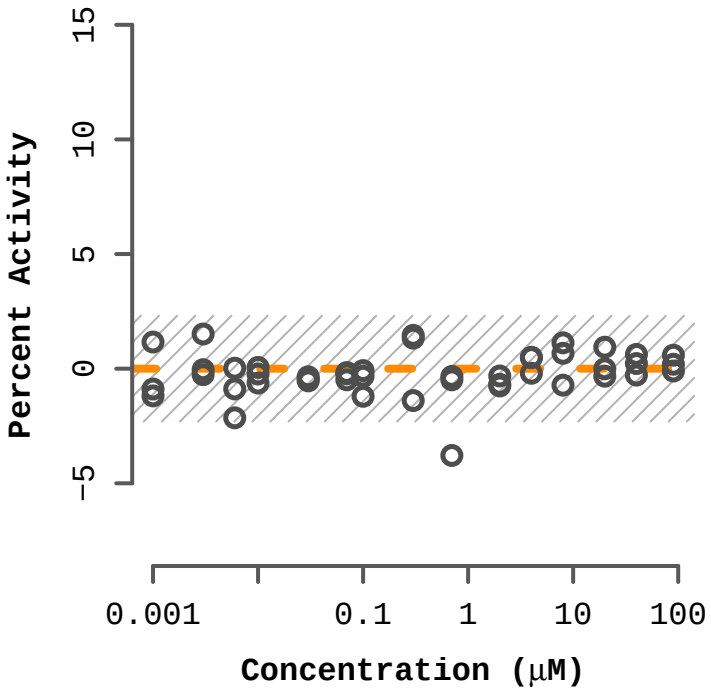
NAME: 2-Methyl-4,6-bis[(octylthio)methyl]phenol
CHID: 44199 **CASRN:** 110553-27-0
SPID(S): Tox21_304010
M4ID: 12475178

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

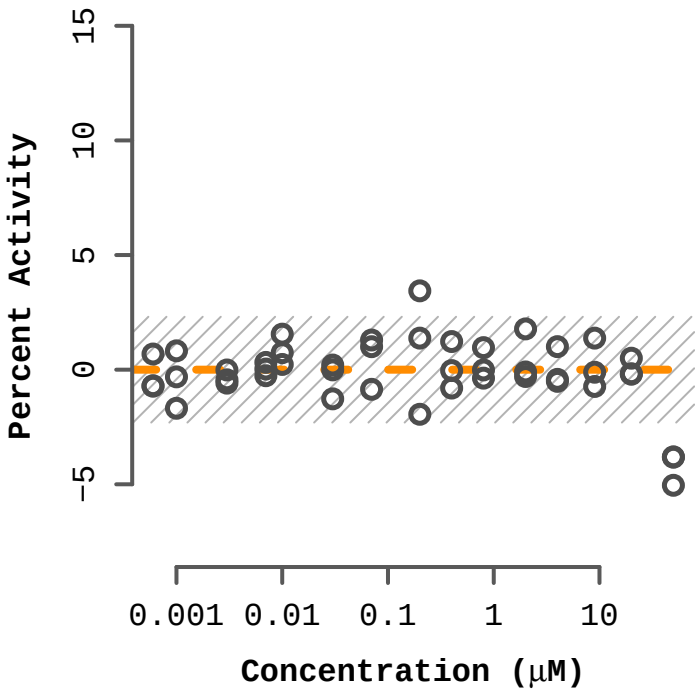
NAME: Bis(2-carboxyethyl) sulfide
CHID: 44200 **CASRN:** 111-17-1
SPID(S): Tox21_300987
M4ID: 12478146

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.466 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

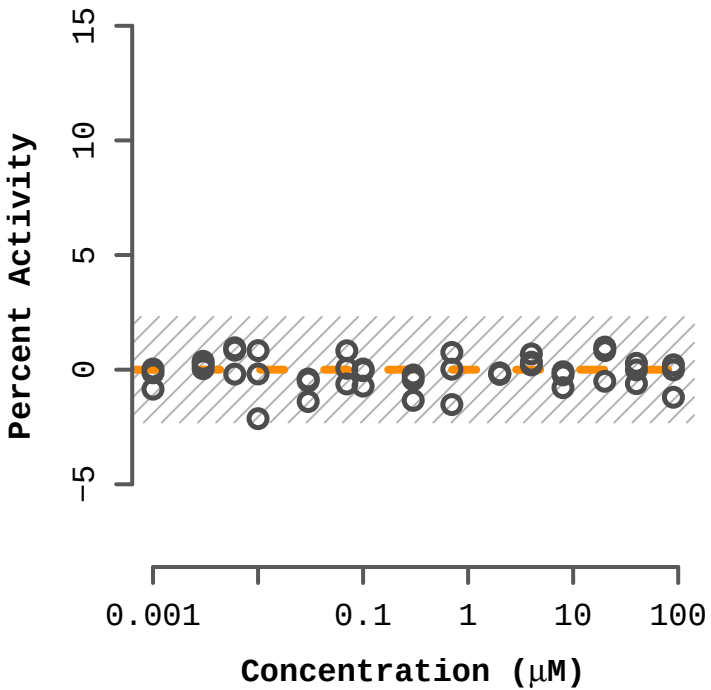
NAME: Quetiapine fumarate
CHID: 44201 CASRN: 111974-72-2
SPID(S): Tox21_302366
M4ID: 12476767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.958 MAX_MED: 1.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

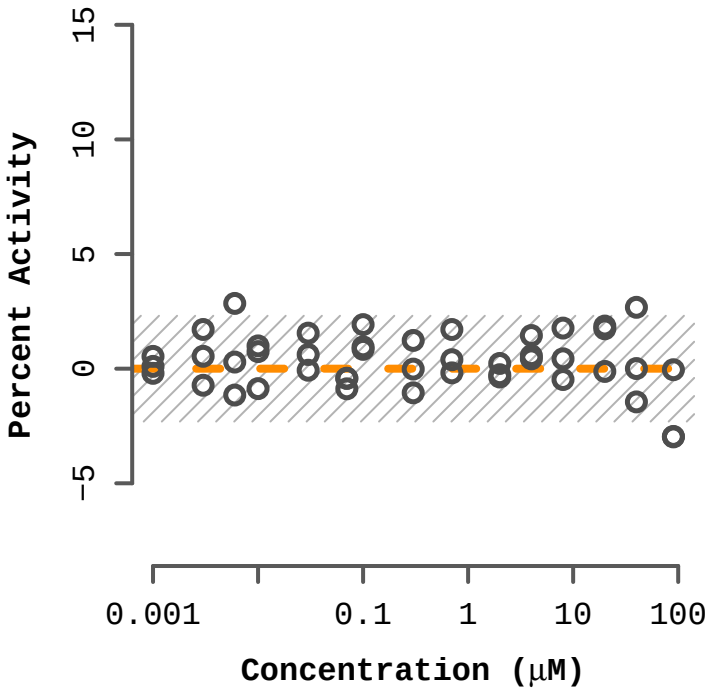
NAME: Octyl acetate
CHID: 44202 CASRN: 112-14-1
SPID(S): Tox21_302296
M4ID: 12476837

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 0.539 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

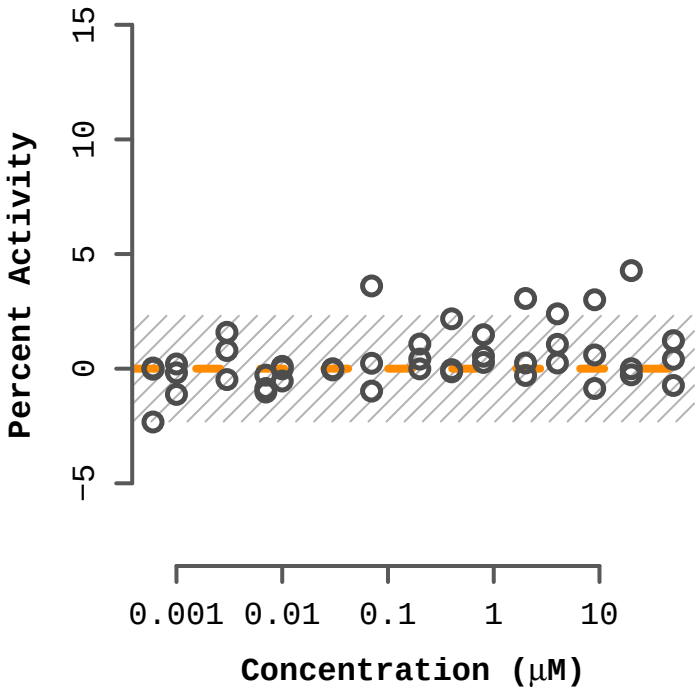
NAME: Pioglitazone hydrochloride
CHID: 44203 CASRN: 112529-15-4
SPID(S): Tox21_300584
M4ID: 12478549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

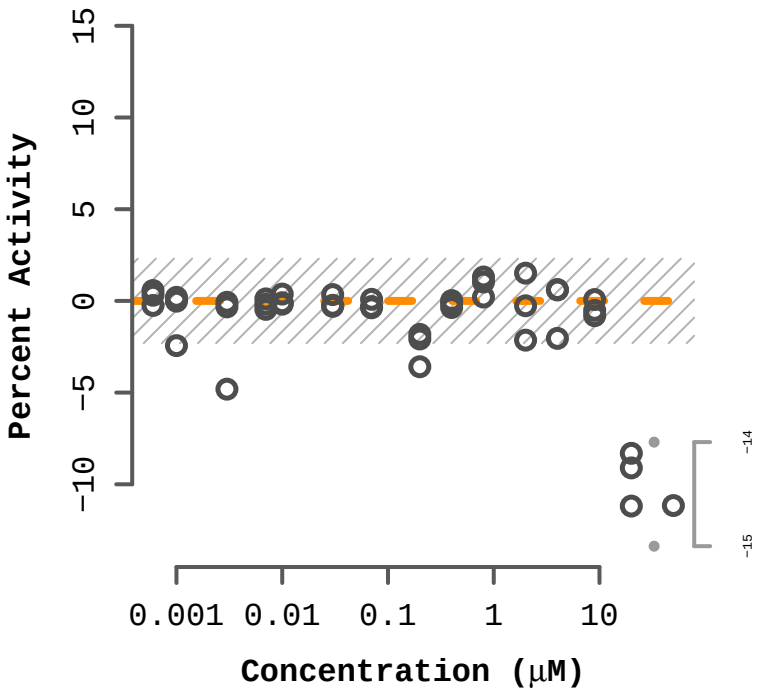
NAME: Pioglitazone hydrochloride
CHID: 44203 CASRN: 112529-15-4
SPID(S): Tox21_111440_1
M4ID: 12483685

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

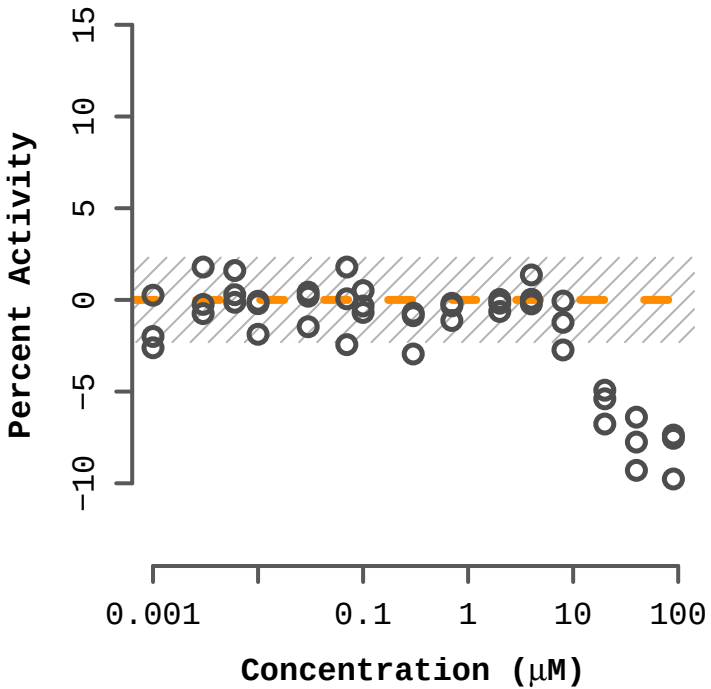
NAME: Mibefradil dihydrochloride
CHID: 44204 **CASRN:** 116666-63-8
SPID(S): Tox21_111244_1
M4ID: 12483819 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.81	NA	NA
PROB:	1	NA	NA
RMSE:	4.4	NA	NA

MAX_MEAN: 0.85 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

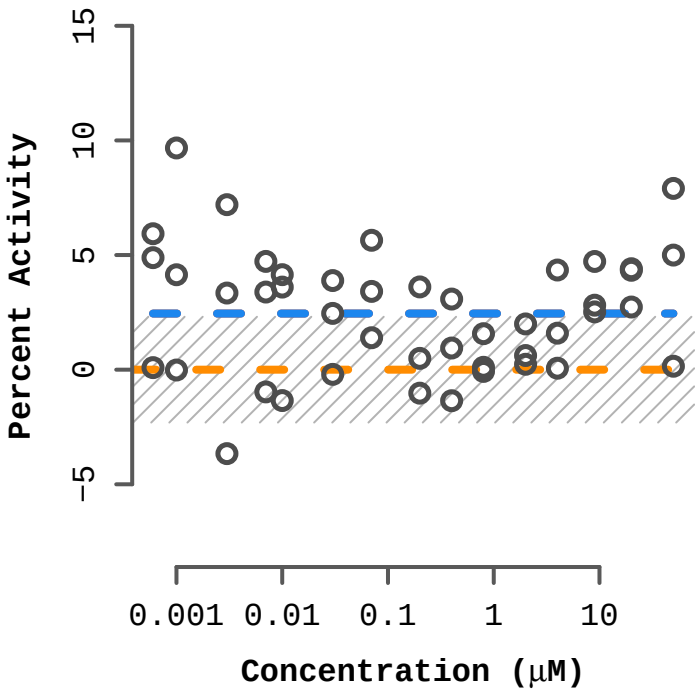
NAME: Rabeprazole sodium
CHID: 44205 **CASRN:** 117976-90-6
SPID(S): Tox21_302317
M4ID: 12476816

HILL MODEL: Not applicable.

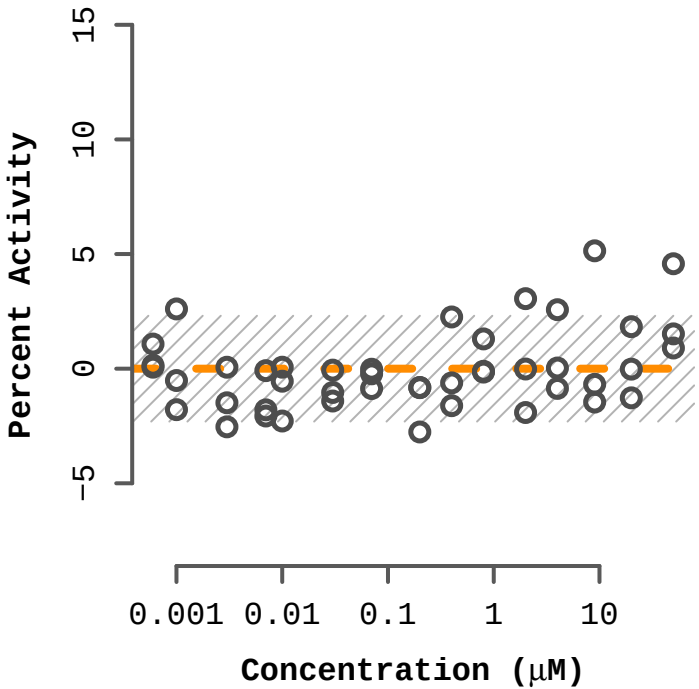
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.43	NA	NA
PROB:	1	NA	NA
RMSE:	3.49	NA	NA

MAX_MEAN: 0.586 **MAX_MED:** 0.285 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Rabeprazole sodium
CHID:    44205   CASRN: 117976-90-6
SPID(S): Tox21_111736_1
M4ID:    12483512

HILL MODEL (in red):
      tp       ga       gw
val:  2.45     -5.22    3.79
sd:   0.409    1750     3290

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.45     -5.21    3.76     3.46     17.6
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  249.57      227.09      231.09
PROB: 0           0.88        0.12
RMSE: 3.66        2.68        2.68

MAX_MEAN: 4.6       MAX_MED: 5         BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

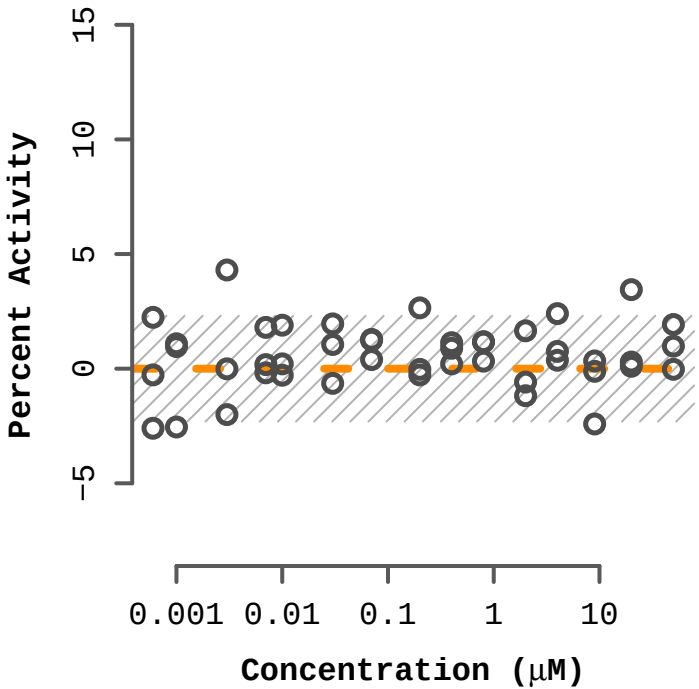
NAME: Bromfenac sodium sesquihydrate
CHID: 44206 CASRN: 120638-55-3
SPID(S): Tox21_112181_1
M4ID: 12483255

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 2.33 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

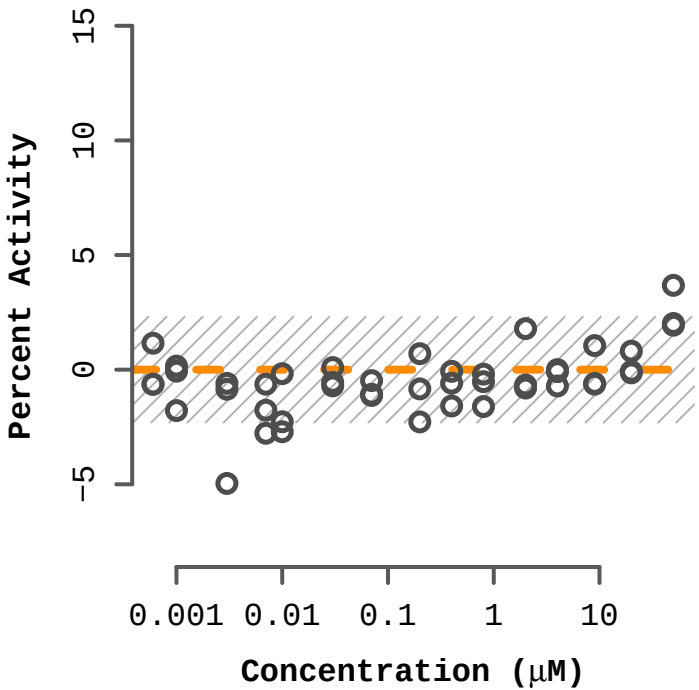
NAME: Alosetron hydrochloride
CHID: 44208 **CASRN:** 122852-69-1
SPID(S): Tox21_112525_1
M4ID: 12483048

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

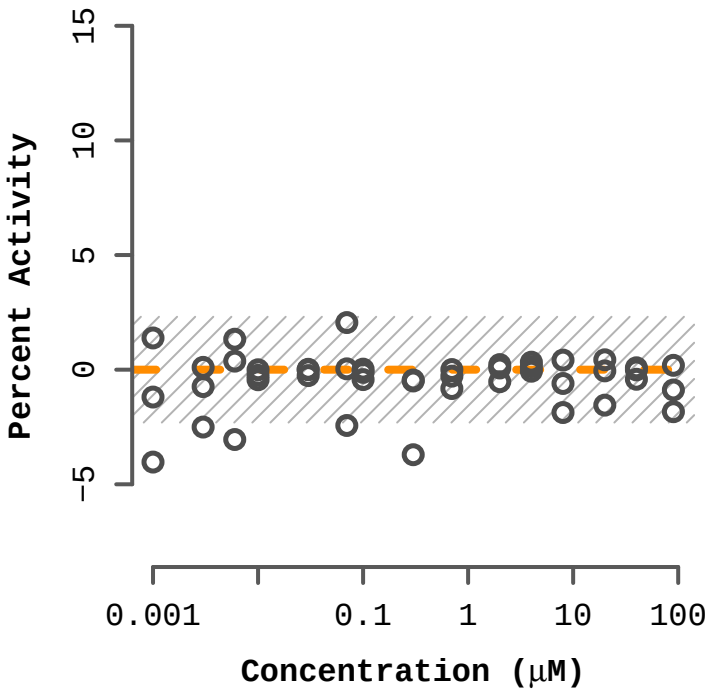
NAME: Valacyclovir hydrochloride
CHID: 44210 CASRN: 124832-27-5
SPID(S): Tox21_111738_1
M4ID: 12483510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.55 **MAX_MED:** 2.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

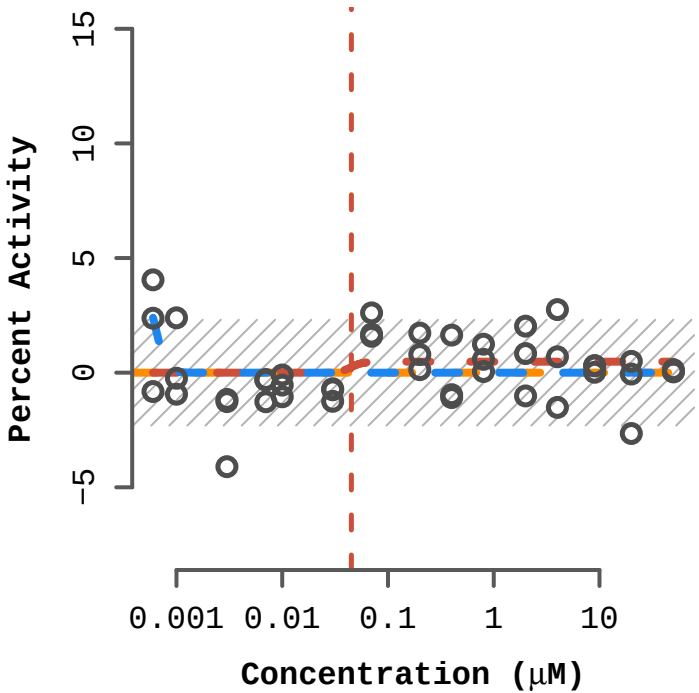
NAME: Pantoprazole sodium
CHID: 44215 **CASRN:** 138786-67-1
SPID(S): Tox21_302362
M4ID: 12476771

HILL MODEL: Not applicable.

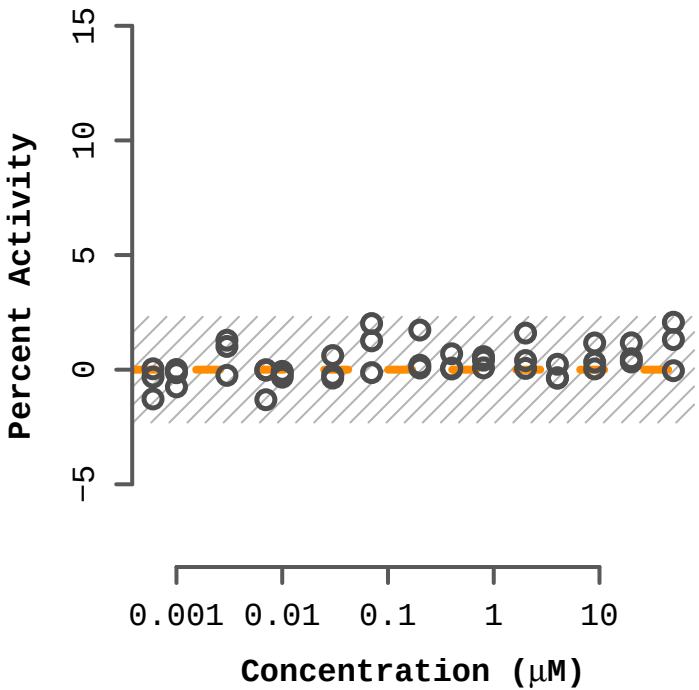
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.133 **MAX_MED:** 0.374 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Eprosartan mesylate
CHID:    44217   CASRN: 144143-96-4
SPID(S): Tox21_112186_1
M4ID:    12483251

HILL MODEL (in red):
      tp       ga       gw
val:  0.479    -1.35    8
sd:   0.248    0.199    8.73

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.58     -4.88    0.317    -3.19    9.6
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  165.42      167.77      171.62
PROB: 0.74        0.23        0.03
RMSE: 1.5         1.46        1.42

MAX_MEAN: 1.96      MAX_MED: 2.38      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

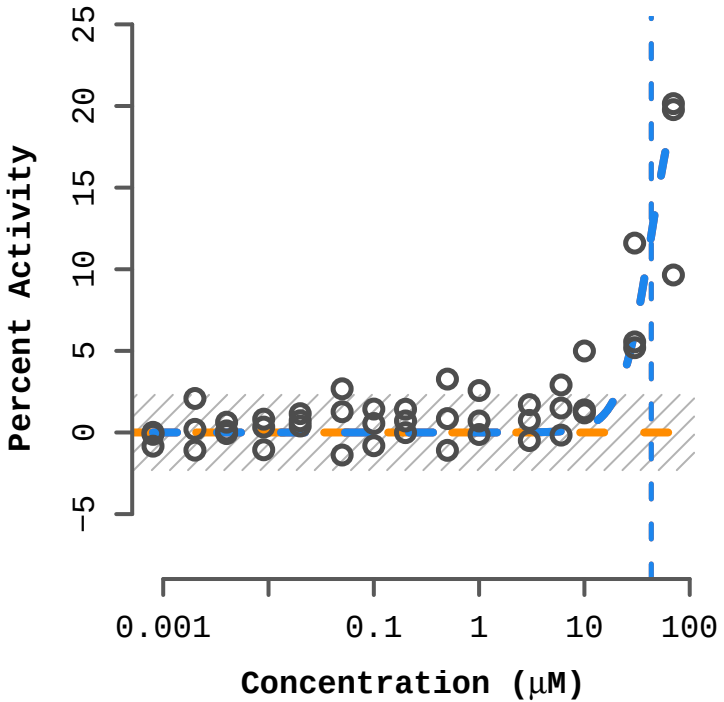
NAME: Tiagabine hydrochloride
CHID: 44218 CASRN: 145821-59-6
SPID(S): Tox21_112245_1
M4ID: 12483206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indinavir sulfate
CHID: 44221 CASRN: 157810-81-6
SPID(S): Tox21_302415
M4ID: 12476718

HILL MODEL (in red):

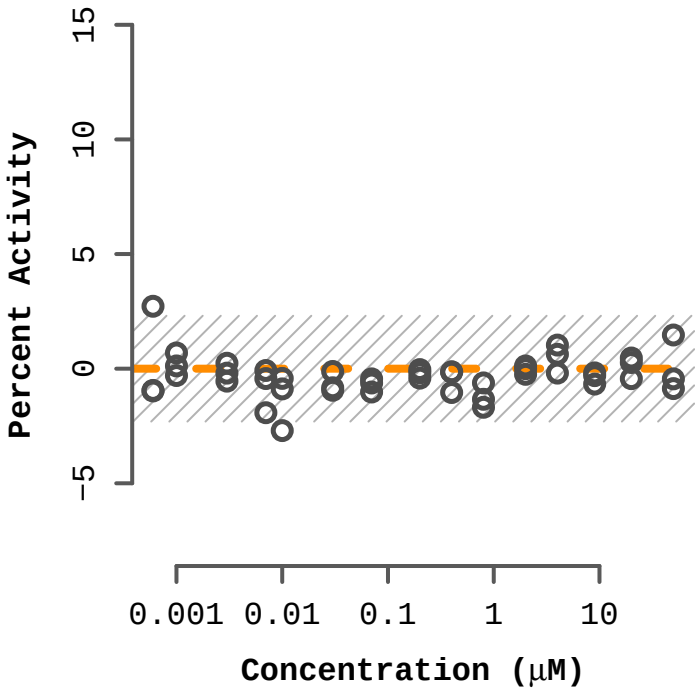
	tp	ga	gw
val:	24.2	1.64	2.93
sd:	10.6	0.18	2.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.2	1.64	2.93	3.14	6.7
sd:	10.4	0.177	2.2	1810	9360

	CNST	HILL	GNLS
AIC:	238.51	185.51	189.51
PROB:	0	0.88	0.12
RMSE:	5.1	2.17	2.17

MAX_MEAN: 16.5 **MAX_MED:** 19.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

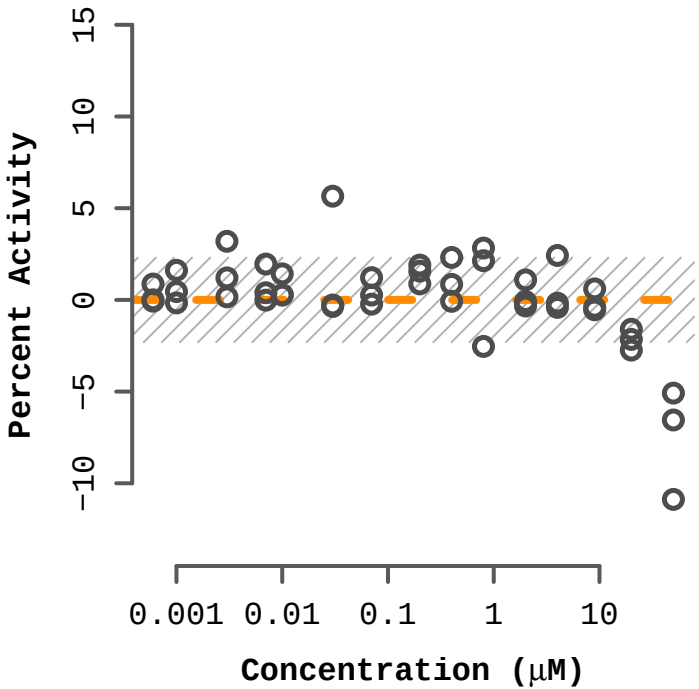
NAME: Indinavir sulfate
CHID: 44221 CASRN: 157810-81-6
SPID(S): Tox21_111687_1
M4ID: 12483534

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.489 **MAX_MED:** 0.629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

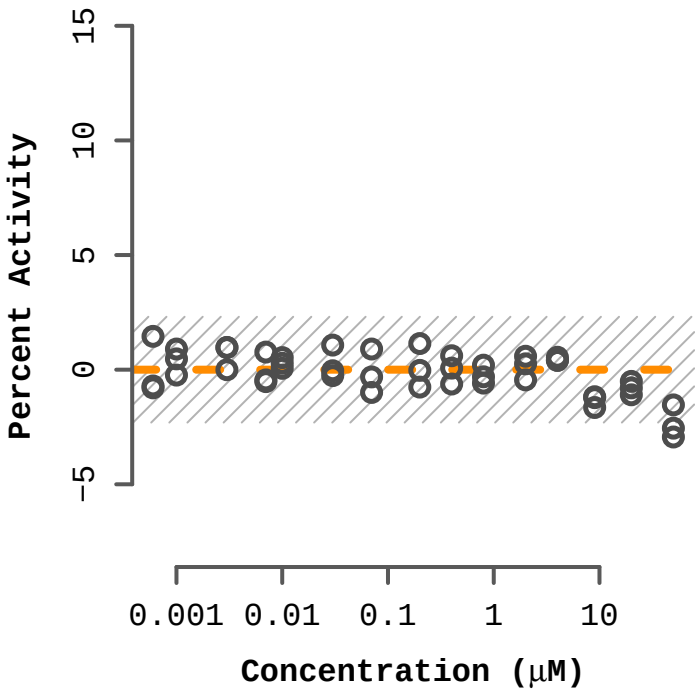
NAME: Ezetimibe
CHID: 44223 CASRN: 163222-33-1
SPID(S): Tox21_111443_1
M4ID: 12483682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.57	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

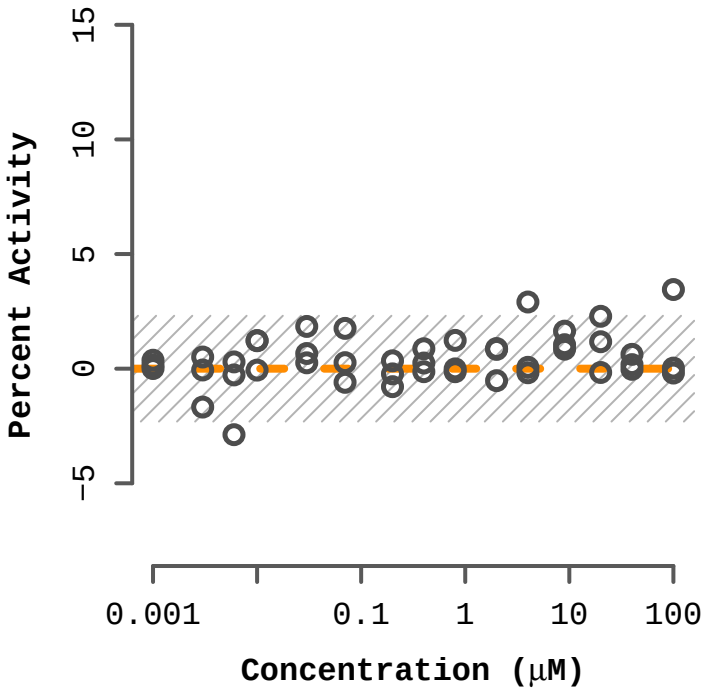
NAME: Valdecoxib
CHID: 44226 **CASRN:** 181695-72-7
SPID(S): Tox21_111438_1
M4ID: 12483687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.646 **MAX_MED:** 0.967 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

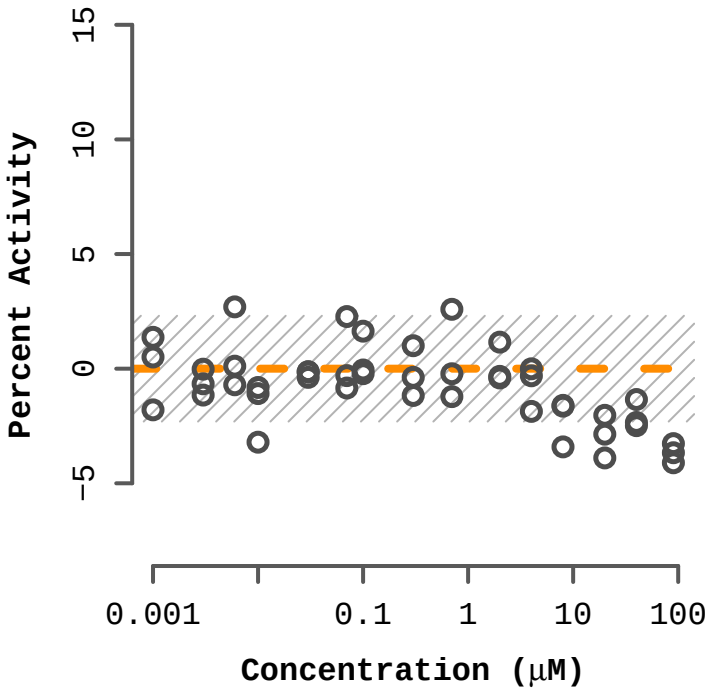
NAME: Pramipexole dihydrochloride monohydrate
CHID: 44227 CASRN: 191217-81-9
SPID(S): Tox21_302316
M4ID: 12476817

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.18 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

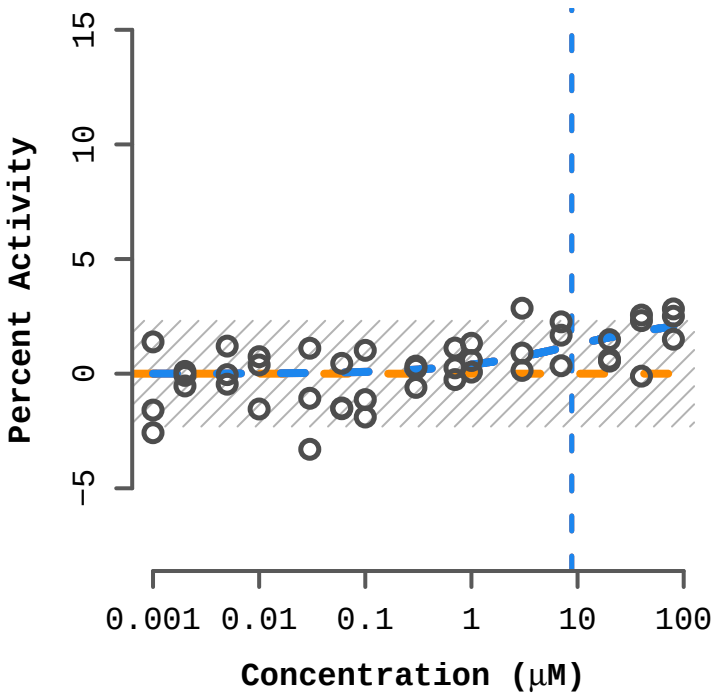
NAME: Antioxidant 1098
CHID: 44233 CASRN: 23128-74-7
SPID(S): Tox21_303983
M4ID: 12475205

HILL MODEL: Not applicable.

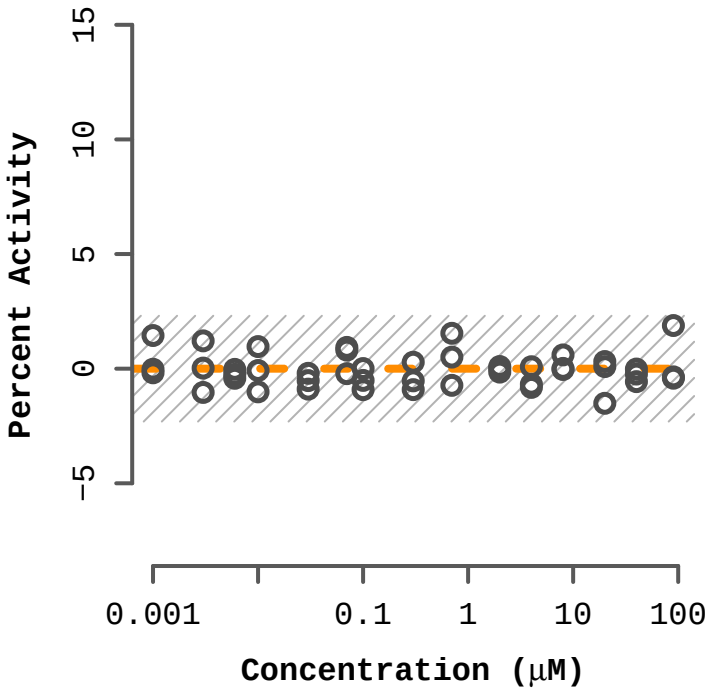
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 0.703 **MAX_MED:** 0.509 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Triethylene glycol bis(3-tert-butyl-4-hydroxy-5
CHID:    44236   CASRN: 36443-68-2
SPID(S): Tox21_302408
M4ID:    12476725

HILL MODEL (in red):
      tp       ga       gw
val:  2.44     0.946    0.757
sd:   2.73     1.9      0.758

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.44     0.946    0.757    3.03     6.95
sd:   2.73     1.9      0.758    1210     7440

      CNST        HILL        GNLS
AIC:  165.1       148.16      152.16
PROB: 0           0.88        0.12
RMSE: 1.43        1.14        1.14

MAX_MEAN: 2.28      MAX_MED: 2.51      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

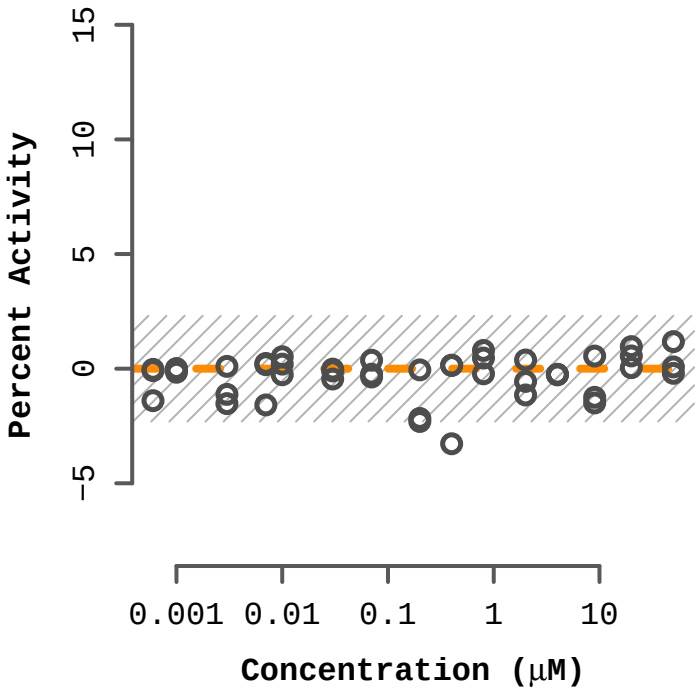
NAME: 2-Methylhexanoic acid
CHID: 44241 **CASRN:** 4536-23-6
SPID(S): Tox21_302640
M4ID: 12476493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.508 **MAX_MED:** 0.811 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

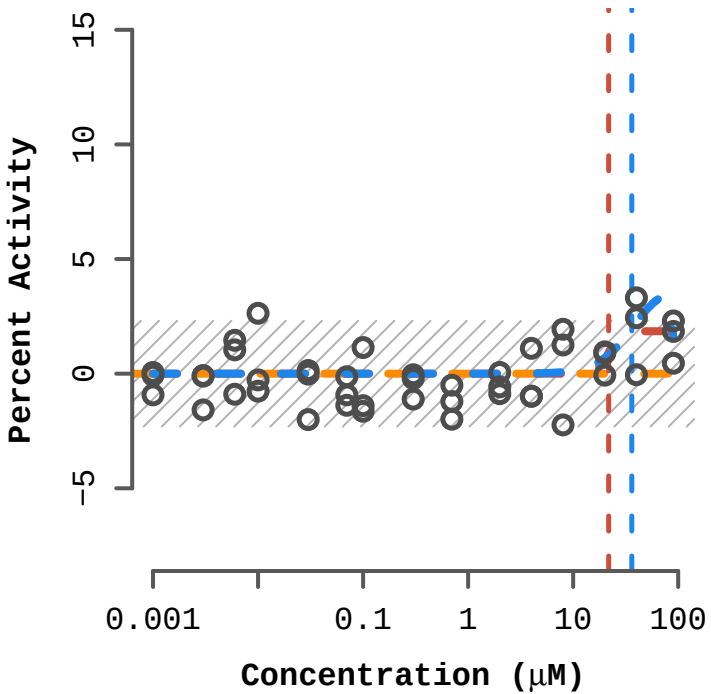
NAME: Lactitol
CHID: 44247 CASRN: 585-86-4
SPID(S): Tox21_112397_1
M4ID: 12483116

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.522 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Ethoxyphenol
CHID: 44251 **CASRN:** 622-62-8
SPID(S): Tox21_302684
M4ID: 12476449

HILL MODEL (in red):

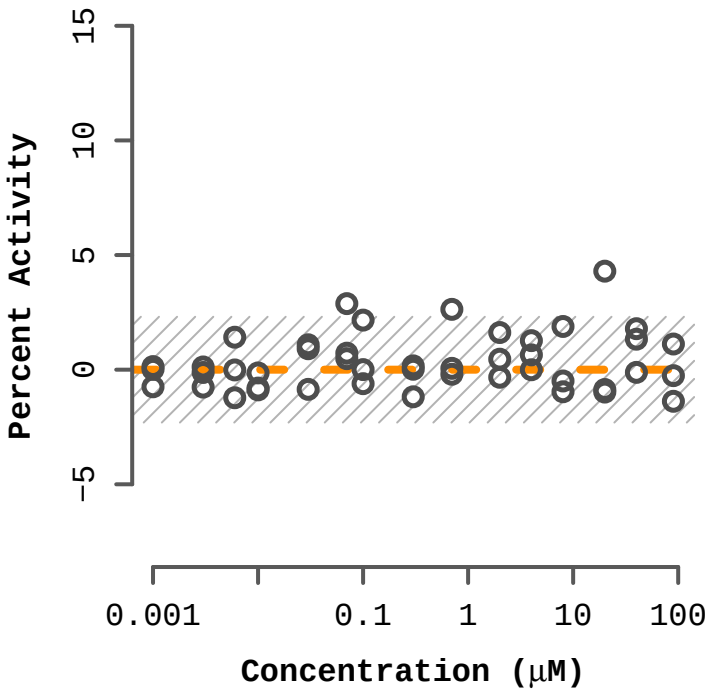
	tp	ga	gw
val:	1.85	1.34	8
sd:	0.507	0.0982	16

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.97	1.56	2.64	1.95	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	156.75	151.35	154.74
PROB:	0.05	0.8	0.15
RMSE:	1.31	1.14	1.14

MAX_MEAN: 1.9 **MAX_MED:** 2.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

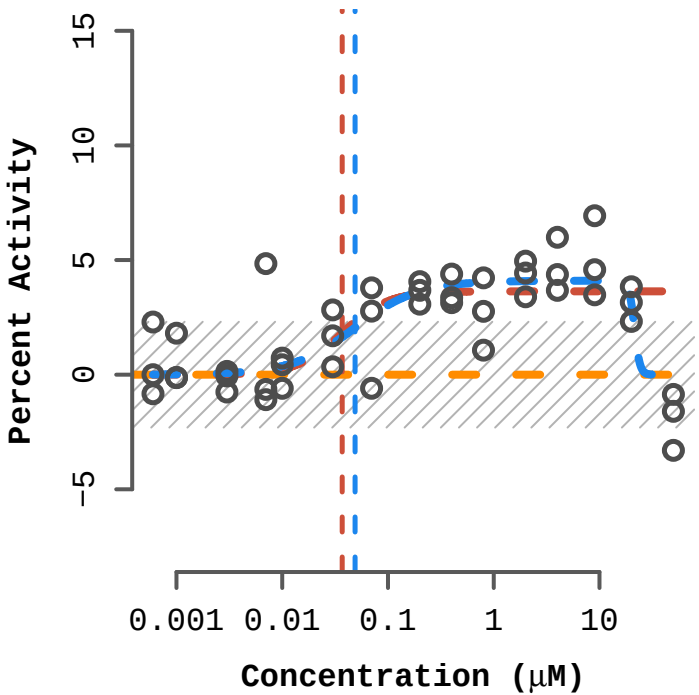
NAME: 5-Methylhexanoic acid
CHID: 44252 **CASRN:** 628-46-6
SPID(S): Tox21_302396
M4ID: 12476737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Atomoxetine hydrochloride
CHID: 44266 CASRN: 82248-59-7
SPID(S): Tox21_110292_1
M4ID: 12484477

HILL MODEL (in red):

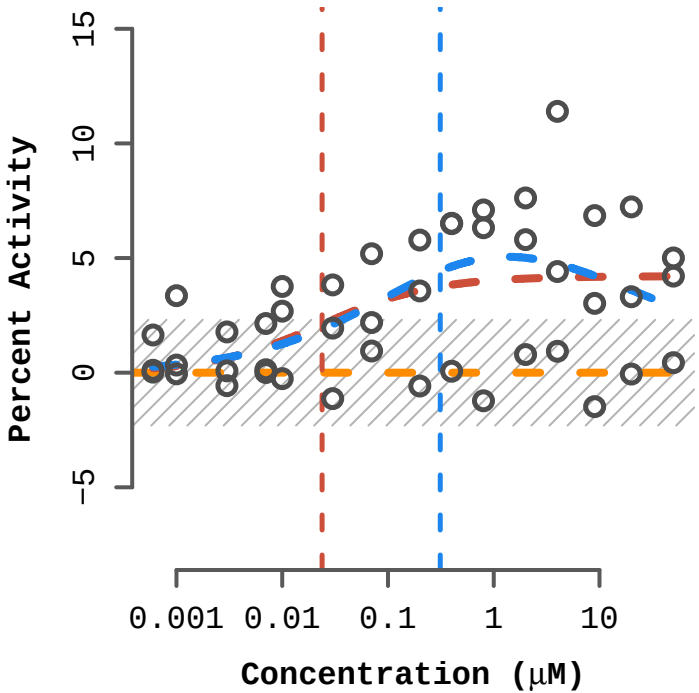
	tp	ga	gw
val:	3.64	−1.43	2.02
sd:	0.311	0.176	1.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.1	−1.31	1.45	1.33	17
sd:	0.437	0.233	0.858	0.0687	39.9

	CNST	HILL	GNLS
AIC:	236.08	185.02	165.57
PROB:	0	0	1
RMSE:	3.08	1.99	1.42

MAX_MEAN: 5 **MAX_MED:** 4.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Moexipril hydrochloride
CHID: 44267 CASRN: 82586-52-5
SPID(S): Tox21_112590_1
M4ID: 12483016

HILL MODEL (in red):

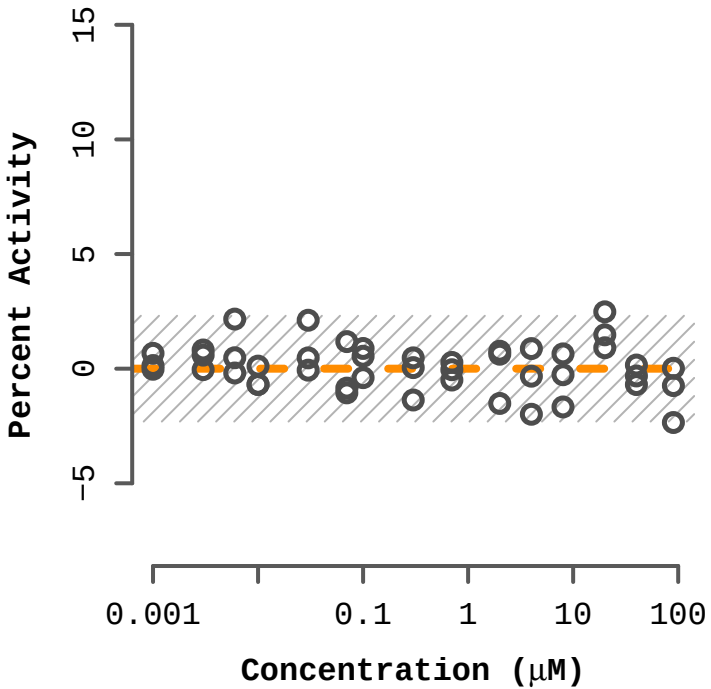
	tp	ga	gw
val:	4.21	−1.62	0.826
sd:	0.75	0.429	0.501

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.7	−0.506	0.622	0.215	0.371
sd:	33.4	1.47	0.42	5.11	0.548

	CNST	HILL	GNLS
AIC:	255.44	226.09	228.21
PROB:	0	0.74	0.26
RMSE:	4.02	2.66	2.64

MAX_MEAN: 5.58 **MAX_MED:** 6.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

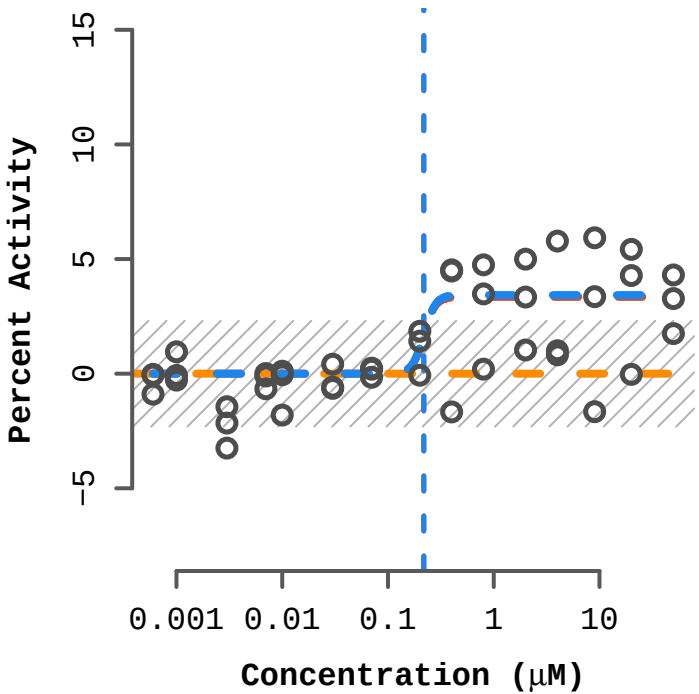
NAME: Cetirizine dihydrochloride
CHID: 44268 **CASRN:** 83881-52-1
SPID(S): Tox21_302261
M4ID: 12476872

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cetirizine dihydrochloride
CHID: 44268 CASRN: 83881-52-1
SPID(S): Tox21_110704_1
M4ID: 12484164

HILL MODEL (in red):

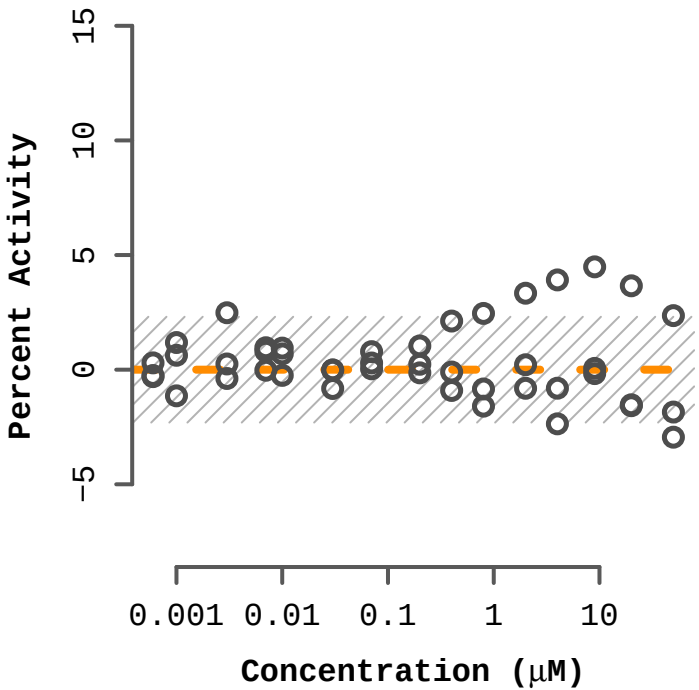
	tp	ga	gw
val:	3.35	−0.662	8
sd:	0.443	0.0732	11.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.43	−0.66	7.97	1.79	11.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	216.23	185.12	189.04
PROB:	0	0.88	0.12
RMSE:	2.62	1.78	1.79

MAX_MEAN: 3.23 MAX_MED: 4.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

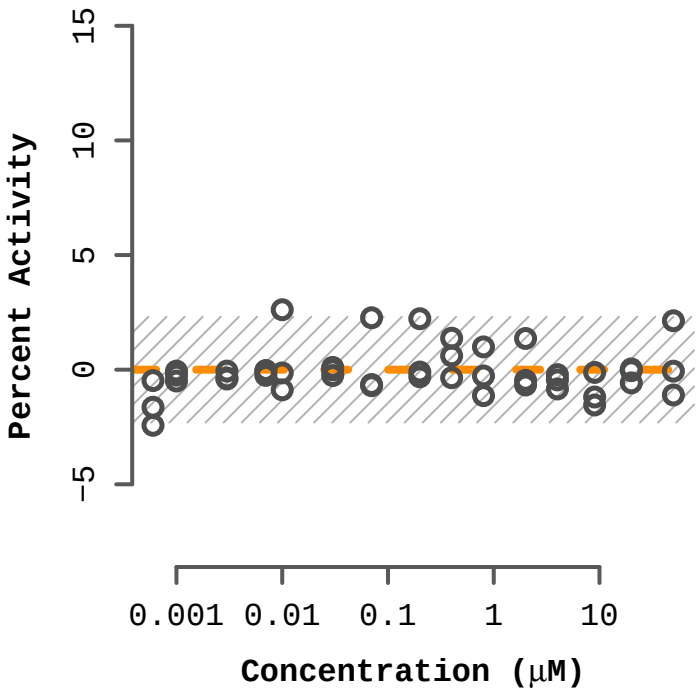
NAME: Quinine
CHID: 44280 **CASRN:** 130-95-0
SPID(S): Tox21_112389_1
M4ID: 12483121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 0.807 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

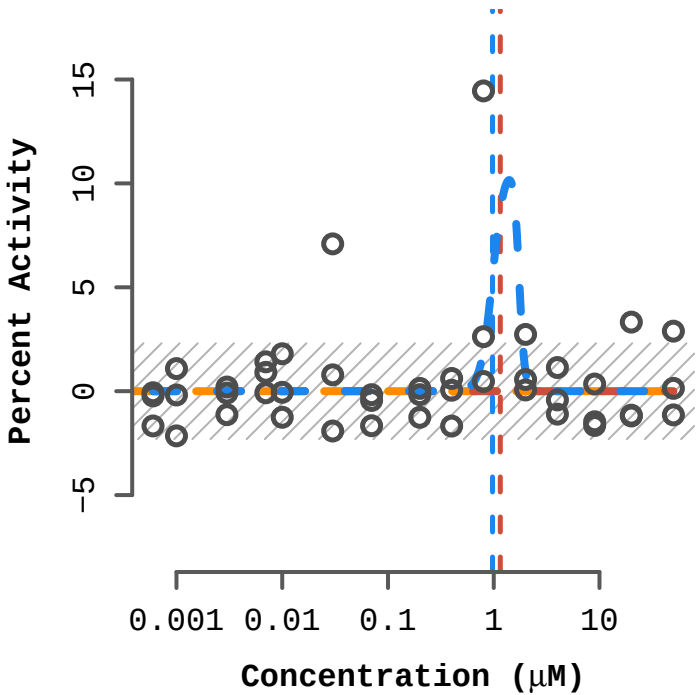
NAME: Almotriptan
CHID: 44289 **CASRN:** 154323-57-6
SPID(S): Tox21_111444_1
M4ID: 12483681

HILL MODEL: Not applicable.

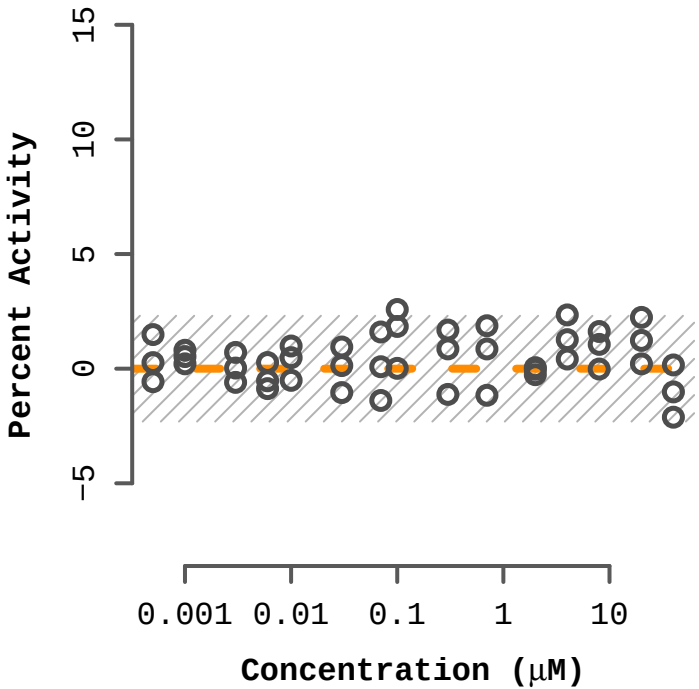
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.605 **MAX_MED:** 0.605 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Fosphenytoin
CHID:    44299   CASRN: 93390-81-9
SPID(S): Tox21_113670
M4ID:    12482544

HILL MODEL (in red):
      tp        ga        gw
val:  2.52e-09  0.0622    1.93
sd:   0.000108  1070      76100

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  11        -0.0115   7.83      0.24      16.9
sd:   NaN       NaN       NaN       NaN       NaN

      CNST          HILL          GNLS
AIC:  184.62        190.62        189.74
PROB: 0.89          0.04          0.07
RMSE: 2.73          2.73          2.47

MAX_MEAN: 5.85      MAX_MED: 2.63      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

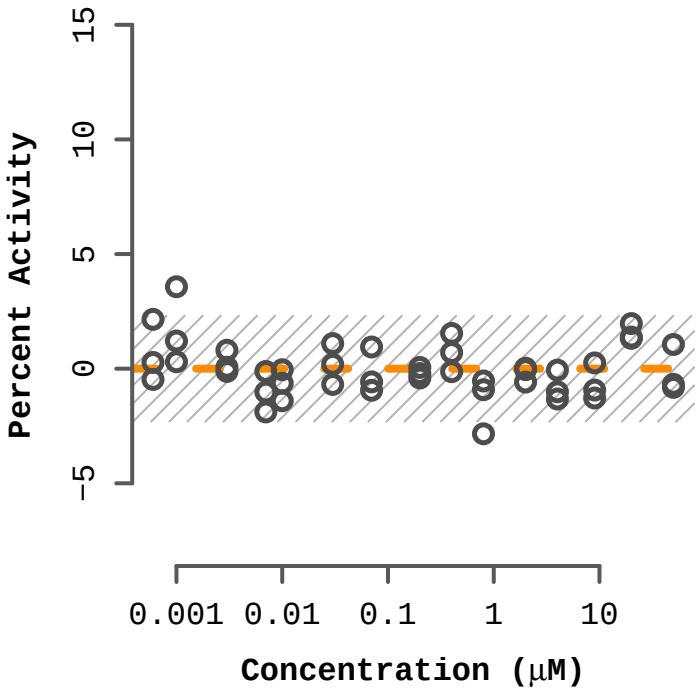
NAME: Atorvastatin calcium
CHID: 44303 **CASRN:** 134523-03-8
SPID(S): Tox21_302373
M4ID: 12476760

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

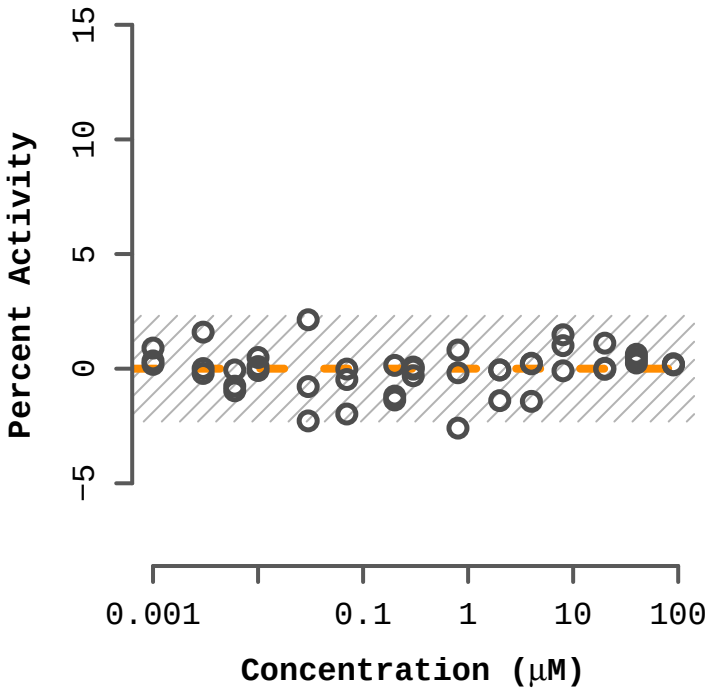
NAME: Atorvastatin calcium
CHID: 44303 **CASRN:** 134523-03-8
SPID(S): Tox21_111685_1
M4ID: 12483536

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

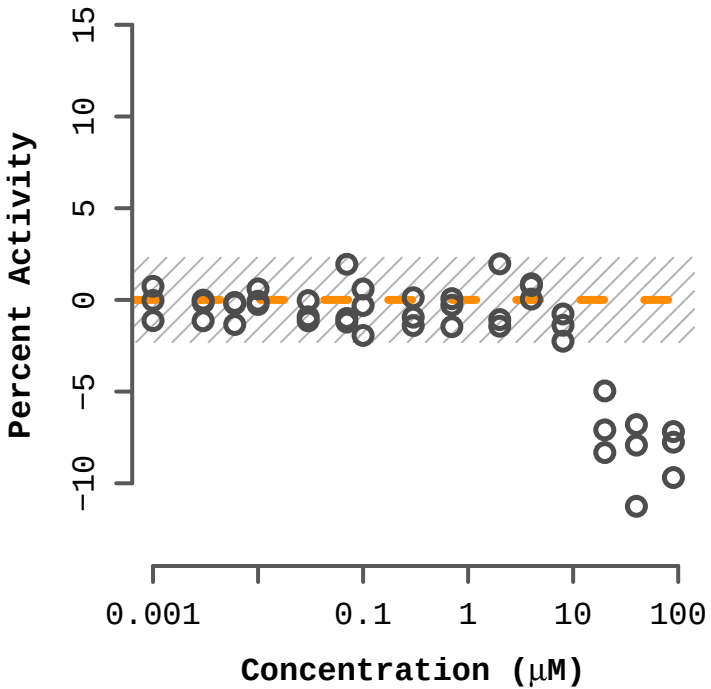
NAME: (1R)−endo−(+)−Fenchyl alcohol
CHID: 44307 **CASRN:** 2217−02−9
SPID(S): Tox21_301348
M4ID: 12477785

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.799 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

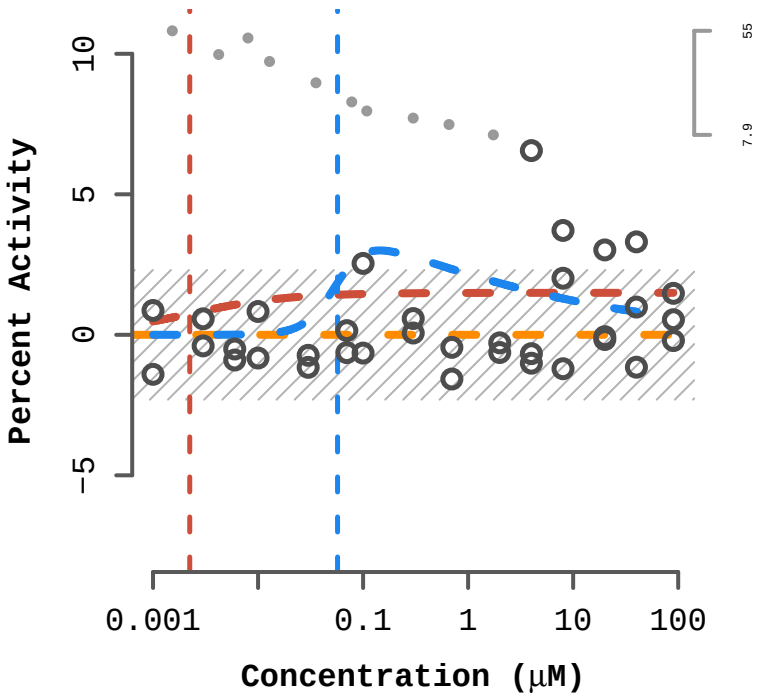
NAME: 1,10-Phenanthroline hydrochloride hydrate
CHID: 44309 **CASRN:** 18851-33-7
SPID(S): Tox21_301286
M4ID: 12477847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.45	NA	NA
PROB:	1	NA	NA
RMSE:	3.72	NA	NA

MAX_MEAN: 0.572 **MAX_MED:** 0.787 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylpentan-1-ol
CHID: 44313 CASRN: 626-89-1
SPID(S): Tox21_301292
M4ID: 12477841 BRK

HILL MODEL (in red):

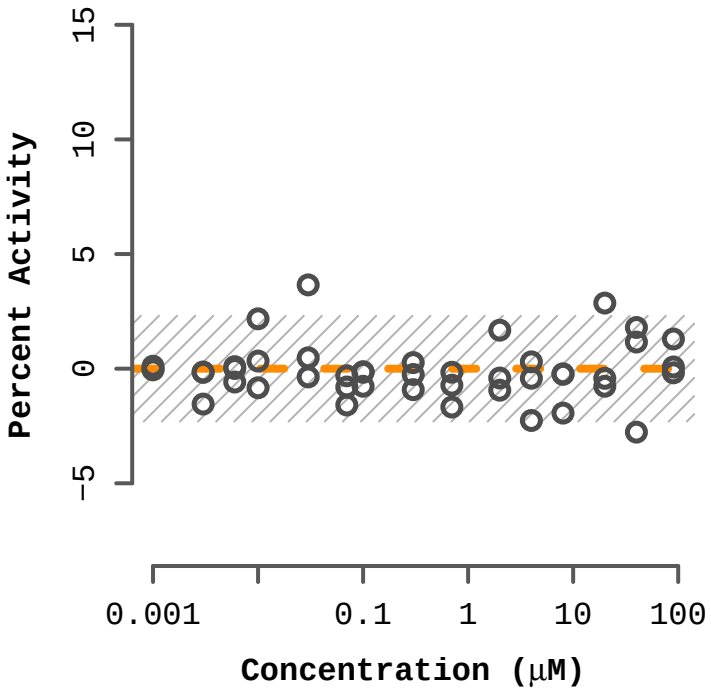
	tp	ga	gw
val:	1.49	−2.65	0.935
sd:	0.999	3.27	2.98

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.78	−1.24	2.99	−0.993	0.332
sd:	52.3	1.17	18.7	17.5	0.923

	CNST	HILL	GNLS
AIC:	344.78	347.83	351.39
PROB:	0.8	0.17	0.03
RMSE:	16.06	15.64	15.82

MAX_MEAN: 18 MAX_MED: 2.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

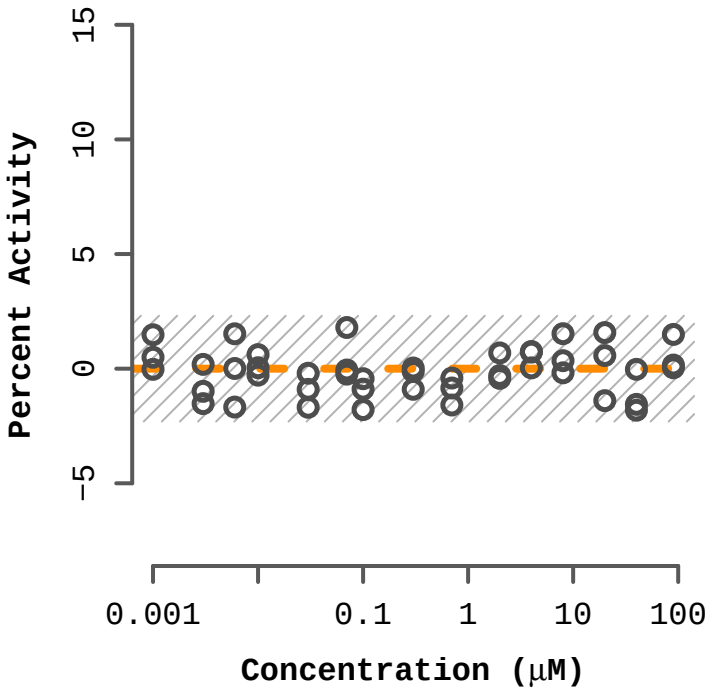
NAME: Methyl (E)−cinnamate
CHID: 44314 **CASRN:** 1754−62−7
SPID(S): Tox21_301384
M4ID: 12477749

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

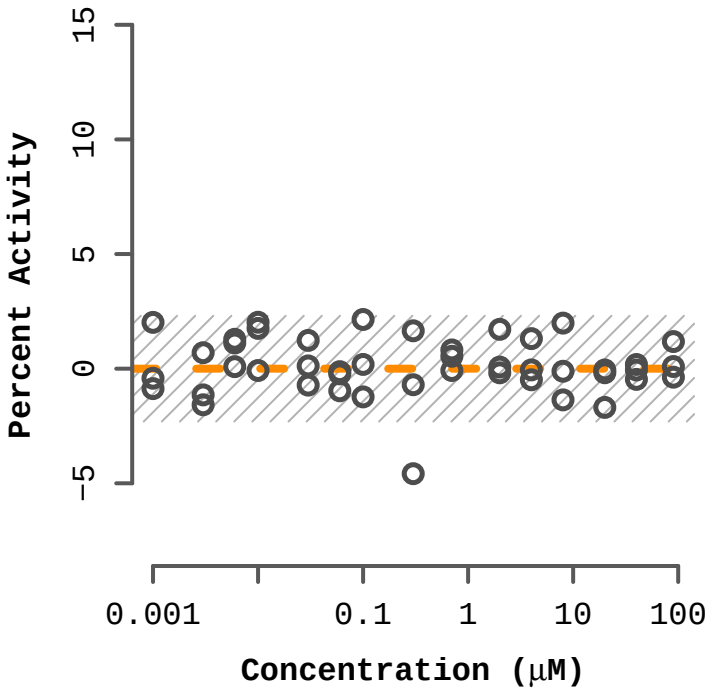
NAME: 1,5−Naphthalenedisulfonic acid, disodium salt |
CHID: 44315 CASRN: 207569−02−6
SPID(S): Tox21_300703
M4ID: 12478430

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.651 MAX_MED: 0.725 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

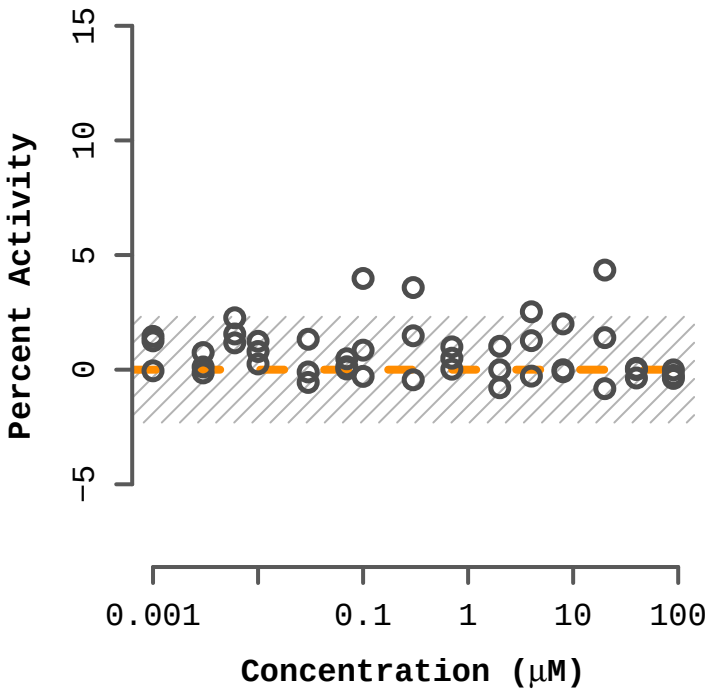
NAME: 4-Methylbenzenesulfonic acid hydrate
CHID: 44316 **CASRN:** 6192-52-5
SPID(S): Tox21_300710
M4ID: 12478423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 8-Hydroxyquinoline-5-sulfonic acid hydrate (1:

CHID: 44317 **CASRN:** 207386-92-3

SPID(S): Tox21_300766

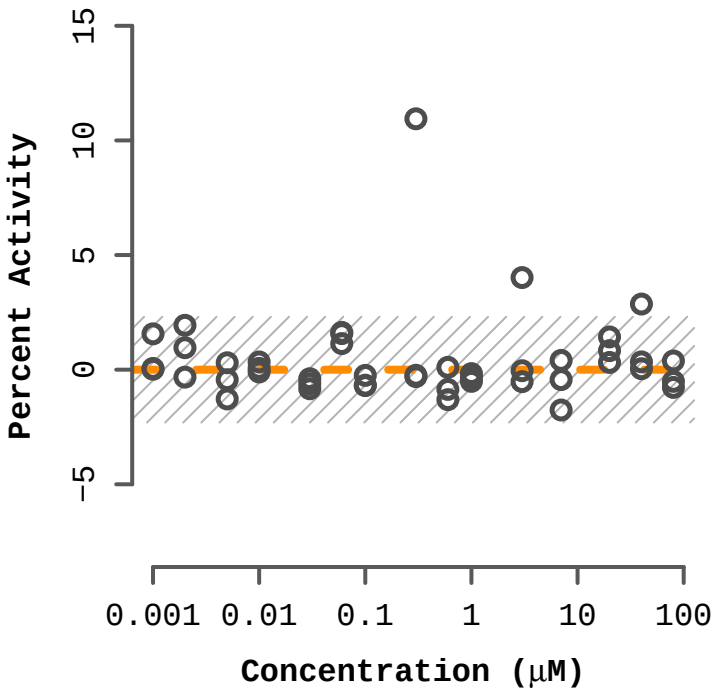
M4ID: 12478367

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

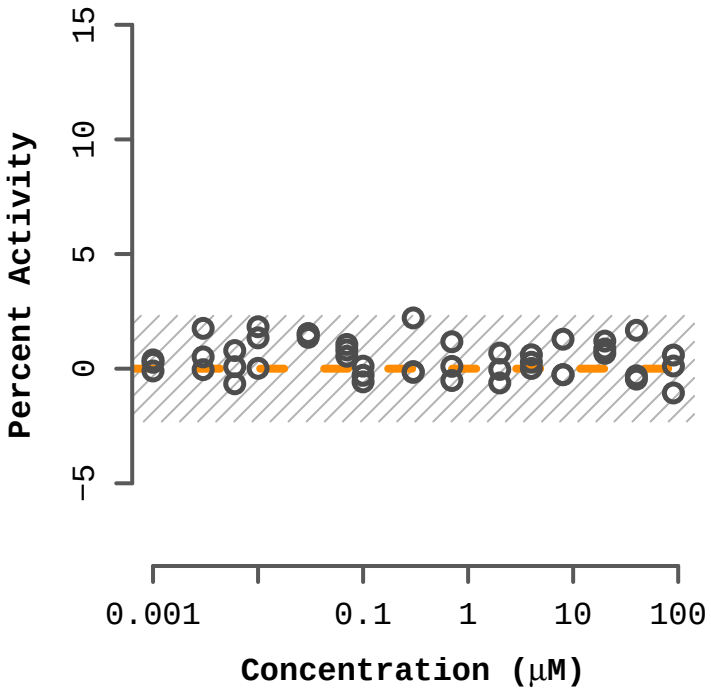
NAME: Chloramine T hydrate (1:x)
CHID: 44318 **CASRN:** 149358-73-6
SPID(S): Tox21_300899
M4ID: 12478234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 3.47 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

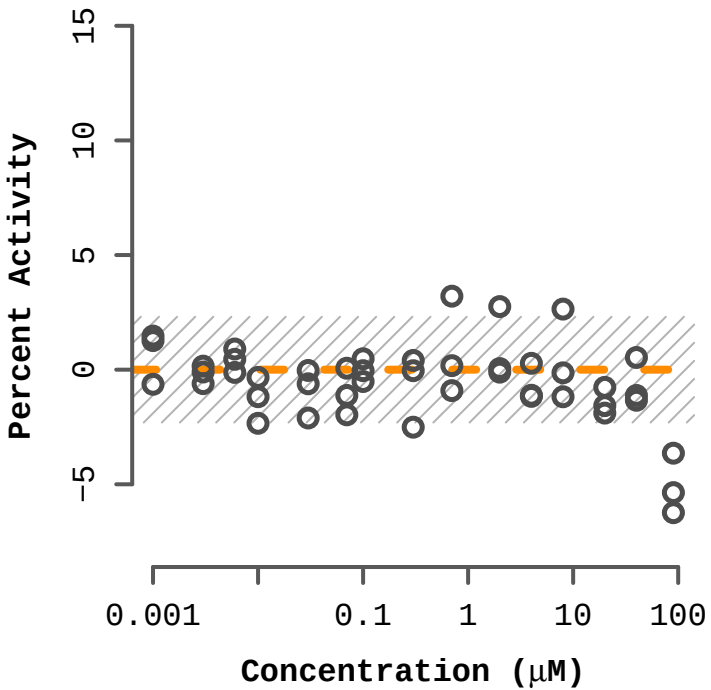
NAME: Diethylamine hydrochloride
CHID: 44320 CASRN: 660-68-4
SPID(S): Tox21_301087
M4ID: 12478046

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.47 MAX_MED: 1.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

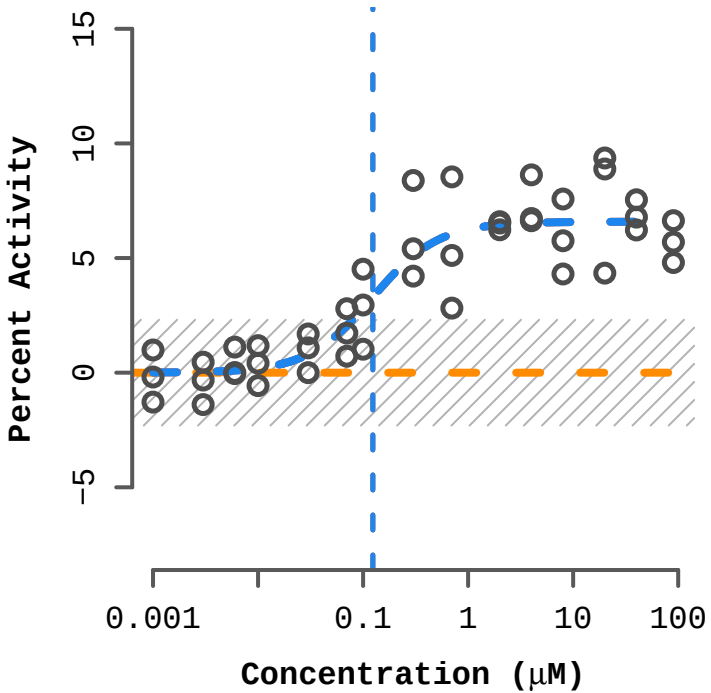
NAME: Dodecylamine hydrochloride
CHID: 44322 CASRN: 929-73-7
SPID(S): Tox21_301702
M4ID: 12477431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 0.899 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzyltrimethylammonium hydroxide
CHID: 44332 CASRN: 100-85-6
SPID(S): Tox21_300756
M4ID: 12478377

HILL MODEL (in red):

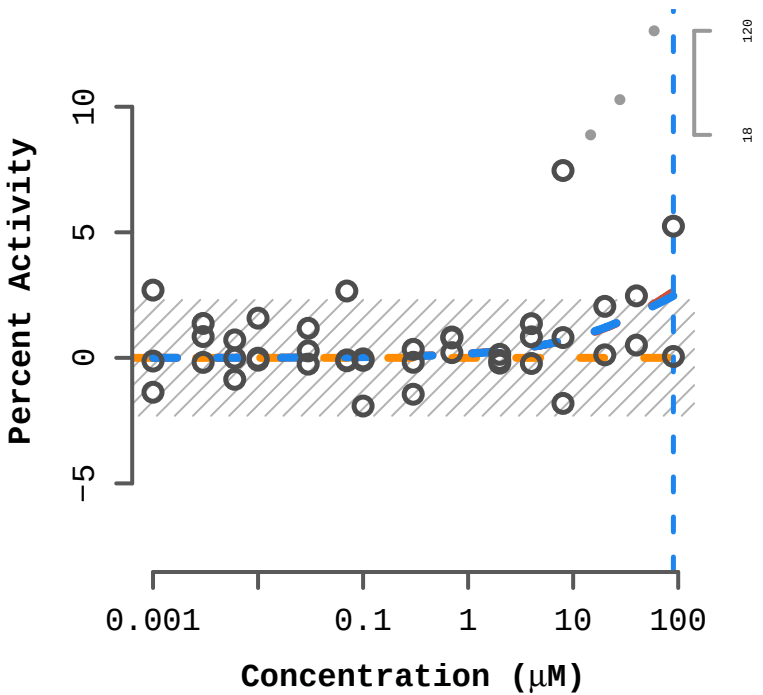
	tp	ga	gw
val:	6.58	−0.907	1.39
sd:	0.325	0.109	0.45

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.58	−0.907	1.39	3.93	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	278.78	162.68	166.68
PROB:	0	0.88	0.12
RMSE:	4.95	1.34	1.34

MAX_MEAN: 7.53 MAX_MED: 8.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methylhexane
CHID: 44334 CASRN: 589-34-4
SPID(S): Tox21_202850
M4ID: 12479402 BRK

HILL MODEL (in red):

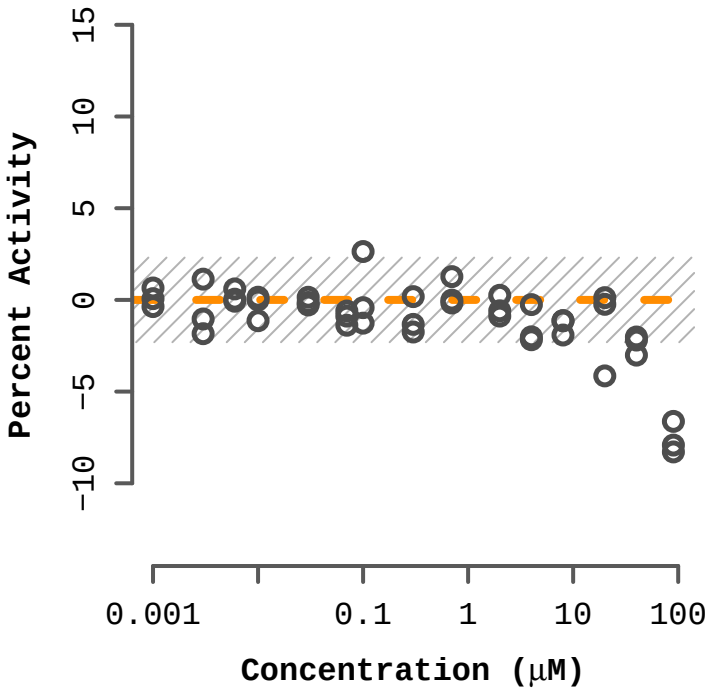
	tp	ga	gw
val:	8.46	2.45	0.684
sd:	112	11.9	1.21

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.93	1.95	0.751	2.86	7.44
sd:	43.6	8.45	1.67	1160	9620

	CNST	HILL	GNLS
AIC:	249.43	249.23	253.24
PROB:	0.44	0.49	0.07
RMSE:	19.97	19.47	19.5

MAX_MEAN: 42.2 MAX_MED: 5.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

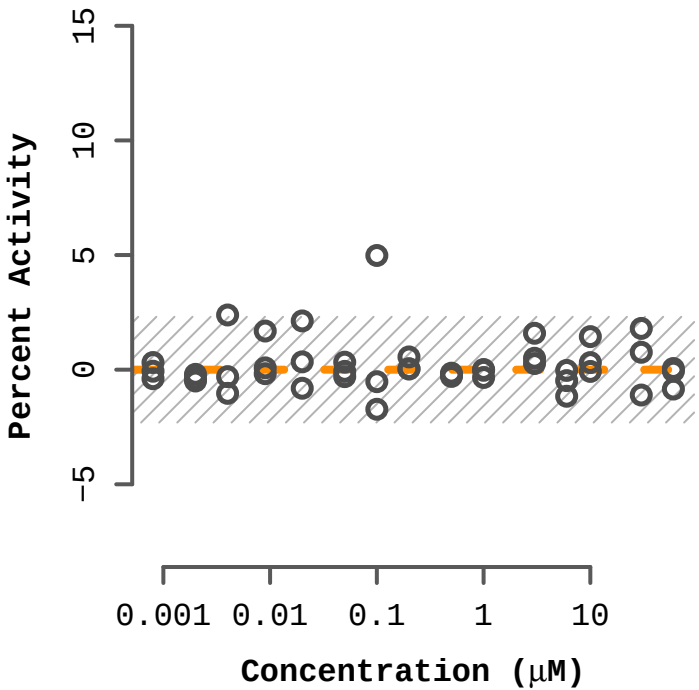
NAME: Pyrasulfotole metabolite (SXX 0665)
CHID: 44338 **CASRN:** 120983-64-4
SPID(S): Tox21_303715
M4ID: 12475473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 0.365 **MAX_MED:** 0.0708 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

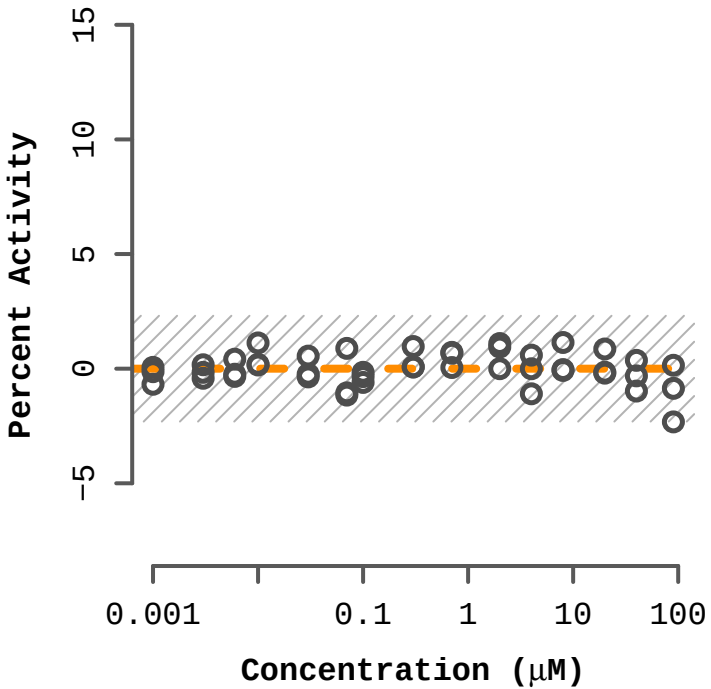
NAME: Florasulam
CHID: 44340 **CASRN:** 145701-23-1
SPID(S): Tox21_302433
M4ID: 12476700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.912 **MAX_MED:** 0.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

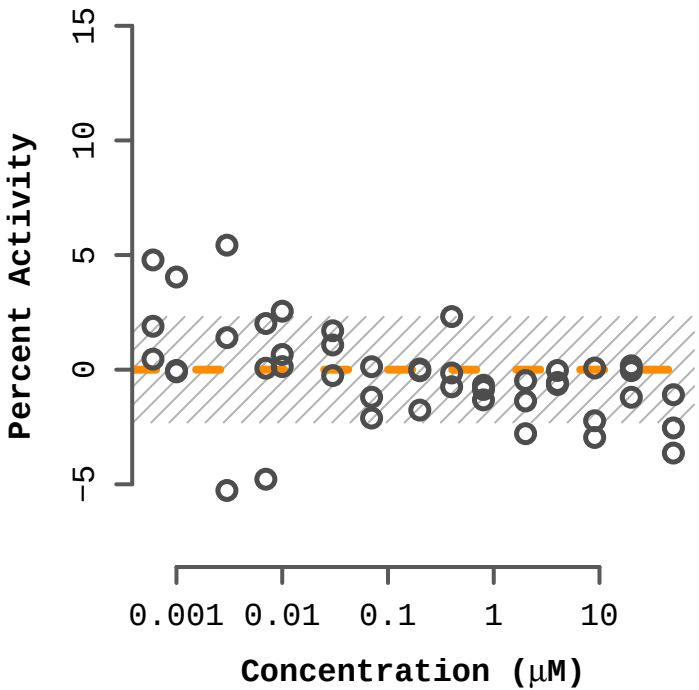
NAME: Spirotetramat
CHID: 44342 CASRN: 203313-25-1
SPID(S): Tox21_302430
M4ID: 12476703

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.681 **MAX_MED:** 0.945 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

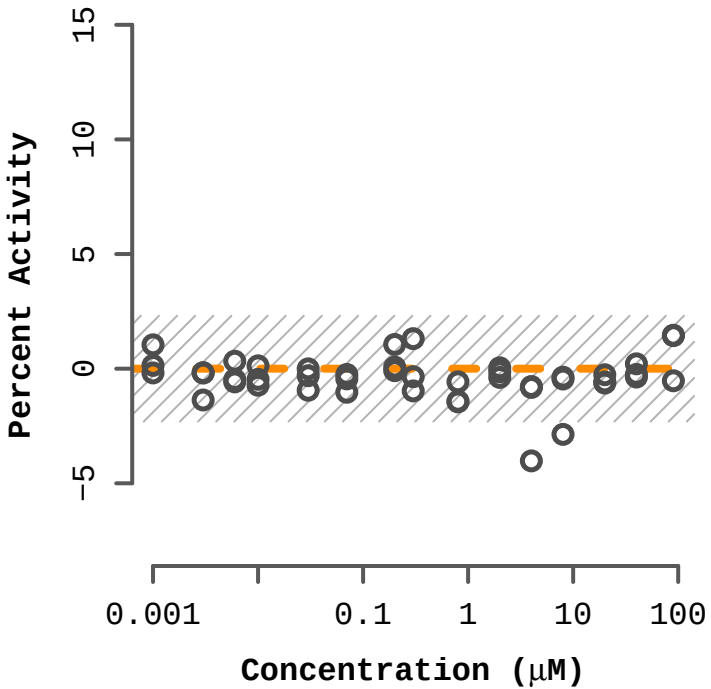
NAME: Vitamin B12
CHID: 44346 **CASRN:** 68-19-9
SPID(S): Tox21_113664
M4ID: 12482549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.13	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

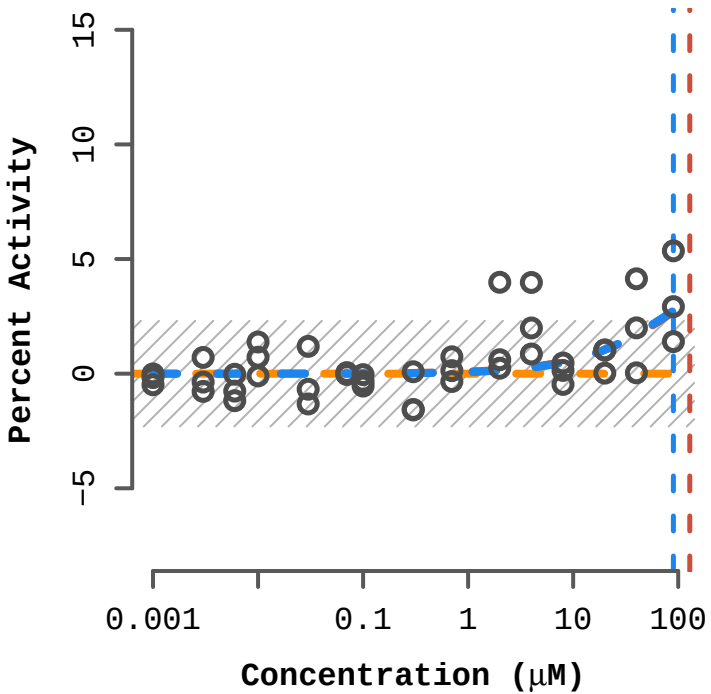
NAME: 4'−Methoxyacetophenone
CHID: 44347 CASRN: 100−06−1
SPID(S): Tox21_300687
M4ID: 12478446

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.792 MAX_MED: 1.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl phenylacetate
CHID: 44352 CASRN: 101-41-7
SPID(S): Tox21_300792
M4ID: 12478341

HILL MODEL (in red):

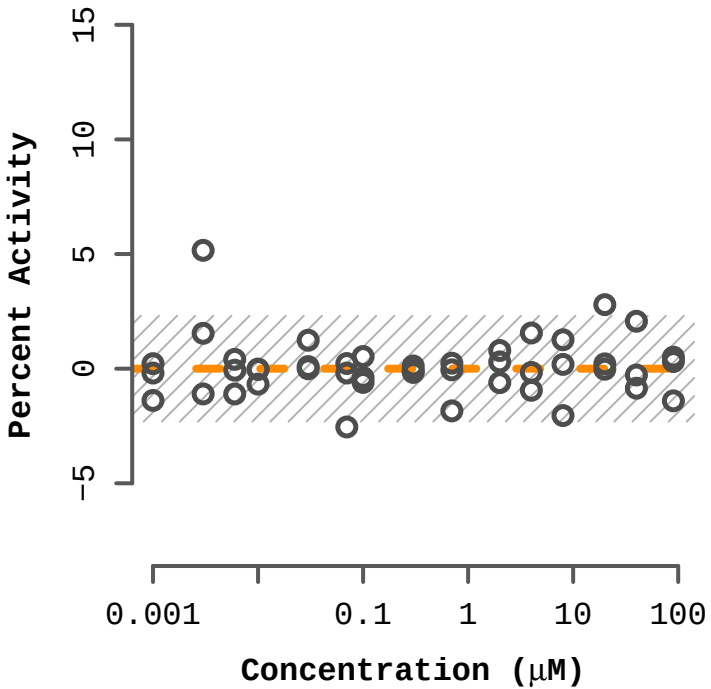
	tp	ga	gw
val:	6.43	2.11	0.88
sd:	7.45	1.01	0.508

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.5	1.95	0.962	2.48	14.8
sd:	6.32	0.957	0.611	813	22600

	CNST	HILL	GNLS
AIC:	160.54	146.44	150.54
PROB:	0	0.89	0.11
RMSE:	1.6	1.22	1.22

MAX_MEAN: 3.23 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

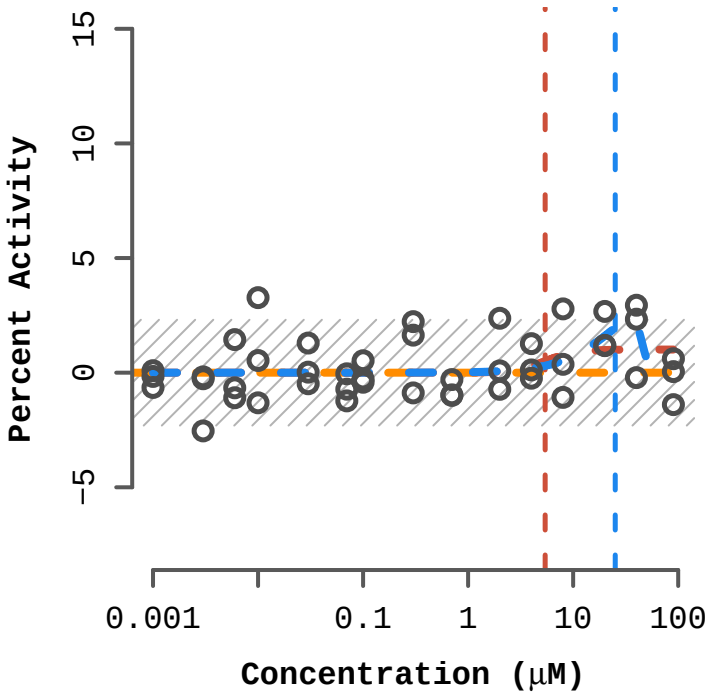
NAME: Ethyl phenylacetate
CHID: 44353 **CASRN:** 101-97-3
SPID(S): Tox21_300810
M4ID: 12478323

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Butyldiethanolamine
CHID: 44354 CASRN: 102-79-4
SPID(S): Tox21_300813
M4ID: 12478320

HILL MODEL (in red):

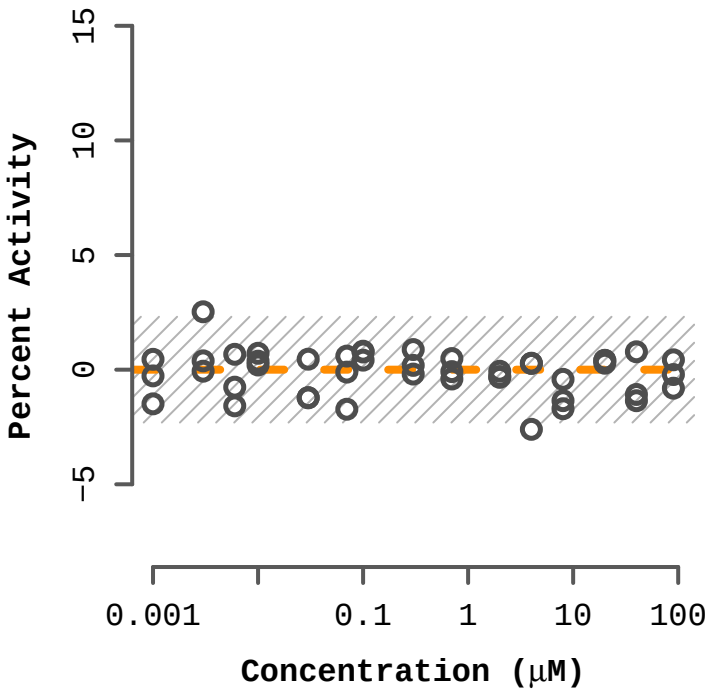
	tp	ga	gw
val:	1.01	0.733	2.92
sd:	0.469	0.46	3.46

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.92	1.4	1.62	1.65	12.1
sd:	55.2	6.62	5.35	0.655	99.1

	CNST	HILL	GNLS
AIC:	157.02	157.31	155.06
PROB:	0.22	0.19	0.59
RMSE:	1.35	1.25	1.19

MAX_MEAN: 1.69 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

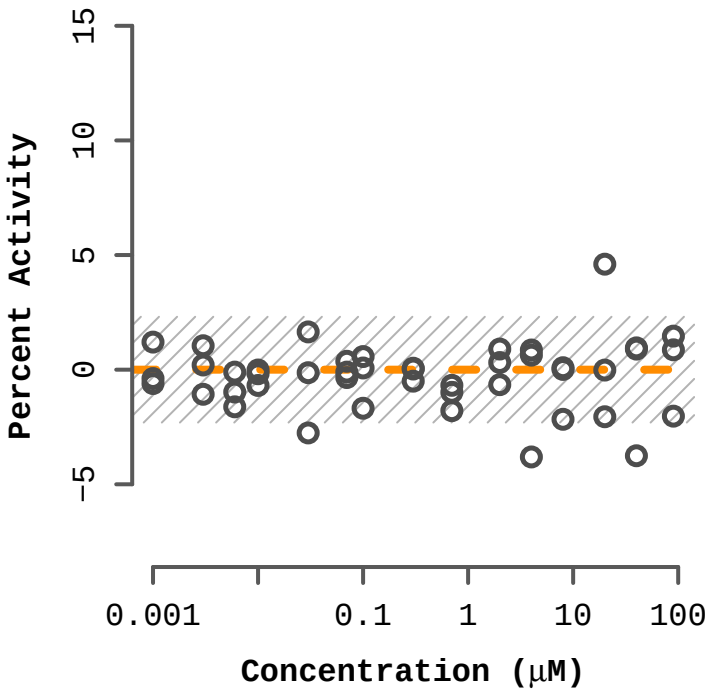
NAME: Dibenzylamine
CHID: 44355 **CASRN:** 103-49-1
SPID(S): Tox21_301089
M4ID: 12478044

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.95 **MAX_MED:** 0.773 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

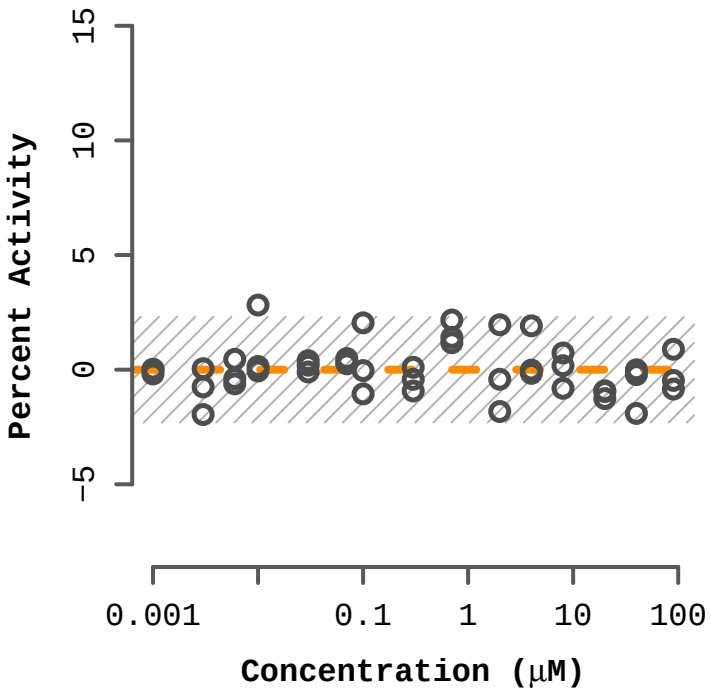
NAME: N-Benzylethanolamine
CHID: 44356 **CASRN:** 104-63-2
SPID(S): Tox21_301199
M4ID: 12477934

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 0.845 **MAX_MED:** 0.898 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

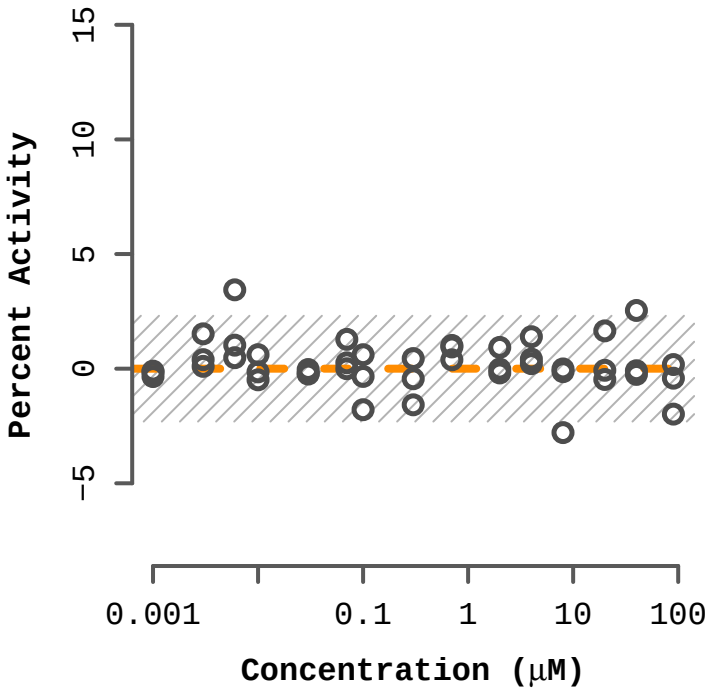
NAME: (4-Methoxyphenyl)methanol
CHID: 44357 **CASRN:** 105-13-5
SPID(S): Tox21_301115
M4ID: 12478018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

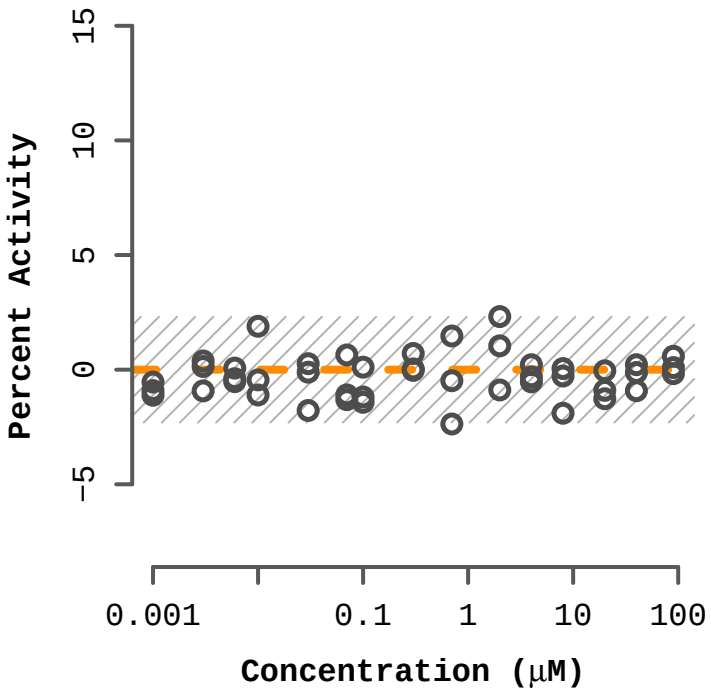
NAME: Pentadecan−15−olide
CHID: 44359 **CASRN:** 106−02−5
SPID(S): Tox21_301123
M4ID: 12478010

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

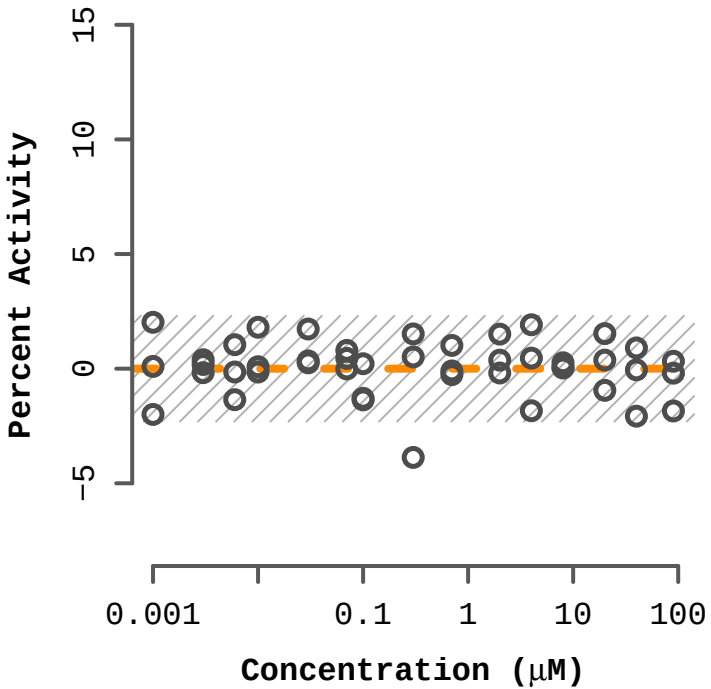
NAME: 3,7-Dimethyloctan-1-ol
CHID: 44360 CASRN: 106-21-8
SPID(S): Tox21_300961
M4ID: 12478172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

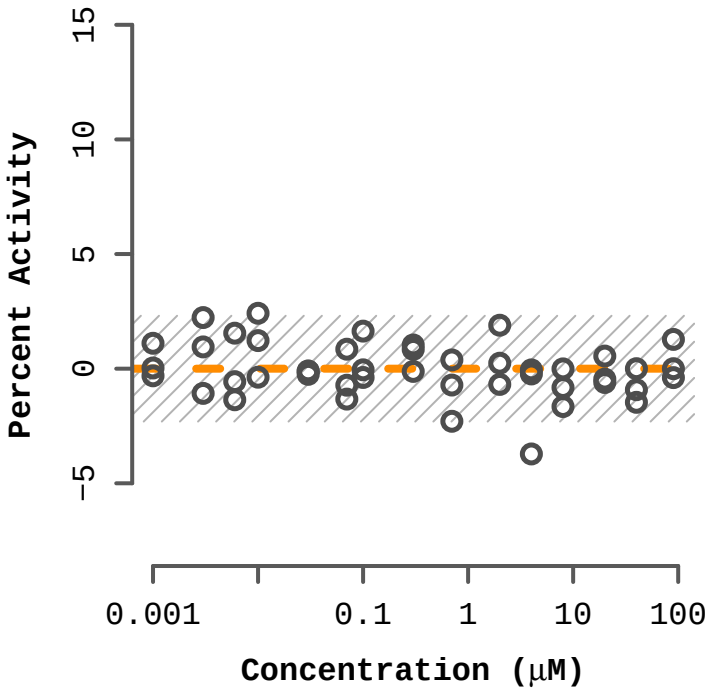
NAME: Hexanedihydrazide
CHID: 44361 **CASRN:** 1071-93-8
SPID(S): Tox21_301067
M4ID: 12478066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.775 **MAX_MED:** 0.514 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

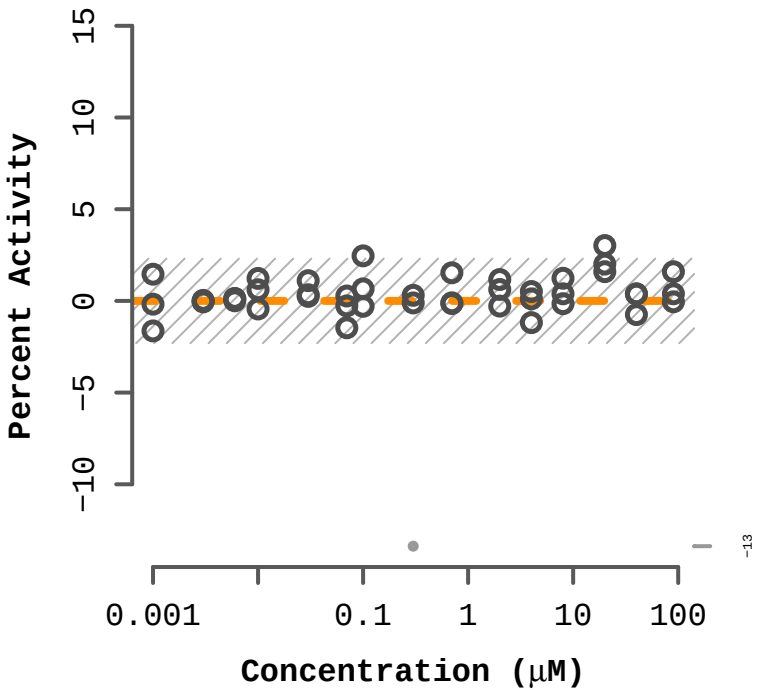
NAME: Glutaric anhydride
CHID: 44362 **CASRN:** 108-55-4
SPID(S): Tox21_300975
M4ID: 12478158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

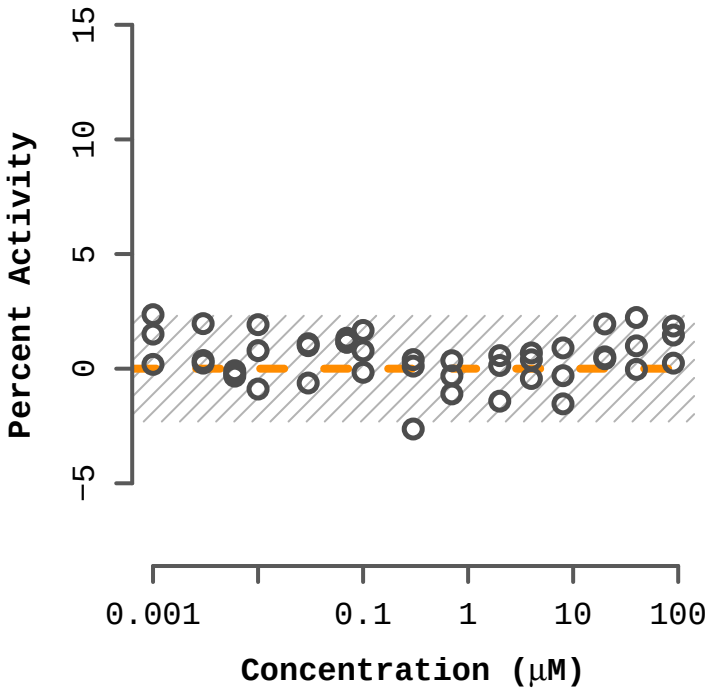
NAME: Ethyl decanoate
CHID: 44363 CASRN: 110-38-3
SPID(S): Tox21_301180
M4ID: 12477953 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

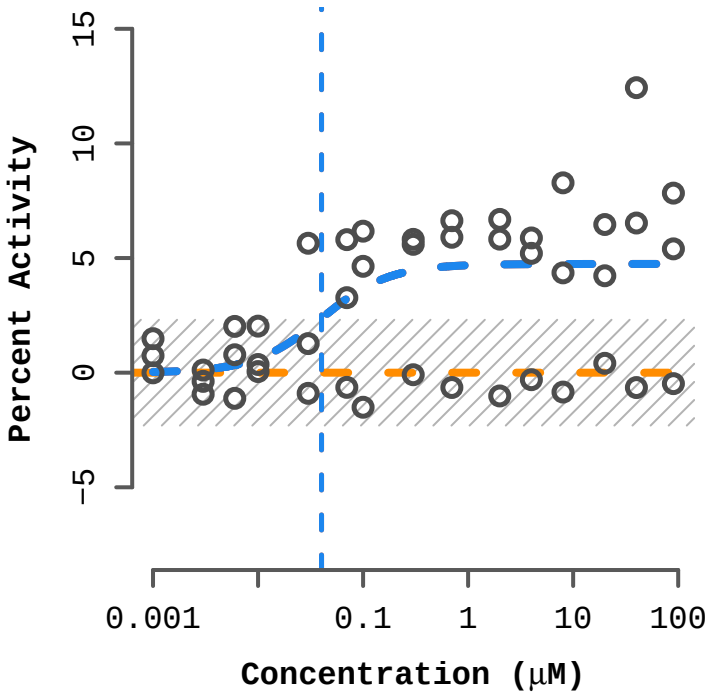
NAME: 1,4−Dibromobutane
CHID: 44364 **CASRN:** 110−52−1
SPID(S): Tox21_301070
M4ID: 12478063

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (1,1−Dimethylethyl)urea
CHID: 44365 CASRN: 1118−12−3
SPID(S): Tox21_302081
M4ID: 12477052

HILL MODEL (in red):

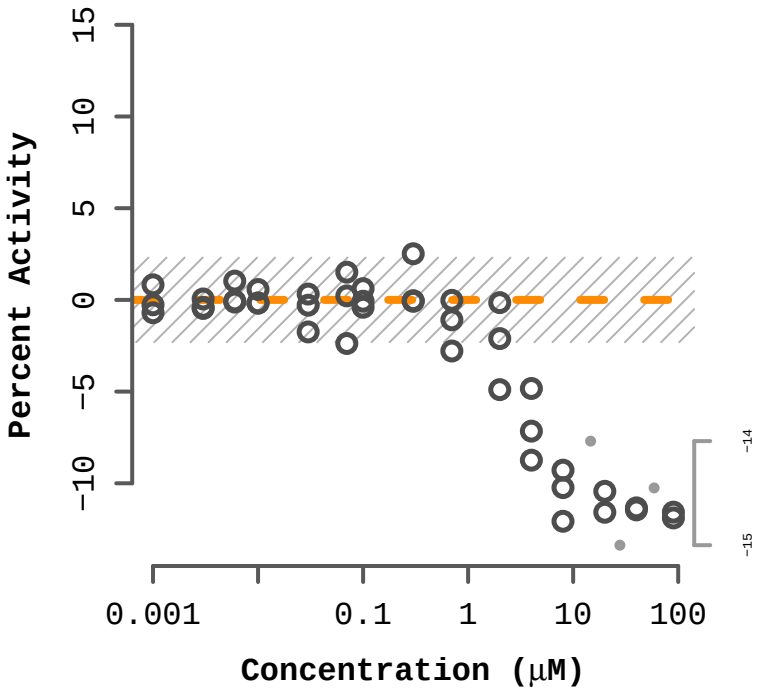
	tp	ga	gw
val:	4.74	−1.4	1.36
sd:	0.725	0.318	1.05

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.74	−1.4	1.36	3.89	5.43
sd:	0.725	0.318	1.05	87200	245000

	CNST	HILL	GNLS
AIC:	265.05	235.85	239.85
PROB:	0	0.88	0.12
RMSE:	4.42	3	3

MAX_MEAN: 6.11 MAX_MED: 6.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

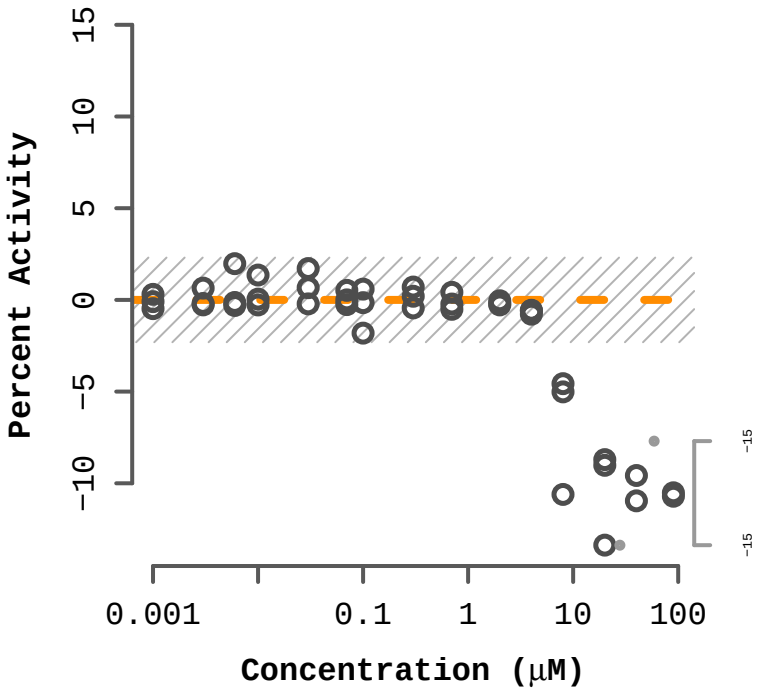
NAME: Dodecyltrimethylammonium bromide
CHID: 44366 **CASRN:** 1119-94-4
SPID(S): Tox21_302084
M4ID: 12477049 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	297.11	NA	NA
PROB:	1	NA	NA
RMSE:	6.63	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.222 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

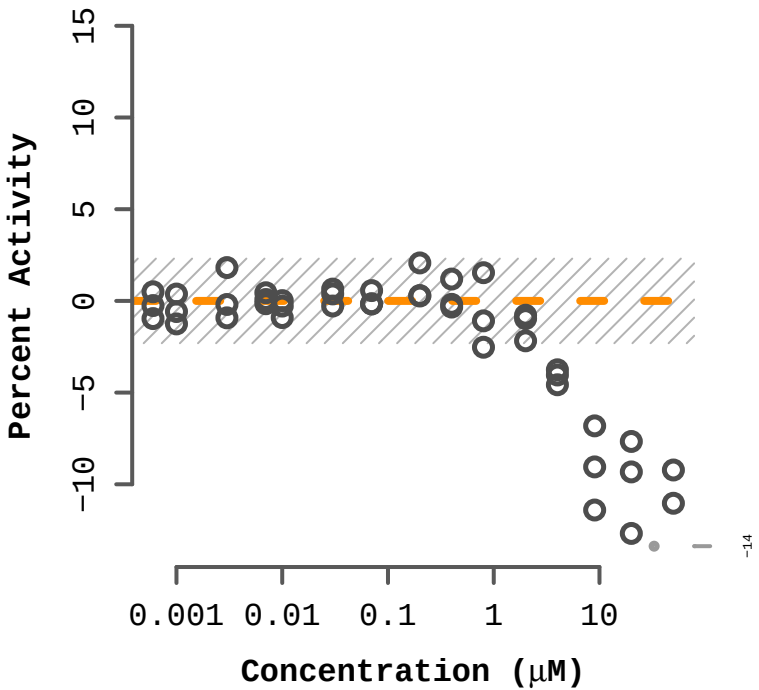
NAME: Tetradonium bromide
CHID: 44367 **CASRN:** 1119-97-7
SPID(S): Tox21_302067
M4ID: 12477066 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	271.14	NA	NA
PROB:	1	NA	NA
RMSE:	5.53	NA	NA

MAX_MEAN: 0.722 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

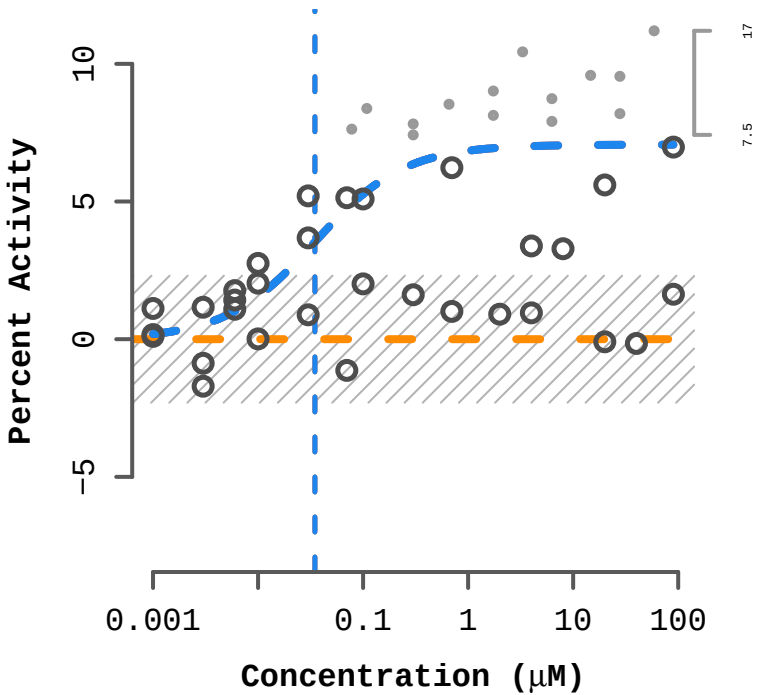
NAME: Tetradonium bromide
CHID: 44367 **CASRN:** 1119-97-7
SPID(S): Tox21_112327_1
M4ID: 12483159 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.51	NA	NA
PROB:	1	NA	NA
RMSE:	4.81	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 0.383 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dodecanoyl chloride
CHID: 44368 CASRN: 112-16-3
SPID(S): Tox21_303812
M4ID: 12475376 BRK

HILL MODEL (in red):

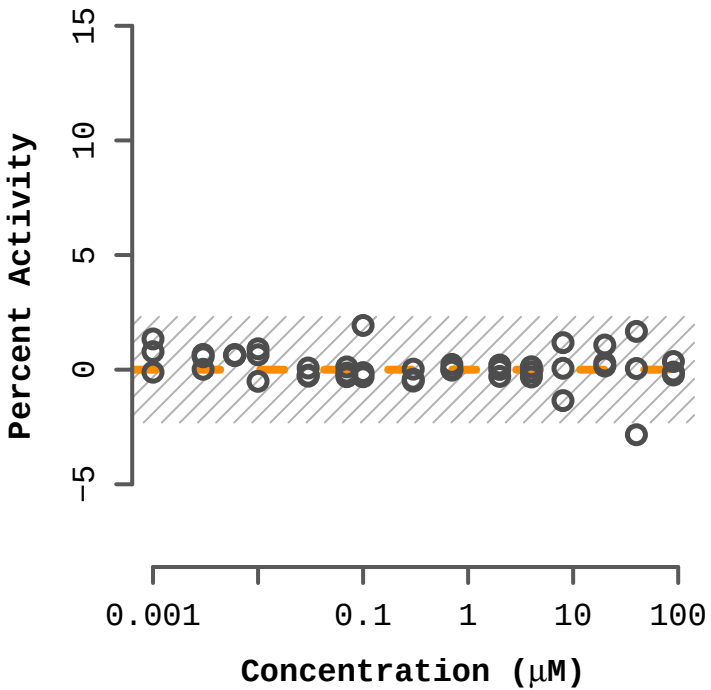
	tp	ga	gw
val:	7.07	-1.46	1.02
sd:	1.21	0.348	0.625

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.07	-1.46	1.02	2.67	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	301.05	260.46	264.46
PROB:	0	0.88	0.12
RMSE:	6.68	3.91	3.91

MAX_MEAN: 8.53 MAX_MED: 9.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

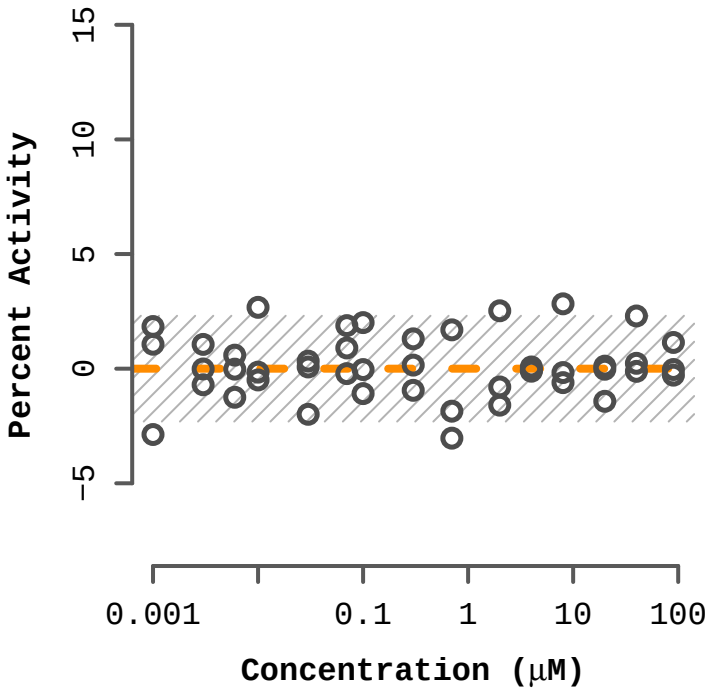
NAME: N,N-dimethylpyridin-4-amine
CHID: 44369 **CASRN:** 1122-58-3
SPID(S): Tox21_302184
M4ID: 12476949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

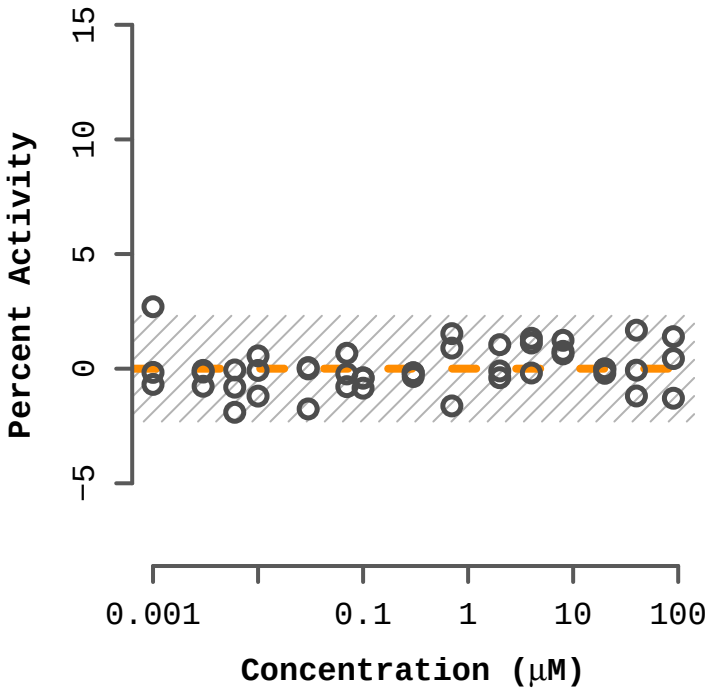
NAME: N-Butylaniline
CHID: 44370 **CASRN:** 1126-78-9
SPID(S): Tox21_302068
M4ID: 12477065

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.857 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

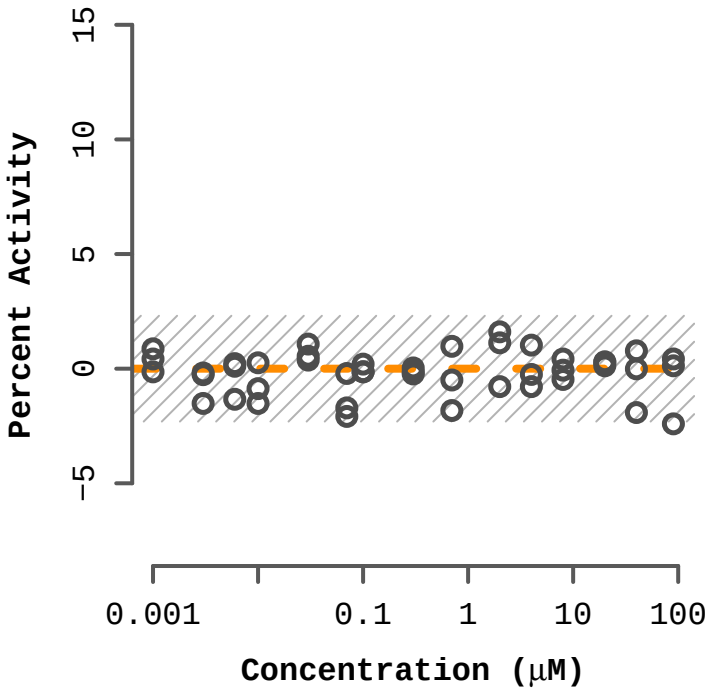
NAME: 4-Morpholinepropanesulfonic acid
CHID: 44371 **CASRN:** 1132-61-2
SPID(S): Tox21_302146
M4ID: 12476987

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

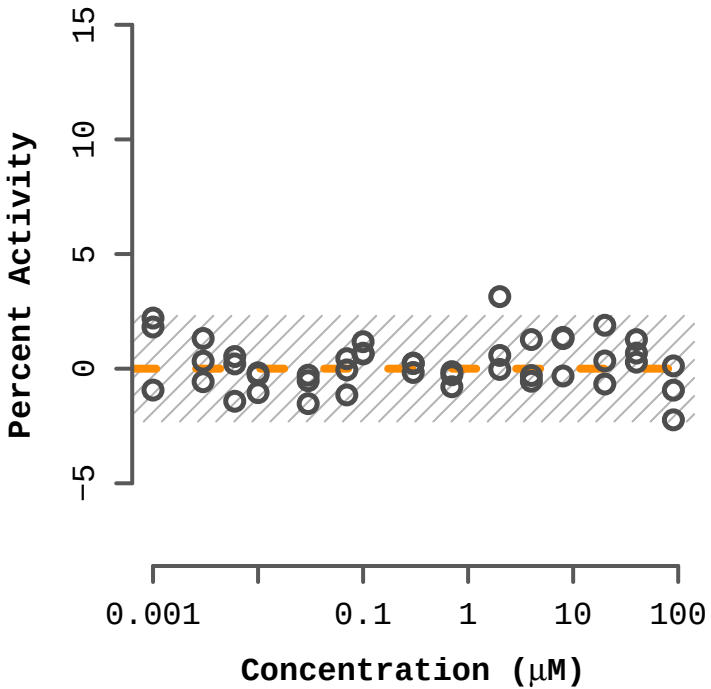
NAME: Tripropan-2-yl phosphite
CHID: 44372 **CASRN:** 116-17-6
SPID(S): Tox21_304011
M4ID: 12475177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.665 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

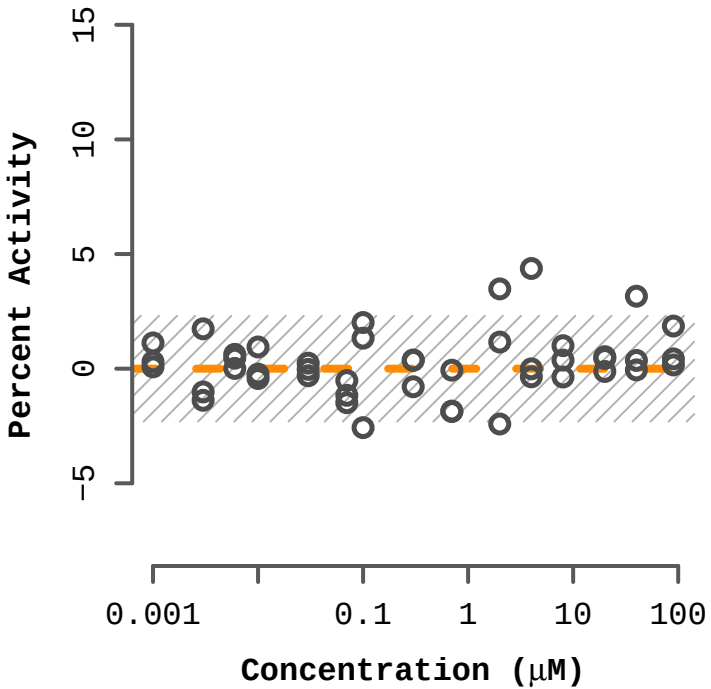
NAME: Tromethamine hydrochloride
CHID: 44373 **CASRN:** 1185-53-1
SPID(S): Tox21_302157
M4ID: 12476976

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

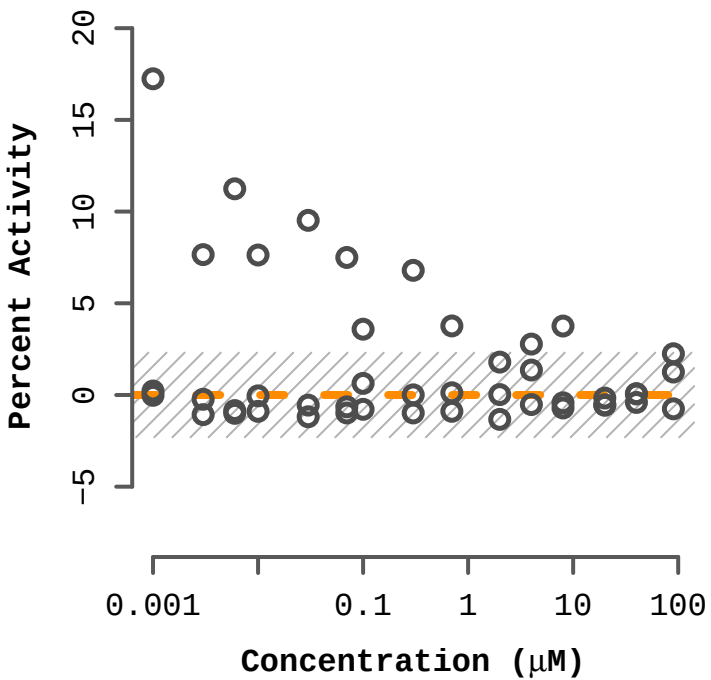
NAME: p-Methylacetophenone
CHID: 44374 **CASRN:** 122-00-9
SPID(S): Tox21_302023
M4ID: 12477110

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

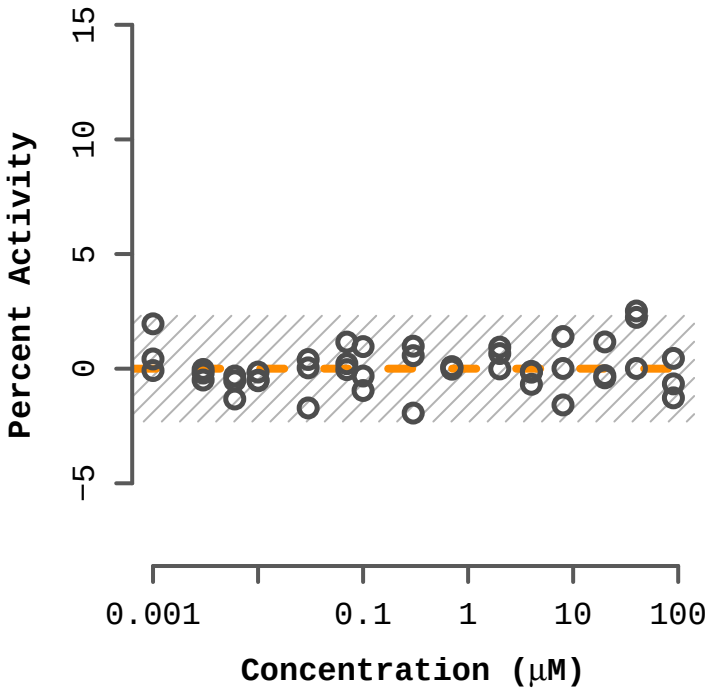
NAME: Glycerol 1-allylether
CHID: 44375 CASRN: 123-34-2
SPID(S): Tox21_302125
M4ID: 12477008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	236.37	NA	NA
PROB:	1	NA	NA
RMSE:	4.24	NA	NA

MAX_MEAN: 5.81 MAX_MED: 1.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

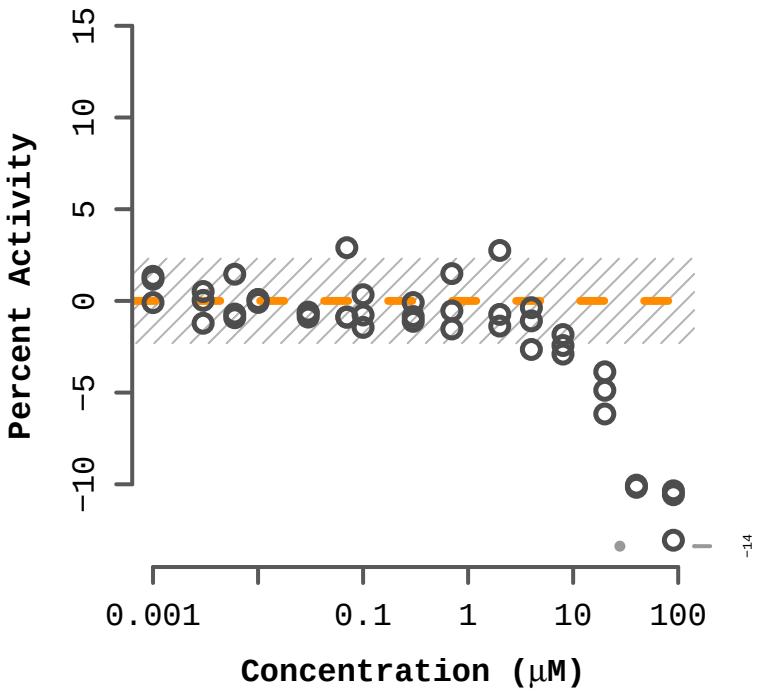
NAME: 2-Ethylhexyl cyanoacetate
CHID: 44378 **CASRN:** 13361-34-7
SPID(S): Tox21_302144
M4ID: 12476989

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

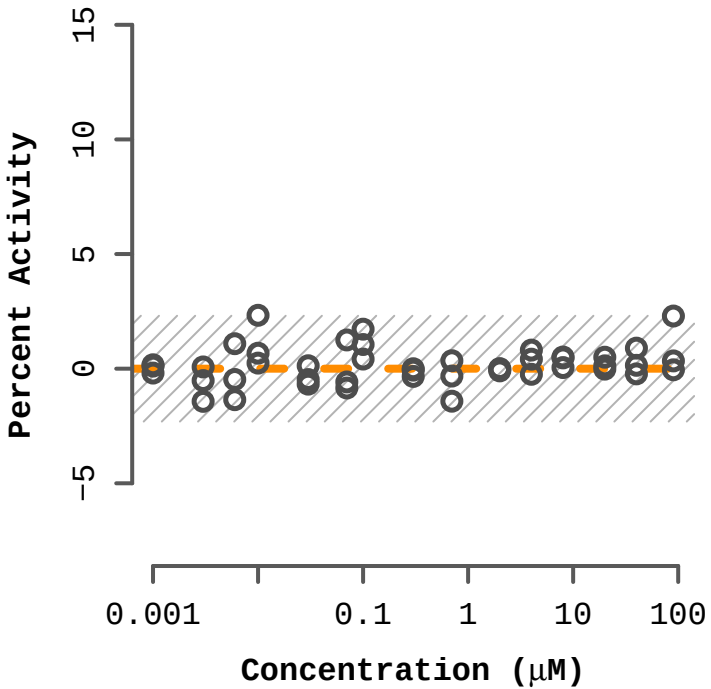
NAME: Gold trichloride
CHID: 44379 **CASRN:** 13453-07-1
SPID(S): Tox21_302116
M4ID: 12477017 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.19	NA	NA
PROB:	1	NA	NA
RMSE:	4.55	NA	NA

MAX_MEAN: 0.811 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

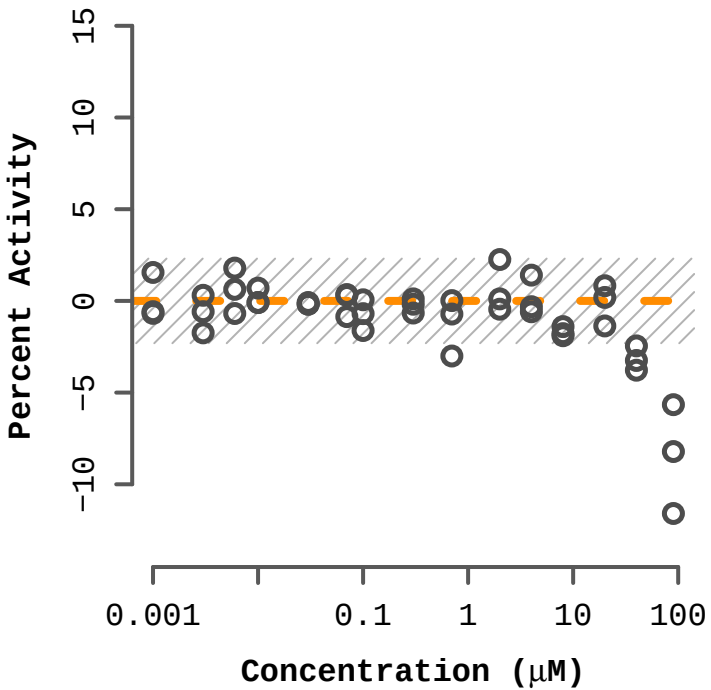
NAME: 1,2−Diphenylethanedione
CHID: 44380 CASRN: 134−81−6
SPID(S): Tox21_302031
M4ID: 12477102

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

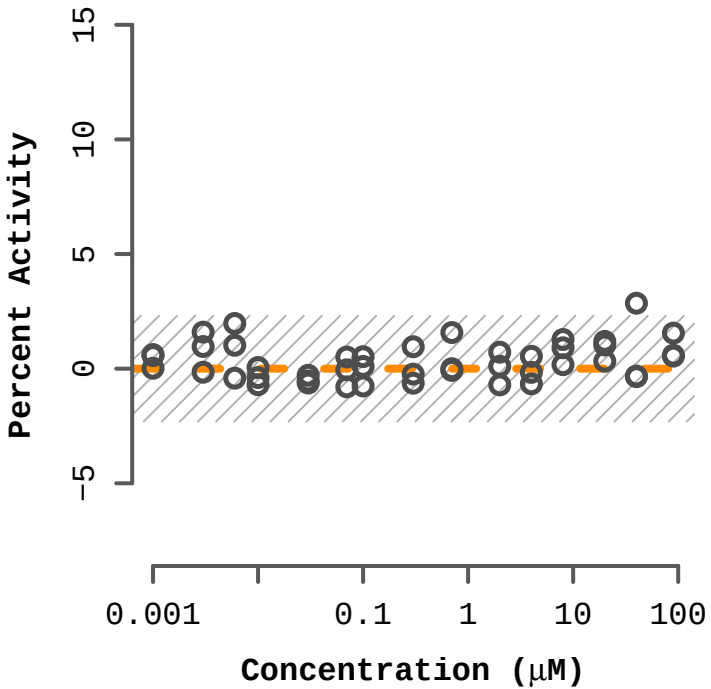
NAME: Bismaleimide
CHID: 44381 **CASRN:** 13676-54-5
SPID(S): Tox21_302064
M4ID: 12477069

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.8	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.632 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

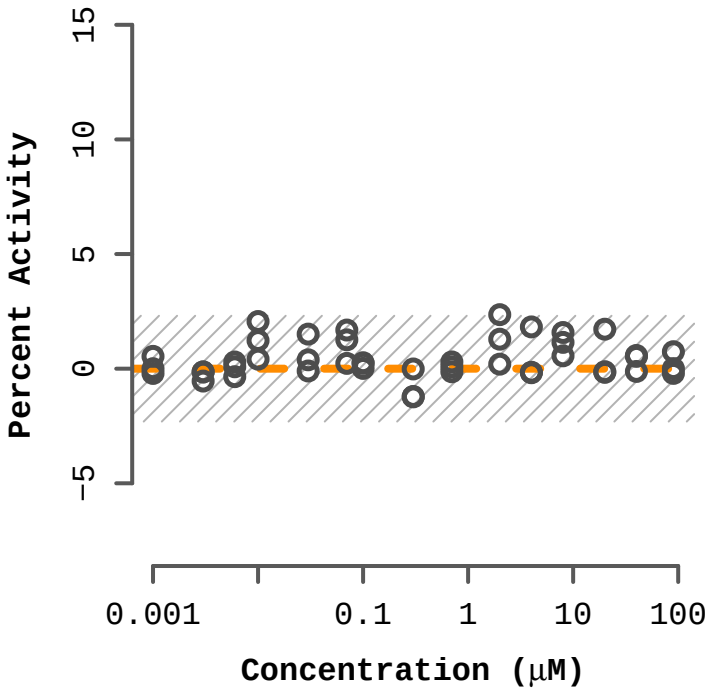
NAME: Thiamine thiozole
CHID: 44382 **CASRN:** 137-00-8
SPID(S): Tox21_302187
M4ID: 12476946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.897 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

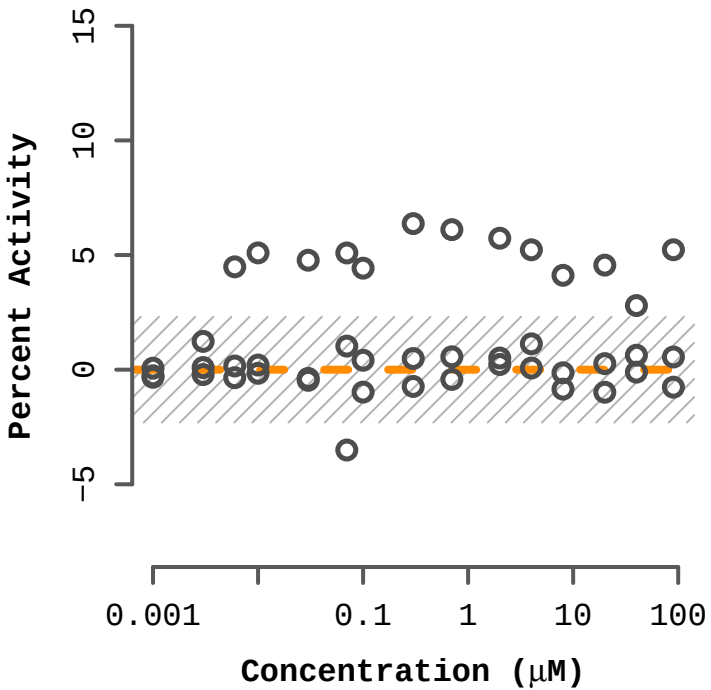
NAME: Diphenyl sulfide
CHID: 44383 **CASRN:** 139-66-2
SPID(S): Tox21_302182
M4ID: 12476951

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

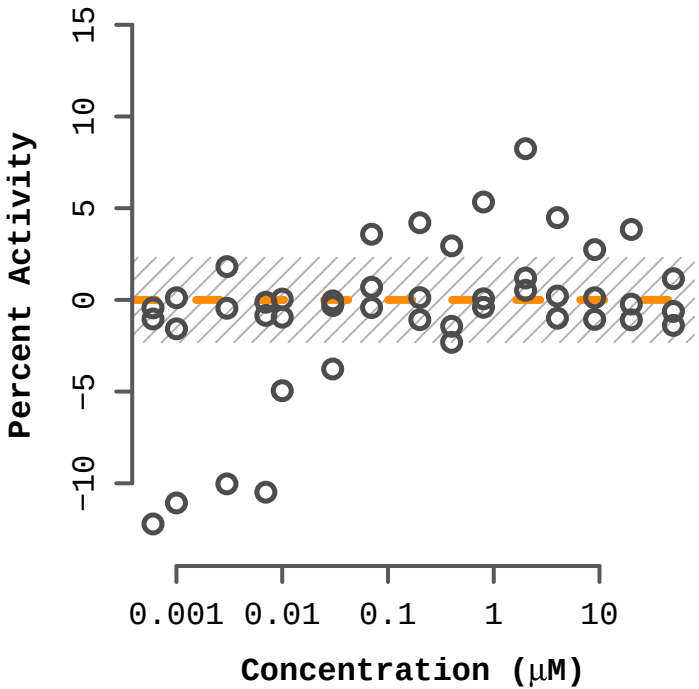
NAME: (2S,5R)-5-Methyl-2-(propan-2-yl)cyclohexanone
CHID: 44384 **CASRN:** 14073-97-3
SPID(S): Tox21_302153
M4ID: 12476980

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.78	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

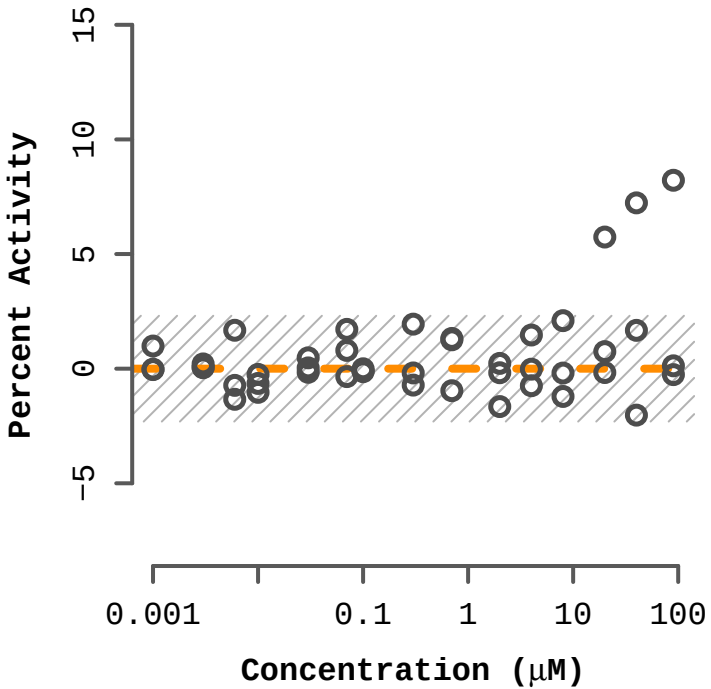
NAME: (2S,5R)-5-Methyl-2-(propan-2-yl)cyclohexanone
CHID: 44384 **CASRN:** 14073-97-3
SPID(S): Tox21_111510_1
M4ID: 12483644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.7	NA	NA
PROB:	1	NA	NA
RMSE:	4.02	NA	NA

MAX_MEAN: 3.32 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

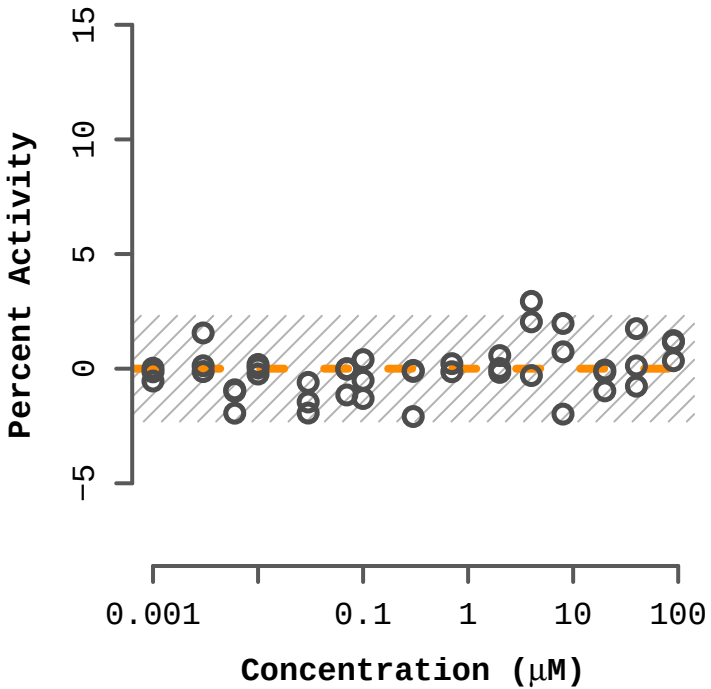
NAME: (2E)−3−Phenylprop−2−enenitrile
CHID: 44385 **CASRN:** 1885−38−7
SPID(S): Tox21_303789
M4ID: 12475399

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

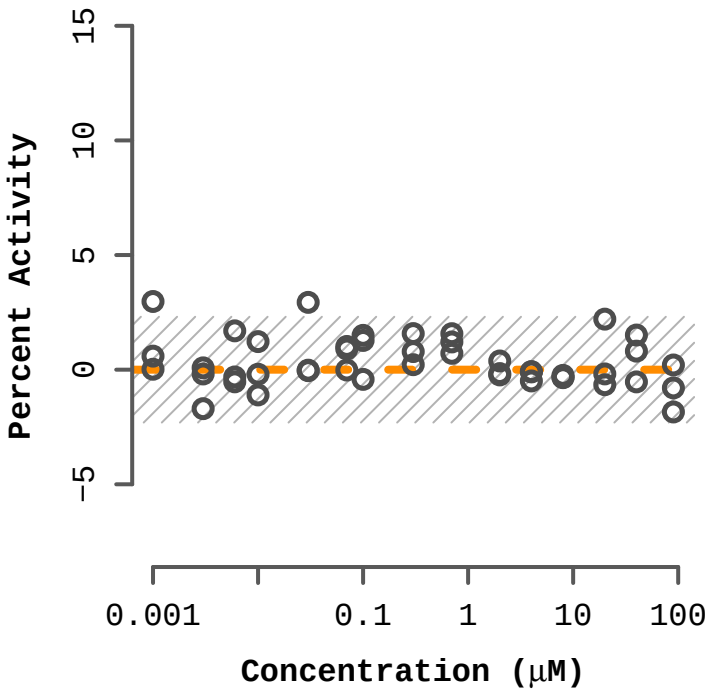
NAME: 2,2,6,6-Tetramethylpiperidin-4-amine
CHID: 44388 **CASRN:** 36768-62-4
SPID(S): Tox21_302132
M4ID: 12477001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

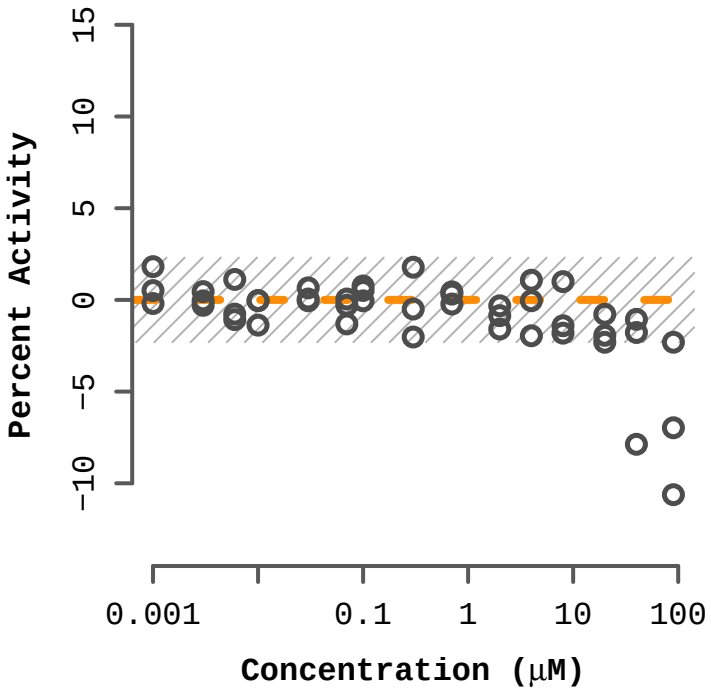
NAME: 3-Methoxy-3-methylbutan-1-ol
CHID: 44389 **CASRN:** 56539-66-3
SPID(S): Tox21_302115
M4ID: 12477018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

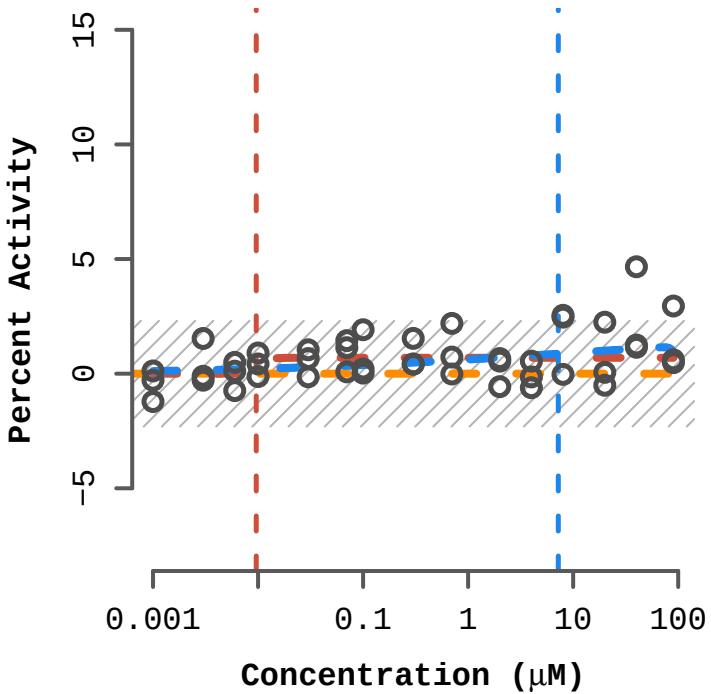
NAME: N-Methylhydrazinecarbothioamide
CHID: 44390 **CASRN:** 6610-29-3
SPID(S): Tox21_302172
M4ID: 12476961

HILL MODEL: Not applicable.

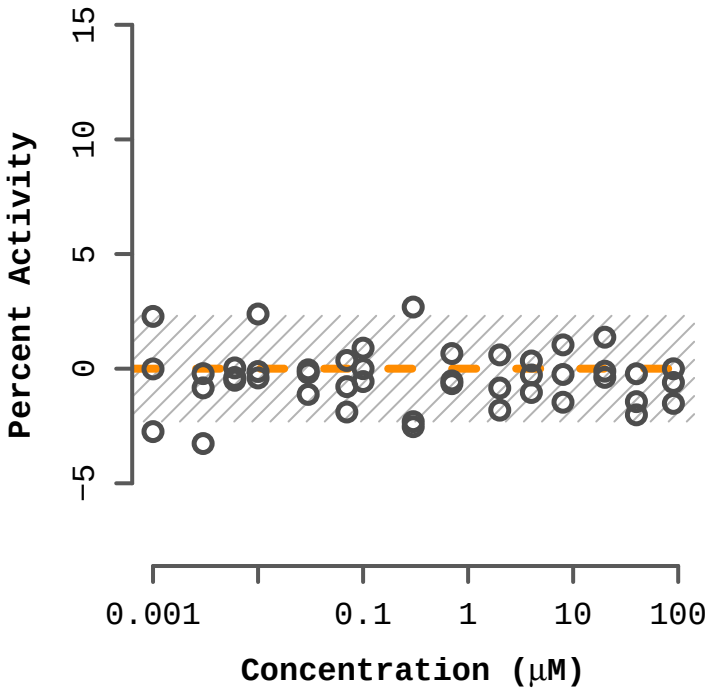
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.85	NA	NA
PROB:	1	NA	NA
RMSE:	2.48	NA	NA

MAX_MEAN: 0.71 **MAX_MED:** 0.517 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Isopropylphenol
CHID:    44391   CASRN: 88-69-7
SPID(S): Tox21_302062
M4ID:    12477071

HILL MODEL (in red):
      tp       ga       gw
val:  0.693    -2.02    8
sd:   0.167    0.152    36.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.74     0.858    0.3      1.99     16.4
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  146.73      135.11      140.35
PROB: 0           0.93        0.07
RMSE: 1.3         1.05        1.03

MAX_MEAN: 2.36      MAX_MED: 2.47      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

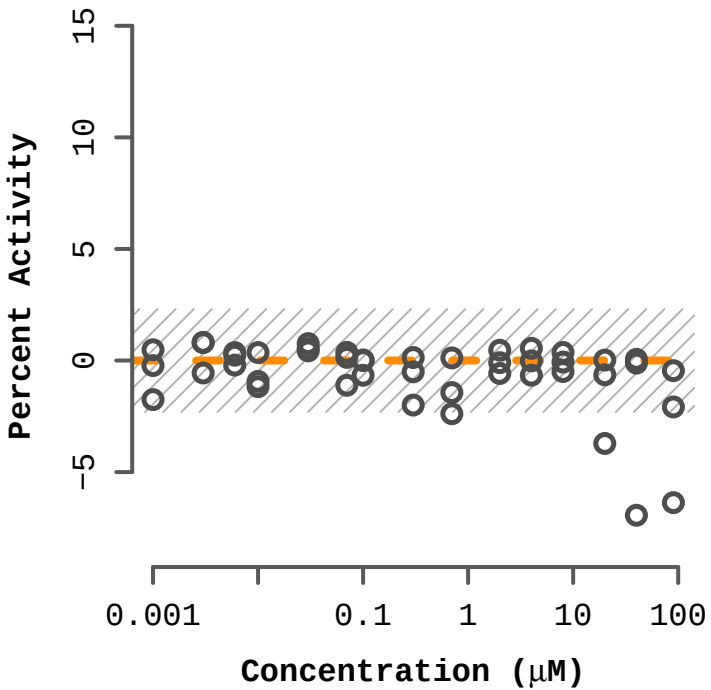
NAME: 2-Methoxynaphthalene
CHID: 44392 **CASRN:** 93-04-9
SPID(S): Tox21_302143
M4ID: 12476990

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.62 **MAX_MED:** 0.0027 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

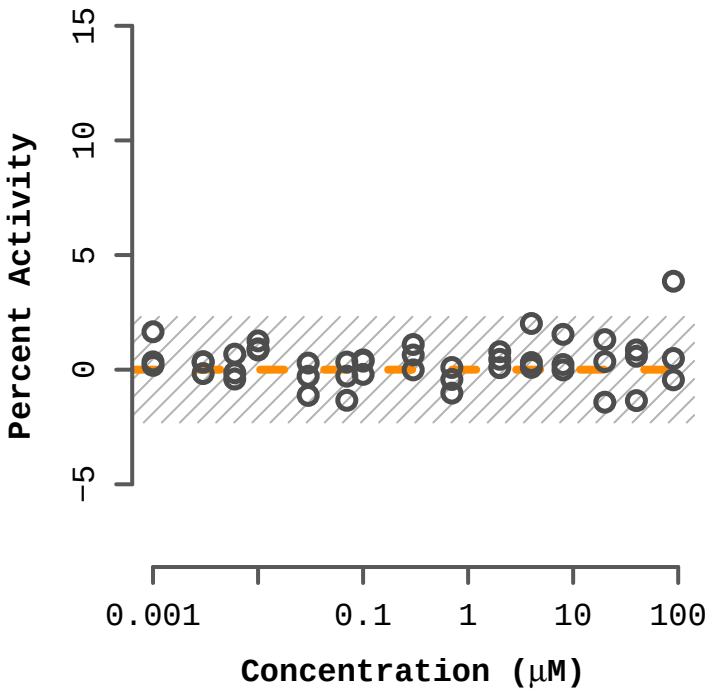
NAME: Dimethylglyoxime
CHID: 44393 CASRN: 95-45-4
SPID(S): Tox21_302169
M4ID: 12476964

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 0.808 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

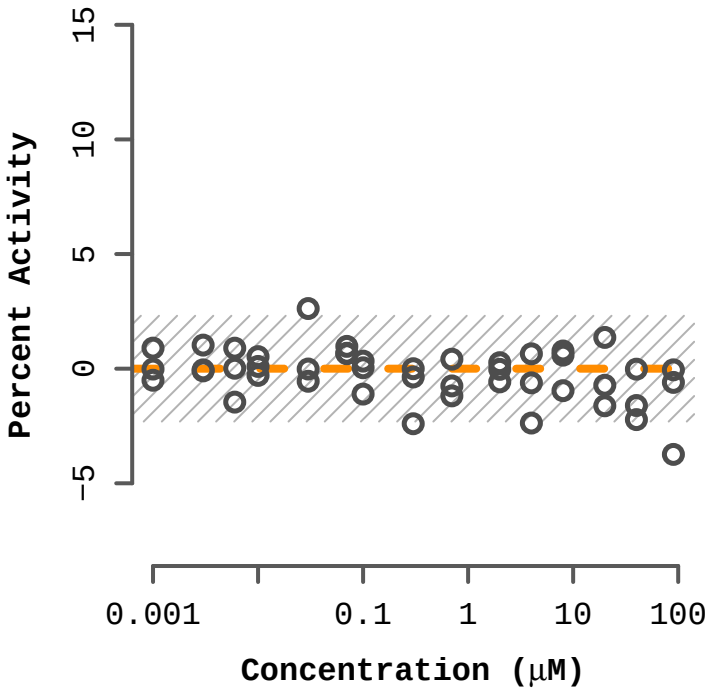
NAME: 4-tert-Butylcyclohexanone
CHID: 44394 **CASRN:** 98-53-3
SPID(S): Tox21_302032
M4ID: 12477101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.911 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

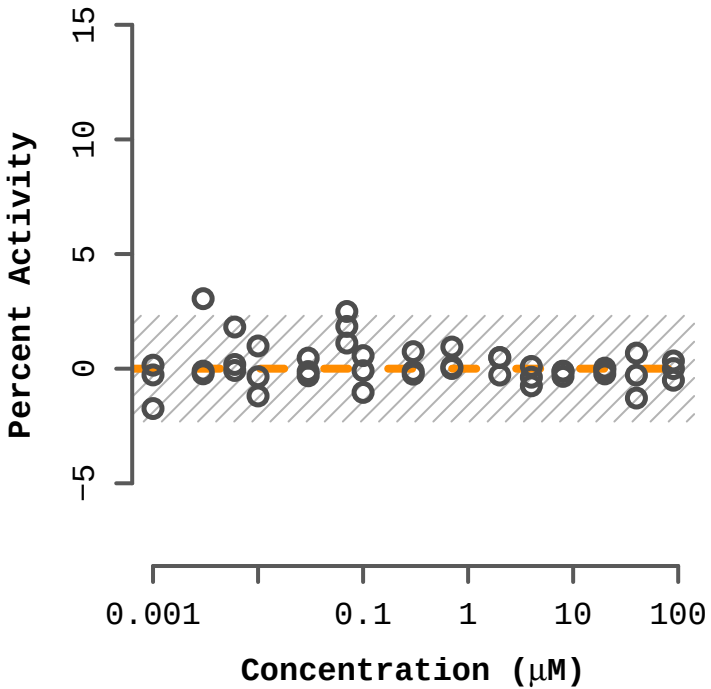
NAME: 1-Bromododecane
CHID: 44395 CASRN: 143-15-7
SPID(S): Tox21_302046
M4ID: 12477087

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.768 **MAX_MED:** 0.674 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

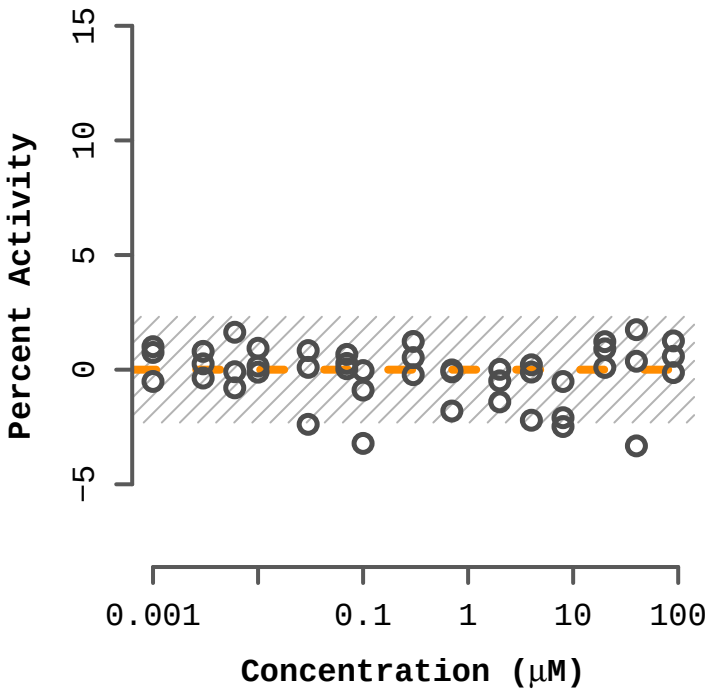
NAME: 2,5,8,11,14−Pentaoxapentadecane
CHID: 44396 CASRN: 143−24−8
SPID(S): Tox21_302147
M4ID: 12476986

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

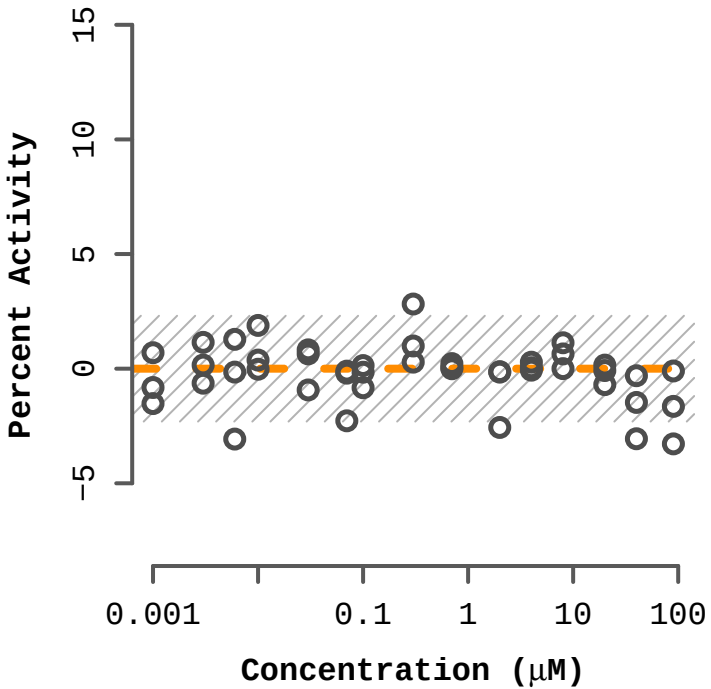
NAME: Trifluoromethanesulfonic acid
CHID: 44397 **CASRN:** 1493-13-6
SPID(S): Tox21_302183
M4ID: 12476950

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.744 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

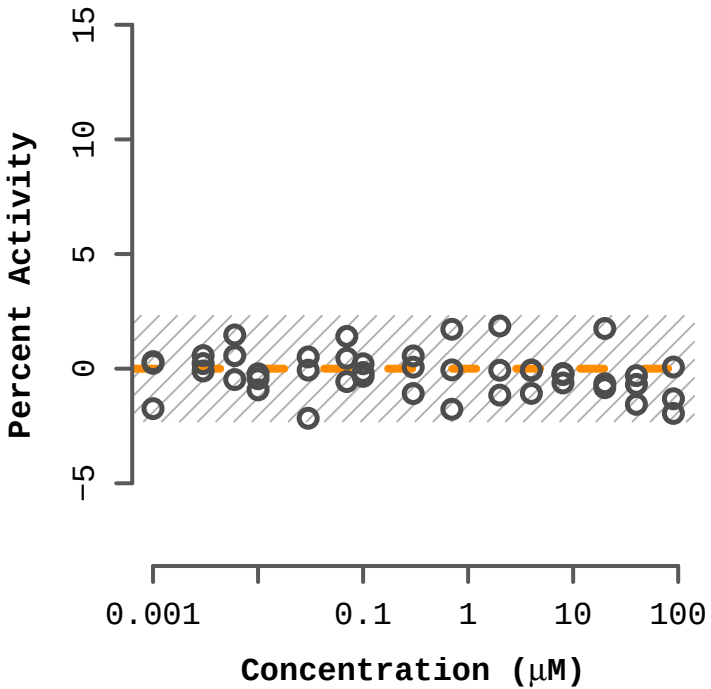
NAME: N,N'−Penta−1,3−dien−1−yl−5−ylidenedianiline hy
CHID: 44398 CASRN: 1497−49−0
SPID(S): Tox21_302102
M4ID: 12477031

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.37 MAX_MED: 0.992 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

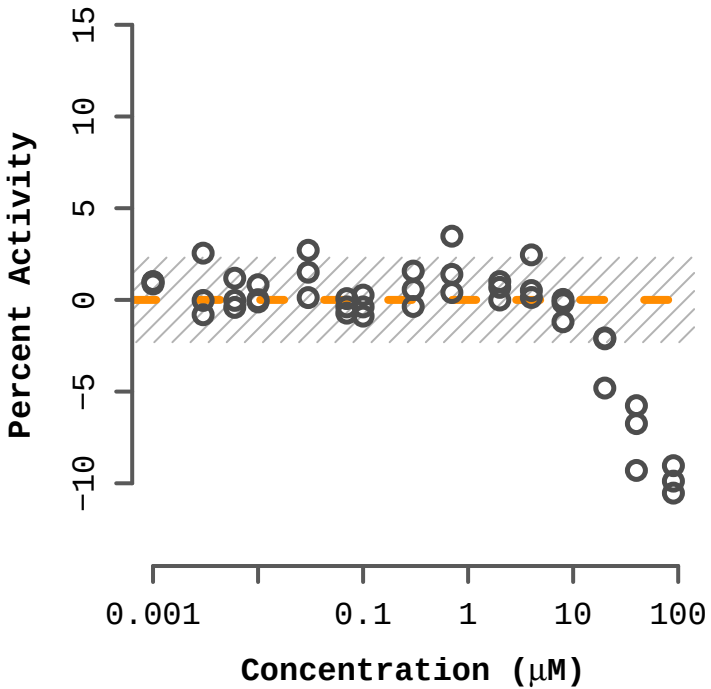
NAME: Phenylphosphonic acid
CHID: 44399 CASRN: 1571-33-1
SPID(S): Tox21_302060
M4ID: 12477073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.523 **MAX_MED:** 0.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

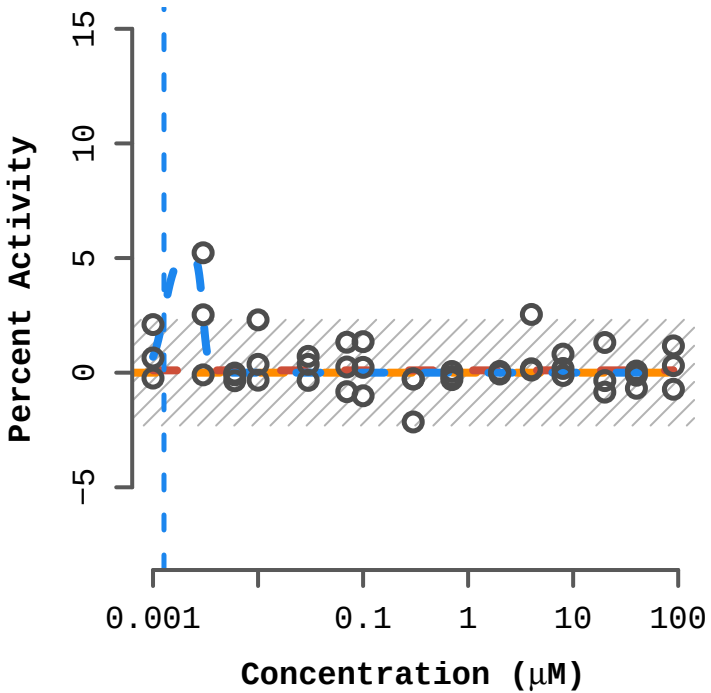
NAME: Tetrabutylammonium bromide
CHID: 44400 CASRN: 1643-19-2
SPID(S): Tox21_302149
M4ID: 12476984

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	223.25	NA	NA
PROB:	1	NA	NA
RMSE:	3.45	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzenecarboximidamide, monohydrochloride
CHID: 44401 CASRN: 1670-14-0
SPID(S): Tox21_302165
M4ID: 12476968

HILL MODEL (in red):

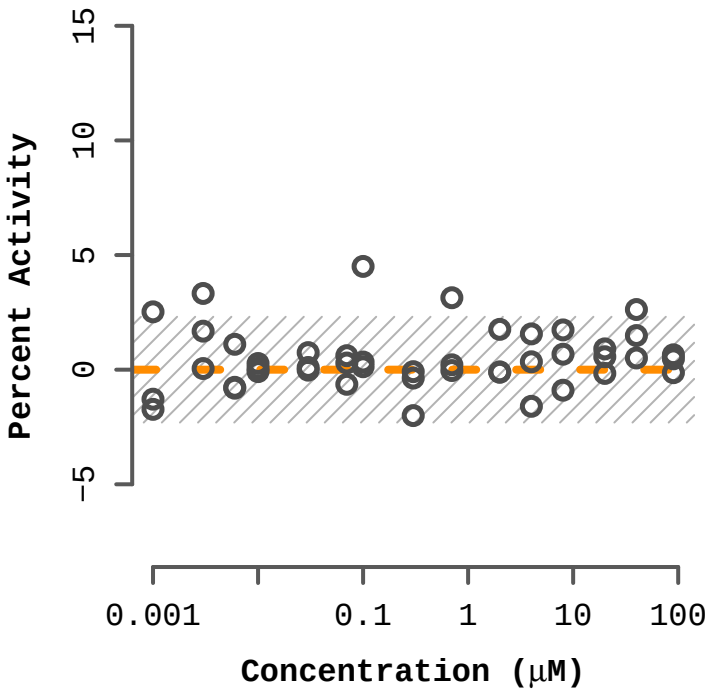
	tp	ga	gw
val:	0.101	−4.89	3.41
sd:	0.123	1270	2280

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.28	−2.9	7.86	−2.53	17.9
sd:	8.81	0.385	33.1	0.0332	537

	CNST	HILL	GNLS
AIC:	131.5	136.8	134.3
PROB:	0.76	0.05	0.19
RMSE:	1.23	1.2	1.01

MAX_MEAN: 2.56 MAX_MED: 2.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

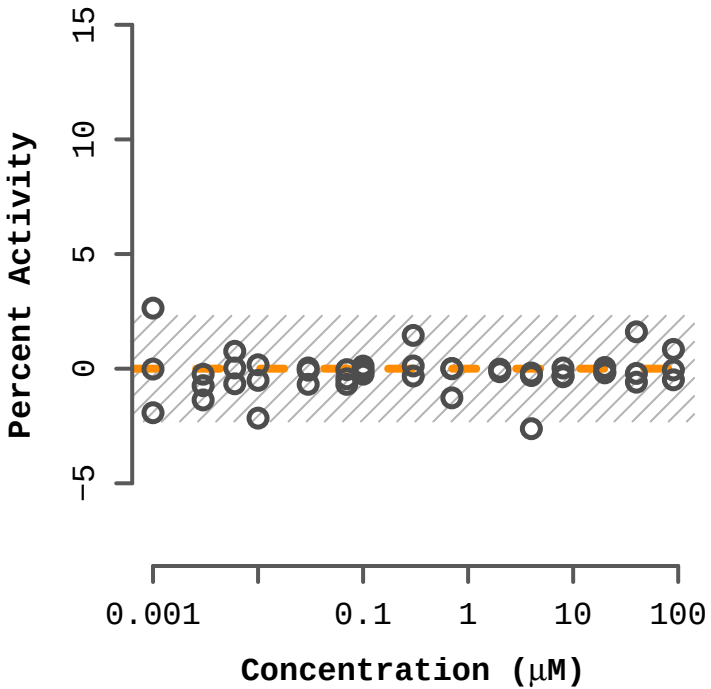
NAME: tert-Butyl 3-oxobutanoate
CHID: 44402 **CASRN:** 1694-31-1
SPID(S): Tox21_302057
M4ID: 12477076

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

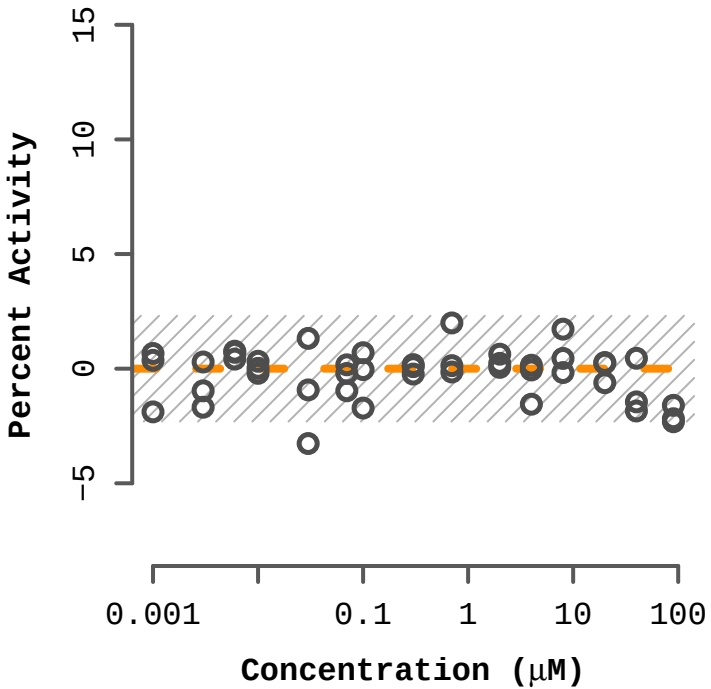
NAME: Phenyl carbonochloridate
CHID: 44403 CASRN: 1885-14-9
SPID(S): Tox21_303763
M4ID: 12475425

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.418 MAX_MED: 0.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

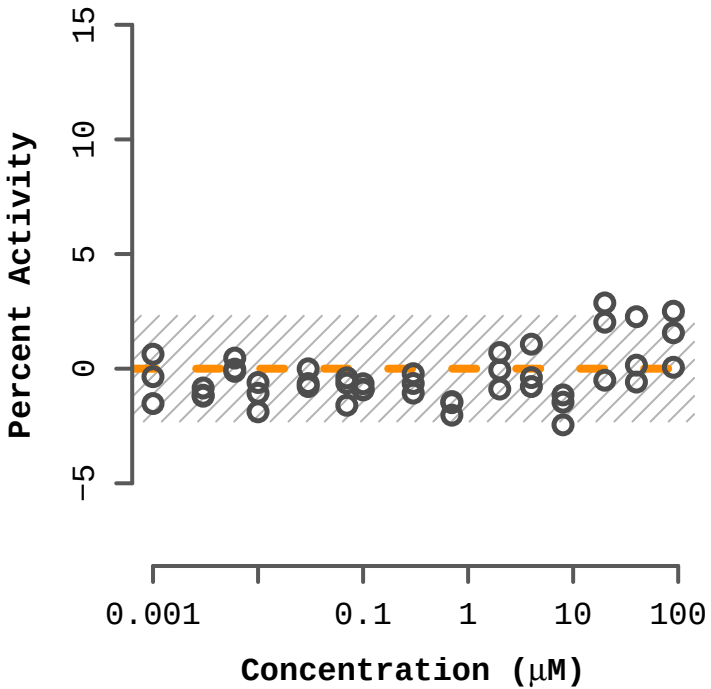
NAME: 2-Hydroxyethyl disulfide
CHID: 44404 CASRN: 1892-29-1
SPID(S): Tox21_302181
M4ID: 12476952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.669 MAX_MED: 0.716 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

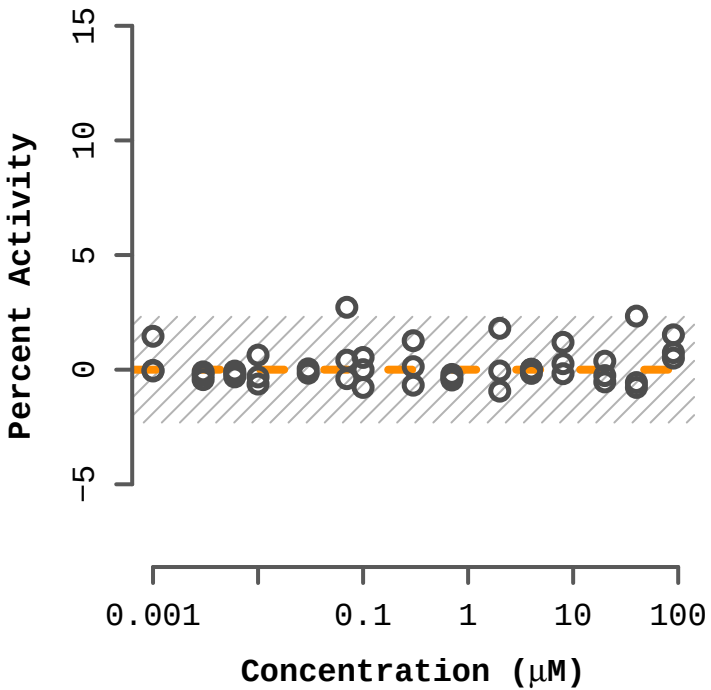
NAME: Aminoguanidine hydrochloride
CHID: 44405 **CASRN:** 1937-19-5
SPID(S): Tox21_302098
M4ID: 12477035

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

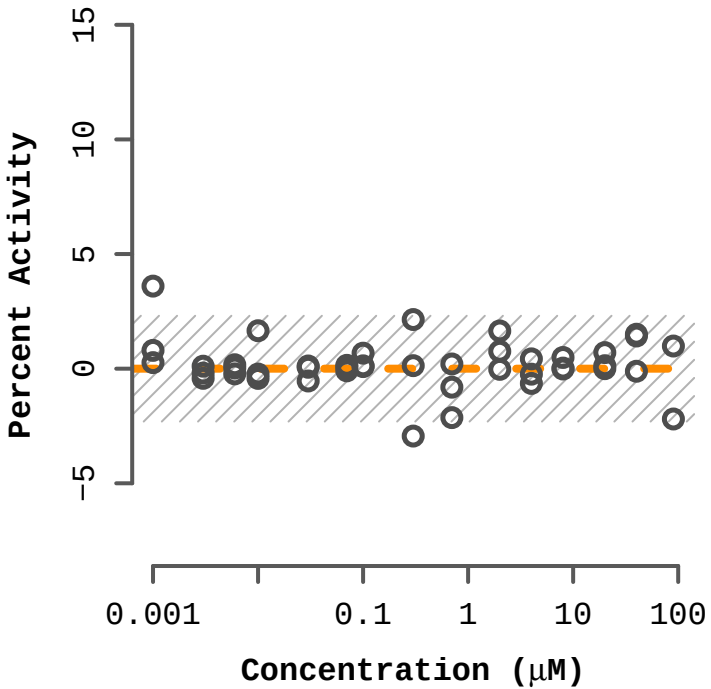
NAME: 3-Amino-4-methylbenzamide
CHID: 44407 **CASRN:** 19406-86-1
SPID(S): Tox21_302118
M4ID: 12477015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.925 **MAX_MED:** 0.747 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

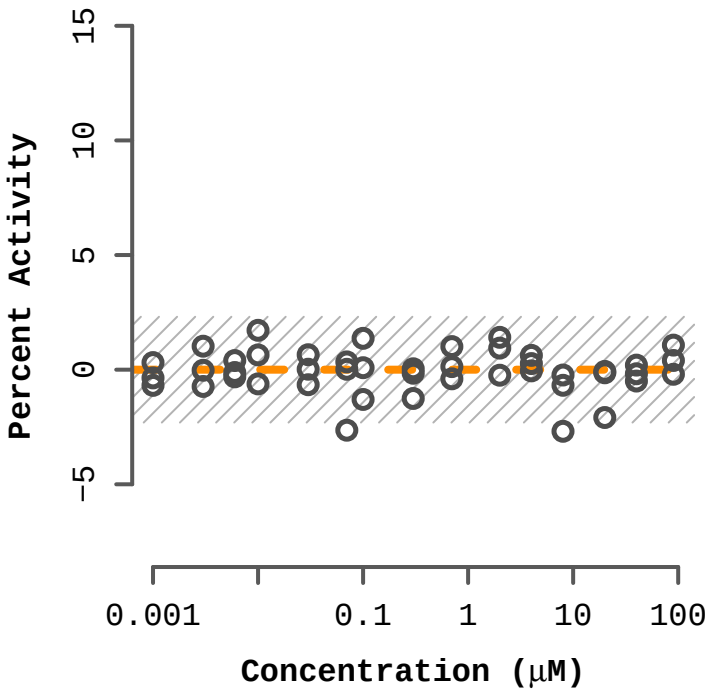
NAME: 2-Morpholinoethylamine
CHID: 44408 **CASRN:** 2038-03-1
SPID(S): Tox21_302071
M4ID: 12477062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

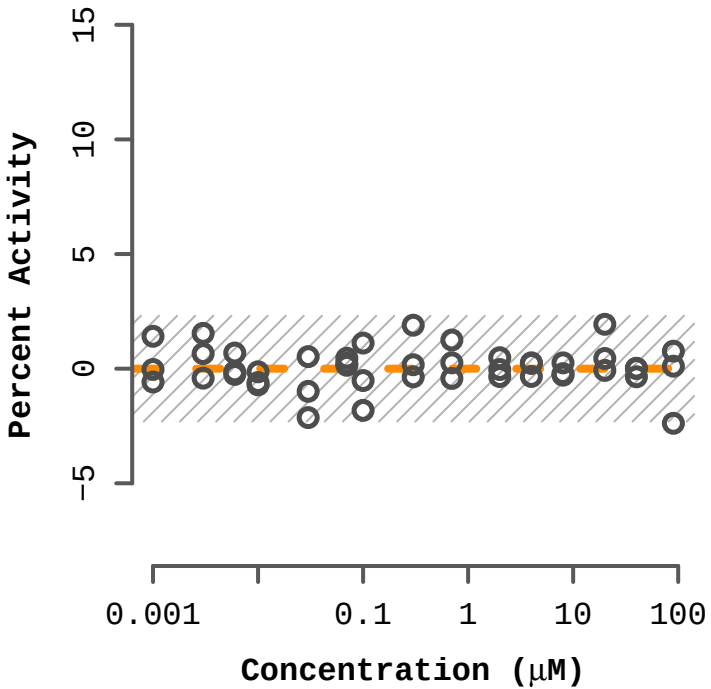
NAME: 1,6-Dichlorohexane
CHID: 44409 **CASRN:** 2163-00-0
SPID(S): Tox21_302121
M4ID: 12477012

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.704 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

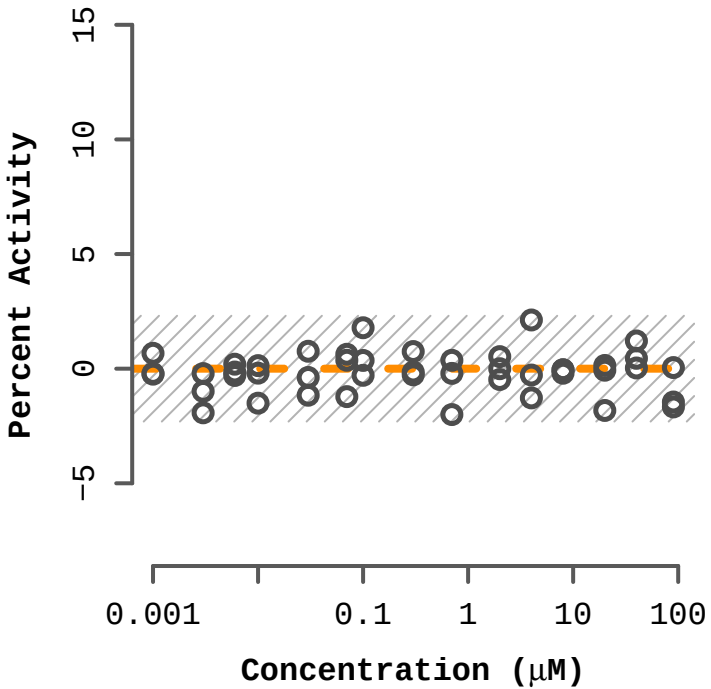
NAME: Potassium 2,5-dihydroxybenzenesulfonate
CHID: 44410 **CASRN:** 21799-87-1
SPID(S): Tox21_302096
M4ID: 12477037

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.769 **MAX_MED:** 0.659 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

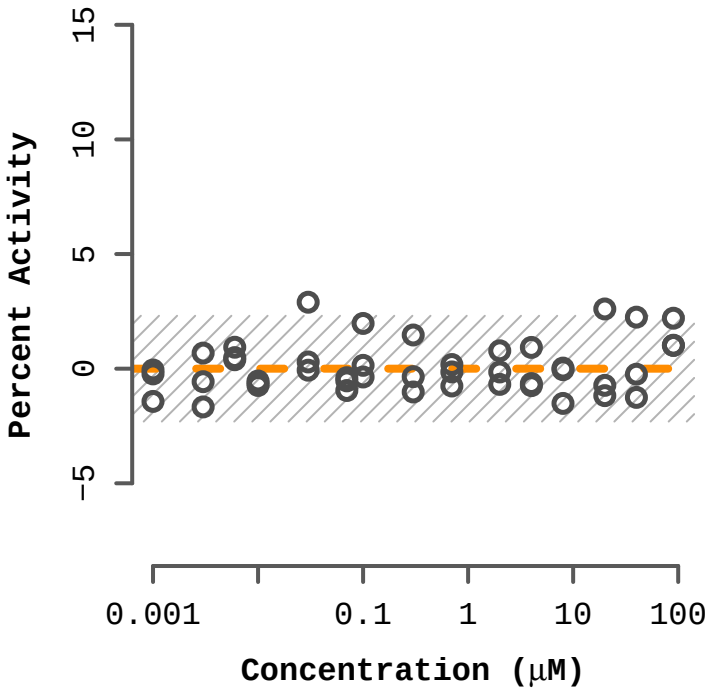
NAME: 1,2,2,6,6-Pentamethylpiperidin-4-ol
CHID: 44411 **CASRN:** 2403-89-6
SPID(S): Tox21_302077
M4ID: 12477056

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.62 **MAX_MED:** 0.452 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

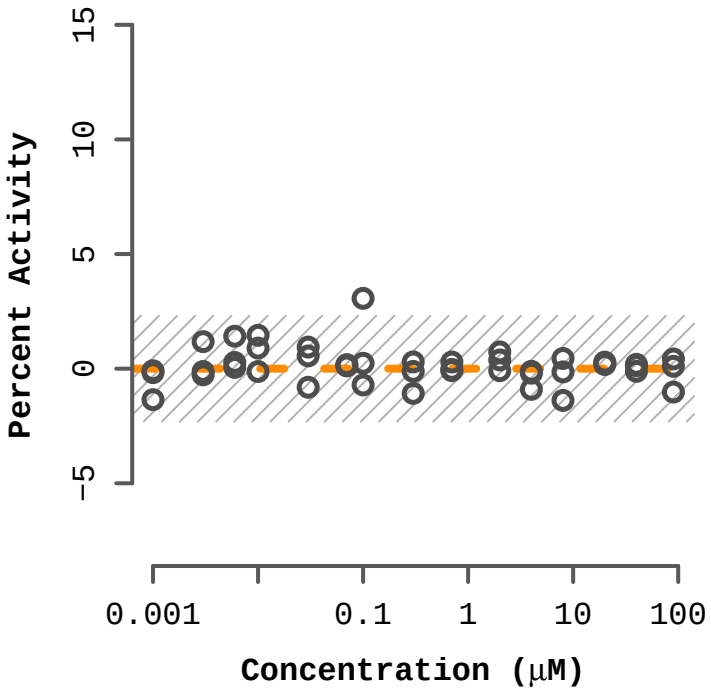
NAME: 4-Methyl-1-phenylpyrazolidin-3-one
CHID: 44412 CASRN: 2654-57-1
SPID(S): Tox21_302042
M4ID: 12477091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

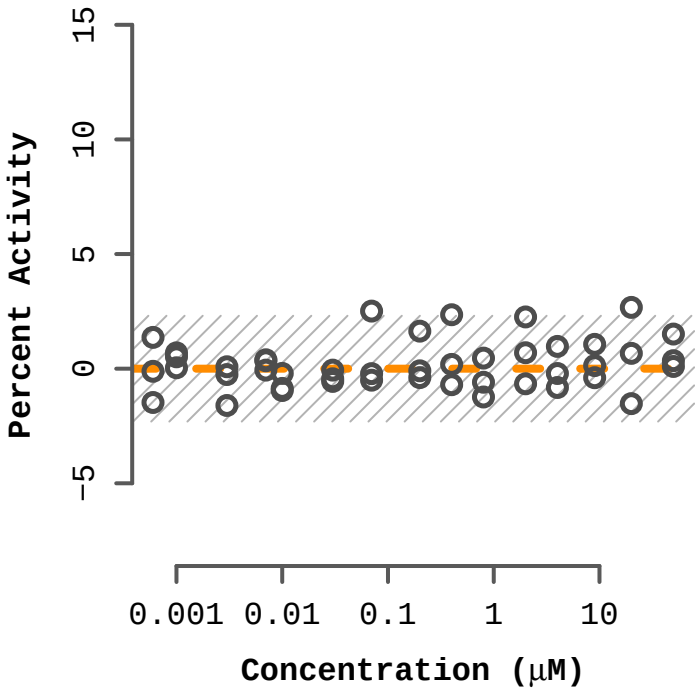
NAME: 1-Ethyl-2-pyrrolidinone
CHID: 44413 **CASRN:** 2687-91-4
SPID(S): Tox21_302140
M4ID: 12476993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.866 **MAX_MED:** 0.901 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

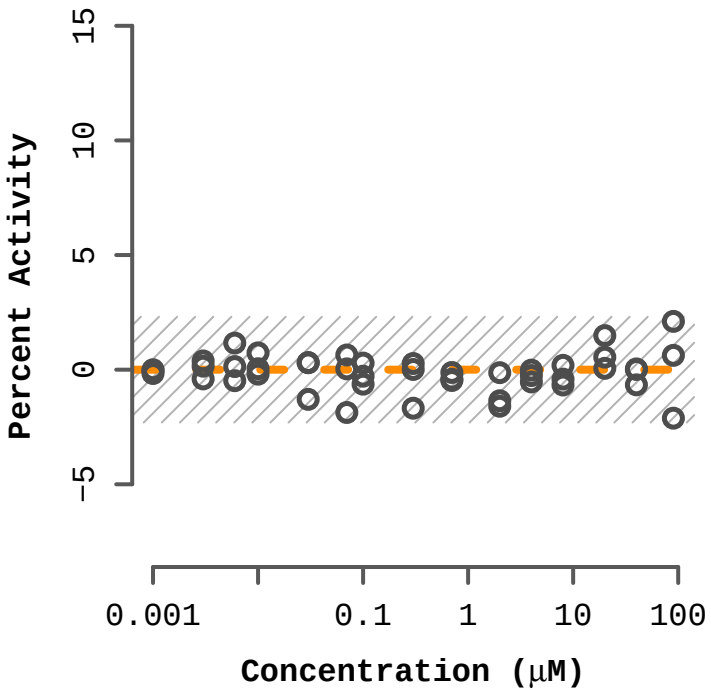
NAME: 1-Ethyl-2-pyrrolidinone
CHID: 44413 **CASRN:** 2687-91-4
SPID(S): Tox21_111935_1
M4ID: 12483423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.766 **MAX_MED:** 0.697 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

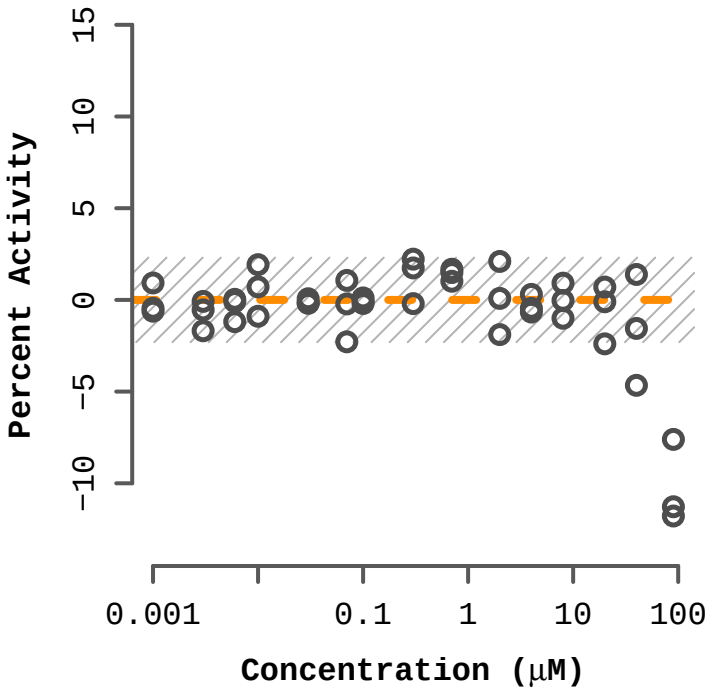
NAME: 3-Amino-4-chlorobenzoic acid
CHID: 44414 **CASRN:** 2840-28-0
SPID(S): Tox21_302124
M4ID: 12477009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.698 **MAX_MED:** 0.626 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

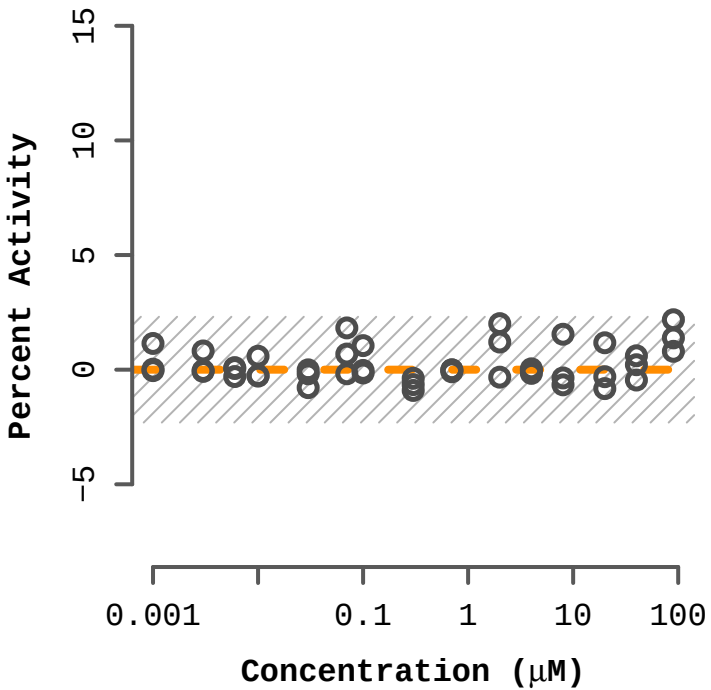
NAME: N,N'−1,3−Phenylenedimaleimide
CHID: 44415 CASRN: 3006−93−7
SPID(S): Tox21_303753
M4ID: 12475435

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.97	NA	NA

MAX_MEAN: 1.4 MAX_MED: 1.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

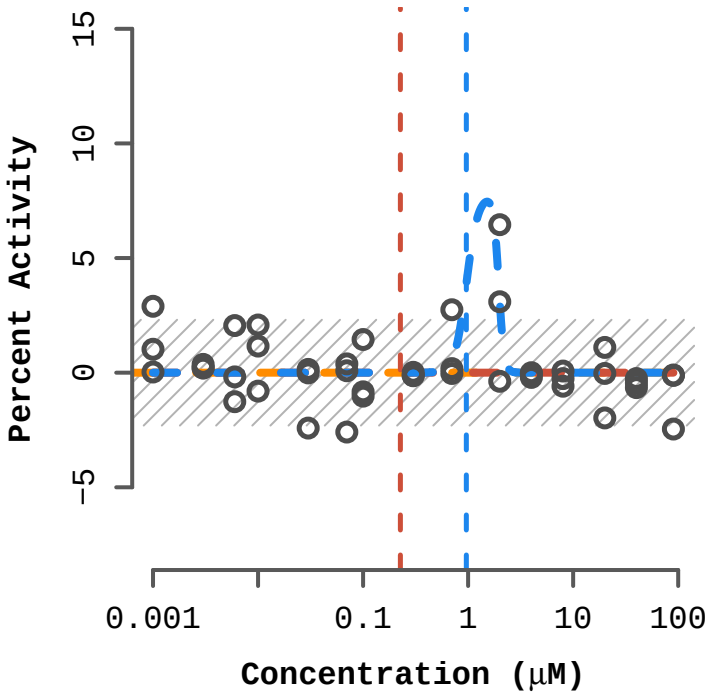
NAME: 1,2,4−Butanetriol
CHID: 44416 **CASRN:** 3068−00−6
SPID(S): Tox21_303969
M4ID: 12475219

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenol Red sodium salt
CHID: 44420 CASRN: 34487-61-1
SPID(S): Tox21_302131
M4ID: 12477002

HILL MODEL (in red):

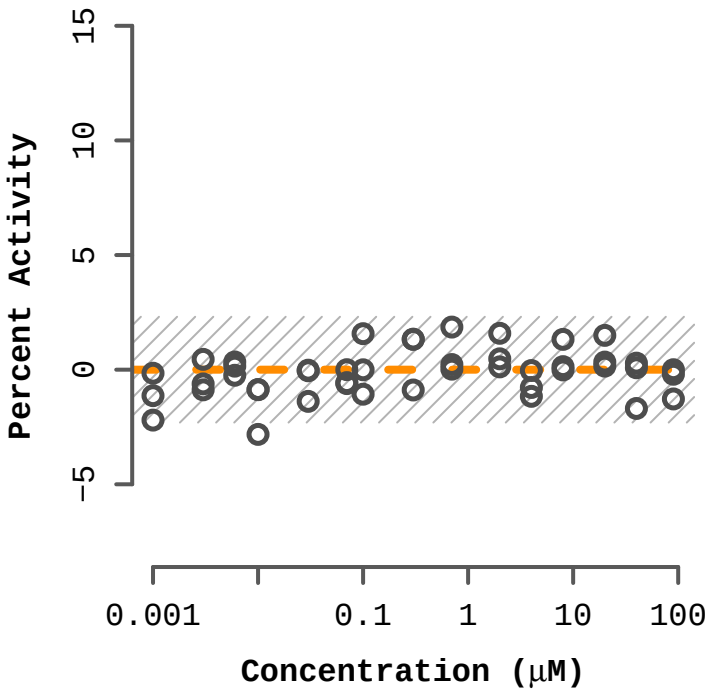
	tp	ga	gw
val:	8.91e-11	-0.645	0.719
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.75	-0.017	7.99	0.291	17.4
sd:	139	1.7	75.4	0.562	504

	CNST	HILL	GNLS
AIC:	156.73	162.73	161.01
PROB:	0.86	0.04	0.1
RMSE:	1.56	1.56	1.33

MAX_MEAN: 3.06 MAX_MED: 3.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

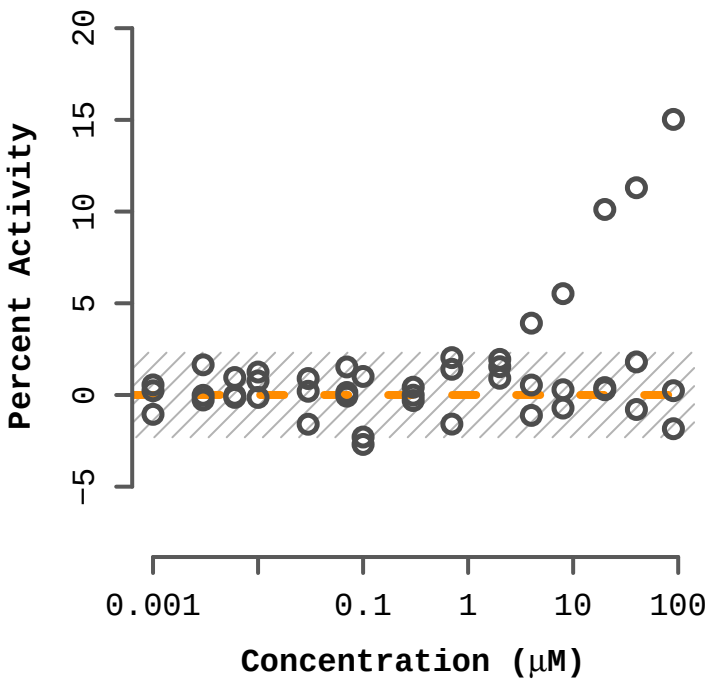
NAME: 3-Acetylpyridine
CHID: 44421 **CASRN:** 350-03-8
SPID(S): Tox21_302119
M4ID: 12477014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.76	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.729 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

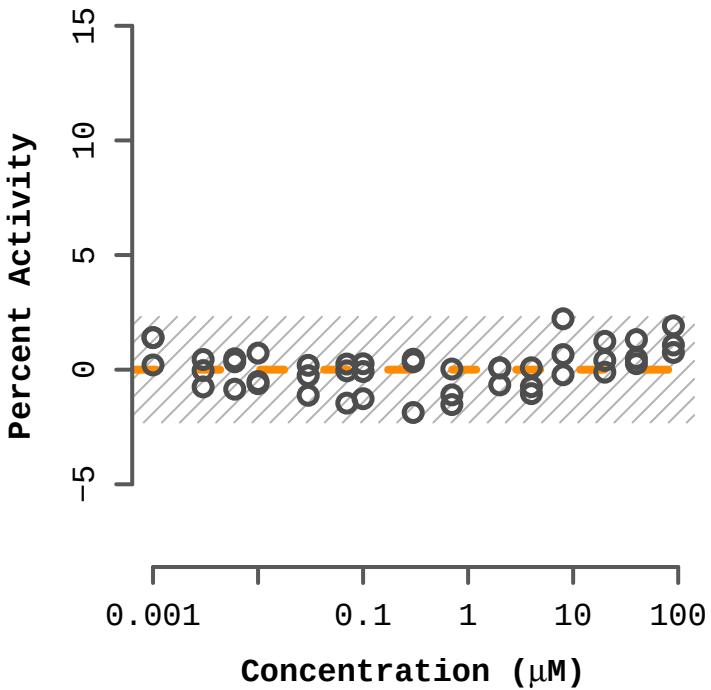
NAME: N-(2-Aminoethyl)-N'-[3-(trimethoxysilyl)propyl]
CHID: 44422 CASRN: 35141-30-1
SPID(S): Tox21_303768
M4ID: 12475420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.31	NA	NA
PROB:	1	NA	NA
RMSE:	3.51	NA	NA

MAX_MEAN: 4.47 MAX_MED: 1.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

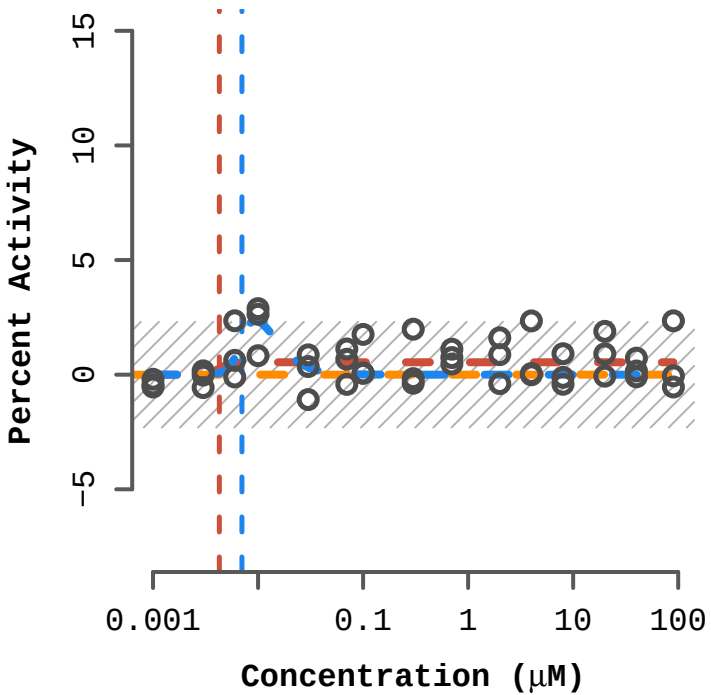
NAME: N−(Chloromethylidene)−N−methylmethanaminium ch
CHID: 44423 CASRN: 3724−43−4
SPID(S): Tox21_302163
M4ID: 12476970

HILL MODEL: Not applicable.

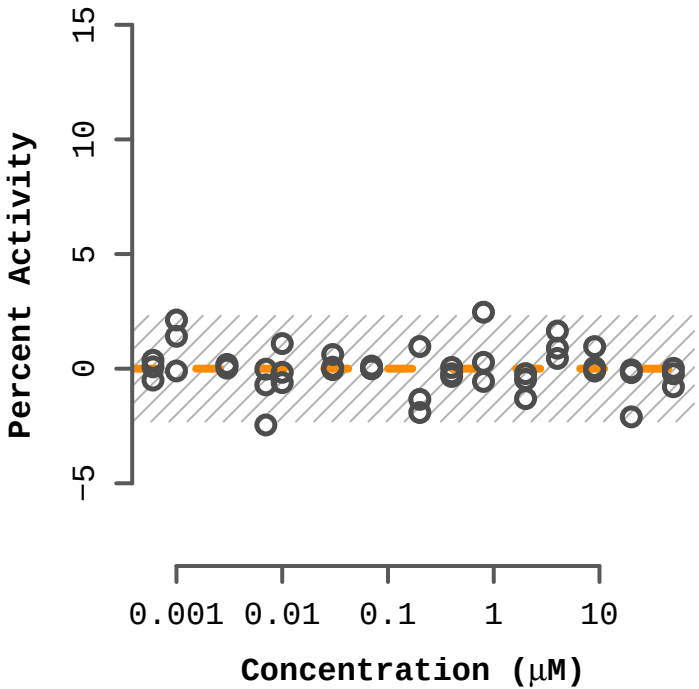
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.4 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-(Aminomethyl)pyridine
CHID:    44424   CASRN: 3731-52-0
SPID(S): Tox21_302074
M4ID:    12477059

HILL MODEL (in red):
      tp       ga       gw
val:  0.541    -2.37    8
sd:   0.153    0.235    11.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.46     -2.15    7.66     -1.86    2.95
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  137.79      131.14      134.46
PROB: 0.03        0.82        0.15
RMSE: 1.12        0.94        0.95

MAX_MEAN: 2.12      MAX_MED: 2.64      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

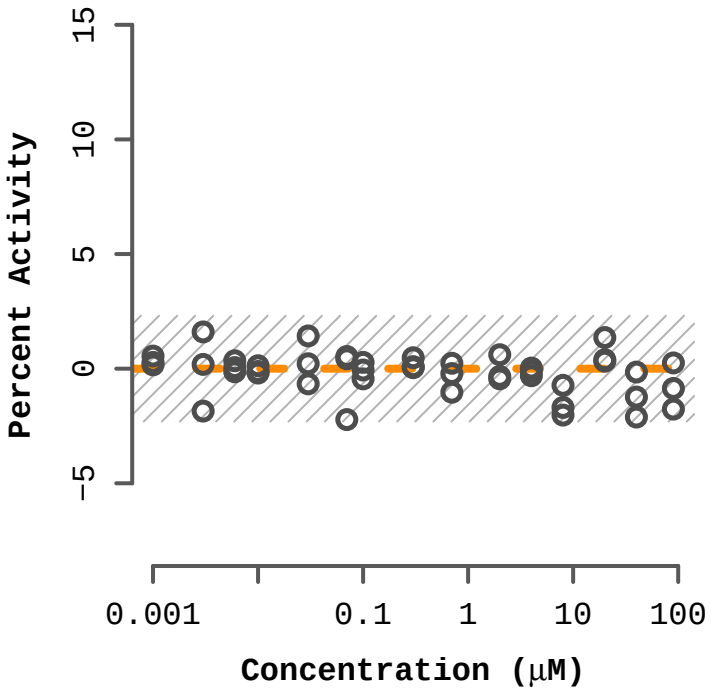
NAME: 3-(Aminomethyl)pyridine
CHID: 44424 **CASRN:** 3731-52-0
SPID(S): Tox21_112325_1
M4ID: 12483161

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

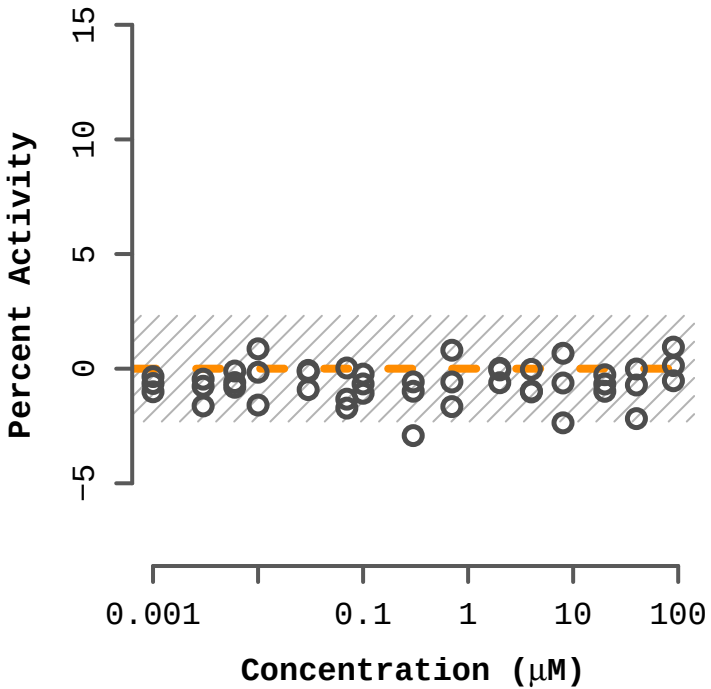
NAME: Monomethyl succinate
CHID: 44425 **CASRN:** 3878-55-5
SPID(S): Tox21_302188
M4ID: 12476945

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.694 **MAX_MED:** 0.432 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

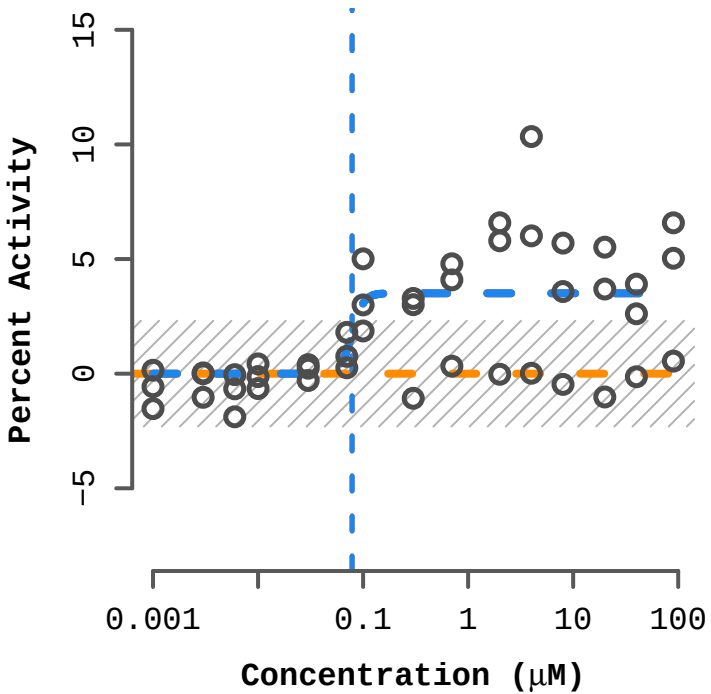
NAME: 4-Morpholinecarboxaldehyde
CHID: 44427 **CASRN:** 4394-85-8
SPID(S): Tox21_302027
M4ID: 12477106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.184 **MAX_MED:** 0.137 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Mercaptopropyltrimethoxysilane
CHID: 44428 CASRN: 4420-74-0
SPID(S): Tox21_302177
M4ID: 12476956

HILL MODEL (in red):

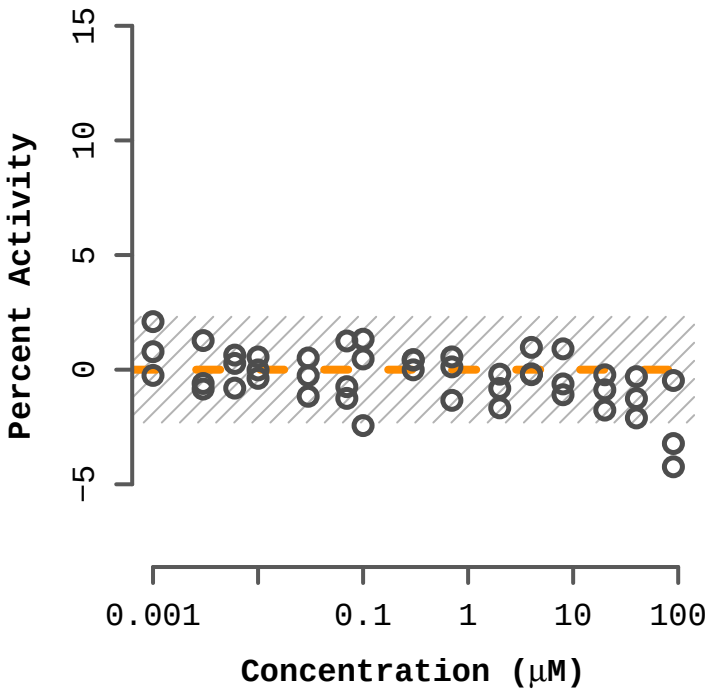
	tp	ga	gw
val:	3.51	-1.1	8
sd:	0.502	0.0653	7.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.51	-1.1	8	2.4	16.9
sd:	0.502	0.0653	7.7	218	8230

	CNST	HILL	GNLS
AIC:	237.11	205.18	209.18
PROB:	0	0.88	0.12
RMSE:	3.38	2.21	2.21

MAX_MEAN: 5.46 MAX_MED: 6.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

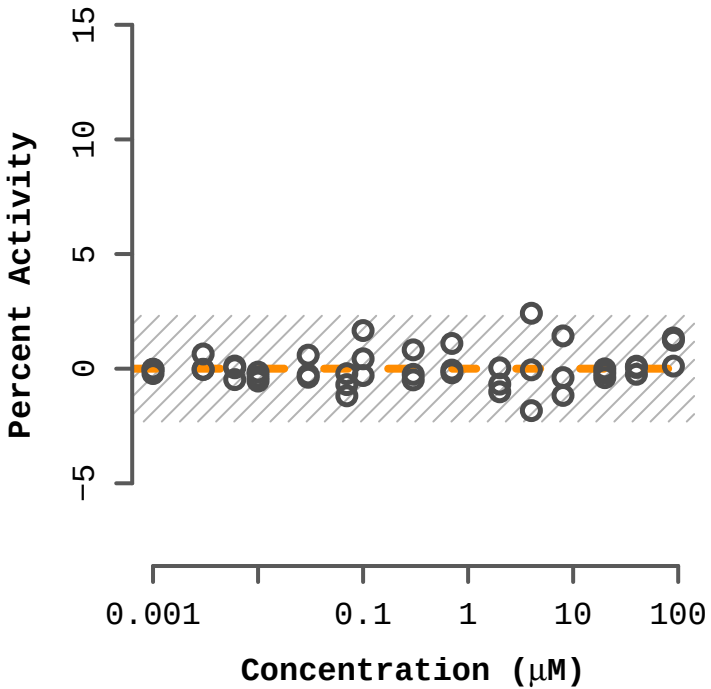
NAME: 1,3,5−Benzenetricarbonyl trichloride
CHID: 44429 **CASRN:** 4422−95−1
SPID(S): Tox21_302180
M4ID: 12476953

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 0.785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

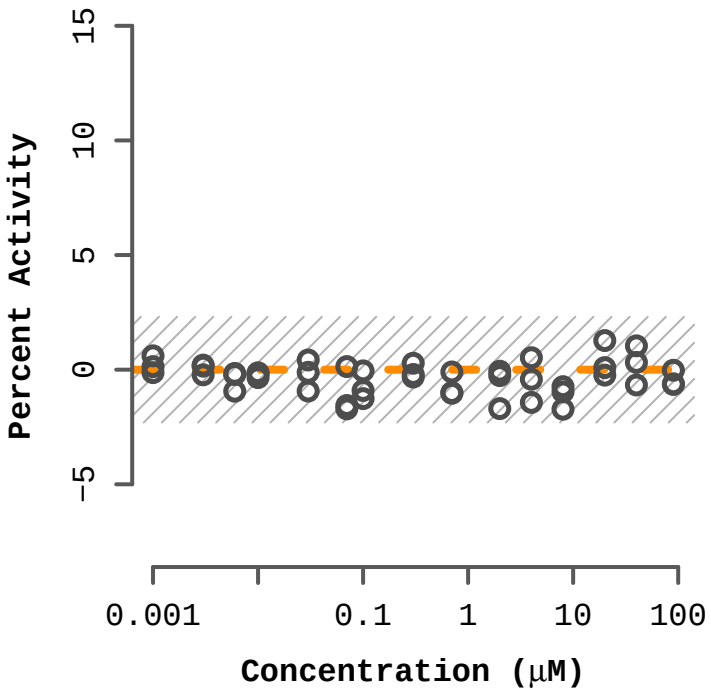
NAME: 1,2−Diphenylethanone
CHID: 44430 **CASRN:** 451−40−1
SPID(S): Tox21_302159
M4ID: 12476974

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.898 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

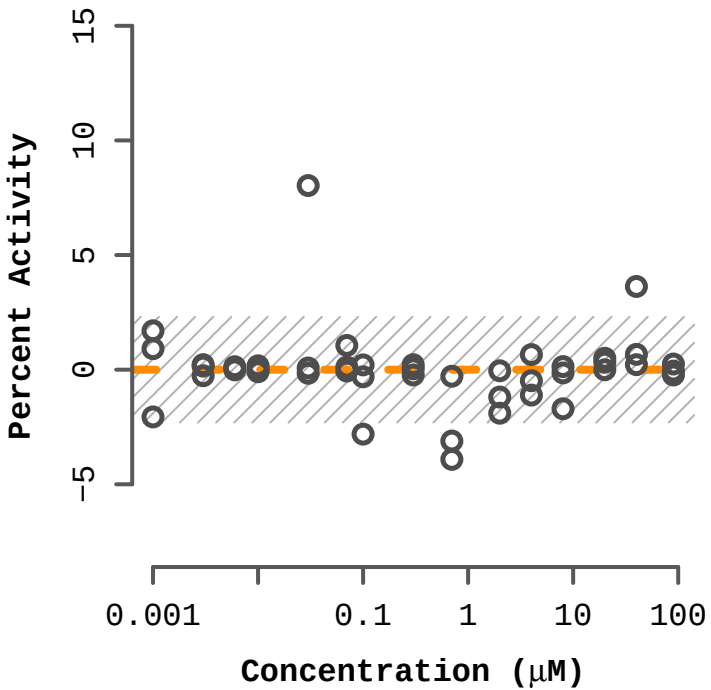
NAME: 2-(tert-Butylamino)ethanol
CHID: 44431 CASRN: 4620-70-6
SPID(S): Tox21_302058
M4ID: 12477075

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.376 **MAX_MED:** 0.318 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

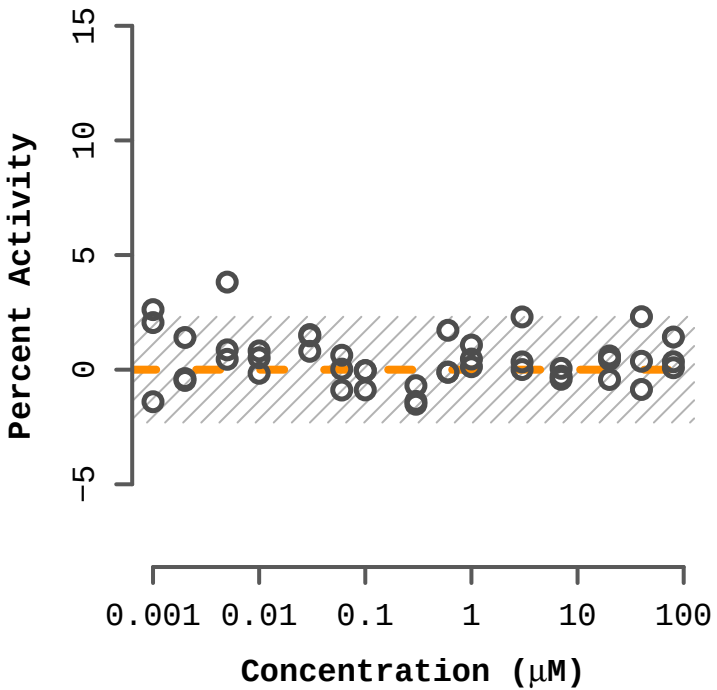
NAME: 1,3-Cyclohexanedione
CHID: 44433 CASRN: 504-02-9
SPID(S): Tox21_302158
M4ID: 12476975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 2.65 MAX_MED: 0.917 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

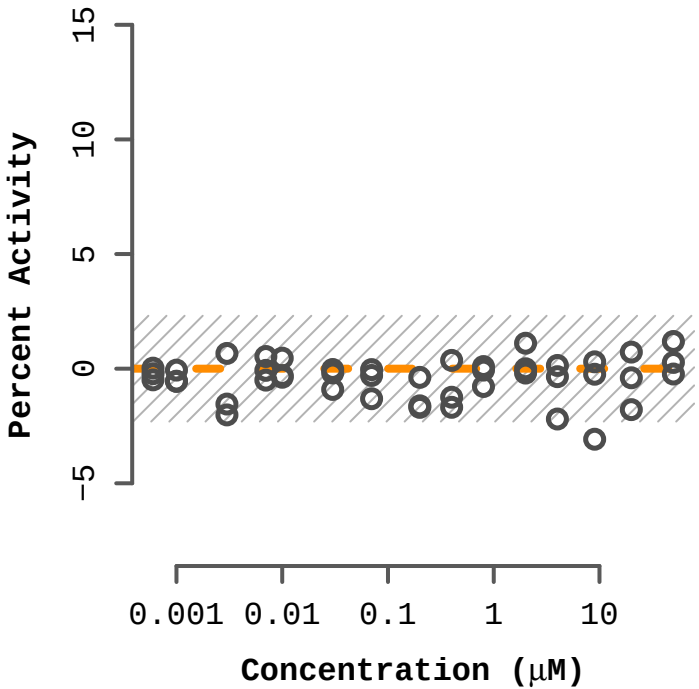
NAME: Procaine hydrochloride
CHID: 44435 CASRN: 51-05-8
SPID(S): Tox21_302114
M4ID: 12477019

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

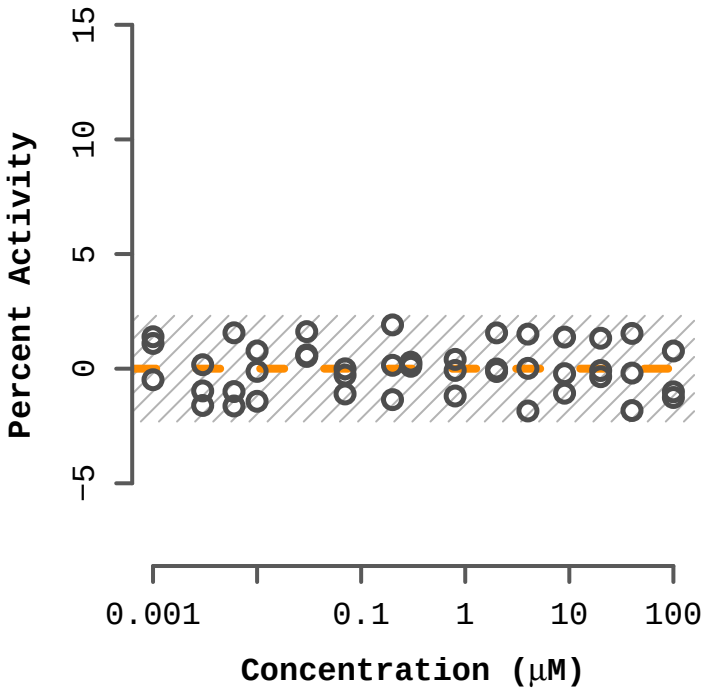
NAME: Procaine hydrochloride
CHID: 44435 **CASRN:** 51-05-8
SPID(S): Tox21_110248_1
M4ID: 12484516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.41 **MAX_MED:** 0.274 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

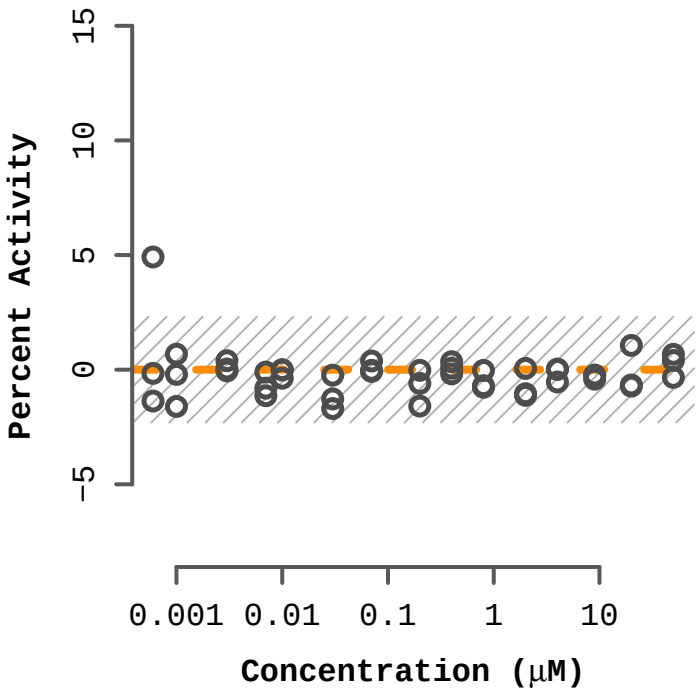
NAME: 3-Acetyldihydro-2(3H)-furanone
CHID: 44436 CASRN: 517-23-7
SPID(S): Tox21_302029
M4ID: 12477104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.92 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

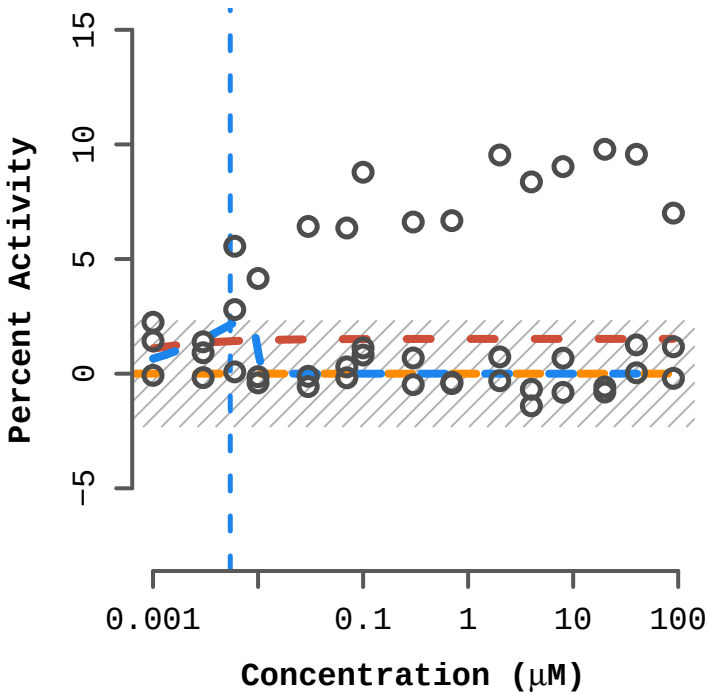
NAME: 3-Acetyldihydro-2(3H)-furanone
CHID: 44436 **CASRN:** 517-23-7
SPID(S): Tox21_113848
M4ID: 12482374

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,5−Diaminobenzoic acid
CHID: 44437 CASRN: 535−87−5
SPID(S): Tox21_302048
M4ID: 12477085

HILL MODEL (in red):

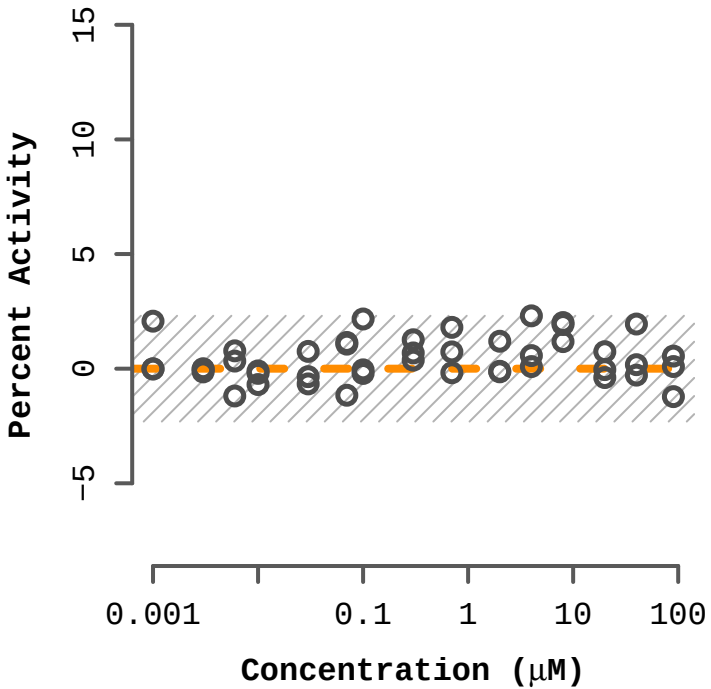
	tp	ga	gw
val:	1.52	−3.42	0.993
sd:	0.641	3.36	4.62

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.26	−2.26	1.01	−2.01	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	253.98	250.52	260.78
PROB:	0.15	0.84	0.01
RMSE:	4.23	3.61	4.15

MAX_MEAN: 3.62 **MAX_MED:** 2.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

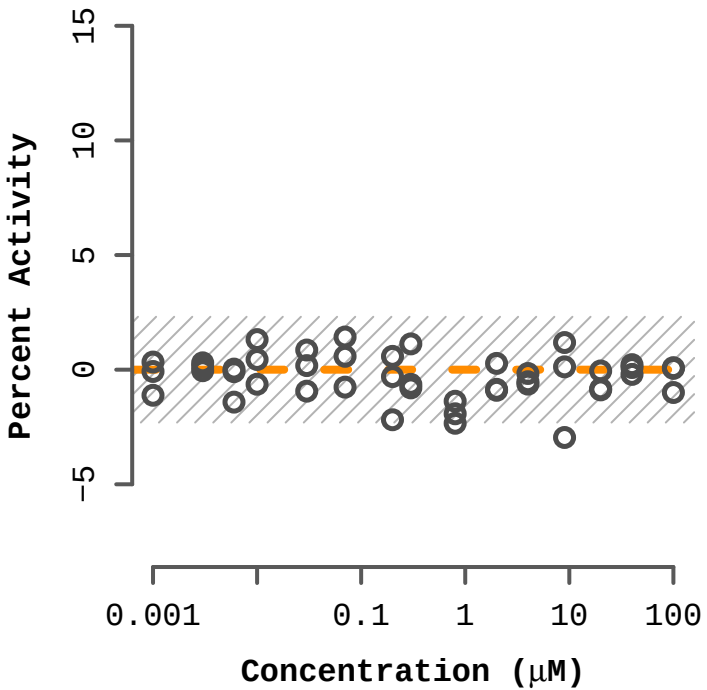
NAME: Tetrahydro-2H-pyran-2-one
CHID: 44438 **CASRN:** 542-28-9
SPID(S): Tox21_302166
M4ID: 12476967

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.39	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

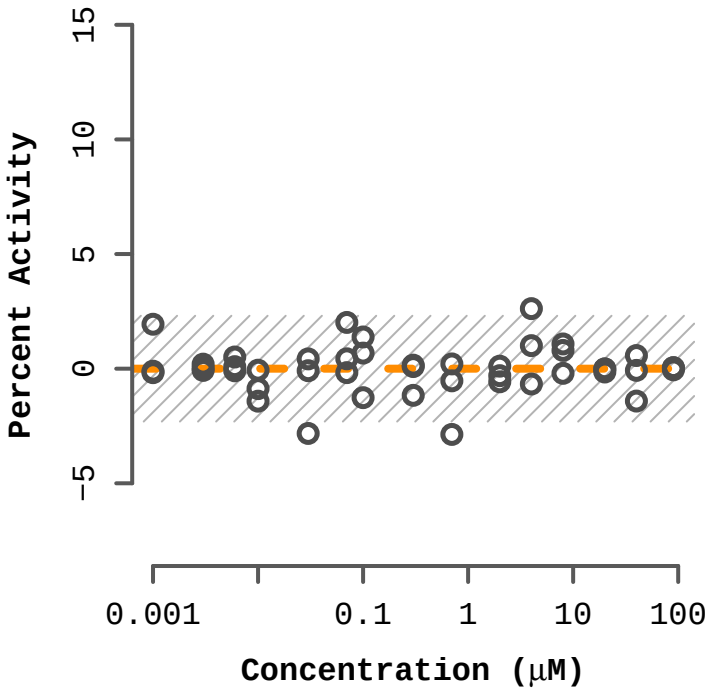
NAME: Butyl cyanoacetate
CHID: 44439 **CASRN:** 5459-58-5
SPID(S): Tox21_302126
M4ID: 12477007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.417 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

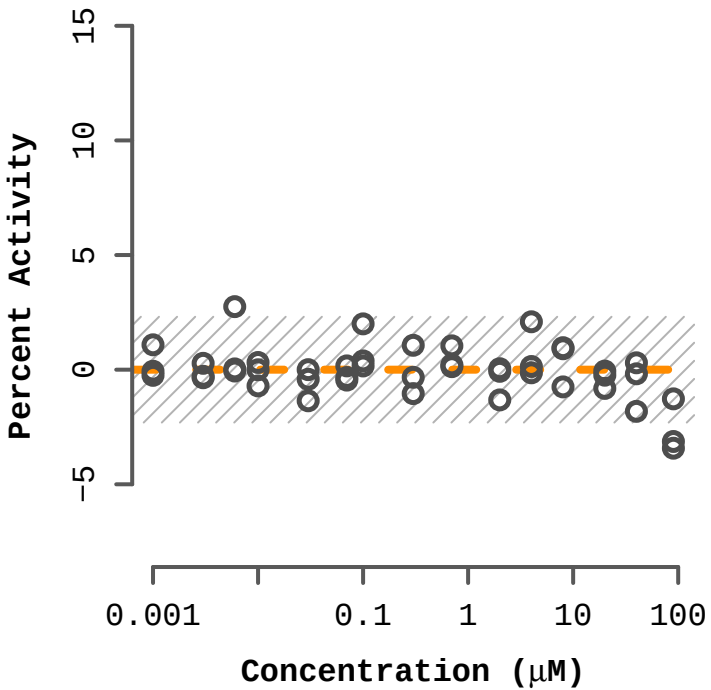
NAME: 2,6-Di(butan-2-yl)phenol
CHID: 44440 CASRN: 5510-99-6
SPID(S): Tox21_302075
M4ID: 12477058

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.987 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

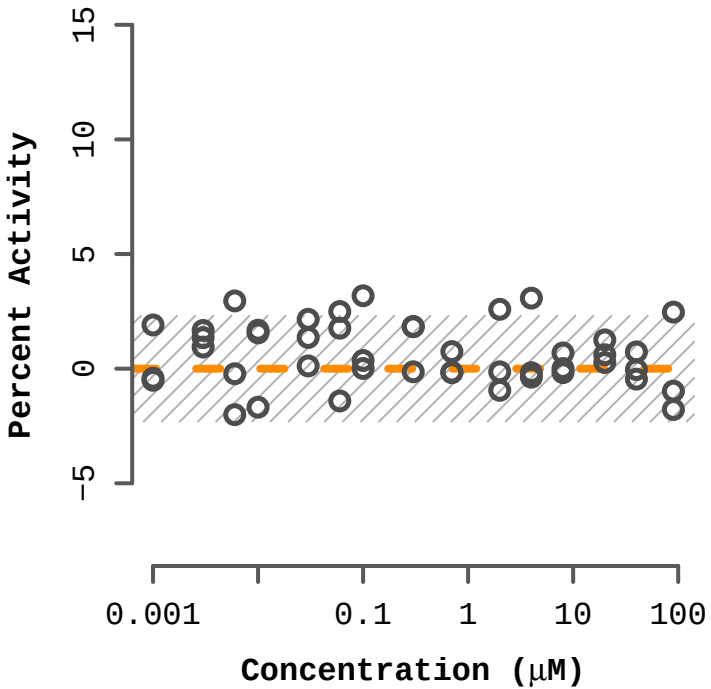
NAME: 1-(Chloromethyl)-2-methylbenzene
CHID: 44441 **CASRN:** 552-45-4
SPID(S): Tox21_302160
M4ID: 12476973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 0.913 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

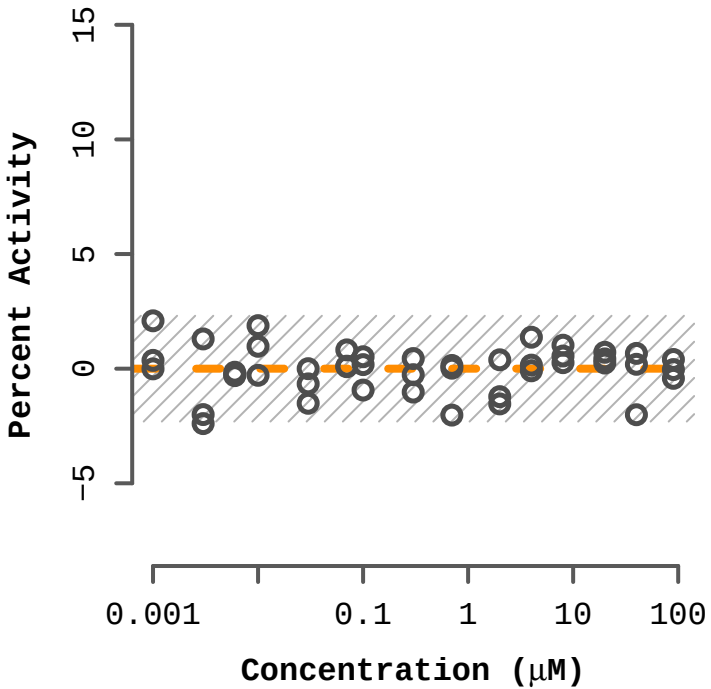
NAME: N,N−Dibutyl−N−methylbutan−1−aminium chloride
CHID: 44443 **CASRN:** 56375−79−2
SPID(S): Tox21_302100
M4ID: 12477033

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

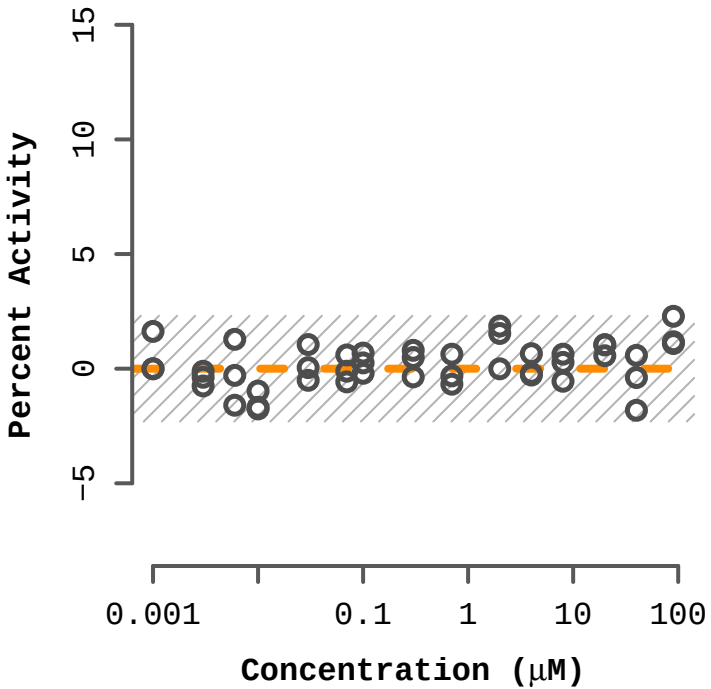
NAME: 4-Bromobenzyl bromide
CHID: 44445 **CASRN:** 589-15-1
SPID(S): Tox21_302061
M4ID: 12477072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.856 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

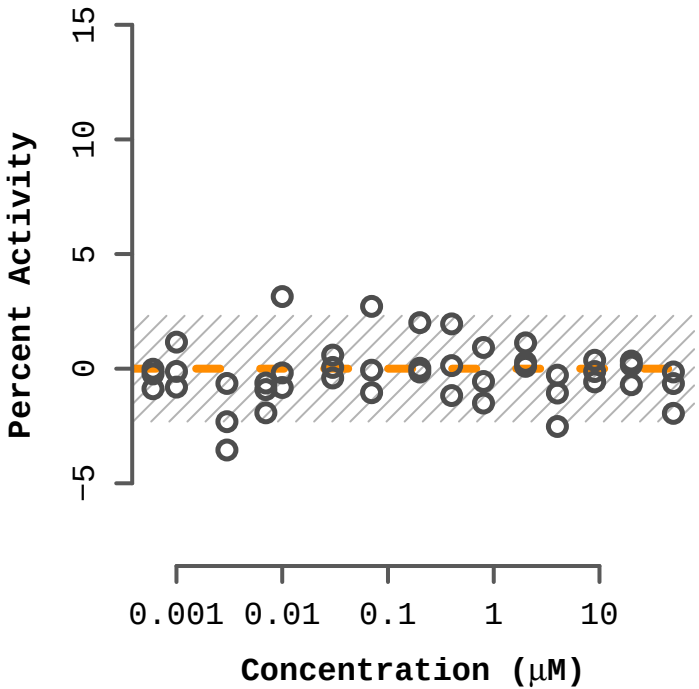
NAME: Betaine hydrochloride
CHID: 44446 CASRN: 590-46-5
SPID(S): Tox21_302142
M4ID: 12476991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.52 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

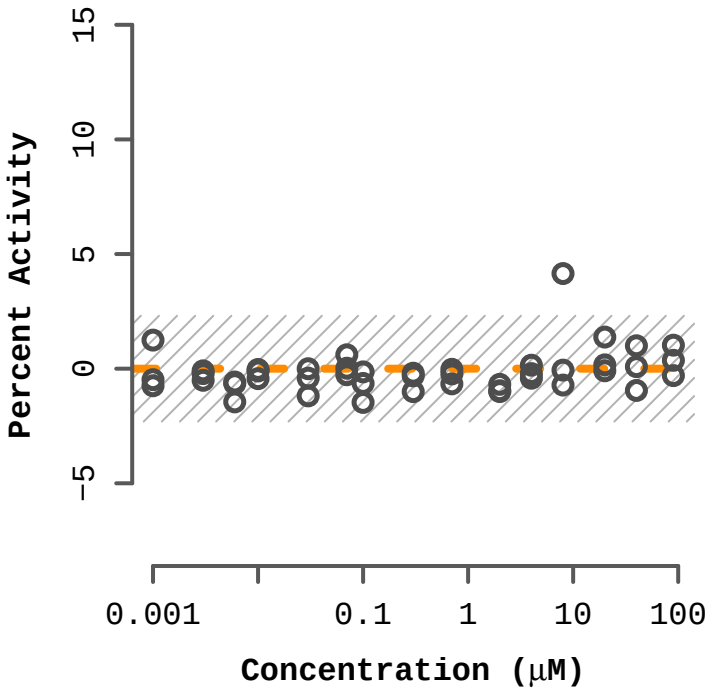
NAME: Betaine hydrochloride
CHID: 44446 **CASRN:** 590-46-5
SPID(S): Tox21_111373_1
M4ID: 12483731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.715 **MAX_MED:** 0.276 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

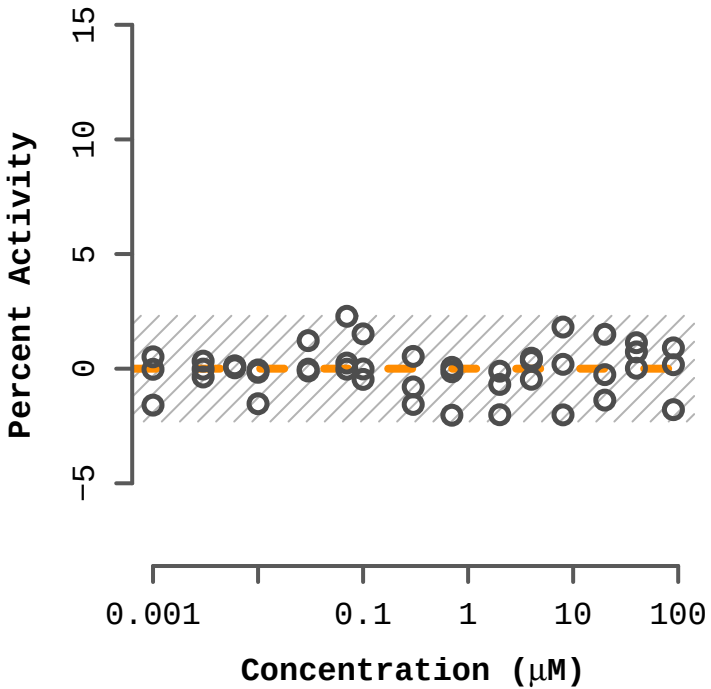
NAME: 3-Methoxybenzaldehyde
CHID: 44447 CASRN: 591-31-1
SPID(S): Tox21_302136
M4ID: 12476997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.13 MAX_MED: 0.366 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

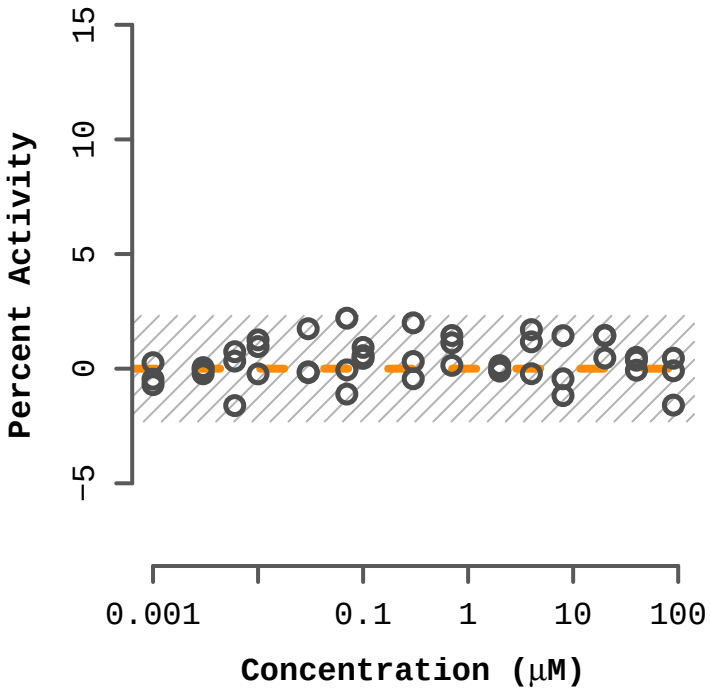
NAME: 4-Pentenoic acid
CHID: 44448 **CASRN:** 591-80-0
SPID(S): Tox21_302069
M4ID: 12477064

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.4	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.837 **MAX_MED:** 0.733 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

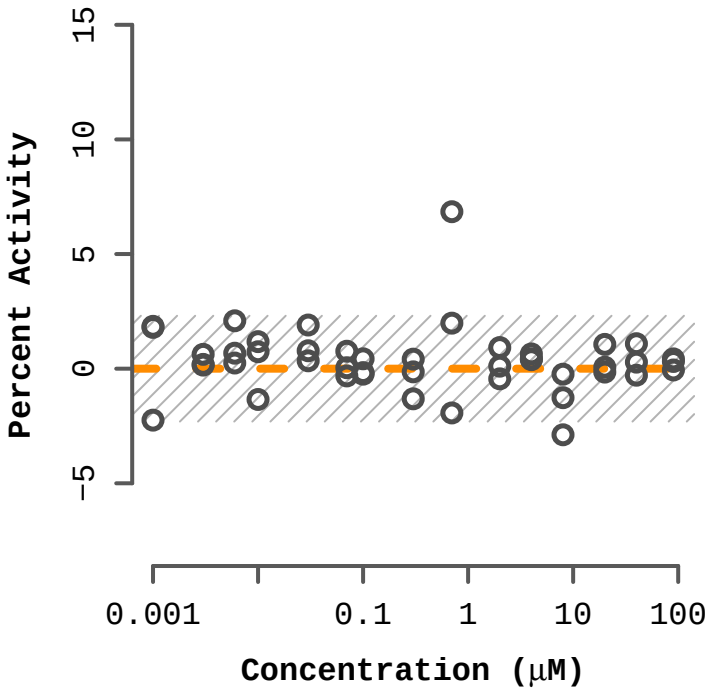
NAME: Tripropyl orthoformate
CHID: 44450 **CASRN:** 621-76-1
SPID(S): Tox21_302099
M4ID: 12477034

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

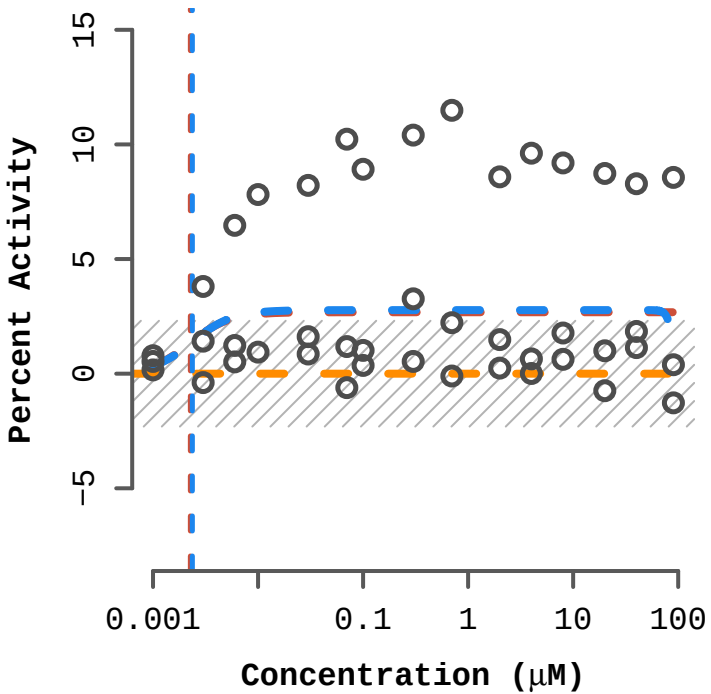
NAME: Methyl hexanedioate
CHID: 44451 **CASRN:** 627-91-8
SPID(S): Tox21_302020
M4ID: 12477113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,6-Dibromohexane
CHID: 44452 CASRN: 629-03-8
SPID(S): Tox21_302059
M4ID: 12477074

HILL MODEL (in red):

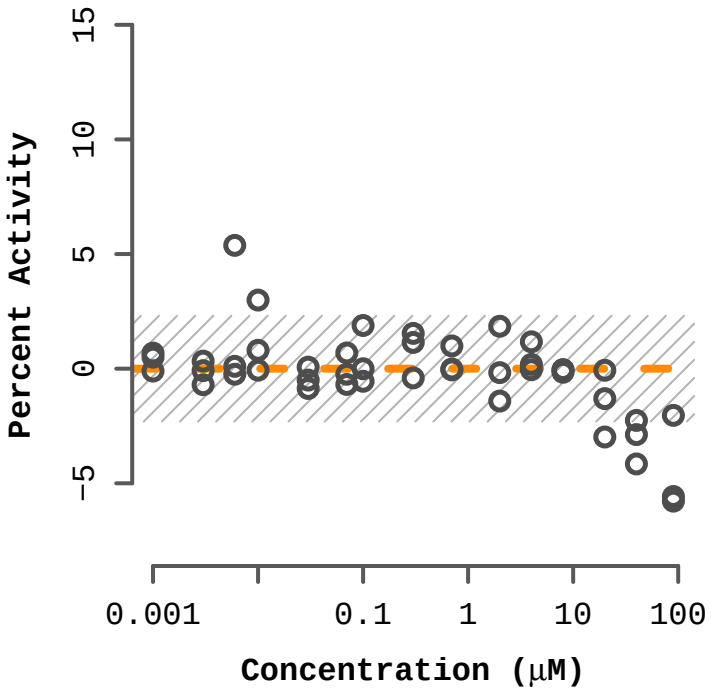
	tp	ga	gw
val:	2.68	−2.64	2.34
sd:	0.718	0.565	4.35

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.77	−2.63	2.28	1.95	15
sd:	0.745	0.538	4.23	0.168	867

	CNST	HILL	GNLS
AIC:	266.87	254.08	257.76
PROB:	0	0.86	0.14
RMSE:	5.05	3.85	3.85

MAX_MEAN: 4.74 MAX_MED: 4.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

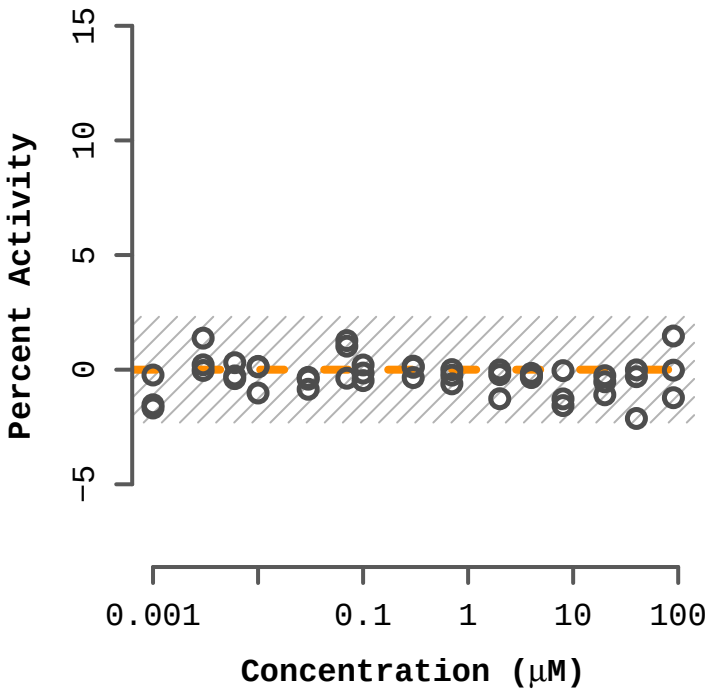
NAME: Ethyl 4-chloro-3-oxobutanoate
CHID: 44454 CASRN: 638-07-3
SPID(S): Tox21_302063
M4ID: 12477070

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.93	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

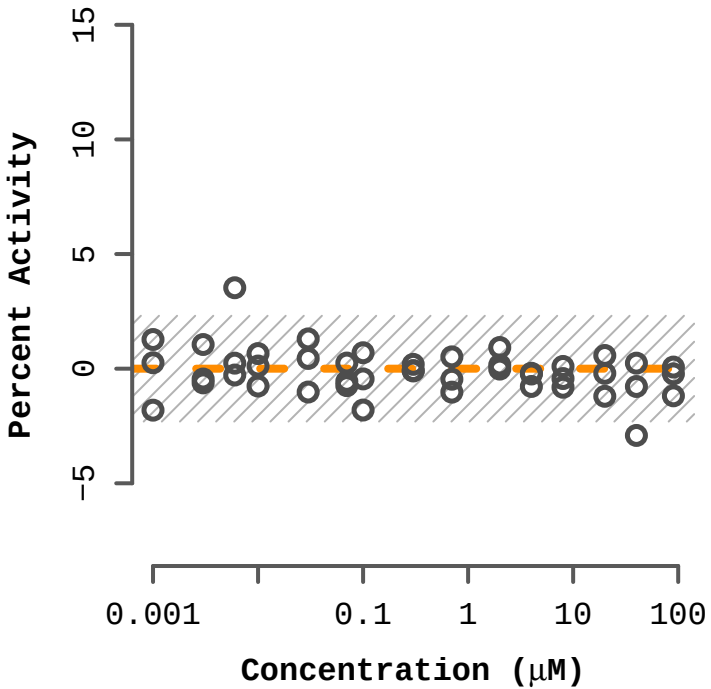
NAME: 1,6-Hexanediol dimethacrylate
CHID: 44455 **CASRN:** 6606-59-3
SPID(S): Tox21_302093
M4ID: 12477040

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.641 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

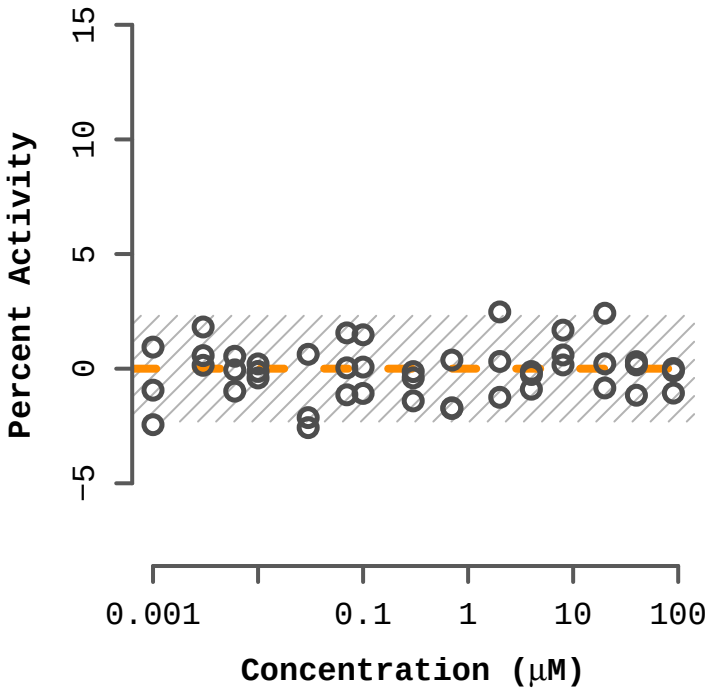
NAME: Cytosine
CHID: 44456 CASRN: 71-30-7
SPID(S): Tox21_302139
M4ID: 12476994

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.17 MAX_MED: 0.447 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

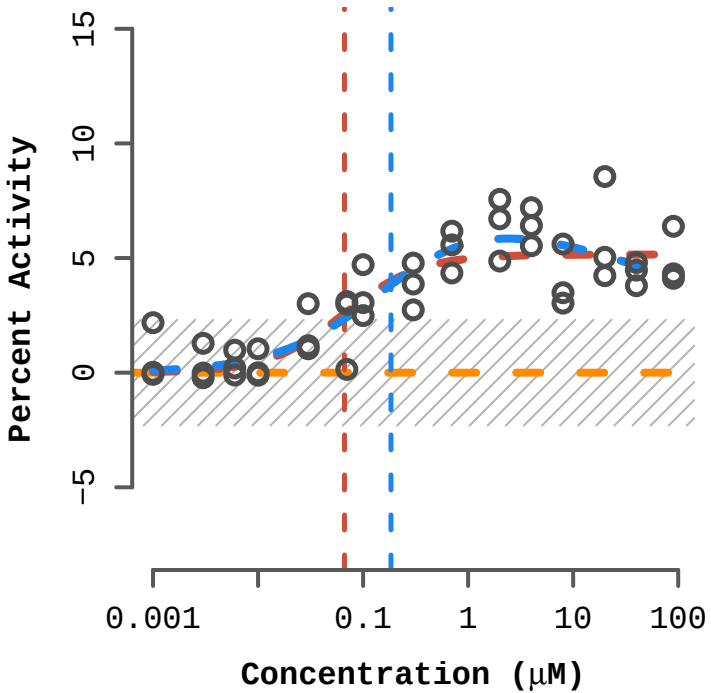
NAME: Tetraethylammonium bromide
CHID: 44457 **CASRN:** 71-91-0
SPID(S): Tox21_302138
M4ID: 12476995

HILL MODEL: Not applicable.

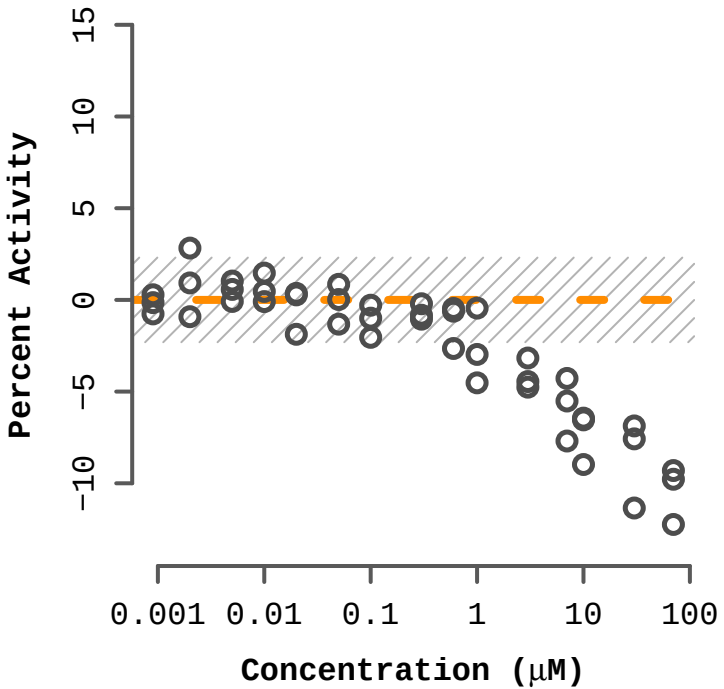
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.847 **MAX_MED:** 0.601 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Sodium 2-[4-(2-hydroxyethyl)piperazin-1-yl]etha
CHID:    44458   CASRN: 75277-39-3
SPID(S): Tox21_302155
M4ID:    12476978

HILL MODEL (in red):
      tp       ga       gw
val:  5.15     -1.18    1.21
sd:   0.303    0.119    0.313

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.06     -0.735   0.859    1.73     0.3
sd:   12.9     0.643    0.222    4.14     0.491

      CNST        HILL        GNLS
AIC:  262.76      153.65      151.76
PROB: 0           0.28        0.72
RMSE: 4.12        1.21        1.17

MAX_MEAN: 6.39      MAX_MED: 6.71      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

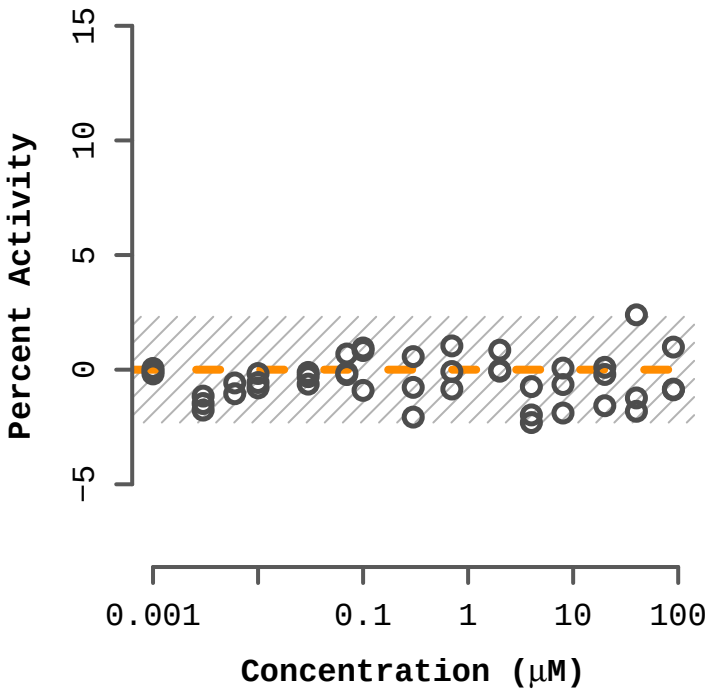
NAME: Bromcresol green
CHID: 44459 **CASRN:** 76-60-8
SPID(S): Tox21_302105
M4ID: 12477028

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	263.6	NA	NA
PROB:	1	NA	NA
RMSE:	4.61	NA	NA

MAX_MEAN: 0.947 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

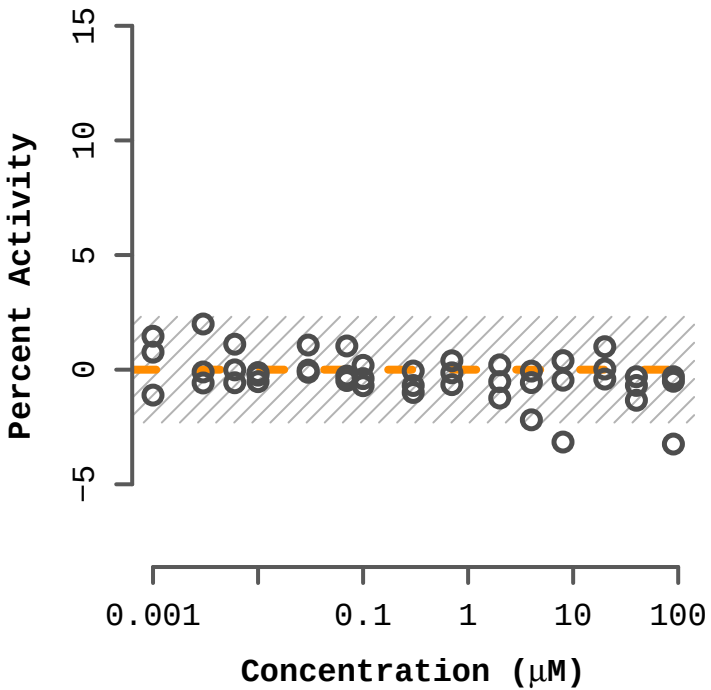
NAME: 5-Methyl-2-(prop-1-en-2-yl)cyclohexanol
CHID: 44461 **CASRN:** 7786-67-6
SPID(S): Tox21_303961
M4ID: 12475227

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.294 **MAX_MED:** 0.836 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

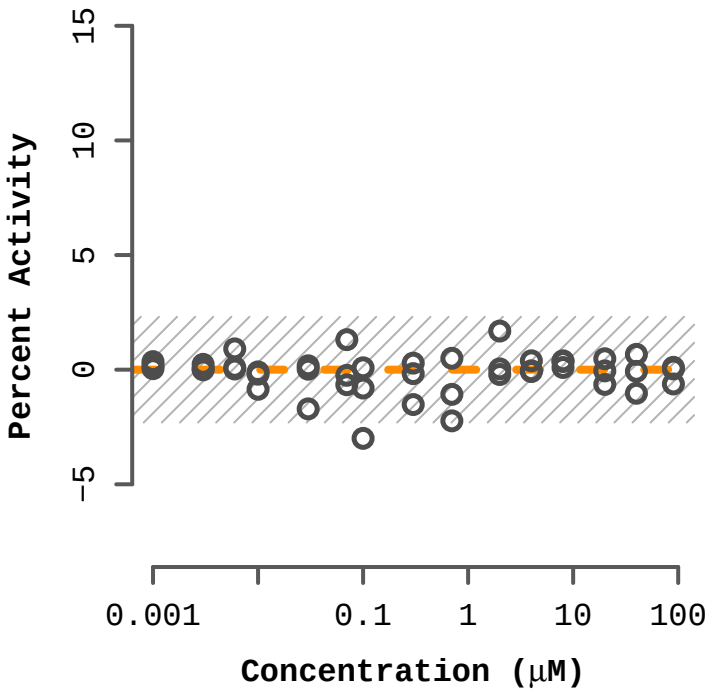
NAME: Triethoxy(phenyl)silane
CHID: 44462 **CASRN:** 780-69-8
SPID(S): Tox21_302168
M4ID: 12476965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.439 **MAX_MED:** 0.764 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

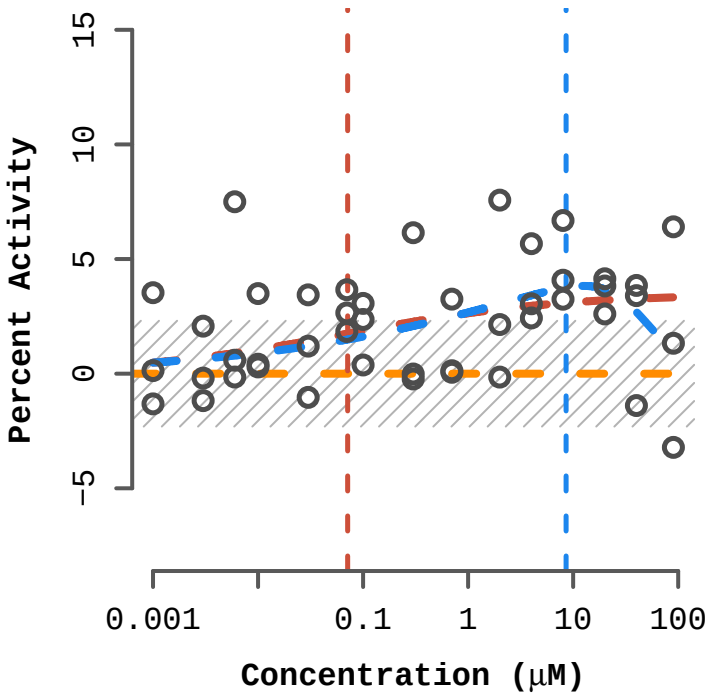
NAME: Ethenyl(triethoxy)silane
CHID: 44463 **CASRN:** 78-08-0
SPID(S): Tox21_302167
M4ID: 12476966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.504 **MAX_MED:** 0.356 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Dihydroxyanthracene−9,10−dione
CHID: 44464 CASRN: 81−64−1
SPID(S): Tox21_302041
M4ID: 12477092

HILL MODEL (in red):

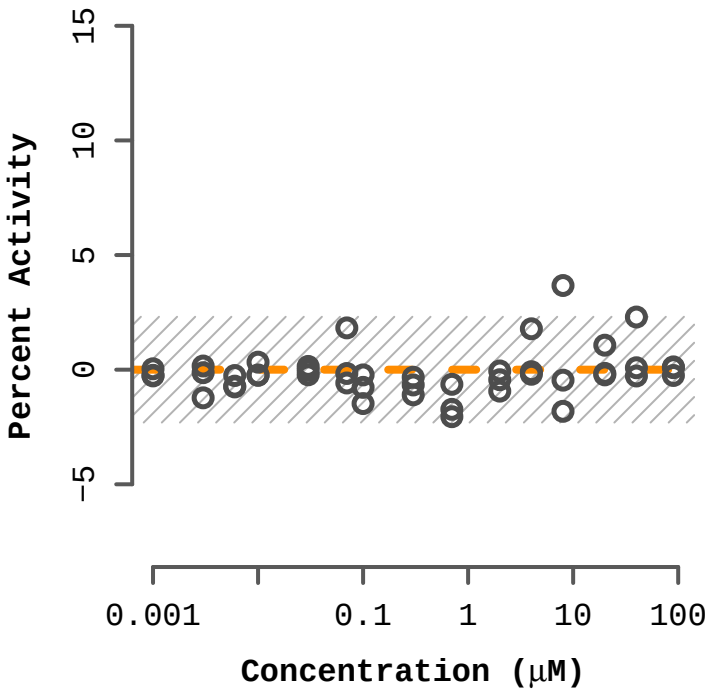
	tp	ga	gw
val:	3.49	−1.15	0.429
sd:	1.2	1.12	0.338

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.76	0.933	0.3	1.66	2.04
sd:	22.8	7.8	0.329	0.443	1.96

	CNST	HILL	GNLS
AIC:	239.84	214.05	215.68
PROB:	0	0.69	0.31
RMSE:	3.31	2.41	2.33

MAX_MEAN: 4.67 MAX_MED: 4.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

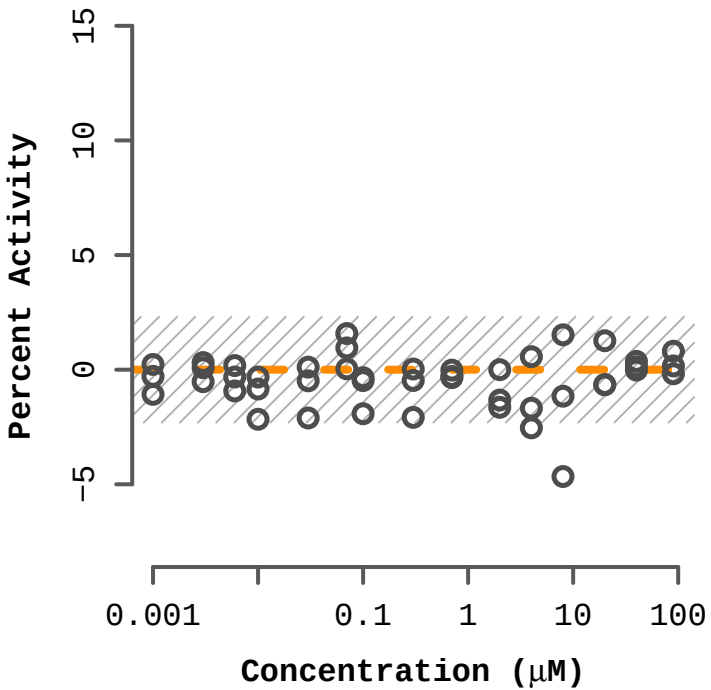
NAME: 2,4−Diaminobenzenesulfonic acid
CHID: 44465 **CASRN:** 88−63−1
SPID(S): Tox21_302078
M4ID: 12477055

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.703 **MAX_MED:** 0.0882 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

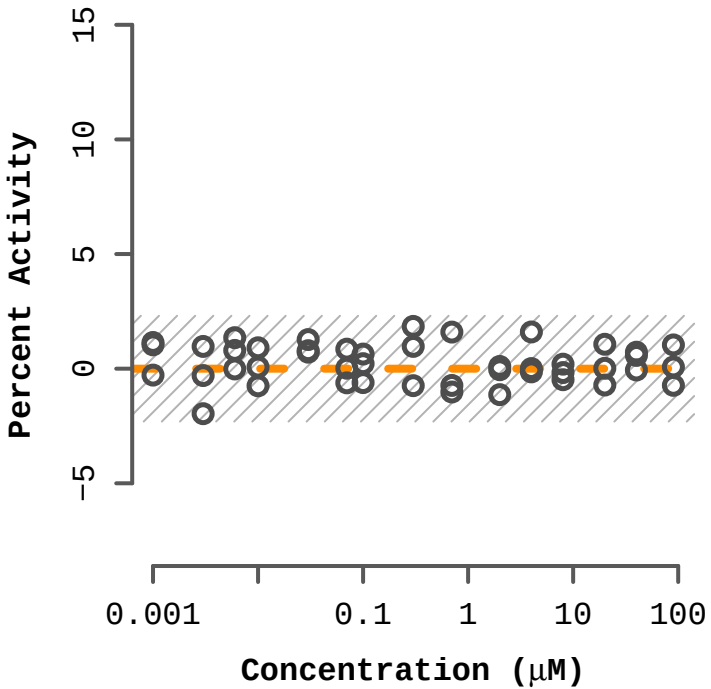
NAME: Pyromellitic acid
CHID: 44466 CASRN: 89-05-4
SPID(S): Tox21_302030
M4ID: 12477103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 0.951 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

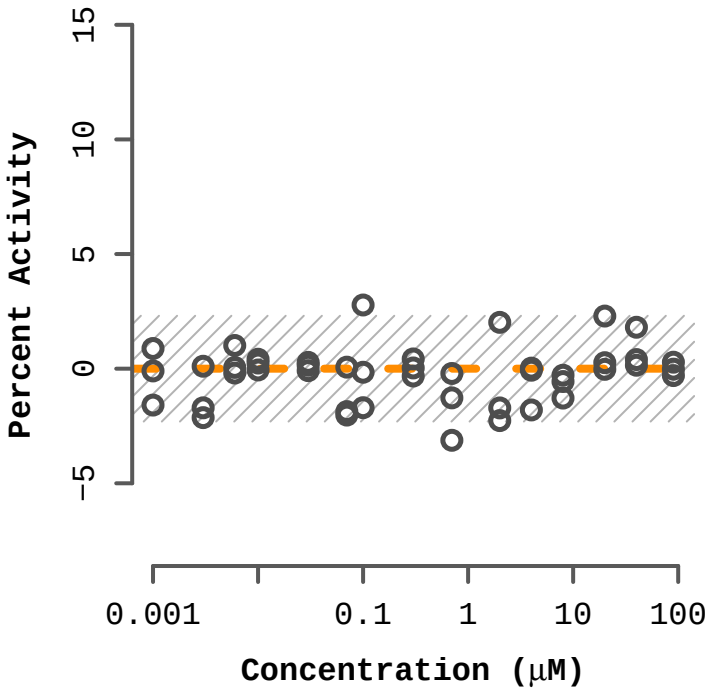
NAME: 2-Aminoethyl hydrogen sulfate
CHID: 44469 **CASRN:** 926-39-6
SPID(S): Tox21_302045
M4ID: 12477088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.927 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

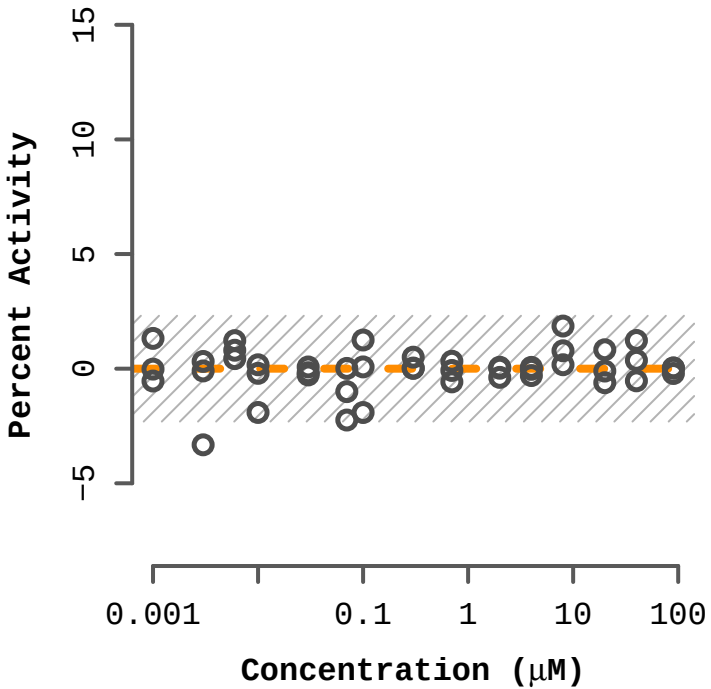
NAME: 1-Phenylpropan-1-one
CHID: 44470 **CASRN:** 93-55-0
SPID(S): Tox21_302025
M4ID: 12477108

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.844 **MAX_MED:** 0.399 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

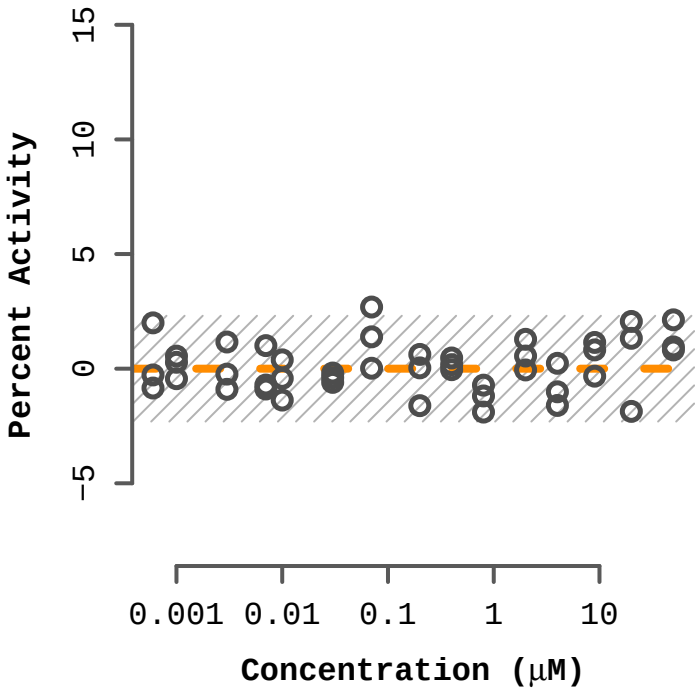
NAME: Methyl nicotinate
CHID: 44471 CASRN: 93-60-7
SPID(S): Tox21_302038
M4ID: 12477095

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 0.806 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

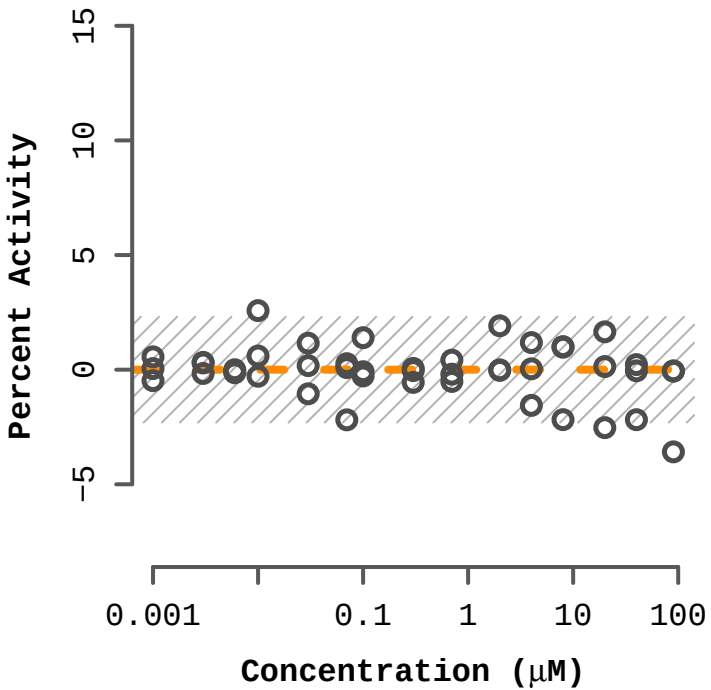
NAME: Methyl nicotinate
CHID: 44471 **CASRN:** 93-60-7
SPID(S): Tox21_111702_1
M4ID: 12483528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

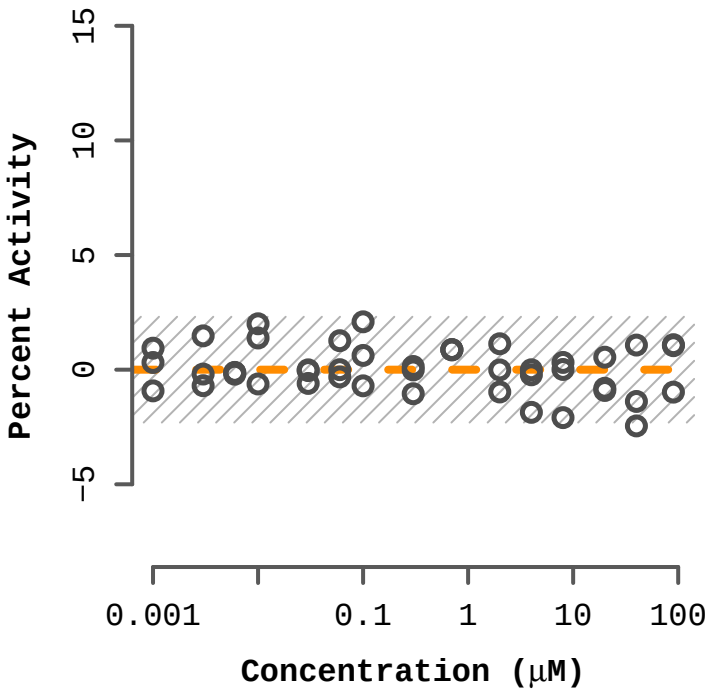
NAME: Diethyl oxalate
CHID: 44472 **CASRN:** 95-92-1
SPID(S): Tox21_302109
M4ID: 12477024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 0.979 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

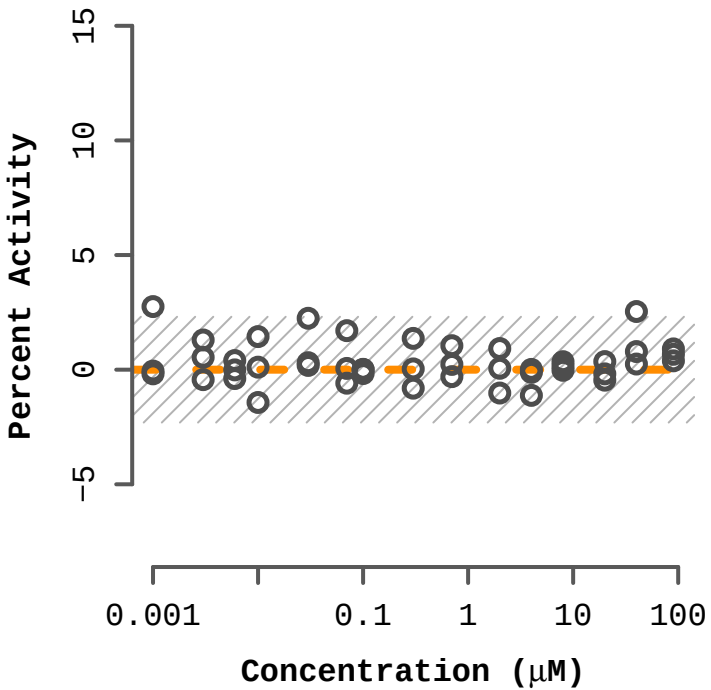
NAME: 4-Chlorobenzenesulfonic acid
CHID: 44473 CASRN: 98-66-8
SPID(S): Tox21_302072
M4ID: 12477061

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.921 MAX_MED: 1.38 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

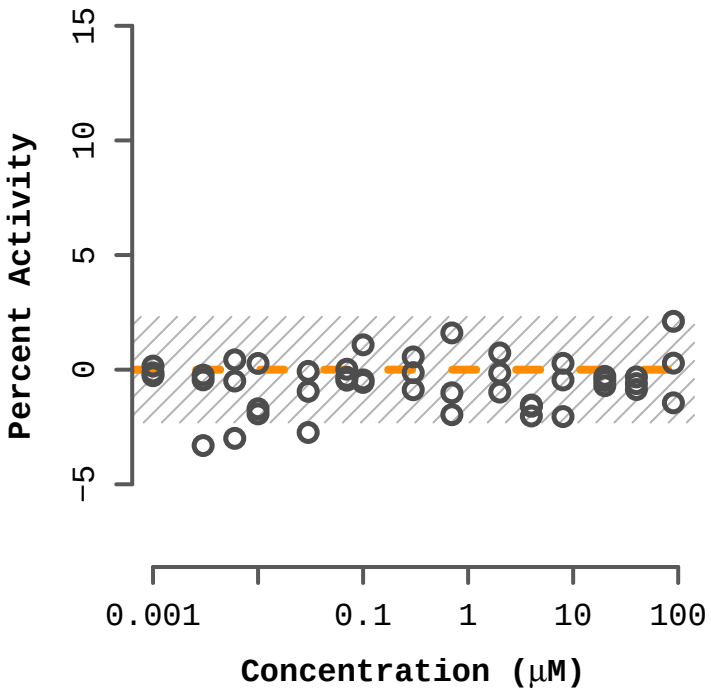
NAME: (2R,5R)-5-Methyl-2-(propan-2-yl)cyclohexanone
CHID: 44475 **CASRN:** 491-07-6
SPID(S): Tox21_301991
M4ID: 12477142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

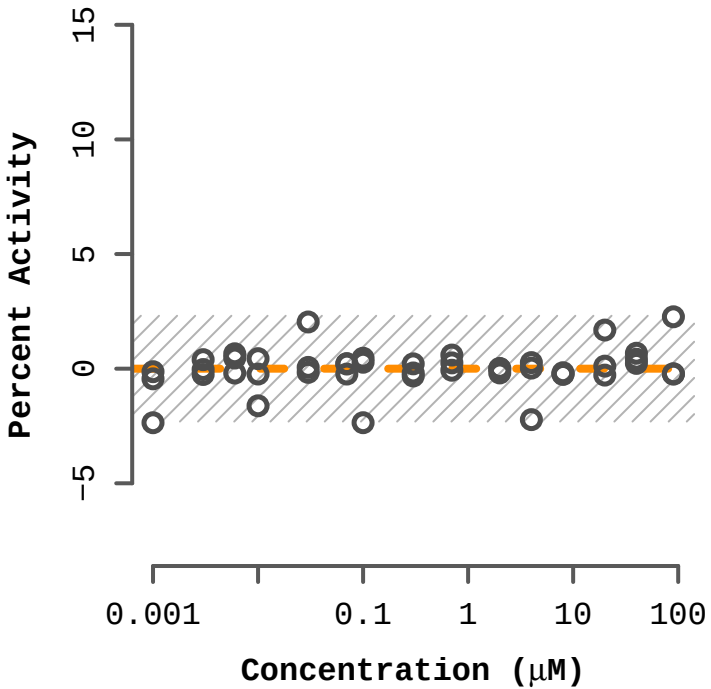
NAME: (S)-(-)-Citronellal
CHID: 44476 **CASRN:** 5949-05-3
SPID(S): Tox21_303980
M4ID: 12475208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.317 **MAX_MED:** 0.286 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

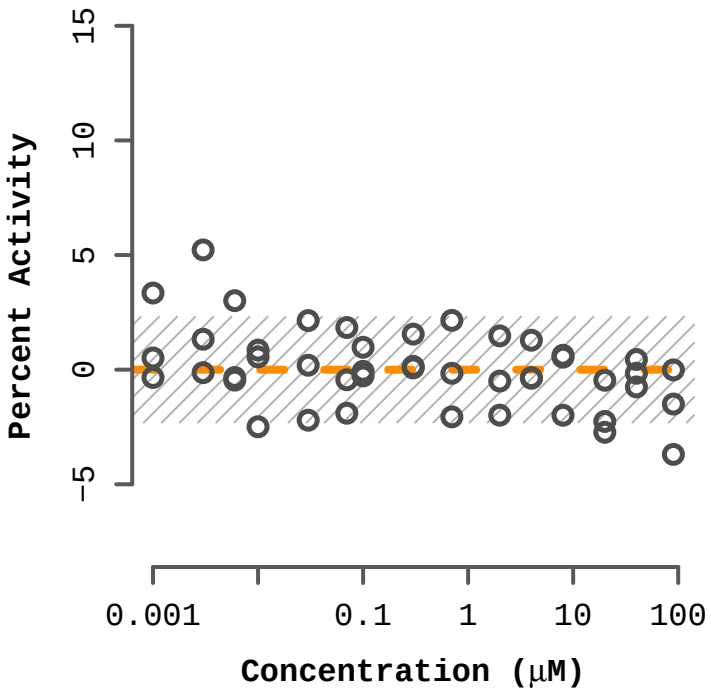
NAME: 3-(Triethoxysilyl)propane-1-thiol
CHID: 44479 **CASRN:** 14814-09-6
SPID(S): Tox21_302193
M4ID: 12476940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.646 **MAX_MED:** 0.465 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

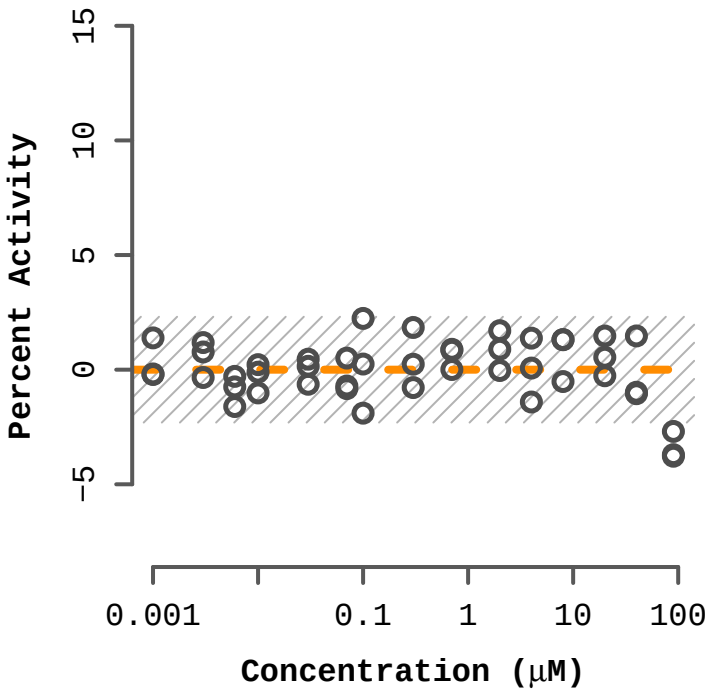
NAME: Acetone thiosemicarbazide
CHID: 44480 **CASRN:** 1752-30-3
SPID(S): Tox21_304003
M4ID: 12475185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

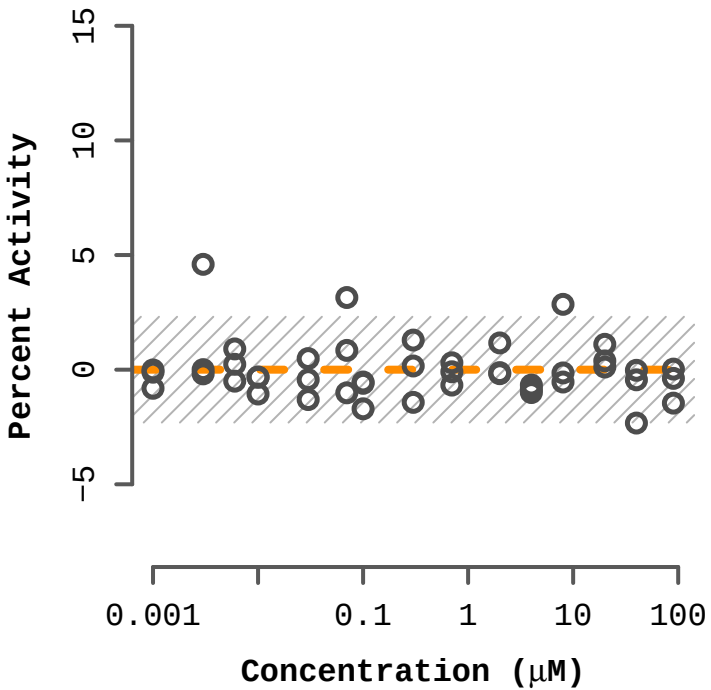
NAME: 1,1'−Disulfanediyldiazepan−2−one
CHID: 44481 CASRN: 23847−08−7
SPID(S): Tox21_301989
M4ID: 12477144

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.853 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

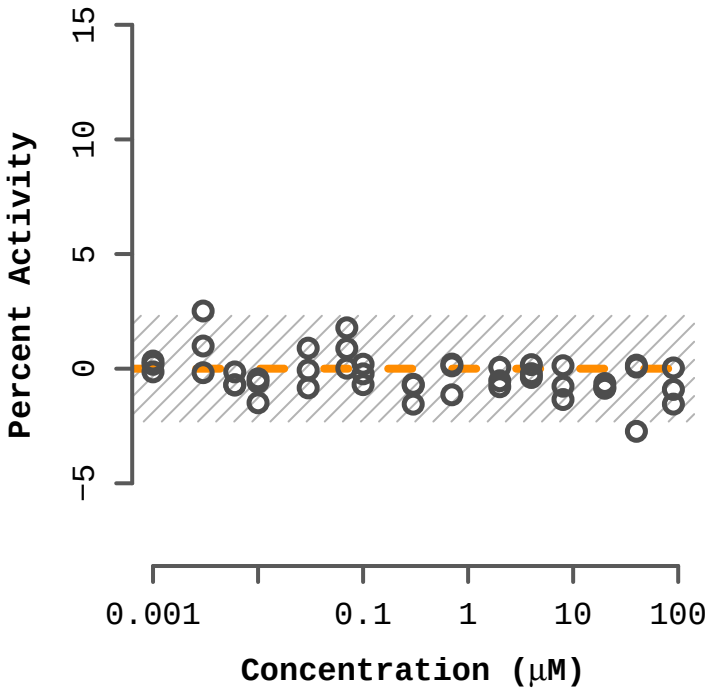
NAME: Isononanamine
CHID: 44484 **CASRN:** 27775-00-4
SPID(S): Tox21_301982
M4ID: 12477151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 0.842 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

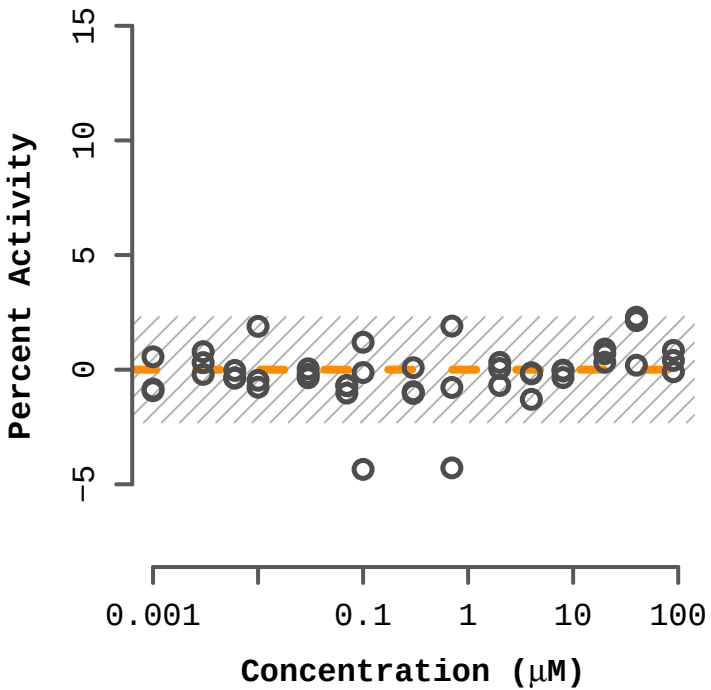
NAME: 4-Ethoxy-4-oxobut-2-enoic acid
CHID: 44485 **CASRN:** 3249-53-4
SPID(S): Tox21_301978
M4ID: 12477155

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

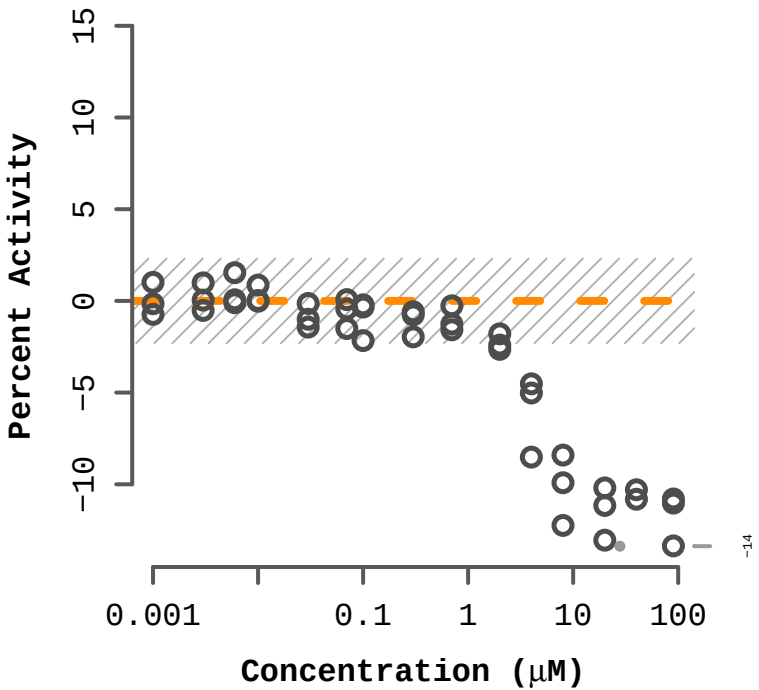
NAME: 1,3-Dipropan-2-ylurea
CHID: 44486 **CASRN:** 4128-37-4
SPID(S): Tox21_301975
M4ID: 12477158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

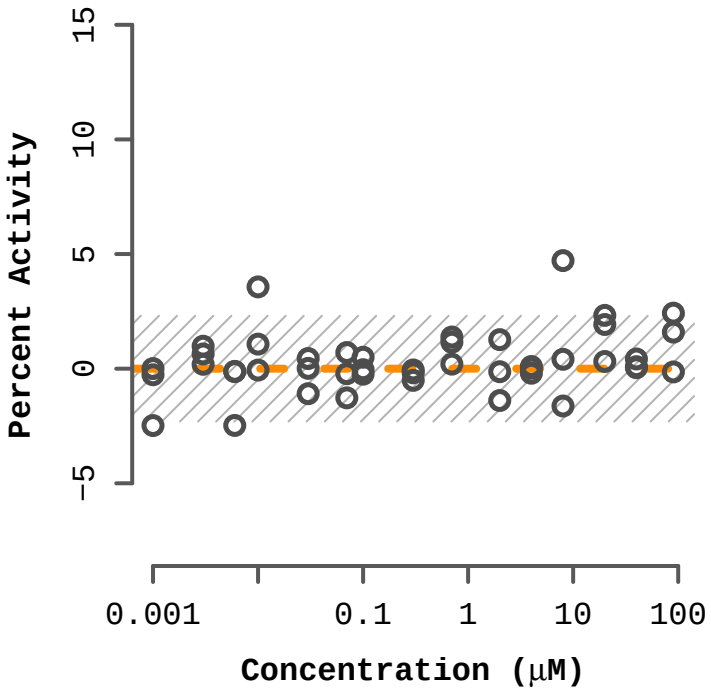
NAME: Methyltrioctylammonium chloride
CHID: 44487 **CASRN:** 5137-55-3
SPID(S): Tox21_302198
M4ID: 12476935 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.08	NA	NA
PROB:	1	NA	NA
RMSE:	6.16	NA	NA

MAX_MEAN: 0.502 **MAX_MED:** 0.0634 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

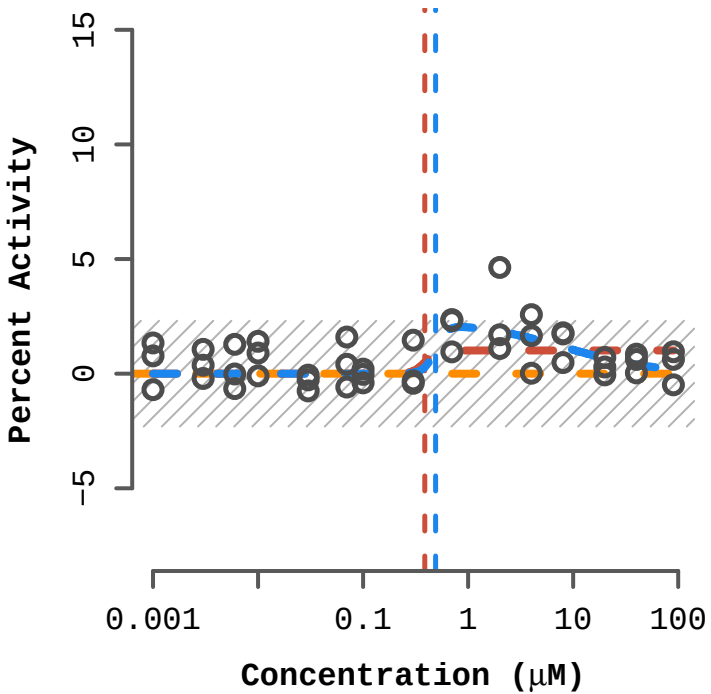
NAME: 1-Aminocyclohexanecarbonitrile
CHID: 44488 **CASRN:** 5496-10-6
SPID(S): Tox21_302194
M4ID: 12476939

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-N,N-dimethyl-3-oxobutanamide
CHID: 44489 CASRN: 5810-11-7
SPID(S): Tox21_301984
M4ID: 12477149

HILL MODEL (in red):

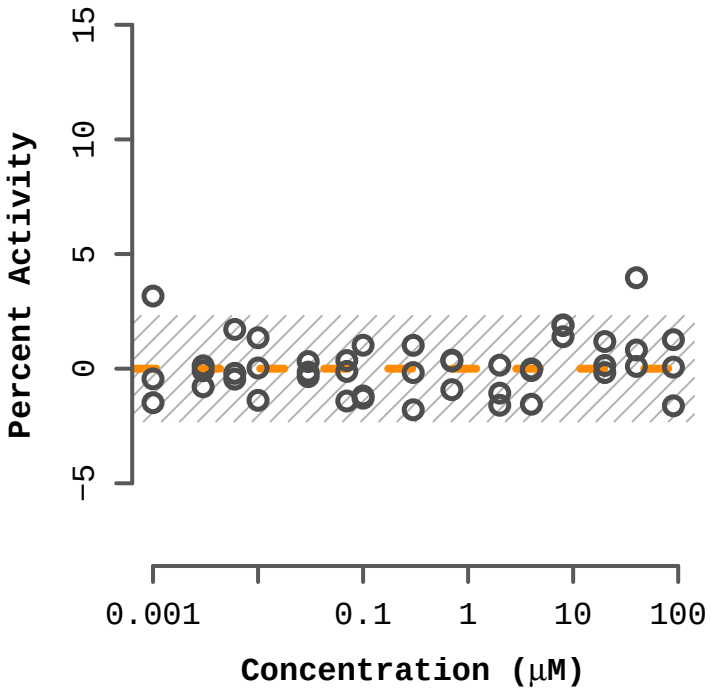
	tp	ga	gw
val:	1.01	-0.413	8
sd:	0.209	0.188	8.76

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.26	-0.31	8	0.931	1
sd:	1.55	0.307	12.7	0.763	1.07

	CNST	HILL	GNLS
AIC:	146.64	131.53	123.71
PROB:	0	0.02	0.98
RMSE:	1.26	0.98	0.84

MAX_MEAN: 2.48 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

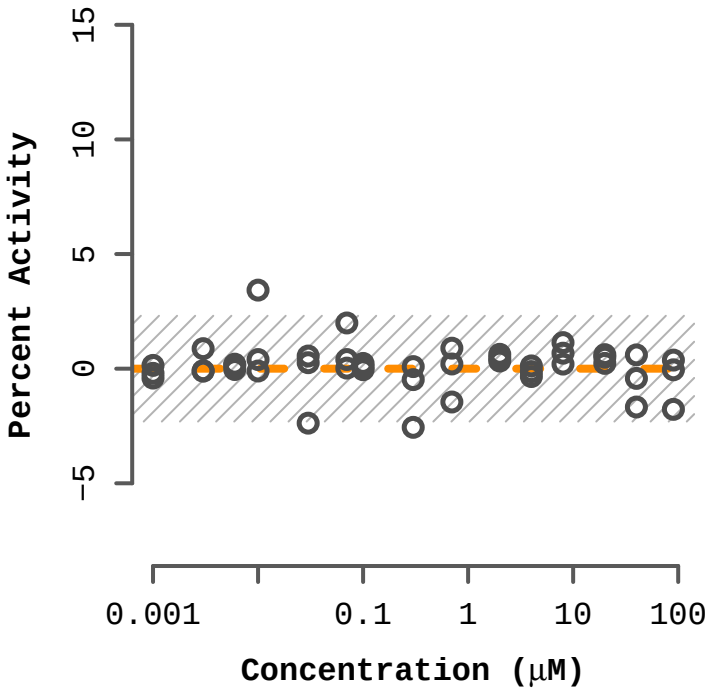
NAME: Methyl 3-sulfamoylthiophene-2-carboxylate
CHID: 44490 CASRN: 59337-93-8
SPID(S): Tox21_301980
M4ID: 12477153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.73 MAX_MED: 1.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

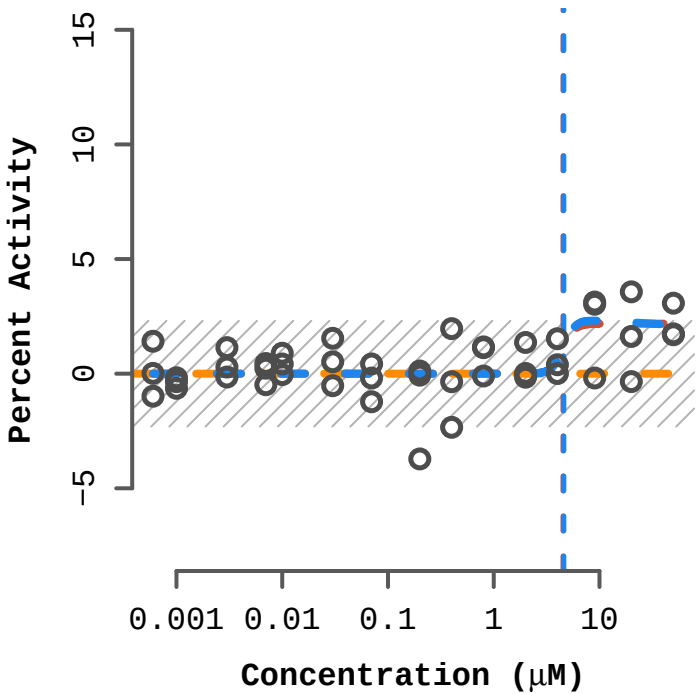
NAME: Piracetam
CHID: 44491 **CASRN:** 7491-74-9
SPID(S): Tox21_301990
M4ID: 12477143

HILL MODEL: Not applicable.

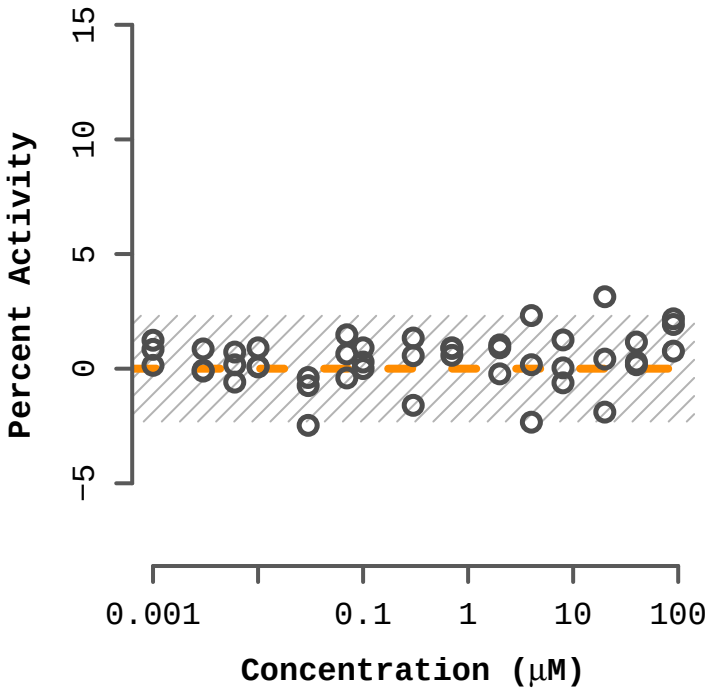
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.677 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Piracetam
CHID:    44491   CASRN: 7491-74-9
SPID(S): Tox21_110229_1
M4ID:    12484532

HILL MODEL (in red):
      tp       ga       gw
val:  2.18     0.655    8
sd:   0.402    0.11     15.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.71     0.663    8        3.54     0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  158.37      142.88      146.66
PROB: 0           0.87        0.13
RMSE: 1.42        1.13        1.13

MAX_MEAN: 2.17      MAX_MED: 3.03      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

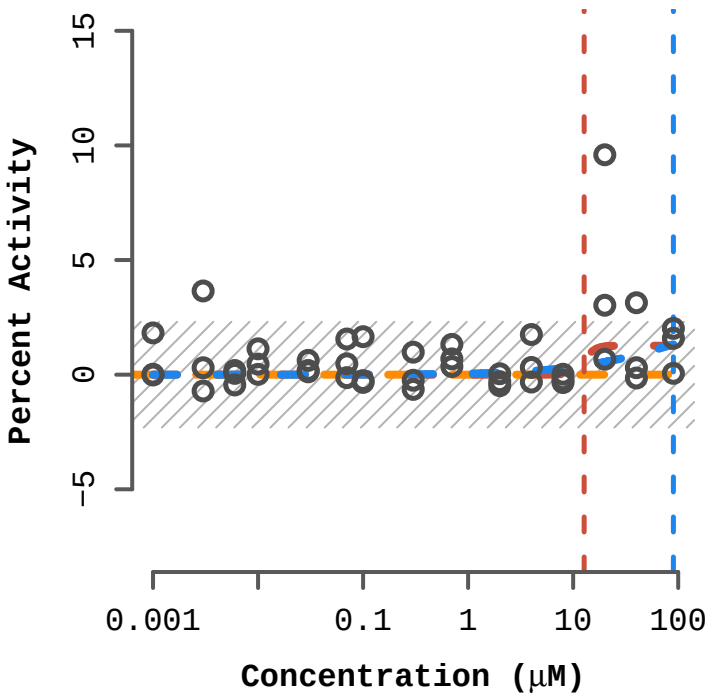
NAME: 1-[3-(Triethoxysilyl)propyl]urea
CHID: 44493 **CASRN:** 23779-32-0
SPID(S): Tox21_300417
M4ID: 12478715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Phenylethyl phenylacetate
CHID: 44494 CASRN: 102-20-5
SPID(S): Tox21_300689
M4ID: 12478444

HILL MODEL (in red):

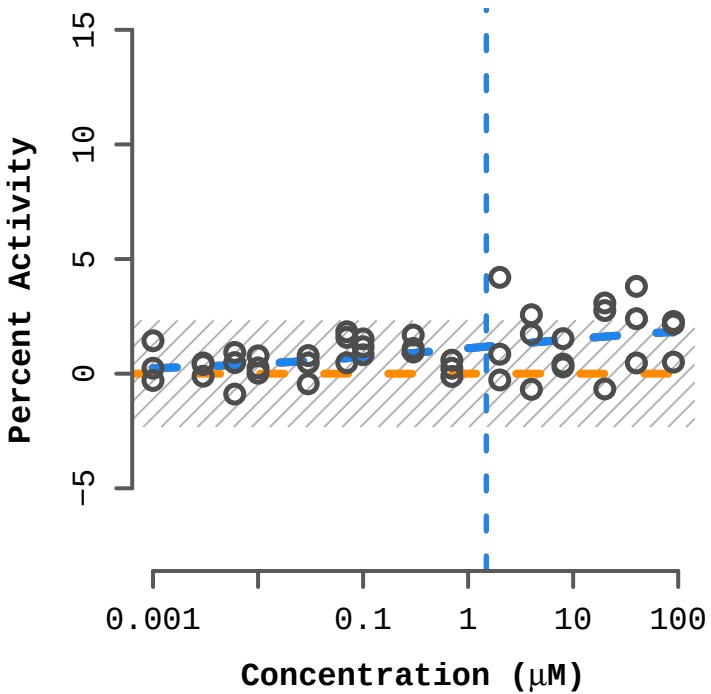
	tp	ga	gw
val:	1.26	1.1	8
sd:	0.453	0.198	8.05

GAIN-LOSS MODEL (in blue):

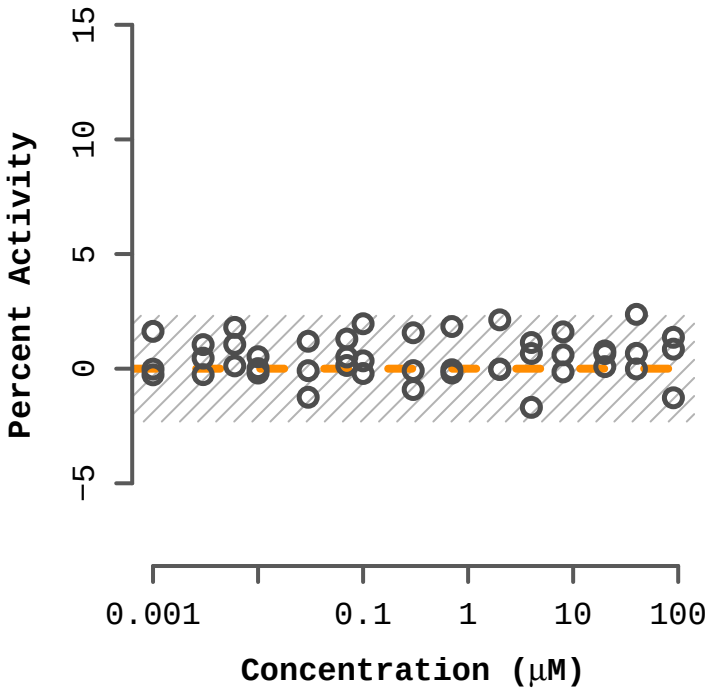
	tp	ga	gw	la	lw
val:	2.64	1.95	0.882	3.49	4.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	150.23	147.01	152.8
PROB:	0.16	0.8	0.04
RMSE:	1.83	1.6	1.69

MAX_MEAN: 4.43 MAX_MED: 3.03 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-(4-Hydroxyphenyl)butan-2-one
CHID:    44495   CASRN: 5471-51-2
SPID(S): Tox21_301459
M4ID:    12477674

HILL MODEL (in red):
      tp       ga       gw
val:  2.36     0.172    0.3
sd:   3.15     4.53     0.347

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.36     0.174    0.3      2.08     13.5
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  164.91      138.89      142.89
PROB: 0           0.88        0.12
RMSE: 1.5         1.03        1.03

MAX_MEAN: 2.23      MAX_MED: 2.75      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

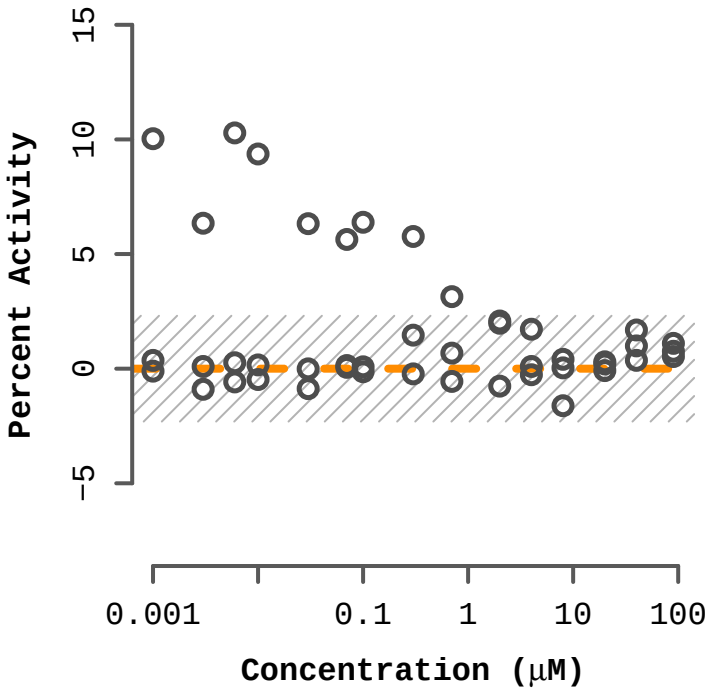
NAME: 6-Pentyltetrahydro-2H-pyran-2-one
CHID: 44496 **CASRN:** 705-86-2
SPID(S): Tox21_301878
M4ID: 12477255

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

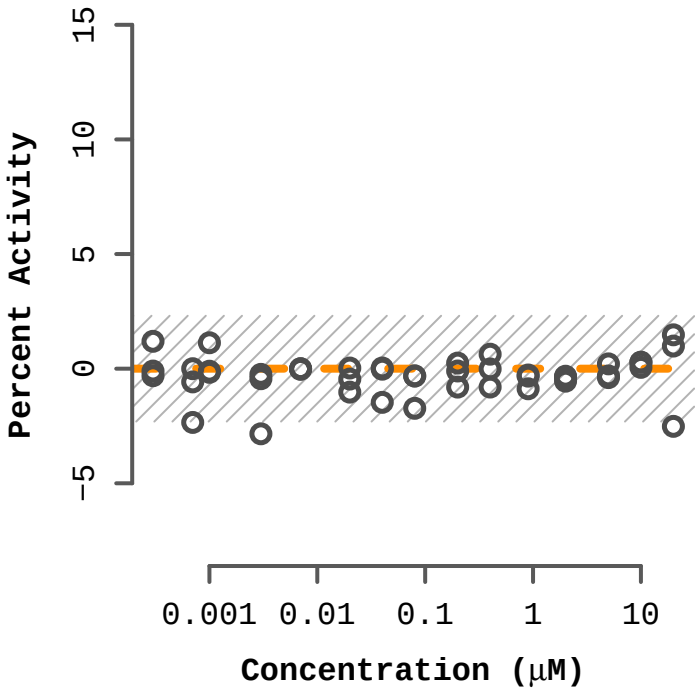
NAME: N,N−Diethyl−N−methylethanaminium chloride
CHID: 44498 **CASRN:** 10052−47−8
SPID(S): Tox21_300798
M4ID: 12478335

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 3.43 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

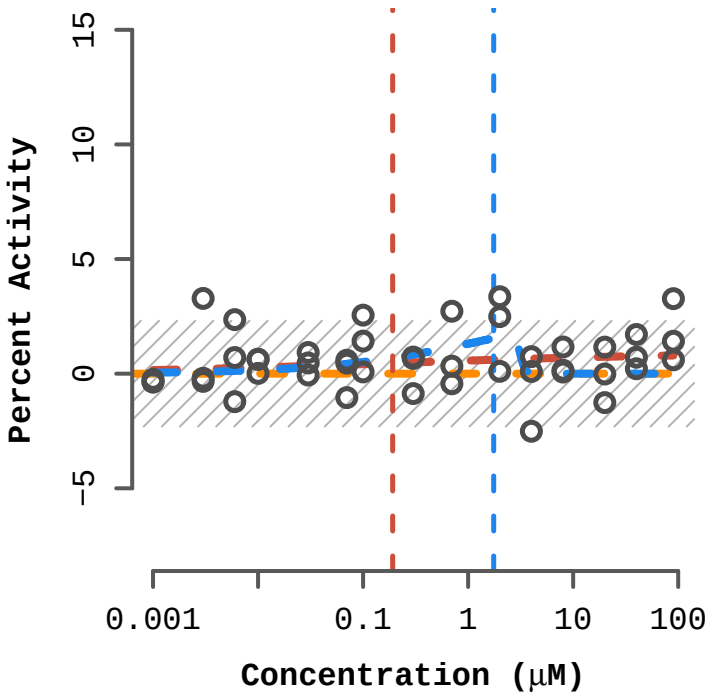
NAME: Dodecane−1−sulfonyl chloride
CHID: 44500 CASRN: 10147−40−7
SPID(S): Tox21_303760
M4ID: 12475428

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.288 **MAX_MED:** 0.988 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'−[Benzene−1,3−diylbis(oxy)]diethanol
CHID: 44502 CASRN: 102−40−9
SPID(S): Tox21_300783
M4ID: 12478350

HILL MODEL (in red):

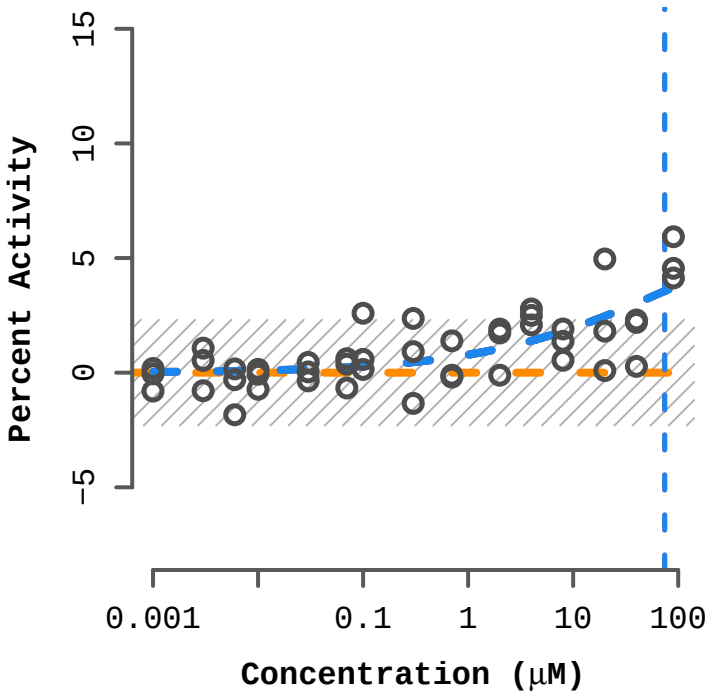
	tp	ga	gw
val:	0.917	−0.718	0.3
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.1	0.243	0.567	0.493	18
sd:	11.2	3.79	0.509	0.344	52.5

	CNST	HILL	GNLS
AIC:	156.29	152.17	158.74
PROB:	0.11	0.86	0.03
RMSE:	1.38	1.24	1.24

MAX_MEAN: 1.98 **MAX_MED:** 2.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Disperse Yellow 64
CHID: 44503 CASRN: 10319-14-9
SPID(S): Tox21_300734
M4ID: 12478399

HILL MODEL (in red):

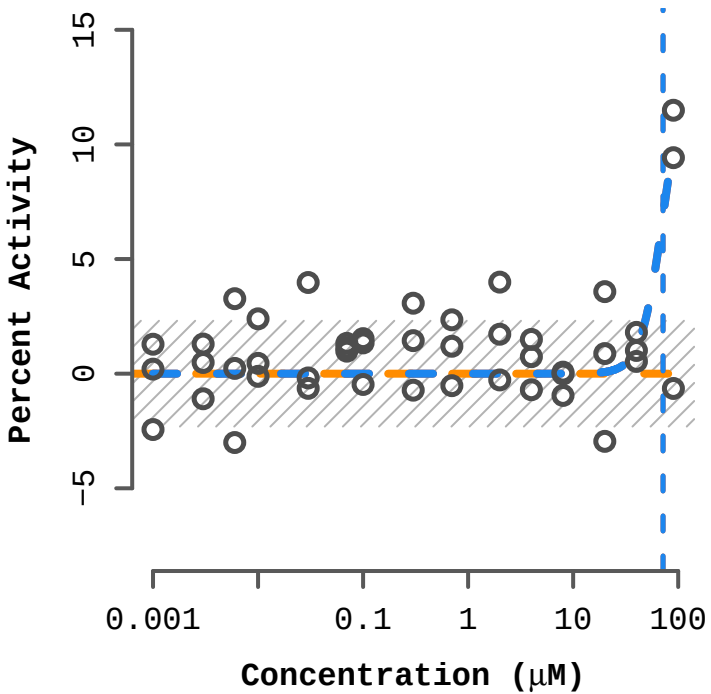
	tp	ga	gw
val:	7.12	1.87	0.485
sd:	4.39	0.989	0.134

GAIN-LOSS MODEL (in blue):

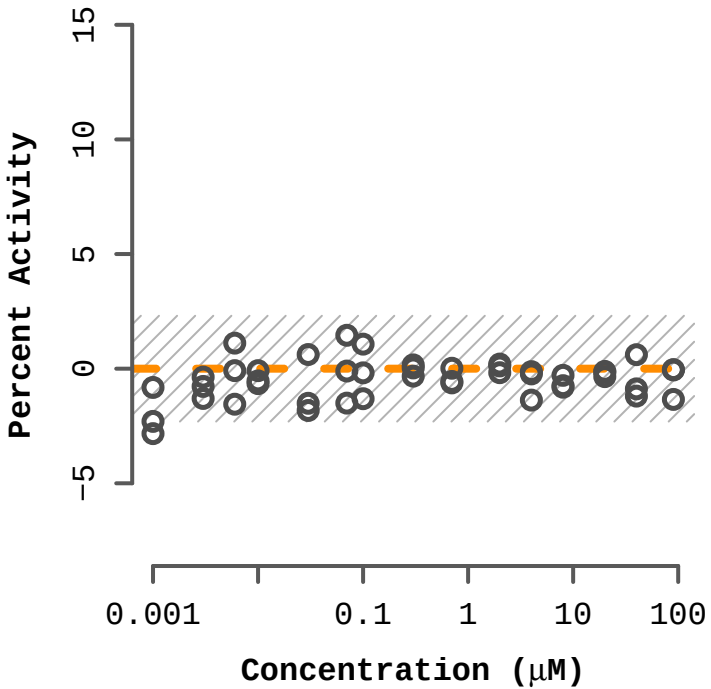
	tp	ga	gw	la	lw
val:	7.12	1.87	0.485	3.36	6.15
sd:	4.39	0.988	0.134	1360	6000

	CNST	HILL	GNLS
AIC:	183.77	147.56	151.56
PROB:	0	0.88	0.12
RMSE:	1.93	1.13	1.13

MAX_MEAN: 4.87 MAX_MED: 4.55 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cadmium dinitrate
CHID:    44504   CASRN: 10325-94-7
SPID(S): Tox21_300771
M4ID:    12478362

HILL MODEL (in red):
      tp       ga       gw
val:  13.8     1.86     4.11
sd:   43.2     0.94     9.71

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.8     1.86     4.11     3.42     4.1
sd:   43.1     0.937    9.68     986      2770

      CNST        HILL        GNLS
AIC:  204.28      197.16      201.16
PROB: 0.02        0.86        0.12
RMSE: 2.8         2.31        2.31

MAX_MEAN: 6.76      MAX_MED: 9.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

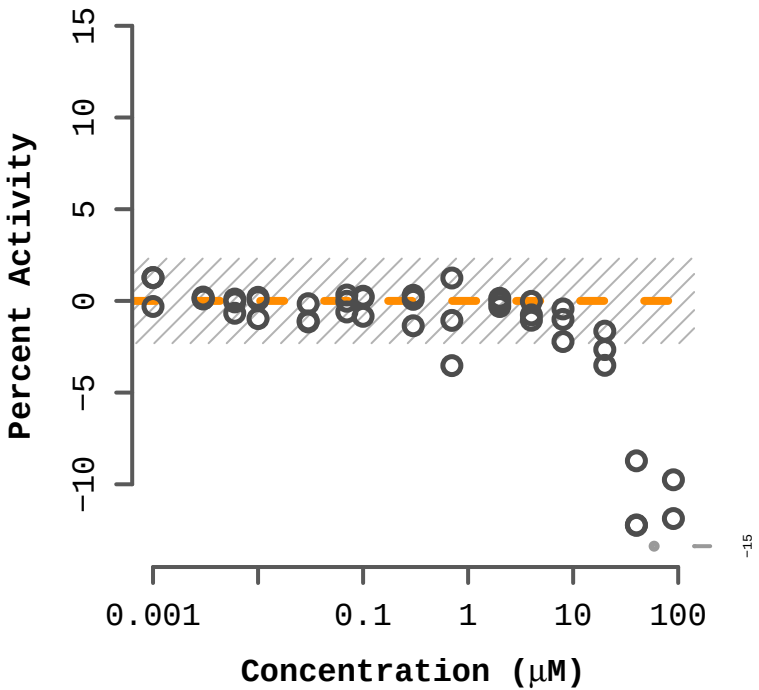
NAME: 2-Phenylethyl acetate
CHID: 44506 **CASRN:** 103-45-7
SPID(S): Tox21_301027
M4ID: 12478106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.05 **MAX_MED:** 0.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

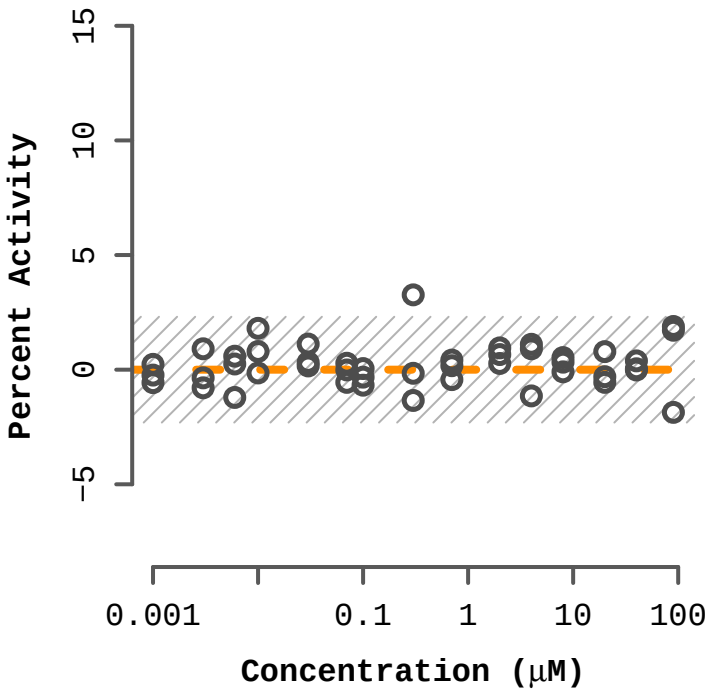
NAME: Maprotiline hydrochloride
CHID: 44507 **CASRN:** 10347-81-6
SPID(S): Tox21_300992
M4ID: 12478141 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.66	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: 0.747 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

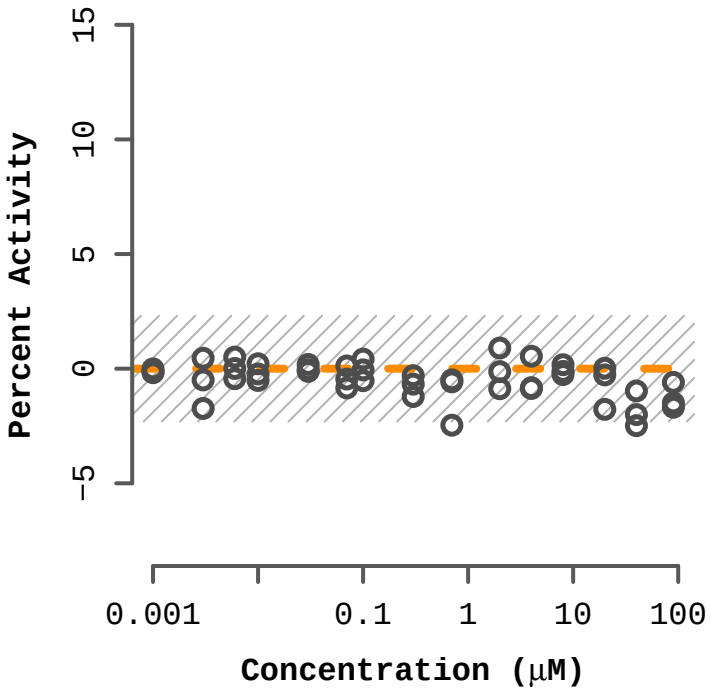
NAME: Barium chloride
CHID: 44508 CASRN: 10361-37-2
SPID(S): Tox21_301015
M4ID: 12478118

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.819 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

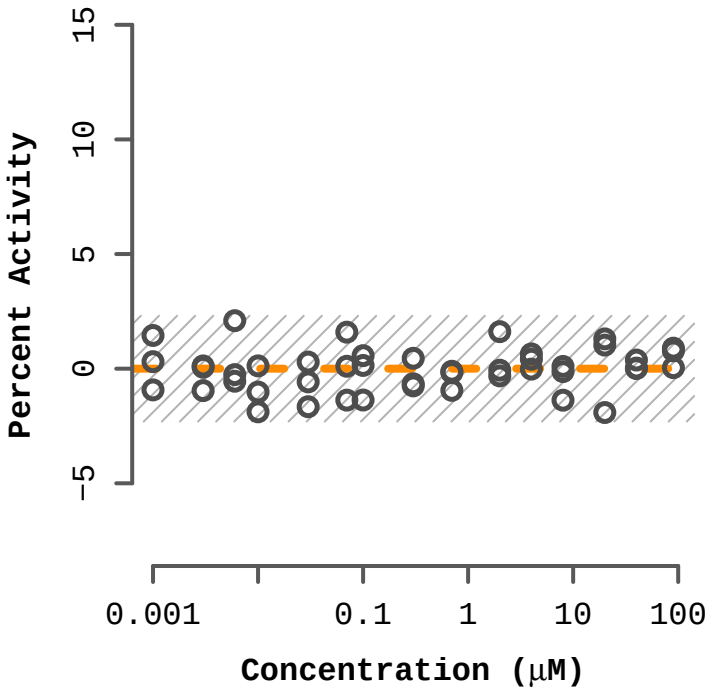
NAME: 3,4,5,6-Tetrachloropyridine-2-carboxylic acid
CHID: 44509 **CASRN:** 10469-09-7
SPID(S): Tox21_300981
M4ID: 12478152

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.0278 **MAX_MED:** 0.0112 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

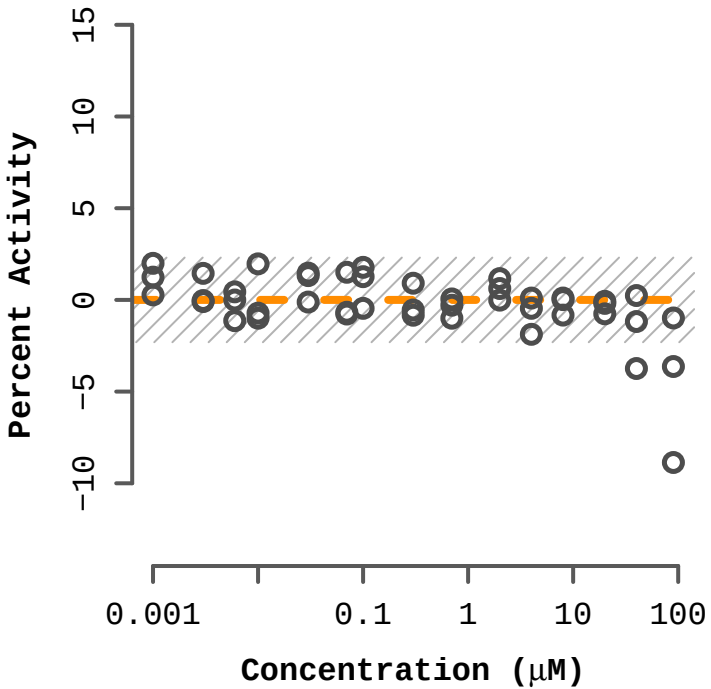
NAME: Dipropyl hexanedioate
CHID: 44511 CASRN: 106-19-4
SPID(S): Tox21_301168
M4ID: 12477965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

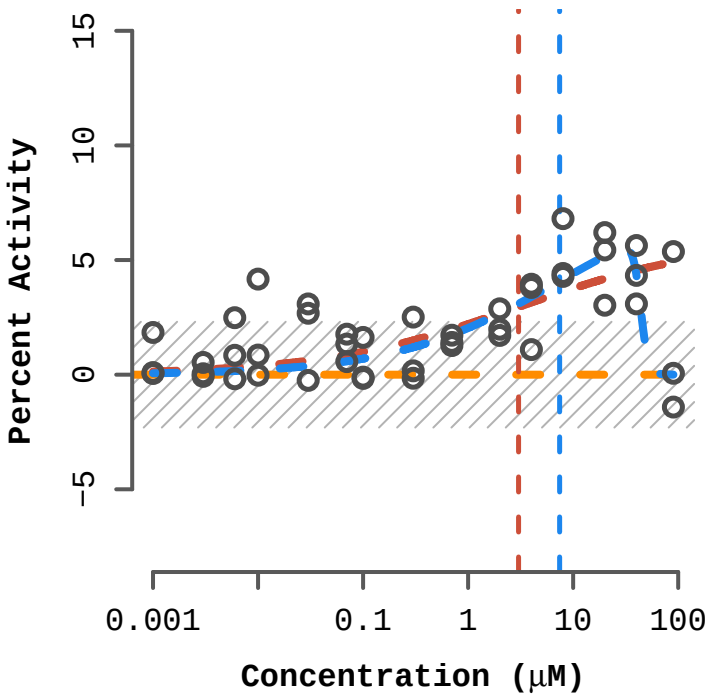
NAME: 3,7-Dimethyloctane-1,7-diol
CHID: 44513 **CASRN:** 107-74-4
SPID(S): Tox21_300934
M4ID: 12478199

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexylparaben
CHID: 44514 CASRN: 1083-27-8
SPID(S): Tox21_303422
M4ID: 12475717

HILL MODEL (in red):

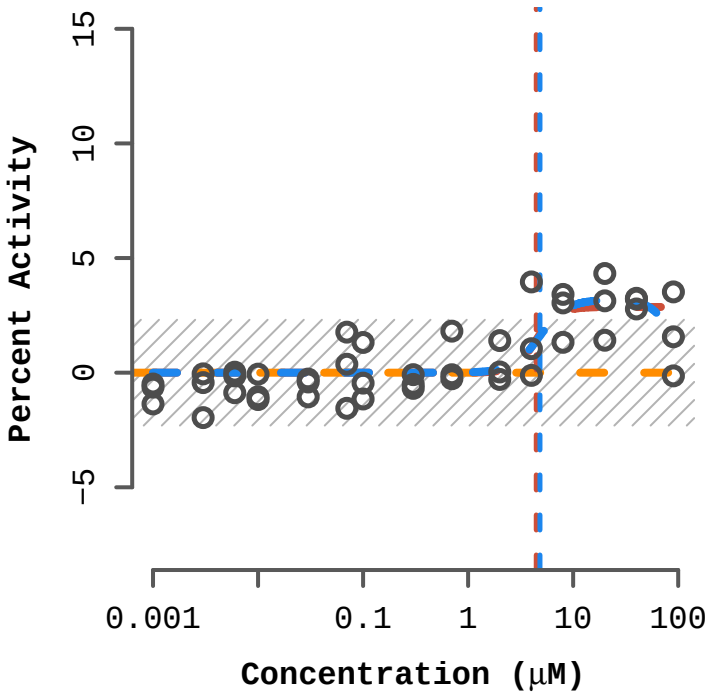
	tp	ga	gw
val:	5.91	0.48	0.469
sd:	2.18	0.81	0.266

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.17	0.871	0.55	1.64	11.9
sd:	3.34	0.674	0.218	0.115	35.5

	CNST	HILL	GNLS
AIC:	225.29	177	169.44
PROB:	0	0.02	0.98
RMSE:	2.85	1.74	1.5

MAX_MEAN: 5.17 MAX_MED: 5.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexylparaben
CHID: 44514 CASRN: 1083-27-8
SPID(S): Tox21_202266
M4ID: 12479986

HILL MODEL (in red):

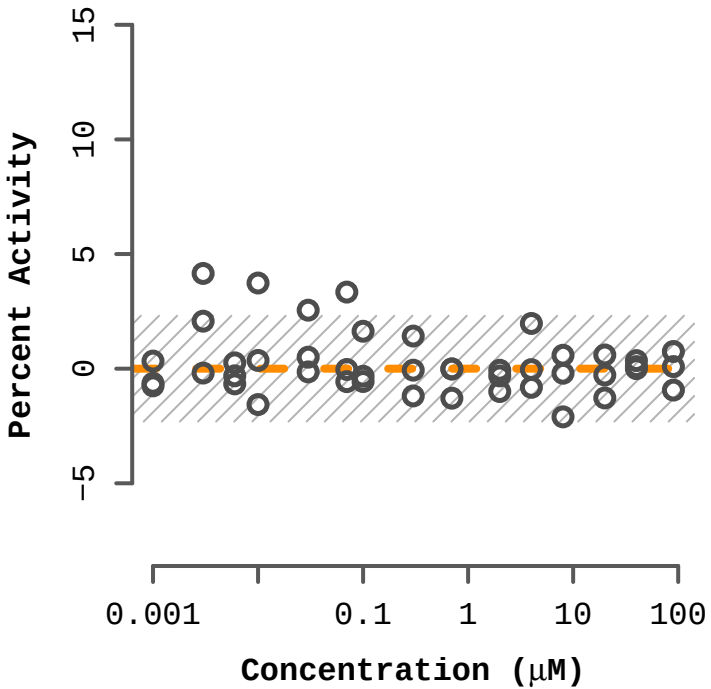
	tp	ga	gw
val:	2.86	0.649	4.32
sd:	0.353	0.108	5.14

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.19	0.684	3.35	1.95	4.15
sd:	0.838	0.14	3.08	0.119	10.6

	CNST	HILL	GNLS
AIC:	180.22	144.22	145.44
PROB:	0	0.65	0.35
RMSE:	1.76	1.09	1.05

MAX_MEAN: 3.08 MAX_MED: 3.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

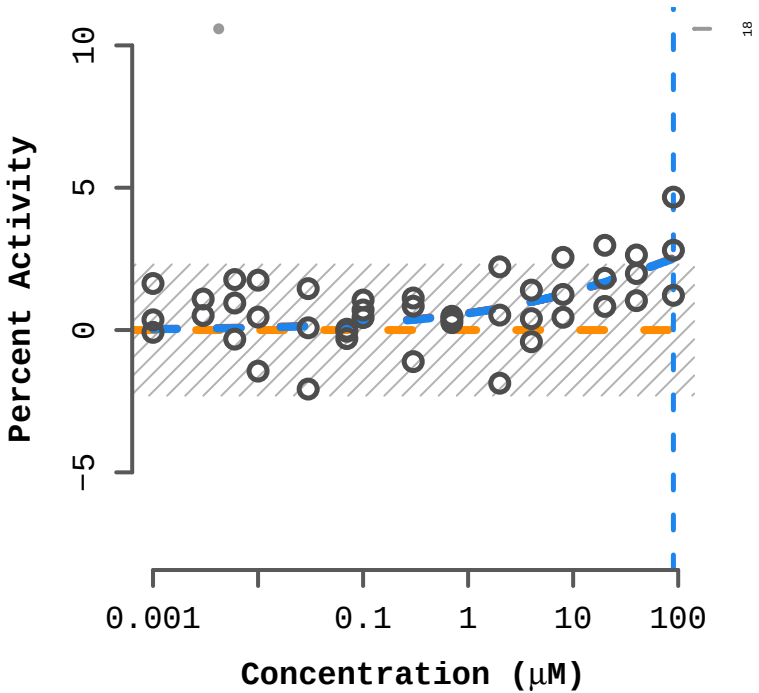
NAME: Tetraethyleneglycol dimethacrylate
CHID: 44515 **CASRN:** 109-17-1
SPID(S): Tox21_300956
M4ID: 12478177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methyl-1-phenyl-1H-pyrazol-5-amine
CHID: 44517 CASRN: 1131-18-6
SPID(S): Tox21_301945
M4ID: 12477188 BRK

HILL MODEL (in red):

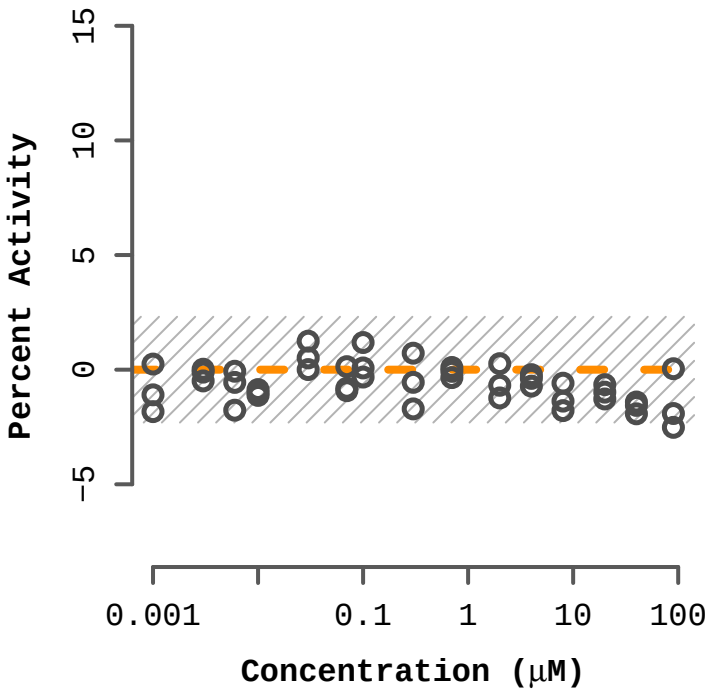
	tp	ga	gw
val:	6.6	2.45	0.408
sd:	10.4	2.81	0.242

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.01	1.95	0.451	3.45	6.64
sd:	5.9	2.08	0.287	18100	80500

	CNST	HILL	GNLS
AIC:	186.27	163.72	167.92
PROB:	0	0.89	0.11
RMSE:	3.1	2.89	2.9

MAX_MEAN: 6.6 MAX_MED: 2.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

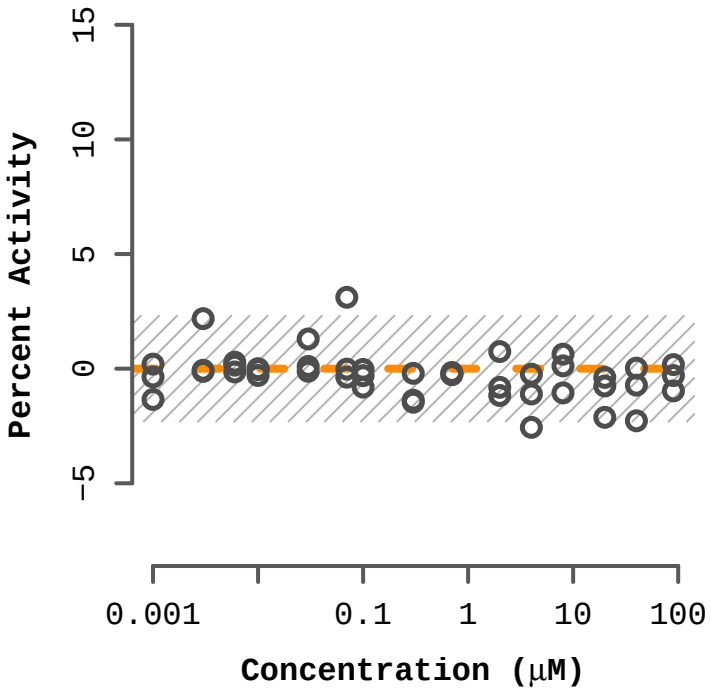
NAME: (−)−Isolongifolene
CHID: 44518 **CASRN:** 1135−66−6
SPID(S): Tox21_302253
M4ID: 12476880

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.588 **MAX_MED:** 0.515 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

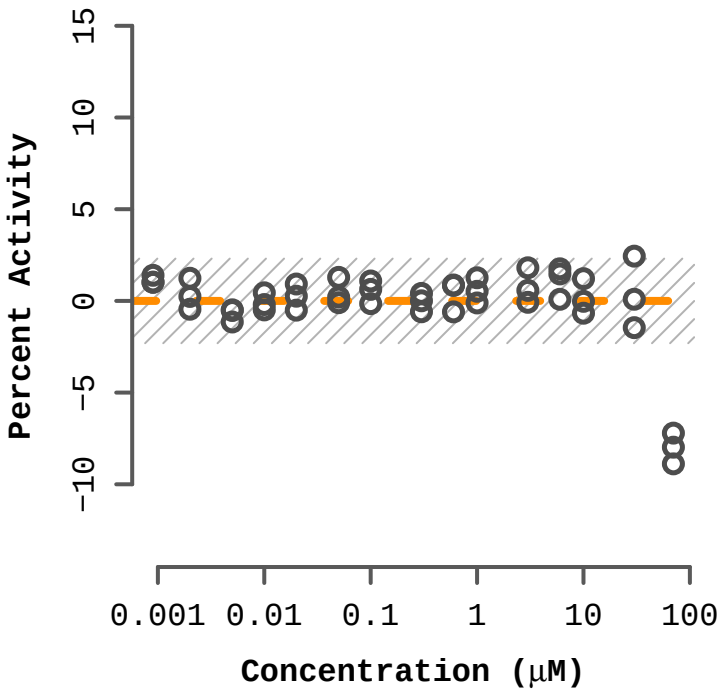
NAME: 1,1,3,3,5-Pentamethyl-4,6-dinitro-2,3-dihydro-1
CHID: 44519 **CASRN:** 116-66-5
SPID(S): Tox21_302237
M4ID: 12476896

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.909 **MAX_MED:** 0.152 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

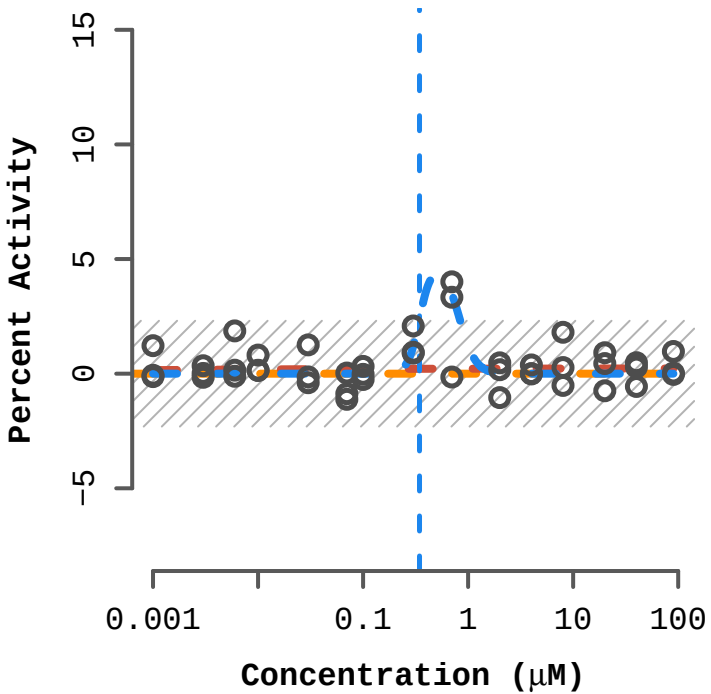
NAME: Tetrabromophenolphthalein ethyl ester
CHID: 44520 CASRN: 1176-74-5
SPID(S): Tox21_301921
M4ID: 12477212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.26	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diatrizoic acid
CHID: 44521 CASRN: 117-96-4
SPID(S): Tox21_301929
M4ID: 12477204

HILL MODEL (in red):

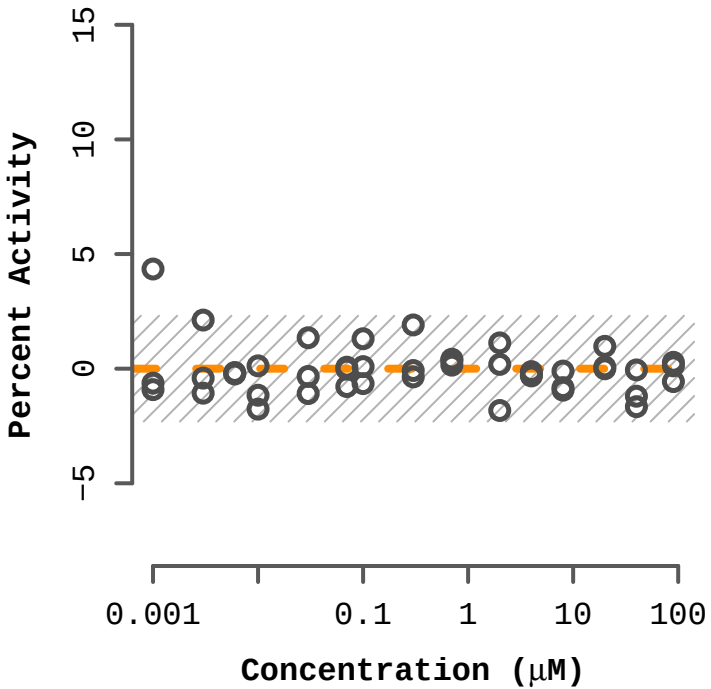
	tp	ga	gw
val:	0.231	−3.99	0.3
sd:	0.316	10.6	2.37

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.81	−0.463	7.98	−0.0813	5.74
sd:	98.8	1.57	91.7	4.87	62.1

	CNST	HILL	GNLS
AIC:	121.72	124.23	111.56
PROB:	0.01	0	0.99
RMSE:	1.07	1.01	0.85

MAX_MEAN: 2.4 MAX_MED: 3.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

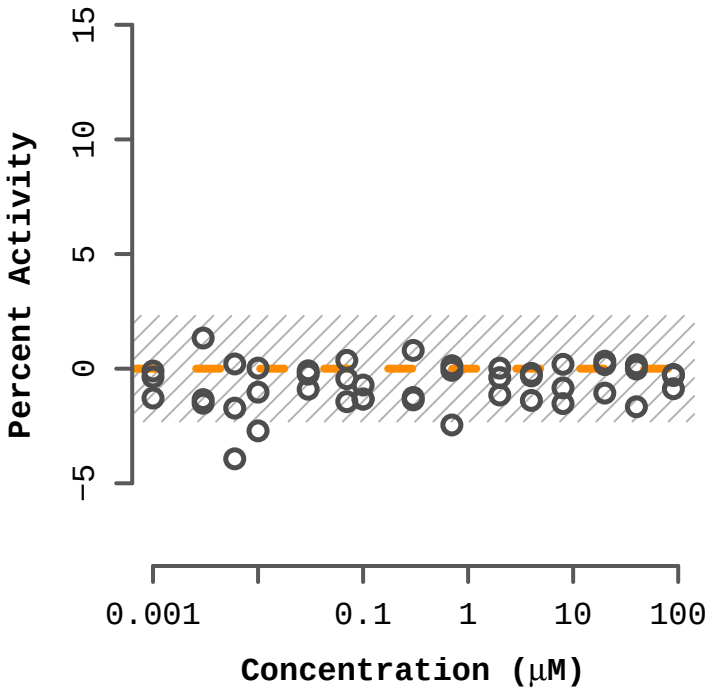
NAME: Tetraethylurea
CHID: 44522 **CASRN:** 1187-03-7
SPID(S): Tox21_301498
M4ID: 12477635

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.352 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

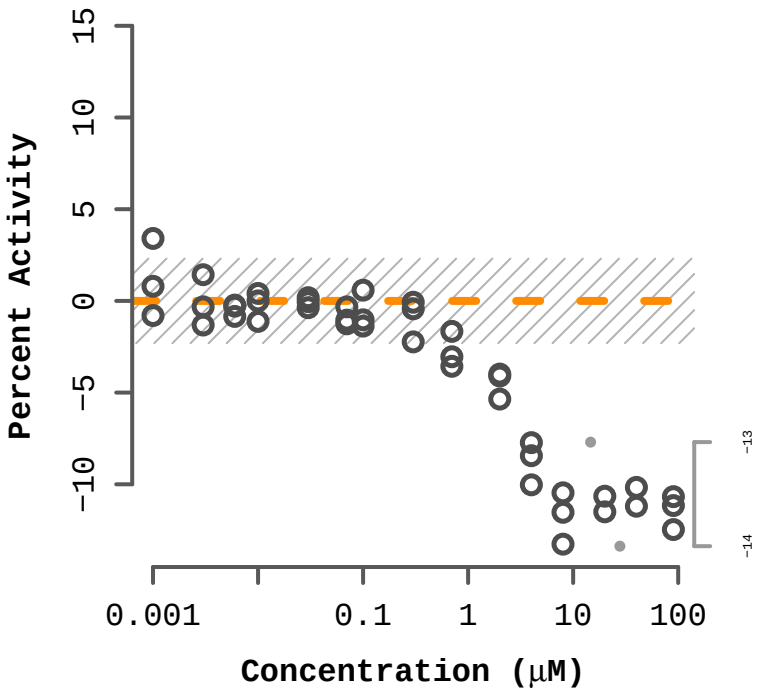
NAME: 5-Amino-2-methylbenzenesulfonic acid
CHID: 44523 **CASRN:** 118-88-7
SPID(S): Tox21_302265
M4ID: 12476868

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: −0.185 **MAX_MED:** 0.179 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

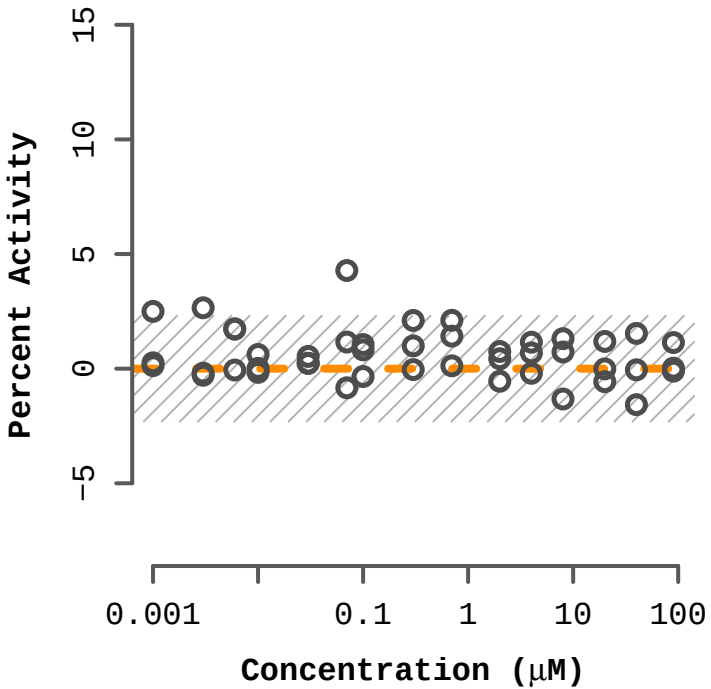
NAME: Phenylmercuric lactate
CHID: 44525 **CASRN:** 122-64-5
SPID(S): Tox21_302004
M4ID: 12477129 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.99	NA	NA
PROB:	1	NA	NA
RMSE:	6.71	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.797 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

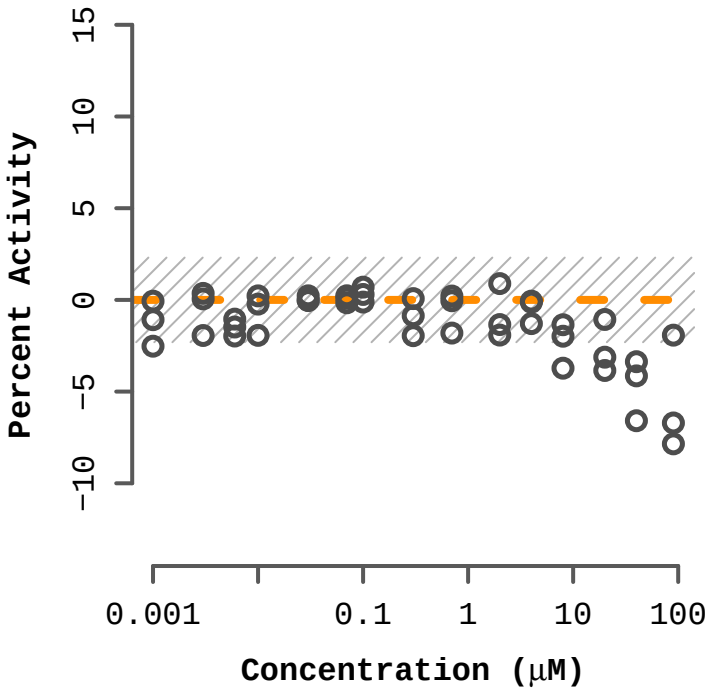
NAME: N-(4-Ethoxyphenyl)-3-oxobutanamide
CHID: 44526 **CASRN:** 122-82-7
SPID(S): Tox21_301551
M4ID: 12477582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

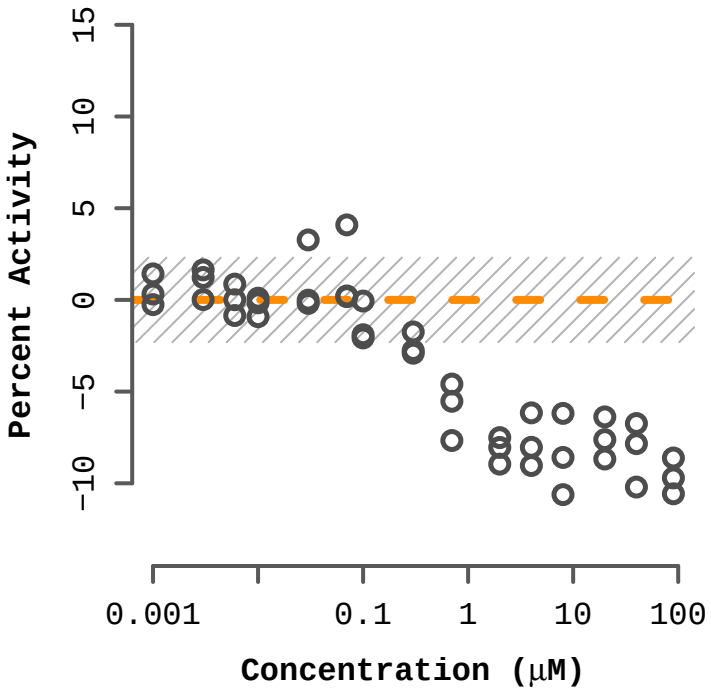
NAME: Ethane−1,2−diyl bis(sulfanylacetate)
CHID: 44527 CASRN: 123−81−9
SPID(S): Tox21_302245
M4ID: 12476888

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.69	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 0.293 MAX_MED: 0.298 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

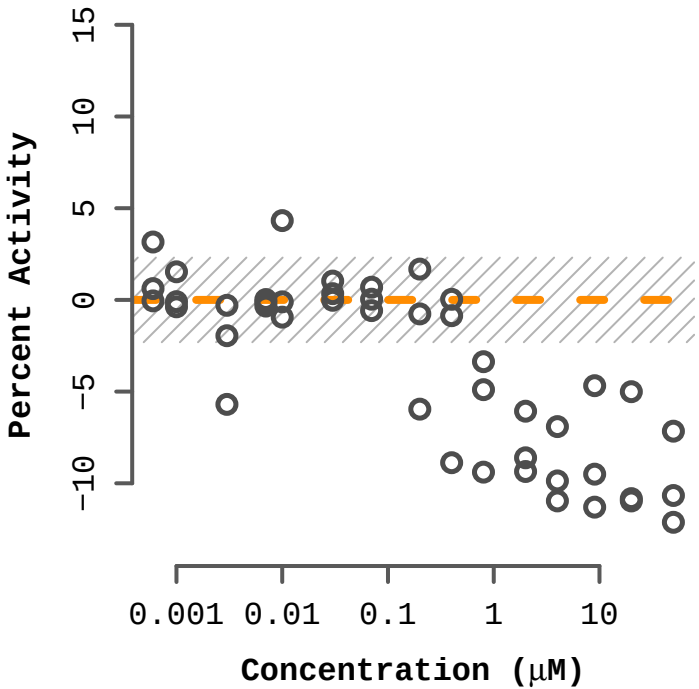
NAME: Oxyphenisatin
CHID: 44528 **CASRN:** 125-13-3
SPID(S): Tox21_301931
M4ID: 12477202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.08	NA	NA
PROB:	1	NA	NA
RMSE:	5.67	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

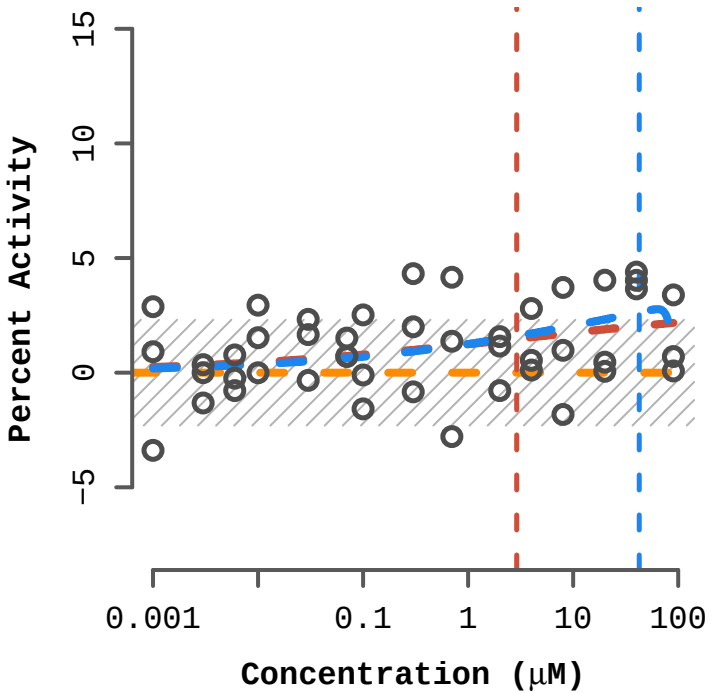
NAME: Oxyphenisatin
CHID: 44528 **CASRN:** 125-13-3
SPID(S): Tox21_113927
M4ID: 12482304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.08	NA	NA
PROB:	1	NA	NA
RMSE:	5.95	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D&C Blue No. 9
CHID: 44532 CASRN: 130-20-1
SPID(S): Tox21_302231
M4ID: 12476902

HILL MODEL (in red):

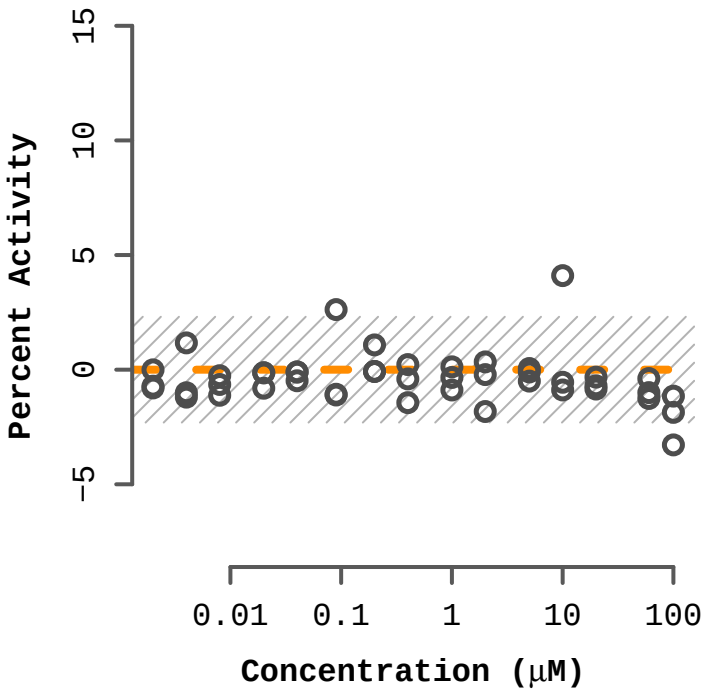
	tp	ga	gw
val:	2.95	0.462	0.3
sd:	6.15	6.74	0.449

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.27	1.63	0.311	1.94	14.4
sd:	4.91	2.12	0.179	0.0705	79.9

	CNST	HILL	GNLS
AIC:	202.74	192.83	195.05
PROB:	0.01	0.75	0.25
RMSE:	2.18	1.79	1.77

MAX_MEAN: 4.03 MAX_MED: 4.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

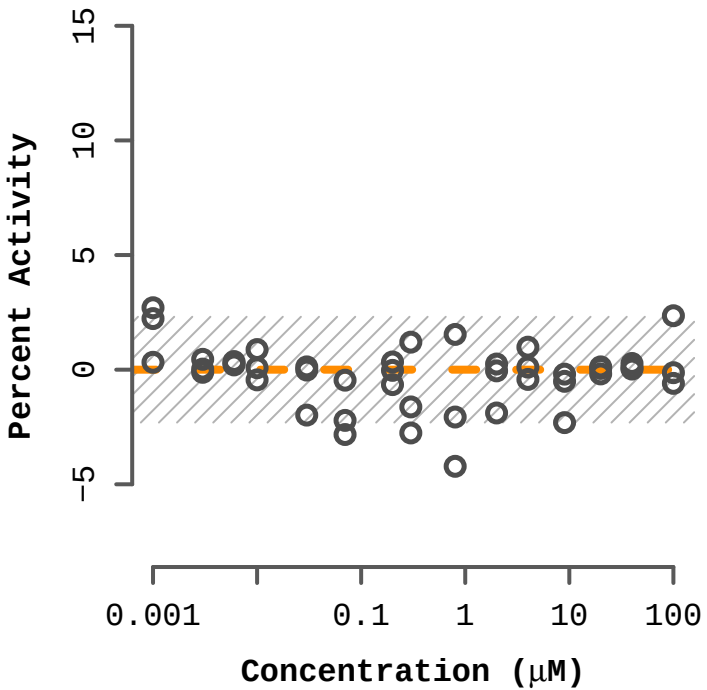
NAME: 2,2'−Dichlorobiphenyl
CHID: 44533 **CASRN:** 13029−08−8
SPID(S): Tox21_202244
M4ID: 12480008

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.891 **MAX_MED:** −0.0755 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

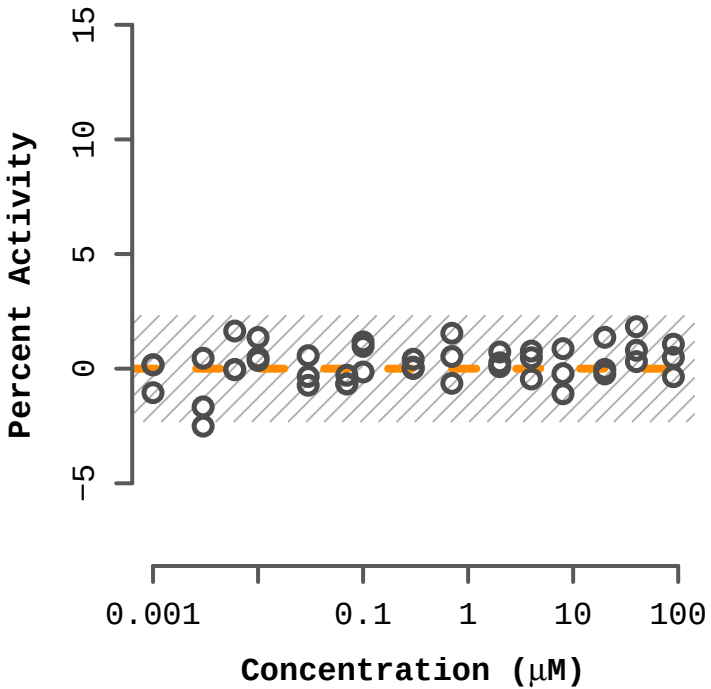
NAME: 4-Acetylphenyl acetate
CHID: 44534 **CASRN:** 13031-43-1
SPID(S): Tox21_302228
M4ID: 12476905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

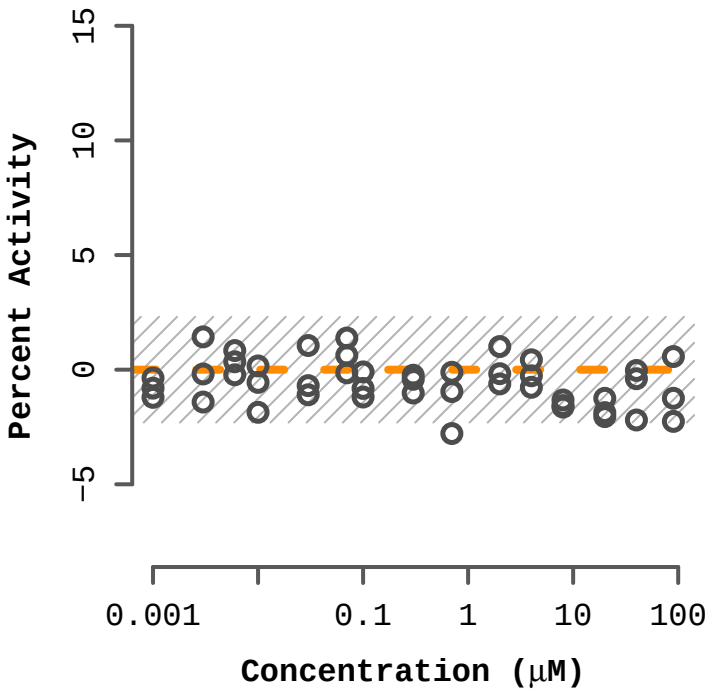
NAME: Sodium 9,10-dioxo-9,10-dihydroanthracene-2-sul
CHID: 44535 **CASRN:** 131-08-8
SPID(S): Tox21_301475
M4ID: 12477658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 0.971 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-(6-tert-Butyl-1,1-dimethyl-2,3-dihydro-1H-in

CHID: 44536 **CASRN:** 13171-00-1

SPID(S): Tox21_301542

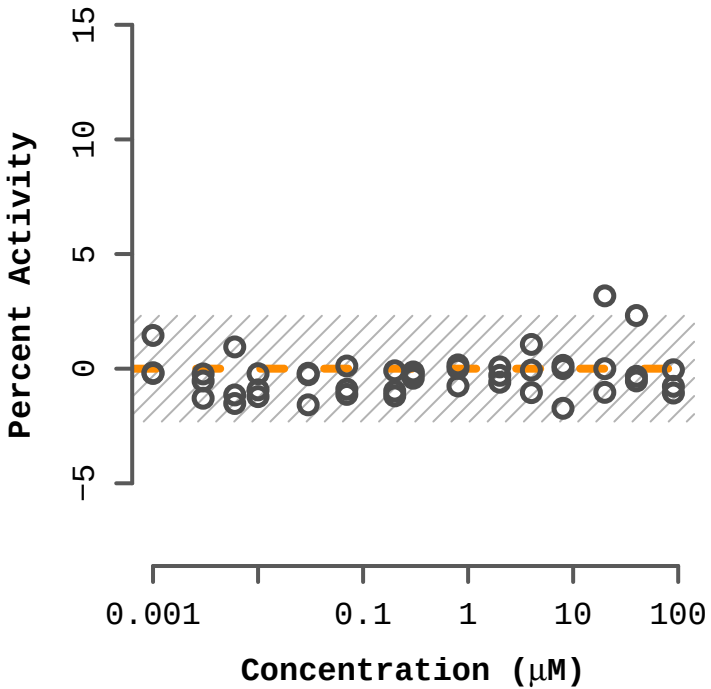
M4ID: 12477591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.624 **MAX_MED:** 0.626 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

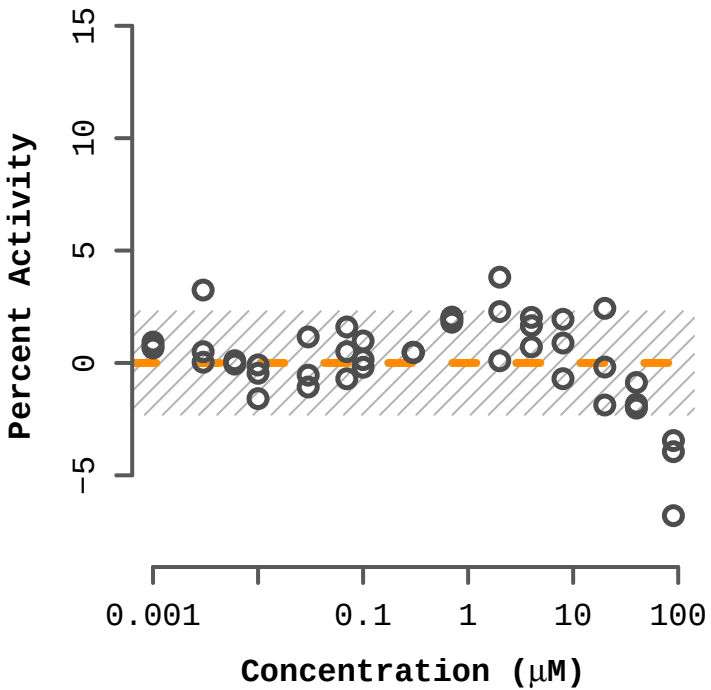
NAME: Sodium triisopropyl naphthalene sulfonate
CHID: 44537 CASRN: 1323-19-9
SPID(S): Tox21_302271
M4ID: 12476862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.716 **MAX_MED:** 0.0192 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

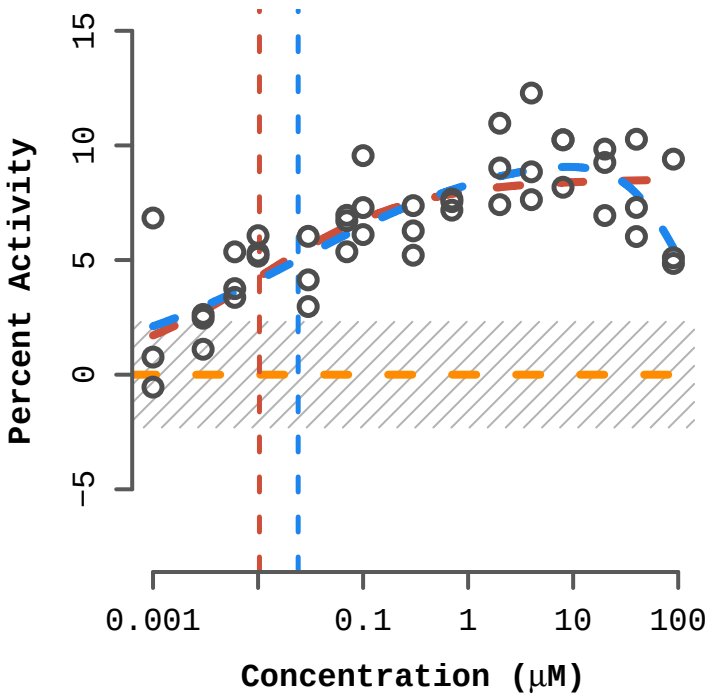
NAME: C.I. Disperse Orange 37
CHID: 44538 **CASRN:** 13301-61-6
SPID(S): Tox21_302225
M4ID: 12476908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.87	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isocyclocitral
CHID: 44541 CASRN: 1335-66-6
SPID(S): Tox21_301863
M4ID: 12477270

HILL MODEL (in red):

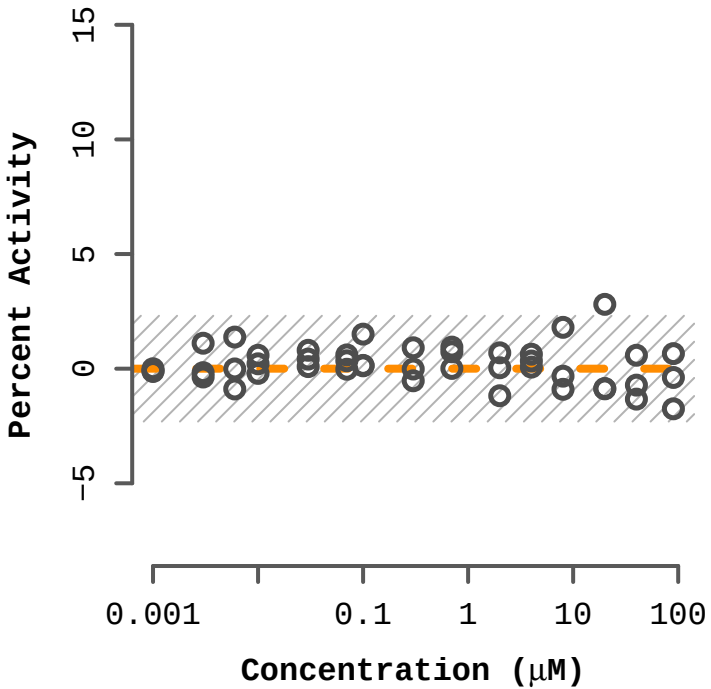
	tp	ga	gw
val:	8.54	−1.99	0.593
sd:	0.572	0.194	0.161

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10	−1.62	0.416	2.03	1.54
sd:	1.94	0.512	0.165	0.14	0.888

	CNST	HILL	GNLS
AIC:	314.21	188.47	186.02
PROB:	0	0.23	0.77
RMSE:	7.07	1.79	1.66

MAX_MEAN: 9.59 MAX_MED: 10.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

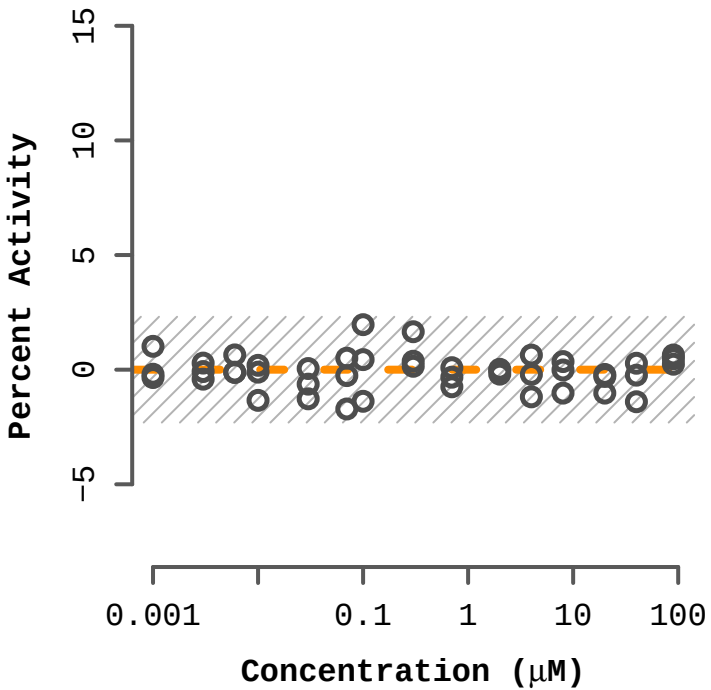
NAME: Citral oxime
CHID: 44542 **CASRN:** 13372-77-5
SPID(S): Tox21_301898
M4ID: 12477235

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.593 **MAX_MED:** 0.739 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

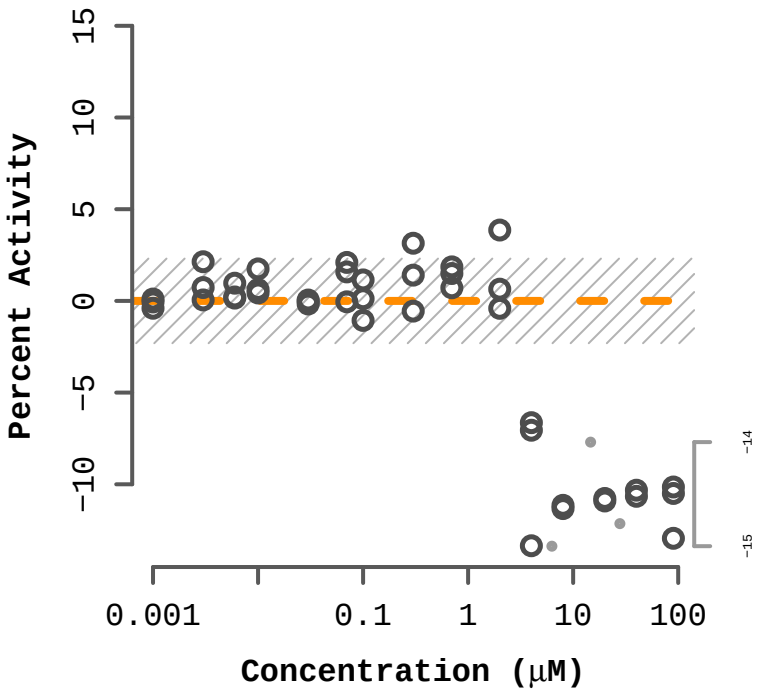
NAME: Disodium 3-hydroxynaphthalene-2,7-disulfonate
CHID: 44543 **CASRN:** 135-51-3
SPID(S): Tox21_301601
M4ID: 12477532

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

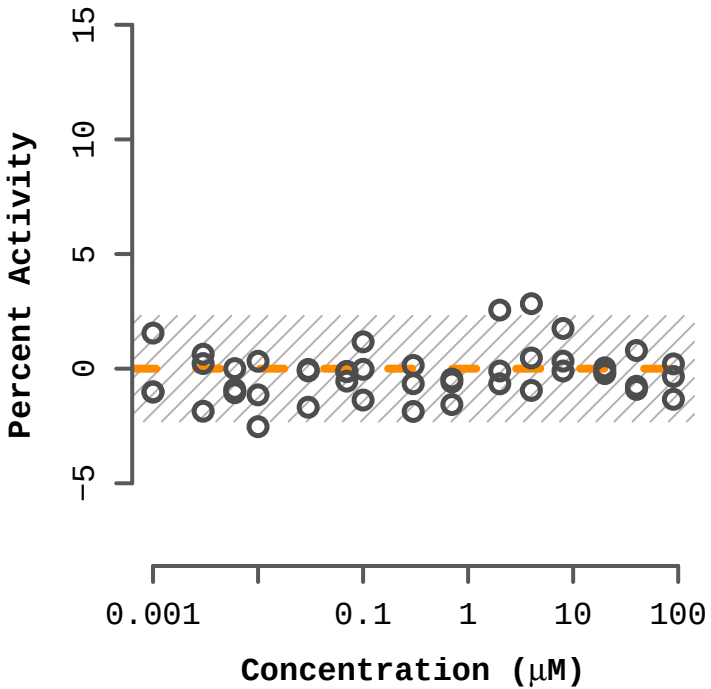
NAME: 3-Hydroxy-N-(3-nitrophenyl)naphthalene-2-carbox
CHID: 44544 CASRN: 135-65-9
SPID(S): Tox21_301464
M4ID: 12477669 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	298.71	NA	NA
PROB:	1	NA	NA
RMSE:	6.7	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

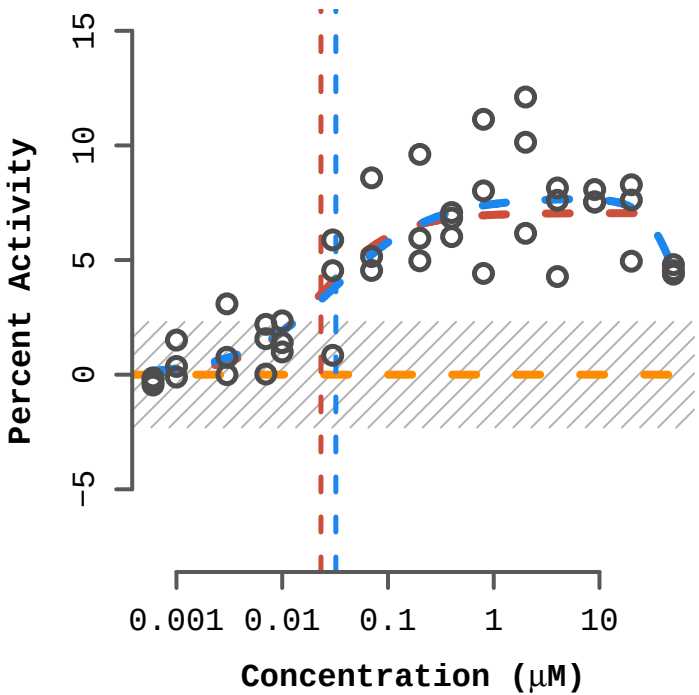
NAME: Minocycline hydrochloride
CHID: 44545 **CASRN:** 13614-98-7
SPID(S): Tox21_301590
M4ID: 12477543

HILL MODEL: Not applicable.

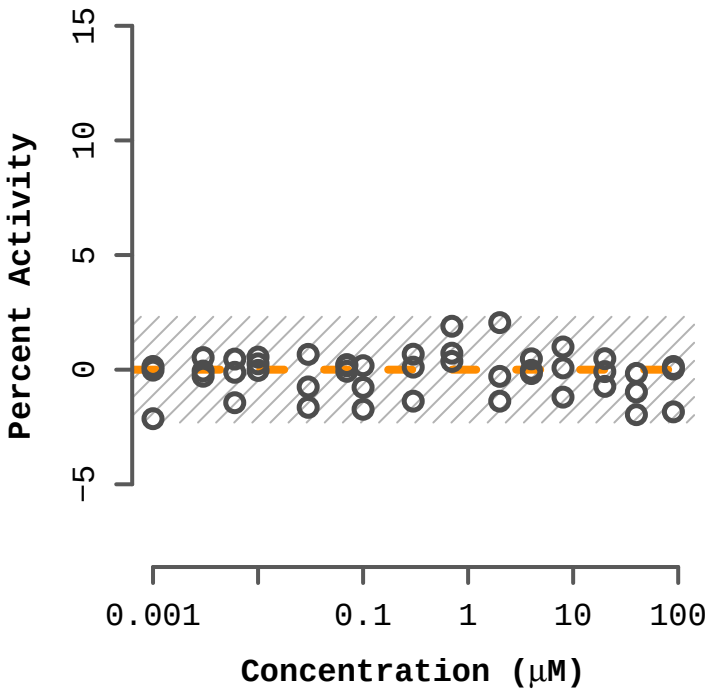
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.785 **MAX_MED:** 0.466 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Minocycline hydrochloride
CHID:    44545   CASRN: 13614-98-7
SPID(S): Tox21_111250_1
M4ID:    12483815

HILL MODEL (in red):
      tp       ga       gw
val:  7.05     -1.63    1.2
sd:   0.432    0.145    0.374

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.72     -1.49    0.957    1.76     2.74
sd:   0.583    0.171    0.252    0.078    2.91

      CNST        HILL        GNLS
AIC:  293.77      188.67      181.3
PROB: 0           0.02        0.98
RMSE: 5.82        1.81        1.65

MAX_MEAN: 9.47      MAX_MED: 10.1      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

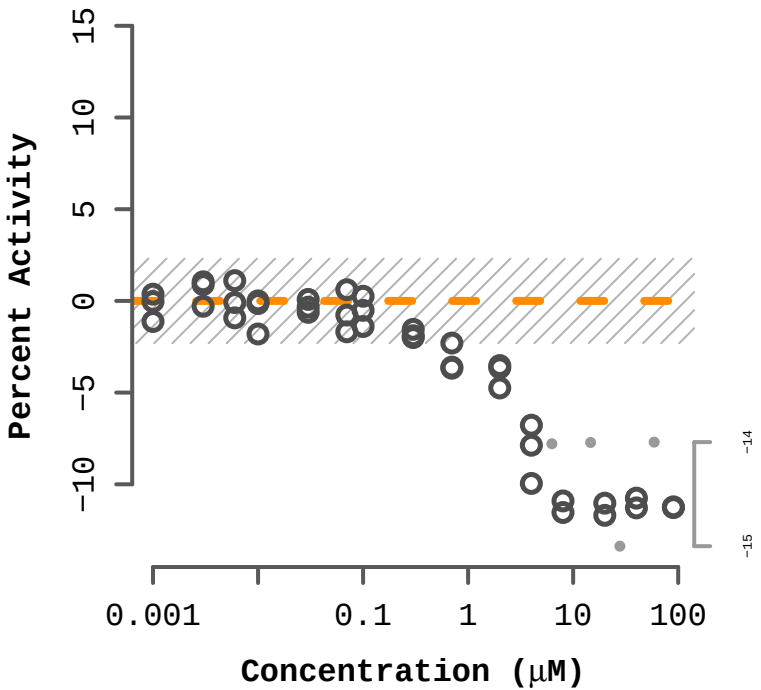
NAME: 2-Heptylcyclopentanone
CHID: 44547 **CASRN:** 137-03-1
SPID(S): Tox21_301923
M4ID: 12477210

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 0.721 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

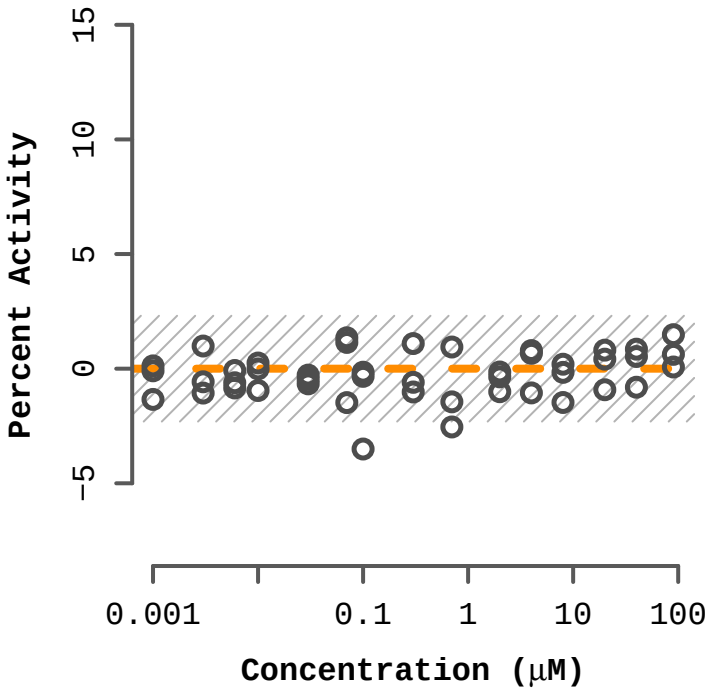
NAME: Potassium dicyanoaurate
CHID: 44549 **CASRN:** 13967-50-5
SPID(S): Tox21_302234
M4ID: 12476899 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	302.55	NA	NA
PROB:	1	NA	NA
RMSE:	6.88	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.892 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

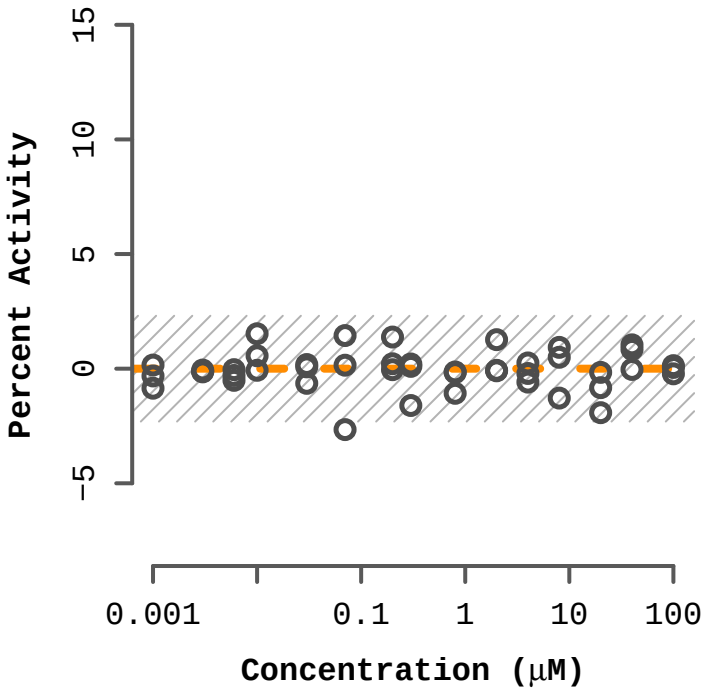
NAME: Aluminum hydroxide acetate (1:1:2)
CHID: 44552 CASRN: 142-03-0
SPID(S): Tox21_301868
M4ID: 12477265

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.729 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

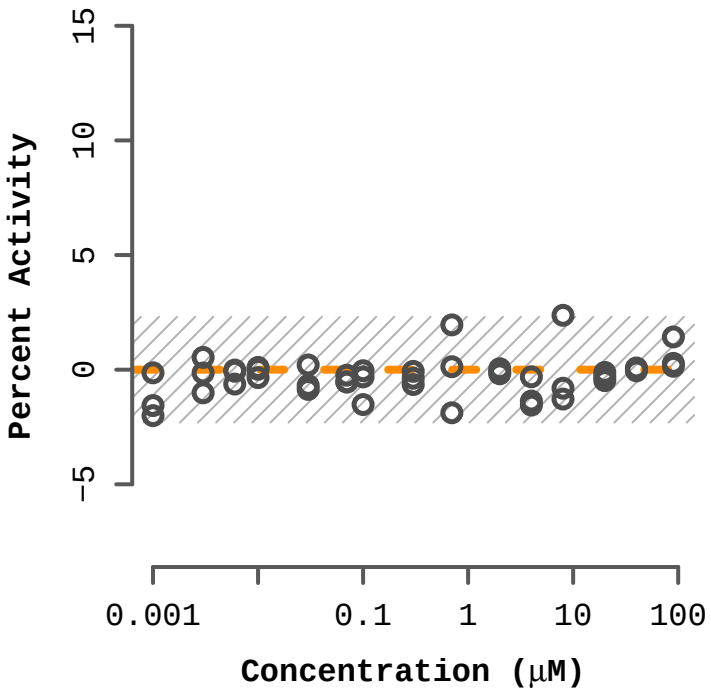
NAME: Sodium 2-methylbenzenesulfonate
CHID: 44553 CASRN: 15046-75-0
SPID(S): Tox21_301897
M4ID: 12477236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.843 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

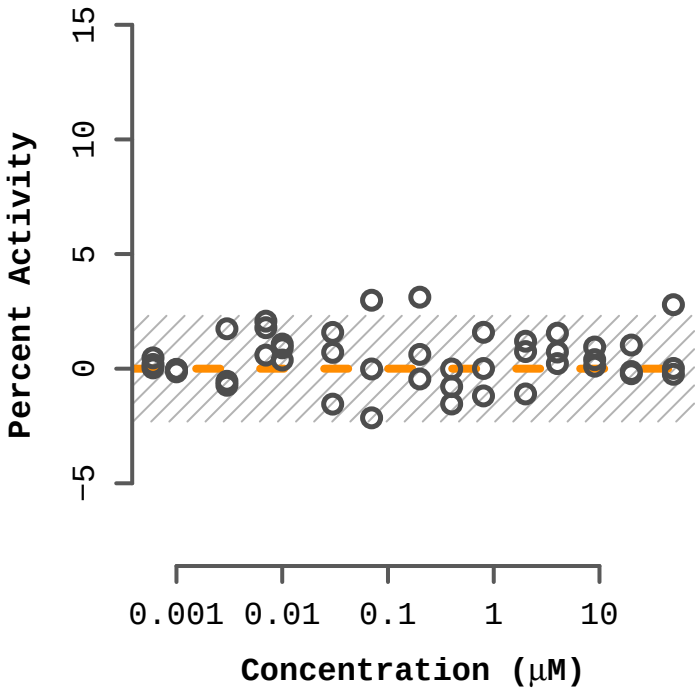
NAME: Cromolyn sodium
CHID: 44554 CASRN: 15826-37-6
SPID(S): Tox21_302003
M4ID: 12477130

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.619 **MAX_MED:** 0.276 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

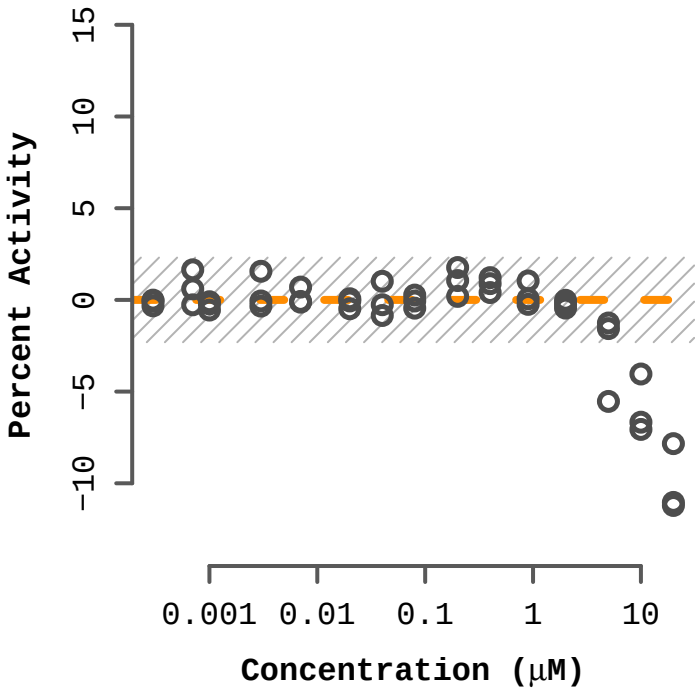
NAME: Cromolyn sodium
CHID: 44554 **CASRN:** 15826-37-6
SPID(S): Tox21_110863_1
M4ID: 12484059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl(4,5,6,7,8,8-hexachloro-1,3-dioxo-1,3,3a,4

CHID: 44558 **CASRN:** 2597-93-5

SPID(S): Tox21_303854

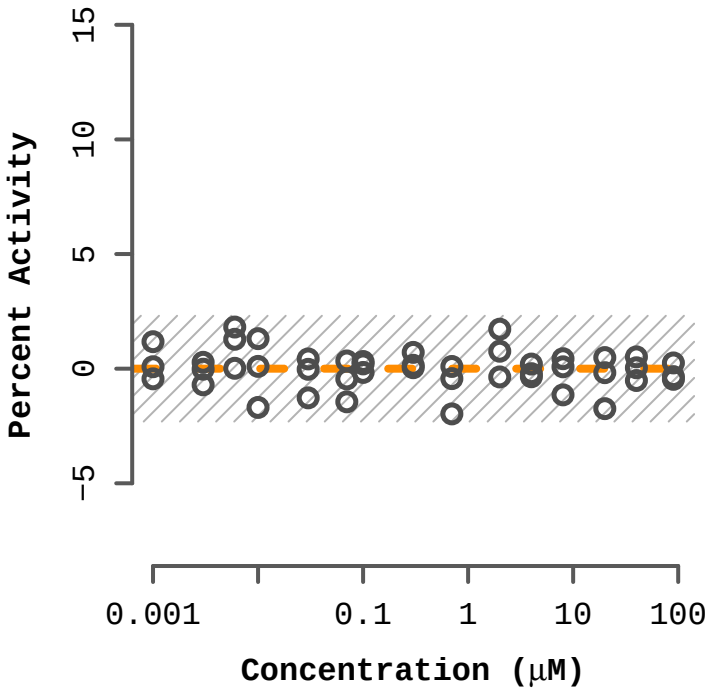
M4ID: 12475334

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.19	NA	NA
PROB:	1	NA	NA
RMSE:	3.24	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

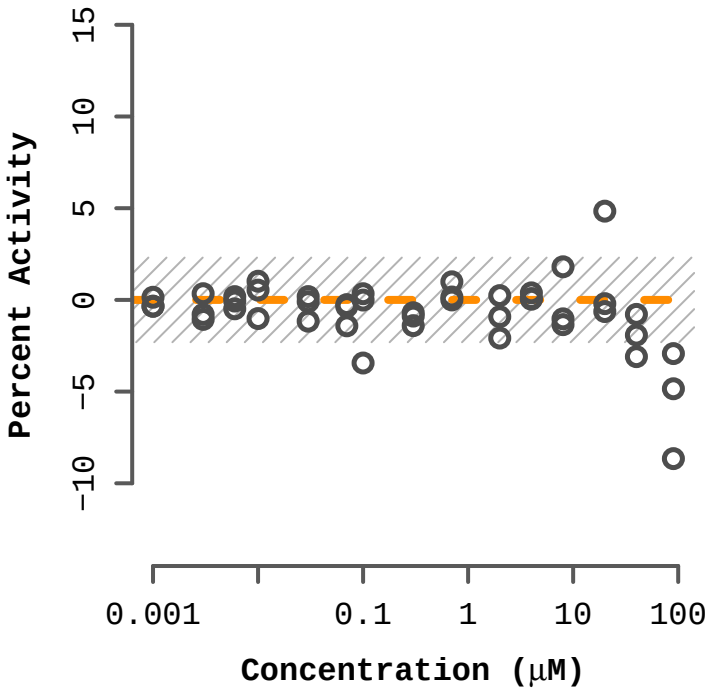
NAME: Profluralin
CHID: 44559 **CASRN:** 26399-36-0
SPID(S): Tox21_301566
M4ID: 12477567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

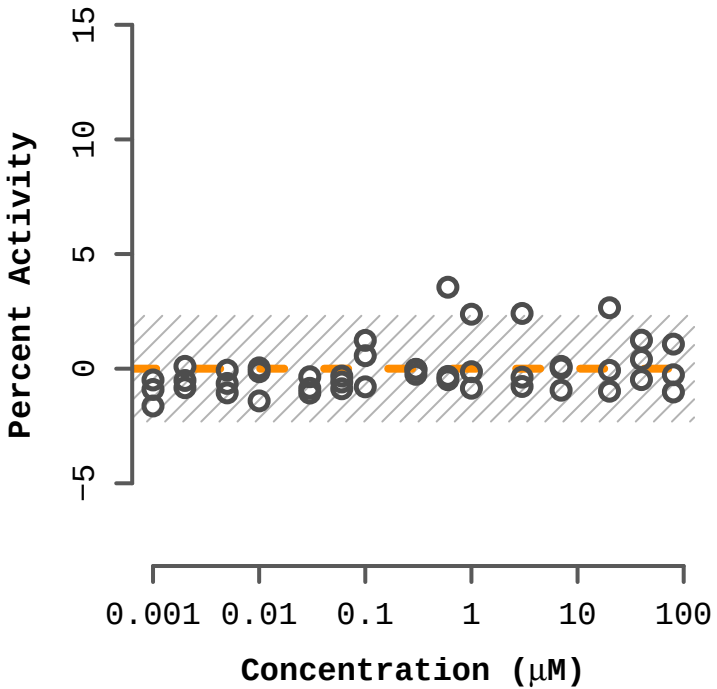
NAME: 5-Bromo-5-nitro-1,3-dioxane
CHID: 44560 **CASRN:** 30007-47-7
SPID(S): Tox21_301588
M4ID: 12477545

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.18	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.535 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

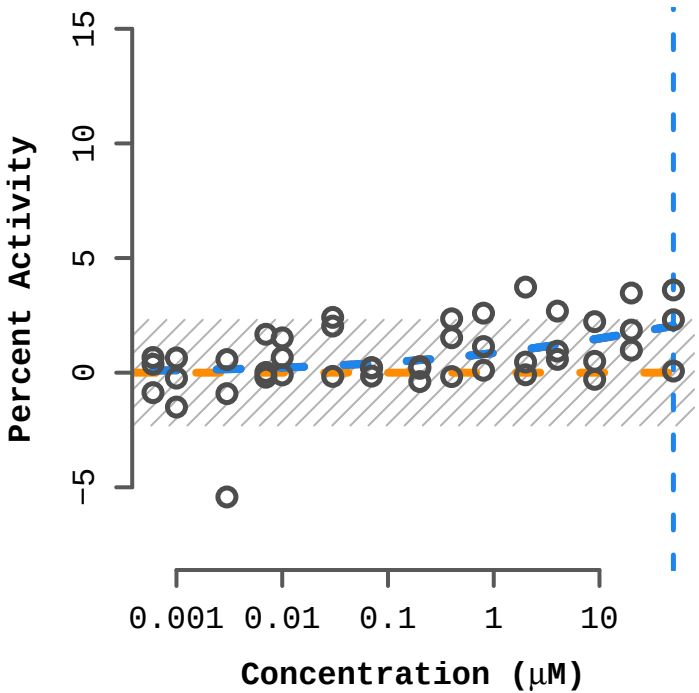
NAME: Bupropion hydrochloride
CHID: 44561 CASRN: 31677-93-7
SPID(S): Tox21_301844
M4ID: 12477289

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.912 **MAX_MED:** 0.568 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bupropion hydrochloride
CHID: 44561 CASRN: 31677-93-7
SPID(S): Tox21_110621_1
M4ID: 12484225

HILL MODEL (in red):

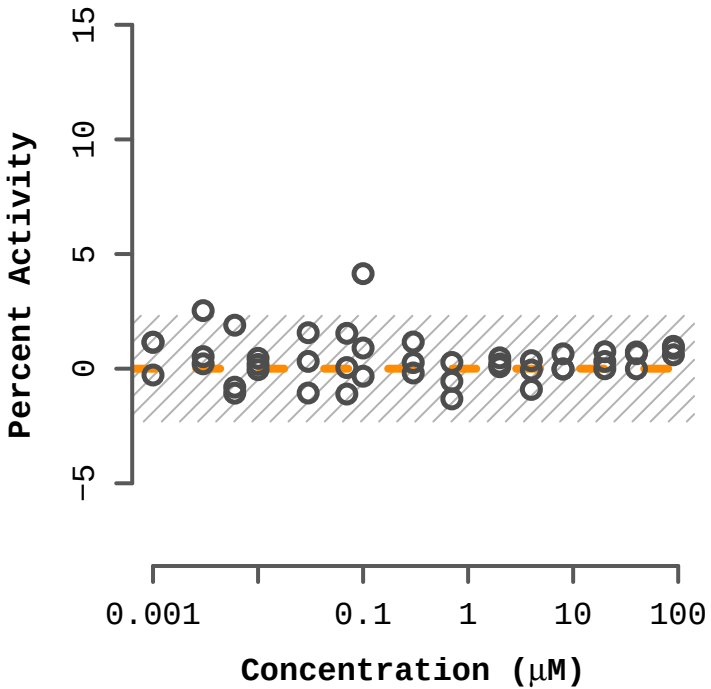
	tp	ga	gw
val:	4.48	1.93	0.325
sd:	7.95	4.09	0.203

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.08	1.7	0.337	3.1	6.22
sd:	7.79	4.35	0.228	6390	28300

	CNST	HILL	GNLS
AIC:	173.18	157.7	161.72
PROB:	0	0.88	0.12
RMSE:	1.69	1.37	1.37

MAX_MEAN: 2.11 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

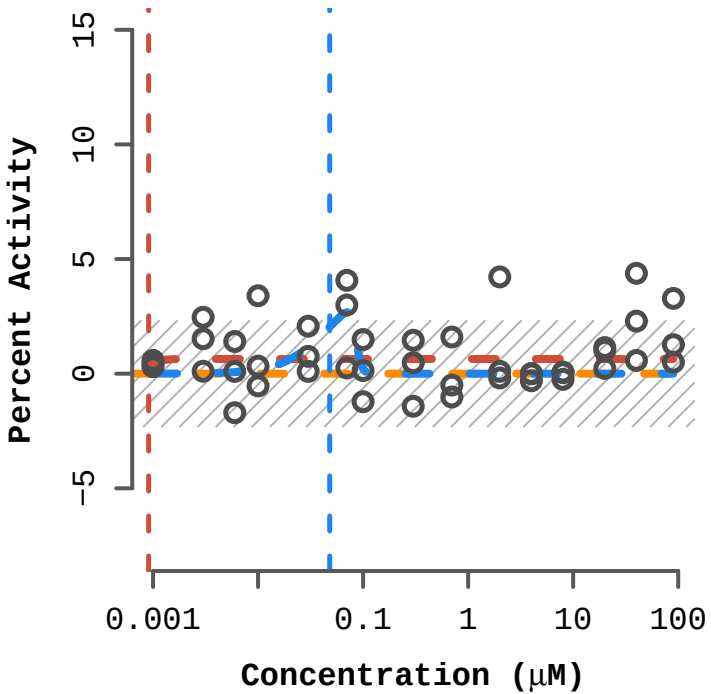
NAME: 6H-Dibenzo[c,e][1,2]oxaphosphinine 6-oxide
CHID: 44563 CASRN: 35948-25-5
SPID(S): Tox21_301503
M4ID: 12477630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.57 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6,10−Trimethyl−2,6,10−triazaundecane
CHID: 44564 CASRN: 3855−32−1
SPID(S): Tox21_300392
M4ID: 12478740

HILL MODEL (in red):

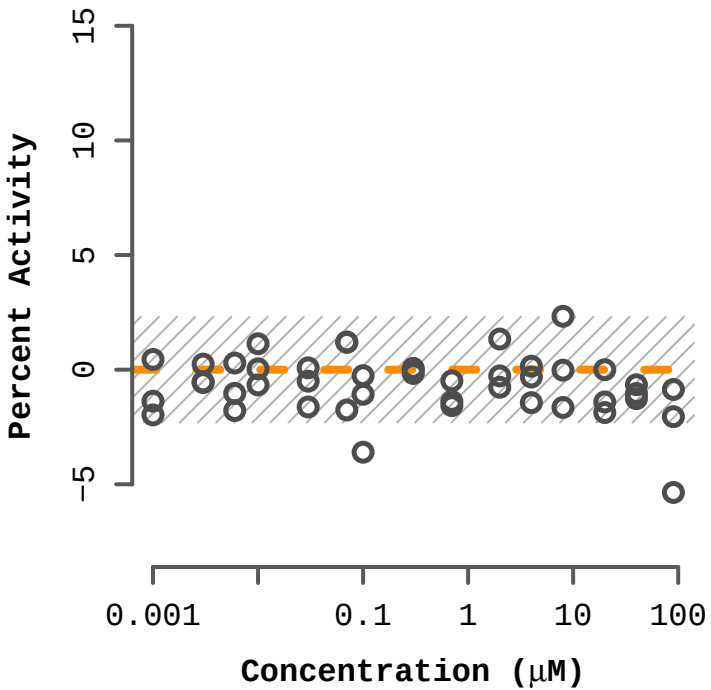
	tp	ga	gw
val:	0.64	−3.04	8
sd:	0.21	0.451	79.9

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.1	−1.32	1.96	−1.07	16.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	172.3	168.27	173.61
PROB:	0.11	0.83	0.06
RMSE:	1.67	1.46	1.52

MAX_MEAN: 2.44 MAX_MED: 3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

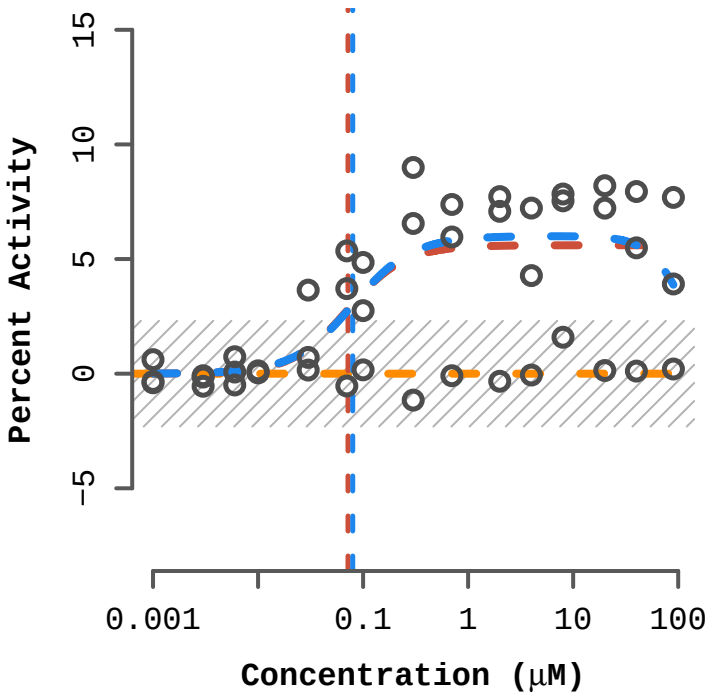
NAME: 3,3'−[Oxybis(ethane−2,1−diyloxy)]dipropan−1−am
CHID: 44565 **CASRN:** 4246−51−9
SPID(S): Tox21_301509
M4ID: 12477624

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.22 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4-Dioxacyclohexadecane-5,16-dione
CHID: 44568 CASRN: 54982-83-1
SPID(S): Tox21_302206
M4ID: 12476927

HILL MODEL (in red):

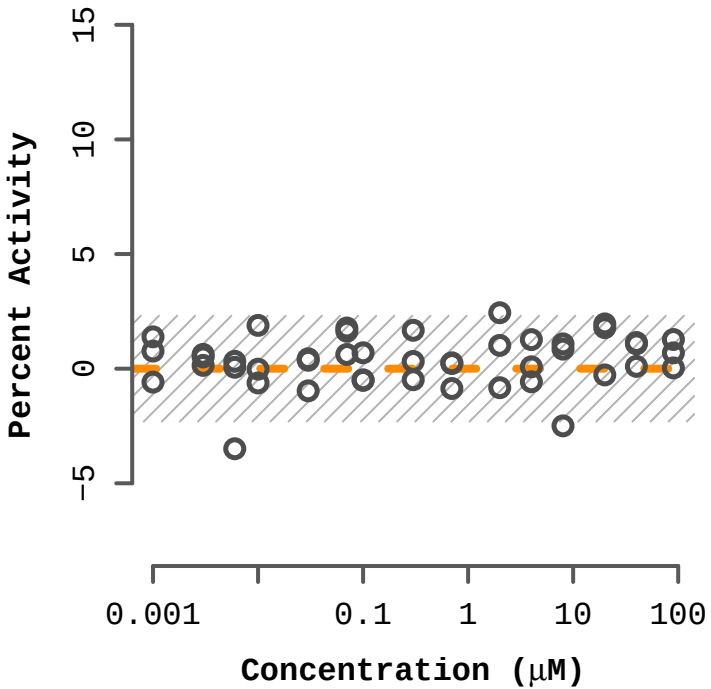
	tp	ga	gw
val:	5.6	−1.14	1.63
sd:	0.718	0.205	0.958

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.01	−1.1	1.54	2.06	2.53
sd:	0.831	0.204	0.907	0.31	4.47

	CNST	HILL	GNLS
AIC:	266.03	227.71	230.6
PROB:	0	0.81	0.19
RMSE:	4.46	2.78	2.79

MAX_MEAN: 5.66 MAX_MED: 7.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

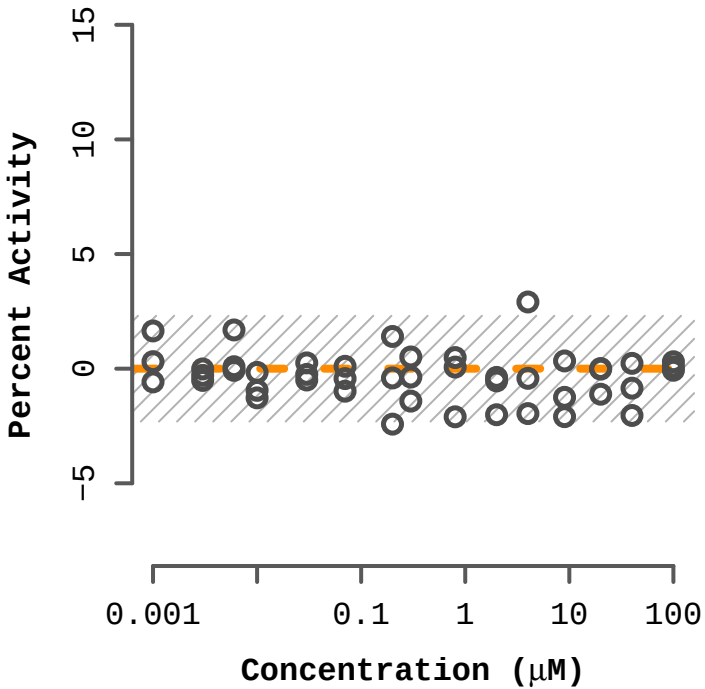
NAME: 1,2-Ethanediamine dihydriodide
CHID: 44570 **CASRN:** 5700-49-2
SPID(S): Tox21_302266
M4ID: 12476867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

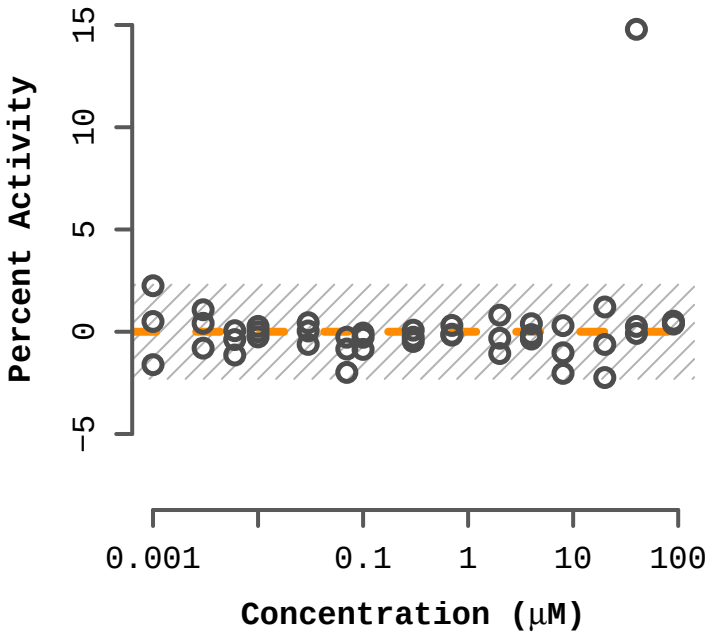
NAME: 3-Isopropylphenol
CHID: 44571 **CASRN:** 618-45-1
SPID(S): Tox21_301558
M4ID: 12477575

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.569 **MAX_MED:** 0.309 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

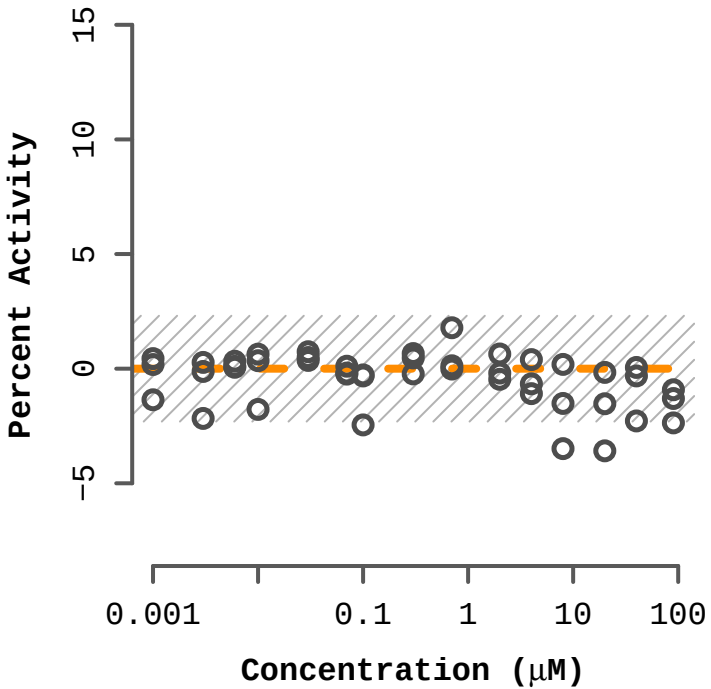
NAME: 3,3,4,4,5,5,6,6,7,7,8,8,8−Tridecafluorooctan−1·
CHID: 44572 CASRN: 647−42−7
SPID(S): Tox21_300519
M4ID: 12478613

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.37	NA	NA

MAX_MEAN: 4.99 MAX_MED: 0.502 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

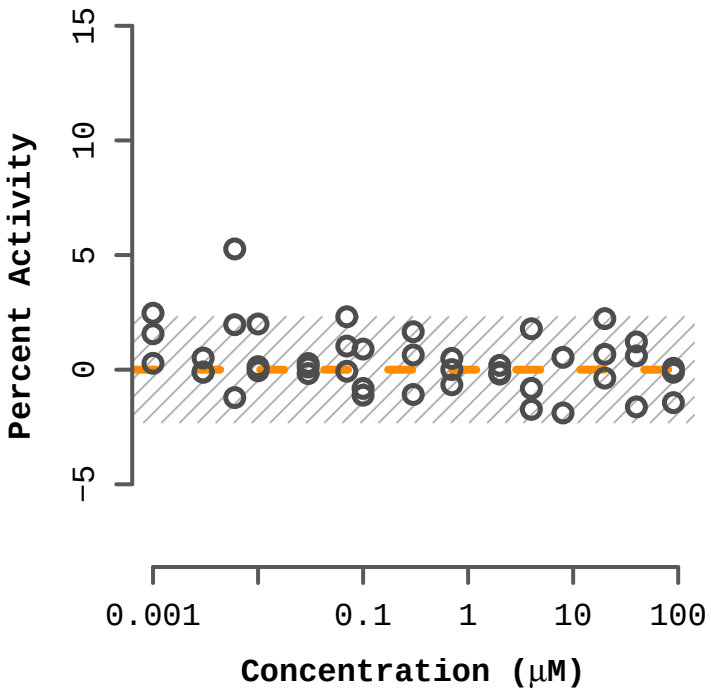
NAME: 2-(2-Methylbutan-2-yl)cyclohexyl acetate
CHID: 44573 **CASRN:** 67874-72-0
SPID(S): Tox21_301888
M4ID: 12477245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.633 **MAX_MED:** 0.488 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

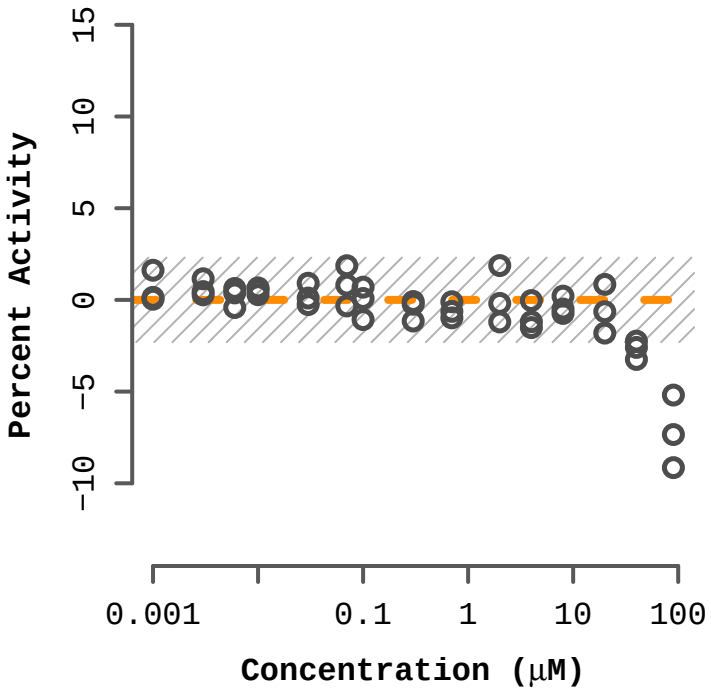
NAME: 2,4-Dimethylcyclohex-3-ene-1-carbaldehyde
CHID: 44574 **CASRN:** 68039-49-6
SPID(S): Tox21_301644
M4ID: 12477489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

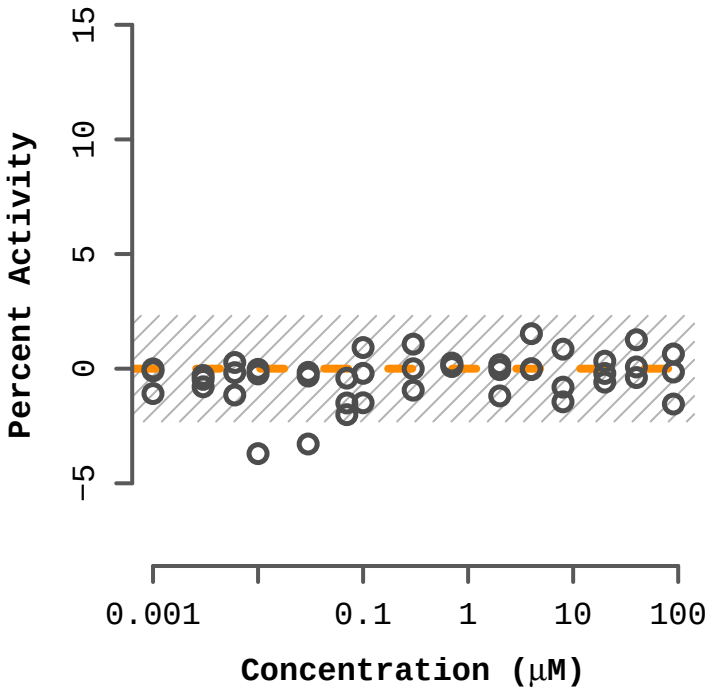
NAME: MON-4660
CHID: 44575 **CASRN:** 71526-07-3
SPID(S): Tox21_302257
M4ID: 12476876

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.35	NA	NA
PROB:	1	NA	NA
RMSE:	2.19	NA	NA

MAX_MEAN: 0.782 **MAX_MED:** 0.809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

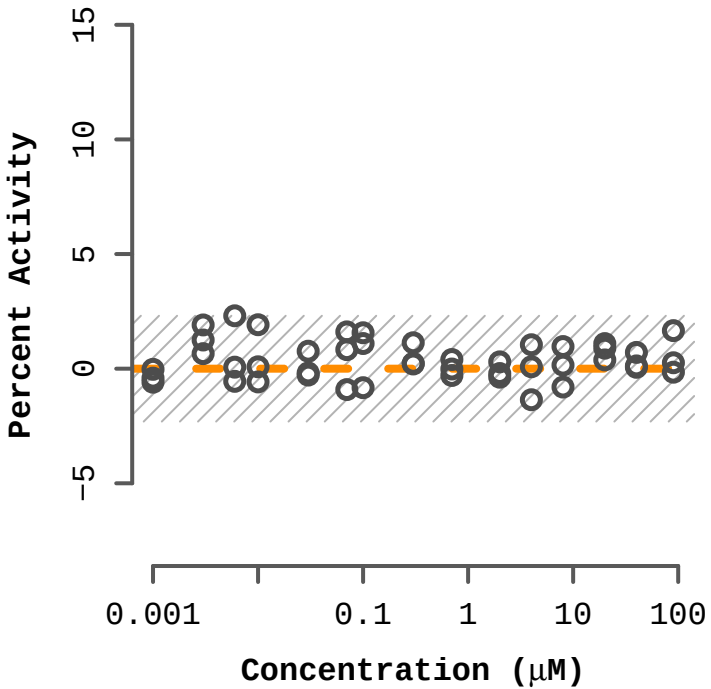
NAME: Acetyltriethyl citrate
CHID: 44576 **CASRN:** 77-89-4
SPID(S): Tox21_301483
M4ID: 12477650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.497 **MAX_MED:** 0.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

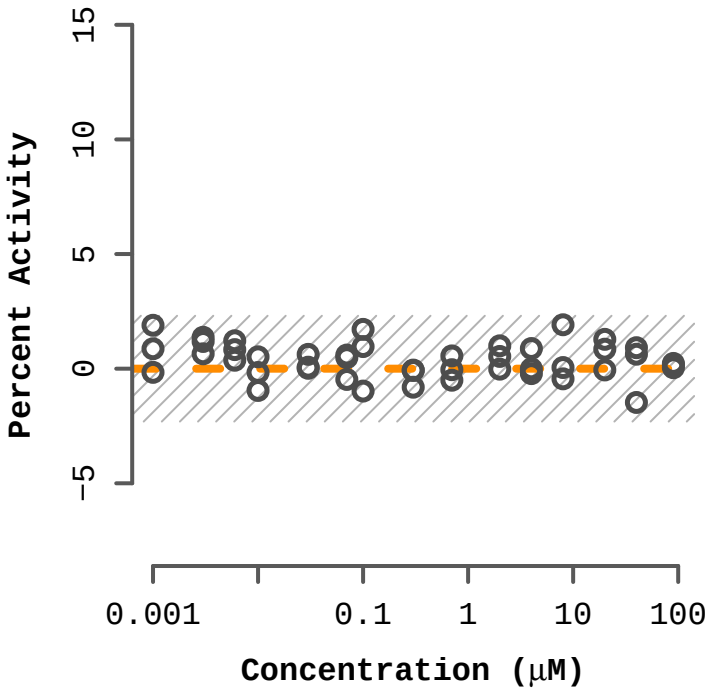
NAME: Calcium bromide
CHID: 44577 **CASRN:** 7789-41-5
SPID(S): Tox21_301859
M4ID: 12477274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

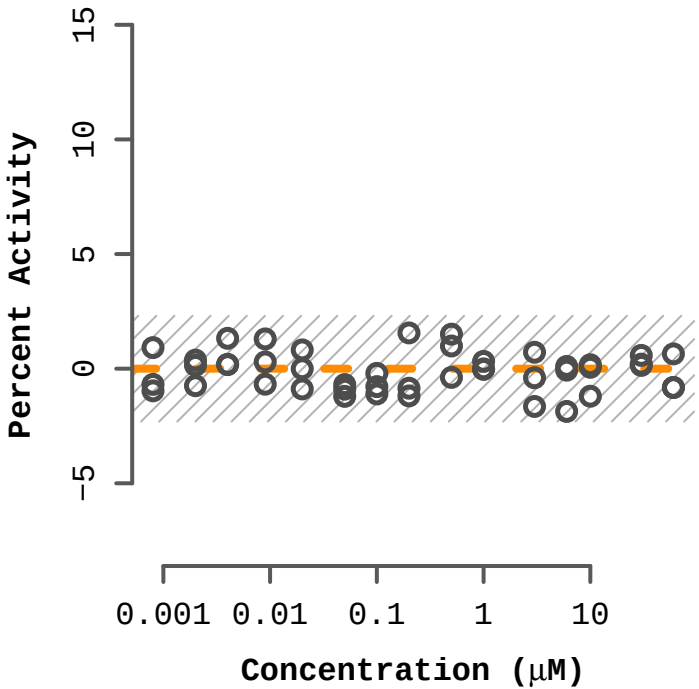
NAME: Sodium 2,5-dimethylbenzenesulfonate
CHID: 44578 **CASRN:** 827-19-0
SPID(S): Tox21_302215
M4ID: 12476918

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

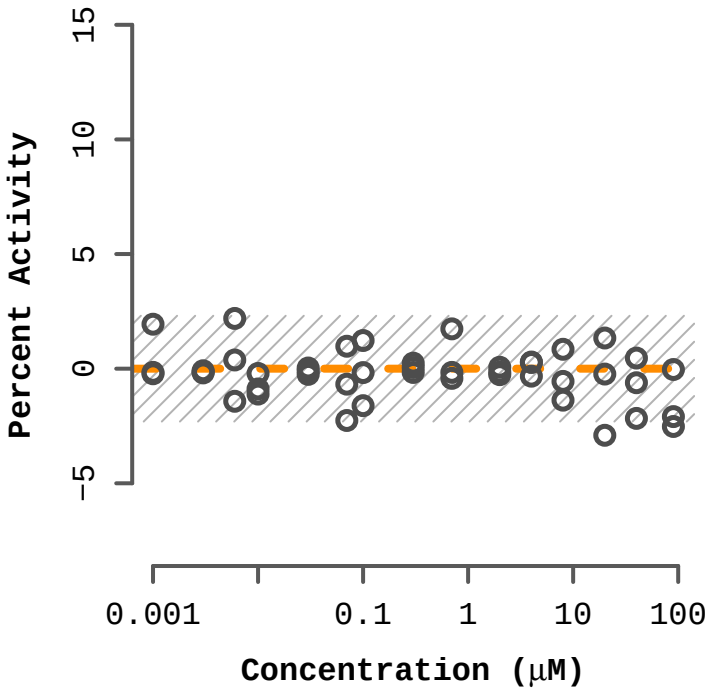
NAME: Pentaerythritol allyl ether
CHID: 44580 **CASRN:** 91648-24-7
SPID(S): Tox21_301451
M4ID: 12477682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.706 **MAX_MED:** 0.991 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

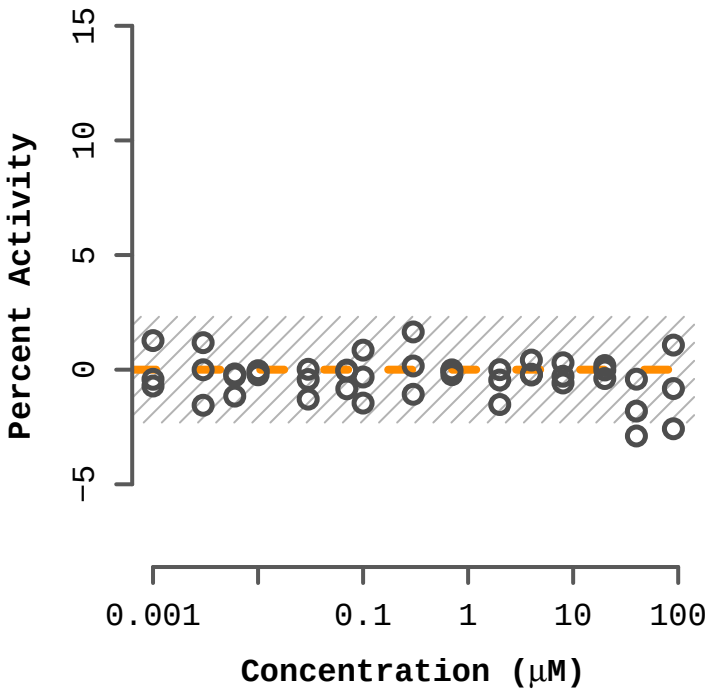
NAME: 2-tert-Butyl-4-ethylphenol
CHID: 44581 **CASRN:** 96-70-8
SPID(S): Tox21_300390
M4ID: 12478742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.52 **MAX_MED:** 0.381 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

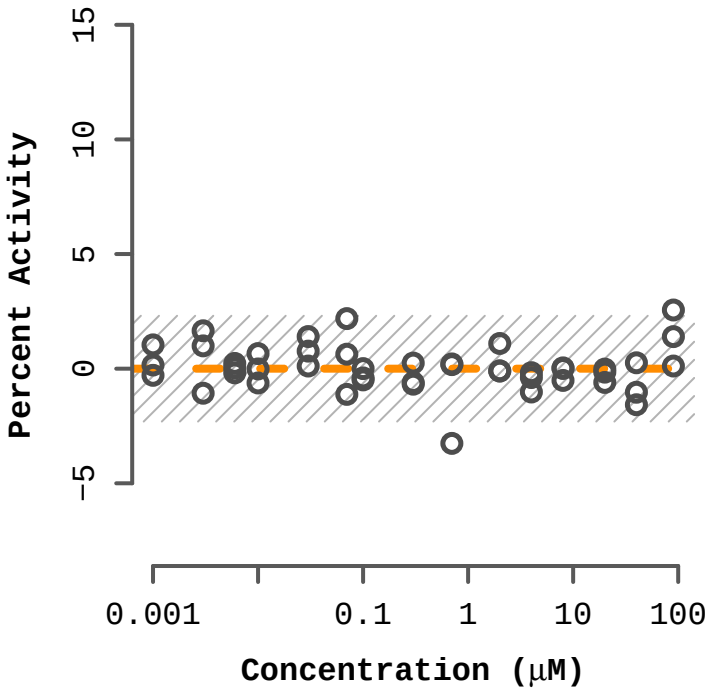
NAME: 1-tert-Butyl-3,4,5-trimethyl-2,6-dinitrobenzene
CHID: 44582 **CASRN:** 145-39-1
SPID(S): Tox21_301938
M4ID: 12477195

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.246 **MAX_MED:** 0.162 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

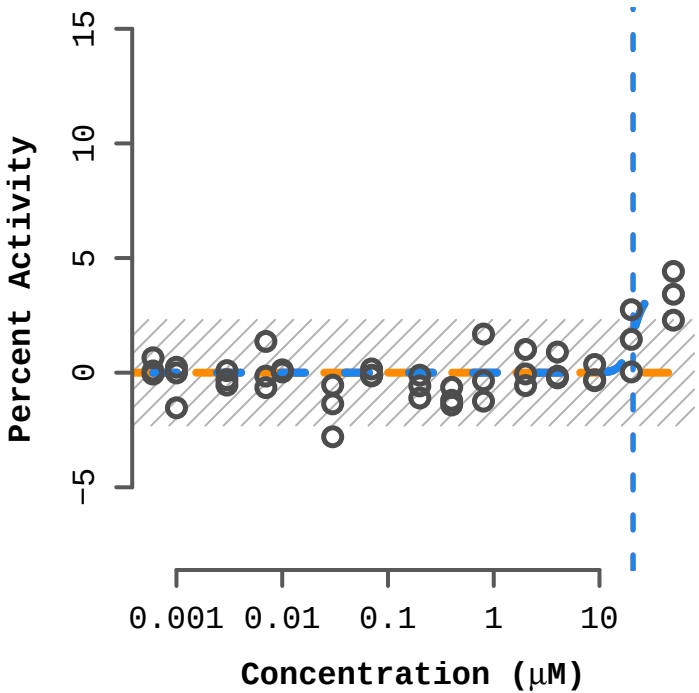
NAME: Selegiline hydrochloride
CHID: 44584 **CASRN:** 14611-52-0
SPID(S): Tox21_301846
M4ID: 12477287

HILL MODEL: Not applicable.

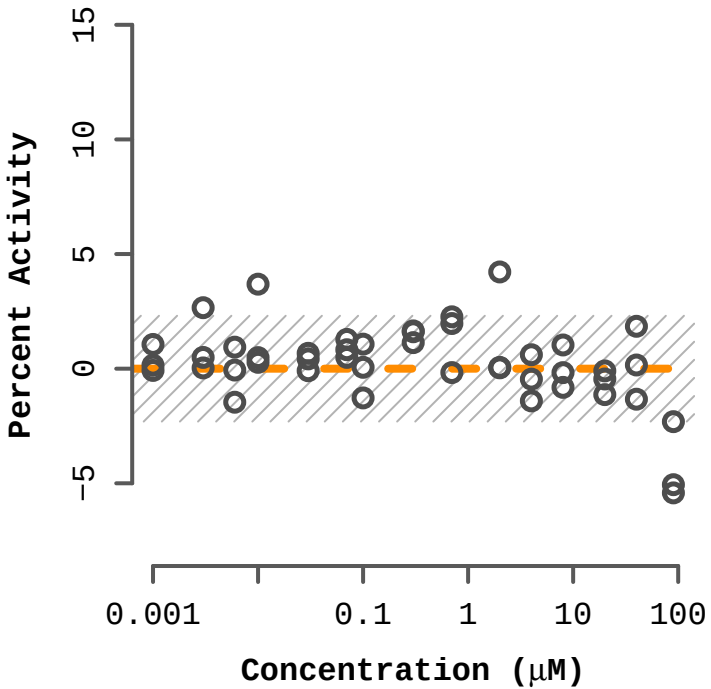
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.4 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Selegiline hydrochloride
CHID:    44584   CASRN: 14611-52-0
SPID(S): Tox21_110572_1
M4ID:    12484259

HILL MODEL (in red):
      tp       ga       gw
val:  3.41     1.32     8
sd:   0.531    0.0613   20.7

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.41     1.32     8        3.58     6.23
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  142.97      121.63      125.63
PROB: 0           0.88        0.12
RMSE: 1.28        0.87        0.87

MAX_MEAN: 3.38      MAX_MED: 3.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

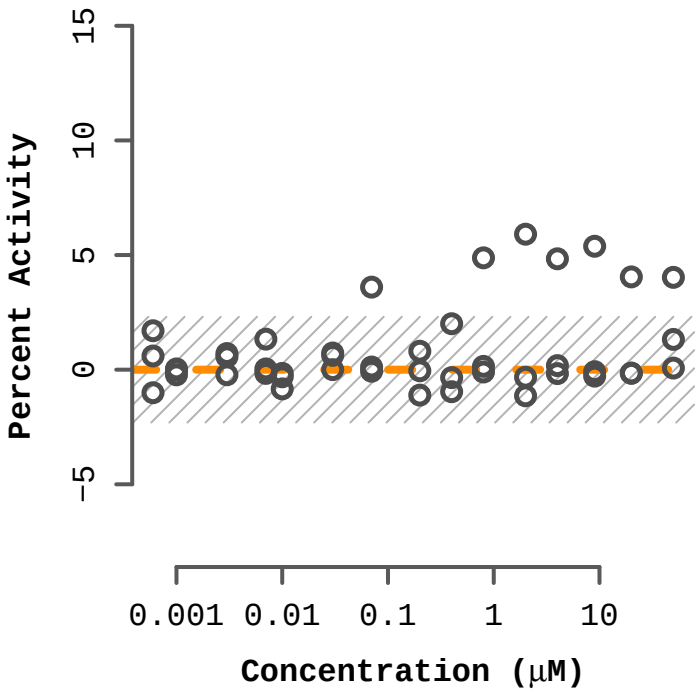
NAME: Dantrolene sodium
CHID: 44585 CASRN: 14663-23-1
SPID(S): Tox21_301997
M4ID: 12477136

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

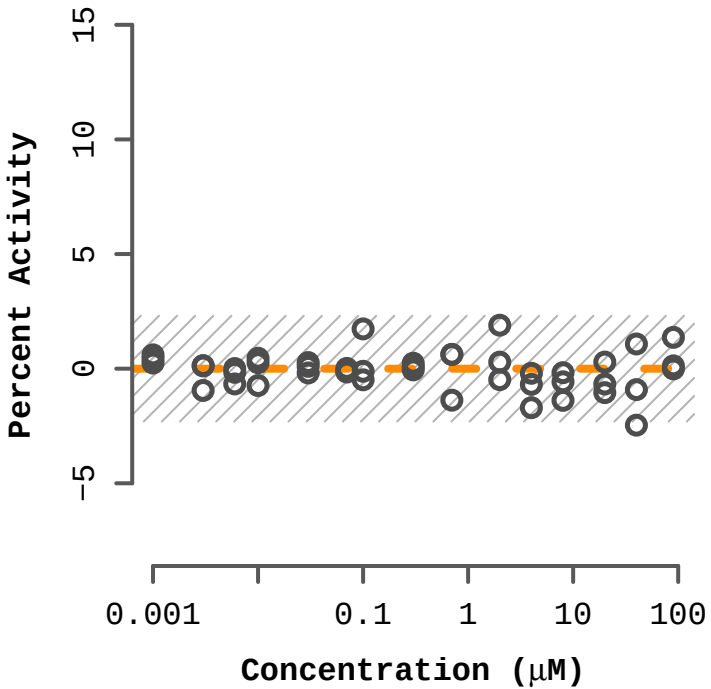
NAME: Dantrolene sodium
CHID: 44585 CASRN: 14663-23-1
SPID(S): Tox21_112013_1
M4ID: 12483372

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

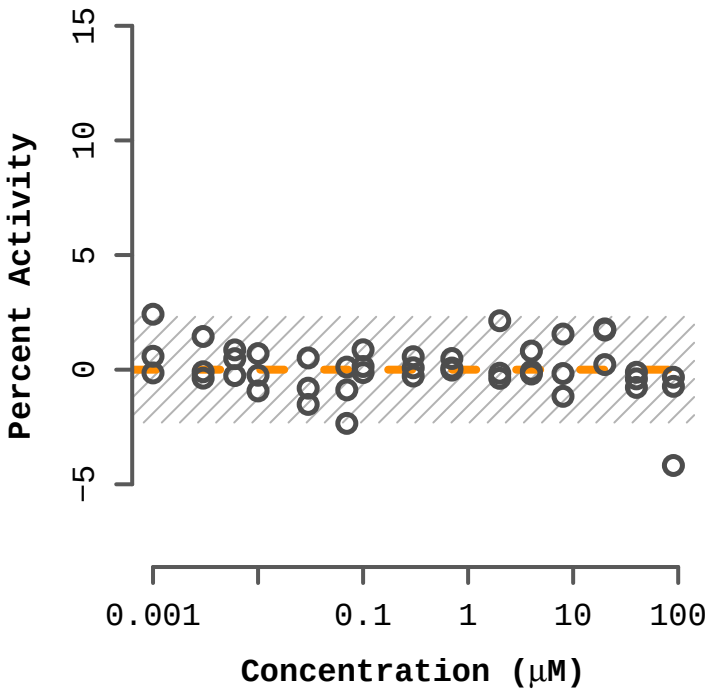
NAME: 3-[Ethyl(phenyl)amino]propanenitrile
CHID: 44587 **CASRN:** 148-87-8
SPID(S): Tox21_301491
M4ID: 12477642

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.569 **MAX_MED:** 0.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

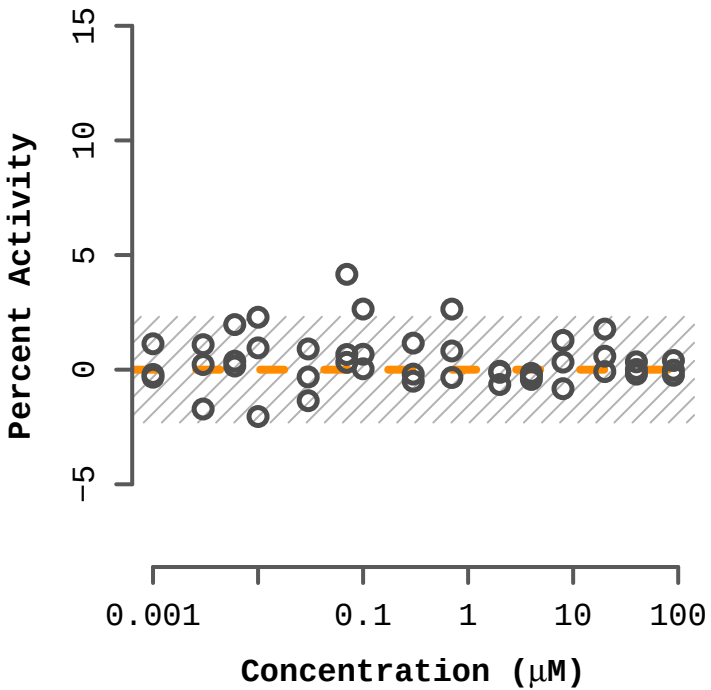
NAME: 2,2'−[Ethane−1,2−diylbis(oxy)]diethanethiol
CHID: 44588 **CASRN:** 14970−87−7
SPID(S): Tox21_301482
M4ID: 12477651

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

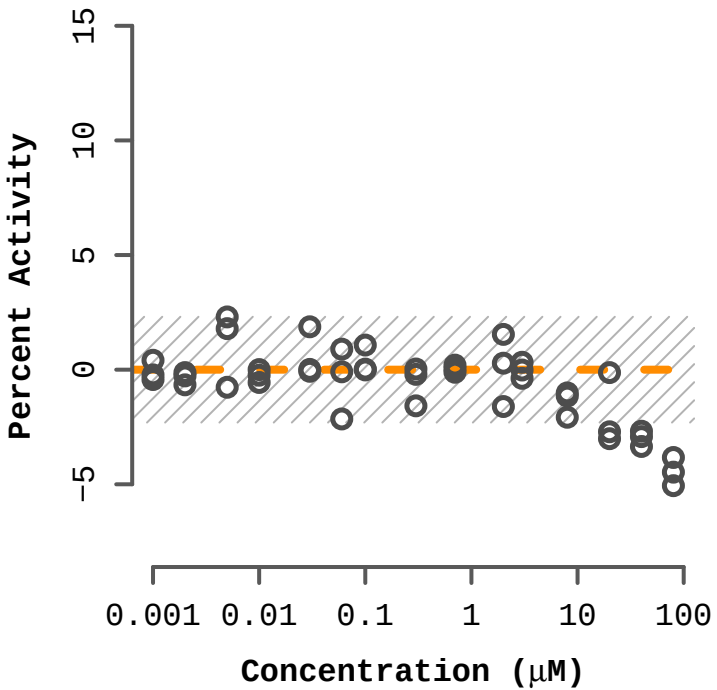
NAME: 5-Methoxy-5-oxopentanoic acid
CHID: 44589 **CASRN:** 1501-27-5
SPID(S): Tox21_301438
M4ID: 12477695

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

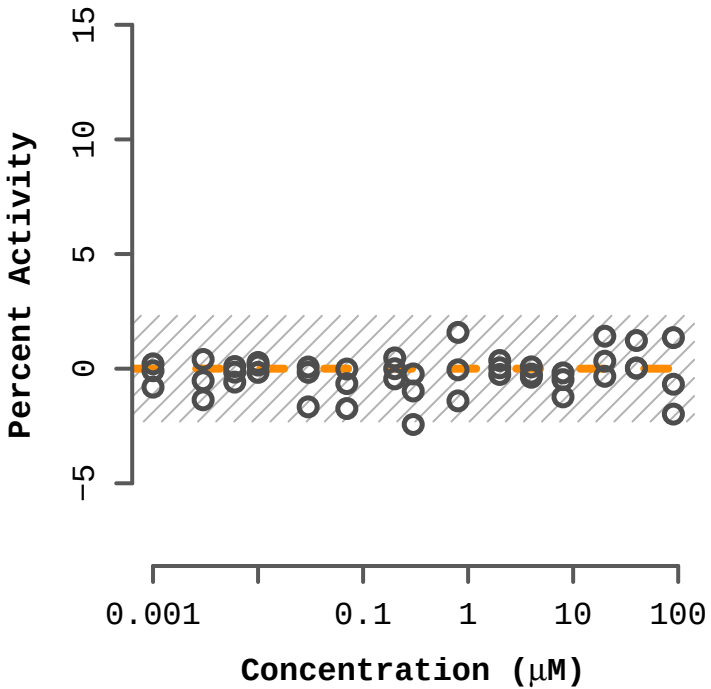
NAME: 2',4',5',7'−Tetrabromofluorescein
CHID: 44590 **CASRN:** 15086−94−9
SPID(S): Tox21_301553
M4ID: 12477580

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

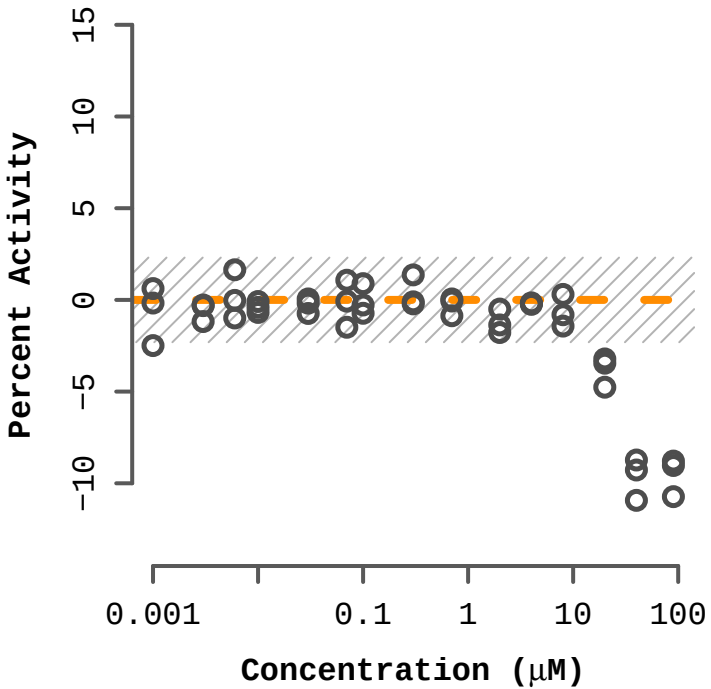
NAME: 2-Butyl-1H-isoindole-1,3(2H)-dione
CHID: 44591 **CASRN:** 1515-72-6
SPID(S): Tox21_301961
M4ID: 12477172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.471 **MAX_MED:** 0.327 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

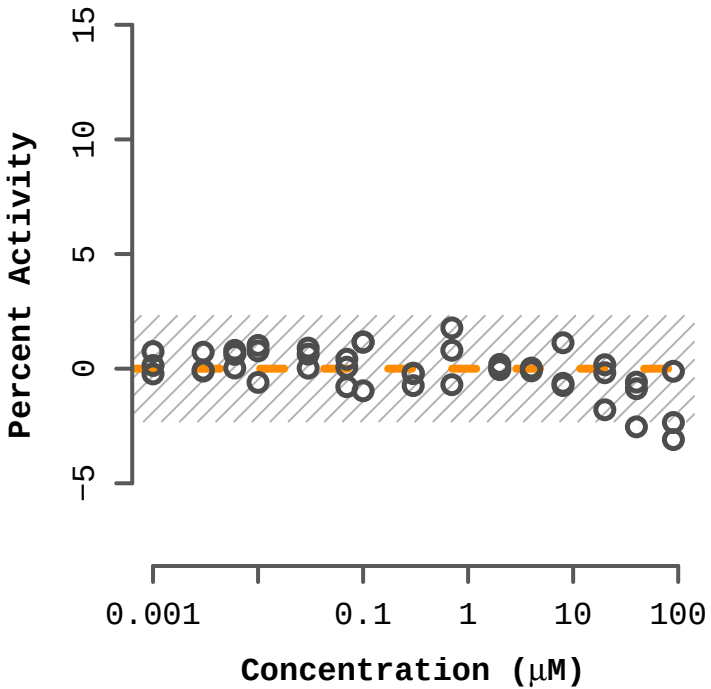
NAME: 1-Benzylquinolinium chloride
CHID: 44593 **CASRN:** 15619-48-4
SPID(S): Tox21_302628
M4ID: 12476505

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.91	NA	NA
PROB:	1	NA	NA
RMSE:	3.74	NA	NA

MAX_MEAN: 0.349 **MAX_MED:** −0.025 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

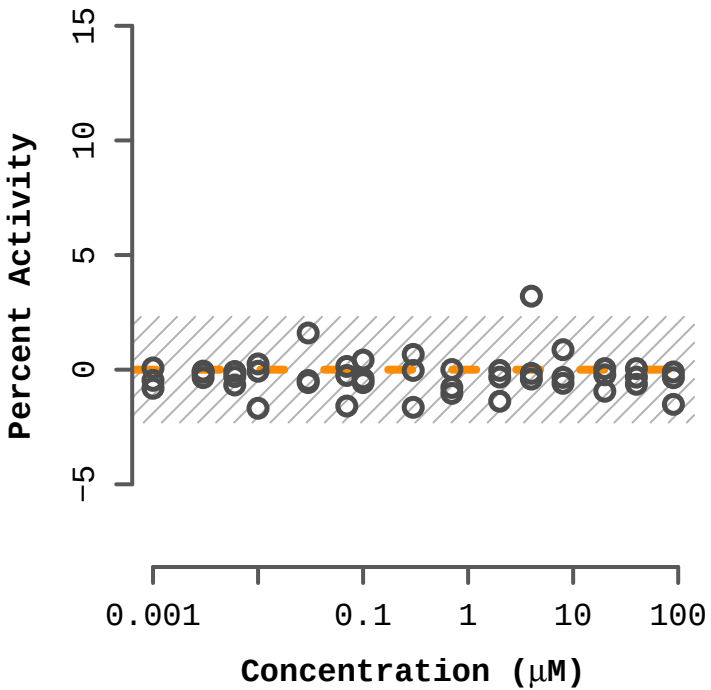
NAME: 1-(4-Chlorophenyl)-4,4-dimethylpent-1-en-3-one
CHID: 44595 **CASRN:** 1577-03-3
SPID(S): Tox21_302525
M4ID: 12476608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.629 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

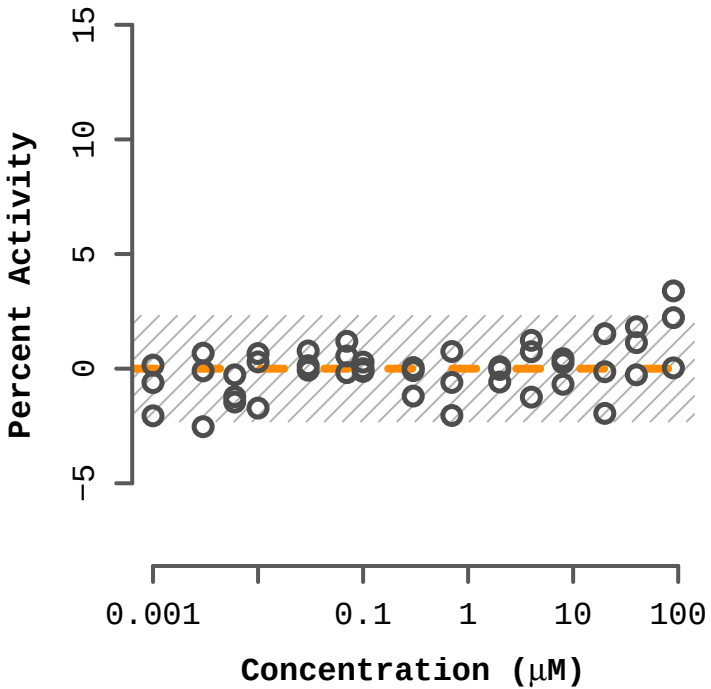
NAME: (Phenylphosphoryl)bis[(2,4,6-trimethylphenyl)m
CHID: 44597 **CASRN:** 162881-26-7
SPID(S): Tox21_302690
M4ID: 12476443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.879 **MAX_MED:** −0.0322 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

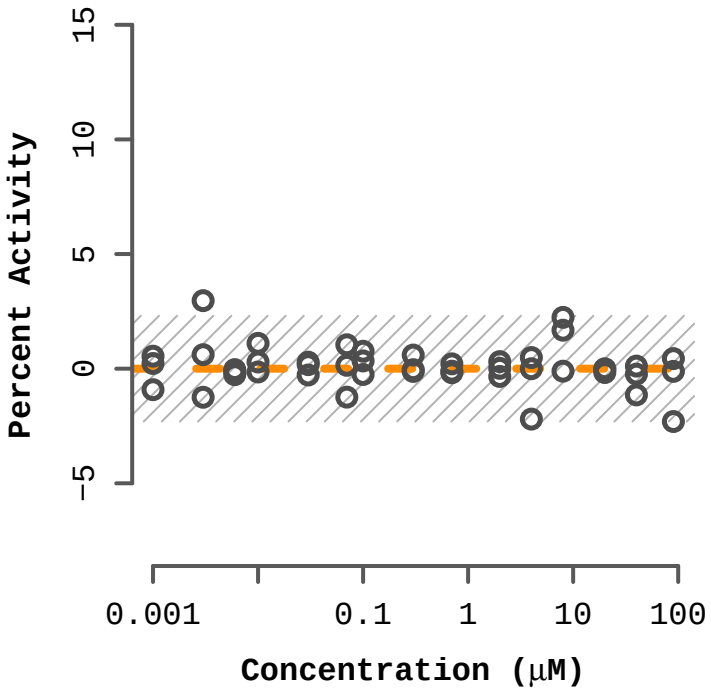
NAME: Panthenol
CHID: 44598 CASRN: 16485-10-2
SPID(S): Tox21_302660
M4ID: 12476473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.89 MAX_MED: 2.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

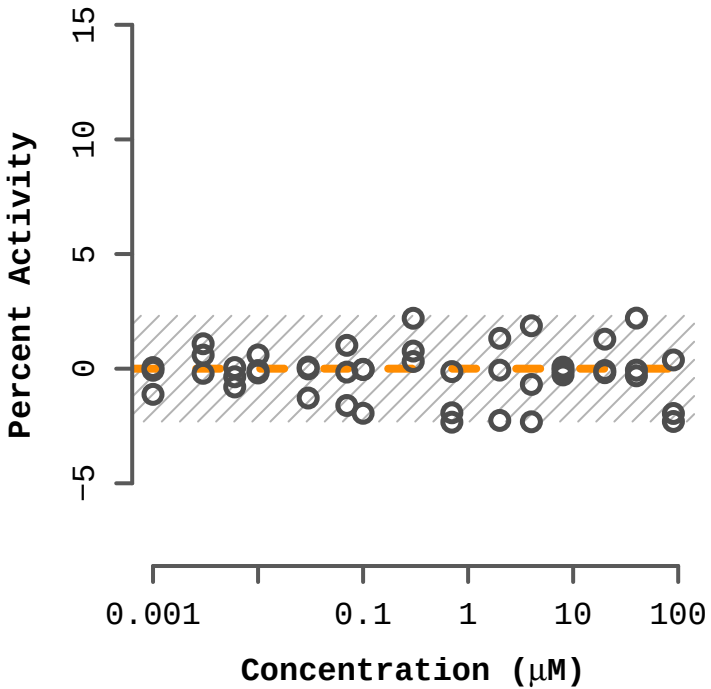
NAME: 3-(Octyloxy)propanenitrile
CHID: 44599 CASRN: 16728-49-7
SPID(S): Tox21_302450
M4ID: 12476683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.27 MAX_MED: 1.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

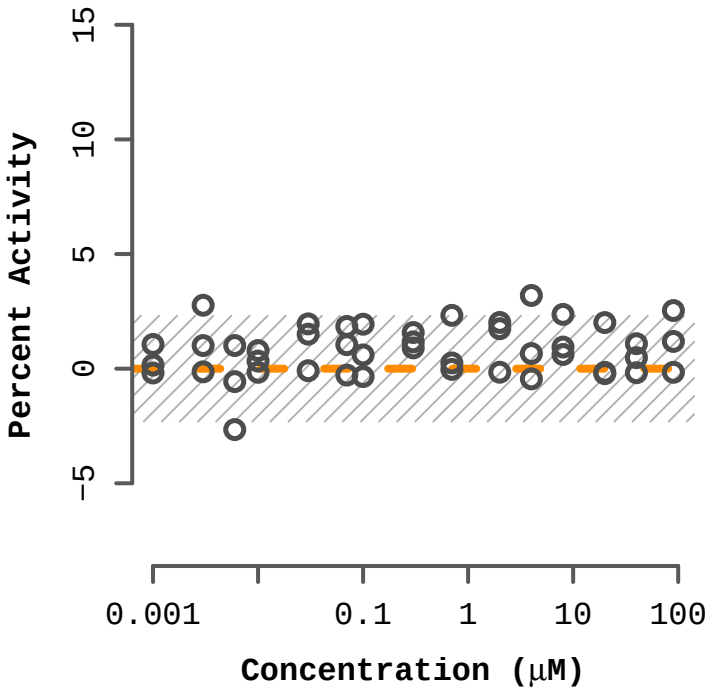
NAME: Cyclohex-3-en-1-ylmethanol
CHID: 44600 **CASRN:** 1679-51-2
SPID(S): Tox21_302637
M4ID: 12476496

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.769 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

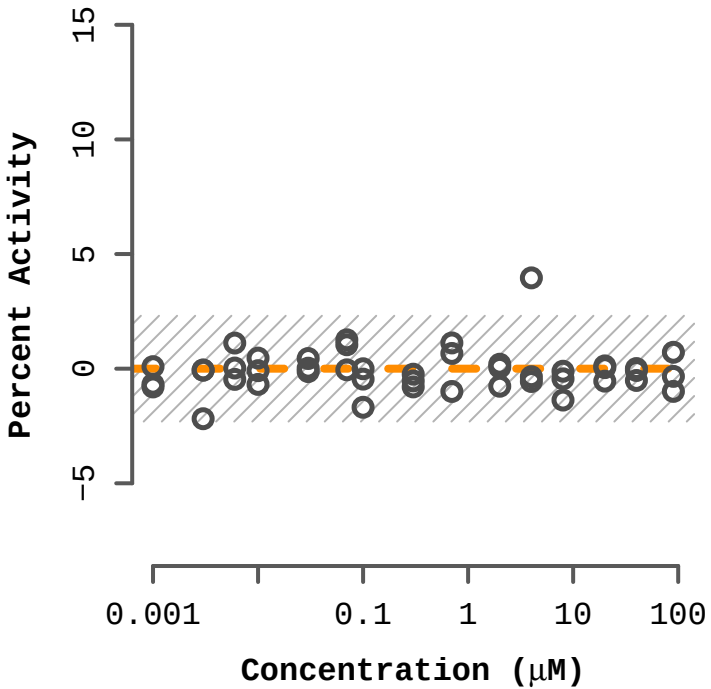
NAME: 3-[Bis(2-hydroxyethyl)amino]propanenitrile
CHID: 44603 **CASRN:** 17209-72-2
SPID(S): Tox21_303618
M4ID: 12475527

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

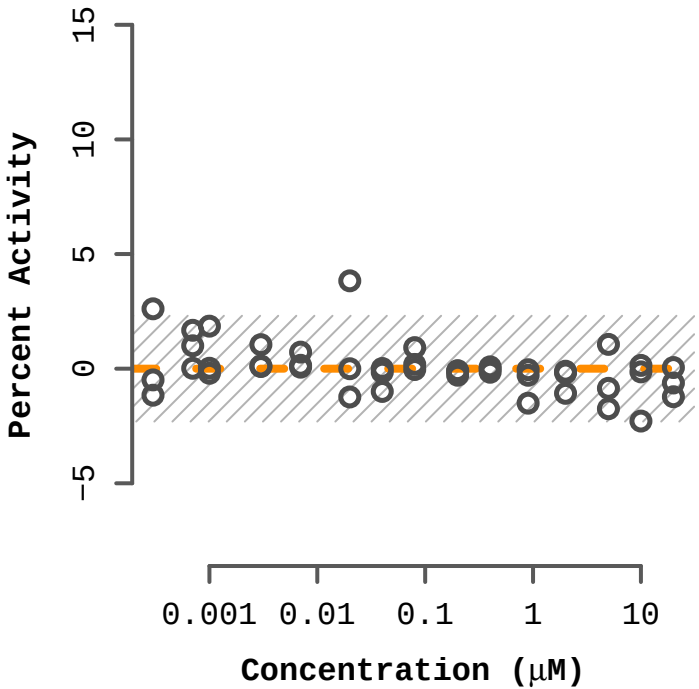
NAME: 1,4-Bis[(ethenyloxy)methyl]cyclohexane
CHID: 44604 CASRN: 17351-75-6
SPID(S): Tox21_302720
M4ID: 12476413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.02 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

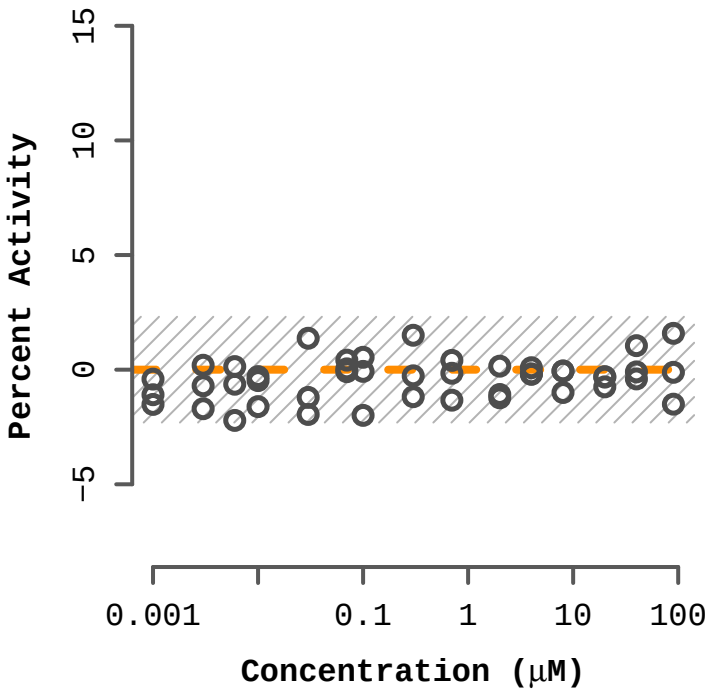
NAME: 1,4-Bis(butylamino)anthracene-9,10-dione
CHID: 44605 **CASRN:** 17354-14-2
SPID(S): Tox21_303986
M4ID: 12475202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.898 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

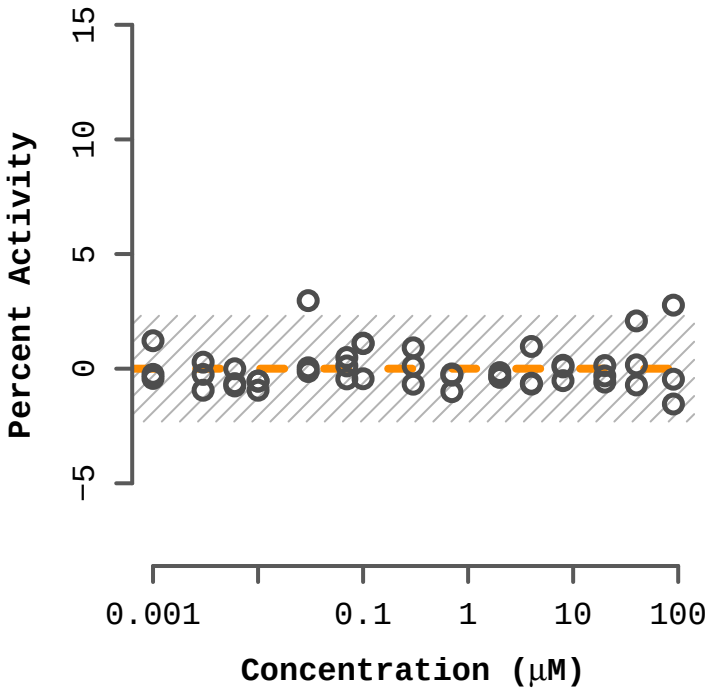
NAME: 3,3'−(4−Methylbenzene−1,3−diyl)bis(1,1−dimethy
CHID: 44606 CASRN: 17526−94−2
SPID(S): Tox21_302673
M4ID: 12476460

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.184 MAX_MED: 0.0375 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

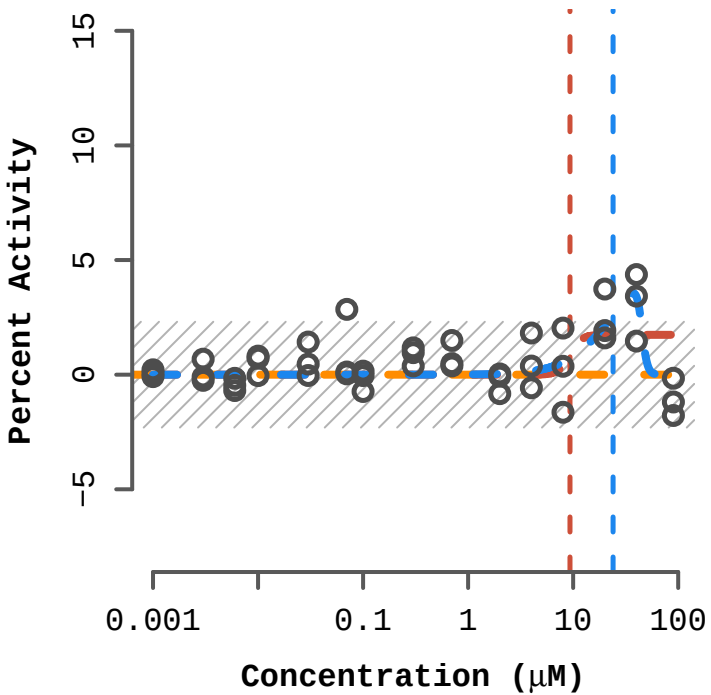
NAME: sec−Butylparaben
CHID: 44607 **CASRN:** 17696−61−6
SPID(S): Tox21_303580
M4ID: 12475565

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.962 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: sec-Butylparaben
CHID: 44607 CASRN: 17696-61-6
SPID(S): Tox21_201970
M4ID: 12480282

HILL MODEL (in red):

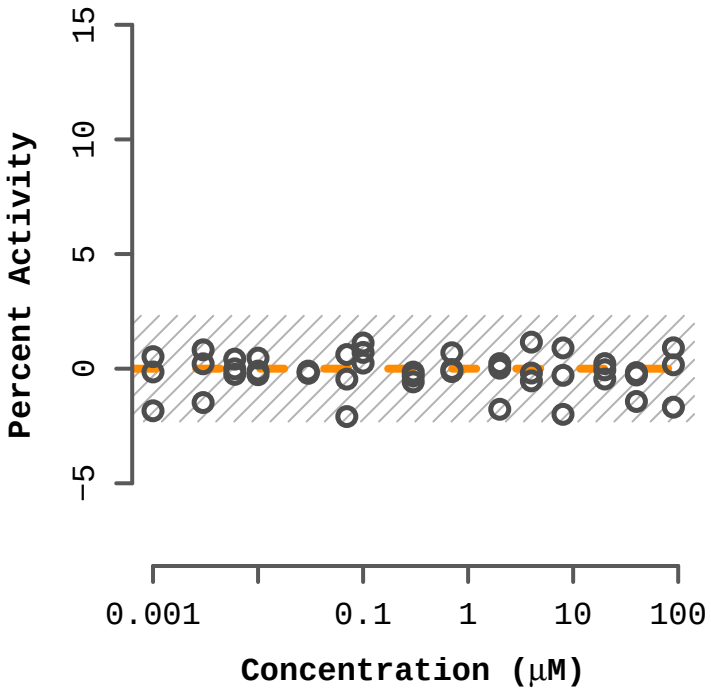
	tp	ga	gw
val:	1.74	0.97	8
sd:	0.5	0.17	16.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.24	1.38	1.97	1.65	17.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	153.19	150.04	134.24
PROB:	0	0	1
RMSE:	1.4	1.23	0.96

MAX_MEAN: 3.09 MAX_MED: 3.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

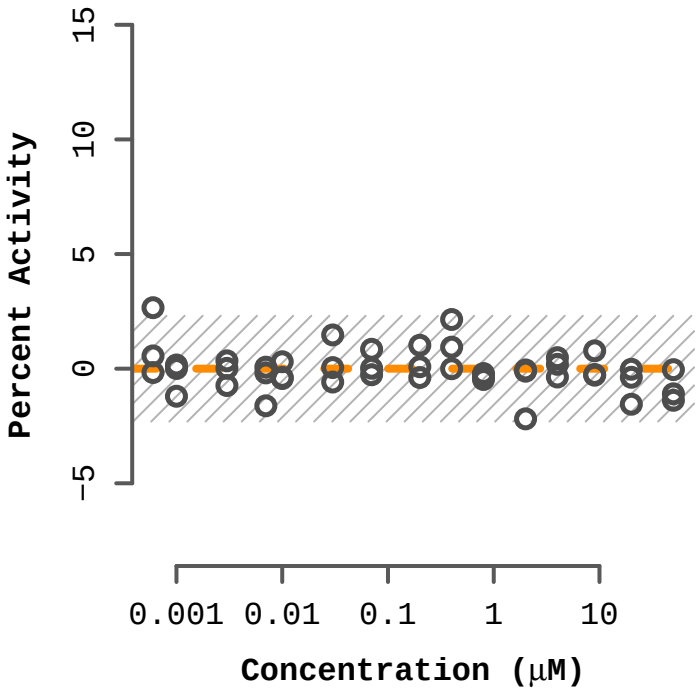
NAME: 2,6-Difluorobenzonitrile
CHID: 44609 **CASRN:** 1897-52-5
SPID(S): Tox21_302519
M4ID: 12476614

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.693 **MAX_MED:** 0.711 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

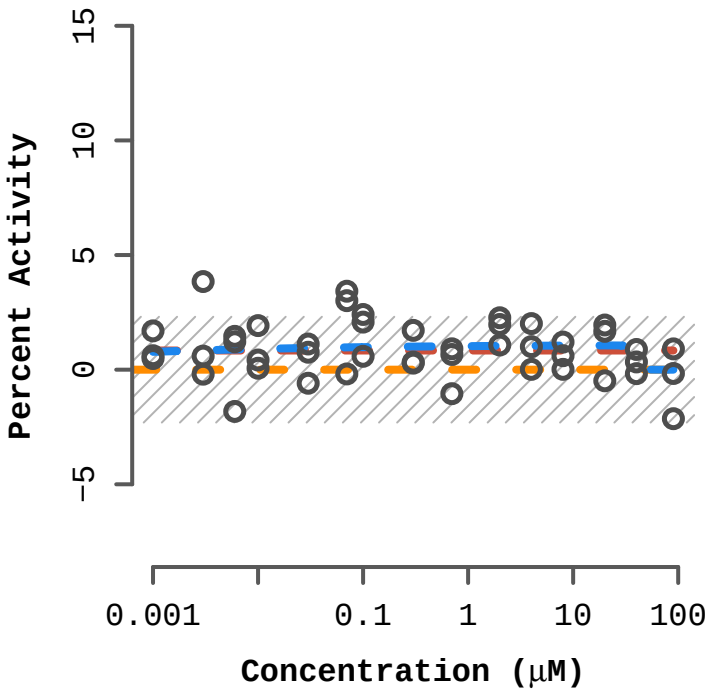
NAME: Sodium 2-amino-5-sulfonaphthalene-1-sulfonate
CHID: 44611 **CASRN:** 19532-03-7
SPID(S): Tox21_303913
M4ID: 12475275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1'−Diazene−1,2−diyldicyclohexanecarbonitrile
CHID: 44613 CASRN: 2094−98−6
SPID(S): Tox21_303619
M4ID: 12475526

HILL MODEL (in red):

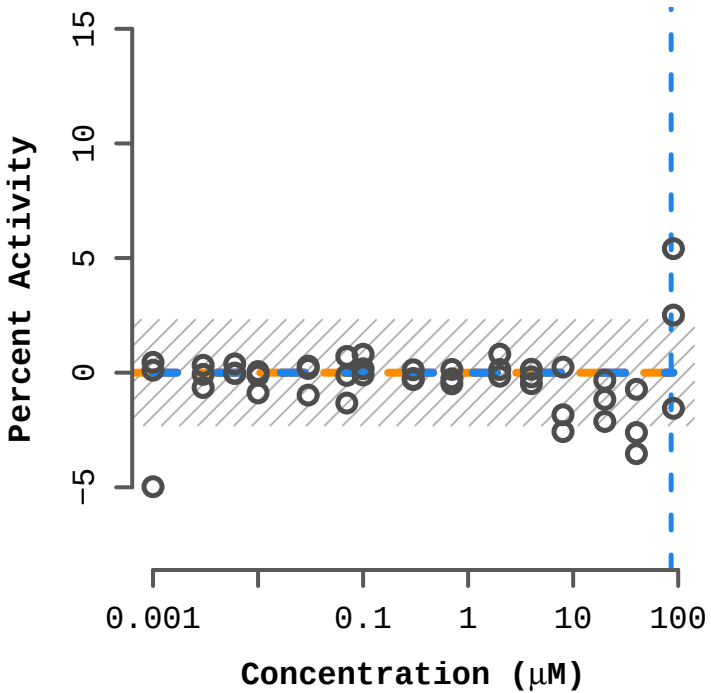
	tp	ga	gw
val:	0.836	−4.69	3.9
sd:	0.169	1480	3430

GAIN−LOSS MODEL (in blue):

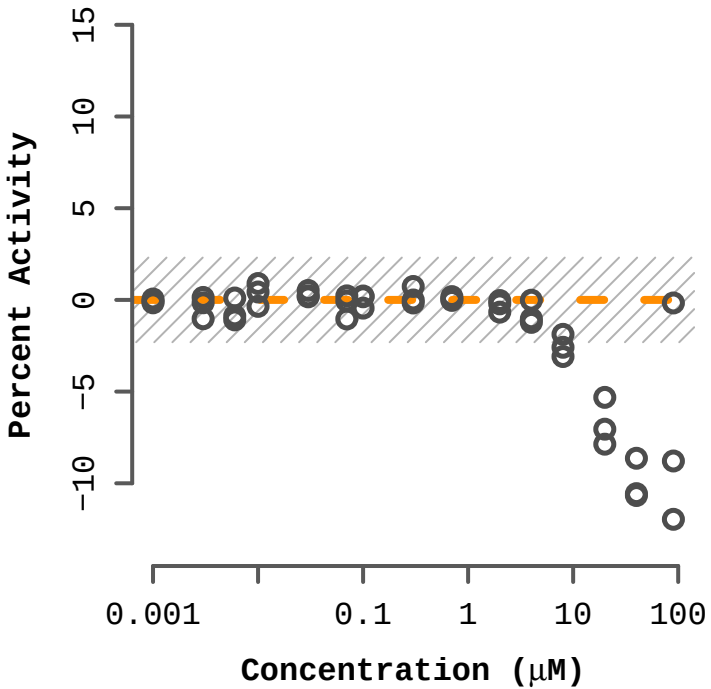
	tp	ga	gw	la	lw
val:	1.08	−4.39	0.3	1.58	17.3
sd:	0.527	6.53	1.28	0.102	98.2

	CNST	HILL	GNLS
AIC:	166.99	152.53	152.65
PROB:	0	0.51	0.49
RMSE:	1.48	1.21	1.15

MAX_MEAN: 2.08 **MAX_MED:** 3.01 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ethylene acrylate
CHID:    44615   CASRN: 2274-11-5
SPID(S): Tox21_302577
M4ID:    12476556

HILL MODEL (in red):
      tp       ga       gw
val:  1.48e-08 2.38     1.65
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.52e-09 1.93     2.13     2.24     5.48
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  150.77      156.77      160.77
PROB: 0.95        0.05        0.01
RMSE: 1.53        1.53        1.53

MAX_MEAN: 2.12      MAX_MED: 2.51      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

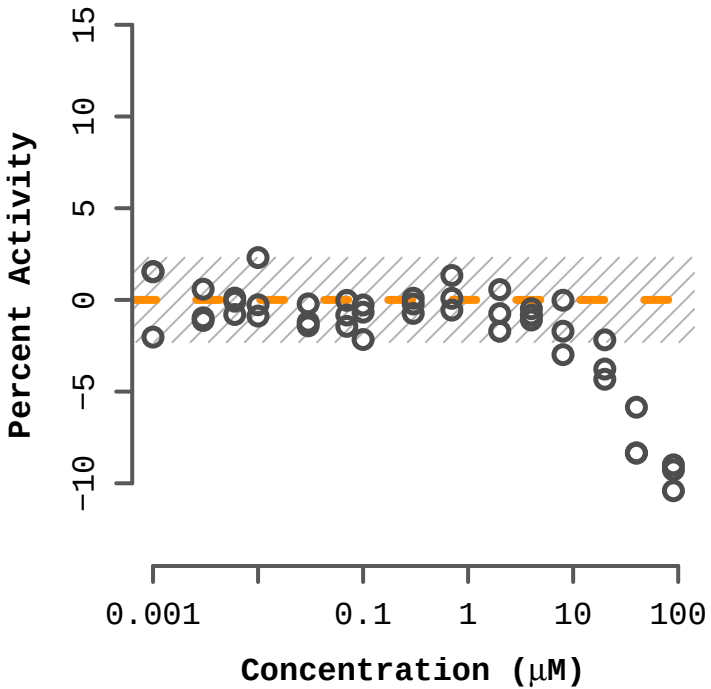
NAME: Tetrabutylphosphonium chloride
CHID: 44616 CASRN: 2304-30-5
SPID(S): Tox21_303484
M4ID: 12475657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.22	NA	NA
PROB:	1	NA	NA
RMSE:	3.91	NA	NA

MAX_MEAN: 0.326 **MAX_MED:** 0.434 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

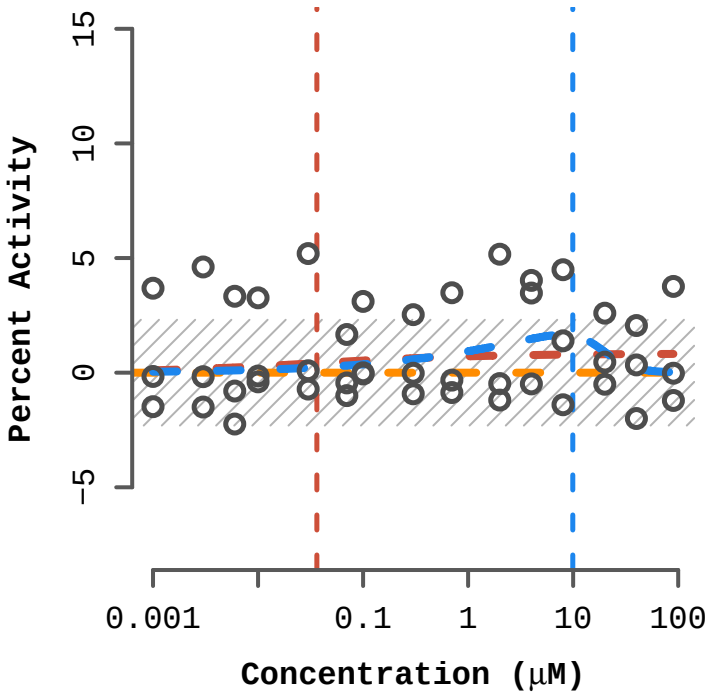
NAME: Tetrabutylphosphonium chloride
CHID: 44616 CASRN: 2304-30-5
SPID(S): Tox21_200765
M4ID: 12481487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.45	NA	NA

MAX_MEAN: 0.389 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: [3-(Trifluoromethyl)phenyl]acetonitrile
CHID: 44617 **CASRN:** 2338-76-3
SPID(S): Tox21_302714
M4ID: 12476419

HILL MODEL (in red):

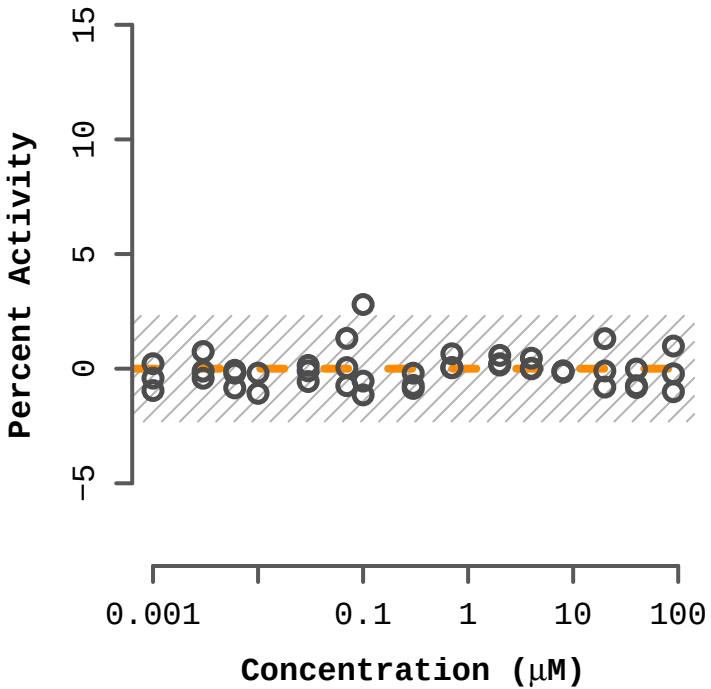
	tp	ga	gw
val:	0.829	−1.44	0.543
sd:	0.677	2.7	1.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.82	0.996	0.49	1.25	3.03
sd:	15.6	5.88	0.816	0.565	7.11

	CNST	HILL	GNLS
AIC:	206.27	209.02	212.04
PROB:	0.76	0.19	0.04
RMSE:	2.31	2.16	2.14

MAX_MEAN: 2.34 **MAX_MED:** 3.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

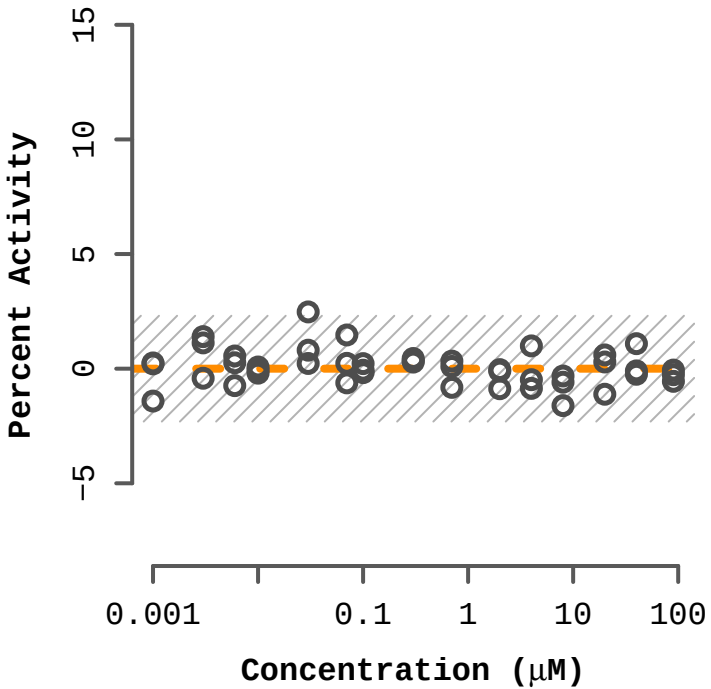
NAME: 1-Bromo-3-methoxybenzene
CHID: 44618 **CASRN:** 2398-37-0
SPID(S): Tox21_302612
M4ID: 12476521

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.217 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

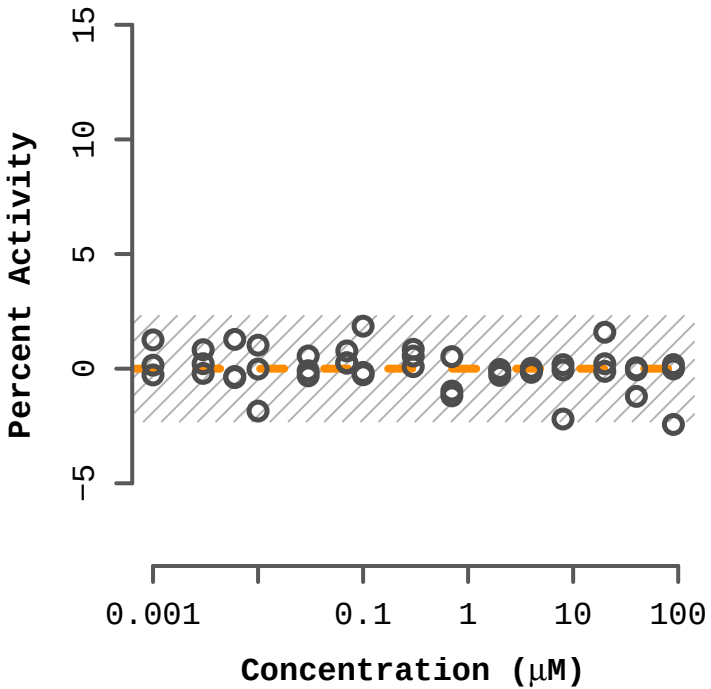
NAME: N-Methyloctan-1-amine
CHID: 44619 **CASRN:** 2439-54-5
SPID(S): Tox21_302511
M4ID: 12476622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

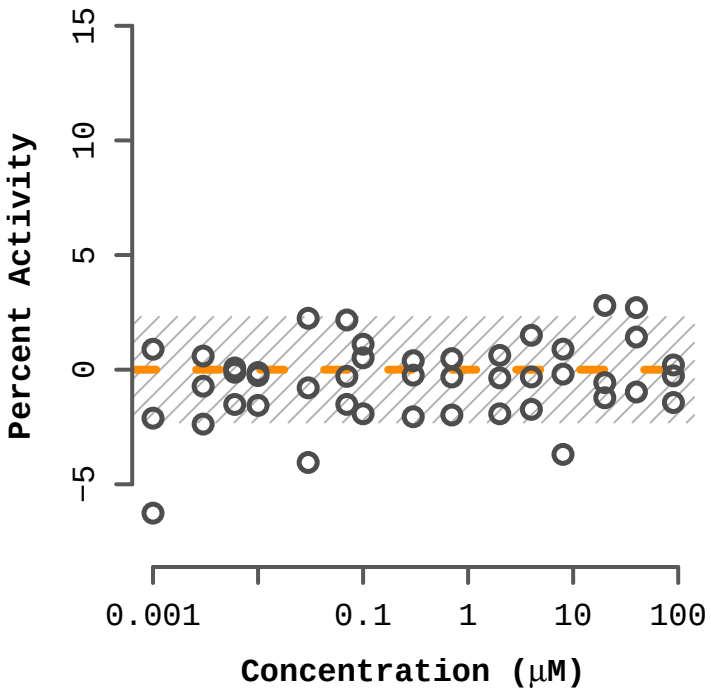
NAME: Trimethyl benzene-1,2,4-tricarboxylate
CHID: 44620 **CASRN:** 2459-10-1
SPID(S): Tox21_302449
M4ID: 12476684

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.564 **MAX_MED:** 0.552 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3'−(1,1,3,3−Tetramethyldisiloxane−1,3−diyl)d

CHID: 44621 **CASRN:** 2469−55−8

SPID(S): Tox21_302715

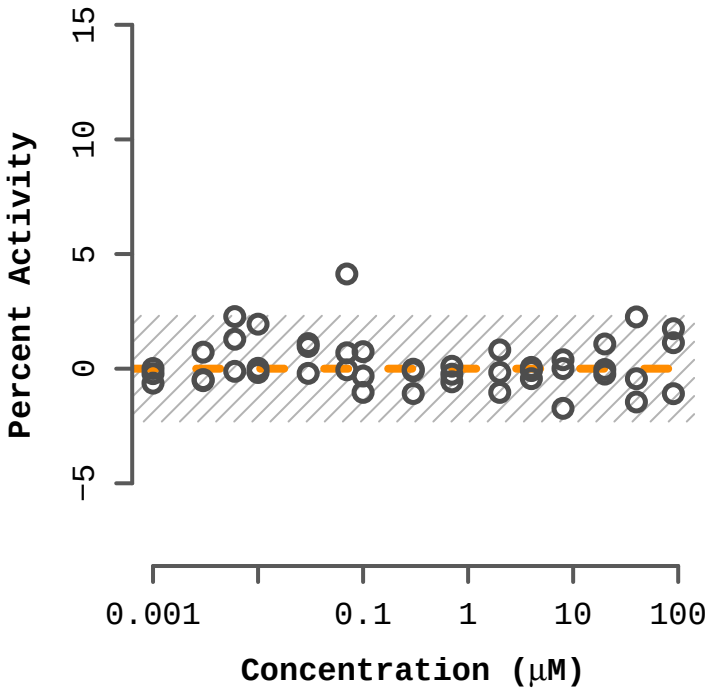
M4ID: 12476418

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

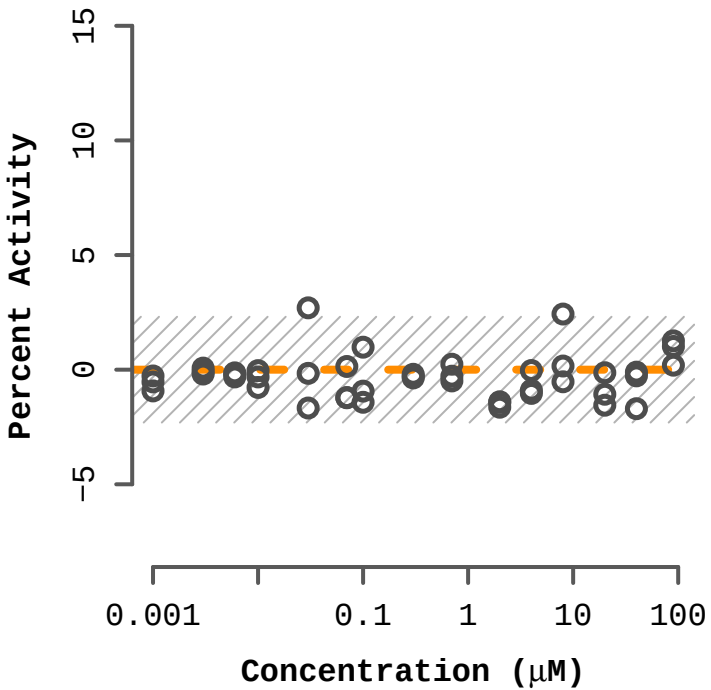
NAME: Aluminum butan-2-olate (2Z)-4-ethoxy-4-oxobut-2
CHID: 44622 **CASRN:** 24772-51-8
SPID(S): Tox21_302693
M4ID: 12476440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

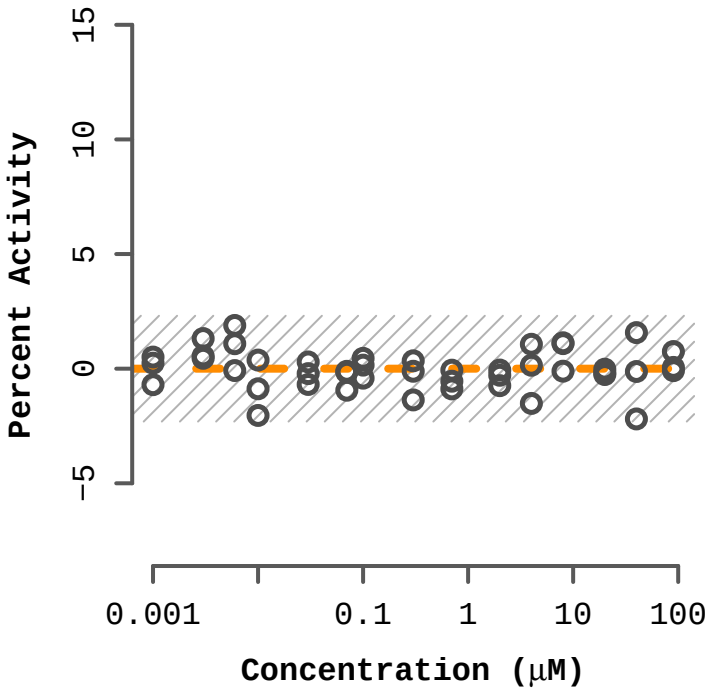
NAME: 4-Hydroxybutyl prop-2-enoate
CHID: 44623 **CASRN:** 2478-10-6
SPID(S): Tox21_302651
M4ID: 12476482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.823 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

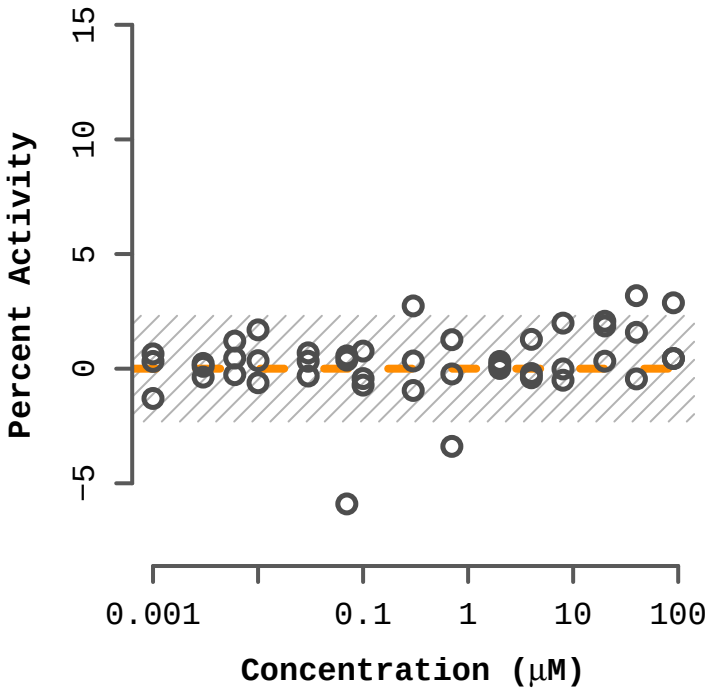
NAME: Octyl prop-2-enoate
CHID: 44624 **CASRN:** 2499-59-4
SPID(S): Tox21_302528
M4ID: 12476605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

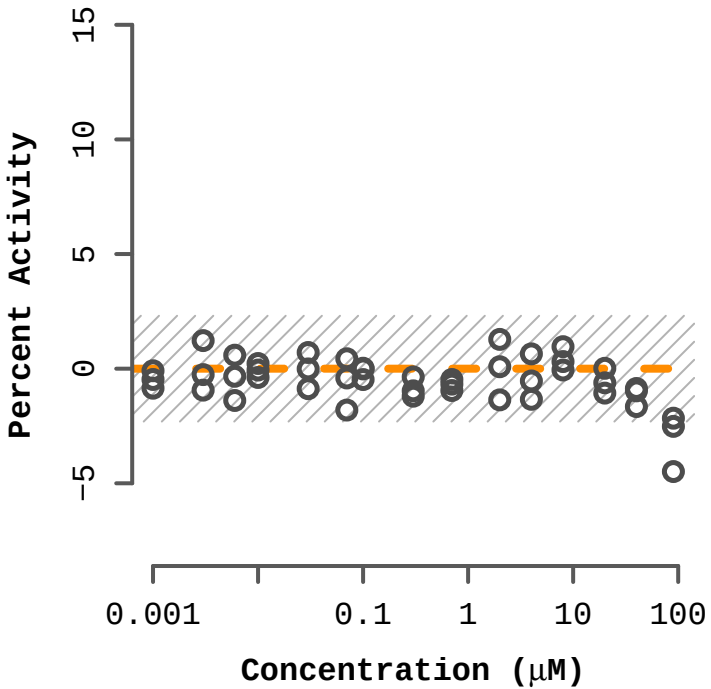
NAME: N,N-Bis(2-hydroxyethyl)formamide
CHID: 44625 **CASRN:** 25209-66-9
SPID(S): Tox21_302644
M4ID: 12476489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

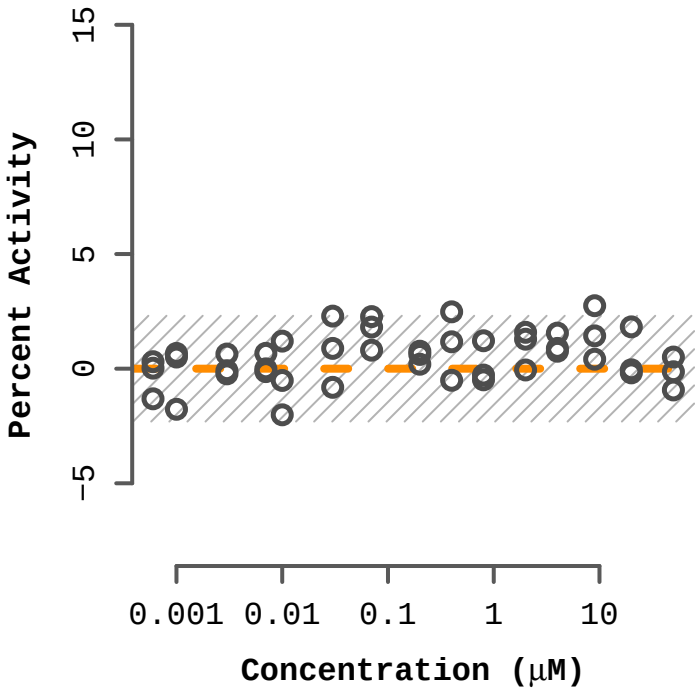
NAME: Trazodone hydrochloride
CHID: 44626 CASRN: 25332-39-2
SPID(S): Tox21_302685
M4ID: 12476448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.405 **MAX_MED:** 0.312 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

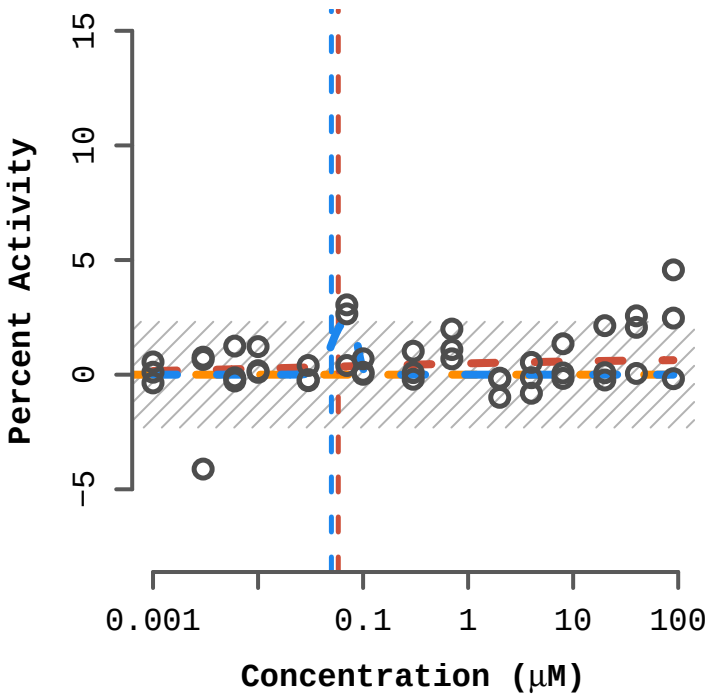
NAME: Trazodone hydrochloride
CHID: 44626 CASRN: 25332-39-2
SPID(S): Tox21_110286_1
M4ID: 12484482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1H-Benzotriazol-1-ol
CHID: 44627 CASRN: 2592-95-2
SPID(S): Tox21_302480
M4ID: 12476653

HILL MODEL (in red):

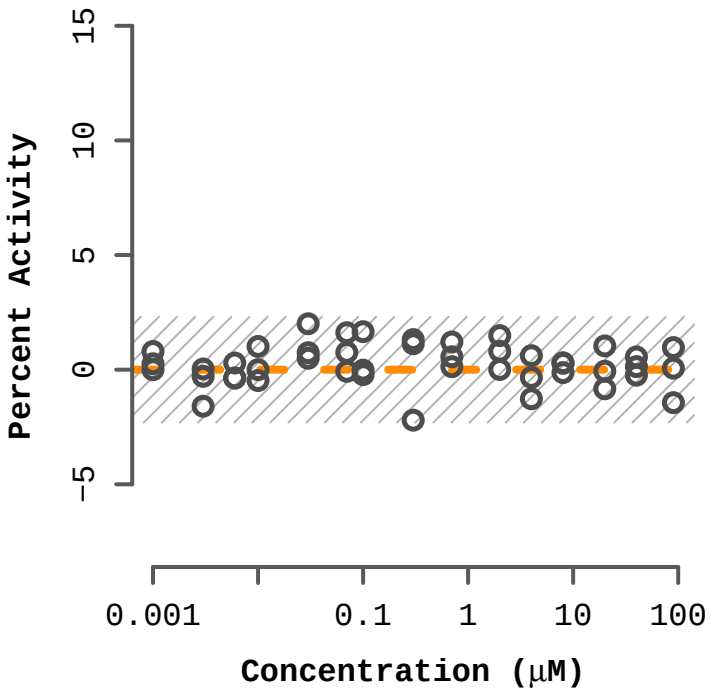
	tp	ga	gw
val:	0.703	-1.24	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.6	-1.3	7.96	-1.05	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	152.5	150.83	153.8
PROB:	0.26	0.6	0.14
RMSE:	1.43	1.29	1.33

MAX_MEAN: 2.29 MAX_MED: 2.65 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

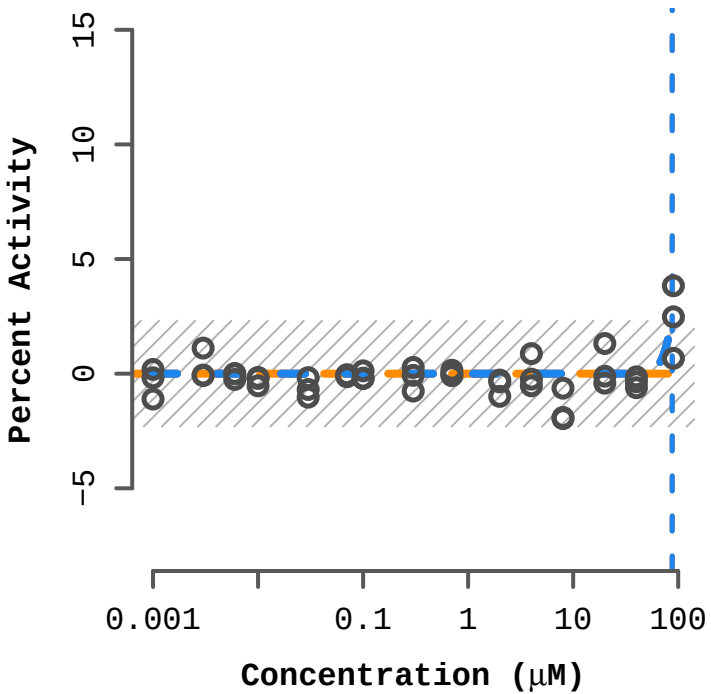
NAME: 4,4'−Diazene−1,2−diylbis(4−cyanopentanoic acid
CHID: 44629 CASRN: 2638−94−0
SPID(S): Tox21_302513
M4ID: 12476620

HILL MODEL: Not applicable.

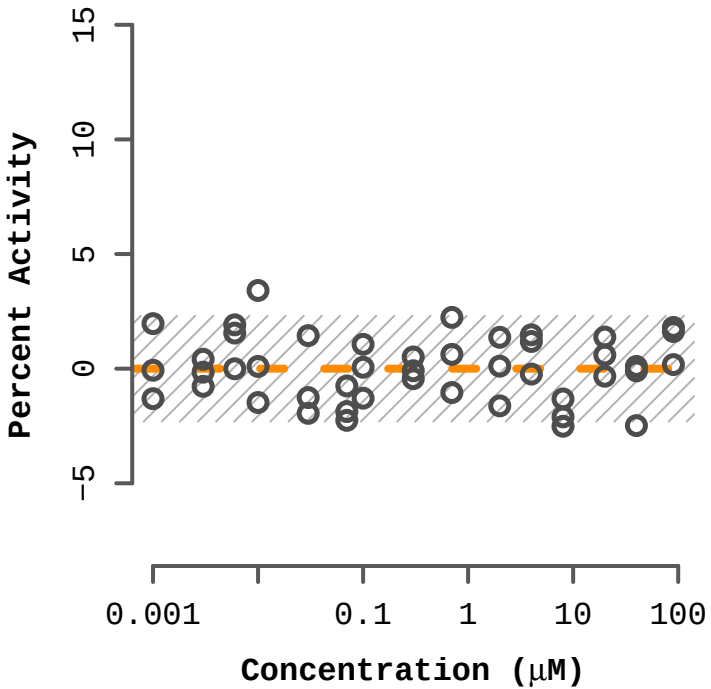
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.08 MAX_MED: 1.13 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-Oxo-N-(2-oxo-2,3-dihydro-1H-benzimidazol-5-y
CHID:    44631   CASRN: 26576-46-5
SPID(S): Tox21_302667
M4ID:    12476466

HILL MODEL (in red):
      tp       ga       gw
val:  4.6      1.94     8
sd:   2.23     0.0577   6.55

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.6      1.94     8        3.91     9.28
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  106.7       99.92       103.92
PROB: 0.03        0.86        0.12
RMSE: 0.93        0.72        0.72

MAX_MEAN: 2.33      MAX_MED: 2.48      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

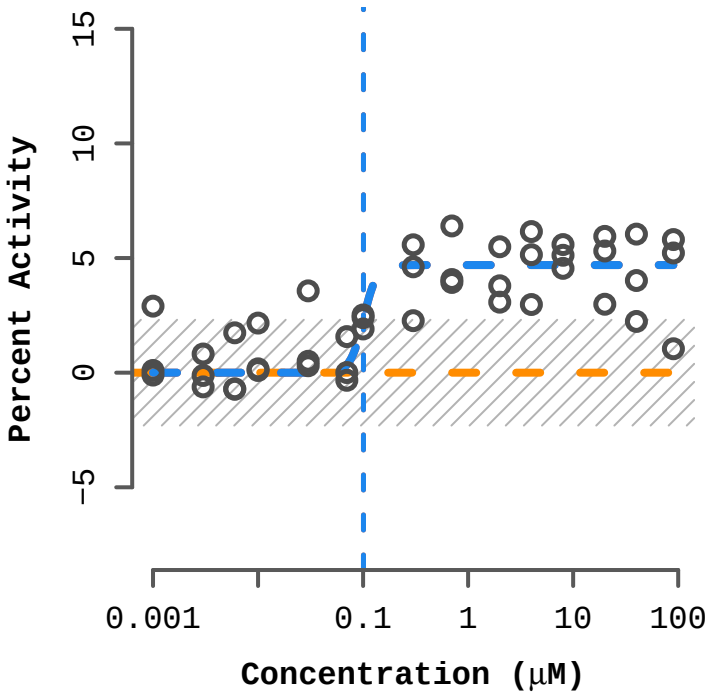
NAME: Dimethyl dihydrogen diphosphate
CHID: 44632 **CASRN:** 26644-00-8
SPID(S): Tox21_302697
M4ID: 12476436

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indapamide
CHID: 44633 CASRN: 26807-65-8
SPID(S): Tox21_302687
M4ID: 12476446

HILL MODEL (in red):

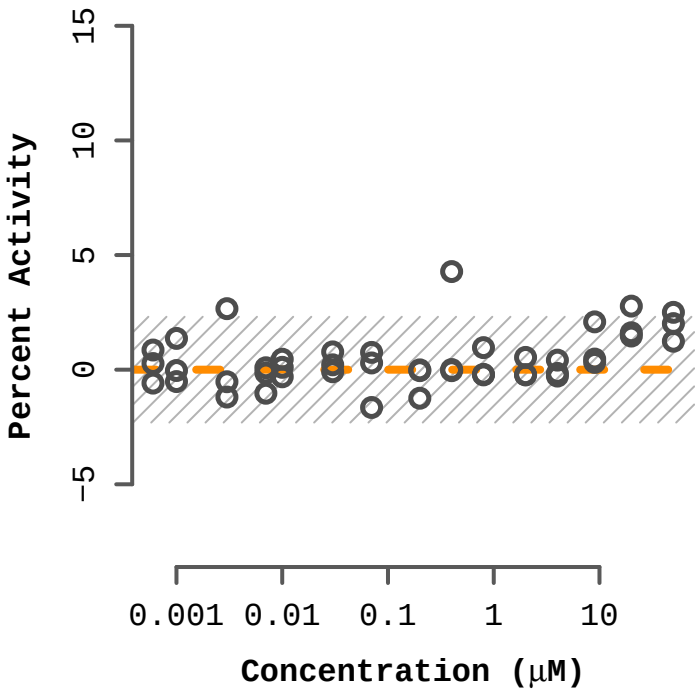
	tp	ga	gw
val:	4.7	−0.996	6.95
sd:	0.278	0.0314	6.28

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.7	−0.996	6.95	3.77	5.17
sd:	0.278	0.0314	6.28	8670	24900

	CNST	HILL	GNLS
AIC:	250.07	161.87	165.87
PROB:	0	0.88	0.12
RMSE:	3.58	1.35	1.35

MAX_MEAN: 5.09 MAX_MED: 5.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

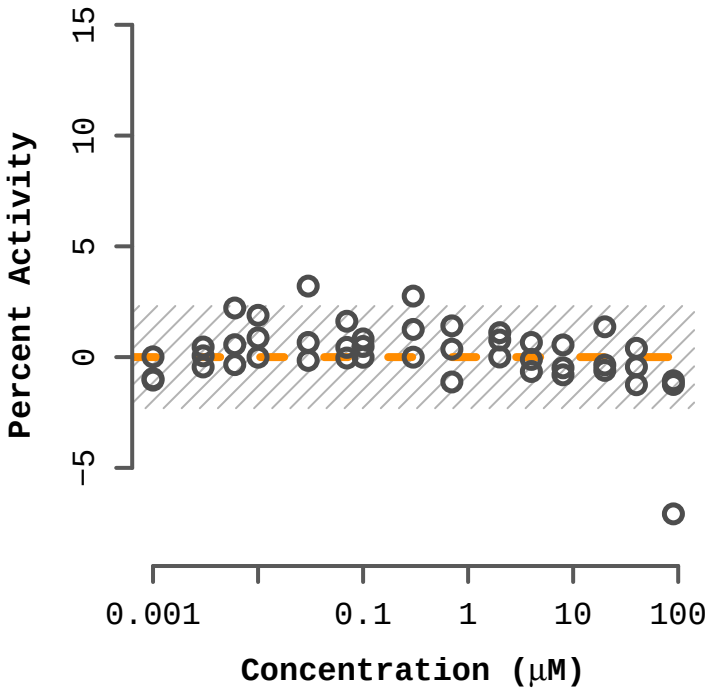
NAME: Indapamide
CHID: 44633 **CASRN:** 26807-65-8
SPID(S): Tox21_110775_1
M4ID: 12484120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

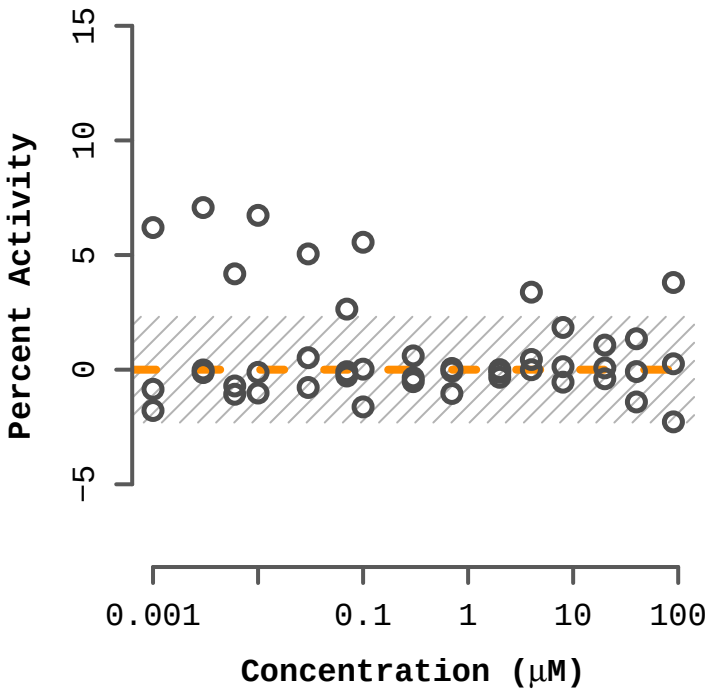
NAME: Sodium 4-vinylbenzenesulfonate
CHID: 44635 CASRN: 2695-37-6
SPID(S): Tox21_302466
M4ID: 12476667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

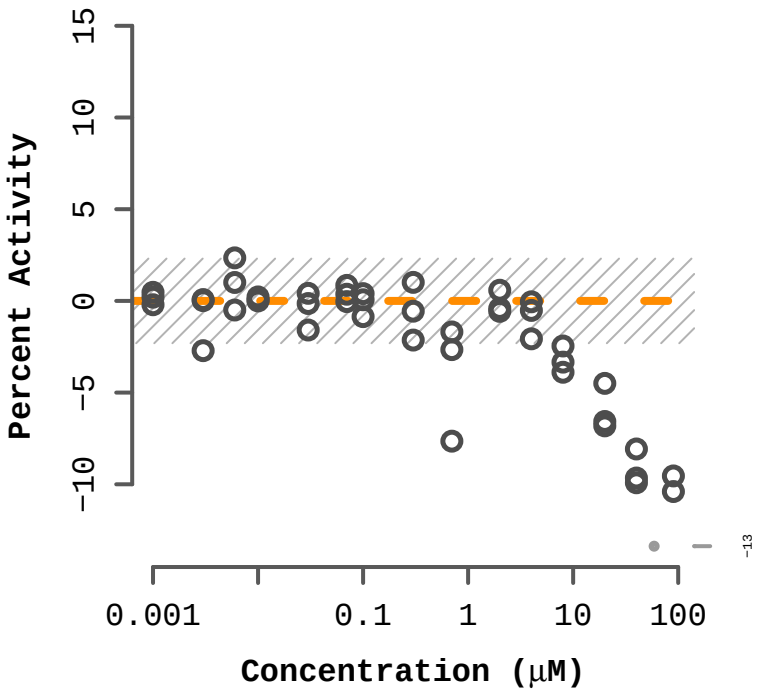
NAME: Diethoxy(methyl)[3-(oxiran-2-ylmethoxy)propyl]s
CHID: 44638 **CASRN:** 2897-60-1
SPID(S): Tox21_302661
M4ID: 12476472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.44	NA	NA

MAX_MEAN: 2.31 **MAX_MED:** 0.524 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

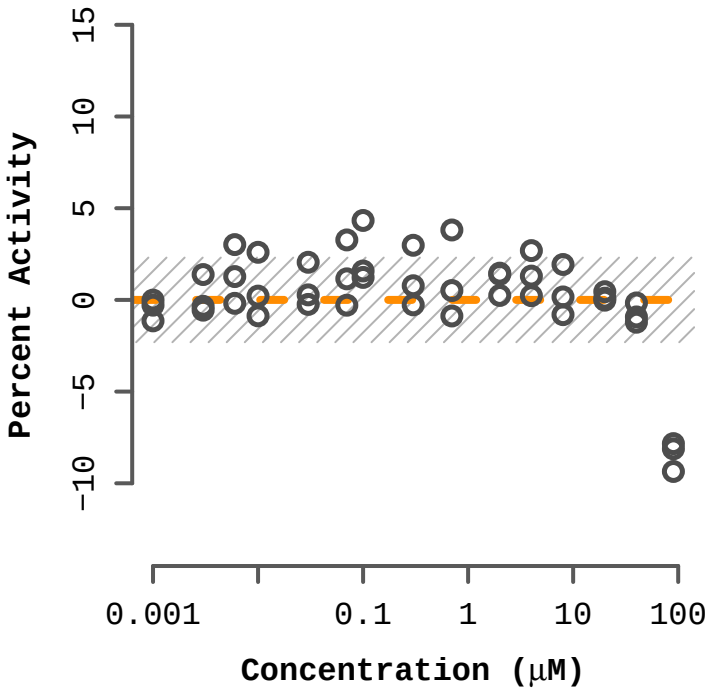
NAME: 2,4-Dichloro-1,3-dinitro-5-(trifluoromethyl)be
CHID: 44639 **CASRN:** 29091-09-6
SPID(S): Tox21_302530
M4ID: 12476603 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	253.25	NA	NA
PROB:	1	NA	NA
RMSE:	4.42	NA	NA

MAX_MEAN: 0.954 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

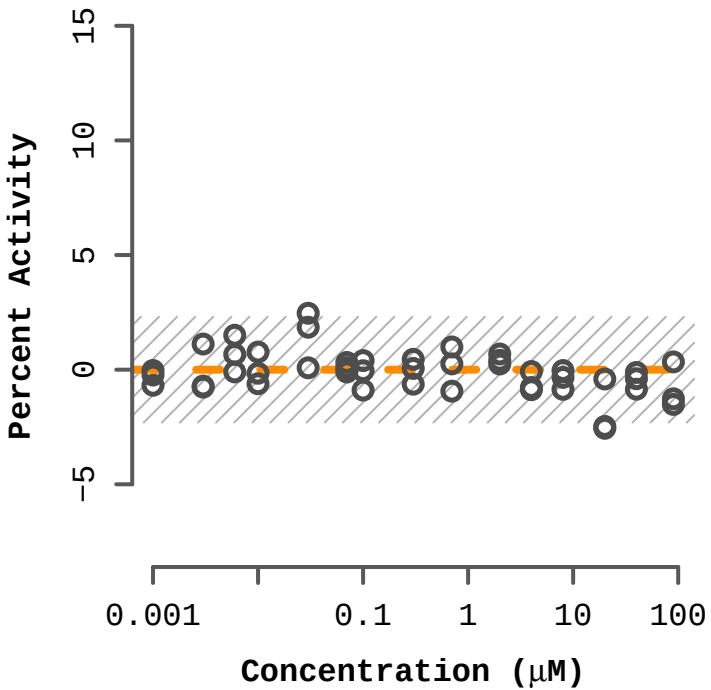
NAME: Disperse Red 82
CHID: 44642 **CASRN:** 30124-94-8
SPID(S): Tox21_302510
M4ID: 12476623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

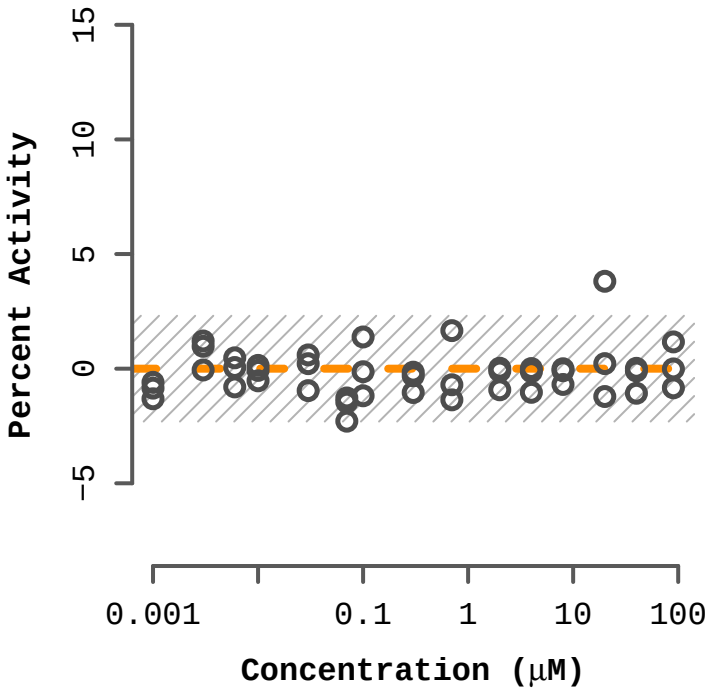
NAME: N,N,N−Trimethyl(oxiran−2−yl)methanaminium chlo
CHID: 44643 **CASRN:** 3033−77−0
SPID(S): Tox21_300176
M4ID: 12478954

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

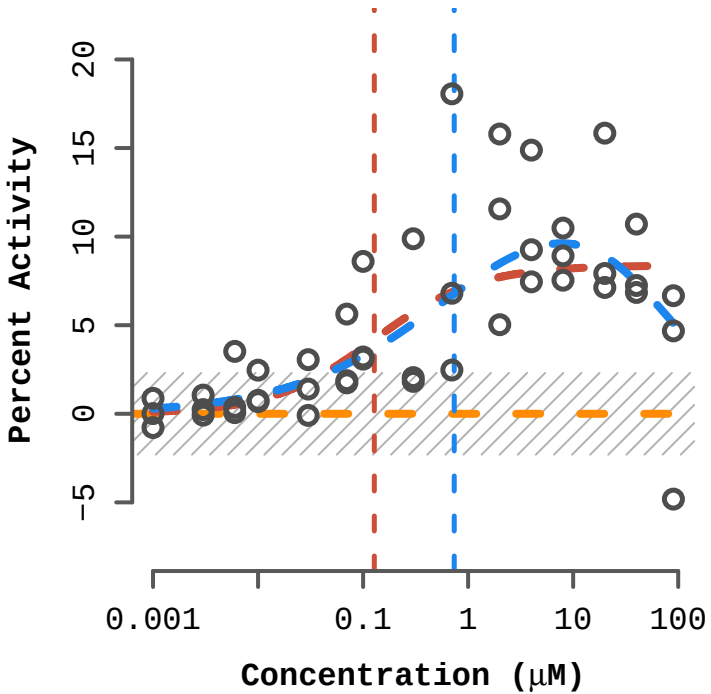
NAME: N-Isopropylphthalimide
CHID: 44644 **CASRN:** 304-17-6
SPID(S): Tox21_302473
M4ID: 12476660

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.941 **MAX_MED:** 0.976 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydralazine hydrochloride
CHID: 44645 CASRN: 304-20-1
SPID(S): Tox21_302496
M4ID: 12476637

HILL MODEL (in red):

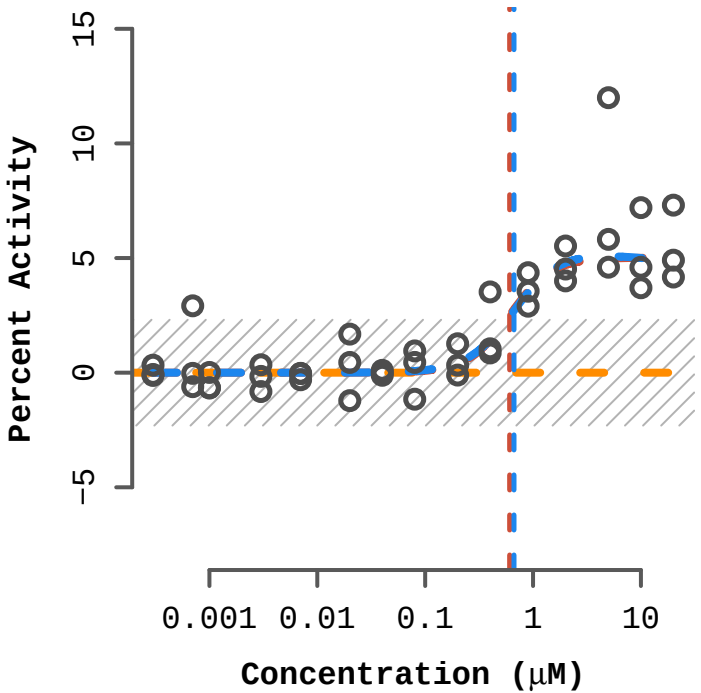
	tp	ga	gw
val:	8.38	−0.893	0.891
sd:	0.789	0.241	0.322

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.7	−0.132	0.576	1.77	0.993
sd:	20.9	2.17	0.383	1.09	1.89

	CNST	HILL	GNLS
AIC:	308.41	244.21	240.9
PROB:	0	0.16	0.84
RMSE:	7.2	3.78	3.42

MAX_MEAN: 10.8 MAX_MED: 11.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydralazine hydrochloride
CHID: 44645 CASRN: 304-20-1
SPID(S): Tox21_110163_1
M4ID: 12484594

HILL MODEL (in red):

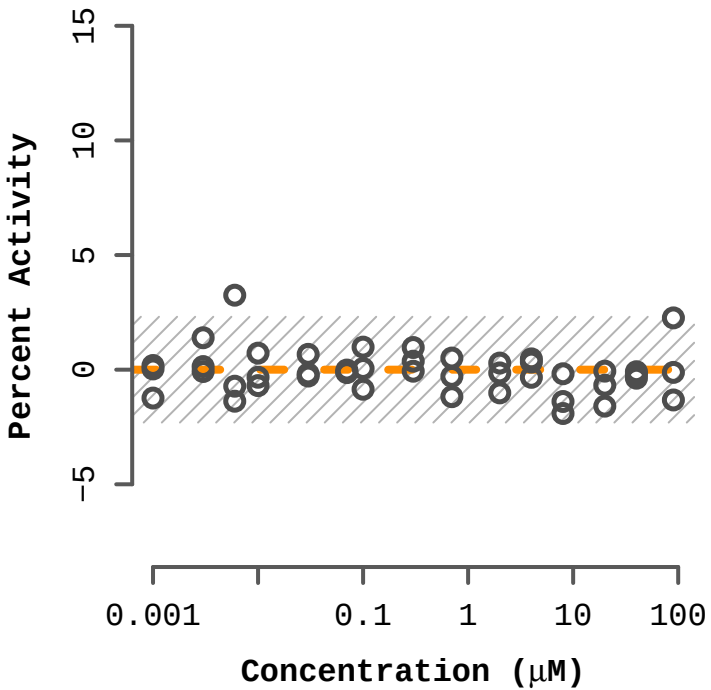
	tp	ga	gw
val:	5.02	−0.217	2.25
sd:	0.36	0.0746	0.716

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.65	−0.177	2.04	3.3	0.393
sd:	8.44	0.24	0.933	11.5	4.43

	CNST	HILL	GNLS
AIC:	233.82	140.83	144.67
PROB:	0	0.87	0.13
RMSE:	3.4	1.4	1.4

MAX_MEAN: 7.47 **MAX_MED:** 5.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

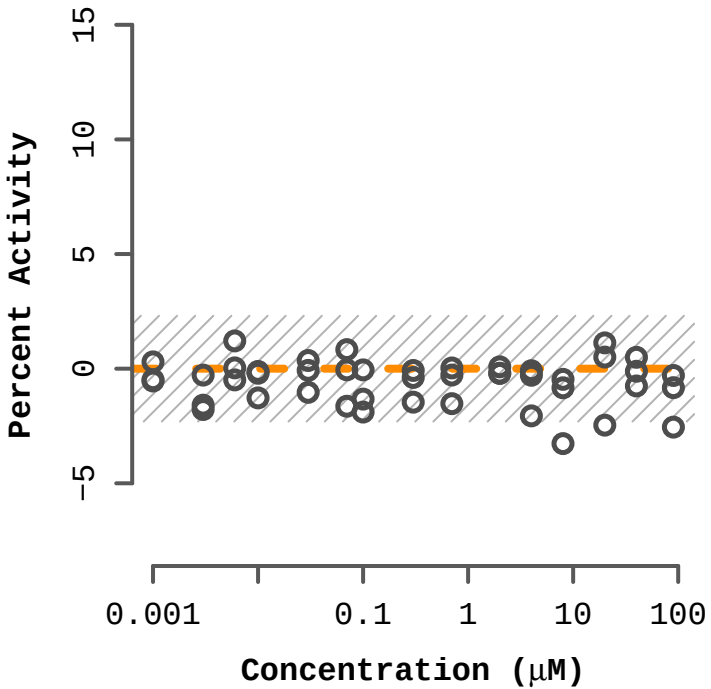
NAME: 5,5-Dimethyl-2-phenoxy-1,3,2-dioxaphosphinane
CHID: 44646 **CASRN:** 3057-08-7
SPID(S): Tox21_302520
M4ID: 12476613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

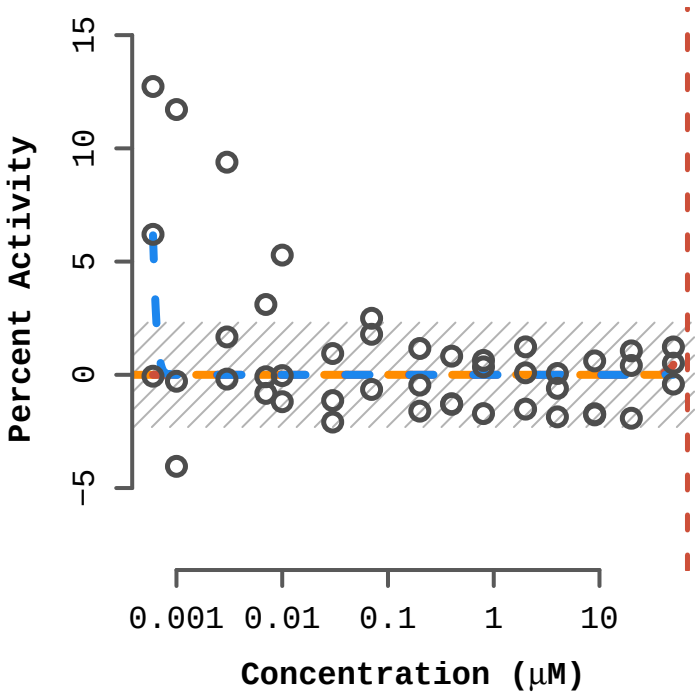
NAME: Pargyline hydrochloride
CHID: 44647 CASRN: 306-07-0
SPID(S): Tox21_302678
M4ID: 12476455

HILL MODEL: Not applicable.

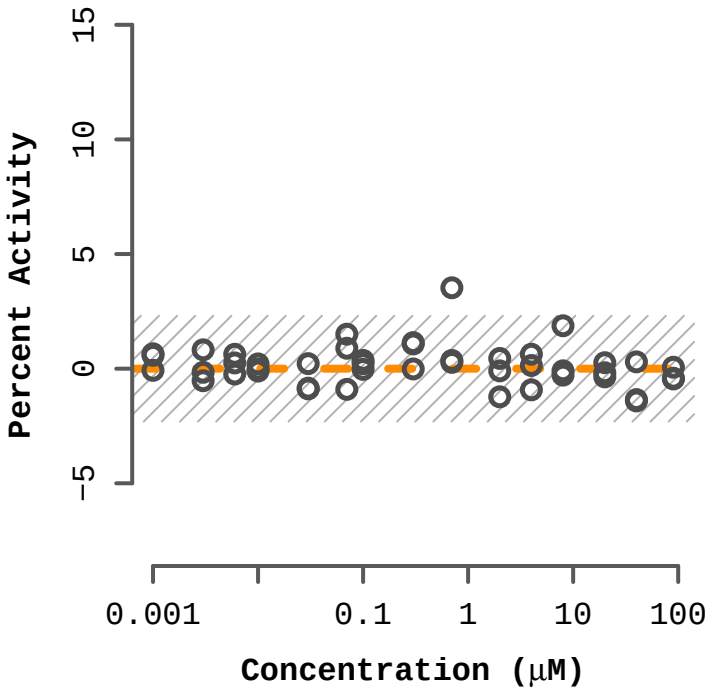
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.253 **MAX_MED:** 0.507 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pargyline hydrochloride
CHID:    44647   CASRN: 306-07-0
SPID(S): Tox21_110241_1
M4ID:    12484522

HILL MODEL (in red):
      tp       ga       gw
val:  5.22     1.83     7.7
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  15.2     -4.83    2.4      -3.23    18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  216.92      222.68      221.16
PROB: 0.85        0.05        0.1
RMSE: 3.44        3.44        3.04

MAX_MEAN: 6.29      MAX_MED: 6.2       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

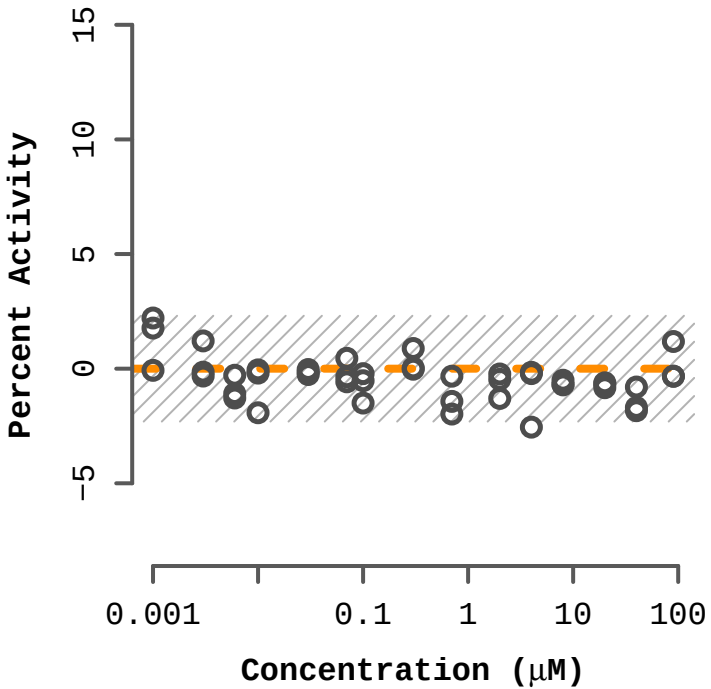
NAME: N-[3-(Trimethoxysilyl)propyl]aniline
CHID: 44648 **CASRN:** 3068-76-6
SPID(S): Tox21_302471
M4ID: 12476662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

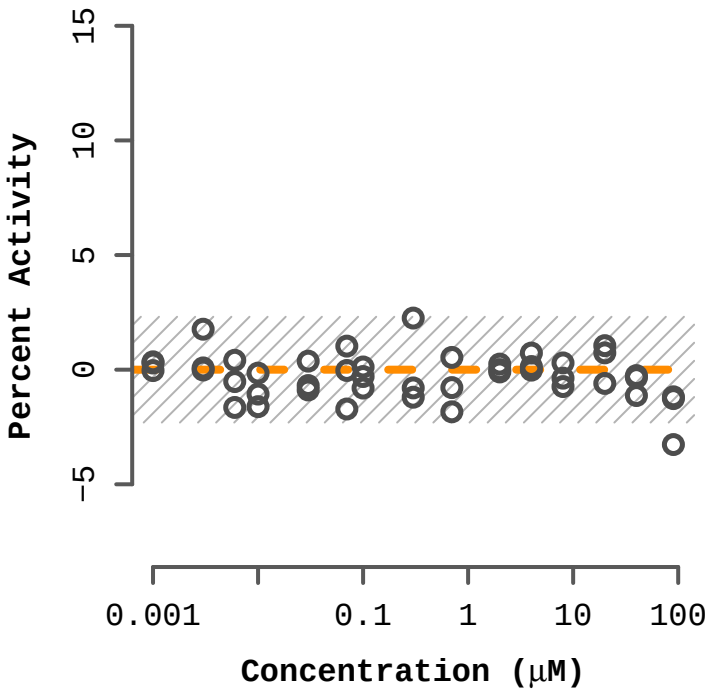
NAME: 2,2'−[(4−Methylphenyl)imino]diethanol
CHID: 44650 **CASRN:** 3077−12−1
SPID(S): Tox21_302653
M4ID: 12476480

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

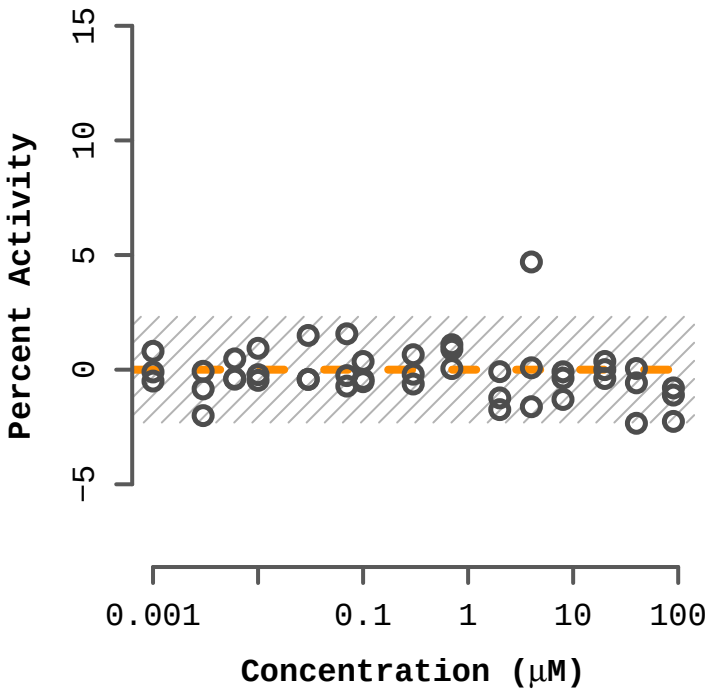
NAME: Labetalol hydrochloride
CHID: 44654 **CASRN:** 32780-64-6
SPID(S): Tox21_302725
M4ID: 12476408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.61 **MAX_MED:** 0.735 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

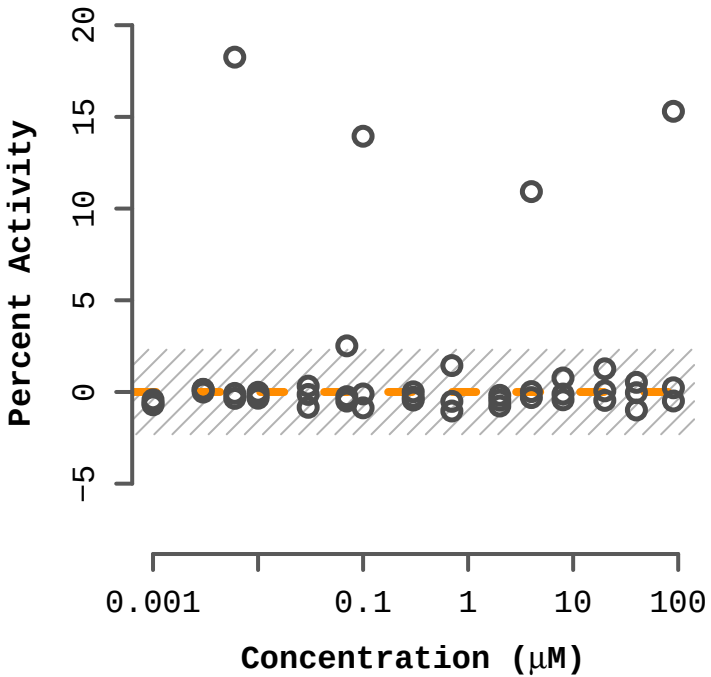
NAME: N,N−Diethyldodecanamide
CHID: 44655 **CASRN:** 3352−87−2
SPID(S): Tox21_302477
M4ID: 12476656

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.891 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

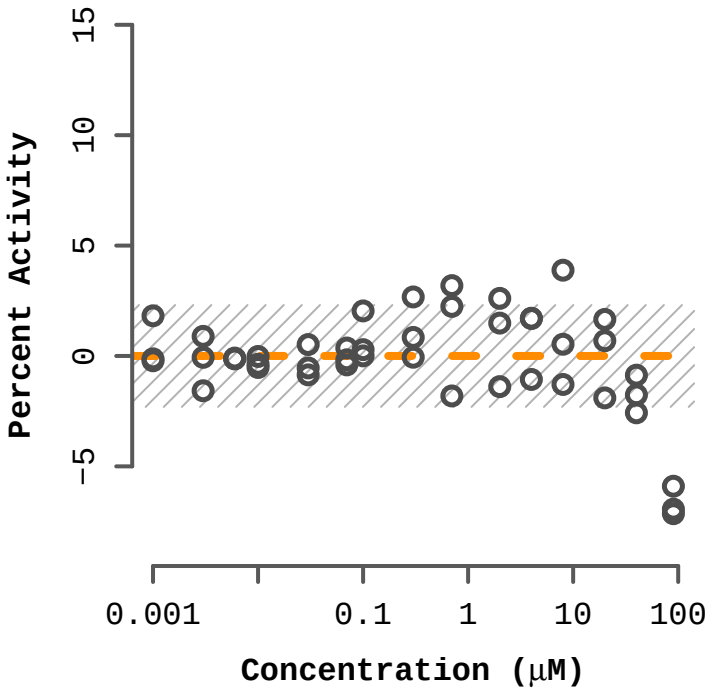
NAME: 3,3'−(Ethylenedioxy)dipropiononitrile
CHID: 44656 CASRN: 3386−87−6
SPID(S): Tox21_301474
M4ID: 12477659

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.01	NA	NA
PROB:	1	NA	NA
RMSE:	4.47	NA	NA

MAX_MEAN: 5.95 **MAX_MED:** 0.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

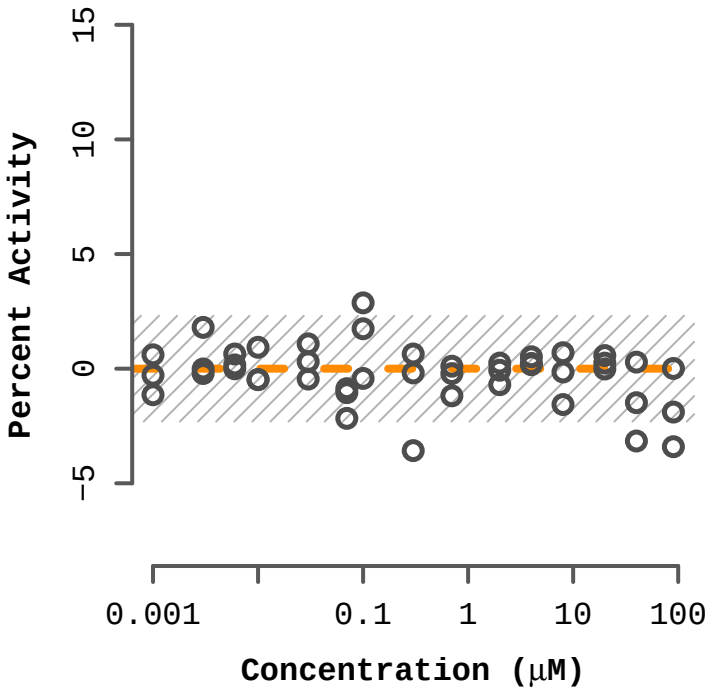
NAME: 1H-Isoindole-1,3(2H)-diimine
CHID: 44658 **CASRN:** 3468-11-9
SPID(S): Tox21_301457
M4ID: 12477676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

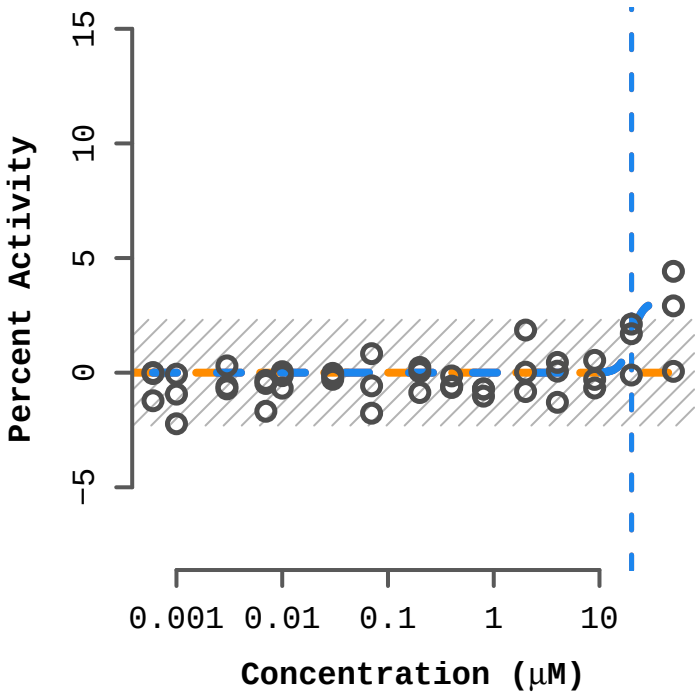
NAME: 2,2'−Sulfanediyldiethanethiol
CHID: 44660 **CASRN:** 3570−55−6
SPID(S): Tox21_301602
M4ID: 12477531

HILL MODEL: Not applicable.

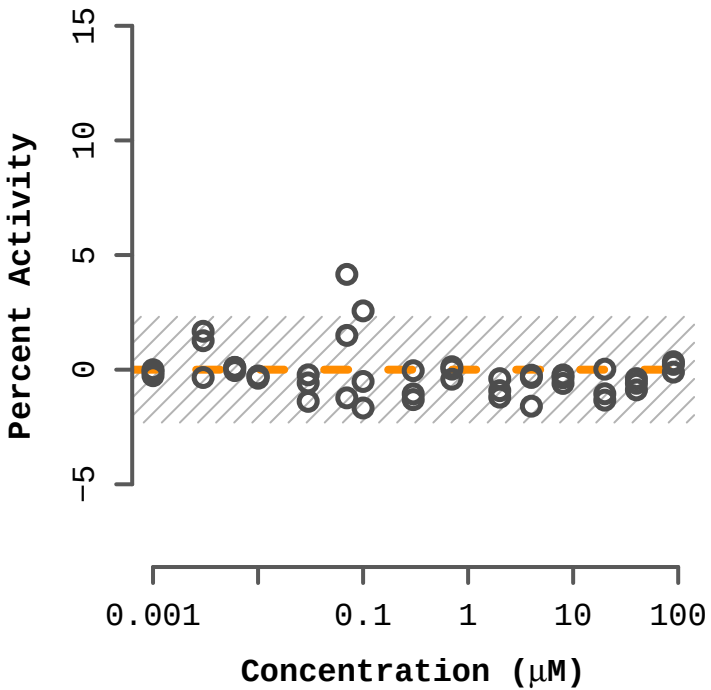
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.74 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-(2H-Benzotriazol-2-yl)-6-(butan-2-yl)-4-tert·
CHID:    44661   CASRN: 36437-37-3
SPID(S): Tox21_303942
M4ID:    12475246

HILL MODEL (in red):
      tp       ga       gw
val:  3.08     1.3      8
sd:   0.682    0.0446   18.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.08     1.3      8        3.68     6.44
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  135.37      128.28      132.28
PROB: 0.02        0.86        0.12
RMSE: 1.17        0.95        0.95

MAX_MEAN: 2.47      MAX_MED: 2.92      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

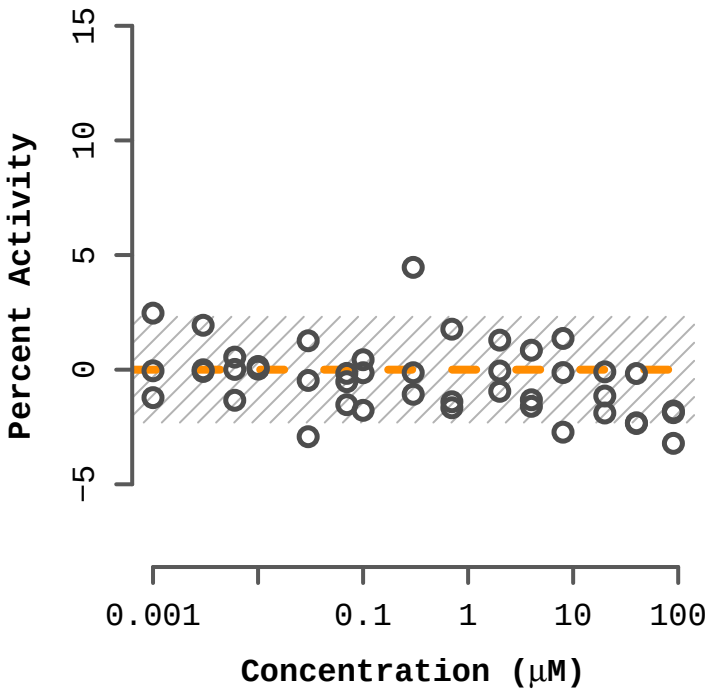
NAME: Ethyl octyl sulfide
CHID: 44662 CASRN: 3698-94-0
SPID(S): Tox21_301893
M4ID: 12477240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

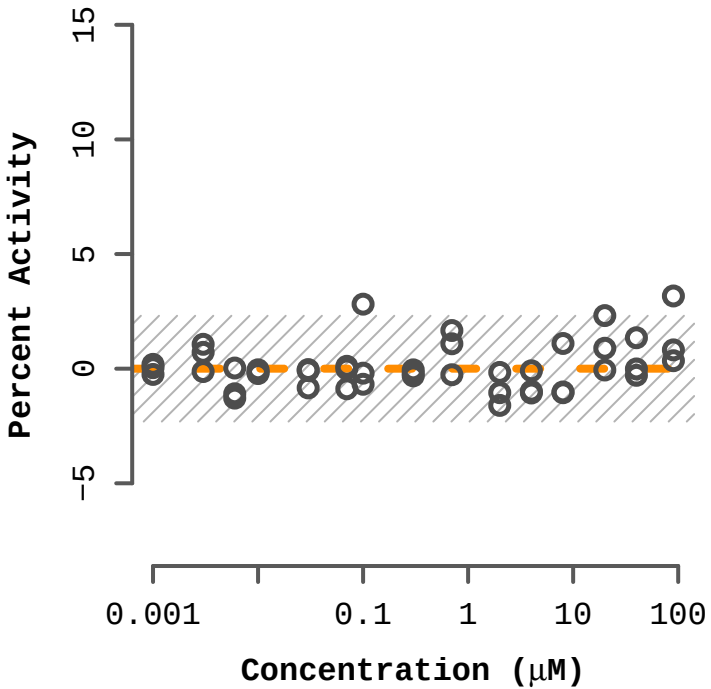
NAME: C.I. Acid Red 1
CHID: 44663 **CASRN:** 3734-67-6
SPID(S): Tox21_301525
M4ID: 12477608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.0495 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

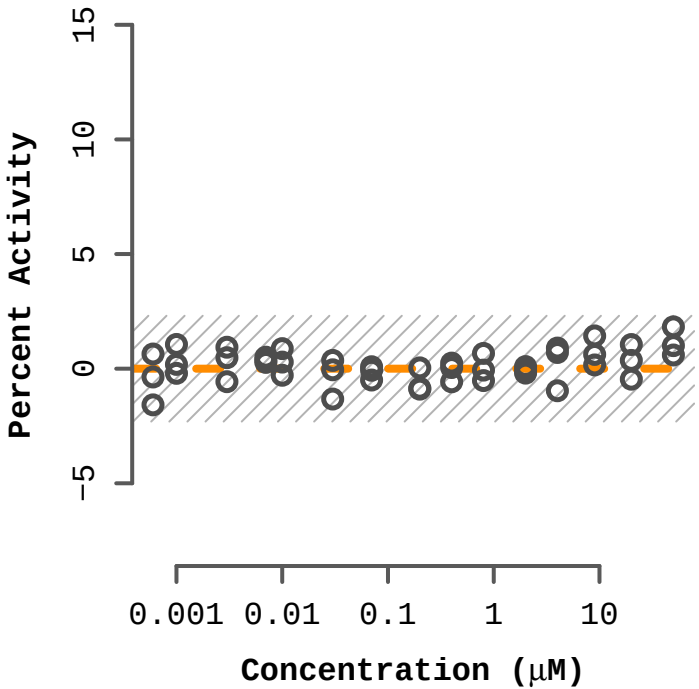
NAME: Todralazine hydrochloride
CHID: 44664 CASRN: 3778-76-5
SPID(S): Tox21_301437
M4ID: 12477696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

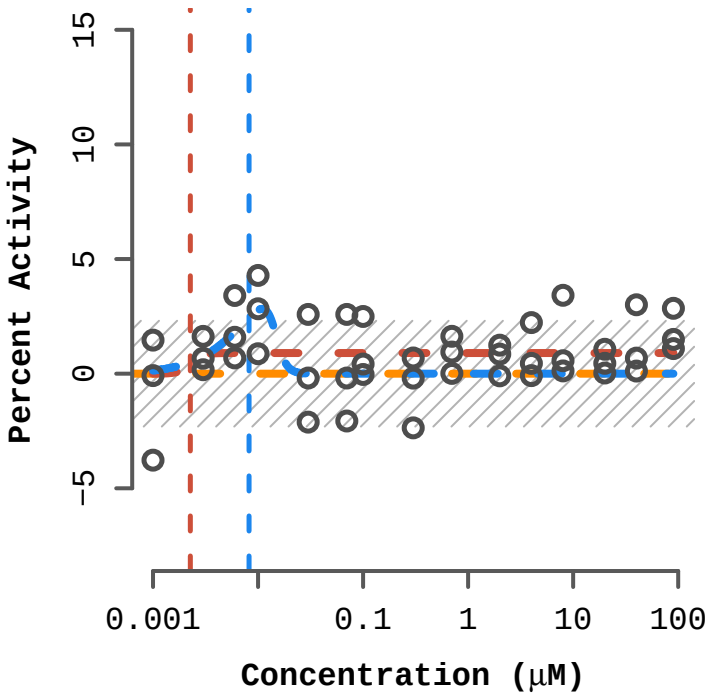
NAME: Todralazine hydrochloride
CHID: 44664 **CASRN:** 3778-76-5
SPID(S): Tox21_113562_1
M4ID: 12482610

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N,N'−Di−tert−butylethane−1,2−diamine
CHID: 44667 CASRN: 4062−60−6
SPID(S): Tox21_301519
M4ID: 12477614

HILL MODEL (in red):

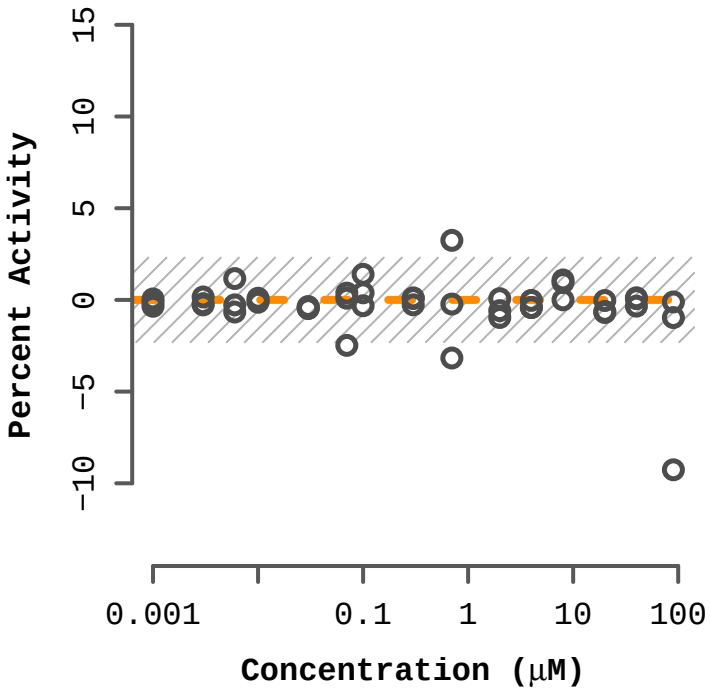
	tp	ga	gw
val:	0.9	−2.64	8
sd:	0.228	1	52.5

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.91	−2.09	1.69	−1.84	8.93
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	182.8	173.36	180.15
PROB:	0.01	0.96	0.03
RMSE:	1.77	1.52	1.55

MAX_MEAN: 2.66 MAX_MED: 2.83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

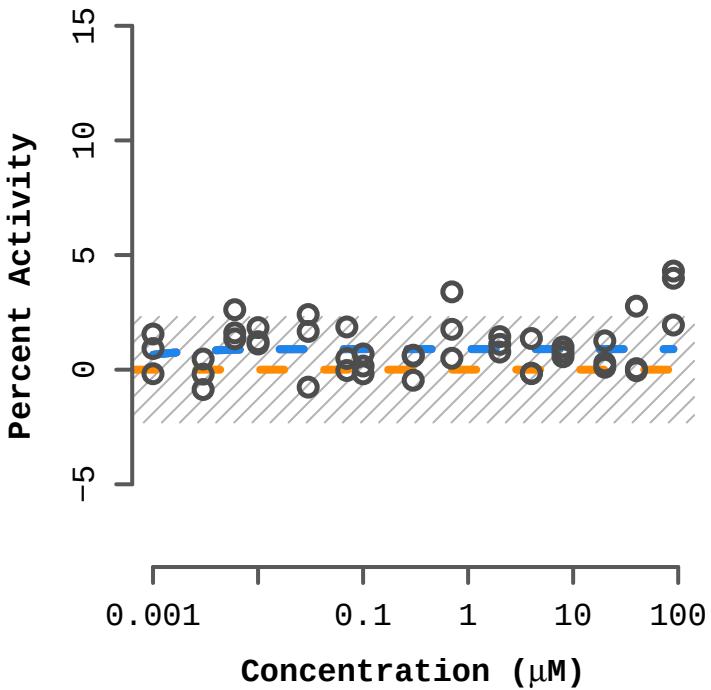
NAME: 1,1,2-Trimethyl-1H-benzo[e]indole
CHID: 44668 **CASRN:** 41532-84-7
SPID(S): Tox21_301959
M4ID: 12477174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 0.682 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clonidine hydrochloride
CHID: 44670 CASRN: 4205-91-8
SPID(S): Tox21_301552
M4ID: 12477581

HILL MODEL (in red):

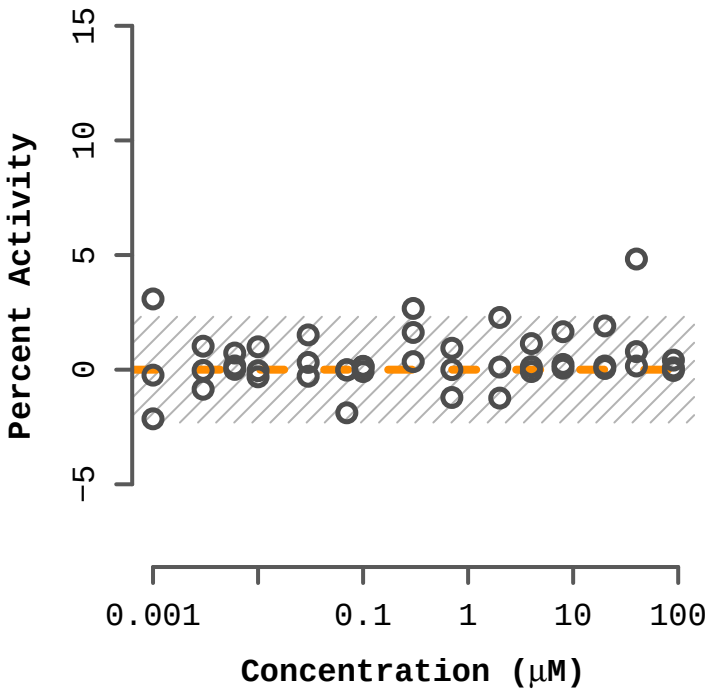
	tp	ga	gw
val:	0.898	−3.3	1.35
sd:	0.179	1.42	2.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.898	−3.3	1.35	3.92	4.06
sd:	0.179	1.42	2.25	1780	3690

	CNST	HILL	GNLS
AIC:	167.07	147.95	151.95
PROB:	0	0.88	0.12
RMSE:	1.54	1.16	1.16

MAX_MEAN: 3.41 **MAX_MED:** 3.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

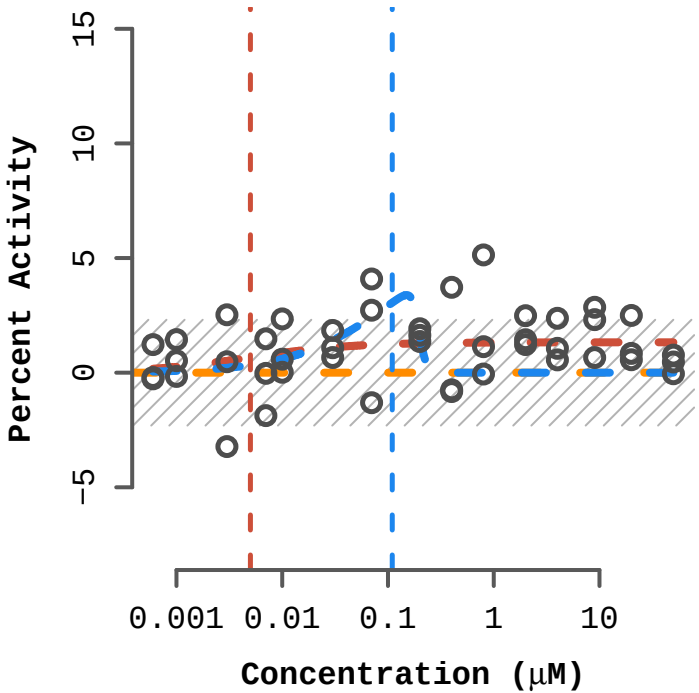
NAME: 2-(Dodecyloxy)ethanol
CHID: 44676 **CASRN:** 4536-30-5
SPID(S): Tox21_301593
M4ID: 12477540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Dodecyloxy)ethanol
CHID: 44676 CASRN: 4536-30-5
SPID(S): Tox21_113966
M4ID: 12482267

HILL MODEL (in red):

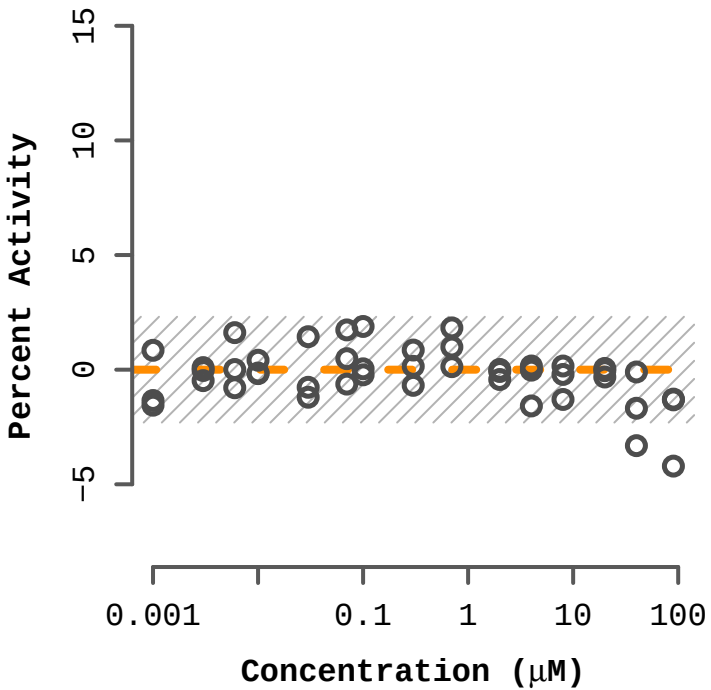
	tp	ga	gw
val:	1.32	-2.3	0.901
sd:	0.271	0.8	0.962

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.11	-0.96	0.926	-0.71	13
sd:	14.6	1.89	0.97	0.152	169

	CNST	HILL	GNLS
AIC:	186.18	168.13	185.03
PROB:	0	1	0
RMSE:	1.85	1.44	1.7

MAX_MEAN: 2.07 MAX_MED: 2.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

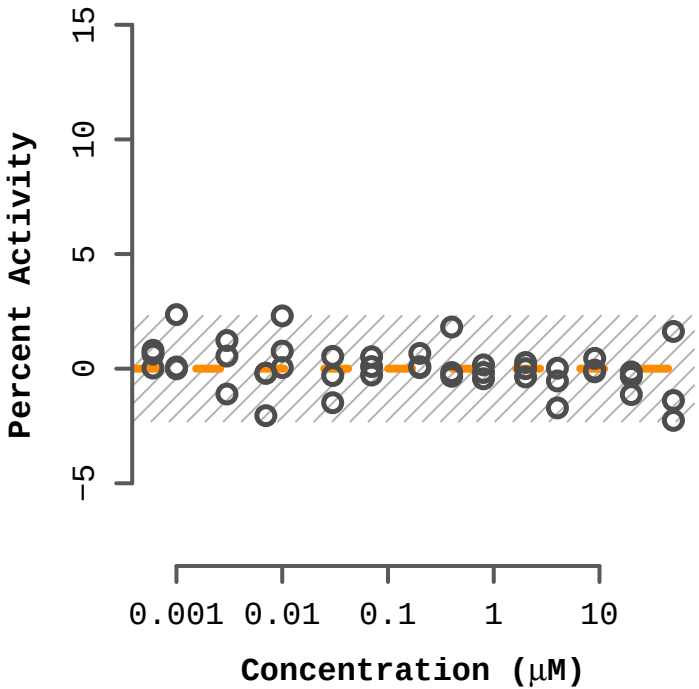
NAME: Orphenadrine dihydrogen citrate
CHID: 44678 CASRN: 4682-36-4
SPID(S): Tox21_301079
M4ID: 12478054

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.982 MAX_MED: 0.989 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

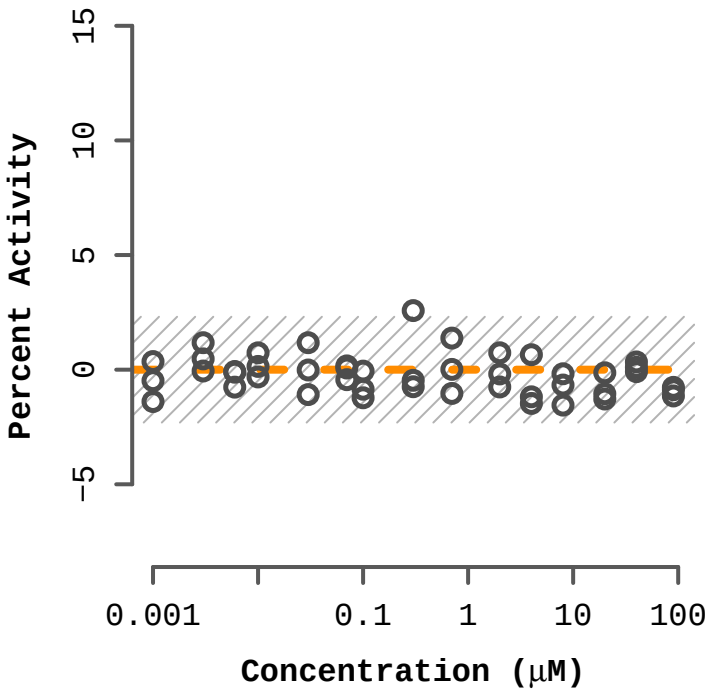
NAME: Orphenadrine dihydrogen citrate
CHID: 44678 CASRN: 4682-36-4
SPID(S): Tox21_111323_1
M4ID: 12483768

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.767 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

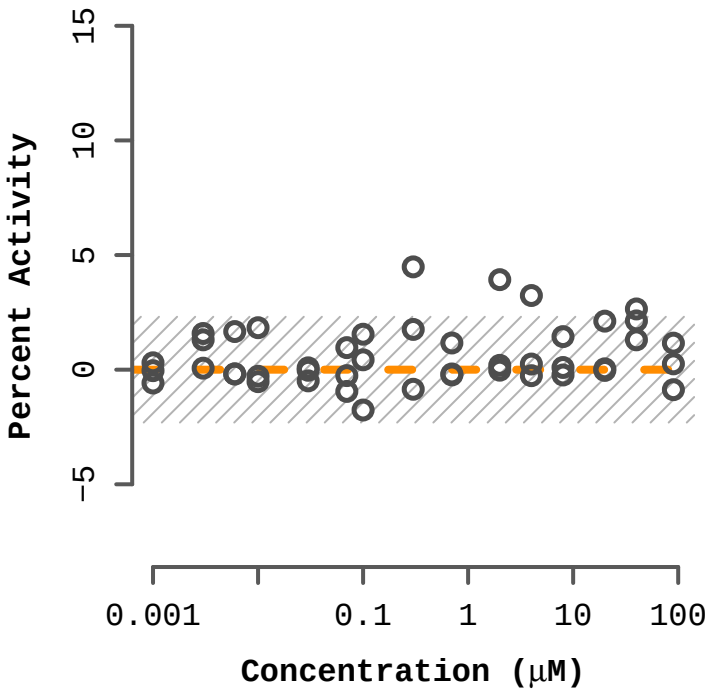
NAME: Octylphosphonic acid
CHID: 44679 CASRN: 4724-48-5
SPID(S): Tox21_302242
M4ID: 12476891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.531 **MAX_MED:** 0.472 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

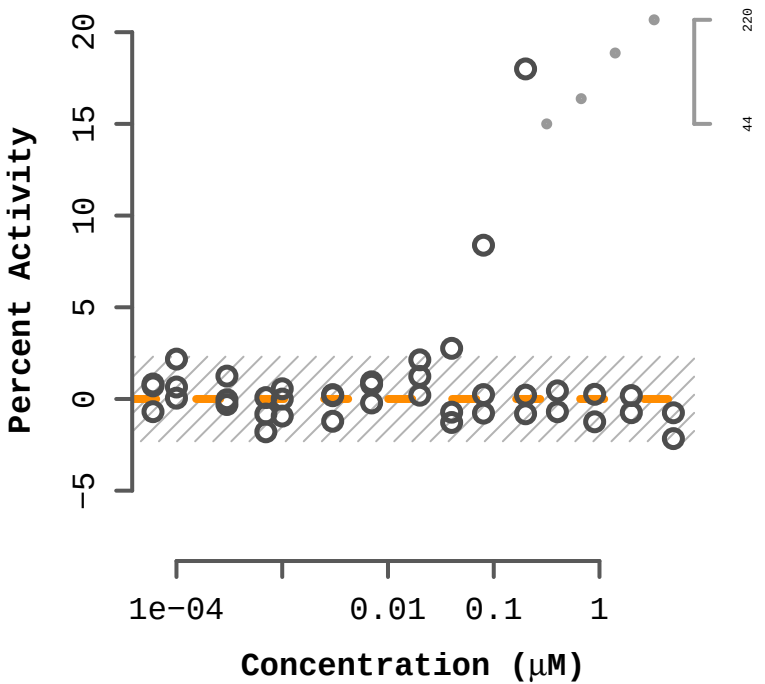
NAME: 2,2'−[(3−Aminopropyl)imino]diethanol
CHID: 44680 **CASRN:** 4985−85−7
SPID(S): Tox21_301510
M4ID: 12477623

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 2.03 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

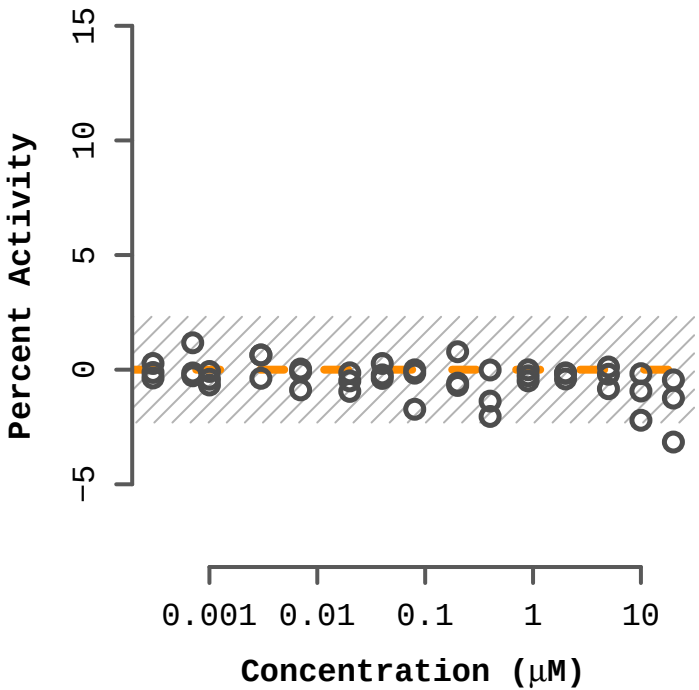
NAME: Chloroquine bis(phosphate)
CHID: 44681 **CASRN:** 50-63-5
SPID(S): Tox21_202838
M4ID: 12479414 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	319.49	NA	NA
PROB:	1	NA	NA
RMSE:	44.07	NA	NA

MAX_MEAN: 73.4 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

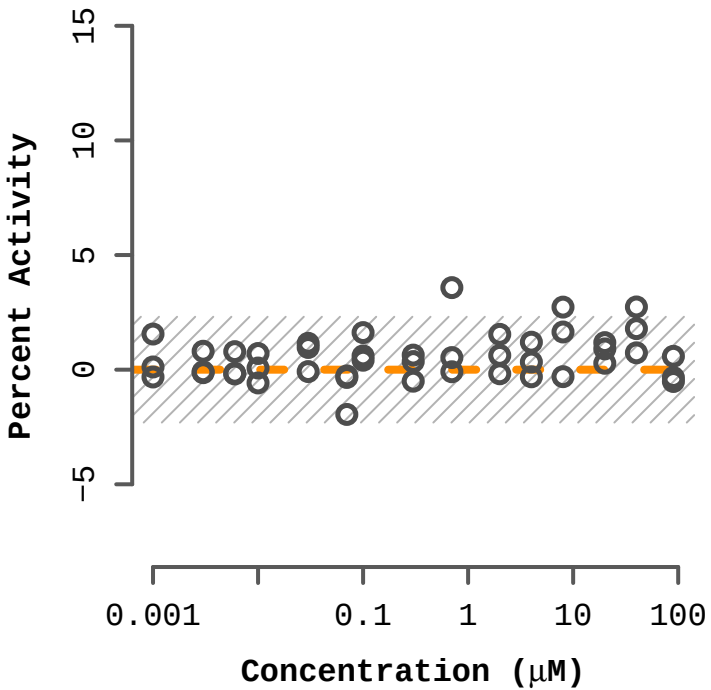
NAME: Chloroquine bis(phosphate)
CHID: 44681 **CASRN:** 50-63-5
SPID(S): Tox21_110115_1
M4ID: 12484638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.303 **MAX_MED:** 0.638 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

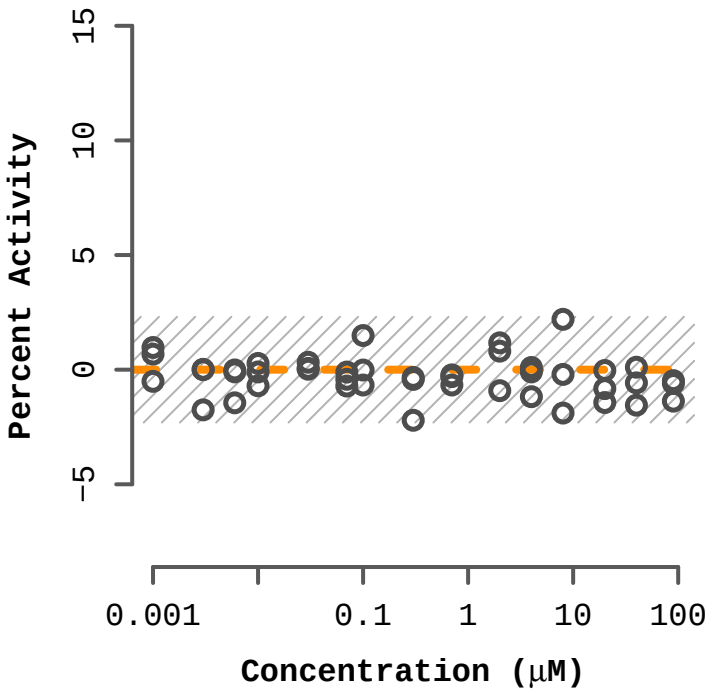
NAME: N,N,N−Trimethyl−3−[(2−methylacryloyl)amino]pro|
CHID: 44682 CASRN: 51410−72−1
SPID(S): Tox21_302211
M4ID: 12476922

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.76 MAX_MED: 1.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

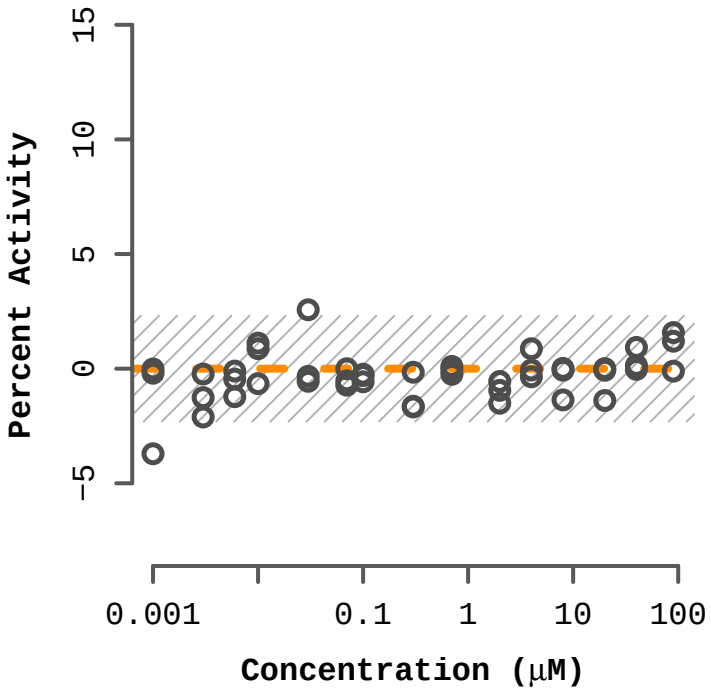
NAME: Sodium 5-oxo-1-(4-sulfophenyl)-4,5-dihydro-1H-p
CHID: 44684 CASRN: 52126-51-9
SPID(S): Tox21_301487
M4ID: 12477646

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.38 MAX_MED: 0.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

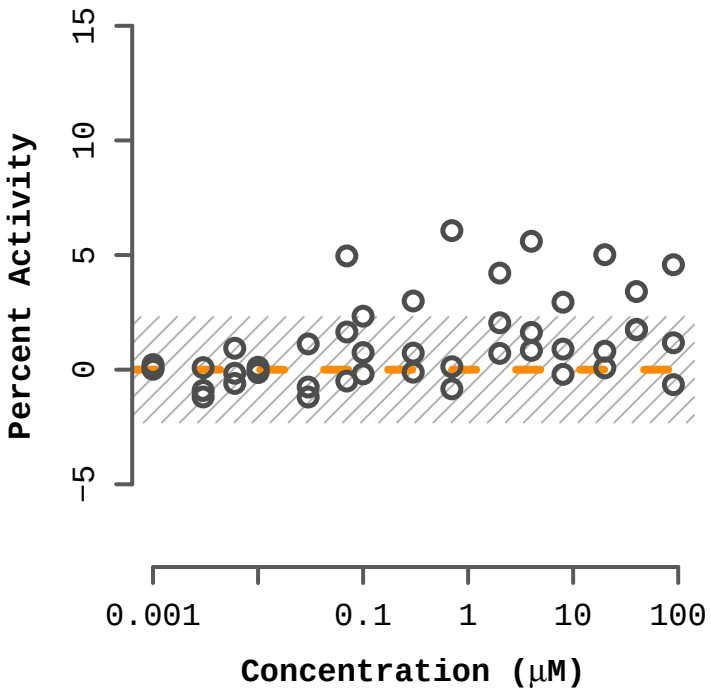
NAME: 2-Chloro-1,4-diethoxybenzene
CHID: 44685 **CASRN:** 52196-74-4
SPID(S): Tox21_301484
M4ID: 12477649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

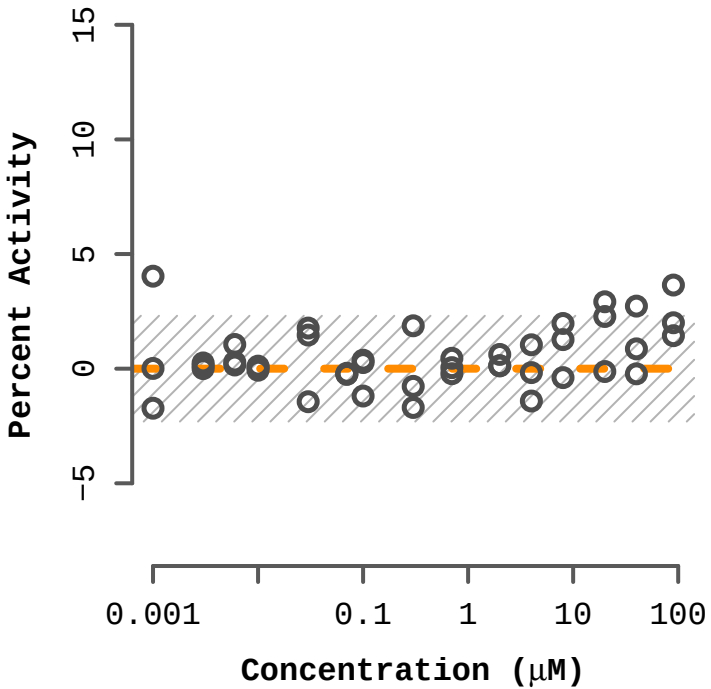
NAME: 4-Amino-2,5-dimethoxy-N-phenylbenzenesulfonami
CHID: 44686 **CASRN:** 52298-44-9
SPID(S): Tox21_301543
M4ID: 12477590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.04	NA	NA
PROB:	1	NA	NA
RMSE:	2.21	NA	NA

MAX_MEAN: 2.69 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

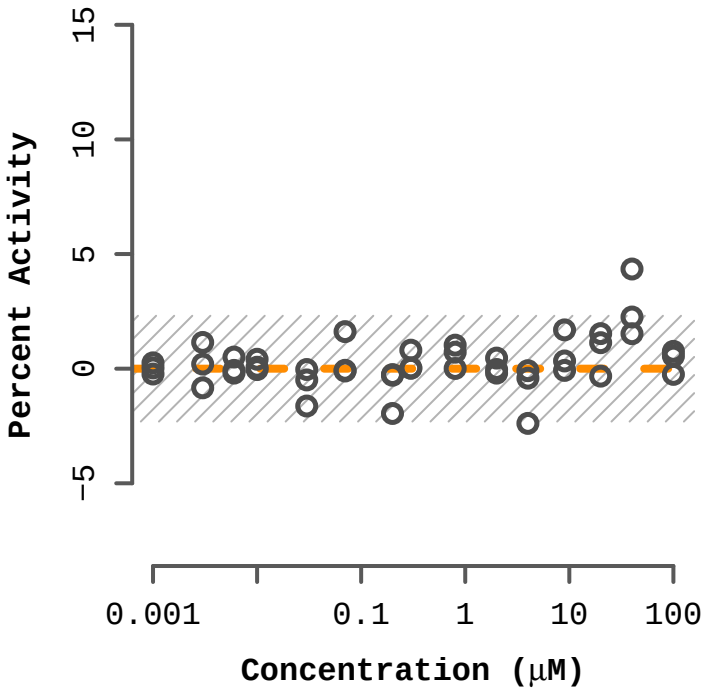
NAME: N-(4-Methoxyphenyl)-3-oxobutanamide
CHID: 44689 **CASRN:** 5437-98-9
SPID(S): Tox21_301481
M4ID: 12477652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 2.36 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

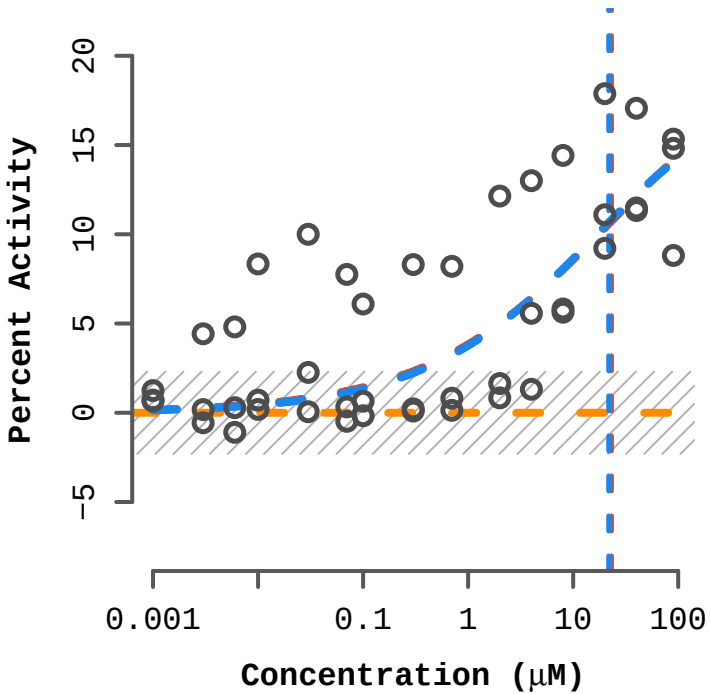
NAME: 1,1'−[Ethane−1,2−diylbis(oxy)]bis(3−methylbenz
CHID: 44690 **CASRN:** 54914−85−1
SPID(S): Tox21_301884
M4ID: 12477249

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 2.71 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Propan-2-yl)-9H-thioxanthen-9-one
CHID: 44691 CASRN: 5495-84-1
SPID(S): Tox21_301537
M4ID: 12477596

HILL MODEL (in red):

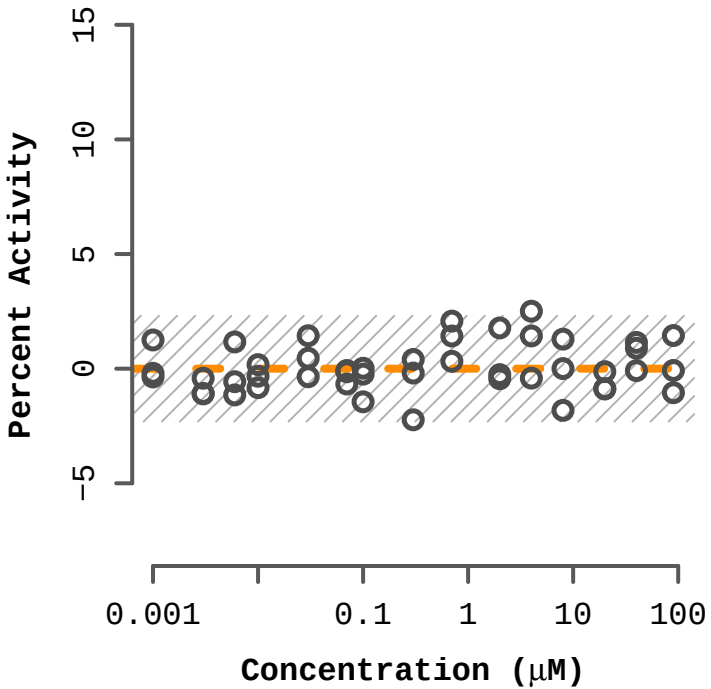
	tp	ga	gw
val:	21.5	1.36	0.486
sd:	11.9	1.08	0.251

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.5	1.34	0.502	3.42	1.08
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	314.59	258.27	262.24
PROB:	0	0.88	0.12
RMSE:	7.74	3.84	3.84

MAX_MEAN: 13.3 MAX_MED: 14.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

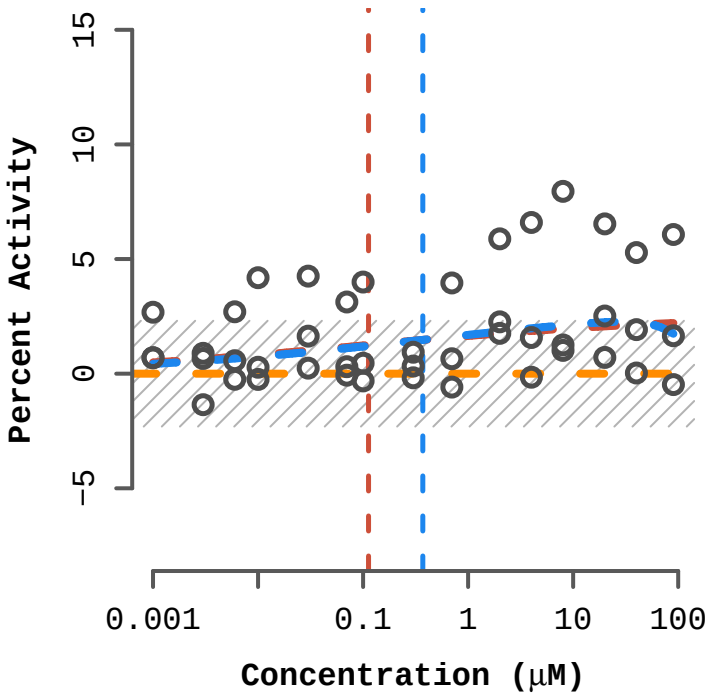
NAME: Scopolamine hydrochloride
CHID: 44692 CASRN: 55-16-3
SPID(S): Tox21_302226
M4ID: 12476907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Magnesium dibenzoate
CHID: 44693 **CASRN:** 553-70-8
SPID(S): Tox21_302263
M4ID: 12476870

HILL MODEL (in red):

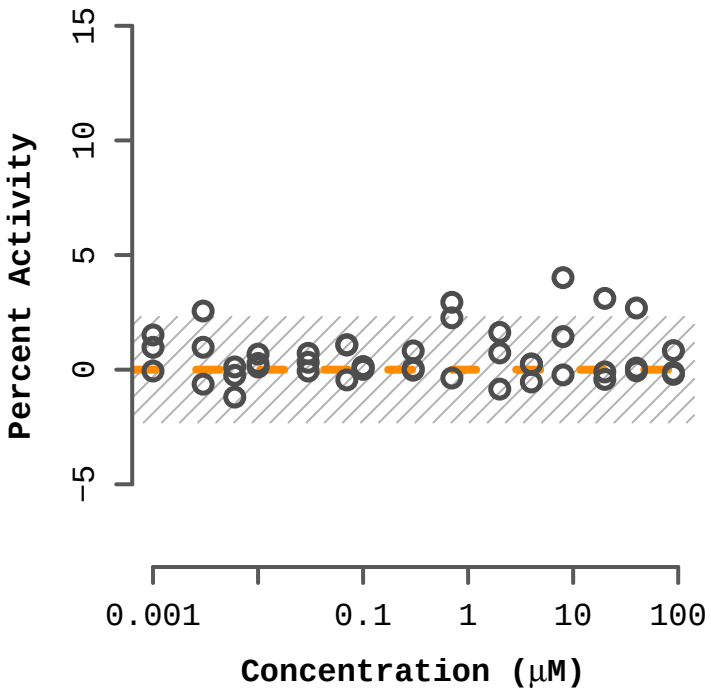
	tp	ga	gw
val:	2.5	−0.948	0.3
sd:	2.24	3.23	0.426

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.95	−0.431	0.3	2.1	2.56
sd:	7.33	8.19	0.716	0.812	13.1

	CNST	HILL	GNLS
AIC:	221.33	205.08	208.93
PROB:	0	0.87	0.13
RMSE:	2.89	2.16	2.15

MAX_MEAN: 3.41 **MAX_MED:** 2.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

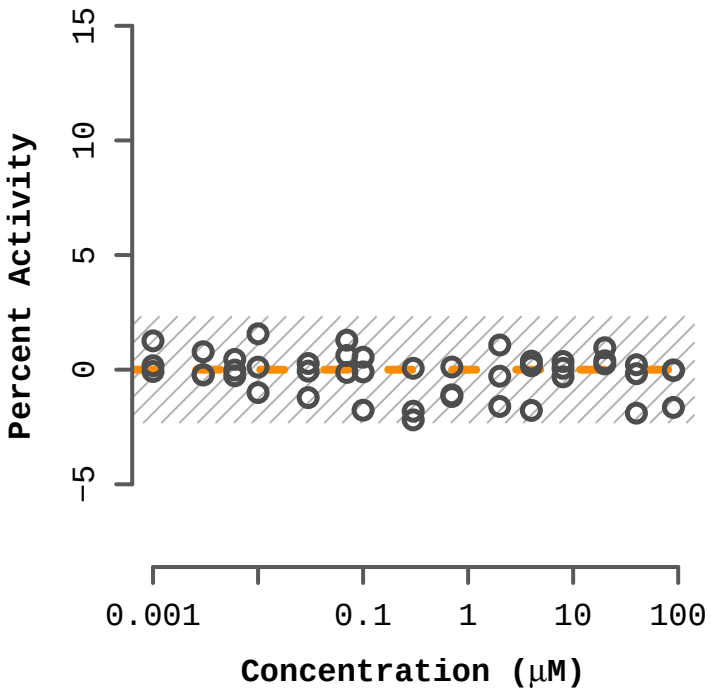
NAME: 3-{[3-(Aziridin-1-yl)propanoyl]oxy}-2-({[3-(az
CHID: 44696 **CASRN:** 57116-45-7
SPID(S): Tox21_302250
M4ID: 12476883

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

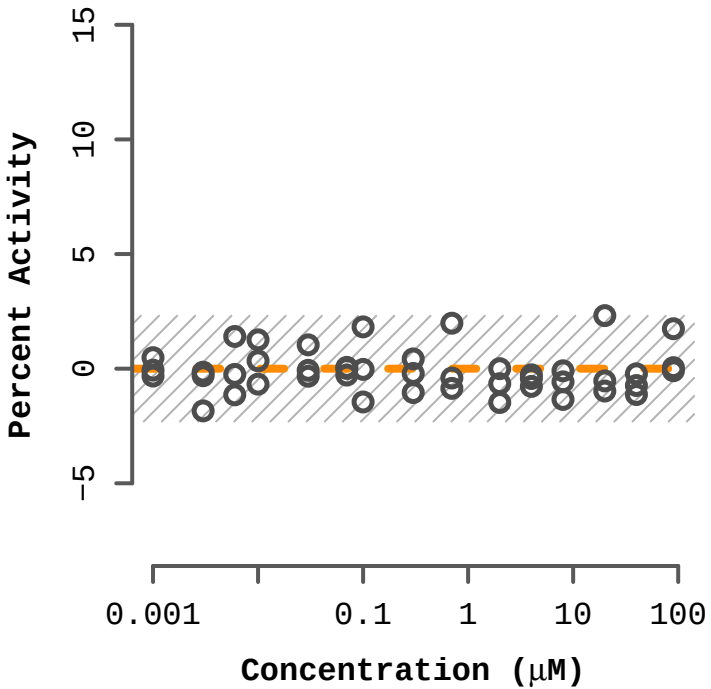
NAME: 4-Ethyloct-1-yn-3-ol
CHID: 44697 **CASRN:** 5877-42-9
SPID(S): Tox21_301468
M4ID: 12477665

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.596 **MAX_MED:** 0.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

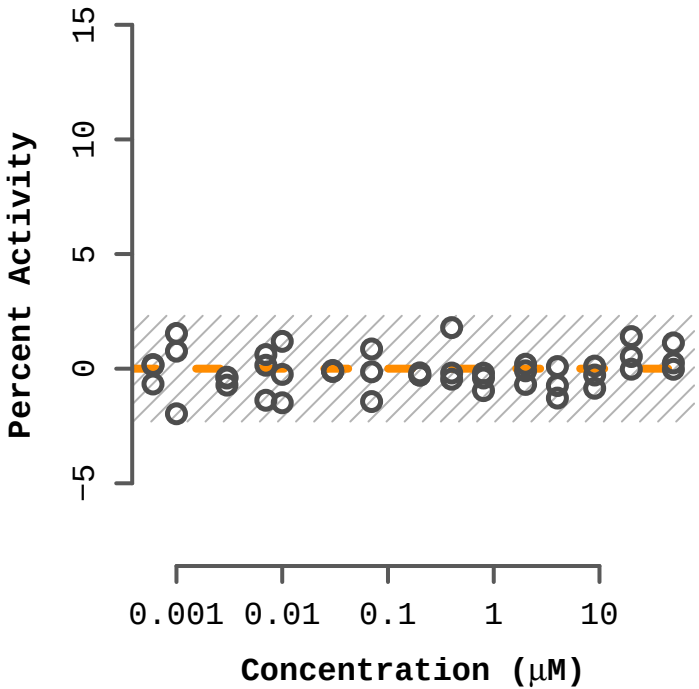
NAME: Dibutan-2-yl disulfide
CHID: 44698 **CASRN:** 5943-30-6
SPID(S): Tox21_301947
M4ID: 12477186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.568 **MAX_MED:** 0.344 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

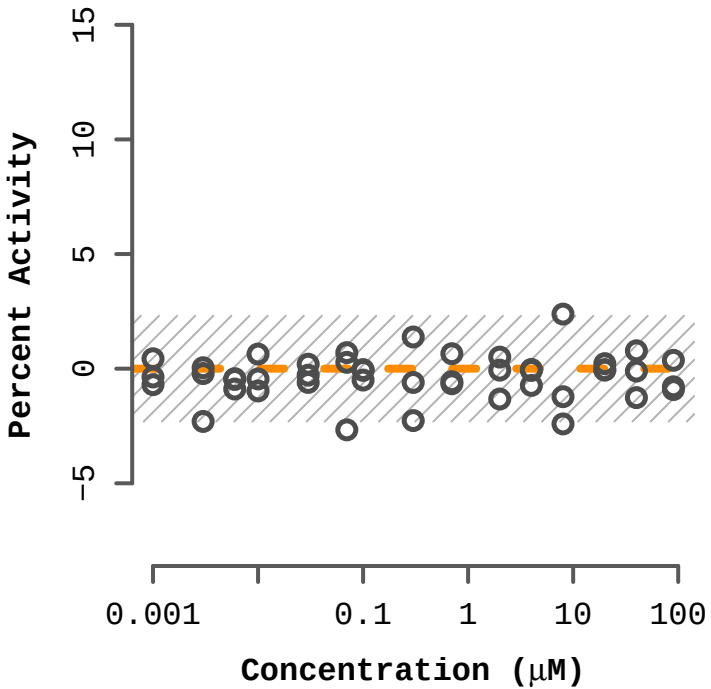
NAME: N,N,N,N',N',N'−Hexamethylhexane−1,6−diaminium (
CHID: 44700 **CASRN:** 60−25−3
SPID(S): Tox21_303898
M4ID: 12475290

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.637 **MAX_MED:** 0.765 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

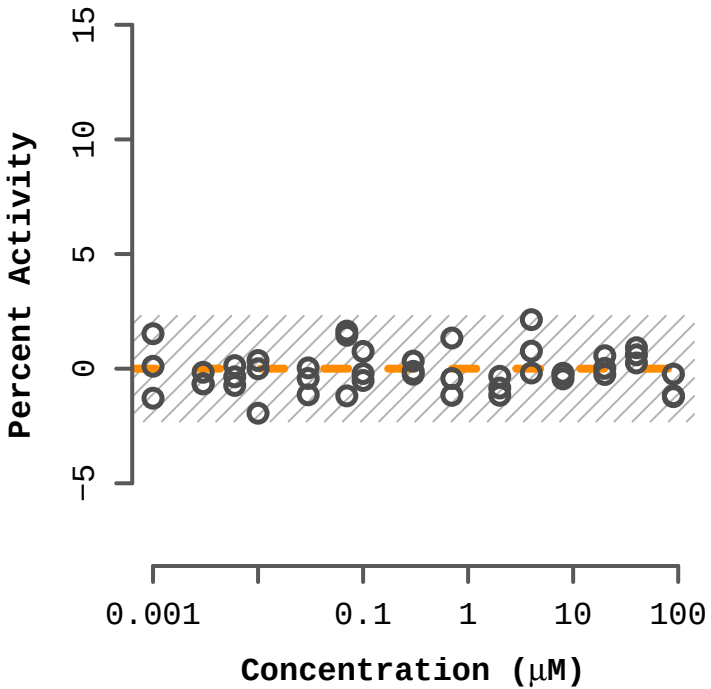
NAME: Methyl 2-chlorobenzoate
CHID: 44701 CASRN: 610-96-8
SPID(S): Tox21_302014
M4ID: 12477119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.32	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.0386 **MAX_MED:** 0.278 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

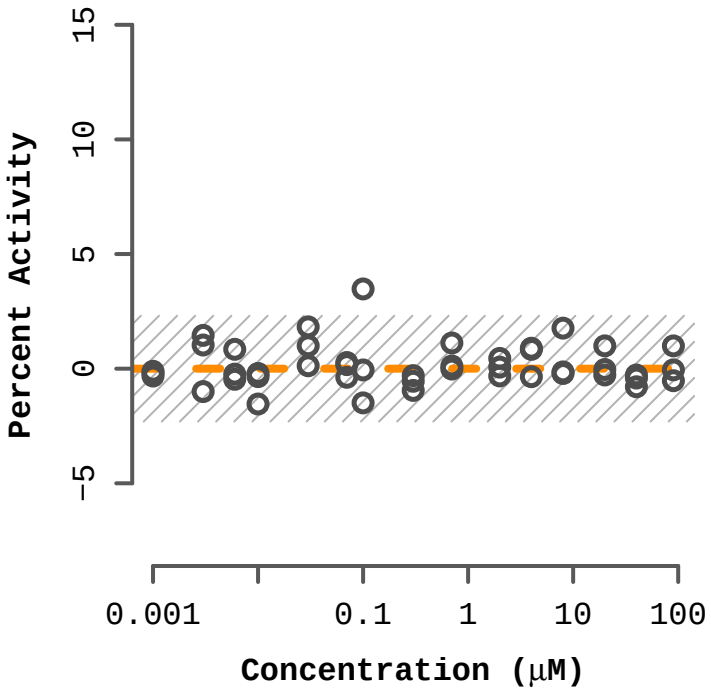
NAME: N-Benzyl-N-hydroxy-1-phenylmethanamine
CHID: 44702 **CASRN:** 621-07-8
SPID(S): Tox21_302001
M4ID: 12477132

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

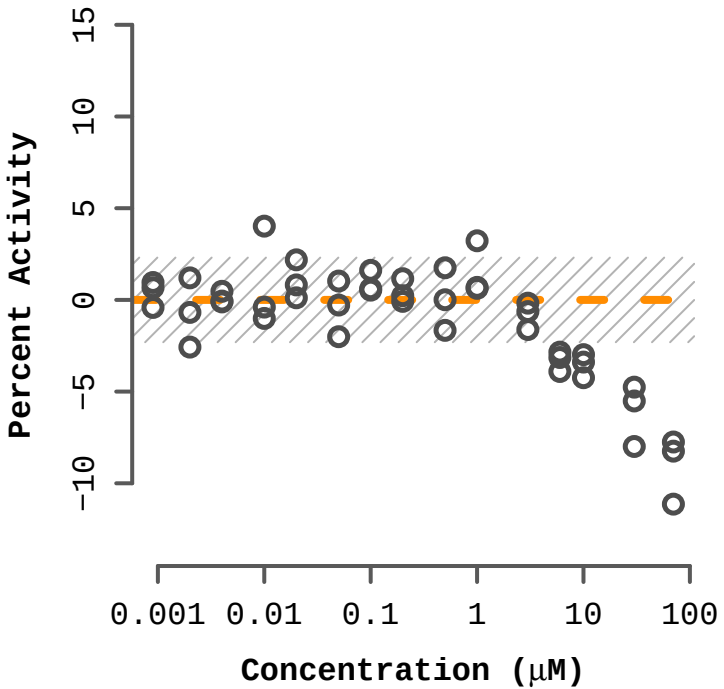
NAME: 4-Chlorobenzonitrile
CHID: 44703 **CASRN:** 623-03-0
SPID(S): Tox21_301477
M4ID: 12477656

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.985 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

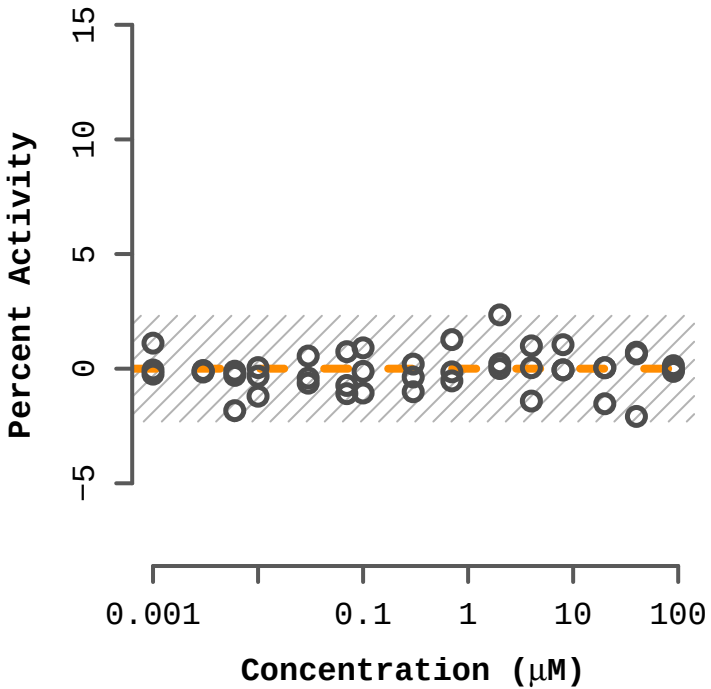
NAME: Bromocresol green sodium salt
CHID: 44704 **CASRN:** 62625-32-5
SPID(S): Tox21_301436
M4ID: 12477697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.82	NA	NA
PROB:	1	NA	NA
RMSE:	3.34	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

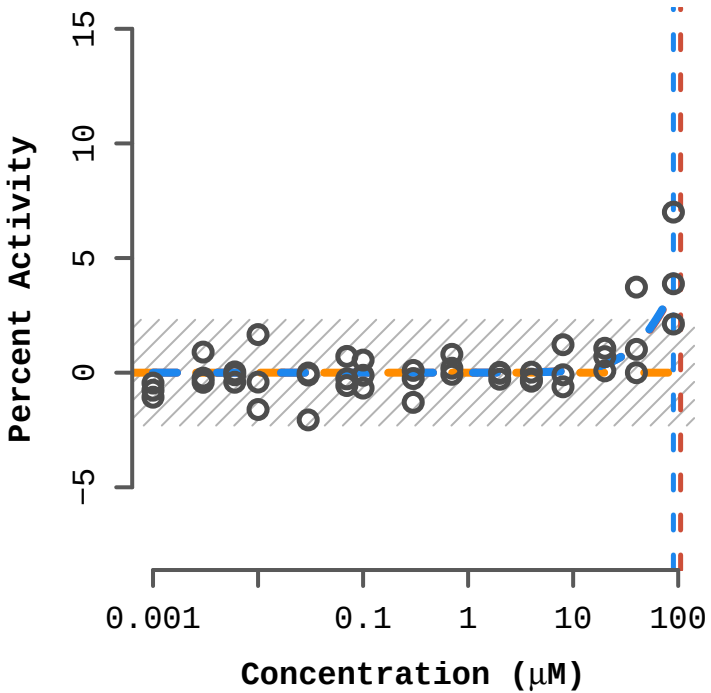
NAME: 1-(2-Aminoethyl)imidazolidin-2-one
CHID: 44706 CASRN: 6281-42-1
SPID(S): Tox21_301958
M4ID: 12477175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.857 MAX_MED: 0.646 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-(2,5-Dimethoxyphenyl)-3-oxobutanamide
CHID: 44709 CASRN: 6375-27-5
SPID(S): Tox21_302213
M4ID: 12476920

HILL MODEL (in red):

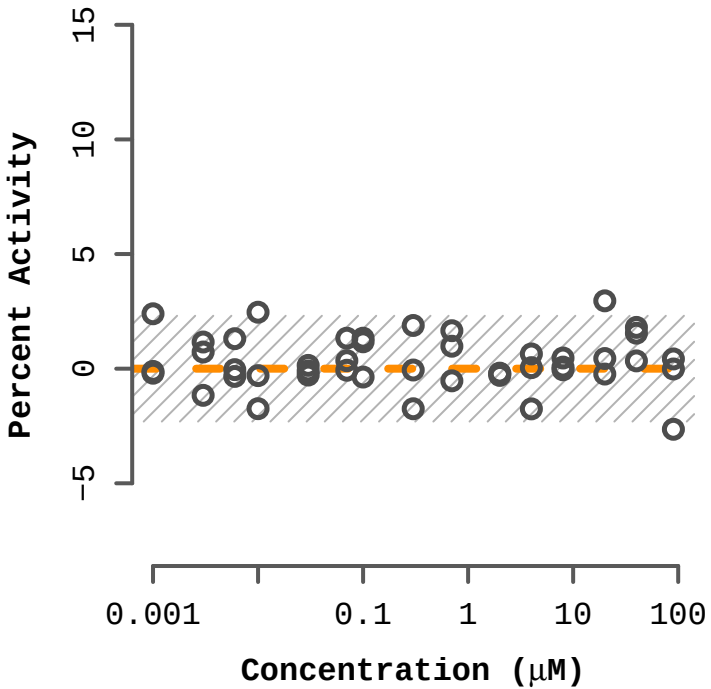
	tp	ga	gw
val:	8.41	2.02	1.85
sd:	11.5	0.579	0.94

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.21	1.95	1.96	3.79	5.91
sd:	9.25	0.551	1.08	78600	253000

	CNST	HILL	GNLS
AIC:	141.77	123.97	128.03
PROB:	0	0.88	0.12
RMSE:	1.52	0.96	0.96

MAX_MEAN: 4.34 MAX_MED: 3.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

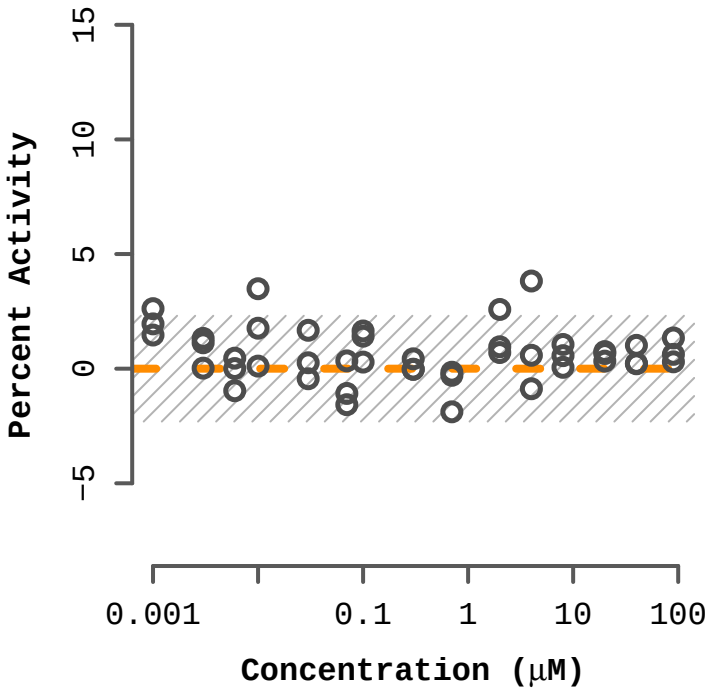
NAME: 2,6-Dichloro-3-methylaniline
CHID: 44710 **CASRN:** 64063-37-2
SPID(S): Tox21_302255
M4ID: 12476878

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

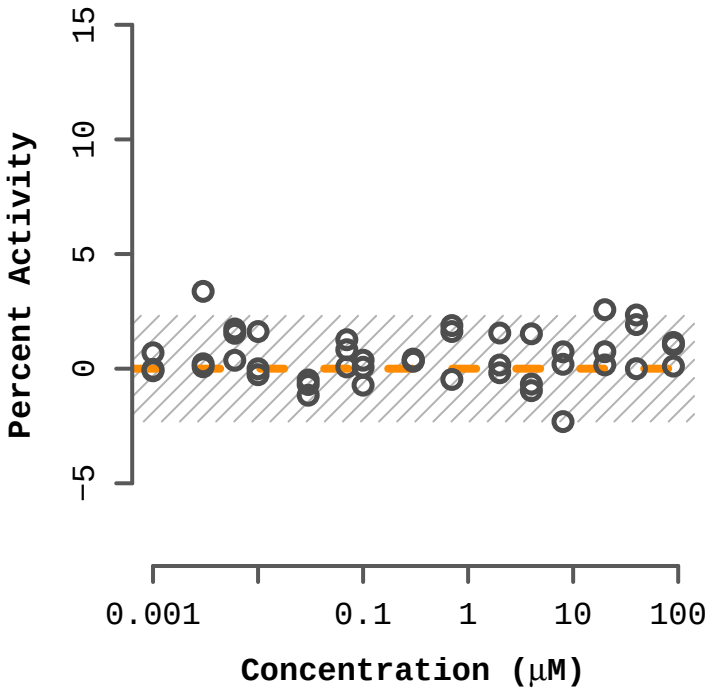
NAME: 1,4-Bis(methoxymethyl)benzene
CHID: 44712 **CASRN:** 6770-38-3
SPID(S): Tox21_301480
M4ID: 12477653

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

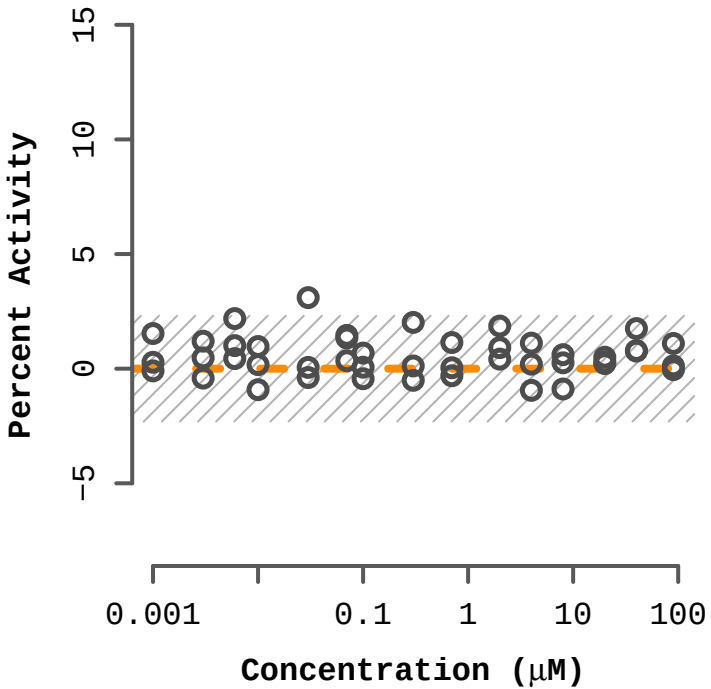
NAME: Acid Red 337
CHID: 44713 **CASRN:** 67786-14-5
SPID(S): Tox21_301899
M4ID: 12477234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

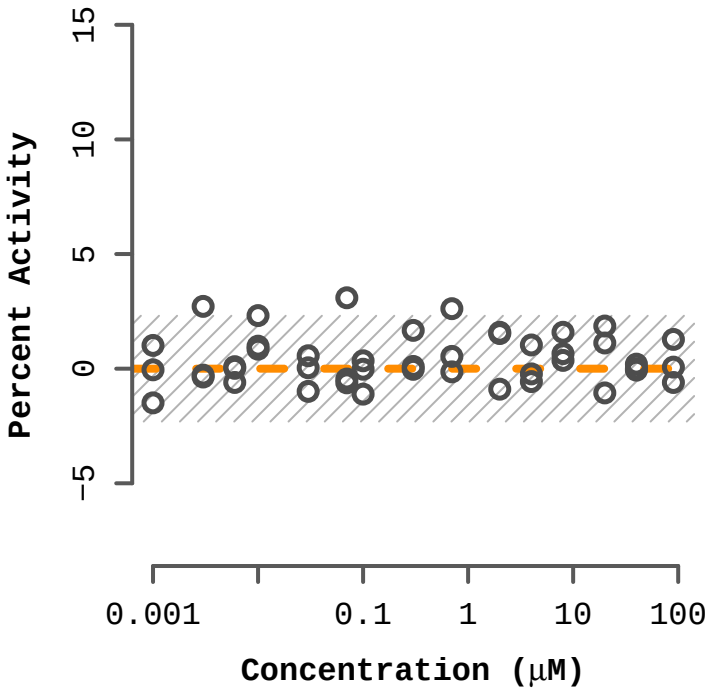
NAME: N2-(4-Nitrophenyl)-L-glutamine hydrochloride
CHID: 44714 CASRN: 67953-08-6
SPID(S): Tox21_302239
M4ID: 12476894

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.21 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

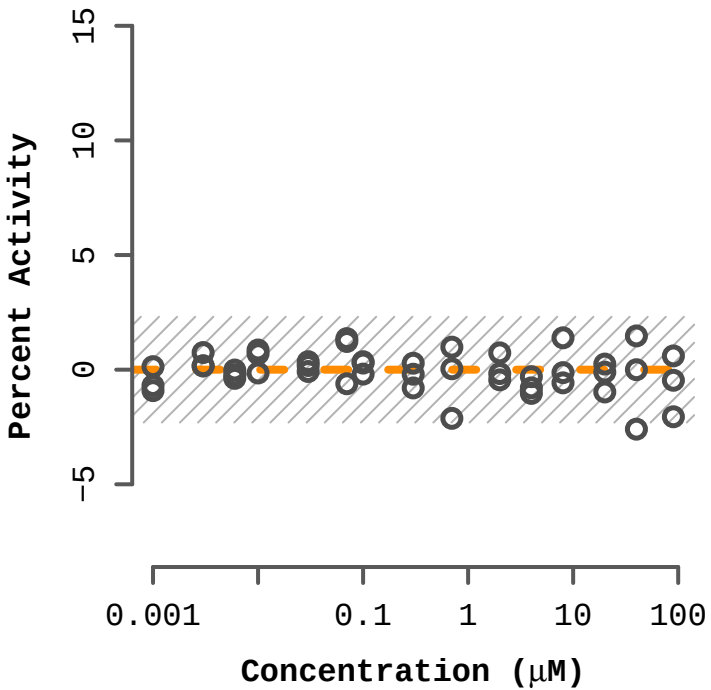
NAME: 2,2-Dimethyl-2,3-dihydro-1-benzofuran-7-amine
CHID: 44715 **CASRN:** 68298-46-4
SPID(S): Tox21_301957
M4ID: 12477176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

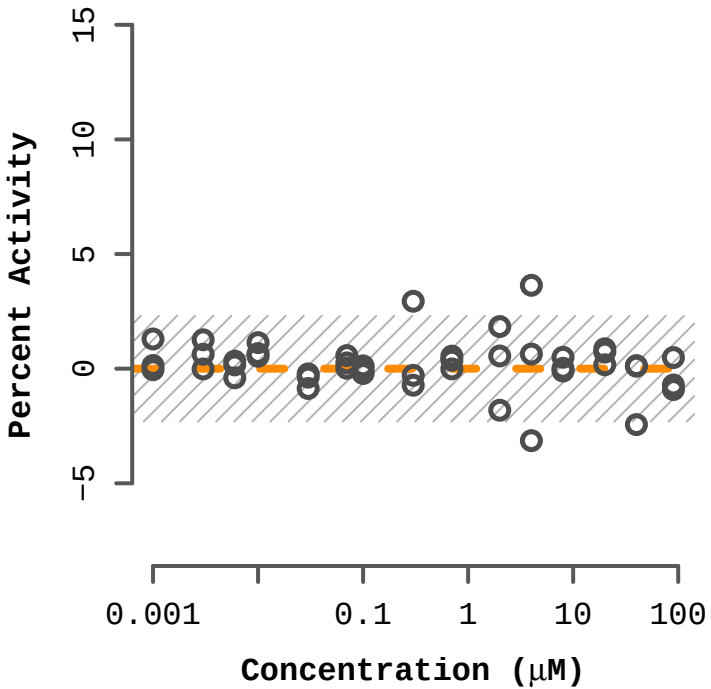
NAME: 1-Cyclohexylpyrrolidin-2-one
CHID: 44716 **CASRN:** 6837-24-7
SPID(S): Tox21_301467
M4ID: 12477666

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.658 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

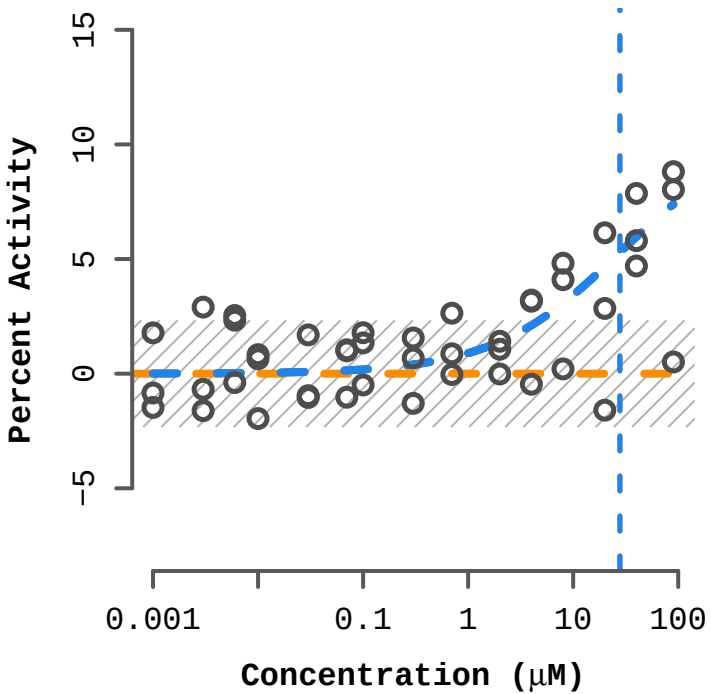
NAME: Dimethoxy(diphenyl)silane
CHID: 44717 **CASRN:** 6843-66-9
SPID(S): Tox21_303725
M4ID: 12475463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.78 **MAX_MED:** 0.726 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acid Orange 156
CHID: 44718 CASRN: 68555-86-2
SPID(S): Tox21_301885
M4ID: 12477248

HILL MODEL (in red):

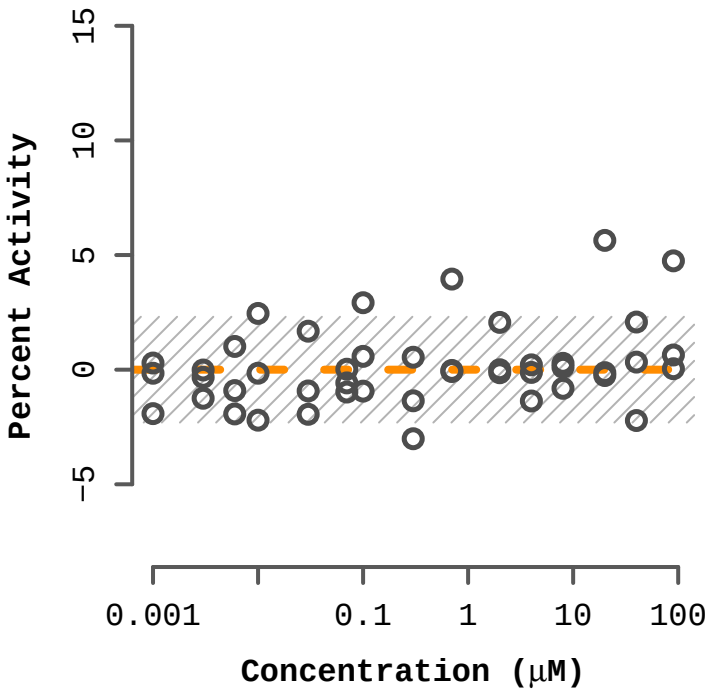
	tp	ga	gw
val:	10.6	1.45	0.716
sd:	4.81	0.616	0.265

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.6	1.44	0.716	3.04	7.2
sd:	4.81	0.617	0.265	904	5970

	CNST	HILL	GNLS
AIC:	226.64	192.63	196.63
PROB:	0	0.88	0.12
RMSE:	3.1	1.99	1.99

MAX_MEAN: 6.12 MAX_MED: 8.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

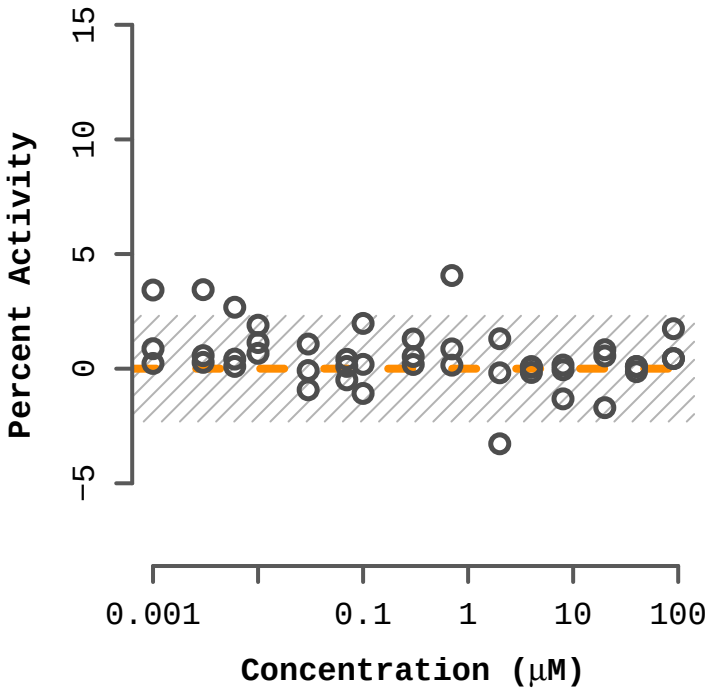
NAME: Dipropyl 3,4,5,6-tetrachlorobenzene-1,2-dicarb
CHID: 44719 **CASRN:** 6928-67-2
SPID(S): Tox21_301501
M4ID: 12477632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

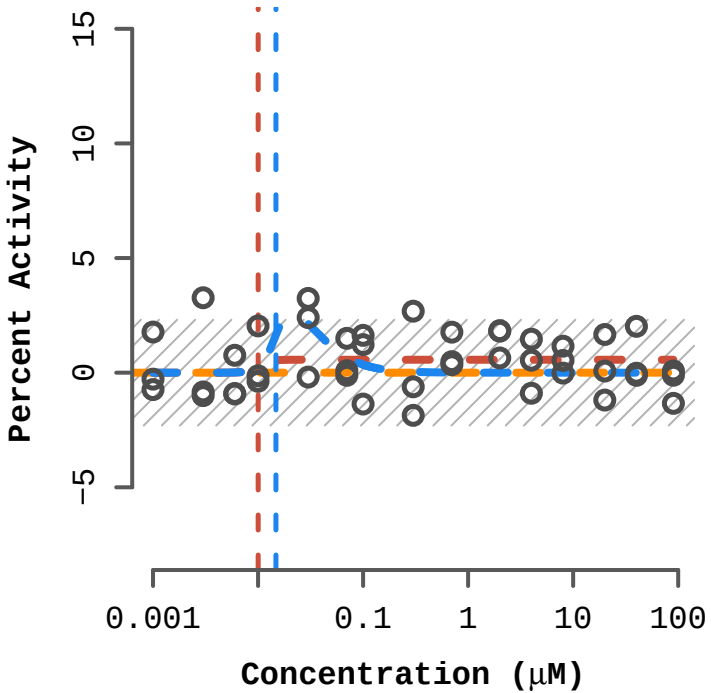
NAME: 4-Methylpyridin-2-amine
CHID: 44720 **CASRN:** 695-34-1
SPID(S): Tox21_301597
M4ID: 12477536

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Dimethylamino)-2-methylpropan-1-ol
CHID: 44721 CASRN: 7005-47-2
SPID(S): Tox21_301516
M4ID: 12477617

HILL MODEL (in red):

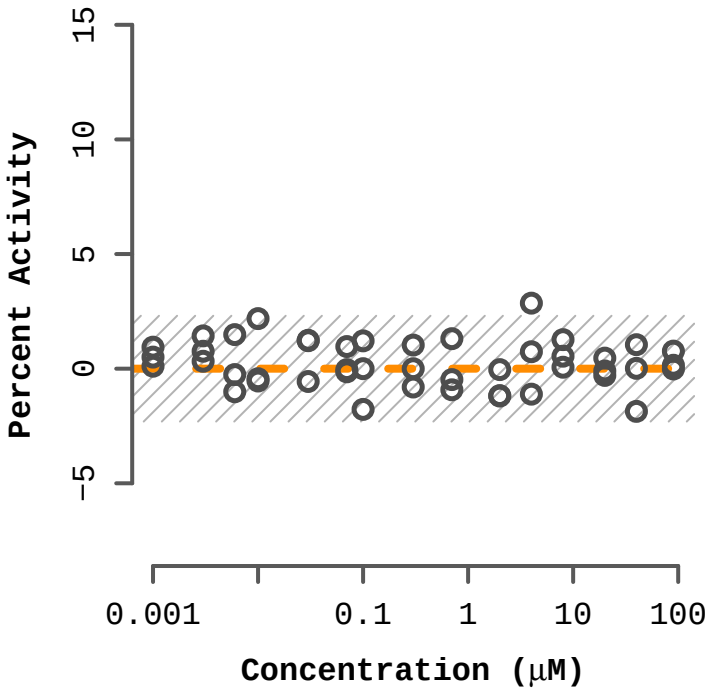
	tp	ga	gw
val:	0.564	-2	8
sd:	0.226	0.278	22.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.92	-1.83	6.6	-1.48	2.09
sd:	9.72	0.851	26.1	1.05	3.32

	CNST	HILL	GNLS
AIC:	160.38	160.2	164.56
PROB:	0.45	0.49	0.06
RMSE:	1.37	1.26	1.27

MAX_MEAN: 1.82 MAX_MED: 2.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

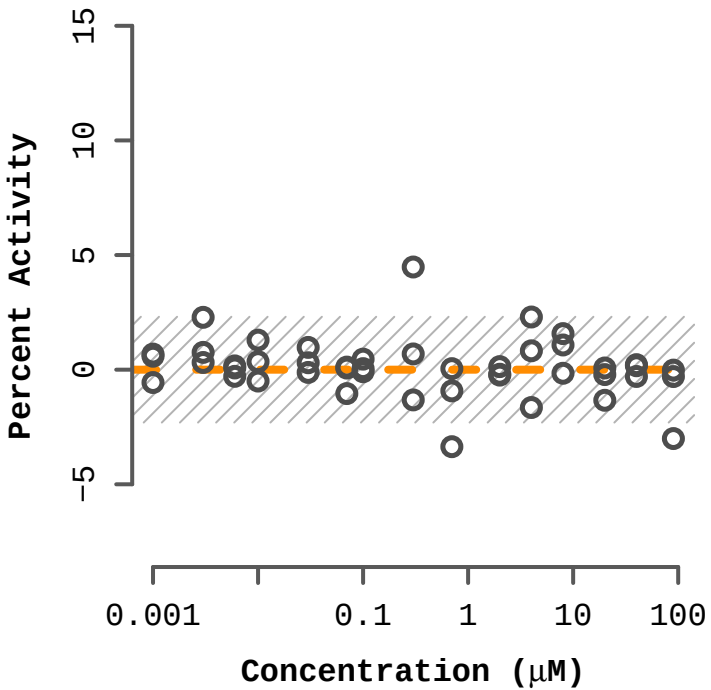
NAME: Potassium 4-[(3-oxobutanoyl)amino]benzenesulfo
CHID: 44722 CASRN: 70321-85-6
SPID(S): Tox21_301900
M4ID: 12477233

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.84 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

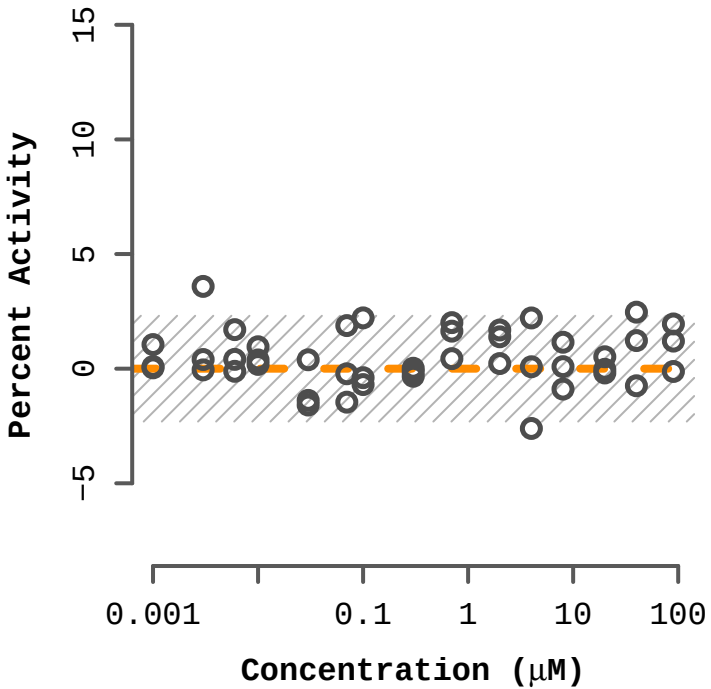
NAME: Aluminum hydroxide acetate (1:2:1)
CHID: 44723 CASRN: 7360-44-3
SPID(S): Tox21_302243
M4ID: 12476890

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

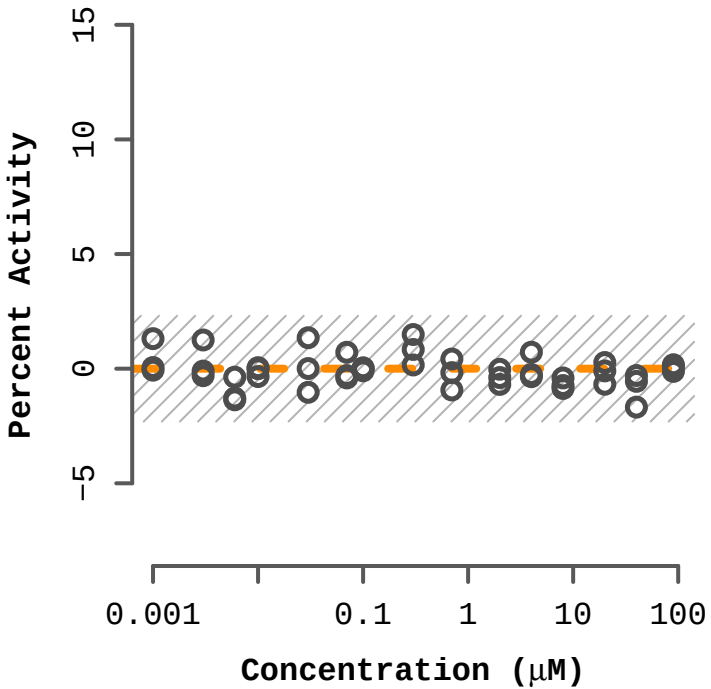
NAME: Aluminum triformate
CHID: 44724 **CASRN:** 7360-53-4
SPID(S): Tox21_302246
M4ID: 12476887

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

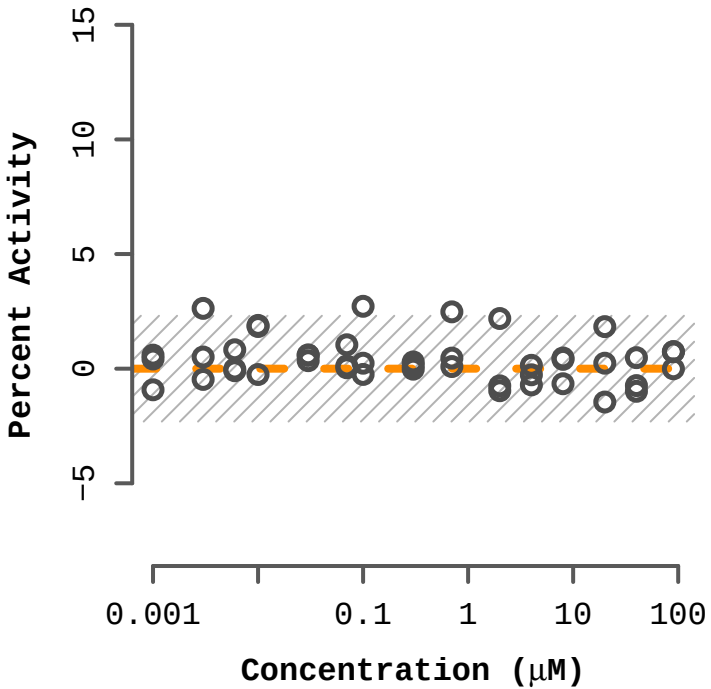
NAME: Butyl hydroxyacetate
CHID: 44725 **CASRN:** 7397-62-8
SPID(S): Tox21_301928
M4ID: 12477205

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.831 **MAX_MED:** 0.839 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

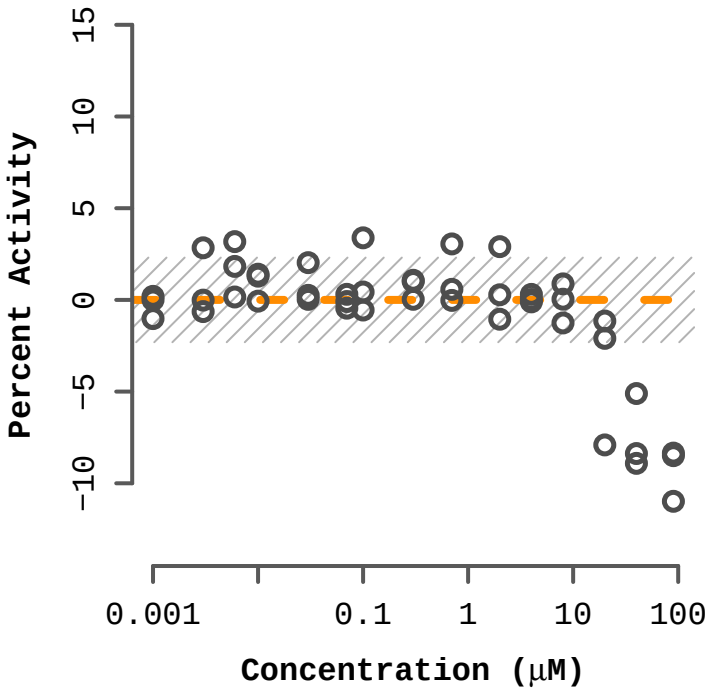
NAME: N-Cyclohexyl-N-methylcyclohexanamine
CHID: 44727 **CASRN:** 7560-83-0
SPID(S): Tox21_301508
M4ID: 12477625

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

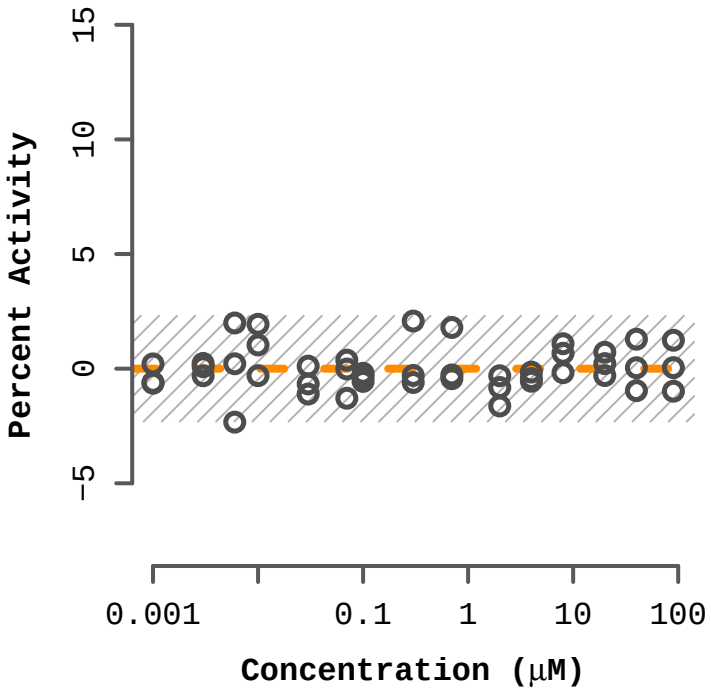
NAME: 3-[(3-Sulfanylpropanoyl)oxy]-2,2-bis{[(3-sulfa
CHID: 44728 **CASRN:** 7575-23-7
SPID(S): Tox21_301513
M4ID: 12477620

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.38	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

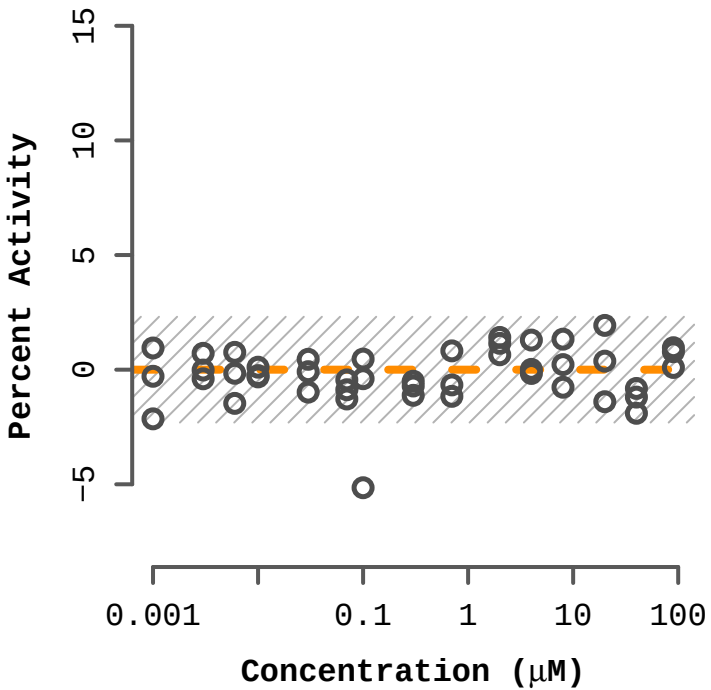
NAME: 1H-Benzo[de]isoquinoline-1,3(2H)-dione
CHID: 44731 CASRN: 81-83-4
SPID(S): Tox21_301585
M4ID: 12477548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.89 MAX_MED: 1.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

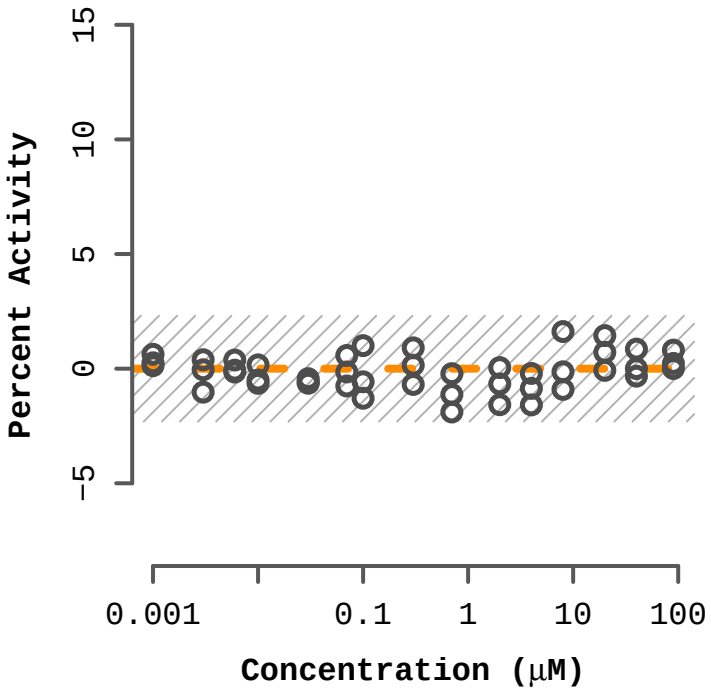
NAME: Phenylphosphonic dichloride
CHID: 44732 **CASRN:** 824-72-6
SPID(S): Tox21_301494
M4ID: 12477639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

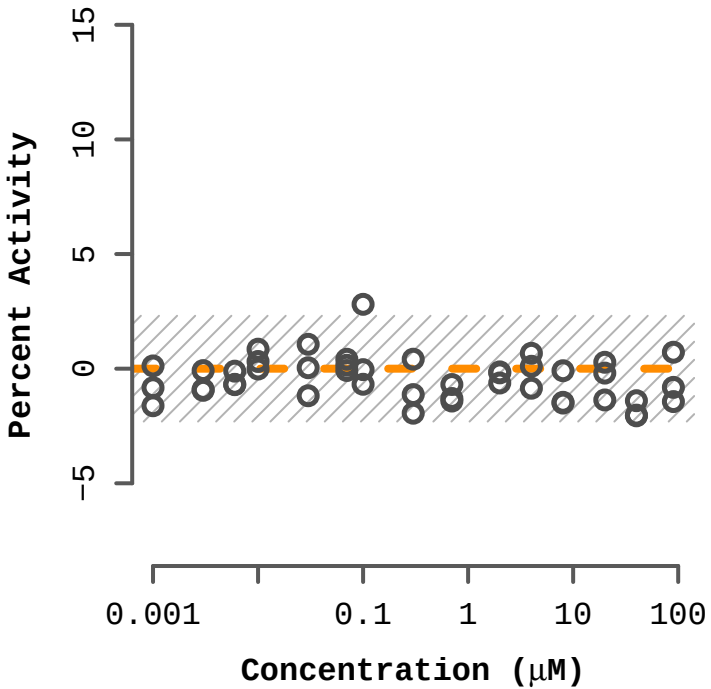
NAME: Sodium 3-nitrobenzoate
CHID: 44733 CASRN: 827-95-2
SPID(S): Tox21_301867
M4ID: 12477266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.695 MAX_MED: 0.712 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

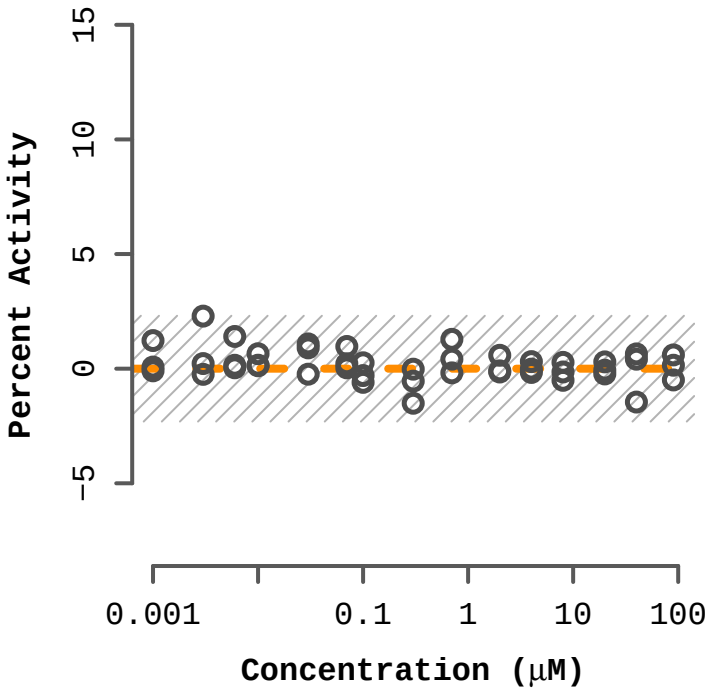
NAME: 2-[{2-[2-(Dimethylamino)ethoxy]ethyl}(methyl)a
CHID: 44734 CASRN: 83016-70-0
SPID(S): Tox21_301511
M4ID: 12477622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.696 MAX_MED: 0.316 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

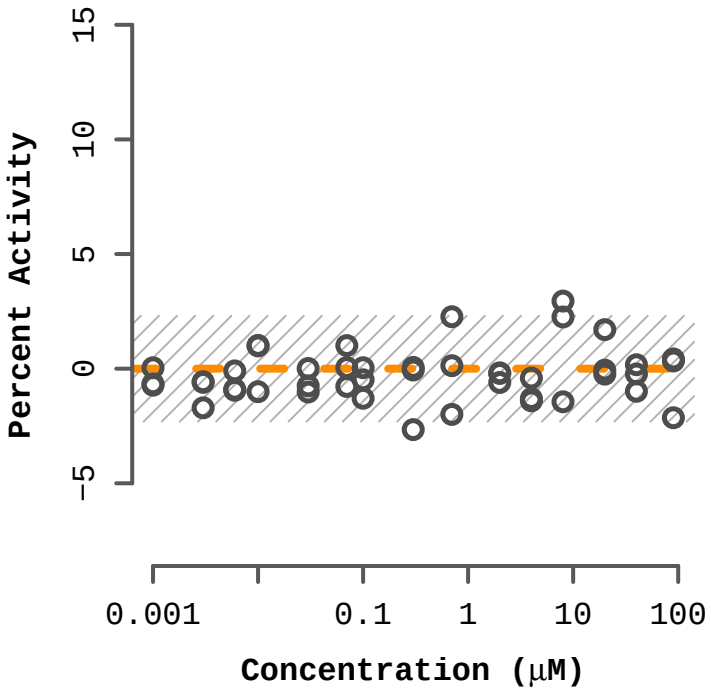
NAME: Disodium benzene-1,3-disulfonate
CHID: 44735 CASRN: 831-59-4
SPID(S): Tox21_301506
M4ID: 12477627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.757 MAX_MED: 0.909 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

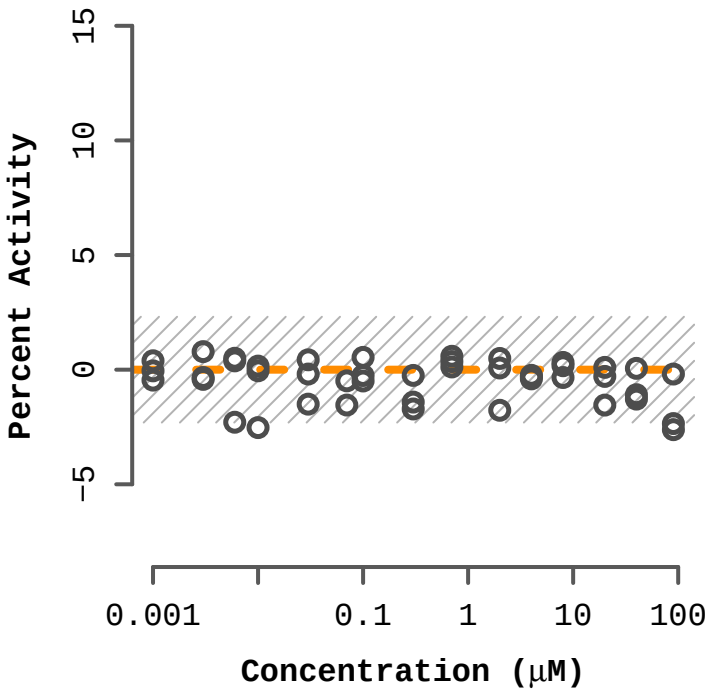
NAME: 4-(2,5-Diethoxy-4-nitrophenyl)morpholine
CHID: 44737 **CASRN:** 86-16-8
SPID(S): Tox21_301452
M4ID: 12477681

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 2.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

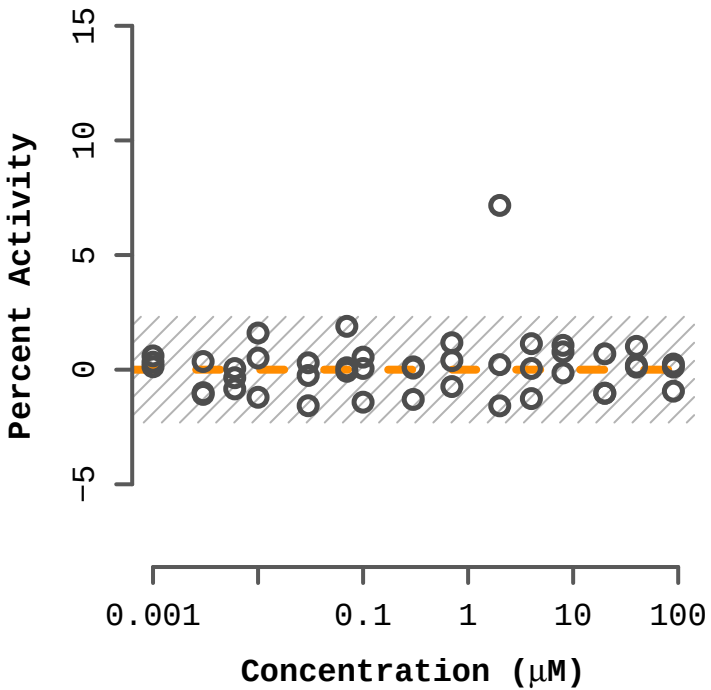
NAME: Ethyl 5-oxo-1-phenyl-4,5-dihydro-1H-pyrazole-3·
CHID: 44738 **CASRN:** 89-33-8
SPID(S): Tox21_301999
M4ID: 12477134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.354 **MAX_MED:** 0.385 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

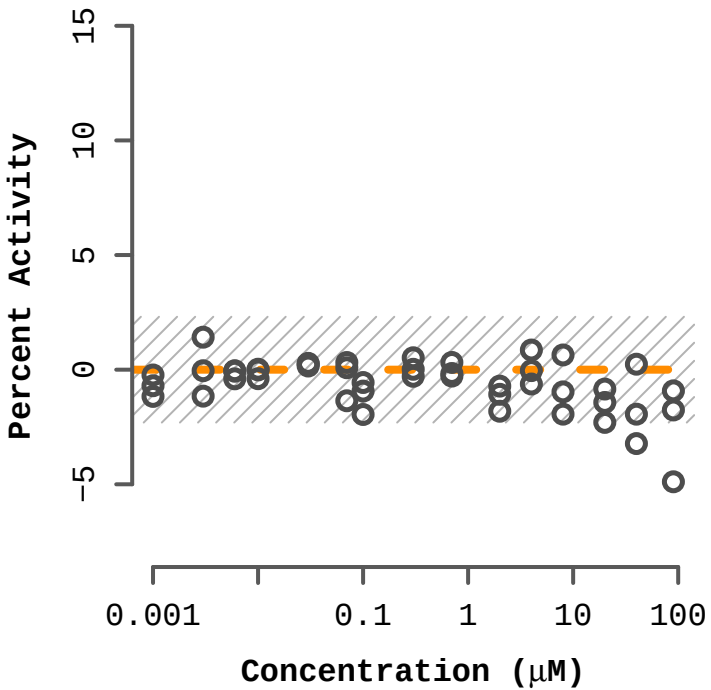
NAME: Dipropan-2-yl butanedioate
CHID: 44740 **CASRN:** 924-88-9
SPID(S): Tox21_301541
M4ID: 12477592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 0.779 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

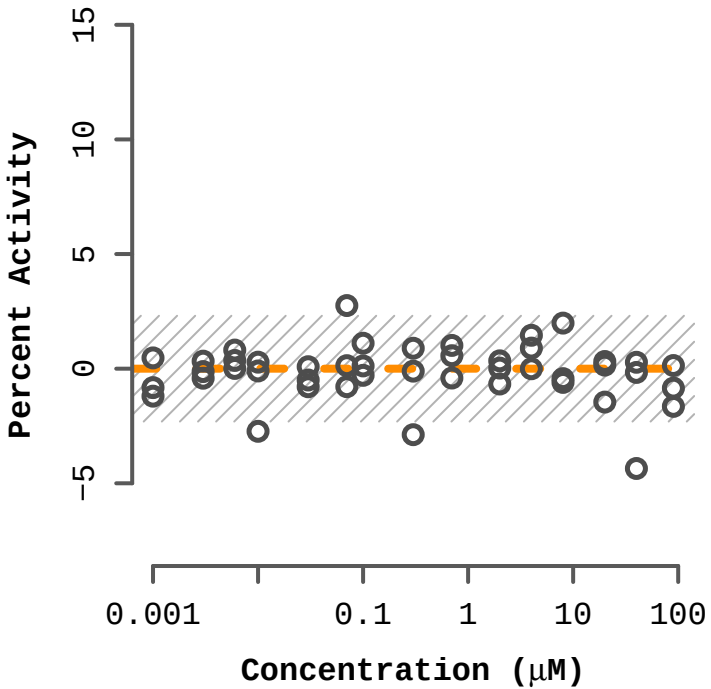
NAME: 2,2'−[Ethane−1,2−diylbis(oxy)]diethanamine
CHID: 44742 **CASRN:** 929−59−9
SPID(S): Tox21_301518
M4ID: 12477615

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.23 **MAX_MED:** 0.253 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

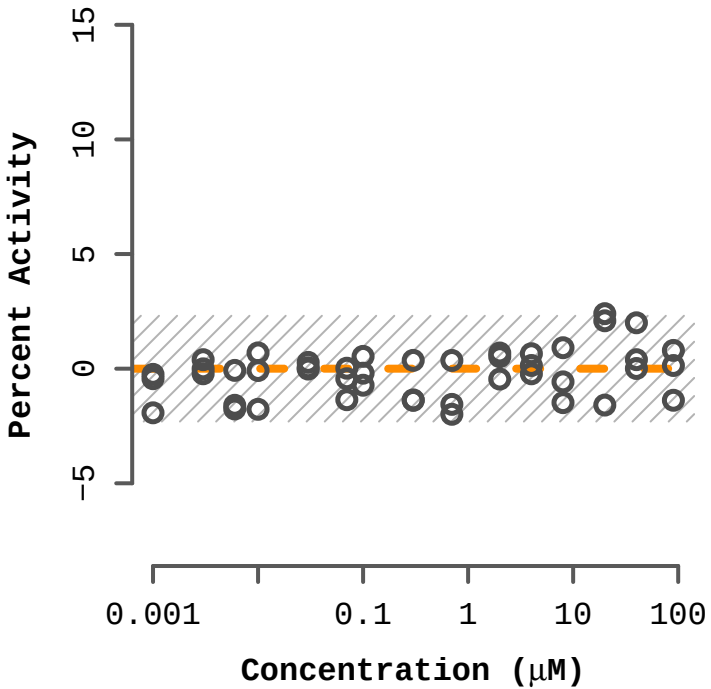
NAME: 6-Aminonaphthalene-2-sulfonic acid
CHID: 44743 **CASRN:** 93-00-5
SPID(S): Tox21_301505
M4ID: 12477628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.785 **MAX_MED:** 0.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

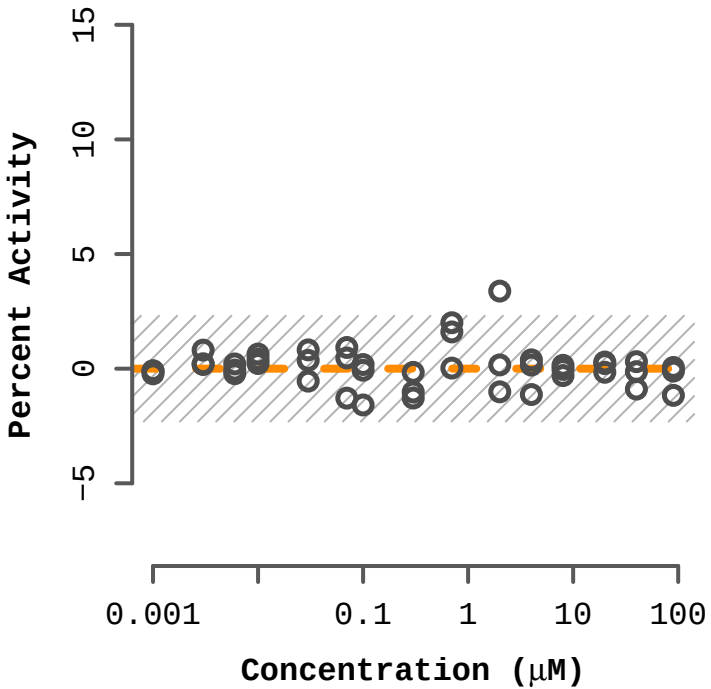
NAME: 2-Ethyl-4-methyl-1H-imidazole
CHID: 44744 **CASRN:** 931-36-2
SPID(S): Tox21_301485
M4ID: 12477648

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.969 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

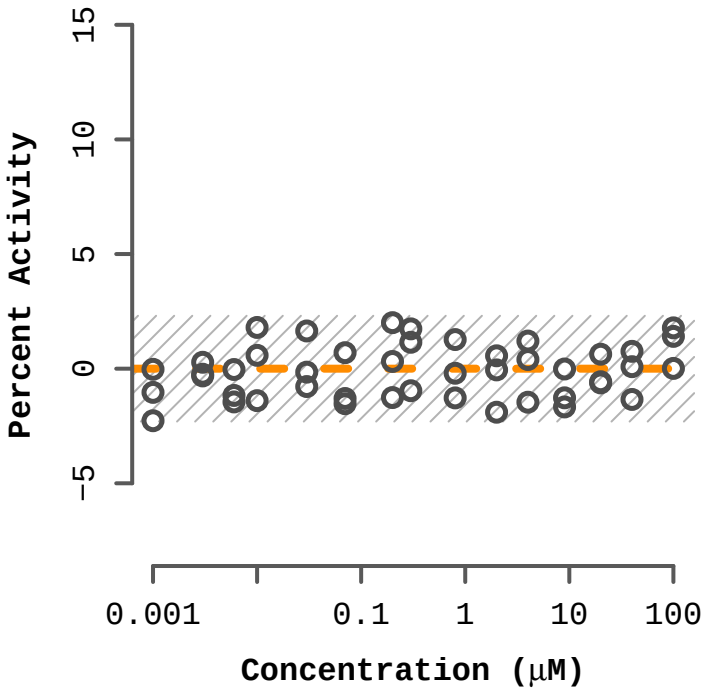
NAME: 2,2,4,4-Tetramethylcyclobutane-1,3-dione
CHID: 44745 **CASRN:** 933-52-8
SPID(S): Tox21_301434
M4ID: 12477699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

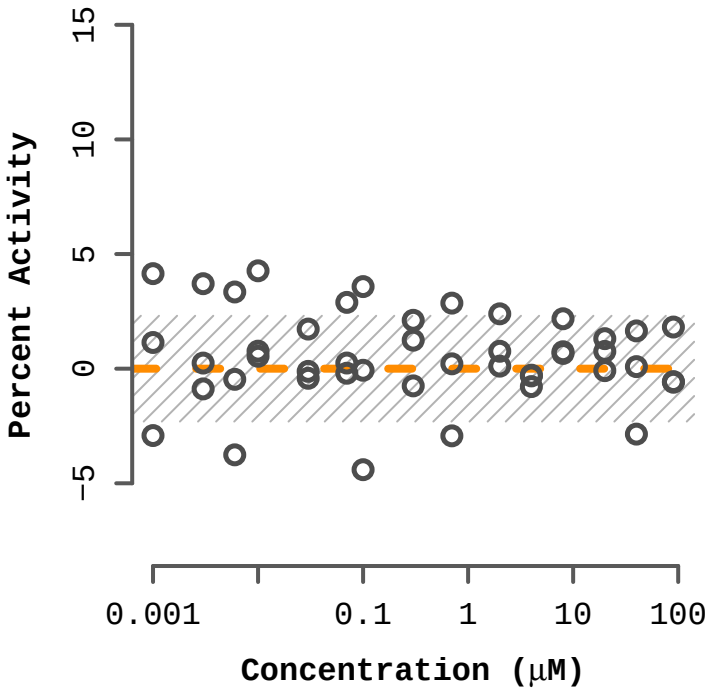
NAME: Propan-2-yl benzoate
CHID: 44746 **CASRN:** 939-48-0
SPID(S): Tox21_301496
M4ID: 12477637

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

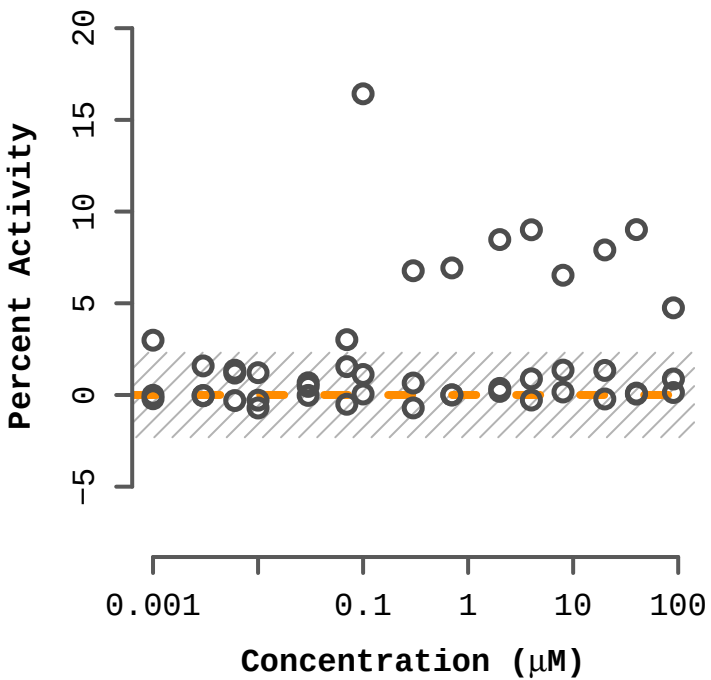
NAME: N-Butylphosphorothioic triamide
CHID: 44747 CASRN: 94317-64-3
SPID(S): Tox21_302015
M4ID: 12477118

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 1.86 MAX_MED: 1.24 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

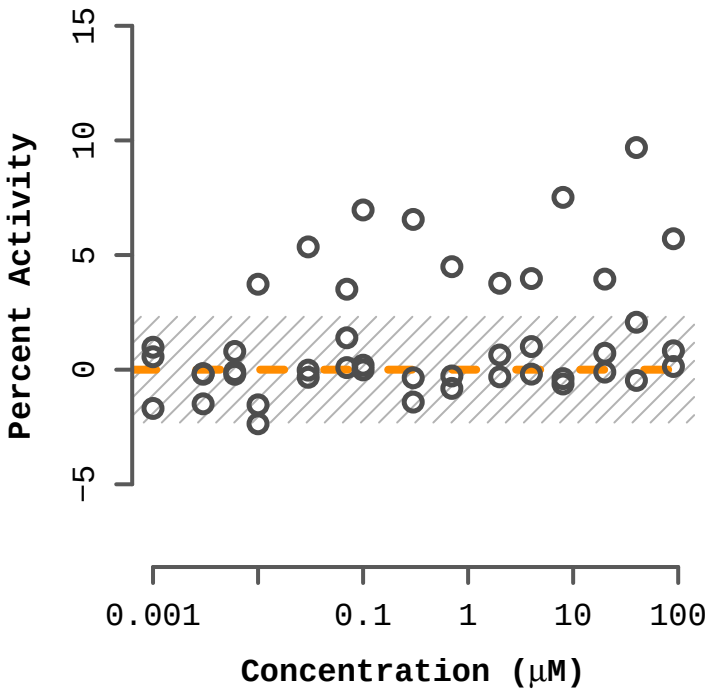
NAME: (1-Hydroxycyclohexyl)(phenyl)methanone
CHID: 44748 CASRN: 947-19-3
SPID(S): Tox21_301462
M4ID: 12477671

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	236.3	NA	NA
PROB:	1	NA	NA
RMSE:	4.12	NA	NA

MAX_MEAN: 5.87 MAX_MED: 1.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

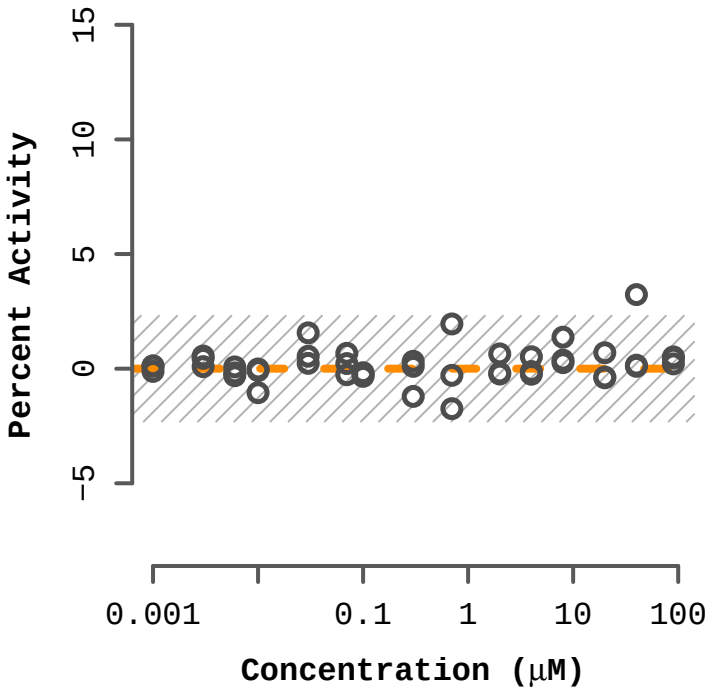
NAME: 4-Methoxy-2-nitroaniline
CHID: 44750 **CASRN:** 96-96-8
SPID(S): Tox21_301596
M4ID: 12477537

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.12	NA	NA
PROB:	1	NA	NA
RMSE:	3.07	NA	NA

MAX_MEAN: 3.76 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

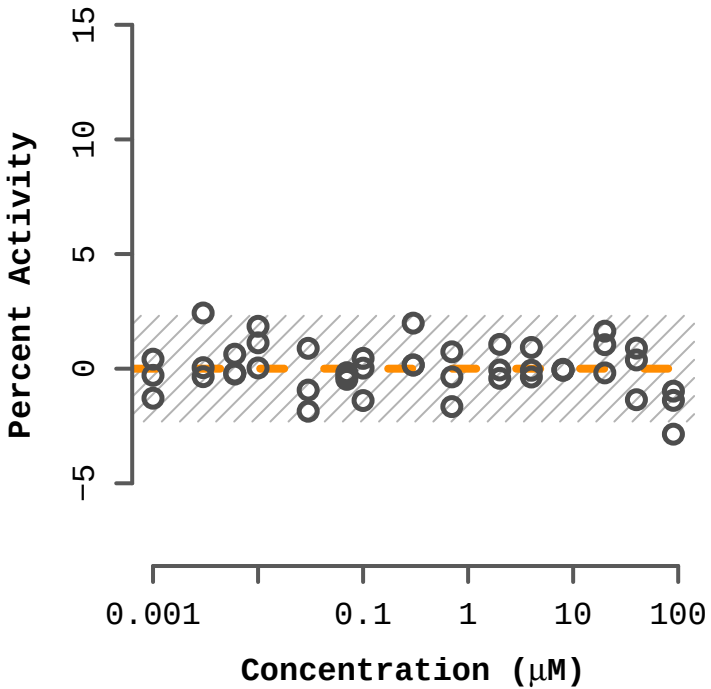
NAME: 2-Aminobenzene-1,4-disulfonic acid
CHID: 44751 **CASRN:** 98-44-2
SPID(S): Tox21_301960
M4ID: 12477173

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.545 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

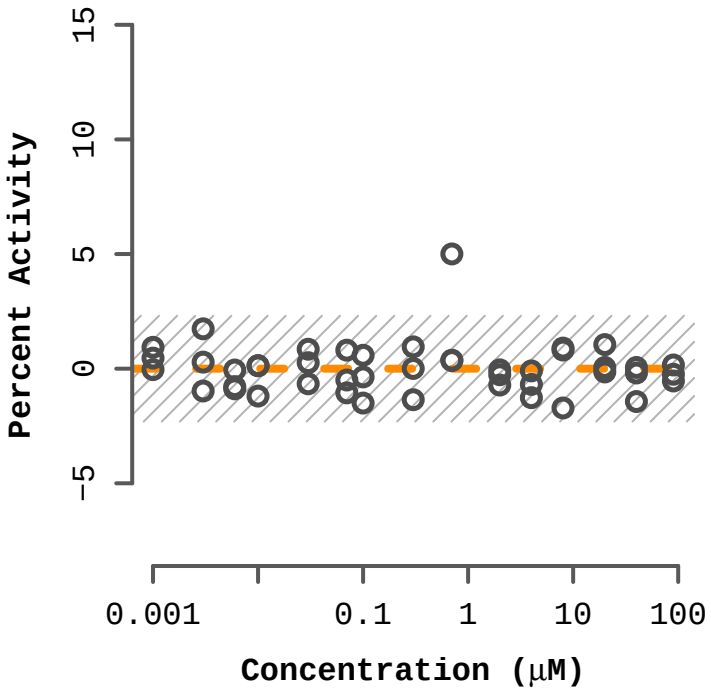
NAME: Diprop-2-en-1-yl (2Z)-but-2-enedioate
CHID: 44752 **CASRN:** 999-21-3
SPID(S): Tox21_301470
M4ID: 12477663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

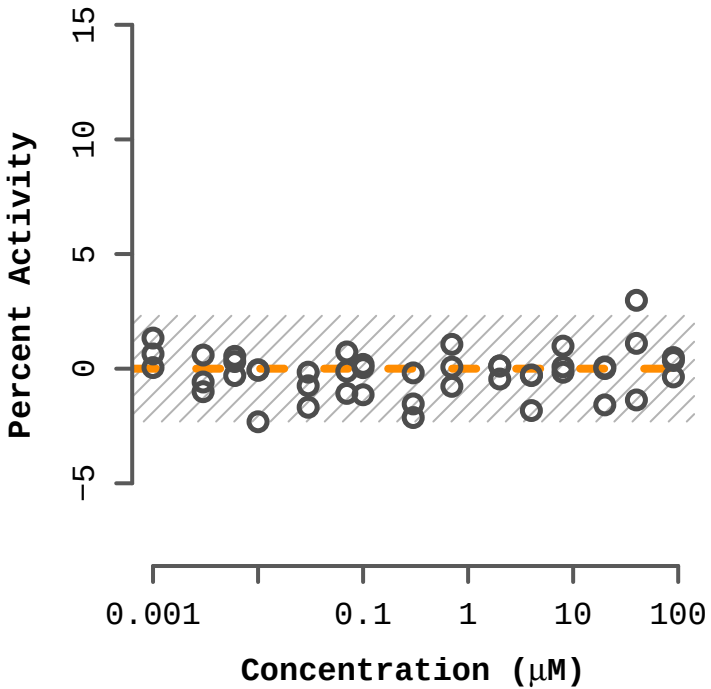
NAME: 2,6-Dimethylhept-5-enal
CHID: 44753 **CASRN:** 106-72-9
SPID(S): Tox21_300941
M4ID: 12478192

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 0.814 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

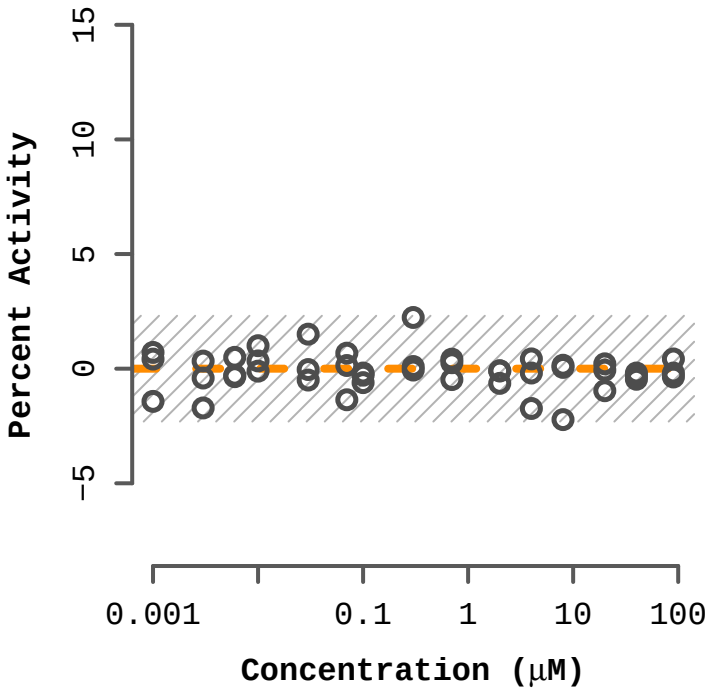
NAME: Prop-2-en-1-yl heptanoate
CHID: 44754 **CASRN:** 142-19-8
SPID(S): Tox21_301779
M4ID: 12477354

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.908 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

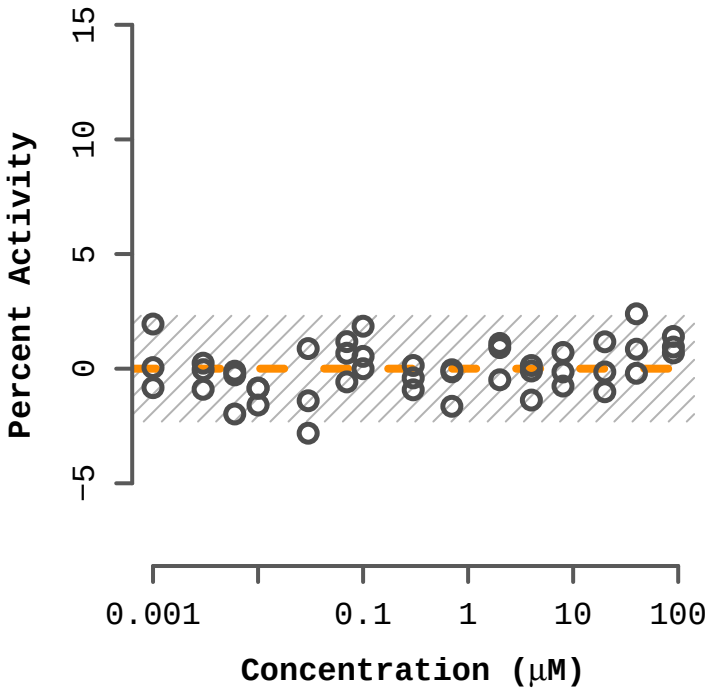
NAME: Prop-2-en-1-yl 3-cyclohexylpropanoate
CHID: 44755 **CASRN:** 2705-87-5
SPID(S): Tox21_301782
M4ID: 12477351

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.757 **MAX_MED:** 0.419 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

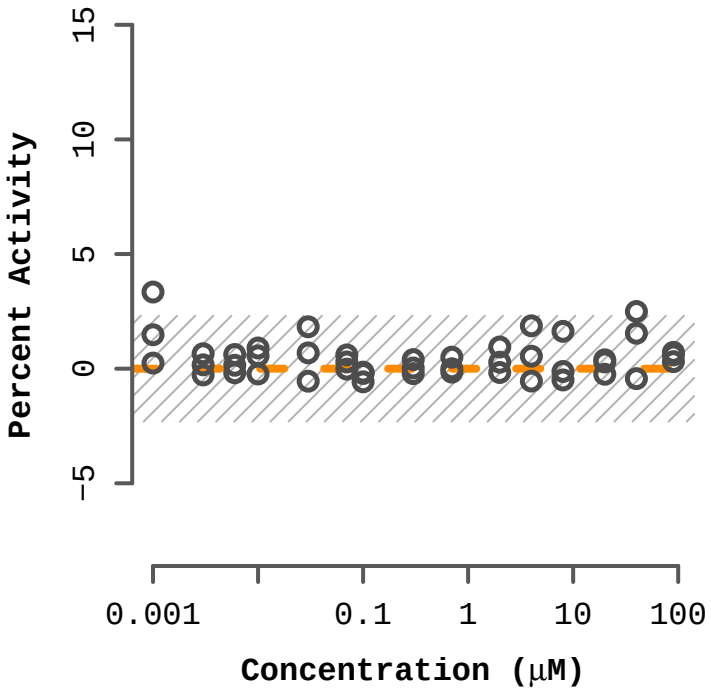
NAME: [(1R)−2,2,3−Trimethylcyclopent−3−en−1−yl]aceta
CHID: 44756 **CASRN:** 4501−58−0
SPID(S): Tox21_301648
M4ID: 12477485

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.944 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

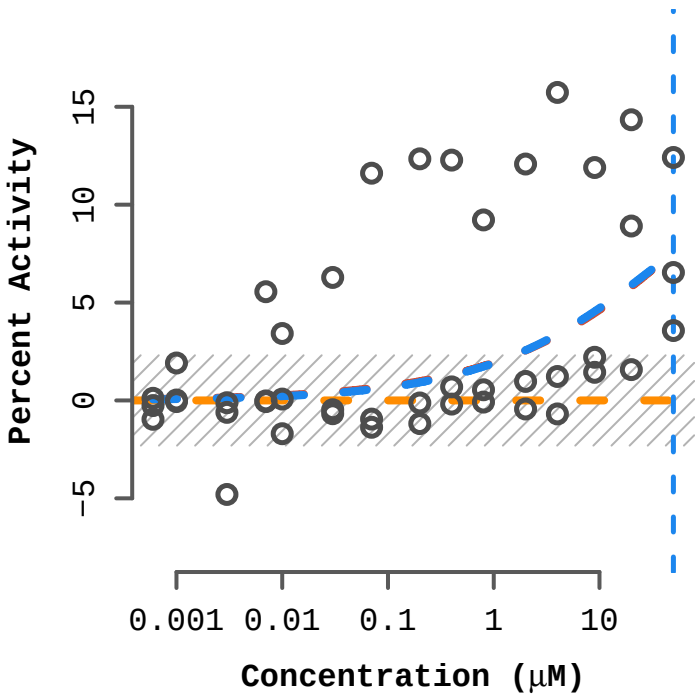
NAME: 3-Methylbutyl 3-methylbutanoate
CHID: 44757 **CASRN:** 659-70-1
SPID(S): Tox21_301620
M4ID: 12477513

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluvastatin sodium
CHID: 44758 CASRN: 93957-55-2
SPID(S): Tox21_112226_1
M4ID: 12483221

HILL MODEL (in red):

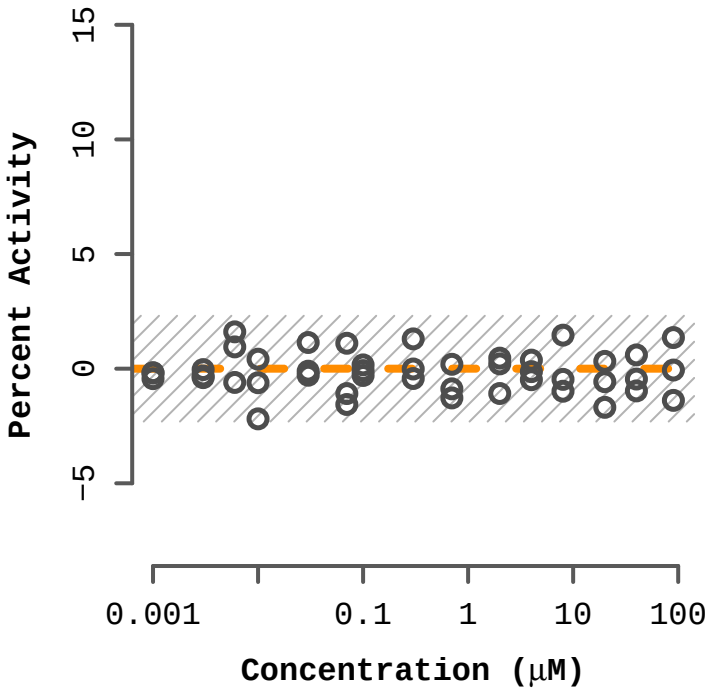
	tp	ga	gw
val:	18.9	2.08	0.454
sd:	47.3	4.15	0.396

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.2	1.7	0.497	3.67	1.05
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	286.34	273.54	277.56
PROB:	0	0.88	0.12
RMSE:	6.12	4.81	4.81

MAX_MEAN: 8.28 **MAX_MED:** 8.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

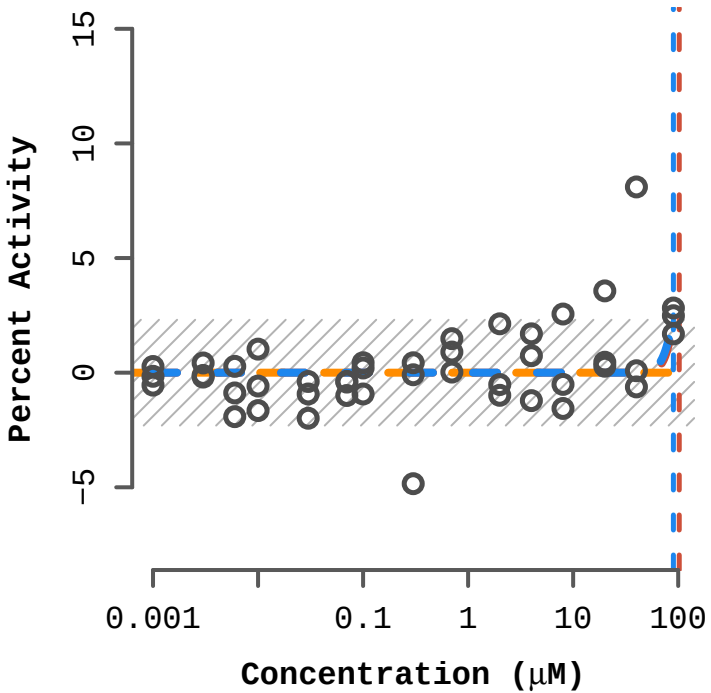
NAME: 1,1,3,3,5,5,7,7-Octamethyltetrasiloxane
CHID: 44759 **CASRN:** 1000-05-1
SPID(S): Tox21_300728
M4ID: 12478405

HILL MODEL: Not applicable.

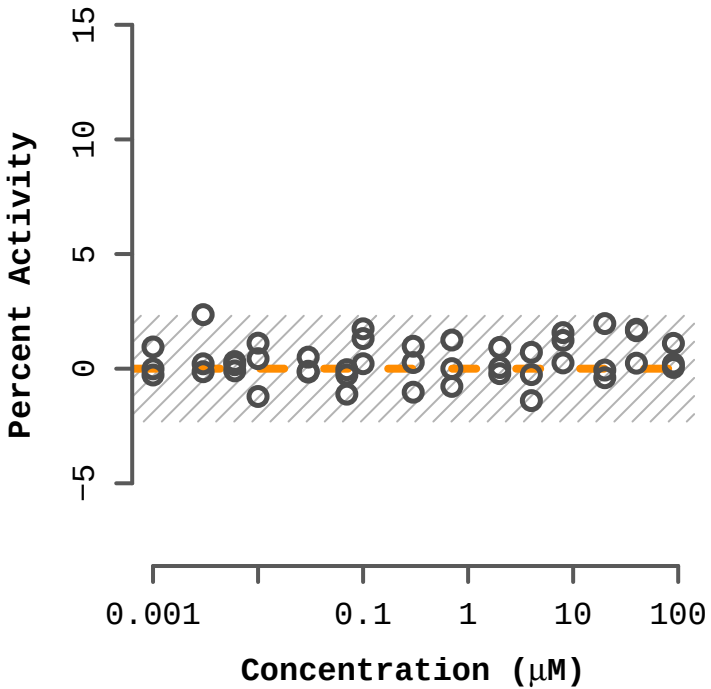
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.654 **MAX_MED:** 0.952 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Neodymium(III) chloride
CHID:    44760   CASRN: 10024-93-8
SPID(S): Tox21_300646
M4ID:    12478487

HILL MODEL (in red):
      tp       ga       gw
val:  8.78     2.01     7.9
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.69     1.95     7.62     3.95     15.5
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  171.64      166.51      170.51
PROB: 0.06        0.82        0.11
RMSE: 1.88        1.78        1.78

MAX_MEAN: 2.52      MAX_MED: 2.49      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triethoxy[2-(7-oxabicyclo[4.1.0]hept-3-yl)ethy

CHID: 44762 **CASRN:** 10217-34-2

SPID(S): Tox21_300751

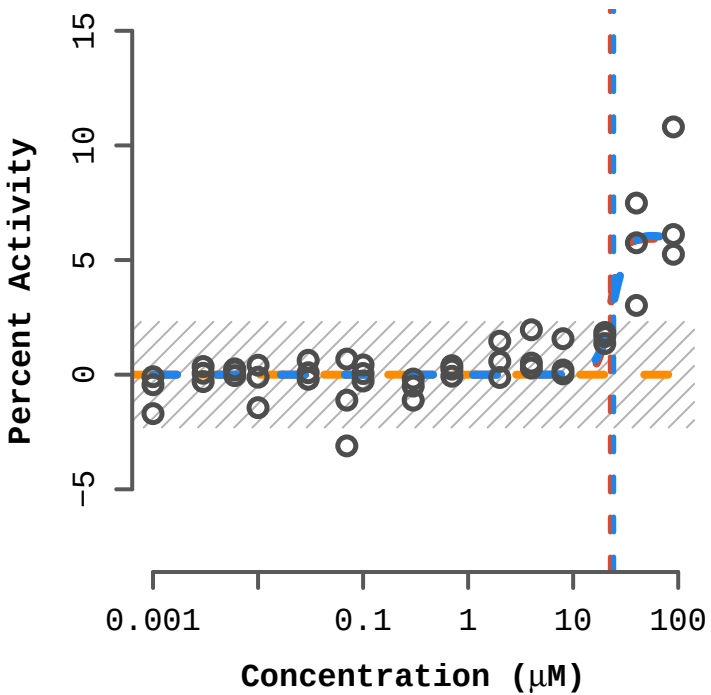
M4ID: 12478382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Parbenate
CHID: 44763 CASRN: 10287-53-3
SPID(S): Tox21_300913
M4ID: 12478220

HILL MODEL (in red):

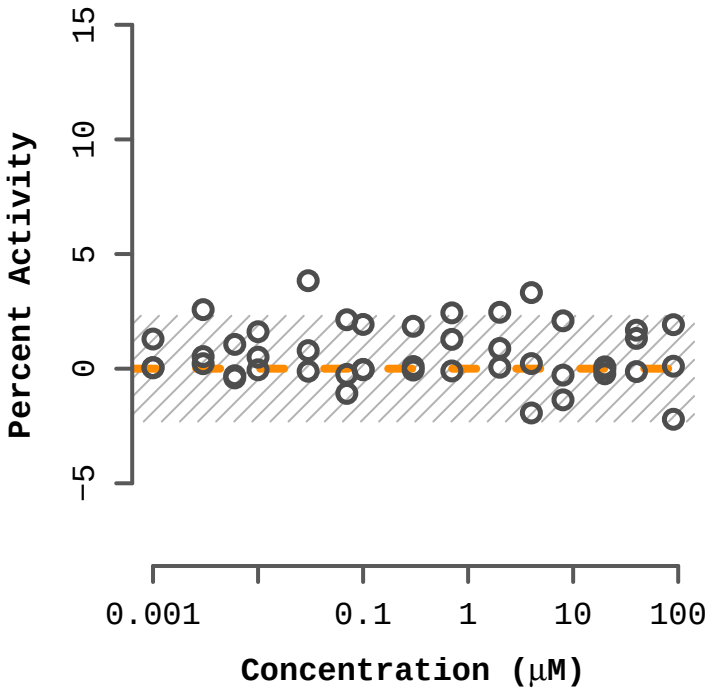
	tp	ga	gw
val:	5.93	1.35	8
sd:	0.436	0.0767	11.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.48	1.39	5.5	3.91	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	191.66	133.31	137.25
PROB:	0	0.88	0.12
RMSE:	2.65	1.19	1.19

MAX_MEAN: 7.39 MAX_MED: 6.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

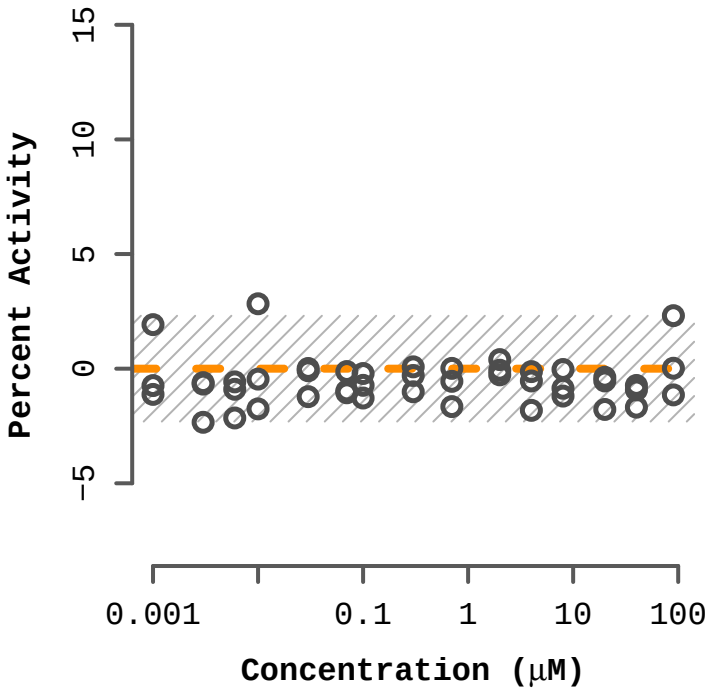
NAME: 2-Phenylethyl 2-methylpropanoate
CHID: 44764 **CASRN:** 103-48-0
SPID(S): Tox21_301122
M4ID: 12478011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

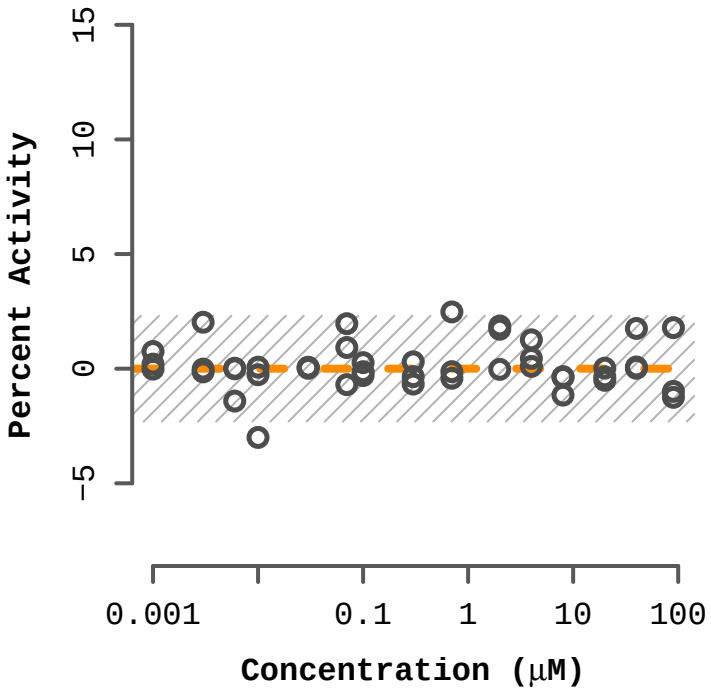
NAME: 3-Phenylprop-2-en-1-yl acetate
CHID: 44765 **CASRN:** 103-54-8
SPID(S): Tox21_301043
M4ID: 12478090

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.397 **MAX_MED:** 0.0198 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

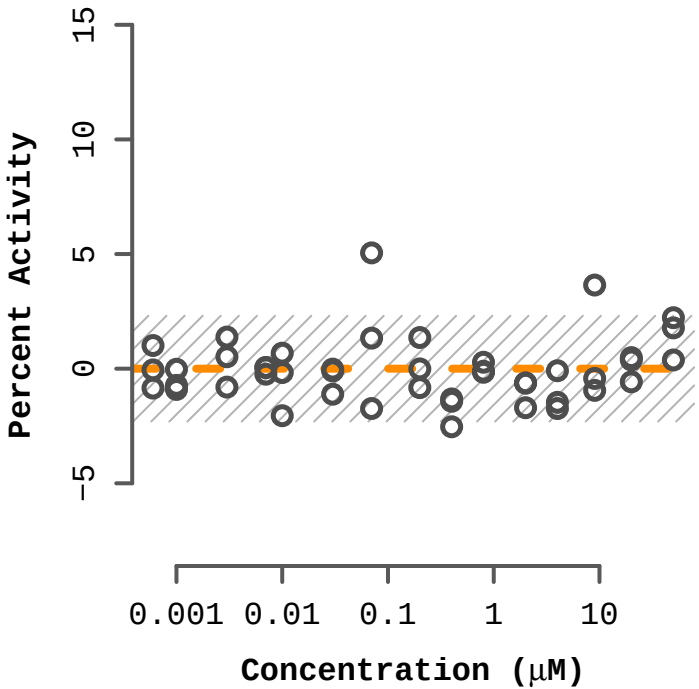
NAME: 2-(Pyridin-2-yl)ethanol
CHID: 44767 **CASRN:** 103-74-2
SPID(S): Tox21_300936
M4ID: 12478197

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

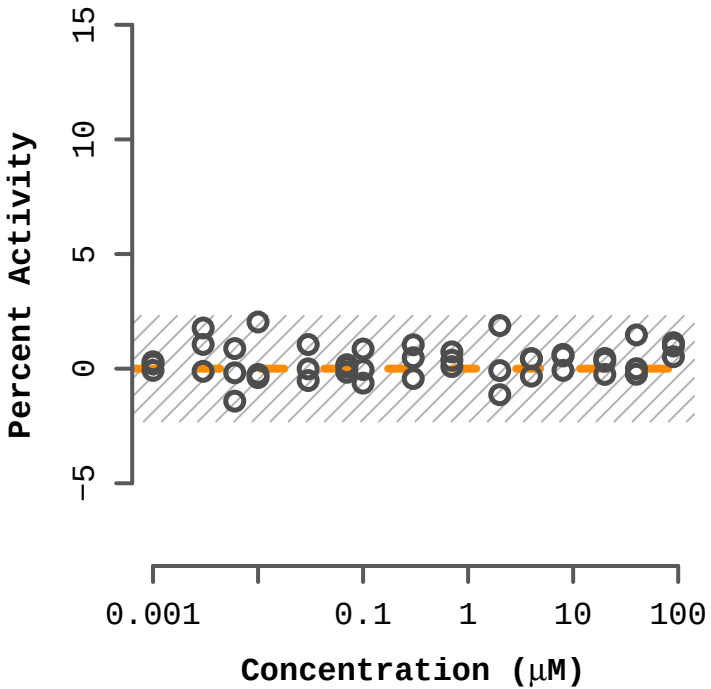
NAME: 8-Bromotheophylline
CHID: 44768 **CASRN:** 10381-75-6
SPID(S): Tox21_112559_1
M4ID: 12483033

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

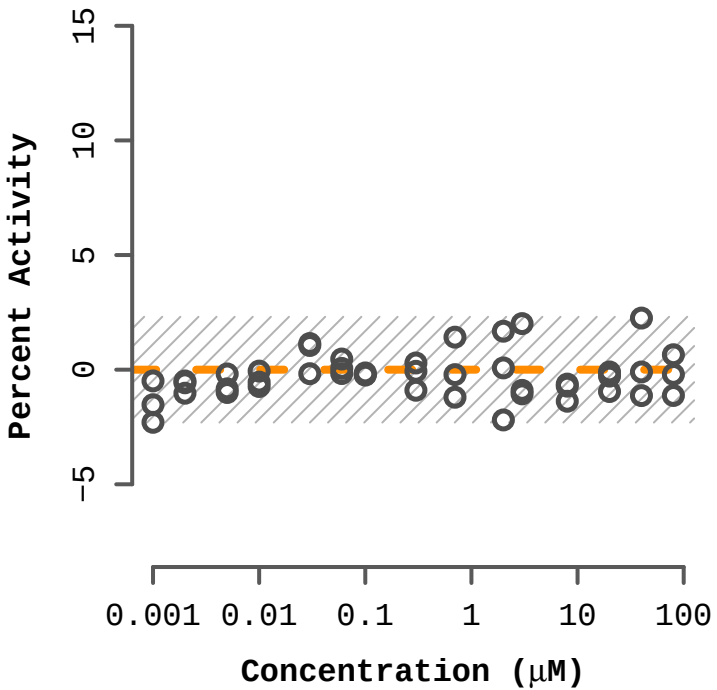
NAME: 2-Methyl-3-[4-(propan-2-yl)phenyl]propanal
CHID: 44769 **CASRN:** 103-95-7
SPID(S): Tox21_301084
M4ID: 12478049

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

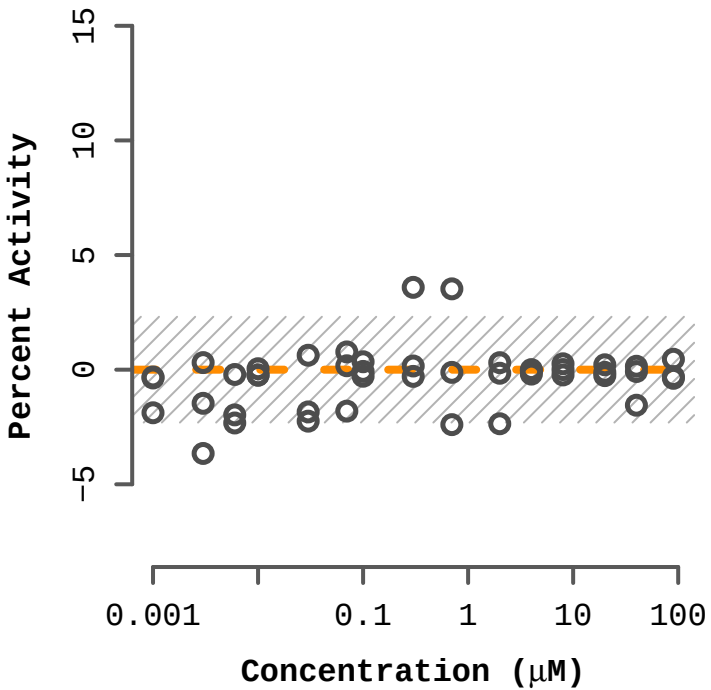
NAME: 4-Methoxybenzyl acetate
CHID: 44770 **CASRN:** 104-21-2
SPID(S): Tox21_301116
M4ID: 12478017

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.38	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.675 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

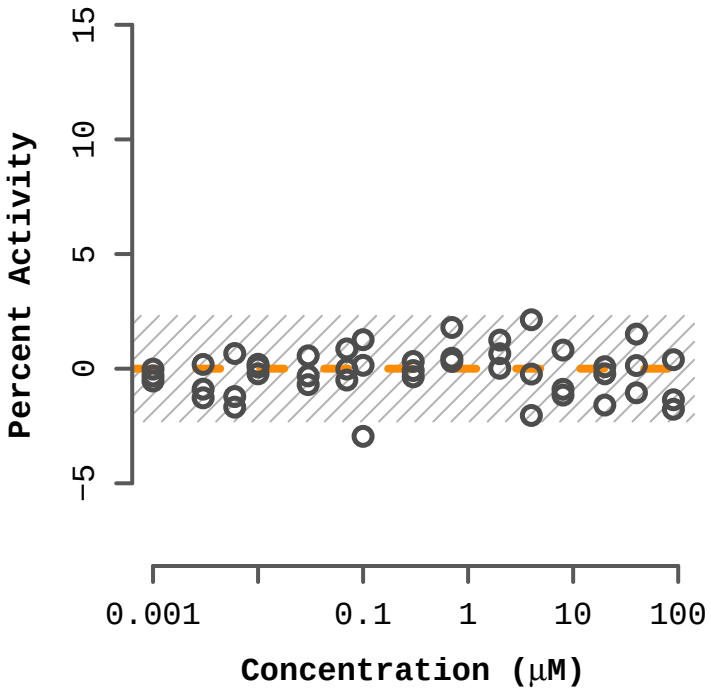
NAME: N-Hydroxy-4-methylpentan-2-imine
CHID: 44771 **CASRN:** 105-44-2
SPID(S): Tox21_301200
M4ID: 12477933

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.173 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

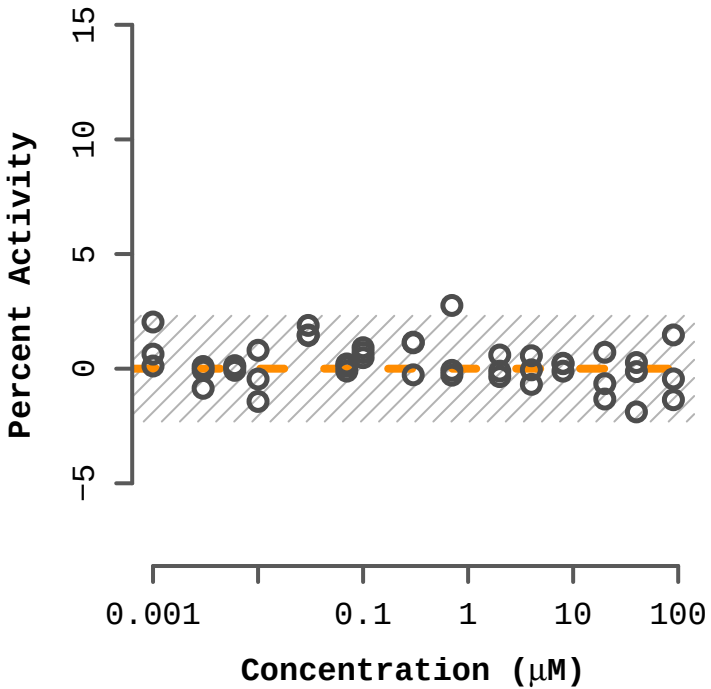
NAME: 3,7-Dimethyloct-6-en-1-yl formate
CHID: 44772 **CASRN:** 105-85-1
SPID(S): Tox21_301031
M4ID: 12478102

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.857 **MAX_MED:** 0.653 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

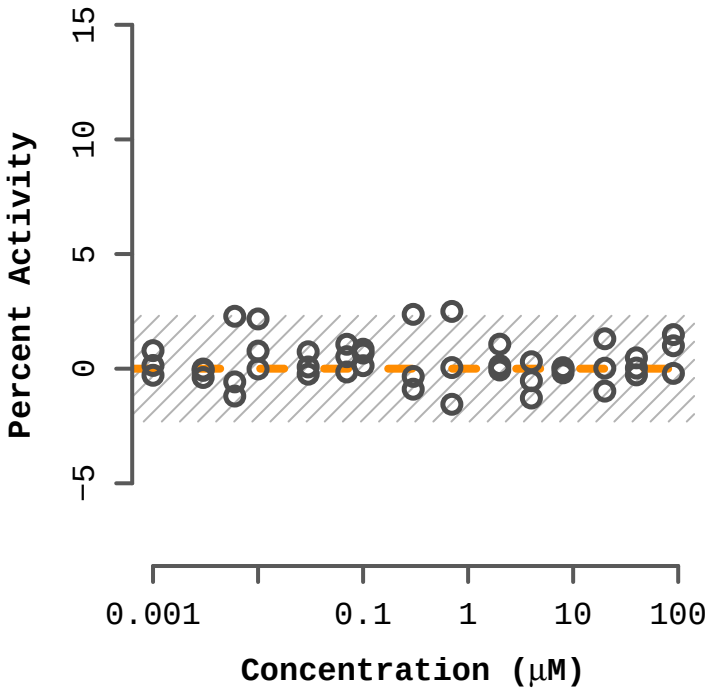
NAME: Ethylene glycol phenyl ether methacrylate
CHID: 44773 **CASRN:** 10595-06-9
SPID(S): Tox21_301053
M4ID: 12478080

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

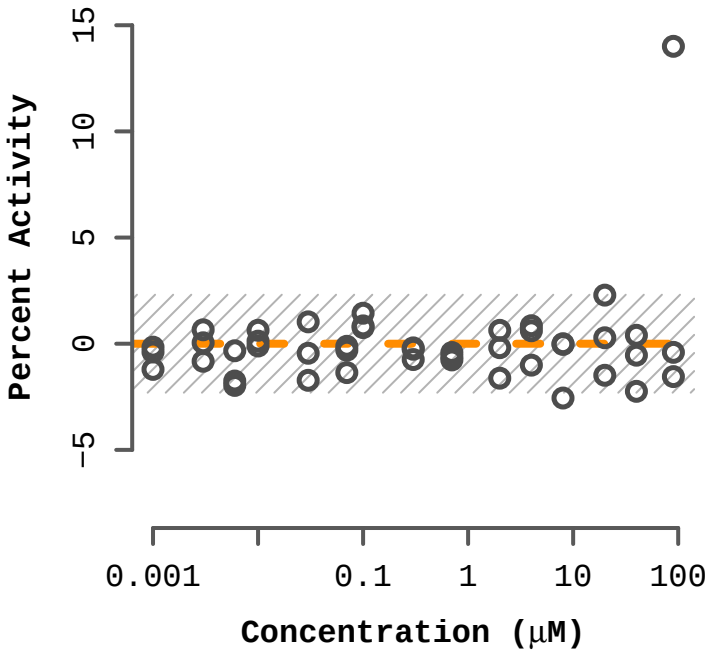
NAME: 1,4-Dioxacycloheptadecane-5,17-dione
CHID: 44774 **CASRN:** 105-95-3
SPID(S): Tox21_300971
M4ID: 12478162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

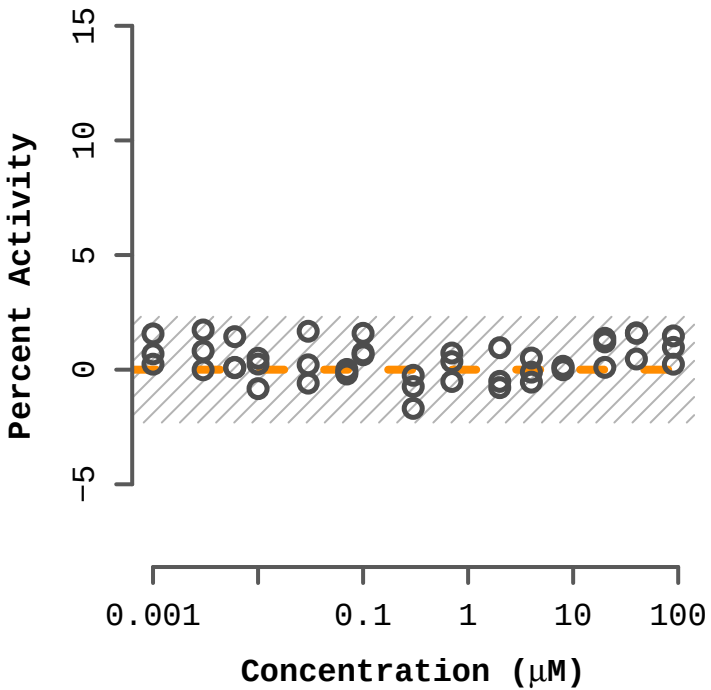
NAME: 2-Cyanoethyl prop-2-enoate
CHID: 44776 CASRN: 106-71-8
SPID(S): Tox21_301205
M4ID: 12477928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.33	NA	NA

MAX_MEAN: 4.02 MAX_MED: 0.842 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

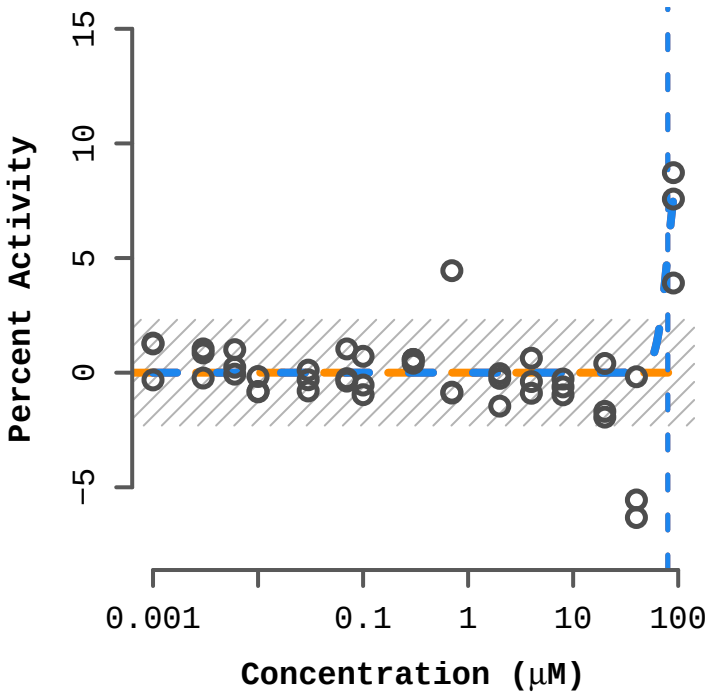
NAME: 2-Hydroxy-1-[4-(2-hydroxyethoxy)phenyl]-2-methy
CHID: 44777 CASRN: 106797-53-9
SPID(S): Tox21_301074
M4ID: 12478059

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Butanediol diacrylate
CHID: 44779 CASRN: 1070−70−8
SPID(S): Tox21_300938
M4ID: 12478195

HILL MODEL (in red):

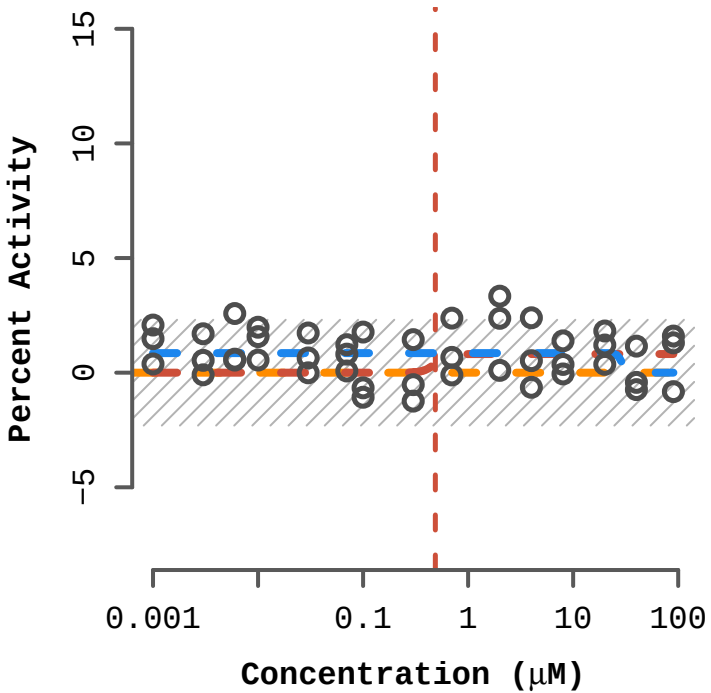
	tp	ga	gw
val:	10.5	1.9	8
sd:	4.78	0.0725	5.28

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.9	8	3.67	3.93
sd:	4.78	0.0725	5.28	1390	3200

	CNST	HILL	GNLS
AIC:	184.99	163.8	167.8
PROB:	0	0.88	0.12
RMSE:	2.43	1.71	1.71

MAX_MEAN: 6.74 **MAX_MED:** 7.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4-Dichloro-2,5-dimethylbenzene
CHID: 44780 **CASRN:** 1124-05-6
SPID(S): Tox21_301811
M4ID: 12477322

HILL MODEL (in red):

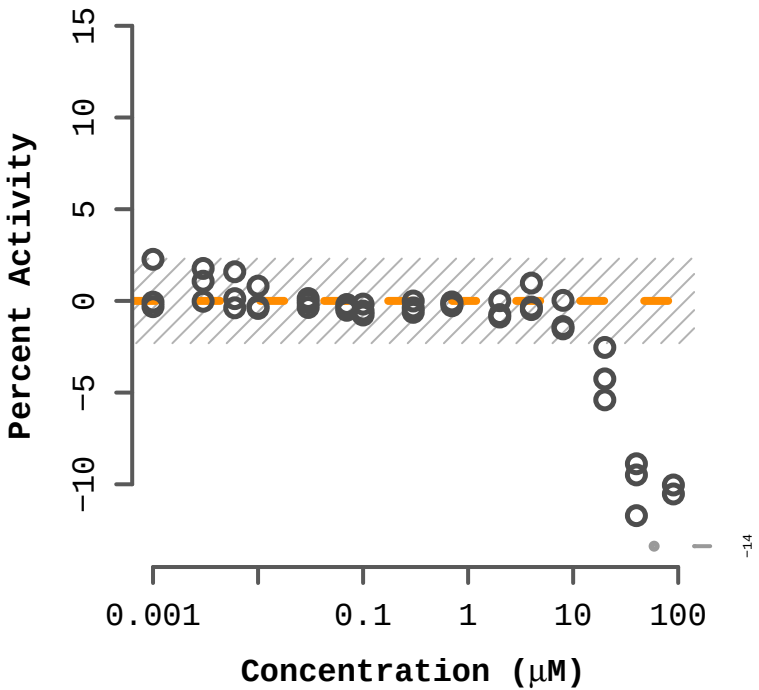
	tp	ga	gw
val:	0.813	−0.312	8
sd:	0.285	0.405	17.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.854	−5	3.59	1.47	18
sd:	0.182	1260	2260	0.58	69.1

	CNST	HILL	GNLS
AIC:	160.05	157.96	150.7
PROB:	0.01	0.03	0.97
RMSE:	1.34	1.21	1.07

MAX_MEAN: 1.94 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

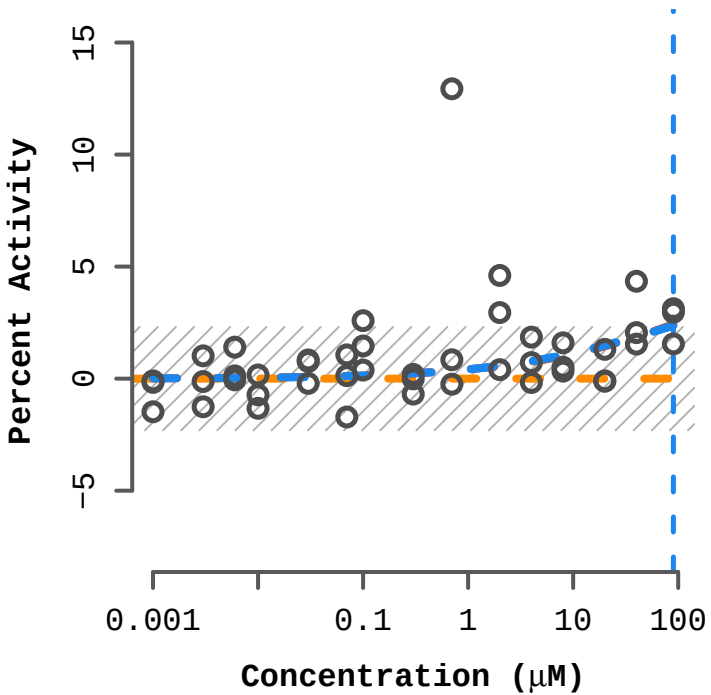
NAME: 2,3,4,5-Tetrachloro-6-(trichloromethyl)pyridine
CHID: 44781 **CASRN:** 1134-04-9
SPID(S): Tox21_301250
M4ID: 12477883 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.33	NA	NA
PROB:	1	NA	NA
RMSE:	4.18	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Amino-4-bromo-9,10-dioxo-9,10-dihydroanthrac
CHID: 44782 CASRN: 116-81-4
SPID(S): Tox21_301752
M4ID: 12477381

HILL MODEL (in red):

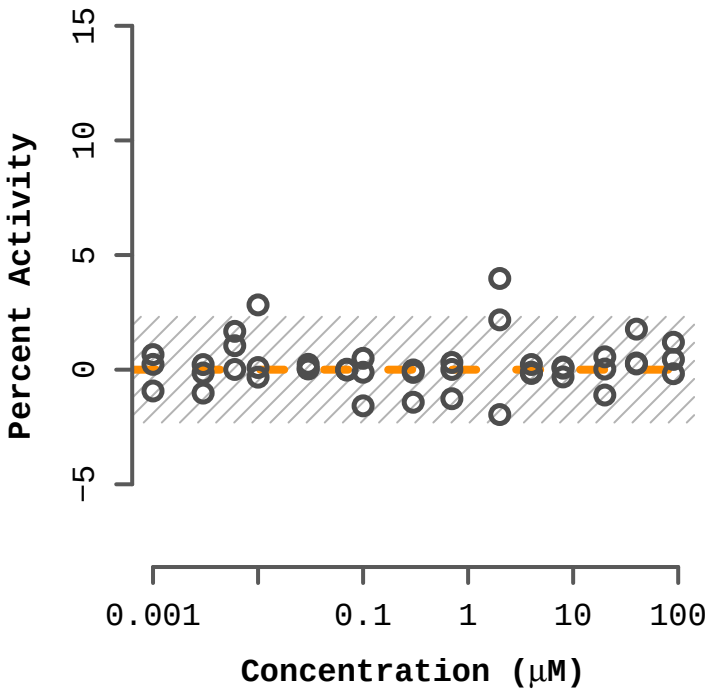
	tp	ga	gw
val:	6.63	2.45	0.48
sd:	10.2	2.15	0.237

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	1.95	0.519	3.94	2.52
sd:	5.35	1.62	0.262	101	127

	CNST	HILL	GNLS
AIC:	183.06	165.5	169.77
PROB:	0	0.89	0.11
RMSE:	2.48	2.21	2.21

MAX_MEAN: 4.51 MAX_MED: 2.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

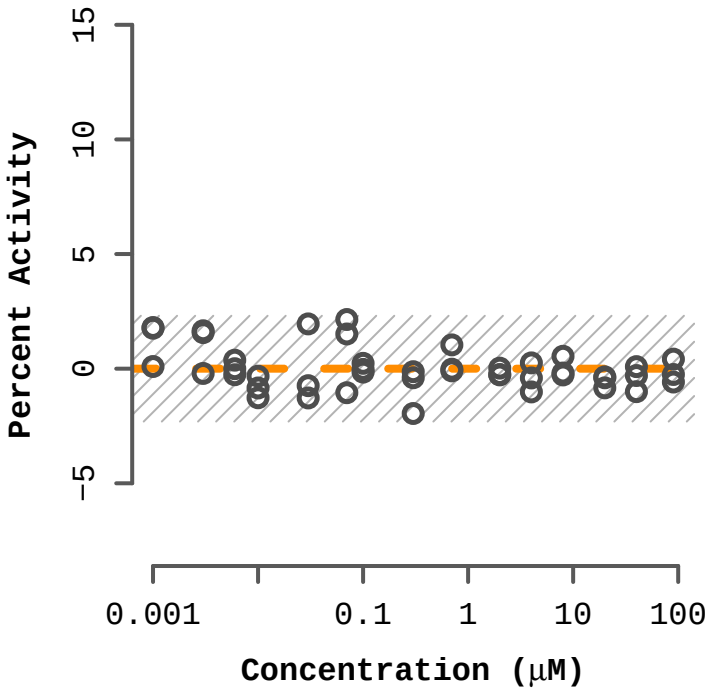
NAME: 2-Silylpropyl-urea, Si-(ethoxy and methoxy) de
CHID: 44783 **CASRN:** 116912-64-2
SPID(S): Tox21_301809
M4ID: 12477324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

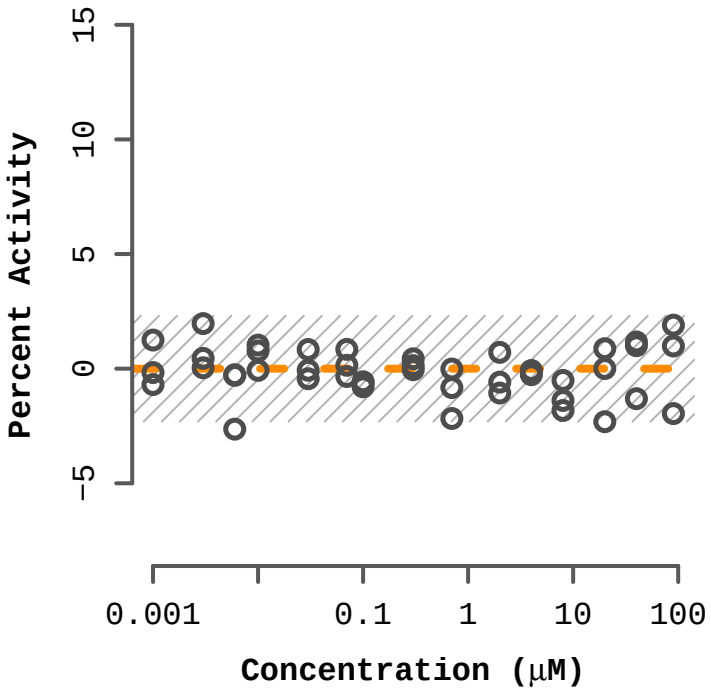
NAME: 1,3-Butyleneglycol dimethacrylate
CHID: 44784 CASRN: 1189-08-8
SPID(S): Tox21_301607
M4ID: 12477526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.77 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

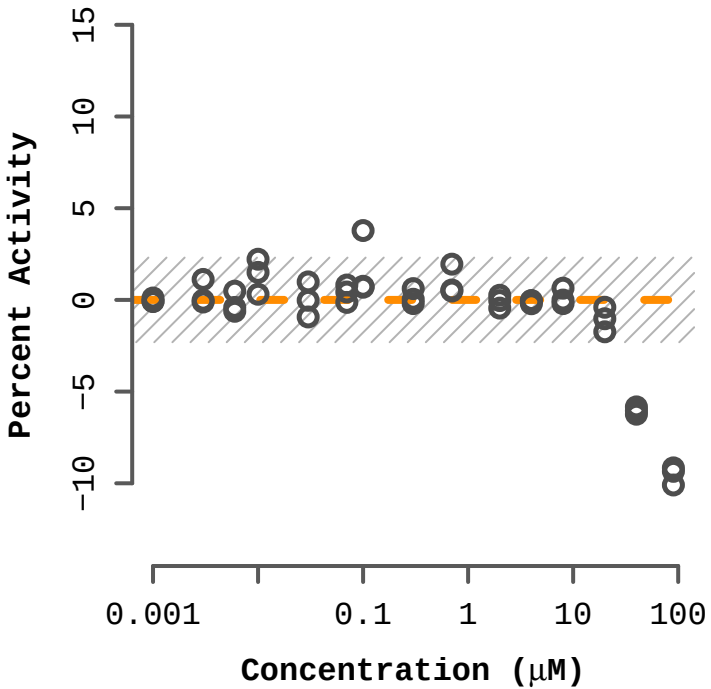
NAME: 3-(3-Methyl-5-oxo-4,5-dihydro-1H-pyrazol-1-yl)|
CHID: 44785 CASRN: 119-17-5
SPID(S): Tox21_301698
M4ID: 12477435

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.82 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

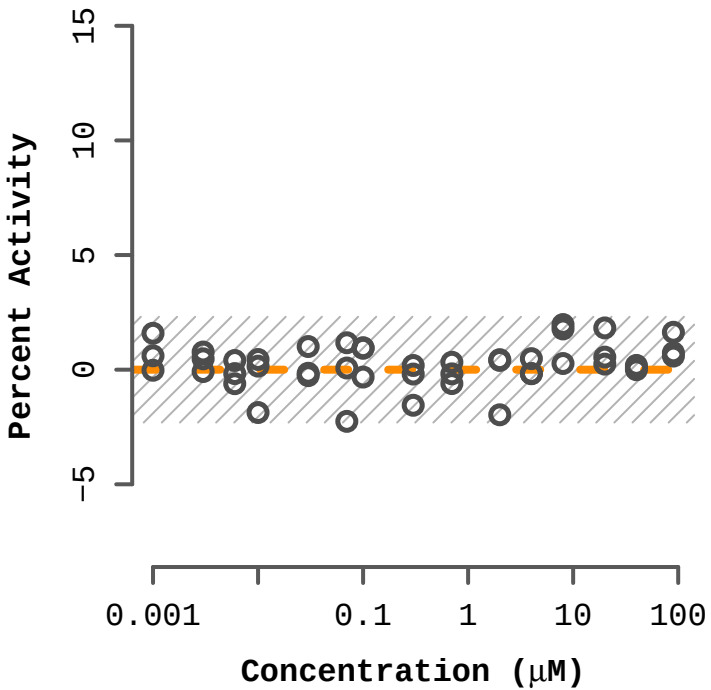
NAME: 2-Benzyl-2-(dimethylamino)-1-[4-(morpholin-4-y
CHID: 44786 CASRN: 119313-12-1
SPID(S): Tox21_301707
M4ID: 12477426

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 1.74 MAX_MED: 1.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

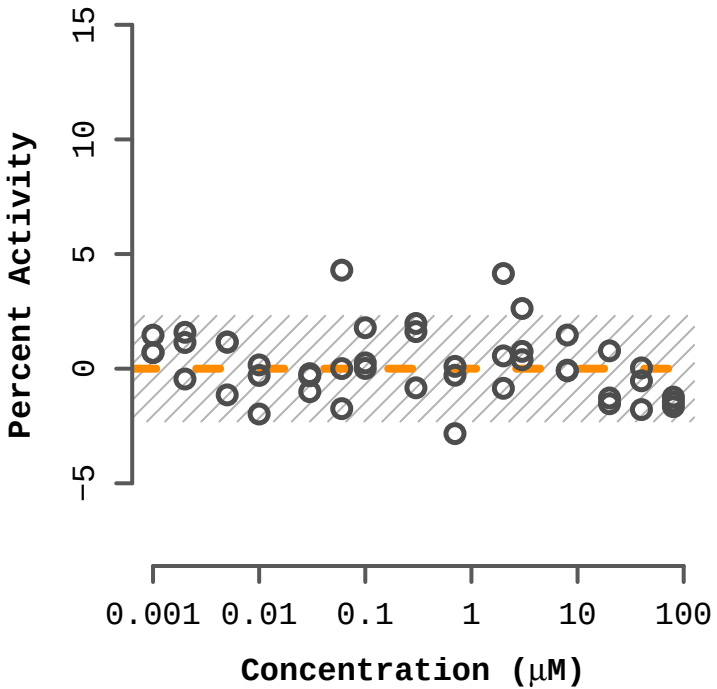
NAME: 4-Hydroxy-7-(phenylamino)naphthalene-2-sulfoni
CHID: 44787 **CASRN:** 119-40-4
SPID(S): Tox21_301802
M4ID: 12477331

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

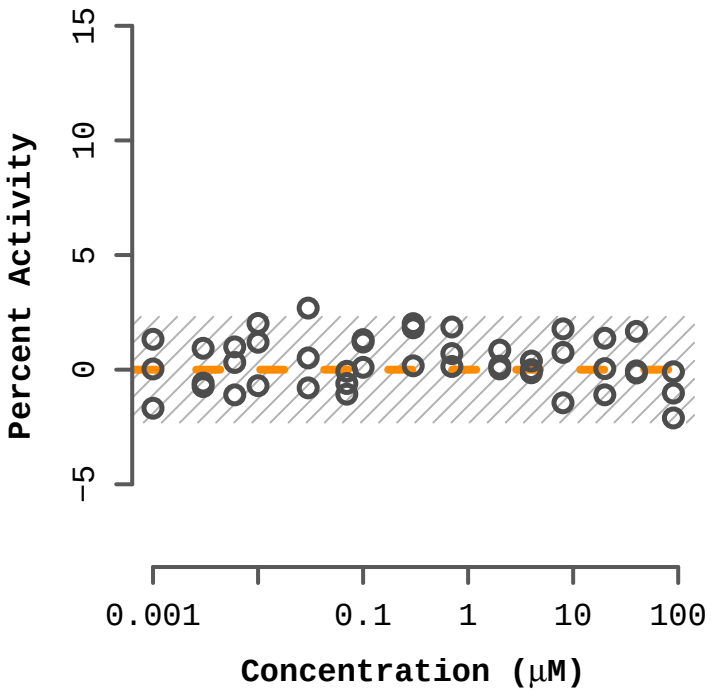
NAME: Naphthalene−2−sulfonic acid
CHID: 44788 **CASRN:** 120−18−3
SPID(S): Tox21_301657
M4ID: 12477476

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

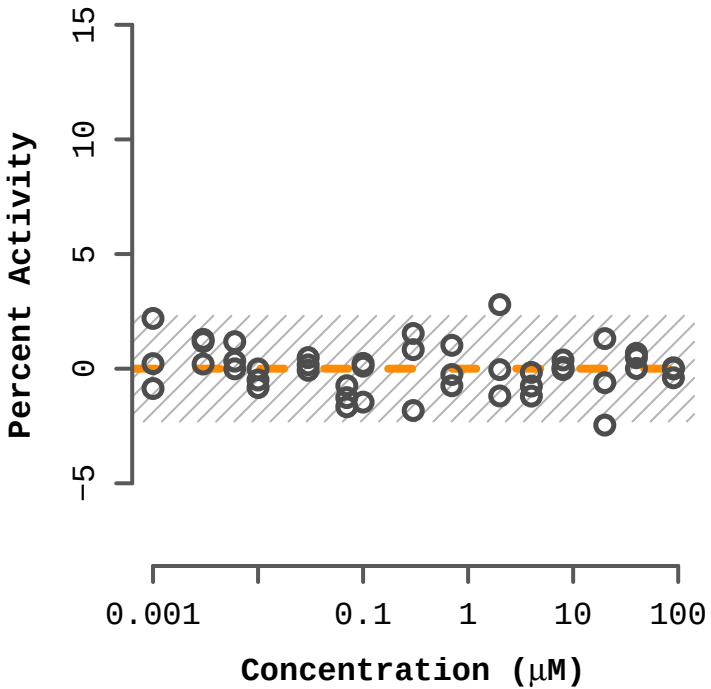
NAME: 3-Methyl-N-phenylaniline
CHID: 44790 **CASRN:** 1205-64-7
SPID(S): Tox21_301615
M4ID: 12477518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

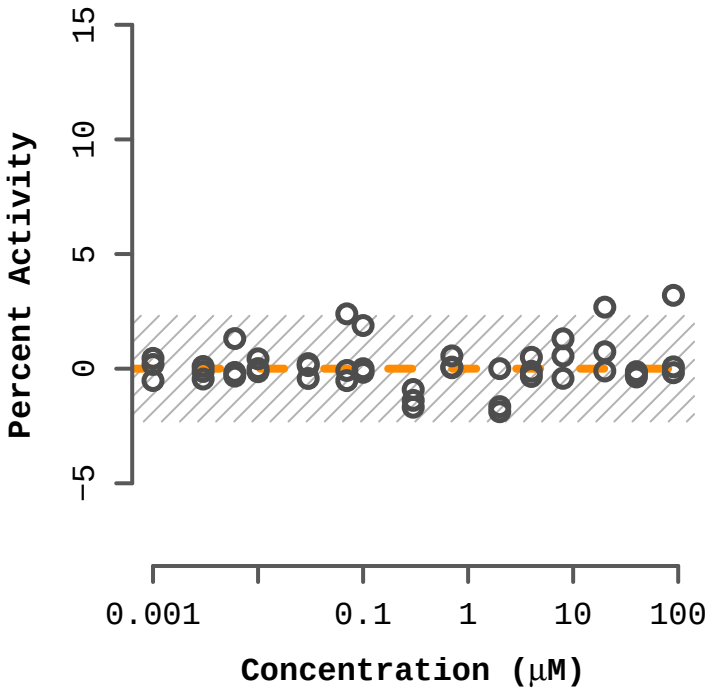
NAME: Benzyl propanoate
CHID: 44791 CASRN: 122-63-4
SPID(S): Tox21_301783
M4ID: 12477350

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

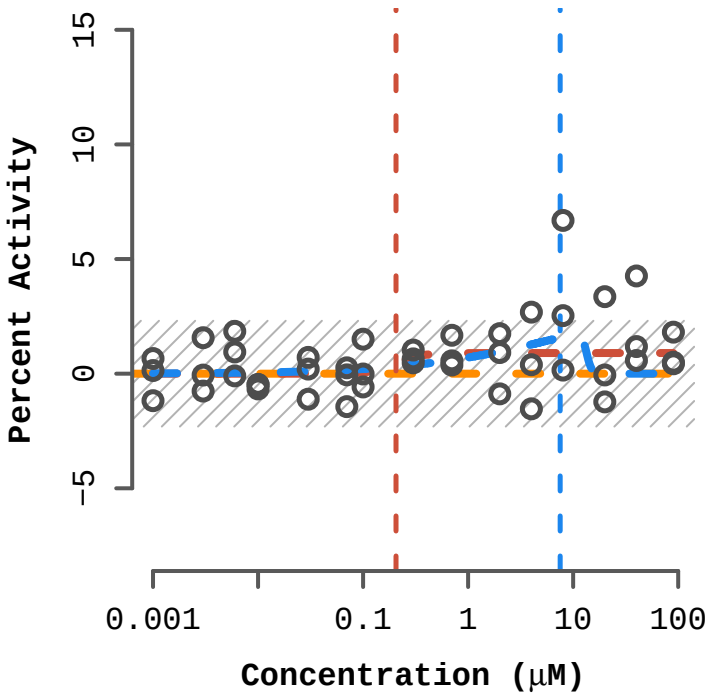
NAME: Sodium 3-chloro-2-hydroxypropane-1-sulfonate
CHID: 44793 **CASRN:** 126-83-0
SPID(S): Tox21_301796
M4ID: 12477337

HILL MODEL: Not applicable.

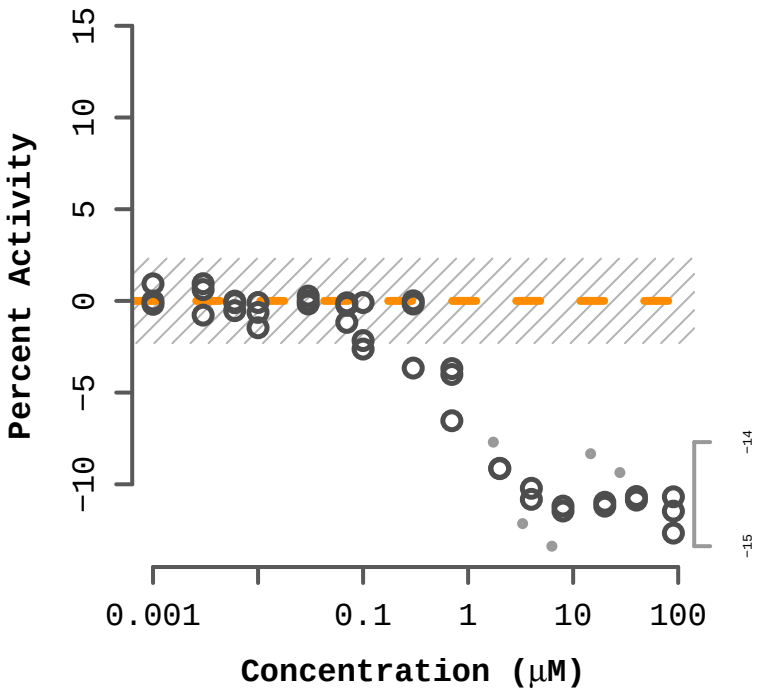
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.739 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-(Hydroxymethyl)-4-methyl-1-phenylpyrazolidin
CHID:    44794   CASRN: 13047-13-7
SPID(S): Tox21_301800
M4ID:    12477333

HILL MODEL (in red):
      tp       ga       gw
val:  0.9      -0.687   3.69
sd:   0.288    0.47     7.27

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.15     0.876    0.619    1.13     18
sd:   19.7     7.52     0.959    1.71     154

      CNST        HILL        GNLS
AIC:  164.16      158.33      167.22
PROB: 0.05        0.94        0.01
RMSE: 1.66        1.43        1.48

MAX_MEAN: 3.13      MAX_MED: 2.53      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

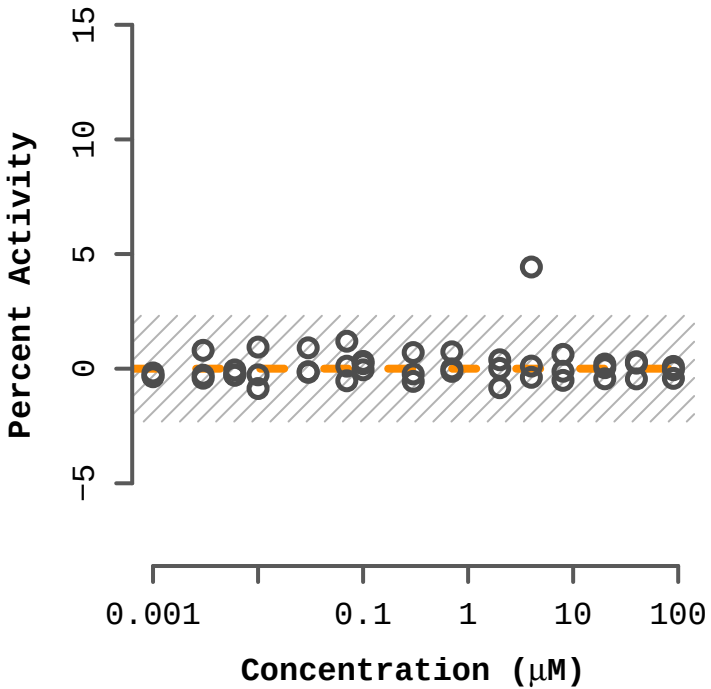
NAME: (Acryloyloxy)(tributyl)stannane
CHID: 44796 **CASRN:** 13331-52-7
SPID(S): Tox21_301795
M4ID: 12477338 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	315.1	NA	NA
PROB:	1	NA	NA
RMSE:	7.64	NA	NA

MAX_MEAN: 0.261 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

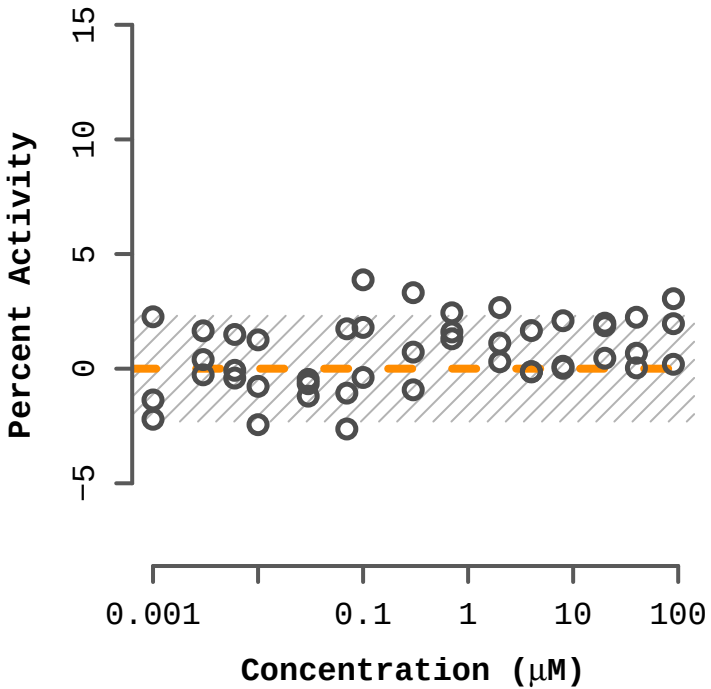
NAME: Sodium bis(2-methylpropyl)phosphinodithioate
CHID: 44798 CASRN: 13360-78-6
SPID(S): Tox21_301761
M4ID: 12477372

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	79.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 0.243 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

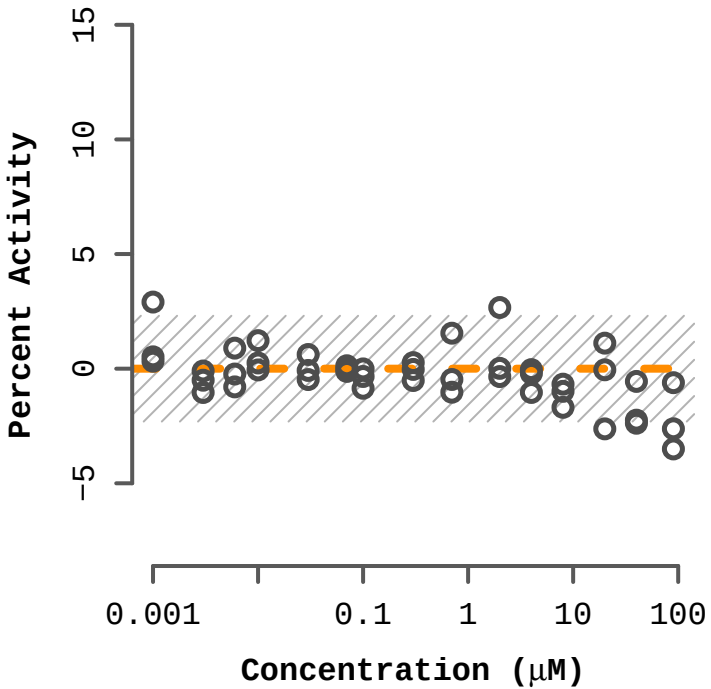
NAME: 2-tert-Butylcyclohexanol
CHID: 44799 **CASRN:** 13491-79-7
SPID(S): Tox21_301280
M4ID: 12477853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

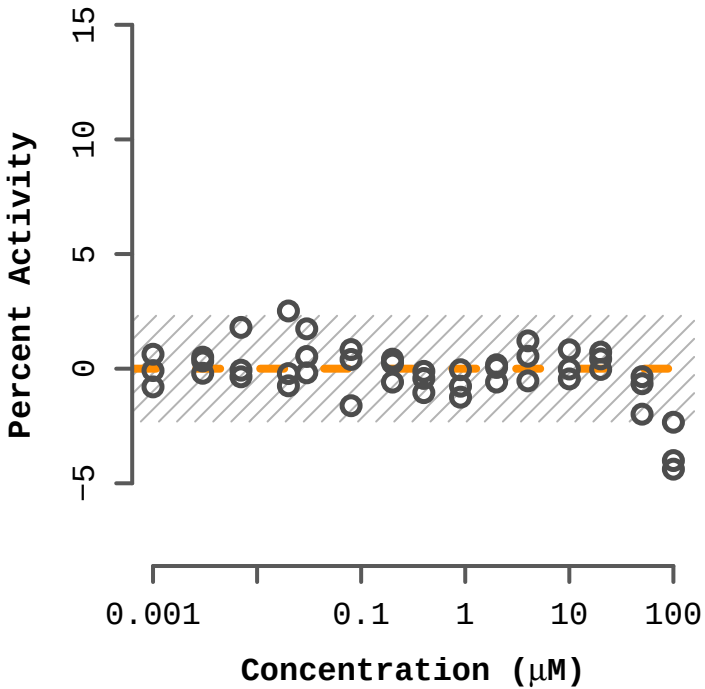
NAME: Sodium dibutylcarbamodithioate
CHID: 44800 CASRN: 136-30-1
SPID(S): Tox21_301797
M4ID: 12477336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.518 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

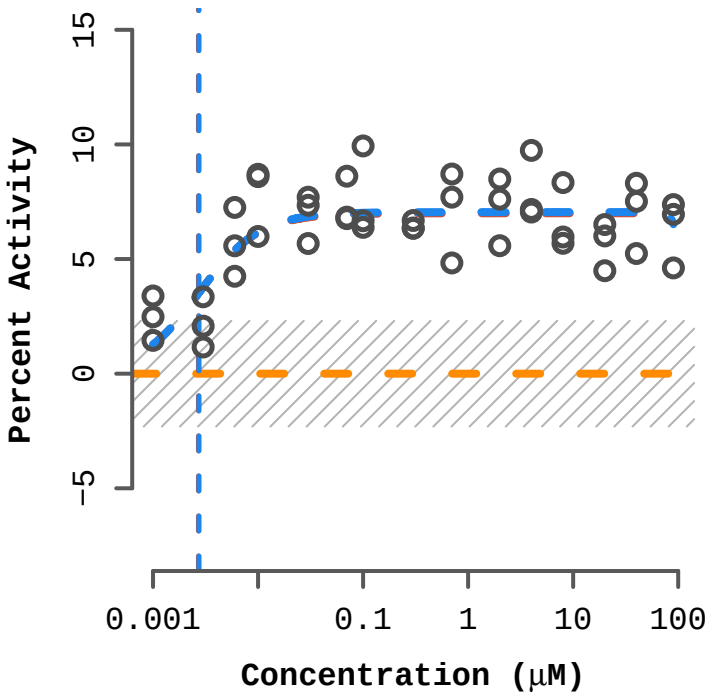
NAME: Sodium O-ethyl carbonodithioate
CHID: 44801 CASRN: 140-90-9
SPID(S): Tox21_301765
M4ID: 12477368

HILL MODEL: Not applicable.

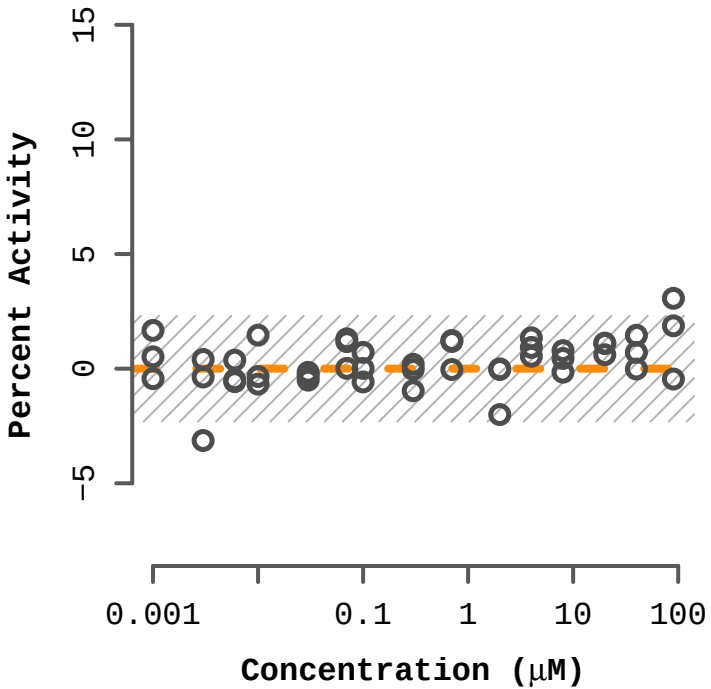
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.698 **MAX_MED:** 0.544 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Bis(2-butoxyethyl) decanedioate
CHID:    44802   CASRN: 141-19-5
SPID(S): Tox21_301302
M4ID:    12477831

HILL MODEL (in red):
      tp       ga       gw
val:  7        -2.57    1.52
sd:   0.249    0.171    0.671

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.05     -2.56    1.5      2.04     12.8
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  309.29      171.78      175.38
PROB: 0           0.86        0.14
RMSE: 6.62        1.43        1.42

MAX_MEAN: 7.99      MAX_MED: 8.6       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

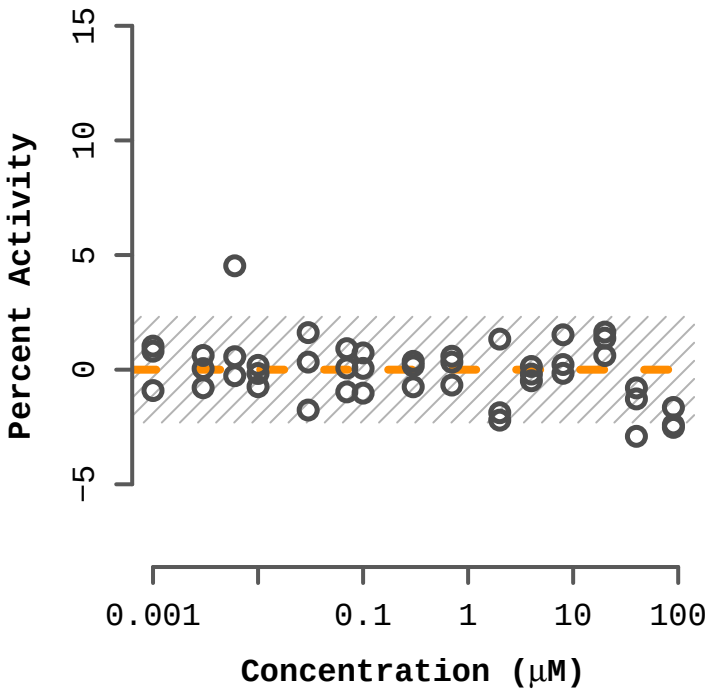
NAME: N-(2-Hydroxyethyl)acetamide
CHID: 44804 CASRN: 142-26-7
SPID(S): Tox21_301724
M4ID: 12477409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,2'−[Cyclohexane−1,4−diylbis(methanediyloxyme

CHID: 44805 **CASRN:** 14228−73−0

SPID(S): Tox21_301709

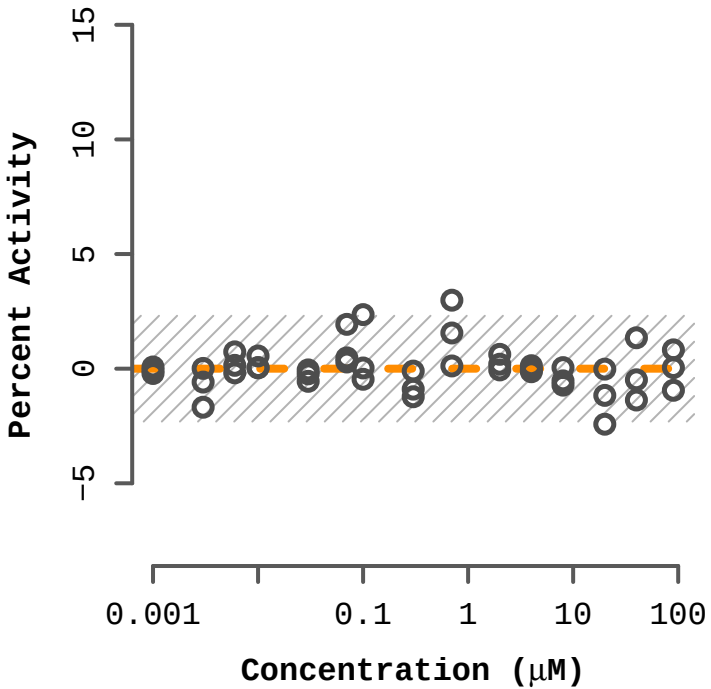
M4ID: 12477424

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

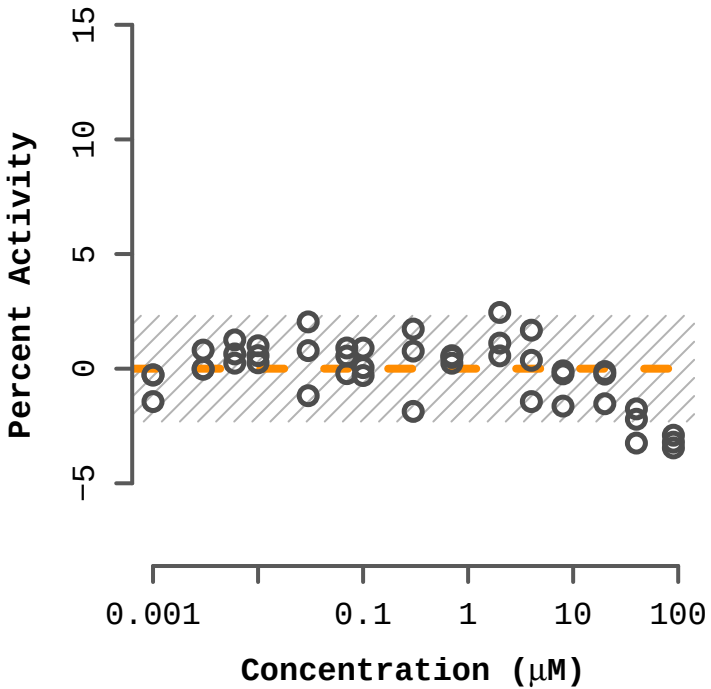
NAME: Dimethyl nonanedioate
CHID: 44807 CASRN: 1732-10-1
SPID(S): Tox21_301713
M4ID: 12477420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

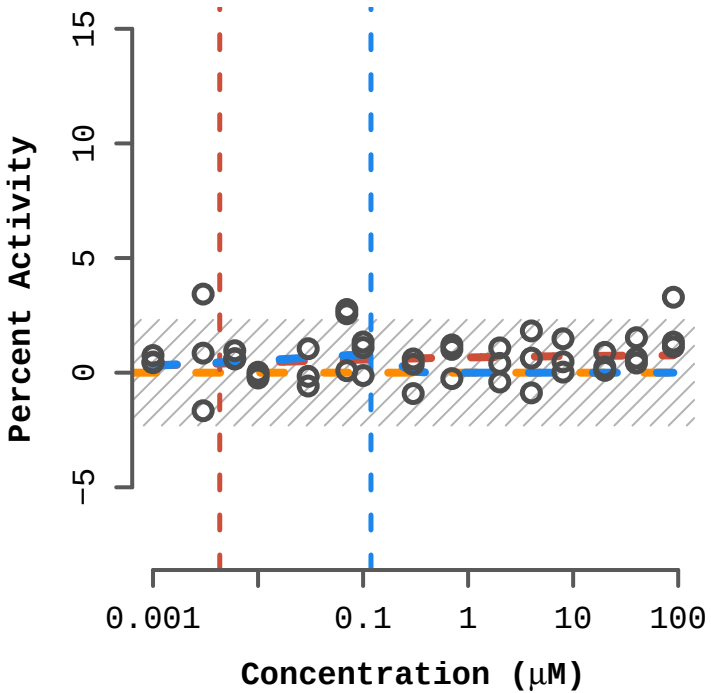
NAME: 3-(4-tert-Butylphenyl)propanal
CHID: 44808 **CASRN:** 18127-01-0
SPID(S): Tox21_301249
M4ID: 12477884

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,7-Dimethyloct-6-en-3-ol
CHID: 44809 CASRN: 18479-51-1
SPID(S): Tox21_301198
M4ID: 12477935

HILL MODEL (in red):

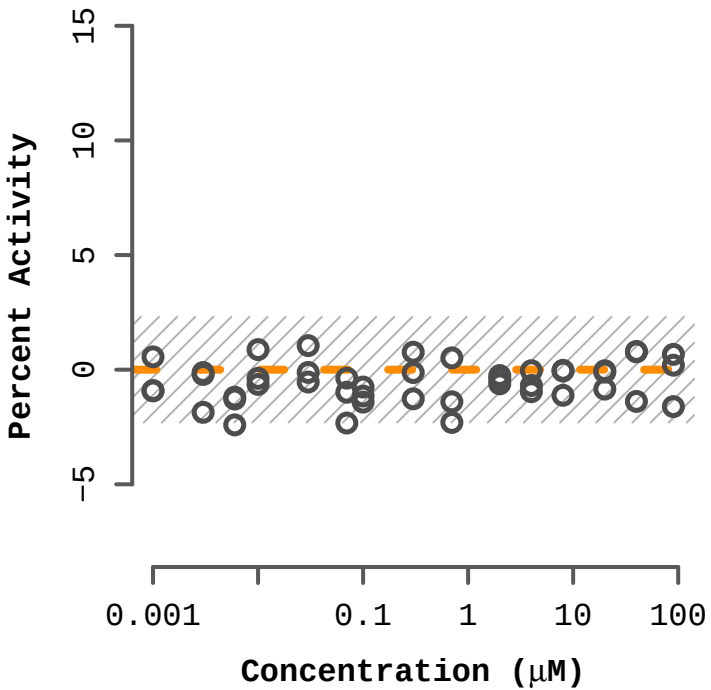
	tp	ga	gw
val:	0.794	−2.36	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.64	−0.925	0.3	−0.675	6.82
sd:	25.1	33.7	0.828	1.11	37.2

	CNST	HILL	GNLS
AIC:	145.06	132.83	148.75
PROB:	0	1	0
RMSE:	1.22	1.01	1.12

MAX_MEAN: 1.92 MAX_MED: 2.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

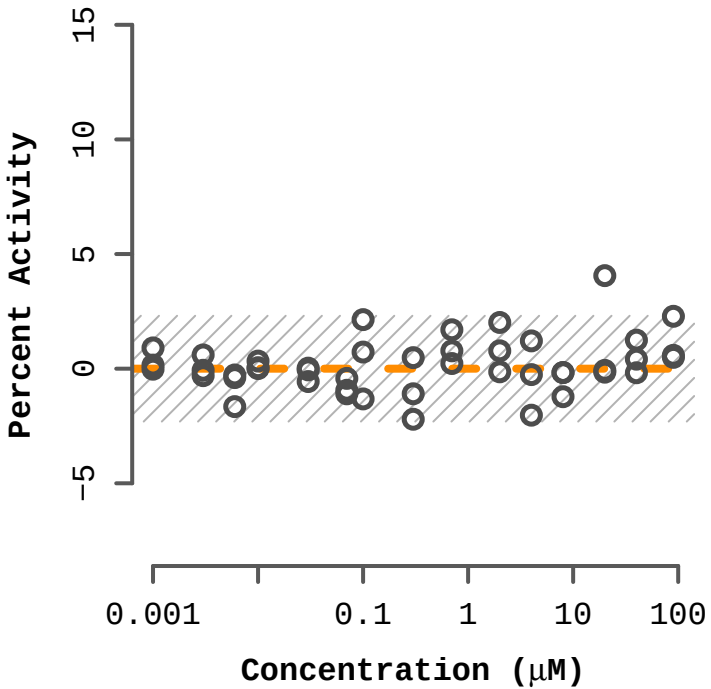
NAME: 2,6-Dimethyloctan-2-ol
CHID: 44810 **CASRN:** 18479-57-7
SPID(S): Tox21_300977
M4ID: 12478156

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.132 **MAX_MED:** 0.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

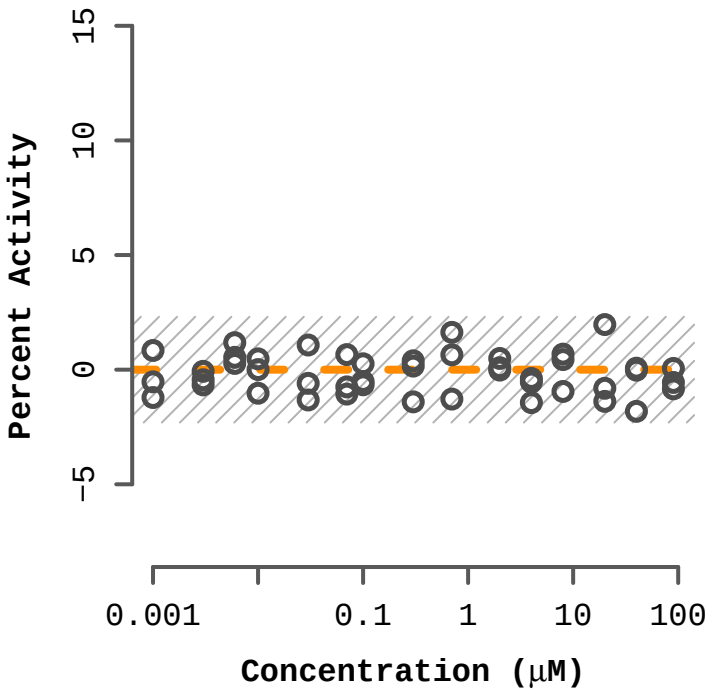
NAME: Chlordimeform hydrochloride
CHID: 44811 **CASRN:** 19750-95-9
SPID(S): Tox21_301412
M4ID: 12477721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 0.781 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

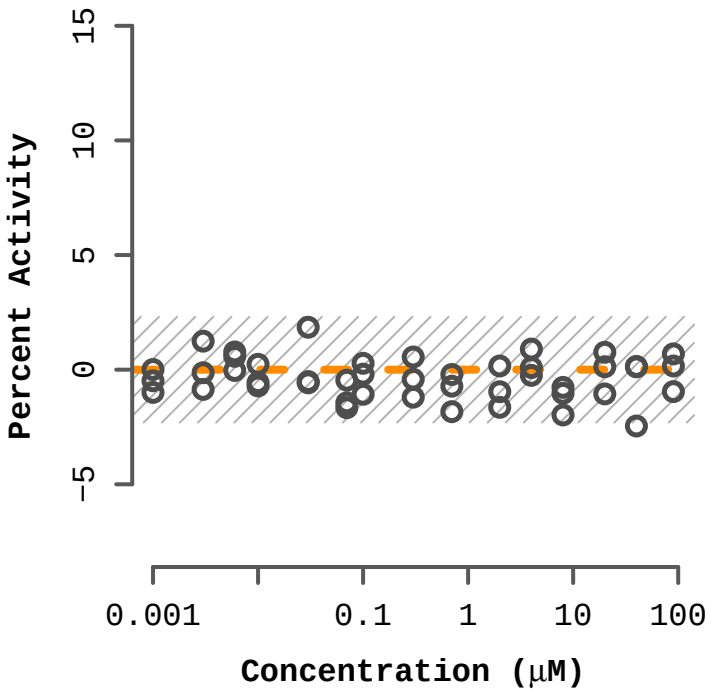
NAME: 3-Methoxybutan-1-ol
CHID: 44812 CASRN: 2517-43-3
SPID(S): Tox21_301623
M4ID: 12477510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.664 MAX_MED: 0.651 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

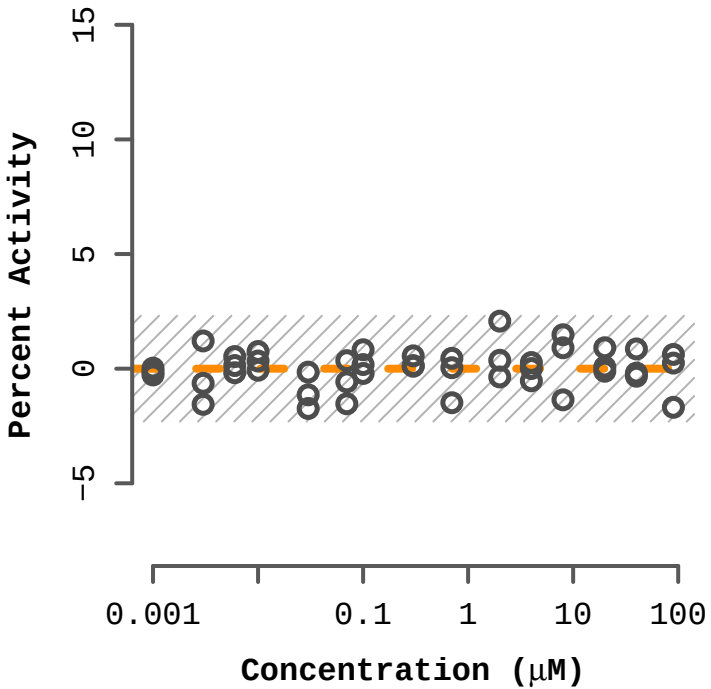
NAME: Dibutyl nonanedioate
CHID: 44815 **CASRN:** 2917-73-9
SPID(S): Tox21_301270
M4ID: 12477863

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.442 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

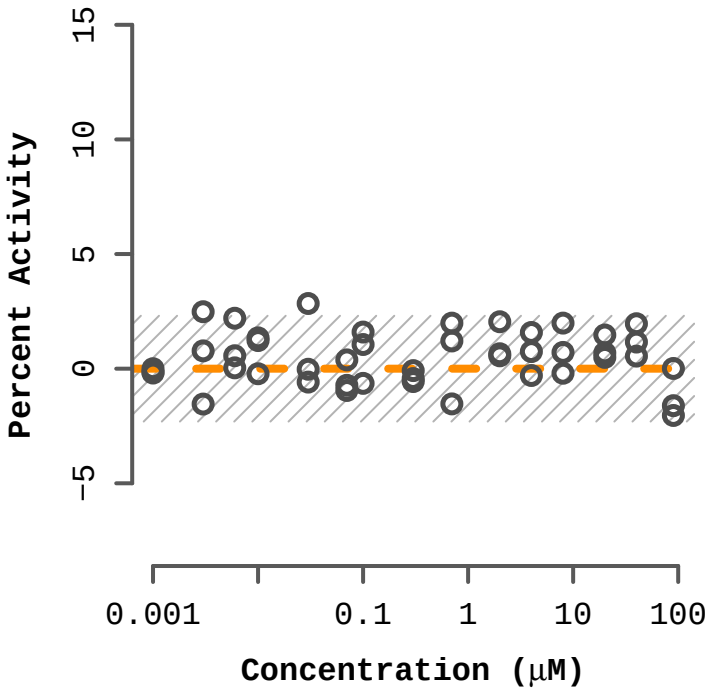
NAME: (2Z)-3,7-Dimethylocta-2,6-dienenitrile
CHID: 44816 CASRN: 31983-27-4
SPID(S): Tox21_301273
M4ID: 12477860

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.695 **MAX_MED:** 0.914 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

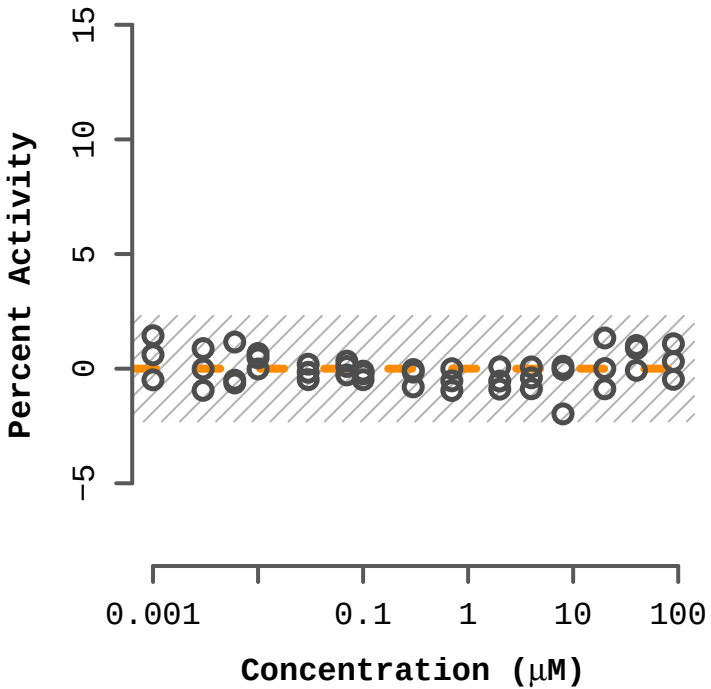
NAME: 3-(5,5,6-Trimethylbicyclo[2.2.1]hept-2-yl)cycl
CHID: 44817 **CASRN:** 3407-42-9
SPID(S): Tox21_301776
M4ID: 12477357

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

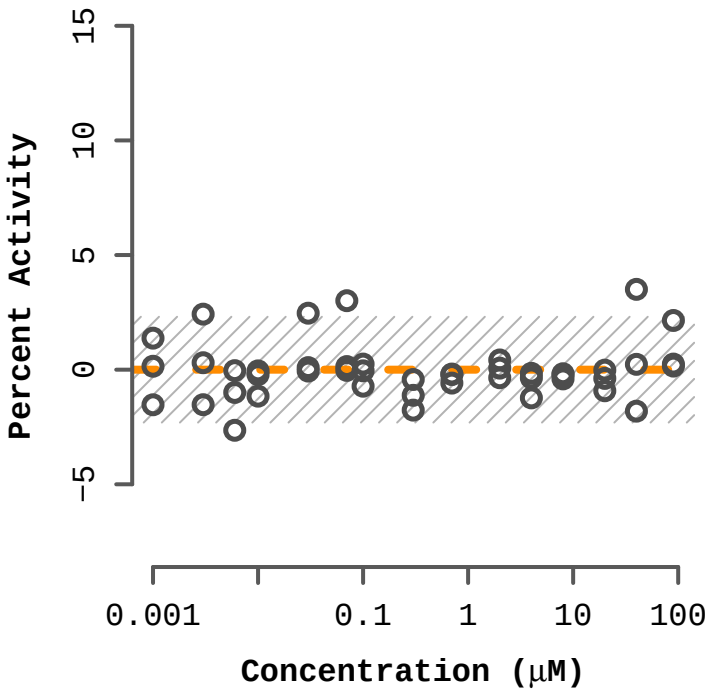
NAME: 2-Butyloctan-1-ol
CHID: 44818 **CASRN:** 3913-02-8
SPID(S): Tox21_301274
M4ID: 12477859

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

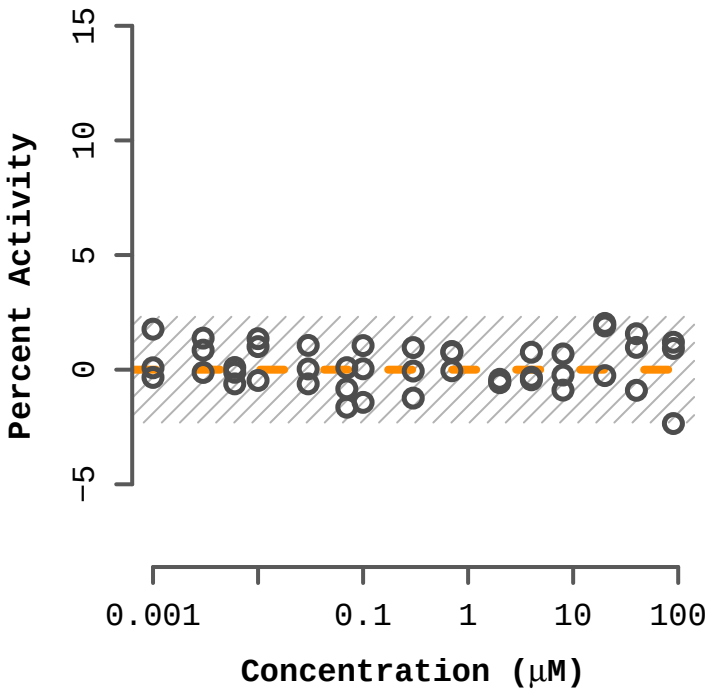
NAME: Lithium 3-carboxy-5-sulfobenzoate
CHID: 44819 CASRN: 46728-75-0
SPID(S): Tox21_301303
M4ID: 12477830

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.04 MAX_MED: 0.305 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

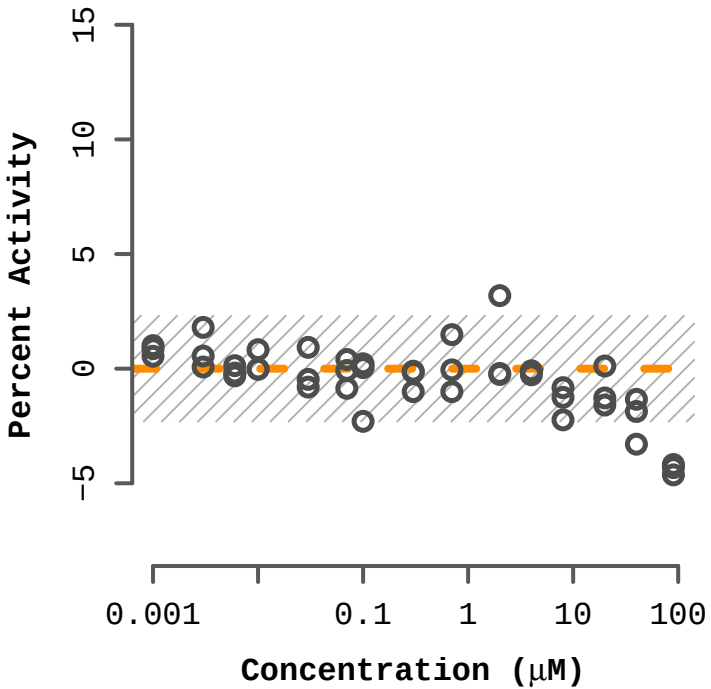
NAME: 4-[2-(Acryloyloxy)ethoxy]-4-oxobutanoic acid
CHID: 44820 **CASRN:** 50940-49-3
SPID(S): Tox21_301669
M4ID: 12477464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

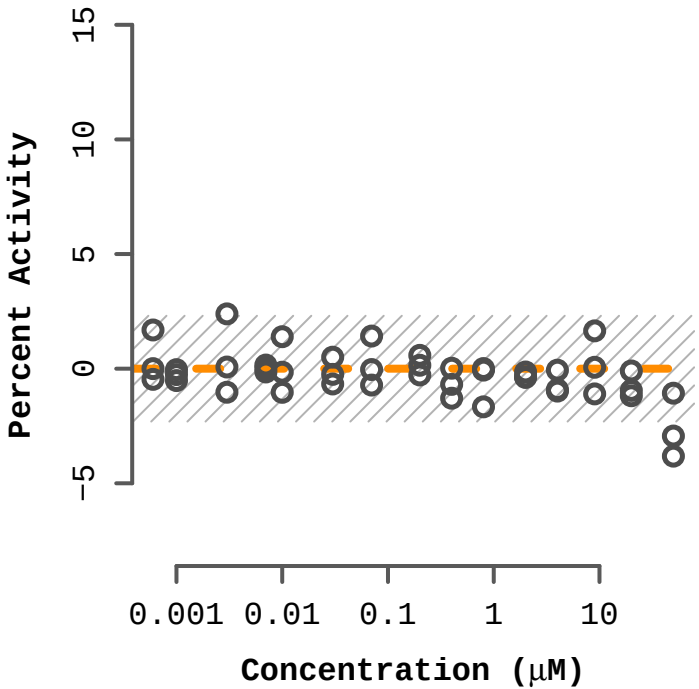
NAME: Ethyl 2-cyano-3,3-diphenylacrylate
CHID: 44821 **CASRN:** 5232-99-5
SPID(S): Tox21_301677
M4ID: 12477456

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

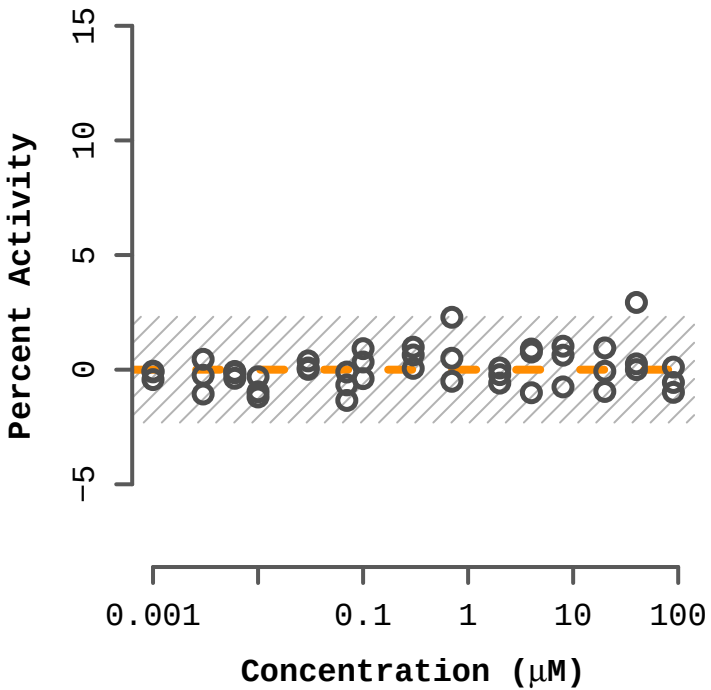
NAME: Ethyl 2-cyano-3,3-diphenylacrylate
CHID: 44821 **CASRN:** 5232-99-5
SPID(S): Tox21_112378_1
M4ID: 12483126

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.48 **MAX_MED:** 0.151 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

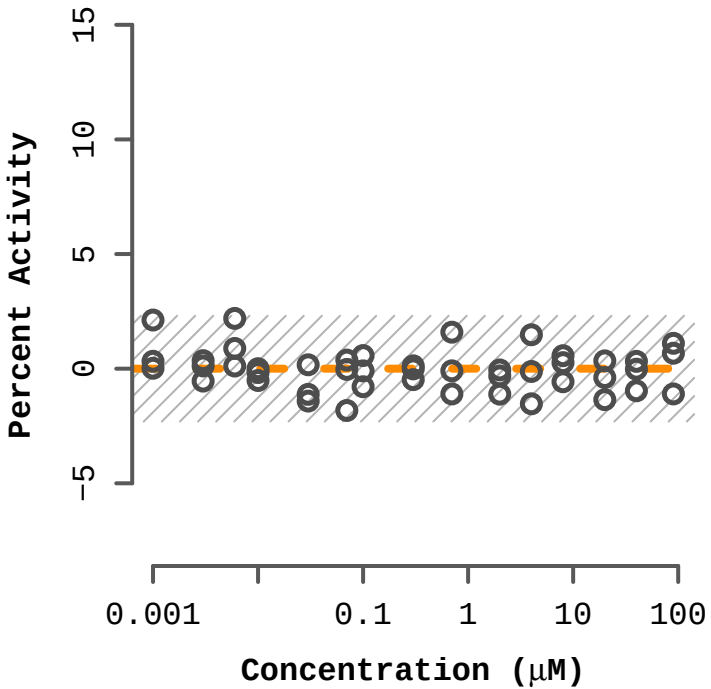
NAME: 3-Methyl-5-phenylpentan-1-ol
CHID: 44822 **CASRN:** 55066-48-3
SPID(S): Tox21_301260
M4ID: 12477873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

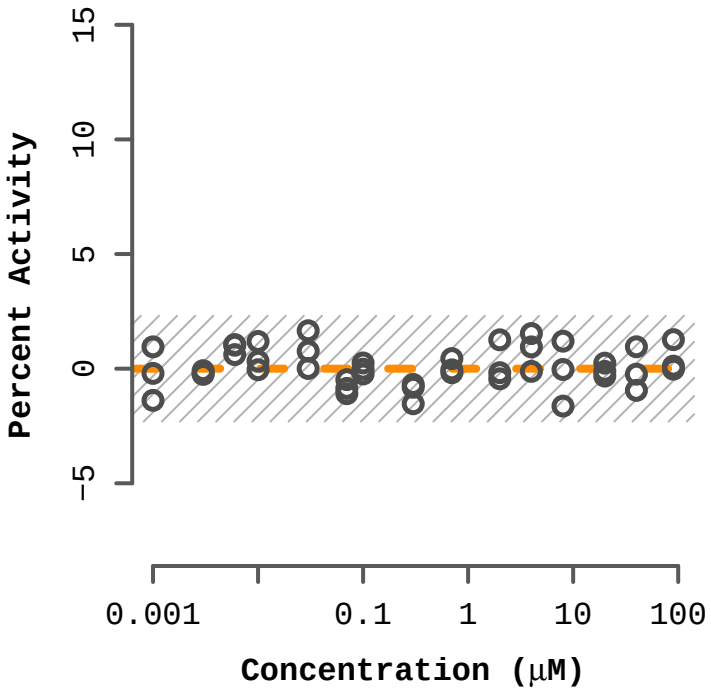
NAME: Sodium methacrylate
CHID: 44823 CASRN: 5536-61-8
SPID(S): Tox21_301636
M4ID: 12477497

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.885 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

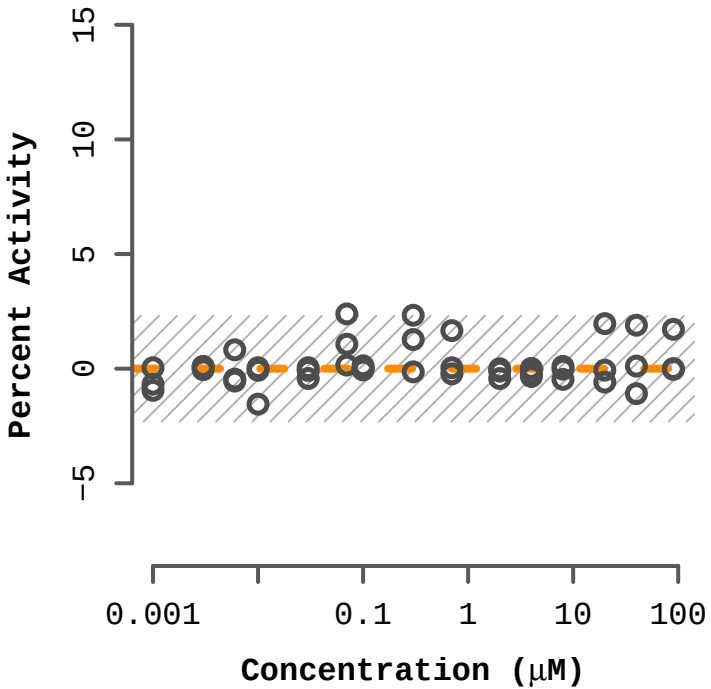
NAME: 4-Methyl-1-(propan-2-yl)cyclohex-3-en-1-ol
CHID: 44824 **CASRN:** 562-74-3
SPID(S): Tox21_301785
M4ID: 12477348

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.898 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

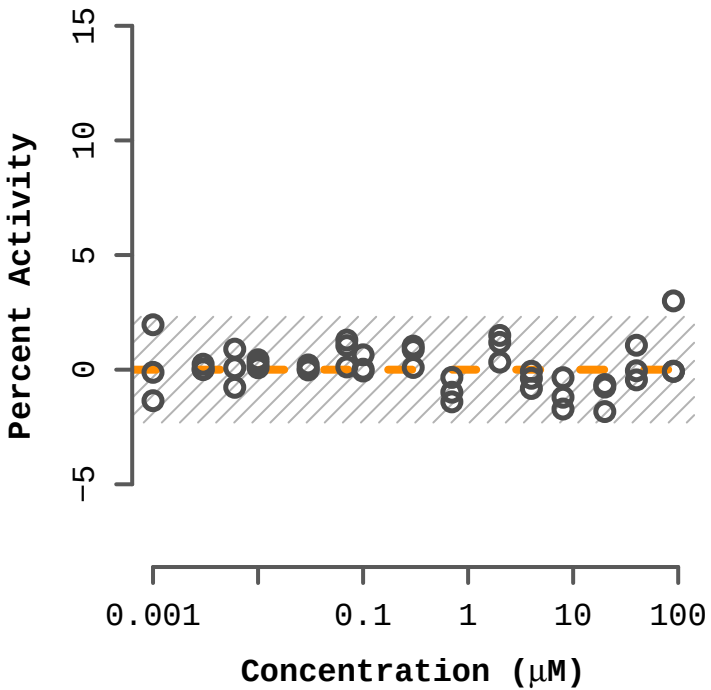
NAME: 3-tert-Butylphenol
CHID: 44825 **CASRN:** 585-34-2
SPID(S): Tox21_301686
M4ID: 12477447

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

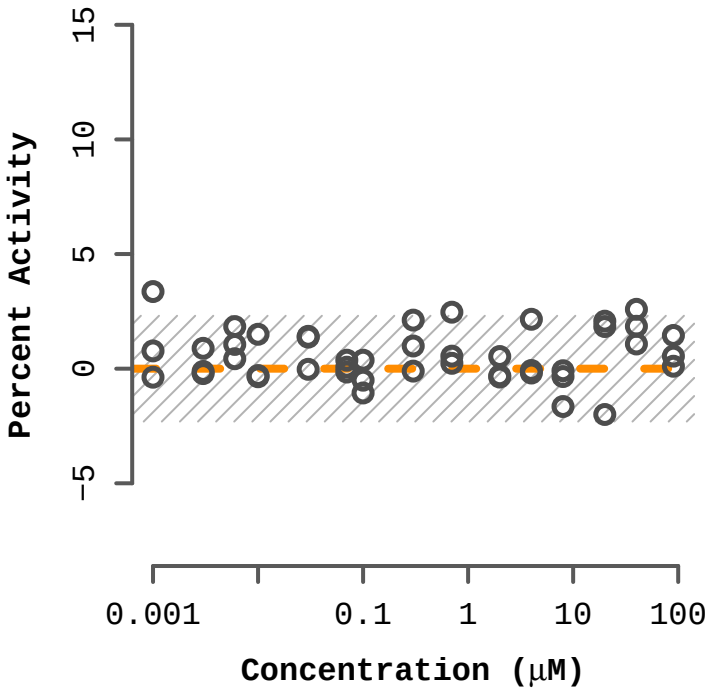
NAME: 3,7-Dimethyloctanal
CHID: 44826 **CASRN:** 5988-91-0
SPID(S): Tox21_301231
M4ID: 12477902

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

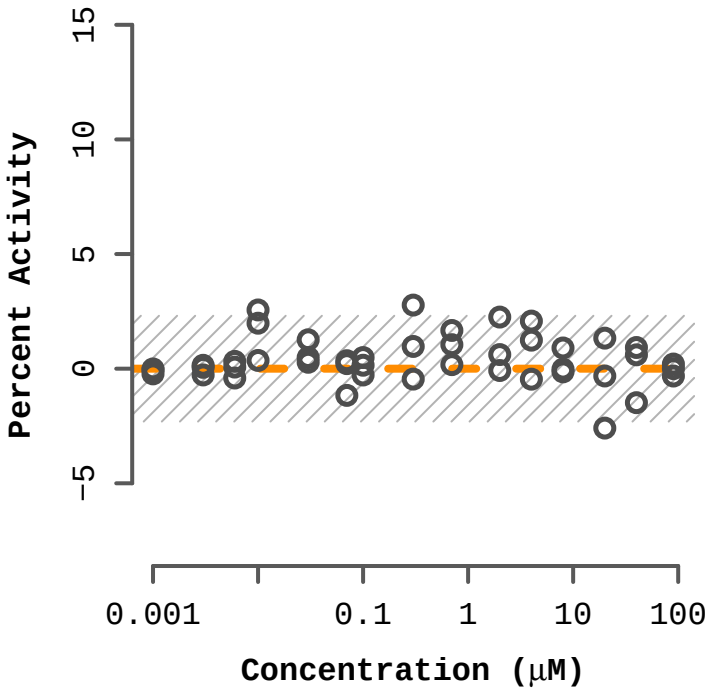
NAME: Propylene glycol diacetate
CHID: 44827 **CASRN:** 623-84-7
SPID(S): Tox21_301689
M4ID: 12477444

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

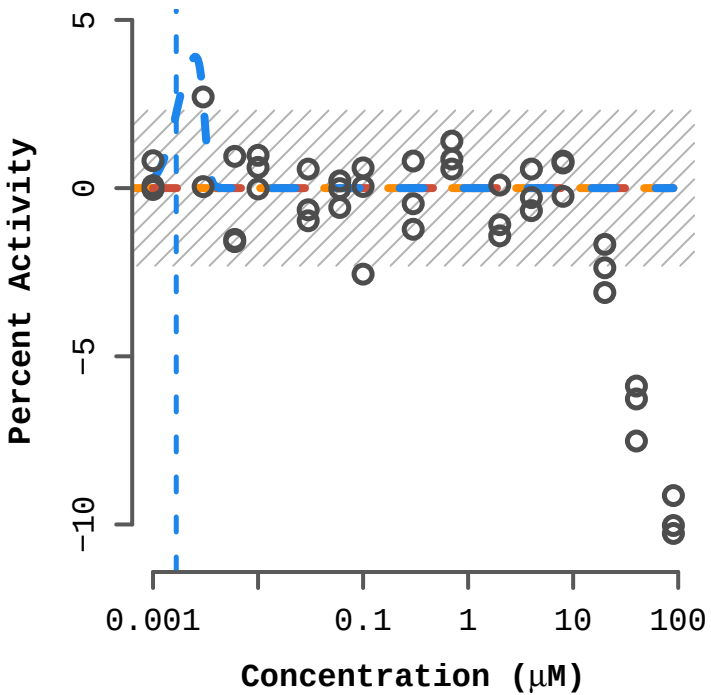
NAME: Ethyl undec−10−enoate
CHID: 44828 CASRN: 692−86−4
SPID(S): Tox21_301705
M4ID: 12477428

HILL MODEL: Not applicable.

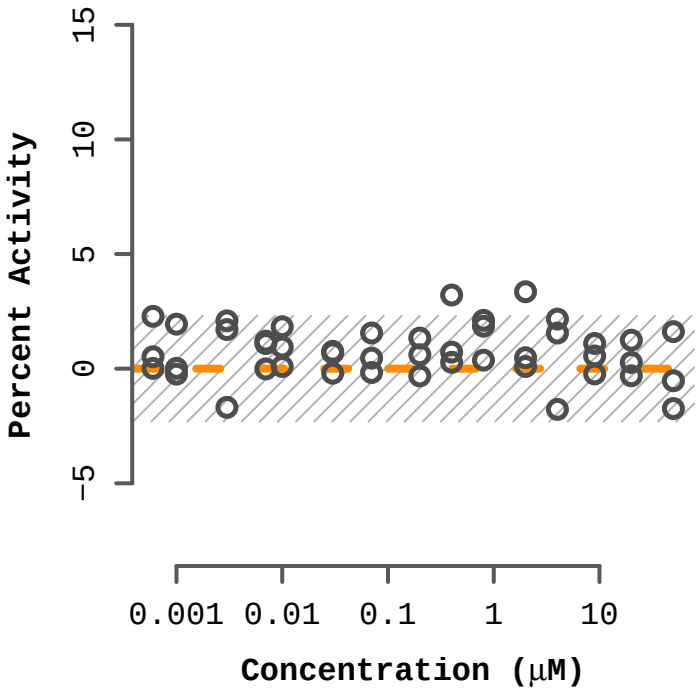
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.98 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)propa
CHID:    44829   CASRN: 70356-09-1
SPID(S): Tox21_202796
M4ID:    12479456

HILL MODEL (in red):
      tp        ga        gw
val:  7.12e-10 -4.51     2.47
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  4.45      -2.78     5.3       -2.51     17.7
sd:   NaN       NaN       NaN       NaN       NaN

      CNST         HILL         GNLS
AIC:  219.62       225.62       225.48
PROB: 0.91         0.05         0.05
RMSE: 3.32         3.32         3.26

MAX_MEAN: 2.55      MAX_MED: 2.71      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

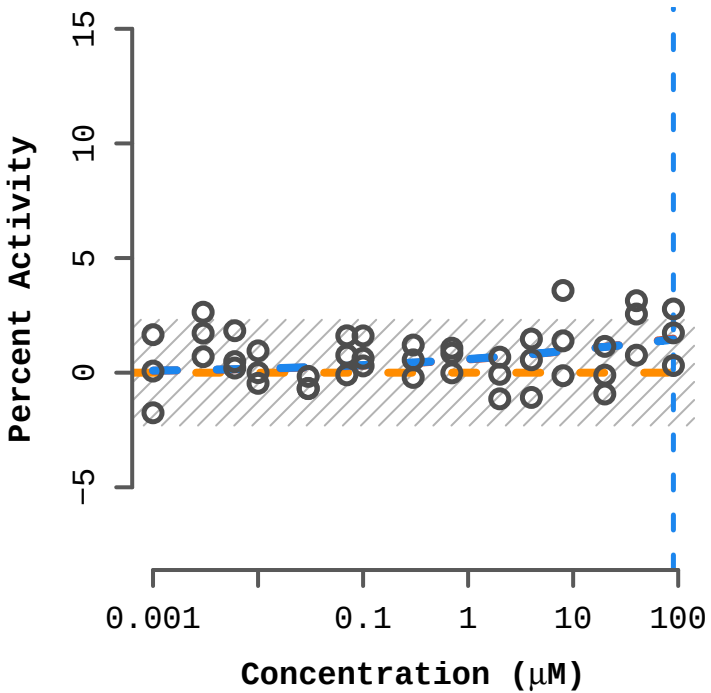
NAME: 1-(4-tert-Butylphenyl)-3-(4-methoxyphenyl)propa
CHID: 44829 **CASRN:** 70356-09-1
SPID(S): Tox21_111427_1
M4ID: 12483696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxy-2-methylpropiophenone
CHID: 44830 CASRN: 7473-98-5
SPID(S): Tox21_301675
M4ID: 12477458

HILL MODEL (in red):

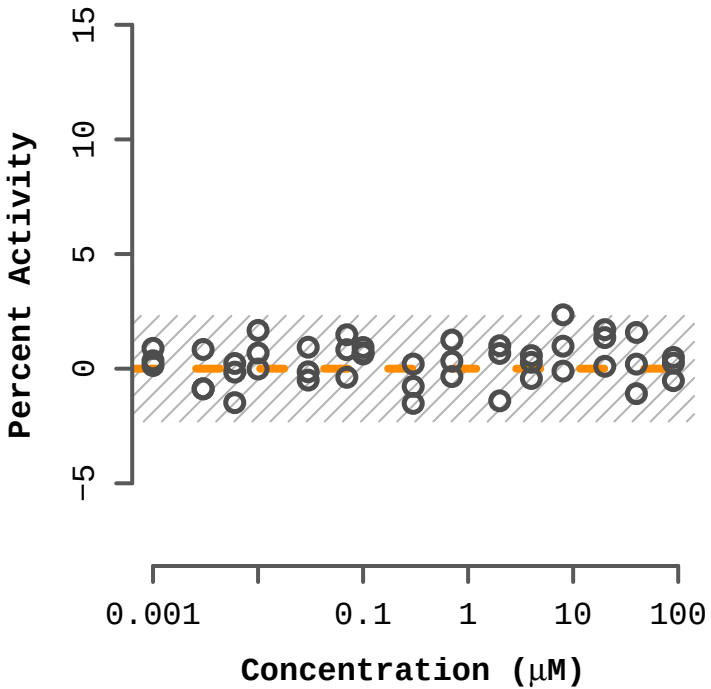
	tp	ga	gw
val:	3.31	2.25	0.3
sd:	7.76	5.55	0.322

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.88	1.95	0.3	3.79	8.75
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	157.41	149.17	153.21
PROB:	0.01	0.87	0.12
RMSE:	1.35	1.13	1.13

MAX_MEAN: 2.16 **MAX_MED:** 2.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

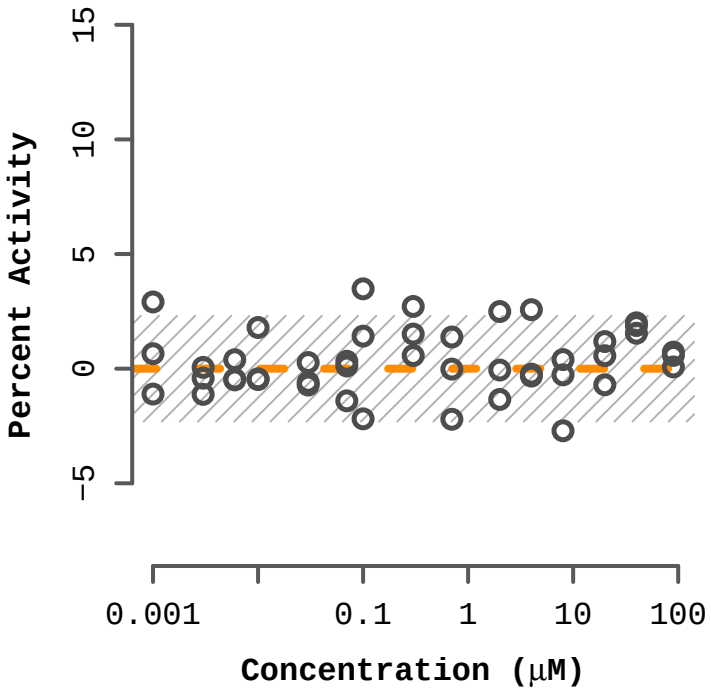
NAME: 1-Butoxy-1-oxopropan-2-yl butanoate
CHID: 44831 **CASRN:** 7492-70-8
SPID(S): Tox21_301784
M4ID: 12477349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

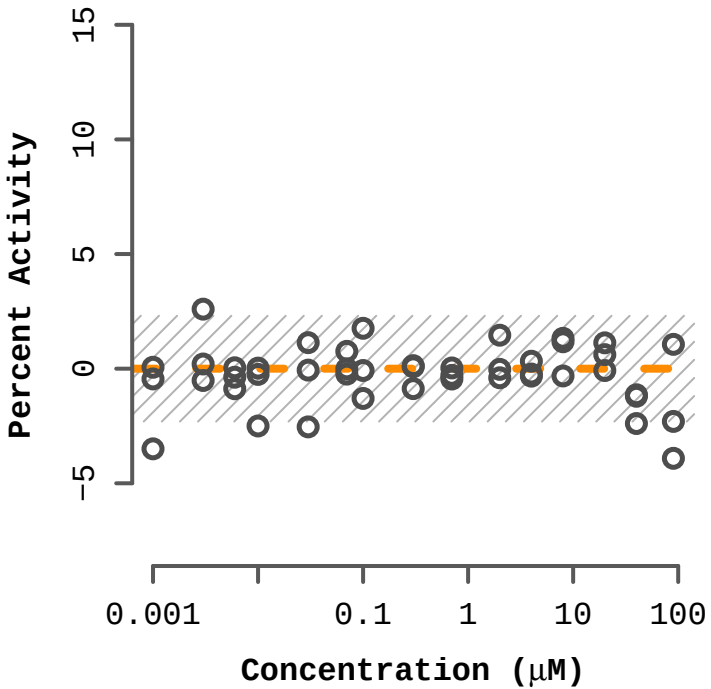
NAME: 1,1-Dimethoxy-3,7-dimethylocta-2,6-diene
CHID: 44832 **CASRN:** 7549-37-3
SPID(S): Tox21_301619
M4ID: 12477514

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

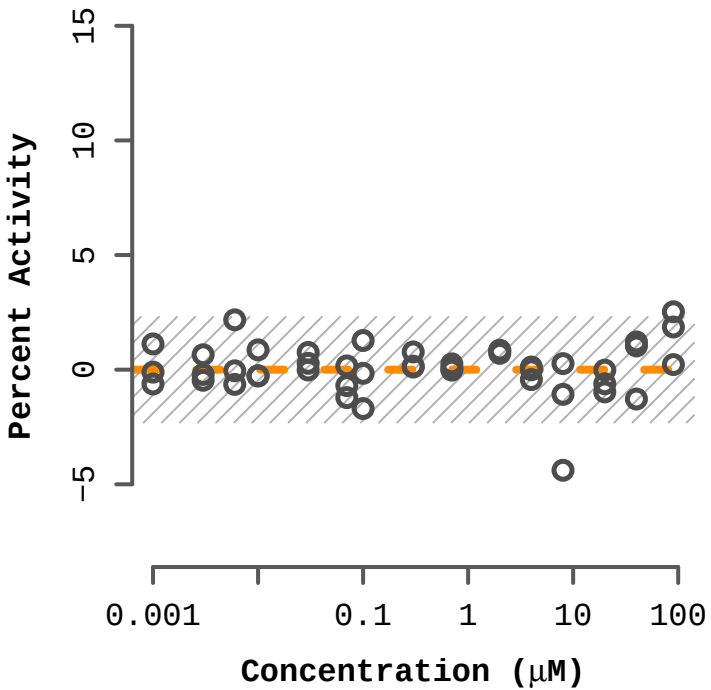
NAME: Terpinyl propionate
CHID: 44833 **CASRN:** 80-27-3
SPID(S): Tox21_301775
M4ID: 12477358

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.763 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

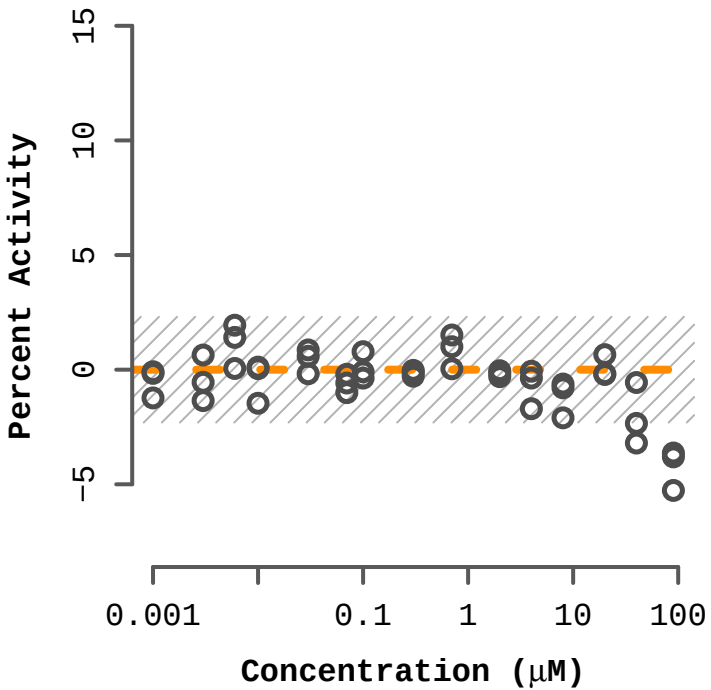
NAME: Sodium 3-(trihydroxysilyl)propyl methylphosphor
CHID: 44834 CASRN: 84962-98-1
SPID(S): Tox21_301789
M4ID: 12477344

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

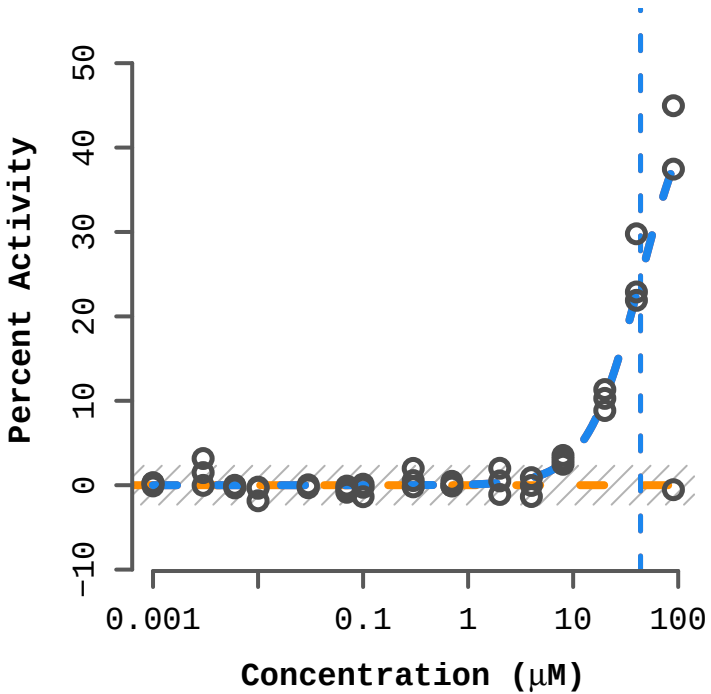
NAME: 4-{2-Oxo-2-[3-(trifluoromethyl)phenyl]ethyl}be
CHID: 44835 **CASRN:** 146653-56-7
SPID(S): Tox21_301222
M4ID: 12477911

HILL MODEL: Not applicable.

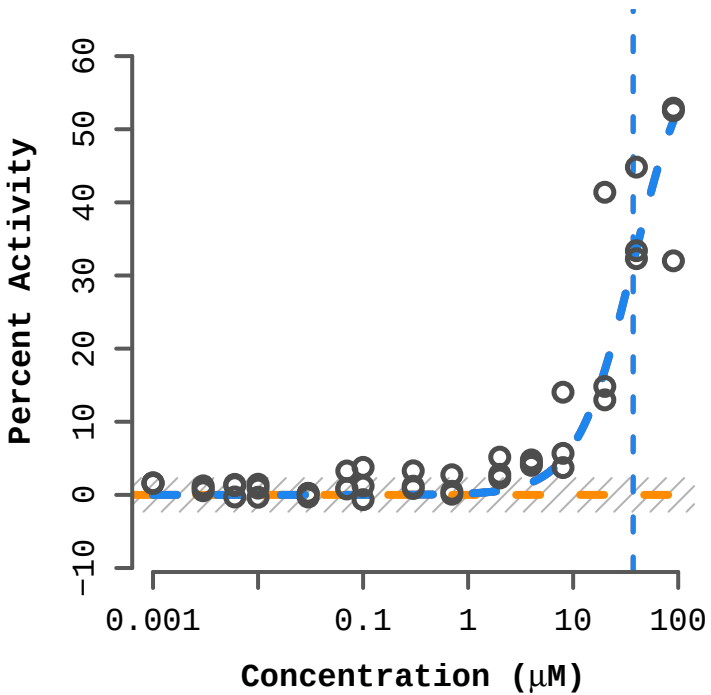
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.41 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,4,4'-Trihydroxybenzophenone
CHID:    44836   CASRN: 1470-79-7
SPID(S): Tox21_303488
M4ID:    12475653

HILL MODEL (in red):
      tp       ga       gw
val:  49       1.64     1.68
sd:   3.3      0.0427   0.124

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  49       1.64     1.68     3.47     3.71
sd:   3.59     0.0448   0.125    2020     3760

      CNST        HILL        GNLS
AIC:  298.41      185.7       189.7
PROB: 0           0.88        0.12
RMSE: 11.24       5.98        5.98

MAX_MEAN: 27.3      MAX_MED: 37.4      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4,4'−Trihydroxybenzophenone
CHID: 44836 CASRN: 1470−79−7
SPID(S): Tox21_202310
M4ID: 12479942

HILL MODEL (in red):

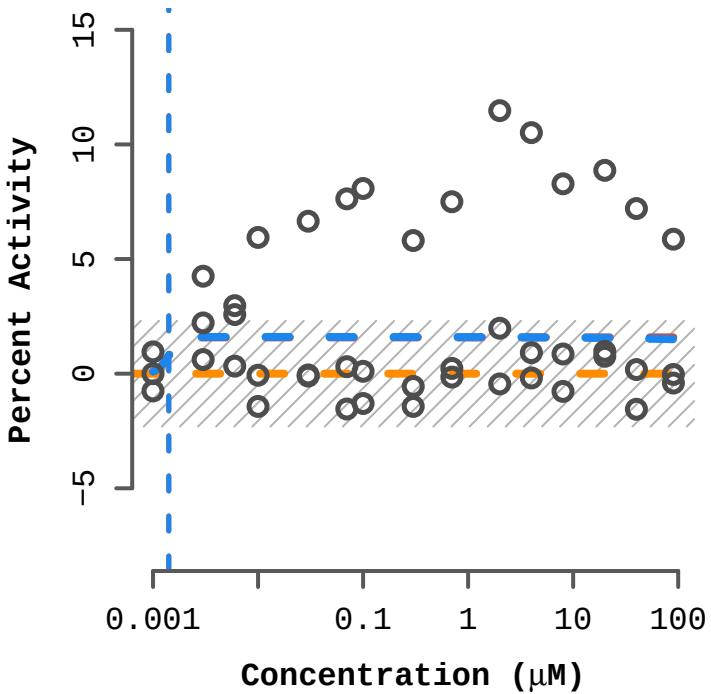
	tp	ga	gw
val:	63.5	1.57	1.61
sd:	6.34	0.0655	0.272

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	63.5	1.57	1.61	2.95	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	359.38	249.03	253.03
PROB:	0	0.88	0.12
RMSE:	17.17	5.41	5.4

MAX_MEAN: 45.8 MAX_MED: 52.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Piperidin-2-yl)ethanol
CHID: 44837 CASRN: 1484-84-0
SPID(S): Tox21_301688
M4ID: 12477445

HILL MODEL (in red):

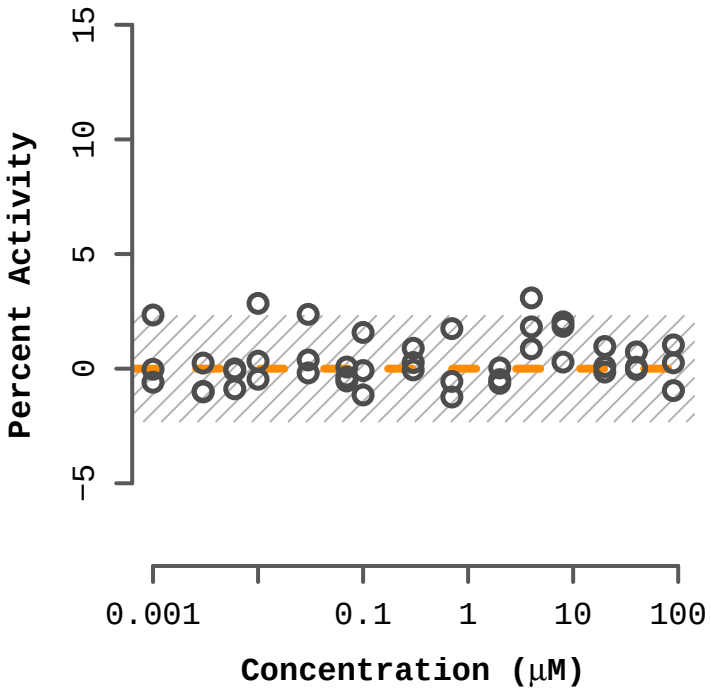
	tp	ga	gw
val:	1.58	−2.85	8
sd:	0.562	0.763	30.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.6	−2.85	8	3.95	0.586
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	255.65	252.41	256.4
PROB:	0.15	0.75	0.1
RMSE:	4.29	3.67	3.67

MAX_MEAN: 4.34 MAX_MED: 2.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

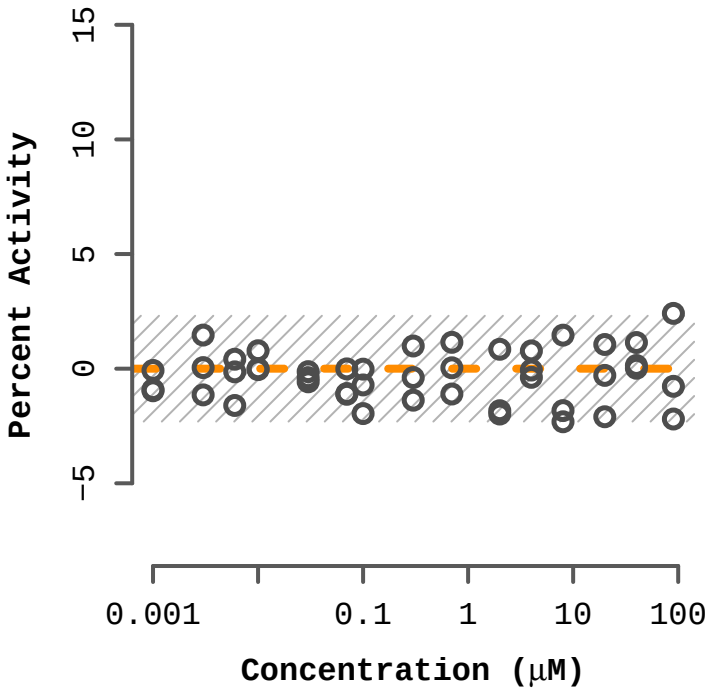
NAME: Ethenyl[tris(prop-1-en-2-yloxy)]silane
CHID: 44839 **CASRN:** 15332-99-7
SPID(S): Tox21_301759
M4ID: 12477374

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

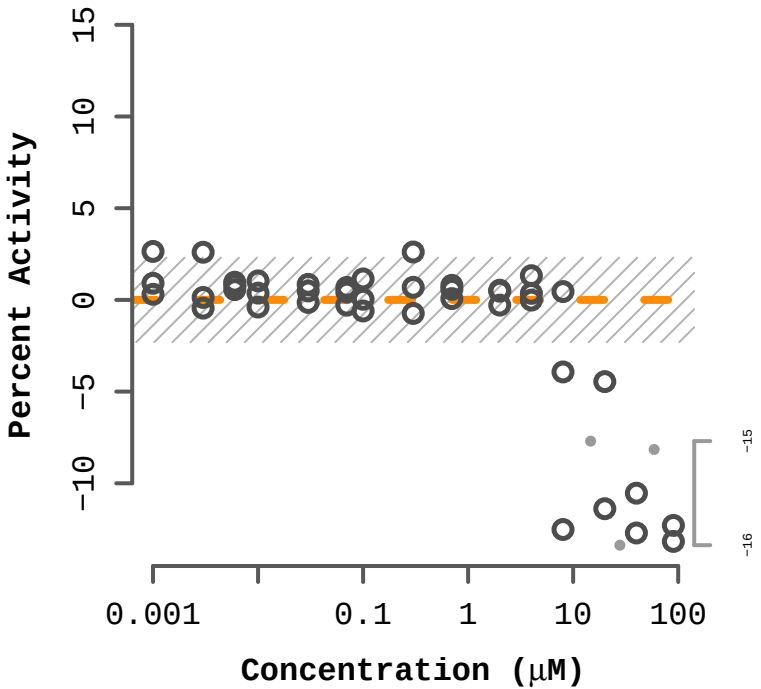
NAME: Sodium 2-methylprop-2-ene-1-sulfonate
CHID: 44840 CASRN: 1561-92-8
SPID(S): Tox21_301717
M4ID: 12477416

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.434 MAX_MED: 0.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

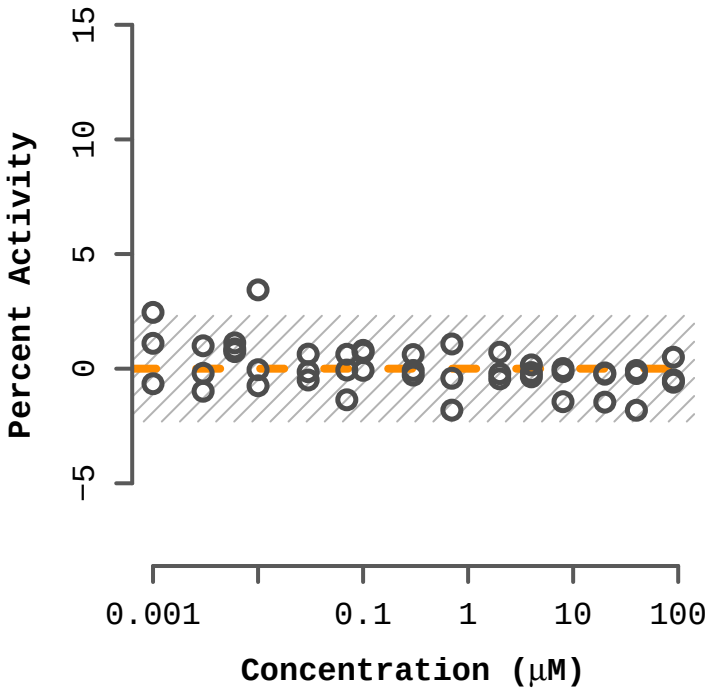
NAME: Bisphenol A glycidyl methacrylate
CHID: 44841 **CASRN:** 1565-94-2
SPID(S): Tox21_301683
M4ID: 12477450 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.75	NA	NA
PROB:	1	NA	NA
RMSE:	6.11	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.908 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

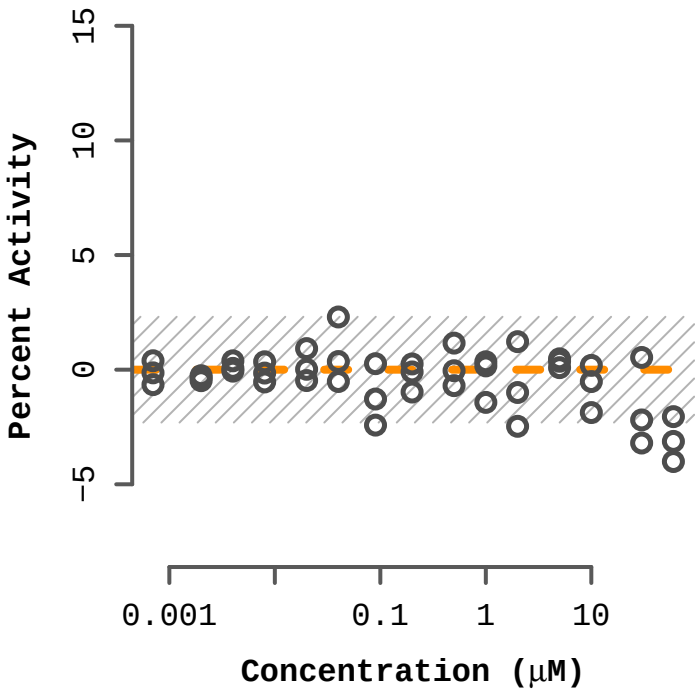
NAME: N,N',N''-Tricyclohexyl-1-methylsilanetriamine
CHID: 44842 **CASRN:** 15901-40-3
SPID(S): Tox21_301786
M4ID: 12477347

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.97 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

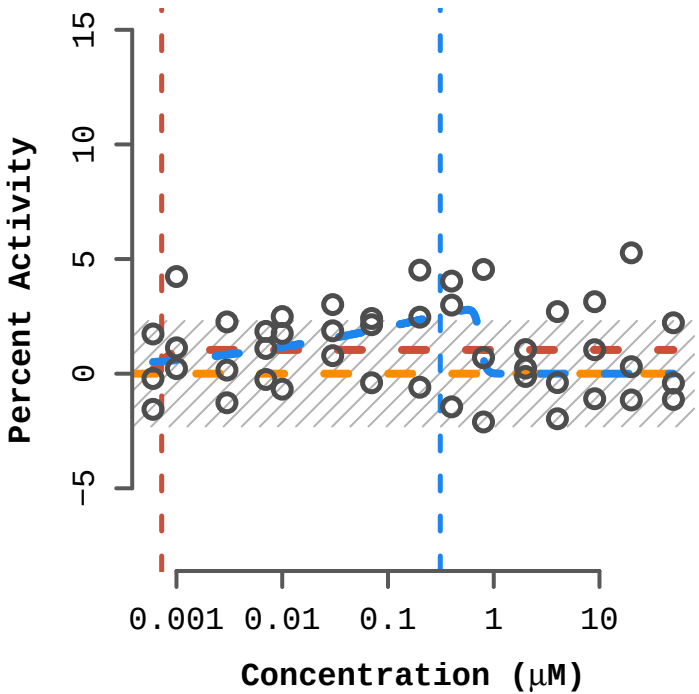
NAME: Erythrosin B
CHID: 44843 CASRN: 15905-32-5
SPID(S): Tox21_301634
M4ID: 12477499

HILL MODEL: Not applicable.

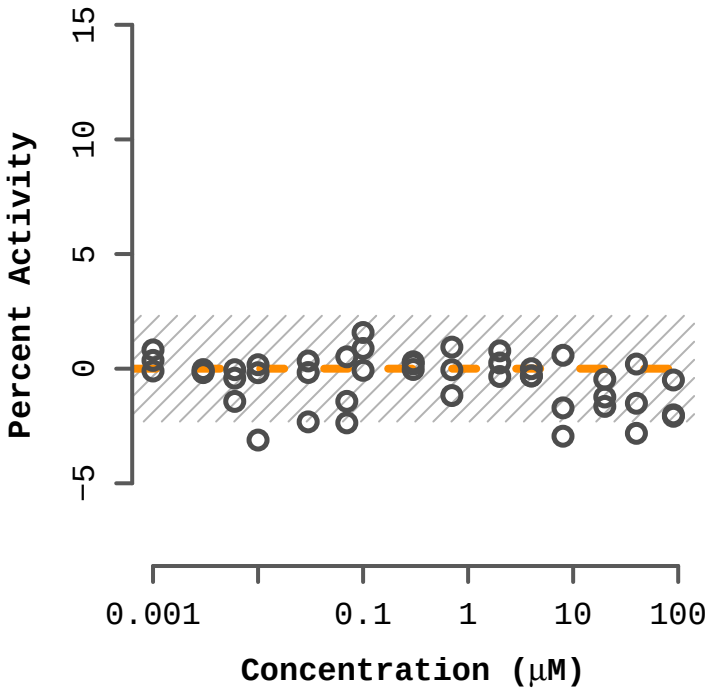
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.714 MAX_MED: 0.367 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Erythrosin B
CHID:    44843   CASRN: 15905-32-5
SPID(S): Tox21_113464_1
M4ID:    12482643

HILL MODEL (in red):
      tp       ga       gw
val:  1.04     -3.14    8
sd:   0.314    0.198    14.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.09     -0.505   0.353    -0.129   17.3
sd:   21.7     10.1     0.741    2.06     1120

      CNST        HILL        GNLS
AIC:  201.29      196.68      196.41
PROB: 0.04        0.45        0.51
RMSE: 2.16        1.86        1.88

MAX_MEAN: 2.13      MAX_MED: 2.99      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

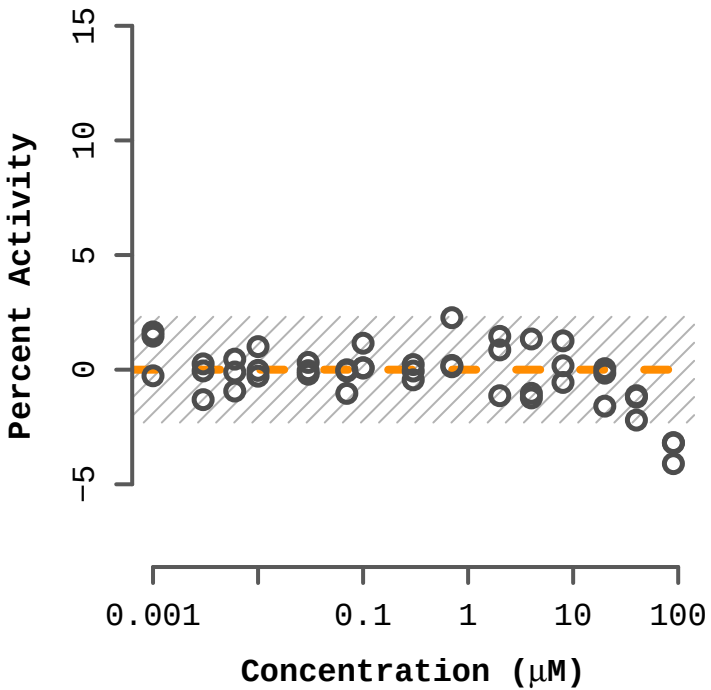
NAME: 3-(Octyloxy)propan-1-amine
CHID: 44844 **CASRN:** 15930-66-2
SPID(S): Tox21_301777
M4ID: 12477356

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.797 **MAX_MED:** 0.883 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

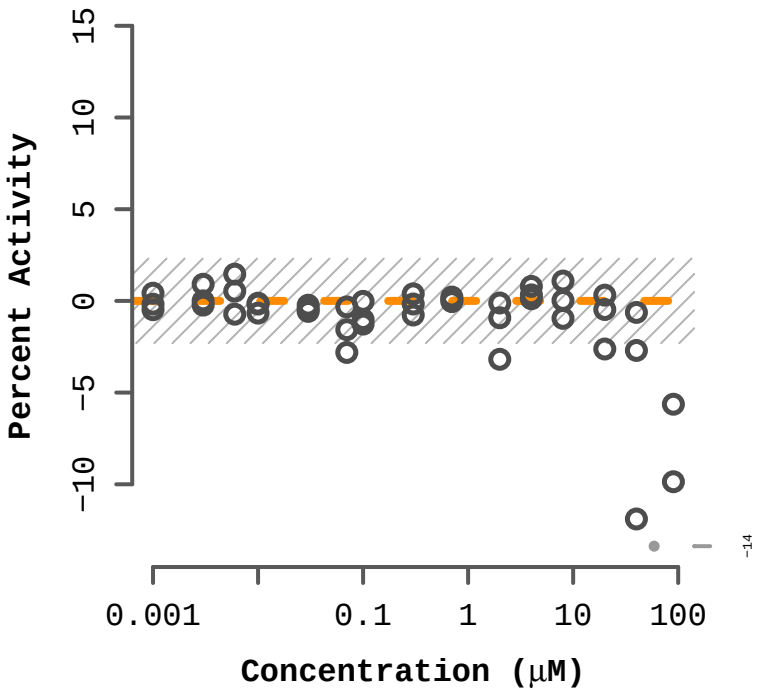
NAME: Butyl 3-mercaptopropionate
CHID: 44845 **CASRN:** 16215-21-7
SPID(S): Tox21_301649
M4ID: 12477484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.949 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

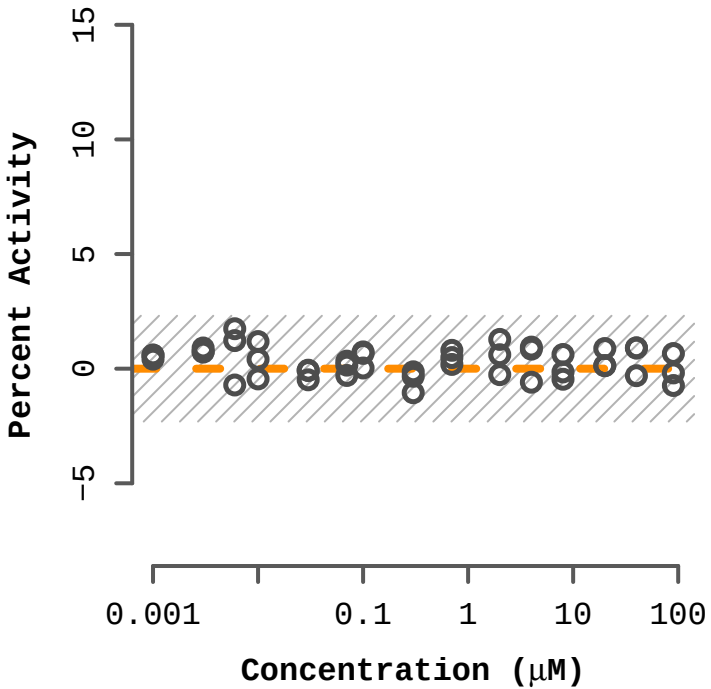
NAME: 4-Chloro-3-nitrobenzaldehyde
CHID: 44846 **CASRN:** 16588-34-4
SPID(S): Tox21_301612
M4ID: 12477521 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.61	NA	NA
PROB:	1	NA	NA
RMSE:	3.34	NA	NA

MAX_MEAN: 0.423 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

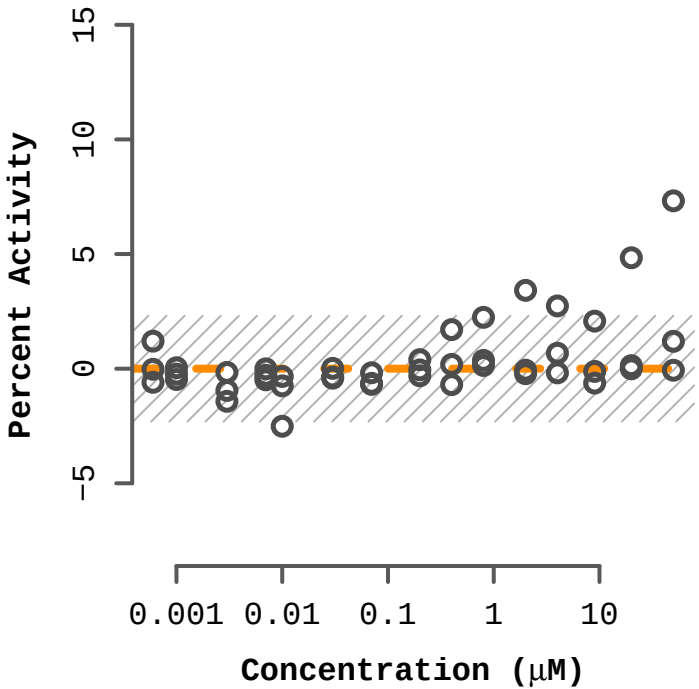
NAME: Tetraisopropyl methylenediphosphonate
CHID: 44847 **CASRN:** 1660-95-3
SPID(S): Tox21_301267
M4ID: 12477866

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.794 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

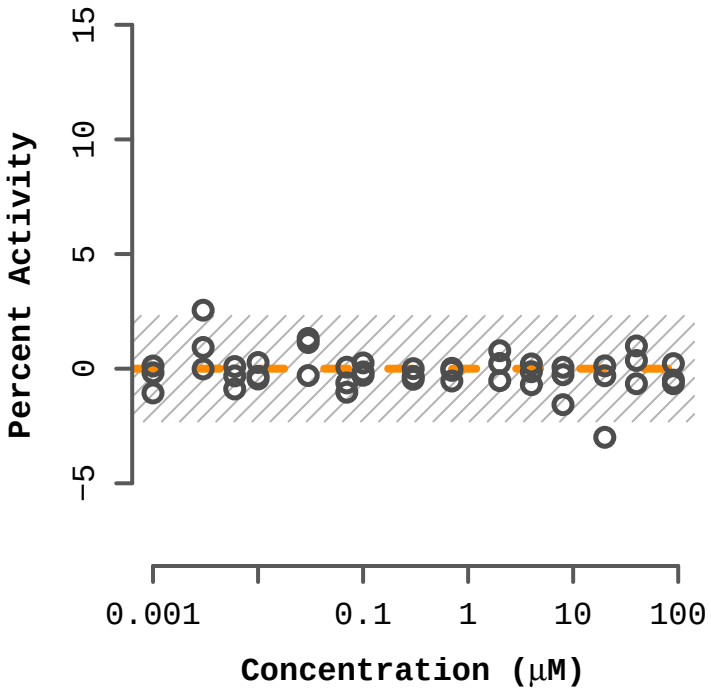
NAME: Tetraisopropyl methylenediphosphonate
CHID: 44847 **CASRN:** 1660-95-3
SPID(S): Tox21_113797
M4ID: 12482422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 2.82 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

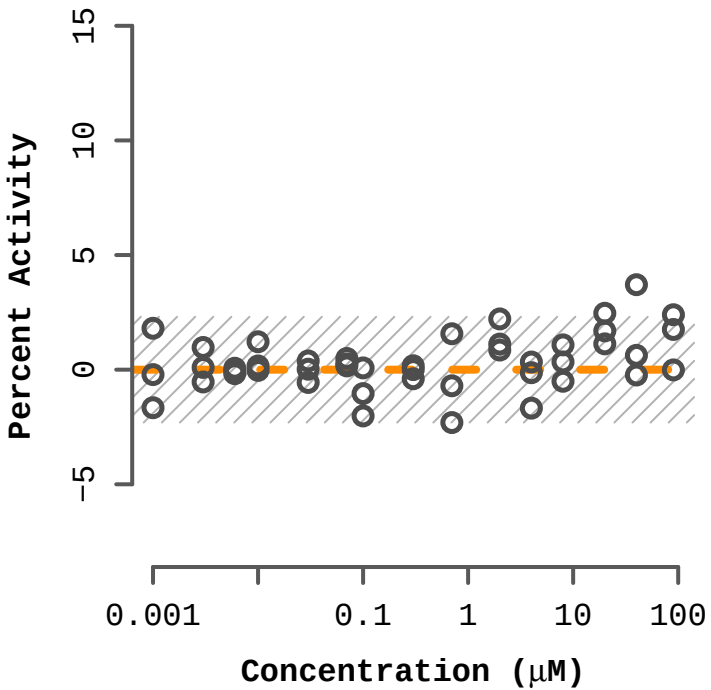
NAME: N-(Isobutoxymethyl)acrylamide
CHID: 44848 **CASRN:** 16669-59-3
SPID(S): Tox21_301403
M4ID: 12477730

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

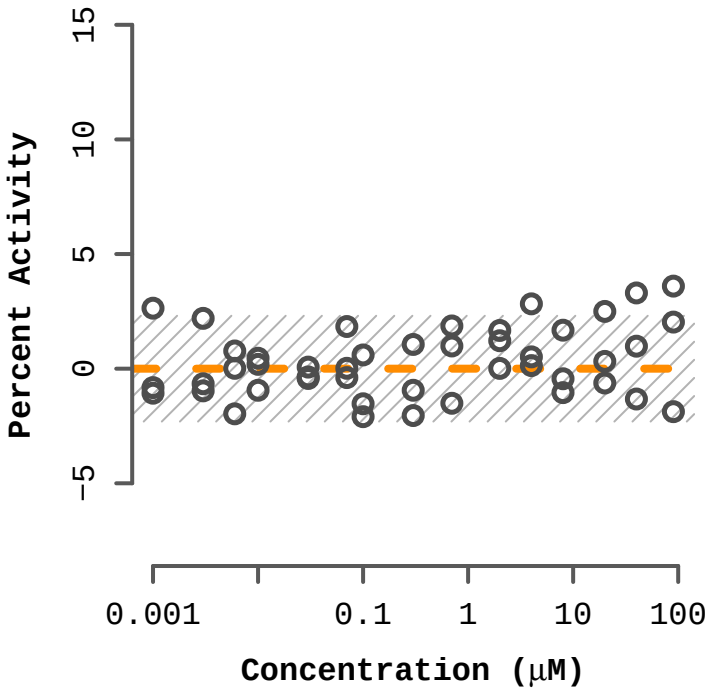
NAME: 5-Amino-1,2-dihydro-3H-1,2,4-triazole-3-thione
CHID: 44849 **CASRN:** 16691-43-3
SPID(S): Tox21_301609
M4ID: 12477524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

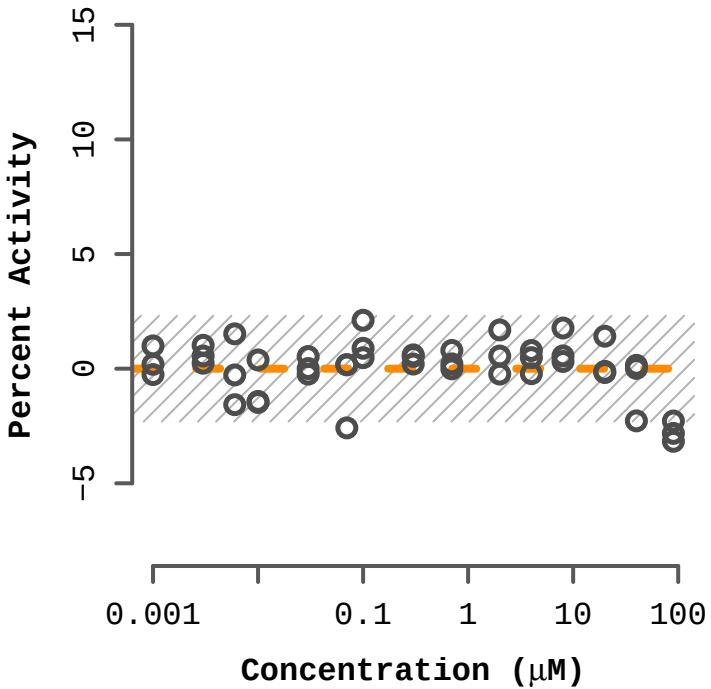
NAME: 2-Hydroxy-3-phenoxypropyl prop-2-enoate
CHID: 44851 CASRN: 16969-10-1
SPID(S): Tox21_301706
M4ID: 12477427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

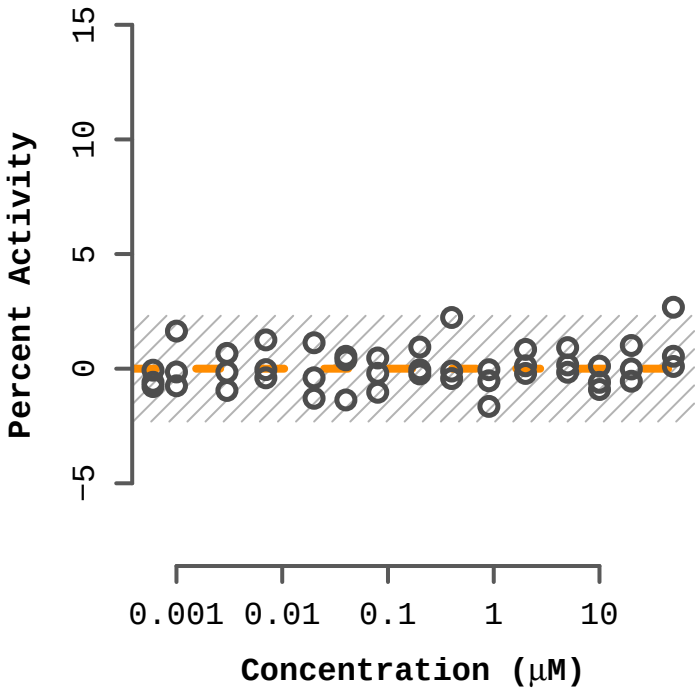
NAME: 4,4'-Propane-1,3-diyldipyridine
CHID: 44852 **CASRN:** 17252-51-6
SPID(S): Tox21_301632
M4ID: 12477501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

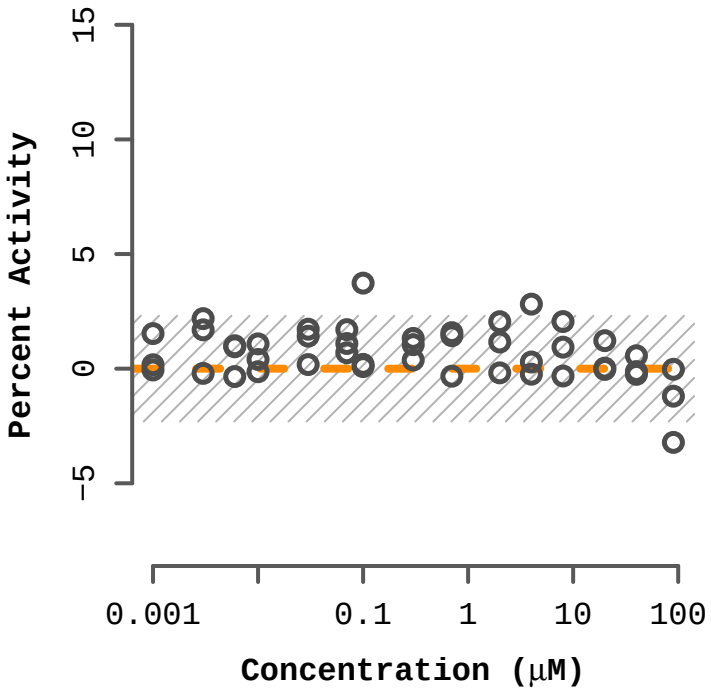
NAME: Trisodium 2,4,6-trithioxo-1,3,5-triazinane-1,3,
CHID: 44853 **CASRN:** 17766-26-6
SPID(S): Tox21_301278
M4ID: 12477855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.542 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

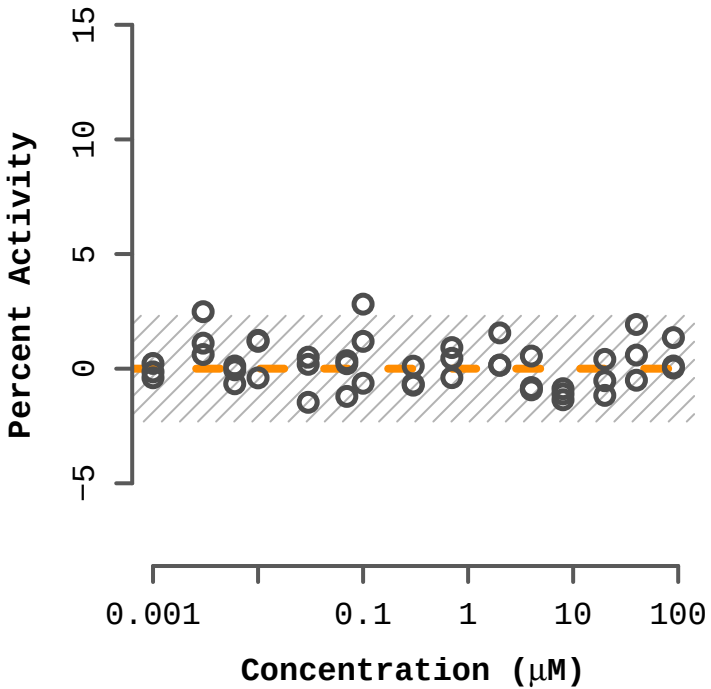
NAME: 4-(Ethenyloxy)butan-1-ol
CHID: 44854 **CASRN:** 17832-28-9
SPID(S): Tox21_301676
M4ID: 12477457

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

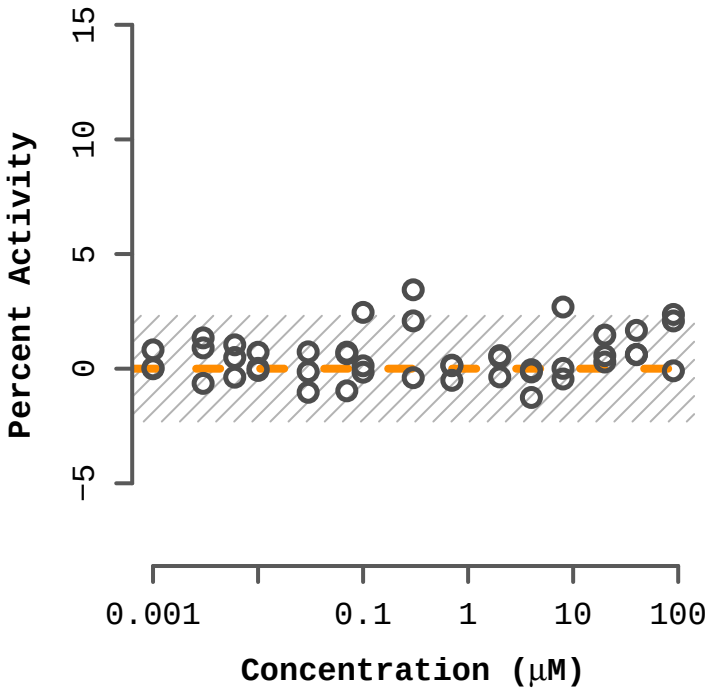
NAME: Ethyl [3-(triethoxysilyl)propyl]carbamate
CHID: 44856 CASRN: 17945-05-0
SPID(S): Tox21_301794
M4ID: 12477339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

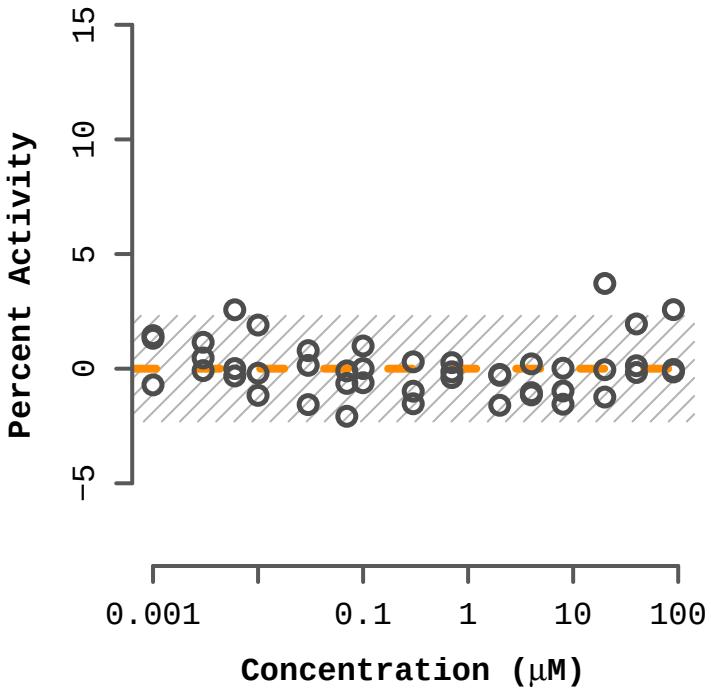
NAME: Triethoxy(2−methylpropyl)silane
CHID: 44857 **CASRN:** 17980−47−1
SPID(S): Tox21_301397
M4ID: 12477736

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.71 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

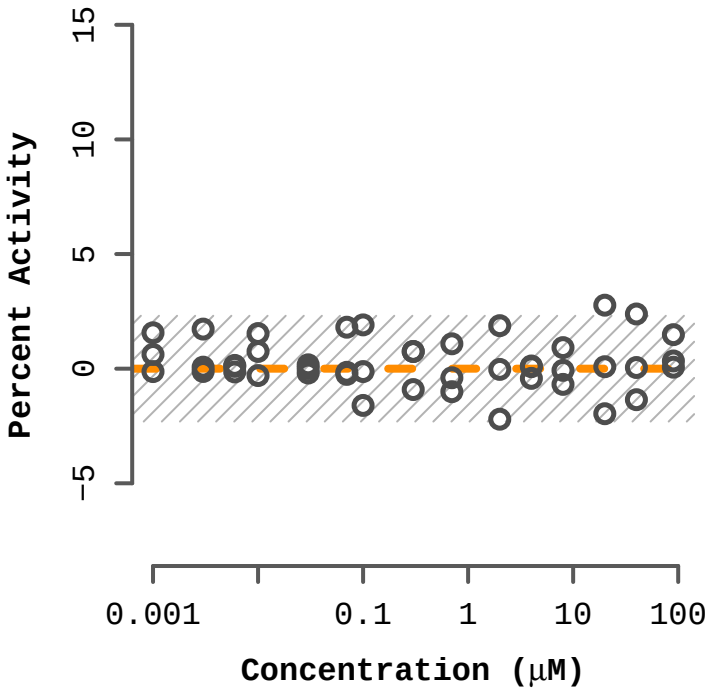
NAME: 5-Phenyl-1H-tetrazole
CHID: 44858 **CASRN:** 18039-42-4
SPID(S): Tox21_301684
M4ID: 12477449

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.812 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

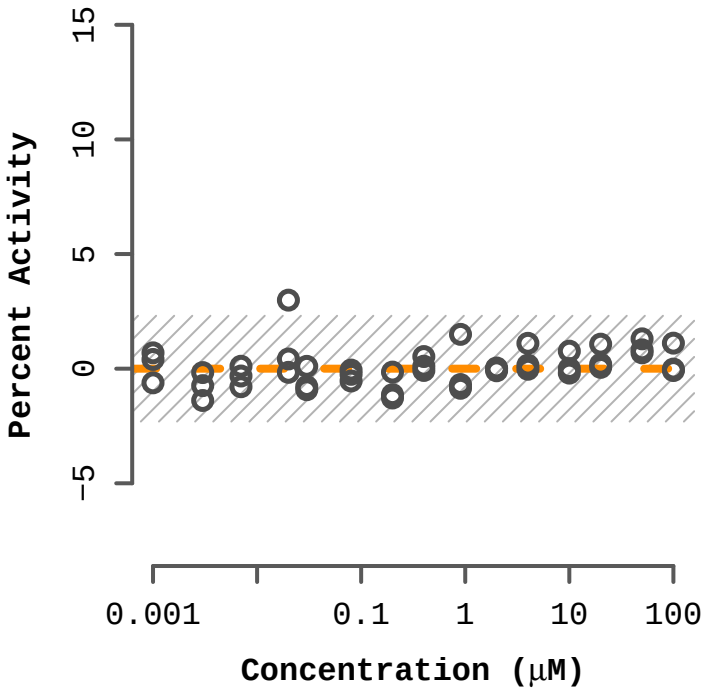
NAME: 5,5'−Oxybis(2−benzofuran−1,3−dione)
CHID: 44859 **CASRN:** 1823−59−2
SPID(S): Tox21_300877
M4ID: 12478256

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

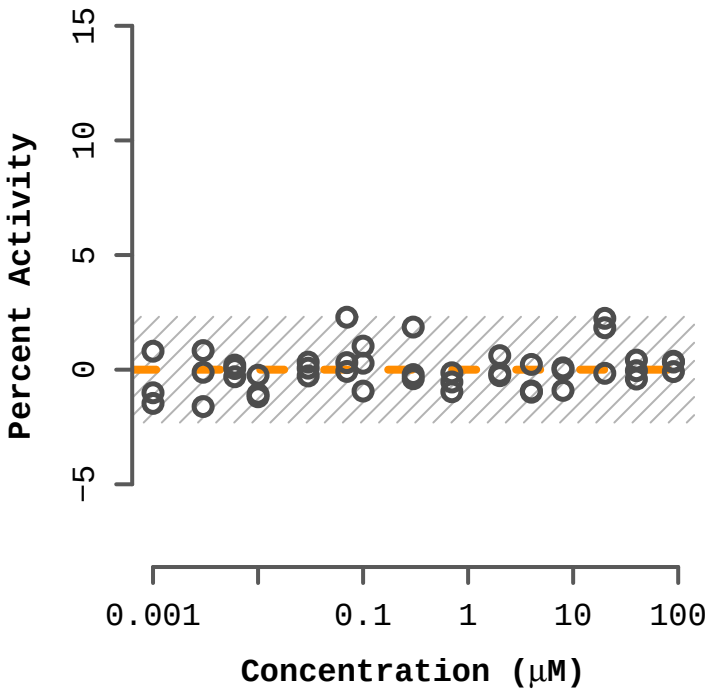
NAME: 6-Methylpyridin-2-amine
CHID: 44860 **CASRN:** 1824-81-3
SPID(S): Tox21_300667
M4ID: 12478466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

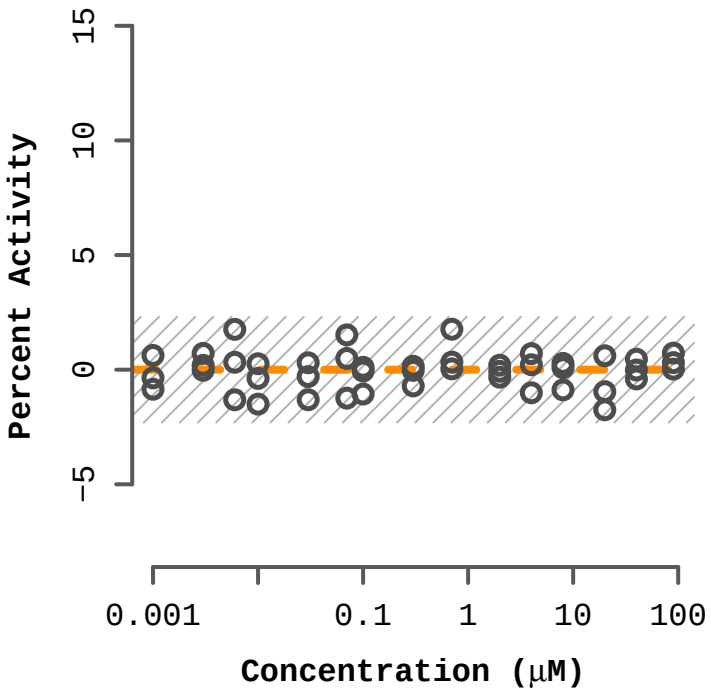
NAME: Undecanedioic acid
CHID: 44862 **CASRN:** 1852-04-6
SPID(S): Tox21_300954
M4ID: 12478179

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

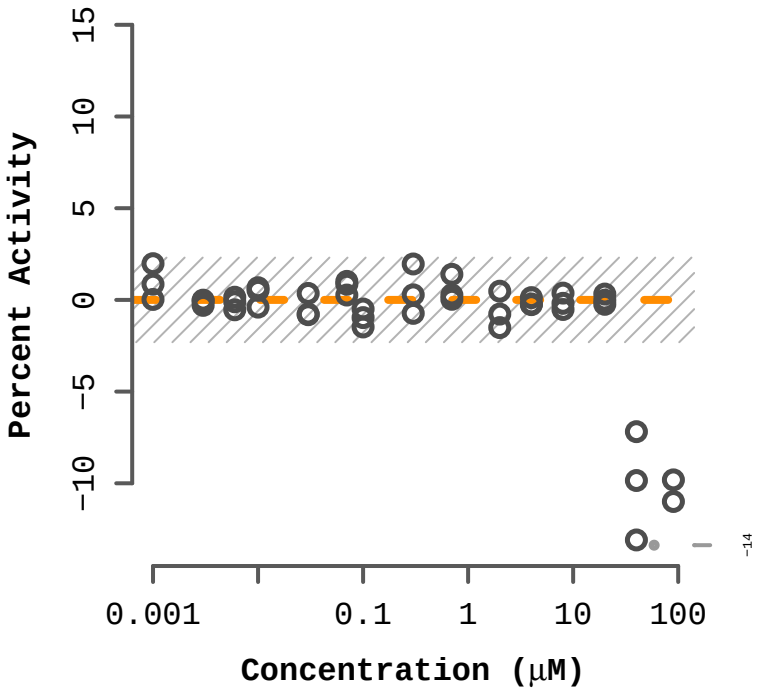
NAME: Ethyl 3-acetyl-4-oxopentanoate
CHID: 44863 **CASRN:** 18835-02-4
SPID(S): Tox21_301225
M4ID: 12477908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.71 **MAX_MED:** 0.489 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

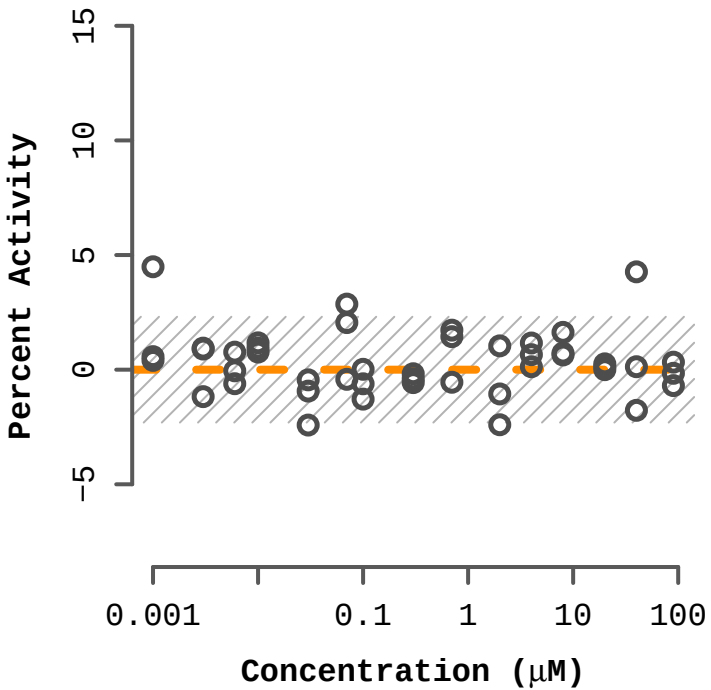
NAME: 2,2'−(Tetradecylimino)diethanol
CHID: 44865 CASRN: 18924−66−8
SPID(S): Tox21_301234
M4ID: 12477899 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.15	NA	NA
PROB:	1	NA	NA
RMSE:	4.09	NA	NA

MAX_MEAN: 0.954 MAX_MED: 0.857 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

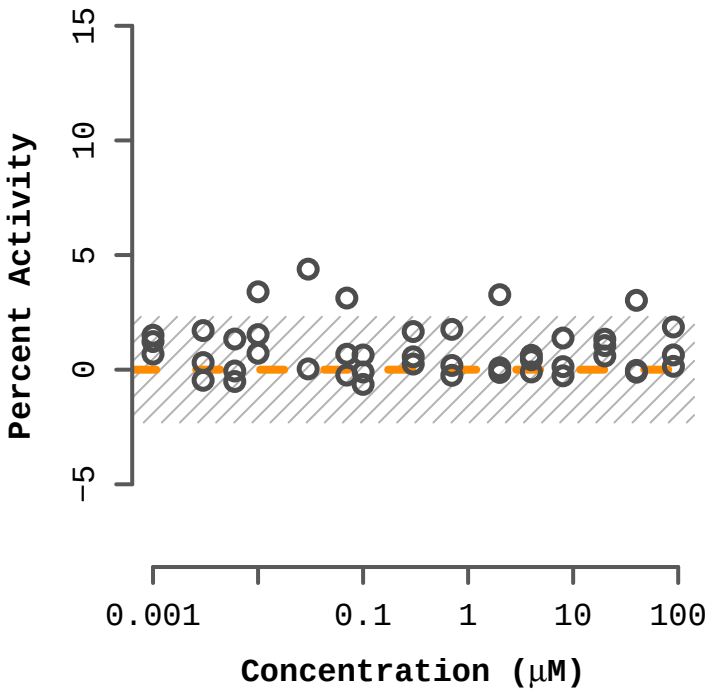
NAME: 2,2−Dimethylpropane−1,3−diyl bis(2−methylprop−2
CHID: 44867 CASRN: 1985−51−9
SPID(S): Tox21_301663
M4ID: 12477470

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.82 MAX_MED: 2.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

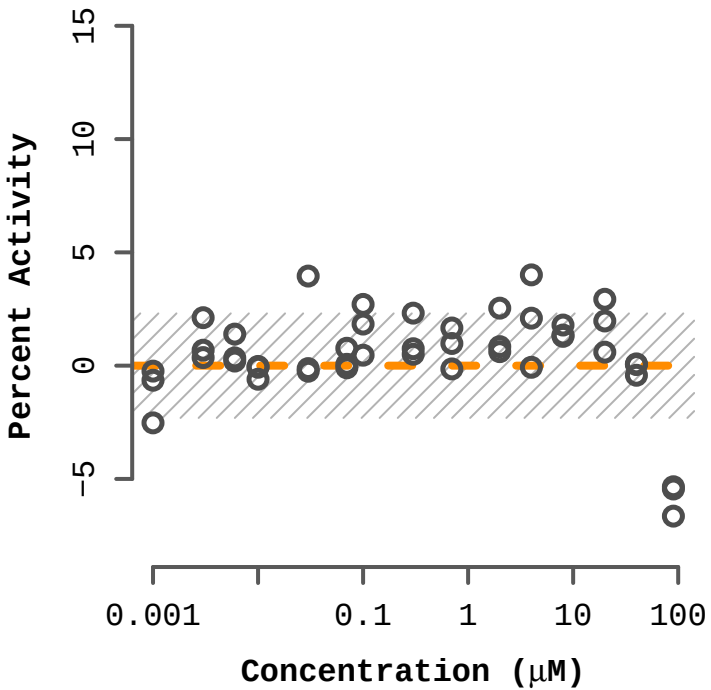
NAME: N-(2,4-Dimethylphenyl)acetamide
CHID: 44868 **CASRN:** 2050-43-3
SPID(S): Tox21_301646
M4ID: 12477487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

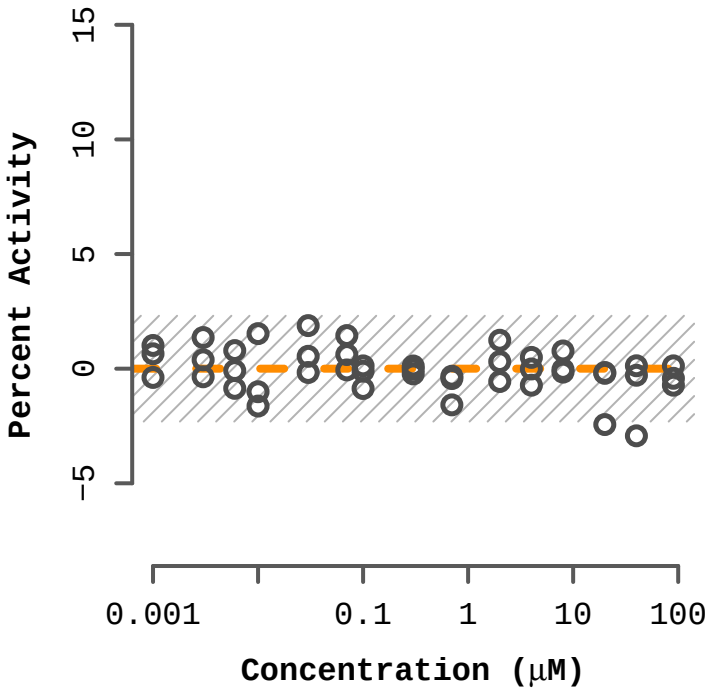
NAME: 4-(3-Phenylpropyl)pyridine
CHID: 44869 **CASRN:** 2057-49-0
SPID(S): Tox21_301719
M4ID: 12477414

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.12	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

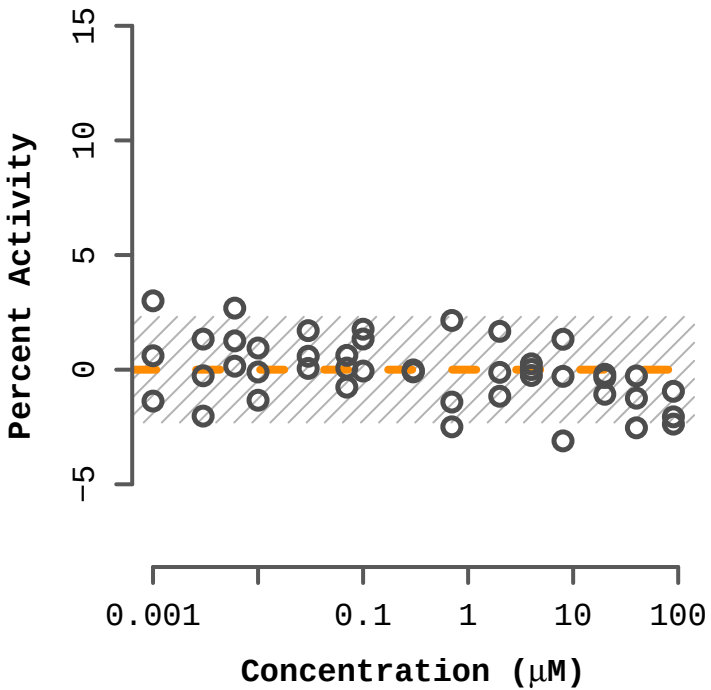
NAME: Butane−1,4−diyl bis(2−methylprop−2−enoate)
CHID: 44870 **CASRN:** 2082−81−7
SPID(S): Tox21_301681
M4ID: 12477452

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.752 **MAX_MED:** 0.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

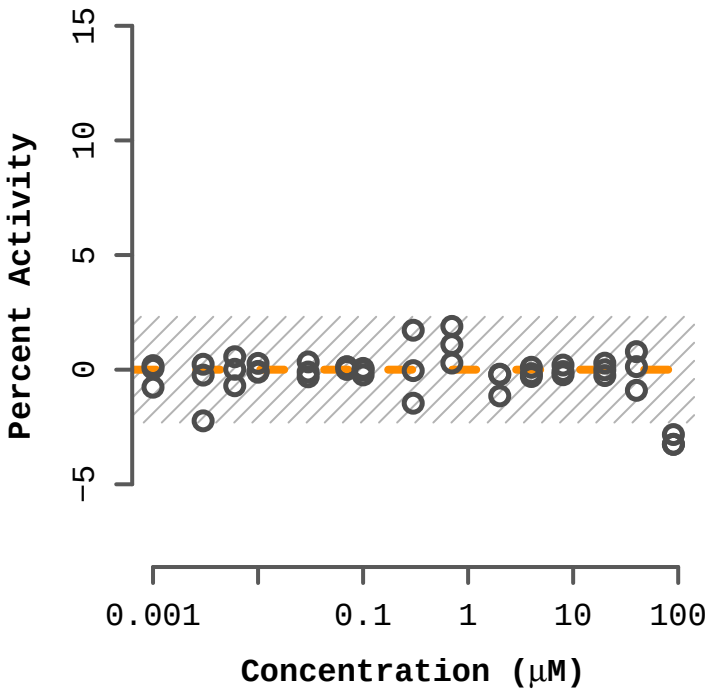
NAME: 1-(2-Isocyanatopropan-2-yl)-3-(prop-1-en-2-yl)|
CHID: 44871 CASRN: 2094-99-7
SPID(S): Tox21_301716
M4ID: 12477417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

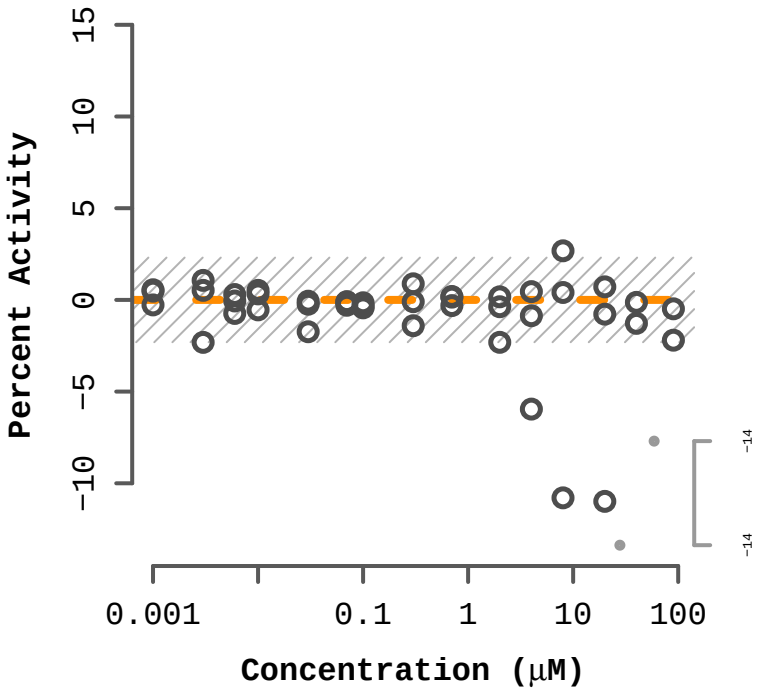
NAME: Bis[4−(glycidyloxy)phenyl]methane
CHID: 44872 CASRN: 2095−03−6
SPID(S): Tox21_303420
M4ID: 12475719

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

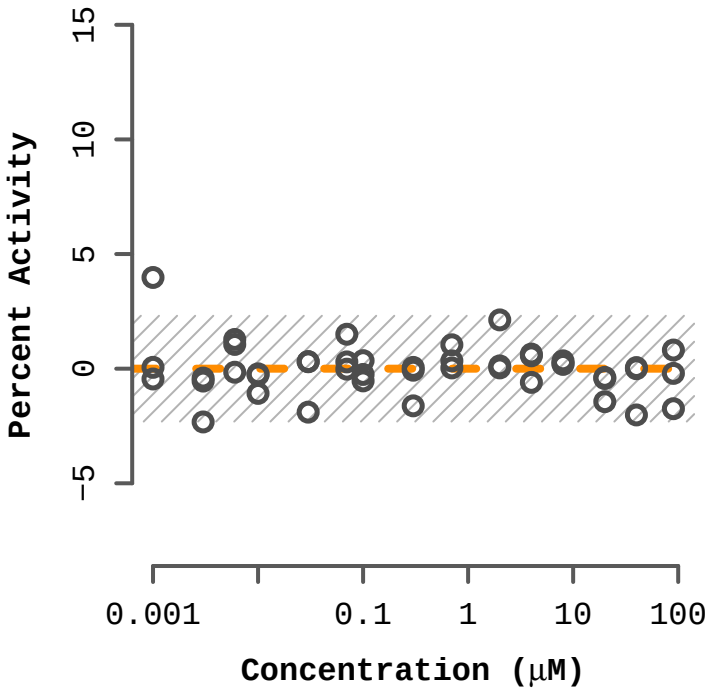
NAME: Bis[4−(glycidyloxy)phenyl]methane
CHID: 44872 **CASRN:** 2095−03−6
SPID(S): Tox21_201598
M4ID: 12480654 **BRK**

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.95	NA	NA
PROB:	1	NA	NA
RMSE:	3.9	NA	NA

MAX_MEAN: 0.255 **MAX_MED:** 0.522 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

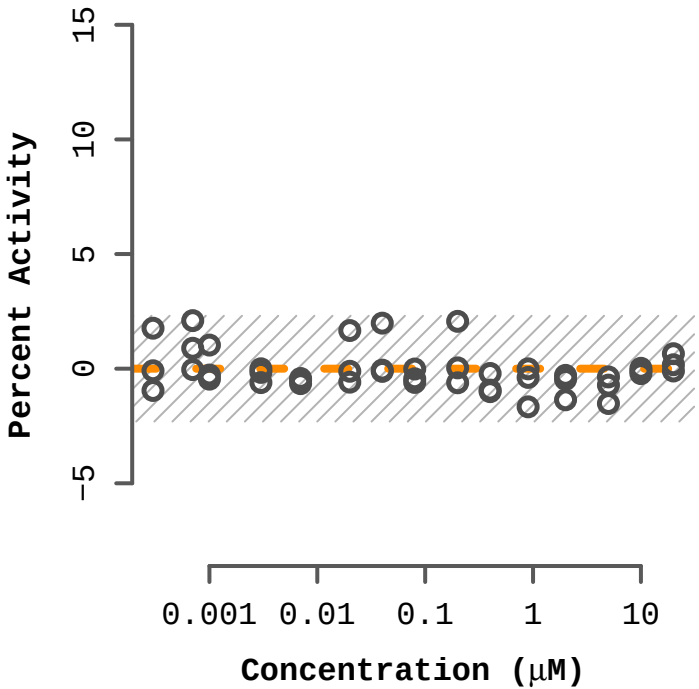
NAME: Decyl prop-2-enoate
CHID: 44873 **CASRN:** 2156-96-9
SPID(S): Tox21_301739
M4ID: 12477394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

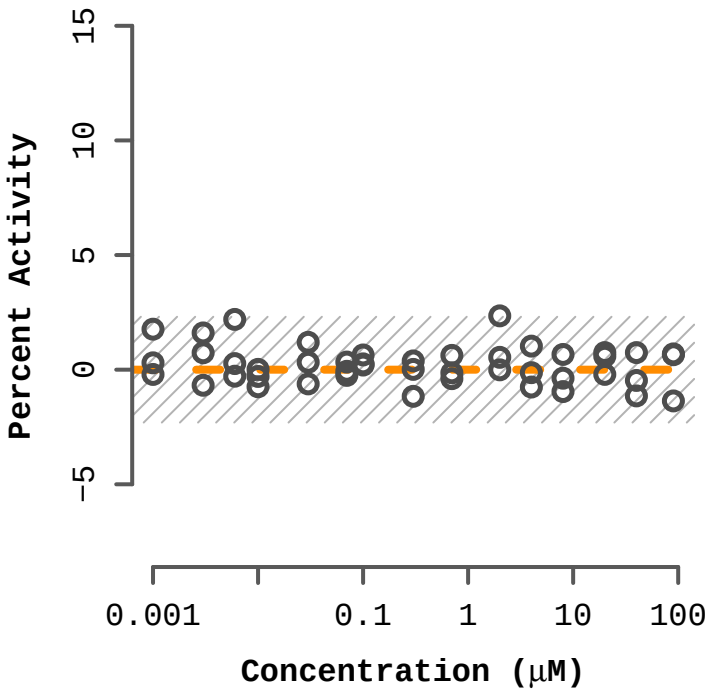
NAME: 2,2-Bis(tert-butylperoxy)butane
CHID: 44874 **CASRN:** 2167-23-9
SPID(S): Tox21_303782
M4ID: 12475406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.983 **MAX_MED:** 0.891 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

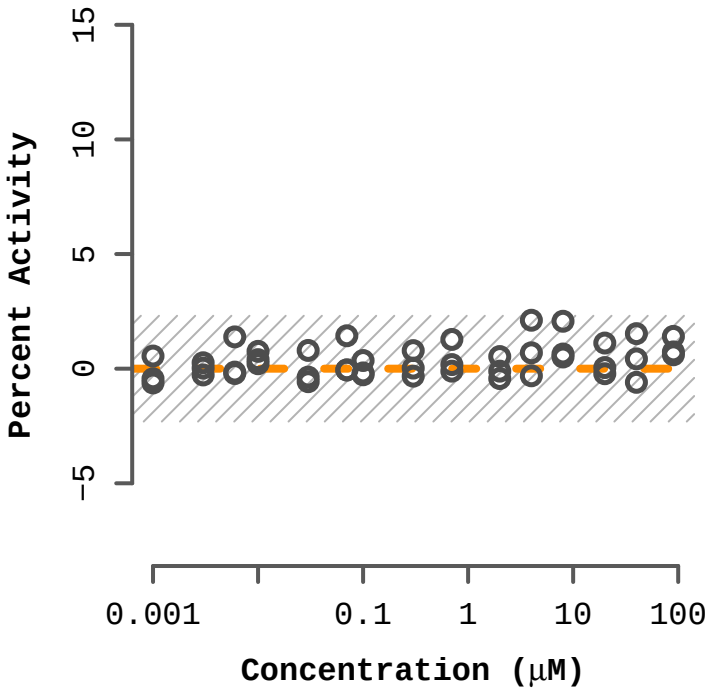
NAME: 2−{[2−(Dimethylamino)ethyl](methyl)amino}ethan
CHID: 44875 CASRN: 2212−32−0
SPID(S): Tox21_301721
M4ID: 12477412

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.961 **MAX_MED:** 0.739 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

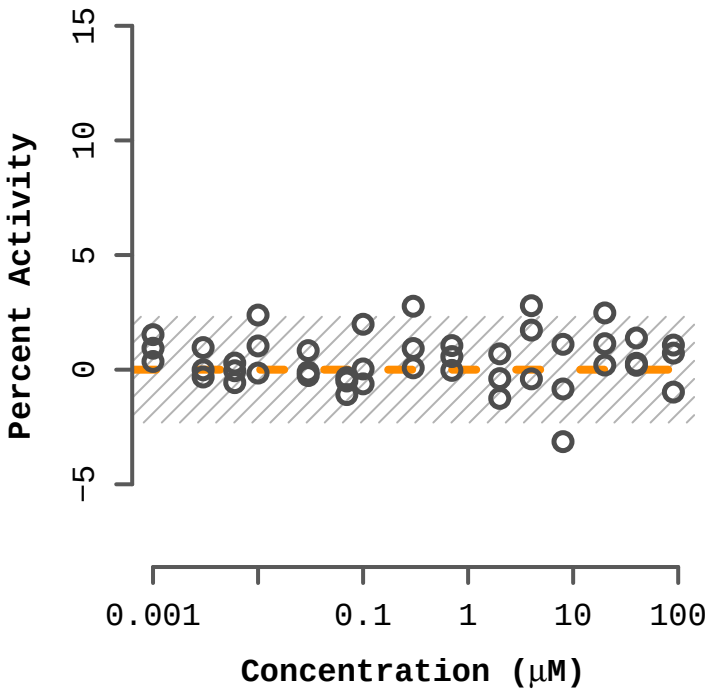
NAME: Ethylene glycol diglycidyl ether
CHID: 44876 CASRN: 2224-15-9
SPID(S): Tox21_301732
M4ID: 12477401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.733 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

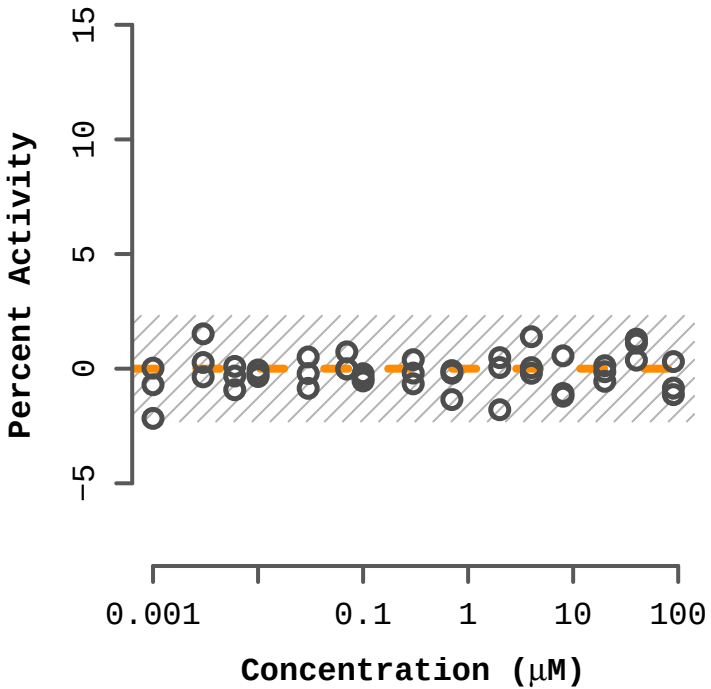
NAME: N-(3-Aminophenyl)propanamide
CHID: 44877 **CASRN:** 22987-10-6
SPID(S): Tox21_301647
M4ID: 12477486

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

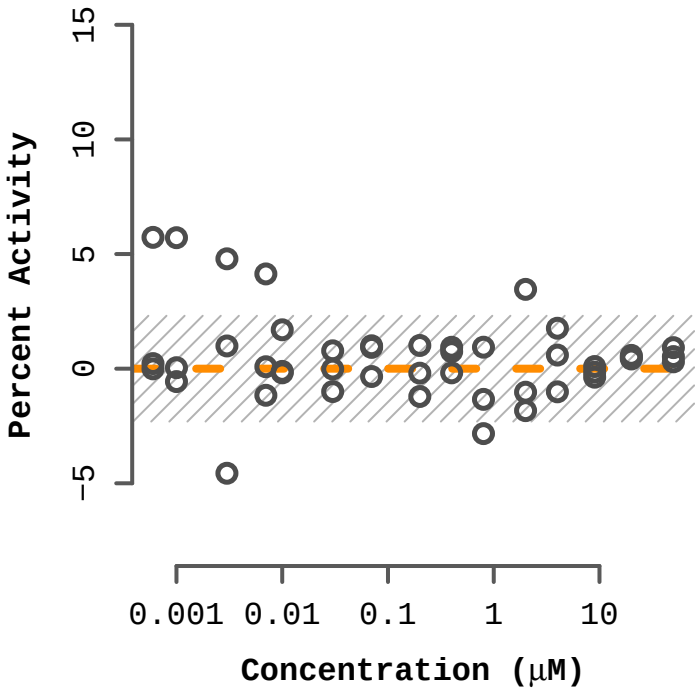
NAME: Propyl benzoate
CHID: 44878 **CASRN:** 2315-68-6
SPID(S): Tox21_301605
M4ID: 12477528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.926 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

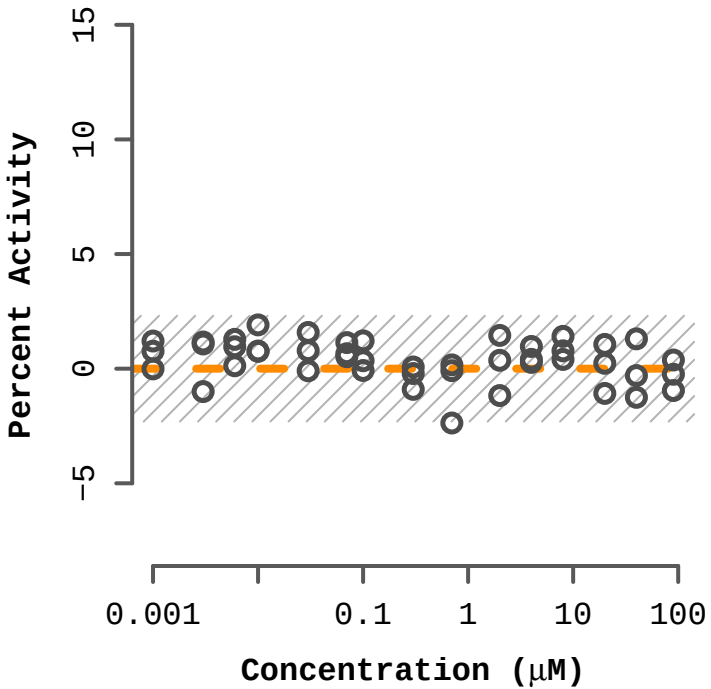
NAME: Propyl benzoate
CHID: 44878 **CASRN:** 2315-68-6
SPID(S): Tox21_111621_1
M4ID: 12483580

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 1.98 **MAX_MED:** 0.992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

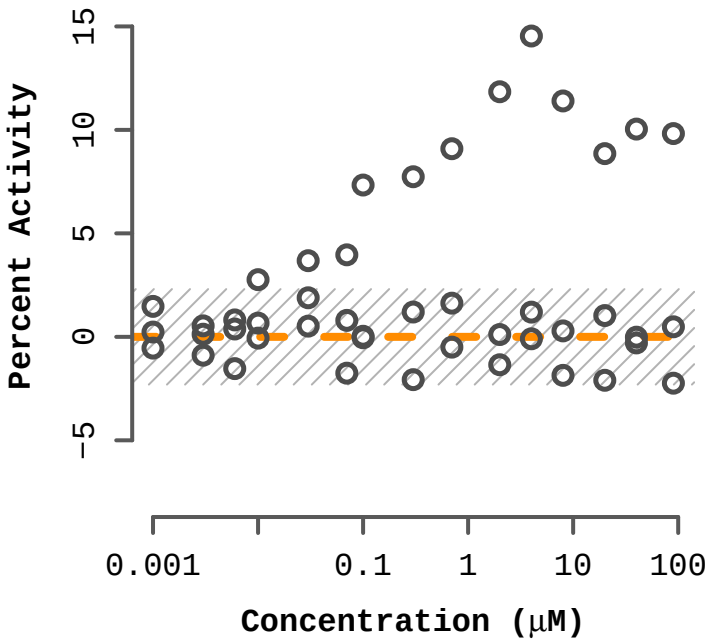
NAME: 2,2'−(Oxydimethanediyl)bis(2−ethylpropane−1,3−(
CHID: 44879 **CASRN:** 23235−61−2
SPID(S): Tox21_301690
M4ID: 12477443

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

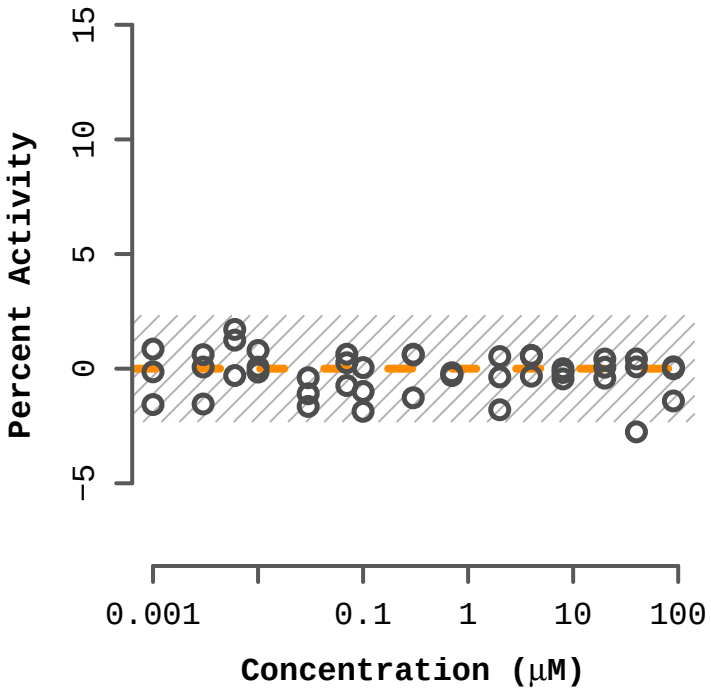
NAME: 2-[2-(2-Propoxyethoxy)ethoxy]ethanol
CHID: 44880 CASRN: 23305-64-8
SPID(S): Tox21_301227
M4ID: 12477906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.25	NA	NA
PROB:	1	NA	NA
RMSE:	4.79	NA	NA

MAX_MEAN: 5.21 MAX_MED: 1.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

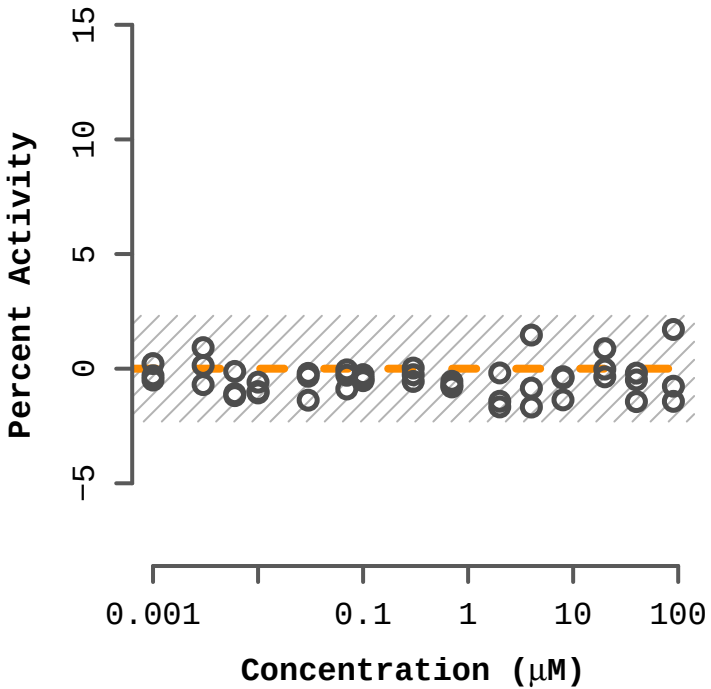
NAME: Methyl [3-(trimethoxysilyl)propyl]carbamate
CHID: 44881 **CASRN:** 23432-62-4
SPID(S): Tox21_301806
M4ID: 12477327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.888 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

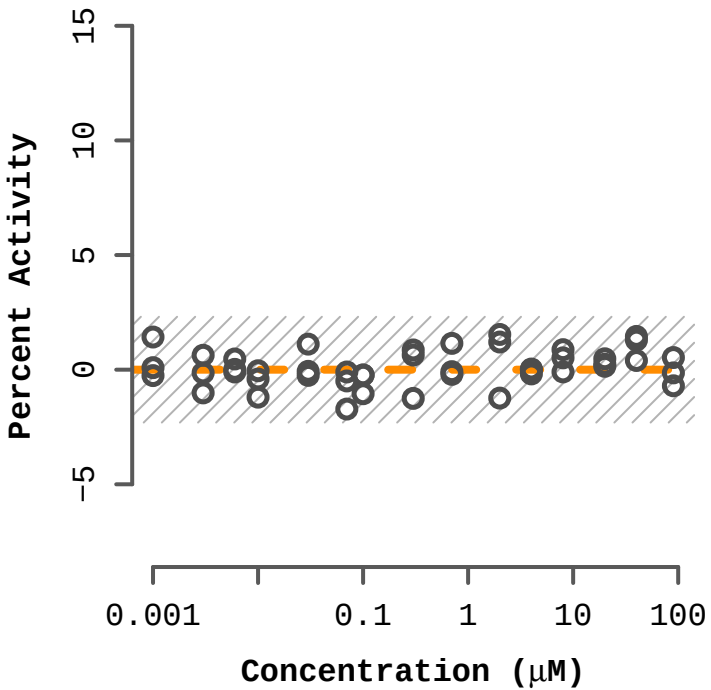
NAME: Di(ethylene glycol) dimethacrylate
CHID: 44882 CASRN: 2358-84-1
SPID(S): Tox21_301734
M4ID: 12477399

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.167 **MAX_MED:** 0.143 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

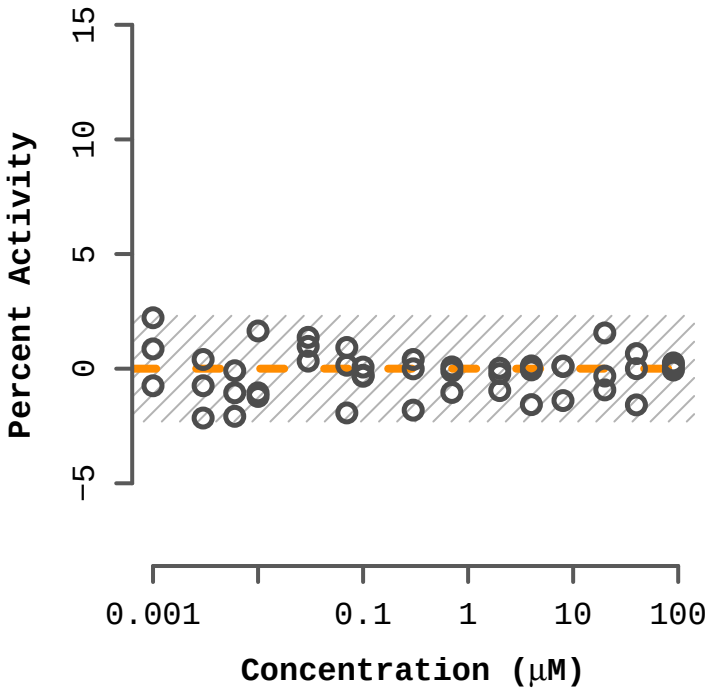
NAME: Butane−1−sulfonyl chloride
CHID: 44883 **CASRN:** 2386−60−9
SPID(S): Tox21_301687
M4ID: 12477446

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

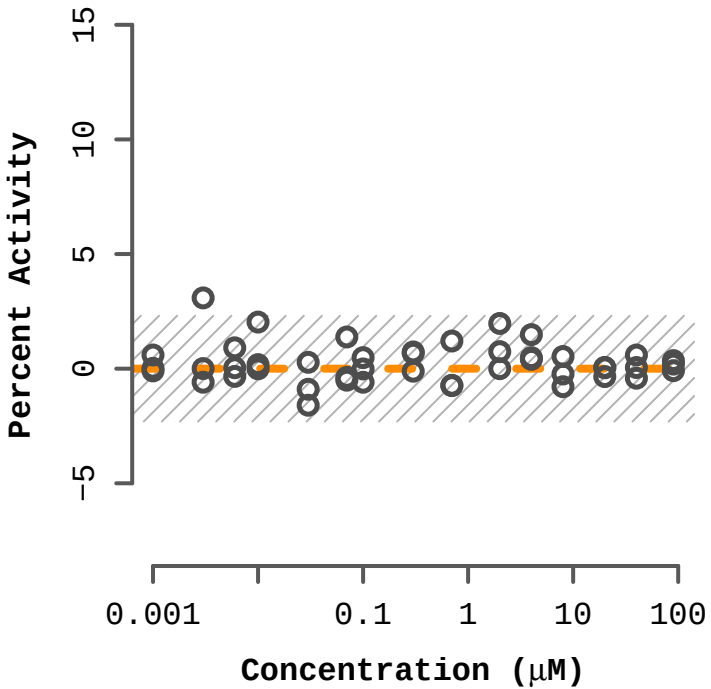
NAME: Tetrahydrofurfuryl acrylate
CHID: 44884 **CASRN:** 2399-48-6
SPID(S): Tox21_301728
M4ID: 12477405

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.891 **MAX_MED:** 0.974 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

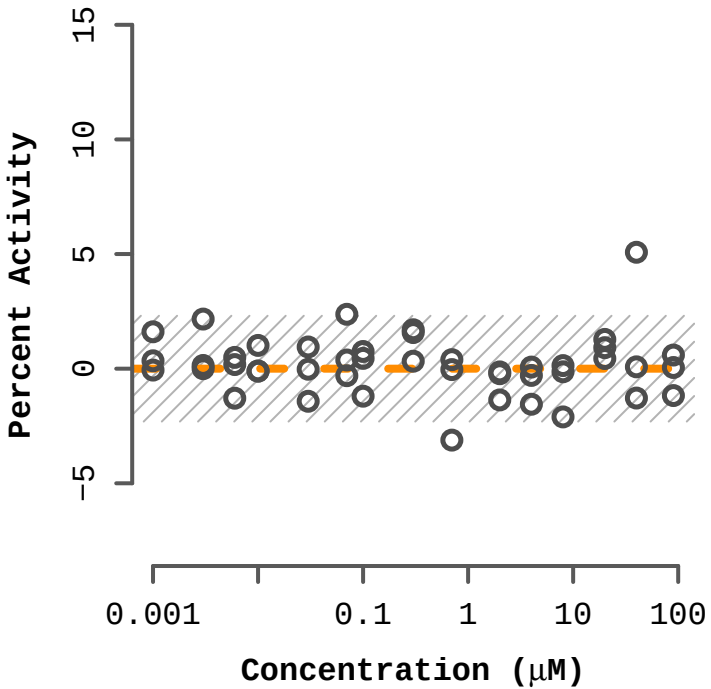
NAME: 5,5'−Bi−2−benzofuran−1,1',3,3'−tetrone
CHID: 44886 **CASRN:** 2420−87−3
SPID(S): Tox21_301695
M4ID: 12477438

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.907 **MAX_MED:** 0.744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

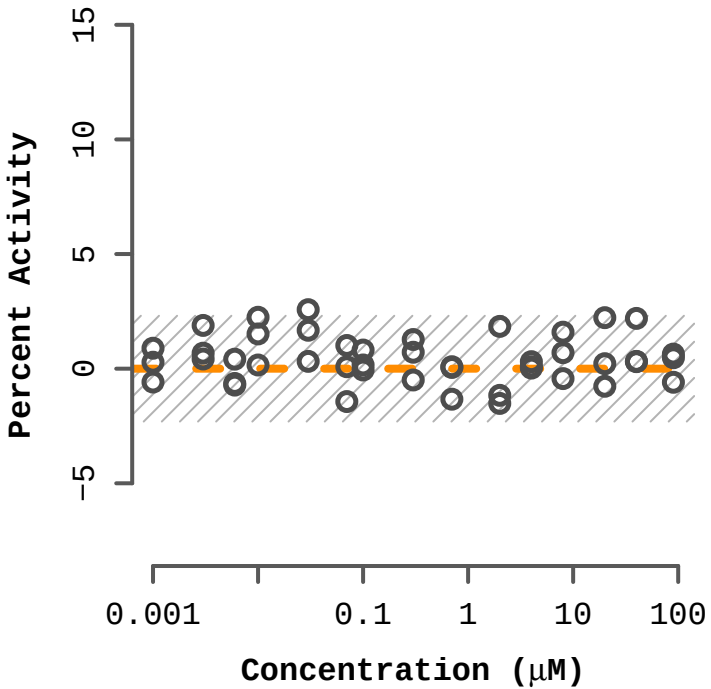
NAME: Dibenzyl diazene-1,2-dicarboxylate
CHID: 44887 **CASRN:** 2449-05-0
SPID(S): Tox21_301610
M4ID: 12477523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

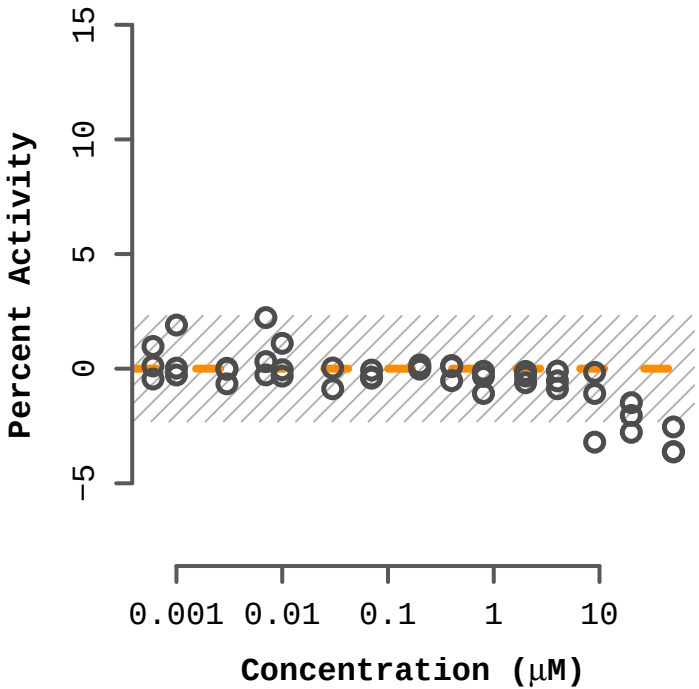
NAME: Barium bis(2-ethylhexanoate)
CHID: 44888 **CASRN:** 2457-01-4
SPID(S): Tox21_301625
M4ID: 12477508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

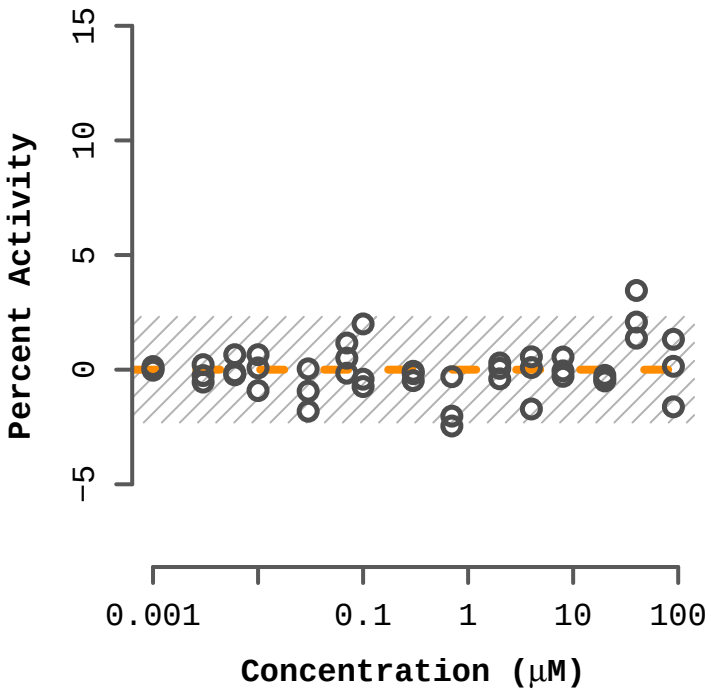
NAME: 2,5-Di-tert-butylcyclohexa-2,5-diene-1,4-dione
CHID: 44889 **CASRN:** 2460-77-7
SPID(S): Tox21_303738
M4ID: 12475450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.757 **MAX_MED:** 0.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

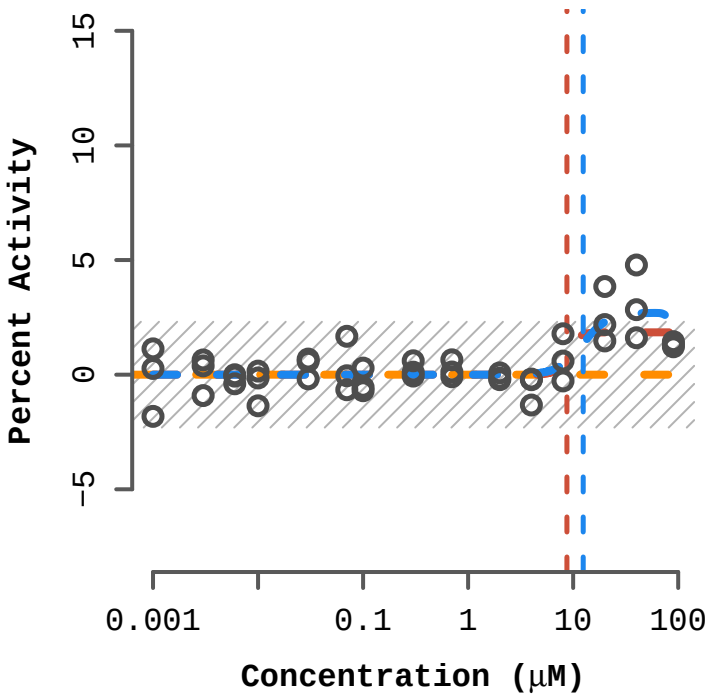
NAME: 2-(4-Hydroxybenzyl)phenol
CHID: 44890 **CASRN:** 2467-03-0
SPID(S): Tox21_303514
M4ID: 12475628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 2.3 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(4-Hydroxybenzyl)phenol
CHID: 44890 CASRN: 2467-03-0
SPID(S): Tox21_201953
M4ID: 12480299

HILL MODEL (in red):

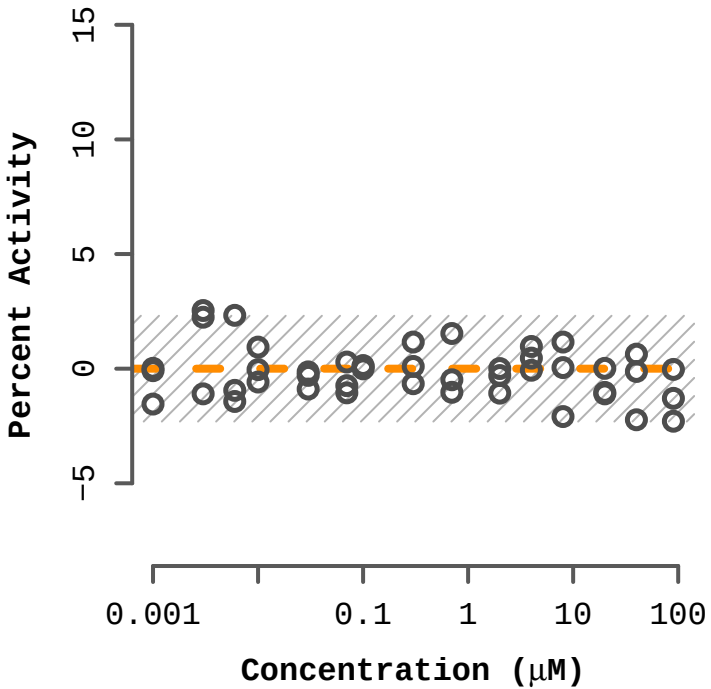
	tp	ga	gw
val:	1.85	0.941	8
sd:	0.274	0.0834	10.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.7	1.1	3.69	1.95	18
sd:	1.14	0.301	3.12	0.0182	398

	CNST	HILL	GNLS
AIC:	146.34	115.8	114.47
PROB:	0	0.34	0.66
RMSE:	1.33	0.85	0.77

MAX_MEAN: 3.08 **MAX_MED:** 2.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

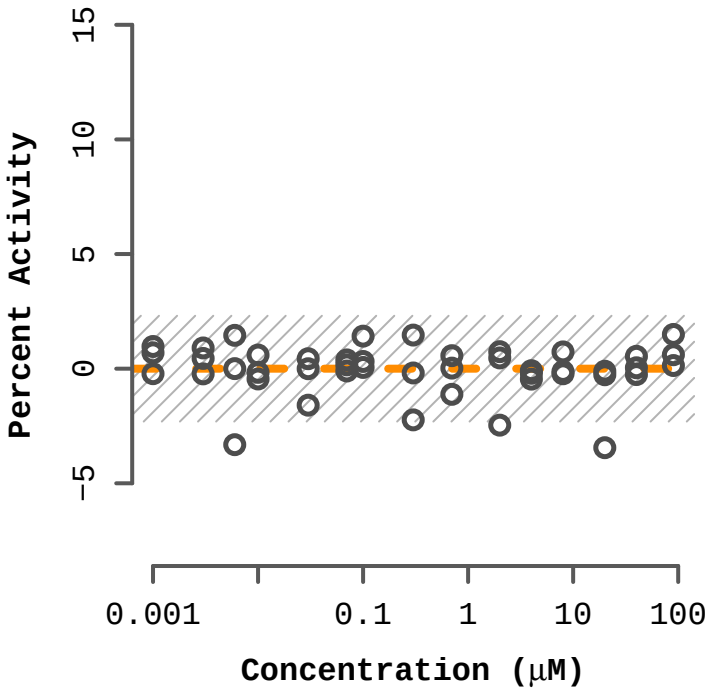
NAME: Diphenyl phosphorochloridate
CHID: 44892 **CASRN:** 2524-64-3
SPID(S): Tox21_301665
M4ID: 12477468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

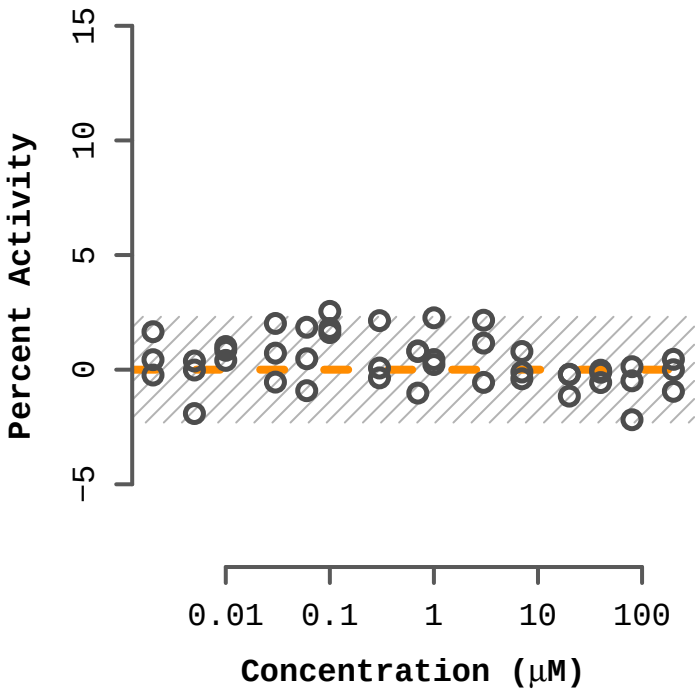
NAME: 2-Hexyldecanoic acid
CHID: 44893 **CASRN:** 25354-97-6
SPID(S): Tox21_301670
M4ID: 12477463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.748 **MAX_MED:** 0.693 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

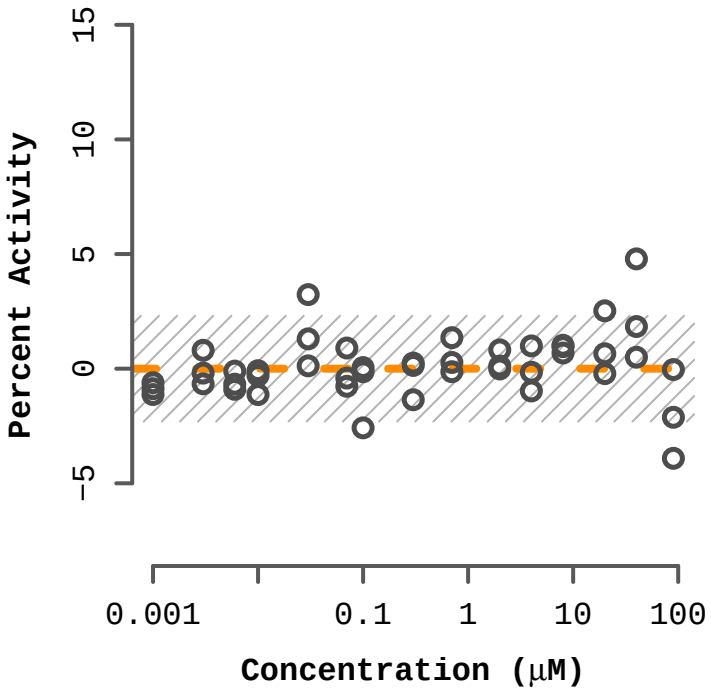
NAME: Trimethylhexane−1,6−diamine
CHID: 44894 **CASRN:** 25620−58−0
SPID(S): Tox21_301729
M4ID: 12477404

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

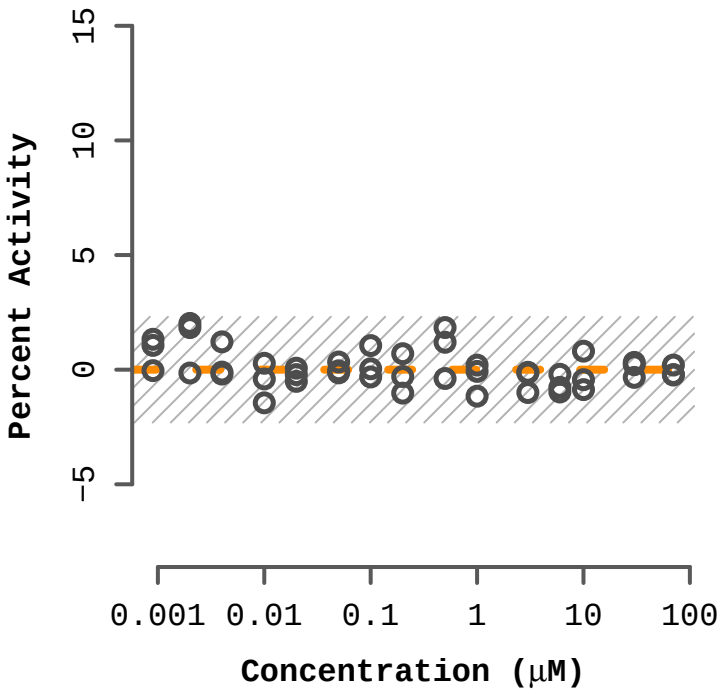
NAME: tert-Butyl 4-hydroxybenzoate
CHID: 44895 **CASRN:** 25804-49-3
SPID(S): Tox21_301248
M4ID: 12477885

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.38 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

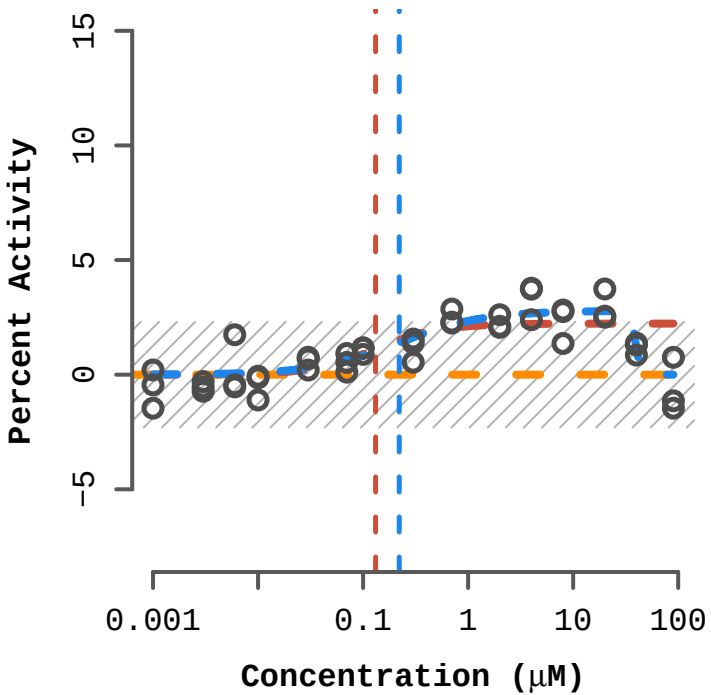
NAME: 1,3,5-Tris[3-(trimethoxysilyl)propyl]-1,3,5-tr
CHID: 44896 **CASRN:** 26115-70-8
SPID(S): Tox21_301284
M4ID: 12477849

HILL MODEL: Not applicable.

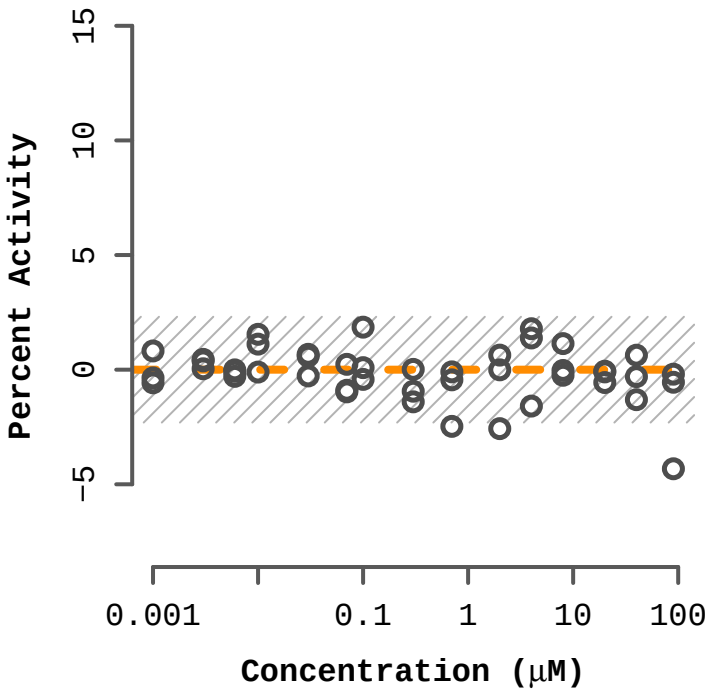
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.84 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Ethylpropane-1,3-diol
CHID:    44897   CASRN: 2612-29-5
SPID(S): Tox21_301262
M4ID:    12477871

HILL MODEL (in red):
      tp       ga       gw
val:  2.23     -0.881   1.44
sd:   0.234    0.175    0.486

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.79     -0.656   1.09     1.59     17.7
sd:   0.247    0.158    0.272    0.0137   32.5

      CNST        HILL        GNLS
AIC:  184.09      132.64      105.71
PROB: 0           0           1
RMSE: 1.76        1.06        0.68

MAX_MEAN: 3.3       MAX_MED: 3.73      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

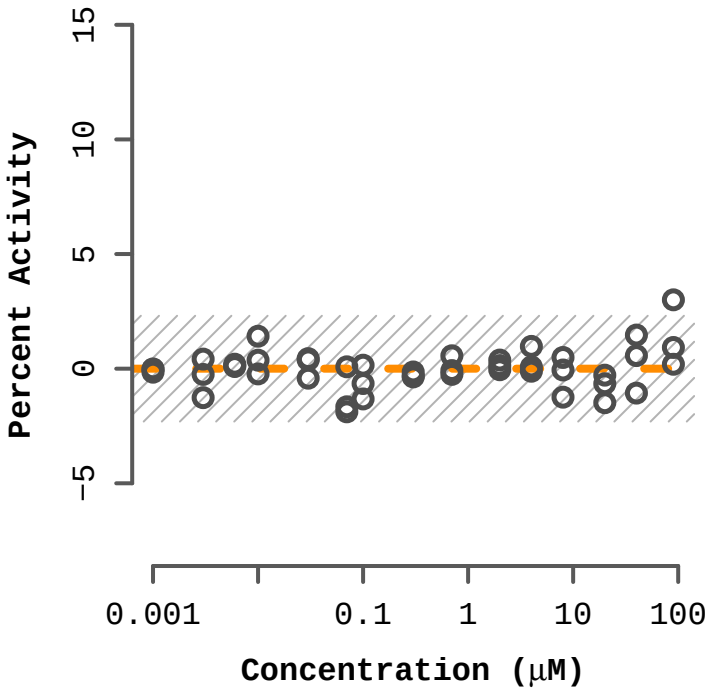
NAME: 4-Ethenylphenyl acetate
CHID: 44898 **CASRN:** 2628-16-2
SPID(S): Tox21_301617
M4ID: 12477516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

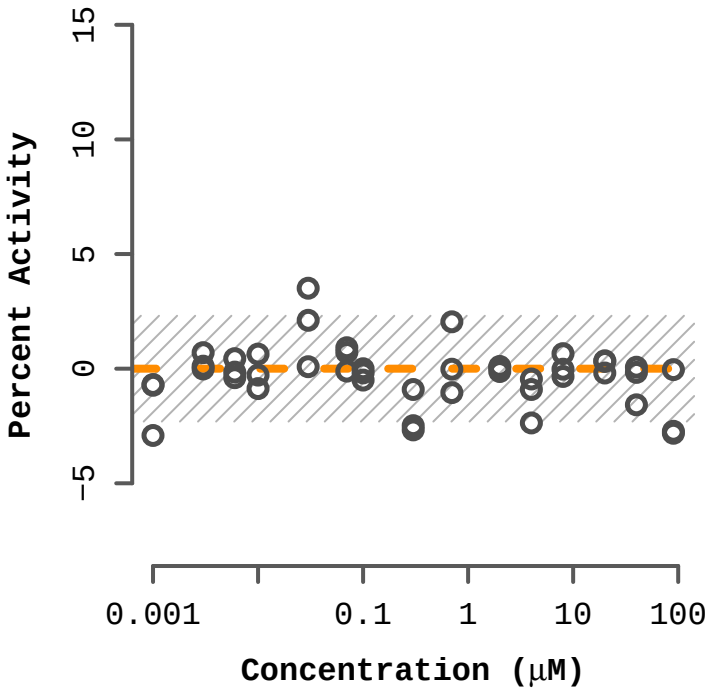
NAME: 2-Amino-2,4-dimethylpentanenitrile
CHID: 44899 **CASRN:** 26842-43-3
SPID(S): Tox21_301813
M4ID: 12477320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

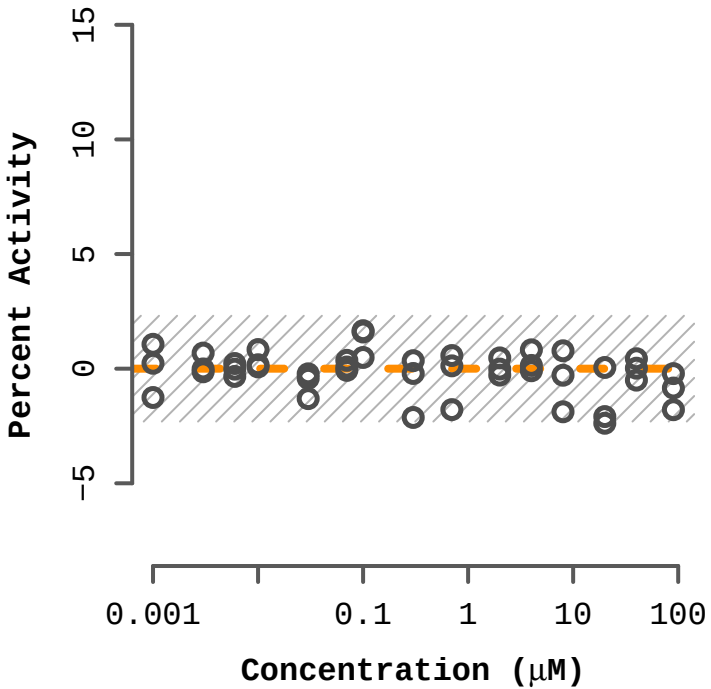
NAME: Tricyclodecanedimethanol
CHID: 44900 CASRN: 26896-48-0
SPID(S): Tox21_301611
M4ID: 12477522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

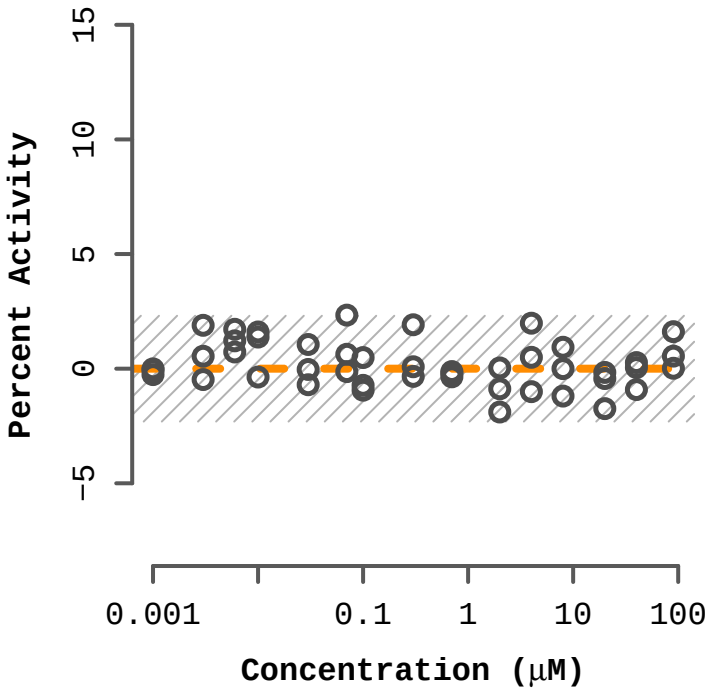
NAME: Triallyl trimellitate
CHID: 44901 **CASRN:** 2694-54-4
SPID(S): Tox21_301788
M4ID: 12477345

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

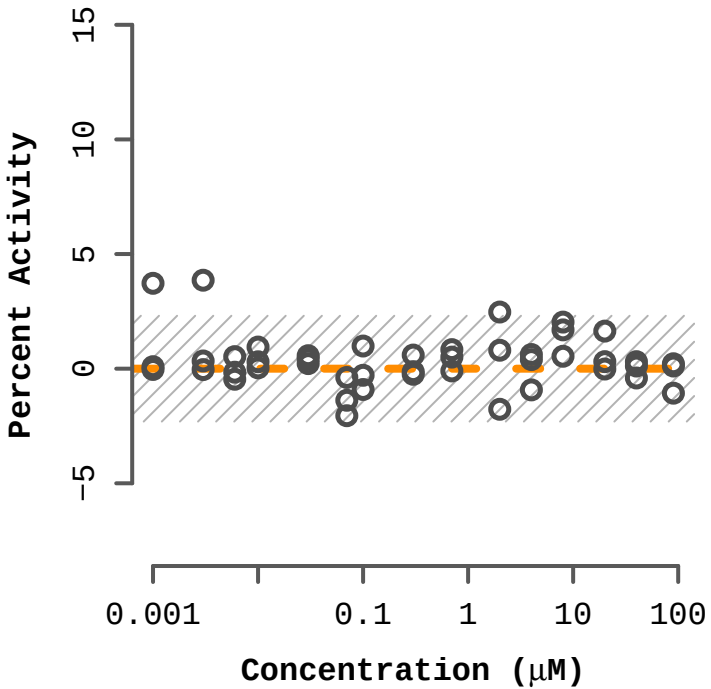
NAME: Calcium neodecanoate
CHID: 44902 **CASRN:** 27253-33-4
SPID(S): Tox21_301791
M4ID: 12477342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

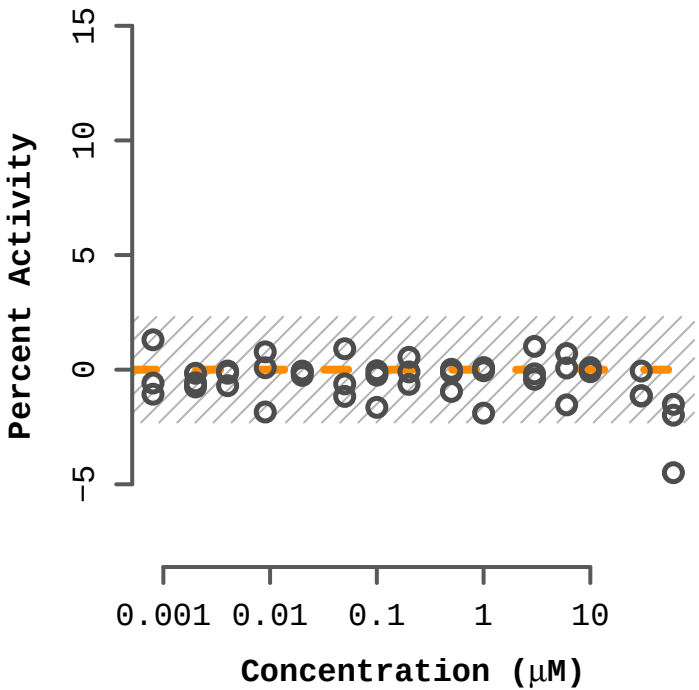
NAME: Titanium(4+) bis[(2E)-4-oxohex-2-en-2-olate] di
CHID: 44903 CASRN: 27858-32-8
SPID(S): Tox21_301787
M4ID: 12477346

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.42 MAX_MED: 1.69 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

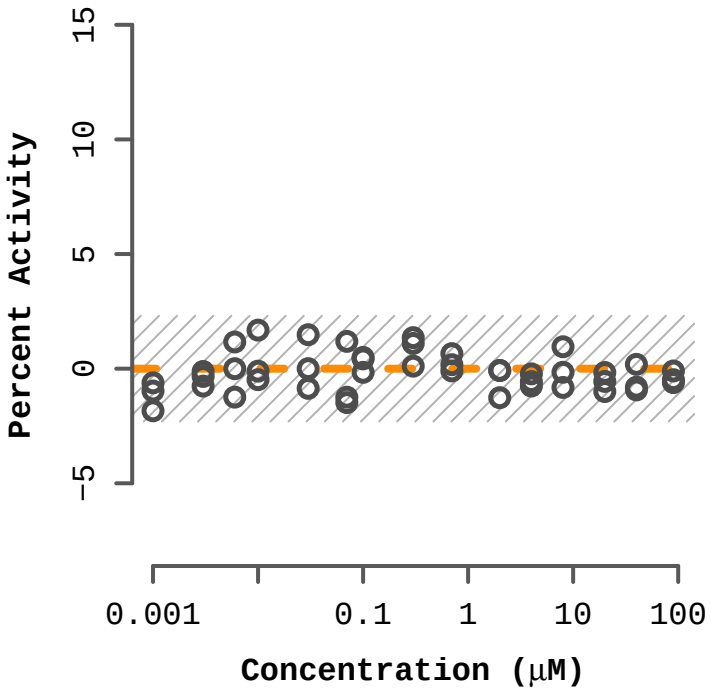
NAME: C.I. Acid Blue 22
CHID: 44904 **CASRN:** 28631-66-5
SPID(S): Tox21_301275
M4ID: 12477858

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.14 **MAX_MED:** 0.0866 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

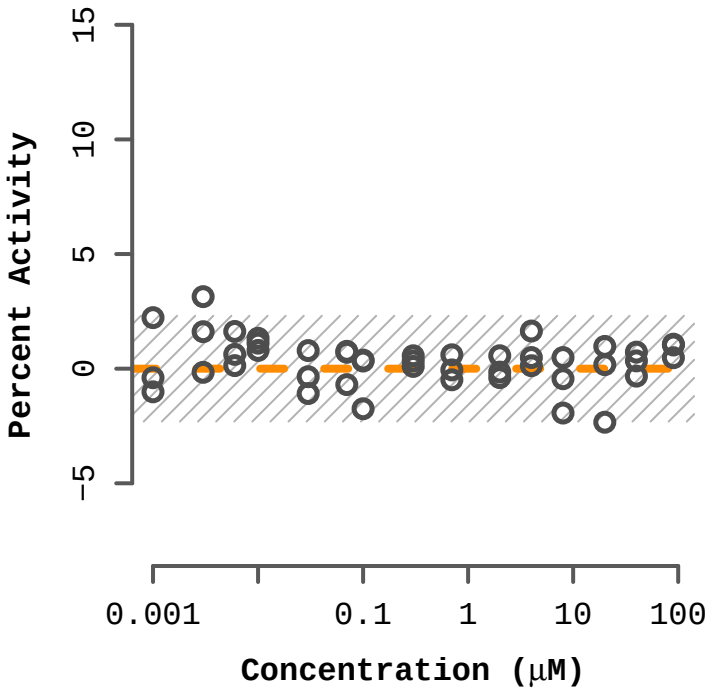
NAME: (2,2,6,6-Tetramethyl-4-oxopiperidin-1-yl)oxidan
CHID: 44905 **CASRN:** 2896-70-0
SPID(S): Tox21_301269
M4ID: 12477864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.856 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

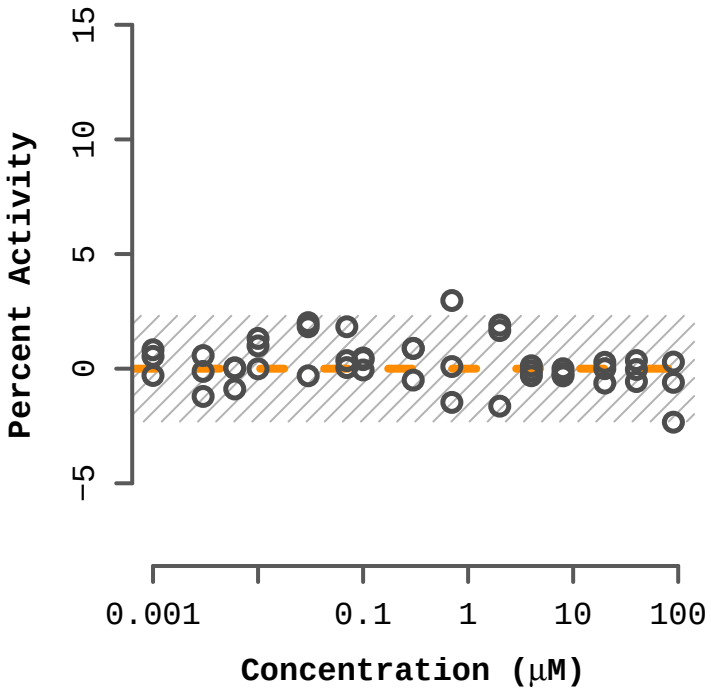
NAME: 2,2,4,4-Tetramethylcyclobutane-1,3-diol
CHID: 44908 **CASRN:** 3010-96-6
SPID(S): Tox21_301614
M4ID: 12477519

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

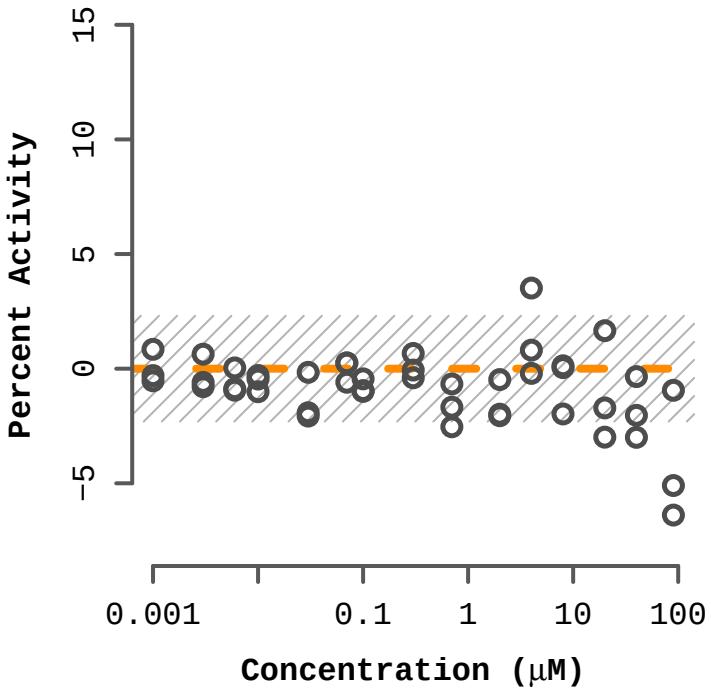
NAME: Dimethoxy(methyl)phenylsilane
CHID: 44909 **CASRN:** 3027-21-2
SPID(S): Tox21_301243
M4ID: 12477890

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

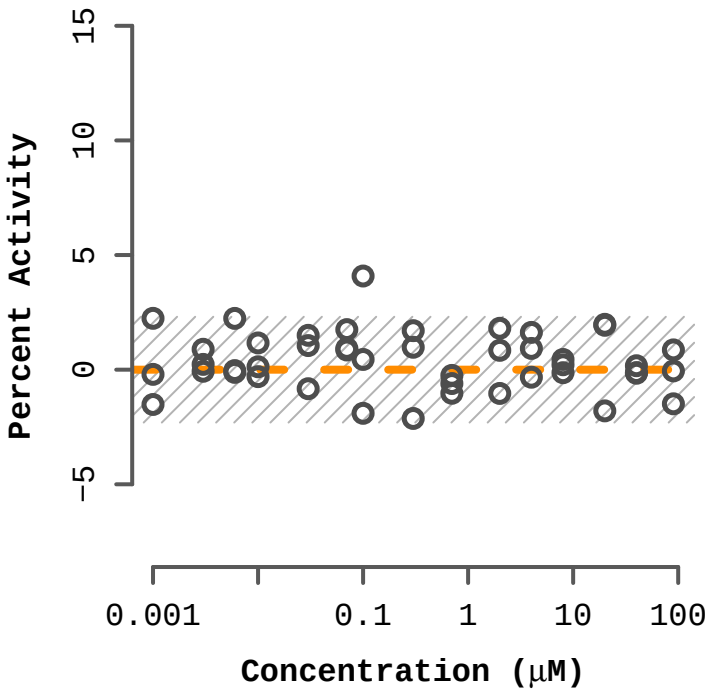
NAME: Hex-3-yne-2,5-diol
CHID: 44910 **CASRN:** 3031-66-1
SPID(S): Tox21_301736
M4ID: 12477397

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

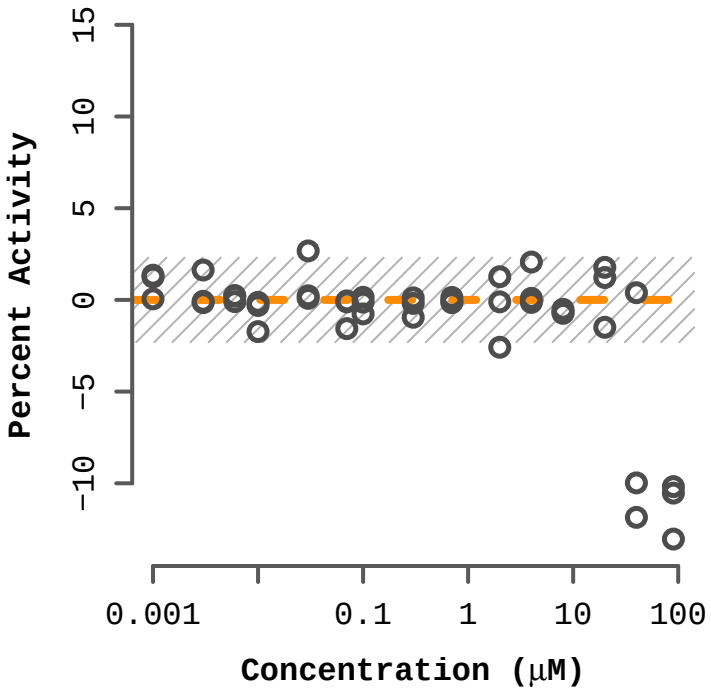
NAME: Isooctyl 3-mercaptopropionate
CHID: 44911 **CASRN:** 30374-01-7
SPID(S): Tox21_301276
M4ID: 12477857

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

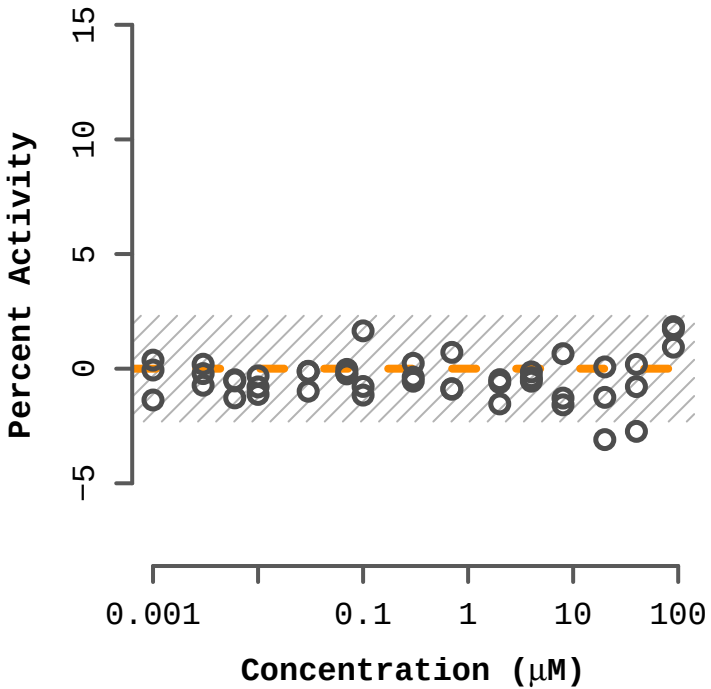
NAME: N-[3-(Dimethylamino)propyl]dodecanamide
CHID: 44913 **CASRN:** 3179-80-4
SPID(S): Tox21_301341
M4ID: 12477792

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.85	NA	NA

MAX_MEAN: 0.994 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

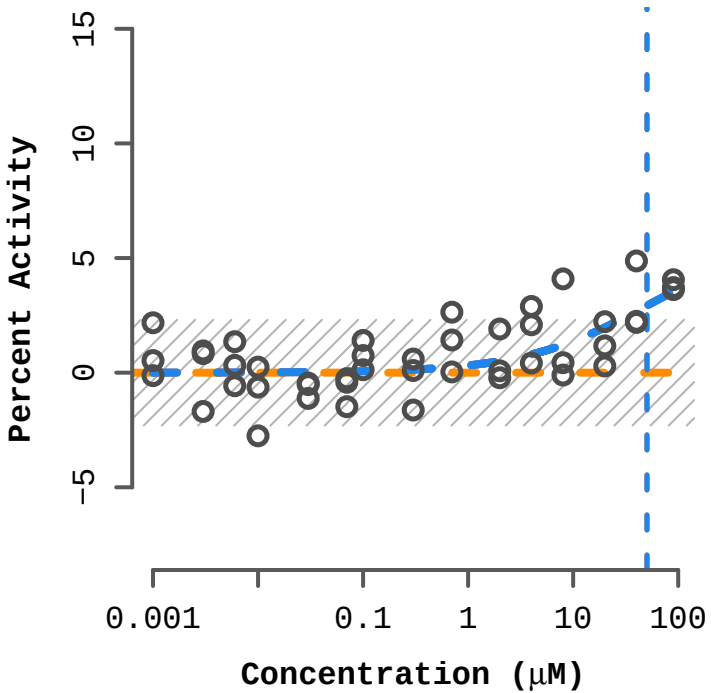
NAME: 3,5-Dichlorosalicylic acid
CHID: 44914 **CASRN:** 320-72-9
SPID(S): Tox21_301696
M4ID: 12477437

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Methyl-3,4-dihydro-2H-1,4-benzoxazine
CHID: 44915 CASRN: 32329-20-7
SPID(S): Tox21_301241
M4ID: 12477892

HILL MODEL (in red):

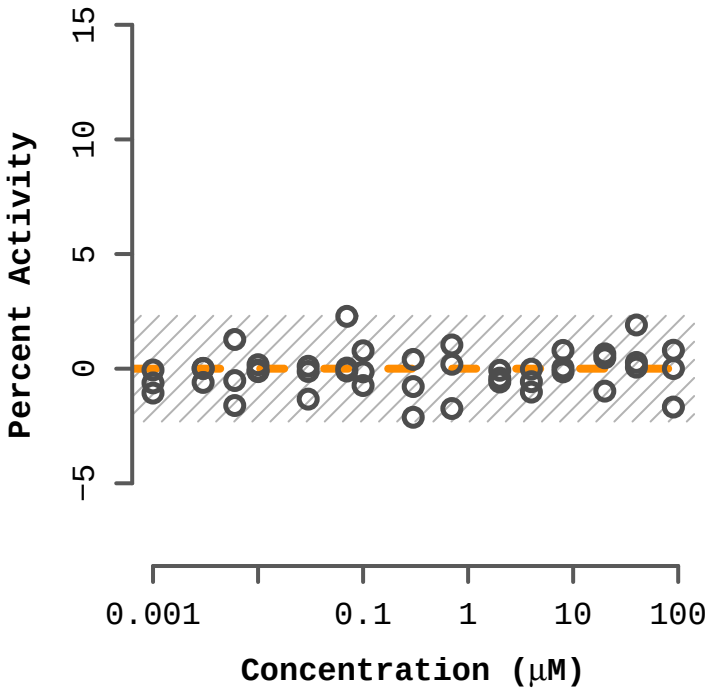
	tp	ga	gw
val:	5.85	1.7	0.731
sd:	2.94	0.616	0.305

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.85	1.7	0.731	3.92	3.26
sd:	2.93	0.616	0.305	321	533

	CNST	HILL	GNLS
AIC:	185.05	154.55	158.55
PROB:	0	0.88	0.12
RMSE:	1.86	1.21	1.21

MAX_MEAN: 3.8 MAX_MED: 3.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

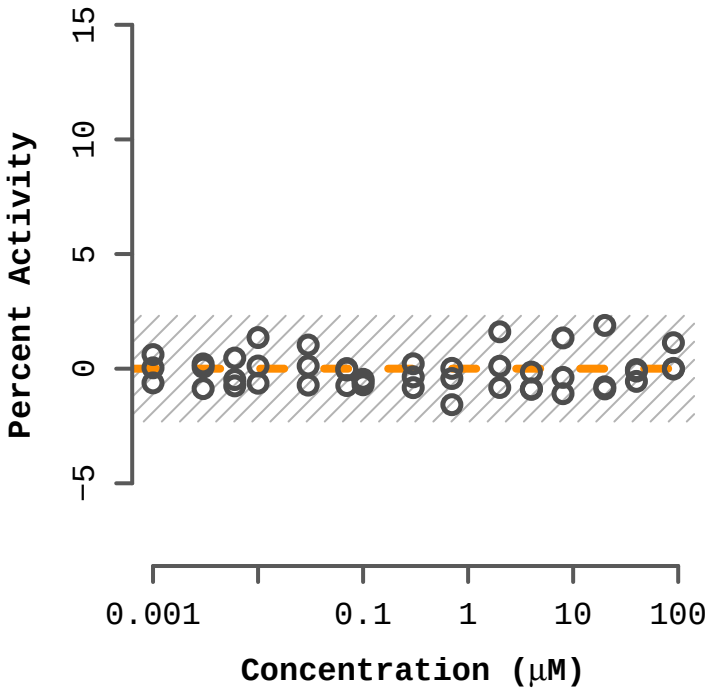
NAME: Bis(methacryloyloxyethyl) hydrogen phosphate
CHID: 44916 **CASRN:** 32435-46-4
SPID(S): Tox21_301651
M4ID: 12477482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.749 **MAX_MED:** 0.476 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

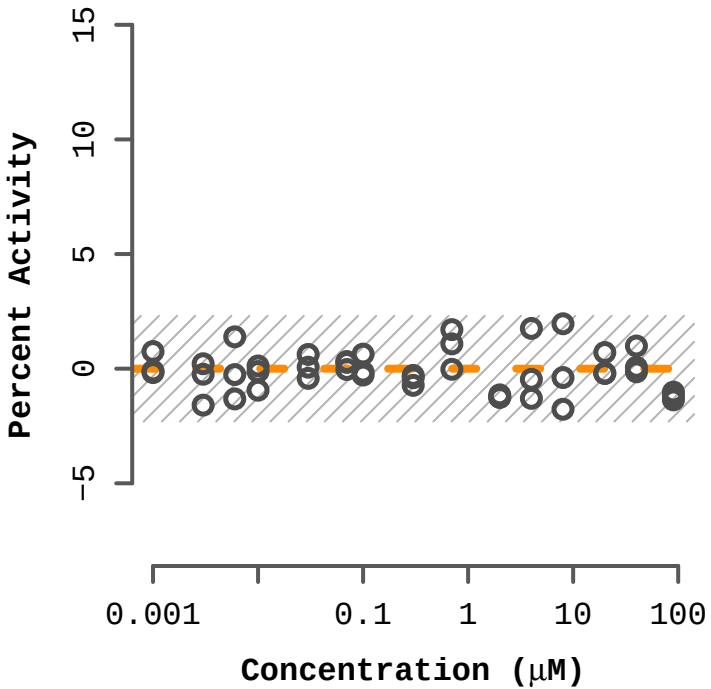
NAME: 1,3,5-Tribromo-2-(prop-2-en-1-yloxy)benzene
CHID: 44918 **CASRN:** 3278-89-5
SPID(S): Tox21_301711
M4ID: 12477422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.378 **MAX_MED:** 0.119 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

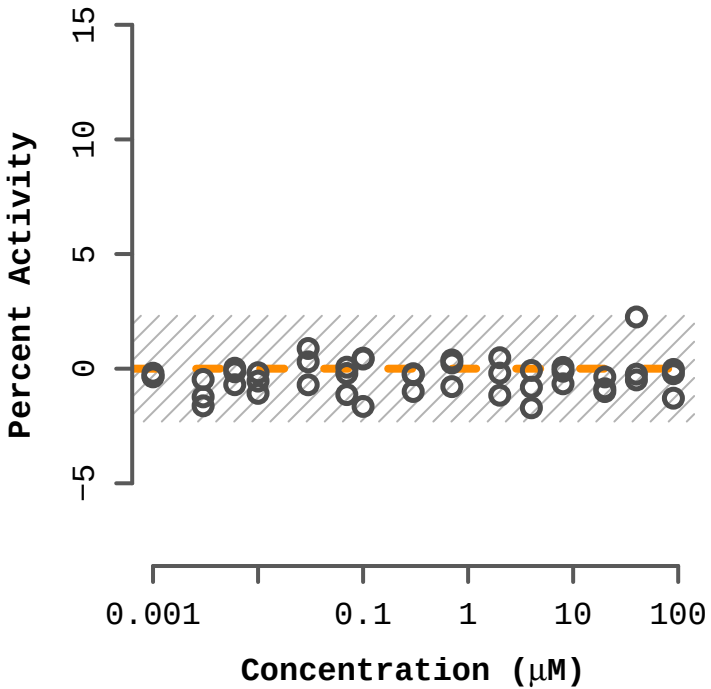
NAME: 2,2-Bis{[(3-sulfanylpropanoyl)oxy]methyl}butyl
CHID: 44919 **CASRN:** 33007-83-9
SPID(S): Tox21_301639
M4ID: 12477494

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.92 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

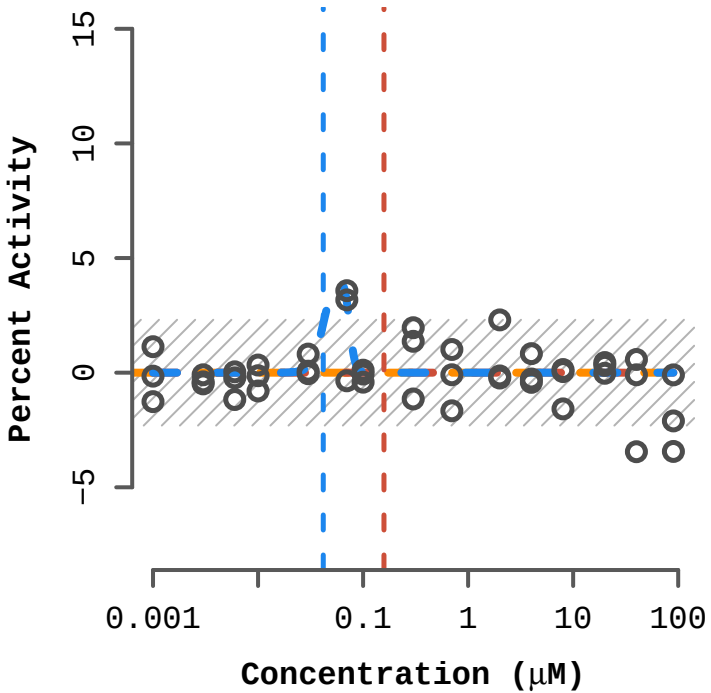
NAME: tert-Butylperoxy 2-ethylhexyl carbonate
CHID: 44921 **CASRN:** 34443-12-4
SPID(S): Tox21_301285
M4ID: 12477848

HILL MODEL: Not applicable.

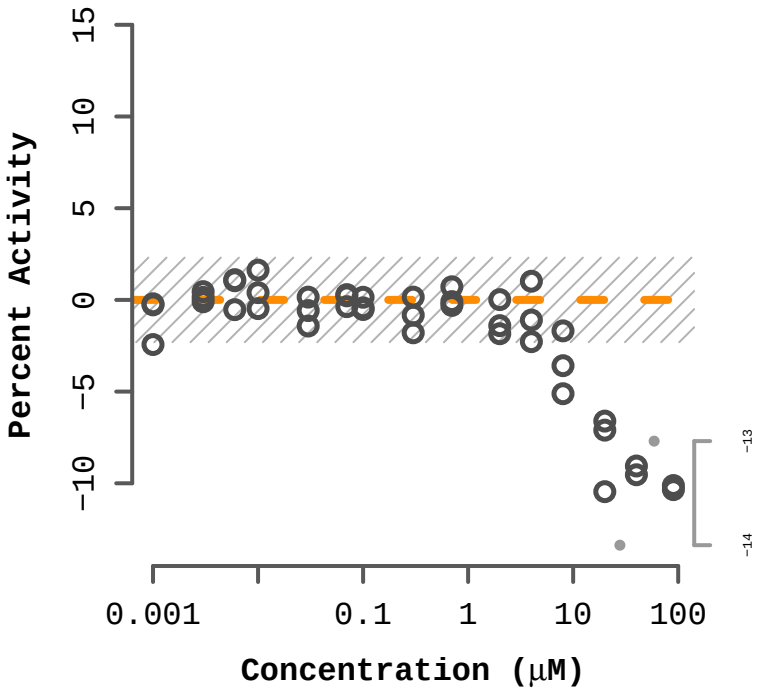
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.51 **MAX_MED:** 0.421 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-(2-Hydroxyethyl)pyrrolidin-2-one
CHID:    44922   CASRN: 3445-11-2
SPID(S): Tox21_301700
M4ID:    12477433

HILL MODEL (in red):
      tp        ga        gw
val:  1.43e-10 -0.801    1.63
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  4.29      -1.38     8         -1.13     16.9
sd:   NaN       NaN       NaN       NaN       NaN

      CNST         HILL         GNLS
AIC:  146.64       152.64       148.47
PROB: 0.69         0.03         0.28
RMSE: 1.31         1.31         1.22

MAX_MEAN: 2.13      MAX_MED: 3.18      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

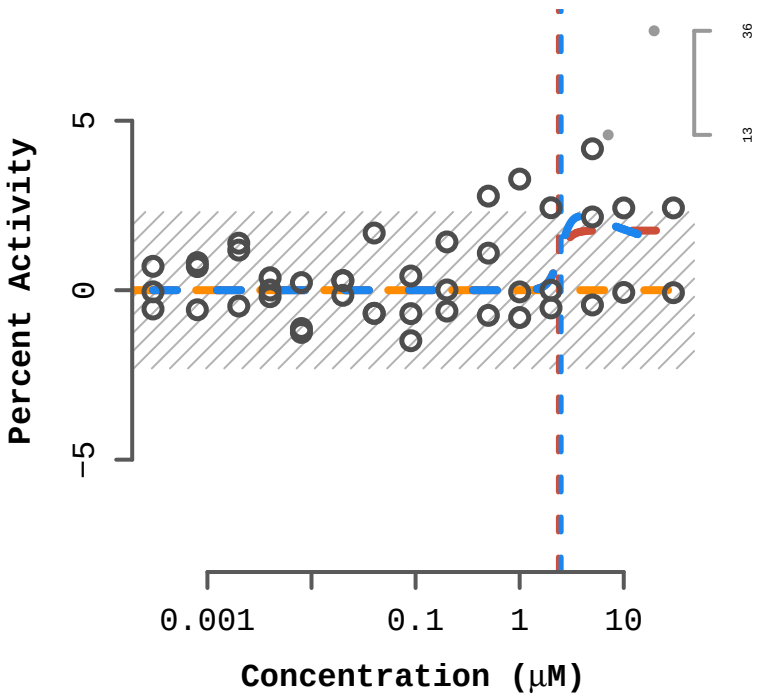
NAME: 3,5-Diethyl-1-phenyl-2-propyl-1,2-dihydropyrid
CHID: 44923 CASRN: 34562-31-7
SPID(S): Tox21_301339
M4ID: 12477794 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	256.68	NA	NA
PROB:	1	NA	NA
RMSE:	4.79	NA	NA

MAX_MEAN: 0.541 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Dibromobenzil
CHID: 44925 CASRN: 35578−47−3
SPID(S): Tox21_202826
M4ID: 12479426 BRK

HILL MODEL (in red):

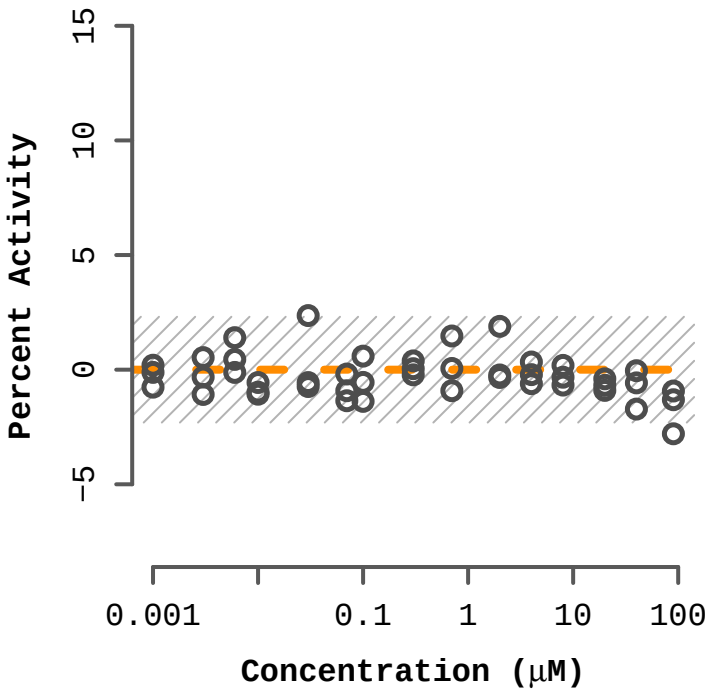
	tp	ga	gw
val:	1.76	0.372	8
sd:	0.623	0.289	30.3

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.36	0.398	7.98	0.648	0.442
sd:	39.4	1.46	119	17.2	2.51

	CNST	HILL	GNLS
AIC:	197.09	195.66	199.37
PROB:	0.3	0.61	0.09
RMSE:	5.82	5.46	5.52

MAX_MEAN: 12.7 MAX_MED: 2.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

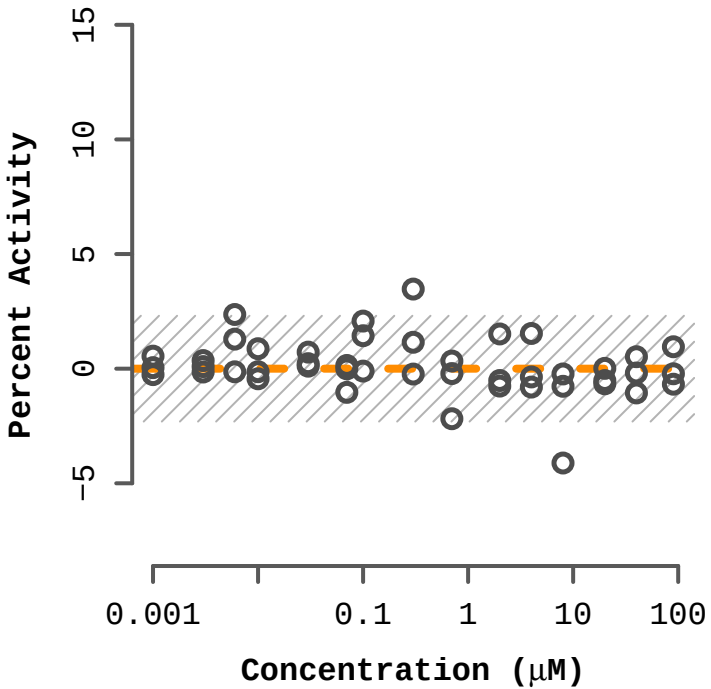
NAME: N-Butyl-2,2,6,6-tetramethylpiperidin-4-amine
CHID: 44926 **CASRN:** 36177-92-1
SPID(S): Tox21_301745
M4ID: 12477388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.576 **MAX_MED:** 0.449 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

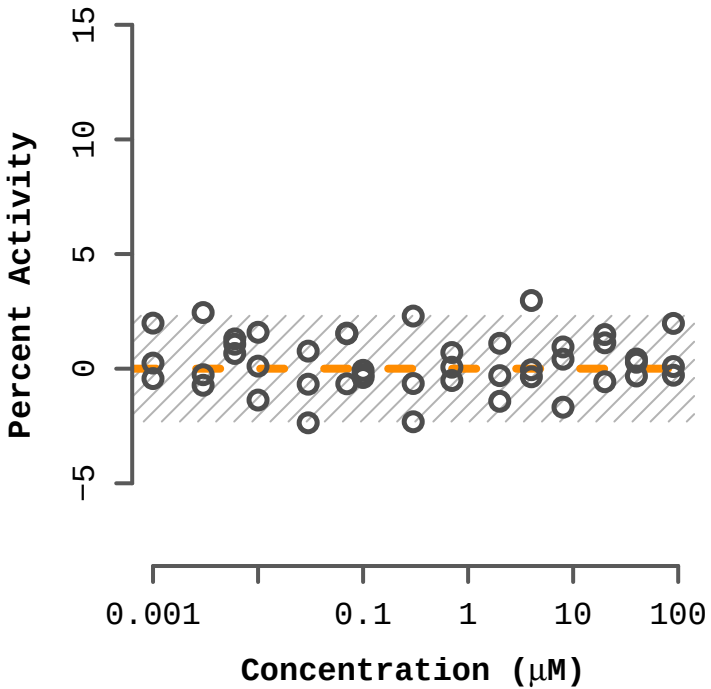
NAME: Bis(2-ethylhexyl) phosphonate
CHID: 44927 **CASRN:** 3658-48-8
SPID(S): Tox21_301682
M4ID: 12477451

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

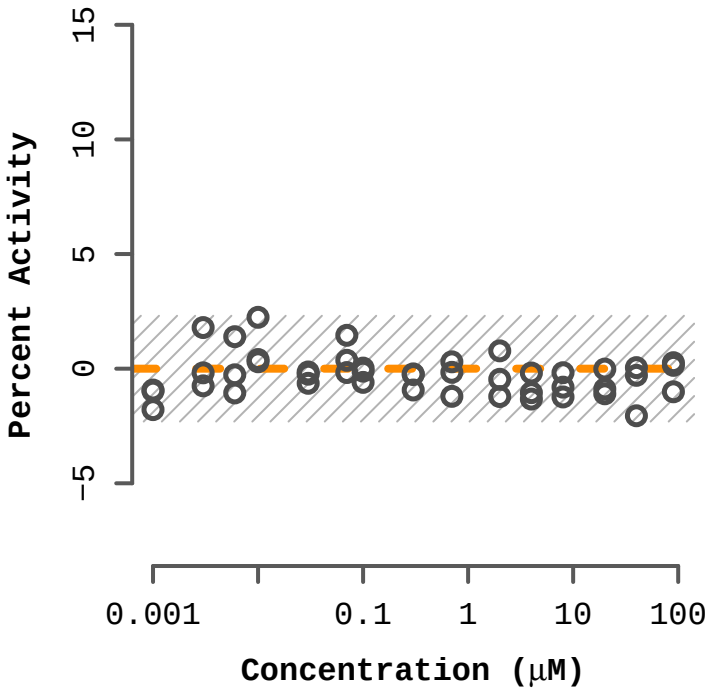
NAME: Isopropyl triethanolamine titanate
CHID: 44928 **CASRN:** 36673-16-2
SPID(S): Tox21_301793
M4ID: 12477340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

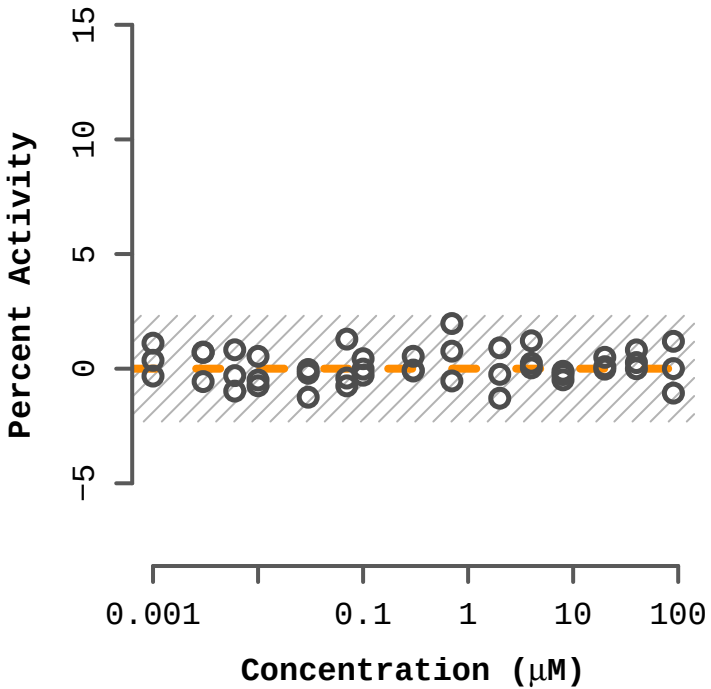
NAME: 1-(Methylsulfanyl)dodecane
CHID: 44929 CASRN: 3698-89-3
SPID(S): Tox21_301265
M4ID: 12477868

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.982 MAX_MED: 0.402 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

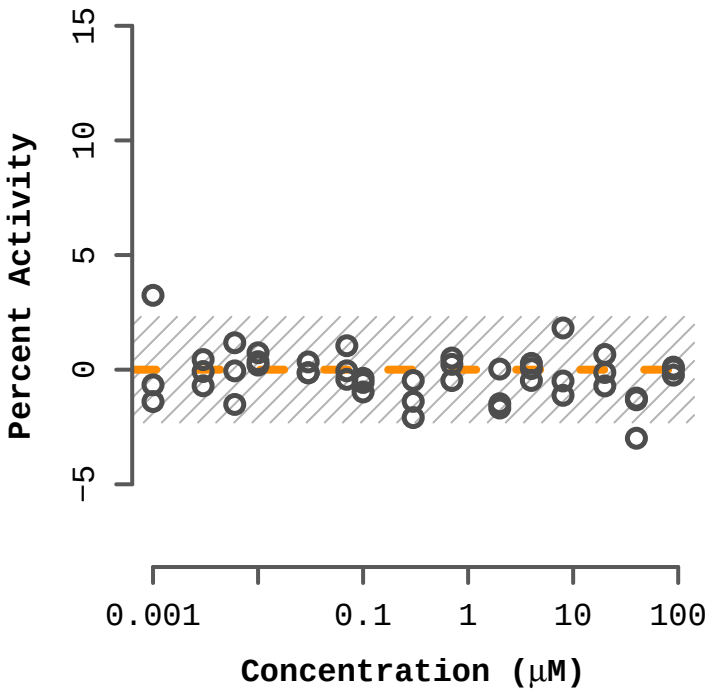
NAME: 2-(Trifluoromethoxy)benzenesulfonamide
CHID: 44930 **CASRN:** 37526-59-3
SPID(S): Tox21_301693
M4ID: 12477440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.734 **MAX_MED:** 0.765 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

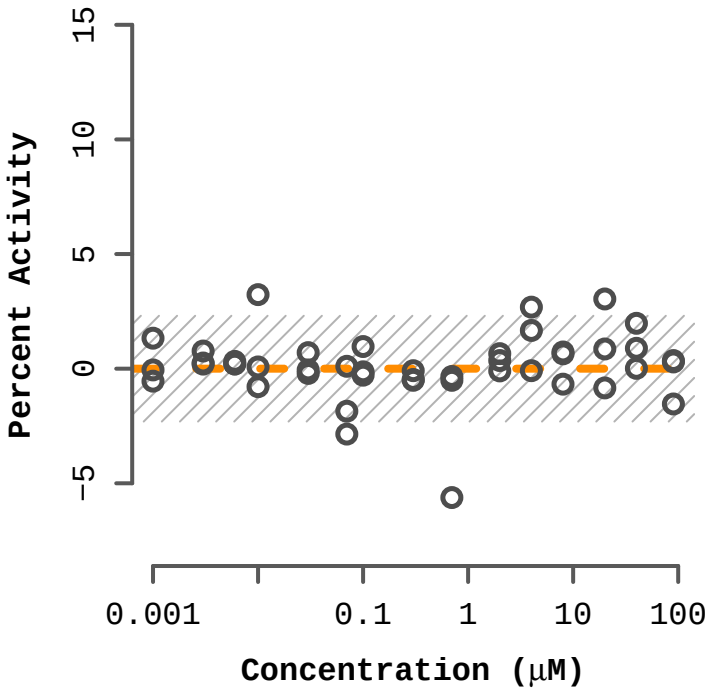
NAME: 2-(tert-Butylamino)ethyl 2-methylprop-2-enoate
CHID: 44931 **CASRN:** 3775-90-4
SPID(S): Tox21_301718
M4ID: 12477415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.431 **MAX_MED:** 0.352 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

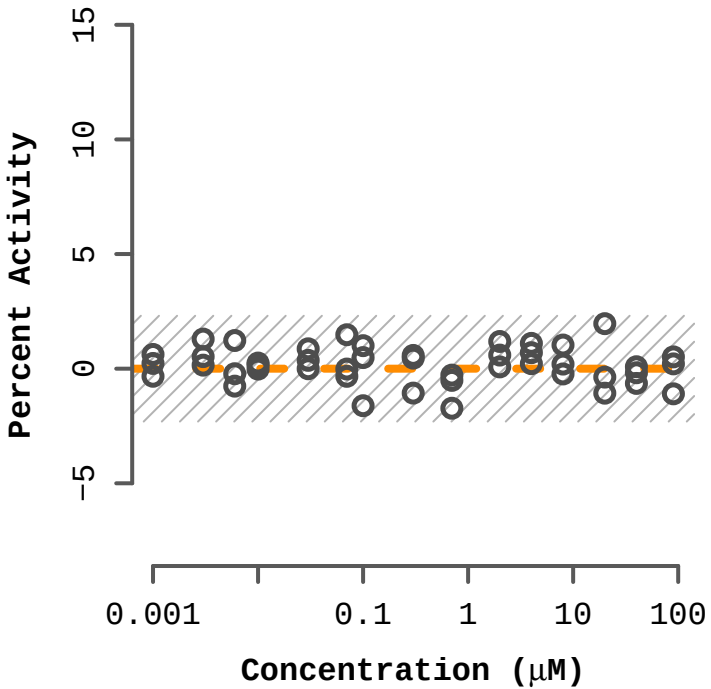
NAME: 4-(Propan-2-yl)benzenesulfonic acid
CHID: 44932 **CASRN:** 16066-35-6
SPID(S): Tox21_301762
M4ID: 12477371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

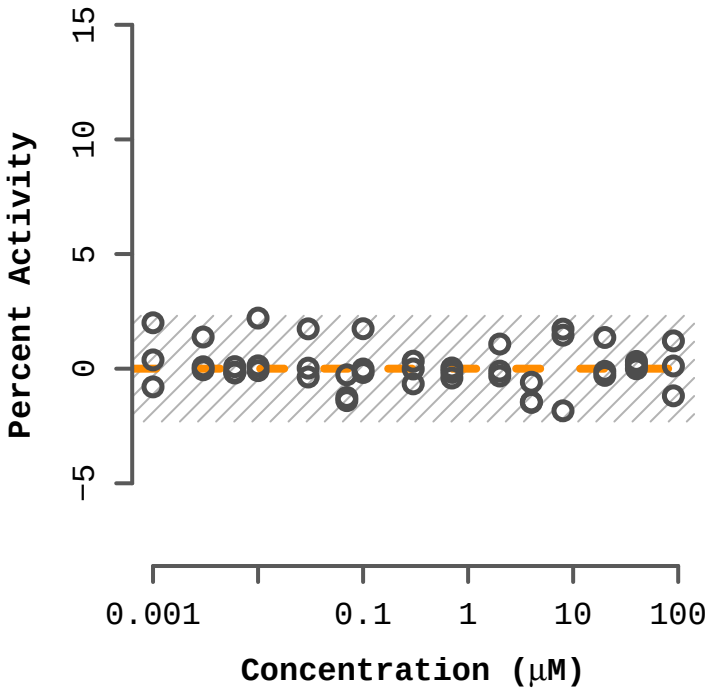
NAME: 1,3-Bis(isocyanatomethyl)cyclohexane
CHID: 44933 **CASRN:** 38661-72-2
SPID(S): Tox21_301661
M4ID: 12477472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.675 **MAX_MED:** 0.699 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

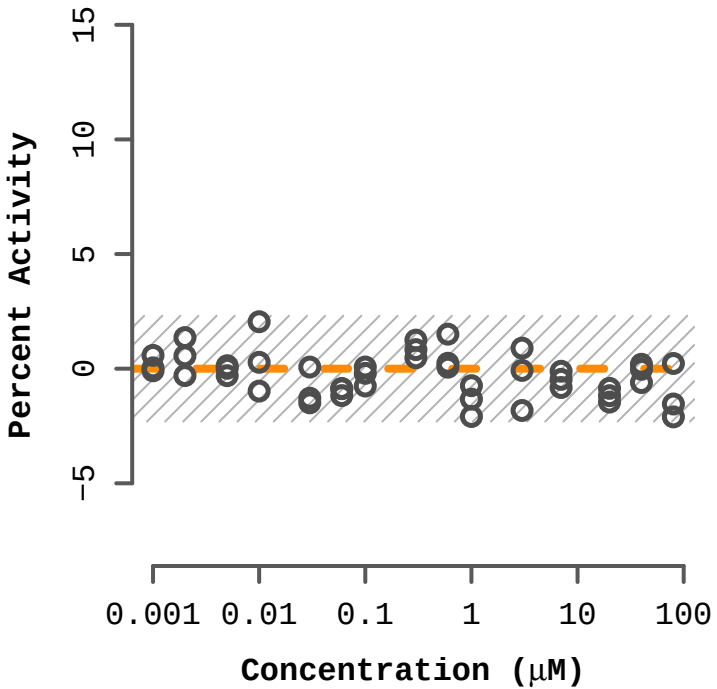
NAME: 4,5-Dihydroxy-1,3-dimethylimidazolidin-2-one
CHID: 44934 **CASRN:** 3923-79-3
SPID(S): Tox21_301257
M4ID: 12477876

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.75 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

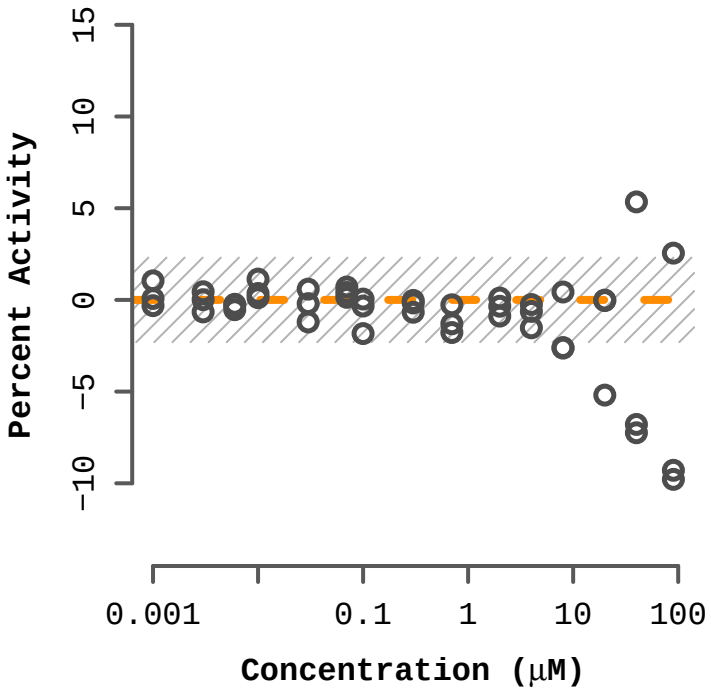
NAME: Chromium acetate, basic
CHID: 44935 CASRN: 39430-51-8
SPID(S): Tox21_301402
M4ID: 12477731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 0.833 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

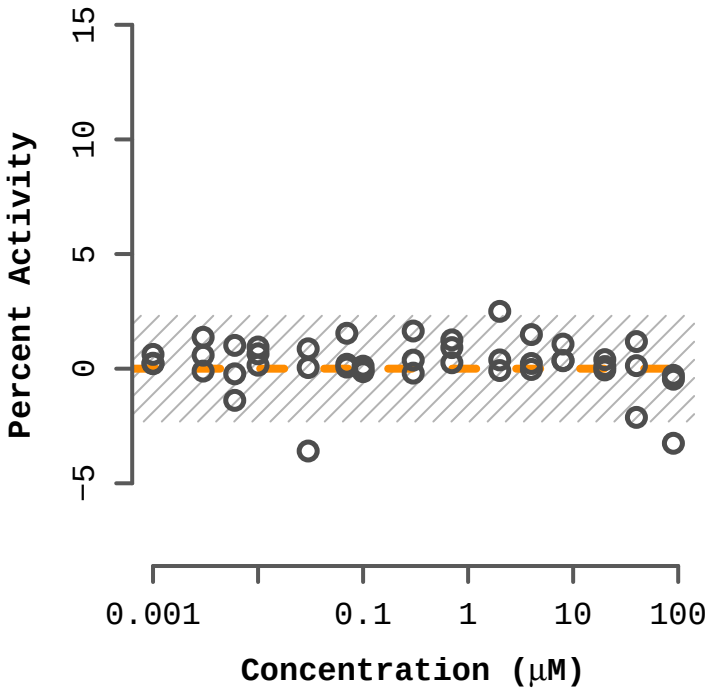
NAME: (2,4,6-Trioxo-1,3,5-triazinane-1,3,5-triyl)tri
CHID: 44936 **CASRN:** 40220-08-4
SPID(S): Tox21_301730
M4ID: 12477403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.76	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 0.537 **MAX_MED:** 0.407 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

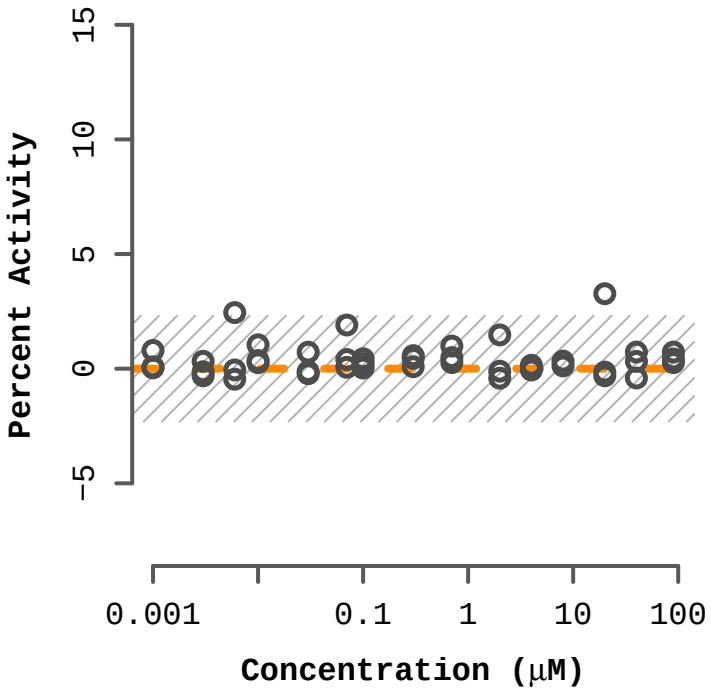
NAME: Ethenylsilanetriyl triacetate
CHID: 44938 **CASRN:** 4130-08-9
SPID(S): Tox21_301283
M4ID: 12477850

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

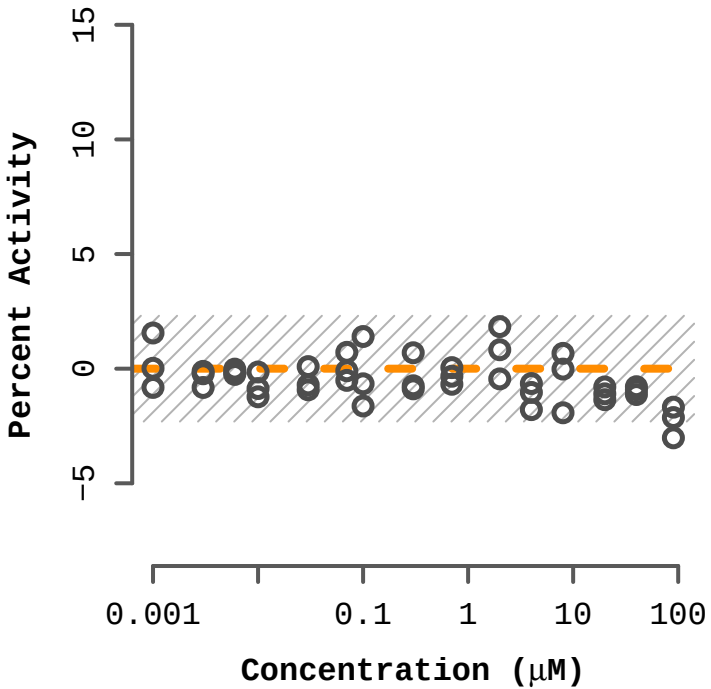
NAME: 1,3,5-Tribromo-2-methoxy-4-methylbenzene
CHID: 44939 CASRN: 41424-36-6
SPID(S): Tox21_301672
M4ID: 12477461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.938 MAX_MED: 0.484 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

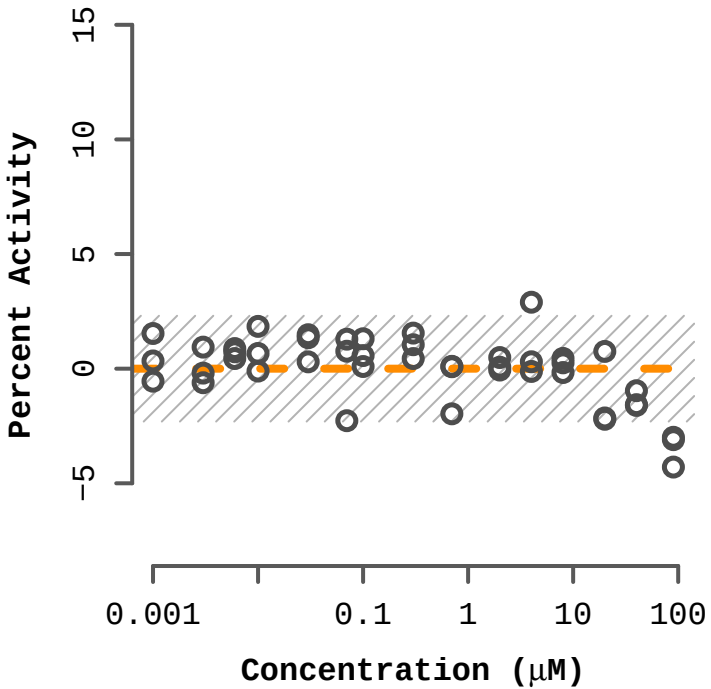
NAME: Octahydro-1H-4,7-methanoindene-1,5-diyldimetha
CHID: 44940 CASRN: 42594-17-2
SPID(S): Tox21_301271
M4ID: 12477862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.74 MAX_MED: 0.827 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

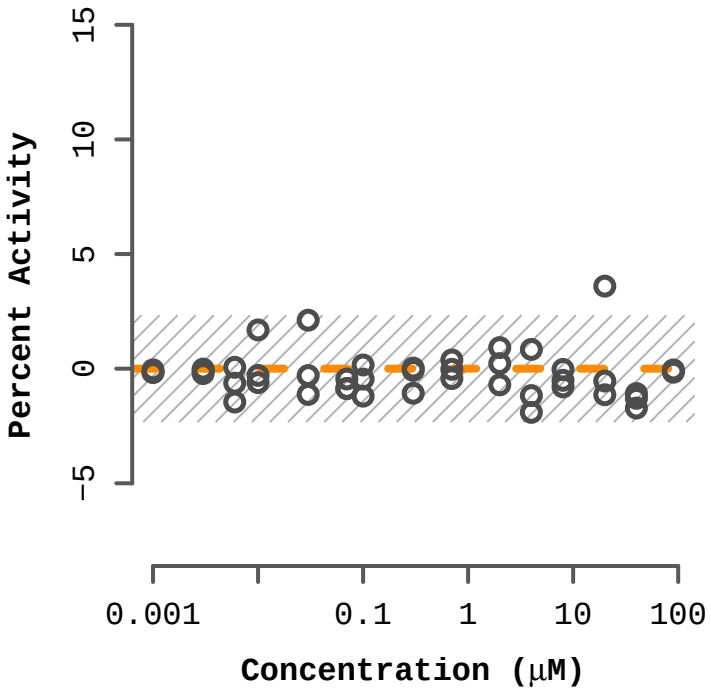
NAME: 2-(Phenylsulfonyl)aniline
CHID: 44941 **CASRN:** 4273-98-7
SPID(S): Tox21_301626
M4ID: 12477507

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

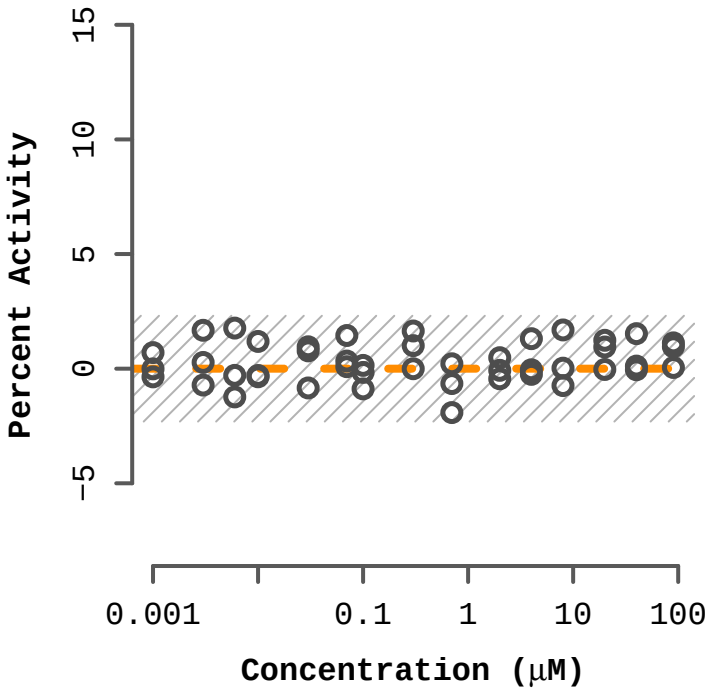
NAME: N,N−Dimethyl−2−(morpholin−4−yl)ethanamine
CHID: 44943 **CASRN:** 4385−05−1
SPID(S): Tox21_303783
M4ID: 12475405

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.3	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.642 **MAX_MED:** 0.223 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

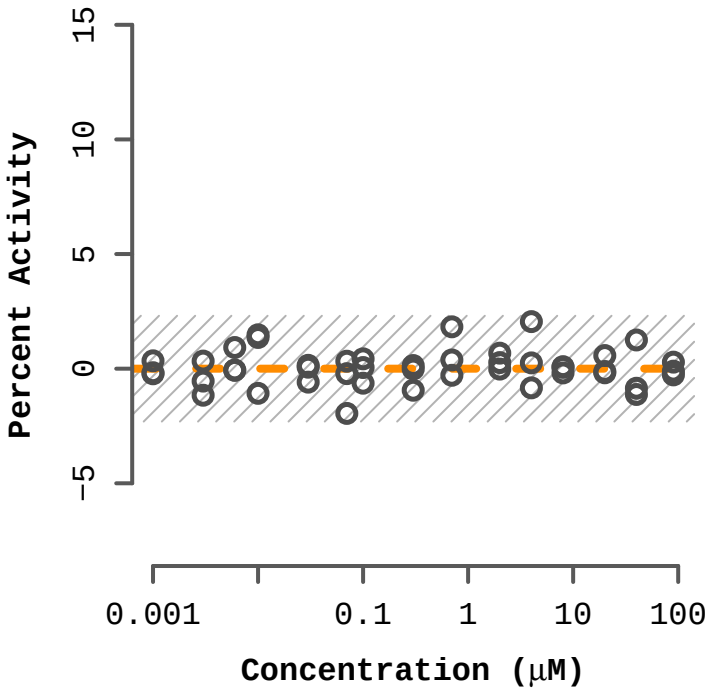
NAME: 2,2'−(Methanediyldisulfanediyl)diethanol
CHID: 44945 **CASRN:** 44860−68−6
SPID(S): Tox21_301758
M4ID: 12477375

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.883 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

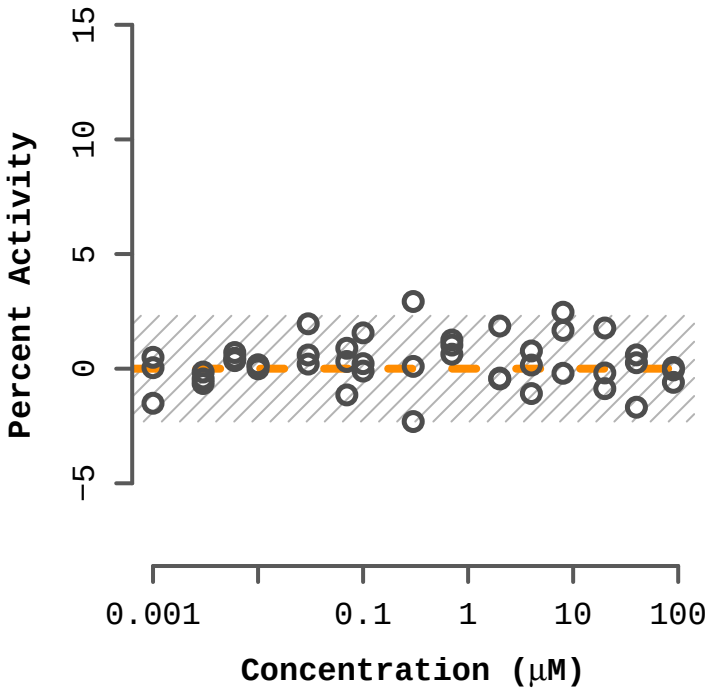
NAME: 1-(Morpholin-4-yl)prop-2-en-1-one
CHID: 44947 **CASRN:** 5117-12-4
SPID(S): Tox21_301658
M4ID: 12477475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.641 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

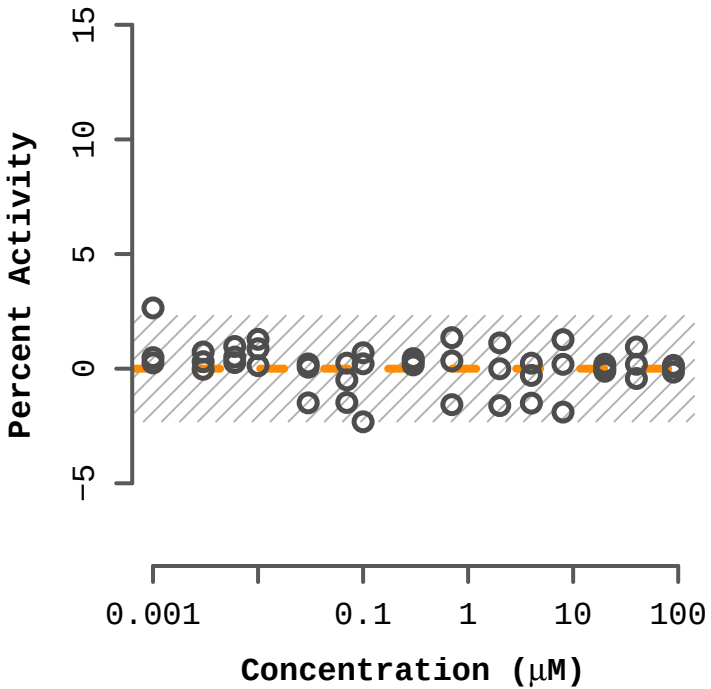
NAME: Methyl 5-chloro-2-nitrobenzoate
CHID: 44948 **CASRN:** 51282-49-6
SPID(S): Tox21_301266
M4ID: 12477867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

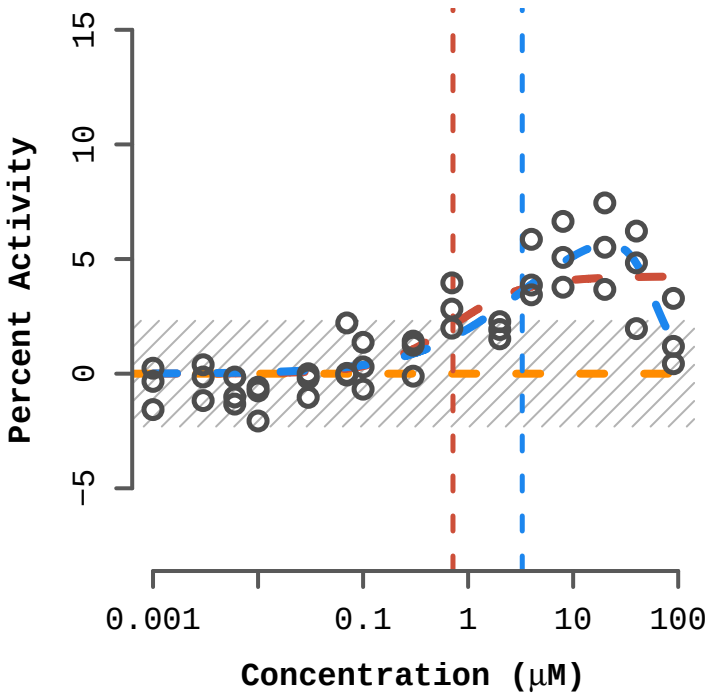
NAME: (5-Ethyl-1,3-dioxan-5-yl)methanol
CHID: 44949 **CASRN:** 5187-23-5
SPID(S): Tox21_301399
M4ID: 12477734

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.874 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Exifone
CHID: 44950 CASRN: 52479-85-3
SPID(S): Tox21_303559
M4ID: 12475586

HILL MODEL (in red):

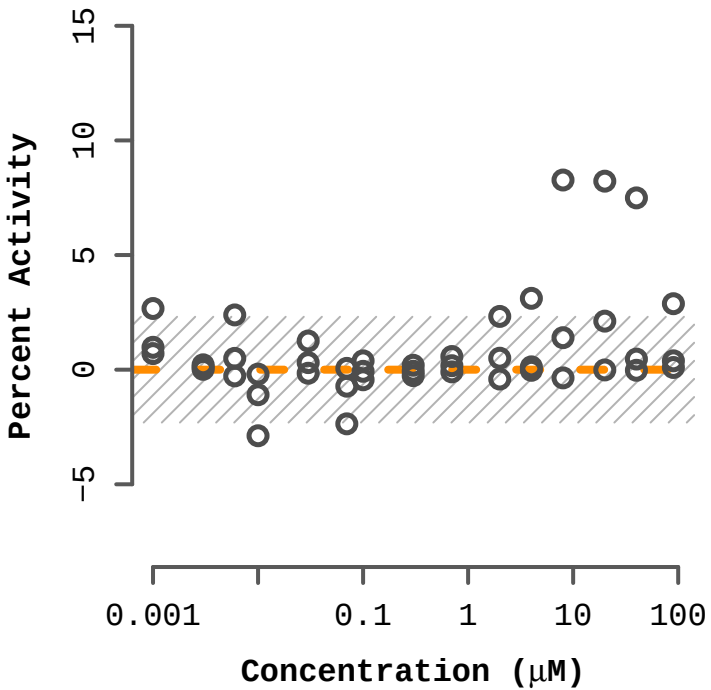
	tp	ga	gw
val:	4.24	−0.144	1.25
sd:	0.579	0.237	0.42

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.2	0.515	0.828	1.76	3.01
sd:	3.05	0.515	0.248	0.142	1.66

	CNST	HILL	GNLS
AIC:	225.69	167.89	157.69
PROB:	0	0.01	0.99
RMSE:	2.93	1.42	1.18

MAX_MEAN: 5.55 **MAX_MED:** 5.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

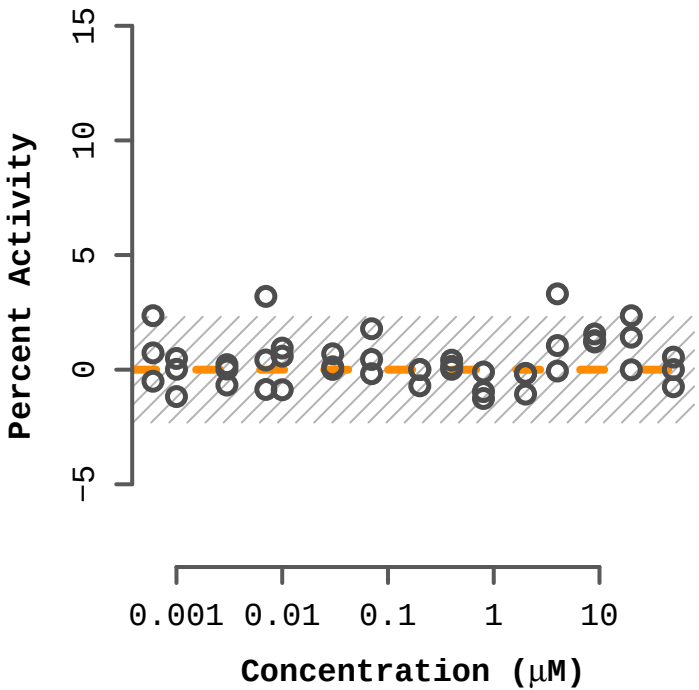
NAME: Exifone
CHID: 44950 CASRN: 52479-85-3
SPID(S): Tox21_201450
M4ID: 12480802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.83	NA	NA
PROB:	1	NA	NA
RMSE:	2.38	NA	NA

MAX_MEAN: 3.44 MAX_MED: 2.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

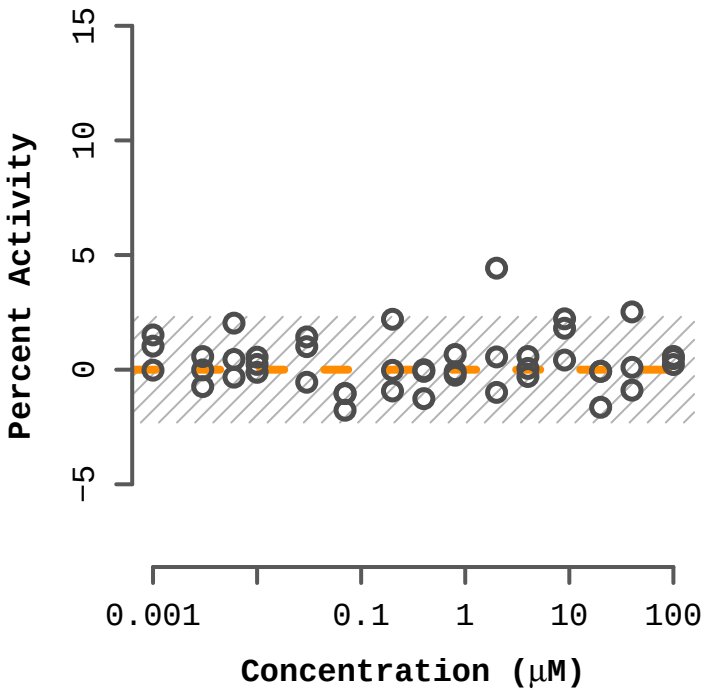
NAME: Exifone
CHID: 44950 **CASRN:** 52479-85-3
SPID(S): Tox21_113656
M4ID: 12482557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

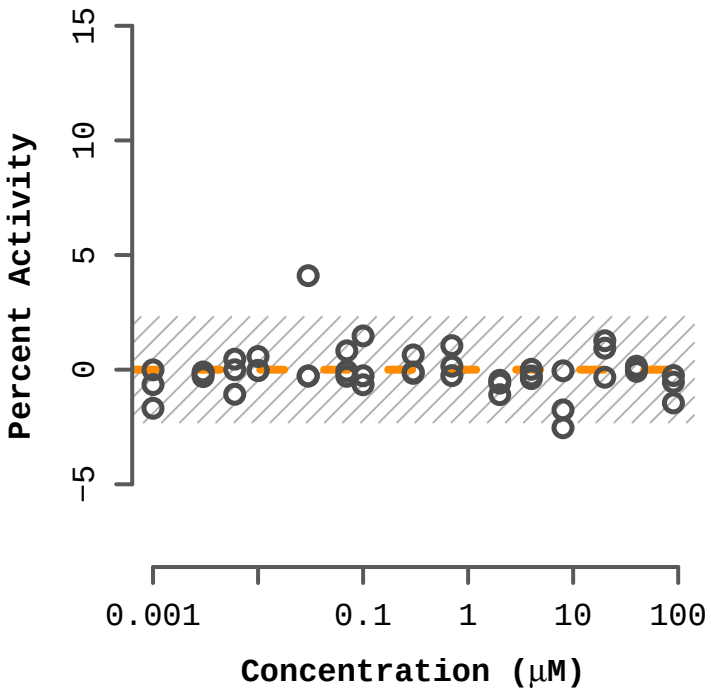
NAME: 2-Hydroxyethyl methacrylate phosphate
CHID: 44951 **CASRN:** 52628-03-2
SPID(S): Tox21_301277
M4ID: 12477856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

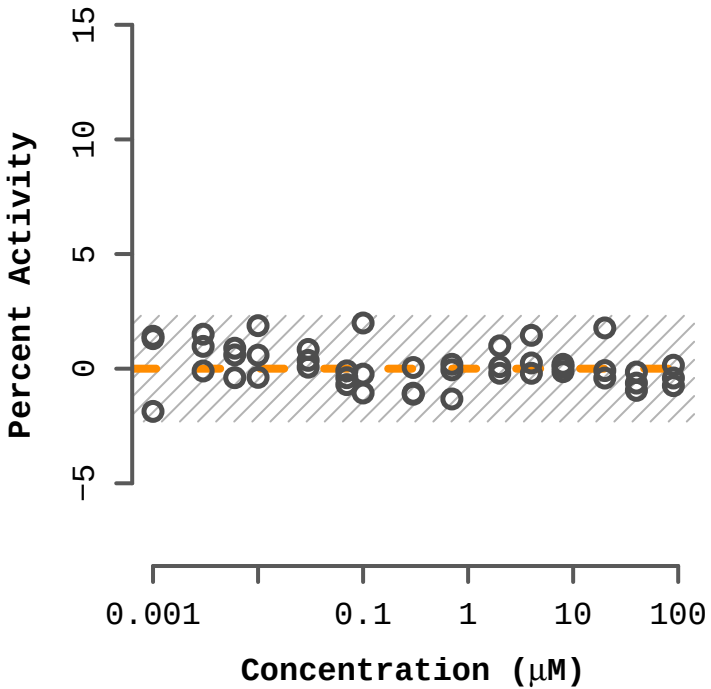
NAME: 2-(Pyridin-4-yl)ethanol
CHID: 44953 **CASRN:** 5344-27-4
SPID(S): Tox21_301621
M4ID: 12477512

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

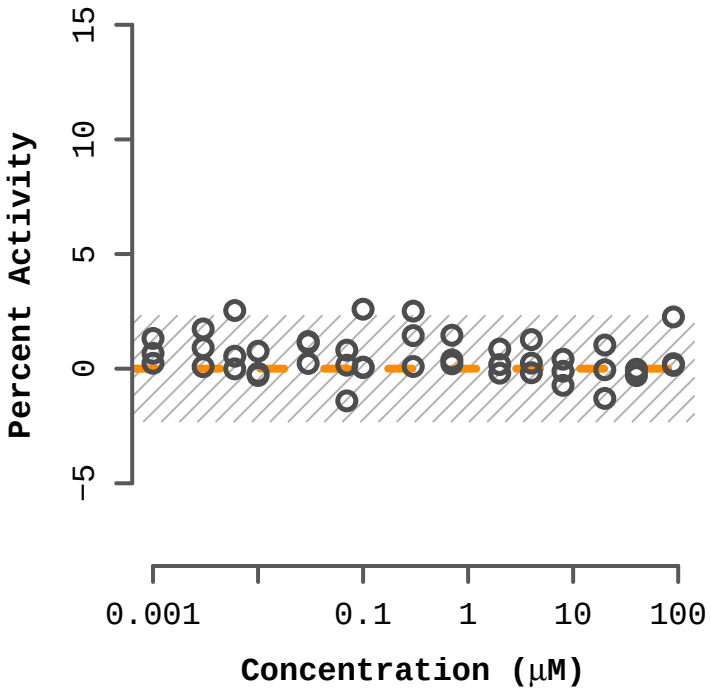
NAME: Sodium nicotinate
CHID: 44955 CASRN: 54-86-4
SPID(S): Tox21_301221
M4ID: 12477912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

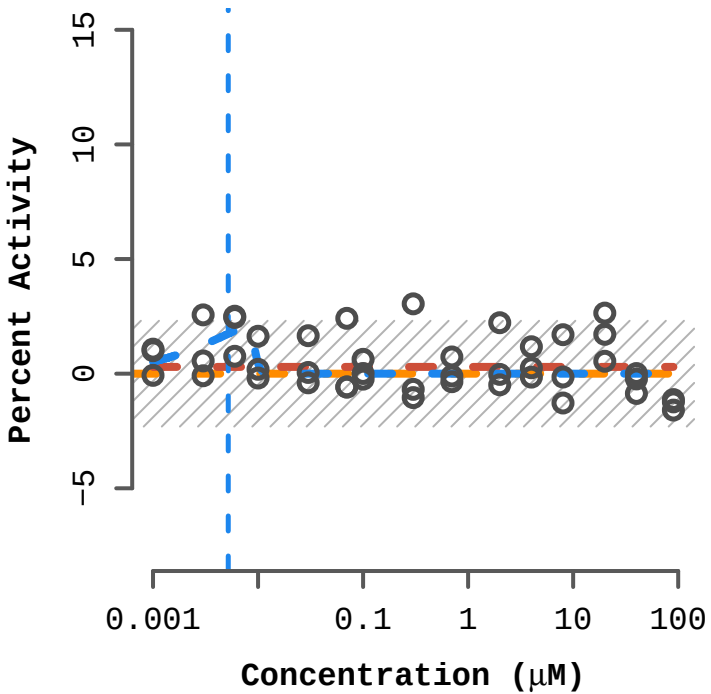
NAME: Trimethylsilyl silicate
CHID: 44958 **CASRN:** 56275-01-5
SPID(S): Tox21_301804
M4ID: 12477329

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propane−1,3−diyl bis(4−aminobenzoate)
CHID: 44960 CASRN: 57609−64−0
SPID(S): Tox21_301701
M4ID: 12477432

HILL MODEL (in red):

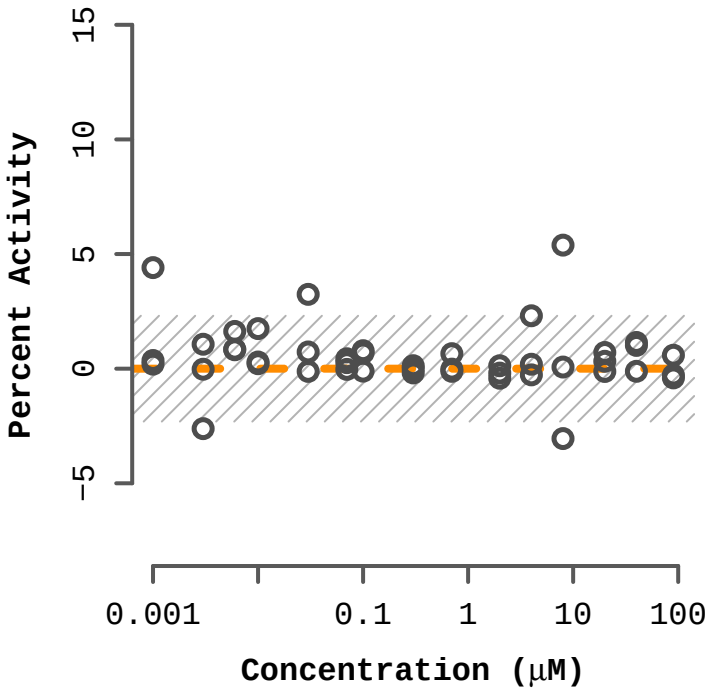
	tp	ga	gw
val:	0.296	−4.24	5.6
sd:	0.184	1170	5240

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.48	−2.28	1.05	−2.03	18
sd:	6.52	1.49	1.02	0.07	36.7

	CNST	HILL	GNLS
AIC:	152.62	155.94	151.43
PROB:	0.33	0.06	0.6
RMSE:	1.28	1.21	1.13

MAX_MEAN: 1.91 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

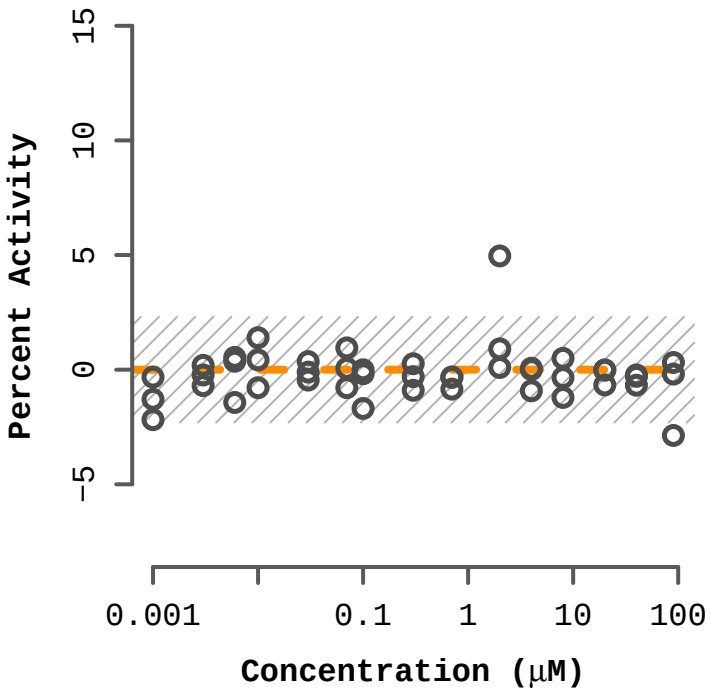
NAME: Bis{2-[2-(propan-2-yl)-1,3-oxazolidin-3-yl]eth
CHID: 44961 **CASRN:** 59719-67-4
SPID(S): Tox21_301668
M4ID: 12477465

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

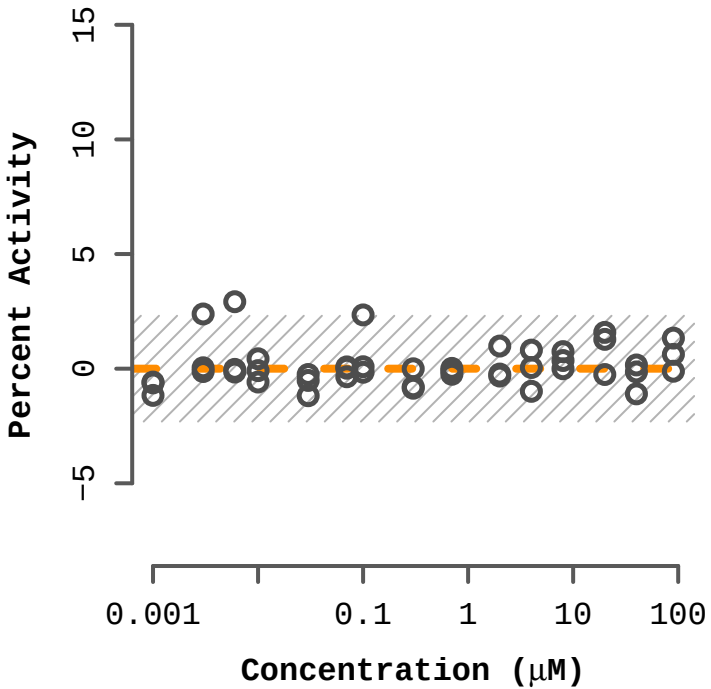
NAME: 3,3'−Sulphonyldianiline
CHID: 44962 CASRN: 599−61−1
SPID(S): Tox21_301737
M4ID: 12477396

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.99 MAX_MED: 0.908 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

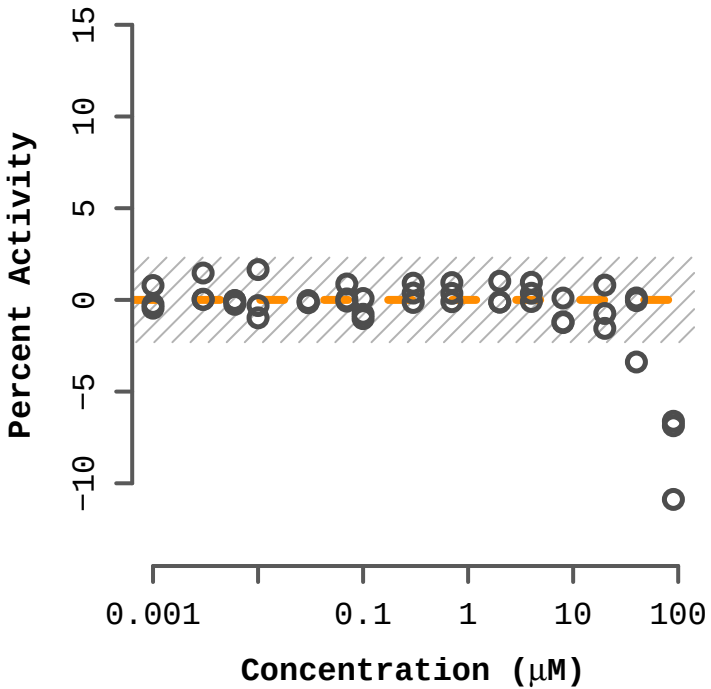
NAME: 4-(3-Methyl-5-oxo-4,5-dihydro-1H-pyrazol-1-yl)|
CHID: 44963 CASRN: 60875-16-3
SPID(S): Tox21_301816
M4ID: 12477317

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.916 MAX_MED: 1.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

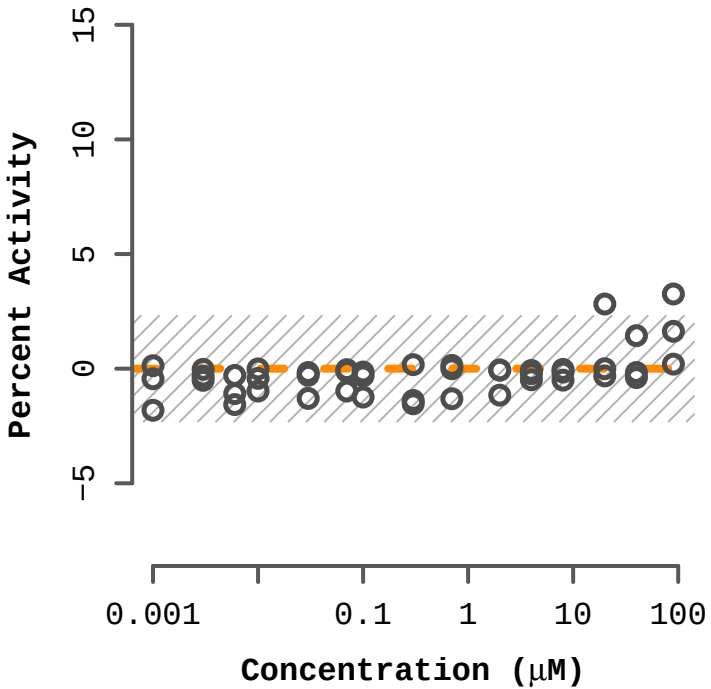
NAME: N-(4-Methylpentan-2-yl)-N-phenylbenzene-1,4-dia
CHID: 44966 CASRN: 61931-82-6
SPID(S): Tox21_301410
M4ID: 12477723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.31	NA	NA

MAX_MEAN: 0.511 MAX_MED: 0.374 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

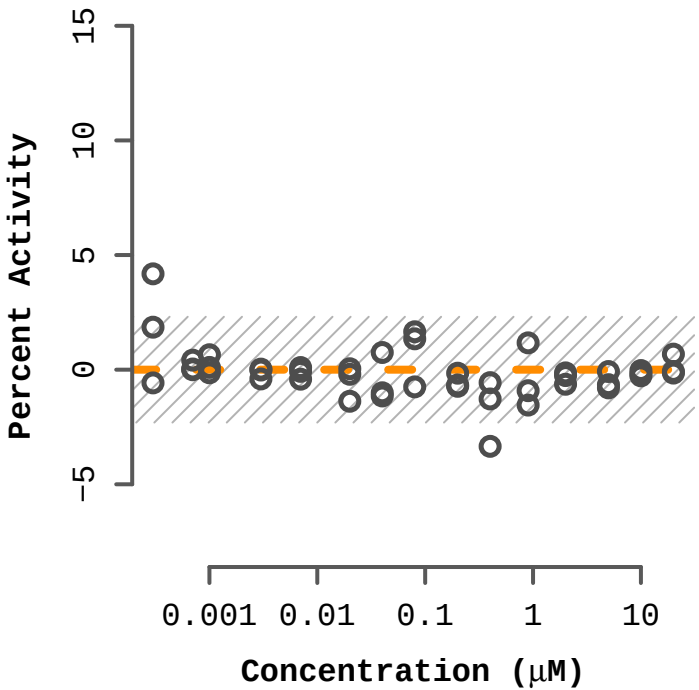
NAME: 1,3-Dioxane-5,5-diyldimethanol
CHID: 44967 **CASRN:** 6228-25-7
SPID(S): Tox21_301652
M4ID: 12477481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.73	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

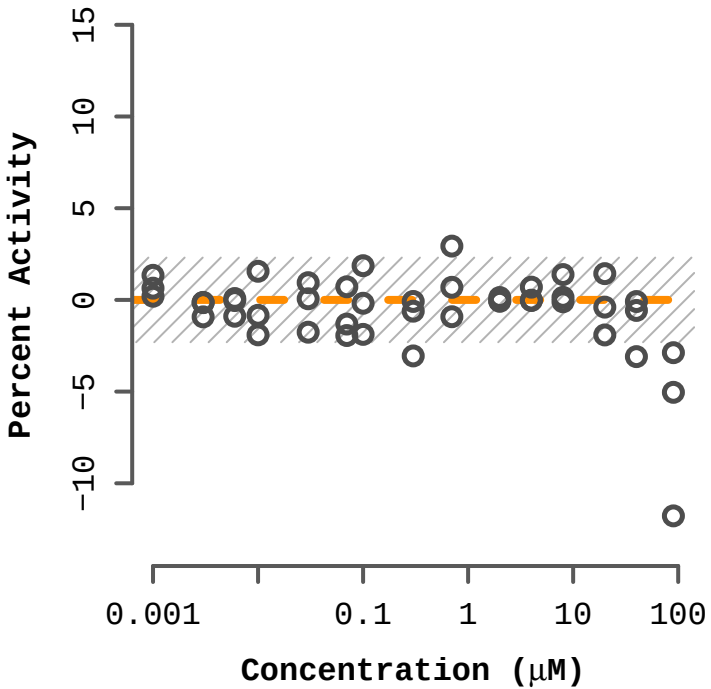
NAME: 2-(3a,4,5,6,7,7a-Hexahydro-1H-4,7-methanoinden-
CHID: 44970 **CASRN:** 65983-31-5
SPID(S): Tox21_303870
M4ID: 12475318

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

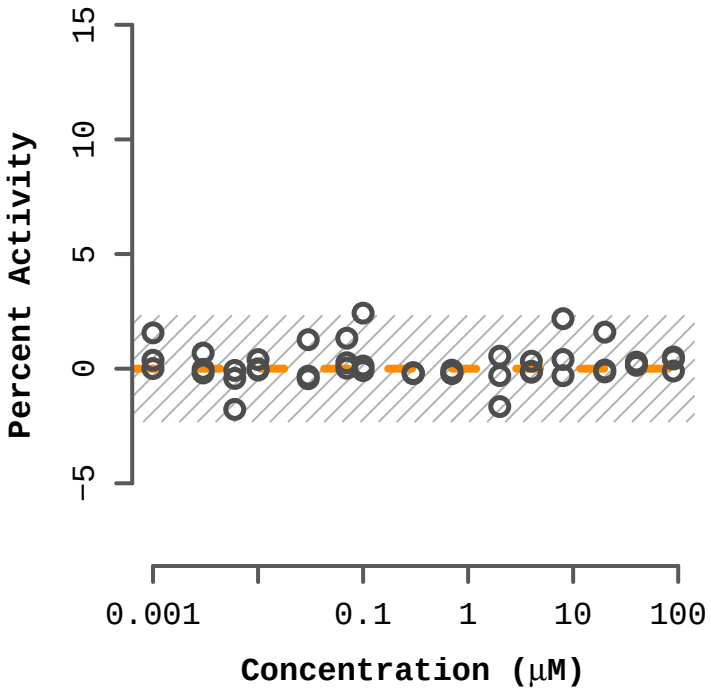
NAME: 2,2',2''-[Methanetriyltris(benzene-4,1-diyloxy
CHID: 44971 CASRN: 66072-38-6
SPID(S): Tox21_301653
M4ID: 12477480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.3	NA	NA

MAX_MEAN: 0.902 MAX_MED: 0.689 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

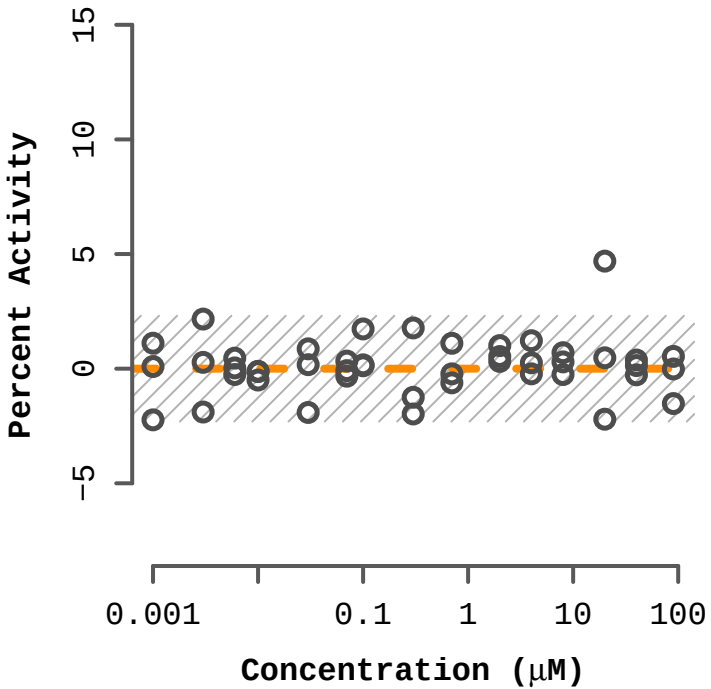
NAME: 1,10−Decanediol dimethacrylate
CHID: 44972 **CASRN:** 6701−13−9
SPID(S): Tox21_301803
M4ID: 12477330

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.821 **MAX_MED:** 0.422 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

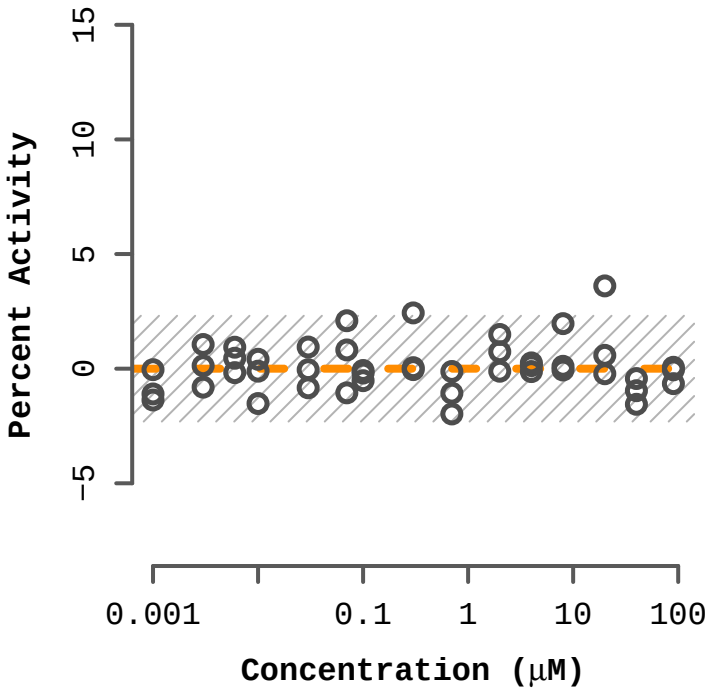
NAME: Propan-2-yl 2-ethylhexanoate
CHID: 44973 **CASRN:** 67024-46-8
SPID(S): Tox21_301232
M4ID: 12477901

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.989 **MAX_MED:** 0.532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

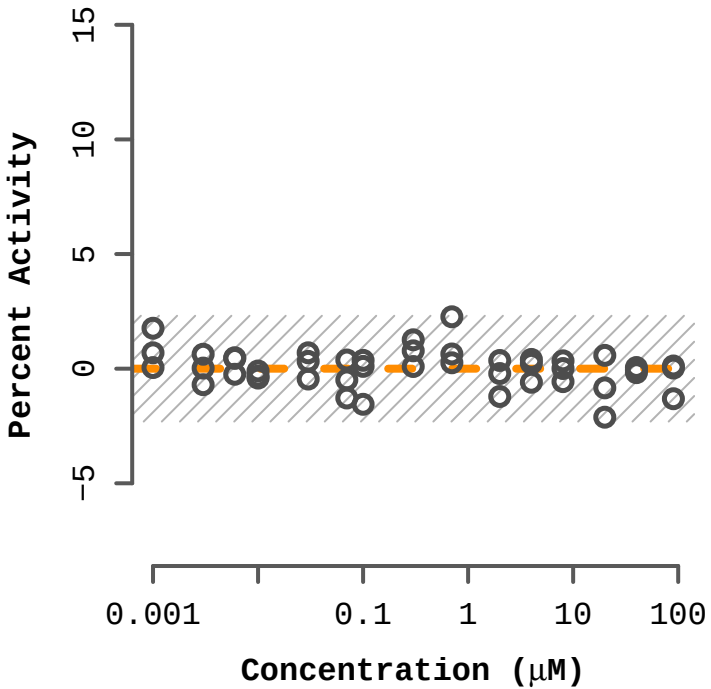
NAME: N'−[3−(Dimethylamino)propyl]−N,N−dimethylpropa
CHID: 44974 CASRN: 6711−48−4
SPID(S): Tox21_301691
M4ID: 12477442

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.33 MAX_MED: 0.819 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

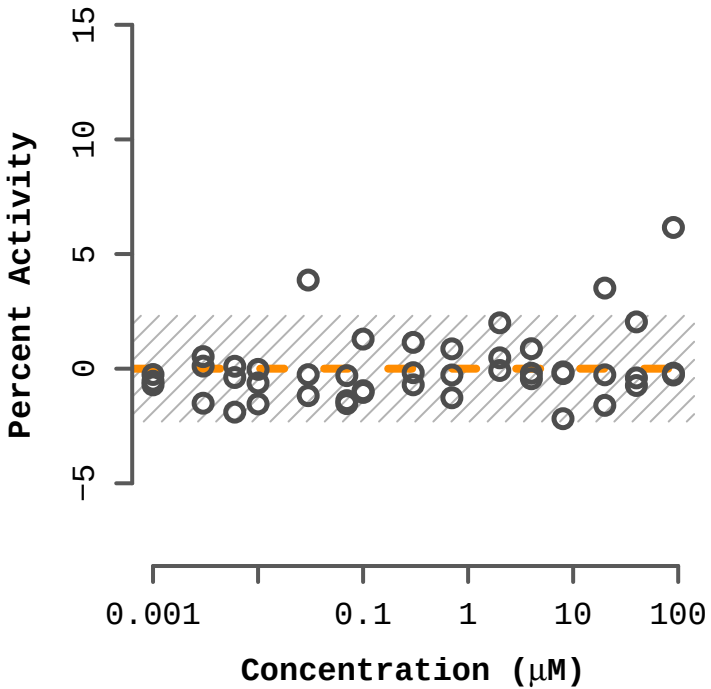
NAME: 1-{Bis[3-(dimethylamino)propyl]amino}propan-2-(
CHID: 44975 **CASRN:** 67151-63-7
SPID(S): Tox21_301306
M4ID: 12477827

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.781 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

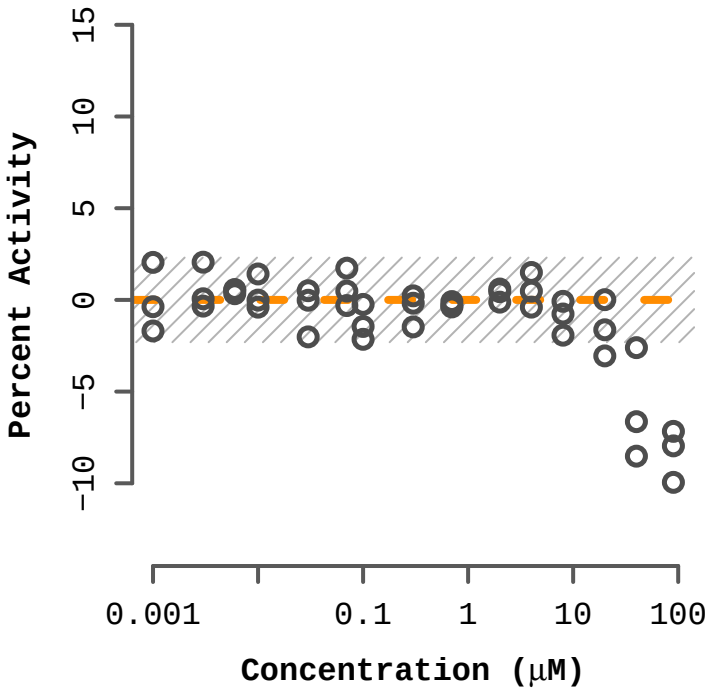
NAME: 2,2-Bis[(prop-2-en-1-yloxy)methyl]butan-1-ol
CHID: 44976 **CASRN:** 682-09-7
SPID(S): Tox21_301662
M4ID: 12477471

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis[(2-ethyl-2,5-dimethylhexanoyl)oxy](dimethy

CHID: 44978 **CASRN:** 68928-76-7

SPID(S): Tox21_301790

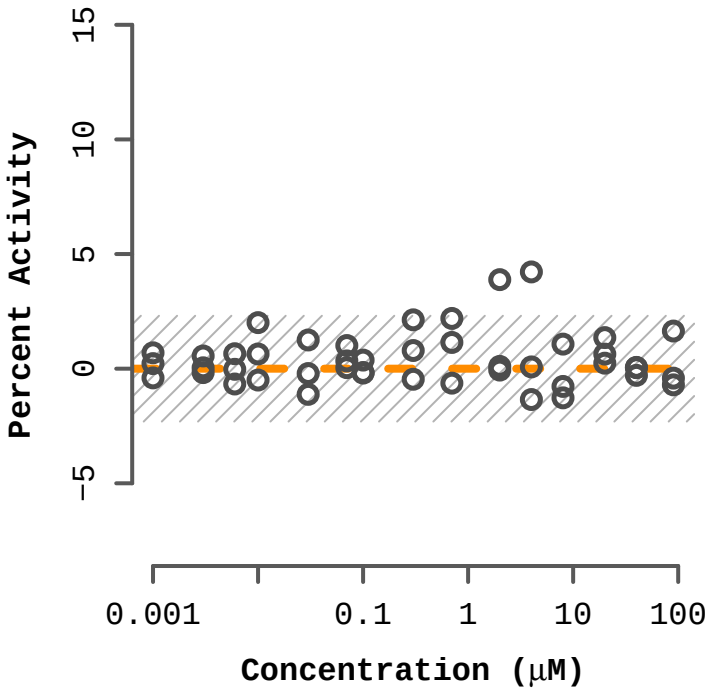
M4ID: 12477343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.94	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 0.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

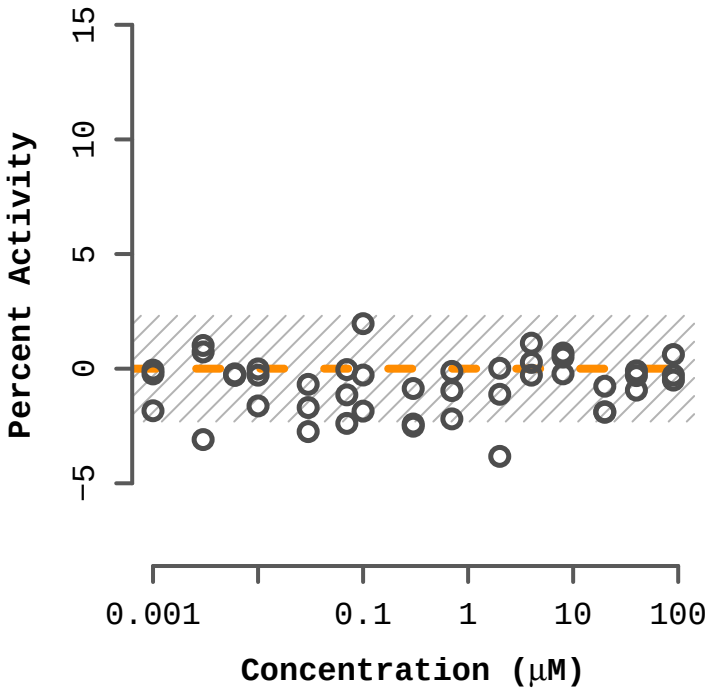
NAME: 2-Chlorobenzenesulfonamide
CHID: 44979 **CASRN:** 6961-82-6
SPID(S): Tox21_301624
M4ID: 12477509

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

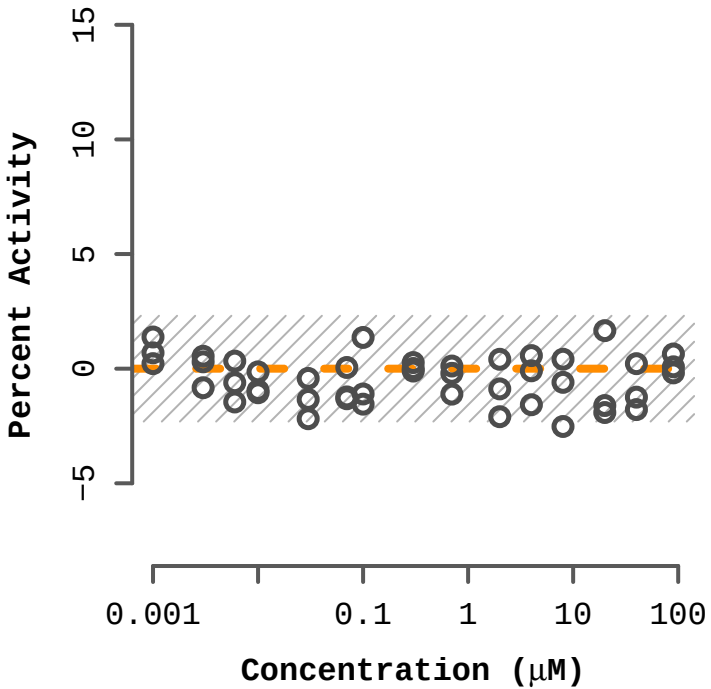
NAME: 3-{[3-(Dimethylamino)propyl]amino}propanenitri
CHID: 44980 CASRN: 69852-45-5
SPID(S): Tox21_301749
M4ID: 12477384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 0.369 **MAX_MED:** 0.732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

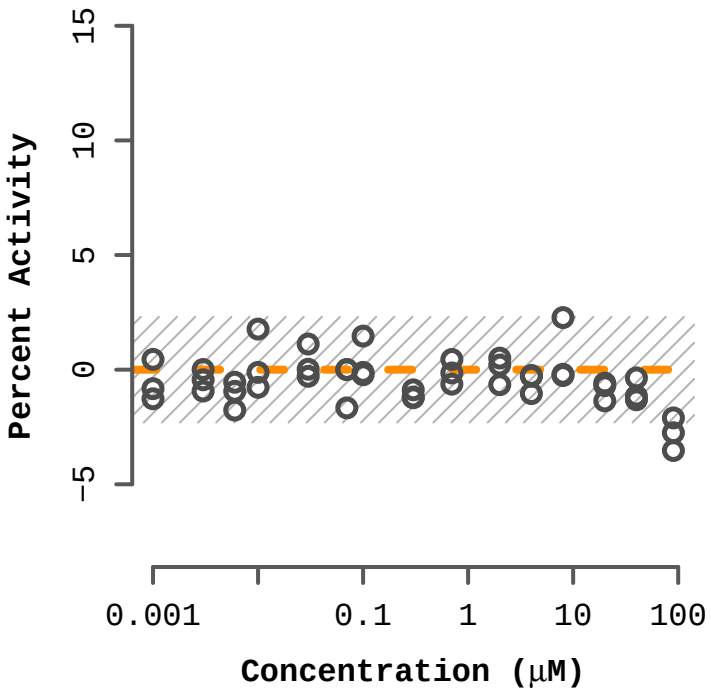
NAME: Phenyl dihydrogen phosphate
CHID: 44981 **CASRN:** 701-64-4
SPID(S): Tox21_301808
M4ID: 12477325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.765 **MAX_MED:** 0.692 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

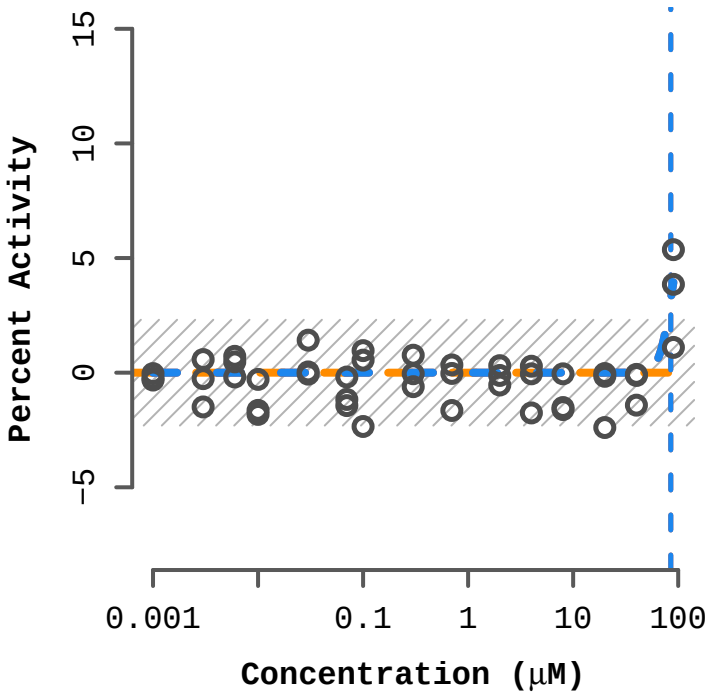
NAME: 2-Amino-N-cyclohexyl-N-methylbenzenesulfonamid
CHID: 44982 **CASRN:** 70693-59-3
SPID(S): Tox21_301697
M4ID: 12477436

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.607 **MAX_MED:** 0.204 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(2-Ethoxyethoxy)ethyl prop-2-enoate
CHID: 44983 CASRN: 7328-17-8
SPID(S): Tox21_301618
M4ID: 12477515

HILL MODEL (in red):

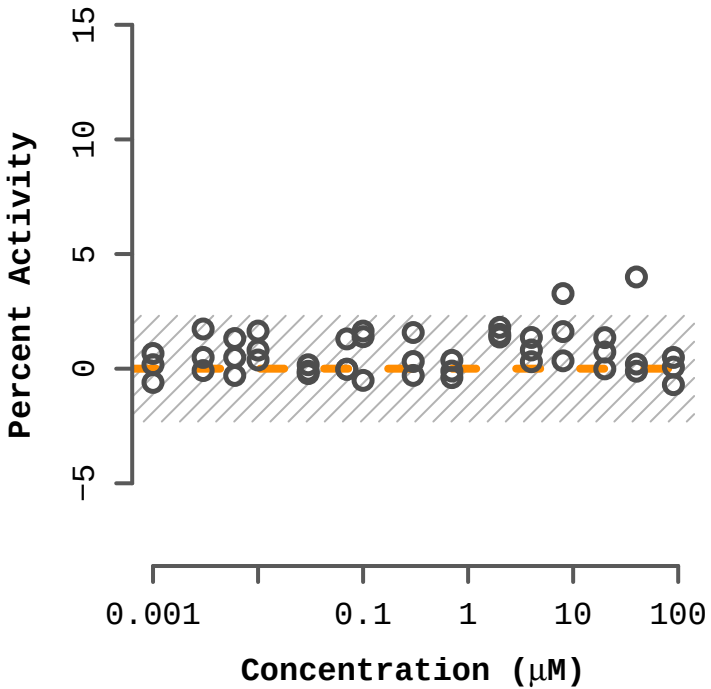
	tp	ga	gw
val:	6.44	1.93	8
sd:	5.34	0.106	7.93

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.44	1.93	8	3.13	7.12
sd:	5.32	0.106	7.93	10400	62900

	CNST	HILL	GNLS
AIC:	148.88	141.59	145.59
PROB:	0.02	0.86	0.12
RMSE:	1.39	1.08	1.08

MAX_MEAN: 3.44 MAX_MED: 3.85 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

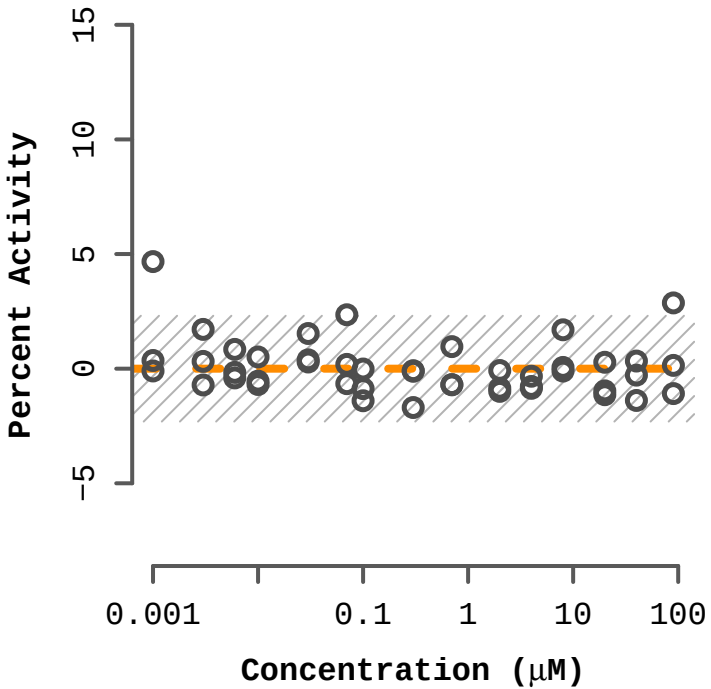
NAME: {2-[2-(Ethenyloxy)ethoxy]ethoxy}ethene
CHID: 44985 **CASRN:** 764-99-8
SPID(S): Tox21_301264
M4ID: 12477869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

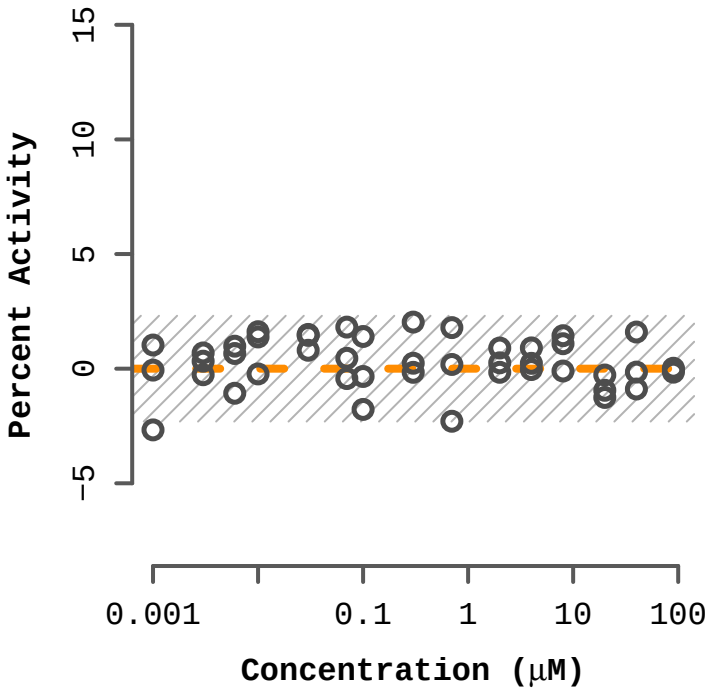
NAME: 3,6,9,12−Tetraoxatetradeca−1,13−diene
CHID: 44986 CASRN: 765−12−8
SPID(S): Tox21_301708
M4ID: 12477425

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 0.388 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

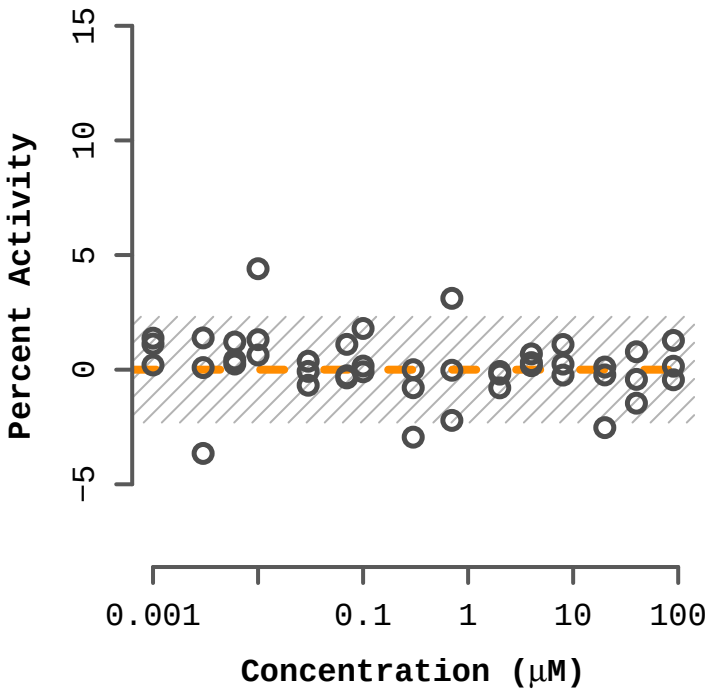
NAME: 3-Bromo-4-fluorobenzaldehyde
CHID: 44989 **CASRN:** 77771-02-9
SPID(S): Tox21_301633
M4ID: 12477500

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

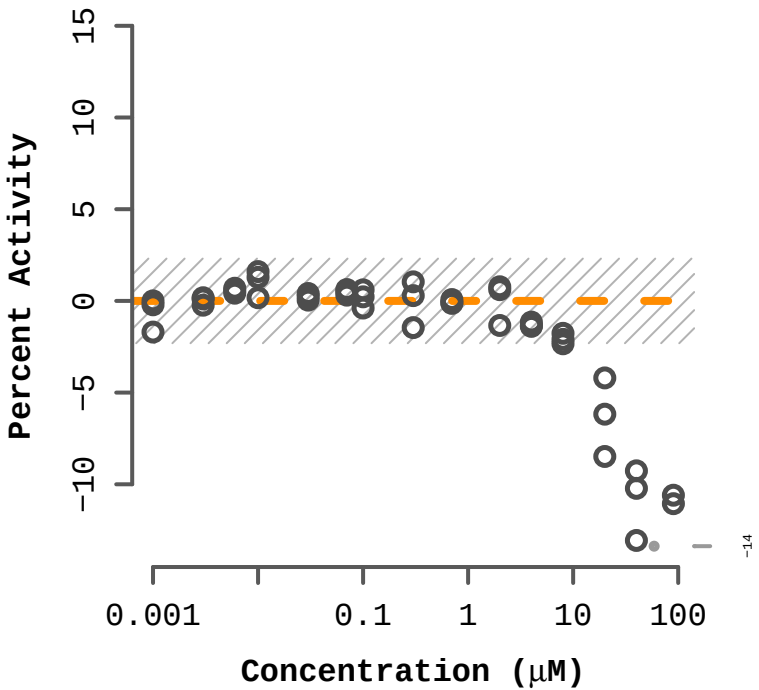
NAME: 3,3,5-Trimethylcyclohexyl 2-methylprop-2-enoat
CHID: 44990 CASRN: 7779-31-9
SPID(S): Tox21_301400
M4ID: 12477733

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 2.12 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

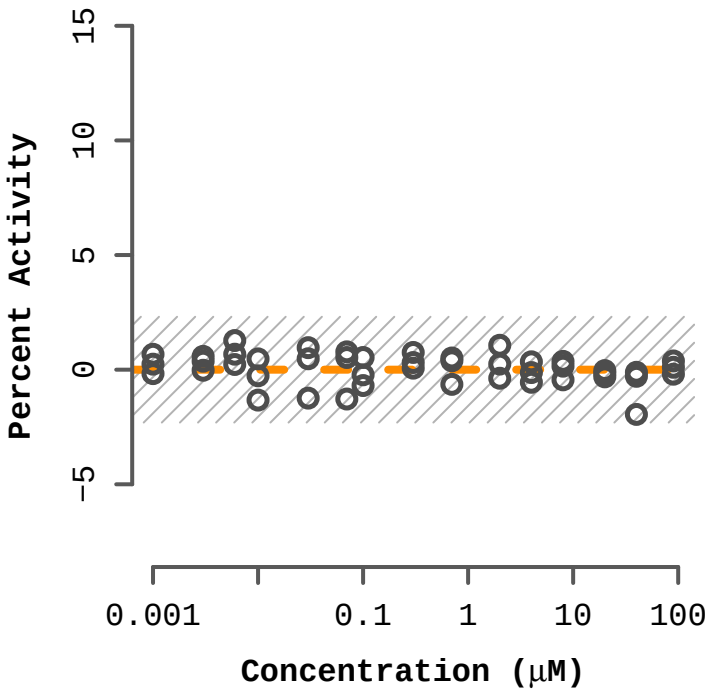
NAME: 2,5-Bis(2-methylbutan-2-yl)benzene-1,4-diol
CHID: 44992 **CASRN:** 79-74-3
SPID(S): Tox21_301767
M4ID: 12477366 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.28	NA	NA
PROB:	1	NA	NA
RMSE:	4.58	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

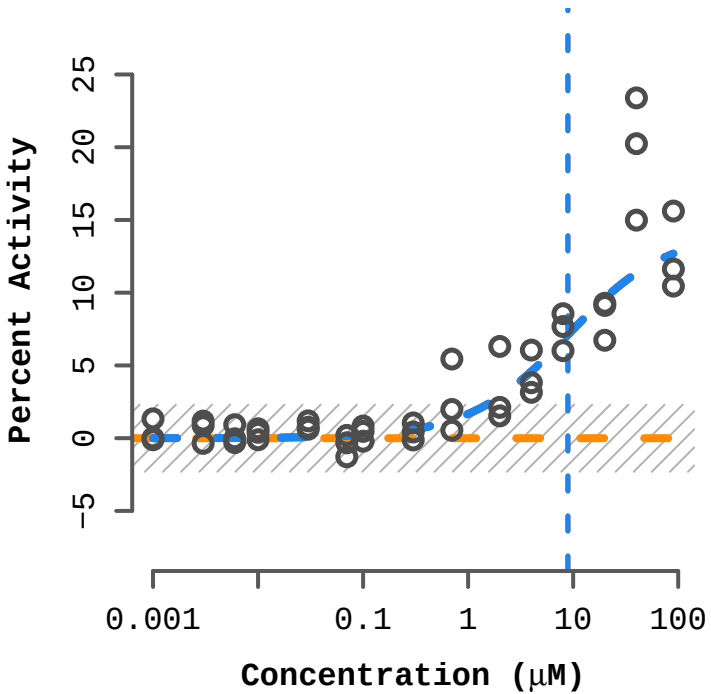
NAME: 4,4'−Propane−2,2−diyldicyclohexanol
CHID: 44993 **CASRN:** 80−04−6
SPID(S): Tox21_301398
M4ID: 12477735

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 0.676 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethylanthracene-9,10-dione
CHID: 44994 CASRN: 84-51-5
SPID(S): Tox21_301694
M4ID: 12477439

HILL MODEL (in red):

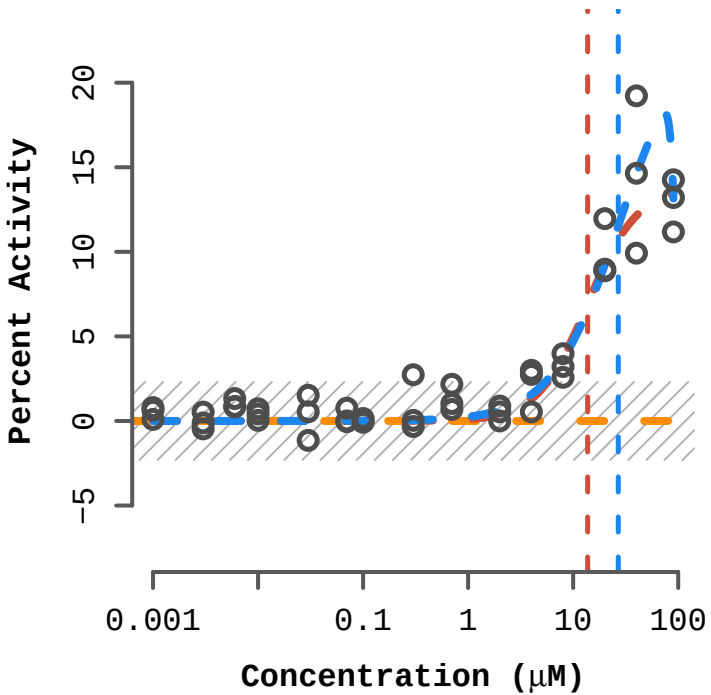
	tp	ga	gw
val:	14.2	0.95	0.922
sd:	2.74	0.218	0.226

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.2	0.95	0.922	3.2	9.77
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	292.85	192.9	196.9
PROB:	0	0.88	0.12
RMSE:	7	2.64	2.64

MAX_MEAN: 19.5 MAX_MED: 20.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9-Ethyl-3-nitro-9H-carbazole
CHID: 44995 CASRN: 86-20-4
SPID(S): Tox21_301272
M4ID: 12477861

HILL MODEL (in red):

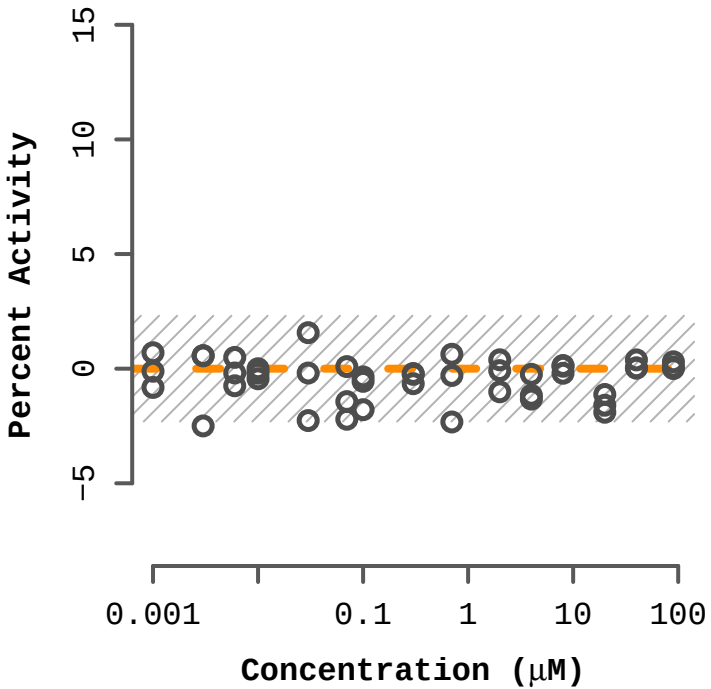
	tp	ga	gw
val:	13.8	1.14	1.84
sd:	0.885	0.0513	0.365

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.1	1.43	1.37	1.97	17.6
sd:	7.48	0.216	0.303	0.00573	12.3

	CNST	HILL	GNLS
AIC:	272.36	157.59	155.98
PROB:	0	0.31	0.69
RMSE:	5.89	1.53	1.37

MAX_MEAN: 14.6 MAX_MED: 14.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

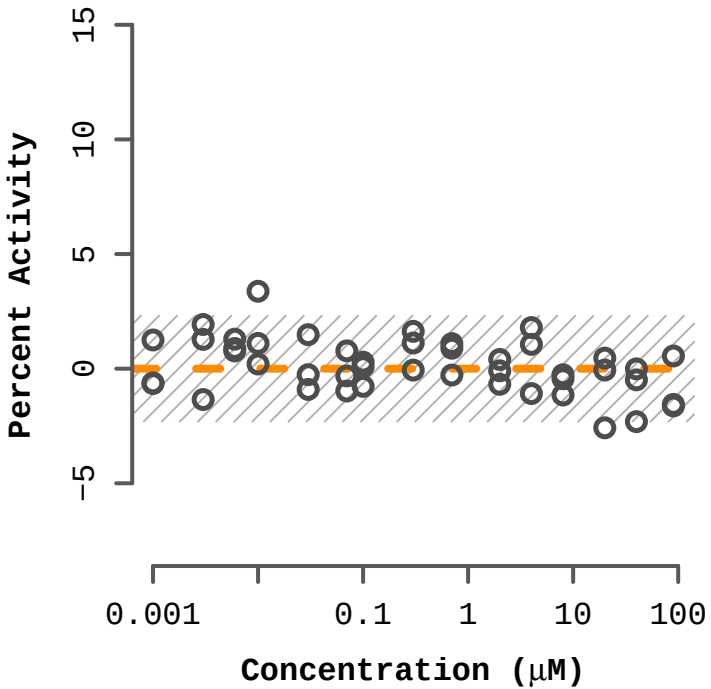
NAME: 3,3,5−Trimethylcyclohexanone
CHID: 44996 CASRN: 873−94−9
SPID(S): Tox21_301727
M4ID: 12477406

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.149 MAX_MED: 0.562 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

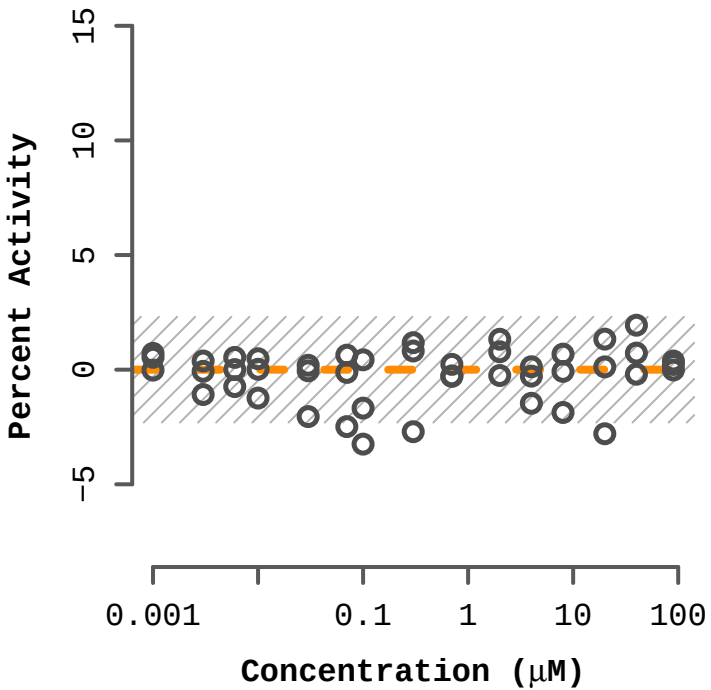
NAME: 2,6-Di-tert-butyl-4-[(dimethylamino)methyl]phe
CHID: 44997 CASRN: 88-27-7
SPID(S): Tox21_301401
M4ID: 12477732

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.56 MAX_MED: 1.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

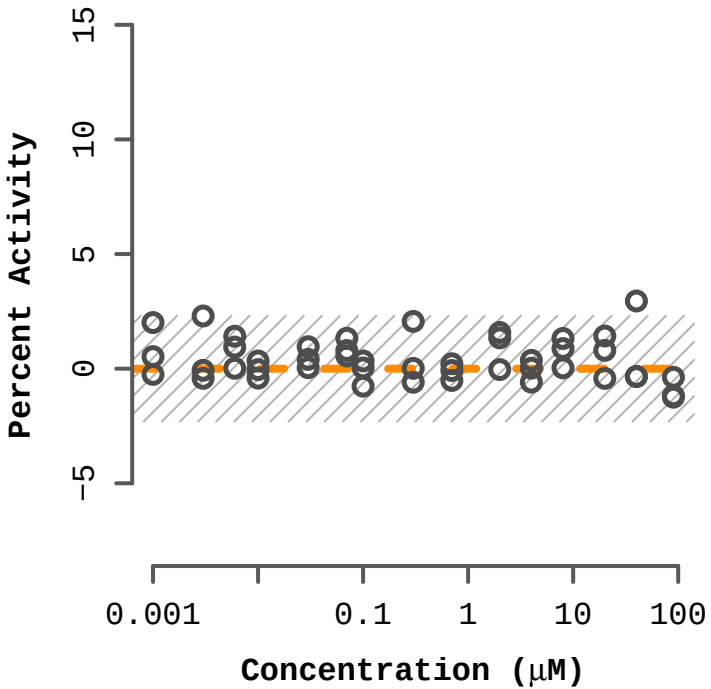
NAME: Fluxofenim
CHID: 44998 **CASRN:** 88485-37-4
SPID(S): Tox21_301792
M4ID: 12477341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.823 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

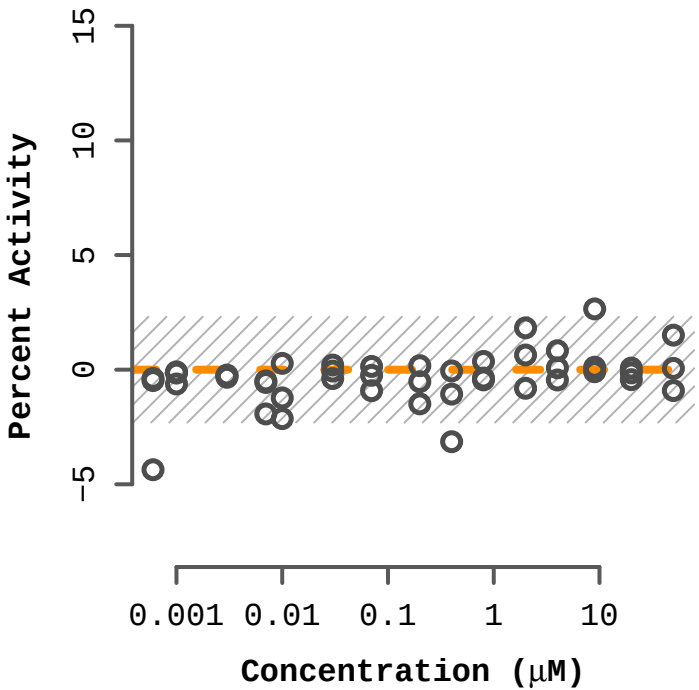
NAME: 4-(3-Methyl-5-oxo-4,5-dihydro-1H-pyrazol-1-yl)|
CHID: 44999 CASRN: 89-36-1
SPID(S): Tox21_301281
M4ID: 12477852

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.72	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.963 MAX_MED: 1.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

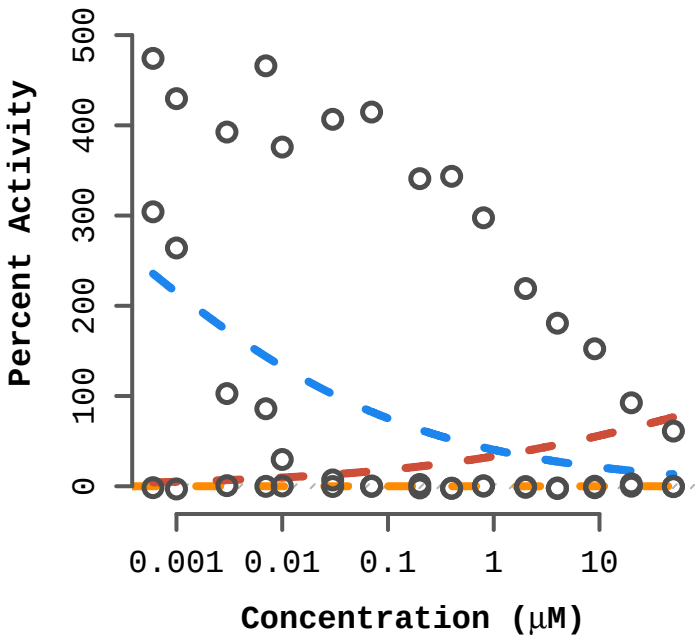
NAME: Verazide
CHID: 45002 **CASRN:** 93-47-0
SPID(S): Tox21_111963_1
M4ID: 12483403

HILL MODEL: Not applicable.

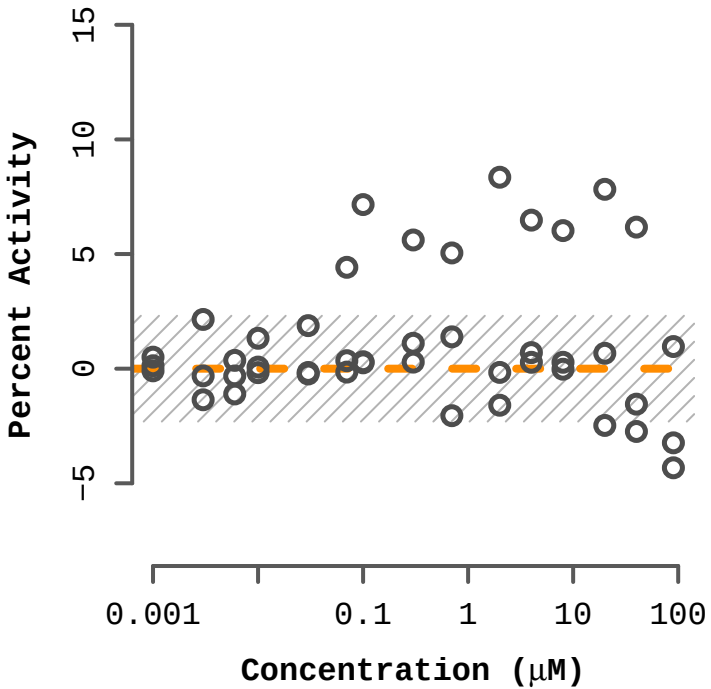
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.891 **MAX_MED:** 0.642 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Suplatast tosylate
CHID:    45003   CASRN: 94055-76-2
SPID(S): Tox21_112652_1
M4ID:    12482996

HILL MODEL (in red):
      tp       ga       gw
val:  184      2.2      0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  568      -3.97    7.32     -3.72    0.3
sd:   766      77.4     751      3.16     0.188

      CNST        HILL        GNLS
AIC:  637.47      606.69      595.96
PROB: 0           0           1
RMSE: 204.38      197.38      155.05

MAX_MEAN: 259       MAX_MED: 304       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

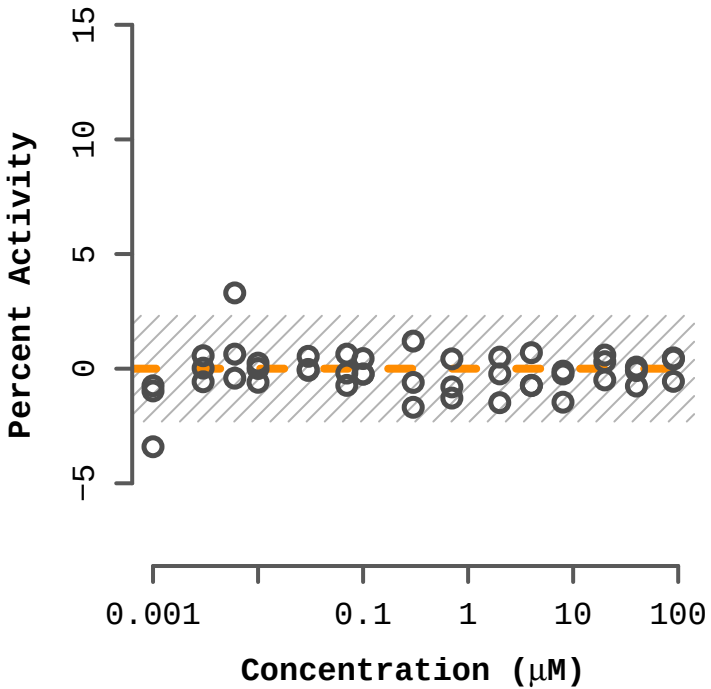
NAME: 2,4-Dichloro-1-(chloromethyl)benzene
CHID: 45005 **CASRN:** 94-99-5
SPID(S): Tox21_301549
M4ID: 12477584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.82	NA	NA
PROB:	1	NA	NA
RMSE:	3.15	NA	NA

MAX_MEAN: 2.57 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

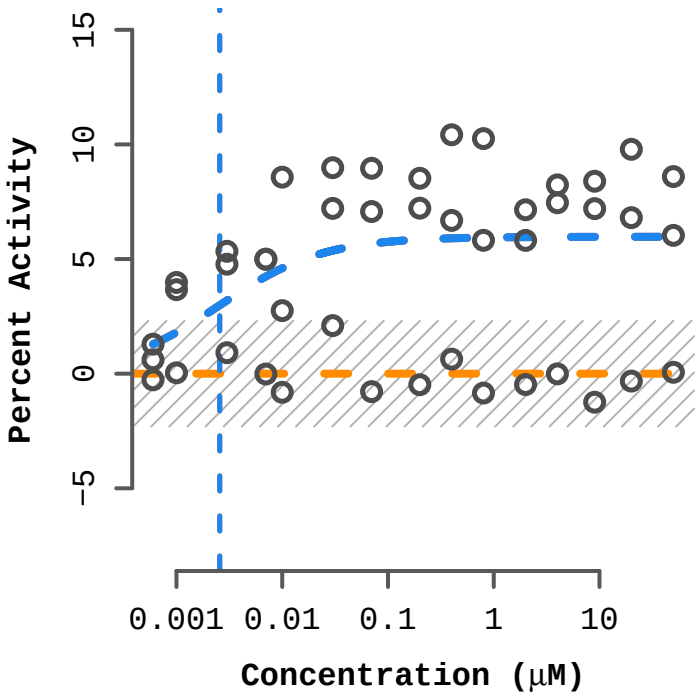
NAME: Nitarsone
CHID: 45007 CASRN: 98-72-6
SPID(S): Tox21_302274
M4ID: 12476859

HILL MODEL: Not applicable.

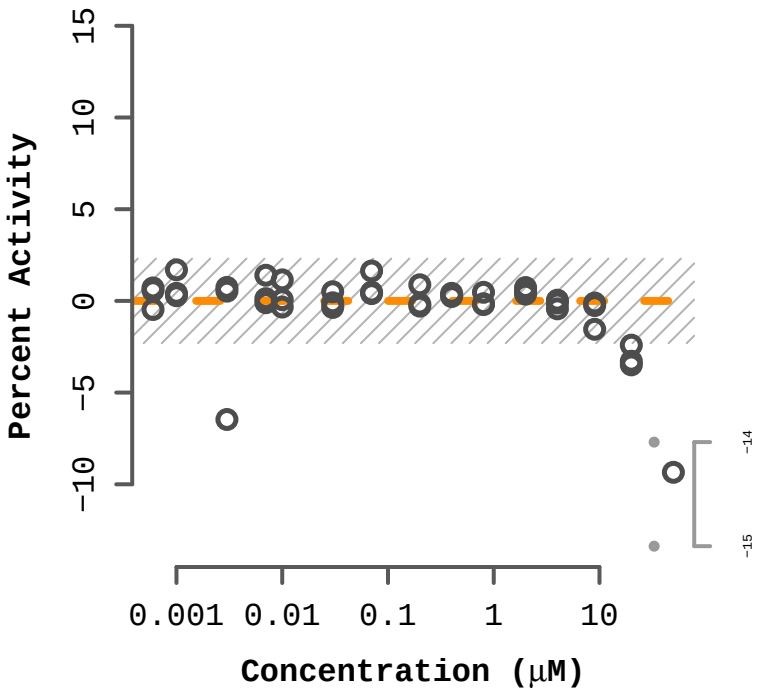
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.18 MAX_MED: 0.637 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Nitarsone
CHID:    45007   CASRN: 98-72-6
SPID(S): Tox21_112758_1
M4ID:    12482967

HILL MODEL (in red):
      tp       ga       gw
val:  5.97     -2.59    0.89
sd:   0.836    0.385    0.577

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.97     -2.59    0.89     2.99     6.27
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  292.78      254.71      258.71
PROB: 0           0.88        0.12
RMSE: 5.75        3.59        3.59

MAX_MEAN: 6.1       MAX_MED: 7.46      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

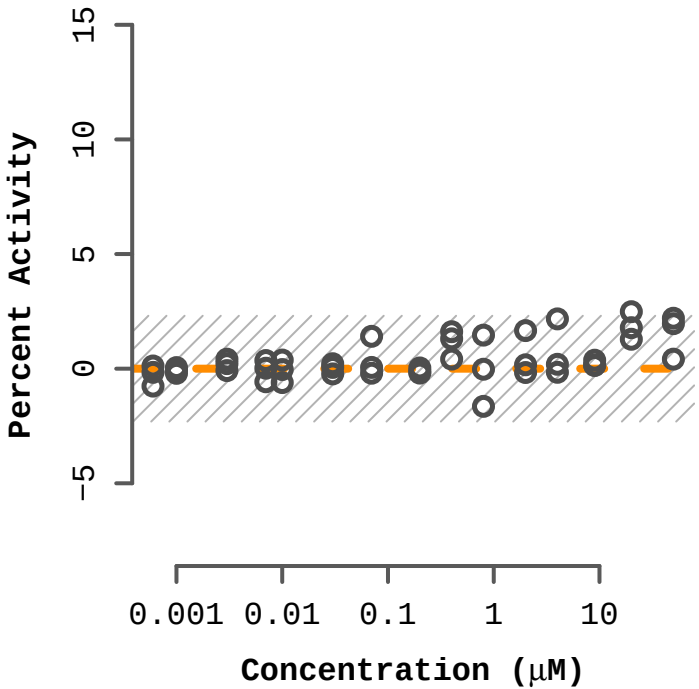
NAME: Maprotiline
CHID: 45029 **CASRN:** 10262-69-8
SPID(S): Tox21_110200_1
M4ID: 12484559 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.7	NA	NA
PROB:	1	NA	NA
RMSE:	3.62	NA	NA

MAX_MEAN: 0.838 **MAX_MED:** 0.559 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

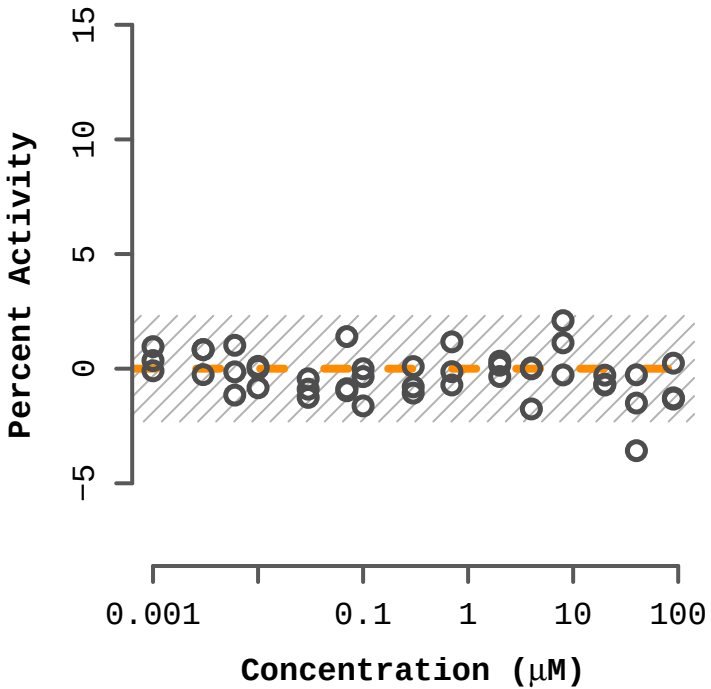
NAME: N,N,N,N',N',N'−Hexamethylhexane−1,6−diaminium
CHID: 45053 **CASRN:** 60−26−4
SPID(S): Tox21_112036_1
M4ID: 12483357

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

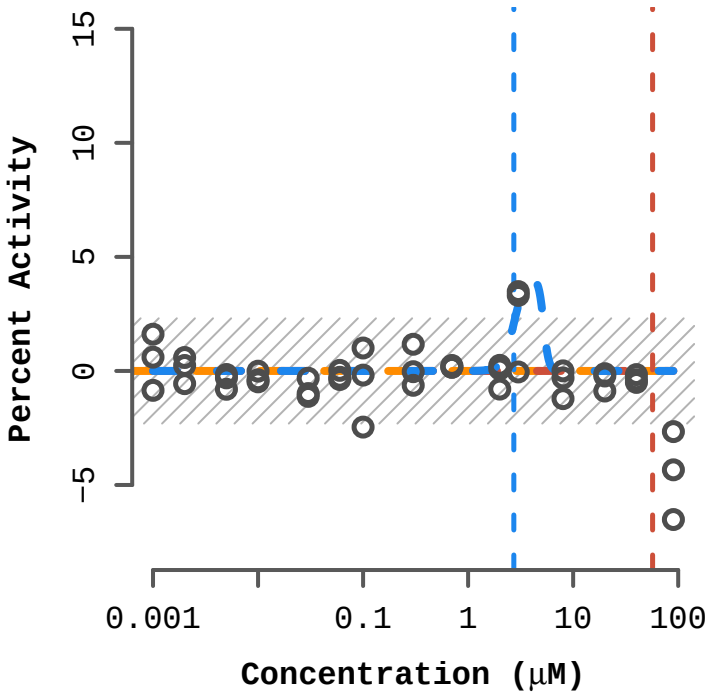
NAME: 2,4,5-Trichlorobenzenesulfonic acid
CHID: 45072 **CASRN:** 6378-25-2
SPID(S): Tox21_301801
M4ID: 12477332

HILL MODEL: Not applicable.

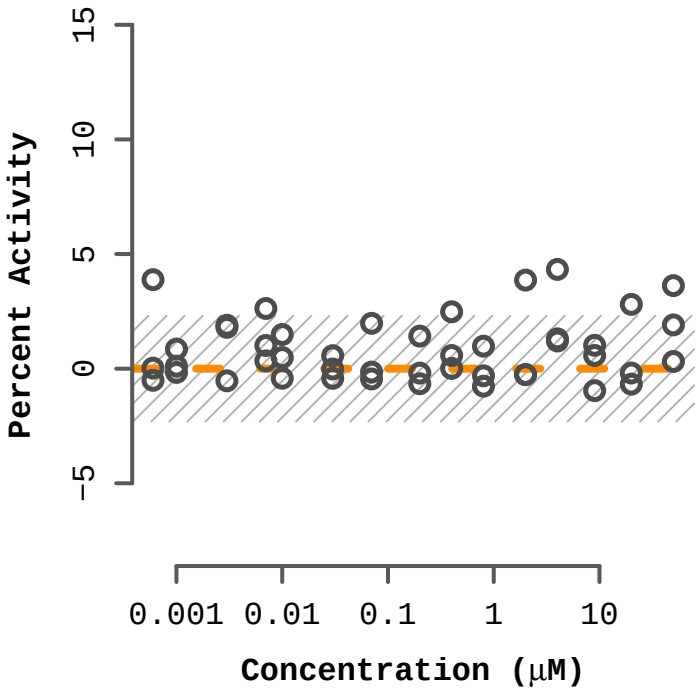
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.985 **MAX_MED:** 1.13 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Chlortetracycline hydrochloride
CHID:    45076   CASRN: 64-72-2
SPID(S): Tox21_301710
M4ID:    12477423

HILL MODEL (in red):
      tp        ga        gw
val:  7.15e-10  1.76      2.45
sd:   8.61e-06  778       115000

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  4.18      0.435     8         0.719     18
sd:   1.85      0.0606    3.36      0.615     59.5

      CNST          HILL          GNLS
AIC:  148.6         154.6         150.6
PROB: 0.71          0.04          0.26
RMSE: 1.58          1.58          1.48

MAX_MEAN: 2.25      MAX_MED: 3.31      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

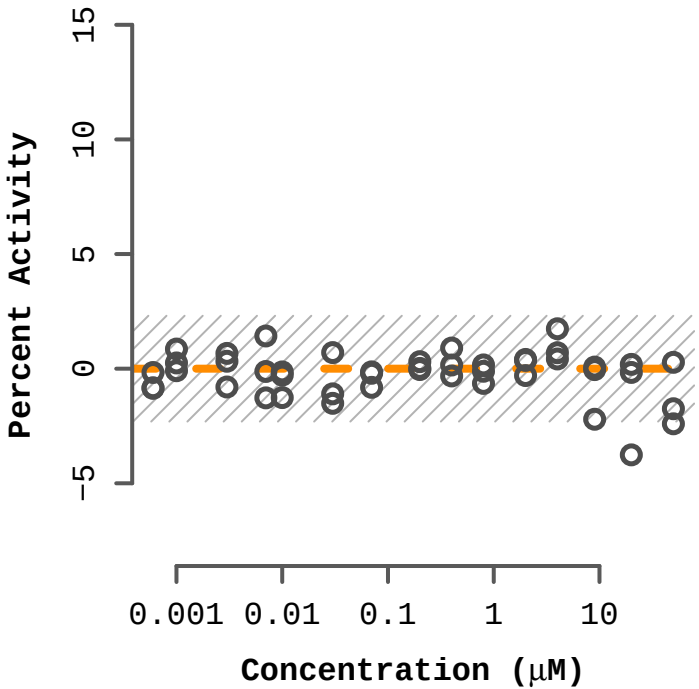
NAME: 8-Quinolinol salicylic acid (1:1)
CHID: 45081 **CASRN:** 2439-07-8
SPID(S): Tox21_110005_1
M4ID: 12484715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

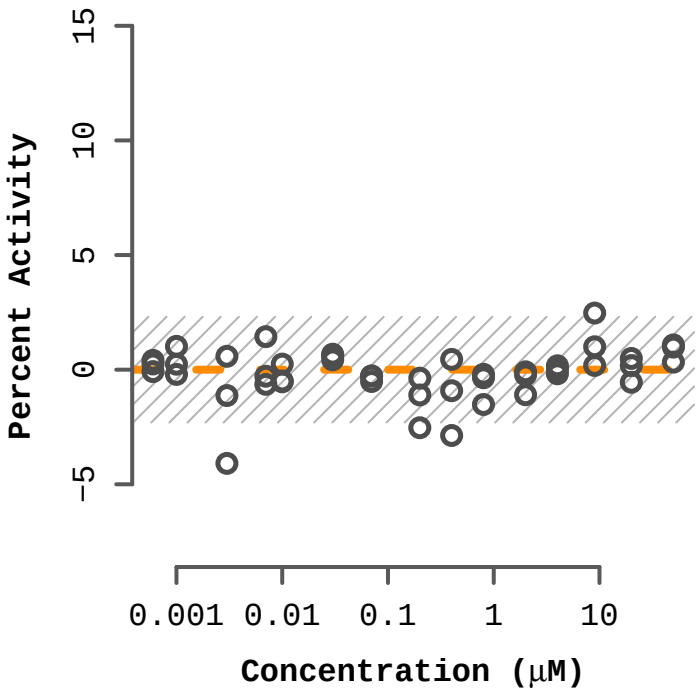
NAME: Aminoquinuride dihydrochloride
CHID: 45083 **CASRN:** 5424-37-3
SPID(S): Tox21_110013_1
M4ID: 12484711

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.954 **MAX_MED:** 0.696 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

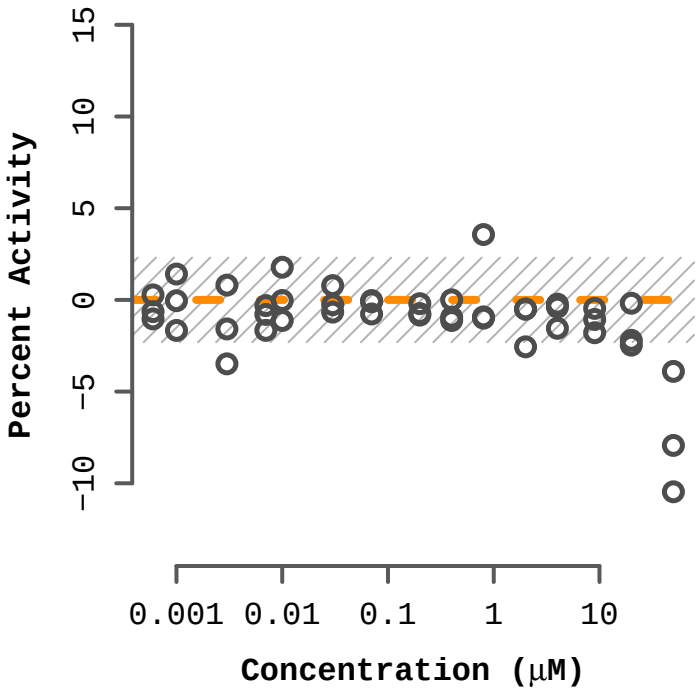
NAME: (2R,3R)−2,3−Dimercaptosuccinic acid
CHID: 45084 **CASRN:** 27887−84−9
SPID(S): Tox21_110015_1
M4ID: 12484710

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

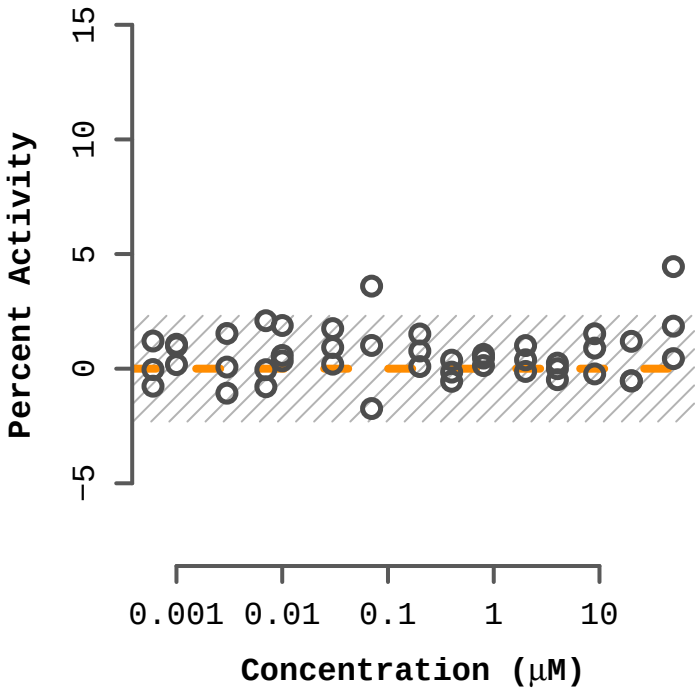
NAME: Fluoperazine dihydrochloride
CHID: 45085 **CASRN:** 440-17-5
SPID(S): Tox21_110017_1
M4ID: 12484709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.41	NA	NA

MAX_MEAN: 0.549 **MAX_MED:** −0.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

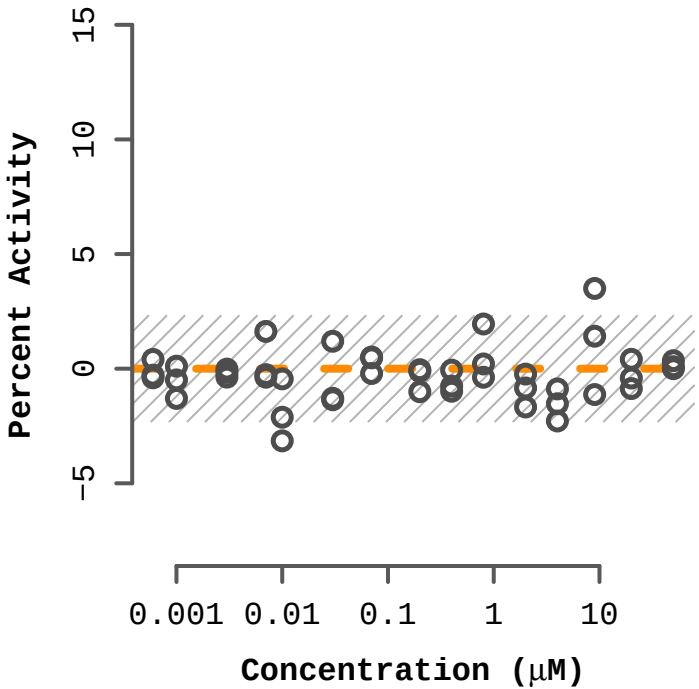
NAME: Pyridoxamine dihydrochloride
CHID: 45088 **CASRN:** 524-36-7
SPID(S): Tox21_110020_1
M4ID: 12484707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

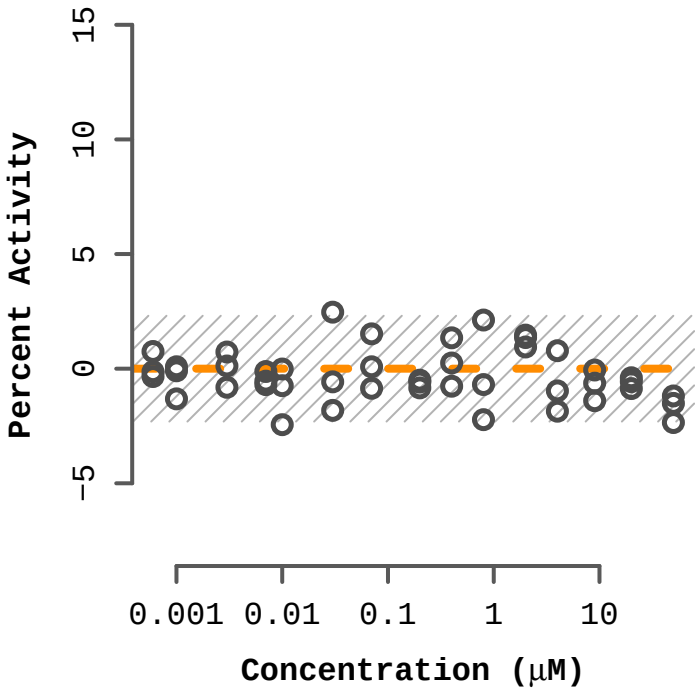
NAME: Carzenide
CHID: 45089 **CASRN:** 138-41-0
SPID(S): Tox21_110021_1
M4ID: 12484706

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

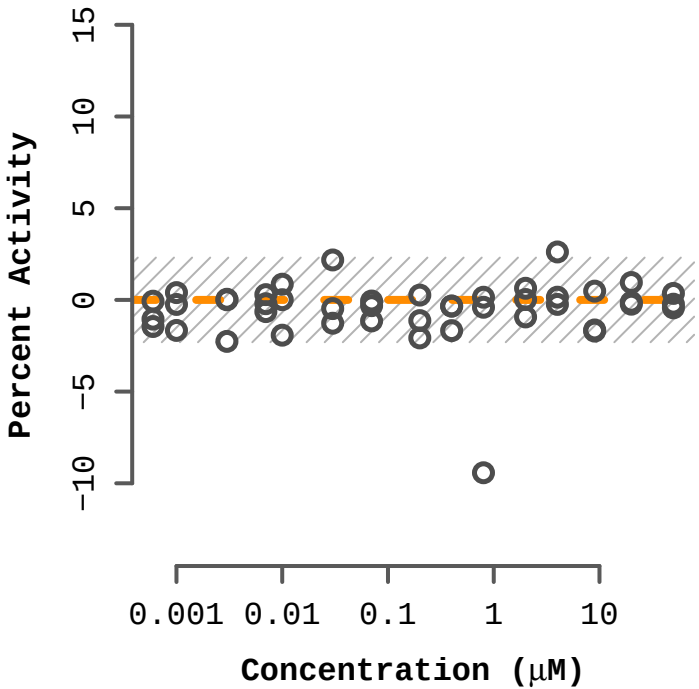
NAME: Pridinol
CHID: 45090 **CASRN:** 511-45-5
SPID(S): Tox21_110022_1
M4ID: 12484705

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

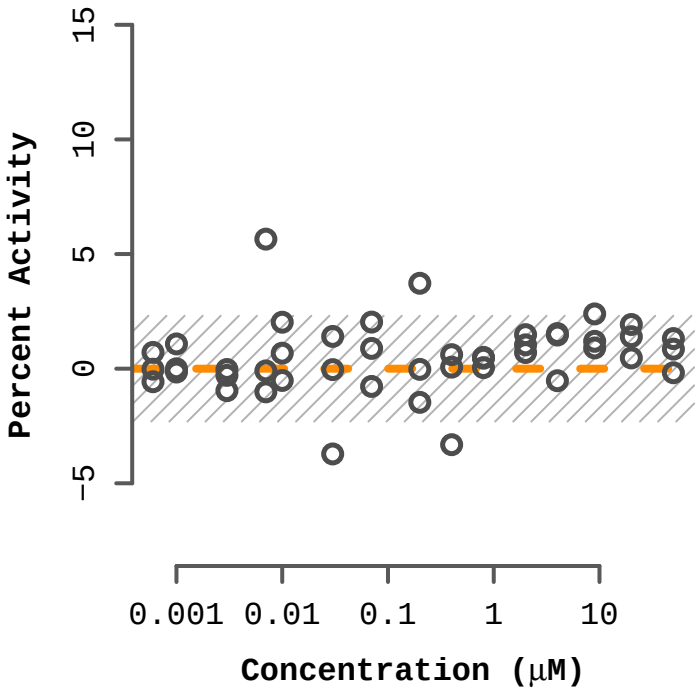
NAME: Procodazole
CHID: 45093 **CASRN:** 23249-97-0
SPID(S): Tox21_110025_1
M4ID: 12484704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 0.841 **MAX_MED:** 0.151 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

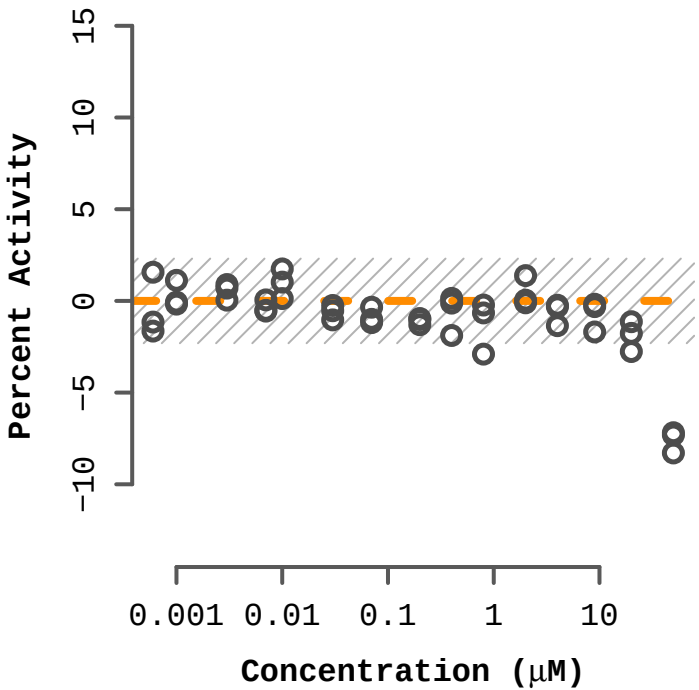
NAME: Homatropine hydrobromide
CHID: 45099 **CASRN:** 51-56-9
SPID(S): Tox21_110318_1
M4ID: 12484460

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

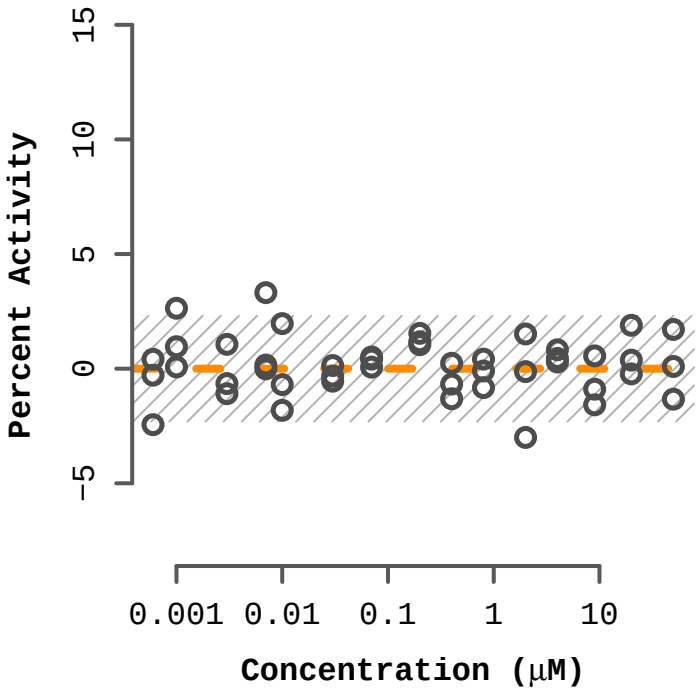
NAME: Cyclobenzaprine hydrochloride
CHID: 45105 **CASRN:** 6202-23-9
SPID(S): Tox21_110040_1
M4ID: 12484698

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

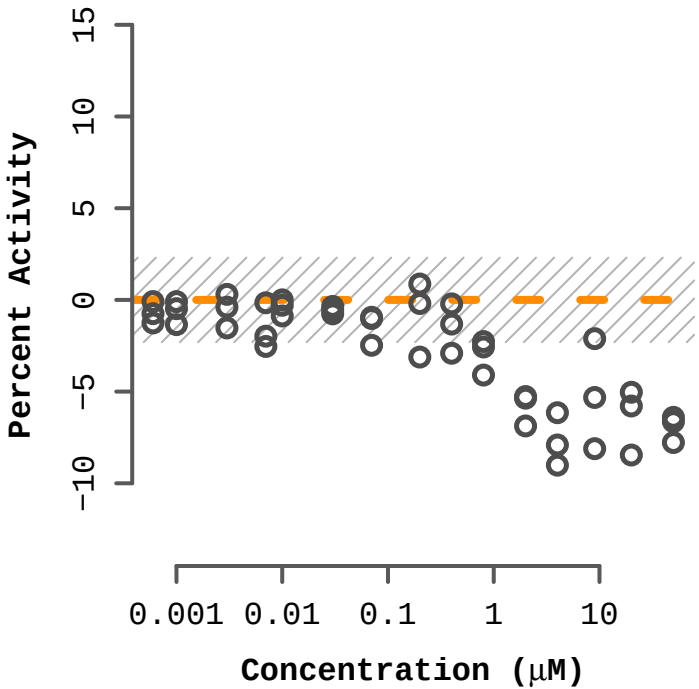
NAME: Phosphonoacetic acid
CHID: 45107 **CASRN:** 4408-78-0
SPID(S): Tox21_110045_1
M4ID: 12484696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

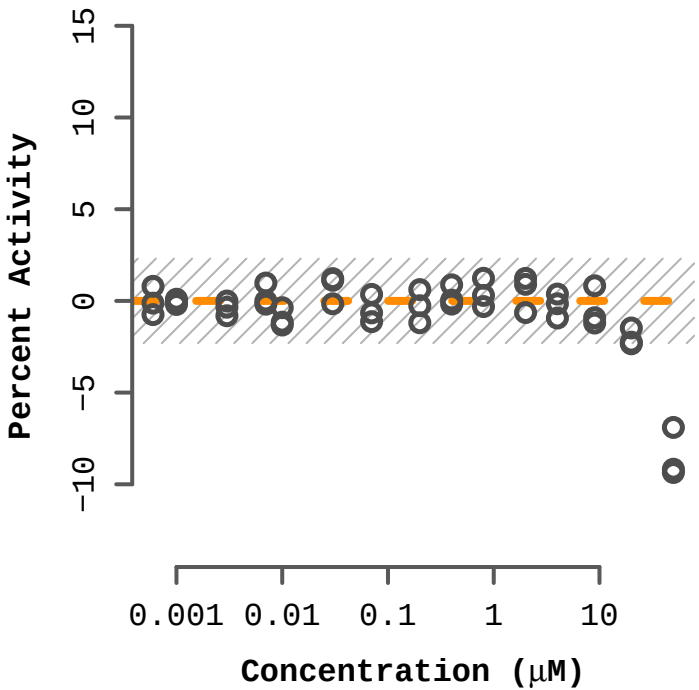
NAME: Adriamycin hydrochloride−DNA complex
CHID: 45111 CASRN: NOCAS_45111
SPID(S): Tox21_110050_1
M4ID: 12484695

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	255.93	NA	NA
PROB:	1	NA	NA
RMSE:	4.04	NA	NA

MAX_MEAN: −0.386 **MAX_MED:** −0.196 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

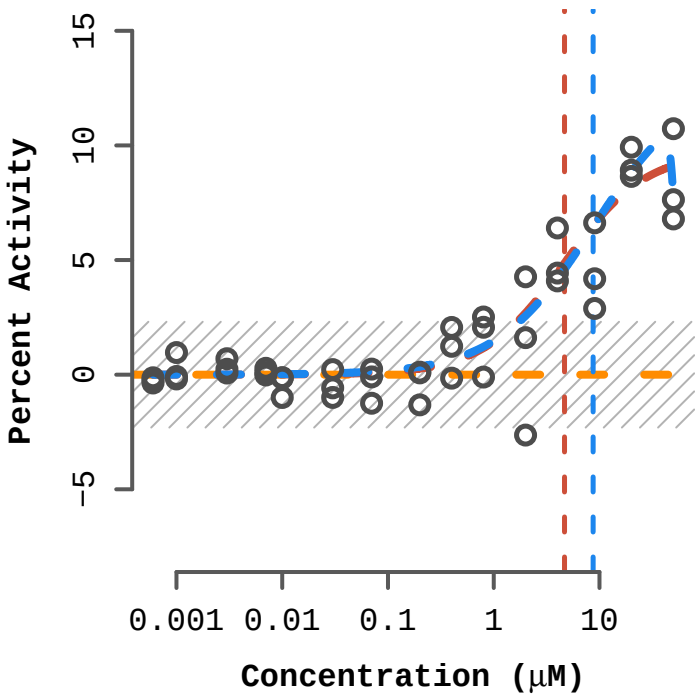
NAME: Domperidone
CHID: 45116 **CASRN:** 57808-66-9
SPID(S): Tox21_110056_1
M4ID: 12484693

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.86	NA	NA
PROB:	1	NA	NA
RMSE:	2.38	NA	NA

MAX_MEAN: 0.728 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pifexole
CHID: 45117 CASRN: 27199-40-2
SPID(S): Tox21_110057_1
M4ID: 12484692

HILL MODEL (in red):

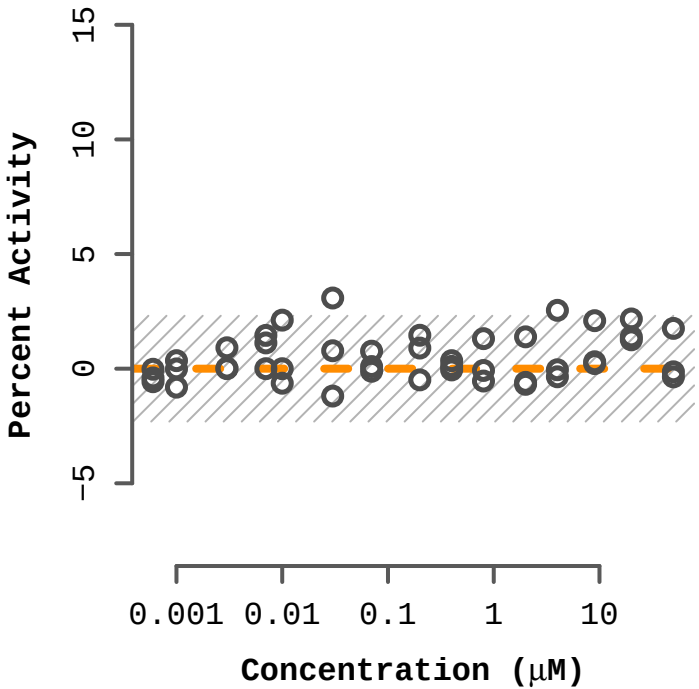
	tp	ga	gw
val:	9.74	0.669	1.13
sd:	1.55	0.169	0.271

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.9	0.94	0.946	1.72	17.2
sd:	3.68	0.307	0.217	0.00862	10.1

	CNST	HILL	GNLS
AIC:	243.08	155.56	154.36
PROB:	0	0.35	0.65
RMSE:	3.86	1.38	1.35

MAX_MEAN: 9.16 MAX_MED: 8.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

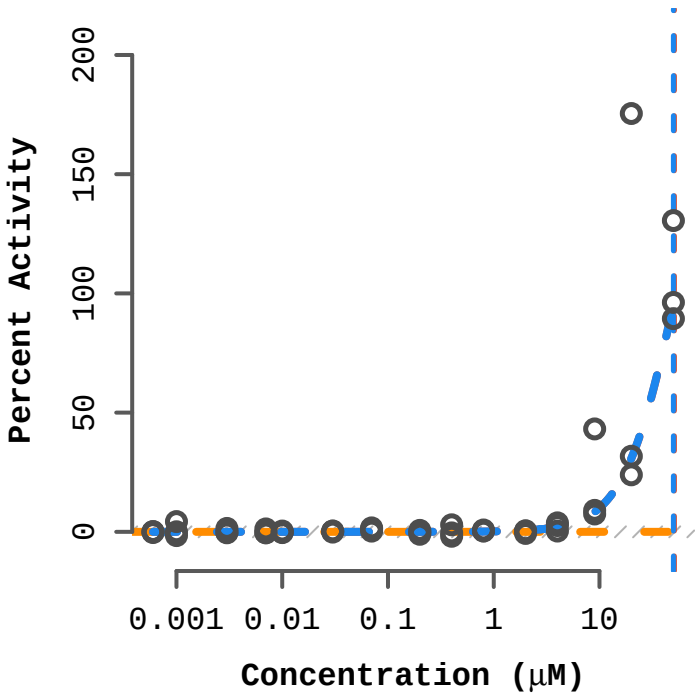
NAME: Oxaprozin
CHID: 45118 **CASRN:** 21256-18-8
SPID(S): Tox21_110059_1
M4ID: 12484690

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (−)−Eburnamonine
CHID: 45119 CASRN: 4880−88−0
SPID(S): Tox21_110060_1
M4ID: 12484689

HILL MODEL (in red):

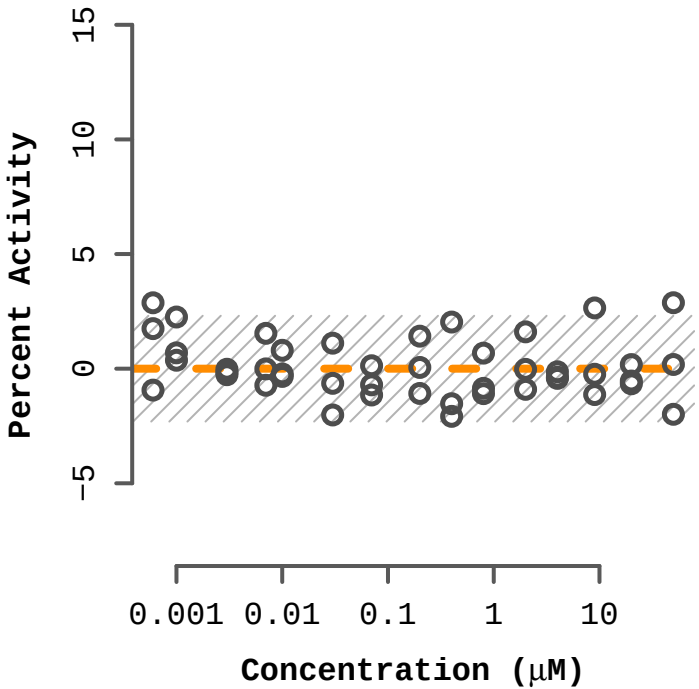
	tp	ga	gw
val:	194	1.71	1.78
sd:	4.65	0.0127	0.0535

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	191	1.7	1.8	3.44	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	377.56	260.57	264.57
PROB:	0	0.88	0.12
RMSE:	39.08	22.87	22.86

MAX_MEAN: 105 MAX_MED: 96.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

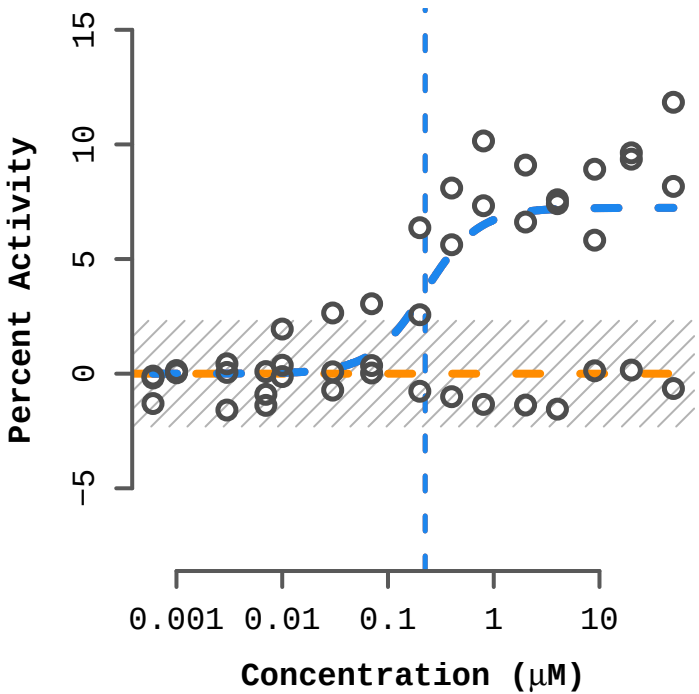
NAME: Alaproclate
CHID: 45122 **CASRN:** 60719-82-6
SPID(S): Tox21_110066_1
M4ID: 12484684

HILL MODEL: Not applicable.

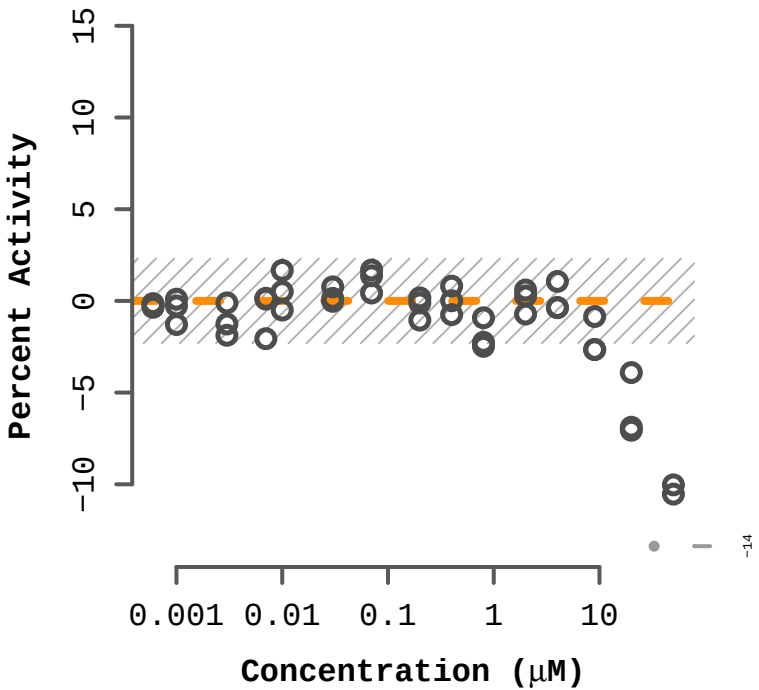
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.75 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-Arachidonylglycine
CHID:    45124   CASRN: 179113-91-8
SPID(S): Tox21_110070_1
M4ID:    12484681

HILL MODEL (in red):
      tp       ga       gw
val:  7.23     -0.648   1.71
sd:   0.901    0.193    1.32

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.23     -0.648   1.71     2.86     7.07
sd:   0.901    0.193    1.32     1710     10400

      CNST        HILL        GNLS
AIC:  271.01      239.44      243.44
PROB: 0           0.88        0.12
RMSE: 4.89        3.41        3.41

MAX_MEAN: 6.45      MAX_MED: 9.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

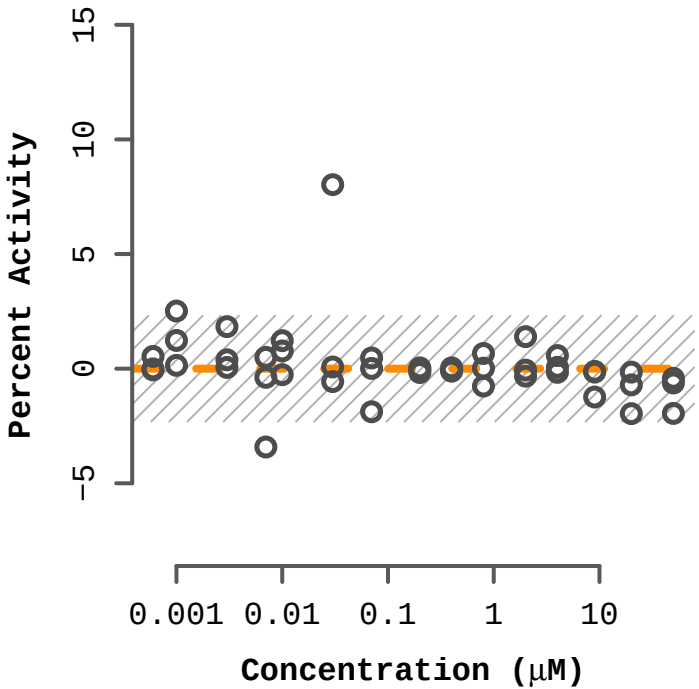
NAME: Docebenone
CHID: 45125 CASRN: 80809-81-0
SPID(S): Tox21_110072_1
M4ID: 12484680 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.1	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

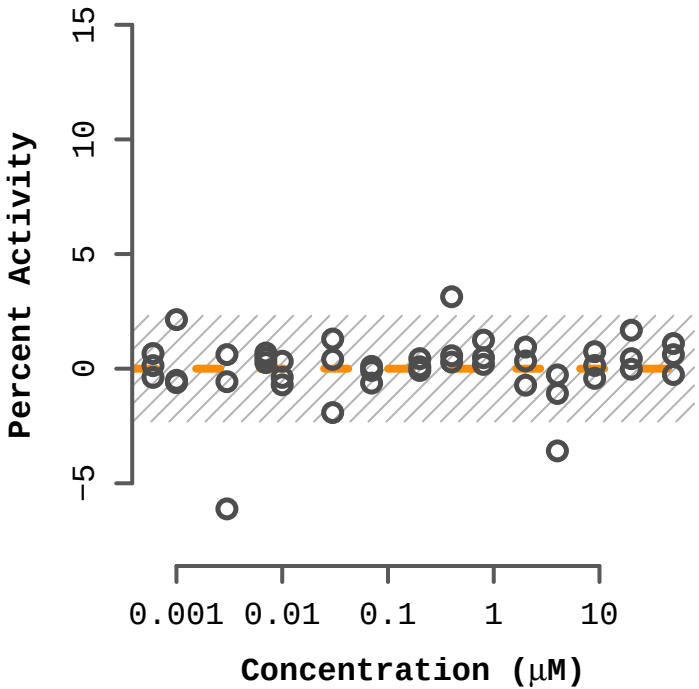
NAME: Alprenolol
CHID: 45127 **CASRN:** 13655-52-2
SPID(S): Tox21_110084_1
M4ID: 12484668

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 2.51 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

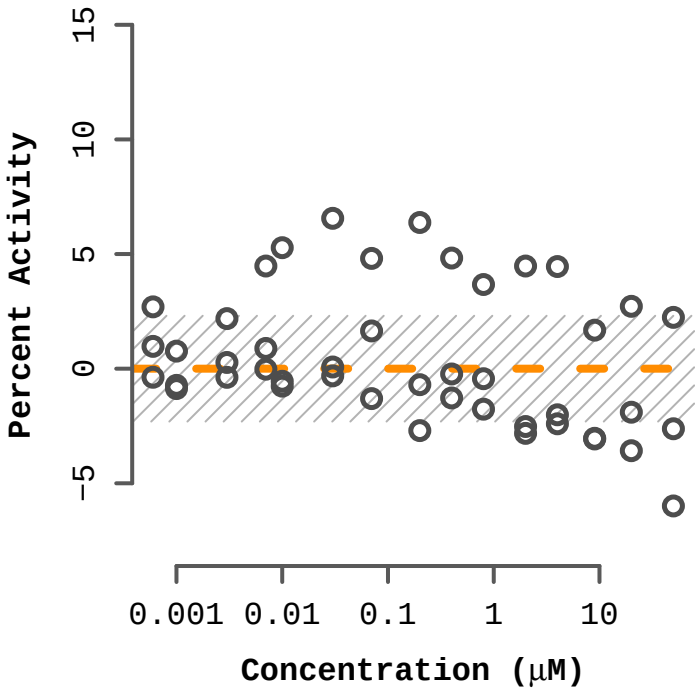
NAME: Aniracetam
CHID: 45128 **CASRN:** 72432-10-1
SPID(S): Tox21_110086_1
M4ID: 12484666

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.614 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

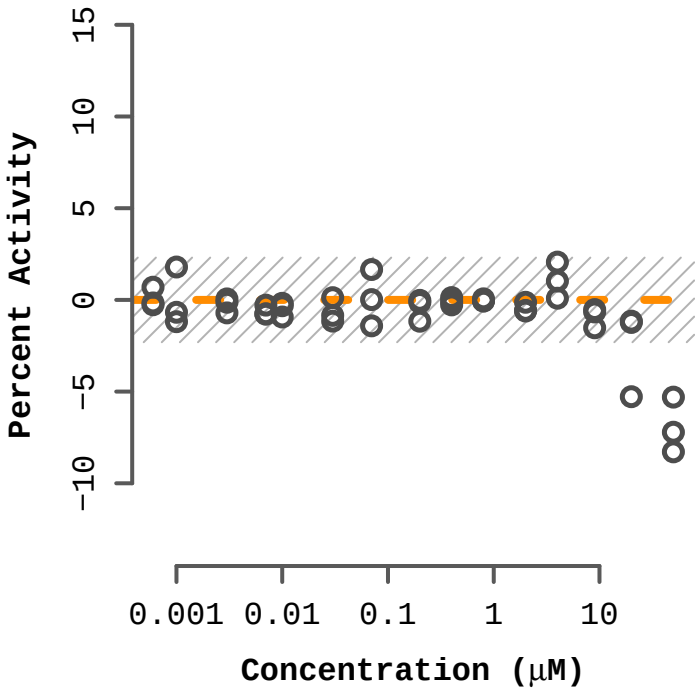
NAME: Cirazoline
CHID: 45131 **CASRN:** 59939-16-1
SPID(S): Tox21_110095_1
M4ID: 12484658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.72	NA	NA
PROB:	1	NA	NA
RMSE:	2.92	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

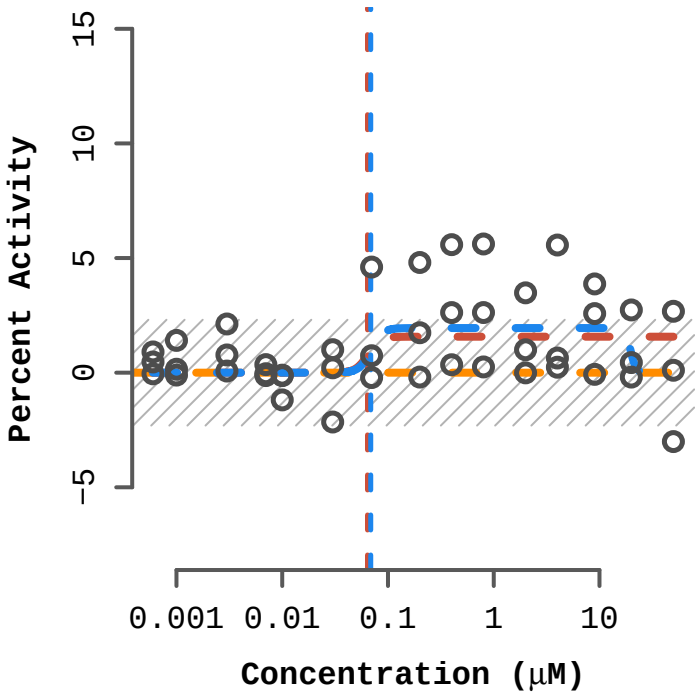
NAME: Cilostazol
CHID: 45132 **CASRN:** 73963-72-1
SPID(S): Tox21_110098_1
M4ID: 12484655

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.87	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (−)−Epicatechin
CHID: 45133 **CASRN:** 490−46−0
SPID(S): Tox21_110101_1
M4ID: 12484652

HILL MODEL (in red):

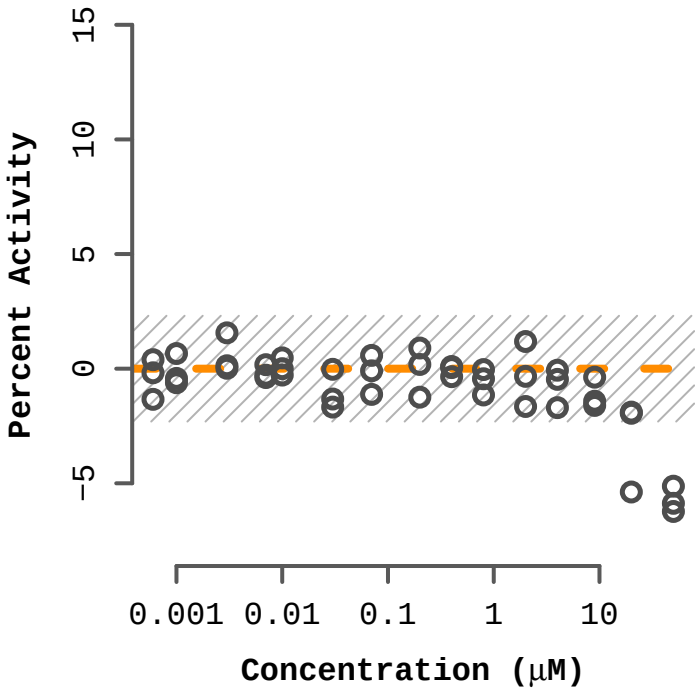
	tp	ga	gw
val:	1.57	−1.19	8
sd:	0.405	0.271	45.9

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.95	−1.16	7.98	1.29	16.7
sd:	0.484	0.133	61	0.127	291

	CNST	HILL	GNLS
AIC:	198.79	187.95	189.36
PROB:	0	0.67	0.33
RMSE:	2.26	1.8	1.7

MAX_MEAN: 2.85 **MAX_MED:** 2.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

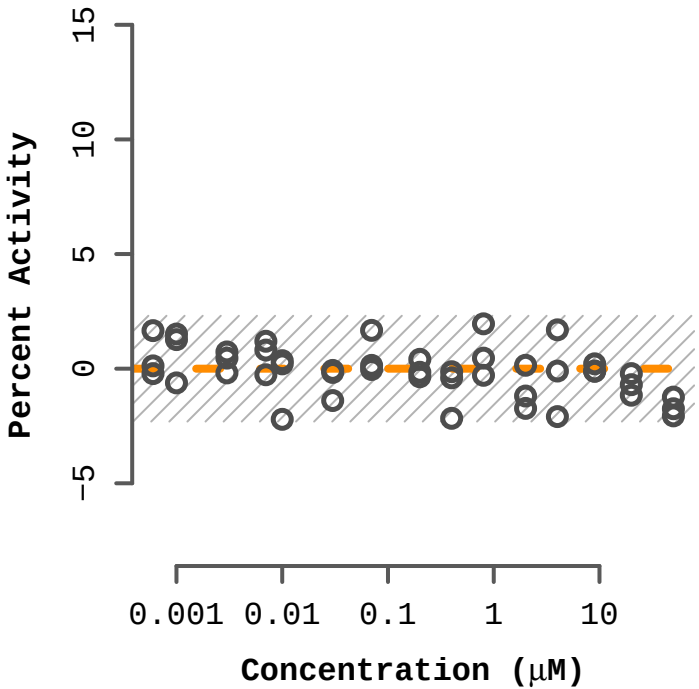
NAME: Clemizole hydrochloride
CHID: 45136 **CASRN:** 1163-36-6
SPID(S): Tox21_110108_1
M4ID: 12484645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.91	NA	NA

MAX_MEAN: 0.571 **MAX_MED:** 0.185 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

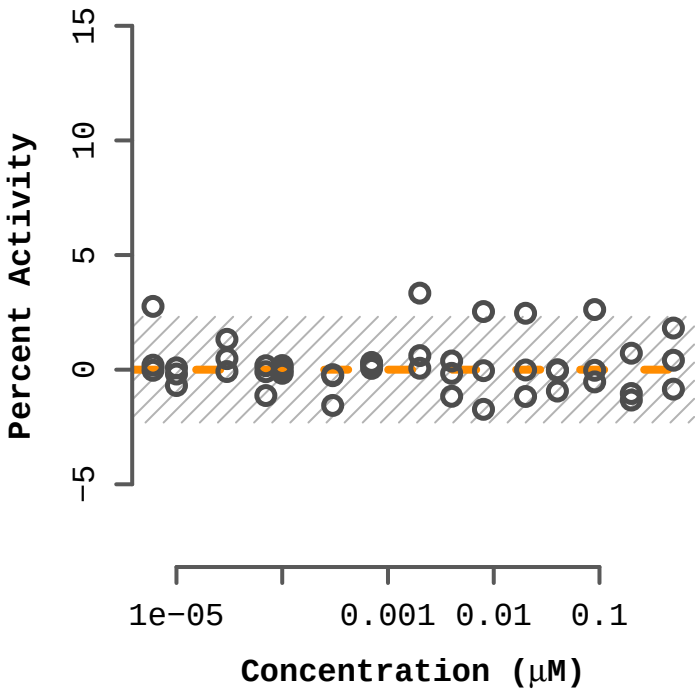
NAME: 1-(3-Chlorophenyl)piperazine
CHID: 45138 **CASRN:** 6640-24-0
SPID(S): Tox21_110110_1
M4ID: 12484643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

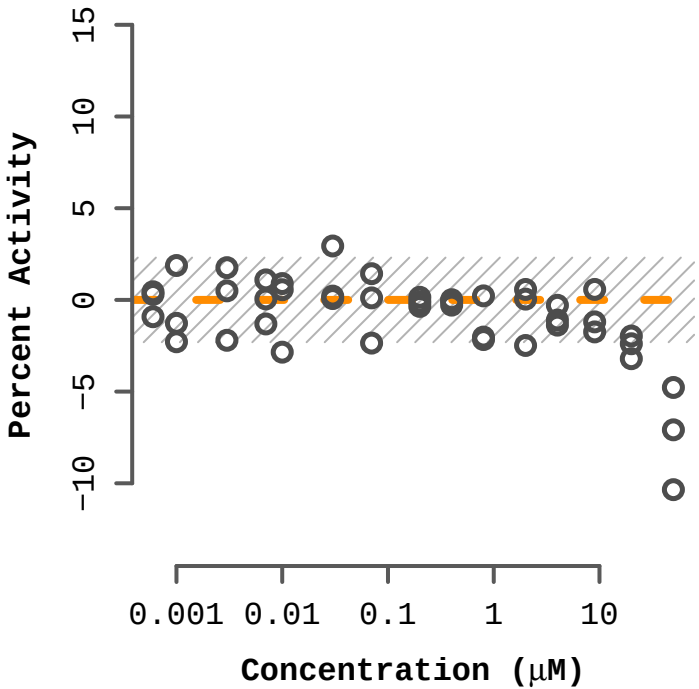
NAME: Fenclonine
CHID: 45139 **CASRN:** 7424-00-2
SPID(S): Tox21_110114_1
M4ID: 12484639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 0.616 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

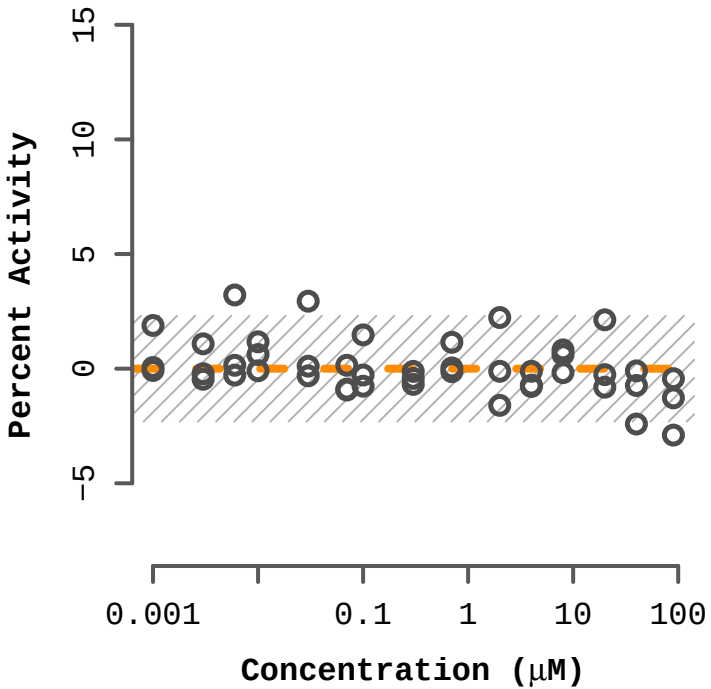
NAME: Cilostamide
CHID: 45140 **CASRN:** 68550-75-4
SPID(S): Tox21_110119_1
M4ID: 12484634

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.5	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.558 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

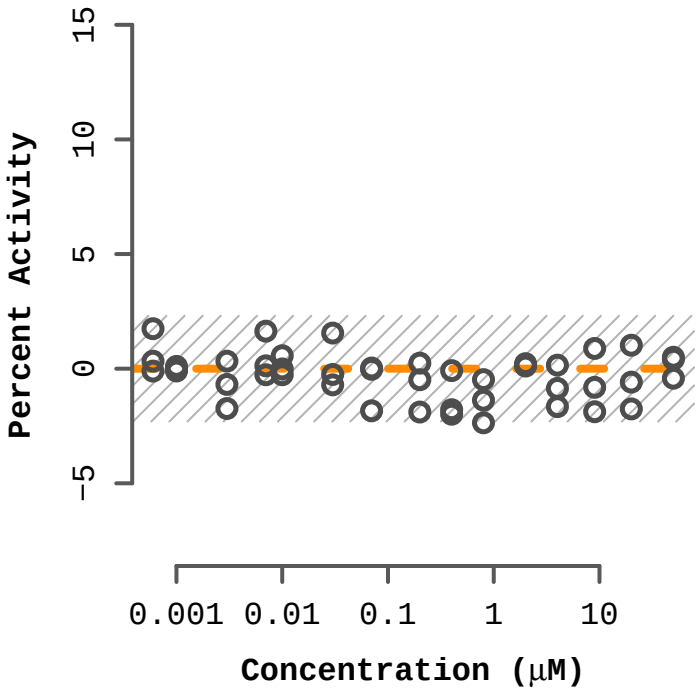
NAME: Meclofenoxate hydrochloride
CHID: 45141 **CASRN:** 3685-84-5
SPID(S): Tox21_302398
M4ID: 12476735

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

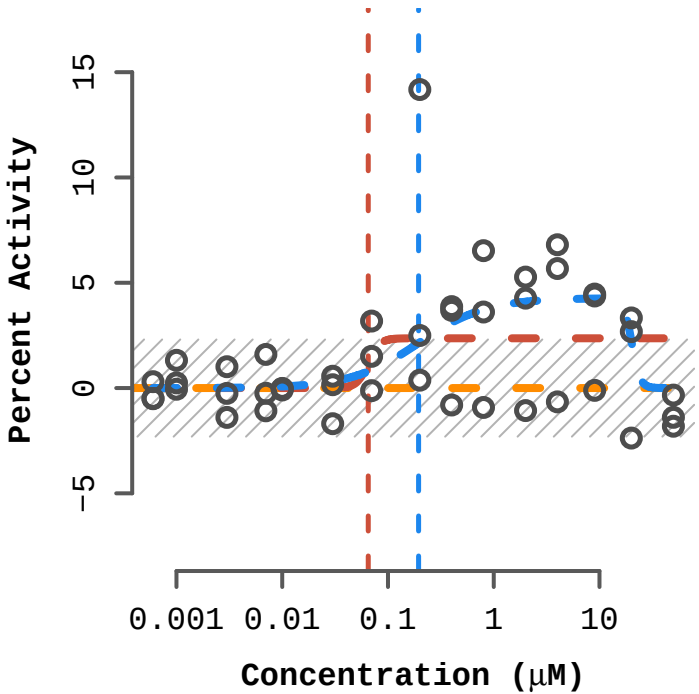
NAME: Meclofenoxate hydrochloride
CHID: 45141 **CASRN:** 3685-84-5
SPID(S): Tox21_110123_1
M4ID: 12484630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 0.414 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Doxepin hydrochloride
CHID: 45145 **CASRN:** 1229-29-4
SPID(S): Tox21_110130_1
M4ID: 12484624

HILL MODEL (in red):

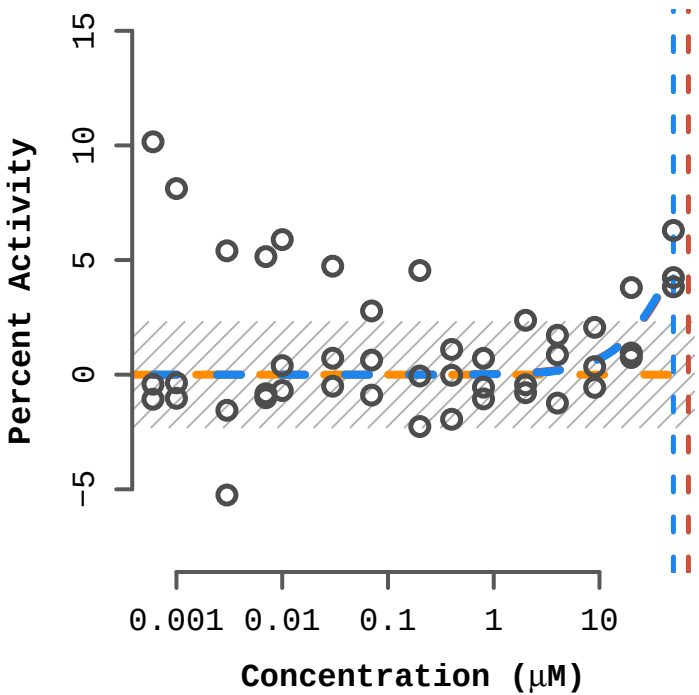
	tp	ga	gw
val:	2.36	−1.19	8
sd:	0.627	0.179	35.2

GAIN-LOSS MODEL (in blue):

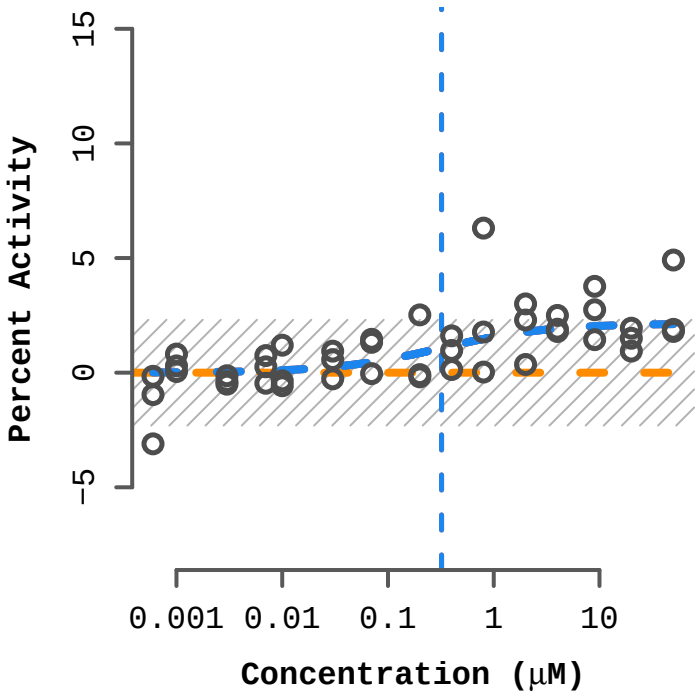
	tp	ga	gw	la	lw
val:	4.27	−0.71	1.36	1.31	11.3
sd:	0.807	0.29	0.735	0.0982	236

	CNST	HILL	GNLS
AIC:	227.39	218.8	209.98
PROB:	0	0.01	0.99
RMSE:	3.37	2.77	2.67

MAX_MEAN: 5.68 **MAX_MED:** 5.68 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Enoximone
CHID:    45147   CASRN: 77671-31-9
SPID(S): Tox21_110137_1
M4ID:    12484618

HILL MODEL (in red):
      tp       ga       gw
val:  12.2     1.84     1.43
sd:   40.1     1.76     1.54

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.4      1.7      1.57     3.66     17.5
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  229.37      220.89      224.91
PROB: 0.01        0.87        0.12
RMSE: 3.21        2.92        2.92

MAX_MEAN: 4.79      MAX_MED: 4.24      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Efaroxan
CHID: 45149 CASRN: 89197-32-0
SPID(S): Tox21_110139_1
M4ID: 12484616

HILL MODEL (in red):

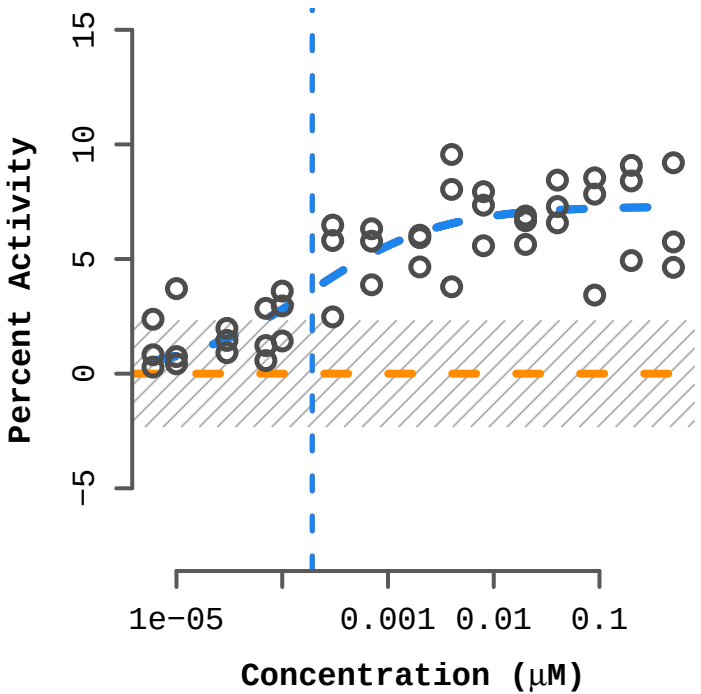
	tp	ga	gw
val:	2.15	−0.493	0.852
sd:	0.354	0.389	0.436

GAIN-LOSS MODEL (in blue):

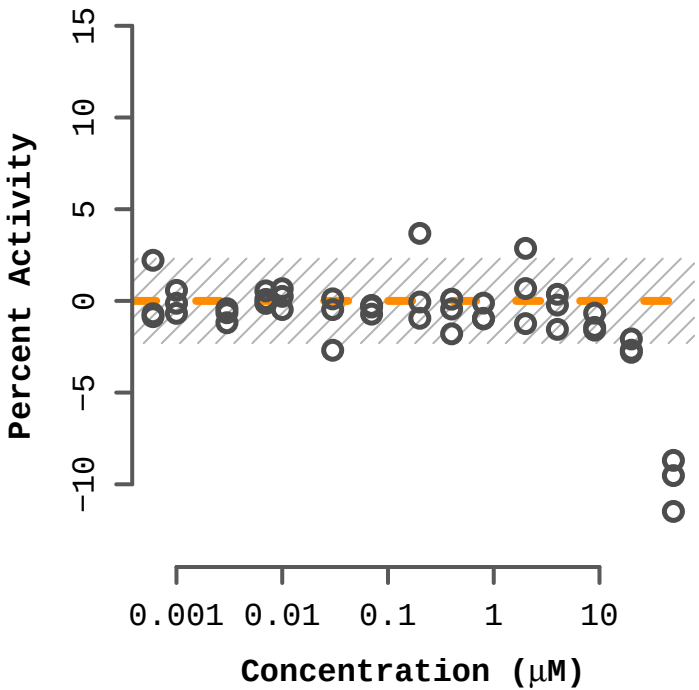
	tp	ga	gw	la	lw
val:	2.15	−0.493	0.852	3.05	5.81
sd:	0.354	0.389	0.436	2330	10200

	CNST	HILL	GNLS
AIC:	183.35	142.95	146.95
PROB:	0	0.88	0.12
RMSE:	1.9	1.22	1.22

MAX_MEAN: 2.87 **MAX_MED:** 2.75 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Egtazic Acid
CHID:    45151   CASRN: 67-42-5
SPID(S): Tox21_110141_1
M4ID:    12484615

HILL MODEL (in red):
      tp       ga       gw
val:  7.29     -3.72    0.716
sd:   0.515    0.192    0.199

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.29     -3.72    0.716    0.98     6.68
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  291.49      175.7       179.7
PROB: 0           0.88        0.12
RMSE: 5.57        1.51        1.51

MAX_MEAN: 7.48      MAX_MED: 8.41      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

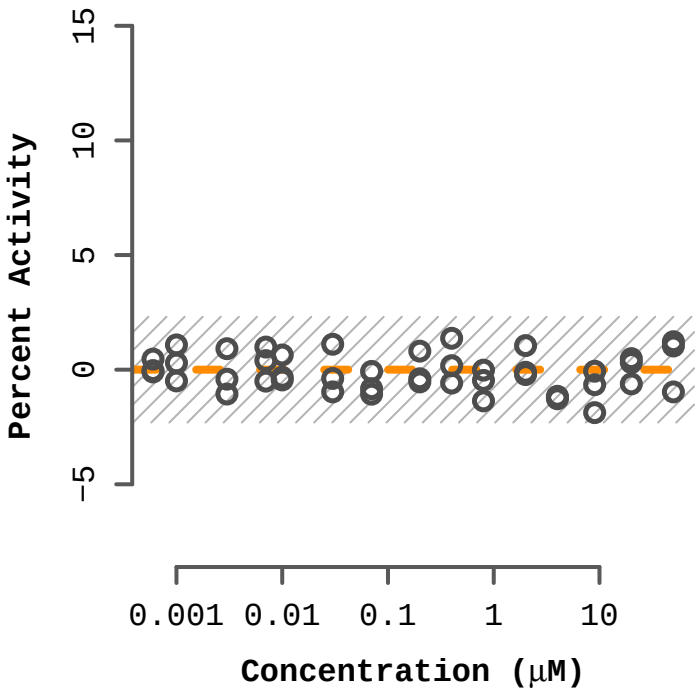
NAME: Fluspirilene
CHID: 45152 **CASRN:** 1841-19-6
SPID(S): Tox21_110142_1
M4ID: 12484614

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 0.893 **MAX_MED:** 0.675 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

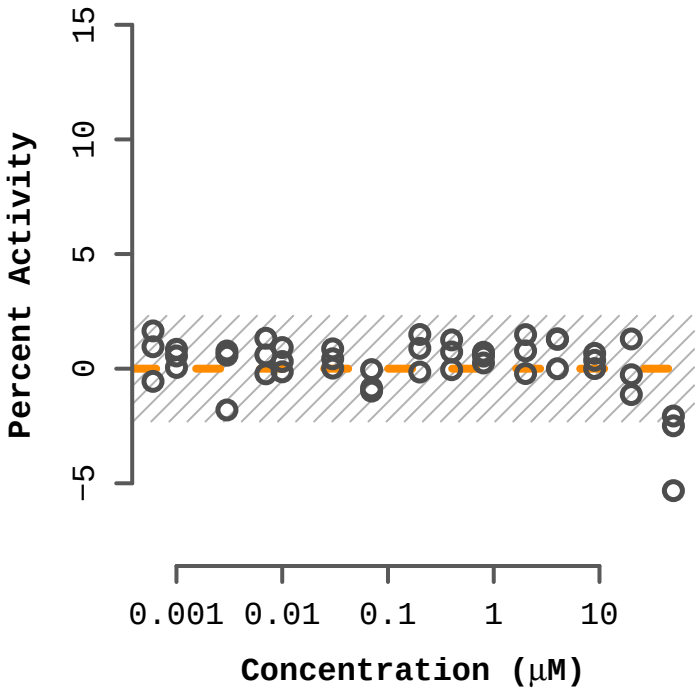
NAME: Furafylline
CHID: 45153 **CASRN:** 80288-49-9
SPID(S): Tox21_110143_1
M4ID: 12484613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.429 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

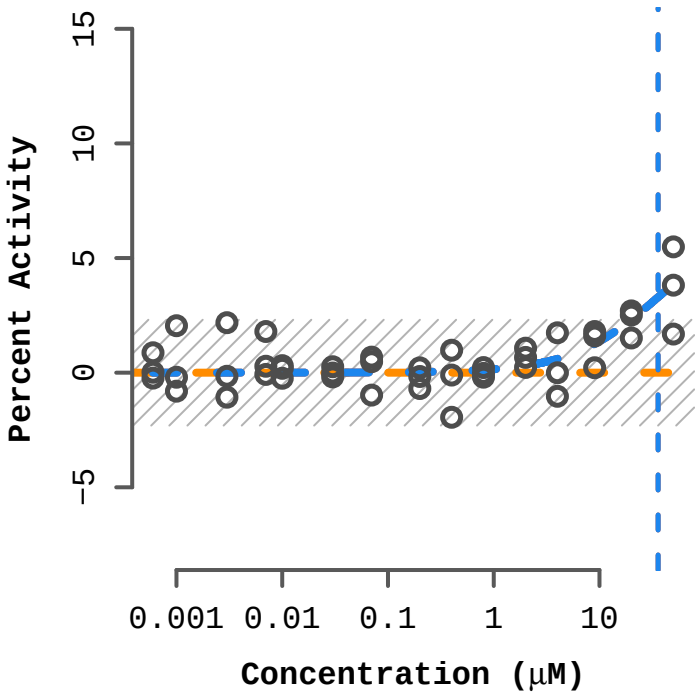
NAME: Guanfacine hydrochloride
CHID: 45157 **CASRN:** 29520-14-7
SPID(S): Tox21_110159_1
M4ID: 12484598

HILL MODEL: Not applicable.

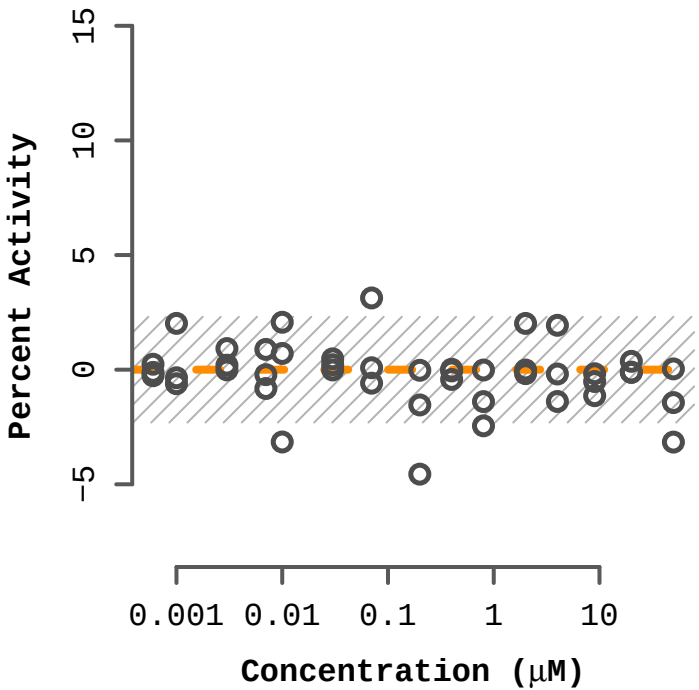
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 1.28 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hydroxytacrine maleate
CHID:    45158   CASRN: 118909-22-1
SPID(S): Tox21_110164_1
M4ID:    12484593

HILL MODEL (in red):
      tp       ga       gw
val:  6.59     1.55     1.05
sd:   6.32     0.797    0.568

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.59     1.55     1.05     3.65     3.82
sd:   6.31     0.796    0.568    4930     9790

      CNST        HILL        GNLS
AIC:  155.92      125         129
PROB: 0           0.88        0.12
RMSE: 1.47        0.91        0.91

MAX_MEAN: 3.66      MAX_MED: 3.82      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

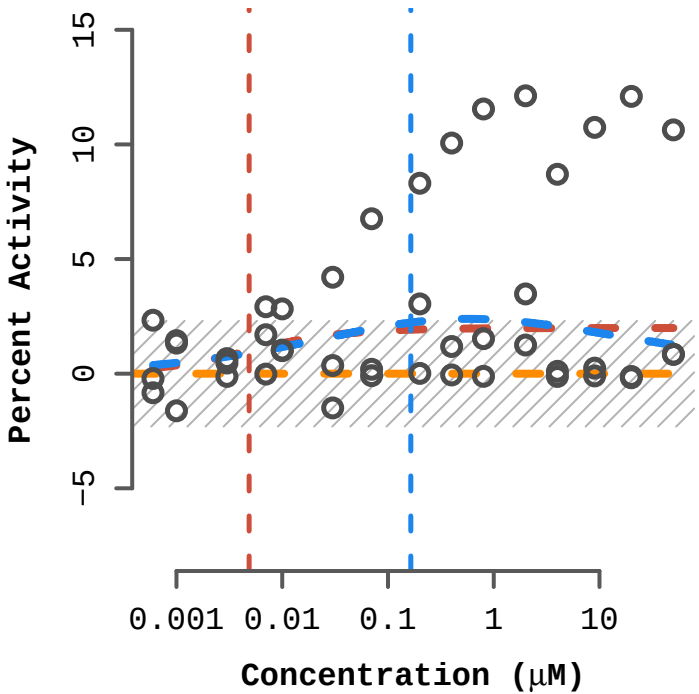
NAME: Idazoxan
CHID: 45161 CASRN: 79944-58-4
SPID(S): Tox21_110173_1
M4ID: 12484585

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Imiloxan
CHID: 45162 **CASRN:** 81167-16-0
SPID(S): Tox21_110175_1
M4ID: 12484583

HILL MODEL (in red):

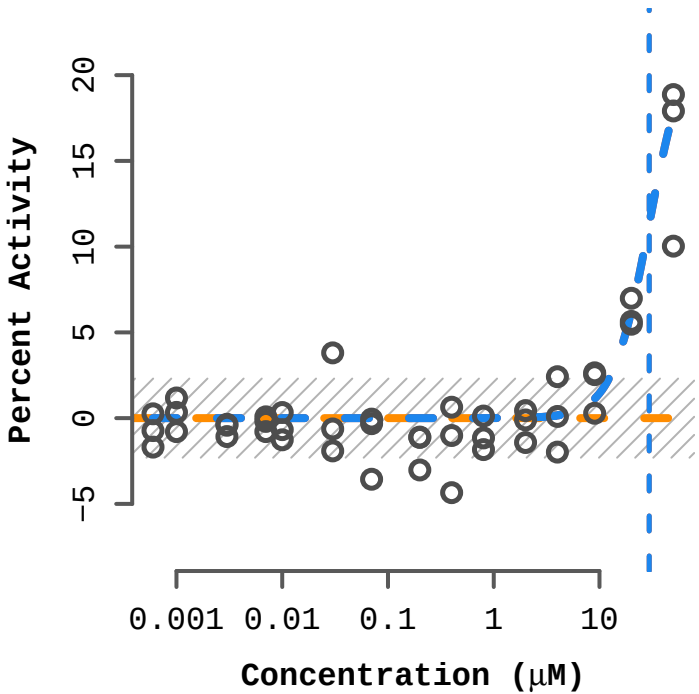
	tp	ga	gw
val:	1.99	−2.31	0.939
sd:	0.816	0.868	1.68

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.17	−0.784	0.516	−0.534	0.321
sd:	131	7.34	1.32	36.3	1.86

	CNST	HILL	GNLS
AIC:	259.33	252.75	256.45
PROB:	0.03	0.84	0.13
RMSE:	4.78	3.98	3.98

MAX_MEAN: 5.62 **MAX_MED:** 3.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linopirdine
CHID: 45163 **CASRN:** 105431-72-9
SPID(S): Tox21_110177_1
M4ID: 12484581

HILL MODEL (in red):

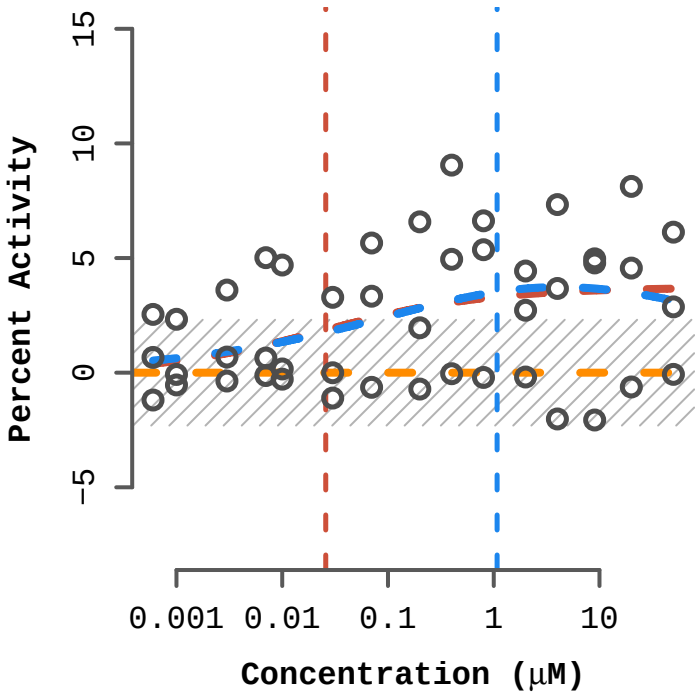
	tp	ga	gw
val:	22.6	1.47	2.48
sd:	4.86	0.104	0.753

GAIN-LOSS MODEL (in blue):

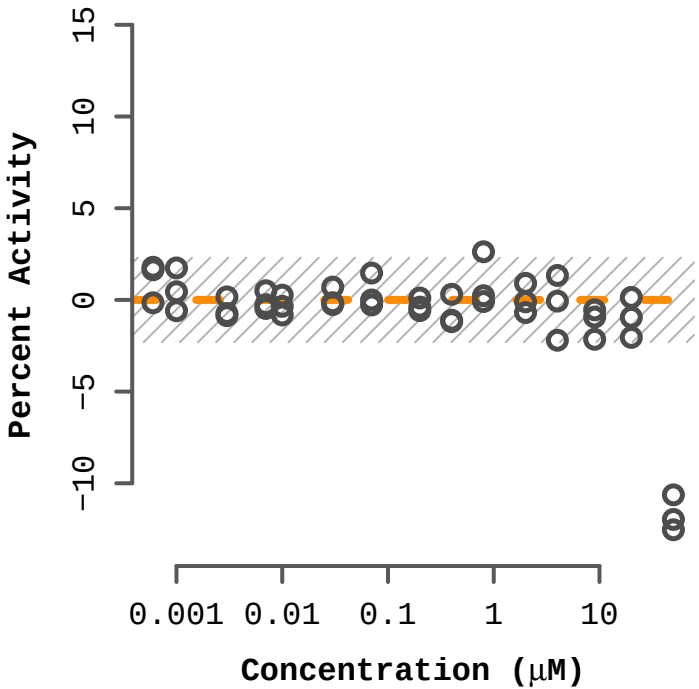
	tp	ga	gw	la	lw
val:	22.6	1.47	2.48	3.42	4.51
sd:	4.85	0.104	0.753	999	2630

	CNST	HILL	GNLS
AIC:	237.08	179.61	183.61
PROB:	0	0.88	0.12
RMSE:	4.69	1.87	1.87

MAX_MEAN: 15.6 **MAX_MED:** 17.9 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Loxoprofen
CHID:    45164   CASRN: 68767-14-6
SPID(S): Tox21_110178_1
M4ID:    12484580

HILL MODEL (in red):
      tp       ga       gw
val:  3.71     -1.59    0.566
sd:   1.03     0.808    0.499

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.9     0.032    0.39     0.874    0.316
sd:   84.3     15.3     1.11     9.56     1.55

      CNST        HILL        GNLS
AIC:  251.33      232.61      236.44
PROB: 0           0.87        0.13
RMSE: 3.78        2.78        2.78

MAX_MEAN: 4.65      MAX_MED: 5.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

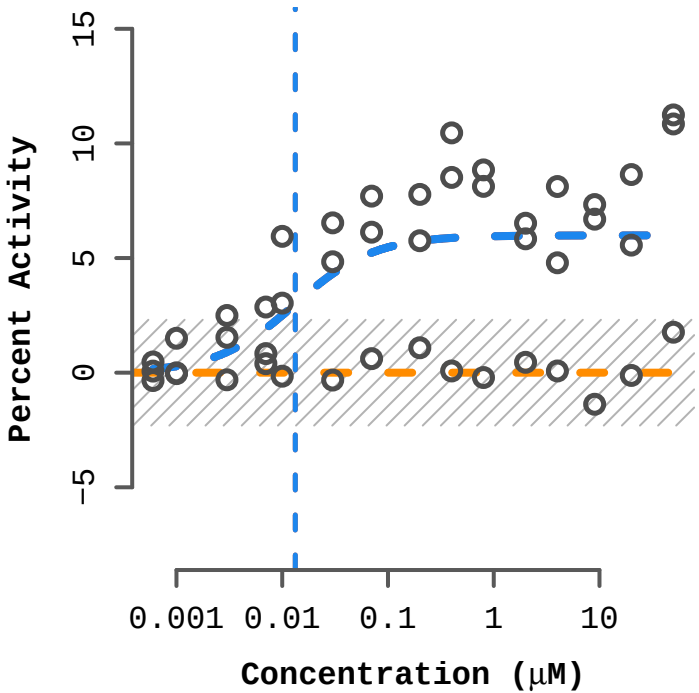
NAME: Loperamide
CHID: 45165 **CASRN:** 53179-11-6
SPID(S): Tox21_110180_1
M4ID: 12484578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.48	NA	NA
PROB:	1	NA	NA
RMSE:	3.19	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lidocaine
CHID: 45166 CASRN: 137-58-6
SPID(S): Tox21_110183_1
M4ID: 12484575

HILL MODEL (in red):

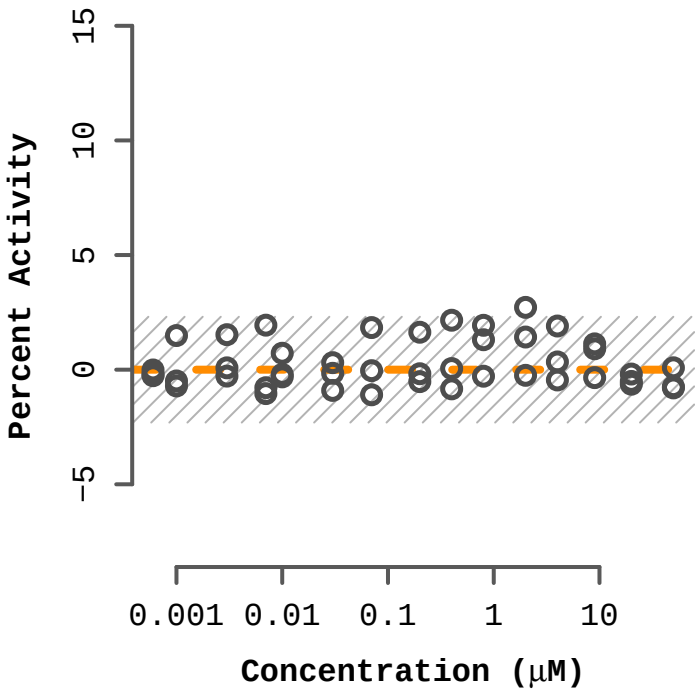
	tp	ga	gw
val:	5.99	−1.88	1.17
sd:	0.809	0.286	0.756

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.99	−1.88	1.17	3.38	4.64
sd:	0.809	0.286	0.756	1300	3610

	CNST	HILL	GNLS
AIC:	282.91	243.05	247.05
PROB:	0	0.88	0.12
RMSE:	5.31	3.22	3.22

MAX_MEAN: 7.95 MAX_MED: 10.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

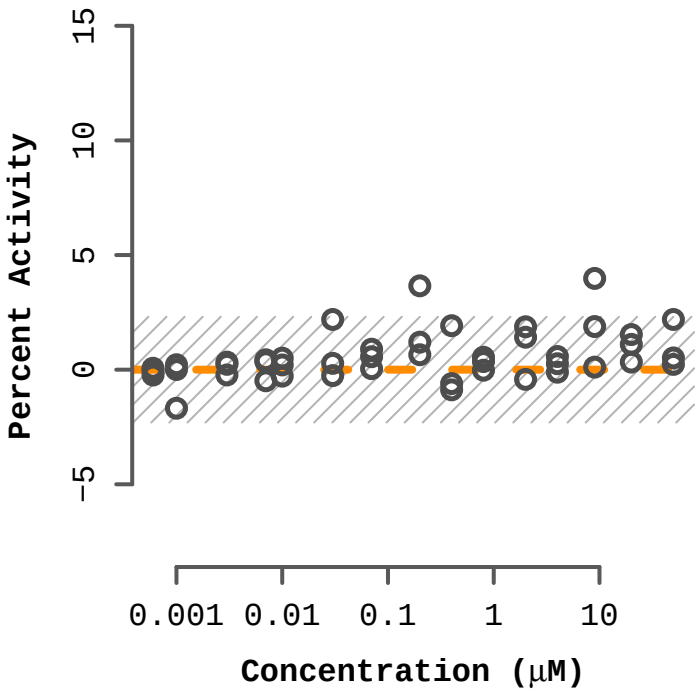
NAME: Metolazone
CHID: 45167 **CASRN:** 17560-51-9
SPID(S): Tox21_110186_1
M4ID: 12484572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

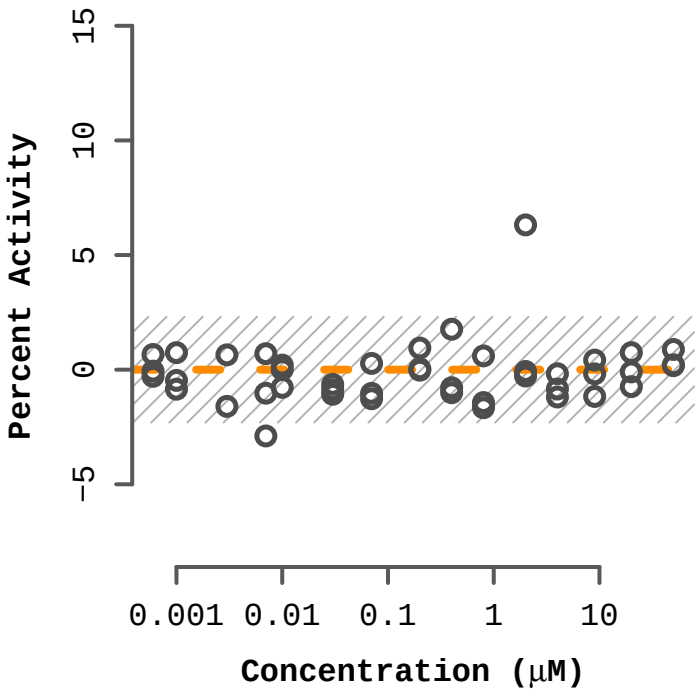
NAME: Metoclopramide
CHID: 45169 **CASRN:** 364-62-5
SPID(S): Tox21_110188_1
M4ID: 12484571

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

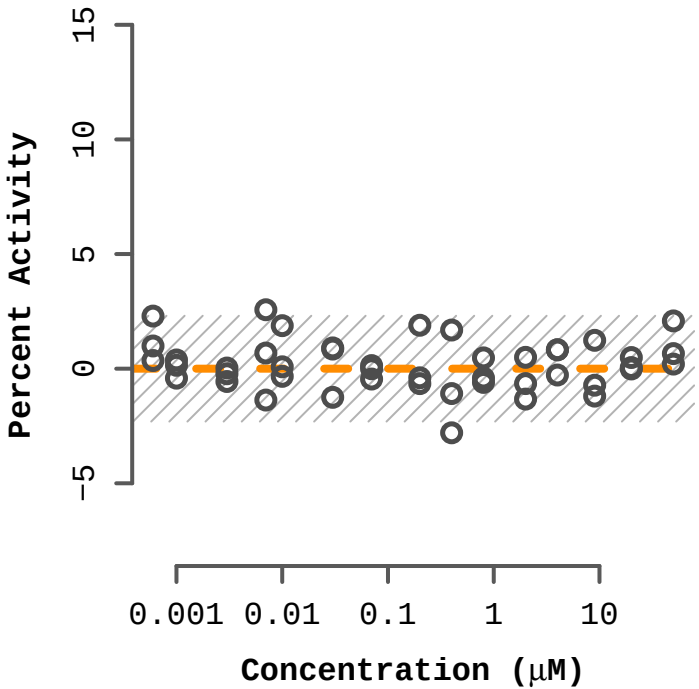
NAME: Moxonidine
CHID: 45170 CASRN: 75438-57-2
SPID(S): Tox21_110190_1
M4ID: 12484569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 0.217 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

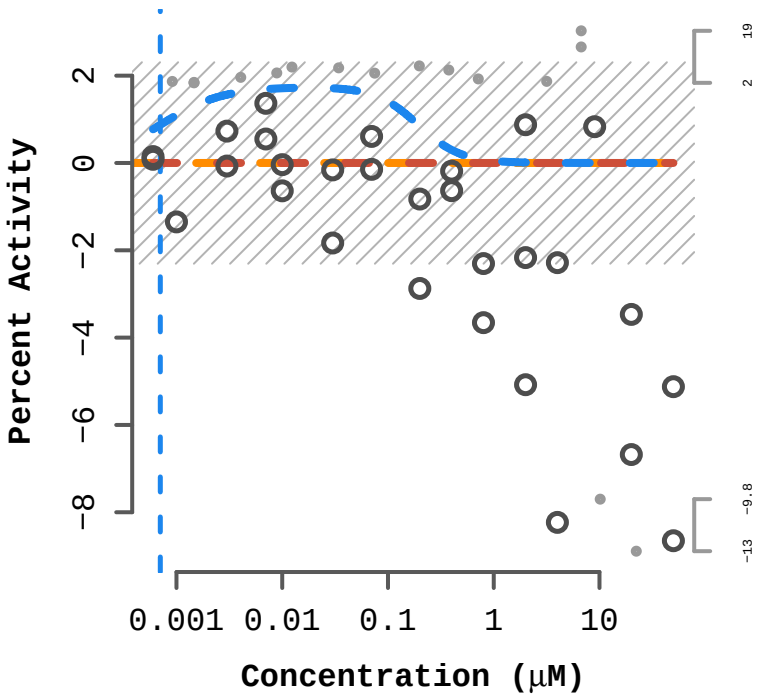
NAME: Molsidomine
CHID: 45171 **CASRN:** 25717-80-0
SPID(S): Tox21_110192_1
M4ID: 12484567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mitoxantrone dihydrochloride
CHID: 45173 **CASRN:** 70476-82-3
SPID(S): Tox21_110197_1
M4ID: 12484562 **BRK**

HILL MODEL (in red):

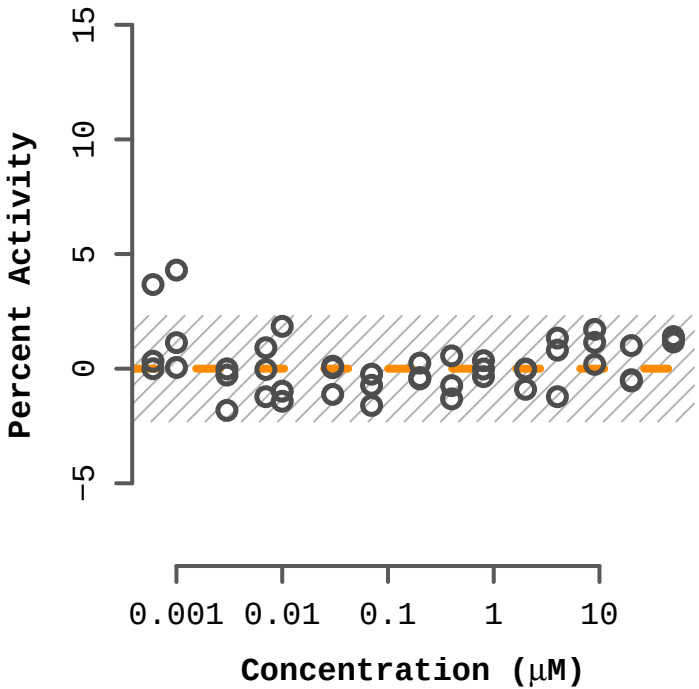
	tp	ga	gw
val:	0.0494	2.19	7.84
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.75	−3.15	1.48	−0.715	2.16
sd:	1.66	1.24	6.36	1.57	5.32

	CNST	HILL	GNLS
AIC:	279.01	285.01	285.96
PROB:	0.93	0.05	0.03
RMSE:	5.65	5.65	5.51

MAX_MEAN: 11.4 **MAX_MED:** 14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

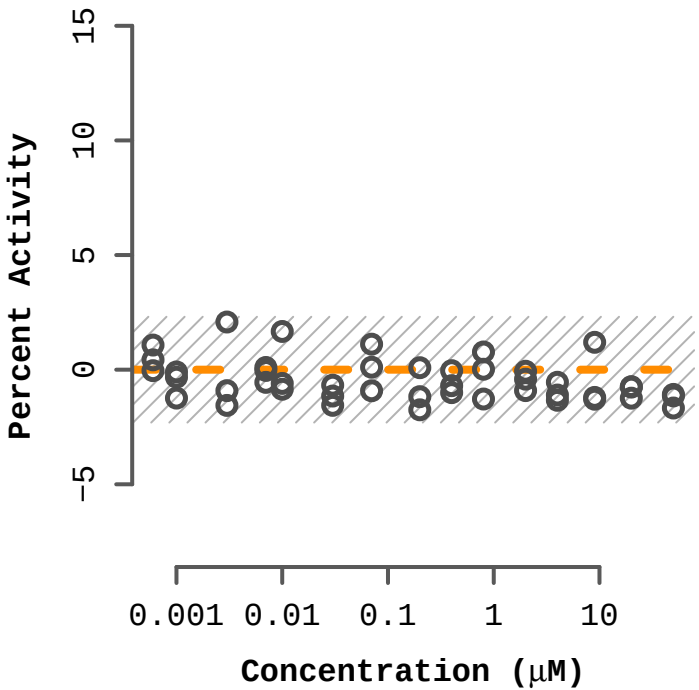
NAME: Memantine
CHID: 45174 **CASRN:** 19982-08-2
SPID(S): Tox21_110199_1
M4ID: 12484560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

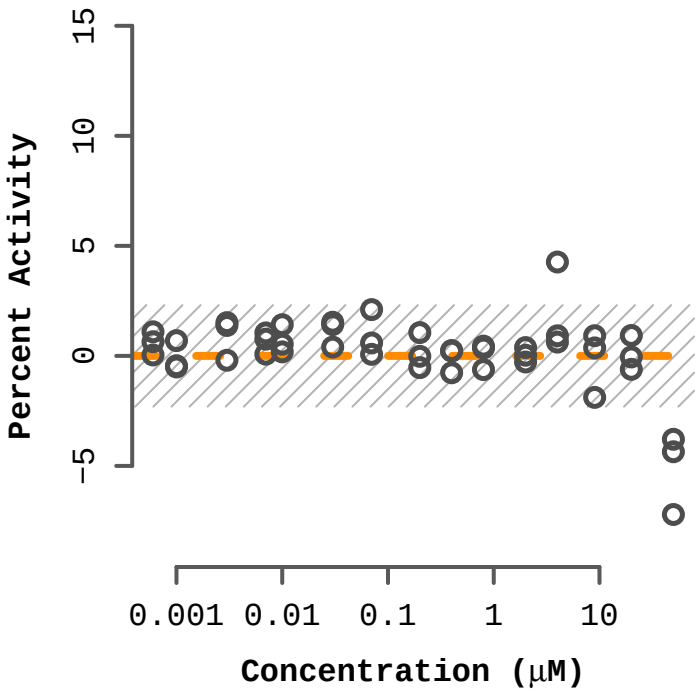
NAME: Nisoxetine
CHID: 45175 **CASRN:** 53179-07-0
SPID(S): Tox21_110203_1
M4ID: 12484556

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.488 **MAX_MED:** 0.431 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

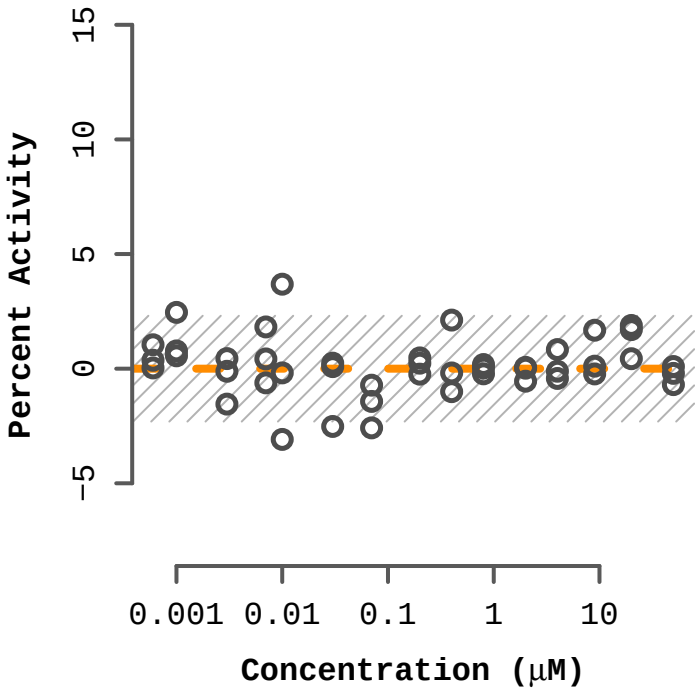
NAME: Naftopidil
CHID: 45176 **CASRN:** 57149-07-2
SPID(S): Tox21_110205_1
M4ID: 12484554

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

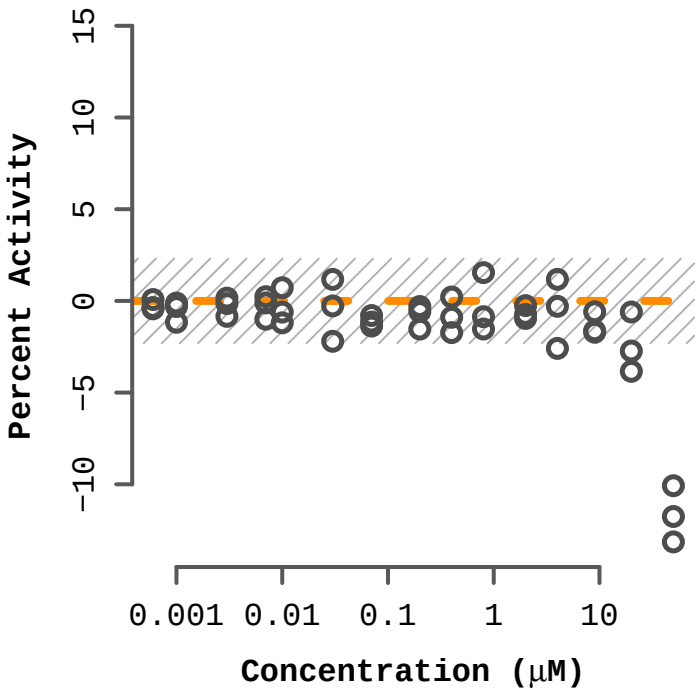
NAME: Nimustine
CHID: 45179 **CASRN:** 42471-28-3
SPID(S): Tox21_110214_1
M4ID: 12484546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

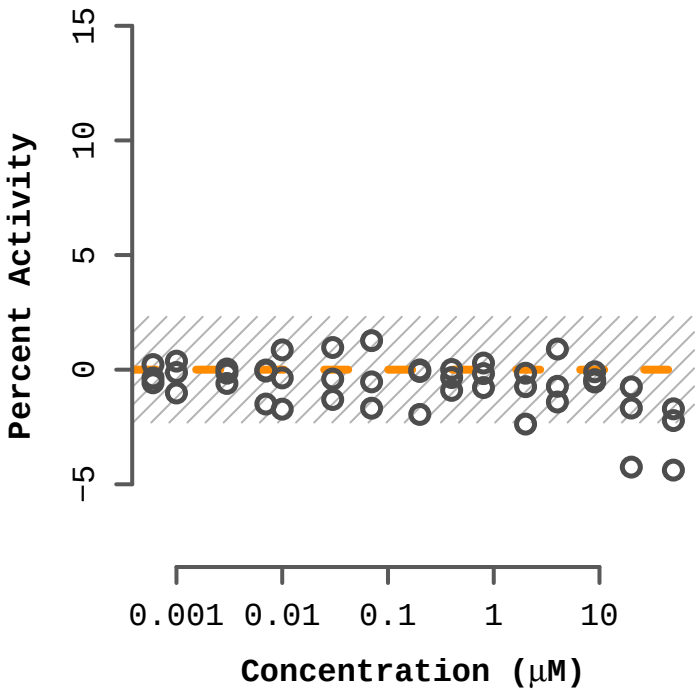
NAME: Oxatomide
CHID: 45181 **CASRN:** 60607-34-3
SPID(S): Tox21_110219_1
M4ID: 12484542

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.5	NA	NA
PROB:	1	NA	NA
RMSE:	3.26	NA	NA

MAX_MEAN: −0.237 **MAX_MED:** −0.108 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

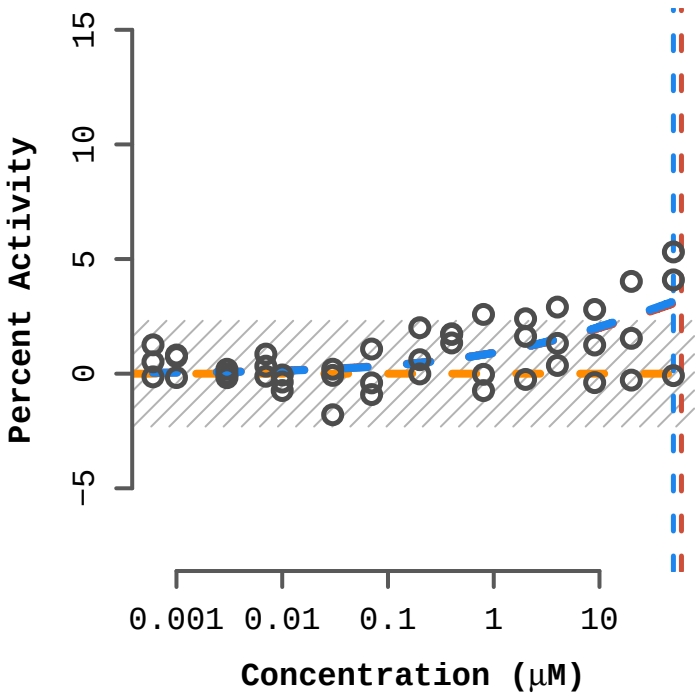
NAME: Pirenperone
CHID: 45182 **CASRN:** 75444-65-4
SPID(S): Tox21_110220_1
M4ID: 12484541

HILL MODEL: Not applicable.

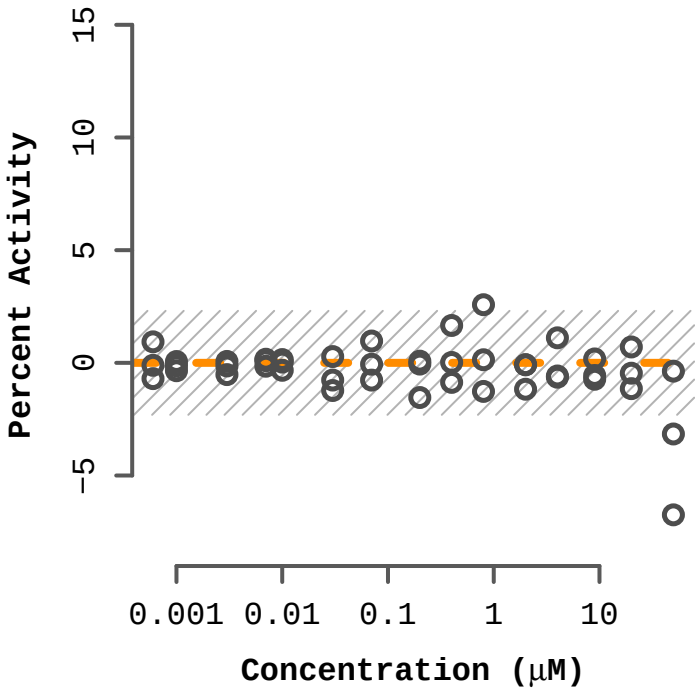
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: −0.219 **MAX_MED:** −0.0623 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pirfenidone
CHID:    45183   CASRN: 53179-13-8
SPID(S): Tox21_110225_1
M4ID:    12484536

HILL MODEL (in red):
      tp       ga       gw
val:  6.37     1.78     0.439
sd:   7.85     1.89     0.182

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.3      1.7      0.456    3.23     8.27
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  168.33      153         157.02
PROB: 0           0.88        0.12
RMSE: 1.64        1.19        1.19

MAX_MEAN: 3.11      MAX_MED: 4.09      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

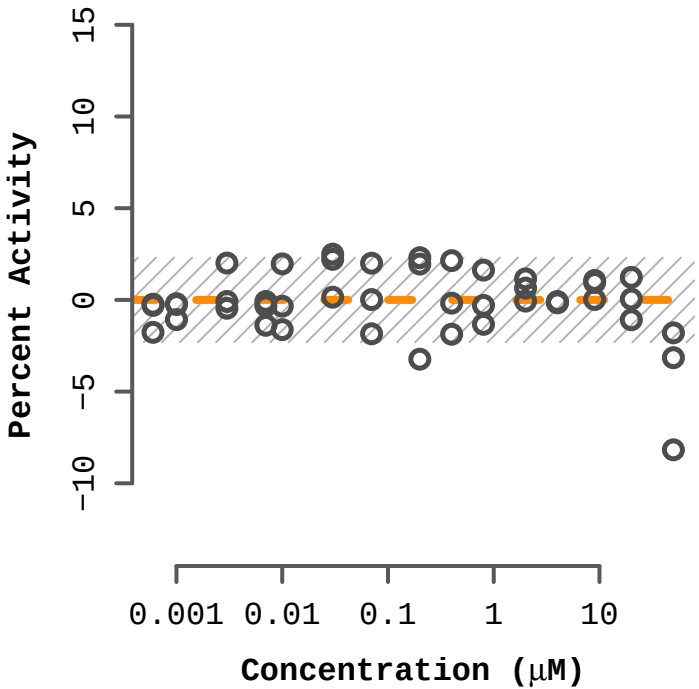
NAME: Propafenone
CHID: 45184 **CASRN:** 54063-53-5
SPID(S): Tox21_110228_1
M4ID: 12484533

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 0.139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

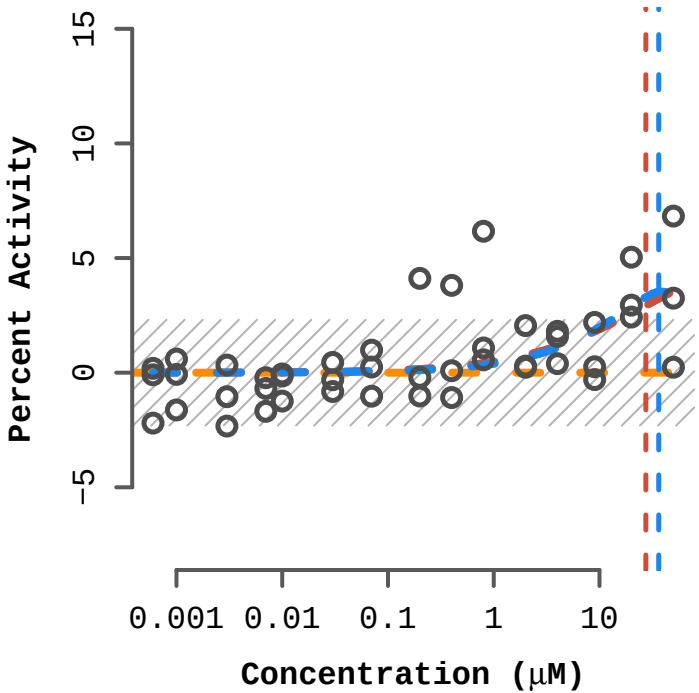
NAME: Propionylpromazine hydrochloride
CHID: 45187 **CASRN:** 7681-67-6
SPID(S): Tox21_110240_1
M4ID: 12484523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 2.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piribedil
CHID: 45188 CASRN: 3605-01-4
SPID(S): Tox21_110245_1
M4ID: 12484519

HILL MODEL (in red):

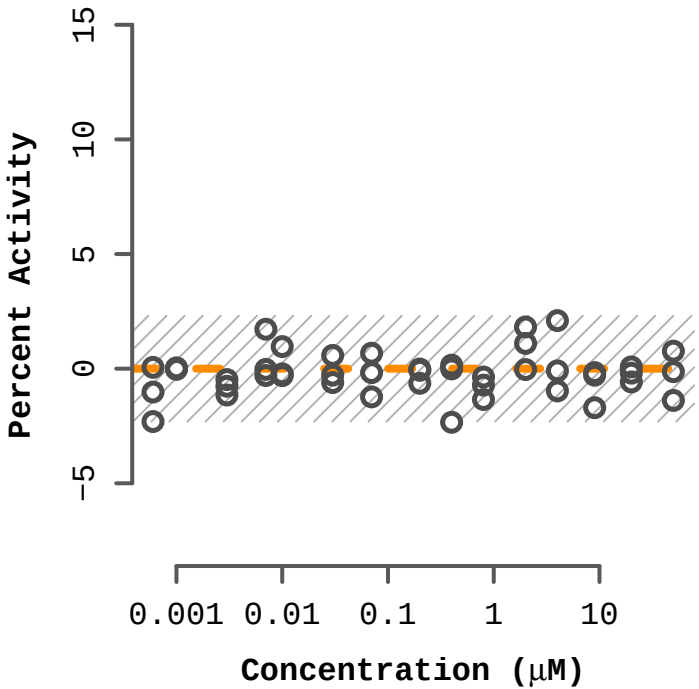
	tp	ga	gw
val:	5.85	1.44	0.729
sd:	6.81	1.35	0.433

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.59	1.56	0.809	1.81	4.46
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	190.4	175.01	178.73
PROB:	0	0.86	0.13
RMSE:	2.15	1.67	1.68

MAX_MEAN: 3.47 **MAX_MED:** 3.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

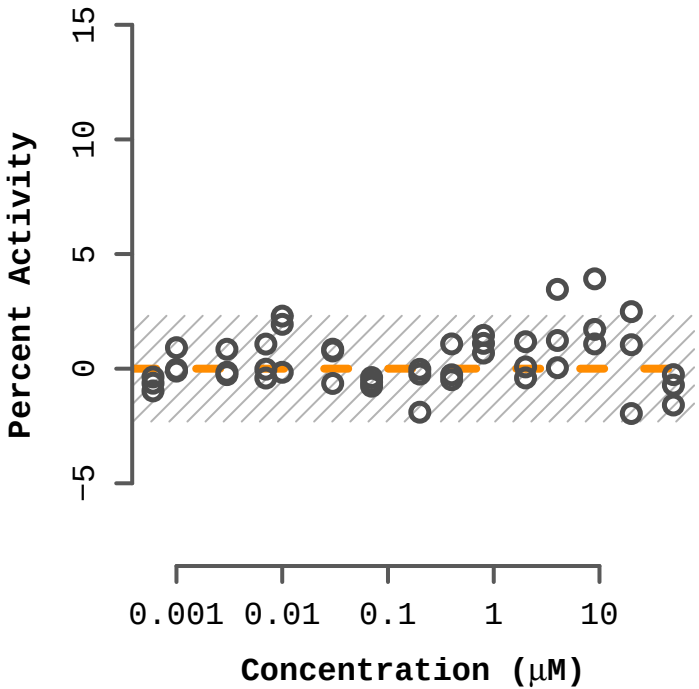
NAME: Propentofylline
CHID: 45189 CASRN: 55242-55-2
SPID(S): Tox21_110247_1
M4ID: 12484517

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.963 MAX_MED: 1.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

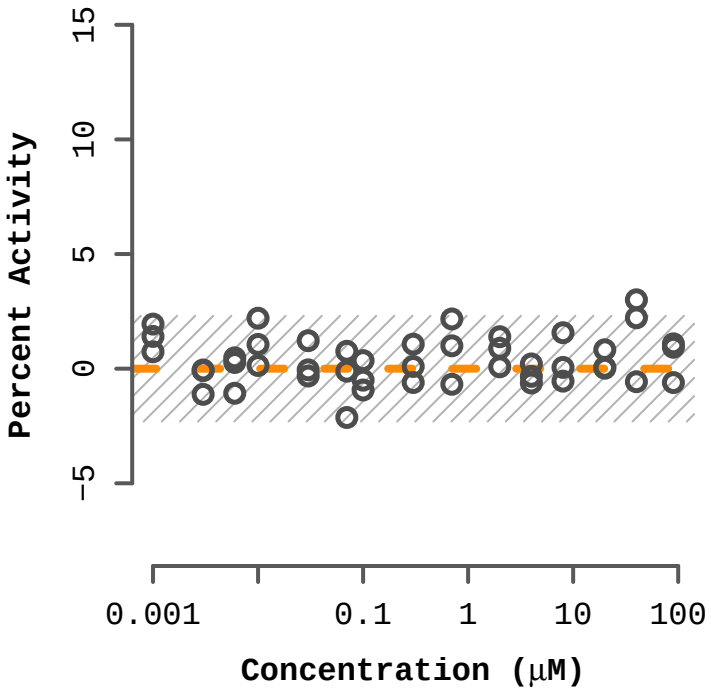
NAME: Quipazine maleate
CHID: 45190 **CASRN:** 5786-68-5
SPID(S): Tox21_110249_1
M4ID: 12484515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

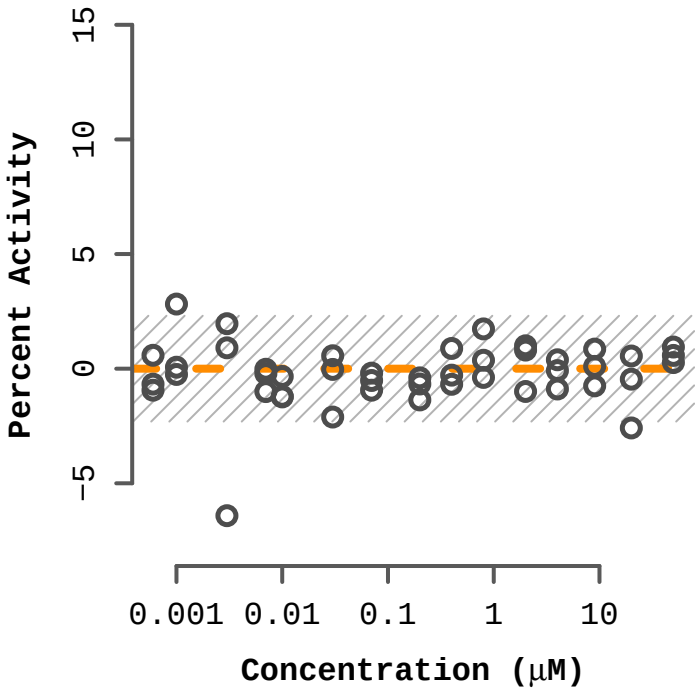
NAME: Ranitidine
CHID: 45191 **CASRN:** 66357-35-5
SPID(S): Tox21_302372
M4ID: 12476761

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

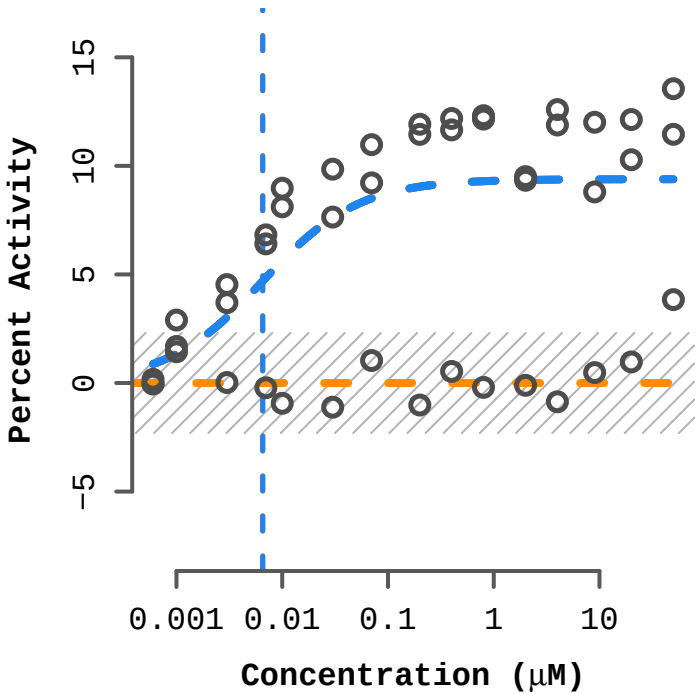
NAME: Ranitidine
CHID: 45191 **CASRN:** 66357-35-5
SPID(S): Tox21_110250_1
M4ID: 12484514

HILL MODEL: Not applicable.

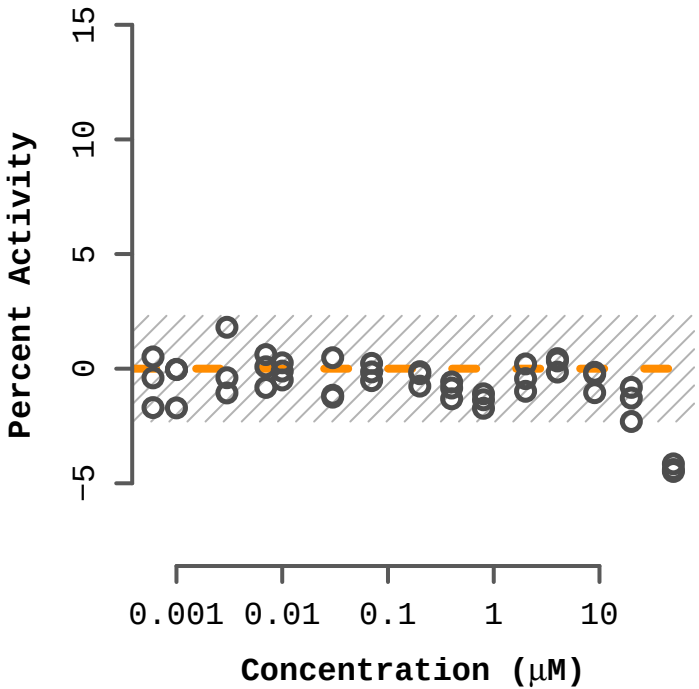
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 0.911 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Riluzole
CHID:    45192   CASRN: 1744-22-5
SPID(S): Tox21_110252_1
M4ID:    12484512

HILL MODEL (in red):
      tp       ga       gw
val:  9.39     -2.18    0.953
sd:   1.1      0.294    0.507

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.39     -2.18    0.953    3.52     4.66
sd:   1.1      0.294    0.507    4530     11600

      CNST        HILL        GNLS
AIC:  320.88      275.09      279.09
PROB: 0           0.88        0.12
RMSE: 7.87        4.7         4.7

MAX_MEAN: 9.62      MAX_MED: 12.2      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

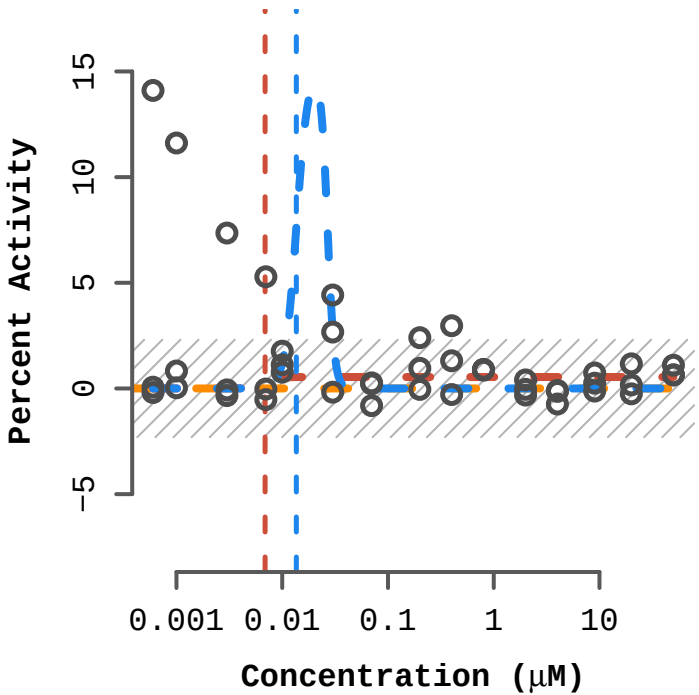
NAME: Risperidone
CHID: 45193 **CASRN:** 106266-06-2
SPID(S): Tox21_110253_1
M4ID: 12484511

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 0.21 **MAX_MED:** 0.339 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Rilmenidine
CHID: 45194 CASRN: 54187-04-1
SPID(S): Tox21_110254_1
M4ID: 12484510

HILL MODEL (in red):

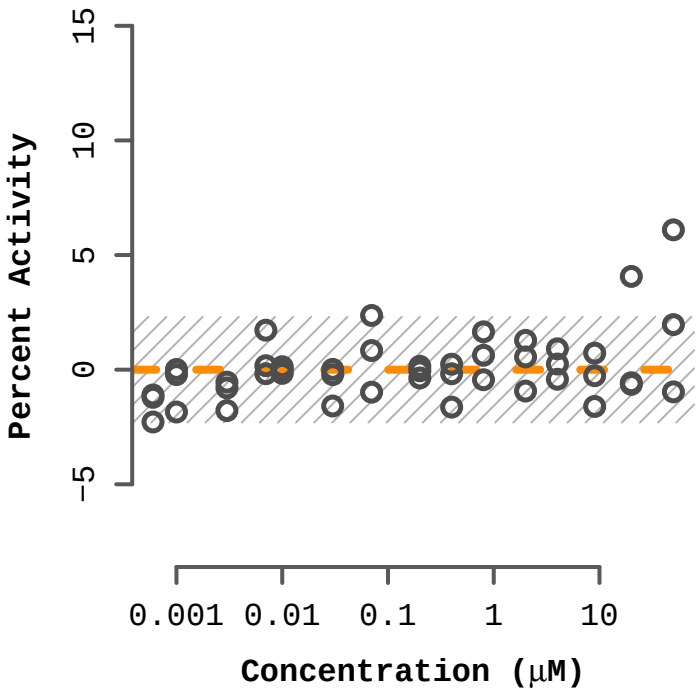
	tp	ga	gw
val:	0.541	−2.16	8
sd:	0.196	0.359	22.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.3	−1.87	7.98	−1.57	13.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	193.72	191.92	194.08
PROB:	0.23	0.57	0.19
RMSE:	3.25	3.18	3.17

MAX_MEAN: 4.66 MAX_MED: 2.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

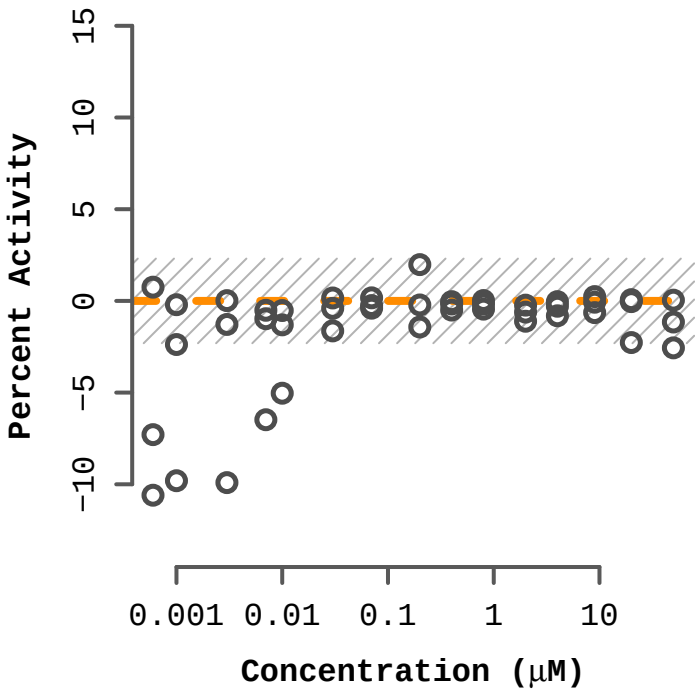
NAME: Ropinirole
CHID: 45195 CASRN: 91374-21-9
SPID(S): Tox21_110256_1
M4ID: 12484508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 2.37 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

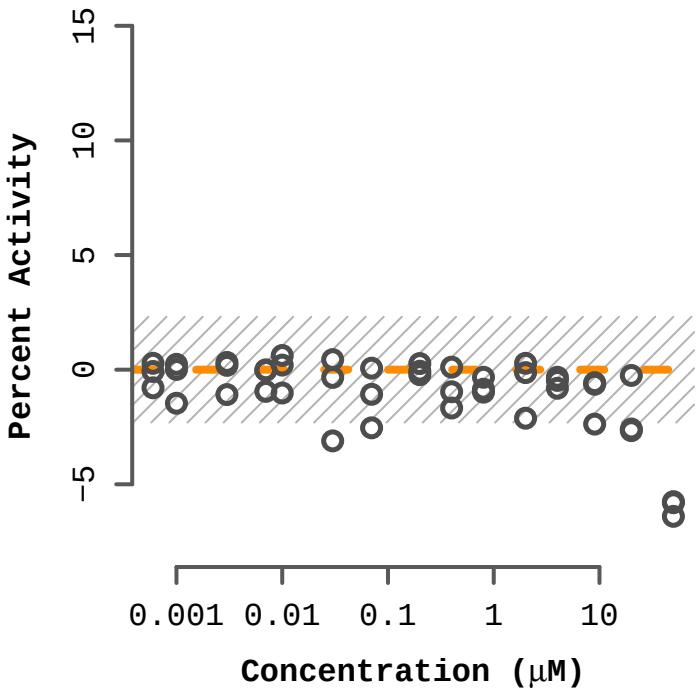
NAME: Ranolazine
CHID: 45196 **CASRN:** 95635-55-5
SPID(S): Tox21_110258_1
M4ID: 12484506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.95	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 0.113 **MAX_MED:** −0.0376 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

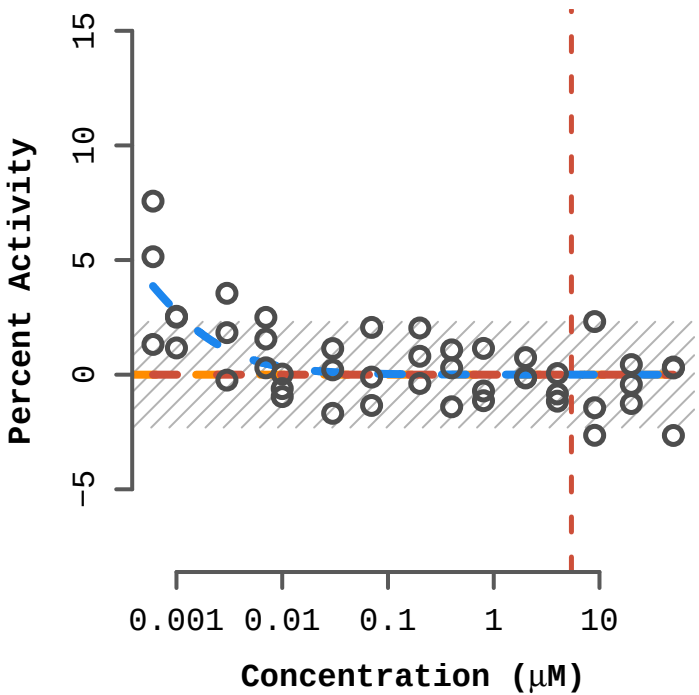
NAME: Spiroxatrine
CHID: 45198 **CASRN:** 1054-88-2
SPID(S): Tox21_110260_1
M4ID: 12484504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: −0.00477 **MAX_MED:** 0.201 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SR 57227A hydrochloride
CHID: 45201 CASRN: 77145-61-0
SPID(S): Tox21_110263_1
M4ID: 12484502

HILL MODEL (in red):

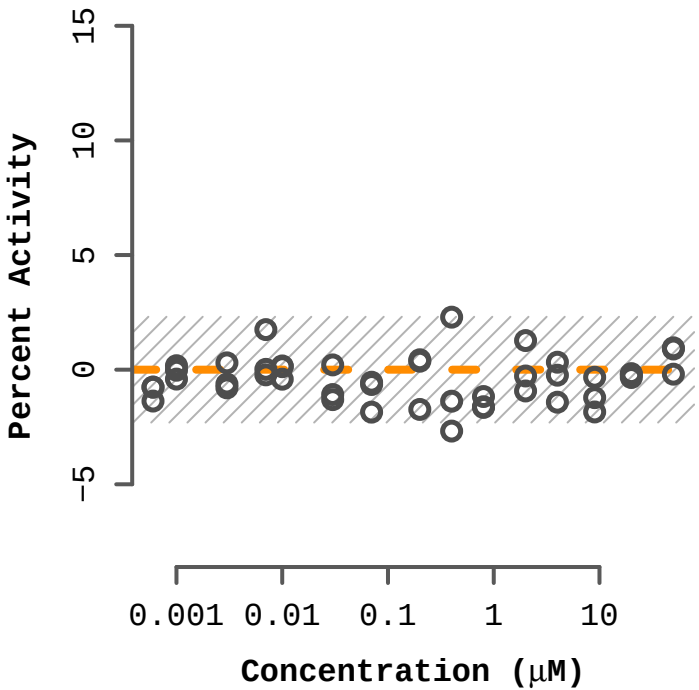
	tp	ga	gw
val:	5.56e-11	0.735	5.62
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.09	-4.68	5.14	-3.35	1.05
sd:	13	827	2970	0.891	0.557

	CNST	HILL	GNLS
AIC:	182.92	188.92	172.79
PROB:	0.01	0	0.99
RMSE:	1.96	1.96	1.4

MAX_MEAN: 4.68 MAX_MED: 5.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

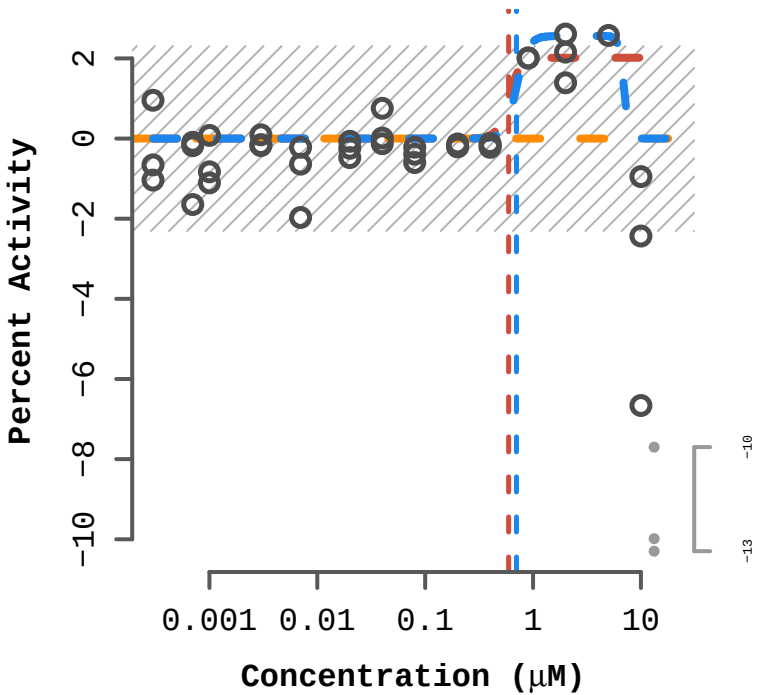
NAME: Siguazodan
CHID: 45202 CASRN: 115344-47-3
SPID(S): Tox21_110264_1
M4ID: 12484501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.554 **MAX_MED:** 0.903 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sanguinarine
CHID: 45204 CASRN: 2447-54-3
SPID(S): Tox21_110268_1
M4ID: 12484499 BRK

HILL MODEL (in red):

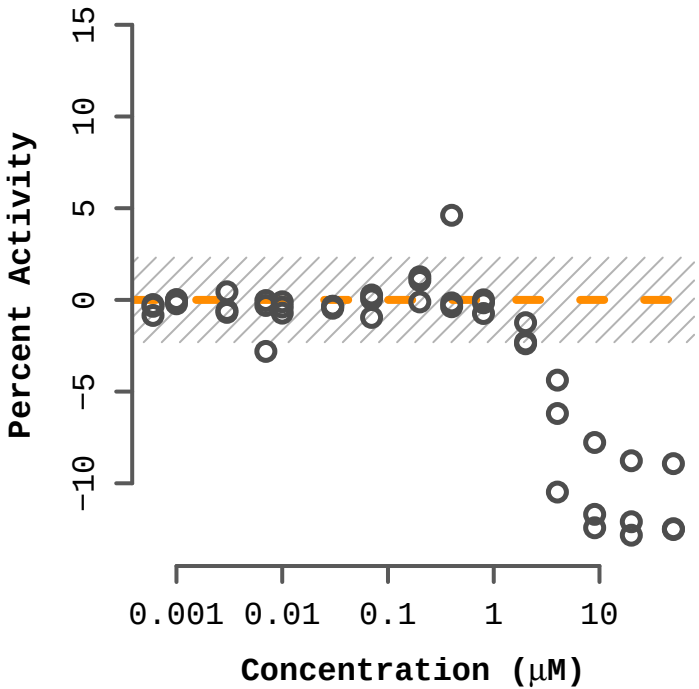
	tp	ga	gw
val:	2.02	−0.227	8
sd:	0.407	0.136	6.08

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.56	−0.154	8	0.842	18
sd:	0.39	0.123	7.55	0.154	18.4

	CNST	HILL	GNLS
AIC:	215.36	210.17	195.36
PROB:	0	0	1
RMSE:	3.65	4.08	3.44

MAX_MEAN: 3.91 MAX_MED: 2.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

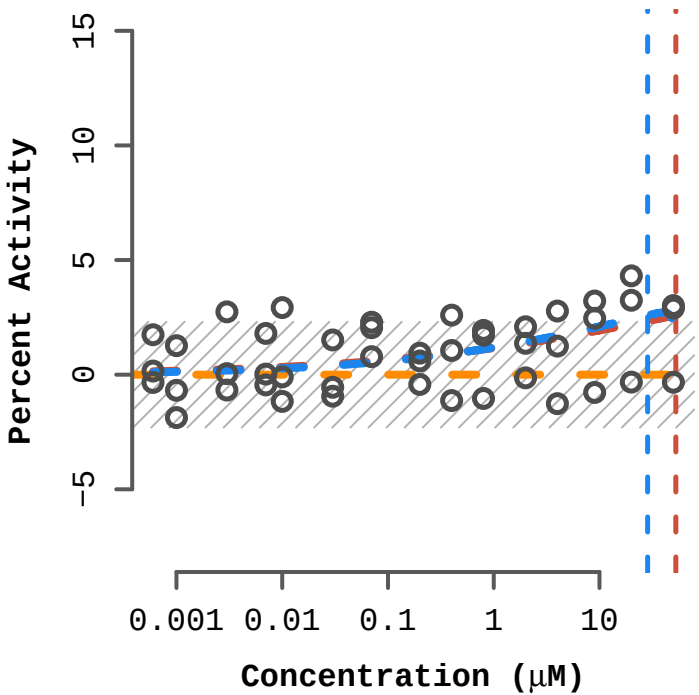
NAME: Spiperone
CHID: 45205 **CASRN:** 749-02-0
SPID(S): Tox21_110269_1
M4ID: 12484498

HILL MODEL: Not applicable.

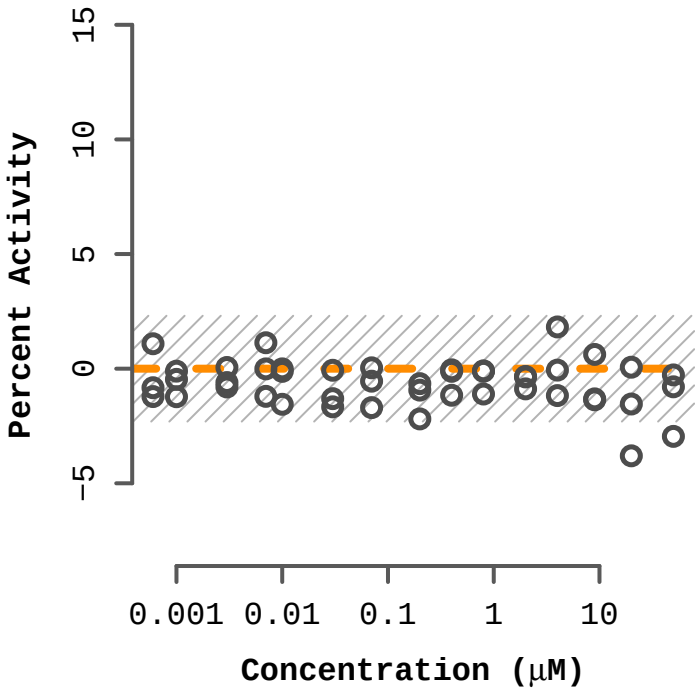
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	273.75	NA	NA
PROB:	1	NA	NA
RMSE:	5.47	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.06 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Gaboxadol
CHID:    45206   CASRN: 64603-91-4
SPID(S): Tox21_110271_1
M4ID:    12484496

HILL MODEL (in red):
      tp       ga       gw
val:  5.18     1.72     0.311
sd:   11.6     5.84     0.299

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.18     1.46     0.362    1.74     13.6
sd:   6.58     2.61     0.219    0.316    96.6

      CNST        HILL        GNLS
AIC:  185.57      173.2       176.99
PROB: 0           0.87        0.13
RMSE: 1.78        1.44        1.45

MAX_MEAN: 2.41      MAX_MED: 3.25      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

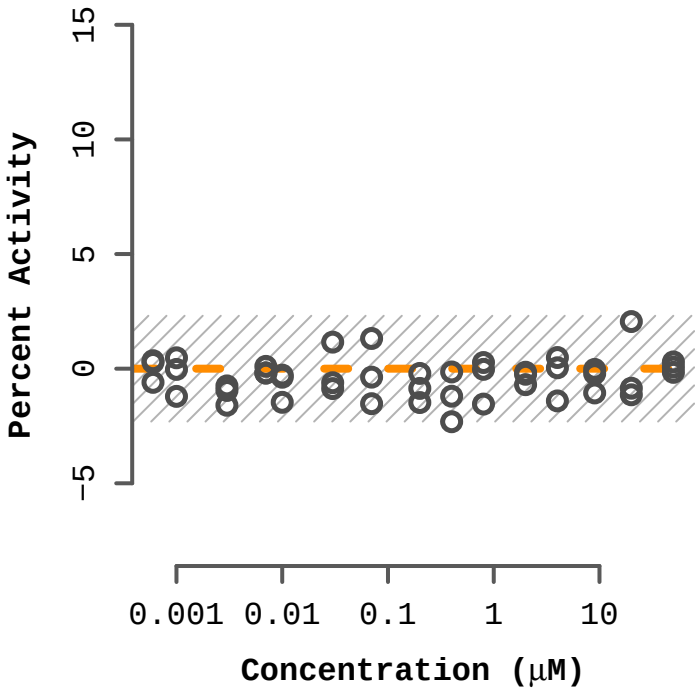
NAME: Tracazolate hydrochloride
CHID: 45208 **CASRN:** NOCAS_45208
SPID(S): Tox21_110273_1
M4ID: 12484494

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.196 **MAX_MED:** −0.00744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

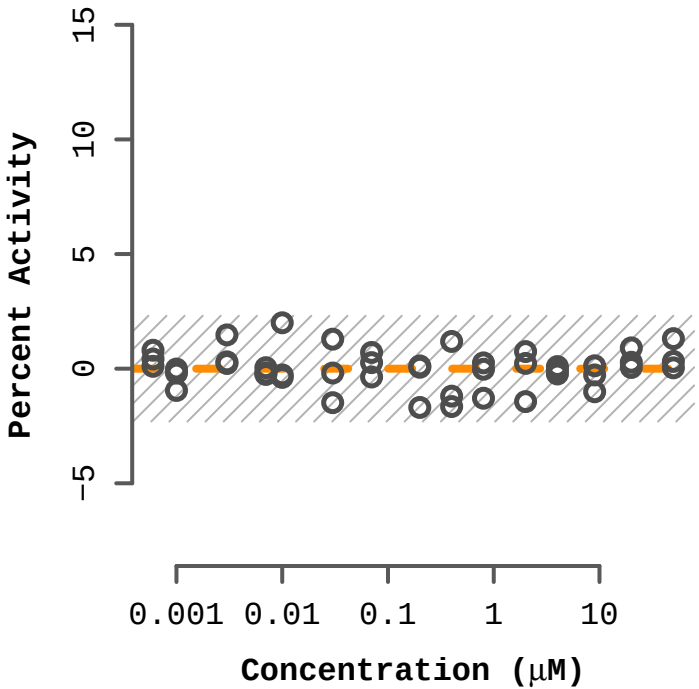
NAME: Telenzepine
CHID: 45209 **CASRN:** 80880-90-6
SPID(S): Tox21_110274_1
M4ID: 12484493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.0678 **MAX_MED:** 0.275 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

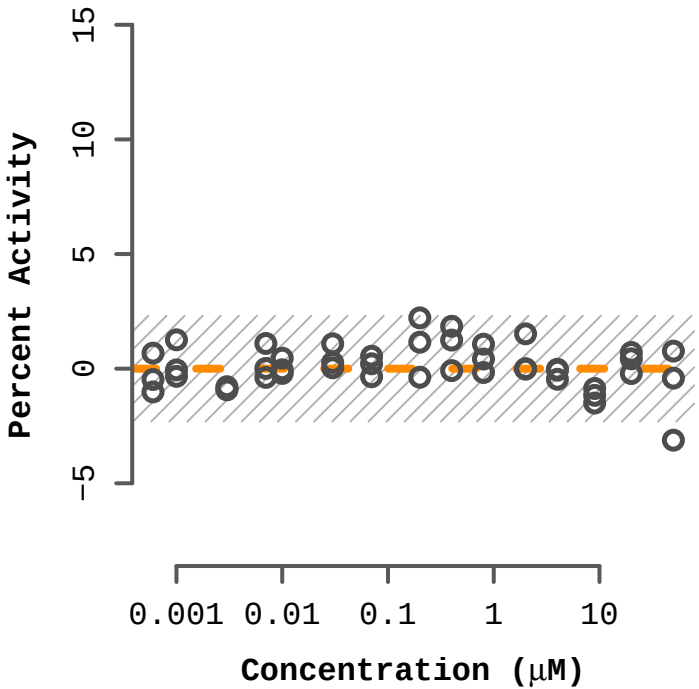
NAME: Tiapride hydrochloride
CHID: 45210 CASRN: 51012-33-0
SPID(S): Tox21_110276_1
M4ID: 12484491

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.667 **MAX_MED:** 0.422 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

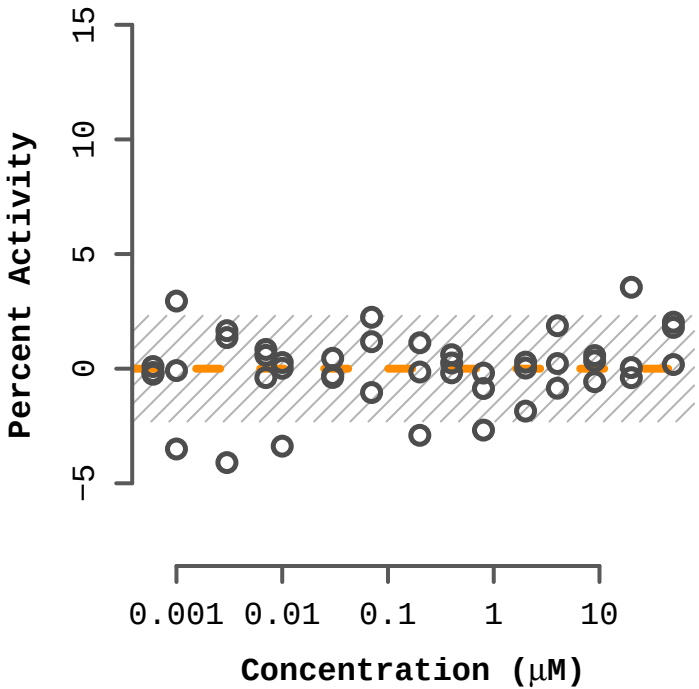
NAME: Tyrphostin 23
CHID: 45215 **CASRN:** 118409-57-7
SPID(S): Tox21_110287_1
M4ID: 12484481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

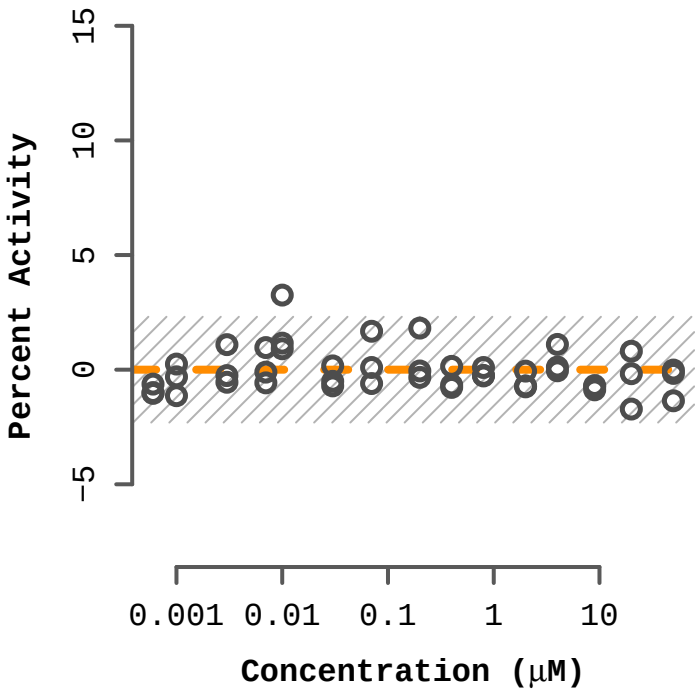
NAME: 1-[2-(Trifluoromethyl)phenyl]-1H-imidazole
CHID: 45217 **CASRN:** 25371-96-4
SPID(S): Tox21_110289_1
M4ID: 12484480

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

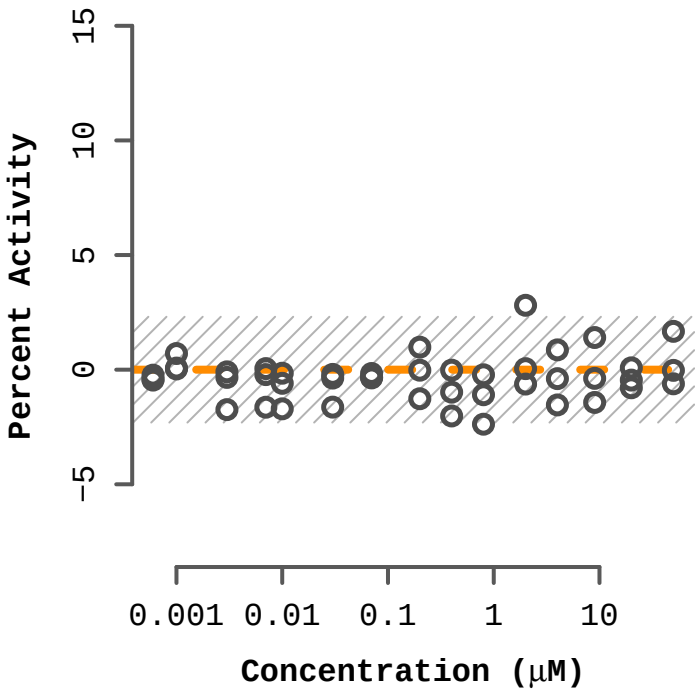
NAME: Tropicamide
CHID: 45220 **CASRN:** 1508-75-4
SPID(S): Tox21_110297_1
M4ID: 12484473

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

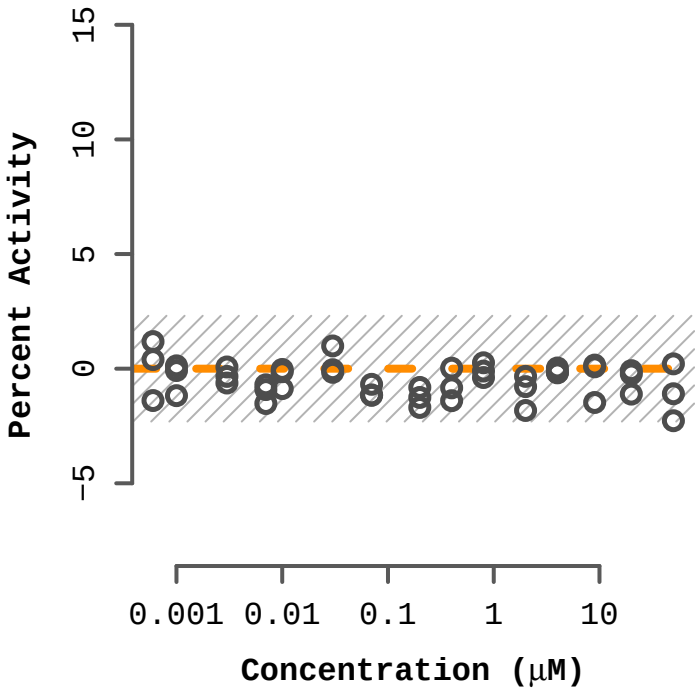
NAME: Brimonidine
CHID: 45221 **CASRN:** 59803-98-4
SPID(S): Tox21_110299_1
M4ID: 12484472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.743 **MAX_MED:** 0.0707 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

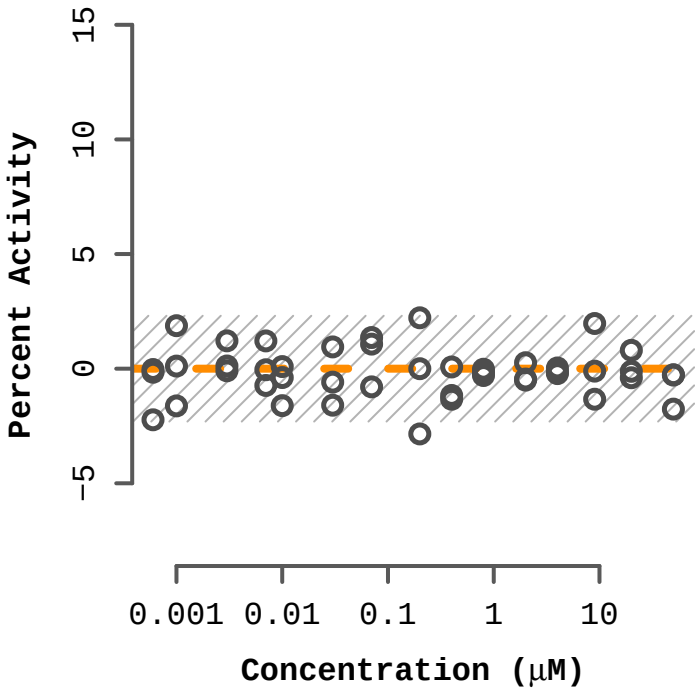
NAME: Xylometazoline hydrochloride
CHID: 45223 CASRN: 1218-35-5
SPID(S): Tox21_110305_1
M4ID: 12484468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.264 **MAX_MED:** 0.399 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

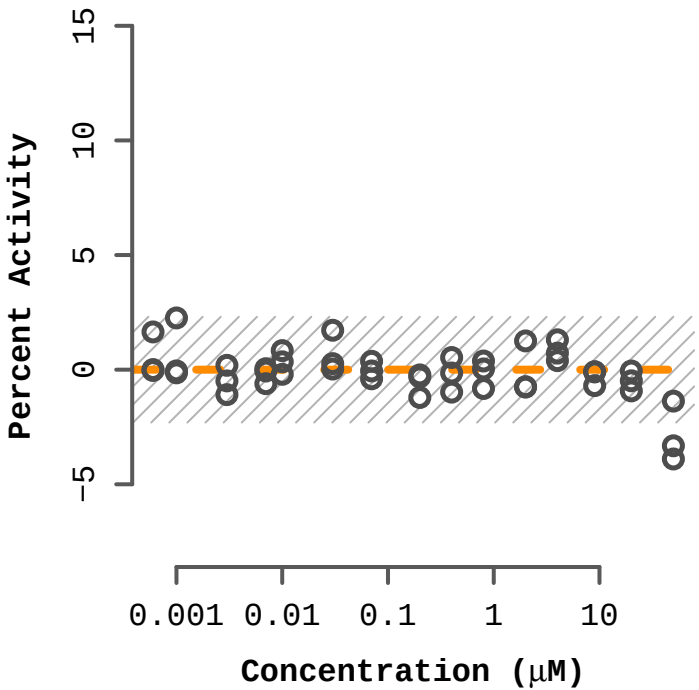
NAME: Zaprinast
CHID: 45224 **CASRN:** 37762-06-4
SPID(S): Tox21_110306_1
M4ID: 12484467

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.547 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

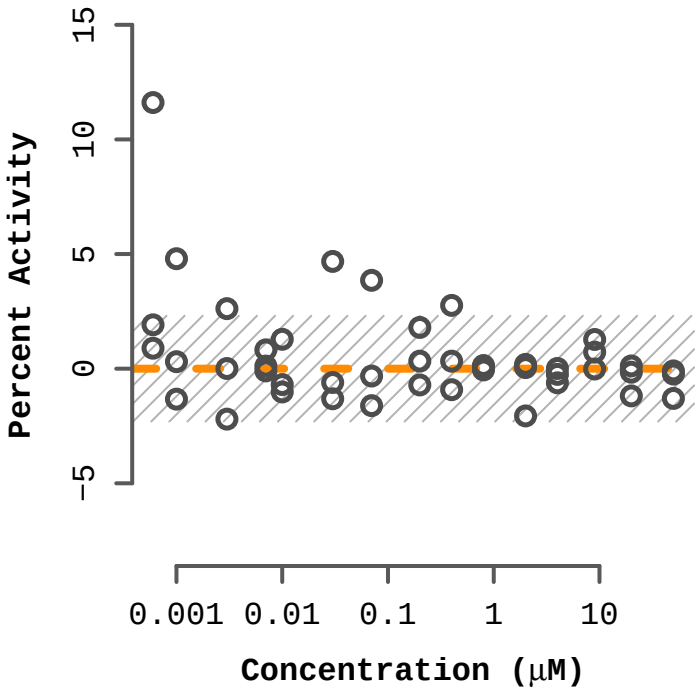
NAME: Loxapine succinate
CHID: 45227 CASRN: 27833-64-3
SPID(S): Tox21_110311_1
M4ID: 12484465

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.808 **MAX_MED:** 0.724 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

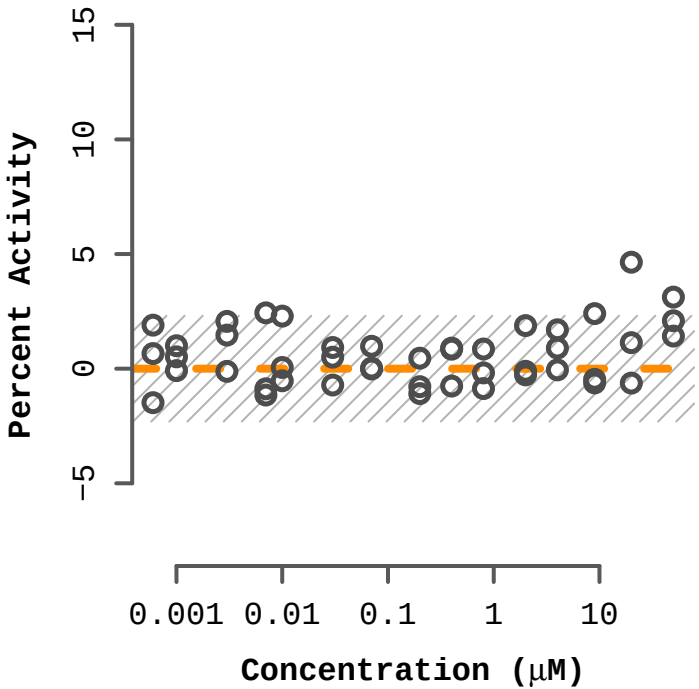
NAME: Lorglumide sodium
CHID: 45228 **CASRN:** 1021868-76-7
SPID(S): Tox21_110312_1
M4ID: 12484464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.02	NA	NA
PROB:	1	NA	NA
RMSE:	2.33	NA	NA

MAX_MEAN: 4.81 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

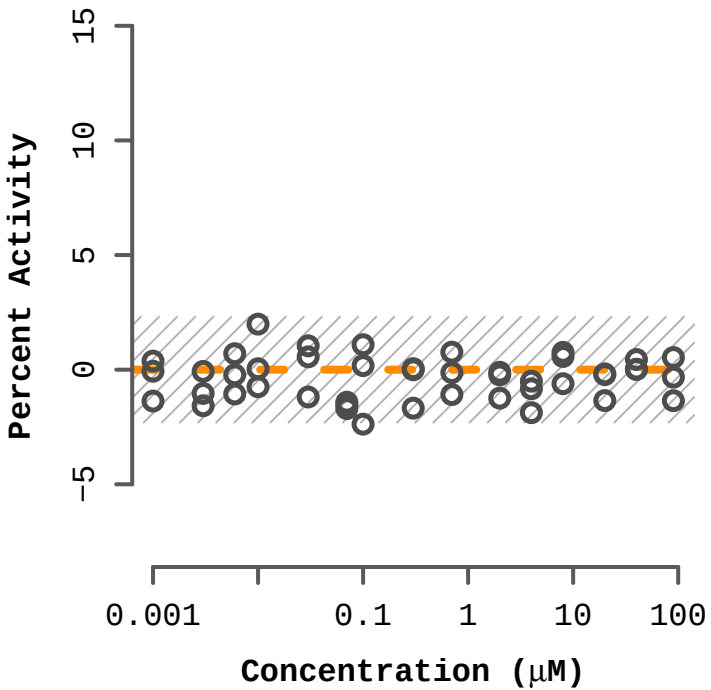
NAME: Pempidine d-tartaric acid
CHID: 45229 **CASRN:** 546-48-5
SPID(S): Tox21_110313_1
M4ID: 12484463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

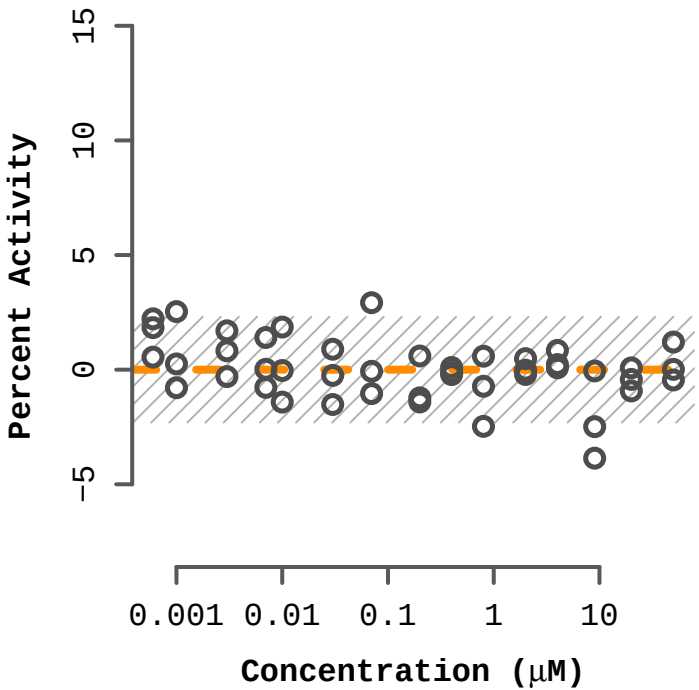
NAME: Tiratricol
CHID: 45232 **CASRN:** 51-24-1
SPID(S): Tox21_303544
M4ID: 12475600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.89	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.43 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

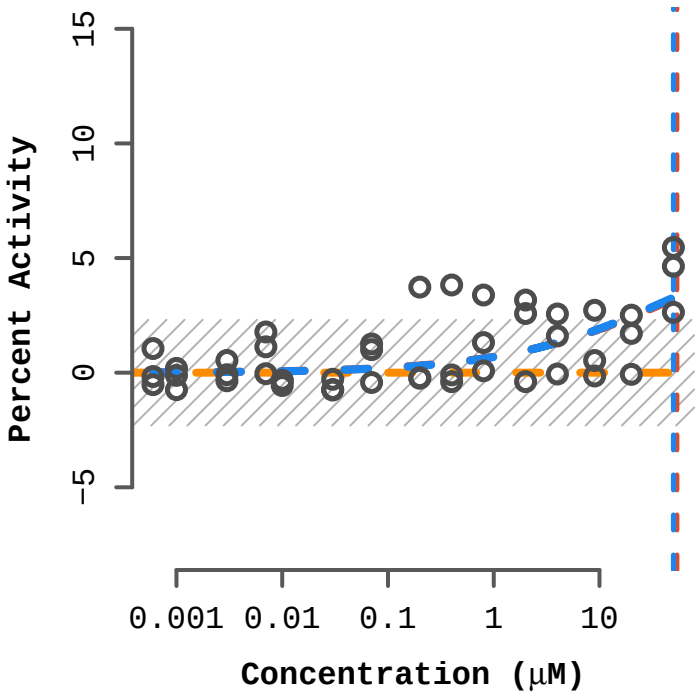
NAME: Idoxuridine
CHID: 45238 **CASRN:** 54-42-2
SPID(S): Tox21_110324_1
M4ID: 12484455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zoxazolamine
CHID: 45245 **CASRN:** 61-80-3
SPID(S): Tox21_110346_1
M4ID: 12484437

HILL MODEL (in red):

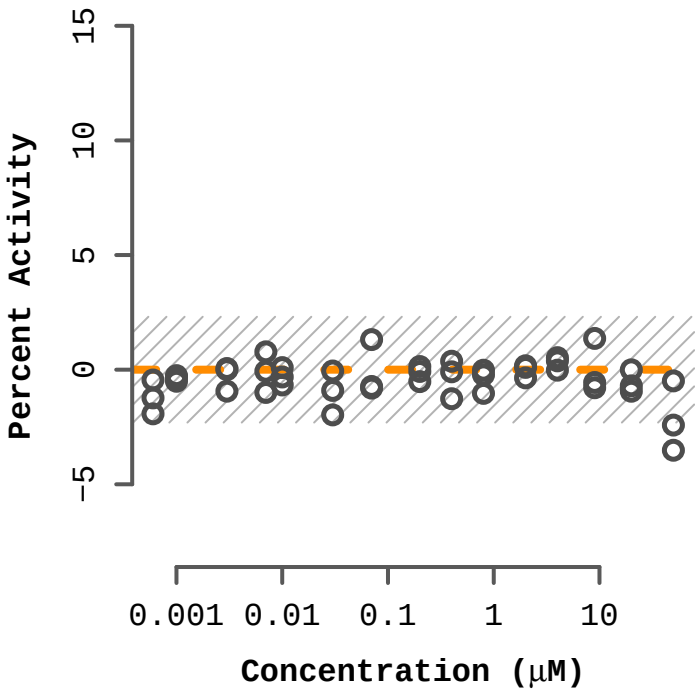
	tp	ga	gw
val:	6.56	1.73	0.534
sd:	5.55	1.14	0.213

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.56	1.7	0.55	3.53	10.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	180.43	160.04	164.05
PROB:	0	0.88	0.12
RMSE:	1.85	1.31	1.32

MAX_MEAN: 4.25 **MAX_MED:** 4.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

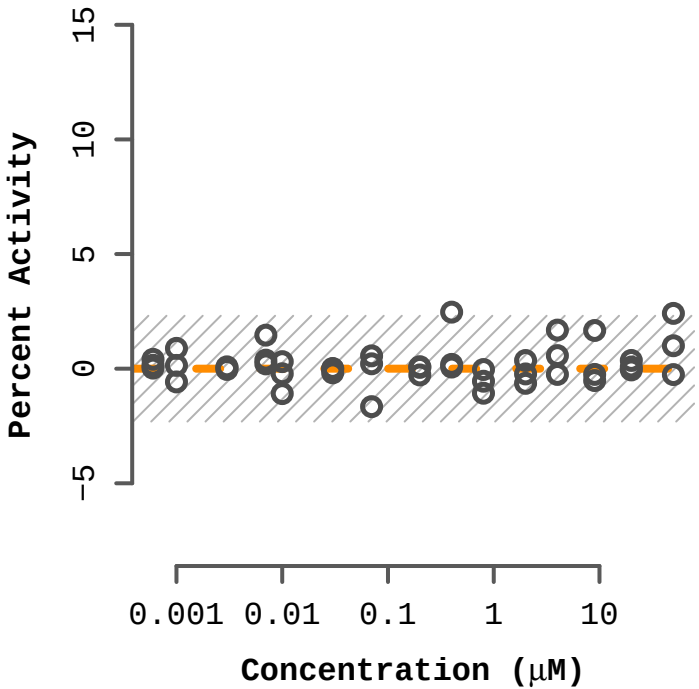
NAME: Primaquine diphosphate
CHID: 45248 **CASRN:** 63-45-6
SPID(S): Tox21_110350_1
M4ID: 12484433

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.04	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.297 **MAX_MED:** 0.386 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

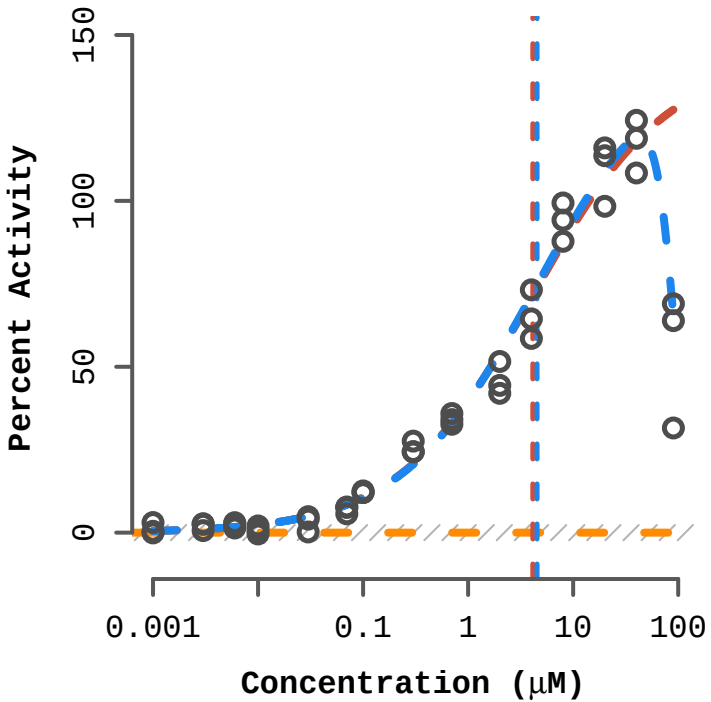
NAME: Demeclocycline hydrochloride
CHID: 45252 CASRN: 64-73-3
SPID(S): Tox21_110354_1
M4ID: 12484431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.05 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 21-Hydroxyprogesterone
CHID: 45254 CASRN: 64-85-7
SPID(S): Tox21_302402
M4ID: 12476731

HILL MODEL (in red):

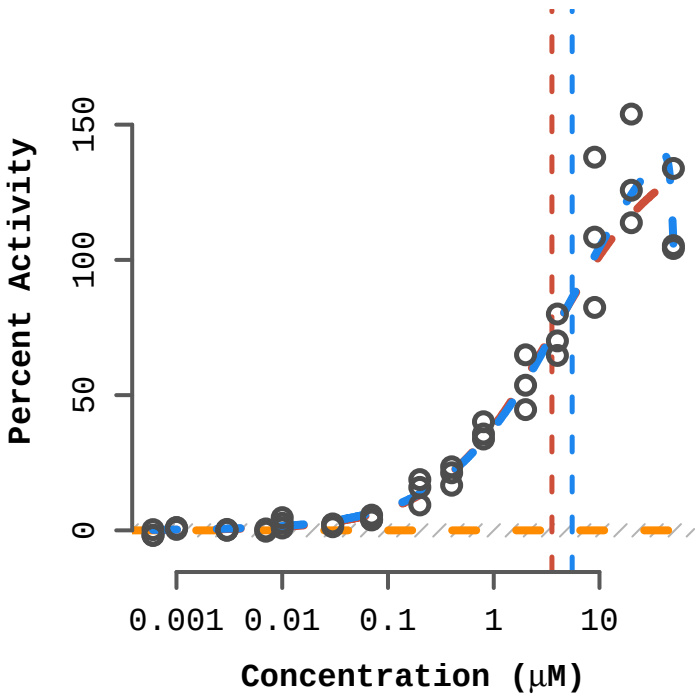
	tp	ga	gw
val:	143	0.616	0.678
sd:	10.9	0.124	0.0549

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	149	0.656	0.674	1.95	4.89
sd:	9.8	0.0992	0.0405	0.00995	2.47

	CNST	HILL	GNLS
AIC:	490.56	341.04	295.57
PROB:	0	0	1
RMSE:	55.61	19.88	7.08

MAX_MEAN: 117 MAX_MED: 119 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 21-Hydroxyprogesterone
CHID: 45254 CASRN: 64-85-7
SPID(S): Tox21_110356_1
M4ID: 12484429

HILL MODEL (in red):

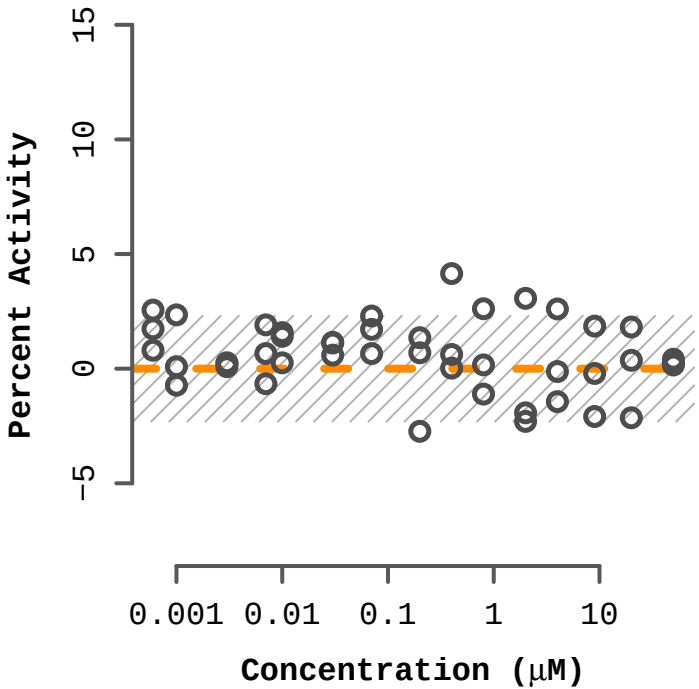
	tp	ga	gw
val:	146	0.55	0.805
sd:	10	0.105	0.071

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	172	0.742	0.742	1.72	17.9
sd:	21	0.17	0.0698	0.00425	4.22

	CNST	HILL	GNLS
AIC:	493.15	323.87	314.94
PROB:	0	0.01	0.99
RMSE:	59.74	10.8	9.52

MAX_MEAN: 131 MAX_MED: 126 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

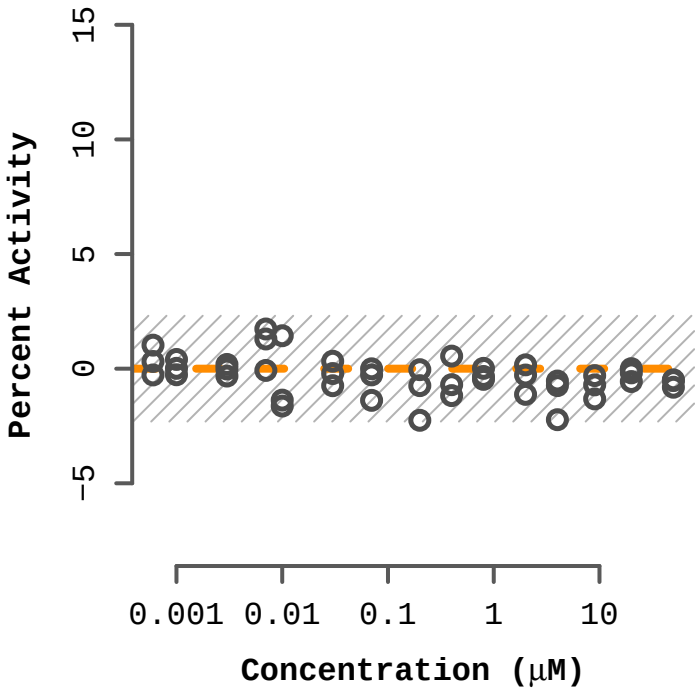
NAME: Pyrithyldione
CHID: 45262 **CASRN:** 77-04-3
SPID(S): Tox21_110368_1
M4ID: 12484420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

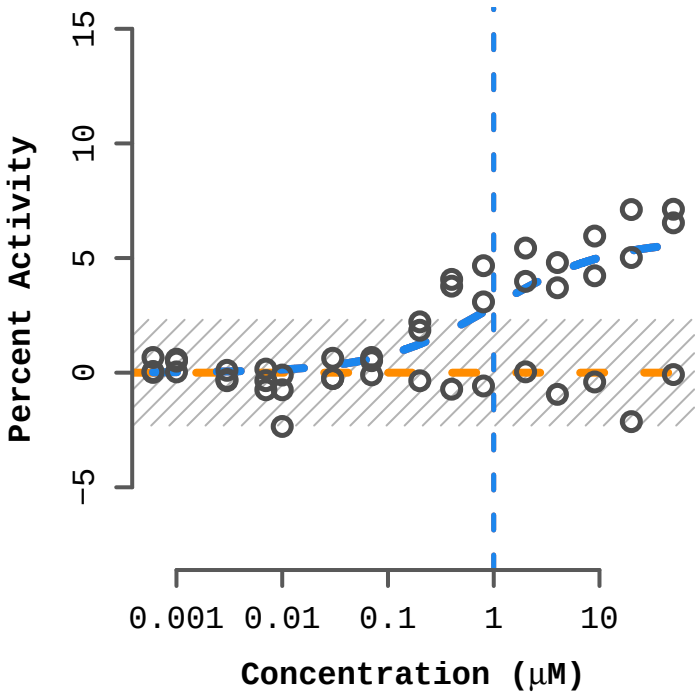
NAME: Sulfachloropyridazine
CHID: 45265 **CASRN:** 80-32-0
SPID(S): Tox21_110372_1
M4ID: 12484416

HILL MODEL: Not applicable.

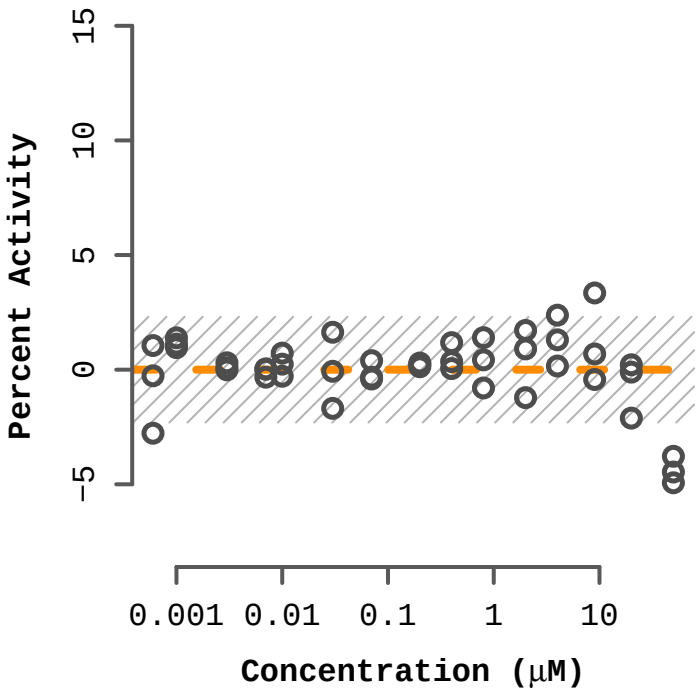
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.984 **MAX_MED:** 1.3 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Khellin
CHID:    45267   CASRN: 82-02-0
SPID(S): Tox21_110374_1
M4ID:    12484414

HILL MODEL (in red):
      tp       ga       gw
val:  5.8      -0.000494 0.805
sd:   1.9      0.661    0.415

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.8      -0.000465 0.805    3.02     6.69
sd:   1.9      0.661    0.415    2780     14000

      CNST        HILL        GNLS
AIC:  224.11      193.62      197.62
PROB: 0           0.88        0.12
RMSE: 2.95        2.18        2.18

MAX_MEAN: 4.53      MAX_MED: 6.54      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

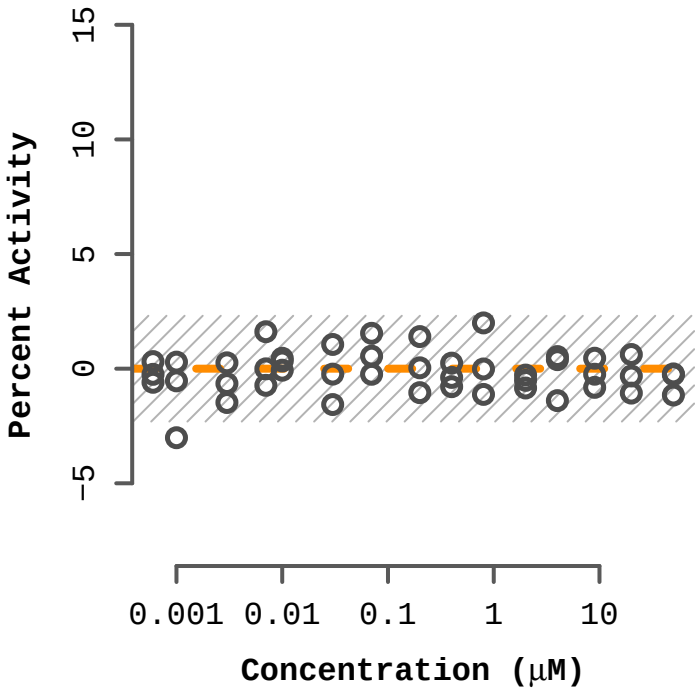
NAME: Dibucaine
CHID: 45271 **CASRN:** 85-79-0
SPID(S): Tox21_110381_1
M4ID: 12484408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

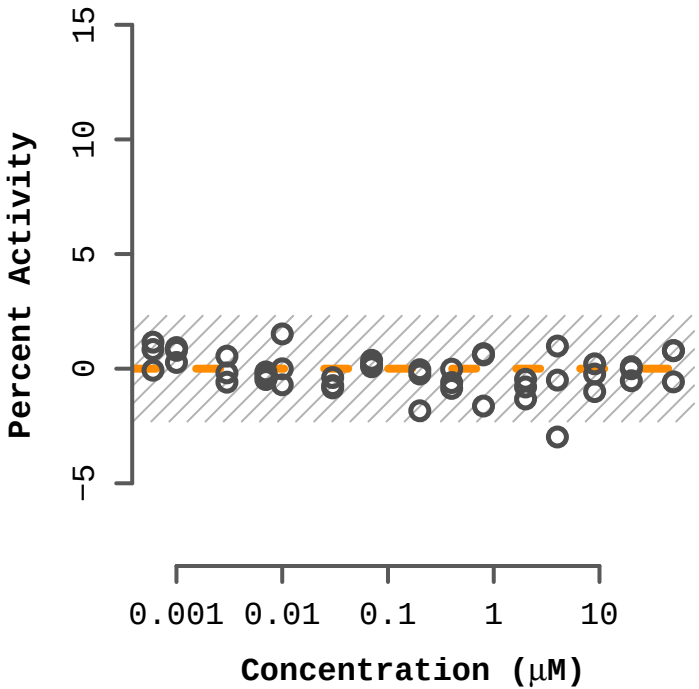
NAME: Azacyclonol
CHID: 45280 **CASRN:** 115-46-8
SPID(S): Tox21_110399_1
M4ID: 12484392

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.616 **MAX_MED:** 0.548 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

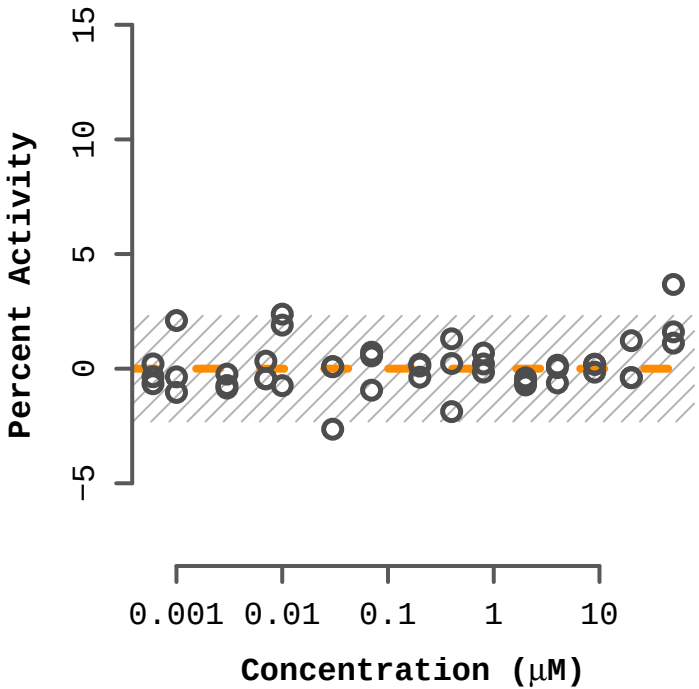
NAME: Succinylsulfathiazole
CHID: 45281 CASRN: 116-43-8
SPID(S): Tox21_110400_1
M4ID: 12484391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.666 **MAX_MED:** 0.838 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

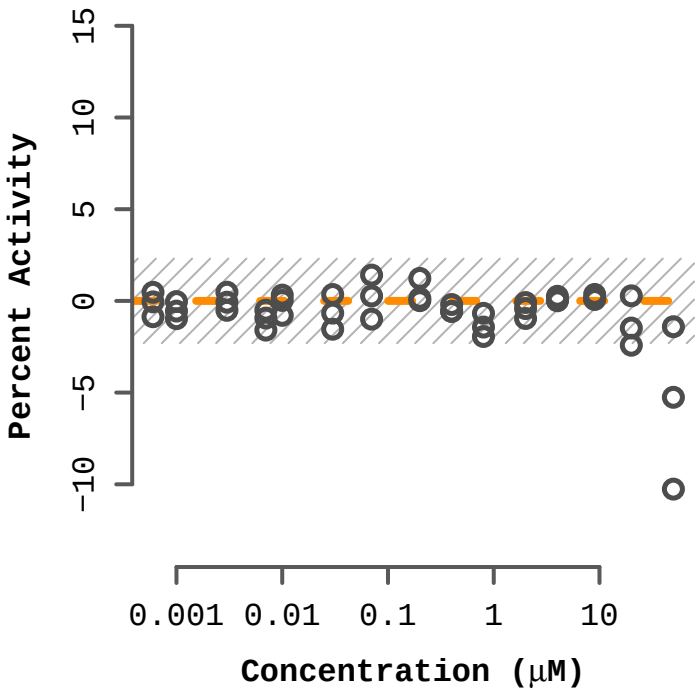
NAME: Sulfabenzamide
CHID: 45287 **CASRN:** 127-71-9
SPID(S): Tox21_110410_1
M4ID: 12484383

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

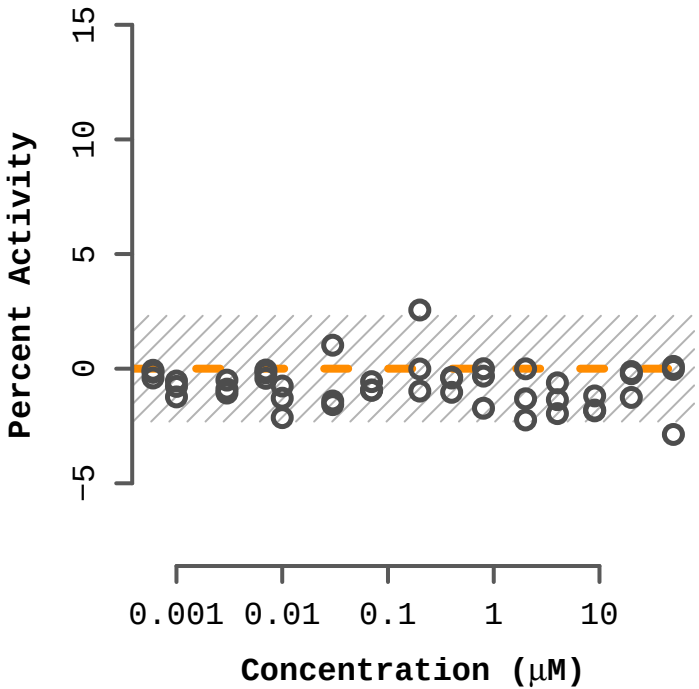
NAME: Oxyphenbutazone
CHID: 45291 **CASRN:** 129-20-4
SPID(S): Tox21_110414_1
M4ID: 12484380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 0.462 **MAX_MED:** 0.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

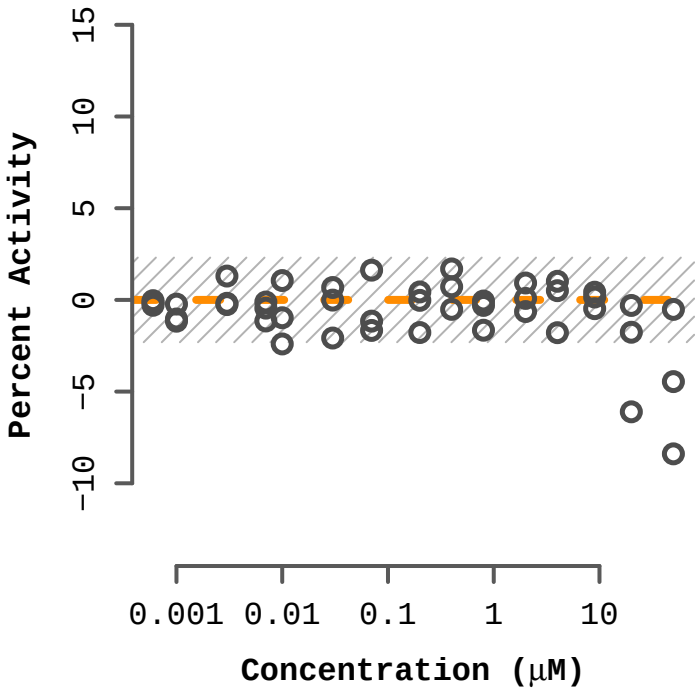
NAME: Piperidolate hydrochloride
CHID: 45292 **CASRN:** 129-77-1
SPID(S): Tox21_110415_1
M4ID: 12484379

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.523 **MAX_MED:** −0.0122 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

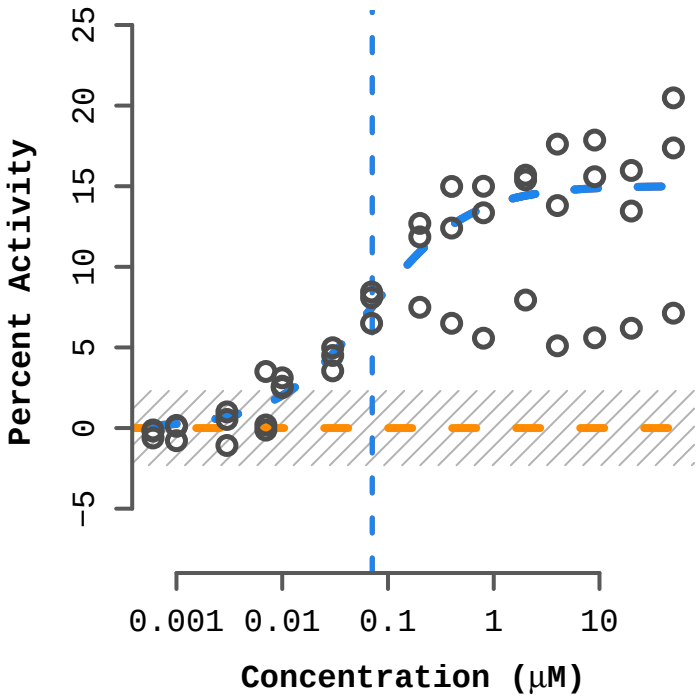
NAME: Benzydamine hydrochloride
CHID: 45293 CASRN: 132-69-4
SPID(S): Tox21_110420_1
M4ID: 12484374

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 0.631 **MAX_MED:** 0.717 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mafenide hydrochloride
CHID: 45296 CASRN: 138-37-4
SPID(S): Tox21_110423_1
M4ID: 12484371

HILL MODEL (in red):

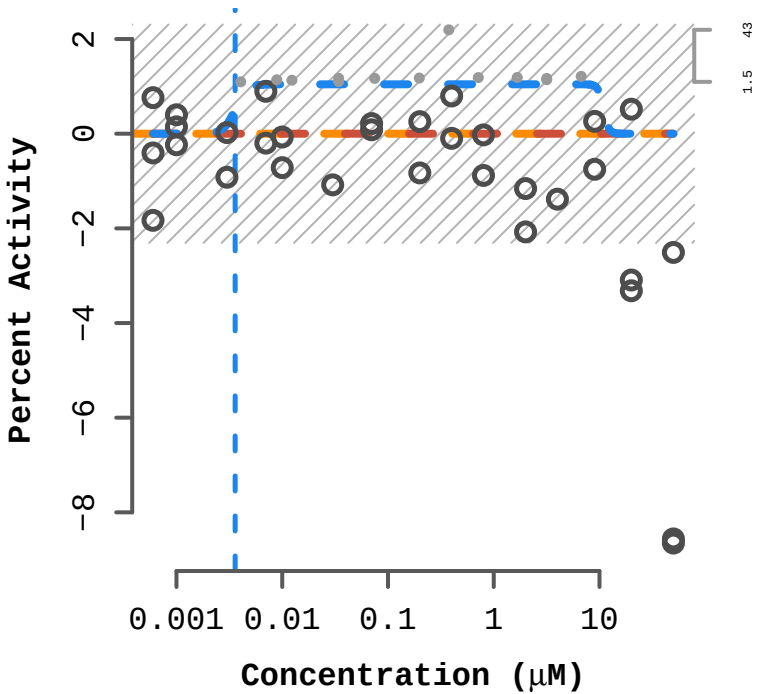
	tp	ga	gw
val:	15	−1.15	0.949
sd:	1.02	0.13	0.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15	−1.15	0.949	2.91	6.92
sd:	1.02	0.13	0.2	1010	5780

	CNST	HILL	GNLS
AIC:	339.92	239.35	243.35
PROB:	0	0.88	0.12
RMSE:	9.89	3.54	3.54

MAX_MEAN: 15 MAX_MED: 17.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexetidine
CHID: 45297 CASRN: 141-94-6
SPID(S): Tox21_110424_1
M4ID: 12484370 BRK

HILL MODEL (in red):

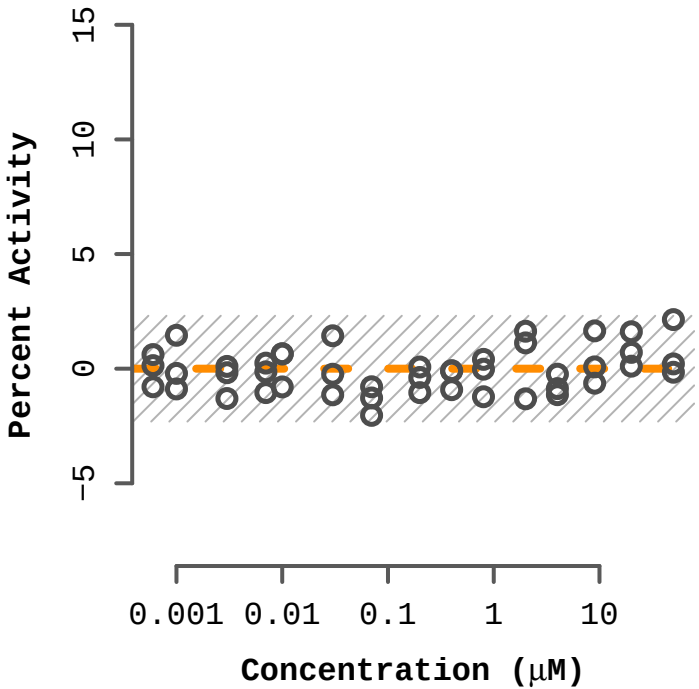
	tp	ga	gw
val:	3.6e-09	2.08	0.761
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.04	-2.45	8	1.04	17.6
sd:	0.529	0.671	61.2	1.59	280

	CNST	HILL	GNLS
AIC:	244.53	250.53	250.01
PROB:	0.9	0.04	0.06
RMSE:	7.07	7.07	6.85

MAX_MEAN: 14.6 MAX_MED: 3.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

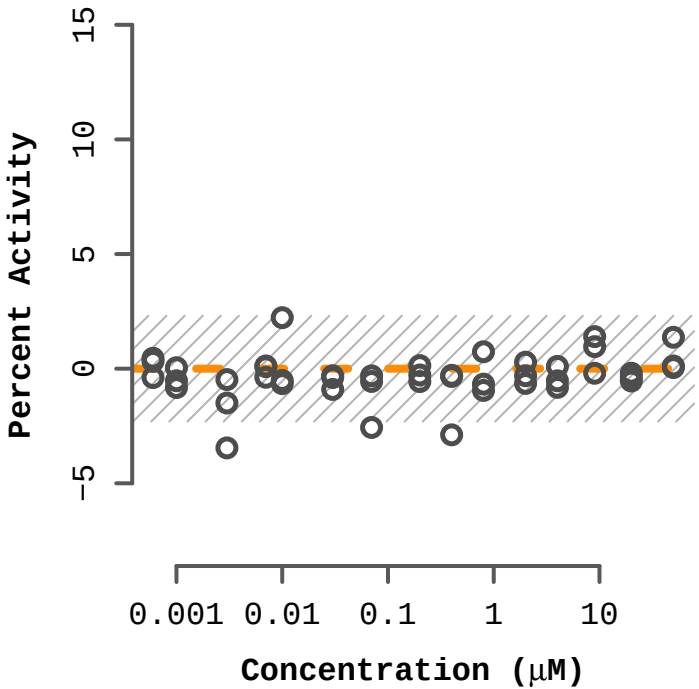
NAME: Butacaine
CHID: 45300 **CASRN:** 149-16-6
SPID(S): Tox21_110428_1
M4ID: 12484366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.812 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

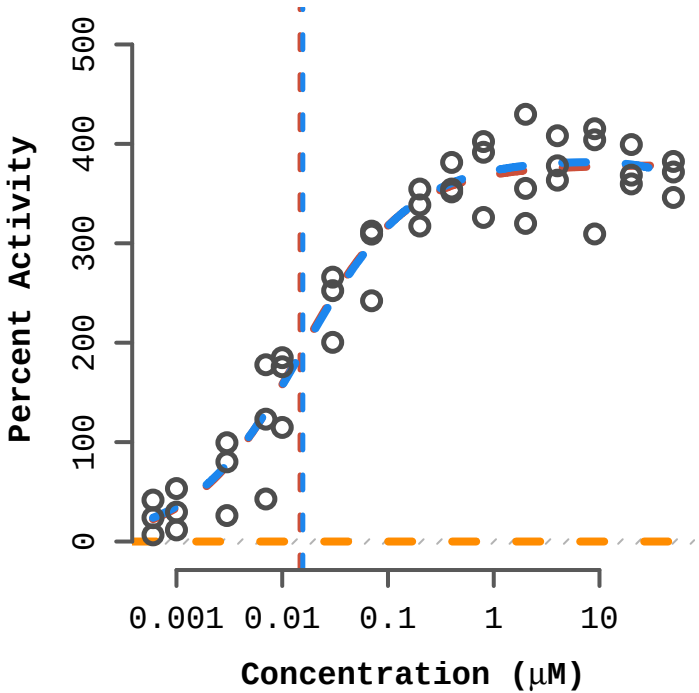
NAME: Dexpropranolol
CHID: 45304 **CASRN:** 5051-22-9
SPID(S): Tox21_110435_1
M4ID: 12484359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 0.963 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoflupredone acetate
CHID: 45306 CASRN: 338-98-7
SPID(S): Tox21_110437_1
M4ID: 12484358

HILL MODEL (in red):

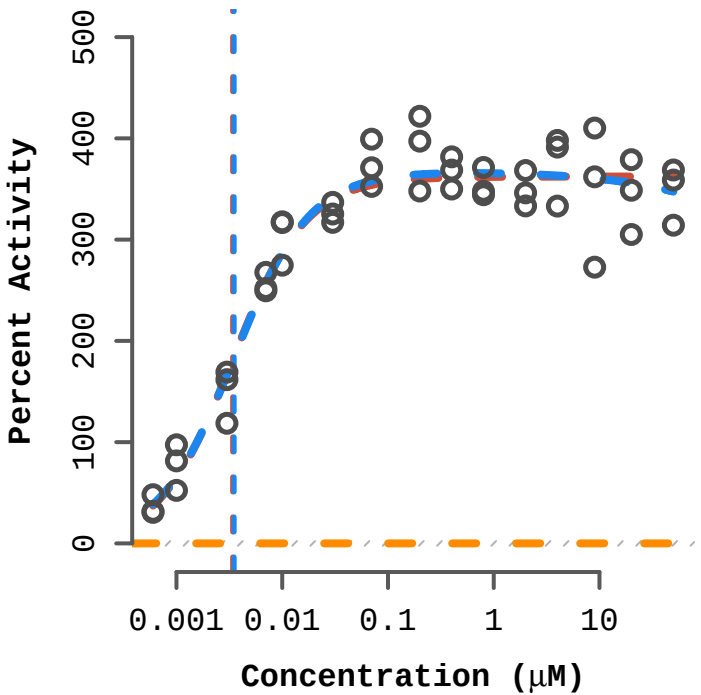
	tp	ga	gw
val:	379	-1.83	0.863
sd:	7.91	0.0632	0.0835

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	385	-1.81	0.833	2.59	1.48
sd:	12.5	0.0761	0.0905	1.88	3.21

	CNST	HILL	GNLS
AIC:	648.94	447.85	450.99
PROB:	0	0.83	0.17
RMSE:	292.49	31.56	31.4

MAX_MEAN: 383 **MAX_MED:** 404 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluocinonide
CHID: 45307 CASRN: 356-12-7
SPID(S): Tox21_110438_1
M4ID: 12484357

HILL MODEL (in red):

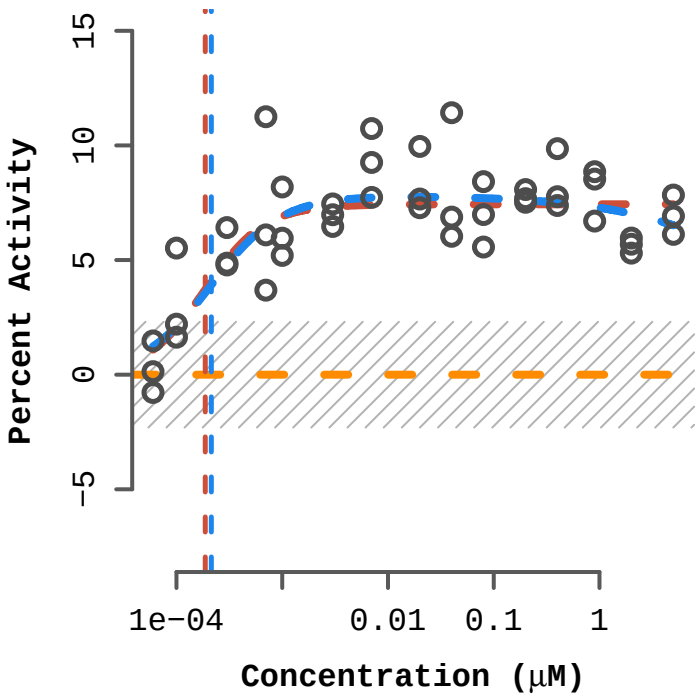
	tp	ga	gw
val:	362	-2.47	1.25
sd:	5.32	0.0357	0.11

GAIN-LOSS MODEL (in blue):

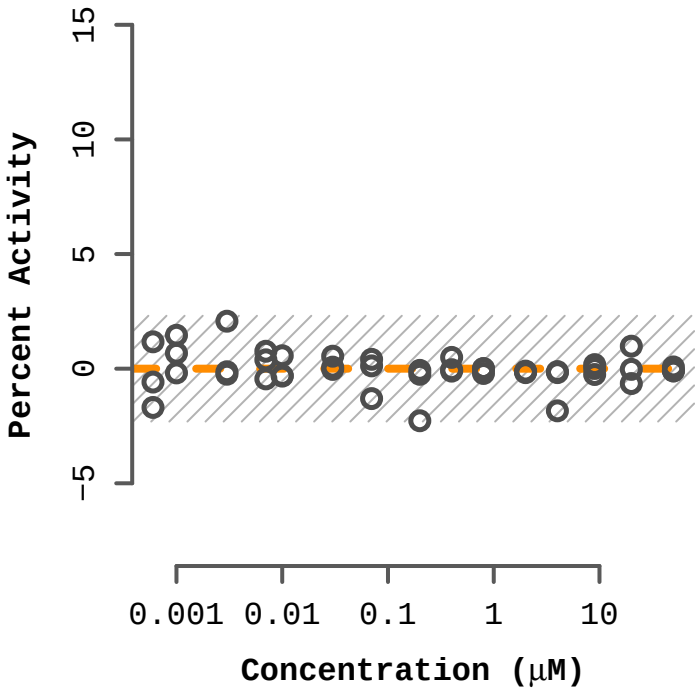
	tp	ga	gw	la	lw
val:	368	-2.45	1.21	3.7	0.616
sd:	14.1	0.0472	0.125	3.9	1.33

	CNST	HILL	GNLS
AIC:	656.5	435.24	437.95
PROB:	0	0.79	0.21
RMSE:	313.78	28.41	27.56

MAX_MEAN: 389 MAX_MED: 397 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hecogenin
CHID:    45310   CASRN: 467-55-0
SPID(S): Tox21_110443_1
M4ID:    12484352

HILL MODEL (in red):
      tp       ga       gw
val:  7.43     -3.73    1.54
sd:   0.276    0.0985   0.477

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.82     -3.67    1.32     1.83     0.616
sd:   0.555    0.123    0.45     1.28     0.661

      CNST        HILL        GNLS
AIC:  314.76      178.95      180.62
PROB: 0           0.7         0.3
RMSE: 7.07        1.65        1.6

MAX_MEAN: 9.24      MAX_MED: 9.26      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

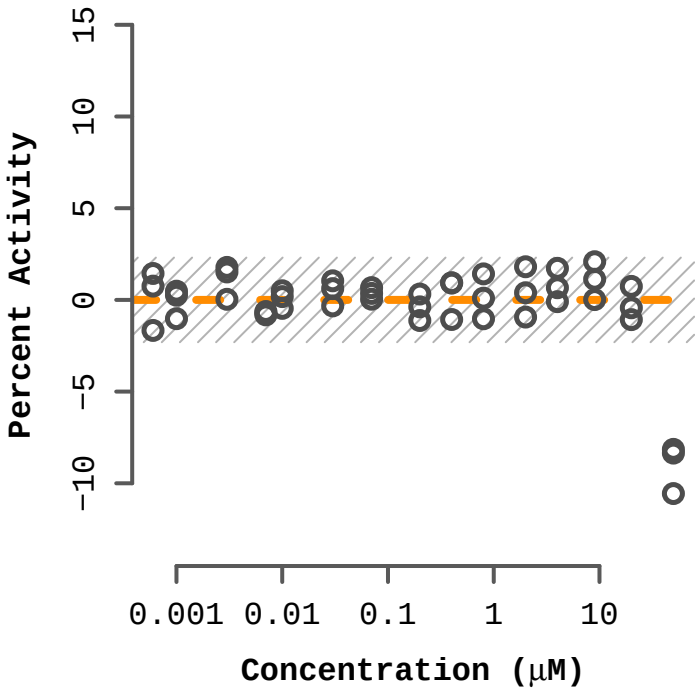
NAME: alpha-Santonin
CHID: 45312 **CASRN:** 481-06-1
SPID(S): Tox21_110445_1
M4ID: 12484350

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.651 **MAX_MED:** 0.675 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

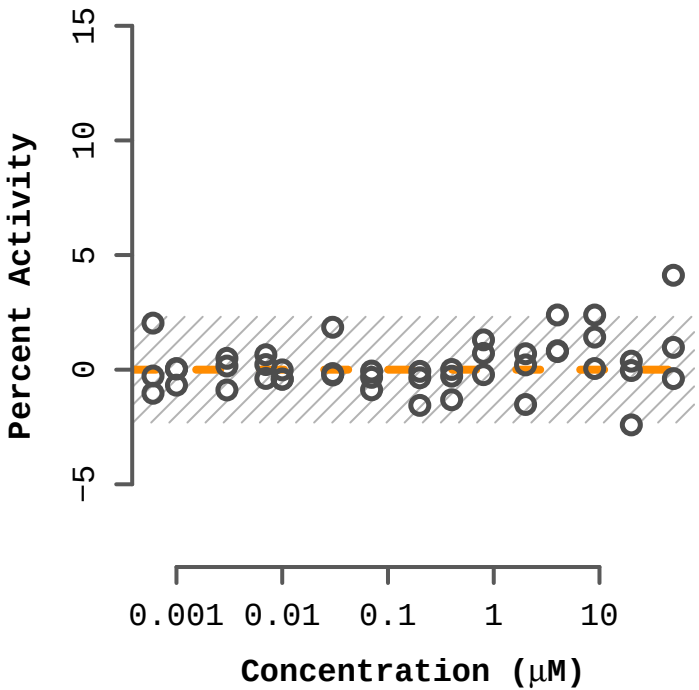
NAME: Trimipramine maleate
CHID: 45315 **CASRN:** 521-78-8
SPID(S): Tox21_110449_1
M4ID: 12484347

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.66	NA	NA
PROB:	1	NA	NA
RMSE:	2.52	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

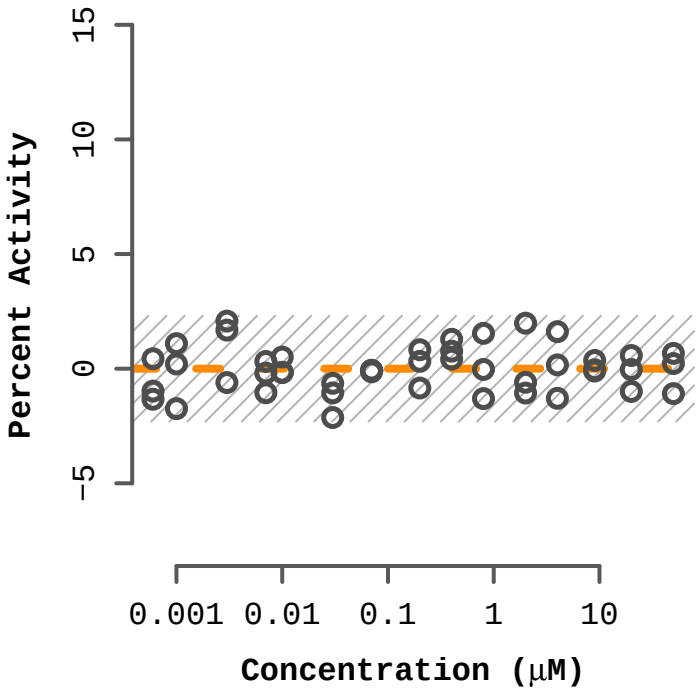
NAME: Tetrahydrozoline hydrochloride
CHID: 45316 **CASRN:** 522-48-5
SPID(S): Tox21_110450_1
M4ID: 12484346

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

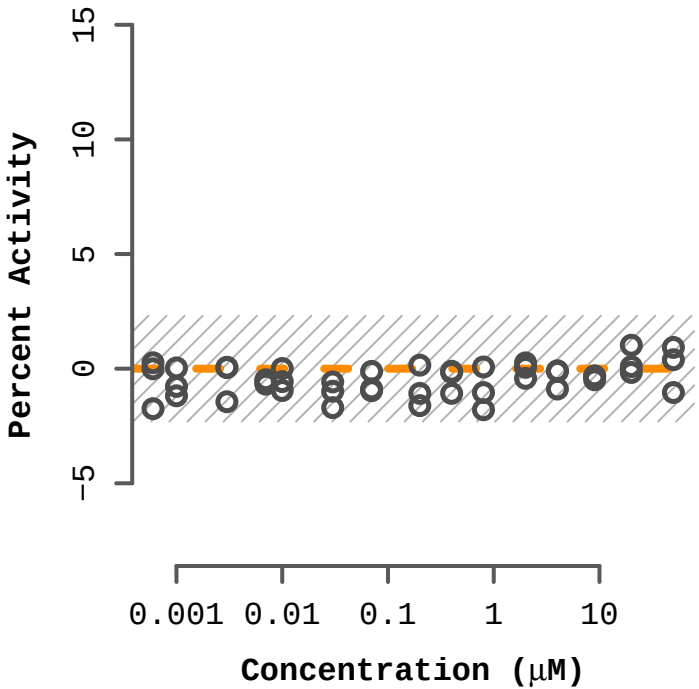
NAME: Amylocaine hydrochloride
CHID: 45320 CASRN: 532-59-2
SPID(S): Tox21_110455_1
M4ID: 12484342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

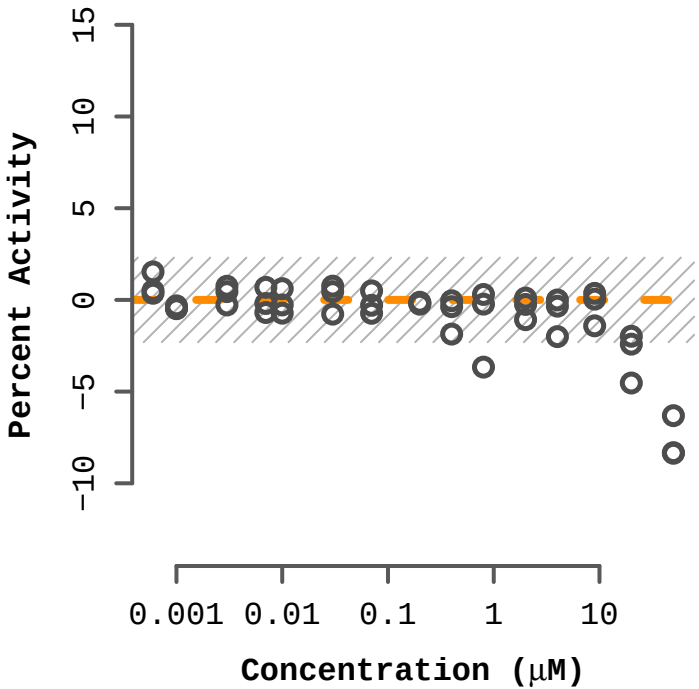
NAME: Hexylcaine hydrochloride
CHID: 45321 **CASRN:** 532-76-3
SPID(S): Tox21_110456_1
M4ID: 12484341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.318 **MAX_MED:** 0.394 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

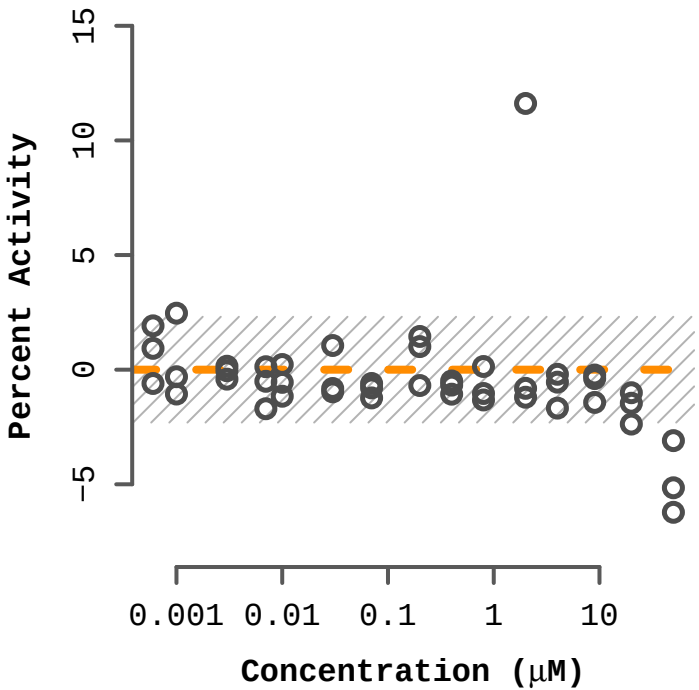
NAME: Dyclonine hydrochloride
CHID: 45323 CASRN: 536-43-6
SPID(S): Tox21_110459_1
M4ID: 12484339

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.81	NA	NA
PROB:	1	NA	NA
RMSE:	2.32	NA	NA

MAX_MEAN: 0.799 **MAX_MED:** 0.506 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

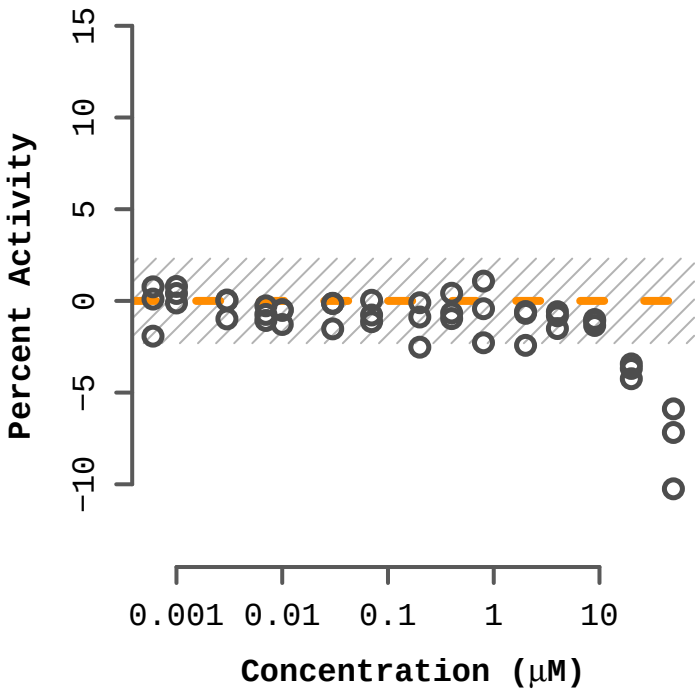
NAME: Diperodon hydrochloride
CHID: 45324 **CASRN:** 537-12-2
SPID(S): Tox21_110460_1
M4ID: 12484338

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 3.2 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

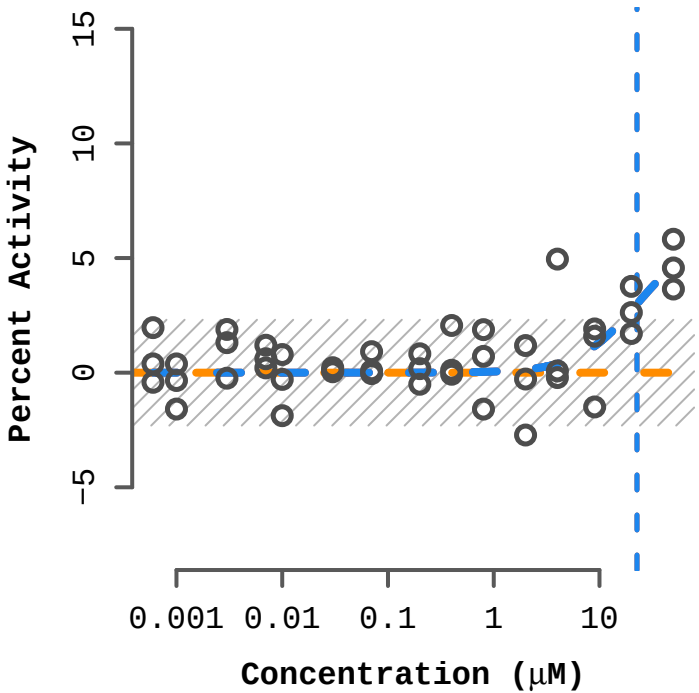
NAME: Thonzonium bromide
CHID: 45326 **CASRN:** 553-08-2
SPID(S): Tox21_110463_1
M4ID: 12484336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.48	NA	NA

MAX_MEAN: 0.361 **MAX_MED:** 0.406 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoxsuprine hydrochloride
CHID: 45328 CASRN: 579-56-6
SPID(S): Tox21_110467_1
M4ID: 12484333

HILL MODEL (in red):

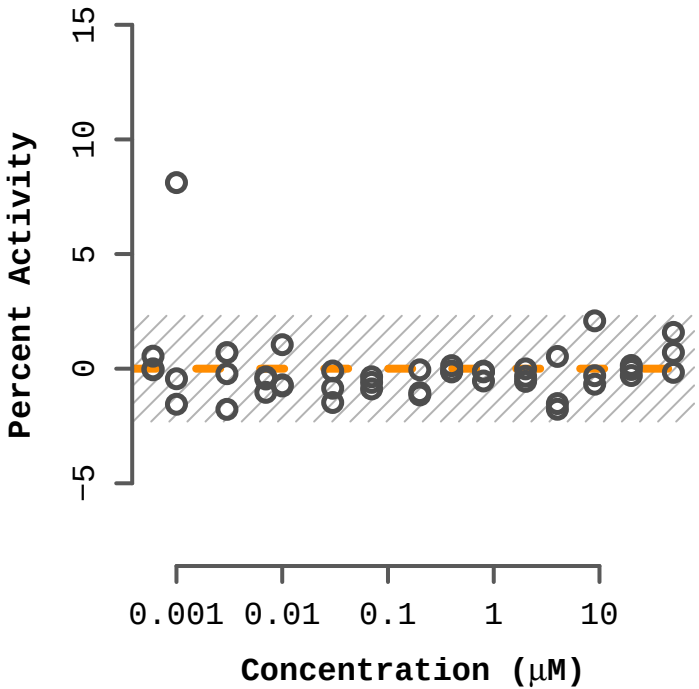
	tp	ga	gw
val:	5.99	1.35	1.55
sd:	3.59	0.43	1.16

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.99	1.35	1.55	2.8	6.11
sd:	3.59	0.43	1.16	1740	9650

	CNST	HILL	GNLS
AIC:	183.05	153.07	157.07
PROB:	0	0.88	0.12
RMSE:	1.92	1.28	1.28

MAX_MEAN: 4.68 **MAX_MED:** 4.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

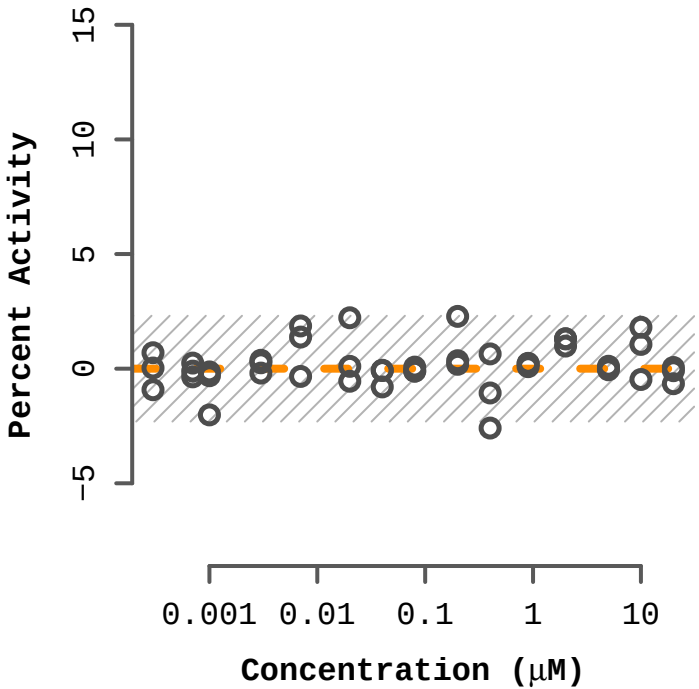
NAME: Meprylcaine hydrochloride
CHID: 45341 **CASRN:** 956-03-6
SPID(S): Tox21_110489_1
M4ID: 12484319

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

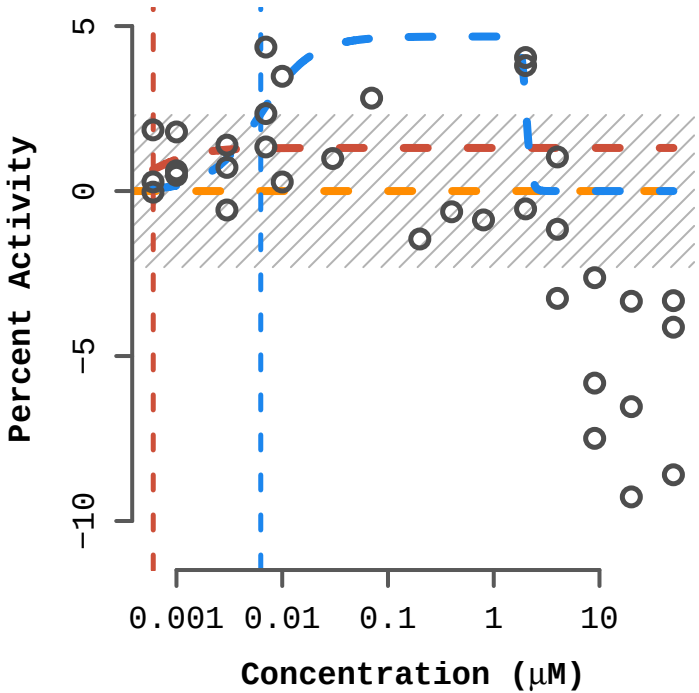
NAME: 7-Aminocephalosporanic acid
CHID: 45342 **CASRN:** 957-68-6
SPID(S): Tox21_110490_1
M4ID: 12484318

HILL MODEL: Not applicable.

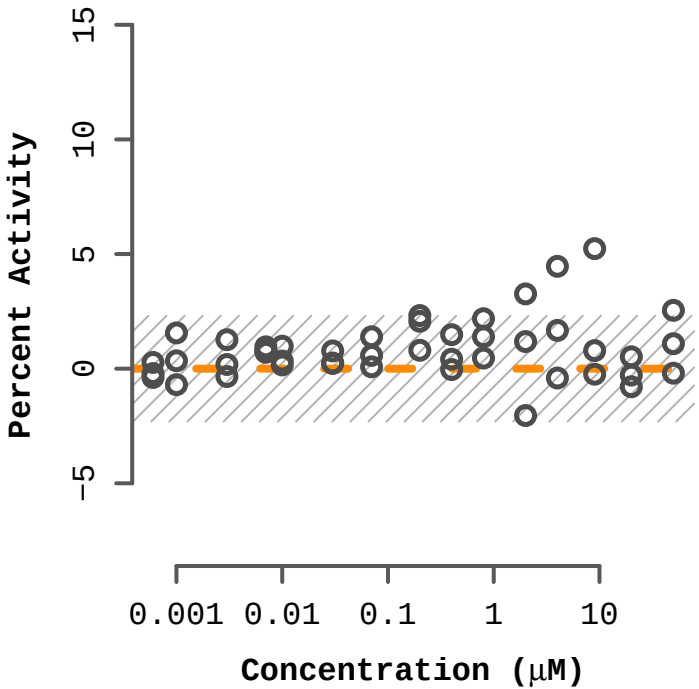
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.38 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Nifuroxazide
CHID:    45343   CASRN: 965-52-6
SPID(S): Tox21_110491_1
M4ID:    12484317

HILL MODEL (in red):
      tp       ga       gw
val:  1.31     -3.22    1.98
sd:   0.754    1.13     6.41

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.68     -2.2     1.79     0.308    17.8
sd:   0.963    0.236    3.36     0.169    404

      CNST        HILL        GNLS
AIC:  266.22      268.85      249.49
PROB: 0           0           1
RMSE: 4.34        4.28        3.45

MAX_MEAN: 4.83      MAX_MED: 5.73      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

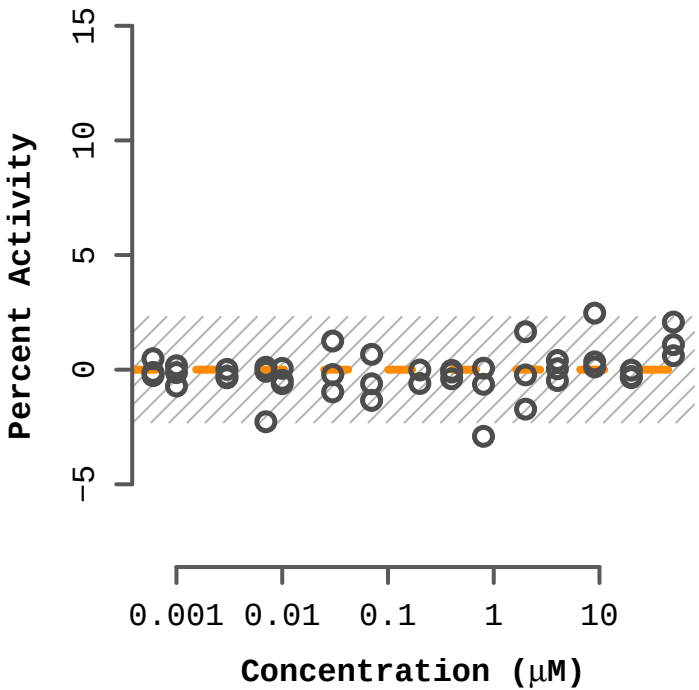
NAME: Ethambutol dihydrochloride
CHID: 45345 CASRN: 1070-11-7
SPID(S): Tox21_110494_1
M4ID: 12484315

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

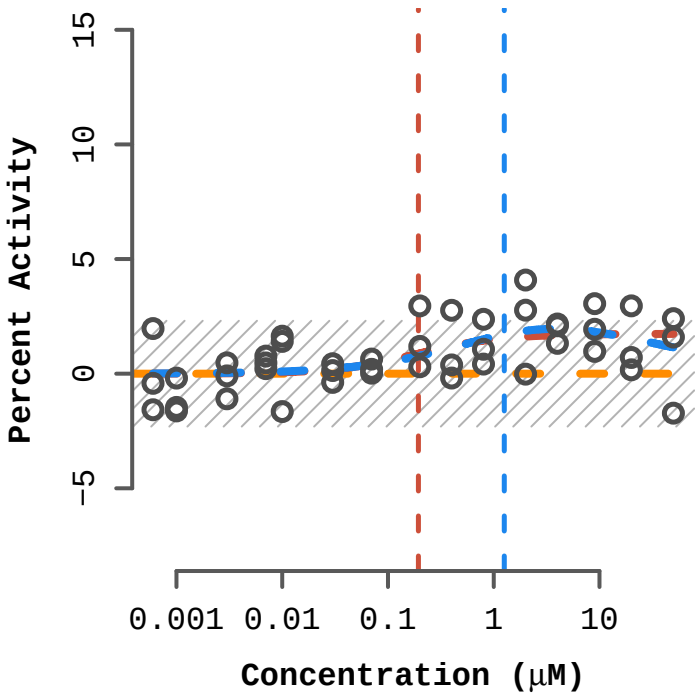
NAME: Meticrane
CHID: 45346 **CASRN:** 1084-65-7
SPID(S): Tox21_110495_1
M4ID: 12484314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethopropazine hydrochloride
CHID: 45347 CASRN: 1094-08-2
SPID(S): Tox21_110496_1
M4ID: 12484313

HILL MODEL (in red):

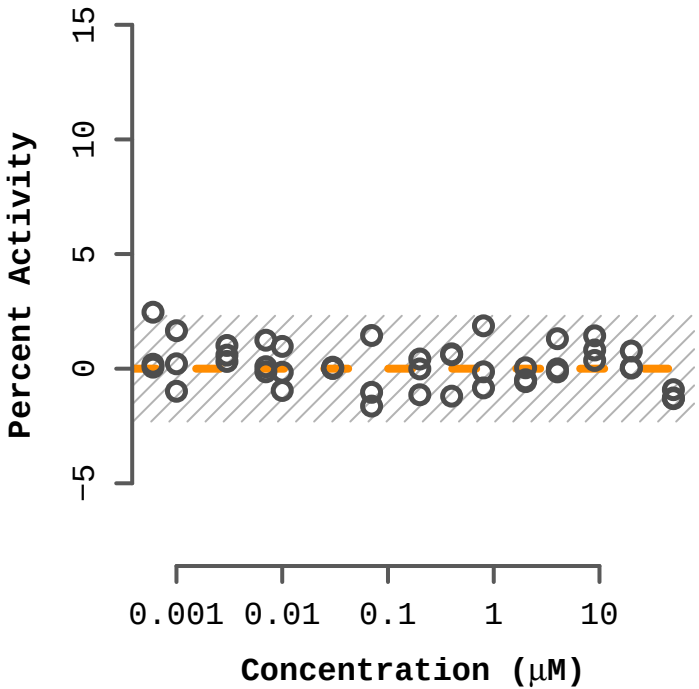
	tp	ga	gw
val:	1.74	−0.712	1.12
sd:	0.362	0.422	0.865

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.9	0.0998	0.806	0.784	0.531
sd:	15.6	1.63	0.627	4.51	1.04

	CNST	HILL	GNLS
AIC:	175.25	153.43	156.46
PROB:	0	0.82	0.18
RMSE:	1.61	1.19	1.16

MAX_MEAN: 2.28 **MAX_MED:** 2.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

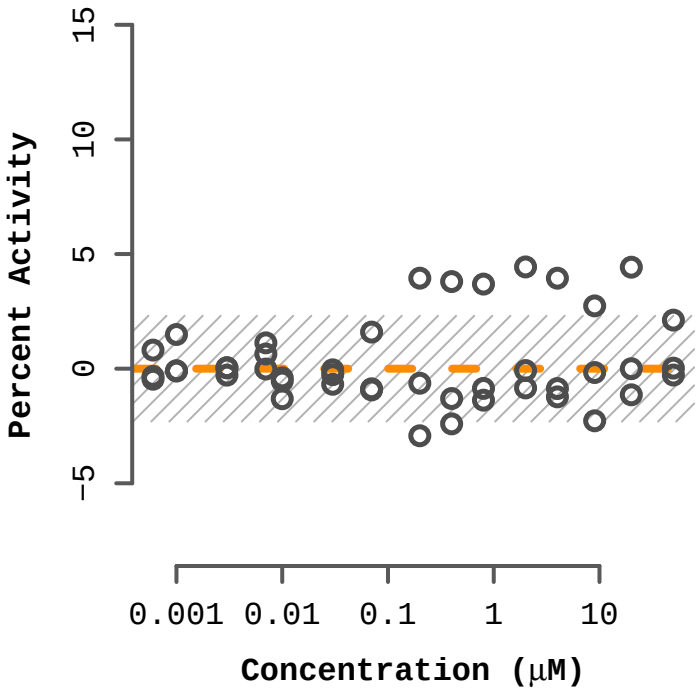
NAME: Meclozine dihydrochloride
CHID: 45348 **CASRN:** 1104-22-9
SPID(S): Tox21_110497_1
M4ID: 12484312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.909 **MAX_MED:** 0.816 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

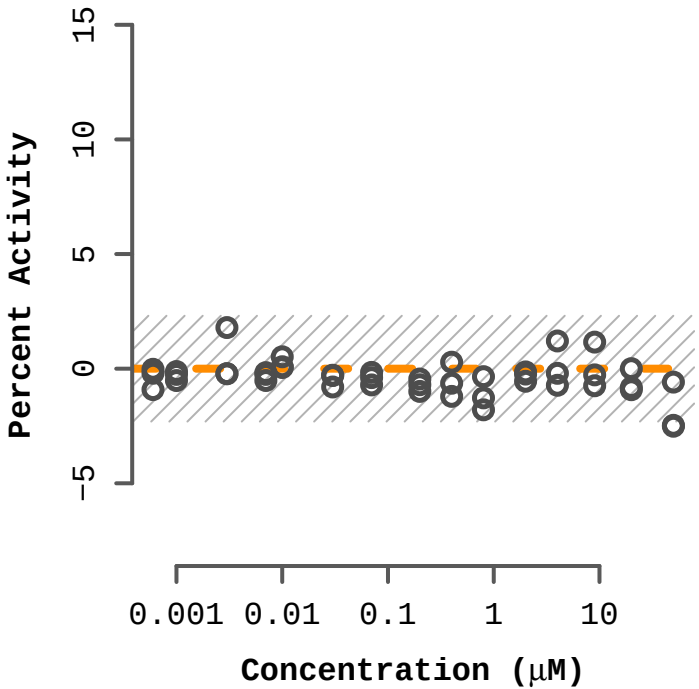
NAME: Sulfamonomethoxine
CHID: 45351 **CASRN:** 1220-83-3
SPID(S): Tox21_110502_1
M4ID: 12484309

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 0.642 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

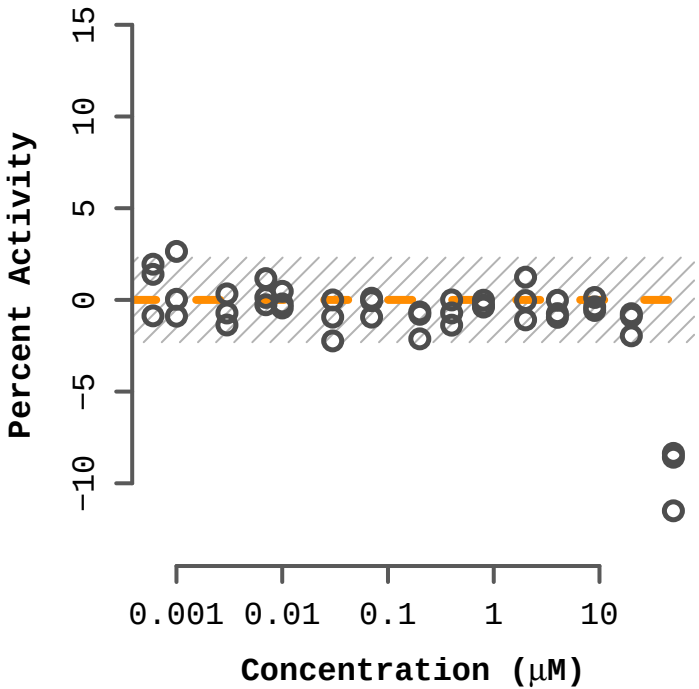
NAME: Procyclidine hydrochloride
CHID: 45357 **CASRN:** 1508-76-5
SPID(S): Tox21_110508_1
M4ID: 12484308

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.453 **MAX_MED:** 0.0869 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

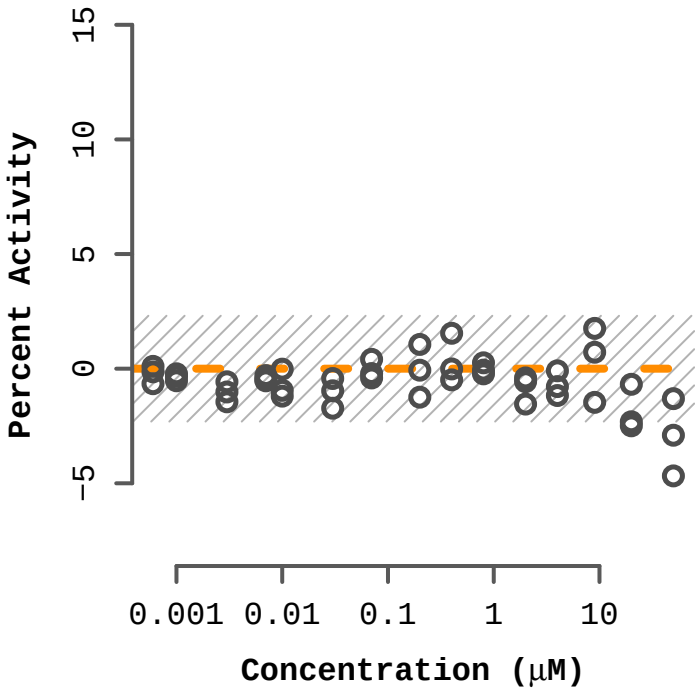
NAME: Metixene hydrochloride
CHID: 45359 **CASRN:** 1553-34-0
SPID(S): Tox21_110510_1
M4ID: 12484306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.13	NA	NA
PROB:	1	NA	NA
RMSE:	2.66	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

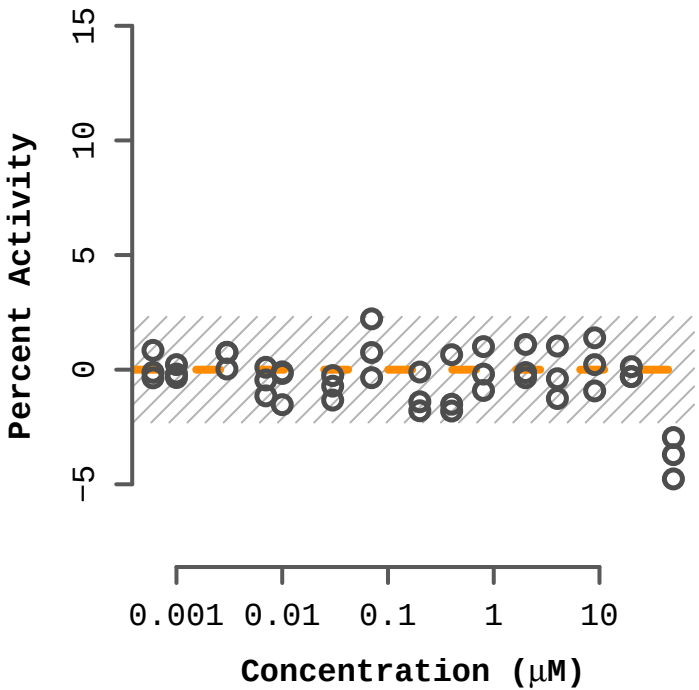
NAME: Azaperone
CHID: 45361 **CASRN:** 1649-18-9
SPID(S): Tox21_110512_1
M4ID: 12484305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.349 **MAX_MED:** 0.717 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

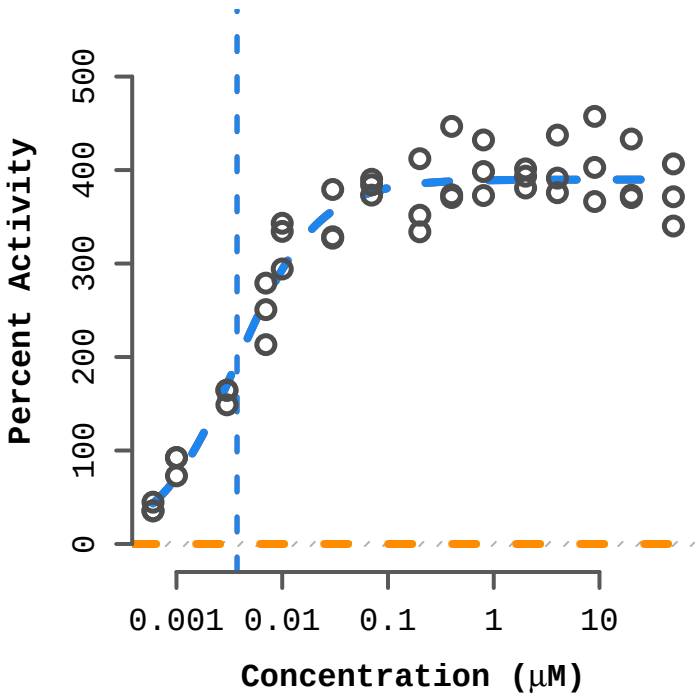
NAME: Benperidol
CHID: 45364 **CASRN:** 2062-84-2
SPID(S): Tox21_110517_1
M4ID: 12484301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.874 **MAX_MED:** 0.756 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flumethasone
CHID: 45365 CASRN: 2135-17-3
SPID(S): Tox21_110518_1
M4ID: 12484300

HILL MODEL (in red):

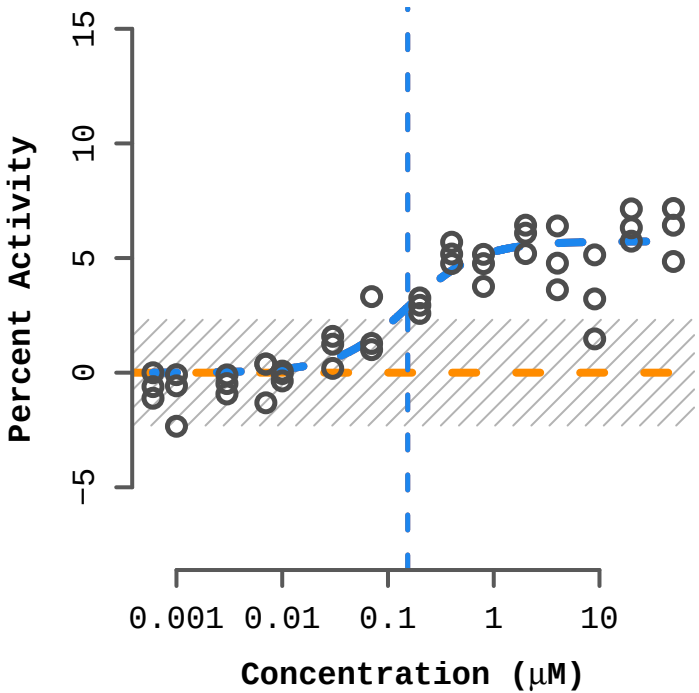
	tp	ga	gw
val:	390	-2.43	1.14
sd:	5.76	0.0384	0.104

GAIN-LOSS MODEL (in blue):

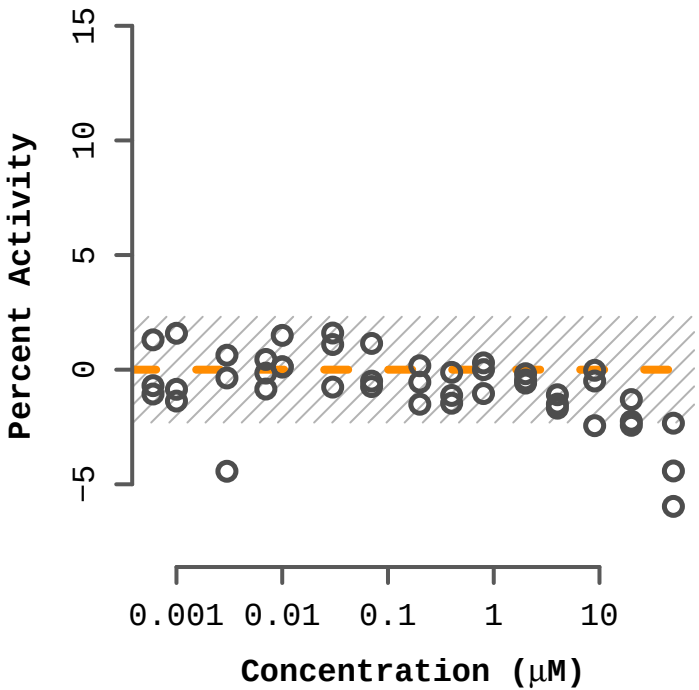
	tp	ga	gw	la	lw
val:	390	-2.43	1.14	3.69	10.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	662.83	437.61	441.61
PROB:	0	0.88	0.12
RMSE:	336.85	27.96	27.96

MAX_MEAN: 409 MAX_MED: 403 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Nifenazone
CHID:    45366   CASRN: 2139-47-1
SPID(S): Tox21_110519_1
M4ID:    12484299

HILL MODEL (in red):
      tp       ga       gw
val:  5.73     -0.813   1.31
sd:   0.32     0.0959   0.302

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.73     -0.813   1.31     2.89     7.35
sd:   0.32     0.0959   0.302    1670     10300

      CNST       HILL       GNLS
AIC:  255.25     141.33     145.33
PROB: 0          0.88       0.12
RMSE: 3.83       1.13       1.13

MAX_MEAN: 6.4       MAX_MED: 6.43      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

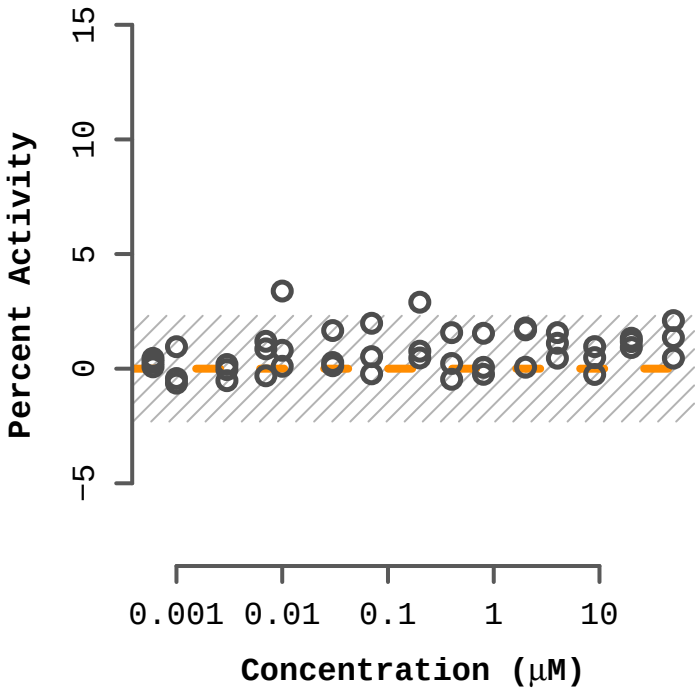
NAME: Bufexamac
CHID: 45368 **CASRN:** 2438-72-4
SPID(S): Tox21_110522_1
M4ID: 12484297

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 0.646 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

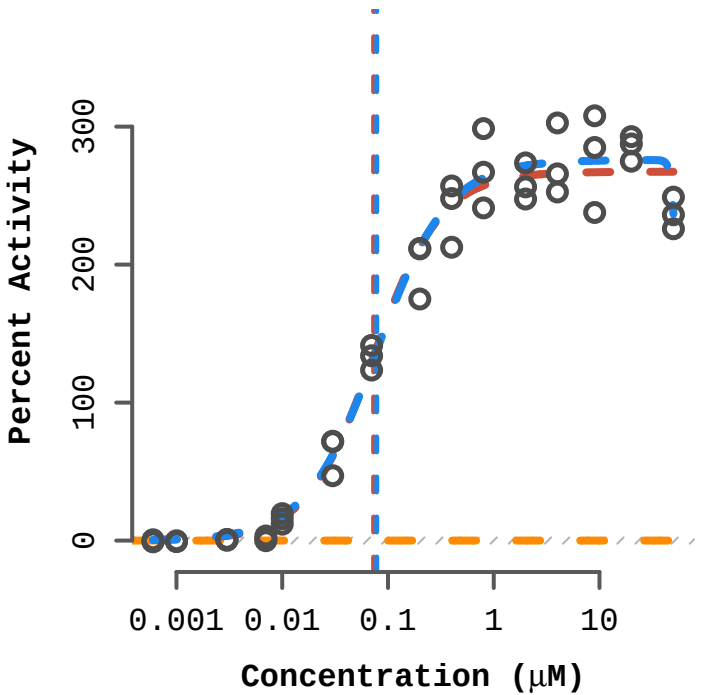
NAME: Methyldopate hydrochloride
CHID: 45370 **CASRN:** 2508-79-4
SPID(S): Tox21_110525_1
M4ID: 12484294

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Medrysone
CHID: 45371 CASRN: 2668-66-8
SPID(S): Tox21_110526_1
M4ID: 12484293

HILL MODEL (in red):

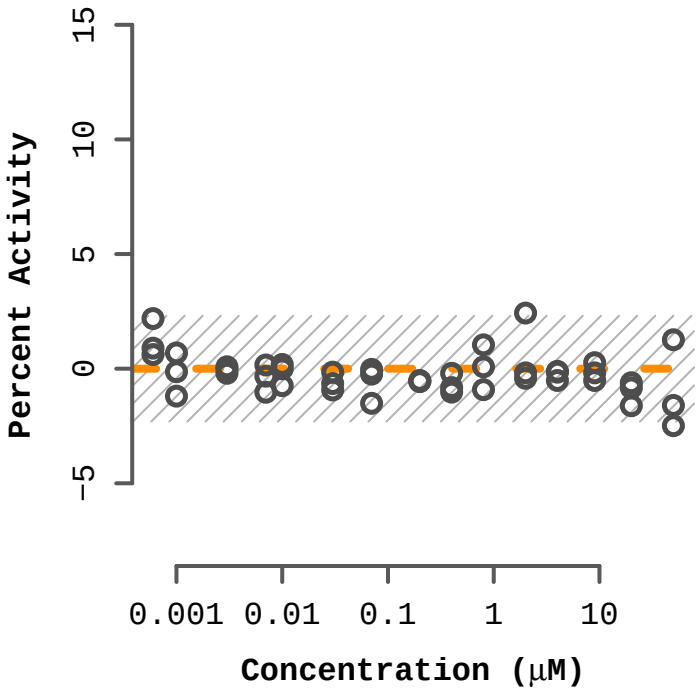
	tp	ga	gw
val:	267	-1.14	1.36
sd:	5.7	0.035	0.113

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	276	-1.11	1.29	1.74	17.9
sd:	5.29	0.032	0.092	0.00667	2.93

	CNST	HILL	GNLS
AIC:	608.94	394.2	384.27
PROB:	0	0.01	0.99
RMSE:	191.56	17.97	15.56

MAX_MEAN: 285 MAX_MED: 287 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

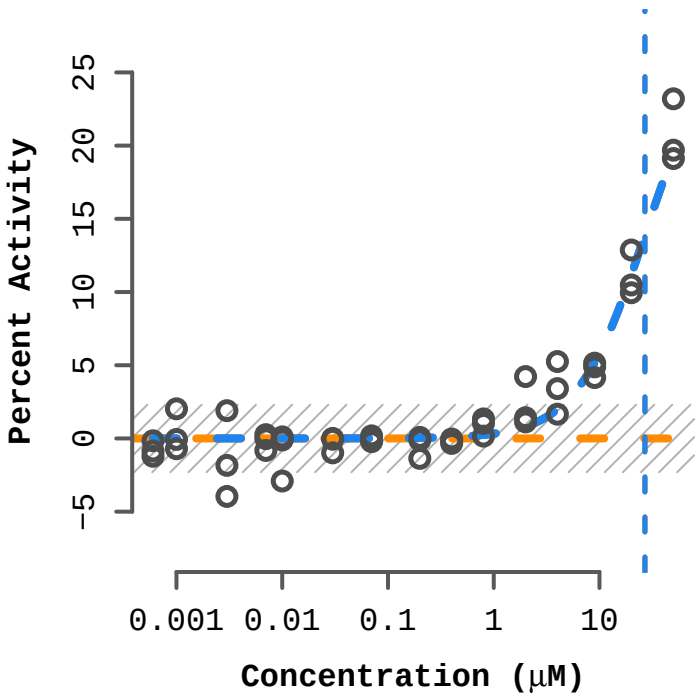
NAME: Mebeverine hydrochloride
CHID: 45372 CASRN: 2753-45-9
SPID(S): Tox21_110527_1
M4ID: 12484292

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.896 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethisoquin hydrochloride
CHID: 45373 **CASRN:** 2773-92-4
SPID(S): Tox21_110528_1
M4ID: 12484291

HILL MODEL (in red):

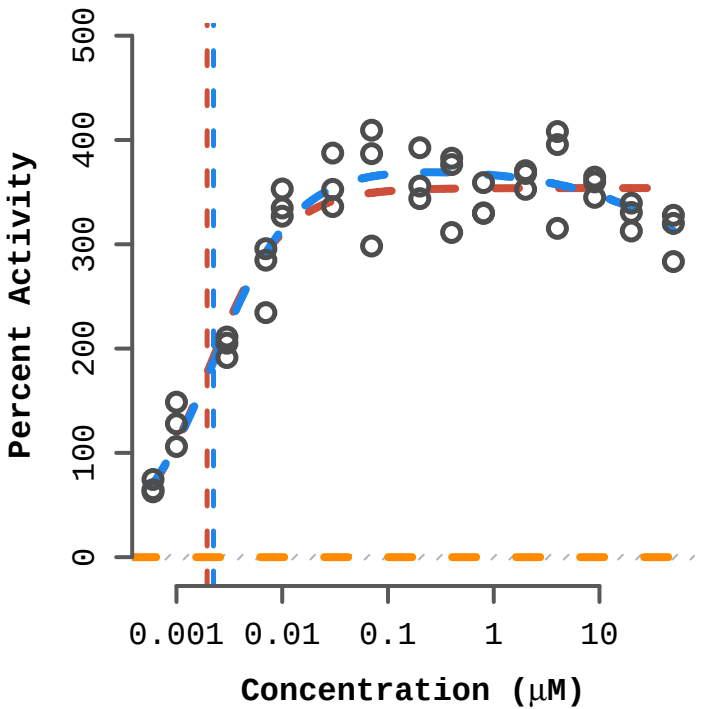
	tp	ga	gw
val:	27.8	1.43	1.35
sd:	3.86	0.108	0.181

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27.8	1.43	1.35	3.37	5.45
sd:	3.87	0.108	0.182	2110	6860

	CNST	HILL	GNLS
AIC:	269.29	158.99	162.99
PROB:	0	0.88	0.12
RMSE:	6.4	1.41	1.41

MAX_MEAN: 20.7 **MAX_MED:** 19.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Halcinonide
CHID: 45375 CASRN: 3093-35-4
SPID(S): Tox21_110530_1
M4ID: 12484289

HILL MODEL (in red):

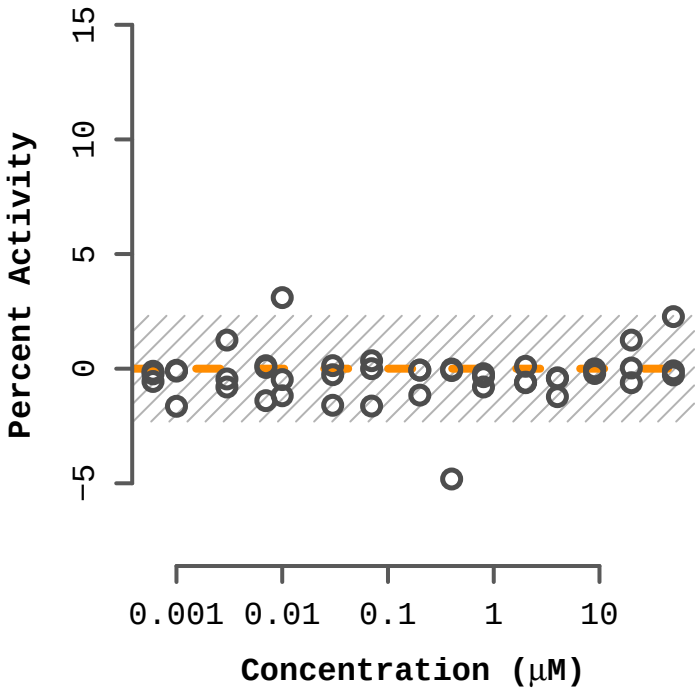
	tp	ga	gw
val:	354	-2.71	1.21
sd:	6.11	0.0455	0.117

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	375	-2.65	1.11	2.95	0.559
sd:	20.1	0.0622	0.117	1.26	0.58

	CNST	HILL	GNLS
AIC:	657.43	446.36	437.37
PROB:	0	0.01	0.99
RMSE:	315.94	30.3	26.88

MAX_MEAN: 373 MAX_MED: 396 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

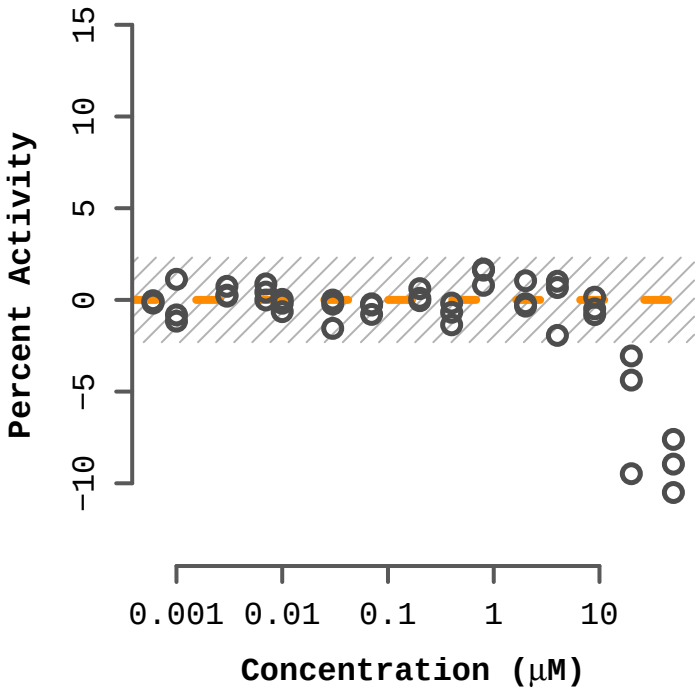
NAME: Moroxidine hydrochloride
CHID: 45376 **CASRN:** 3160-91-6
SPID(S): Tox21_110532_1
M4ID: 12484287

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 0.054 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

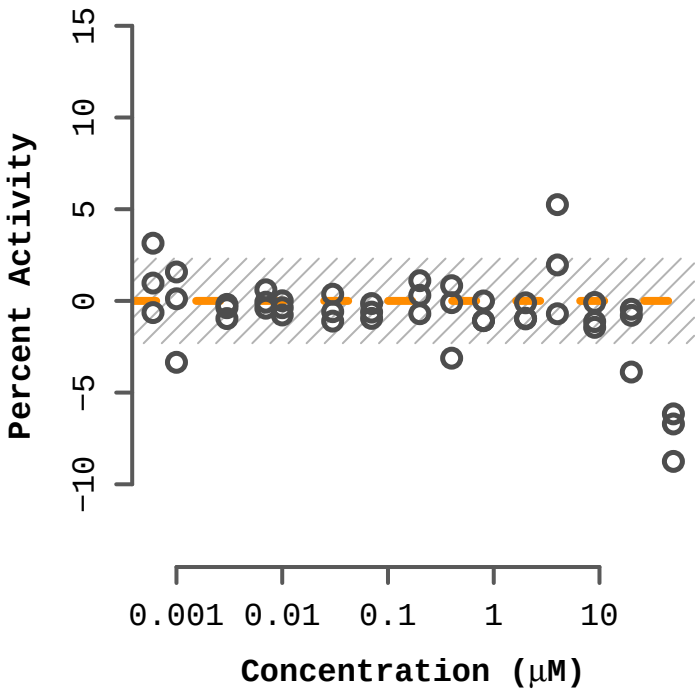
NAME: Lidoflazine
CHID: 45377 **CASRN:** 3416-26-0
SPID(S): Tox21_110533_1
M4ID: 12484286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.87	NA	NA
PROB:	1	NA	NA
RMSE:	2.95	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

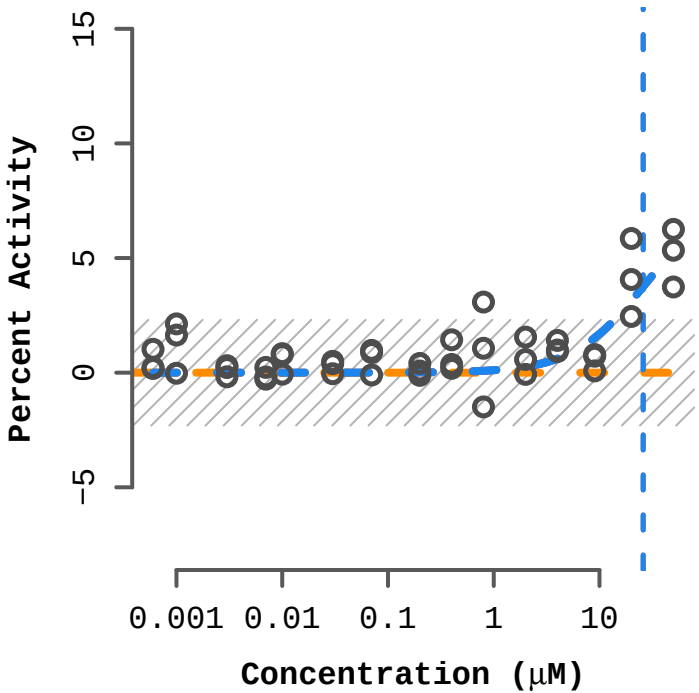
NAME: Furaltadone hydrochloride
CHID: 45380 CASRN: 3759-92-0
SPID(S): Tox21_110538_1
M4ID: 12484282

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.19	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 2.17 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methacycline hydrochloride
CHID: 45382 CASRN: 3963-95-9
SPID(S): Tox21_110542_1
M4ID: 12484278

HILL MODEL (in red):

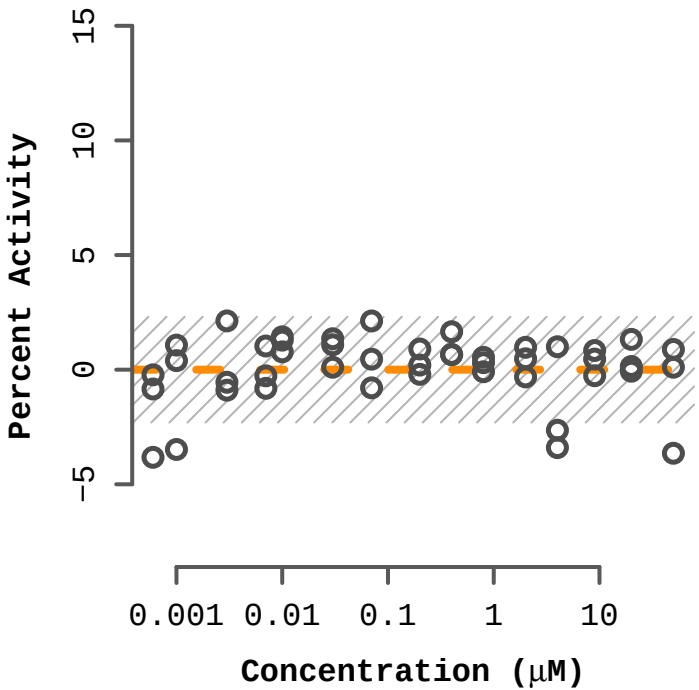
	tp	ga	gw
val:	7.5	1.41	1.3
sd:	4.78	0.508	1.08

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.5	1.41	1.3	3.39	3.98
sd:	4.78	0.508	1.08	1140	2490

	CNST	HILL	GNLS
AIC:	175.94	132.51	136.51
PROB:	0	0.88	0.12
RMSE:	1.96	1	1

MAX_MEAN: 5.11 **MAX_MED:** 5.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

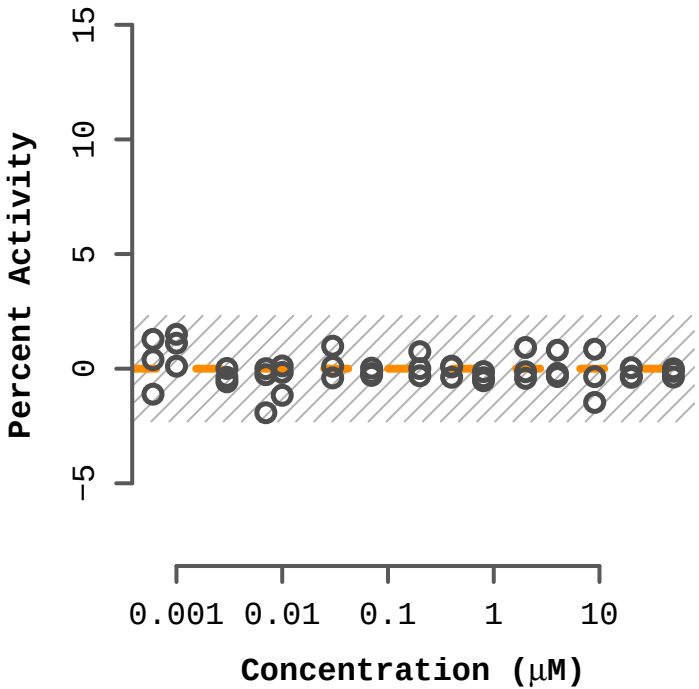
NAME: Bromopride
CHID: 45383 CASRN: 4093-35-0
SPID(S): Tox21_110543_1
M4ID: 12484277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.17 MAX_MED: 1.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

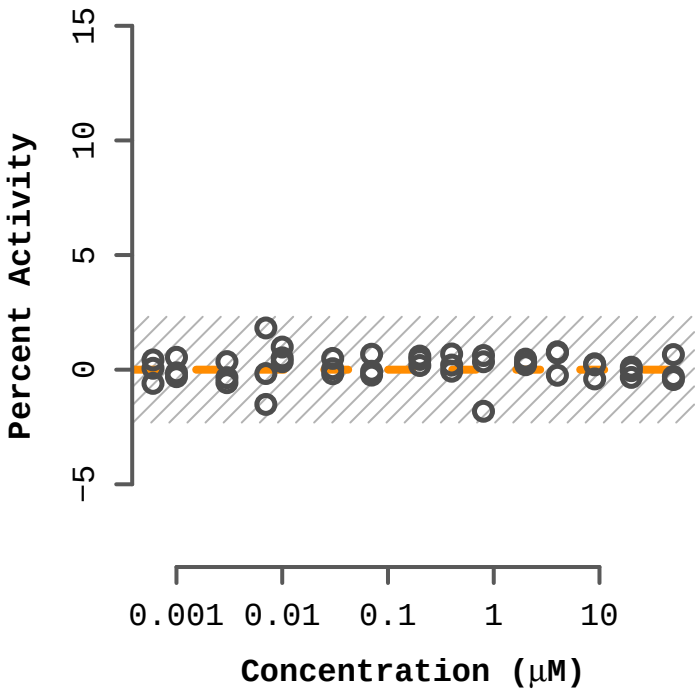
NAME: cis−Nanophine hydrochloride
CHID: 45386 **CASRN:** 5072−45−7
SPID(S): Tox21_110546_1
M4ID: 12484276

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.907 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

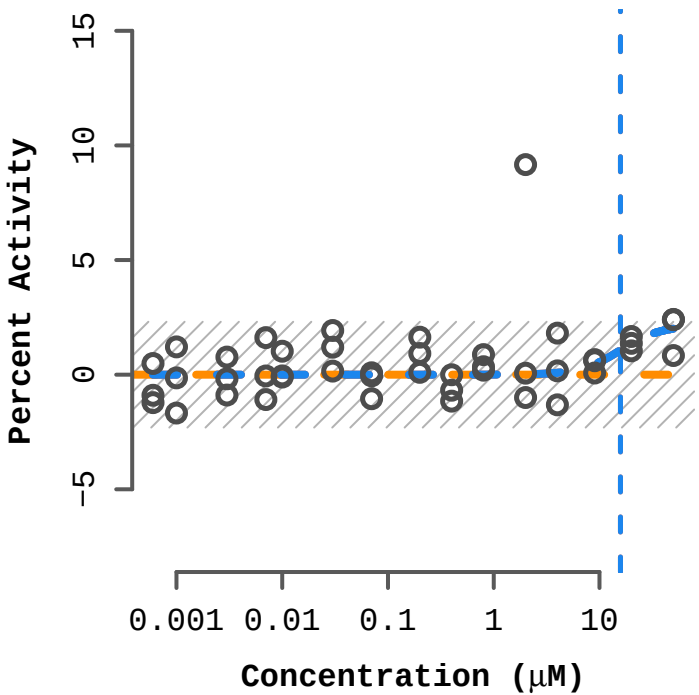
NAME: Cefalonium
CHID: 45388 **CASRN:** 5575-21-3
SPID(S): Tox21_110548_1
M4ID: 12484275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	81.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.619 **MAX_MED:** 0.728 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Felbinac
CHID: 45389 **CASRN:** 5728-52-9
SPID(S): Tox21_110549_1
M4ID: 12484274

HILL MODEL (in red):

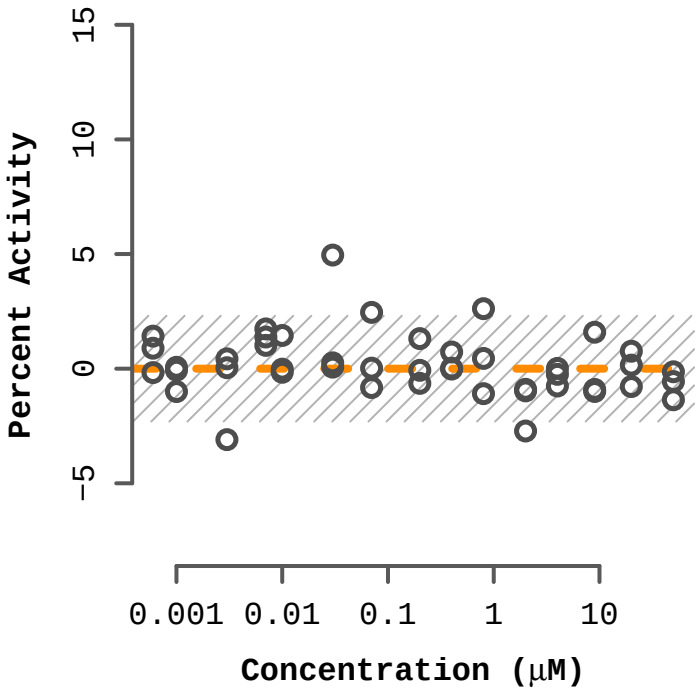
	tp	ga	gw
val:	2.14	1.2	2.33
sd:	0.868	0.236	2.15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.14	1.2	2.33	3.24	3.67
sd:	0.876	0.237	2.16	5860	14100

	CNST	HILL	GNLS
AIC:	154.45	143.54	147.54
PROB:	0	0.88	0.12
RMSE:	1.73	1.62	1.62

MAX_MEAN: 2.75 **MAX_MED:** 2.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

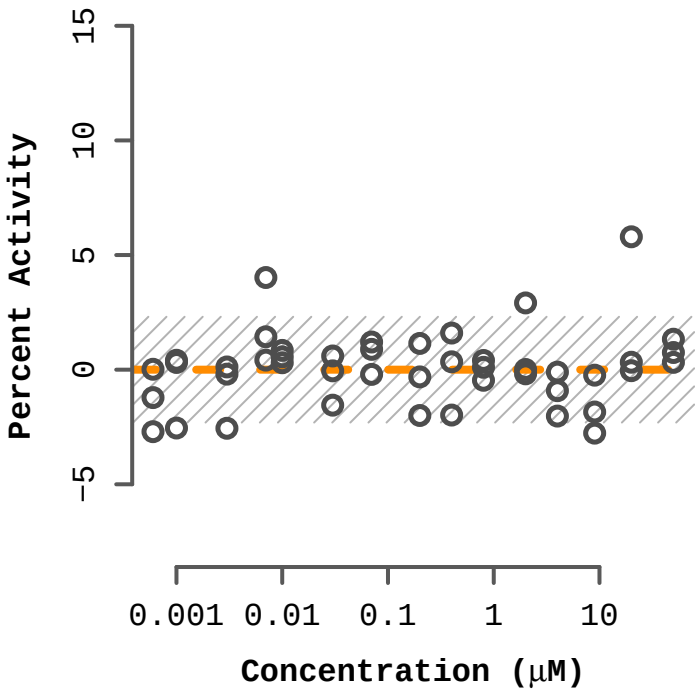
NAME: Cyclopentolate hydrochloride
CHID: 45390 **CASRN:** 5870-29-1
SPID(S): Tox21_110550_1
M4ID: 12484273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

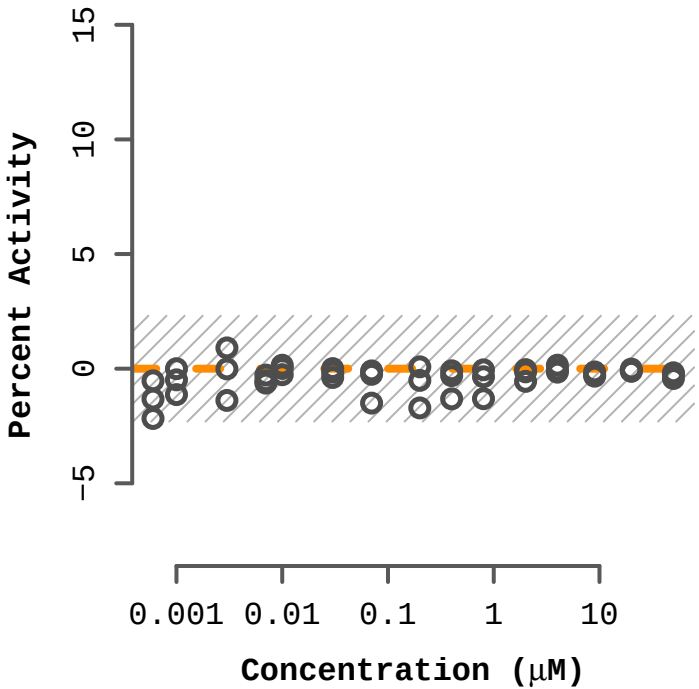
NAME: Orciprenaline sulfate
CHID: 45391 **CASRN:** 5874-97-5
SPID(S): Tox21_110551_1
M4ID: 12484272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.03 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

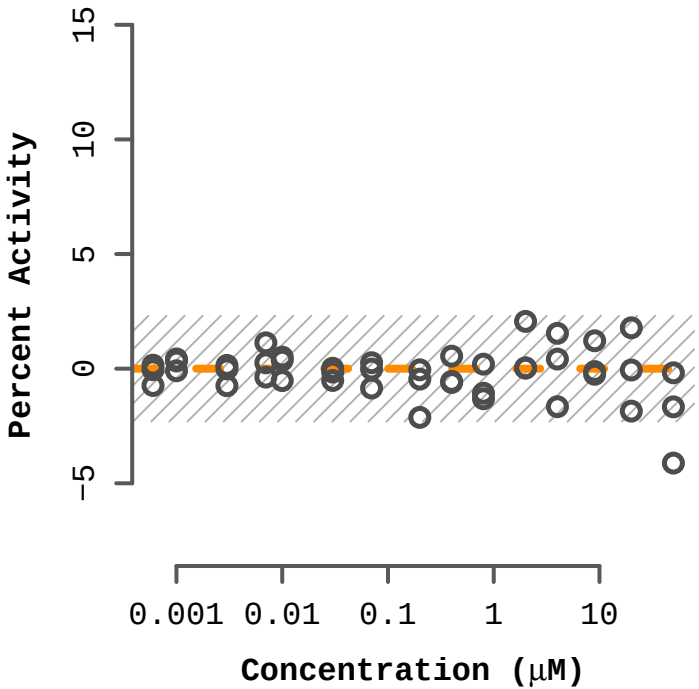
NAME: Hydrocotarnine hydrobromide
CHID: 45392 **CASRN:** 5985-00-2
SPID(S): Tox21_110552_1
M4ID: 12484271

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: −0.0171 **MAX_MED:** 0.0115 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

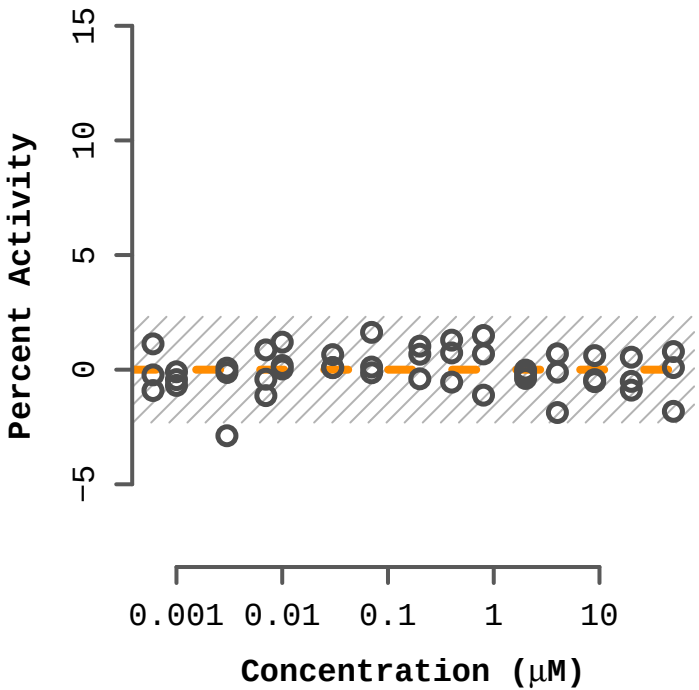
NAME: Benoxinate hydrochloride
CHID: 45393 **CASRN:** 5987-82-6
SPID(S): Tox21_110553_1
M4ID: 12484270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.708 **MAX_MED:** 0.421 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

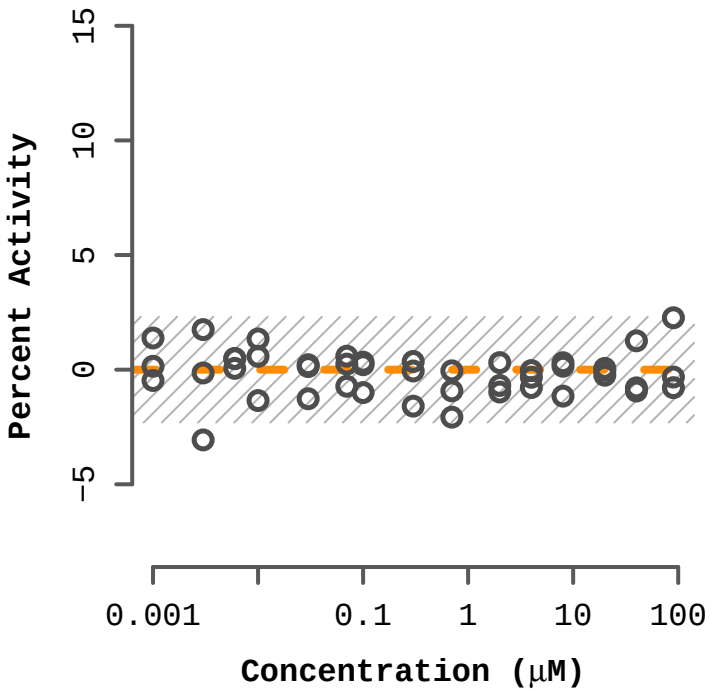
NAME: Salicylic acid dihydrogen phosphate
CHID: 45394 **CASRN:** 6064-83-1
SPID(S): Tox21_110554_1
M4ID: 12484269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.537 **MAX_MED:** 0.732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

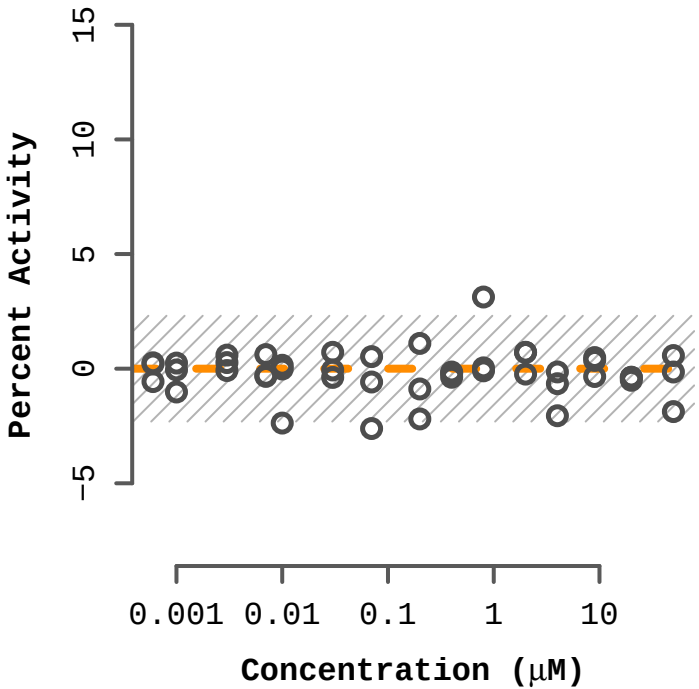
NAME: Ronidazole
CHID: 45400 CASRN: 7681-76-7
SPID(S): Tox21_303404
M4ID: 12475735

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.388 MAX_MED: 0.582 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

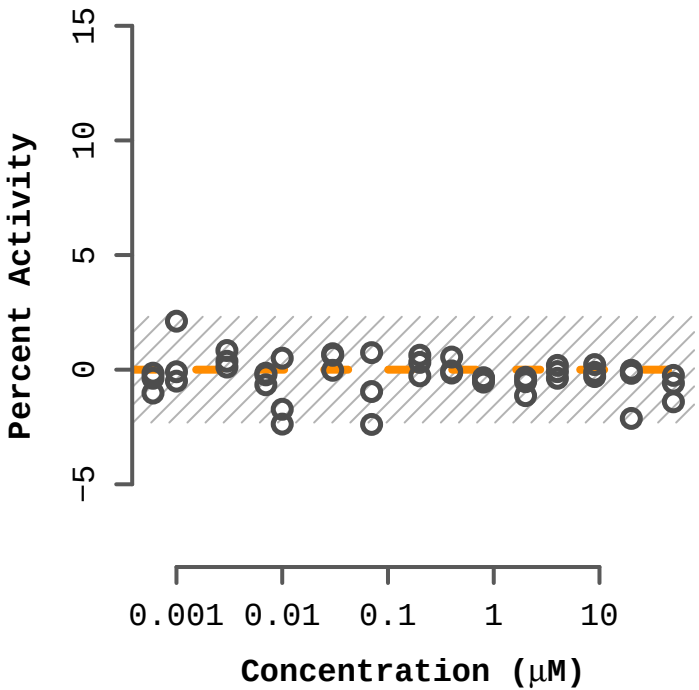
NAME: Ronidazole
CHID: 45400 **CASRN:** 7681-76-7
SPID(S): Tox21_110560_1
M4ID: 12484266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

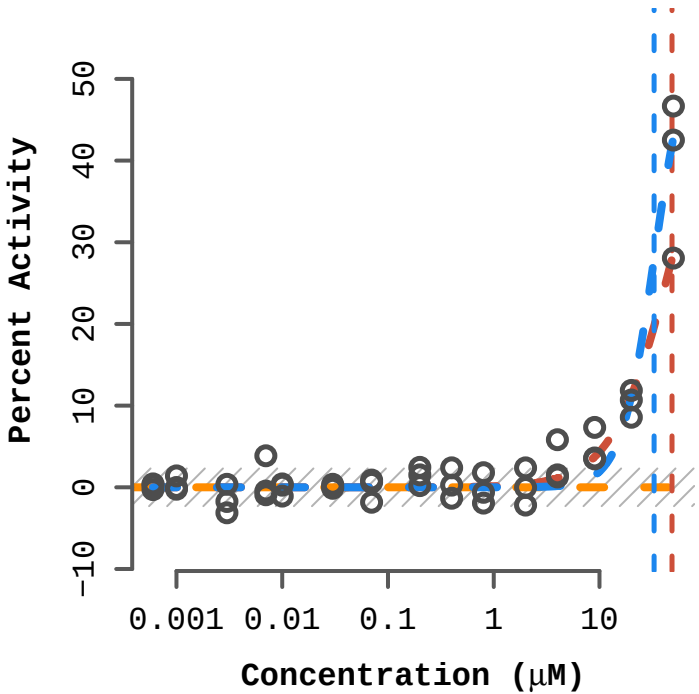
NAME: Doxycycline hydrochloride
CHID: 45405 CASRN: 10592-13-9
SPID(S): Tox21_110566_1
M4ID: 12484263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.509 **MAX_MED:** 0.628 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trimetazidine dihydrochloride
CHID: 45407 CASRN: 13171-25-0
SPID(S): Tox21_110568_1
M4ID: 12484262

HILL MODEL (in red):

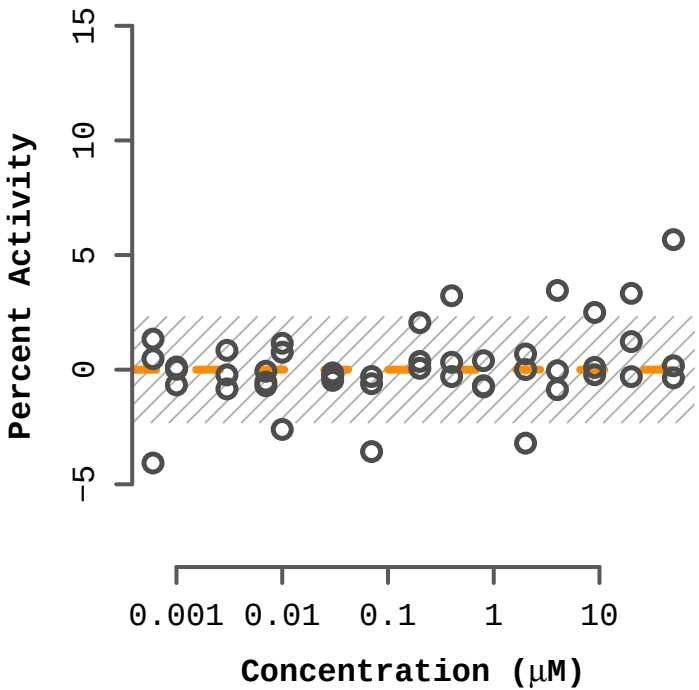
	tp	ga	gw
val:	56	1.69	1.57
sd:	16.4	0.161	0.24

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	56	1.52	2.8	3.69	4.32
sd:	9.69	0.0755	0.629	1730	3770

	CNST	HILL	GNLS
AIC:	285.99	210.63	211.96
PROB:	0	0.66	0.34
RMSE:	10.84	3.74	2.94

MAX_MEAN: 39.1 **MAX_MED:** 42.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

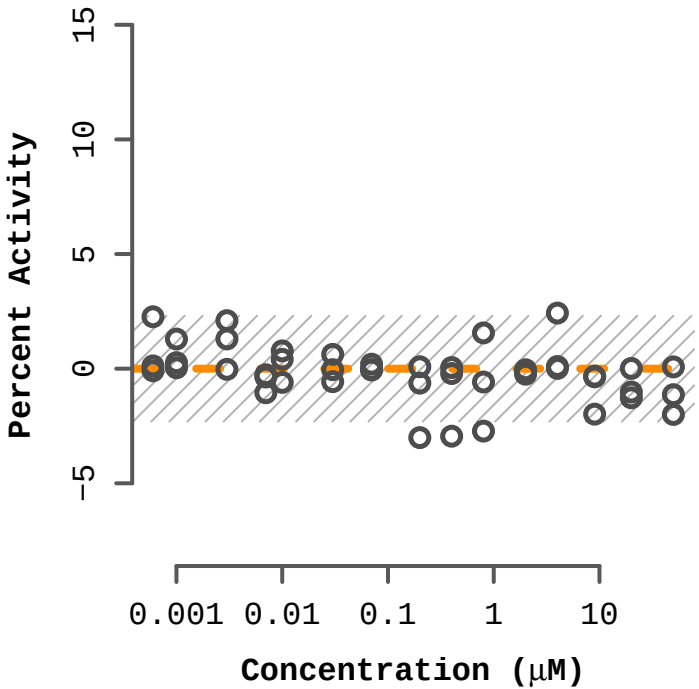
NAME: Tolfenamic acid
CHID: 45409 **CASRN:** 13710-19-5
SPID(S): Tox21_110570_1
M4ID: 12484261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

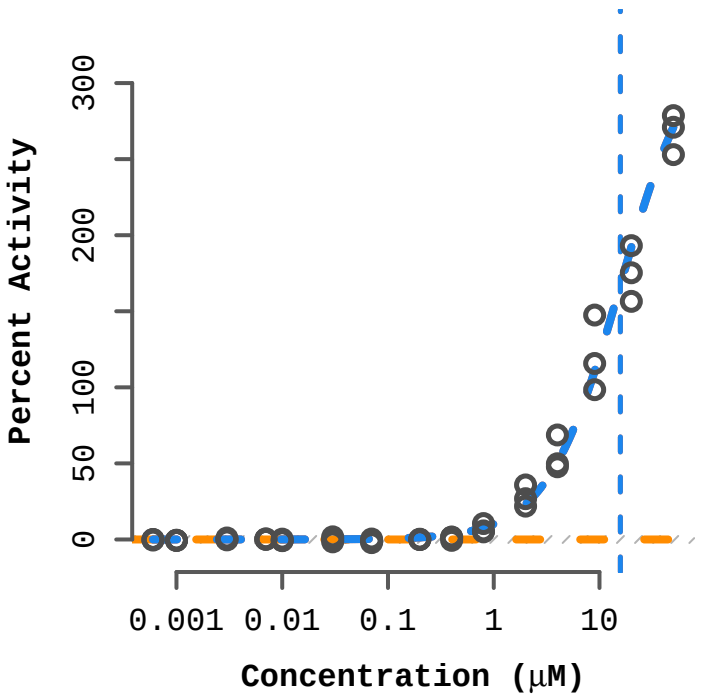
NAME: Parbendazole
CHID: 45410 **CASRN:** 14255-87-9
SPID(S): Tox21_110571_1
M4ID: 12484260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benserazide hydrochloride
CHID: 45412 CASRN: 14919-77-8
SPID(S): Tox21_110573_1
M4ID: 12484258

HILL MODEL (in red):

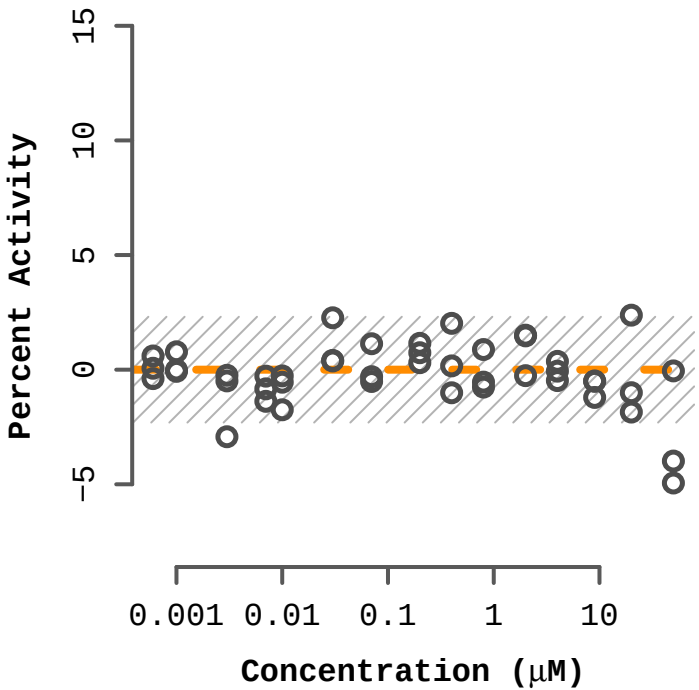
	tp	ga	gw
val:	334	1.2	1.26
sd:	9.08	0.0272	0.0383

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	334	1.2	1.26	3.69	7.79
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	532.63	300.24	304.24
PROB:	0	0.88	0.12
RMSE:	90.02	9.46	9.46

MAX_MEAN: 268 **MAX_MED:** 271 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

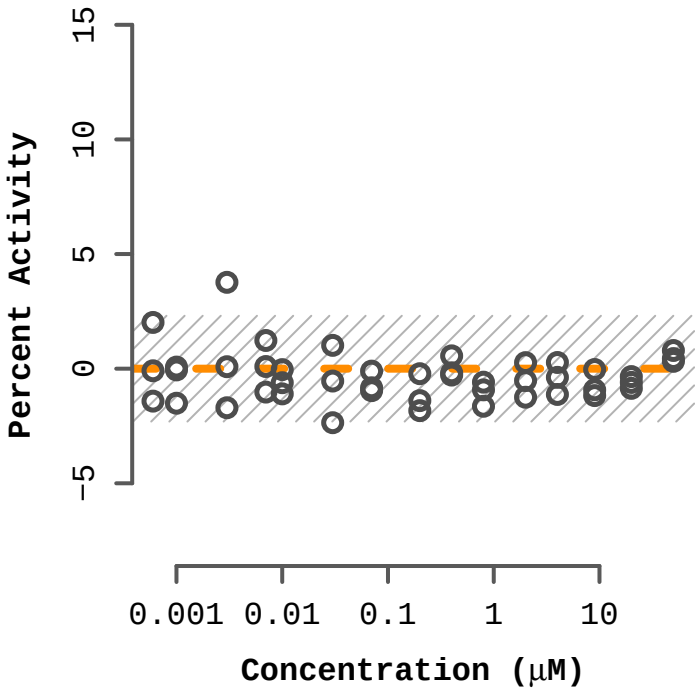
NAME: Cloperastine hydrochloride
CHID: 45413 **CASRN:** 14984-68-0
SPID(S): Tox21_110575_1
M4ID: 12484256

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

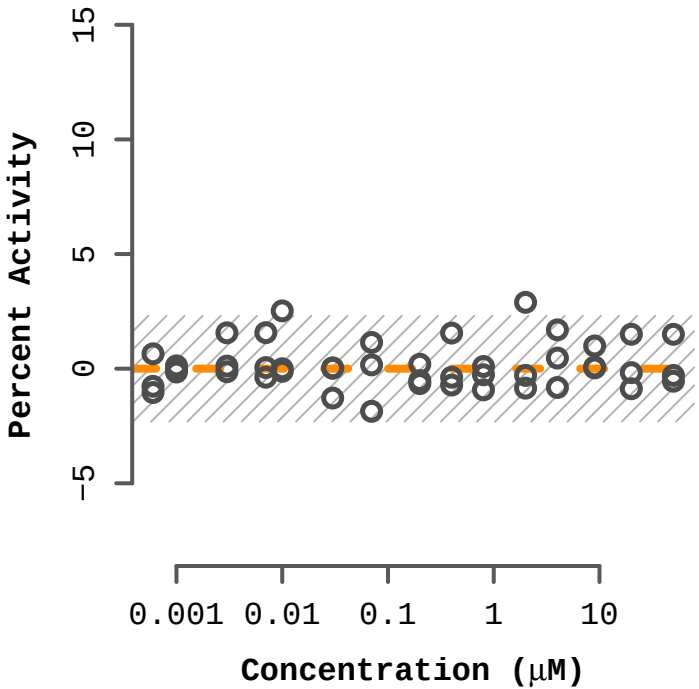
NAME: Trapidil
CHID: 45416 **CASRN:** 15421-84-8
SPID(S): Tox21_110578_1
M4ID: 12484254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.442 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

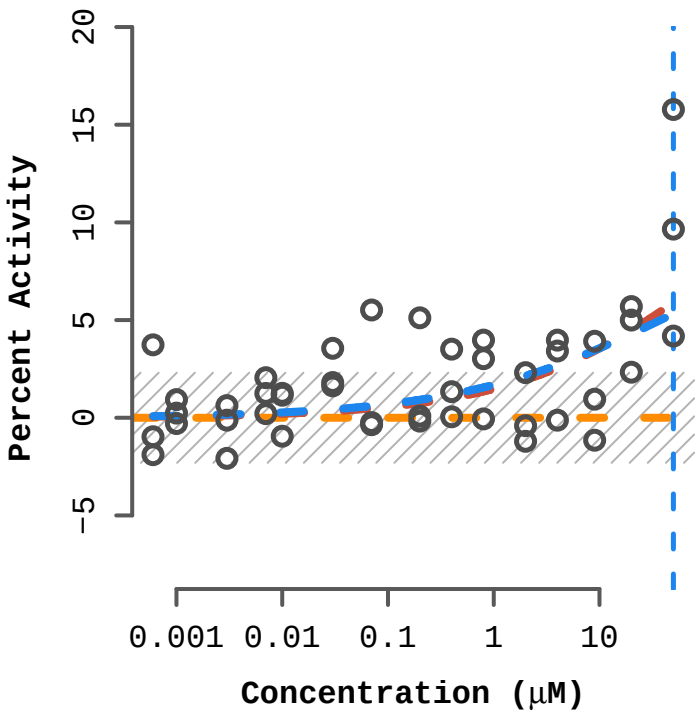
NAME: Molindone hydrochloride
CHID: 45417 **CASRN:** 15622-65-8
SPID(S): Tox21_110579_1
M4ID: 12484253

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.803 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenoterol hydrobromide
CHID: 45419 CASRN: 1944-12-3
SPID(S): Tox21_110581_1
M4ID: 12484252

HILL MODEL (in red):

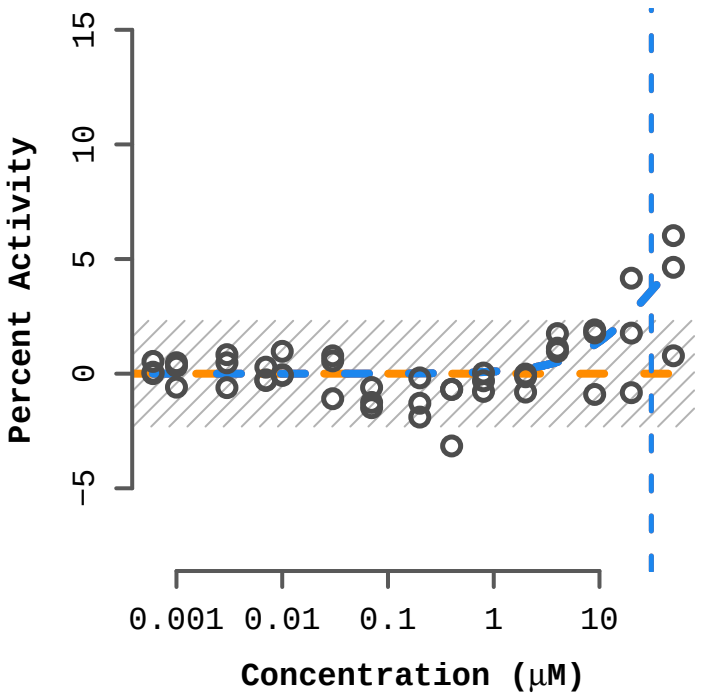
	tp	ga	gw
val:	15.8	2.2	0.449
sd:	28.9	1.99	0.311

GAIN-LOSS MODEL (in blue):

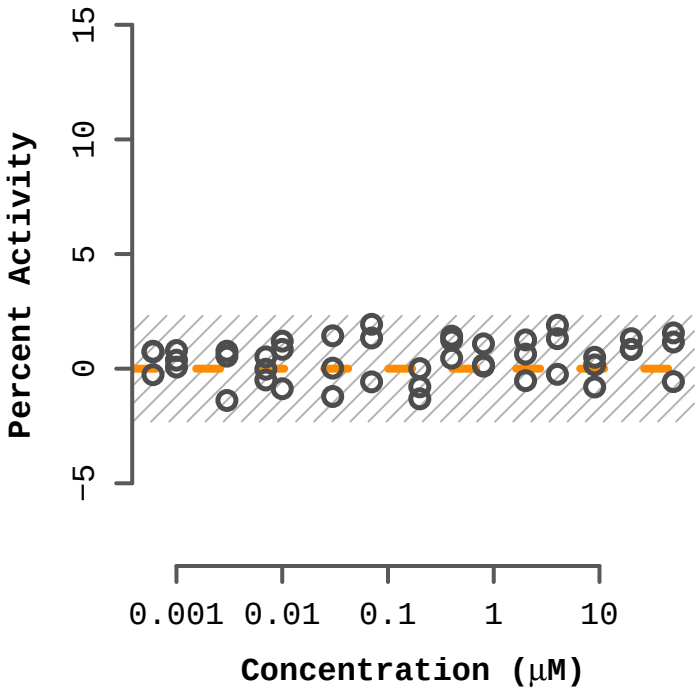
	tp	ga	gw	la	lw
val:	10.6	1.7	0.427	3.52	17.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	235.21	213.02	217.5
PROB:	0	0.9	0.1
RMSE:	3.72	2.52	2.58

MAX_MEAN: 9.87 **MAX_MED:** 9.66 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ornidazole
CHID:    45420   CASRN: 16773-42-5
SPID(S): Tox21_110582_1
M4ID:    12484251

HILL MODEL (in red):
      tp       ga       gw
val:  7.23     1.49     1.26
sd:   5.39     0.592    0.494

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.23     1.49     1.26     2.61     8.88
sd:   5.39     0.592    0.494    1470     14400

      CNST        HILL        GNLS
AIC:  160.85      147.72      151.72
PROB: 0           0.88        0.12
RMSE: 1.63        1.23        1.23

MAX_MEAN: 3.82      MAX_MED: 4.64      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

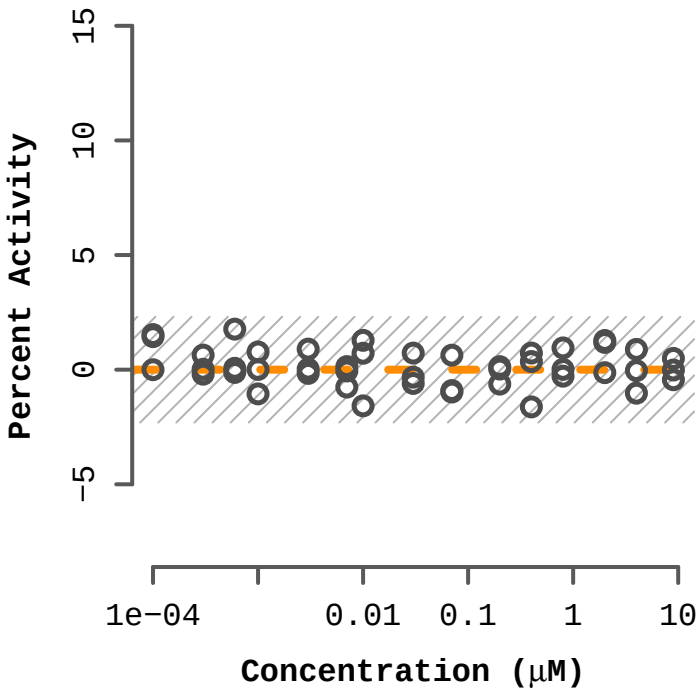
NAME: Epirizole
CHID: 45422 **CASRN:** 18694-40-1
SPID(S): Tox21_110584_1
M4ID: 12484250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

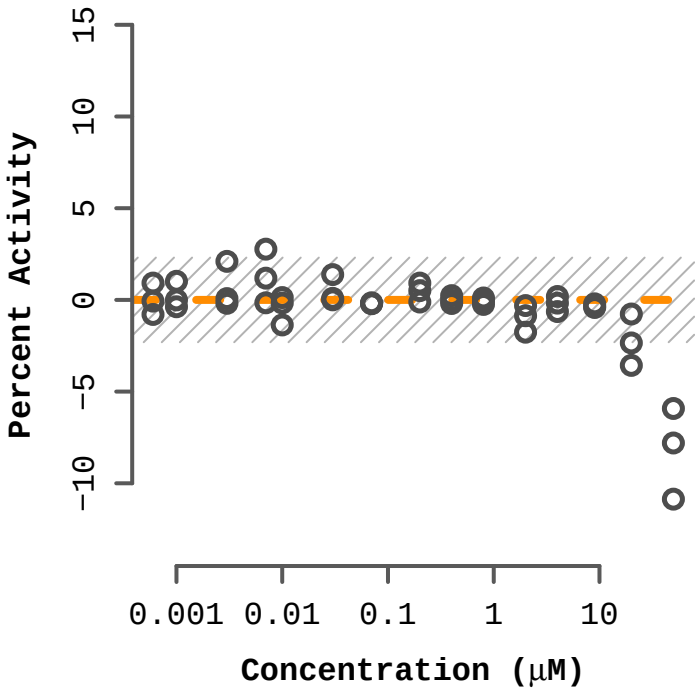
NAME: Piromidic acid
CHID: 45424 **CASRN:** 19562-30-2
SPID(S): Tox21_110587_1
M4ID: 12484247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.992 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

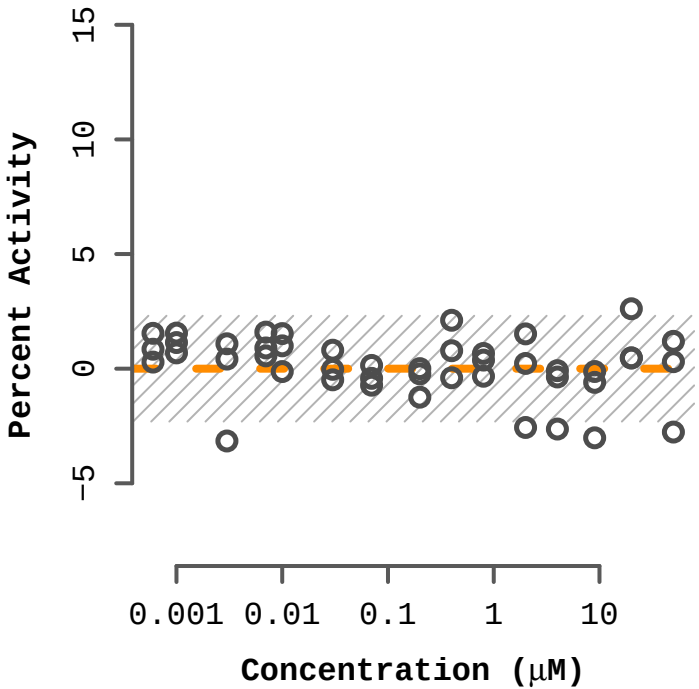
NAME: Dilazep
CHID: 45425 **CASRN:** 35898-87-4
SPID(S): Tox21_110588_1
M4ID: 12484246

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.18	NA	NA
PROB:	1	NA	NA
RMSE:	2.4	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

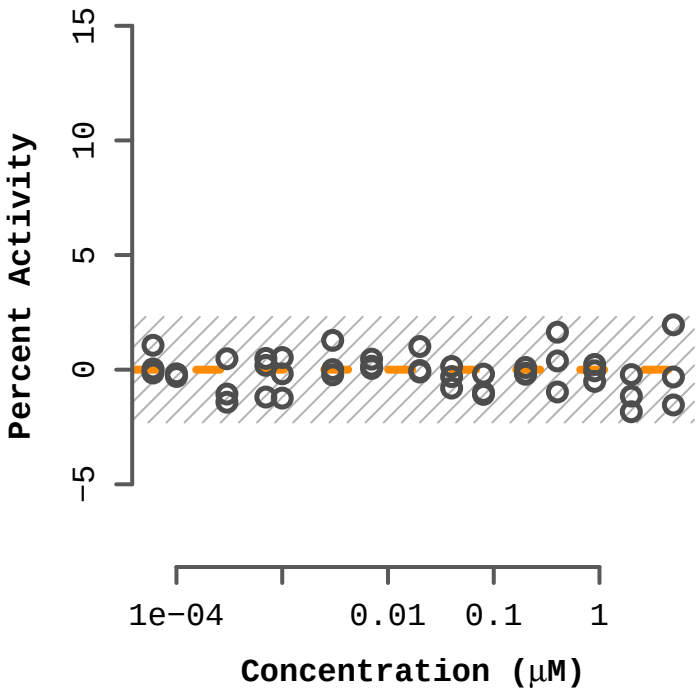
NAME: Spectinomycin dihydrochloride
CHID: 45429 **CASRN:** 21736-83-4
SPID(S): Tox21_110592_1
M4ID: 12484244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

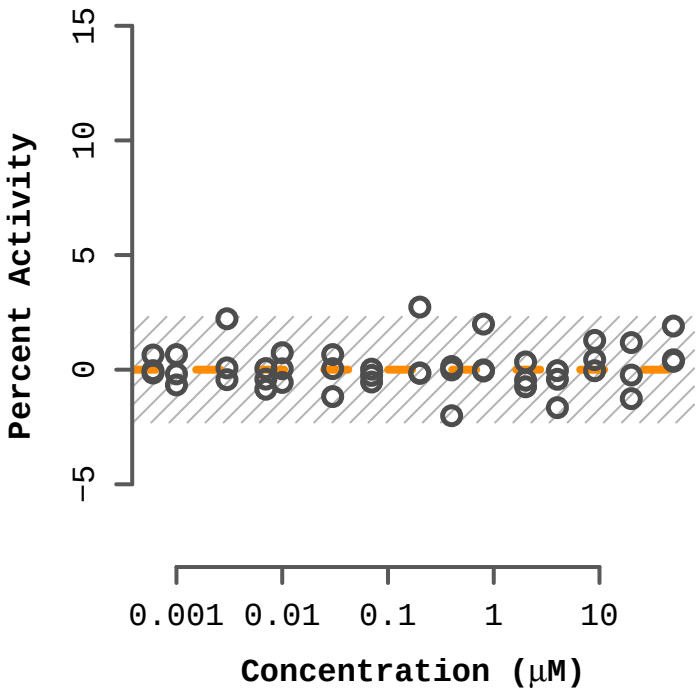
NAME: Benfotiamine
CHID: 45433 **CASRN:** 22457-89-2
SPID(S): Tox21_110597_1
M4ID: 12484241

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.355 **MAX_MED:** 0.383 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

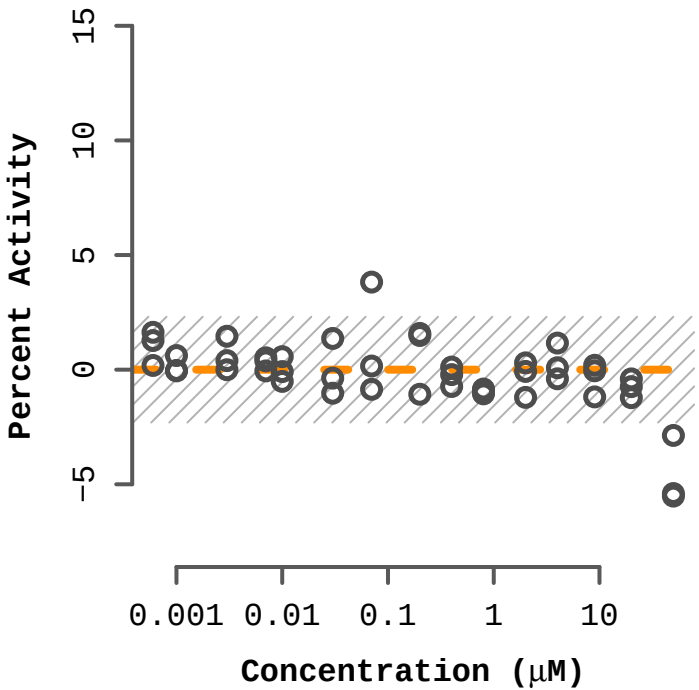
NAME: Etandazole
CHID: 45434 **CASRN:** 22668-01-5
SPID(S): Tox21_110599_1
M4ID: 12484239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.901 **MAX_MED:** 0.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

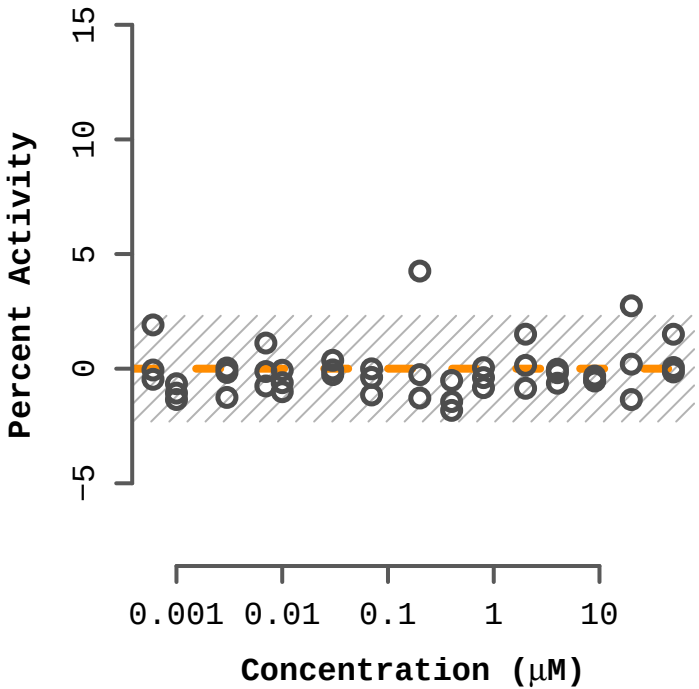
NAME: Famprofazone
CHID: 45435 **CASRN:** 22881-35-2
SPID(S): Tox21_110600_1
M4ID: 12484238

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

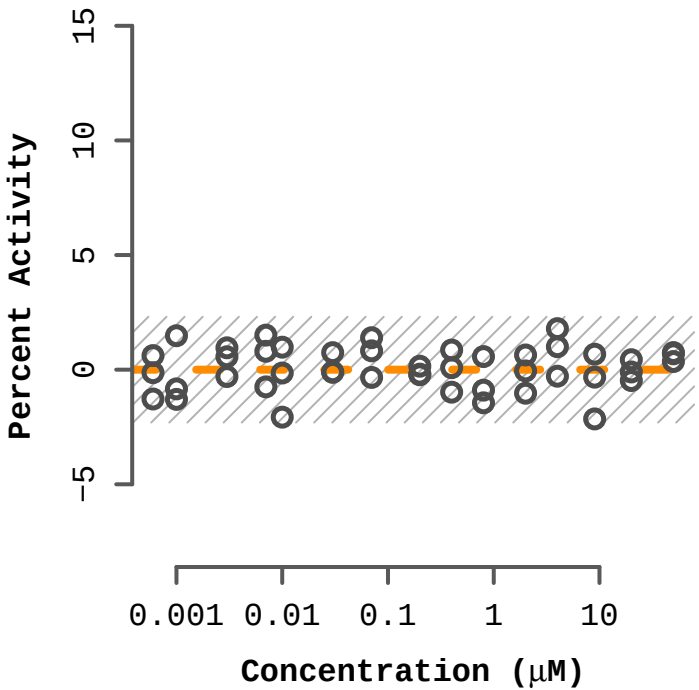
NAME: Terbutaline hemisulfate
CHID: 45437 **CASRN:** 23031-32-5
SPID(S): Tox21_110602_1
M4ID: 12484237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.908 **MAX_MED:** 0.199 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

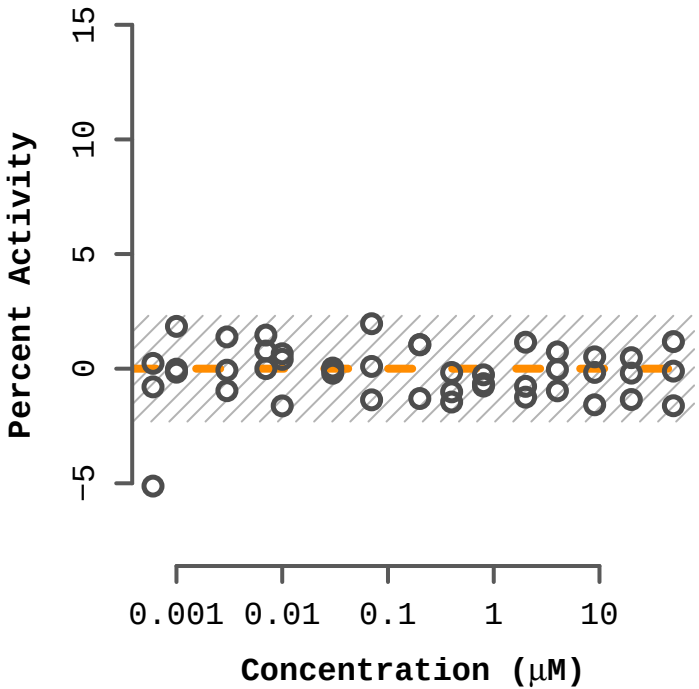
NAME: Probucol
CHID: 45440 **CASRN:** 23288-49-5
SPID(S): Tox21_110605_1
M4ID: 12484236

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.837 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

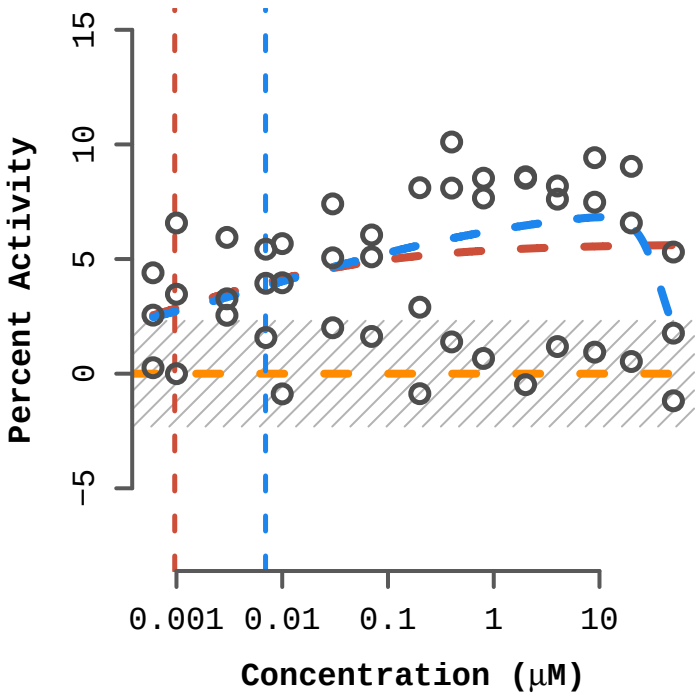
NAME: Nefopam hydrochloride
CHID: 45441 **CASRN:** 23327-57-3
SPID(S): Tox21_110606_1
M4ID: 12484235

HILL MODEL: Not applicable.

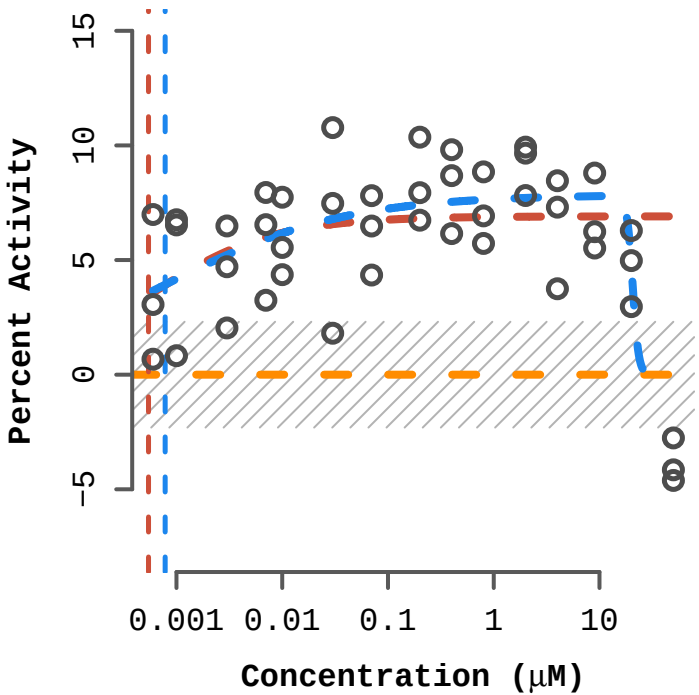
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

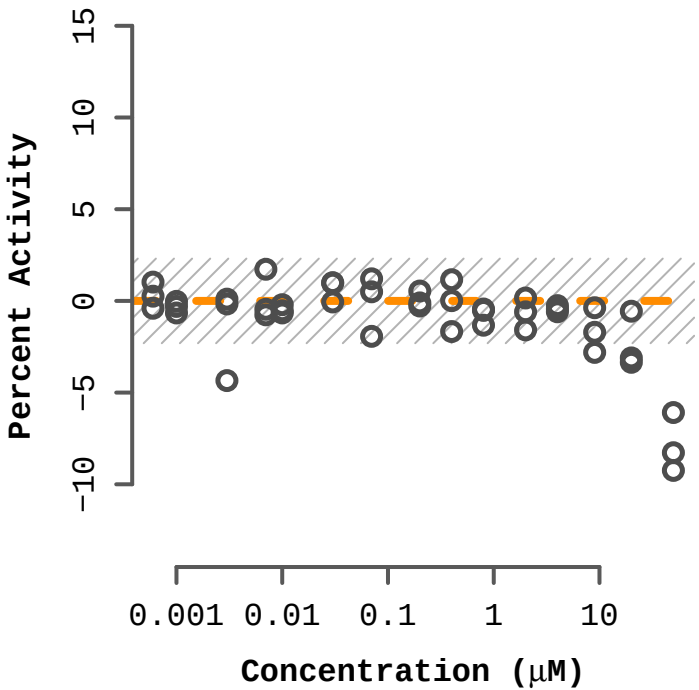
MAX_MEAN: 0.747 **MAX_MED:** 1.04 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Articaine hydrochloride
CHID:    45444   CASRN: 23964-57-0
SPID(S): Tox21_110609_1
M4ID:    12484234

HILL MODEL (in red):
      tp       ga       gw
val:  5.66     -3.02    0.429
sd:   1.14     0.816    0.363

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.63     -2.16    0.302    1.59     3.63
sd:   3.9      1.72     0.3      0.226    5.9

      CNST        HILL        GNLS
AIC:  287.94      245.89      244.87
PROB: 0           0.38        0.62
RMSE: 5.44        3.19        3.1

MAX_MEAN: 6.53      MAX_MED: 8.52      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Isoconazole
CHID:    45447   CASRN: 27523-40-6
SPID(S): Tox21_110616_1
M4ID:    12484229

HILL MODEL (in red):
      tp       ga       gw
val:  6.91     -3.26    0.738
sd:   0.565    0.469    0.447

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.85     -3.11    0.509    1.31     15.6
sd:   0.738    0.456    0.304    0.0473   57.2

      CNST        HILL        GNLS
AIC:  308.66      239.67      218.2
PROB: 0           0           1
RMSE: 6.64        3.52        2.27

MAX_MEAN: 9.14      MAX_MED: 9.66      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

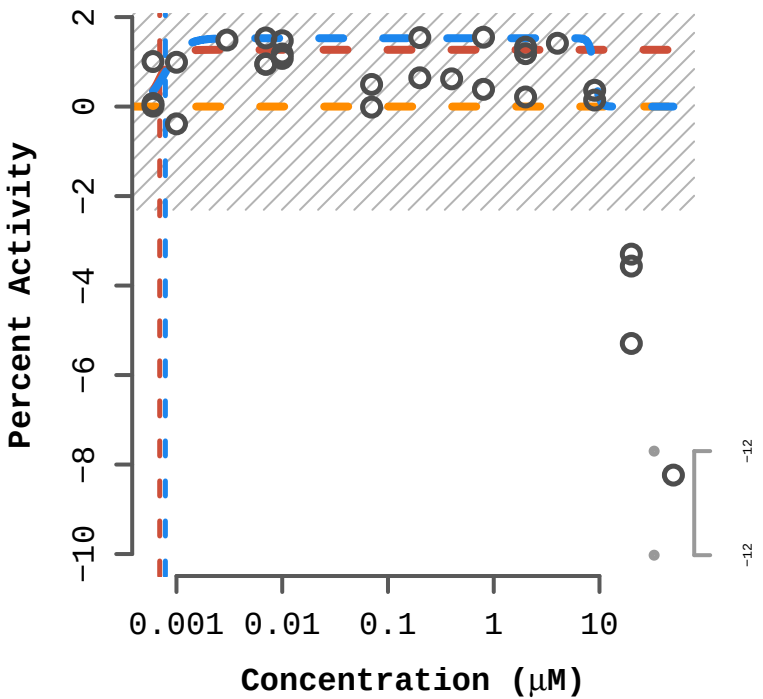
NAME: Etofenamate
CHID: 45448 **CASRN:** 30544-47-9
SPID(S): Tox21_110618_1
M4ID: 12484227

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.43	NA	NA

MAX_MEAN: 0.637 **MAX_MED:** 0.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butoconazole nitrate
CHID: 45452 CASRN: 64872-77-1
SPID(S): Tox21_110624_1
M4ID: 12484223 BRK

HILL MODEL (in red):

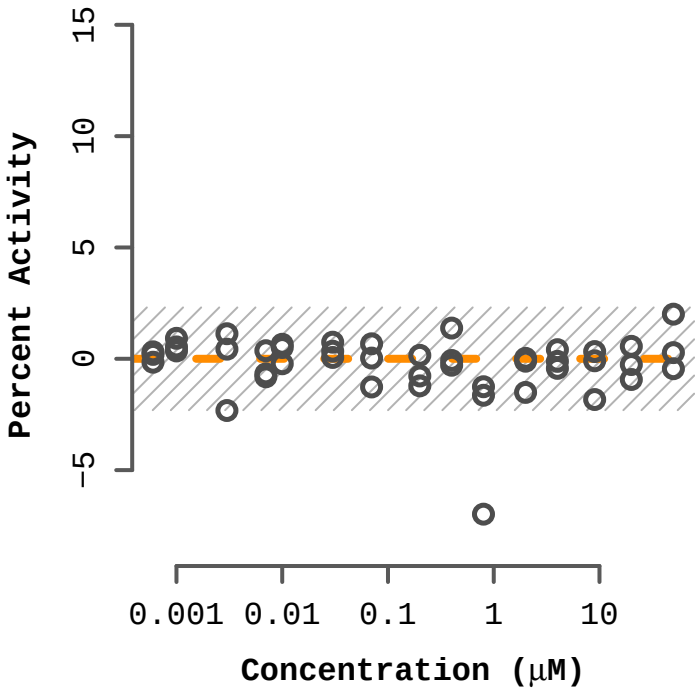
	tp	ga	gw
val:	1.27	−3.16	6.56
sd:	0.243	0.234	20

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.53	−3.1	4.64	0.954	18
sd:	0.234	0.202	7.26	0.0509	728

	CNST	HILL	GNLS
AIC:	224.61	213.62	206.46
PROB:	0	0.03	0.97
RMSE:	3.38	3.52	3.1

MAX_MEAN: 2.48 **MAX_MED:** 2.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

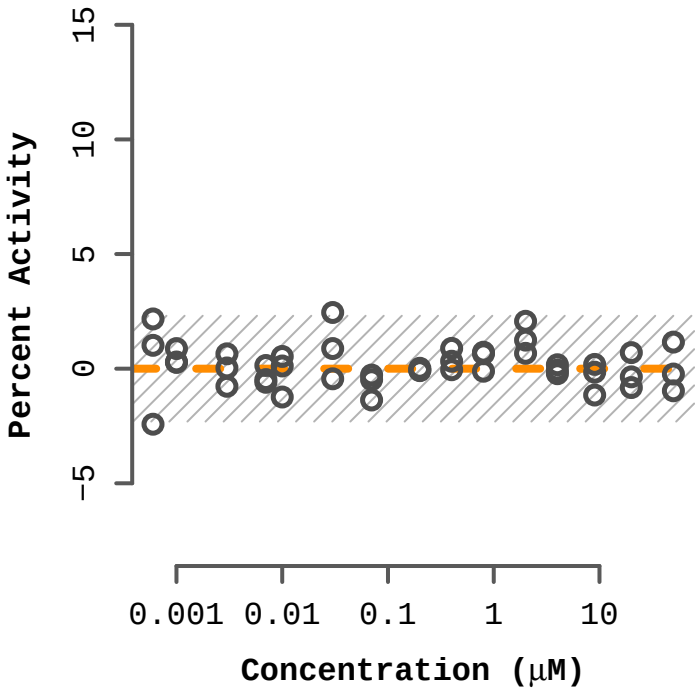
NAME: Pivampicillin
CHID: 45459 **CASRN:** 33817-20-8
SPID(S): Tox21_110631_1
M4ID: 12484219

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.614 **MAX_MED:** 0.535 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

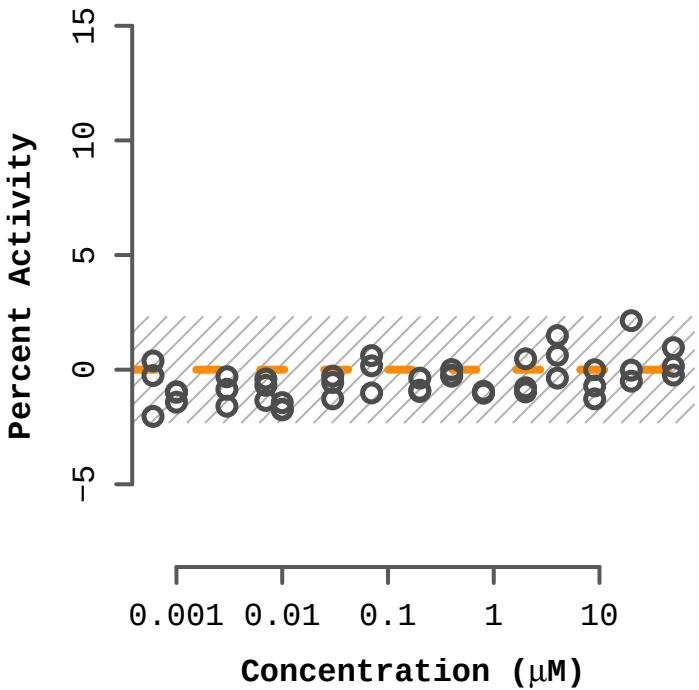
NAME: Acebutolol hydrochloride
CHID: 45461 **CASRN:** 34381-68-5
SPID(S): Tox21_110633_1
M4ID: 12484218

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

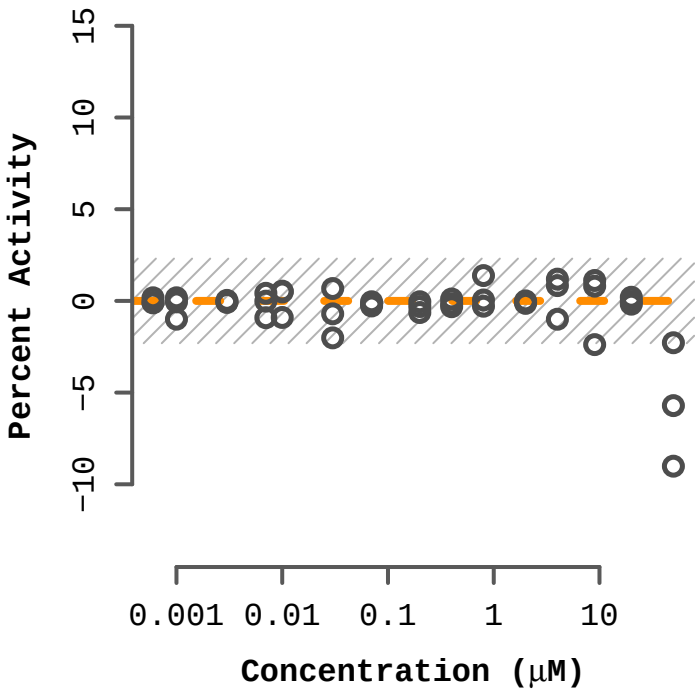
NAME: Isoxicam
CHID: 45462 **CASRN:** 34552-84-6
SPID(S): Tox21_110634_1
M4ID: 12484217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.583 **MAX_MED:** 0.627 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

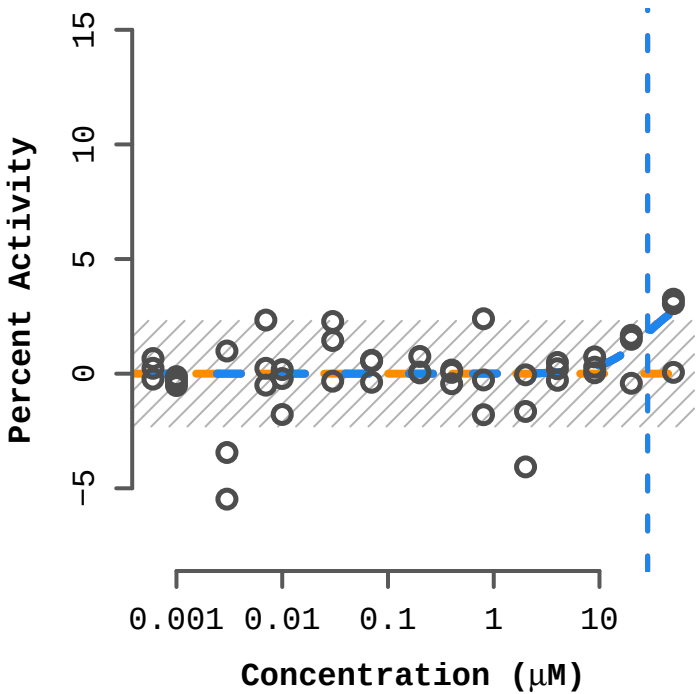
NAME: Halofantrine hydrochloride
CHID: 45464 **CASRN:** 36167-63-2
SPID(S): Tox21_110637_1
M4ID: 12484215

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 0.383 **MAX_MED:** 0.836 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bacampicillin hydrochloride
CHID: 45466 CASRN: 37661-08-8
SPID(S): Tox21_110640_1
M4ID: 12484213

HILL MODEL (in red):

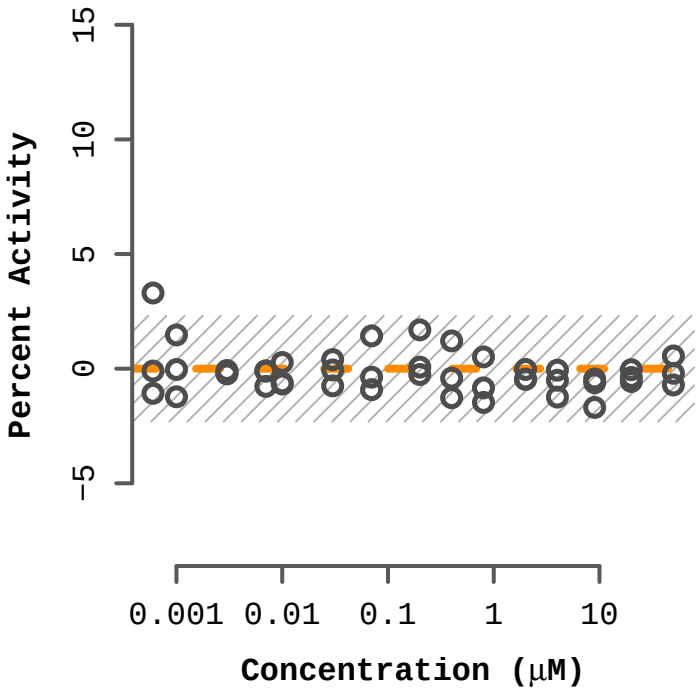
	tp	ga	gw
val:	3.55	1.46	2.09
sd:	3.28	0.522	2.06

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.55	1.46	2.09	2.72	5.79
sd:	3.28	0.522	2.06	1060	6060

	CNST	HILL	GNLS
AIC:	163.05	158.97	162.97
PROB:	0.1	0.79	0.11
RMSE:	1.61	1.5	1.5

MAX_MEAN: 2.12 **MAX_MED:** 3.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

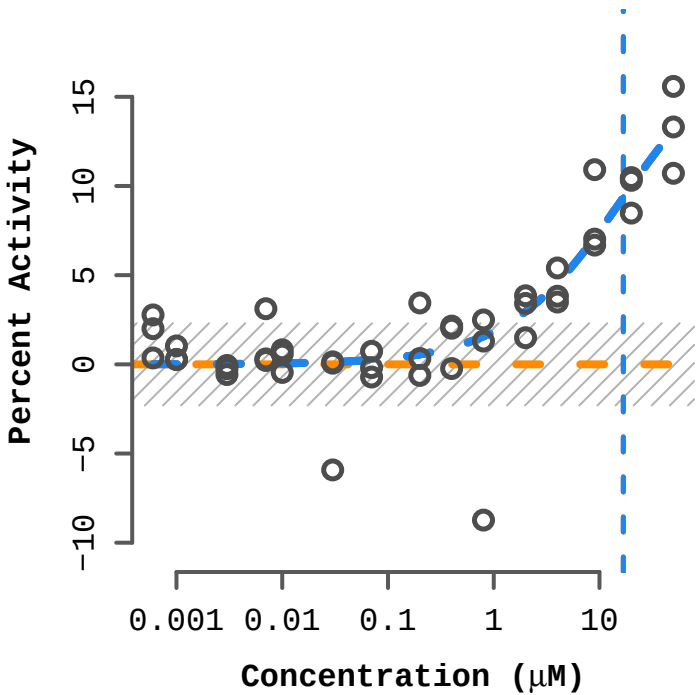
NAME: Suprofen
CHID: 45469 **CASRN:** 40828-46-4
SPID(S): Tox21_110643_1
M4ID: 12484212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.709 **MAX_MED:** 0.0694 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nabumetone
CHID: 45472 CASRN: 42924-53-8
SPID(S): Tox21_110647_1
M4ID: 12484208

HILL MODEL (in red):

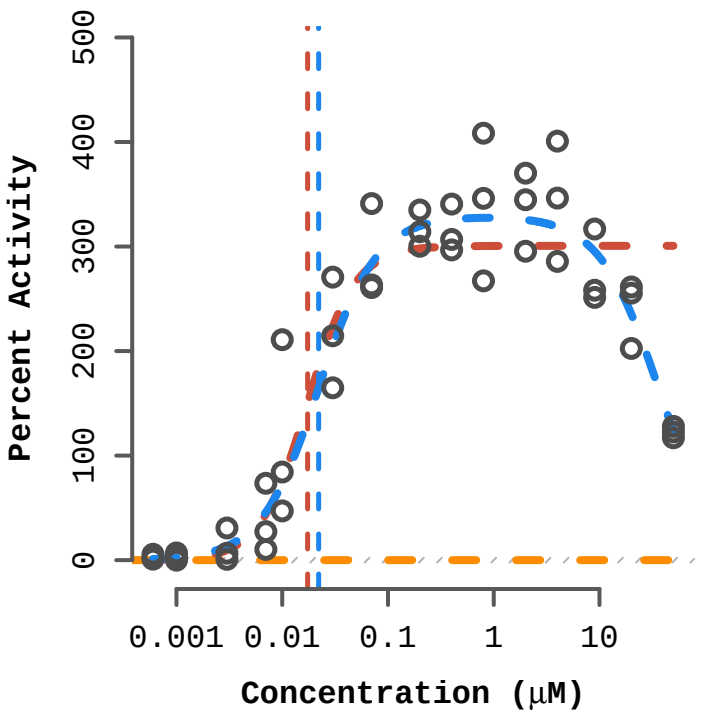
	tp	ga	gw
val:	18.7	1.23	0.785
sd:	5.26	0.339	0.169

GAIN-LOSS MODEL (in blue):

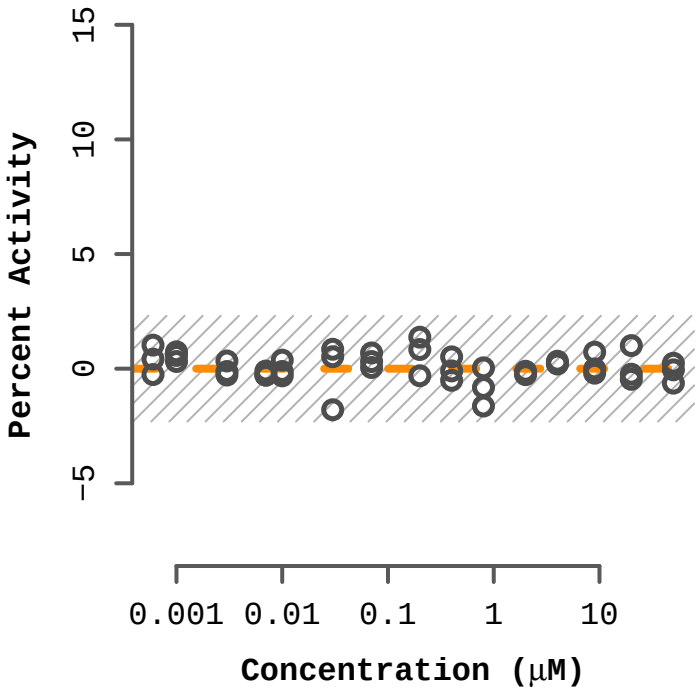
	tp	ga	gw	la	lw
val:	18.7	1.23	0.785	3.63	4.96
sd:	5.27	0.339	0.169	12000	30900

	CNST	HILL	GNLS
AIC:	274.62	181.95	185.95
PROB:	0	0.88	0.12
RMSE:	5.35	2.2	2.2

MAX_MEAN: 13.2 **MAX_MED:** 13.3 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Rimexolone
CHID:    45474   CASRN: 49697-38-3
SPID(S): Tox21_110650_1
M4ID:    12484205

HILL MODEL (in red):
      tp       ga       gw
val:  301      -1.76    1.94
sd:   11.4     0.0787   0.427

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  329      -1.66    1.59     1.56     1.55
sd:   12.1     0.0693   0.284    0.0503   0.333

      CNST        HILL        GNLS
AIC:  629.58      501.25      460.51
PROB: 0           0           1
RMSE: 239.19      63.62       37.57

MAX_MEAN: 344       MAX_MED: 346       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

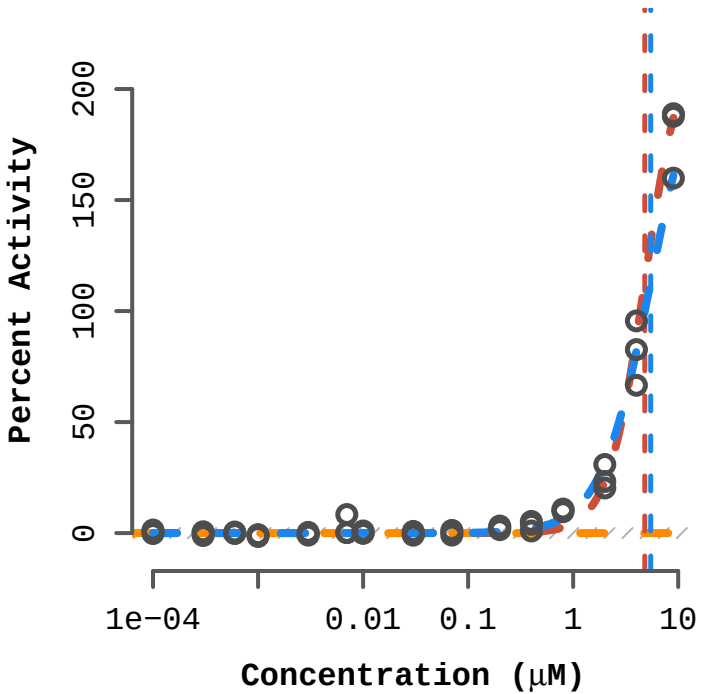
NAME: Carteolol hydrochloride
CHID: 45478 **CASRN:** 51781-21-6
SPID(S): Tox21_110654_1
M4ID: 12484203

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	83.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.635 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ribostamycin sulfate
CHID: 45480 CASRN: 53797-35-6
SPID(S): Tox21_110657_1
M4ID: 12484201

HILL MODEL (in red):

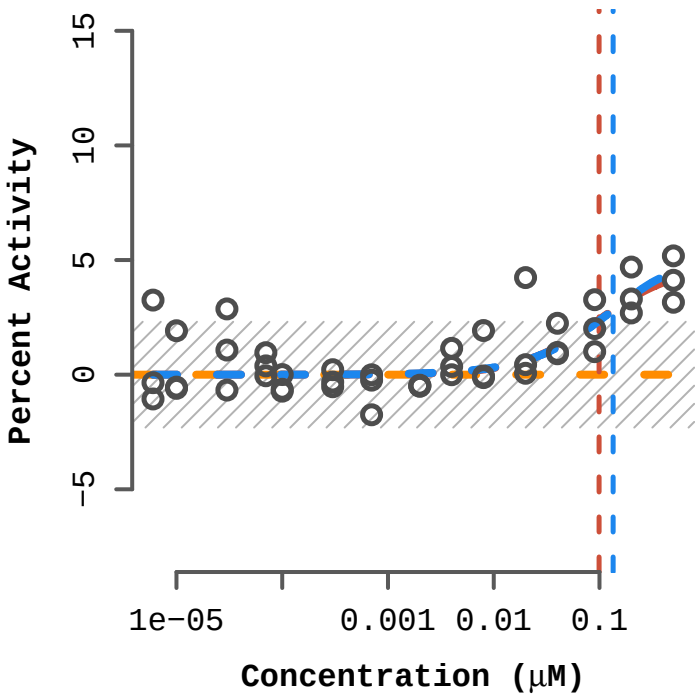
	tp	ga	gw
val:	227	0.682	2.47
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	227	0.739	1.81	2.12	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	425.06	264.6	275.54
PROB:	0	1	0
RMSE:	51.48	6.09	7.06

MAX_MEAN: 179 **MAX_MED:** 188 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Netilmicin sulfate
CHID: 45484 CASRN: 56391-57-2
SPID(S): Tox21_110663_1
M4ID: 12484195

HILL MODEL (in red):

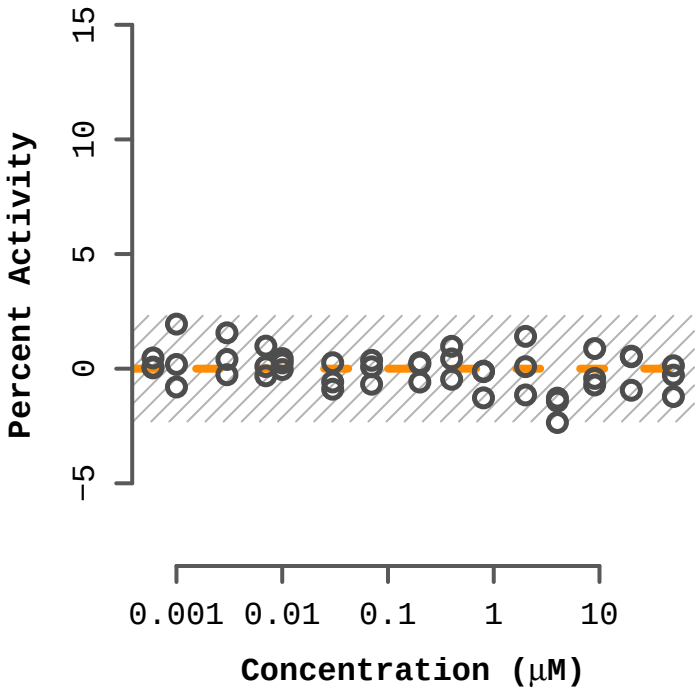
	tp	ga	gw
val:	4.78	−1	1.19
sd:	1.32	0.286	0.493

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.64	−0.871	1.09	−0.174	7.91
sd:	5.66	0.847	0.642	2.32	144

	CNST	HILL	GNLS
AIC:	187.14	140.7	144.66
PROB:	0	0.88	0.12
RMSE:	1.96	1.14	1.14

MAX_MEAN: 4.15 **MAX_MED:** 4.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

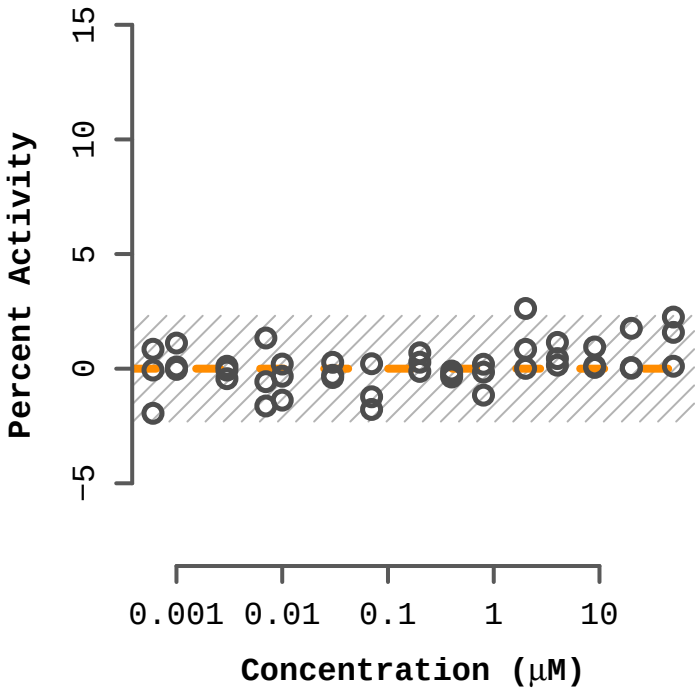
NAME: Meptazinol hydrochloride
CHID: 45485 CASRN: 59263-76-2
SPID(S): Tox21_110665_1
M4ID: 12484194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.569 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

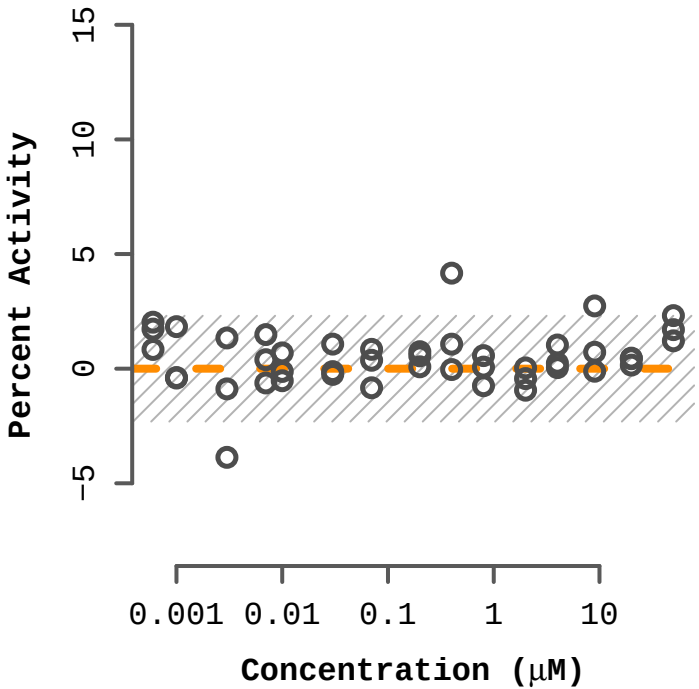
NAME: Tenoxicam
CHID: 45486 **CASRN:** 59804-37-4
SPID(S): Tox21_110666_1
M4ID: 12484193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

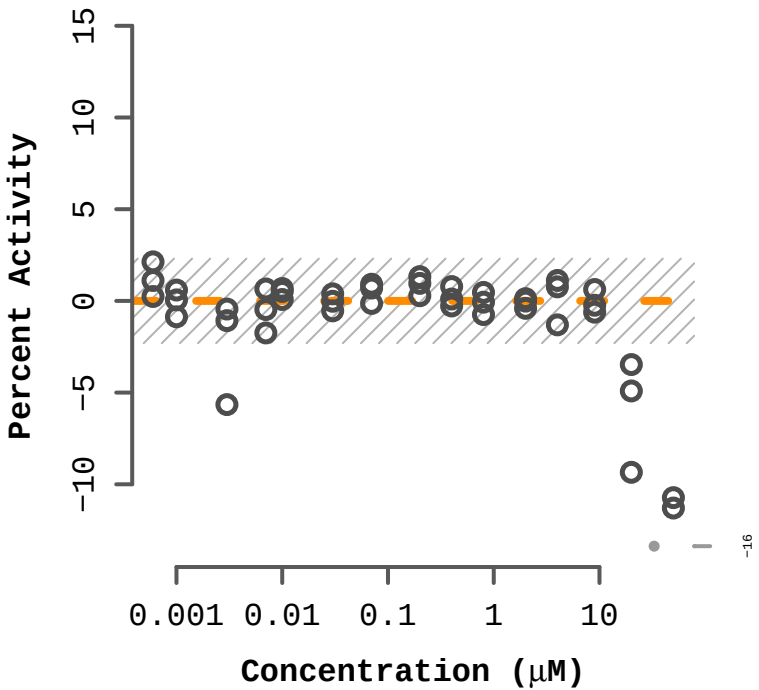
NAME: Clorsulon
CHID: 45488 CASRN: 60200-06-8
SPID(S): Tox21_110669_1
M4ID: 12484190

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.75 MAX_MED: 1.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

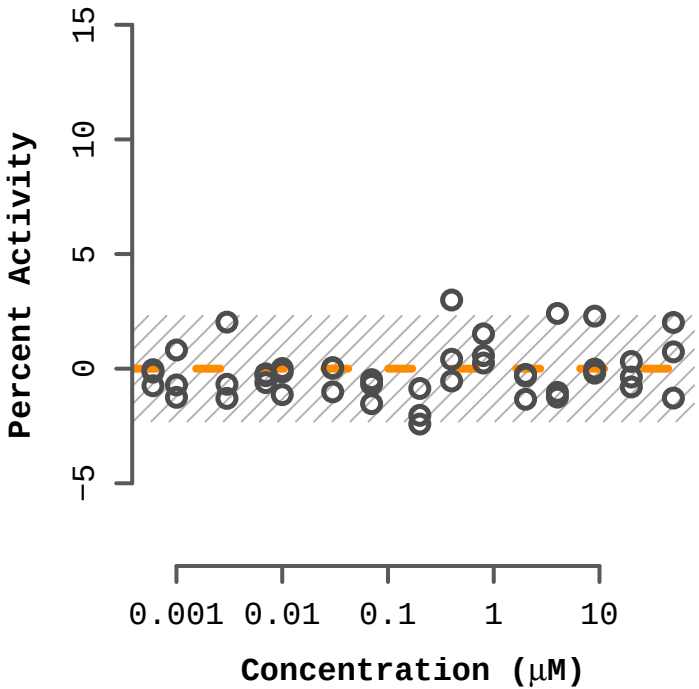
NAME: Sulconazole nitrate
CHID: 45490 **CASRN:** 61318-91-0
SPID(S): Tox21_110671_1
M4ID: 12484189 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.32	NA	NA
PROB:	1	NA	NA
RMSE:	3.86	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

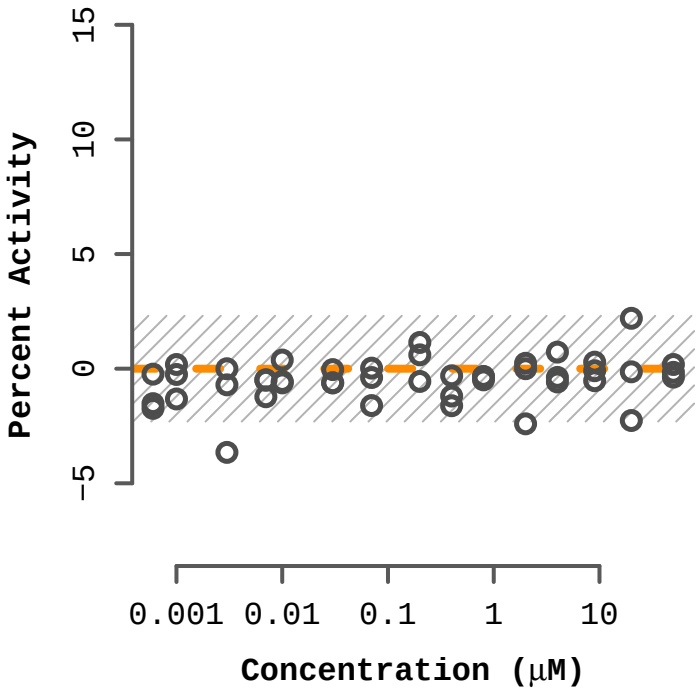
NAME: Etifenin
CHID: 45492 CASRN: 63245-28-3
SPID(S): Tox21_110673_1
M4ID: 12484187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.958 **MAX_MED:** 0.734 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

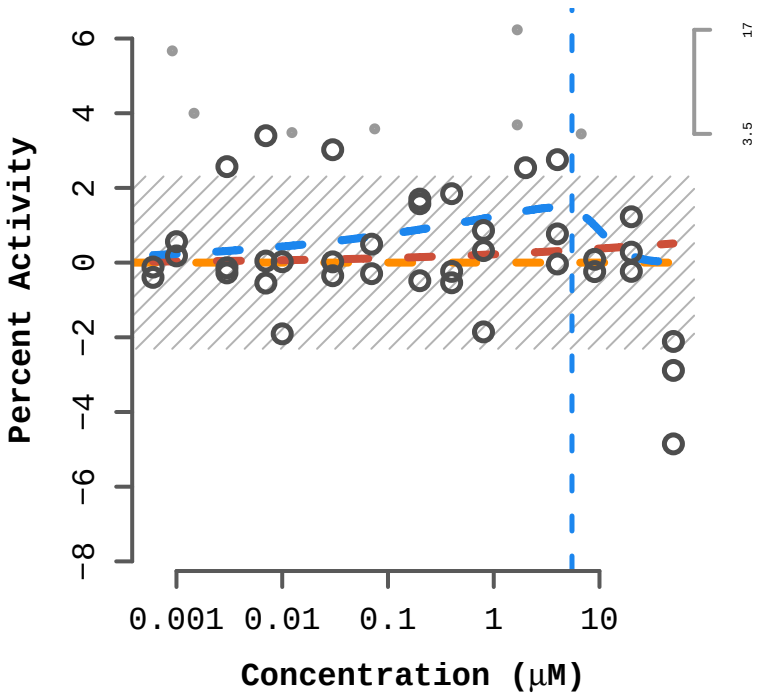
NAME: Terazosin hydrochloride
CHID: 45493 **CASRN:** 63074-08-8
SPID(S): Tox21_110674_1
M4ID: 12484186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.398 **MAX_MED:** 0.605 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Naftifine hydrochloride
CHID: 45496 **CASRN:** 65473-14-5
SPID(S): Tox21_110677_1
M4ID: 12484185 **BRK**

HILL MODEL (in red):

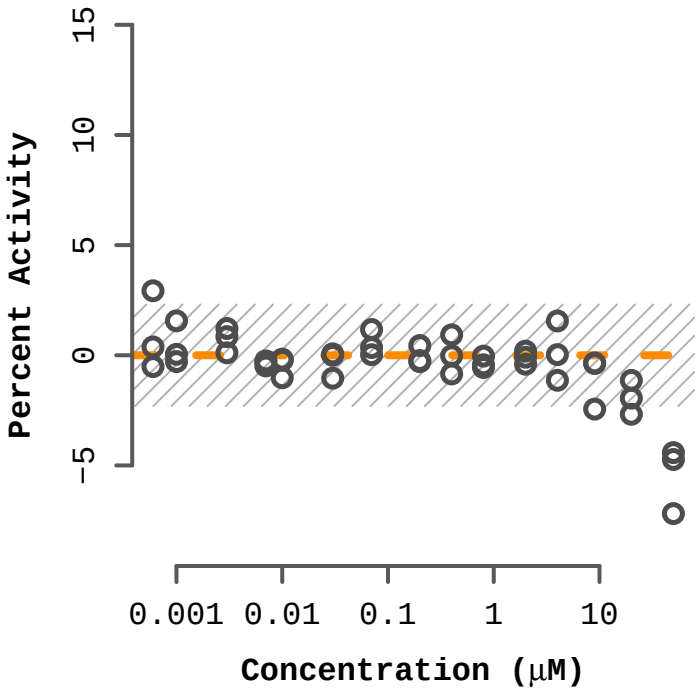
	tp	ga	gw
val:	1.23	2.2	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.28	0.74	0.3	0.99	3.17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	225.02	230.54	228.39
PROB:	0.8	0.05	0.15
RMSE:	3.97	3.94	3.72

MAX_MEAN: 8.16 **MAX_MED:** 4.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

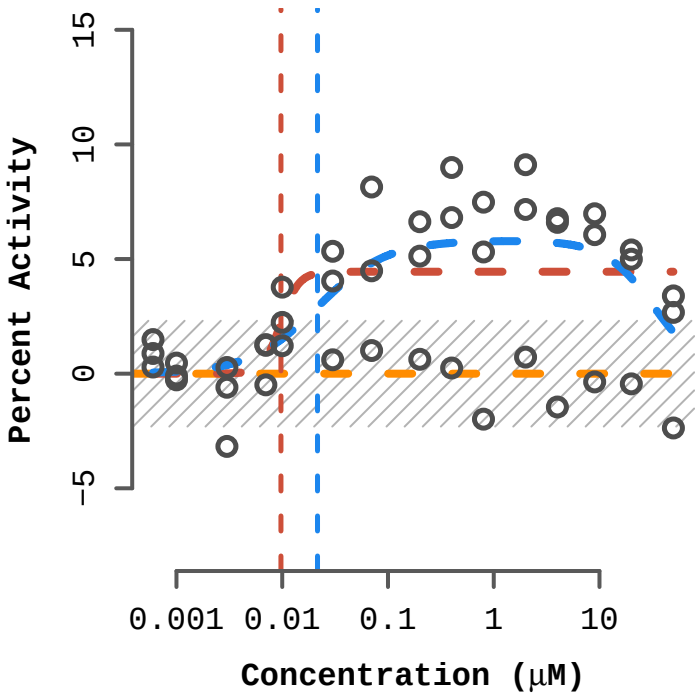
NAME: Glafenine hydrochloride
CHID: 45497 **CASRN:** 65513-72-6
SPID(S): Tox21_110678_1
M4ID: 12484184

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 0.932 **MAX_MED:** 0.848 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Florfenicol
CHID: 45500 **CASRN:** 73231-34-2
SPID(S): Tox21_110683_1
M4ID: 12484181

HILL MODEL (in red):

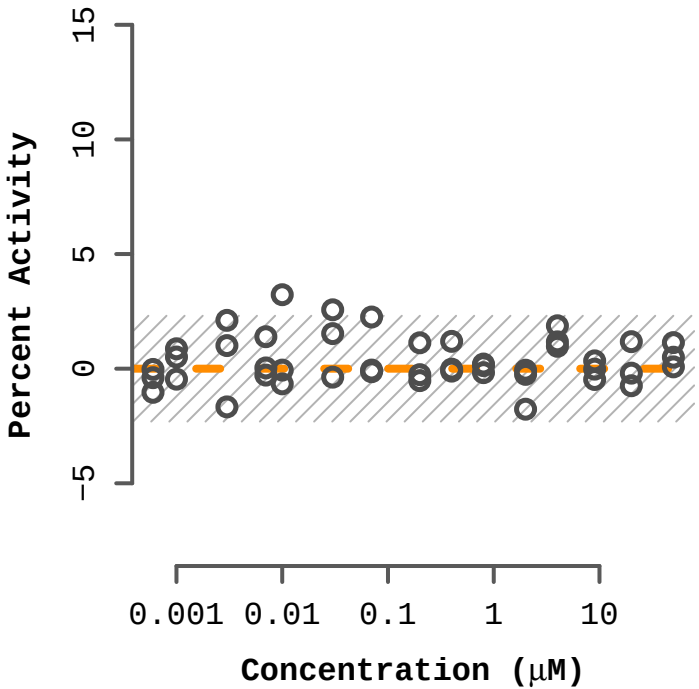
	tp	ga	gw
val:	4.45	−2.01	5.19
sd:	0.611	0.0982	7.04

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.82	−1.67	1.34	1.52	1.87
sd:	1.05	0.337	0.951	0.23	1.61

	CNST	HILL	GNLS
AIC:	264.74	232.53	231.64
PROB:	0	0.39	0.61
RMSE:	4.34	2.87	2.85

MAX_MEAN: 5.67 **MAX_MED:** 7.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

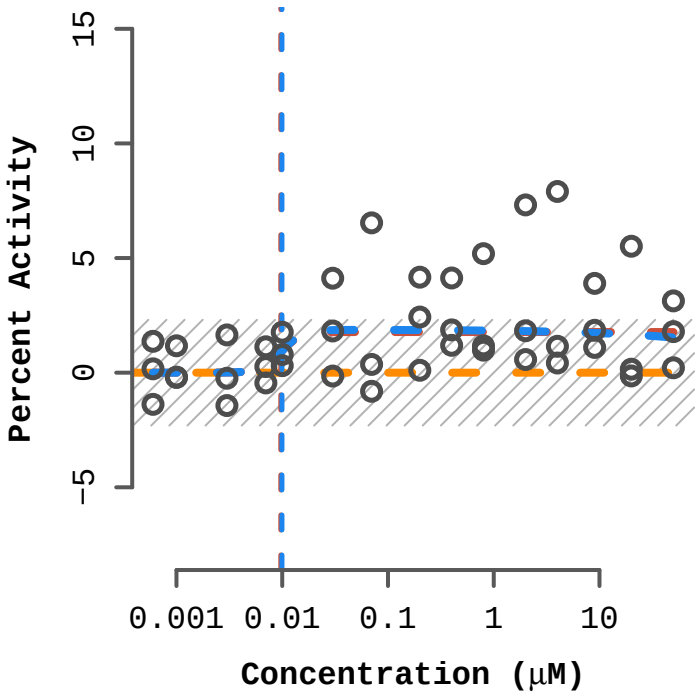
NAME: Ozagrel hydrochloride
CHID: 45506 **CASRN:** 78712-43-3
SPID(S): Tox21_110693_1
M4ID: 12484173

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Levocabastine hydrochloride
CHID: 45508 CASRN: 79547-78-7
SPID(S): Tox21_110695_1
M4ID: 12484172

HILL MODEL (in red):

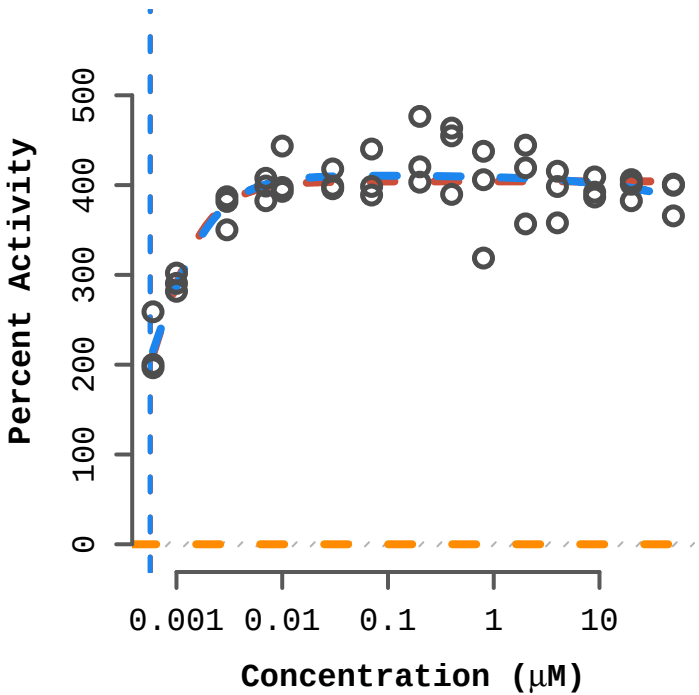
	tp	ga	gw
val:	1.77	−2.01	4.81
sd:	0.356	0.156	9.78

GAIN-LOSS MODEL (in blue):

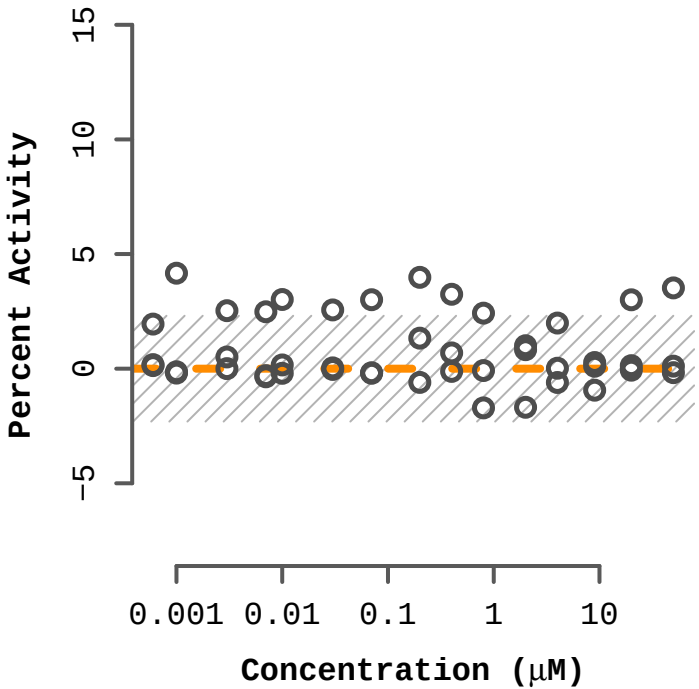
	tp	ga	gw	la	lw
val:	1.87	−2	4.6	2.81	0.588
sd:	0.581	0.171	9.9	5.16	2.24

	CNST	HILL	GNLS
AIC:	214.42	194.18	198.08
PROB:	0	0.88	0.12
RMSE:	2.74	2.01	2.01

MAX_MEAN: 3.24 **MAX_MED:** 2.43 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Fluticasone propionate
CHID:    45511   CASRN: 80474-14-2
SPID(S): Tox21_110698_1
M4ID:    12484170

HILL MODEL (in red):
      tp       ga       gw
val:  404      -3.25    1.63
sd:   4.31     0.0381   0.287

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  411      -3.25    1.45     3.7      0.6
sd:   7.79     0.0439   0.304    1.68     0.503

      CNST        HILL        GNLS
AIC:  726.01      433.67      434.6
PROB: 0           0.61        0.39
RMSE: 387.31      28.63       27.65

MAX_MEAN: 436       MAX_MED: 455       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

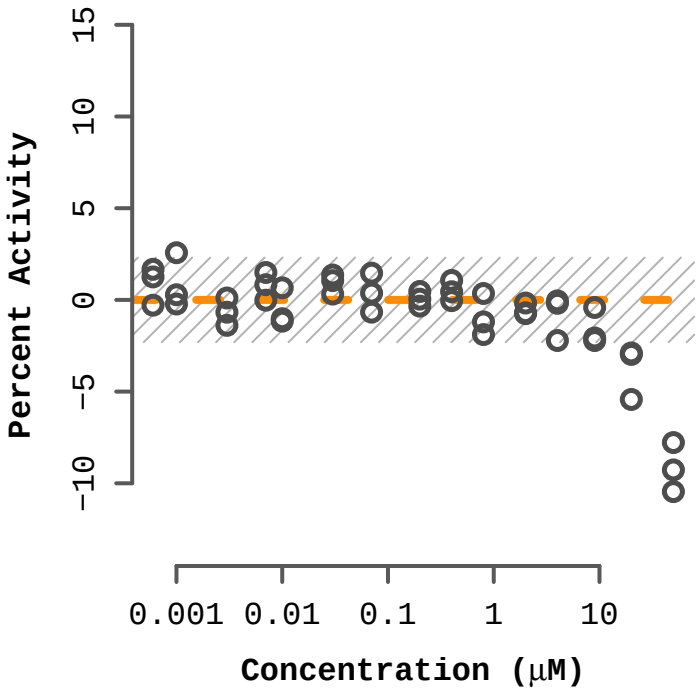
NAME: Racecadotril
CHID: 45513 **CASRN:** 81110-73-8
SPID(S): Tox21_110700_1
M4ID: 12484168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

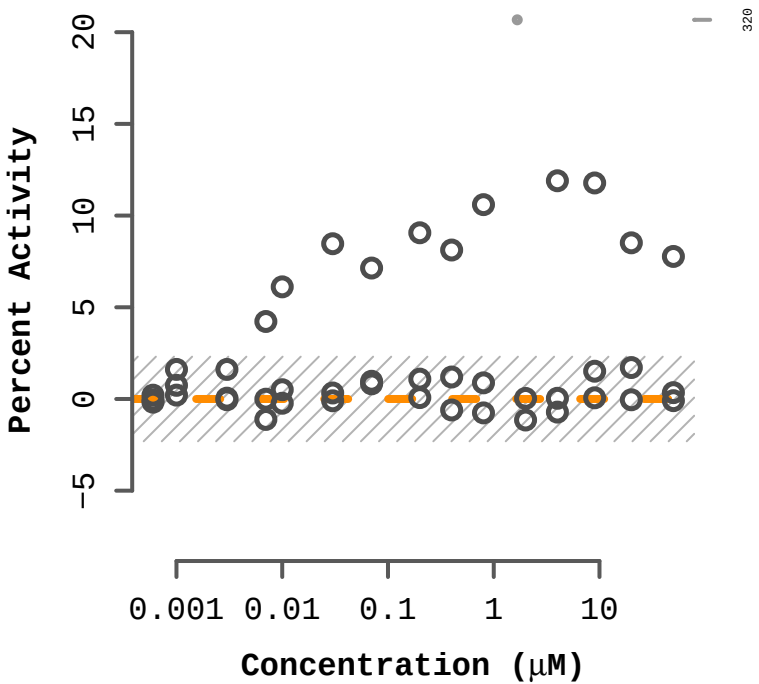
NAME: Alfuzosin hydrochloride
CHID: 45514 **CASRN:** 81403-68-1
SPID(S): Tox21_110701_1
M4ID: 12484167

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.86	NA	NA
PROB:	1	NA	NA
RMSE:	2.79	NA	NA

MAX_MEAN: 0.91 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

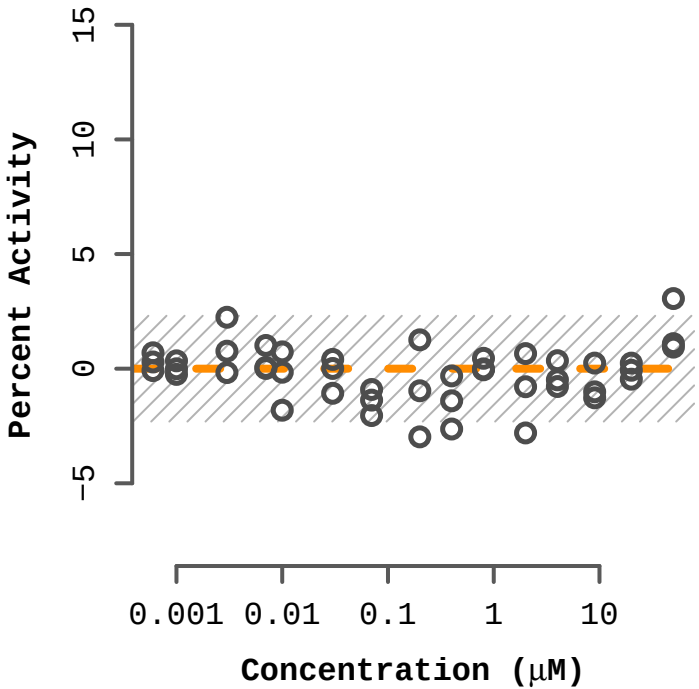
NAME: Bambuterol hydrochloride
CHID: 45515 **CASRN:** 81732-46-9
SPID(S): Tox21_110702_1
M4ID: 12484166 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	291.55	NA	NA
PROB:	1	NA	NA
RMSE:	47.58	NA	NA

MAX_MEAN: 106 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

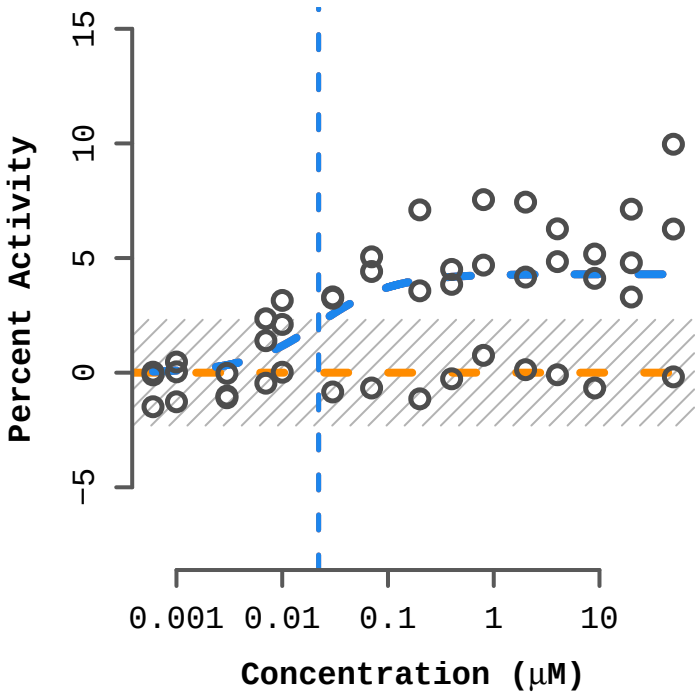
NAME: (−)−Quinpirole hydrochloride
CHID: 45519 **CASRN:** 85798−08−9
SPID(S): Tox21_110707_1
M4ID: 12484161

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ioversol
CHID: 45521 CASRN: 87771-40-2
SPID(S): Tox21_110709_1
M4ID: 12484159

HILL MODEL (in red):

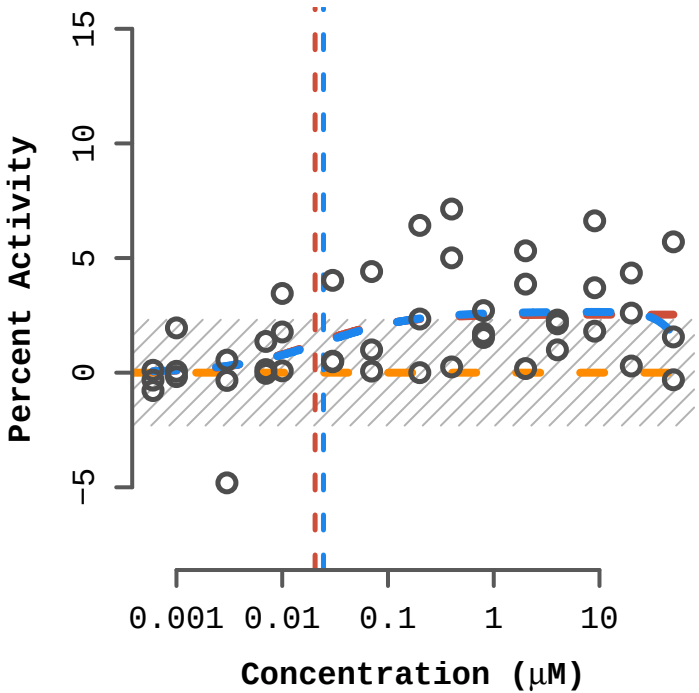
	tp	ga	gw
val:	4.29	−1.66	1.24
sd:	0.65	0.393	0.908

GAIN-LOSS MODEL (in blue):

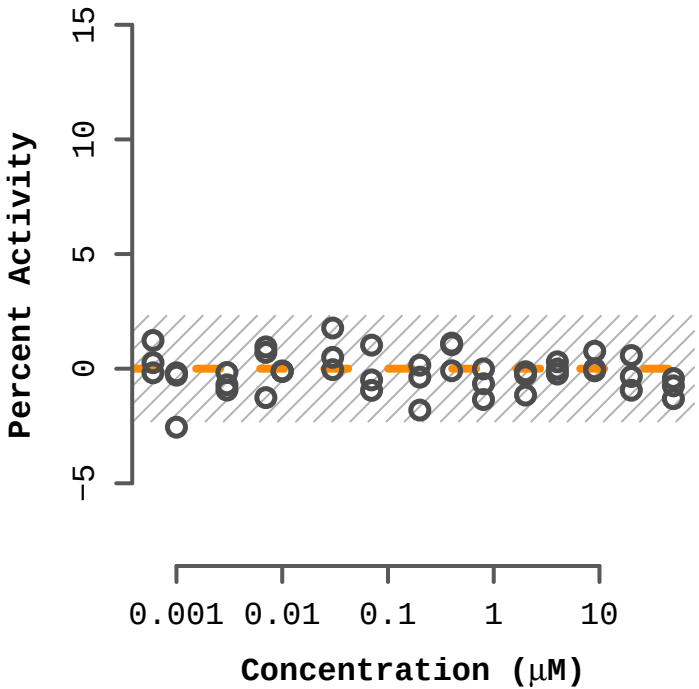
	tp	ga	gw	la	lw
val:	4.29	−1.66	1.24	3.65	4.73
sd:	0.65	0.393	0.908	8370	20300

	CNST	HILL	GNLS
AIC:	253.66	217.87	221.87
PROB:	0	0.88	0.12
RMSE:	3.88	2.46	2.46

MAX_MEAN: 5.35 **MAX_MED:** 6.27 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Aceclofenac
CHID:    45522   CASRN: 89796-99-6
SPID(S): Tox21_110710_1
M4ID:    12484158

HILL MODEL (in red):
      tp       ga       gw
val:  2.53     -1.69    1.09
sd:   0.488    0.531    0.91

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.66     -1.61    0.992    1.76     3.61
sd:   0.58     0.57     0.827    0.364    14.6

      CNST        HILL        GNLS
AIC:  227.02      199.21      202.77
PROB: 0           0.86        0.14
RMSE: 2.96        2           2

MAX_MEAN: 4.13      MAX_MED: 5.01      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

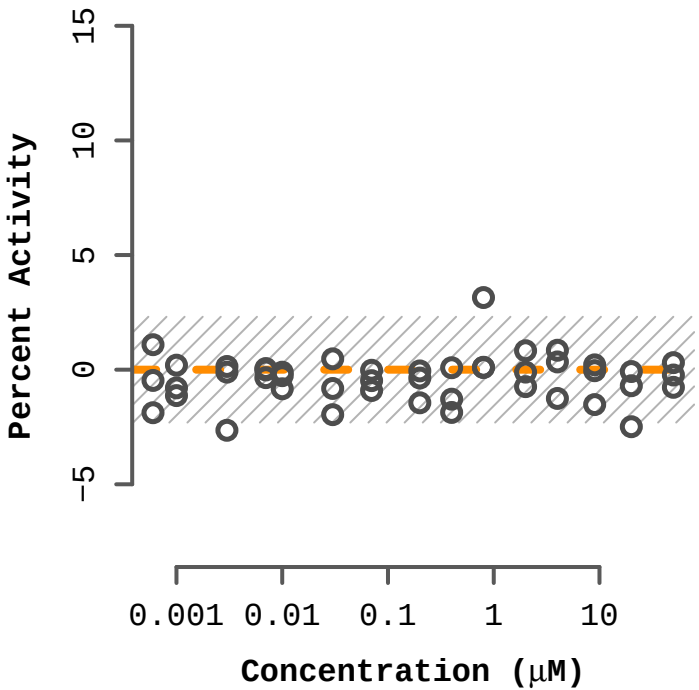
NAME: Iodixanol
CHID: 45523 **CASRN:** 92339-11-2
SPID(S): Tox21_110711_1
M4ID: 12484157

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.743 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

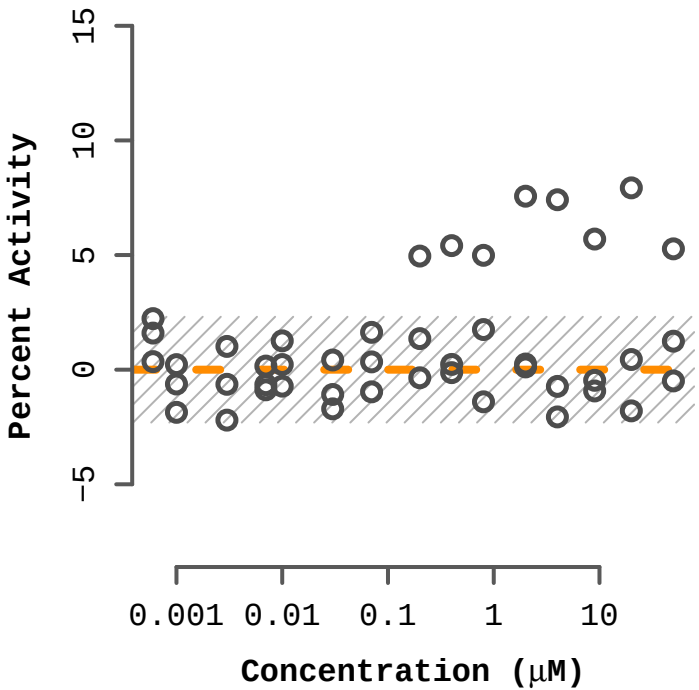
NAME: Meropenem
CHID: 45526 **CASRN:** 96036-03-2
SPID(S): Tox21_113794
M4ID: 12482425

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.339 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

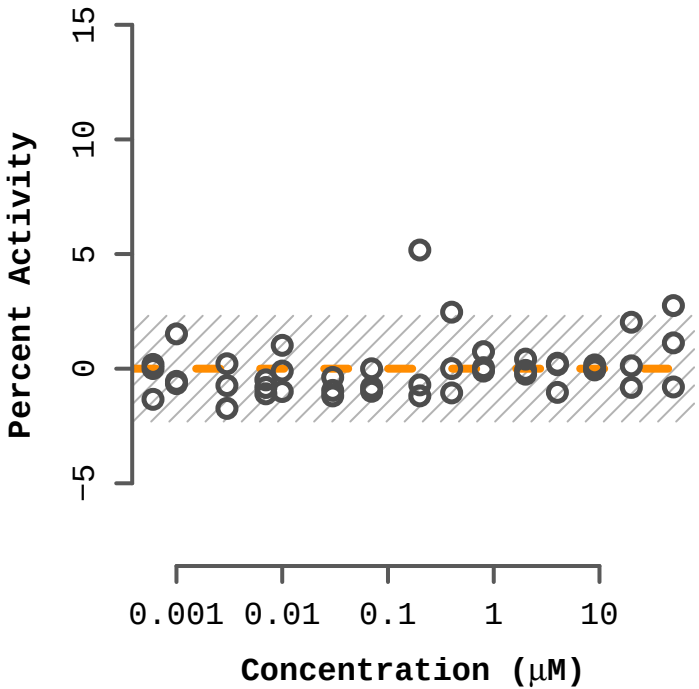
NAME: Meropenem
CHID: 45526 **CASRN:** 96036-03-2
SPID(S): Tox21_110715_1
M4ID: 12484153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.85	NA	NA
PROB:	1	NA	NA
RMSE:	2.83	NA	NA

MAX_MEAN: 2.65 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

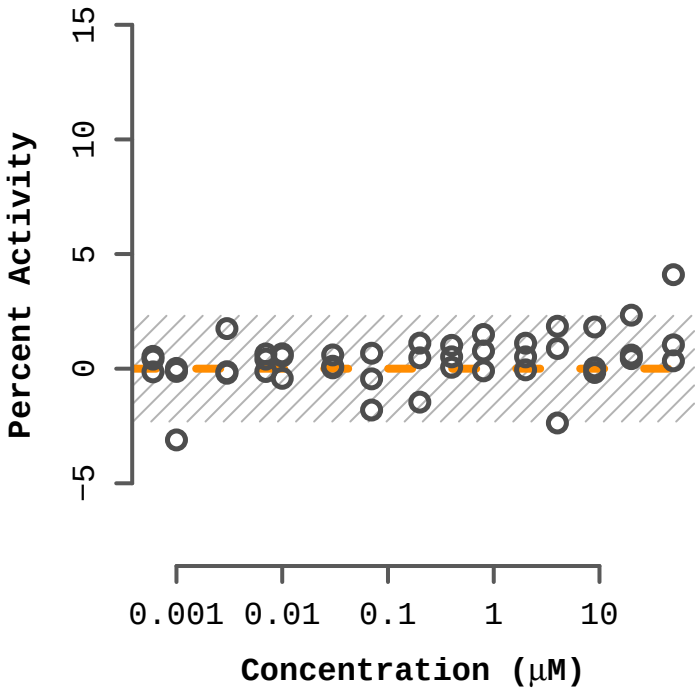
NAME: Lomefloxacin hydrochloride
CHID: 45527 **CASRN:** 98079-52-8
SPID(S): Tox21_110716_1
M4ID: 12484152

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

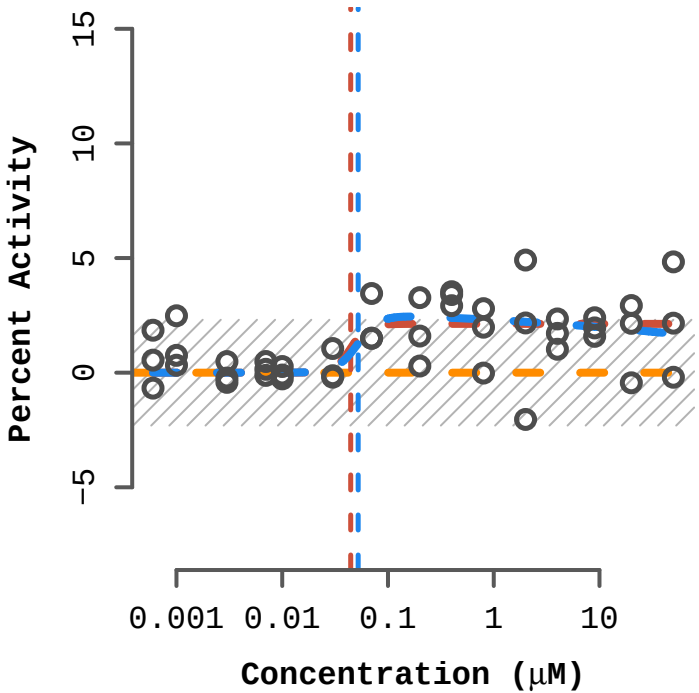
NAME: Dorzolamide hydrochloride
CHID: 45530 **CASRN:** 130693-82-2
SPID(S): Tox21_110720_1
M4ID: 12484150

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Brinzolamide
CHID: 45531 **CASRN:** 138890-62-7
SPID(S): Tox21_110722_1
M4ID: 12484149

HILL MODEL (in red):

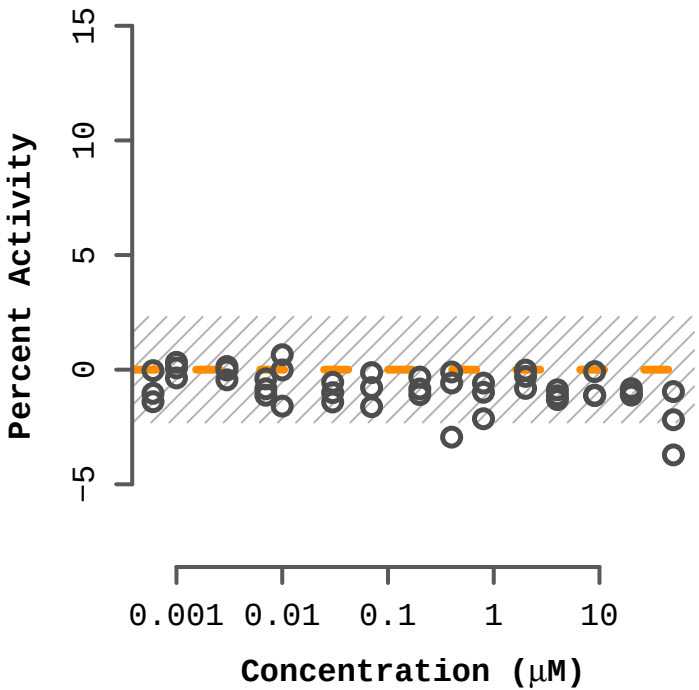
	tp	ga	gw
val:	2.13	−1.35	5.73
sd:	0.244	0.212	6.78

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.74	−1.28	4.29	2.41	0.3
sd:	3.52	0.2	4.44	2.68	1.24

	CNST	HILL	GNLS
AIC:	195.15	155.06	158.42
PROB:	0	0.84	0.16
RMSE:	2.02	1.31	1.31

MAX_MEAN: 3.29 **MAX_MED:** 3.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

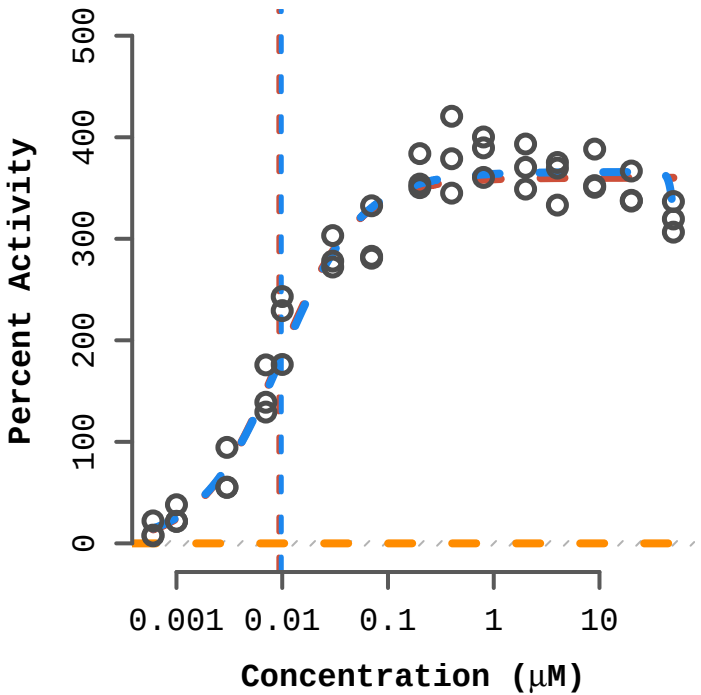
NAME: Nafronyl oxalate
CHID: 45533 **CASRN:** 3200-06-4
SPID(S): Tox21_110724_1
M4ID: 12484148

HILL MODEL: Not applicable.

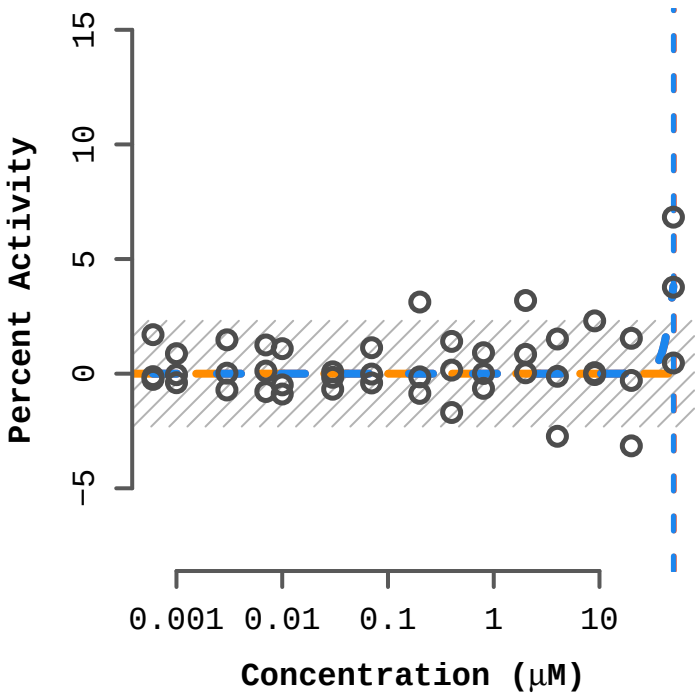
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

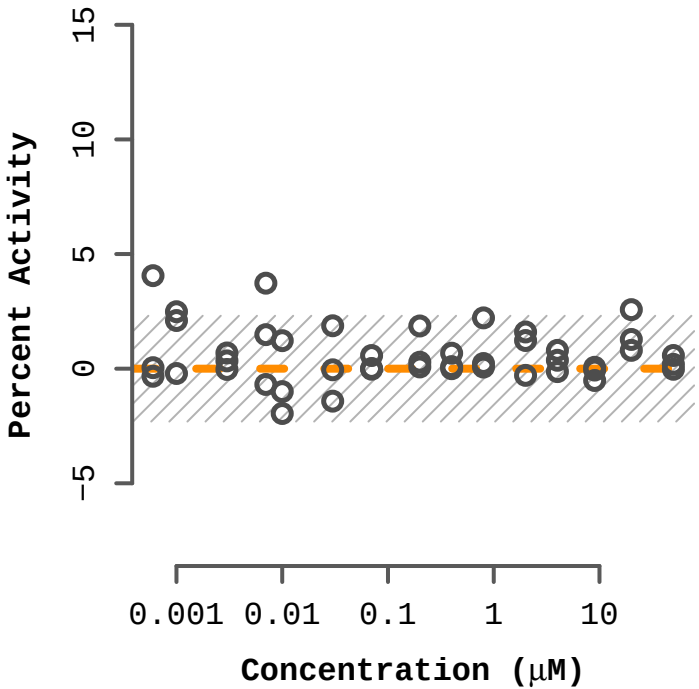
MAX_MEAN: 0.0139 **MAX_MED:** 0.0776 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Flunisolide
CHID:    45534   CASRN: 3385-03-3
SPID(S): Tox21_110725_1
M4ID:    12484147

HILL MODEL (in red):
      tp       ga       gw
val:  360      -2.03    1.18
sd:   5.81     0.0432   0.111

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  366      -2.01    1.14     1.75     15.9
sd:   5.6      0.0408   0.097    0.0124   3.87

      CNST        HILL        GNLS
AIC:  649.88      431.87      426.31
PROB: 0           0.06        0.94
RMSE: 294         26.24       23.94

MAX_MEAN: 383       MAX_MED: 390       BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Disopyramide
CHID:    45536   CASRN: 3737-09-5
SPID(S): Tox21_110727_1
M4ID:    12484146

HILL MODEL (in red):
      tp       ga       gw
val:  8.17     1.71     7.84
sd:   8.81     0.11     27.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.05     1.7      8        3.43     0.726
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  165.17      163.38      167.38
PROB: 0.26        0.65        0.09
RMSE: 1.69        1.4         1.4

MAX_MEAN: 3.69      MAX_MED: 3.77      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

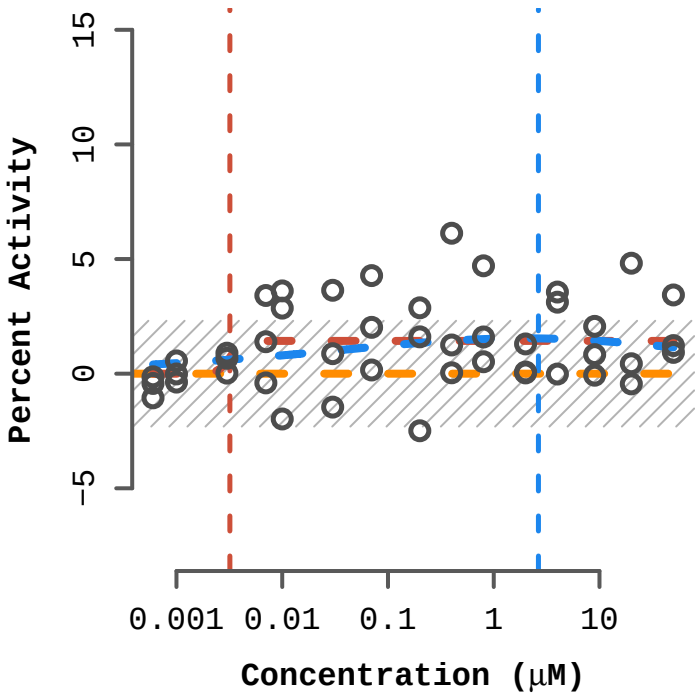
NAME: Cefotiam hydrochloride
CHID: 45538 CASRN: 66309-69-1
SPID(S): Tox21_110730_1
M4ID: 12484144

HILL MODEL: Not applicable.

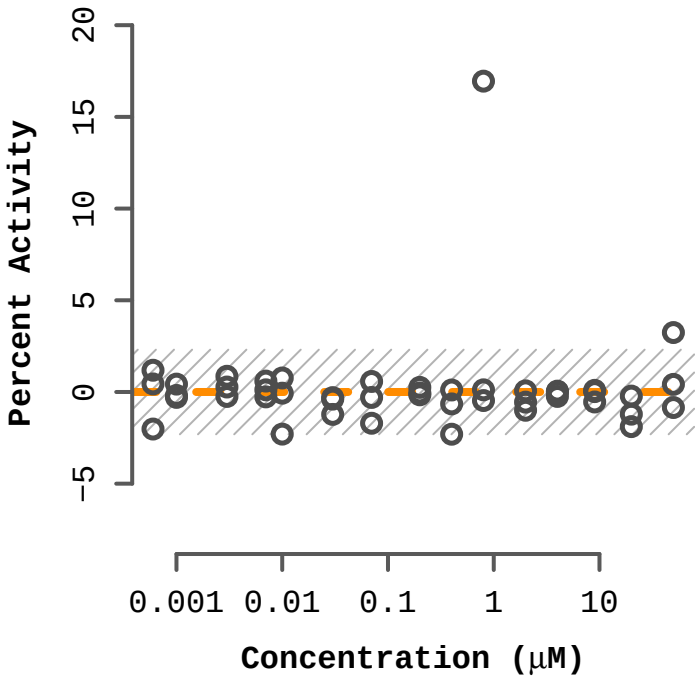
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 2.1 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tocainide hydrochloride
CHID:    45540   CASRN: 35891-93-1
SPID(S): Tox21_110732_1
M4ID:    12484143

HILL MODEL (in red):
      tp       ga       gw
val:  1.43     -2.49    8
sd:   0.309    0.247    64.8

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.55     0.423    0.3      0.673    0.376
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  202.41      188.1       195.24
PROB: 0           0.97        0.03
RMSE: 2.25        1.77        1.81

MAX_MEAN: 2.47      MAX_MED: 3.12      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

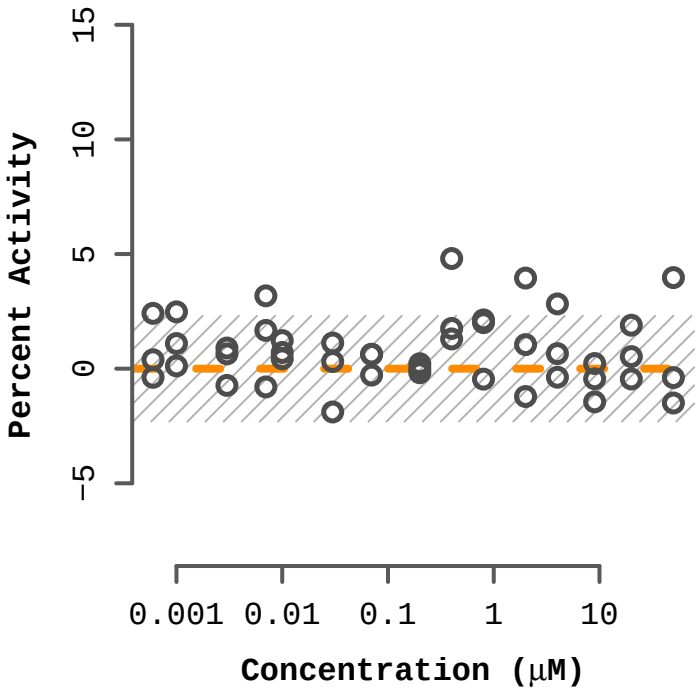
NAME: Methylatropine nitrate
CHID: 45543 **CASRN:** 52-88-0
SPID(S): Tox21_110735_1
M4ID: 12484142

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.79	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 5.53 **MAX_MED:** 0.441 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

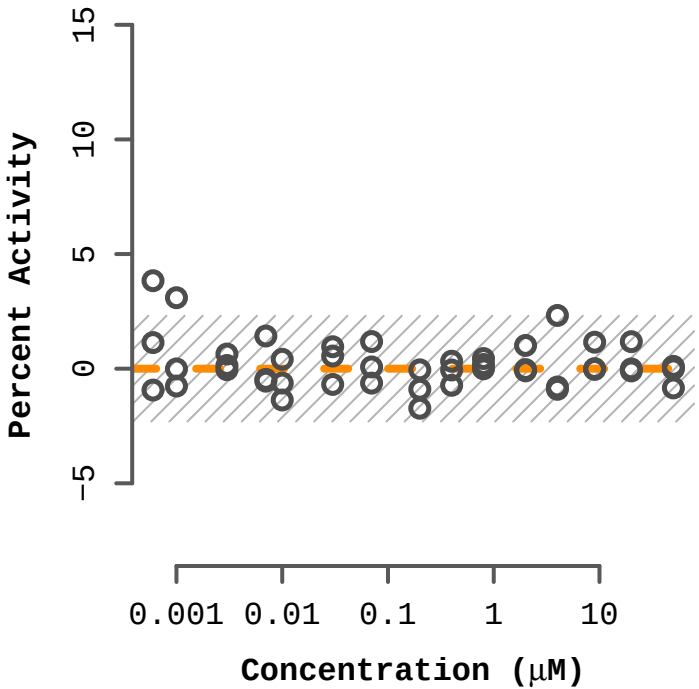
NAME: Amprolium hydrochloride
CHID: 45547 CASRN: 137-88-2
SPID(S): Tox21_110740_1
M4ID: 12484141

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 2.62 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

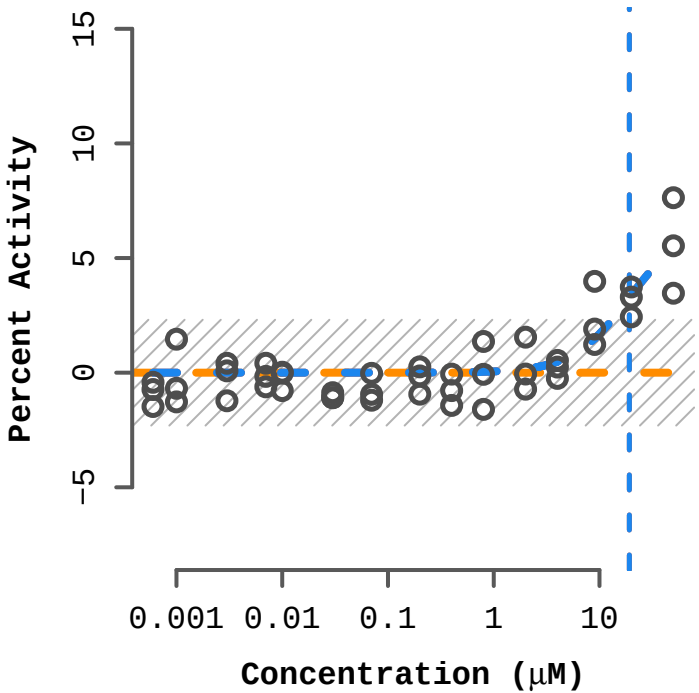
NAME: Cloxacillin sodium
CHID: 45551 CASRN: 642-78-4
SPID(S): Tox21_110744_1
M4ID: 12484138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethylcarbamazine citrate
CHID: 45555 **CASRN:** 1642-54-2
SPID(S): Tox21_110748_1
M4ID: 12484136

HILL MODEL (in red):

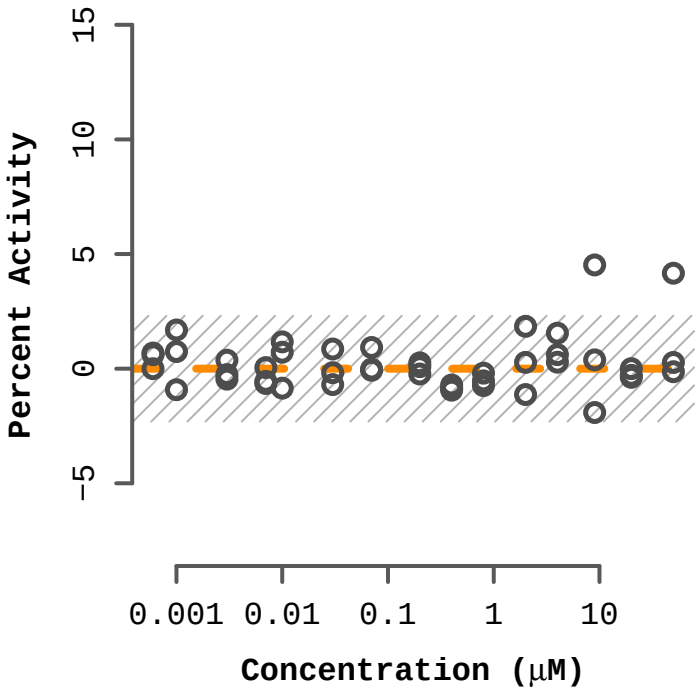
	tp	ga	gw
val:	6.53	1.28	1.62
sd:	2.3	0.234	0.57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.53	1.28	1.62	3.1	5.61
sd:	2.3	0.234	0.57	1870	7530

	CNST	HILL	GNLS
AIC:	179.34	136.01	140.01
PROB:	0	0.88	0.12
RMSE:	2	0.98	0.98

MAX_MEAN: 5.55 **MAX_MED:** 5.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

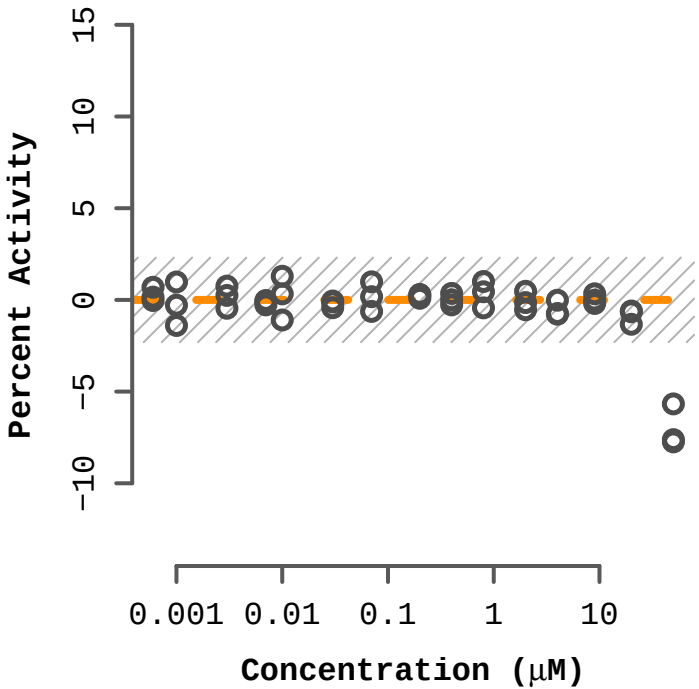
NAME: Oxalamine citrate
CHID: 45556 **CASRN:** 1949-20-8
SPID(S): Tox21_110749_1
M4ID: 12484135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.748 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

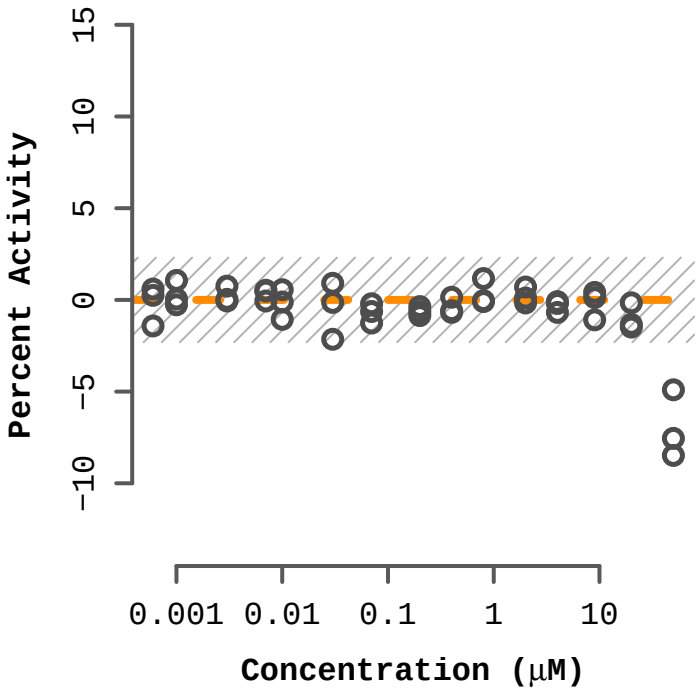
NAME: Thioproperazine dimethanesulfonate
CHID: 45558 **CASRN:** 2347-80-0
SPID(S): Tox21_110751_1
M4ID: 12484134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 0.34 **MAX_MED:** 0.447 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

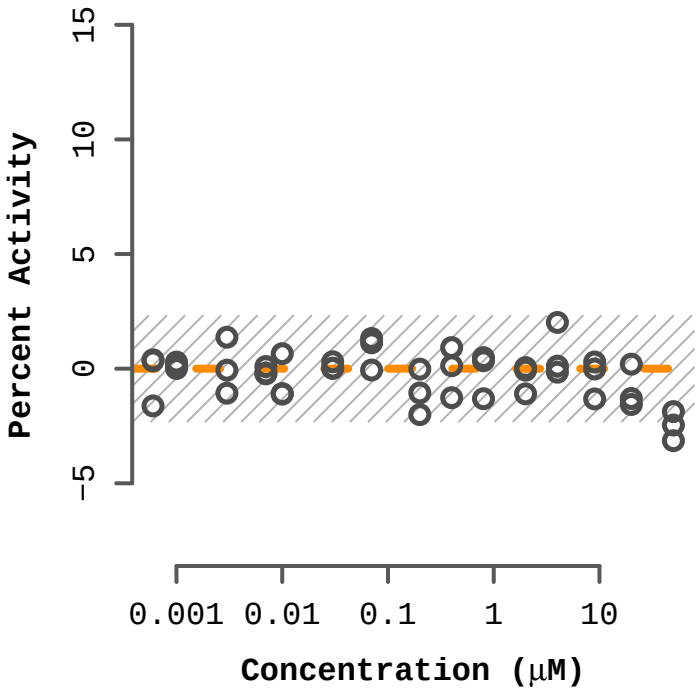
NAME: Trimeprazine tartrate
CHID: 45560 **CASRN:** 4330-99-8
SPID(S): Tox21_110755_1
M4ID: 12484132

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 0.348 **MAX_MED:** 0.482 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

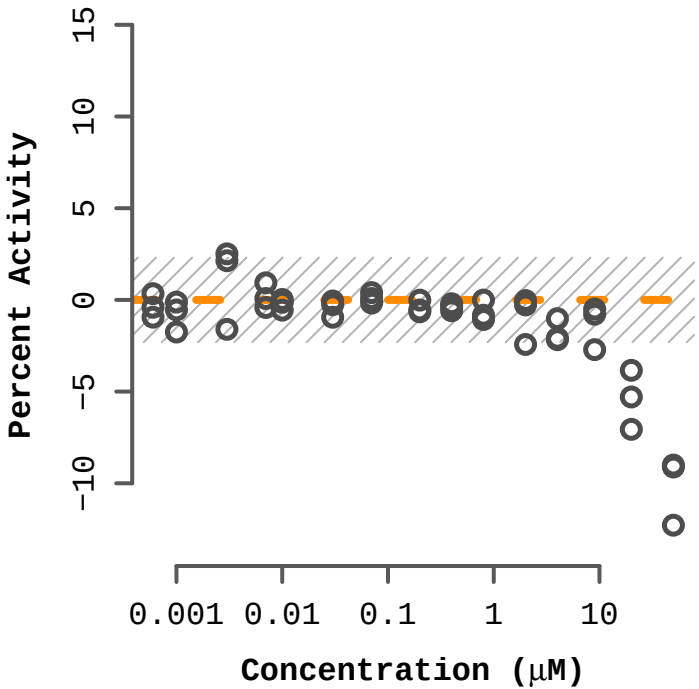
NAME: Alverine citrate
CHID: 45562 **CASRN:** 5560-59-8
SPID(S): Tox21_110757_1
M4ID: 12484131

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.796 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

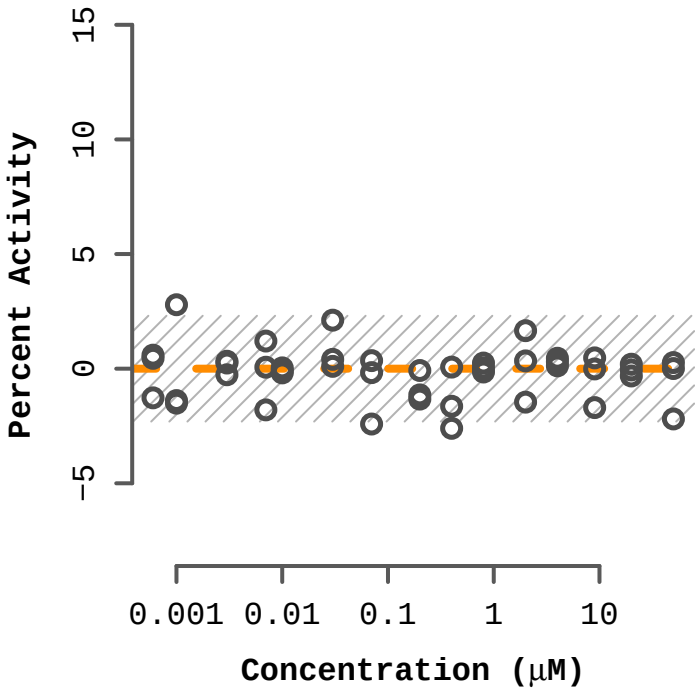
NAME: Quinacrine dihydrochloride dihydrate
CHID: 45565 **CASRN:** 6151-30-0
SPID(S): Tox21_110762_1
M4ID: 12484128

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.18	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

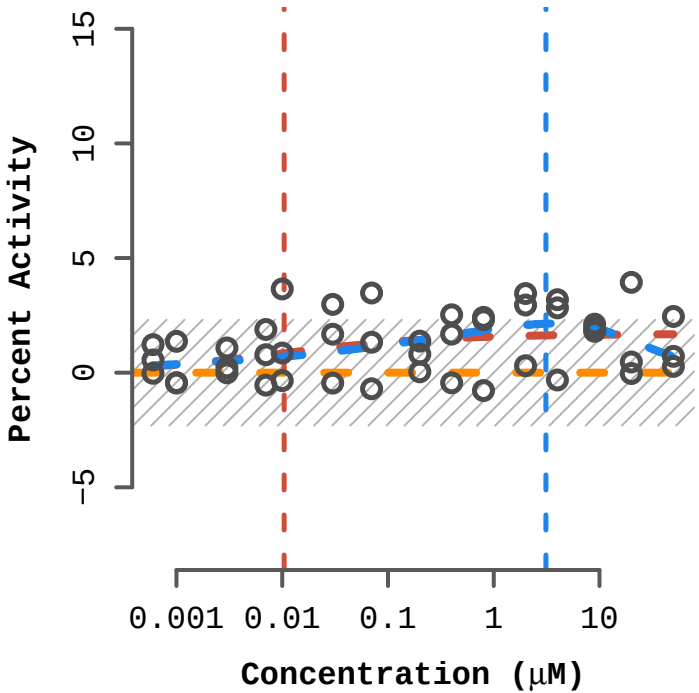
NAME: Meclofenamate sodium
CHID: 45567 **CASRN:** 6385-02-0
SPID(S): Tox21_110764_1
M4ID: 12484127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 0.452 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nafcillin sodium monohydrate
CHID: 45570 CASRN: 7177-50-6
SPID(S): Tox21_110767_1
M4ID: 12484126

HILL MODEL (in red):

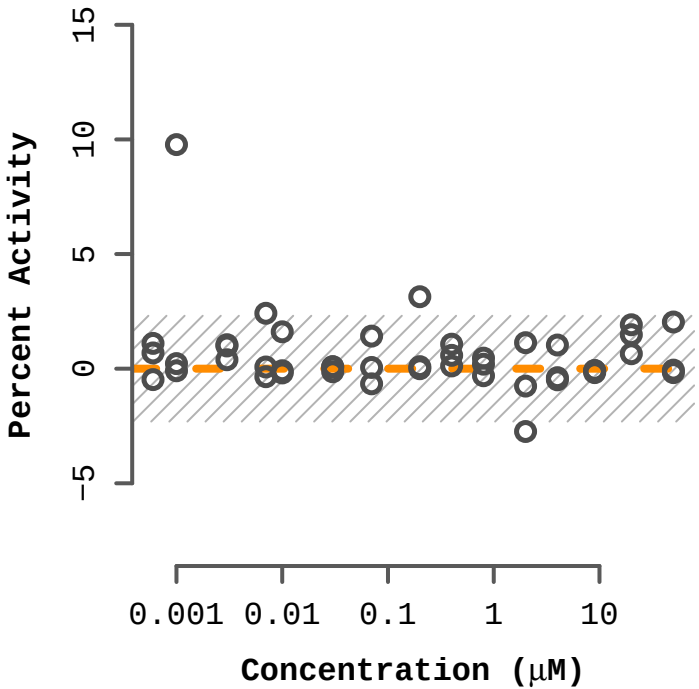
	tp	ga	gw
val:	1.69	−1.98	0.572
sd:	0.442	0.83	0.507

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.73	0.493	0.307	1.25	1.28
sd:	6.58	3.42	0.182	0.482	0.88

	CNST	HILL	GNLS
AIC:	185.57	162.8	164.25
PROB:	0	0.67	0.33
RMSE:	1.81	1.28	1.28

MAX_MEAN: 2.24 **MAX_MED:** 2.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

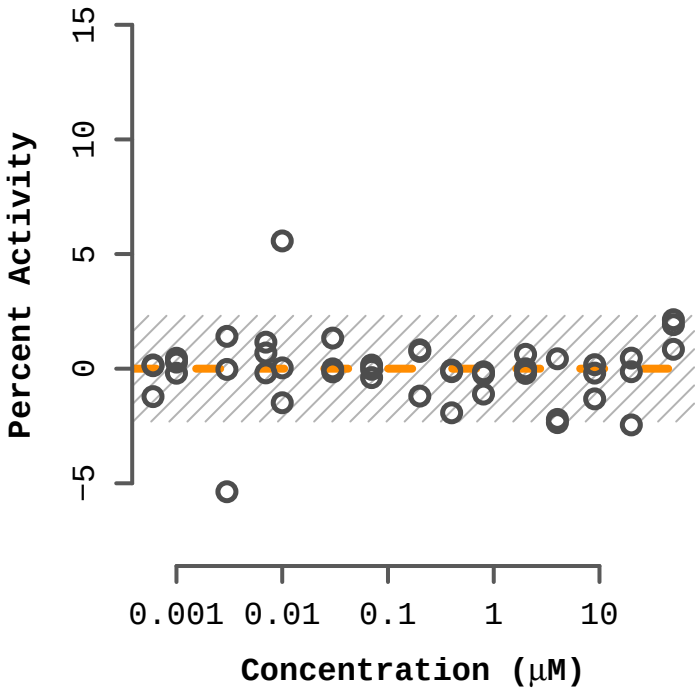
NAME: Carbenoxolone sodium
CHID: 45572 **CASRN:** 7421-40-1
SPID(S): Tox21_110769_1
M4ID: 12484125

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 3.3 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

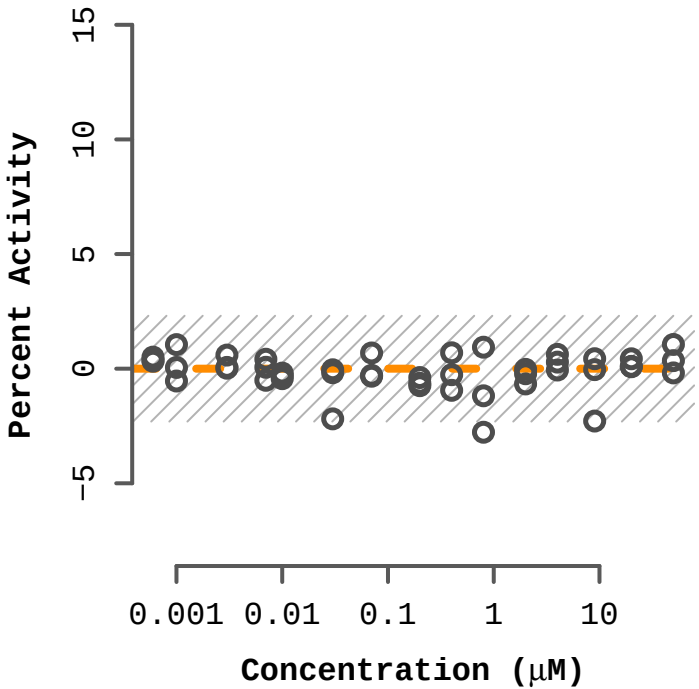
NAME: Cephapirin sodium
CHID: 45574 **CASRN:** 24356-60-3
SPID(S): Tox21_110772_1
M4ID: 12484123

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

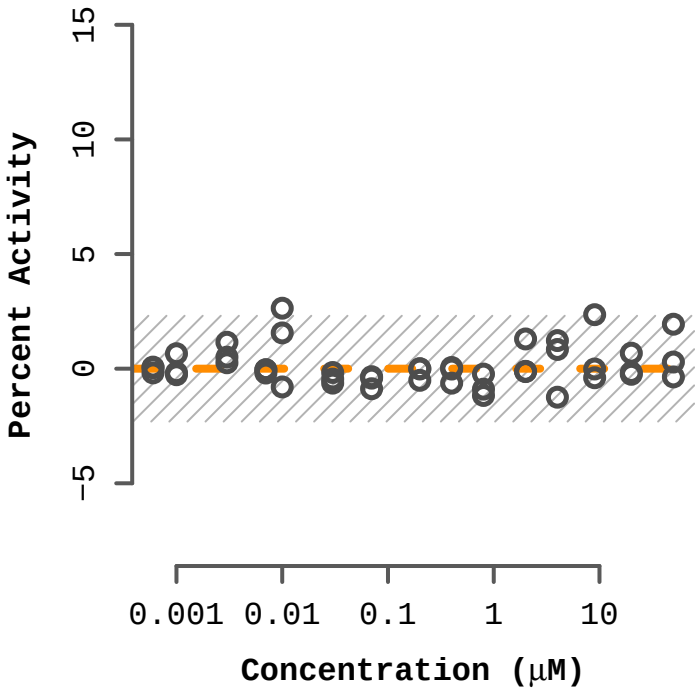
NAME: Morantel tartrate
CHID: 45575 **CASRN:** 26155-31-7
SPID(S): Tox21_110773_1
M4ID: 12484122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.409 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

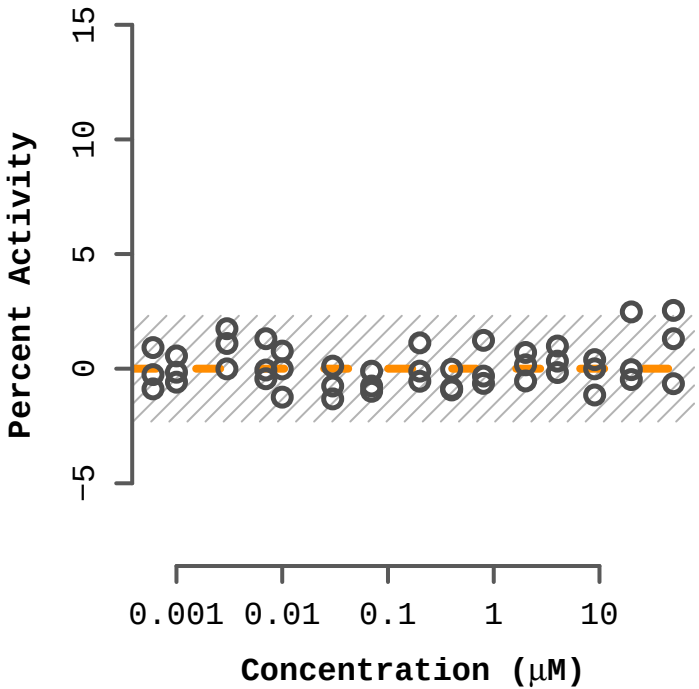
NAME: Naproxen sodium
CHID: 45576 **CASRN:** 26159-34-2
SPID(S): Tox21_110774_1
M4ID: 12484121

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

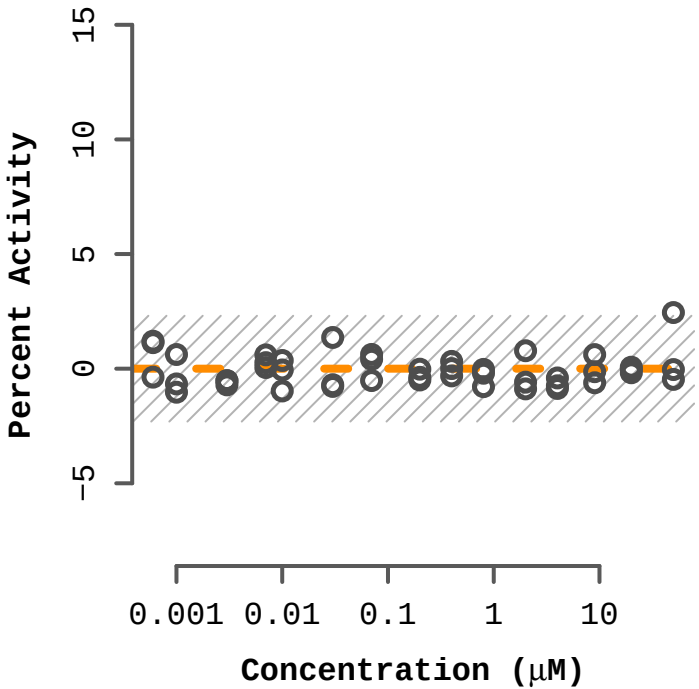
NAME: Yohimbic acid monohydrate
CHID: 45578 **CASRN:** 207801-27-2
SPID(S): Tox21_110776_1
M4ID: 12484119

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

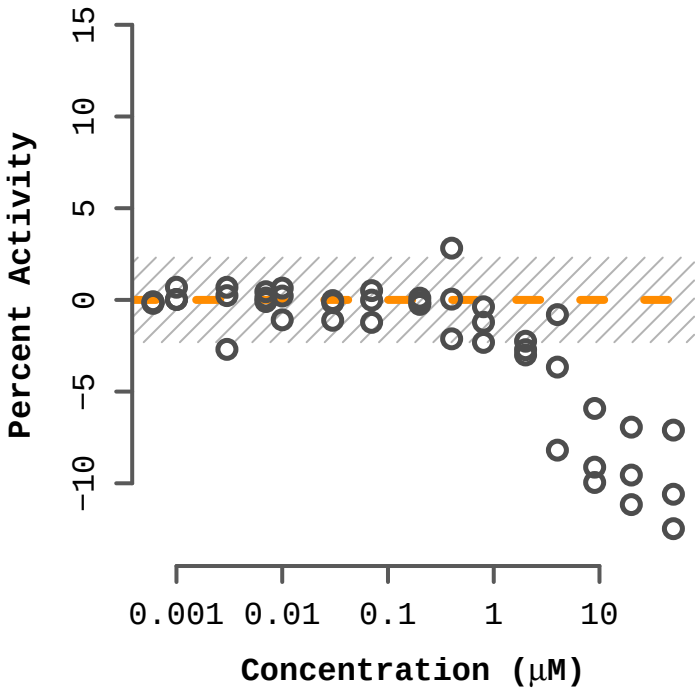
NAME: Metaraminol bitartrate
CHID: 45580 **CASRN:** 33402-03-8
SPID(S): Tox21_110778_1
M4ID: 12484118

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.656 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

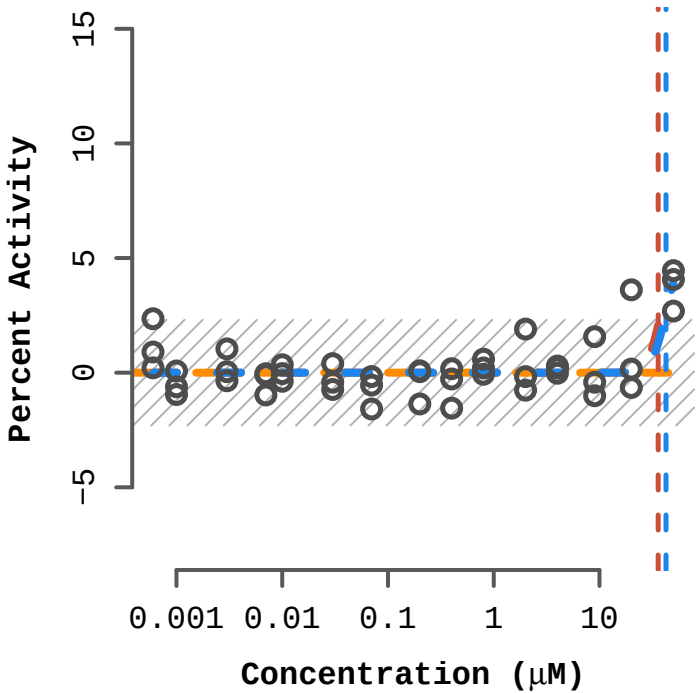
NAME: Ciclopirox olamine
CHID: 45583 **CASRN:** 41621-49-2
SPID(S): Tox21_110781_1
M4ID: 12484117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	256.58	NA	NA
PROB:	1	NA	NA
RMSE:	4.56	NA	NA

MAX_MEAN: 0.248 **MAX_MED:** 0.236 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flunixin meglumine
CHID: 45584 CASRN: 42461-84-7
SPID(S): Tox21_110782_1
M4ID: 12484116

HILL MODEL (in red):

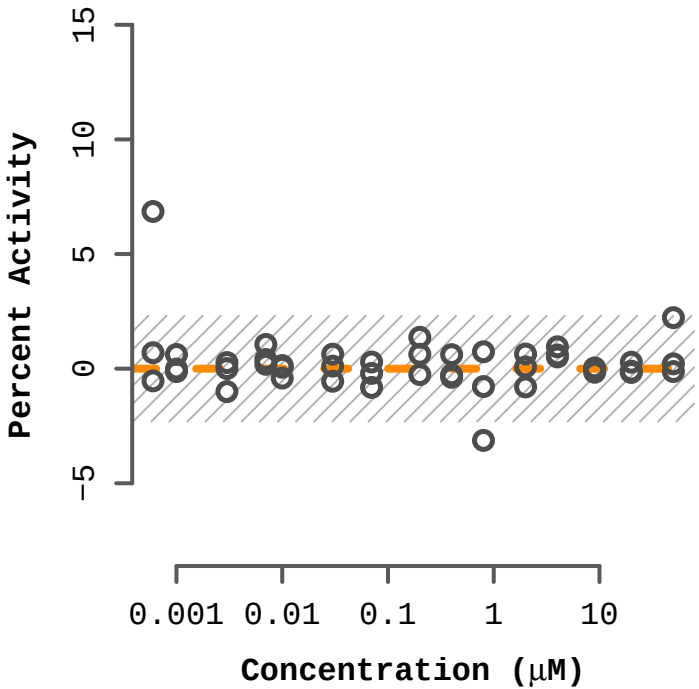
	tp	ga	gw
val:	4.16	1.56	8
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.32	1.63	6.6	3.46	1.03
sd:	37.1	0.421	20	294	168

	CNST	HILL	GNLS
AIC:	144.81	124.16	128.16
PROB:	0	0.88	0.12
RMSE:	1.36	0.96	0.96

MAX_MEAN: 3.74 **MAX_MED:** 4.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

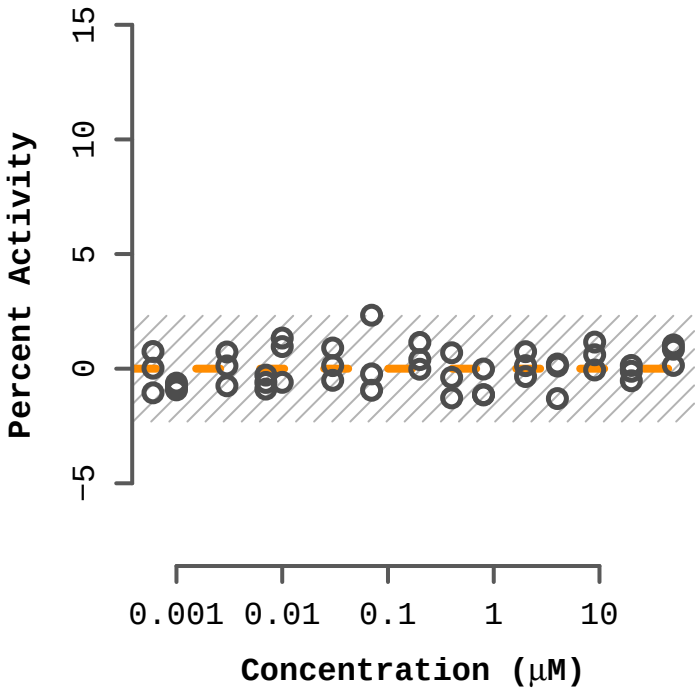
NAME: Fenoprofen calcium salt dihydrate
CHID: 45587 CASRN: 71720-56-4
SPID(S): Tox21_110785_1
M4ID: 12484115

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

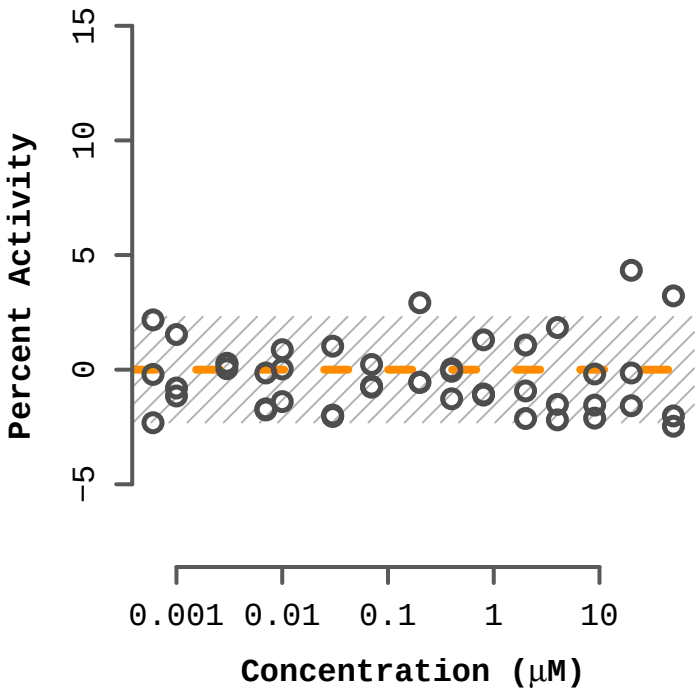
NAME: Betahistine mesylate
CHID: 45588 **CASRN:** 54856-23-4
SPID(S): Tox21_110786_1
M4ID: 12484114

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.677 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

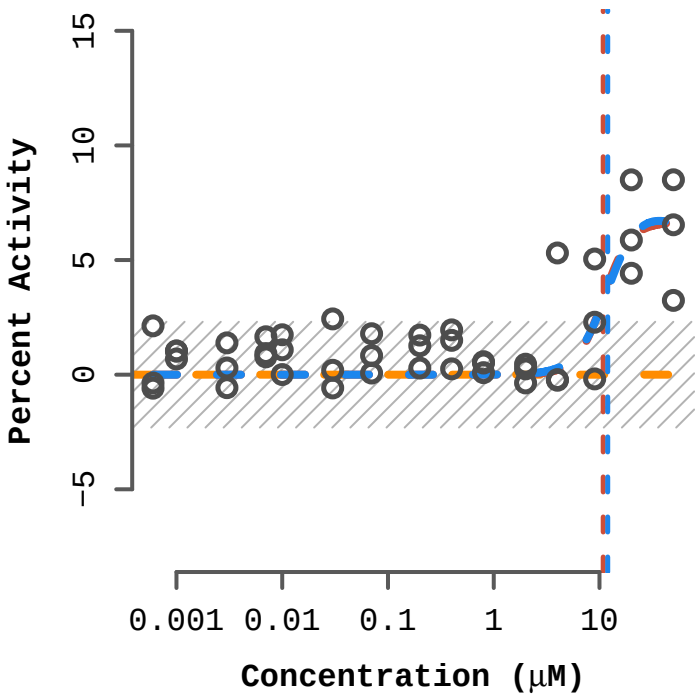
NAME: Cefmetazole sodium
CHID: 45590 **CASRN:** 56796-39-5
SPID(S): Tox21_110788_1
M4ID: 12484112

HILL MODEL: Not applicable.

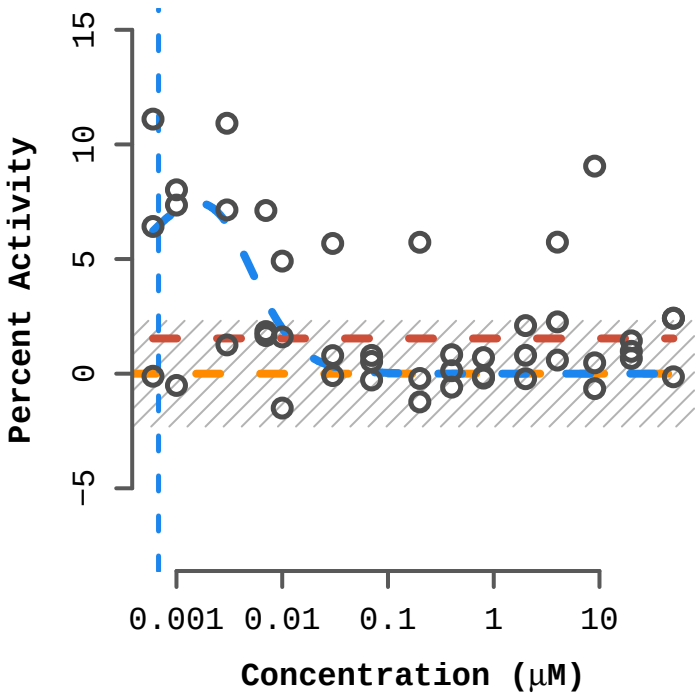
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

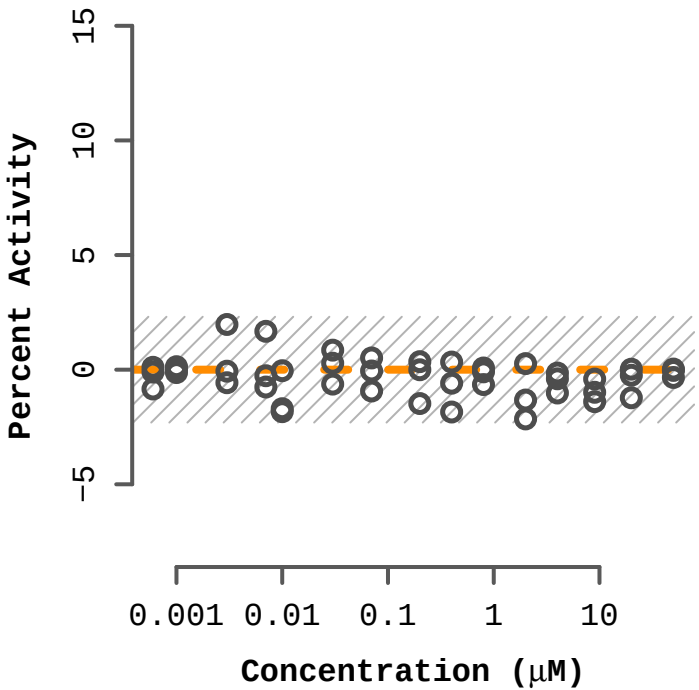
MAX_MEAN: 0.874 **MAX_MED:** 0.252 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Gabexate mesilate
CHID:    45591   CASRN: 56974-61-9
SPID(S): Tox21_110789_1
M4ID:    12484111

HILL MODEL (in red):
      tp       ga       gw
val:  6.66     1.04     3.44
sd:   1.1      0.109    2.43

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.58     1.08     2.94     2.39     1.26
sd:   30       0.663    5.2      21.1     56.3

      CNST        HILL        GNLS
AIC:  210.16      171.12      175.11
PROB: 0           0.88        0.12
RMSE: 2.79        1.52        1.52

MAX_MEAN: 6.27      MAX_MED: 6.54      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tolmetin sodium
CHID:    45594   CASRN: 64490-92-2
SPID(S): Tox21_110792_1
M4ID:    12484110

HILL MODEL (in red):
      tp       ga       gw
val:  1.54     -5.05    4.07
sd:   0.448    1630     3580

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.3     -3.17    0.71     -2.37    1.87
sd:   29.7     2.7      2.25     0.651    3.01

      CNST        HILL        GNLS
AIC:  249.76      242.44      234.11
PROB: 0           0.02        0.98
RMSE: 4.09        3.42        3.05

MAX_MEAN: 6.44      MAX_MED: 7.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

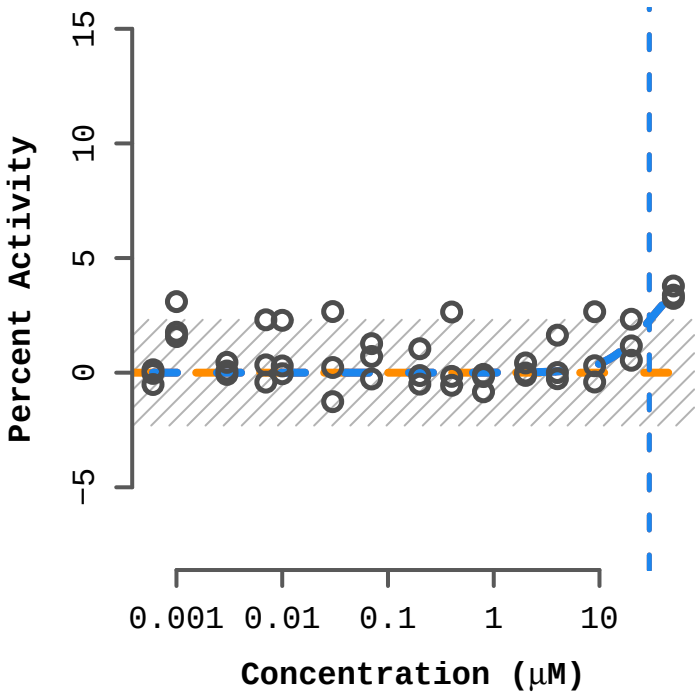
NAME: Moxalactam disodium
CHID: 45595 **CASRN:** 64953-12-4
SPID(S): Tox21_110793_1
M4ID: 12484109

HILL MODEL: Not applicable.

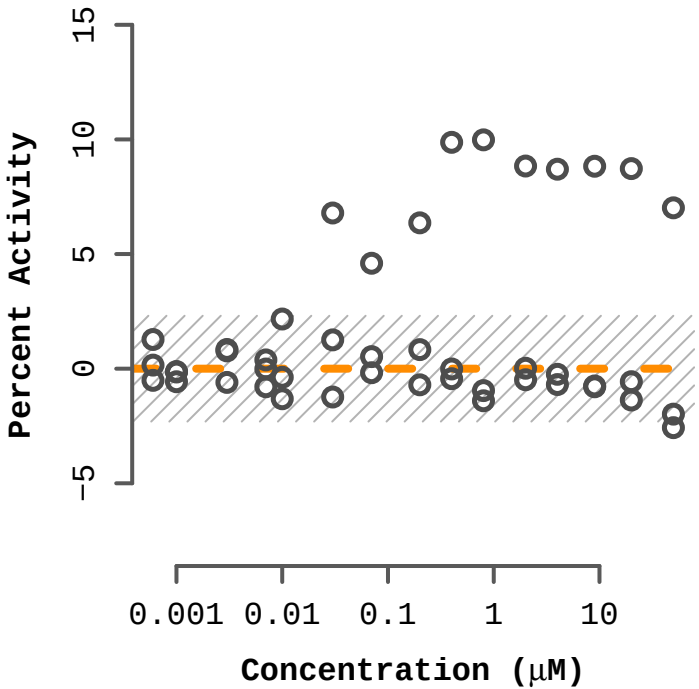
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.447 **MAX_MED:** 0.283 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ketorolac tromethamine
CHID:    45597   CASRN: 74103-07-4
SPID(S): Tox21_110795_1
M4ID:    12484108

HILL MODEL (in red):
      tp       ga       gw
val:  4.54     1.47     2.17
sd:   3.11     0.363    1.99

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.54     1.47     2.17     3.12     5.37
sd:   3.11     0.363    1.99     2040     7740

      CNST        HILL        GNLS
AIC:  163.18      141.25      145.25
PROB: 0           0.88        0.12
RMSE: 1.5         1.13        1.13

MAX_MEAN: 3.47      MAX_MED: 3.38      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

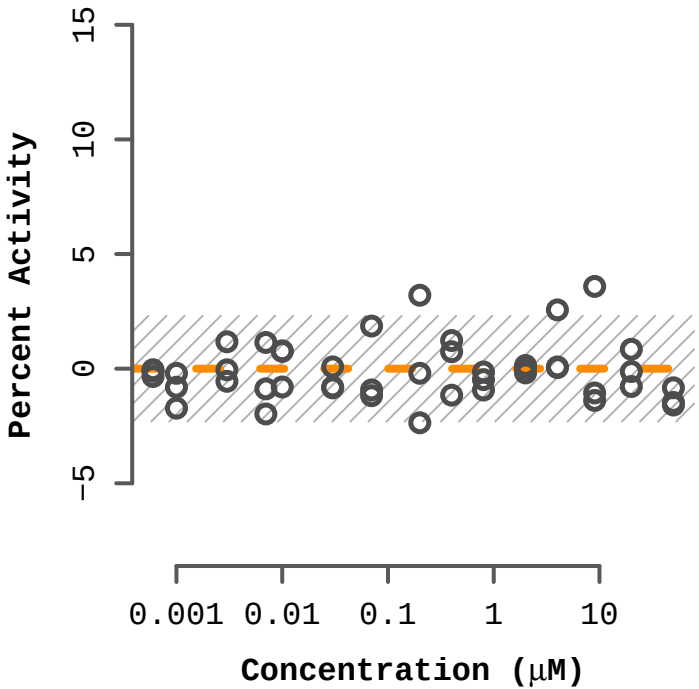
NAME: Doxazosin mesylate
CHID: 45598 **CASRN:** 77883-43-3
SPID(S): Tox21_110796_1
M4ID: 12484107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.25	NA	NA
PROB:	1	NA	NA
RMSE:	3.93	NA	NA

MAX_MEAN: 3.14 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

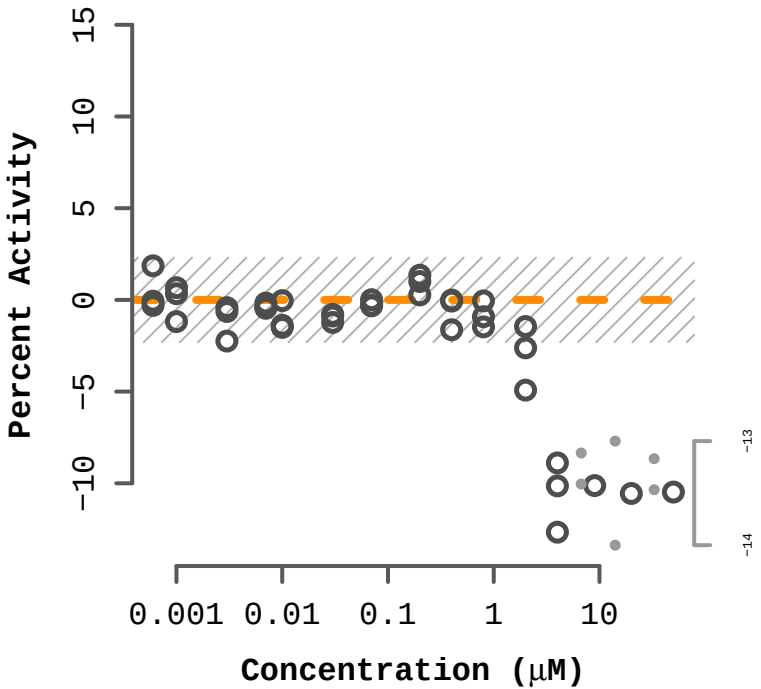
NAME: Lisinopril dihydrate
CHID: 45600 CASRN: 83915-83-7
SPID(S): Tox21_110798_1
M4ID: 12484106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.898 **MAX_MED:** 0.755 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

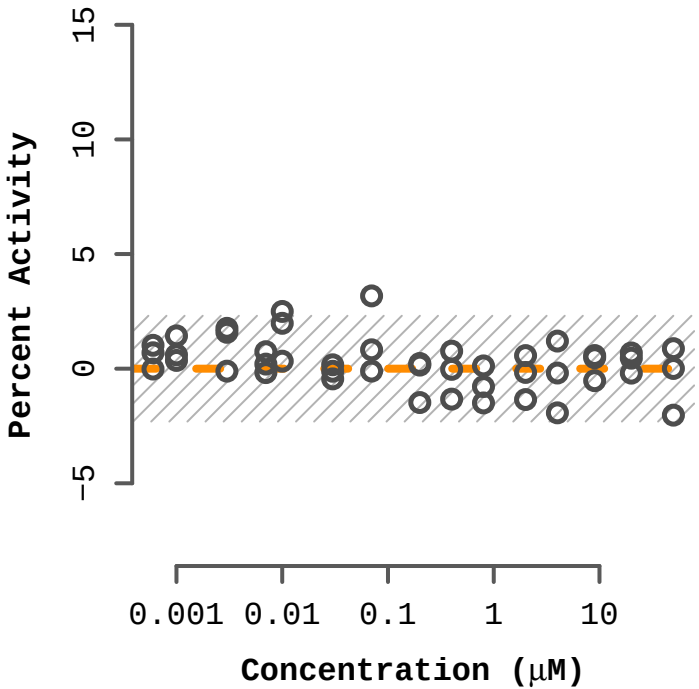
NAME: Clofilium tosylate
CHID: 45601 **CASRN:** 92953-10-1
SPID(S): Tox21_110799_1
M4ID: 12484105 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.72	NA	NA
PROB:	1	NA	NA
RMSE:	6.45	NA	NA

MAX_MEAN: 0.875 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

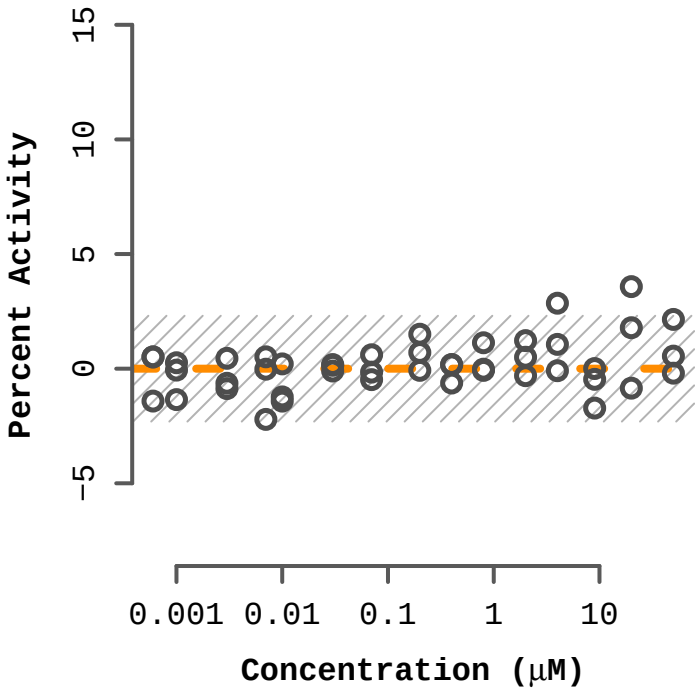
NAME: Nicergoline
CHID: 45607 **CASRN:** 27848-84-6
SPID(S): Tox21_110810_1
M4ID: 12484101

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

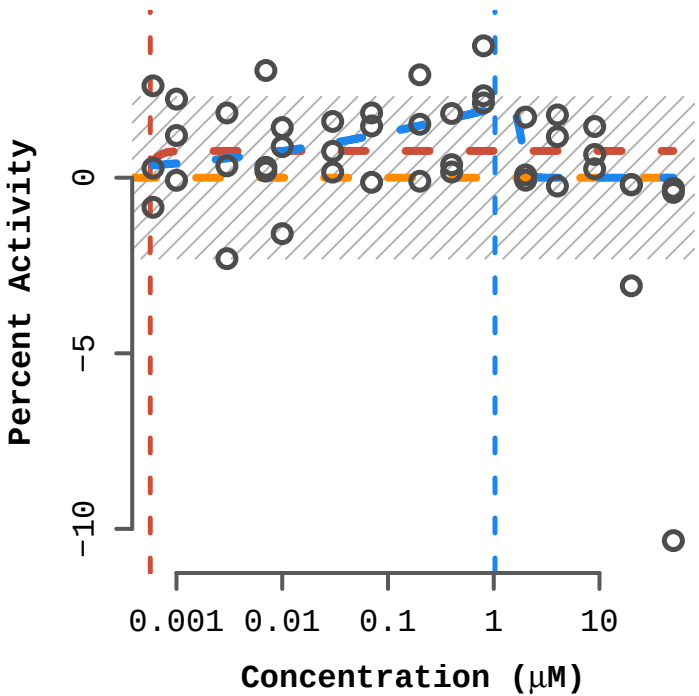
NAME: (1S,9R)-beta-Hydrastine
CHID: 45611 **CASRN:** 29617-43-4
SPID(S): Tox21_110815_1
M4ID: 12484098

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dihydroergotamine
CHID: 45614 **CASRN:** 511-12-6
SPID(S): Tox21_110821_1
M4ID: 12484095

HILL MODEL (in red):

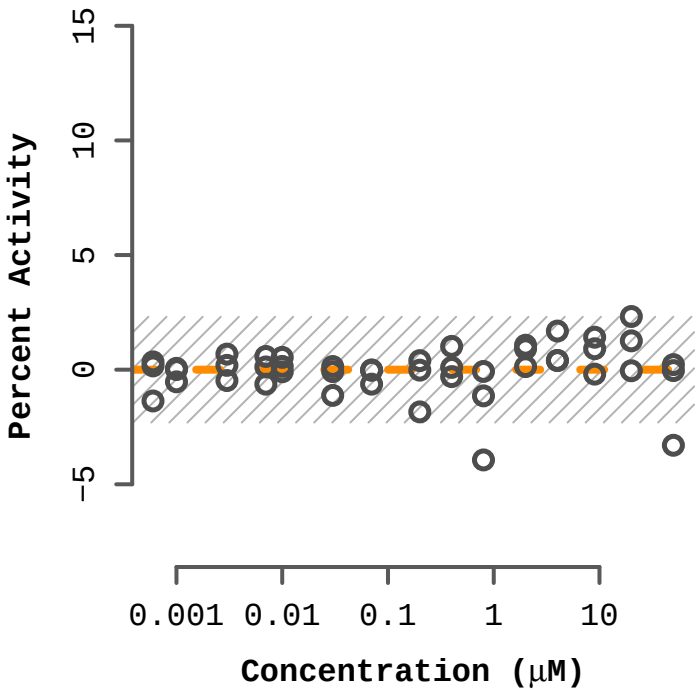
	tp	ga	gw
val:	0.762	−3.25	8
sd:	0.213	0.306	27.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.96	0.0121	0.312	0.262	13.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	184.01	178.3	175.15
PROB:	0.01	0.17	0.82
RMSE:	2.17	2.13	1.97

MAX_MEAN: 2.74 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

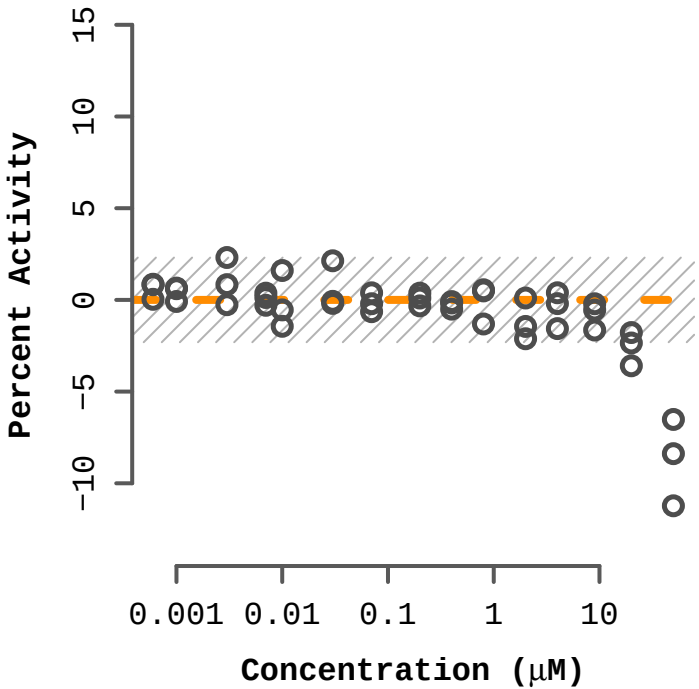
NAME: Fasudil hydrochloride
CHID: 45615 **CASRN:** 105628-07-7
SPID(S): Tox21_110824_1
M4ID: 12484092

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

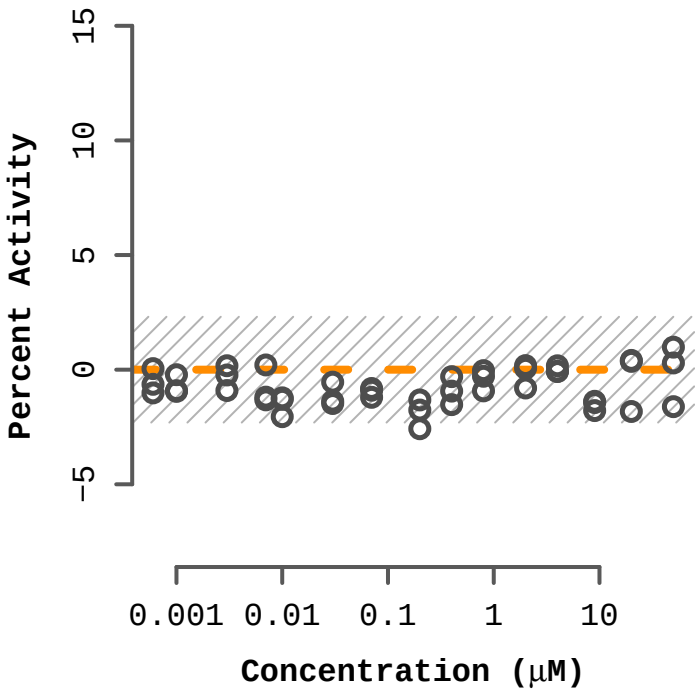
NAME: Flunarizine
CHID: 45616 **CASRN:** 52468-60-7
SPID(S): Tox21_110825_1
M4ID: 12484091

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.8	NA	NA
PROB:	1	NA	NA
RMSE:	2.56	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 0.835 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

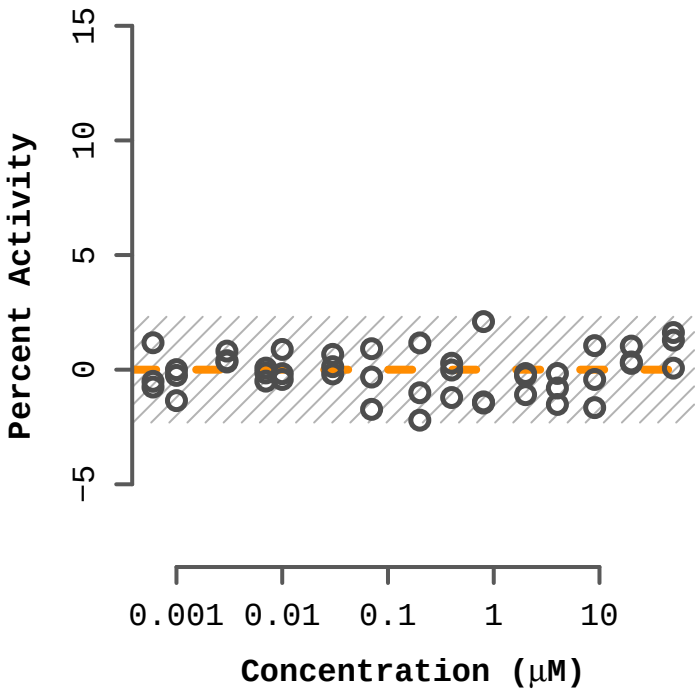
NAME: Miglustat
CHID: 45618 **CASRN:** 72599-27-0
SPID(S): Tox21_110830_1
M4ID: 12484086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.00746 **MAX_MED:** 0.363 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

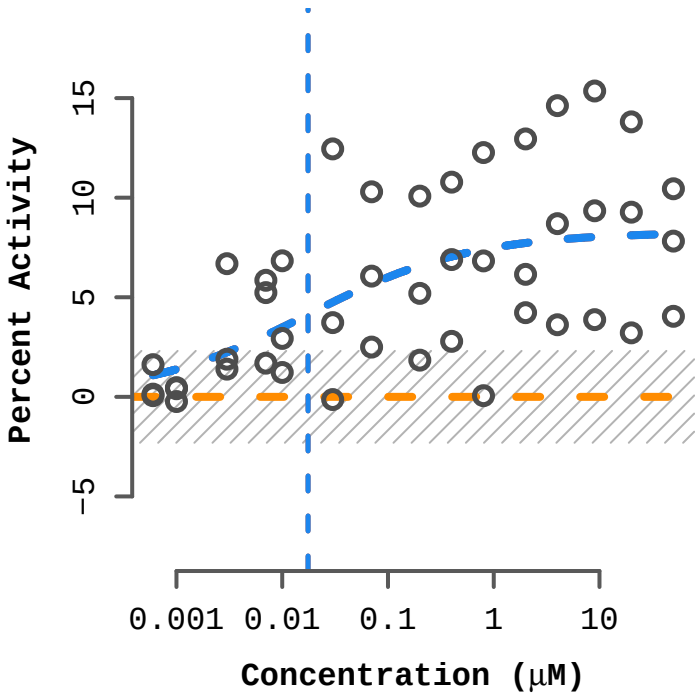
NAME: Enrofloxacin
CHID: 45619 **CASRN:** 93106-60-6
SPID(S): Tox21_110831_1
M4ID: 12484085

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flumequine
CHID: 45623 CASRN: 42835-25-6
SPID(S): Tox21_110840_1
M4ID: 12484079

HILL MODEL (in red):

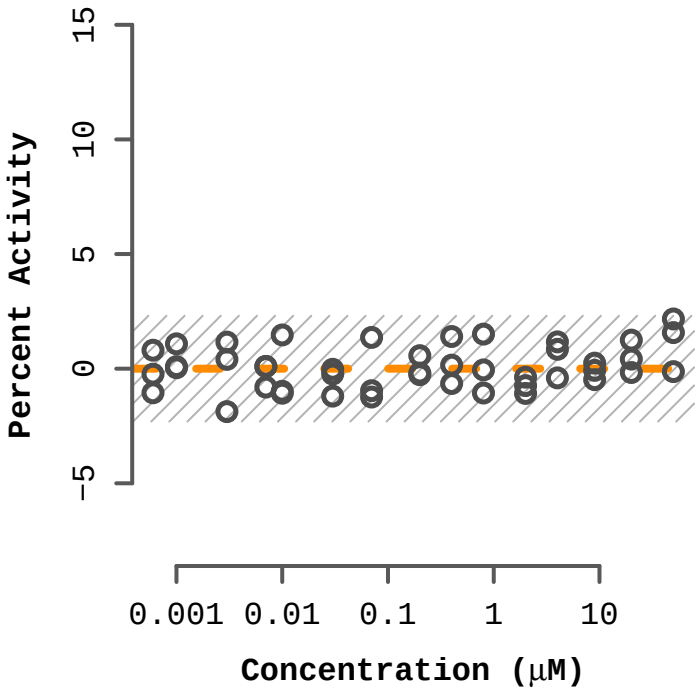
	tp	ga	gw
val:	8.27	−1.76	0.561
sd:	1.56	0.596	0.314

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.27	−1.76	0.561	3.7	9.61
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	310.91	254.51	258.51
PROB:	0	0.88	0.12
RMSE:	7.2	3.59	3.59

MAX_MEAN: 9.53 MAX_MED: 9.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

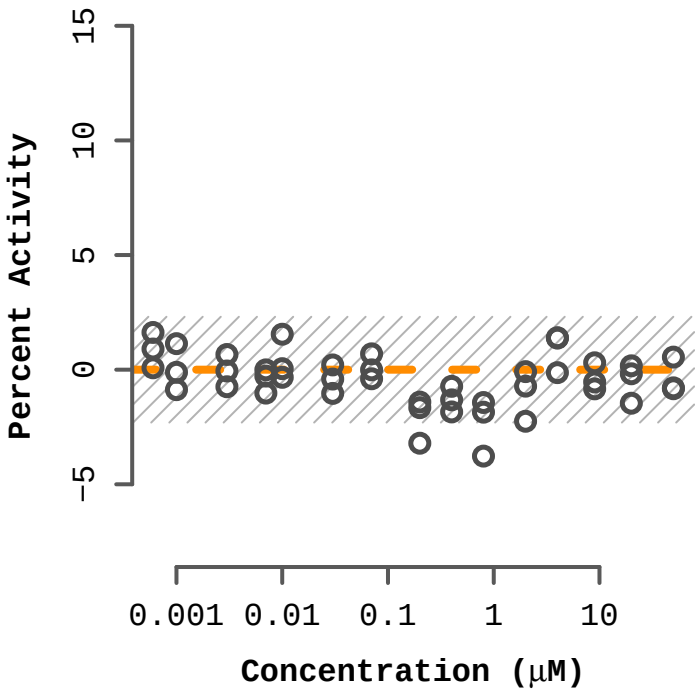
NAME: Dropropizine
CHID: 45624 CASRN: 17692-31-8
SPID(S): Tox21_110842_1
M4ID: 12484077

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

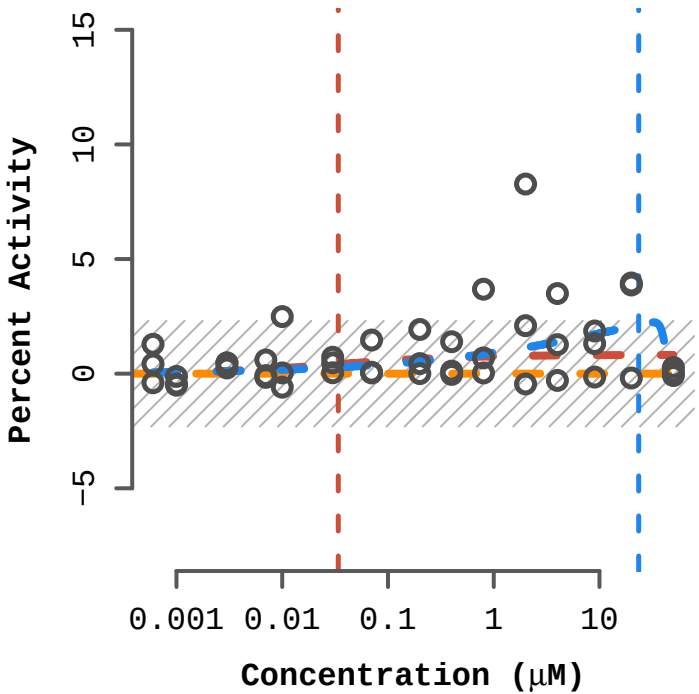
NAME: Oxibendazole
CHID: 45625 **CASRN:** 20559-55-1
SPID(S): Tox21_110844_1
M4ID: 12484075

HILL MODEL: Not applicable.

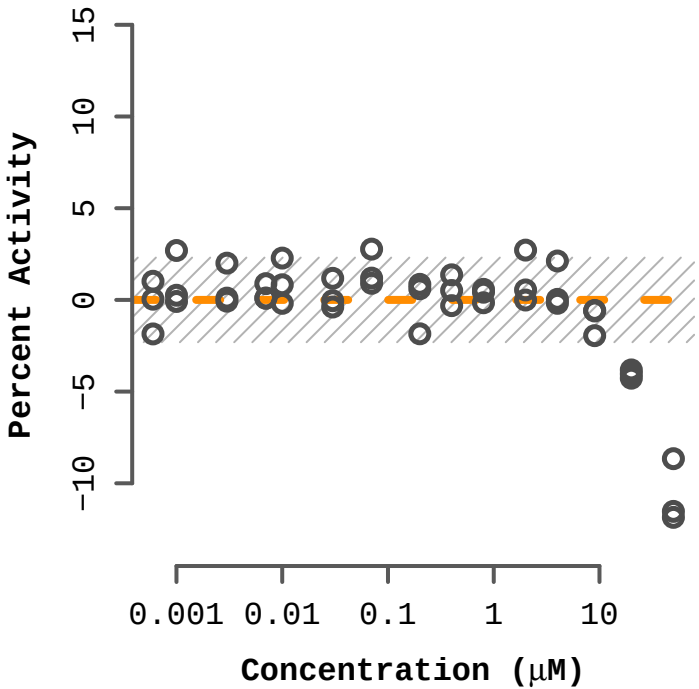
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.882 **MAX_MED:** 1.38 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Betamipron
CHID:    45626   CASRN: 3440-28-6
SPID(S): Tox21_110845_1
M4ID:    12484074

HILL MODEL (in red):
      tp       ga       gw
val:  0.821    -1.47    0.721
sd:   0.363    1.04     0.781

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.25     1.37     0.408    1.62     18
sd:   11.6     4.31     0.205    0.355    79.9

      CNST        HILL        GNLS
AIC:  163.66      157.95      156.65
PROB: 0.02        0.34        0.64
RMSE: 1.86        1.6         1.49

MAX_MEAN: 3.31      MAX_MED: 3.87      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

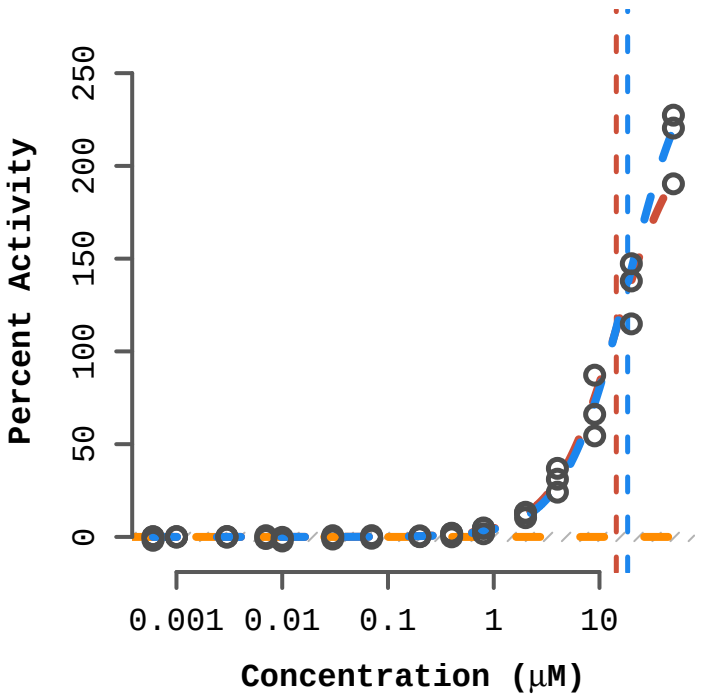
NAME: Bifonazole
CHID: 45631 CASRN: 60628-96-8
SPID(S): Tox21_110850_1
M4ID: 12484070

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.42	NA	NA
PROB:	1	NA	NA
RMSE:	3.18	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxyphenonium bromide
CHID: 45632 CASRN: 50-10-2
SPID(S): Tox21_110851_1
M4ID: 12484069

HILL MODEL (in red):

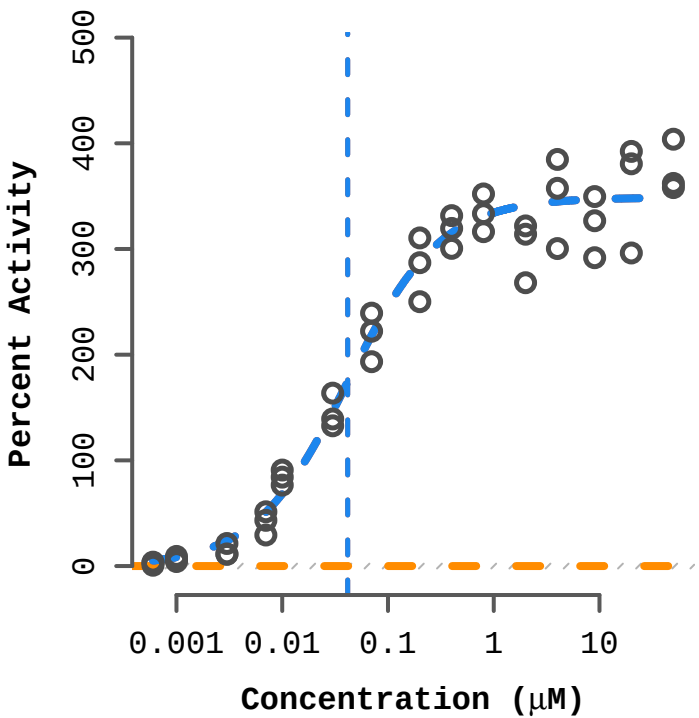
	tp	ga	gw
val:	224	1.16	1.44
sd:	7.89	0.0337	0.0605

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	273	1.27	1.43	2.56	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	479.11	285.67	277.08
PROB:	0	0.01	0.99
RMSE:	68.12	8.72	7.53

MAX_MEAN: 213 MAX_MED: 220 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone valerate
CHID: 45633 **CASRN:** 57524-89-7
SPID(S): Tox21_110853_1
M4ID: 12484067

HILL MODEL (in red):

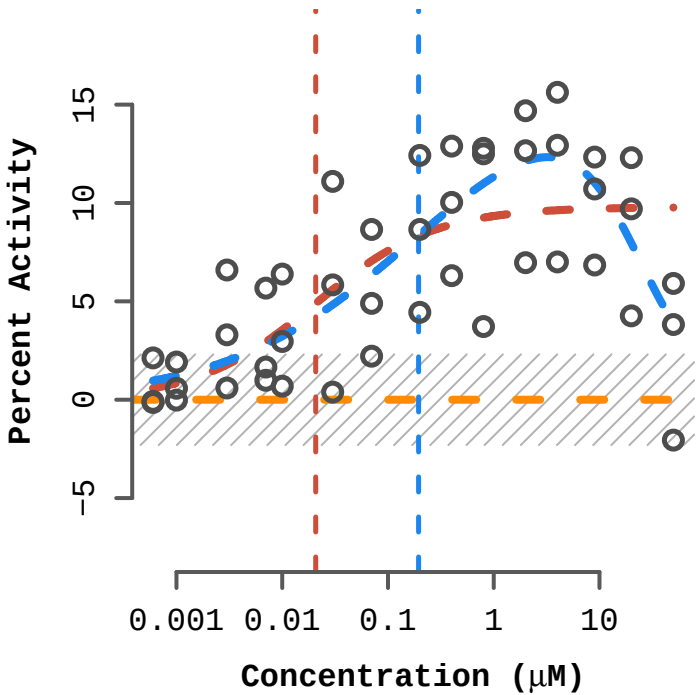
	tp	ga	gw
val:	349	-1.38	0.99
sd:	8.33	0.0502	0.0835

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	349	-1.38	0.99	2.78	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	634.73	425.59	429.59
PROB:	0	0.88	0.12
RMSE:	252.89	25.47	25.47

MAX_MEAN: 375 **MAX_MED:** 381 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Homochlorcyclizine
CHID: 45635 CASRN: 848-53-3
SPID(S): Tox21_110855_1
M4ID: 12484065

HILL MODEL (in red):

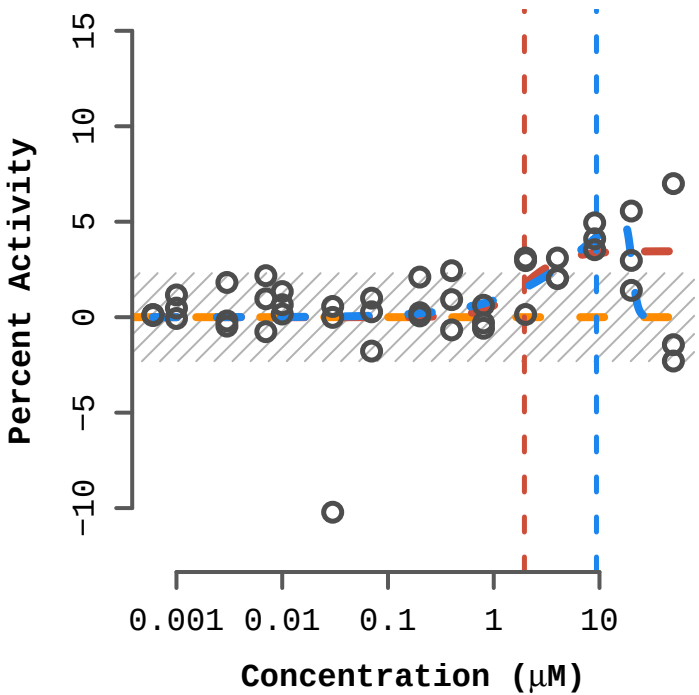
	tp	ga	gw
val:	9.79	−1.68	0.779
sd:	1.05	0.287	0.26

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.8	−0.71	0.483	1.33	1.32
sd:	11.9	1.39	0.235	0.403	0.941

	CNST	HILL	GNLS
AIC:	320.72	253.77	244.1
PROB:	0	0.01	0.99
RMSE:	7.91	3.65	3.07

MAX_MEAN: 11.9 MAX_MED: 12.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diacerein
CHID: 45636 **CASRN:** 13739-02-1
SPID(S): Tox21_110856_1
M4ID: 12484064

HILL MODEL (in red):

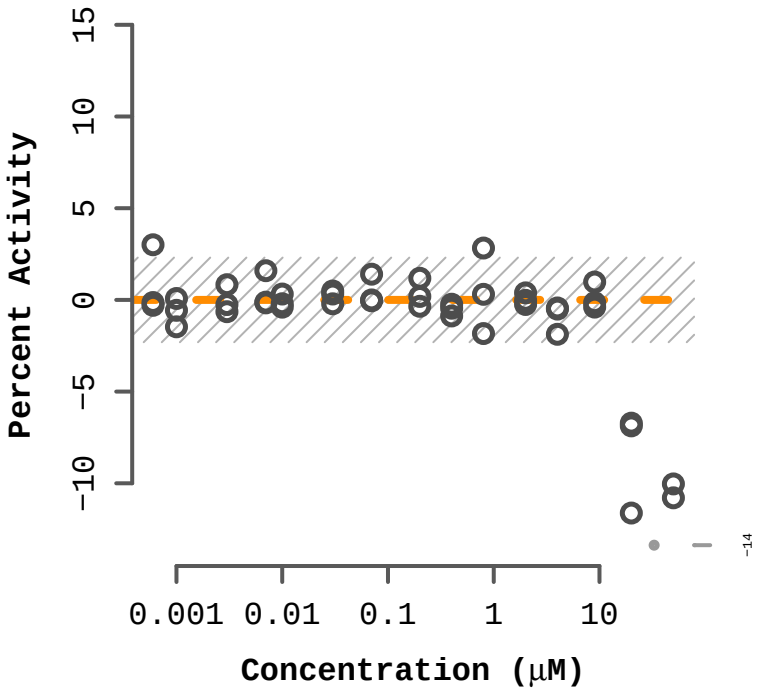
	tp	ga	gw
val:	3.45	0.29	2.3
sd:	0.897	0.234	1.95

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.4	0.972	0.961	1.3	16.4
sd:	14.6	1.51	0.849	0.0271	136

	CNST	HILL	GNLS
AIC:	208.16	186.14	180.41
PROB:	0	0.05	0.95
RMSE:	2.68	2.23	2.15

MAX_MEAN: 4.2 **MAX_MED:** 4.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

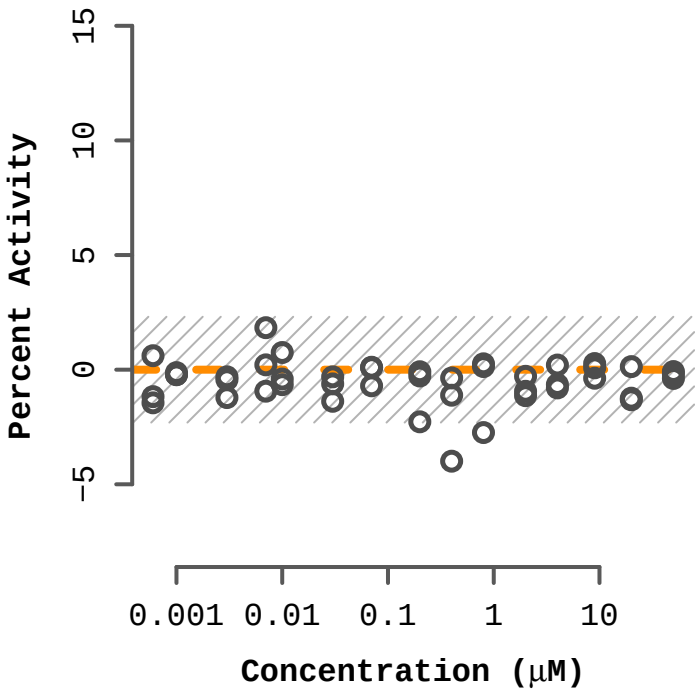
NAME: Suloctdil
CHID: 45638 **CASRN:** 54767-75-8
SPID(S): Tox21_110858_1
M4ID: 12484063 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.23	NA	NA
PROB:	1	NA	NA
RMSE:	3.87	NA	NA

MAX_MEAN: 0.859 **MAX_MED:** 0.323 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

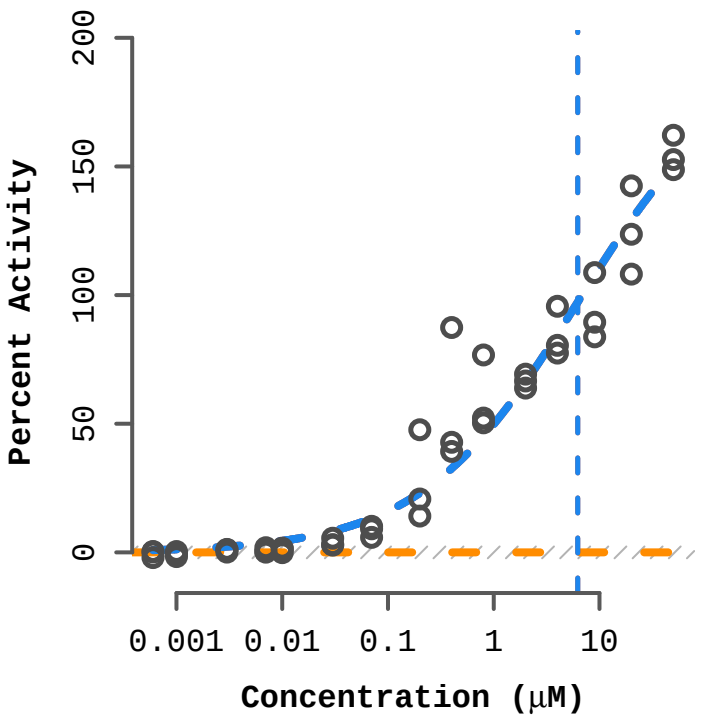
NAME: Butetamate
CHID: 45640 **CASRN:** 14007-64-8
SPID(S): Tox21_110860_1
M4ID: 12484062

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.369 **MAX_MED:** 0.212 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cortodoxone
CHID: 45642 **CASRN:** 152-58-9
SPID(S): Tox21_110867_1
M4ID: 12484057

HILL MODEL (in red):

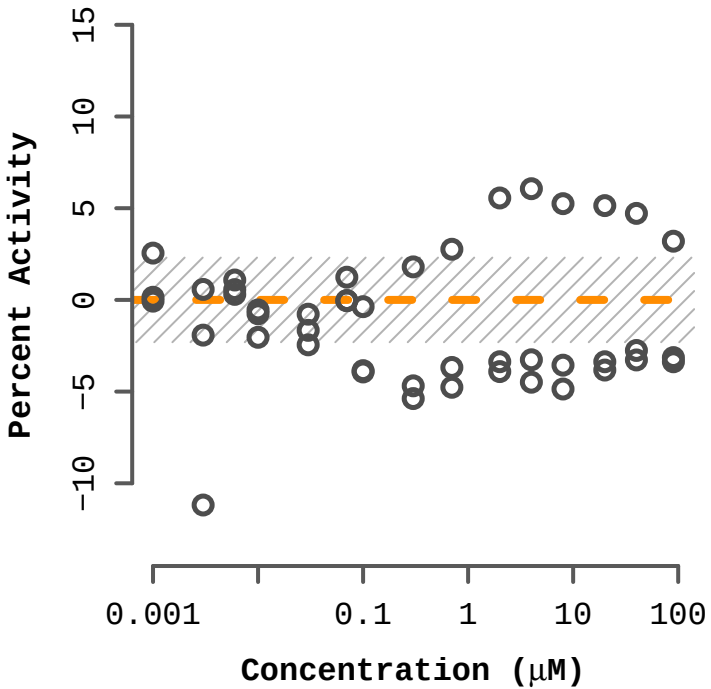
	tp	ga	gw
val:	195	0.794	0.583
sd:	17.8	0.167	0.0529

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	195	0.794	0.583	3.03	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	508.3	342.9	346.9
PROB:	0	0.88	0.12
RMSE:	67.69	12.53	12.53

MAX_MEAN: 155 **MAX_MED:** 153 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

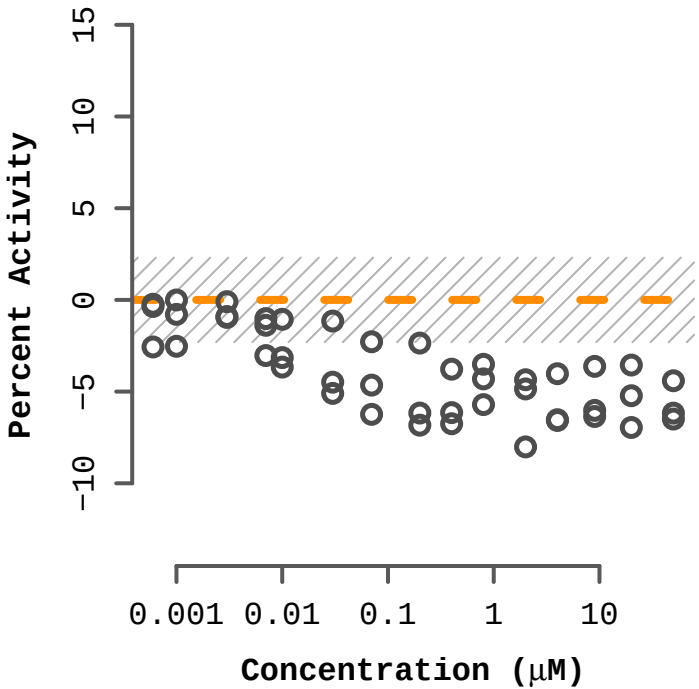
NAME: Podofilox
CHID: 45645 CASRN: 518-28-5
SPID(S): Tox21_202922
M4ID: 12479330

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 0.877 **MAX_MED:** 0.563 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

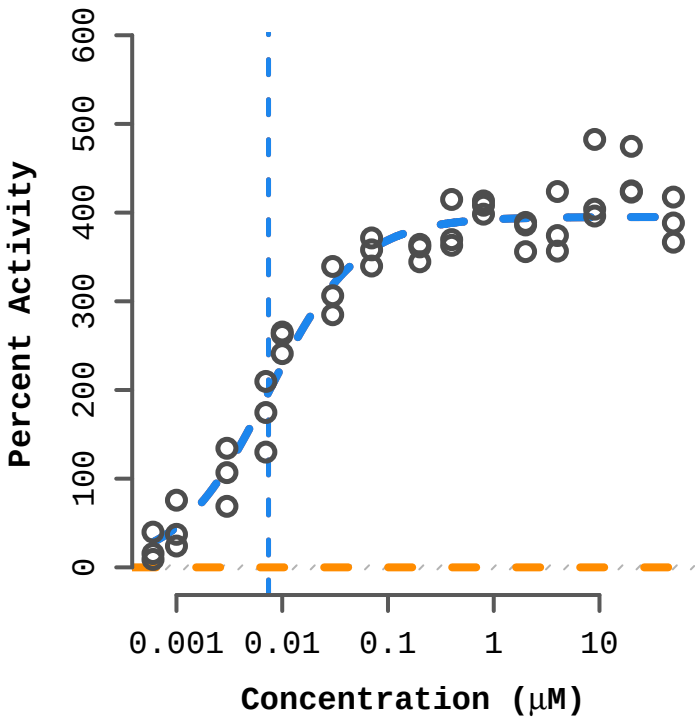
NAME: Podofilox
CHID: 45645 **CASRN:** 518-28-5
SPID(S): Tox21_110874_1
M4ID: 12484053

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	271.81	NA	NA
PROB:	1	NA	NA
RMSE:	4.48	NA	NA

MAX_MEAN: −0.651 **MAX_MED:** −0.356 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diflorasone diacetate
CHID: 45646 CASRN: 33564-31-7
SPID(S): Tox21_110875_1
M4ID: 12484052

HILL MODEL (in red):

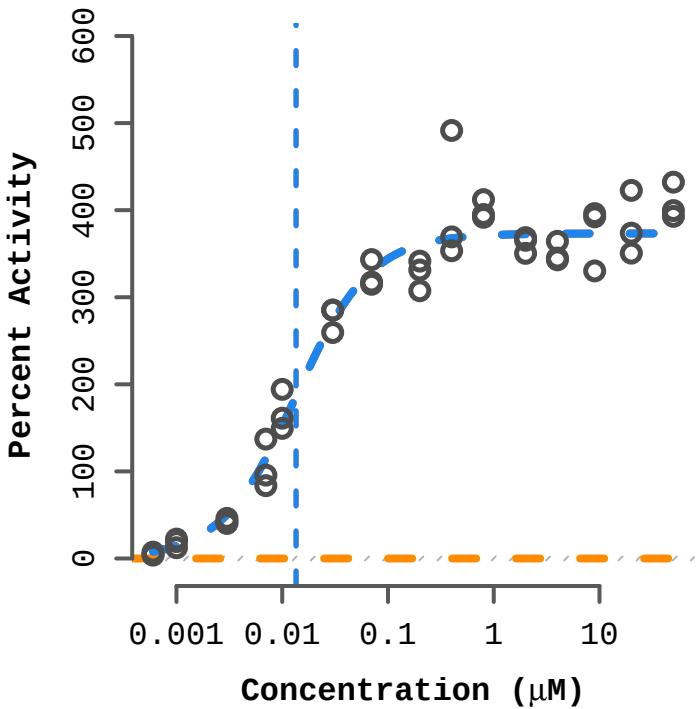
	tp	ga	gw
val:	395	-2.13	1.02
sd:	6.87	0.0497	0.107

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	395	-2.13	1.02	3.66	17.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	659.42	441.61	445.61
PROB:	0	0.88	0.12
RMSE:	326.41	29.82	29.82

MAX_MEAN: 441 **MAX_MED:** 425 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Desoximetasone
CHID: 45647 CASRN: 382-67-2
SPID(S): Tox21_110889_1
M4ID: 12484038

HILL MODEL (in red):

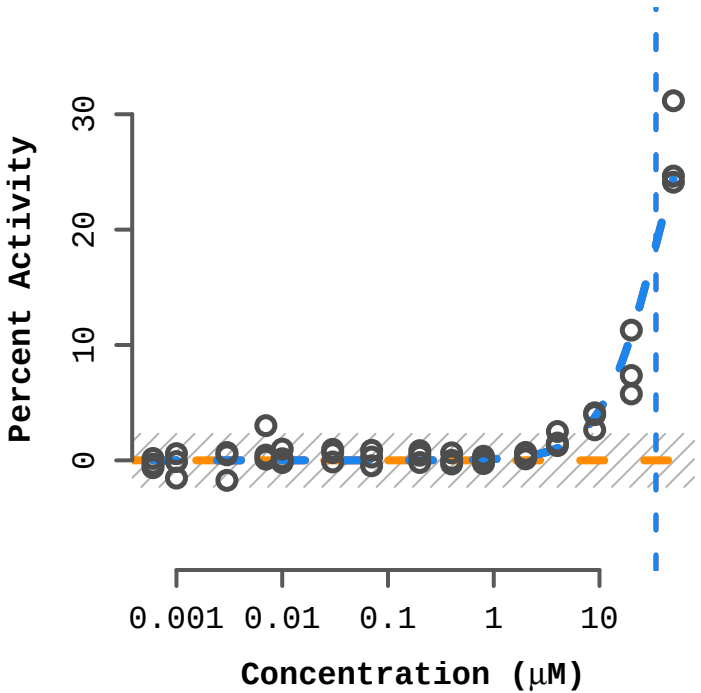
	tp	ga	gw
val:	373	-1.87	1.23
sd:	6.36	0.0368	0.109

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	373	-1.87	1.23	3.41	16.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	651.77	432.55	436.55
PROB:	0	0.88	0.12
RMSE:	301.94	29.77	29.77

MAX_MEAN: 408 MAX_MED: 400 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (E)-4-amino-2-butenoic acid
CHID: 45648 CASRN: 38090-53-8
SPID(S): Tox21_110902_1
M4ID: 12484028

HILL MODEL (in red):

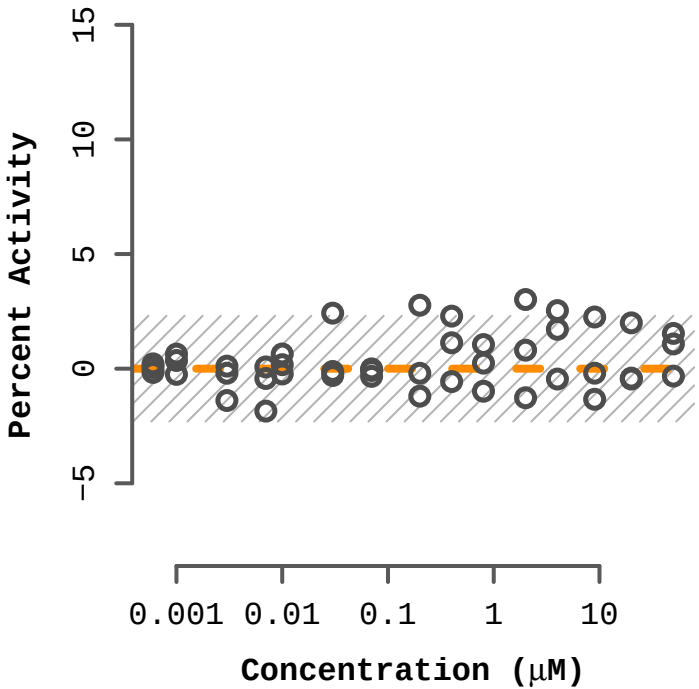
	tp	ga	gw
val:	37.4	1.53	1.65
sd:	4.67	0.0784	0.163

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	37.4	1.53	1.65	2.59	10.6
sd:	4.68	0.0785	0.164	1620	19200

	CNST	HILL	GNLS
AIC:	250.87	144.75	148.75
PROB:	0	0.88	0.12
RMSE:	7.37	1.57	1.57

MAX_MEAN: 26.6 MAX_MED: 24.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

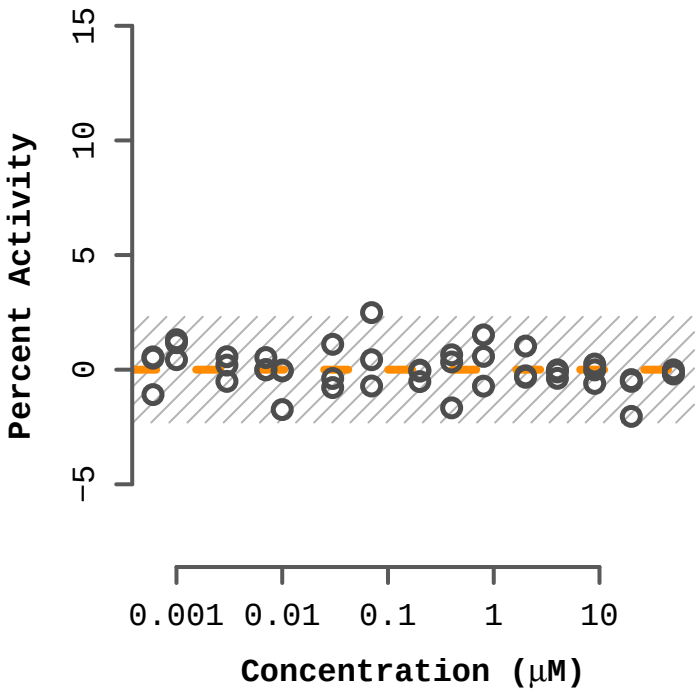
NAME: D-Alanine
CHID: 45649 **CASRN:** 338-69-2
SPID(S): Tox21_110903_1
M4ID: 12484027

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

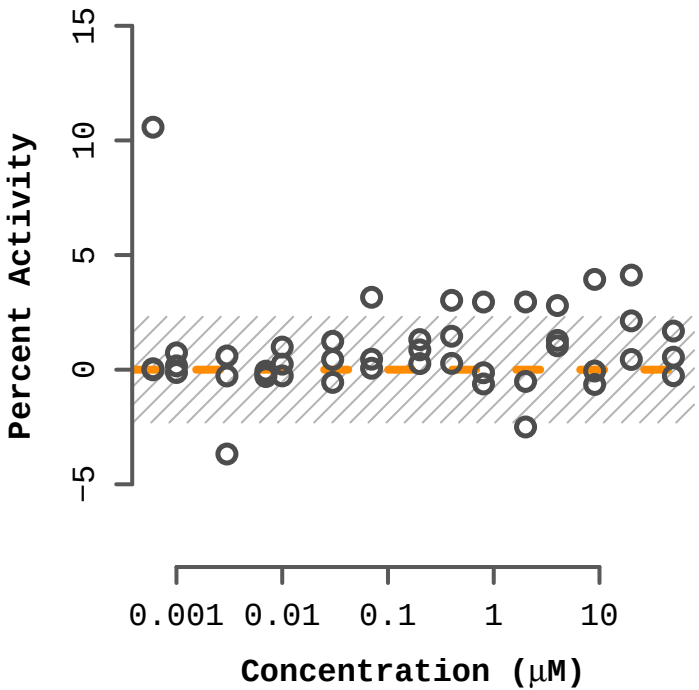
NAME: Azasetron
CHID: 45651 **CASRN:** 123040-69-7
SPID(S): Tox21_110906_1
M4ID: 12484025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.975 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

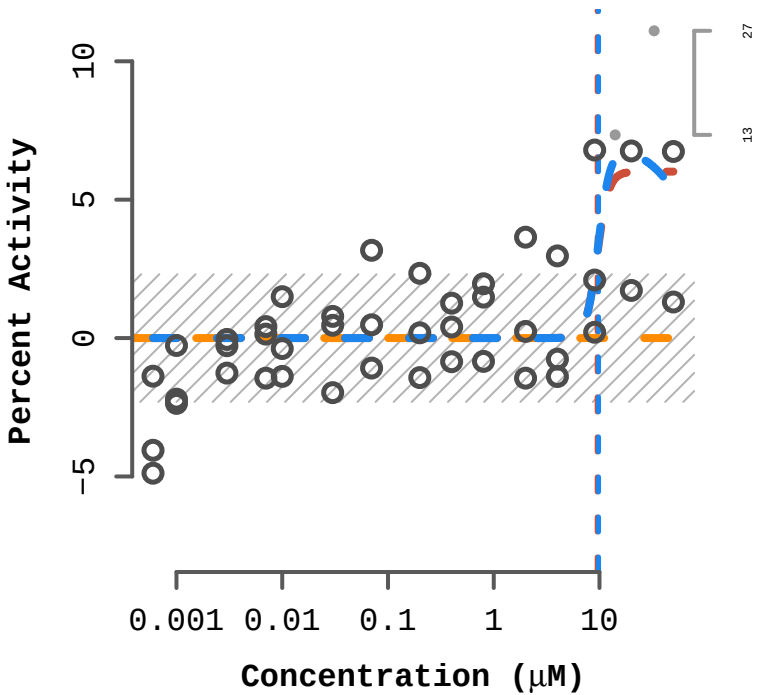
NAME: Cimaterol
CHID: 45652 **CASRN:** 54239-37-1
SPID(S): Tox21_110908_1
M4ID: 12484024

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.26	NA	NA

MAX_MEAN: 3.54 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cinanserin
CHID: 45653 CASRN: 1166-34-3
SPID(S): Tox21_110911_1
M4ID: 12484022 BRK

HILL MODEL (in red):

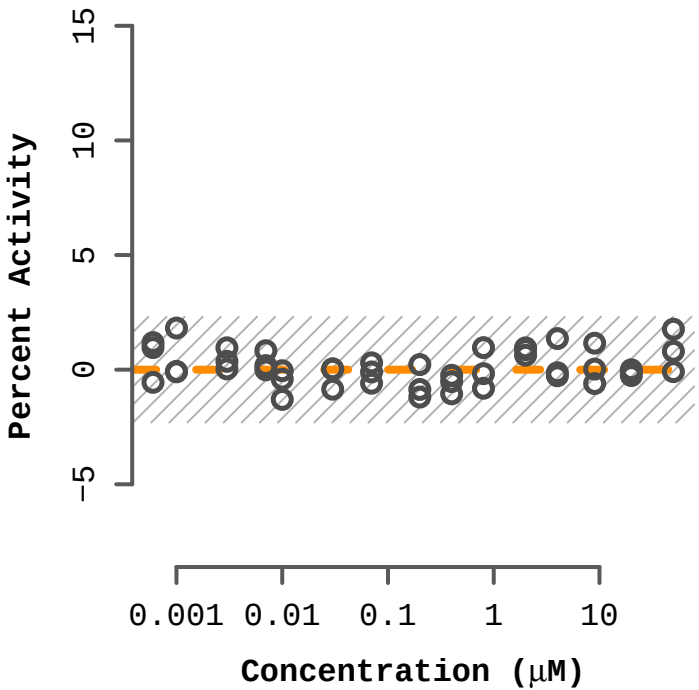
	tp	ga	gw
val:	6.01	0.978	8
sd:	1.39	0.0907	23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.99	0.991	7.88	1.94	2.05
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	236.09	225.16	228.94
PROB:	0	0.87	0.13
RMSE:	5.07	3.87	3.93

MAX_MEAN: 11.7 MAX_MED: 6.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

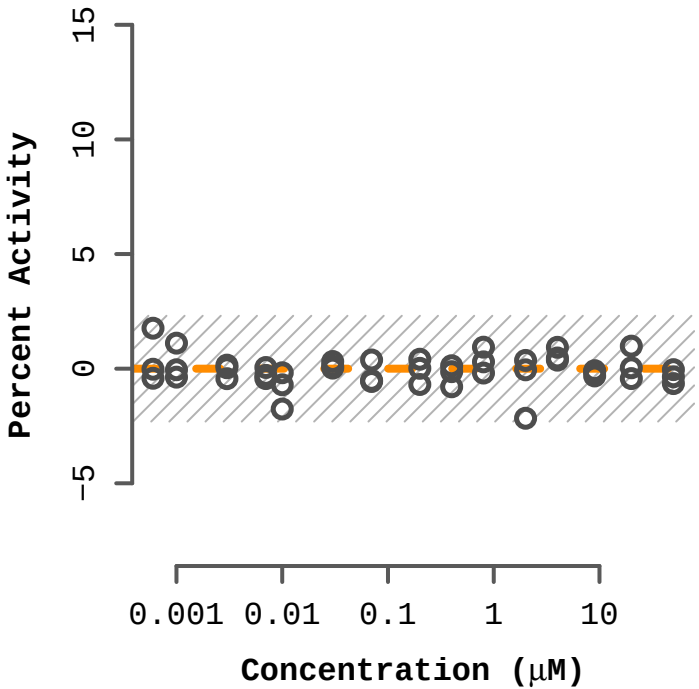
NAME: Flurofamide
CHID: 45654 **CASRN:** 70788-28-2
SPID(S): Tox21_110912_1
M4ID: 12484021

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.828 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

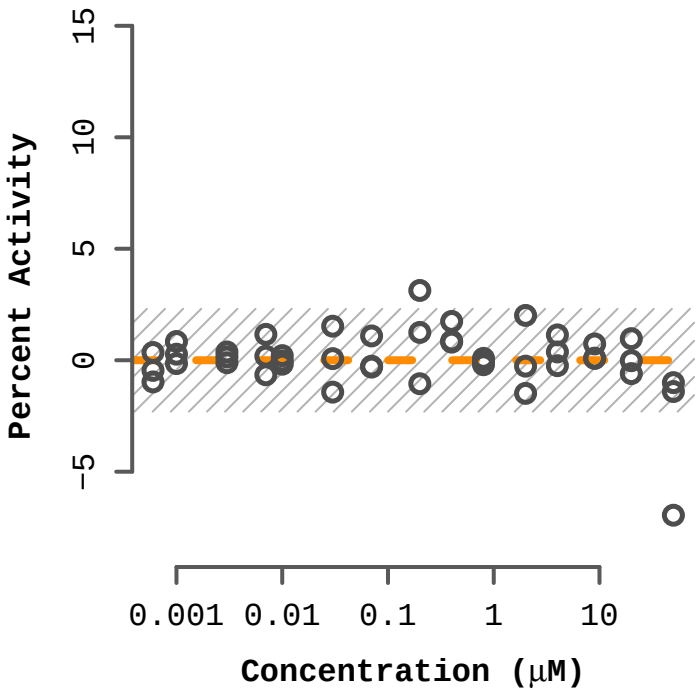
NAME: Alrestatin
CHID: 45655 **CASRN:** 51411-04-2
SPID(S): Tox21_110913_1
M4ID: 12484020

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	85.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.591 **MAX_MED:** 0.468 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

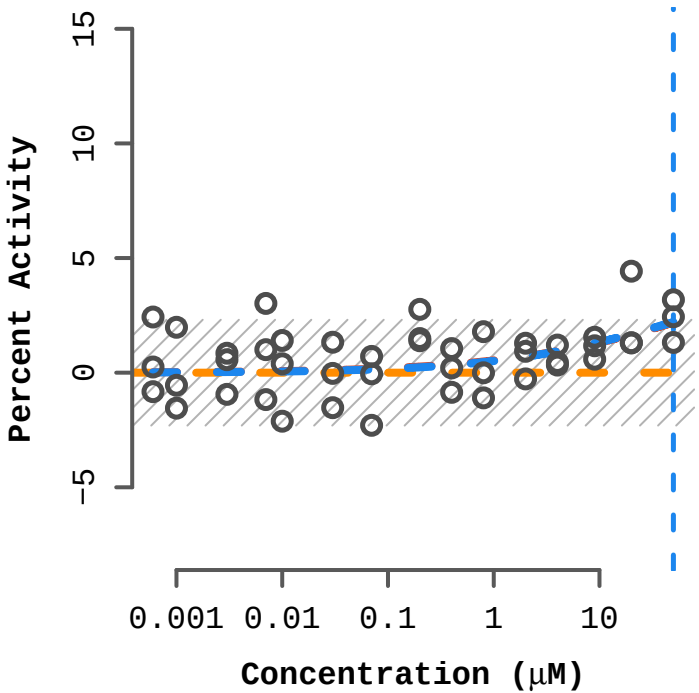
NAME: Ifenprodil
CHID: 45656 **CASRN:** 23210-56-2
SPID(S): Tox21_110915_1
M4ID: 12484018

HILL MODEL: Not applicable.

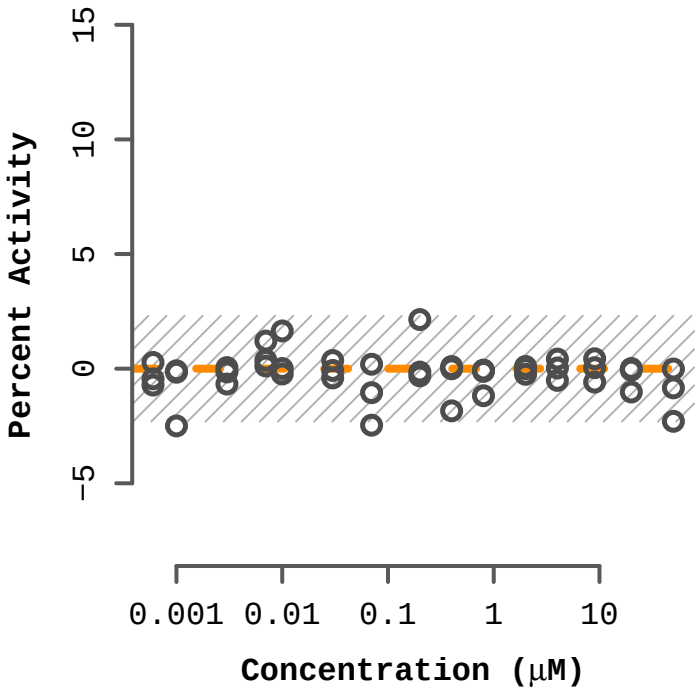
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.25 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Anpirtoline
CHID:    45659   CASRN: 98330-05-3
SPID(S): Tox21_110922_1
M4ID:    12484013

HILL MODEL (in red):
      tp       ga       gw
val:  5.31     2.03     0.468
sd:   6.8      2.12     0.326

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.42     1.7      0.523    3.32     6.7
sd:   5.62     1.94     0.379    73100    3e+05

      CNST        HILL        GNLS
AIC:  172.75      158.5       162.6
PROB: 0           0.89        0.11
RMSE: 1.57        1.26        1.26

MAX_MEAN: 2.35      MAX_MED: 2.44      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

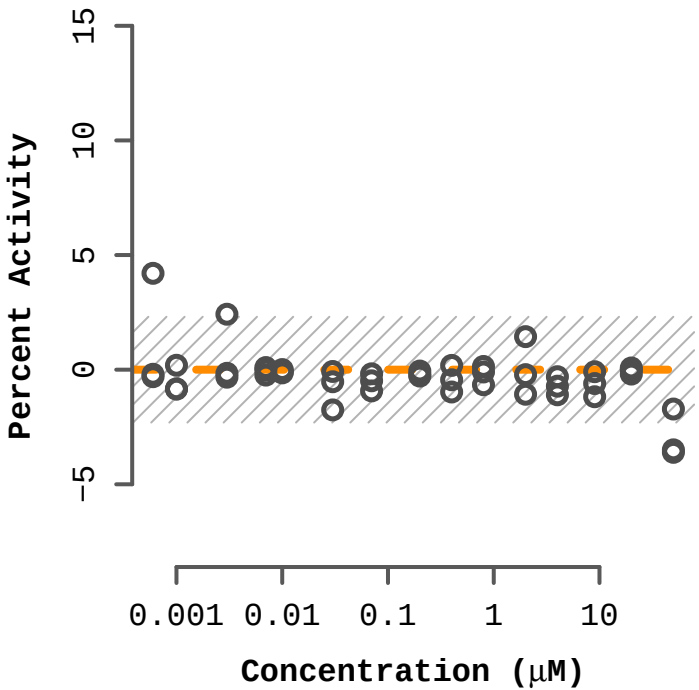
NAME: Pirlindole mesylate
CHID: 45660 **CASRN:** 207572-66-5
SPID(S): Tox21_110923_1
M4ID: 12484012

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.564 **MAX_MED:** 0.368 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

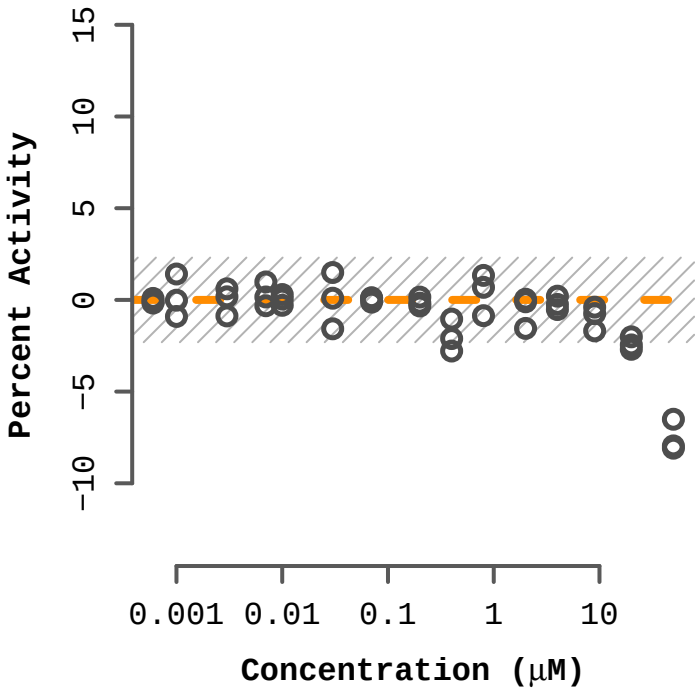
NAME: Tesmilifene
CHID: 45661 **CASRN:** 98774-23-3
SPID(S): Tox21_110924_1
M4ID: 12484011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** −5e-06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

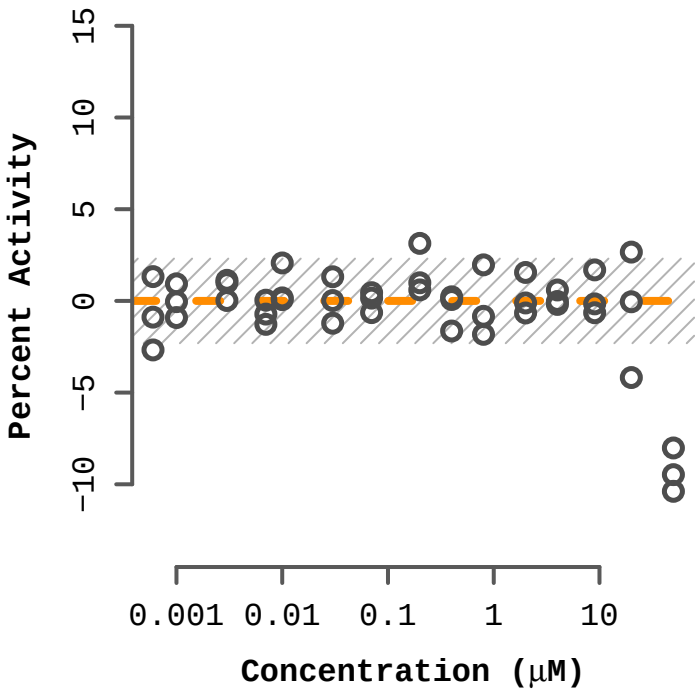
NAME: SNC 80
CHID: 45662 CASRN: 156727-74-1
SPID(S): Tox21_110925_1
M4ID: 12484010

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.69	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 0.389 **MAX_MED:** 0.686 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

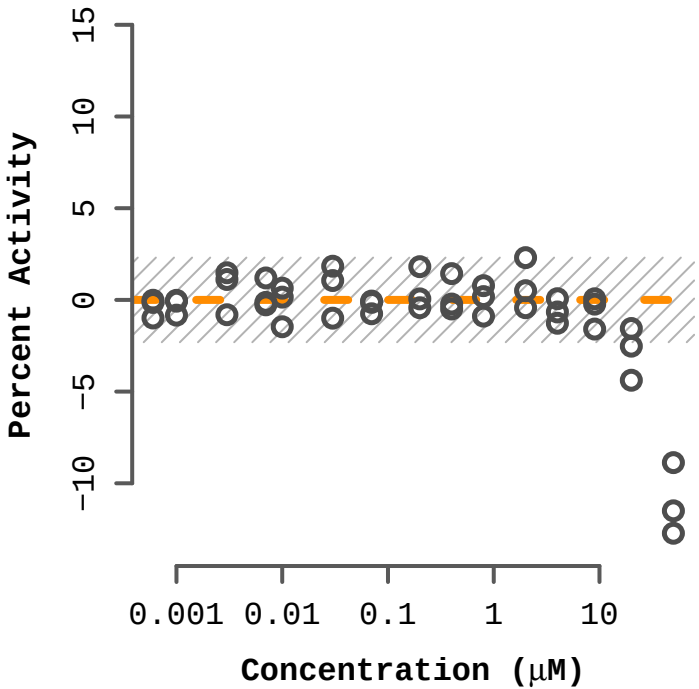
NAME: Bifemelane
CHID: 45663 **CASRN:** 90293-01-9
SPID(S): Tox21_110926_1
M4ID: 12484009

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.72	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

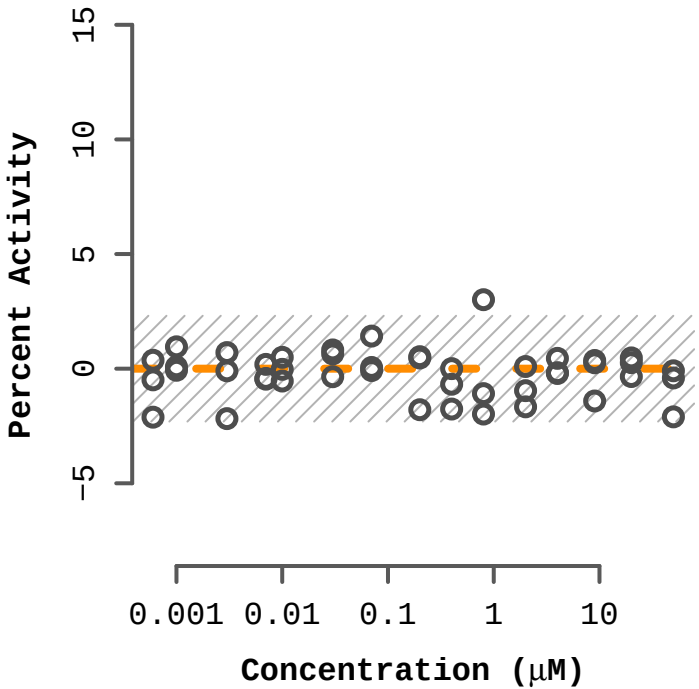
NAME: Guanabenz
CHID: 45666 **CASRN:** 5051-62-7
SPID(S): Tox21_110932_1
M4ID: 12484005

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.11	NA	NA

MAX_MEAN: 0.795 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

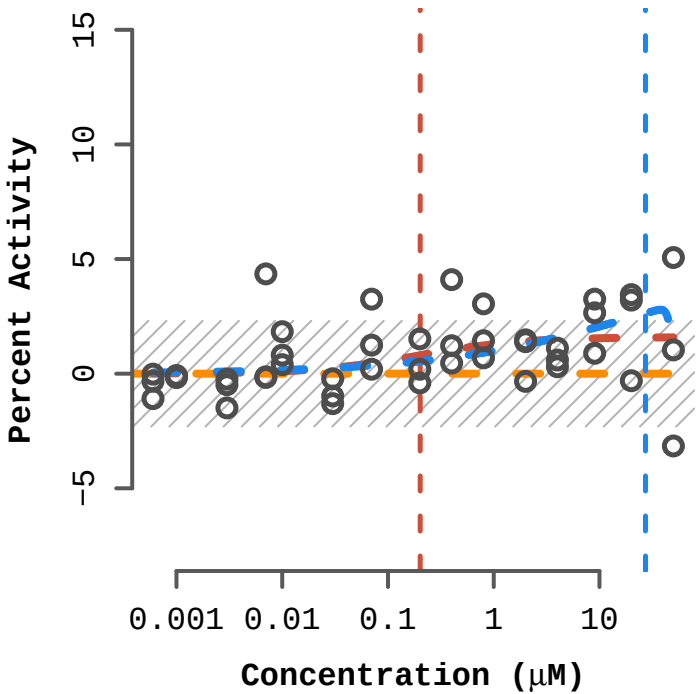
NAME: Remoxipride
CHID: 45668 **CASRN:** 80125-14-0
SPID(S): Tox21_110934_1
M4ID: 12484003

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.466 **MAX_MED:** 0.646 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Olvanil
CHID: 45669 **CASRN:** 58493-49-5
SPID(S): Tox21_110935_1
M4ID: 12484002

HILL MODEL (in red):

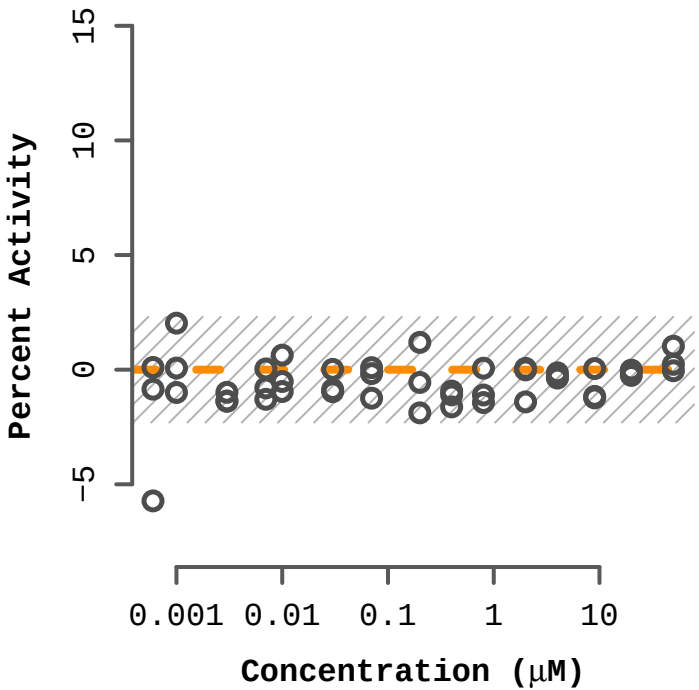
	tp	ga	gw
val:	1.6	−0.695	0.878
sd:	1.46	1.74	2.17

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.26	1.43	0.44	1.68	18
sd:	11.3	3.48	0.238	0.055	68.1

	CNST	HILL	GNLS
AIC:	183.82	170.8	173.75
PROB:	0	0.81	0.19
RMSE:	1.87	1.56	1.56

MAX_MEAN: 2.27 **MAX_MED:** 3.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

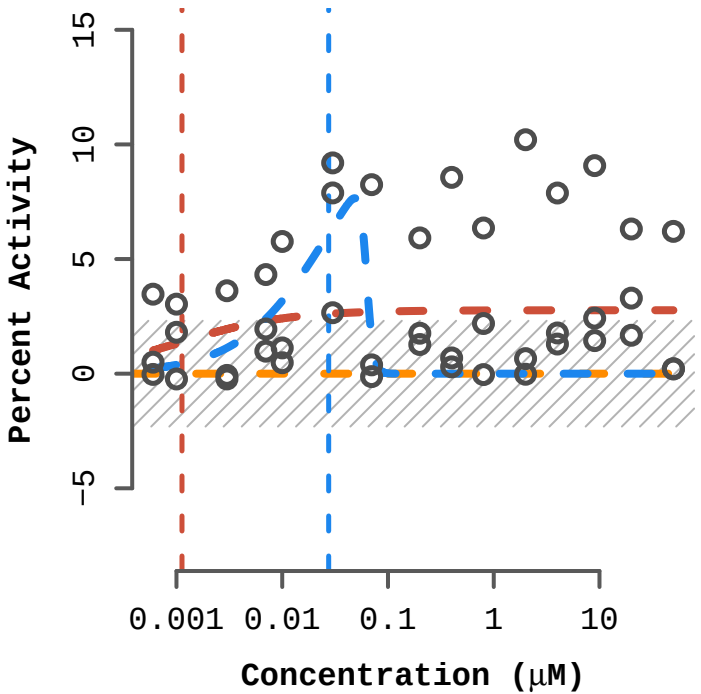
NAME: SCH 50911
CHID: 45670 **CASRN:** 160415-07-6
SPID(S): Tox21_110936_1
M4ID: 12484001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.405 **MAX_MED:** 0.234 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Procaterol
CHID: 45673 CASRN: 72332-33-3
SPID(S): Tox21_110941_1
M4ID: 12483997

HILL MODEL (in red):

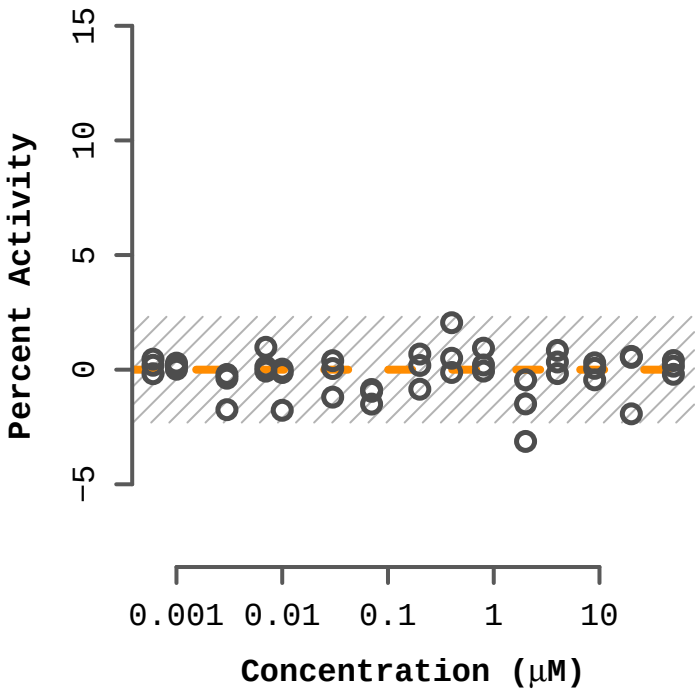
	tp	ga	gw
val:	2.77	−2.95	0.876
sd:	0.633	0.754	1.01

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.2	−1.56	1.04	−1.2	13.8
sd:	12.6	0.858	0.884	0.839	241

	CNST	HILL	GNLS
AIC:	259.66	238.27	255.8
PROB:	0	1	0
RMSE:	4.3	3.05	3.77

MAX_MEAN: 6.58 MAX_MED: 7.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

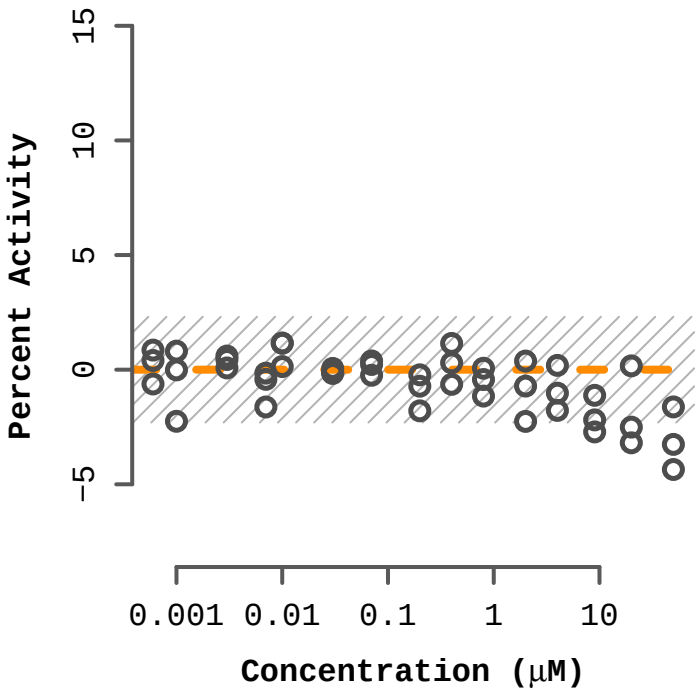
NAME: AF-DX 116
CHID: 45674 **CASRN:** 102394-31-0
SPID(S): Tox21_110942_1
M4ID: 12483996

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.81 **MAX_MED:** 0.537 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

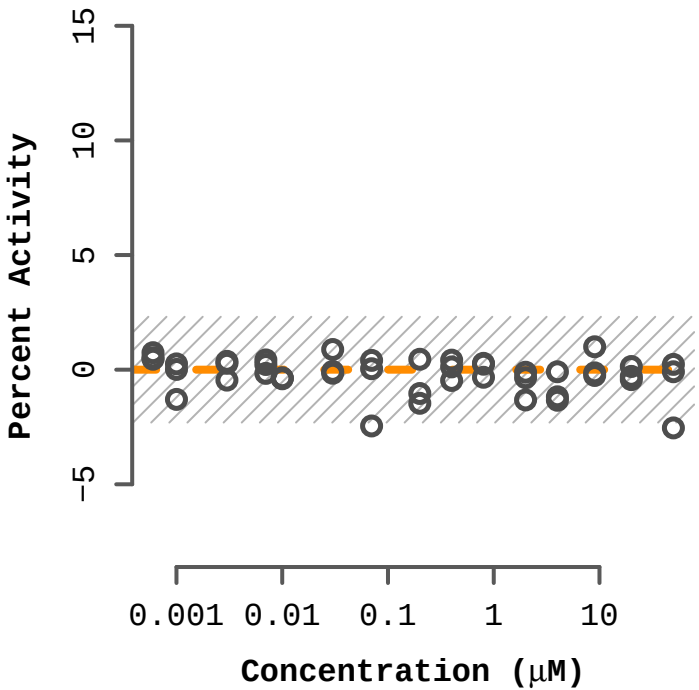
NAME: Loreclezole hydrochloride
CHID: 45676 CASRN: NOCAS_45676
SPID(S): Tox21_110946_1
M4ID: 12483993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

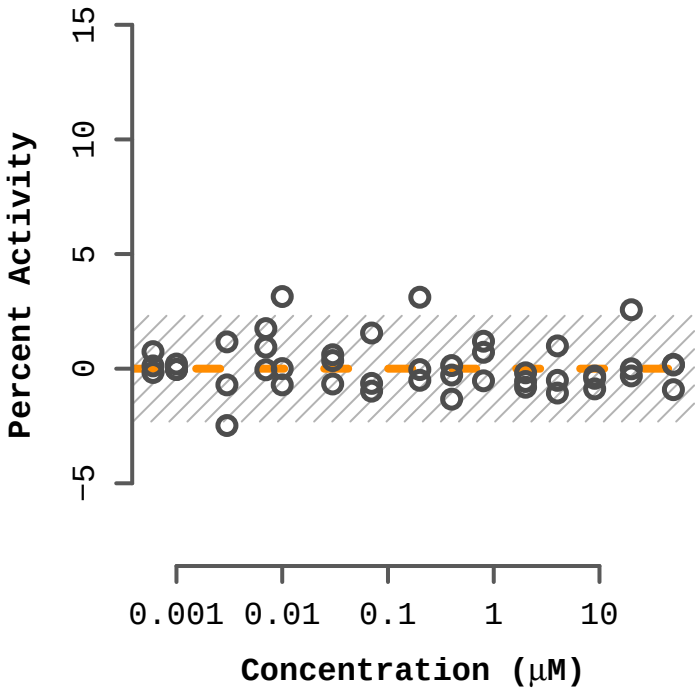
NAME: Levcromakalim
CHID: 45677 CASRN: 94535-50-9
SPID(S): Tox21_110948_1
M4ID: 12483991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

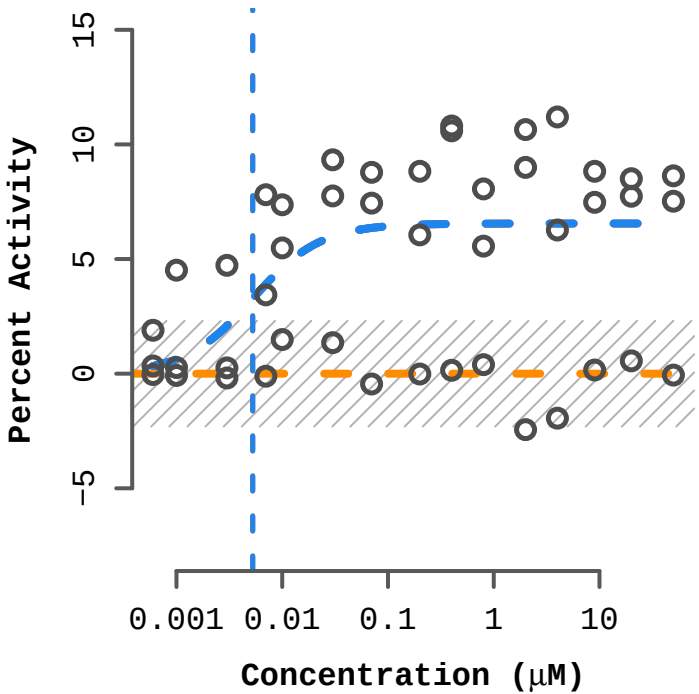
NAME: Roquinimex
CHID: 45680 **CASRN:** 84088-42-6
SPID(S): Tox21_110951_1
M4ID: 12483990

HILL MODEL: Not applicable.

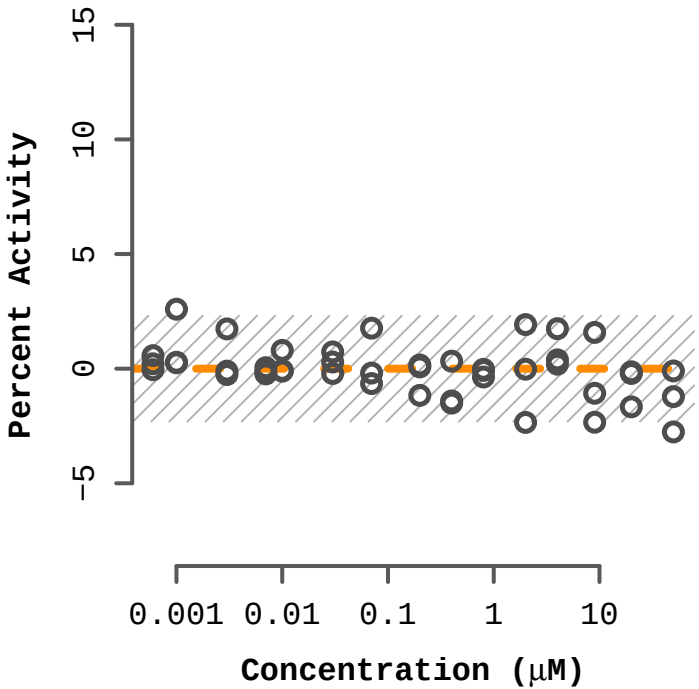
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 0.939 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pinacidil monohydrate
CHID:    45682   CASRN: 85371-64-8
SPID(S): Tox21_110954_1
M4ID:    12483987

HILL MODEL (in red):
      tp       ga       gw
val:  6.55     -2.28    1.35
sd:   0.849    0.278    1.29

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.55     -2.28    1.35     2.61     18
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  298.24      260.31      264.31
PROB: 0           0.88        0.12
RMSE: 6.14        3.86        3.86

MAX_MEAN: 7.18      MAX_MED: 10.6      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

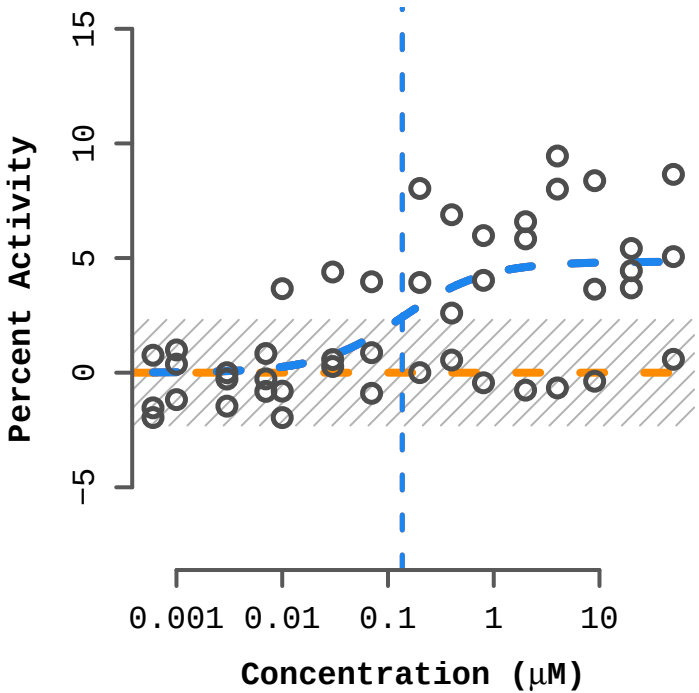
NAME: Remacemide hydrochloride
CHID: 45683 **CASRN:** 111686-79-4
SPID(S): Tox21_110956_1
M4ID: 12483985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.385 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acifran
CHID: 45685 CASRN: 72420-38-3
SPID(S): Tox21_110958_1
M4ID: 12483984

HILL MODEL (in red):

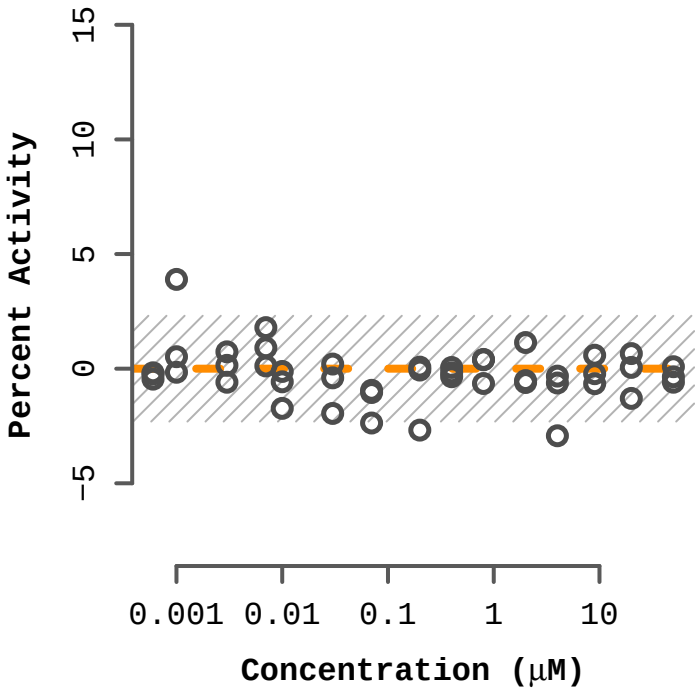
	tp	ga	gw
val:	4.84	−0.865	1.11
sd:	0.876	0.41	0.664

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.84	−0.865	1.11	2.94	5.72
sd:	0.876	0.41	0.664	1550	7200

	CNST	HILL	GNLS
AIC:	255.49	225.34	229.34
PROB:	0	0.88	0.12
RMSE:	4.04	2.63	2.63

MAX_MEAN: 5.6 MAX_MED: 8.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

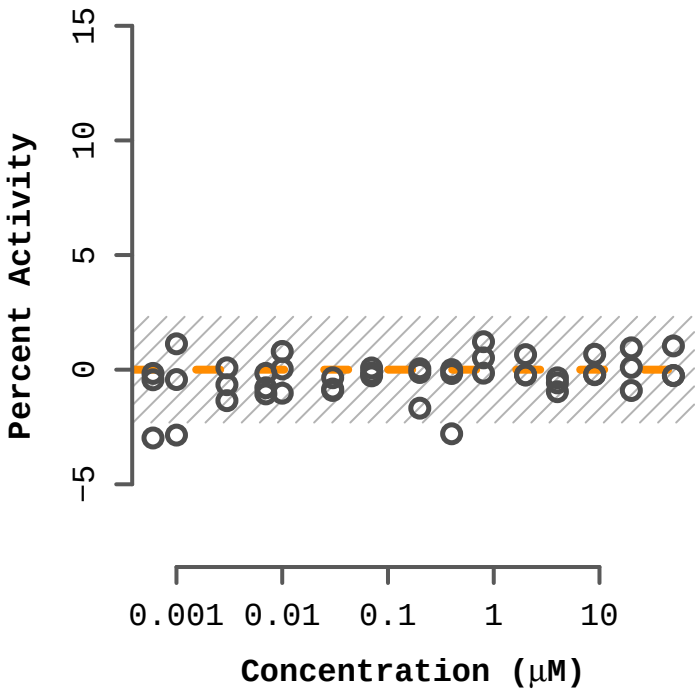
NAME: Zacopride hydrochloride
CHID: 45686 **CASRN:** 99617-34-2
SPID(S): Tox21_110959_1
M4ID: 12483983

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 0.911 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

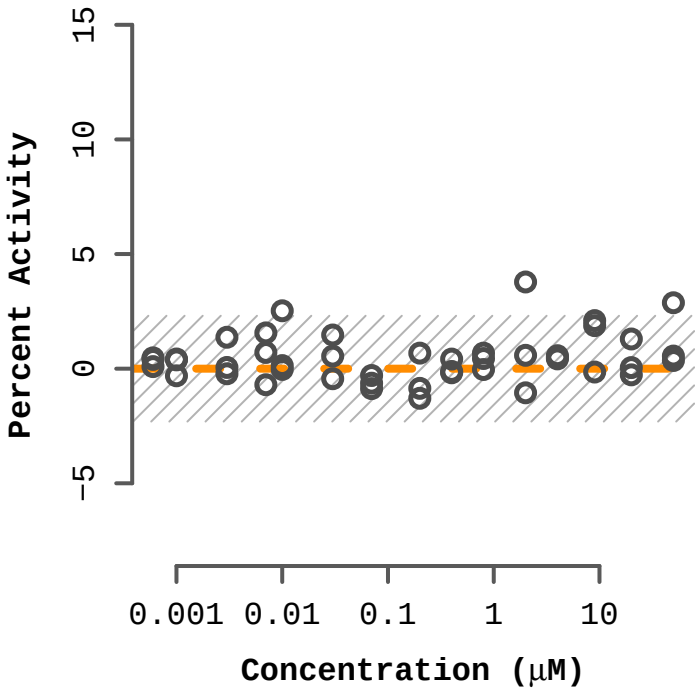
NAME: Raclopride
CHID: 45687 CASRN: 84225-95-6
SPID(S): Tox21_110961_1
M4ID: 12483981

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

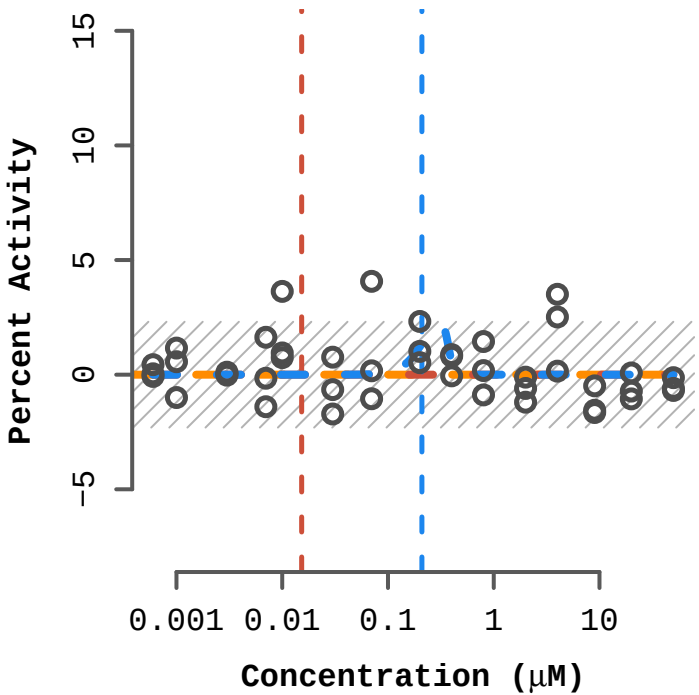
NAME: Ipsapirone
CHID: 45688 **CASRN:** 95847-70-4
SPID(S): Tox21_110962_1
M4ID: 12483980

HILL MODEL: Not applicable.

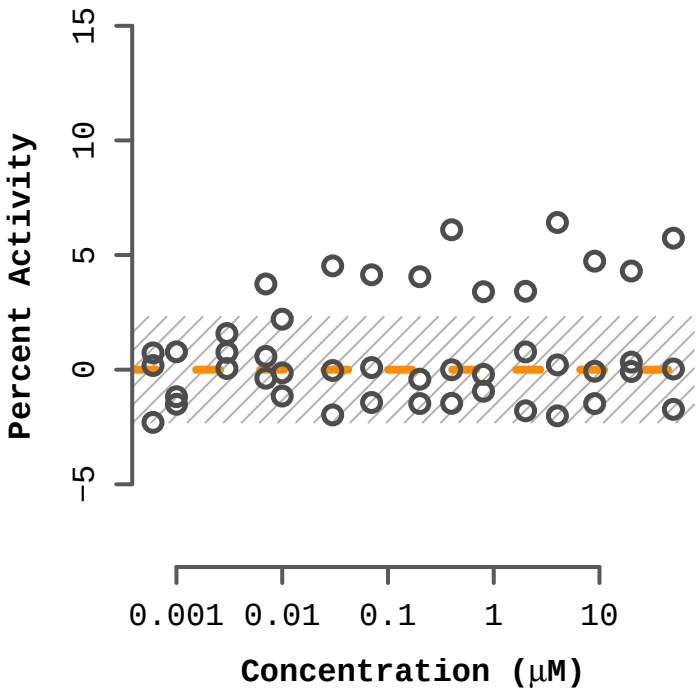
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.88 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Reboxetine mesylate
CHID:    45690   CASRN: 98769-84-7
SPID(S): Tox21_110964_1
M4ID:    12483979

HILL MODEL (in red):
      tp       ga       gw
val:  1.6e-09  -1.82    2.26
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.71     -0.679   4.41     -0.429   17.7
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  152.65      158.65      157.47
PROB: 0.88        0.04        0.08
RMSE: 1.36        1.36        1.31

MAX_MEAN: 2.06      MAX_MED: 2.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

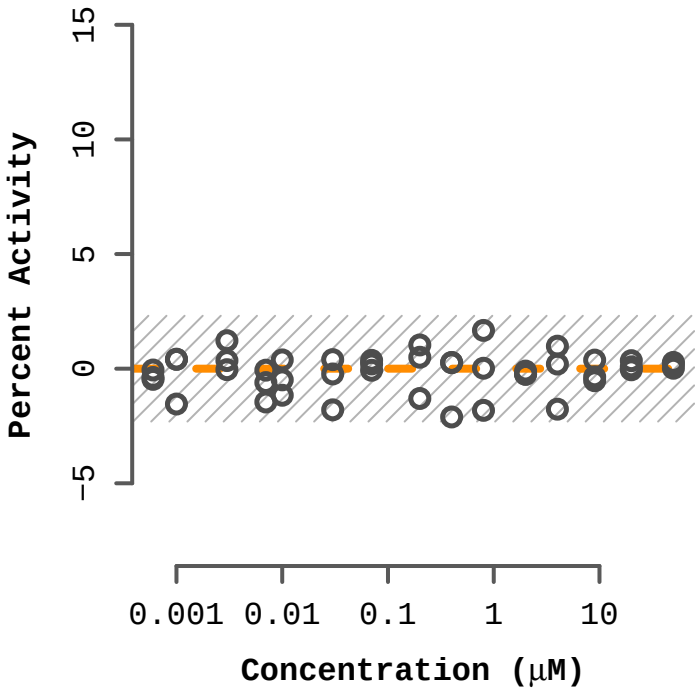
NAME: Nicorandil
CHID: 45692 **CASRN:** 65141-46-0
SPID(S): Tox21_110968_1
M4ID: 12483977

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.53	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 0.776 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

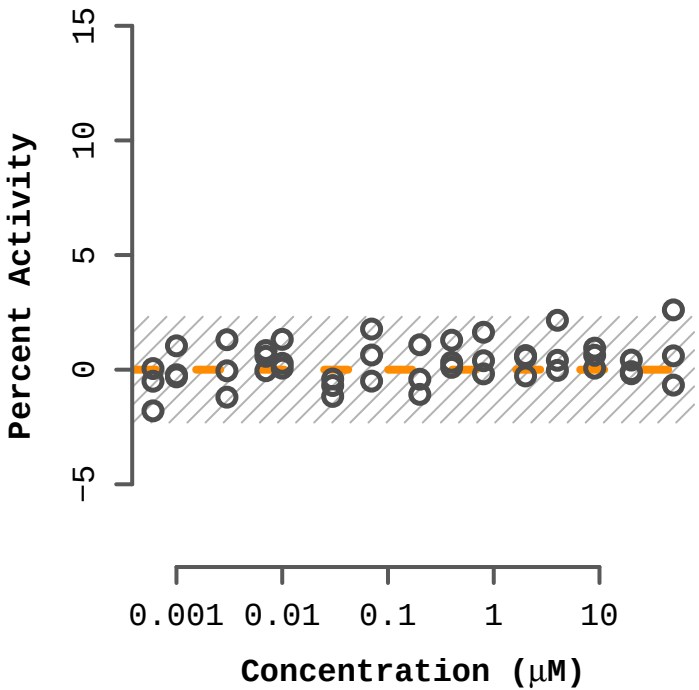
NAME: Capobenic acid
CHID: 45695 **CASRN:** 21434-91-3
SPID(S): Tox21_110972_1
M4ID: 12483975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.512 **MAX_MED:** 0.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

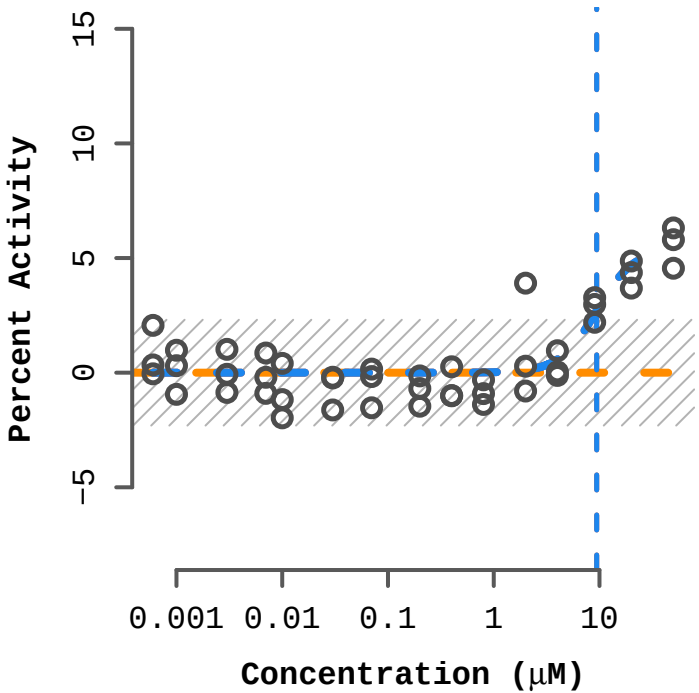
NAME: Afalanine
CHID: 45697 **CASRN:** 2901-75-9
SPID(S): Tox21_110975_1
M4ID: 12483974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.847 **MAX_MED:** 0.641 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nicotredole
CHID: 45698 **CASRN:** 29876-14-0
SPID(S): Tox21_110977_1
M4ID: 12483972

HILL MODEL (in red):

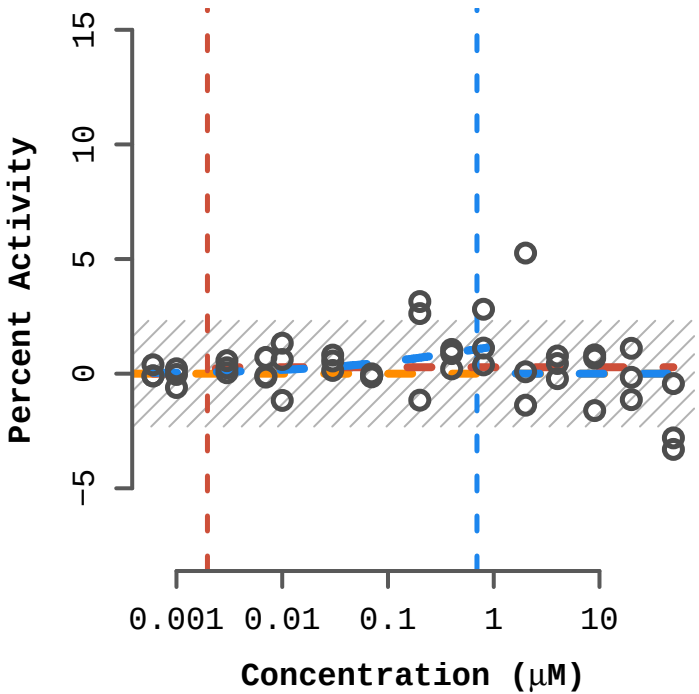
	tp	ga	gw
val:	5.42	0.974	2.48
sd:	0.743	0.0988	1.01

GAIN-LOSS MODEL (in blue):

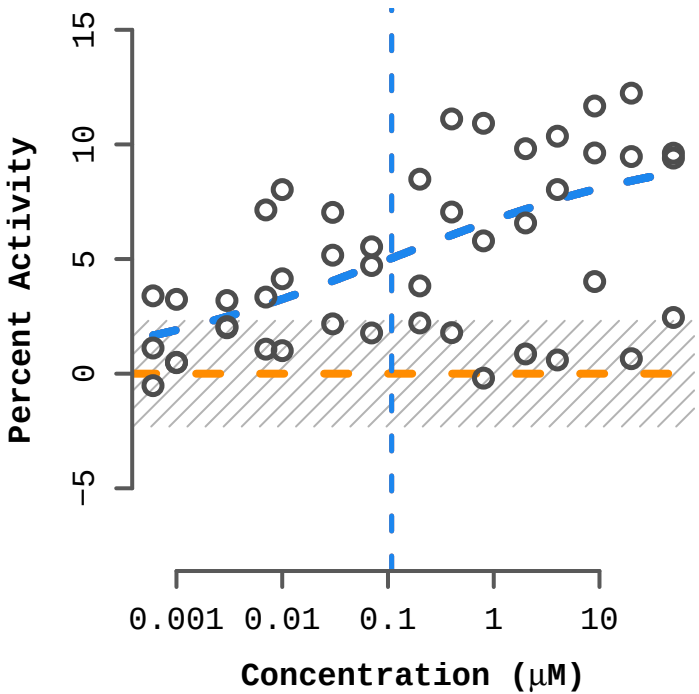
	tp	ga	gw	la	lw
val:	5.42	0.974	2.48	3.19	5.68
sd:	0.743	0.0988	1.01	1710	6550

	CNST	HILL	GNLS
AIC:	194.92	135.36	139.36
PROB:	0	0.88	0.12
RMSE:	2.21	1.03	1.03

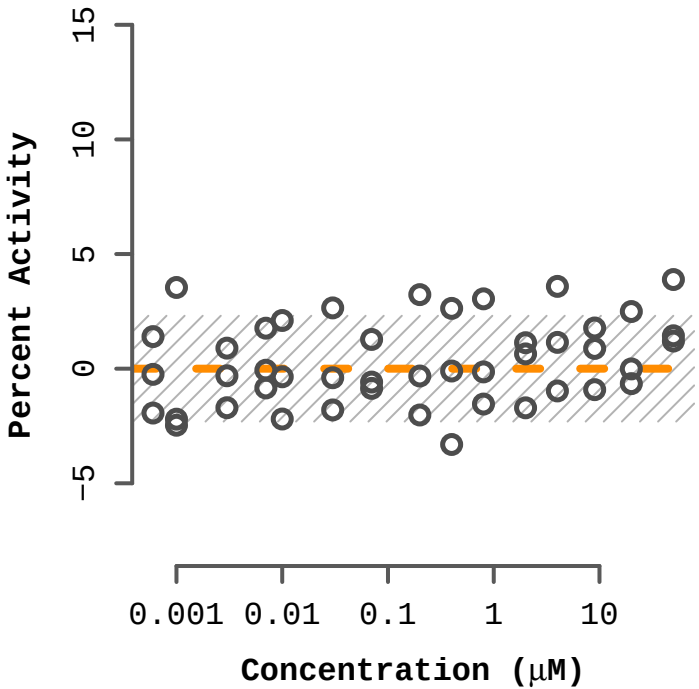
MAX_MEAN: 5.56 **MAX_MED:** 5.8 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4,5-Diphenylimidazole
CHID:    45700   CASRN: 668-94-0
SPID(S): Tox21_110979_1
M4ID:    12483971

HILL MODEL (in red):
      tp       ga       gw
val:  0.281    -2.71    8
sd:   0.166    1.27     43.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.13     -0.159   0.582    0.0915   18
sd:   4.61     2.99     0.589    1.42     130

      CNST        HILL        GNLS
AIC:  150.48      153.66      152.21
PROB: 0.62        0.13        0.26
RMSE: 1.42        1.39        1.32

MAX_MEAN: 1.54      MAX_MED: 2.62      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Trovafloxacin mesylate
CHID:    45701   CASRN: 147059-75-4
SPID(S): Tox21_110980_1
M4ID:    12483970

HILL MODEL (in red):
      tp       ga       gw
val:  10.1     -0.965   0.311
sd:   3.79     1.36     0.171

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.1     -0.965   0.311    3.49     5.55
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  298.27      243.14      247.14
PROB: 0           0.88        0.12
RMSE: 6.2         3.24        3.24

MAX_MEAN: 8.44      MAX_MED: 9.63      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

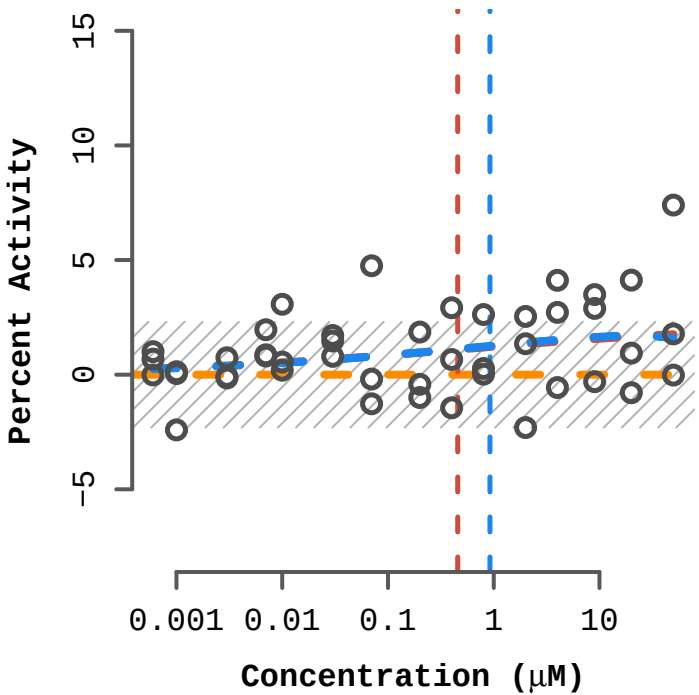
NAME: Trimecaine monohydrochloride
CHID: 45702 CASRN: 1027-14-1
SPID(S): Tox21_110981_1
M4ID: 12483969

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 2.18 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxcarbazepine
CHID: 45703 **CASRN:** 28721-07-5
SPID(S): Tox21_110983_1
M4ID: 12483967

HILL MODEL (in red):

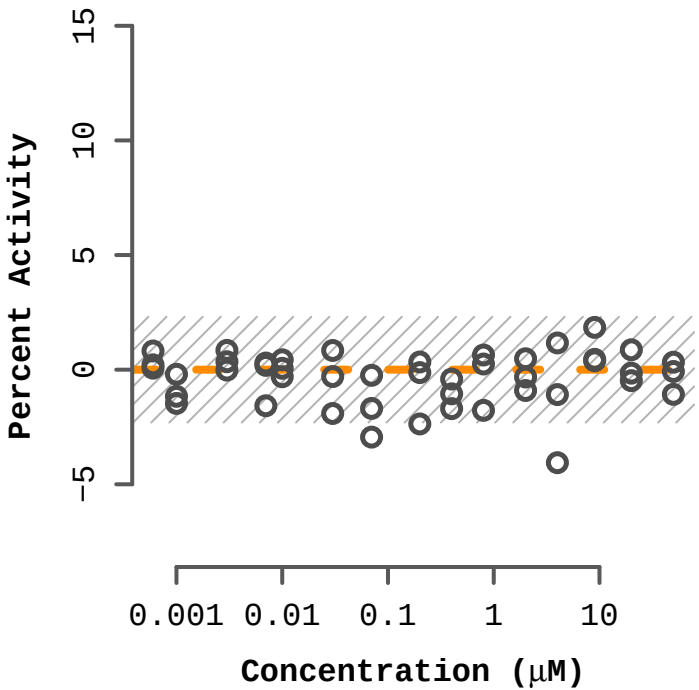
	tp	ga	gw
val:	2.19	−0.341	0.3
sd:	3.76	5.9	0.492

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.5	−0.0357	0.3	2.12	1.56
sd:	12.3	14.5	0.698	3.62	5.96

	CNST	HILL	GNLS
AIC:	195.62	188.17	192.13
PROB:	0.02	0.86	0.12
RMSE:	2.17	1.8	1.81

MAX_MEAN: 3.05 **MAX_MED:** 2.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

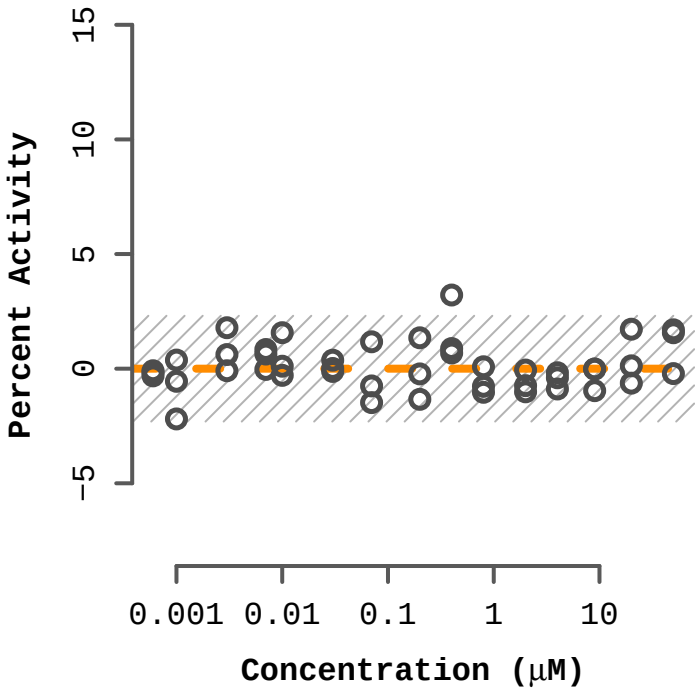
NAME: Gatifloxacin
CHID: 45704 **CASRN:** 112811-59-3
SPID(S): Tox21_110984_1
M4ID: 12483966

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.895 **MAX_MED:** 0.452 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

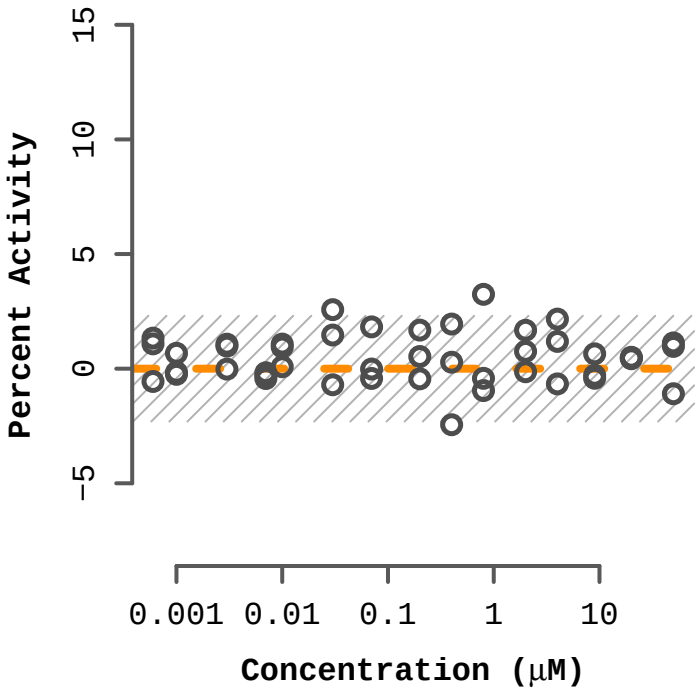
NAME: Metralindole
CHID: 45705 **CASRN:** 54188-38-4
SPID(S): Tox21_110986_1
M4ID: 12483964

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

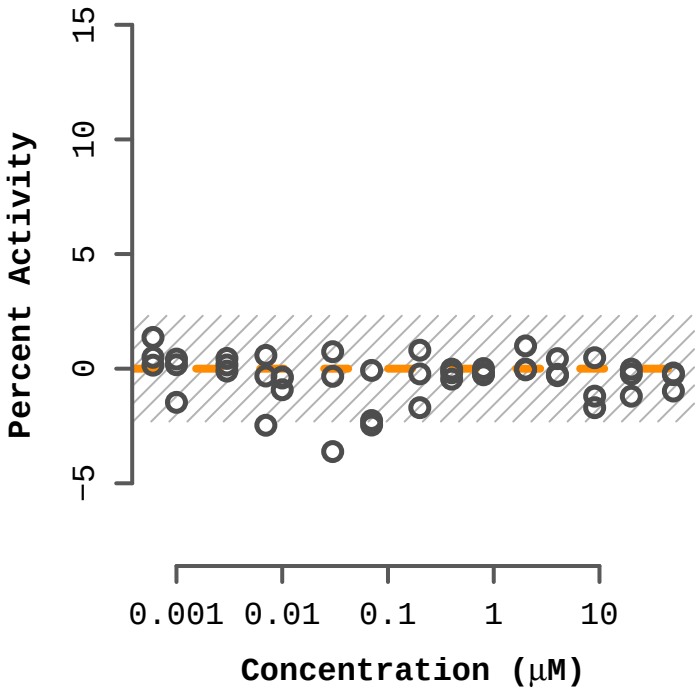
NAME: Metomidate hydrochloride
CHID: 45707 CASRN: 35944-74-2
SPID(S): Tox21_110988_1
M4ID: 12483963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

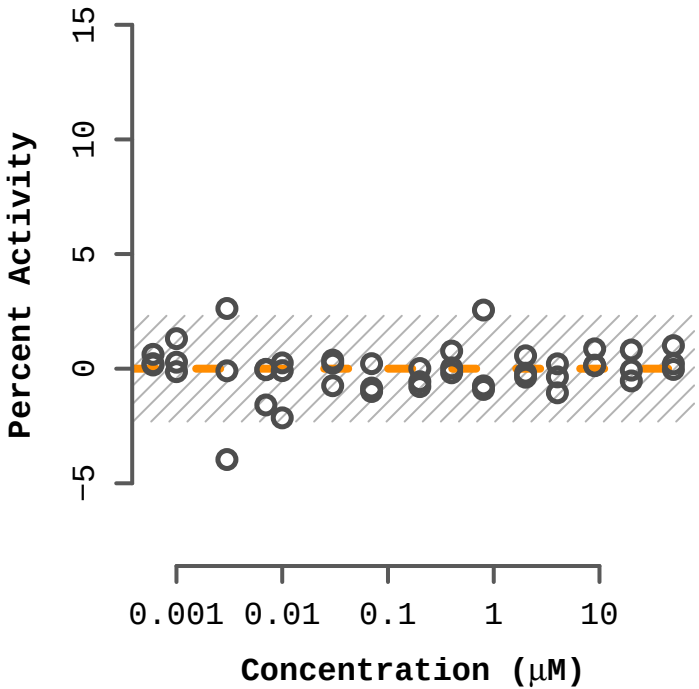
NAME: Rufloxacin hydrochloride
CHID: 45709 CASRN: 106017-08-7
SPID(S): Tox21_110990_1
M4ID: 12483962

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.672 **MAX_MED:** 0.496 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

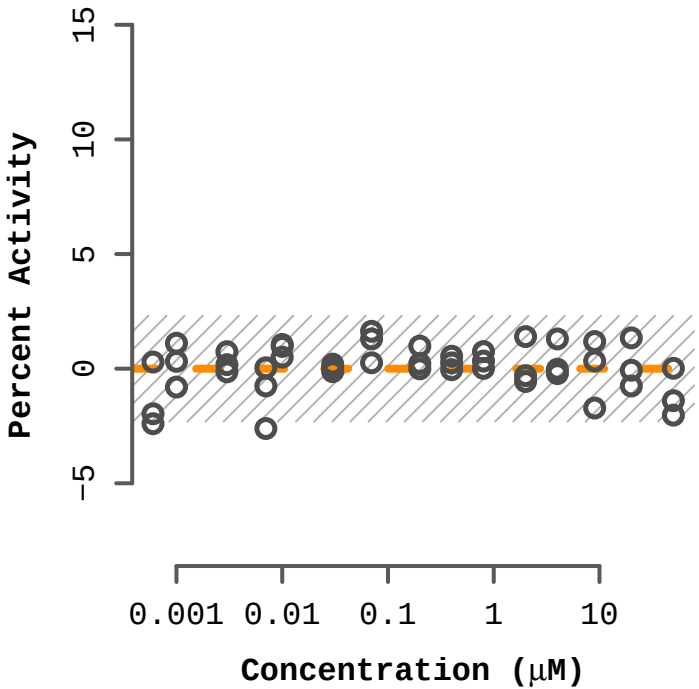
NAME: Eterobarb
CHID: 45710 **CASRN:** 27511-99-5
SPID(S): Tox21_110991_1
M4ID: 12483961

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.489 **MAX_MED:** 0.283 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

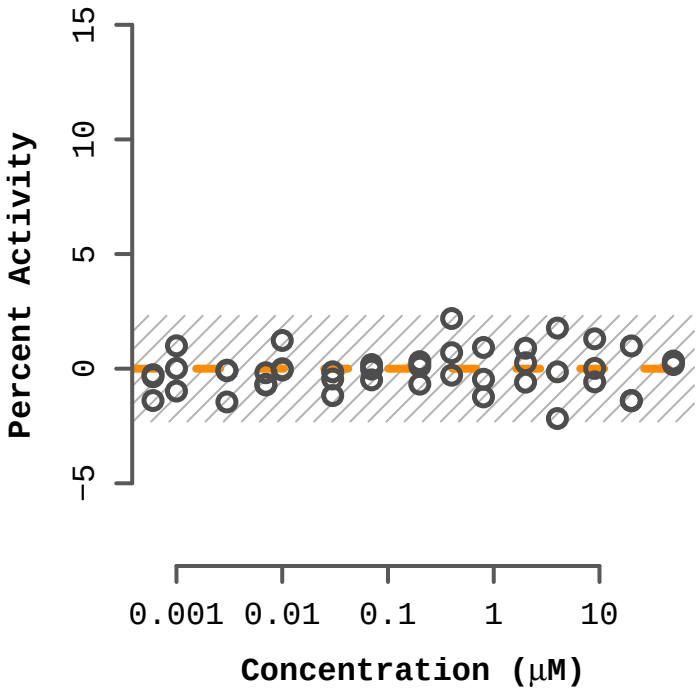
NAME: Cochineal
CHID: 45735 **CASRN:** 1343-78-8
SPID(S): Tox21_111163_1
M4ID: 12483866

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

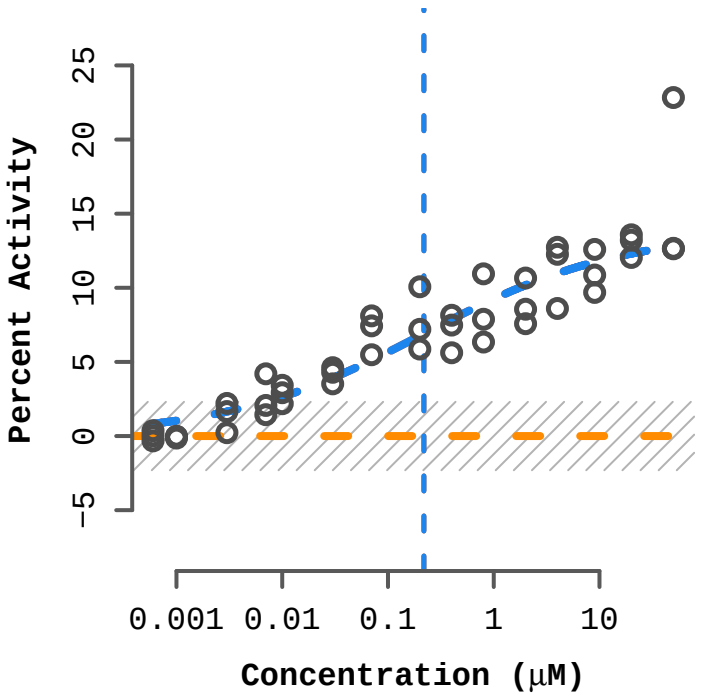
NAME: Mifobate
CHID: 45741 **CASRN:** 76541-72-5
SPID(S): Tox21_111190_1
M4ID: 12483856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.868 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cinalukast
CHID: 45742 **CASRN:** 128312-51-6
SPID(S): Tox21_111191_1
M4ID: 12483855

HILL MODEL (in red):

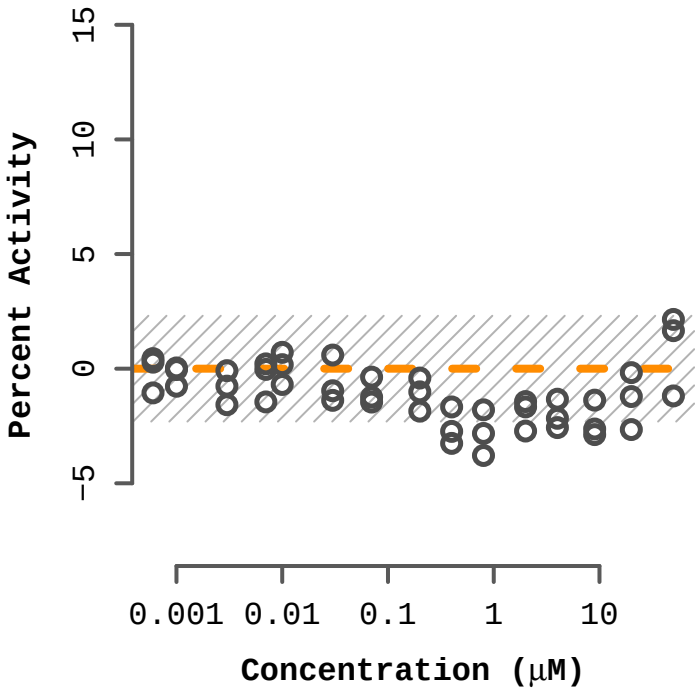
	tp	ga	gw
val:	13.8	−0.66	0.466
sd:	1.16	0.252	0.0689

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.8	−0.66	0.466	3.14	5.61
sd:	1.16	0.252	0.0689	1440	5560

	CNST	HILL	GNLS
AIC:	325.28	181.78	185.78
PROB:	0	0.88	0.12
RMSE:	8.39	2.04	2.04

MAX_MEAN: 16 **MAX_MED:** 13.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

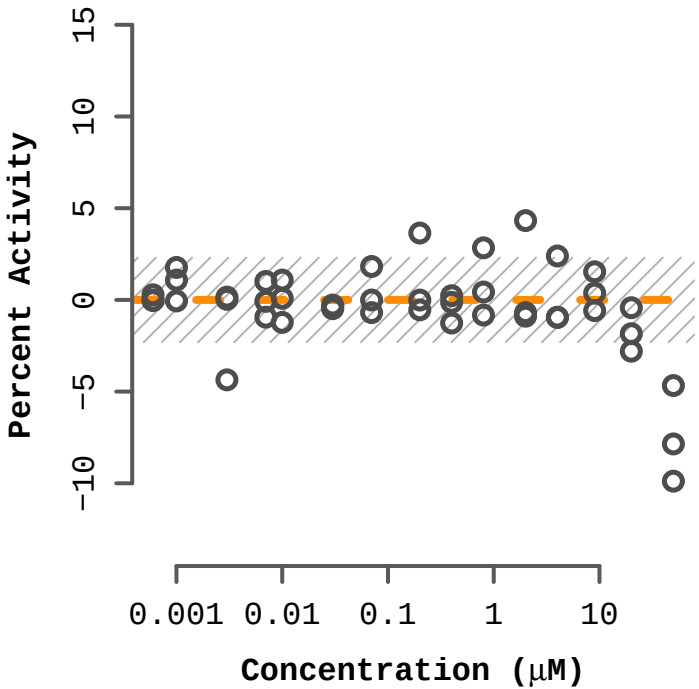
NAME: Tricirbine
CHID: 45743 **CASRN:** 35943-35-2
SPID(S): Tox21_111192_1
M4ID: 12483854

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.874 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

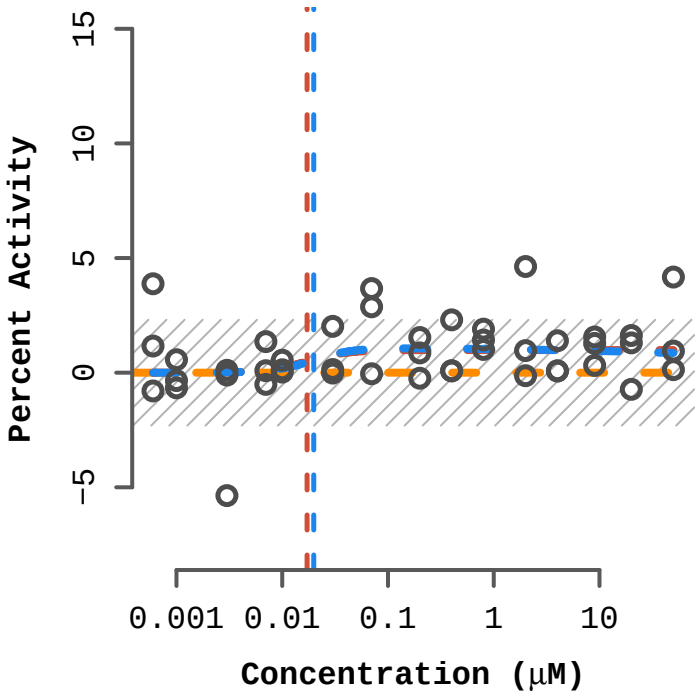
NAME: Eliprodil
CHID: 45744 **CASRN:** 119431-25-3
SPID(S): Tox21_111194_1
M4ID: 12483852

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.49	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zatebradine hydrochloride
CHID: 45745 CASRN: 91940-87-3
SPID(S): Tox21_111195_1
M4ID: 12483851

HILL MODEL (in red):

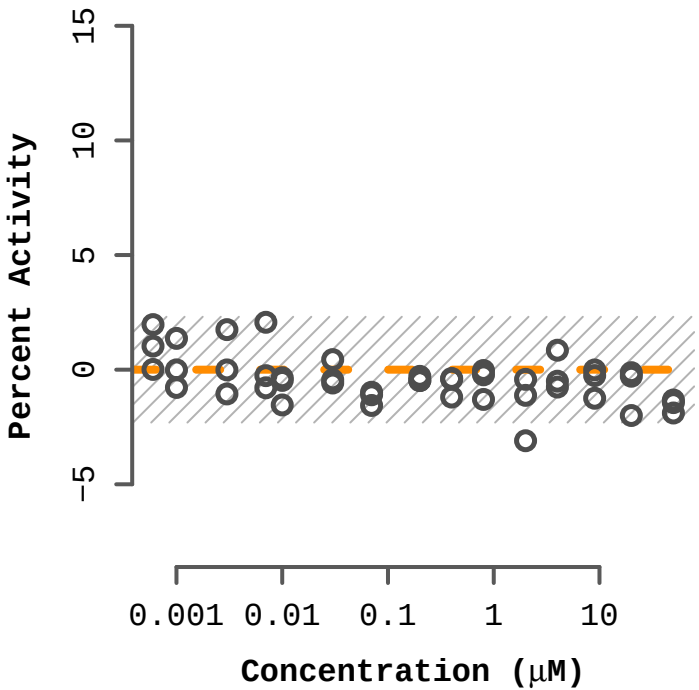
	tp	ga	gw
val:	0.987	−1.76	2.36
sd:	0.226	0.47	2.63

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.13	−1.7	2.33	3.38	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	174.26	161.73	165.7
PROB:	0	0.88	0.12
RMSE:	1.78	1.5	1.5

MAX_MEAN: 2.17 **MAX_MED:** 2.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

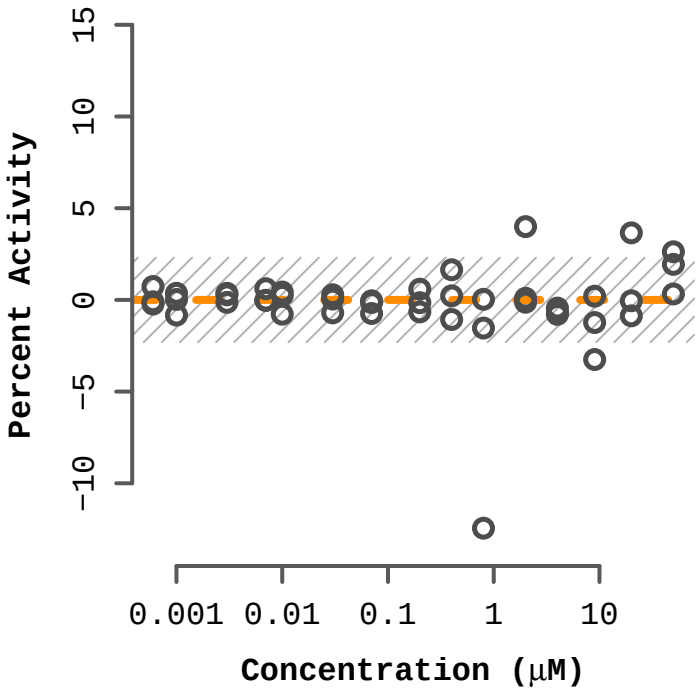
NAME: Relcovaptan
CHID: 45746 **CASRN:** 150375-75-0
SPID(S): Tox21_111198_1
M4ID: 12483848

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

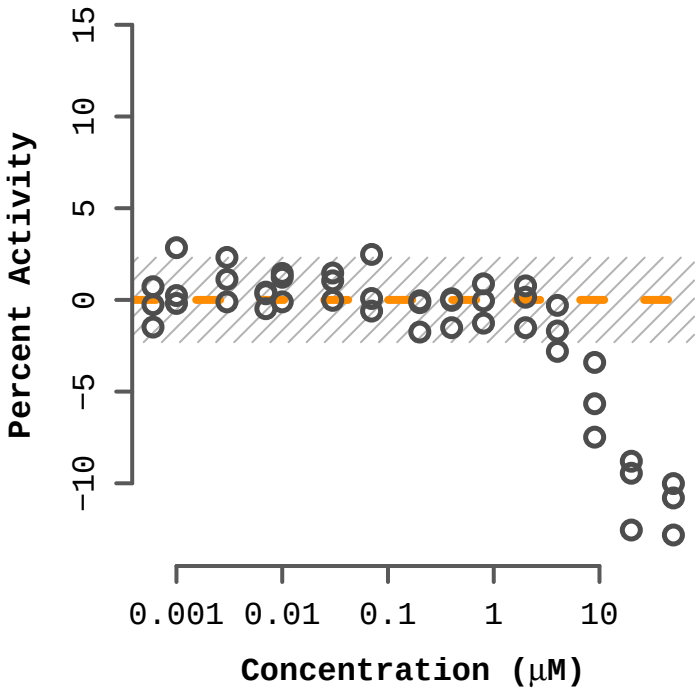
NAME: Acecainide hydrochloride
CHID: 45748 **CASRN:** 34118-92-8
SPID(S): Tox21_111206_1
M4ID: 12483841

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.7	NA	NA
PROB:	1	NA	NA
RMSE:	2.21	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

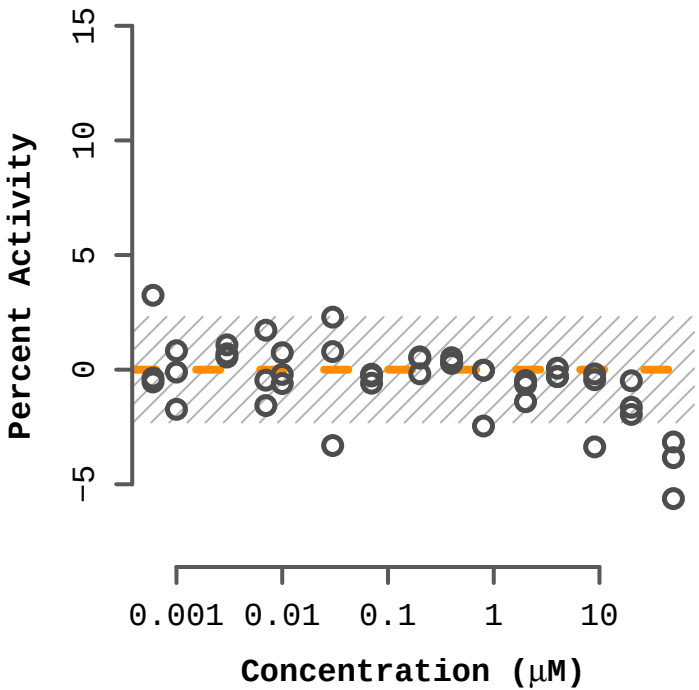
NAME: Amperozide hydrochloride
CHID: 45750 **CASRN:** 75529-73-6
SPID(S): Tox21_111208_1
M4ID: 12483840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	245.43	NA	NA
PROB:	1	NA	NA
RMSE:	4.37	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

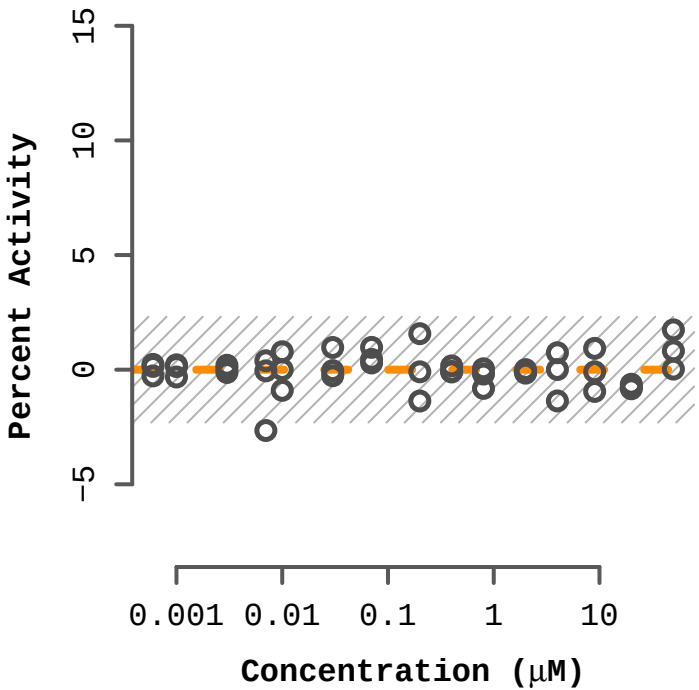
NAME: Opipramol dihydrochloride
CHID: 45752 CASRN: 909-39-7
SPID(S): Tox21_111210_1
M4ID: 12483839

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

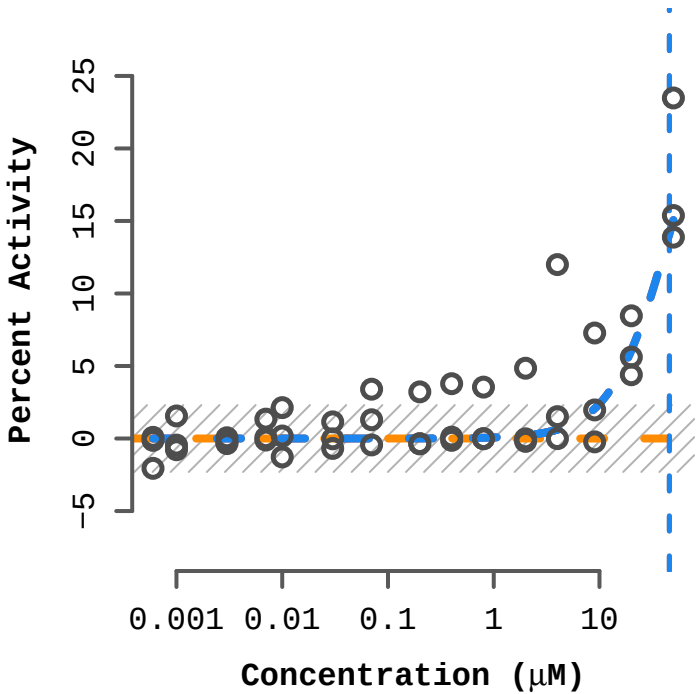
NAME: R−(+)−Atenolol
CHID: 45753 **CASRN:** 56715−13−0
SPID(S): Tox21_111211_1
M4ID: 12483838

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.862 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Azepexole hydrochloride
CHID: 45756 CASRN: 36067-72-8
SPID(S): Tox21_111214_1
M4ID: 12483837

HILL MODEL (in red):

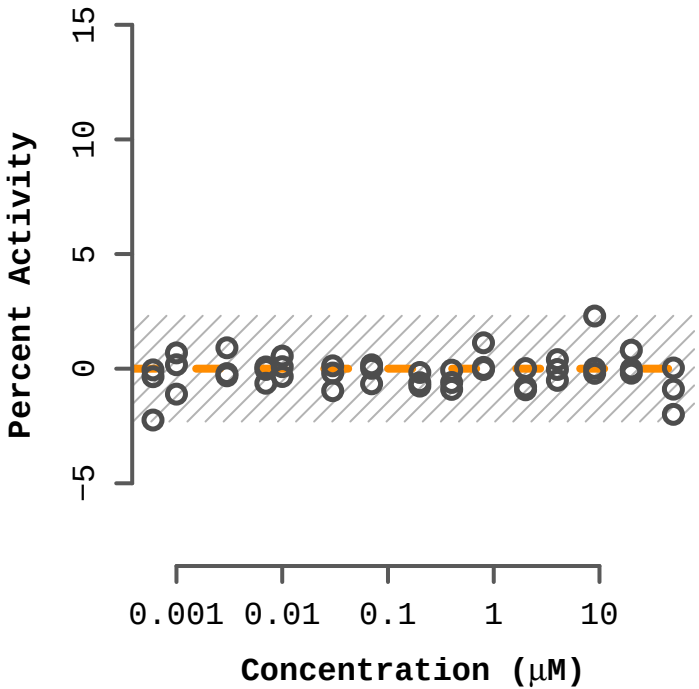
	tp	ga	gw
val:	28.2	1.66	1.56
sd:	19.5	0.396	0.64

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	28.2	1.66	1.56	3.31	5.02
sd:	19.5	0.396	0.641	2380	7430

	CNST	HILL	GNLS
AIC:	256.03	204.55	208.55
PROB:	0	0.88	0.12
RMSE:	5.57	2.72	2.72

MAX_MEAN: 17.6 **MAX_MED:** 15.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

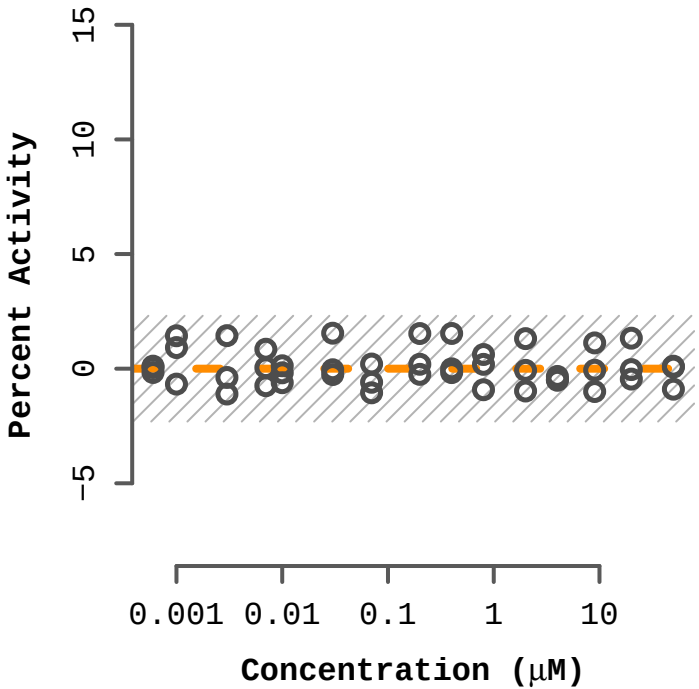
NAME: Aptiganel hydrochloride
CHID: 45762 **CASRN:** 137160-11-3
SPID(S): Tox21_111220_1
M4ID: 12483835

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.702 **MAX_MED:** 0.173 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

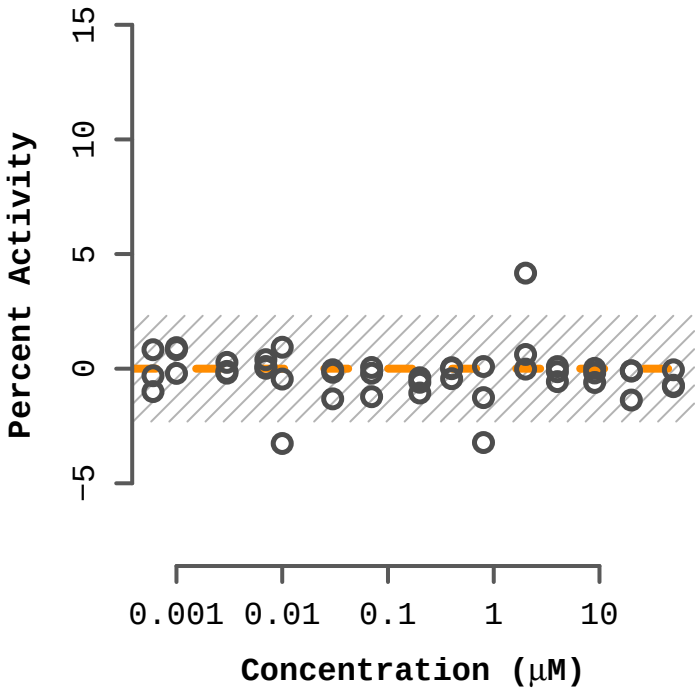
NAME: Methyl L−DOPA hydrochloride
CHID: 45763 **CASRN:** 1421−65−4
SPID(S): Tox21_111221_1
M4ID: 12483834

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.562 **MAX_MED:** 0.923 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

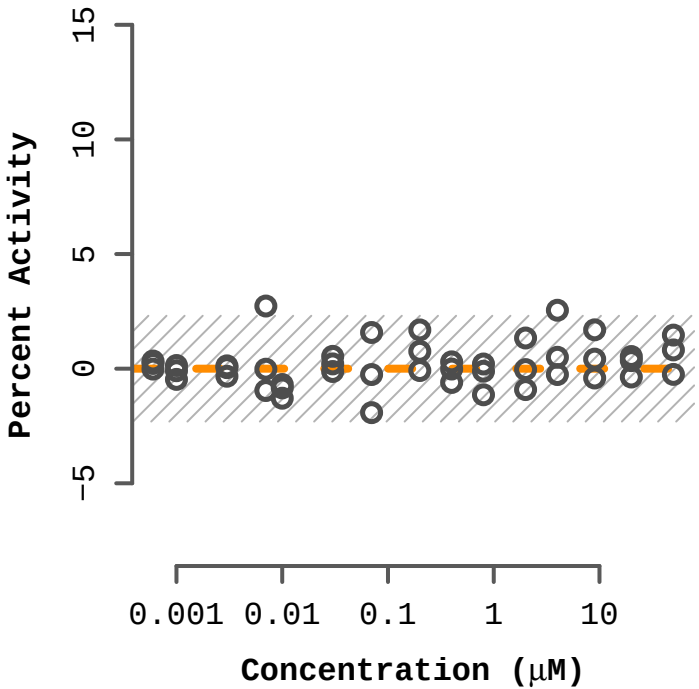
NAME: Eflornithine hydrochloride
CHID: 45765 **CASRN:** 96020-91-6
SPID(S): Tox21_111224_1
M4ID: 12483832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 0.837 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

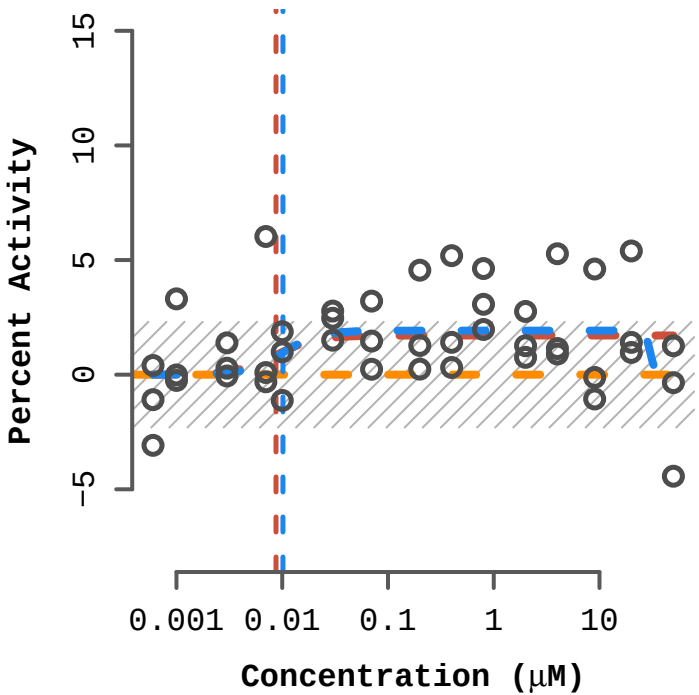
NAME: Etazolate hydrochloride
CHID: 45767 **CASRN:** 35838-58-5
SPID(S): Tox21_111226_1
M4ID: 12483831

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.931 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Safingol
CHID: 45768 CASRN: 15639-50-6
SPID(S): Tox21_111227_1
M4ID: 12483830

HILL MODEL (in red):

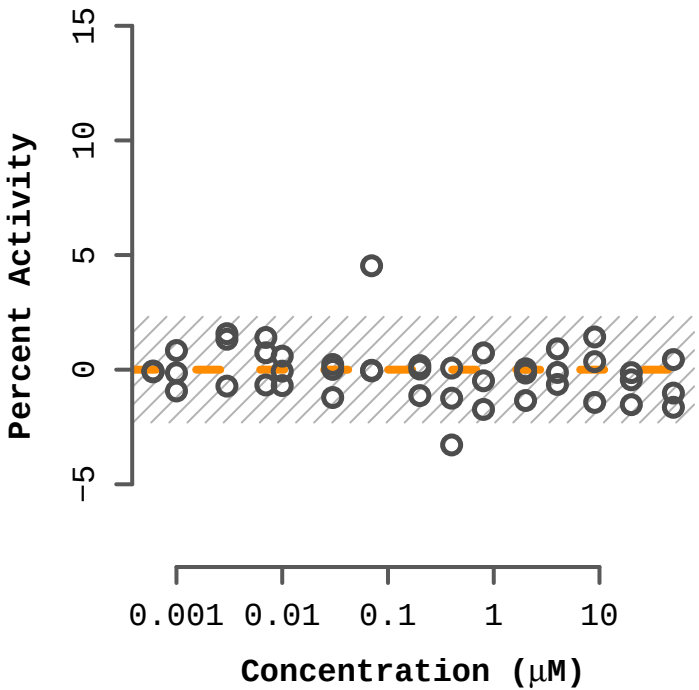
	tp	ga	gw
val:	1.71	−2.06	2.33
sd:	0.355	0.589	6.42

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.92	−1.99	2.55	1.48	17.8
sd:	0.372	0.356	7.75	1.81	162

	CNST	HILL	GNLS
AIC:	214.91	198.72	198.83
PROB:	0	0.51	0.49
RMSE:	2.57	2.07	1.94

MAX_MEAN: 3.23 **MAX_MED:** 3.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

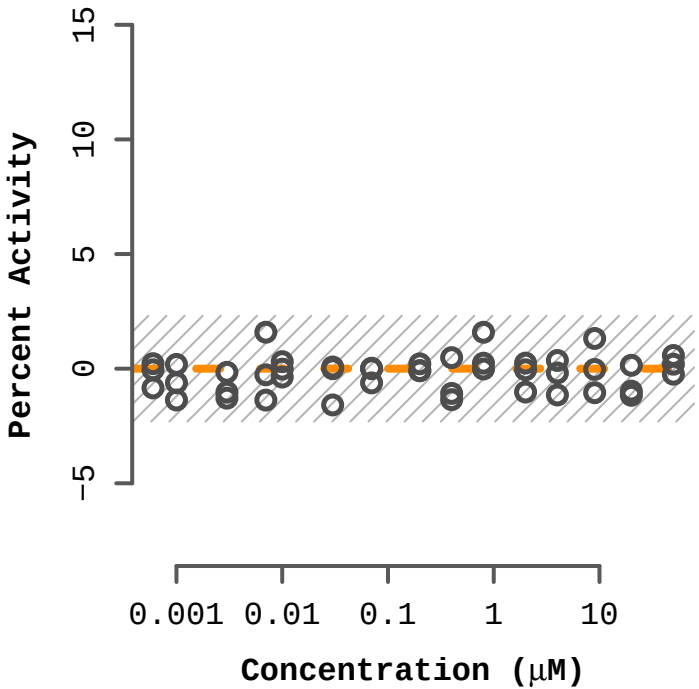
NAME: Eticlopride hydrochloride
CHID: 45769 **CASRN:** 97612-24-3
SPID(S): Tox21_111229_1
M4ID: 12483828

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

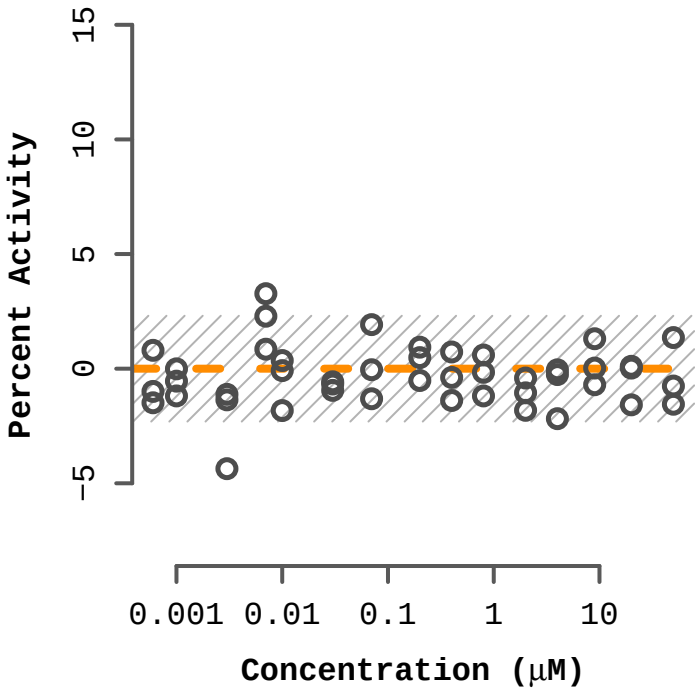
NAME: Fenspiride hydrochloride
CHID: 45770 **CASRN:** 5053-08-7
SPID(S): Tox21_111230_1
M4ID: 12483827

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.606 **MAX_MED:** 0.241 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

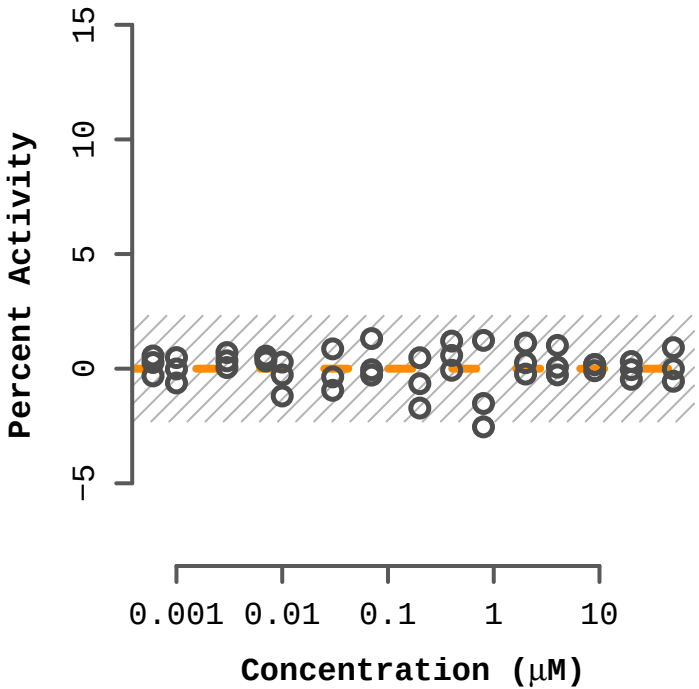
NAME: Flupirtine maleate
CHID: 45771 **CASRN:** 75507-68-5
SPID(S): Tox21_111232_1
M4ID: 12483825

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

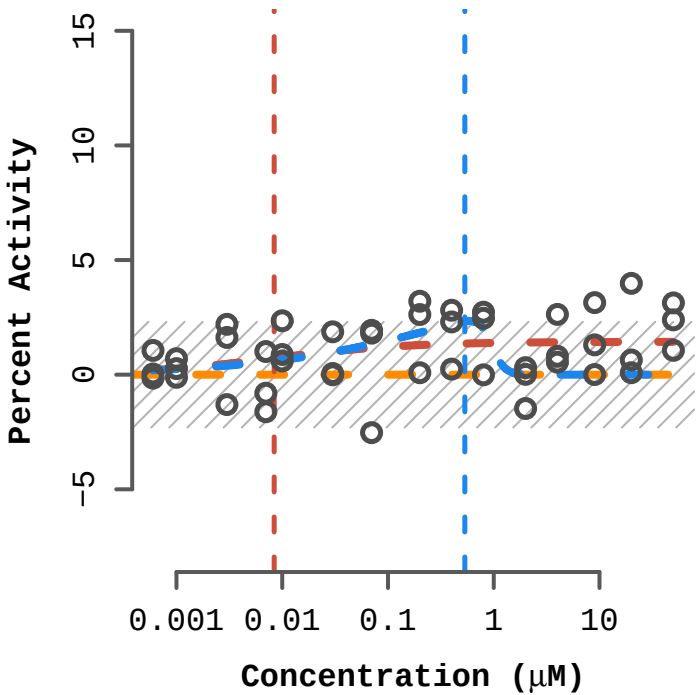
NAME: 4-Methylpyrazole hydrochloride
CHID: 45776 **CASRN:** 56010-88-9
SPID(S): Tox21_111241_1
M4ID: 12483822

HILL MODEL: Not applicable.

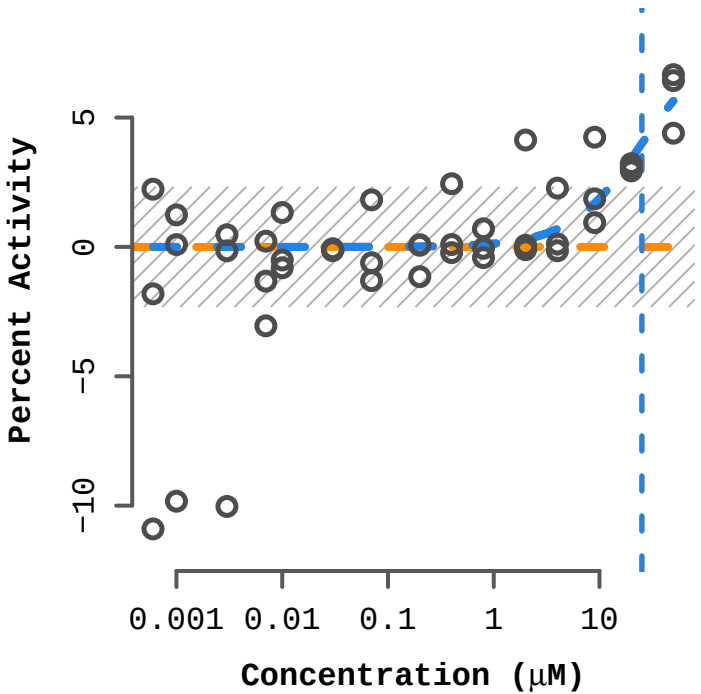
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.571 **MAX_MED:** 0.578 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Mizoribine
CHID:    45777   CASRN: 50924-49-7
SPID(S): Tox21_111242_1
M4ID:    12483821

HILL MODEL (in red):
      tp       ga       gw
val:  1.43     -2.08    0.695
sd:   0.363    0.785    0.757

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.72     -0.273   0.463    -0.0232  7.32
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  183.6       167.87      178.01
PROB: 0           0.99        0.01
RMSE: 1.75        1.37        1.53

MAX_MEAN: 2.2       MAX_MED: 2.62      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clorgyline hydrochloride
CHID: 45778 CASRN: 17780-75-5
SPID(S): Tox21_111243_1
M4ID: 12483820

HILL MODEL (in red):

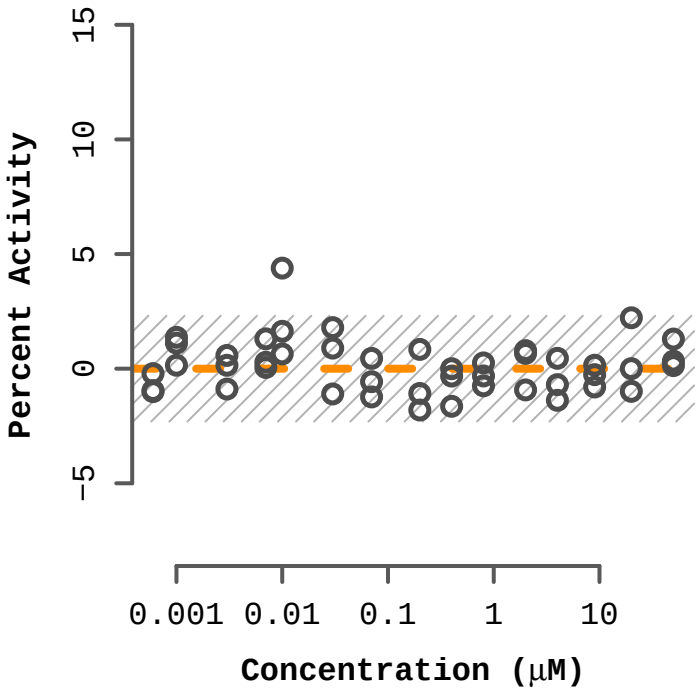
	tp	ga	gw
val:	7.99	1.4	1.28
sd:	3.42	0.329	0.536

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.99	1.4	1.28	2.9	6.7
sd:	3.42	0.329	0.535	1290	7200

	CNST	HILL	GNLS
AIC:	227.26	197.43	201.43
PROB:	0	0.88	0.12
RMSE:	3.44	2.91	2.91

MAX_MEAN: 5.83 **MAX_MED:** 6.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

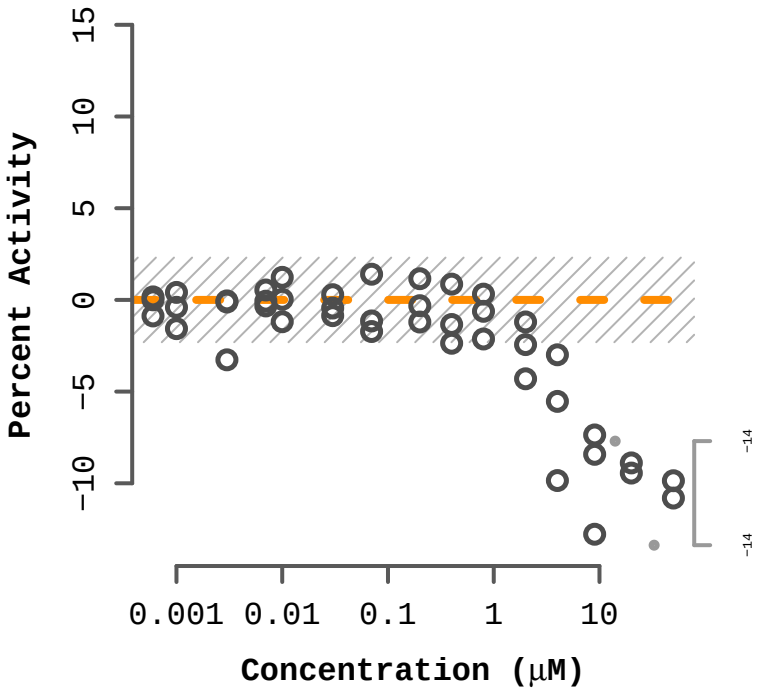
NAME: Cysteamine hydrochloride
CHID: 45779 **CASRN:** 156-57-0
SPID(S): Tox21_111245_1
M4ID: 12483818

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

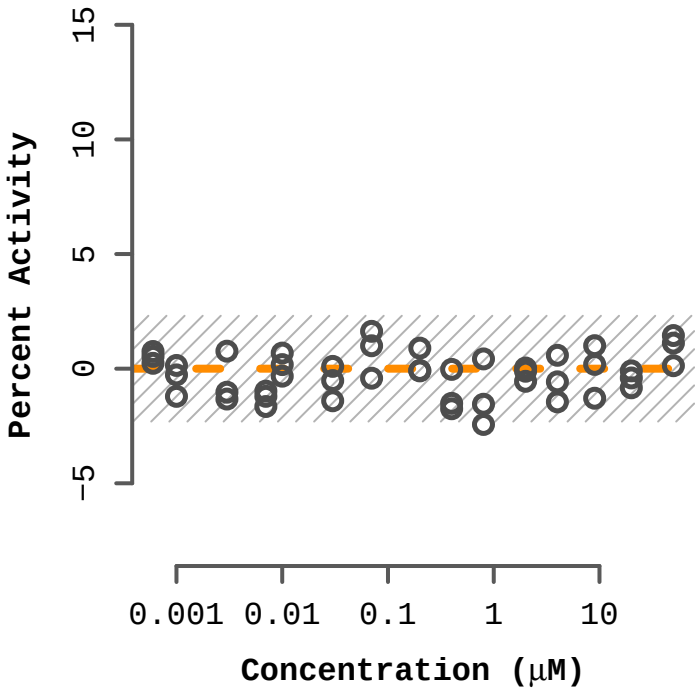
NAME: Stilonium iodide
CHID: 45781 **CASRN:** 77257-42-2
SPID(S): Tox21_111247_1
M4ID: 12483817 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.89	NA	NA
PROB:	1	NA	NA
RMSE:	5.29	NA	NA

MAX_MEAN: 0.0486 **MAX_MED:** 0.0345 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

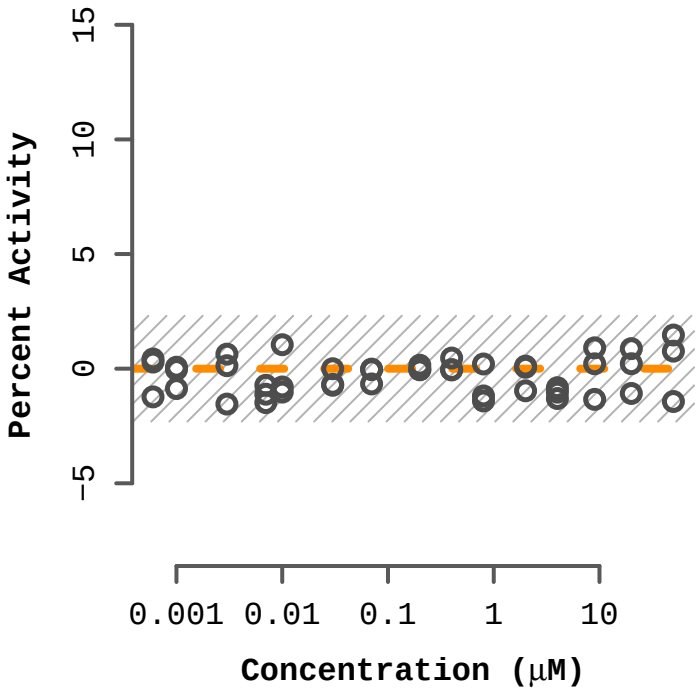
NAME: Mexiletene hydrochloride
CHID: 45783 **CASRN:** 5370-01-4
SPID(S): Tox21_111249_2
M4ID: 12483816

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.898 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

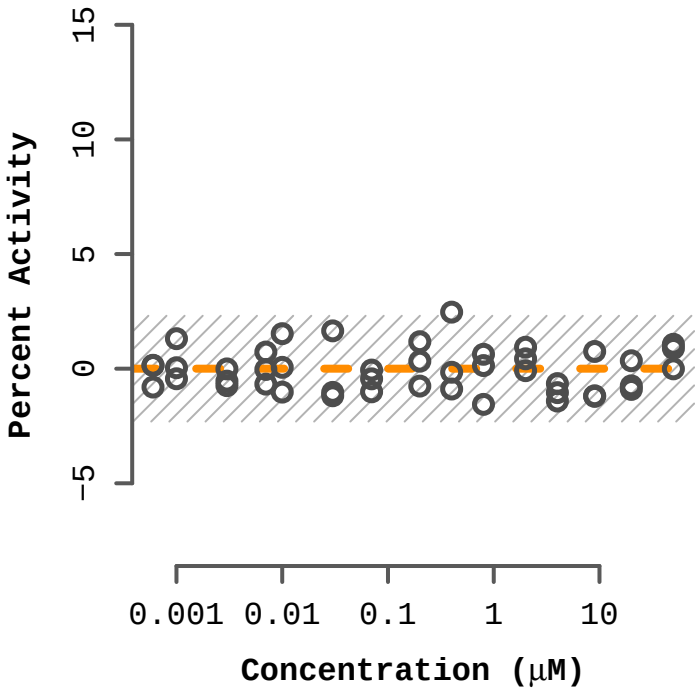
NAME: Naphazoline hydrochloride
CHID: 45788 CASRN: 550-99-2
SPID(S): Tox21_111255_1
M4ID: 12483813

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.268 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

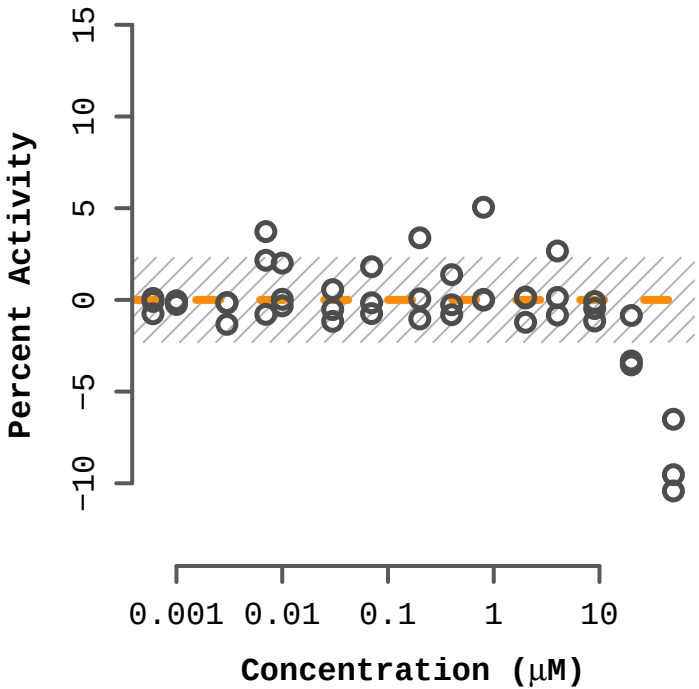
NAME: Nomifensine maleate
CHID: 45790 CASRN: 32795-47-4
SPID(S): Tox21_111258_1
M4ID: 12483811

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.648 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

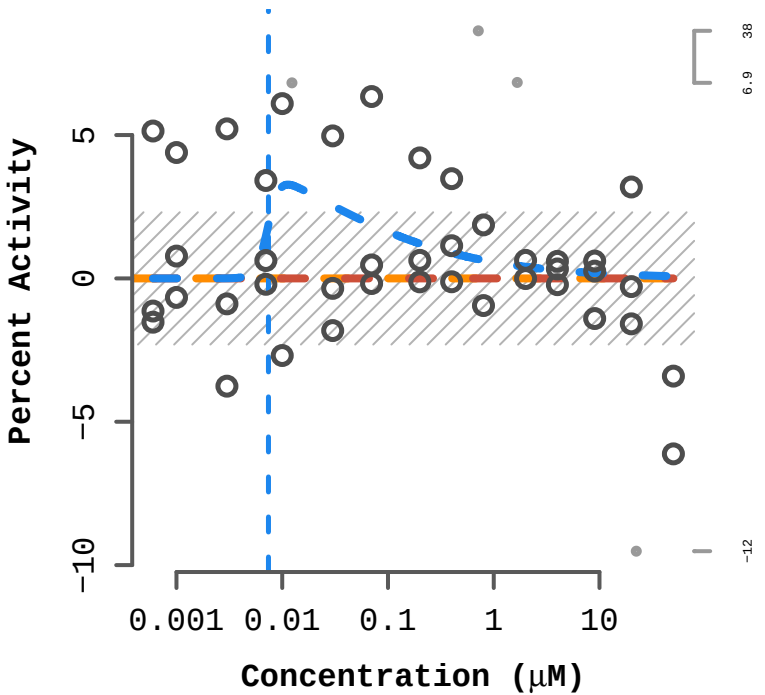
NAME: Octoclothepine maleate
CHID: 45791 **CASRN:** 4789-68-8
SPID(S): Tox21_111259_1
M4ID: 12483810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.79	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Proadifen hydrochloride
CHID: 45792 CASRN: 62-68-0
SPID(S): Tox21_111260_1
M4ID: 12483809 BRK

HILL MODEL (in red):

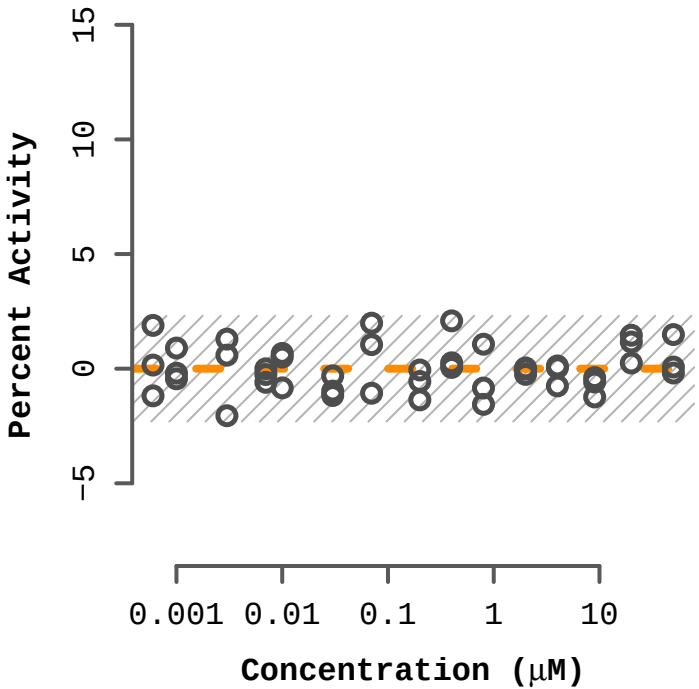
	tp	ga	gw
val:	1.58e-07	2.17	0.309
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.5	−2.13	8	−1.88	0.541
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	258.52	264.52	263.44
PROB:	0.88	0.04	0.08
RMSE:	6.65	6.65	6.46

MAX_MEAN: 12.9 **MAX_MED:** 6.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

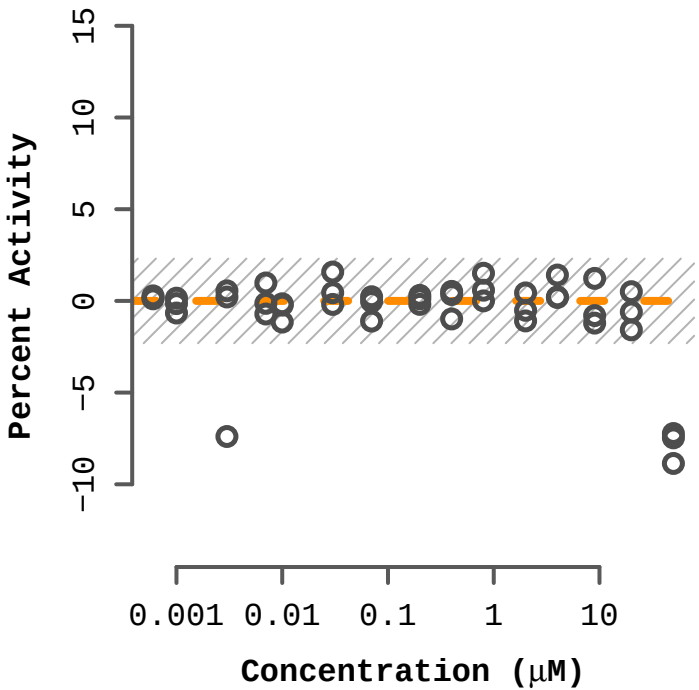
NAME: Bisoprolol fumarate
CHID: 45794 **CASRN:** 104344-23-2
SPID(S): Tox21_111262_1
M4ID: 12483808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.958 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

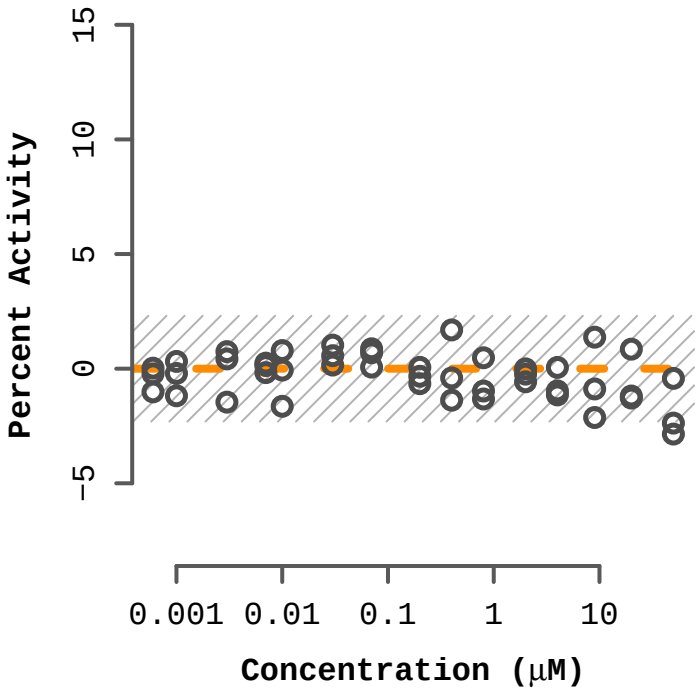
NAME: Salmeterol xinafoate
CHID: 45798 **CASRN:** 94749-08-3
SPID(S): Tox21_111270_1
M4ID: 12483804

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.42	NA	NA

MAX_MEAN: 0.699 **MAX_MED:** 0.585 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

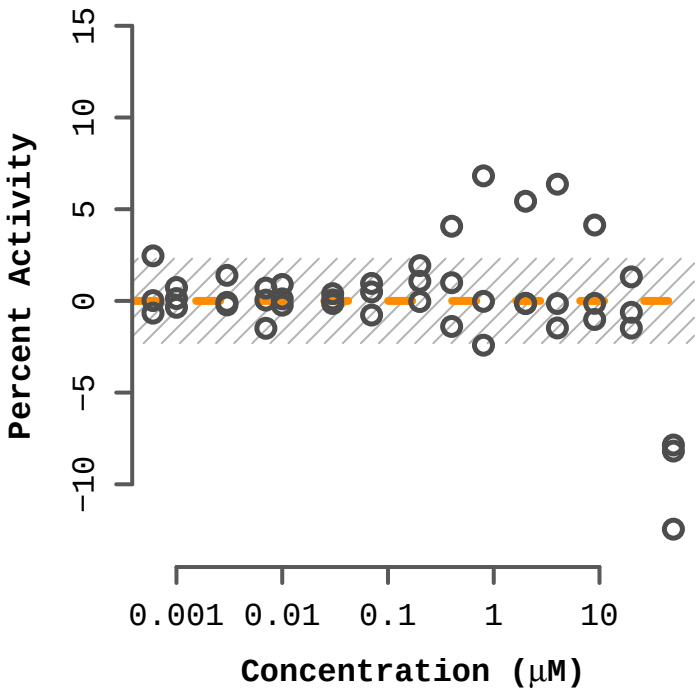
NAME: Trihexyphenidyl hydrochloride
CHID: 45802 **CASRN:** 52-49-3
SPID(S): Tox21_111274_1
M4ID: 12483801

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.585 **MAX_MED:** 0.694 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

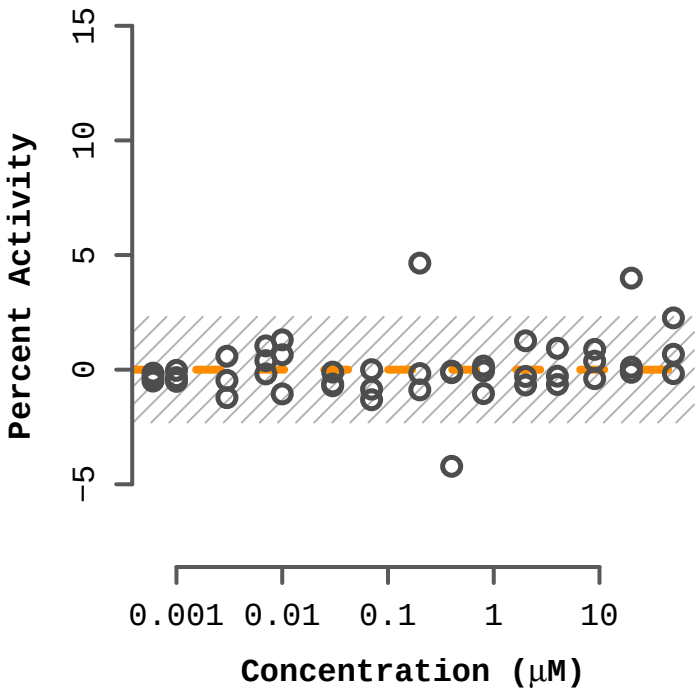
NAME: Triflupromazine hydrochloride
CHID: 45804 **CASRN:** 1098-60-8
SPID(S): Tox21_111276_1
M4ID: 12483800

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.77	NA	NA
PROB:	1	NA	NA
RMSE:	3.23	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

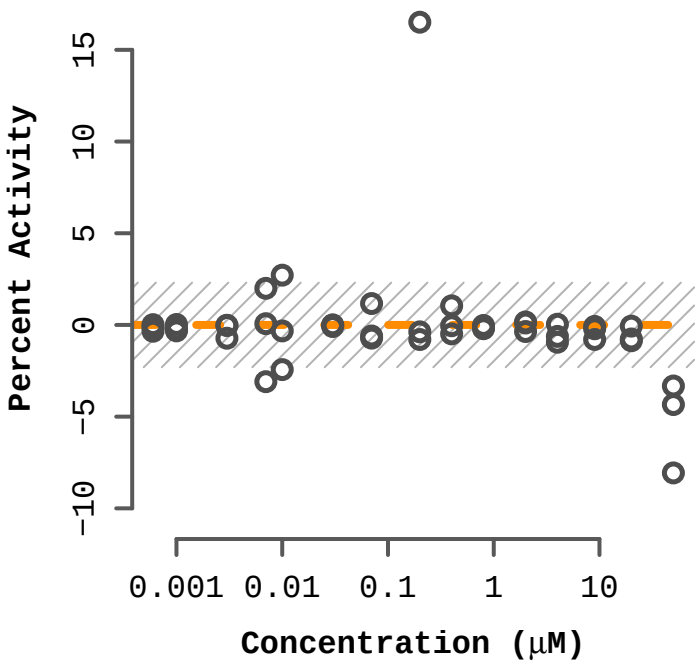
NAME: Tulobuterol hydrochloride
CHID: 45805 CASRN: 56776-01-3
SPID(S): Tox21_111277_1
M4ID: 12483799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.674 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

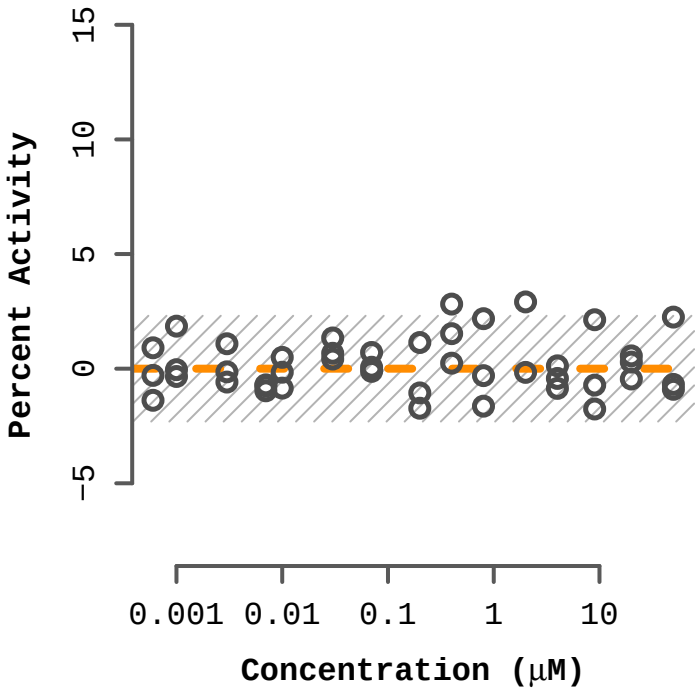
NAME: Trequinsin hydrochloride
CHID: 45806 **CASRN:** 78416-81-6
SPID(S): Tox21_111279_1
M4ID: 12483797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 5.11 **MAX_MED:** 0.107 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

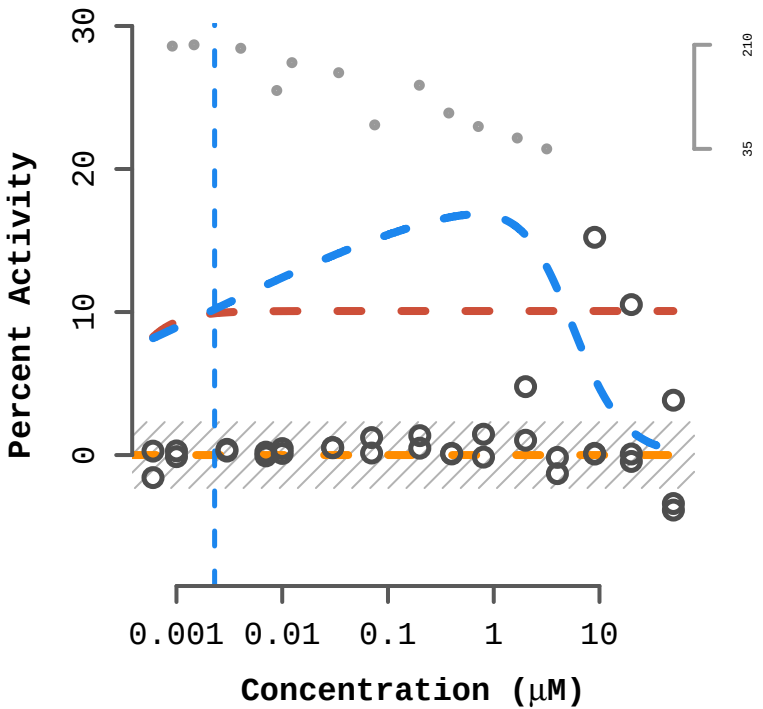
NAME: N-alpha-p-Tosyl-L-lysine chloromethyl ketone hy
CHID: 45807 CASRN: 4272-74-6
SPID(S): Tox21_111280_1
M4ID: 12483796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trifluperidol hydrochloride
CHID: 45810 CASRN: 2062-77-3
SPID(S): Tox21_111284_1
M4ID: 12483793 BRK

HILL MODEL (in red):

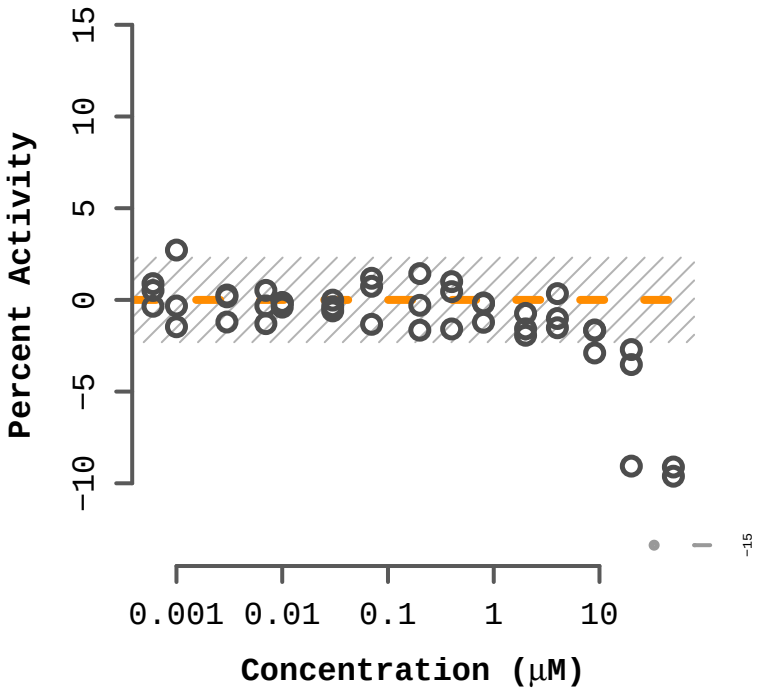
	tp	ga	gw
val:	10.1	-3.56	1.96
sd:	5.91	6.86	32.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	20.4	-2.64	0.3	0.73	1.78
sd:	58.6	9.18	1.73	1.04	4.65

	CNST	HILL	GNLS
AIC:	516.35	498.44	501.27
PROB:	0	0.8	0.2
RMSE:	75.18	71.07	70.16

MAX_MEAN: 70.6 MAX_MED: 4.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

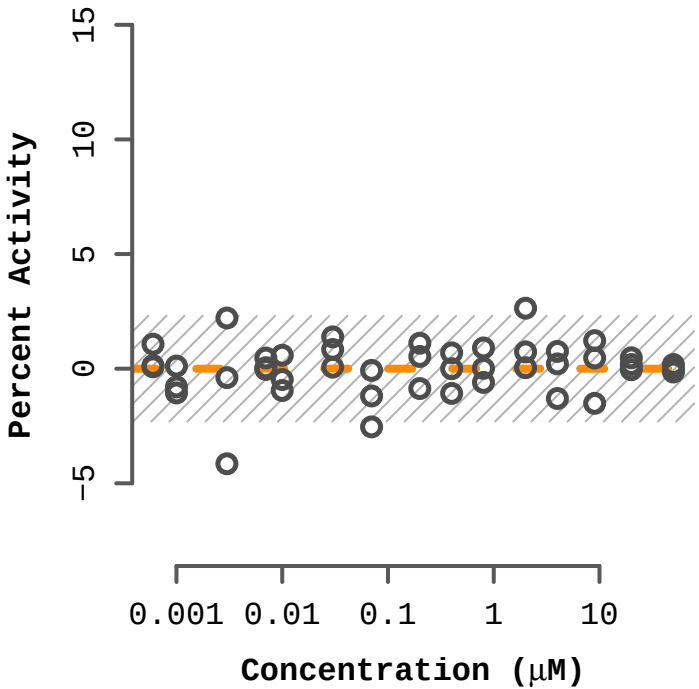
NAME: Zolantidine dimaleate
CHID: 45811 CASRN: 104076-39-3
SPID(S): Tox21_111285_1
M4ID: 12483792 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.77	NA	NA
PROB:	1	NA	NA
RMSE:	3.54	NA	NA

MAX_MEAN: 0.353 **MAX_MED:** 0.743 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

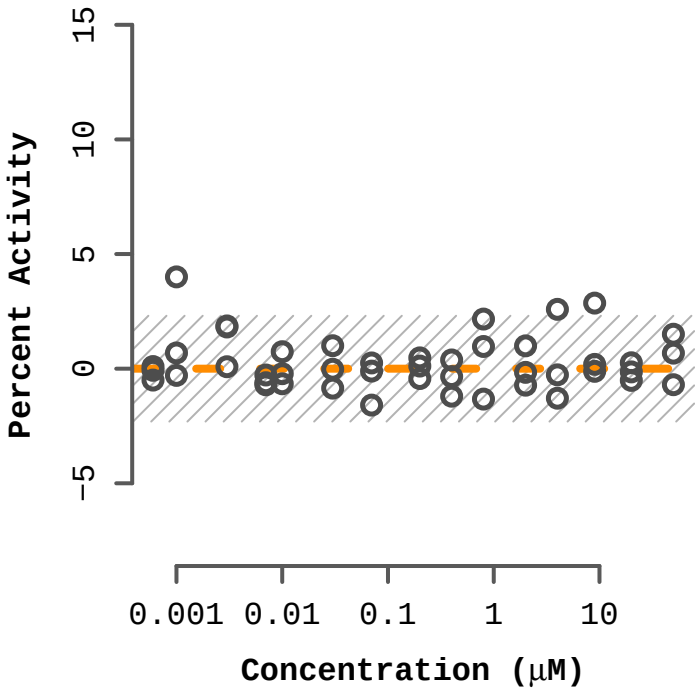
NAME: Urapidil hydrochloride
CHID: 45812 **CASRN:** 64887-14-5
SPID(S): Tox21_111286_1
M4ID: 12483791

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.839 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

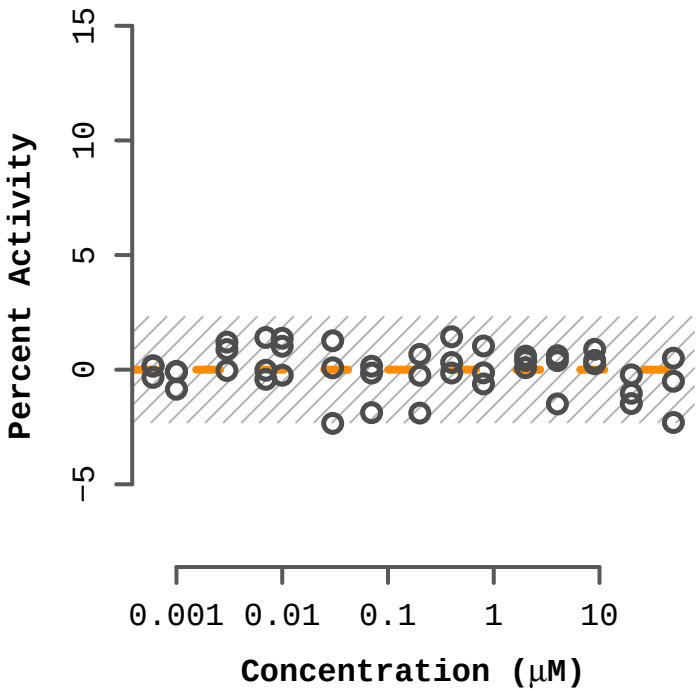
NAME: Olprinone hydrochloride
CHID: 45813 **CASRN:** 119615-63-3
SPID(S): Tox21_111287_1
M4ID: 12483790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

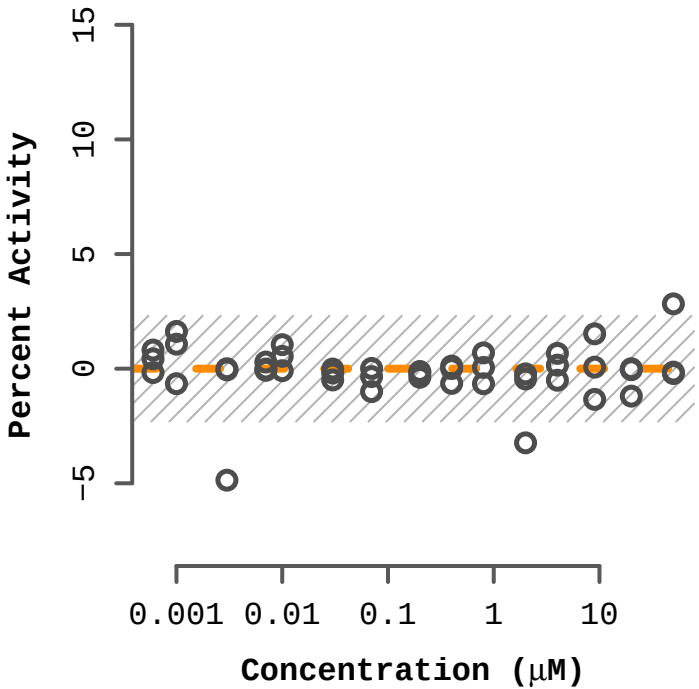
NAME: Zimeldine dihydrochloride hydrate
CHID: 45815 **CASRN:** 61129-30-4
SPID(S): Tox21_111289_1
M4ID: 12483789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.717 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

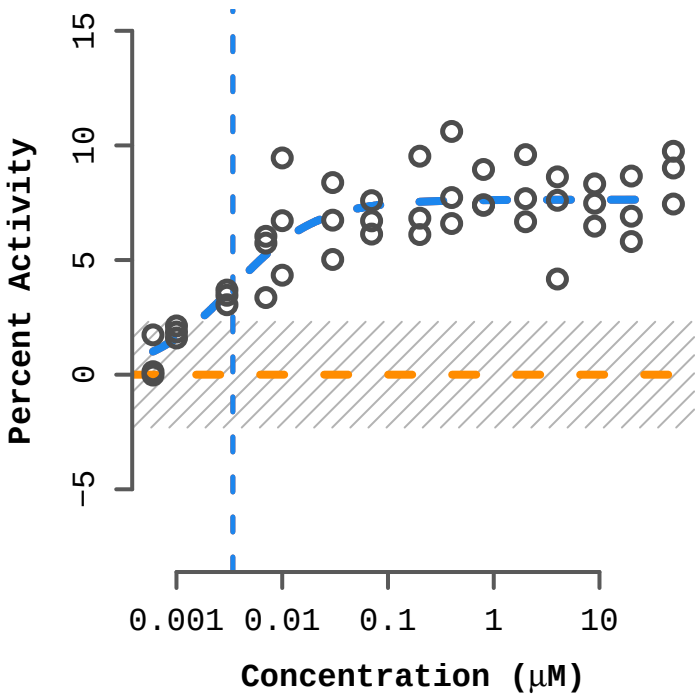
NAME: Carbenicillin disodium
CHID: 45820 **CASRN:** 4800-94-6
SPID(S): Tox21_111304_1
M4ID: 12483779

HILL MODEL: Not applicable.

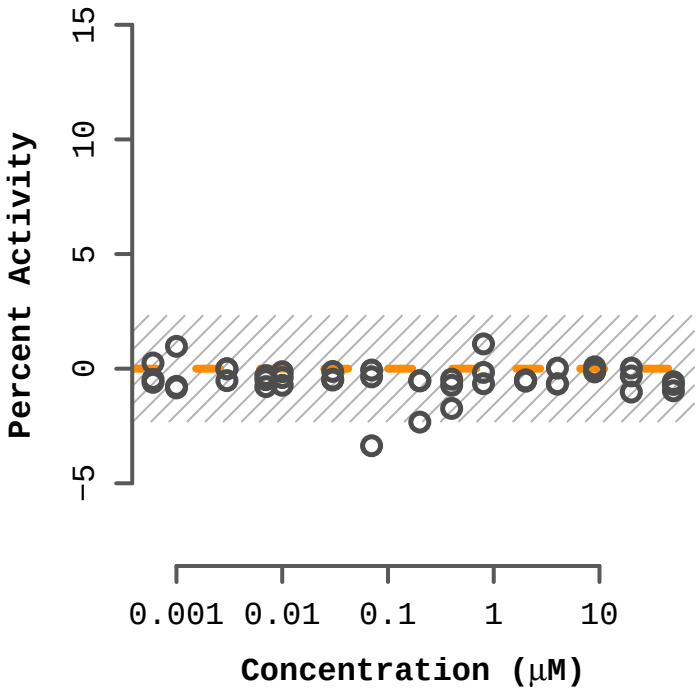
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.824 **MAX_MED:** 1.07 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ephedrine hydrochloride
CHID:    45825   CASRN: 50-98-6
SPID(S): Tox21_111310_1
M4ID:    12483776

HILL MODEL (in red):
      tp       ga       gw
val:  7.63     -2.47    1.08
sd:   0.27     0.0932   0.262

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.63     -2.47    1.08     3.46     4.97
sd:   0.27     0.0932   0.262    1690     4780

      CNST        HILL        GNLS
AIC:  310.26      161.87      165.87
PROB: 0           0.88        0.12
RMSE: 6.74        1.34        1.34

MAX_MEAN: 8.74      MAX_MED: 9.02      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

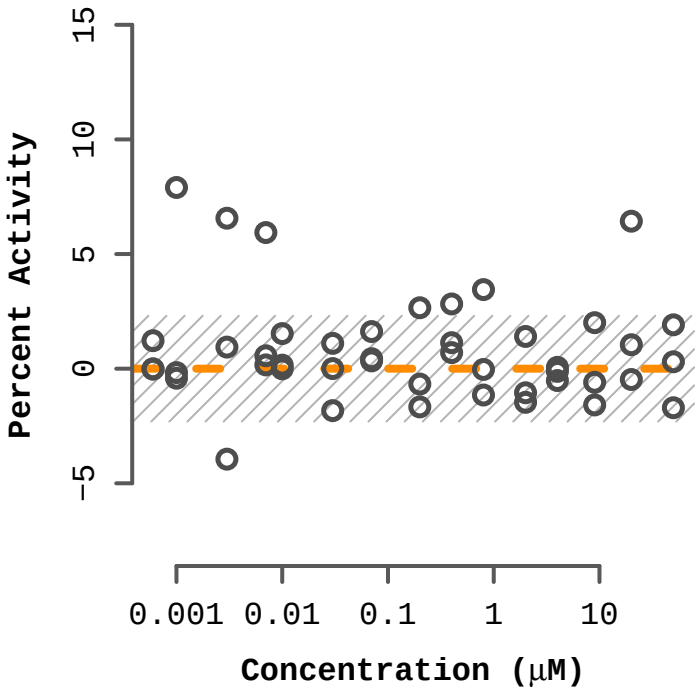
NAME: Eucatropine hydrochloride
CHID: 45828 CASRN: 536-93-6
SPID(S): Tox21_113348_1
M4ID: 12482681

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.0894 **MAX_MED:** −0.00487 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

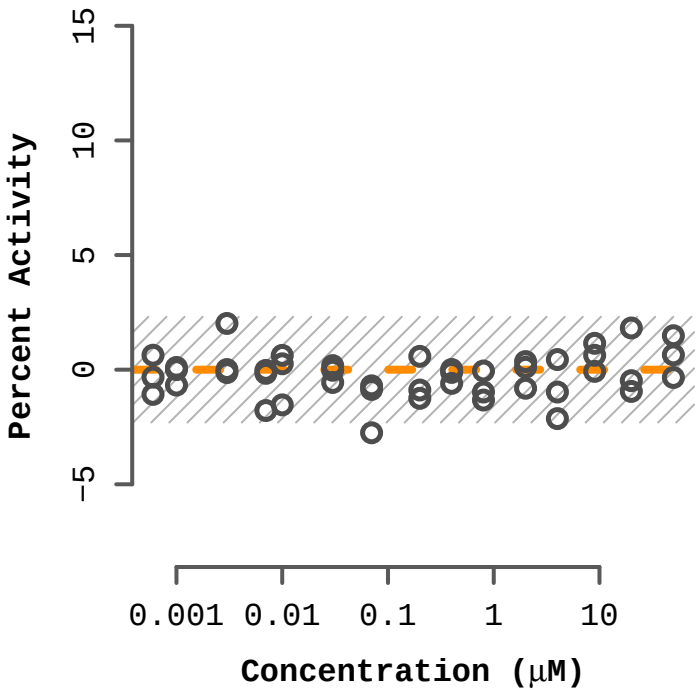
NAME: Isosorbide dinitrate
CHID: 45832 **CASRN:** 87-33-2
SPID(S): Tox21_111317_1
M4ID: 12483774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.42	NA	NA

MAX_MEAN: 2.44 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

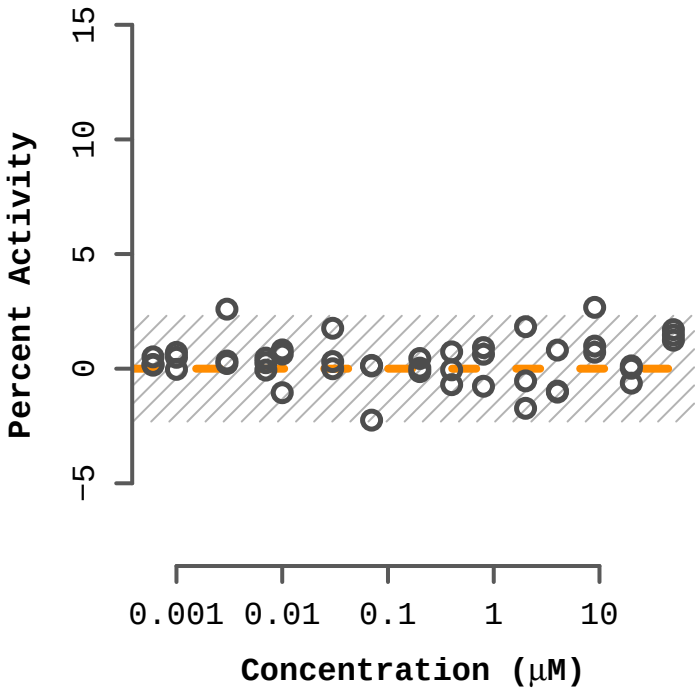
NAME: Lactulose
CHID: 45833 **CASRN:** 4618-18-2
SPID(S): Tox21_111318_1
M4ID: 12483773

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.633 **MAX_MED:** 0.647 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

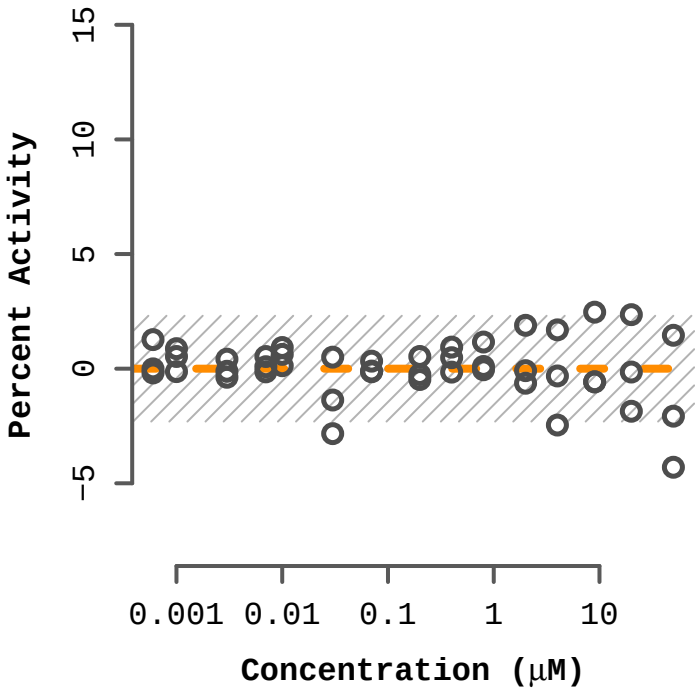
NAME: Methicillin sodium hydrate
CHID: 45835 **CASRN:** 7246-14-2
SPID(S): Tox21_111320_1
M4ID: 12483771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

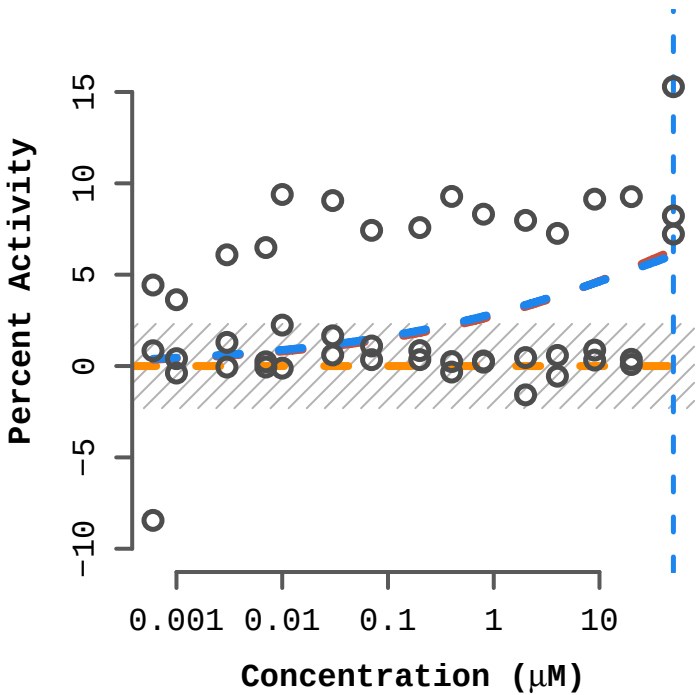
NAME: Nitromide
CHID: 45836 **CASRN:** 121-81-3
SPID(S): Tox21_111321_1
M4ID: 12483770

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.56 **MAX_MED:** 0.625 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxidopamine hydrochloride
CHID: 45838 CASRN: 28094-15-7
SPID(S): Tox21_111324_1
M4ID: 12483767

HILL MODEL (in red):

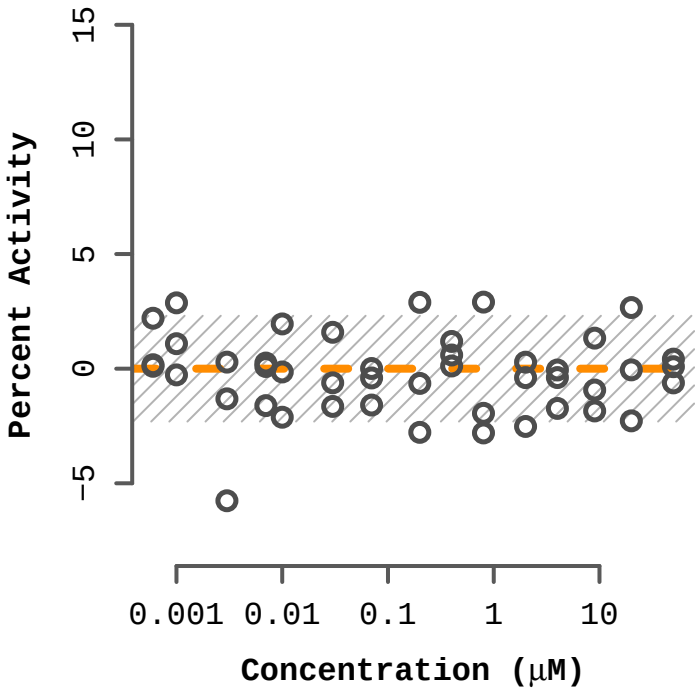
	tp	ga	gw
val:	15.3	2.2	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.1	1.7	0.3	3	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	279.09	268.22	272.31
PROB:	0	0.88	0.11
RMSE:	5.33	4.19	4.19

MAX_MEAN: 10.2 **MAX_MED:** 8.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

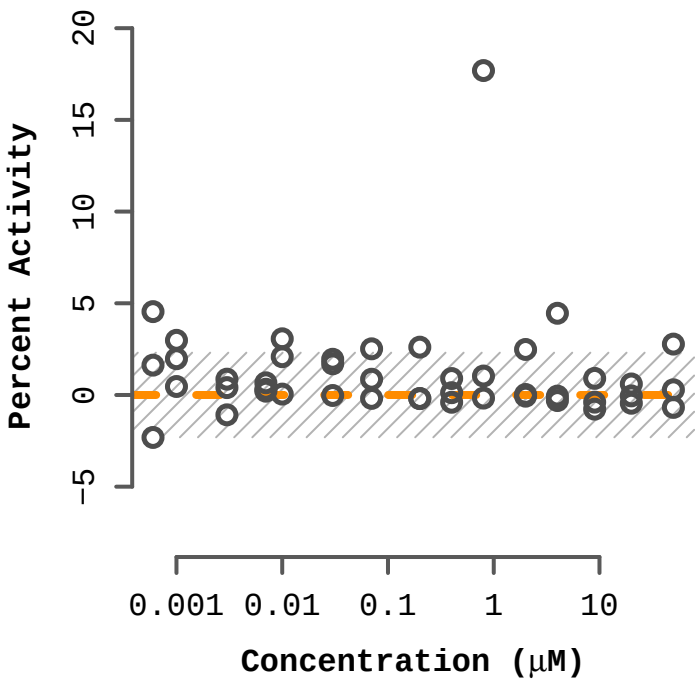
NAME: Salicyl alcohol
CHID: 45843 **CASRN:** 90-01-7
SPID(S): Tox21_111330_1
M4ID: 12483762

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

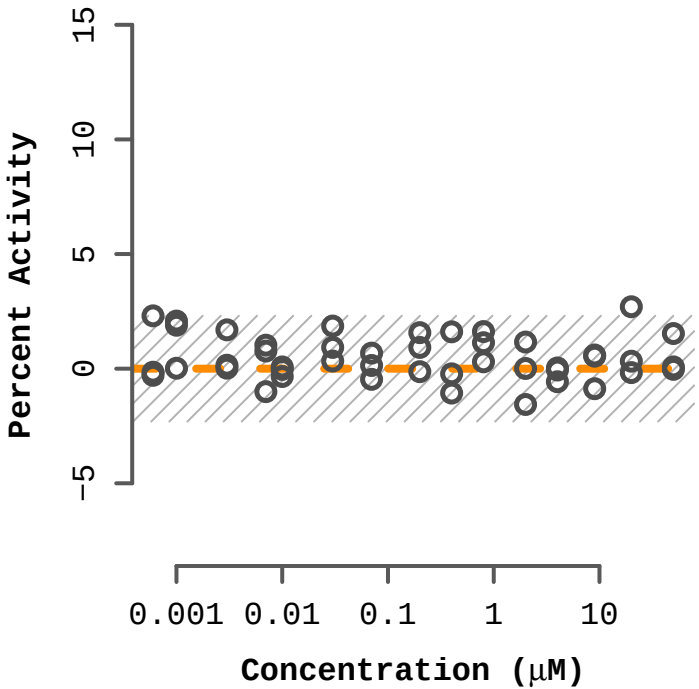
NAME: 2-Aminoheptane sulfate
CHID: 45845 CASRN: 6411-75-2
SPID(S): Tox21_111333_1
M4ID: 12483759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.81	NA	NA
PROB:	1	NA	NA
RMSE:	3.09	NA	NA

MAX_MEAN: 6.19 MAX_MED: 2.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

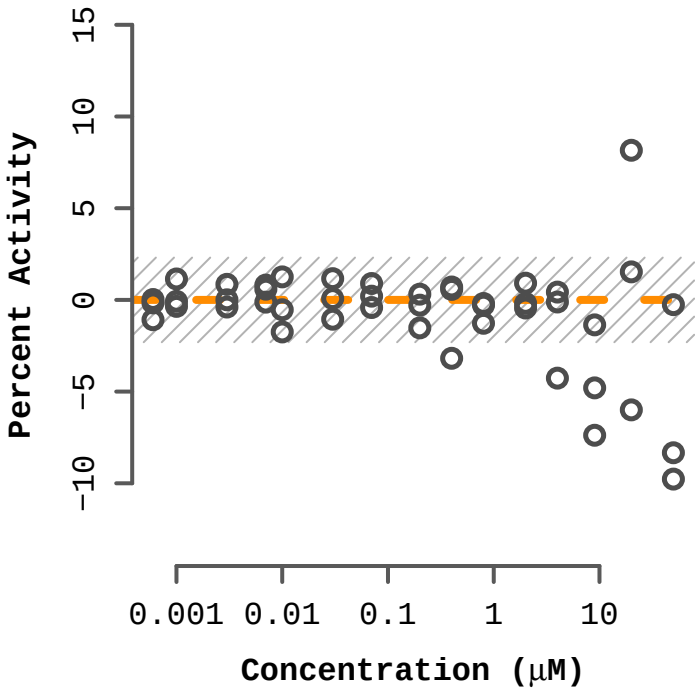
NAME: Acetarsol
CHID: 45847 CASRN: 97-44-9
SPID(S): Tox21_111336_1
M4ID: 12483758

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.33 MAX_MED: 1.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

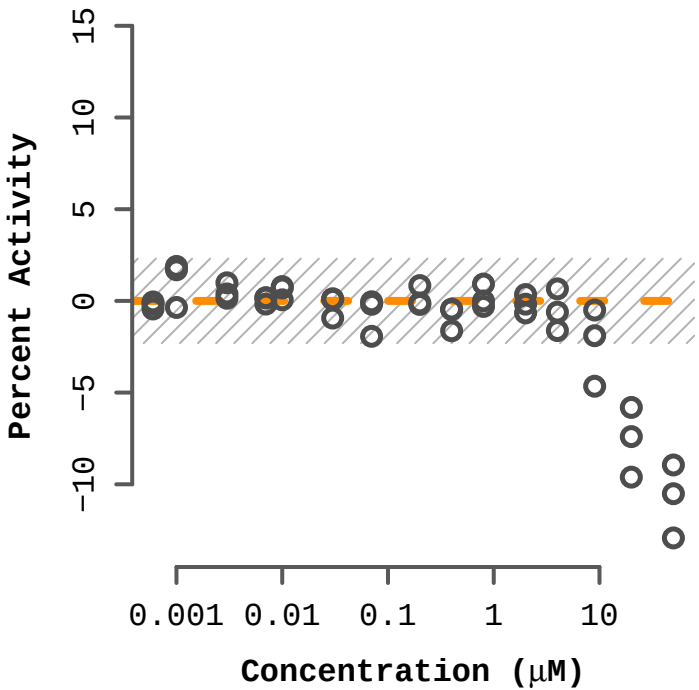
NAME: Acriflavine hydrochloride
CHID: 45848 **CASRN:** 69235-50-3
SPID(S): Tox21_111337_1
M4ID: 12483757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.76	NA	NA
PROB:	1	NA	NA
RMSE:	2.97	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

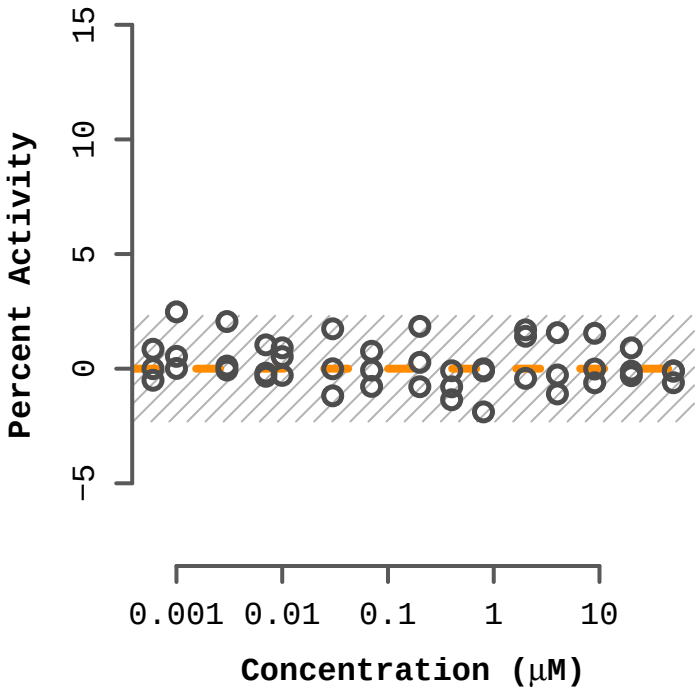
NAME: Broxyquinoline
CHID: 45849 **CASRN:** 521-74-4
SPID(S): Tox21_111338_1
M4ID: 12483756

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.44	NA	NA
PROB:	1	NA	NA
RMSE:	3.61	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

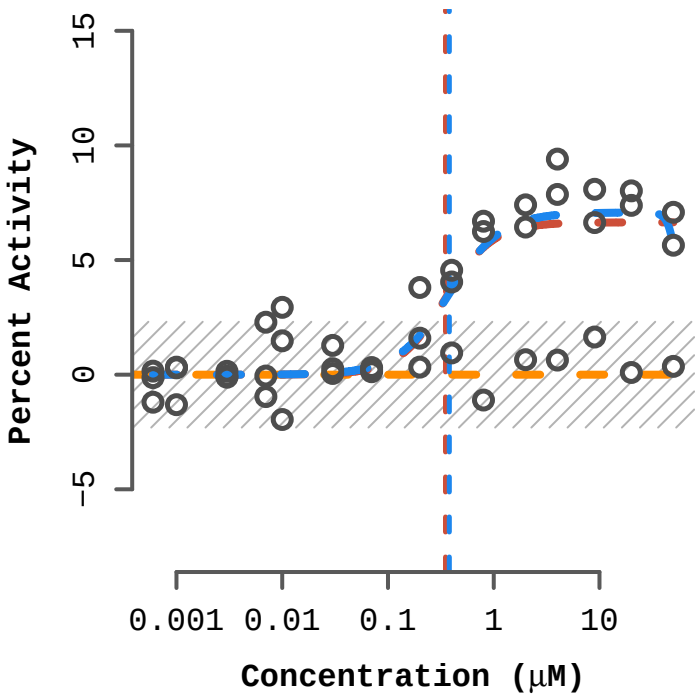
NAME: Carnitine hydrochloride
CHID: 45850 **CASRN:** 461-05-2
SPID(S): Tox21_111339_1
M4ID: 12483755

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flopropione
CHID: 45851 **CASRN:** 2295-58-1
SPID(S): Tox21_111340_1
M4ID: 12483754

HILL MODEL (in red):

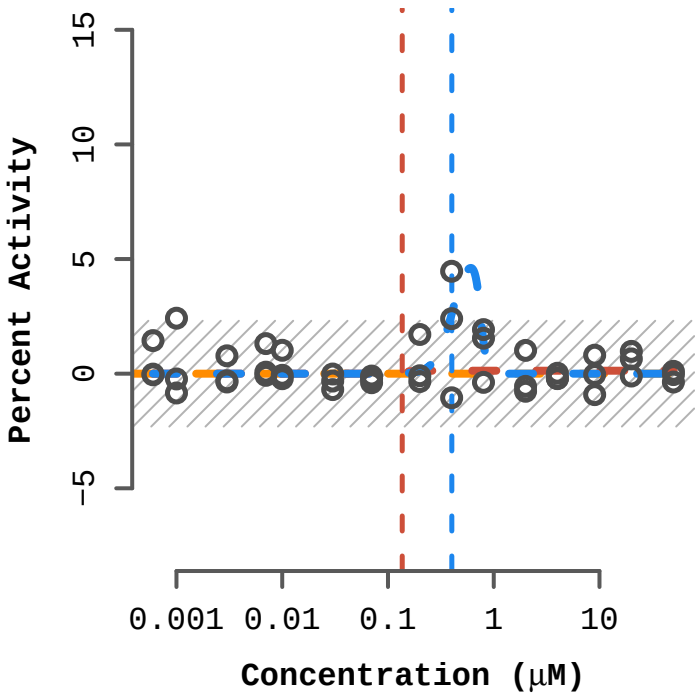
	tp	ga	gw
val:	6.64	−0.456	1.97
sd:	0.604	0.112	0.929

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.08	−0.42	1.77	1.75	10.2
sd:	0.675	0.116	0.818	0.191	35.2

	CNST	HILL	GNLS
AIC:	253.35	207.6	210.25
PROB:	0	0.79	0.21
RMSE:	4.02	2.49	2.5

MAX_MEAN: 5.97 **MAX_MED:** 7.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Iproniazid sulfate
CHID: 45852 CASRN: 36504-56-0
SPID(S): Tox21_111341_1
M4ID: 12483753

HILL MODEL (in red):

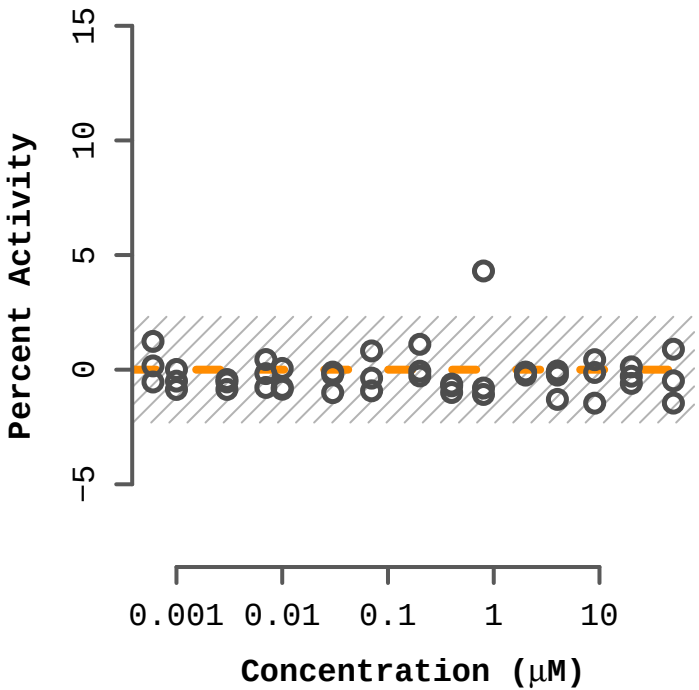
	tp	ga	gw
val:	0.128	−0.865	8
sd:	0.186	1.22	40.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.26	−0.396	5.49	−0.124	15.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	126.23	131.74	125.67
PROB:	0.42	0.03	0.56
RMSE:	1.1	1.08	0.96

MAX_MEAN: 1.94 **MAX_MED:** 2.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

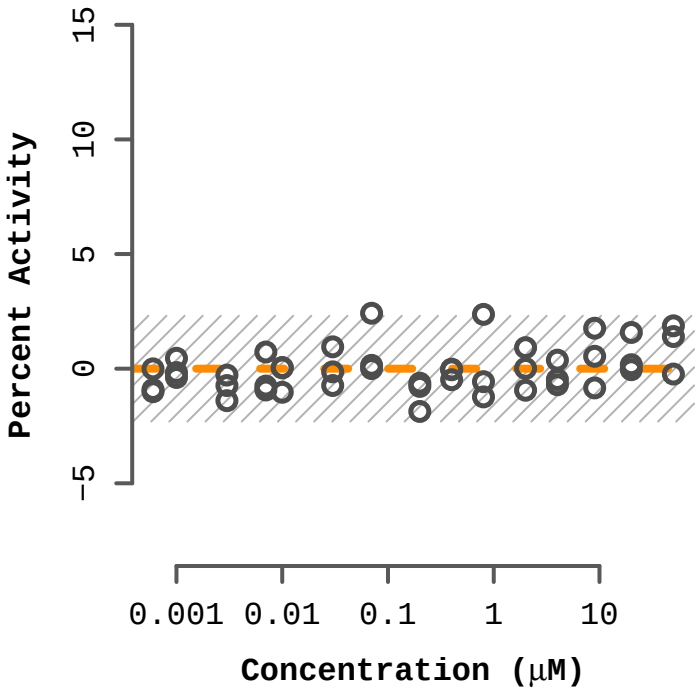
NAME: Benfluorex hydrochloride
CHID: 45854 **CASRN:** 23642-66-2
SPID(S): Tox21_111343_1
M4ID: 12483751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.809 **MAX_MED:** 0.165 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

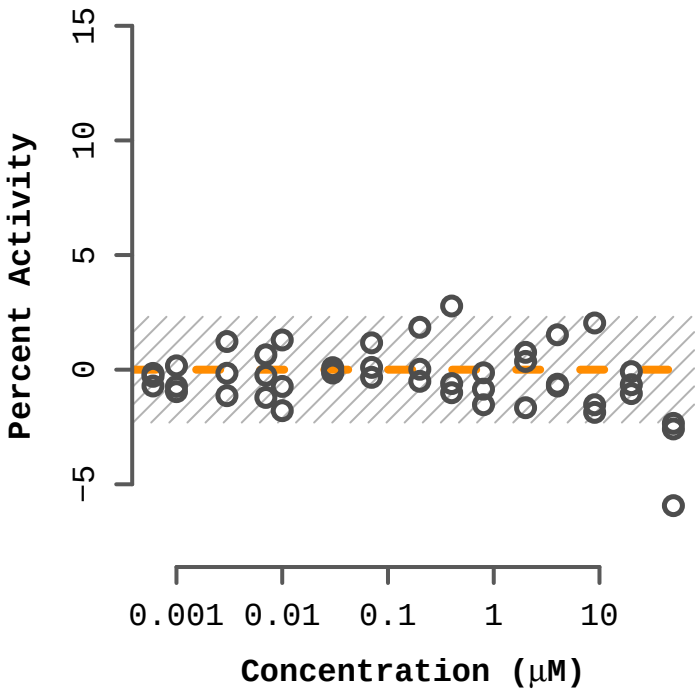
NAME: Althiazide
CHID: 45857 **CASRN:** 5588-16-9
SPID(S): Tox21_111347_1
M4ID: 12483749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

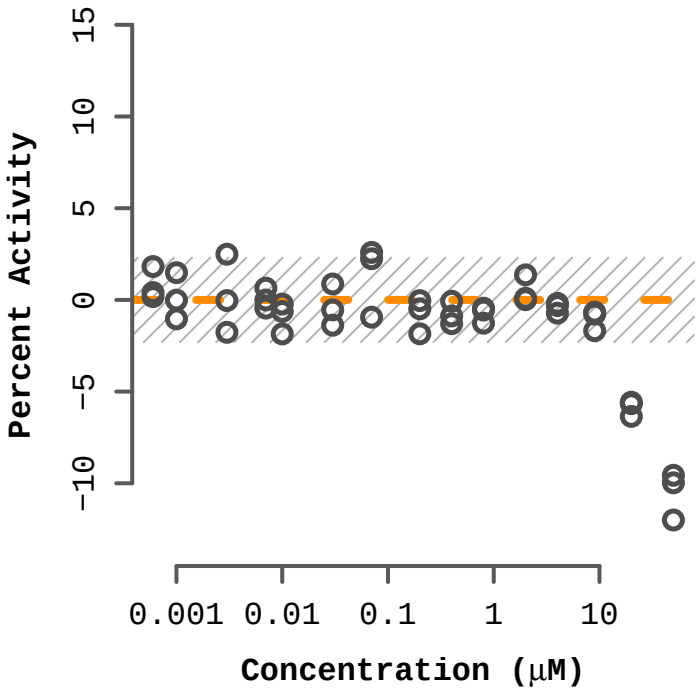
NAME: Drofenine hydrochloride
CHID: 45859 CASRN: 548-66-3
SPID(S): Tox21_111350_1
M4ID: 12483747

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 0.454 **MAX_MED:** 0.363 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

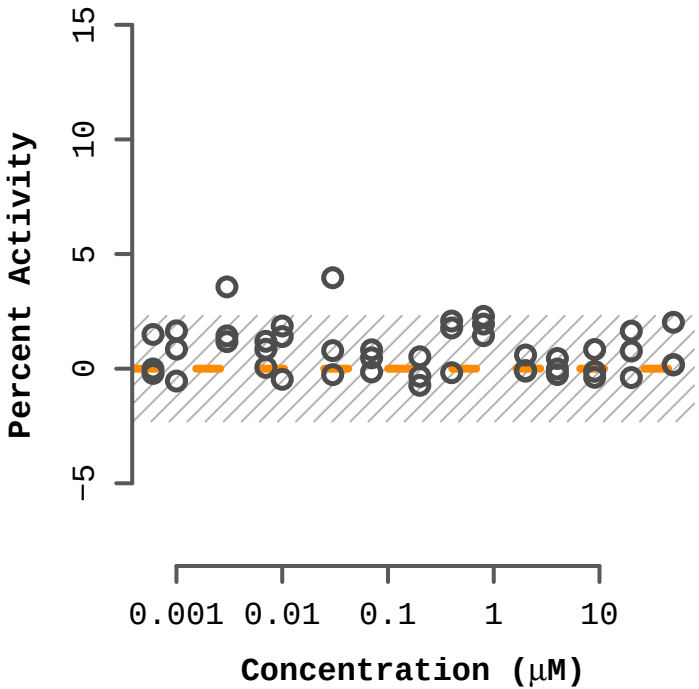
NAME: Fendiline hydrochloride
CHID: 45860 **CASRN:** 13636-18-5
SPID(S): Tox21_111351_1
M4ID: 12483746

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.91	NA	NA
PROB:	1	NA	NA
RMSE:	3.3	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

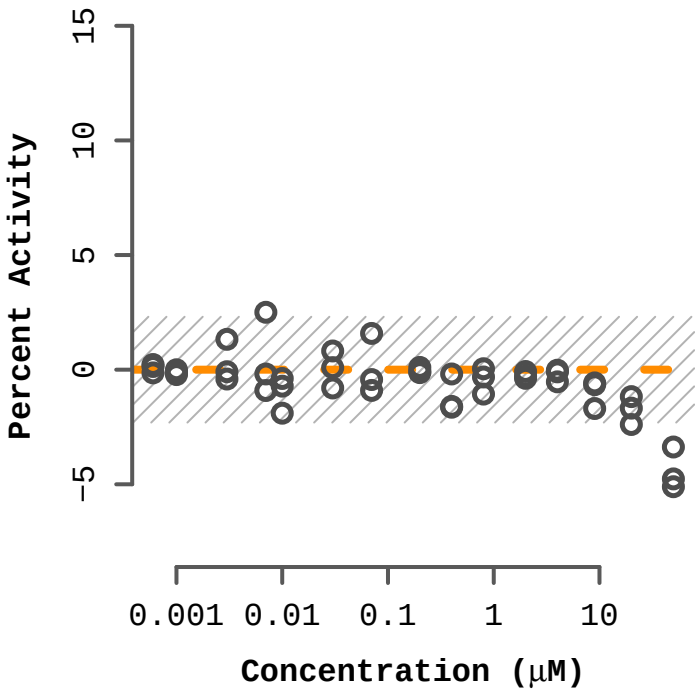
NAME: Mefexamide hydrochloride
CHID: 45862 **CASRN:** 3413-64-7
SPID(S): Tox21_111353_1
M4ID: 12483745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

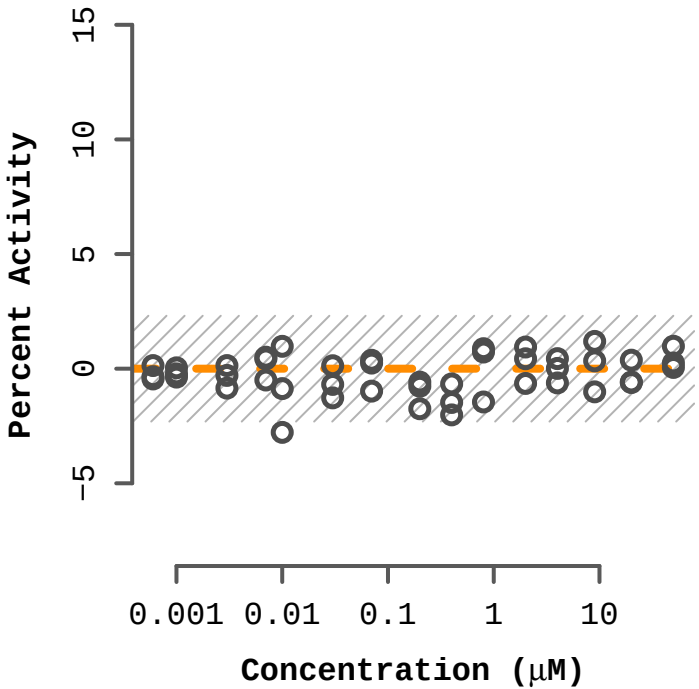
NAME: Pimethixene maleate
CHID: 45863 **CASRN:** 13187-06-9
SPID(S): Tox21_111354_1
M4ID: 12483744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.47 **MAX_MED:** 0.141 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

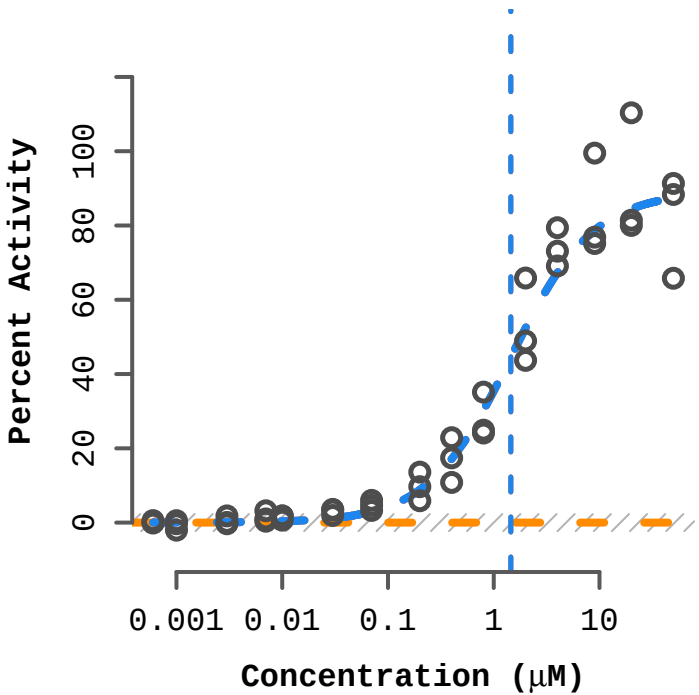
NAME: Minaprine dihydrochloride
CHID: 45864 **CASRN:** 25953-17-7
SPID(S): Tox21_111355_1
M4ID: 12483743

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.429 **MAX_MED:** 0.727 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Estradiol acetate
CHID: 45867 **CASRN:** 4245-41-4
SPID(S): Tox21_113661
M4ID: 12482552

HILL MODEL (in red):

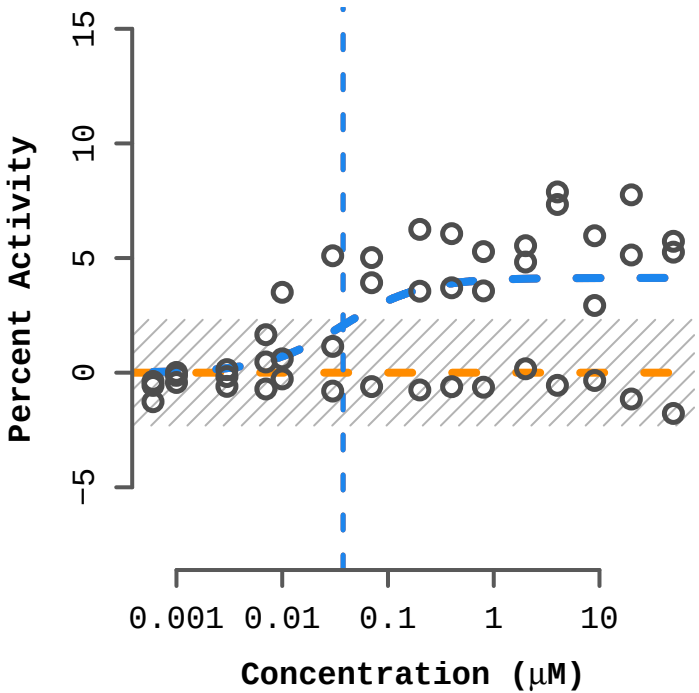
	tp	ga	gw
val:	89	0.162	1.11
sd:	2.99	0.0588	0.117

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	89	0.162	1.11	2.7	8.15
sd:	2.99	0.0588	0.117	569	4630

	CNST	HILL	GNLS
AIC:	472.78	294.05	298.05
PROB:	0	0.88	0.12
RMSE:	46.2	7.18	7.18

MAX_MEAN: 90.6 **MAX_MED:** 88.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tolperisone hydrochloride
CHID: 45868 CASRN: 3644-61-9
SPID(S): Tox21_111360_1
M4ID: 12483740

HILL MODEL (in red):

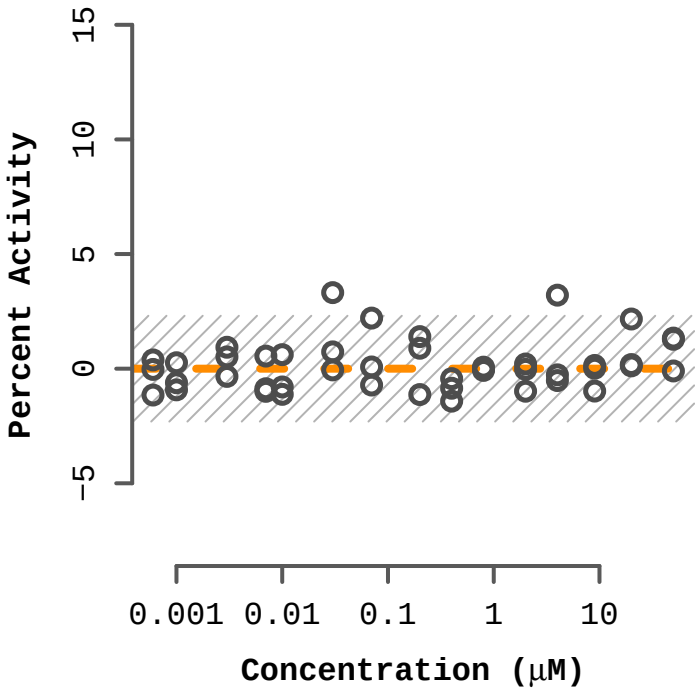
	tp	ga	gw
val:	4.13	−1.42	1.18
sd:	0.819	0.488	1.04

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.13	−1.42	1.18	2.74	7.33
sd:	0.819	0.488	1.04	1570	11000

	CNST	HILL	GNLS
AIC:	247.94	222.38	226.38
PROB:	0	0.88	0.12
RMSE:	3.65	2.56	2.56

MAX_MEAN: 4.89 MAX_MED: 7.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

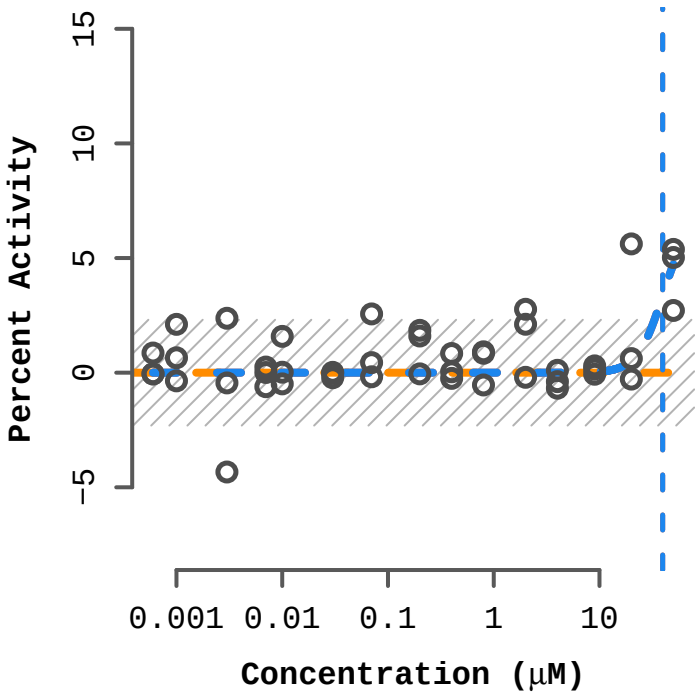
NAME: Acetyl-L-leucine
CHID: 45870 **CASRN:** 1188-21-2
SPID(S): Tox21_111362_1
M4ID: 12483739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carprofen
CHID: 45871 CASRN: 53716-49-7
SPID(S): Tox21_111363_1
M4ID: 12483738

HILL MODEL (in red):

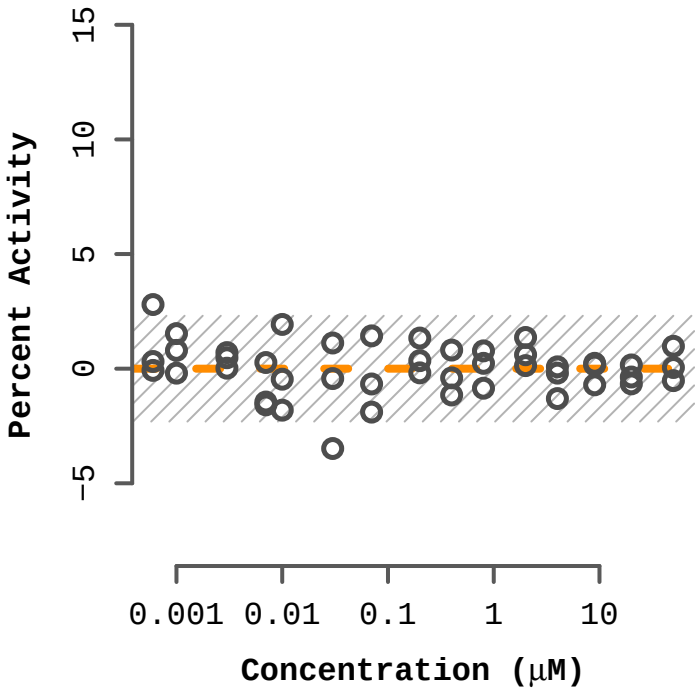
	tp	ga	gw
val:	6.74	1.6	3.65
sd:	22.6	1.1	8.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.74	1.6	3.65	3.19	7.88
sd:	23.3	1.14	8.77	325000	1030000

	CNST	HILL	GNLS
AIC:	172.82	156.03	160.03
PROB:	0	0.88	0.12
RMSE:	1.86	1.44	1.44

MAX_MEAN: 4.37 **MAX_MED:** 5.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

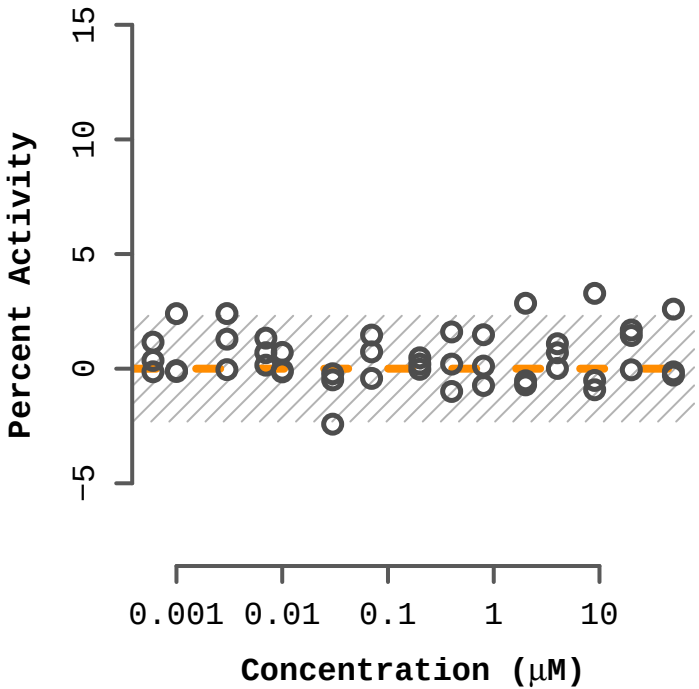
NAME: Cefoperazone sodium
CHID: 45874 **CASRN:** 62893-20-3
SPID(S): Tox21_111367_1
M4ID: 12483736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.799 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

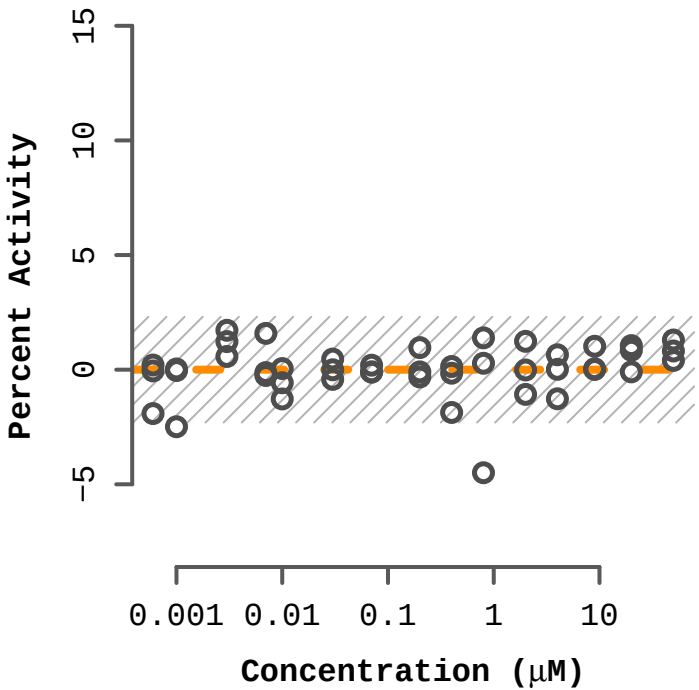
NAME: Chromocarb
CHID: 45878 **CASRN:** 4940-39-0
SPID(S): Tox21_111376_1
M4ID: 12483729

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

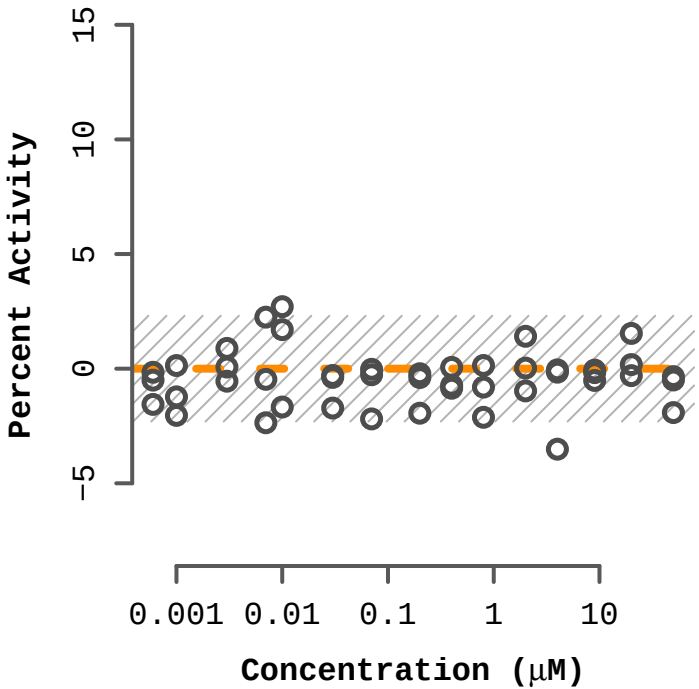
NAME: Acexamic acid
CHID: 45879 **CASRN:** 57-08-9
SPID(S): Tox21_111377_1
M4ID: 12483728

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

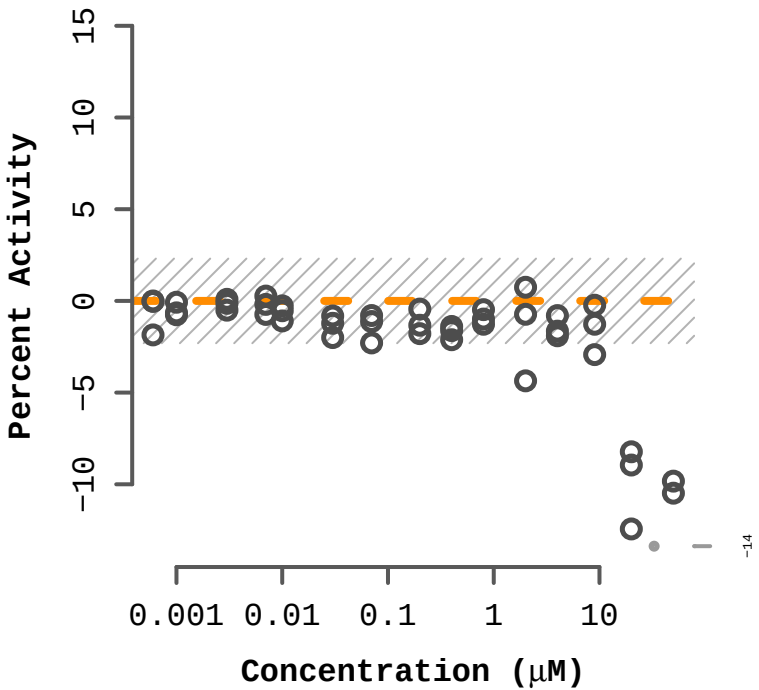
NAME: Adiphenine hydrochloride
CHID: 45880 **CASRN:** 50-42-0
SPID(S): Tox21_111379_1
M4ID: 12483726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

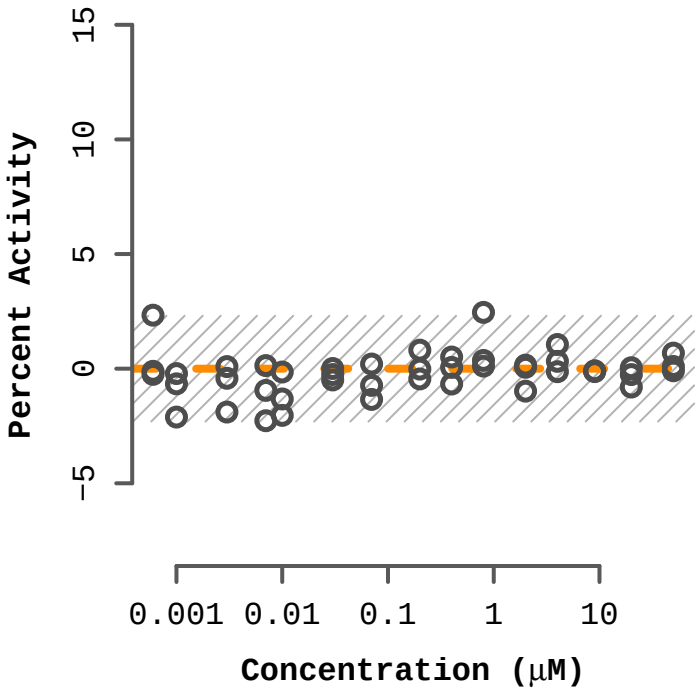
NAME: Alexidine dihydrochloride
CHID: 45881 **CASRN:** 1715-30-6
SPID(S): Tox21_111380_1
M4ID: 12483725 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.01	NA	NA
PROB:	1	NA	NA
RMSE:	4.14	NA	NA

MAX_MEAN: −0.182 **MAX_MED:** −0.0259 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

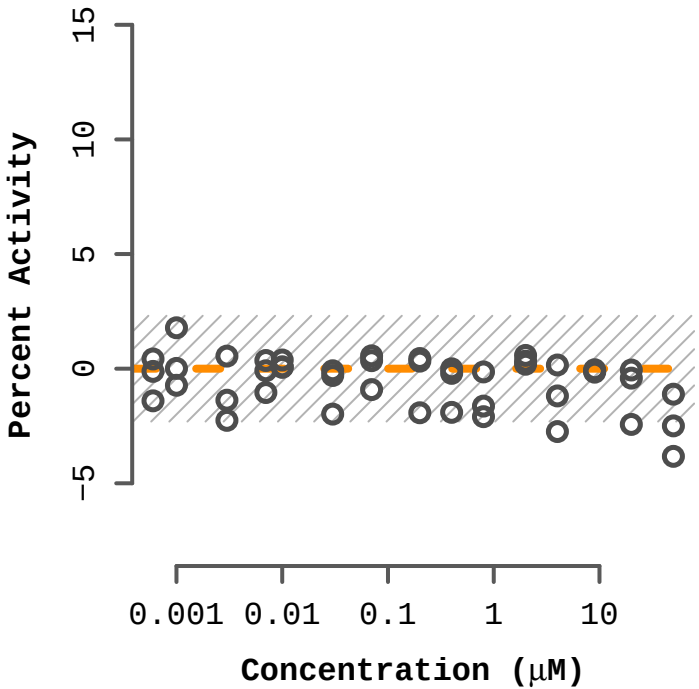
NAME: Amiprilose hydrochloride
CHID: 45883 **CASRN:** 60414-06-4
SPID(S): Tox21_111382_1
M4ID: 12483723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.977 **MAX_MED:** 0.361 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

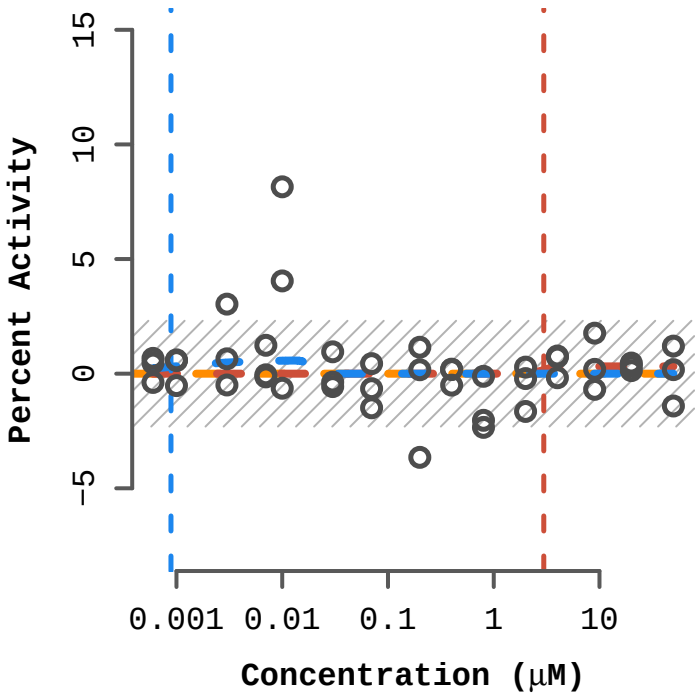
NAME: Bromhexine hydrochloride
CHID: 45886 **CASRN:** 611-75-6
SPID(S): Tox21_111385_1
M4ID: 12483721

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.368 **MAX_MED:** 0.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ceftriaxone disodium trihydrate
CHID: 45887 **CASRN:** 104376-79-6
SPID(S): Tox21_111386_1
M4ID: 12483720

HILL MODEL (in red):

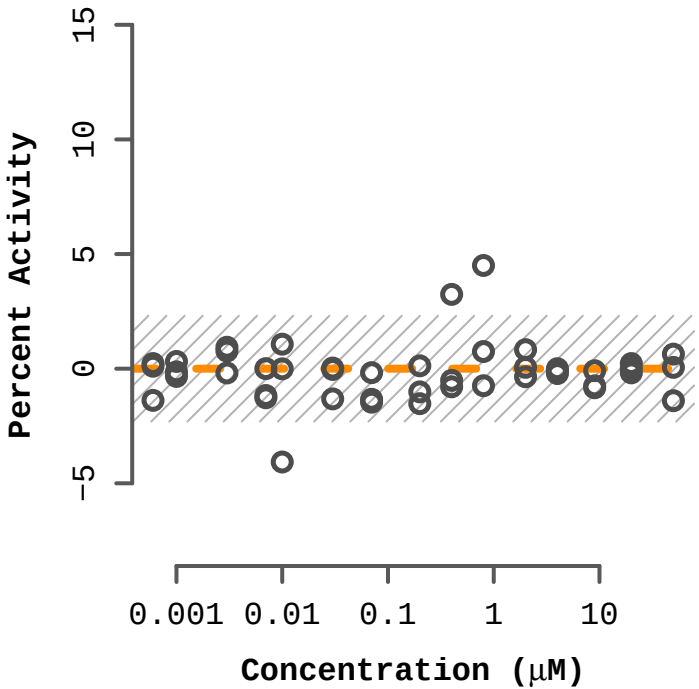
	tp	ga	gw
val:	0.318	0.473	8
sd:	0.287	0.313	16.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.599	−3.05	1.18	−1.75	18
sd:	2.18	3.11	14.2	5.84	439

	CNST	HILL	GNLS
AIC:	156.69	161.47	164.59
PROB:	0.9	0.08	0.02
RMSE:	1.74	1.74	1.64

MAX_MEAN: 3.85 **MAX_MED:** 4.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

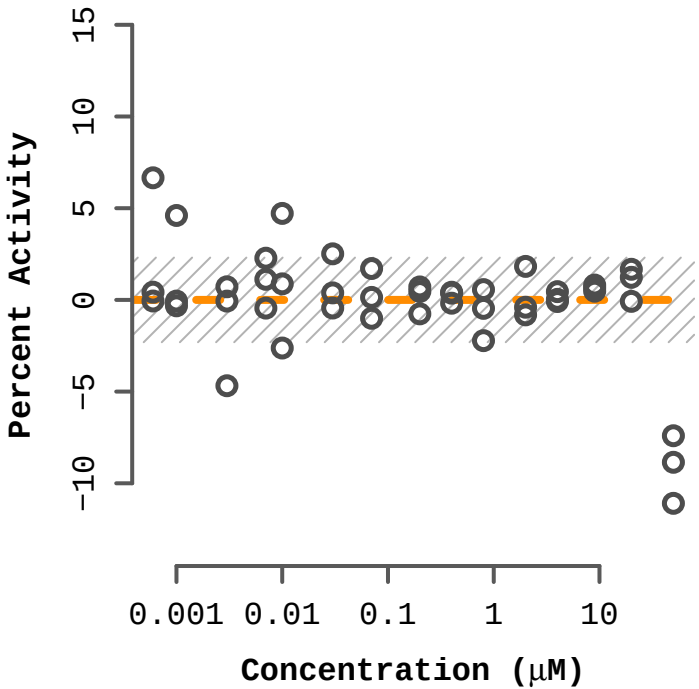
NAME: Citiolone
CHID: 45888 **CASRN:** 1195-16-0
SPID(S): Tox21_113346_1
M4ID: 12482683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 0.769 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

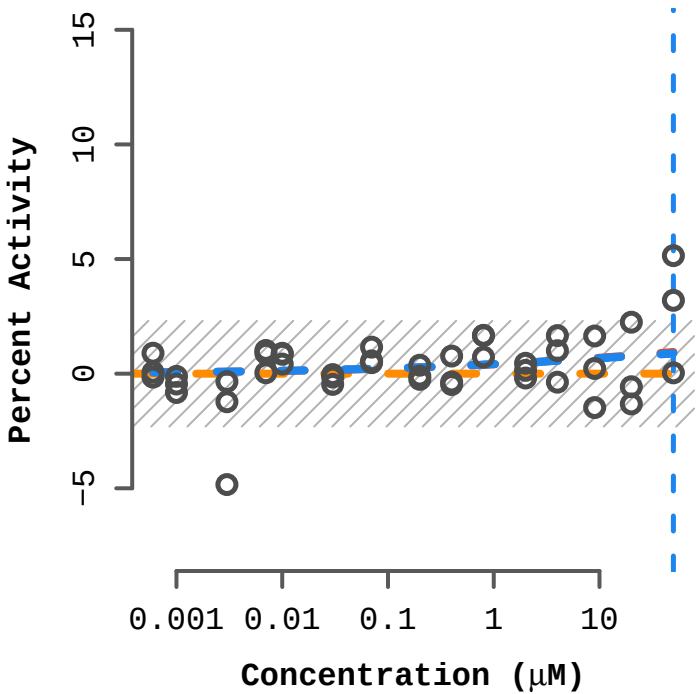
NAME: Clofoctol
CHID: 45889 **CASRN:** 37693-01-9
SPID(S): Tox21_111389_1
M4ID: 12483718

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.57	NA	NA
PROB:	1	NA	NA
RMSE:	3.01	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Heptaminol hydrochloride
CHID: 45891 **CASRN:** 543-15-7
SPID(S): Tox21_111391_1
M4ID: 12483717

HILL MODEL (in red):

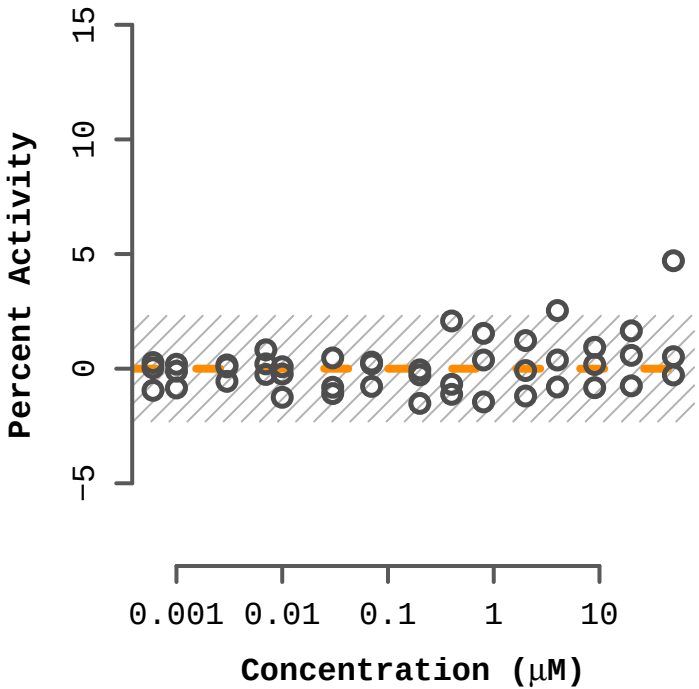
	tp	ga	gw
val:	2.28	2.2	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.76	1.7	0.3	3.7	4.54
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	148.46	149.4	153.41
PROB:	0.59	0.37	0.05
RMSE:	1.43	1.32	1.32

MAX_MEAN: 2.8 **MAX_MED:** 3.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

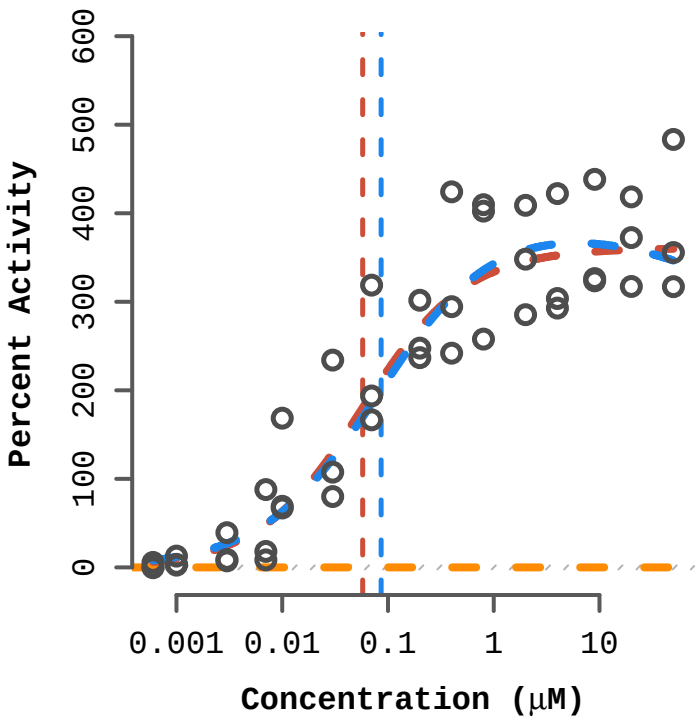
NAME: Diosmin
CHID: 45892 **CASRN:** 520-27-4
SPID(S): Tox21_111392_1
M4ID: 12483716

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 0.582 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone 17-butyrate
CHID: 45896 **CASRN:** 13609-67-1
SPID(S): Tox21_111397_1
M4ID: 12483713

HILL MODEL (in red):

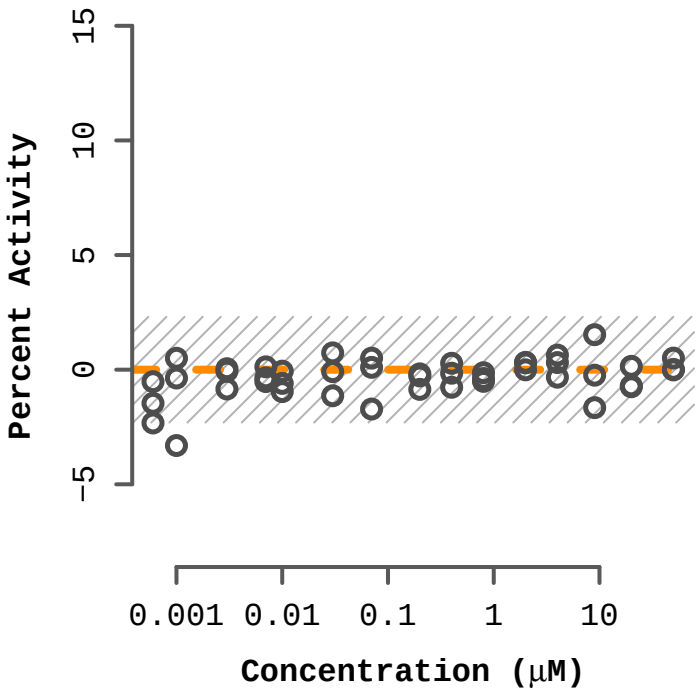
	tp	ga	gw
val:	361	-1.24	0.885
sd:	17.2	0.117	0.15

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	407	-1.06	0.787	3.7	0.389
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	639.14	497.09	502.14
PROB:	0	0.93	0.07
RMSE:	267.61	54.49	55.79

MAX_MEAN: 385 **MAX_MED:** 402 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

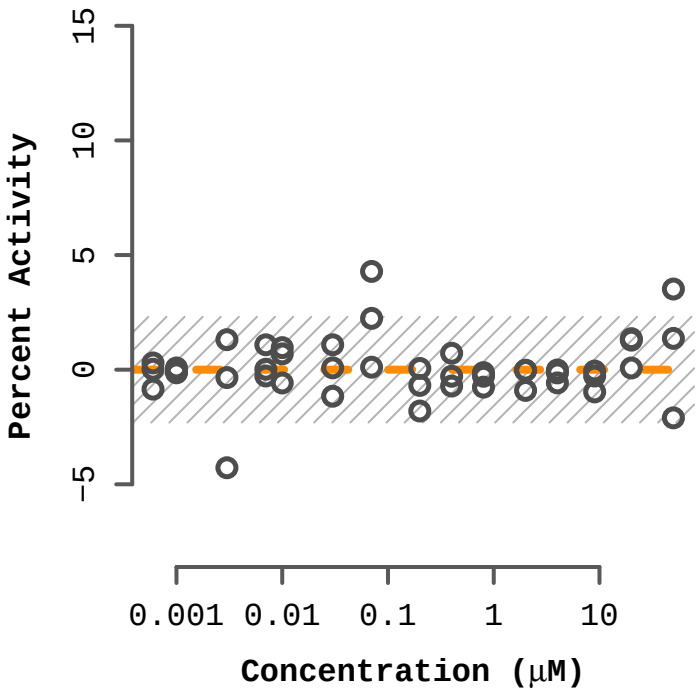
NAME: Tetroquinone
CHID: 45897 **CASRN:** 319-89-1
SPID(S): Tox21_111400_1
M4ID: 12483711

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.208 **MAX_MED:** 0.312 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

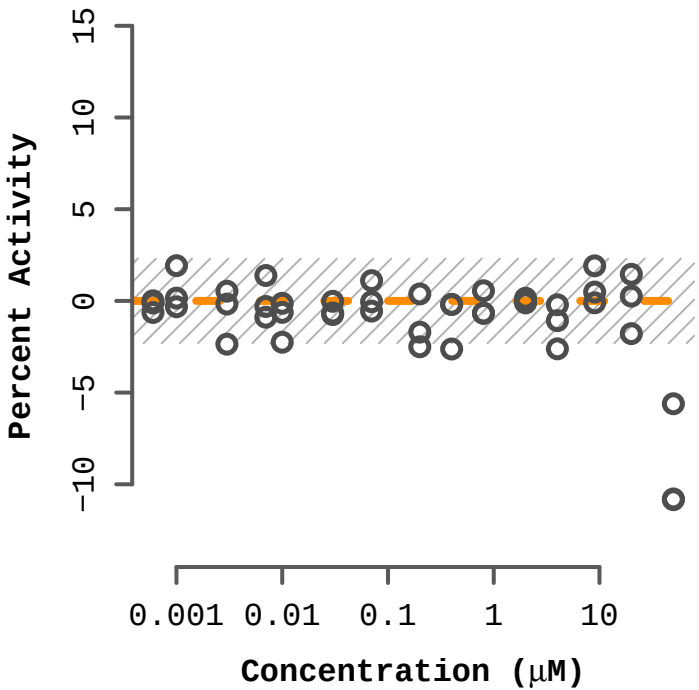
NAME: Sulfanitran
CHID: 45898 **CASRN:** 122-16-7
SPID(S): Tox21_111401_1
M4ID: 12483710

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

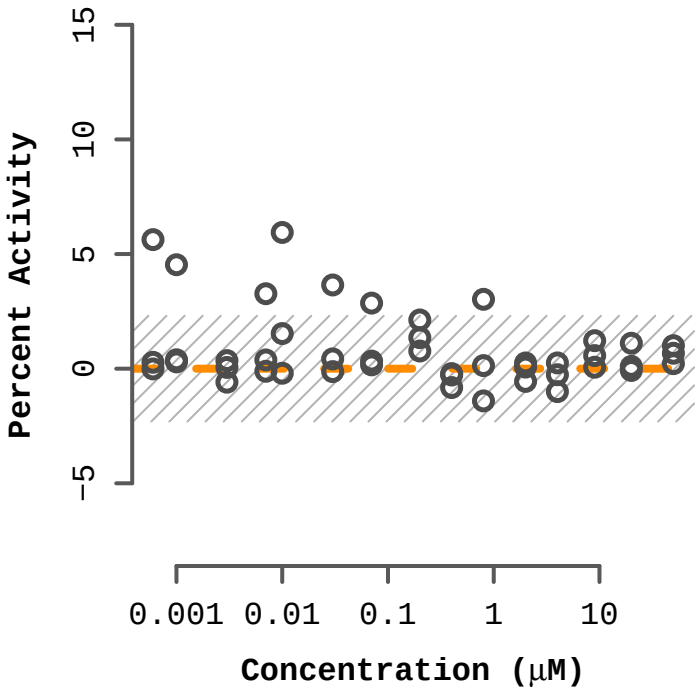
NAME: Exalamide
CHID: 45899 **CASRN:** 53370-90-4
SPID(S): Tox21_111403_1
M4ID: 12483708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 0.766 **MAX_MED:** 0.485 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

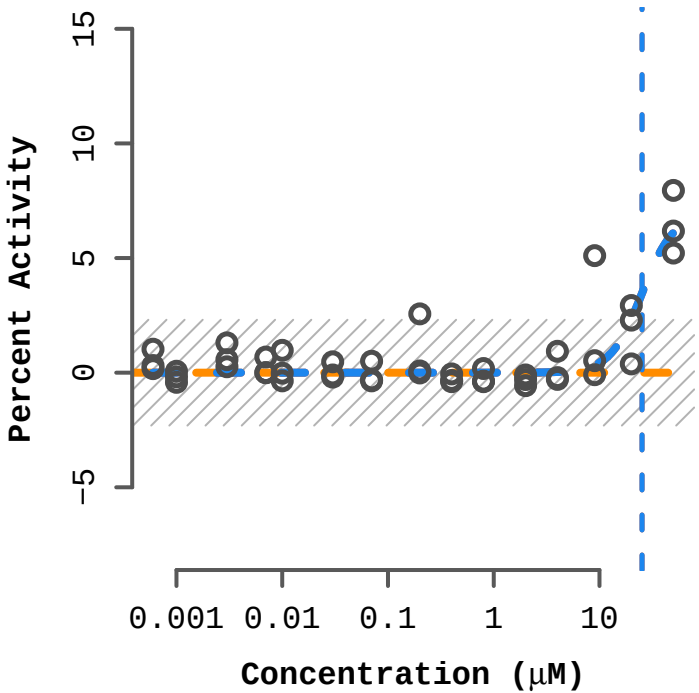
NAME: Resorcinol monoacetate
CHID: 45901 CASRN: 102-29-4
SPID(S): Tox21_111406_1
M4ID: 12483707

HILL MODEL: Not applicable.

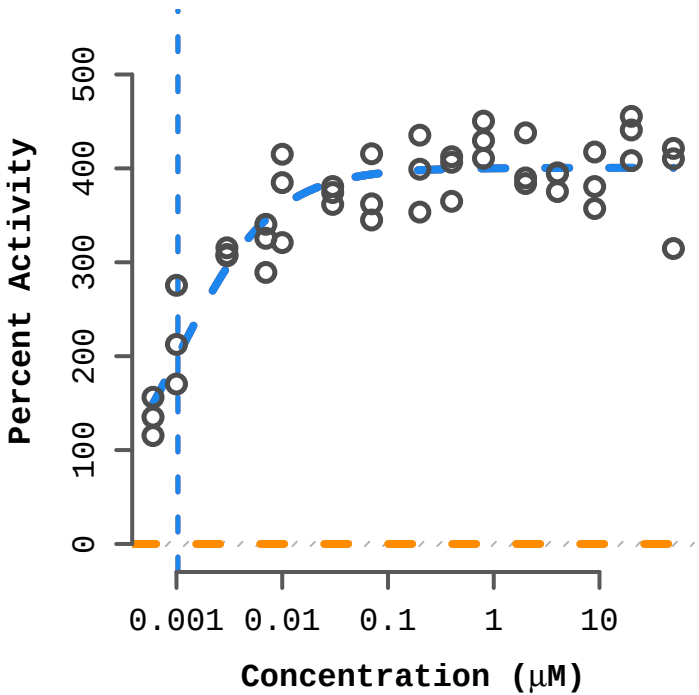
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

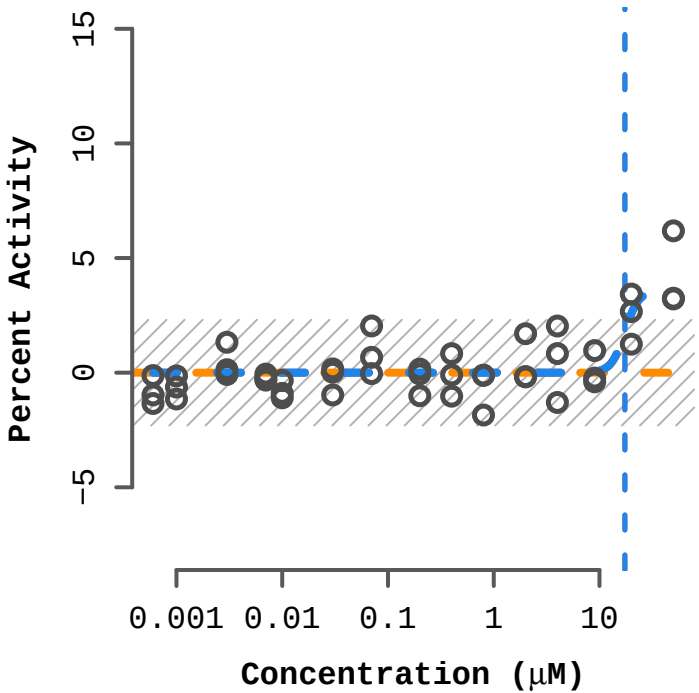
MAX_MEAN: 2.43 **MAX_MED:** 1.53 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ramifenazone
CHID:    45906   CASRN: 3615-24-5
SPID(S): Tox21_111412_1
M4ID:    12483705

HILL MODEL (in red):
      tp       ga       gw
val:  6.94     1.4      2.91
sd:   1.64     0.12     1.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.94     1.4      2.91     2.71     4.94
sd:   1.65     0.12     1.5      470      2320

      CNST        HILL        GNLS
AIC:  157.78      110.26      114.26
PROB: 0           0.88        0.12
RMSE: 2.02        1.01        1.01

MAX_MEAN: 6.45      MAX_MED: 6.18      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Clobetasol propionate
CHID:    45907   CASRN: 25122-46-7
SPID(S): Tox21_111414_1
M4ID:    12483703

HILL MODEL (in red):
      tp       ga       gw
val:  401      -2.99    0.957
sd:   6.77     0.0545   0.148

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  401      -2.99    0.957    3.68     4
sd:   6.77     0.0545   0.148    1820     3410

      CNST        HILL        GNLS
AIC:  670.57      452.27      456.27
PROB: 0           0.88        0.12
RMSE: 364.11      32.84       32.84

MAX_MEAN: 435       MAX_MED: 441       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxyphencyclimine hydrochloride
CHID: 45909 CASRN: 125-52-0
SPID(S): Tox21_111416_1
M4ID: 12483702

HILL MODEL (in red):

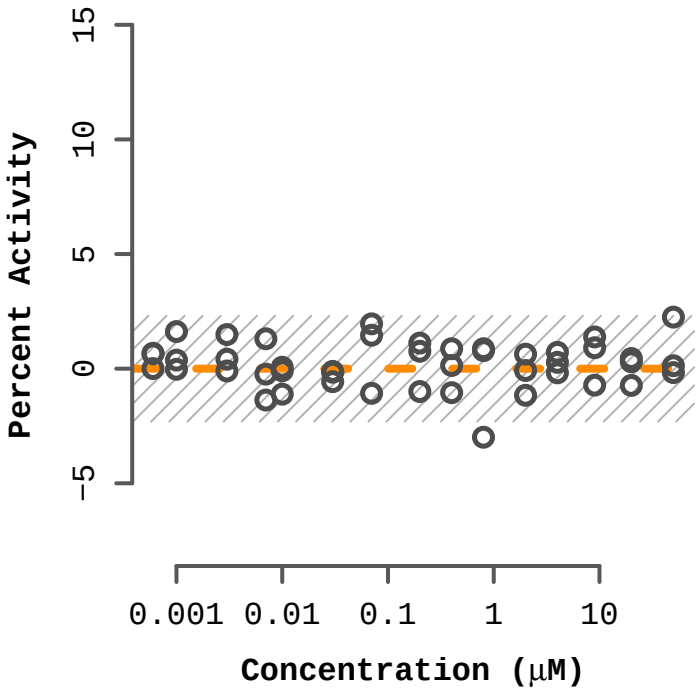
	tp	ga	gw
val:	3.57	1.24	6.74
sd:	0.538	0.14	14.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.57	1.24	6.74	3.49	12.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	159.47	130.95	134.95
PROB:	0	0.88	0.12
RMSE:	1.57	0.95	0.95

MAX_MEAN: 4.22 **MAX_MED:** 3.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

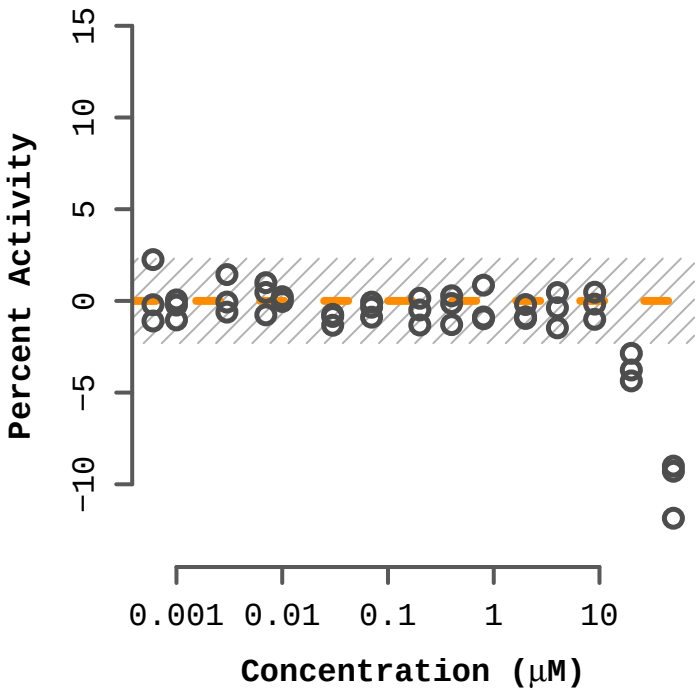
NAME: Aminolevulinic acid hydrochloride
CHID: 45914 **CASRN:** 5451-09-2
SPID(S): Tox21_111426_1
M4ID: 12483697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.33	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

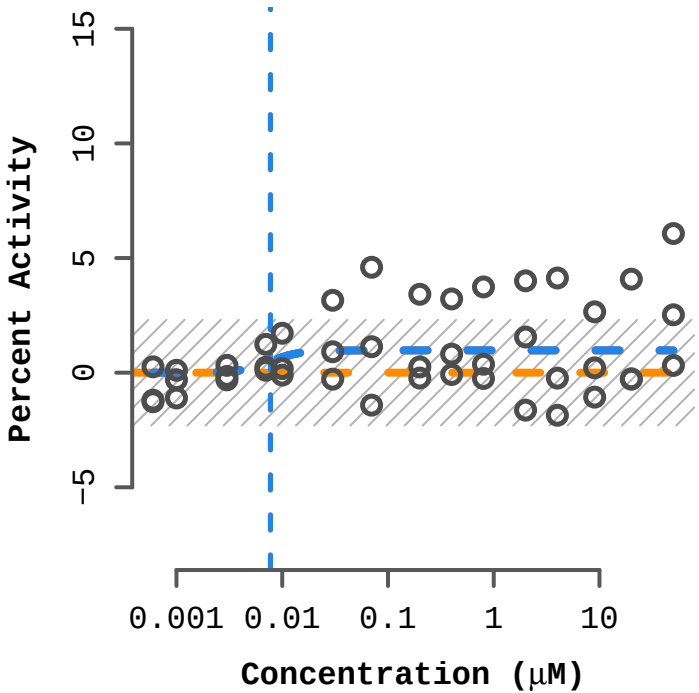
NAME: Carvedilol tartrate
CHID: 45916 **CASRN:** NOCAS_45916
SPID(S): Tox21_111431_1
M4ID: 12483694

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.75	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 0.318 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Moxifloxacin hydrochloride
CHID: 45921 CASRN: 186826-86-8
SPID(S): Tox21_111439_1
M4ID: 12483686

HILL MODEL (in red):

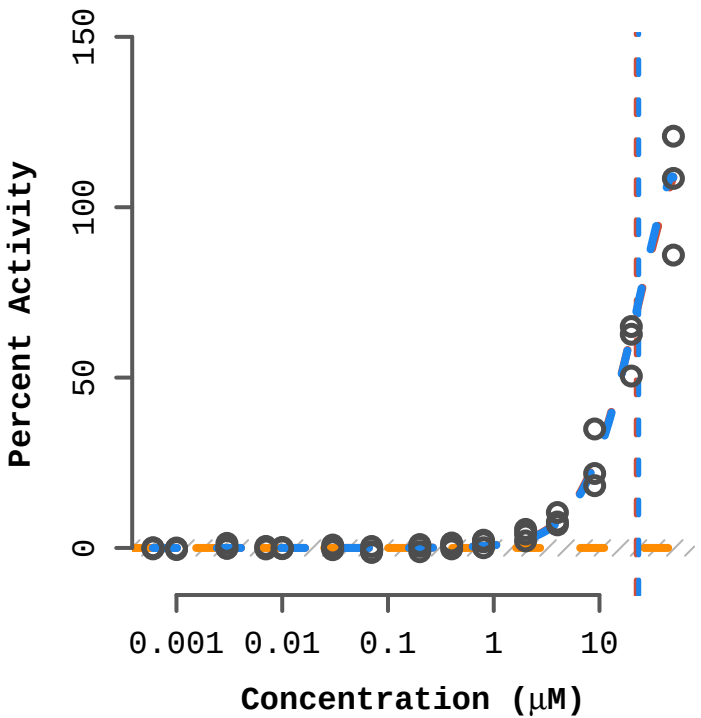
	tp	ga	gw
val:	0.972	−2.11	3.18
sd:	0.373	0.379	6.49

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.972	−2.11	3.18	2.82	17.7
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	190.86	188.1	192.1
PROB:	0.18	0.72	0.1
RMSE:	2.06	1.77	1.77

MAX_MEAN: 2.97 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benazepril hydrochloride
CHID: 45922 CASRN: 86541-74-4
SPID(S): Tox21_111441_1
M4ID: 12483684

HILL MODEL (in red):

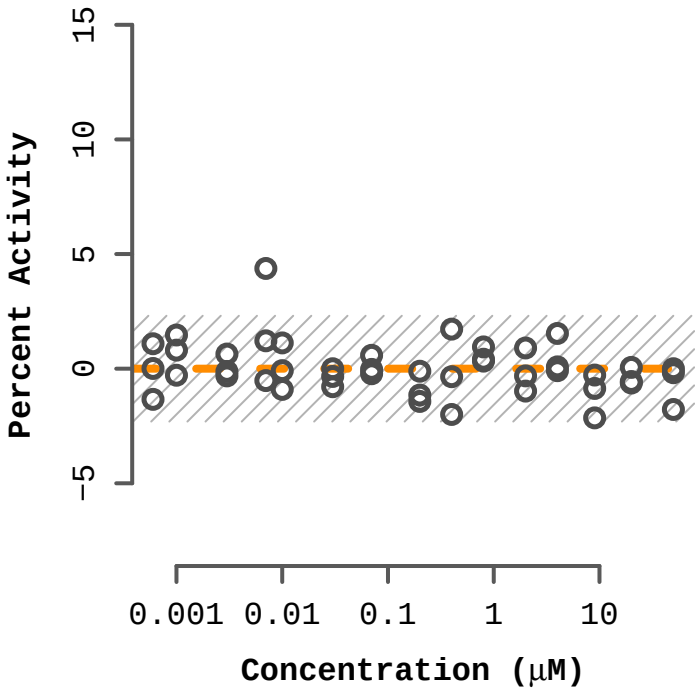
	tp	ga	gw
val:	138	1.35	1.65
sd:	3.86	0.0199	0.0718

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	145	1.37	1.65	1.78	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	397.2	225.51	228.72
PROB:	0	0.83	0.17
RMSE:	32.24	4.75	4.75

MAX_MEAN: 105 MAX_MED: 108 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

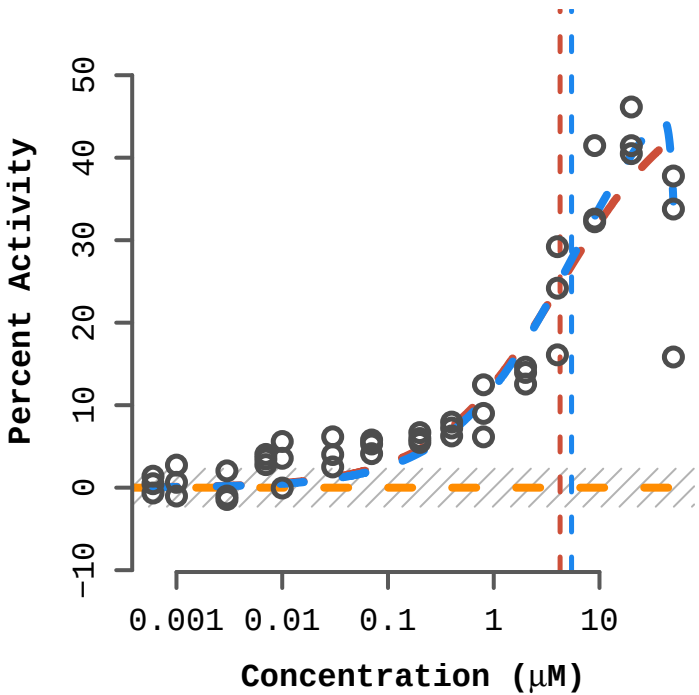
NAME: Sibutramine hydrochloride
CHID: 45927 CASRN: 84485-00-7
SPID(S): Tox21_111448_1
M4ID: 12483680

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Canrenone
CHID: 45930 **CASRN:** 976-71-6
SPID(S): Tox21_111451_1
M4ID: 12483679

HILL MODEL (in red):

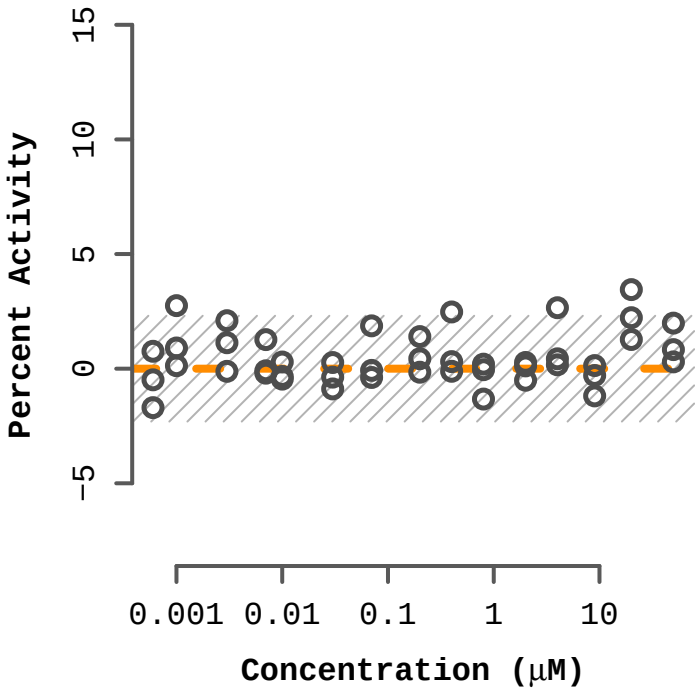
	tp	ga	gw
val:	49.3	0.628	0.737
sd:	8.28	0.229	0.143

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	55.4	0.736	0.754	1.73	14.6
sd:	6.83	0.165	0.0997	0.0104	5.3

	CNST	HILL	GNLS
AIC:	386.58	268.94	256.81
PROB:	0	0	1
RMSE:	18.36	5.45	4.23

MAX_MEAN: 42.7 **MAX_MED:** 41.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

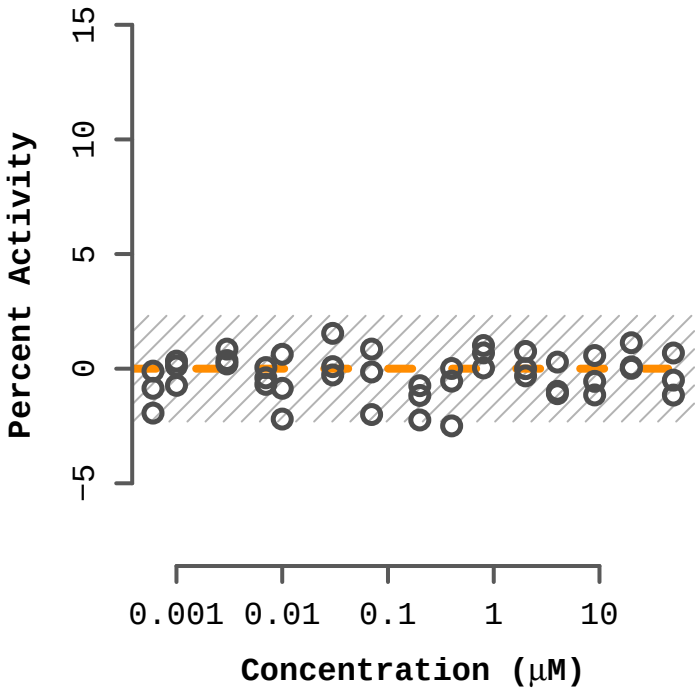
NAME: Zolmitriptan
CHID: 45933 **CASRN:** 139264-17-8
SPID(S): Tox21_111455_1
M4ID: 12483677

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

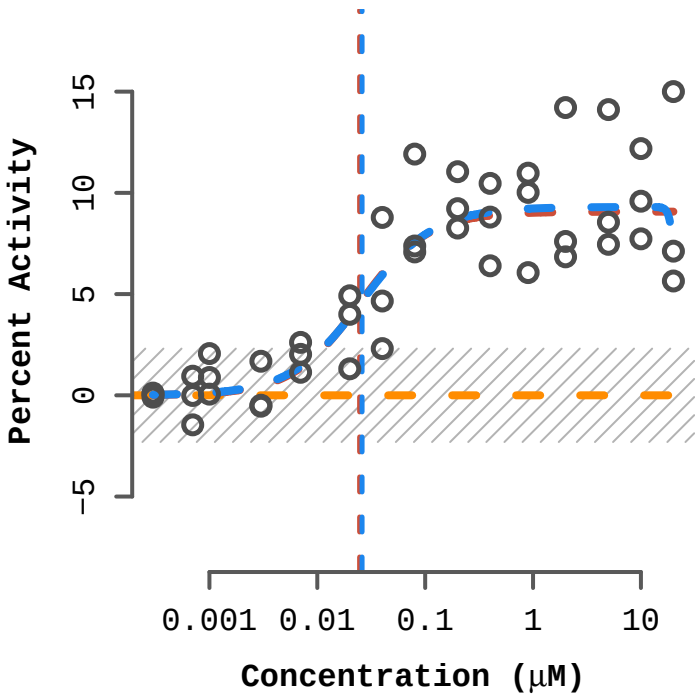
NAME: Secnidazole
CHID: 45934 **CASRN:** 3366-95-8
SPID(S): Tox21_111457_1
M4ID: 12483675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.578 **MAX_MED:** 0.688 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pefloxacin mesylate
CHID: 45935 CASRN: 70458-95-6
SPID(S): Tox21_111458_1
M4ID: 12483674

HILL MODEL (in red):

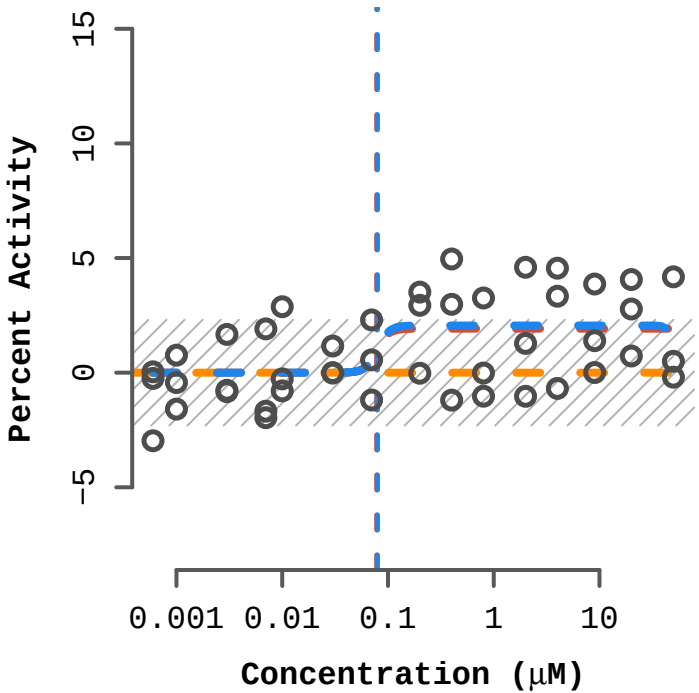
	tp	ga	gw
val:	9.07	−1.61	1.38
sd:	0.56	0.122	0.401

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.3	−1.59	1.31	1.33	17.7
sd:	0.585	0.12	0.366	0.0448	28.8

	CNST	HILL	GNLS
AIC:	313.9	205.49	207.38
PROB:	0	0.72	0.28
RMSE:	7.33	2.19	2.25

MAX_MEAN: 10 **MAX_MED:** 10 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Rebamipide
CHID: 45937 CASRN: 90098-04-7
SPID(S): Tox21_111460_1
M4ID: 12483673

HILL MODEL (in red):

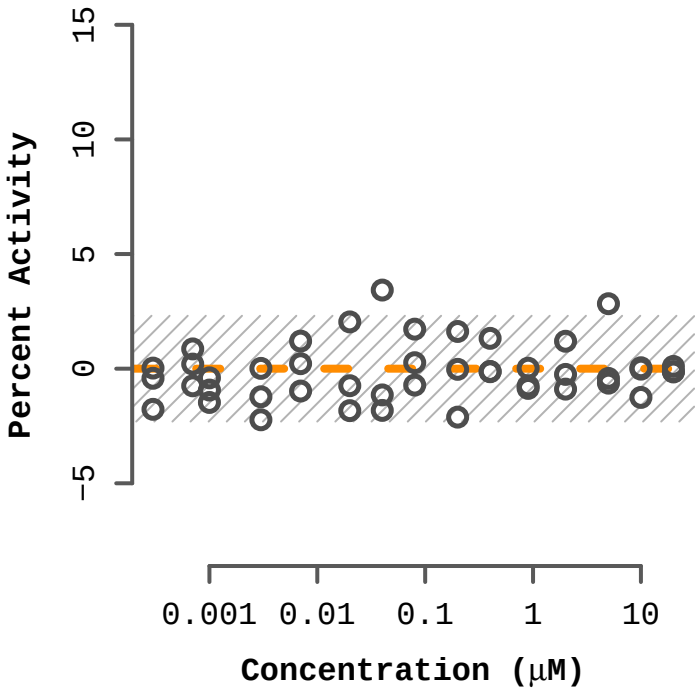
	tp	ga	gw
val:	1.92	−1.11	8
sd:	0.465	0.535	89.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.06	−1.1	7.73	1.7	15.4
sd:	0.494	0.633	90.6	0.0665	1160

	CNST	HILL	GNLS
AIC:	204.72	194.3	197.7
PROB:	0	0.84	0.15
RMSE:	2.25	1.78	1.78

MAX_MEAN: 2.52 **MAX_MED:** 3.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

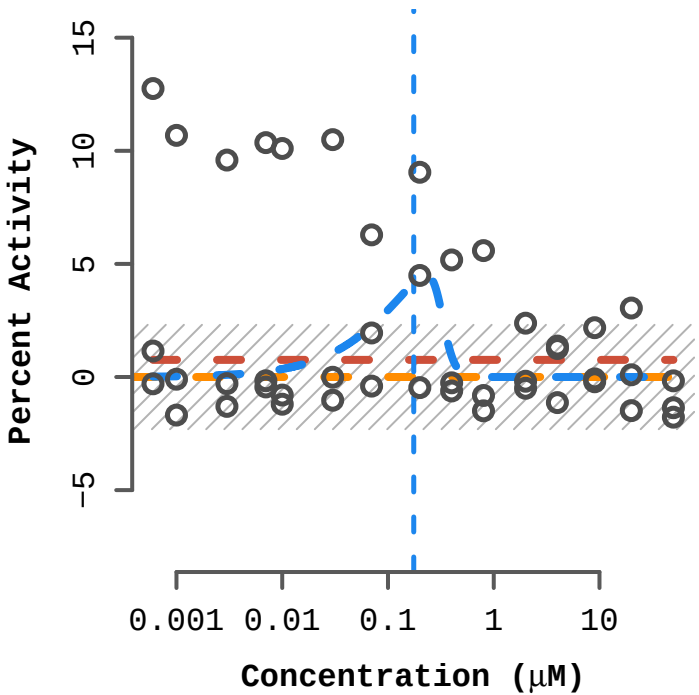
NAME: Sarafloxacin hydrochloride
CHID: 45939 **CASRN:** 91296-87-6
SPID(S): Tox21_111462_1
M4ID: 12483672

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.594 **MAX_MED:** 0.263 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prothionamide
CHID: 45940 CASRN: 14222-60-7
SPID(S): Tox21_111463_1
M4ID: 12483671

HILL MODEL (in red):

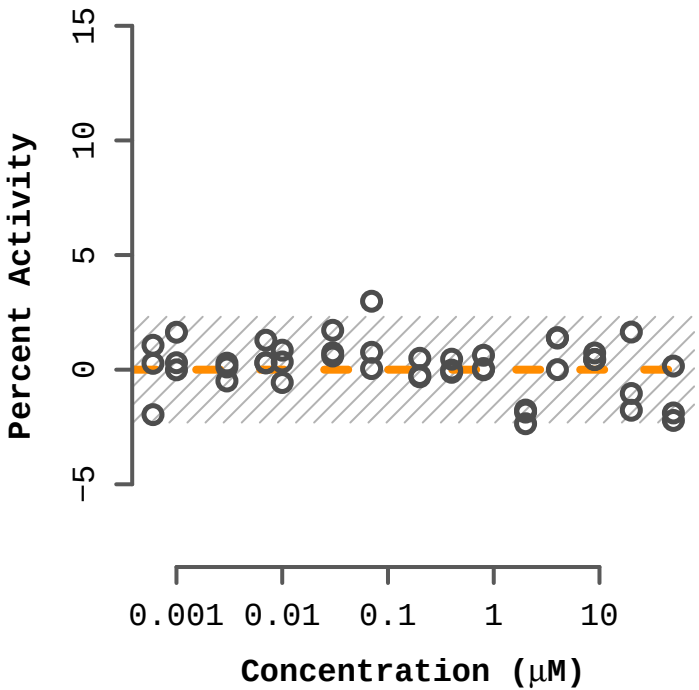
	tp	ga	gw
val:	0.758	−5.19	3.36
sd:	0.507	1730	2980

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.43	−0.756	1.09	−0.491	7.93
sd:	34.9	3.35	3.35	0.867	67.3

	CNST	HILL	GNLS
AIC:	255.59	259.05	259.74
PROB:	0.77	0.14	0.1
RMSE:	4.56	4.29	4.28

MAX_MEAN: 4.54 **MAX_MED:** 4.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

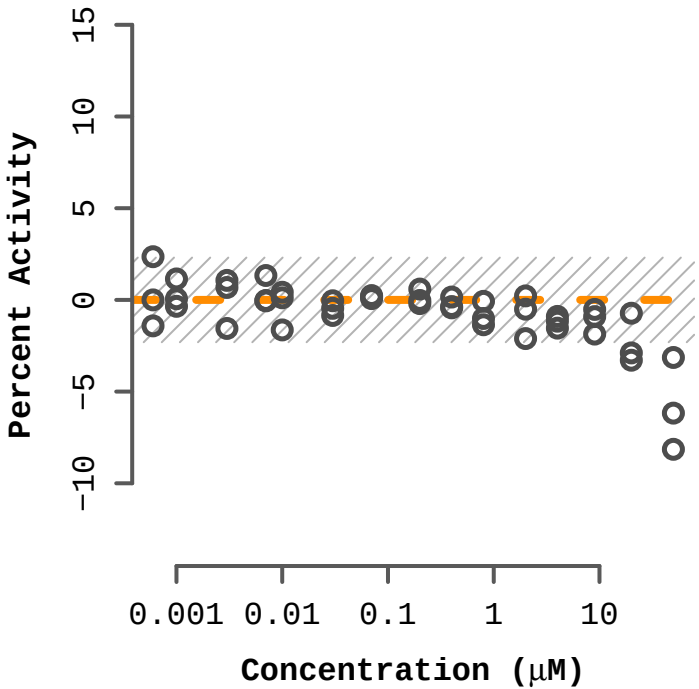
NAME: Carmofur
CHID: 45941 CASRN: 61422-45-5
SPID(S): Tox21_111464_1
M4ID: 12483670

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

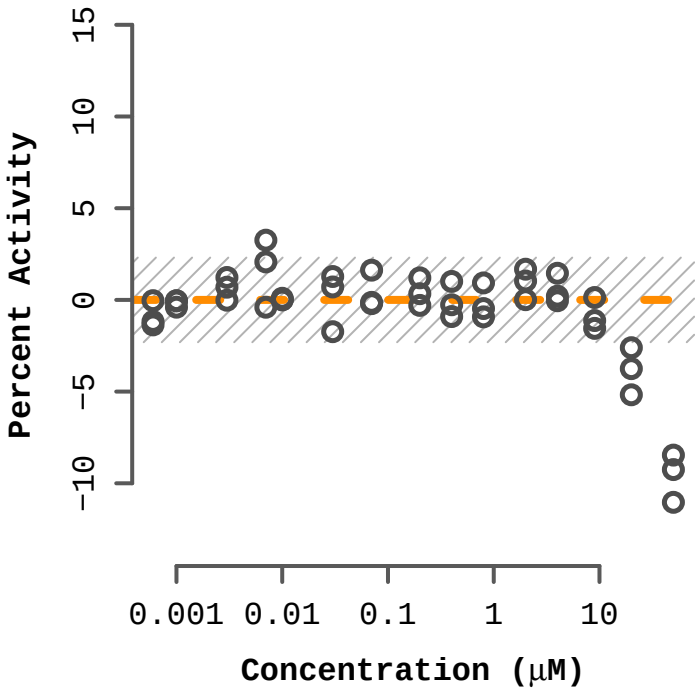
NAME: Miltefosine
CHID: 45942 **CASRN:** 58066-85-6
SPID(S): Tox21_111466_1
M4ID: 12483668

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.94	NA	NA

MAX_MEAN: 0.417 **MAX_MED:** 0.679 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

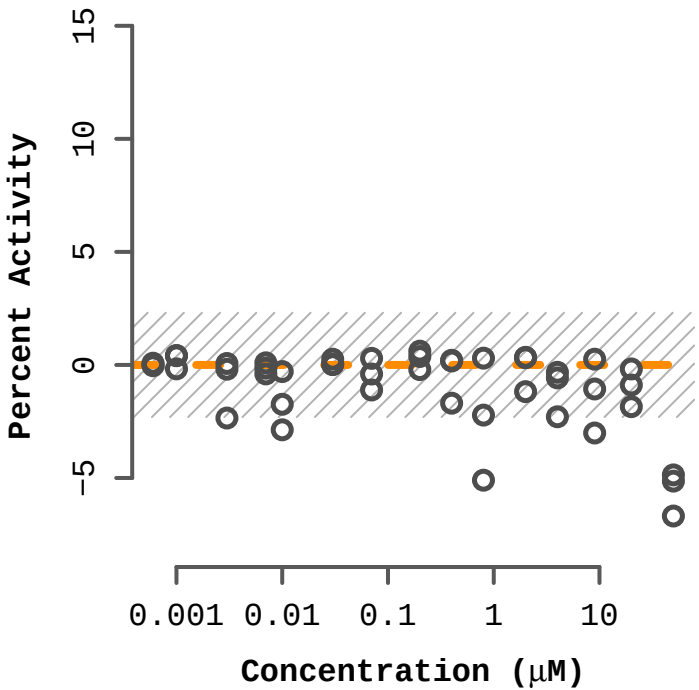
NAME: Oxiconazole nitrate
CHID: 45943 **CASRN:** 64211-46-7
SPID(S): Tox21_111467_1
M4ID: 12483667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.87	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

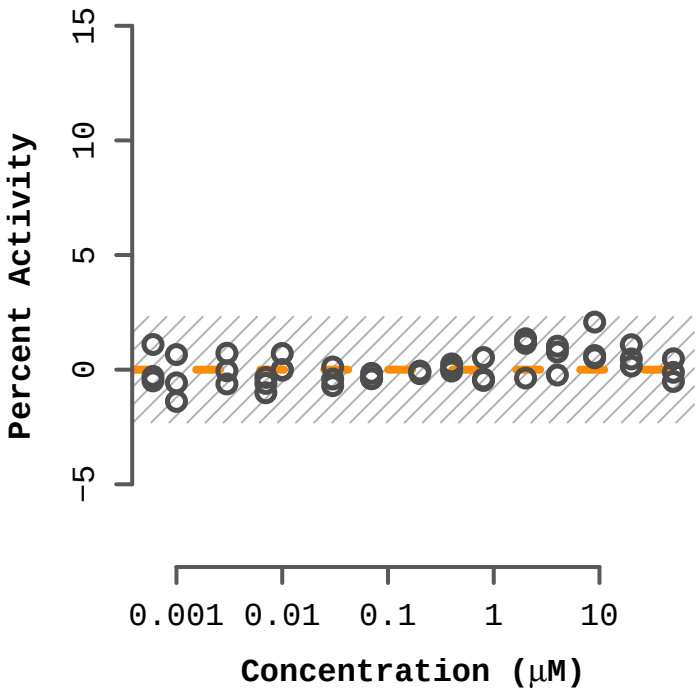
NAME: Azelastine hydrochloride
CHID: 45945 CASRN: 79307-93-0
SPID(S): Tox21_111469_1
M4ID: 12483666

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.94	NA	NA

MAX_MEAN: 0.26 **MAX_MED:** 0.408 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

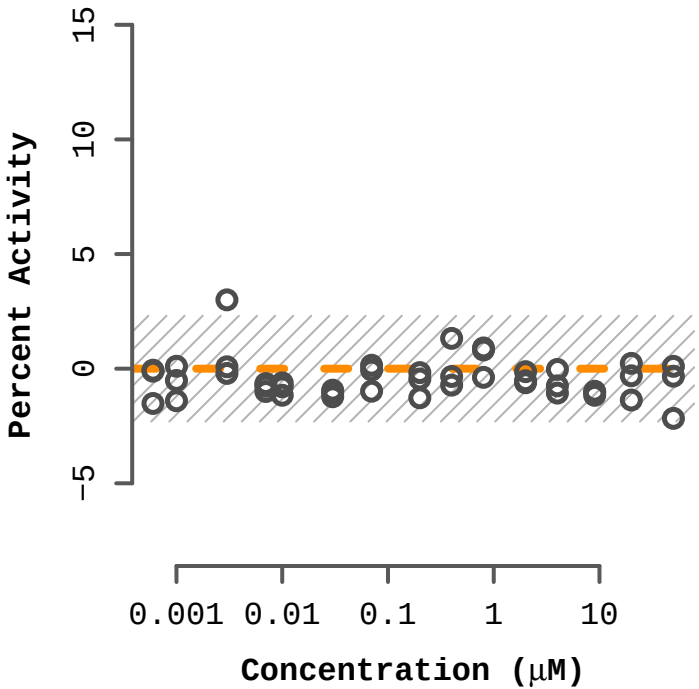
NAME: Zolpidem
CHID: 45946 **CASRN:** 82626-48-0
SPID(S): Tox21_111471_1
M4ID: 12483664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

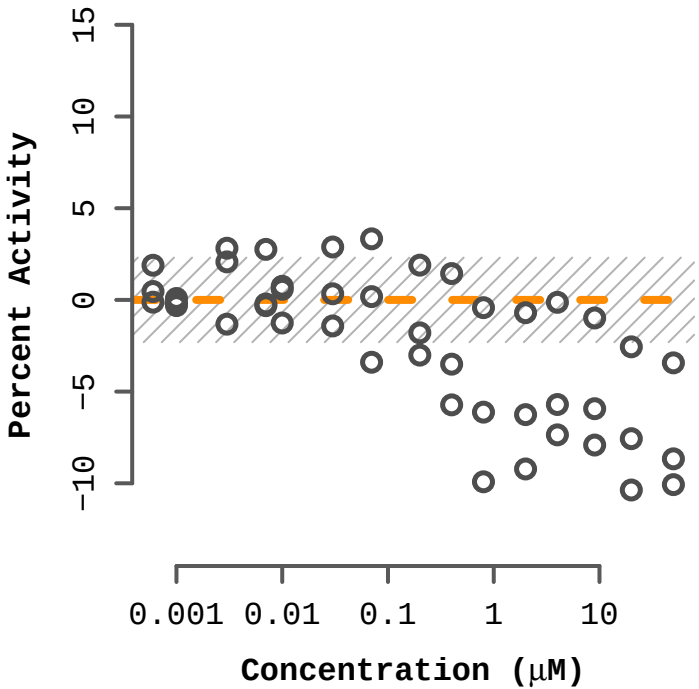
NAME: Gemifloxacin mesylate
CHID: 45948 **CASRN:** 204519-65-3
SPID(S): Tox21_111473_1
M4ID: 12483662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.961 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

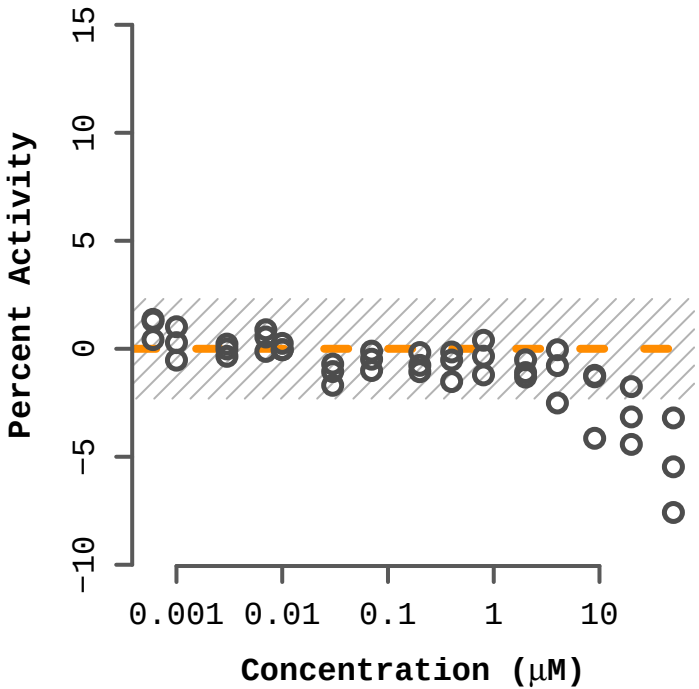
NAME: Topotecan hydrochloride
CHID: 45952 **CASRN:** 119413-54-6
SPID(S): Tox21_111478_1
M4ID: 12483660

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.41	NA	NA
PROB:	1	NA	NA
RMSE:	4.54	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

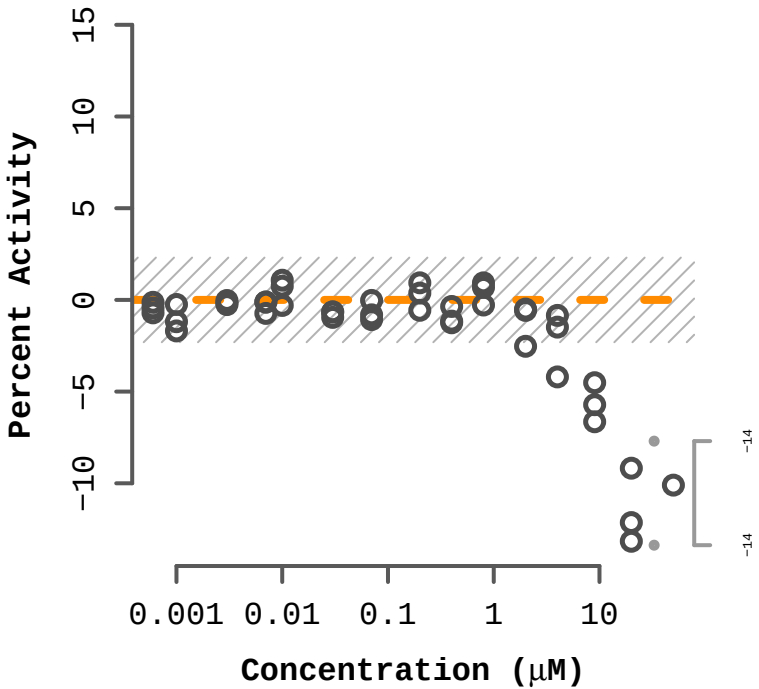
NAME: Irinotecan hydrochloride
CHID: 45953 **CASRN:** 100286-90-6
SPID(S): Tox21_111479_1
M4ID: 12483659

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

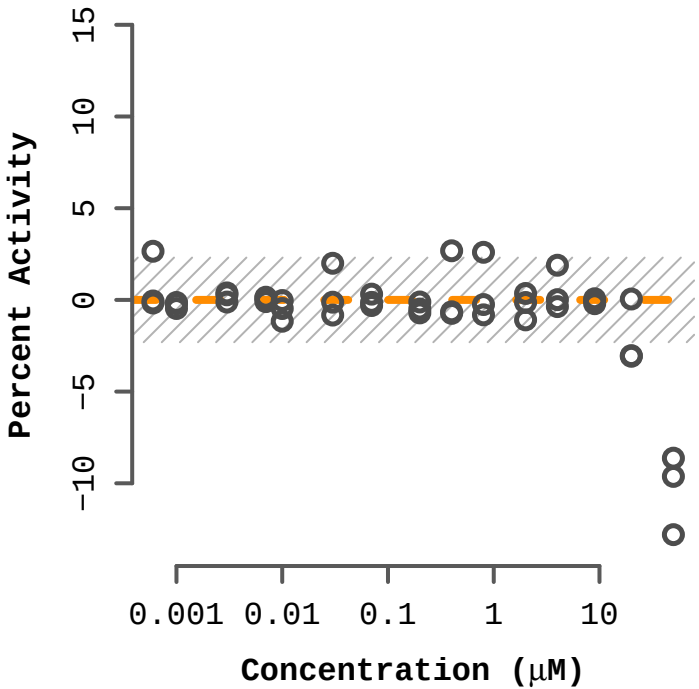
NAME: Tegaserod
CHID: 45955 **CASRN:** 145158-71-0
SPID(S): Tox21_111481_1
M4ID: 12483658 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.97	NA	NA
PROB:	1	NA	NA
RMSE:	4.77	NA	NA

MAX_MEAN: 0.508 **MAX_MED:** 0.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

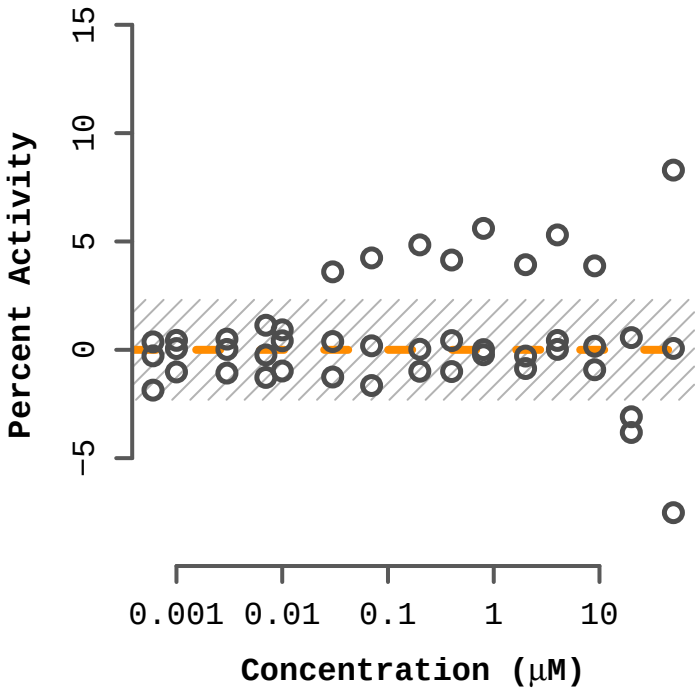
NAME: Cepharanthine
CHID: 45957 **CASRN:** 481-49-2
SPID(S): Tox21_111483_1
M4ID: 12483657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 0.81 **MAX_MED:** 0.279 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

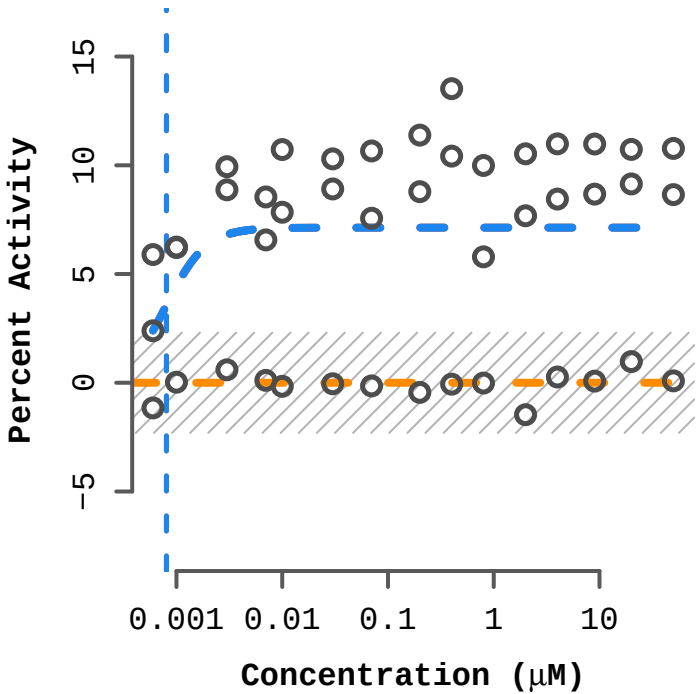
NAME: Tilorone
CHID: 45958 **CASRN:** 27591-97-5
SPID(S): Tox21_111484_1
M4ID: 12483656

HILL MODEL: Not applicable.

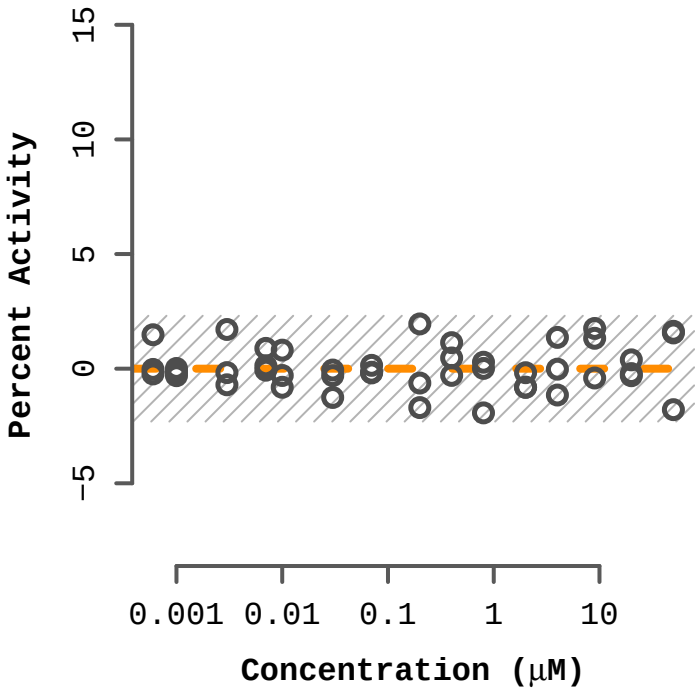
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 0.434 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Alizarin
CHID:    45960   CASRN: 72-48-0
SPID(S): Tox21_111486_1
M4ID:    12483655

HILL MODEL (in red):
      tp       ga       gw
val:  7.13     -3.09    2.32
sd:   0.882    0.206    4.48

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.13     -3.09    2.32     3.55     6.12
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  317.79      277.67      281.67
PROB: 0           0.88        0.12
RMSE: 7.5         4.55        4.55

MAX_MEAN: 7.96      MAX_MED: 10.4      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

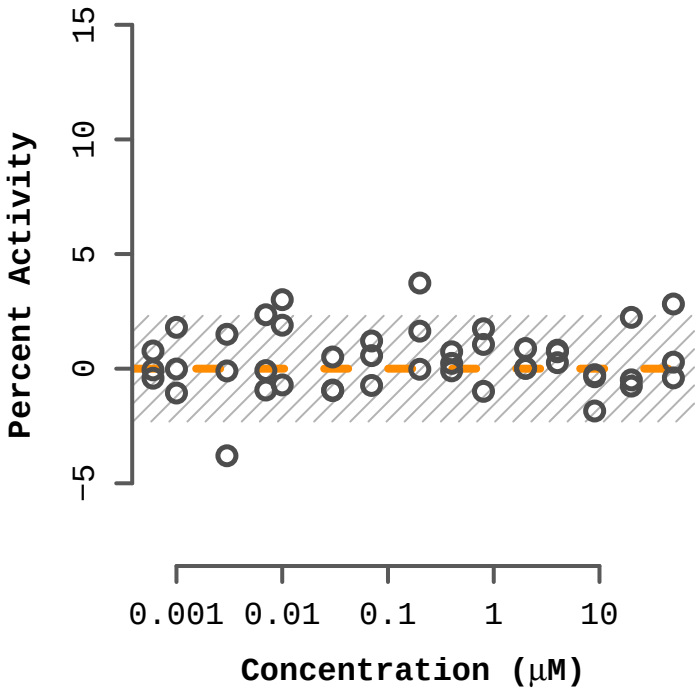
NAME: 1,3,5-Trimethoxybenzene
CHID: 45963 **CASRN:** 621-23-8
SPID(S): Tox21_111489_1
M4ID: 12483654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

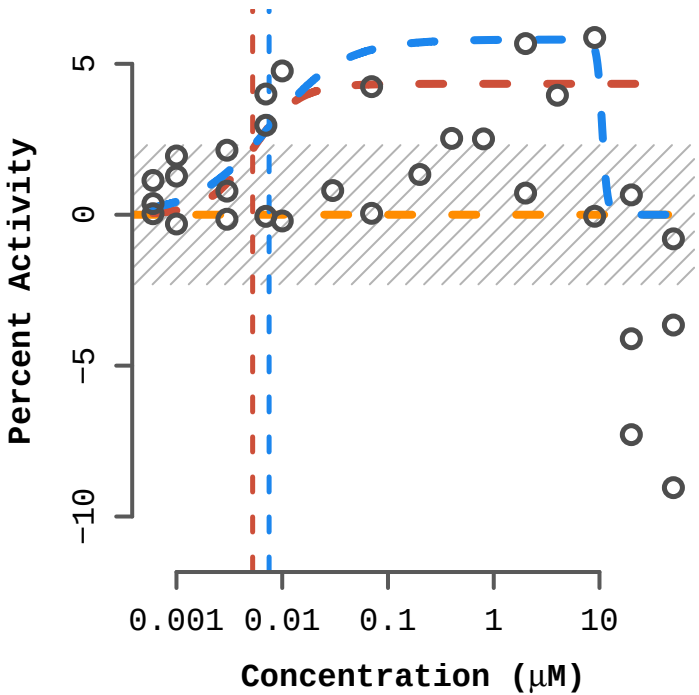
NAME: Bisabolol
CHID: 45964 **CASRN:** 515-69-5
SPID(S): Tox21_111490_1
M4ID: 12483653

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cloxyquin
CHID: 45973 CASRN: 130-16-5
SPID(S): Tox21_111501_1
M4ID: 12483648

HILL MODEL (in red):

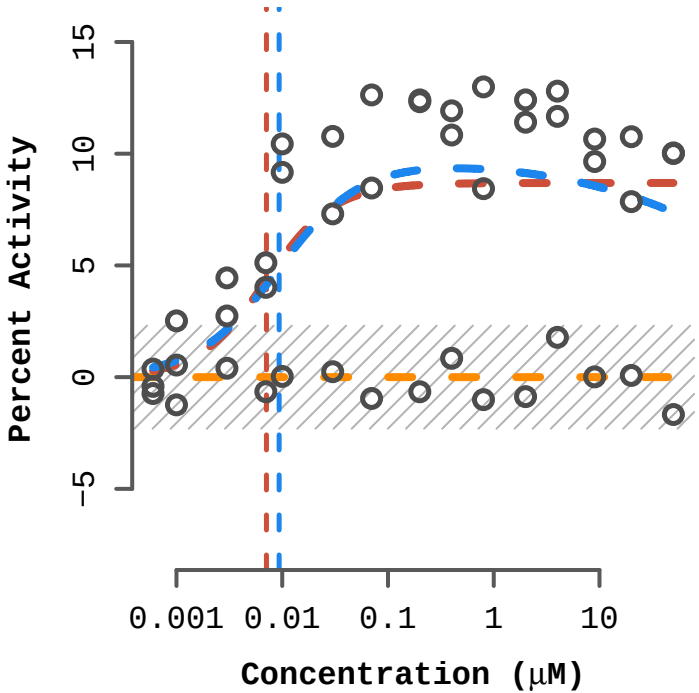
	tp	ga	gw
val:	4.34	−2.28	2.04
sd:	0.754	0.306	3.07

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.8	−2.12	1.25	1.03	17.8
sd:	0.759	0.253	1.21	0.606	148

	CNST	HILL	GNLS
AIC:	278.02	256.86	237.41
PROB:	0	0	1
RMSE:	4.92	4.05	2.99

MAX_MEAN: 6.55 MAX_MED: 6.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Deracoxib
CHID: 45975 CASRN: 169590-41-4
SPID(S): Tox21_111503_1
M4ID: 12483646

HILL MODEL (in red):

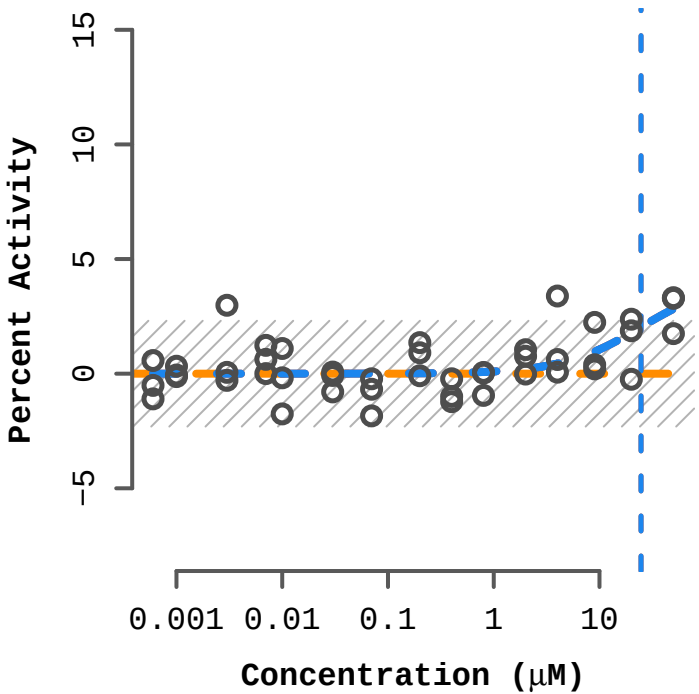
	tp	ga	gw
val:	8.69	−2.15	1.36
sd:	1.08	0.258	0.96

GAIN-LOSS MODEL (in blue):

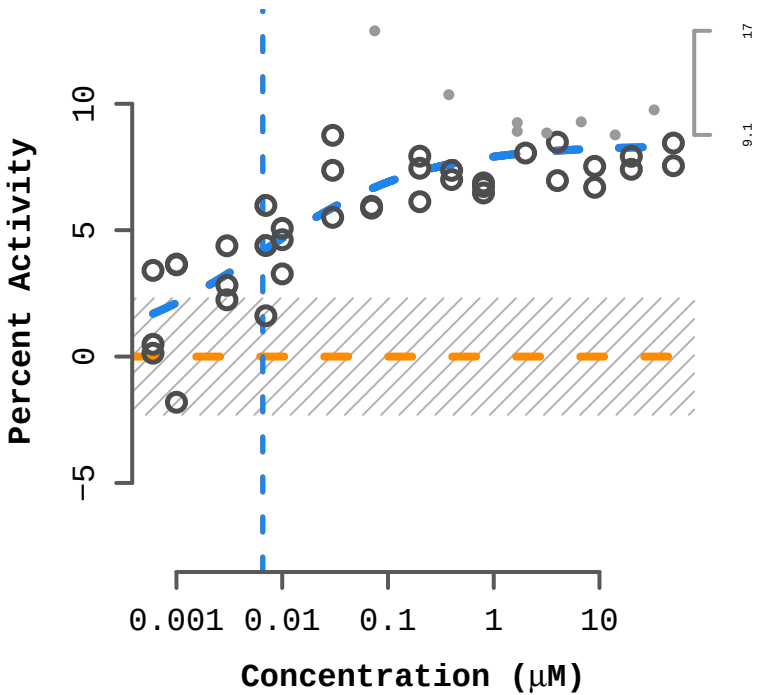
	tp	ga	gw	la	lw
val:	9.78	−2.03	1.12	2.7	0.485
sd:	3.94	0.465	0.851	3.12	1.55

	CNST	HILL	GNLS
AIC:	318.2	278.68	282.24
PROB:	0	0.86	0.14
RMSE:	7.69	4.81	4.81

MAX_MEAN: 8.75 MAX_MED: 12.3 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hypoxanthine
CHID:    45983   CASRN: 68-94-0
SPID(S): Tox21_111511_1
M4ID:    12483643

HILL MODEL (in red):
      tp       ga       gw
val:  4.07     1.39     1.16
sd:   2.46     0.525    0.581

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.07     1.39     1.16     3.28     4.18
sd:   2.46     0.525    0.582    590      1570

      CNST        HILL        GNLS
AIC:  152.75      134.08      138.08
PROB: 0           0.88        0.12
RMSE: 1.34        1.02        1.02

MAX_MEAN: 2.78      MAX_MED: 3.29      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Limoni
CHID: 45985 CASRN: 1180-71-8
SPID(S): Tox21_111513_1
M4ID: 12483642 BRK

HILL MODEL (in red):

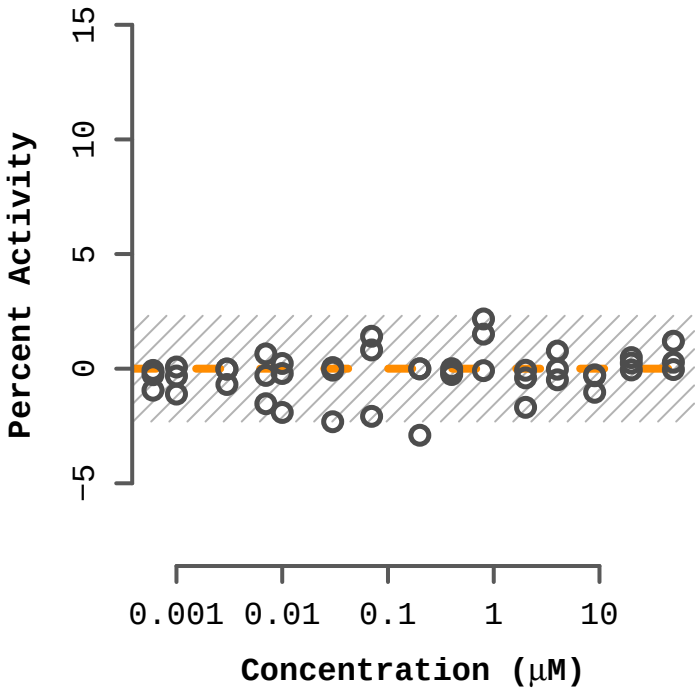
	tp	ga	gw
val:	8.35	−2.18	0.573
sd:	0.494	0.185	0.173

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.35	−2.18	0.573	2.29	15.5
sd:	0.494	0.185	0.173	1190	31200

	CNST	HILL	GNLS
AIC:	315.25	187.52	191.52
PROB:	0	0.88	0.12
RMSE:	7.25	2.18	2.18

MAX_MEAN: 9.65 MAX_MED: 9.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

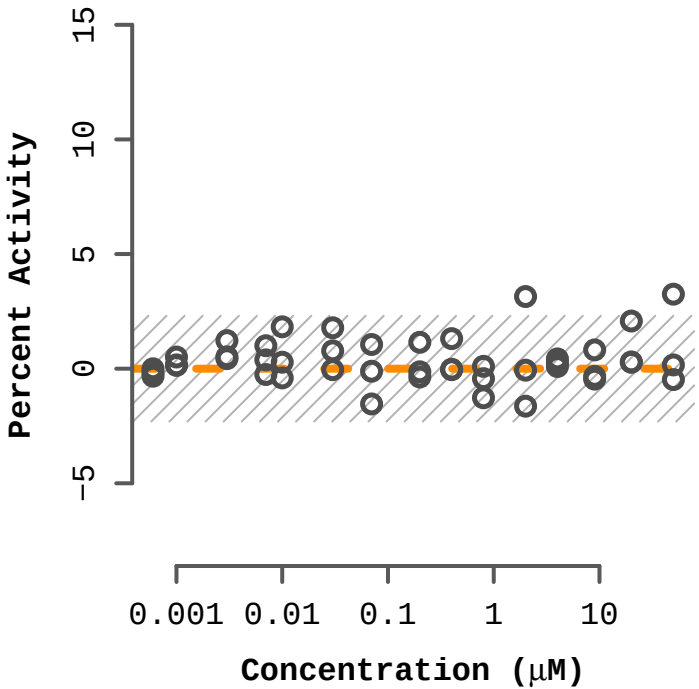
NAME: Creatinine
CHID: 45987 **CASRN:** 60-27-5
SPID(S): Tox21_111516_1
M4ID: 12483640

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

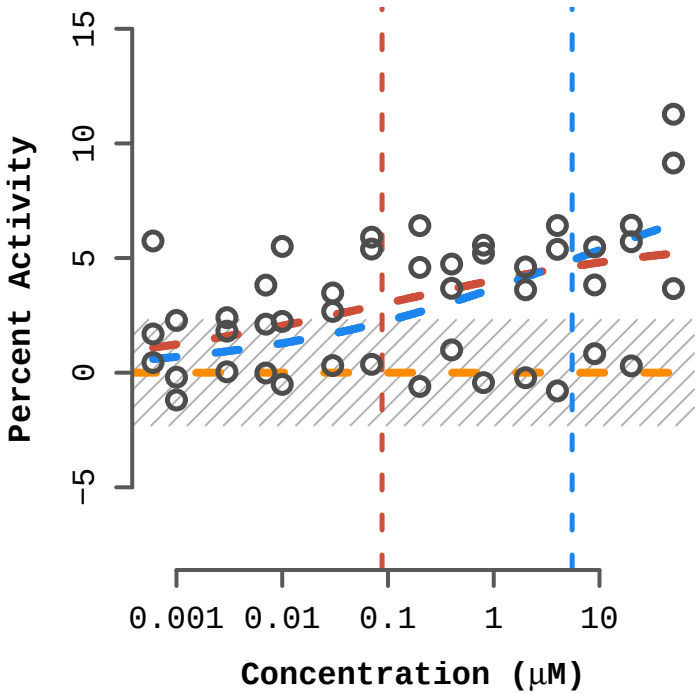
NAME: Tripelennamine citrate
CHID: 45989 **CASRN:** 6138-56-3
SPID(S): Tox21_111518_1
M4ID: 12483639

HILL MODEL: Not applicable.

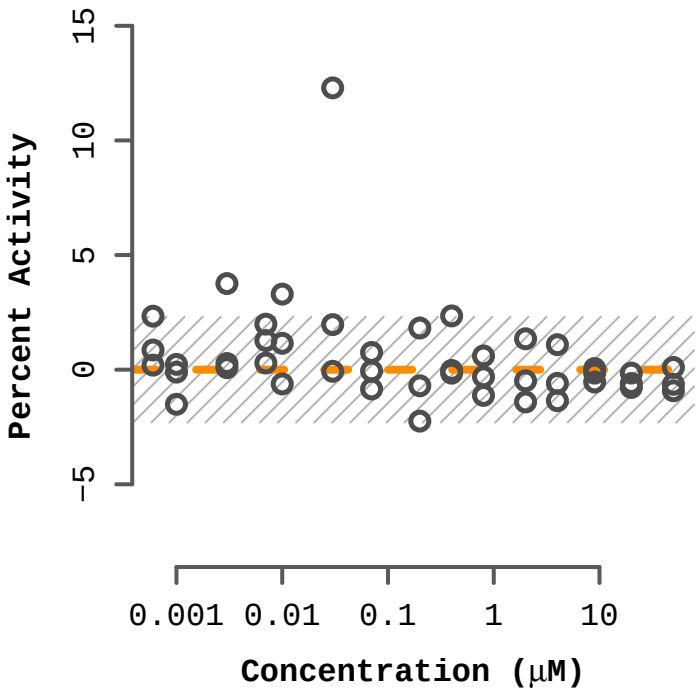
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.981 **MAX_MED:** 0.78 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Inosine
CHID:    45993   CASRN: 58-63-9
SPID(S): Tox21_111522_1
M4ID:    12483637

HILL MODEL (in red):
      tp       ga       gw
val:  5.97     -1.06    0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.82     0.742    0.3      2.82     6.78
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  262.08      223.28      229.46
PROB: 0           0.96        0.04
RMSE: 4.21        2.57        2.61

MAX_MEAN: 8.03      MAX_MED: 9.15      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

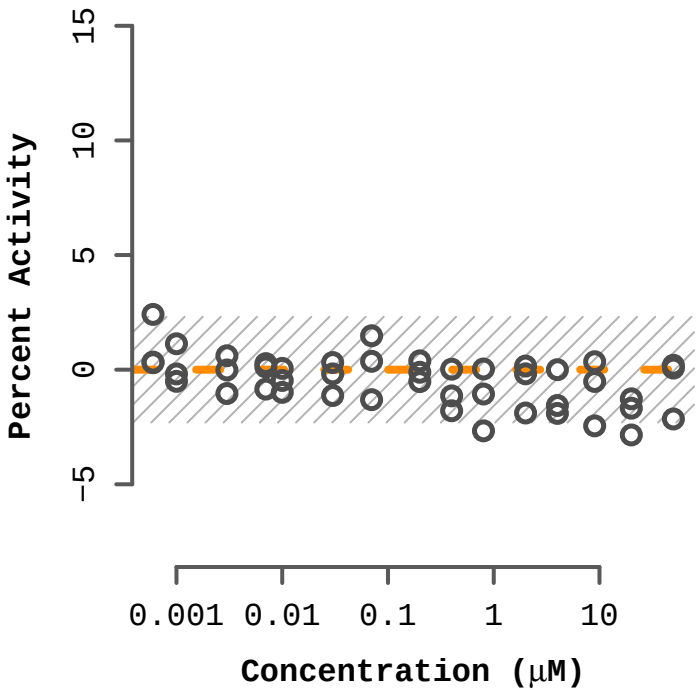
NAME: Guaiazulene
CHID: 45996 **CASRN:** 489-84-9
SPID(S): Tox21_111526_1
M4ID: 12483635

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 4.73 **MAX_MED:** 1.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

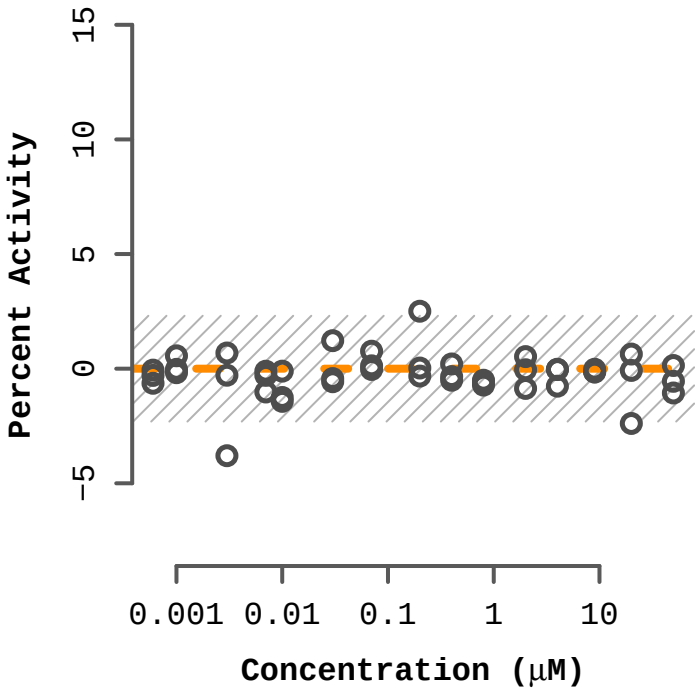
NAME: Conessine
CHID: 46000 **CASRN:** 546-06-5
SPID(S): Tox21_111531_1
M4ID: 12483633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.365 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

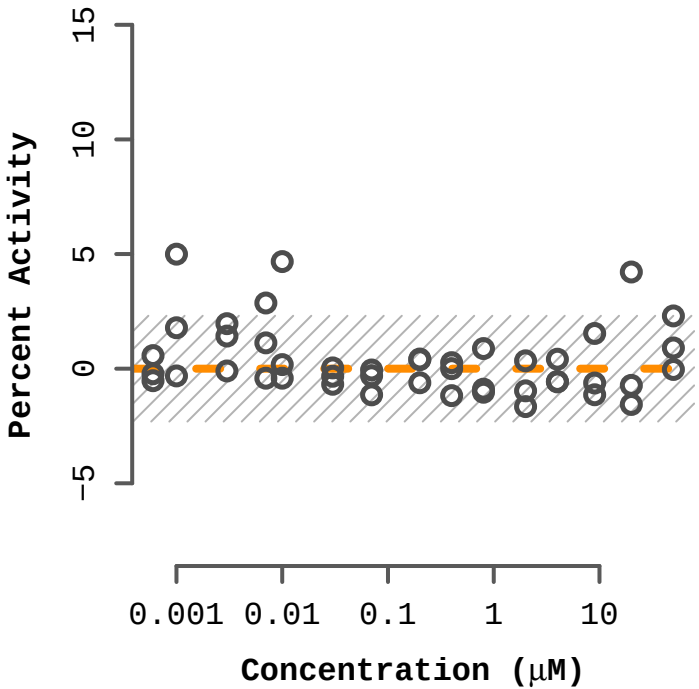
NAME: Escitalopram oxalate
CHID: 46003 **CASRN:** 219861-08-2
SPID(S): Tox21_111535_1
M4ID: 12483631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.738 **MAX_MED:** 0.126 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

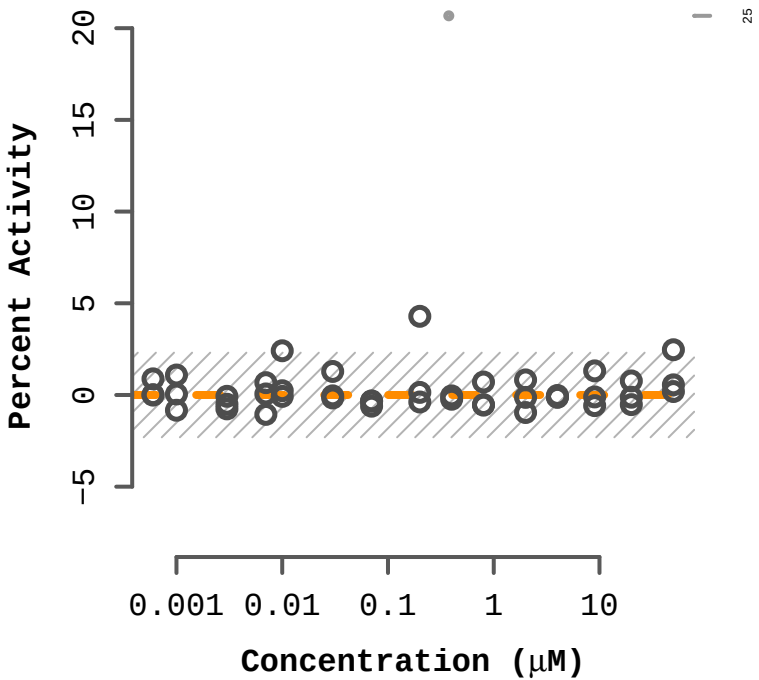
NAME: N-Methylbenzylamine hydrochloride
CHID: 46007 **CASRN:** 13426-94-3
SPID(S): Tox21_111541_1
M4ID: 12483627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 2.16 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

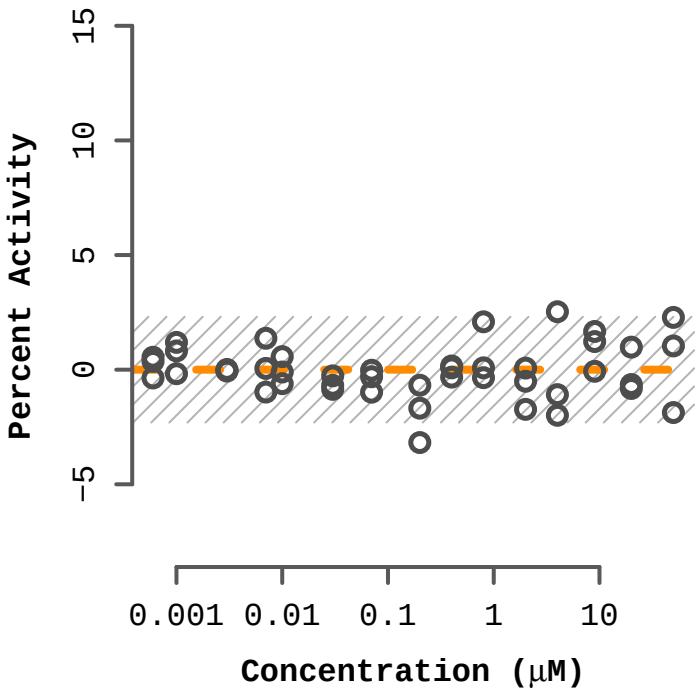
NAME: Acadesine
CHID: 46015 **CASRN:** 2627-69-2
SPID(S): Tox21_111551_1
M4ID: 12483624 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.4	NA	NA
PROB:	1	NA	NA
RMSE:	3.92	NA	NA

MAX_MEAN: 8.39 **MAX_MED:** 0.555 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

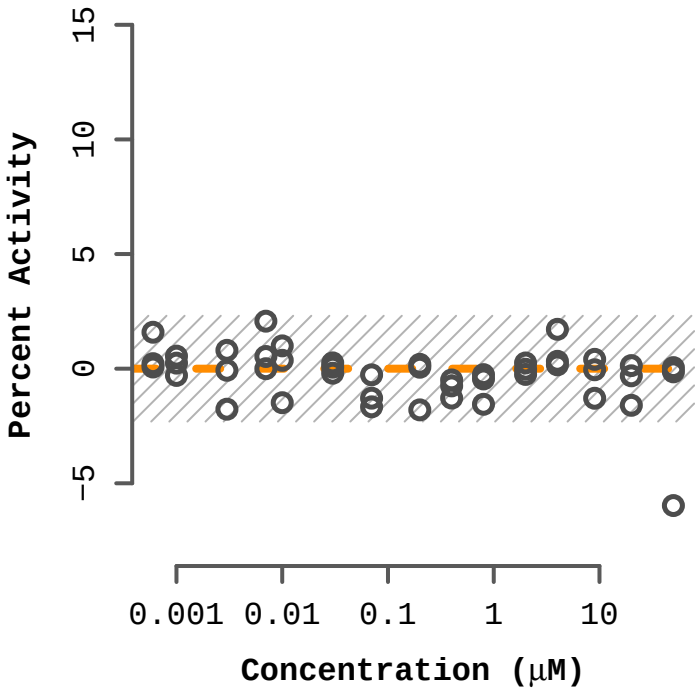
NAME: Aminoguanidine hemisulfate
CHID: 46016 **CASRN:** 996-19-0
SPID(S): Tox21_111552_1
M4ID: 12483623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.942 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

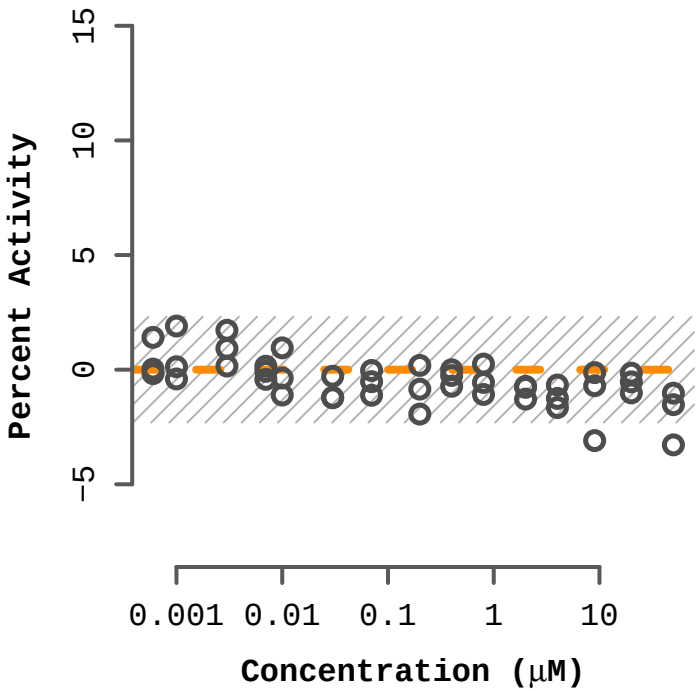
NAME: Trimebutine maleate
CHID: 46017 CASRN: 34140-59-5
SPID(S): Tox21_111554_1
M4ID: 12483621

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.868 MAX_MED: 0.533 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

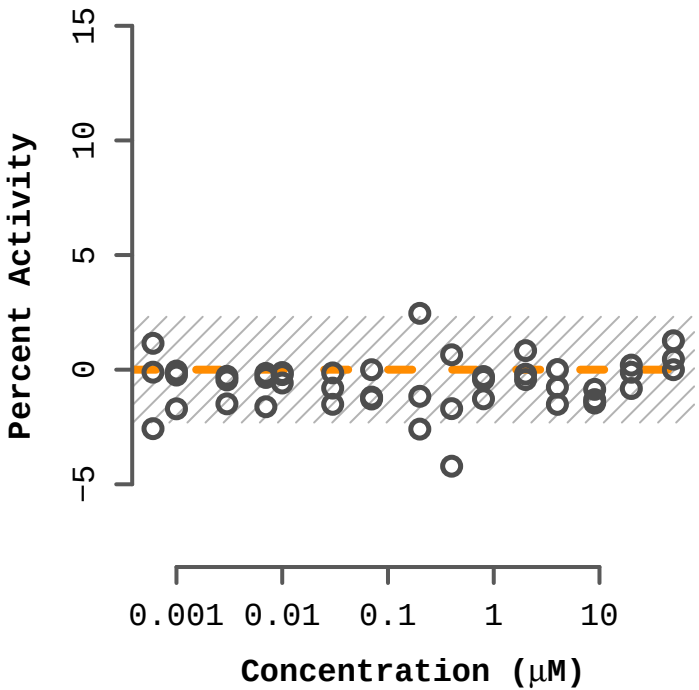
NAME: Thioinosine
CHID: 46019 **CASRN:** 574-25-4
SPID(S): Tox21_111558_1
M4ID: 12483619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

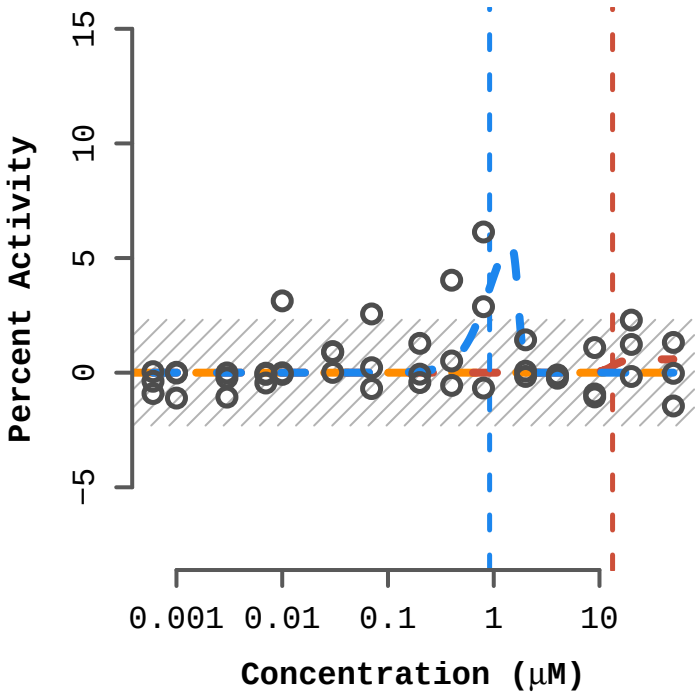
NAME: Pyridoxal
CHID: 46020 CASRN: 66-72-8
SPID(S): Tox21_111561_1
M4ID: 12483617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.574 **MAX_MED:** 0.459 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zonisamide
CHID: 46023 CASRN: 68291-97-4
SPID(S): Tox21_111569_1
M4ID: 12483613

HILL MODEL (in red):

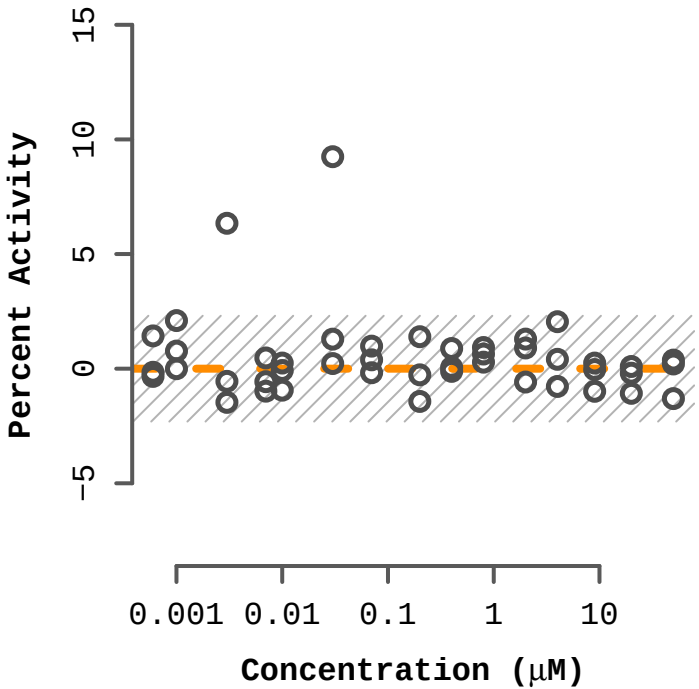
	tp	ga	gw
val:	0.582	1.12	8
sd:	0.511	0.234	10.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.37	−0.0391	3.18	0.231	17.7
sd:	40.6	1.34	5.57	9.71	2440

	CNST	HILL	GNLS
AIC:	151.28	155.97	155.79
PROB:	0.83	0.08	0.09
RMSE:	1.51	1.5	1.3

MAX_MEAN: 2.78 **MAX_MED:** 2.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

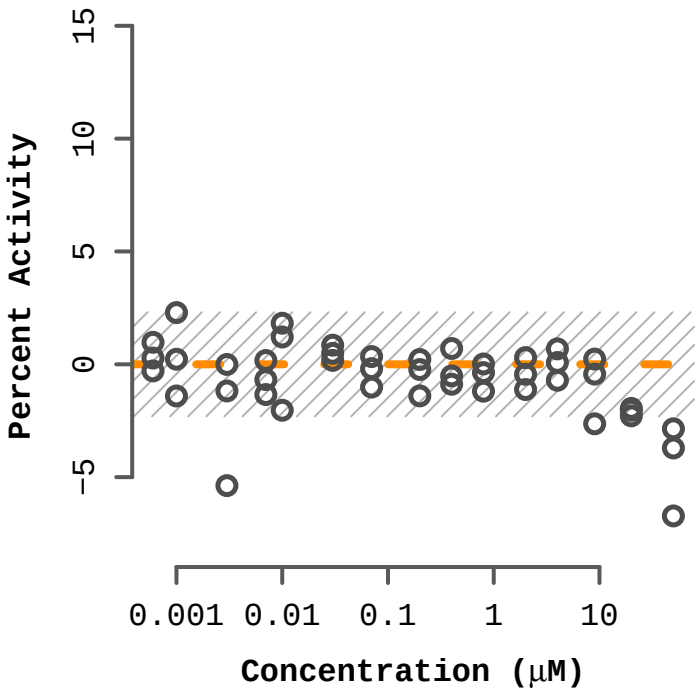
NAME: Clopidogrel hydrogen sulfate
CHID: 46024 CASRN: 135046-48-9
SPID(S): Tox21_111570_1
M4ID: 12483612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 3.59 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

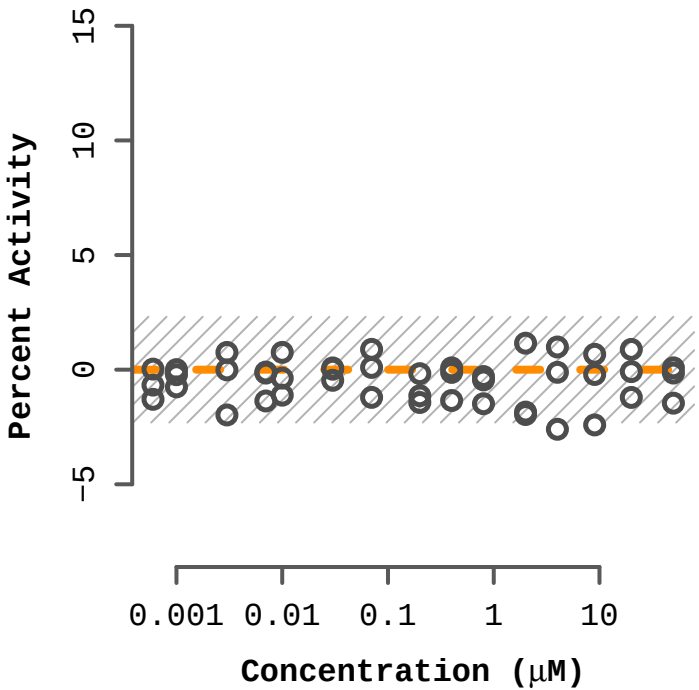
NAME: Efavirenz
CHID: 46029 **CASRN:** 154598-52-4
SPID(S): Tox21_111582_1
M4ID: 12483605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 0.504 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

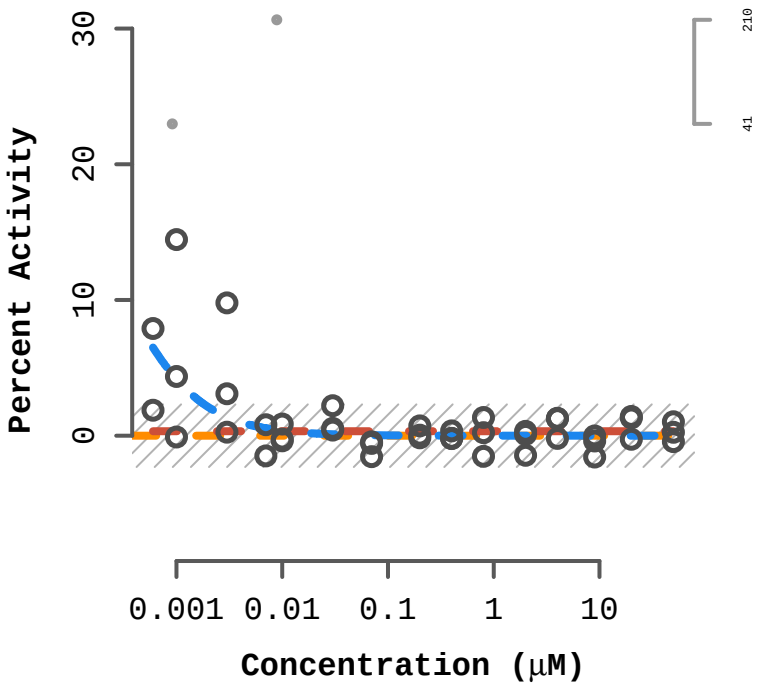
NAME: Tazobactam sodium
CHID: 46030 **CASRN:** 89785-84-2
SPID(S): Tox21_111584_1
M4ID: 12483604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: −0.0736 **MAX_MED:** 0.0987 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Acarbose
CHID: 46034 CASRN: 56180-94-0
SPID(S): Tox21_111597_1
M4ID: 12483596 BRK

HILL MODEL (in red):

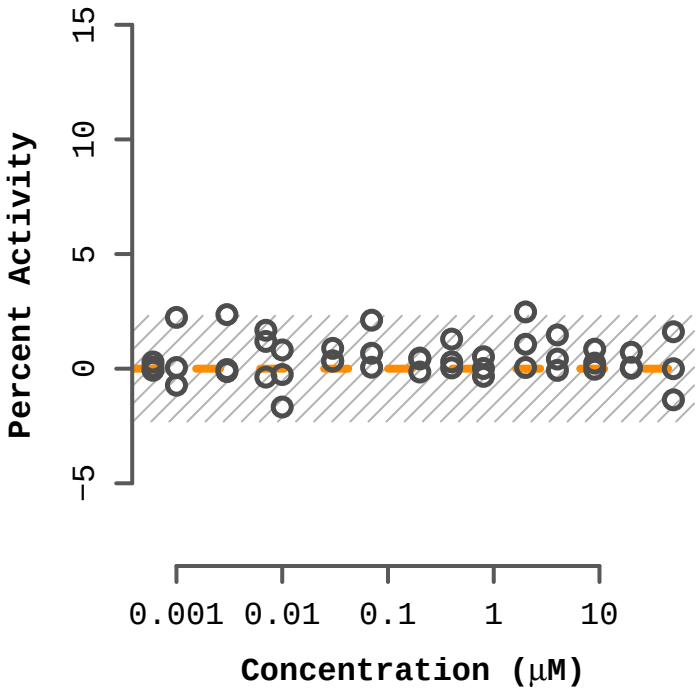
	tp	ga	gw
val:	0.33	-5.2	3.52
sd:	0.244	1540	2700

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.9	-4.81	7.35	-3.55	1.14
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	259.8	263.93	257.03
PROB:	0.2	0.02	0.78
RMSE:	31.6	31.54	31.29

MAX_MEAN: 68.8 MAX_MED: 7.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

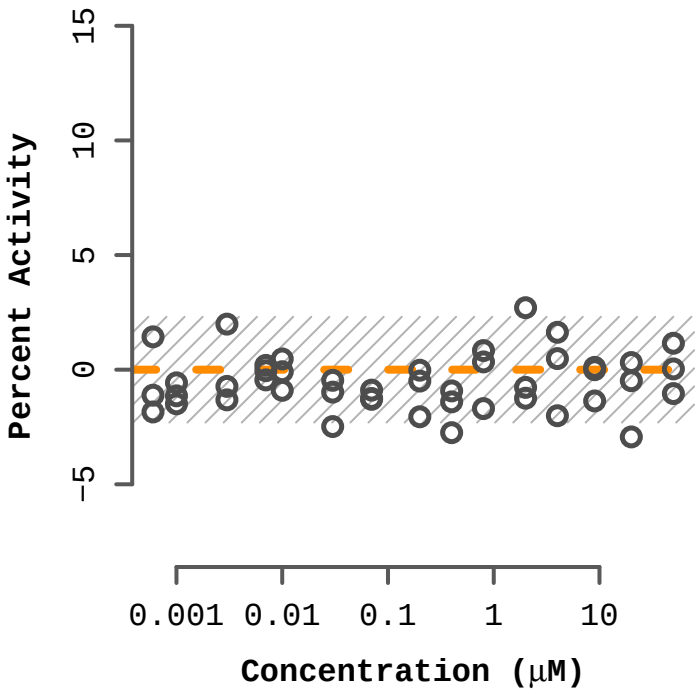
NAME: Huperzine A
CHID: 46038 **CASRN:** 102518-79-6
SPID(S): Tox21_111603_1
M4ID: 12483594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

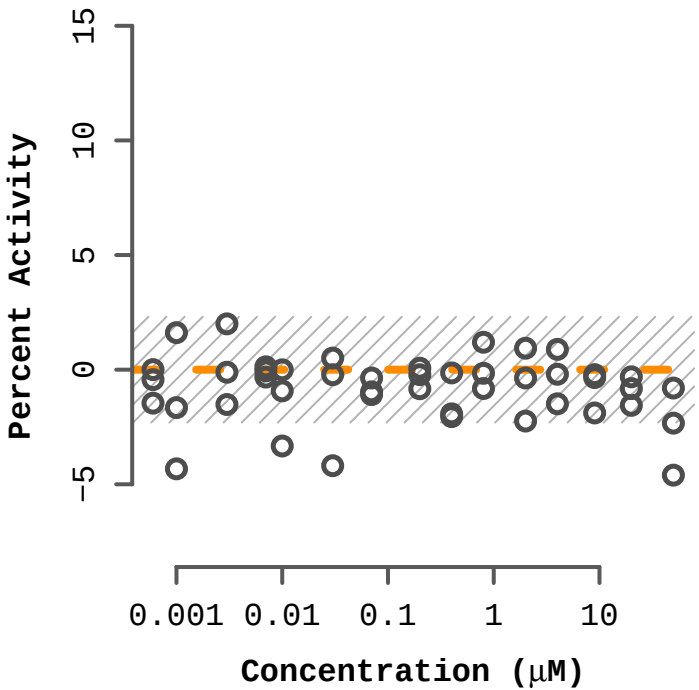
NAME: m-Cresyl acetate
CHID: 46041 **CASRN:** 122-46-3
SPID(S): Tox21_111606_1
M4ID: 12483592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.23 **MAX_MED:** 0.485 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

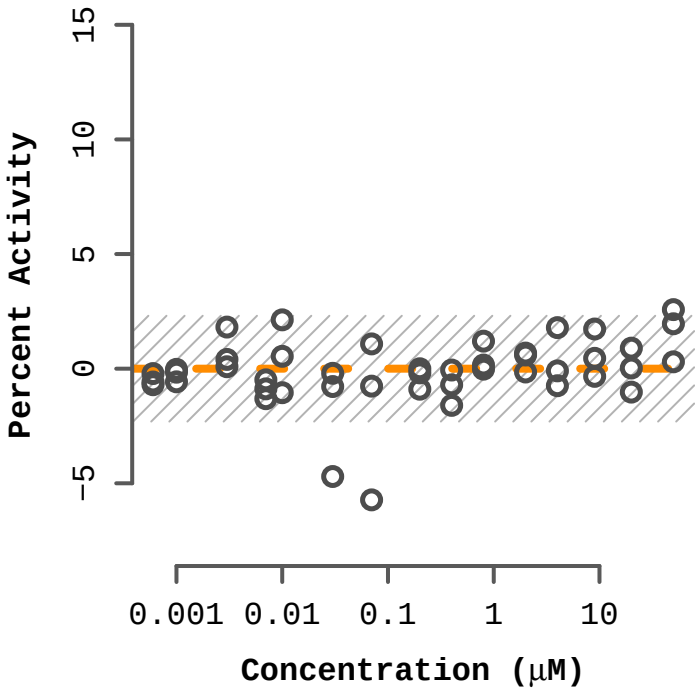
NAME: Laureth 10s
CHID: 46042 **CASRN:** 13081-34-0
SPID(S): Tox21_111623_1
M4ID: 12483578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 0.124 **MAX_MED:** −0.052 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

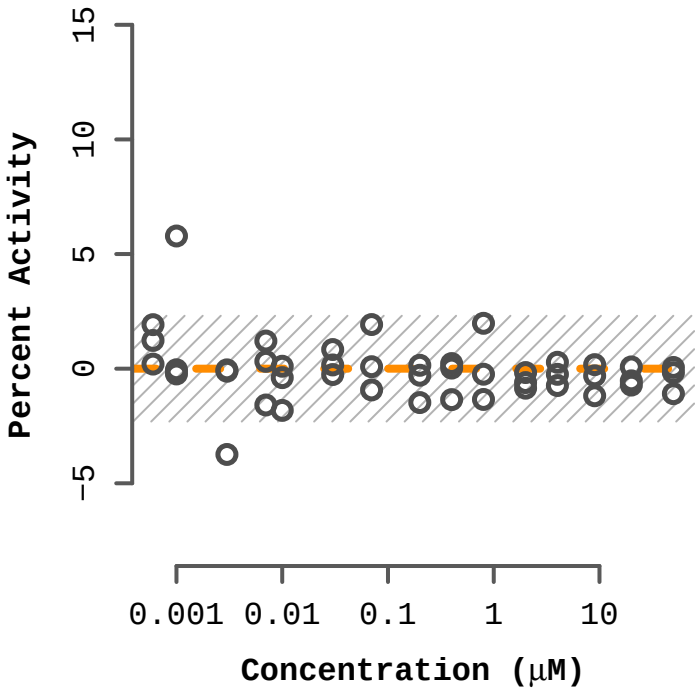
NAME: N-Acetyl-L-tyrosine
CHID: 46045 **CASRN:** 537-55-3
SPID(S): Tox21_111630_1
M4ID: 12483574

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

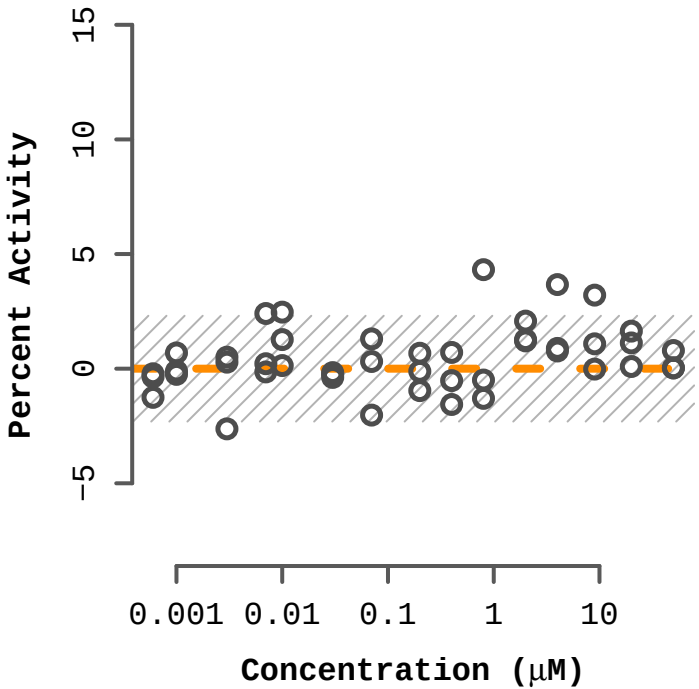
NAME: Iodoantipyrine
CHID: 46047 **CASRN:** 129-81-7
SPID(S): Tox21_111636_1
M4ID: 12483571

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

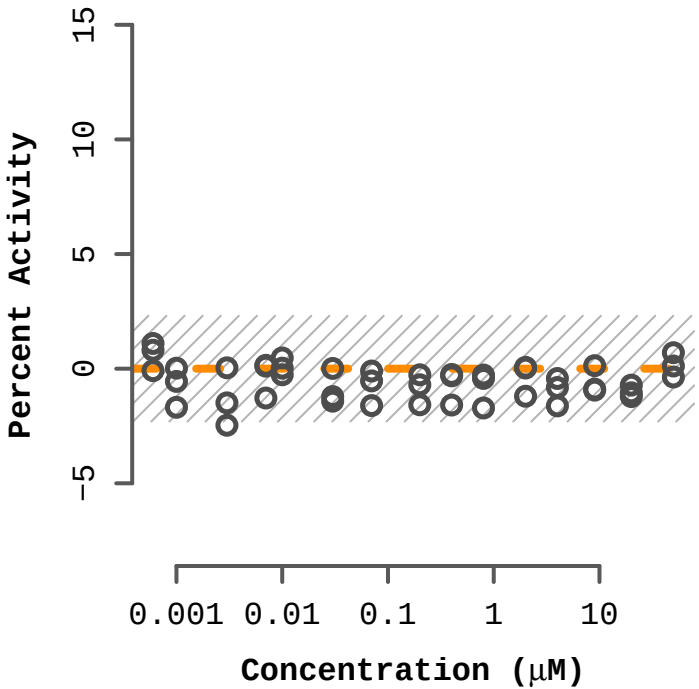
NAME: D-Galactitol
CHID: 46051 **CASRN:** 608-66-2
SPID(S): Tox21_111644_1
M4ID: 12483563

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

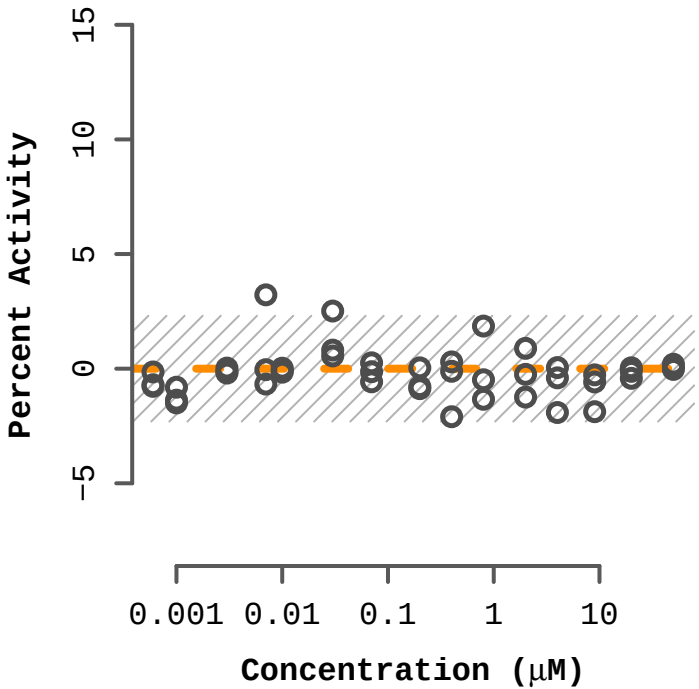
NAME: D-Galactitol
CHID: 46051 **CASRN:** 608-66-2
SPID(S): Tox21_111643_1
M4ID: 12483564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.807 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

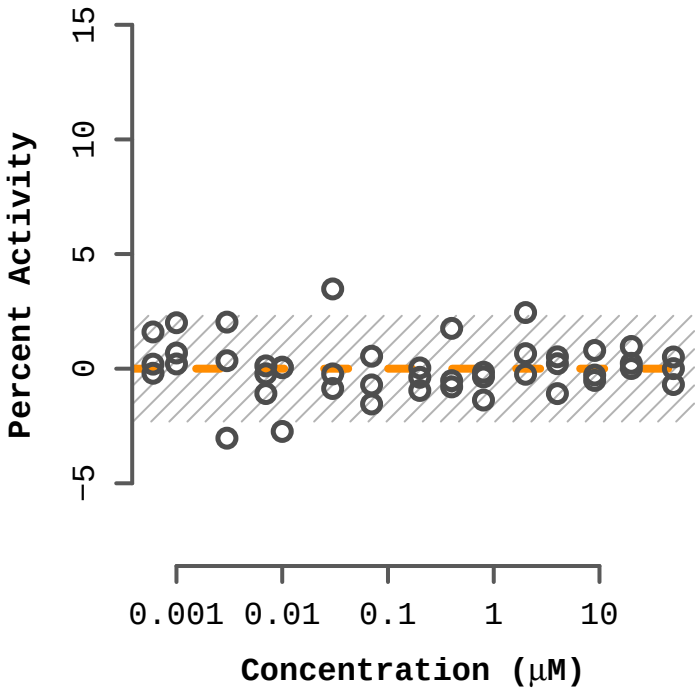
NAME: Parethoxycaine
CHID: 46060 **CASRN:** 94-23-5
SPID(S): Tox21_111677_1
M4ID: 12483542

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.812 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

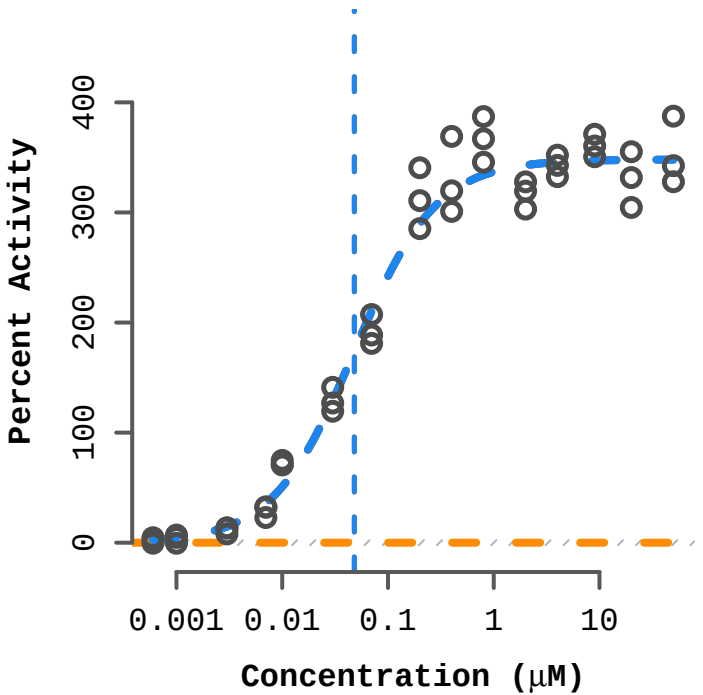
NAME: Sodium 4-aminosalicylate
CHID: 46066 **CASRN:** 133-10-8
SPID(S): Tox21_111696_1
M4ID: 12483532

HILL MODEL: Not applicable.

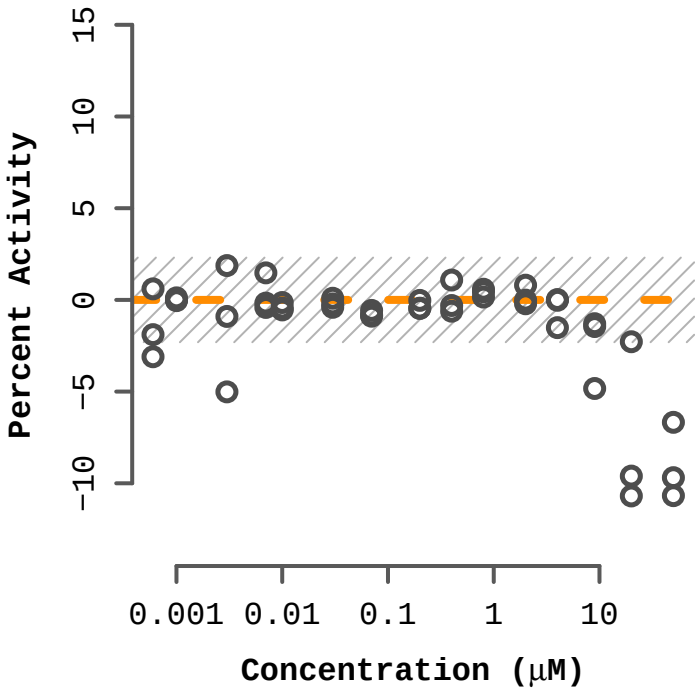
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.685 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Fluprednisolone
CHID:    46067   CASRN: 53-34-9
SPID(S): Tox21_111698_1
M4ID:    12483531

HILL MODEL (in red):
      tp       ga       gw
val:  348      -1.32    1.12
sd:   5.31     0.0354   0.0815

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  348      -1.32    1.12     3.38     17.7
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  635.82      410.26      414.26
PROB: 0           0.88        0.12
RMSE: 256.27      21.45       21.45

MAX_MEAN: 367       MAX_MED: 367       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

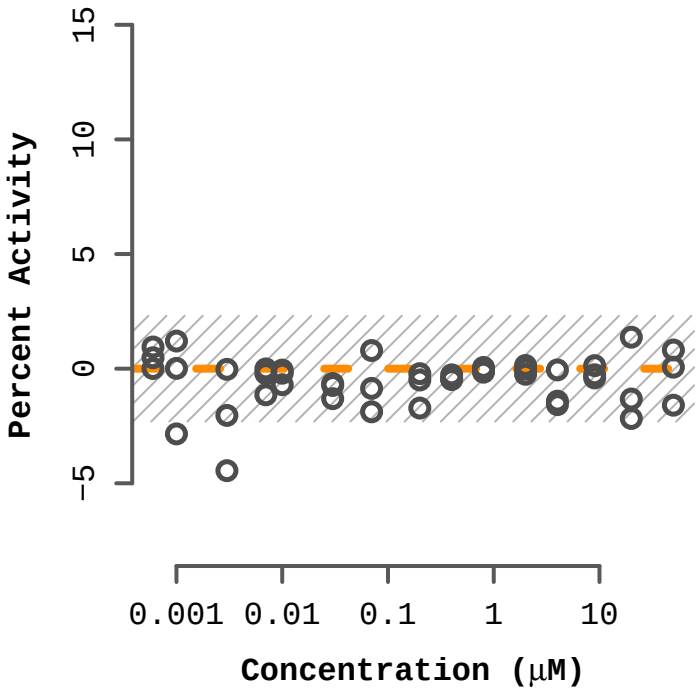
NAME: Benzoxiquine
CHID: 46069 **CASRN:** 86-75-9
SPID(S): Tox21_111701_1
M4ID: 12483529

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.41	NA	NA
PROB:	1	NA	NA
RMSE:	3.48	NA	NA

MAX_MEAN: 0.394 **MAX_MED:** 0.444 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

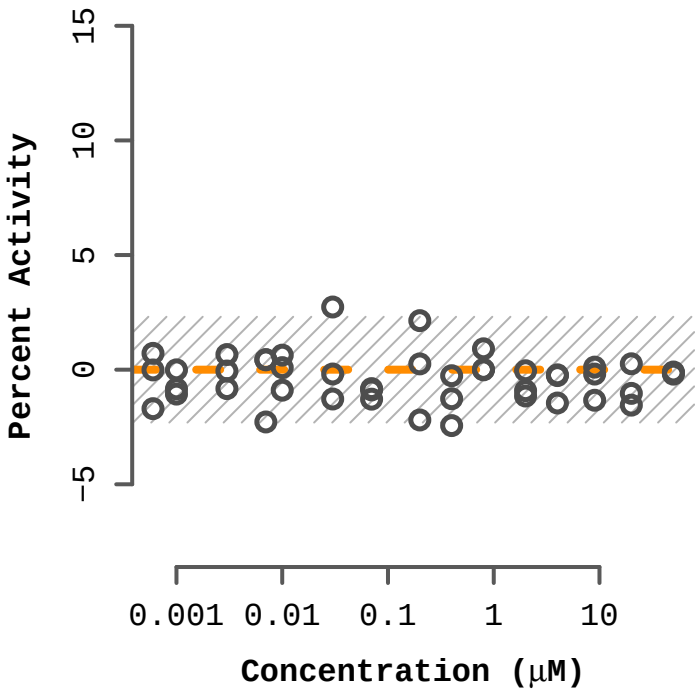
NAME: Levobupivacaine hydrochloride
CHID: 46071 CASRN: 27262-48-2
SPID(S): Tox21_111706_1
M4ID: 12483526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.478 **MAX_MED:** 0.479 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

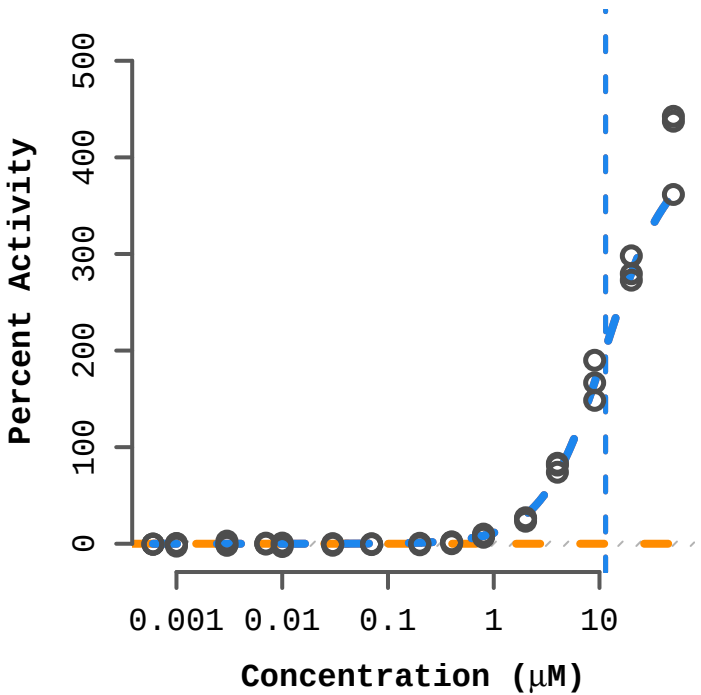
NAME: Hippuric acid
CHID: 46073 **CASRN:** 495-69-2
SPID(S): Tox21_111710_1
M4ID: 12483524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.424 **MAX_MED:** 0.435 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sildenafil citrate
CHID: 46076 CASRN: 171599-83-0
SPID(S): Tox21_111717_1
M4ID: 12483521

HILL MODEL (in red):

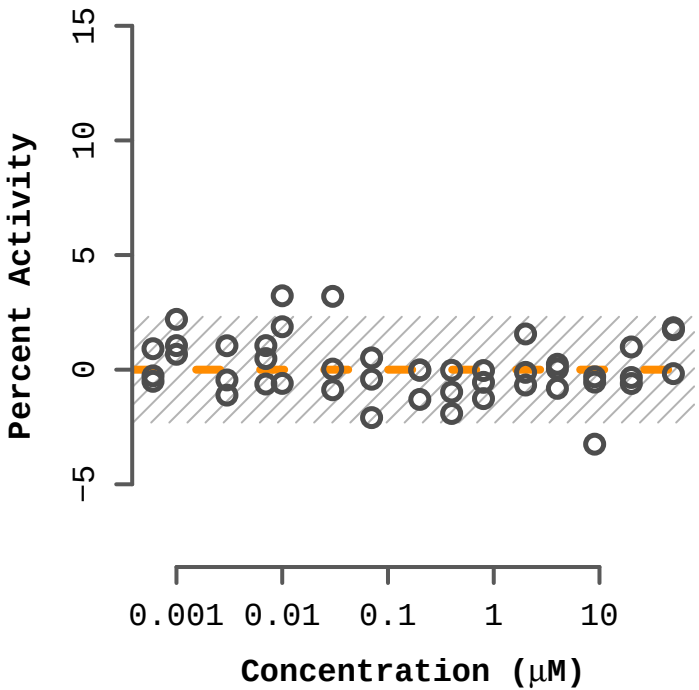
	tp	ga	gw
val:	404	1.06	1.45
sd:	4.72	0.0114	0.0308

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	404	1.06	1.45	3.66	16.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	558.31	315.82	319.82
PROB:	0	0.88	0.12
RMSE:	138.78	17.55	17.55

MAX_MEAN: 414 **MAX_MED:** 437 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

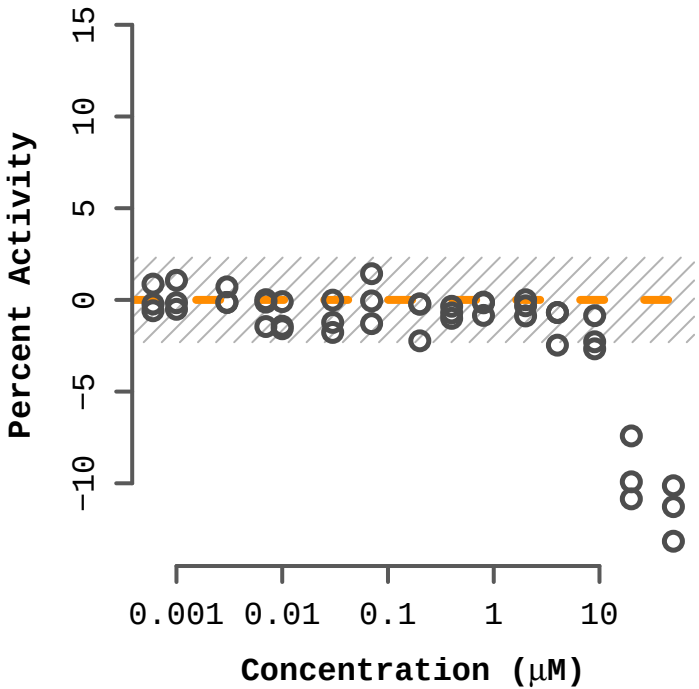
NAME: Thymol iodide
CHID: 46081 **CASRN:** 552-22-7
SPID(S): Tox21_111723_1
M4ID: 12483519

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

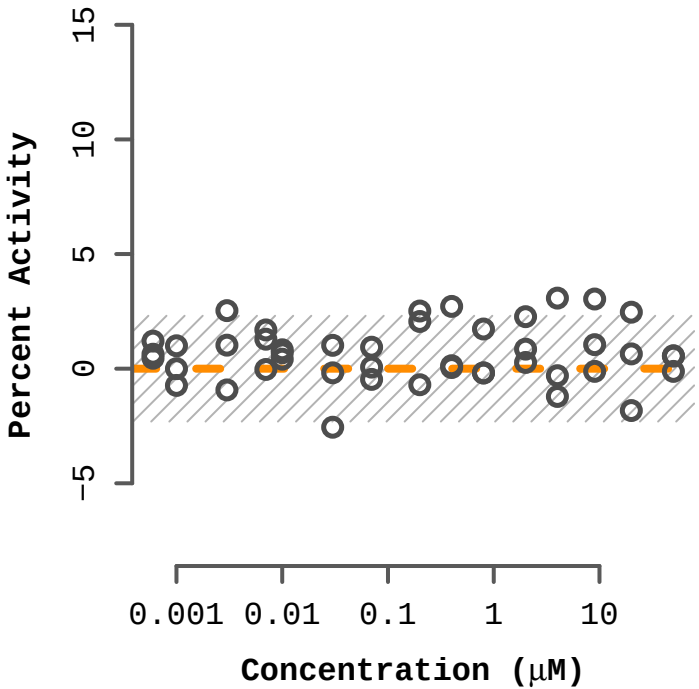
NAME: Aripiprazole
CHID: 46083 **CASRN:** 129722-12-9
SPID(S): Tox21_111728_1
M4ID: 12483518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.13	NA	NA
PROB:	1	NA	NA
RMSE:	4	NA	NA

MAX_MEAN: 0.147 **MAX_MED:** −0.0532 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

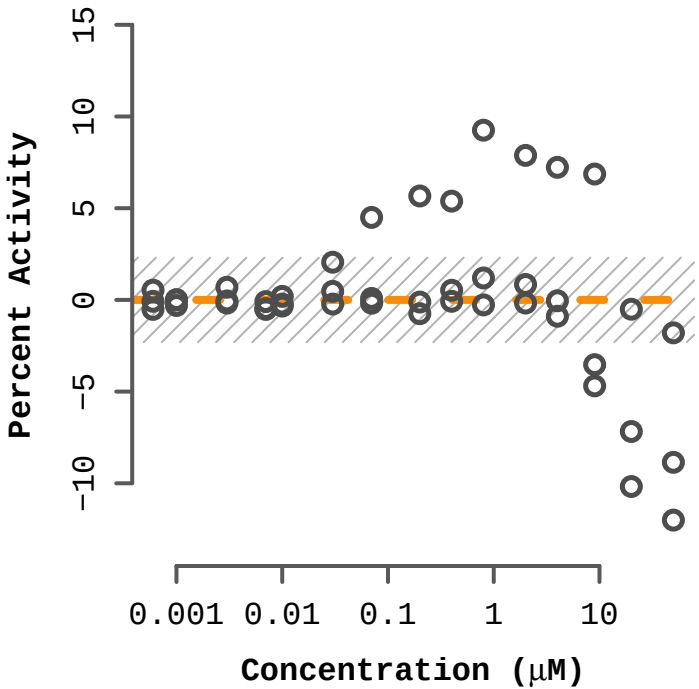
NAME: Eszopiclone
CHID: 46086 **CASRN:** 138729-47-2
SPID(S): Tox21_111733_1
M4ID: 12483515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

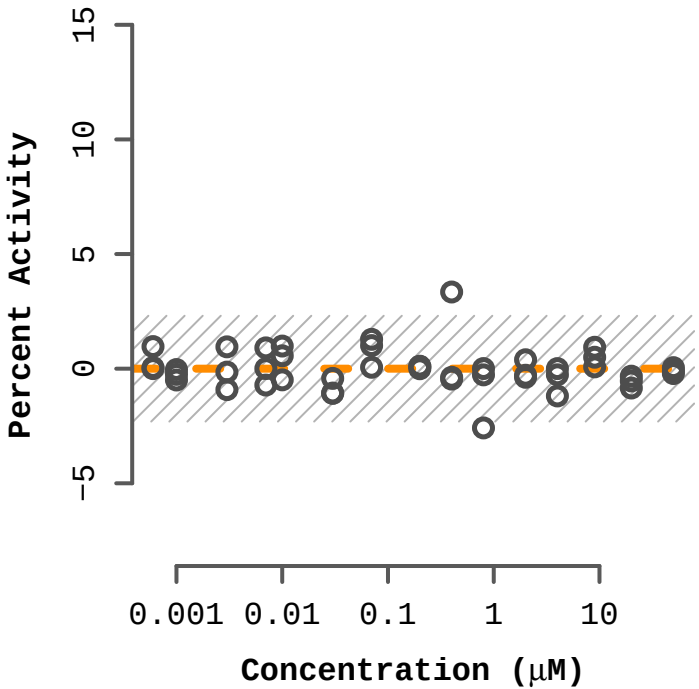
NAME: Nefazodone hydrochloride
CHID: 46088 **CASRN:** 82752-99-6
SPID(S): Tox21_111735_1
M4ID: 12483513

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.51	NA	NA
PROB:	1	NA	NA
RMSE:	4.09	NA	NA

MAX_MEAN: 3.39 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

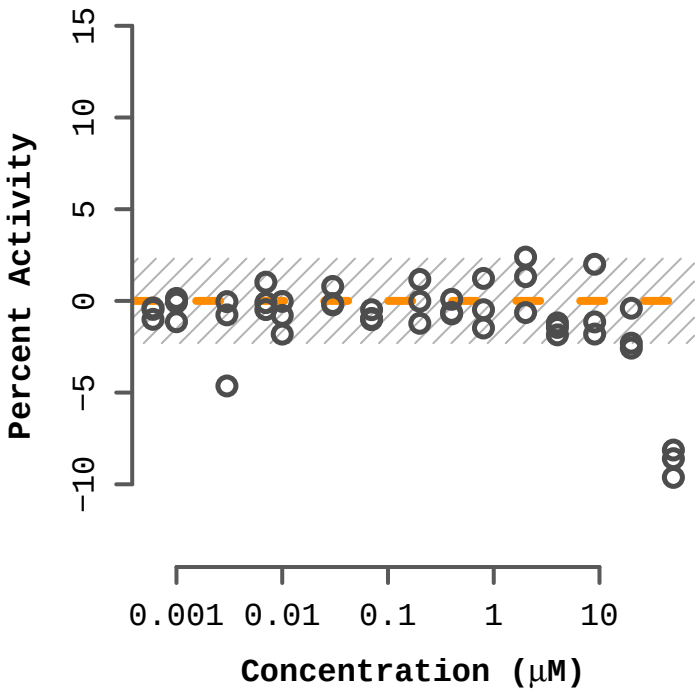
NAME: Eltoprazine hydrochloride
CHID: 46090 **CASRN:** 98206-09-8
SPID(S): Tox21_111742_1
M4ID: 12483507

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.84 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

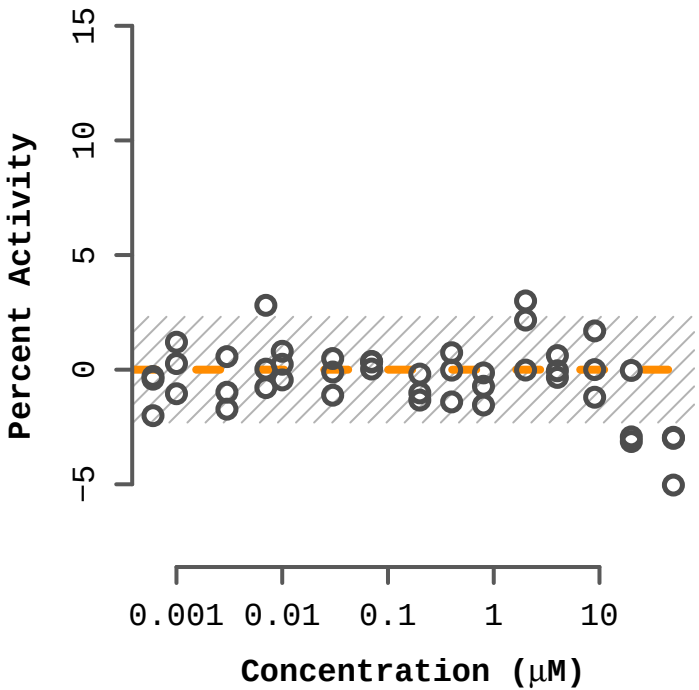
NAME: Zaldaride
CHID: 46091 **CASRN:** 109826-26-8
SPID(S): Tox21_111743_1
M4ID: 12483506

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

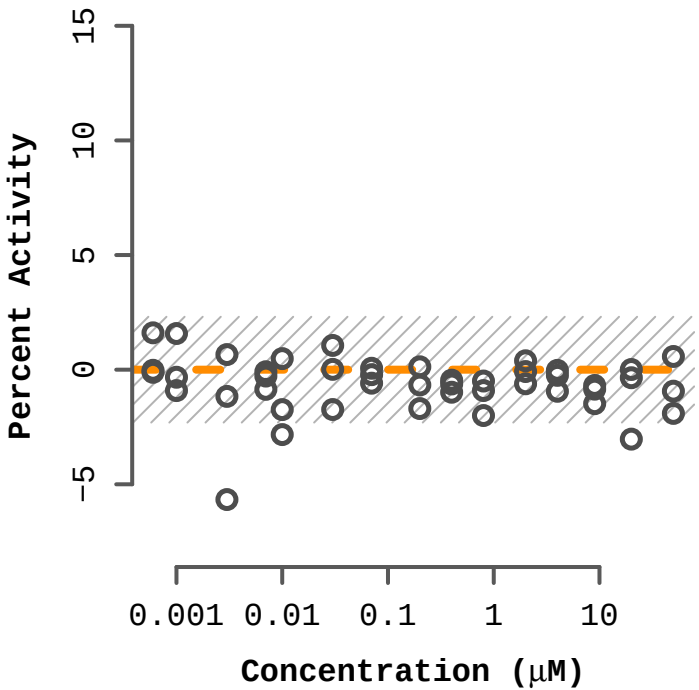
NAME: Devazepide
CHID: 46092 **CASRN:** 103420-77-5
SPID(S): Tox21_111744_1
M4ID: 12483505

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

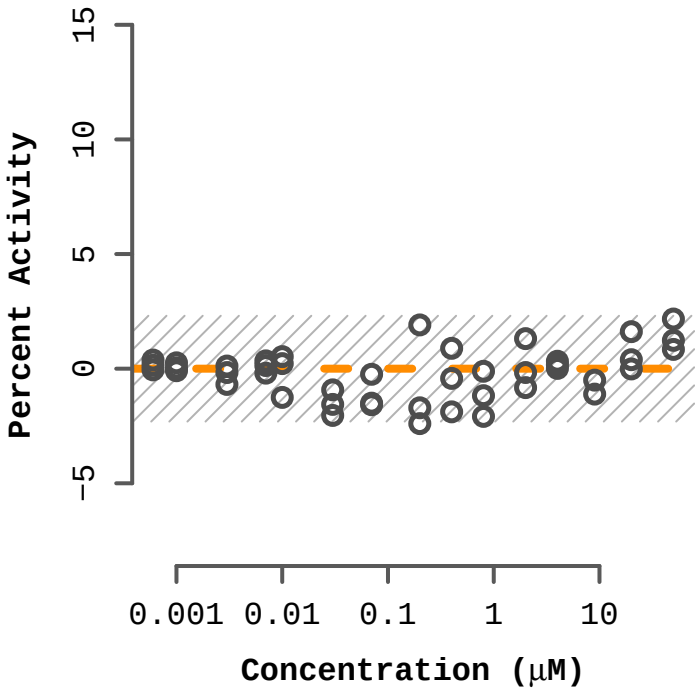
NAME: Fanapanel
CHID: 46093 **CASRN:** 161605-73-8
SPID(S): Tox21_111745_1
M4ID: 12483504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.49 **MAX_MED:** 0.0158 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

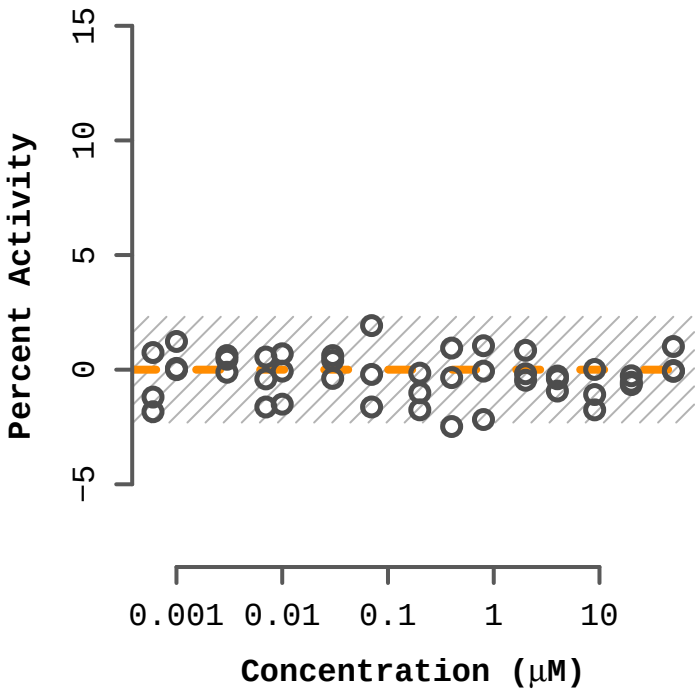
NAME: Eplerenone
CHID: 46094 **CASRN:** 107724-20-9
SPID(S): Tox21_111746_1
M4ID: 12483503

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

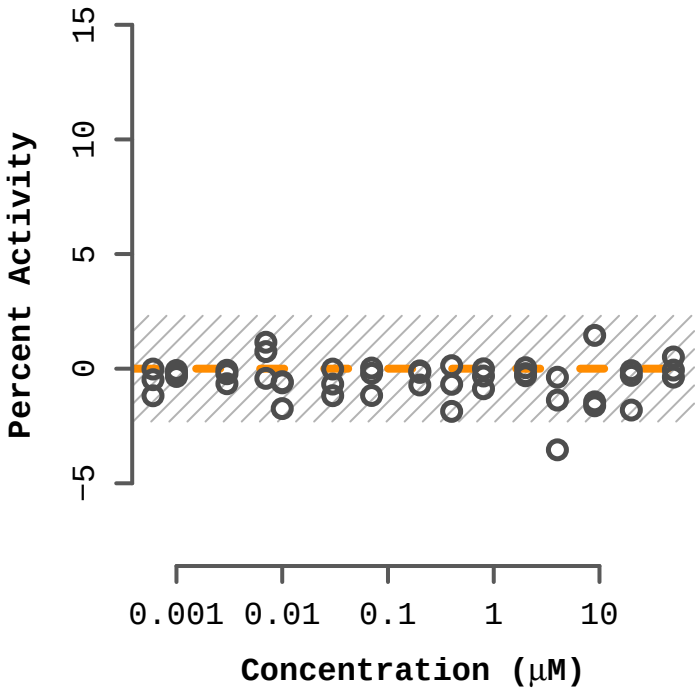
NAME: Pepstatin
CHID: 46095 **CASRN:** 26305-03-3
SPID(S): Tox21_111747_1
M4ID: 12483502

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.431 **MAX_MED:** 0.455 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

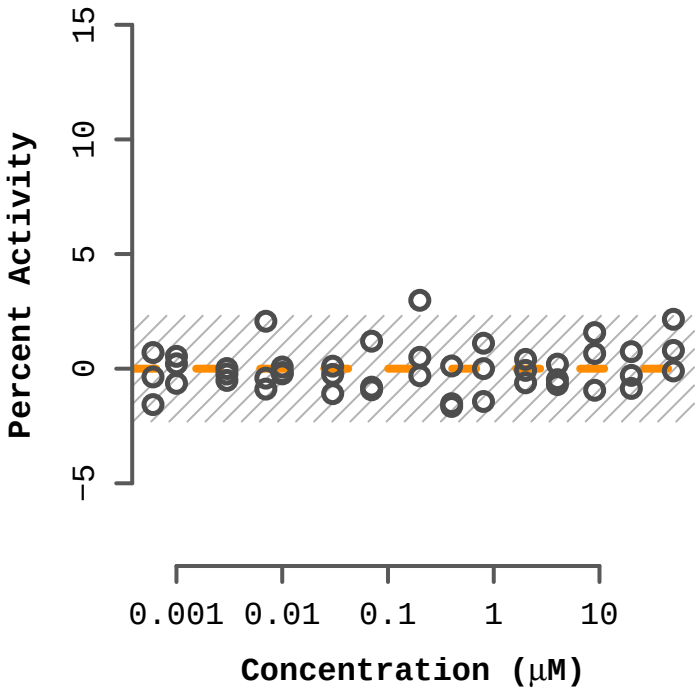
NAME: Hordenine
CHID: 46096 **CASRN:** 539-15-1
SPID(S): Tox21_111748_1
M4ID: 12483501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.493 **MAX_MED:** 0.747 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

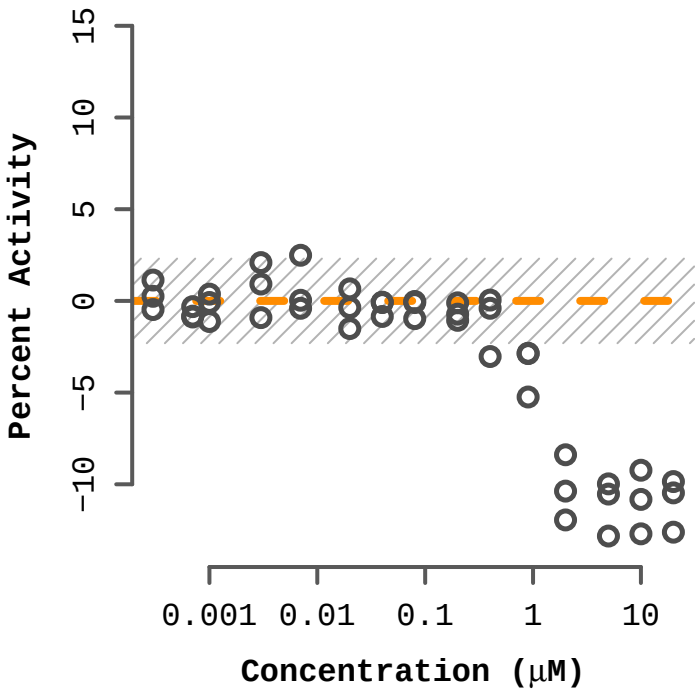
NAME: 6,7-Dimethoxyquinazoline-2,4(1H,3H)-dione
CHID: 46100 **CASRN:** 28888-44-0
SPID(S): Tox21_111752_1
M4ID: 12483499

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.798 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

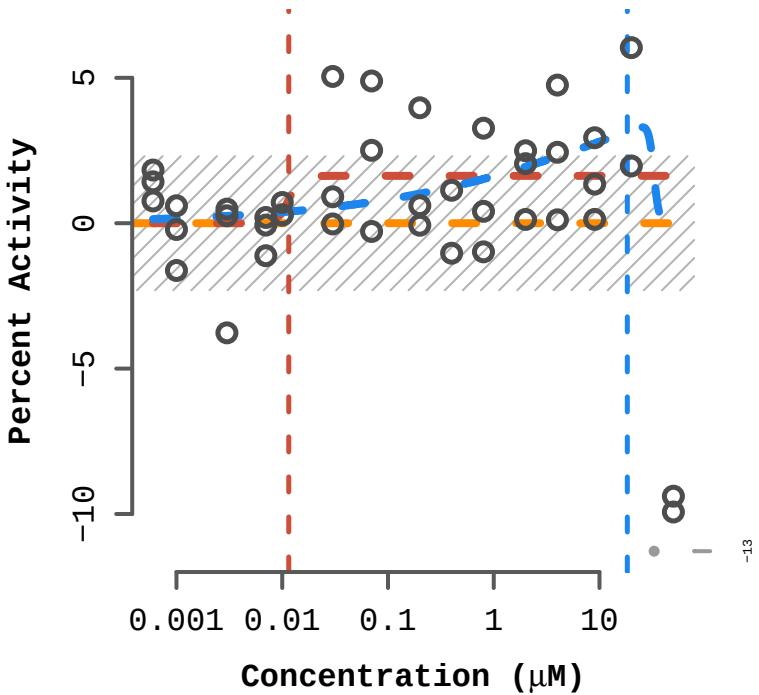
NAME: Geliomycin
CHID: 46101 CASRN: 20004-62-0
SPID(S): Tox21_111753_1
M4ID: 12483498

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	282.55	NA	NA
PROB:	1	NA	NA
RMSE:	5.77	NA	NA

MAX_MEAN: 0.708 **MAX_MED:** 0.921 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tenidap
CHID: 46104 CASRN: 120210-48-2
SPID(S): Tox21_111757_1
M4ID: 12483497 BRK

HILL MODEL (in red):

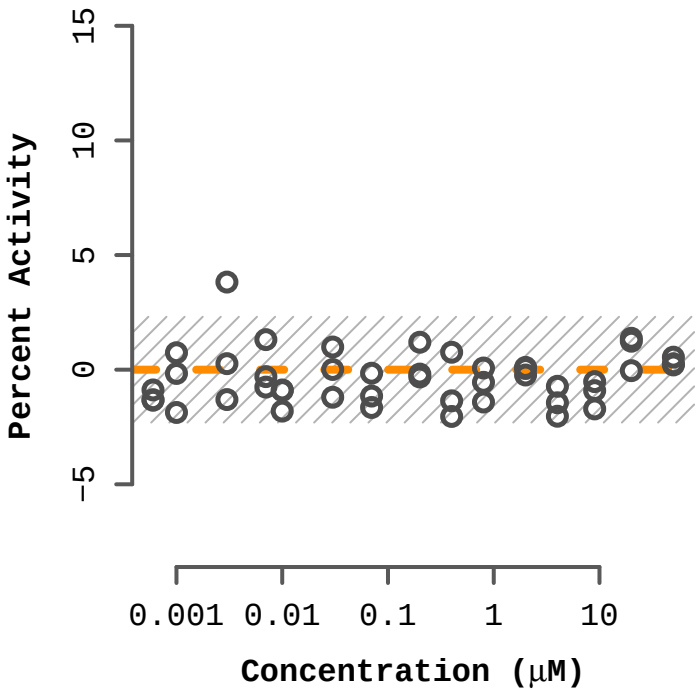
	tp	ga	gw
val:	1.63	−1.94	8
sd:	0.472	0.361	31.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.3	1.26	0.365	1.51	18
sd:	12.7	3.91	0.214	0.574	54.2

	CNST	HILL	GNLS
AIC:	241.62	236.76	236.15
PROB:	0.04	0.41	0.55
RMSE:	3.9	3.87	3.52

MAX_MEAN: 4.9 MAX_MED: 6.04 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

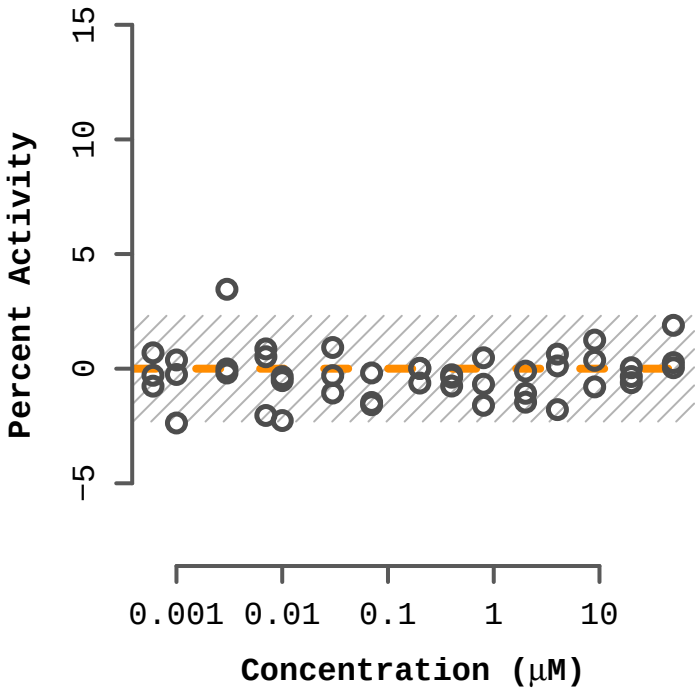
NAME: Vanitiolide
CHID: 46107 **CASRN:** 17692-71-6
SPID(S): Tox21_111762_1
M4ID: 12483496

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.928 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

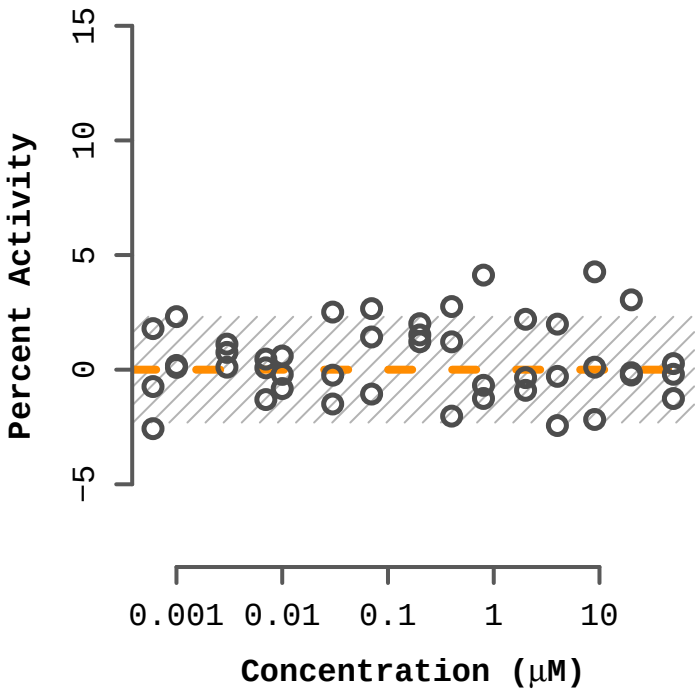
NAME: Acetylsalicylamide
CHID: 46108 **CASRN:** 5663-71-8
SPID(S): Tox21_111763_1
M4ID: 12483495

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

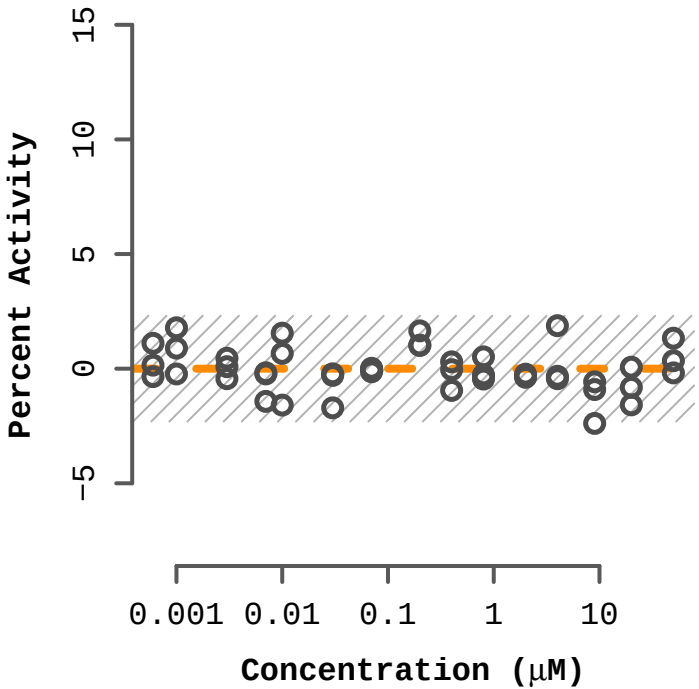
NAME: Bumecaine
CHID: 46109 **CASRN:** 30103-44-7
SPID(S): Tox21_111764_1
M4ID: 12483494

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

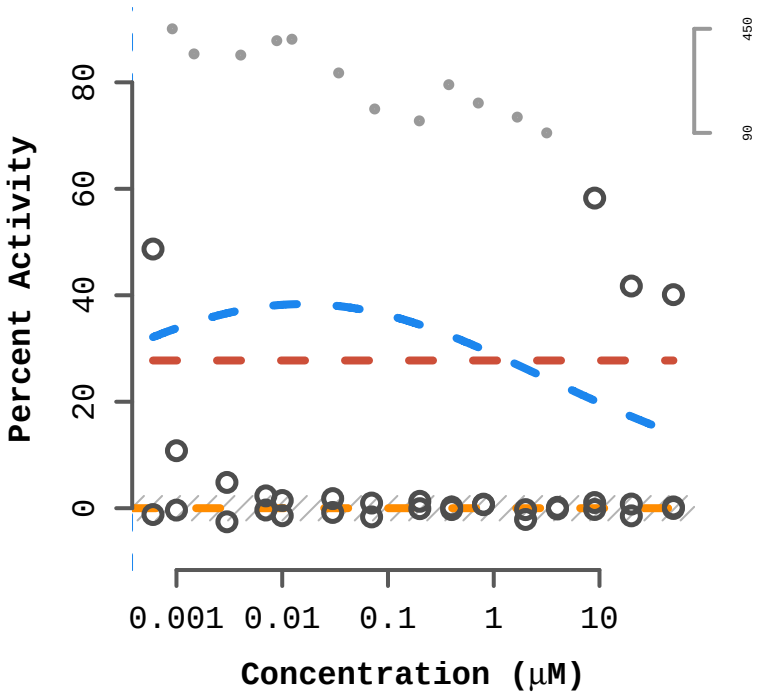
NAME: Benzylsulfamide
CHID: 46110 CASRN: 104-22-3
SPID(S): Tox21_111765_1
M4ID: 12483493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Crotoniazide
CHID: 46113 CASRN: 7007-96-7
SPID(S): Tox21_111768_1
M4ID: 12483491 BRK

HILL MODEL (in red):

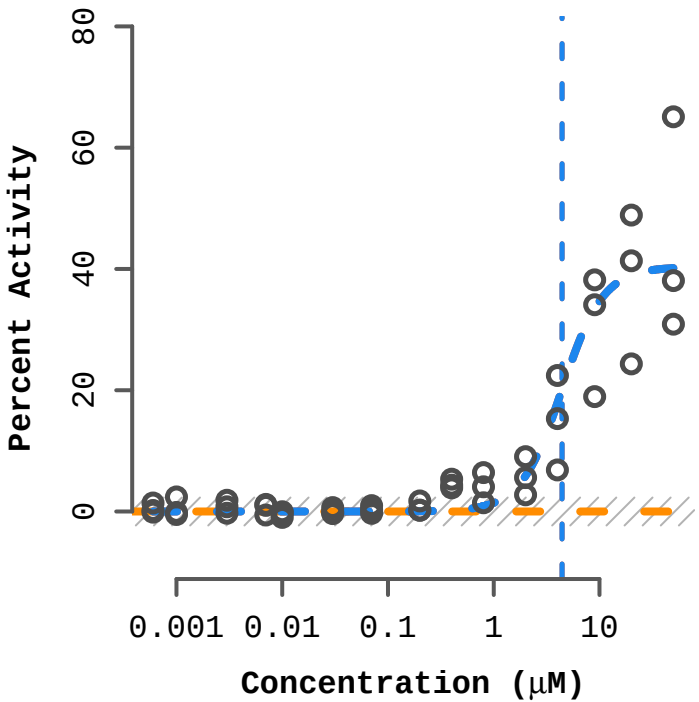
	tp	ga	gw
val:	27.7	-4.16	6.92
sd:	12.8	622	4580

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	67.1	-3.43	0.3	-0.166	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	583.37	564.24	567.93
PROB:	0	0.86	0.14
RMSE:	154.52	142.68	140.04

MAX_MEAN: 166 MAX_MED: 48.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dianiline
CHID: 46114 CASRN: 58338-59-3
SPID(S): Tox21_111769_1
M4ID: 12483490

HILL MODEL (in red):

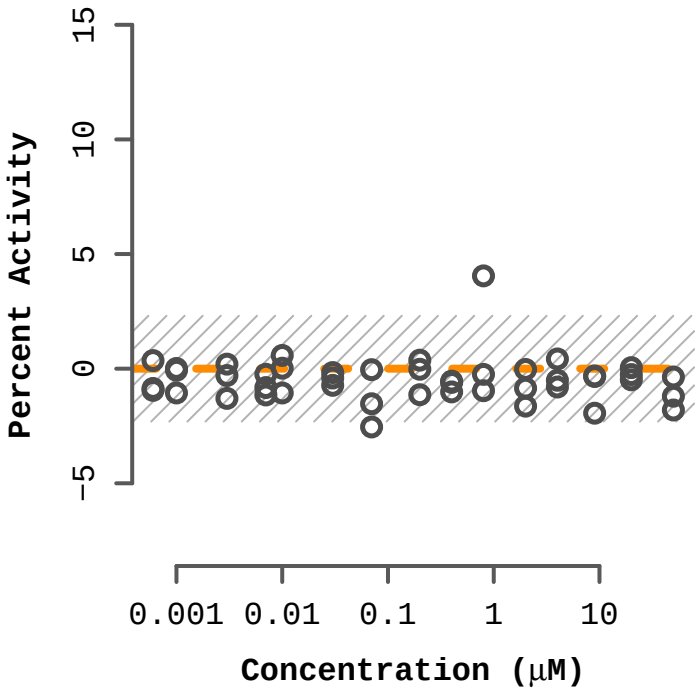
	tp	ga	gw
val:	40.3	0.646	2.22
sd:	2.81	0.0557	0.509

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	40.3	0.646	2.22	3.43	6.02
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	373.42	271.8	275.8
PROB:	0	0.88	0.12
RMSE:	18.48	5.87	5.87

MAX_MEAN: 44.7 MAX_MED: 41.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

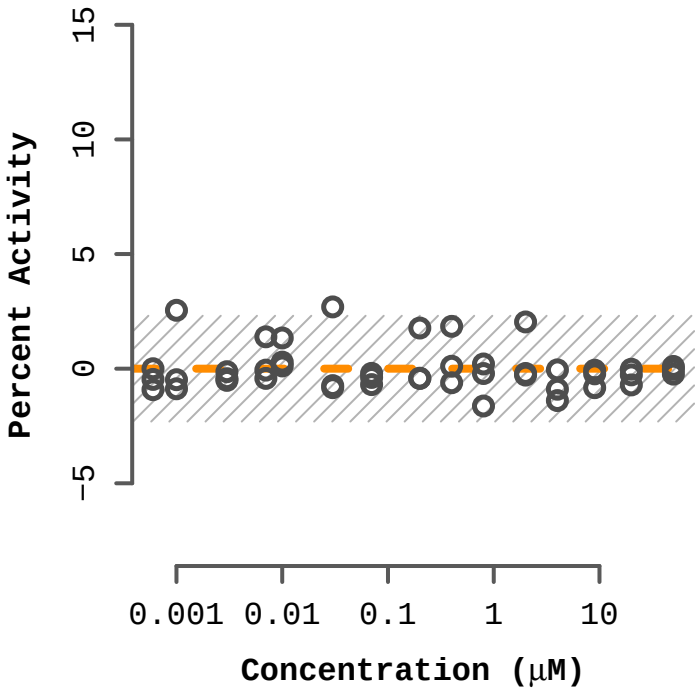
NAME: Metocinium iodide
CHID: 46117 **CASRN:** 2424-71-7
SPID(S): Tox21_111772_1
M4ID: 12483489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.947 **MAX_MED:** 0.022 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

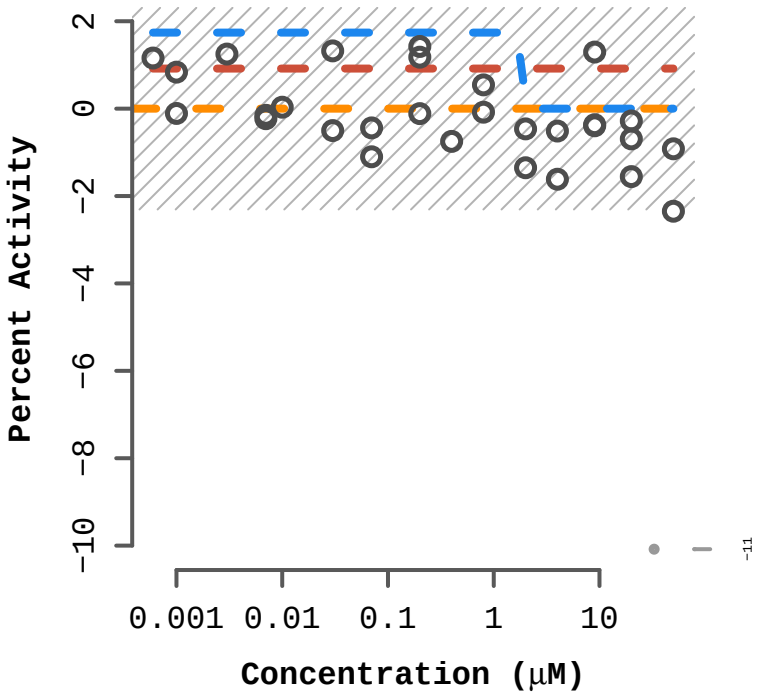
NAME: Pranolium chloride
CHID: 46119 CASRN: 42879-47-0
SPID(S): Tox21_111774_1
M4ID: 12483488

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.583 **MAX_MED:** 0.288 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluperlapine
CHID: 46123 **CASRN:** 67121-76-0
SPID(S): Tox21_111780_1
M4ID: 12483486 **BRK**

HILL MODEL (in red):

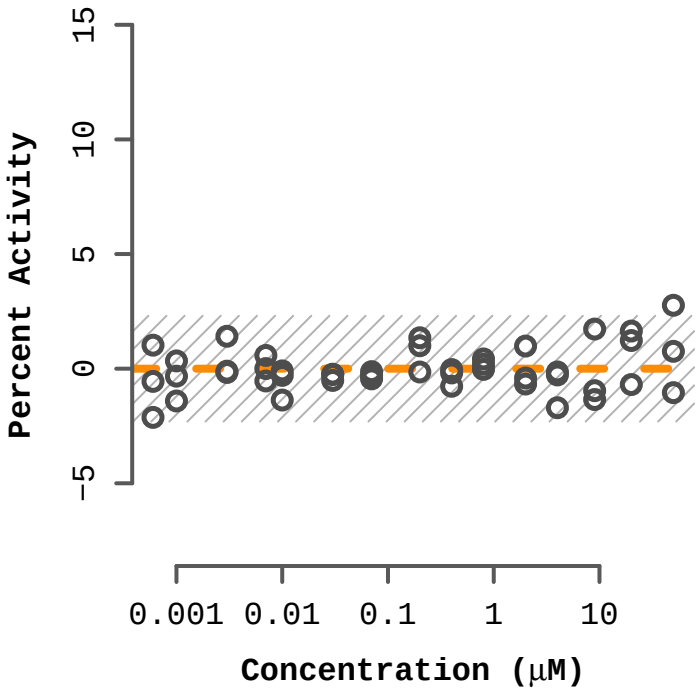
	tp	ga	gw
val:	0.917	−5.21	4.52
sd:	0.446	12000	27200

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.74	−5.18	4.1	0.266	17.9
sd:	0.564	4190	8790	34.9	17600

	CNST	HILL	GNLS
AIC:	249	250.45	247.98
PROB:	0.32	0.15	0.53
RMSE:	4.17	3.93	3.6

MAX_MEAN: 4.41 **MAX_MED:** 2.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

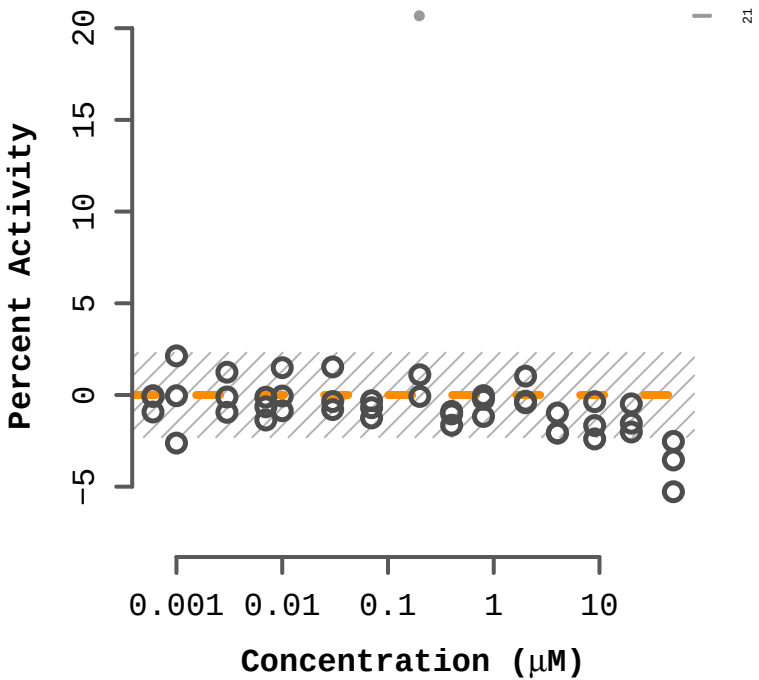
NAME: (S)−Mephenytoin
CHID: 46126 **CASRN:** 70989−04−7
SPID(S): Tox21_111783_1
M4ID: 12483485

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.827 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

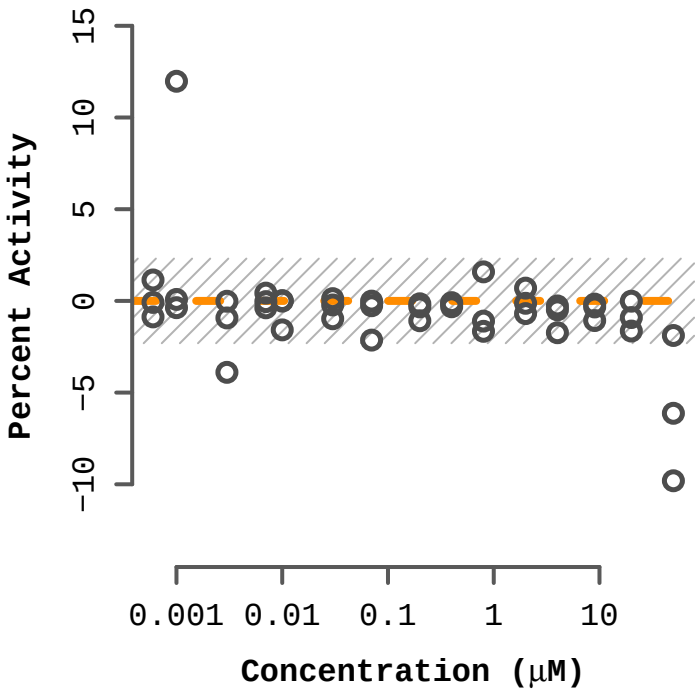
NAME: Pravadoline
CHID: 46127 **CASRN:** 92623-83-1
SPID(S): Tox21_111785_1
M4ID: 12483483 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.46	NA	NA

MAX_MEAN: 7.28 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

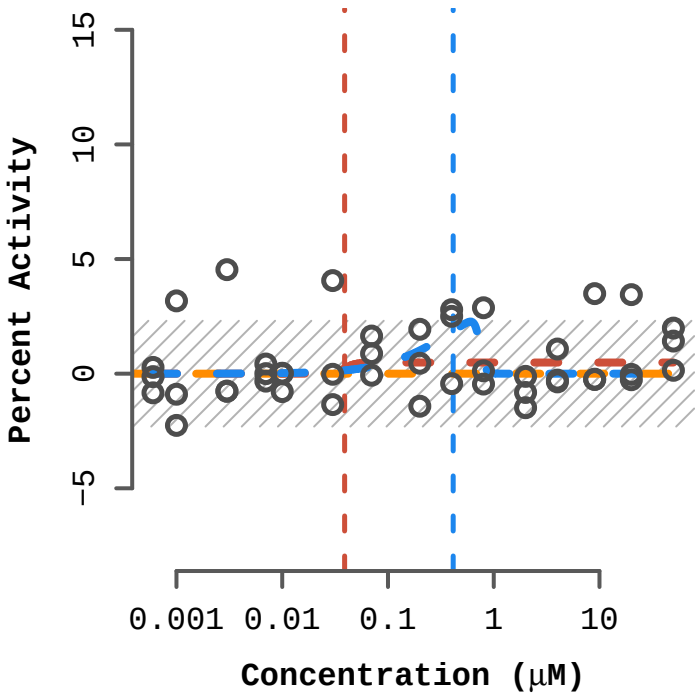
NAME: Nafamostat mesylate
CHID: 46128 **CASRN:** 82956-11-4
SPID(S): Tox21_111787_1
M4ID: 12483481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 3.9 **MAX_MED:** 0.082 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetridamine
CHID: 46130 **CASRN:** 17289-49-5
SPID(S): Tox21_111789_1
M4ID: 12483479

HILL MODEL (in red):

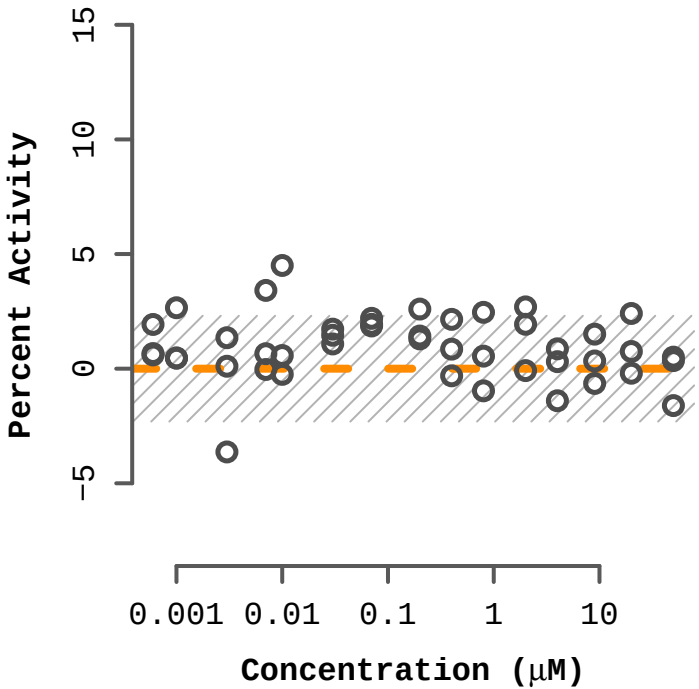
	tp	ga	gw
val:	0.485	−1.41	8
sd:	0.284	0.62	27.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.74	−0.384	1.36	−0.134	18
sd:	9.87	1.44	1.39	0.293	143

	CNST	HILL	GNLS
AIC:	172.01	174.92	177.2
PROB:	0.76	0.18	0.06
RMSE:	1.66	1.58	1.59

MAX_MEAN: 1.62 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

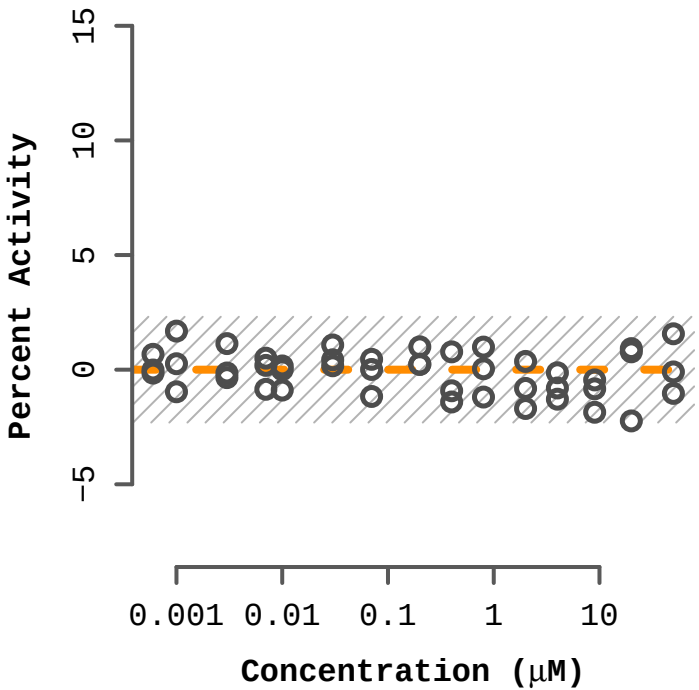
NAME: Iodoalphionic acid
CHID: 46131 **CASRN:** 577-91-3
SPID(S): Tox21_111790_1
M4ID: 12483478

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

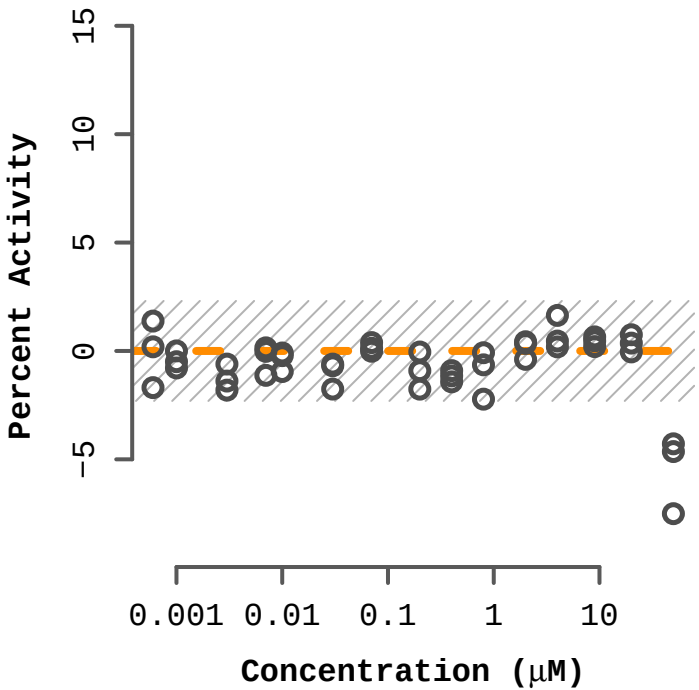
NAME: Risedronate sodium
CHID: 46132 **CASRN:** 115436-72-1
SPID(S): Tox21_111791_1
M4ID: 12483477

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.561 **MAX_MED:** 0.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

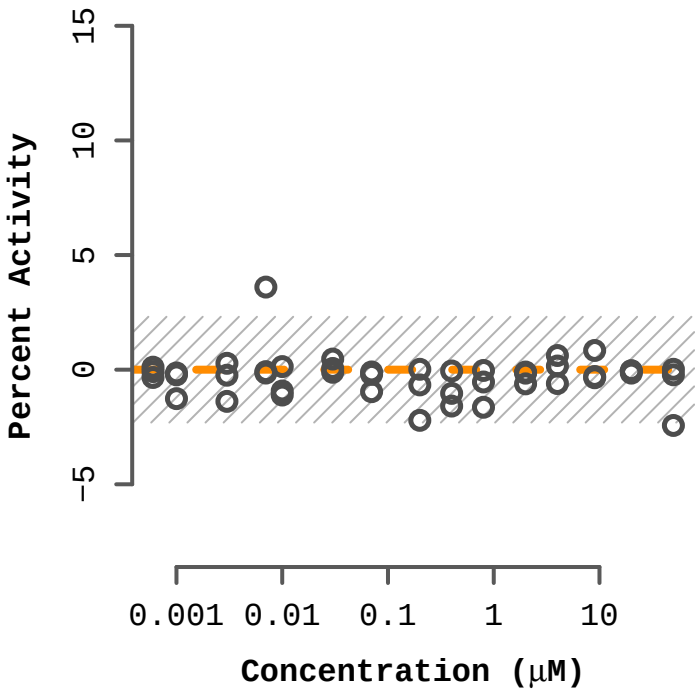
NAME: Benziodarone
CHID: 46134 **CASRN:** 68-90-6
SPID(S): Tox21_111793_1
M4ID: 12483476

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 0.763 **MAX_MED:** 0.468 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

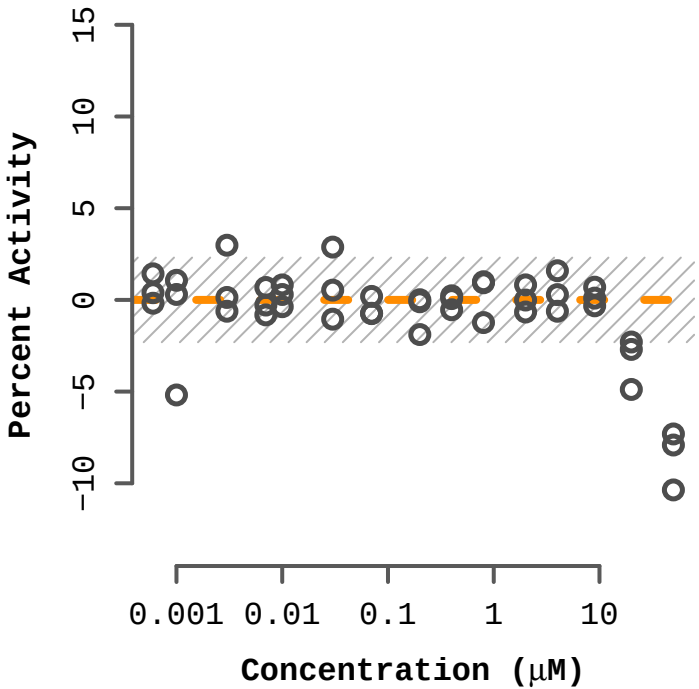
NAME: Loretin
CHID: 46136 **CASRN:** 547-91-1
SPID(S): Tox21_111795_1
M4ID: 12483475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.161 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

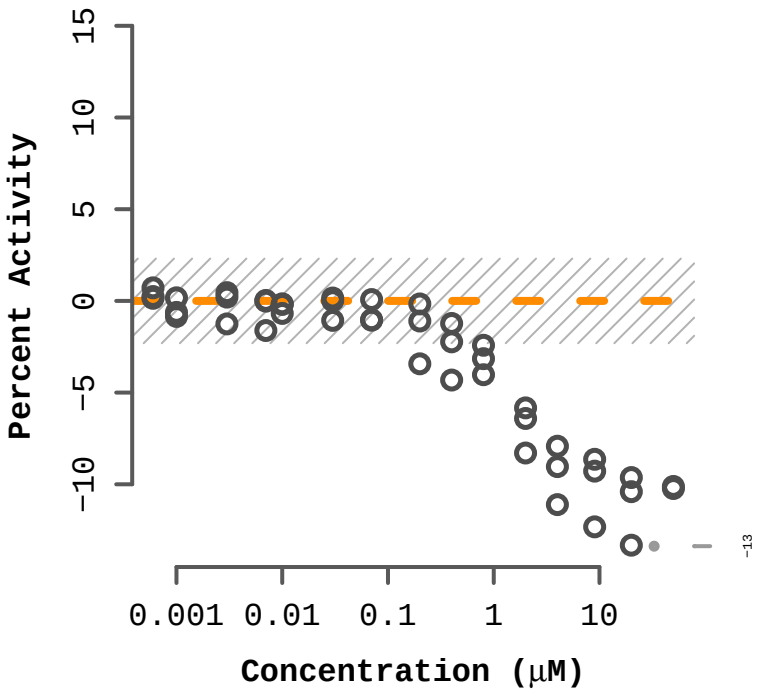
NAME: Indocate
CHID: 46137 **CASRN:** 31386-25-1
SPID(S): Tox21_111796_1
M4ID: 12483474

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.68	NA	NA

MAX_MEAN: 0.833 **MAX_MED:** 0.935 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

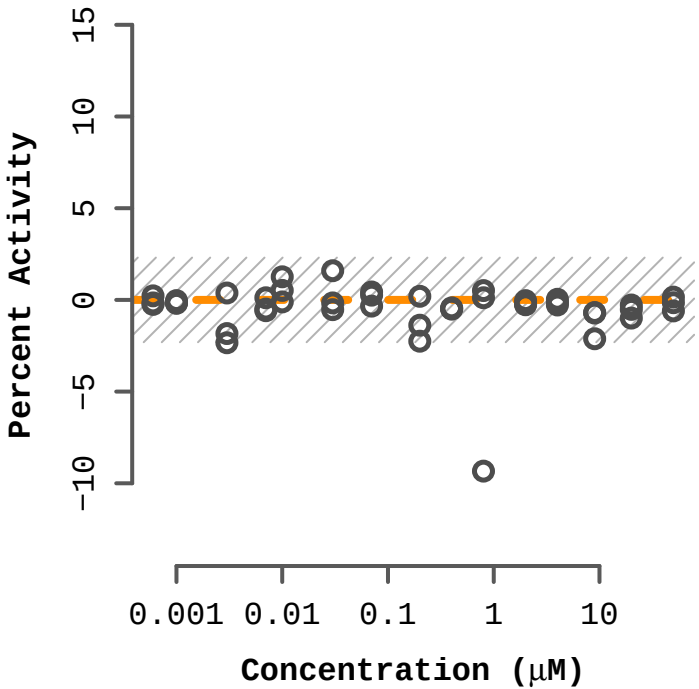
NAME: Chlormidazole
CHID: 46140 **CASRN:** 3689-76-7
SPID(S): Tox21_111799_1
M4ID: 12483473 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	288.23	NA	NA
PROB:	1	NA	NA
RMSE:	5.91	NA	NA

MAX_MEAN: 0.366 **MAX_MED:** 0.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

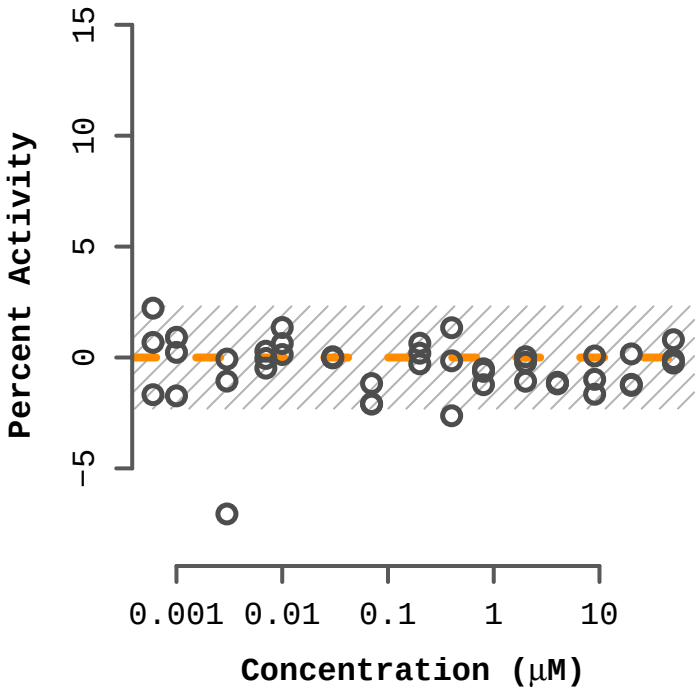
NAME: Pincainide
CHID: 46142 **CASRN:** 83471-41-4
SPID(S): Tox21_111801_1
M4ID: 12483472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 0.558 **MAX_MED:** 0.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

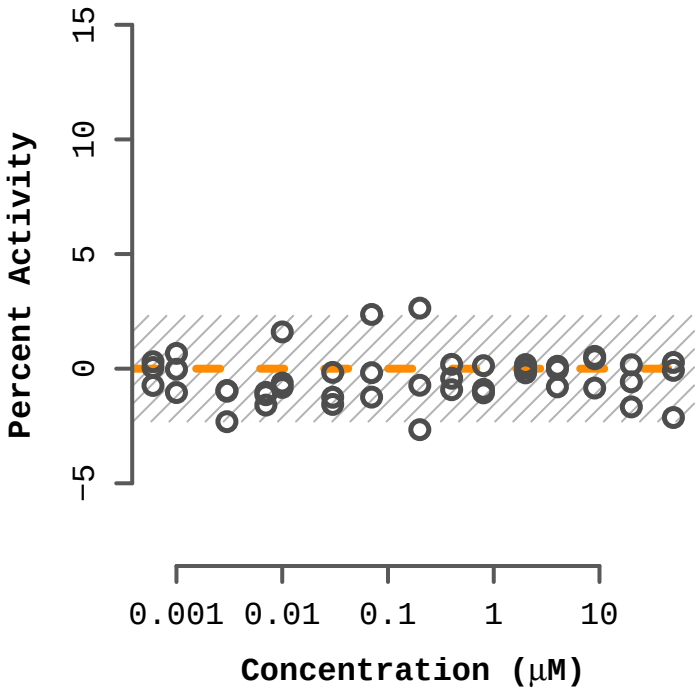
NAME: Clobenzorex hydrochloride
CHID: 46145 CASRN: 5843-53-8
SPID(S): Tox21_111806_1
M4ID: 12483469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 0.707 **MAX_MED:** 0.682 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

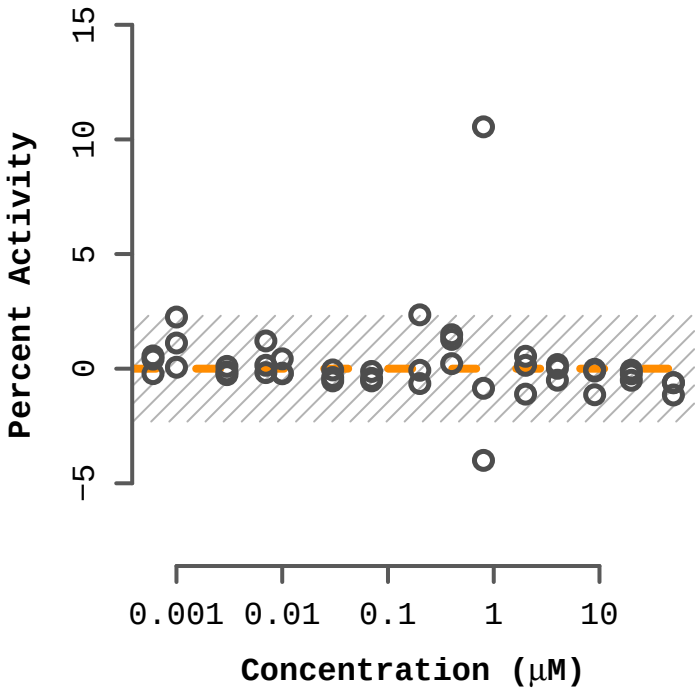
NAME: Esaprazole
CHID: 46147 CASRN: 64204-55-3
SPID(S): Tox21_111808_1
M4ID: 12483468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.318 **MAX_MED:** 0.434 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

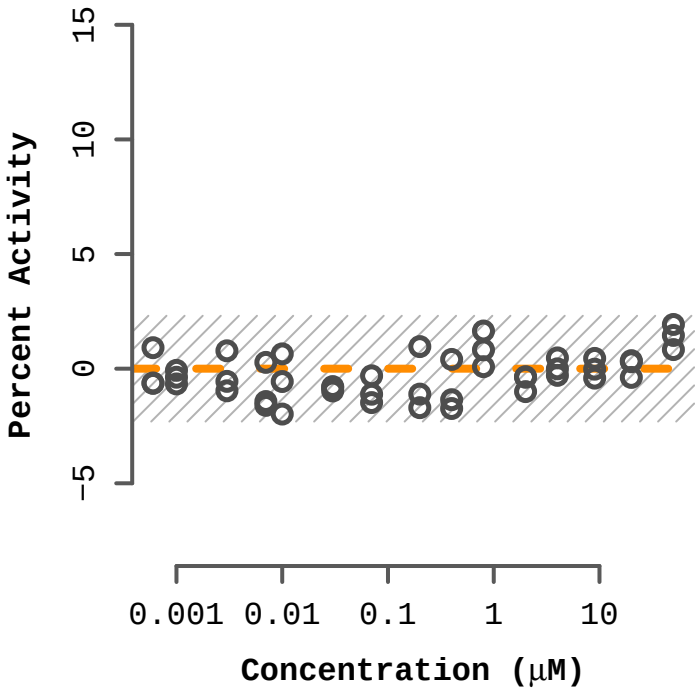
NAME: Riodipine
CHID: 46148 **CASRN:** 71653-63-9
SPID(S): Tox21_111809_1
M4ID: 12483467

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

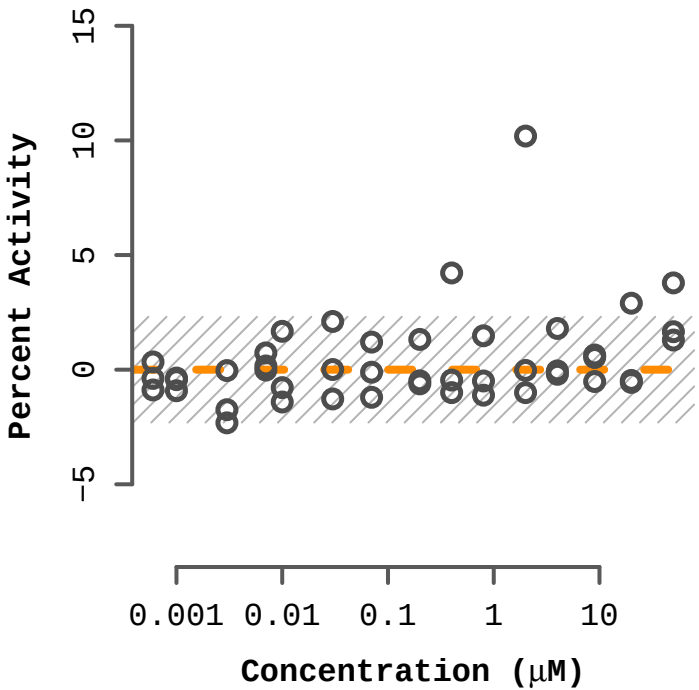
NAME: Pyrrocaine
CHID: 46150 **CASRN:** 2210-77-7
SPID(S): Tox21_111811_1
M4ID: 12483465

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

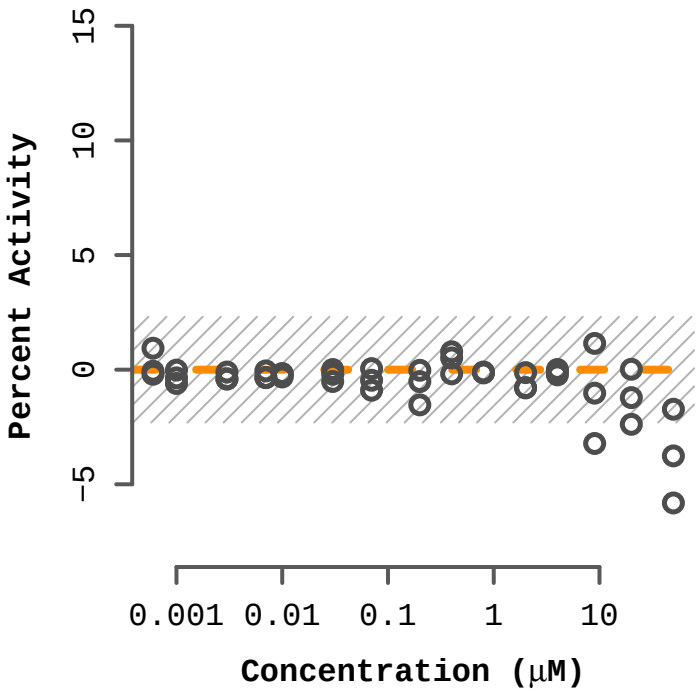
NAME: Lonazolac
CHID: 46151 CASRN: 53808-88-1
SPID(S): Tox21_111812_1
M4ID: 12483464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 3.05 MAX_MED: 1.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

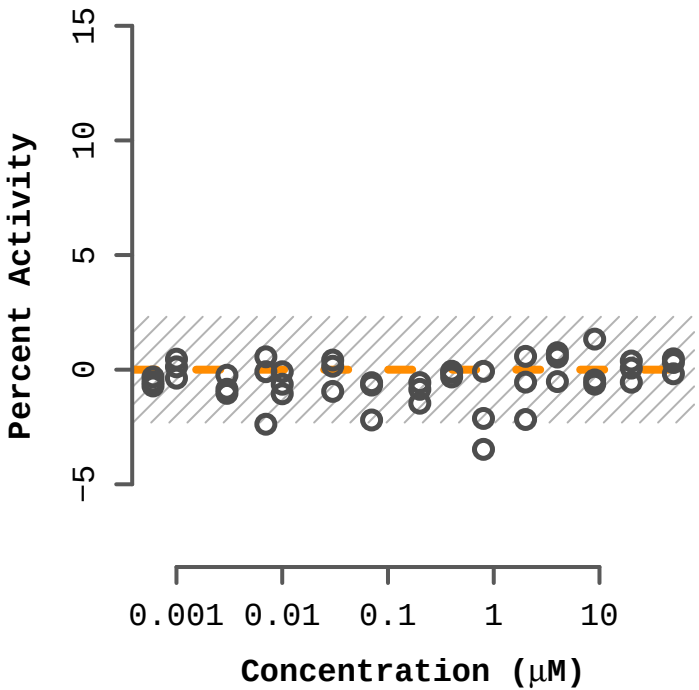
NAME: Metochalcone
CHID: 46152 **CASRN:** 18493-30-6
SPID(S): Tox21_111813_1
M4ID: 12483463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.372 **MAX_MED:** 0.515 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

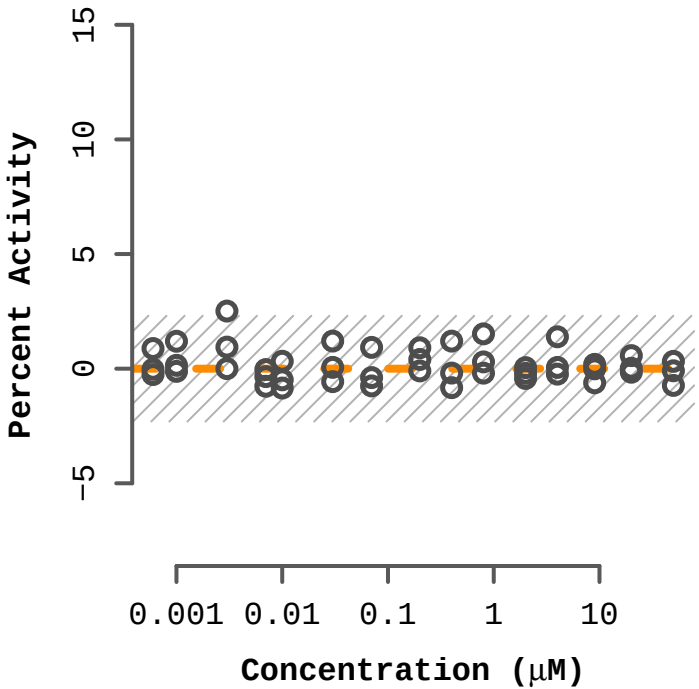
NAME: Clofenamide
CHID: 46153 **CASRN:** 671-95-4
SPID(S): Tox21_111814_1
M4ID: 12483462

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.259 **MAX_MED:** 0.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

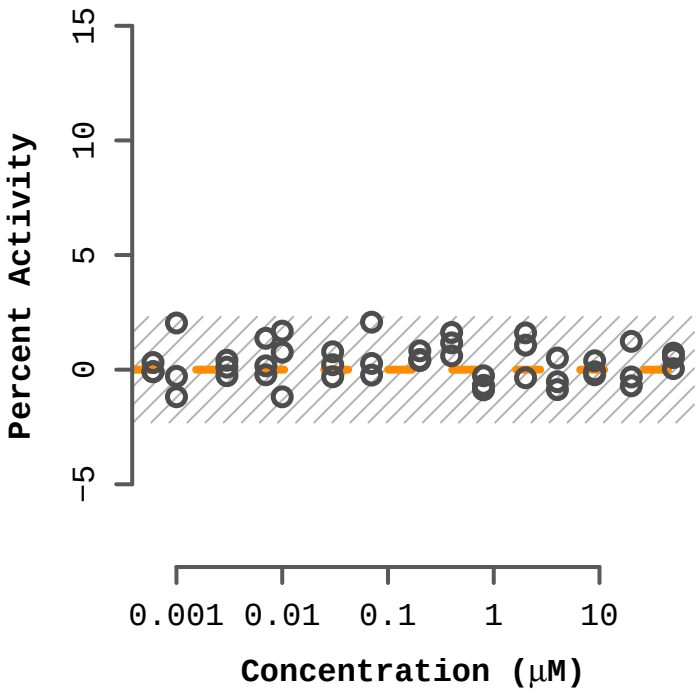
NAME: Fenclozic acid
CHID: 46157 **CASRN:** 17969-20-9
SPID(S): Tox21_111819_1
M4ID: 12483460

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.942 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

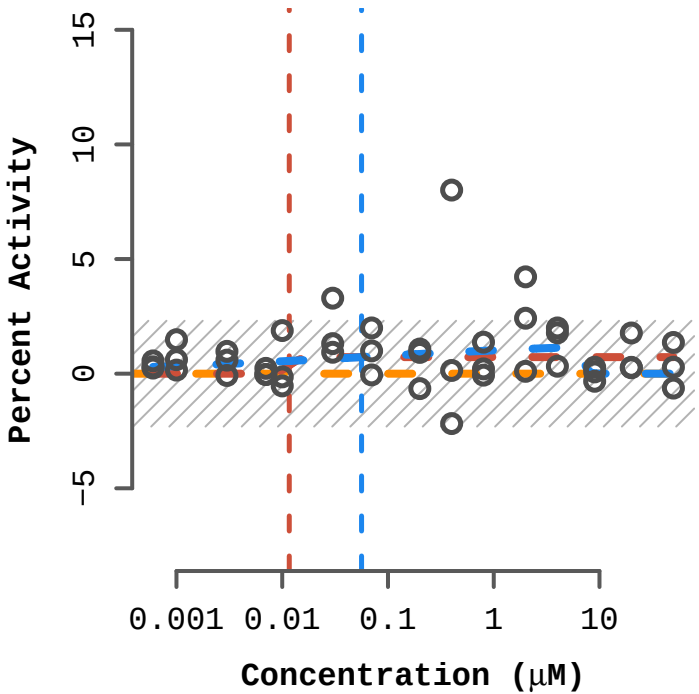
NAME: Clopirac
CHID: 46158 CASRN: 42779-82-8
SPID(S): Tox21_111822_1
M4ID: 12483457

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.13 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Morphazinamide
CHID: 46159 **CASRN:** 952-54-5
SPID(S): Tox21_111823_1
M4ID: 12483456

HILL MODEL (in red):

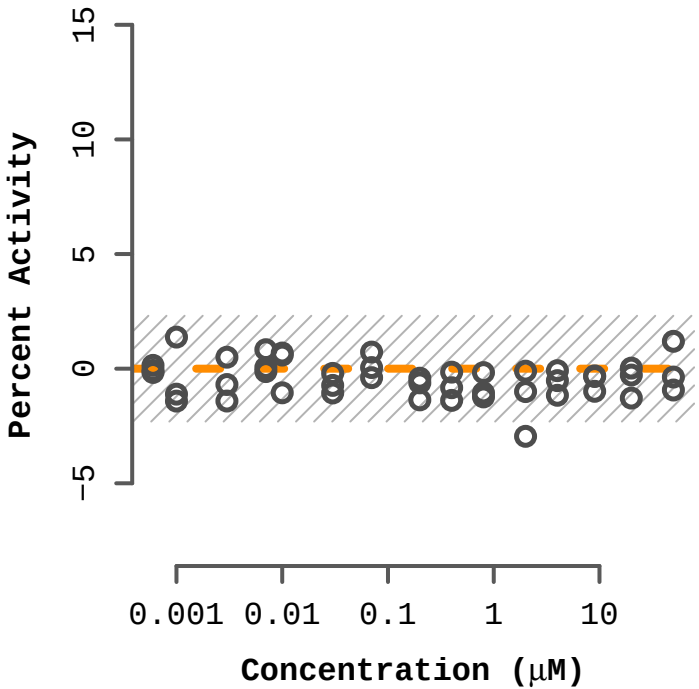
	tp	ga	gw
val:	0.722	−1.93	8
sd:	0.202	0.343	34.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.45	−1.25	0.3	0.847	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	160.71	154.24	155.33
PROB:	0.02	0.62	0.36
RMSE:	1.74	1.54	1.5

MAX_MEAN: 2.25 **MAX_MED:** 2.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

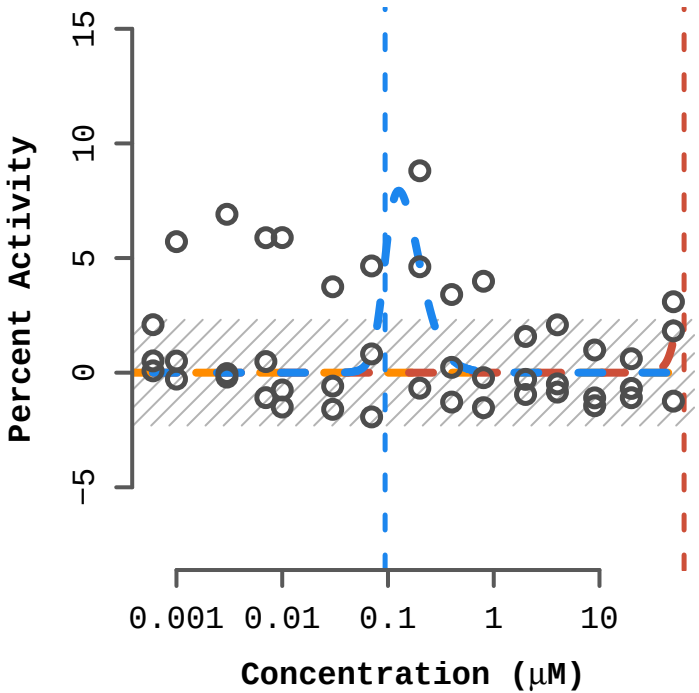
NAME: 2-Iodohippuric acid
CHID: 46161 **CASRN:** 147-58-0
SPID(S): Tox21_111826_1
M4ID: 12483455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.252 **MAX_MED:** 0.595 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pivagabine
CHID: 46162 CASRN: 69542-93-4
SPID(S): Tox21_111827_1
M4ID: 12483454

HILL MODEL (in red):

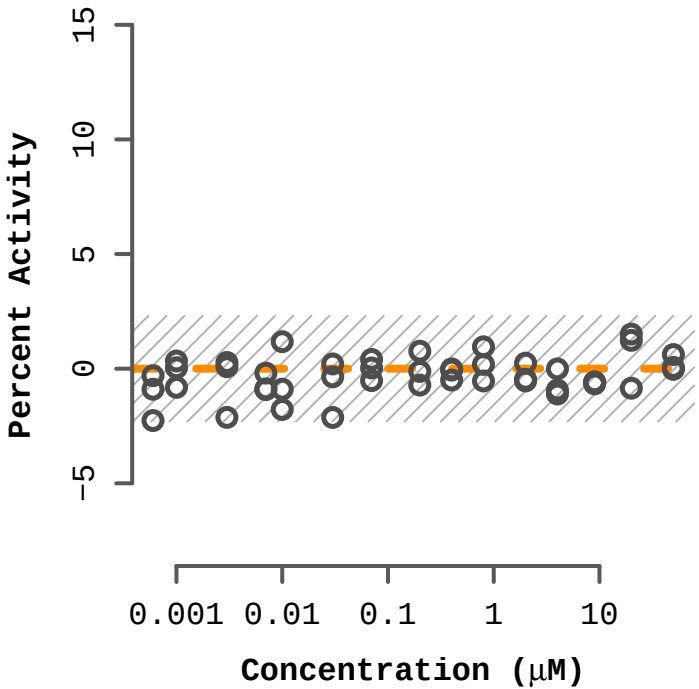
	tp	ga	gw
val:	10.6	1.8	7.98
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.6	−1.03	8	−0.723	3.77
sd:	113	2.89	178	2.31	12.6

	CNST	HILL	GNLS
AIC:	217.6	222.48	222.49
PROB:	0.85	0.07	0.07
RMSE:	2.84	2.82	2.6

MAX_MEAN: 4.25 MAX_MED: 4.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

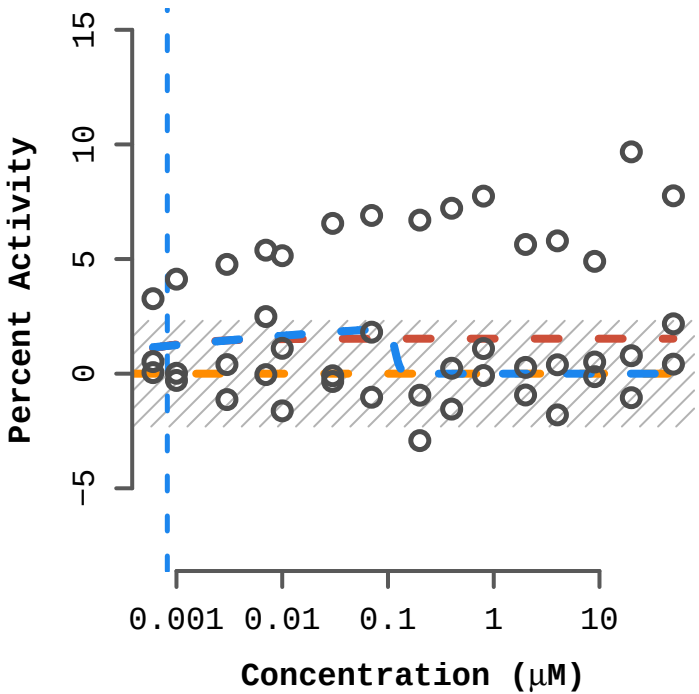
NAME: Lozilurea
CHID: 46163 **CASRN:** 71475-35-9
SPID(S): Tox21_111828_1
M4ID: 12483453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.633 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norletimol
CHID: 46174 **CASRN:** 886-08-8
SPID(S): Tox21_111839_1
M4ID: 12483452

HILL MODEL (in red):

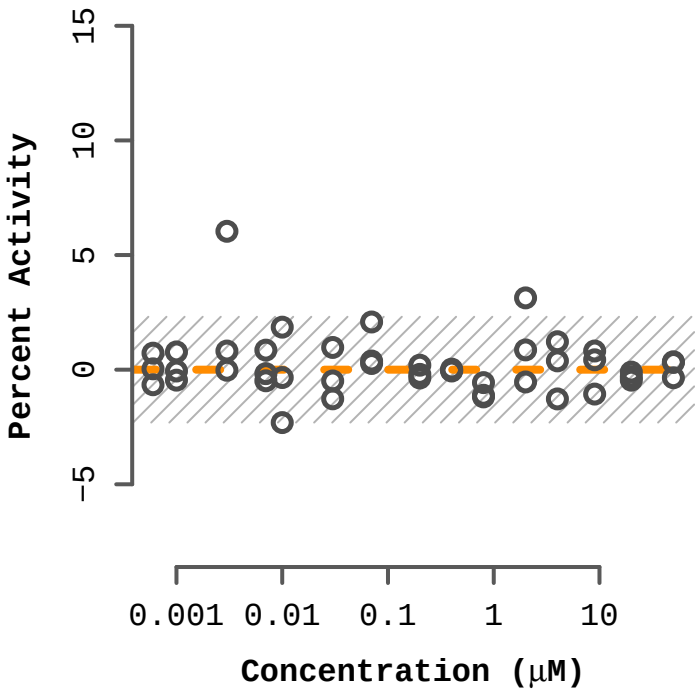
	tp	ga	gw
val:	1.53	−3.57	1.22
sd:	0.593	2.71	5.89

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.42	−3.09	0.306	−0.932	17.5
sd:	13.7	15.4	3.35	4.69	359

	CNST	HILL	GNLS
AIC:	247.59	244.39	252.42
PROB:	0.17	0.82	0.01
RMSE:	3.76	3.22	3.55

MAX_MEAN: 3.45 **MAX_MED:** 2.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

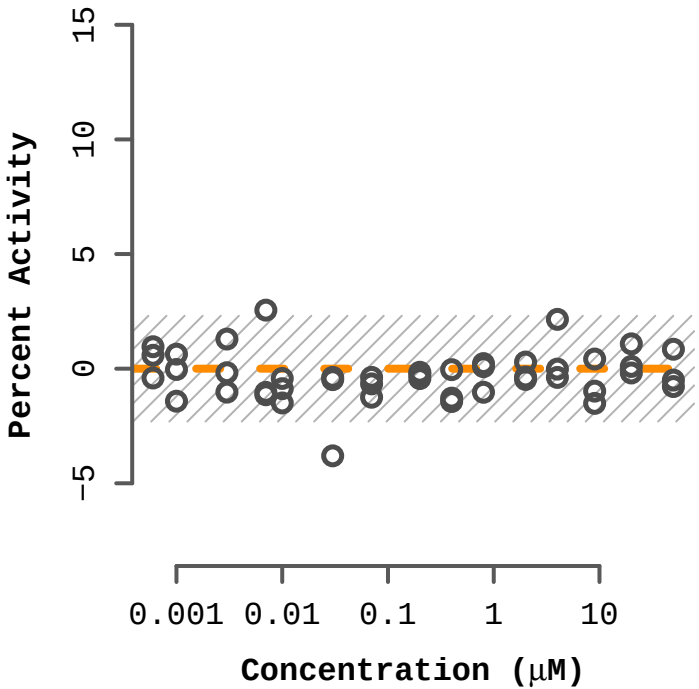
NAME: Ftorpropazine
CHID: 46176 **CASRN:** 33414-36-7
SPID(S): Tox21_111841_1
M4ID: 12483451

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 0.864 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

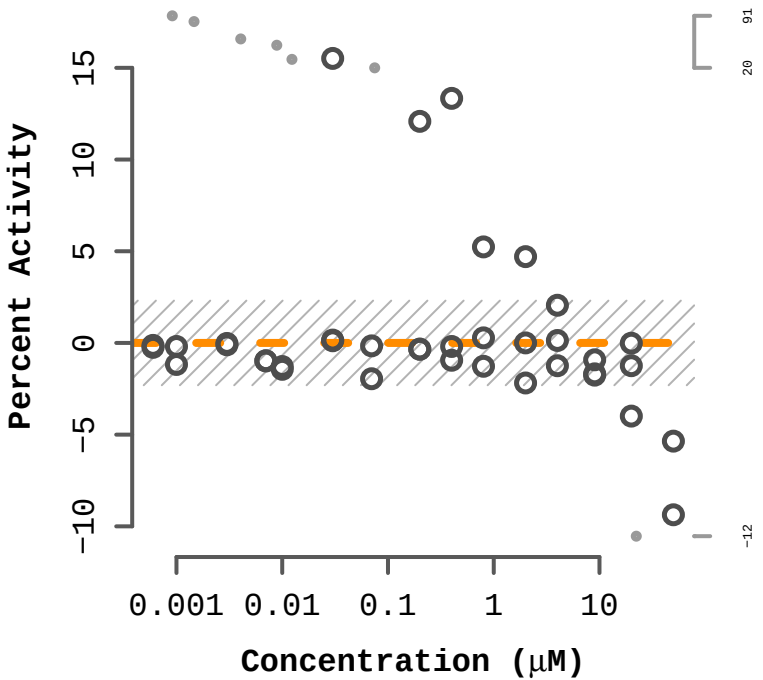
NAME: Sulfalene
CHID: 46179 CASRN: 152-47-6
SPID(S): Tox21_111844_1
M4ID: 12483450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.585 **MAX_MED:** 0.585 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

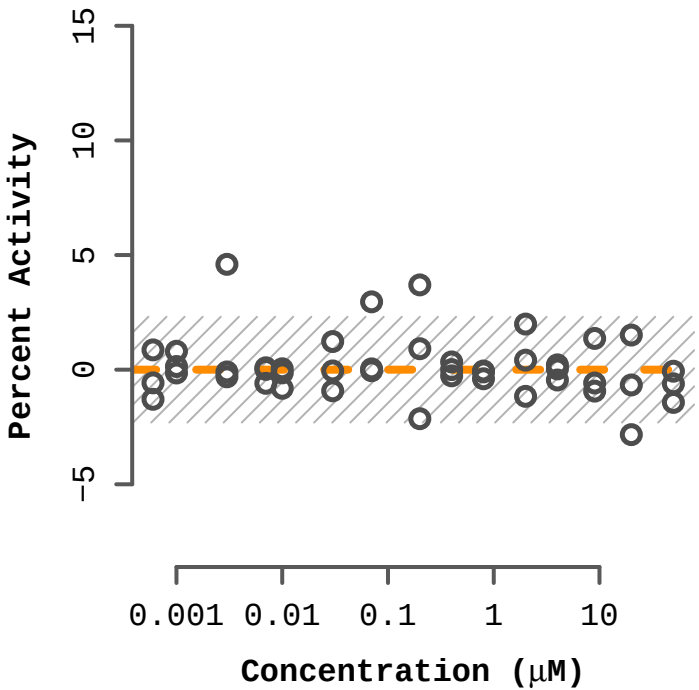
NAME: Ftormetazine
CHID: 46180 **CASRN:** 33414-30-1
SPID(S): Tox21_111845_1
M4ID: 12483449 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	362.14	NA	NA
PROB:	1	NA	NA
RMSE:	23	NA	NA

MAX_MEAN: 30.3 **MAX_MED:** 0.279 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

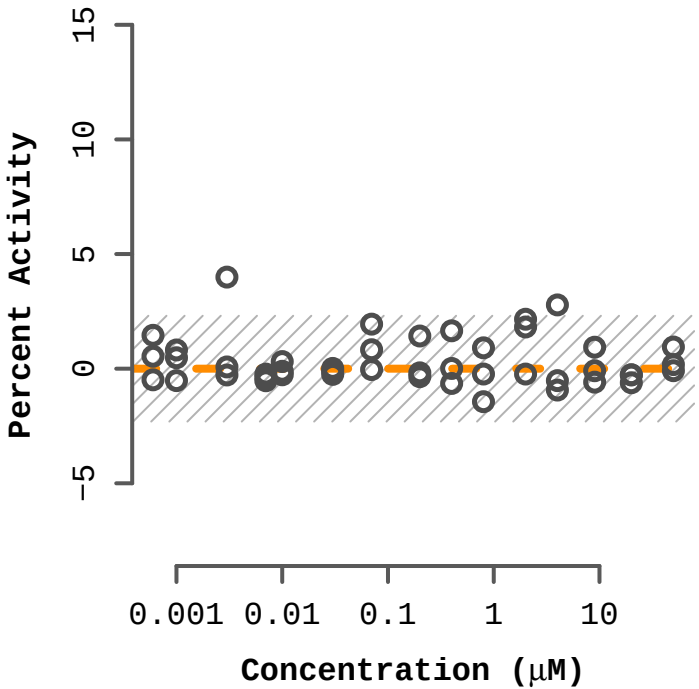
NAME: Etafenone
CHID: 46181 **CASRN:** 90-54-0
SPID(S): Tox21_111846_1
M4ID: 12483448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.916 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

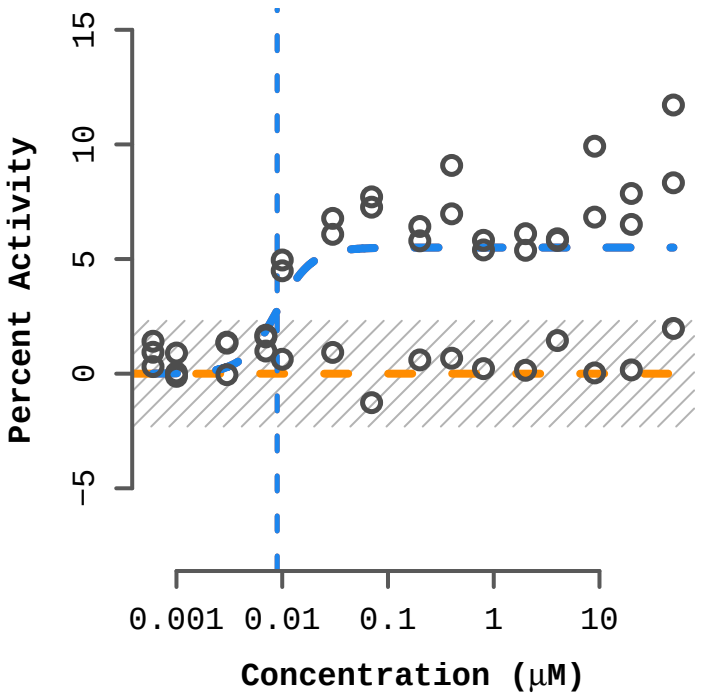
NAME: Fosenazide
CHID: 46188 CASRN: 16543-10-5
SPID(S): Tox21_111853_1
M4ID: 12483447

HILL MODEL: Not applicable.

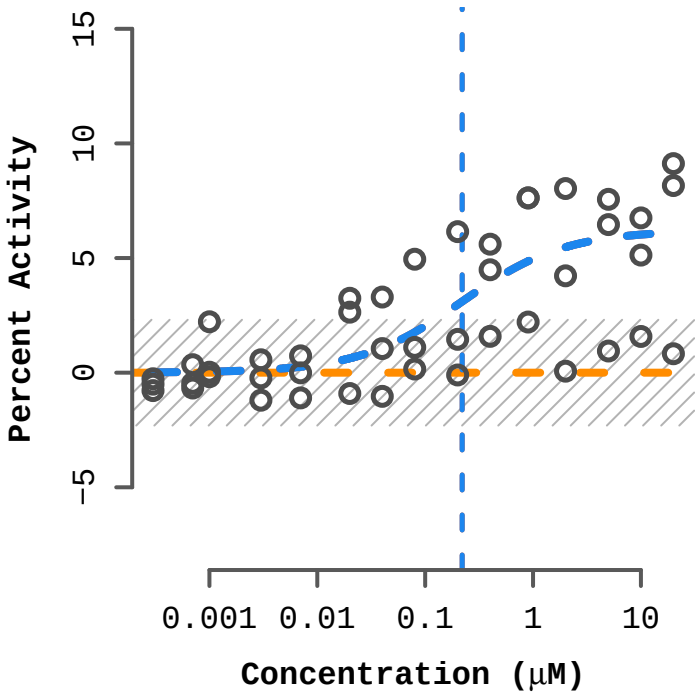
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

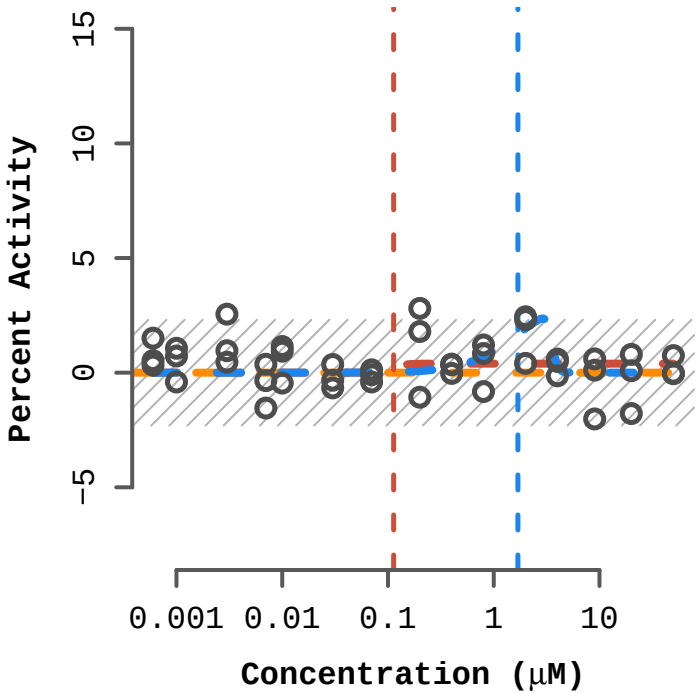
MAX_MEAN: 1.27 **MAX_MED:** 1.82 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Amanozine
CHID:    46190   CASRN: 537-17-7
SPID(S): Tox21_111855_1
M4ID:    12483446

HILL MODEL (in red):
      tp       ga       gw
val:  5.5      -2.05    2.64
sd:   0.61     0.14     6.51

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.5      -2.05    2.64     3.17     7.6
sd:   0.61     0.14     6.51     47100    244000

      CNST        HILL        GNLS
AIC:  277.75      231.59      235.59
PROB: 0           0.88        0.12
RMSE: 5           2.89        2.89

MAX_MEAN: 7.34      MAX_MED: 8.33      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dicarbine
CHID:    46193   CASRN: 17411-19-7
SPID(S): Tox21_111858_1
M4ID:    12483445

HILL MODEL (in red):
      tp       ga       gw
val:  6.21     -0.657   0.911
sd:   1.19     0.349    0.517

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.21     -0.657   0.911    3.05     7.03
sd:   1.19     0.349    0.517    208000   810000

      CNST        HILL        GNLS
AIC:  251.36      210.27      214.27
PROB: 0           0.88        0.12
RMSE: 3.92        2.24        2.24

MAX_MEAN: 6.04      MAX_MED: 8.16      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tritiozine
CHID: 46195 **CASRN:** 35619-65-9
SPID(S): Tox21_111860_1
M4ID: 12483444

HILL MODEL (in red):

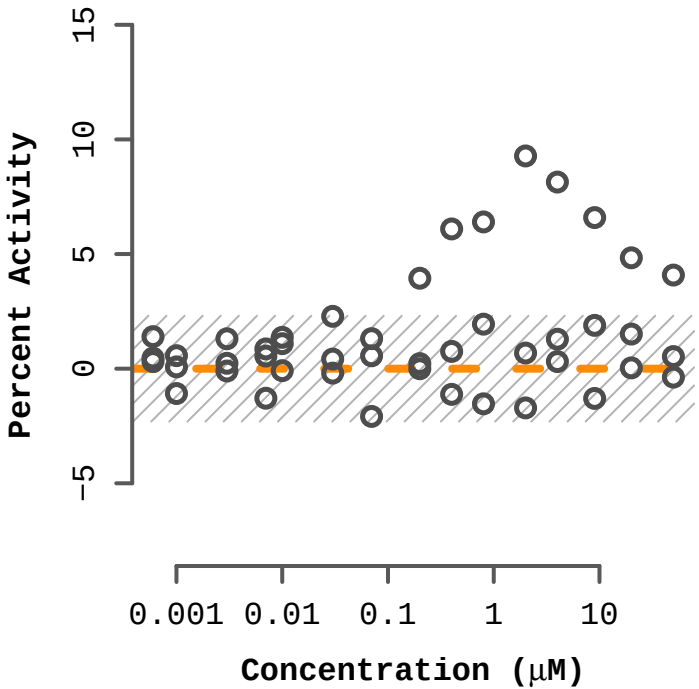
	tp	ga	gw
val:	0.393	−0.946	8
sd:	0.195	0.507	17.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.37	0.229	1.78	0.551	17.2
sd:	5.33	0.825	1.89	1.17	394

	CNST	HILL	GNLS
AIC:	137.35	139.46	137.42
PROB:	0.43	0.15	0.42
RMSE:	1.1	1.06	0.99

MAX_MEAN: 1.72 **MAX_MED:** 2.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

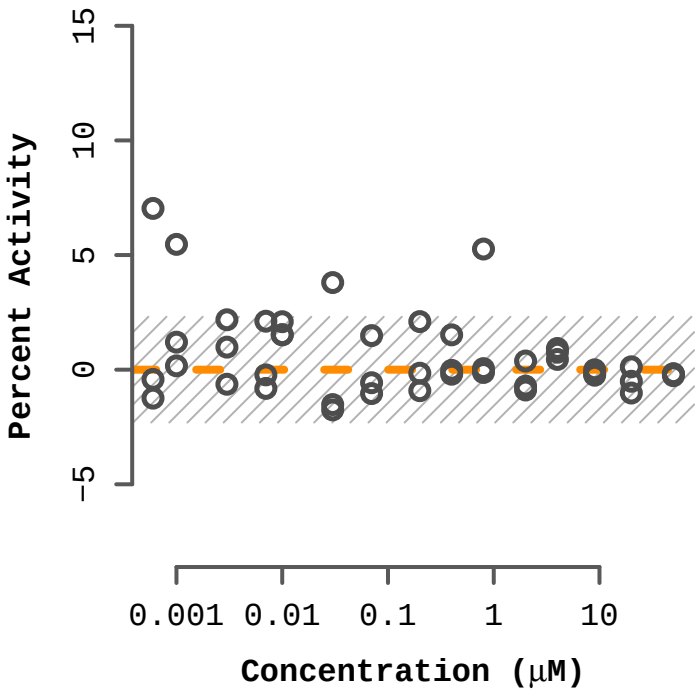
NAME: Isosorbide
CHID: 46196 CASRN: 652-67-5
SPID(S): Tox21_111861_1
M4ID: 12483443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.31	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 3.25 MAX_MED: 1.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

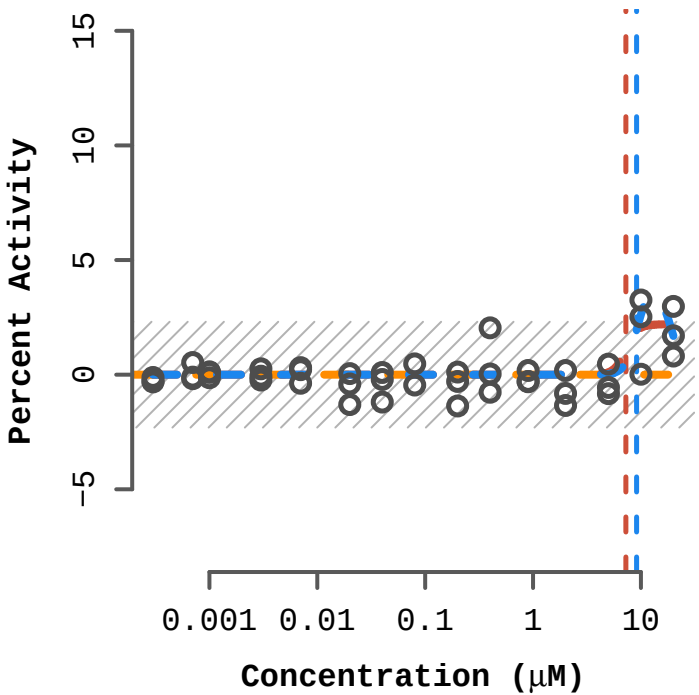
NAME: Diaveridine
CHID: 46200 CASRN: 5355-16-8
SPID(S): Tox21_111866_1
M4ID: 12483441

HILL MODEL: Not applicable.

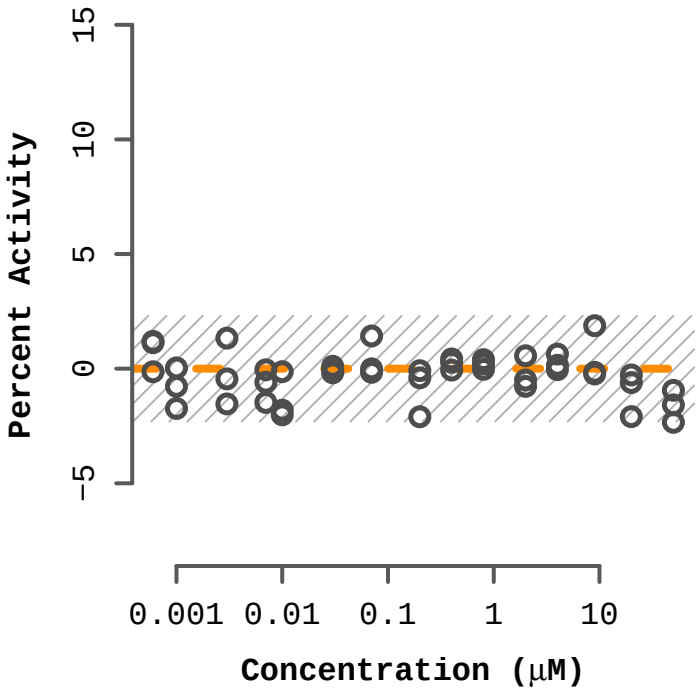
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 2.28 MAX_MED: 1.53 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Orbifloxacin
CHID:    46201   CASRN: 113617-63-3
SPID(S): Tox21_111867_1
M4ID:    12483440

HILL MODEL (in red):
      tp       ga       gw
val:  2.2      0.86     8
sd:   0.5      0.0704   3.75

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.91     0.96     8        1.28     6.99
sd:   4.3      0.172    5.86     0.129    25.8

      CNST        HILL        GNLS
AIC:  115.74      103.23      104.22
PROB: 0           0.62        0.38
RMSE: 1.01        0.74        0.75

MAX_MEAN: 1.93      MAX_MED: 2.53      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

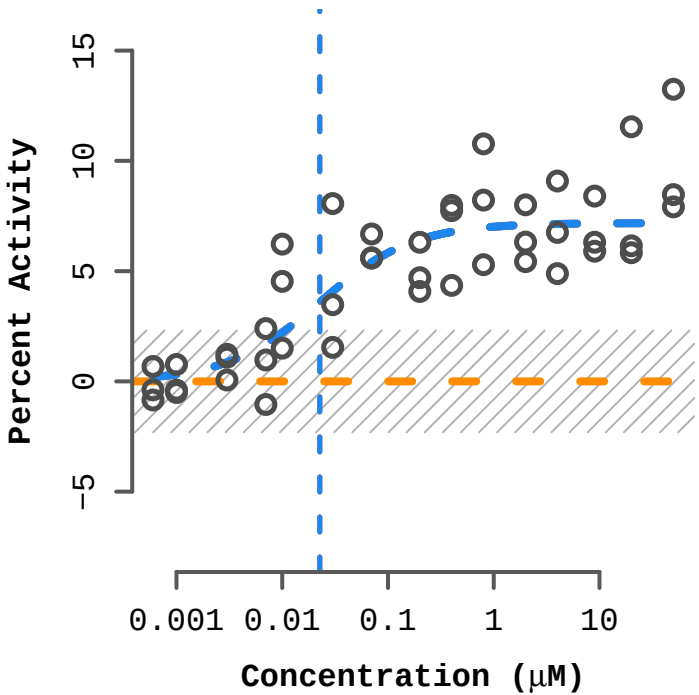
NAME: Mosapride citrate
CHID: 46207 CASRN: 112885-42-4
SPID(S): Tox21_111874_1
M4ID: 12483438

HILL MODEL: Not applicable.

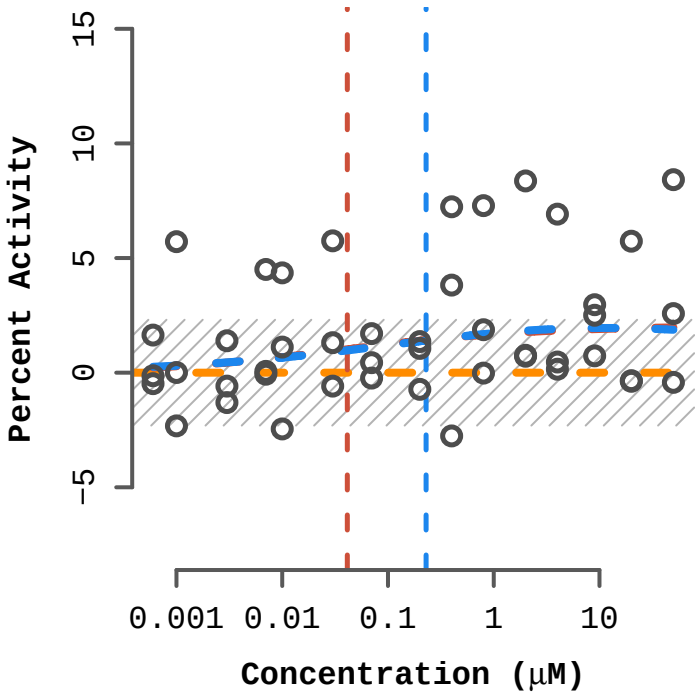
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.731 **MAX_MED:** 1.13 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ethiazide
CHID:    46215   CASRN: 1824-58-4
SPID(S): Tox21_111883_1
M4ID:    12483436

HILL MODEL (in red):
      tp       ga       gw
val:  7.18     -1.64    0.985
sd:   0.5      0.195    0.303

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.18     -1.64    0.985    3.55     6.35
sd:   0.5      0.195    0.303    51000    175000

      CNST        HILL        GNLS
AIC:  297.4       194.19      198.19
PROB: 0           0.88        0.12
RMSE: 6.04        1.96        1.96

MAX_MEAN: 9.88      MAX_MED: 8.47      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Romazarit
CHID: 46216 **CASRN:** 109543-76-2
SPID(S): Tox21_111884_1
M4ID: 12483435

HILL MODEL (in red):

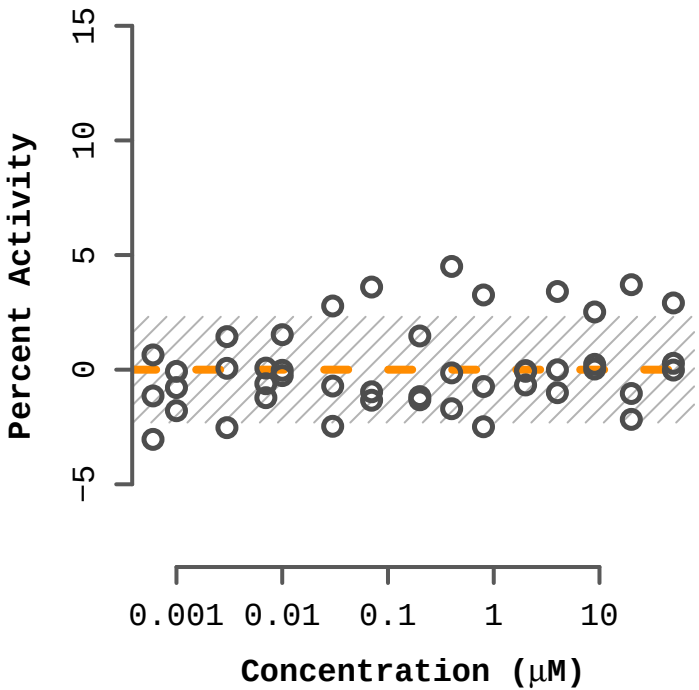
	tp	ga	gw
val:	2.03	−1.38	0.492
sd:	1.25	1.81	0.742

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.07	−0.64	0.4	2.8	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	234.97	229.25	233.27
PROB:	0.05	0.84	0.11
RMSE:	3.37	2.82	2.82

MAX_MEAN: 3.53 **MAX_MED:** 3.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

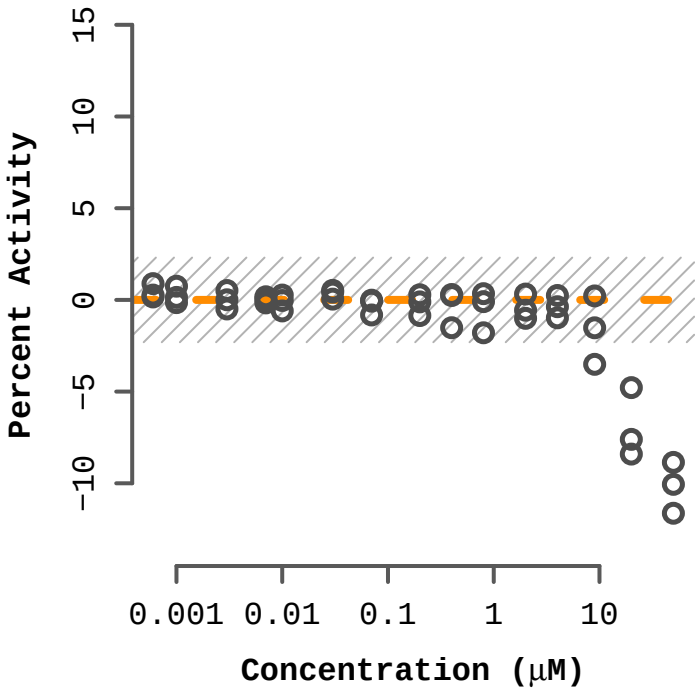
NAME: Haloxon
CHID: 46221 **CASRN:** 321-55-1
SPID(S): Tox21_111889_1
M4ID: 12483433

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.278 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

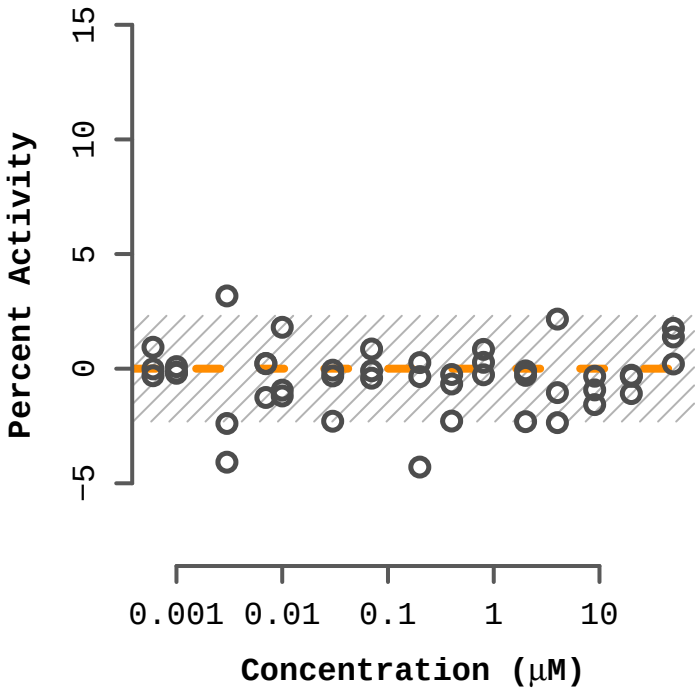
NAME: Fomocaine
CHID: 46222 **CASRN:** 17692-39-6
SPID(S): Tox21_111890_1
M4ID: 12483432

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.39	NA	NA
PROB:	1	NA	NA
RMSE:	3.31	NA	NA

MAX_MEAN: 0.439 **MAX_MED:** 0.426 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

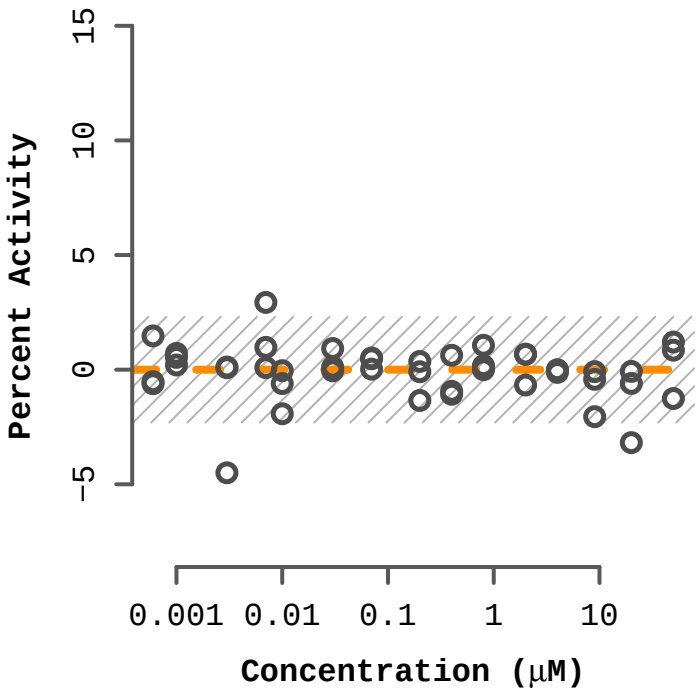
NAME: Bithionoloxide
CHID: 46225 **CASRN:** 844-26-8
SPID(S): Tox21_111894_1
M4ID: 12483430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

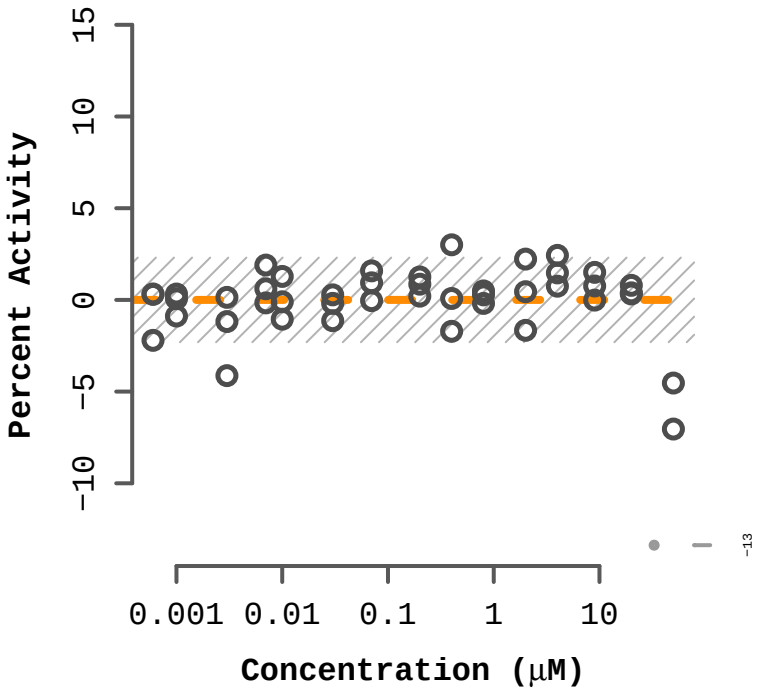
NAME: Nifursol
CHID: 46226 CASRN: 16915-70-1
SPID(S): Tox21_111895_1
M4ID: 12483429

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.975 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

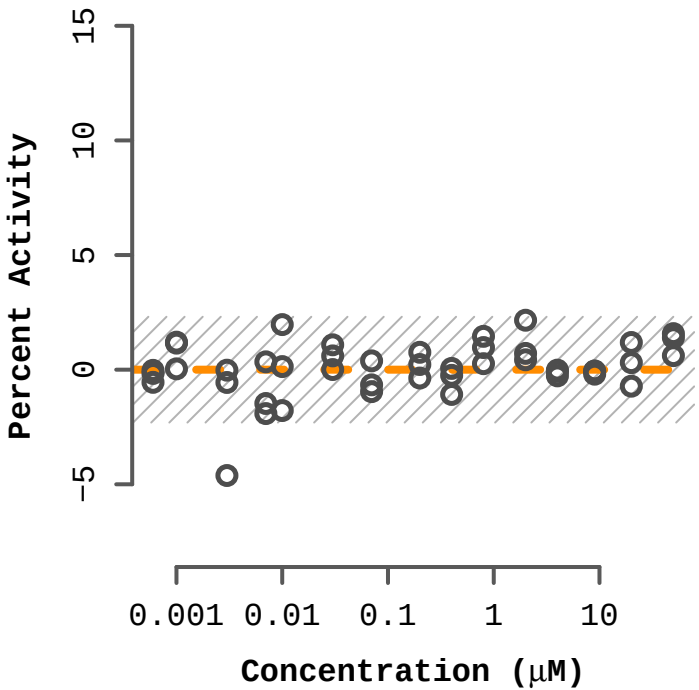
NAME: Rafoxanide
CHID: 46227 **CASRN:** 22662-39-1
SPID(S): Tox21_111896_1
M4ID: 12483428 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.99	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

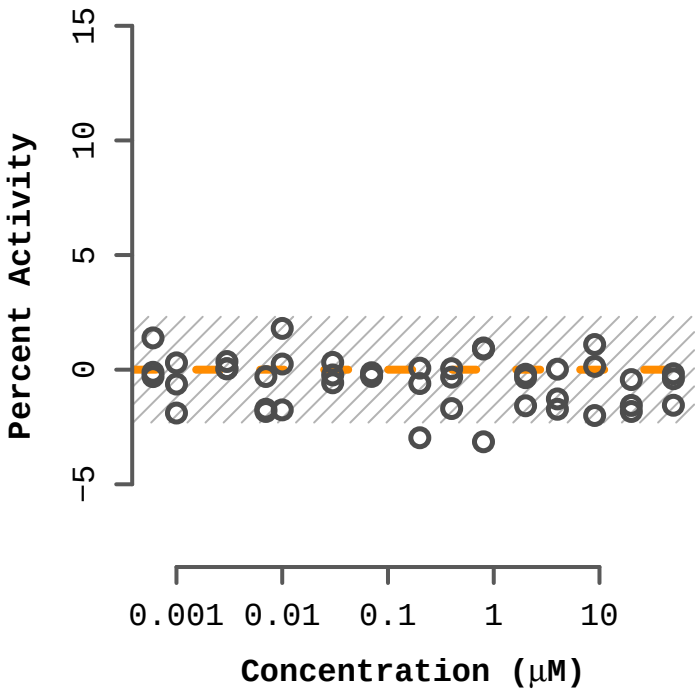
NAME: Diamfenetide
CHID: 46229 **CASRN:** 36141-82-9
SPID(S): Tox21_111898_1
M4ID: 12483427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

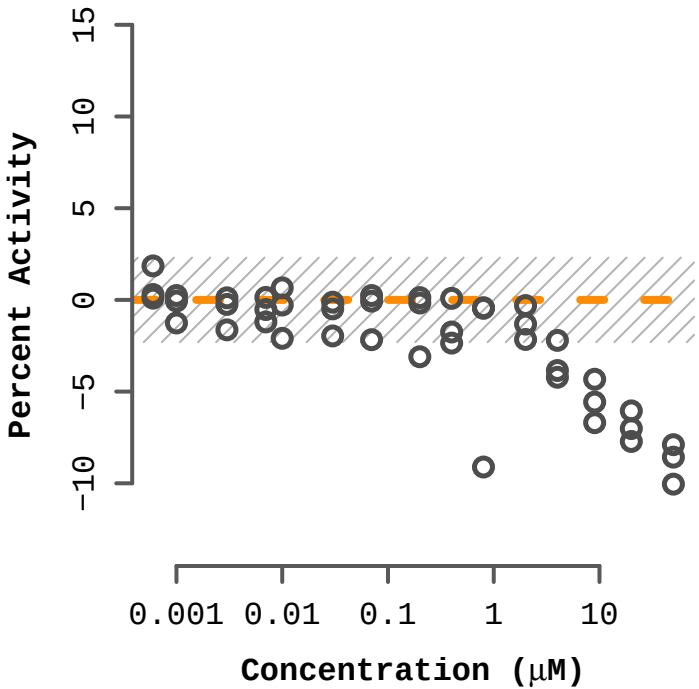
NAME: Carbocloral
CHID: 46233 **CASRN:** 541-79-7
SPID(S): Tox21_111902_1
M4ID: 12483426

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.325 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

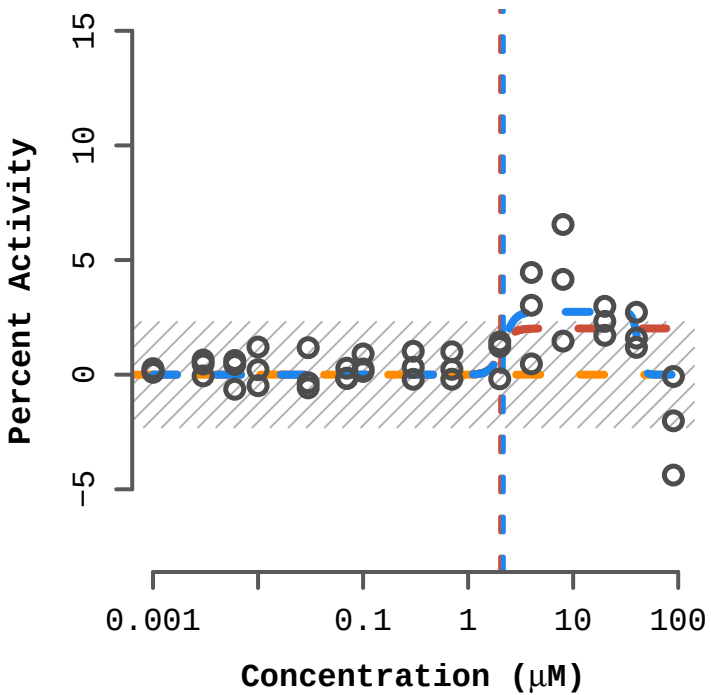
NAME: Broquinaldol
CHID: 46235 **CASRN:** 15599-52-7
SPID(S): Tox21_111904_1
M4ID: 12483425

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	244.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.79	NA	NA

MAX_MEAN: 0.75 **MAX_MED:** 0.297 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mexenone
CHID: 46242 CASRN: 1641-17-4
SPID(S): Tox21_200930
M4ID: 12481322

HILL MODEL (in red):

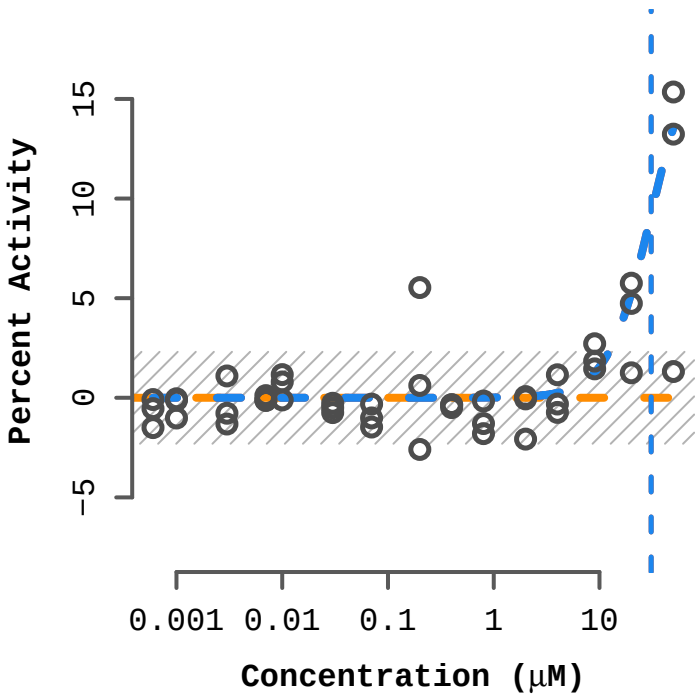
	tp	ga	gw
val:	2.02	0.31	8
sd:	0.346	0.0606	14.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.74	0.335	8	1.62	18
sd:	0.416	0.0639	11.7	0.0258	32.5

	CNST	HILL	GNLS
AIC:	175.09	154.5	141.22
PROB:	0	0	1
RMSE:	1.86	1.56	1.18

MAX_MEAN: 4.06 MAX_MED: 4.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bromindione
CHID: 46244 CASRN: 1146-98-1
SPID(S): Tox21_111919_1
M4ID: 12483424

HILL MODEL (in red):

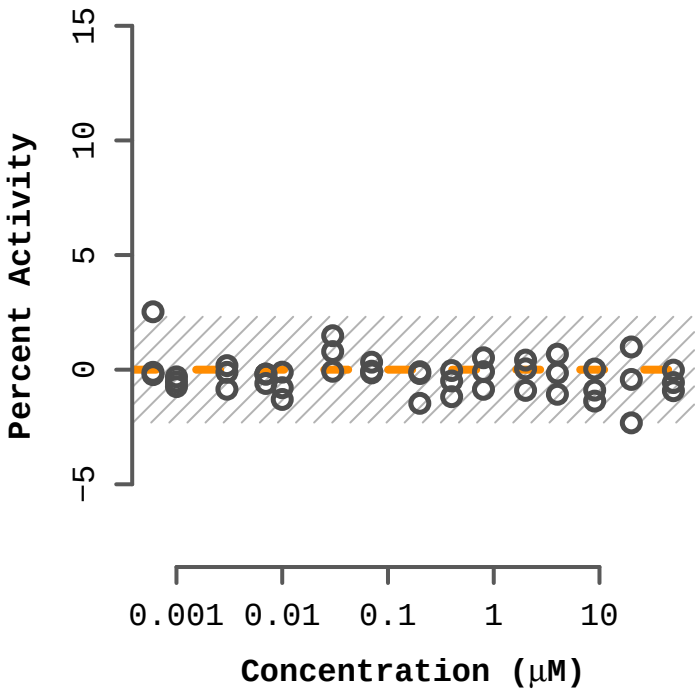
	tp	ga	gw
val:	18.4	1.49	2.12
sd:	3.84	0.108	0.477

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.4	1.49	2.12	3.69	3.98
sd:	3.84	0.108	0.477	1220	2450

	CNST	HILL	GNLS
AIC:	202.14	170.82	174.82
PROB:	0	0.88	0.12
RMSE:	3.48	2.29	2.29

MAX_MEAN: 9.97 **MAX_MED:** 13.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

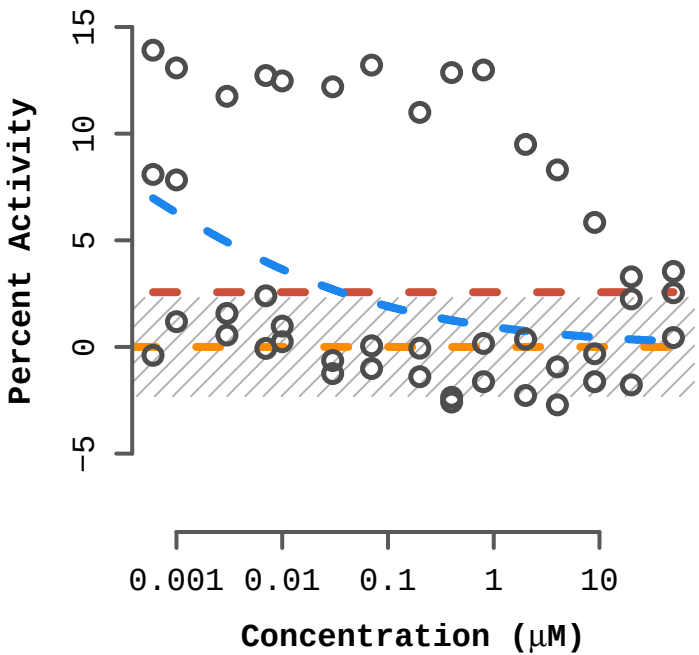
NAME: Pidolic acid
CHID: 46260 **CASRN:** 98-79-3
SPID(S): Tox21_111936_1
M4ID: 12483422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.735 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: D-delta-Tocopherol
CHID: 46263 CASRN: 119-13-1
SPID(S): Tox21_111941_1
M4ID: 12483420

HILL MODEL (in red):

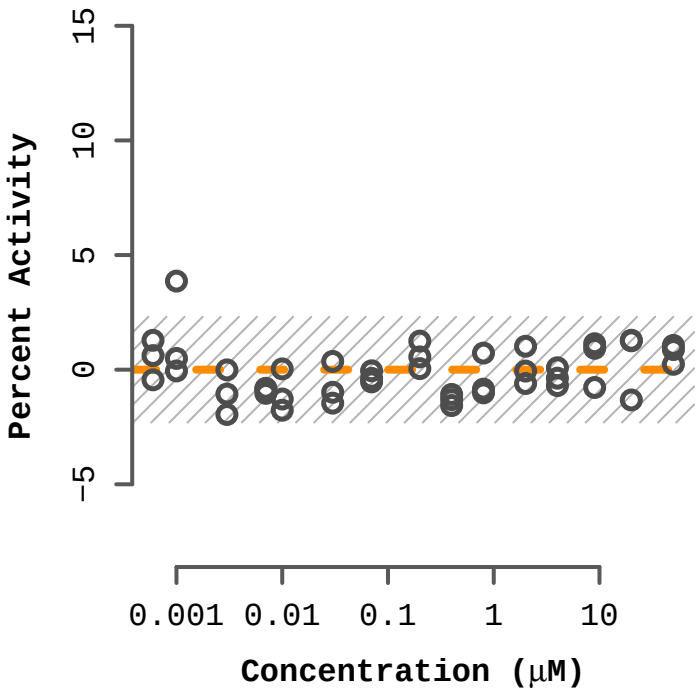
	tp	ga	gw
val:	2.57	−4.25	7.18
sd:	0.901	961	6630

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.7	−5.16	3.49	−3.65	0.336
sd:	25	1160	2030	3.4	0.32

	CNST	HILL	GNLS
AIC:	299.08	295.88	295.5
PROB:	0.08	0.41	0.5
RMSE:	6.67	5.69	5.46

MAX_MEAN: 7.37 **MAX_MED:** 8.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

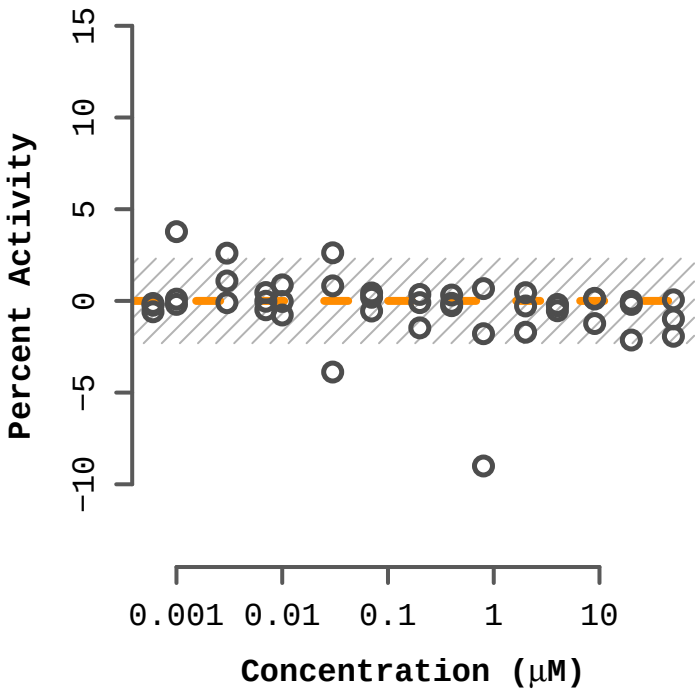
NAME: Ethopabate
CHID: 46264 **CASRN:** 59-06-3
SPID(S): Tox21_111943_1
M4ID: 12483418

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

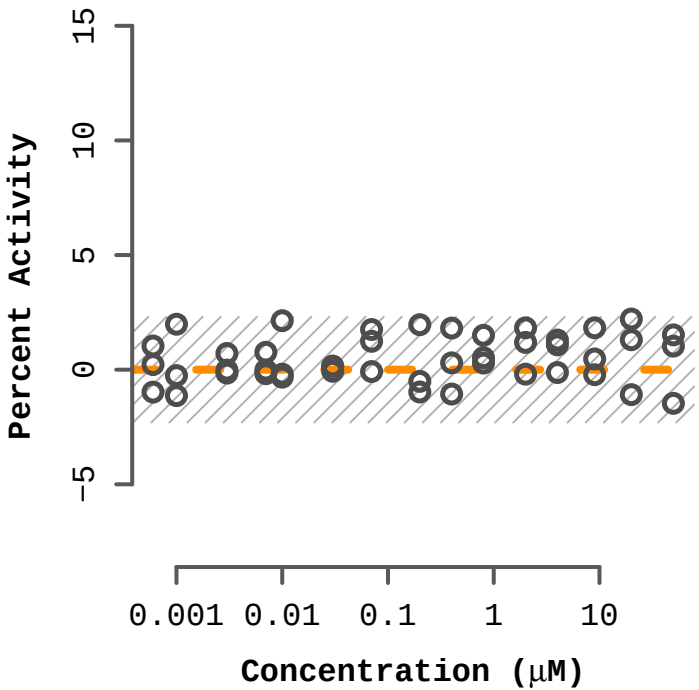
NAME: Bretazenil
CHID: 46266 **CASRN:** 84379-13-5
SPID(S): Tox21_111947_1
M4ID: 12483415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

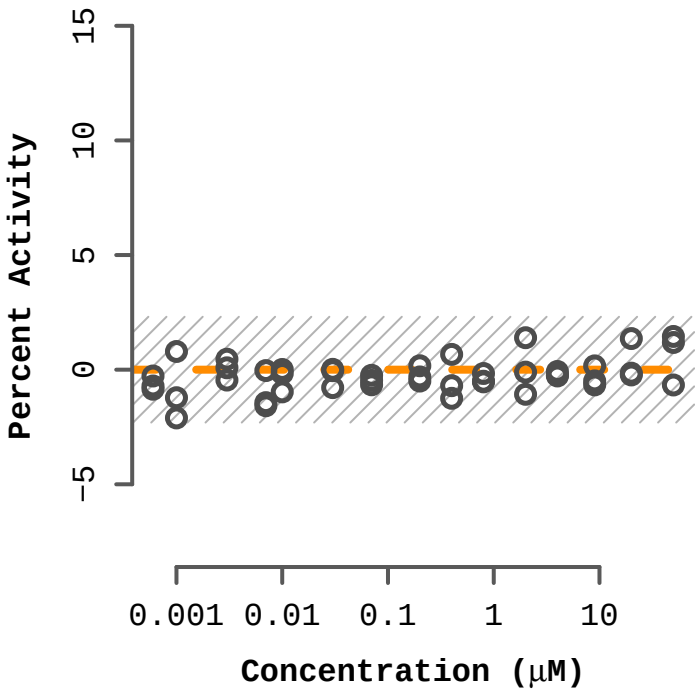
NAME: Sulazepam
CHID: 46267 **CASRN:** 2898-13-7
SPID(S): Tox21_111948
M4ID: 12483414

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

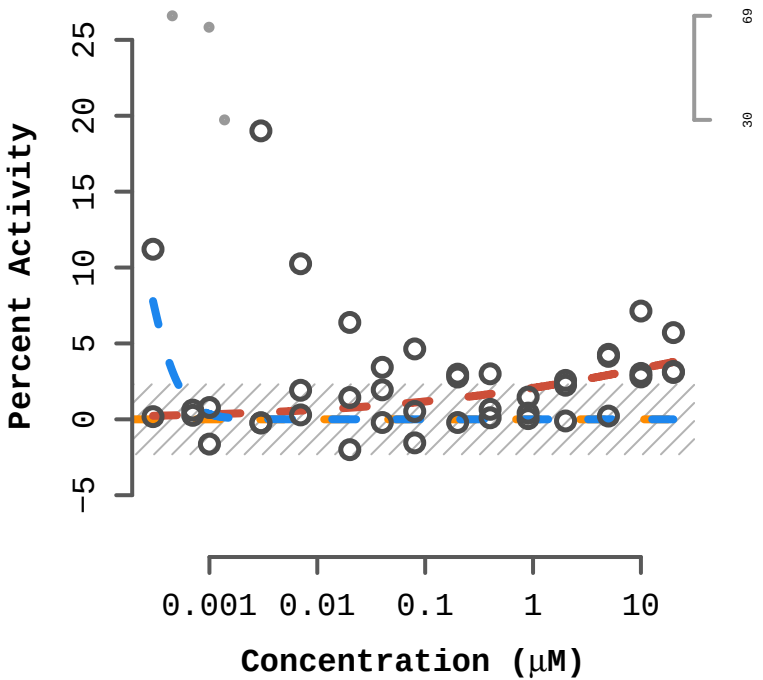
NAME: Butamirate citrate
CHID: 46270 CASRN: 18109-81-4
SPID(S): Tox21_111952_1
M4ID: 12483413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.657 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pipofezine
CHID: 46271 CASRN: 24886-52-0
SPID(S): Tox21_111953_1
M4ID: 12483412 BRK

HILL MODEL (in red):

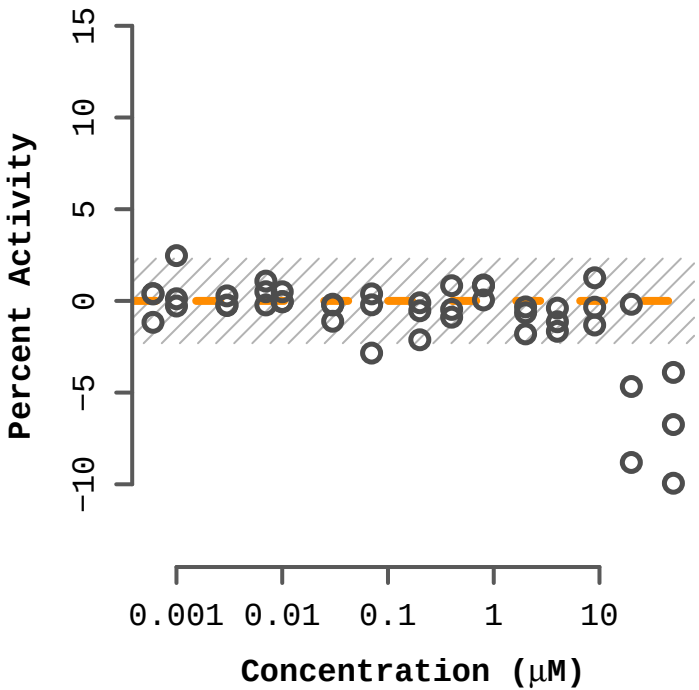
	tp	ga	gw
val:	8.73	1.69	0.3
sd:	23	6.62	0.33

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	18.8	−5.52	7.92	−3.57	3.01
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	310.15	300.28	317.41
PROB:	0.01	0.99	0
RMSE:	15.51	15.3	14.6

MAX_MEAN: 26.9 **MAX_MED:** 11.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

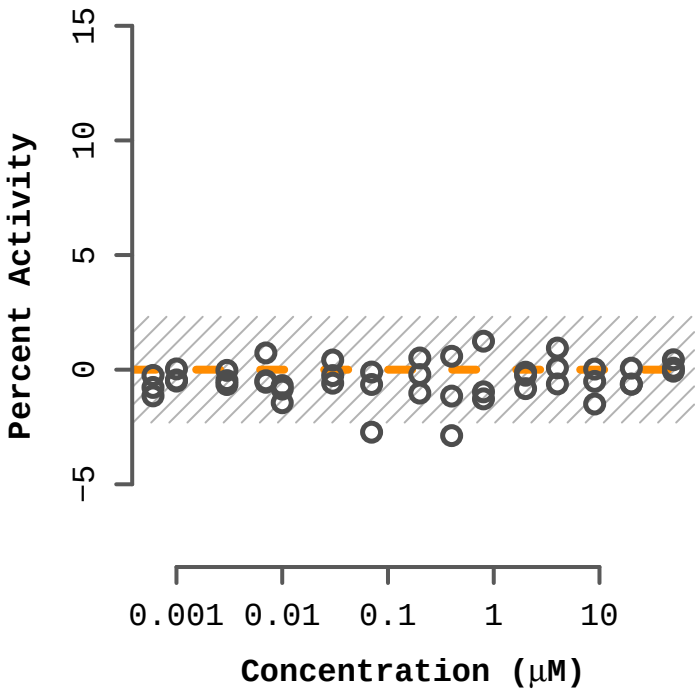
NAME: Salinazid
CHID: 46272 CASRN: 495-84-1
SPID(S): Tox21_111955_1
M4ID: 12483410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.89	NA	NA
PROB:	1	NA	NA
RMSE:	2.57	NA	NA

MAX_MEAN: 0.77 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

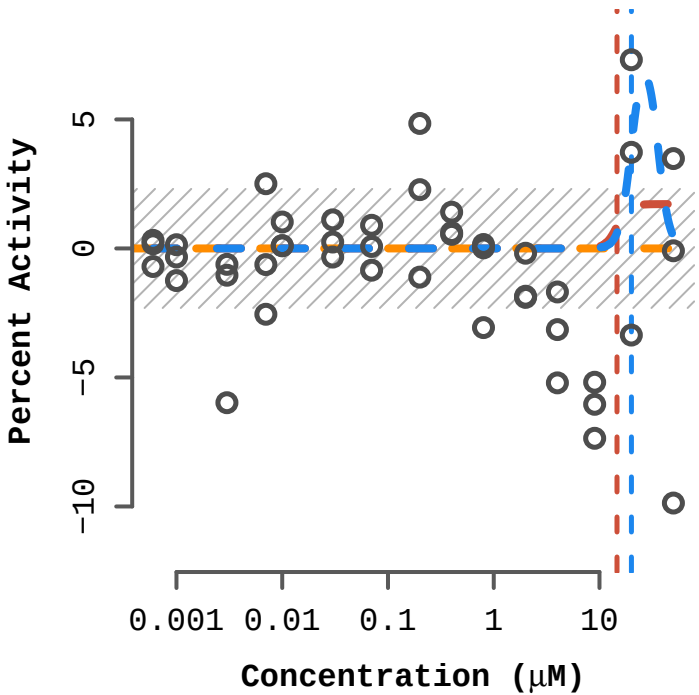
NAME: Glycyclamide
CHID: 46273 **CASRN:** 664-95-9
SPID(S): Tox21_111956_1
M4ID: 12483409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.146 **MAX_MED:** 0.0818 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethacridine lactate hydrate
CHID: 46274 CASRN: 6402-23-9
SPID(S): Tox21_111957_1
M4ID: 12483408

HILL MODEL (in red):

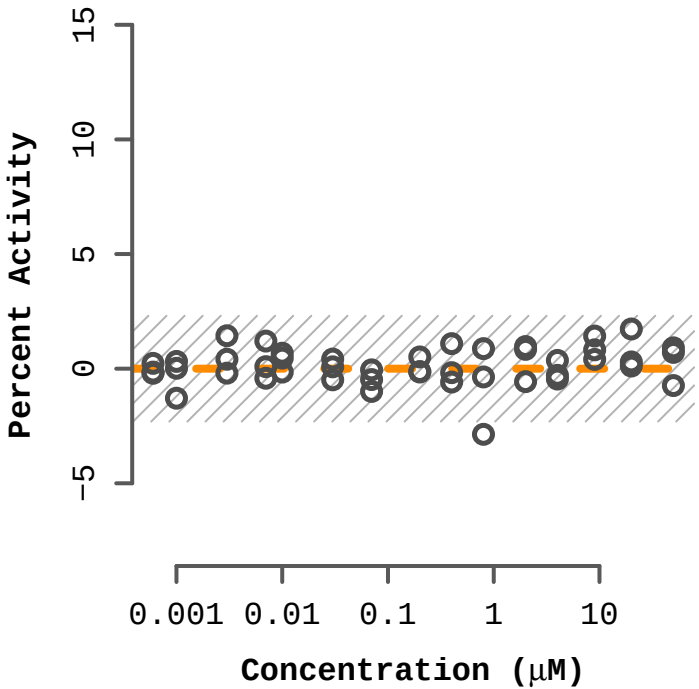
	tp	ga	gw
val:	1.72	1.17	8
sd:	1.71	0.177	8.25

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.03	1.3	8	1.55	8.2
sd:	30.5	0.407	9.68	1.02	55.4

	CNST	HILL	GNLS
AIC:	227.64	232.64	234.77
PROB:	0.9	0.07	0.03
RMSE:	3.17	3.22	3.14

MAX_MEAN: 2.56 **MAX_MED:** 3.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

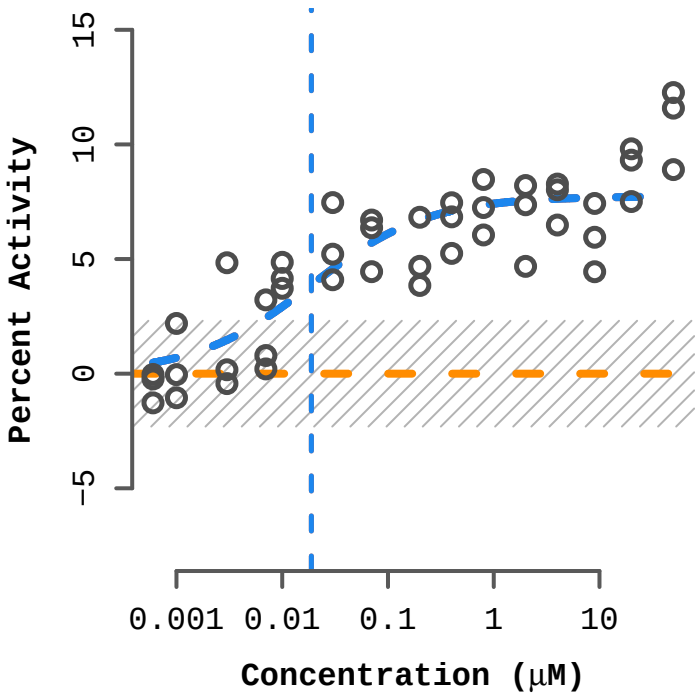
NAME: Sulfasuccinamide
CHID: 46275 **CASRN:** 3563-14-2
SPID(S): Tox21_111958_1
M4ID: 12483407

HILL MODEL: Not applicable.

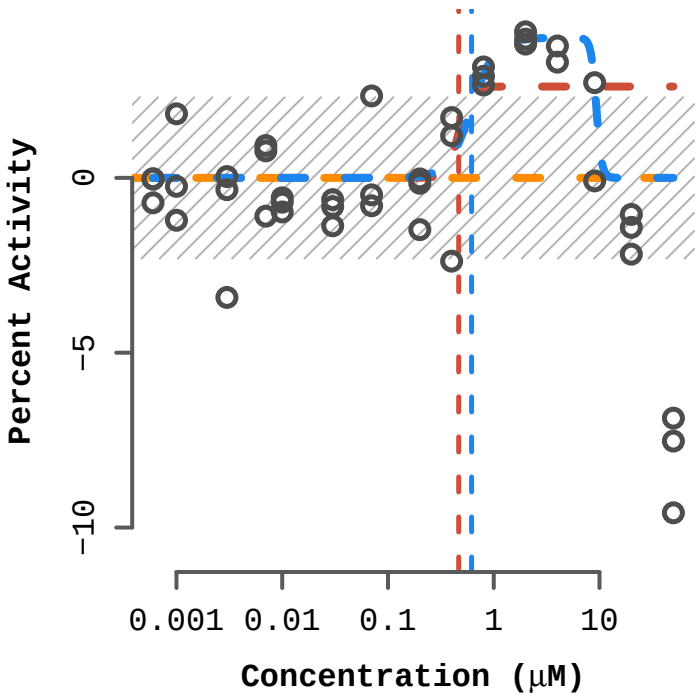
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 0.843 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Glysobuzole
CHID:    46276   CASRN: 3567-08-6
SPID(S): Tox21_111959_1
M4ID:    12483406

HILL MODEL (in red):
      tp       ga       gw
val:  7.74     -1.72    0.789
sd:   0.829    0.303    0.399

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.74     -1.72    0.789    3.11     15.5
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  300.3       188.97      192.97
PROB: 0           0.88        0.12
RMSE: 6.16        1.76        1.76

MAX_MEAN: 10.9      MAX_MED: 11.6      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tenonitrozole
CHID: 46277 CASRN: 3810-35-3
SPID(S): Tox21_111962_1
M4ID: 12483404

HILL MODEL (in red):

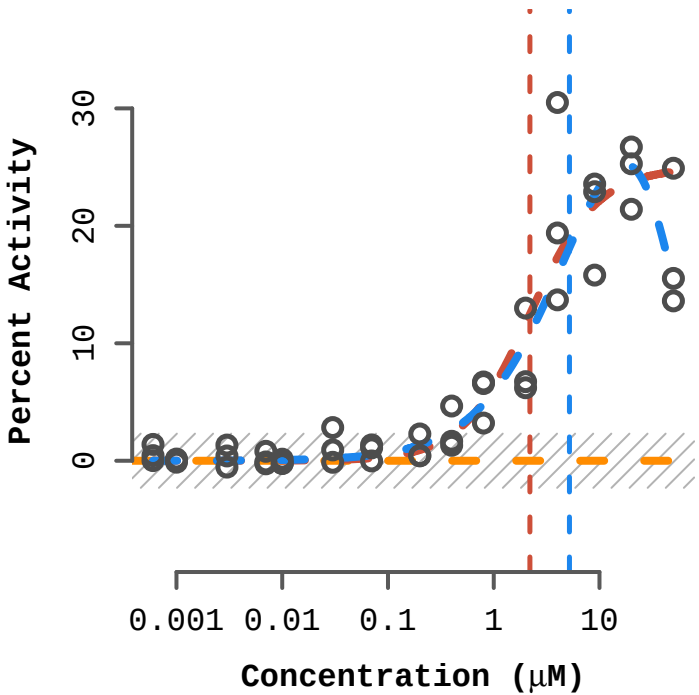
	tp	ga	gw
val:	2.61	−0.331	8
sd:	0.609	0.145	11.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.01	−0.21	3.93	0.97	17.2
sd:	0.509	0.101	2.42	0.124	131

	CNST	HILL	GNLS
AIC:	225.7	220.37	198.1
PROB:	0	0	1
RMSE:	3.05	3.24	2.45

MAX_MEAN: 4.02 MAX_MED: 3.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Frentizole
CHID: 46279 CASRN: 26130-02-9
SPID(S): Tox21_111964_1
M4ID: 12483402

HILL MODEL (in red):

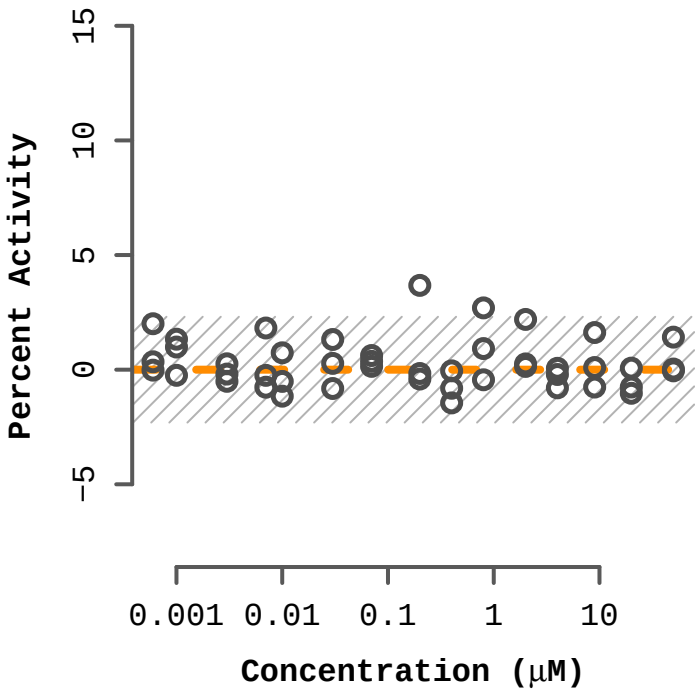
	tp	ga	gw
val:	24.9	0.342	1.36
sd:	1.42	0.0861	0.22

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	36.6	0.716	1.01	1.66	2.19
sd:	18.6	0.464	0.243	0.154	1.24

	CNST	HILL	GNLS
AIC:	343.99	225.79	216.18
PROB:	0	0.01	0.99
RMSE:	11.63	3.47	3.2

MAX_MEAN: 24.5 MAX_MED: 25.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

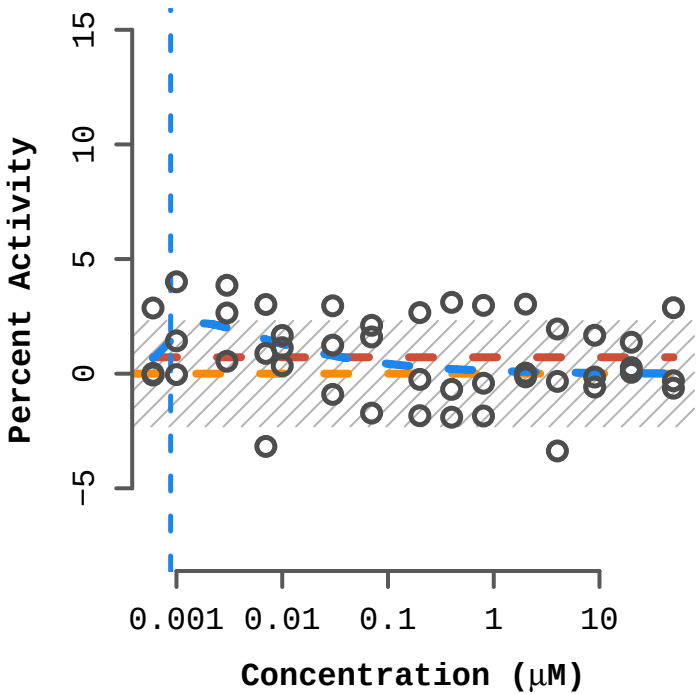
NAME: Dazmegrel
CHID: 46281 CASRN: 76894-77-4
SPID(S): Tox21_111966_1
M4ID: 12483401

HILL MODEL: Not applicable.

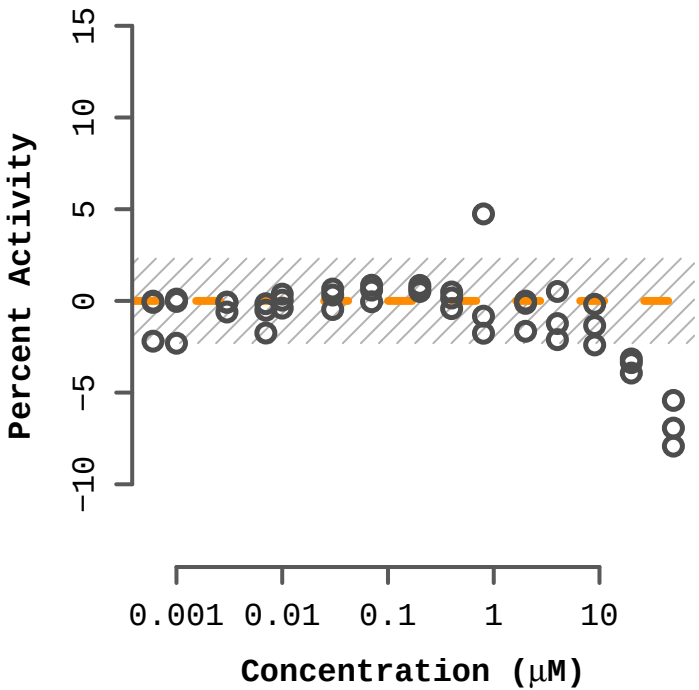
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.06 MAX_MED: 0.988 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ambrisentan
CHID:    46282   CASRN: 177036-94-1
SPID(S): Tox21_111967_1
M4ID:    12483400

HILL MODEL (in red):
      tp       ga       gw
val:  0.715    -4.93    3.78
sd:   0.284    1670     3330

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.81     -3.05    3.36     -2.75    0.575
sd:   11.5     0.302    4.17     3.1      0.697

      CNST        HILL        GNLS
AIC:  193.36      193.18      192.76
PROB: 0.29        0.32        0.39
RMSE: 1.94        1.8         1.74

MAX_MEAN: 2.35      MAX_MED: 2.65      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

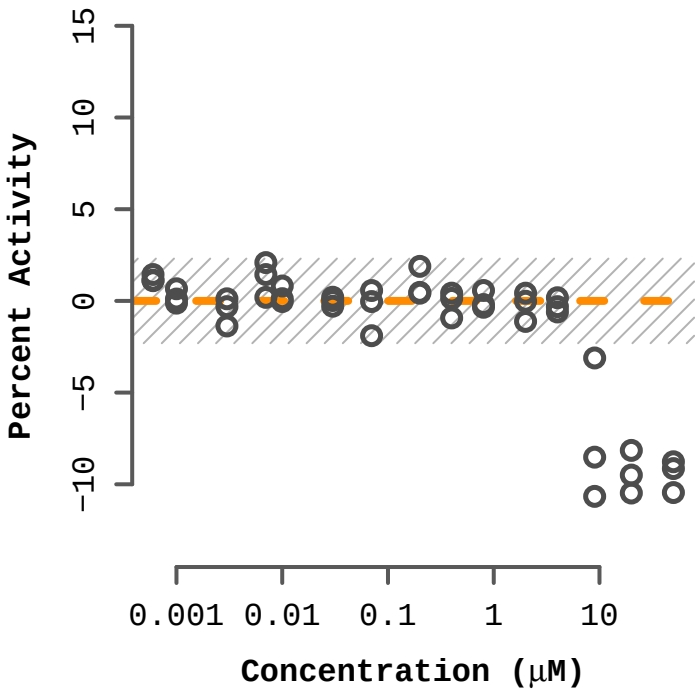
NAME: Flazalone
CHID: 46283 **CASRN:** 21221-18-1
SPID(S): Tox21_111968_1
M4ID: 12483399

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.06	NA	NA
PROB:	1	NA	NA
RMSE:	2.3	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.675 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

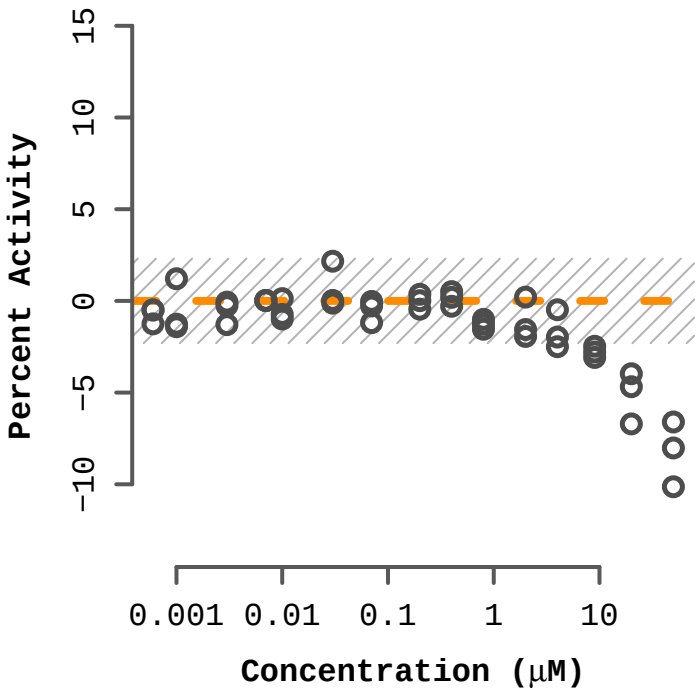
NAME: Nitroxoline
CHID: 46284 **CASRN:** 4008-48-4
SPID(S): Tox21_111969_1
M4ID: 12483398

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.47	NA	NA
PROB:	1	NA	NA
RMSE:	4.1	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

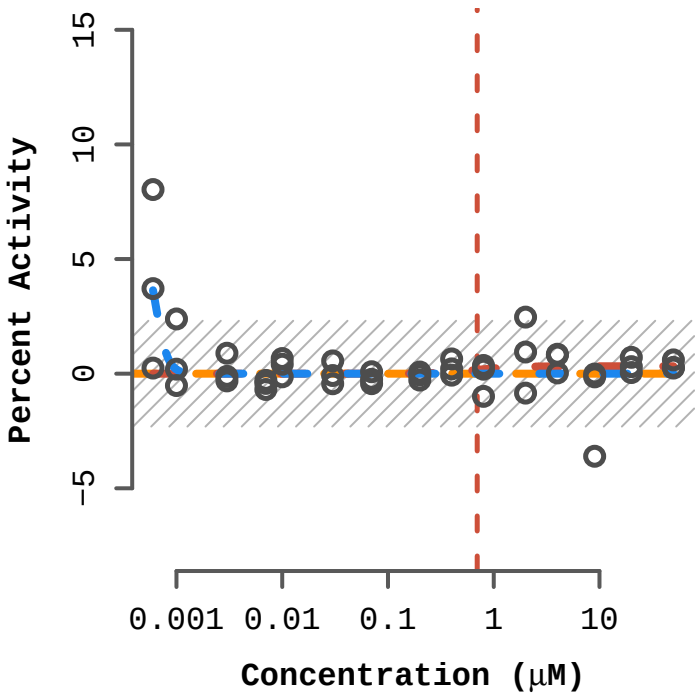
NAME: Proroxan
CHID: 46285 **CASRN:** 33743-96-3
SPID(S): Tox21_111970_1
M4ID: 12483397

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.66	NA	NA
PROB:	1	NA	NA
RMSE:	2.81	NA	NA

MAX_MEAN: 0.691 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfaethidole
CHID: 46286 **CASRN:** 94-19-9
SPID(S): Tox21_111971_1
M4ID: 12483396

HILL MODEL (in red):

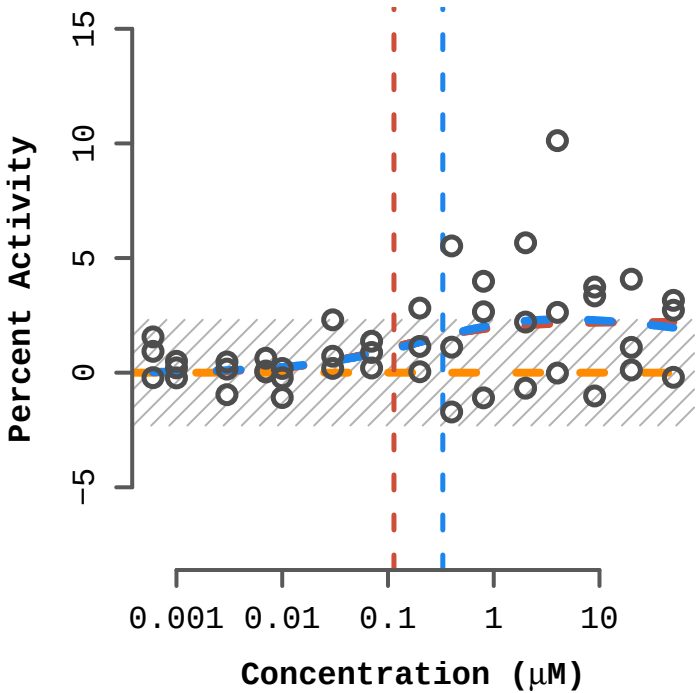
	tp	ga	gw
val:	0.323	−0.156	2.44
sd:	0.181	1.1	4.64

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.96	−5.08	1.45	−3.2	7.65
sd:	12	956	578	0.085	8.65

	CNST	HILL	GNLS
AIC:	130.25	132.65	133.33
PROB:	0.66	0.2	0.14
RMSE:	1.58	1.58	1.19

MAX_MEAN: 4 **MAX_MED:** 3.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfabenz
CHID: 46287 CASRN: 127-77-5
SPID(S): Tox21_111972_1
M4ID: 12483395

HILL MODEL (in red):

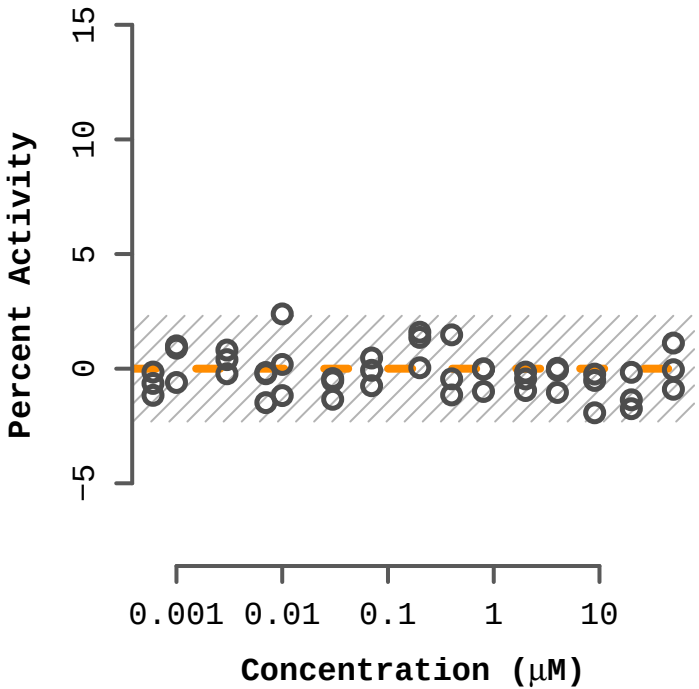
	tp	ga	gw
val:	2.22	−0.943	0.924
sd:	0.587	0.541	0.742

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.83	−0.482	0.746	1.84	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	203.07	187.75	191.63
PROB:	0	0.87	0.13
RMSE:	2.55	1.97	1.96

MAX_MEAN: 4.25 **MAX_MED:** 3.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

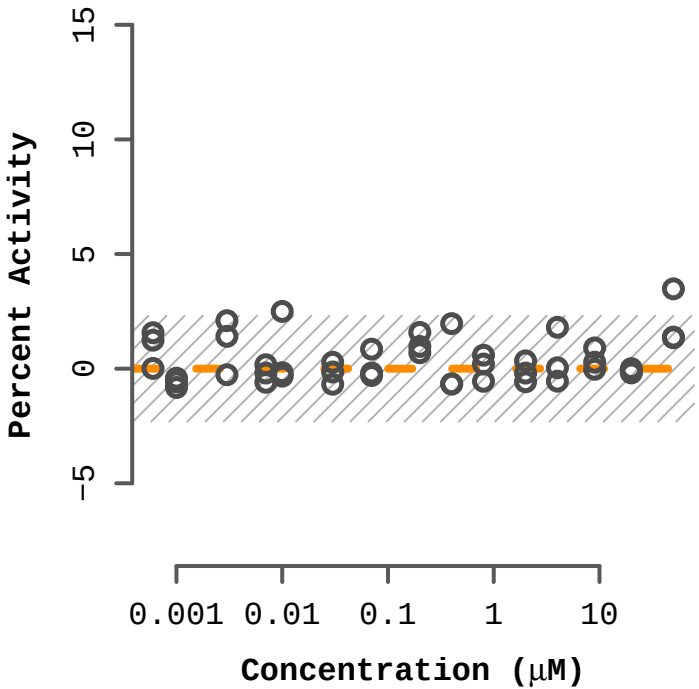
NAME: Pexantel
CHID: 46288 **CASRN:** 10001-13-5
SPID(S): Tox21_111973_1
M4ID: 12483394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.999 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

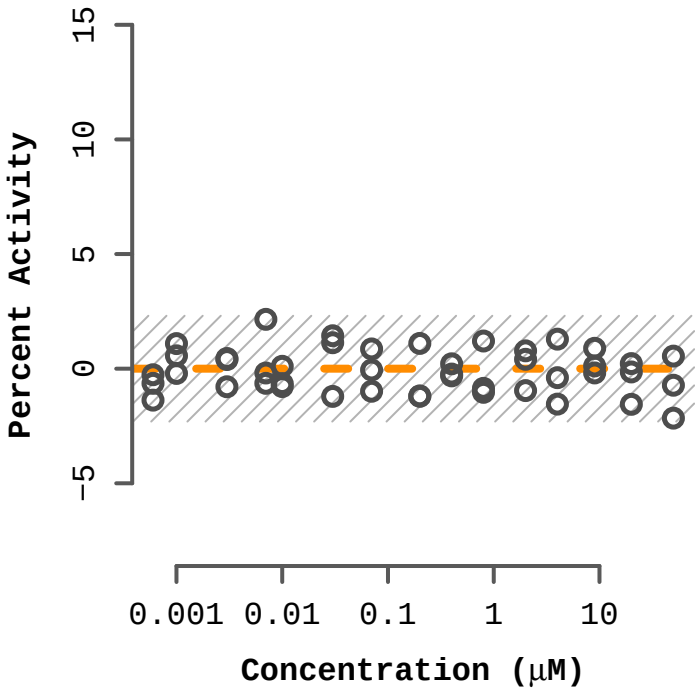
NAME: Mecarbinate
CHID: 46289 **CASRN:** 15574-49-9
SPID(S): Tox21_111974_1
M4ID: 12483393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

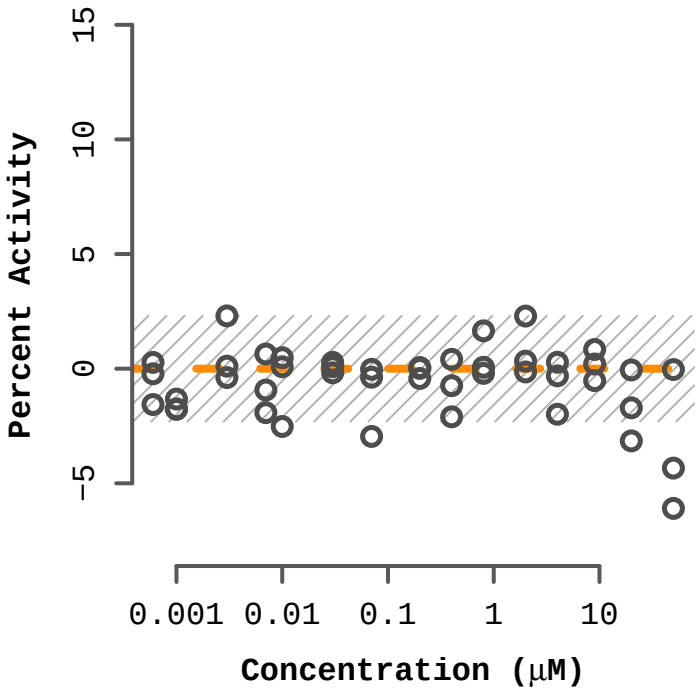
NAME: Aprofene
CHID: 46294 **CASRN:** 3563-01-7
SPID(S): Tox21_111979_1
M4ID: 12483392

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

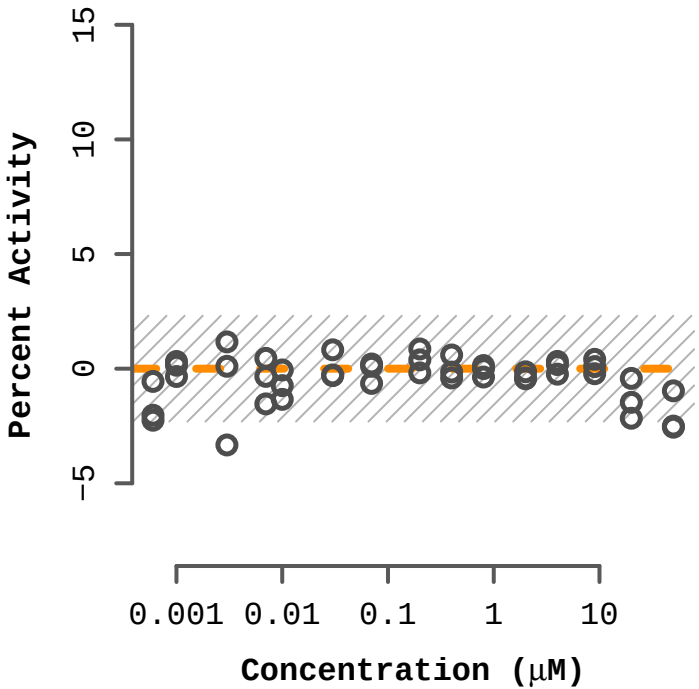
NAME: Butinoline
CHID: 46295 **CASRN:** 968-61-6
SPID(S): Tox21_111980_1
M4ID: 12483391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 0.829 **MAX_MED:** 0.332 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

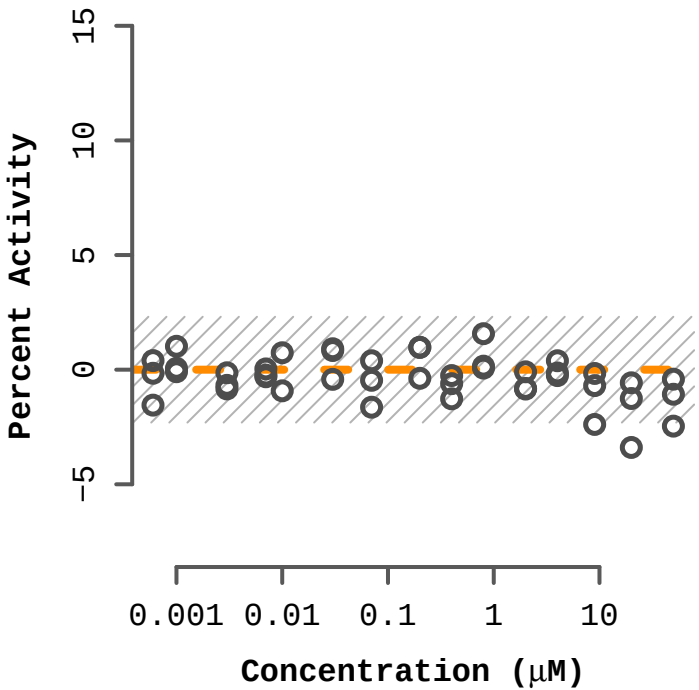
NAME: Fenoverine
CHID: 46296 **CASRN:** 37561-27-6
SPID(S): Tox21_111981_1
M4ID: 12483390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.356 **MAX_MED:** 0.388 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

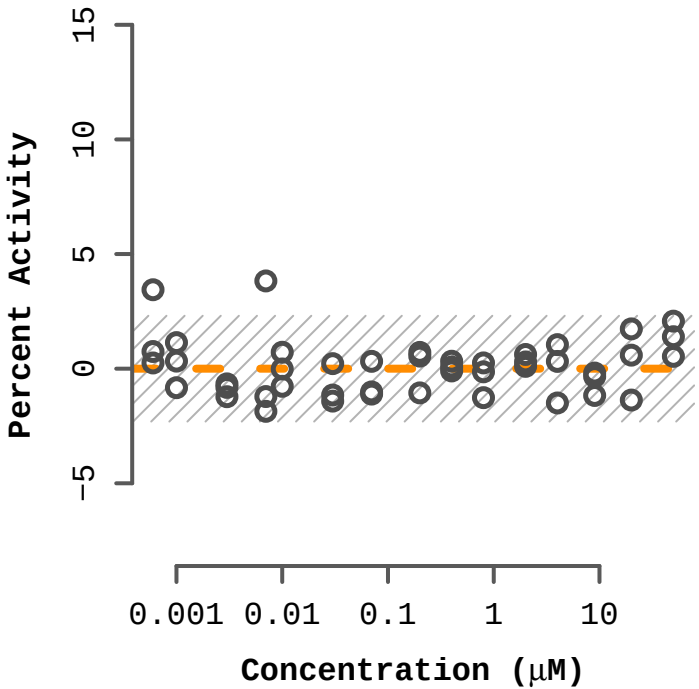
NAME: Dinsed
CHID: 46297 **CASRN:** 96-62-8
SPID(S): Tox21_111982_1
M4ID: 12483389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.599 **MAX_MED:** 0.976 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

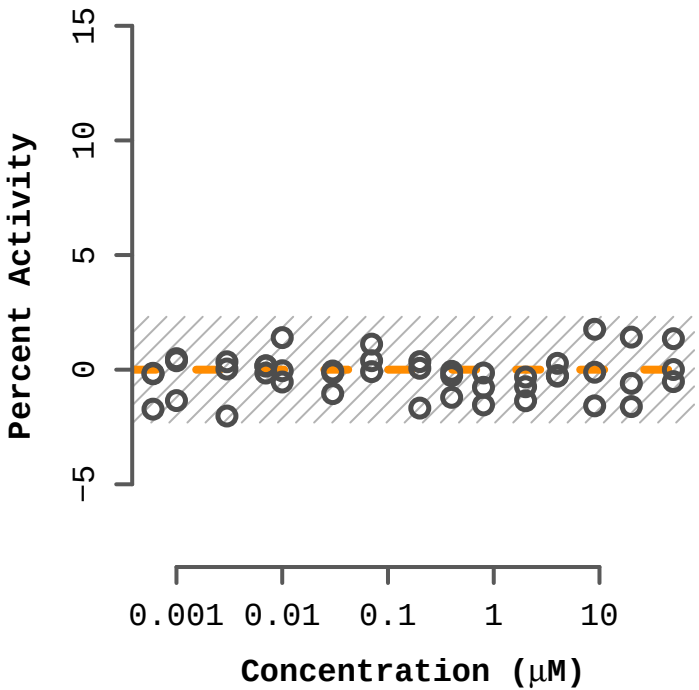
NAME: Risocaine
CHID: 46299 **CASRN:** 94-12-2
SPID(S): Tox21_111984_1
M4ID: 12483388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

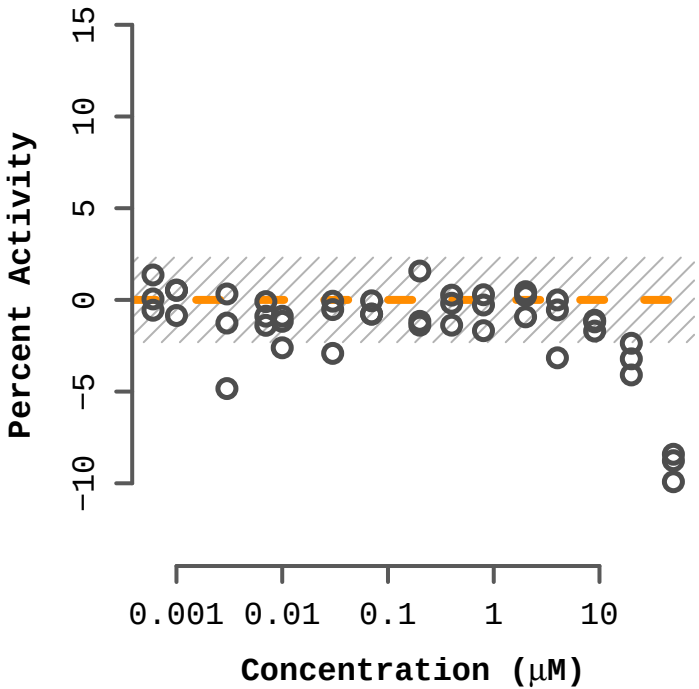
NAME: Ftaxilide
CHID: 46300 CASRN: 19368-18-4
SPID(S): Tox21_111986_1
M4ID: 12483386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.475 MAX_MED: 0.393 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

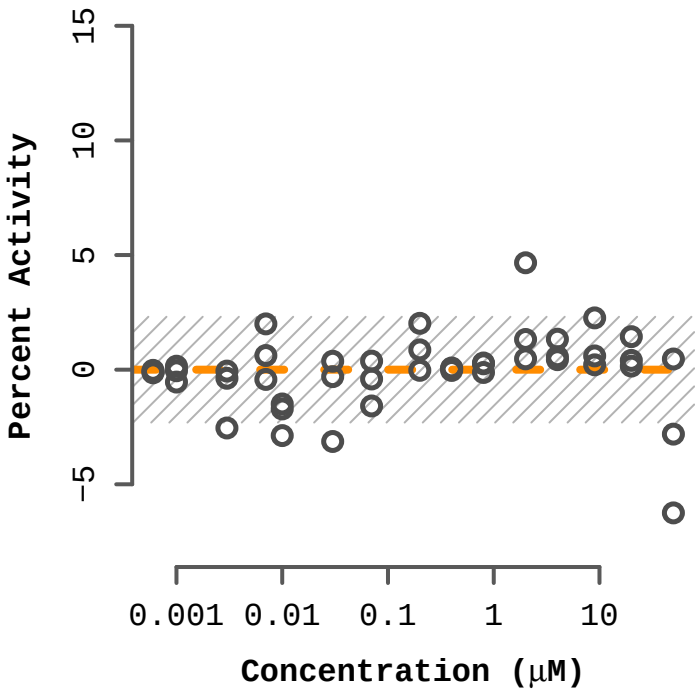
NAME: Pinokalant hydrochloride
CHID: 46305 **CASRN:** 143482-60-4
SPID(S): Tox21_111993_1
M4ID: 12483385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.81	NA	NA

MAX_MEAN: 0.284 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

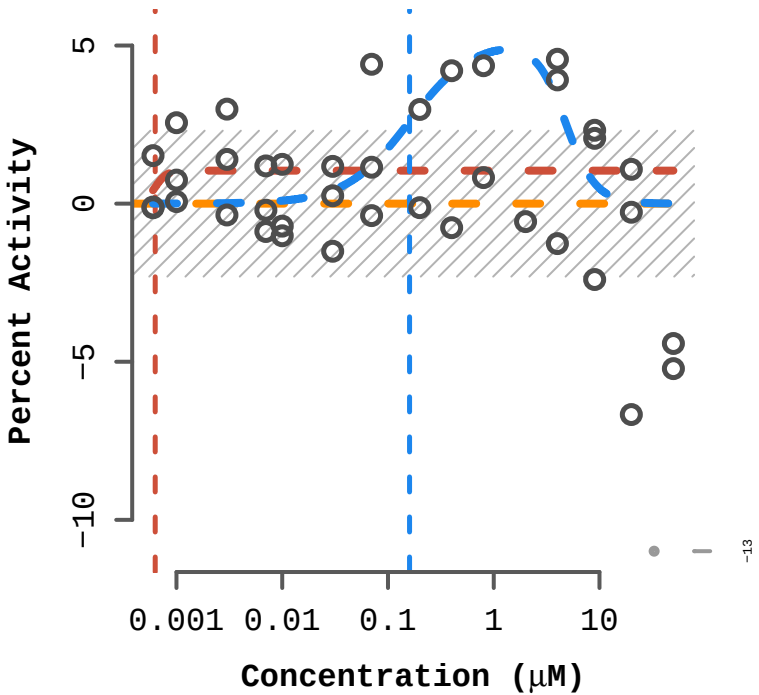
NAME: Falnidamol dihydrochloride
CHID: 46307 CASRN: 1216920-18-1
SPID(S): Tox21_111996_1
M4ID: 12483383

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cilnidipine
CHID: 46309 CASRN: 132203-70-4
SPID(S): Tox21_112001_1
M4ID: 12483379 BRK

HILL MODEL (in red):

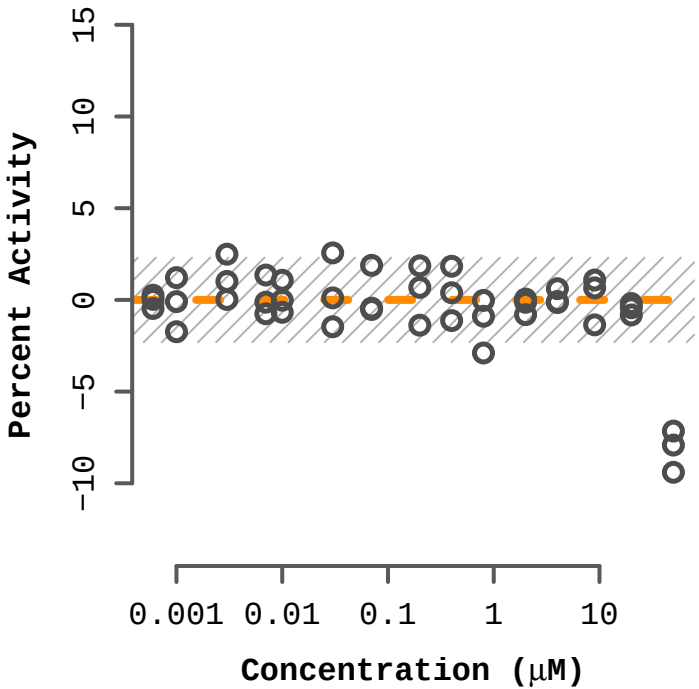
	tp	ga	gw
val:	1.04	−3.2	8
sd:	0.487	0.308	55.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.21	−0.796	1.45	0.677	3.05
sd:	3.01	0.591	1.66	0.268	2.72

	CNST	HILL	GNLS
AIC:	247.49	248.81	238.18
PROB:	0.01	0	0.99
RMSE:	3.93	3.82	3.25

MAX_MEAN: 5.27 MAX_MED: 5.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

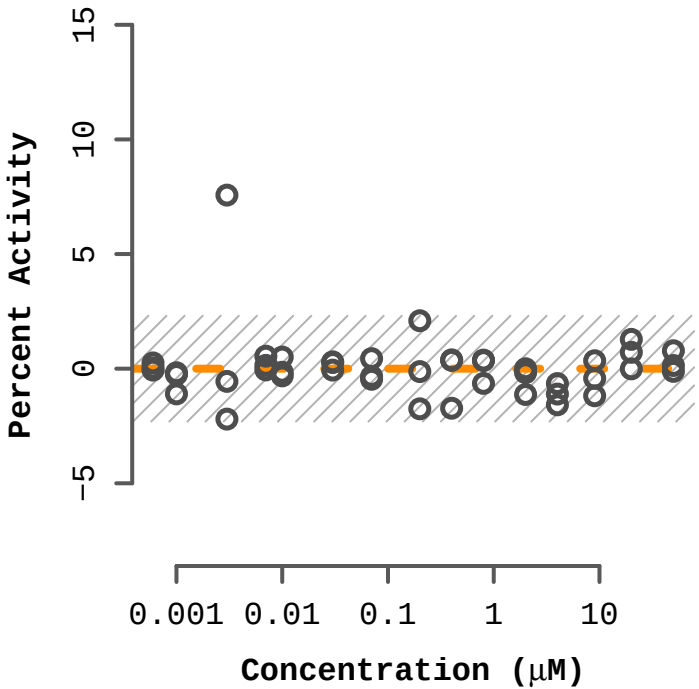
NAME: cis-Flupentixol
CHID: 46310 **CASRN:** 53772-82-0
SPID(S): Tox21_112003_1
M4ID: 12483378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

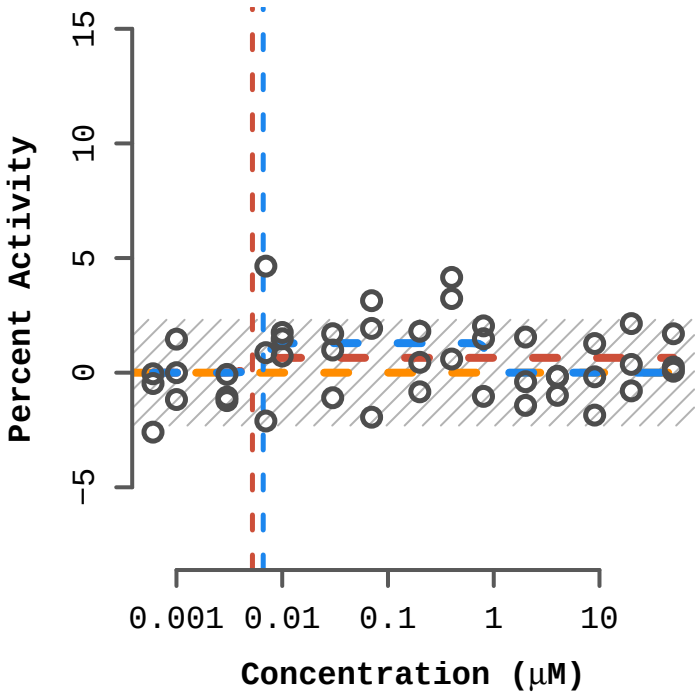
NAME: Naltrexone
CHID: 46313 CASRN: 16590-41-3
SPID(S): Tox21_112007_1
M4ID: 12483375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 0.715 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Quinelorane
CHID: 46315 CASRN: 97466-90-5
SPID(S): Tox21_112009_1
M4ID: 12483374

HILL MODEL (in red):

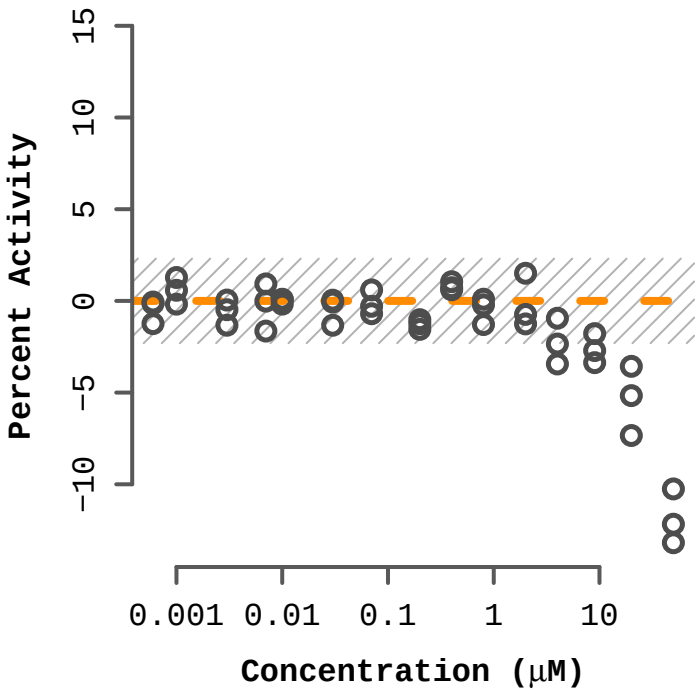
	tp	ga	gw
val:	0.647	−2.28	8
sd:	0.27	0.365	13.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.29	−2.18	8	−0.0503	16.5
sd:	0.402	0.207	15.2	1.85	651

	CNST	HILL	GNLS
AIC:	177.68	178.13	176.6
PROB:	0.28	0.23	0.49
RMSE:	1.68	1.56	1.49

MAX_MEAN: 2.66 **MAX_MED:** 3.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

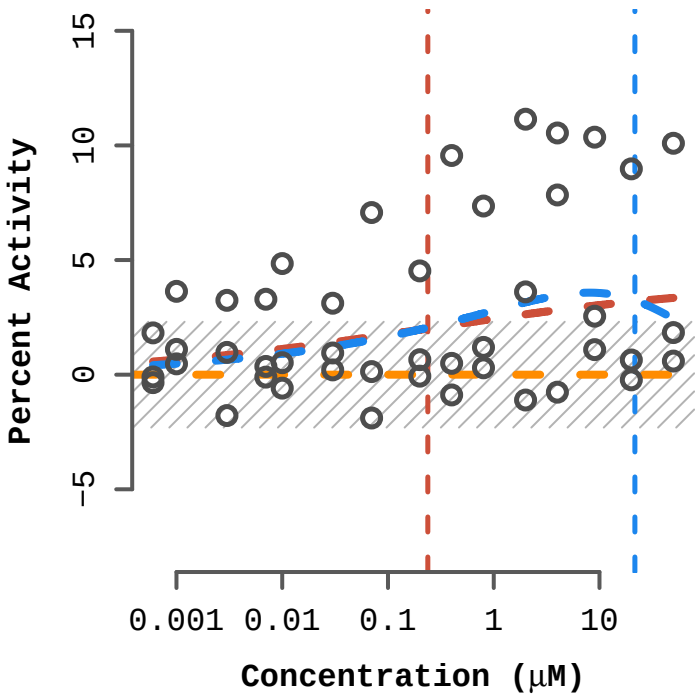
NAME: Niguldipine hydrochloride
CHID: 46318 **CASRN:** 102992-93-8
SPID(S): Tox21_112014_1
M4ID: 12483371

HILL MODEL: Not applicable.

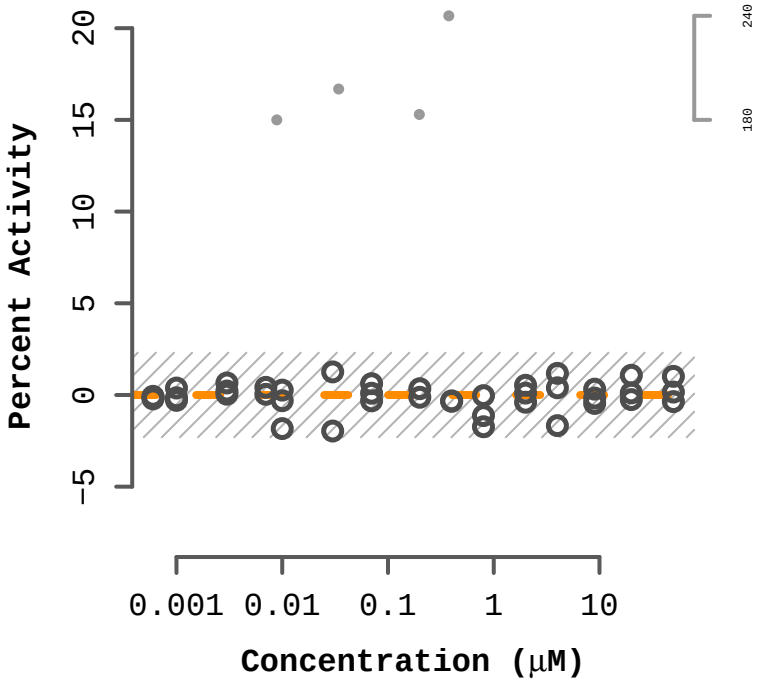
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.61	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 0.722 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (−)−(5S,8R)−Lisuride
CHID:    46320   CASRN: 159701−44−7
SPID(S): Tox21_112019_1
M4ID:    12483368

HILL MODEL (in red):
      tp       ga       gw
val:  4.02     −0.623   0.3
sd:   NaN      NaN      NaN

GAIN−LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.1     1.33     0.3      1.58     1.03
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  259.2       249.94      253.53
PROB: 0.01        0.85        0.14
RMSE: 4.51        3.52        3.48

MAX_MEAN: 5.87      MAX_MED: 7.84      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

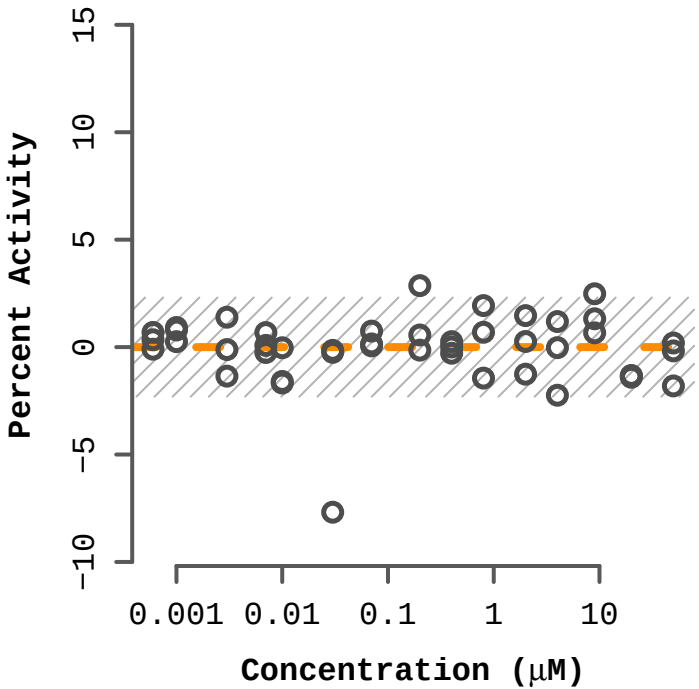
NAME: Talipexole
CHID: 46321 **CASRN:** 101626-70-4
SPID(S): Tox21_112020_1
M4ID: 12483367 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	295.52	NA	NA
PROB:	1	NA	NA
RMSE:	60.17	NA	NA

MAX_MEAN: 80.2 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

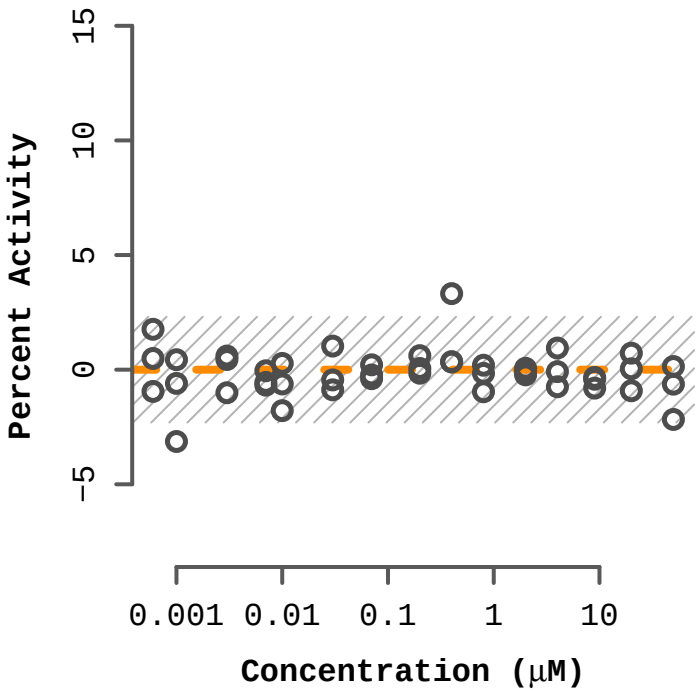
NAME: Mesulergine
CHID: 46324 **CASRN:** 64795-35-3
SPID(S): Tox21_112023_1
M4ID: 12483366

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

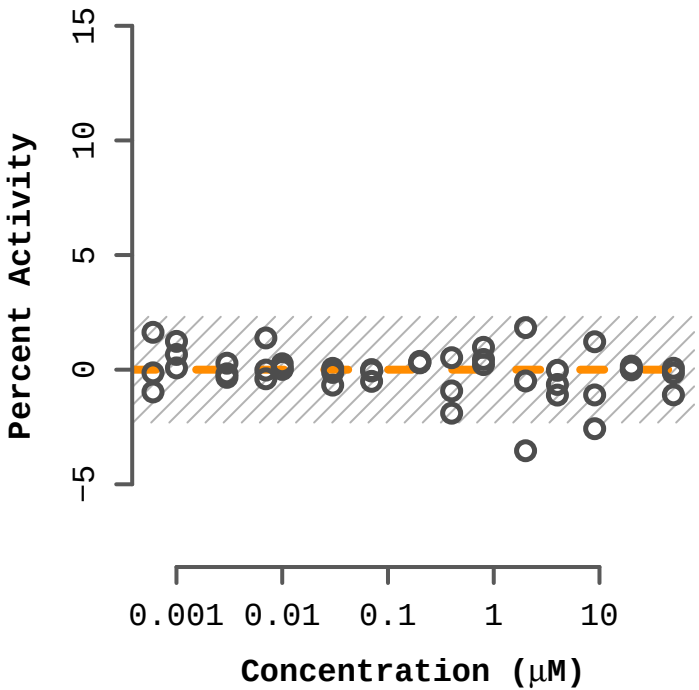
NAME: U-69593
CHID: 46326 **CASRN:** 96744-75-1
SPID(S): Tox21_112026_1
M4ID: 12483364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

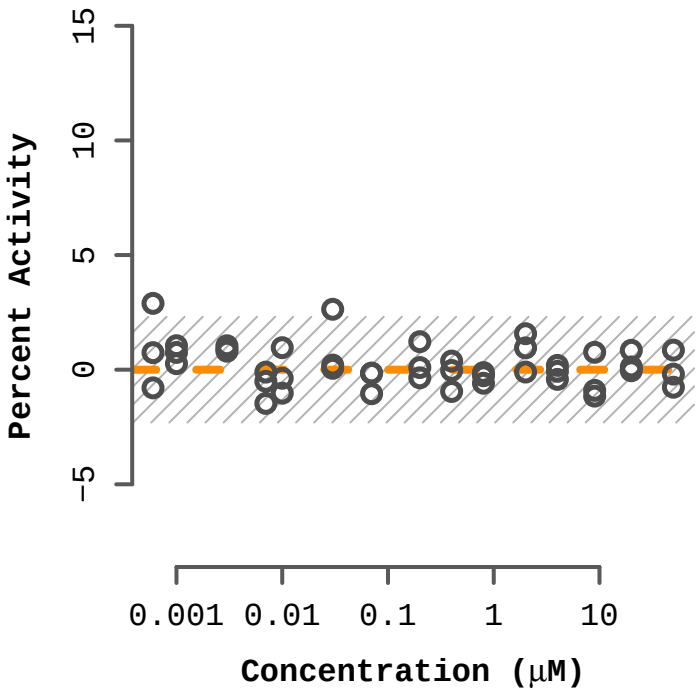
NAME: Chlorisondamine chloride
CHID: 46332 **CASRN:** 69-27-2
SPID(S): Tox21_112032_1
M4ID: 12483359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.66 **MAX_MED:** 0.666 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

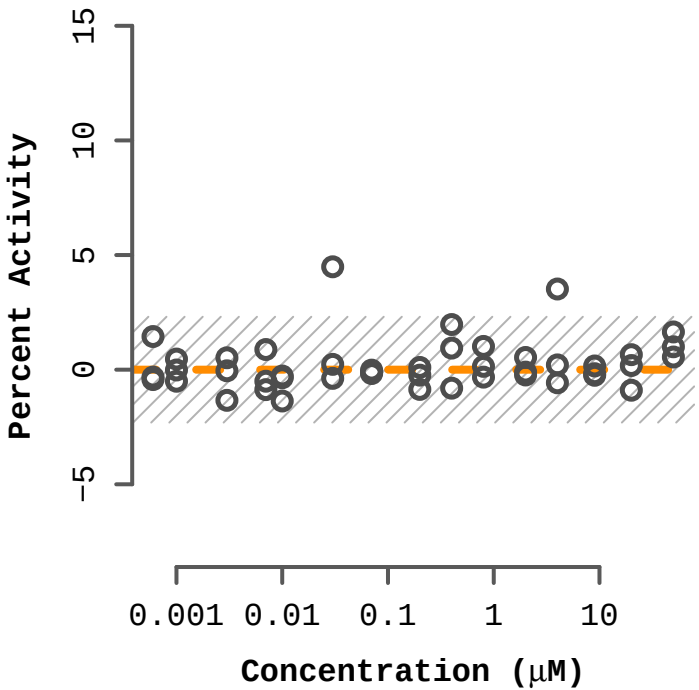
NAME: Tiotidine
CHID: 46341 **CASRN:** 69014-14-8
SPID(S): Tox21_112041_1
M4ID: 12483353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

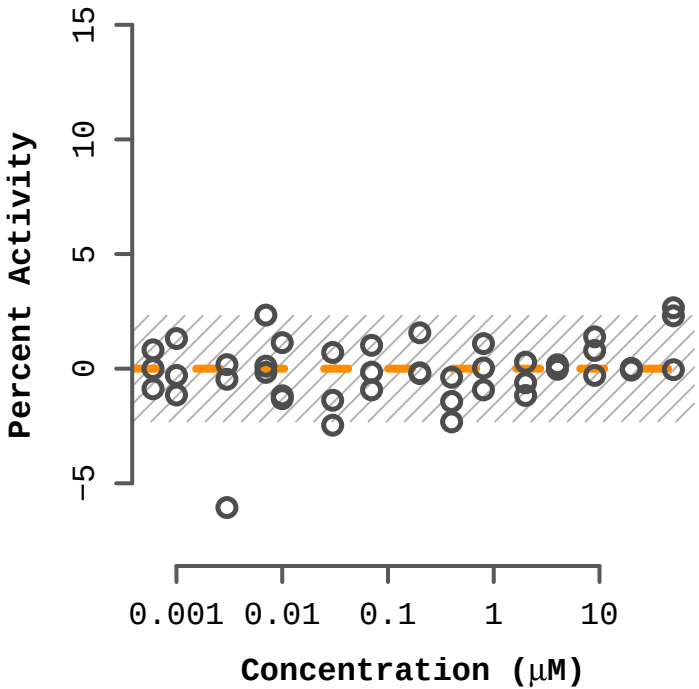
NAME: Lisofylline
CHID: 46343 **CASRN:** 6493-06-7
SPID(S): Tox21_112043_1
M4ID: 12483352

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

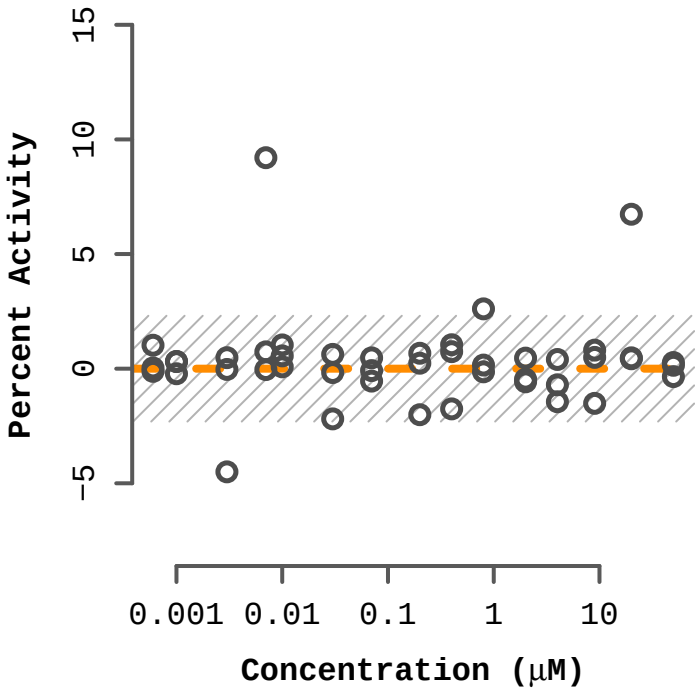
NAME: Suramin
CHID: 46344 **CASRN:** 145-63-1
SPID(S): Tox21_112045_1
M4ID: 12483351

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

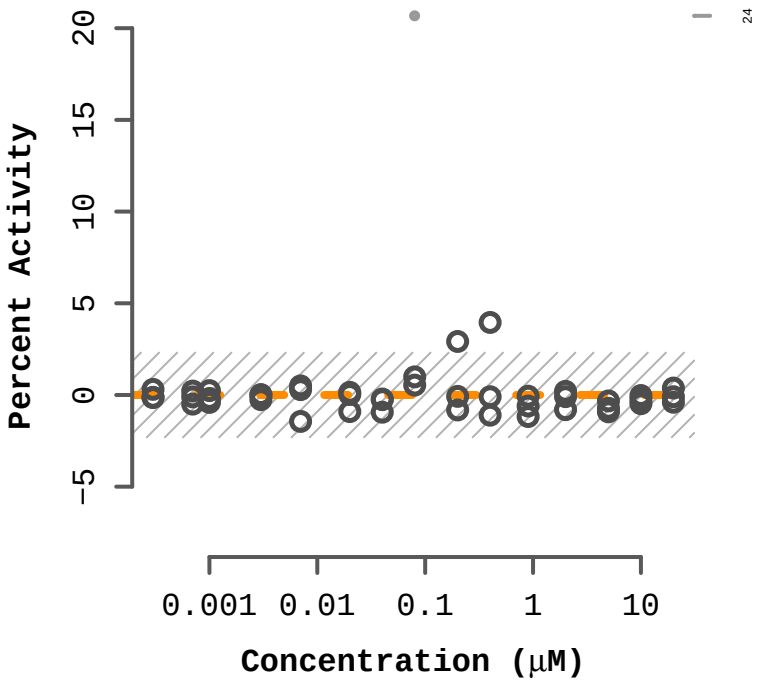
NAME: D-Glutamine
CHID: 46345 **CASRN:** 5959-95-5
SPID(S): Tox21_112047_1
M4ID: 12483349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.77	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 3.3 **MAX_MED:** 0.744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

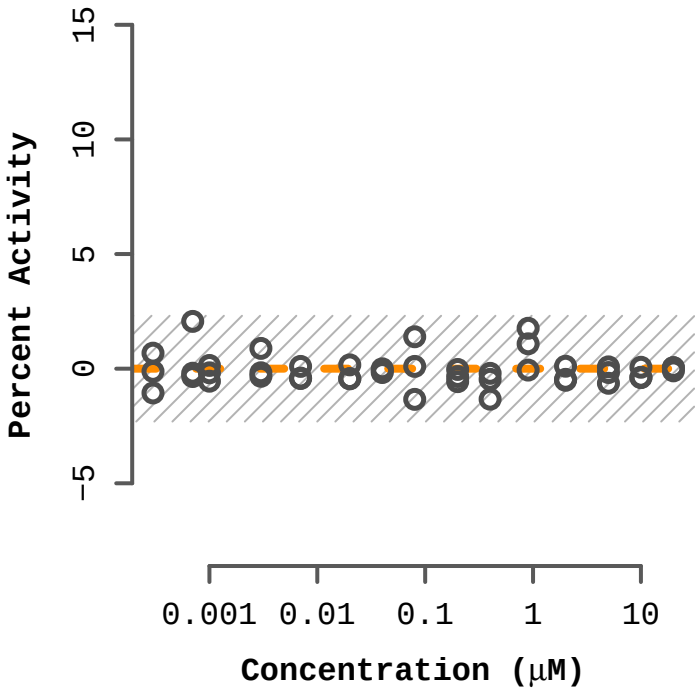
NAME: D−Leucine
CHID: 46347 **CASRN:** 328−38−1
SPID(S): Tox21_112049_1
M4ID: 12483348 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.37	NA	NA
PROB:	1	NA	NA
RMSE:	3.71	NA	NA

MAX_MEAN: 8.57 **MAX_MED:** 0.989 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

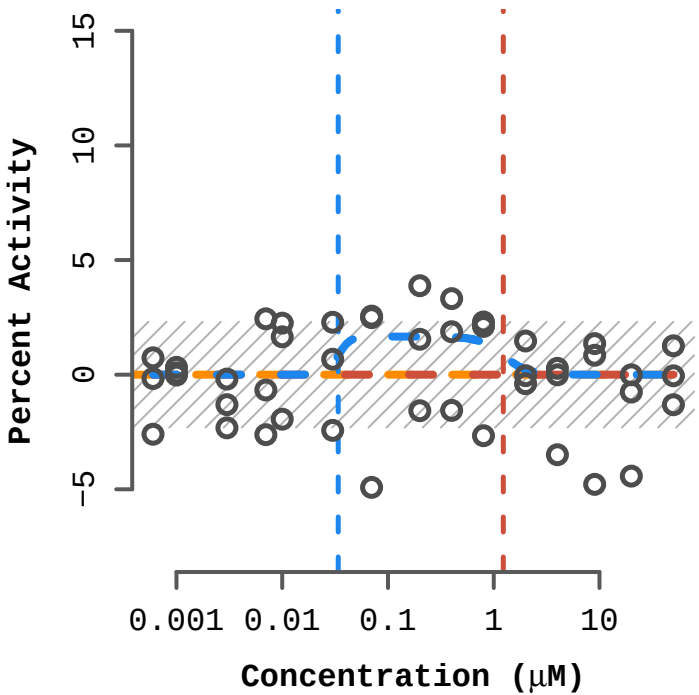
NAME: Dexfosfoserine
CHID: 46348 **CASRN:** 407-41-0
SPID(S): Tox21_112050_1
M4ID: 12483347

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	86.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Levonordefrin
CHID: 46349 CASRN: 829-74-3
SPID(S): Tox21_112051_1
M4ID: 12483346

HILL MODEL (in red):

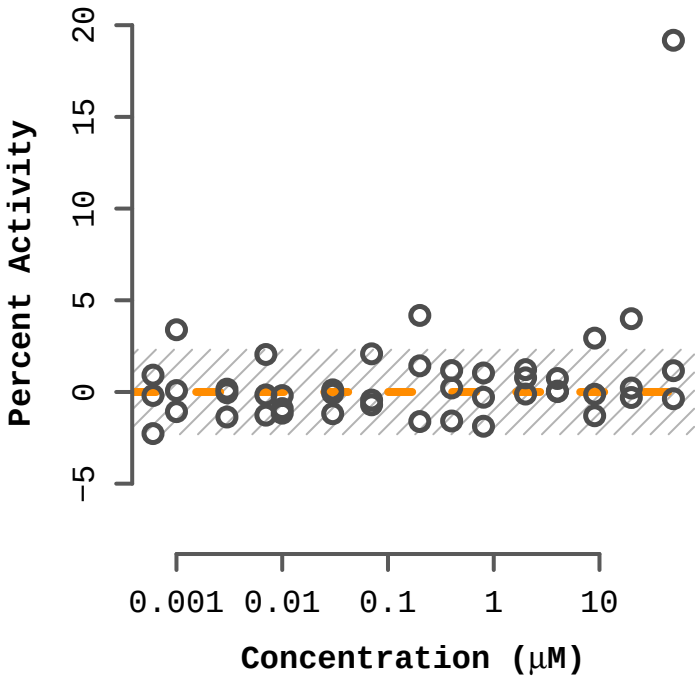
	tp	ga	gw
val:	1.14e-09	0.0903	0.72
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.66	−1.47	8	0.093	3.83
sd:	0.796	0.341	45.3	0.534	7.07

	CNST	HILL	GNLS
AIC:	201.23	207.23	206.17
PROB:	0.88	0.04	0.07
RMSE:	2.13	2.13	2.14

MAX_MEAN: 1.29 MAX_MED: 2.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

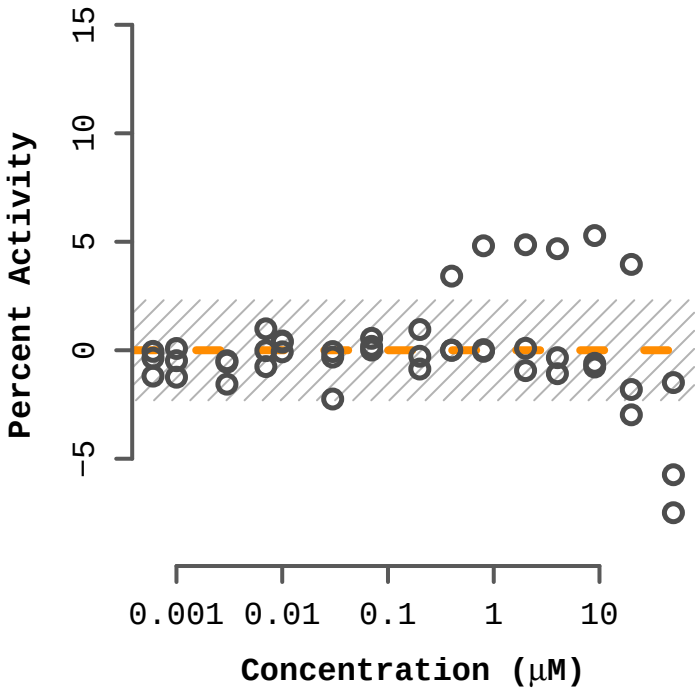
NAME: D−Nicotine
CHID: 46351 CASRN: 25162−00−9
SPID(S): Tox21_112053_1
M4ID: 12483344

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.92	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 6.66 MAX_MED: 1.43 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

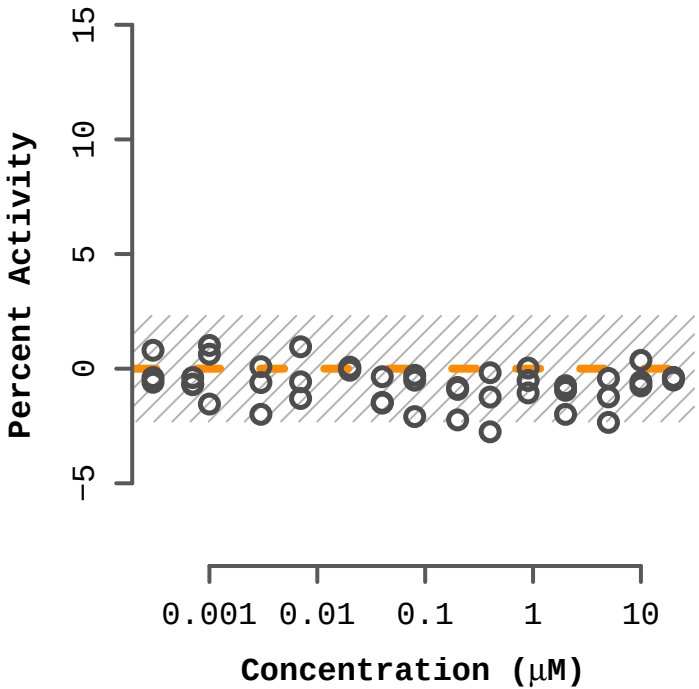
NAME: Otilonium bromide
CHID: 46357 CASRN: 26095-59-0
SPID(S): Tox21_112059_1
M4ID: 12483342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.68	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 1.6 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

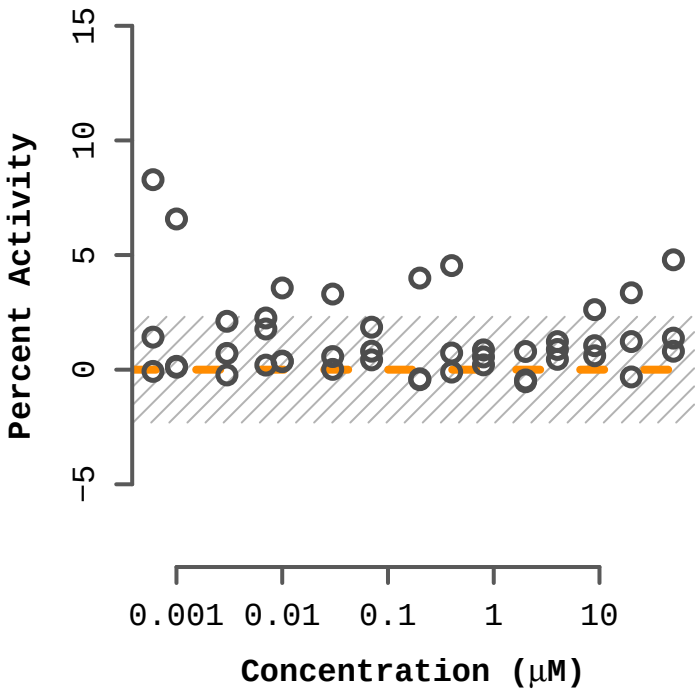
NAME: Myriocin
CHID: 46360 CASRN: 35891-70-4
SPID(S): Tox21_112062_1
M4ID: 12483341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.0358 **MAX_MED:** 0.634 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

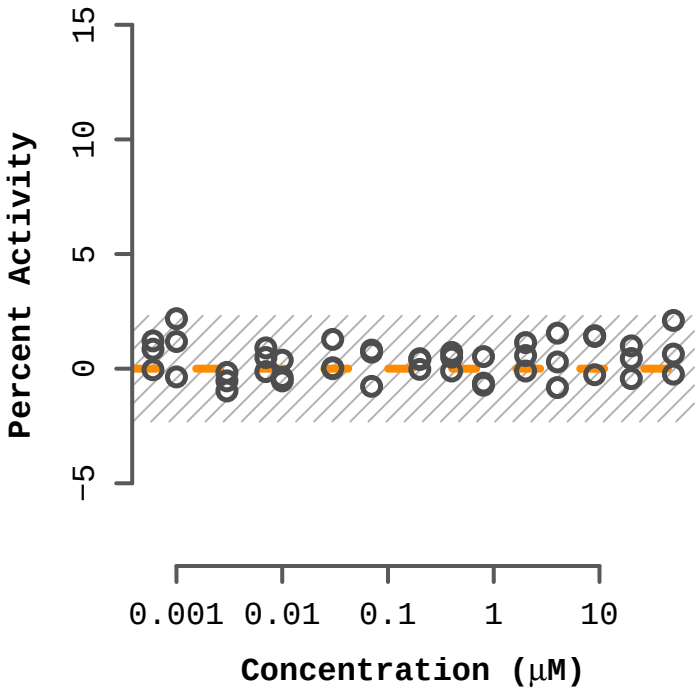
NAME: Mecloralurea
CHID: 46383 **CASRN:** 1954-79-6
SPID(S): Tox21_112123_1
M4ID: 12483304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.31	NA	NA
PROB:	1	NA	NA
RMSE:	2.33	NA	NA

MAX_MEAN: 3.21 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

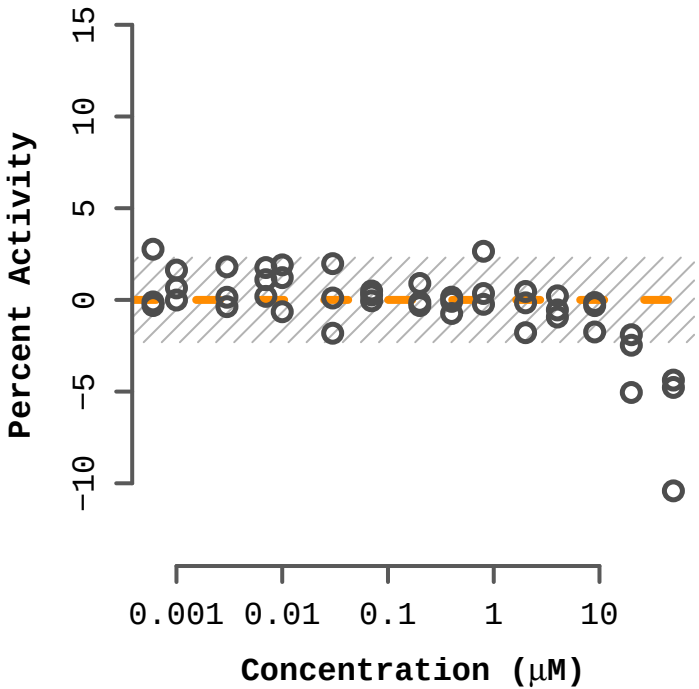
NAME: Molracetam
CHID: 46384 **CASRN:** 94746-78-8
SPID(S): Tox21_112124_1
M4ID: 12483303

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

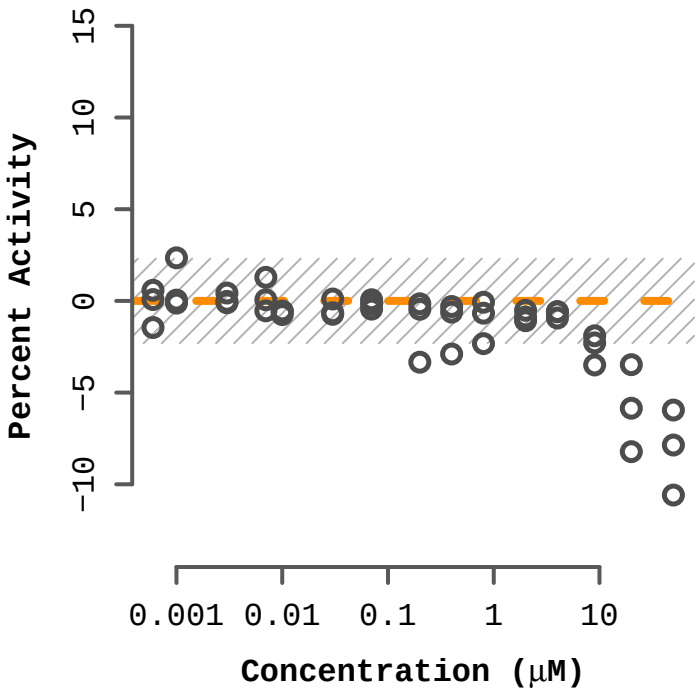
NAME: Amindocate
CHID: 46385 **CASRN:** 31386-24-0
SPID(S): Tox21_112125_1
M4ID: 12483302

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.53	NA	NA
PROB:	1	NA	NA
RMSE:	2.28	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

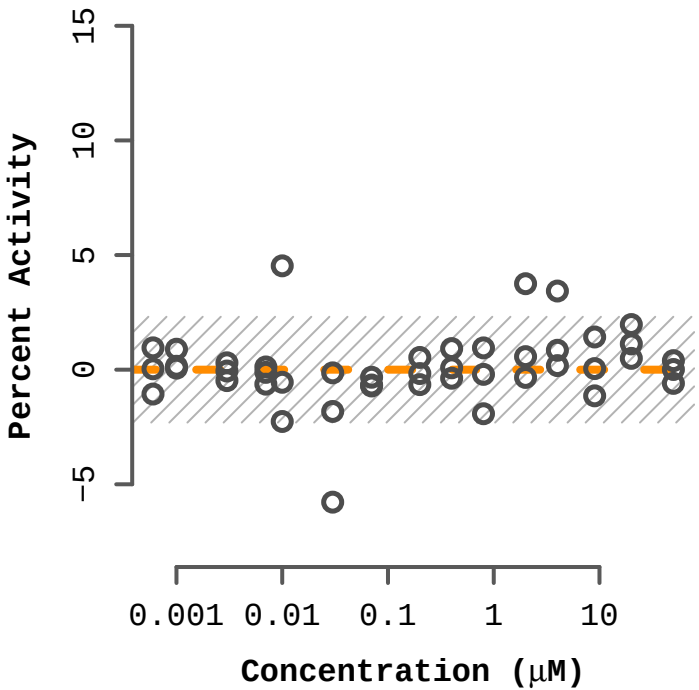
NAME: Cyclovalone
CHID: 46386 **CASRN:** 579-23-7
SPID(S): Tox21_112126_1
M4ID: 12483301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.46	NA	NA
PROB:	1	NA	NA
RMSE:	2.93	NA	NA

MAX_MEAN: 0.759 **MAX_MED:** 0.0742 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

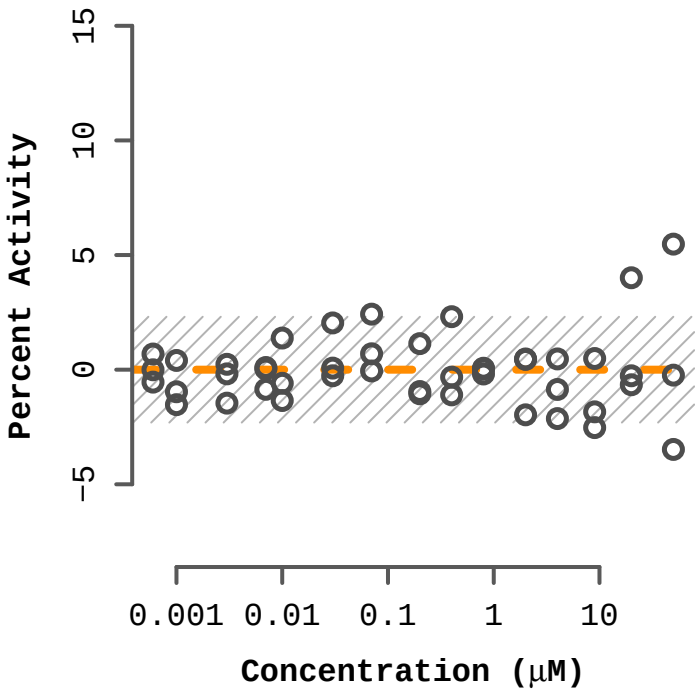
NAME: Amiphenazole
CHID: 46388 **CASRN:** 490-55-1
SPID(S): Tox21_112128_1
M4ID: 12483299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

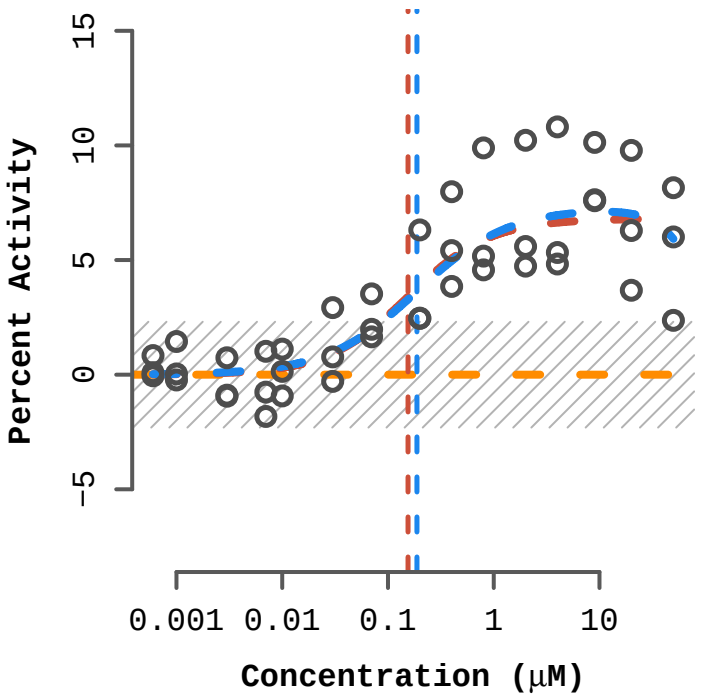
NAME: Lidofenin
CHID: 46389 **CASRN:** 59160-29-1
SPID(S): Tox21_112129_1
M4ID: 12483298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.695 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfisomidine
CHID: 46390 **CASRN:** 515-64-0
SPID(S): Tox21_112130_1
M4ID: 12483297

HILL MODEL (in red):

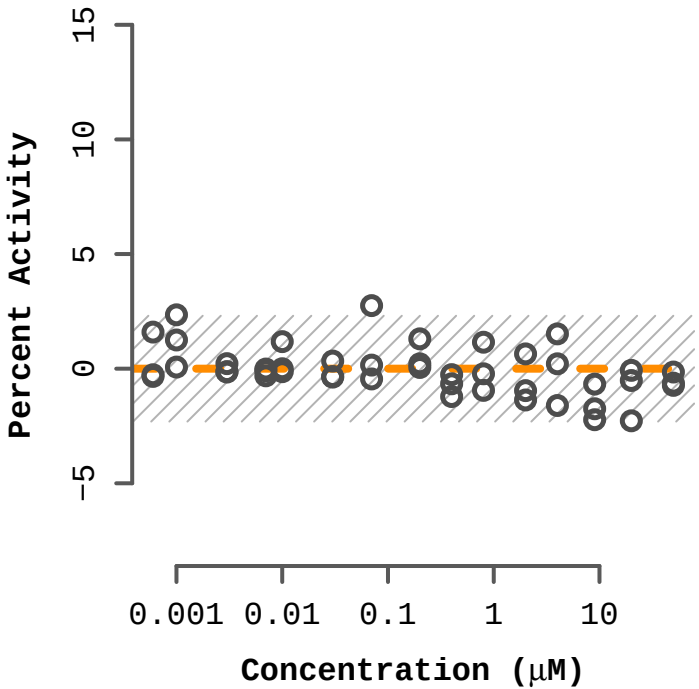
	tp	ga	gw
val:	6.81	−0.81	1.12
sd:	0.653	0.189	0.368

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.28	−0.726	1.01	1.99	2.27
sd:	1.05	0.242	0.363	0.57	4.33

	CNST	HILL	GNLS
AIC:	277.81	191.72	195
PROB:	0	0.84	0.16
RMSE:	5.05	1.85	1.8

MAX_MEAN: 8.45 **MAX_MED:** 7.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

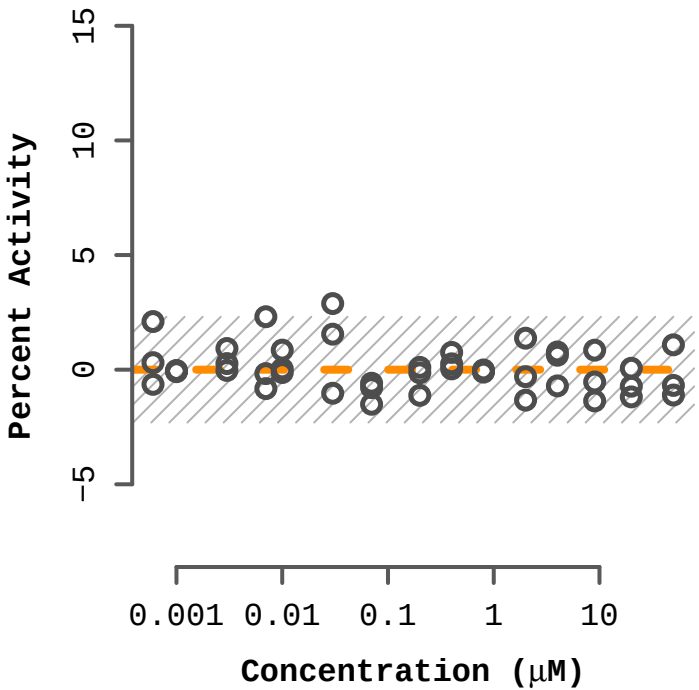
NAME: Nithiamide
CHID: 46391 **CASRN:** 140-40-9
SPID(S): Tox21_112132_1
M4ID: 12483295

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

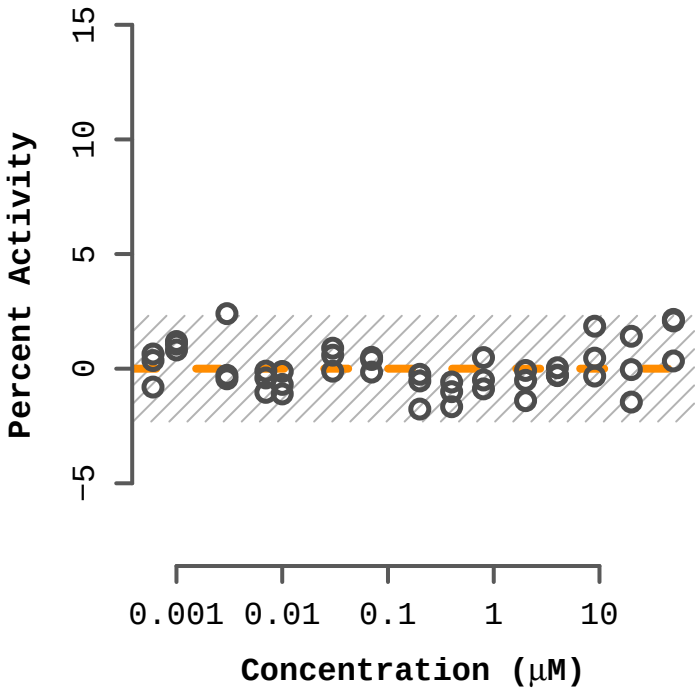
NAME: Nicothiazone
CHID: 46392 **CASRN:** 555-90-8
SPID(S): Tox21_112133_1
M4ID: 12483294

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

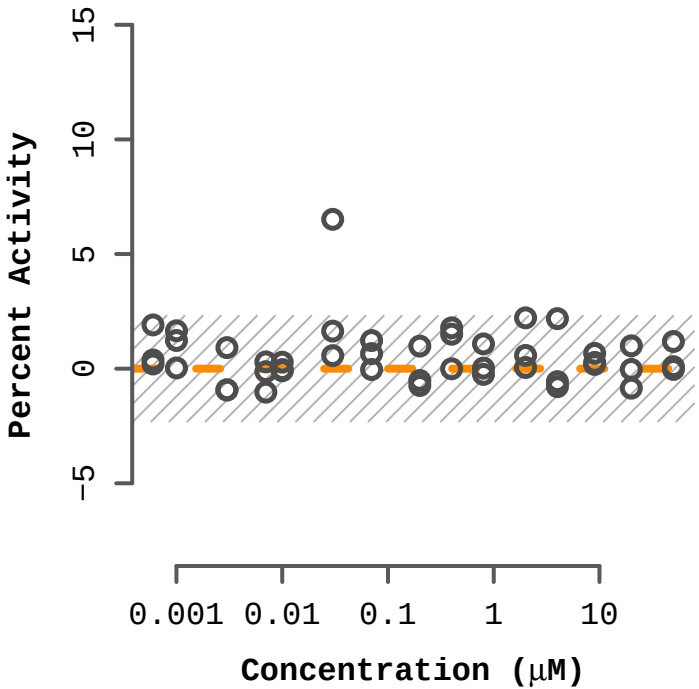
NAME: Glyoctamide
CHID: 46394 **CASRN:** 1038-59-1
SPID(S): Tox21_112135_1
M4ID: 12483293

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

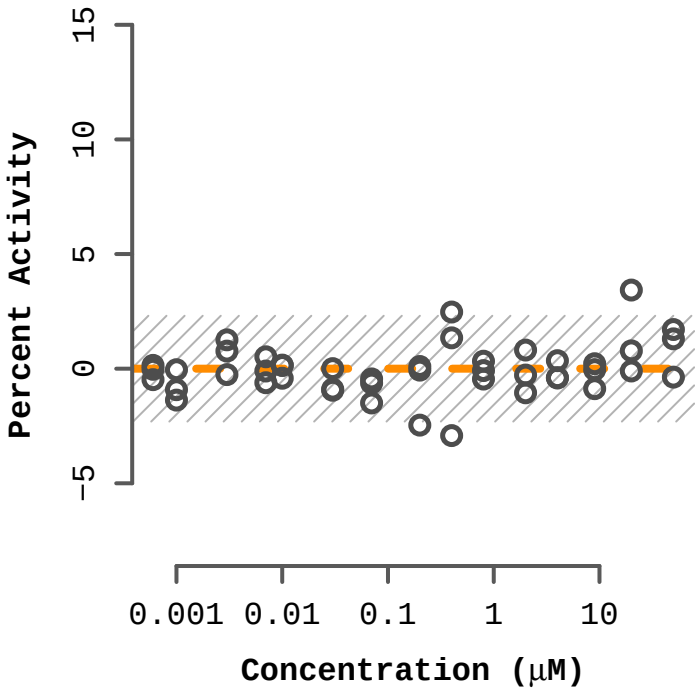
NAME: Tolpentamide
CHID: 46395 **CASRN:** 1027-87-8
SPID(S): Tox21_112136_1
M4ID: 12483292

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 2.91 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

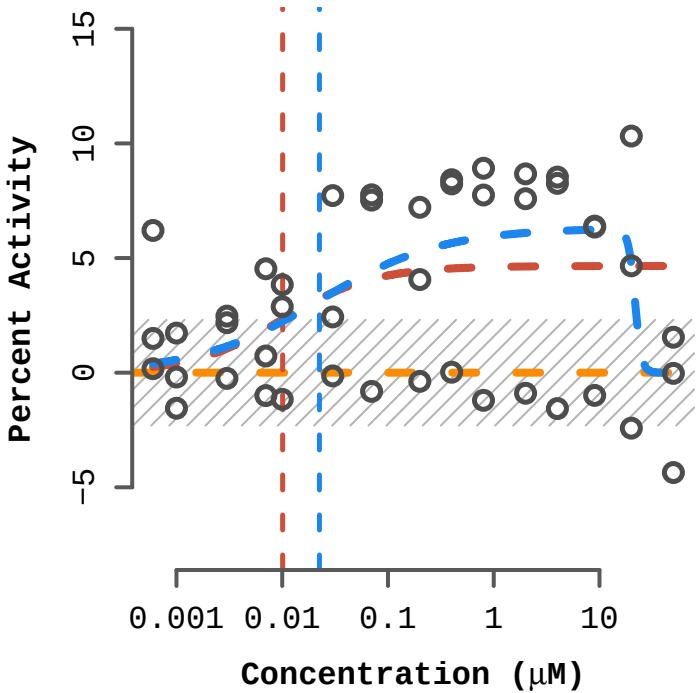
NAME: DL-alpha Tocopheryl nicotinate
CHID: 46396 CASRN: 43119-47-7
SPID(S): Tox21_112137_1
M4ID: 12483291

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nihydrazone
CHID: 46398 **CASRN:** 67-28-7
SPID(S): Tox21_112139_1
M4ID: 12483290

HILL MODEL (in red):

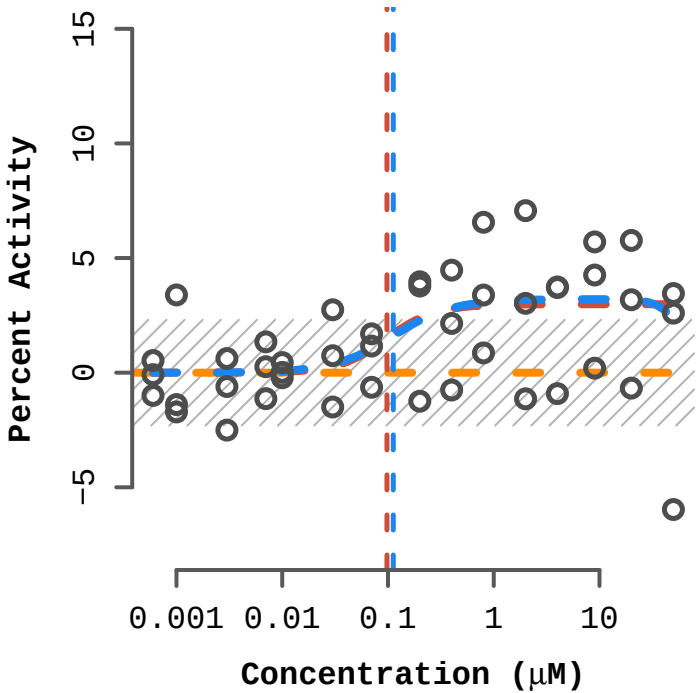
	tp	ga	gw
val:	4.65	−2	1.01
sd:	1.02	0.487	0.951

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.31	−1.65	0.748	1.34	13.8
sd:	1.36	0.5	0.552	0.497	198

	CNST	HILL	GNLS
AIC:	279.12	262.08	258.03
PROB:	0	0.12	0.88
RMSE:	5.06	3.82	3.61

MAX_MEAN: 5.56 **MAX_MED:** 8.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nifuraldezone
CHID: 46399 CASRN: 3270-71-1
SPID(S): Tox21_112140_1
M4ID: 12483289

HILL MODEL (in red):

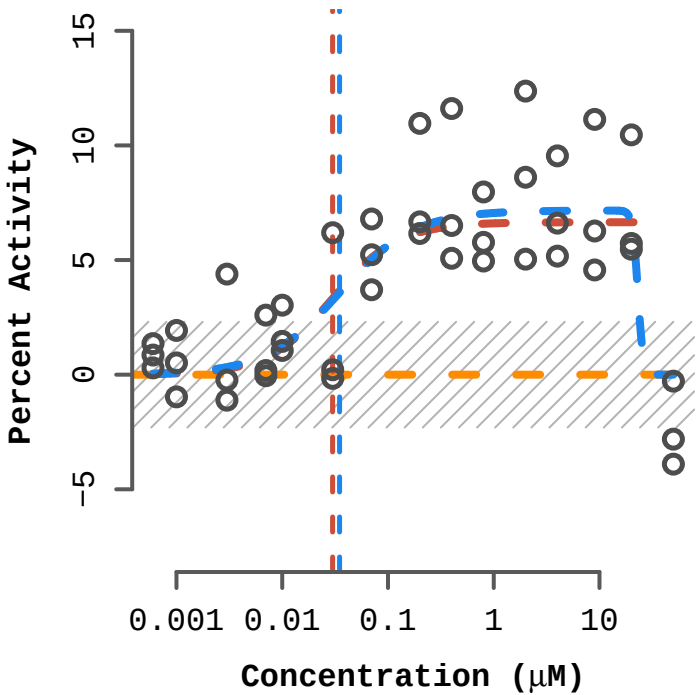
	tp	ga	gw
val:	2.99	−1.01	1.91
sd:	0.587	0.318	3.07

GAIN-LOSS MODEL (in blue):

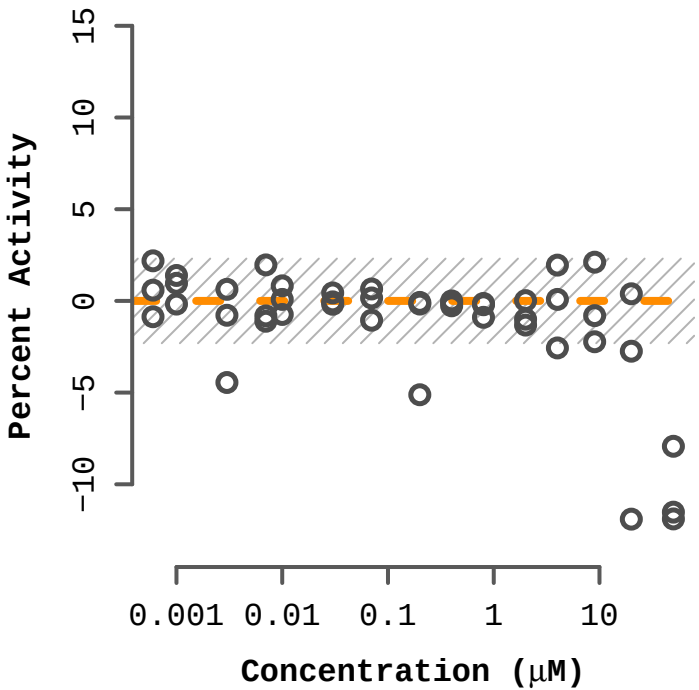
	tp	ga	gw	la	lw
val:	3.21	−0.95	1.54	1.81	3.84
sd:	0.787	0.394	1.88	0.882	30.5

	CNST	HILL	GNLS
AIC:	228.71	210.64	214.26
PROB:	0	0.86	0.14
RMSE:	2.96	2.41	2.36

MAX_MEAN: 3.6 MAX_MED: 4.26 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Myralact
CHID:    46400   CASRN: 15518-87-3
SPID(S): Tox21_112141_1
M4ID:    12483288

HILL MODEL (in red):
      tp       ga       gw
val:  6.65     -1.52    1.4
sd:   0.604    0.228    0.641

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.16     -1.46    1.24     1.36     17.2
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  291.25      233.21      215.2
PROB: 0           0           1
RMSE: 5.76        3.22        2.26

MAX_MEAN: 8.67      MAX_MED: 8.61      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

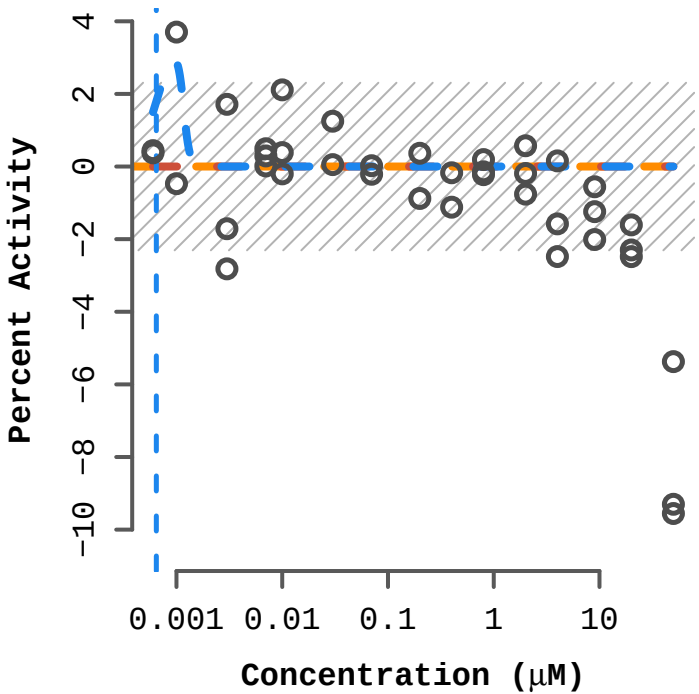
NAME: Tiliquinol
CHID: 46401 **CASRN:** 5541-67-3
SPID(S): Tox21_112142_1
M4ID: 12483287

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.96	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 0.726 **MAX_MED:** 0.962 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nifuroxime
CHID: 46402 CASRN: 6236-05-1
SPID(S): Tox21_112143_1
M4ID: 12483286

HILL MODEL (in red):

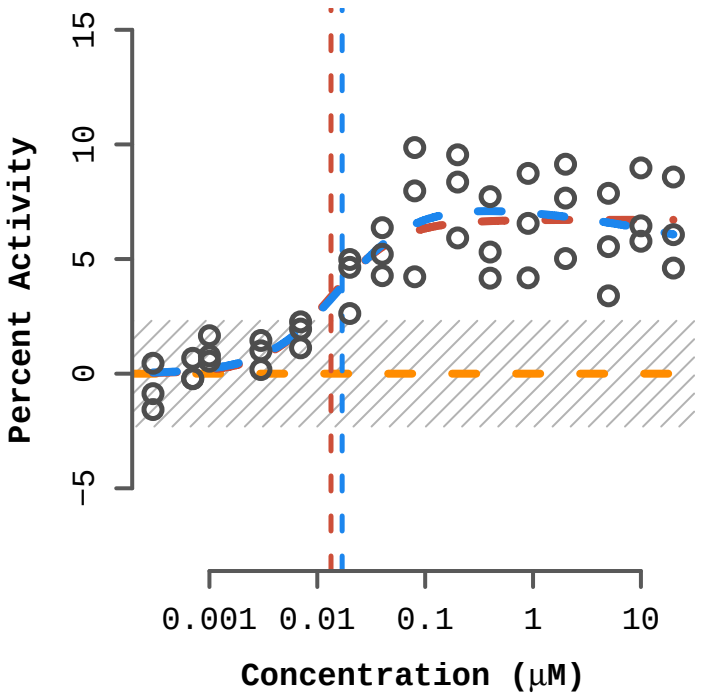
	tp	ga	gw
val:	4.4e-09	−3.69	4.43
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.59	−3.19	4.59	−2.93	15.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	232.4	238.4	237.91
PROB:	0.9	0.04	0.06
RMSE:	3.49	3.49	3.39

MAX_MEAN: 3.65 **MAX_MED:** 3.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxfenicine
CHID: 46403 CASRN: 32462-30-9
SPID(S): Tox21_112144_1
M4ID: 12483285

HILL MODEL (in red):

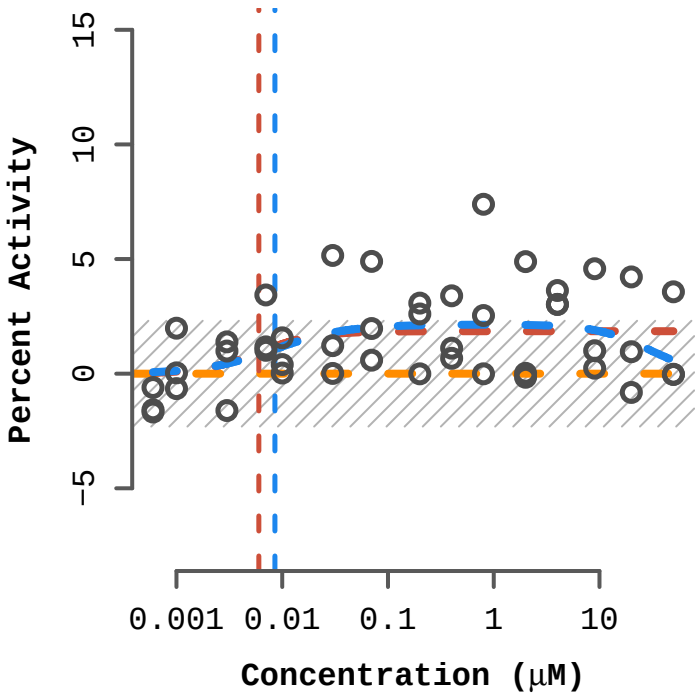
	tp	ga	gw
val:	6.71	−1.87	1.41
sd:	0.406	0.109	0.393

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.9	−1.77	1.25	3.04	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	288.35	176.85	180
PROB:	0	0.83	0.17
RMSE:	5.45	1.52	1.51

MAX_MEAN: 7.94 **MAX_MED:** 8.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Idrocilamide
CHID: 46404 CASRN: 6961-46-2
SPID(S): Tox21_112145_1
M4ID: 12483284

HILL MODEL (in red):

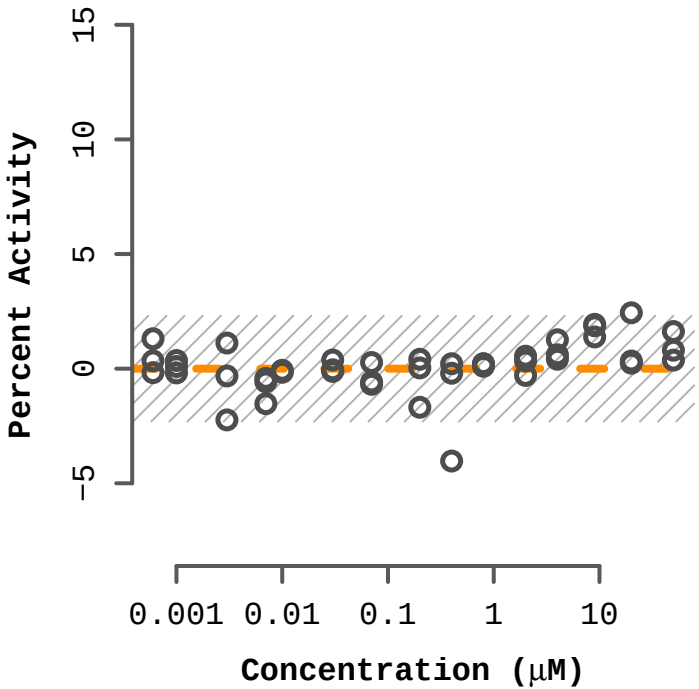
	tp	ga	gw
val:	1.85	−2.22	1.65
sd:	0.412	0.431	1.66

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.15	−2.07	1.3	1.46	1.76
sd:	0.552	0.5	1.29	0.5	1.92

	CNST	HILL	GNLS
AIC:	212.7	193.22	195.8
PROB:	0	0.78	0.22
RMSE:	2.53	1.83	1.81

MAX_MEAN: 3.31 **MAX_MED:** 3.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

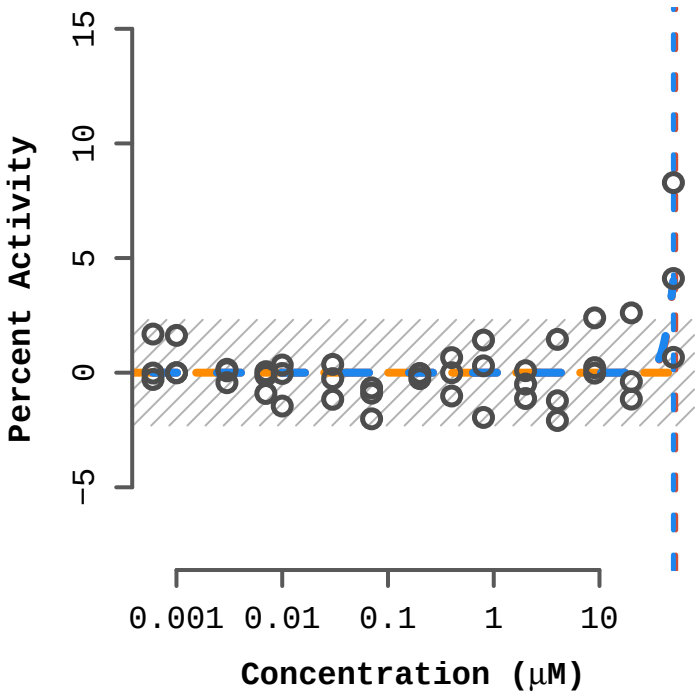
NAME: Guaiacol carbonate
CHID: 46405 CASRN: 553-17-3
SPID(S): Tox21_112147_1
M4ID: 12483283

HILL MODEL: Not applicable.

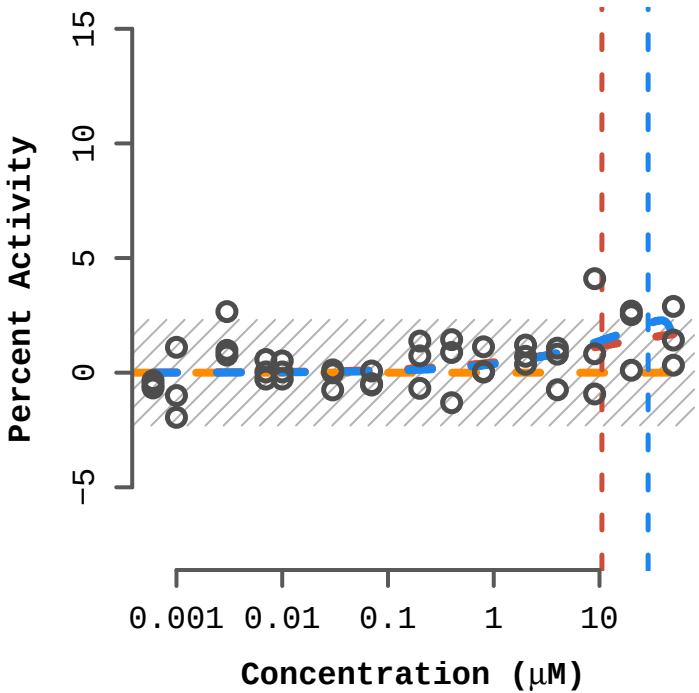
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.87 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Benzoylpas
CHID:    46406   CASRN: 13898-58-3
SPID(S): Tox21_112148_1
M4ID:    12483282

HILL MODEL (in red):
      tp       ga       gw
val:  9.93     1.72     7.9
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.99     1.7      8        3.12     2.39
sd:   7.83     0.0981   22.1     380      662

      CNST        HILL        GNLS
AIC:  156.27      154.04      158.04
PROB: 0.22        0.68        0.09
RMSE: 1.72        1.3         1.3

MAX_MEAN: 4.36      MAX_MED: 4.11      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Eprobemide
CHID: 46409 CASRN: 87940-60-1
SPID(S): Tox21_112151_1
M4ID: 12483280

HILL MODEL (in red):

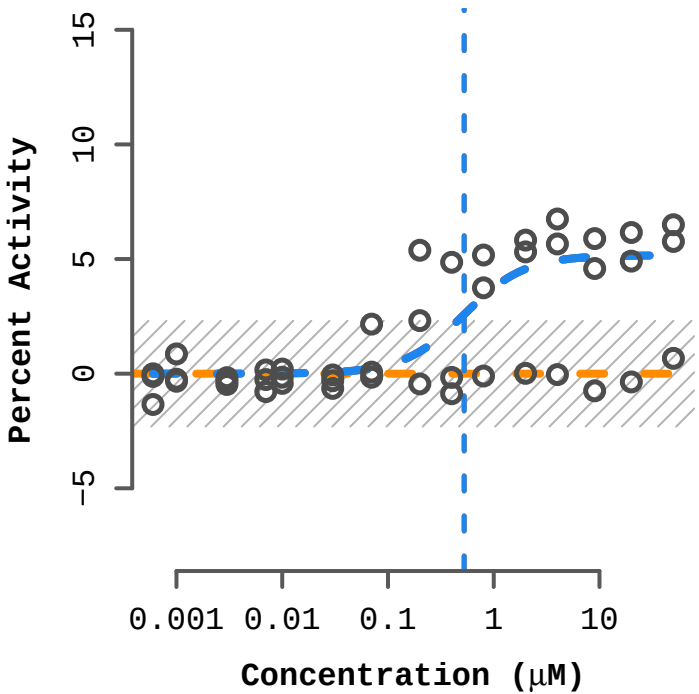
	tp	ga	gw
val:	2.33	1.02	0.613
sd:	2.64	1.81	0.576

GAIN-LOSS MODEL (in blue):

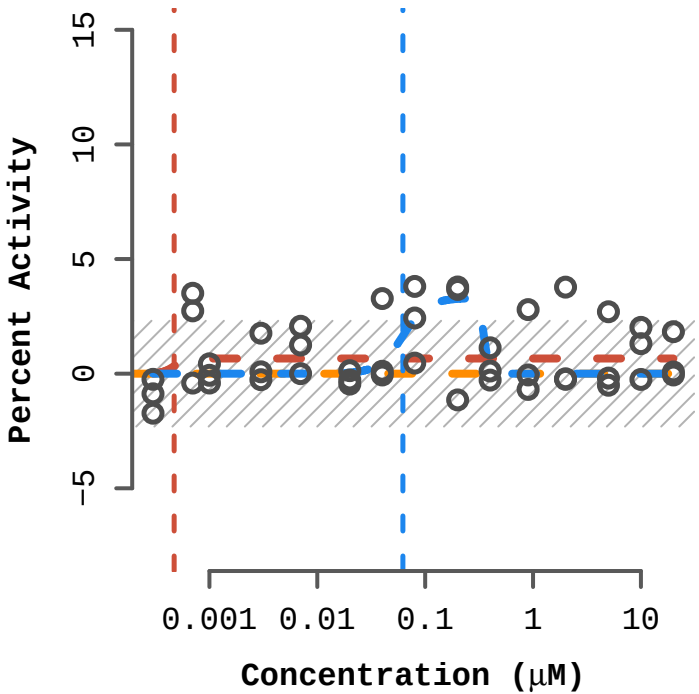
	tp	ga	gw	la	lw
val:	4.26	1.46	0.699	1.71	12.6
sd:	8.24	1.88	0.417	0.0834	96.4

	CNST	HILL	GNLS
AIC:	148.04	139.53	142.94
PROB:	0.01	0.84	0.15
RMSE:	1.27	1.05	1.04

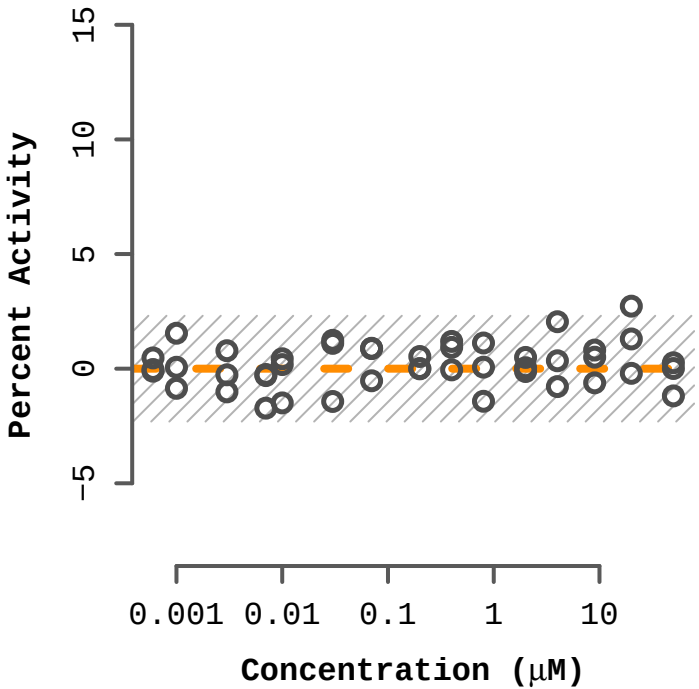
MAX_MEAN: 1.78 **MAX_MED:** 2.53 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Oxaceprol
CHID:    46410   CASRN: 33996-33-7
SPID(S): Tox21_112152_1
M4ID:    12483279

HILL MODEL (in red):
      tp       ga       gw
val:  5.16     -0.28    1.52
sd:   0.6      0.265    1.06

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.16     -0.28    1.52     3.12     5.12
sd:   0.6      0.265    1.06     981      3550

      CNST        HILL        GNLS
AIC:  230.42      197.99      201.99
PROB: 0           0.88        0.12
RMSE: 3.14        2.15        2.15

MAX_MEAN: 4.31      MAX_MED: 5.77      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    L-Threonine
CHID:    46412   CASRN: 72-19-5
SPID(S): Tox21_112154_1
M4ID:    12483278

HILL MODEL (in red):
      tp       ga       gw
val:  0.662    -3.33    8
sd:   0.245    0.231    10.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.3      -1.21    3.8      -0.456   17.3
sd:   0.873    0.151    2.99     2.1      627

      CNST        HILL        GNLS
AIC:  177.41      175.3       174.86
PROB: 0.13        0.39        0.48
RMSE: 1.73        1.5         1.55

MAX_MEAN: 2.23      MAX_MED: 3.68      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

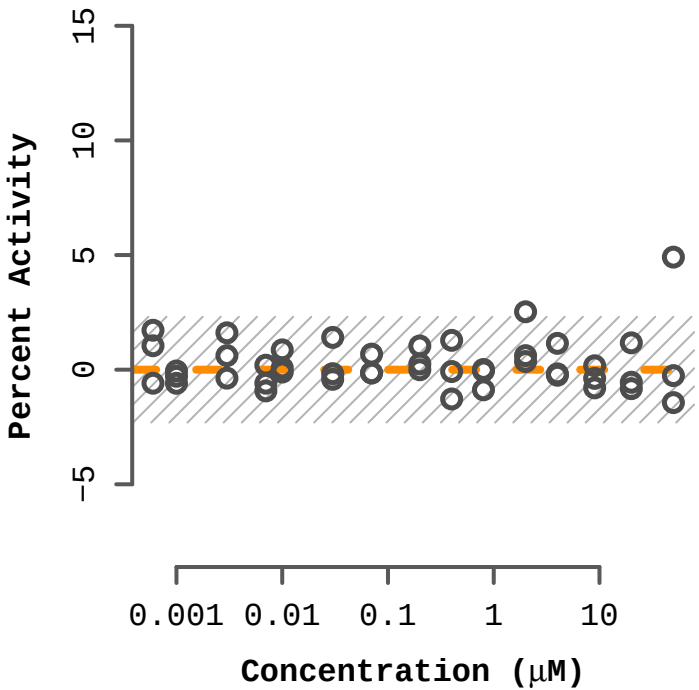
NAME: Muromonab-CD3
CHID: 46414 **CASRN:** 140608-64-6
SPID(S): Tox21_112156_1
M4ID: 12483277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

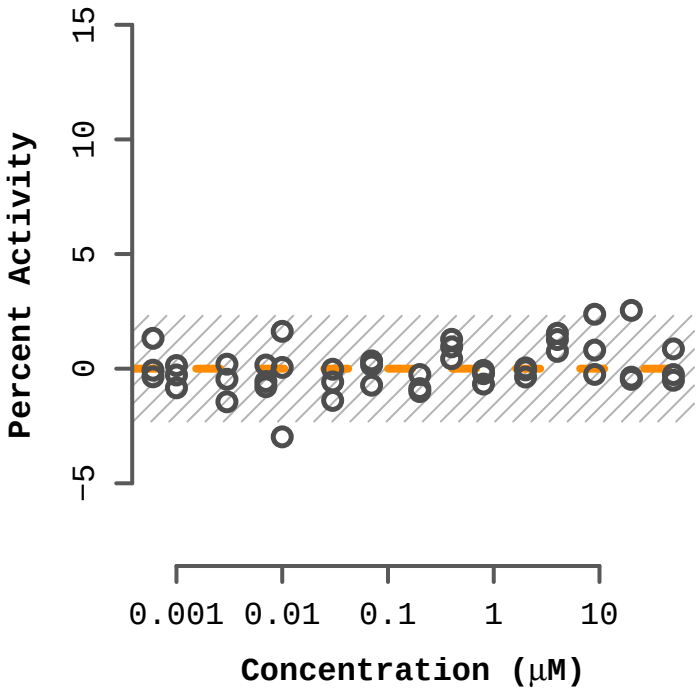
NAME: Camylofin
CHID: 46415 **CASRN:** 54-30-8
SPID(S): Tox21_112157_1
M4ID: 12483276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

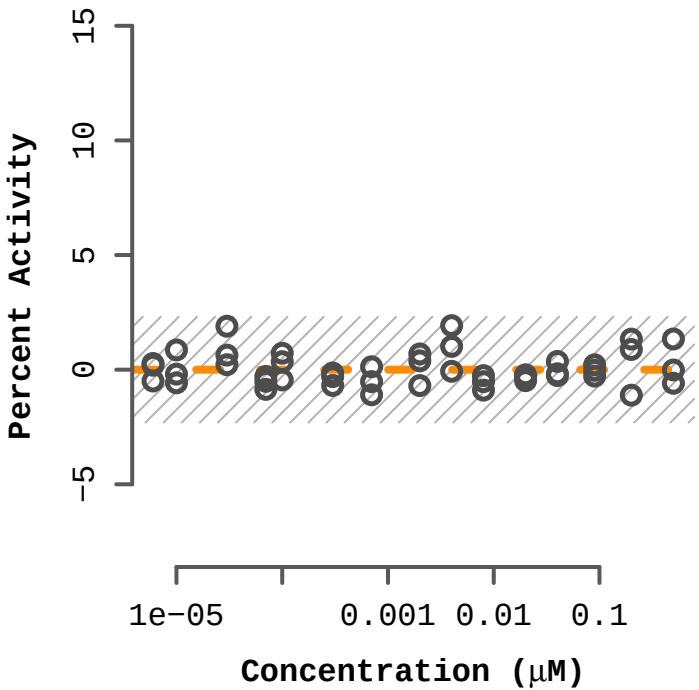
NAME: Cinromide
CHID: 46417 **CASRN:** 58473-74-8
SPID(S): Tox21_112161_1
M4ID: 12483274

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

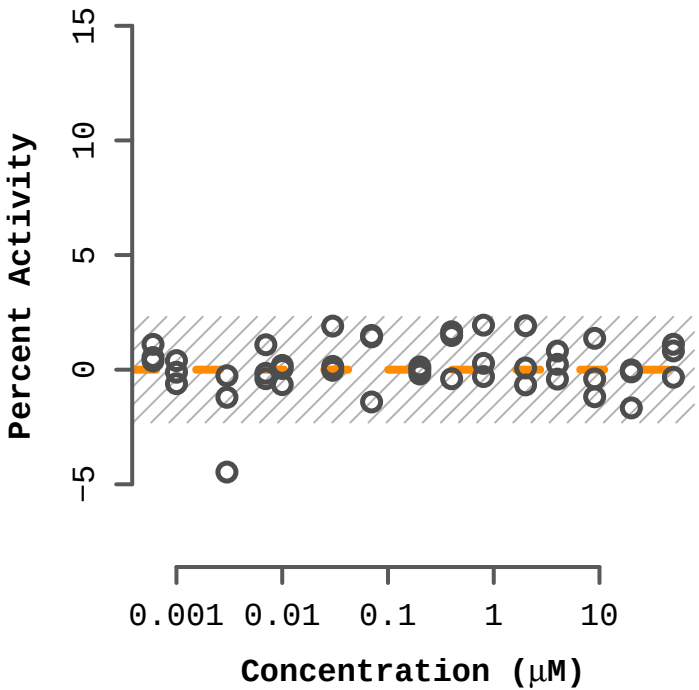
NAME: L-Cystine
CHID: 46418 **CASRN:** 56-89-3
SPID(S): Tox21_112162_1
M4ID: 12483273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.957 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

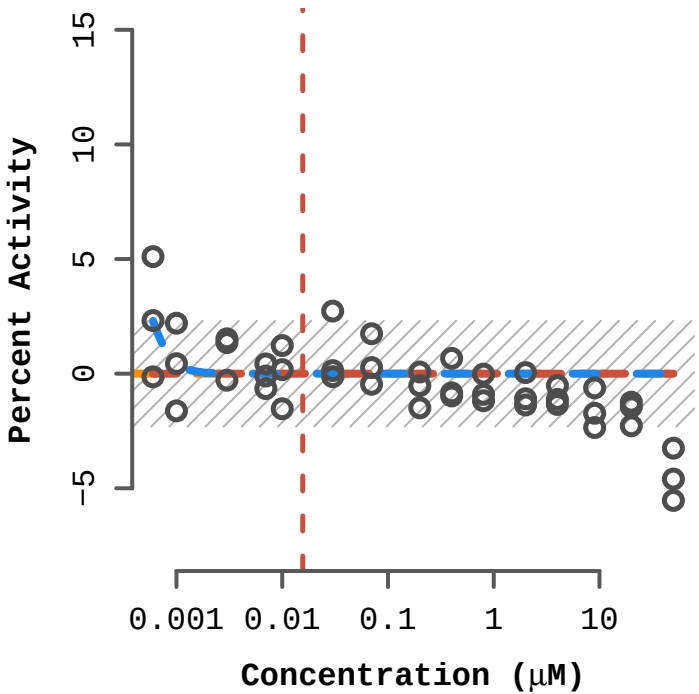
NAME: Parapropamol
CHID: 46419 **CASRN:** 1693-37-4
SPID(S): Tox21_112163_1
M4ID: 12483272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Buformin
CHID: 46420 CASRN: 692-13-7
SPID(S): Tox21_112164_1
M4ID: 12483271

HILL MODEL (in red):

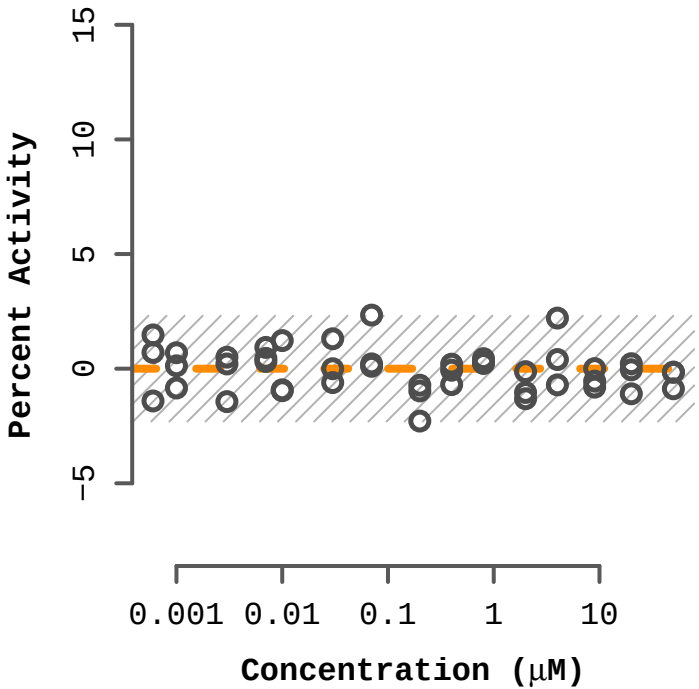
	tp	ga	gw
val:	2.77e-11	-1.81	1.24
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.13	-4.31	7.08	-3.28	3.9
sd:	38.7	7300	47800	1.26	10.2

	CNST	HILL	GNLS
AIC:	180.13	186.13	186.18
PROB:	0.91	0.05	0.04
RMSE:	1.84	1.84	1.72

MAX_MEAN: 2.43 MAX_MED: 2.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

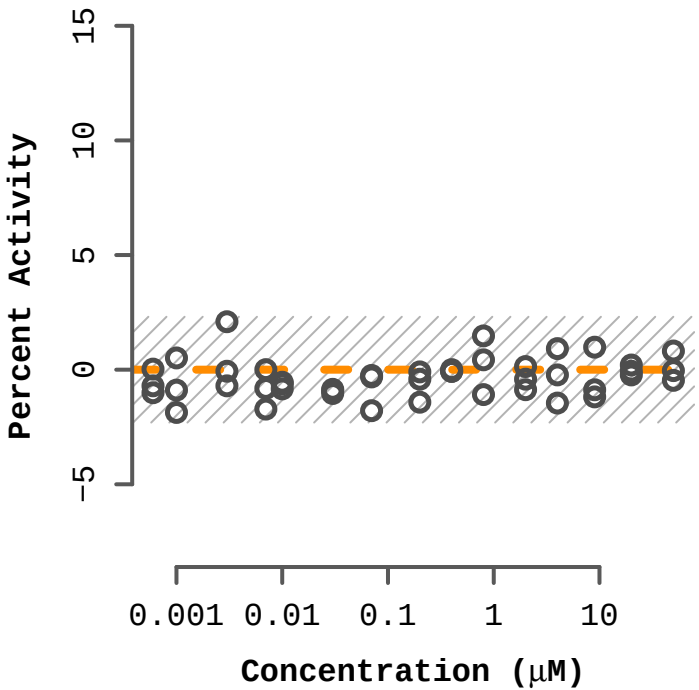
NAME: 4-Phenolsulfonic acid
CHID: 46421 **CASRN:** 98-67-9
SPID(S): Tox21_112165_1
M4ID: 12483270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.885 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

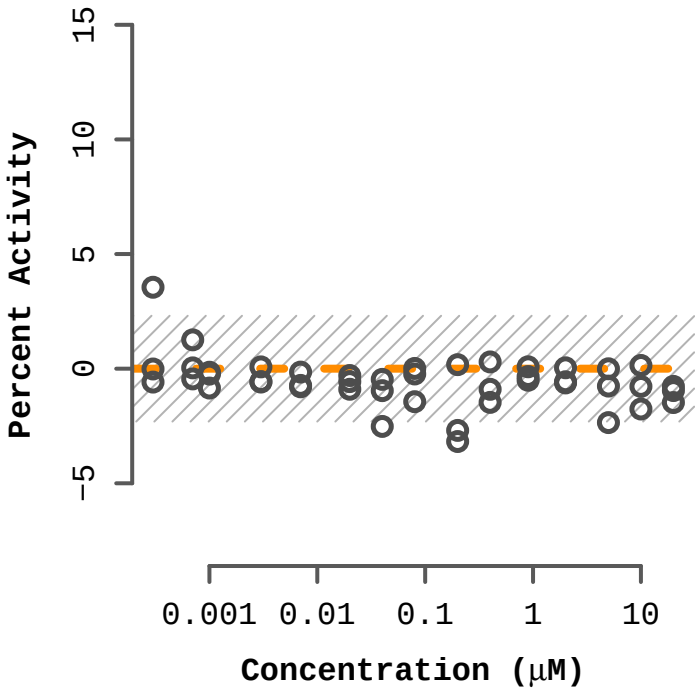
NAME: Droxidopa
CHID: 46422 CASRN: 23651-95-8
SPID(S): Tox21_112167_1
M4ID: 12483268

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.44 **MAX_MED:** 0.432 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

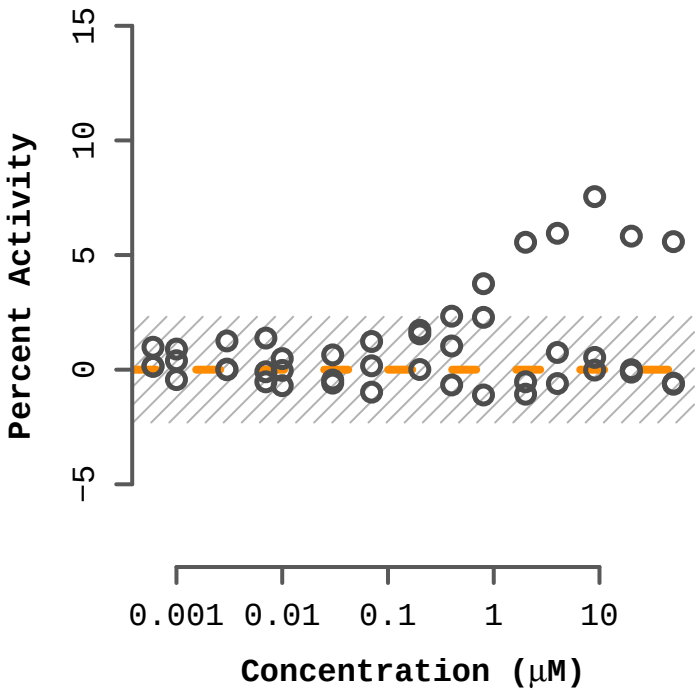
NAME: Azaclorzine
CHID: 46423 **CASRN:** 49864-70-2
SPID(S): Tox21_112168_1
M4ID: 12483267

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.986 **MAX_MED:** 0.036 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

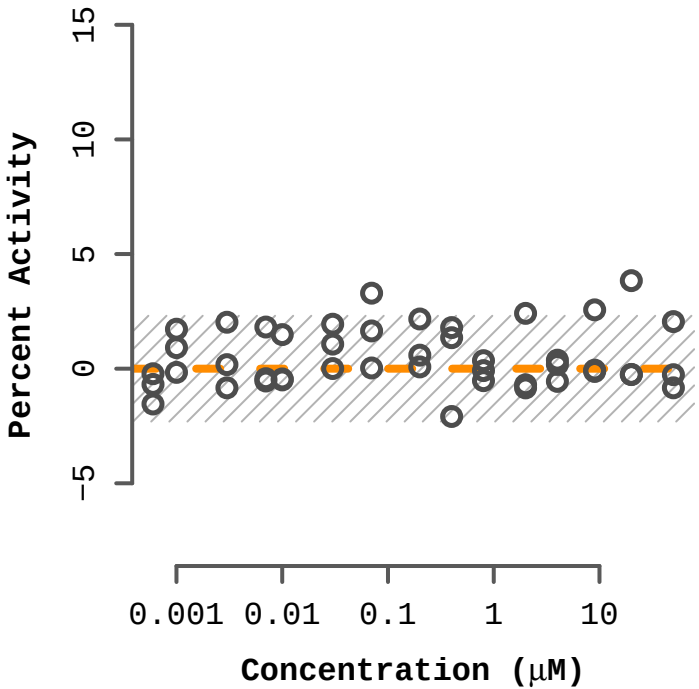
NAME: Clofexamide
CHID: 46424 **CASRN:** 1223-36-5
SPID(S): Tox21_112169_1
M4ID: 12483266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.23	NA	NA
PROB:	1	NA	NA
RMSE:	2.28	NA	NA

MAX_MEAN: 2.69 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

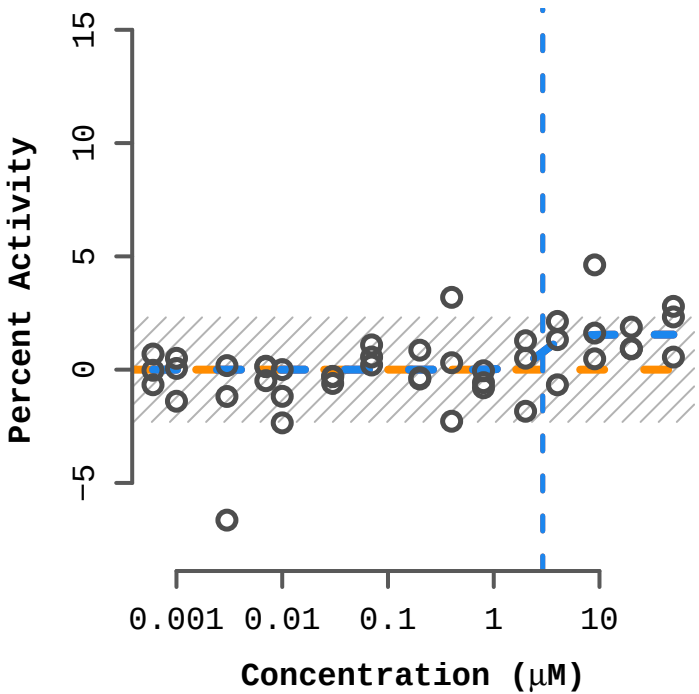
NAME: Sulfacarbamide
CHID: 46425 **CASRN:** 547-44-4
SPID(S): Tox21_112170_1
M4ID: 12483265

HILL MODEL: Not applicable.

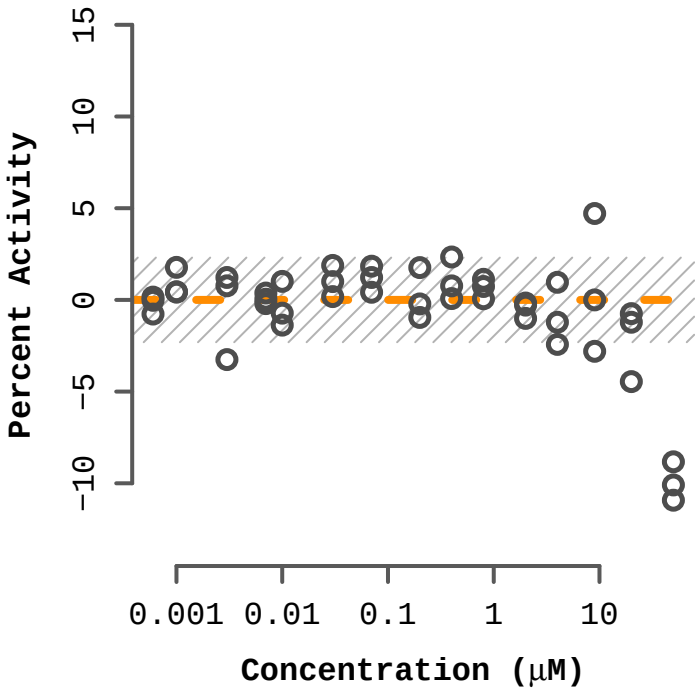
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.65 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Talinolol
CHID:    46426   CASRN: 57460-41-0
SPID(S): Tox21_112171_1
M4ID:    12483264

HILL MODEL (in red):
      tp       ga       gw
val:  1.55     0.463    4.05
sd:   0.382    0.246    4.55

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.55     0.463    4.05     3.04     6.05
sd:   0.382    0.246    4.55     1930     8710

      CNST        HILL        GNLS
AIC:  167.02      155.51      159.51
PROB: 0           0.88        0.12
RMSE: 1.7         1.49        1.49

MAX_MEAN: 2.24      MAX_MED: 2.33      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

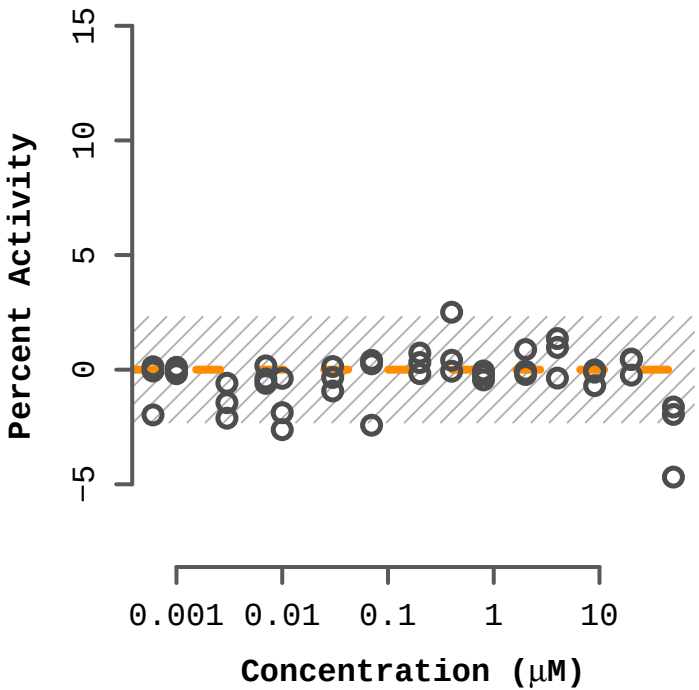
NAME: Lomerizine dihydrochloride
CHID: 46427 **CASRN:** 101477-54-7
SPID(S): Tox21_112172_1
M4ID: 12483263

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

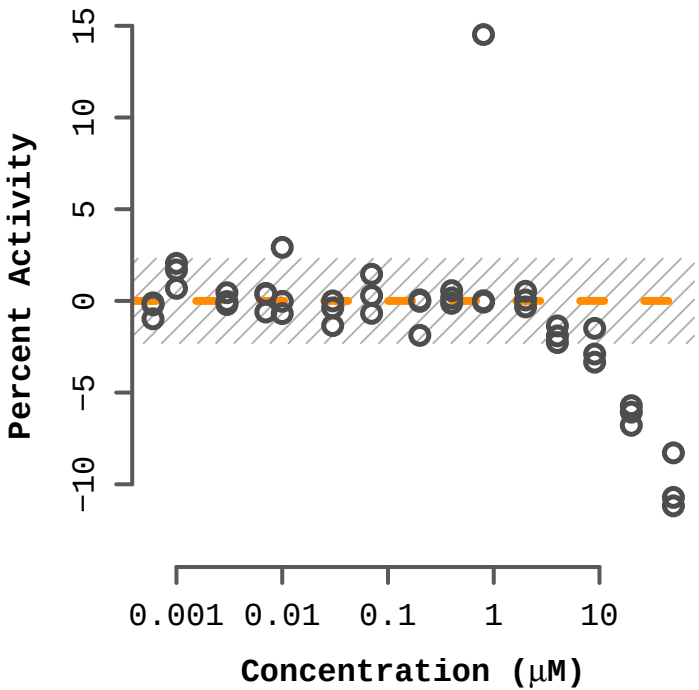
NAME: Lanoconazole
CHID: 46428 **CASRN:** 101530-10-3
SPID(S): Tox21_112173_1
M4ID: 12483262

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.951 **MAX_MED:** 0.973 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

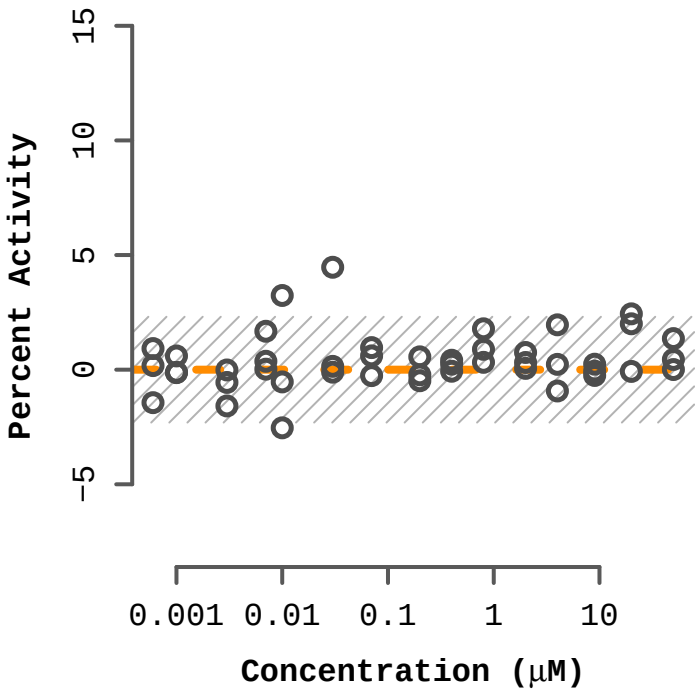
NAME: Lacidipine
CHID: 46429 **CASRN:** 103890-78-4
SPID(S): Tox21_112174_1
M4ID: 12483261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.6	NA	NA
PROB:	1	NA	NA
RMSE:	3.93	NA	NA

MAX_MEAN: 4.82 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

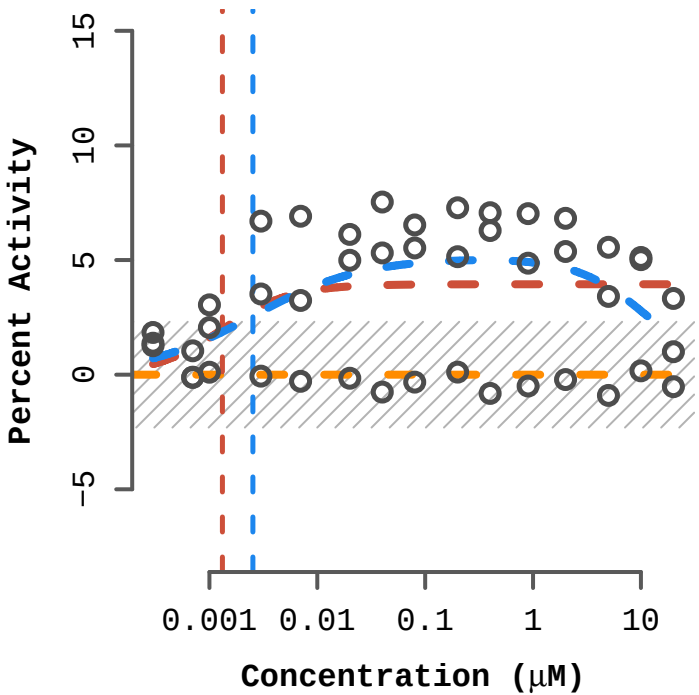
NAME: Fropenem
CHID: 46430 CASRN: 106560-14-9
SPID(S): Tox21_112175_1
M4ID: 12483260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.5 MAX_MED: 2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Danofloxacin
CHID: 46432 CASRN: 112398-08-0
SPID(S): Tox21_112177_1
M4ID: 12483258

HILL MODEL (in red):

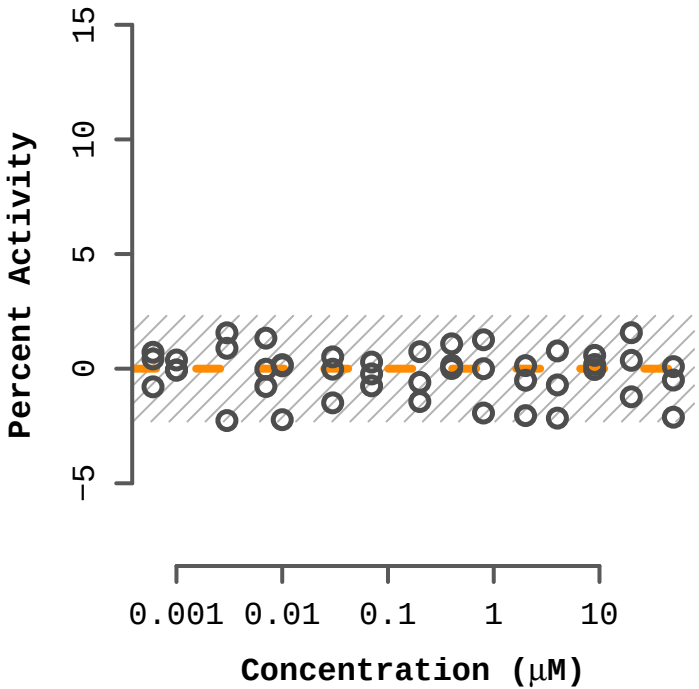
	tp	ga	gw
val:	3.94	−2.88	1.36
sd:	0.613	0.321	1.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.12	−2.6	0.853	1.06	1.32
sd:	1.42	0.539	0.741	0.363	1.72

	CNST	HILL	GNLS
AIC:	262.93	233.19	232.75
PROB:	0	0.45	0.55
RMSE:	4.17	2.76	2.73

MAX_MEAN: 4.18 MAX_MED: 6.29 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

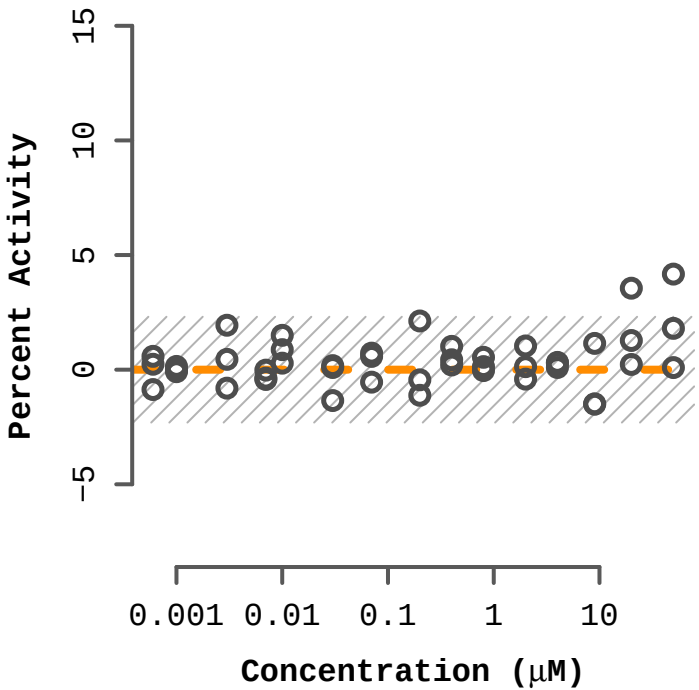
NAME: Dofetilide
CHID: 46433 **CASRN:** 115256-11-6
SPID(S): Tox21_112178_1
M4ID: 12483257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.414 **MAX_MED:** 0.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

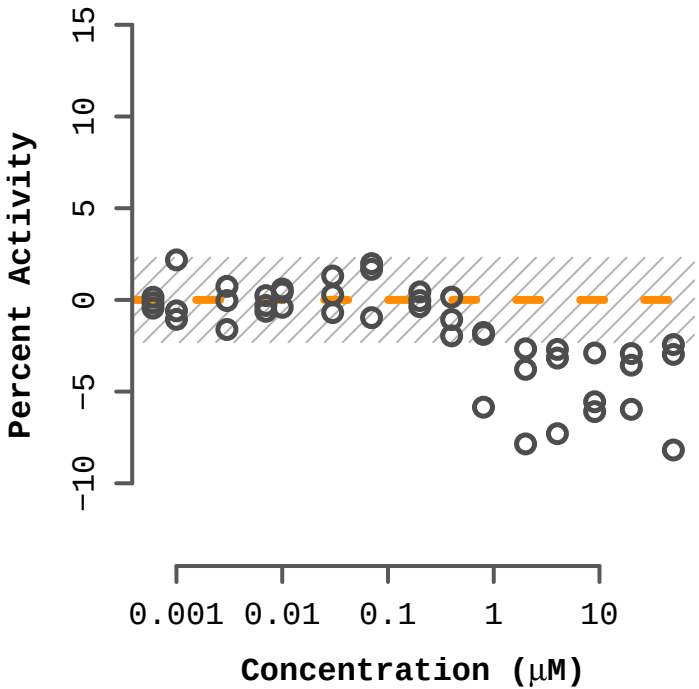
NAME: Lafutidine
CHID: 46434 **CASRN:** 118288-08-7
SPID(S): Tox21_112179_1
M4ID: 12483256

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

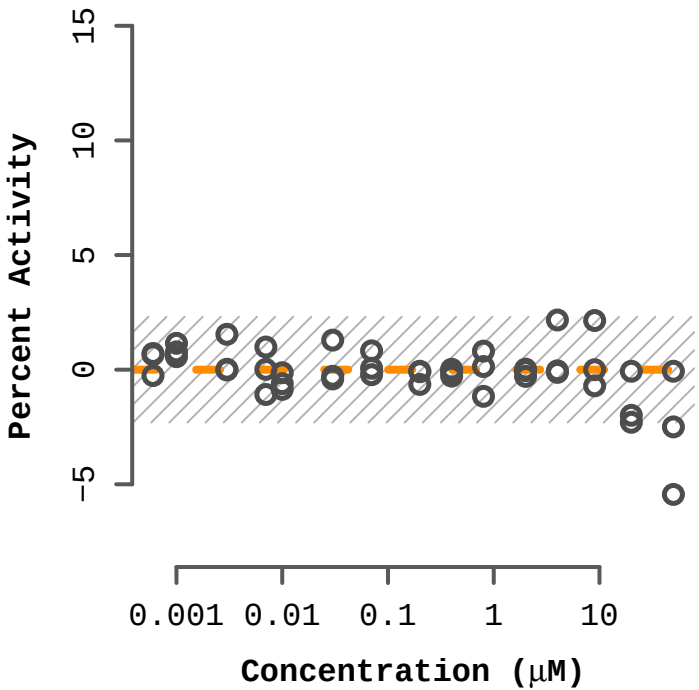
NAME: Clofarabine
CHID: 46437 **CASRN:** 123318-82-1
SPID(S): Tox21_112182_1
M4ID: 12483254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.13	NA	NA
PROB:	1	NA	NA
RMSE:	3.11	NA	NA

MAX_MEAN: 0.894 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

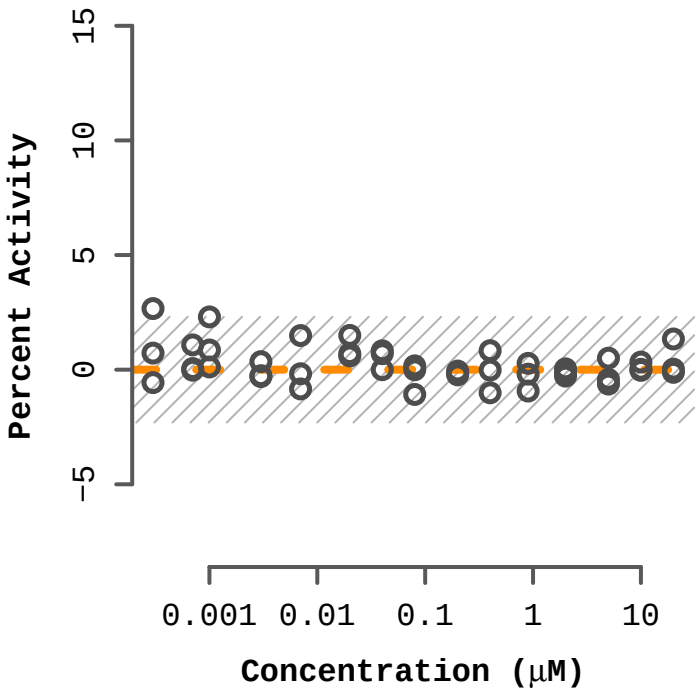
NAME: Entacapone
CHID: 46439 **CASRN:** 130929-57-6
SPID(S): Tox21_112184_1
M4ID: 12483253

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.832 **MAX_MED:** 0.777 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

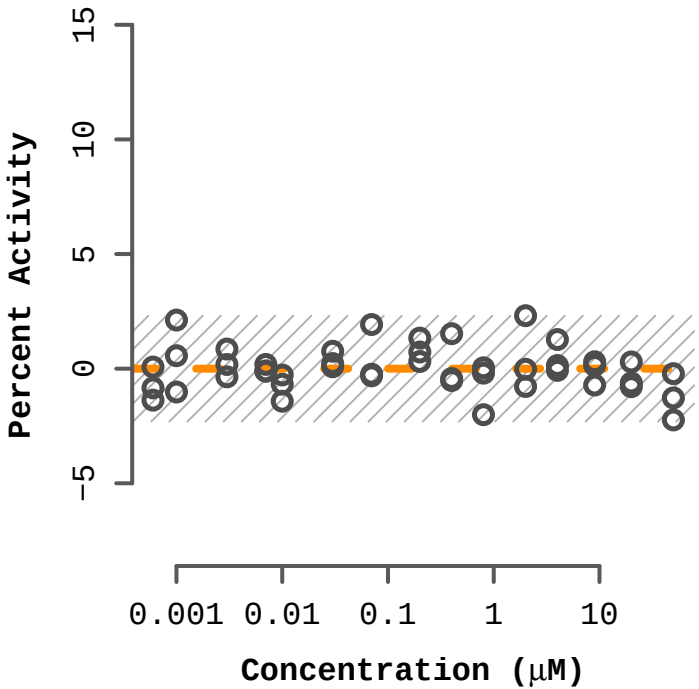
NAME: Fudosteine
CHID: 46440 **CASRN:** 13189-98-5
SPID(S): Tox21_112185_1
M4ID: 12483252

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

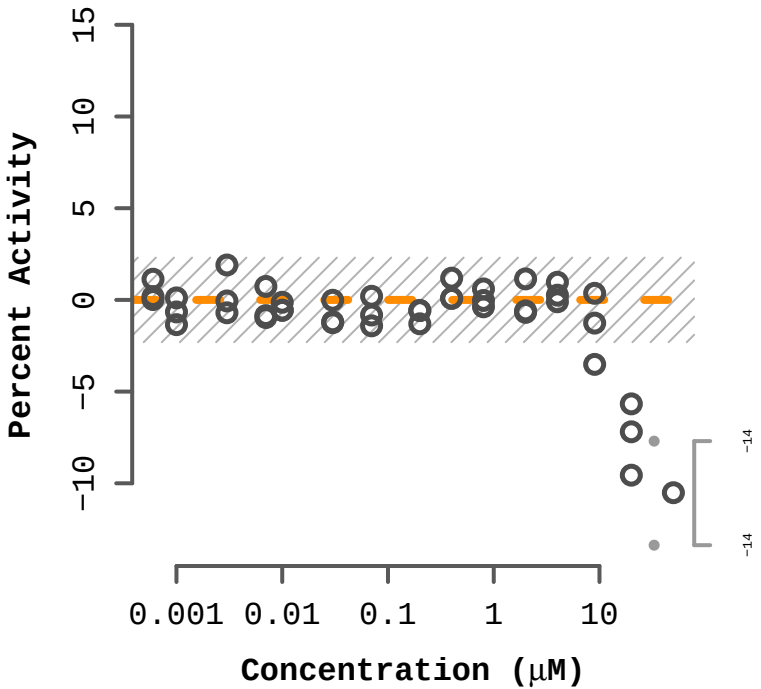
NAME: Pargeverine hydrochloride
CHID: 46442 **CASRN:** 2765-97-1
SPID(S): Tox21_112187_1
M4ID: 12483250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 0.729 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

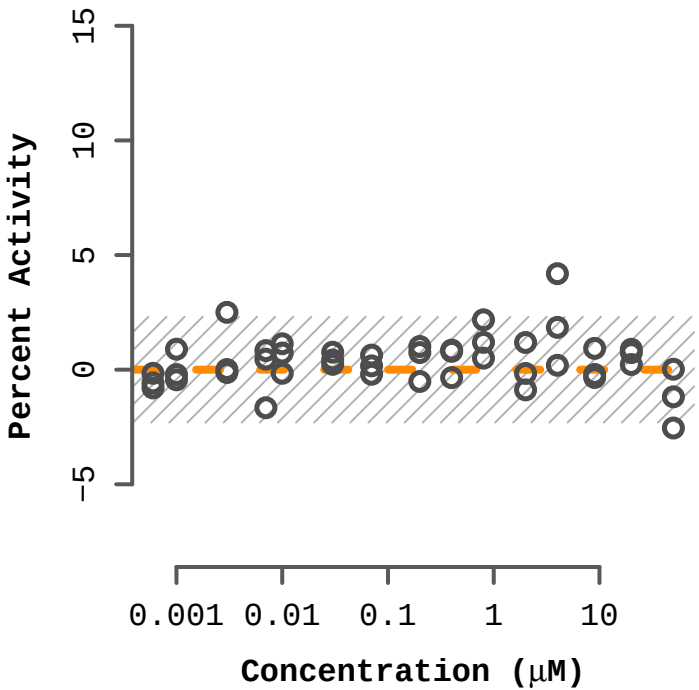
NAME: Duloxetine hydrochloride
CHID: 46443 **CASRN:** 136434-34-9
SPID(S): Tox21_112188_1
M4ID: 12483249 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 0.455 **MAX_MED:** 0.259 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

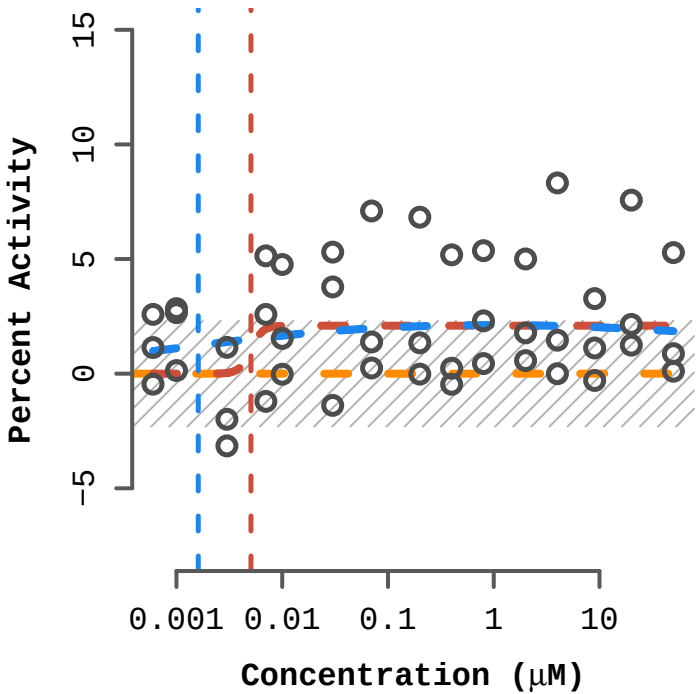
NAME: Levosimendan
CHID: 46445 **CASRN:** 141505-33-1
SPID(S): Tox21_113768
M4ID: 12482447

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Levosimendan
CHID: 46445 **CASRN:** 141505-33-1
SPID(S): Tox21_112191_1
M4ID: 12483247

HILL MODEL (in red):

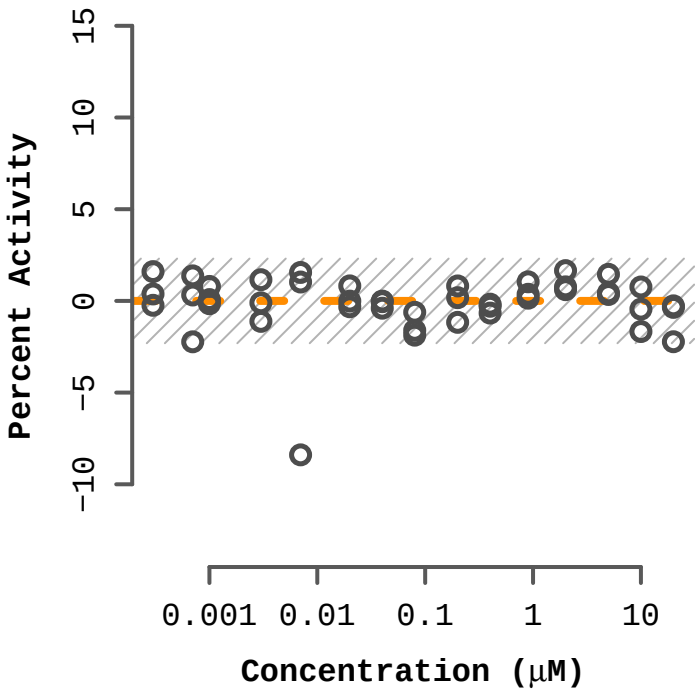
	tp	ga	gw
val:	2.09	−2.3	8
sd:	0.468	0.259	11.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.49	−2.79	0.417	3.32	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	238.87	224.44	228.88
PROB:	0	0.9	0.1
RMSE:	3.36	2.56	2.6

MAX_MEAN: 3.66 **MAX_MED:** 3.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

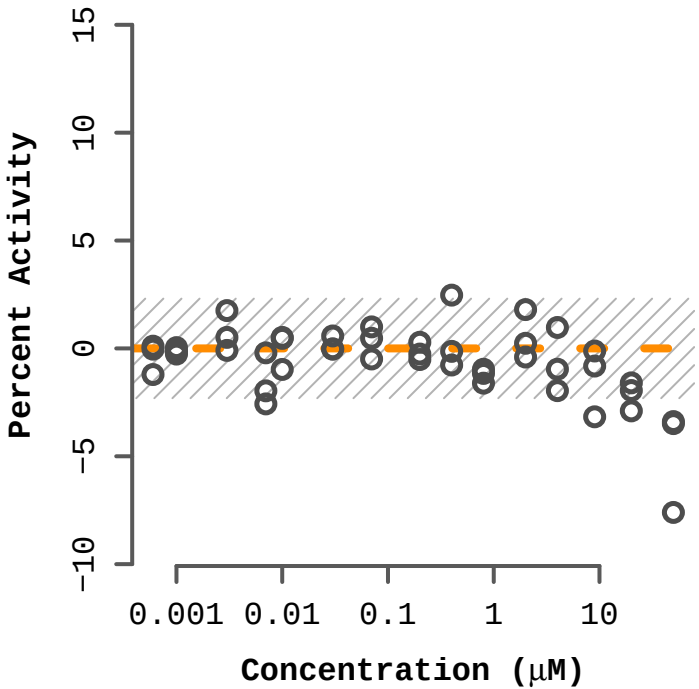
NAME: Pitavastatin calcium
CHID: 46448 **CASRN:** 147526-32-7
SPID(S): Tox21_303926
M4ID: 12475262

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

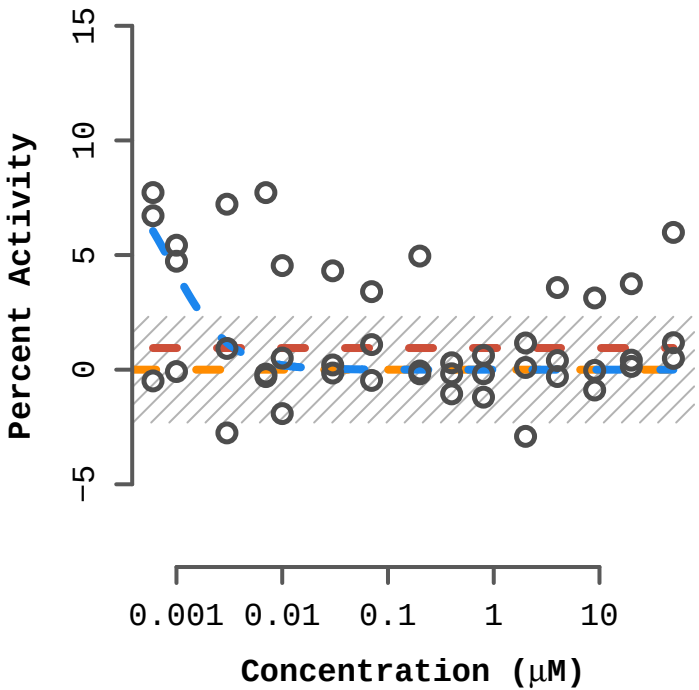
NAME: Perospirone hydrochloride
CHID: 46449 **CASRN:** 129273-38-7
SPID(S): Tox21_112196_1
M4ID: 12483245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 0.726 **MAX_MED:** 0.512 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Montelukast sodium
CHID: 46450 CASRN: 151767-02-1
SPID(S): Tox21_112197_1
M4ID: 12483244

HILL MODEL (in red):

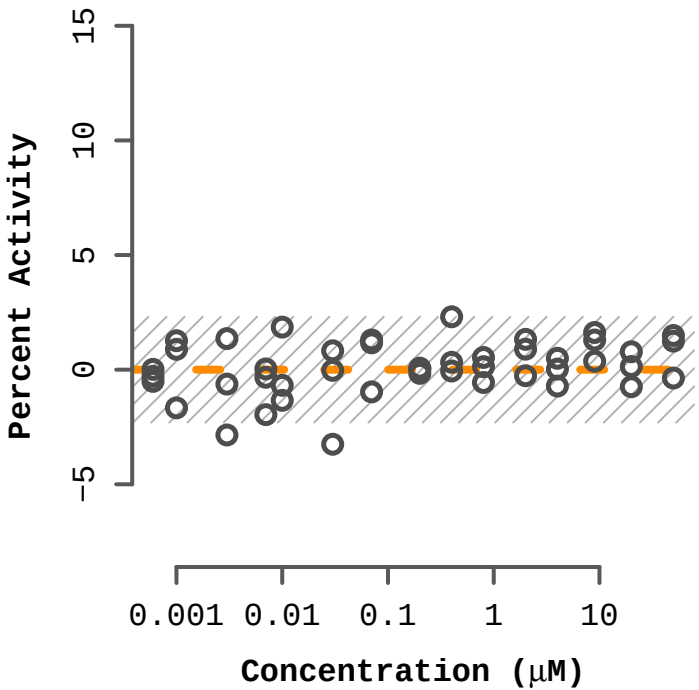
	tp	ga	gw
val:	0.944	−5.19	3.55
sd:	0.402	1210	2140

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.27	−3.79	7.96	−3.05	1.59
sd:	10.3	28.1	393	0.653	2.4

	CNST	HILL	GNLS
AIC:	229.25	229.14	226.89
PROB:	0.19	0.2	0.61
RMSE:	3.15	2.83	2.75

MAX_MEAN: 4.65 **MAX_MED:** 6.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

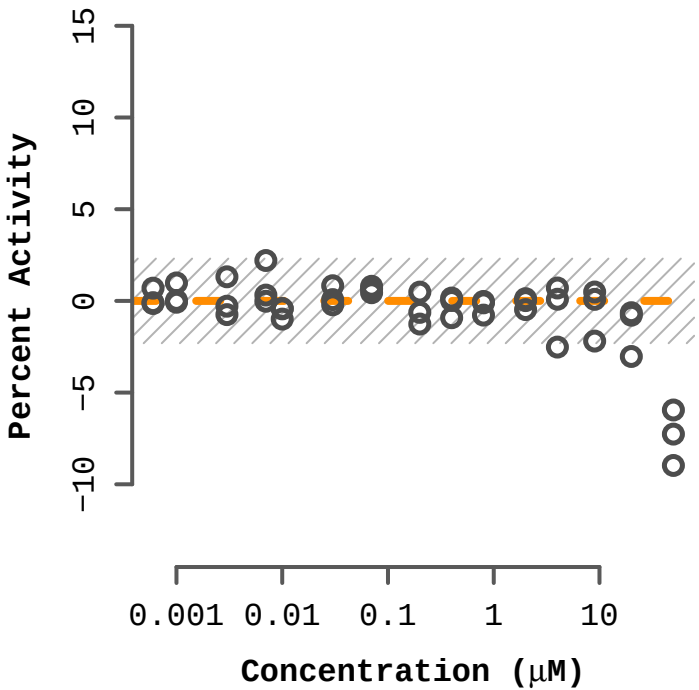
NAME: Capecitabine
CHID: 46451 **CASRN:** 154361-50-9
SPID(S): Tox21_112198_1
M4ID: 12483243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

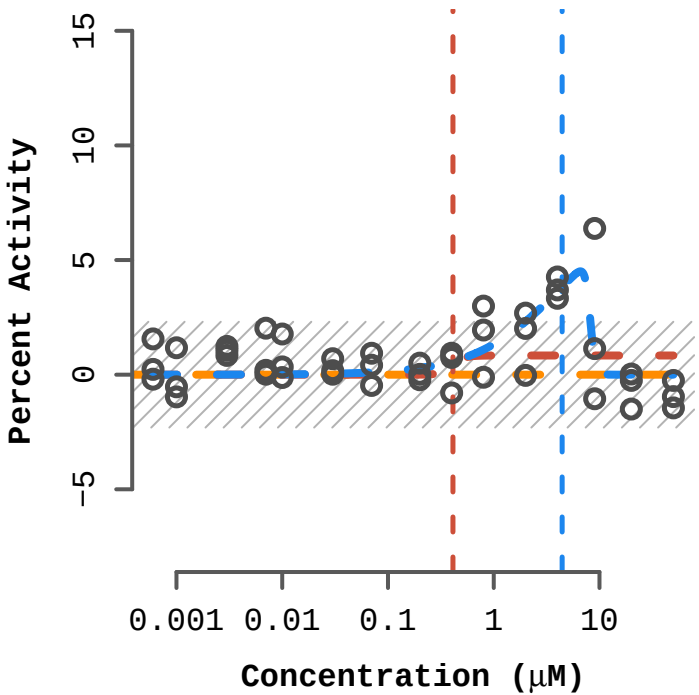
NAME: Rimonabant
CHID: 46453 **CASRN:** 168273-06-1
SPID(S): Tox21_112200_1
M4ID: 12483242

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.71	NA	NA
PROB:	1	NA	NA
RMSE:	2.14	NA	NA

MAX_MEAN: 0.835 **MAX_MED:** 0.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Erlotinib
CHID: 46454 CASRN: 183321-74-6
SPID(S): Tox21_112202_1
M4ID: 12483240

HILL MODEL (in red):

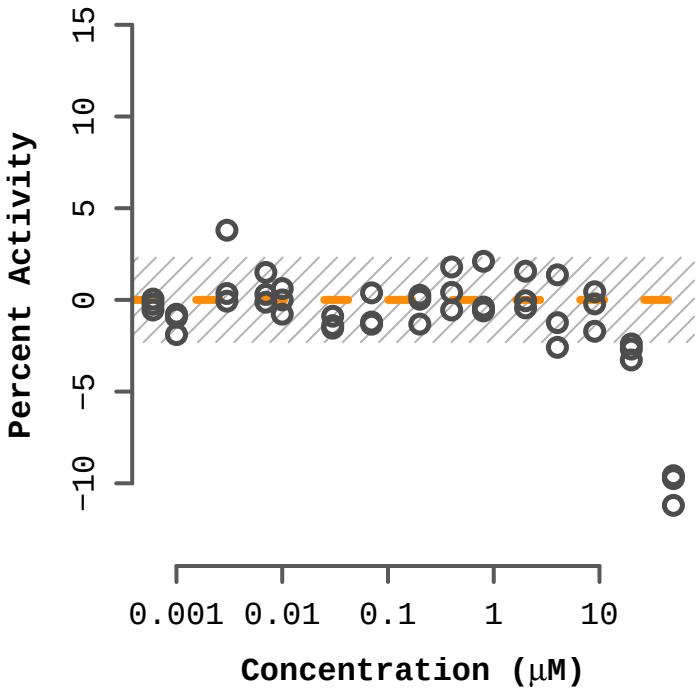
	tp	ga	gw
val:	0.836	−0.386	8
sd:	0.471	0.189	23.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.66	0.647	1.05	0.911	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	170.54	172.65	149.1
PROB:	0	0	1
RMSE:	1.74	1.56	1.27

MAX_MEAN: 3.76 MAX_MED: 3.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

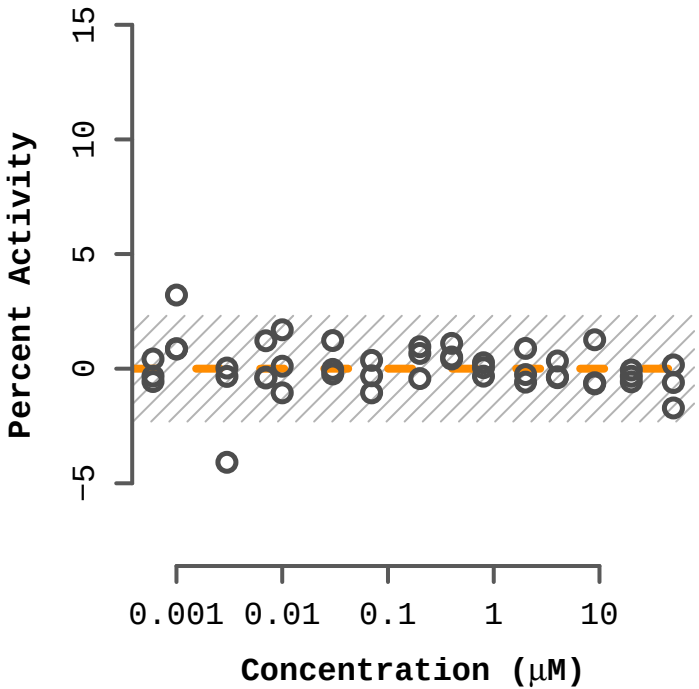
NAME: Lopinavir
CHID: 46456 **CASRN:** 192725-17-0
SPID(S): Tox21_112204_1
M4ID: 12483239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.96	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.413 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

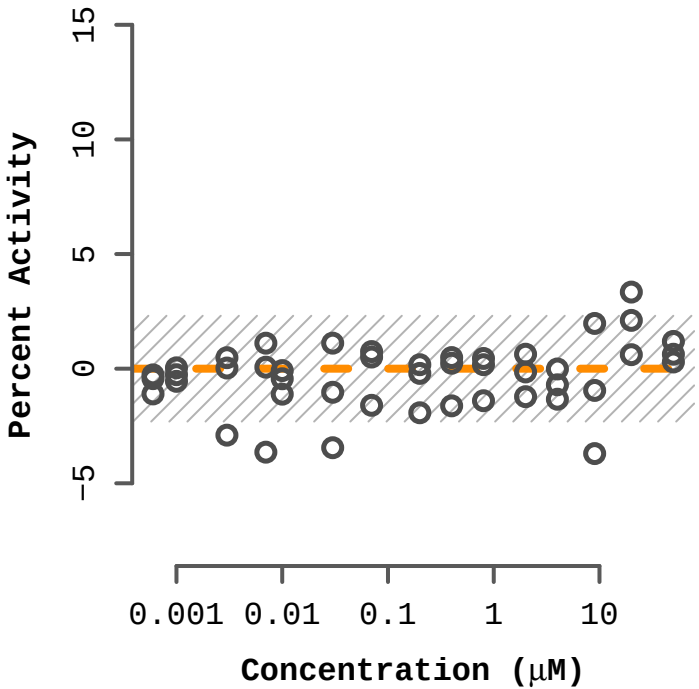
NAME: Etoricoxib
CHID: 46457 CASRN: 202409-33-4
SPID(S): Tox21_112206_1
M4ID: 12483237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 0.872 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

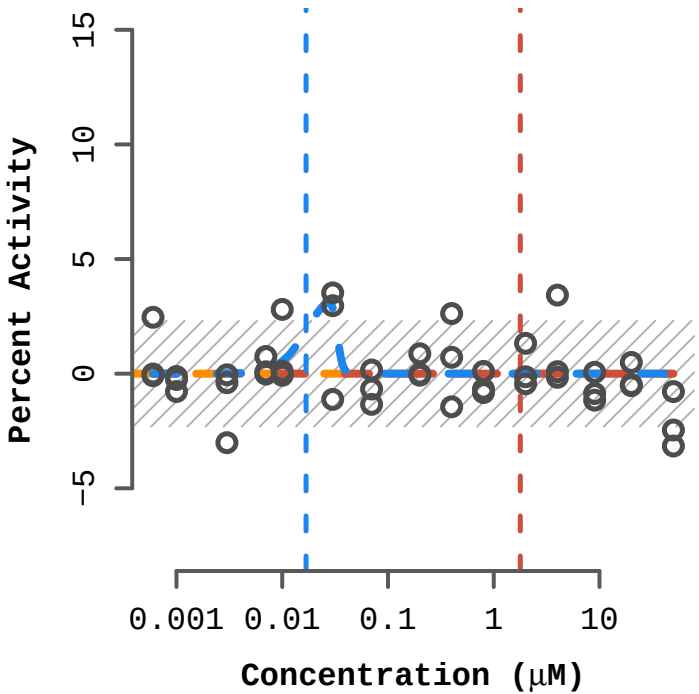
NAME: Estramustine
CHID: 46458 **CASRN:** 2998-57-4
SPID(S): Tox21_112207_1
M4ID: 12483236

HILL MODEL: Not applicable.

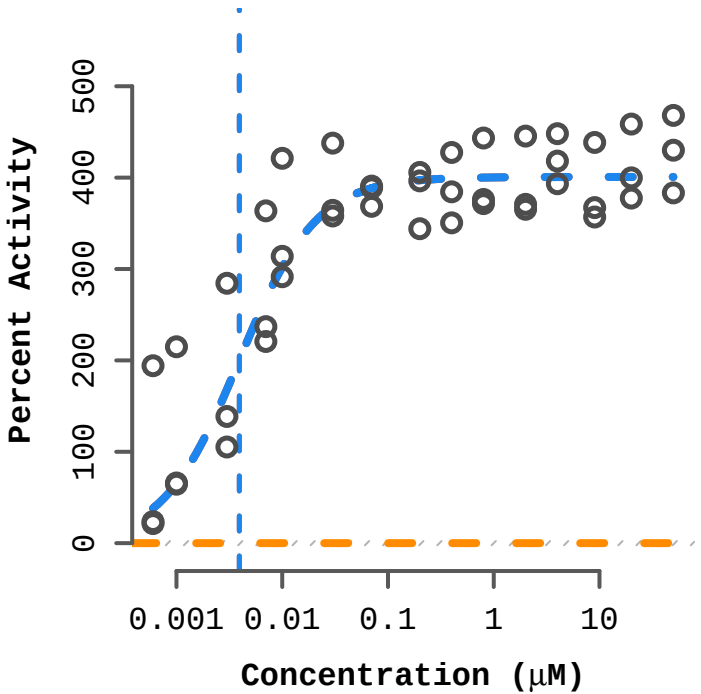
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 2.11 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cetraxate hydrochloride
CHID:    46459   CASRN: 27724-96-5
SPID(S): Tox21_112210_1
M4ID:    12483233

HILL MODEL (in red):
      tp        ga        gw
val:  3.19e-10  0.251     2.05
sd:   3.49e-05  24400     16600

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.78      -1.77     3.47      -1.48     18
sd:   NaN       NaN       NaN       NaN       NaN

      CNST          HILL          GNLS
AIC:  158.2         164.2         161.29
PROB: 0.79          0.04          0.17
RMSE: 1.44          1.44          1.38

MAX_MEAN: 1.79      MAX_MED: 2.97      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Halometasone hydrate
CHID: 46460 CASRN: 1310709-74-0
SPID(S): Tox21_112211_1
M4ID: 12483232

HILL MODEL (in red):

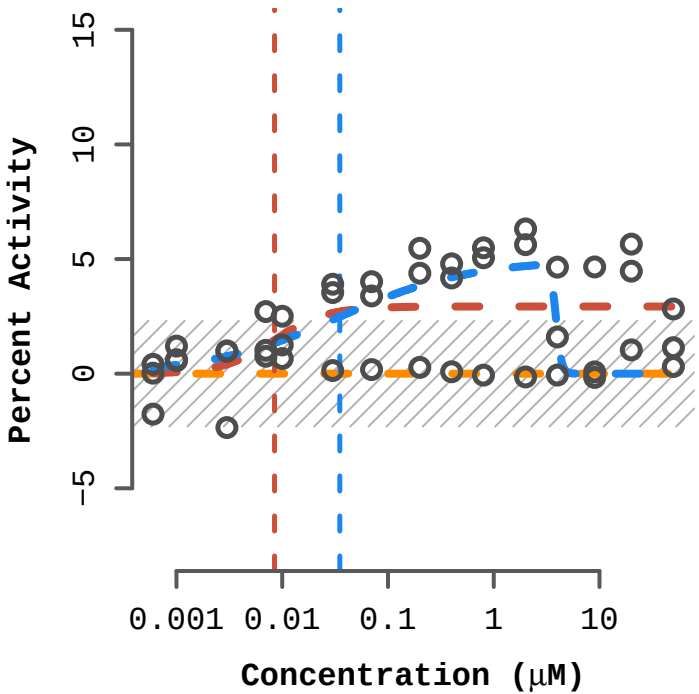
	tp	ga	gw
val:	401	-2.41	1.2
sd:	8.71	0.0764	0.195

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	401	-2.41	1.2	3.69	14
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	667.01	488.87	492.87
PROB:	0	0.88	0.12
RMSE:	352.24	53.35	53.35

MAX_MEAN: 427 **MAX_MED:** 430 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pitofenone hydrochloride
CHID: 46461 CASRN: 1248-42-6
SPID(S): Tox21_112212_1
M4ID: 12483231

HILL MODEL (in red):

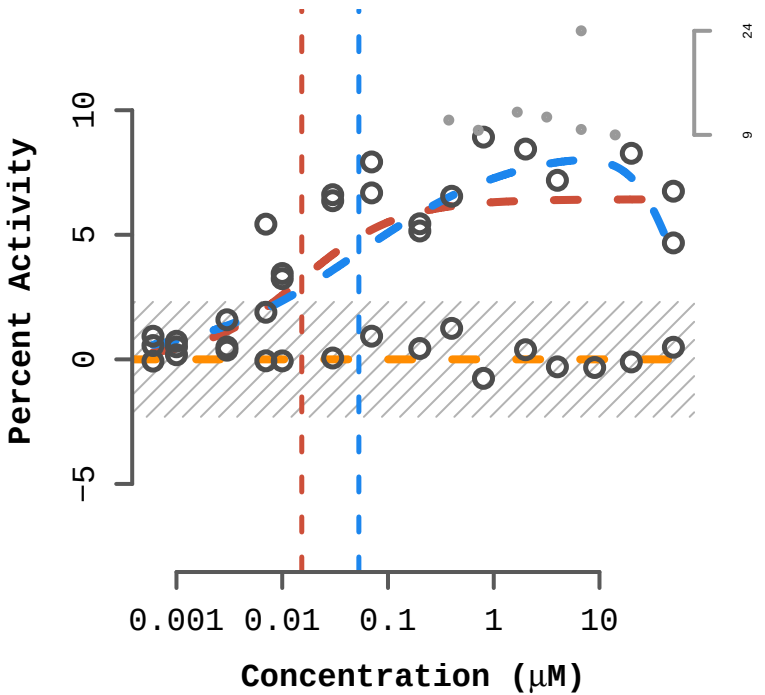
	tp	ga	gw
val:	2.93	−2.07	1.74
sd:	0.513	0.25	1.96

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.97	−1.46	0.7	0.589	16.9
sd:	1.85	0.744	0.476	0.243	317

	CNST	HILL	GNLS
AIC:	231.79	202.34	207.73
PROB:	0	0.94	0.06
RMSE:	3.02	1.94	2.18

MAX_MEAN: 3.93 **MAX_MED:** 5.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Malotilate
CHID: 46463 CASRN: 59937-28-9
SPID(S): Tox21_112214_1
M4ID: 12483230 BRK

HILL MODEL (in red):

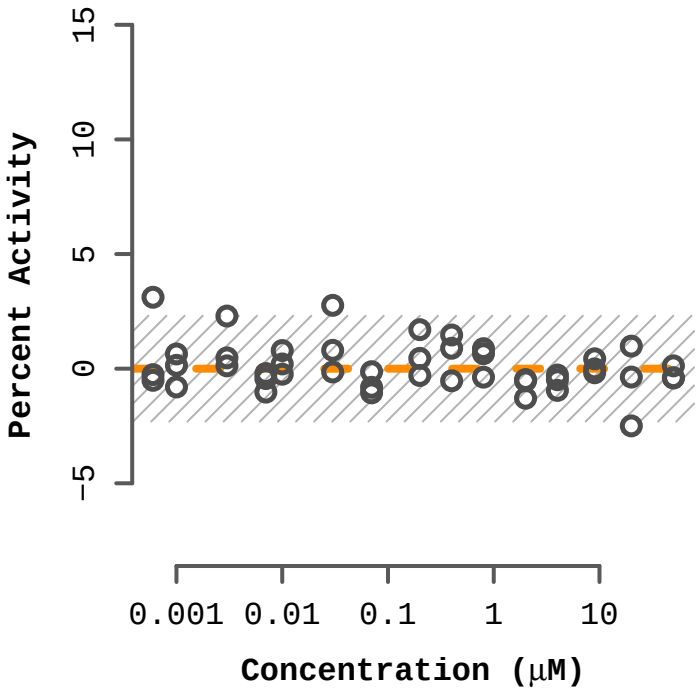
	tp	ga	gw
val:	6.43	−1.82	0.952
sd:	1.14	0.404	0.708

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.58	−1.28	0.584	1.69	2.16
sd:	3.52	0.941	0.373	0.232	3.17

	CNST	HILL	GNLS
AIC:	295.09	259.71	261.47
PROB:	0	0.71	0.29
RMSE:	6.54	4.26	4.18

MAX_MEAN: 11 MAX_MED: 9.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

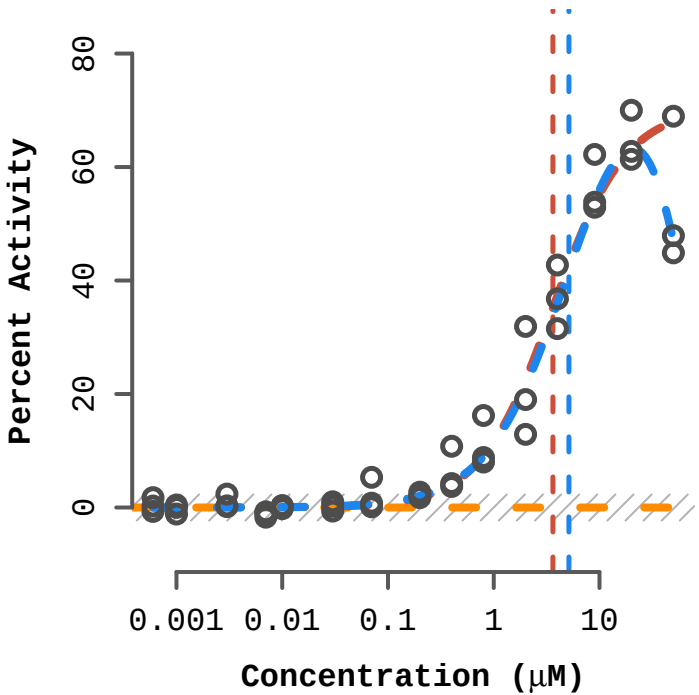
NAME: Phenprobamate
CHID: 46464 **CASRN:** 673-31-4
SPID(S): Tox21_112215_1
M4ID: 12483229

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.892 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Drospirenone
CHID: 46465 **CASRN:** 67392-87-4
SPID(S): Tox21_112216_1
M4ID: 12483228

HILL MODEL (in red):

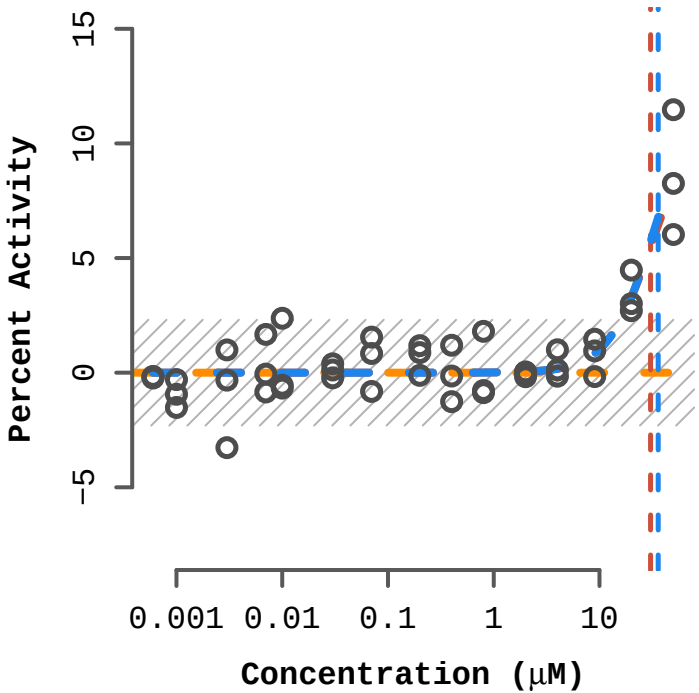
	tp	ga	gw
val:	70.4	0.56	1.26
sd:	2.63	0.0481	0.108

GAIN-LOSS MODEL (in blue):

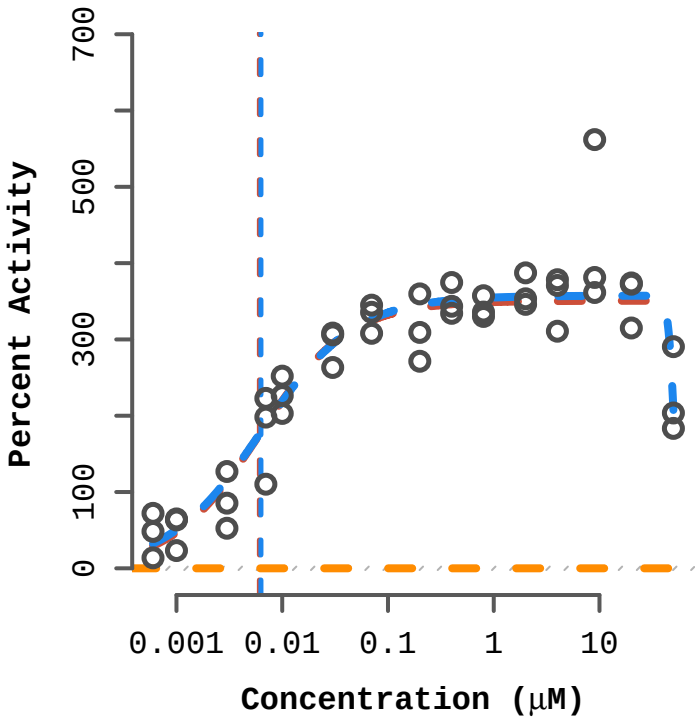
	tp	ga	gw	la	lw
val:	84	0.711	1.14	1.78	2.13
sd:	17.8	0.165	0.128	0.0529	1.09

	CNST	HILL	GNLS
AIC:	425.83	264.92	252.51
PROB:	0	0	1
RMSE:	28.9	5.69	4.7

MAX_MEAN: 64.7 **MAX_MED:** 62.8 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Argatroban
CHID:    46467   CASRN: 74863-84-6
SPID(S): Tox21_112218_1
M4ID:    12483227

HILL MODEL (in red):
      tp       ga       gw
val:  11       1.48     2.05
sd:   5.25     0.254    0.984

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.8     1.56     1.98     1.85     6.07
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  190.43      144.32      148.32
PROB: 0           0.88        0.12
RMSE: 2.65        1.14        1.14

MAX_MEAN: 8.59      MAX_MED: 8.26      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Loteprednol etabonate
CHID: 46468 CASRN: 82034-46-6
SPID(S): Tox21_112219_1
M4ID: 12483226

HILL MODEL (in red):

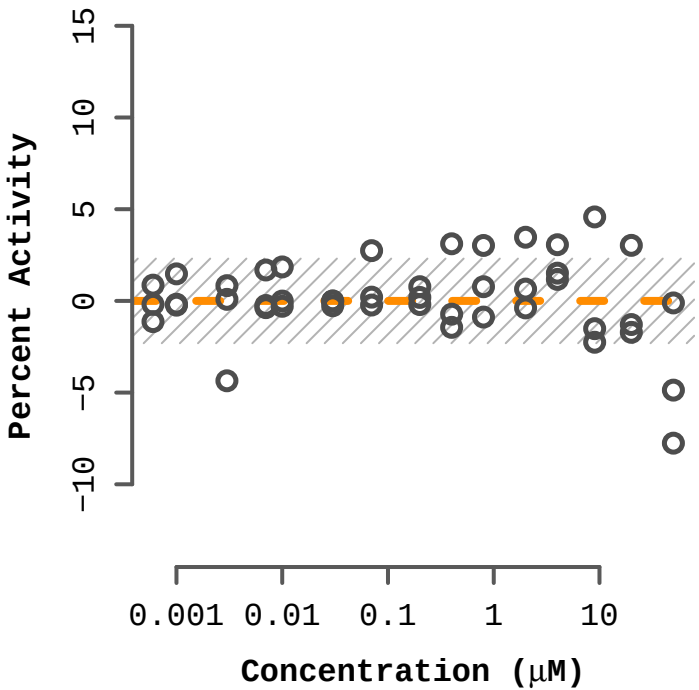
	tp	ga	gw
val:	351	-2.22	1.03
sd:	8.2	0.0615	0.147

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	357	-2.2	0.981	1.71	14.8
sd:	7.42	0.0566	0.123	0.0074	10.8

	CNST	HILL	GNLS
AIC:	648.57	476.72	461.3
PROB:	0	0	1
RMSE:	290.74	54.26	43.3

MAX_MEAN: 435 MAX_MED: 381 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

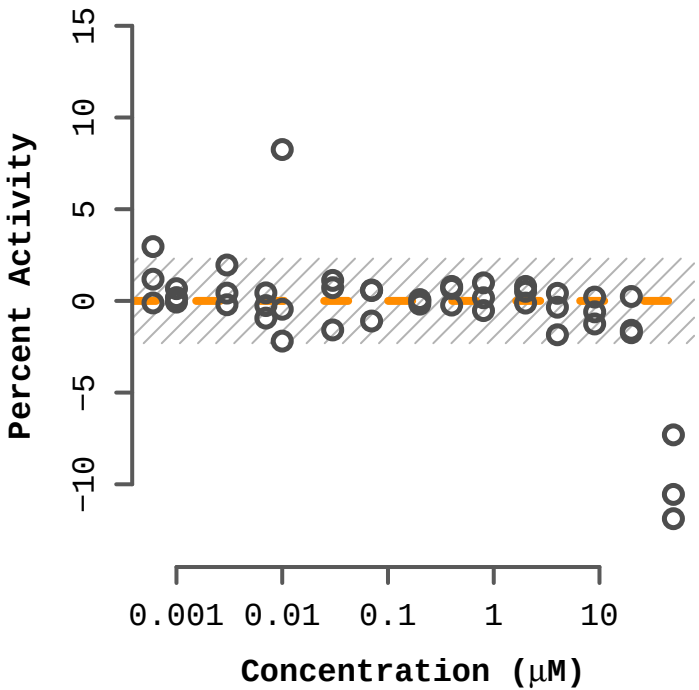
NAME: Liranaftate
CHID: 46470 **CASRN:** 88678-31-3
SPID(S): Tox21_112223_1
M4ID: 12483223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

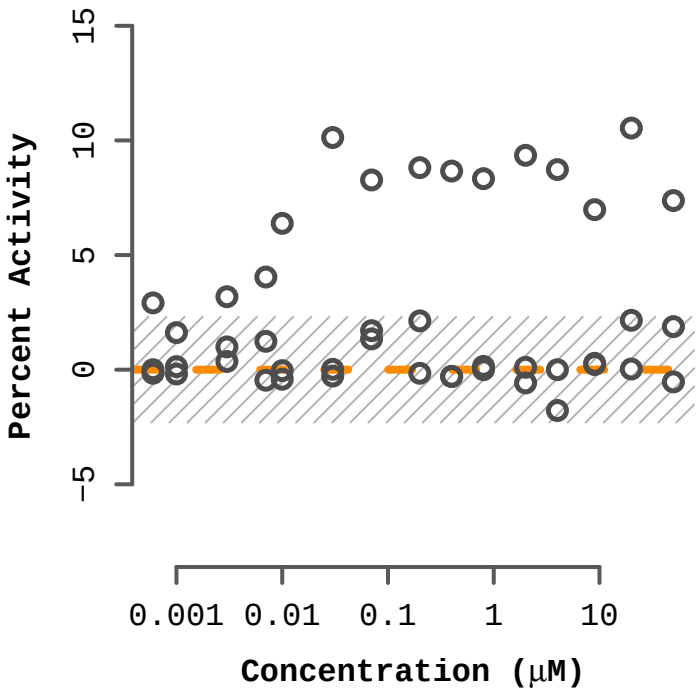
NAME: Ebastine
CHID: 46472 **CASRN:** 90729-43-4
SPID(S): Tox21_112225_1
M4ID: 12483222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	190.76	NA	NA
PROB:	1	NA	NA
RMSE:	3.04	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

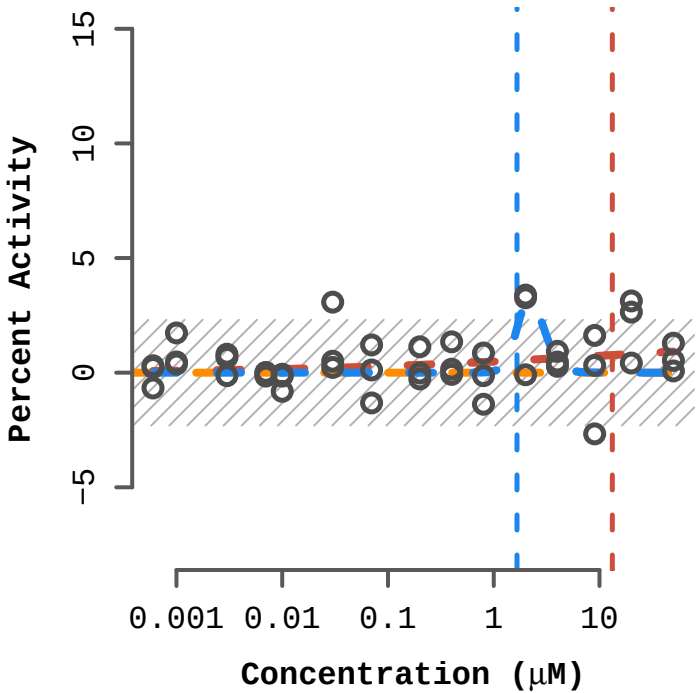
NAME: Ampiroxicam
CHID: 46474 **CASRN:** 99464-64-9
SPID(S): Tox21_112227_1
M4ID: 12483220

HILL MODEL: Not applicable.

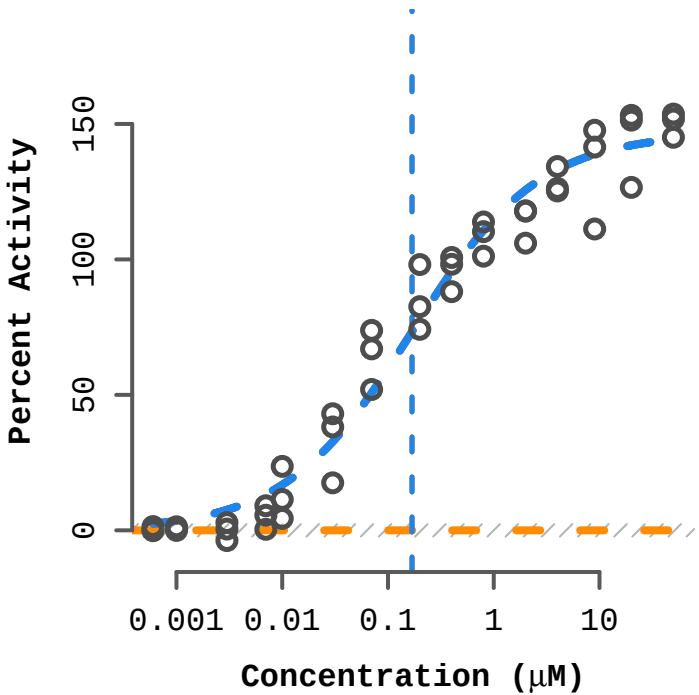
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	257.28	NA	NA
PROB:	1	NA	NA
RMSE:	4.41	NA	NA

MAX_MEAN: 4.24 **MAX_MED:** 2.15 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Trocimine
CHID:    46475   CASRN: 14368-24-2
SPID(S): Tox21_112228_1
M4ID:    12483219

HILL MODEL (in red):
      tp       ga       gw
val:  1.53     1.12     0.3
sd:   4.53     8.95     0.641

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.02     0.22     8        0.47     5.99
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  147.73      143.72      148.07
PROB: 0.11        0.8         0.09
RMSE: 1.31        1.17        1.19

MAX_MEAN: 2.19      MAX_MED: 3.27      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Gestodene
CHID: 46478 CASRN: 60282-87-3
SPID(S): Tox21_112232_1
M4ID: 12483218

HILL MODEL (in red):

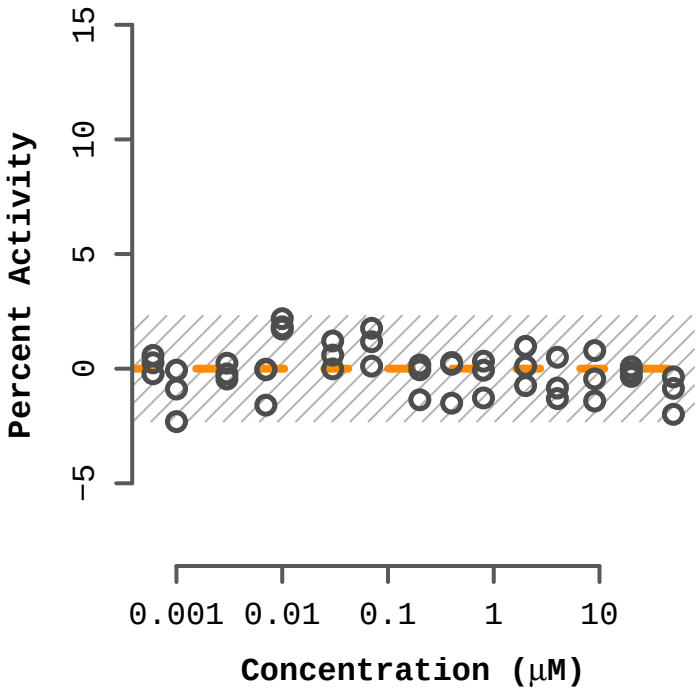
	tp	ga	gw
val:	147	-0.773	0.723
sd:	4.86	0.0769	0.0622

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	147	-0.773	0.723	2.4	17.9
sd:	4.86	0.0769	0.0622	8340	207000

	CNST	HILL	GNLS
AIC:	541.73	344.82	348.82
PROB:	0	0.88	0.12
RMSE:	91.29	10.08	10.08

MAX_MEAN: 150 MAX_MED: 152 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

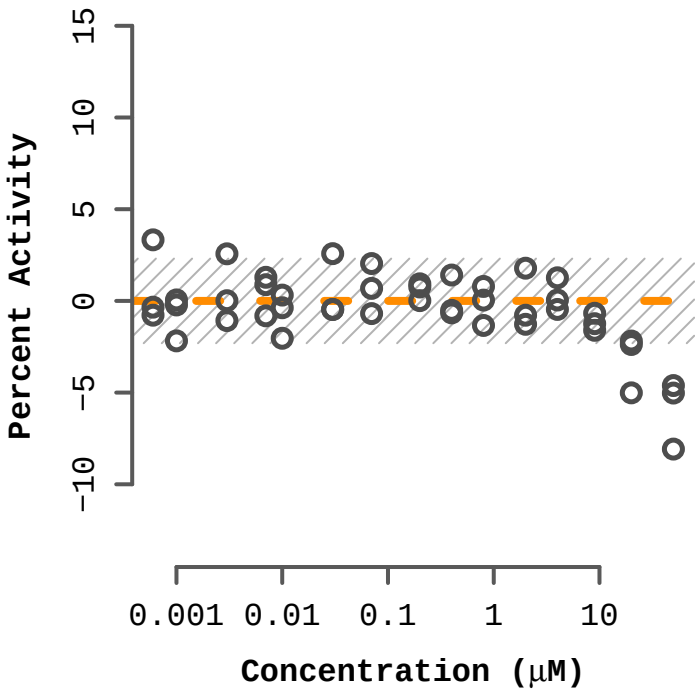
NAME: Prulifloxacin
CHID: 46480 **CASRN:** 123447-62-1
SPID(S): Tox21_112235_1
M4ID: 12483216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.8	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

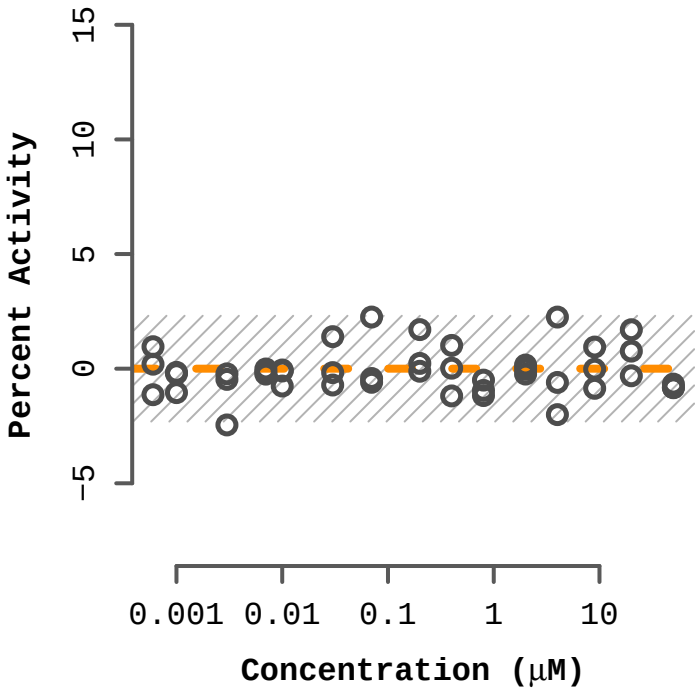
NAME: Adapalene
CHID: 46481 **CASRN:** 106685-40-9
SPID(S): Tox21_112236_1
M4ID: 12483215

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.42	NA	NA
PROB:	1	NA	NA
RMSE:	2.16	NA	NA

MAX_MEAN: 0.738 **MAX_MED:** 0.886 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

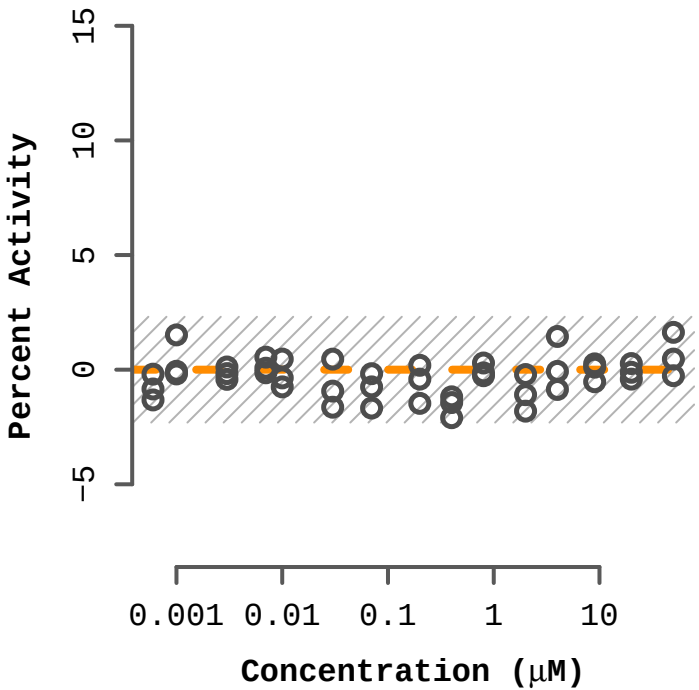
NAME: Raltitrexed
CHID: 46482 **CASRN:** 112887-68-0
SPID(S): Tox21_112237_1
M4ID: 12483214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.719 **MAX_MED:** 0.767 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

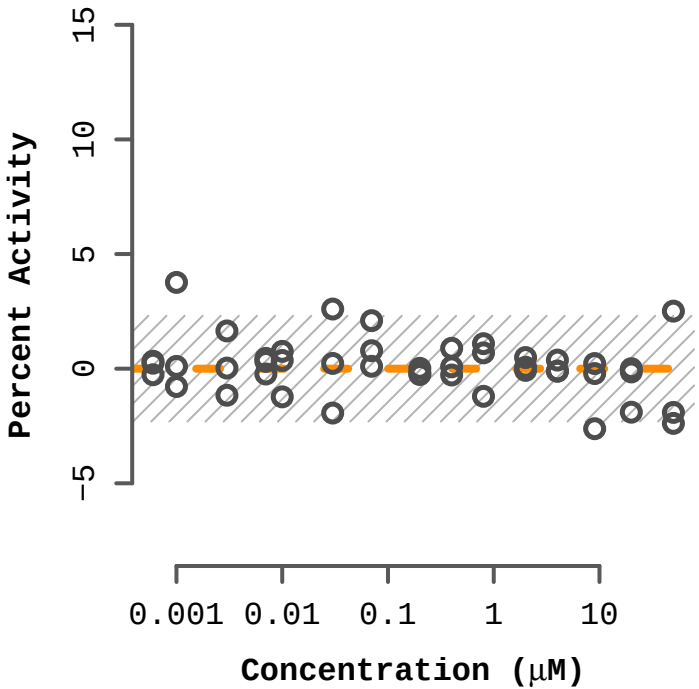
NAME: Nadifloxacin
CHID: 46483 **CASRN:** 124858-35-1
SPID(S): Tox21_112239_1
M4ID: 12483212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.611 **MAX_MED:** 0.463 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

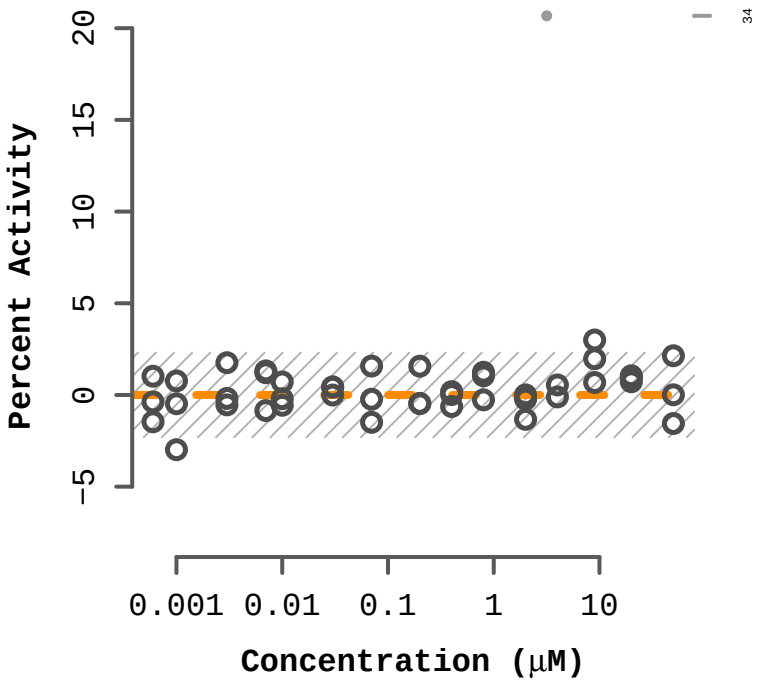
NAME: Fenpiverinium bromide
CHID: 46484 **CASRN:** 125-60-0
SPID(S): Tox21_112240_1
M4ID: 12483211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

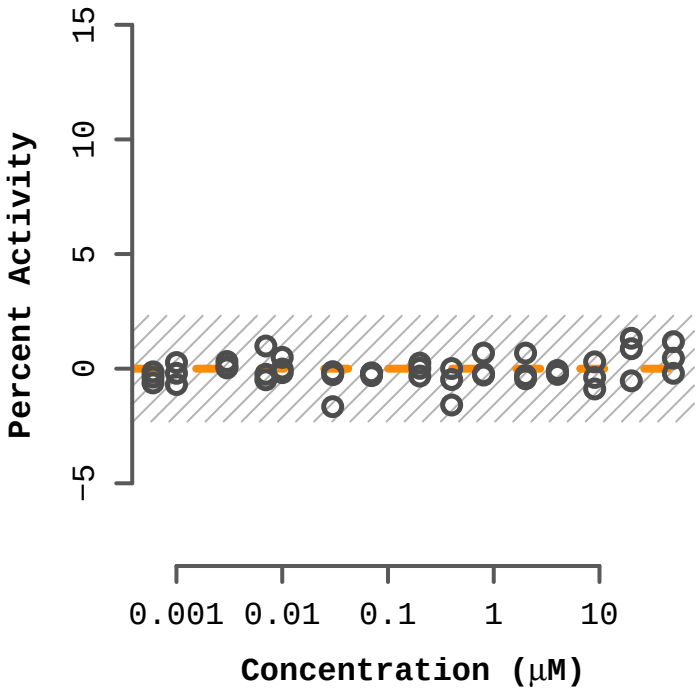
NAME: Voriconazole
CHID: 46485 CASRN: 137234-62-9
SPID(S): Tox21_112241_1
M4ID: 12483210 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.97	NA	NA
PROB:	1	NA	NA
RMSE:	5.19	NA	NA

MAX_MEAN: 11.5 MAX_MED: 1.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

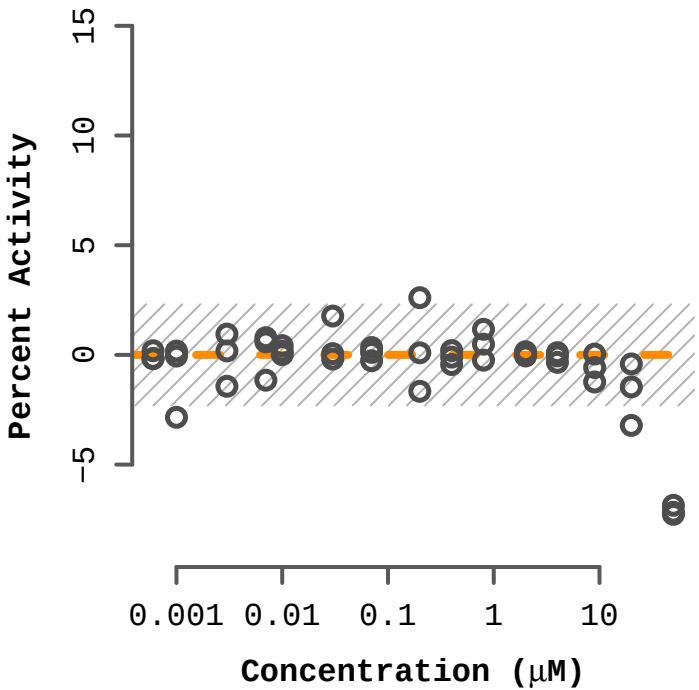
NAME: Olopatadine hydrochloride
CHID: 46486 CASRN: 140462-76-6
SPID(S): Tox21_112242_1
M4ID: 12483209

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	79.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.59	NA	NA

MAX_MEAN: 0.558 **MAX_MED:** 0.873 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

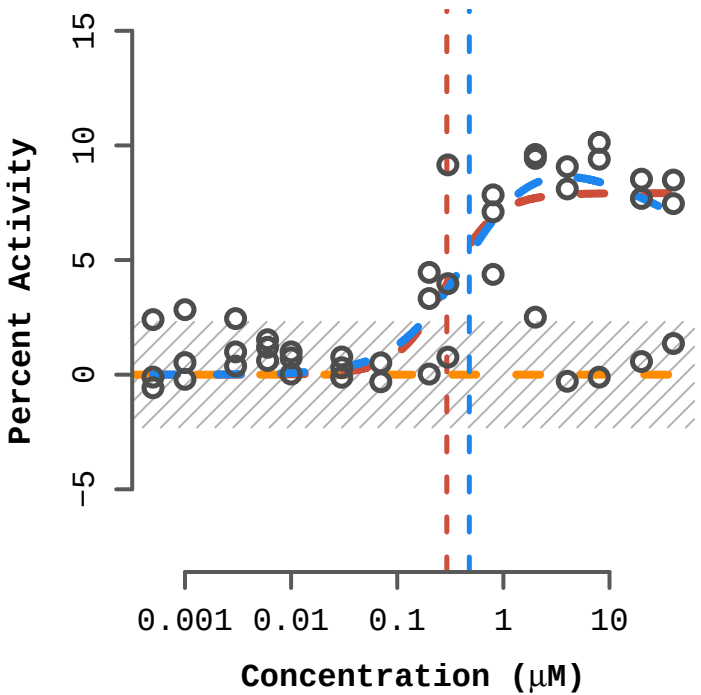
NAME: Adefovir dipivoxil
CHID: 46487 **CASRN:** 142340-99-6
SPID(S): Tox21_112243_1
M4ID: 12483208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.594 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cerivastatin sodium
CHID: 46488 CASRN: 143201-11-0
SPID(S): Tox21_303882
M4ID: 12475306

HILL MODEL (in red):

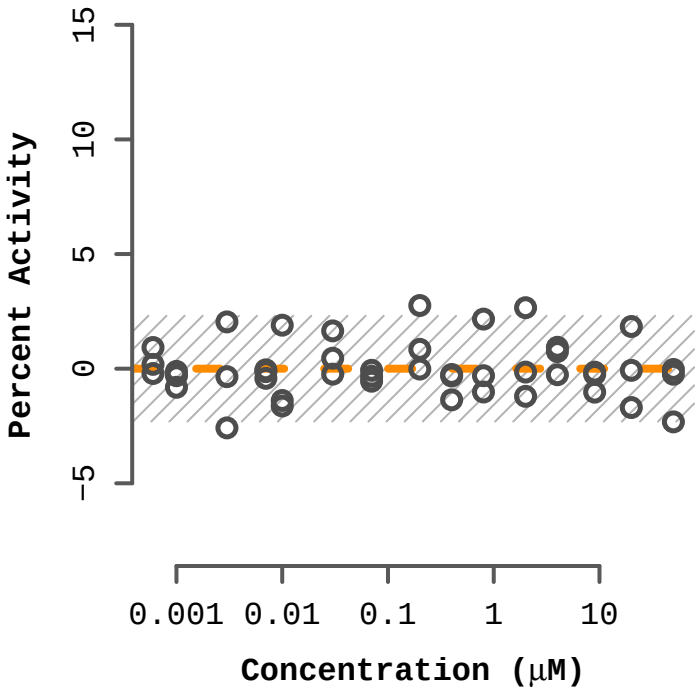
	tp	ga	gw
val:	7.92	−0.533	1.86
sd:	0.669	0.129	0.849

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.7	−0.321	1.29	2.08	0.386
sd:	51.9	1.2	1.09	7.9	3.62

	CNST	HILL	GNLS
AIC:	267.59	214.41	217.12
PROB:	0	0.8	0.2
RMSE:	4.95	2.84	2.87

MAX_MEAN: 7.18 **MAX_MED:** 9.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

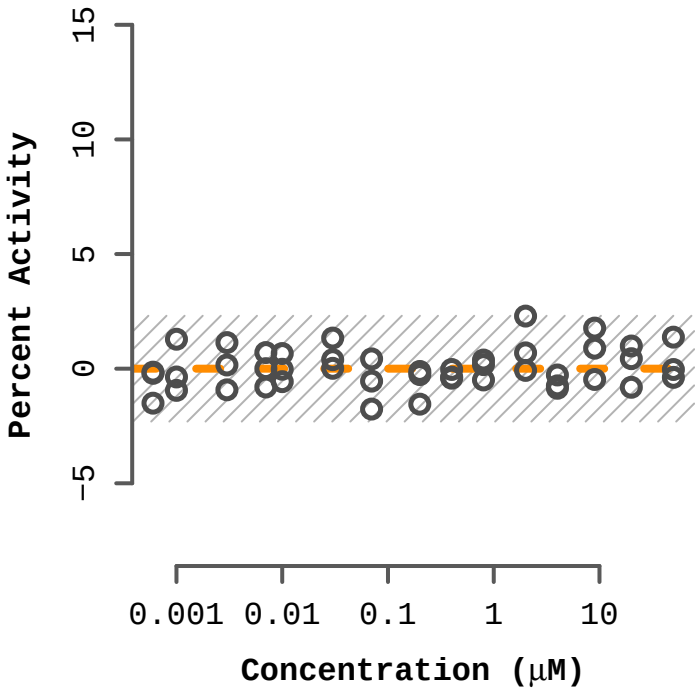
NAME: Cerivastatin sodium
CHID: 46488 **CASRN:** 143201-11-0
SPID(S): Tox21_112244_1
M4ID: 12483207

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.844 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

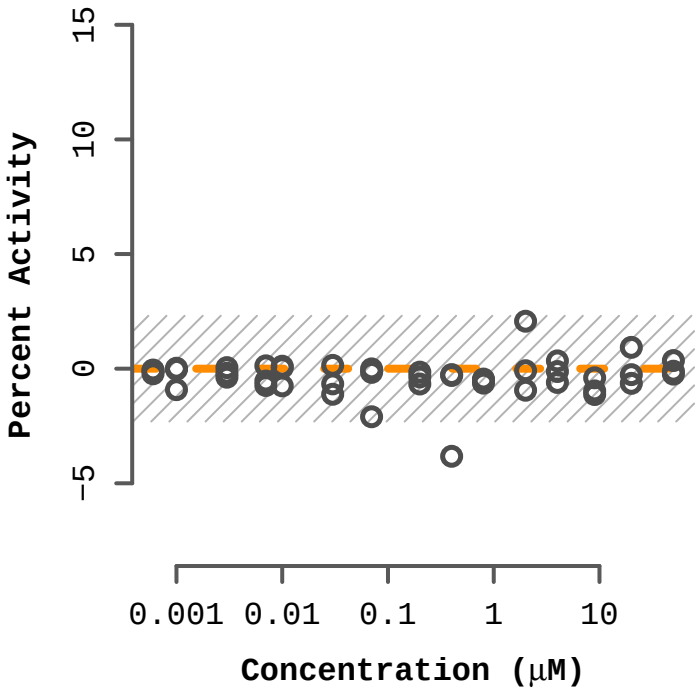
NAME: Alibendol
CHID: 46490 **CASRN:** 26750-81-2
SPID(S): Tox21_112247_1
M4ID: 12483205

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 0.895 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

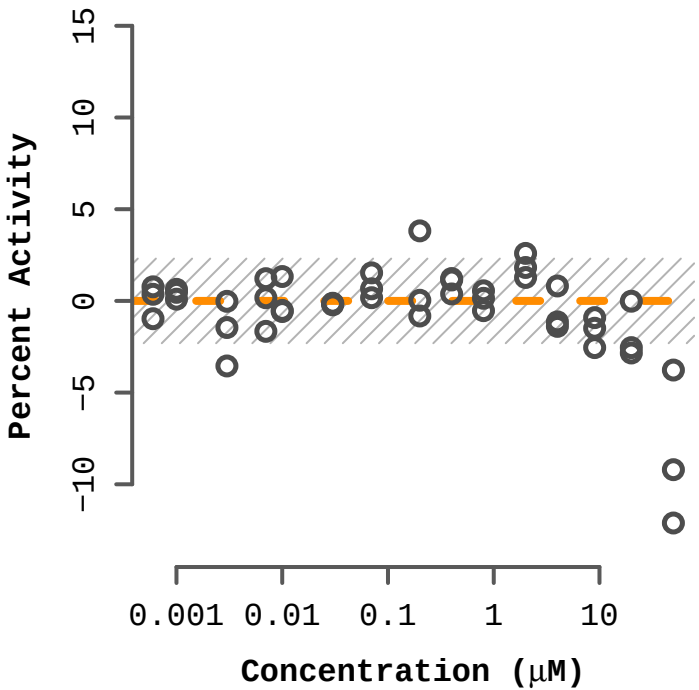
NAME: Penciclovir
CHID: 46491 **CASRN:** 39809-25-1
SPID(S): Tox21_112248_1
M4ID: 12483204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.348 **MAX_MED:** 0.0446 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

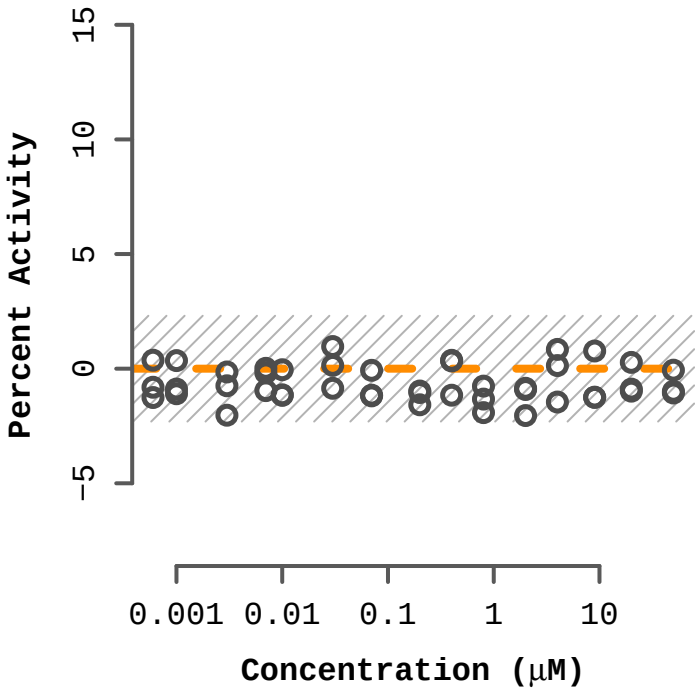
NAME: Sunitinib malate
CHID: 46492 **CASRN:** 341031-54-7
SPID(S): Tox21_112249_1
M4ID: 12483203

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.92	NA	NA
PROB:	1	NA	NA
RMSE:	2.71	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

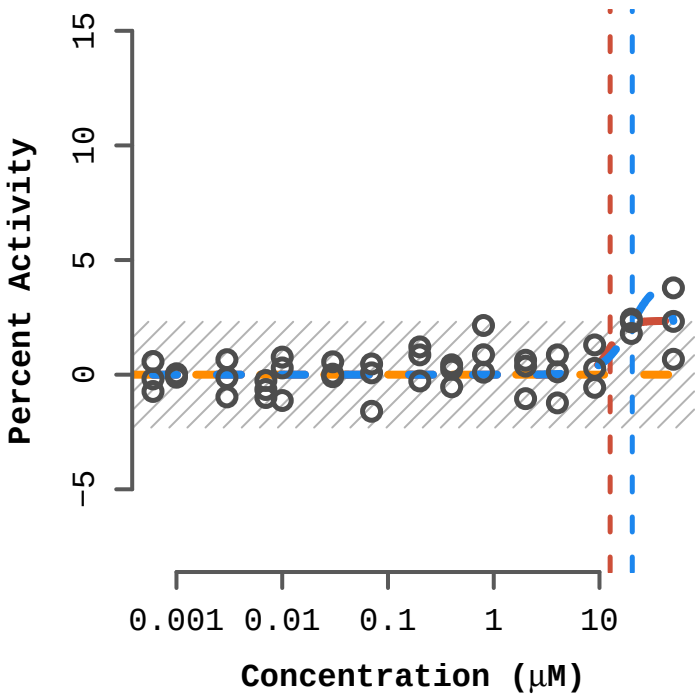
NAME: Nifekalant hydrochloride
CHID: 46495 **CASRN:** 130636-43-0
SPID(S): Tox21_112254_1
M4ID: 12483199

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.0857 **MAX_MED:** 0.337 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cloricromen hydrochloride
CHID: 46499 **CASRN:** 74697-28-2
SPID(S): Tox21_112260_1
M4ID: 12483196

HILL MODEL (in red):

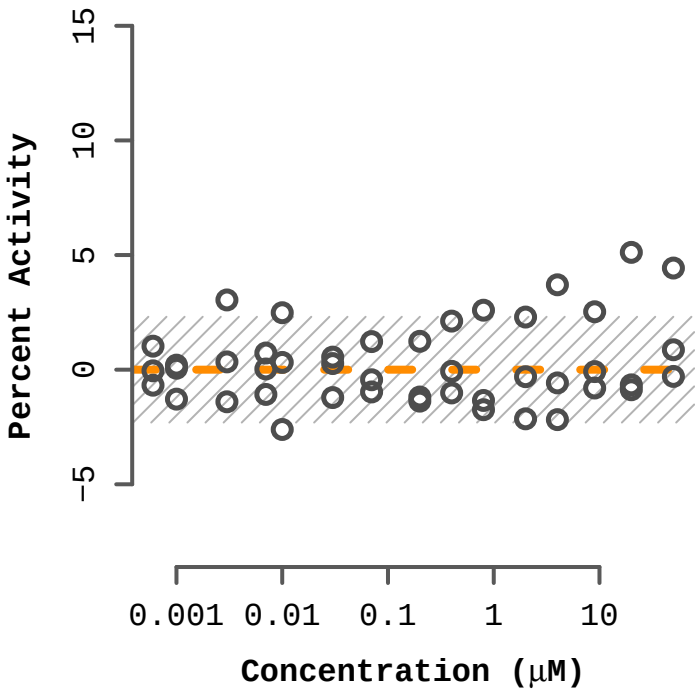
	tp	ga	gw
val:	2.35	1.1	5.63
sd:	0.627	0.177	5.84

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.52	1.31	3.16	1.71	7.77
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	136.78	115.34	119.32
PROB:	0	0.88	0.12
RMSE:	1.13	0.79	0.79

MAX_MEAN: 2.26 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

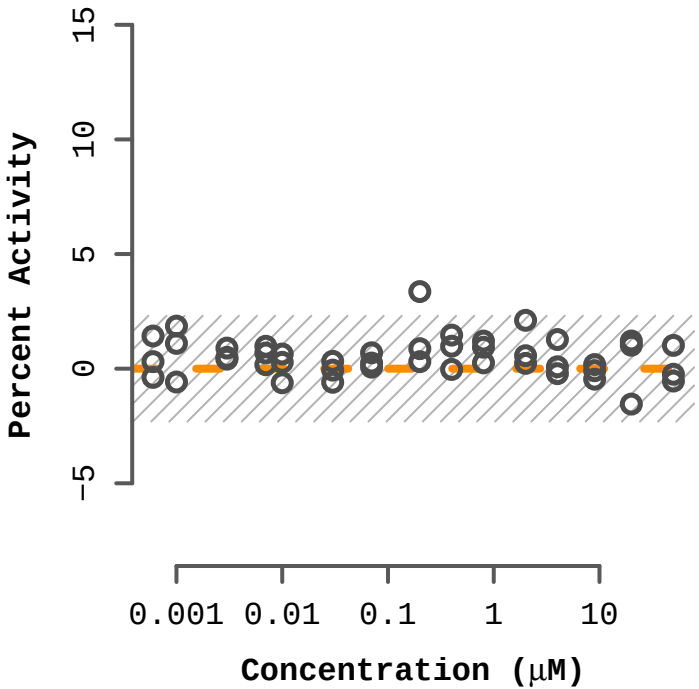
NAME: Daltroban
CHID: 46501 CASRN: 79094-20-5
SPID(S): Tox21_112262_1
M4ID: 12483195

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

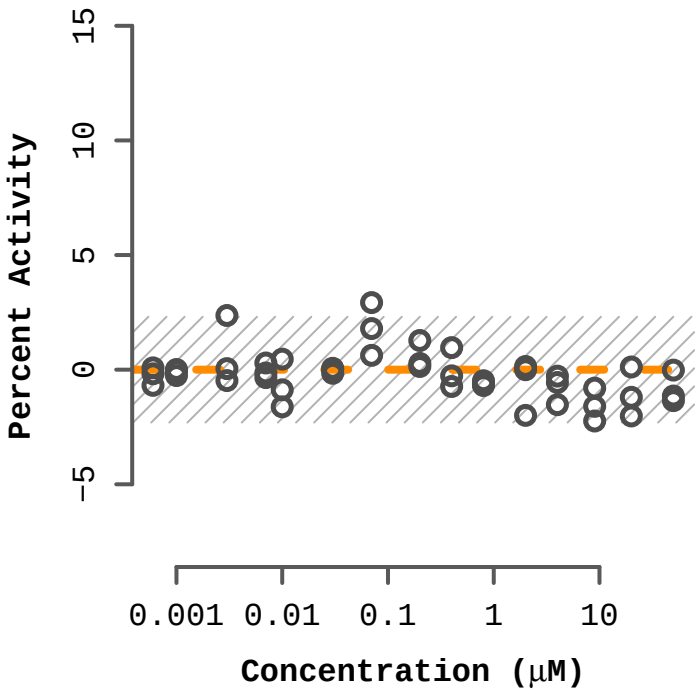
NAME: Epinastine hydrochloride
CHID: 46502 CASRN: 108929-04-0
SPID(S): Tox21_112263_1
M4ID: 12483194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

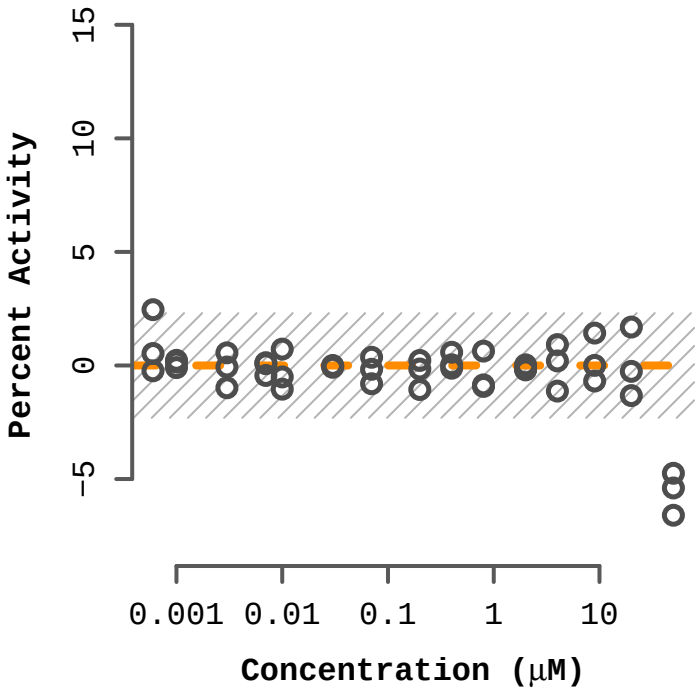
NAME: Ganaxolone
CHID: 46503 **CASRN:** 38398-32-2
SPID(S): Tox21_112264_1
M4ID: 12483193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

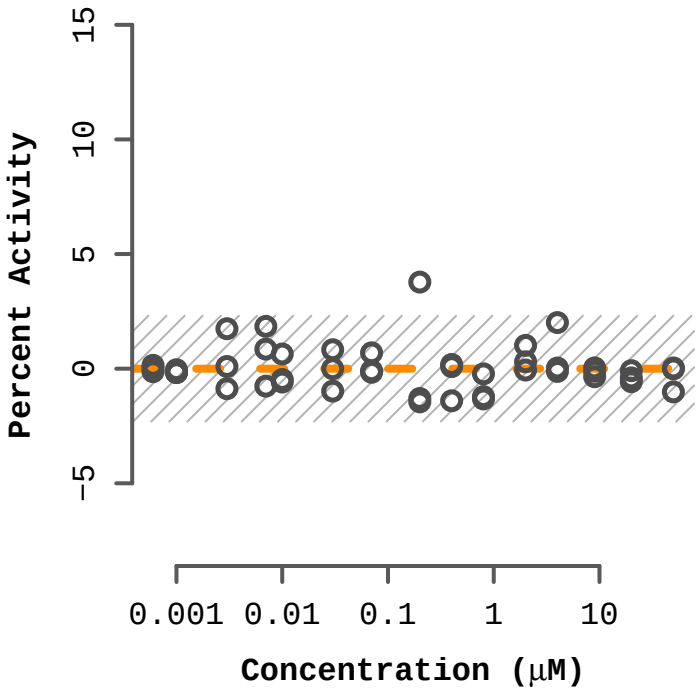
NAME: Indoramin hydrochloride
CHID: 46504 **CASRN:** 38821-52-2
SPID(S): Tox21_112265_1
M4ID: 12483192

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 0.528 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

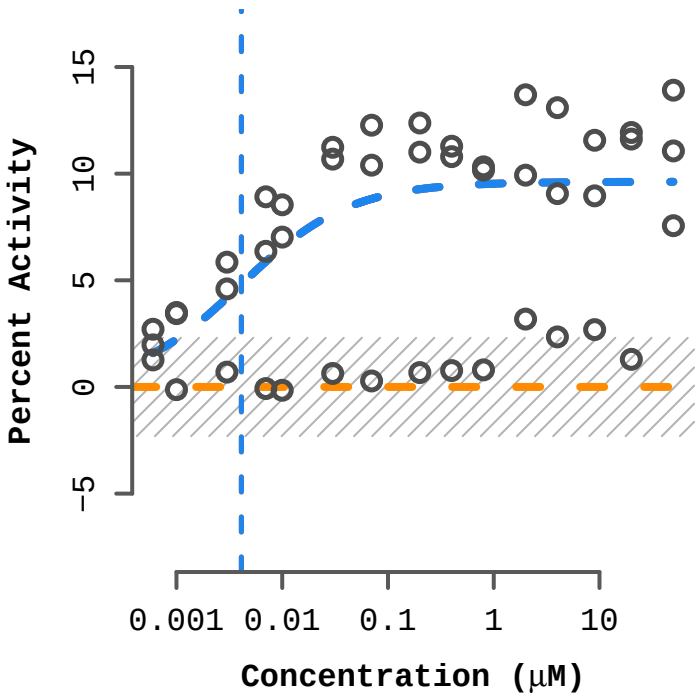
NAME: Pipamperone dihydrochloride
CHID: 46505 **CASRN:** 2448-68-2
SPID(S): Tox21_112266_1
M4ID: 12483191

HILL MODEL: Not applicable.

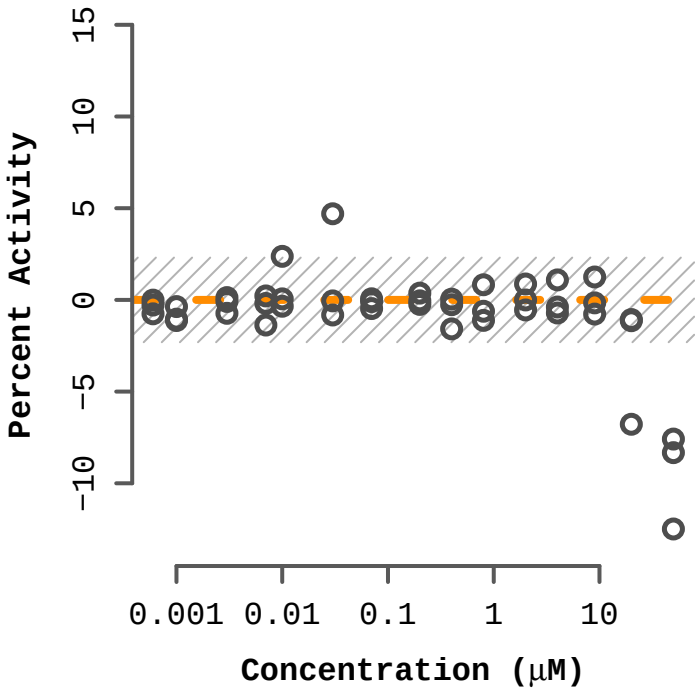
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.647 **MAX_MED:** 0.855 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Rufinamide
CHID:    46506   CASRN: 106308-44-5
SPID(S): Tox21_112267_1
M4ID:    12483190

HILL MODEL (in red):
      tp       ga       gw
val:  9.62     -2.39    0.845
sd:   0.921    0.265    0.414

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.62     -2.39    0.845    2.78     9.71
sd:   0.921    0.265    0.414    14600    131000

      CNST        HILL        GNLS
AIC:  324.9       266.28      270.28
PROB: 0           0.88        0.12
RMSE: 8.16        4.22        4.22

MAX_MEAN: 10.8      MAX_MED: 11.6      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

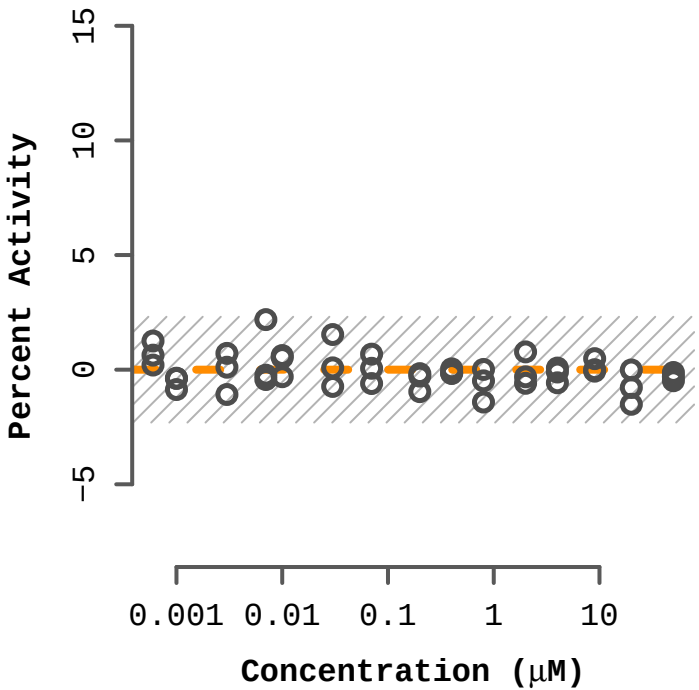
NAME: Triparanol
CHID: 46507 **CASRN:** 78-41-1
SPID(S): Tox21_112268_1
M4ID: 12483189

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.43	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 0.0582 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

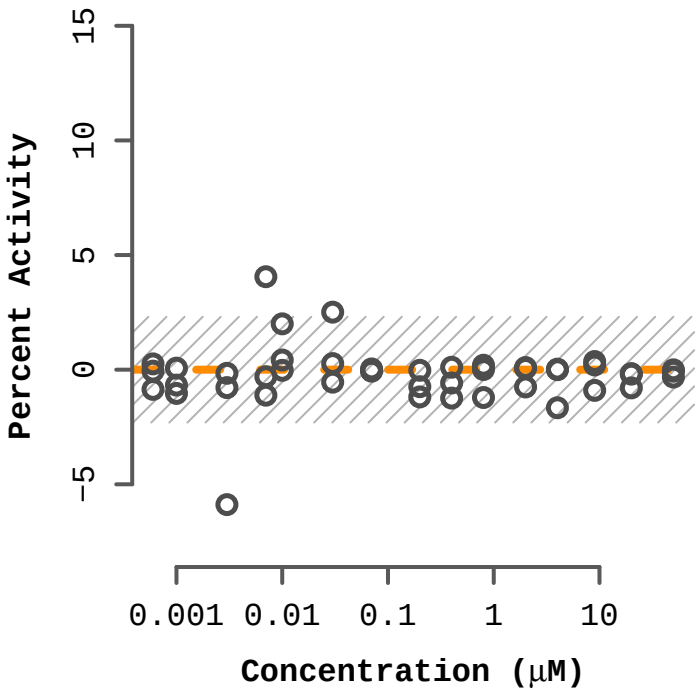
NAME: Etiracetam
CHID: 46510 **CASRN:** 33996-58-6
SPID(S): Tox21_112273_1
M4ID: 12483187

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.697 **MAX_MED:** 0.635 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

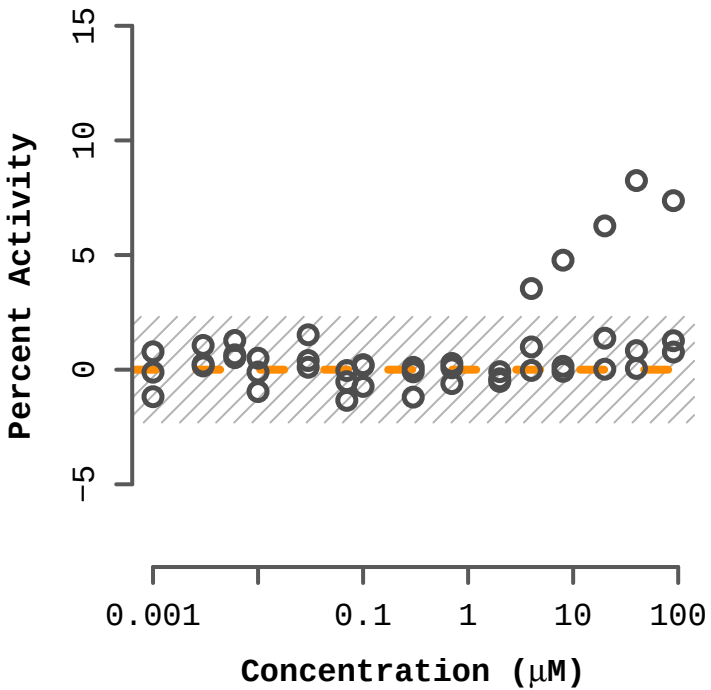
NAME: Perflunafene
CHID: 46511 **CASRN:** 306-94-5
SPID(S): Tox21_112274_1
M4ID: 12483186

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.88 **MAX_MED:** 0.423 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

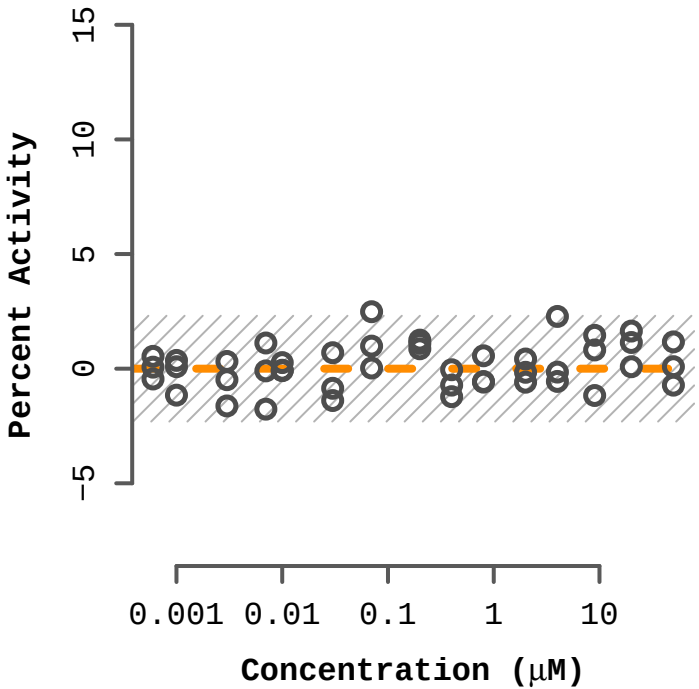
NAME: 1-Thioglycerol
CHID: 46512 **CASRN:** 96-27-5
SPID(S): Tox21_202881
M4ID: 12479371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.91	NA	NA
PROB:	1	NA	NA
RMSE:	2.2	NA	NA

MAX_MEAN: 3.14 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

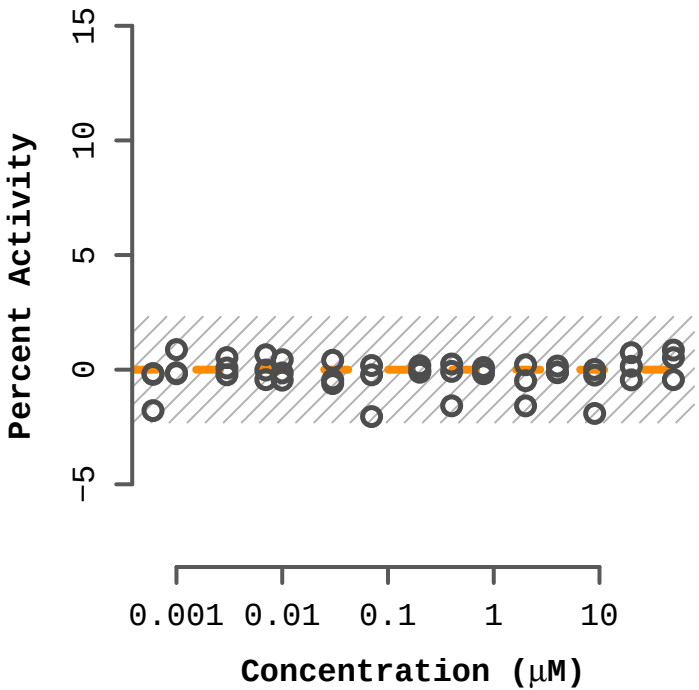
NAME: 1-Thioglycerol
CHID: 46512 **CASRN:** 96-27-5
SPID(S): Tox21_112276_1
M4ID: 12483185

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

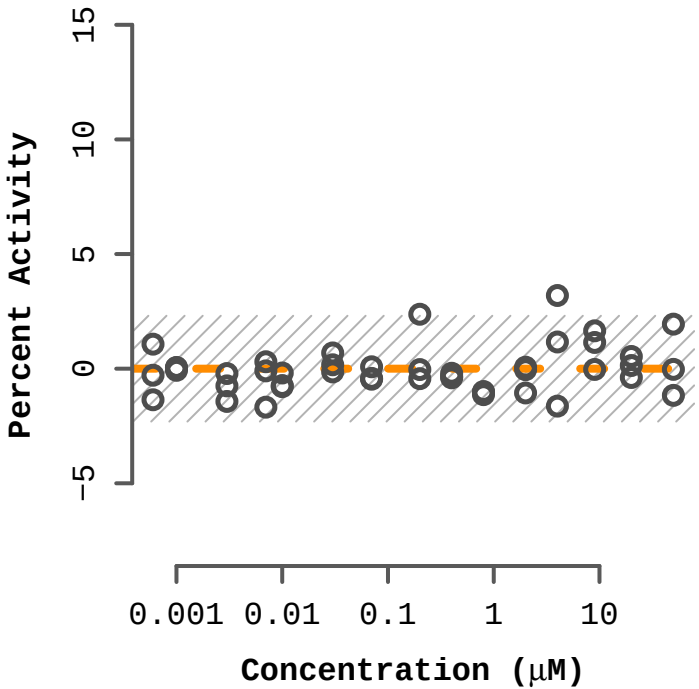
NAME: Squalane
CHID: 46513 **CASRN:** 111-01-3
SPID(S): Tox21_112277_1
M4ID: 12483184

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	86.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.69	NA	NA

MAX_MEAN: 0.316 **MAX_MED:** 0.522 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

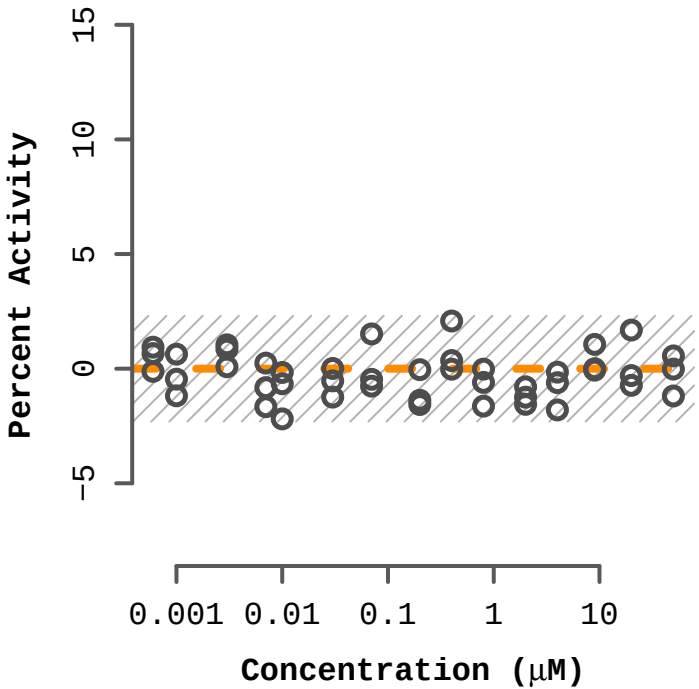
NAME: D−(−)−Mandelic acid
CHID: 46523 **CASRN:** 611−71−2
SPID(S): Tox21_112292_1
M4ID: 12483179

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.31	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.922 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

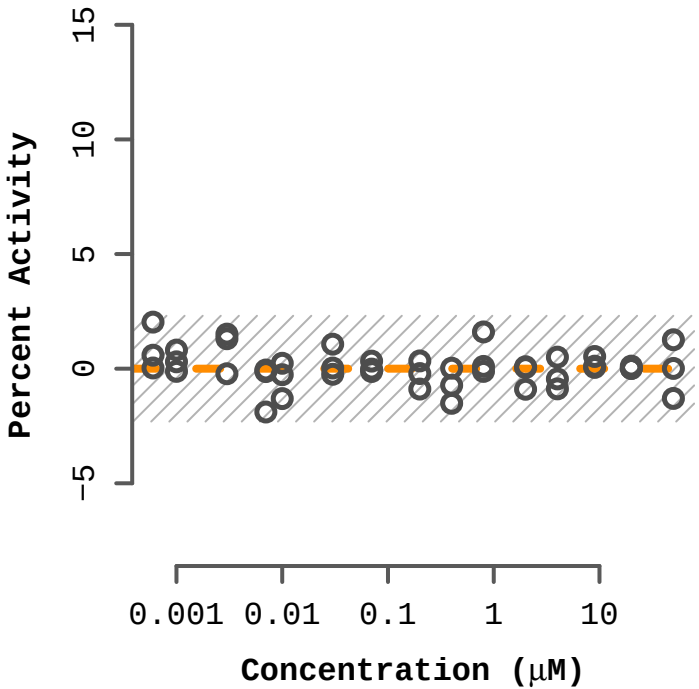
NAME: Flamenol
CHID: 46525 **CASRN:** 2174-64-3
SPID(S): Tox21_112298_1
M4ID: 12483177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.69	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

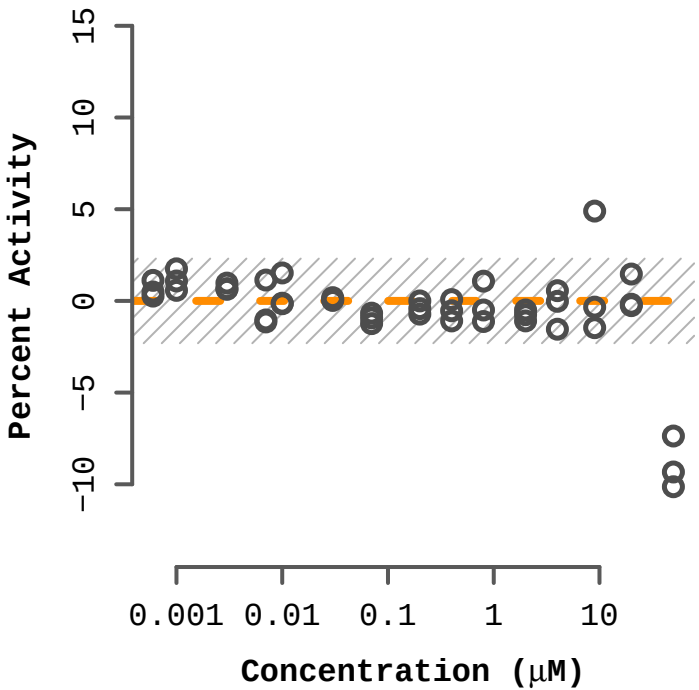
NAME: Ethyl nicotinate
CHID: 46526 **CASRN:** 614-18-6
SPID(S): Tox21_112299_1
M4ID: 12483176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

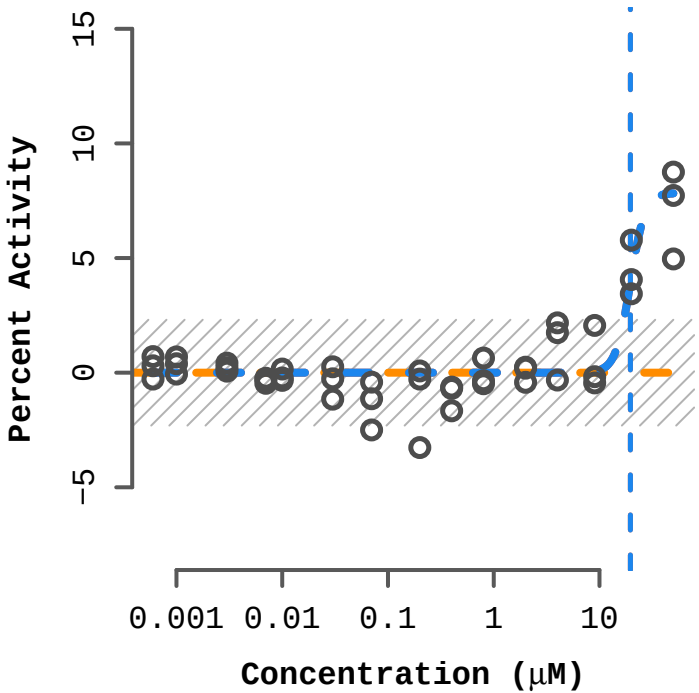
NAME: Decominol hydrochloride
CHID: 46529 **CASRN:** 60812-23-9
SPID(S): Tox21_112303_1
M4ID: 12483175

HILL MODEL: Not applicable.

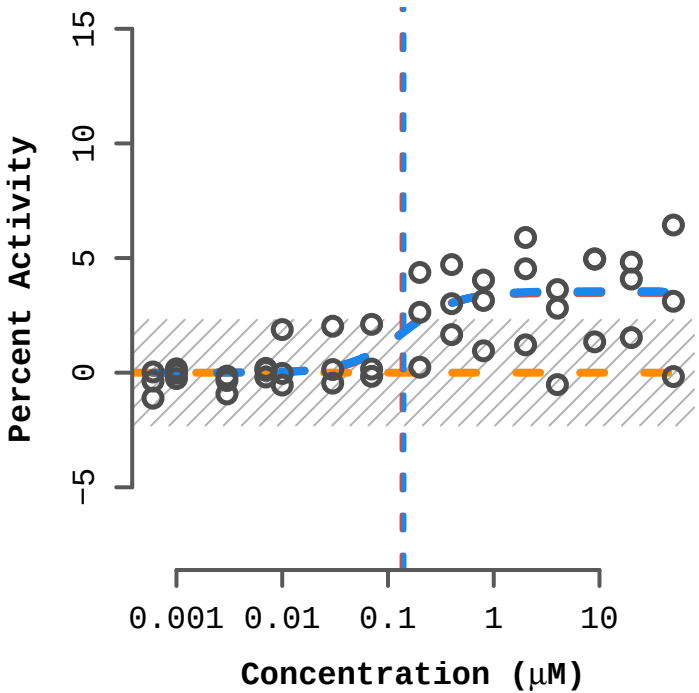
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.58	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.09 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Piconol
CHID:    46531   CASRN: 586-98-1
SPID(S): Tox21_112305_1
M4ID:    12483174

HILL MODEL (in red):
      tp       ga       gw
val:  7.84     1.29     6.28
sd:   0.648    0.0247   11.6

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.9      1.29     6.28     3.68     1.1
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  187.15      133.47      137.47
PROB: 0           0.88        0.12
RMSE: 2.41        1.06        1.06

MAX_MEAN: 7.15      MAX_MED: 7.73      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Acetyl-L-glutamic acid
CHID: 46534 CASRN: 1188-37-0
SPID(S): Tox21_112308_1
M4ID: 12483172

HILL MODEL (in red):

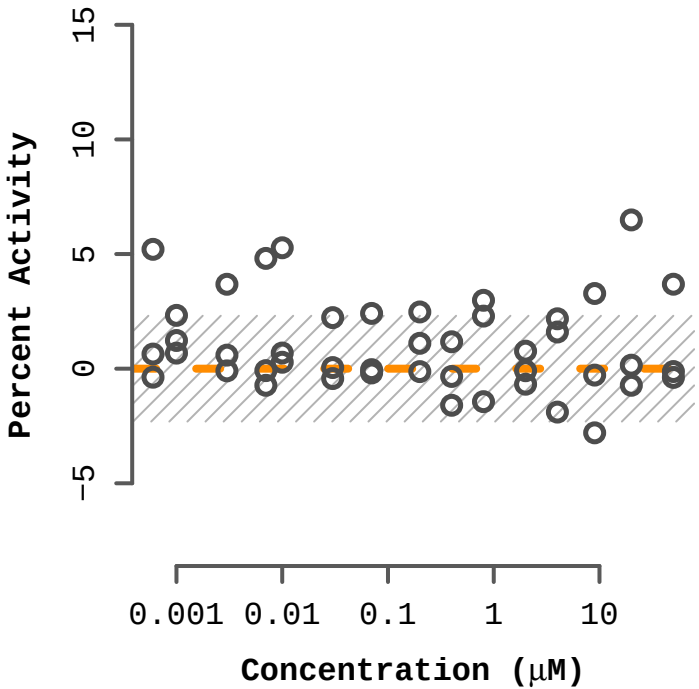
	tp	ga	gw
val:	3.48	−0.867	1.8
sd:	0.477	0.221	1.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.55	−0.849	1.68	1.76	13.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	219.05	170.95	174.83
PROB:	0	0.87	0.13
RMSE:	2.69	1.48	1.48

MAX_MEAN: 3.88 **MAX_MED:** 4.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

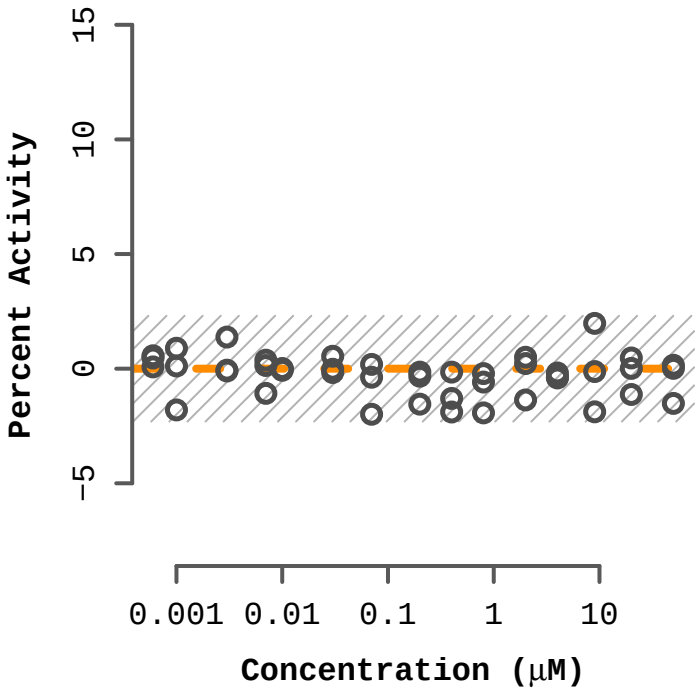
NAME: 2-Amino-6-methylheptane
CHID: 46535 **CASRN:** 543-82-8
SPID(S): Tox21_112309_1
M4ID: 12483171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.08	NA	NA
PROB:	1	NA	NA
RMSE:	2.24	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

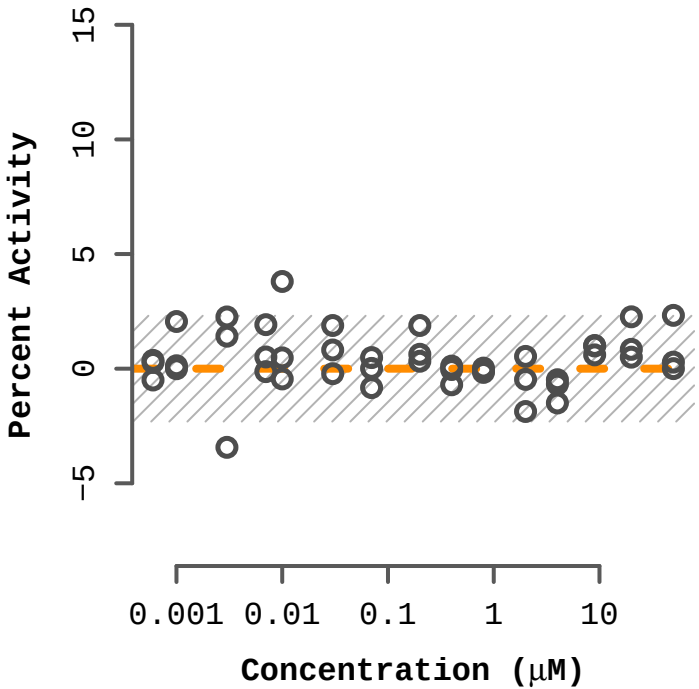
NAME: L−Thioproline
CHID: 46536 **CASRN:** 34592−47−7
SPID(S): Tox21_112310_1
M4ID: 12483170

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.406 **MAX_MED:** 0.467 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

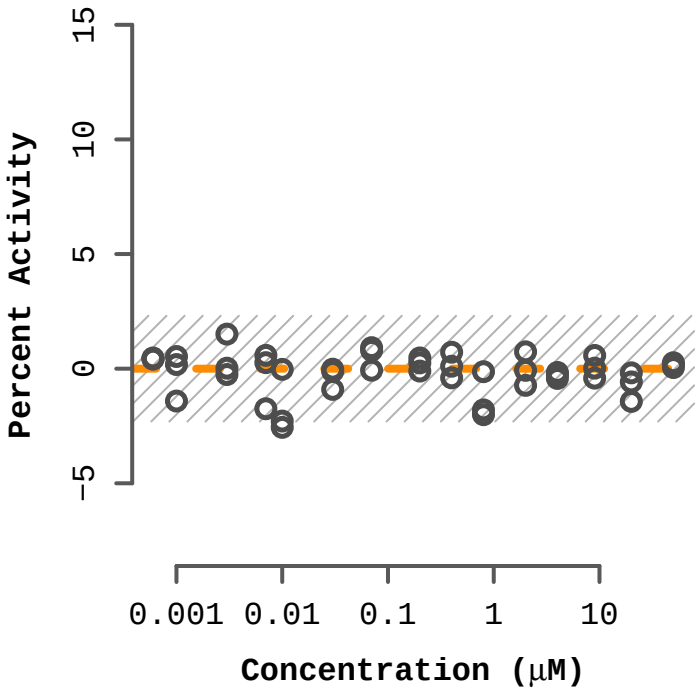
NAME: Calcium levulinate
CHID: 46539 **CASRN:** 5743-49-7
SPID(S): Tox21_112315_1
M4ID: 12483168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

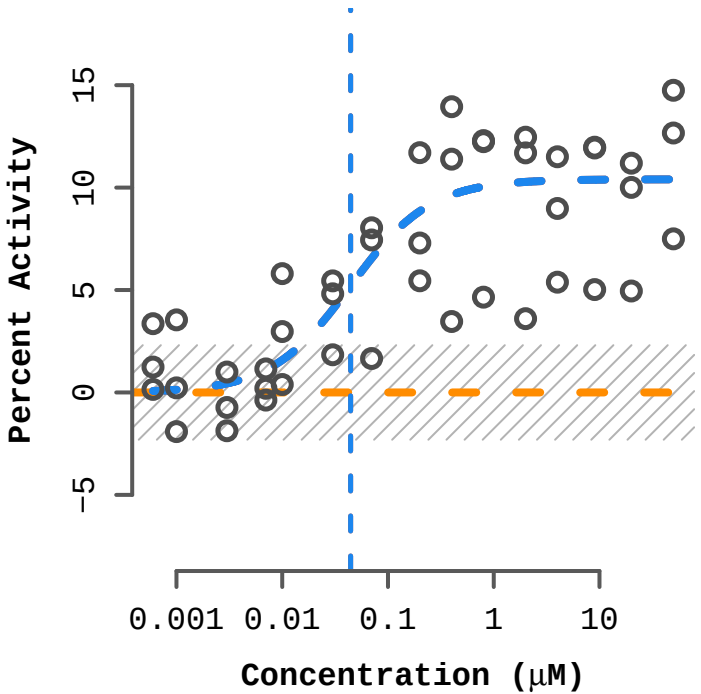
NAME: alpha-Lipoic acid amide
CHID: 46541 **CASRN:** 940-69-2
SPID(S): Tox21_112317_1
M4ID: 12483167

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.4	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.551 **MAX_MED:** 0.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nicotinic acid 1-oxide
CHID: 46543 CASRN: 2398-81-4
SPID(S): Tox21_112319_1
M4ID: 12483166

HILL MODEL (in red):

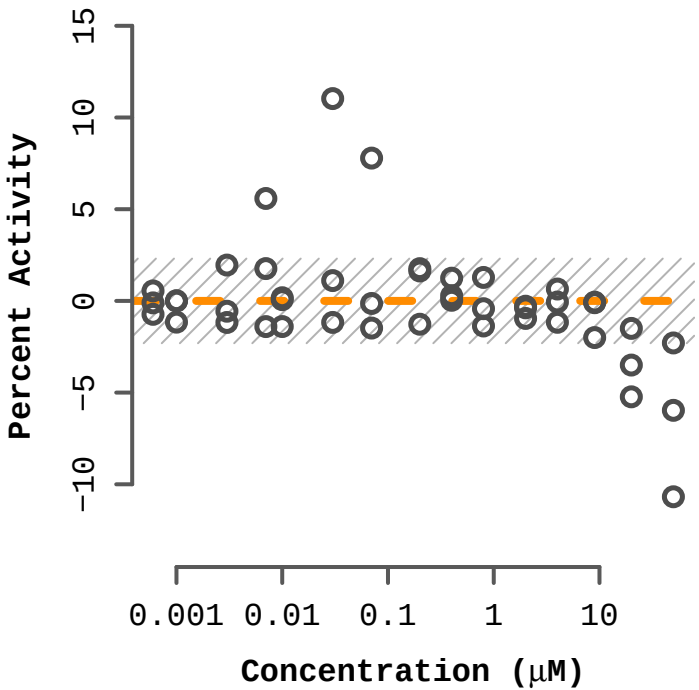
	tp	ga	gw
val:	10.4	−1.35	1.15
sd:	0.816	0.173	0.401

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.4	−1.35	1.15	2.51	11
sd:	0.816	0.173	0.401	1610	22000

	CNST	HILL	GNLS
AIC:	318.44	235.9	239.9
PROB:	0	0.88	0.12
RMSE:	7.72	2.94	2.94

MAX_MEAN: 11.6 MAX_MED: 12.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

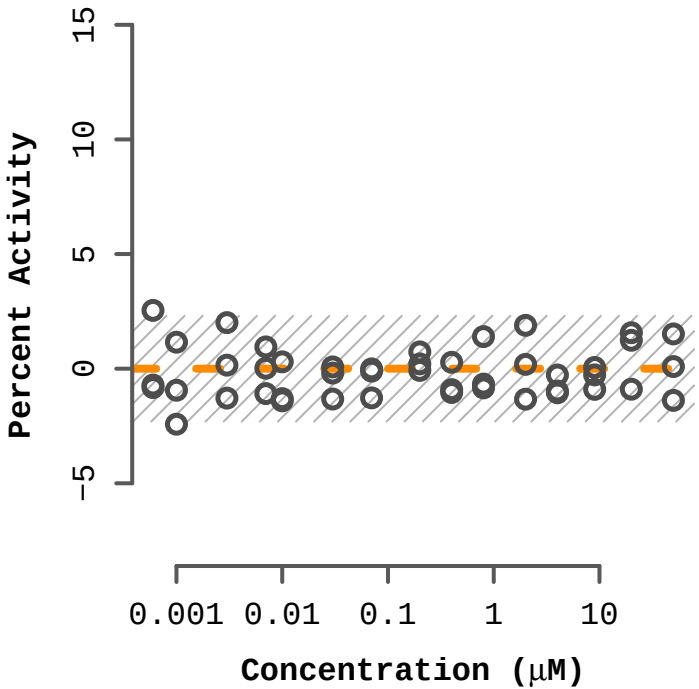
NAME: Diphenylcyclopropenone
CHID: 46545 **CASRN:** 886-38-4
SPID(S): Tox21_112322_1
M4ID: 12483164

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.75	NA	NA
PROB:	1	NA	NA
RMSE:	3.16	NA	NA

MAX_MEAN: 3.66 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

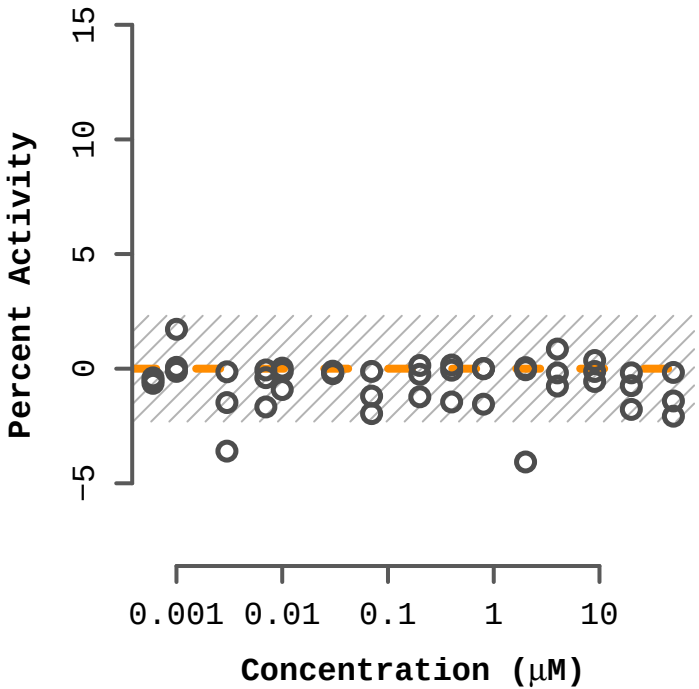
NAME: Pyrithioxin dihydrochloride
CHID: 46550 CASRN: 10049-83-9
SPID(S): Tox21_112335_1
M4ID: 12483153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.639 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

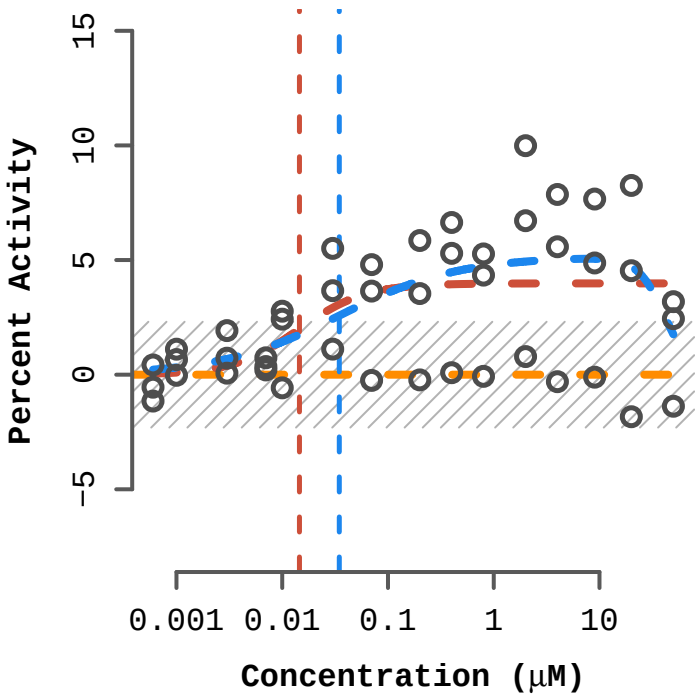
NAME: Quinestrol
CHID: 46553 **CASRN:** 152-43-2
SPID(S): Tox21_112340_1
M4ID: 12483150

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.554 **MAX_MED:** 0.0594 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Climbazole
CHID: 46555 **CASRN:** 38083-17-9
SPID(S): Tox21_112343_1
M4ID: 12483148

HILL MODEL (in red):

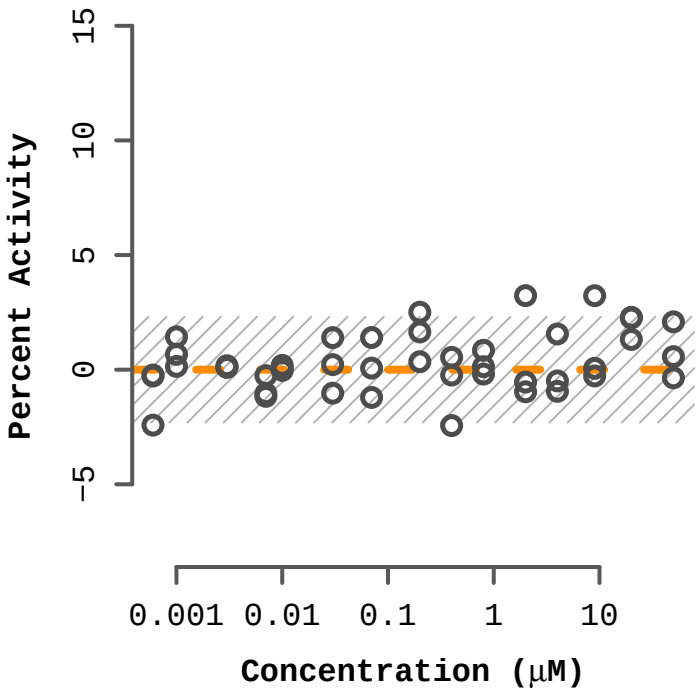
	tp	ga	gw
val:	3.98	−1.84	1.39
sd:	0.713	0.328	1.58

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.15	−1.46	0.769	1.62	3.41
sd:	1.51	0.64	0.546	0.235	7.08

	CNST	HILL	GNLS
AIC:	254.09	224.23	224.3
PROB:	0	0.51	0.49
RMSE:	3.95	2.62	2.56

MAX_MEAN: 5.83 **MAX_MED:** 6.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

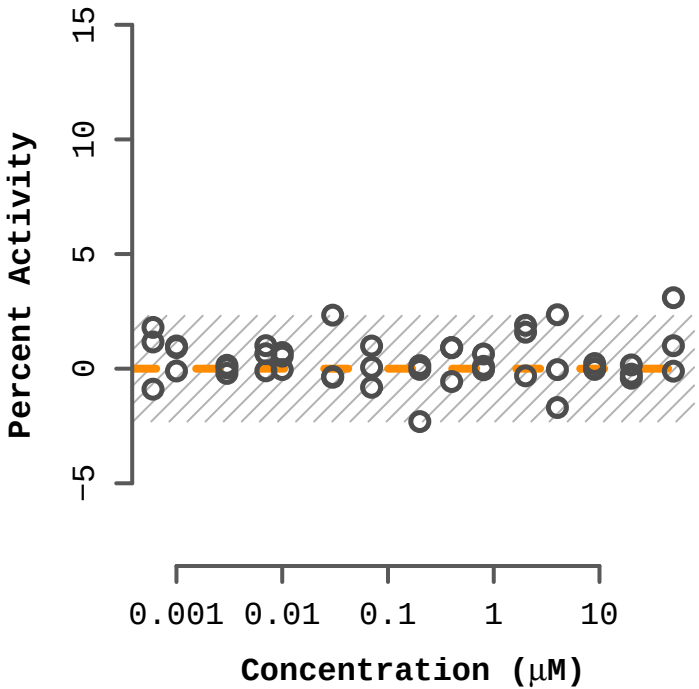
NAME: Cridanimod
CHID: 46557 CASRN: 38609-97-1
SPID(S): Tox21_112348_1
M4ID: 12483144

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

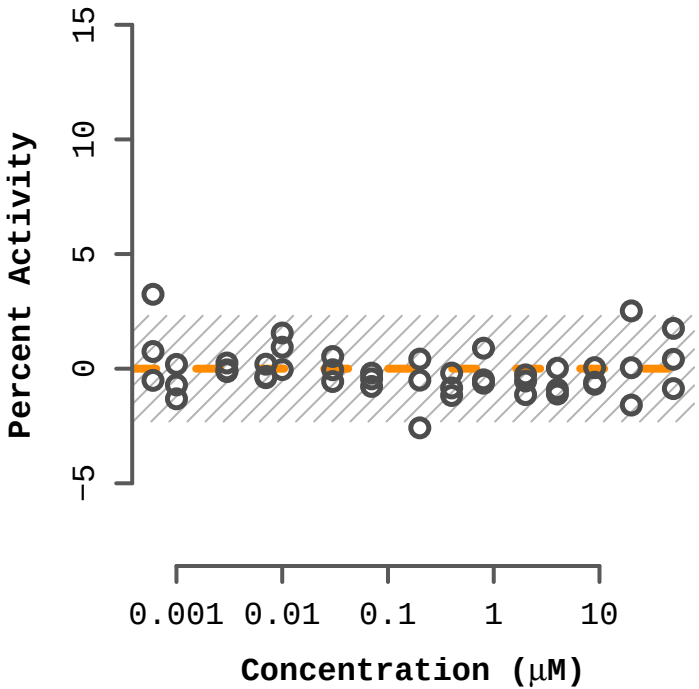
NAME: 2-Chloro-5-methylphenol
CHID: 46558 **CASRN:** 615-74-7
SPID(S): Tox21_112350_1
M4ID: 12483143

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

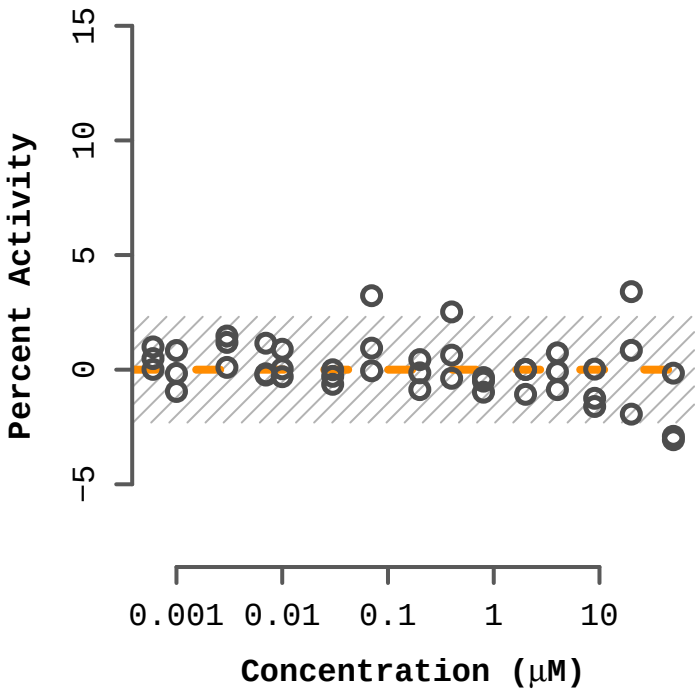
NAME: 1-Bromoheptadecafluorooctane
CHID: 46560 **CASRN:** 423-55-2
SPID(S): Tox21_112353_1
M4ID: 12483140

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.938 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

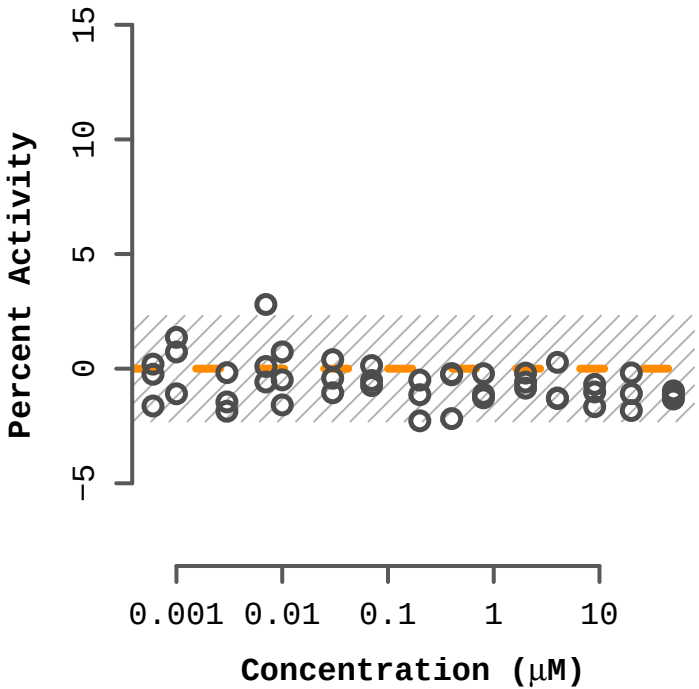
NAME: Bipenamol
CHID: 46561 CASRN: 79467-22-4
SPID(S): Tox21_112355_1
M4ID: 12483138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N,N'−Dibenzylethane−1,2−diamine dihydrochlorid

CHID: 46563 **CASRN:** 3412−76−8

SPID(S): Tox21_112357_1

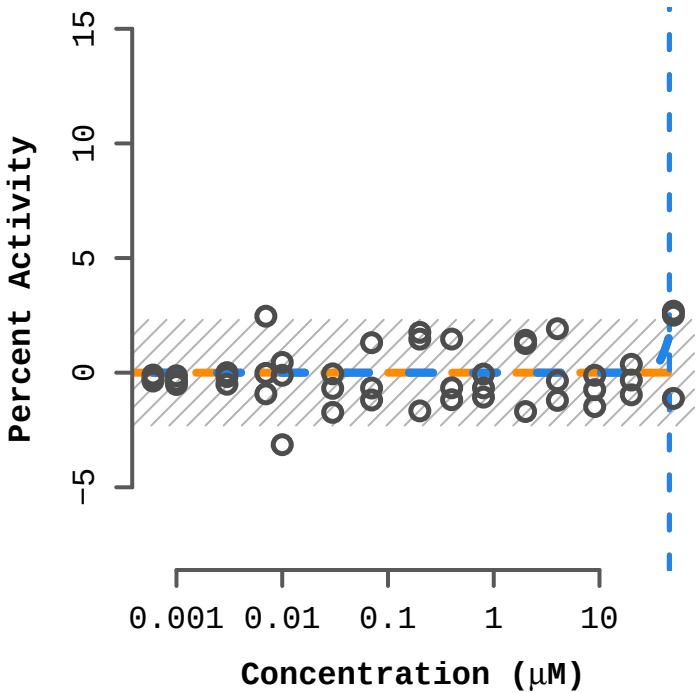
M4ID: 12483137

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.772 **MAX_MED:** 0.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Xenalipin
CHID: 46565 CASRN: 84392-17-6
SPID(S): Tox21_112359_1
M4ID: 12483136

HILL MODEL (in red):

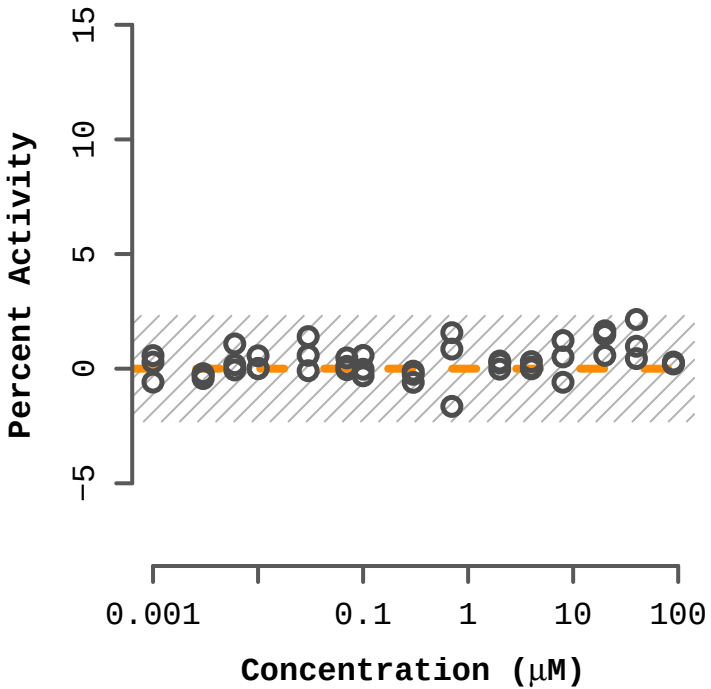
	tp	ga	gw
val:	3.22	1.66	8
sd:	14.3	0.67	20.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.22	1.66	8	2.45	13.3
sd:	14.1	0.663	20.6	45600	749000

	CNST	HILL	GNLS
AIC:	151.01	152.7	156.7
PROB:	0.67	0.29	0.04
RMSE:	1.24	1.2	1.2

MAX_MEAN: 1.36 MAX_MED: 2.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

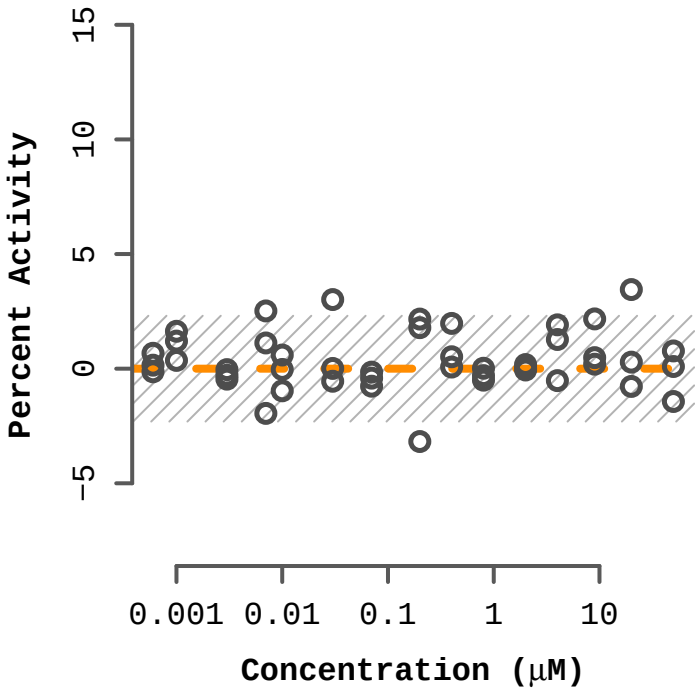
NAME: 4-Tolyl acetate
CHID: 46567 **CASRN:** 140-39-6
SPID(S): Tox21_302350
M4ID: 12476783

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

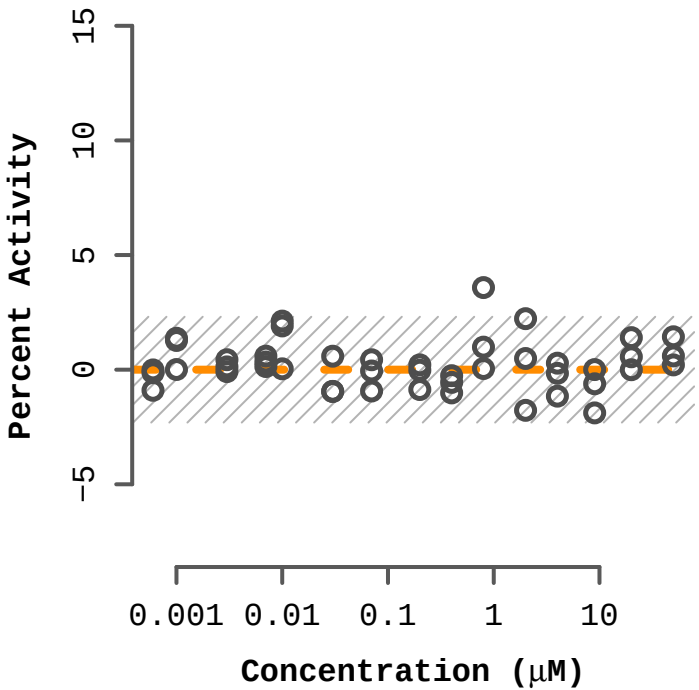
NAME: 4-Tolyl acetate
CHID: 46567 **CASRN:** 140-39-6
SPID(S): Tox21_112361_1
M4ID: 12483135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

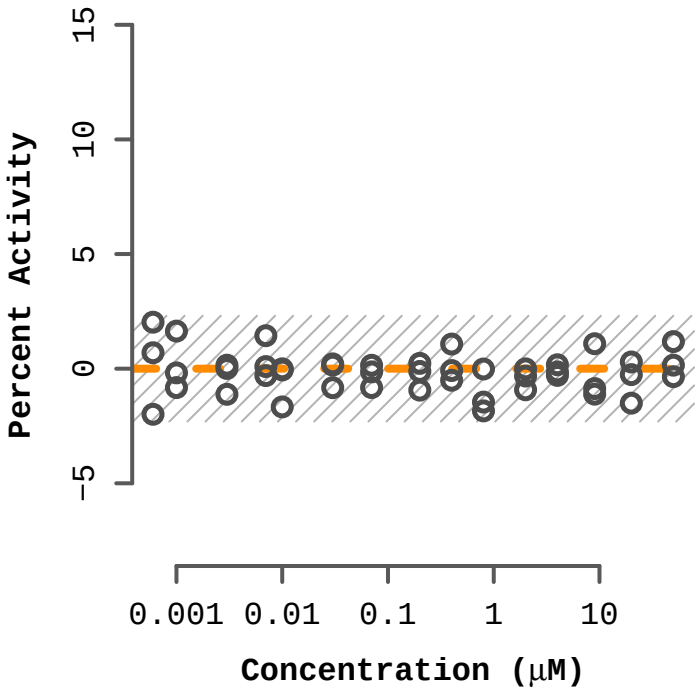
NAME: Mepiroxol
CHID: 46569 **CASRN:** 6968-72-5
SPID(S): Tox21_112363_1
M4ID: 12483134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

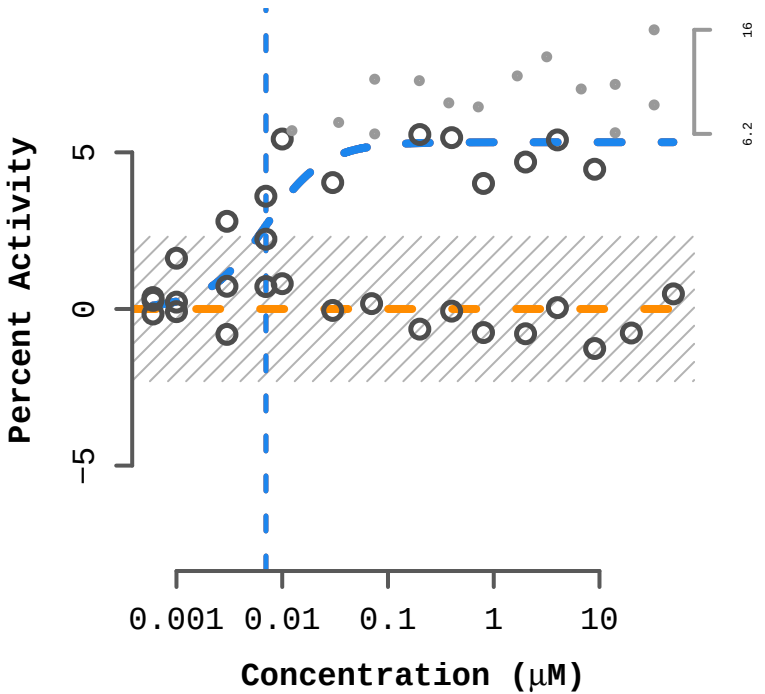
NAME: Benznidazole
CHID: 46570 CASRN: 22994-85-0
SPID(S): Tox21_112364_1
M4ID: 12483133

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.411 **MAX_MED:** 0.697 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyacetacide
CHID: 46572 CASRN: 140-87-4
SPID(S): Tox21_112366_1
M4ID: 12483132 BRK

HILL MODEL (in red):

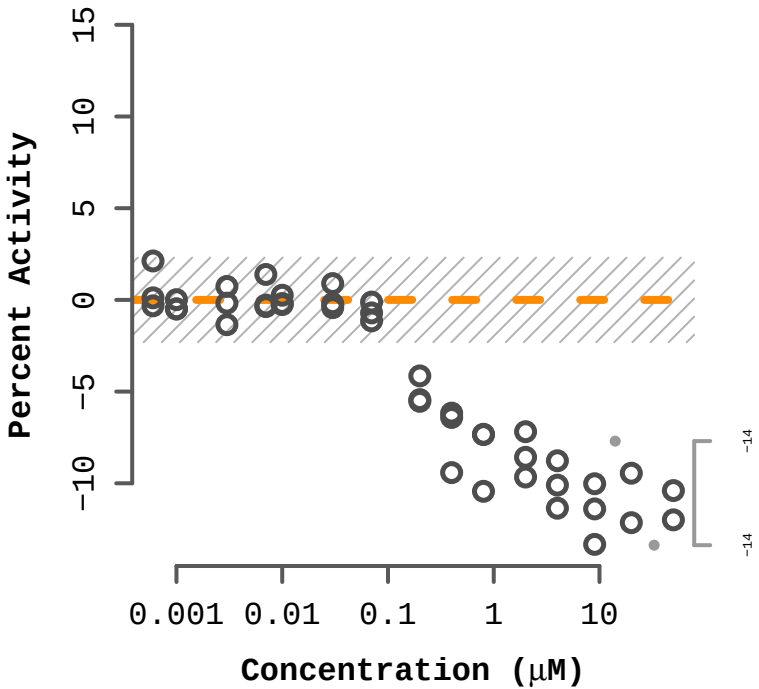
	tp	ga	gw
val:	5.32	−2.15	1.57
sd:	0.988	0.293	2.29

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.32	−2.15	1.57	2.83	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	291.76	263.77	267.77
PROB:	0	0.88	0.12
RMSE:	6.05	4.02	4.02

MAX_MEAN: 8.31 MAX_MED: 8.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

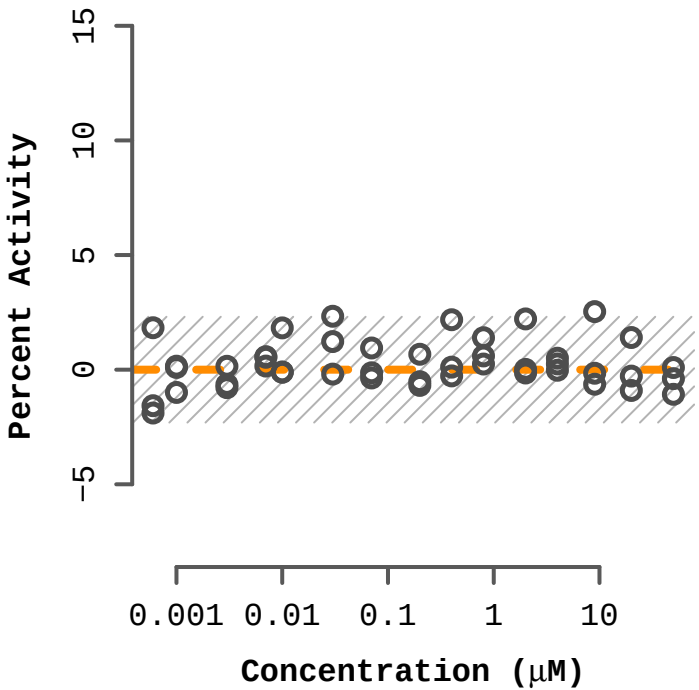
NAME: Carbocyanine
CHID: 46576 **CASRN:** 605-91-4
SPID(S): Tox21_112373_1
M4ID: 12483129 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	309.91	NA	NA
PROB:	1	NA	NA
RMSE:	7.12	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.116 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

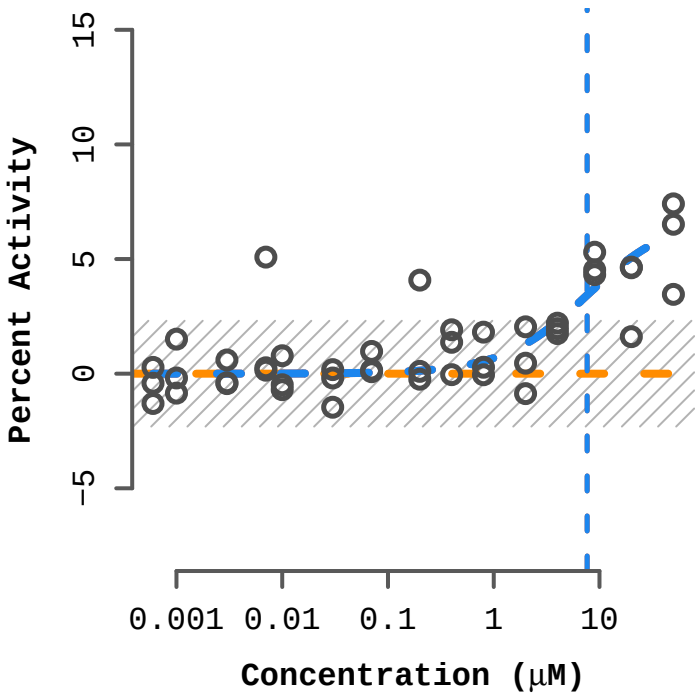
NAME: Alovudine
CHID: 46579 **CASRN:** 25526-93-6
SPID(S): Tox21_112376_1
M4ID: 12483128

HILL MODEL: Not applicable.

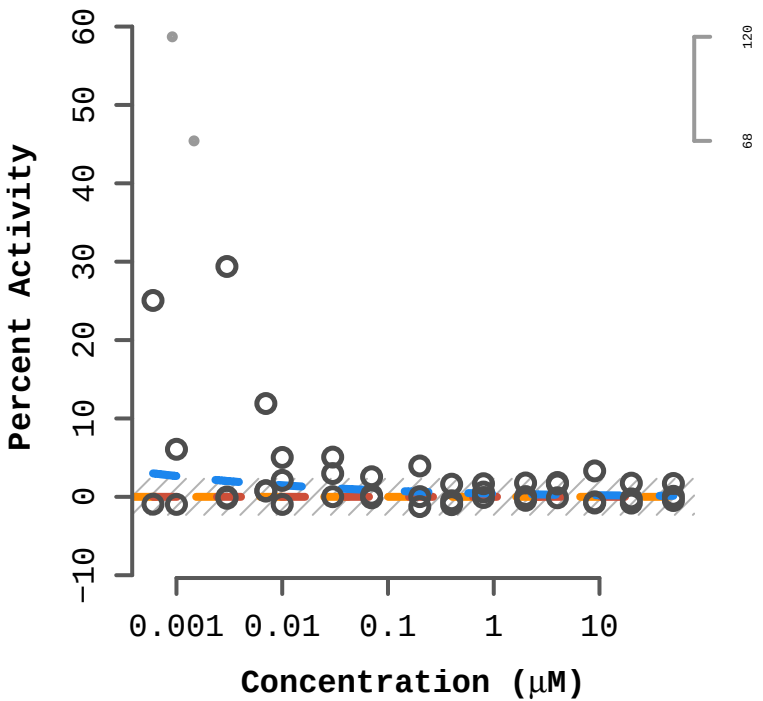
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.23 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Padimate
CHID:    46580   CASRN: 21245-01-2
SPID(S): Tox21_112377_1
M4ID:    12483127

HILL MODEL (in red):
      tp       ga       gw
val:  6.86     0.883    1.08
sd:   3.43     0.531    0.923

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.86     0.883    1.08     3.15     5.42
sd:   3.43     0.531    0.923    1050     3930

      CNST        HILL        GNLS
AIC:  209.86      154.86      158.86
PROB: 0           0.88        0.12
RMSE: 2.59        1.4         1.4

MAX_MEAN: 5.8       MAX_MED: 6.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carsalam
CHID: 46584 **CASRN:** 2037-95-8
SPID(S): Tox21_112383_1
M4ID: 12483123 **BRK**

HILL MODEL (in red):

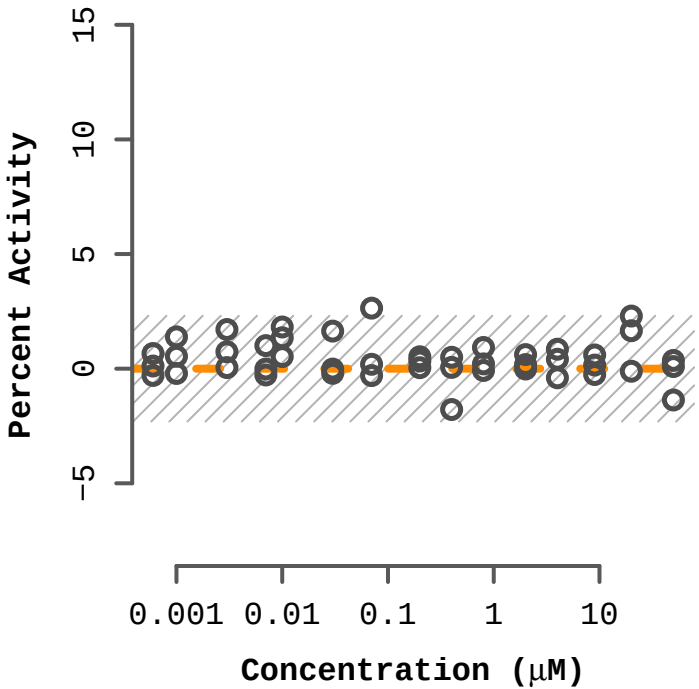
	tp	ga	gw
val:	43.3	2	6.64
sd:	1920	3.8	185

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13	−5.22	2.74	−4.97	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	299.53	305.43	304.85
PROB:	0.89	0.05	0.06
RMSE:	21.91	21.91	21.18

MAX_MEAN: 49.2 **MAX_MED:** 25.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

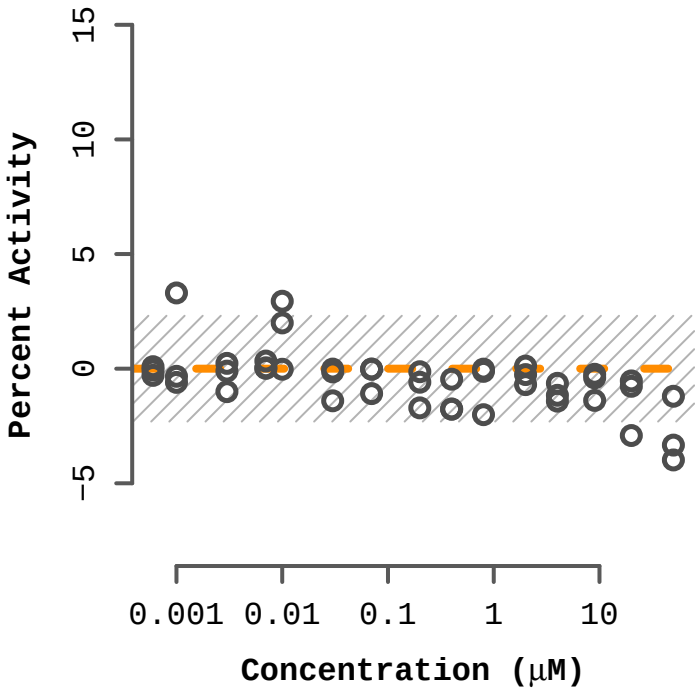
NAME: 1,3-Bis(4-carboxyphenoxy)propane
CHID: 46585 **CASRN:** 3753-81-9
SPID(S): Tox21_112384_1
M4ID: 12483122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

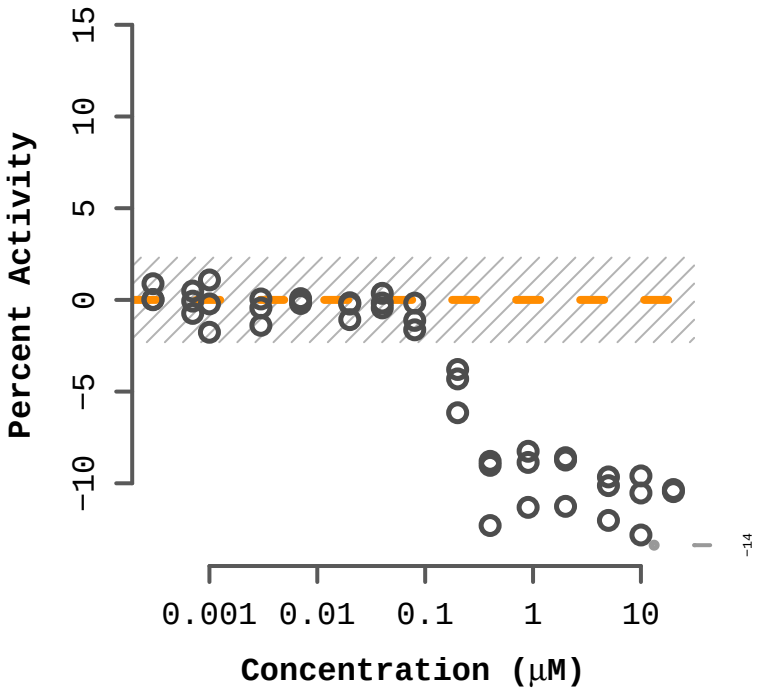
NAME: Protoporphyrin disodium
CHID: 46589 **CASRN:** 50865-01-5
SPID(S): Tox21_112390_1
M4ID: 12483120

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

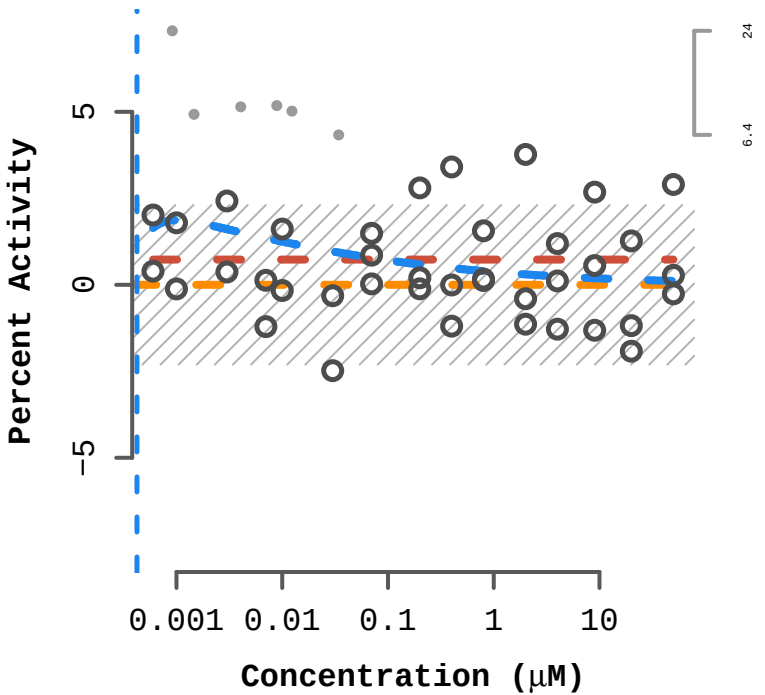
NAME: 3,3'−Diethylthiacarbocyanine iodide
CHID: 46591 CASRN: 905−97−5
SPID(S): Tox21_112392_1
M4ID: 12483118 BRK

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.99	NA	NA
PROB:	1	NA	NA
RMSE:	6.76	NA	NA

MAX_MEAN: 0.307 **MAX_MED:** 0.0272 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pyridoxal phosphate hydrate
CHID: 46594 **CASRN:** 41468-25-1
SPID(S): Tox21_112399_1
M4ID: 12483115 **BRK**

HILL MODEL (in red):

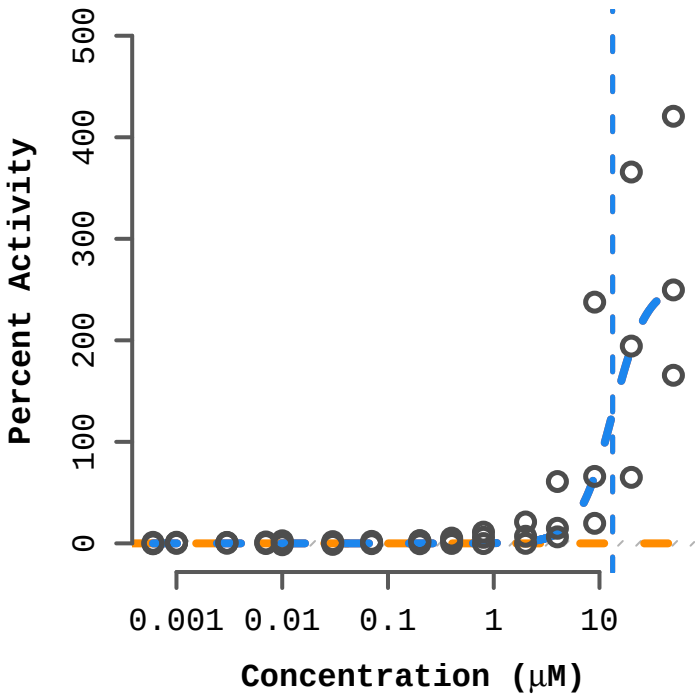
	tp	ga	gw
val:	0.729	−5.2	3.37
sd:	0.354	1250	2080

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.13	−3.37	3.4	−3.12	0.322
sd:	16.8	1.31	25.2	9.04	0.423

	CNST	HILL	GNLS
AIC:	243.01	244.54	246.15
PROB:	0.6	0.28	0.12
RMSE:	5.06	4.82	4.59

MAX_MEAN: 8.73 **MAX_MED:** 2.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Difloxacin hydrochloride
CHID: 46599 CASRN: 91296-86-5
SPID(S): Tox21_112405_1
M4ID: 12483114

HILL MODEL (in red):

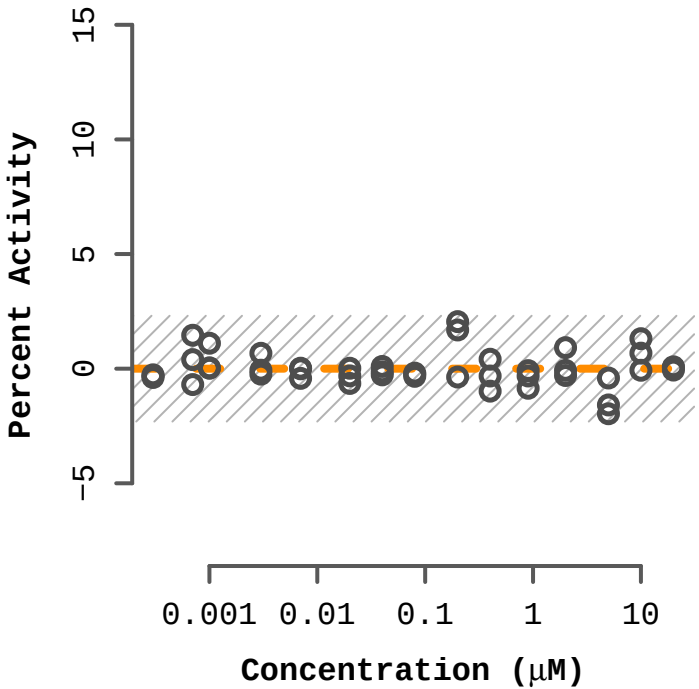
	tp	ga	gw
val:	257	1.12	2.68
sd:	7.5	0.0194	0.245

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	257	1.12	2.68	3.66	12.6
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	495.44	424.93	428.93
PROB:	0	0.88	0.12
RMSE:	106.3	51.08	51.08

MAX_MEAN: 279 **MAX_MED:** 250 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

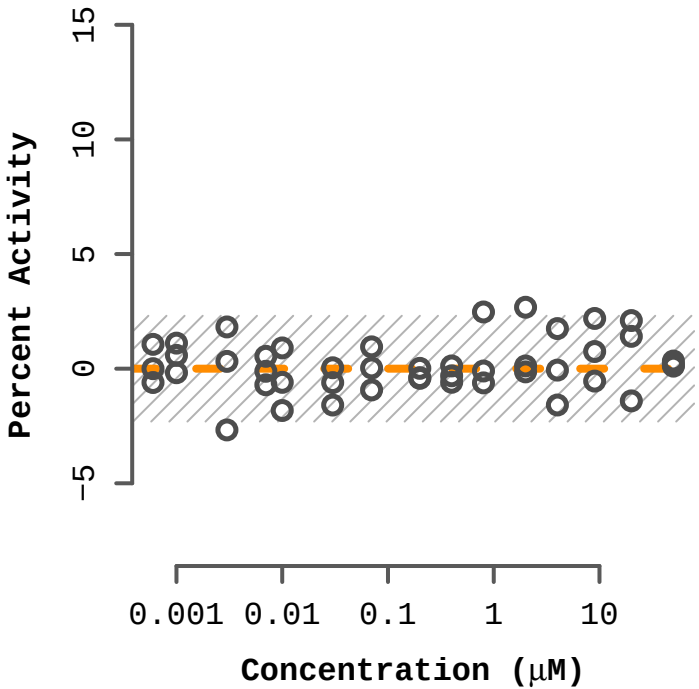
NAME: Marbofloxacin
CHID: 46600 **CASRN:** 115550-35-1
SPID(S): Tox21_112406_1
M4ID: 12483113

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

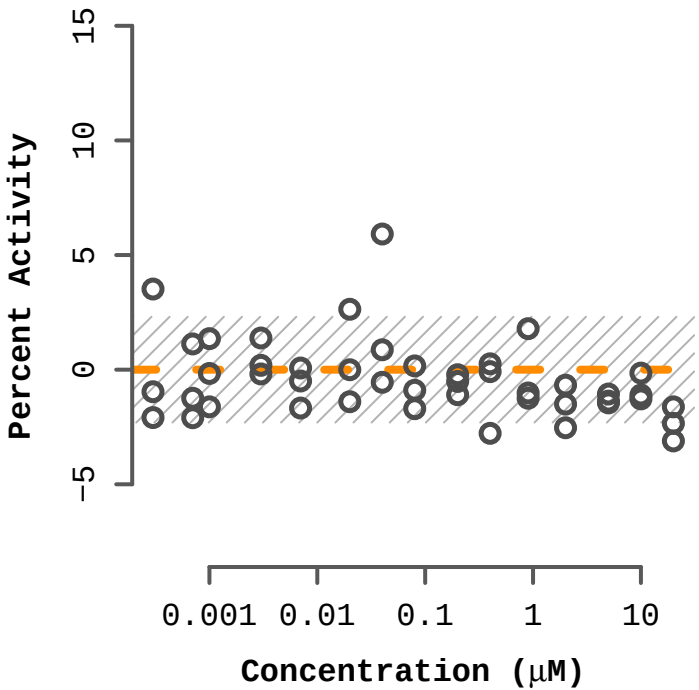
NAME: Trifluridine
CHID: 46602 **CASRN:** 70-00-8
SPID(S): Tox21_112411_1
M4ID: 12483111

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.887 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

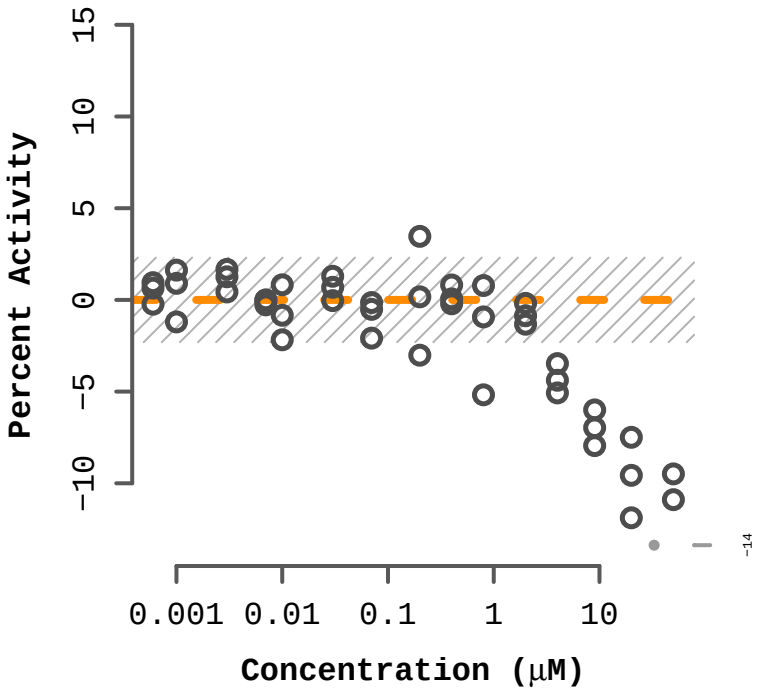
NAME: Imidocarb dipropionate
CHID: 46604 CASRN: 55750-06-6
SPID(S): Tox21_112415_1
M4ID: 12483109

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 0.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

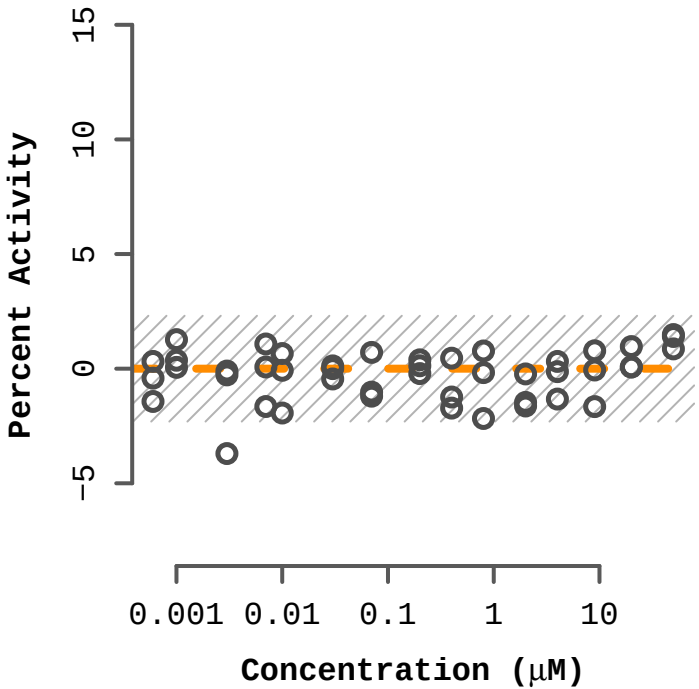
NAME: Benzyldimethyltetradecylammonium chloride dihy
CHID: 46606 CASRN: 147228-81-7
SPID(S): Tox21_112417_1
M4ID: 12483108 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	259.16	NA	NA
PROB:	1	NA	NA
RMSE:	4.65	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

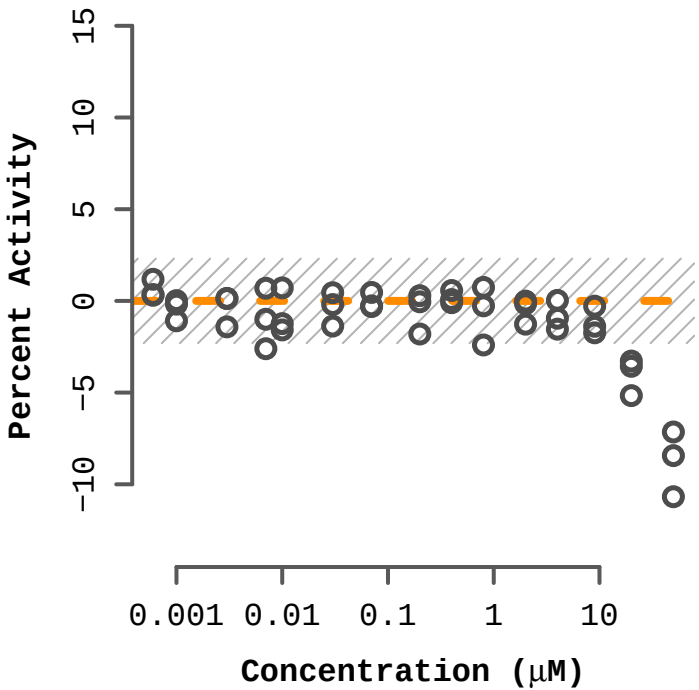
NAME: Palonosetron hydrochloride
CHID: 46610 **CASRN:** 135729-62-3
SPID(S): Tox21_112421_1
M4ID: 12483107

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

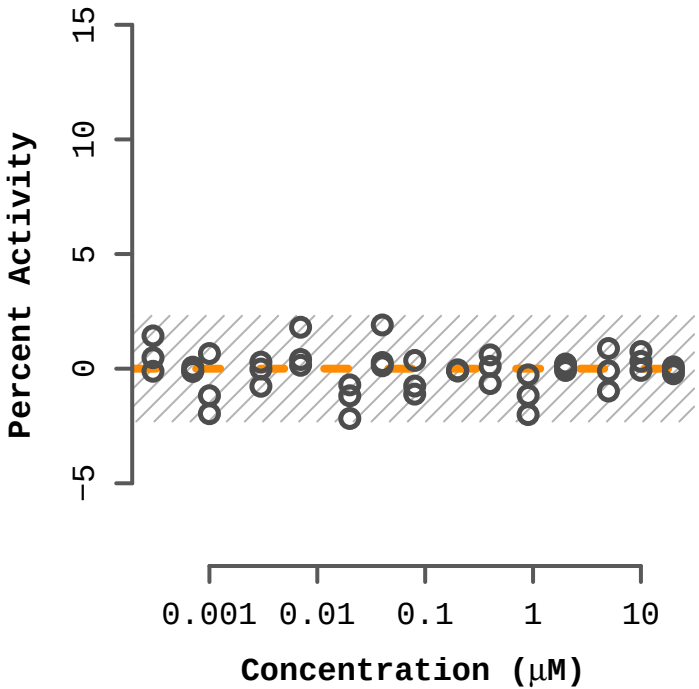
NAME: Tioconazole
CHID: 46619 **CASRN:** 65899-73-2
SPID(S): Tox21_112434_1
M4ID: 12483104

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.69	NA	NA

MAX_MEAN: 0.612 **MAX_MED:** 0.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

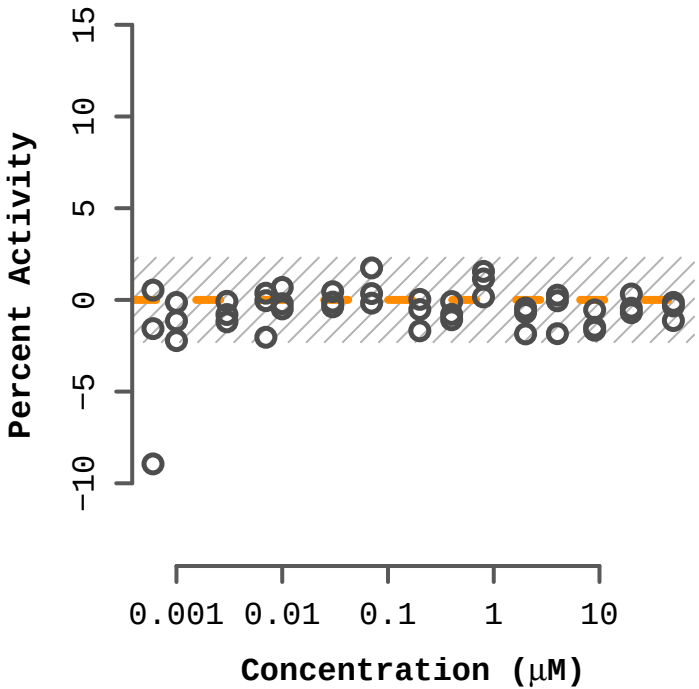
NAME: Pemirolast potassium
CHID: 46623 **CASRN:** 100299-08-9
SPID(S): Tox21_112438_1
M4ID: 12483103

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.786 **MAX_MED:** 0.479 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

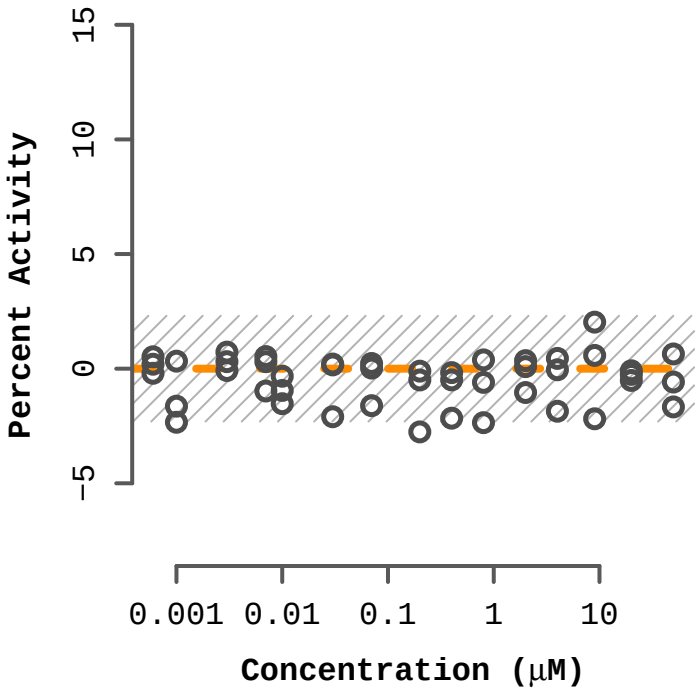
NAME: Bosentan
CHID: 46627 **CASRN:** 147536-97-8
SPID(S): Tox21_112444_1
M4ID: 12483099

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 0.954 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

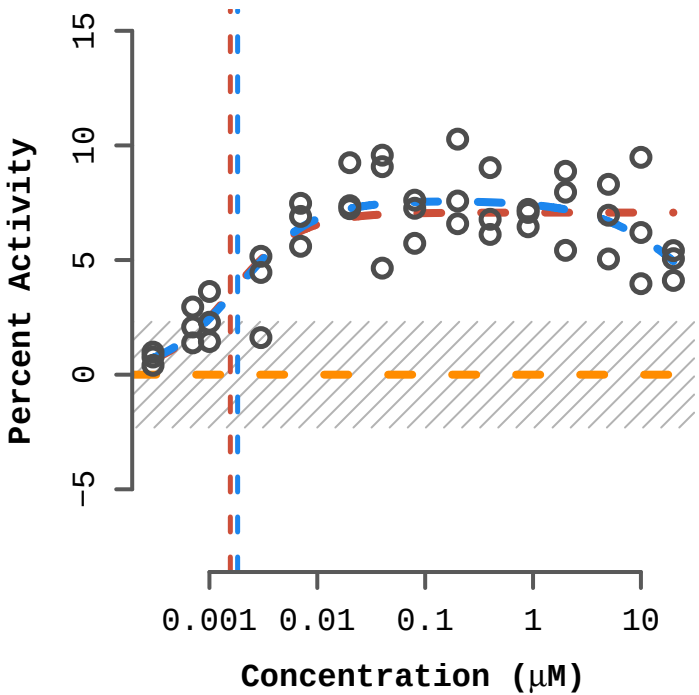
NAME: Tamsulosin hydrochloride
CHID: 46628 CASRN: 106463-17-6
SPID(S): Tox21_112446_1
M4ID: 12483097

HILL MODEL: Not applicable.

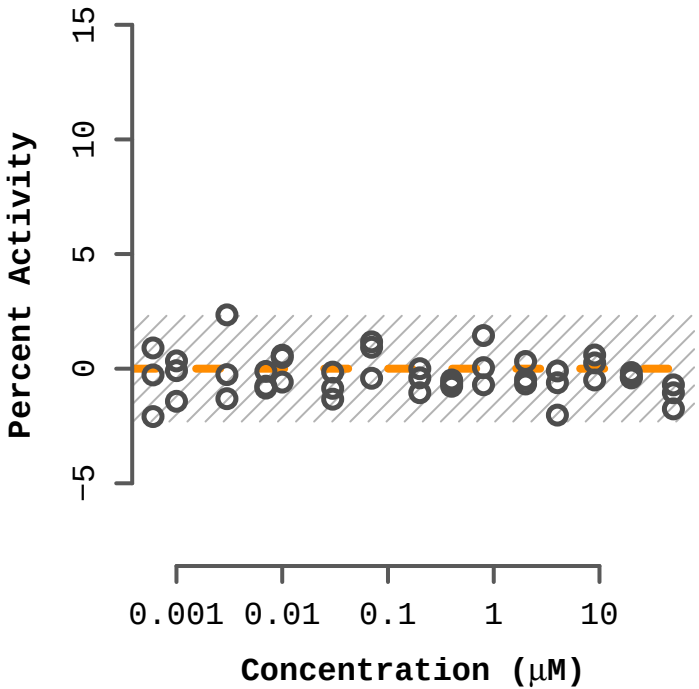
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.317 **MAX_MED:** 0.58 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Eprazinone dihydrochloride
CHID:    46631   CASRN: 10402-53-6
SPID(S): Tox21_112449_1
M4ID:    12483096

HILL MODEL (in red):
      tp       ga       gw
val:  7.07     -2.81    1.37
sd:   0.297    0.0984   0.292

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.62     -2.74    1.24     1.58     0.978
sd:   0.64     0.115    0.265    0.407    1.27

      CNST        HILL        GNLS
AIC:  304.04      175.2       167.75
PROB: 0           0.02        0.98
RMSE: 6.32        1.52        1.36

MAX_MEAN: 8.15      MAX_MED: 9.07      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

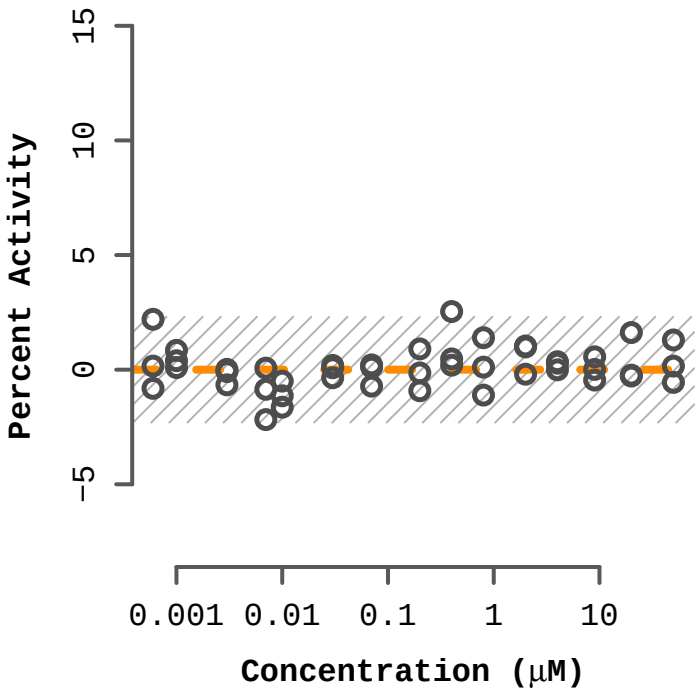
NAME: Prosultiamine
CHID: 46633 **CASRN:** 59-58-5
SPID(S): Tox21_112451_1
M4ID: 12483094

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.563 **MAX_MED:** 0.935 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

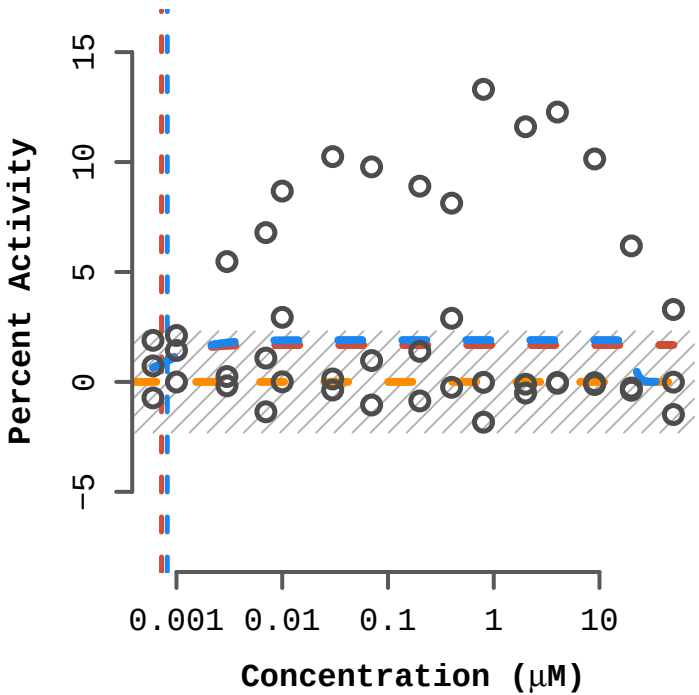
NAME: Trepibutone
CHID: 46634 **CASRN:** 41826-92-0
SPID(S): Tox21_112452_1
M4ID: 12483093

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.993 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clinofibrate
CHID: 46638 **CASRN:** 30299-08-2
SPID(S): Tox21_112457_1
M4ID: 12483091

HILL MODEL (in red):

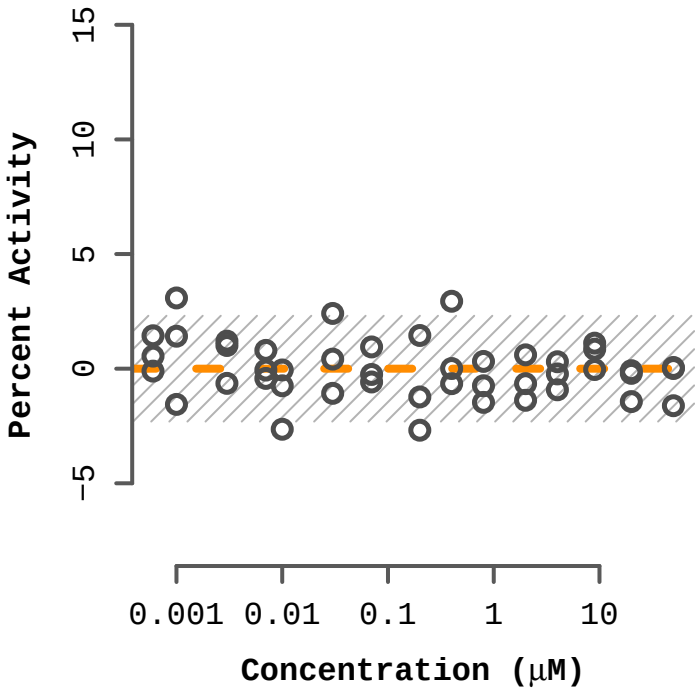
	tp	ga	gw
val:	1.68	−3.14	2.72
sd:	0.688	0.552	11.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.9	−3.09	2.09	1.32	16.5
sd:	0.821	0.615	7.33	0.512	382

	CNST	HILL	GNLS
AIC:	268.25	266.11	269.7
PROB:	0.23	0.66	0.11
RMSE:	5.06	4.4	4.34

MAX_MEAN: 4.06 **MAX_MED:** 2.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

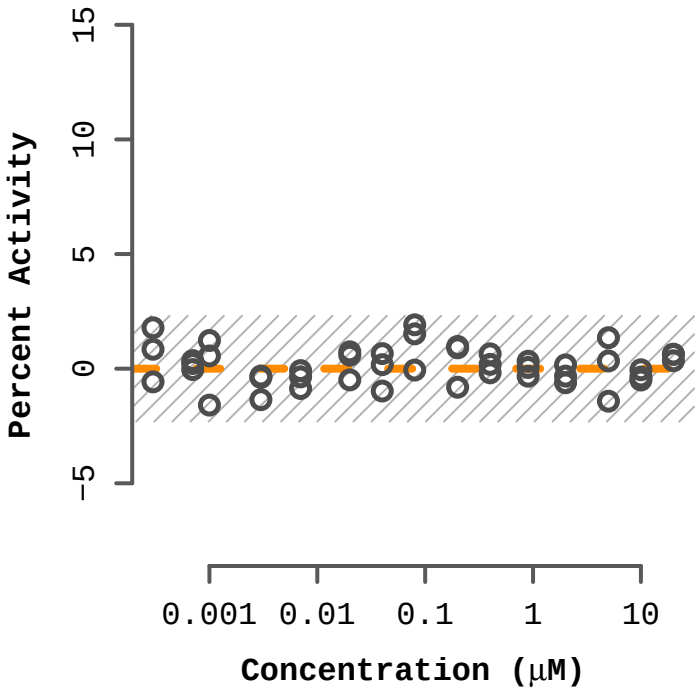
NAME: Pilsicainide
CHID: 46639 **CASRN:** 88069-67-4
SPID(S): Tox21_112458_1
M4ID: 12483090

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

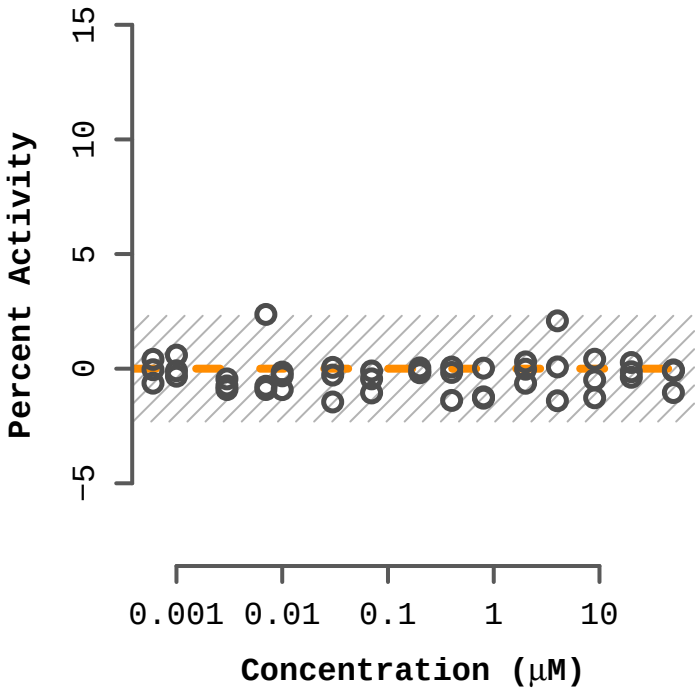
NAME: Zofenopril
CHID: 46640 **CASRN:** 81872-10-8
SPID(S): Tox21_112459_1
M4ID: 12483089

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

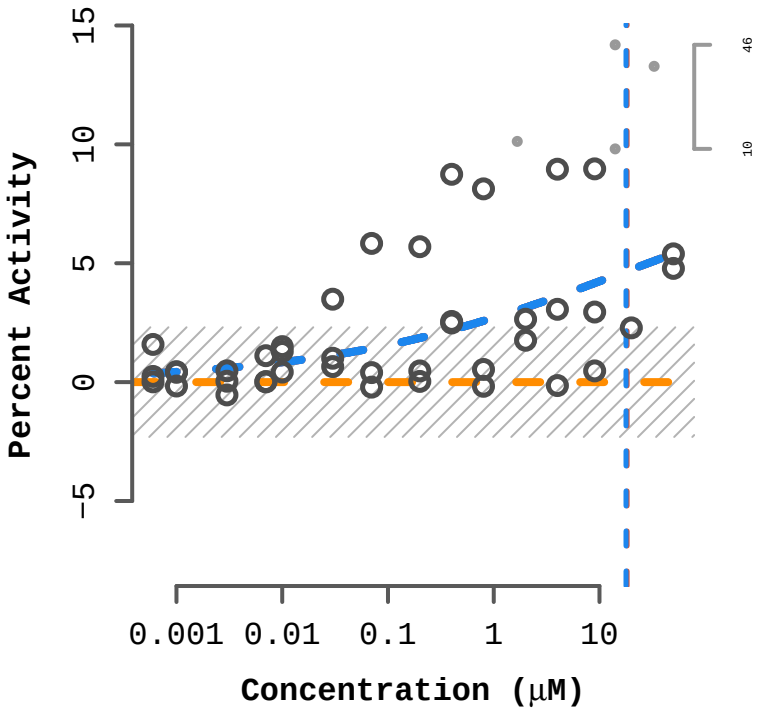
NAME: Bisibutiamine
CHID: 46641 **CASRN:** 3286-46-2
SPID(S): Tox21_112460_1
M4ID: 12483088

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.256 **MAX_MED:** 0.0785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bendazac sodium
CHID: 46644 **CASRN:** 23255-99-4
SPID(S): Tox21_112465_1
M4ID: 12483085 **BRK**

HILL MODEL (in red):

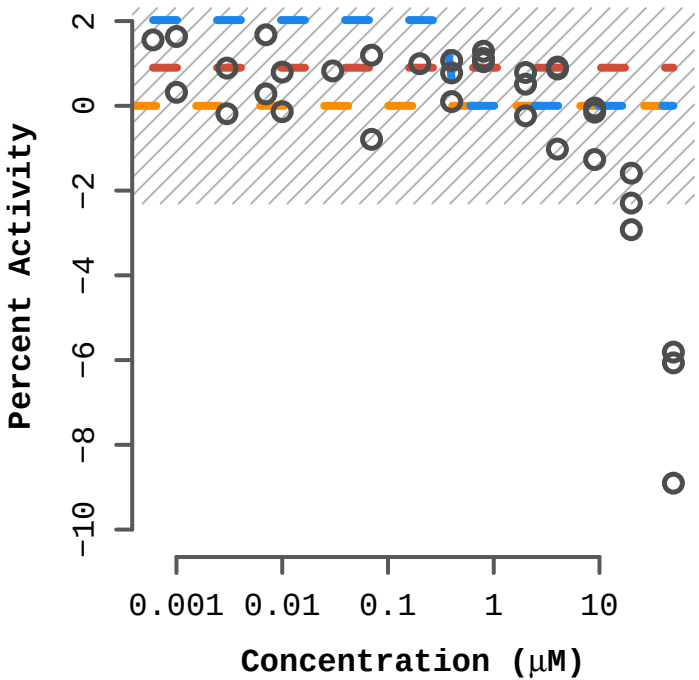
	tp	ga	gw
val:	9.34	1.26	0.309
sd:	16.7	5.02	0.264

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.31	1.25	0.31	3.13	4
sd:	16.5	4.97	0.264	714	1850

	CNST	HILL	GNLS
AIC:	287.24	264.63	268.63
PROB:	0	0.88	0.12
RMSE:	9.92	8.45	8.45

MAX_MEAN: 19.7 **MAX_MED:** 10.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Calcipotriene
CHID: 46648 CASRN: 112965-21-6
SPID(S): Tox21_112469_1
M4ID: 12483084

HILL MODEL (in red):

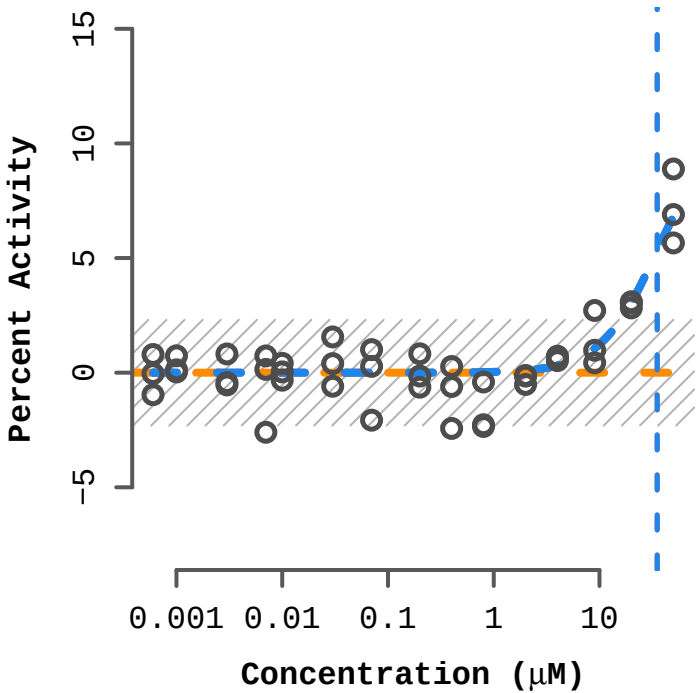
	tp	ga	gw
val:	0.9	−5.18	3.6
sd:	0.33	1060	1930

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.02	−4.49	5.46	−0.416	17.4
sd:	0.417	719	3090	0.775	728

	CNST	HILL	GNLS
AIC:	224.77	224.02	213.67
PROB:	0	0.01	0.99
RMSE:	3.05	2.96	2.54

MAX_MEAN: 4.61 MAX_MED: 3.82 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Anethole trithione
CHID: 46651 **CASRN:** 532-11-6
SPID(S): Tox21_112475_1
M4ID: 12483080

HILL MODEL (in red):

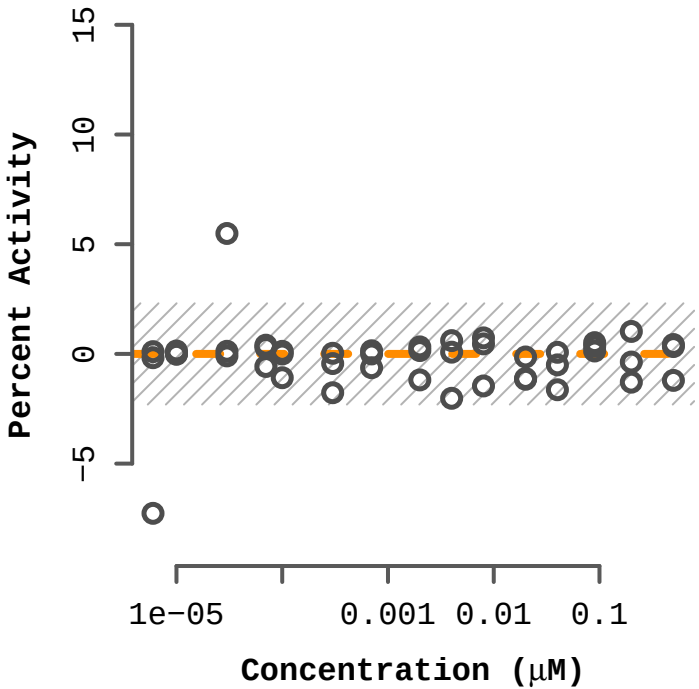
	tp	ga	gw
val:	10.7	1.55	1.62
sd:	4.68	0.256	0.52

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.7	1.55	1.62	3.69	3.56
sd:	4.68	0.256	0.52	1270	2300

	CNST	HILL	GNLS
AIC:	185.59	134.05	138.05
PROB:	0	0.88	0.12
RMSE:	2.28	1.03	1.03

MAX_MEAN: 7.15 **MAX_MED:** 6.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

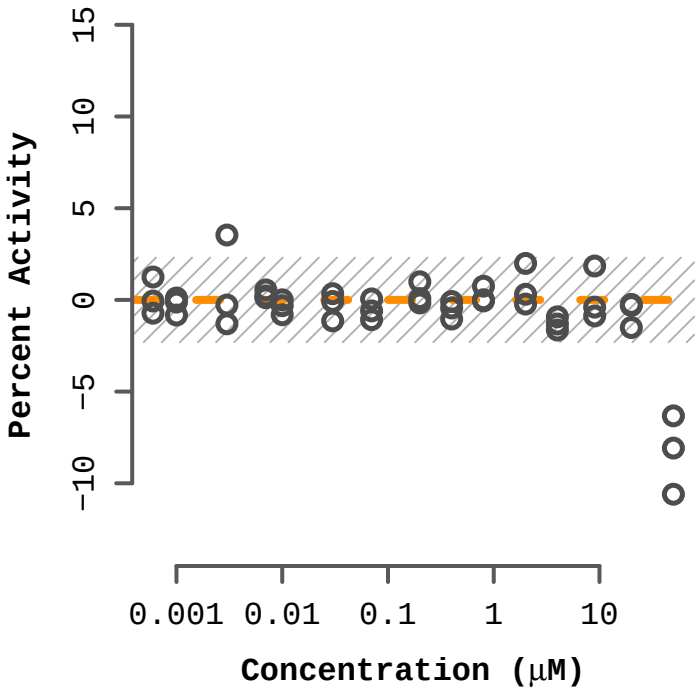
NAME: Capreomycin IB
CHID: 46652 **CASRN:** 33490-33-4
SPID(S): Tox21_112477_1
M4ID: 12483078

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.84 **MAX_MED:** 0.459 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

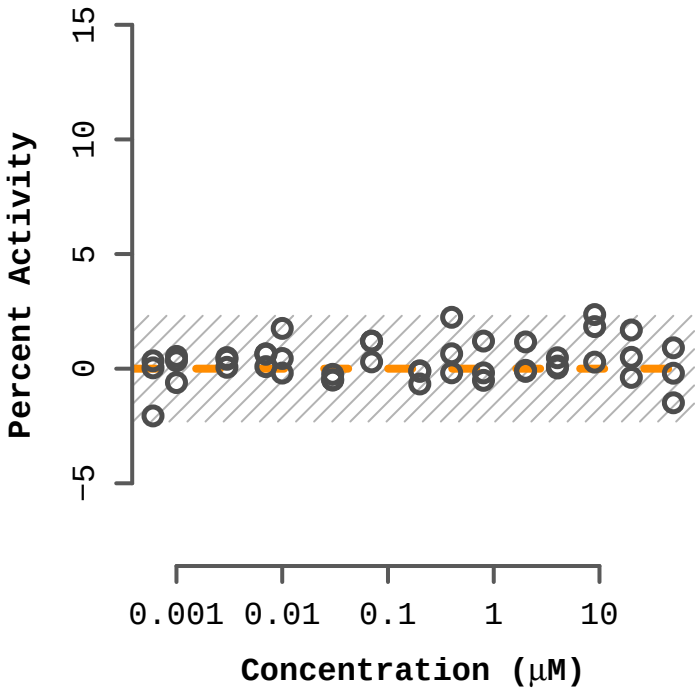
NAME: Sarpogrelate hydrochloride
CHID: 46662 **CASRN:** 135159-51-2
SPID(S): Tox21_112490_1
M4ID: 12483073

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.47	NA	NA
PROB:	1	NA	NA
RMSE:	2.39	NA	NA

MAX_MEAN: 0.691 **MAX_MED:** 0.308 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

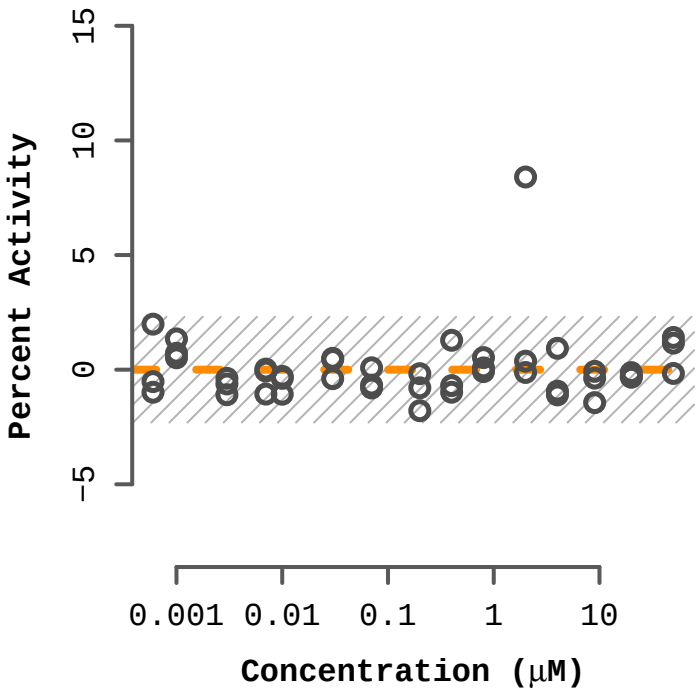
NAME: Lumefantrine
CHID: 46663 **CASRN:** 82186-77-4
SPID(S): Tox21_112491_1
M4ID: 12483072

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

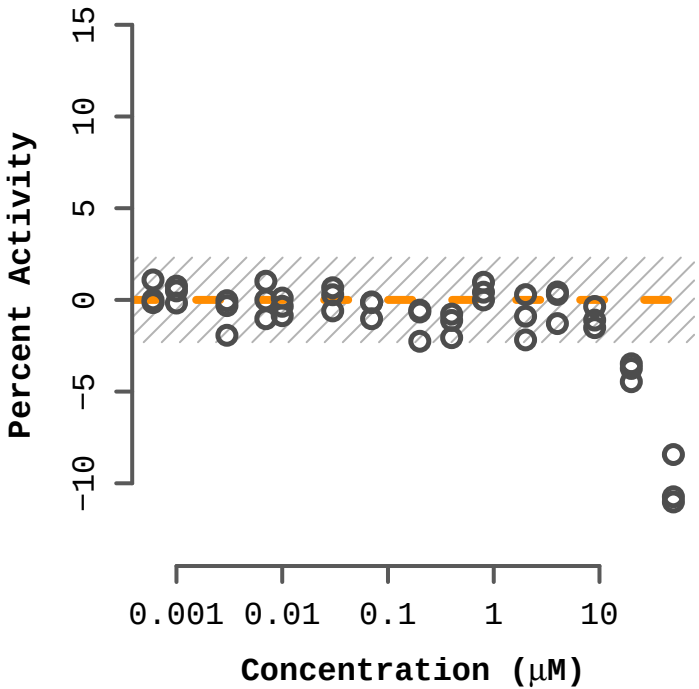
NAME: Lenalidomide
CHID: 46664 **CASRN:** 191732-72-6
SPID(S): Tox21_112492_1
M4ID: 12483071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 2.89 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

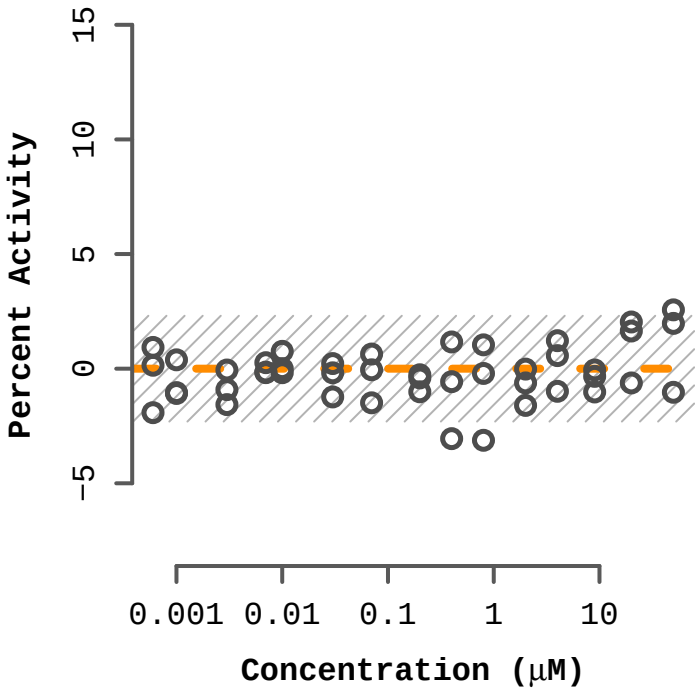
NAME: Lercanidipine hydrochloride
CHID: 46665 **CASRN:** 132866-11-6
SPID(S): Tox21_112493_1
M4ID: 12483070

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.67	NA	NA
PROB:	1	NA	NA
RMSE:	2.94	NA	NA

MAX_MEAN: 0.463 **MAX_MED:** 0.493 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

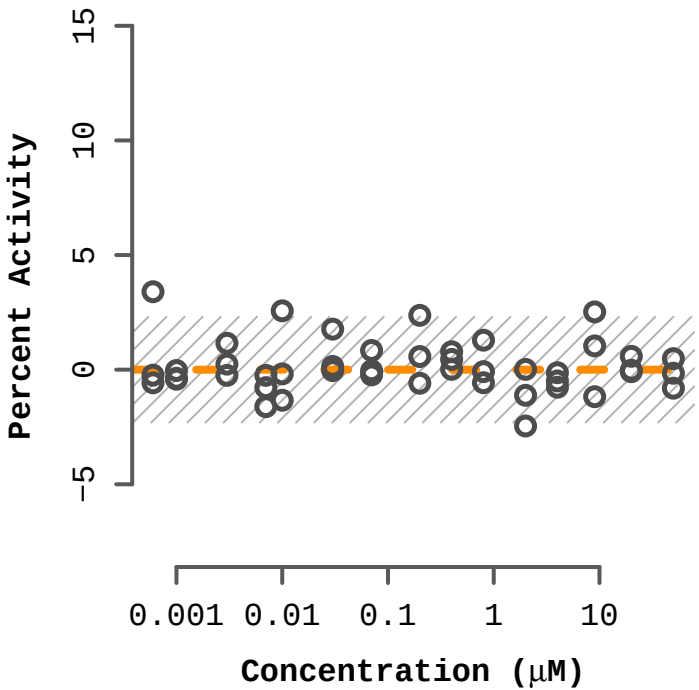
NAME: Roxatidine acetate hydrochloride
CHID: 46670 CASRN: 93793-83-0
SPID(S): Tox21_112500_1
M4ID: 12483066

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

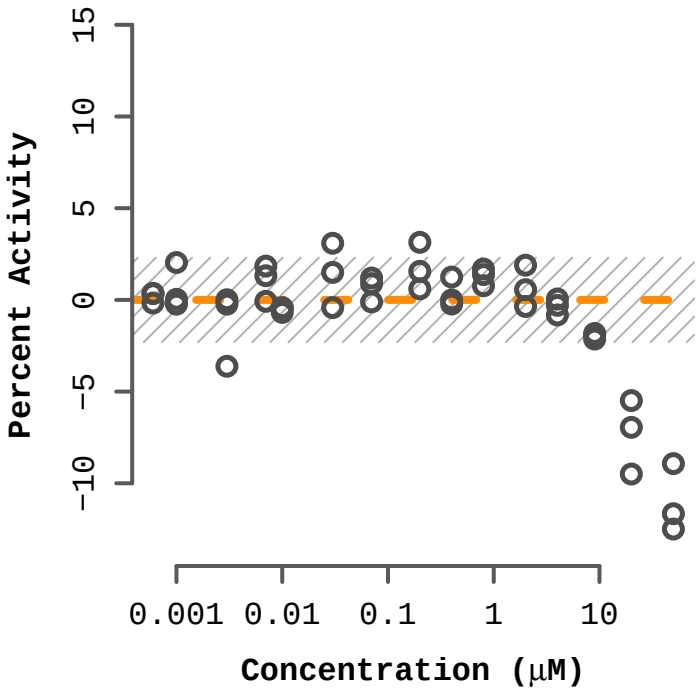
NAME: Eptifibatide
CHID: 46673 **CASRN:** 188627-80-7
SPID(S): Tox21_112503_1
M4ID: 12483064

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.864 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

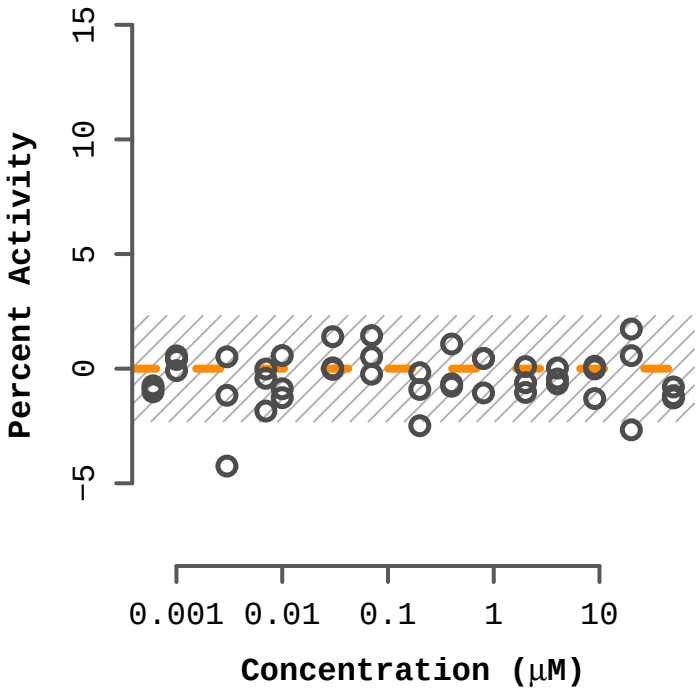
NAME: Lapatinib
CHID: 46675 CASRN: 231277-92-2
SPID(S): Tox21_112505_1
M4ID: 12483063

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.69	NA	NA
PROB:	1	NA	NA
RMSE:	3.69	NA	NA

MAX_MEAN: 1.77 MAX_MED: 1.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

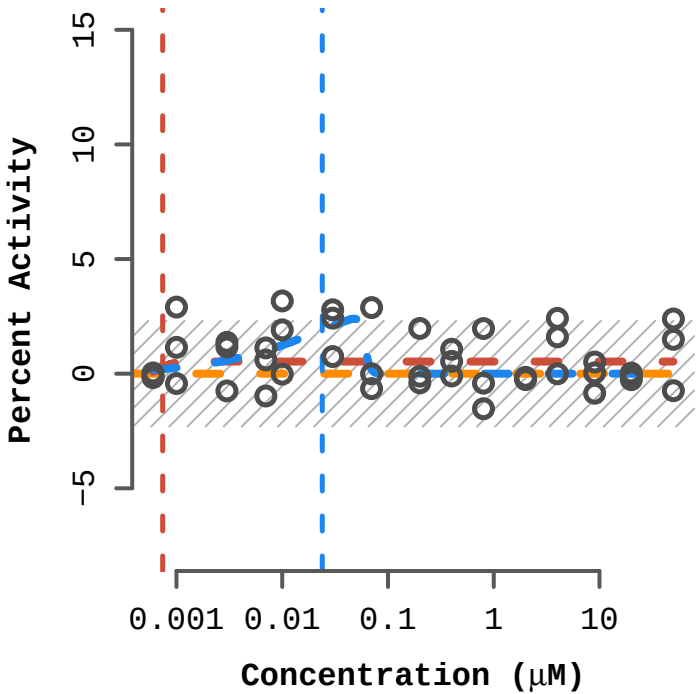
NAME: Pipethanate ethylbromide
CHID: 46677 **CASRN:** 23182-46-9
SPID(S): Tox21_112507_1
M4ID: 12483061

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.577 **MAX_MED:** 0.569 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Doripenem
CHID: 46678 CASRN: 148016-81-3
SPID(S): Tox21_112508_1
M4ID: 12483060

HILL MODEL (in red):

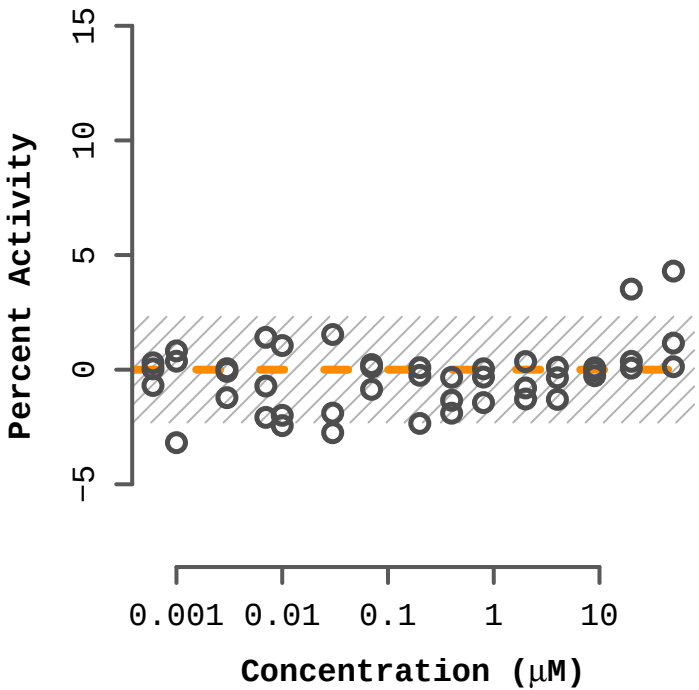
	tp	ga	gw
val:	0.527	−3.13	8
sd:	0.203	0.192	13.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.81	−1.62	0.83	−1.22	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.44	156.26	154.26
PROB:	0.13	0.23	0.64
RMSE:	1.36	1.2	1.17

MAX_MEAN: 1.99 MAX_MED: 2.42 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

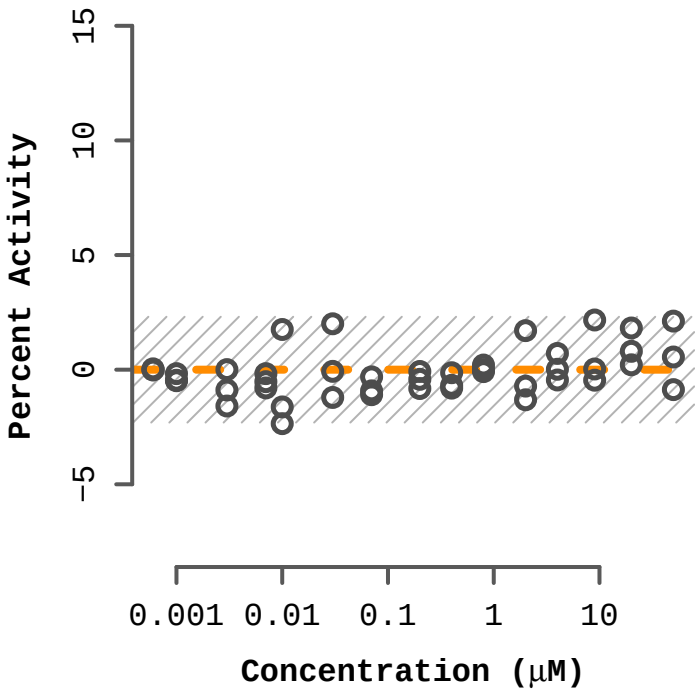
NAME: Vandetanib
CHID: 46681 CASRN: 443913-73-3
SPID(S): Tox21_112511_1
M4ID: 12483058

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.86 MAX_MED: 1.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

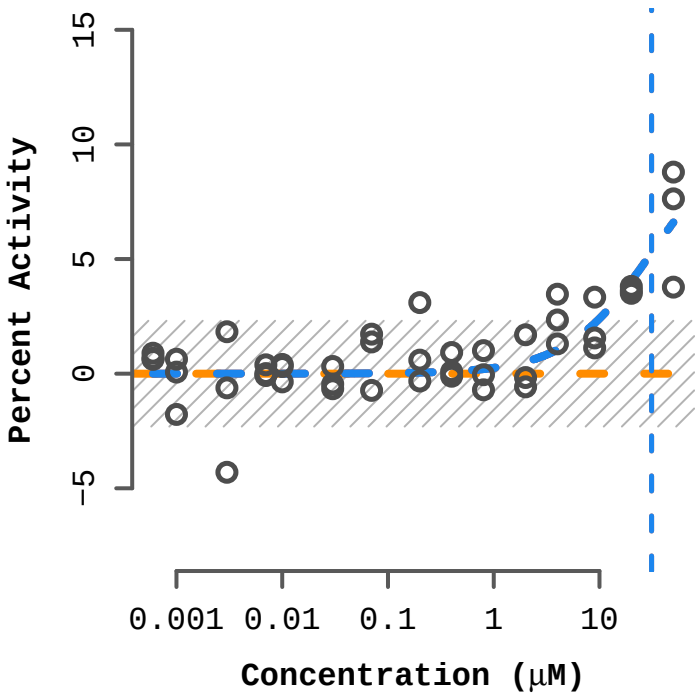
NAME: Ramatroban
CHID: 46685 **CASRN:** 116649-85-5
SPID(S): Tox21_112516_1
M4ID: 12483056

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.945 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tenatoprazole
CHID: 46687 CASRN: 113712-98-4
SPID(S): Tox21_112518_1
M4ID: 12483055

HILL MODEL (in red):

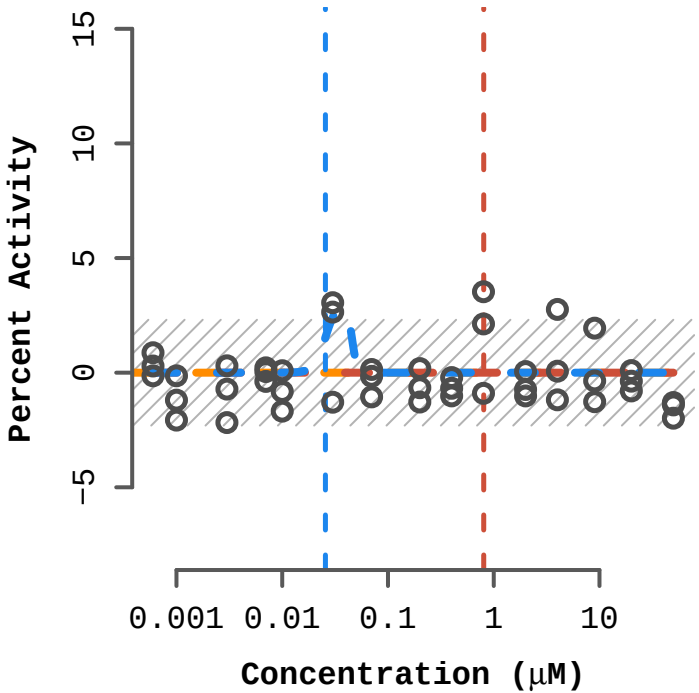
	tp	ga	gw
val:	10.6	1.49	1.08
sd:	5.01	0.318	0.351

GAIN-LOSS MODEL (in blue):

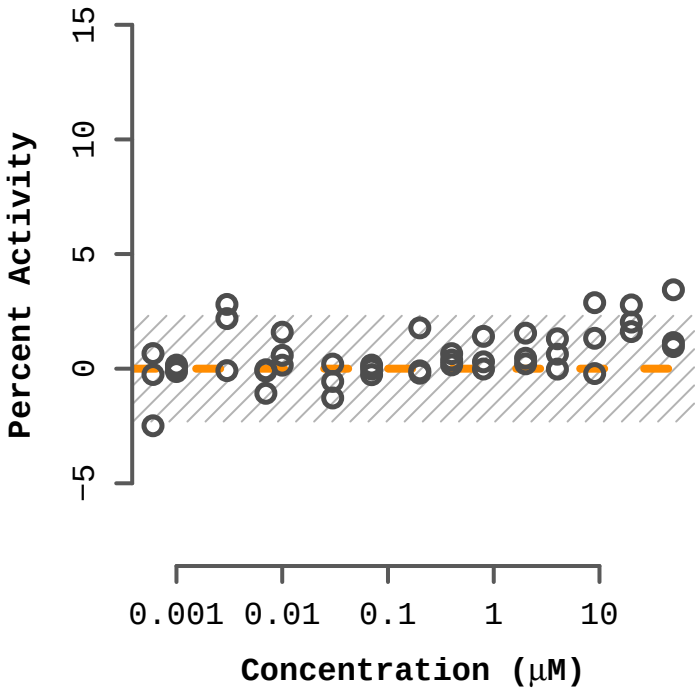
	tp	ga	gw	la	lw
val:	10.6	1.49	1.08	2.99	6.73
sd:	5.01	0.318	0.351	1610	8410

	CNST	HILL	GNLS
AIC:	199.89	153.63	157.63
PROB:	0	0.88	0.12
RMSE:	2.47	1.28	1.28

MAX_MEAN: 6.73 MAX_MED: 7.63 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hexoprenaline sulfate
CHID:    46688   CASRN: 32266-10-7
SPID(S): Tox21_112519_1
M4ID:    12483054

HILL MODEL (in red):
      tp        ga        gw
val:  1.59e-10 -0.0947  1.97
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.09      -1.59     8         -1.34     18
sd:   20.4      1.46      25.3      1.28      123

      CNST         HILL         GNLS
AIC:  156.35       162.35       161.71
PROB: 0.89         0.04         0.06
RMSE: 1.34         1.34         1.31

MAX_MEAN: 1.59      MAX_MED: 2.64      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

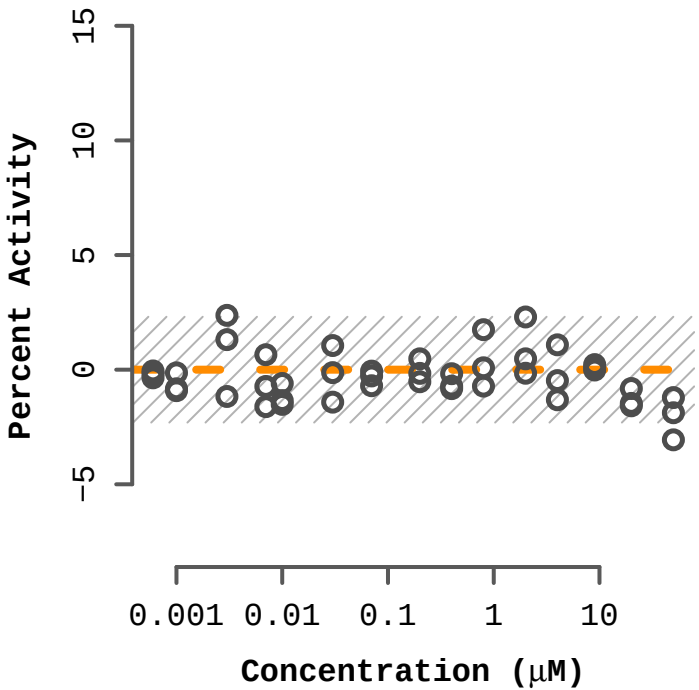
NAME: Ormetoprim
CHID: 46689 **CASRN:** 6981-18-6
SPID(S): Tox21_112520_1
M4ID: 12483053

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

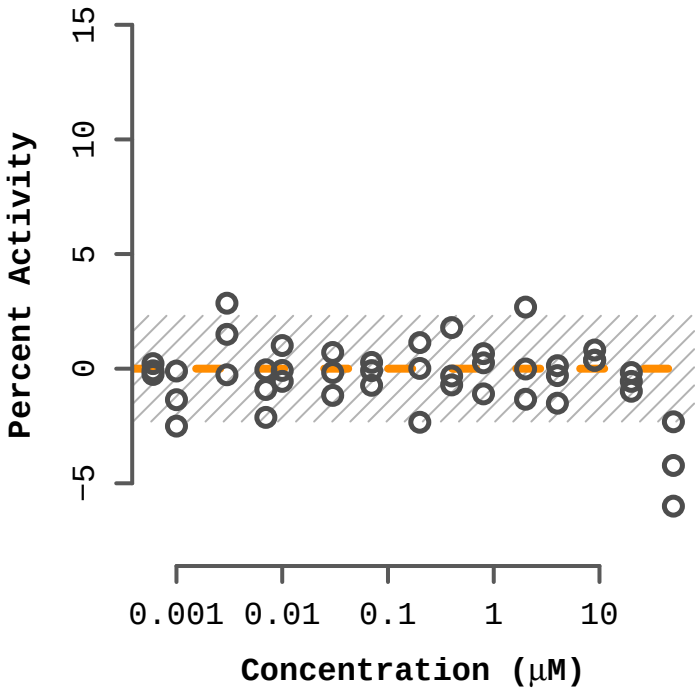
NAME: Amorolfine
CHID: 46690 **CASRN:** 78613-35-1
SPID(S): Tox21_112521_1
M4ID: 12483052

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.873 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

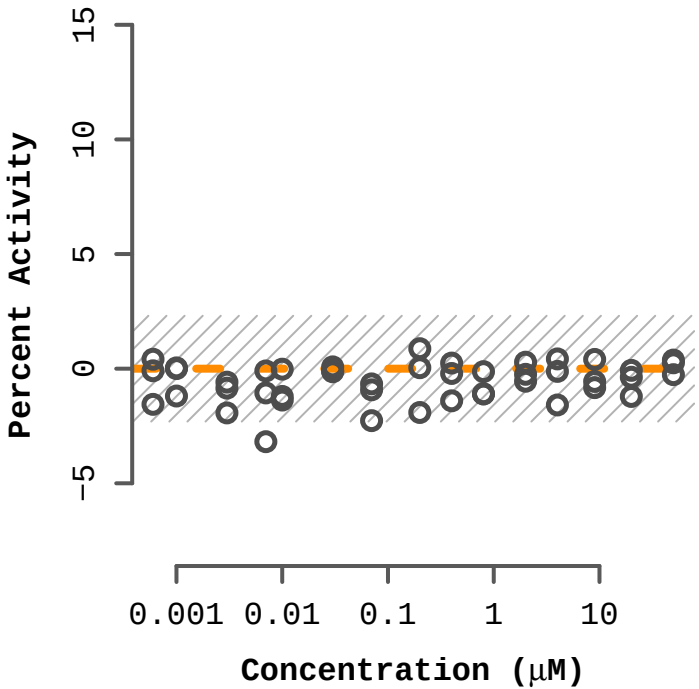
NAME: Tazarotene
CHID: 46691 **CASRN:** 118292-40-3
SPID(S): Tox21_112522_1
M4ID: 12483051

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

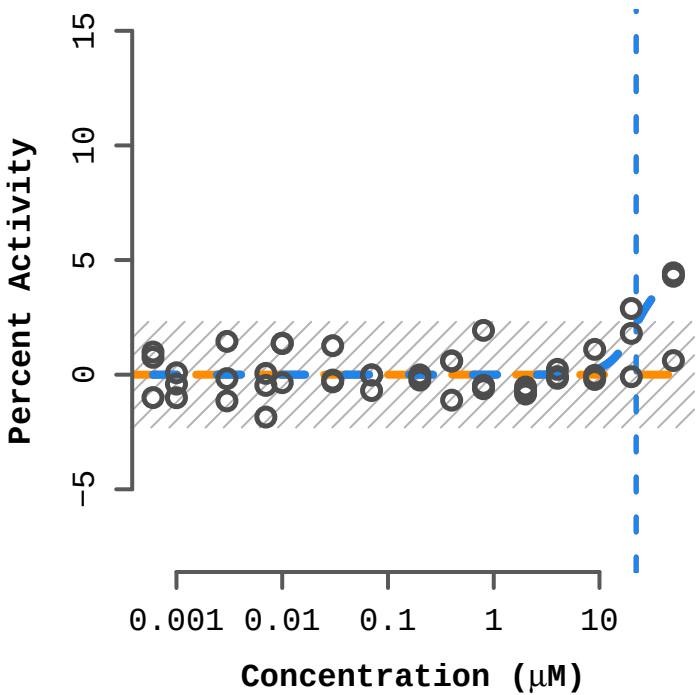
NAME: Grepafloxacin hydrochloride
CHID: 46692 **CASRN:** 161967-81-3
SPID(S): Tox21_112524_1
M4ID: 12483049

HILL MODEL: Not applicable.

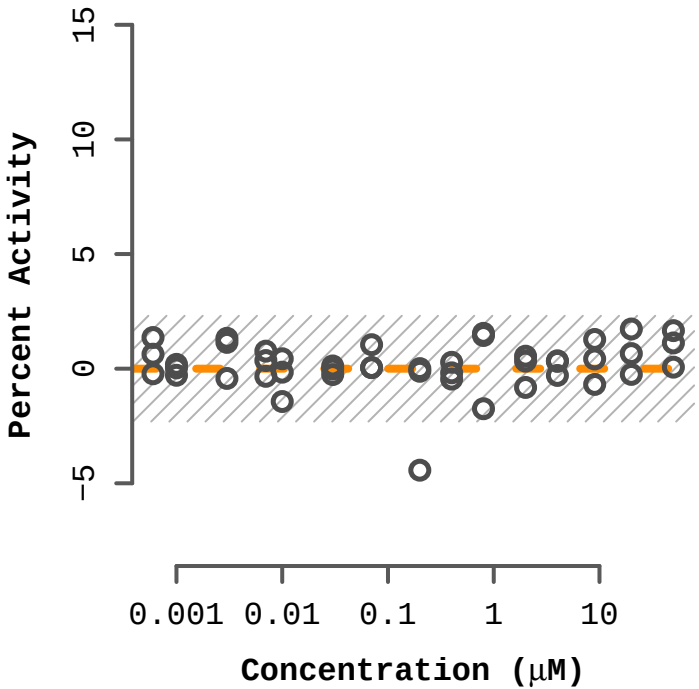
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.24	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.126 **MAX_MED:** 0.258 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Itopride hydrochloride
CHID:    46693   CASRN: 122892-31-3
SPID(S): Tox21_112526_1
M4ID:    12483047

HILL MODEL (in red):
      tp       ga       gw
val:  4.37     1.35     3.34
sd:   1.06     0.134    2.86

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.37     1.35     3.34     3.6      1.97
sd:   1.27     0.137    2.86     356      392

      CNST        HILL        GNLS
AIC:  142.6       129.93      133.93
PROB: 0           0.88        0.12
RMSE: 1.3         0.98        0.98

MAX_MEAN: 3.12      MAX_MED: 4.29      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

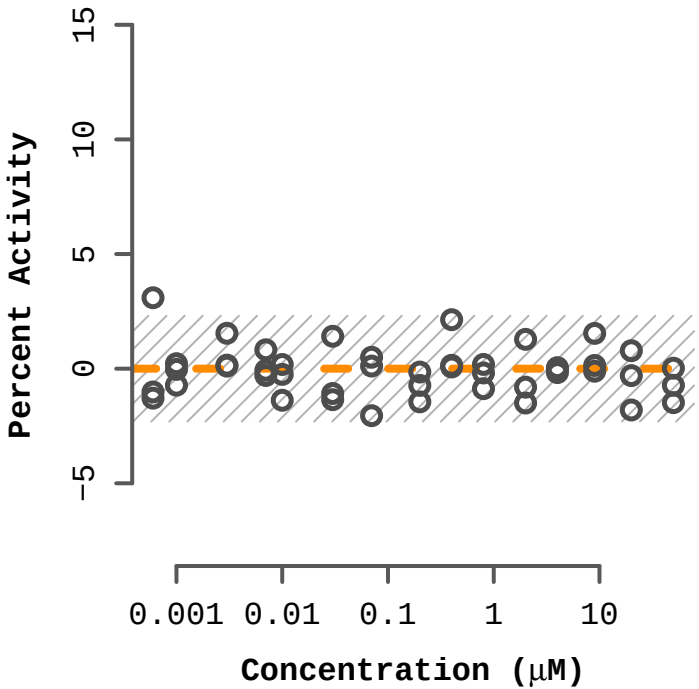
NAME: Balofloxacin
CHID: 46695 **CASRN:** 127294-70-6
SPID(S): Tox21_112529_1
M4ID: 12483045

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.951 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

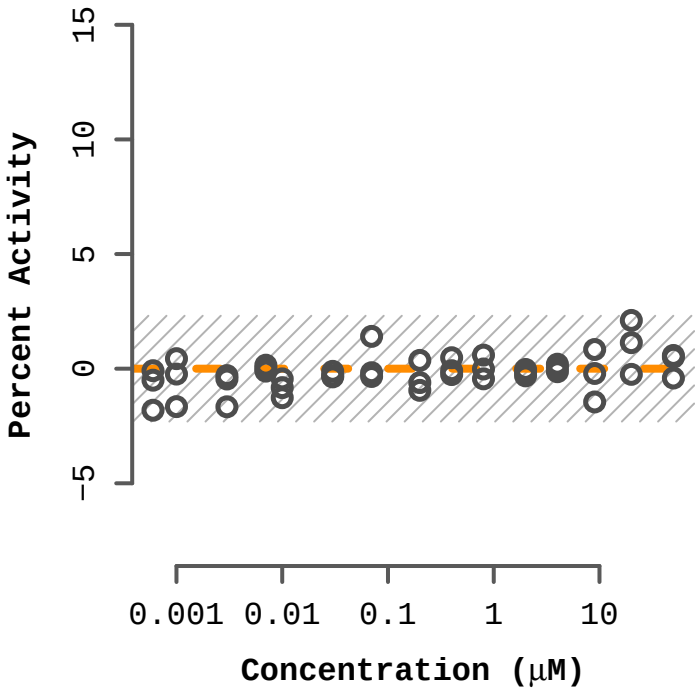
NAME: Vardenafil citrate
CHID: 46696 **CASRN:** 1193386-64-9
SPID(S): Tox21_112530_1
M4ID: 12483044

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.787 **MAX_MED:** 0.156 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

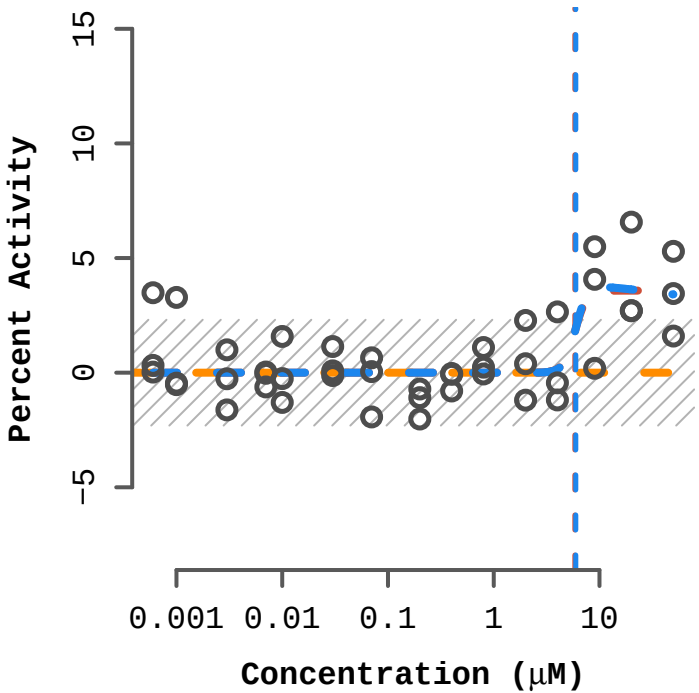
NAME: Pazufloxacin
CHID: 46697 **CASRN:** 127045-41-4
SPID(S): Tox21_112531_1
M4ID: 12483043

HILL MODEL: Not applicable.

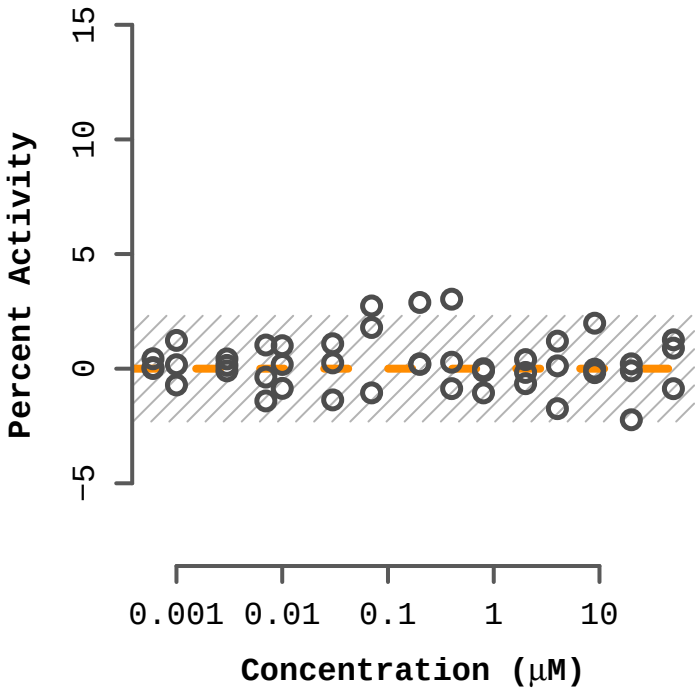
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.999 **MAX_MED:** 1.14 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Donepezil hydrochloride
CHID:    46698   CASRN: 120011-70-3
SPID(S): Tox21_112534_1
M4ID:    12483041

HILL MODEL (in red):
      tp       ga       gw
val:  3.58     0.767    8
sd:   0.575    0.137    6.34

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.54     0.776    8        3.3      0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  192.6       168.24      172.05
PROB: 0           0.87        0.13
RMSE: 2.15        1.44        1.44

MAX_MEAN: 3.99      MAX_MED: 4.07      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

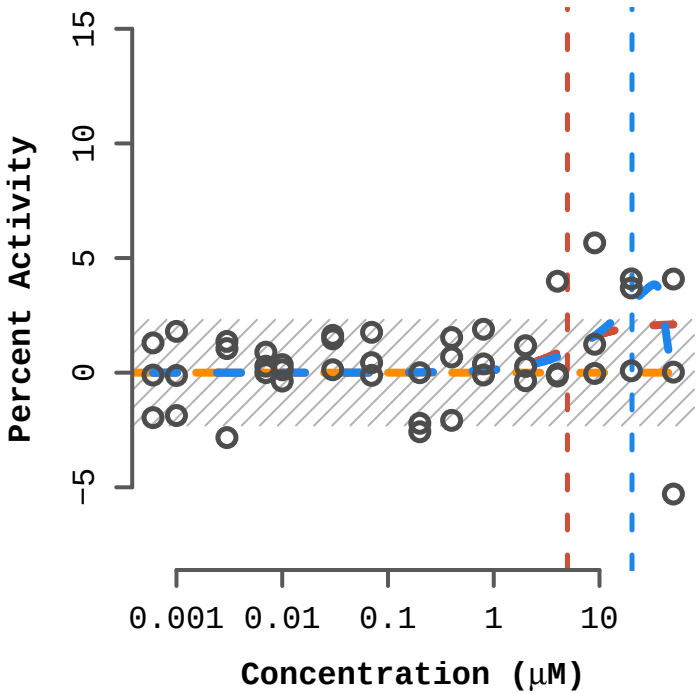
NAME: Clorprenaline hydrochloride
CHID: 46699 CASRN: 6933-90-0
SPID(S): Tox21_112535_1
M4ID: 12483040

HILL MODEL: Not applicable.

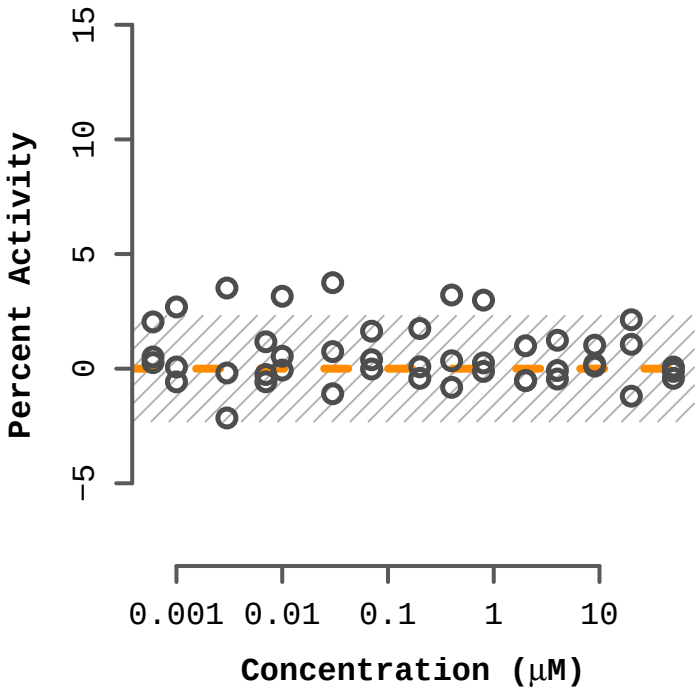
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.8 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Agaric acid
CHID:    46705   CASRN: 666-99-9
SPID(S): Tox21_112543_1
M4ID:    12483037

HILL MODEL (in red):
      tp       ga       gw
val:  2.14     0.697    1.79
sd:   1.3      0.479    2.65

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.1      1.31     1.27     1.62     15.6
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  188.4       188.16      189.64
PROB: 0.38        0.42        0.2
RMSE: 2.01        1.89        1.78

MAX_MEAN: 2.62      MAX_MED: 3.7       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

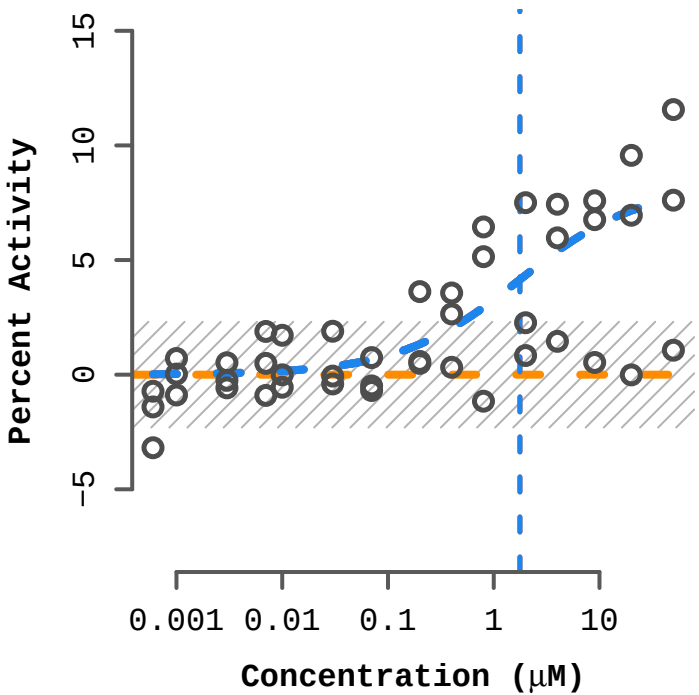
NAME: N-Carbamyl-L-glutamic acid
CHID: 46706 **CASRN:** 1188-38-1
SPID(S): Tox21_112544_1
M4ID: 12483036

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fleroxacin
CHID: 46714 CASRN: 79660-72-3
SPID(S): Tox21_112553_1
M4ID: 12483035

HILL MODEL (in red):

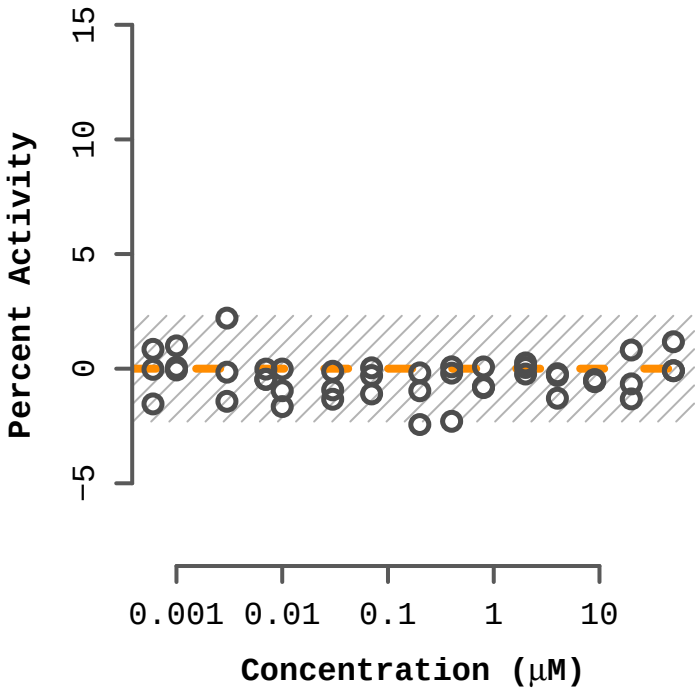
	tp	ga	gw
val:	8.29	0.248	0.759
sd:	2.59	0.579	0.338

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.29	0.248	0.759	3.01	5.4
sd:	2.59	0.579	0.338	1040	4260

	CNST	HILL	GNLS
AIC:	249.22	213.15	217.15
PROB:	0	0.88	0.12
RMSE:	4.01	2.46	2.46

MAX_MEAN: 6.75 MAX_MED: 7.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

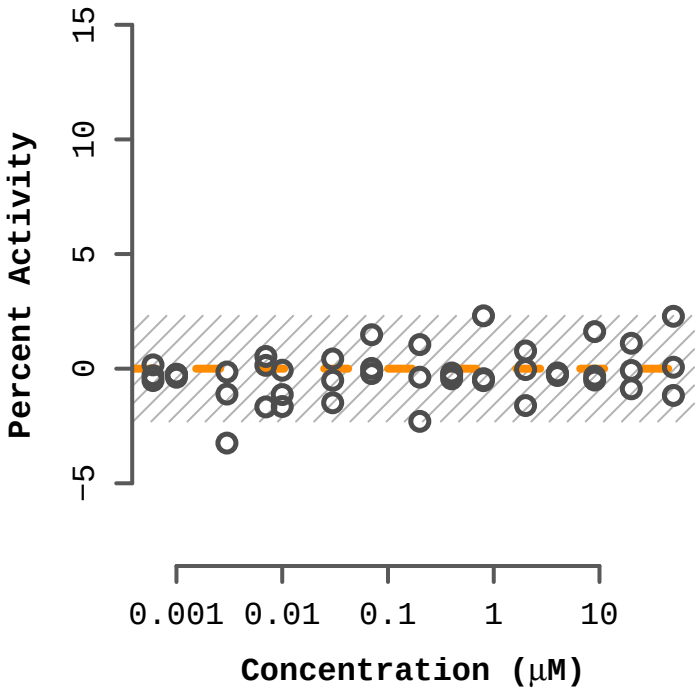
NAME: 3,4−Diaminopyridine
CHID: 46715 **CASRN:** 54−96−6
SPID(S): Tox21_112555_1
M4ID: 12483034

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.334 **MAX_MED:** 0.0604 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

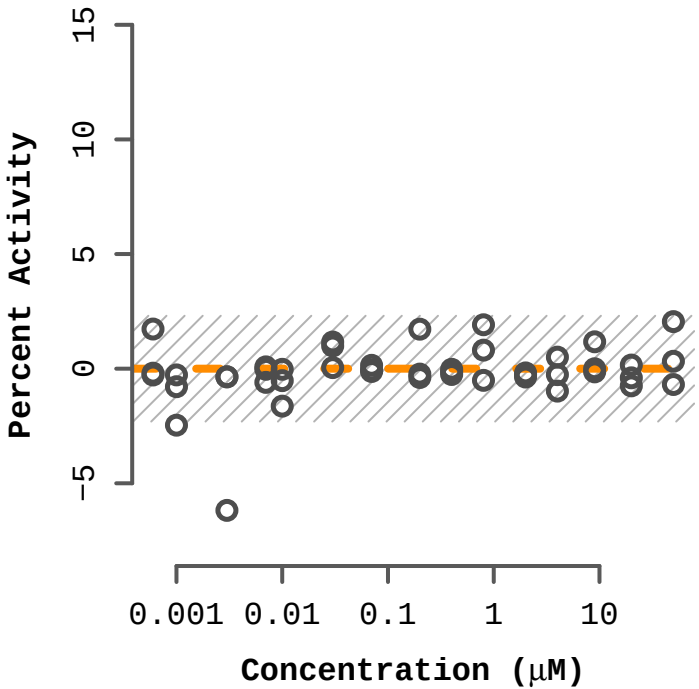
NAME: Mefeserpine
CHID: 46721 **CASRN:** 3735-85-1
SPID(S): Tox21_112564
M4ID: 12483031

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.451 **MAX_MED:** 0.146 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

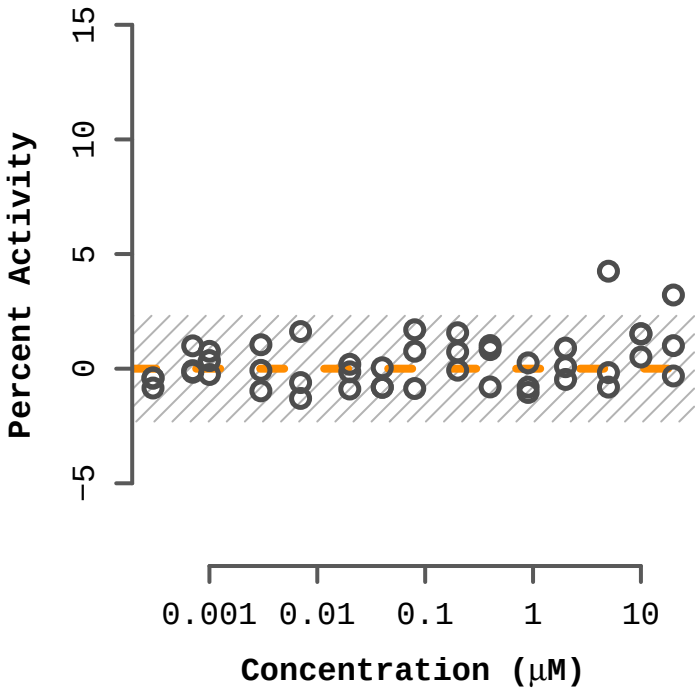
NAME: Xaliproden hydrochloride
CHID: 46724 **CASRN:** 90494-79-4
SPID(S): Tox21_112567_1
M4ID: 12483030

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.74 **MAX_MED:** 0.992 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

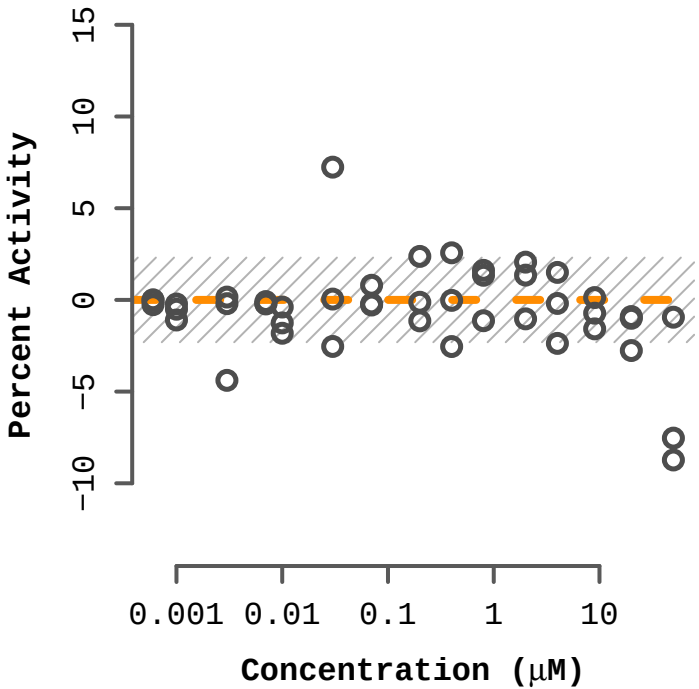
NAME: Anagrelide hydrochloride
CHID: 46725 CASRN: 58579-51-4
SPID(S): Tox21_112568_1
M4ID: 12483029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

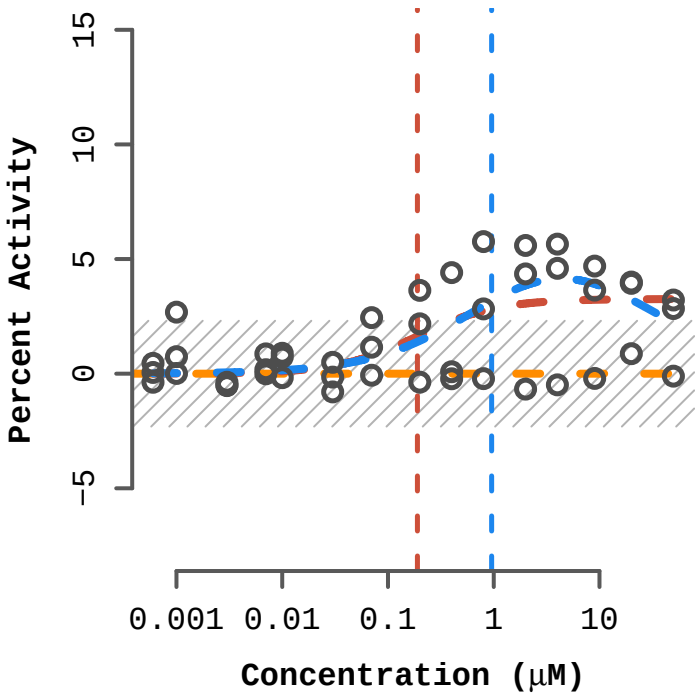
NAME: Aprindine hydrochloride
CHID: 46726 **CASRN:** 33237-74-0
SPID(S): Tox21_112569_1
M4ID: 12483028

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.99	NA	NA
PROB:	1	NA	NA
RMSE:	2.46	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sivelestat sodium tetrahydrate
CHID: 46727 CASRN: 201677-61-4
SPID(S): Tox21_112570_1
M4ID: 12483027

HILL MODEL (in red):

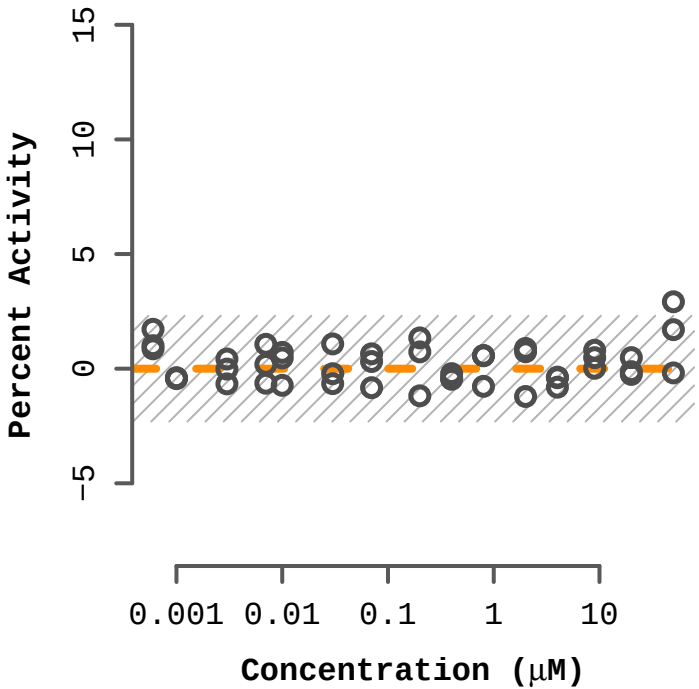
	tp	ga	gw
val:	3.26	−0.721	1.16
sd:	0.544	0.362	0.66

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.92	−0.0197	0.835	1.31	0.773
sd:	7.68	0.922	0.46	1.15	0.751

	CNST	HILL	GNLS
AIC:	211.99	186.32	187.33
PROB:	0	0.62	0.38
RMSE:	2.53	1.72	1.74

MAX_MEAN: 3.25 **MAX_MED:** 4.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

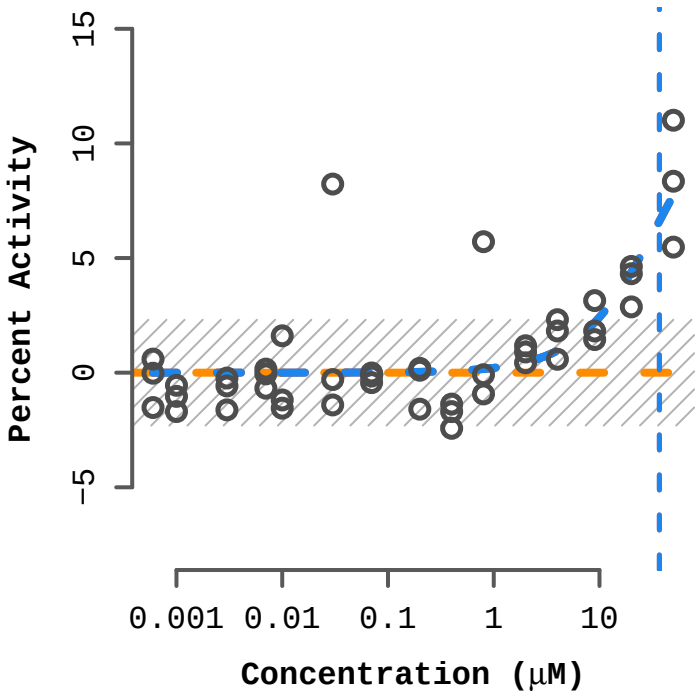
NAME: Ipidacrine hydrochloride hydrate
CHID: 46734 **CASRN:** 118499-70-0
SPID(S): Tox21_112577_1
M4ID: 12483025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lintitript
CHID: 46738 CASRN: 136381-85-6
SPID(S): Tox21_112581_1
M4ID: 12483024

HILL MODEL (in red):

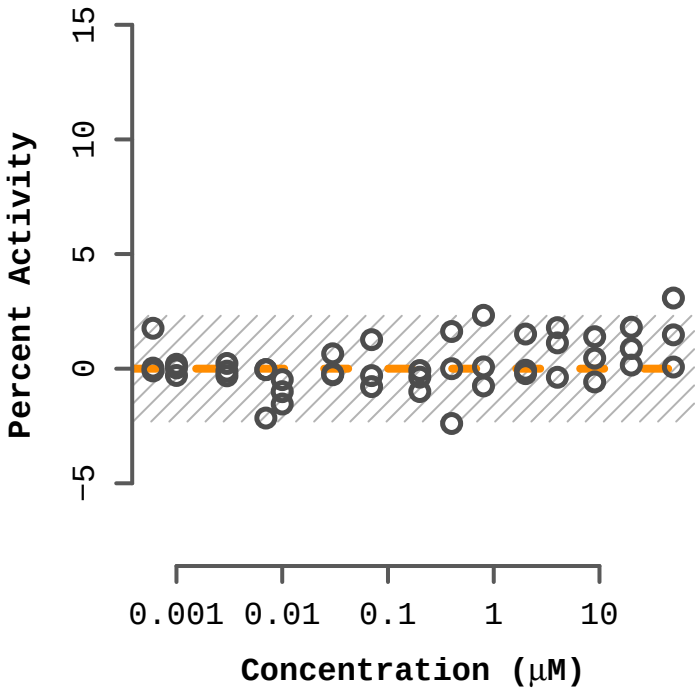
	tp	ga	gw
val:	13.2	1.57	1.15
sd:	6.29	0.343	0.299

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13.2	1.57	1.15	3.7	3.84
sd:	6.29	0.343	0.3	1200	2320

	CNST	HILL	GNLS
AIC:	217.55	173.13	177.13
PROB:	0	0.88	0.12
RMSE:	3.09	1.87	1.87

MAX_MEAN: 8.28 **MAX_MED:** 8.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

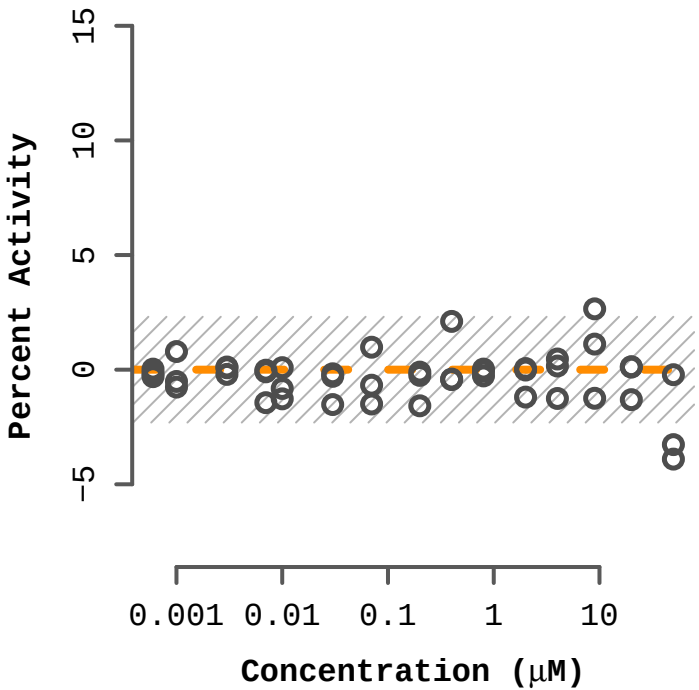
NAME: Lazabemide hydrochloride
CHID: 46739 **CASRN:** 103878-83-7
SPID(S): Tox21_112582_1
M4ID: 12483023

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

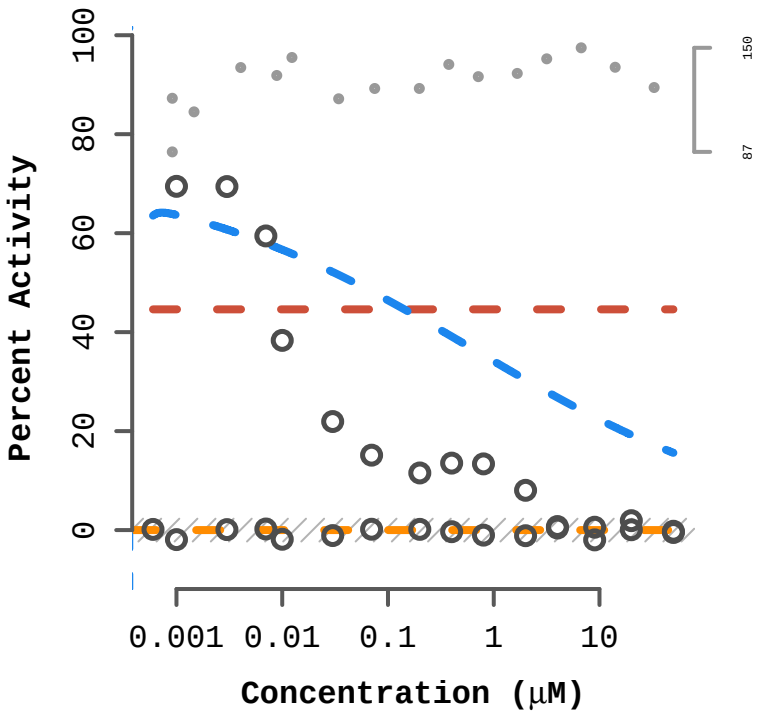
NAME: Talniflumate
CHID: 46740 **CASRN:** 66898-62-2
SPID(S): Tox21_112584_1
M4ID: 12483021

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Carboplatin
CHID: 46742 **CASRN:** 41575-94-4
SPID(S): Tox21_112586_1
M4ID: 12483020 **BRK**

HILL MODEL (in red):

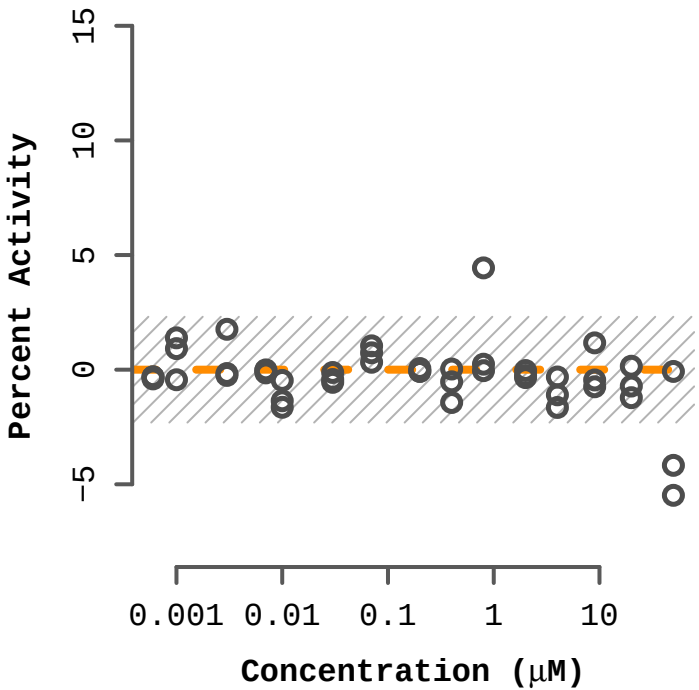
	tp	ga	gw
val:	44.6	-4.43	7.38
sd:	10.7	5650	34400

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	72.8	-3.43	8	-0.18	0.3
sd:	134	0.756	28.9	7.02	0.911

	CNST	HILL	GNLS
AIC:	525.96	512.83	515.07
PROB:	0	0.75	0.25
RMSE:	80.56	60.97	61.68

MAX_MEAN: 69.7 **MAX_MED:** 86.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

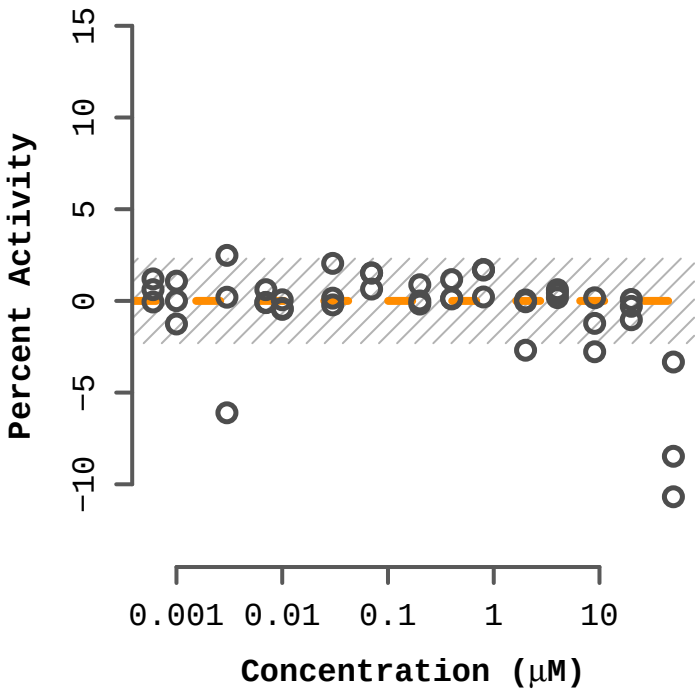
NAME: Fananserin
CHID: 46743 **CASRN:** 127625-29-0
SPID(S): Tox21_112587_1
M4ID: 12483019

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

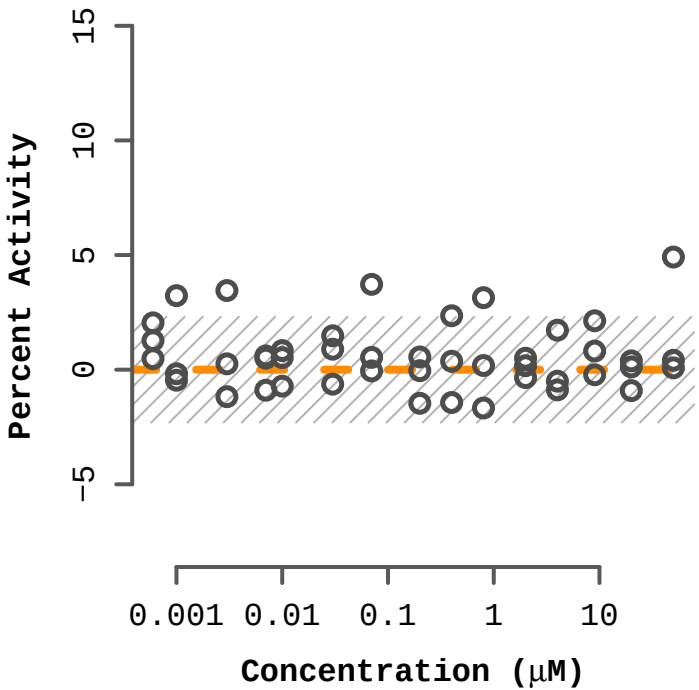
NAME: Bucindolol
CHID: 46744 **CASRN:** 71119-11-4
SPID(S): Tox21_112588_1
M4ID: 12483018

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.5	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

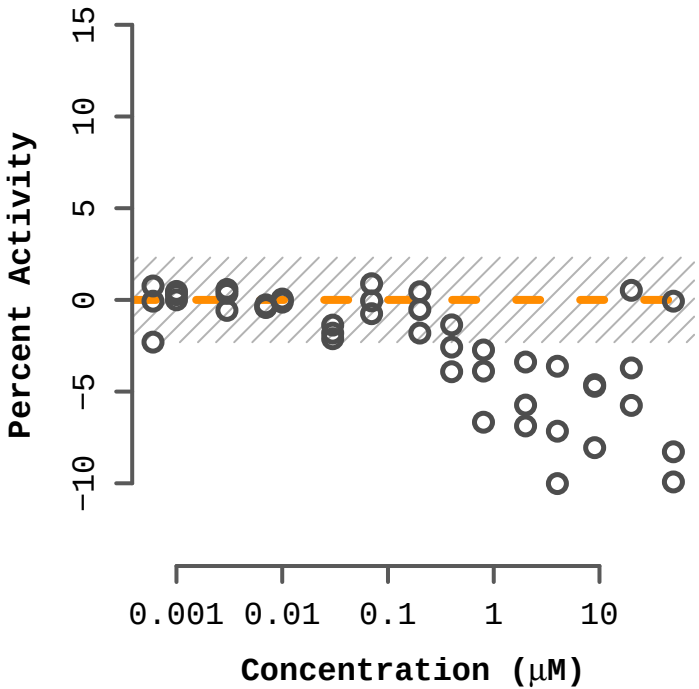
NAME: Loxoribine
CHID: 46748 **CASRN:** 121288-39-9
SPID(S): Tox21_112592_1
M4ID: 12483015

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

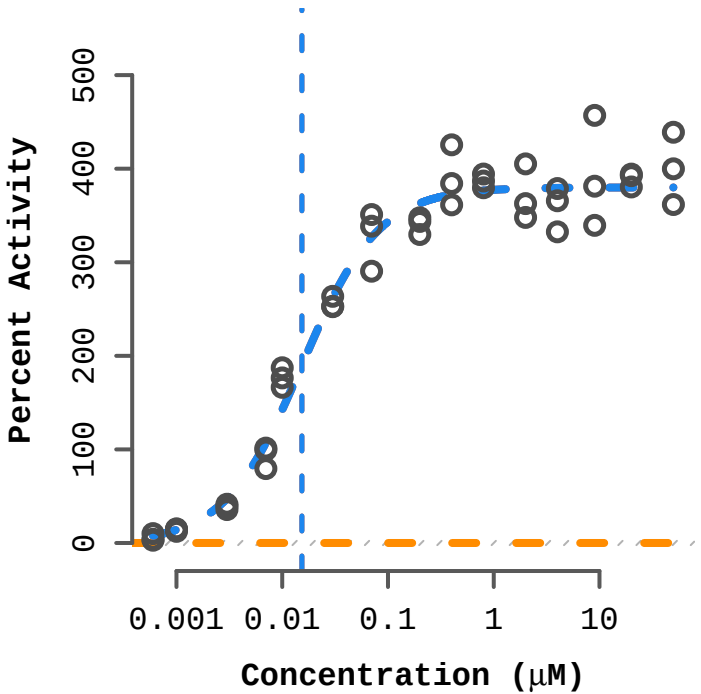
NAME: Pirarubicin
CHID: 46755 **CASRN:** 72496-41-4
SPID(S): Tox21_112602_1
M4ID: 12483011

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.92	NA	NA

MAX_MEAN: 0.253 **MAX_MED:** 0.356 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Desonide
CHID: 46756 CASRN: 638-94-8
SPID(S): Tox21_112603_1
M4ID: 12483010

HILL MODEL (in red):

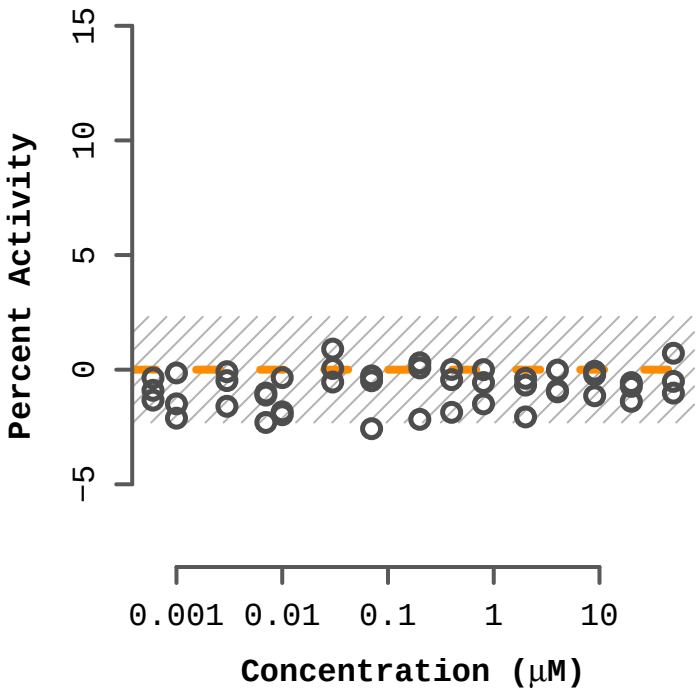
	tp	ga	gw
val:	380	-1.81	1.19
sd:	5.47	0.0358	0.0905

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	380	-1.81	1.19	2.39	14.7
sd:	5.47	0.0358	0.0905	1900	40200

	CNST	HILL	GNLS
AIC:	651.89	424.15	428.15
PROB:	0	0.88	0.12
RMSE:	302.34	25.3	25.3

MAX_MEAN: 400 **MAX_MED:** 400 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

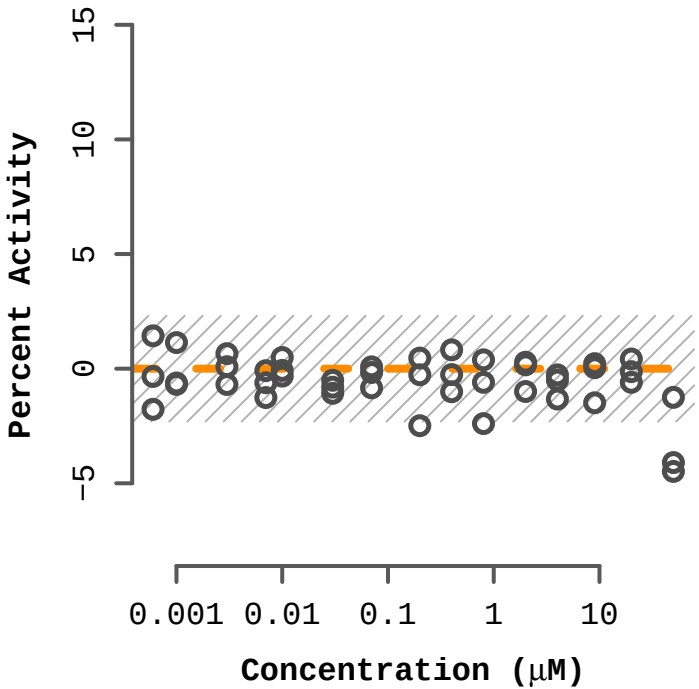
NAME: Isbufylline
CHID: 46767 **CASRN:** 90162-60-0
SPID(S): Tox21_112621_1
M4ID: 12483007

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.138 **MAX_MED:** 0.077 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

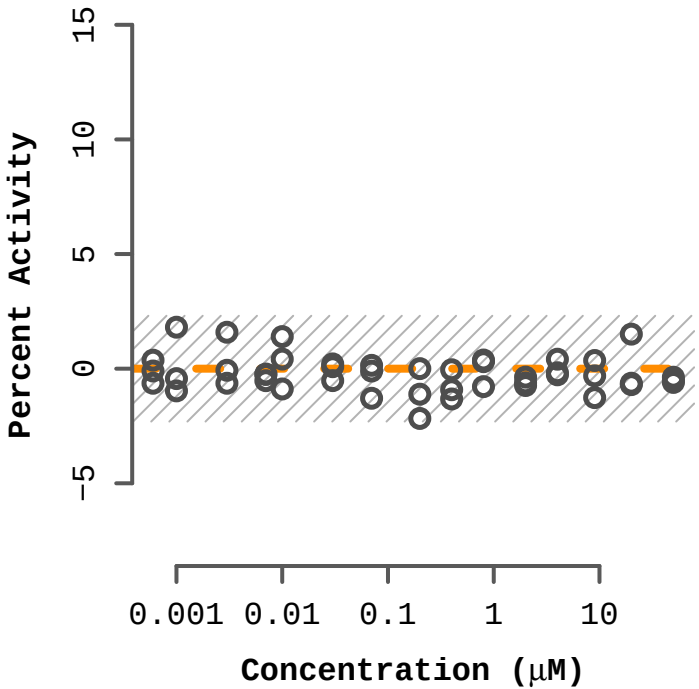
NAME: Iodophthalein sodium
CHID: 46768 **CASRN:** 2217-44-9
SPID(S): Tox21_112622_1
M4ID: 12483006

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.0299 **MAX_MED:** 0.169 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

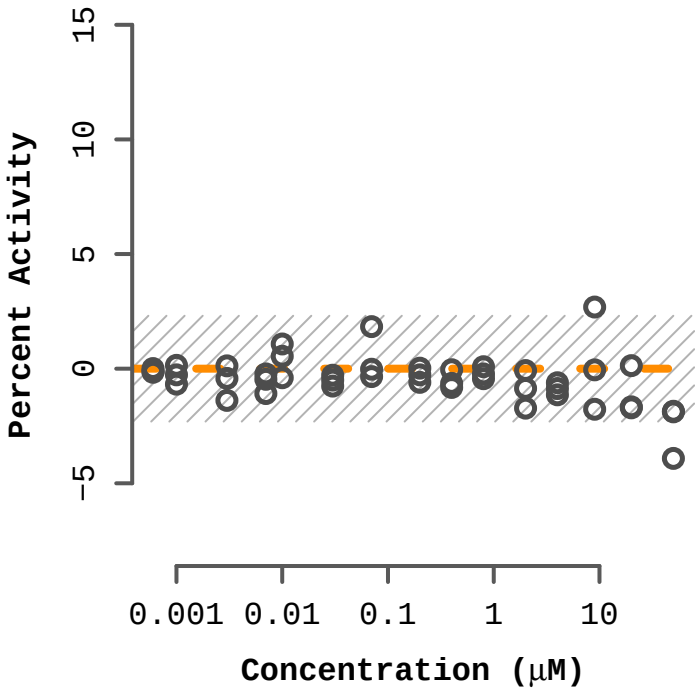
NAME: Fenobam
CHID: 46770 **CASRN:** 57653-26-6
SPID(S): Tox21_112624_1
M4ID: 12483004

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.312 **MAX_MED:** 0.419 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

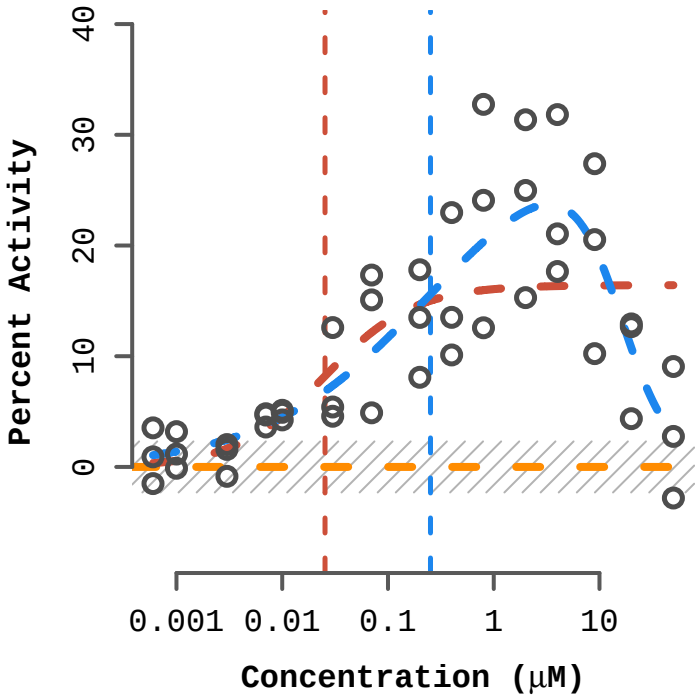
NAME: Rotigotine
CHID: 46772 CASRN: 99755-59-6
SPID(S): Tox21_112627_1
M4ID: 12483003

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.49 **MAX_MED:** 0.543 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ataluren
CHID: 46776 CASRN: 775304-57-9
SPID(S): Tox21_112631_1
M4ID: 12483002

HILL MODEL (in red):

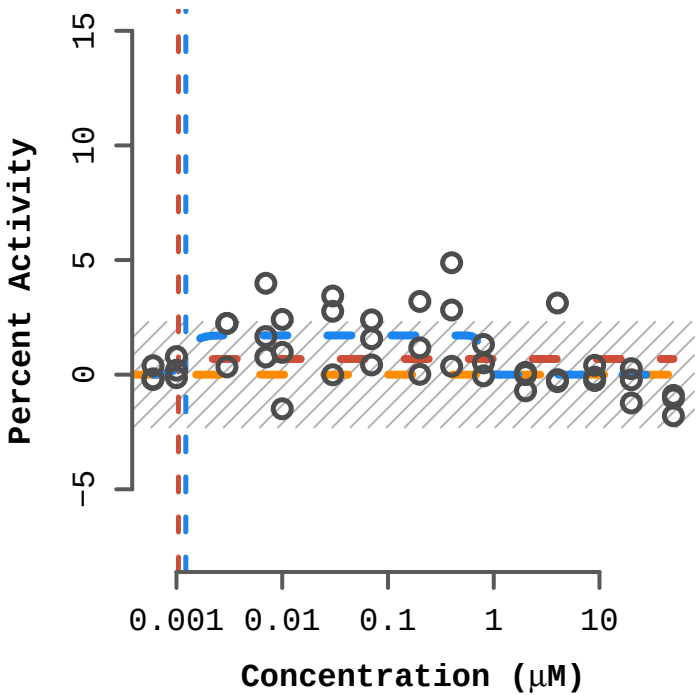
	tp	ga	gw
val:	16.4	−1.6	1.03
sd:	1.83	0.225	0.36

GAIN-LOSS MODEL (in blue):

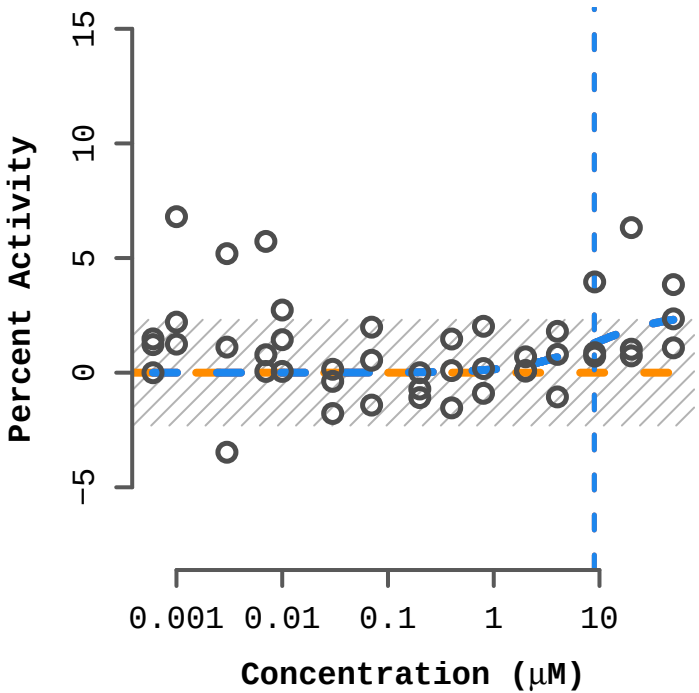
	tp	ga	gw	la	lw
val:	31.2	−0.598	0.554	1.18	1.83
sd:	15.5	0.883	0.197	0.216	1.03

	CNST	HILL	GNLS
AIC:	372.06	307.5	285.06
PROB:	0	0	1
RMSE:	14.49	6.98	4.87

MAX_MEAN: 23.9 MAX_MED: 25 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Darifenacin hydrobromide
CHID:    46780   CASRN: 133099-07-7
SPID(S): Tox21_112636_1
M4ID:    12483000

HILL MODEL (in red):
      tp       ga       gw
val:  0.684    -2.98    8
sd:   0.244    0.235    49.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.71     -2.91    8        -0.113   18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  174.92      172.5       154.96
PROB: 0           0           1
RMSE: 1.7         1.49        1.21

MAX_MEAN: 2.69      MAX_MED: 2.82      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tadalafil
CHID: 46786 CASRN: 171596-29-5
SPID(S): Tox21_112642_1
M4ID: 12482998

HILL MODEL (in red):

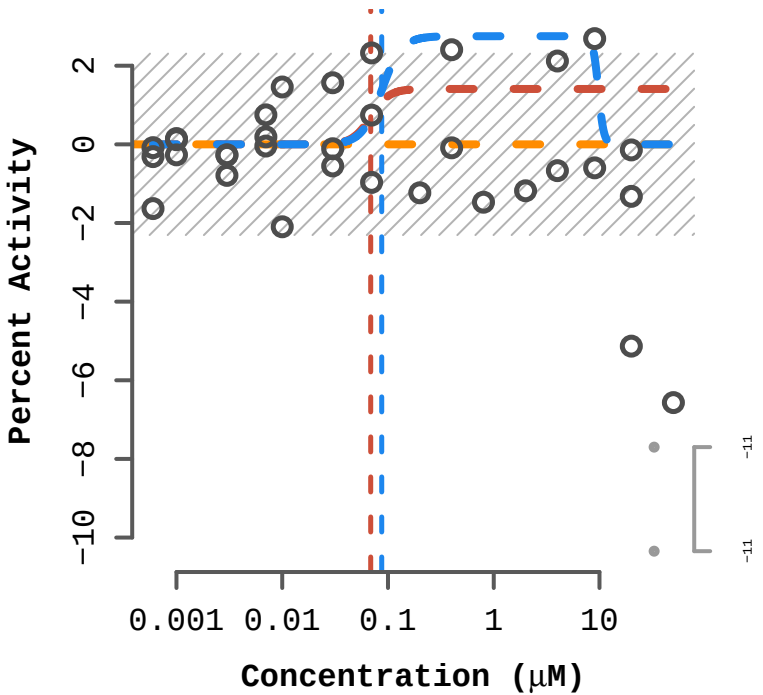
	tp	ga	gw
val:	2.57	0.951	1.27
sd:	2.14	0.9	1.79

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.57	0.951	1.27	3.19	4.61
sd:	2.14	0.9	1.79	1400	4350

	CNST	HILL	GNLS
AIC:	199.96	194.67	198.67
PROB:	0.06	0.83	0.11
RMSE:	2.34	2.1	2.1

MAX_MEAN: 3.42 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cinacalcet hydrochloride
CHID: 46792 CASRN: 364782-34-3
SPID(S): Tox21_112654_1
M4ID: 12482995 BRK

HILL MODEL (in red):

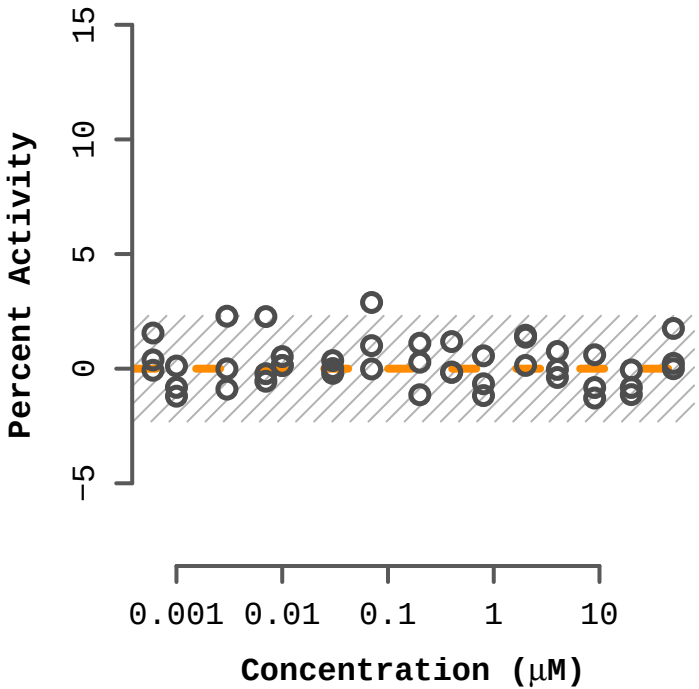
	tp	ga	gw
val:	1.41	−1.16	5.06
sd:	0.681	0.496	42.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.75	−1.06	4.61	0.99	17
sd:	0.701	0.469	24	0.856	410

	CNST	HILL	GNLS
AIC:	227.12	228.62	221.44
PROB:	0.05	0.03	0.92
RMSE:	3.41	3.52	3.12

MAX_MEAN: 2.65 MAX_MED: 4.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

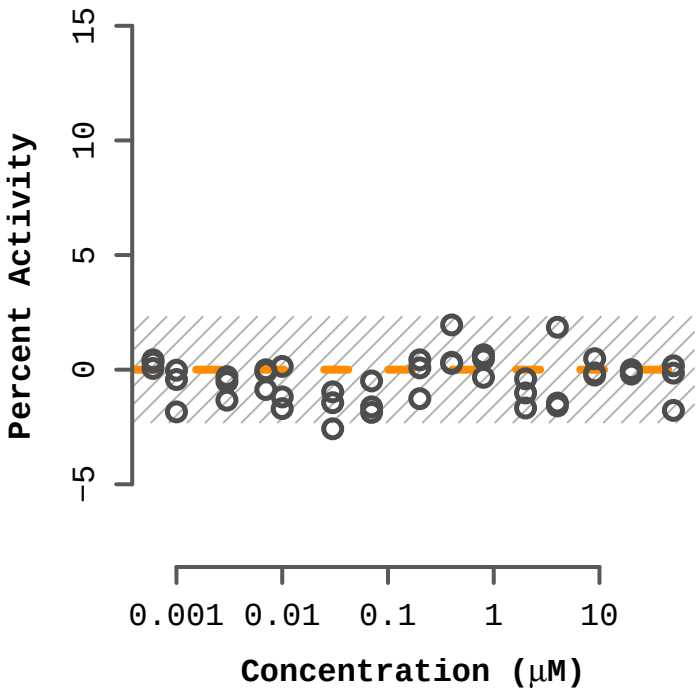
NAME: Mabuterol hydrochloride
CHID: 46798 CASRN: 54240-36-7
SPID(S): Tox21_112660_1
M4ID: 12482993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.7	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

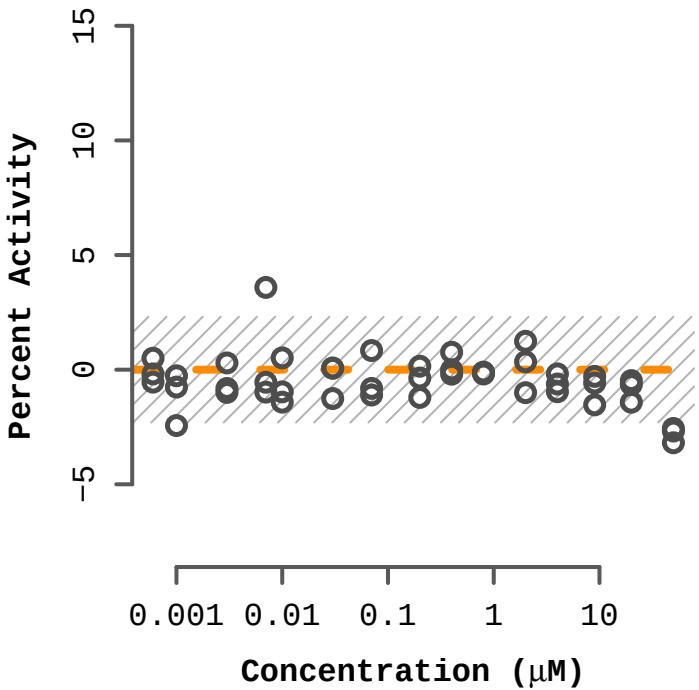
NAME: Gimeracil
CHID: 46799 **CASRN:** 103766-25-2
SPID(S): Tox21_112661_1
M4ID: 12482992

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 0.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

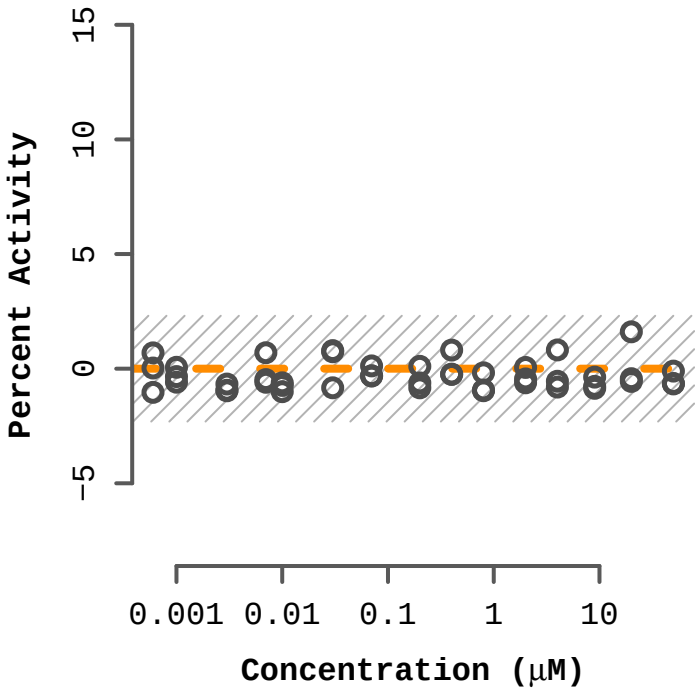
NAME: Mizolastine
CHID: 46801 CASRN: 108612-45-9
SPID(S): Tox21_112663_1
M4ID: 12482991

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.345 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

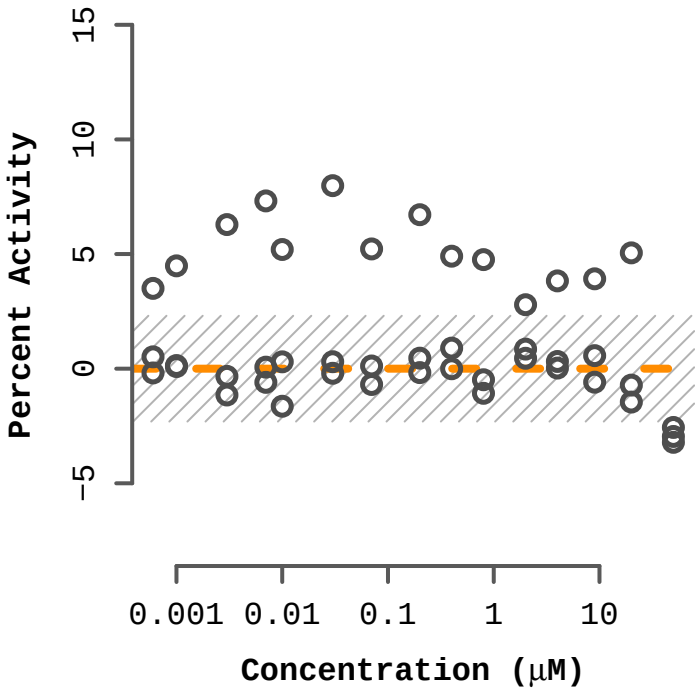
NAME: Bropirimine
CHID: 46803 CASRN: 56741-95-8
SPID(S): Tox21_112665_1
M4ID: 12482990

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.232 MAX_MED: 0.738 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

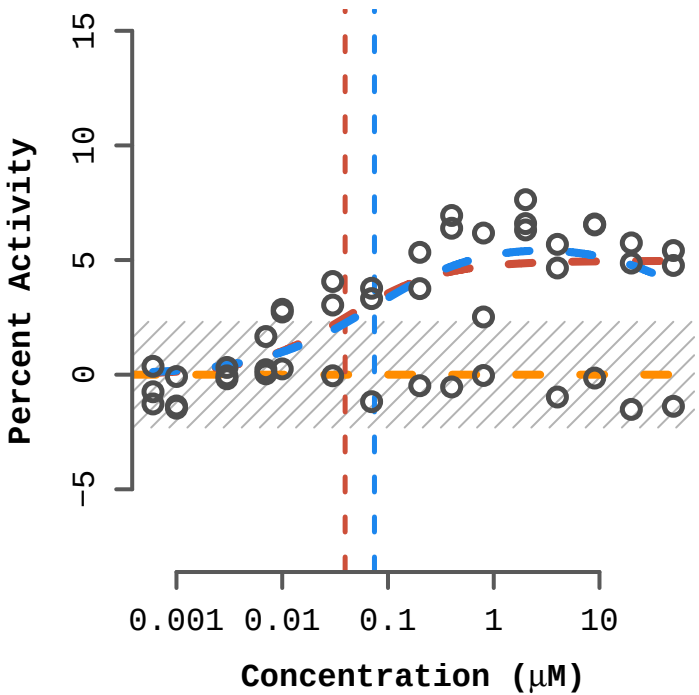
NAME: Pimobendan hydrochloride
CHID: 46804 CASRN: 77469-98-8
SPID(S): Tox21_112667_1
M4ID: 12482988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	229.56	NA	NA
PROB:	1	NA	NA
RMSE:	3.12	NA	NA

MAX_MEAN: 2.7 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nolatrexed dihydrochloride
CHID: 46810 CASRN: 152946-68-4
SPID(S): Tox21_112673_1
M4ID: 12482986

HILL MODEL (in red):

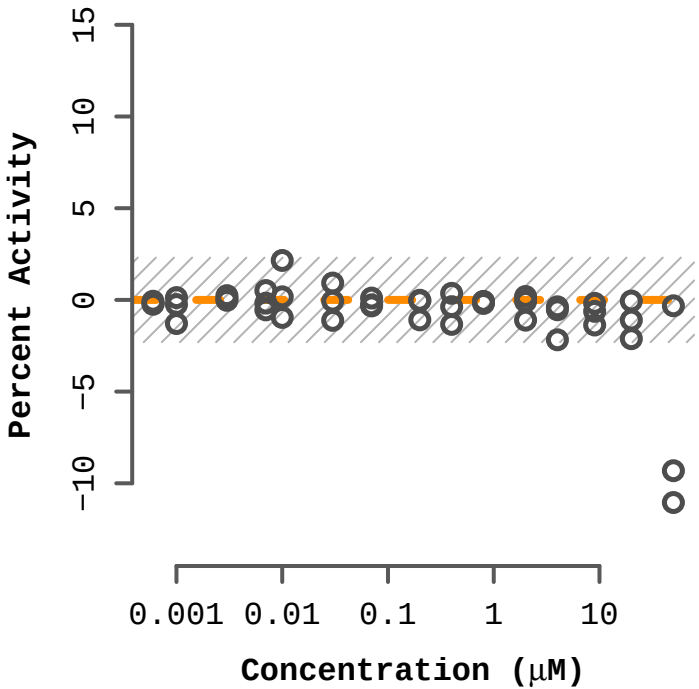
	tp	ga	gw
val:	4.96	−1.41	0.982
sd:	0.635	0.325	0.39

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.02	−1.13	0.809	2.11	0.751
sd:	3.08	0.734	0.411	0.955	1.71

	CNST	HILL	GNLS
AIC:	253.33	216.89	219.98
PROB:	0	0.82	0.18
RMSE:	3.8	2.56	2.54

MAX_MEAN: 6.85 **MAX_MED:** 6.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

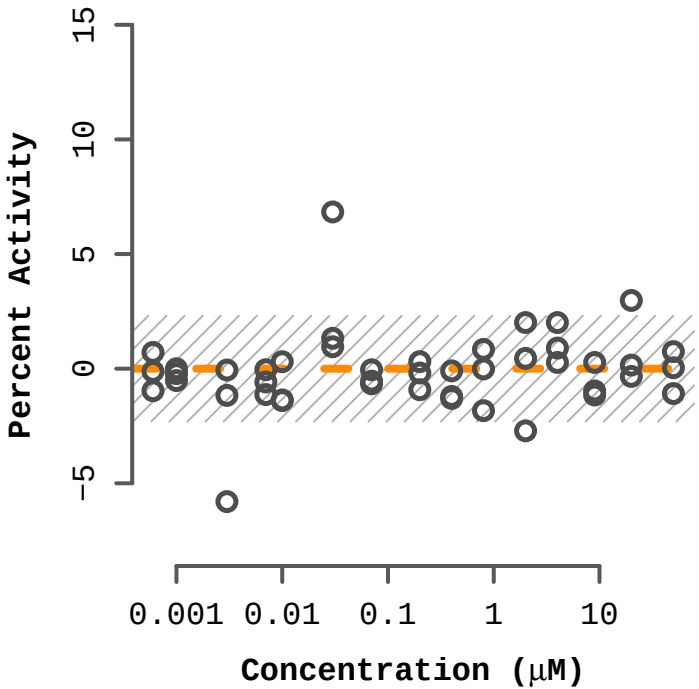
NAME: Robenidine
CHID: 46813 **CASRN:** 25875-51-8
SPID(S): Tox21_112676_1
M4ID: 12482985

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.76	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 0.456 **MAX_MED:** 0.169 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

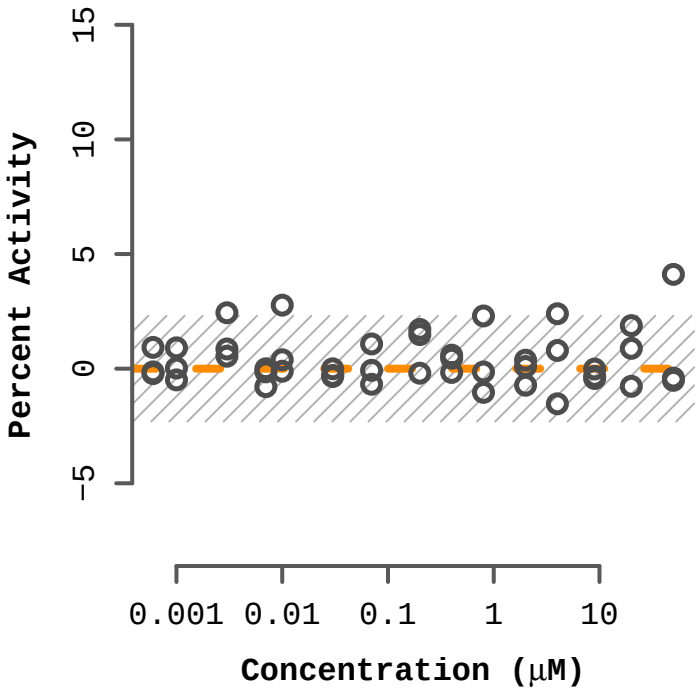
NAME: Liarozole hydrochloride
CHID: 46817 **CASRN:** 145858-50-0
SPID(S): Tox21_112683_1
M4ID: 12482983

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 3.04 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

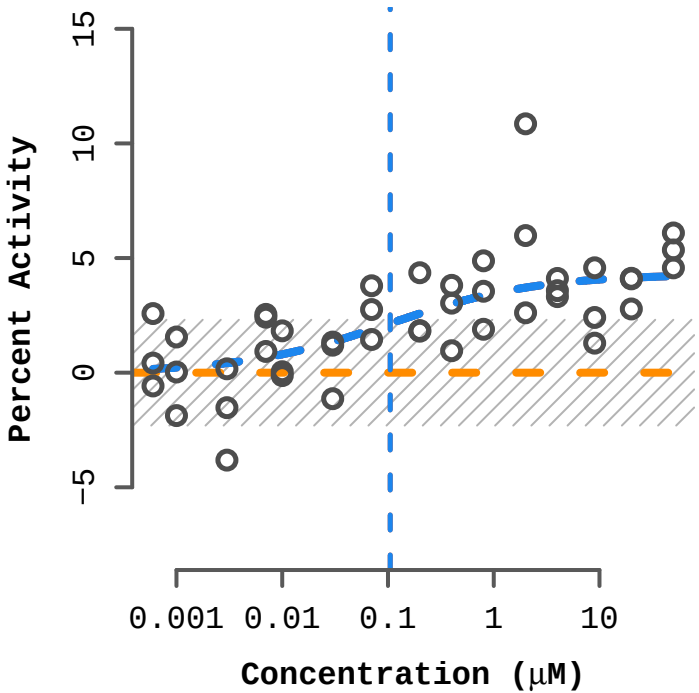
NAME: Ethyl linoleate
CHID: 46820 CASRN: 6114-21-2
SPID(S): Tox21_112687_1
M4ID: 12482982

HILL MODEL: Not applicable.

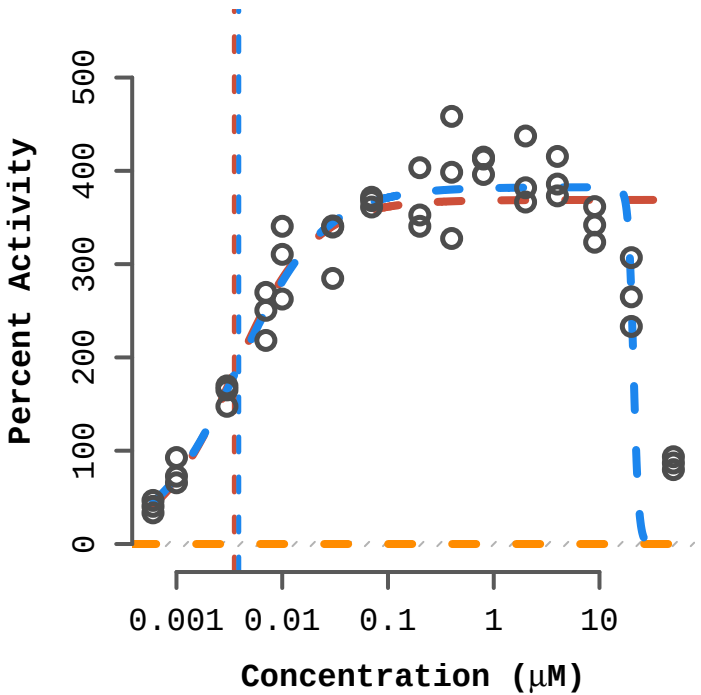
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

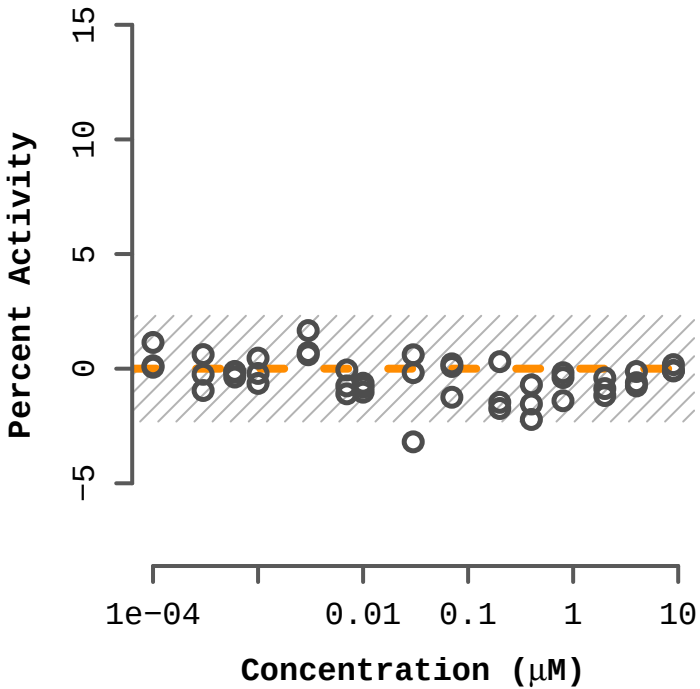
MAX_MEAN: 1.28 **MAX_MED:** 1.49 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    dl-Coniine
CHID:    46821   CASRN: 3238-60-6
SPID(S): Tox21_112688_1
M4ID:    12482981

HILL MODEL (in red):
      tp       ga       gw
val:  4.3      -0.979   0.626
sd:   0.745    0.45     0.326

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.3      -0.979   0.626    3.64     3.92
sd:   0.745    0.45     0.326    755      1530

      CNST        HILL        GNLS
AIC:  242.09      180.88      184.88
PROB: 0           0.88        0.12
RMSE: 3.41        1.78        1.78

MAX_MEAN: 6.48      MAX_MED: 5.98      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Clobetasone butyrate
CHID:    46823   CASRN: 25122-57-0
SPID(S): Tox21_112691_1
M4ID:    12482980

HILL MODEL (in red):
      tp       ga       gw
val:  369      -2.45    1.17
sd:   9.99     0.0593   0.16

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  382      -2.41    1.08     1.32     17.9
sd:   8.29     0.0481   0.116    0.00879  7.83

      CNST        HILL        GNLS
AIC:  653.2       505.77      462.88
PROB: 0           0           1
RMSE: 305.05      83.05       36.64

MAX_MEAN: 408       MAX_MED: 413       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

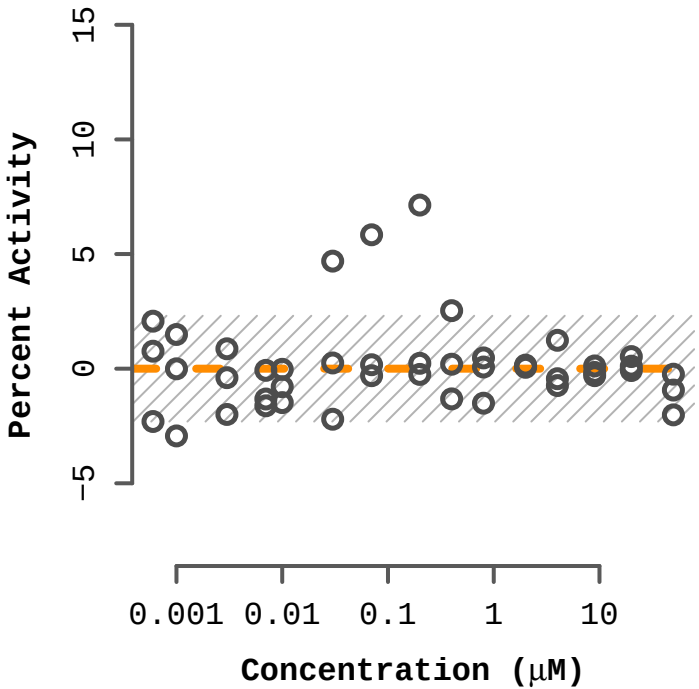
NAME: Sodium urate
CHID: 46828 **CASRN:** 1198-77-2
SPID(S): Tox21_112696_1
M4ID: 12482979

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.993 **MAX_MED:** 0.705 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

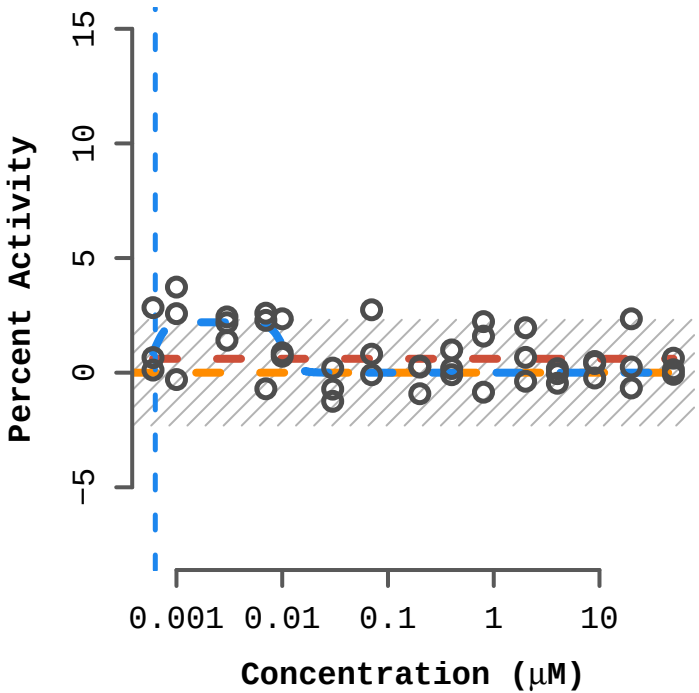
NAME: Disodium 2-hydroxybutanedioate
CHID: 46831 **CASRN:** 676-46-0
SPID(S): Tox21_112699_1
M4ID: 12482978

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.91	NA	NA

MAX_MEAN: 2.37 **MAX_MED:** 0.763 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nelarabine
CHID: 46842 CASRN: 121032-29-9
SPID(S): Tox21_112714_1
M4ID: 12482977

HILL MODEL (in red):

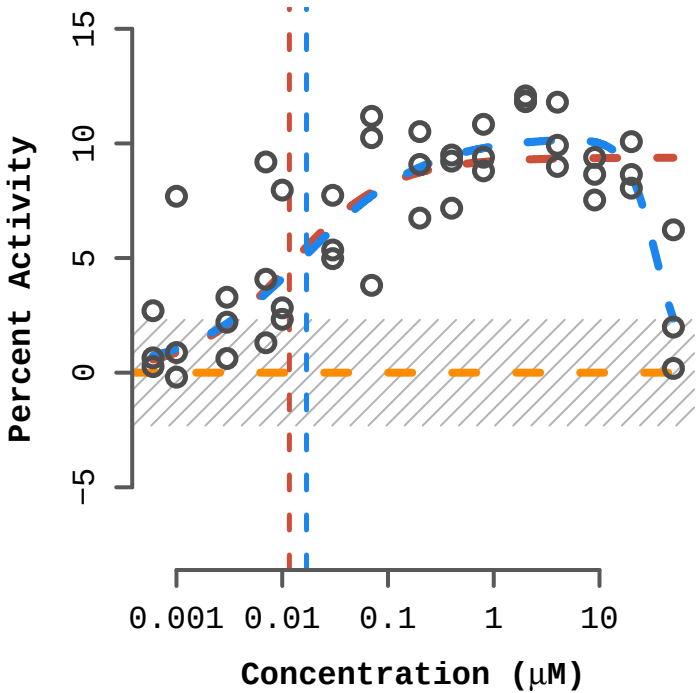
	tp	ga	gw
val:	0.606	−5.15	3.6
sd:	0.192	1310	2380

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.2	−3.2	8	−1.99	7.28
sd:	0.408	0.0649	9.29	0.065	13.7

	CNST	HILL	GNLS
AIC:	162.55	158.18	146.42
PROB:	0	0	1
RMSE:	1.44	1.23	1.11

MAX_MEAN: 2.01 **MAX_MED:** 2.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propiverine hydrochloride
CHID: 46847 CASRN: 54556-98-8
SPID(S): Tox21_112719_1
M4ID: 12482976

HILL MODEL (in red):

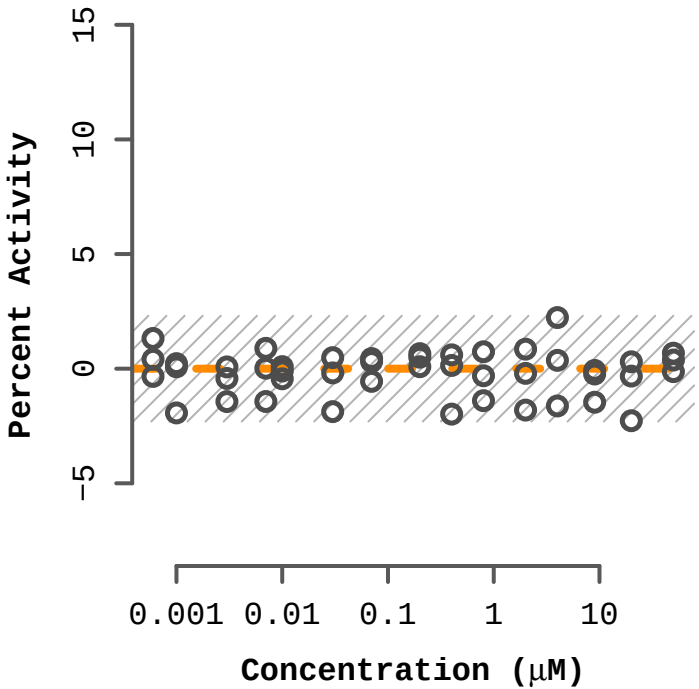
	tp	ga	gw
val:	9.38	−1.93	0.92
sd:	0.514	0.169	0.256

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.3	−1.77	0.771	1.53	3.14
sd:	0.77	0.194	0.216	0.0768	1.53

	CNST	HILL	GNLS
AIC:	320.18	221.1	207.23
PROB:	0	0	1
RMSE:	7.63	2.78	2.16

MAX_MEAN: 11.9 **MAX_MED:** 11.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

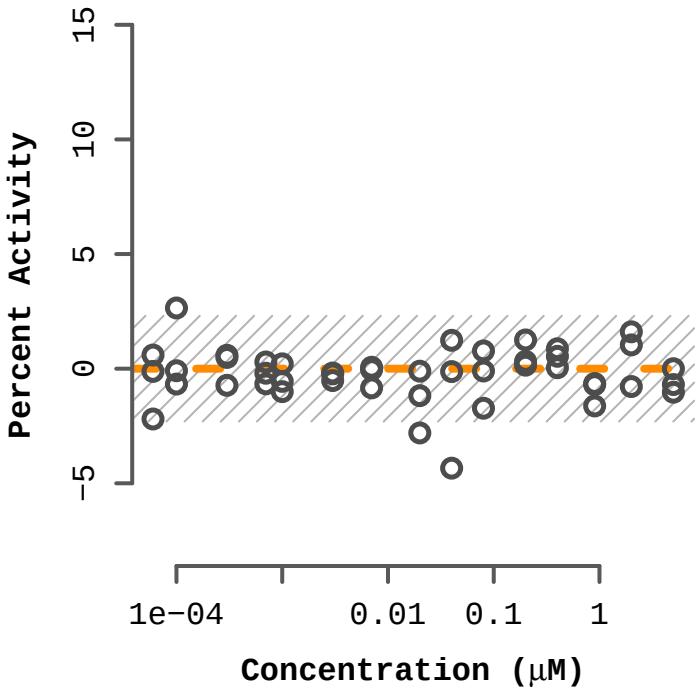
NAME: Celiprolol hydrochloride
CHID: 46850 CASRN: 57470-78-7
SPID(S): Tox21_112722_1
M4ID: 12482975

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.464 **MAX_MED:** 0.501 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

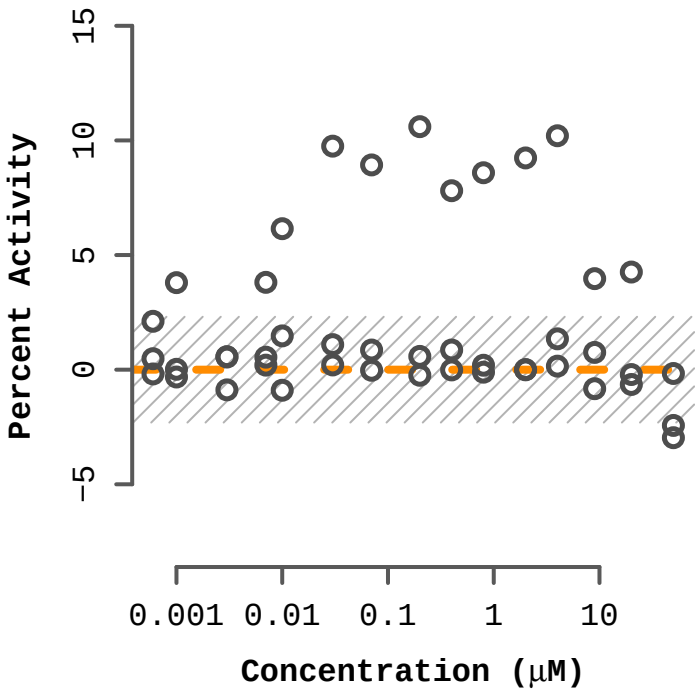
NAME: Decoquinate
CHID: 46851 **CASRN:** 18507-89-6
SPID(S): Tox21_112723_1
M4ID: 12482974

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.63 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

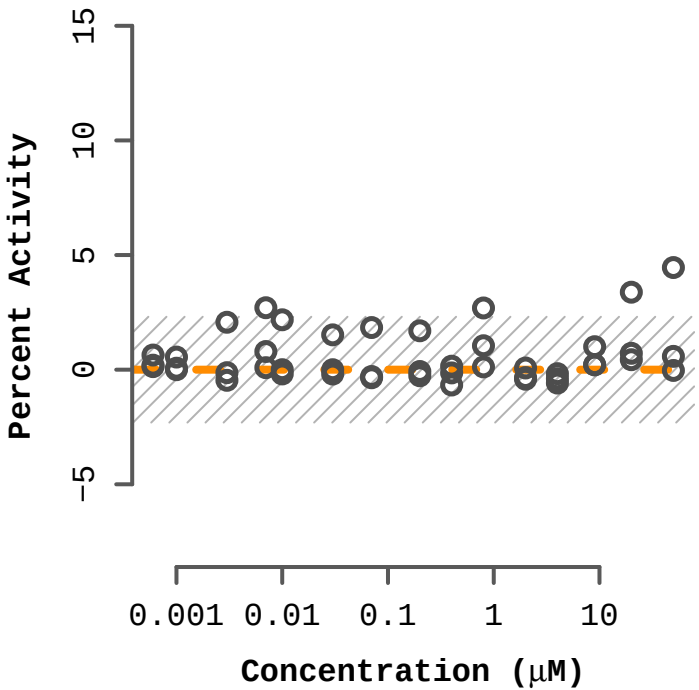
NAME: Tamibarotene
CHID: 46853 CASRN: 94497-51-5
SPID(S): Tox21_112725_1
M4ID: 12482973

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	244.9	NA	NA
PROB:	1	NA	NA
RMSE:	4.06	NA	NA

MAX_MEAN: 3.9 MAX_MED: 1.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

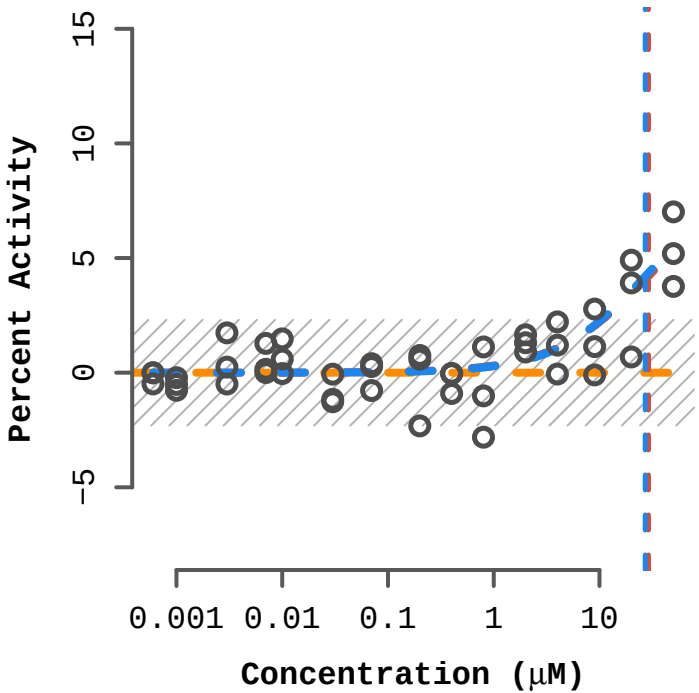
NAME: Eletriptan
CHID: 46861 CASRN: 143322-58-1
SPID(S): Tox21_112737_1
M4ID: 12482970

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.67 MAX_MED: 1.05 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Desmopressin acetate
CHID: 46864 CASRN: 62288-83-9
SPID(S): Tox21_112740_1
M4ID: 12482969

HILL MODEL (in red):

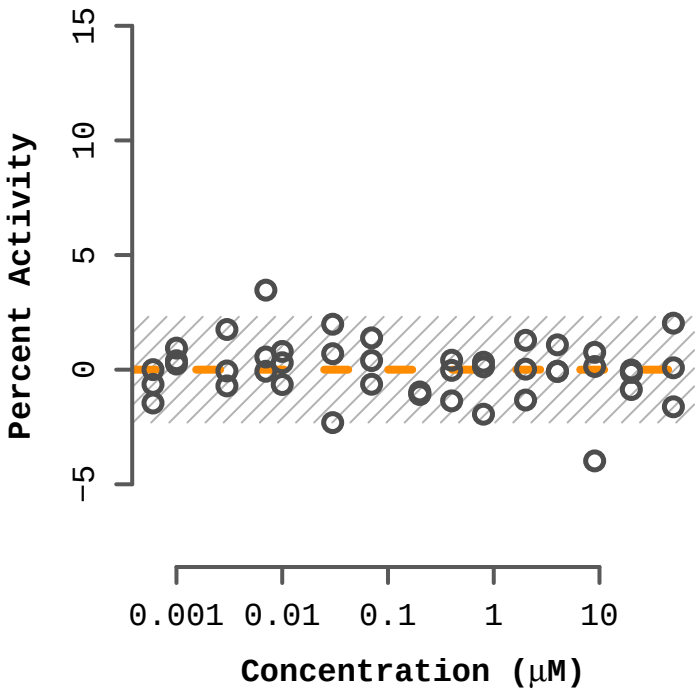
	tp	ga	gw
val:	8.42	1.46	0.968
sd:	6.33	0.736	0.462

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.42	1.43	1.02	1.77	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	181.56	146.87	150.84
PROB:	0	0.88	0.12
RMSE:	2	1.13	1.13

MAX_MEAN: 5.32 **MAX_MED:** 5.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

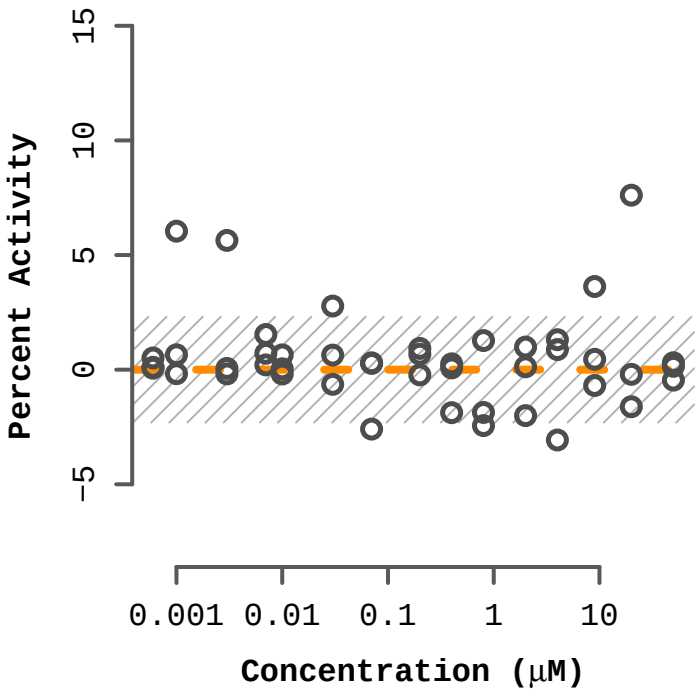
NAME: DL-Isoleucine
CHID: 46882 CASRN: 443-79-8
SPID(S): Tox21_112765_1
M4ID: 12482965

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.32 MAX_MED: 0.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

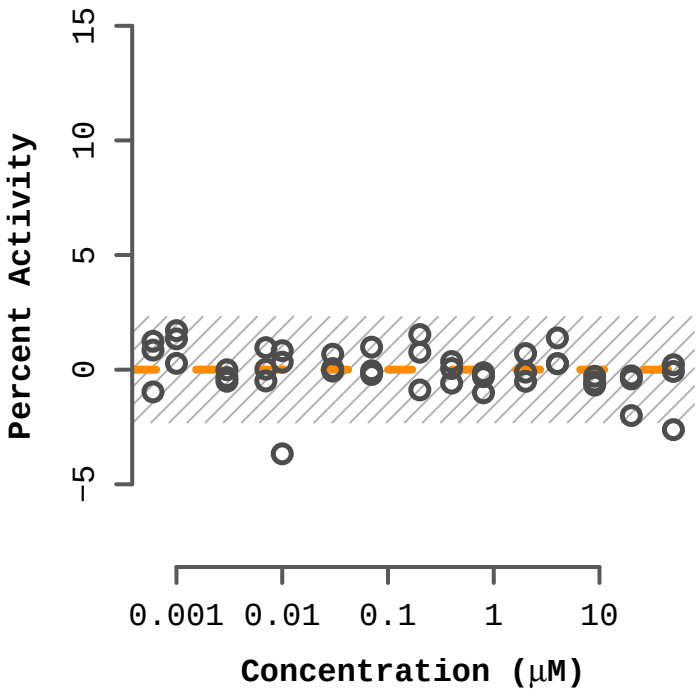
NAME: Pentisomicin
CHID: 46887 **CASRN:** 55870-64-9
SPID(S): Tox21_112770_1
M4ID: 12482963

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.8	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 2.17 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

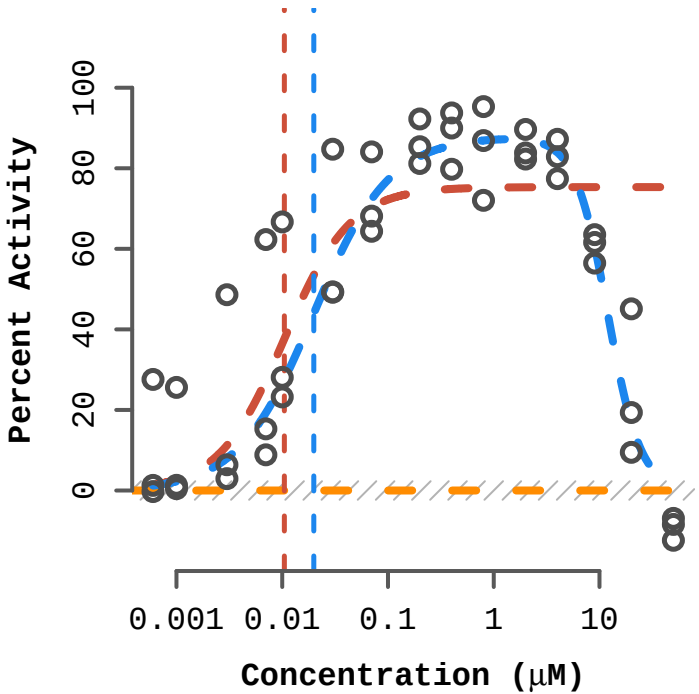
NAME: Bendamustine
CHID: 46888 CASRN: 16506-27-7
SPID(S): Tox21_112771_1
M4ID: 12482962

HILL MODEL: Not applicable.

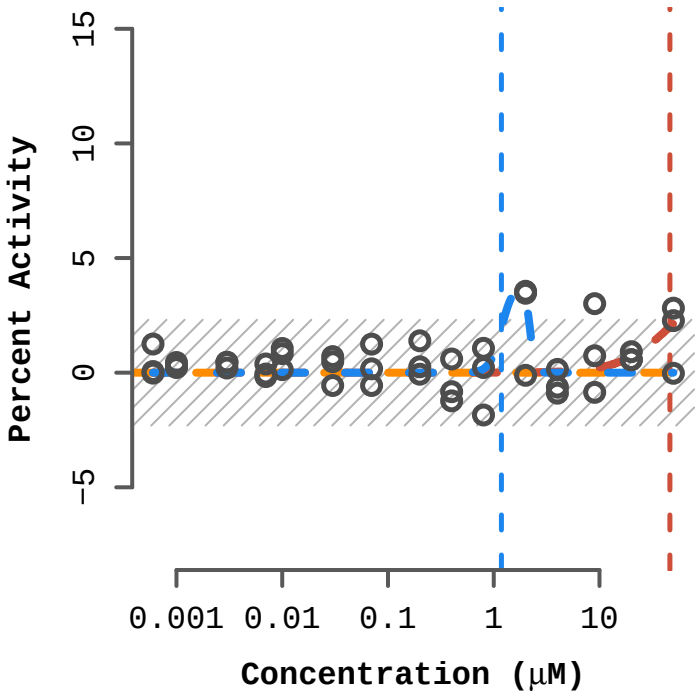
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.95	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.11 MAX_MED: 1.34 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Furazabol
CHID:    46889   CASRN: 1239-29-8
SPID(S): Tox21_112772
M4ID:    12482961

HILL MODEL (in red):
      tp       ga       gw
val:  75.3     -1.98    1.4
sd:   4.8      0.156    0.525

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  87.9     -1.7     1.22     1.08     2.81
sd:   3.19     0.0793   0.212    0.0389   0.577

      CNST        HILL        GNLS
AIC:  506.01      430.78      369.19
PROB: 0           0           1
RMSE: 60.6        29.58       14.57

MAX_MEAN: 87.8      MAX_MED: 90        BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Thiamine disulfide
CHID: 46890 CASRN: 67-16-3
SPID(S): Tox21_112773
M4ID: 12482960

HILL MODEL (in red):

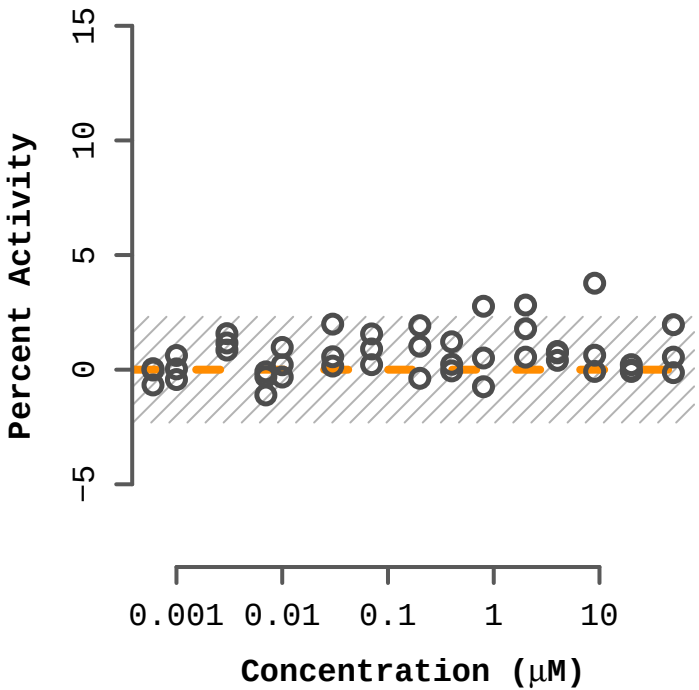
	tp	ga	gw
val:	4	1.67	1.84
sd:	14.6	1.77	3.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.85	0.0727	8	0.342	18
sd:	22.6	0.947	38.6	0.823	116

	CNST	HILL	GNLS
AIC:	140.25	136.76	141.17
PROB:	0.14	0.78	0.09
RMSE:	1.22	1.12	1.1

MAX_MEAN: 2.3 **MAX_MED:** 3.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

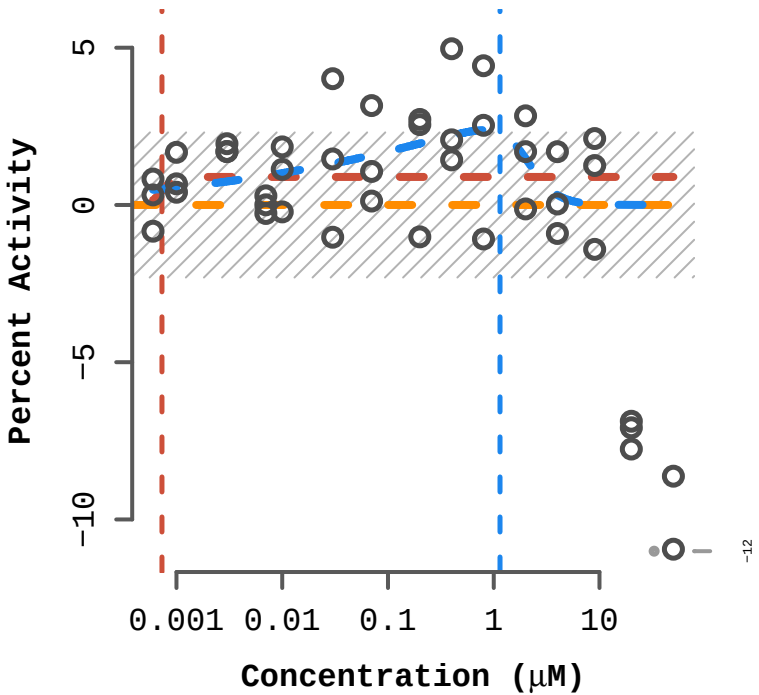
NAME: Mebrofenin
CHID: 46891 CASRN: 78266-06-5
SPID(S): Tox21_112775
M4ID: 12482958

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Riboflavin tetrabutyrate
CHID: 46892 CASRN: 752-56-7
SPID(S): Tox21_112776
M4ID: 12482957 BRK

HILL MODEL (in red):

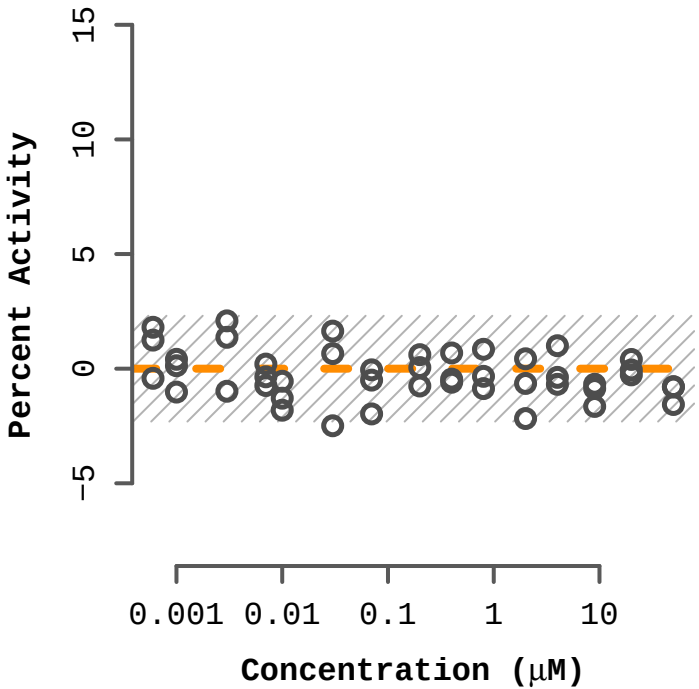
	tp	ga	gw
val:	0.891	−3.14	8
sd:	0.383	0.371	28.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.27	0.0595	0.303	0.311	3.25
sd:	16.8	8.03	0.368	0.294	5.82

	CNST	HILL	GNLS
AIC:	239.2	240.53	236.56
PROB:	0.19	0.1	0.71
RMSE:	3.77	3.91	3.57

MAX_MEAN: 2.83 MAX_MED: 2.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

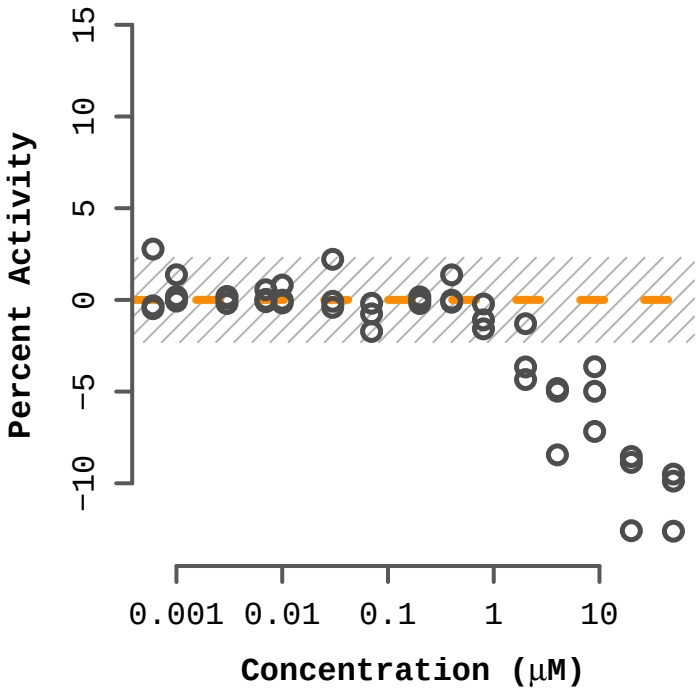
NAME: Magnesium salicylate tetrahydrate
CHID: 46896 **CASRN:** 18917-95-8
SPID(S): Tox21_112780
M4ID: 12482955

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.878 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

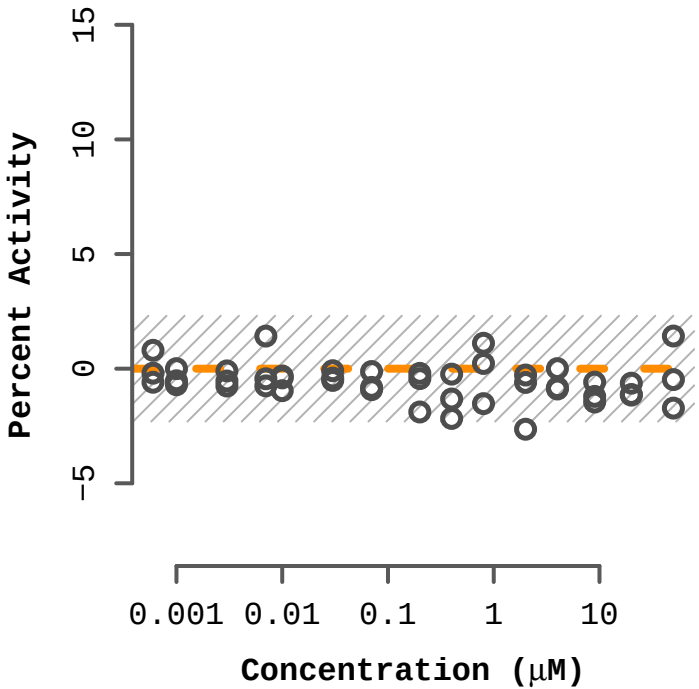
NAME: Nitrovin
CHID: 46903 **CASRN:** 804-36-4
SPID(S): Tox21_112791_1
M4ID: 12482952

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	256.42	NA	NA
PROB:	1	NA	NA
RMSE:	4.53	NA	NA

MAX_MEAN: 0.659 **MAX_MED:** 0.185 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

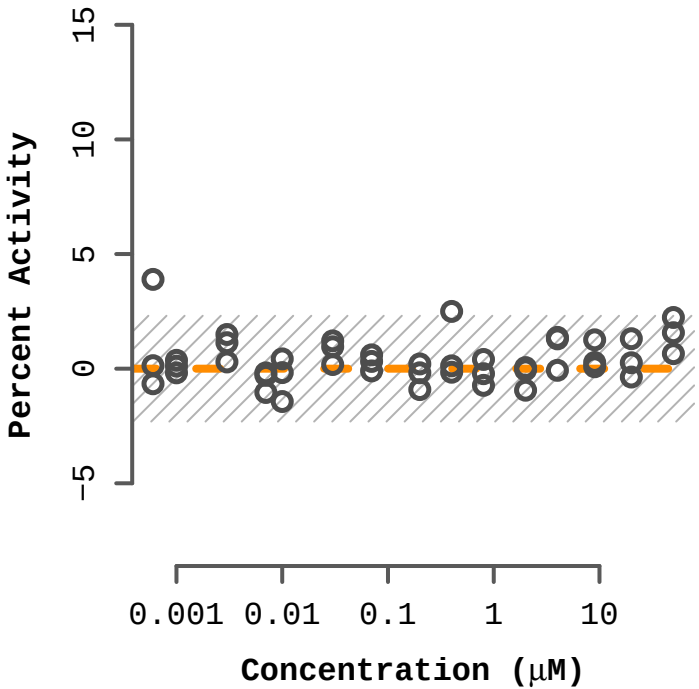
NAME: 3,3',5'−Triiodo−L−thyronine
CHID: 46908 **CASRN:** 5817−39−0
SPID(S): Tox21_112797_1
M4ID: 12482950

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.0779 **MAX_MED:** 0.228 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

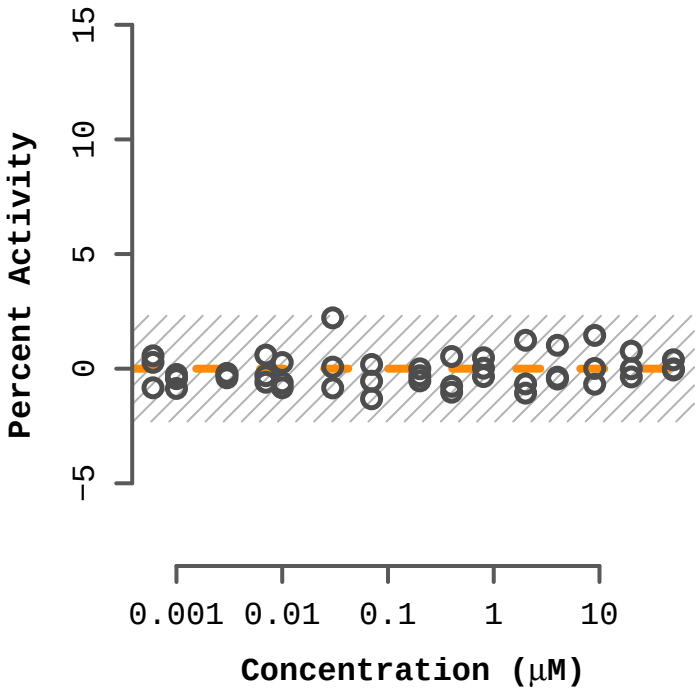
NAME: Azosemide
CHID: 46910 **CASRN:** 27589-33-9
SPID(S): Tox21_112799_1
M4ID: 12482949

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

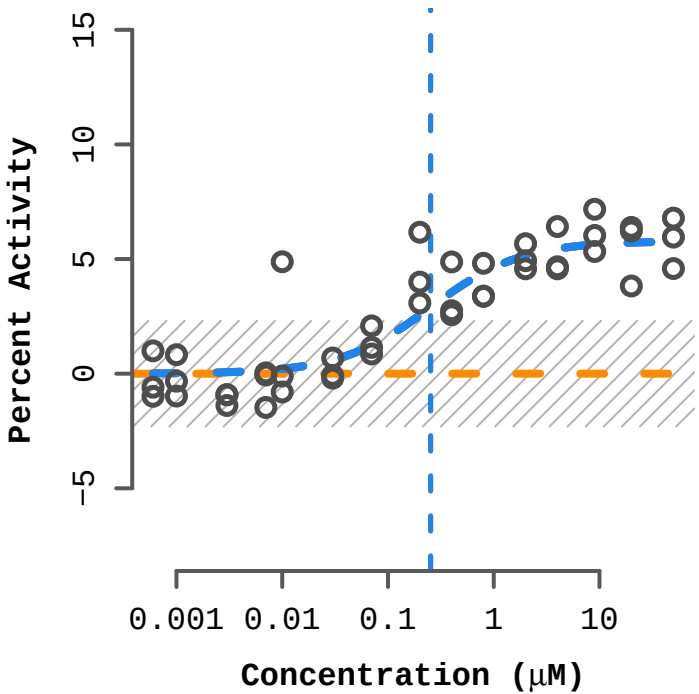
NAME: Emedastine difumarate
CHID: 46911 CASRN: 87233-62-3
SPID(S): Tox21_112800_1
M4ID: 12482948

HILL MODEL: Not applicable.

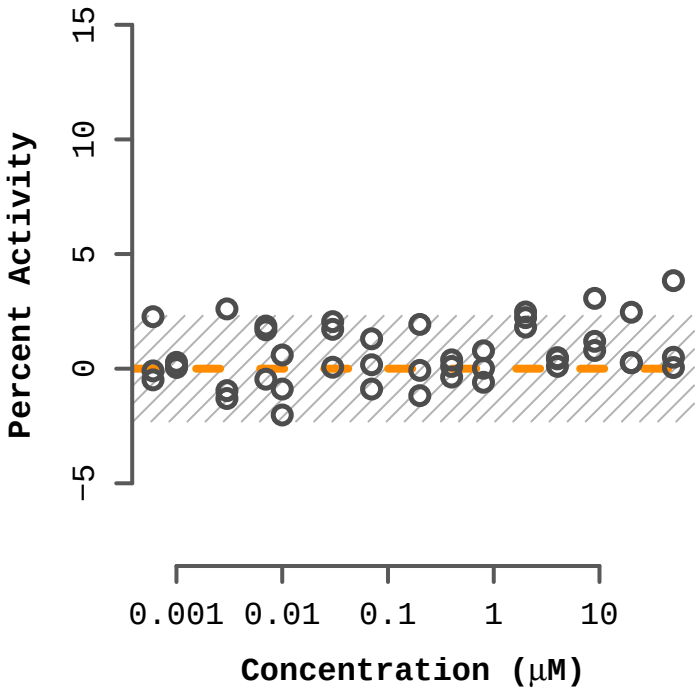
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 0.278 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Imidapril hydrochloride
CHID:    46912   CASRN: 89396-94-1
SPID(S): Tox21_112801_1
M4ID:    12482947

HILL MODEL (in red):
      tp       ga       gw
val:  5.78     -0.597   1.01
sd:   0.435    0.182    0.231

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.78     -0.597   1.01     3.33     6.12
sd:   0.435    0.182    0.231    20000    75100

      CNST        HILL        GNLS
AIC:  255.89      148.82      152.82
PROB: 0           0.88        0.12
RMSE: 3.84        1.24        1.24

MAX_MEAN: 6.18      MAX_MED: 6.23      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

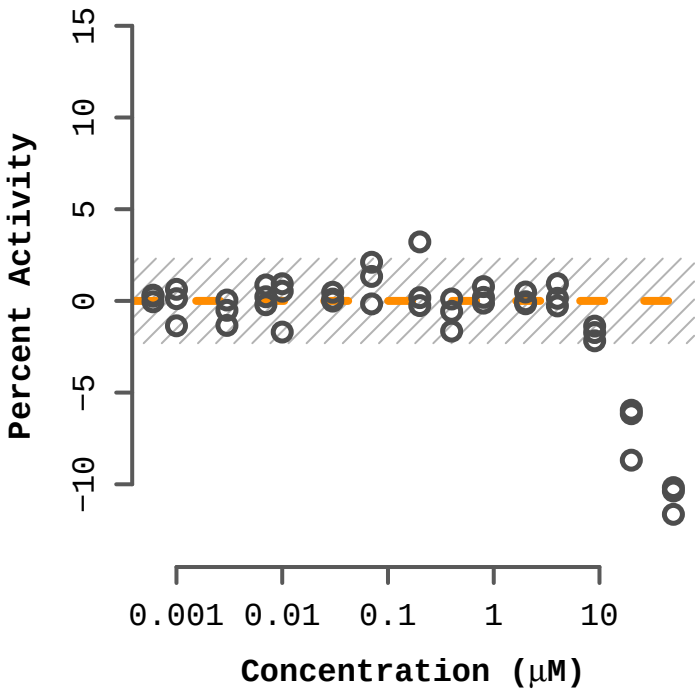
NAME: Temocapril hydrochloride
CHID: 46914 CASRN: 110221-44-8
SPID(S): Tox21_112803_1
M4ID: 12482946

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.17 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

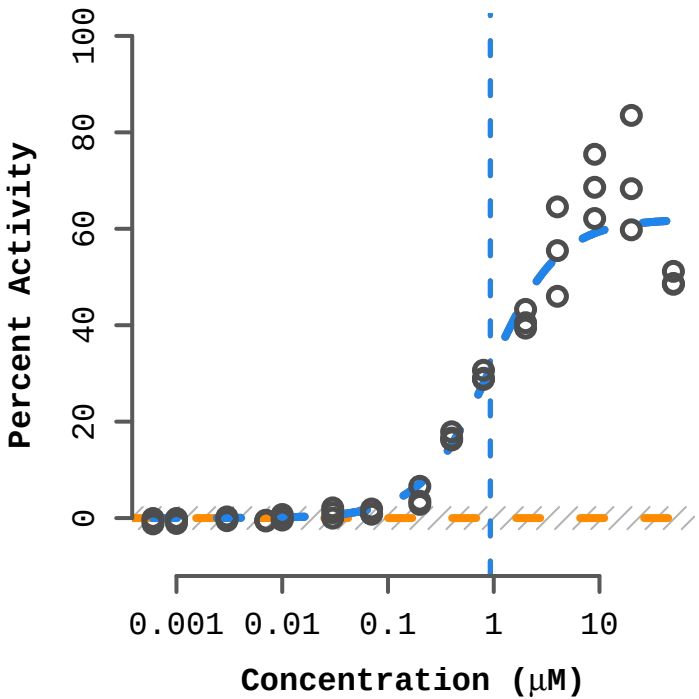
NAME: Vatalanib
CHID: 46919 **CASRN:** 212141-54-3
SPID(S): Tox21_112808_1
M4ID: 12482945

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.45	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norgestimate
CHID: 46922 **CASRN:** 35189-28-7
SPID(S): Tox21_112811_1
M4ID: 12482944

HILL MODEL (in red):

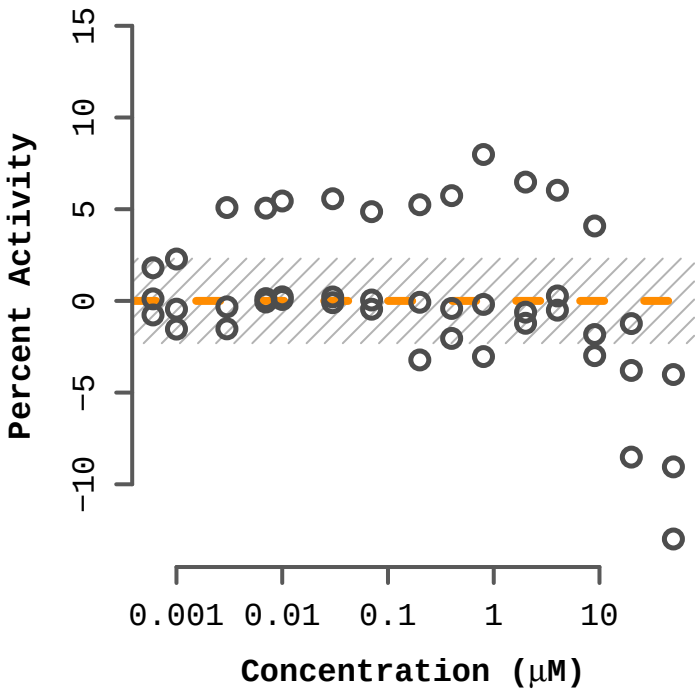
	tp	ga	gw
val:	62	-0.0322	1.33
sd:	3.8	0.0609	0.147

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	62	-0.0322	1.33	3.34	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	448.38	282.69	286.69
PROB:	0	0.88	0.12
RMSE:	34.9	6.13	6.13

MAX_MEAN: 70.5 **MAX_MED:** 68.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

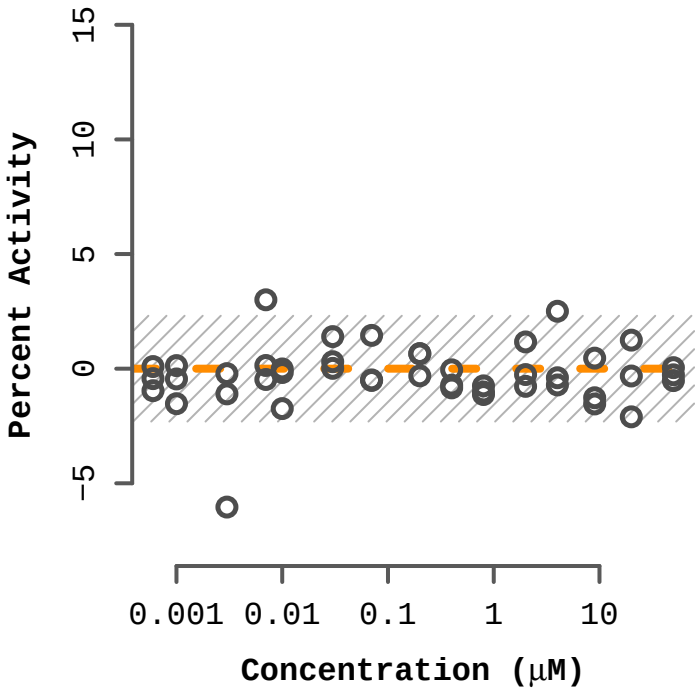
NAME: Oxapium iodide
CHID: 46925 **CASRN:** 6577-41-9
SPID(S): Tox21_112814_1
M4ID: 12482943

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.24	NA	NA
PROB:	1	NA	NA
RMSE:	4.12	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 0.272 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

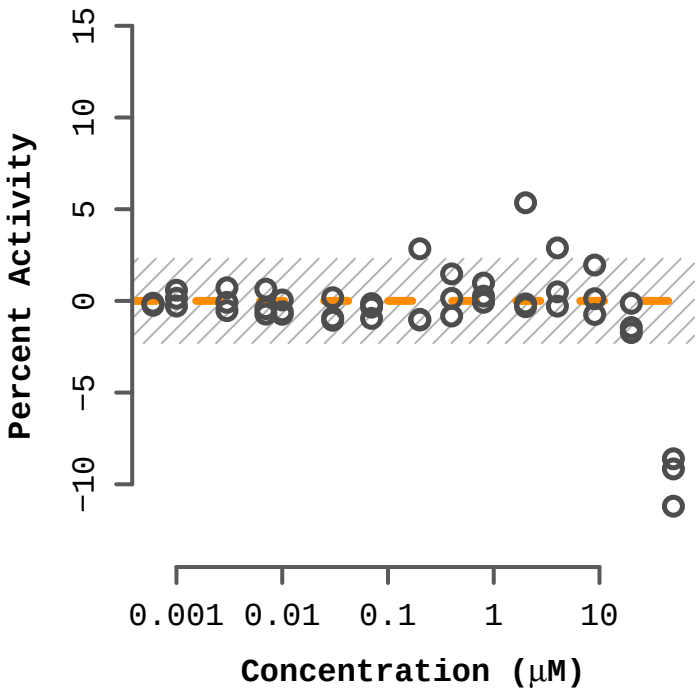
NAME: Caffeine, citrated
CHID: 46938 **CASRN:** 69-22-7
SPID(S): Tox21_110099_1
M4ID: 12484654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 0.648 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

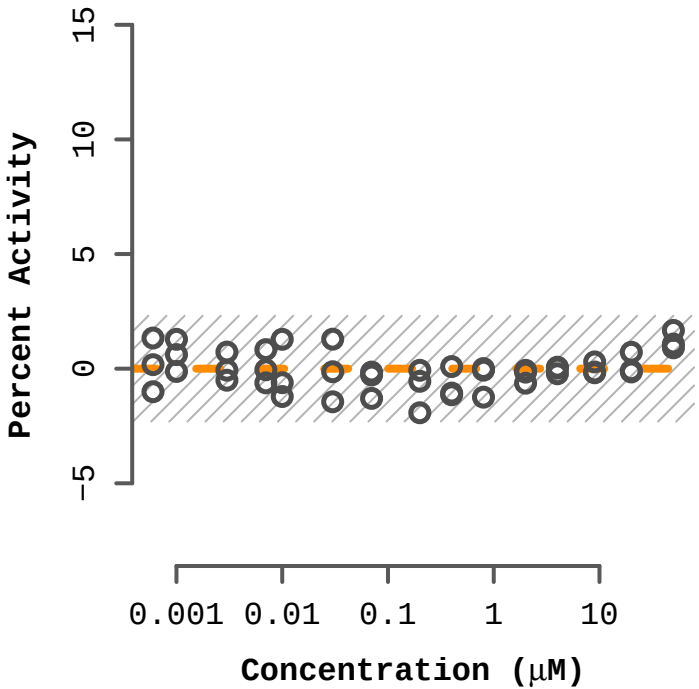
NAME: Desipramine hydrochloride
CHID: 46942 **CASRN:** 58-28-6
SPID(S): Tox21_110129_1
M4ID: 12484625

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.79	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 0.497 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

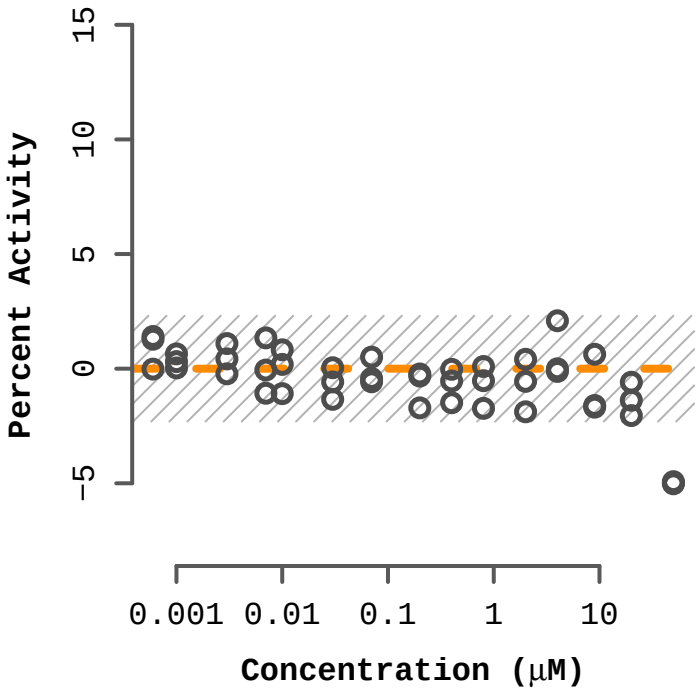
NAME: Moxisylyte hydrochloride
CHID: 46946 CASRN: 964-52-3
SPID(S): Tox21_110194_1
M4ID: 12484565

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

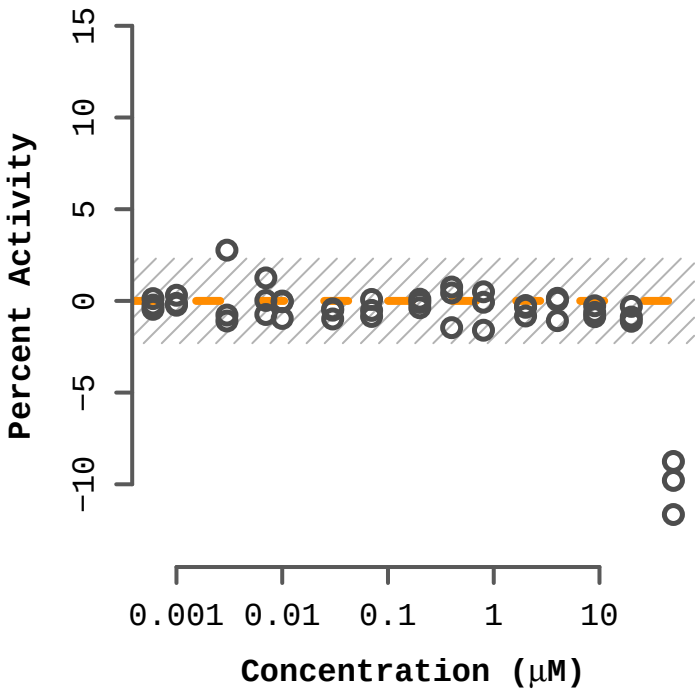
NAME: Promazine hydrochloride
CHID: 46949 **CASRN:** 53-60-1
SPID(S): Tox21_110235_1
M4ID: 12484528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 0.891 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

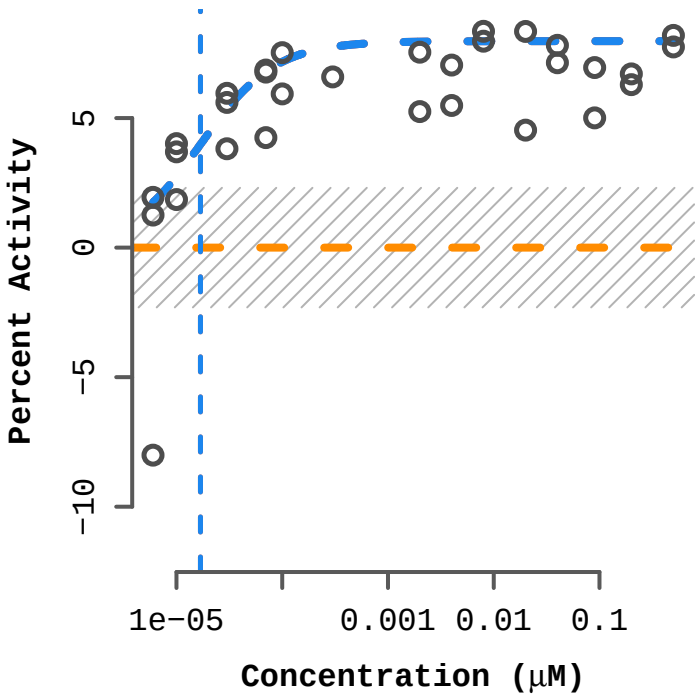
NAME: Protriptyline hydrochloride
CHID: 46951 **CASRN:** 1225-55-4
SPID(S): Tox21_110244_1
M4ID: 12484520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 0.301 **MAX_MED:** 0.435 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Guanethidine sulfate
CHID: 46966 **CASRN:** 60-02-6
SPID(S): Tox21_110340_1
M4ID: 12484442

HILL MODEL (in red):

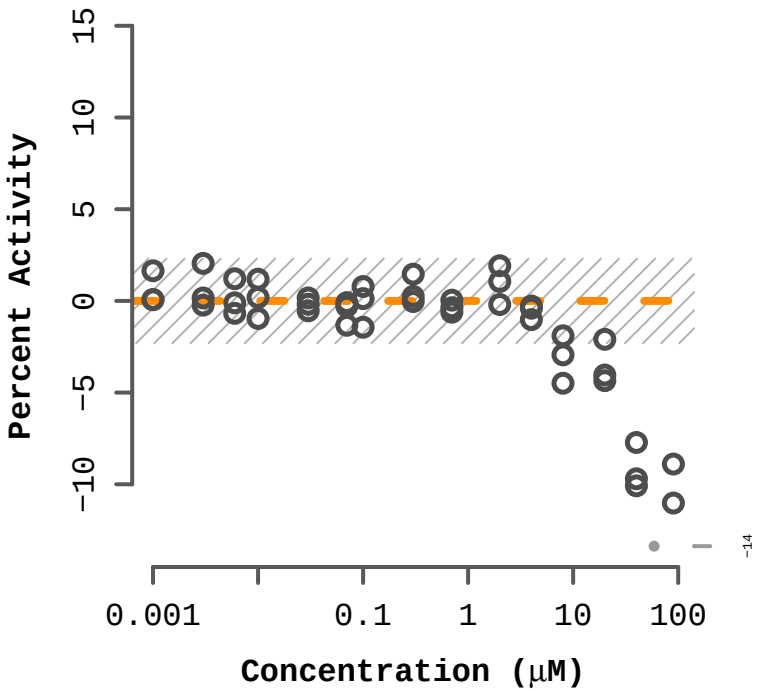
	tp	ga	gw
val:	7.97	−4.77	1.23
sd:	0.249	0.0904	0.251

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.97	−4.77	1.23	0.949	6.74
sd:	0.249	0.0904	0.251	1620	8750

	CNST	HILL	GNLS
AIC:	316.44	172.26	176.26
PROB:	0	0.88	0.12
RMSE:	7.15	1.92	1.92

MAX_MEAN: 8.81 **MAX_MED:** 8.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

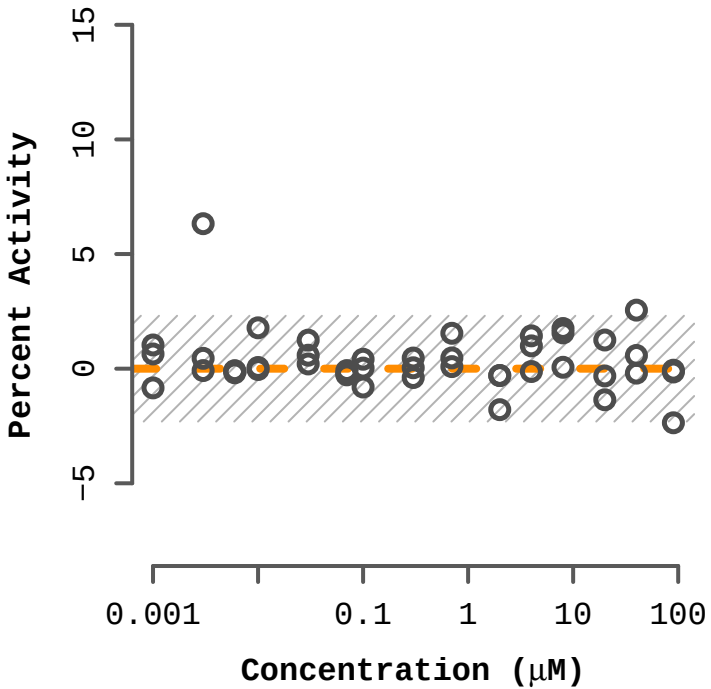
NAME: 5HPP-33
CHID: 46970 CASRN: 105624-86-0
SPID(S): Tox21_300631
M4ID: 12478502 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	235.6	NA	NA
PROB:	1	NA	NA
RMSE:	4.06	NA	NA

MAX_MEAN: 0.929 MAX_MED: 1.06 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

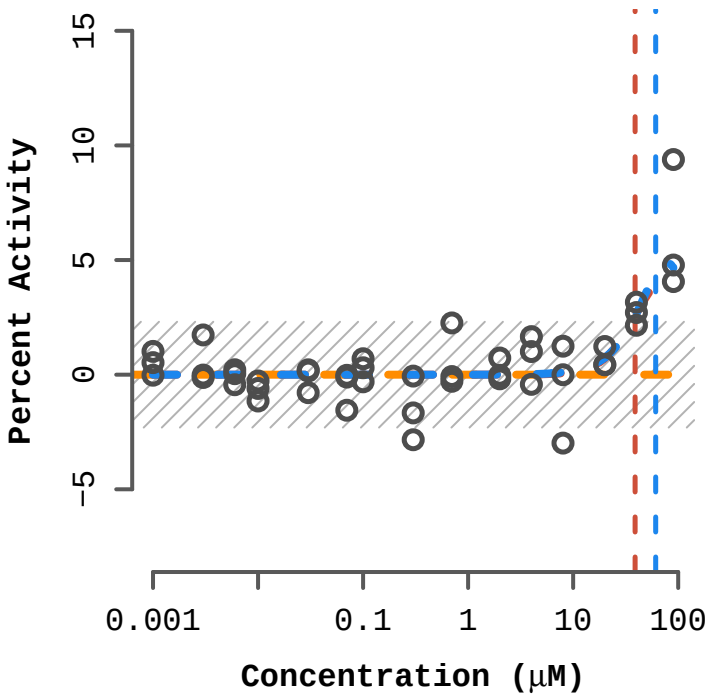
NAME: 2-Phenylmercaptoethanol
CHID: 46974 **CASRN:** 699-12-7
SPID(S): Tox21_301520
M4ID: 12477613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.23 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methylumbelliferone hydrate
CHID: 46976 CASRN: 103764-33-6
SPID(S): Tox21_301068
M4ID: 12478065

HILL MODEL (in red):

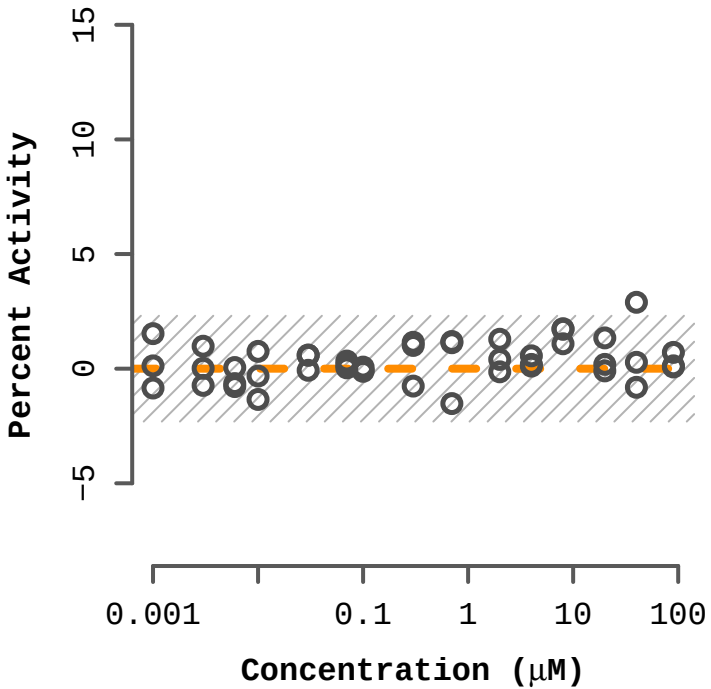
	tp	ga	gw
val:	5.14	1.59	2.74
sd:	1.1	0.1	1.34

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.65	1.79	2.23	2.04	4.18
sd:	32.2	0.999	1.86	0.543	19.4

	CNST	HILL	GNLS
AIC:	175.41	137.48	141.42
PROB:	0	0.88	0.12
RMSE:	2.07	1.2	1.2

MAX_MEAN: 6.08 MAX_MED: 4.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

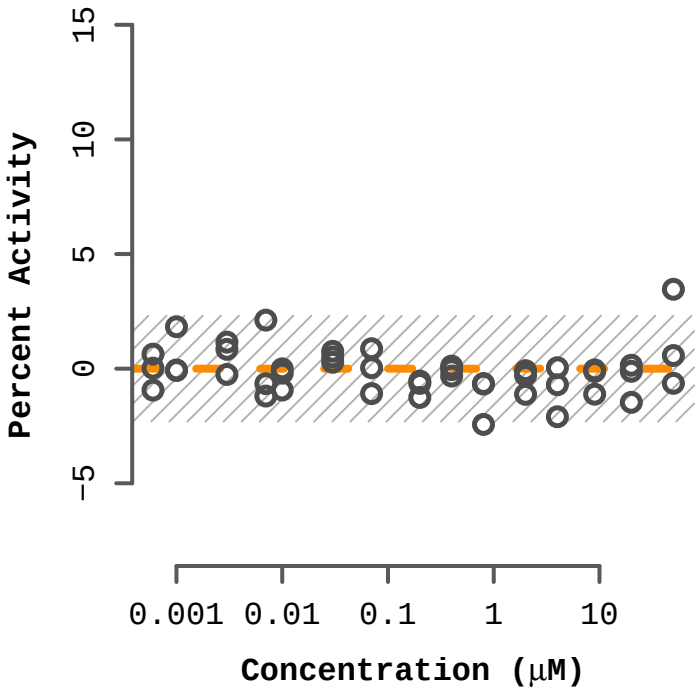
NAME: Buflomedil hydrochloride
CHID: 46977 CASRN: 35543-24-9
SPID(S): Tox21_301435
M4ID: 12477698

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.52 MAX_MED: 1.72 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

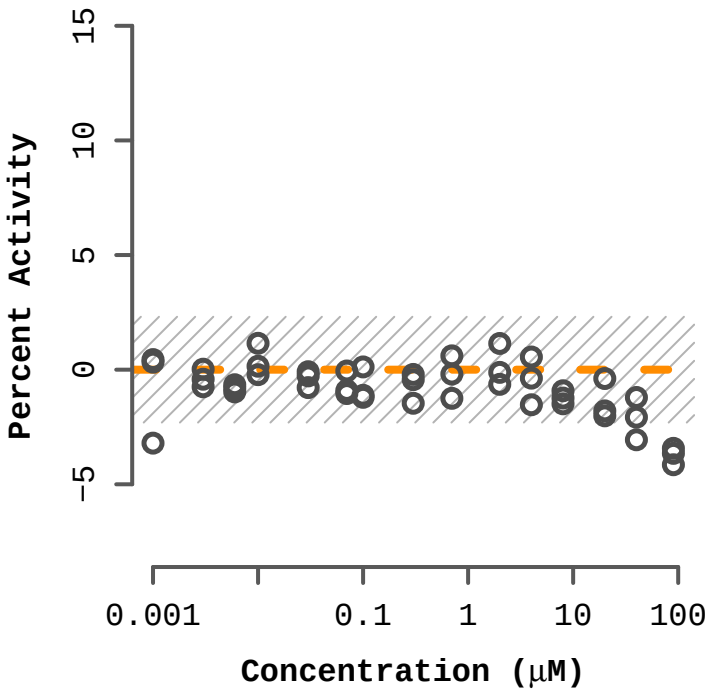
NAME: Buflomedil hydrochloride
CHID: 46977 CASRN: 35543-24-9
SPID(S): Tox21_110636_1
M4ID: 12484216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.845 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

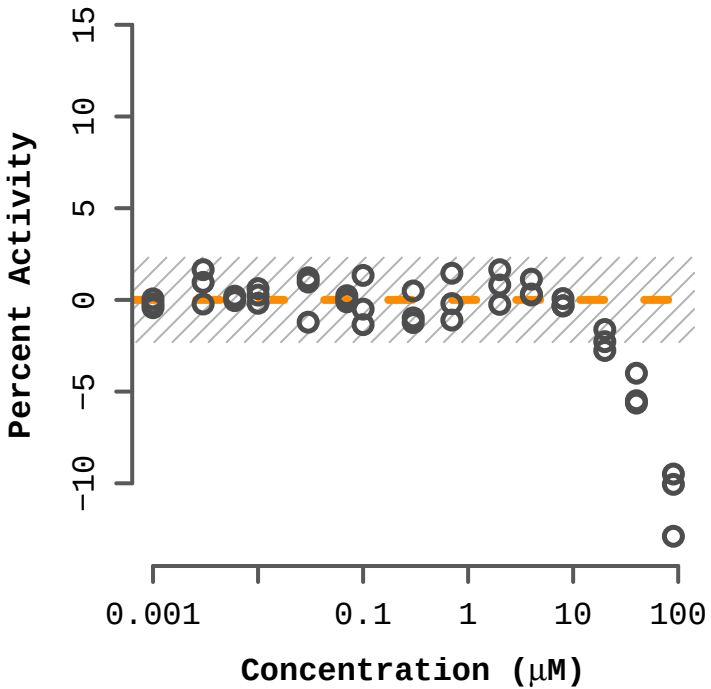
NAME: N-(Alkyl C10-C16)-N,N-dimethylglycine betaine
CHID: 46978 **CASRN:** 66455-29-6
SPID(S): Tox21_301433
M4ID: 12477700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 0.363 **MAX_MED:** 0.329 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

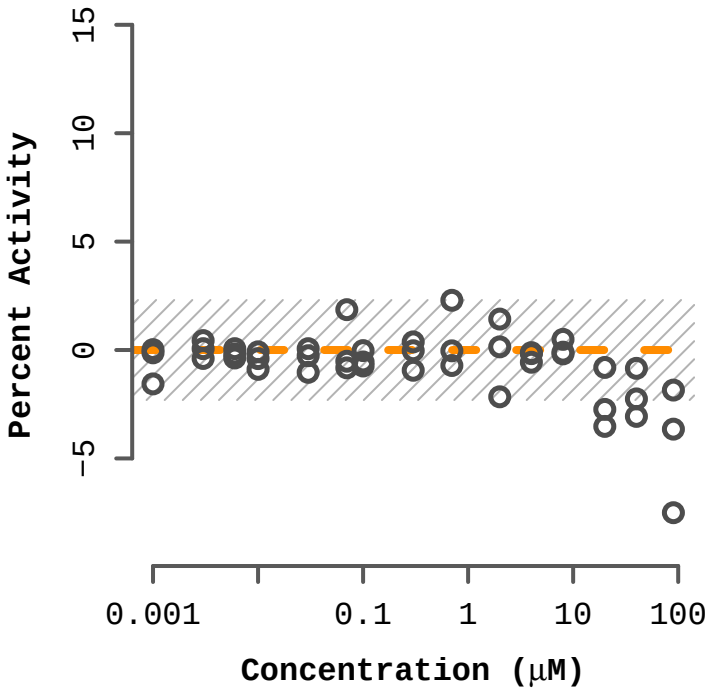
NAME: 1-(2,6-Dichlorophenyl)-2-indolinone
CHID: 46979 **CASRN:** 15362-40-0
SPID(S): Tox21_301756
M4ID: 12477377

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.26	NA	NA
PROB:	1	NA	NA
RMSE:	3.25	NA	NA

MAX_MEAN: 0.795 **MAX_MED:** 0.976 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

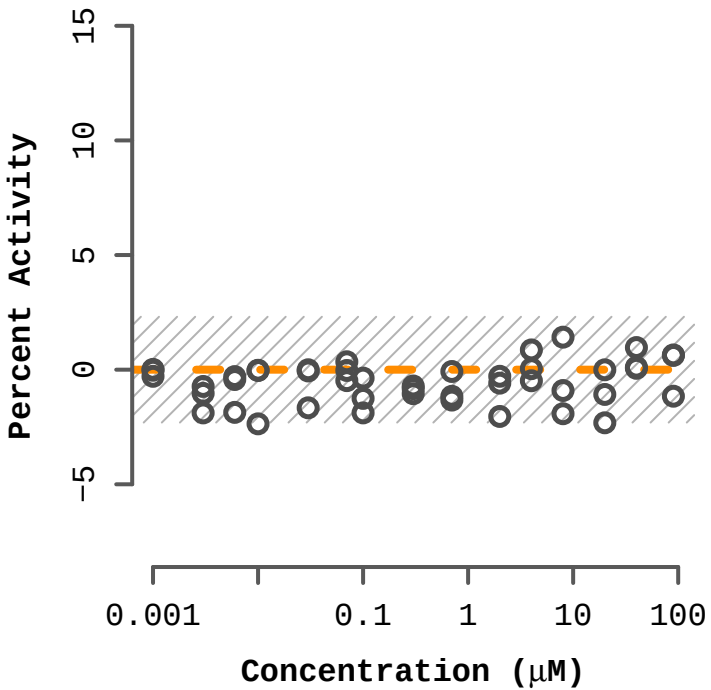
NAME: Monosodium 8-amino-1-naphthol-3,6-disulfonate
CHID: 46980 CASRN: 312693-54-2
SPID(S): Tox21_301413
M4ID: 12477720

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 0.515 MAX_MED: 0.147 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

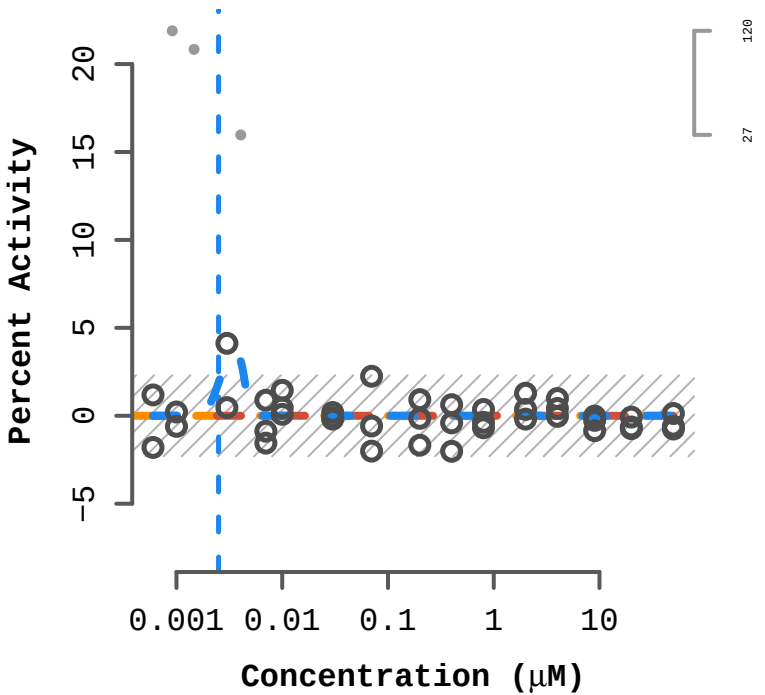
NAME: dl-Tartaric acid
CHID: 46986 **CASRN:** 133-37-9
SPID(S): Tox21_302052
M4ID: 12477081

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.379 **MAX_MED:** 0.623 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: DL−Cysteine
CHID: 46988 CASRN: 3374−22−9
SPID(S): Tox21_111766_1
M4ID: 12483492 BRK

HILL MODEL (in red):

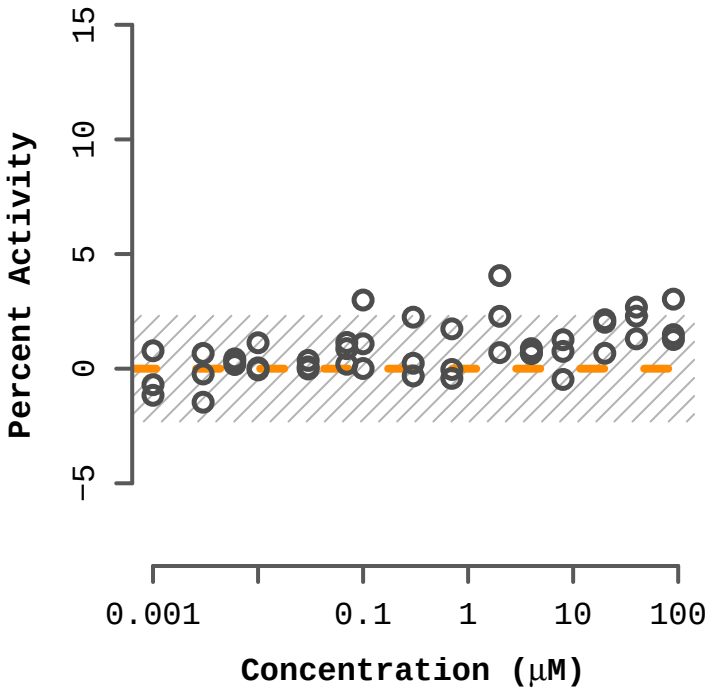
	tp	ga	gw
val:	15.2	2.2	8
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.76	−2.6	8	−2.35	18
sd:	16.5	0.97	43.9	1.49	138

	CNST	HILL	GNLS
AIC:	239.66	245.67	246.12
PROB:	0.92	0.05	0.04
RMSE:	23.82	23.82	23.74

MAX_MEAN: 39.5 MAX_MED: 4.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

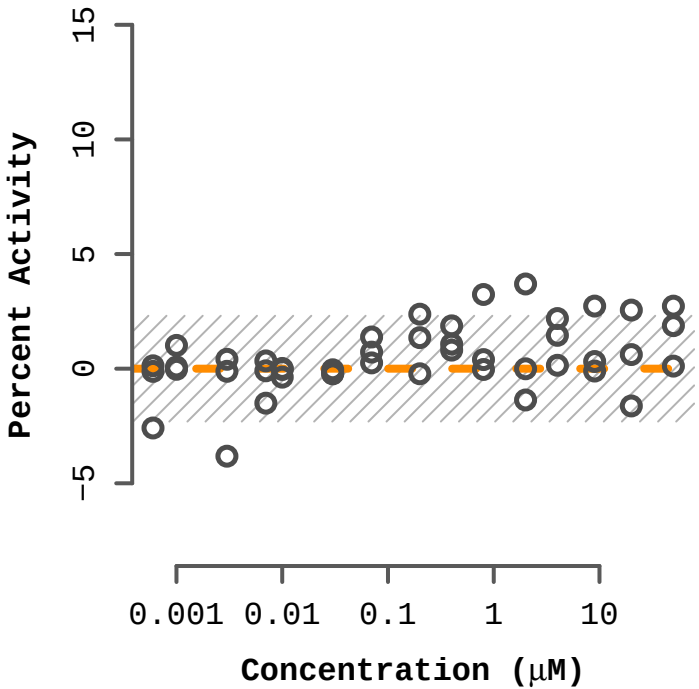
NAME: d−Tryptophan
CHID: 46989 **CASRN:** 153−94−6
SPID(S): Tox21_301300
M4ID: 12477833

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.35 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

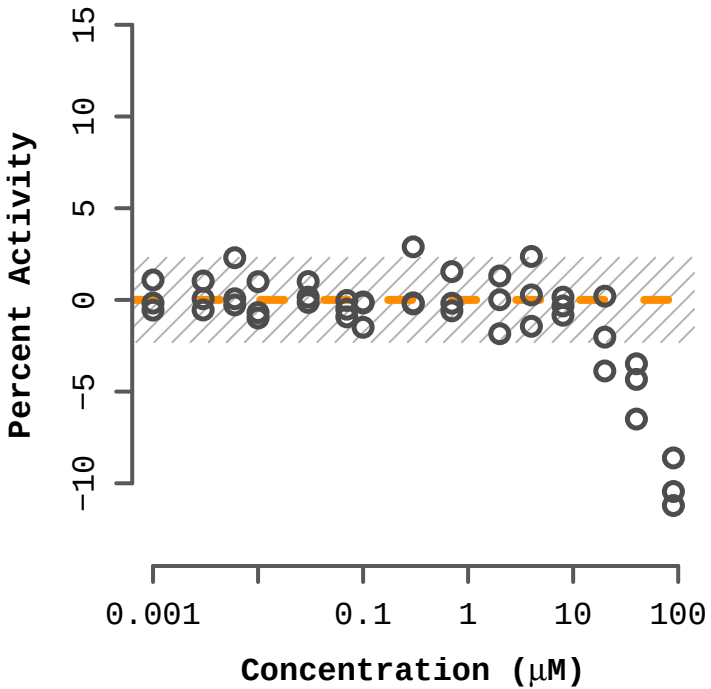
NAME: d-Tryptophan
CHID: 46989 **CASRN:** 153-94-6
SPID(S): Tox21_111205_1
M4ID: 12483842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

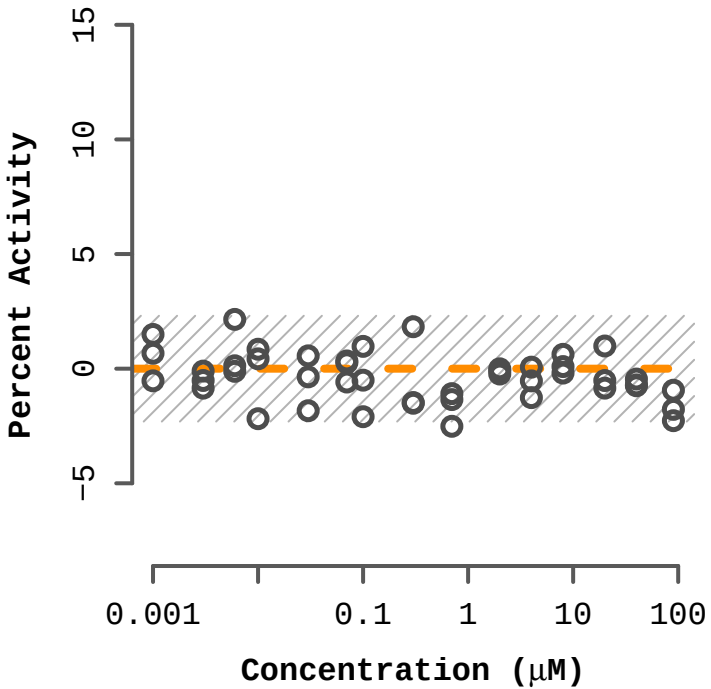
NAME: Nicardipine hydrochloride
CHID: 46992 **CASRN:** 54527-84-3
SPID(S): Tox21_301832
M4ID: 12477301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.28	NA	NA
PROB:	1	NA	NA
RMSE:	3.13	NA	NA

MAX_MEAN: 0.84 **MAX_MED:** 0.274 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

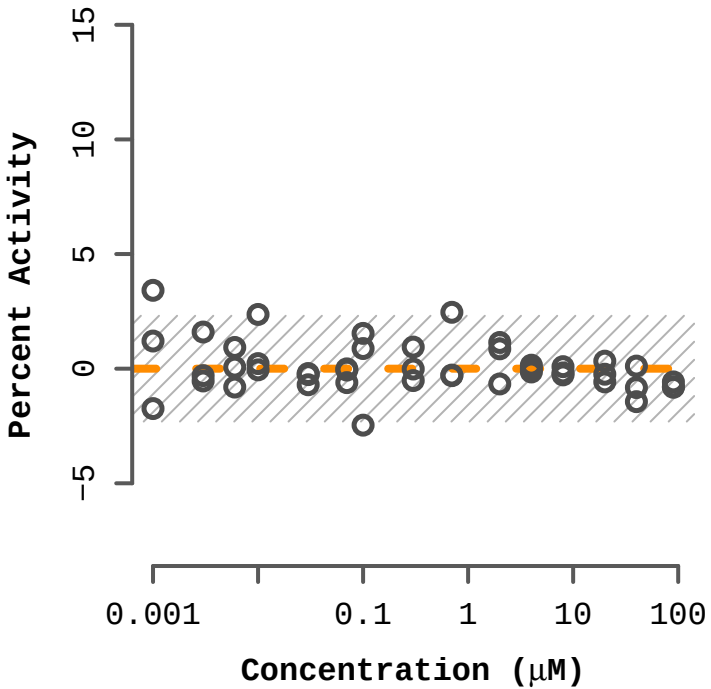
NAME: Ethyl 3-ethoxy-3-iminopropionate hydrochloride
CHID: 46994 CASRN: 2318-25-4
SPID(S): Tox21_301583
M4ID: 12477550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.721 MAX_MED: 0.673 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

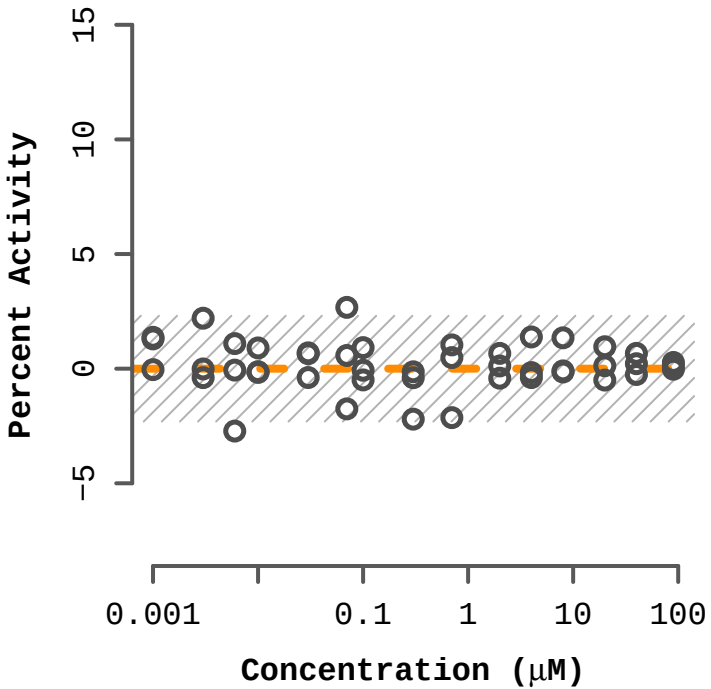
NAME: Tributylphosphine
CHID: 46998 CASRN: 998-40-3
SPID(S): Tox21_301600
M4ID: 12477533

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.962 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

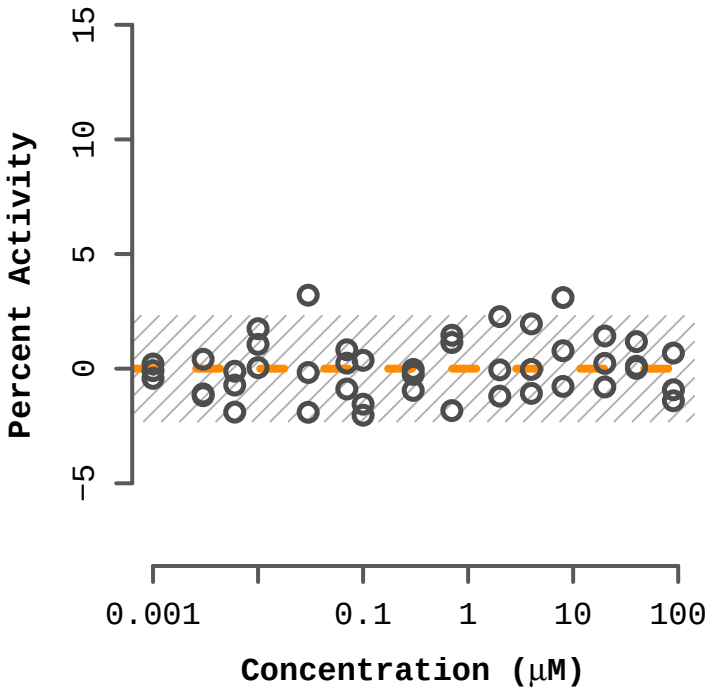
NAME: 2,6-Dimethoxybenzoic acid
CHID: 46999 **CASRN:** 1466-76-8
SPID(S): Tox21_301998
M4ID: 12477135

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

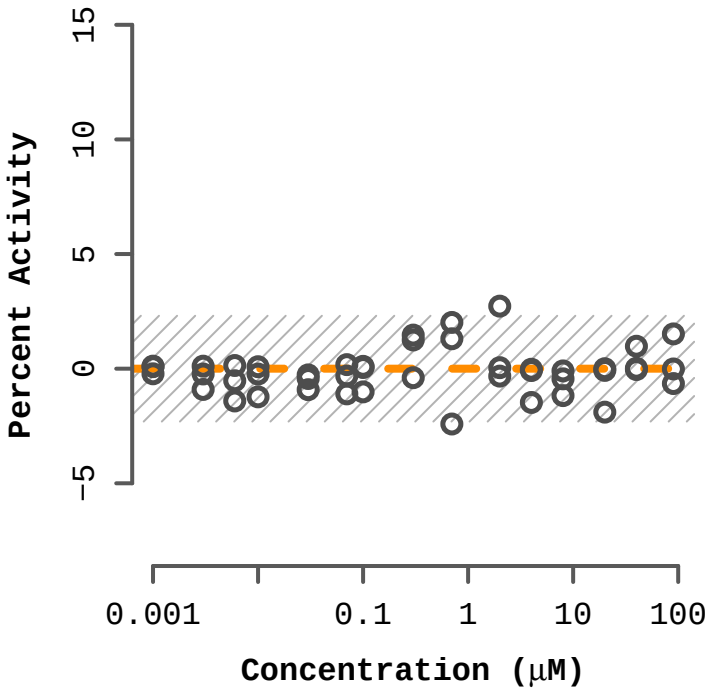
NAME: 1,2-Bis(2-chloroethoxy)ethane
CHID: 47000 **CASRN:** 112-26-5
SPID(S): Tox21_302011
M4ID: 12477122

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

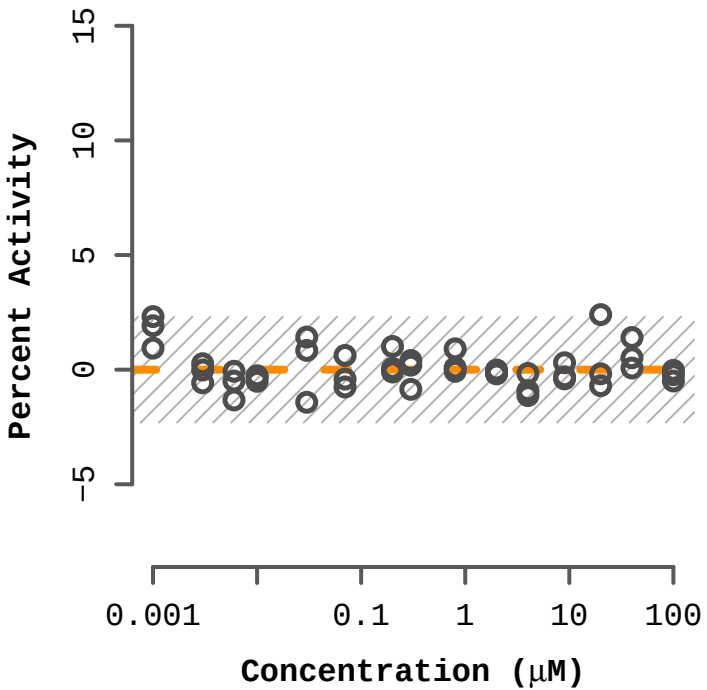
NAME: (2,2−Dimethoxyethyl)benzene
CHID: 47001 **CASRN:** 101−48−4
SPID(S): Tox21_300675
M4ID: 12478458

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.817 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

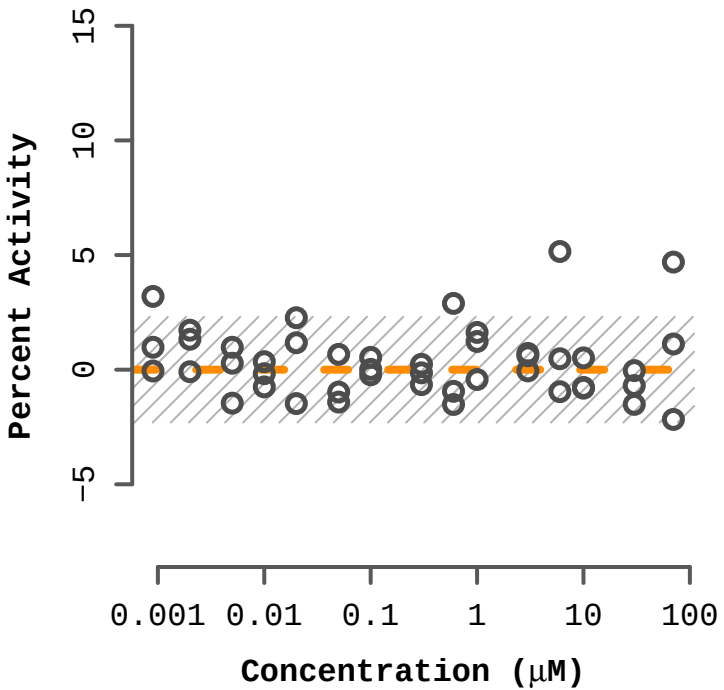
NAME: Potassium perchlorate
CHID: 47003 **CASRN:** 7778-74-7
SPID(S): Tox21_302192
M4ID: 12476941

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

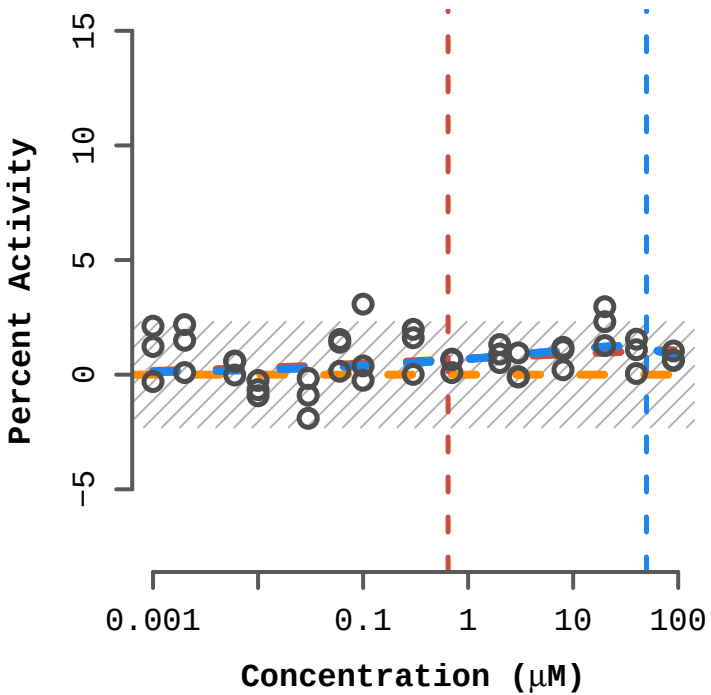
NAME: Glycyrrhizin
CHID: 47006 **CASRN:** 1405-86-3
SPID(S): Tox21_303493
M4ID: 12475648

HILL MODEL: Not applicable.

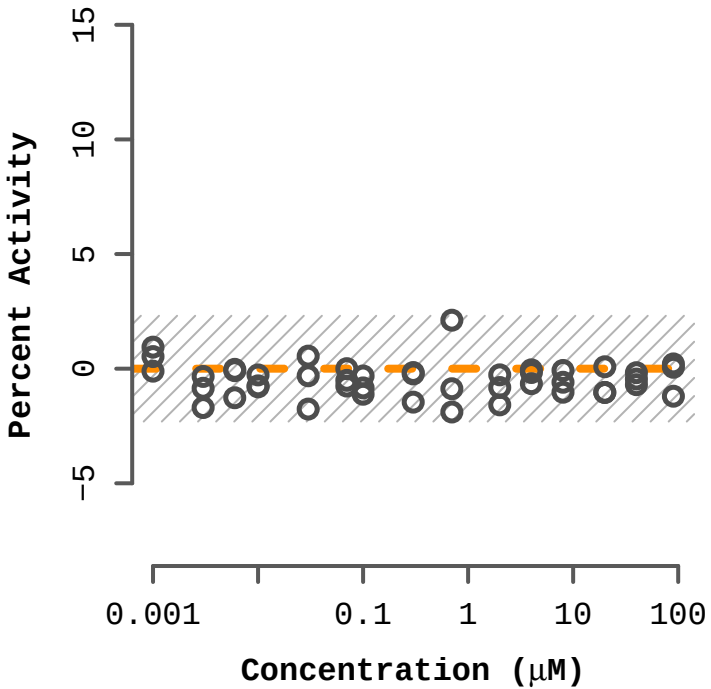
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.33 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ditridecyl phthalate (mixture of branched chai
CHID:    47027   CASRN: 75359-31-8
SPID(S): Tox21_301830
M4ID:    12477303

HILL MODEL (in red):
      tp       ga       gw
val:  1.31     -0.191   0.3
sd:   1.89     4.56     0.808

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.91     1.7      0.3      1.95     2.4
sd:   7.41     6.15     0.283    0.364    2.65

      CNST        HILL        GNLS
AIC:  150.69      135.37      137.99
PROB: 0           0.79        0.21
RMSE: 1.24        0.99        0.98

MAX_MEAN: 2.18      MAX_MED: 2.31      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

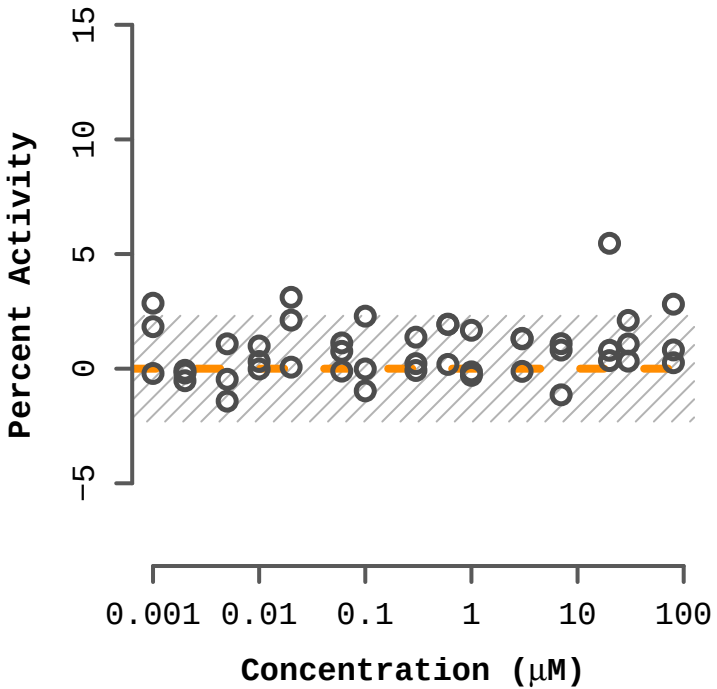
NAME: D−Lactitol monohydrate
CHID: 47028 **CASRN:** 81025−04−9
SPID(S): Tox21_302283
M4ID: 12476850

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.454 **MAX_MED:** 0.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

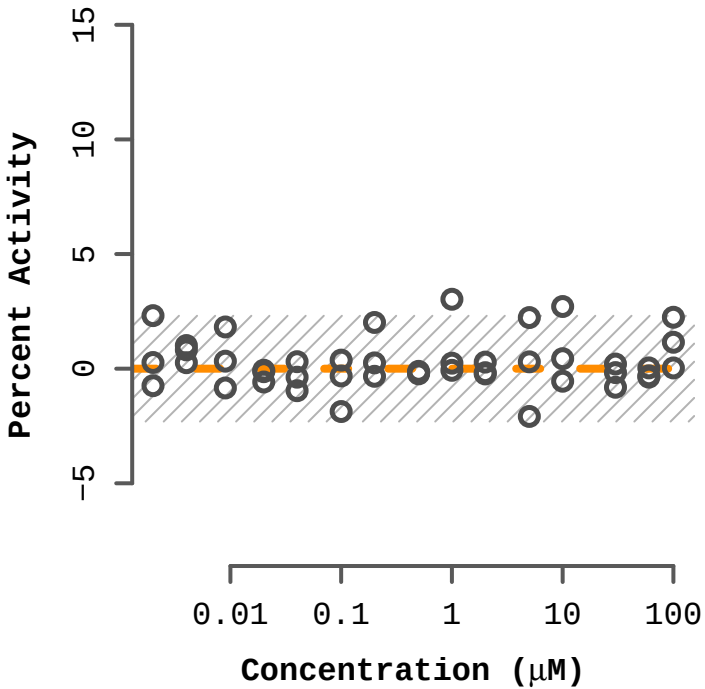
NAME: Tetracosafluorotetradecahydrophenanthrene
CHID: 47029 **CASRN:** 306-91-2
SPID(S): Tox21_302291
M4ID: 12476842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 2.21 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

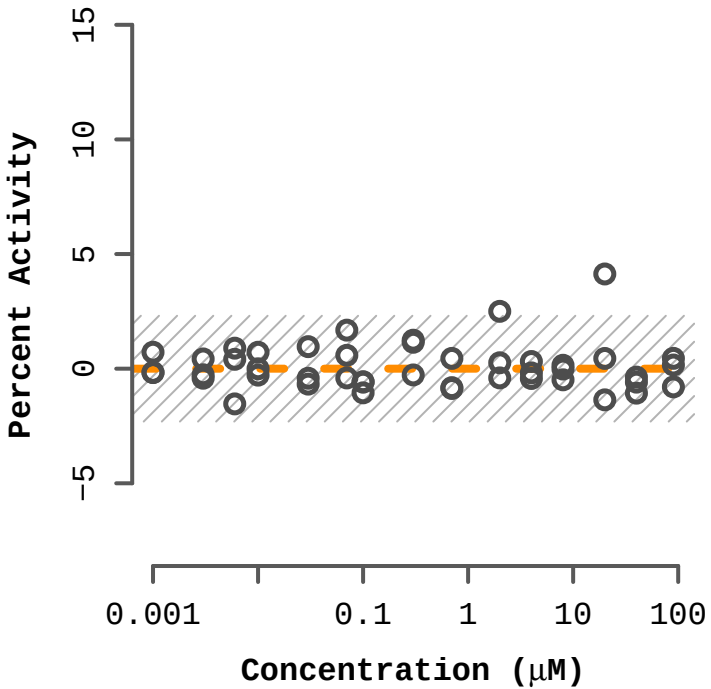
NAME: D−Lactic acid
CHID: 47030 **CASRN:** 10326−41−7
SPID(S): Tox21_300843
M4ID: 12478290

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

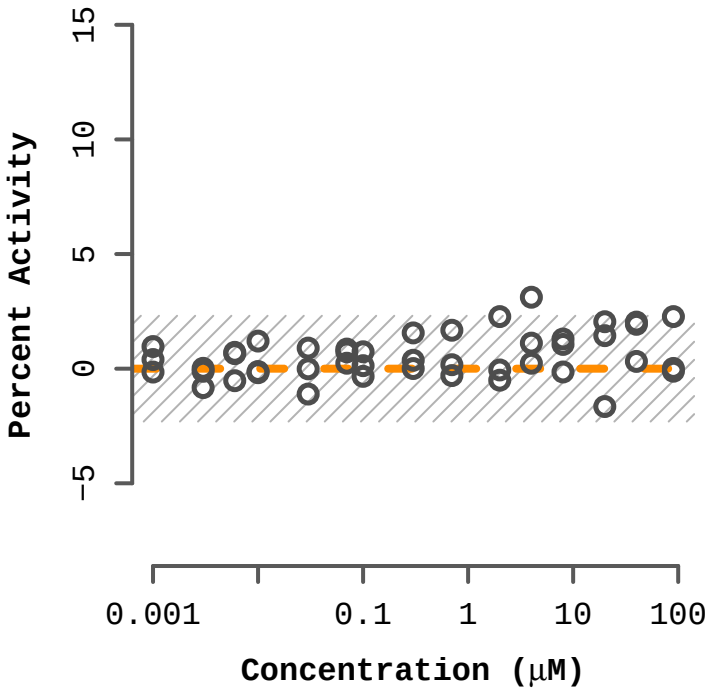
NAME: Tribenzylamine
CHID: 47031 **CASRN:** 620-40-6
SPID(S): Tox21_302339
M4ID: 12476794

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.75	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

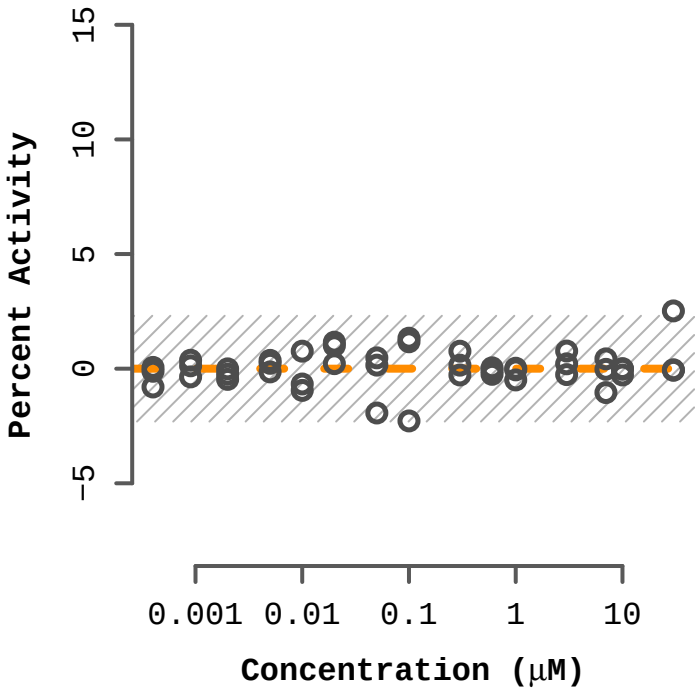
NAME: alpha−Cedrene
CHID: 47032 **CASRN:** 469−61−4
SPID(S): Tox21_302305
M4ID: 12476828

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

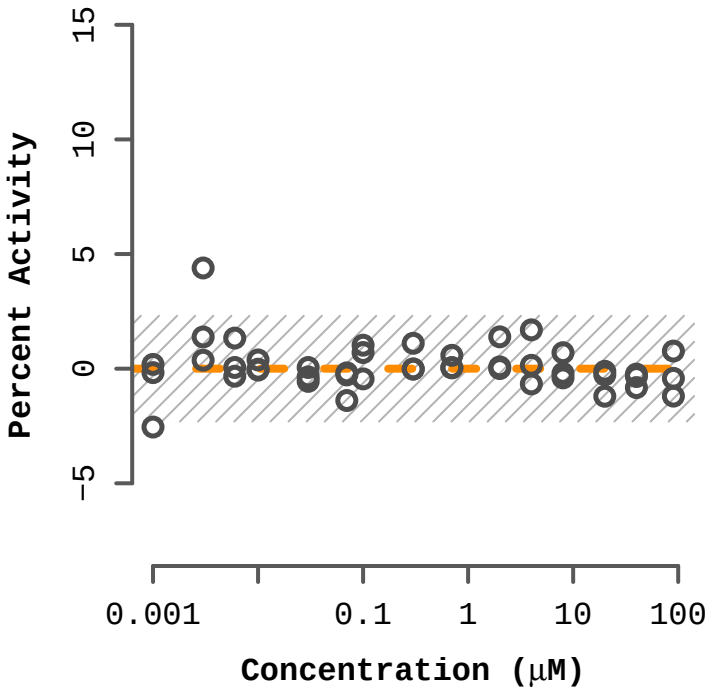
NAME: gamma-Cyclodextrin
CHID: 47033 **CASRN:** 17465-86-0
SPID(S): Tox21_302303
M4ID: 12476830

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

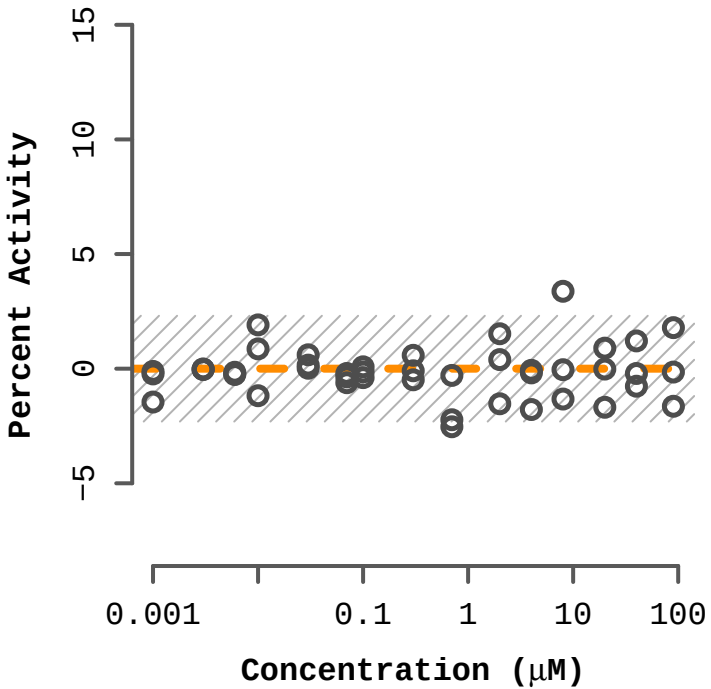
NAME: (2E,6Z)-1,1-diethoxynona-2,6-diene
CHID: 47034 **CASRN:** 67674-36-6
SPID(S): Tox21_302392
M4ID: 12476741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

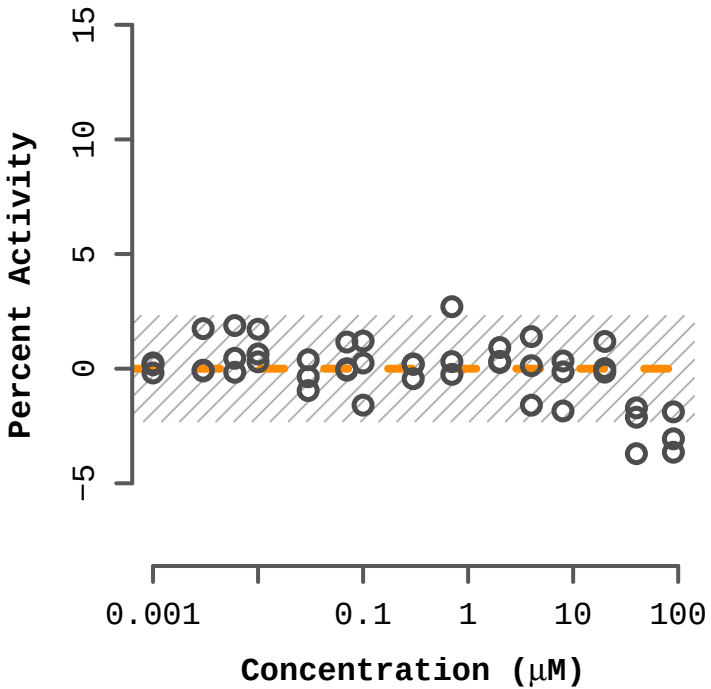
NAME: (2E)-2-Decenal
CHID: 47035 **CASRN:** 3913-81-3
SPID(S): Tox21_302302
M4ID: 12476831

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.671 **MAX_MED:** 0.865 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

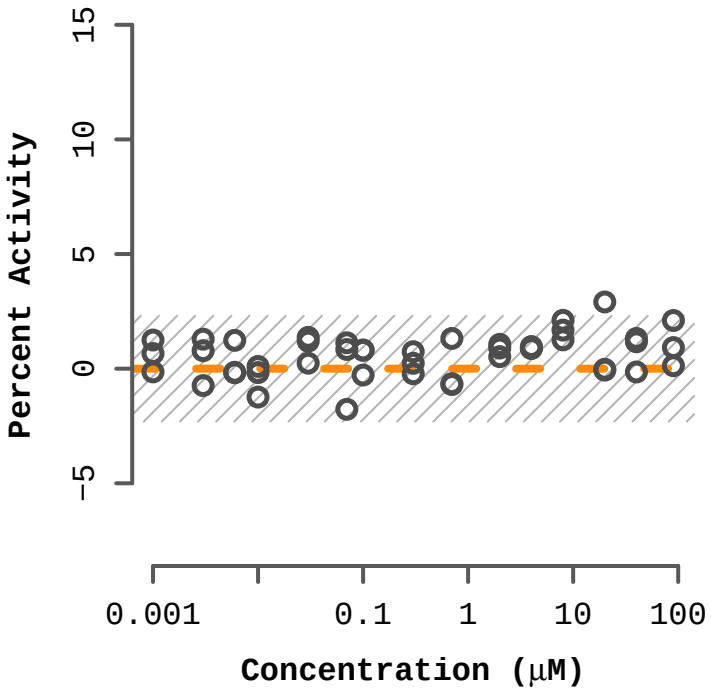
NAME: Thiocyclam oxalate
CHID: 47036 **CASRN:** 31895-22-4
SPID(S): Tox21_302381
M4ID: 12476752

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 0.922 **MAX_MED:** 0.644 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

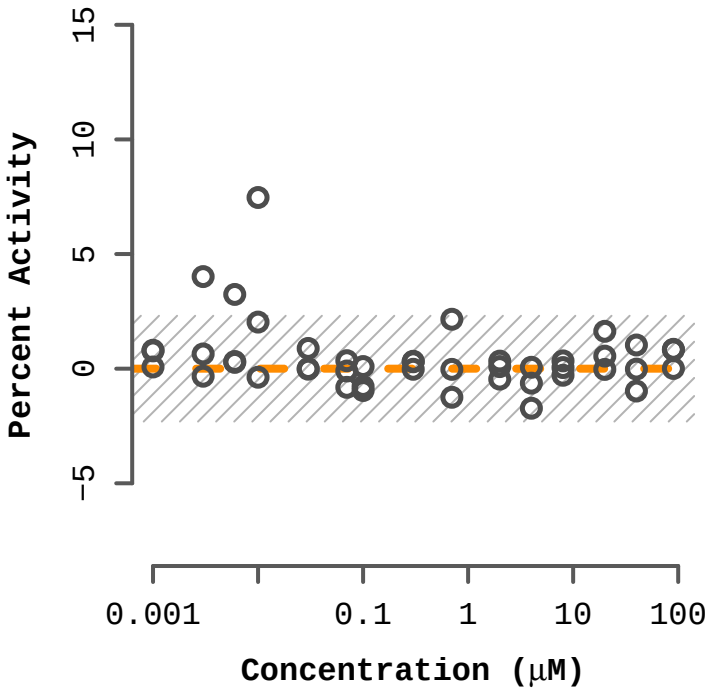
NAME: Tembotrione
CHID: 47037 **CASRN:** 335104-84-2
SPID(S): Tox21_302382
M4ID: 12476751

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

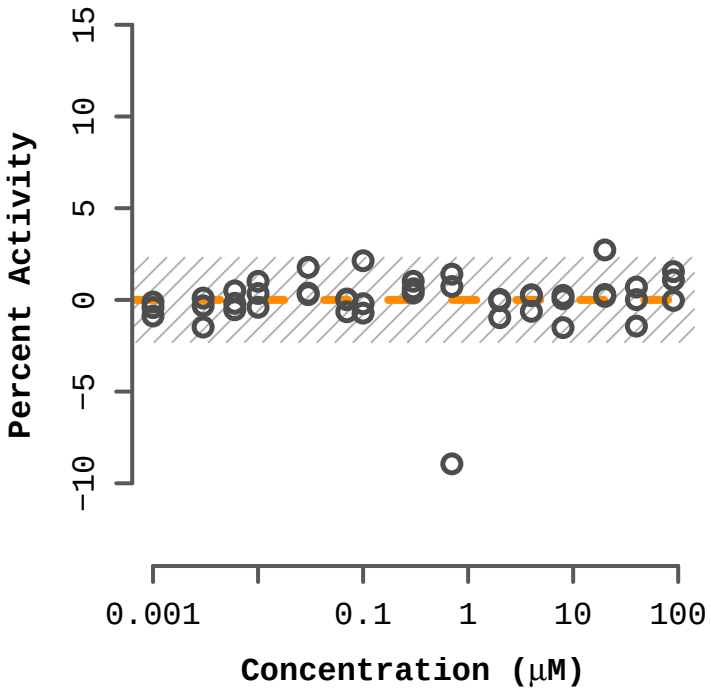
NAME: 4-Ethyl-2-methoxyphenol
CHID: 47038 **CASRN:** 2785-89-9
SPID(S): Tox21_302308
M4ID: 12476825

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 3.04 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

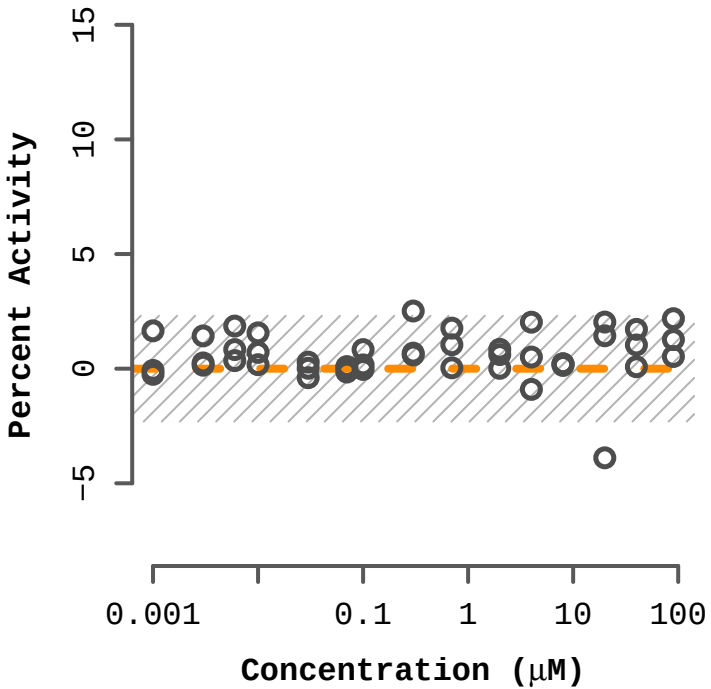
NAME: N-Ethyl-4-menthane-3-carboxamide
CHID: 47039 CASRN: 39711-79-0
SPID(S): Tox21_302336
M4ID: 12476797

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 1.07 MAX_MED: 1.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

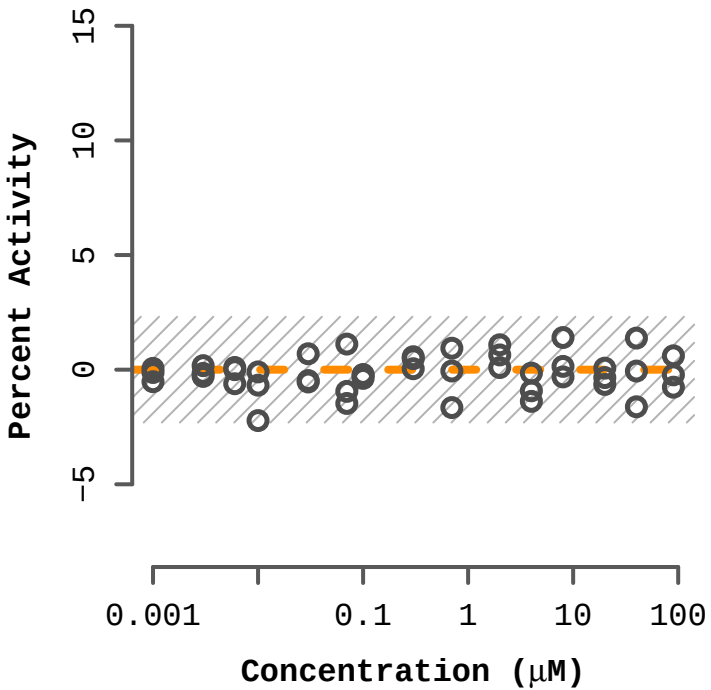
NAME: Zinc neodecanoate
CHID: 47040 **CASRN:** 27253-29-8
SPID(S): Tox21_302394
M4ID: 12476739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

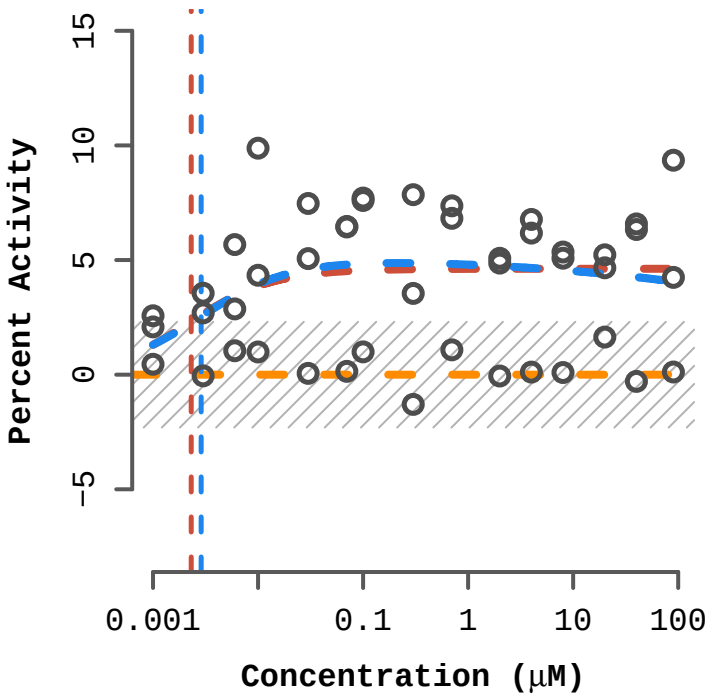
NAME: Alloxydim-sodium
CHID: 47041 **CASRN:** 55635-13-7
SPID(S): Tox21_302387
M4ID: 12476746

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.609 **MAX_MED:** 0.644 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: alpha-Irone
CHID: 47042 CASRN: 79-69-6
SPID(S): Tox21_302306
M4ID: 12476827

HILL MODEL (in red):

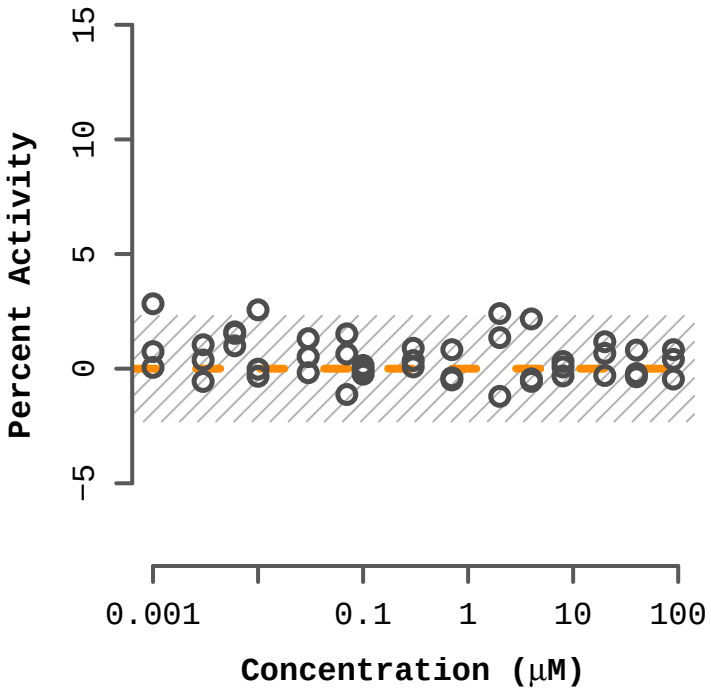
	tp	ga	gw
val:	4.62	−2.64	1.11
sd:	0.586	0.374	0.85

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.15	−2.54	1.01	3.87	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	278.25	236.38	240.08
PROB:	0	0.86	0.14
RMSE:	4.9	2.9	2.9

MAX_MEAN: 5.43 MAX_MED: 7.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

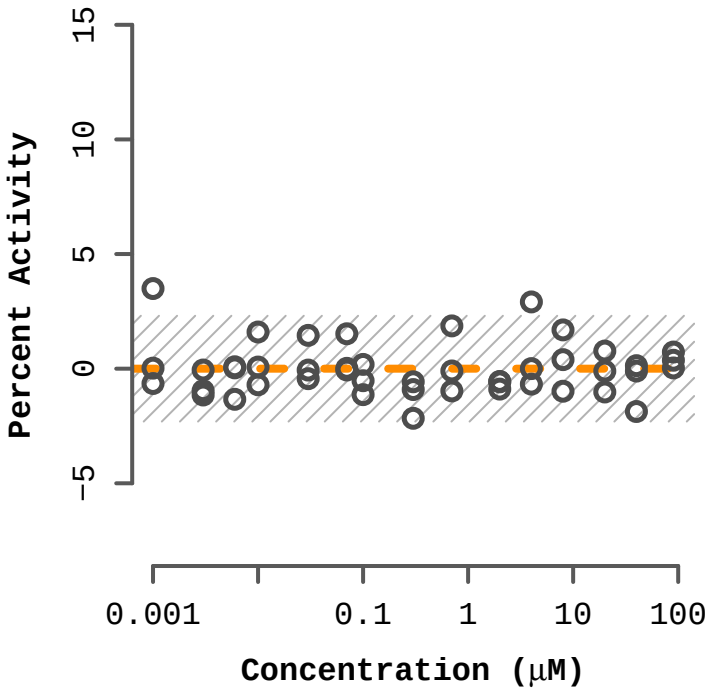
NAME: Potassium tetrathionate
CHID: 47043 **CASRN:** 13932-13-3
SPID(S): Tox21_302315
M4ID: 12476818

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

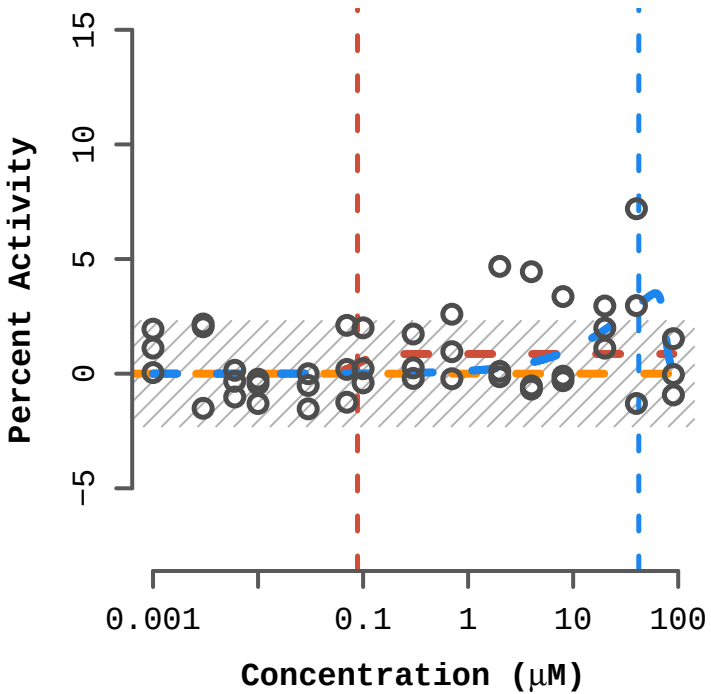
NAME: Ethyl dodecanoate
CHID: 47044 **CASRN:** 106-33-2
SPID(S): Tox21_300967
M4ID: 12478166

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.959 **MAX_MED:** 0.395 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Longifolene
CHID: 47045 CASRN: 475-20-7
SPID(S): Tox21_302307
M4ID: 12476826

HILL MODEL (in red):

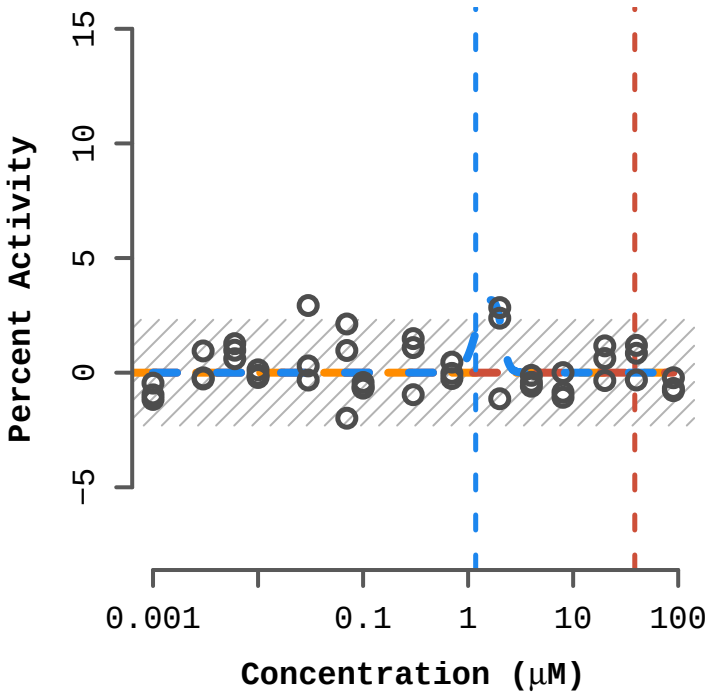
	tp	ga	gw
val:	0.861	-1.05	4.88
sd:	0.37	0.344	13.1

GAIN-LOSS MODEL (in blue):

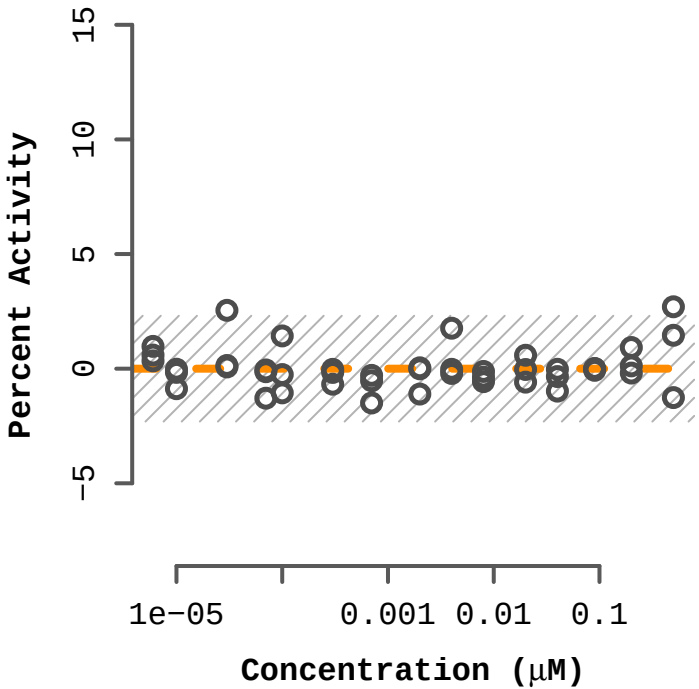
	tp	ga	gw	la	lw
val:	6.05	1.62	1.04	1.87	18
sd:	64	9.87	10.8	0.844	180

	CNST	HILL	GNLS
AIC:	184.28	183.78	184.72
PROB:	0.32	0.42	0.26
RMSE:	1.98	1.75	1.7

MAX_MEAN: 2.96 MAX_MED: 2.97 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Butyl 2-methylbutyrate
CHID:    47046   CASRN: 15706-73-7
SPID(S): Tox21_302310
M4ID:    12476823

HILL MODEL (in red):
      tp       ga       gw
val:  2.45e-10 1.59     1.89
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.52     0.072    7.88     0.322    13.7
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  136.48      142.48      140.84
PROB: 0.86        0.04        0.1
RMSE: 1.09        1.09        1.05

MAX_MEAN: 1.36      MAX_MED: 2.38      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

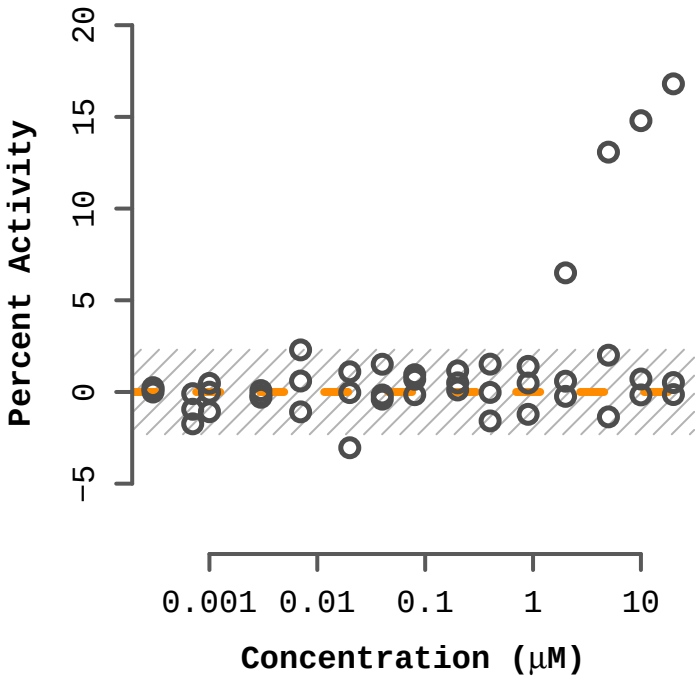
NAME: 5-Methyl-3-heptanone
CHID: 47047 **CASRN:** 541-85-5
SPID(S): Tox21_303912
M4ID: 12475276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

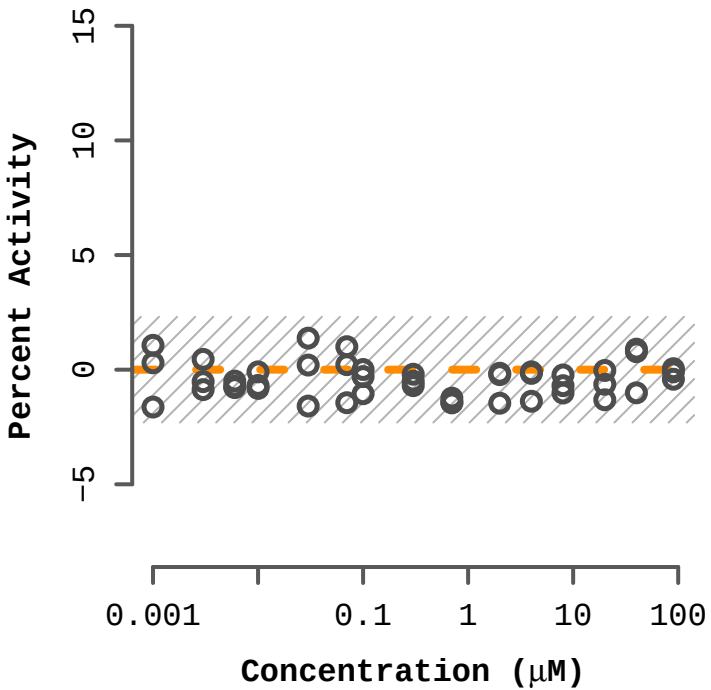
NAME: trans-beta-Farnesene
CHID: 47049 **CASRN:** 18794-84-8
SPID(S): Tox21_303792
M4ID: 12475396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.13	NA	NA
PROB:	1	NA	NA
RMSE:	4.11	NA	NA

MAX_MEAN: 5.73 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

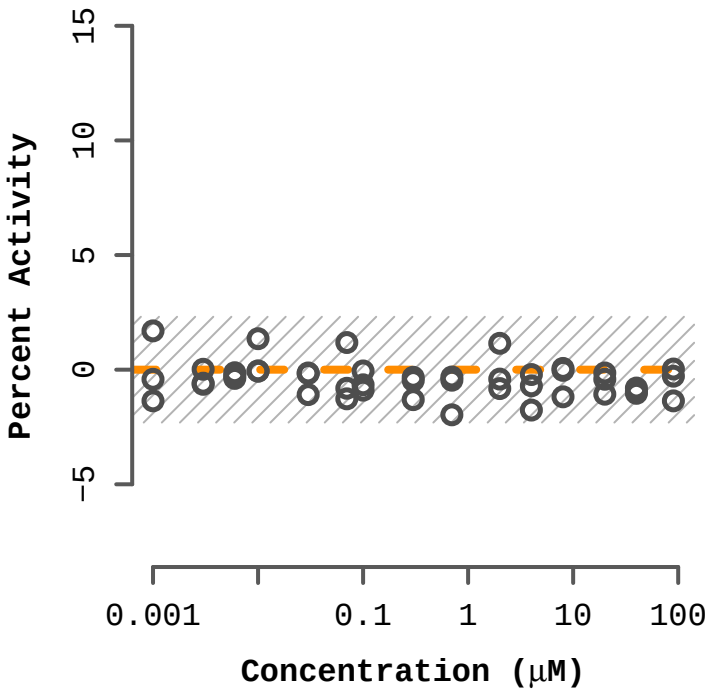
NAME: Nootkatone
CHID: 47050 **CASRN:** 4674-50-4
SPID(S): Tox21_302385
M4ID: 12476748

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.224 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

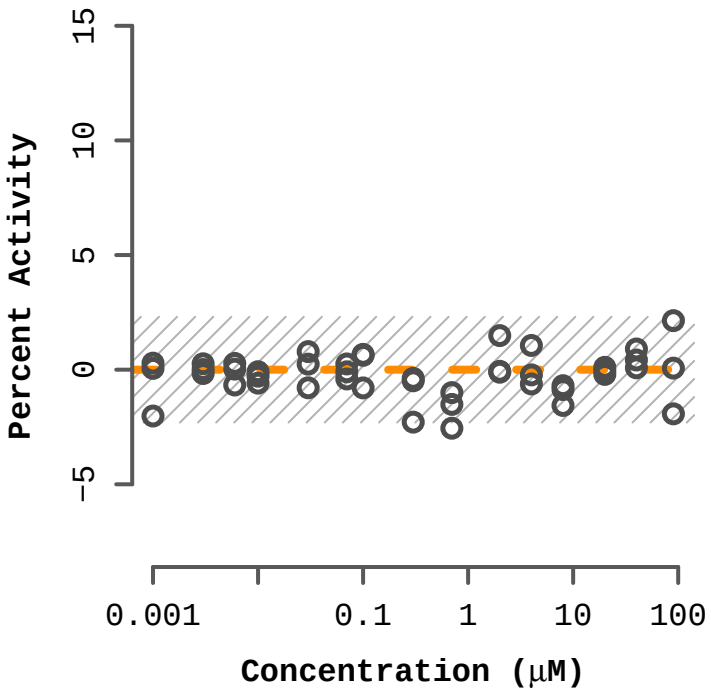
NAME: Ocimene−Limonene mixture
CHID: 47051 **CASRN:** NOCAS_47051
SPID(S): Tox21_302304
M4ID: 12476829

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.412 **MAX_MED:** −0.0284 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

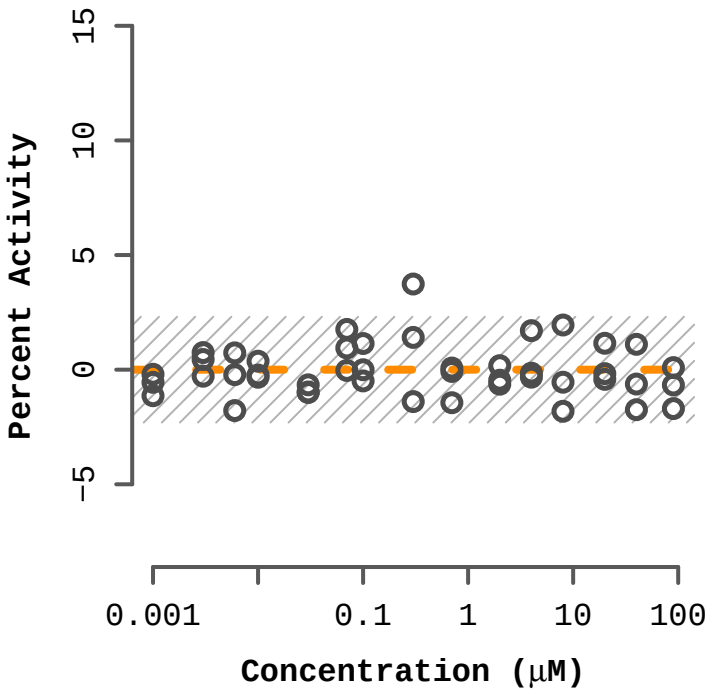
NAME: Valencene
CHID: 47052 **CASRN:** 4630-07-3
SPID(S): Tox21_302397
M4ID: 12476736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.469 **MAX_MED:** 0.627 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

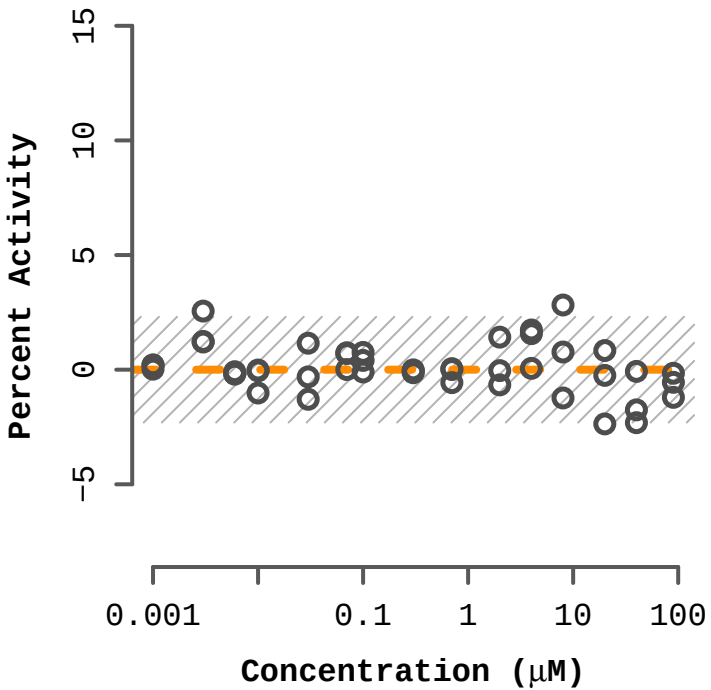
NAME: (R)−alpha−Phellandrene
CHID: 47053 **CASRN:** 4221−98−1
SPID(S): Tox21_302301
M4ID: 12476832

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

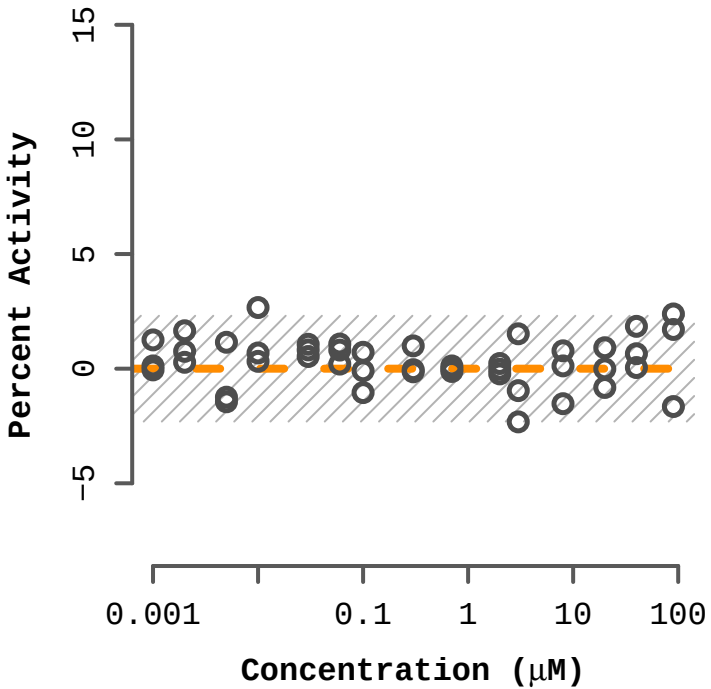
NAME: Theaspirane
CHID: 47055 **CASRN:** 36431-72-8
SPID(S): Tox21_302289
M4ID: 12476844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

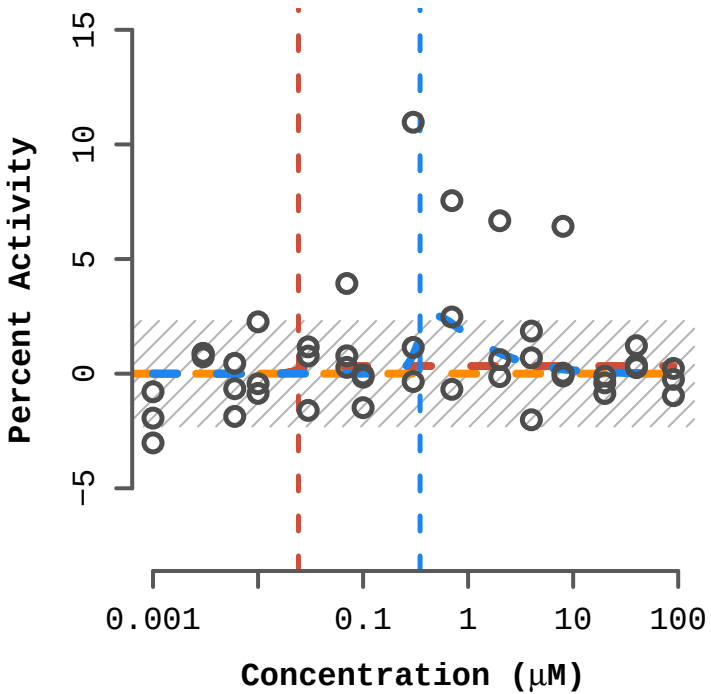
NAME: Tridodecylamine
CHID: 47056 **CASRN:** 102-87-4
SPID(S): Tox21_300664
M4ID: 12478469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl isovalerate
CHID: 47057 CASRN: 108-64-5
SPID(S): Tox21_301194
M4ID: 12477939

HILL MODEL (in red):

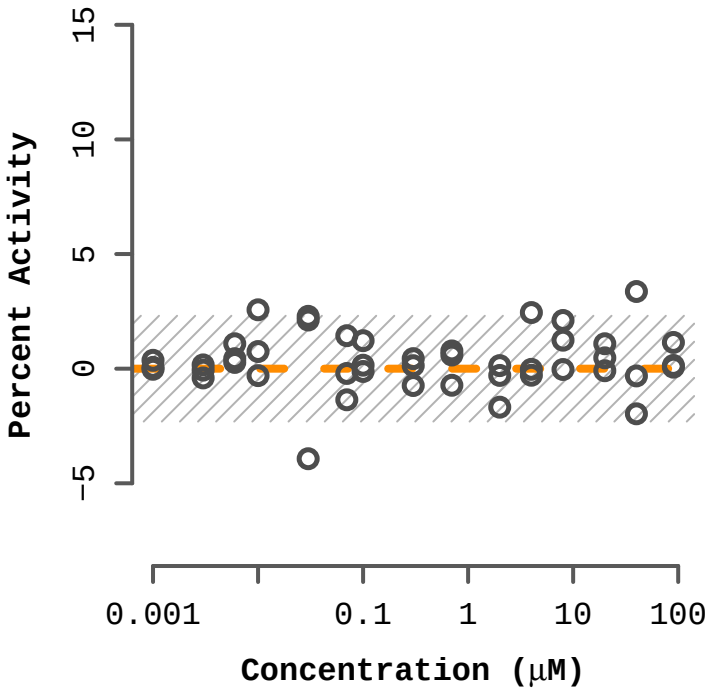
	tp	ga	gw
val:	0.332	−1.62	8
sd:	0.292	2.96	200

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.76	−0.458	7.43	−0.208	1.25
sd:	25.2	0.454	44.2	3.39	2.4

	CNST	HILL	GNLS
AIC:	196.91	201.43	202.71
PROB:	0.86	0.09	0.05
RMSE:	2.72	2.62	2.47

MAX_MEAN: 3.93 **MAX_MED:** 2.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

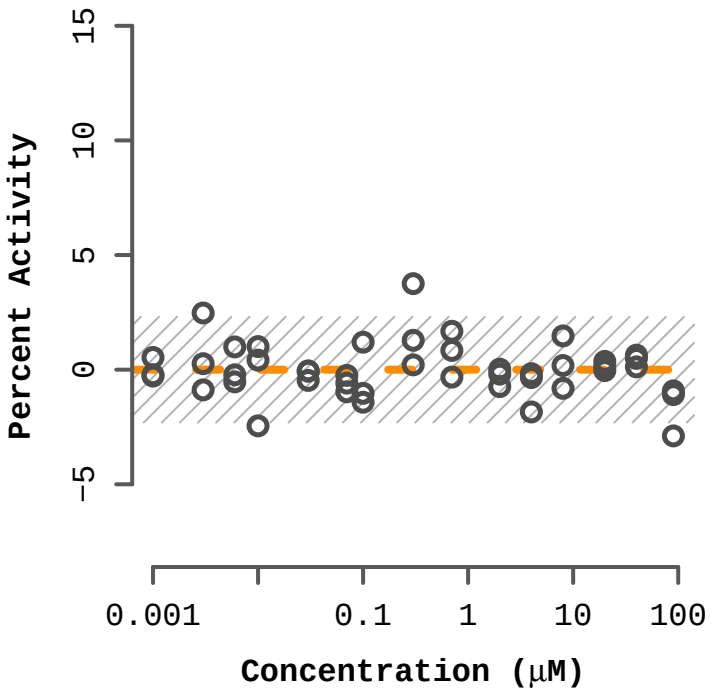
NAME: Ethyl levulinate
CHID: 47058 **CASRN:** 539-88-8
SPID(S): Tox21_302292
M4ID: 12476841

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

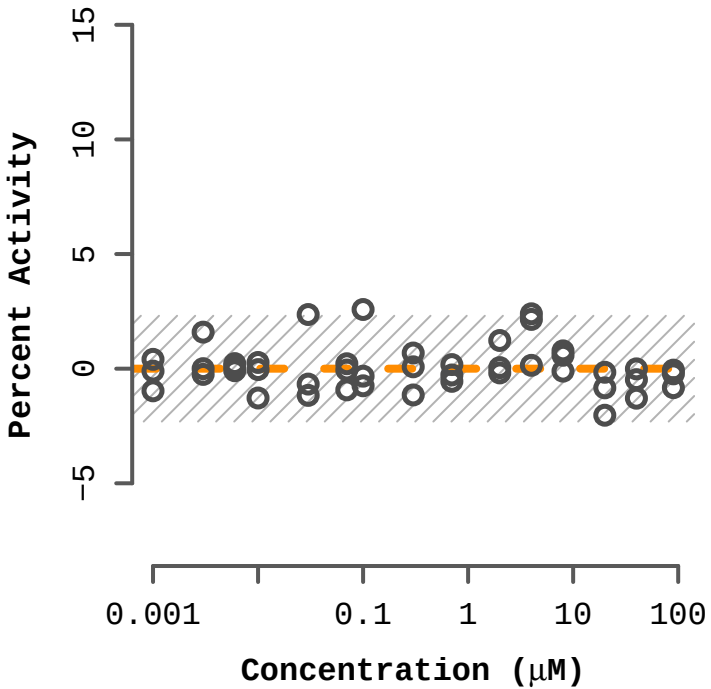
NAME: Butyrophenone
CHID: 47059 **CASRN:** 495-40-9
SPID(S): Tox21_302345
M4ID: 12476788

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

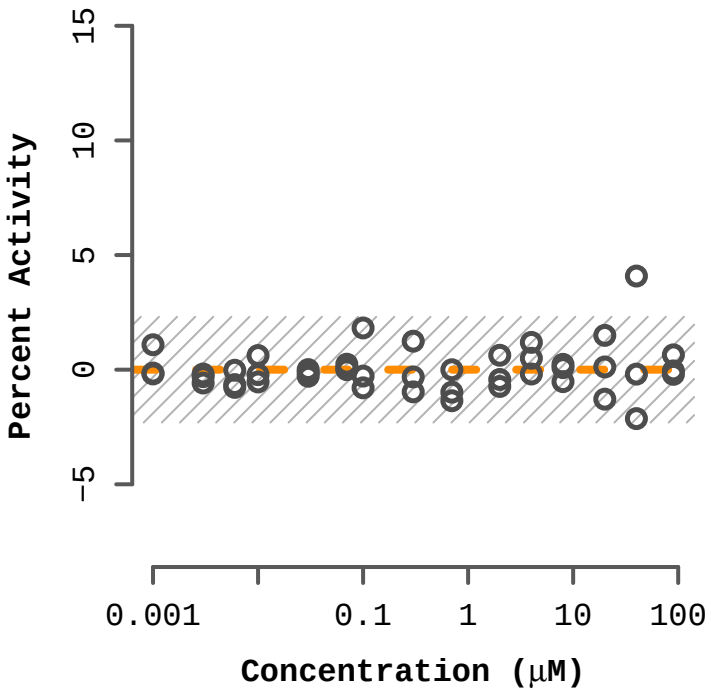
NAME: 1,3−Dimethoxybenzene
CHID: 47060 **CASRN:** 151−10−0
SPID(S): Tox21_302348
M4ID: 12476785

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

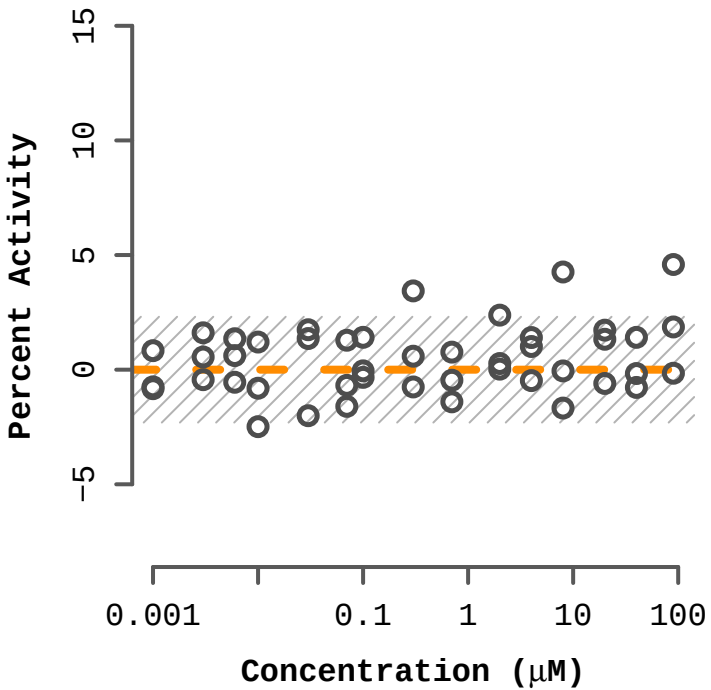
NAME: Heptadecane
CHID: 47061 CASRN: 629-78-7
SPID(S): Tox21_302278
M4ID: 12476855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.587 MAX_MED: 0.499 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

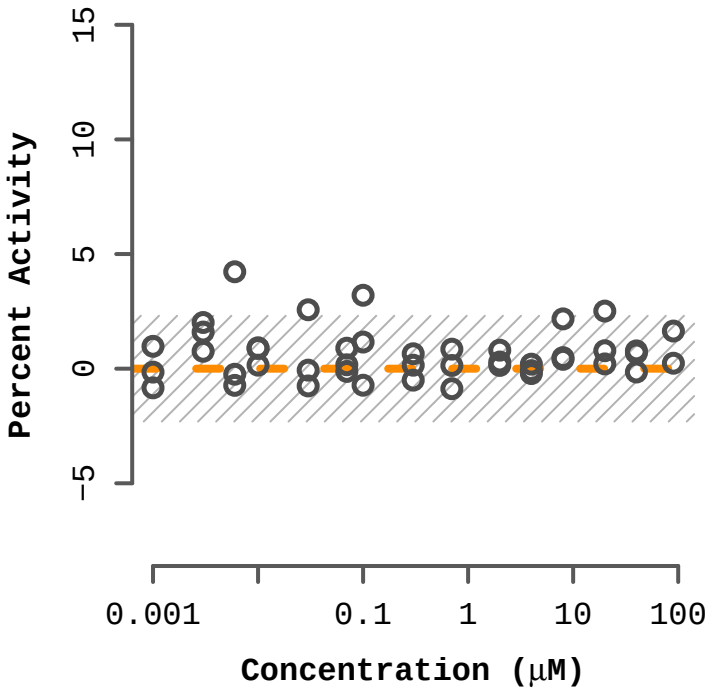
NAME: (E)−2−Hexen−1−ol
CHID: 47062 **CASRN:** 928−95−0
SPID(S): Tox21_301839
M4ID: 12477294

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

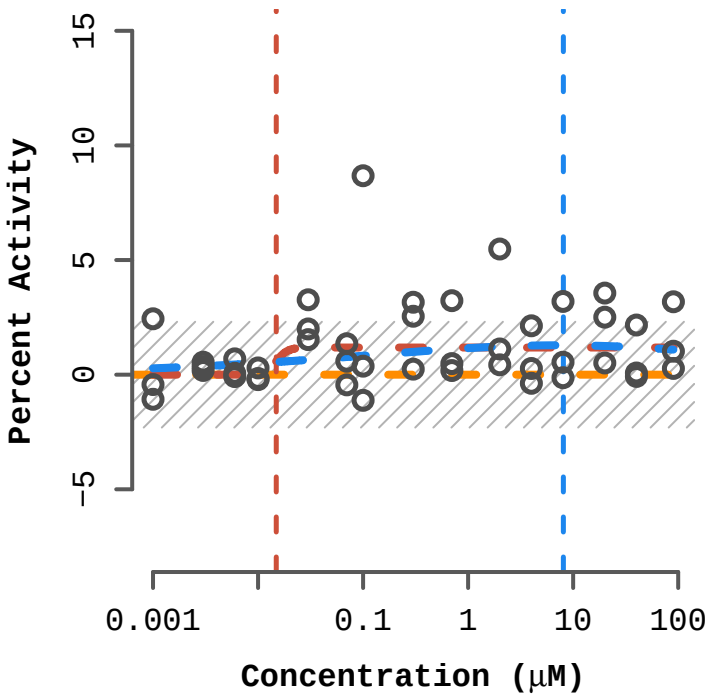
NAME: Hydrocinnamic acid
CHID: 47064 **CASRN:** 501-52-0
SPID(S): Tox21_302329
M4ID: 12476804

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2−Dimethoxybenzene
CHID: 47065 CASRN: 91−16−7
SPID(S): Tox21_302297
M4ID: 12476836

HILL MODEL (in red):

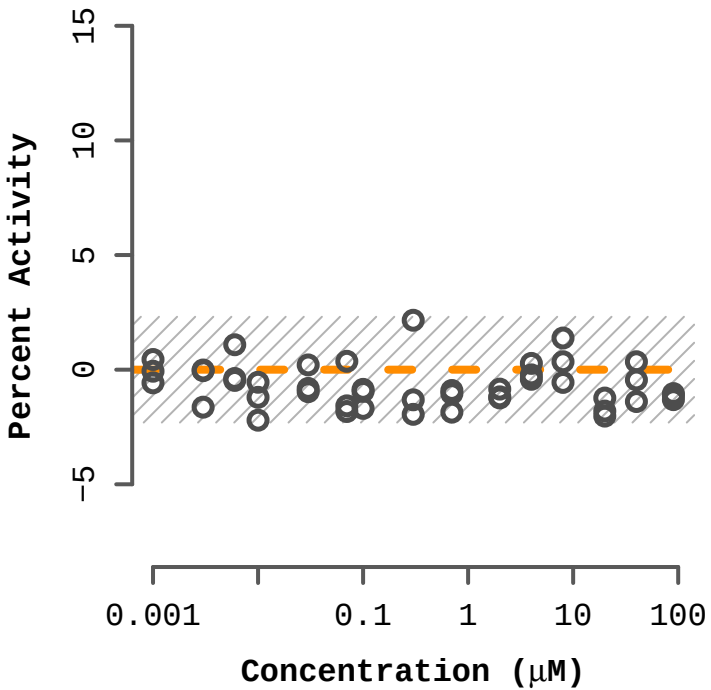
	tp	ga	gw
val:	1.18	−1.83	8
sd:	0.268	0.367	12.9

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.67	0.907	0.303	1.16	0.344
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	188.75	174.78	180.91
PROB:	0	0.95	0.04
RMSE:	2.18	1.74	1.79

MAX_MEAN: 2.64 MAX_MED: 2.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

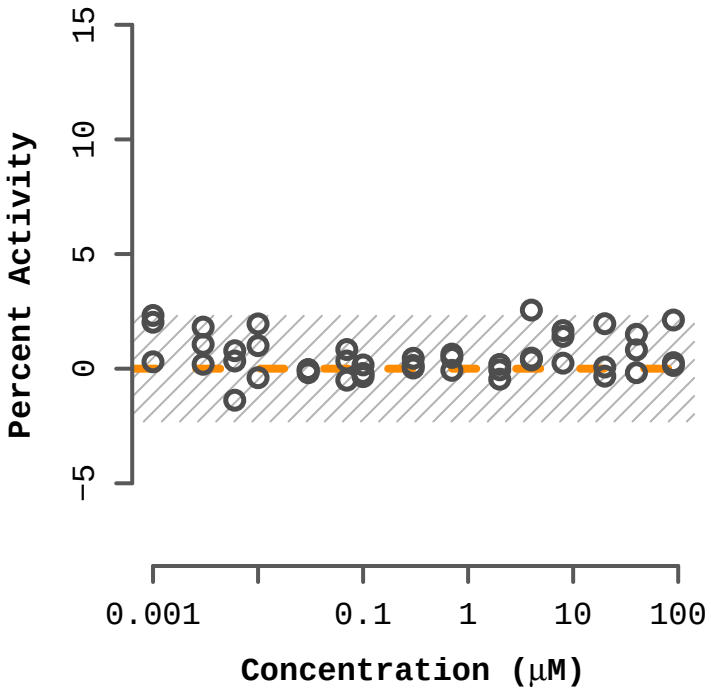
NAME: 2,3-Hexanedione
CHID: 47066 **CASRN:** 3848-24-6
SPID(S): Tox21_302349
M4ID: 12476784

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.392 **MAX_MED:** 0.348 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

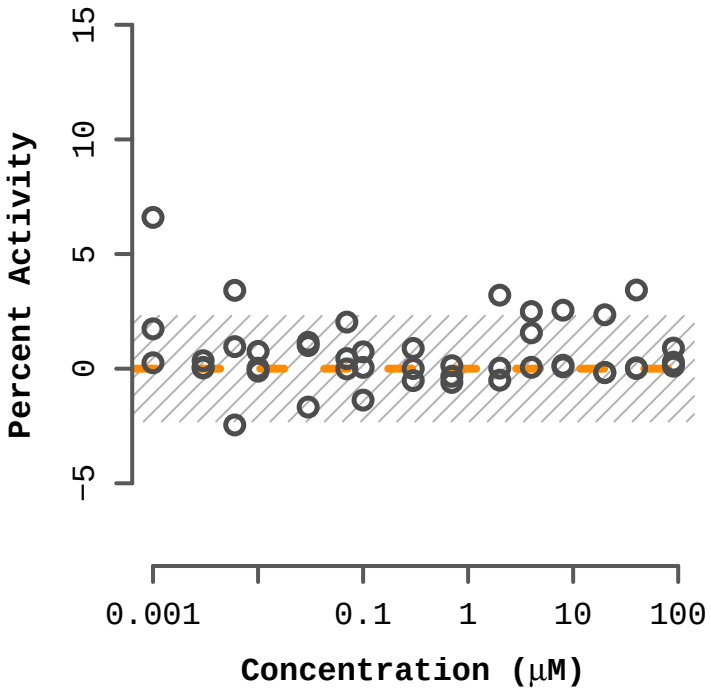
NAME: Lepidine
CHID: 47067 CASRN: 491-35-0
SPID(S): Tox21_301829
M4ID: 12477304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

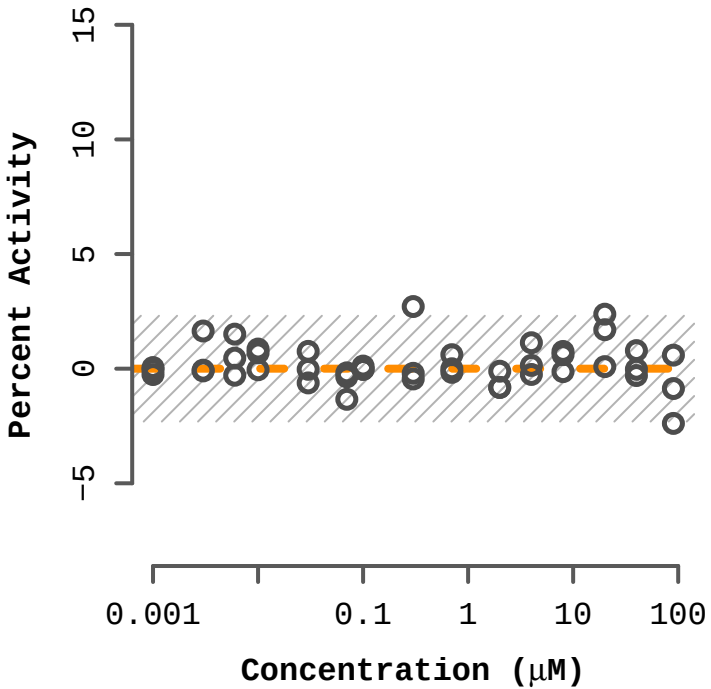
NAME: cis-3,7-Dimethyl-2,6-octadien-1-yl acetate
CHID: 47068 **CASRN:** 141-12-8
SPID(S): Tox21_301974
M4ID: 12477159

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 2.87 **MAX_MED:** 1.74 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

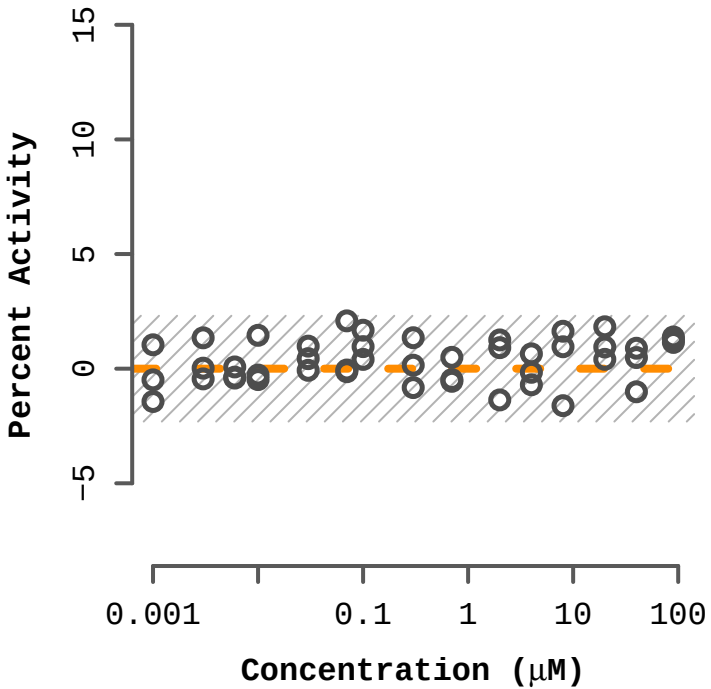
NAME: Tetramethylpyrazine
CHID: 47070 **CASRN:** 1124-11-4
SPID(S): Tox21_302313
M4ID: 12476820

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

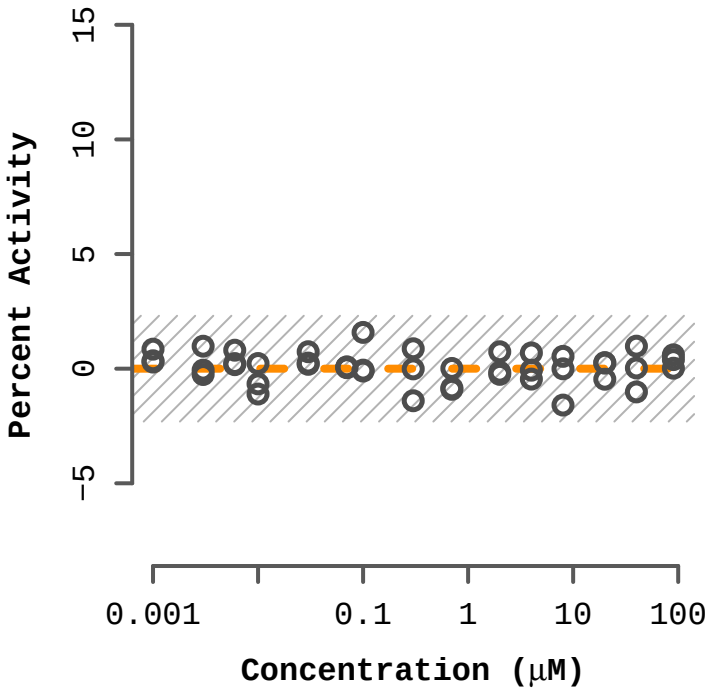
NAME: 2-Methylphenethyl alcohol
CHID: 47071 CASRN: 19819-98-8
SPID(S): Tox21_302287
M4ID: 12476846

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.27 MAX_MED: 1.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

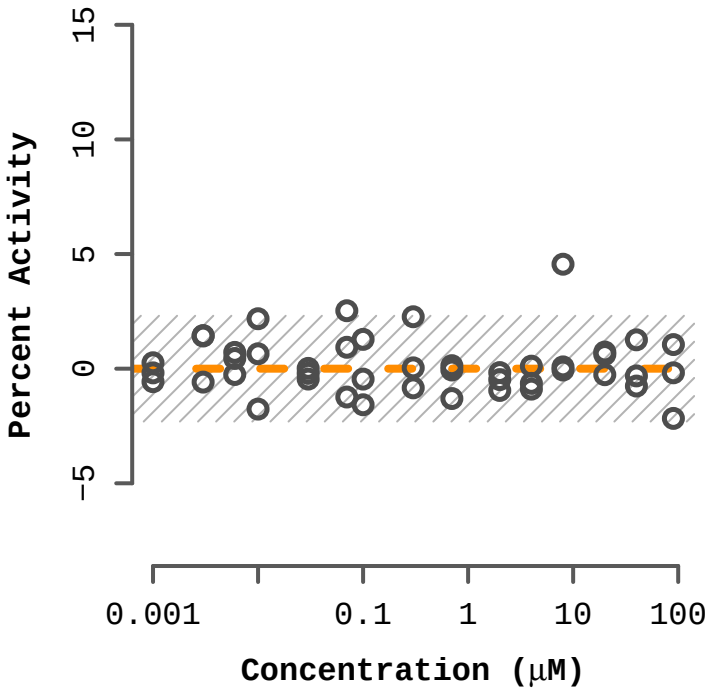
NAME: 3,5,5-Trimethyl-2-cyclohexen-1-ol
CHID: 47072 **CASRN:** 470-99-5
SPID(S): Tox21_302344
M4ID: 12476789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	91.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.496 **MAX_MED:** 0.397 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

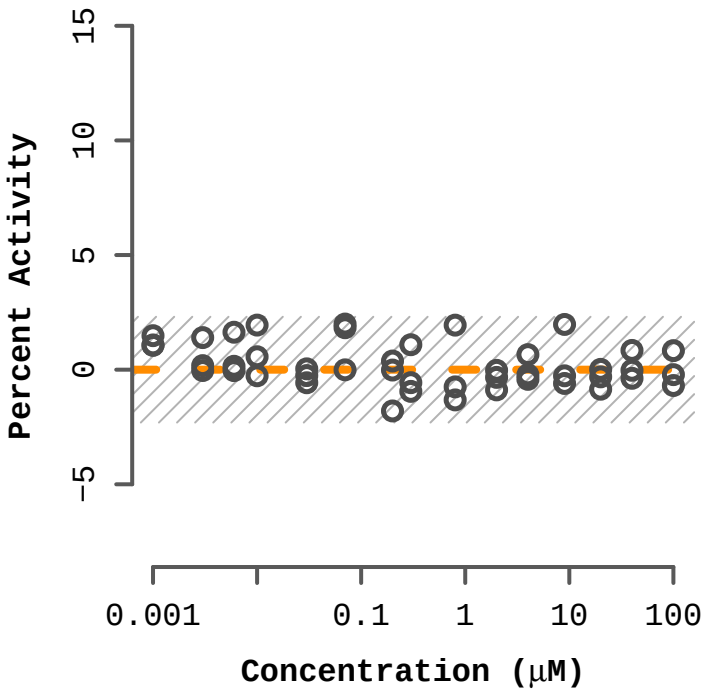
NAME: Isobutyl benzoate
CHID: 47074 **CASRN:** 120-50-3
SPID(S): Tox21_302327
M4ID: 12476806

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

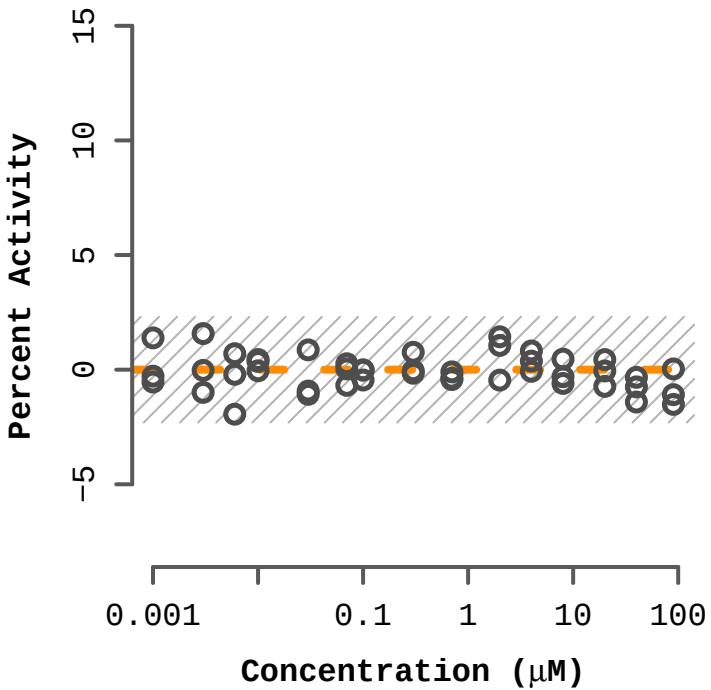
NAME: 2,3,5-Trimethylpyrazine
CHID: 47075 **CASRN:** 14667-55-1
SPID(S): Tox21_302314
M4ID: 12476819

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

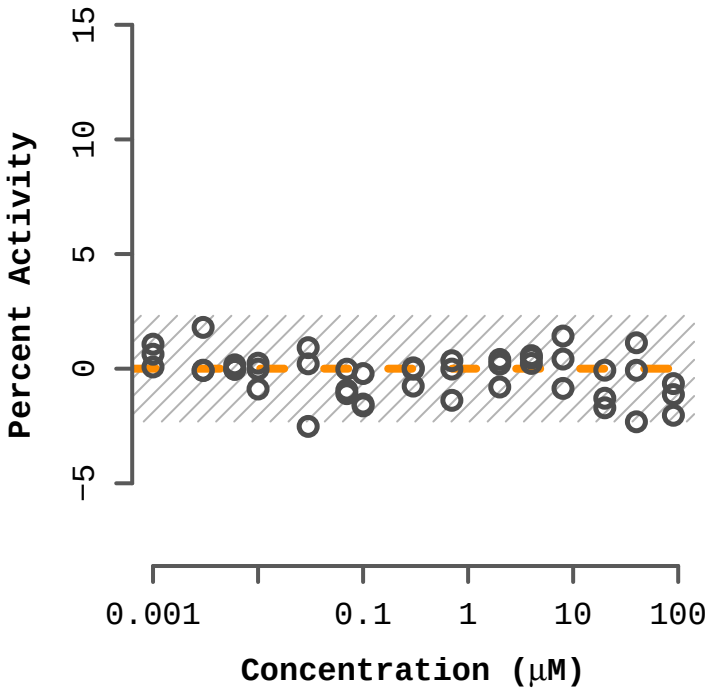
NAME: (S)−Limonene
CHID: 47078 **CASRN:** 5989−54−8
SPID(S): Tox21_302295
M4ID: 12476838

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.681 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

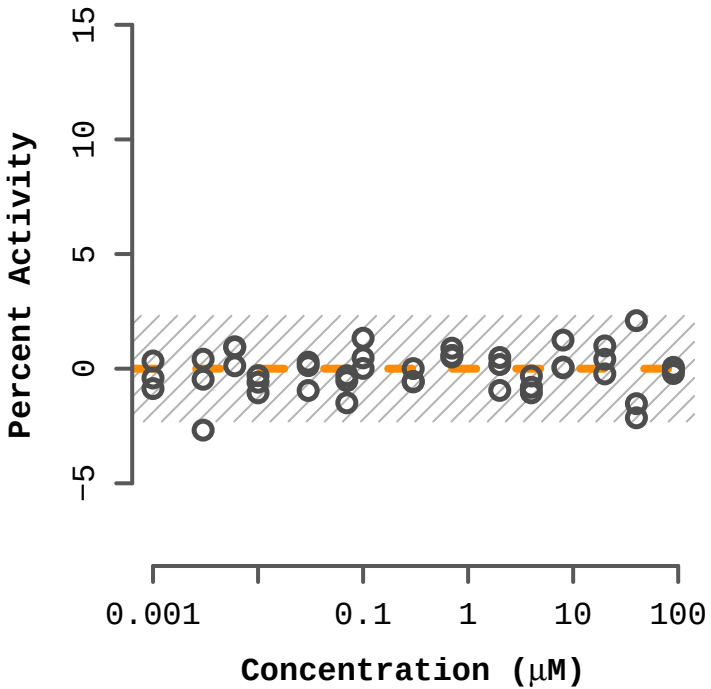
NAME: 4-Ethylbenzaldehyde
CHID: 47080 **CASRN:** 4748-78-1
SPID(S): Tox21_302332
M4ID: 12476801

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.12	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.593 **MAX_MED:** 0.632 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

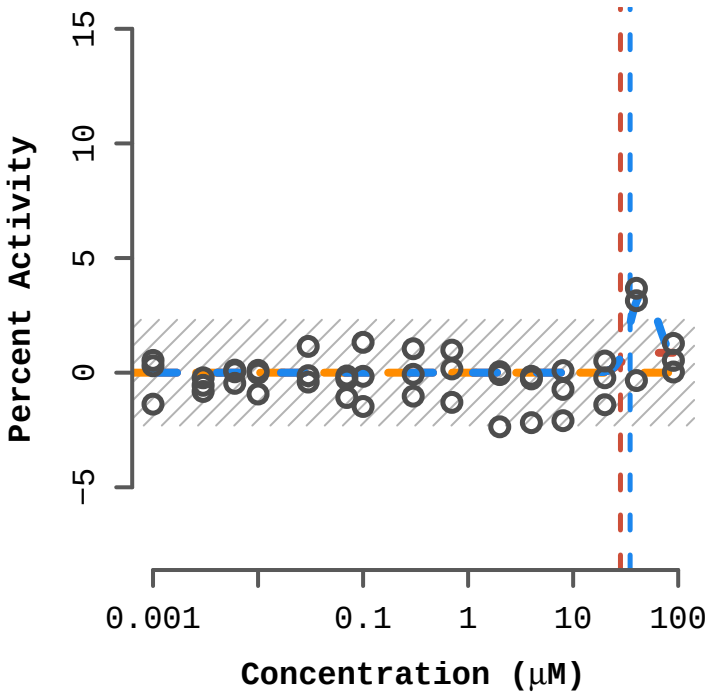
NAME: 2-tert-Butylcyclohexanone
CHID: 47081 **CASRN:** 1728-46-7
SPID(S): Tox21_302281
M4ID: 12476852

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.67 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-sec-Butyl-3-methoxypyrazine
CHID: 47082 CASRN: 24168-70-5
SPID(S): Tox21_301823
M4ID: 12477310

HILL MODEL (in red):

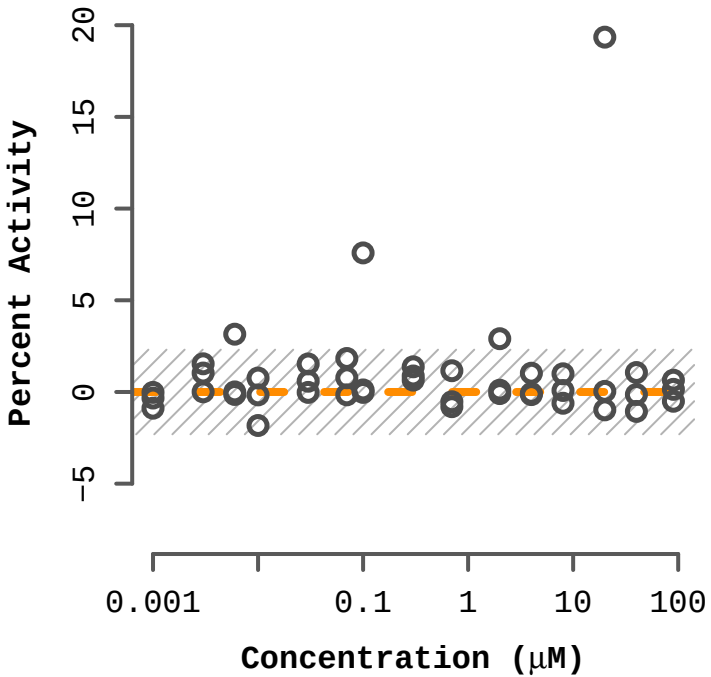
	tp	ga	gw
val:	0.867	1.45	8
sd:	0.509	0.16	8.69

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.42	1.54	8	1.81	5.53
sd:	5.03	0.191	6.95	0.327	10.6

	CNST	HILL	GNLS
AIC:	136.18	138.67	136.2
PROB:	0.44	0.13	0.43
RMSE:	1.14	1.05	1.02

MAX_MEAN: 2.16 MAX_MED: 3.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

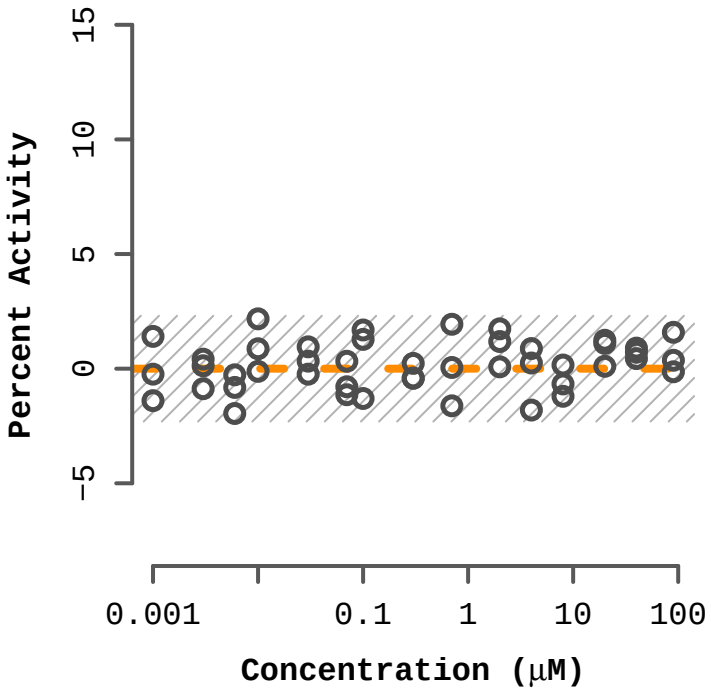
NAME: Methyl butyrate
CHID: 47083 CASRN: 623-42-7
SPID(S): Tox21_301821
M4ID: 12477312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.87	NA	NA
PROB:	1	NA	NA
RMSE:	3.26	NA	NA

MAX_MEAN: 6.14 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

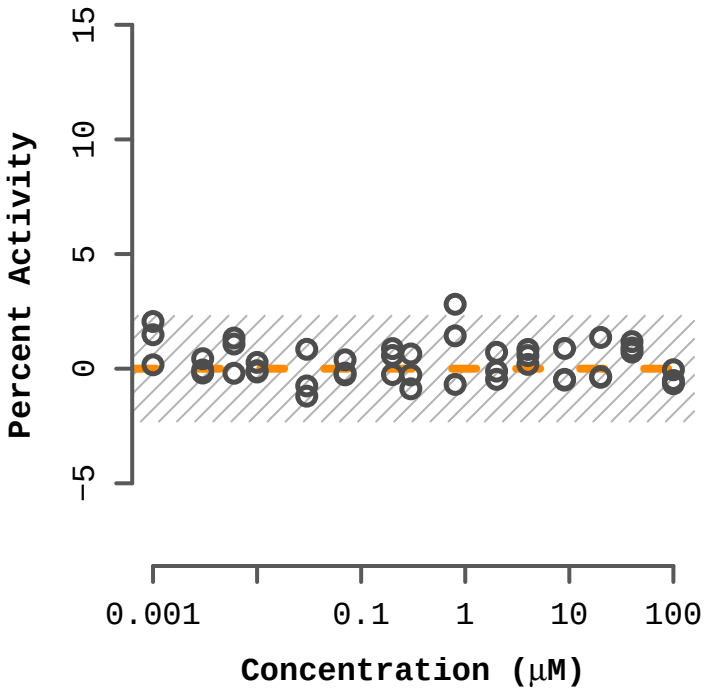
NAME: 2-Acetylpyrrole
CHID: 47084 **CASRN:** 1072-83-9
SPID(S): Tox21_300952
M4ID: 12478181

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

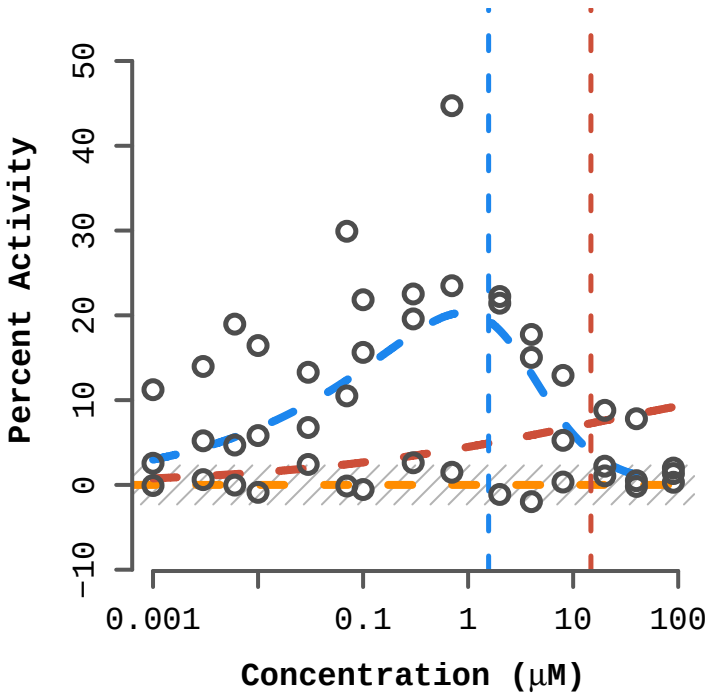
NAME: Acetylpyrazine
CHID: 47085 **CASRN:** 22047-25-2
SPID(S): Tox21_302309
M4ID: 12476824

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (E)−2−Nonenal
CHID: 47086 CASRN: 18829−56−6
SPID(S): Tox21_300815
M4ID: 12478318

HILL MODEL (in red):

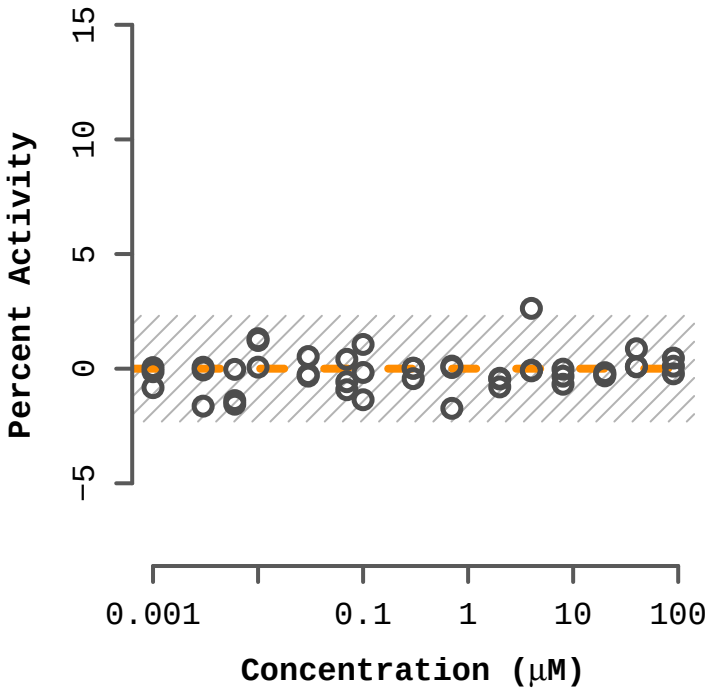
	tp	ga	gw
val:	14.5	1.17	0.3
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	53.5	0.195	0.385	0.496	1.39
sd:	73.1	2.54	0.194	0.333	0.659

	CNST	HILL	GNLS
AIC:	361.35	356.7	332.45
PROB:	0	0	1
RMSE:	13.58	11.94	8.7

MAX_MEAN: 23.2 MAX_MED: 23.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

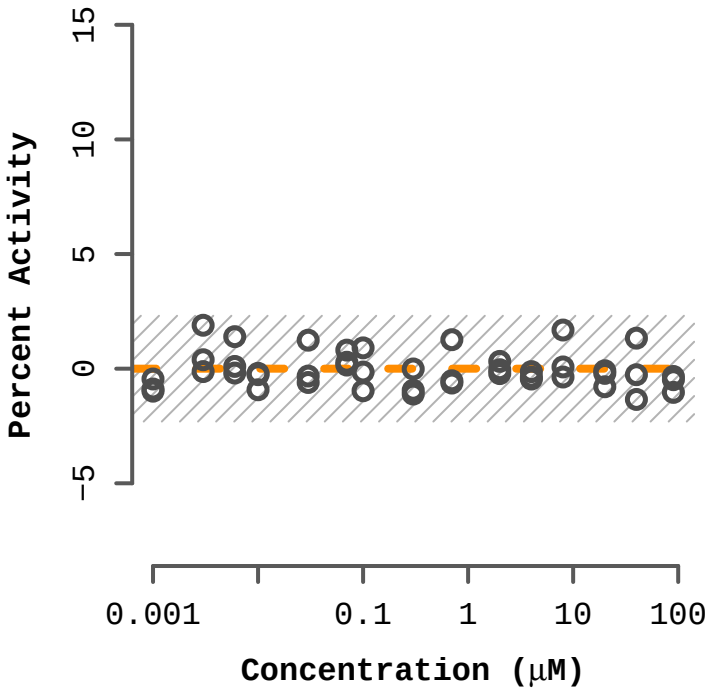
NAME: Methyl 2-methoxybenzoate
CHID: 47087 CASRN: 606-45-1
SPID(S): Tox21_302334
M4ID: 12476799

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.869 MAX_MED: 1.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

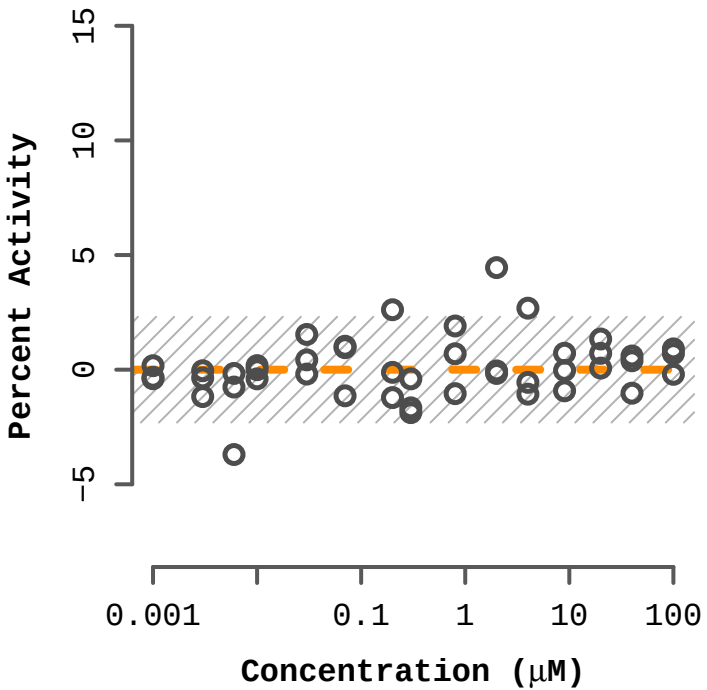
NAME: 2,6,6-Trimethyl-1-cyclohexene-1-acetaldehyde
CHID: 47088 **CASRN:** 472-66-2
SPID(S): Tox21_302284
M4ID: 12476849

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.721 **MAX_MED:** 0.392 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

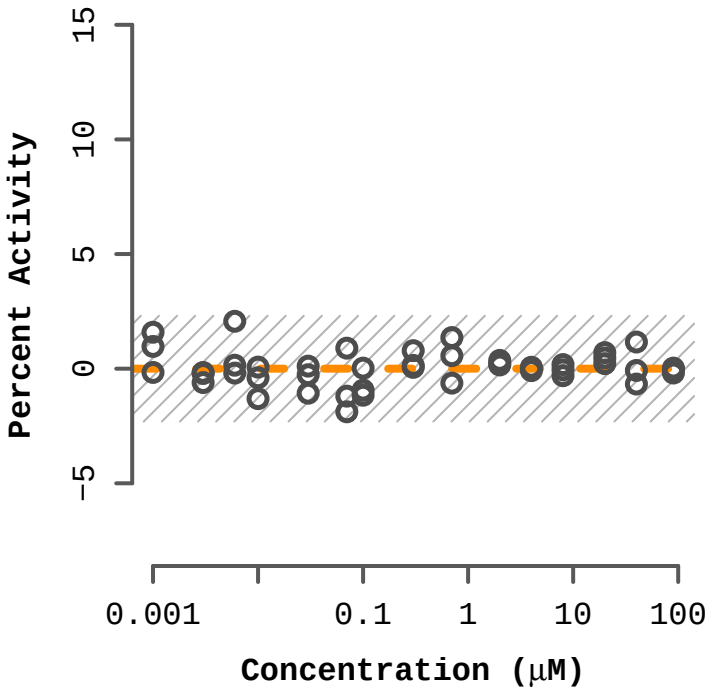
NAME: 2,3-Butanedithiol
CHID: 47089 **CASRN:** 4532-64-3
SPID(S): Tox21_301822
M4ID: 12477311

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 0.962 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

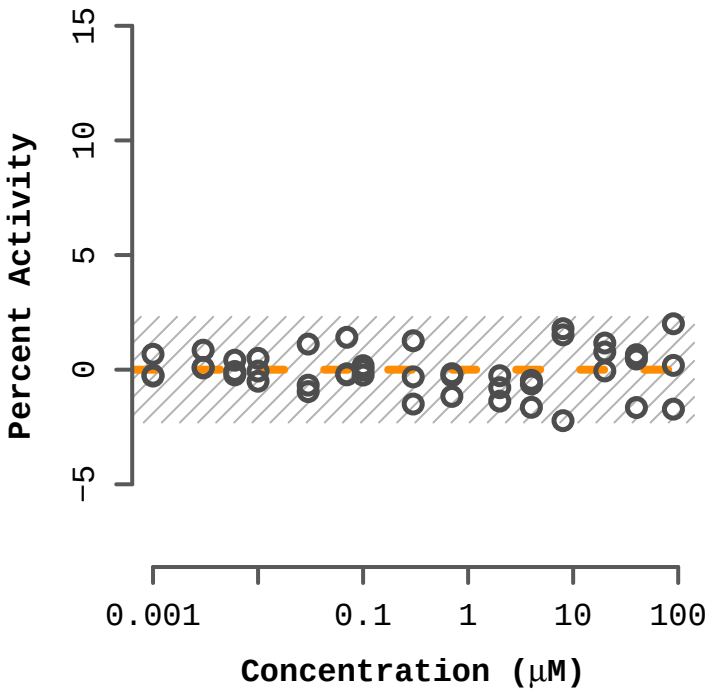
NAME: 5-Methylquinoxaline
CHID: 47090 **CASRN:** 13708-12-8
SPID(S): Tox21_302282
M4ID: 12476851

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.799 **MAX_MED:** 0.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

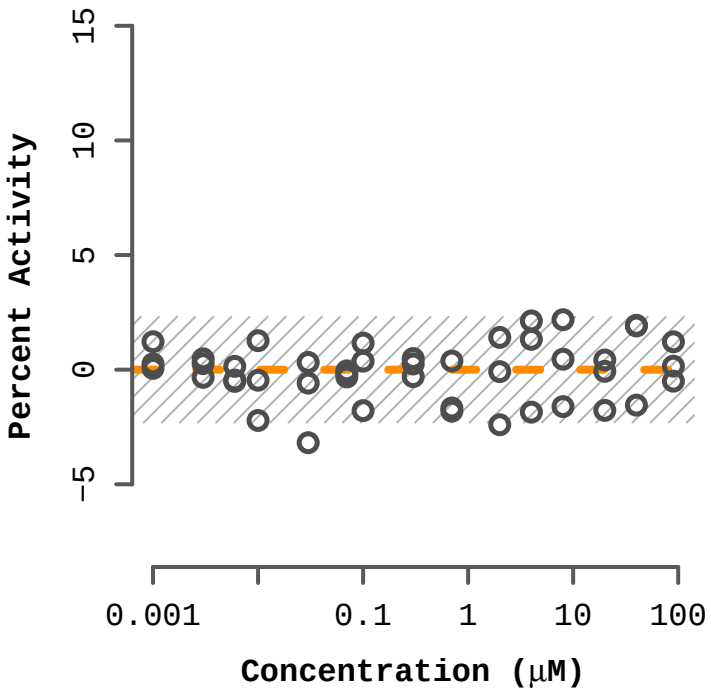
NAME: 1-Phenylethyl propionate
CHID: 47091 **CASRN:** 120-45-6
SPID(S): Tox21_302346
M4ID: 12476787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.628 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

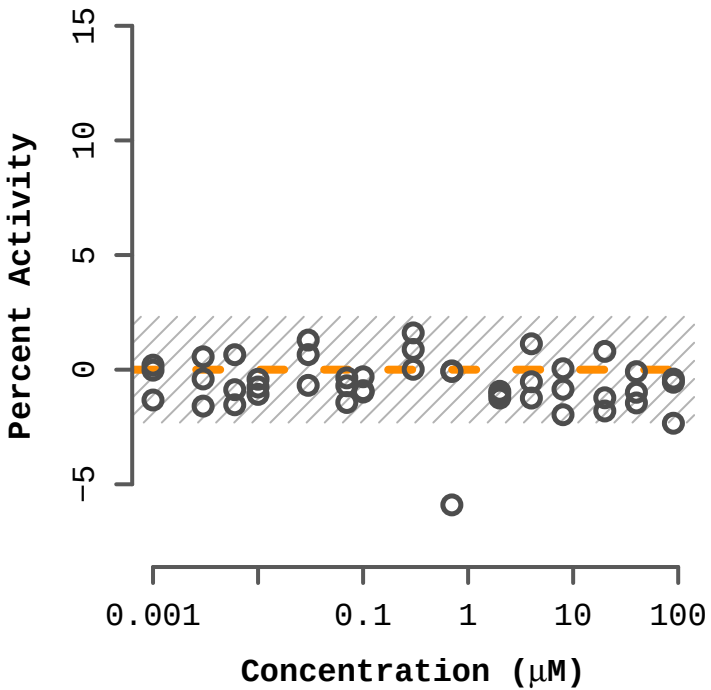
NAME: Jasmone
CHID: 47092 **CASRN:** 488-10-8
SPID(S): Tox21_301825
M4ID: 12477308

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.766 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

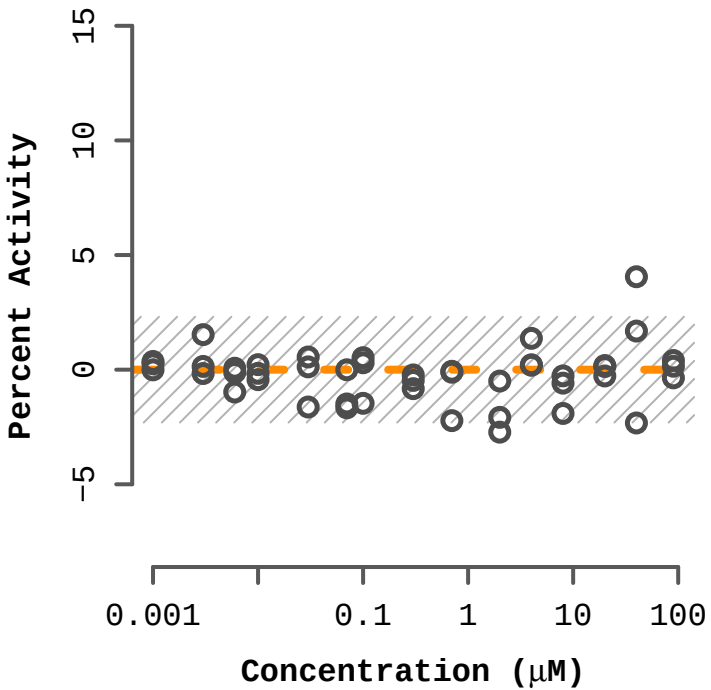
NAME: Methyl 2-octynoate
CHID: 47093 **CASRN:** 111-12-6
SPID(S): Tox21_300979
M4ID: 12478154

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.836 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

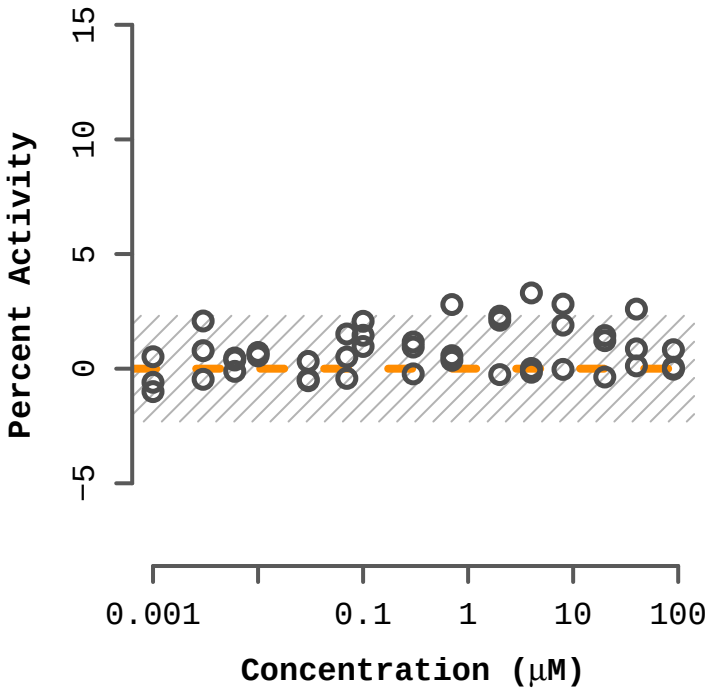
NAME: Ethyl benzoylacetate
CHID: 47094 **CASRN:** 94-02-0
SPID(S): Tox21_302326
M4ID: 12476807

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

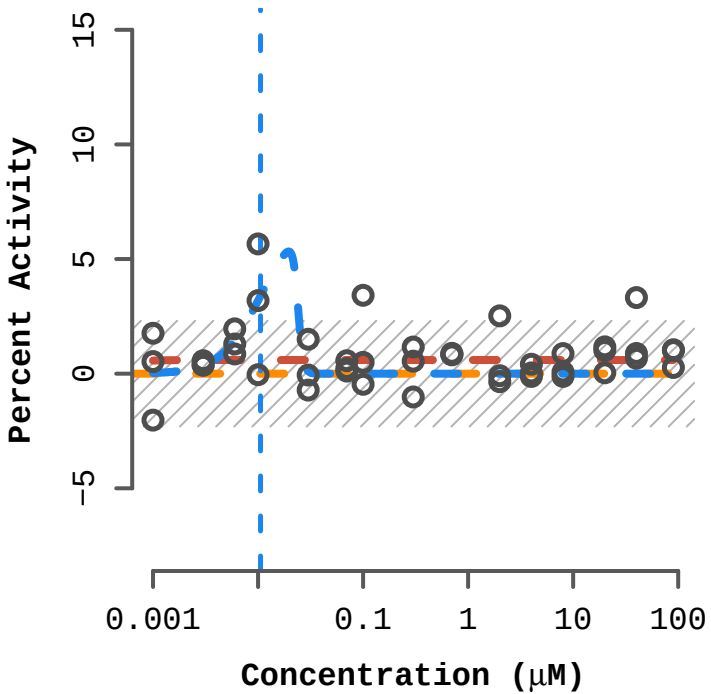
NAME: Ethyl hydrocinnamate
CHID: 47095 **CASRN:** 2021-28-5
SPID(S): Tox21_302337
M4ID: 12476796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piperazine dihydrochloride
CHID: 47096 **CASRN:** 142-64-3
SPID(S): Tox21_302343
M4ID: 12476790

HILL MODEL (in red):

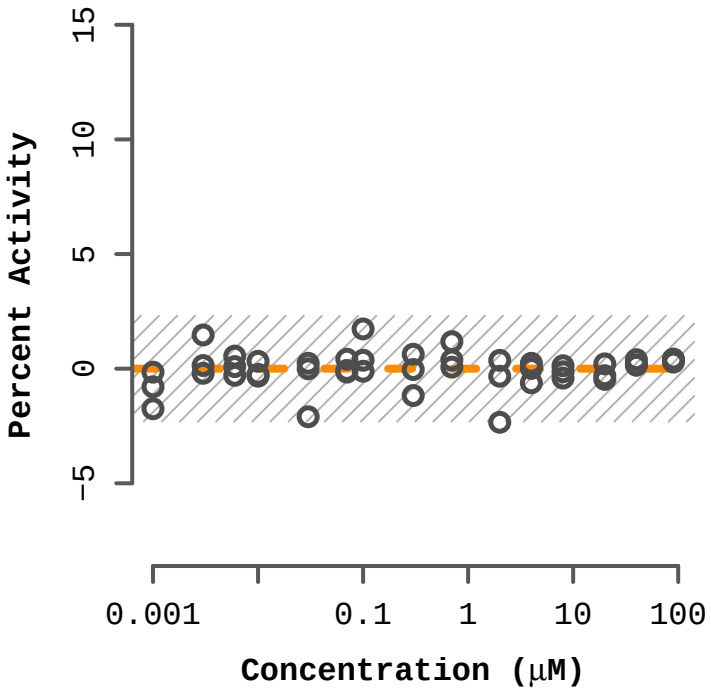
	tp	ga	gw
val:	0.595	−3.51	2.72
sd:	0.143	8.07	33.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.79	−1.98	2.3	−1.62	17.9
sd:	10.2	0.53	1.73	0.26	47.7

	CNST	HILL	GNLS
AIC:	156.36	146.12	153.11
PROB:	0.01	0.96	0.03
RMSE:	1.5	1.29	1.24

MAX_MEAN: 2.94 **MAX_MED:** 3.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

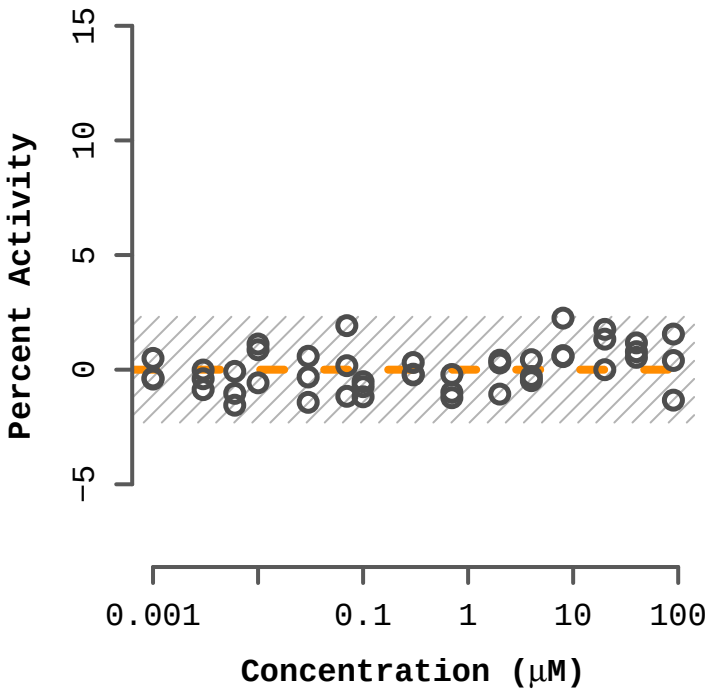
NAME: 3-Phenylbutyraldehyde
CHID: 47098 **CASRN:** 16251-77-7
SPID(S): Tox21_302323
M4ID: 12476810

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.664 **MAX_MED:** 0.389 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

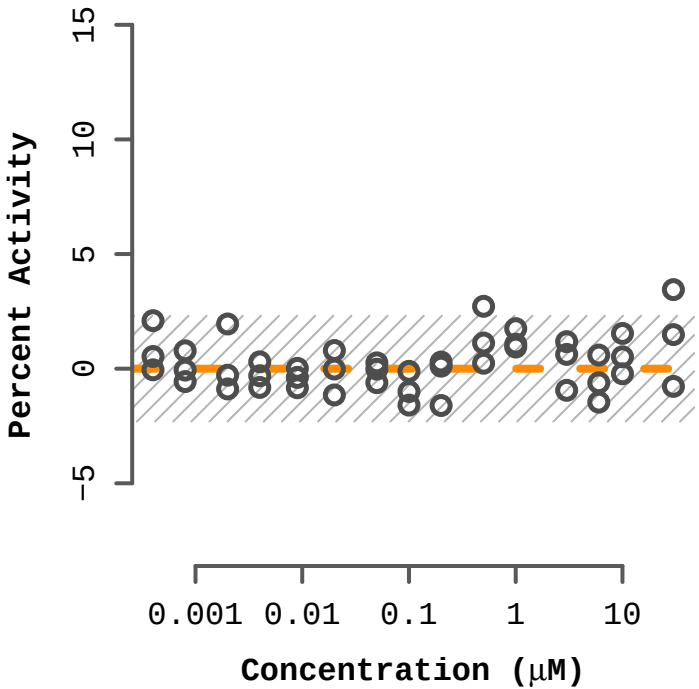
NAME: Undecanoic delta-lactone
CHID: 47099 **CASRN:** 710-04-3
SPID(S): Tox21_302328
M4ID: 12476805

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

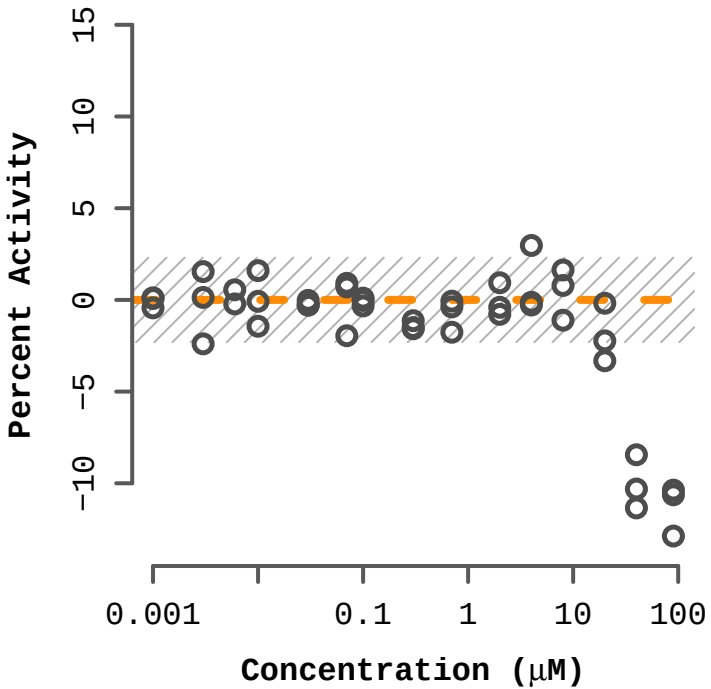
NAME: 2,3-Diethylpyrazine
CHID: 47101 **CASRN:** 15707-24-1
SPID(S): Tox21_301820
M4ID: 12477313

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

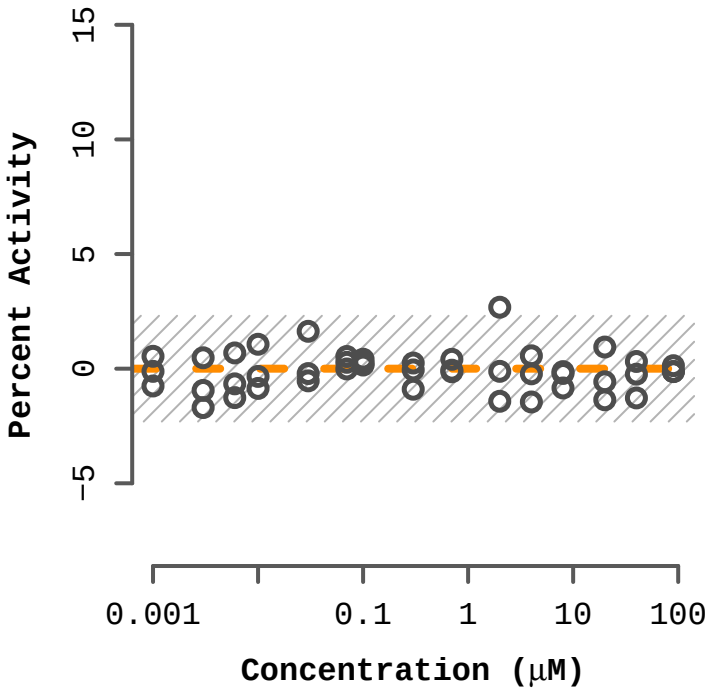
NAME: Dehydroabietylamine acetate
CHID: 47102 **CASRN:** 2026-24-6
SPID(S): Tox21_302299
M4ID: 12476834

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.37	NA	NA
PROB:	1	NA	NA
RMSE:	4.13	NA	NA

MAX_MEAN: 0.854 **MAX_MED:** 0.788 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

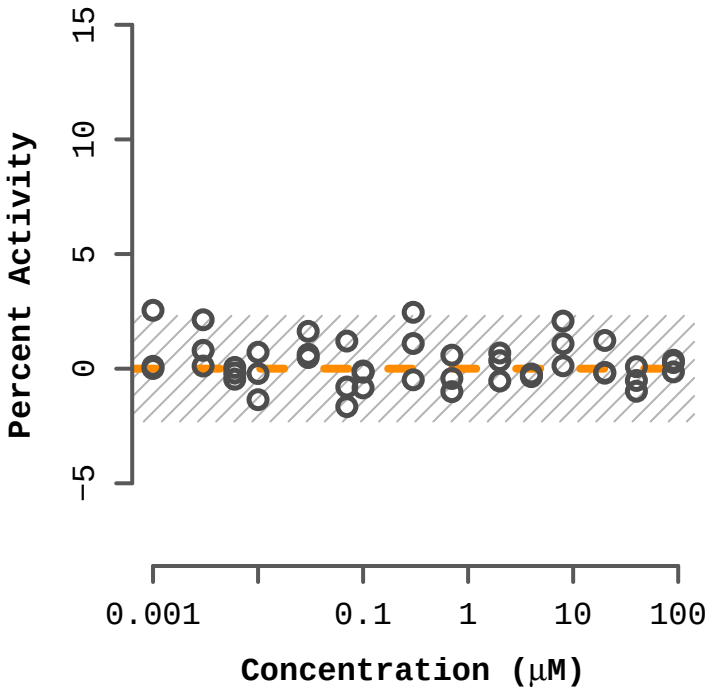
NAME: Octadecyl sulfate sodium salt
CHID: 47103 **CASRN:** 1120-04-3
SPID(S): Tox21_302384
M4ID: 12476749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.382 **MAX_MED:** 0.278 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

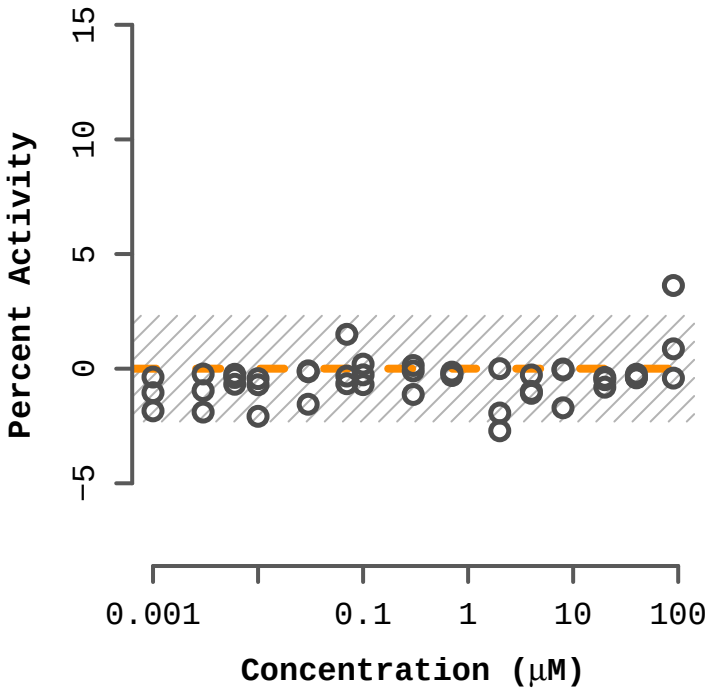
NAME: trans−2,cis−6−Nonadienal
CHID: 47104 **CASRN:** 557−48−2
SPID(S): Tox21_301826
M4ID: 12477307

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

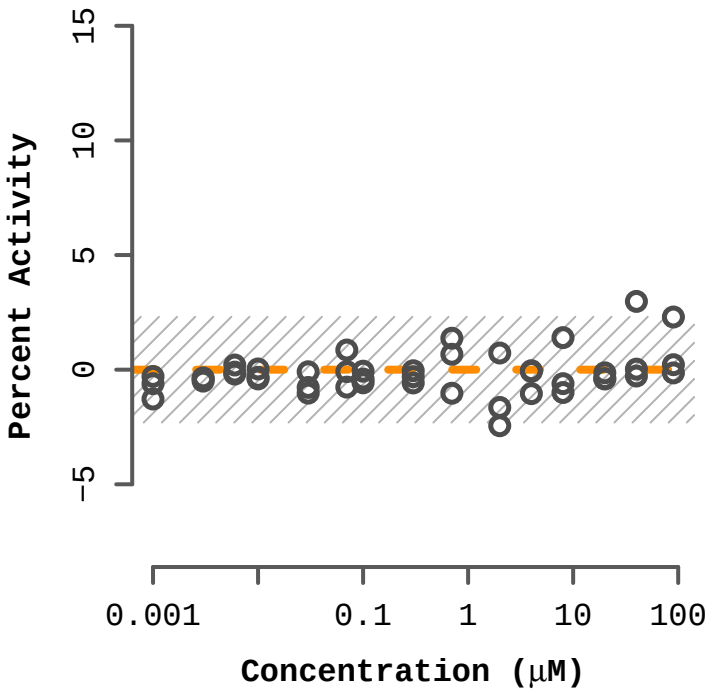
NAME: 2-Methoxy-4-methylphenol
CHID: 47105 **CASRN:** 93-51-6
SPID(S): Tox21_302681
M4ID: 12476452

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.866 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

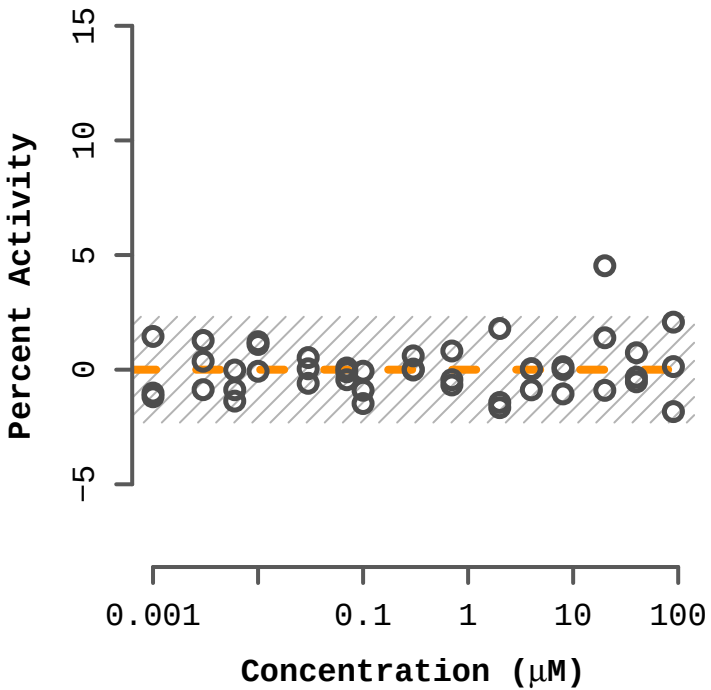
NAME: Citronellic acid
CHID: 47106 CASRN: 502-47-6
SPID(S): Tox21_302694
M4ID: 12476439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.909 **MAX_MED:** 0.674 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

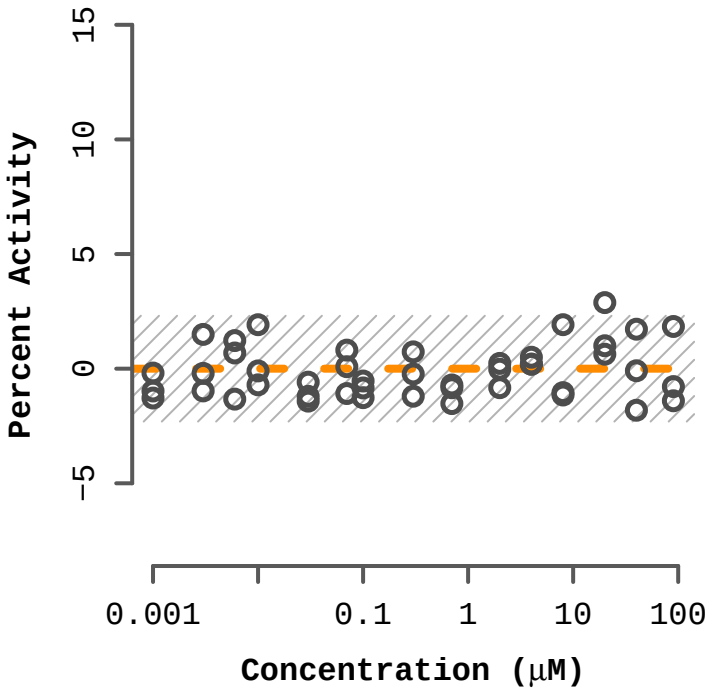
NAME: 3,5,5-Trimethylhexanal
CHID: 47107 **CASRN:** 5435-64-3
SPID(S): Tox21_302701
M4ID: 12476432

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

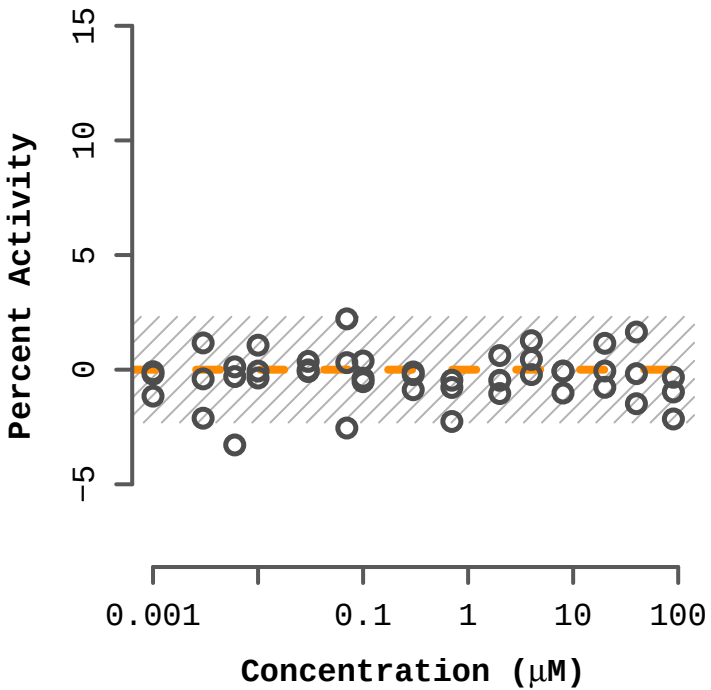
NAME: Cyclopentanethiol
CHID: 47108 CASRN: 1679-07-8
SPID(S): Tox21_302675
M4ID: 12476458

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.51 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

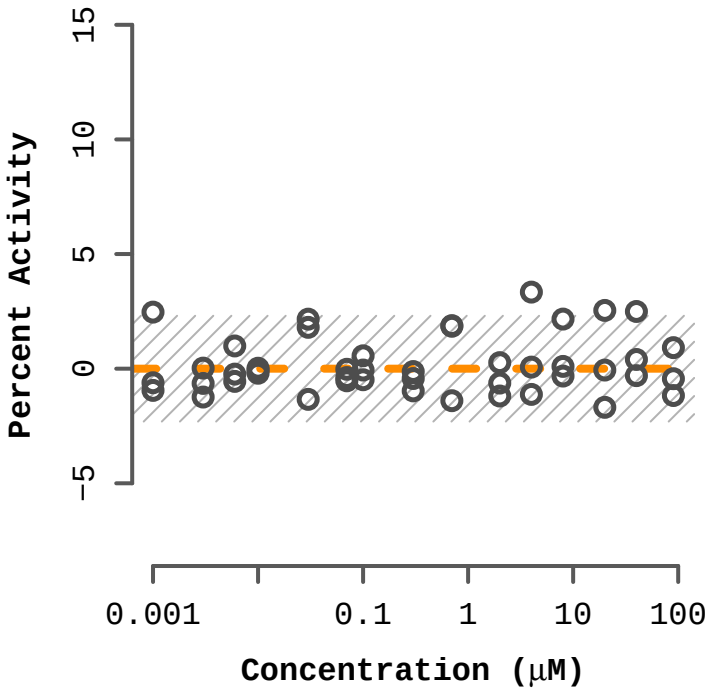
NAME: 2-Phenylpropionaldehyde dimethyl acetal
CHID: 47109 **CASRN:** 90-87-9
SPID(S): Tox21_302706
M4ID: 12476427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.501 **MAX_MED:** 0.448 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

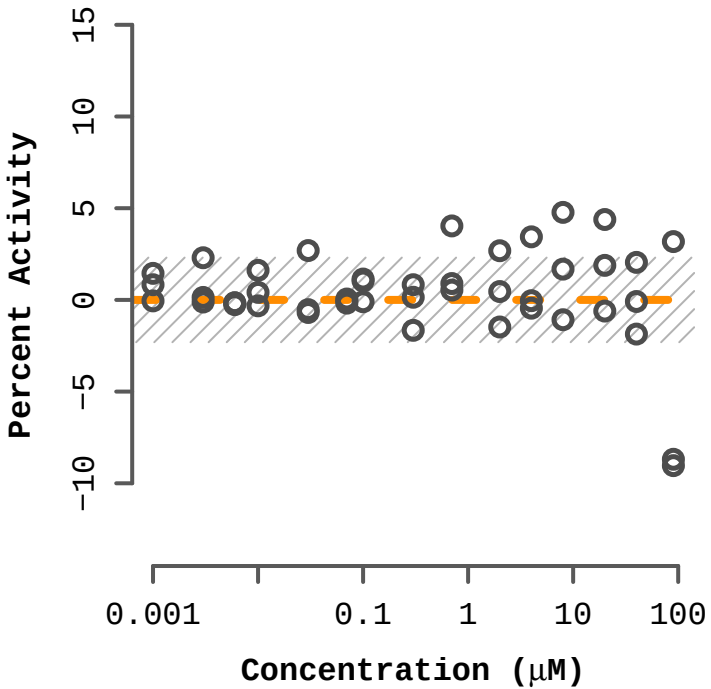
NAME: trans,trans-Farnesyl acetate
CHID: 47110 **CASRN:** 4128-17-0
SPID(S): Tox21_302688
M4ID: 12476445

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

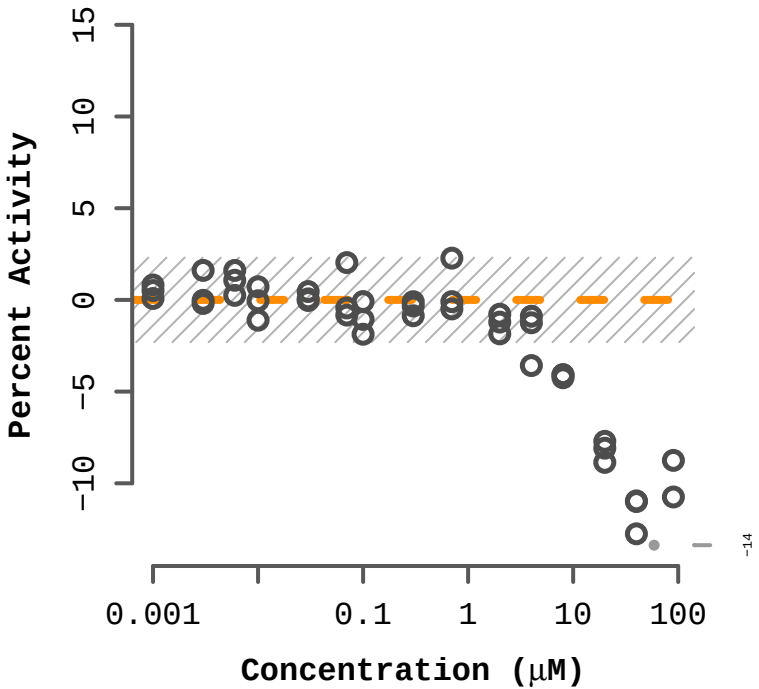
NAME: Sclareol
CHID: 47111 **CASRN:** 515-03-7
SPID(S): Tox21_302727
M4ID: 12476406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.44	NA	NA
PROB:	1	NA	NA
RMSE:	2.53	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

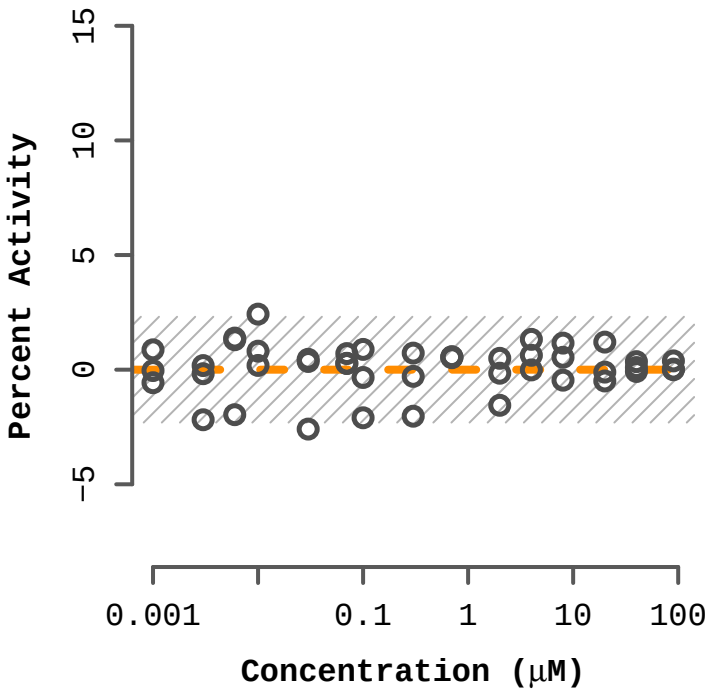
NAME: Didodecyldimethylammonium bromide
CHID: 47112 **CASRN:** 3282-73-3
SPID(S): Tox21_302608
M4ID: 12476525 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	261.96	NA	NA
PROB:	1	NA	NA
RMSE:	4.91	NA	NA

MAX_MEAN: 0.978 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

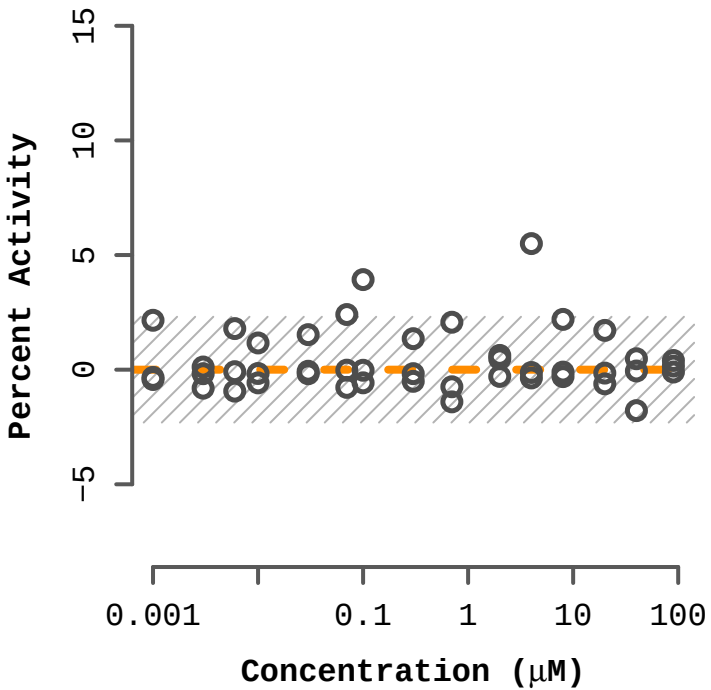
NAME: (−)−Ambroxide
CHID: 47113 **CASRN:** 6790−58−5
SPID(S): Tox21_302674
M4ID: 12476459

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

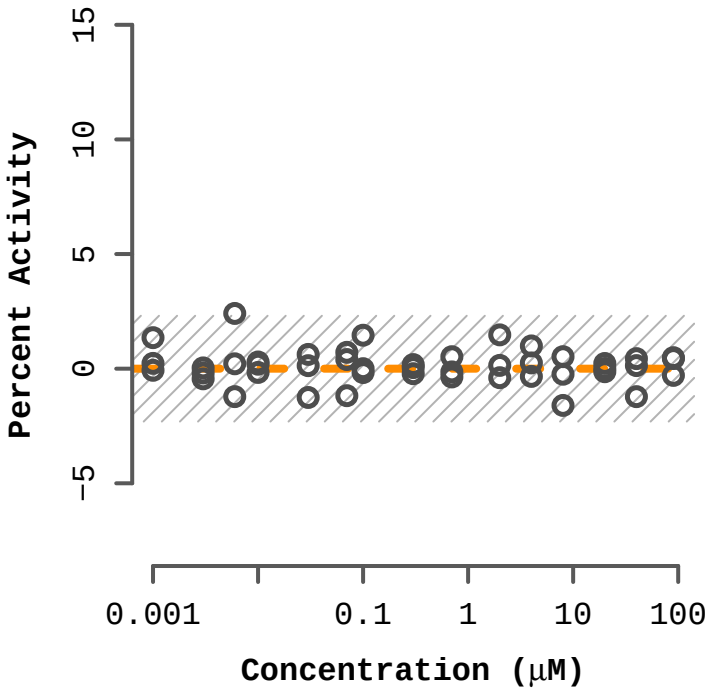
NAME: Geranic acid
CHID: 47115 **CASRN:** 459-80-3
SPID(S): Tox21_302708
M4ID: 12476425

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 0.474 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

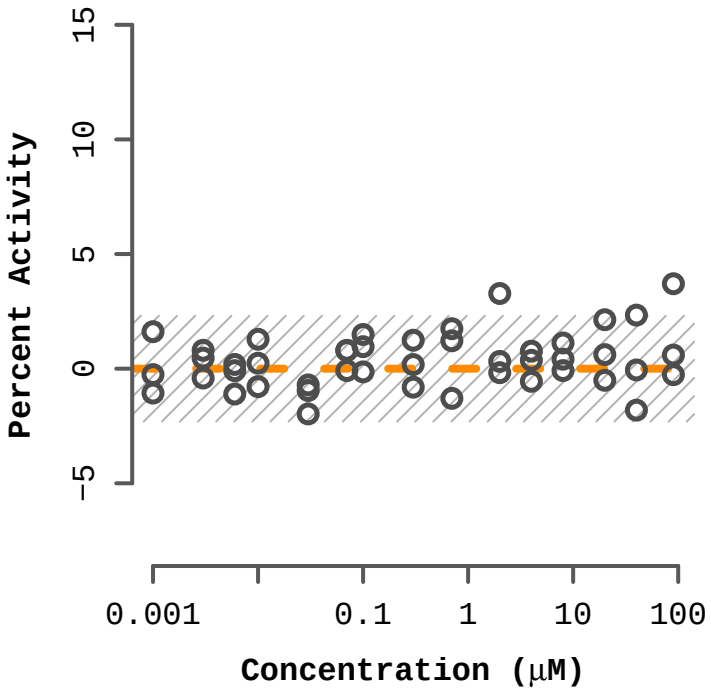
NAME: Isopulegol
CHID: 47116 **CASRN:** 89-79-2
SPID(S): Tox21_302529
M4ID: 12476604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.506 **MAX_MED:** 0.443 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

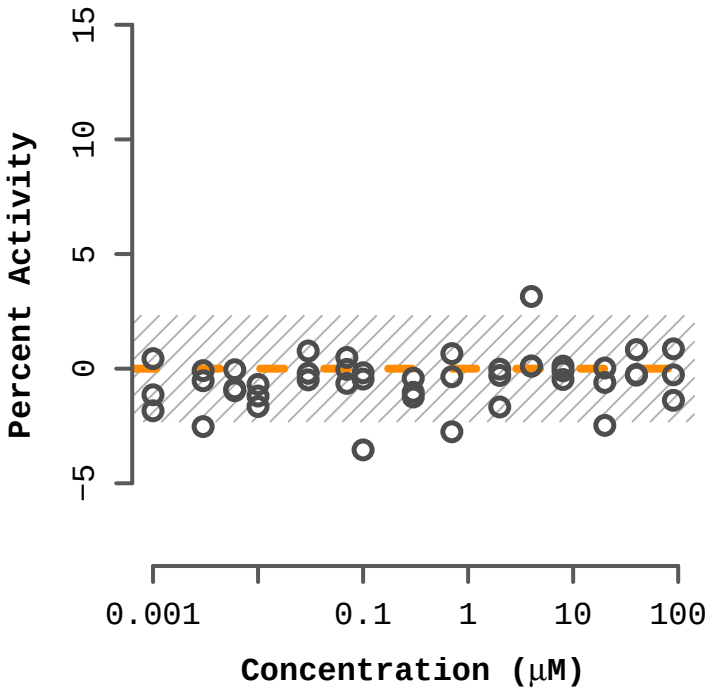
NAME: Ytterbium(III) chloride
CHID: 47117 **CASRN:** 10361-91-8
SPID(S): Tox21_301062
M4ID: 12478071

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

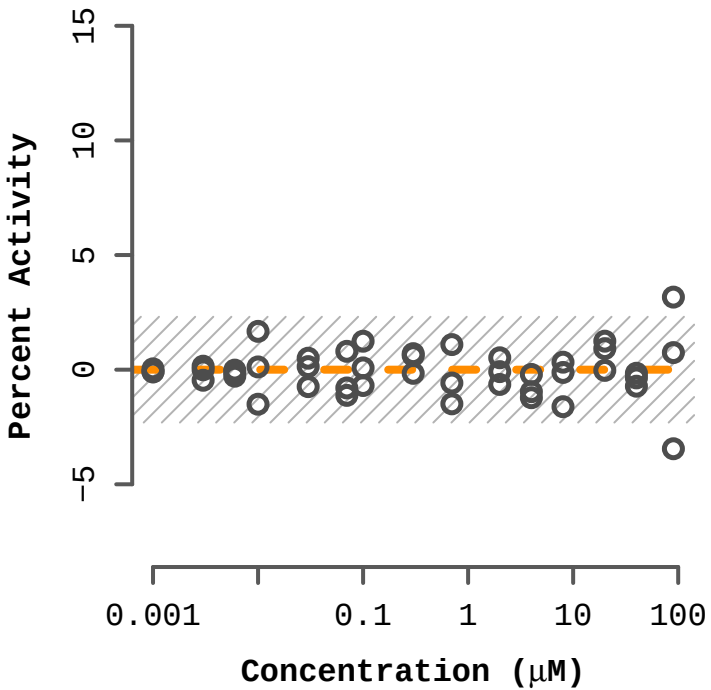
NAME: 2-Methyl-3-furanthiol
CHID: 47118 **CASRN:** 28588-74-1
SPID(S): Tox21_302709
M4ID: 12476424

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.118 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

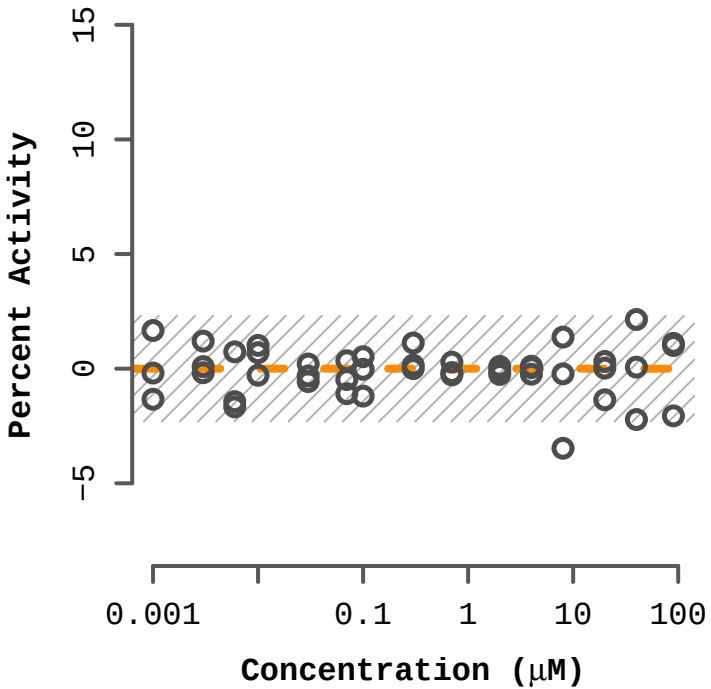
NAME: 4'−tert−Butyl−2',6'−dimethylacetophenone
CHID: 47120 **CASRN:** 2040−10−0
SPID(S): Tox21_302639
M4ID: 12476494

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.712 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

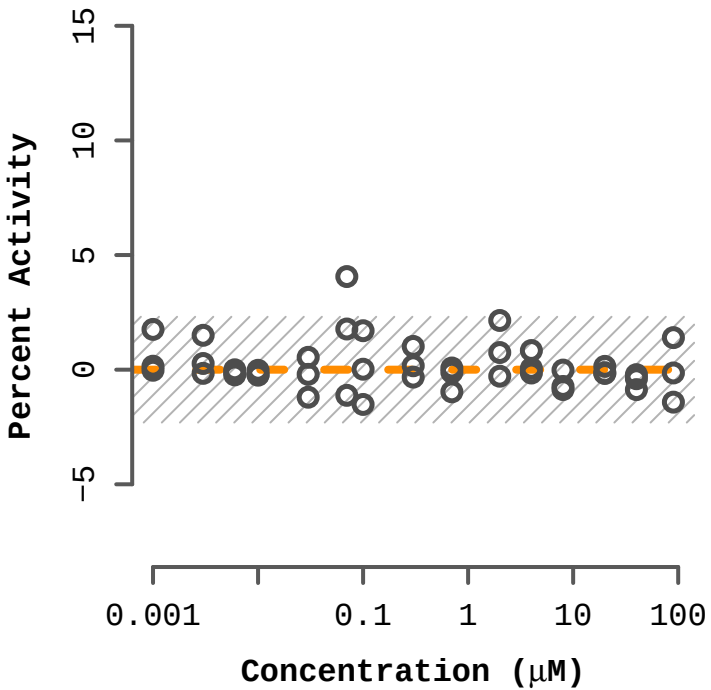
NAME: 2-Benzofurancarboxaldehyde
CHID: 47121 CASRN: 4265-16-1
SPID(S): Tox21_302448
M4ID: 12476685

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.477 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

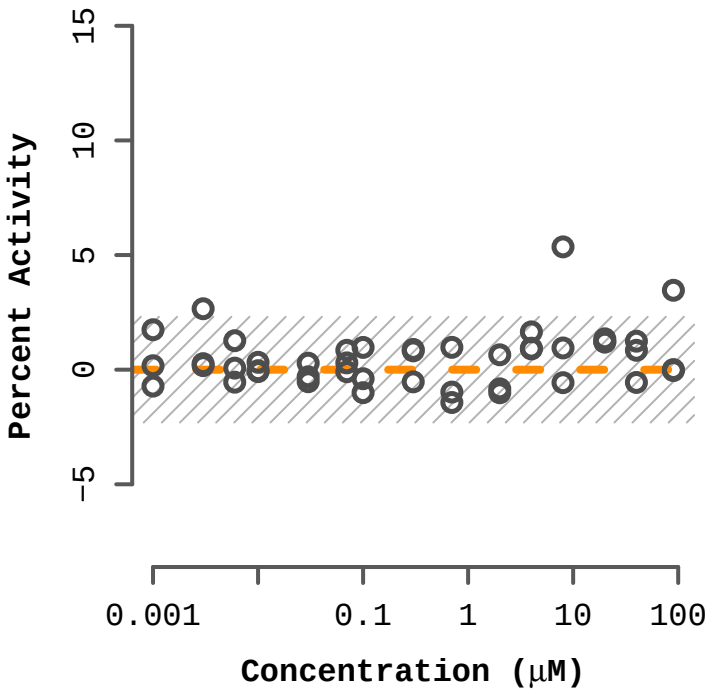
NAME: Nonyl acetate
CHID: 47123 **CASRN:** 143-13-5
SPID(S): Tox21_302536
M4ID: 12476597

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

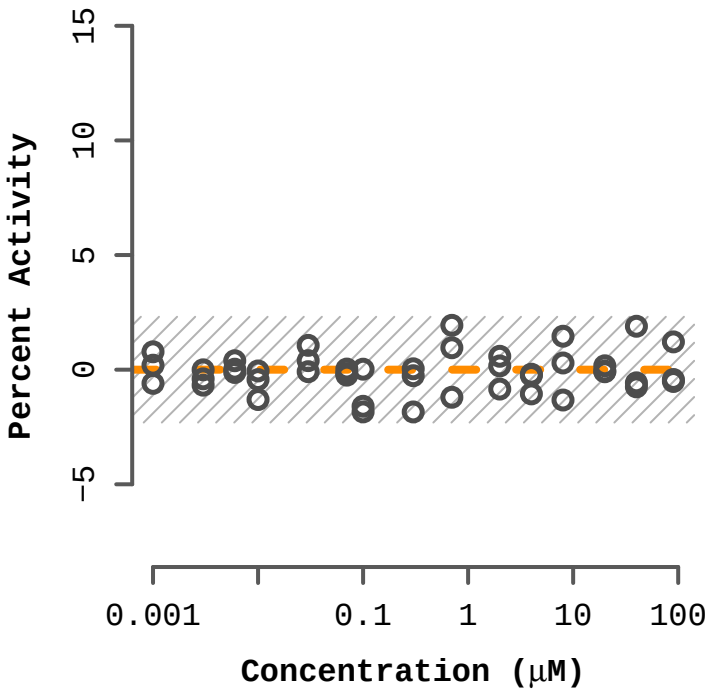
NAME: Heptyl acetate
CHID: 47124 CASRN: 112-06-1
SPID(S): Tox21_302615
M4ID: 12476518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.91 MAX_MED: 1.22 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

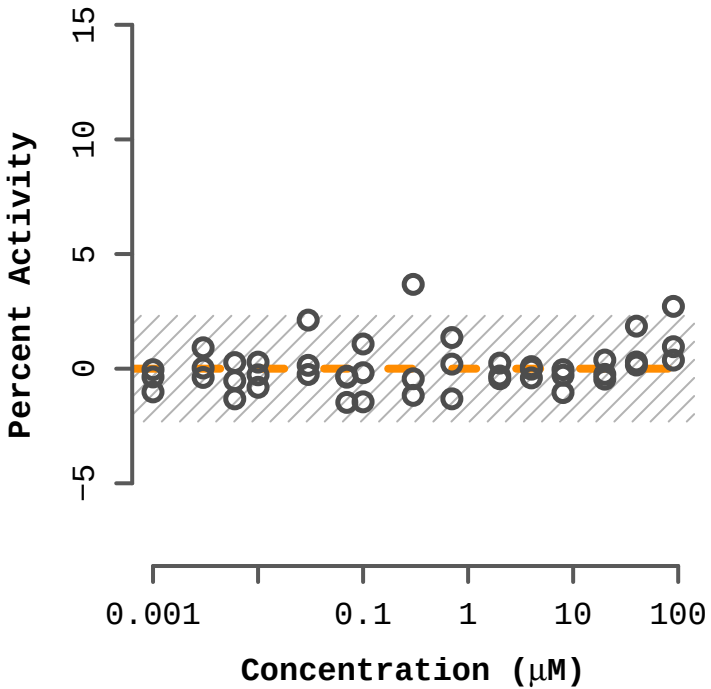
NAME: 9-Decenyl acetate
CHID: 47125 **CASRN:** 50816-18-7
SPID(S): Tox21_302671
M4ID: 12476462

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.564 **MAX_MED:** 0.958 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

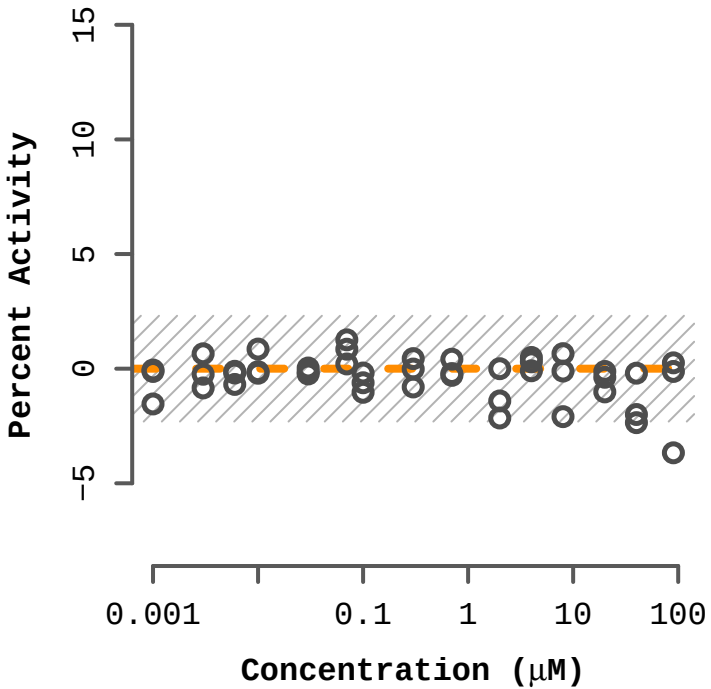
NAME: Ethyl 2-methoxybenzoate
CHID: 47126 **CASRN:** 7335-26-4
SPID(S): Tox21_302680
M4ID: 12476453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

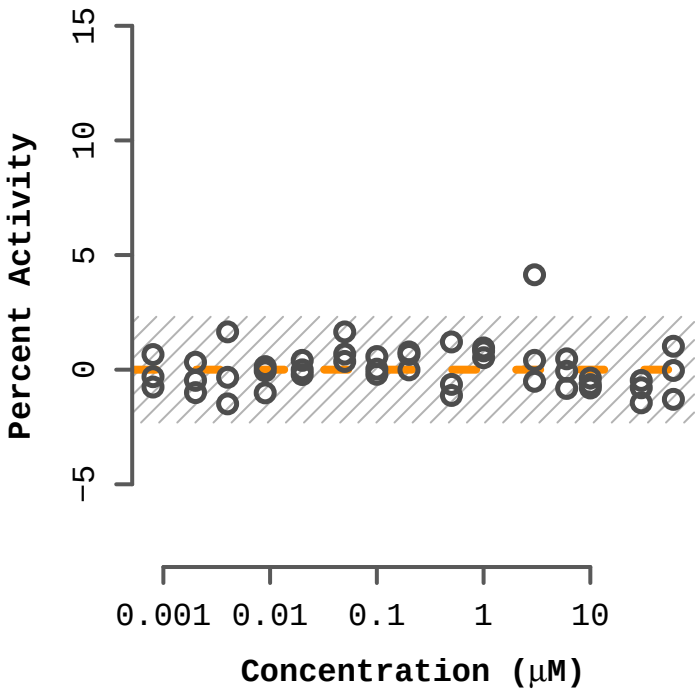
NAME: 4-(tert-Pentyl)-cyclohexanone
CHID: 47127 **CASRN:** 16587-71-6
SPID(S): Tox21_302460
M4ID: 12476673

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.773 **MAX_MED:** 0.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

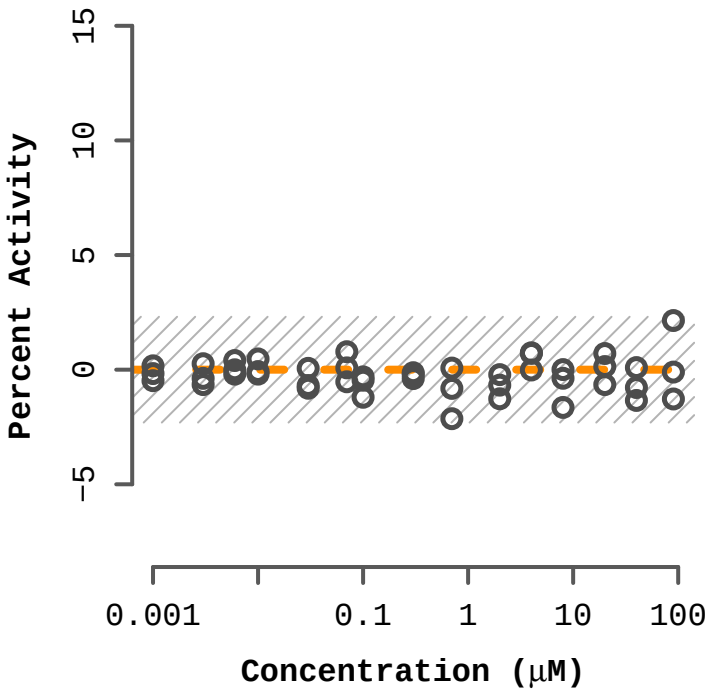
NAME: 3,3-Dimethylallyl acetate
CHID: 47128 **CASRN:** 1191-16-8
SPID(S): Tox21_302724
M4ID: 12476409

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 0.821 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

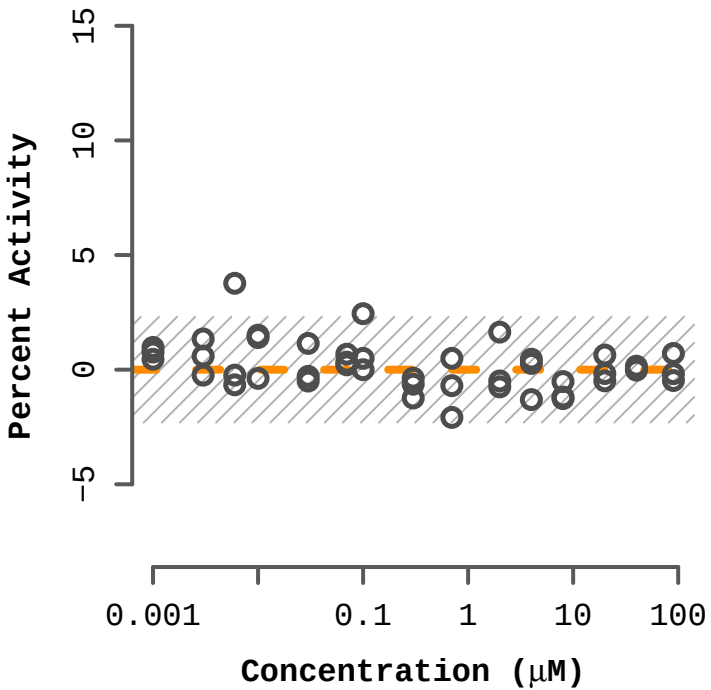
NAME: Methyl geranate
CHID: 47129 **CASRN:** NOCAS_47129
SPID(S): Tox21_302707
M4ID: 12476426

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.479 **MAX_MED:** 0.711 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

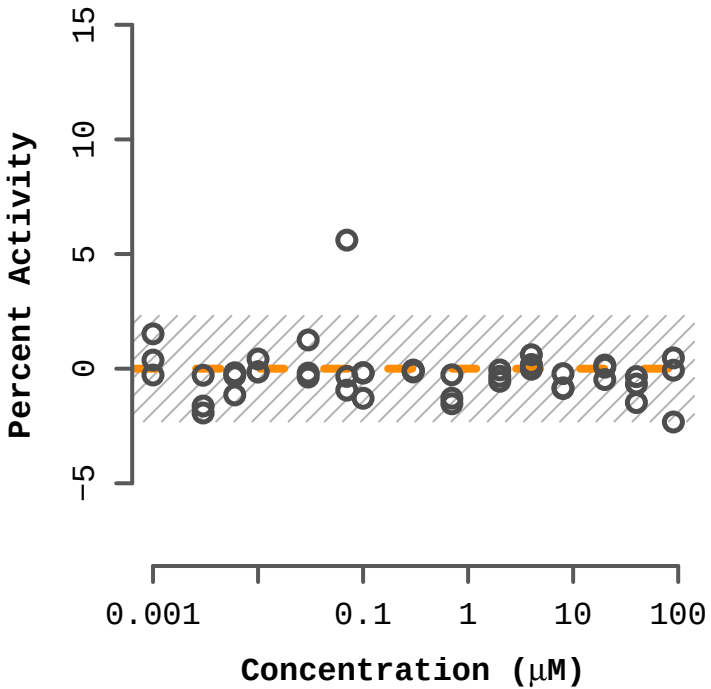
NAME: Benzyl tiglate
CHID: 47130 **CASRN:** 37526-88-8
SPID(S): Tox21_302648
M4ID: 12476485

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.979 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

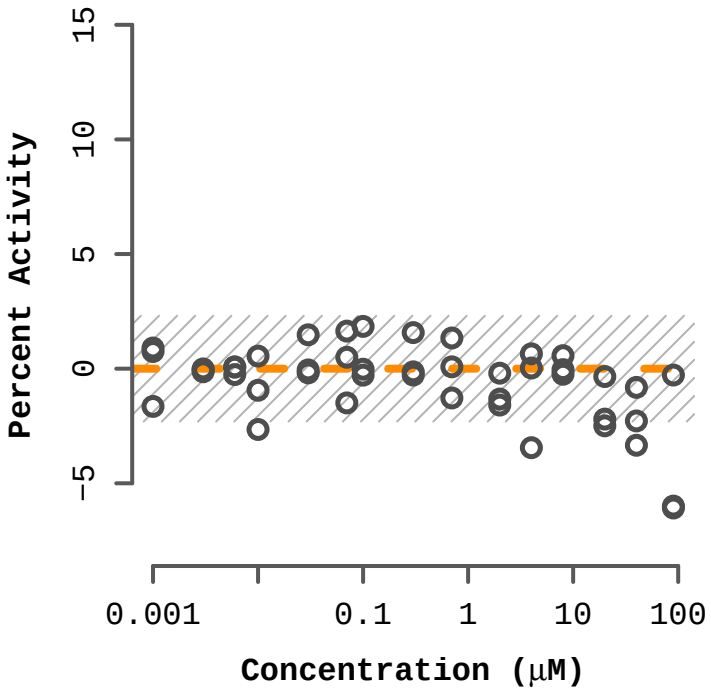
NAME: 3-Methyl-2-butenyl benzoate
CHID: 47131 **CASRN:** 5205-11-8
SPID(S): Tox21_302705
M4ID: 12476428

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 0.377 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

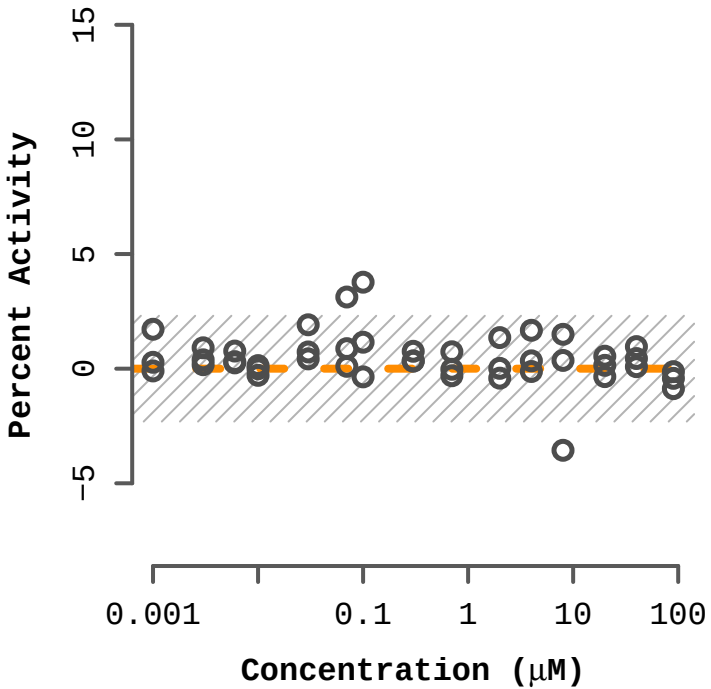
NAME: 3-(Methylthio)propyl isothiocyanate
CHID: 47132 **CASRN:** 505-79-3
SPID(S): Tox21_302609
M4ID: 12476524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 0.514 **MAX_MED:** 0.751 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

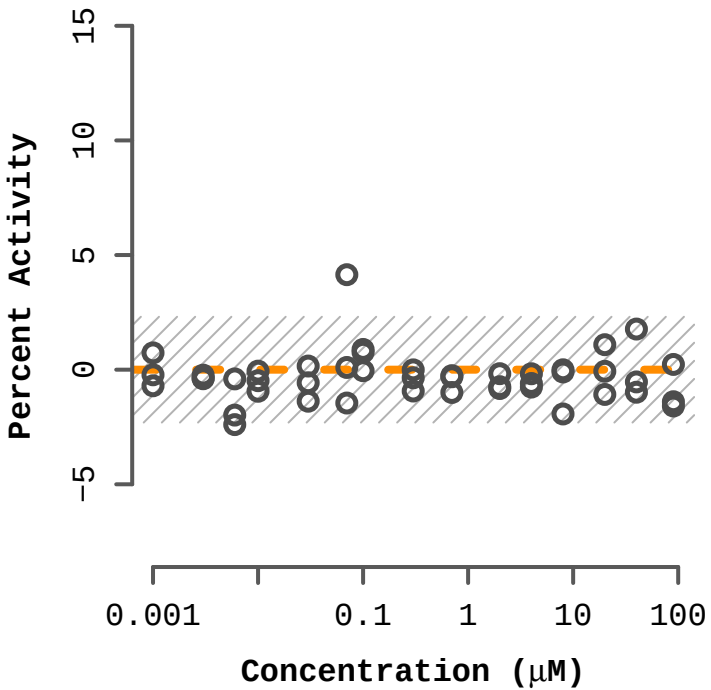
NAME: 2,4,5-Trimethyl-3-oxazoline
CHID: 47133 **CASRN:** 22694-96-8
SPID(S): Tox21_303617
M4ID: 12475528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

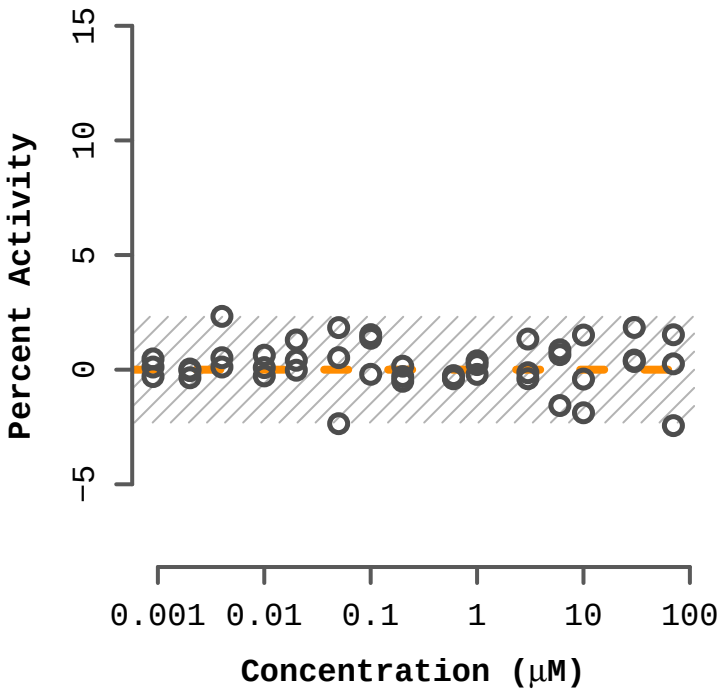
NAME: 2-Octen-4-one
CHID: 47134 **CASRN:** 4643-27-0
SPID(S): Tox21_302717
M4ID: 12476416

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.93 **MAX_MED:** 0.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

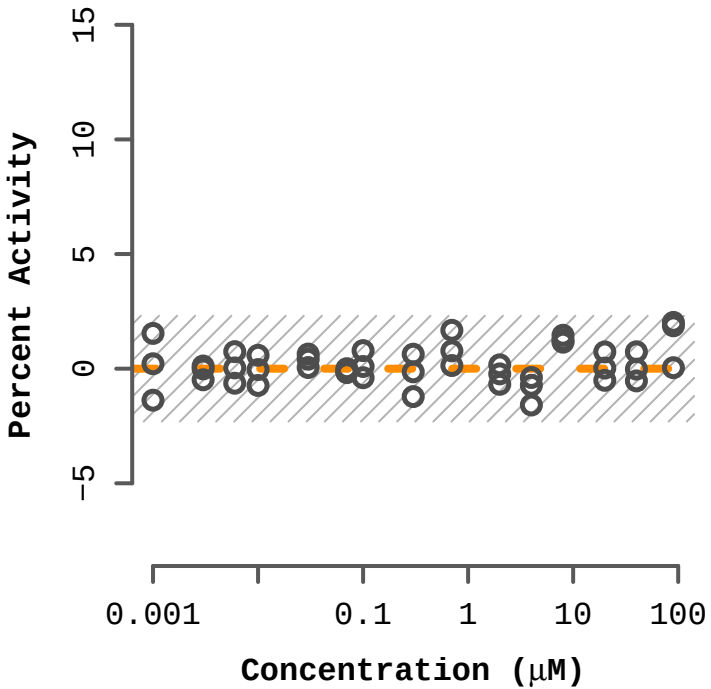
NAME: 2-Methylbenzenethiol
CHID: 47135 **CASRN:** 137-06-4
SPID(S): Tox21_302483
M4ID: 12476650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.989 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

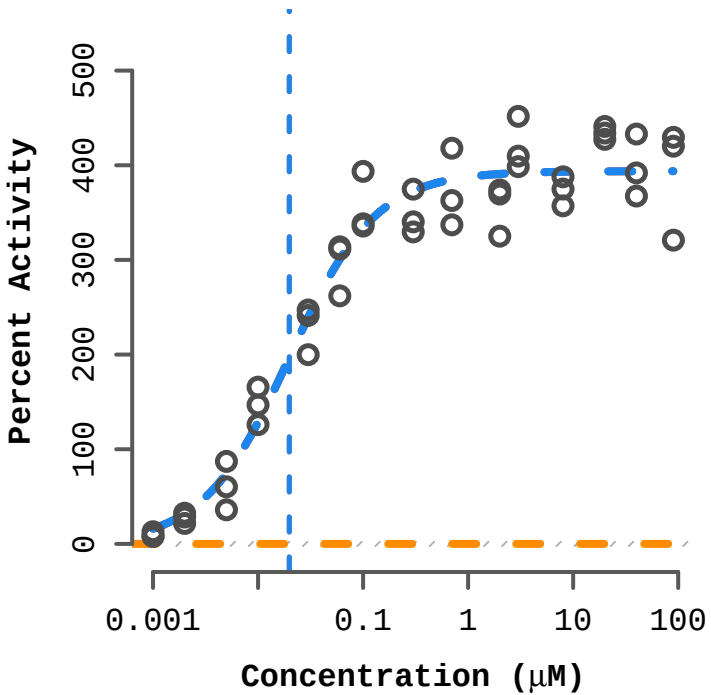
NAME: Bromopentafluorobenzene
CHID: 47136 **CASRN:** 344-04-7
SPID(S): Tox21_302507
M4ID: 12476626

HILL MODEL: Not applicable.

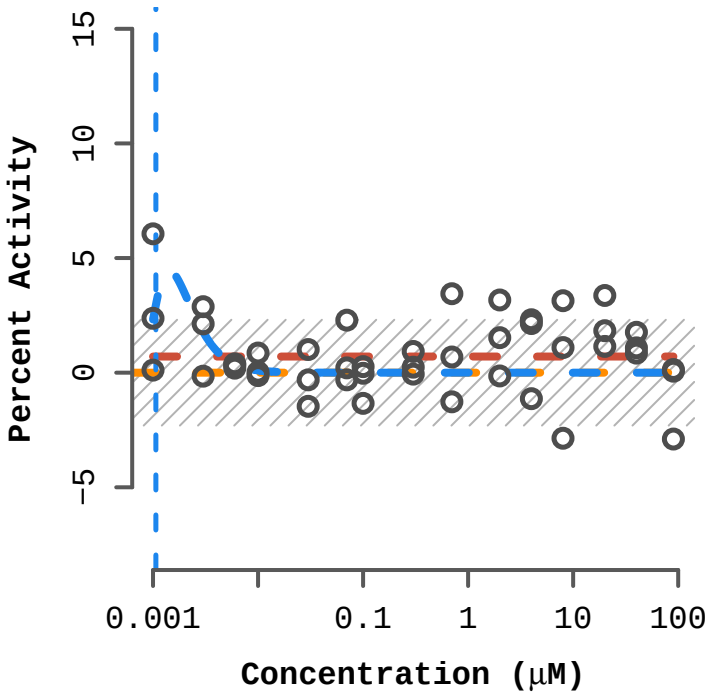
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.87 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Betamethasone 21-phosphate disodium
CHID:    47137   CASRN: 151-73-5
SPID(S): Tox21_302467
M4ID:    12476666

HILL MODEL (in red):
      tp       ga       gw
val:  394      -1.7     1.06
sd:   8.2      0.0472   0.0974

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  394      -1.7     1.06     3.7      5.01
sd:   8.2      0.0472   0.0974   1620     4660

      CNST        HILL        GNLS
AIC:  656.37      447.24      451.24
PROB: 0           0.88        0.12
RMSE: 316.5       30.85       30.85

MAX_MEAN: 434       MAX_MED: 434       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: tert-Butylbenzene
CHID: 47138 **CASRN:** 98-06-6
SPID(S): Tox21_300540
M4ID: 12478592

HILL MODEL (in red):

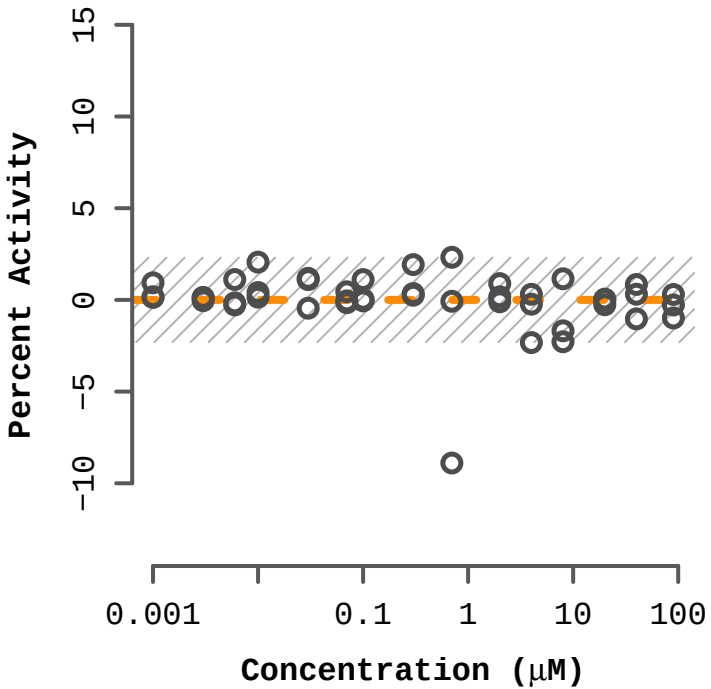
	tp	ga	gw
val:	0.704	−4.78	4.09
sd:	0.228	1480	3400

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.05	−2.97	7.6	−2.7	2.63
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	183.48	180.34	186.05
PROB:	0.16	0.79	0.05
RMSE:	1.85	1.67	1.65

MAX_MEAN: 2.85 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

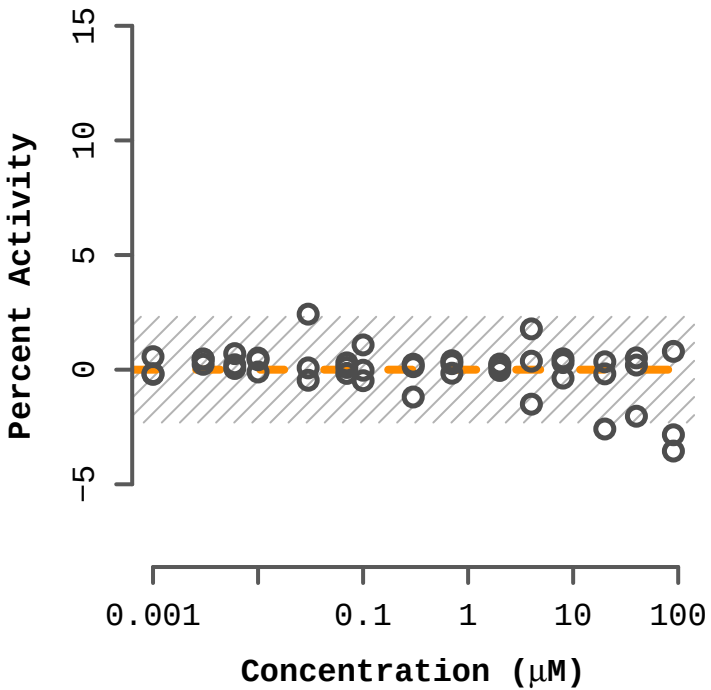
NAME: 5-Cyclohexadecen-1-one
CHID: 47139 **CASRN:** 37609-25-9
SPID(S): Tox21_302532
M4ID: 12476601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 0.872 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

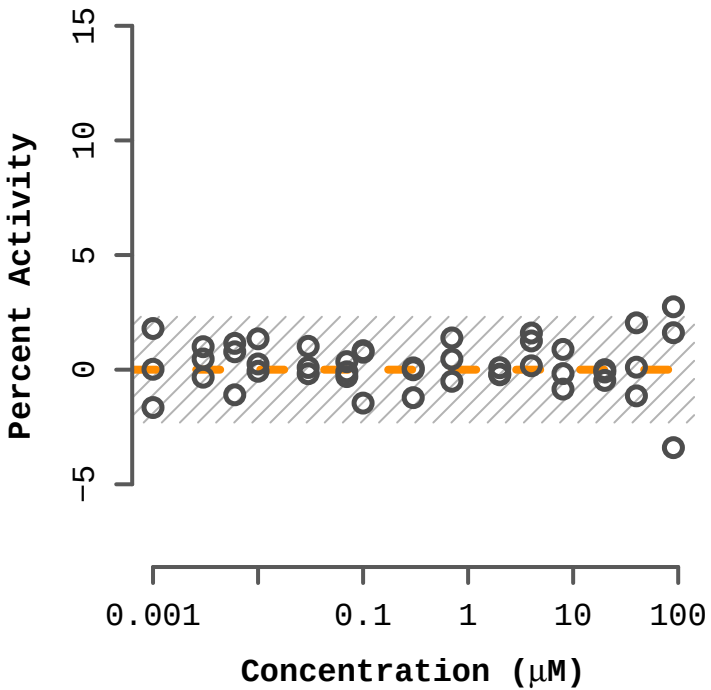
NAME: Isopropyl citrate (Mixture)
CHID: 47140 **CASRN:** NOCAS_47140
SPID(S): Tox21_302479
M4ID: 12476654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.681 **MAX_MED:** 0.455 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

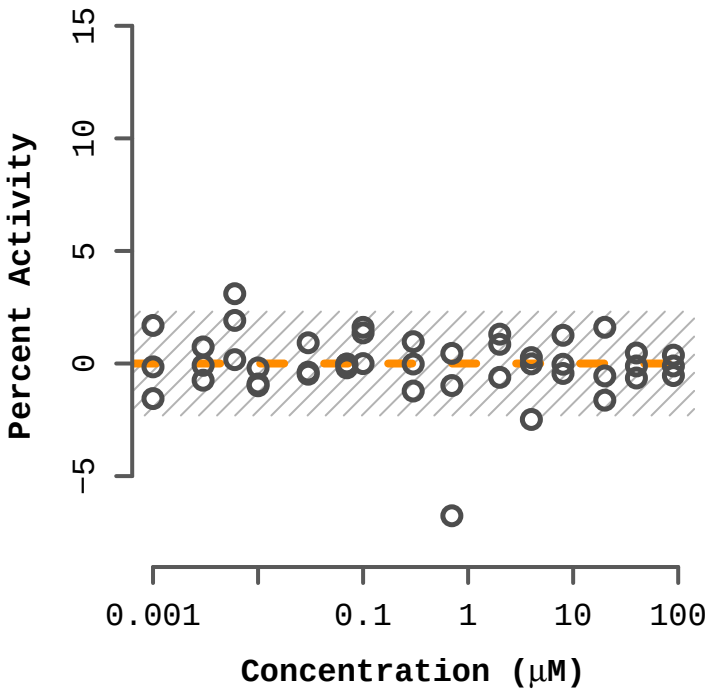
NAME: Cyclopentadecanone
CHID: 47141 **CASRN:** 502-72-7
SPID(S): Tox21_302465
M4ID: 12476668

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

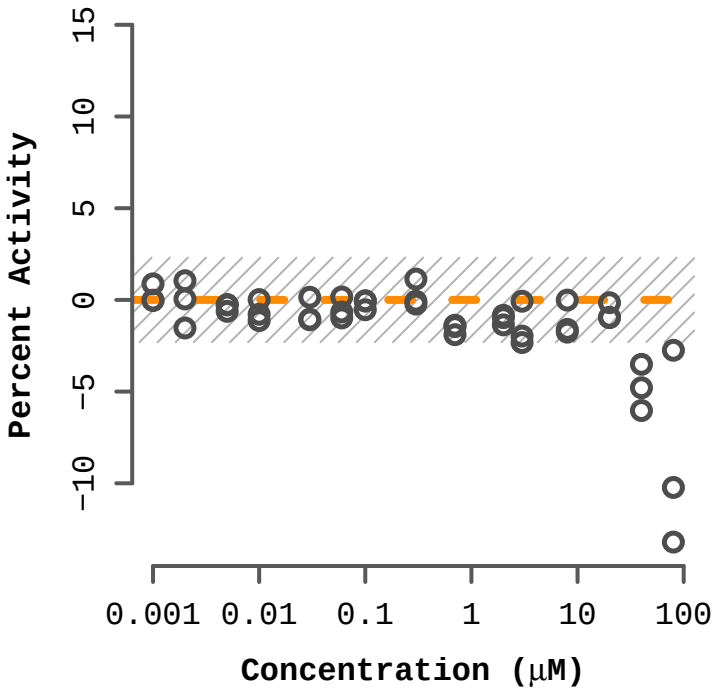
NAME: beta-Cyclocitral
CHID: 47142 **CASRN:** 432-25-7
SPID(S): Tox21_302524
M4ID: 12476609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

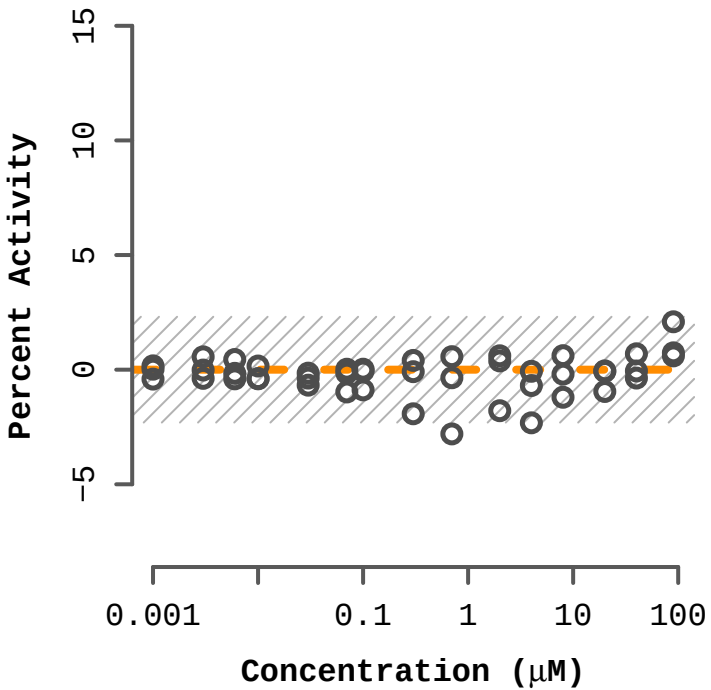
NAME: Chlorhexidine dihydrochloride
CHID: 47144 **CASRN:** 3697-42-5
SPID(S): Tox21_302689
M4ID: 12476444

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.97	NA	NA

MAX_MEAN: 0.282 **MAX_MED:** 0.0522 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

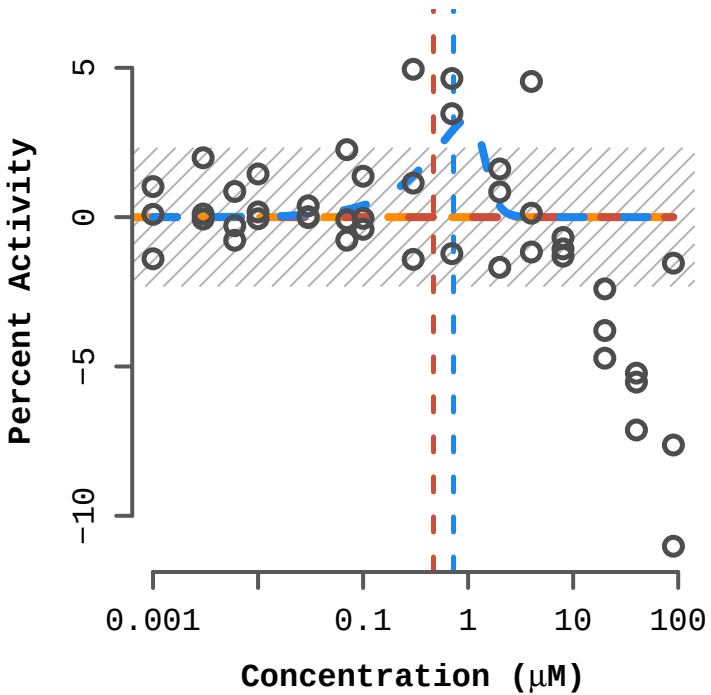
NAME: 3,3-Dimethylacrylic acid
CHID: 47145 **CASRN:** 541-47-9
SPID(S): Tox21_302475
M4ID: 12476658

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.737 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethylstilbestrol dipropionate
CHID: 47146 CASRN: 130-80-3
SPID(S): Tox21_302713
M4ID: 12476420

HILL MODEL (in red):

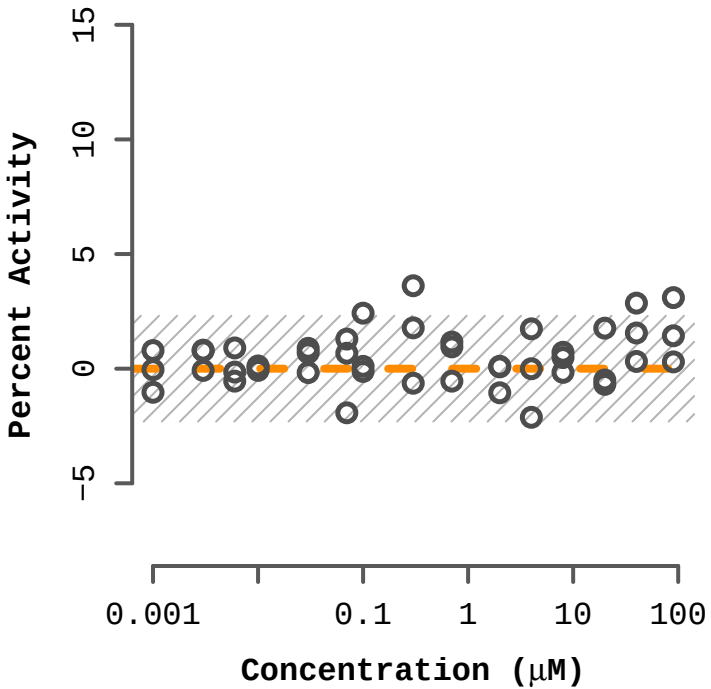
	tp	ga	gw
val:	1.53e-10	-0.33	2.37
sd:	2.63e-05	6970	568000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.94	-0.139	1.34	0.149	6.98
sd:	19.6	2.05	2.3	1.24	57.4

	CNST	HILL	GNLS
AIC:	224.07	230.07	230.15
PROB:	0.91	0.05	0.04
RMSE:	3.15	3.15	3.06

MAX_MEAN: 2.3 MAX_MED: 3.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

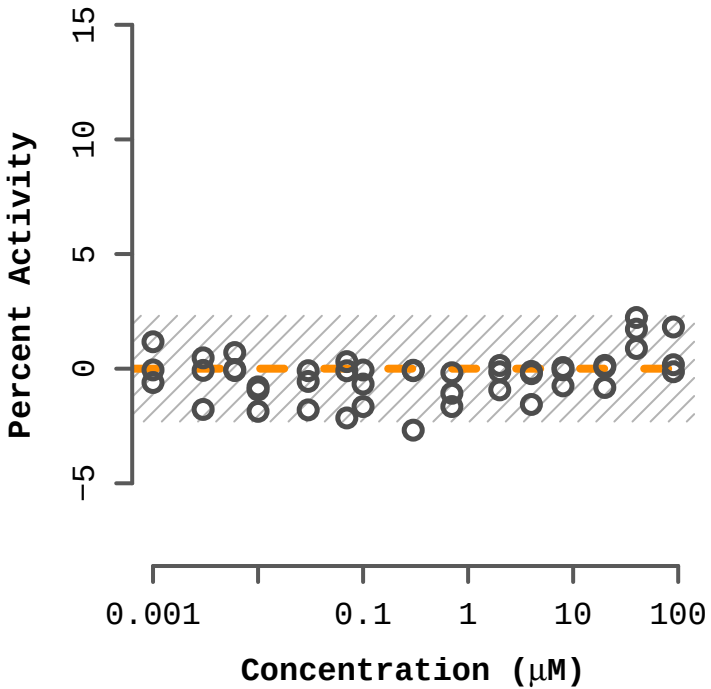
NAME: 4-Isopropylcyclohexanol
CHID: 47149 **CASRN:** 4621-04-9
SPID(S): Tox21_302454
M4ID: 12476679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

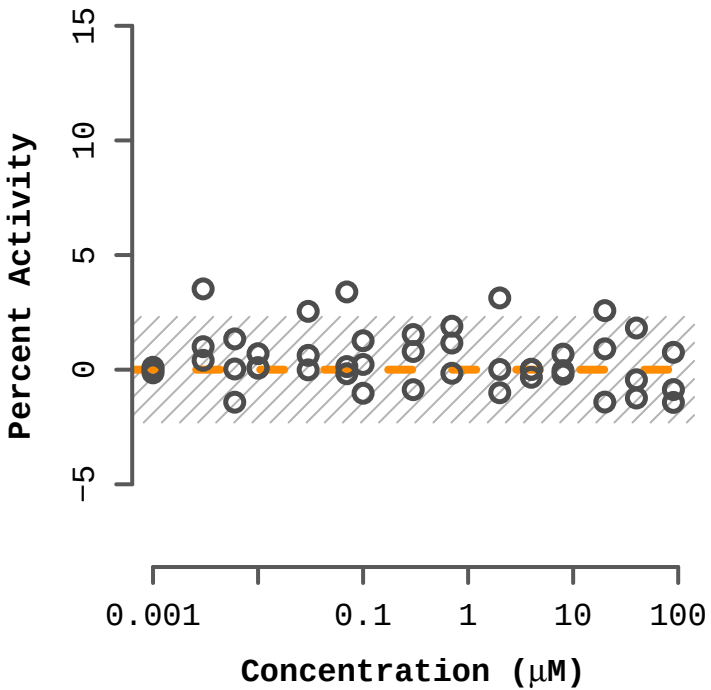
NAME: tert-Butyl hydrogen phthalate
CHID: 47150 **CASRN:** 33693-84-4
SPID(S): Tox21_302695
M4ID: 12476438

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

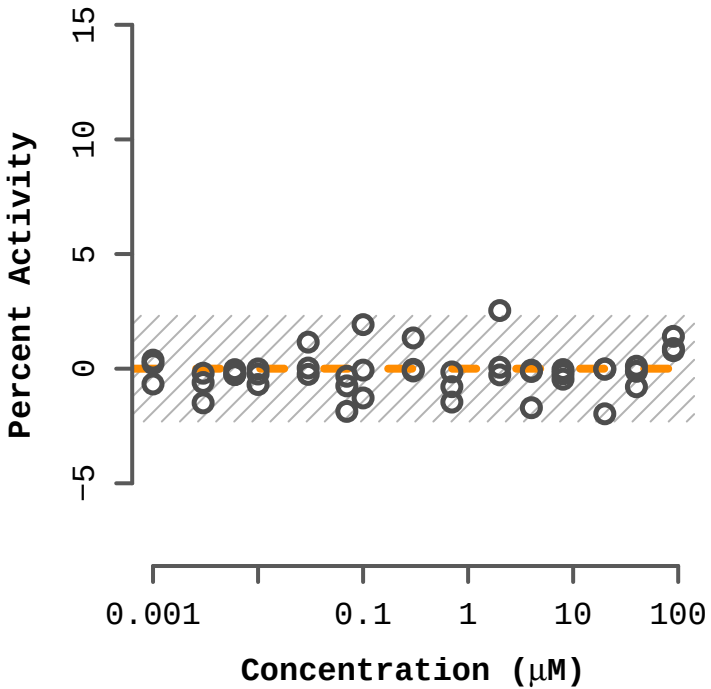
NAME: Geranyl butyrate
CHID: 47152 **CASRN:** 106-29-6
SPID(S): Tox21_301108
M4ID: 12478025

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

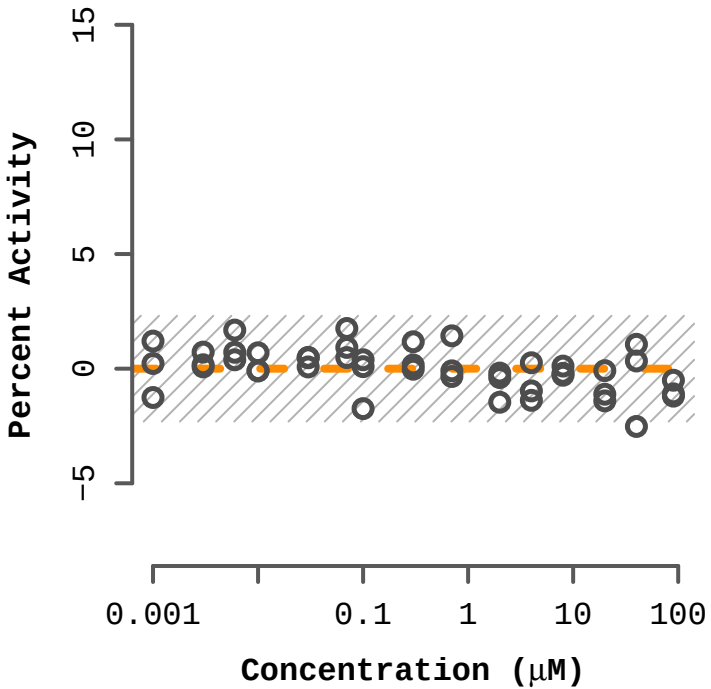
NAME: L-Glutamic acid hydrochloride
CHID: 47155 **CASRN:** 138-15-8
SPID(S): Tox21_302652
M4ID: 12476481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

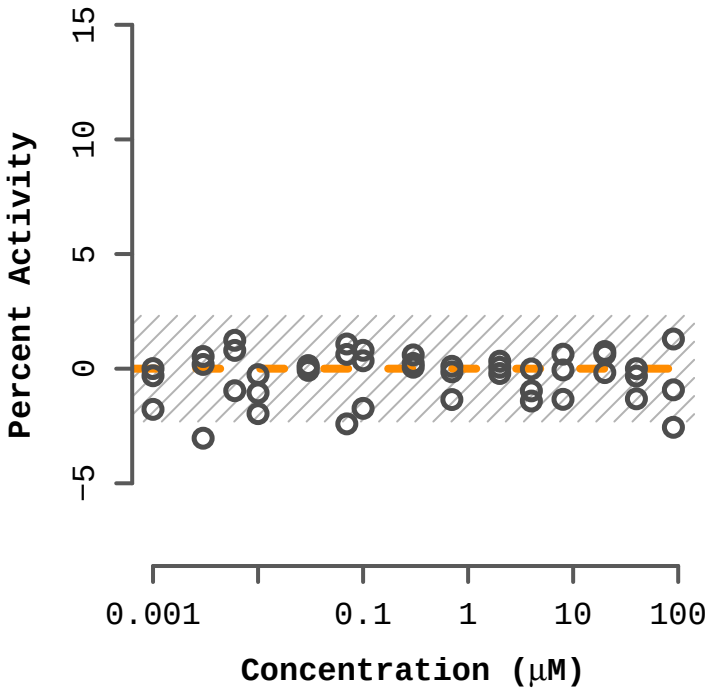
NAME: 2-(2-Butyl)-4,5-dimethyl-3-thiazoline
CHID: 47156 **CASRN:** 65894-82-8
SPID(S): Tox21_302459
M4ID: 12476674

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.928 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

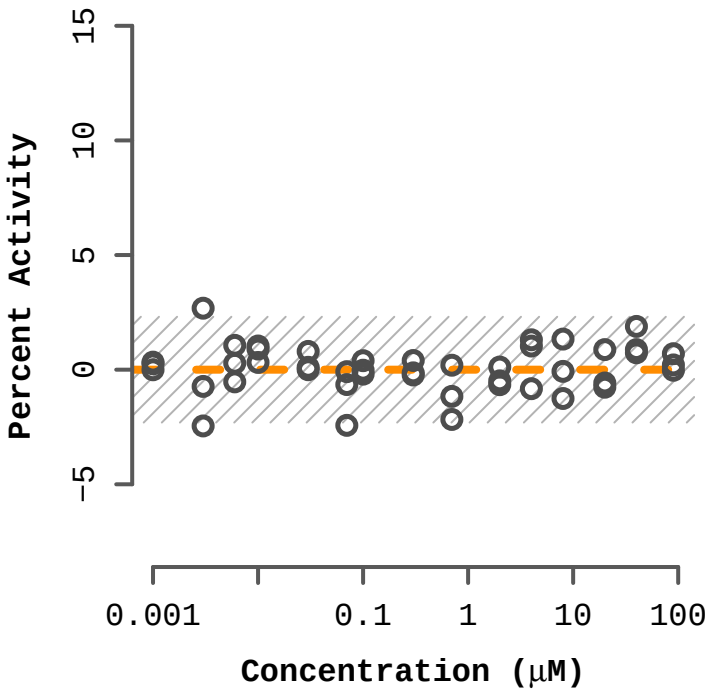
NAME: 3-(2-Methyl-3-furylthio)-4-heptanone
CHID: 47157 **CASRN:** 61295-41-8
SPID(S): Tox21_302502
M4ID: 12476631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.403 **MAX_MED:** 0.798 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

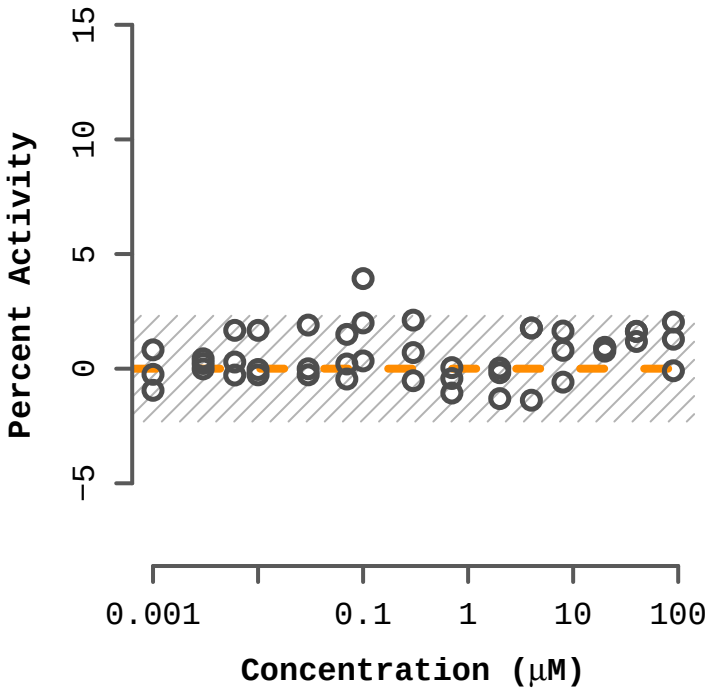
NAME: 2-Heptanol
CHID: 47158 **CASRN:** 543-49-7
SPID(S): Tox21_302517
M4ID: 12476616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

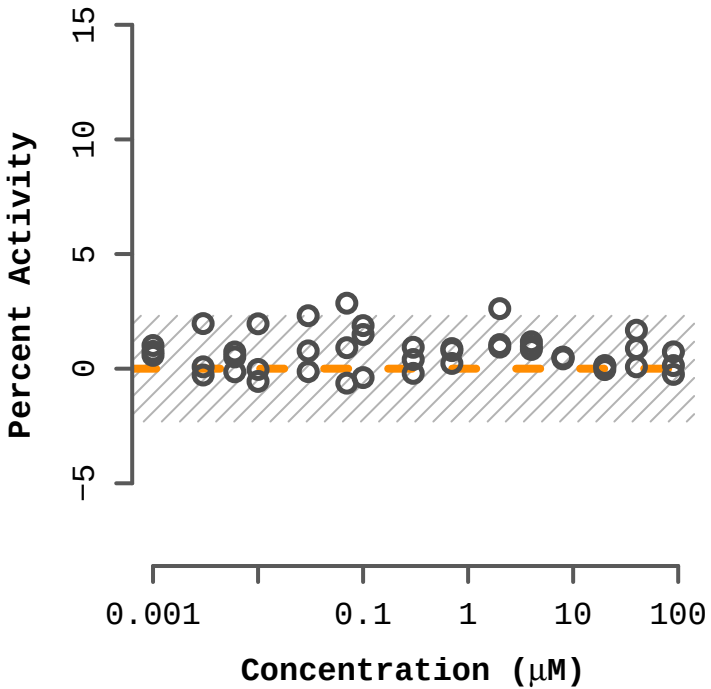
NAME: 4-Methylphenyl 3-methylbutanoate
CHID: 47159 **CASRN:** 55066-56-3
SPID(S): Tox21_302643
M4ID: 12476490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

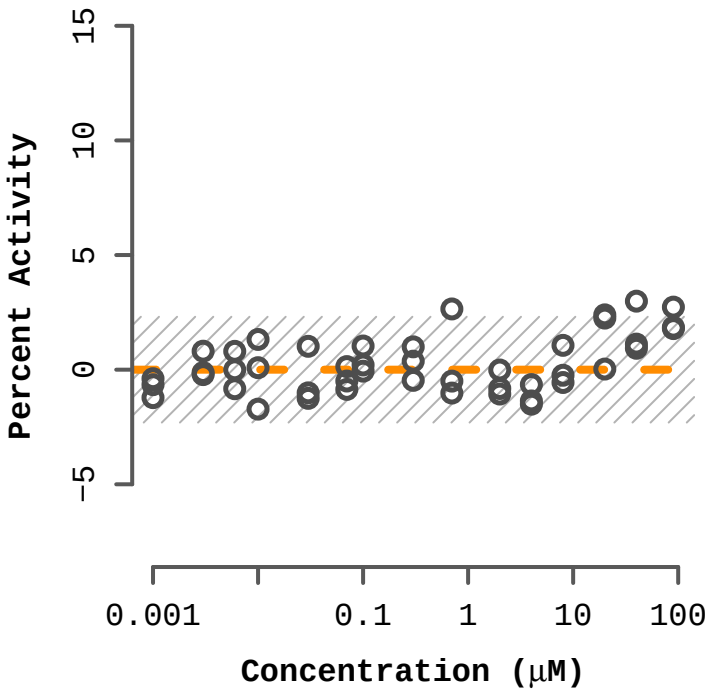
NAME: Linalyl isovalerate
CHID: 47160 **CASRN:** 1118-27-0
SPID(S): Tox21_303620
M4ID: 12475525

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

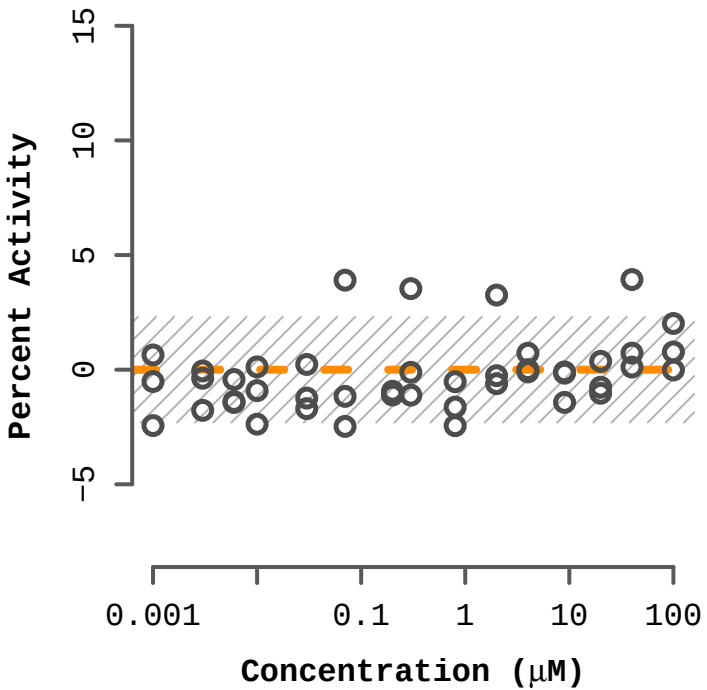
NAME: Piperonyl acetone
CHID: 47161 **CASRN:** 55418-52-5
SPID(S): Tox21_302658
M4ID: 12476475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 2.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

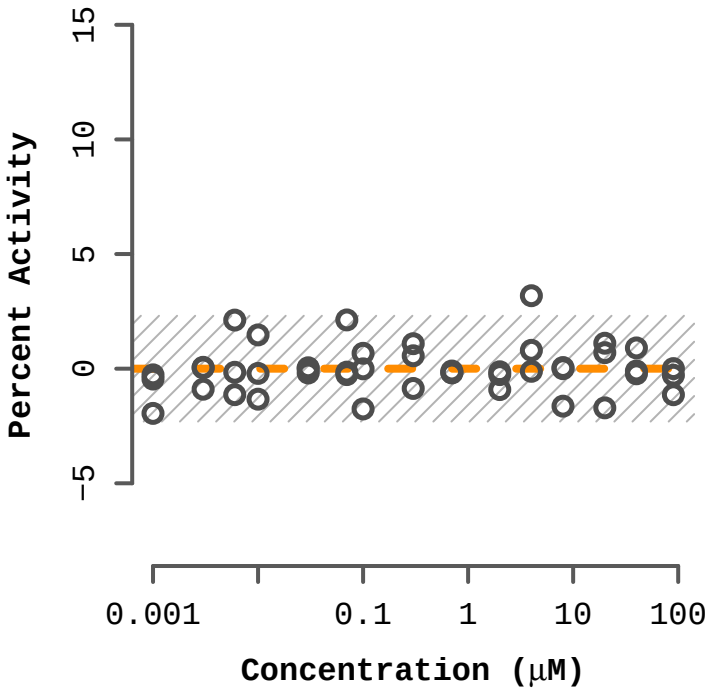
NAME: 1-Octen-3-one
CHID: 47162 **CASRN:** 4312-99-6
SPID(S): Tox21_302710
M4ID: 12476423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 0.774 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

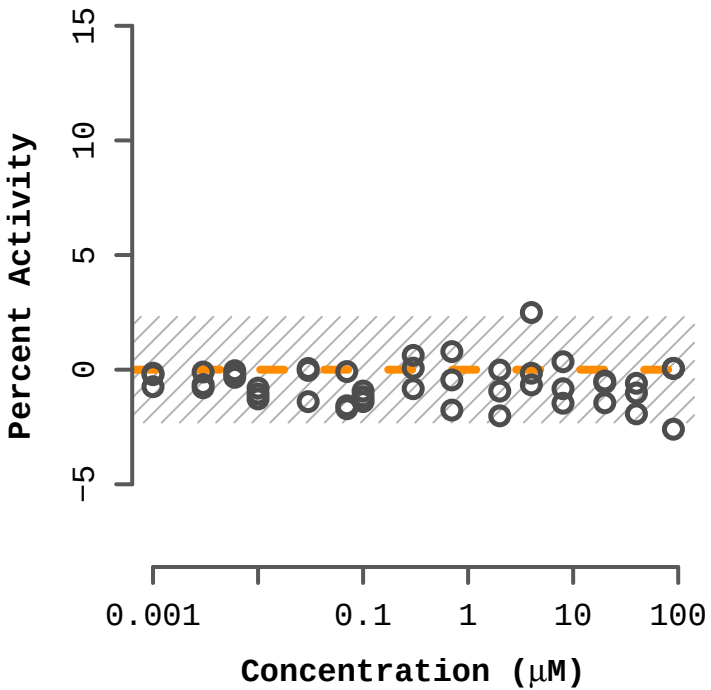
NAME: 6-Acetyl-1,2,3,4-tetrahydronaphthalene
CHID: 47163 **CASRN:** 774-55-0
SPID(S): Tox21_302669
M4ID: 12476464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

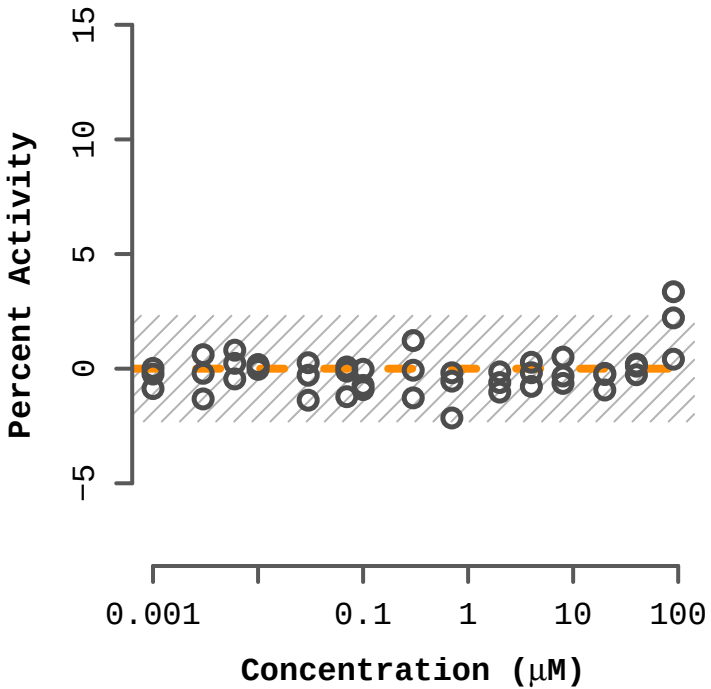
NAME: delta-Octanolactone
CHID: 47164 **CASRN:** 698-76-0
SPID(S): Tox21_302699
M4ID: 12476434

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.561 **MAX_MED:** 0.0686 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

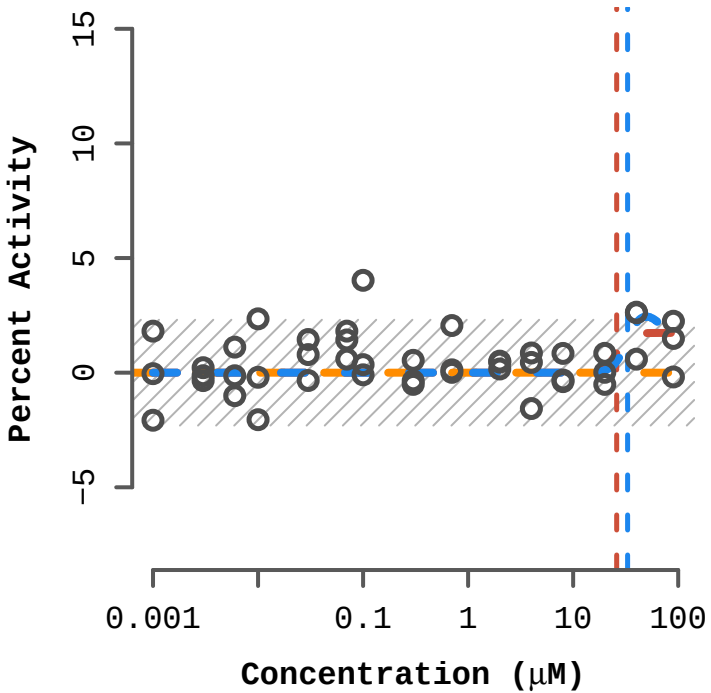
NAME: 7-Methyl-2H-1,5-benzodioxepin-3(4H)-one
CHID: 47165 **CASRN:** 28940-11-6
SPID(S): Tox21_302683
M4ID: 12476450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 2 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(4-Methoxyphenyl)-2-butanone
CHID: 47166 **CASRN:** 104-20-1
SPID(S): Tox21_301165
M4ID: 12477968

HILL MODEL (in red):

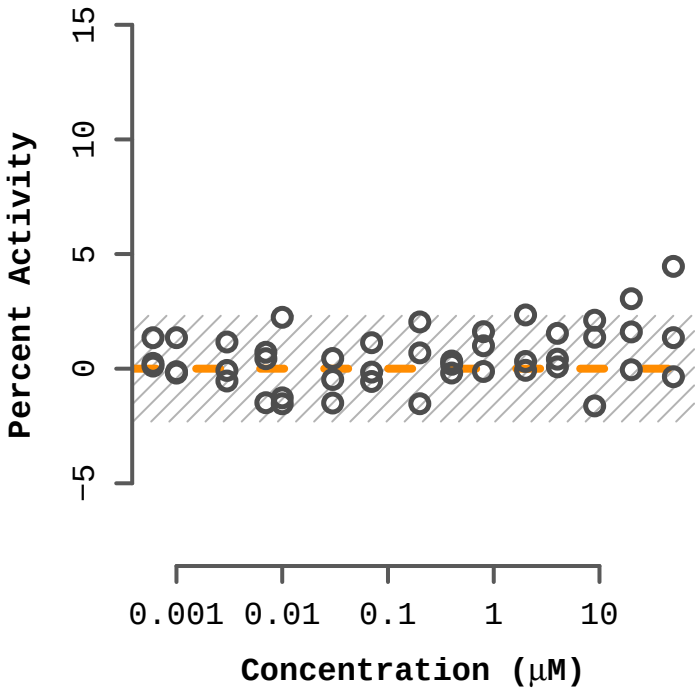
	tp	ga	gw
val:	1.73	1.41	8
sd:	0.476	0.123	7.08

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.91	1.52	6.63	1.94	3.88
sd:	109	9.44	212	7.26	297

	CNST	HILL	GNLS
AIC:	151.92	147.26	150.25
PROB:	0.07	0.76	0.17
RMSE:	1.31	1.18	1.17

MAX_MEAN: 1.95 **MAX_MED:** 2.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

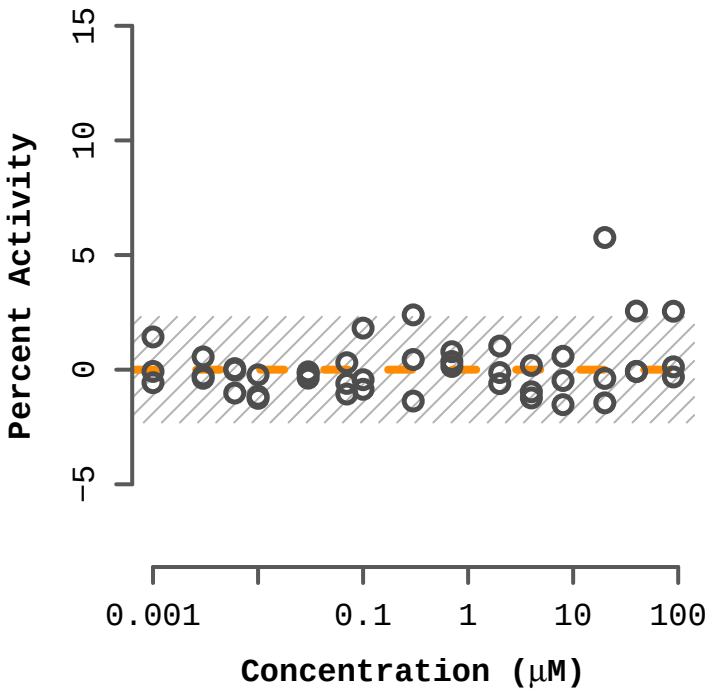
NAME: 4-(4-Methoxyphenyl)-2-butanone
CHID: 47166 **CASRN:** 104-20-1
SPID(S): Tox21_113654
M4ID: 12482558

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.82 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

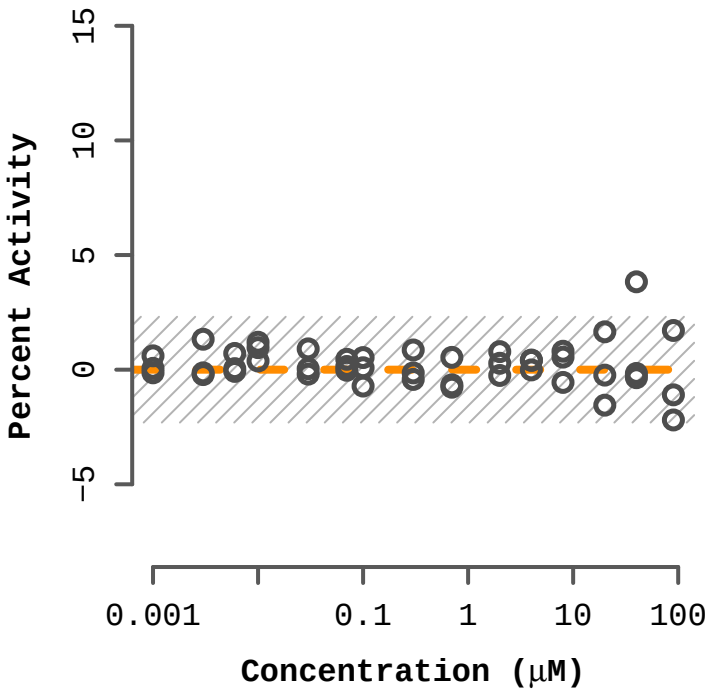
NAME: N-Methylacetamide
CHID: 47167 **CASRN:** 79-16-3
SPID(S): Tox21_300192
M4ID: 12478938

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.445 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

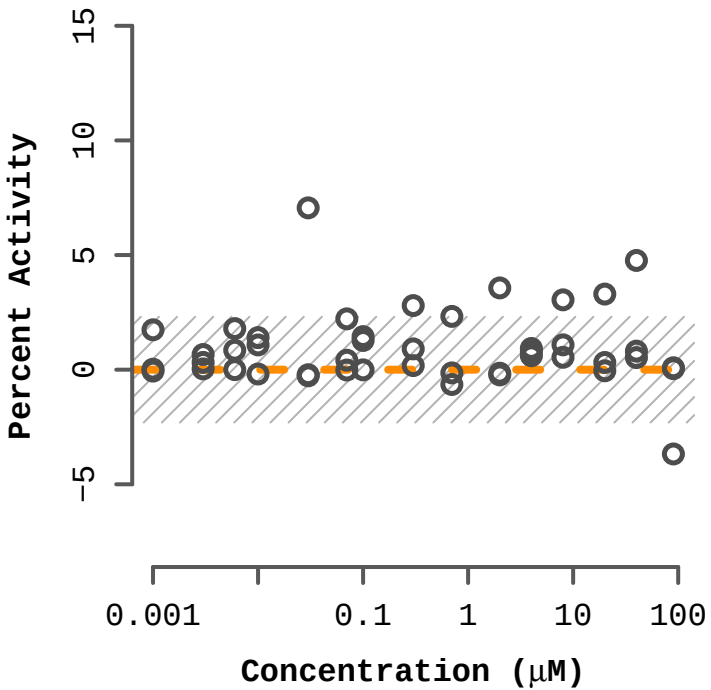
NAME: Isolongifolanone
CHID: 47168 **CASRN:** 29461-14-1
SPID(S): Tox21_302470
M4ID: 12476663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.964 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

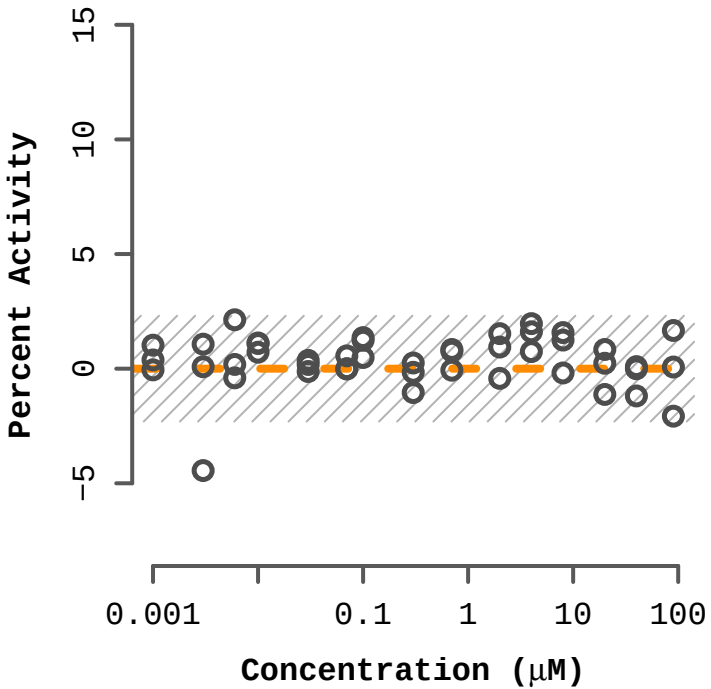
NAME: 5-Methyl-2-thiophenecarboxaldehyde
CHID: 47169 **CASRN:** 13679-70-4
SPID(S): Tox21_302636
M4ID: 12476497

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.87	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

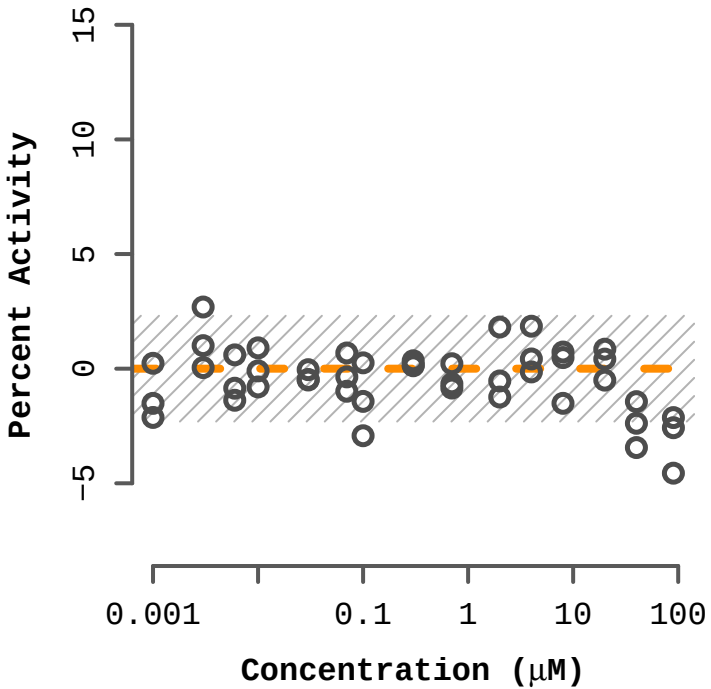
NAME: Sodium pantothenate
CHID: 47173 **CASRN:** 867-81-2
SPID(S): Tox21_302487
M4ID: 12476646

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

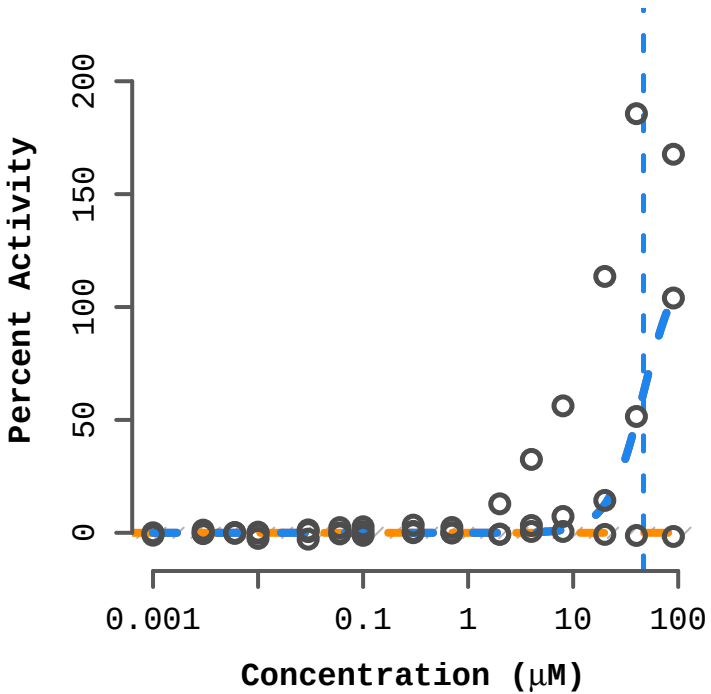
NAME: Bis(2−butoxyethyl) phthalate
CHID: 47174 **CASRN:** 117−83−9
SPID(S): Tox21_303550
M4ID: 12475595

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(2-butoxyethyl) phthalate
CHID: 47174 CASRN: 117-83-9
SPID(S): Tox21_201843
M4ID: 12480409

HILL MODEL (in red):

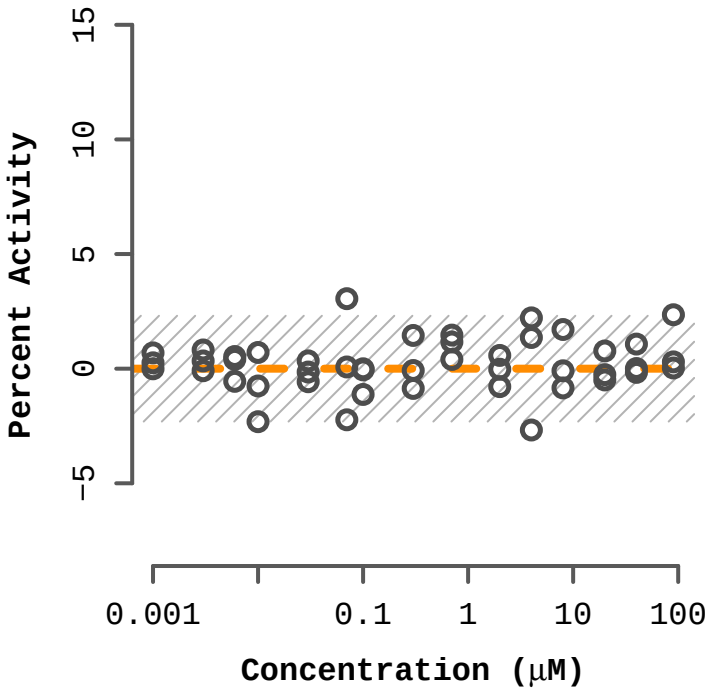
	tp	ga	gw
val:	124	1.67	2.57
sd:	22	0.0874	0.884

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	124	1.67	2.57	3.3	17.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	402.47	393.25	397.25
PROB:	0.01	0.87	0.12
RMSE:	45.62	33.67	33.67

MAX_MEAN: 90 **MAX_MED:** 104 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

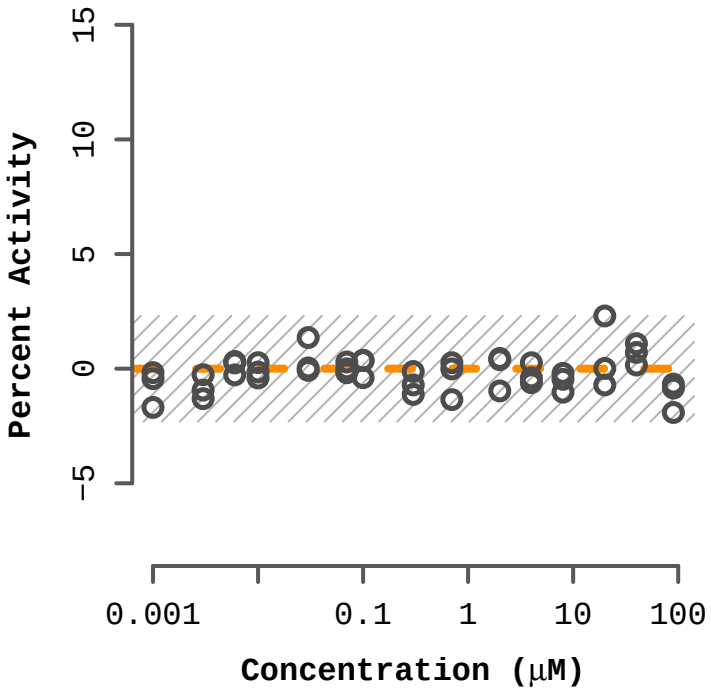
NAME: 4-Phenyl-1-cyclohexene
CHID: 47176 **CASRN:** 4994-16-5
SPID(S): Tox21_302516
M4ID: 12476617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

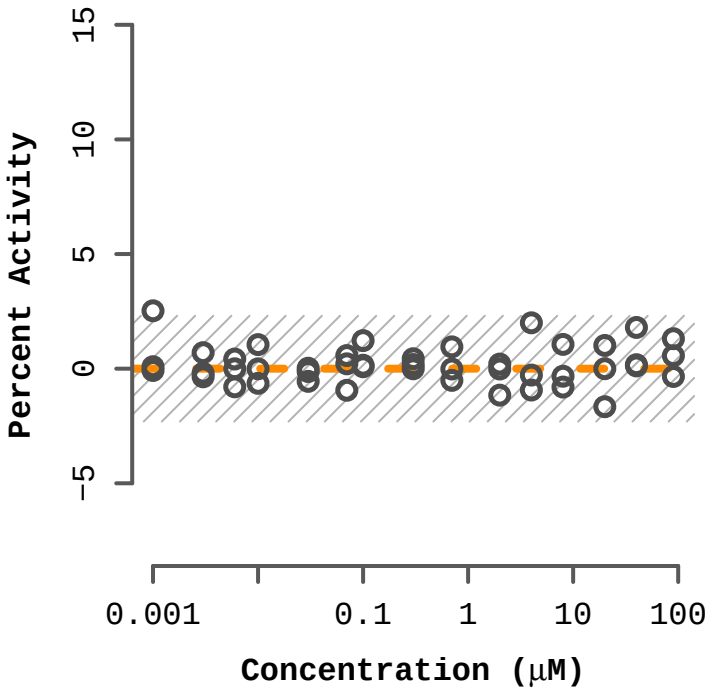
NAME: 4-Phenyltoluene
CHID: 47177 **CASRN:** 644-08-6
SPID(S): Tox21_302610
M4ID: 12476523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.654 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

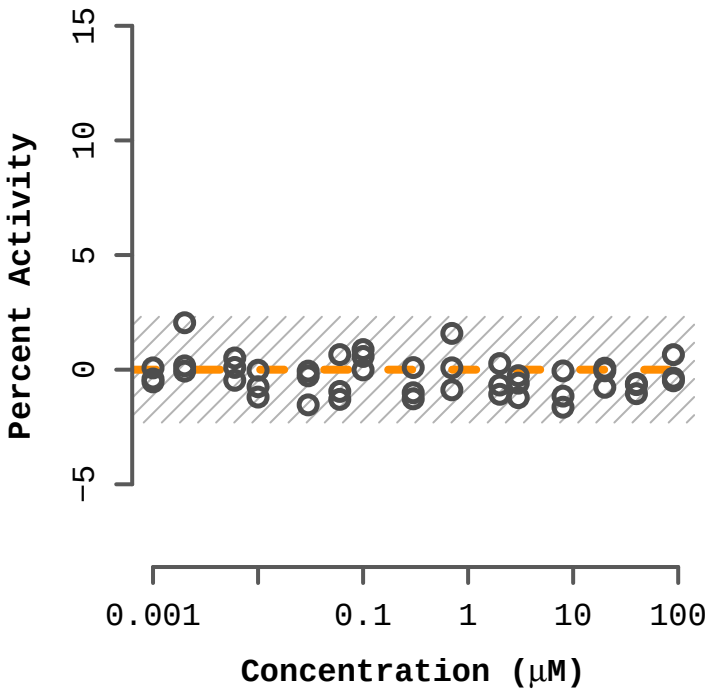
NAME: 2-Ethylhexyl octadecanoate
CHID: 47178 **CASRN:** 22047-49-0
SPID(S): Tox21_302619
M4ID: 12476514

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.846 **MAX_MED:** 0.567 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

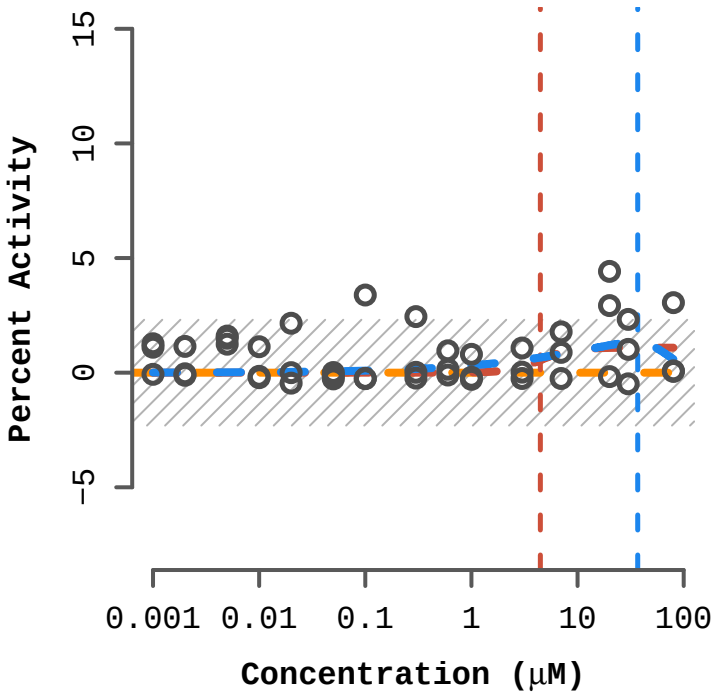
NAME: Isocetyl stearate
CHID: 47179 **CASRN:** 25339-09-7
SPID(S): Tox21_303638
M4ID: 12475507

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triisodecyl trimellitate
CHID: 47180 **CASRN:** 36631-30-8
SPID(S): Tox21_302650
M4ID: 12476483

HILL MODEL (in red):

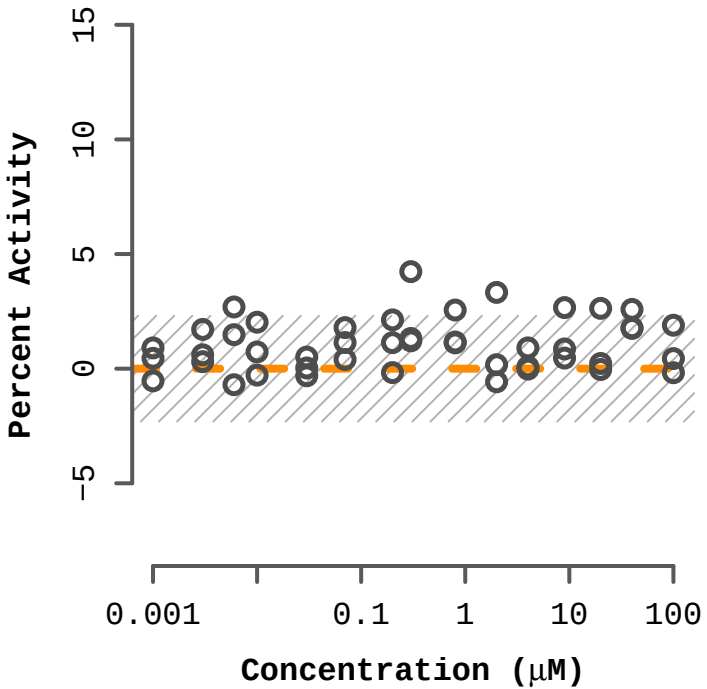
	tp	ga	gw
val:	1.09	0.65	3.07
sd:	0.536	0.365	5.01

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.95	1.57	0.589	1.82	3.64
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	151.7	150.5	153.45
PROB:	0.31	0.56	0.13
RMSE:	1.38	1.21	1.19

MAX_MEAN: 2.39 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

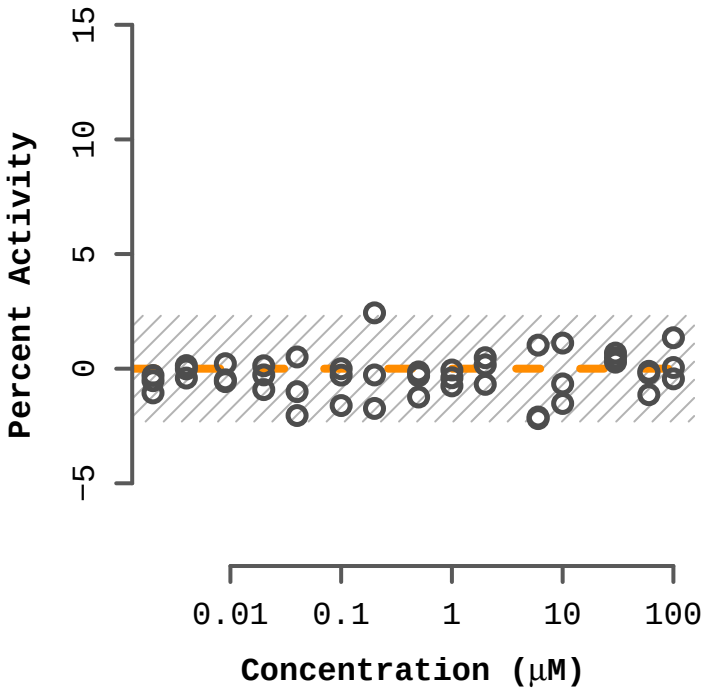
NAME: Propylene glycol dipelargonate
CHID: 47182 **CASRN:** 41395-83-9
SPID(S): Tox21_303622
M4ID: 12475523

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 2.26 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

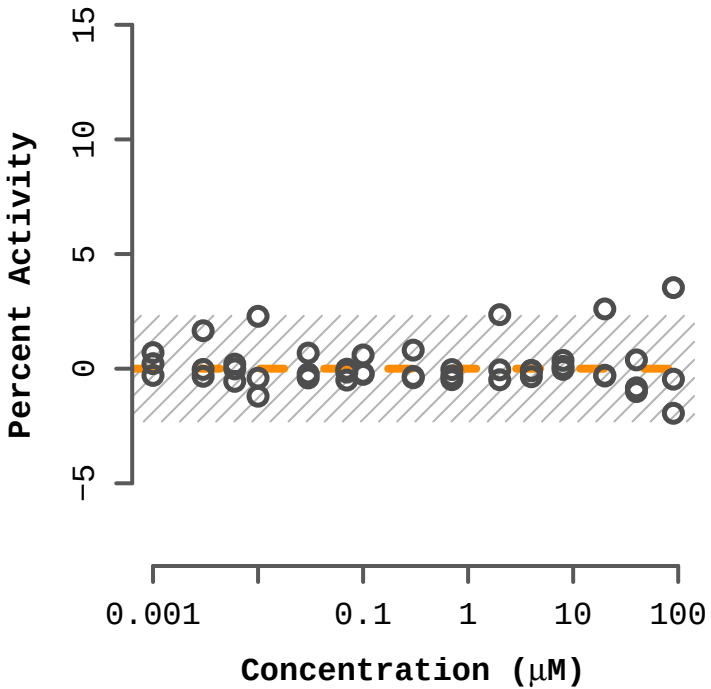
NAME: Triethanolamine Laurate
CHID: 47183 **CASRN:** 2224-49-9
SPID(S): Tox21_302696
M4ID: 12476437

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** 0.475 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

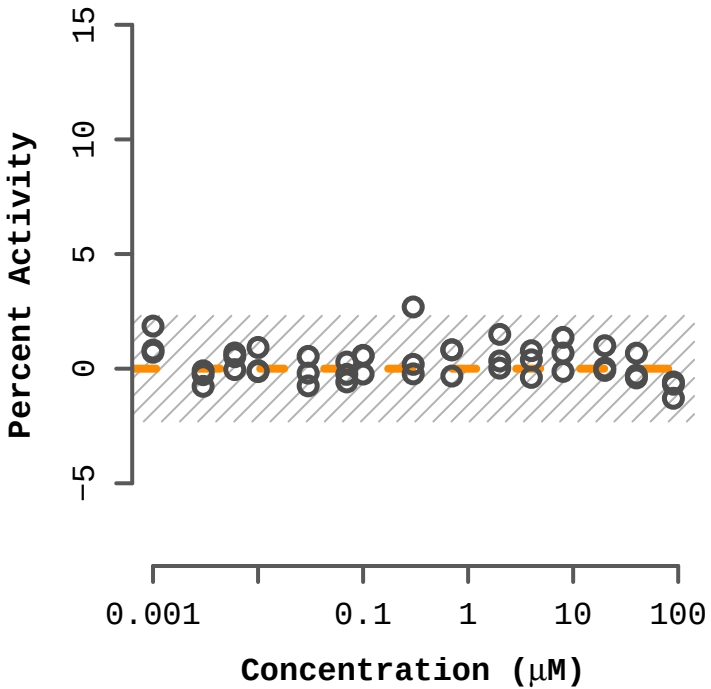
NAME: 2,3,5-Trimethylphenol
CHID: 47184 **CASRN:** 697-82-5
SPID(S): Tox21_302716
M4ID: 12476417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.44	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.668 **MAX_MED:** 0.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

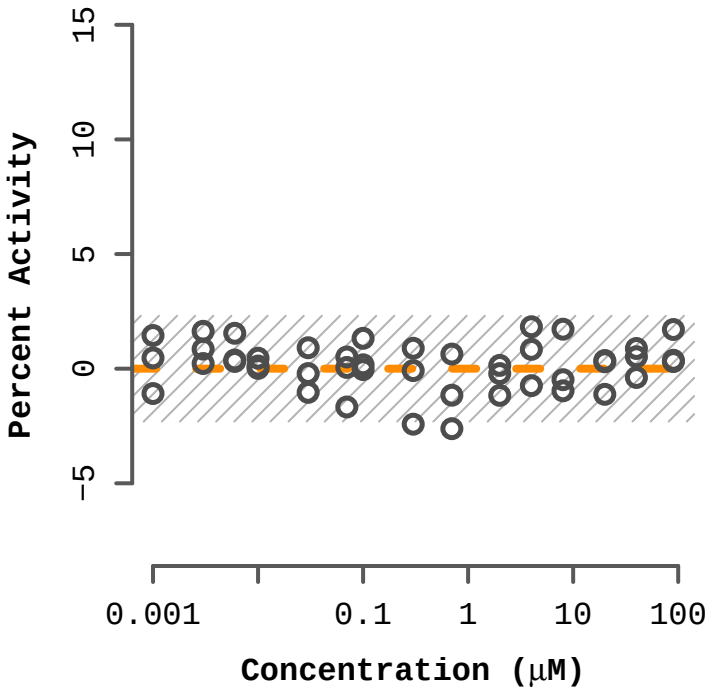
NAME: Isopentyl benzoate
CHID: 47185 **CASRN:** 94-46-2
SPID(S): Tox21_302461
M4ID: 12476672

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

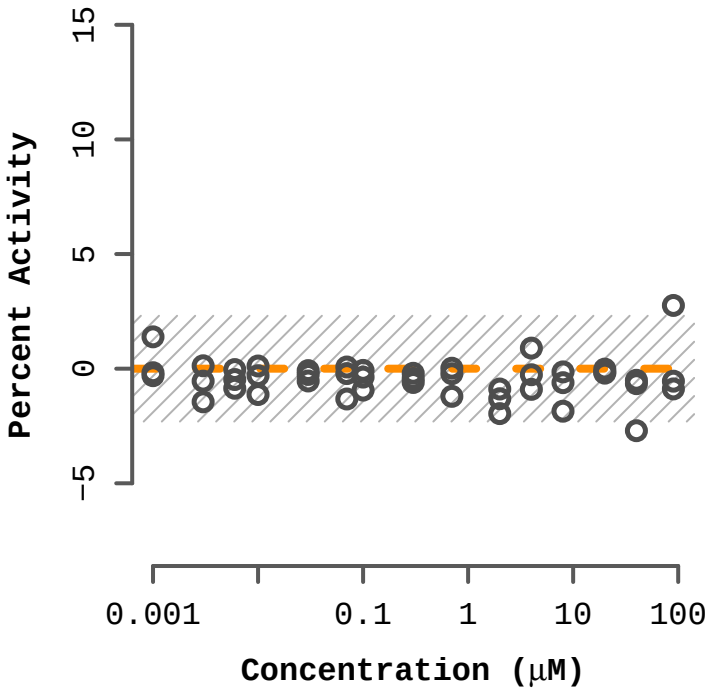
NAME: Isobutyl salicylate
CHID: 47186 **CASRN:** 87-19-4
SPID(S): Tox21_302515
M4ID: 12476618

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.904 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

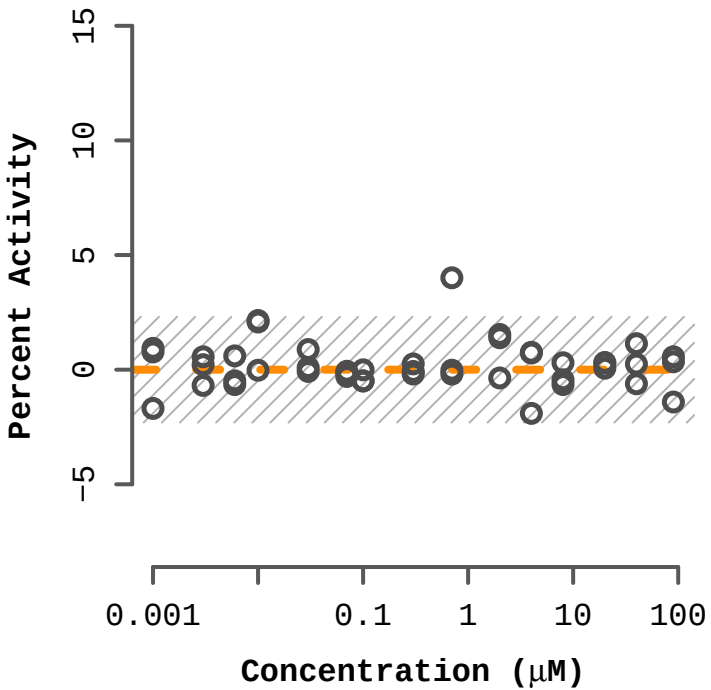
NAME: Citronellyl propionate
CHID: 47187 CASRN: 141-14-0
SPID(S): Tox21_302679
M4ID: 12476454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.445 MAX_MED: −0.144 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

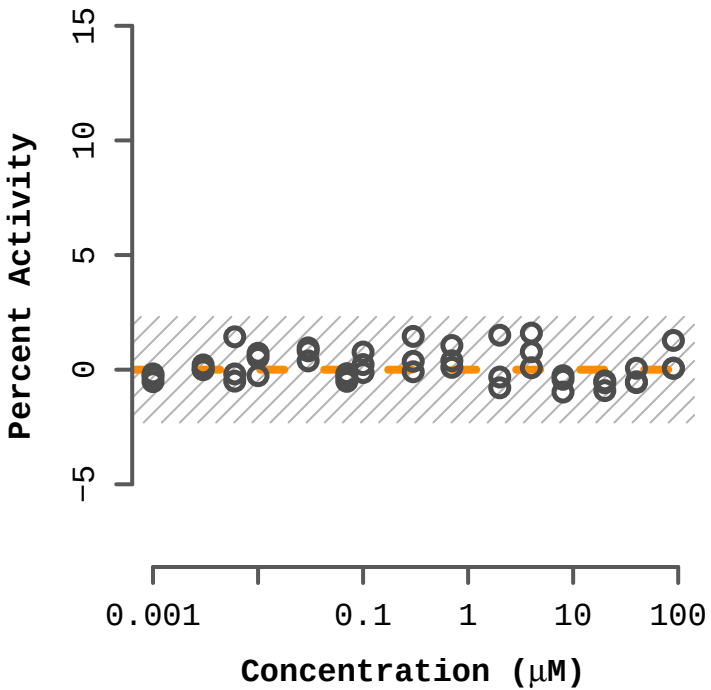
NAME: 2-Cyclohexylethyl acetate
CHID: 47188 CASRN: 21722-83-8
SPID(S): Tox21_302452
M4ID: 12476681

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.4 MAX_MED: 2.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

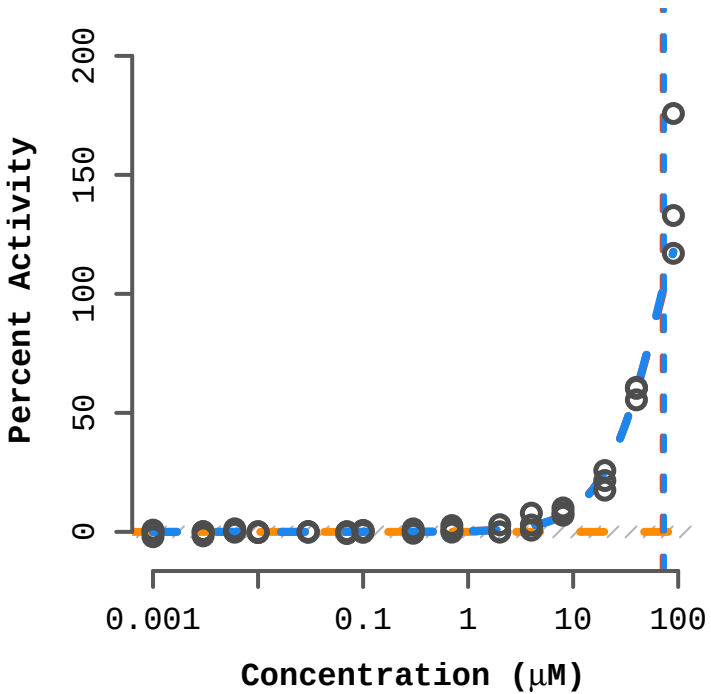
NAME: Decyl acetate
CHID: 47189 **CASRN:** 112-17-4
SPID(S): Tox21_302572
M4ID: 12476561

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.823 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: gamma-Dodecalactone
CHID: 47190 CASRN: 2305-05-7
SPID(S): Tox21_302617
M4ID: 12476516

HILL MODEL (in red):

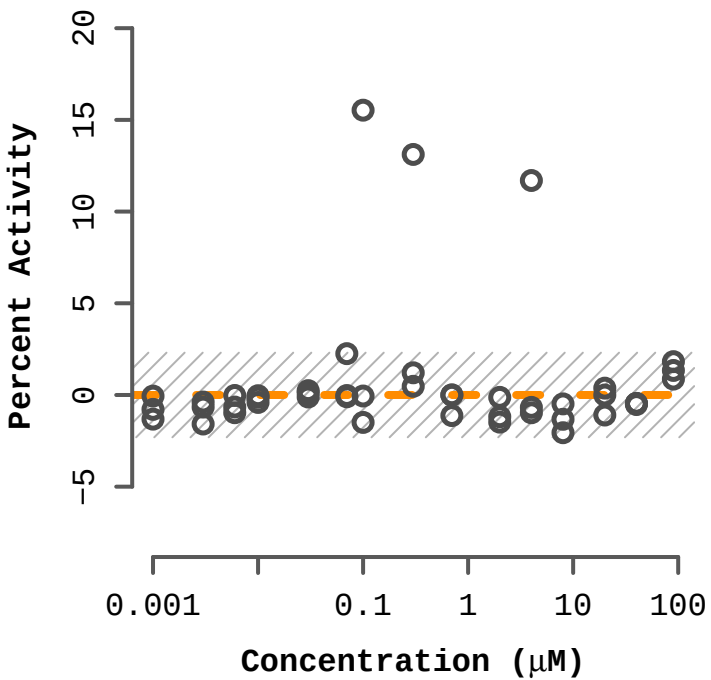
	tp	ga	gw
val:	199	1.85	1.52
sd:	4.17	0.014	0.0417

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	211	1.87	1.52	2.15	7.88
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	403.65	225.48	229.02
PROB:	0	0.85	0.15
RMSE:	40.67	9.15	9.17

MAX_MEAN: 142 MAX_MED: 133 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

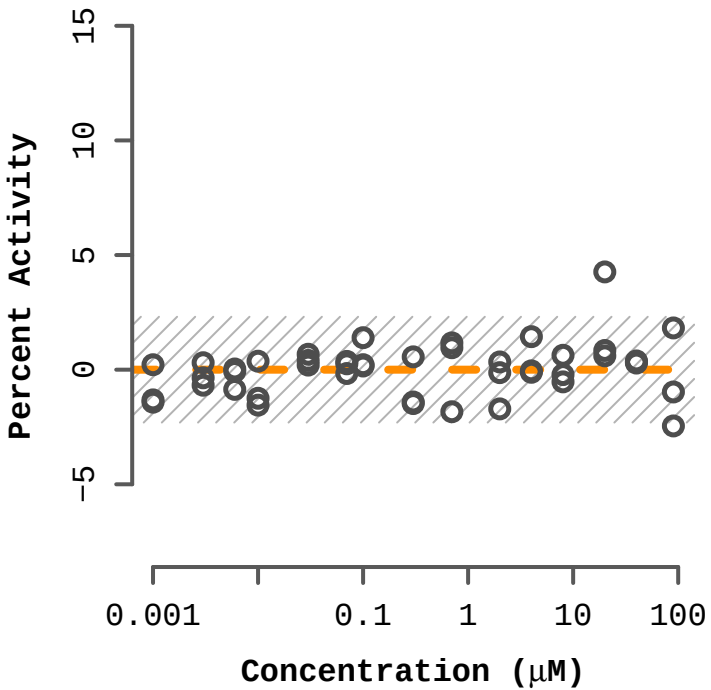
NAME: Linalyl benzoate
CHID: 47191 **CASRN:** 126-64-7
SPID(S): Tox21_302668
M4ID: 12476465

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.61	NA	NA

MAX_MEAN: 4.93 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

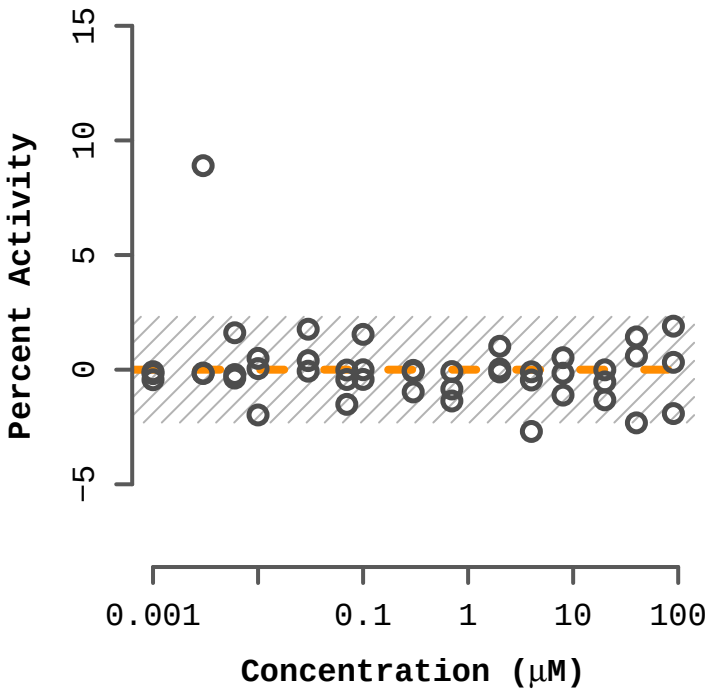
NAME: trans−2,cis−6−Nonadien−1−ol
CHID: 47192 **CASRN:** 28069−72−9
SPID(S): Tox21_302474
M4ID: 12476659

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 0.959 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

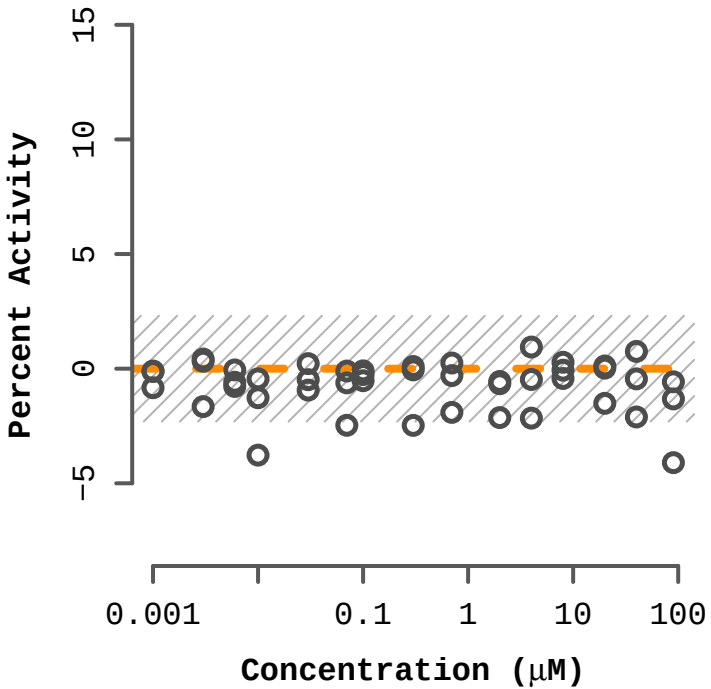
NAME: Rhodinol
CHID: 47193 **CASRN:** 141-25-3
SPID(S): Tox21_302625
M4ID: 12476508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.67	NA	NA

MAX_MEAN: 2.86 **MAX_MED:** 0.592 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

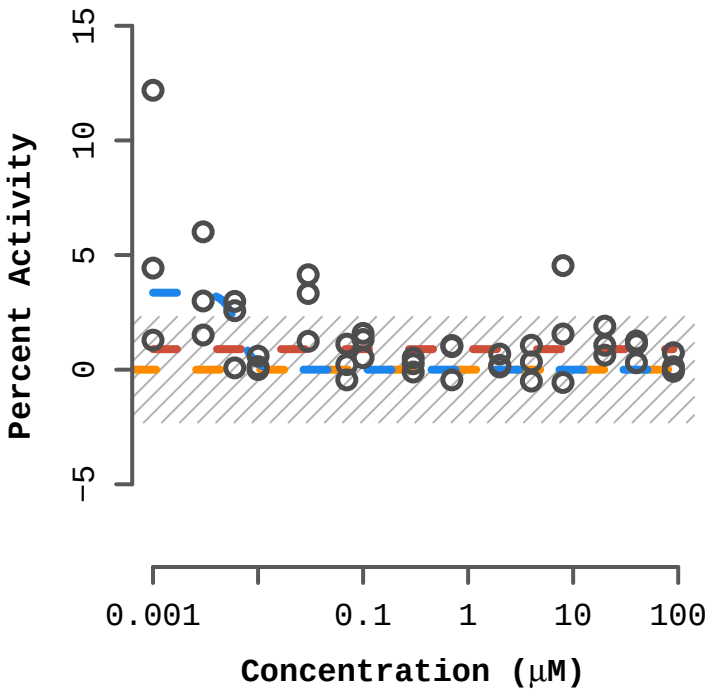
NAME: p-Mentha-8-thiol-3-one
CHID: 47195 **CASRN:** 38462-22-5
SPID(S): Tox21_302579
M4ID: 12476554

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: −0.0704 **MAX_MED:** 0.328 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5H-5-Methyl-6,7-dihydrocyclopenta[b]pyrazine
CHID: 47196 **CASRN:** 23747-48-0
SPID(S): Tox21_302522
M4ID: 12476611

HILL MODEL (in red):

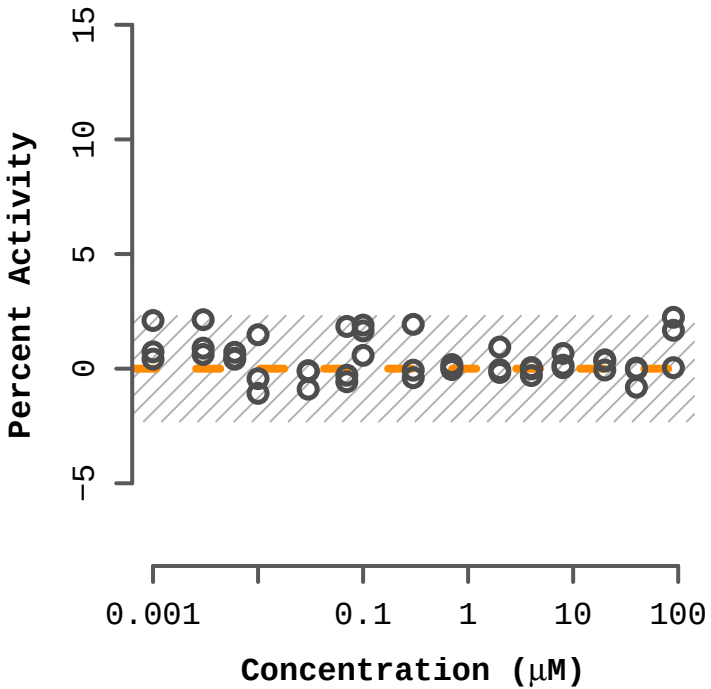
	tp	ga	gw
val:	0.894	−4.94	3.93
sd:	0.191	1670	3370

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.36	−4.99	3.39	−2.18	5.9
sd:	0.877	894	1530	0.0849	5.85

	CNST	HILL	GNLS
AIC:	193.83	179.3	181.5
PROB:	0	0.75	0.25
RMSE:	2.61	2.24	1.95

MAX_MEAN: 5.97 **MAX_MED:** 4.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

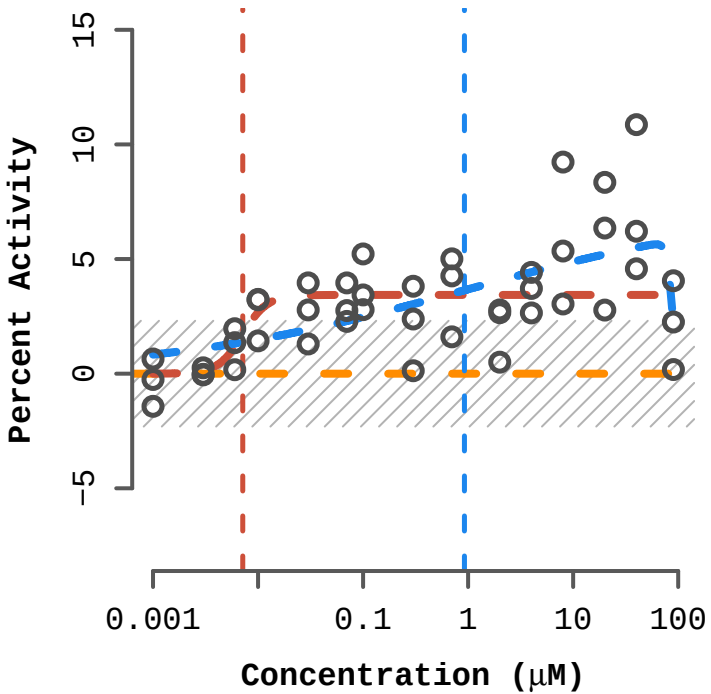
NAME: Fenchyl acetate
CHID: 47197 **CASRN:** 13851-11-1
SPID(S): Tox21_302571
M4ID: 12476562

HILL MODEL: Not applicable.

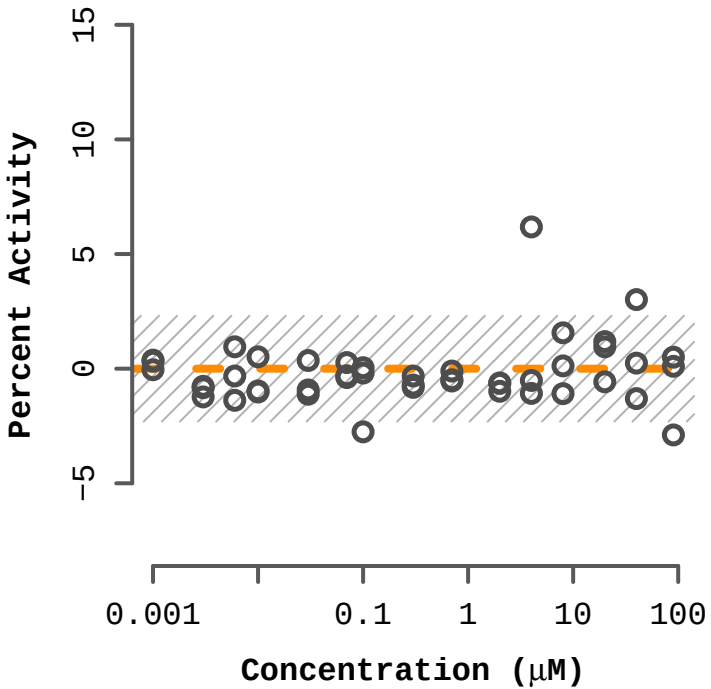
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.68 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ethyl 2-methylpentanoate
CHID:    47198   CASRN: 39255-32-8
SPID(S): Tox21_302712
M4ID:    12476421

HILL MODEL (in red):
      tp       ga       gw
val:  3.44     -2.15    3.73
sd:   0.3      0.0974   3.23

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.28     -0.0353  0.3      1.94     15.7
sd:   12.9     5.87     0.413    0.0337   36.2

      CNST        HILL        GNLS
AIC:  254.49      191.5       193.42
PROB: 0           0.72        0.28
RMSE: 3.93        2.08        1.81

MAX_MEAN: 7.22      MAX_MED: 6.35      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

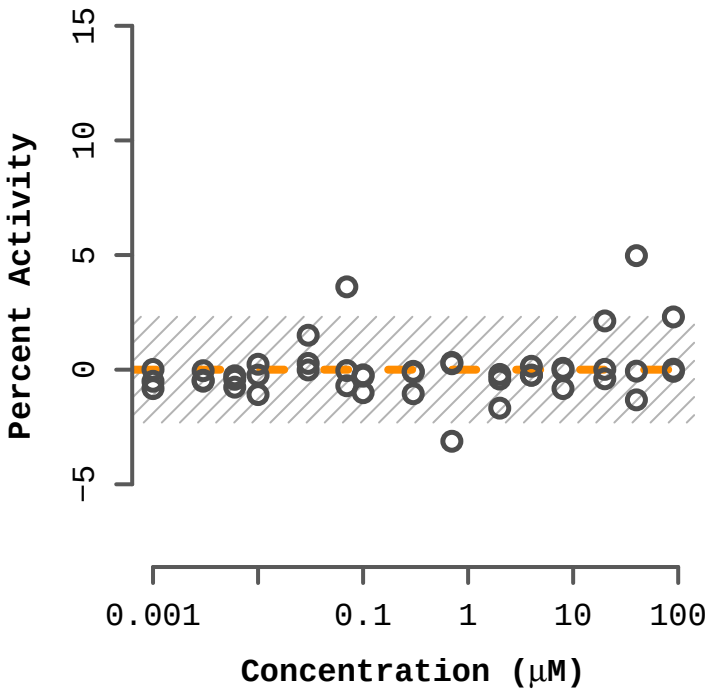
NAME: 2-Methoxy-4-propylphenol
CHID: 47199 **CASRN:** 2785-87-7
SPID(S): Tox21_302722
M4ID: 12476411

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 0.954 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

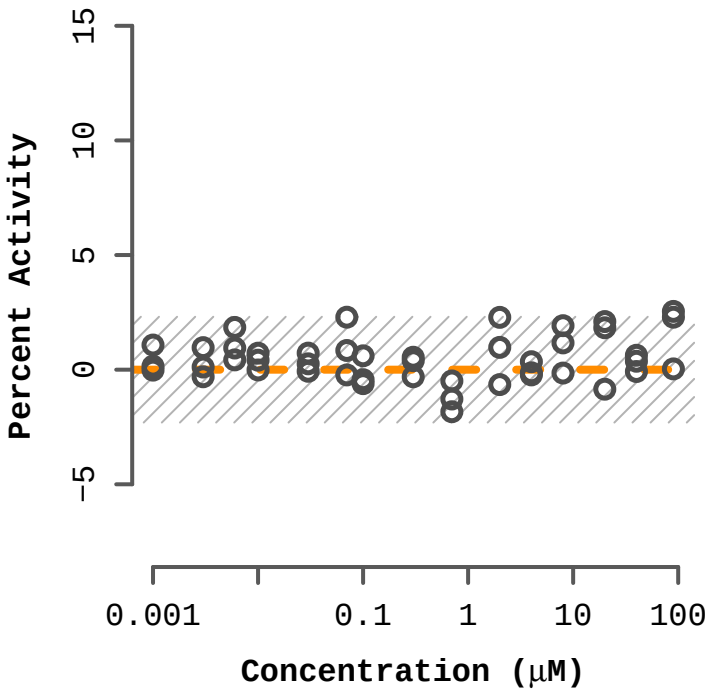
NAME: Dihydro-beta-ionone
CHID: 47200 **CASRN:** 17283-81-7
SPID(S): Tox21_302666
M4ID: 12476467

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.275 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

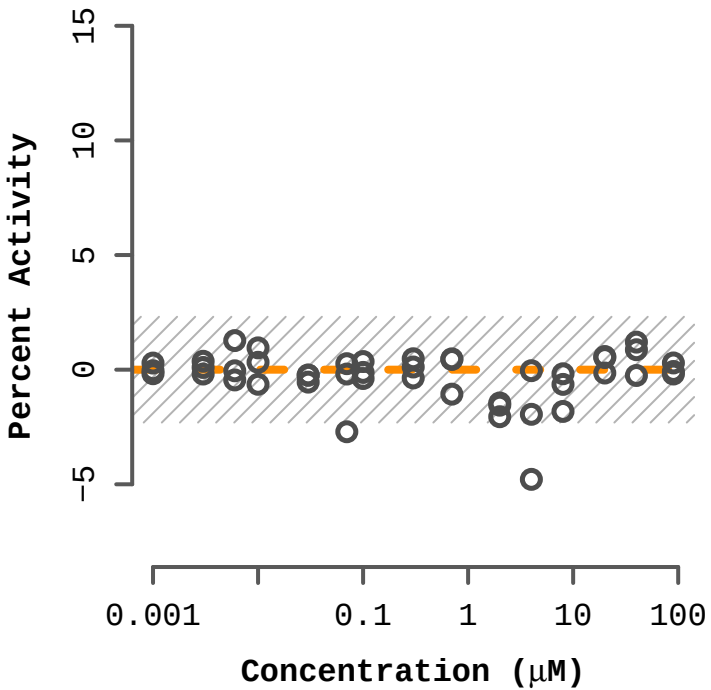
NAME: Vanillin isobutyrate
CHID: 47201 **CASRN:** 20665-85-4
SPID(S): Tox21_302542
M4ID: 12476591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

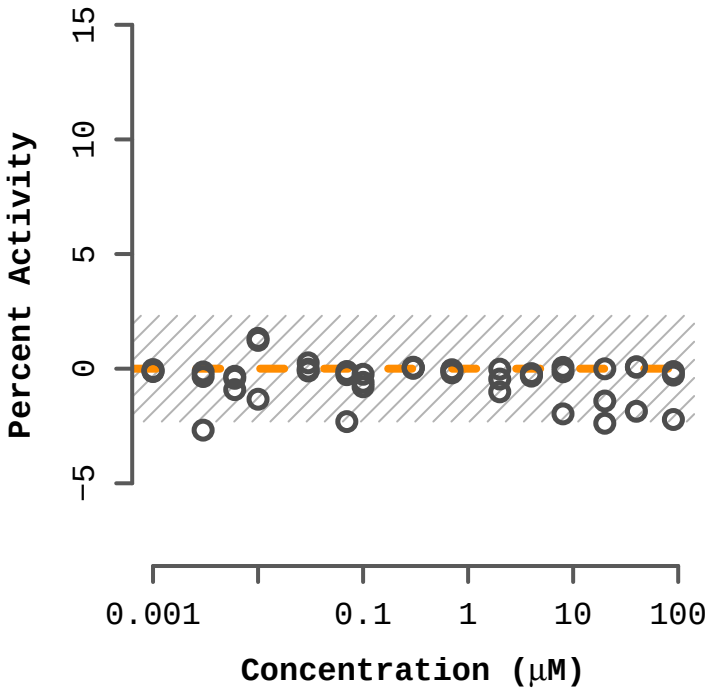
NAME: alpha−Farnesene
CHID: 47202 **CASRN:** 502−61−4
SPID(S): Tox21_303626
M4ID: 12475519

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

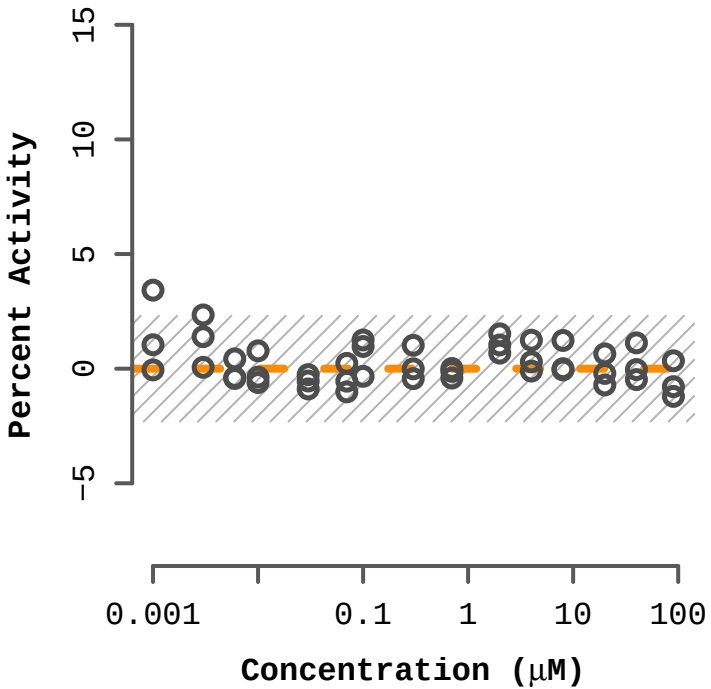
NAME: Phenoxyethyl propionate
CHID: 47203 CASRN: 23495-12-7
SPID(S): Tox21_302718
M4ID: 12476415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.409 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

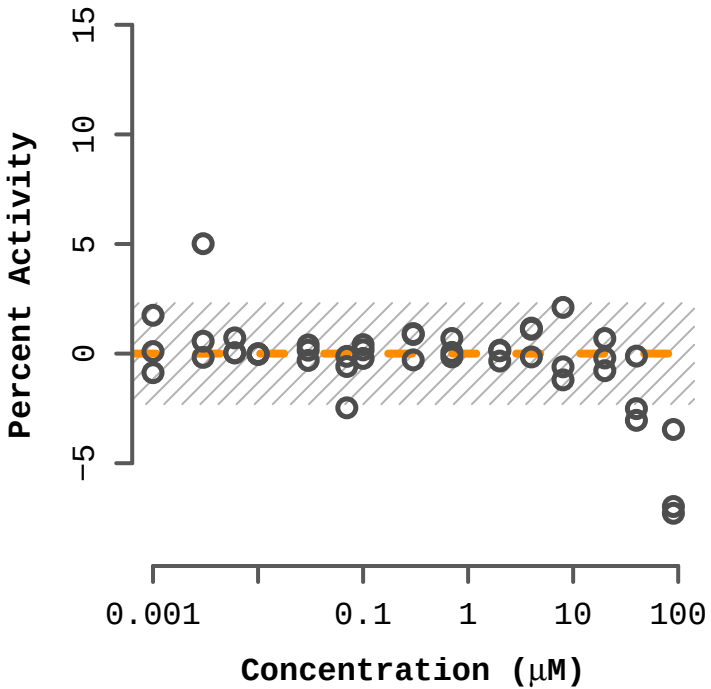
NAME: 2-Ethylhexyl trans-4-methoxycinnamate
CHID: 47205 **CASRN:** 83834-59-7
SPID(S): Tox21_302576
M4ID: 12476557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

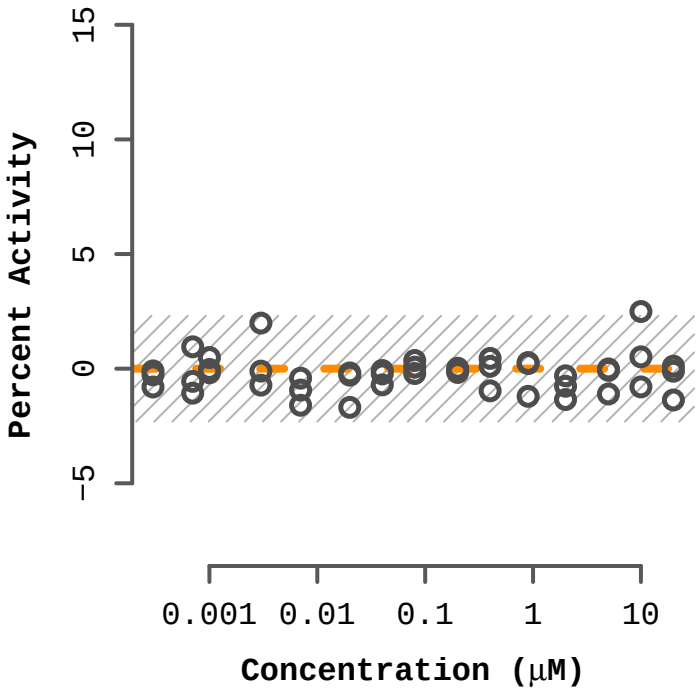
NAME: trans-2-Methoxycinnamaldehyde
CHID: 47206 **CASRN:** 60125-24-8
SPID(S): Tox21_303635
M4ID: 12475510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	166.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.99	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

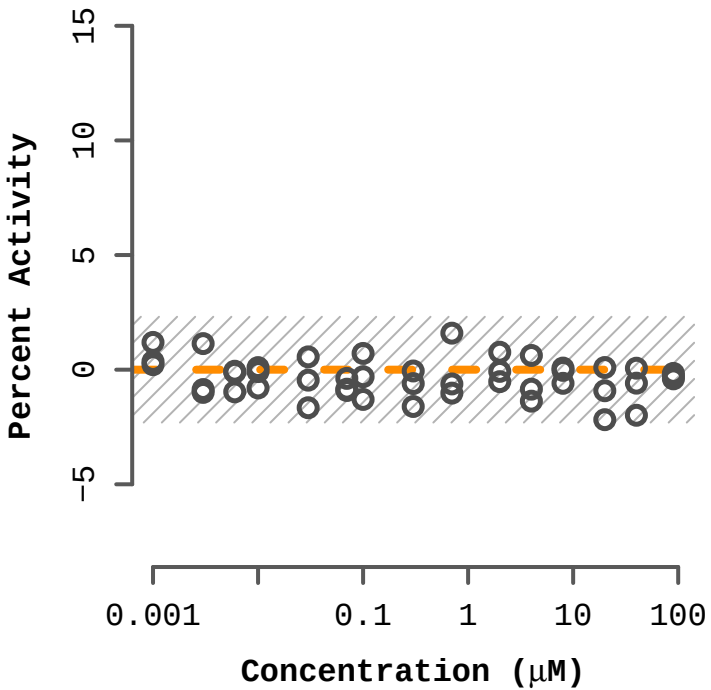
NAME: Sodium bisulfite, mixture of NaHSO3 and Na2S2O5
CHID: 47218 CASRN: NOCAS_47218
SPID(S): Tox21_303826
M4ID: 12475362

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.739 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

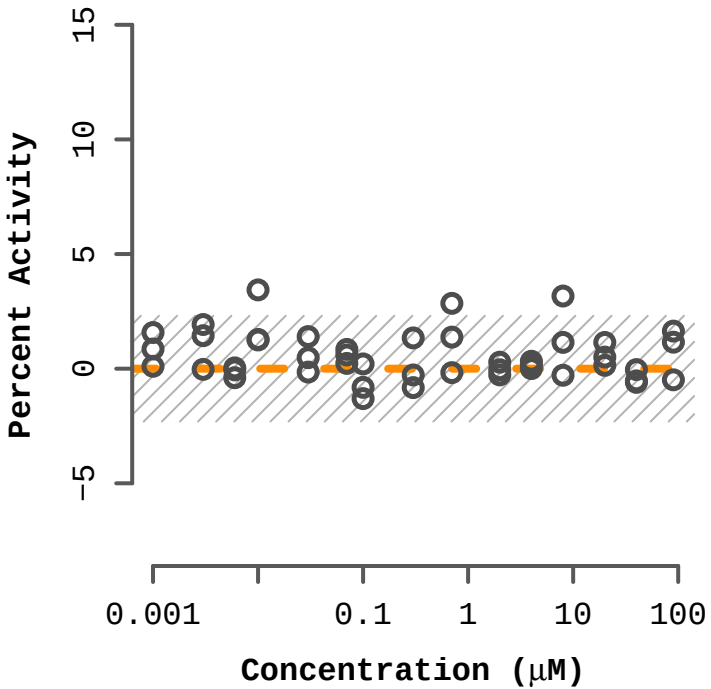
NAME: Farnesyl acetate
CHID: 47222 **CASRN:** 29548-30-9
SPID(S): Tox21_303761
M4ID: 12475427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.59 **MAX_MED:** 0.358 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

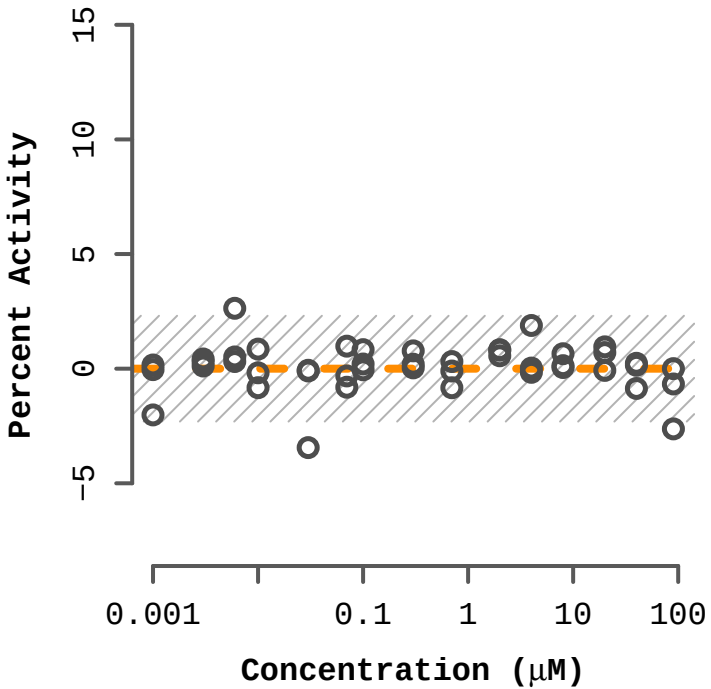
NAME: (S)-Citronellene
CHID: 47236 **CASRN:** 10281-55-7
SPID(S): Tox21_300803
M4ID: 12478330

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

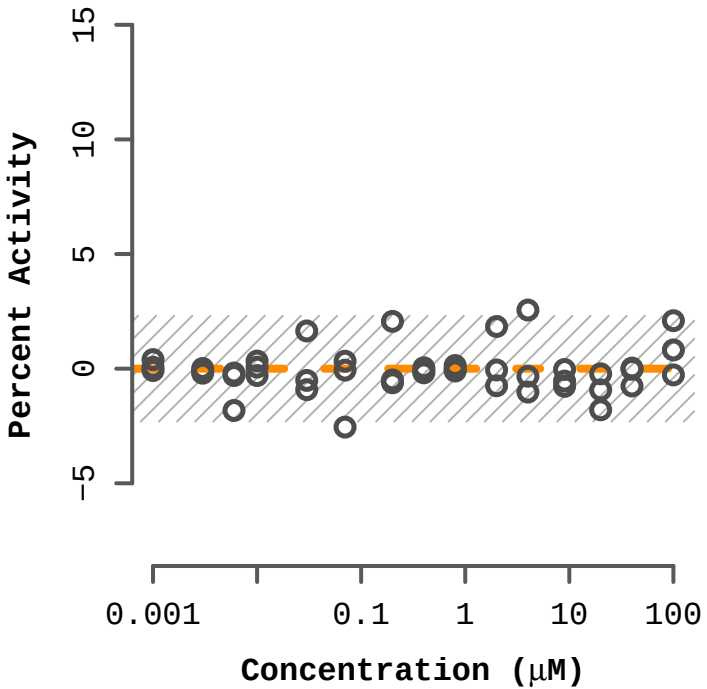
NAME: cis−Nerolidol
CHID: 47239 **CASRN:** 3790−78−1
SPID(S): Tox21_302456
M4ID: 12476677

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

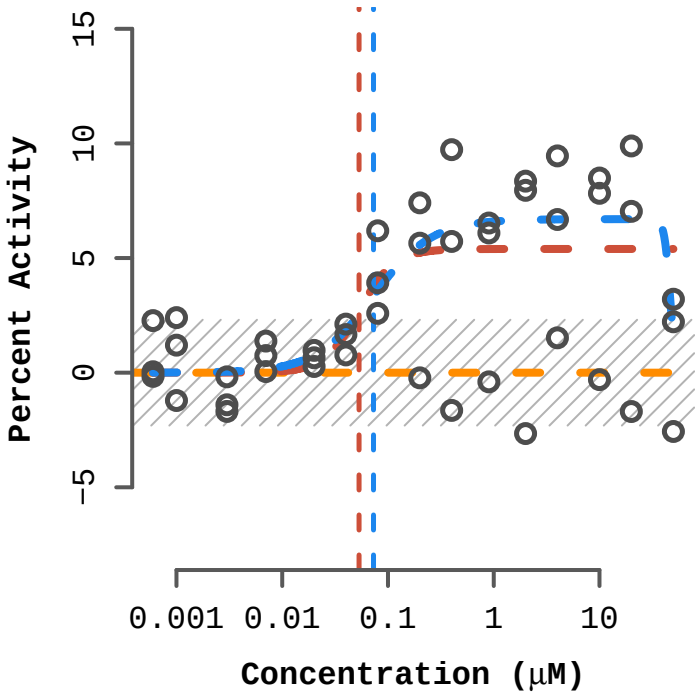
NAME: Pyrimidine−2,4,5,6(1H,3H)−tetrone tetrahydrate
CHID: 47241 **CASRN:** 6010−91−9
SPID(S): Tox21_302662
M4ID: 12476471

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 0.819 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4−Diaminoanisole sulfate hydrate
CHID: 47242 CASRN: 123333−56−2
SPID(S): Tox21_302700
M4ID: 12476433

HILL MODEL (in red):

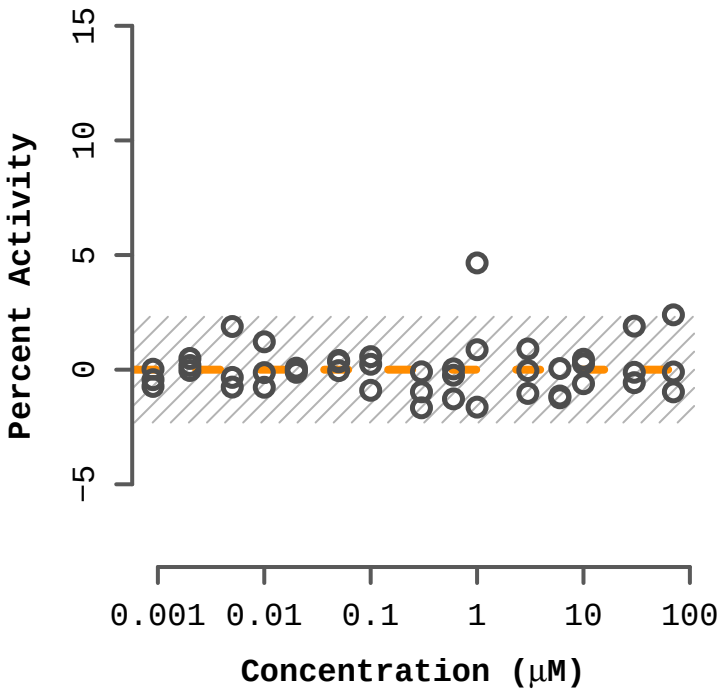
	tp	ga	gw
val:	5.4	−1.27	2.63
sd:	0.853	0.154	2.55

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.7	−1.14	1.59	1.67	16.2
sd:	0.889	0.208	1.2	0.164	83.9

	CNST	HILL	GNLS
AIC:	269.06	240.93	236.81
PROB:	0	0.11	0.89
RMSE:	4.64	3.27	3.24

MAX_MEAN: 5.89 MAX_MED: 7.96 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

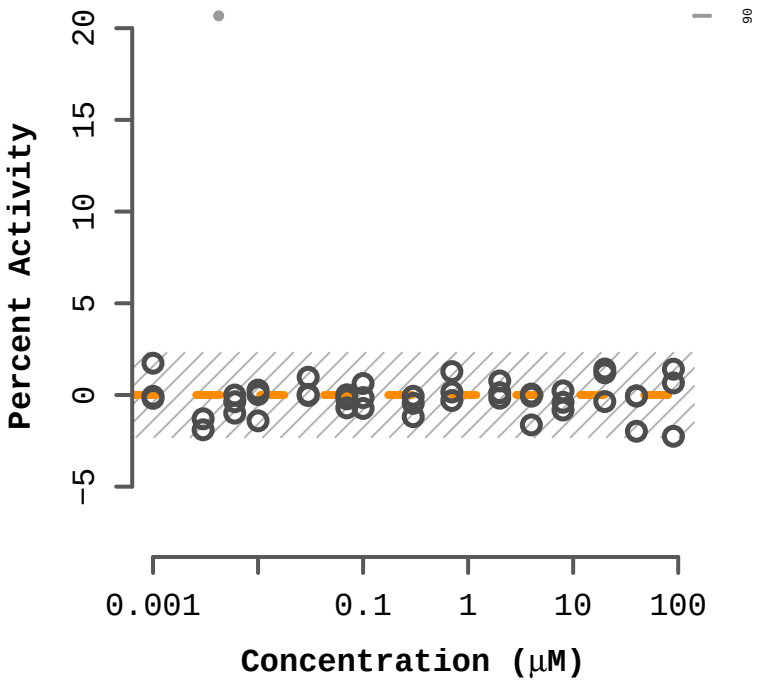
NAME: Ammonium glycyrrhizinate trihydrate
CHID: 47243 **CASRN:** 911217-00-0
SPID(S): Tox21_302526
M4ID: 12476607

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.872 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

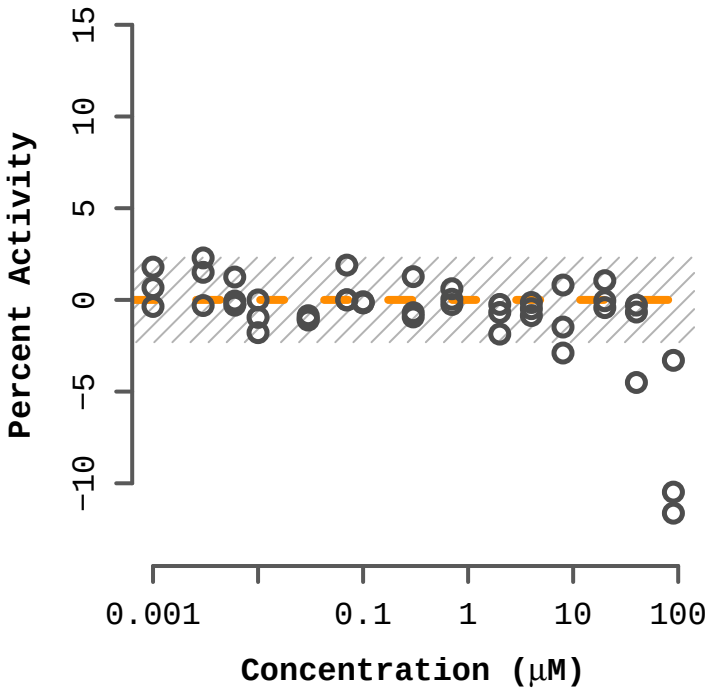
NAME: 3-Cyclohexylpropan-1-ol
CHID: 47244 CASRN: 1124-63-6
SPID(S): Tox21_303632
M4ID: 12475513 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.12	NA	NA
PROB:	1	NA	NA
RMSE:	13.47	NA	NA

MAX_MEAN: 29 MAX_MED: 1.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

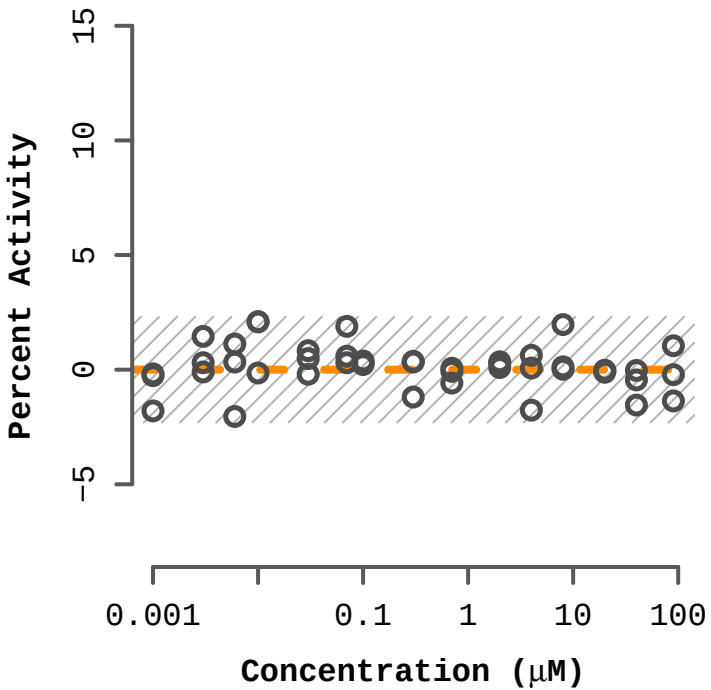
NAME: Darbufelone mesylate
CHID: 47246 **CASRN:** 139340-56-0
SPID(S): Tox21_300202
M4ID: 12478928

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.67	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

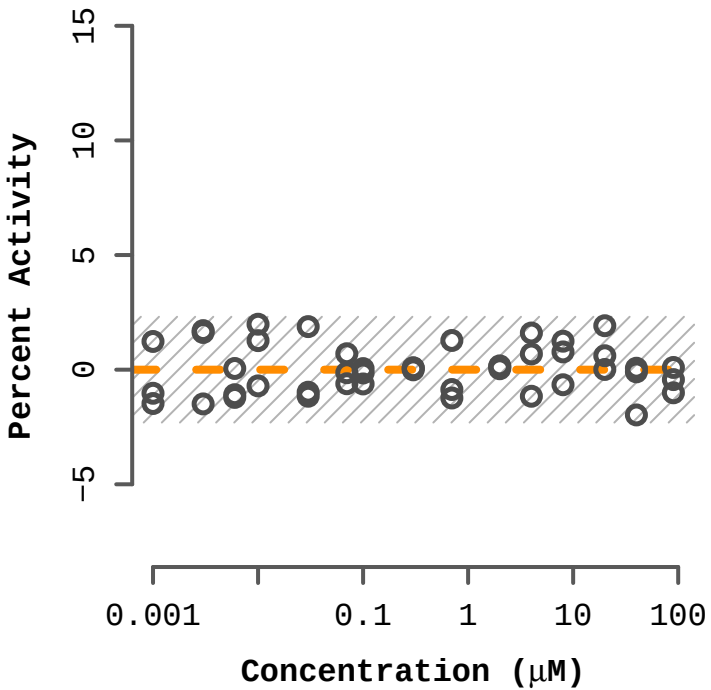
NAME: CI−1018
CHID: 47248 CASRN: NOCAS_47248
SPID(S): Tox21_300203
M4ID: 12478927

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.35 MAX_MED: 2.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

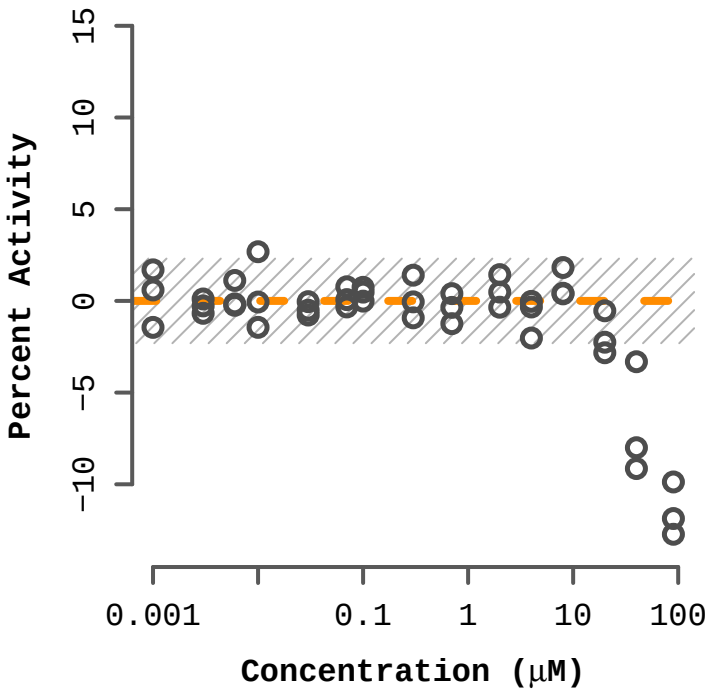
NAME: Fandosentan potassium salt
CHID: 47249 **CASRN:** 221246-12-4
SPID(S): Tox21_300204
M4ID: 12478926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

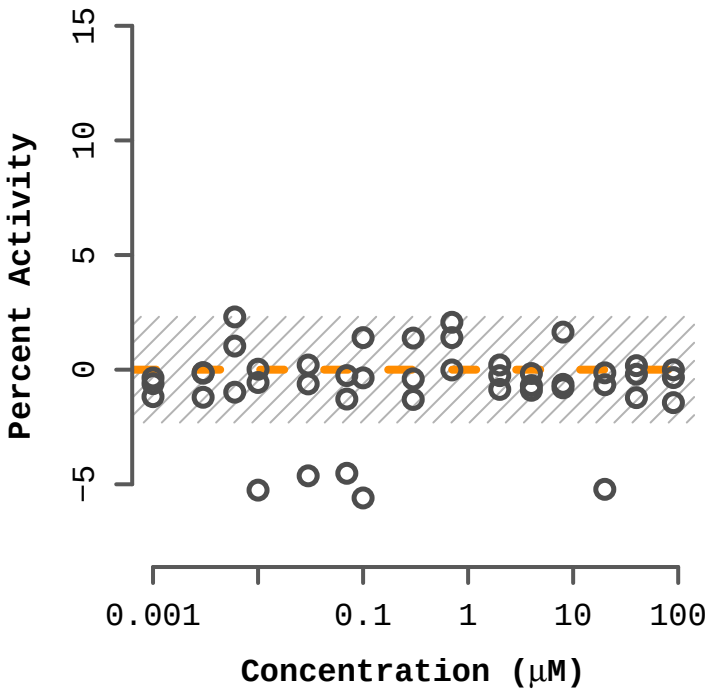
NAME: CP−122721
CHID: 47251 **CASRN:** 145742−28−5
SPID(S): Tox21_300205
M4ID: 12478925

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.69	NA	NA
PROB:	1	NA	NA
RMSE:	3.67	NA	NA

MAX_MEAN: 0.876 **MAX_MED:** 0.599 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

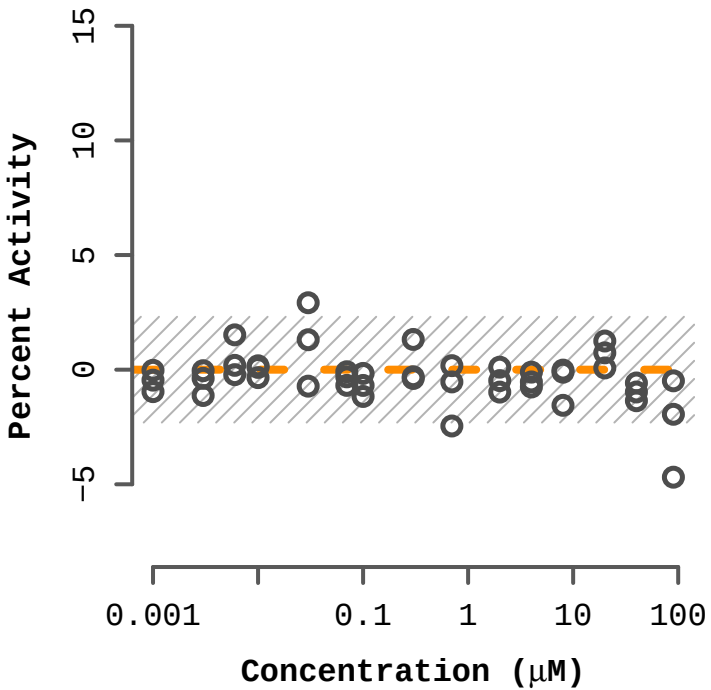
NAME: Ingliforib
CHID: 47252 **CASRN:** 186392-65-4
SPID(S): Tox21_300206
M4ID: 12478924

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

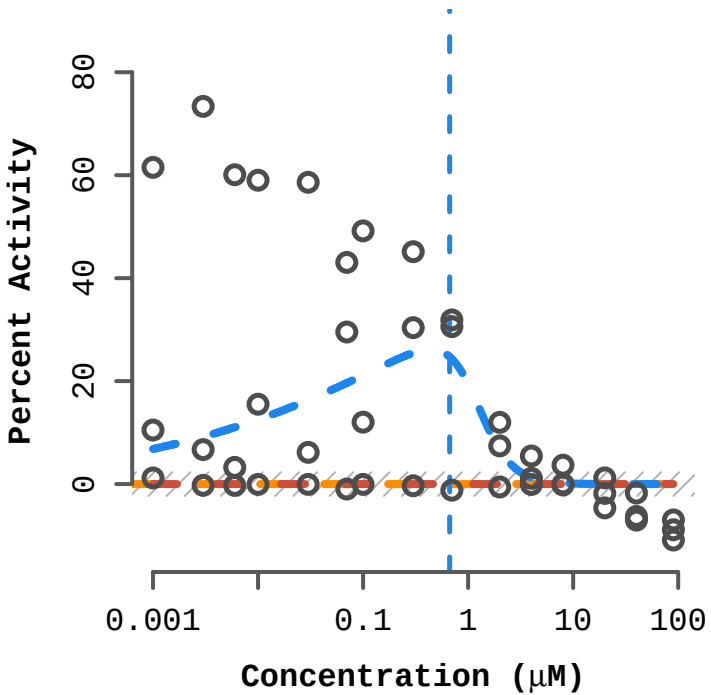
NAME: CP-401387
CHID: 47253 **CASRN:** 199171-88-5
SPID(S): Tox21_300207
M4ID: 12478923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: CP-457920
CHID: 47254 CASRN: 220860-50-4
SPID(S): Tox21_300208
M4ID: 12478922

HILL MODEL (in red):

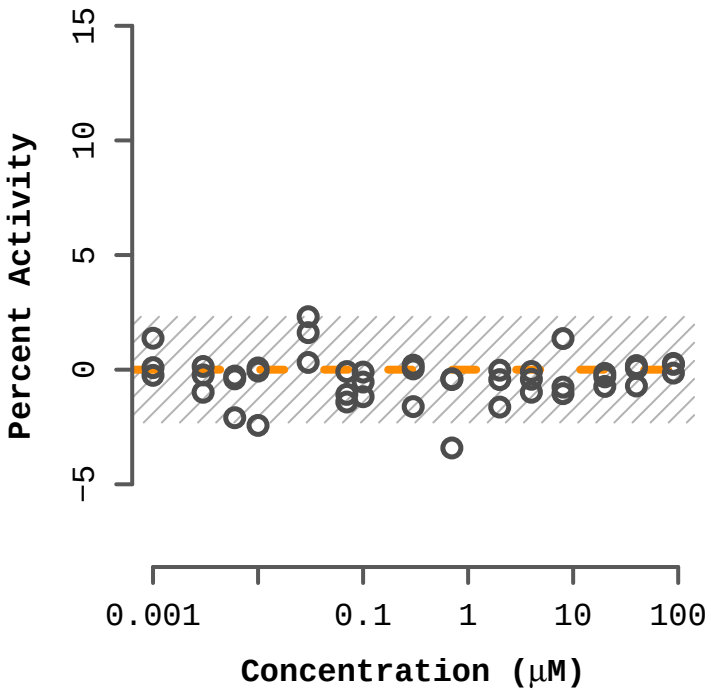
	tp	ga	gw
val:	1.72	2.45	7.83
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	59.5	-0.176	0.315	0.0741	2.76
sd:	159	6.31	0.325	0.356	2.68

	CNST	HILL	GNLS
AIC:	414.27	420.27	402.72
PROB:	0	0	1
RMSE:	26.23	26.23	20.56

MAX_MEAN: 26.6 MAX_MED: 30.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

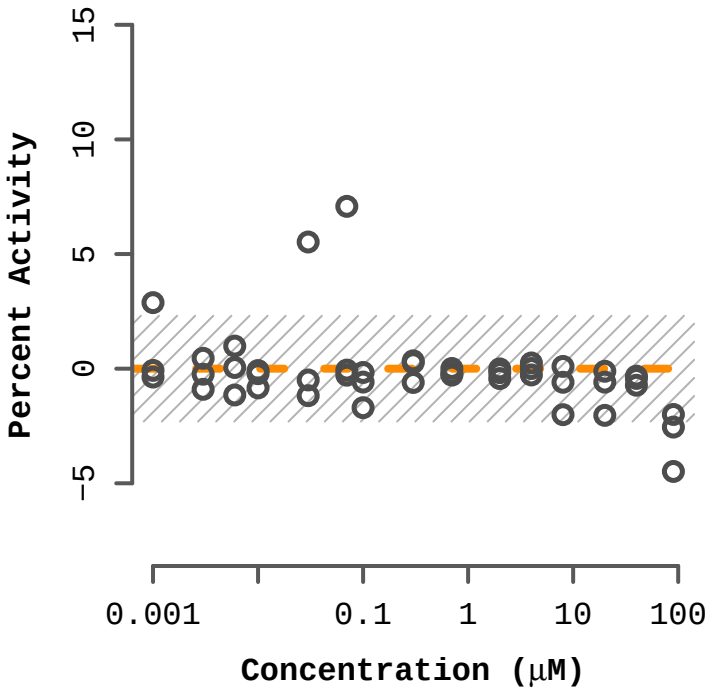
NAME: CP−465394
CHID: 47255 **CASRN:** NOCAS_47255
SPID(S): Tox21_300209
M4ID: 12478921

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

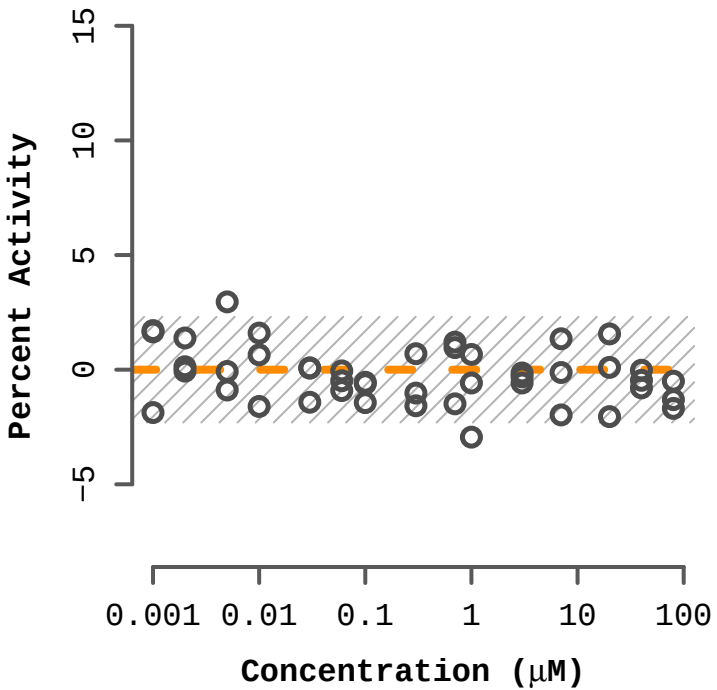
NAME: Zamifenacin
CHID: 47257 CASRN: 127308-82-1
SPID(S): Tox21_300210
M4ID: 12478920

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 2.25 MAX_MED: 0.263 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

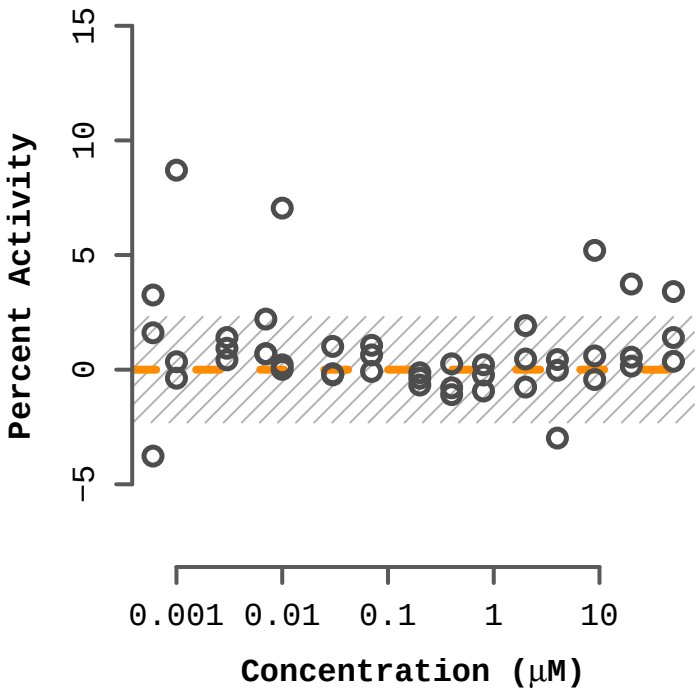
NAME: Enadoline
CHID: 47258 **CASRN:** 124378-77-4
SPID(S): Tox21_300426
M4ID: 12478706

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.666 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

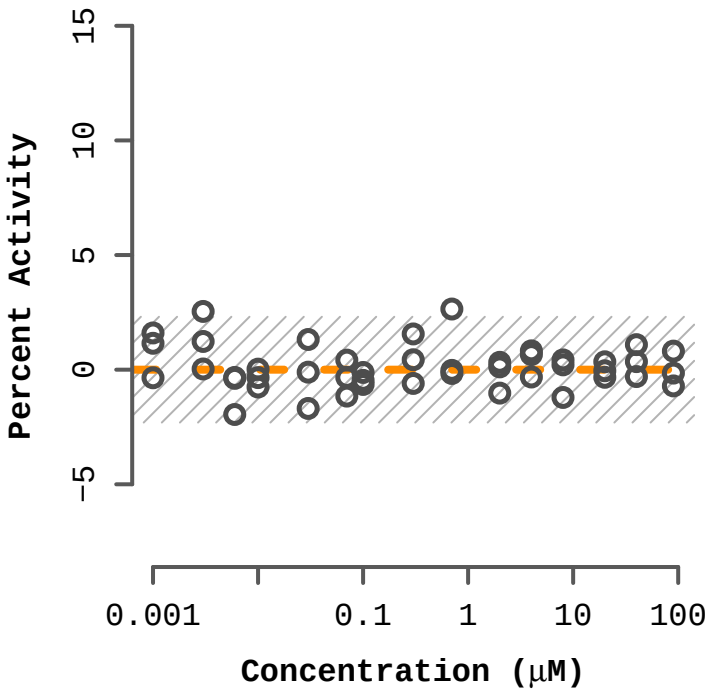
NAME: PharmaGSID_47259
CHID: 47259 **CASRN:** 149062-75-9
SPID(S): Tox21_300427
M4ID: 12478705

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.3	NA	NA

MAX_MEAN: 2.89 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

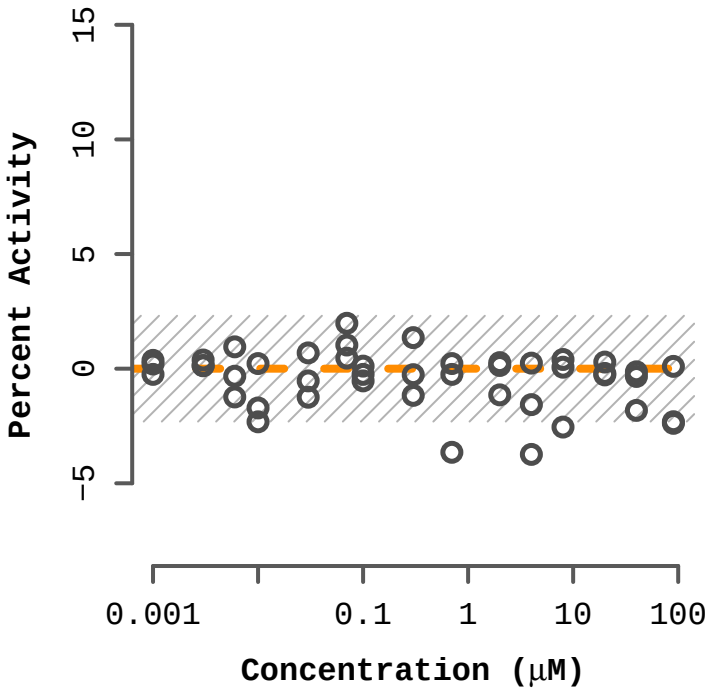
NAME: PharmaGSID_47261
CHID: 47261 **CASRN:** 177785-47-6
SPID(S): Tox21_300428
M4ID: 12478704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

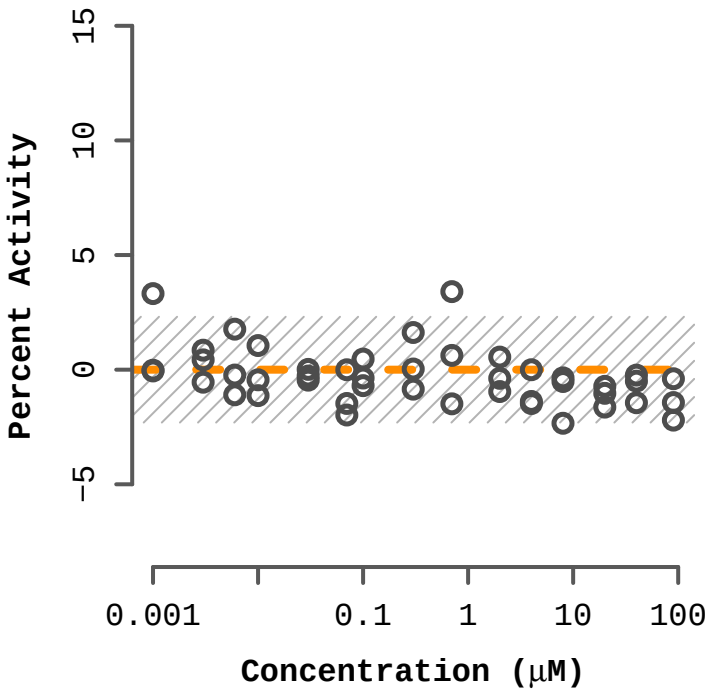
NAME: CI-1029
CHID: 47262 CASRN: 207736-05-8
SPID(S): Tox21_300429
M4ID: 12478703

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.16 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

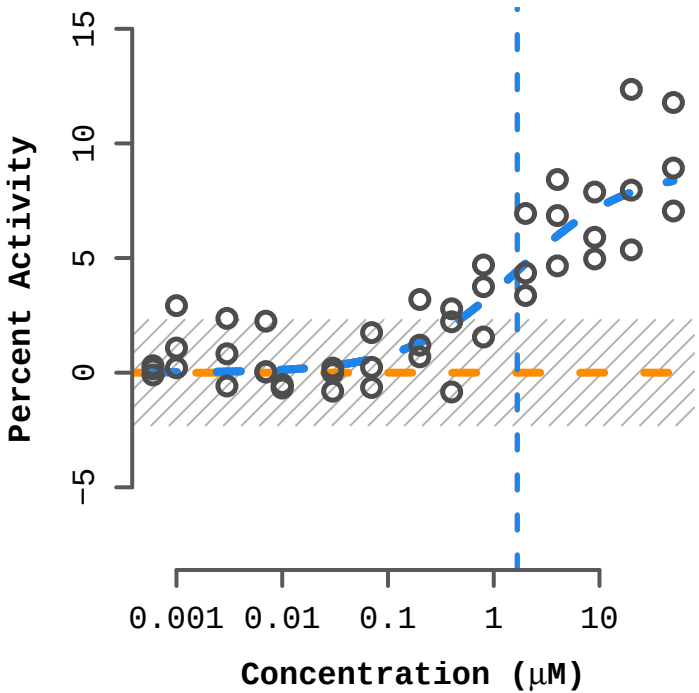
NAME: PharmaGSID_47263
CHID: 47263 **CASRN:** 349495-42-7
SPID(S): Tox21_300430
M4ID: 12478702

HILL MODEL: Not applicable.

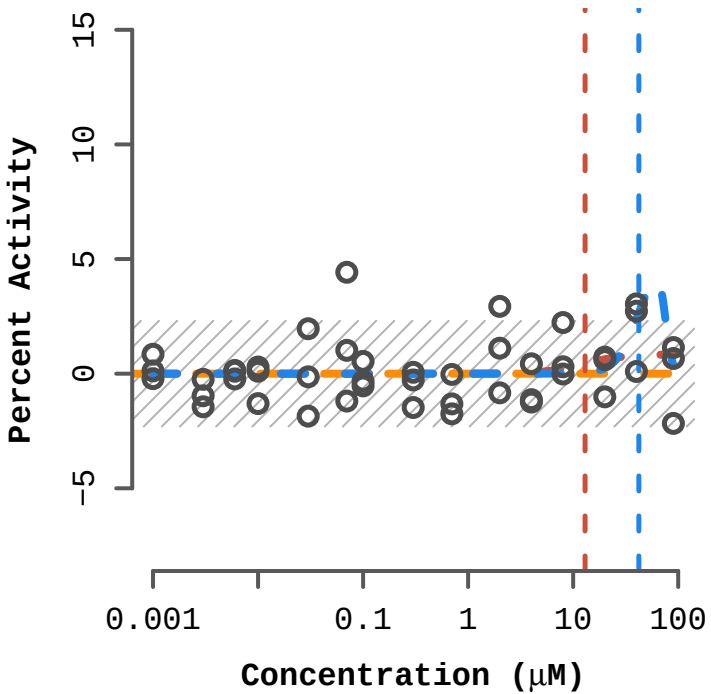
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.624 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    CP-283097
CHID:    47264   CASRN: 171866-31-2
SPID(S): Tox21_300431
M4ID:    12478701

HILL MODEL (in red):
      tp       ga       gw
val:  8.87     0.223    0.829
sd:   1.47     0.277    0.25

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.87     0.223    0.829    2.93     6.17
sd:   1.47     0.277    0.25     604      3030

      CNST        HILL        GNLS
AIC:  264.57      174.66      178.66
PROB: 0           0.88        0.12
RMSE: 4.58        1.54        1.54

MAX_MEAN: 9.26      MAX_MED: 8.93      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: CP−471358
CHID: 47265 CASRN: NOCAS_47265
SPID(S): Tox21_300432
M4ID: 12478700

HILL MODEL (in red):

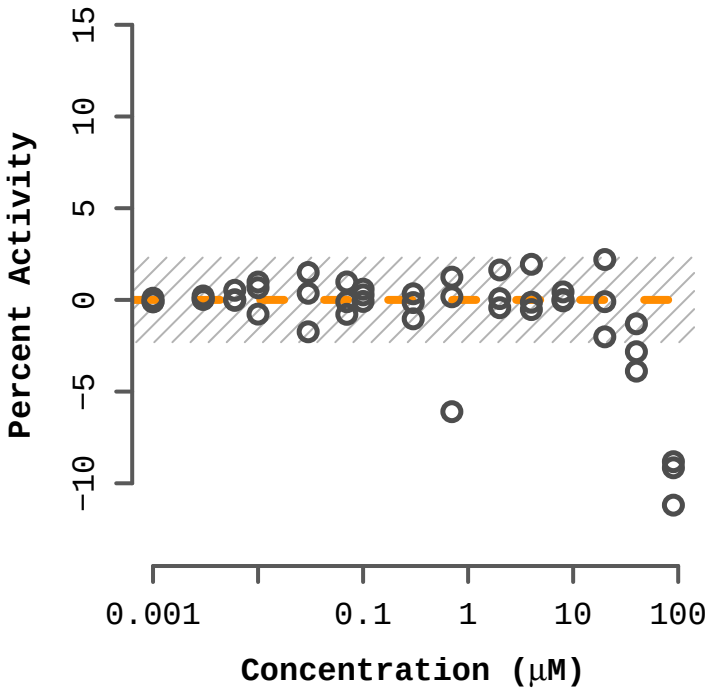
	tp	ga	gw
val:	0.842	1.11	2.37
sd:	0.717	0.908	2.75

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.31	1.63	4.07	1.88	14
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	156.66	159.65	159.92
PROB:	0.7	0.16	0.14
RMSE:	1.39	1.35	1.3

MAX_MEAN: 1.96 MAX_MED: 2.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

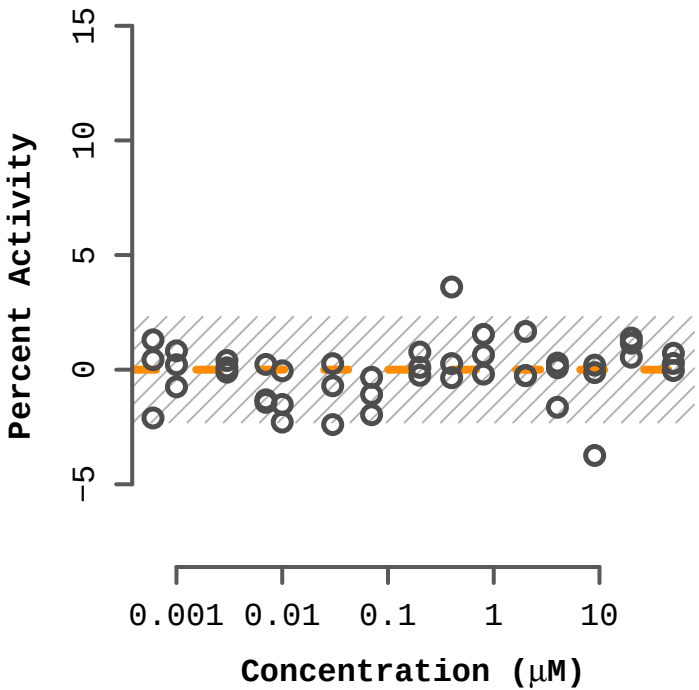
NAME: CP−544439
CHID: 47266 CASRN: 230954−09−3
SPID(S): Tox21_300433
M4ID: 12478699

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	191.73	NA	NA
PROB:	1	NA	NA
RMSE:	2.9	NA	NA

MAX_MEAN: 0.43 **MAX_MED:** 0.661 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

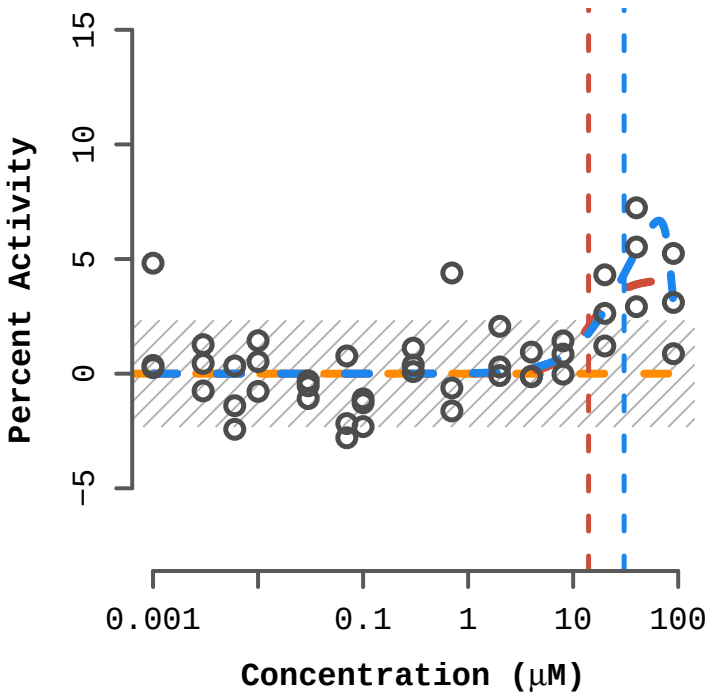
NAME: CP−642931
CHID: 47267 CASRN: NOCAS_47267
SPID(S): Tox21_300434
M4ID: 12478698

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: CI-959
CHID: 47268 CASRN: 104795-68-8
SPID(S): Tox21_300435
M4ID: 12478697

HILL MODEL (in red):

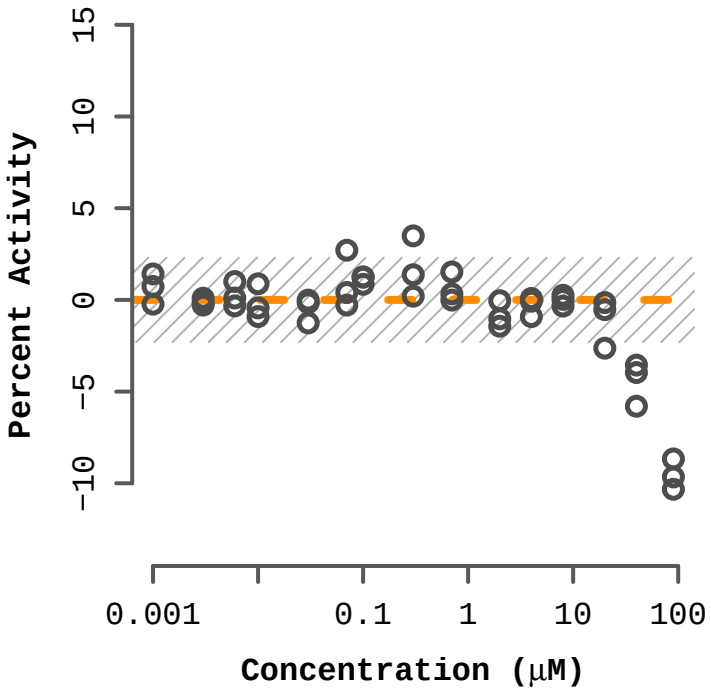
	tp	ga	gw
val:	4.11	1.15	2.77
sd:	0.886	0.156	1.58

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.68	1.49	1.76	1.94	12.1
sd:	8.2	0.5	1.15	0.0403	38.1

	CNST	HILL	GNLS
AIC:	201.67	178.23	179.05
PROB:	0	0.6	0.4
RMSE:	2.35	1.65	1.58

MAX_MEAN: 5.23 MAX_MED: 5.53 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

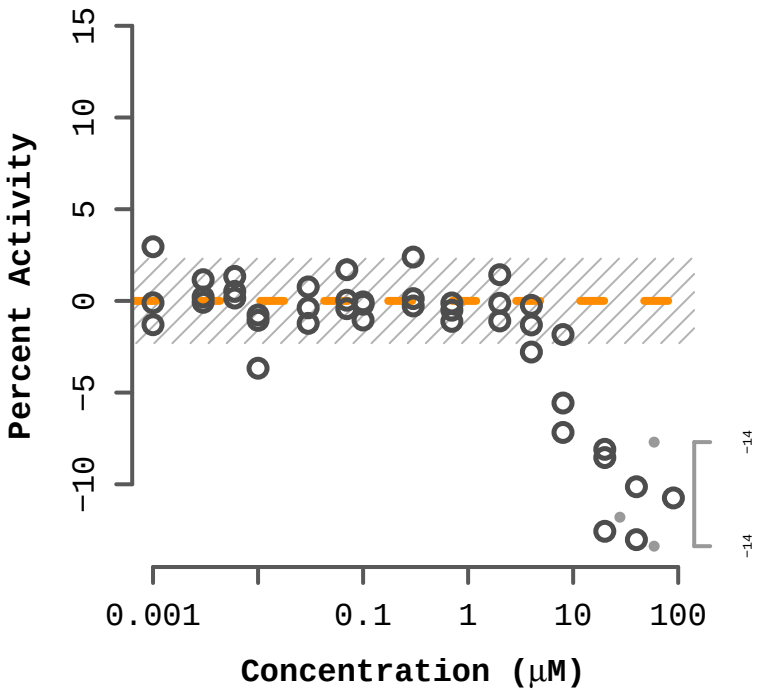
NAME: Besonprodil
CHID: 47270 **CASRN:** 253450-09-8
SPID(S): Tox21_300436
M4ID: 12478696

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.92	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

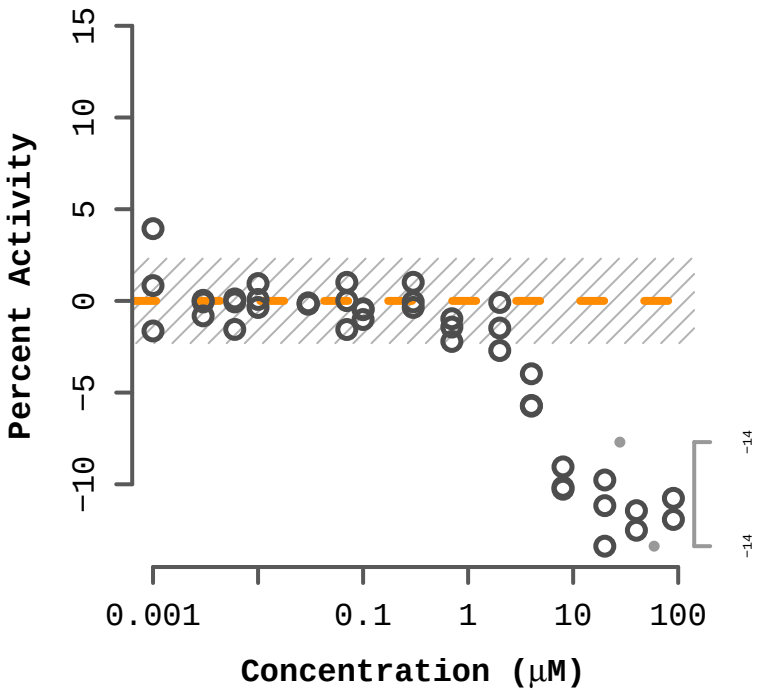
NAME: PD 0343701
CHID: 47271 **CASRN:** 676116-04-4
SPID(S): Tox21_300437
M4ID: 12478695 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	273.96	NA	NA
PROB:	1	NA	NA
RMSE:	5.62	NA	NA

MAX_MEAN: 0.748 **MAX_MED:** 0.519 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

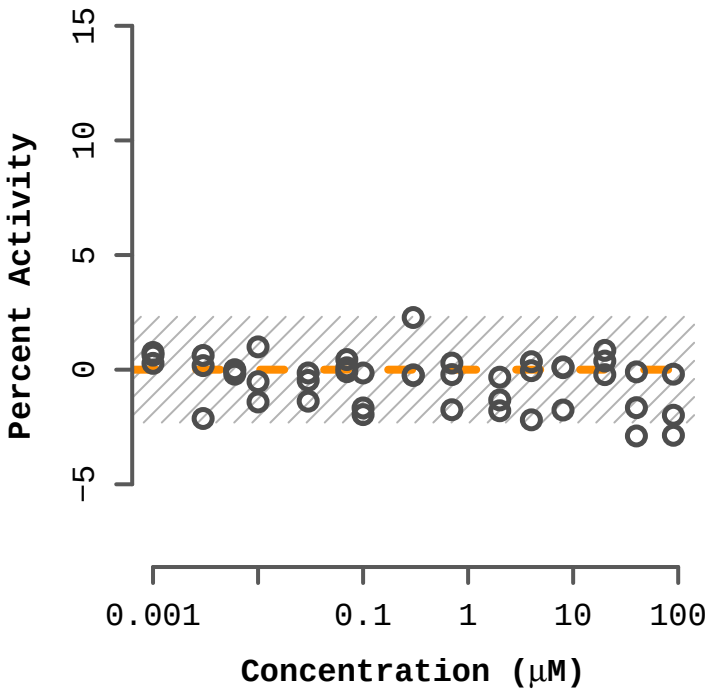
NAME: CJ-013610
CHID: 47272 CASRN: 249296-43-3
SPID(S): Tox21_300438
M4ID: 12478694 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.62	NA	NA
PROB:	1	NA	NA
RMSE:	6.23	NA	NA

MAX_MEAN: 1.05 MAX_MED: 0.837 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

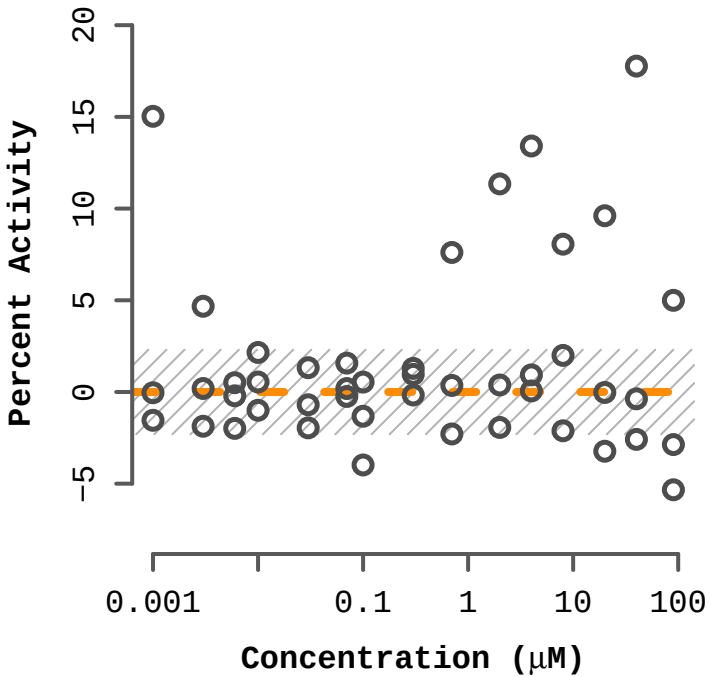
NAME: CP−114271
CHID: 47274 **CASRN:** 113734−18−2
SPID(S): Tox21_300439
M4ID: 12478693

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.601 **MAX_MED:** 0.634 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

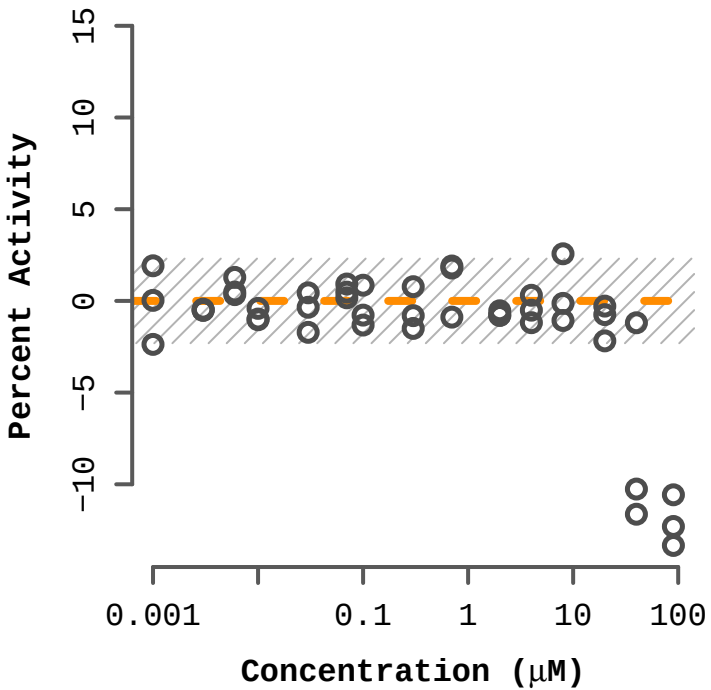
NAME: CP-409092
CHID: 47276 CASRN: 194098-25-4
SPID(S): Tox21_300440
M4ID: 12478692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	262.54	NA	NA
PROB:	1	NA	NA
RMSE:	5.23	NA	NA

MAX_MEAN: 4.94 MAX_MED: 2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

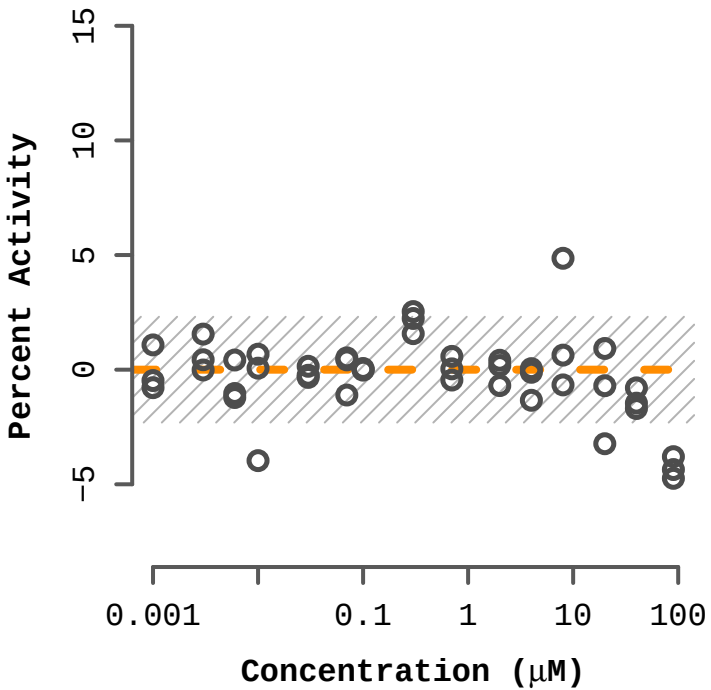
NAME: Elzasonan
CHID: 47277 **CASRN:** 361343-19-3
SPID(S): Tox21_300441
M4ID: 12478691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.08	NA	NA
PROB:	1	NA	NA
RMSE:	4.03	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

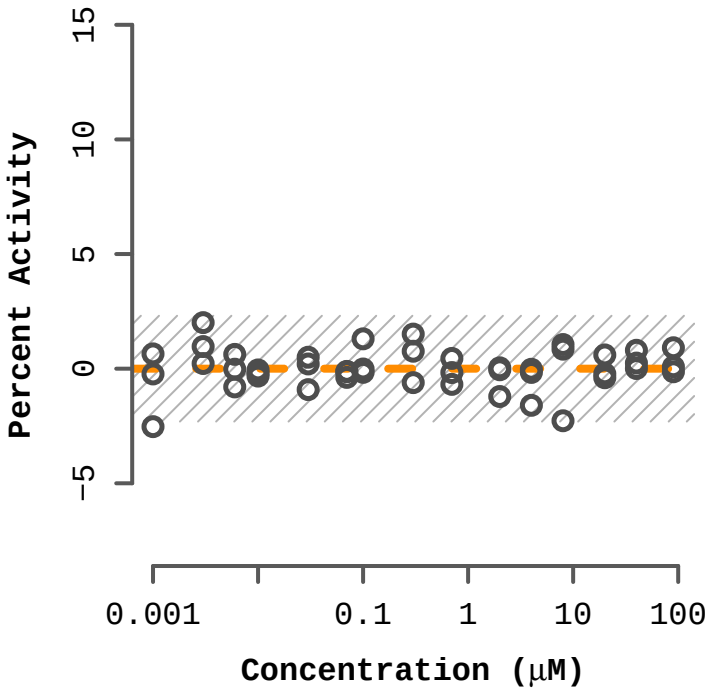
NAME: CP−457677
CHID: 47278 **CASRN:** 214535−77−0
SPID(S): Tox21_300442
M4ID: 12478690

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 2.11 **MAX_MED:** 2.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

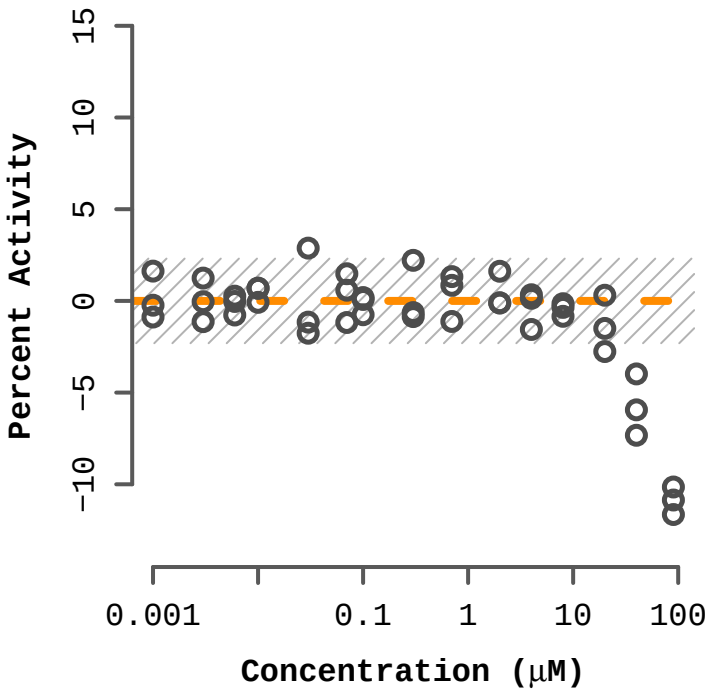
NAME: CP−532623
CHID: 47279 **CASRN:** 261947−38−0
SPID(S): Tox21_300443
M4ID: 12478689

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.967 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

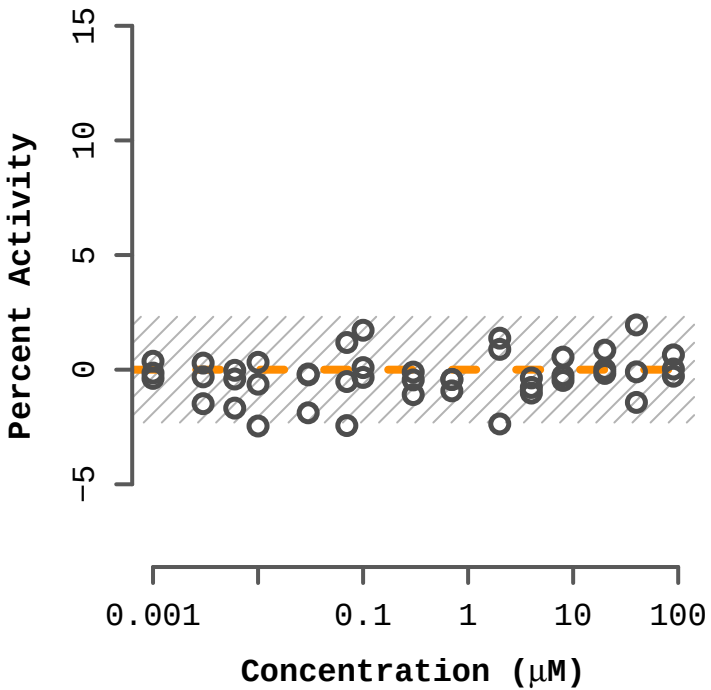
NAME: CP-607366
CHID: 47280 **CASRN:** 289716-94-5
SPID(S): Tox21_300444
M4ID: 12478688

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.99	NA	NA
PROB:	1	NA	NA
RMSE:	3.37	NA	NA

MAX_MEAN: 0.467 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

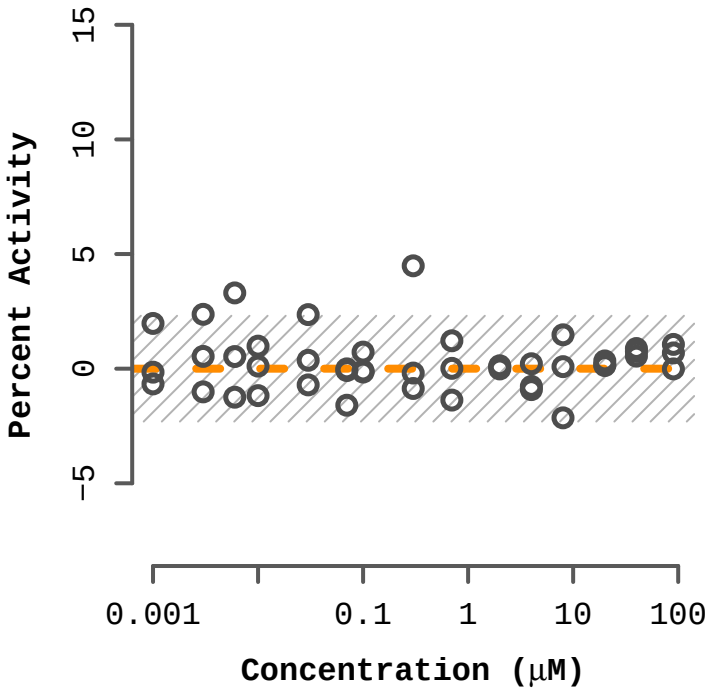
NAME: CP−612372
CHID: 47281 **CASRN:** 353280−07−6
SPID(S): Tox21_300445
M4ID: 12478687

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.492 **MAX_MED:** 0.887 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

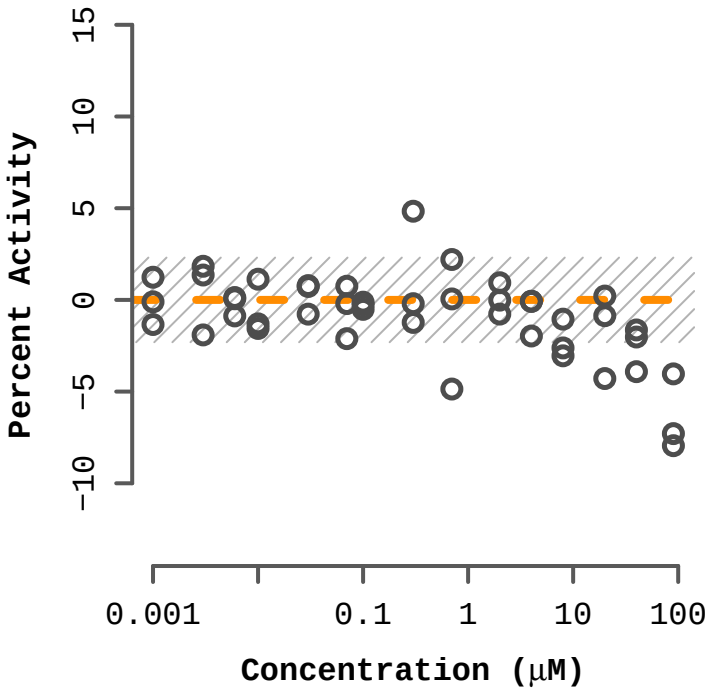
NAME: CP-671305
CHID: 47282 CASRN: 445295-04-5
SPID(S): Tox21_300446
M4ID: 12478686

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.15 MAX_MED: 0.757 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

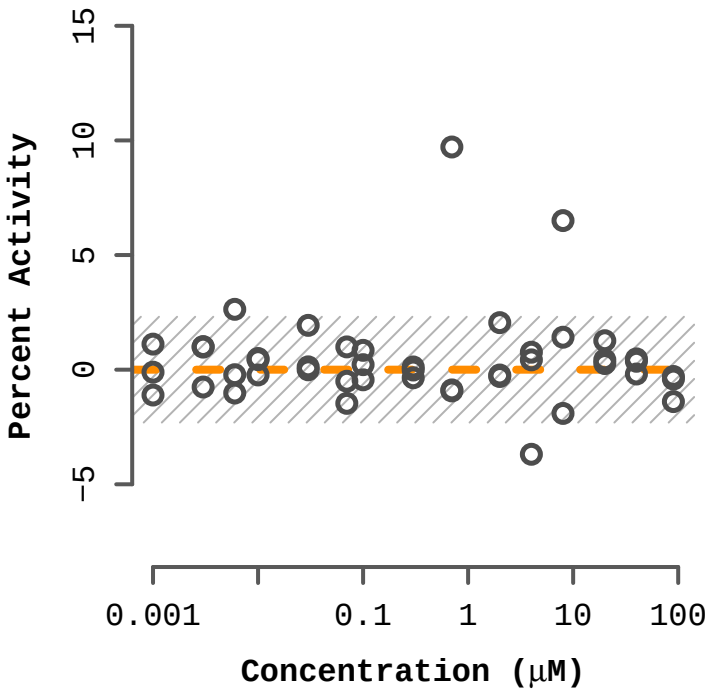
NAME: CP−728663
CHID: 47283 **CASRN:** 368832−42−2
SPID(S): Tox21_300447
M4ID: 12478685

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.46	NA	NA
PROB:	1	NA	NA
RMSE:	2.47	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

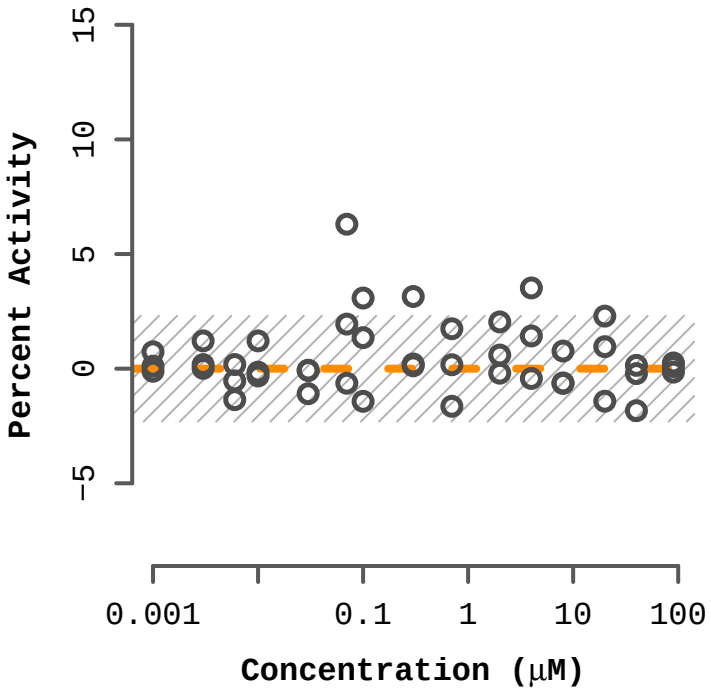
NAME: PHA-00543613
CHID: 47284 **CASRN:** 478149-53-0
SPID(S): Tox21_300448
M4ID: 12478684

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.05	NA	NA
PROB:	1	NA	NA
RMSE:	2.05	NA	NA

MAX_MEAN: 2.64 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

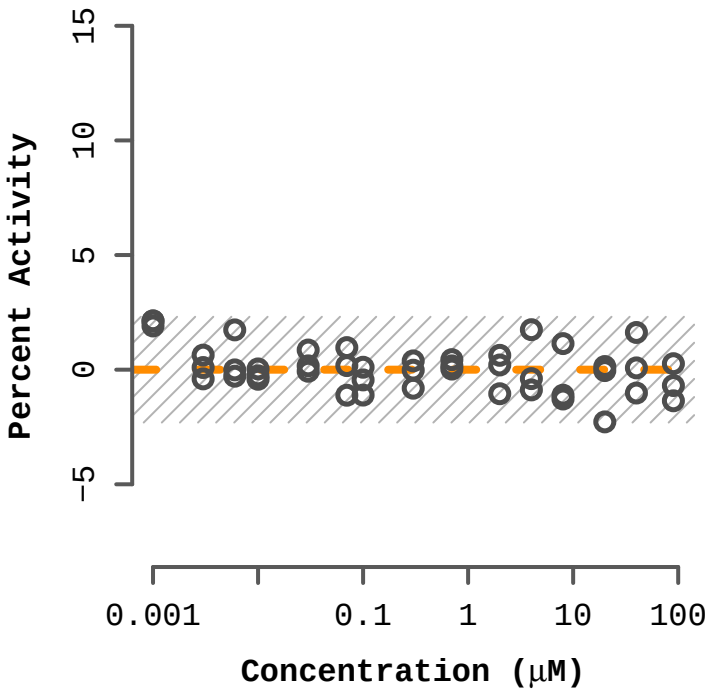
NAME: PHA-00568487
CHID: 47285 CASRN: 527680-56-4
SPID(S): Tox21_300449
M4ID: 12478683

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 2.54 MAX_MED: 1.94 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

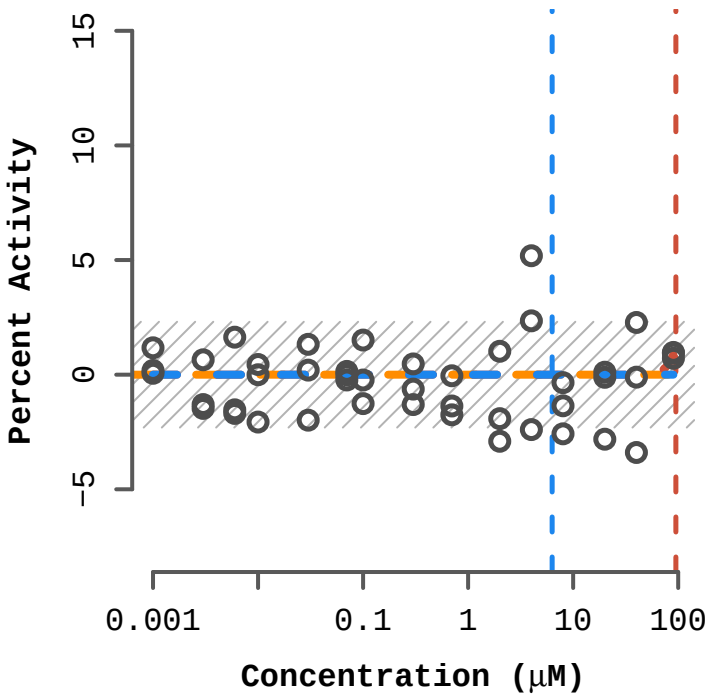
NAME: Candoxatril
CHID: 47286 **CASRN:** 123122-55-4
SPID(S): Tox21_300450
M4ID: 12478682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: UK-333747
CHID: 47287 CASRN: 197077-55-7
SPID(S): Tox21_300451
M4ID: 12478681

HILL MODEL (in red):

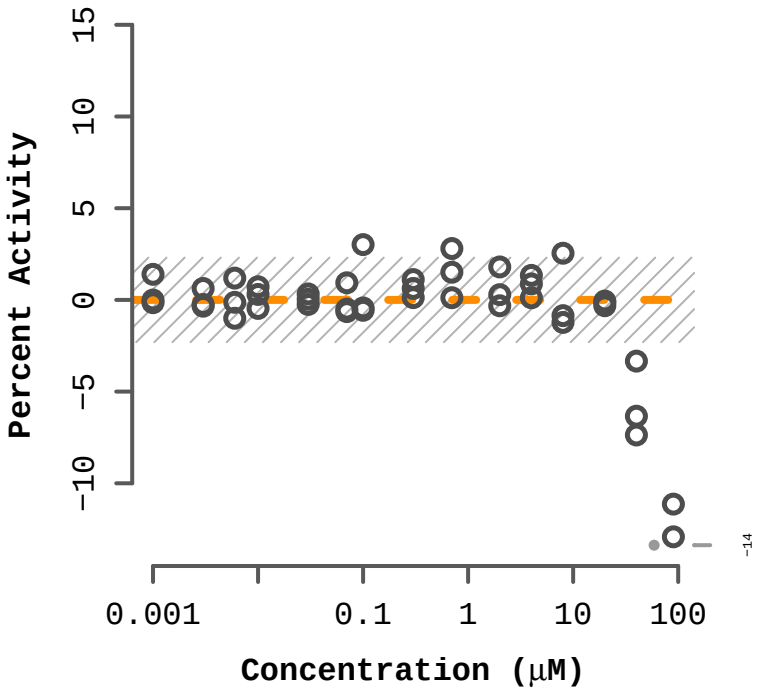
	tp	ga	gw
val:	2.21	1.98	7.88
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.92e-10	0.8	1.54	1.3	5.82
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	174.97	179.38	184.97
PROB:	0.9	0.1	0.01
RMSE:	1.65	1.63	1.65

MAX_MEAN: 1.72 MAX_MED: 2.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

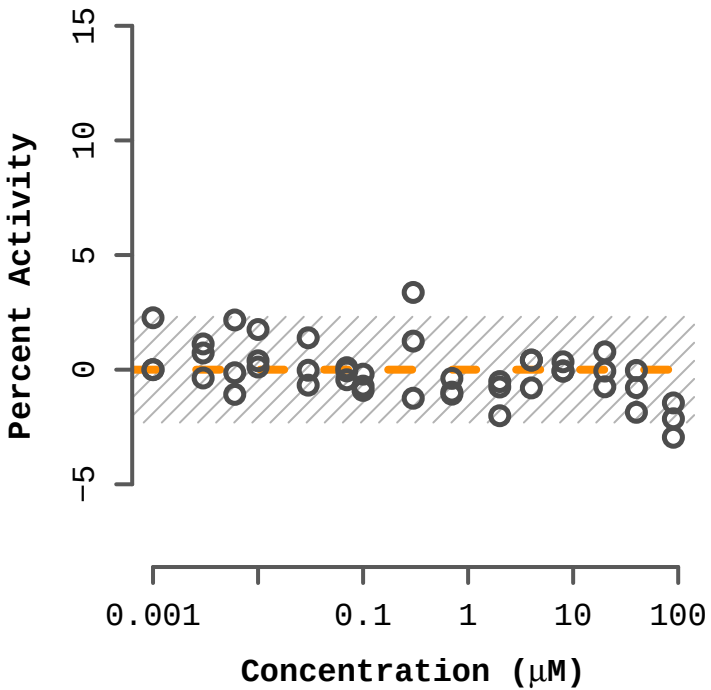
NAME: UK-337312
CHID: 47288 CASRN: 203942-49-8
SPID(S): Tox21_300452
M4ID: 12478680 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.73	NA	NA
PROB:	1	NA	NA
RMSE:	3.8	NA	NA

MAX_MEAN: 1.48 MAX_MED: 1.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

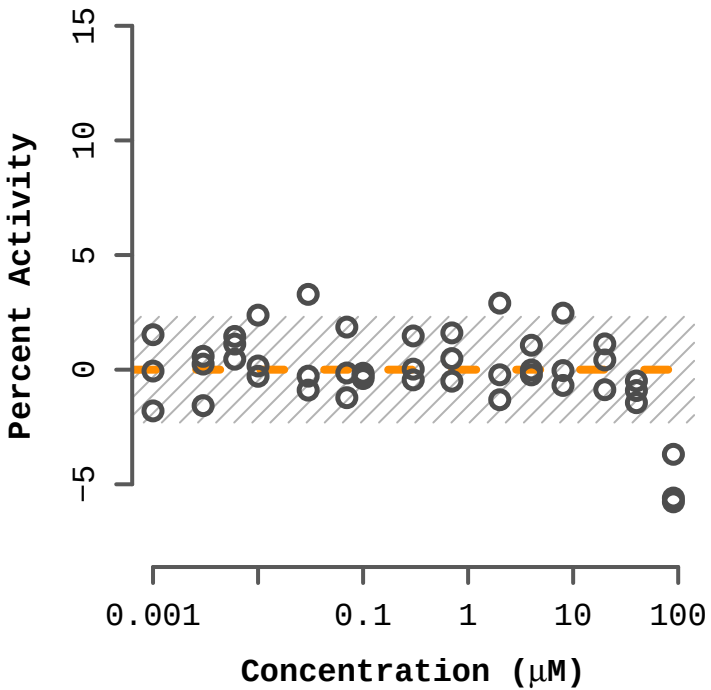
NAME: UK-343664
CHID: 47289 CASRN: 215297-27-1
SPID(S): Tox21_300453
M4ID: 12478679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.87	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.12 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

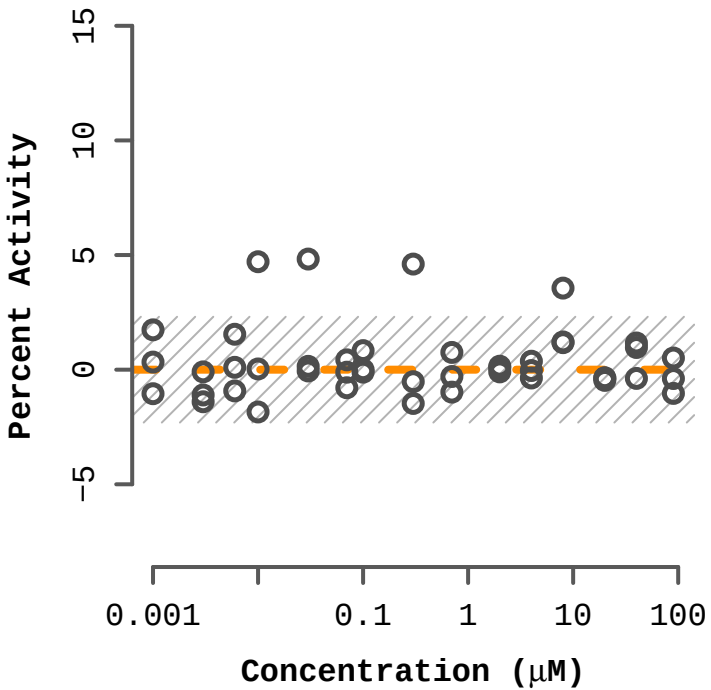
NAME: UK-416244
CHID: 47290 **CASRN:** 402910-27-4
SPID(S): Tox21_300454
M4ID: 12478678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

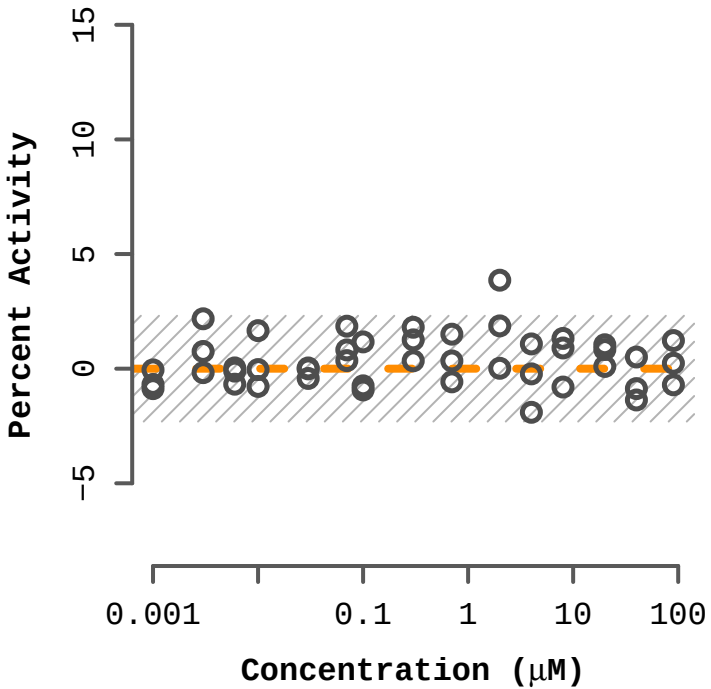
NAME: CI−1044
CHID: 47291 **CASRN:** NOCAS_47291
SPID(S): Tox21_300455
M4ID: 12478677

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 1.98 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

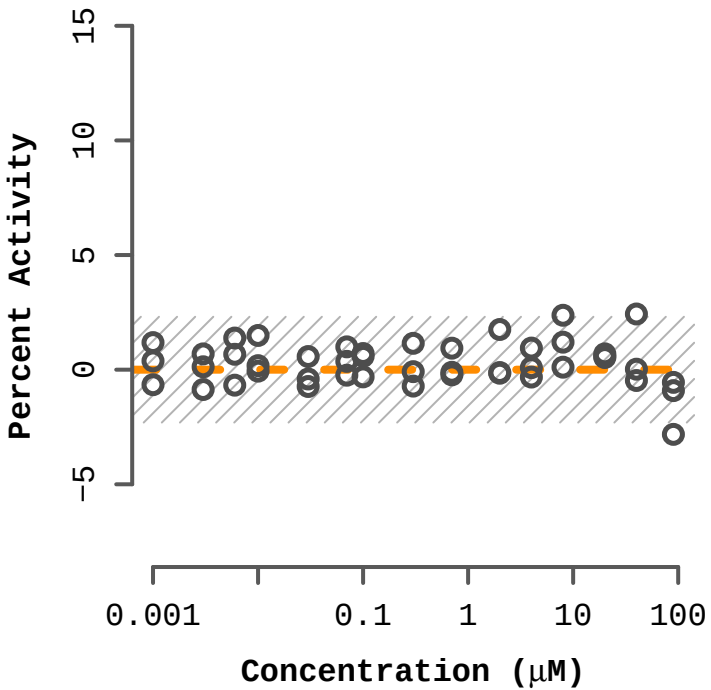
NAME: PD 0200347
CHID: 47292 **CASRN:** NOCAS_47292
SPID(S): Tox21_300456
M4ID: 12478676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

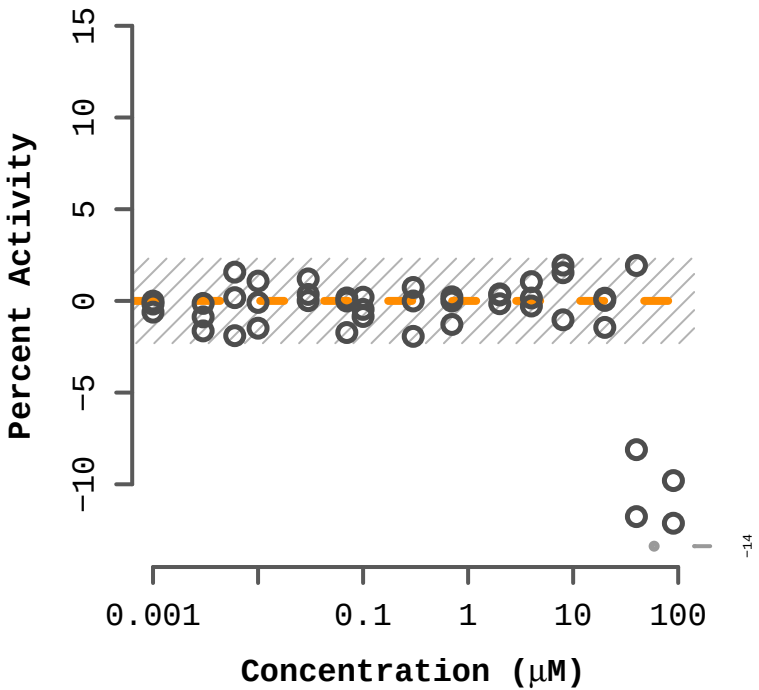
NAME: CP−863187
CHID: 47294 CASRN: 668981−02−0
SPID(S): Tox21_300457
M4ID: 12478675

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

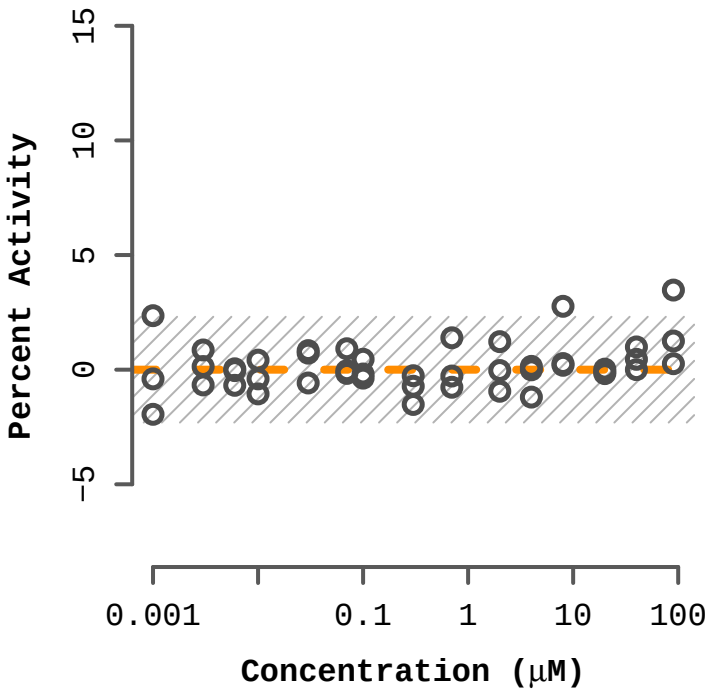
NAME: UK-373911
CHID: 47295 CASRN: 291305-06-1
SPID(S): Tox21_300458
M4ID: 12478674 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.4	NA	NA
PROB:	1	NA	NA
RMSE:	3.93	NA	NA

MAX_MEAN: 0.822 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

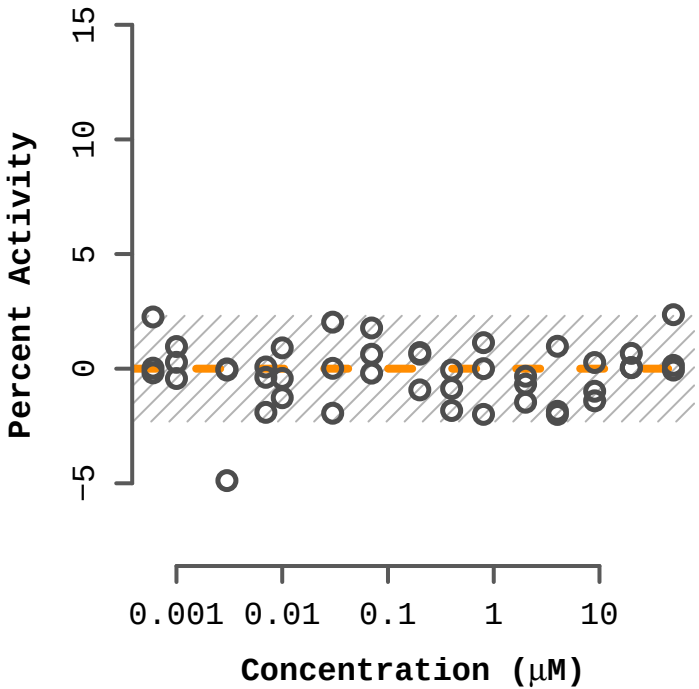
NAME: Zenarestat
CHID: 47296 **CASRN:** 112733-06-9
SPID(S): Tox21_300459
M4ID: 12478673

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

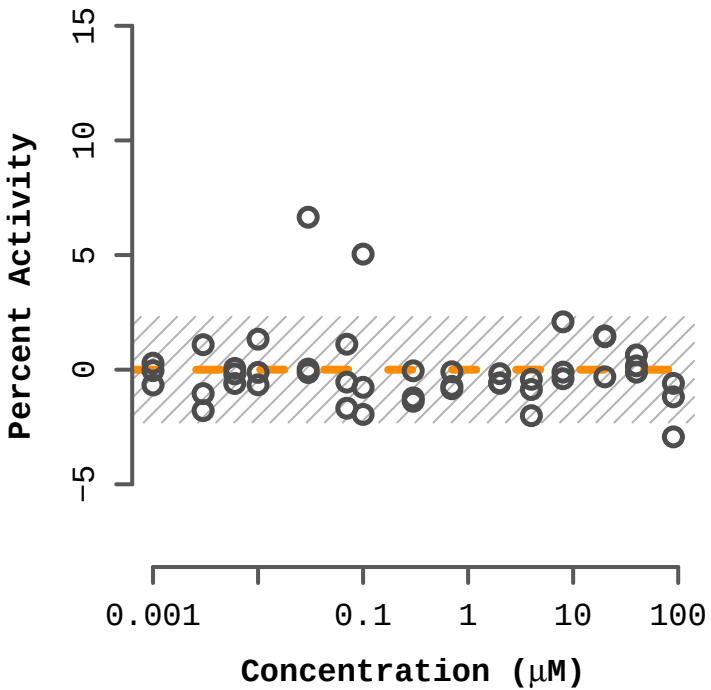
NAME: Zenarestat
CHID: 47296 **CASRN:** 112733-06-9
SPID(S): Tox21_113652
M4ID: 12482560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.814 **MAX_MED:** 0.634 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

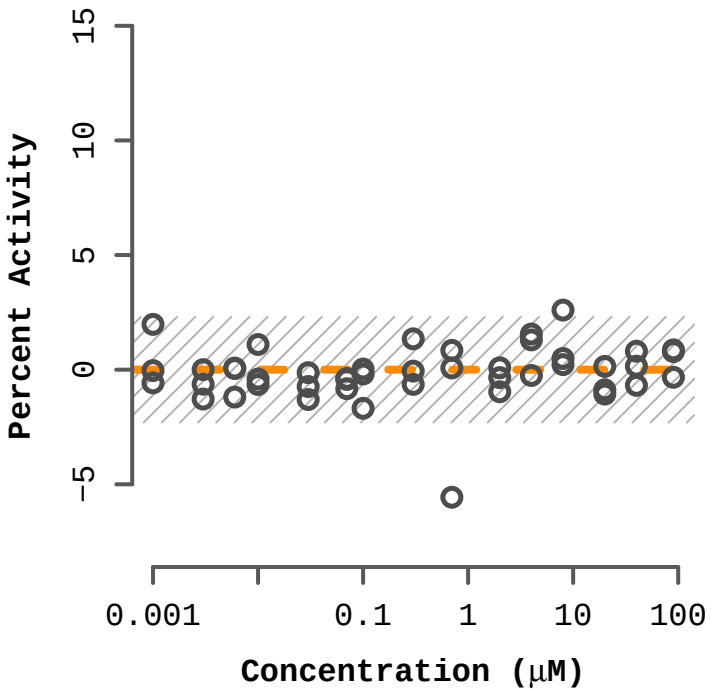
NAME: CP−085958
CHID: 47297 **CASRN:** 134002−60−1
SPID(S): Tox21_300460
M4ID: 12478672

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

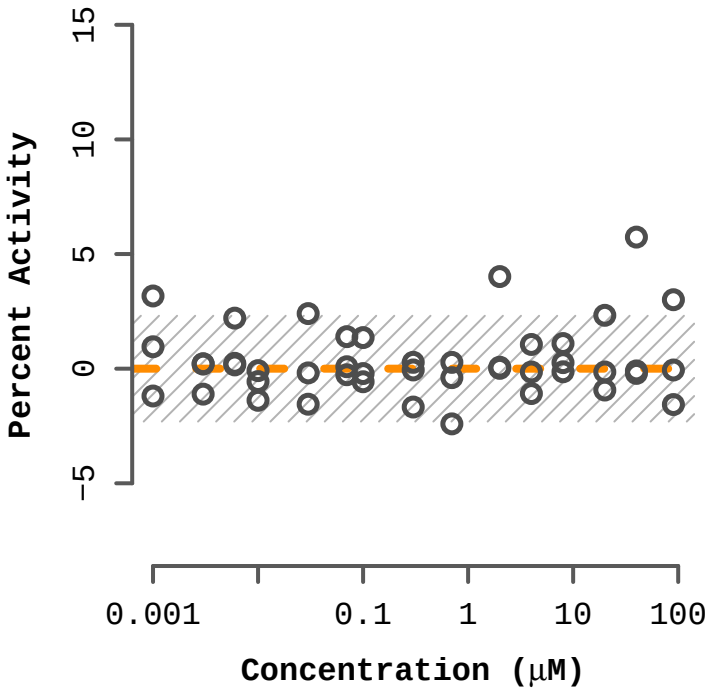
NAME: CP−422935
CHID: 47299 CASRN: NOCAS_47299
SPID(S): Tox21_300461
M4ID: 12478671

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

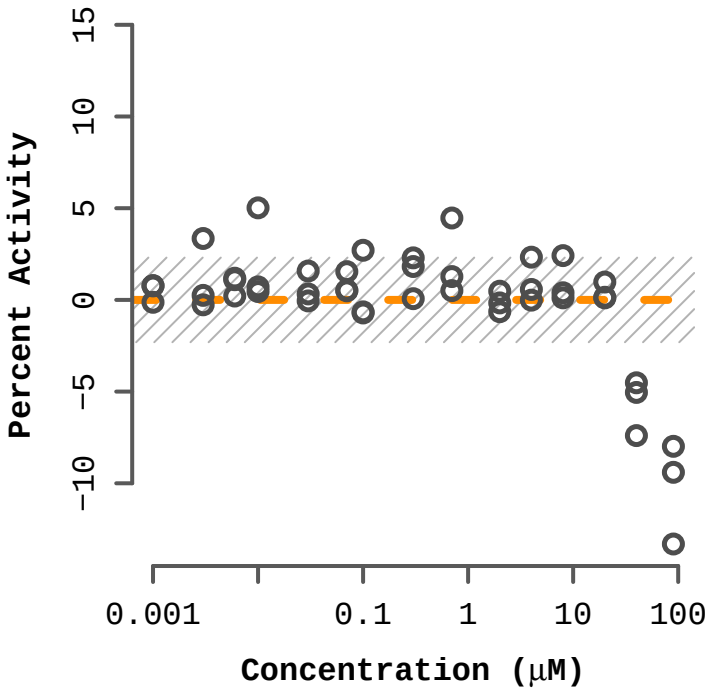
NAME: CP−456773
CHID: 47301 **CASRN:** 210826−40−7
SPID(S): Tox21_300462
M4ID: 12478670

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 0.957 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

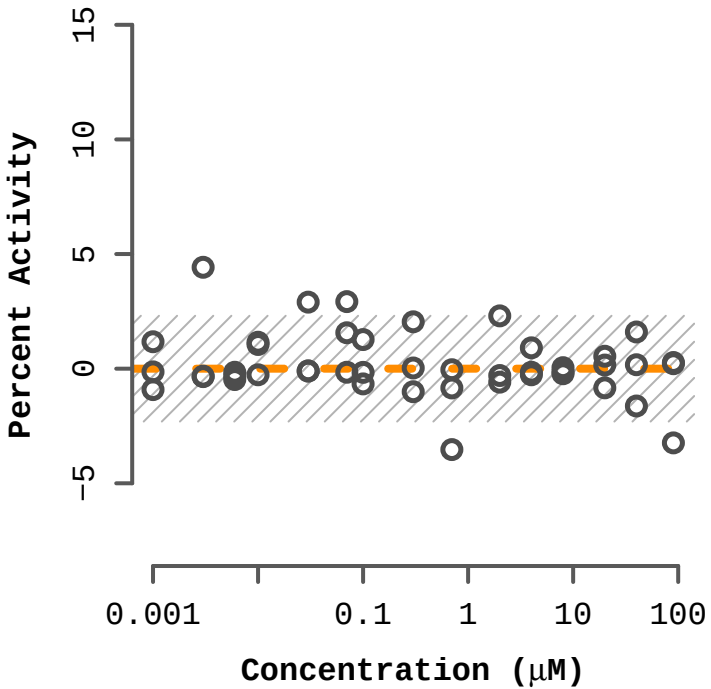
NAME: CJ-013790
CHID: 47303 CASRN: 179465-71-5
SPID(S): Tox21_300463
M4ID: 12478669

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.66	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 2.08 MAX_MED: 1.82 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

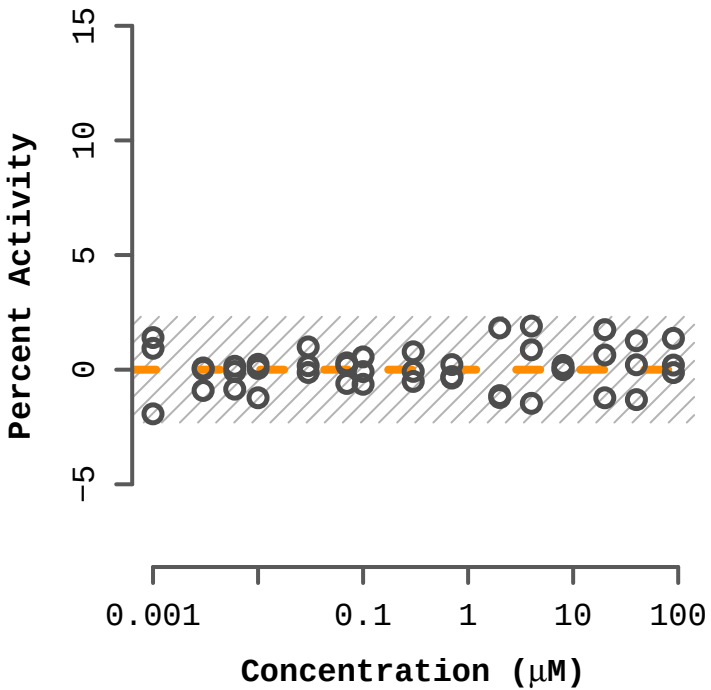
NAME: CP−100829
CHID: 47304 CASRN: 135080−03−4
SPID(S): Tox21_300464
M4ID: 12478668

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.45 MAX_MED: 1.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

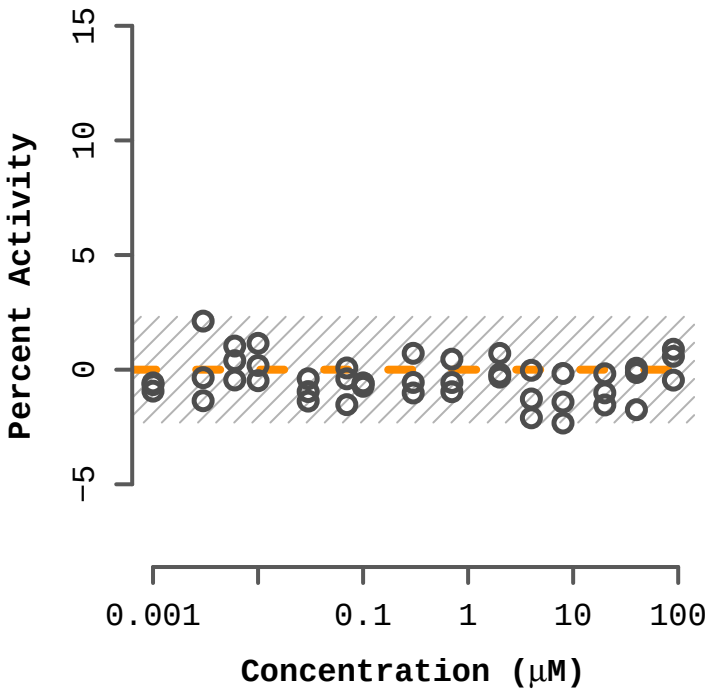
NAME: CP−608039
CHID: 47305 CASRN: NOCAS_47305
SPID(S): Tox21_300465
M4ID: 12478667

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.481 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

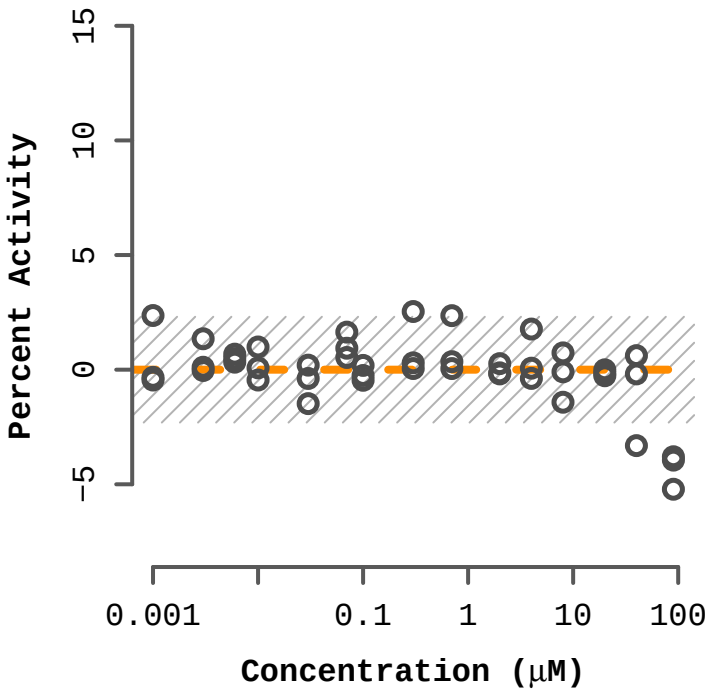
NAME: CP−634384
CHID: 47306 CASRN: 290352−28−2
SPID(S): Tox21_300466
M4ID: 12478666

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.34 MAX_MED: 0.583 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

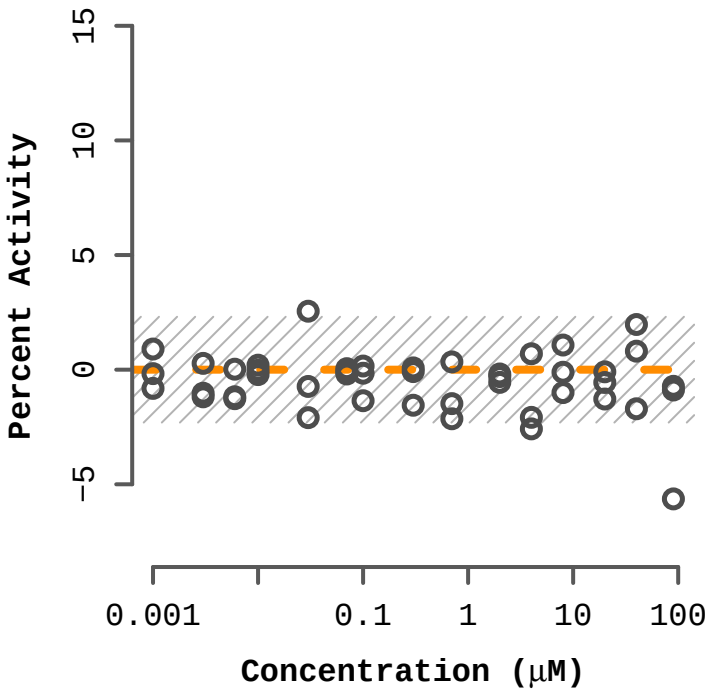
NAME: PD−0333941
CHID: 47307 **CASRN:** 501027−49−2
SPID(S): Tox21_300467
M4ID: 12478665

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

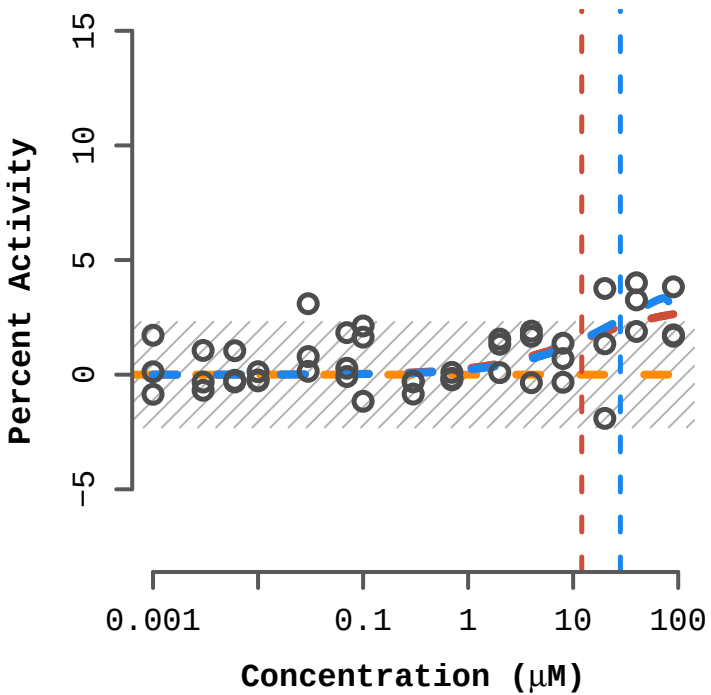
NAME: CP−105696
CHID: 47308 CASRN: 158081−99−3
SPID(S): Tox21_300468
M4ID: 12478664

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.359 MAX_MED: 0.809 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: UK-156819
CHID: 47309 CASRN: 162706-14-1
SPID(S): Tox21_300469
M4ID: 12478663

HILL MODEL (in red):

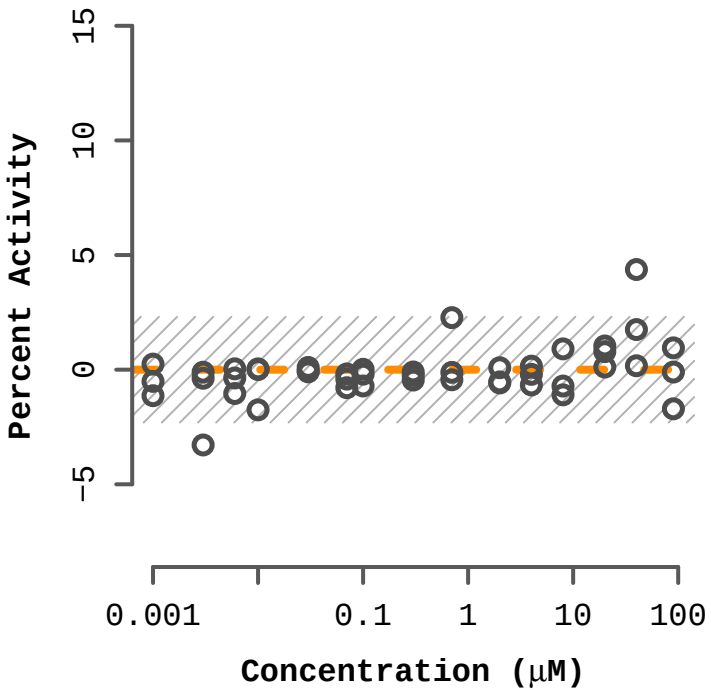
	tp	ga	gw
val:	3.05	1.08	0.923
sd:	1.44	0.606	0.659

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.81	1.45	0.909	1.97	17.9
sd:	5.49	0.967	0.479	0.033	61

	CNST	HILL	GNLS
AIC:	170.61	149.66	152.12
PROB:	0	0.77	0.23
RMSE:	1.59	1.19	1.18

MAX_MEAN: 3.05 MAX_MED: 3.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

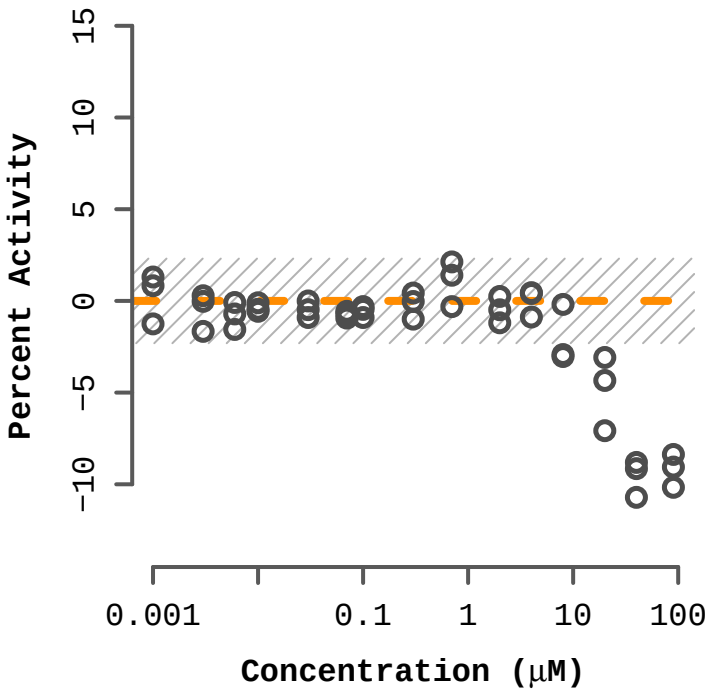
NAME: Farglitazar
CHID: 47310 **CASRN:** 196808-45-4
SPID(S): Tox21_300218
M4ID: 12478912

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

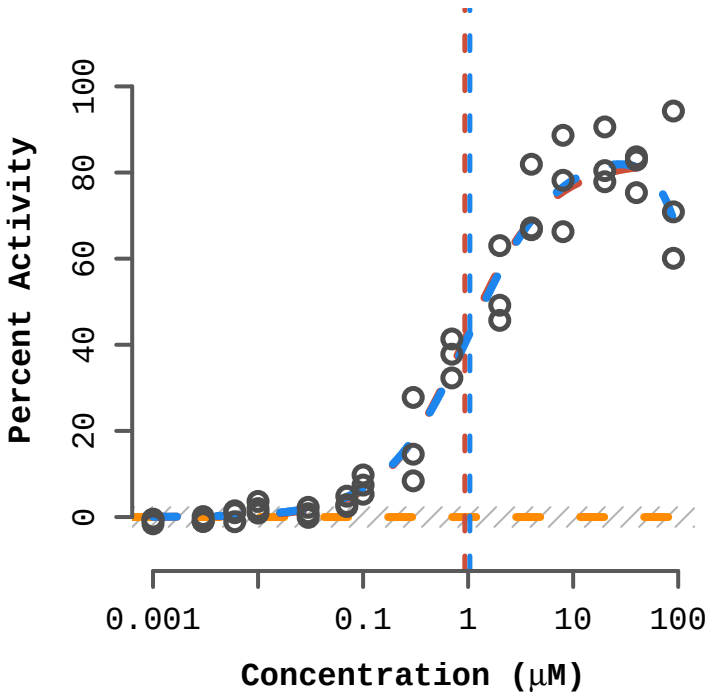
NAME: GSK163929B
CHID: 47311 **CASRN:** NOCAS_47311
SPID(S): Tox21_300215
M4ID: 12478915

HILL MODEL: Not applicable.

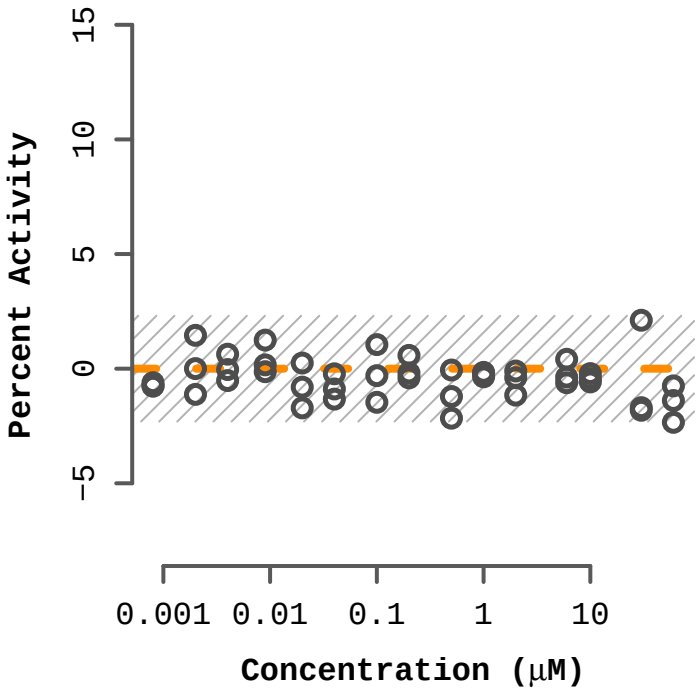
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233.65	NA	NA
PROB:	1	NA	NA
RMSE:	3.81	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.4 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    GSK232420A
CHID:    47312   CASRN: 864283-48-7
SPID(S): Tox21_300220
M4ID:    12478910

HILL MODEL (in red):
      tp       ga       gw
val:  82.4     -0.0313  1.12
sd:   2.61     0.0611   0.116

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  85.5     0.0167   1.06     2.22     2.46
sd:   5.42     0.0938   0.125    0.215    2.28

      CNST        HILL        GNLS
AIC:  481.45      298.16      296.25
PROB: 0           0.28        0.72
RMSE: 48.5        6.52        6.39

MAX_MEAN: 83        MAX_MED: 82.9      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

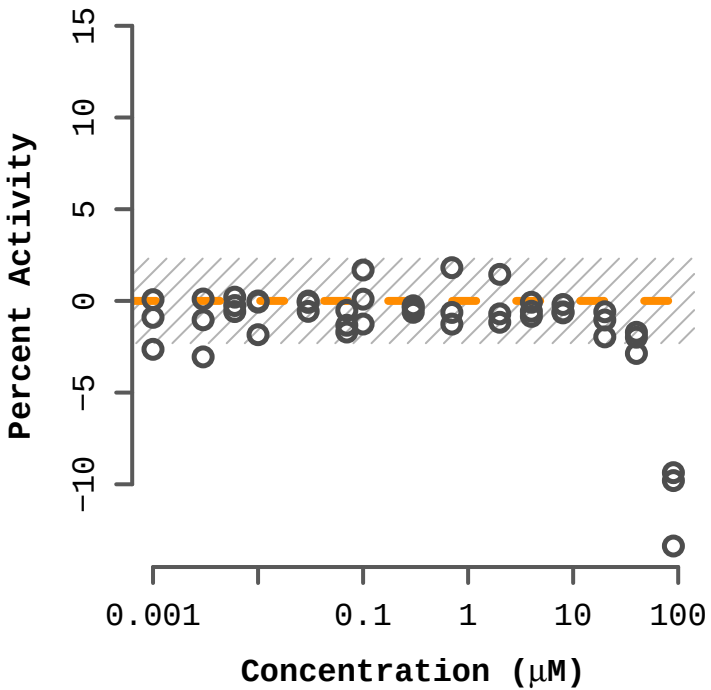
NAME: GW473178E methyl benzene sulphonic acid
CHID: 47313 **CASRN:** 263553-33-9
SPID(S): Tox21_300219
M4ID: 12478911

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.65	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.428 **MAX_MED:** 0.168 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

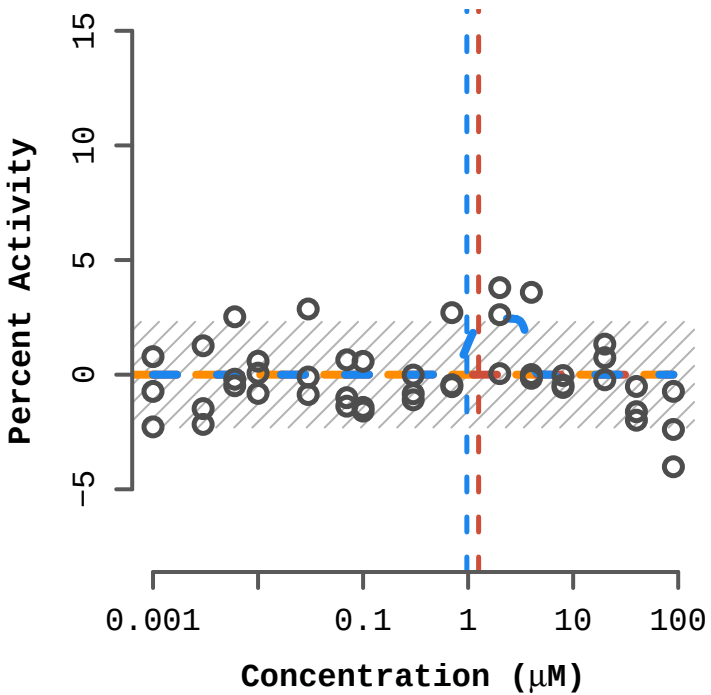
NAME: PharmaGSID_47315
CHID: 47315 **CASRN:** 444610-91-7
SPID(S): Tox21_300222
M4ID: 12478908

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.9	NA	NA
PROB:	1	NA	NA
RMSE:	3.08	NA	NA

MAX_MEAN: 0.174 **MAX_MED:** 0.0968 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Aplaviroc hydrochloride
CHID: 47316 **CASRN:** 461023-63-2
SPID(S): Tox21_300211
M4ID: 12478919

HILL MODEL (in red):

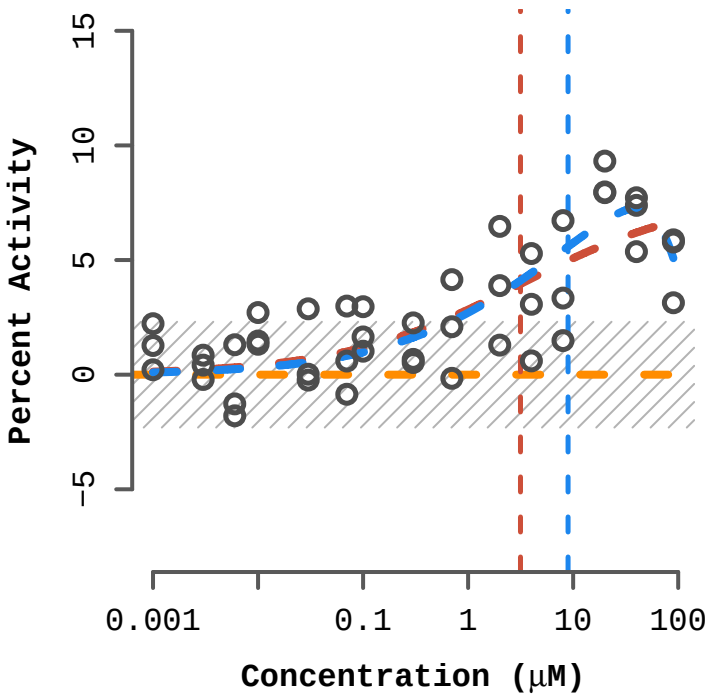
	tp	ga	gw
val:	1.07e-10	0.0999	2.38
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.45	−0.0122	7.99	0.571	17.3
sd:	1.08	1.31	69.2	1.65	914

	CNST	HILL	GNLS
AIC:	172.21	178.21	176.52
PROB:	0.86	0.04	0.1
RMSE:	1.6	1.6	1.48

MAX_MEAN: 2.16 **MAX_MED:** 2.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SB202235
CHID: 47318 CASRN: 139149-55-6
SPID(S): Tox21_300217
M4ID: 12478913

HILL MODEL (in red):

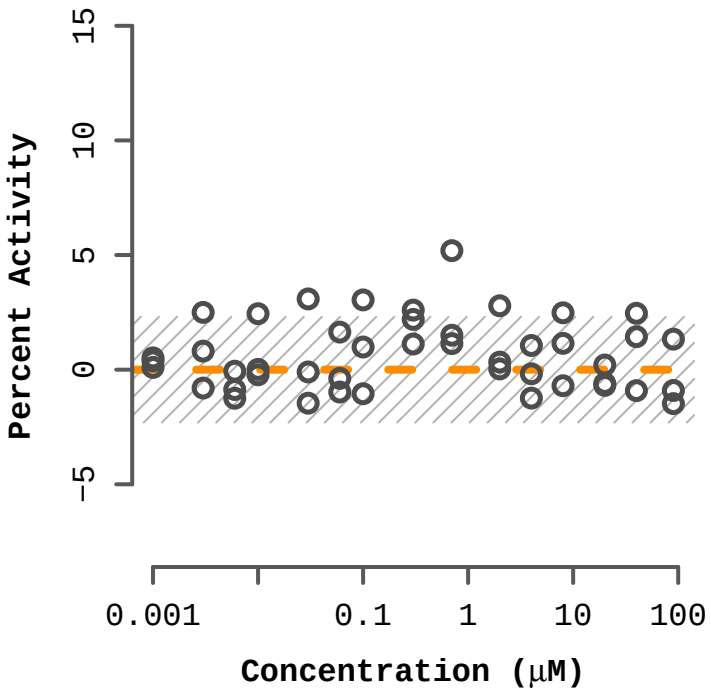
	tp	ga	gw
val:	7.91	0.498	0.506
sd:	2.24	0.639	0.225

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.2	0.951	0.522	2.01	3.08
sd:	3.99	0.604	0.156	0.087	2.8

	CNST	HILL	GNLS
AIC:	251.9	191.59	189.27
PROB:	0	0.24	0.76
RMSE:	3.87	1.77	1.66

MAX_MEAN: 8.41 MAX_MED: 7.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

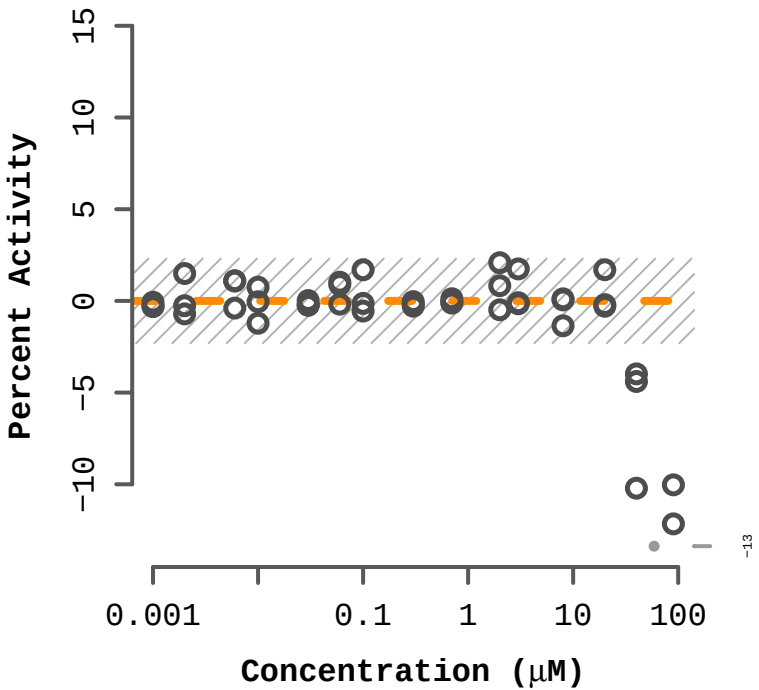
NAME: Carabersat
CHID: 47319 **CASRN:** 184653-84-7
SPID(S): Tox21_300213
M4ID: 12478917

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.61 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

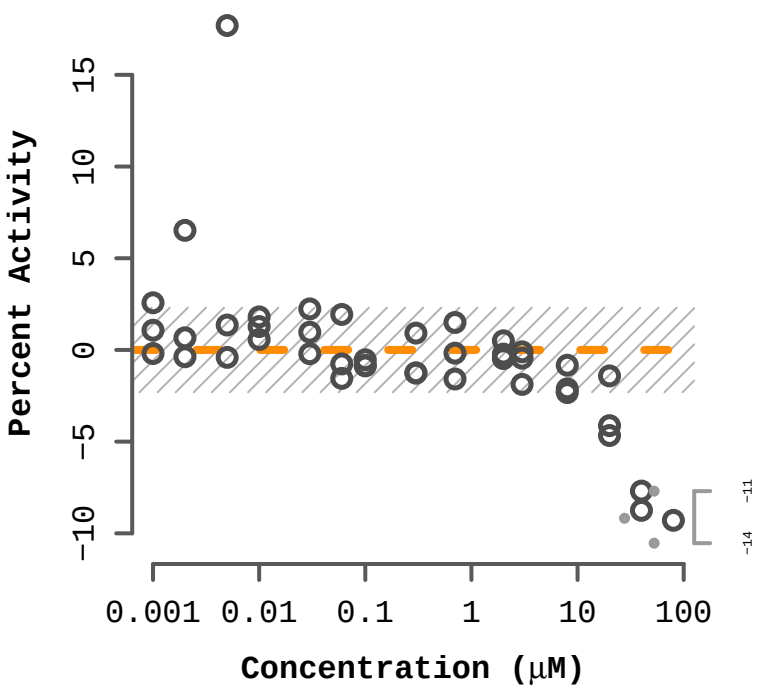
NAME: SB236057A
CHID: 47320 CASRN: 180084-01-9
SPID(S): Tox21_300212
M4ID: 12478918 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	202.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 0.811 MAX_MED: 1.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

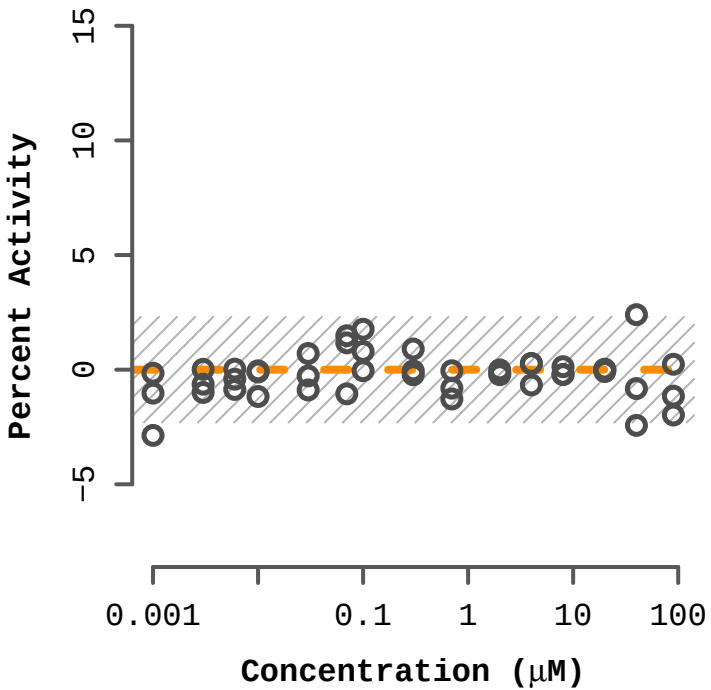
NAME: SB243213A
CHID: 47322 CASRN: 200940-23-4
SPID(S): Tox21_300216
M4ID: 12478914 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	256.96	NA	NA
PROB:	1	NA	NA
RMSE:	5.04	NA	NA

MAX_MEAN: 6.22 MAX_MED: 1.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

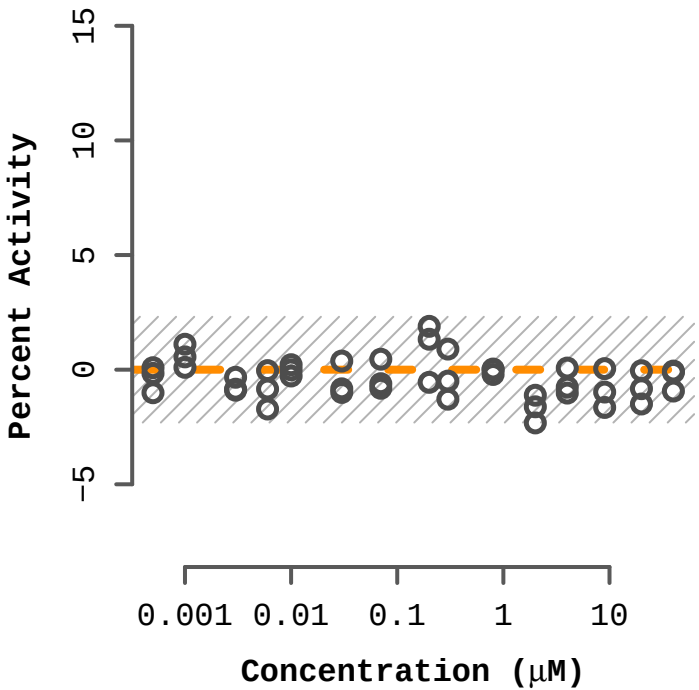
NAME: SB281832
CHID: 47324 CASRN: 219790-72-4
SPID(S): Tox21_300221
M4ID: 12478909

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.84 MAX_MED: 1.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

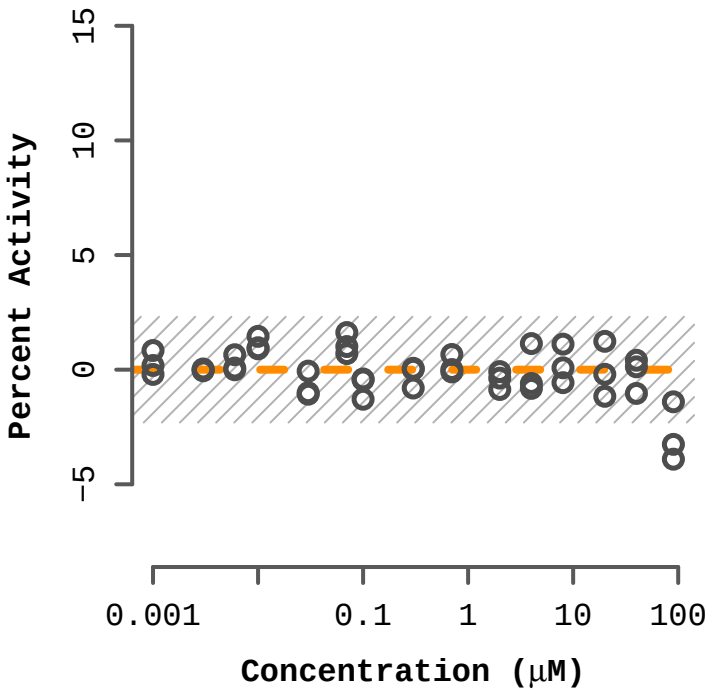
NAME: SB413217A
CHID: 47325 **CASRN:** NOCAS_47325
SPID(S): Tox21_300214
M4ID: 12478916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

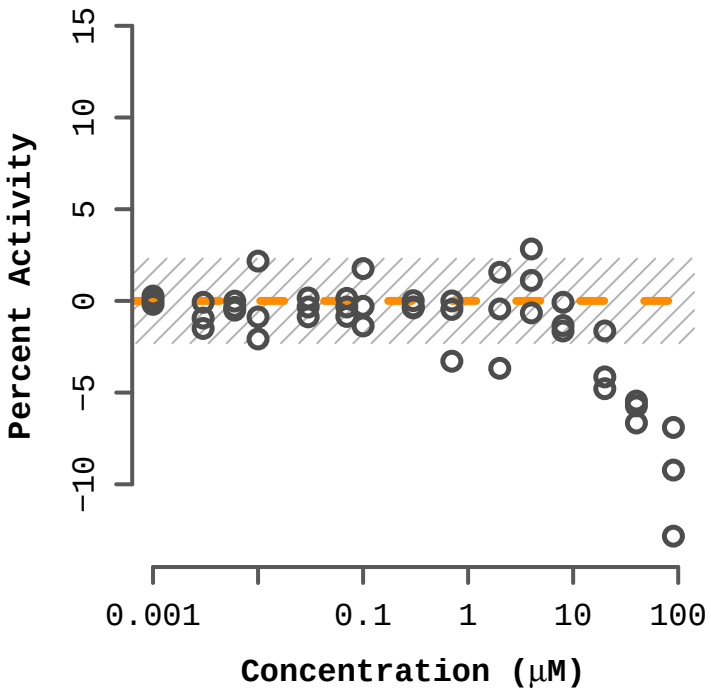
NAME: MK-578
CHID: 47327 **CASRN:** 313994-79-5
SPID(S): Tox21_300223
M4ID: 12478907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

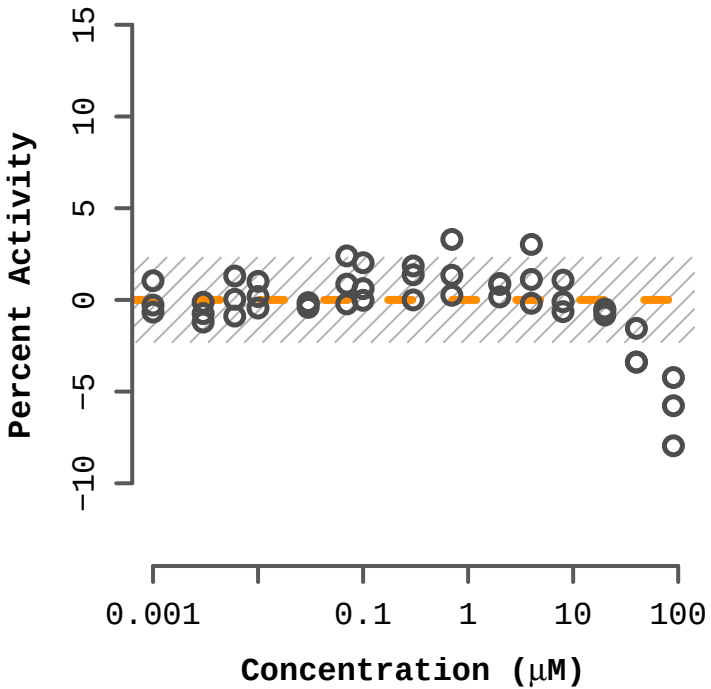
NAME: MK-274
CHID: 47328 **CASRN:** NOCAS_47328
SPID(S): Tox21_300224
M4ID: 12478906

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	223.29	NA	NA
PROB:	1	NA	NA
RMSE:	3.36	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

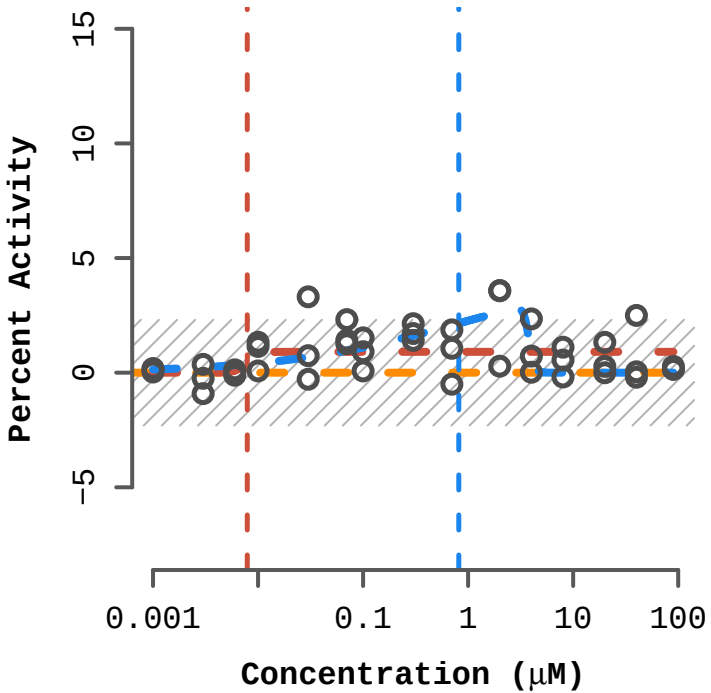
NAME: PharmaGSID_47330
CHID: 47330 **CASRN:** NOCAS_47330
SPID(S): Tox21_300225
M4ID: 12478905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.35	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: MK-547
CHID: 47331 CASRN: 331623-06-4
SPID(S): Tox21_300226
M4ID: 12478904

HILL MODEL (in red):

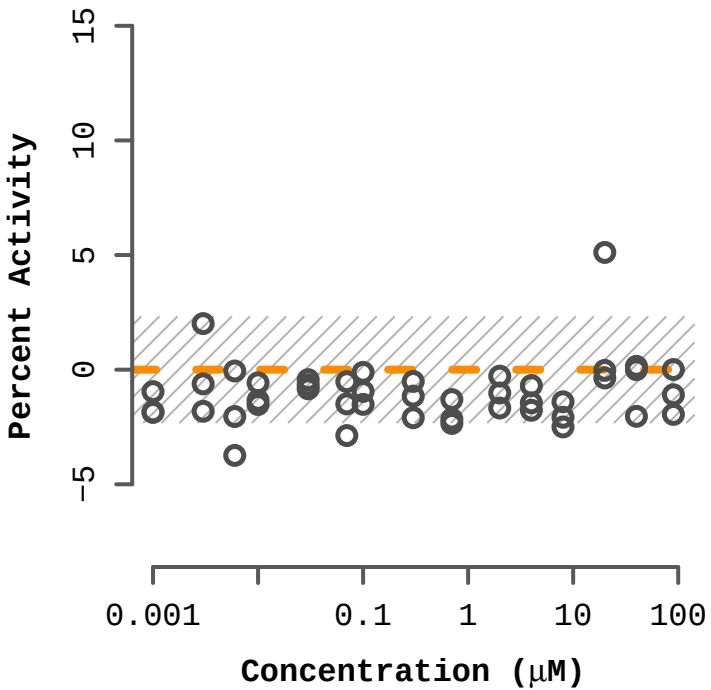
	tp	ga	gw
val:	0.909	−2.1	8
sd:	0.175	0.137	9.61

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.3	−0.0891	0.508	0.578	17.4
sd:	8.1	2.95	0.338	0.233	165

	CNST	HILL	GNLS
AIC:	154.61	134.33	132.08
PROB:	0	0.25	0.75
RMSE:	1.36	0.99	0.98

MAX_MEAN: 2.48 MAX_MED: 3.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

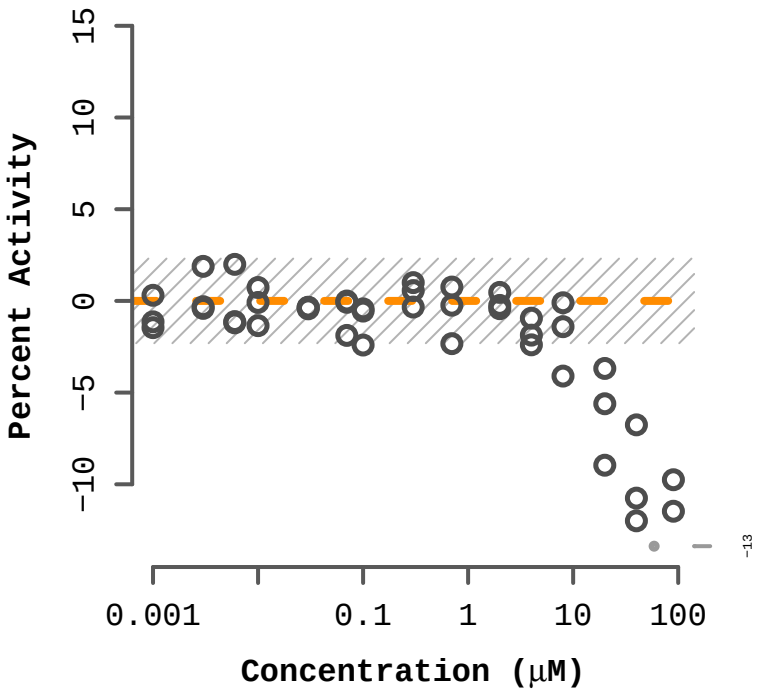
NAME: PharmaGSID_47333
CHID: 47333 **CASRN:** NOCAS_47333
SPID(S): Tox21_300261
M4ID: 12478869

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 0.00151 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

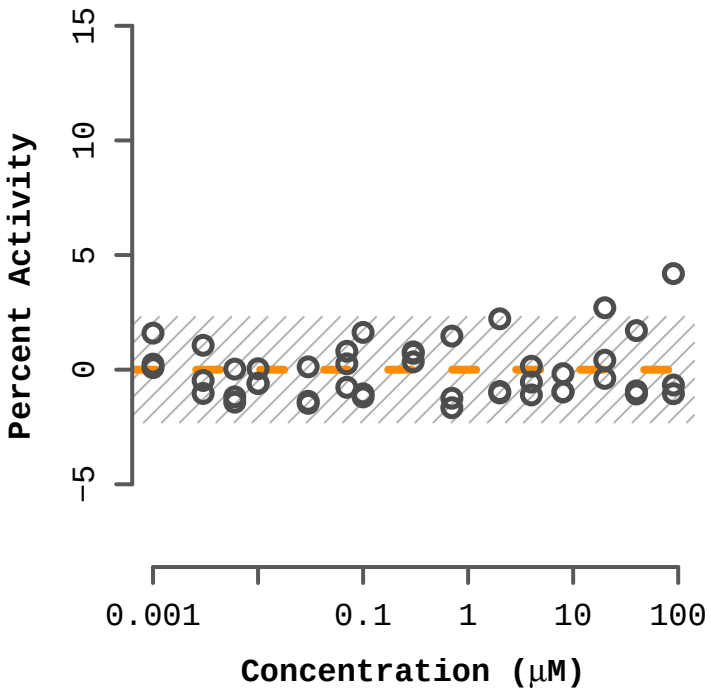
NAME: MK-968
CHID: 47334 CASRN: NOCAS_47334
SPID(S): Tox21_300262
M4ID: 12478868 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.22	NA	NA
PROB:	1	NA	NA
RMSE:	4.47	NA	NA

MAX_MEAN: 0.411 MAX_MED: 0.566 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

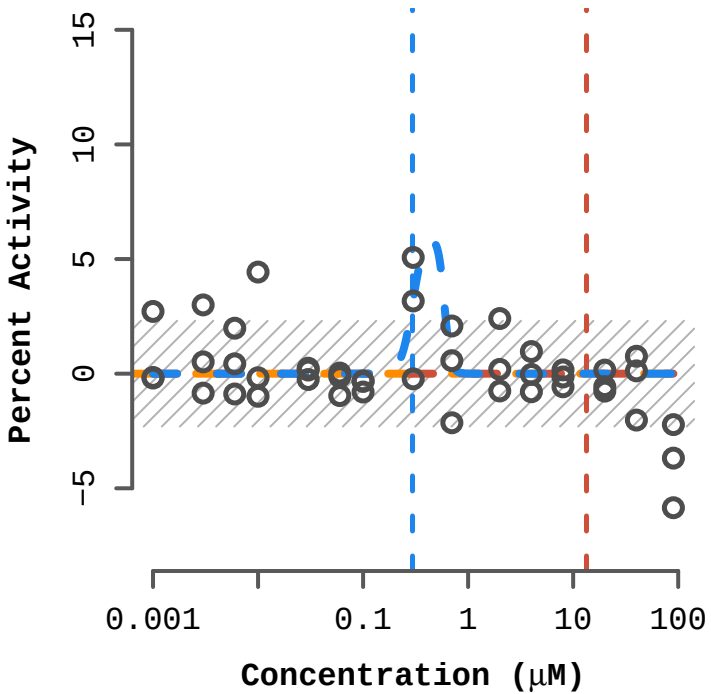
NAME: MK-812
CHID: 47335 **CASRN:** 851916-42-2
SPID(S): Tox21_300263
M4ID: 12478867

HILL MODEL: Not applicable.

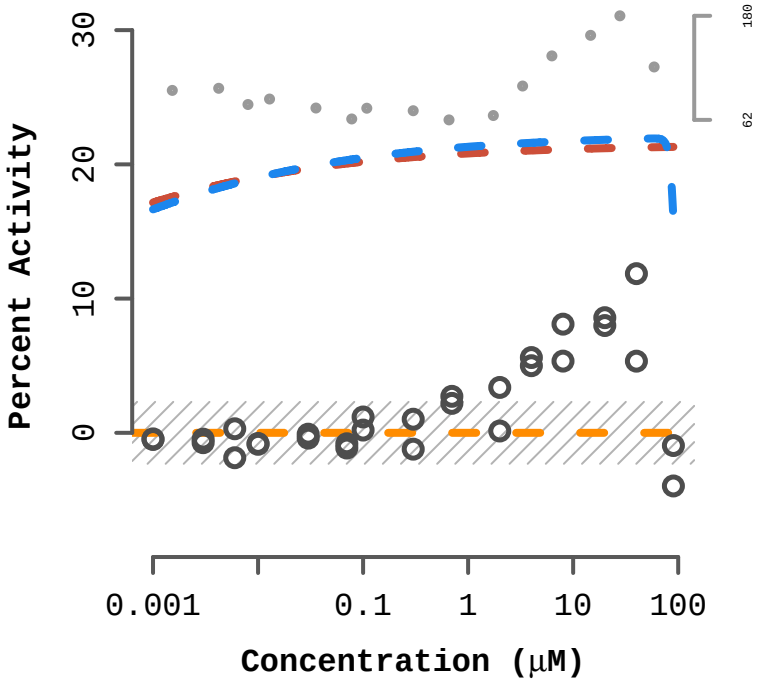
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.38	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 0.712 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    PharmaGSID_47337
CHID:    47337   CASRN: 1061517-62-1
SPID(S): Tox21_300264
M4ID:    12478866

HILL MODEL (in red):
      tp        ga        gw
val:  6.97e-11  1.13      1.46
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  6.08      -0.53     8         -0.226    14.6
sd:   106       2.01      29.6      3.51      720

      CNST        HILL        GNLS
AIC:  177.51      183.51      181.52
PROB: 0.84        0.04        0.11
RMSE: 1.87        1.87        1.74

MAX_MEAN: 2.67      MAX_MED: 3.17      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: HMR1426
CHID: 47338 CASRN: 262376-75-0
SPID(S): Tox21_300227
M4ID: 12478903 BRK

HILL MODEL (in red):

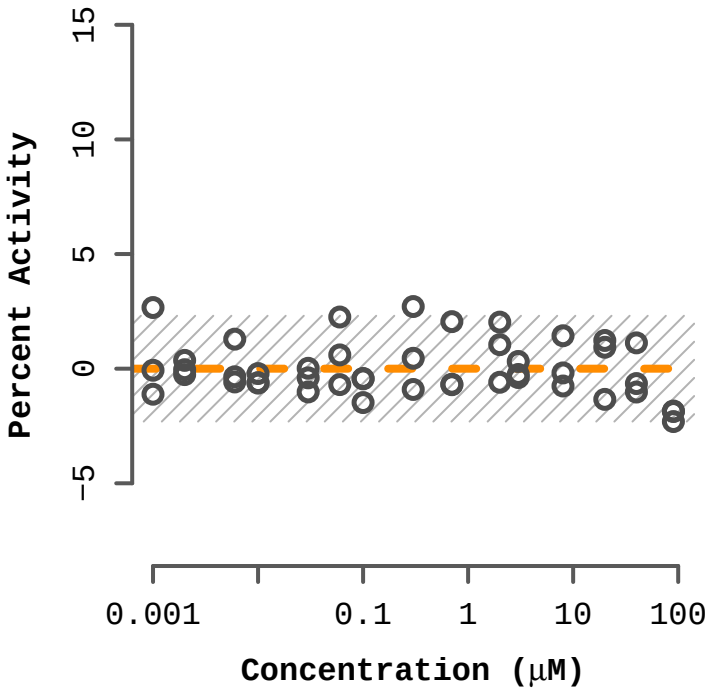
	tp	ga	gw
val:	21.5	-5	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.2	-4.59	0.3	1.98	17.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	490.09	485.71	489.67
PROB:	0.09	0.8	0.11
RMSE:	60.18	51.49	51.55

MAX_MEAN: 66 MAX_MED: 11.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

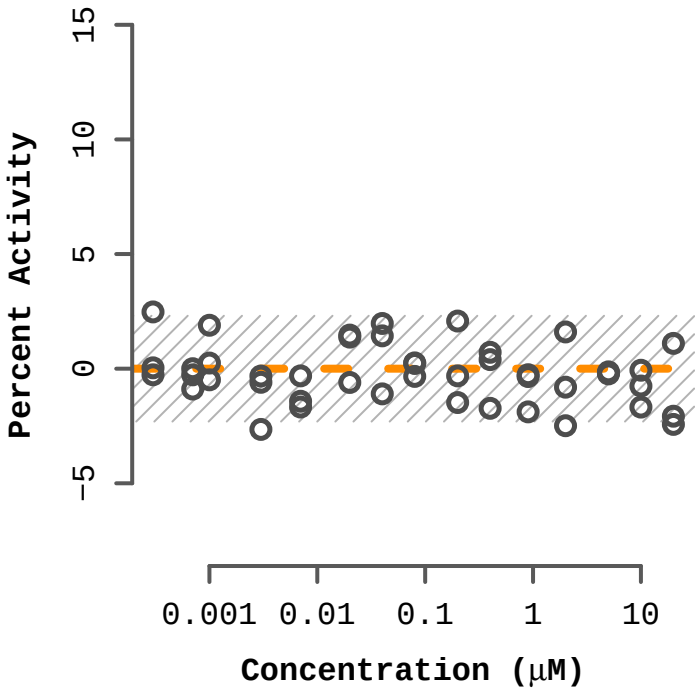
NAME: SR144190
CHID: 47339 **CASRN:** 181640-09-5
SPID(S): Tox21_300228
M4ID: 12478902

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.83 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

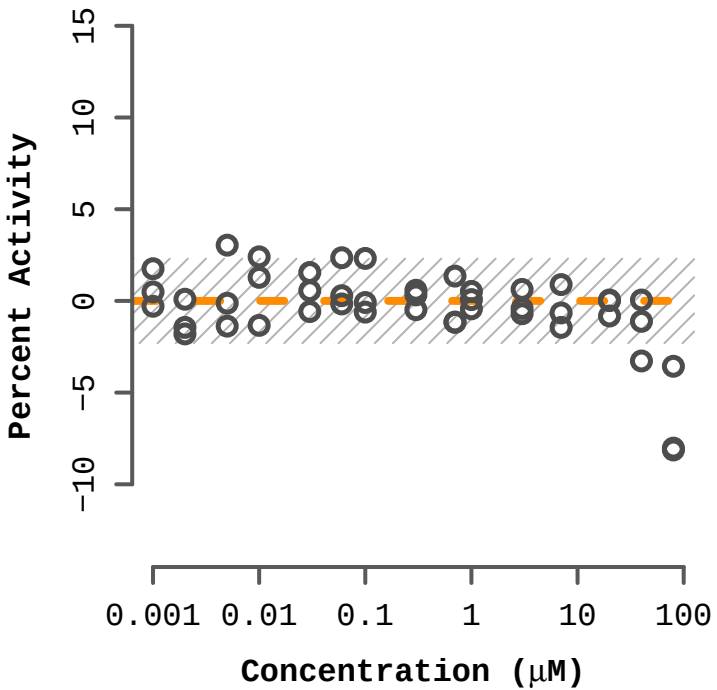
NAME: SSR146977
CHID: 47341 **CASRN:** 264618-44-2
SPID(S): Tox21_300229
M4ID: 12478901

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.769 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

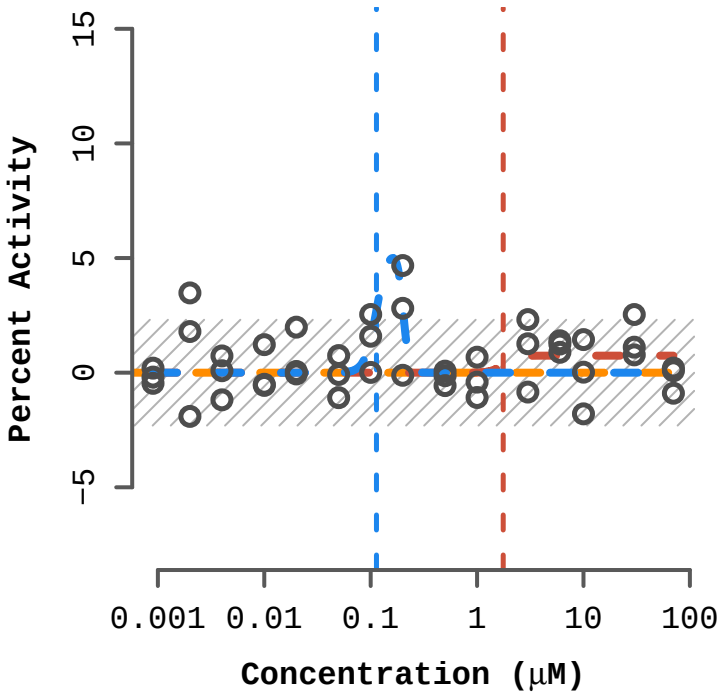
NAME: SR125047
CHID: 47342 CASRN: NOCAS_47342
SPID(S): Tox21_300230
M4ID: 12478900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.13	NA	NA
PROB:	1	NA	NA
RMSE:	2.16	NA	NA

MAX_MEAN: 0.826 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cariporide mesylate
CHID: 47344 CASRN: 159138-81-5
SPID(S): Tox21_300231
M4ID: 12478899

HILL MODEL (in red):

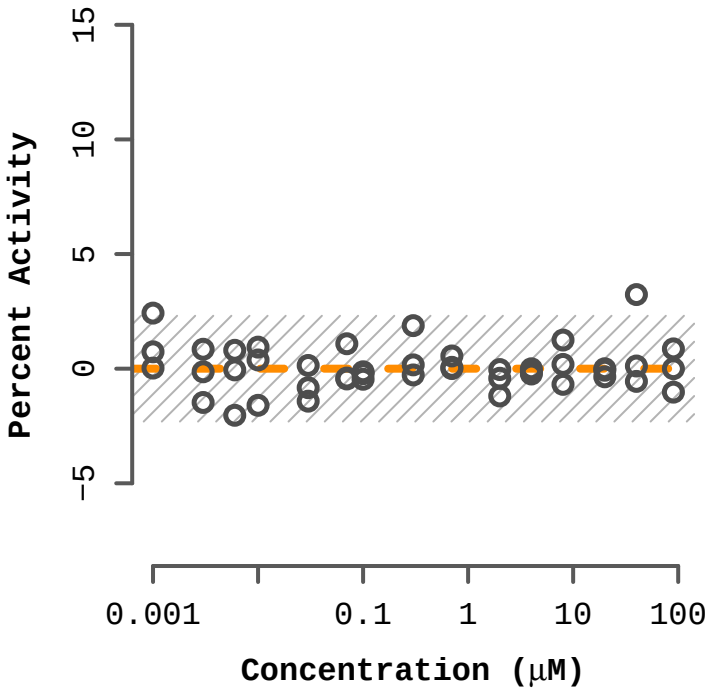
	tp	ga	gw
val:	0.743	0.246	8
sd:	0.312	0.492	16.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.46	−0.946	8	−0.696	15.8
sd:	141	2.01	30	0.861	2990

	CNST	HILL	GNLS
AIC:	161.7	162.64	162.41
PROB:	0.43	0.27	0.3
RMSE:	1.46	1.41	1.27

MAX_MEAN: 2.46 **MAX_MED:** 2.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

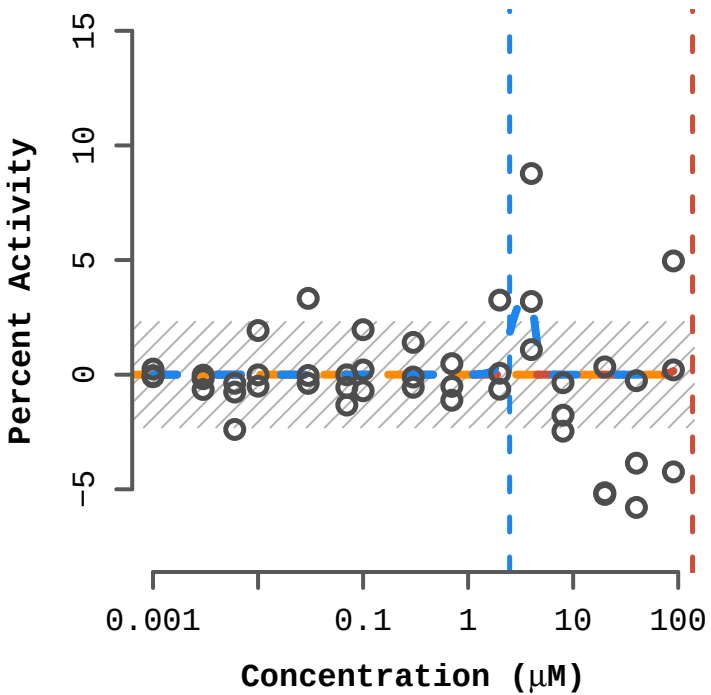
NAME: SSR162369
CHID: 47346 CASRN: NOCAS_47346
SPID(S): Tox21_300232
M4ID: 12478898

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.06 MAX_MED: 0.736 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SR271425
CHID: 47347 CASRN: 155990-20-8
SPID(S): Tox21_300233
M4ID: 12478897

HILL MODEL (in red):

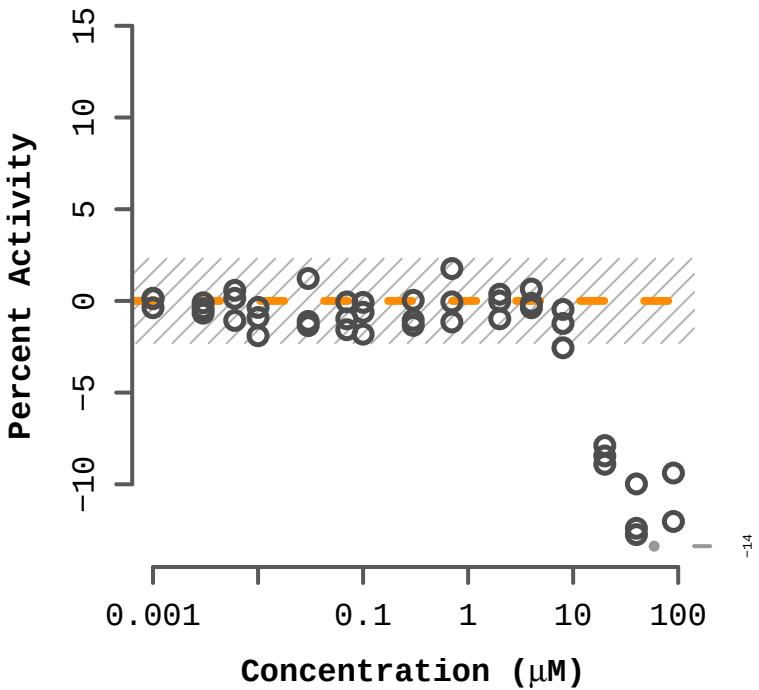
	tp	ga	gw
val:	4.69	2.14	7.97
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.66	0.395	8	0.645	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	203.55	209.54	207.17
PROB:	0.82	0.04	0.13
RMSE:	2.52	2.52	2.27

MAX_MEAN: 4.35 MAX_MED: 3.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

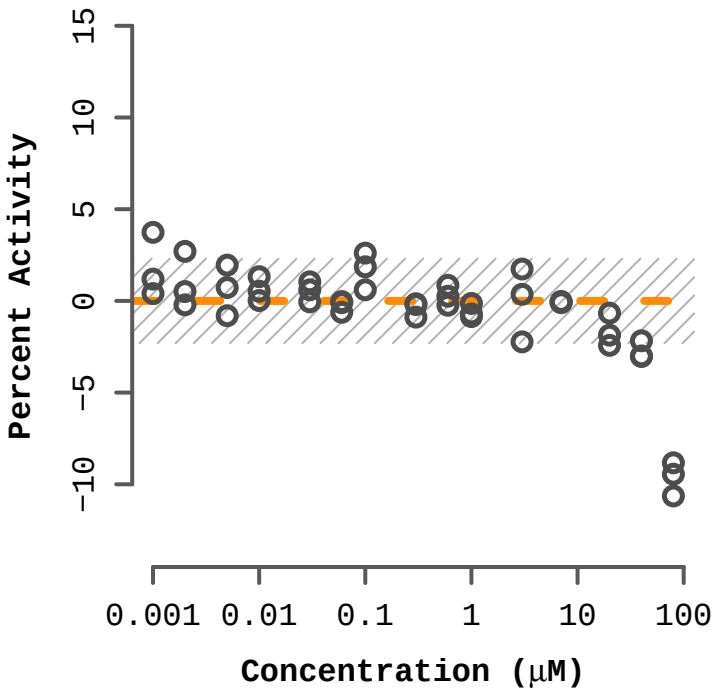
NAME: SSR504734
CHID: 47348 **CASRN:** 742693-38-5
SPID(S): Tox21_300234
M4ID: 12478896 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	255.19	NA	NA
PROB:	1	NA	NA
RMSE:	4.91	NA	NA

MAX_MEAN: 0.189 **MAX_MED:** 0.143 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

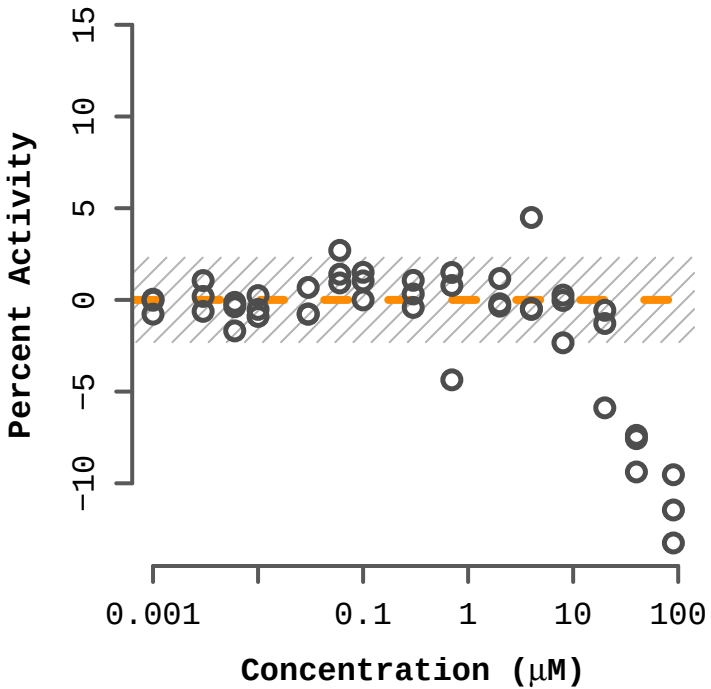
NAME: AVE8488
CHID: 47349 **CASRN:** NOCAS_47349
SPID(S): Tox21_300471
M4ID: 12478661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	199.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.85	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

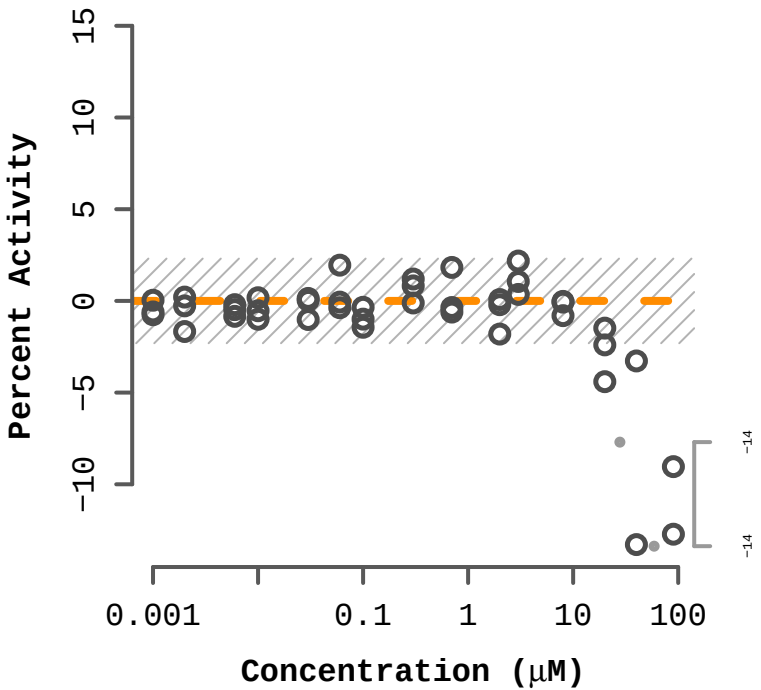
NAME: SSR240612
CHID: 47351 CASRN: NOCAS_47351
SPID(S): Tox21_300235
M4ID: 12478895

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233.77	NA	NA
PROB:	1	NA	NA
RMSE:	3.96	NA	NA

MAX_MEAN: 1.68 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

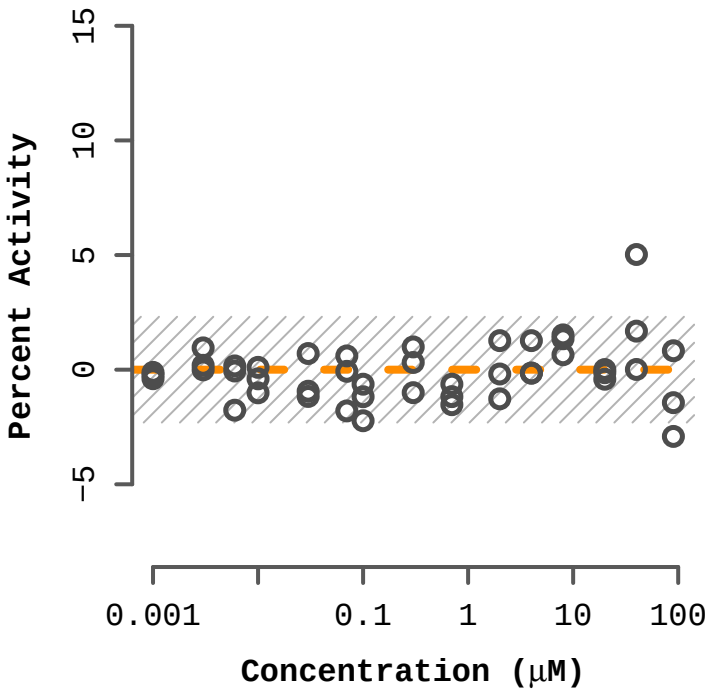
NAME: SSR241586
CHID: 47353 **CASRN:** NOCAS_47353
SPID(S): Tox21_300236
M4ID: 12478894 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.49	NA	NA
PROB:	1	NA	NA
RMSE:	4.43	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

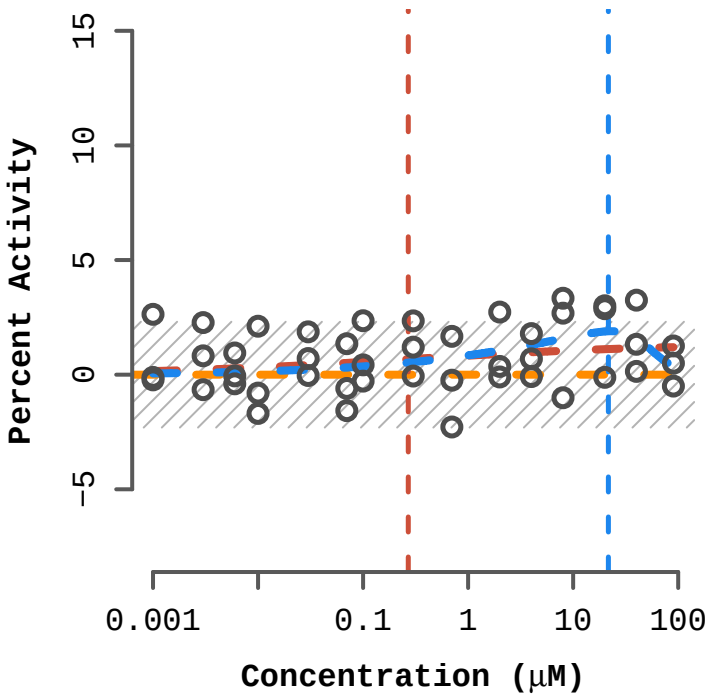
NAME: Trelanserin
CHID: 47355 **CASRN:** 189003-92-7
SPID(S): Tox21_300237
M4ID: 12478893

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.24 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ilepatril
CHID: 47356 CASRN: 473289-62-2
SPID(S): Tox21_300238
M4ID: 12478892

HILL MODEL (in red):

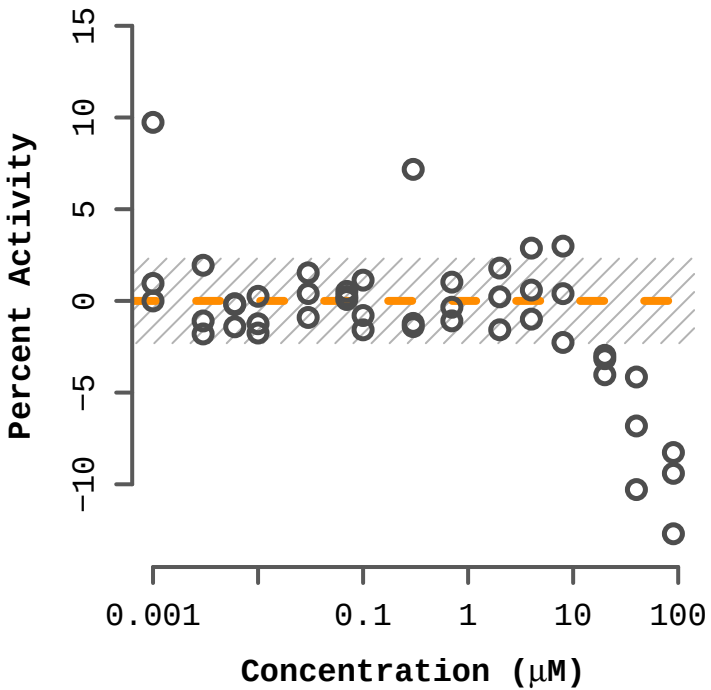
	tp	ga	gw
val:	1.35	−0.57	0.361
sd:	1	2.31	0.544

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4	1.34	0.431	1.72	3.27
sd:	5.22	2.18	0.415	0.314	3.06

	CNST	HILL	GNLS
AIC:	174.63	169.42	170.73
PROB:	0.05	0.63	0.33
RMSE:	1.59	1.37	1.34

MAX_MEAN: 1.92 MAX_MED: 2.88 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

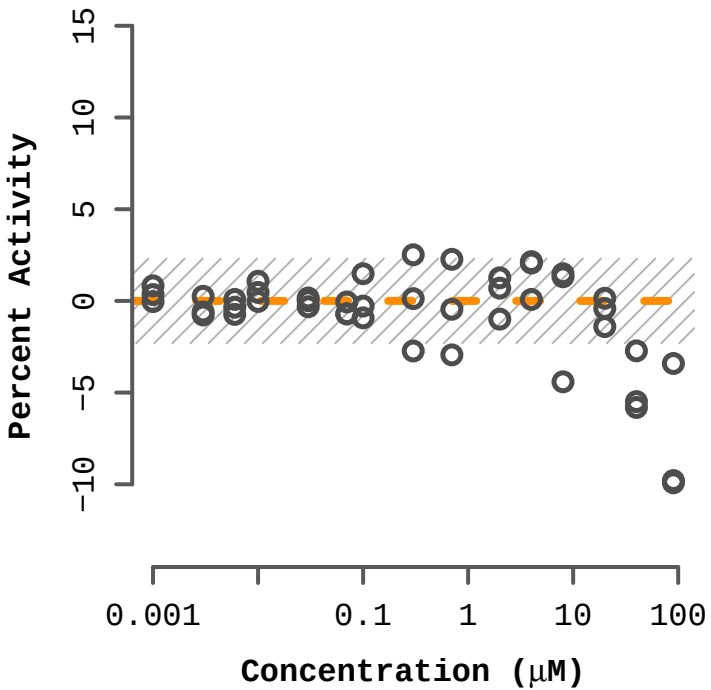
NAME: Surinabant
CHID: 47357 CASRN: 288104-79-0
SPID(S): Tox21_300239
M4ID: 12478891

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	243.08	NA	NA
PROB:	1	NA	NA
RMSE:	4.02	NA	NA

MAX_MEAN: 3.56 **MAX_MED:** 0.954 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

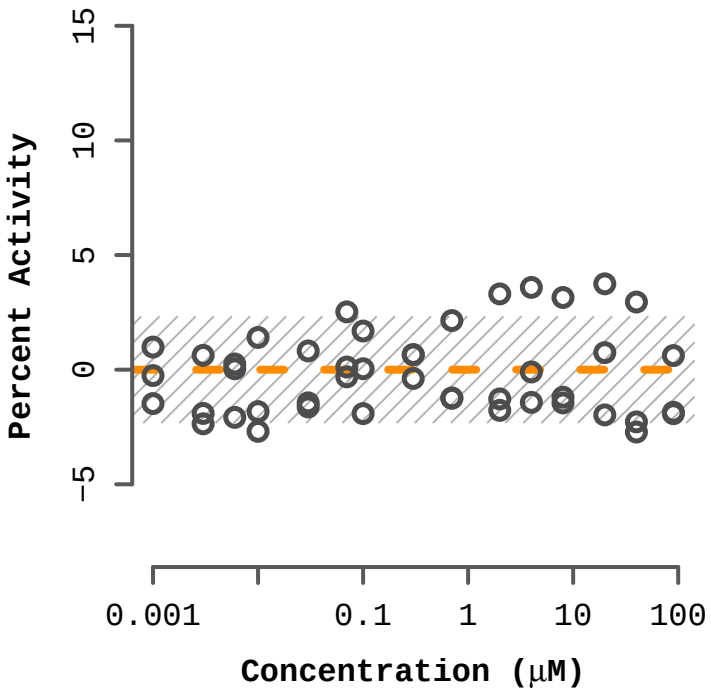
NAME: Nelivaptan
CHID: 47358 **CASRN:** 439687-69-1
SPID(S): Tox21_300240
M4ID: 12478890

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	203.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.79	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

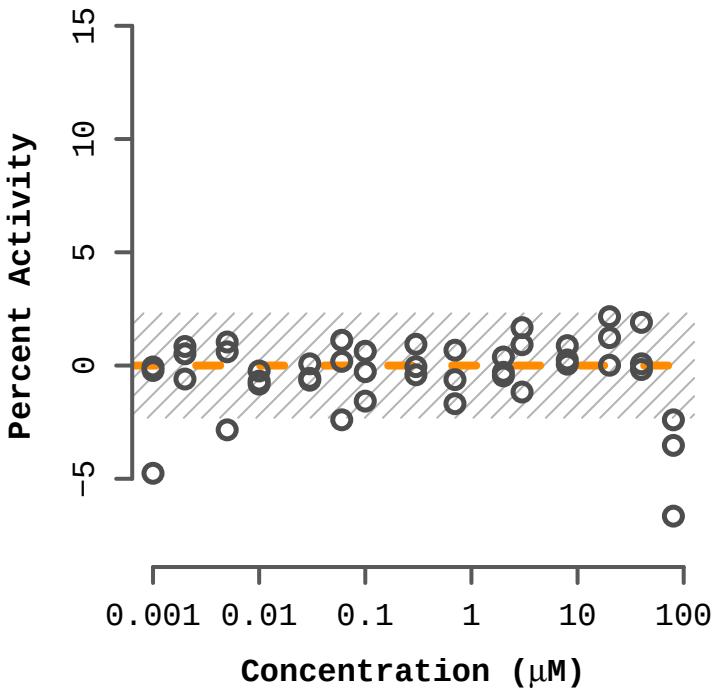
NAME: SSR180711
CHID: 47359 **CASRN:** 298198-52-4
SPID(S): Tox21_300241
M4ID: 12478889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 0.84 **MAX_MED:** 0.744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

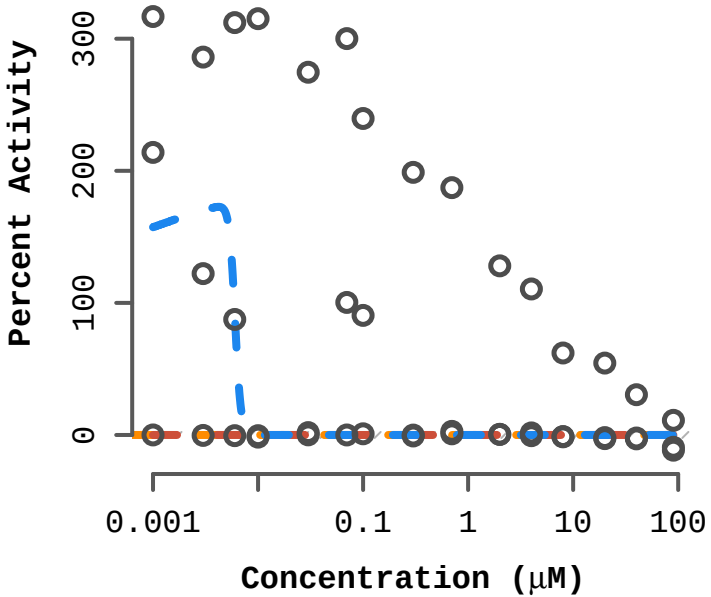
NAME: SR58611
CHID: 47360 **CASRN:** 929601-09-2
SPID(S): Tox21_300242
M4ID: 12478888

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SSR150106
CHID: 47362 CASRN: NOCAS_47362
SPID(S): Tox21_300243
M4ID: 12478887

HILL MODEL (in red):

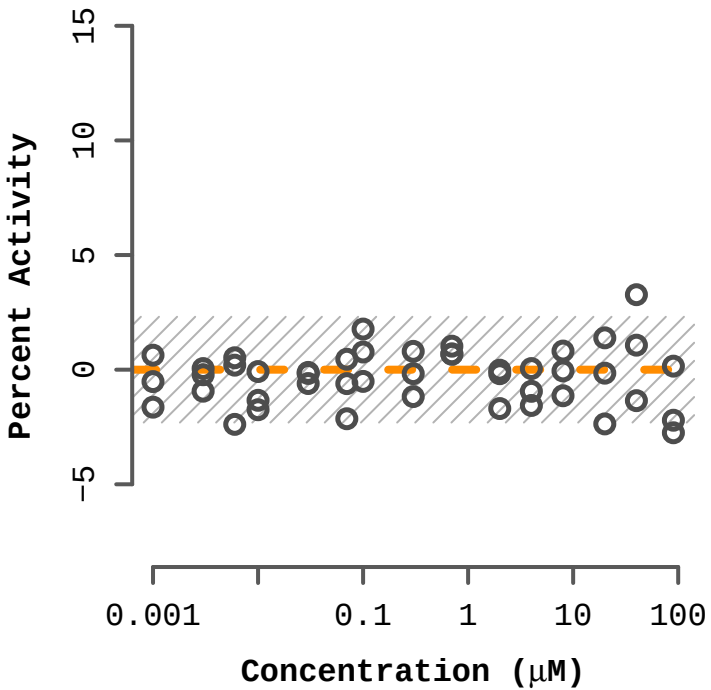
	tp	ga	gw
val:	9.65	2.45	5.83
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	214	-4.48	0.3	-2.22	15.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	571.95	568.49	561.28
PROB:	0	0.03	0.97
RMSE:	133.34	133.34	116.16

MAX_MEAN: 177 MAX_MED: 214 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

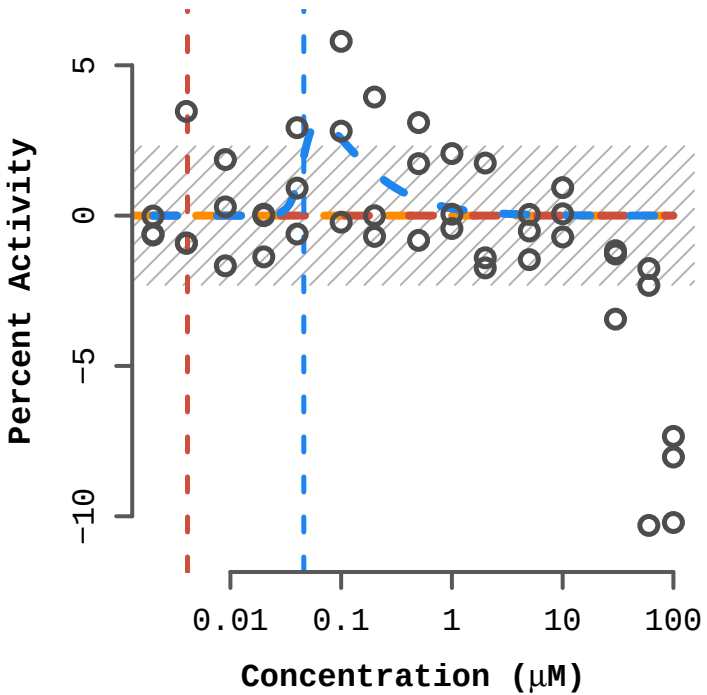
NAME: Volinanserin
CHID: 47363 **CASRN:** 139290-65-6
SPID(S): Tox21_300244
M4ID: 12478886

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 0.997 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SSR103800
CHID: 47364 CASRN: NOCAS_47364
SPID(S): Tox21_300245
M4ID: 12478885

HILL MODEL (in red):

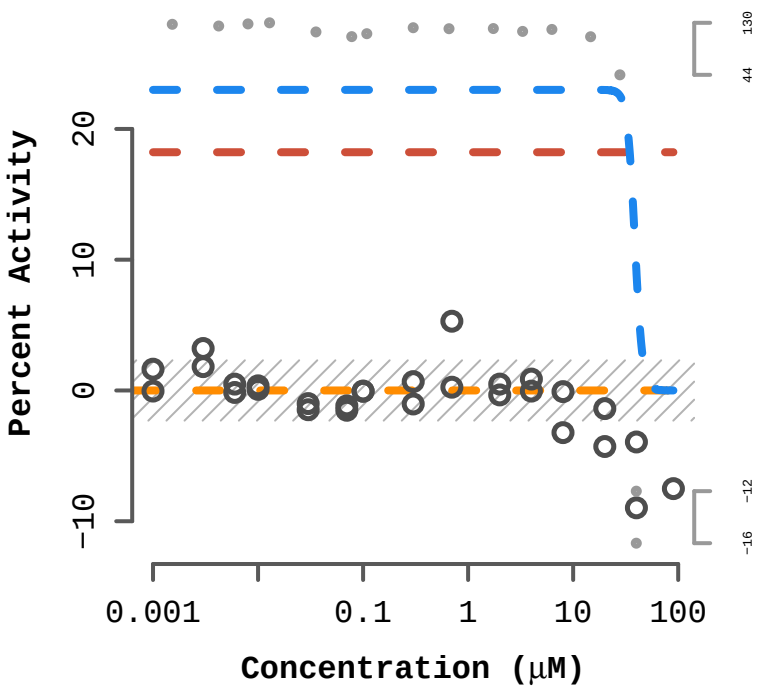
	tp	ga	gw
val:	1.38e−09	−2.39	3.96
sd:	NaN	NaN	NaN

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.85	−1.34	7.89	−1.09	1.26
sd:	28.5	0.259	22	2.79	1.26

	CNST	HILL	GNLS
AIC:	222.06	228.06	227.21
PROB:	0.89	0.04	0.07
RMSE:	3.24	3.24	3.12

MAX_MEAN: 2.8 MAX_MED: 2.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SAR115740
CHID: 47366 CASRN: NOCAS_47366
SPID(S): Tox21_300246
M4ID: 12478884 BRK

HILL MODEL (in red):

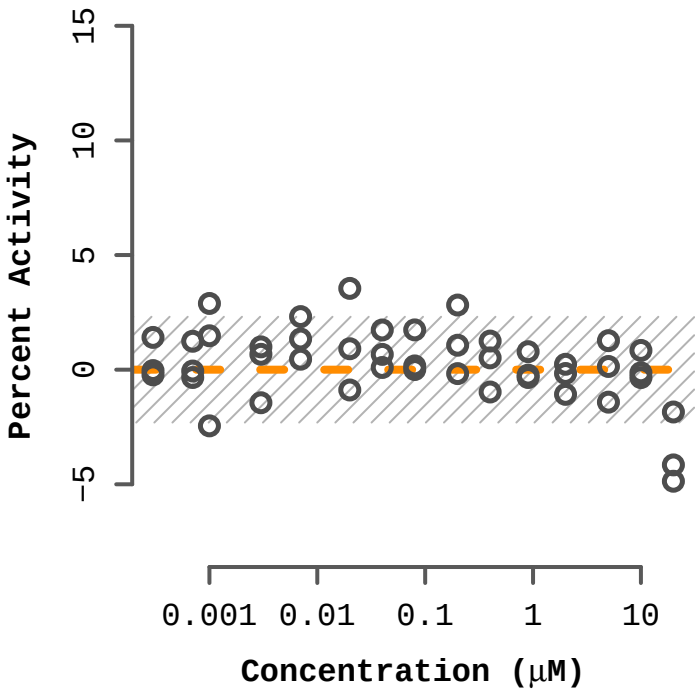
	tp	ga	gw
val:	18.2	−4.62	3.98
sd:	8.24	1530	3720

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23	−4.53	7.82	1.59	12
sd:	9.38	380000	574000	0.494	374

	CNST	HILL	GNLS
AIC:	500.24	497.9	500
PROB:	0.19	0.6	0.21
RMSE:	63.23	55.74	53.87

MAX_MEAN: 42.5 MAX_MED: 5.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

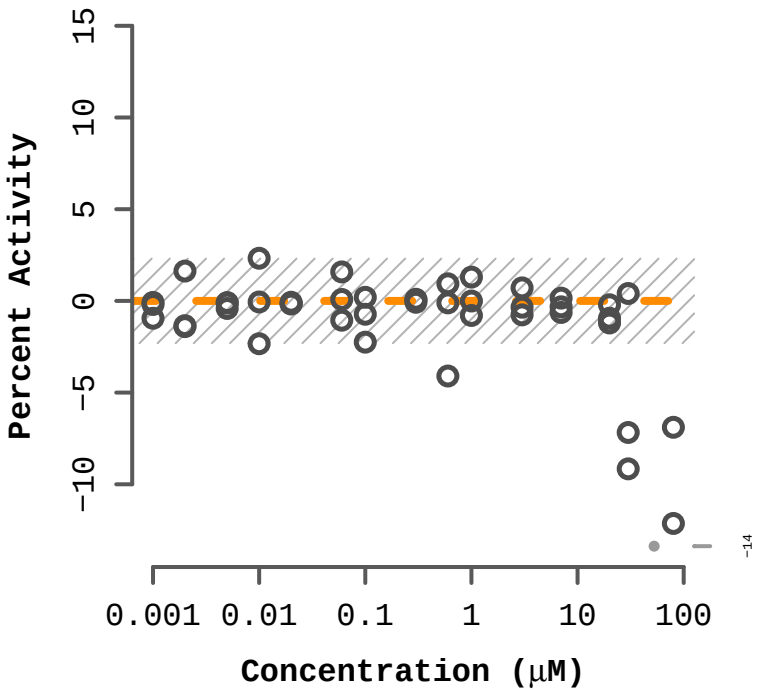
NAME: SSR69071
CHID: 47368 **CASRN:** 344930-95-6
SPID(S): Tox21_300247
M4ID: 12478883

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

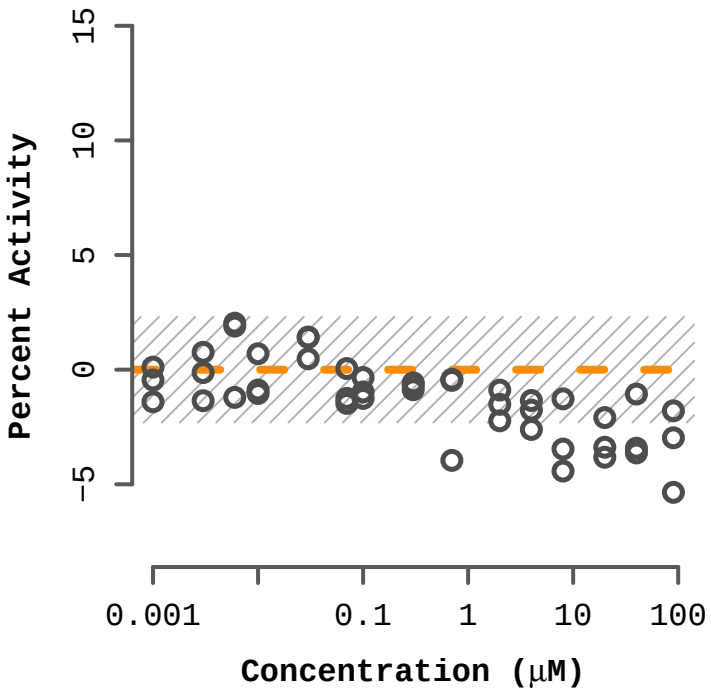
NAME: SR146131
CHID: 47369 CASRN: 221671-62-1
SPID(S): Tox21_300248
M4ID: 12478882 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.67	NA	NA
PROB:	1	NA	NA
RMSE:	3.61	NA	NA

MAX_MEAN: 0.204 **MAX_MED:** 0.0809 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

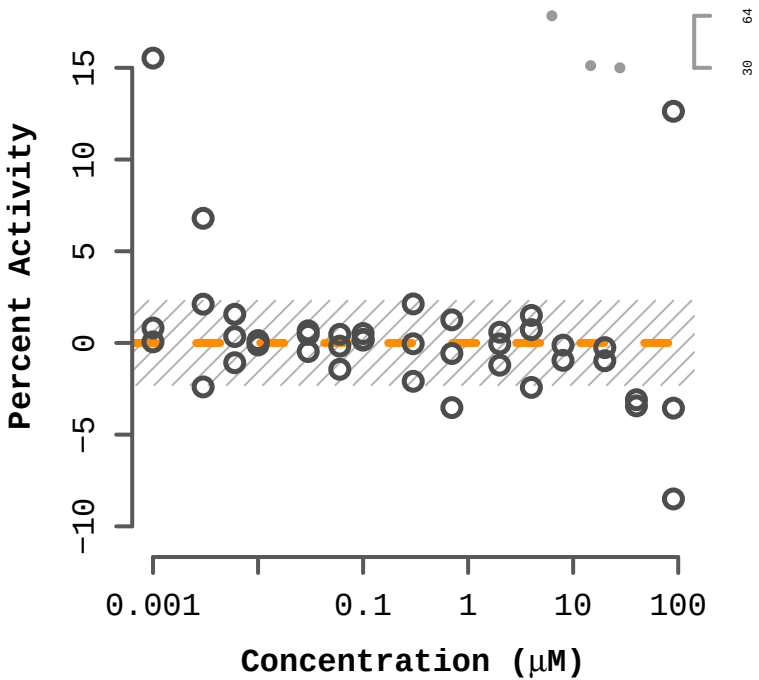
NAME: AVE5638
CHID: 47371 CASRN: 725228-45-5
SPID(S): Tox21_300249
M4ID: 12478881

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.3	NA	NA
PROB:	1	NA	NA
RMSE:	2.08	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

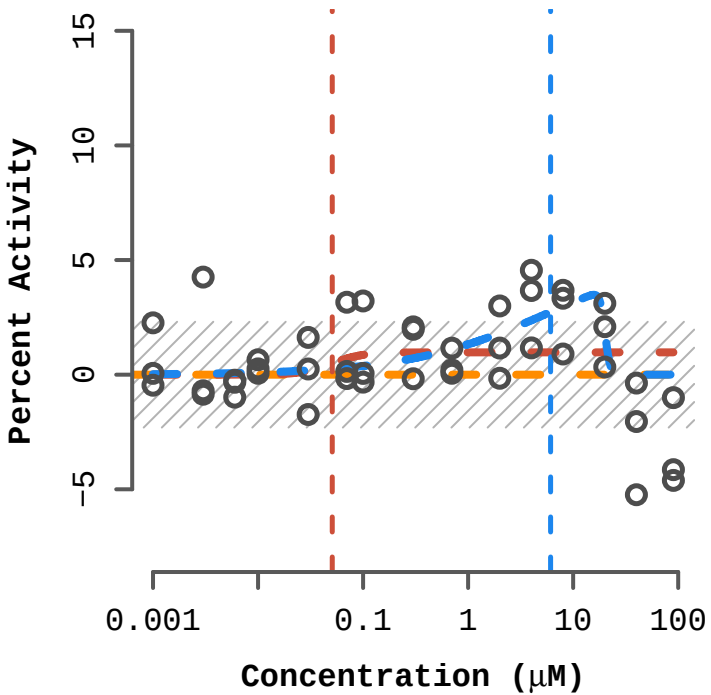
NAME: AVE3295
CHID: 47372 **CASRN:** 478263-98-8
SPID(S): Tox21_300250
M4ID: 12478880 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	283.74	NA	NA
PROB:	1	NA	NA
RMSE:	12.06	NA	NA

MAX_MEAN: 21 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SSR161421
CHID: 47374 CASRN: NOCAS_47374
SPID(S): Tox21_300251
M4ID: 12478879

HILL MODEL (in red):

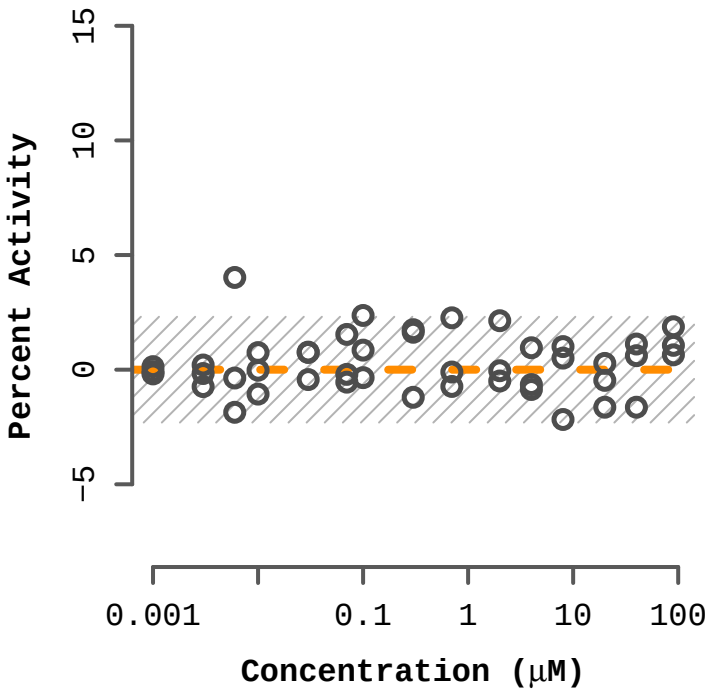
	tp	ga	gw
val:	0.974	−1.29	3.02
sd:	0.425	0.621	10.2

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.47	0.785	0.631	1.3	17.9
sd:	6.64	1.63	0.454	0.0411	263

	CNST	HILL	GNLS
AIC:	201.24	201.16	190.01
PROB:	0	0	0.99
RMSE:	2.21	2.15	1.82

MAX_MEAN: 3.13 MAX_MED: 3.67 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

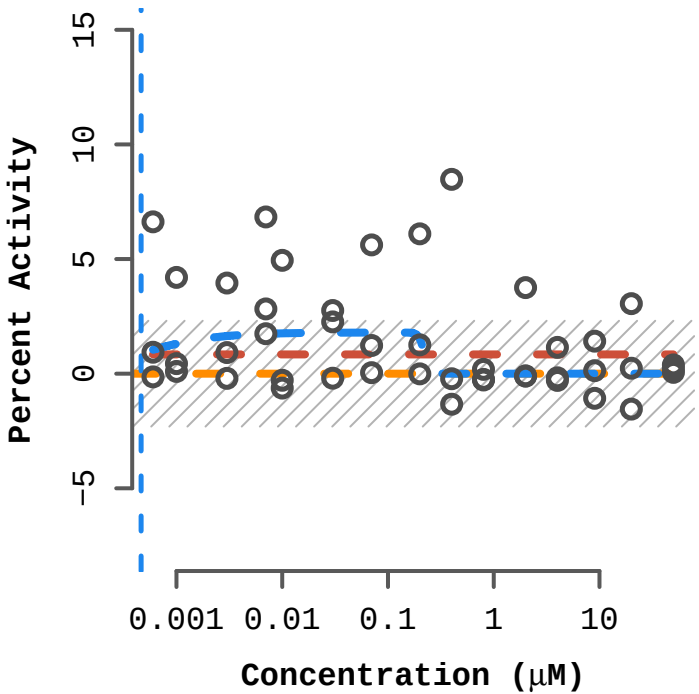
NAME: AVE9423
CHID: 47375 **CASRN:** 862243-29-6
SPID(S): Tox21_300252
M4ID: 12478878

HILL MODEL: Not applicable.

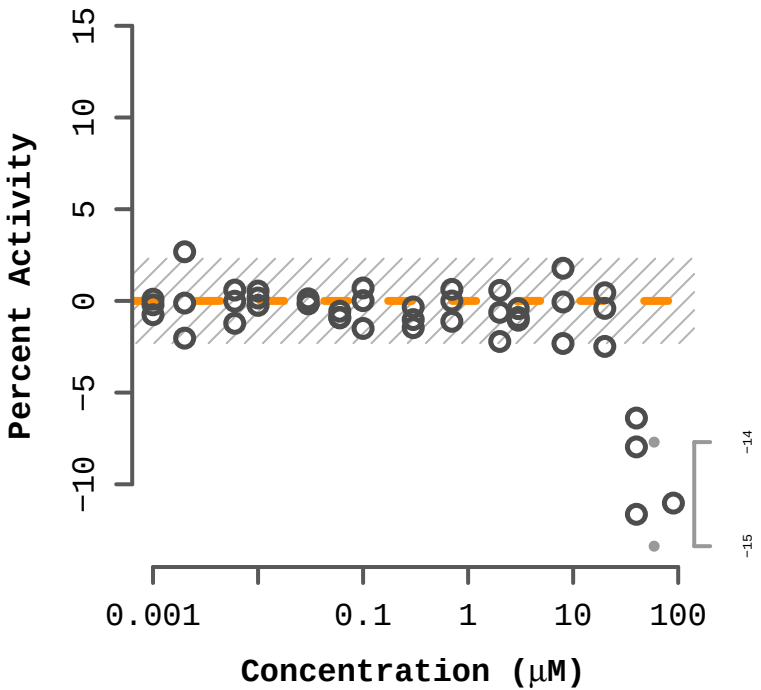
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.63 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    AVE2865
CHID:    47376   CASRN: 648917-13-9
SPID(S): Tox21_300253
M4ID:    12478877

HILL MODEL (in red):
      tp       ga       gw
val:  0.84     -4.63    5.1
sd:   0.31     1850     6630

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.79     -3.33    1.26     -0.657   17.5
sd:   0.665    0.978    3.12     1.45     609

      CNST        HILL        GNLS
AIC:  213.33      211.1       209.1
PROB: 0.08        0.25        0.67
RMSE: 2.79        2.47        2.36

MAX_MEAN: 3.8       MAX_MED: 2.83      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

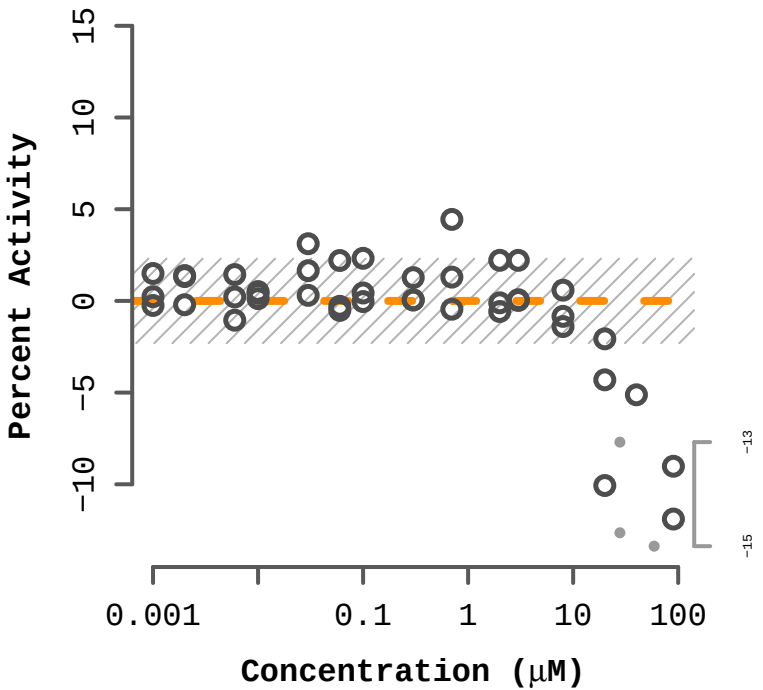
NAME: AVE6324
CHID: 47377 **CASRN:** NOCAS_47377
SPID(S): Tox21_300254
M4ID: 12478876 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.15	NA	NA
PROB:	1	NA	NA
RMSE:	4.25	NA	NA

MAX_MEAN: 0.178 **MAX_MED:** 0.161 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

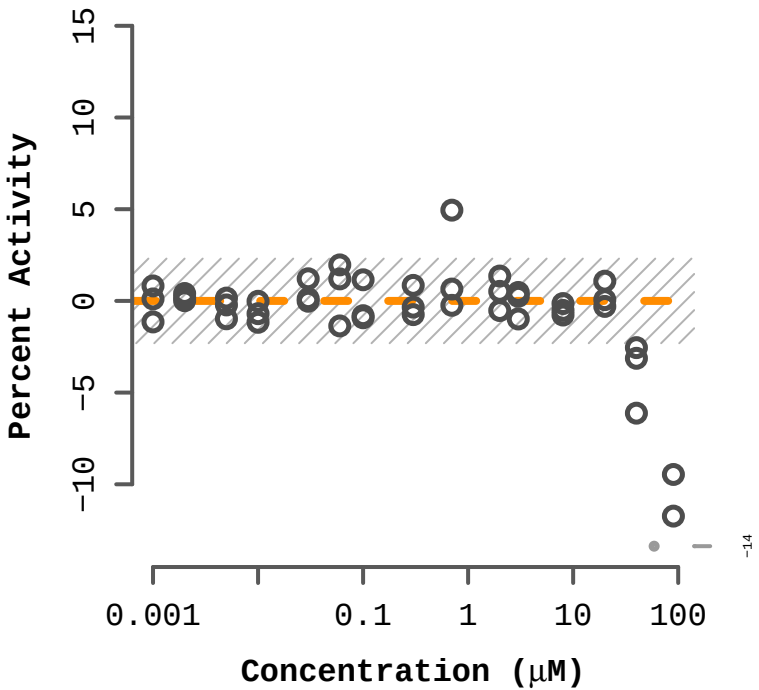
NAME: SSR126768
CHID: 47379 CASRN: NOCAS_47379
SPID(S): Tox21_300255
M4ID: 12478875 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.78	NA	NA
PROB:	1	NA	NA
RMSE:	4.86	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

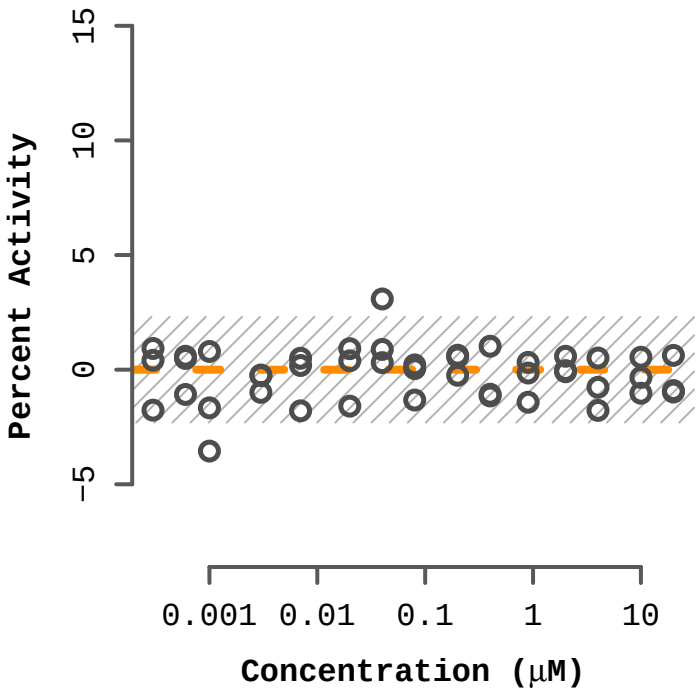
NAME: AVE8923
CHID: 47381 CASRN: NOCAS_47381
SPID(S): Tox21_300472
M4ID: 12478660 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	200.25	NA	NA
PROB:	1	NA	NA
RMSE:	3.41	NA	NA

MAX_MEAN: 1.79 MAX_MED: 1.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

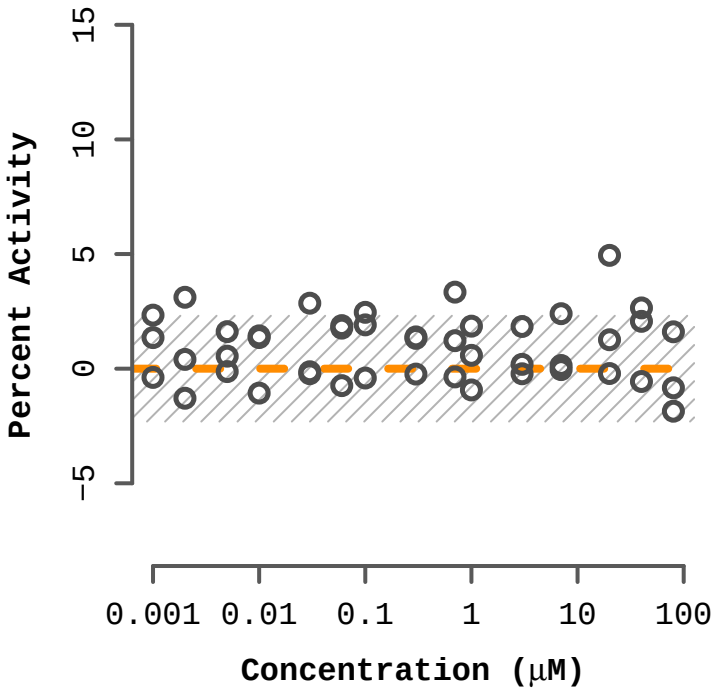
NAME: AVE3247
CHID: 47383 CASRN: NOCAS_47383
SPID(S): Tox21_300256
M4ID: 12478874

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.884 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

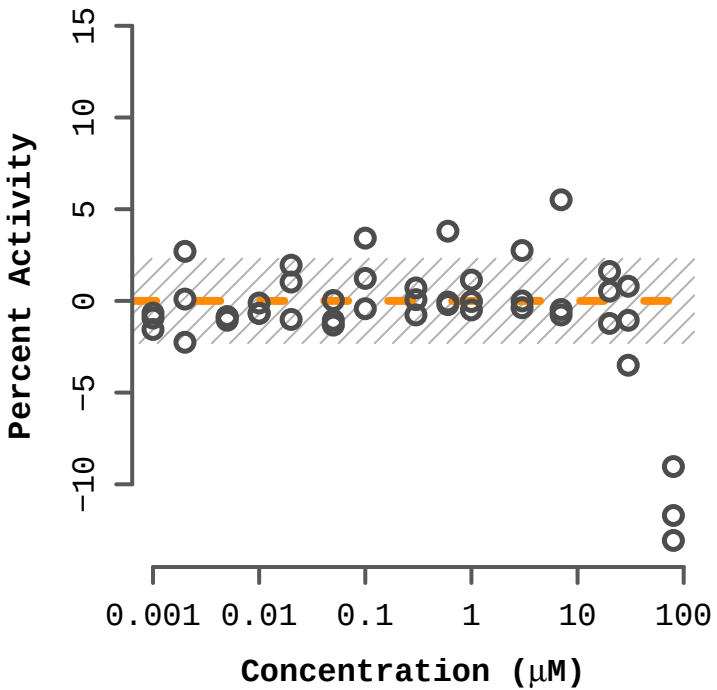
NAME: SAR377142
CHID: 47385 **CASRN:** NOCAS_47385
SPID(S): Tox21_300257
M4ID: 12478873

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

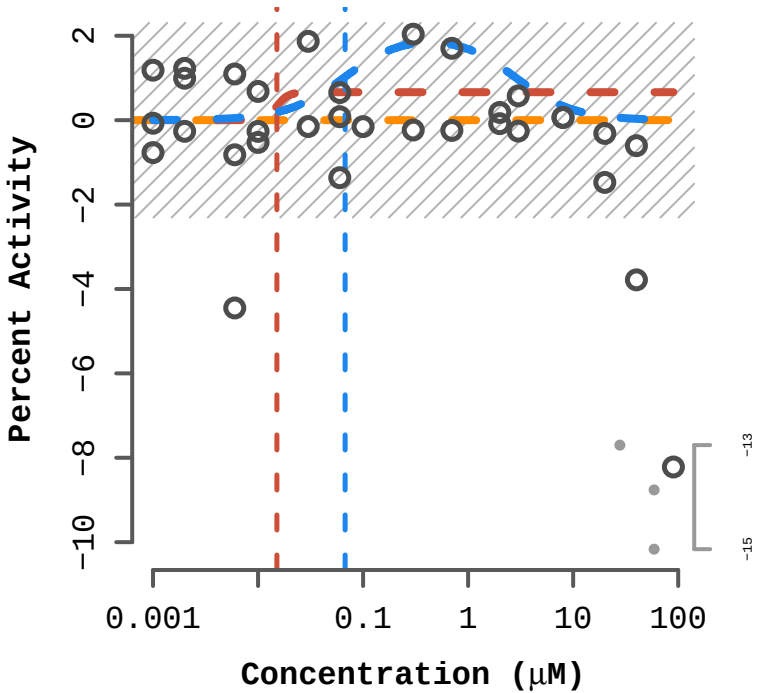
NAME: SAR102779
CHID: 47387 **CASRN:** NOCAS_47387
SPID(S): Tox21_300258
M4ID: 12478872

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.12	NA	NA
PROB:	1	NA	NA
RMSE:	3.35	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: SAR150640
CHID: 47389 CASRN: NOCAS_47389
SPID(S): Tox21_300259
M4ID: 12478871 BRK

HILL MODEL (in red):

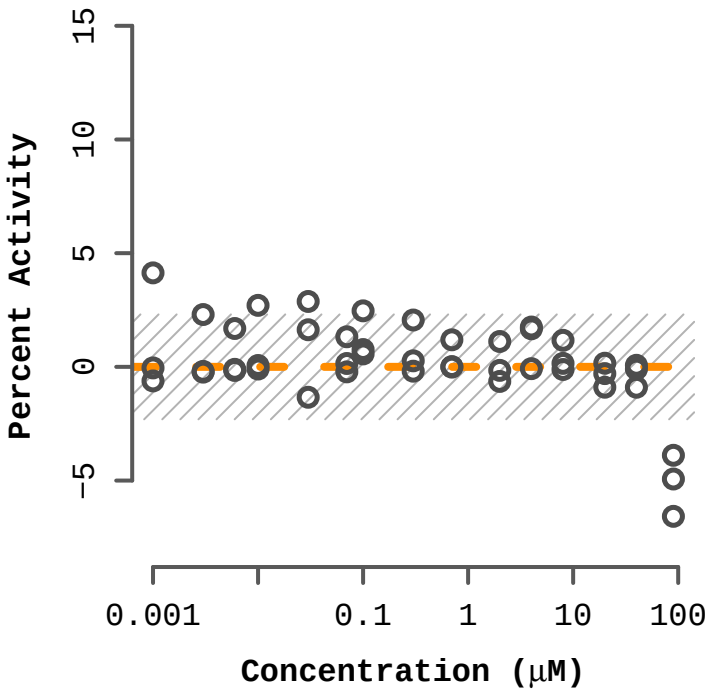
	tp	ga	gw
val:	0.663	−1.82	8
sd:	0.418	0.921	28.8

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.06	−1.17	1.53	0.443	1.55
sd:	1.99	0.755	2.49	0.927	1.87

	CNST	HILL	GNLS
AIC:	236.28	239.89	238.95
PROB:	0.7	0.12	0.18
RMSE:	4.21	4.32	4.1

MAX_MEAN: 2.19 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

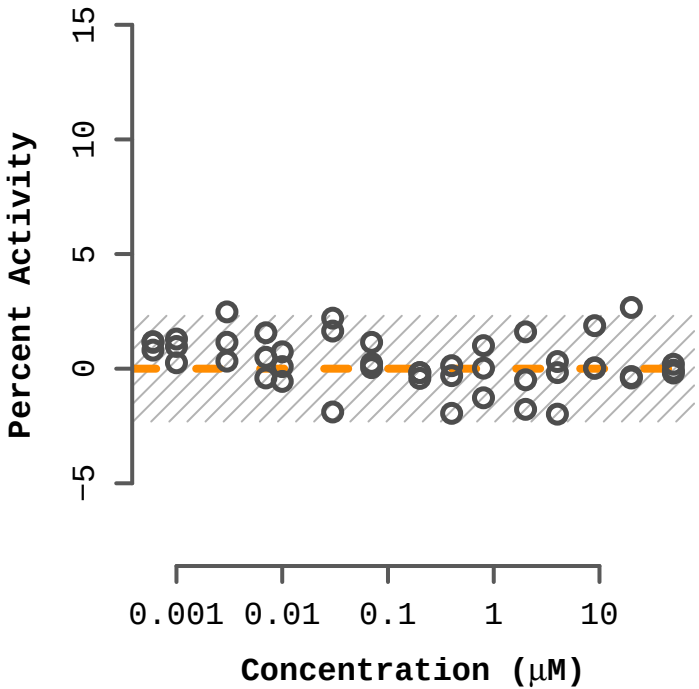
NAME: SAR102608
CHID: 47391 CASRN: 1068967-96-3
SPID(S): Tox21_300260
M4ID: 12478870

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.27 MAX_MED: 1.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

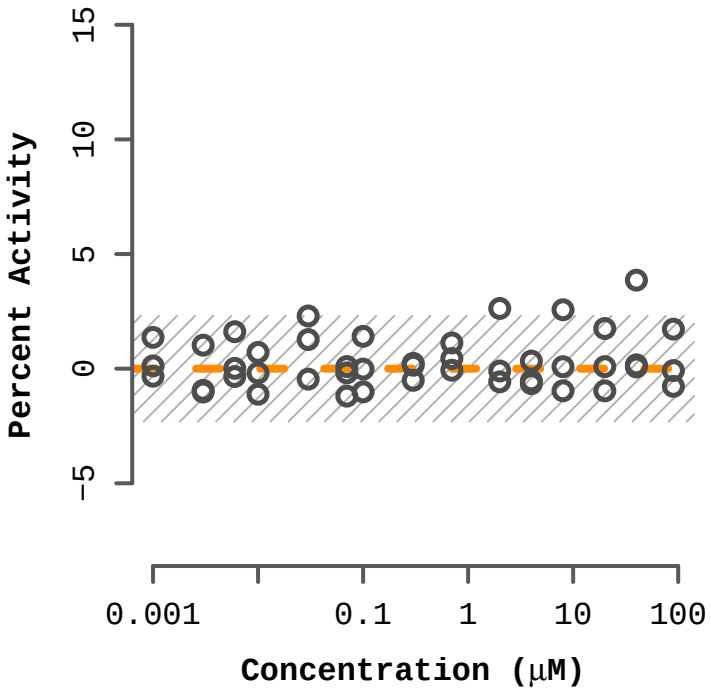
NAME: Grinstad Soft−N−Safe
CHID: 47394 **CASRN:** NOCAS_47394
SPID(S): Tox21_300630
M4ID: 12478503

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

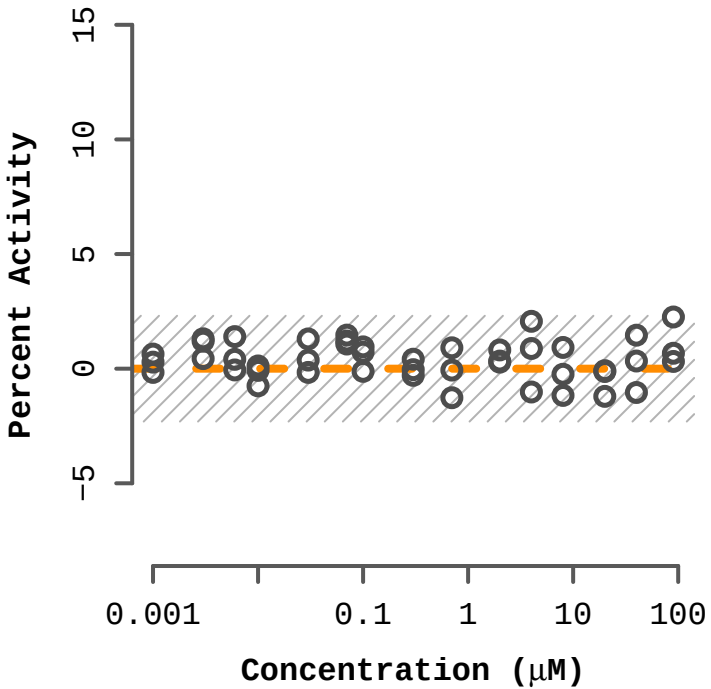
NAME: Diisononyl cyclohexane-1,2-dicarboxylate
CHID: 47395 **CASRN:** 166412-78-8
SPID(S): Tox21_300638
M4ID: 12478495

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

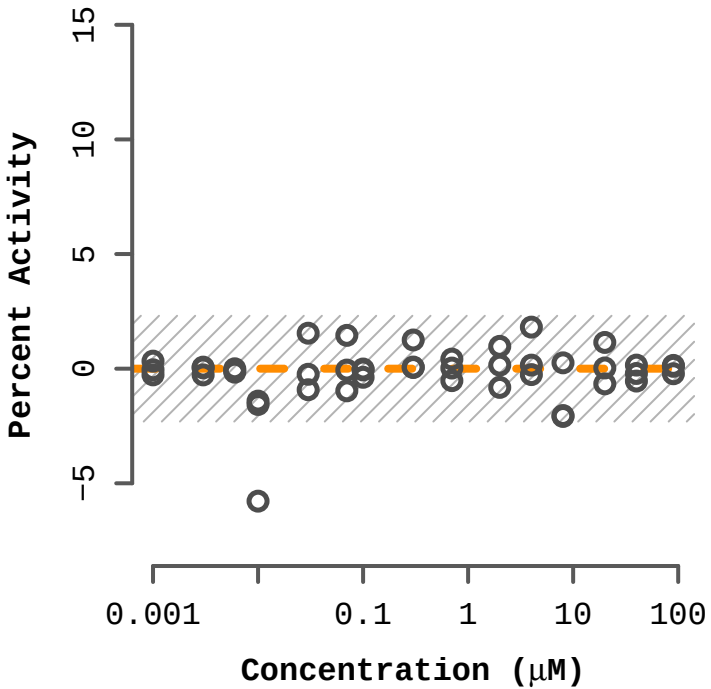
NAME: Venlafaxine hydrochloride
CHID: 47397 **CASRN:** 99300-78-4
SPID(S): Tox21_302508
M4ID: 12476625

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

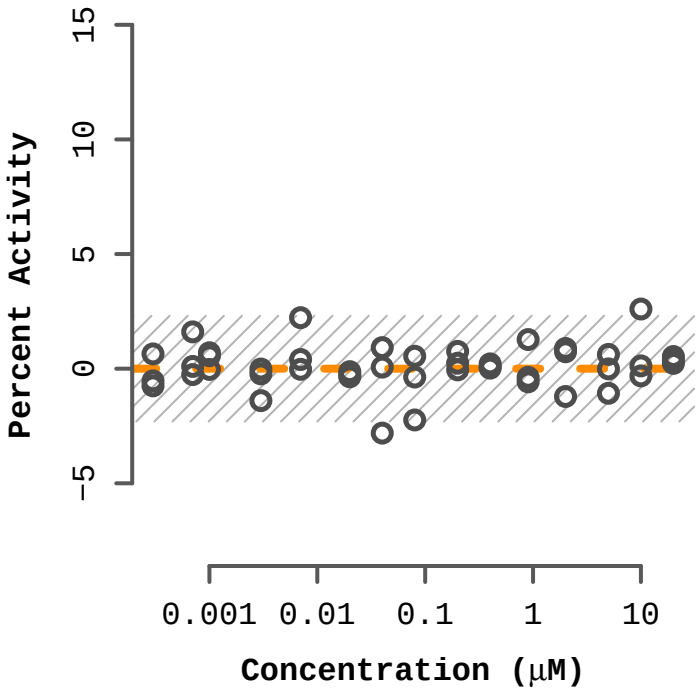
NAME: Dihydro-1,1,2,3,3-pentamethyl-4(5H)-indanone
CHID: 47399 **CASRN:** 33704-61-9
SPID(S): Tox21_302677
M4ID: 12476456

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.571 **MAX_MED:** 0.156 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

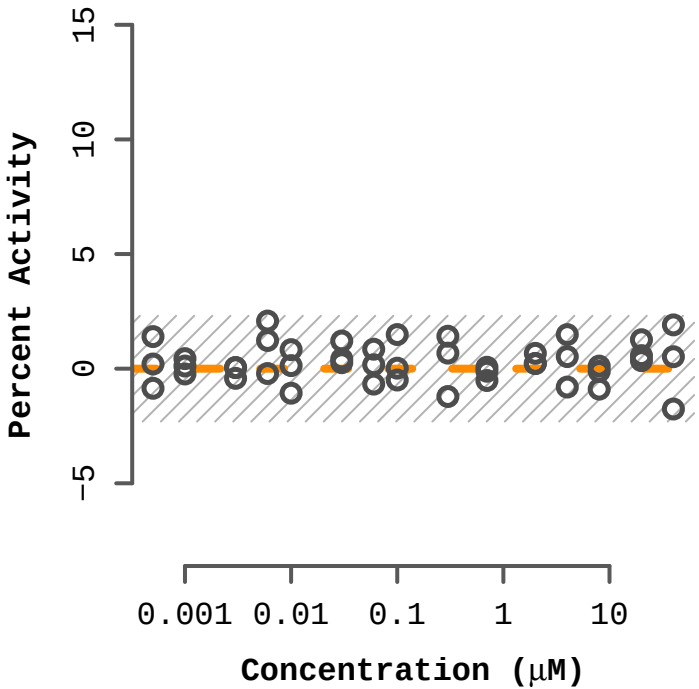
NAME: Carvacryl methyl ether
CHID: 47400 **CASRN:** 6379-73-3
SPID(S): Tox21_303748
M4ID: 12475440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.867 **MAX_MED:** 0.739 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

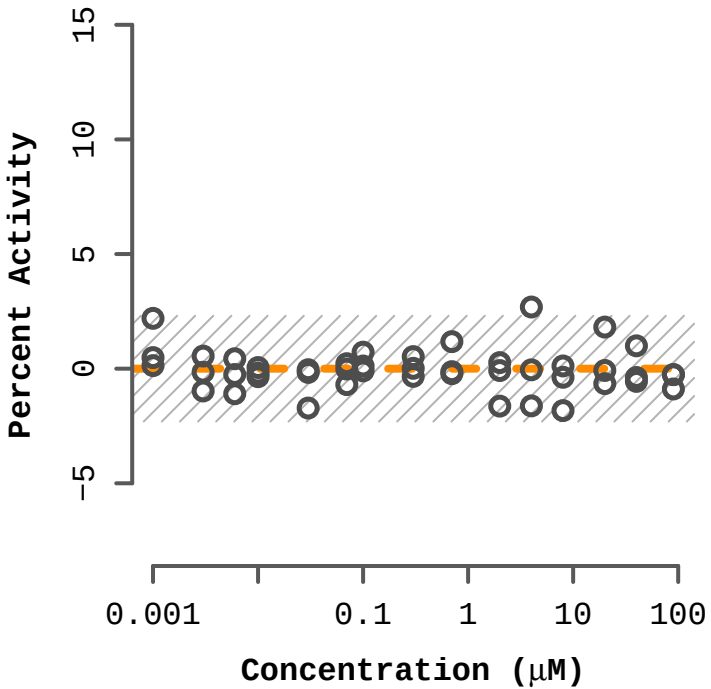
NAME: Methapyrilene fumarate
CHID: 47404 CASRN: 33032-12-1
SPID(S): Tox21_303631
M4ID: 12475514

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

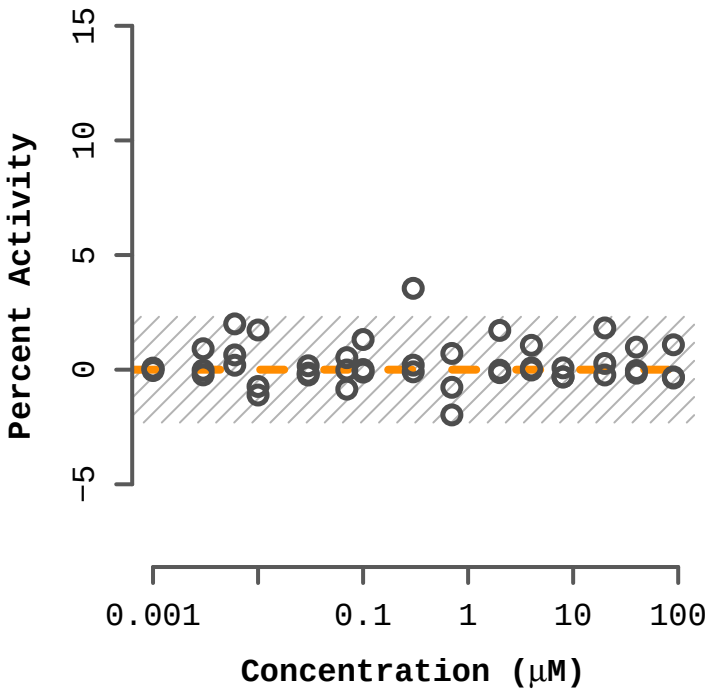
NAME: Citronellyl butyrate
CHID: 47405 **CASRN:** 141-16-2
SPID(S): Tox21_302488
M4ID: 12476645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 0.486 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

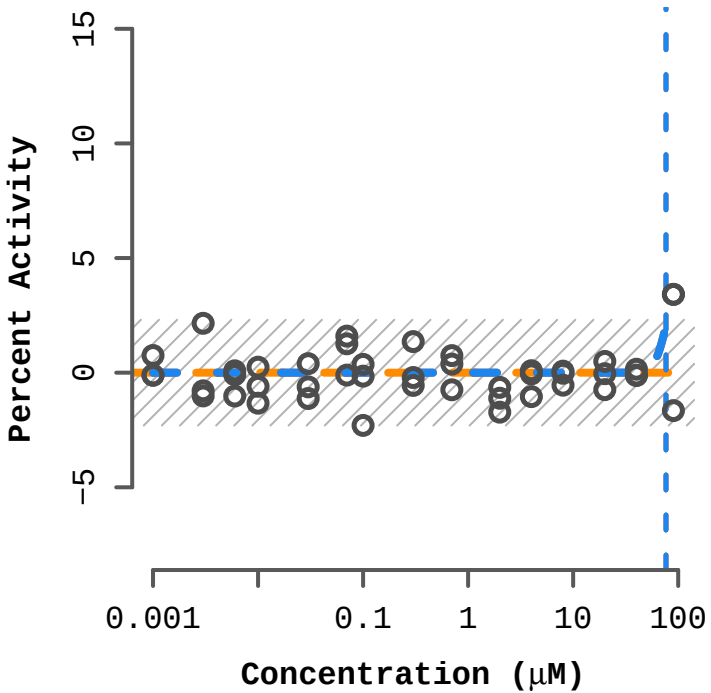
NAME: Eugenyl phenylacetate
CHID: 47406 **CASRN:** 10402-33-2
SPID(S): Tox21_301203
M4ID: 12477930

HILL MODEL: Not applicable.

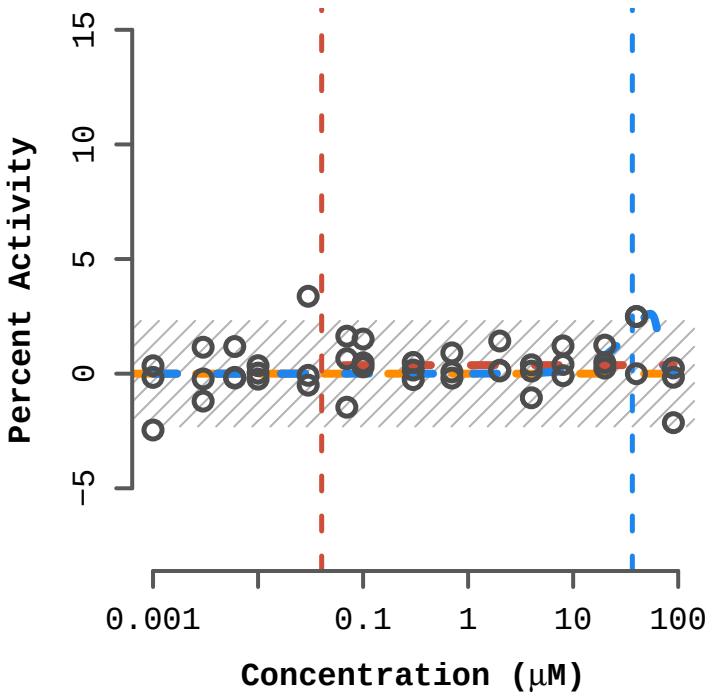
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 0.645 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Methyl citronellate
CHID:    47408   CASRN: 2270-60-2
SPID(S): Tox21_302649
M4ID:    12476484

HILL MODEL (in red):
      tp       ga       gw
val:  4.1      1.88     7.98
sd:   6.84     0.335    15.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.1      1.88     8        3.44     12.9
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  135.89      132.22      136.22
PROB: 0.12        0.77        0.1
RMSE: 1.13        1.11        1.11

MAX_MEAN: 1.73      MAX_MED: 3.42      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Linalyl cinnamate
CHID: 47410 **CASRN:** 78-37-5
SPID(S): Tox21_302635
M4ID: 12476498

HILL MODEL (in red):

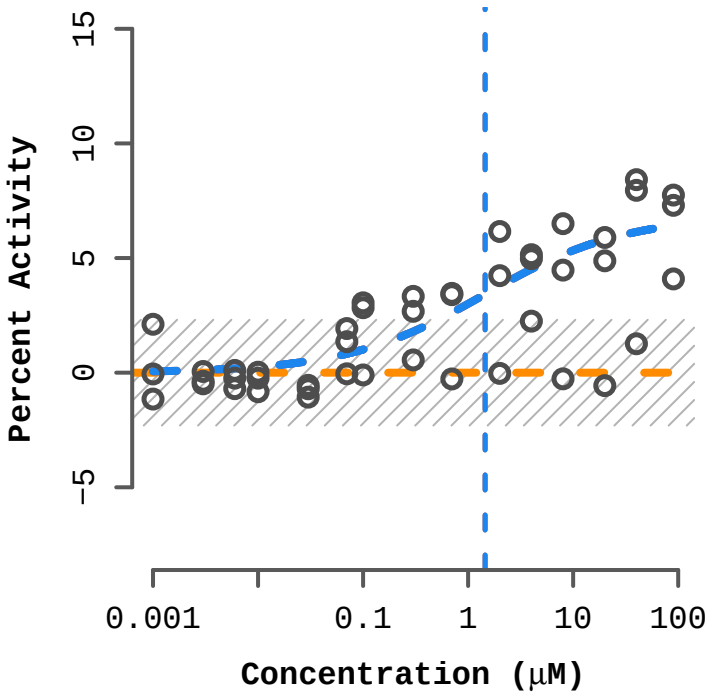
	tp	ga	gw
val:	0.373	−1.39	8
sd:	0.151	0.552	23.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.83	1.56	2.24	1.81	18
sd:	5.74	0.598	2.59	0.345	44.2

	CNST	HILL	GNLS
AIC:	134.02	134.19	134.15
PROB:	0.35	0.32	0.33
RMSE:	1.11	1.06	1.01

MAX_MEAN: 1.66 **MAX_MED:** 2.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Phenylpropyl cinnamate
CHID: 47411 CASRN: 122-68-9
SPID(S): Tox21_302672
M4ID: 12476461

HILL MODEL (in red):

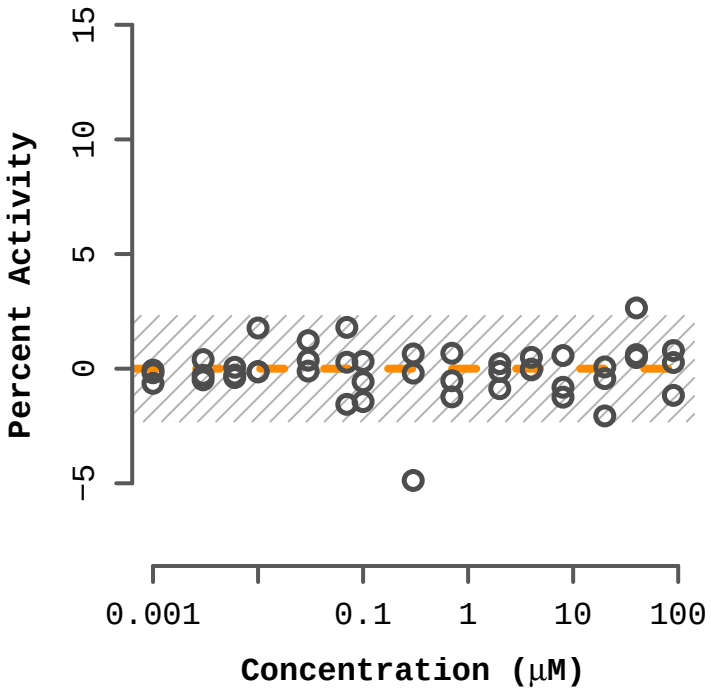
	tp	ga	gw
val:	6.84	0.162	0.655
sd:	1.69	0.533	0.233

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.84	0.162	0.655	3.21	6.53
sd:	1.69	0.533	0.233	1800	9300

	CNST	HILL	GNLS
AIC:	243.88	192.46	196.46
PROB:	0	0.88	0.12
RMSE:	3.57	1.99	1.99

MAX_MEAN: 6.38 MAX_MED: 7.96 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

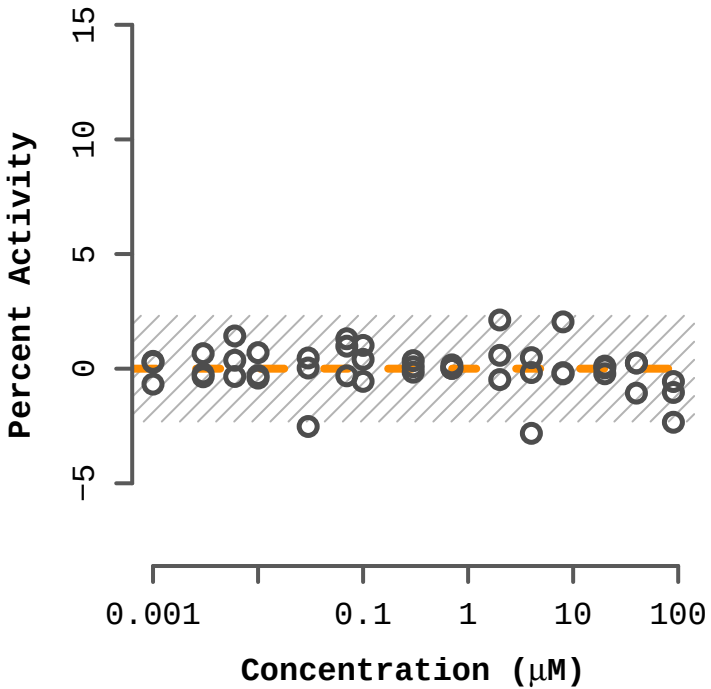
NAME: 1-(4-Methoxyphenyl)-1-pentene-3-one
CHID: 47412 **CASRN:** 104-27-8
SPID(S): Tox21_300928
M4ID: 12478205

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.616 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

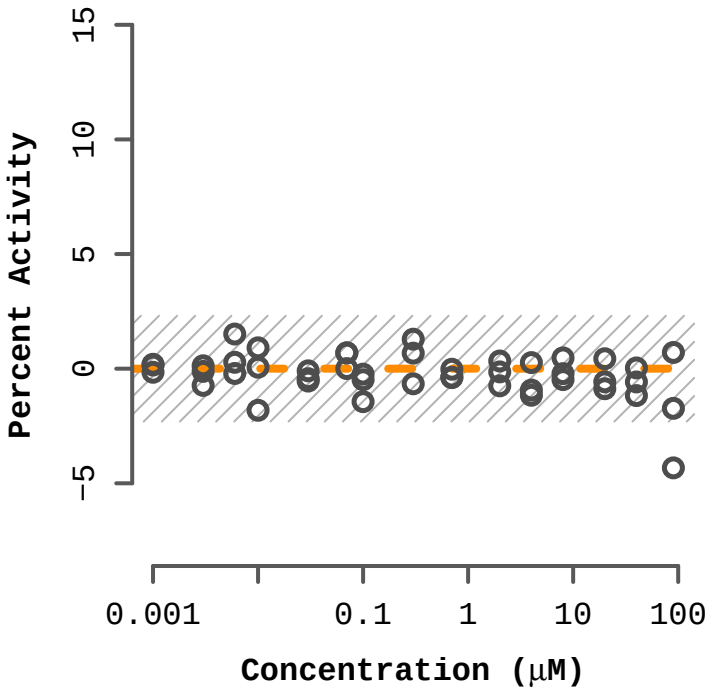
NAME: Geranyl tiglate
CHID: 47413 **CASRN:** 7785-33-3
SPID(S): Tox21_302492
M4ID: 12476641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.745 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

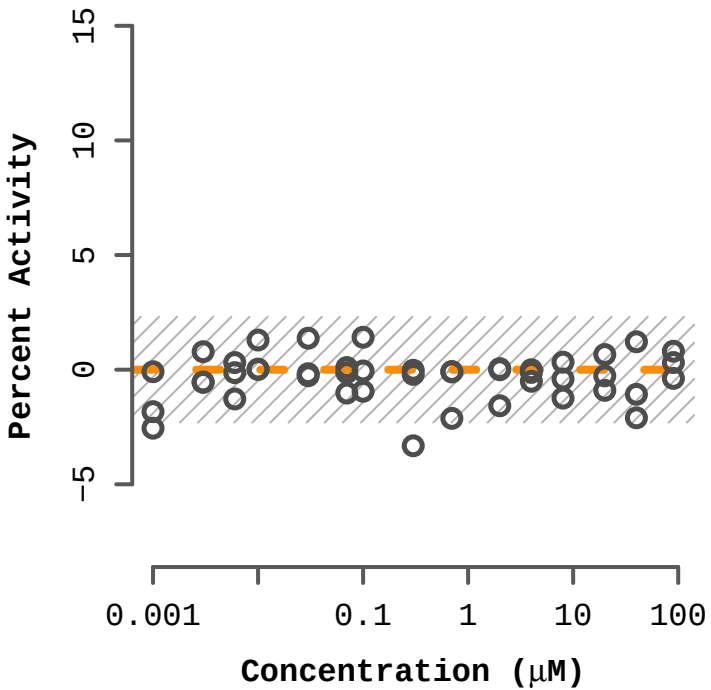
NAME: 2,4-Hexadienyl isobutyrate
CHID: 47414 **CASRN:** 16491-24-0
SPID(S): Tox21_302558
M4ID: 12476575

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.528 **MAX_MED:** 0.685 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

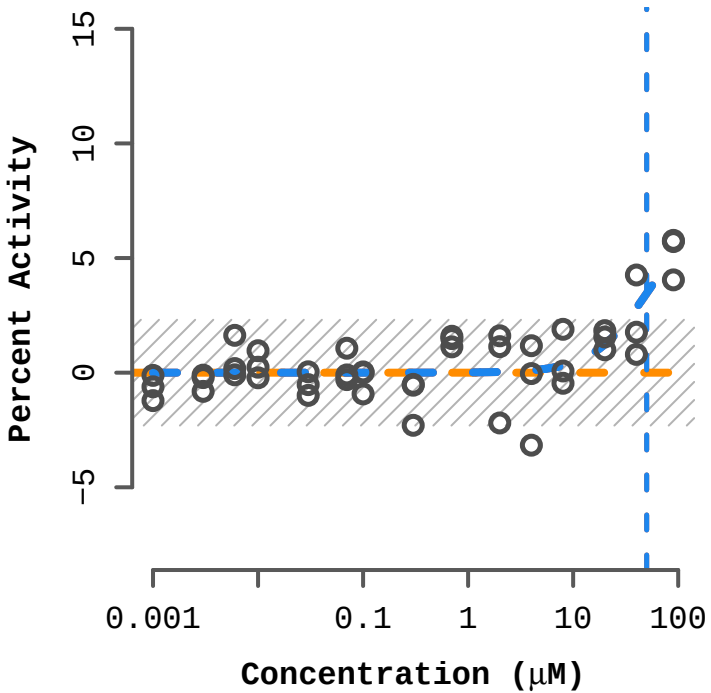
NAME: Ethyl linalool
CHID: 47415 **CASRN:** 10339-55-6
SPID(S): Tox21_300812
M4ID: 12478321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.444 **MAX_MED:** 0.312 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-methyl-6-methylideneoct-7-en-2-yl acetate
CHID: 47416 CASRN: 1118-39-4
SPID(S): Tox21_302568
M4ID: 12476565

HILL MODEL (in red):

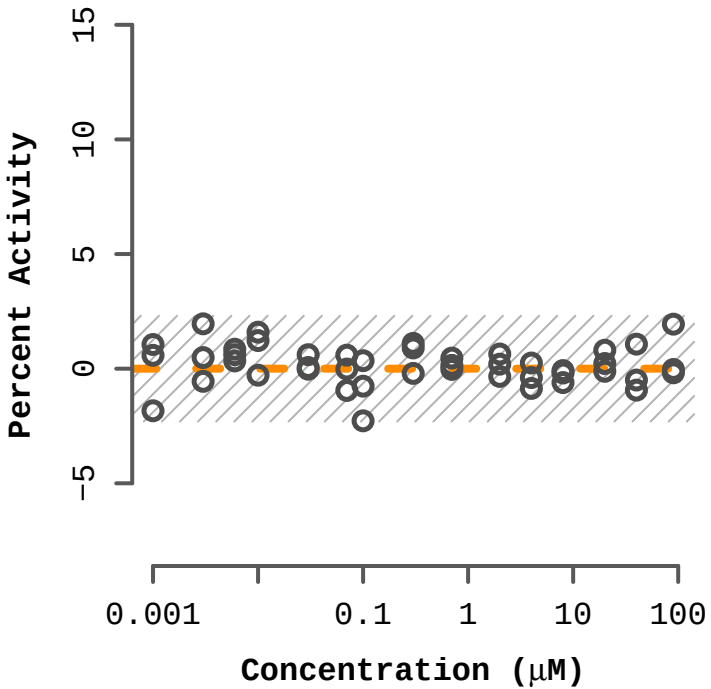
	tp	ga	gw
val:	6.93	1.7	1.66
sd:	2.62	0.251	0.663

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.93	1.7	1.66	3.39	5.24
sd:	2.62	0.251	0.663	727	2670

	CNST	HILL	GNLS
AIC:	177.41	145.34	149.34
PROB:	0	0.88	0.12
RMSE:	1.87	1.1	1.1

MAX_MEAN: 5.18 MAX_MED: 5.72 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

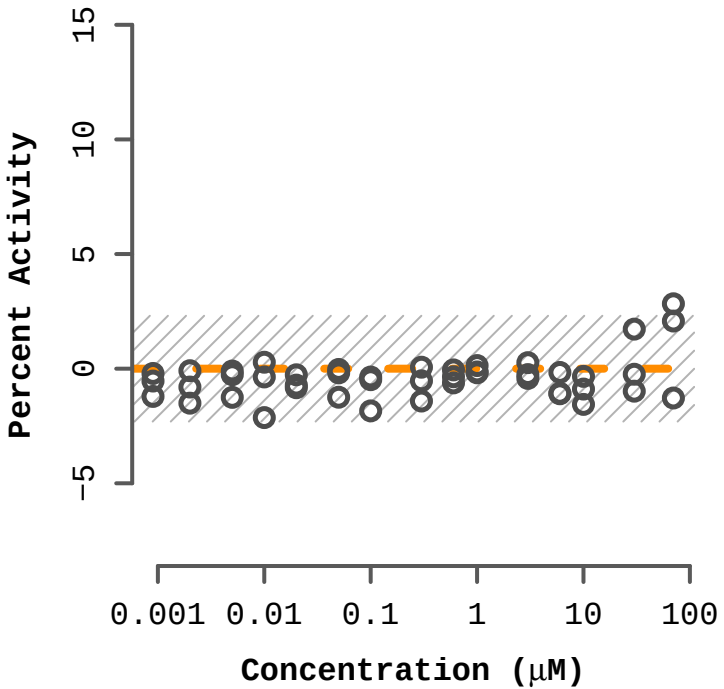
NAME: 4-Hydroxy-5-methyl-3-furanone
CHID: 47417 **CASRN:** 19322-27-1
SPID(S): Tox21_302541
M4ID: 12476592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.846 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

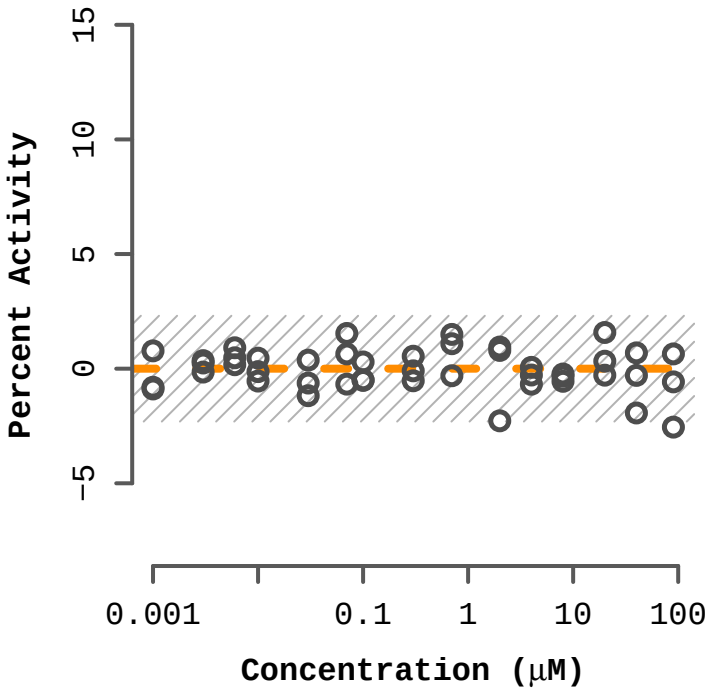
NAME: Acetaldehyde ethyl cis-3-hexenyl acetal
CHID: 47418 **CASRN:** 28069-74-1
SPID(S): Tox21_302692
M4ID: 12476441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 2.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

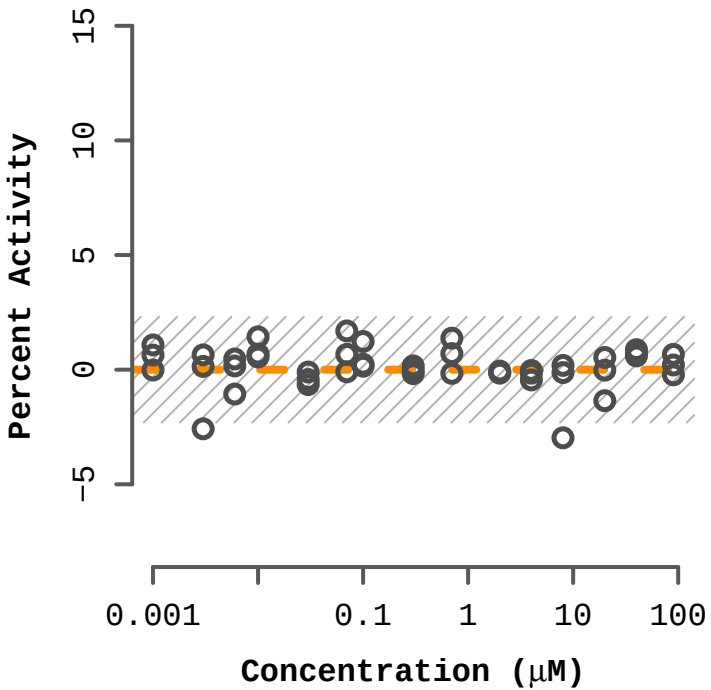
NAME: 5-Methyl-2-phenyl-2-hexenal
CHID: 47419 **CASRN:** 21834-92-4
SPID(S): Tox21_302458
M4ID: 12476675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.76 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

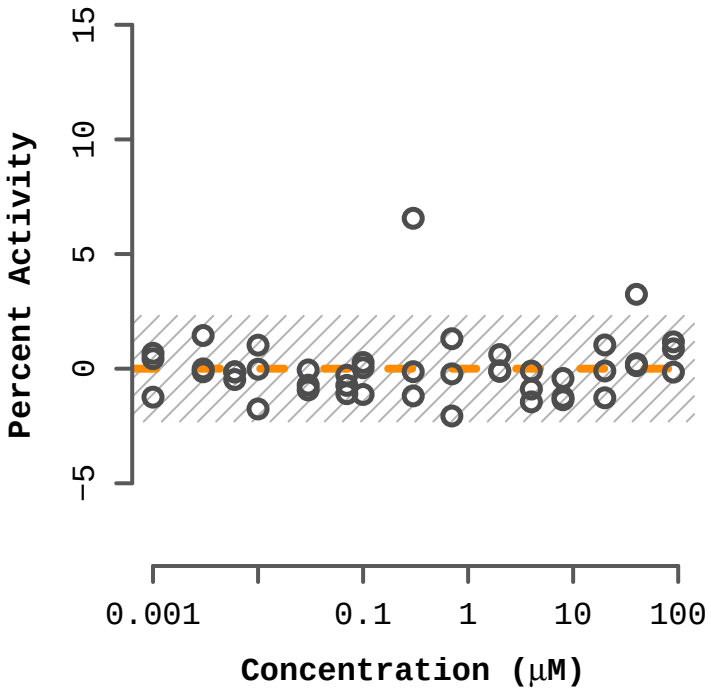
NAME: 4-(4-Hydroxy-3-methoxyphenyl)-2-butanone
CHID: 47420 CASRN: 122-48-5
SPID(S): Tox21_302493
M4ID: 12476640

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.89 MAX_MED: 0.717 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-(5-Isopropyl-2-methyl-cyclohex-2-enyl)-propa

CHID: 47422 **CASRN:** 31375-17-4

SPID(S): Tox21_303629

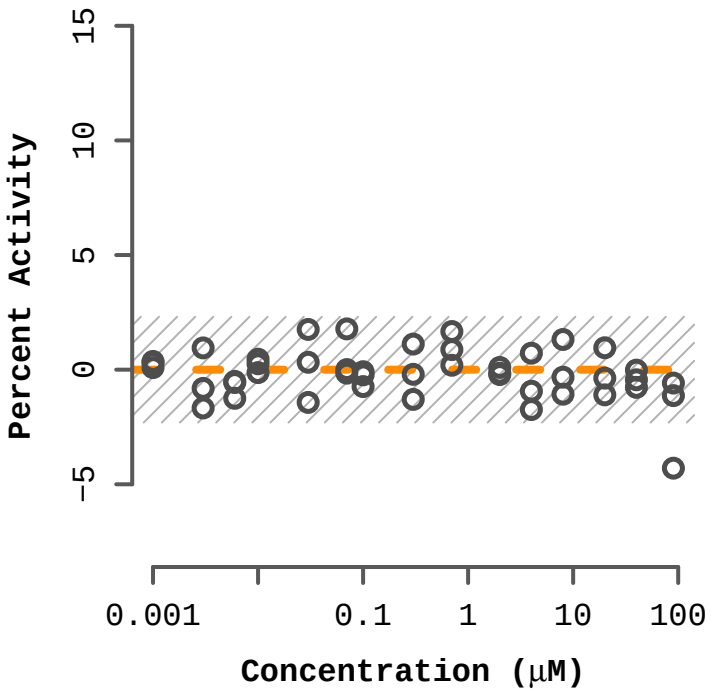
M4ID: 12475516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 1.75 **MAX_MED:** 0.867 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

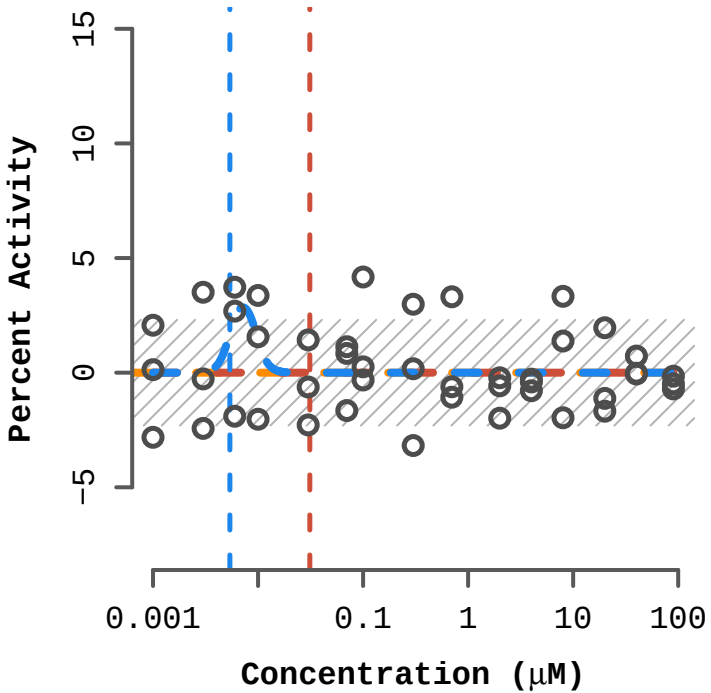
NAME: 2-Acetoxy-5-nitrobenzyl chloride
CHID: 47423 **CASRN:** 5174-32-3
SPID(S): Tox21_302564
M4ID: 12476569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.913 **MAX_MED:** 0.879 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1'-Bi(cyclohexyl)-2-one
CHID: 47424 **CASRN:** 90-42-6
SPID(S): Tox21_302728
M4ID: 12476405

HILL MODEL (in red):

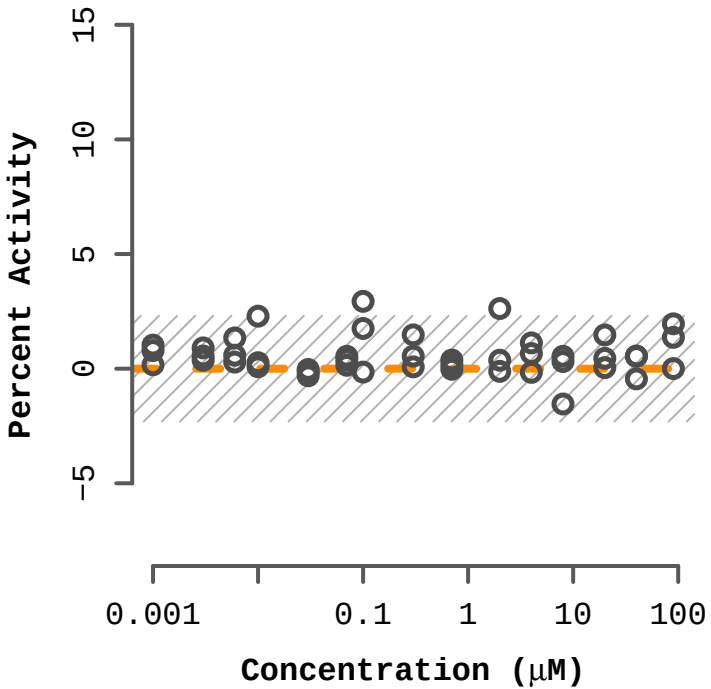
	tp	ga	gw
val:	4.67e-09	-1.51	2.7
sd:	0.00149	3020	71700

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.46	-2.27	8	-2.02	7.86
sd:	33.9	1.55	45.1	0.849	59.5

	CNST	HILL	GNLS
AIC:	191.99	197.99	198.38
PROB:	0.92	0.05	0.04
RMSE:	1.92	1.92	1.88

MAX_MEAN: 1.5 **MAX_MED:** 2.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

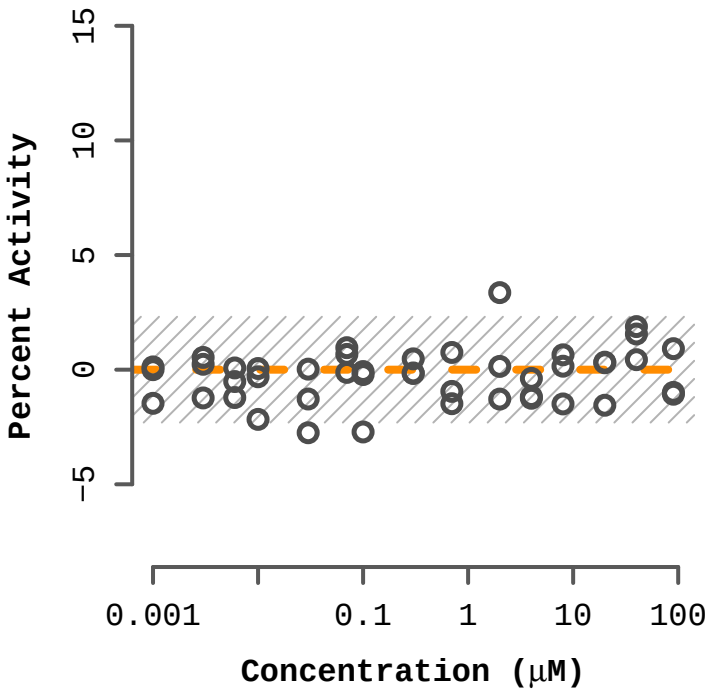
NAME: 4-Butylphenol
CHID: 47425 **CASRN:** 1638-22-8
SPID(S): Tox21_302594
M4ID: 12476539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

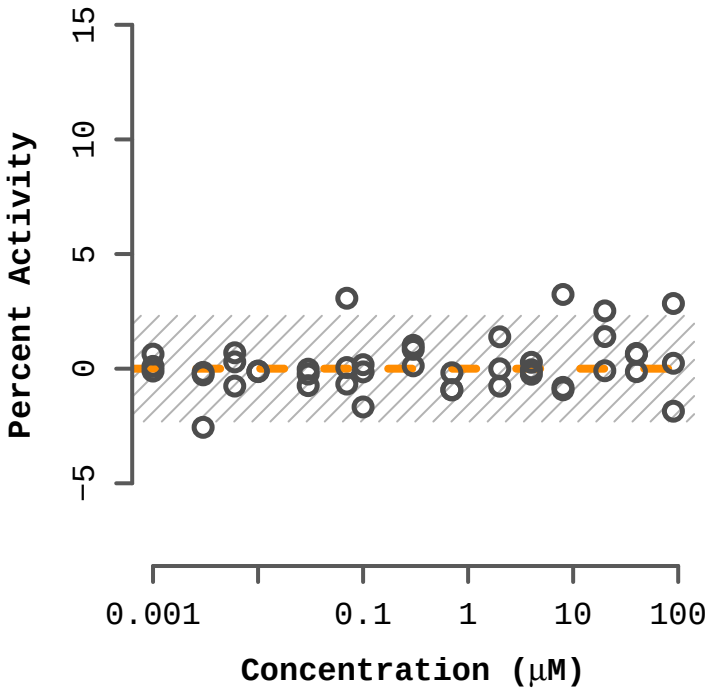
NAME: dl−Carvone
CHID: 47426 **CASRN:** 99−49−0
SPID(S): Tox21_302547
M4ID: 12476586

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

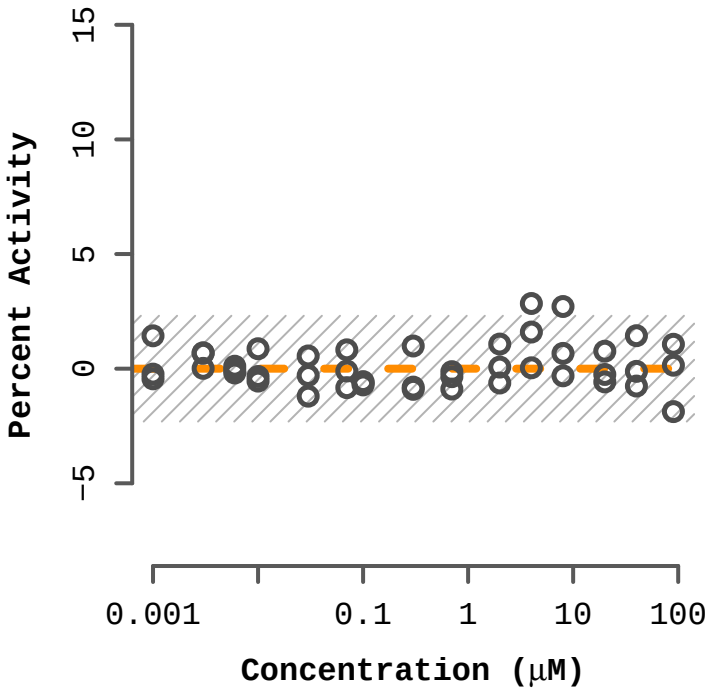
NAME: 2,4-DB-isooctyl ester
CHID: 47427 **CASRN:** 1320-15-6
SPID(S): Tox21_302495
M4ID: 12476638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

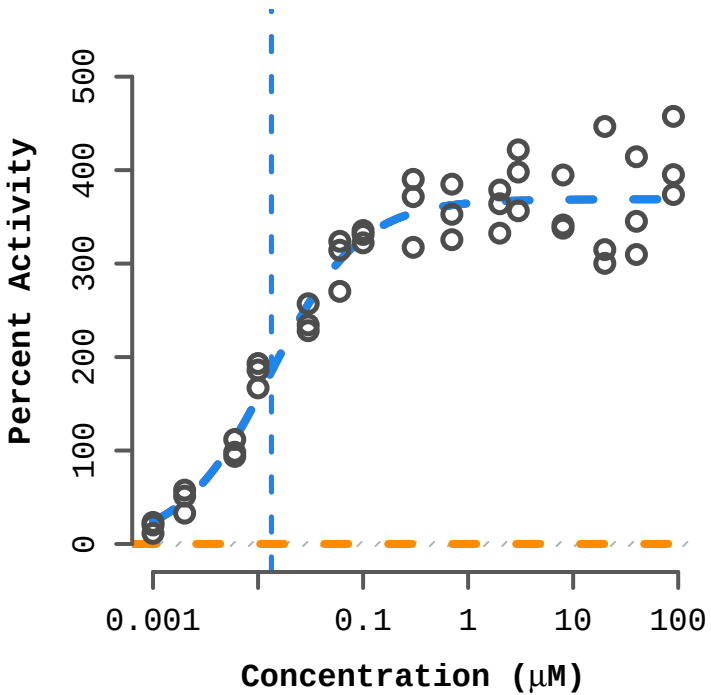
NAME: (4-Methylphenoxy) acetic acid ethyl ester
CHID: 47428 **CASRN:** 67028-40-4
SPID(S): Tox21_302634
M4ID: 12476499

HILL MODEL: Not applicable.

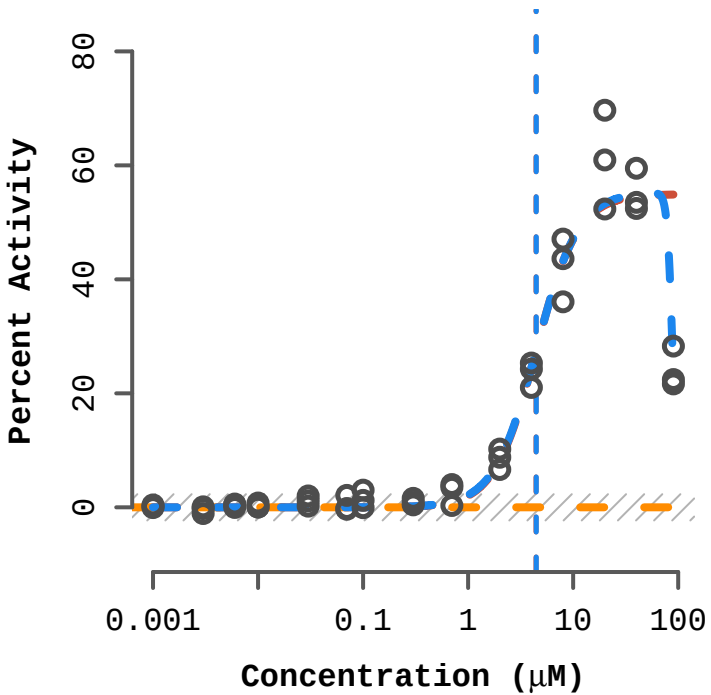
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.6 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dexamethasone sodium phosphate
CHID:    47429   CASRN: 2392-39-4
SPID(S): Tox21_302586
M4ID:    12476547

HILL MODEL (in red):
      tp       ga       gw
val:  369      -1.87    1.02
sd:   8.34     0.0517   0.0948

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  369      -1.87    1.02     2.89     8.92
sd:   8.34     0.0517   0.0948   374      3580

      CNST        HILL        GNLS
AIC:  653.49      449.23      453.23
PROB: 0           0.88        0.12
RMSE: 305.61      32.43       32.43

MAX_MEAN: 409       MAX_MED: 398       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Equilin
CHID: 47433 CASRN: 474-86-2
SPID(S): Tox21_302641
M4ID: 12476492

HILL MODEL (in red):

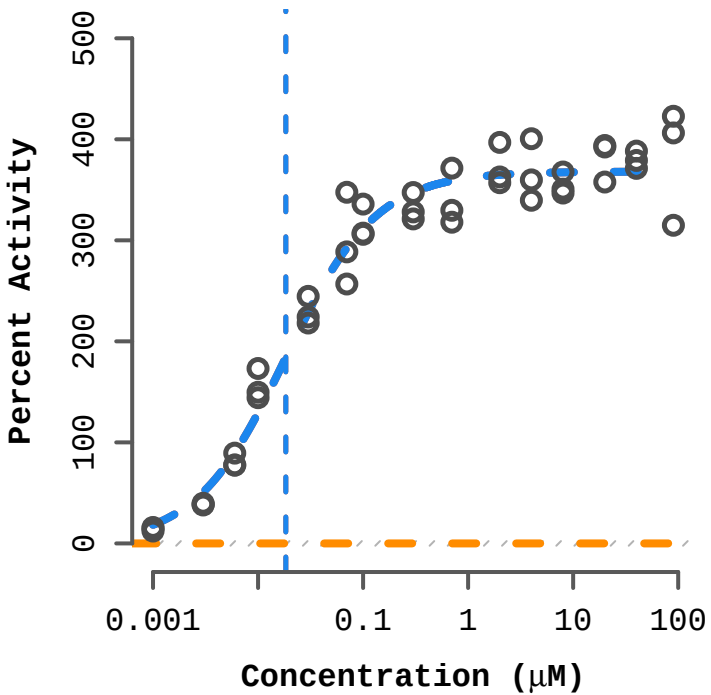
	tp	ga	gw
val:	55	0.646	2.19
sd:	1.58	0.0226	0.226

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	55.4	0.649	2.15	1.95	17.4
sd:	1.61	0.0208	0.193	0.00383	4.94

	CNST	HILL	GNLS
AIC:	413.08	275.11	221.97
PROB:	0	0	1
RMSE:	25.65	8.64	3.38

MAX_MEAN: 61 MAX_MED: 61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flurandrenolide
CHID: 47434 CASRN: 1524-88-5
SPID(S): Tox21_302611
M4ID: 12476522

HILL MODEL (in red):

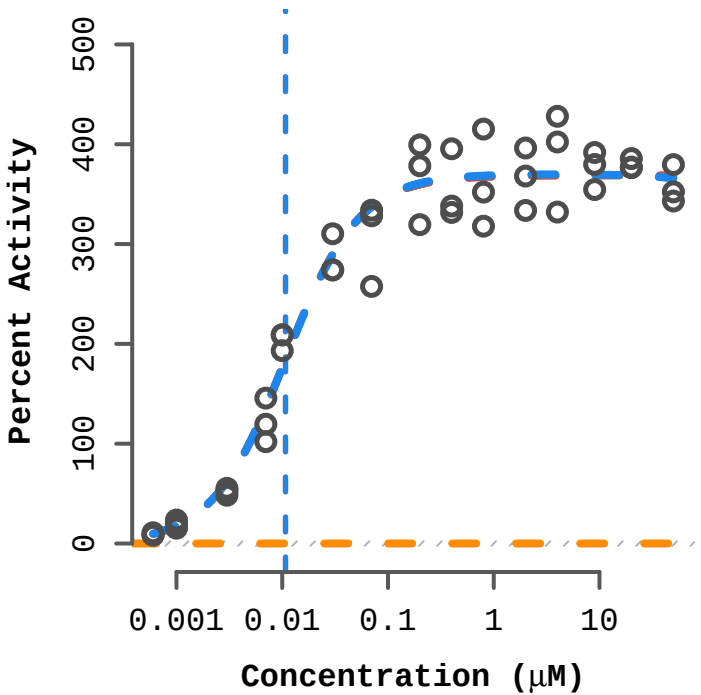
	tp	ga	gw
val:	368	-1.74	1.01
sd:	5.88	0.0402	0.0759

GAIN-LOSS MODEL (in blue):

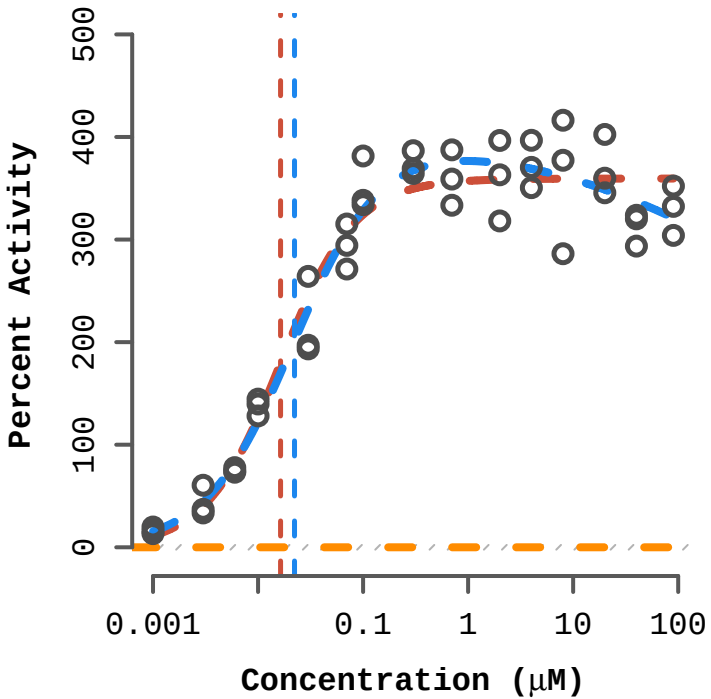
	tp	ga	gw	la	lw
val:	368	-1.74	1.01	2.5	17.6
sd:	5.88	0.0402	0.0759	485	15200

	CNST	HILL	GNLS
AIC:	651.44	422.41	426.41
PROB:	0	0.88	0.12
RMSE:	298.86	23.77	23.77

MAX_MEAN: 381 MAX_MED: 406 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Flurandrenolide
CHID:    47434   CASRN: 1524-88-5
SPID(S): Tox21_110509_1
M4ID:    12484307

HILL MODEL (in red):
      tp       ga       gw
val:  369      -1.97    1.26
sd:   6.44     0.0415   0.125

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  370      -1.97    1.25     3.4      1.13
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  650.9       434.15      438
PROB: 0           0.87        0.13
RMSE: 298.04      27.15       27.12

MAX_MEAN: 387       MAX_MED: 402       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluorometholone
CHID: 47435 CASRN: 426-13-1
SPID(S): Tox21_302593
M4ID: 12476540

HILL MODEL (in red):

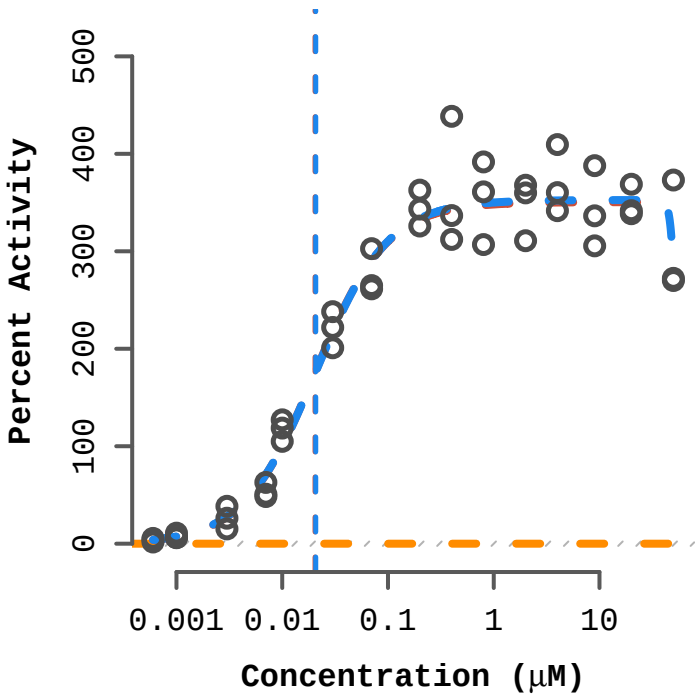
	tp	ga	gw
val:	359	-1.79	1.23
sd:	7.04	0.0466	0.113

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	412	-1.65	1.04	3.78	0.3
sd:	79.5	0.119	0.118	1.45	0.4

	CNST	HILL	GNLS
AIC:	650.05	444.84	435.58
PROB:	0	0.01	0.99
RMSE:	294.54	30.39	26.95

MAX_MEAN: 373 MAX_MED: 377 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluorometholone
CHID: 47435 CASRN: 426-13-1
SPID(S): Tox21_110440_1
M4ID: 12484355

HILL MODEL (in red):

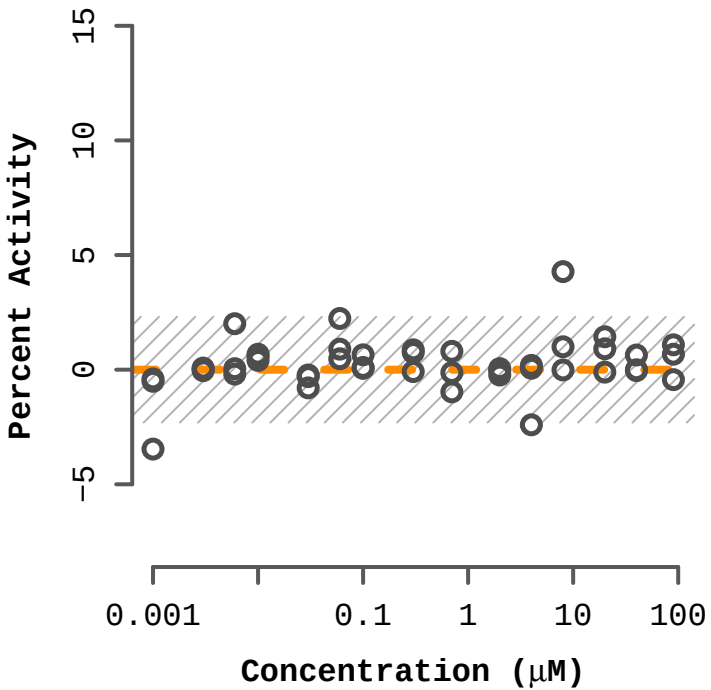
	tp	ga	gw
val:	350	-1.69	1.28
sd:	6.76	0.0411	0.12

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	353	-1.68	1.27	1.73	17.9
sd:	6.54	0.0393	0.112	0.00675	3.61

	CNST	HILL	GNLS
AIC:	642.21	438.74	435.44
PROB:	0	0.16	0.84
RMSE:	272.95	30.77	29.14

MAX_MEAN: 370 MAX_MED: 361 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

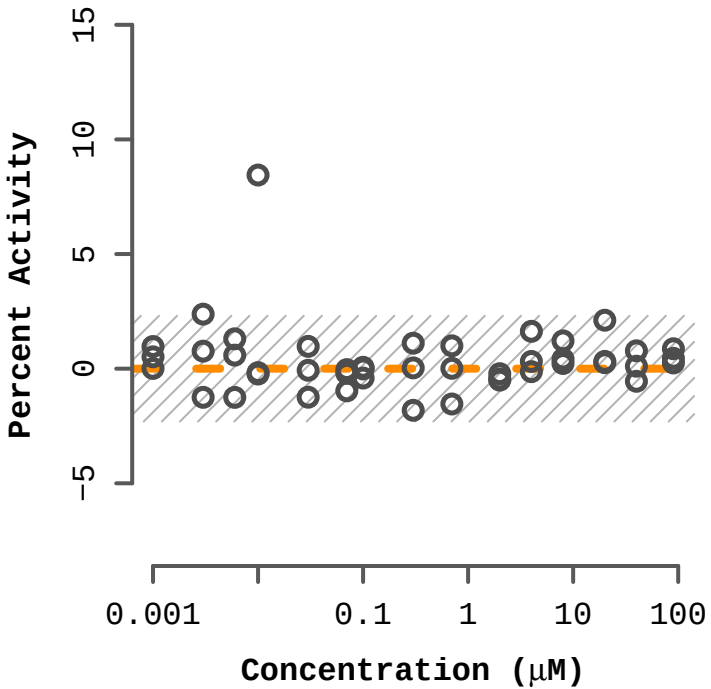
NAME: Glycocholic acid
CHID: 47436 CASRN: 475-31-0
SPID(S): Tox21_302549
M4ID: 12476584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

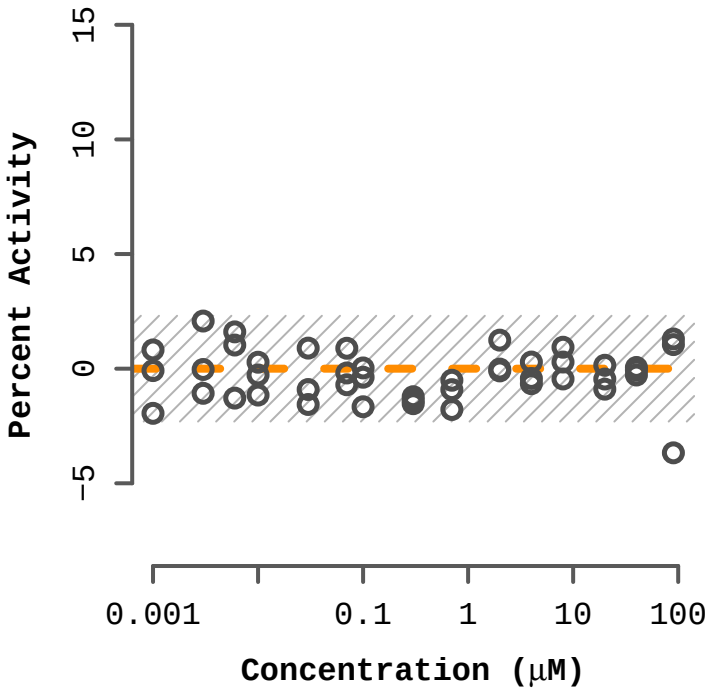
NAME: alpha-Hexyl-gamma-butyrolactone
CHID: 47437 **CASRN:** 18436-37-8
SPID(S): Tox21_301140
M4ID: 12477993

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.54	NA	NA

MAX_MEAN: 2.68 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

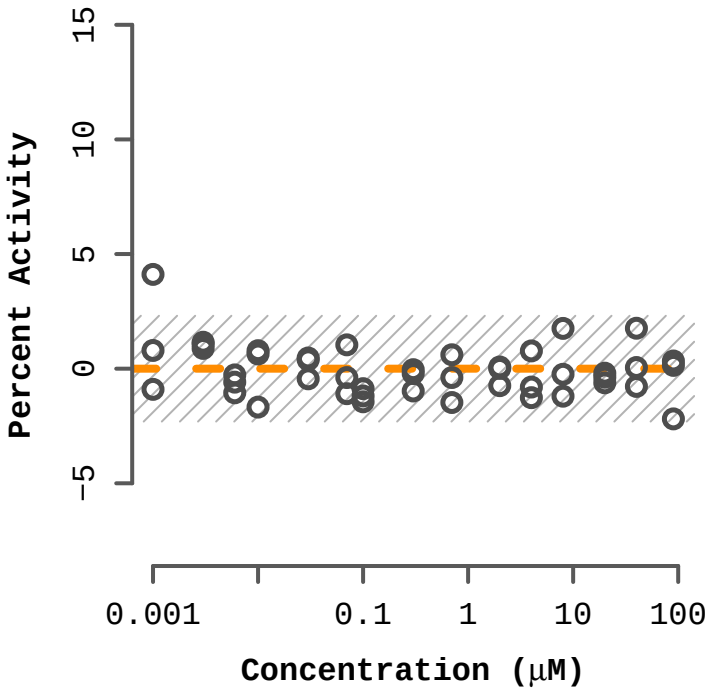
NAME: Benzyl 3-methylbutyl ether
CHID: 47439 **CASRN:** 122-73-6
SPID(S): Tox21_303630
M4ID: 12475515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.452 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

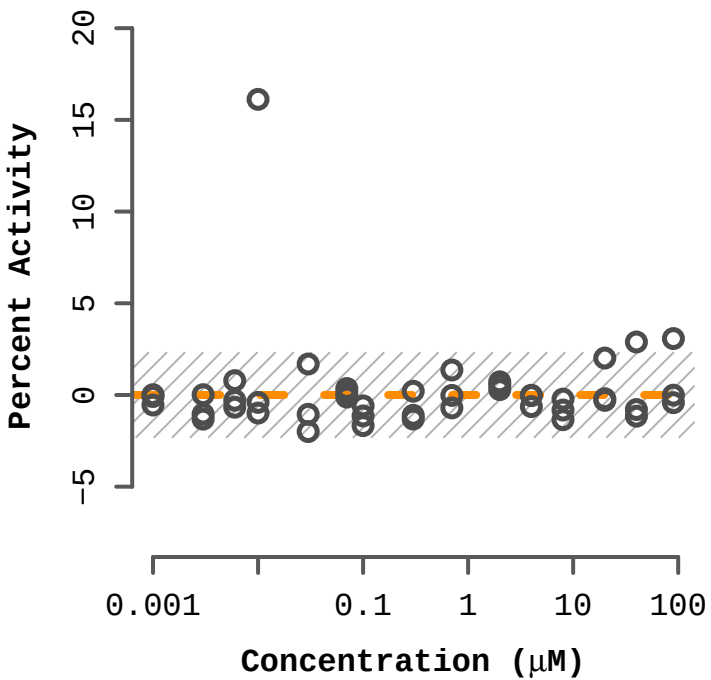
NAME: 4-Isopropylbenzonitrile
CHID: 47440 **CASRN:** 13816-33-6
SPID(S): Tox21_302580
M4ID: 12476553

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

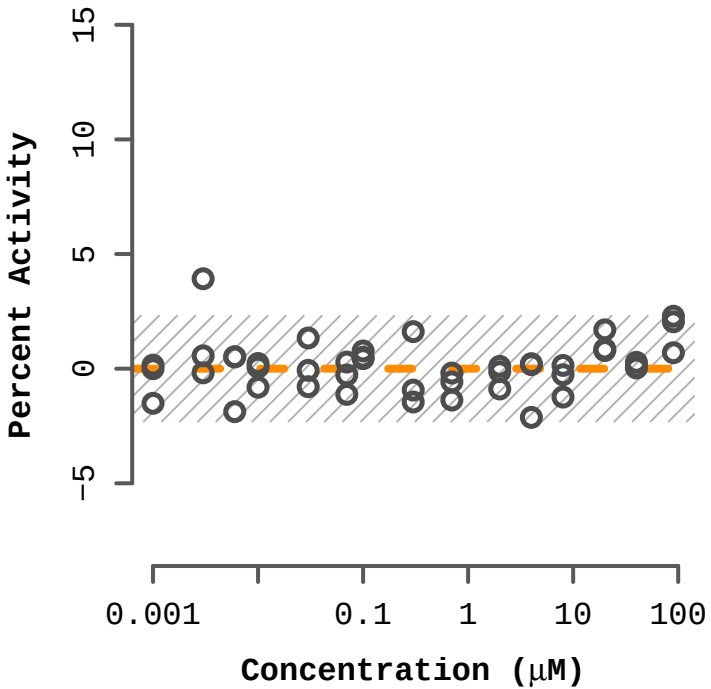
NAME: 3-Methoxy-5-methylphenol
CHID: 47443 CASRN: 3209-13-0
SPID(S): Tox21_302551
M4ID: 12476582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.63	NA	NA

MAX_MEAN: 4.91 MAX_MED: 0.548 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

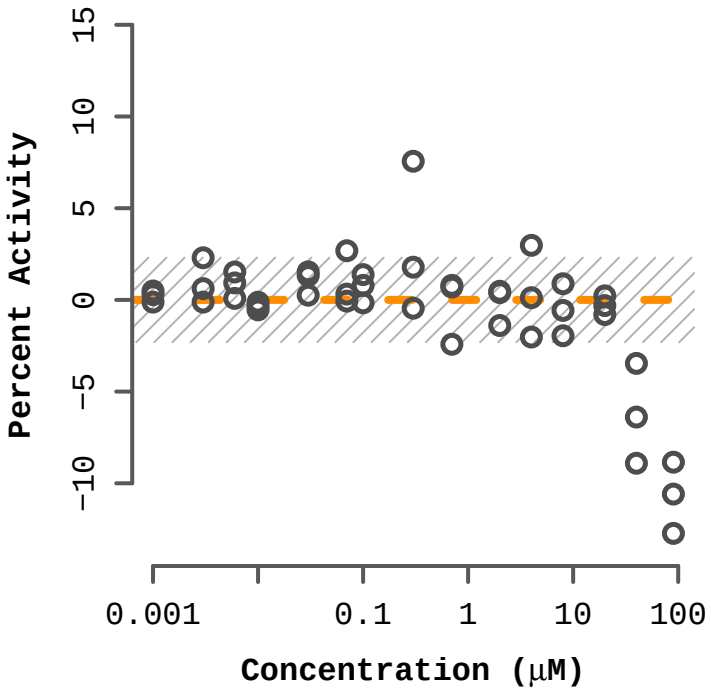
NAME: 6-Methyl-1,2,3,4-tetrahydroquinoline
CHID: 47444 **CASRN:** 91-61-2
SPID(S): Tox21_302506
M4ID: 12476627

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.68 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

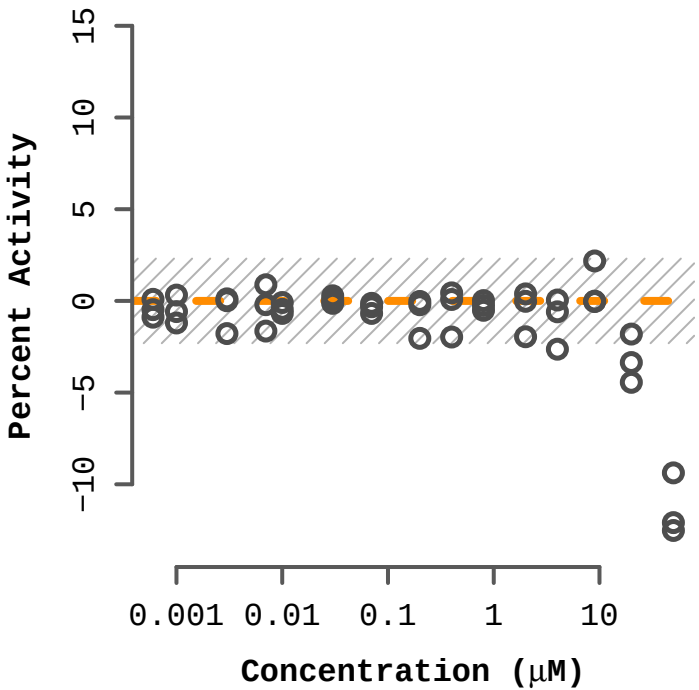
NAME: Fipexide hydrochloride
CHID: 47446 **CASRN:** 34161-23-4
SPID(S): Tox21_302469
M4ID: 12476664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.17	NA	NA
PROB:	1	NA	NA
RMSE:	3.64	NA	NA

MAX_MEAN: 2.96 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

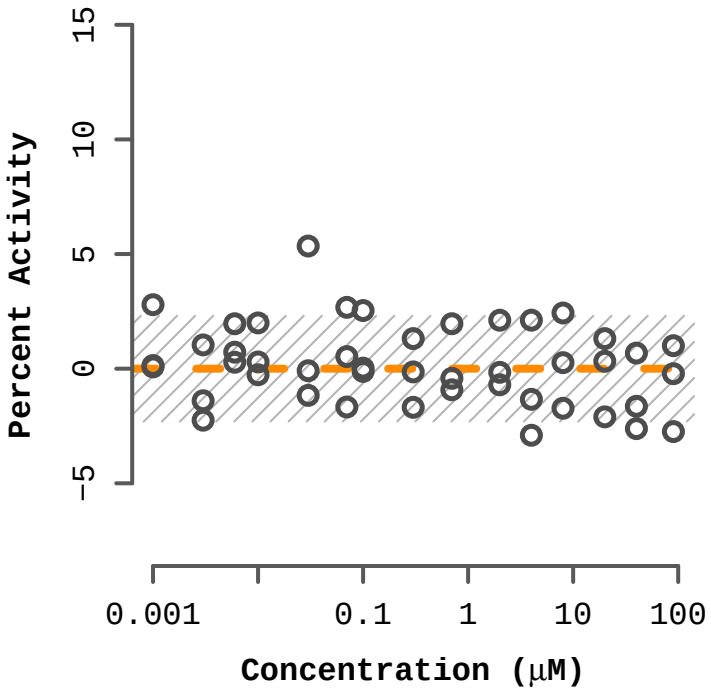
NAME: Fipexide hydrochloride
CHID: 47446 **CASRN:** 34161-23-4
SPID(S): Tox21_111394_1
M4ID: 12483715

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.58	NA	NA
PROB:	1	NA	NA
RMSE:	3.2	NA	NA

MAX_MEAN: 0.711 **MAX_MED:** 0.0785 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

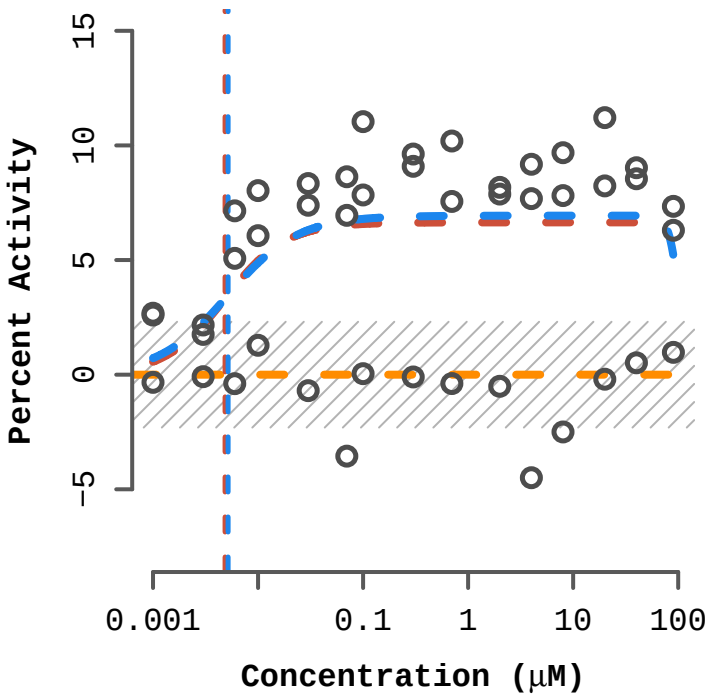
NAME: Hydrazinecarboxylic acid, phenylmethyl ester
CHID: 47447 **CASRN:** 5331-43-1
SPID(S): Tox21_302719
M4ID: 12476414

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.721 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Potassium chlorate
CHID: 47448 **CASRN:** 3811-04-9
SPID(S): Tox21_302523
M4ID: 12476610

HILL MODEL (in red):

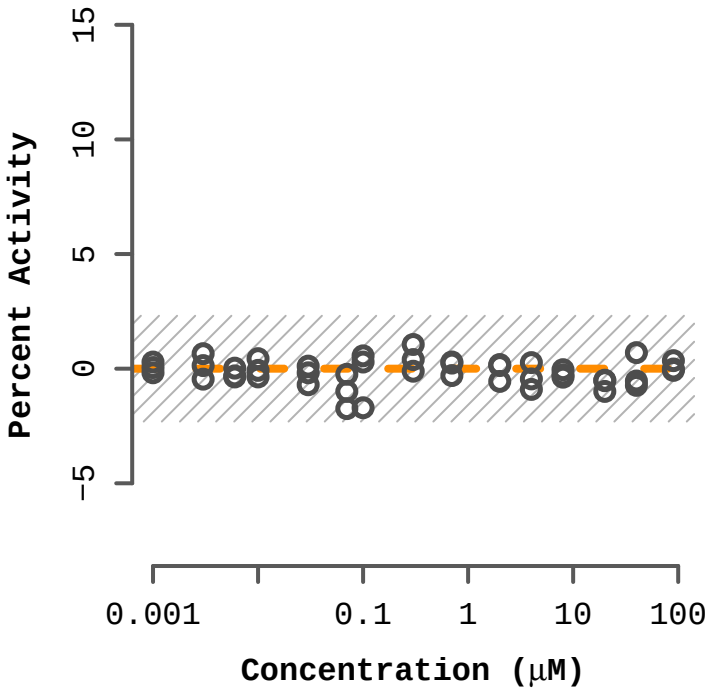
	tp	ga	gw
val:	6.64	−2.31	1.5
sd:	0.861	0.249	1.97

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.94	−2.29	1.31	2.01	9.18
sd:	0.947	0.264	1.49	0.535	95.6

	CNST	HILL	GNLS
AIC:	304.25	268.53	271.97
PROB:	0	0.85	0.15
RMSE:	6.46	4.34	4.36

MAX_MEAN: 6.42 **MAX_MED:** 9.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

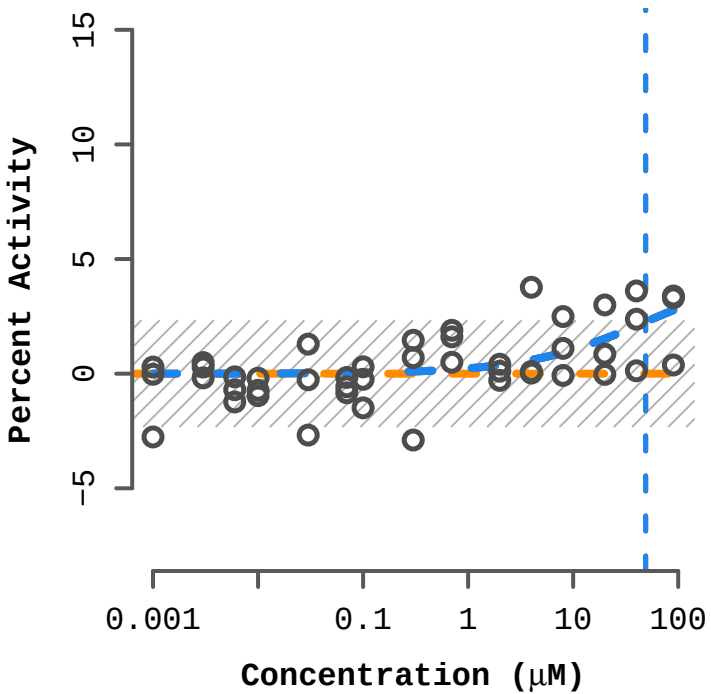
NAME: 5-Chlorobenzotriazole
CHID: 47450 **CASRN:** 94-97-3
SPID(S): Tox21_302472
M4ID: 12476661

HILL MODEL: Not applicable.

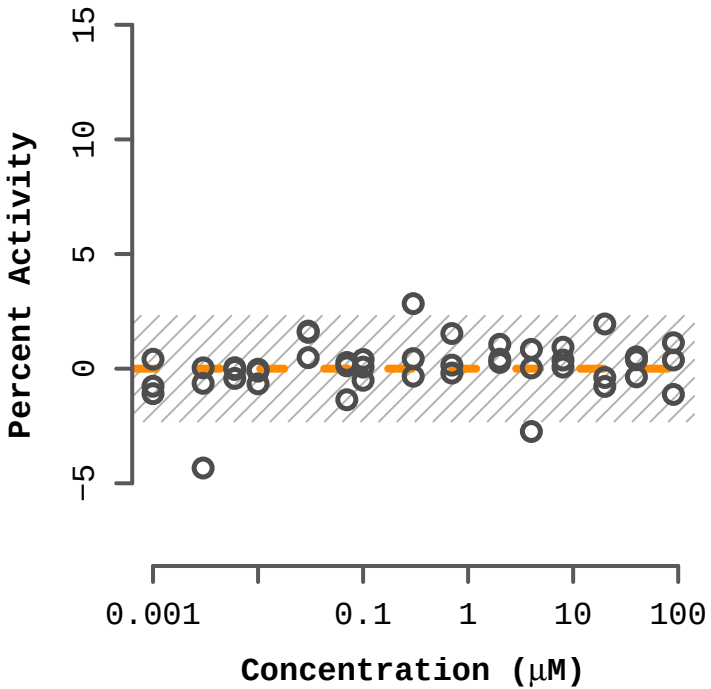
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	78.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.58	NA	NA

MAX_MEAN: 0.449 **MAX_MED:** 0.4 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Acid Yellow 11
CHID:    47451   CASRN: 6359-82-6
SPID(S): Tox21_302596
M4ID:    12476537

HILL MODEL (in red):
      tp       ga       gw
val:  4.52     1.69     0.752
sd:   4.57     1.21     0.458

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.52     1.69     0.753    3.82     2.55
sd:   4.59     1.21     0.459    164      220

      CNST        HILL        GNLS
AIC:  169.66      157.29      161.29
PROB: 0           0.88        0.12
RMSE: 1.59        1.27        1.27

MAX_MEAN: 2.36      MAX_MED: 3.31      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

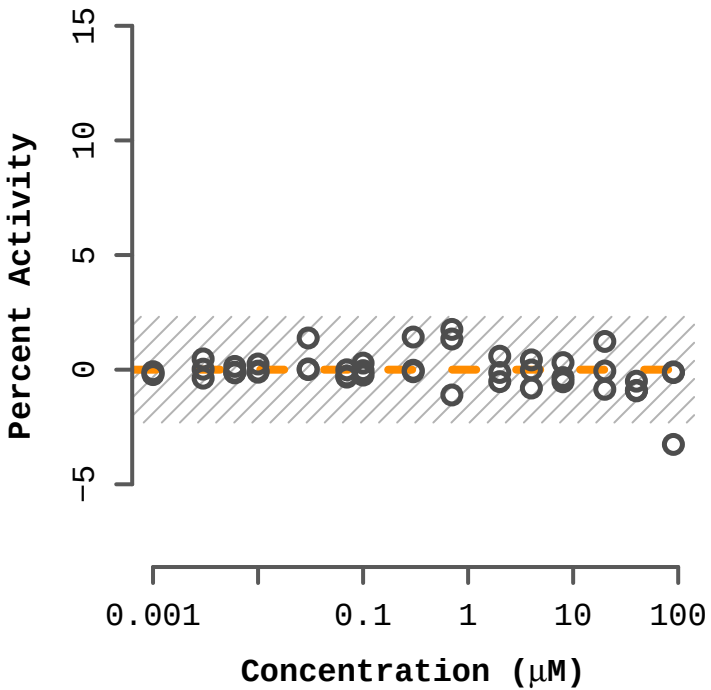
NAME: Dipiperidinomethane
CHID: 47453 **CASRN:** 880-09-1
SPID(S): Tox21_302484
M4ID: 12476649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

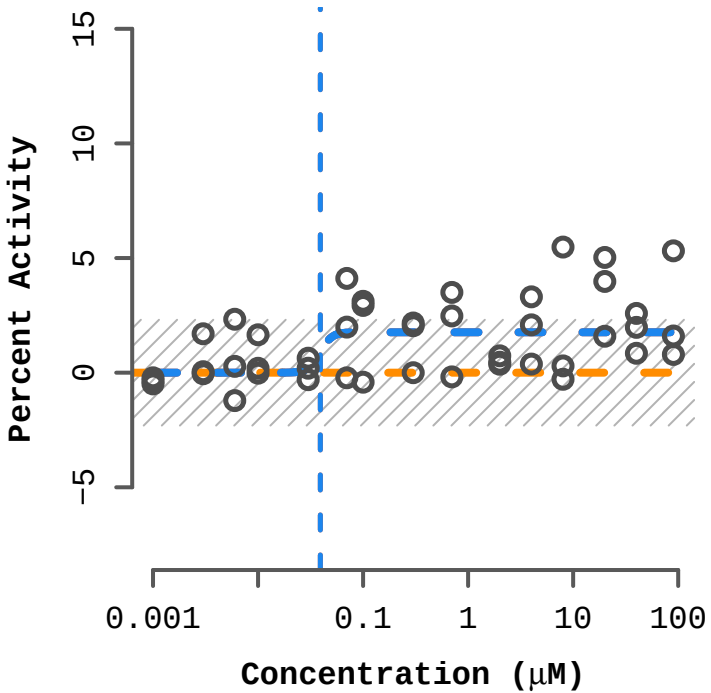
NAME: Dikegulac
CHID: 47454 CASRN: 18467-77-1
SPID(S): Tox21_300935
M4ID: 12478198

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.665 MAX_MED: 1.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2−Norbornene−5,6−dicarboxylic anhydride
CHID: 47456 CASRN: 826−62−0
SPID(S): Tox21_300273
M4ID: 12478857

HILL MODEL (in red):

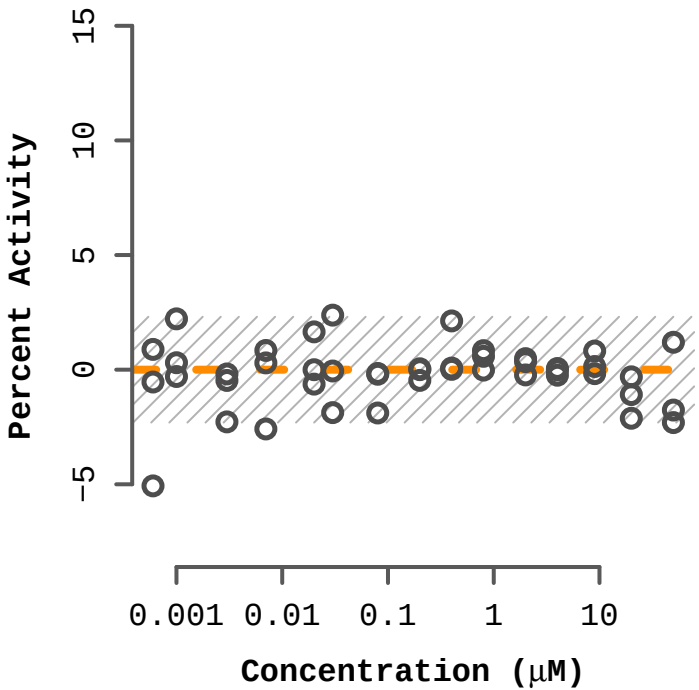
	tp	ga	gw
val:	1.76	−1.41	8
sd:	0.3	0.282	17.1

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.76	−1.41	8	3.51	3.93
sd:	0.3	0.282	17.1	691	1690

	CNST	HILL	GNLS
AIC:	198.52	174.31	178.31
PROB:	0	0.88	0.12
RMSE:	2.18	1.5	1.5

MAX_MEAN: 3.53 MAX_MED: 3.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

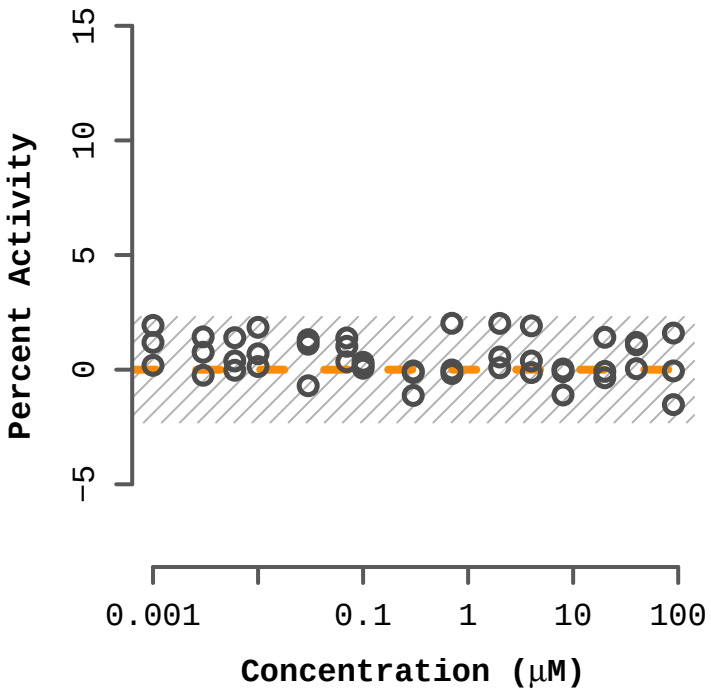
NAME: Calcium saccharin hydrate
CHID: 47459 **CASRN:** 6381-91-5
SPID(S): Tox21_302447
M4ID: 12476686

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

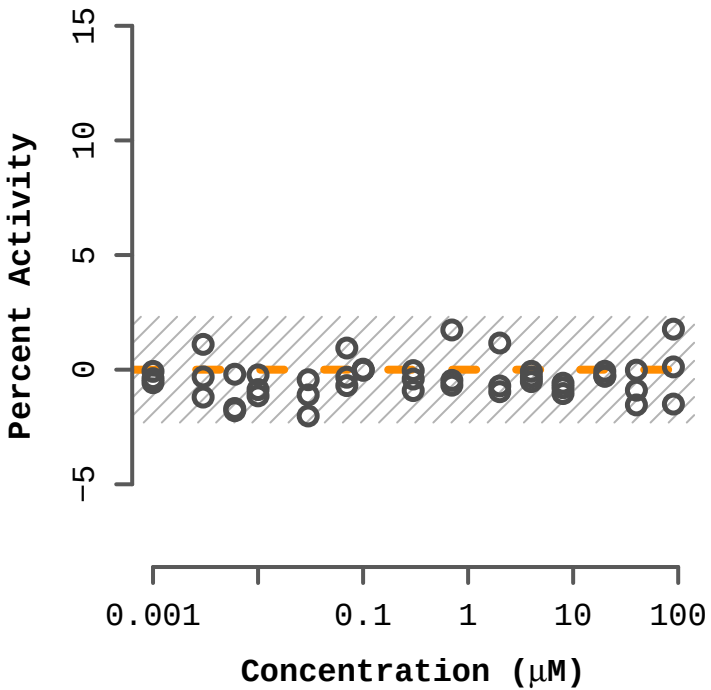
NAME: 3-Pyridinamine
CHID: 47461 **CASRN:** 462-08-8
SPID(S): Tox21_303451
M4ID: 12475689

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.51	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

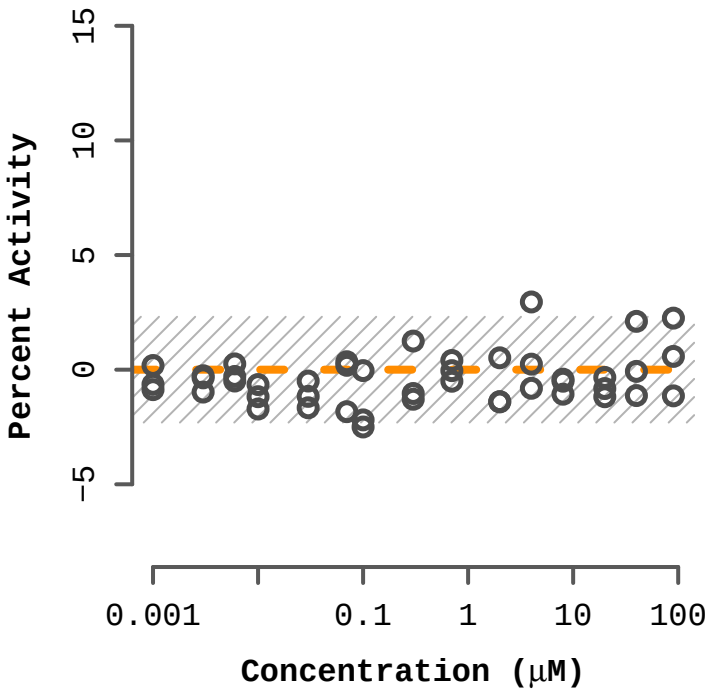
NAME: 3-Pyridinamine
CHID: 47461 **CASRN:** 462-08-8
SPID(S): Tox21_201650
M4ID: 12480602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.198 **MAX_MED:** 0.122 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

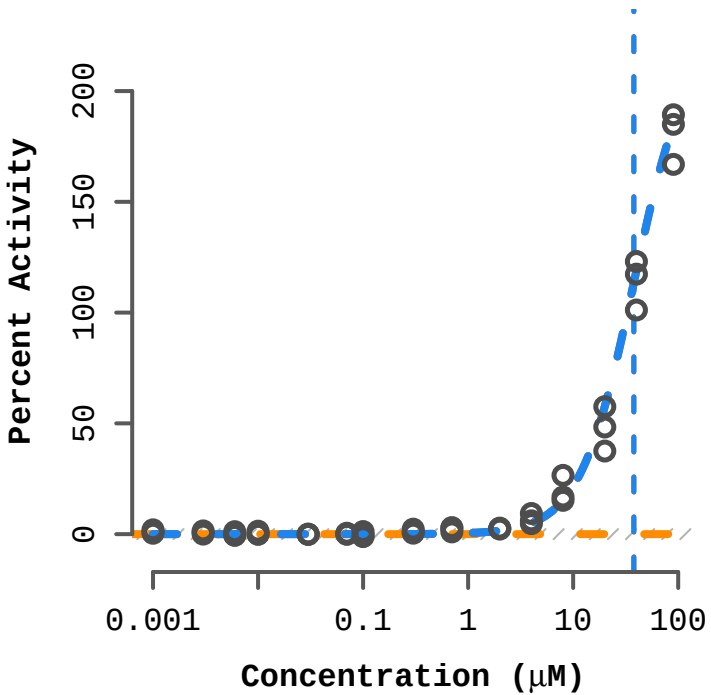
NAME: 3-Carene
CHID: 47462 **CASRN:** 13466-78-9
SPID(S): Tox21_302632
M4ID: 12476501

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.795 **MAX_MED:** 0.579 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Corodane
CHID: 47463 CASRN: 13380-94-4
SPID(S): Tox21_302627
M4ID: 12476506

HILL MODEL (in red):

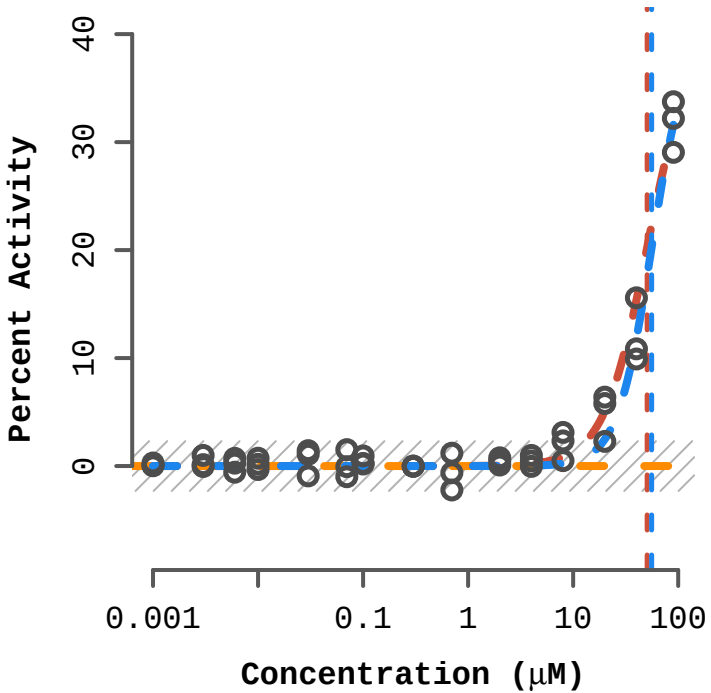
	tp	ga	gw
val:	227	1.58	1.69
sd:	3.98	0.0129	0.0381

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	227	1.58	1.69	3.95	7.38
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	454.45	249.17	253.17
PROB:	0	0.88	0.12
RMSE:	56.88	5.47	5.48

MAX_MEAN: 180 MAX_MED: 185 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Ethyl-2-methylpyrazine
CHID: 47464 CASRN: 15707-23-0
SPID(S): Tox21_302613
M4ID: 12476520

HILL MODEL (in red):

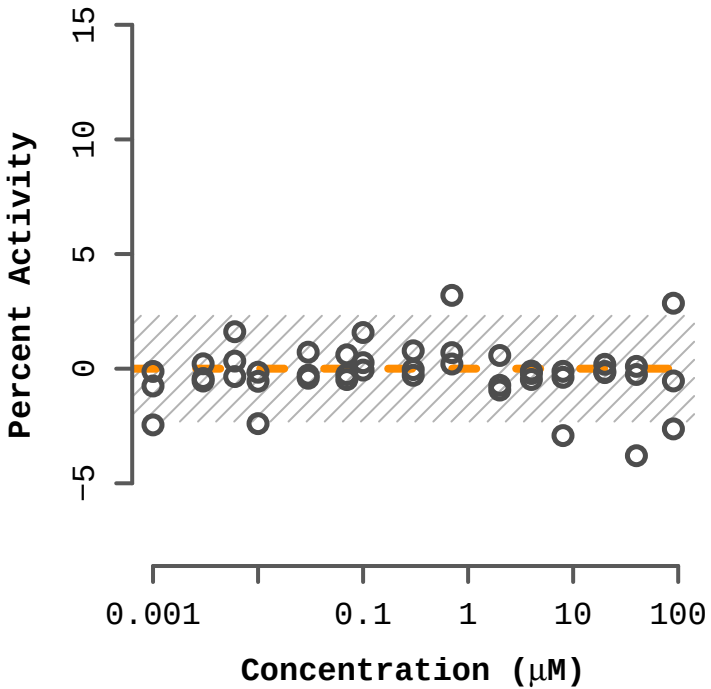
	tp	ga	gw
val:	40.5	1.7	2.09
sd:	3.91	0.0441	0.258

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	40.5	1.75	2.66	2.57	17.7
sd:	13.2	0.142	1.37	1520	42500

	CNST	HILL	GNLS
AIC:	272.41	159.62	165.21
PROB:	0	0.94	0.06
RMSE:	8.94	1.48	1.41

MAX_MEAN: 31.7 MAX_MED: 32.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

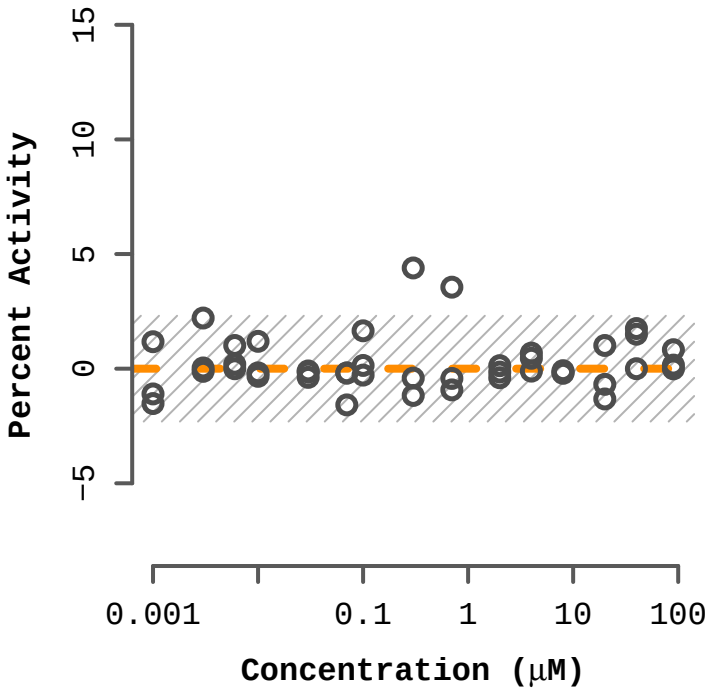
NAME: 6-(1-Methylethyl)quinoline
CHID: 47465 **CASRN:** 135-79-5
SPID(S): Tox21_302711
M4ID: 12476422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.701 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

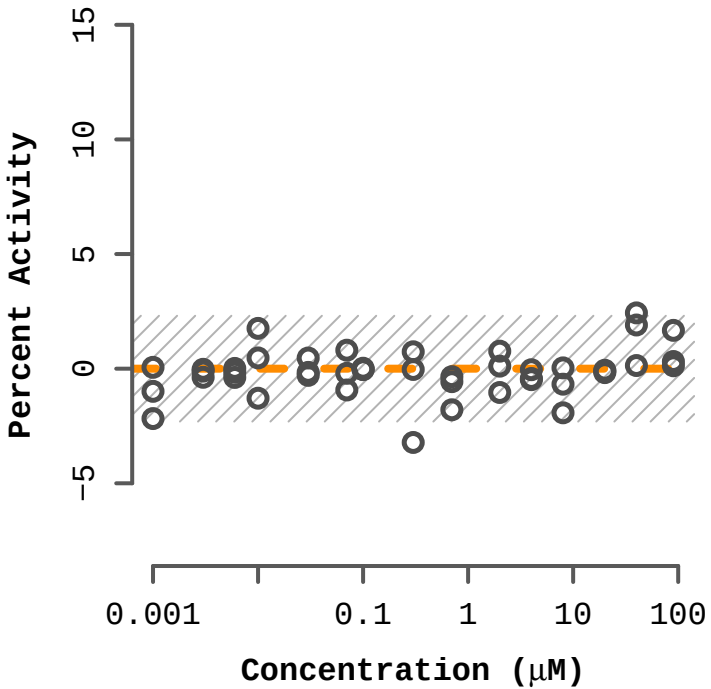
NAME: 2-Isopropoxyethanol
CHID: 47466 **CASRN:** 109-59-1
SPID(S): Tox21_301136
M4ID: 12477997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

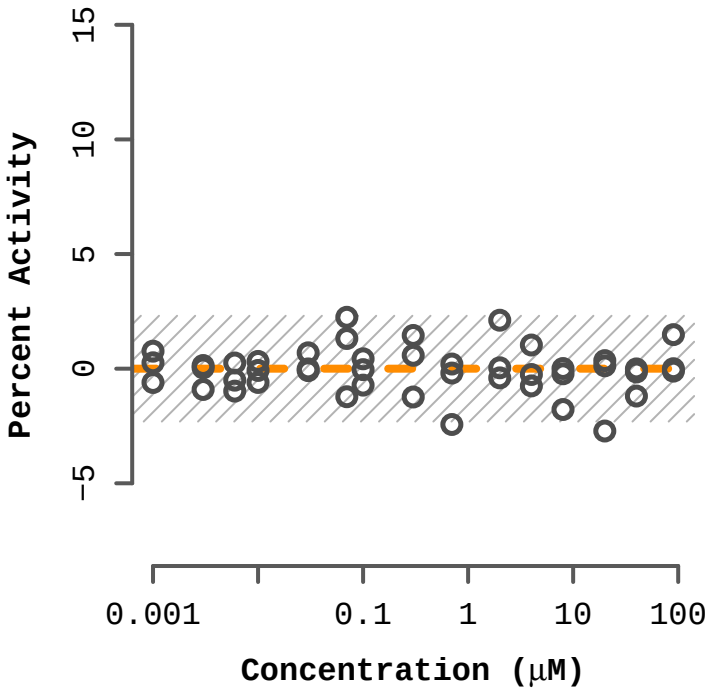
NAME: Choline hydroxide
CHID: 47467 **CASRN:** 123-41-1
SPID(S): Tox21_302647
M4ID: 12476486

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

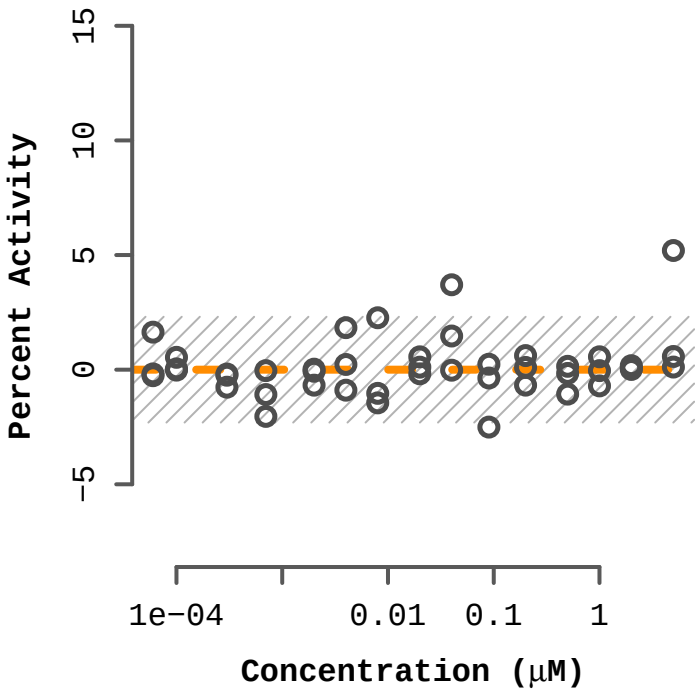
NAME: 2-tert-Butyl-6-methylphenol
CHID: 47468 CASRN: 2219-82-1
SPID(S): Tox21_302562
M4ID: 12476571

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.779 MAX_MED: 1.32 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

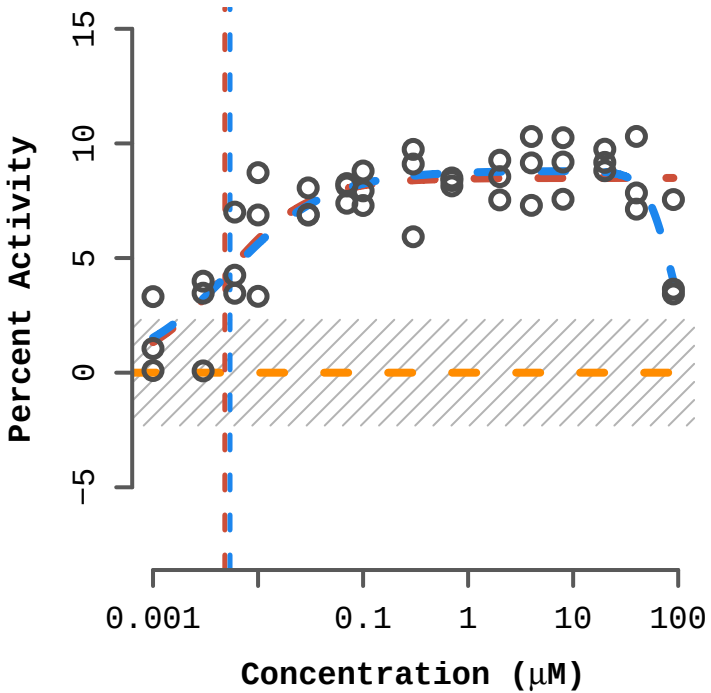
NAME: N,N,N',N'−Tetramethyl−1,3−propanediamine
CHID: 47469 **CASRN:** 110−95−2
SPID(S): Tox21_300932
M4ID: 12478201

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methoxybenzyl acetate
CHID: 47470 **CASRN:** 1331-83-5
SPID(S): Tox21_302726
M4ID: 12476407

HILL MODEL (in red):

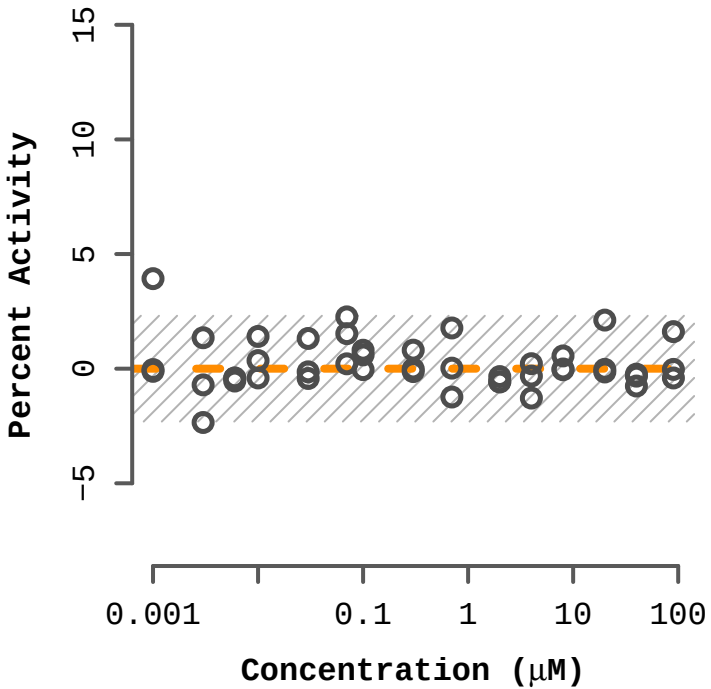
	tp	ga	gw
val:	8.49	−2.32	1.07
sd:	0.294	0.109	0.283

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.8	−2.27	0.926	1.93	3.58
sd:	0.324	0.11	0.218	0.043	1.82

	CNST	HILL	GNLS
AIC:	319.42	174.67	165.76
PROB:	0	0.01	0.99
RMSE:	7.43	1.62	1.35

MAX_MEAN: 9.25 **MAX_MED:** 9.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

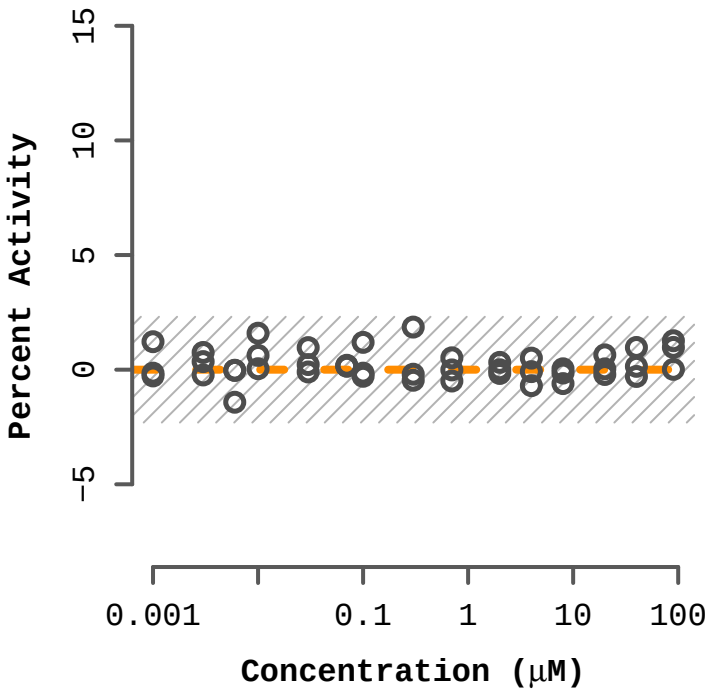
NAME: 2-Methyl-3-buten-2-ol
CHID: 47471 **CASRN:** 115-18-4
SPID(S): Tox21_303823
M4ID: 12475365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

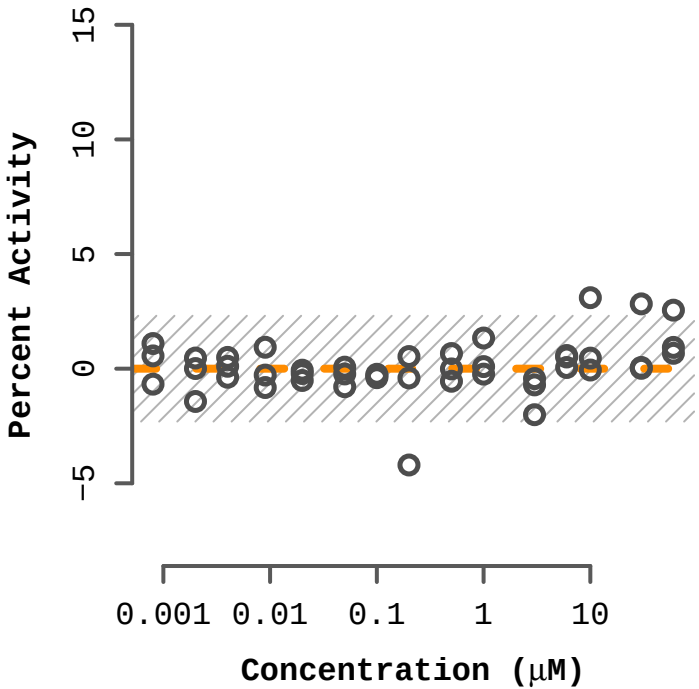
NAME: N,N−Dimethylbutylamine
CHID: 47472 **CASRN:** 927−62−8
SPID(S): Tox21_303901
M4ID: 12475287

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.66	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 0.972 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

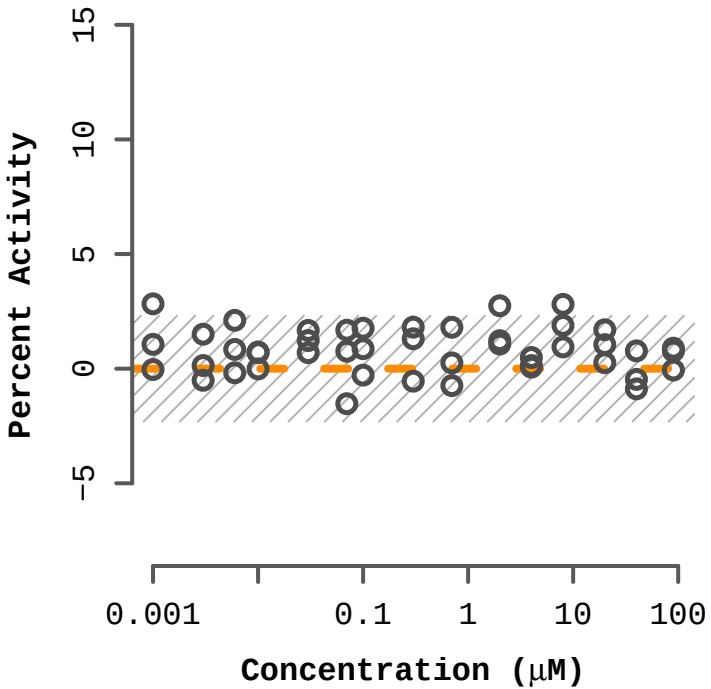
NAME: Polymethylene polyphenyl isocynate
CHID: 47473 **CASRN:** 9016-87-9
SPID(S): Tox21_302585
M4ID: 12476548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

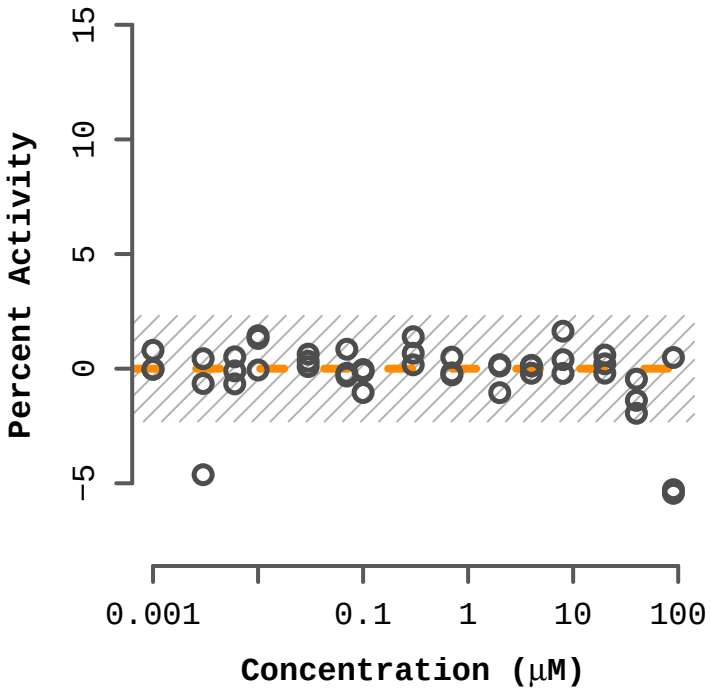
NAME: 1,8-Octanedithiol
CHID: 47474 **CASRN:** 1191-62-4
SPID(S): Tox21_303621
M4ID: 12475524

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.88 **MAX_MED:** 1.89 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

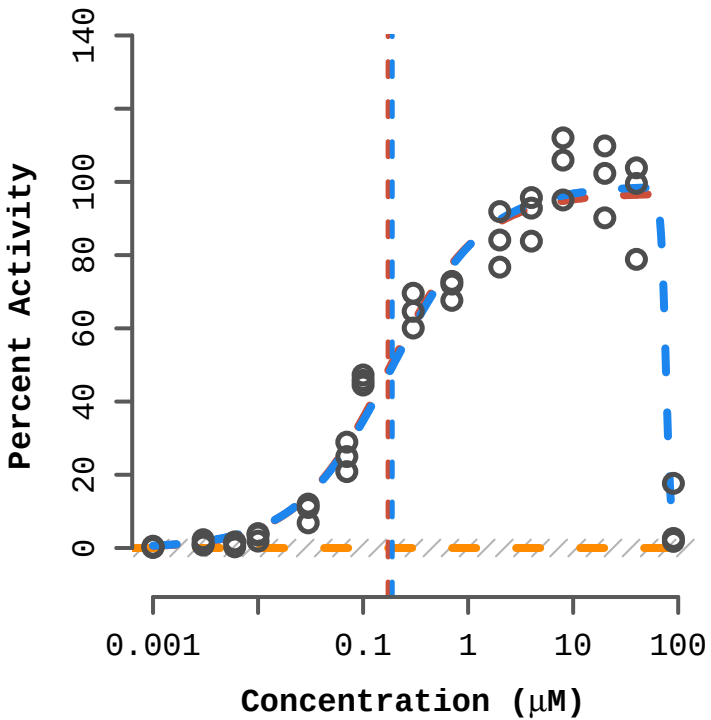
NAME: 2-Thienyl disulfide
CHID: 47476 **CASRN:** 6911-51-9
SPID(S): Tox21_302478
M4ID: 12476655

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 0.9 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: dl-Norgestrel
CHID: 47477 CASRN: 6533-00-2
SPID(S): Tox21_303623
M4ID: 12475522

HILL MODEL (in red):

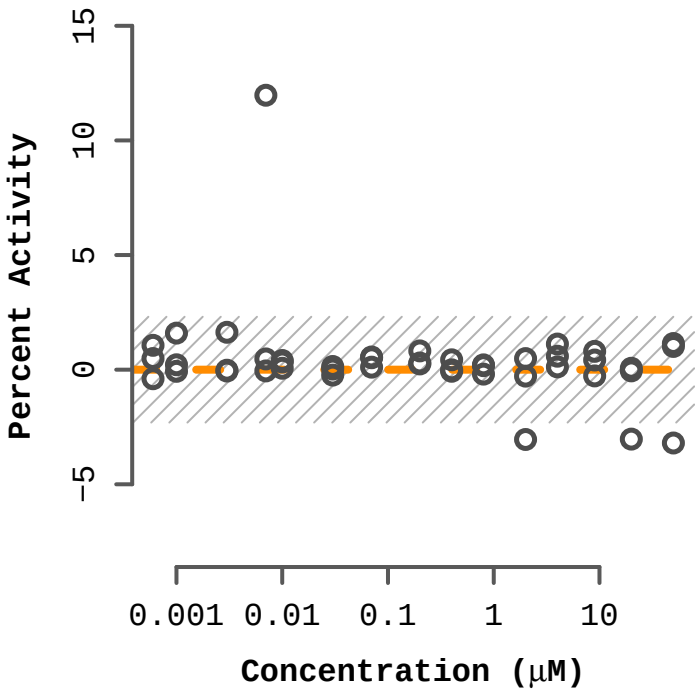
	tp	ga	gw
val:	96.9	-0.762	0.994
sd:	3.45	0.0747	0.117

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	98.9	-0.723	0.962	1.88	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	505.77	366.81	315.21
PROB:	0	0	1
RMSE:	62.05	24.12	7.05

MAX_MEAN: 104 MAX_MED: 106 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

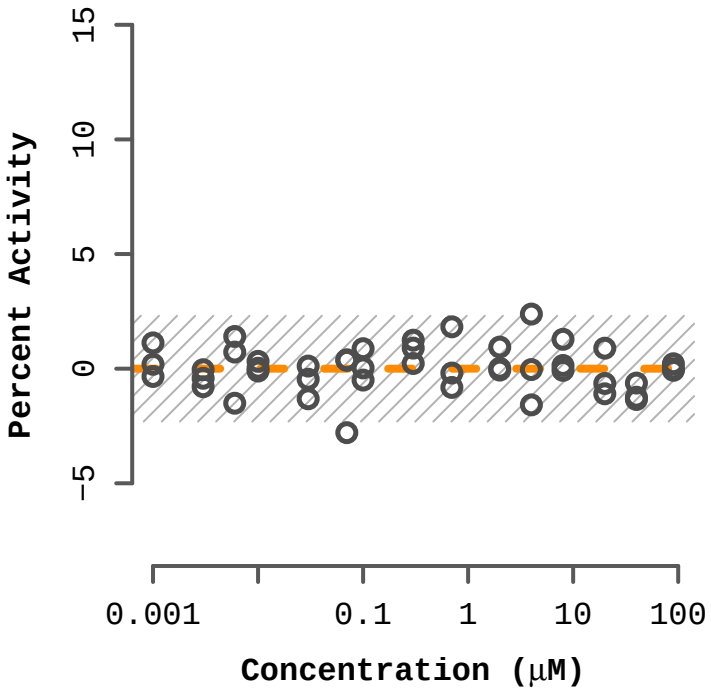
NAME: Nitric acid, magnesium salt
CHID: 47484 **CASRN:** 13446-18-9
SPID(S): Tox21_302464
M4ID: 12476669

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.63	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 4.13 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

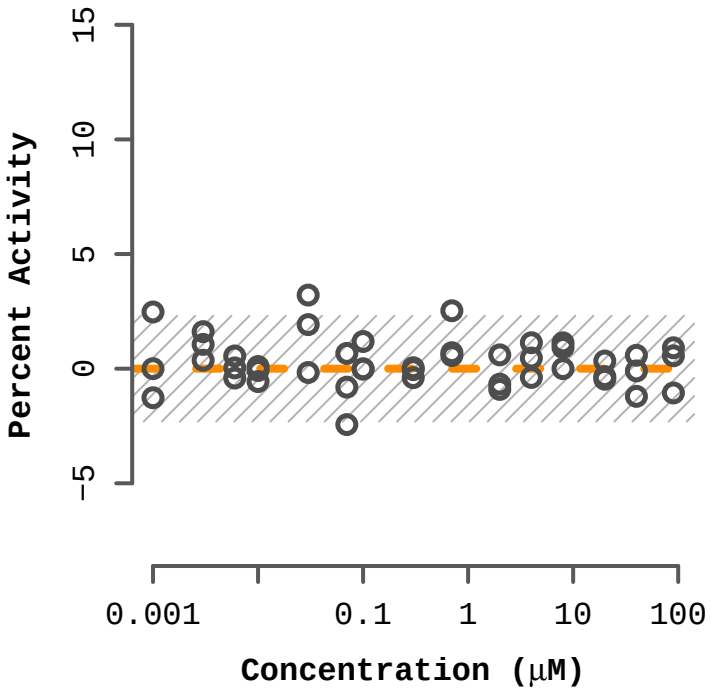
NAME: Methoxybenzyl alcohol
CHID: 47486 **CASRN:** 1331-81-3
SPID(S): Tox21_302521
M4ID: 12476612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.899 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

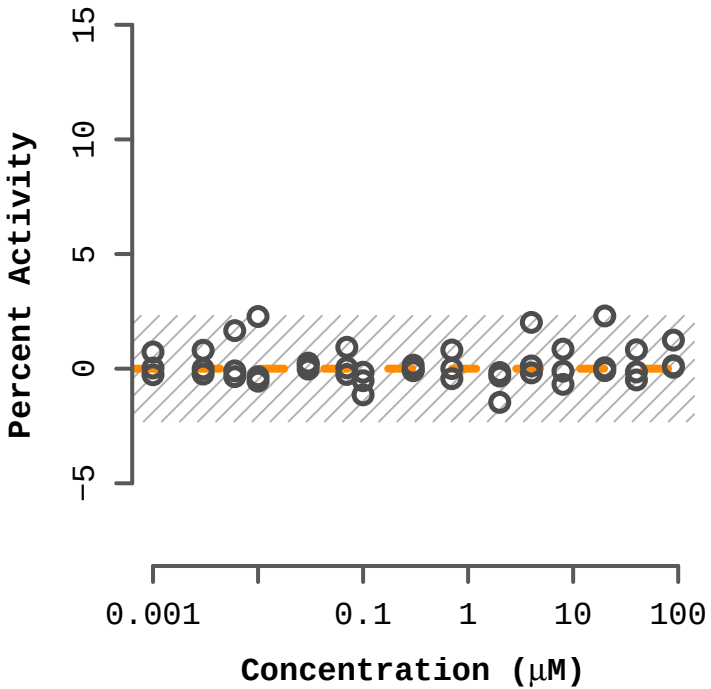
NAME: Sulfuric acid, monononyl ester, sodium salt
CHID: 47487 CASRN: 1072-15-7
SPID(S): Tox21_301006
M4ID: 12478127

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.66 MAX_MED: 1.92 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

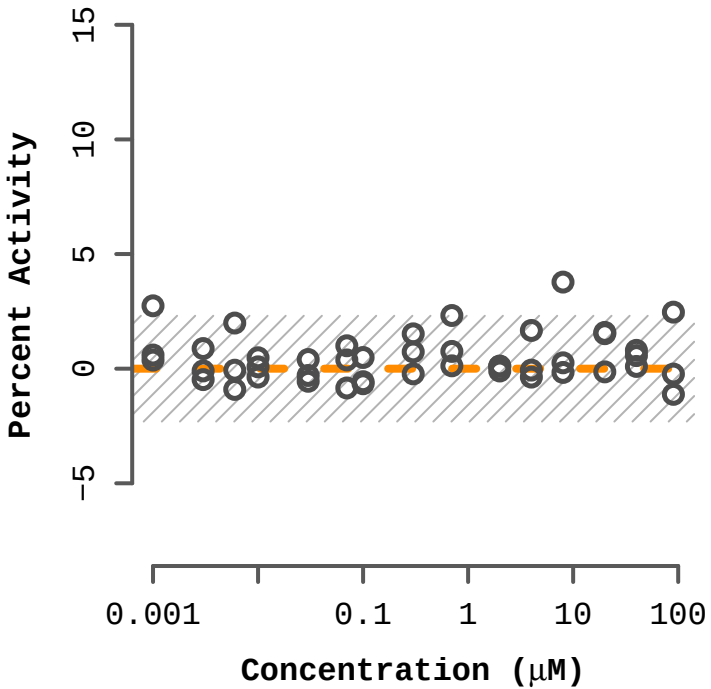
NAME: Linalyl isobutyrate
CHID: 47490 CASRN: 78-35-3
SPID(S): Tox21_302721
M4ID: 12476412

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.753 MAX_MED: 0.17 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

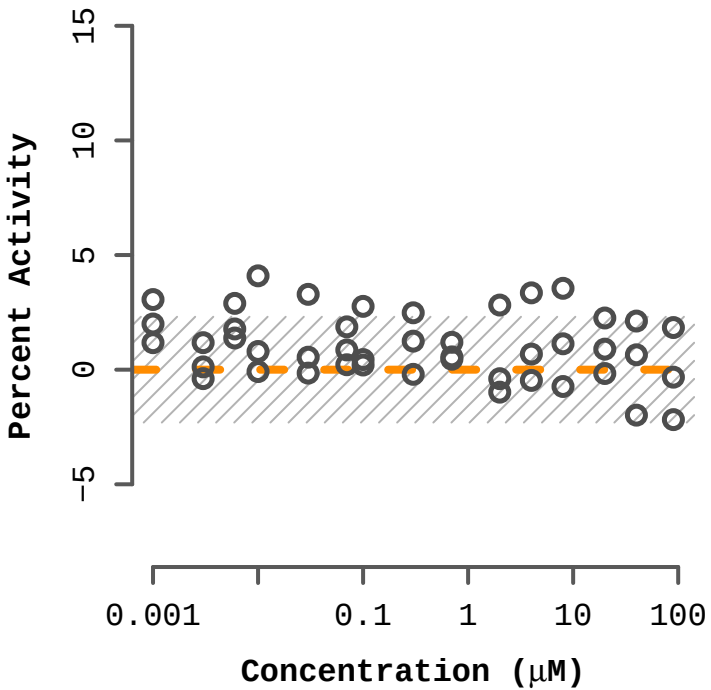
NAME: Pyrazinyl methyl sulfide
CHID: 47491 **CASRN:** 21948-70-9
SPID(S): Tox21_302534
M4ID: 12476599

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

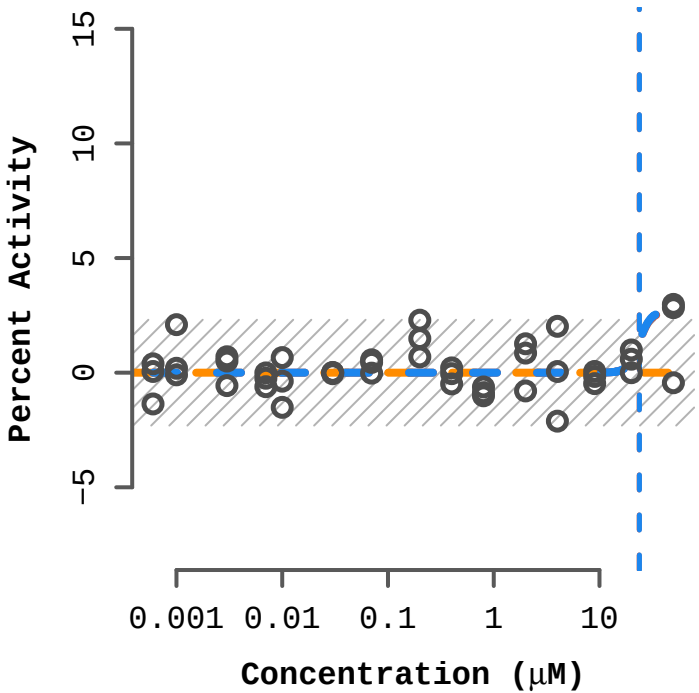
NAME: Midodrine hydrochloride
CHID: 47493 **CASRN:** 3092-17-9
SPID(S): Tox21_302723
M4ID: 12476410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Midodrine hydrochloride
CHID: 47493 CASRN: 3092-17-9
SPID(S): Tox21_110529_1
M4ID: 12484290

HILL MODEL (in red):

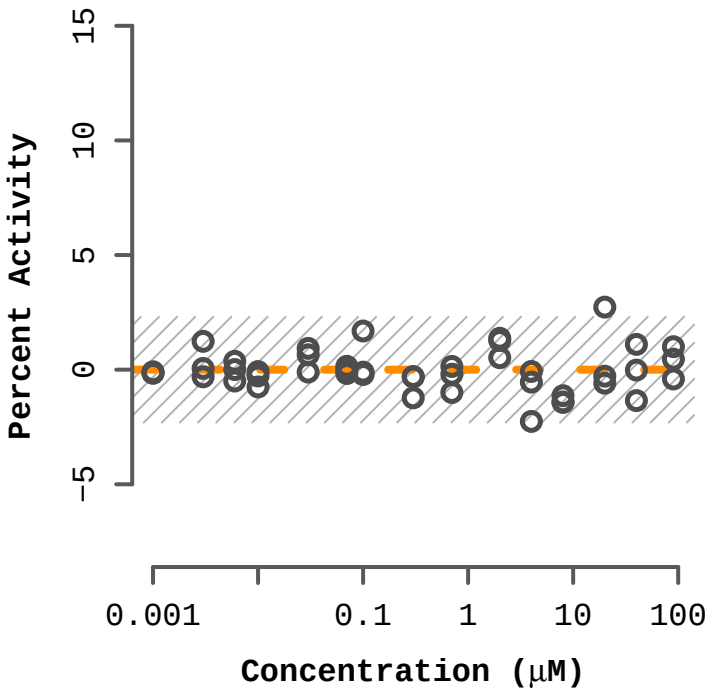
	tp	ga	gw
val:	2.65	1.38	8
sd:	0.53	0.316	32.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.77	1.38	8	2.87	1.12
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	132.25	129.09	133.09
PROB:	0.15	0.75	0.1
RMSE:	1.07	0.98	0.98

MAX_MEAN: 1.79 **MAX_MED:** 2.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

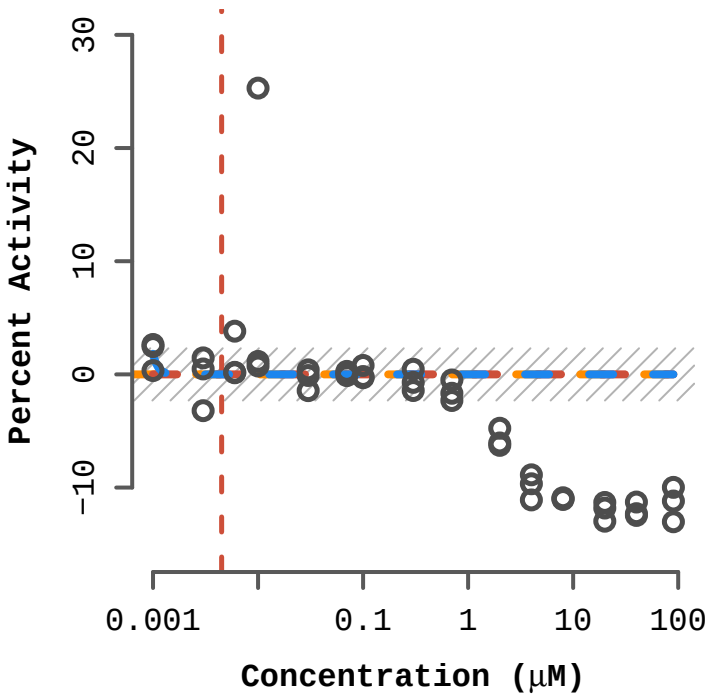
NAME: Octyl decyl phthalate
CHID: 47497 CASRN: 119-07-3
SPID(S): Tox21_302603
M4ID: 12476530

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triphenyllead acetate
CHID: 47498 **CASRN:** 1162-06-7
SPID(S): Tox21_302482
M4ID: 12476651

HILL MODEL (in red):

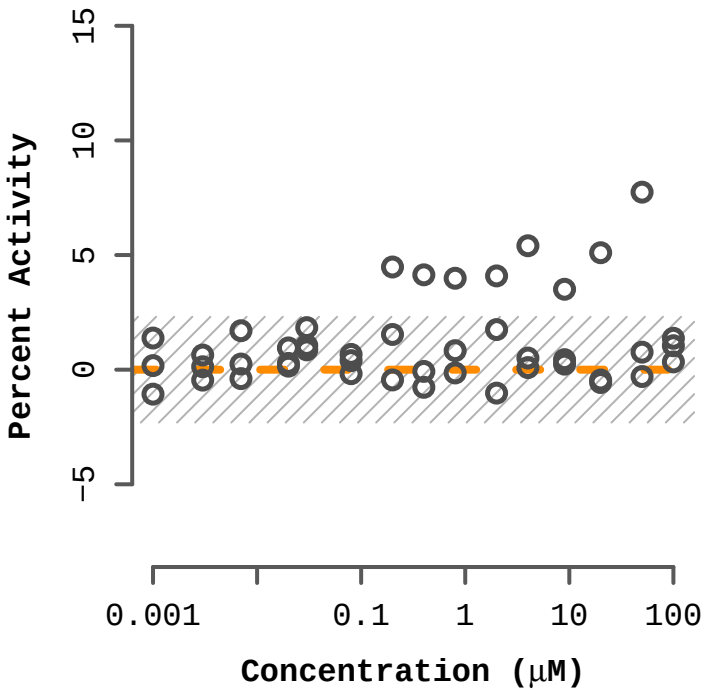
	tp	ga	gw
val:	4.85e-09	-2.35	0.305
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	23.6	-4.72	3.87	-3.11	9.79
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	312.32	318.32	321.96
PROB:	0.95	0.05	0.01
RMSE:	7.77	7.77	7.75

MAX_MEAN: 9.06 **MAX_MED:** 2.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

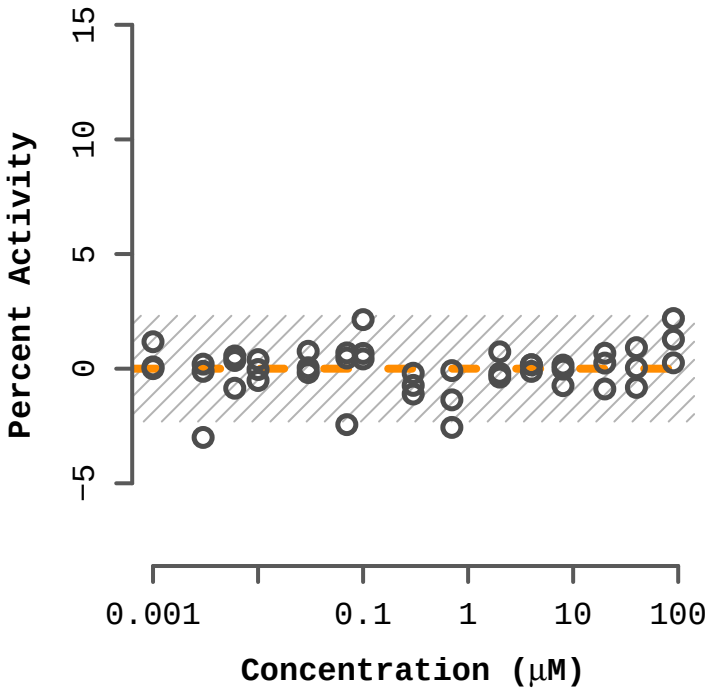
NAME: Methylpolysilicone
CHID: 47501 **CASRN:** 9004-73-3
SPID(S): Tox21_302481
M4ID: 12476652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.23	NA	NA

MAX_MEAN: 2.74 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

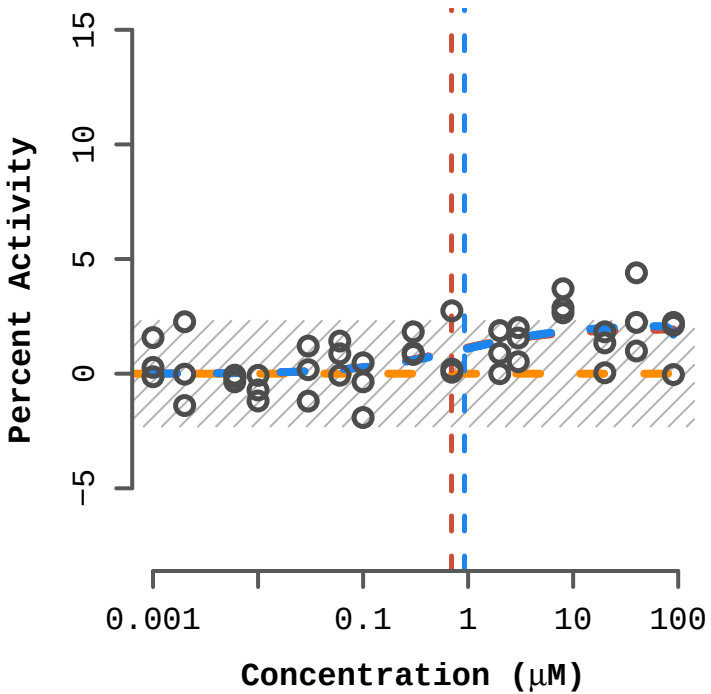
NAME: Timolol maleate salt
CHID: 47504 **CASRN:** 26921-17-5
SPID(S): Tox21_302468
M4ID: 12476665

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.75	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3,3',5-Triiodo-l-thyronine sodium salt
CHID: 47505 CASRN: 55-06-1
SPID(S): Tox21_302514
M4ID: 12476619

HILL MODEL (in red):

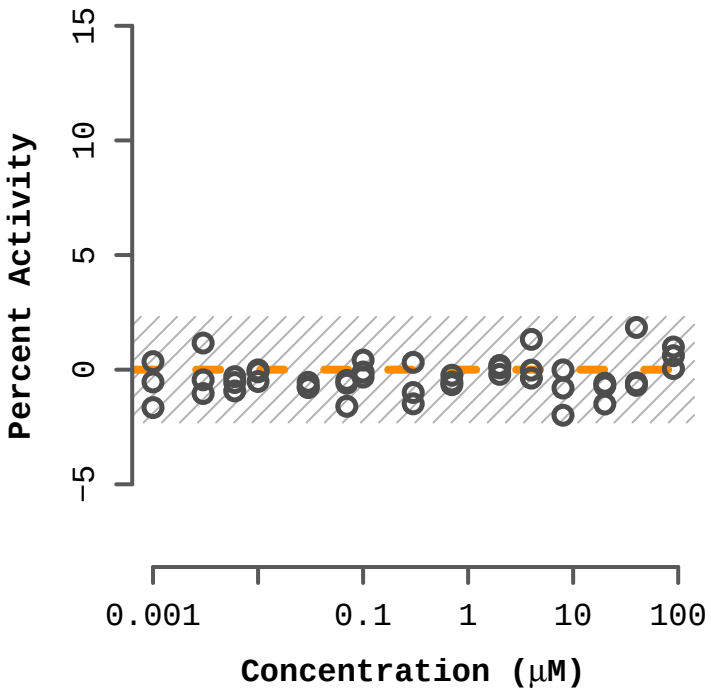
	tp	ga	gw
val:	1.95	−0.158	0.925
sd:	0.408	0.458	0.47

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.13	−0.0347	0.863	2	14.9
sd:	0.611	0.518	0.461	0.168	60.7

	CNST	HILL	GNLS
AIC:	172.62	145.04	148.79
PROB:	0	0.87	0.13
RMSE:	1.59	1.08	1.07

MAX_MEAN: 3.08 **MAX_MED:** 2.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

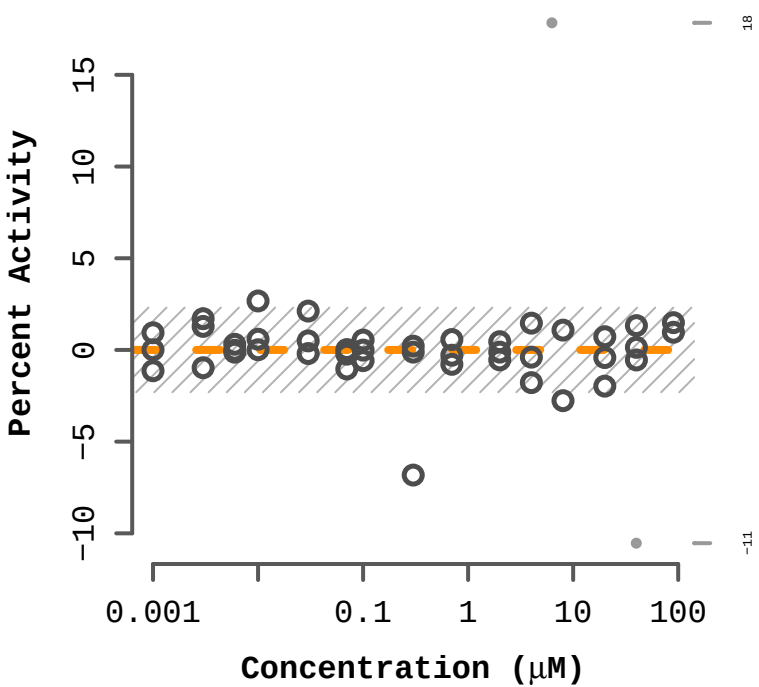
NAME: Salicylic acid p-tolyl ester
CHID: 47508 **CASRN:** 607-88-5
SPID(S): Tox21_302616
M4ID: 12476517

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 0.551 **MAX_MED:** 0.611 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

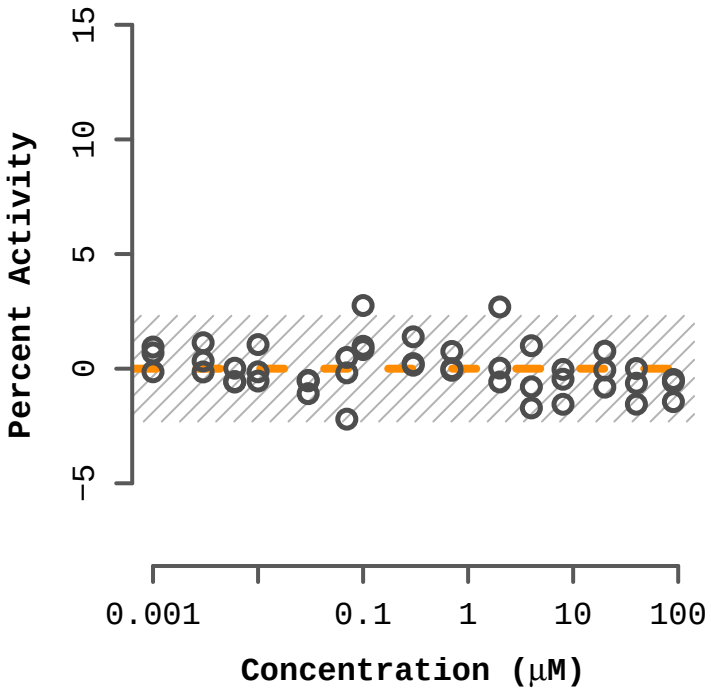
NAME: Benzyl butyrate
CHID: 47510 **CASRN:** 103-37-7
SPID(S): Tox21_300891
M4ID: 12478242 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.55	NA	NA
PROB:	1	NA	NA
RMSE:	3.52	NA	NA

MAX_MEAN: 5.55 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

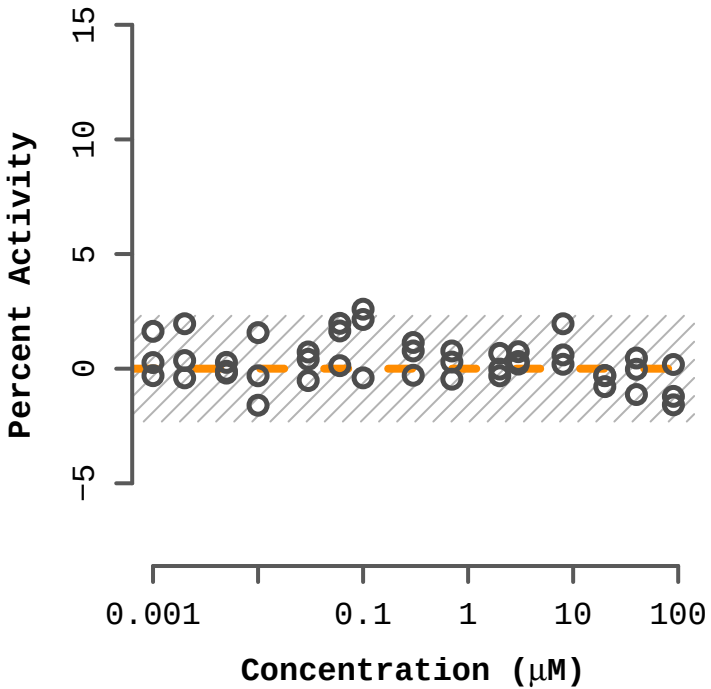
NAME: Ethyl hexadecanoate
CHID: 47511 CASRN: 628-97-7
SPID(S): Tox21_302505
M4ID: 12476628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.53	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 0.979 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

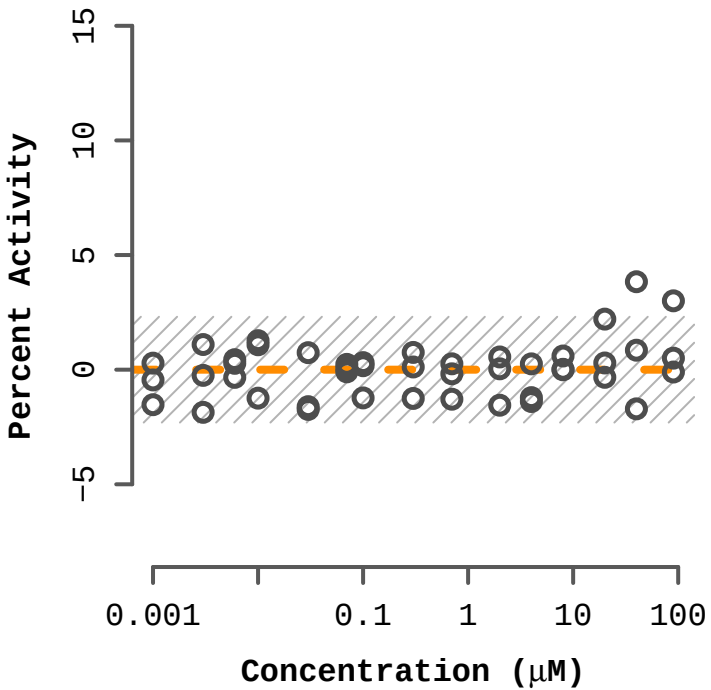
NAME: Indium(III) chloride hydrate
CHID: 47512 **CASRN:** 143983-91-9
SPID(S): Tox21_302501
M4ID: 12476632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

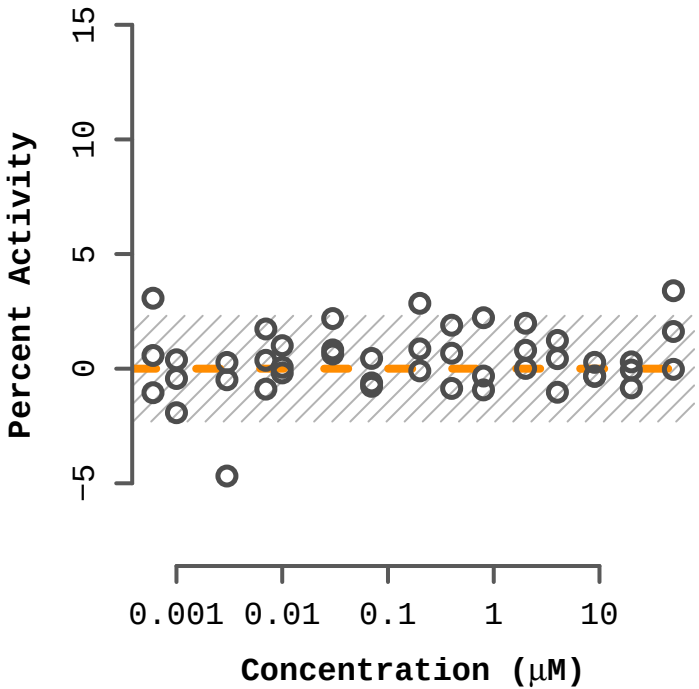
NAME: Hexanedioic acid, di-C7-9-branched and linear a
CHID: 47517 CASRN: 68515-75-3
SPID(S): Tox21_302605
M4ID: 12476528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.14 MAX_MED: 1.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

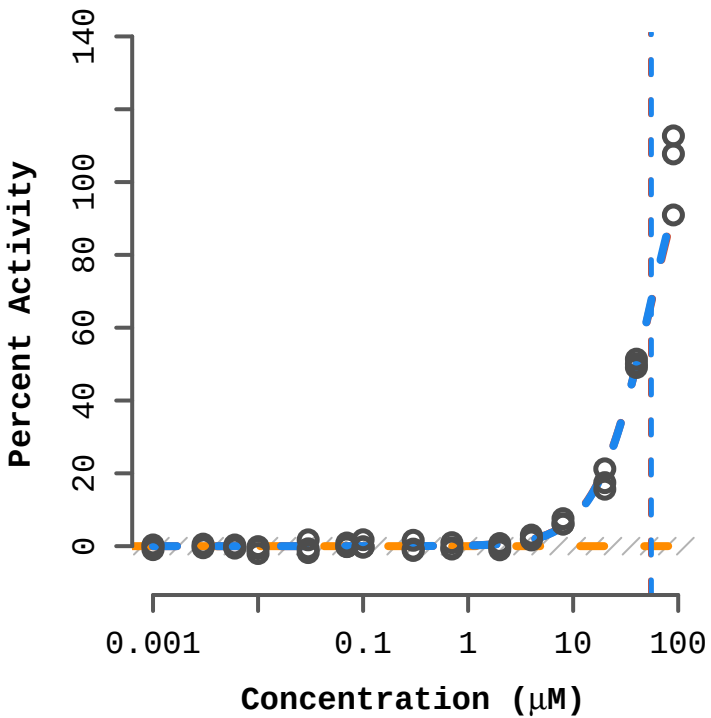
NAME: Levamisole hydrochloride
CHID: 47518 **CASRN:** 16595-80-5
SPID(S): Tox21_111282_1
M4ID: 12483794

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexyl isobutyrate
CHID: 47519 CASRN: 2349-07-7
SPID(S): Tox21_302491
M4ID: 12476642

HILL MODEL (in red):

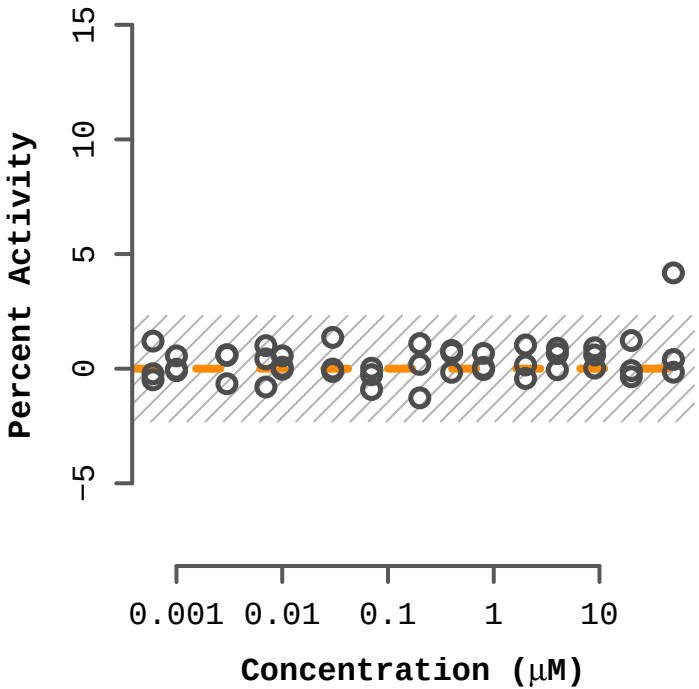
	tp	ga	gw
val:	132	1.74	1.63
sd:	2.62	0.0117	0.0402

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	135	1.74	1.64	2.09	13.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	383.2	196.82	200.46
PROB:	0	0.86	0.14
RMSE:	30.3	4.18	4.21

MAX_MEAN: 104 MAX_MED: 108 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

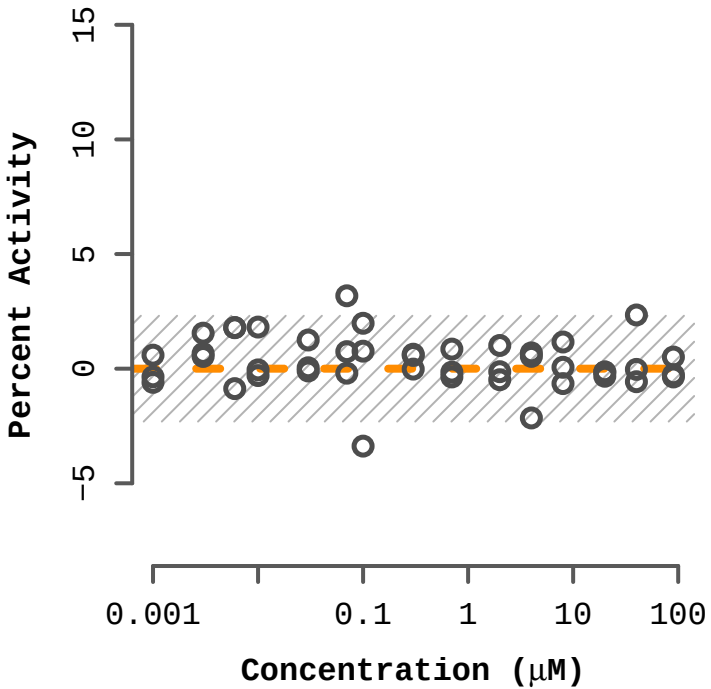
NAME: 1,1-Dimethoxyoctane
CHID: 47520 **CASRN:** 10022-28-3
SPID(S): Tox21_303766
M4ID: 12475422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 0.711 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

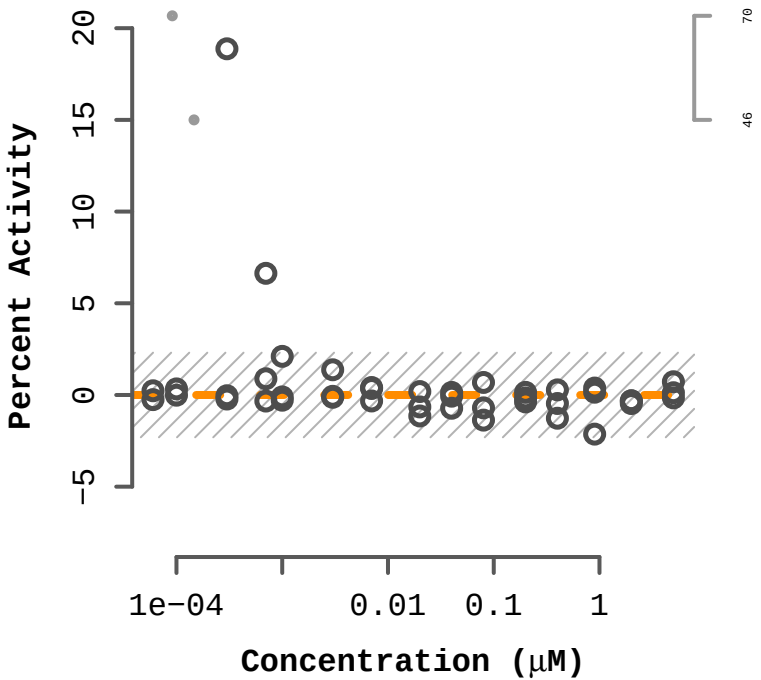
NAME: Sodium 4-isopropylbenzenesulfonate
CHID: 47523 **CASRN:** 15763-76-5
SPID(S): Tox21_303637
M4ID: 12475508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

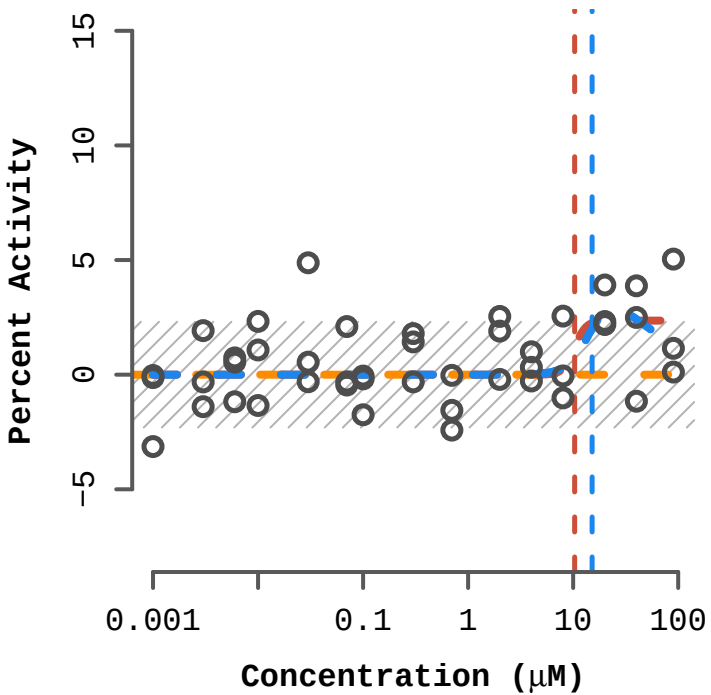
NAME: Kanamycin A sulfate
CHID: 47524 **CASRN:** 25389-94-0
SPID(S): Tox21_202817
M4ID: 12479435 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.39	NA	NA
PROB:	1	NA	NA
RMSE:	12.88	NA	NA

MAX_MEAN: 23.5 **MAX_MED:** 0.888 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pravastatin sodium
CHID: 47525 **CASRN:** 81131-70-6
SPID(S): Tox21_300270
M4ID: 12478860

HILL MODEL (in red):

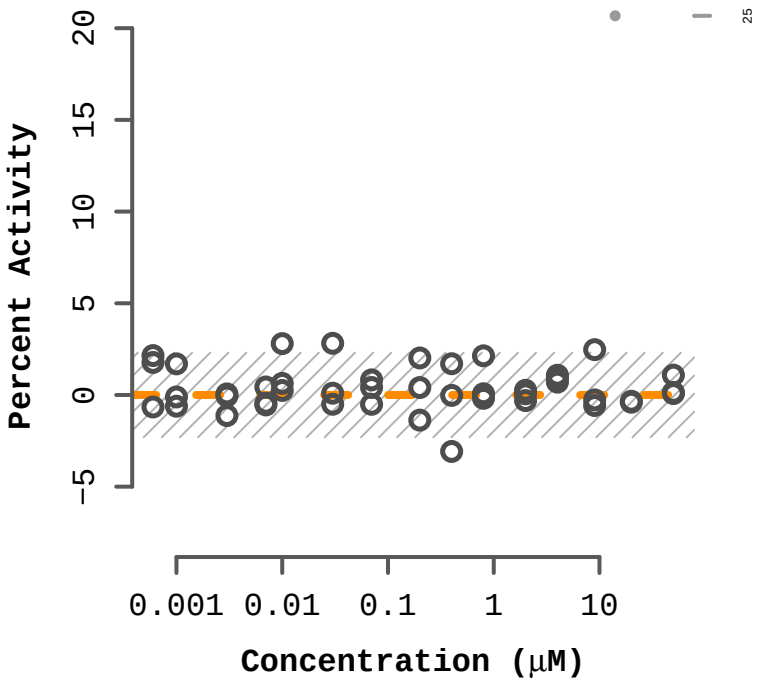
	tp	ga	gw
val:	2.36	1.01	8
sd:	0.577	0.223	13.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.04	1.18	4.22	1.45	1.09
sd:	50.3	0.677	7.56	5.98	4.05

	CNST	HILL	GNLS
AIC:	188.29	180.81	183.66
PROB:	0.02	0.79	0.19
RMSE:	1.92	1.64	1.65

MAX_MEAN: 2.81 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

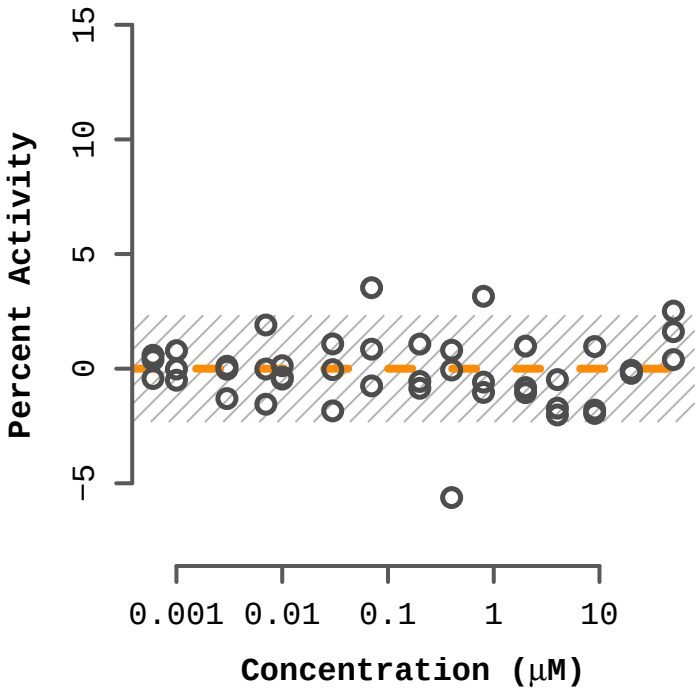
NAME: C10-21 sulfonic acids phenyl esters
CHID: 47526 CASRN: 91082-17-6
SPID(S): Tox21_300331
M4ID: 12478801 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.2	NA	NA
PROB:	1	NA	NA
RMSE:	3.86	NA	NA

MAX_MEAN: 7.96 MAX_MED: 1.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

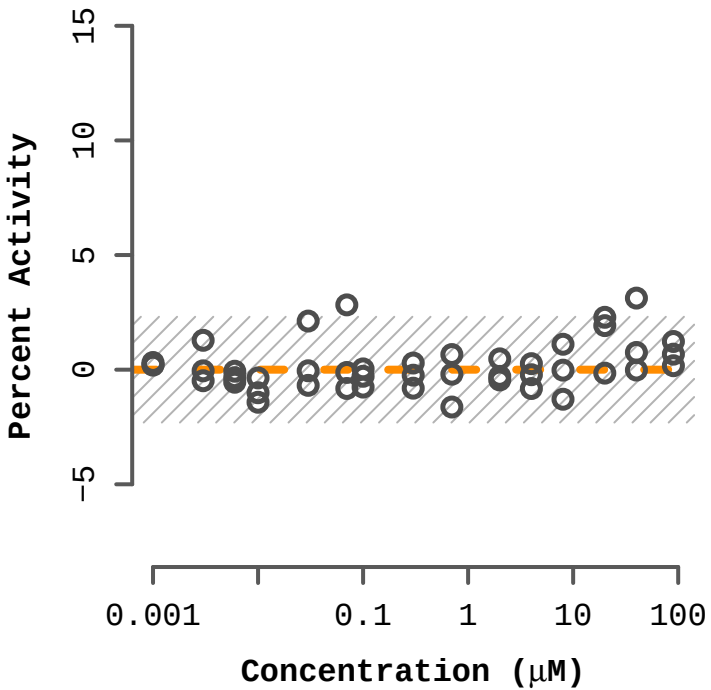
NAME: Adipic acid, polypropyleneglycol, laurate
CHID: 47527 **CASRN:** 66456-53-9
SPID(S): Tox21_300330
M4ID: 12478802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

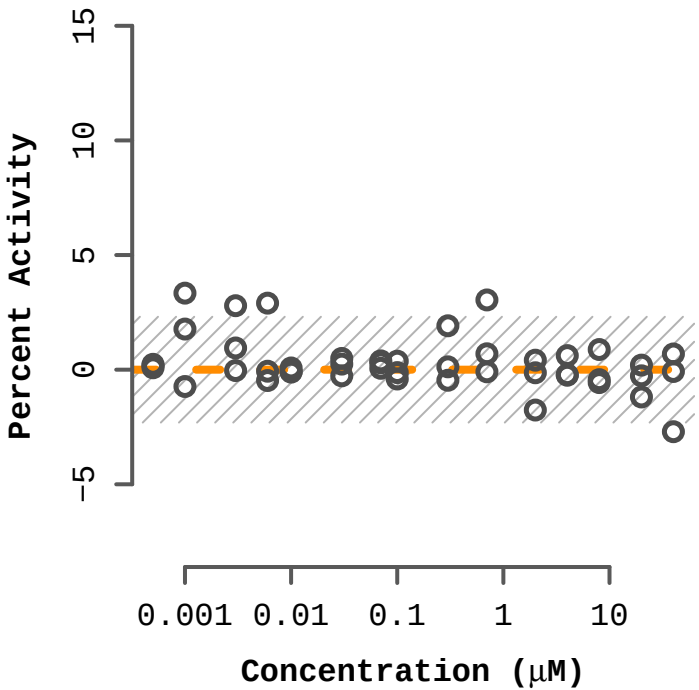
NAME: Benzyloctyl adipate
CHID: 47528 **CASRN:** 58394-64-2
SPID(S): Tox21_300324
M4ID: 12478808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

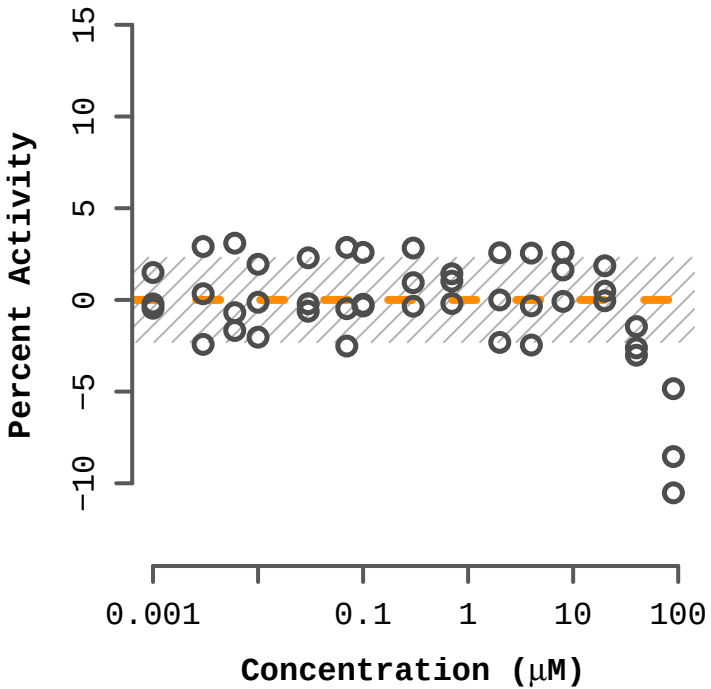
NAME: Acamprosate calcium
CHID: 47529 **CASRN:** 77337-73-6
SPID(S): Tox21_302606
M4ID: 12476527

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

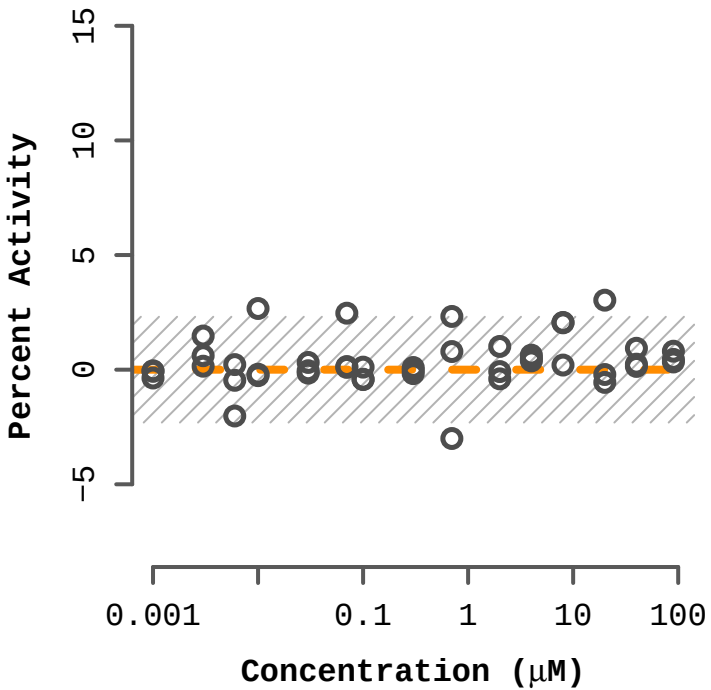
NAME: Hydroxyzine hydrochloride
CHID: 47530 **CASRN:** 1244-76-4
SPID(S): Tox21_302563
M4ID: 12476570

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	210.99	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

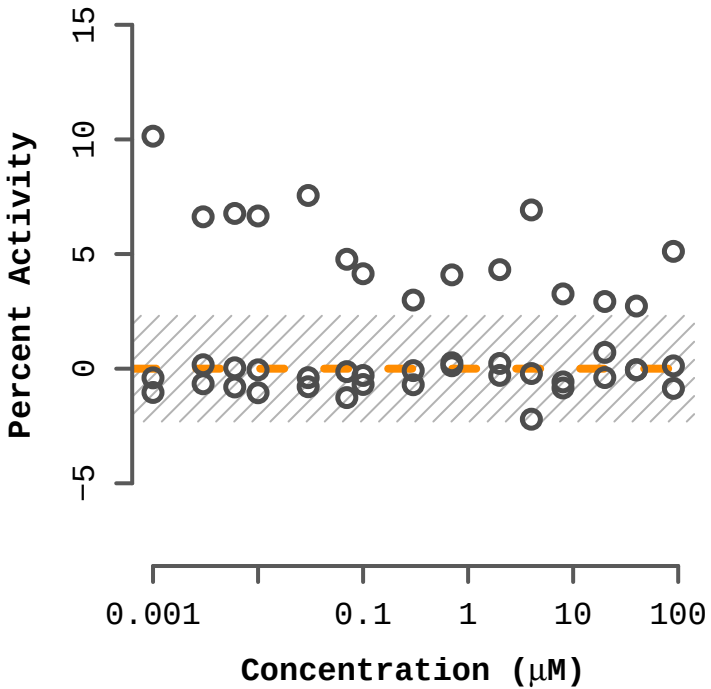
NAME: Trioctyl trimellitate
CHID: 47533 **CASRN:** 89-04-3
SPID(S): Tox21_300640
M4ID: 12478493

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

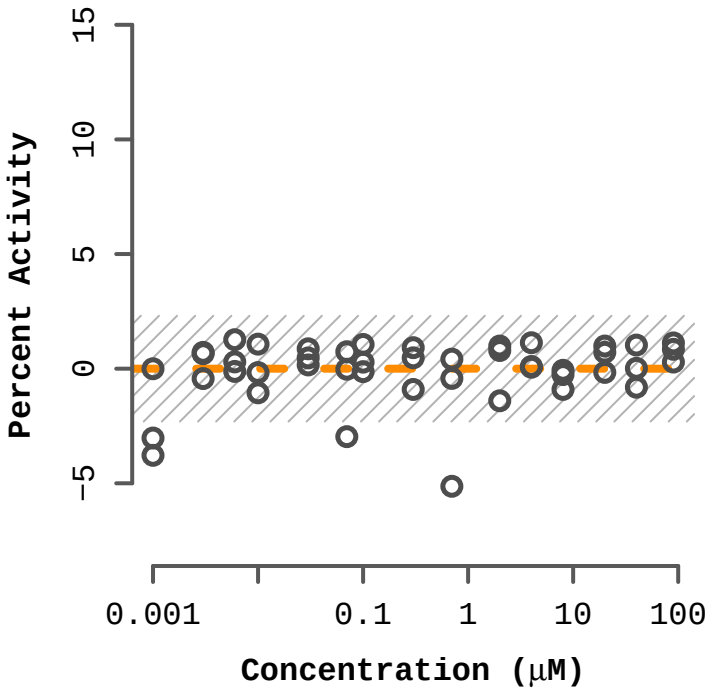
NAME: Butyryl trihexyl citrate
CHID: 47535 **CASRN:** 82469-79-2
SPID(S): Tox21_300521
M4ID: 12478611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.43	NA	NA
PROB:	1	NA	NA
RMSE:	3.31	NA	NA

MAX_MEAN: 2.9 **MAX_MED:** 0.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

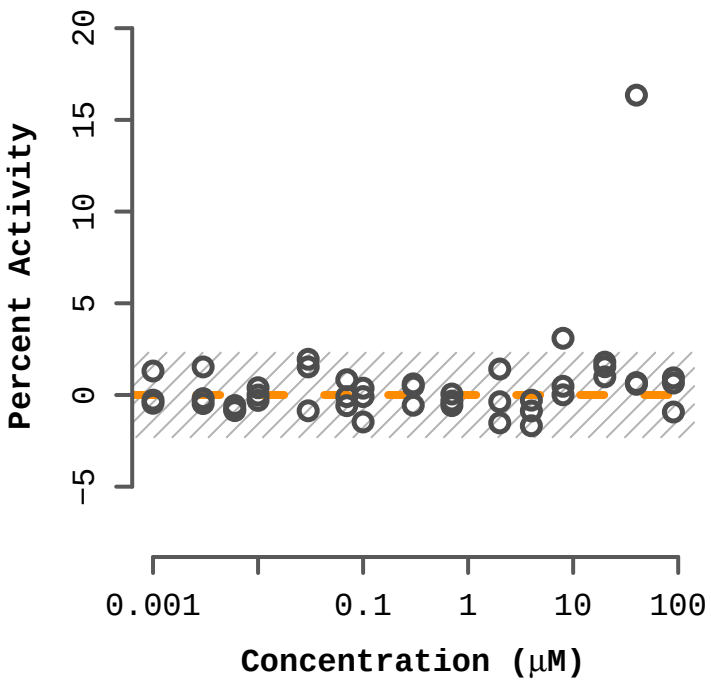
NAME: Dioctyl succinate
CHID: 47537 **CASRN:** 2432-87-3
SPID(S): Tox21_300523
M4ID: 12478609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.754 **MAX_MED:** 0.846 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

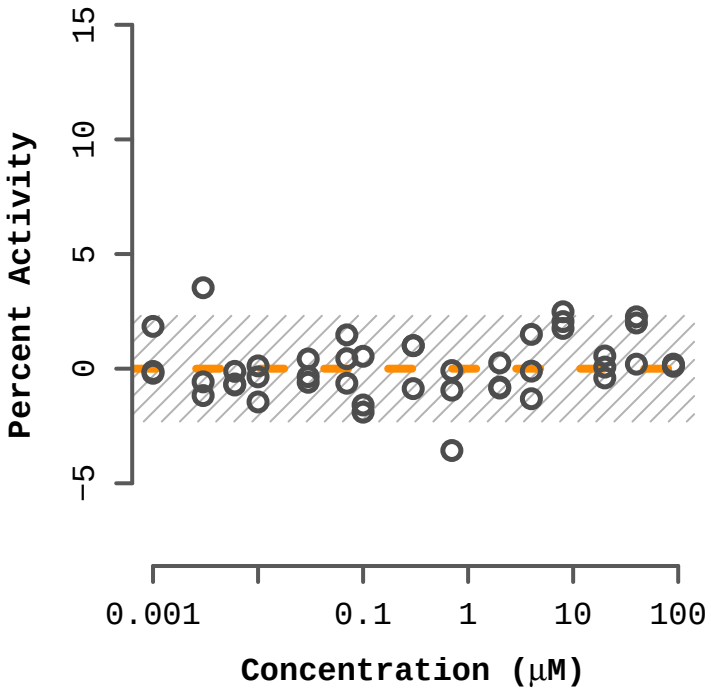
NAME: Pentane−1,5−diyl dibenzoate
CHID: 47538 CASRN: 6624−73−3
SPID(S): Tox21_300524
M4ID: 12478608

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.65	NA	NA
PROB:	1	NA	NA
RMSE:	2.64	NA	NA

MAX_MEAN: 5.87 MAX_MED: 1.54 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

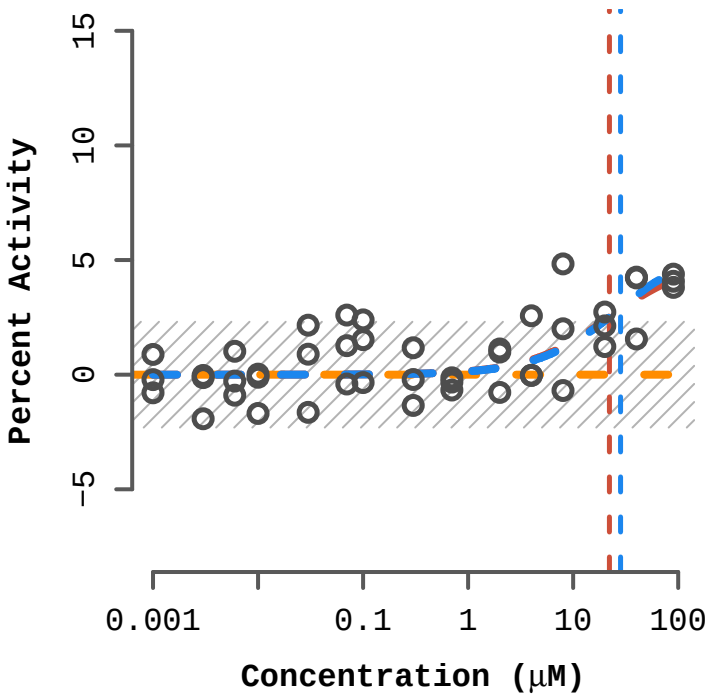
NAME: Hexane−1,6−diyl dibenzoate
CHID: 47539 **CASRN:** 22915−73−7
SPID(S): Tox21_300525
M4ID: 12478607

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Hydroxyfluorene
CHID: 47540 **CASRN:** 6344-67-8
SPID(S): Tox21_300628
M4ID: 12478505

HILL MODEL (in red):

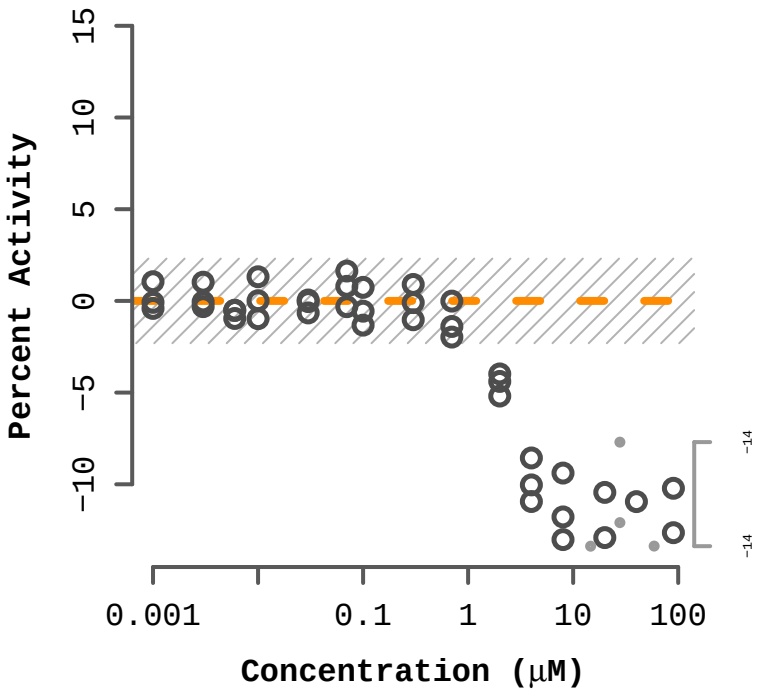
	tp	ga	gw
val:	5	1.35	1.12
sd:	1.9	0.401	0.655

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.8	1.45	1.1	2.06	9.15
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	191.3	156.33	160.21
PROB:	0	0.87	0.13
RMSE:	1.99	1.24	1.25

MAX_MEAN: 4.09 **MAX_MED:** 4.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

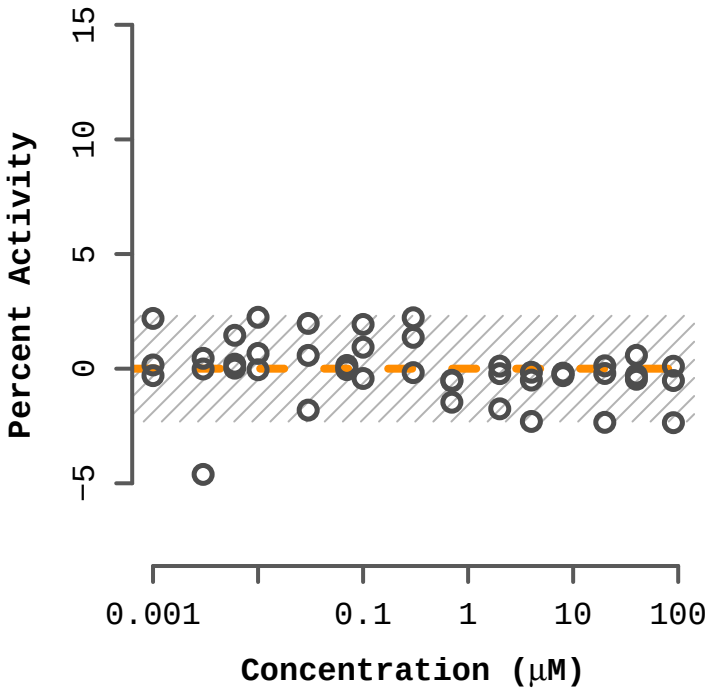
NAME: Picoxystrobin
CHID: 47542 **CASRN:** 117428-22-5
SPID(S): Tox21_300625
M4ID: 12478508 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	304.4	NA	NA
PROB:	1	NA	NA
RMSE:	7.05	NA	NA

MAX_MEAN: 0.704 **MAX_MED:** 0.795 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

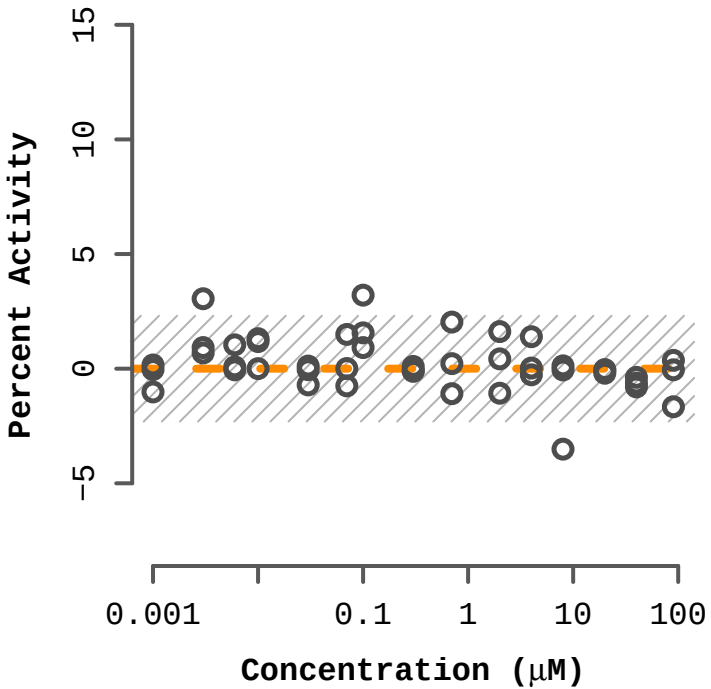
NAME: Furalaxyl
CHID: 47543 **CASRN:** 57646-30-7
SPID(S): Tox21_302489
M4ID: 12476644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

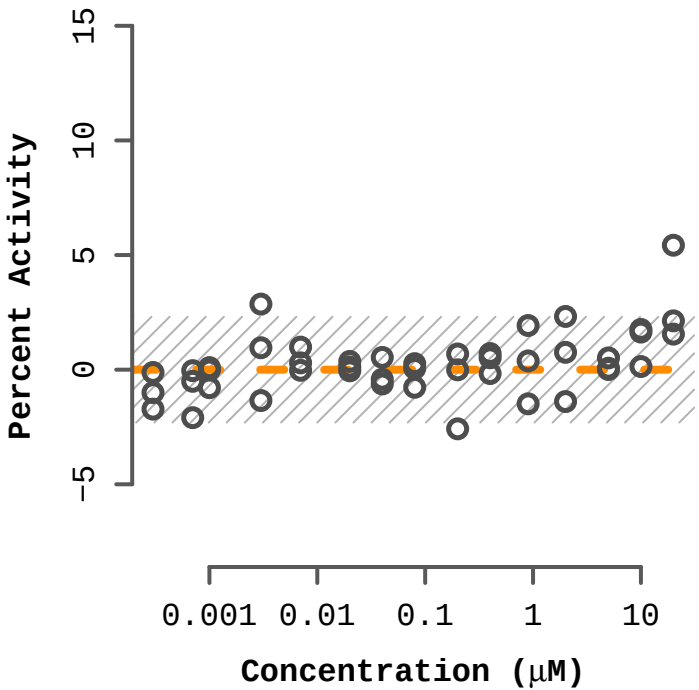
NAME: 3-Thiatetradecanoic acid
CHID: 47545 **CASRN:** 116296-31-2
SPID(S): Tox21_302618
M4ID: 12476515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.9 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

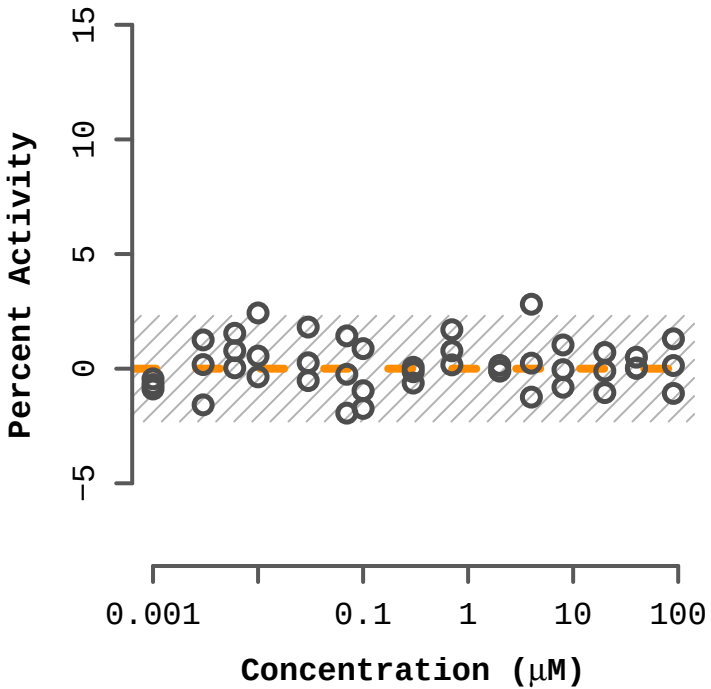
NAME: 1,3,5-Undecatriene
CHID: 47546 **CASRN:** 16356-11-9
SPID(S): Tox21_303704
M4ID: 12475484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 3.04 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

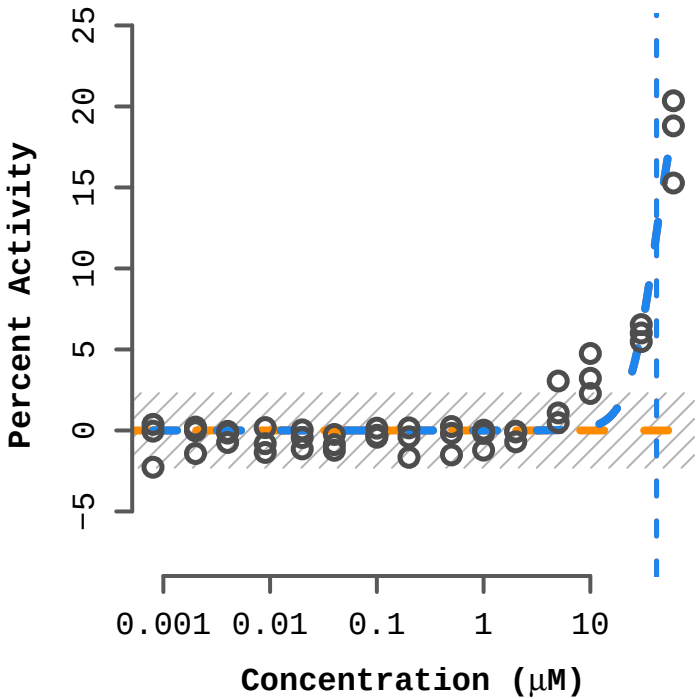
NAME: Hydroxycitronellal dimethyl acetal
CHID: 47547 **CASRN:** 141-92-4
SPID(S): Tox21_302540
M4ID: 12476593

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.883 **MAX_MED:** 0.787 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1'−Oxybis(2,3,4,5−tetrabromobenzene)
CHID: 47548 CASRN: 85446−17−9
SPID(S): Tox21_302453
M4ID: 12476680

HILL MODEL (in red):

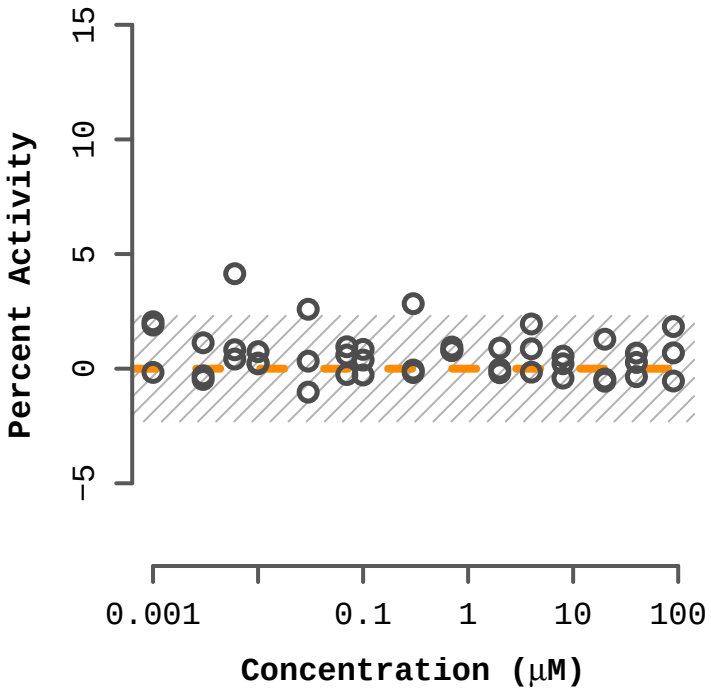
	tp	ga	gw
val:	24.4	1.62	3.31
sd:	5.3	0.0779	1.03

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24.4	1.62	3.31	2.6	10.9
sd:	5.3	0.0779	1.03	1390	18400

	CNST	HILL	GNLS
AIC:	232.4	153.43	157.43
PROB:	0	0.88	0.12
RMSE:	5.12	1.35	1.35

MAX_MEAN: 18.1 MAX_MED: 18.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

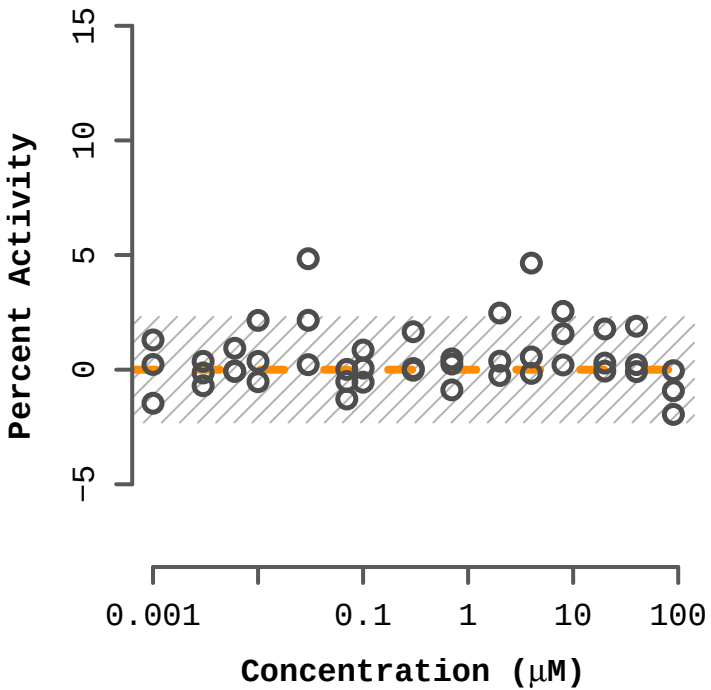
NAME: Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate
CHID: 47549 **CASRN:** 6290-17-1
SPID(S): Tox21_302457
M4ID: 12476676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

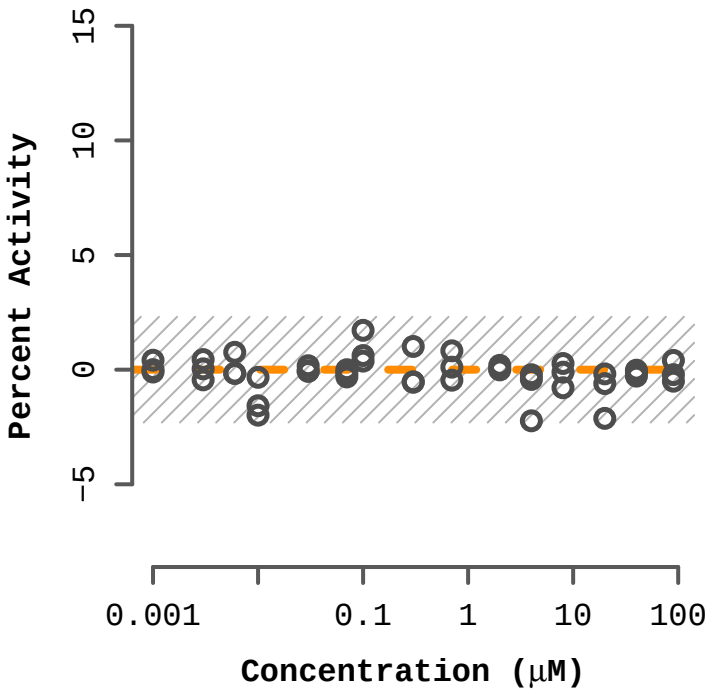
NAME: epsilon-Decalactone
CHID: 47551 **CASRN:** 5579-78-2
SPID(S): Tox21_302462
M4ID: 12476671

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.41 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

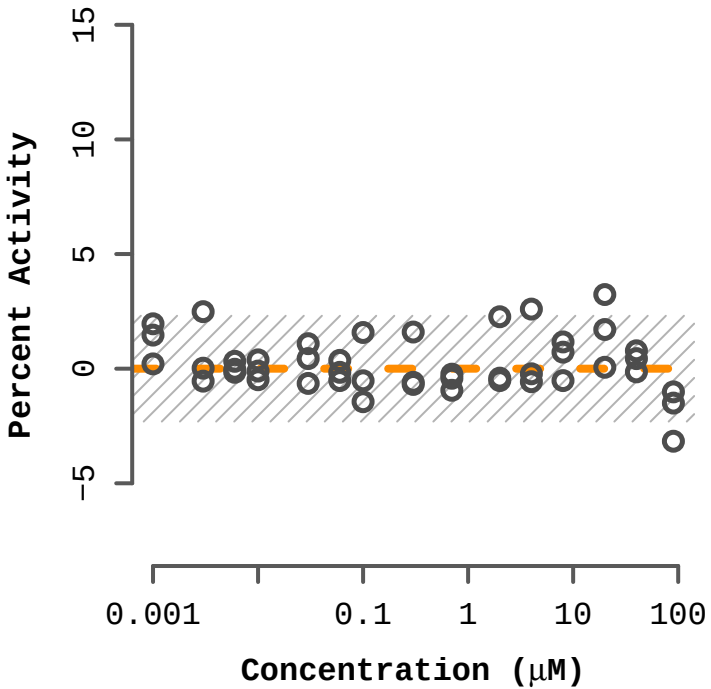
NAME: Hexyl hexanoate
CHID: 47552 **CASRN:** 6378-65-0
SPID(S): Tox21_302574
M4ID: 12476559

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	93.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.903 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

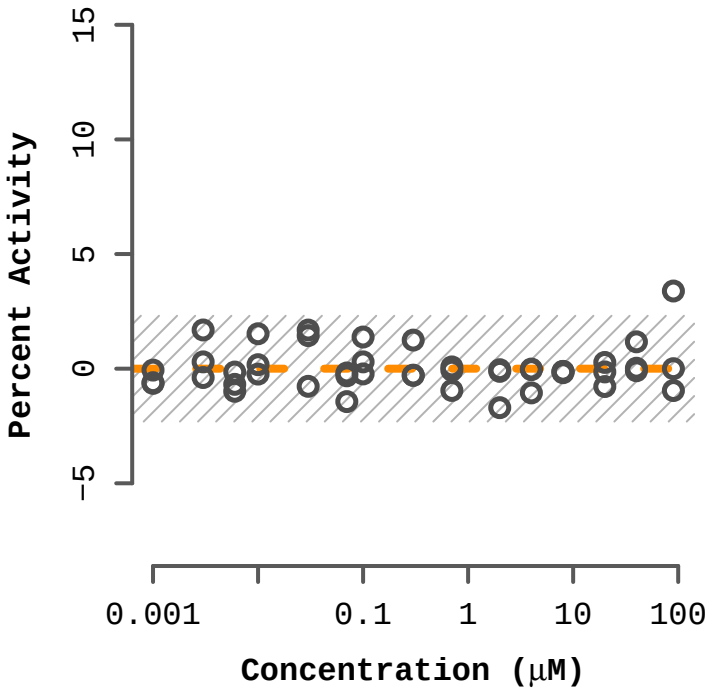
NAME: Perfluoroundecanoic acid
CHID: 47553 **CASRN:** 2058-94-8
SPID(S): Tox21_300606
M4ID: 12478527

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

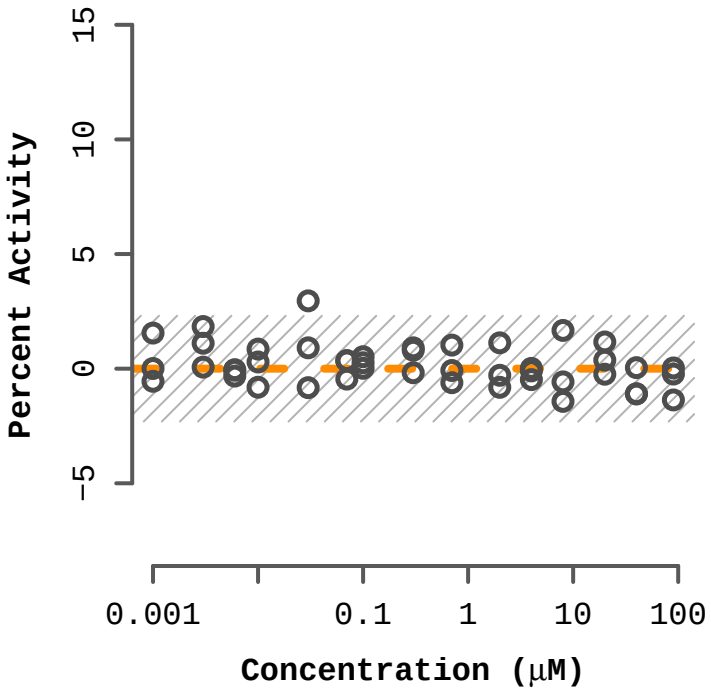
NAME: (3Z)-Hex-3-en-1-yl benzoate
CHID: 47554 **CASRN:** 25152-85-6
SPID(S): Tox21_302663
M4ID: 12476470

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.813 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

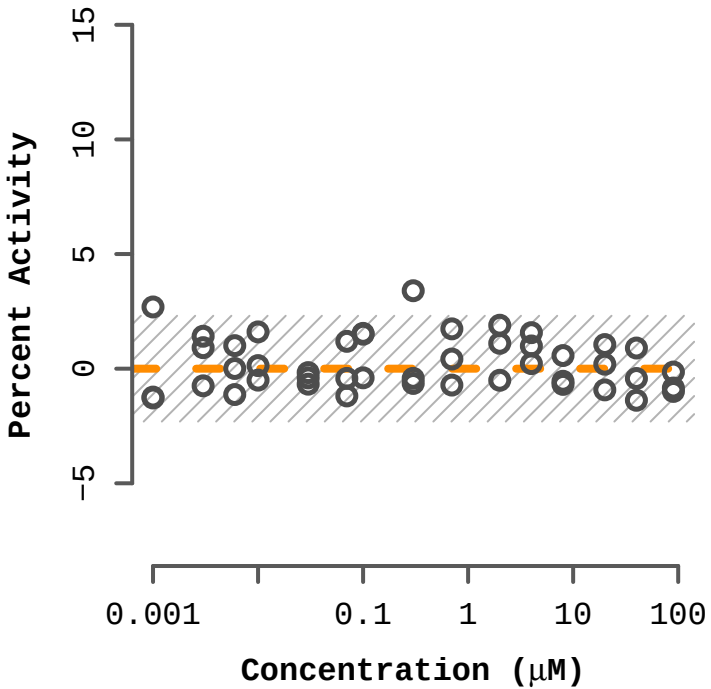
NAME: 3,7-Dimethyloct-6-en-1-yl 2-methylbut-2-enoate
CHID: 47556 **CASRN:** 255714-11-5
SPID(S): Tox21_302553
M4ID: 12476580

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

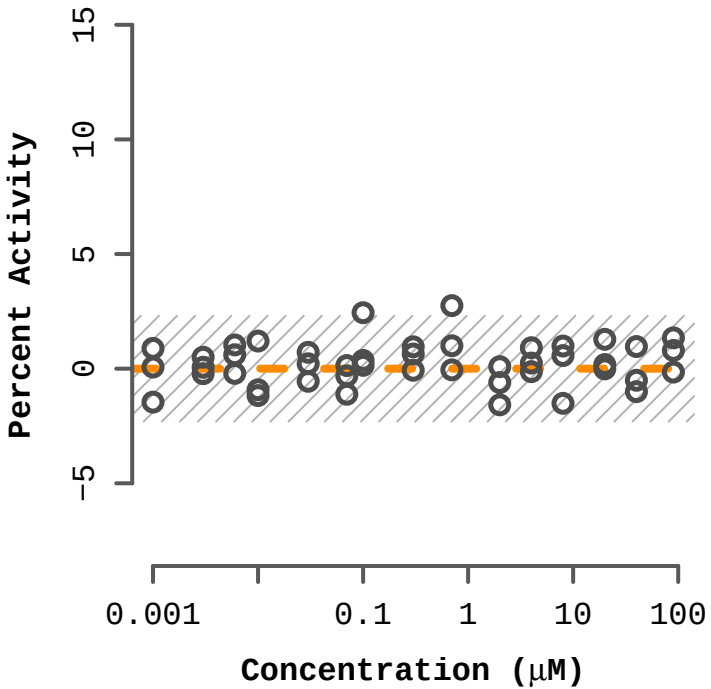
NAME: Tridecafluorohexylethyl methacrylate
CHID: 47558 **CASRN:** 2144-53-8
SPID(S): Tox21_300607
M4ID: 12478526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.929 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

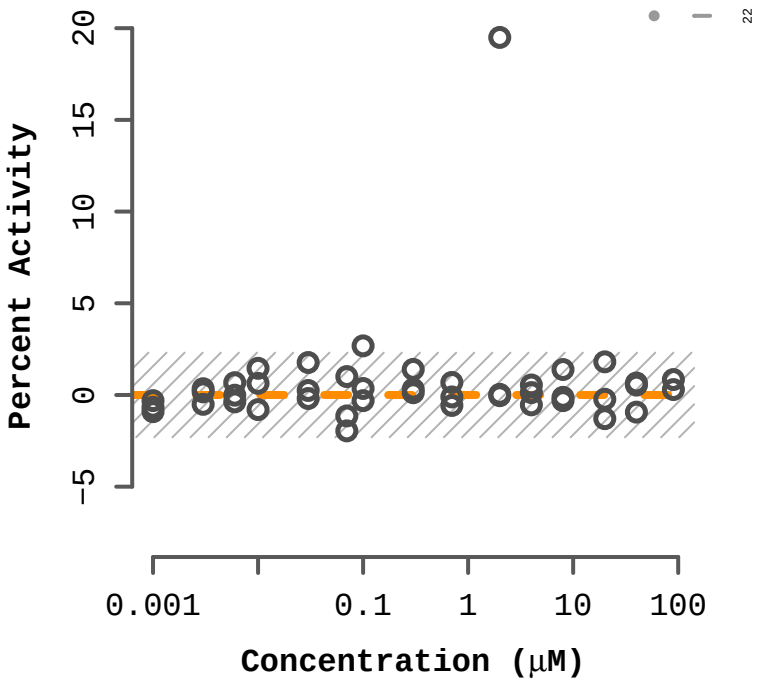
NAME: Hexyl butyrate
CHID: 47559 **CASRN:** 2639-63-6
SPID(S): Tox21_302445
M4ID: 12476688

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

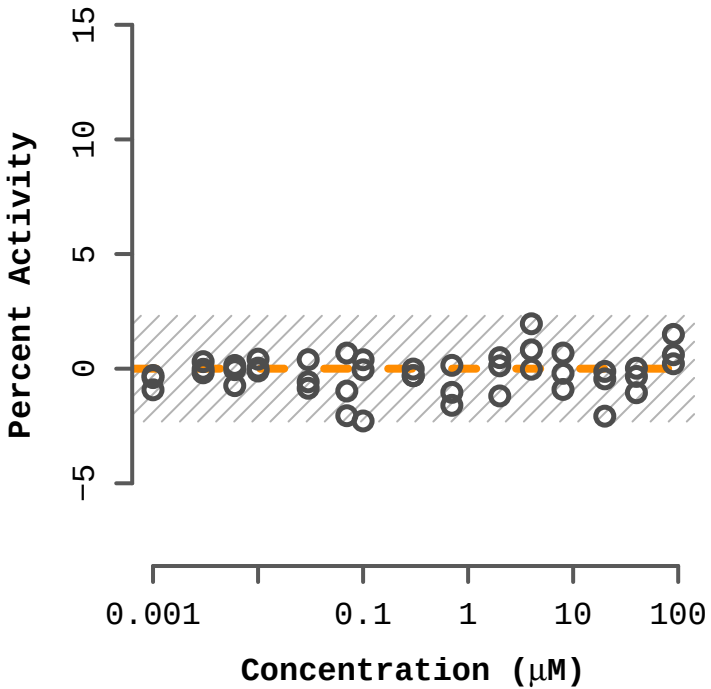
NAME: (3Z)-Hex-3-en-1-yl hexanoate
CHID: 47560 **CASRN:** 31501-11-8
SPID(S): Tox21_302626
M4ID: 12476507 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	169.6	NA	NA
PROB:	1	NA	NA
RMSE:	4.46	NA	NA

MAX_MEAN: 7.69 **MAX_MED:** 0.843 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

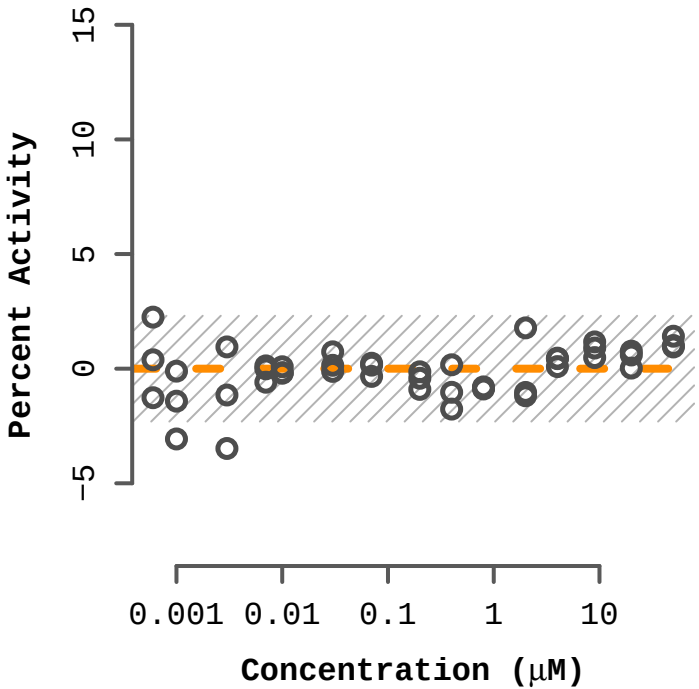
NAME: (3Z)-Hex-3-en-1-yl (2E)-2-methylbut-2-enoate
CHID: 47562 **CASRN:** 67883-79-8
SPID(S): Tox21_302573
M4ID: 12476560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.92 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

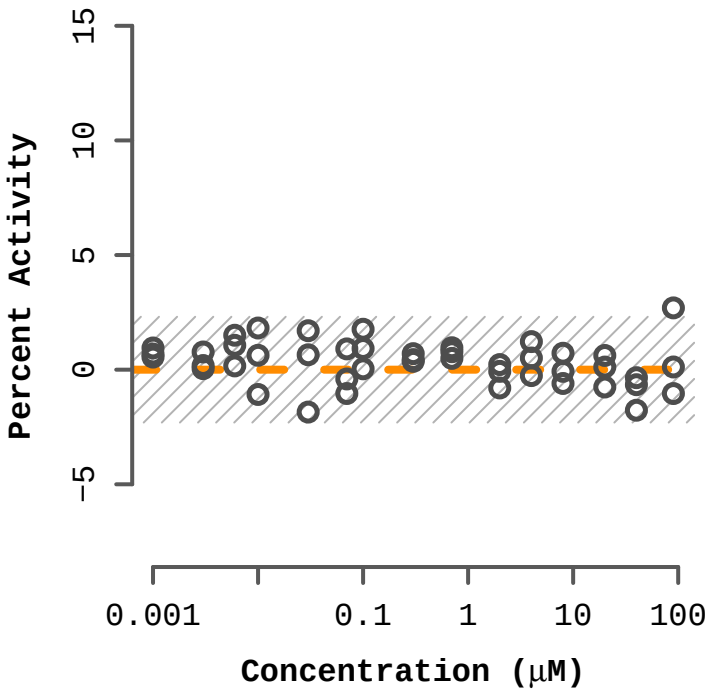
NAME: 1H,1H,2H,2H−Perfluorooctyl iodide
CHID: 47565 **CASRN:** 2043−57−4
SPID(S): Tox21_300609
M4ID: 12478524

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

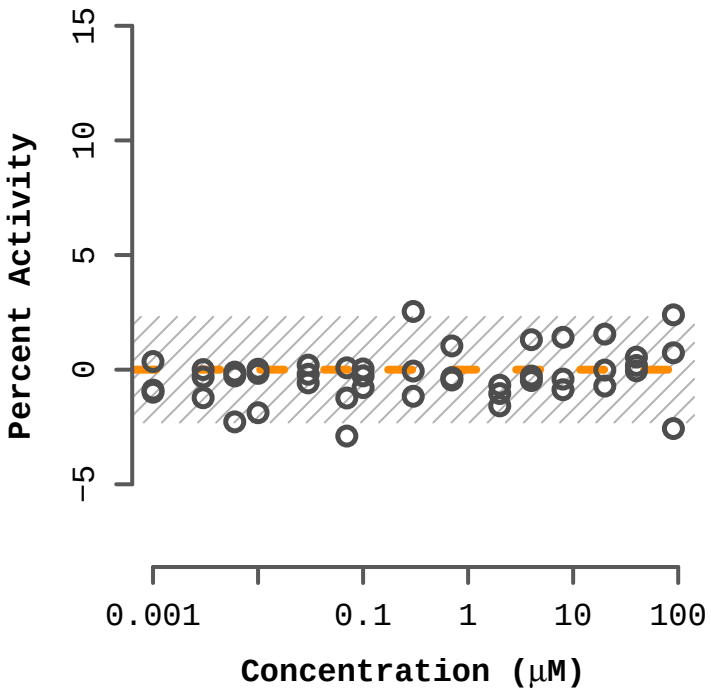
NAME: 2-Phenylethyl 2-methylbutanoate
CHID: 47567 **CASRN:** 24817-51-4
SPID(S): Tox21_302498
M4ID: 12476635

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.911 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

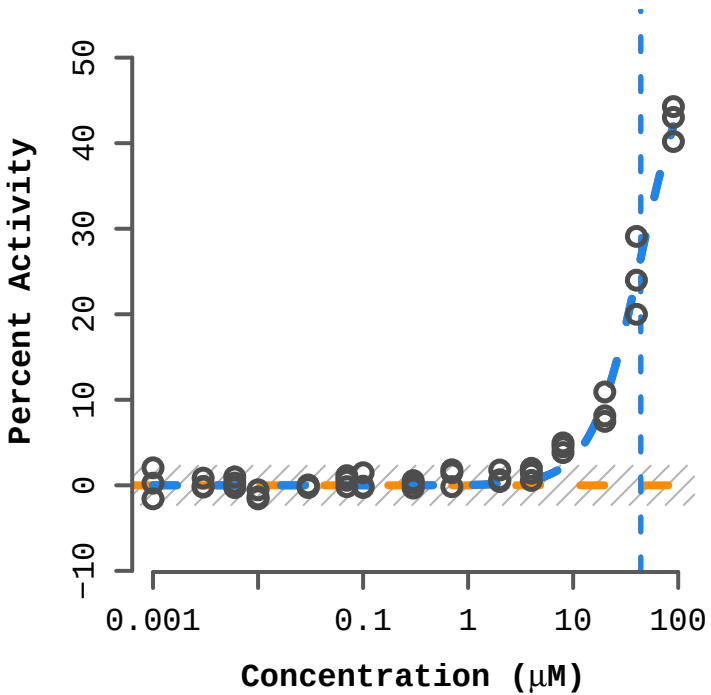
NAME: Metamitron
CHID: 47568 **CASRN:** 41394-05-2
SPID(S): Tox21_302665
M4ID: 12476468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.44 **MAX_MED:** 0.739 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxyfluorene
CHID: 47569 **CASRN:** 2443-58-5
SPID(S): Tox21_302595
M4ID: 12476538

HILL MODEL (in red):

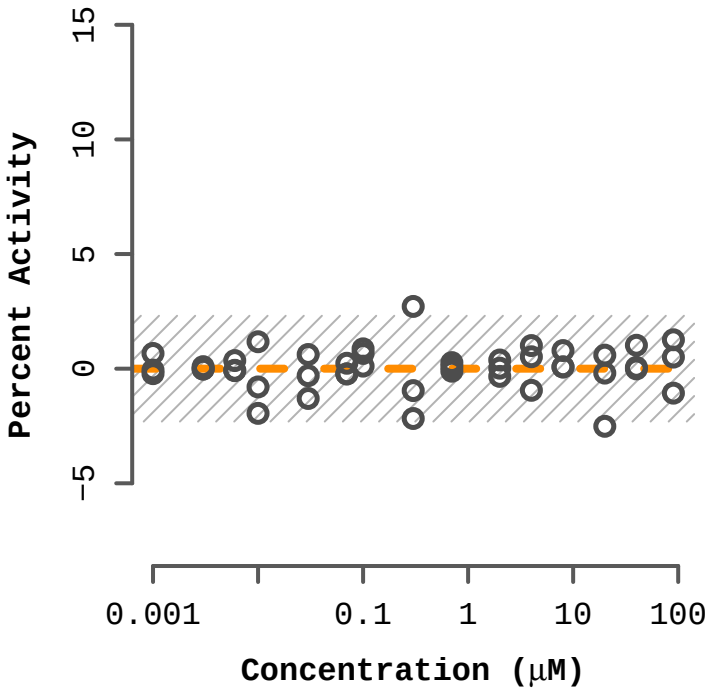
	tp	ga	gw
val:	53.1	1.64	1.85
sd:	4.9	0.0532	0.301

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	53.1	1.64	1.85	3.32	9.94
sd:	4.9	0.0532	0.301	102000	775000

	CNST	HILL	GNLS
AIC:	318.49	171.46	175.46
PROB:	0	0.88	0.12
RMSE:	12.98	1.54	1.54

MAX_MEAN: 42.5 **MAX_MED:** 43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

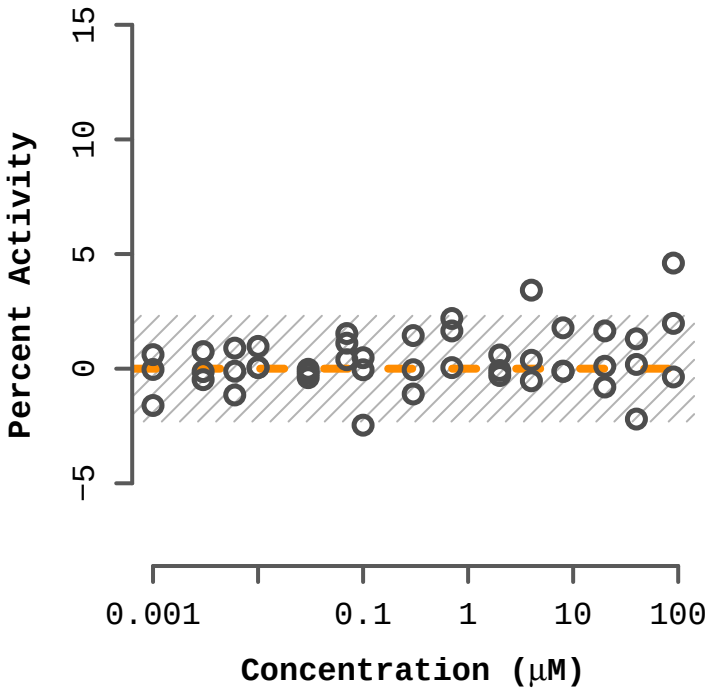
NAME: (1R,5R)-3,3,5-trimethylcyclohexanol
CHID: 47570 **CASRN:** 933-48-2
SPID(S): Tox21_302583
M4ID: 12476550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.548 **MAX_MED:** 0.666 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

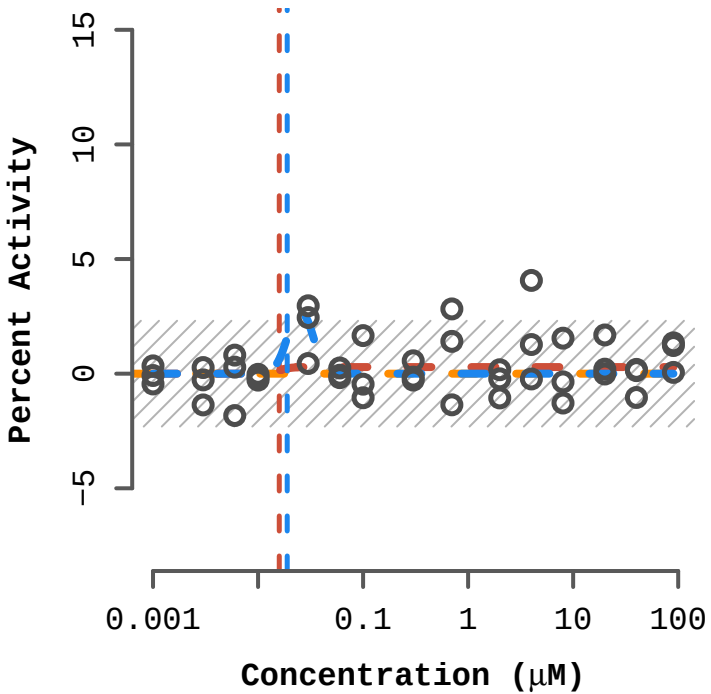
NAME: 3,7-Dimethylocta-1,6-dien-3-yl propanoate
CHID: 47574 **CASRN:** 144-39-8
SPID(S): Tox21_302590
M4ID: 12476543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cotinine
CHID: 47576 CASRN: 486-56-6
SPID(S): Tox21_300615
M4ID: 12478518

HILL MODEL (in red):

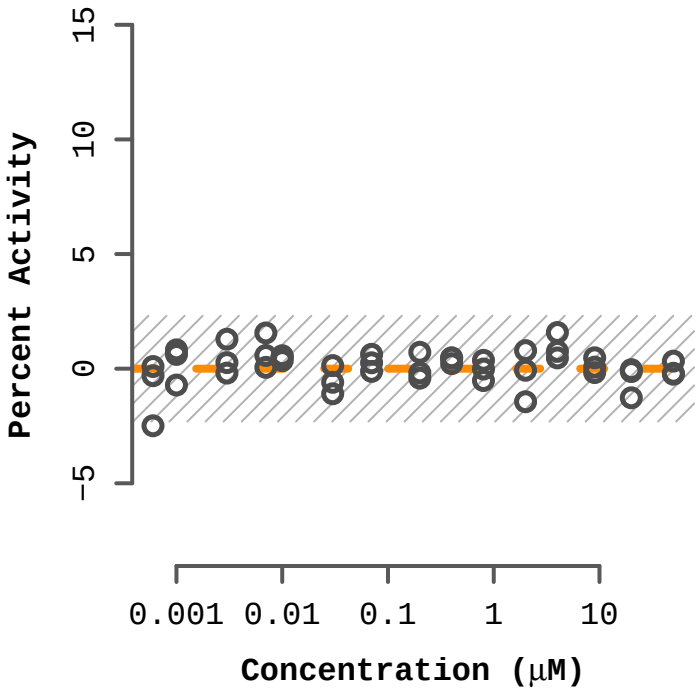
	tp	ga	gw
val:	0.289	−1.8	8
sd:	0.194	0.539	17.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.18	−1.72	8	−1.47	8.47
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	143.7	147.36	145.35
PROB:	0.63	0.1	0.27
RMSE:	1.24	1.17	1.13

MAX_MEAN: 1.95 MAX_MED: 2.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

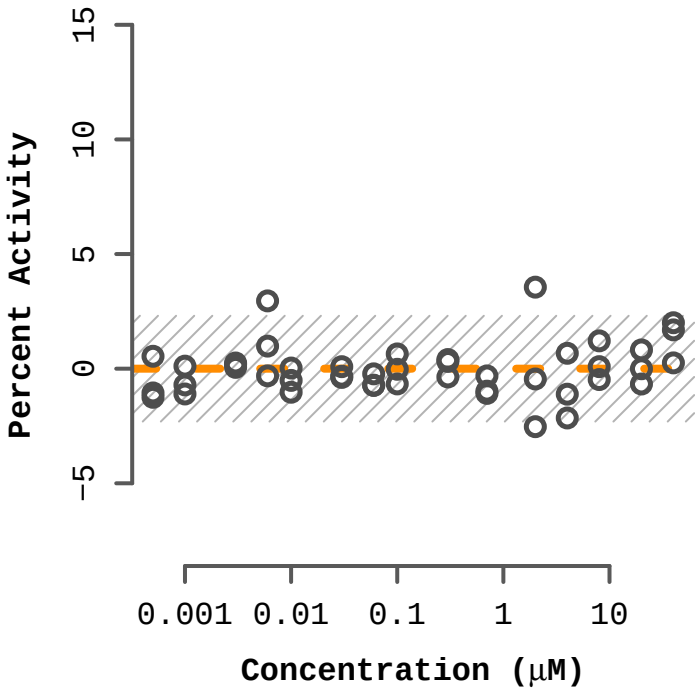
NAME: Cotinine
CHID: 47576 **CASRN:** 486-56-6
SPID(S): Tox21_111219_1
M4ID: 12483836

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.935 **MAX_MED:** 0.755 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

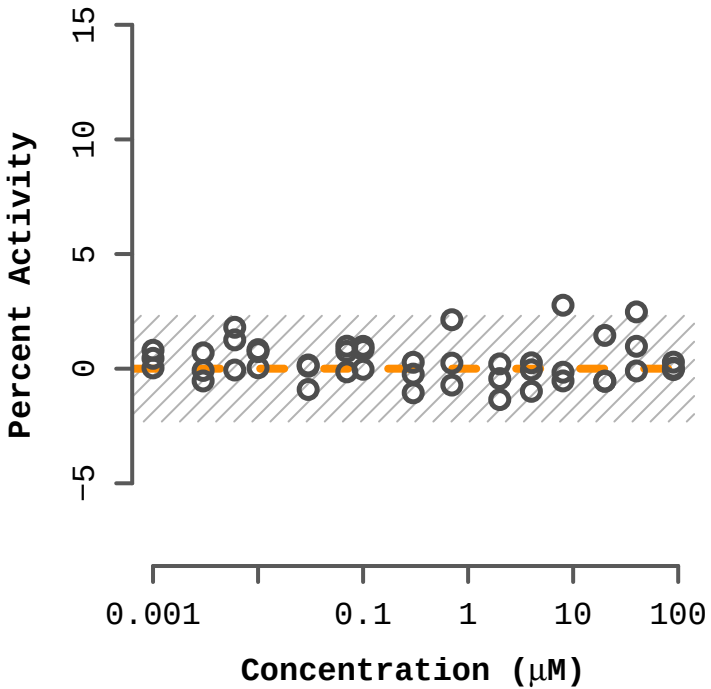
NAME: 1,1,1,2,2,3,3,4,4−Nonafluoro−6−iodohexane
CHID: 47578 **CASRN:** 2043−55−2
SPID(S): Tox21_302584
M4ID: 12476549

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

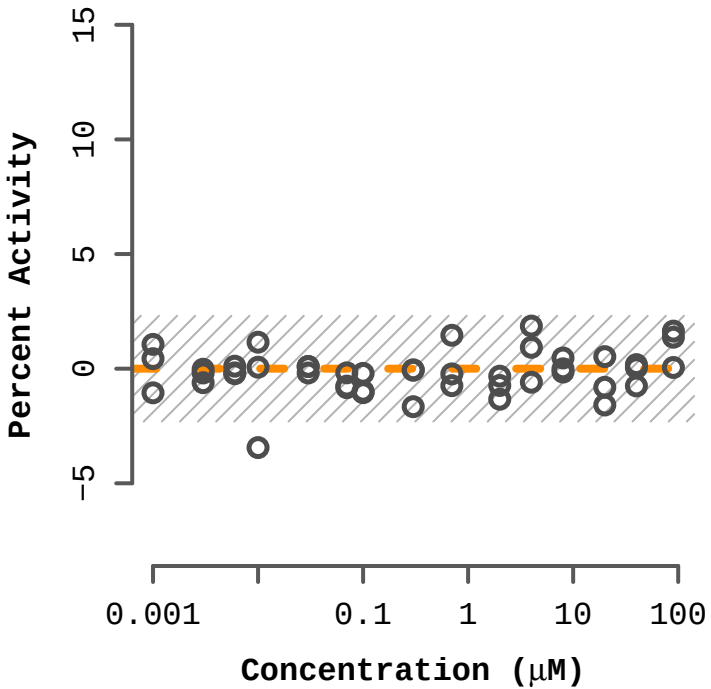
NAME: (3Z)-Hex-3-en-1-yl propanoate
CHID: 47579 **CASRN:** 33467-74-2
SPID(S): Tox21_303627
M4ID: 12475518

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

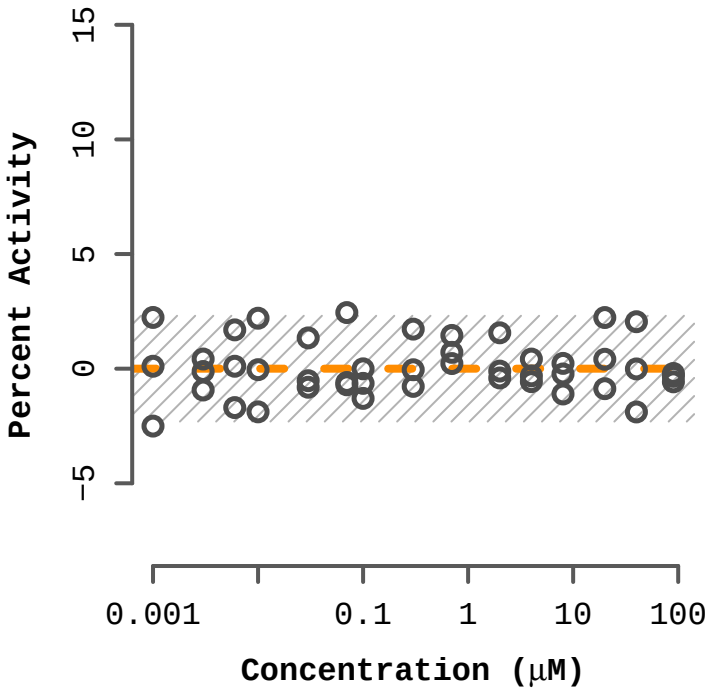
NAME: Pentyl hexanoate
CHID: 47581 **CASRN:** 540-07-8
SPID(S): Tox21_302698
M4ID: 12476435

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

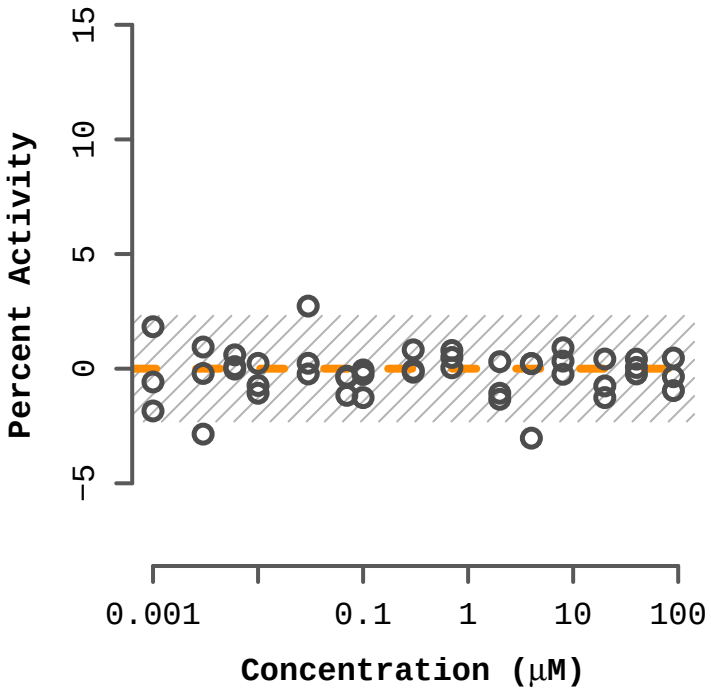
NAME: Hexyl propanoate
CHID: 47582 **CASRN:** 2445-76-3
SPID(S): Tox21_302443
M4ID: 12476690

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.797 **MAX_MED:** 0.715 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

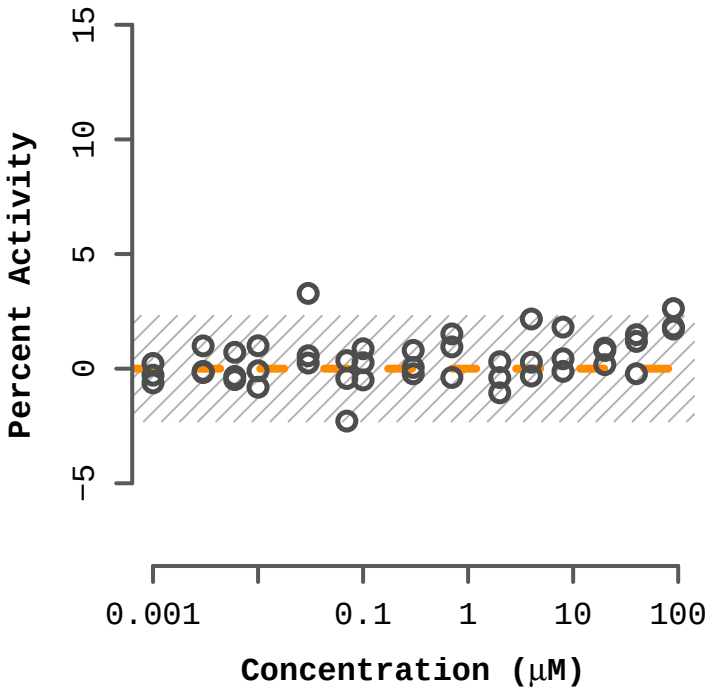
NAME: 2-Phenylethyl hexanoate
CHID: 47584 CASRN: 6290-37-5
SPID(S): Tox21_302527
M4ID: 12476606

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.913 MAX_MED: 0.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

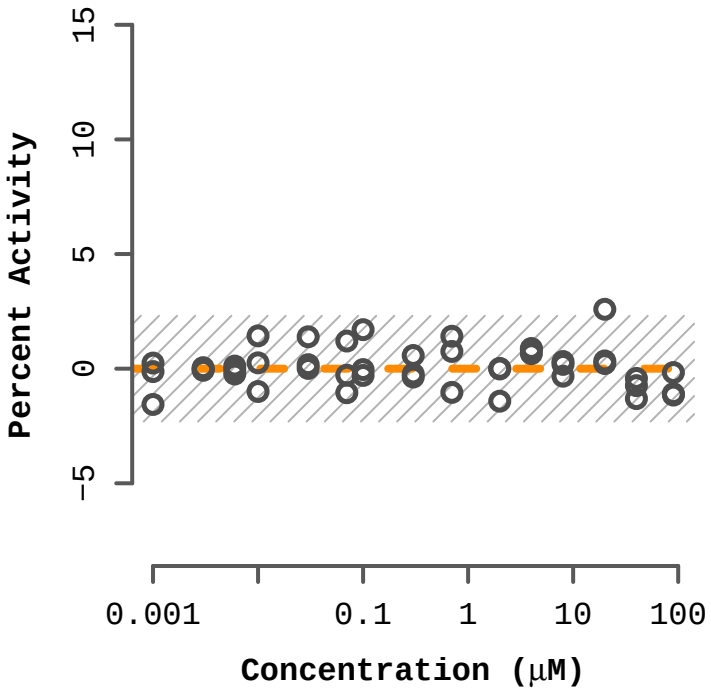
NAME: (3Z)-Hex-3-en-1-yl 2-methylpropanoate
CHID: 47585 **CASRN:** 41519-23-7
SPID(S): Tox21_302630
M4ID: 12476503

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

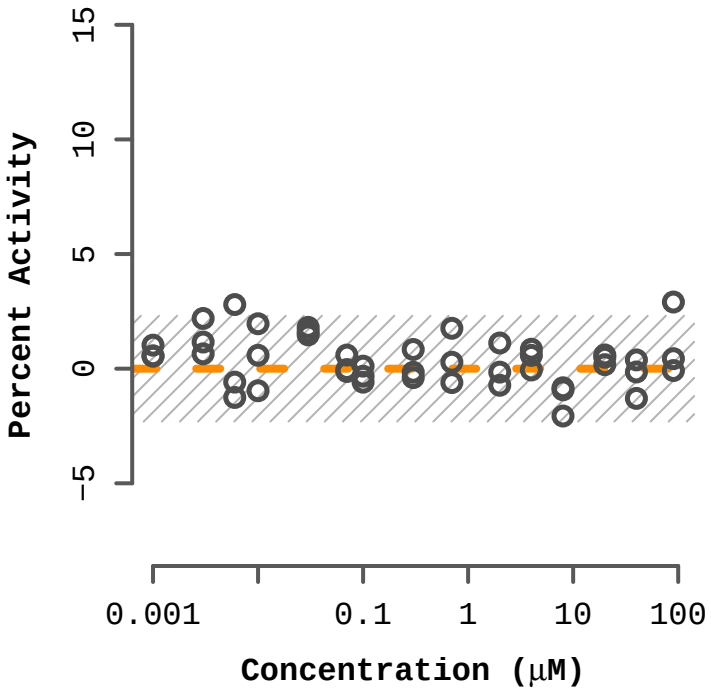
NAME: (6Z)-Non-6-en-1-ol
CHID: 47587 **CASRN:** 35854-86-5
SPID(S): Tox21_303624
M4ID: 12475521

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

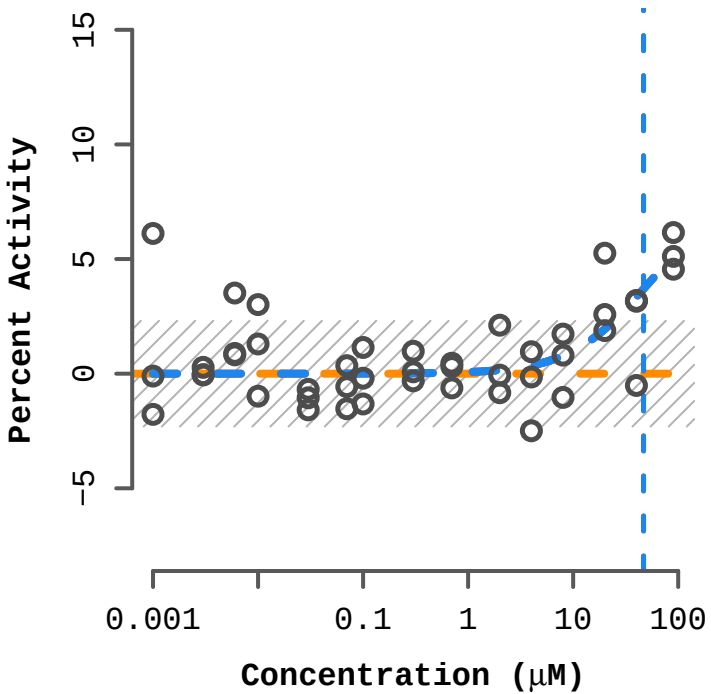
NAME: 6-Pentyl-2H-pyran-2-one
CHID: 47589 **CASRN:** 27593-23-3
SPID(S): Tox21_302570
M4ID: 12476563

HILL MODEL: Not applicable.

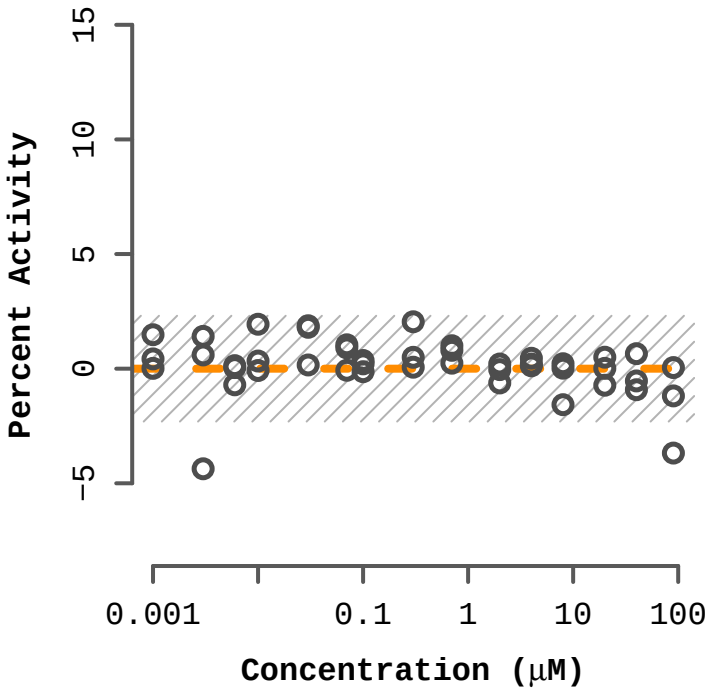
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.6 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Phenylethyl benzoate
CHID:    47590   CASRN: 94-47-3
SPID(S): Tox21_302622
M4ID:    12476511

HILL MODEL (in red):
      tp       ga       gw
val:  7.39     1.67     1.21
sd:   4.61     0.522    0.599

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.39     1.67     1.21     3.19     6.29
sd:   4.61     0.522    0.599    1140     5820

      CNST        HILL        GNLS
AIC:  200.15      171.77      175.77
PROB: 0           0.88        0.12
RMSE: 2.3         1.66        1.66

MAX_MEAN: 5.28      MAX_MED: 5.12      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

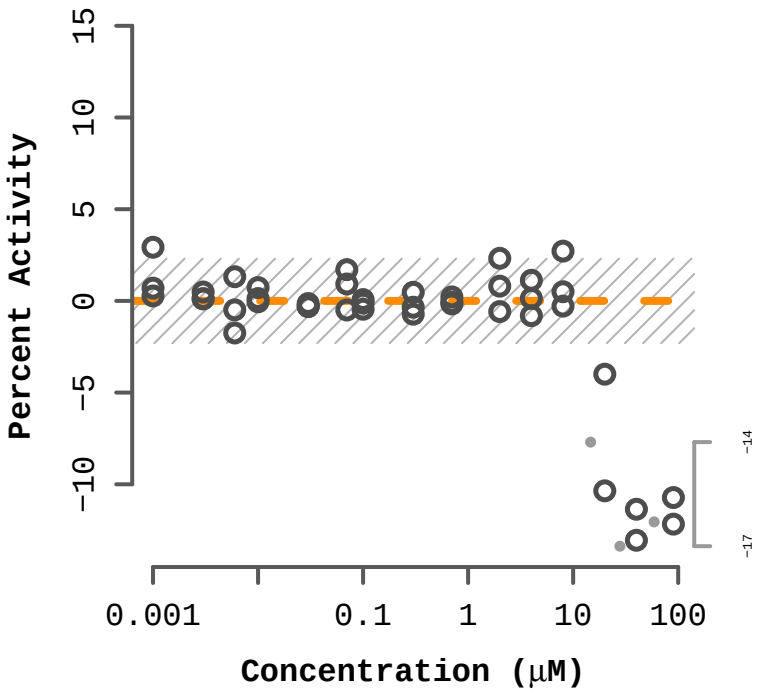
NAME: Allyl Ionone
CHID: 47591 **CASRN:** 79-78-7
SPID(S): Tox21_302463
M4ID: 12476670

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

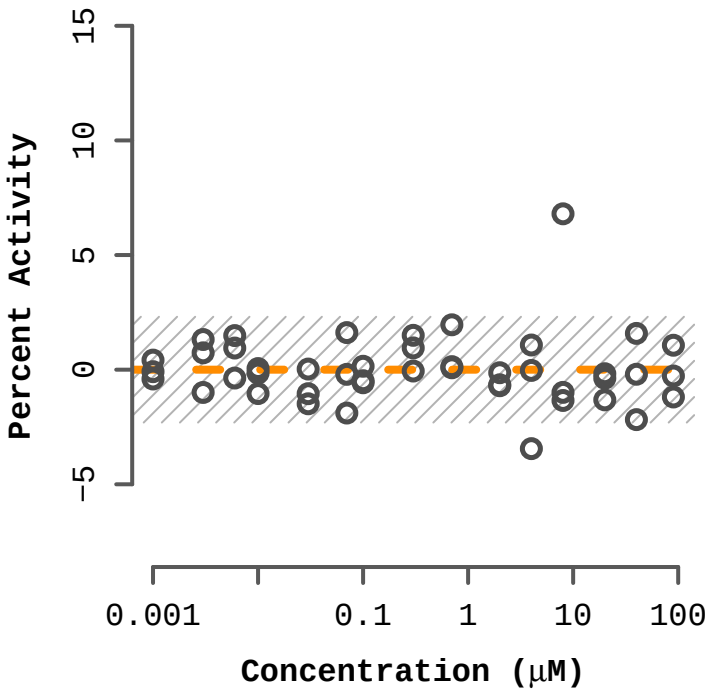
NAME: 9-Phenanthrol
CHID: 47592 **CASRN:** 484-17-3
SPID(S): Tox21_300618
M4ID: 12478515 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	263.57	NA	NA
PROB:	1	NA	NA
RMSE:	5.73	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.924 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

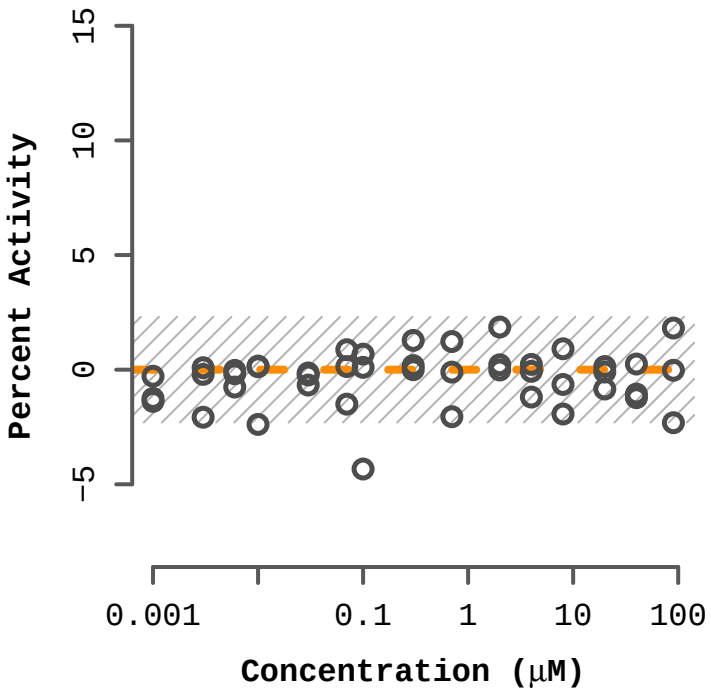
NAME: alpha-Phellandrene
CHID: 47593 **CASRN:** 99-83-2
SPID(S): Tox21_302550
M4ID: 12476583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 0.951 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

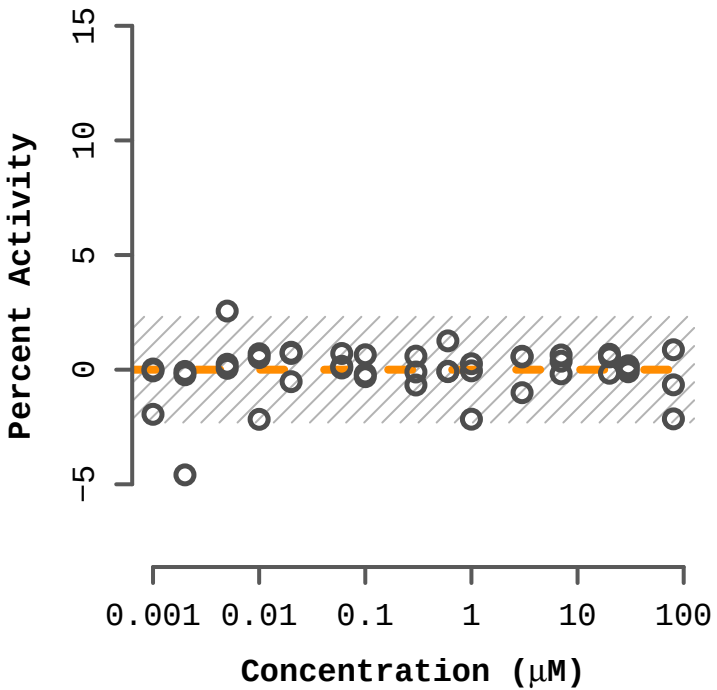
NAME: Sodium 4-octylbenzenesulfonate
CHID: 47594 **CASRN:** 6149-03-7
SPID(S): Tox21_303628
M4ID: 12475517

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.688 **MAX_MED:** 0.215 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

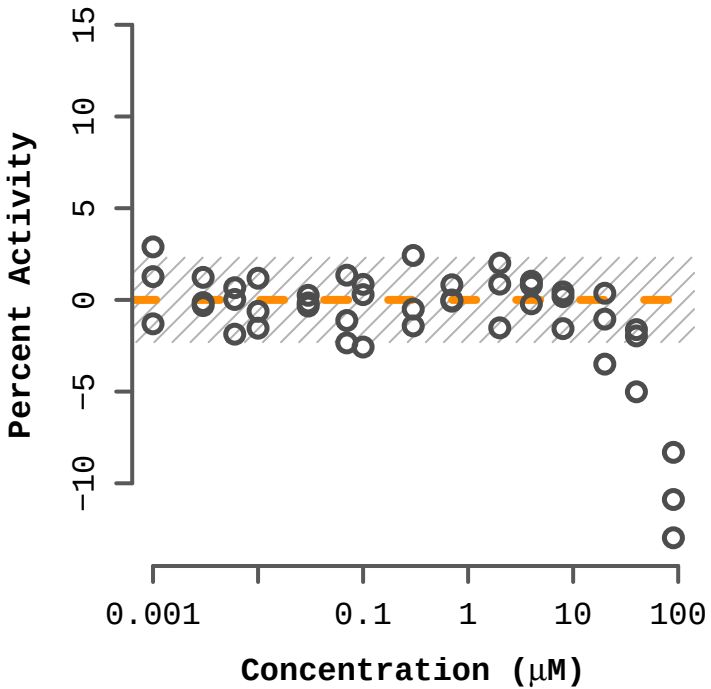
NAME: Pluronic F−127
CHID: 47597 **CASRN:** 9003−11−6
SPID(S): Tox21_302499
M4ID: 12476634

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.952 **MAX_MED:** 0.709 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

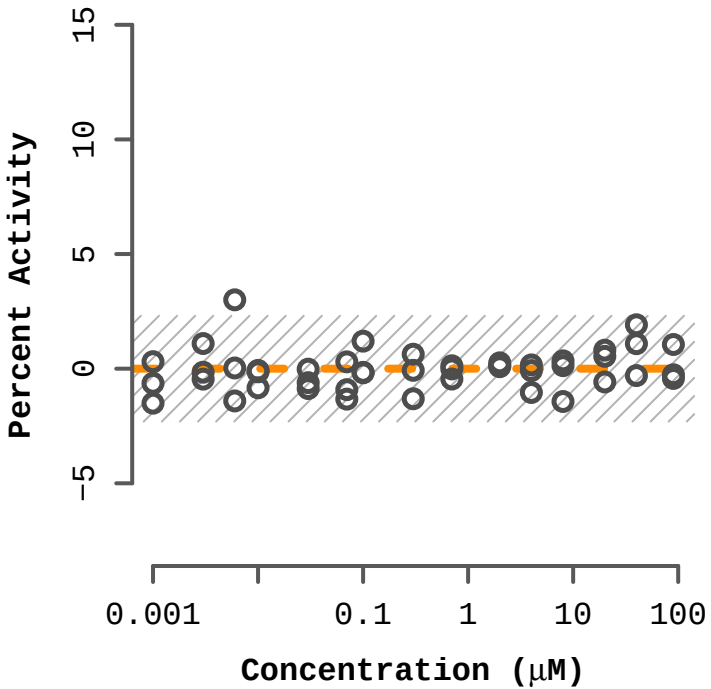
NAME: 4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol]
CHID: 47598 **CASRN:** 41481-66-7
SPID(S): Tox21_300629
M4ID: 12478504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.05	NA	NA
PROB:	1	NA	NA
RMSE:	3.19	NA	NA

MAX_MEAN: 0.954 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

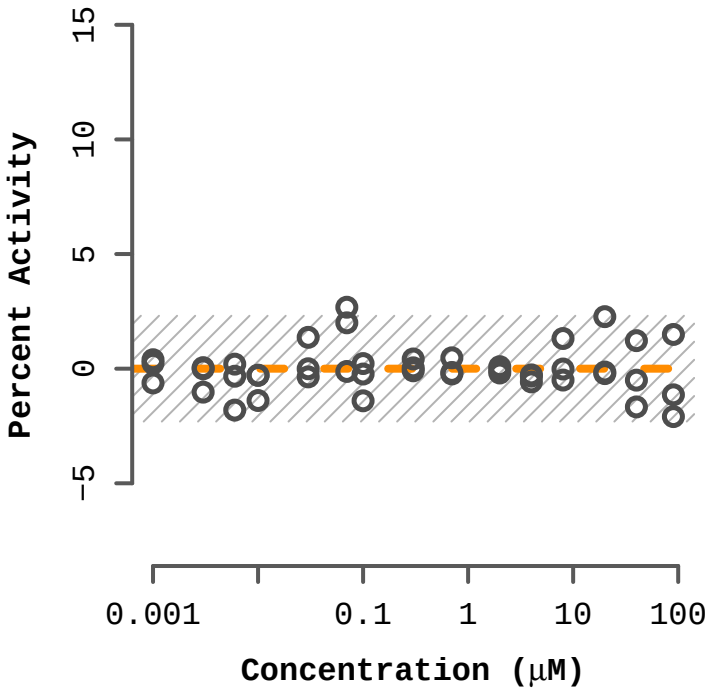
NAME: Hexyl 2-methylbutanoate
CHID: 47599 **CASRN:** 10032-15-2
SPID(S): Tox21_302599
M4ID: 12476534

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.903 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

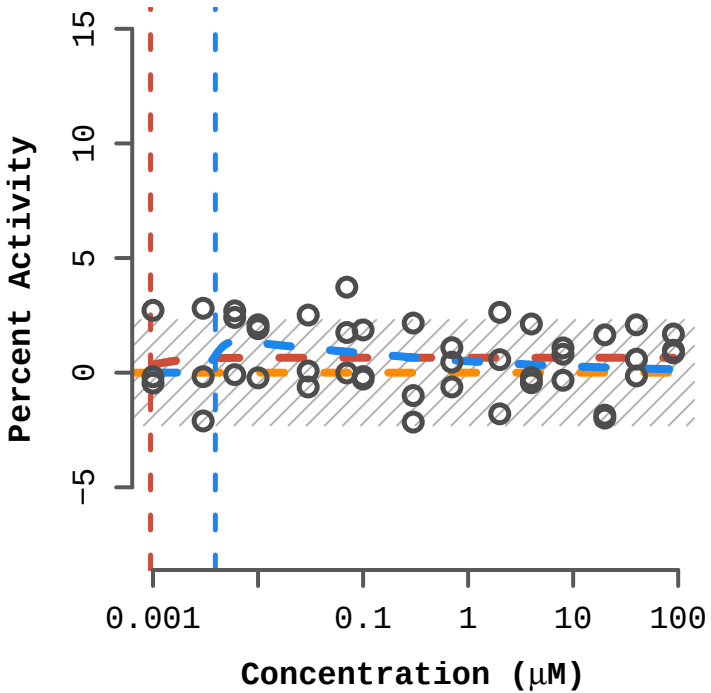
NAME: 2-Methyl-1-phenylpropan-2-ol
CHID: 47601 **CASRN:** 100-86-7
SPID(S): Tox21_302533
M4ID: 12476600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzyl 2-methylpropanoate
CHID: 47602 **CASRN:** 103-28-6
SPID(S): Tox21_303852
M4ID: 12475336

HILL MODEL (in red):

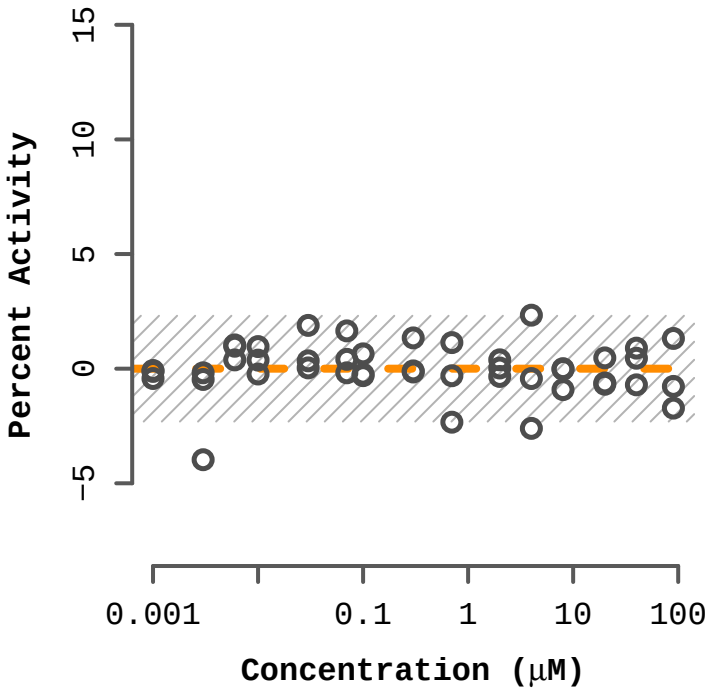
	tp	ga	gw
val:	0.652	−3.02	2.47
sd:	0.249	1.09	7.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.74	−2.41	7.97	−2.16	0.302
sd:	6.51	0.214	11	5.03	0.444

	CNST	HILL	GNLS
AIC:	177.26	176.4	179.1
PROB:	0.34	0.52	0.14
RMSE:	1.61	1.49	1.46

MAX_MEAN: 1.82 **MAX_MED:** 2.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

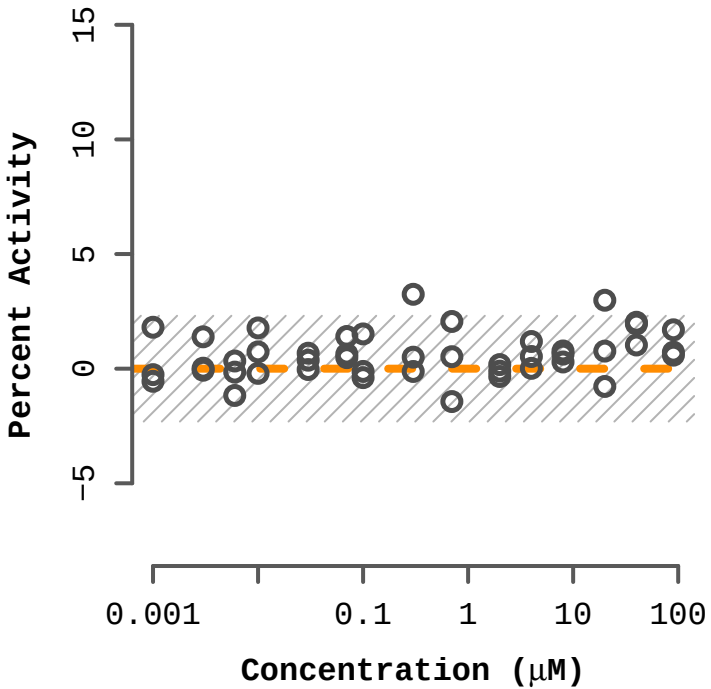
NAME: Benzyl 3-methylbutanoate
CHID: 47603 **CASRN:** 103-38-8
SPID(S): Tox21_302504
M4ID: 12476629

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

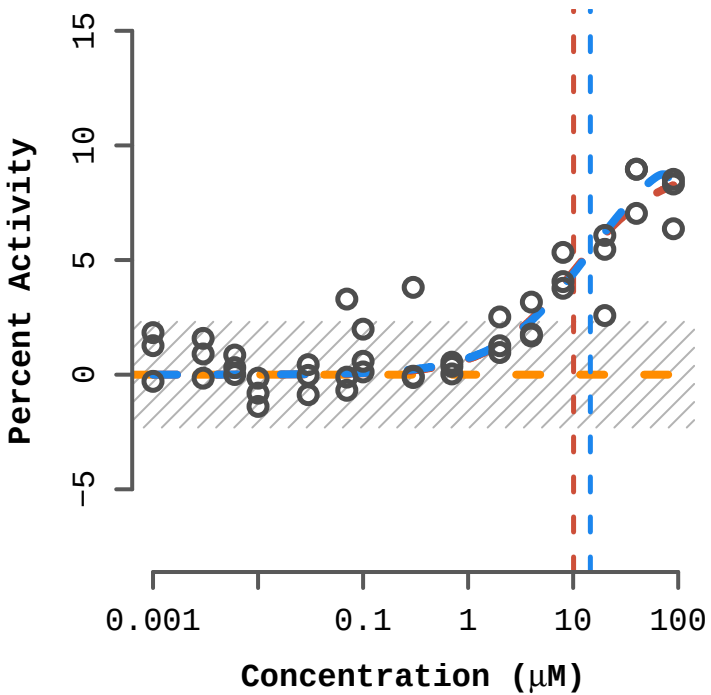
NAME: 2-Phenylethyl butanoate
CHID: 47604 **CASRN:** 103-52-6
SPID(S): Tox21_302607
M4ID: 12476526

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Phenylethyl 3-phenylprop-2-enoate
CHID: 47605 CASRN: 103-53-7
SPID(S): Tox21_302633
M4ID: 12476500

HILL MODEL (in red):

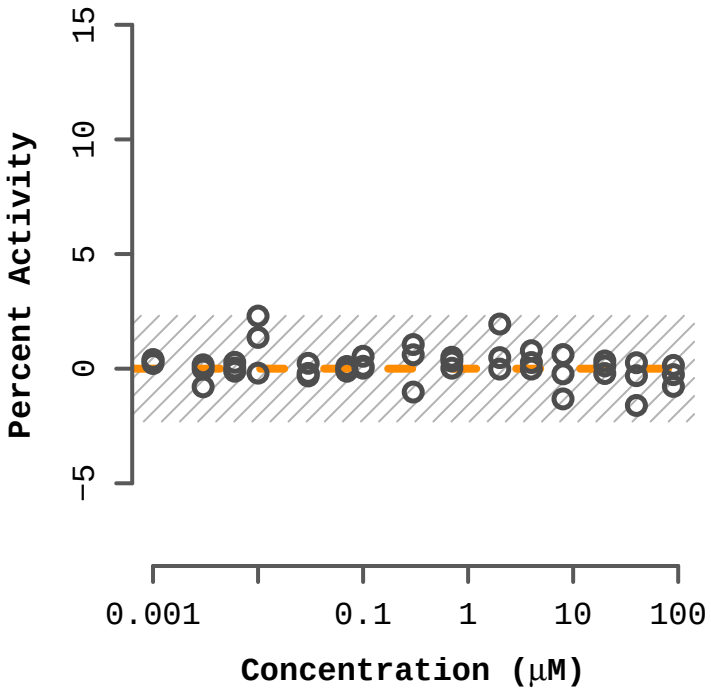
	tp	ga	gw
val:	9.03	1	1.08
sd:	1.02	0.137	0.235

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.8	1.16	0.982	2.04	9.59
sd:	3.02	0.285	0.233	0.0818	10.7

	CNST	HILL	GNLS
AIC:	241.06	147.98	150.48
PROB:	0	0.78	0.22
RMSE:	3.63	1.23	1.21

MAX_MEAN: 8.32 MAX_MED: 8.96 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

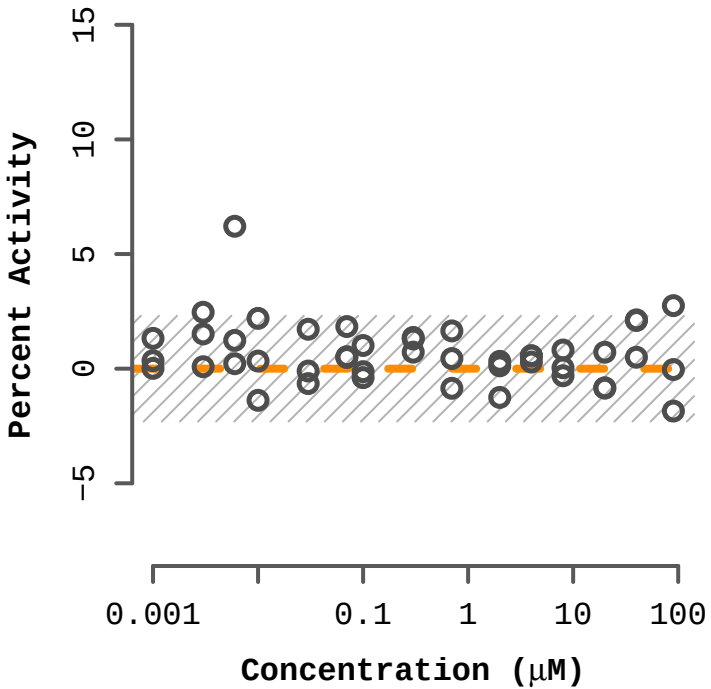
NAME: (2E)-3-Phenylprop-2-en-1-yl propanoate
CHID: 47606 CASRN: 78761-38-3
SPID(S): Tox21_302444
M4ID: 12476689

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	88.98	NA	NA
PROB:	1	NA	NA
RMSE:	0.7	NA	NA

MAX_MEAN: 1.16 MAX_MED: 1.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

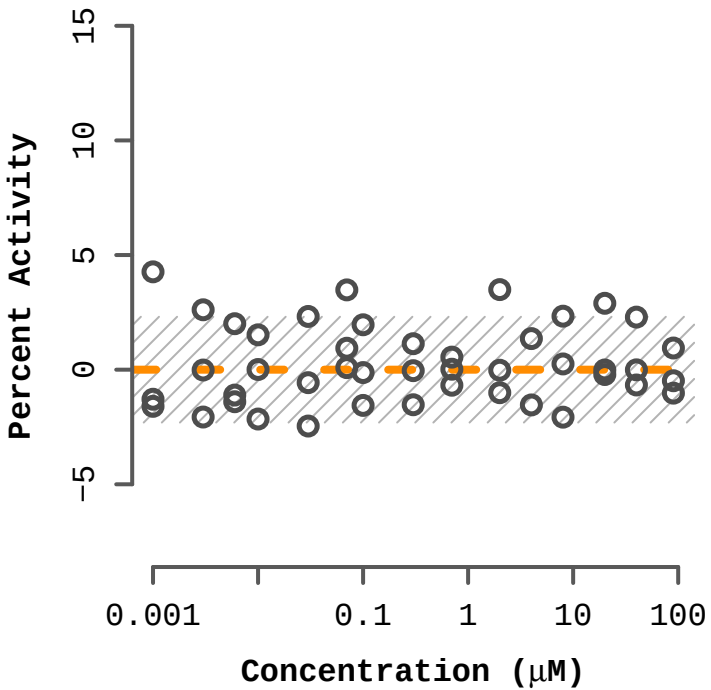
NAME: 3-Phenylprop-2-en-1-yl propanoate
CHID: 47607 **CASRN:** 103-56-0
SPID(S): Tox21_303749
M4ID: 12475439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.48	NA	NA

MAX_MEAN: 2.56 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

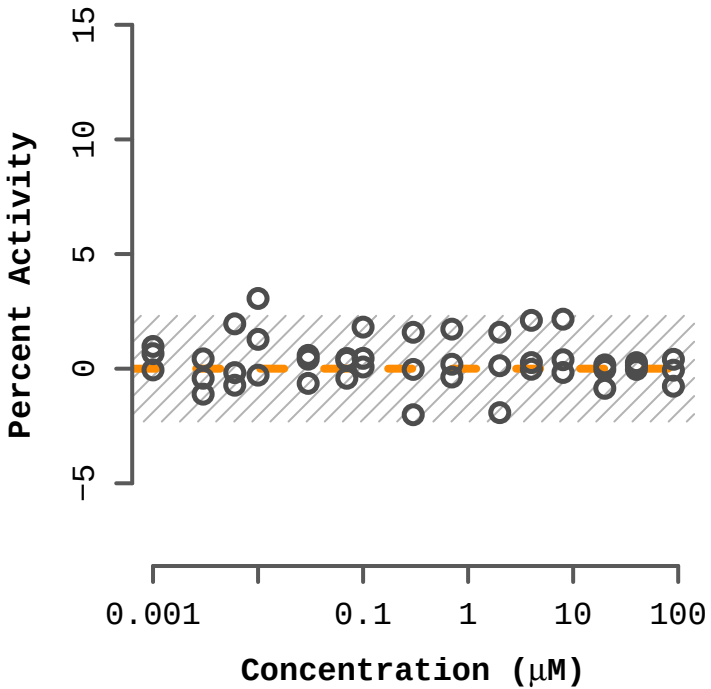
NAME: 3-Phenylprop-2-en-1-yl 2-methylpropanoate
CHID: 47608 **CASRN:** 103-59-3
SPID(S): Tox21_302702
M4ID: 12476431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.7	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 0.936 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

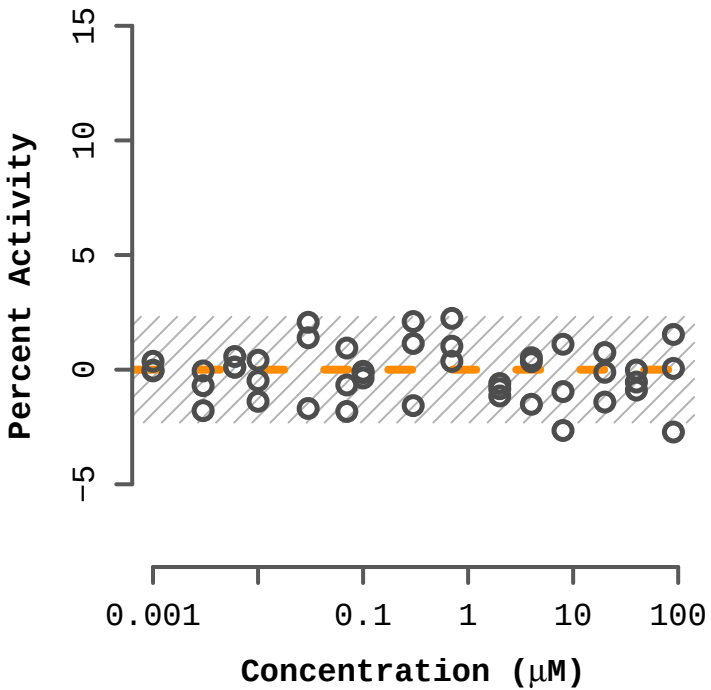
NAME: 4-Octanolide
CHID: 47609 **CASRN:** 104-50-7
SPID(S): Tox21_302569
M4ID: 12476564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

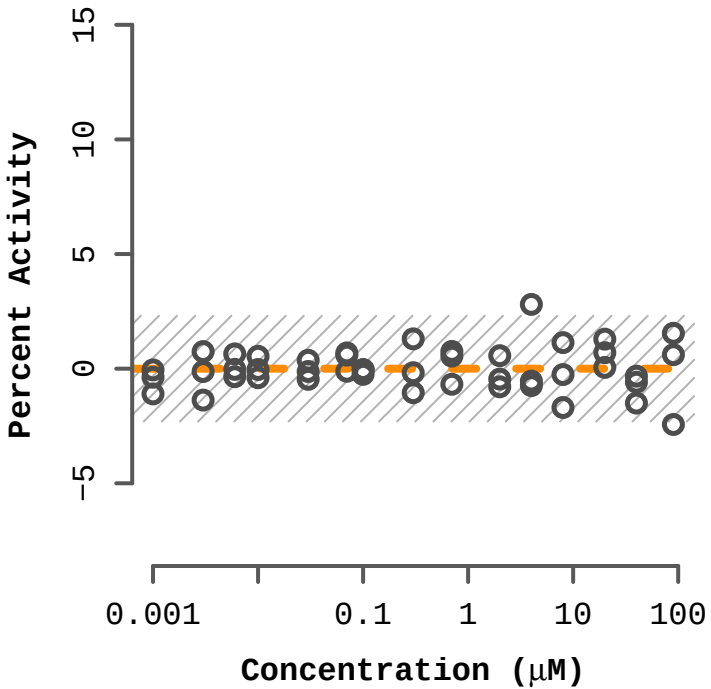
NAME: 3-Phenylpropanal
CHID: 47610 **CASRN:** 104-53-0
SPID(S): Tox21_302494
M4ID: 12476639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

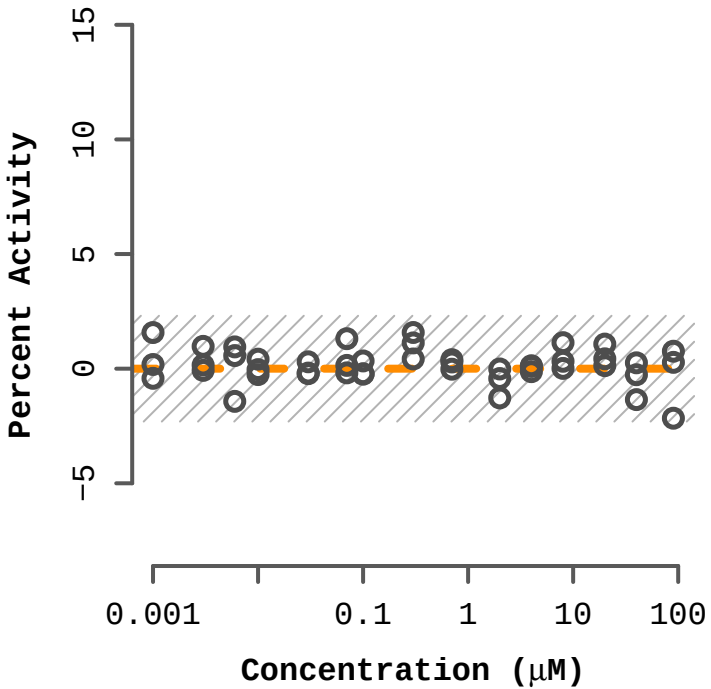
NAME: 1,4-Heptanolide
CHID: 47611 **CASRN:** 105-21-5
SPID(S): Tox21_302676
M4ID: 12476457

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.682 **MAX_MED:** 0.698 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

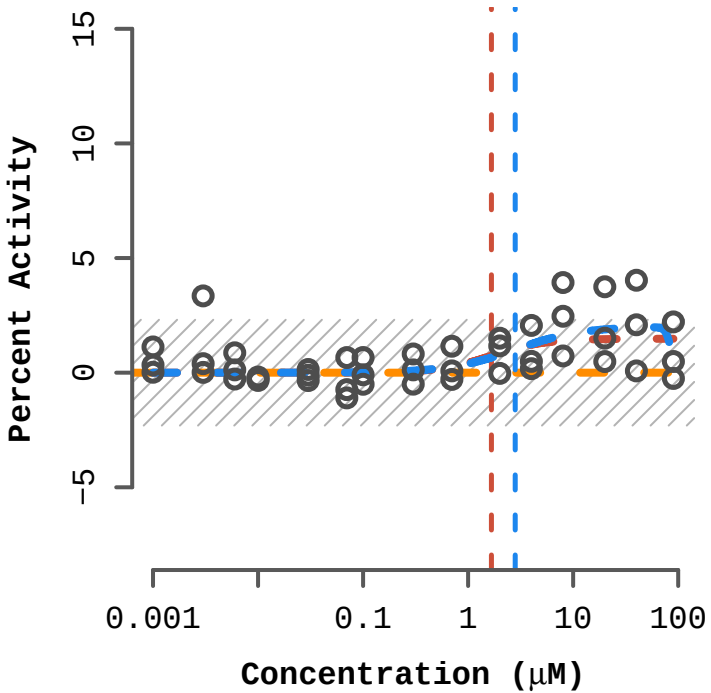
NAME: (2E)-3,7-Dimethylocta-2,6-dien-1-yl formate
CHID: 47614 **CASRN:** 105-86-2
SPID(S): Tox21_302545
M4ID: 12476588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Methoxy-4-methyl-1-(propan-2-yl)benzene
CHID: 47617 **CASRN:** 1076-56-8
SPID(S): Tox21_302575
M4ID: 12476558

HILL MODEL (in red):

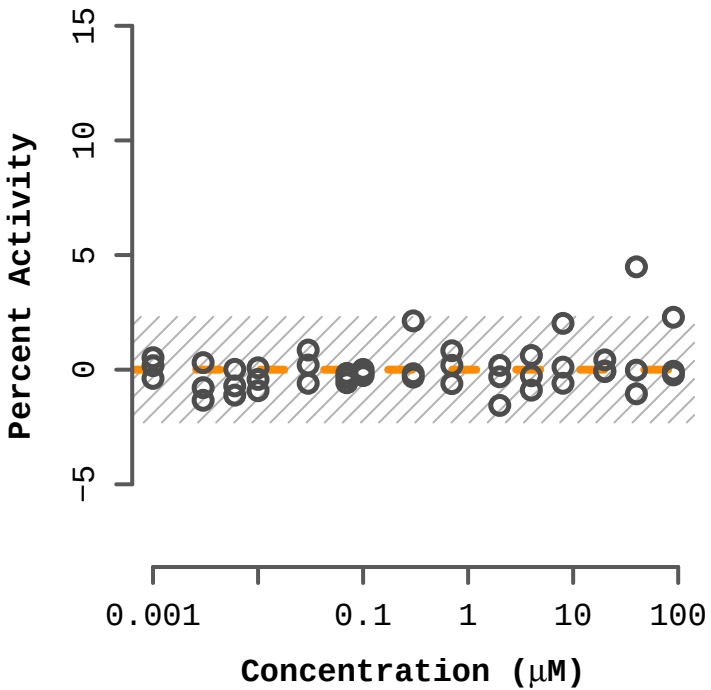
	tp	ga	gw
val:	1.48	0.222	1.77
sd:	0.414	0.337	1.38

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.01	0.448	1.38	1.93	16.6
sd:	0.682	0.366	1.01	0.0568	42.3

	CNST	HILL	GNLS
AIC:	152.8	136.42	137.77
PROB:	0	0.66	0.34
RMSE:	1.43	1.06	1.01

MAX_MEAN: 2.38 **MAX_MED:** 2.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

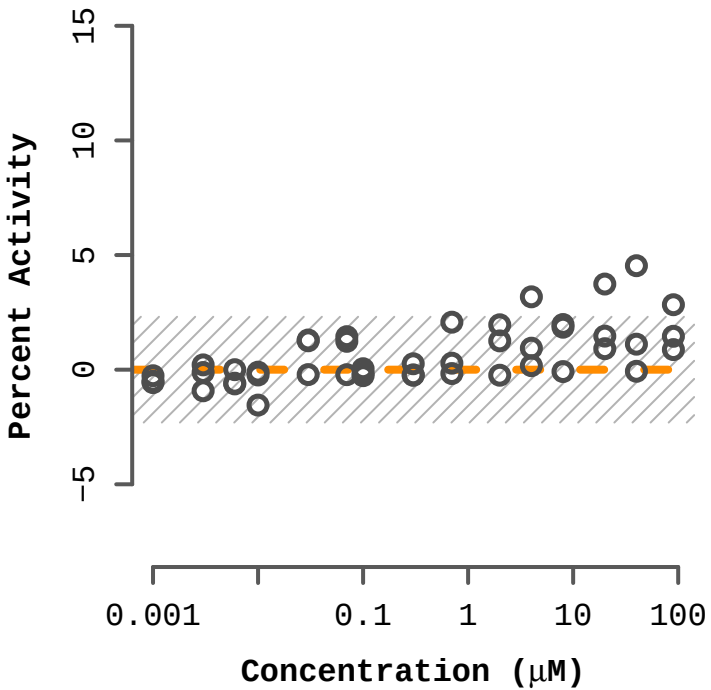
NAME: 4-Pentanolide
CHID: 47618 **CASRN:** 108-29-2
SPID(S): Tox21_302624
M4ID: 12476509

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.203 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

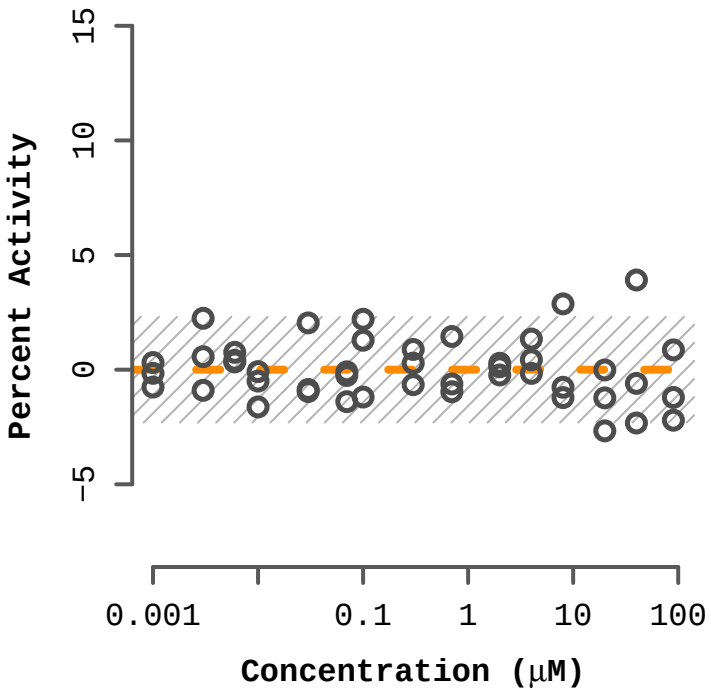
NAME: 2-Methylpyrazine
CHID: 47620 **CASRN:** 109-08-0
SPID(S): Tox21_303776
M4ID: 12475412

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

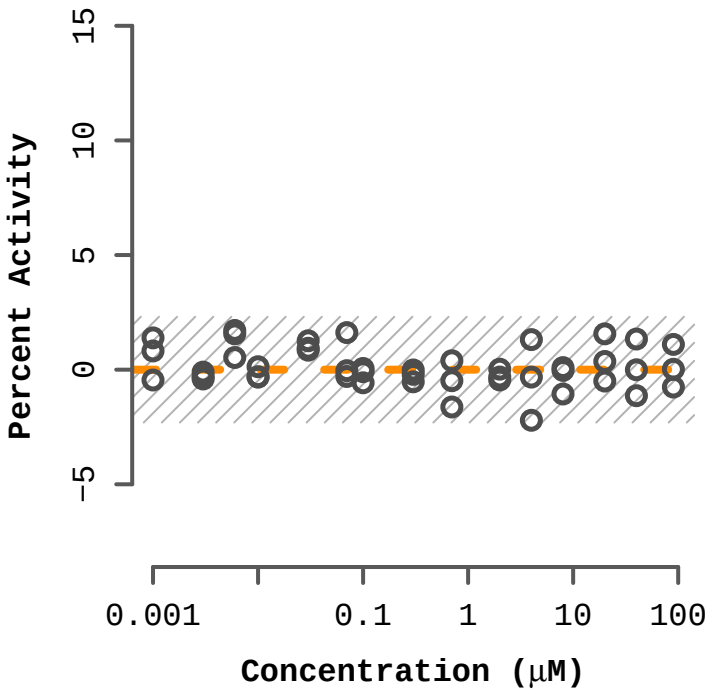
NAME: Oxacycloheptadecan-2-one
CHID: 47622 **CASRN:** 109-29-5
SPID(S): Tox21_302621
M4ID: 12476512

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 0.764 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

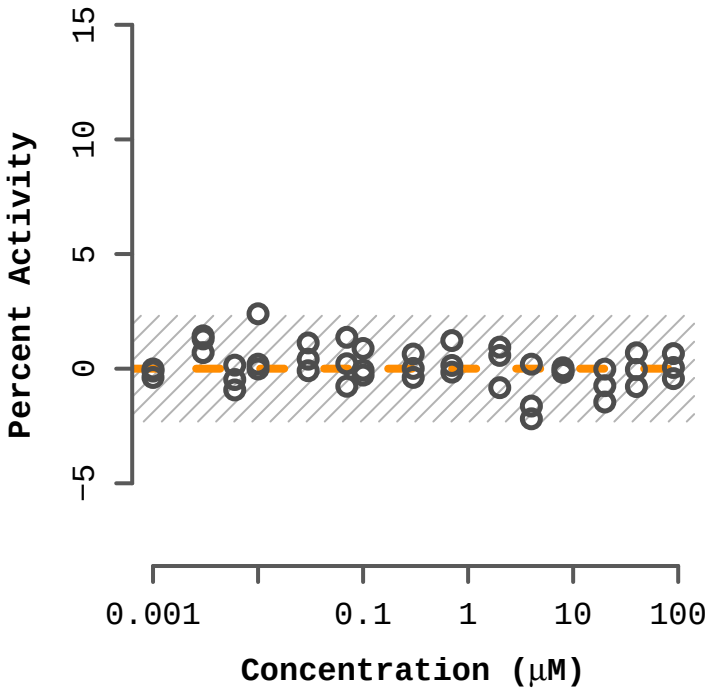
NAME: Dihexyl nonanedioate
CHID: 47623 **CASRN:** 109-31-9
SPID(S): Tox21_303465
M4ID: 12475675

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.78	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.56 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

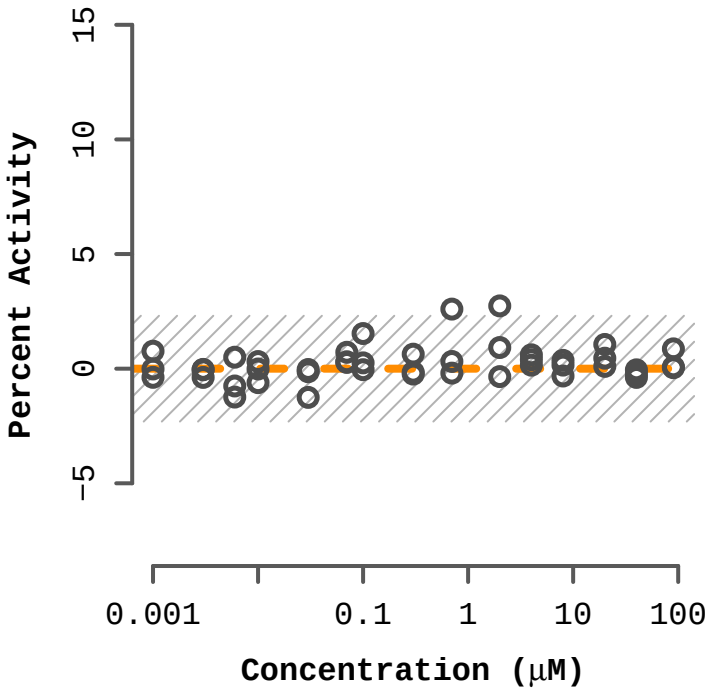
NAME: Butyl undec−10−enoate
CHID: 47624 **CASRN:** 109−42−2
SPID(S): Tox21_302561
M4ID: 12476572

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

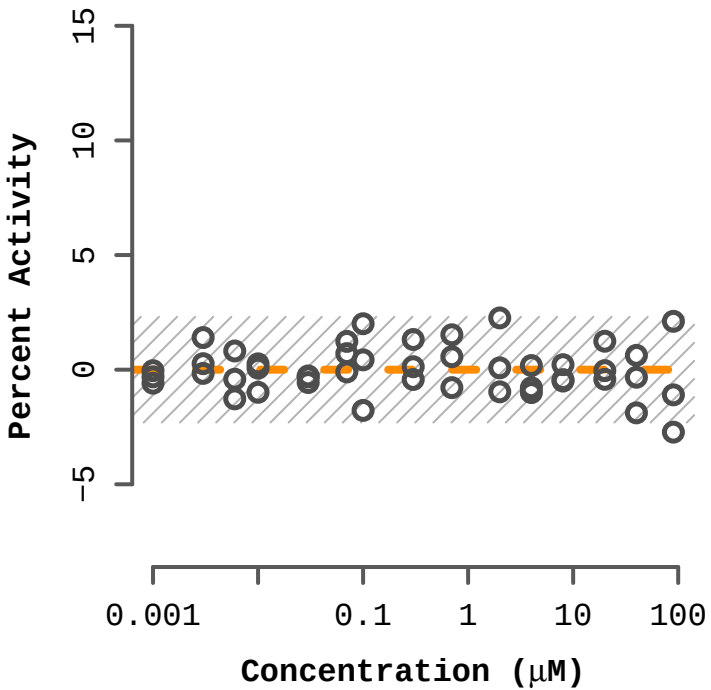
NAME: Dicyclohexyl disulfide
CHID: 47628 CASRN: 2550-40-5
SPID(S): Tox21_300619
M4ID: 12478514

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 1.11 MAX_MED: 0.924 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

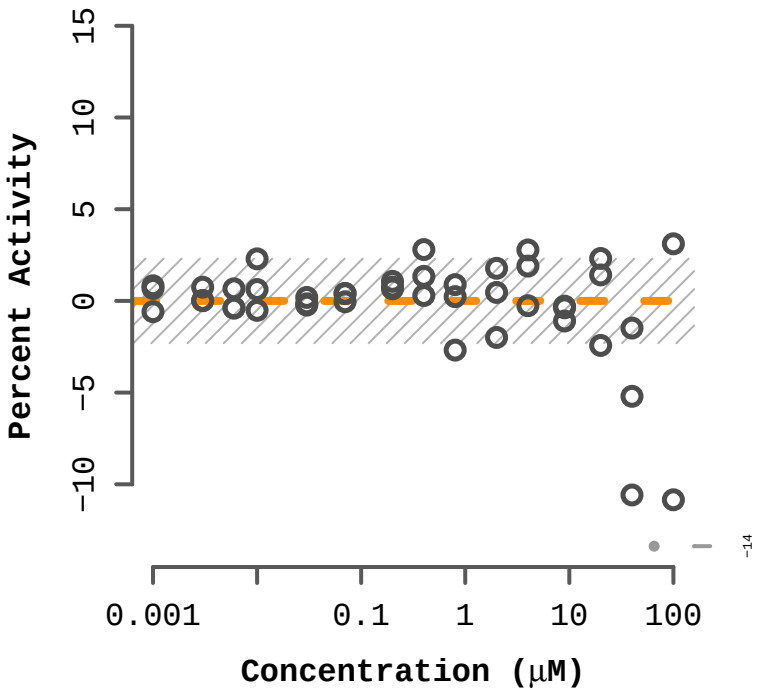
NAME: 2-Methylundecanal
CHID: 47629 **CASRN:** 110-41-8
SPID(S): Tox21_302620
M4ID: 12476513

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.614 **MAX_MED:** 0.701 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

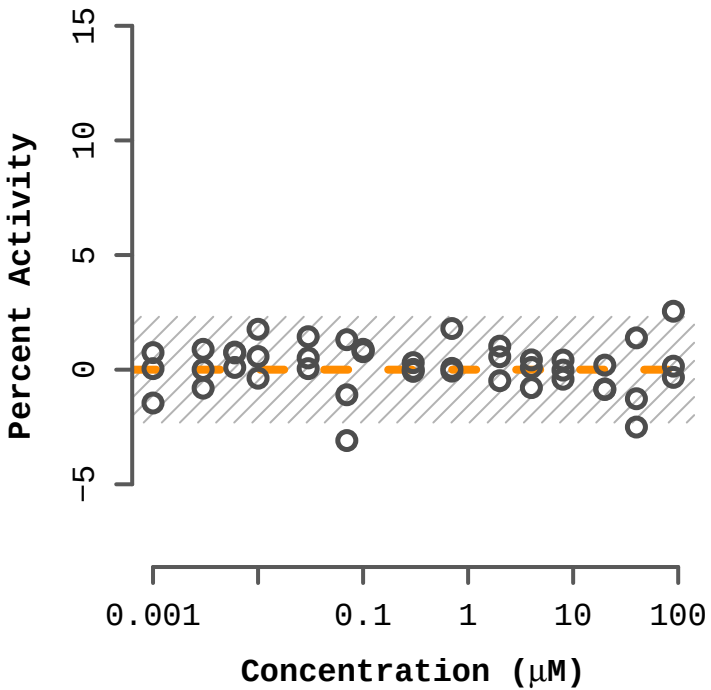
NAME: Tetronic 701
CHID: 47630 **CASRN:** 11111-34-5
SPID(S): Tox21_302455
M4ID: 12476678 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.31	NA	NA
PROB:	1	NA	NA
RMSE:	3.44	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

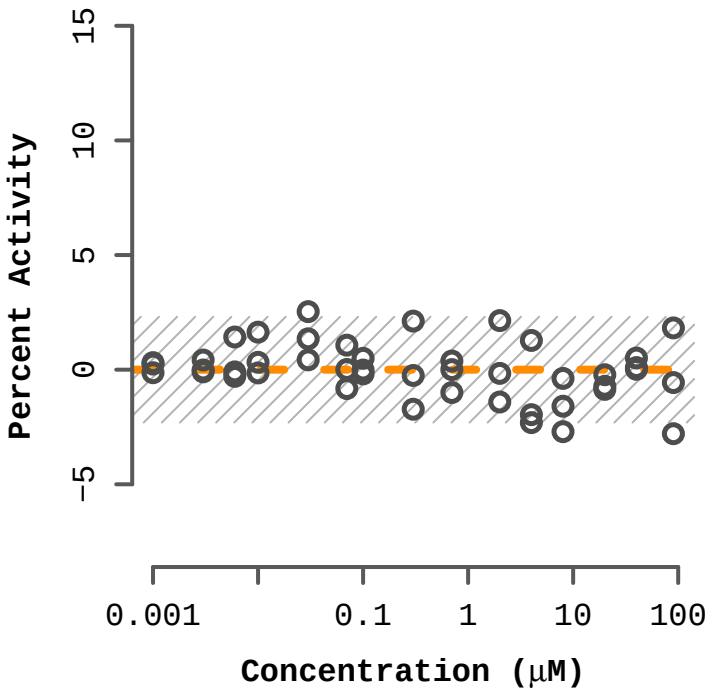
NAME: (2E,4E)-Hexa-2,4-dien-1-ol
CHID: 47631 **CASRN:** 17102-64-6
SPID(S): Tox21_302548
M4ID: 12476585

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.837 **MAX_MED:** 0.833 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

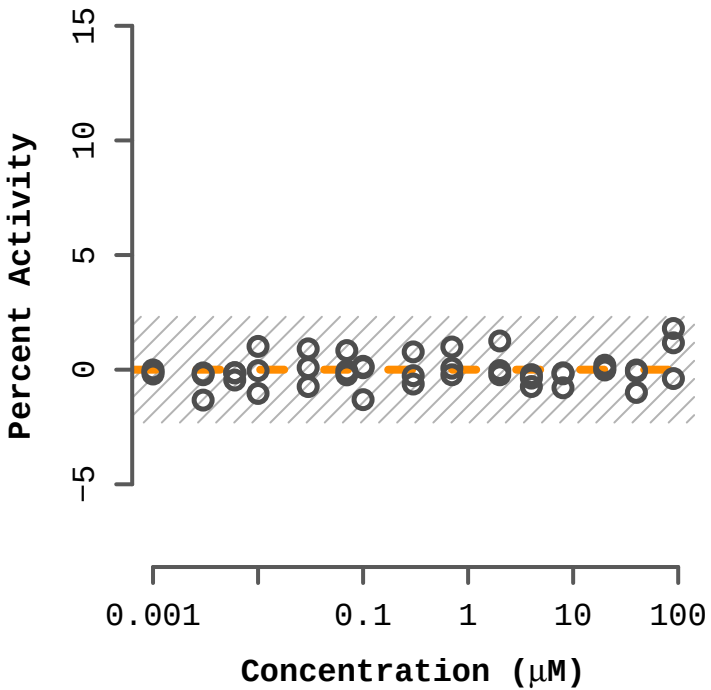
NAME: Ethyl oleate
CHID: 47633 **CASRN:** 111-62-6
SPID(S): Tox21_303521
M4ID: 12475622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

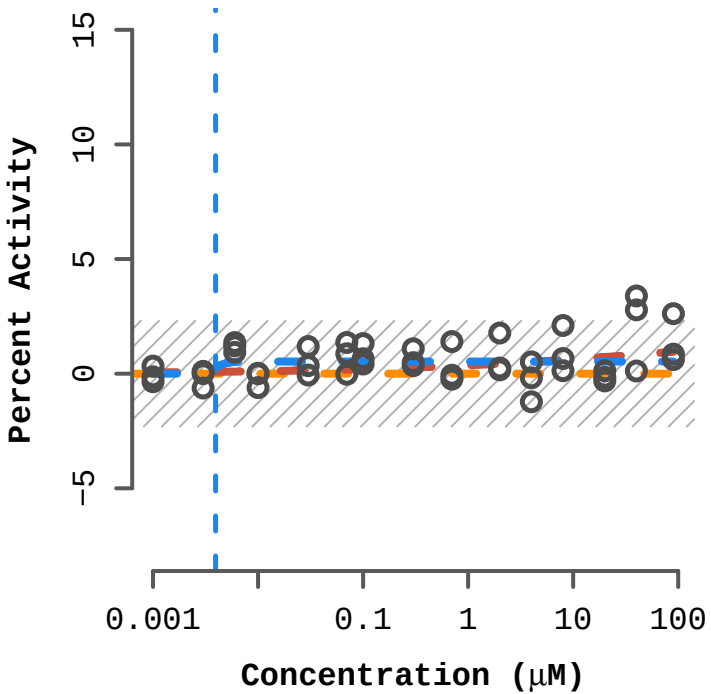
NAME: Hexyl octanoate
CHID: 47636 **CASRN:** 1117-55-1
SPID(S): Tox21_302578
M4ID: 12476555

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl (2E)-non-2-enoate
CHID: 47637 **CASRN:** 14952-06-8
SPID(S): Tox21_302582
M4ID: 12476551

HILL MODEL (in red):

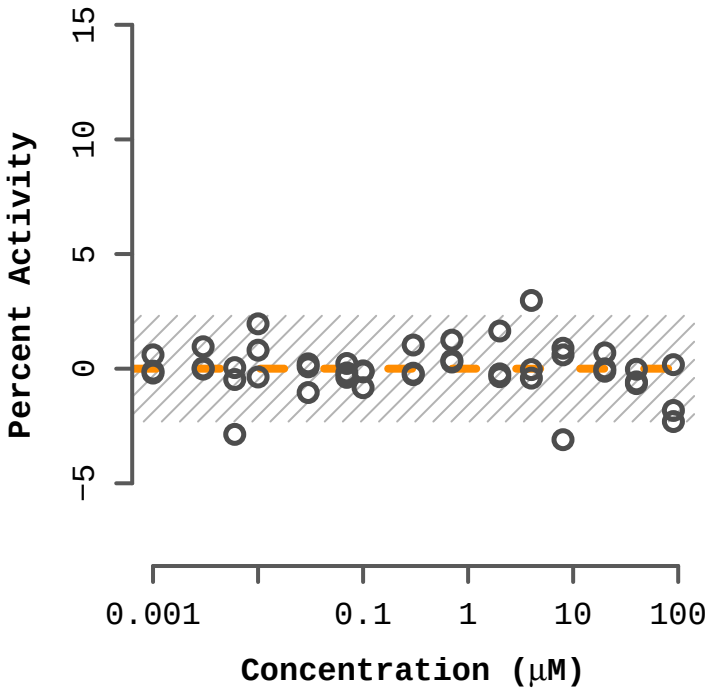
	tp	ga	gw
val:	2.2	2.33	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.529	−2.4	8	3.29	9.1
sd:	0.129	0.143	7.71	103000	686000

	CNST	HILL	GNLS
AIC:	131.22	125.6	124.99
PROB:	0.02	0.41	0.56
RMSE:	1.08	0.89	0.89

MAX_MEAN: 2.1 **MAX_MED:** 2.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

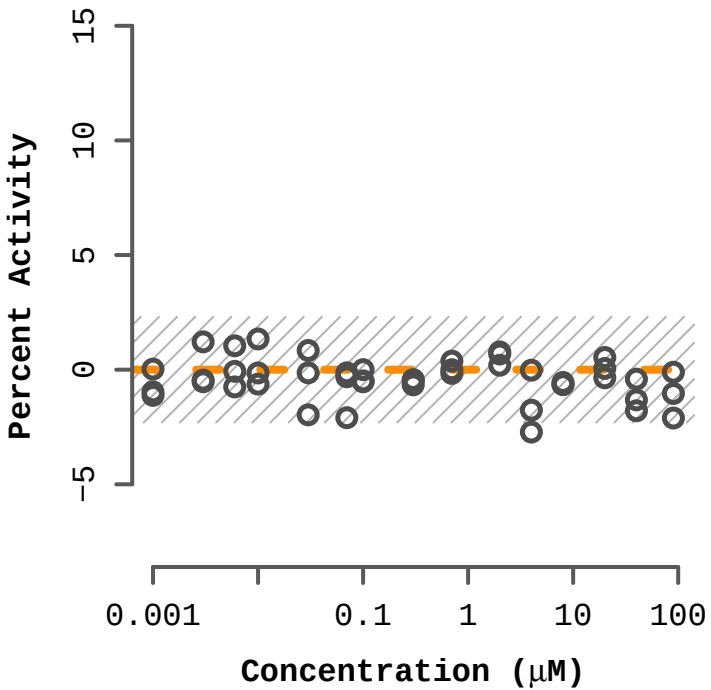
NAME: Methyl 2-nonynoate
CHID: 47639 CASRN: 111-80-8
SPID(S): Tox21_302446
M4ID: 12476687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.842 MAX_MED: 0.808 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

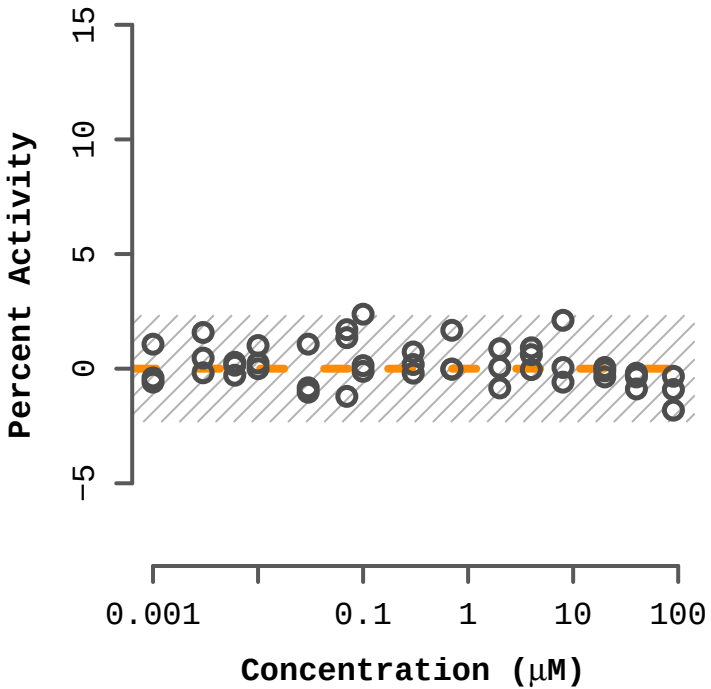
NAME: Dodecyl acetate
CHID: 47641 **CASRN:** 112-66-3
SPID(S): Tox21_303459
M4ID: 12475681

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.551 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

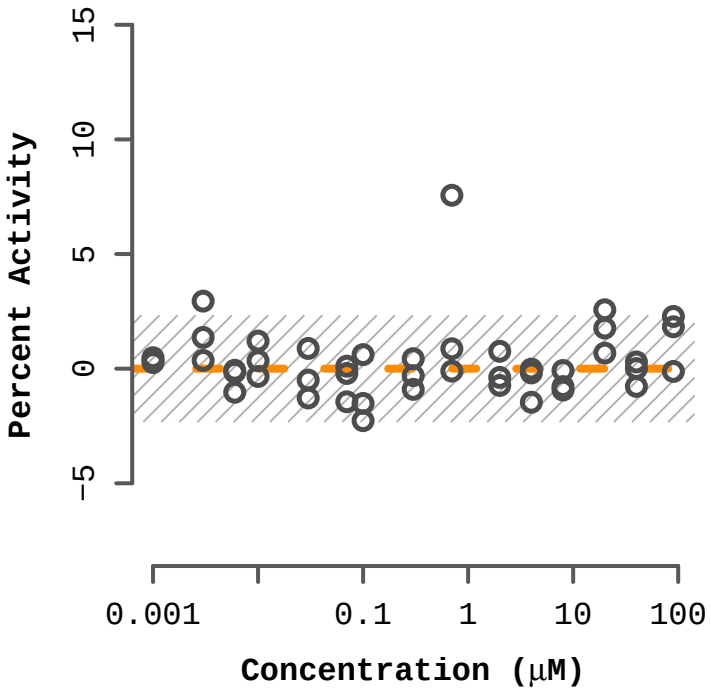
NAME: Linalyl formate
CHID: 47642 **CASRN:** 115-99-1
SPID(S): Tox21_303366
M4ID: 12475769

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.799 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

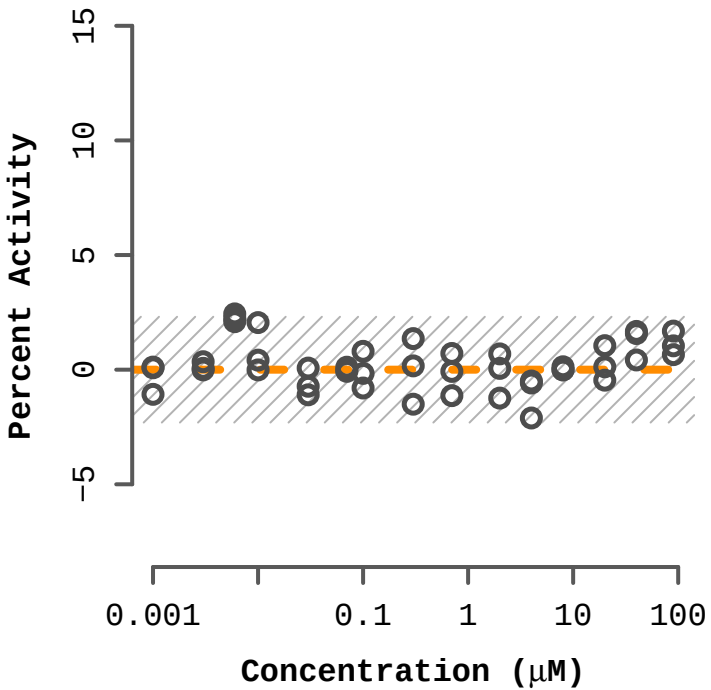
NAME: 1-Cyclohexylethanol
CHID: 47643 **CASRN:** 1193-81-3
SPID(S): Tox21_302512
M4ID: 12476621

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.78 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

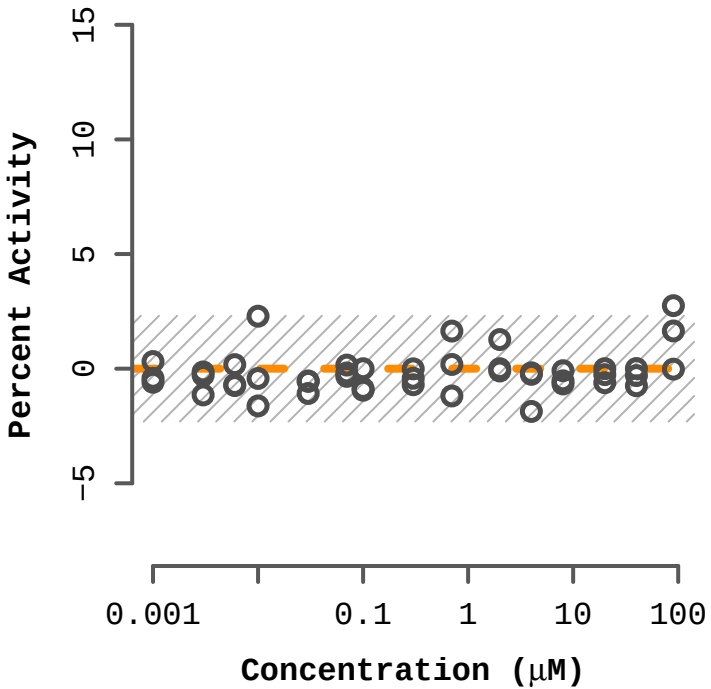
NAME: Isoquinoline
CHID: 47644 **CASRN:** 119-65-3
SPID(S): Tox21_302503
M4ID: 12476630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 2.26 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

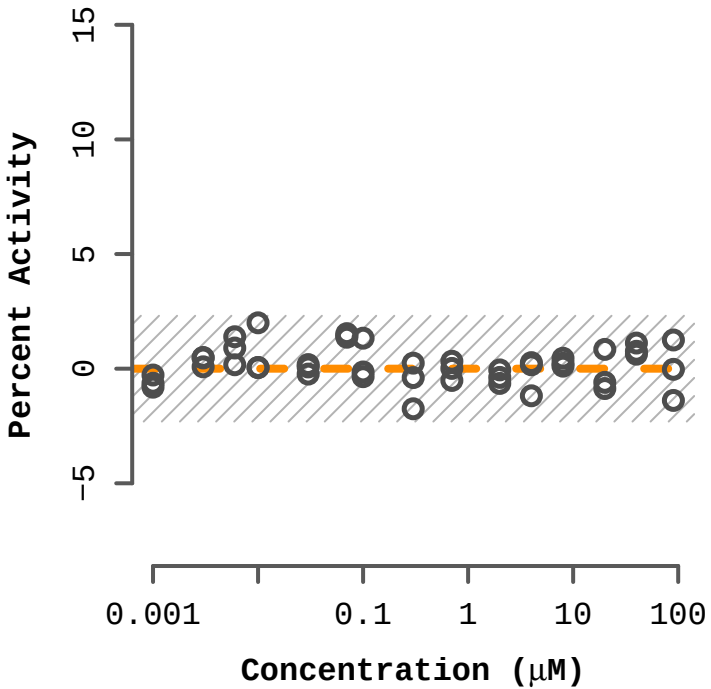
NAME: Methyl 4-methoxybenzoate
CHID: 47645 **CASRN:** 121-98-2
SPID(S): Tox21_302682
M4ID: 12476451

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

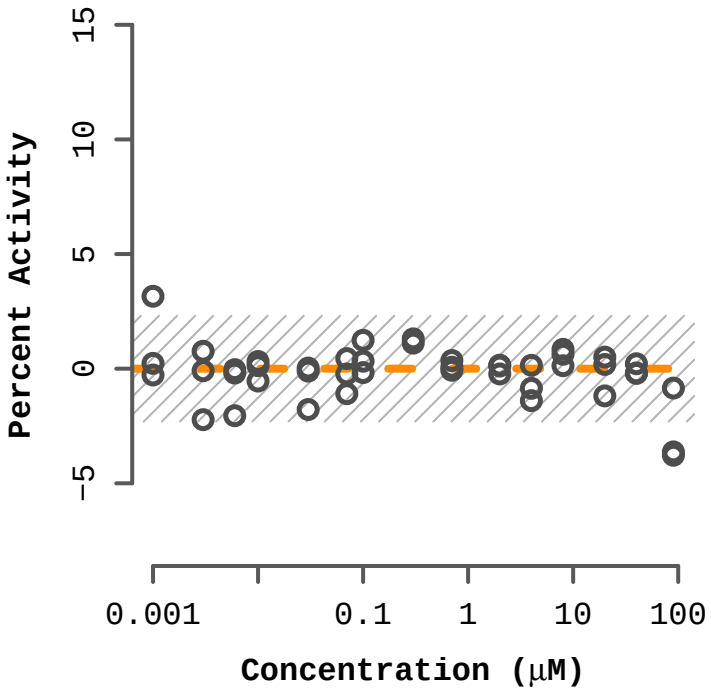
NAME: Isobutyl 3-phenylacrylate
CHID: 47646 **CASRN:** 122-67-8
SPID(S): Tox21_302557
M4ID: 12476576

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

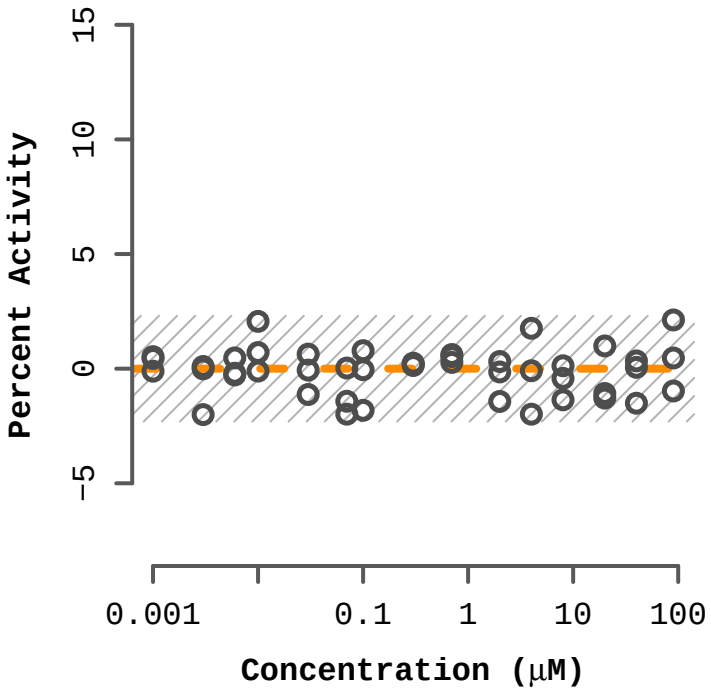
NAME: 3-Phenyl-2-propen-1-yl 3-phenylacrylate
CHID: 47647 **CASRN:** 122-69-0
SPID(S): Tox21_302485
M4ID: 12476648

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

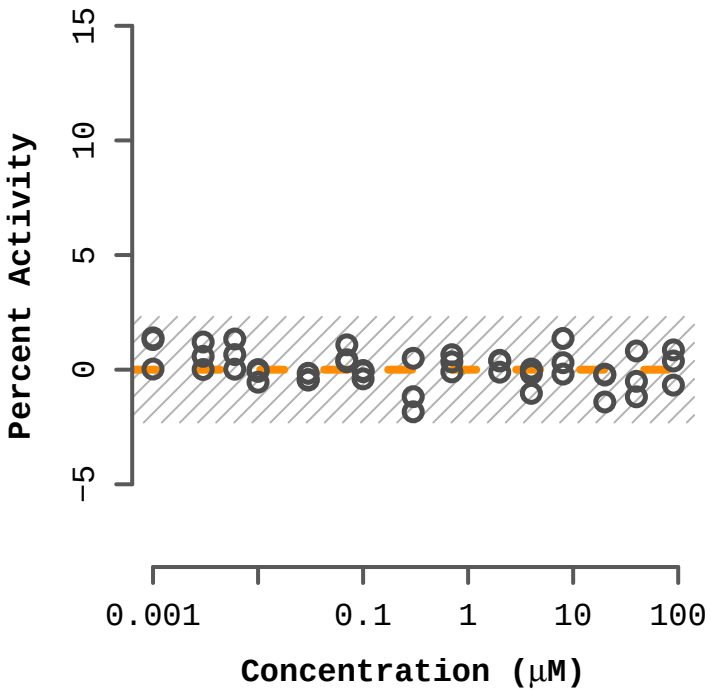
NAME: 3-Phenylpropyl acetate
CHID: 47648 **CASRN:** 122-72-5
SPID(S): Tox21_302587
M4ID: 12476546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.72	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.889 **MAX_MED:** 0.705 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

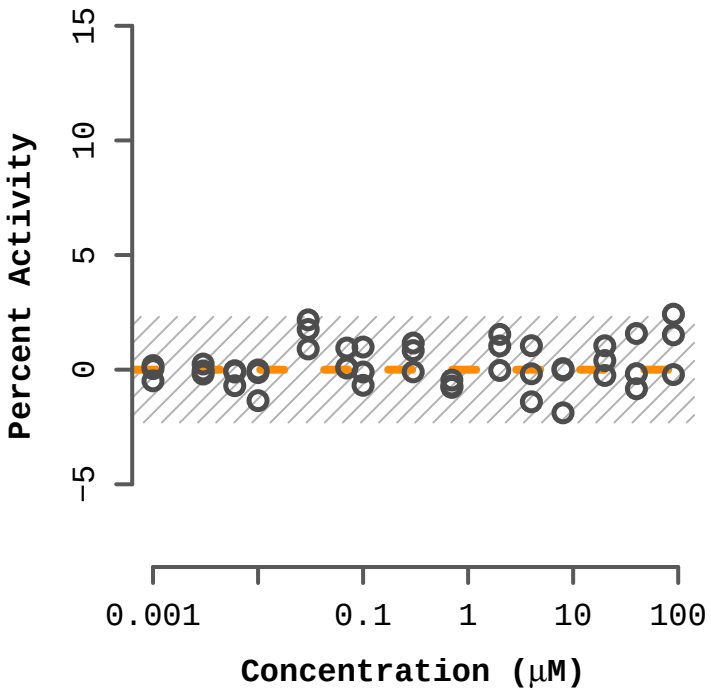
NAME: 4-Methoxybenzyl formate
CHID: 47649 **CASRN:** 122-91-8
SPID(S): Tox21_302535
M4ID: 12476598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.911 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

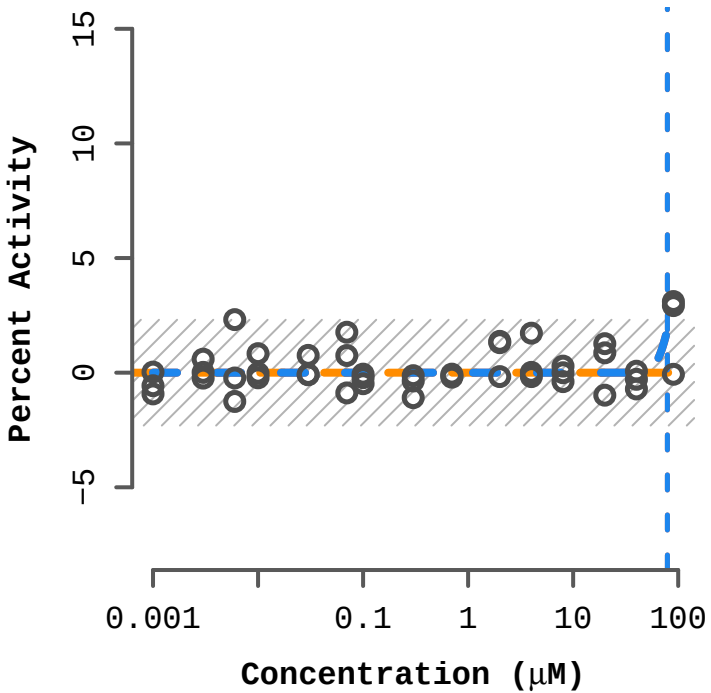
NAME: Ethyl nonanoate
CHID: 47651 **CASRN:** 123-29-5
SPID(S): Tox21_302588
M4ID: 12476545

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl tetradecanoate
CHID: 47654 CASRN: 124-06-1
SPID(S): Tox21_303520
M4ID: 12475623

HILL MODEL (in red):

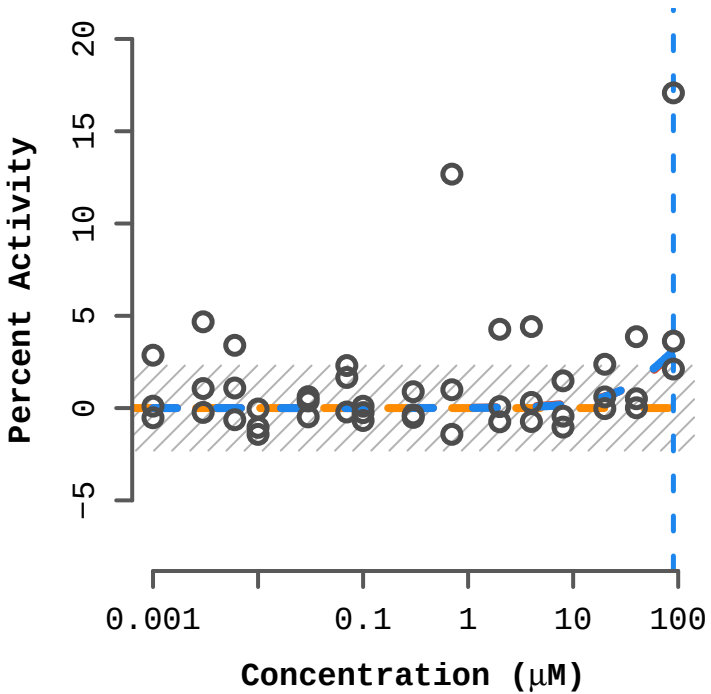
	tp	ga	gw
val:	3.73	1.9	8
sd:	3.83	0.185	7.71

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.73	1.9	8	3.71	2.7
sd:	3.85	0.186	7.72	234	362

	CNST	HILL	GNLS
AIC:	122.67	119.37	123.37
PROB:	0.14	0.75	0.1
RMSE:	1	0.88	0.88

MAX_MEAN: 1.99 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Octanenitrile
CHID: 47655 **CASRN:** 124-12-9
SPID(S): Tox21_302546
M4ID: 12476587

HILL MODEL (in red):

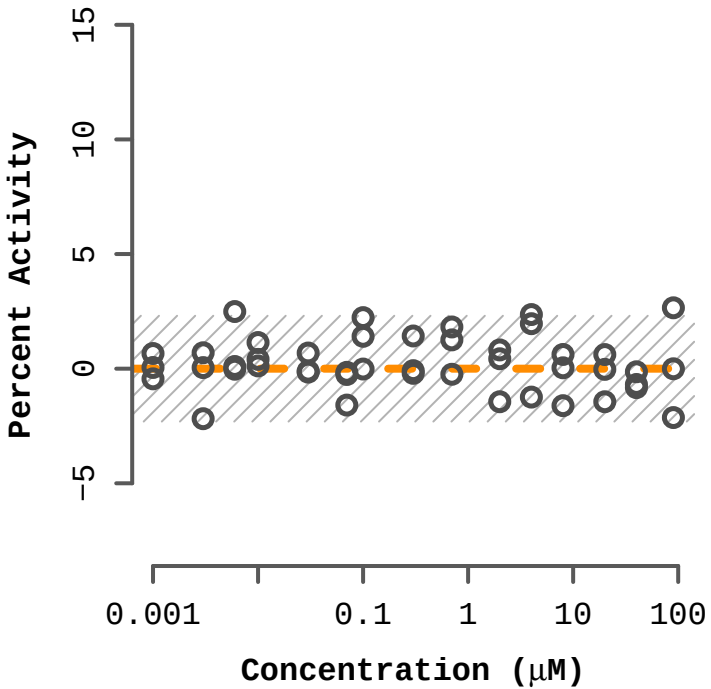
	tp	ga	gw
val:	15.3	2.45	1.18
sd:	91	3.1	1.17

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.21	1.95	1.48	3.95	1.92
sd:	13.2	1.21	1.58	86.2	90.2

	CNST	HILL	GNLS
AIC:	210.15	206	210.1
PROB:	0.1	0.8	0.1
RMSE:	3.64	3.24	3.24

MAX_MEAN: 7.61 **MAX_MED:** 3.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

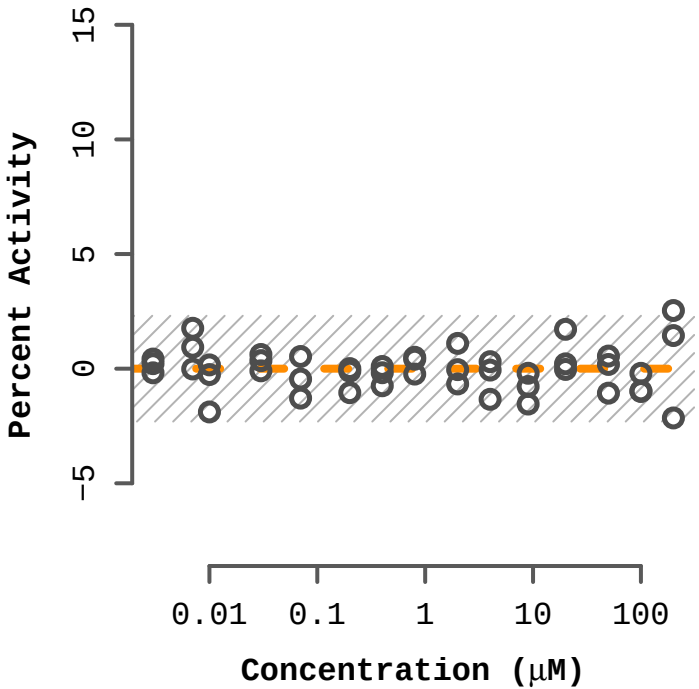
NAME: 9-Decen-1-ol
CHID: 47656 **CASRN:** 13019-22-2
SPID(S): Tox21_302537
M4ID: 12476596

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

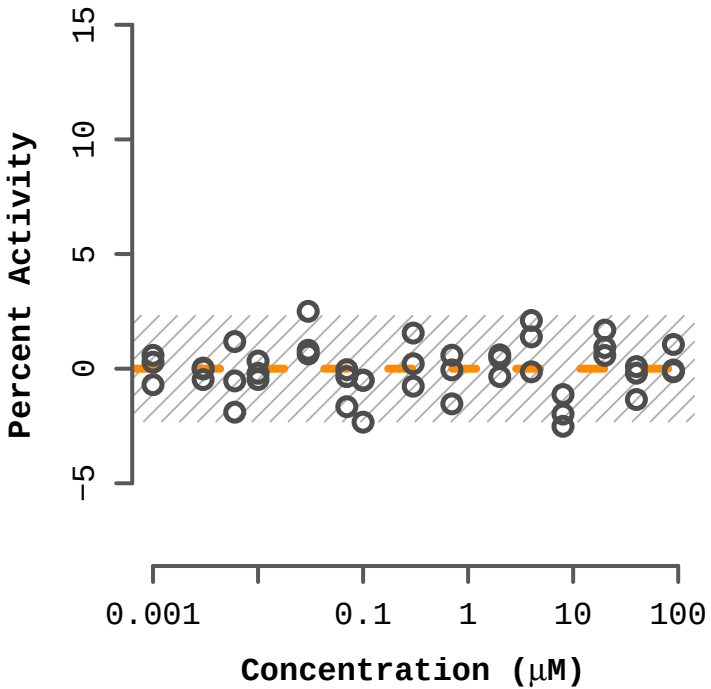
NAME: 1,3−Nonanediol monoacetate
CHID: 47657 **CASRN:** 1322−17−4
SPID(S): Tox21_302555
M4ID: 12476578

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.895 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

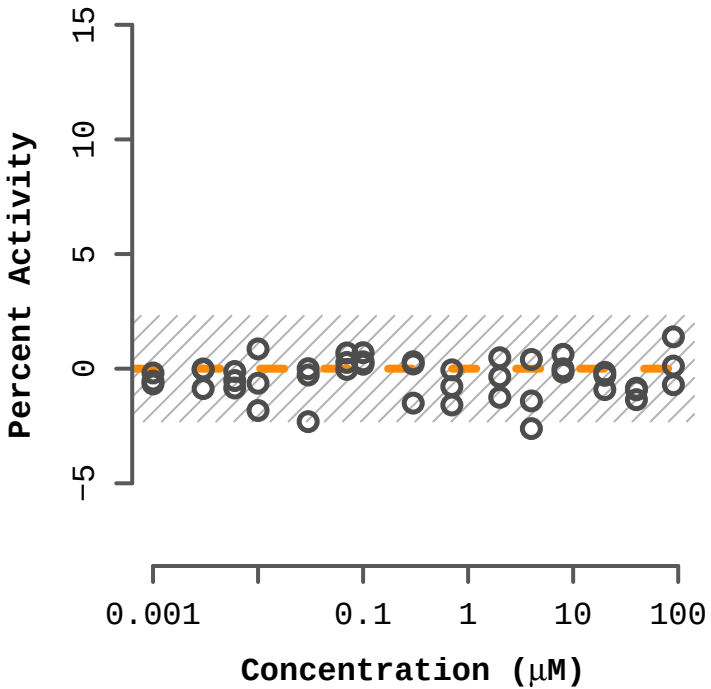
NAME: Methyl 3-nonenoate
CHID: 47659 **CASRN:** 13481-87-3
SPID(S): Tox21_302559
M4ID: 12476574

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

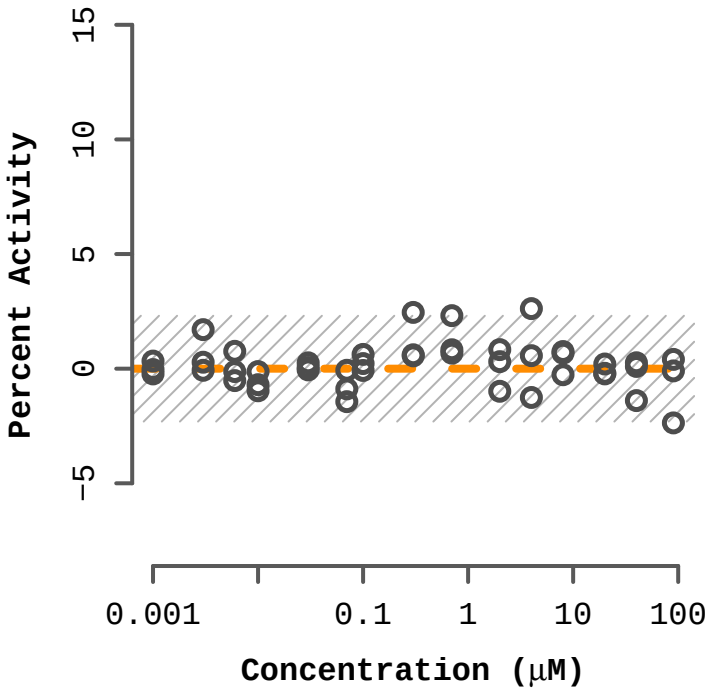
NAME: 3,5-Dimethyl-1,2-cyclopentanedione
CHID: 47660 **CASRN:** 13494-07-0
SPID(S): Tox21_302565
M4ID: 12476568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.85	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.399 **MAX_MED:** 0.301 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

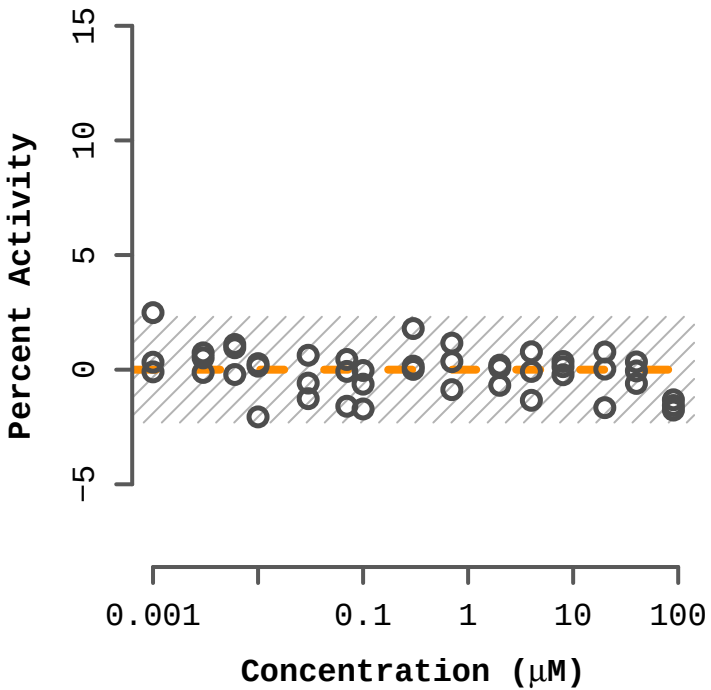
NAME: S-Furfuryl thioacetate
CHID: 47661 CASRN: 13678-68-7
SPID(S): Tox21_302486
M4ID: 12476647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.27 MAX_MED: 0.828 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

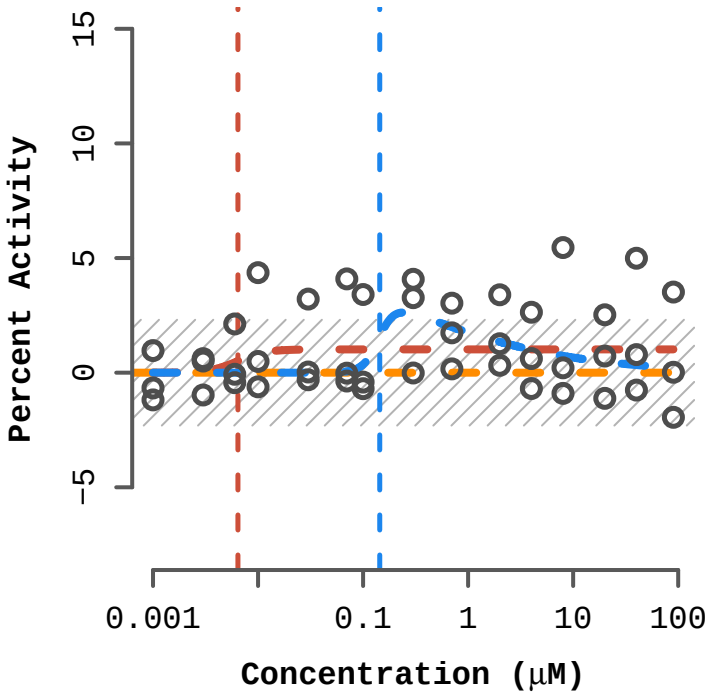
NAME: Iprovalicarb
CHID: 47662 CASRN: 140923-17-7
SPID(S): Tox21_303633
M4ID: 12475512

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.908 MAX_MED: 0.957 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Furfurylpyrrole
CHID: 47663 CASRN: 1438-94-4
SPID(S): Tox21_302604
M4ID: 12476529

HILL MODEL (in red):

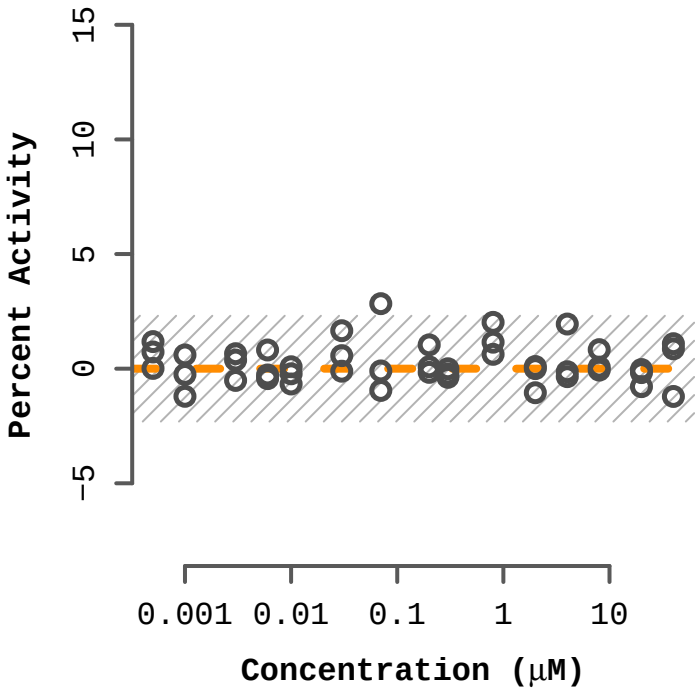
	tp	ga	gw
val:	1.01	−2.19	3.38
sd:	0.365	0.453	14.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.42	−0.841	5.85	−0.591	0.539
sd:	13.4	0.333	16	3.52	0.536

	CNST	HILL	GNLS
AIC:	197.84	194.5	196.2
PROB:	0.12	0.62	0.26
RMSE:	2.16	1.84	1.9

MAX_MEAN: 2.44 MAX_MED: 3.27 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

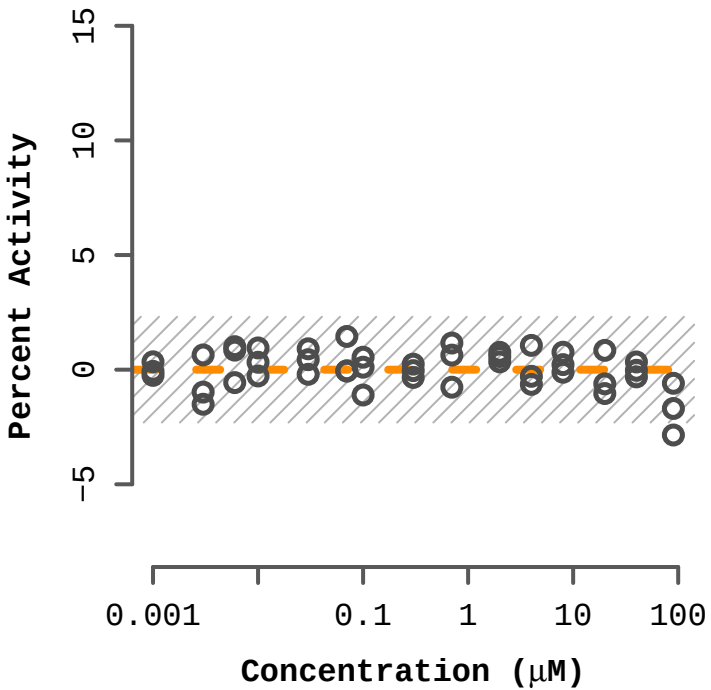
NAME: Furfuryl isopropyl sulfide
CHID: 47665 **CASRN:** 1883-78-9
SPID(S): Tox21_303491
M4ID: 12475650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

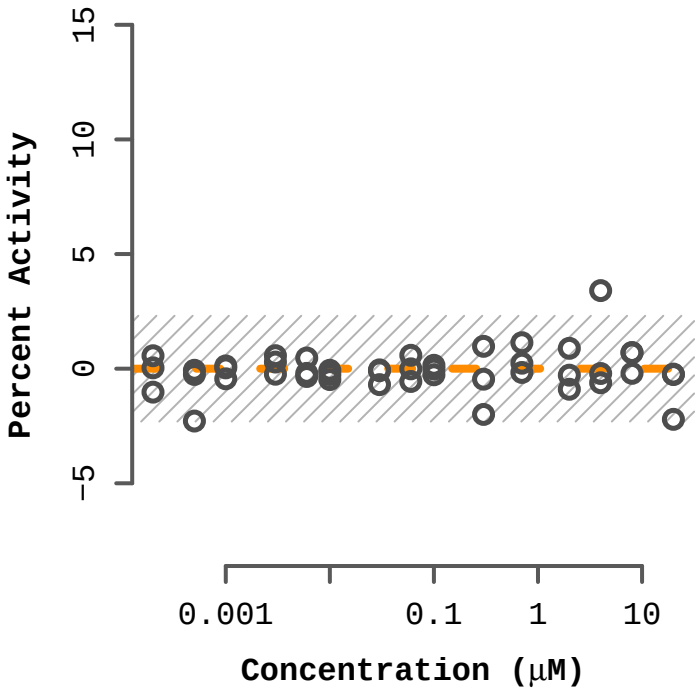
NAME: Tridec-2-enenitrile
CHID: 47667 **CASRN:** 22629-49-8
SPID(S): Tox21_302490
M4ID: 12476643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.559 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

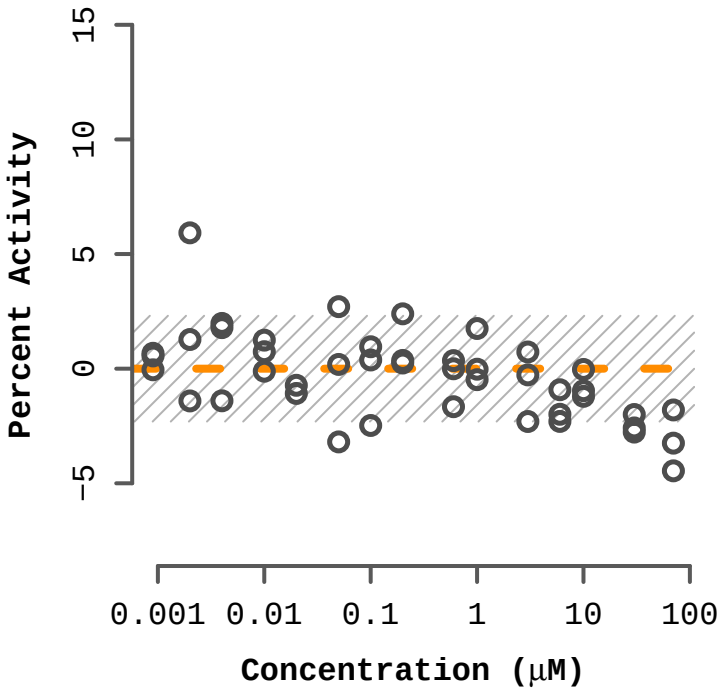
NAME: 4-Hexen-3-one
CHID: 47670 **CASRN:** 2497-21-4
SPID(S): Tox21_303442
M4ID: 12475698

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.862 **MAX_MED:** 0.694 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

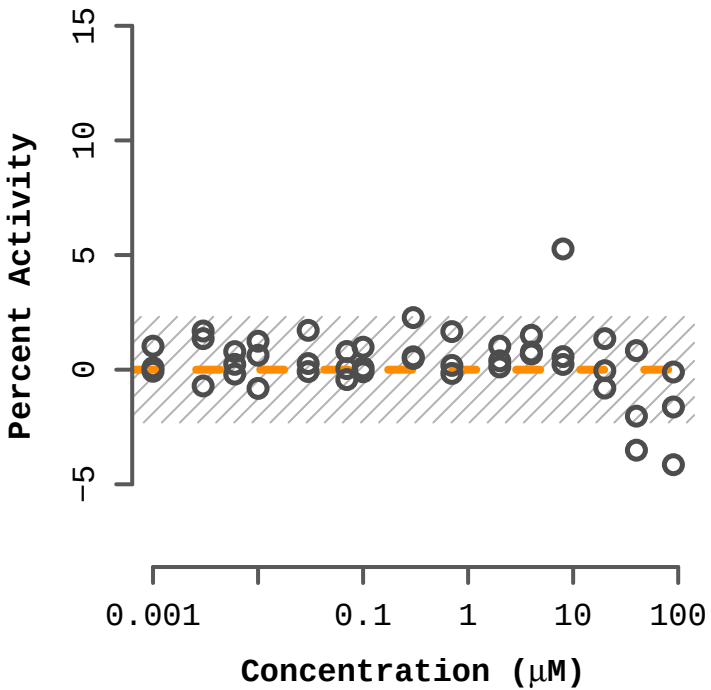
NAME: Flubendiamide
CHID: 47672 **CASRN:** 272451-65-7
SPID(S): Tox21_303432
M4ID: 12475707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

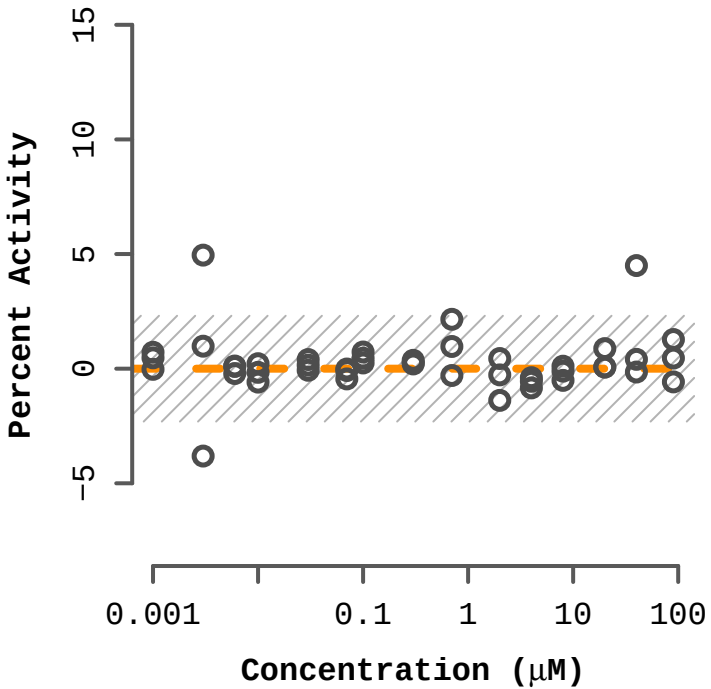
NAME: Bis(2-methyl-3-furyl)disulfide
CHID: 47673 **CASRN:** 28588-75-2
SPID(S): Tox21_302589
M4ID: 12476544

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

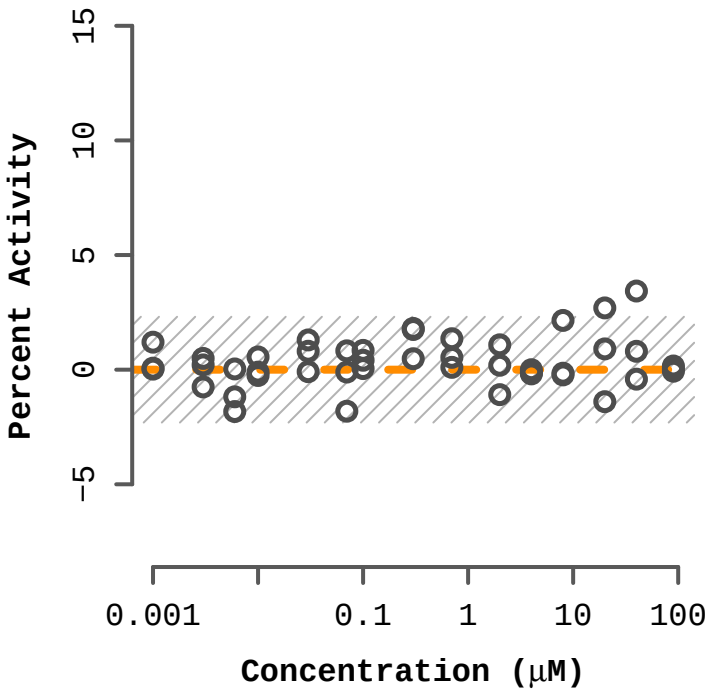
NAME: 4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one
CHID: 47674 **CASRN:** 28664-35-9
SPID(S): Tox21_302500
M4ID: 12476633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

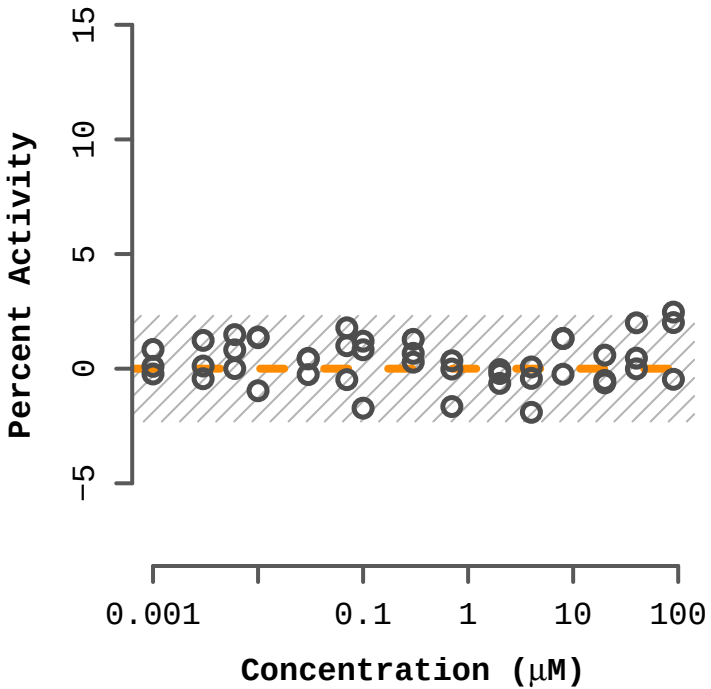
NAME: 3-Methylcyclohexane-1,2-dione
CHID: 47675 **CASRN:** 3008-43-3
SPID(S): Tox21_303634
M4ID: 12475511

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

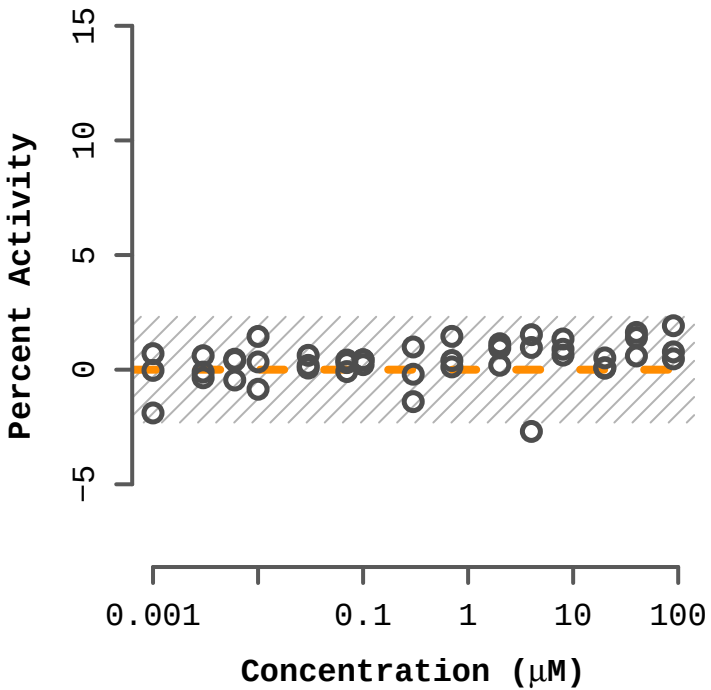
NAME: 2-Methyldihydrofuran-3(2H)-one
CHID: 47677 **CASRN:** 3188-00-9
SPID(S): Tox21_302600
M4ID: 12476533

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

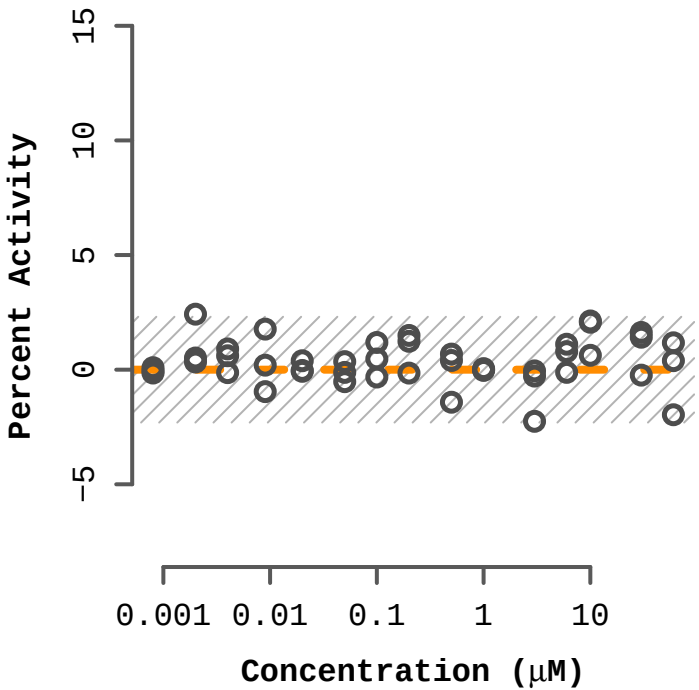
NAME: 5,6,7,8−Tetrahydroquinoxaline
CHID: 47678 **CASRN:** 34413−35−9
SPID(S): Tox21_302592
M4ID: 12476541

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

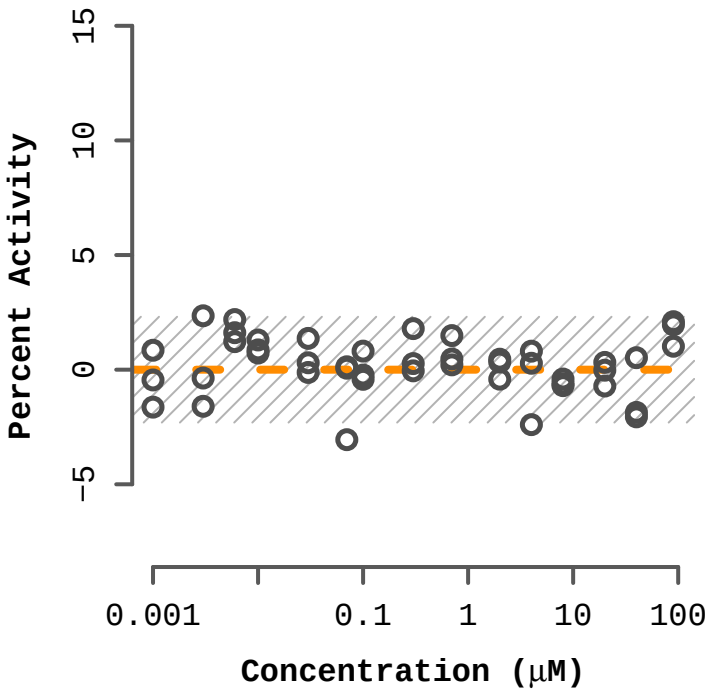
NAME: 2-Pentylfuran
CHID: 47679 **CASRN:** 3777-69-3
SPID(S): Tox21_303542
M4ID: 12475602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 2.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

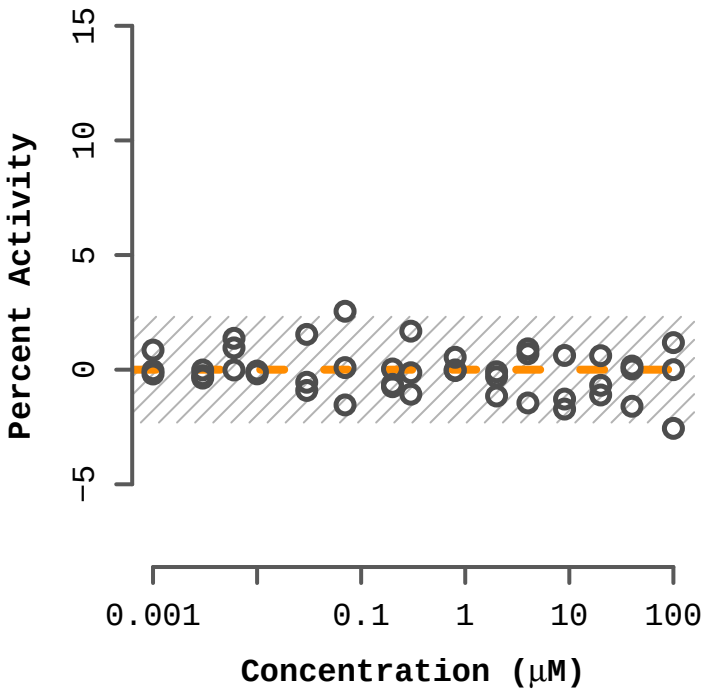
NAME: 5-Acetyl-2,4-dimethylthiazole
CHID: 47680 **CASRN:** 38205-60-6
SPID(S): Tox21_302567
M4ID: 12476566

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

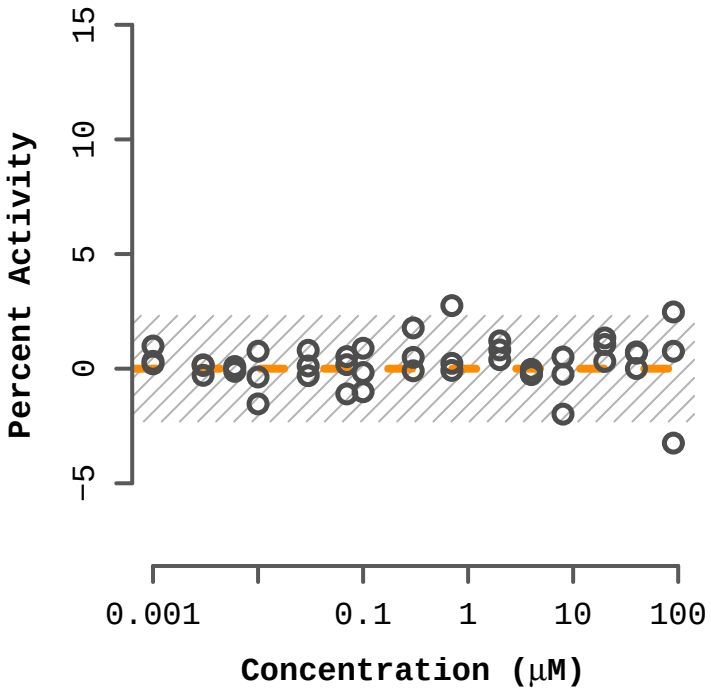
NAME: 3,4−Hexanedione
CHID: 47681 **CASRN:** 4437−51−8
SPID(S): Tox21_302566
M4ID: 12476567

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.77 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

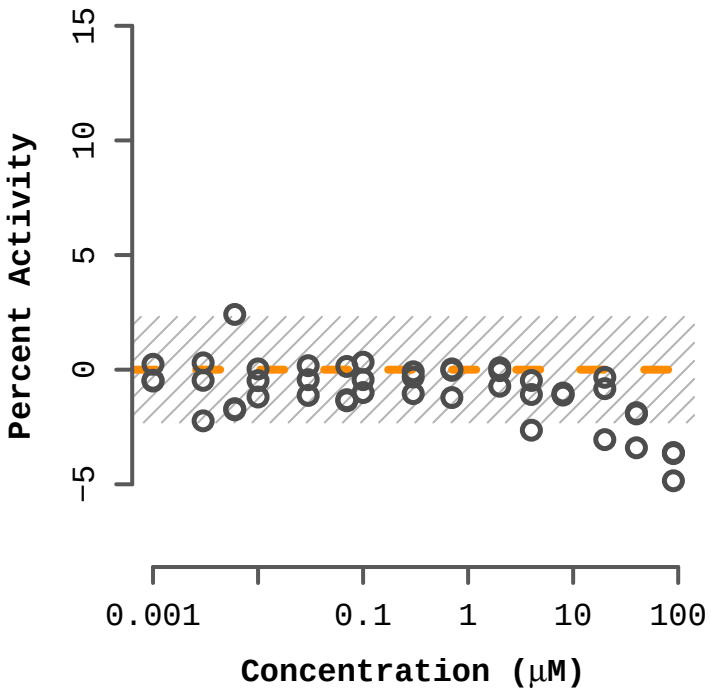
NAME: 4-Cyclohexyl-4-methyl-pentan-2-one
CHID: 47682 **CASRN:** 4927-39-3
SPID(S): Tox21_303636
M4ID: 12475509

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

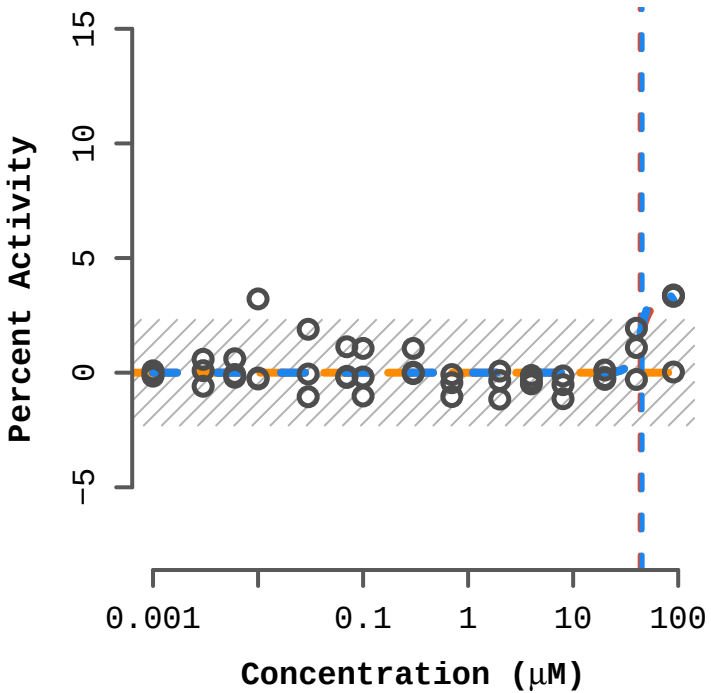
NAME: 2,5-Dimethyl-1,4-dithiane-2,5-diol
CHID: 47683 **CASRN:** 55704-78-4
SPID(S): Tox21_302432
M4ID: 12476701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: −0.227 **MAX_MED:** −0.029 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phenethyl tiglate
CHID: 47684 **CASRN:** 55719-85-2
SPID(S): Tox21_302686
M4ID: 12476447

HILL MODEL (in red):

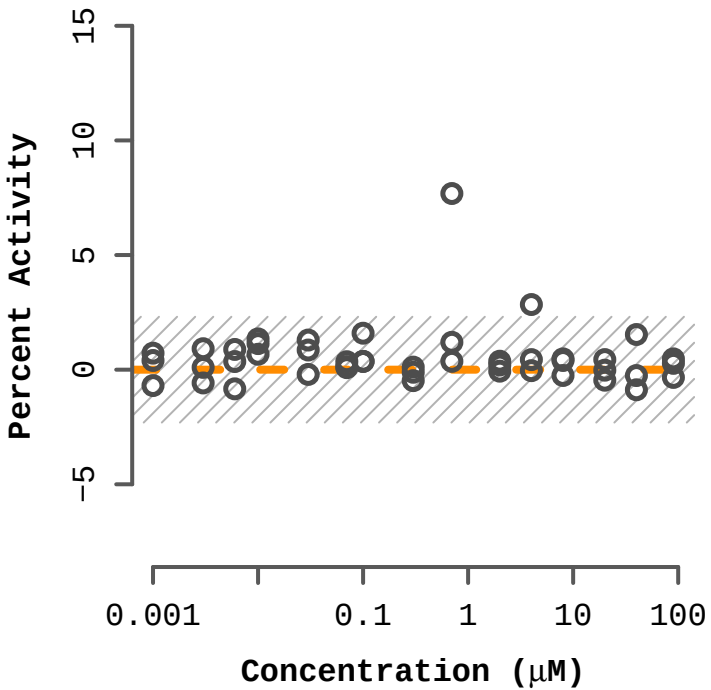
	tp	ga	gw
val:	3.18	1.64	8
sd:	0.402	0.0767	13.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.06	1.66	8	2.07	4.72
sd:	23.3	0.372	14.6	0.737	84.6

	CNST	HILL	GNLS
AIC:	124.13	115.53	119.53
PROB:	0.01	0.87	0.12
RMSE:	1.09	0.92	0.92

MAX_MEAN: 2.25 **MAX_MED:** 3.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

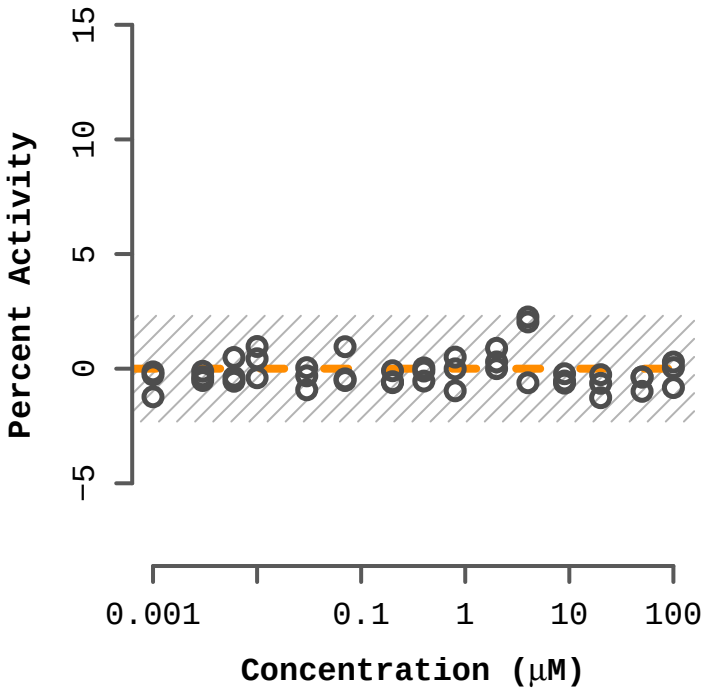
NAME: (3aR)−(+)−Sclareolide
CHID: 47686 CASRN: 564−20−5
SPID(S): Tox21_302544
M4ID: 12476589

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 3.08 MAX_MED: 1.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

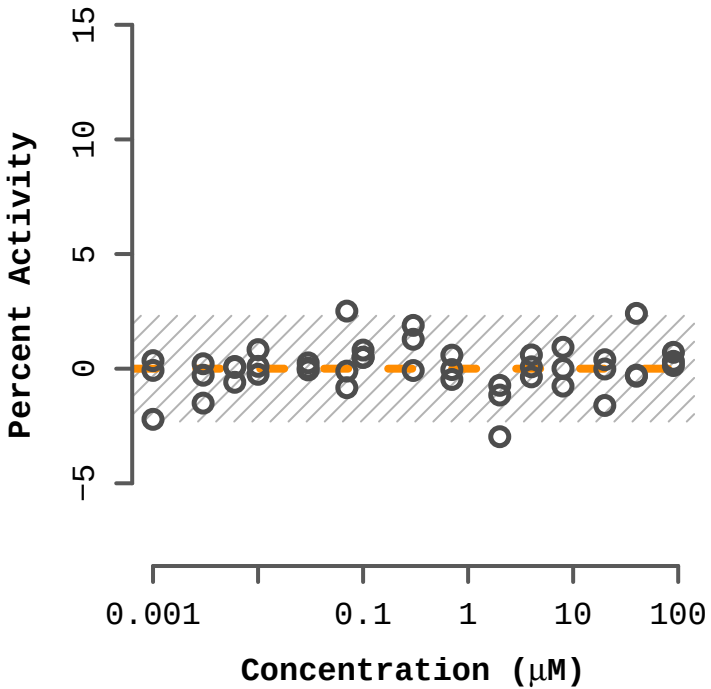
NAME: Calcium L−ascorbate dihydrate
CHID: 47687 **CASRN:** 5743−28−2
SPID(S): Tox21_303536
M4ID: 12475608

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	99.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

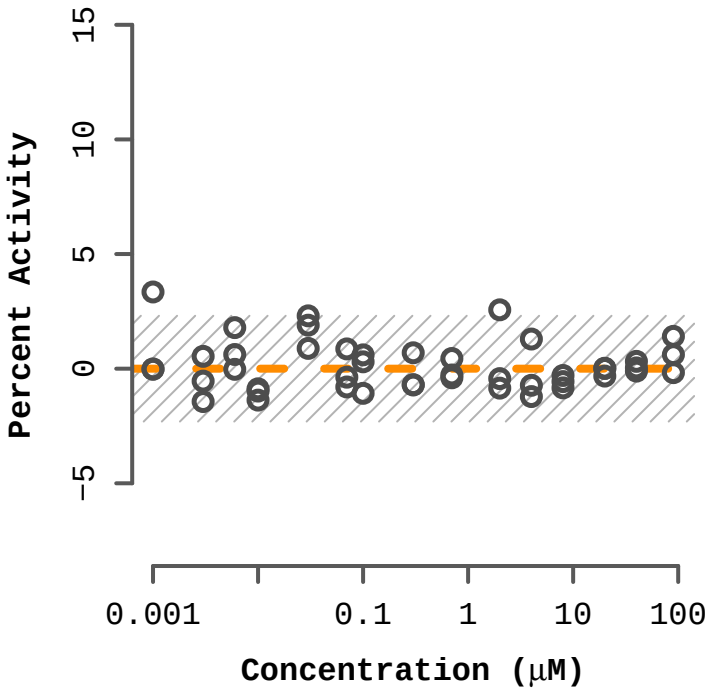
NAME: 2-Methylpropyl but-2-enoate
CHID: 47691 **CASRN:** 589-66-2
SPID(S): Tox21_303966
M4ID: 12475222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

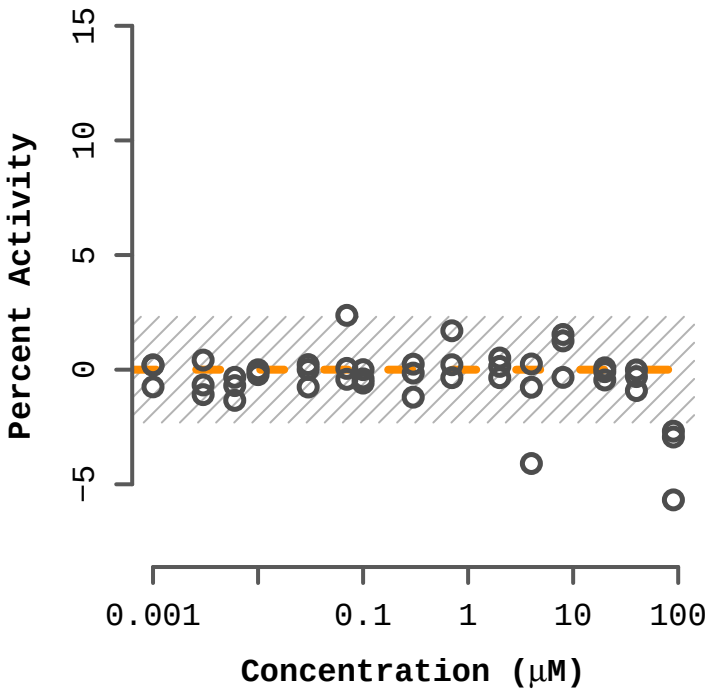
NAME: alpha−Angelica lactone
CHID: 47693 **CASRN:** 591−12−8
SPID(S): Tox21_303997
M4ID: 12475191

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

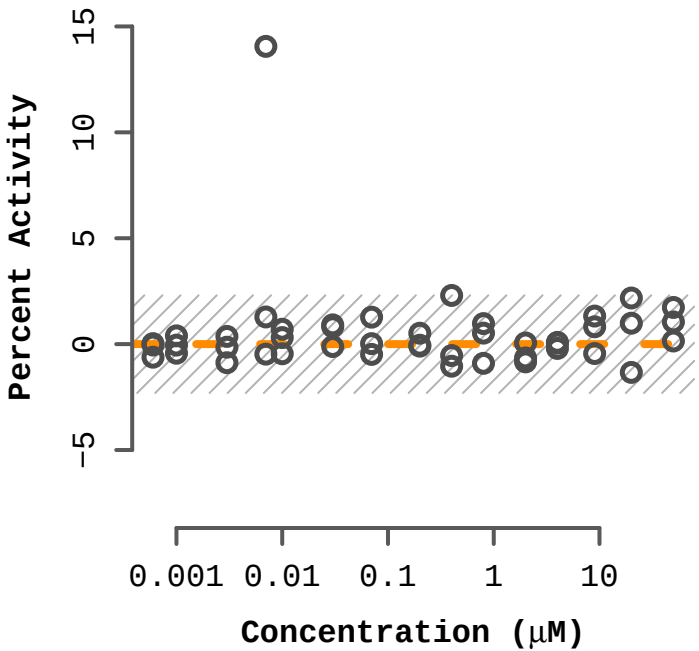
NAME: Quinine hydrochloride dihydrate
CHID: 47694 **CASRN:** 6119-47-7
SPID(S): Tox21_303565
M4ID: 12475580

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.82 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

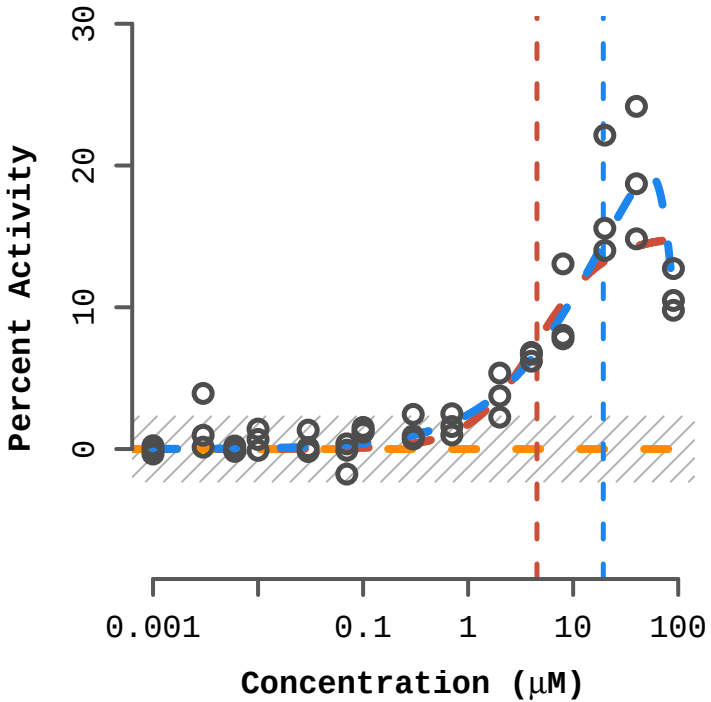
NAME: Cremophor EL
CHID: 47696 CASRN: 61791-12-6
SPID(S): Tox21_302543
M4ID: 12476590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.81	NA	NA
PROB:	1	NA	NA
RMSE:	2.26	NA	NA

MAX_MEAN: 4.96 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Naphthalen-2-yl 2-aminobenzoate
CHID: 47697 CASRN: 63449-68-3
SPID(S): Tox21_302560
M4ID: 12476573

HILL MODEL (in red):

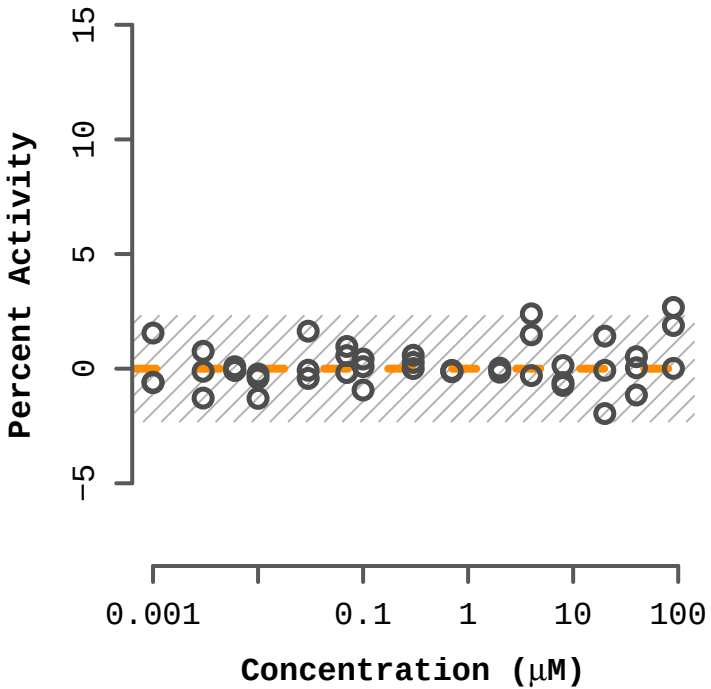
	tp	ga	gw
val:	15.1	0.655	1.34
sd:	1.48	0.0889	0.314

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29	1.29	0.807	1.95	6.27
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	310.01	205.02	179.3
PROB:	0	0	1
RMSE:	8.13	2.63	1.89

MAX_MEAN: 19.2 MAX_MED: 18.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

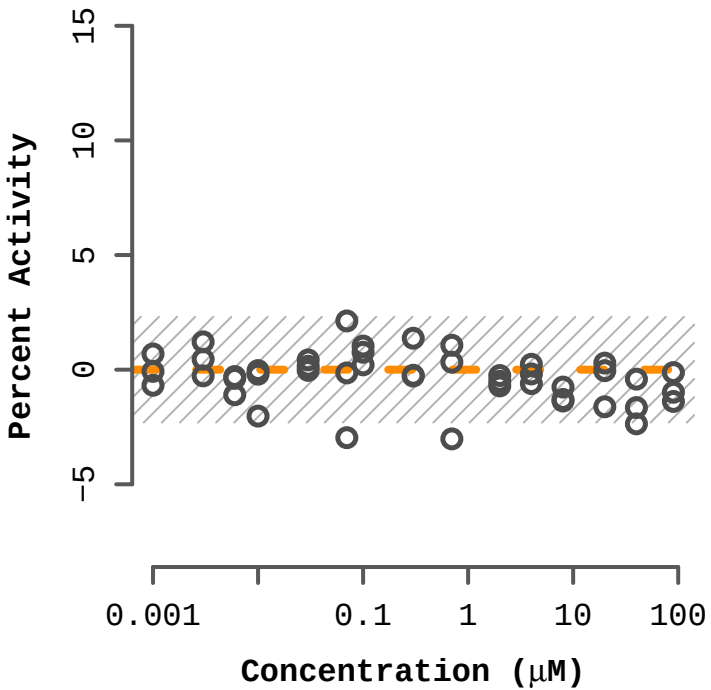
NAME: cis-5-Octen-1-ol
CHID: 47700 **CASRN:** 64275-73-6
SPID(S): Tox21_302602
M4ID: 12476531

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

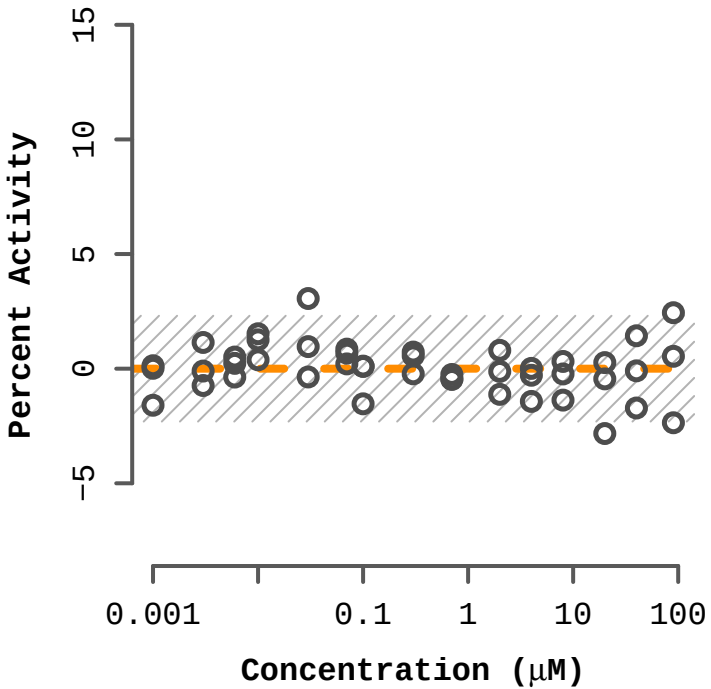
NAME: 2-Propylphenol
CHID: 47702 **CASRN:** 644-35-9
SPID(S): Tox21_302552
M4ID: 12476581

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.669 **MAX_MED:** 0.761 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

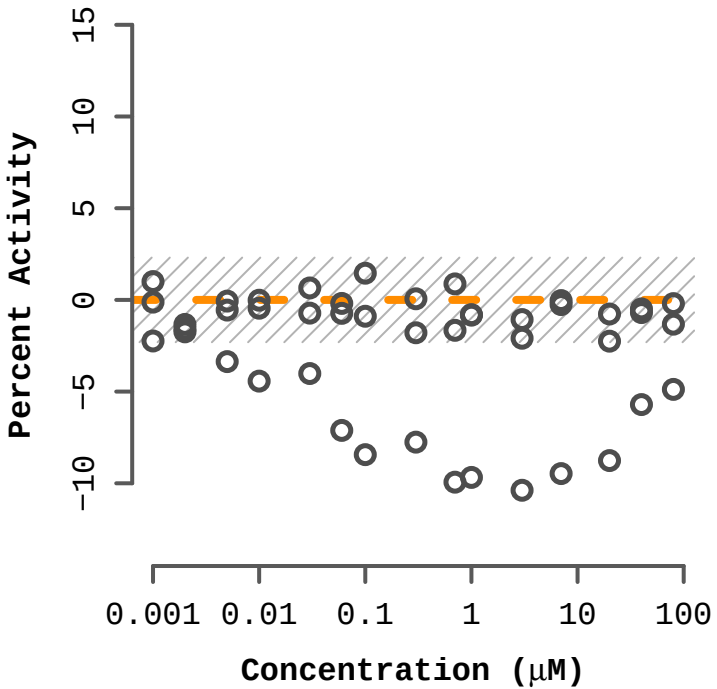
NAME: Maltol isobutyrate
CHID: 47703 **CASRN:** 65416-14-0
SPID(S): Tox21_302601
M4ID: 12476532

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

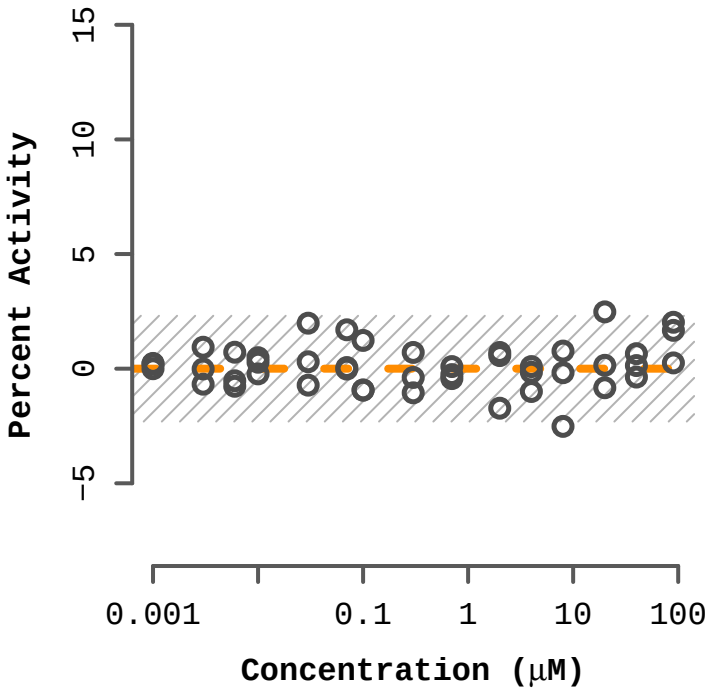
NAME: Methyl 2-methyl-3-furyl disulfide
CHID: 47704 **CASRN:** 65505-17-1
SPID(S): Tox21_303594
M4ID: 12475551

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.94	NA	NA
PROB:	1	NA	NA
RMSE:	4.19	NA	NA

MAX_MEAN: −0.452 **MAX_MED:** −0.119 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

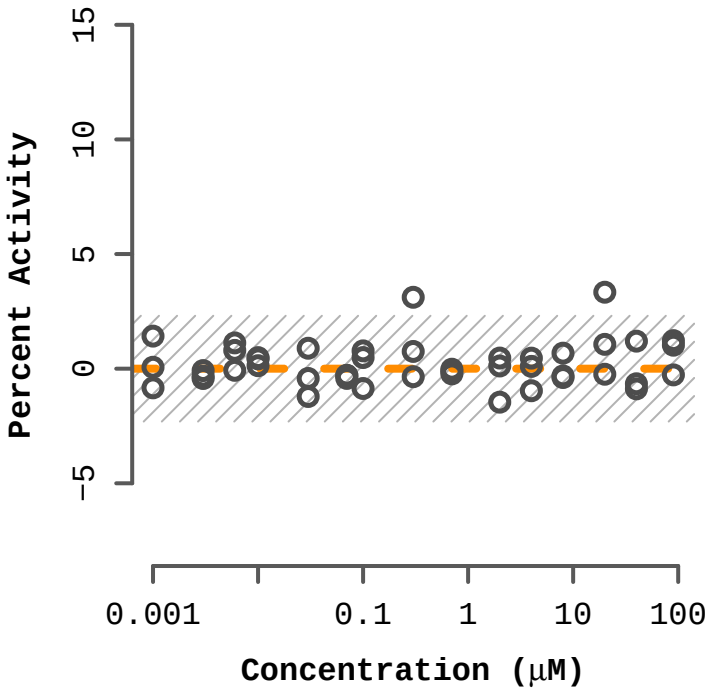
NAME: 12-Oxahexadecanolide
CHID: 47705 **CASRN:** 6707-60-4
SPID(S): Tox21_302556
M4ID: 12476577

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

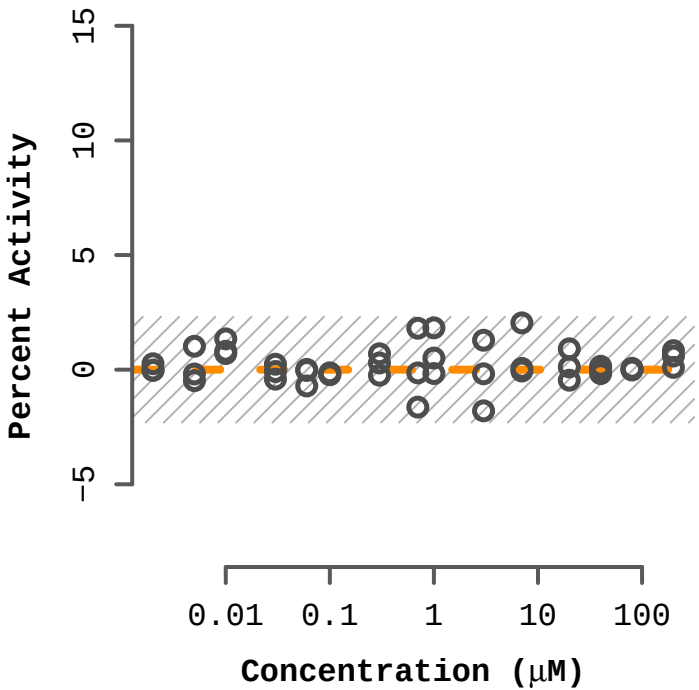
NAME: 2-Methyl-4-propyl-1,3-oxathiane
CHID: 47706 **CASRN:** 67715-80-4
SPID(S): Tox21_303625
M4ID: 12475520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

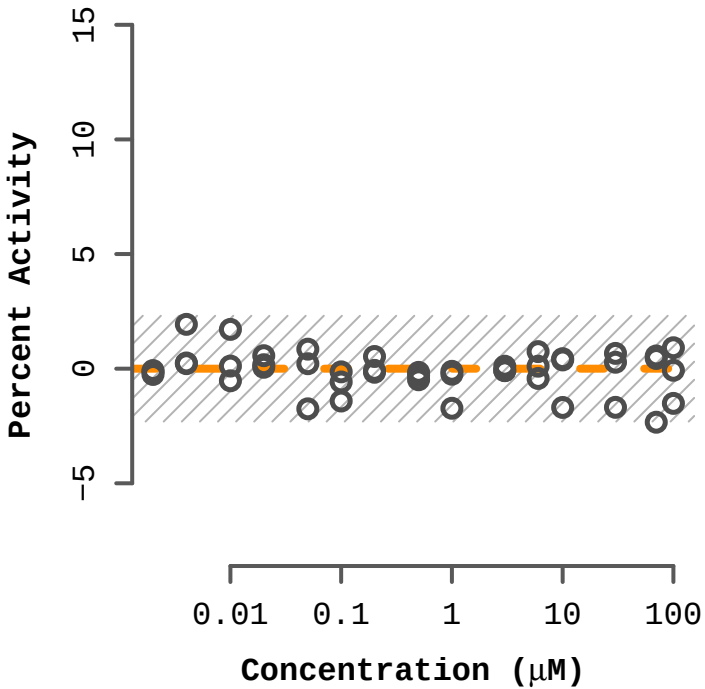
NAME: (Methylthio)methylpyrazine
CHID: 47707 **CASRN:** 67952-65-2
SPID(S): Tox21_302591
M4ID: 12476542

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.952 **MAX_MED:** 0.805 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

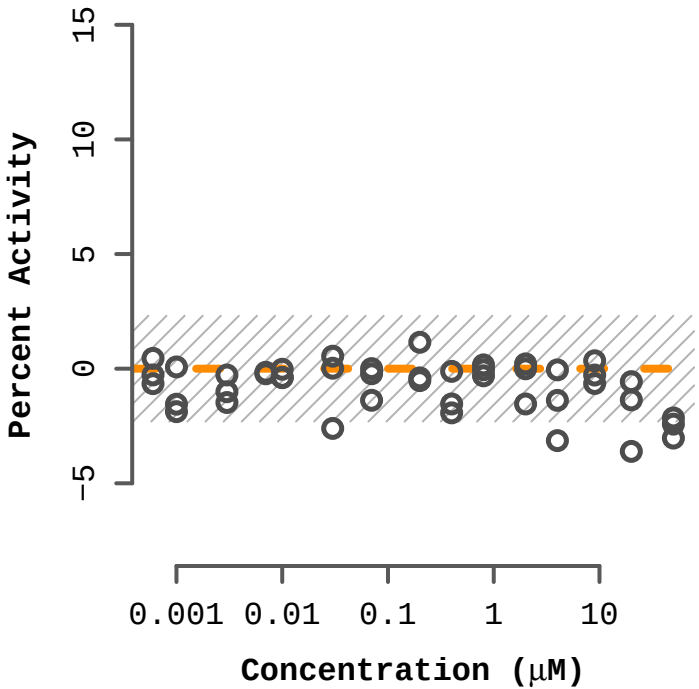
NAME: Igepal CO−890
CHID: 47708 CASRN: NOCAS_47708
SPID(S): Tox21_302531
M4ID: 12476602

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.445 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

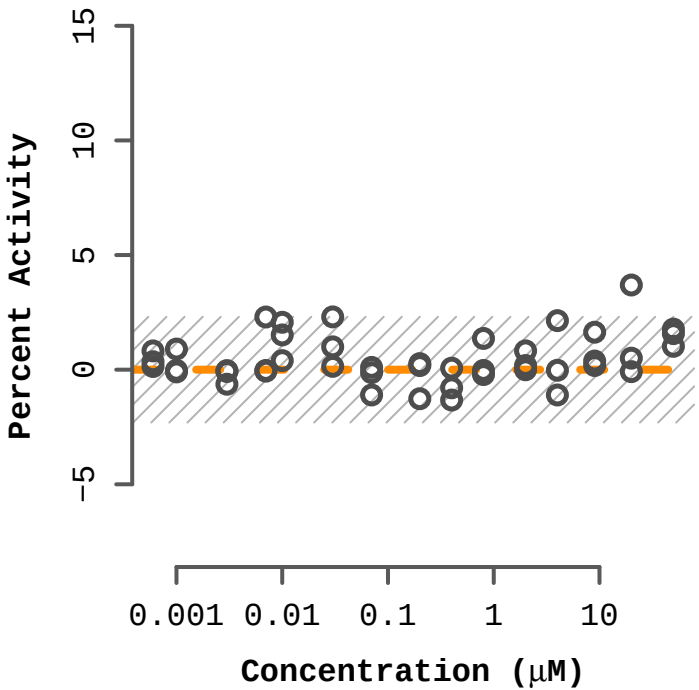
NAME: Cananga oil
CHID: 47709 **CASRN:** 68606-83-7
SPID(S): Tox21_302703
M4ID: 12476430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.0777 **MAX_MED:** 0.0217 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

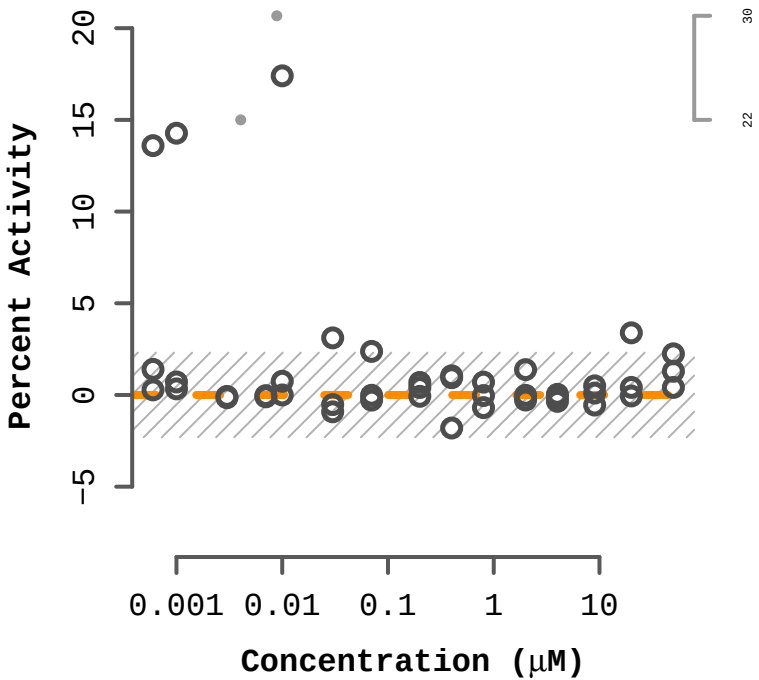
NAME: Bran
CHID: 47711 **CASRN:** 68916-76-7
SPID(S): Tox21_301291
M4ID: 12477842

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

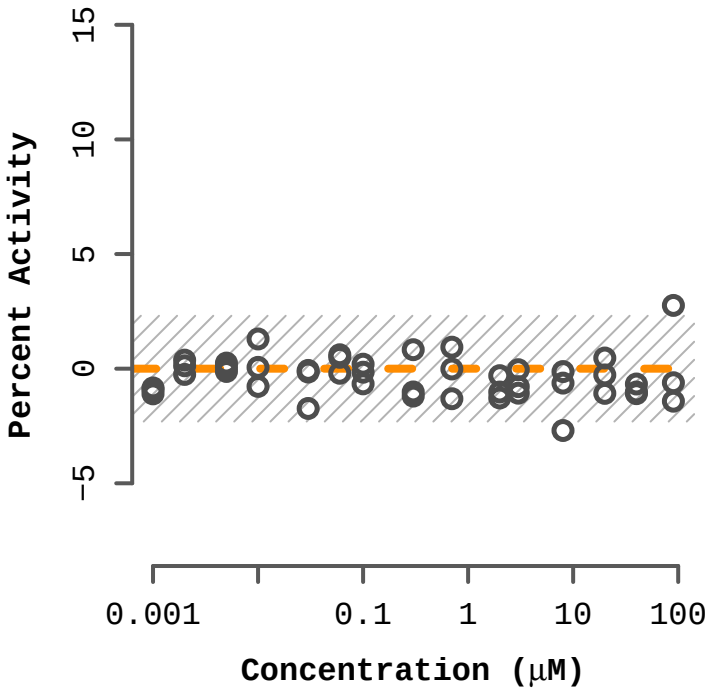
NAME: Cornmint oil
CHID: 47712 **CASRN:** 68917-18-0
SPID(S): Tox21_302670
M4ID: 12476463 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	238.54	NA	NA
PROB:	1	NA	NA
RMSE:	6.83	NA	NA

MAX_MEAN: 9.95 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

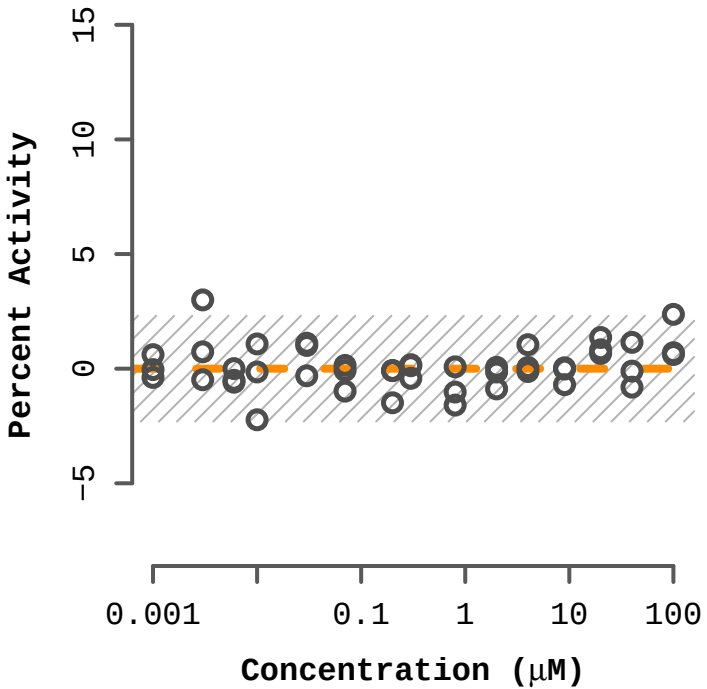
NAME: Anisyl propionate
CHID: 47713 **CASRN:** 7549-33-9
SPID(S): Tox21_302554
M4ID: 12476579

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.302 **MAX_MED:** 0.497 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

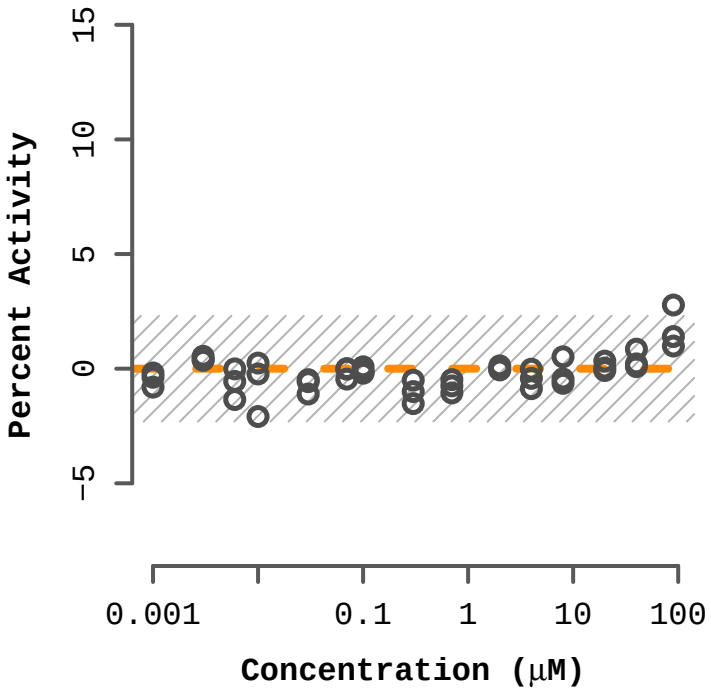
NAME: 3-Methyl-1,2-cyclopentanedione
CHID: 47716 **CASRN:** 765-70-8
SPID(S): Tox21_302629
M4ID: 12476504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

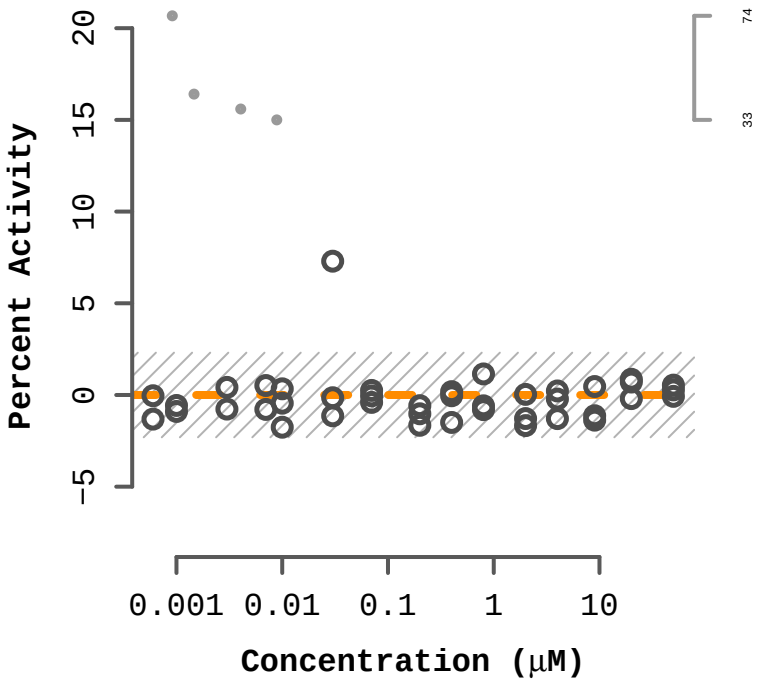
NAME: 4-Methyl-1-phenyl-2-pentanol
CHID: 47717 **CASRN:** 7779-78-4
SPID(S): Tox21_302657
M4ID: 12476476

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

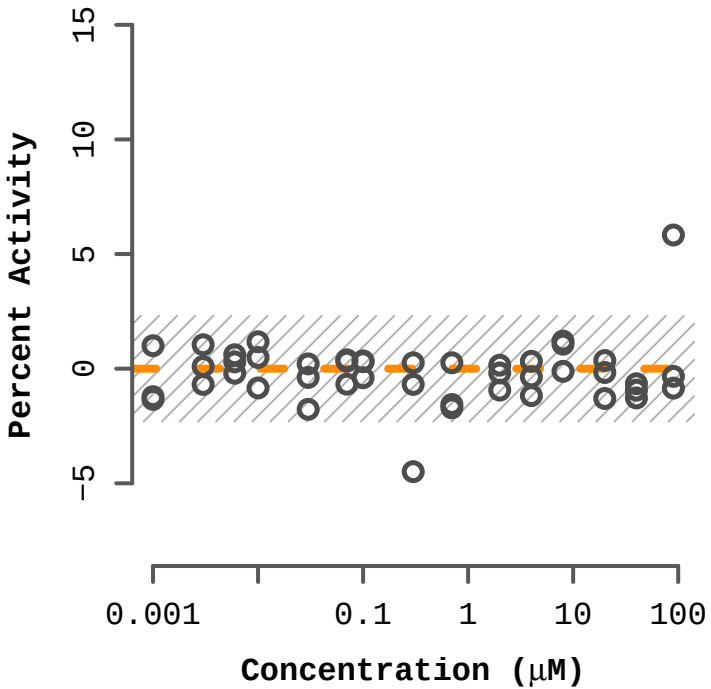
NAME: Petitgrain oil
CHID: 47721 **CASRN:** 8014-17-3
SPID(S): Tox21_301290
M4ID: 12477843 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	257.78	NA	NA
PROB:	1	NA	NA
RMSE:	14.88	NA	NA

MAX_MEAN: 24.2 **MAX_MED:** 0.707 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

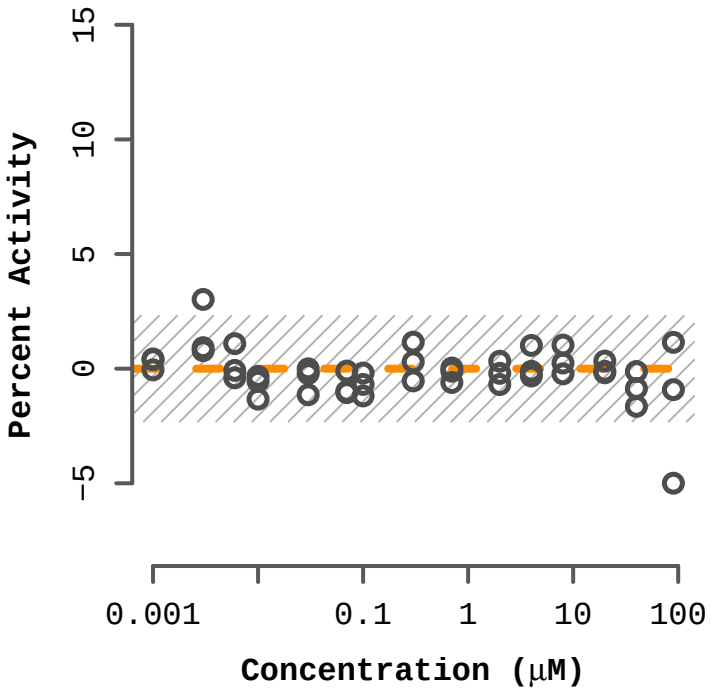
NAME: Trithioacetone
CHID: 47723 **CASRN:** 828-26-2
SPID(S): Tox21_302581
M4ID: 12476552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

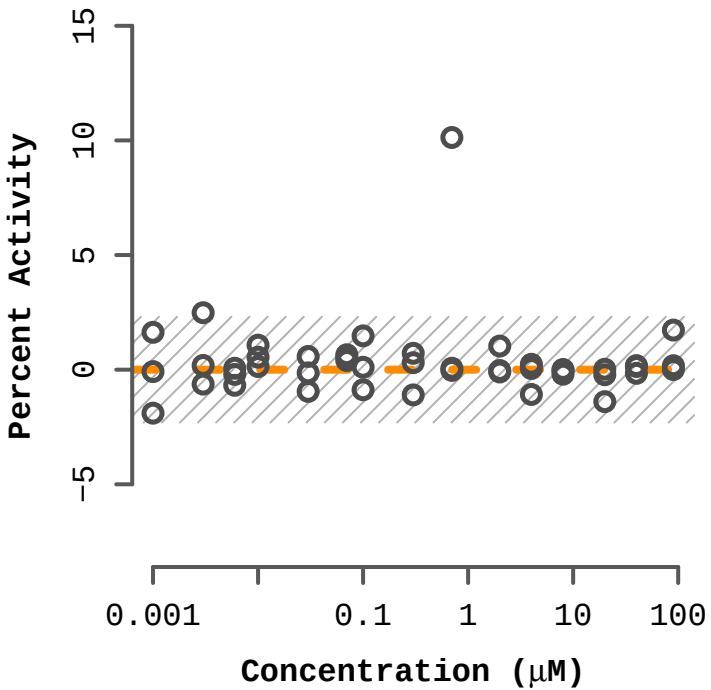
NAME: 2,2,2-Trichloro-1-phenylethyl acetate
CHID: 47725 **CASRN:** 90-17-5
SPID(S): Tox21_302598
M4ID: 12476535

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.918 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

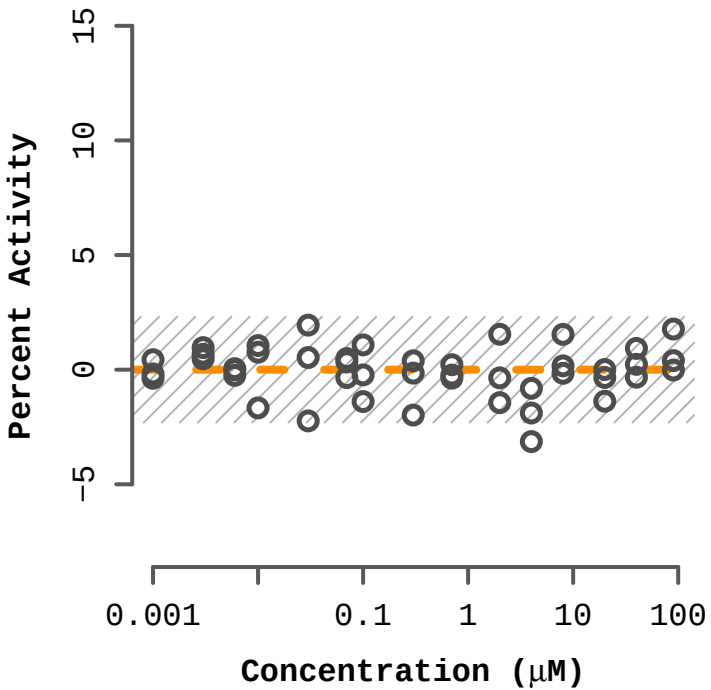
NAME: trans-2-Ethoxy-5-(1-propenyl)phenol
CHID: 47726 CASRN: NOCAS_47726
SPID(S): Tox21_302539
M4ID: 12476594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 3.39 MAX_MED: 0.547 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

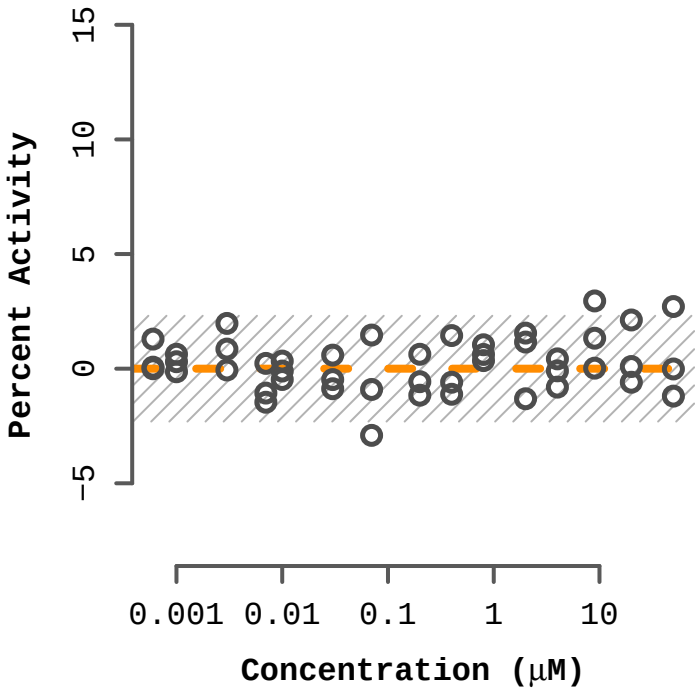
NAME: 2-Ethoxy-5-(1-propenyl)phenol
CHID: 47727 **CASRN:** 94-86-0
SPID(S): Tox21_303945
M4ID: 12475243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.719 **MAX_MED:** 0.765 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

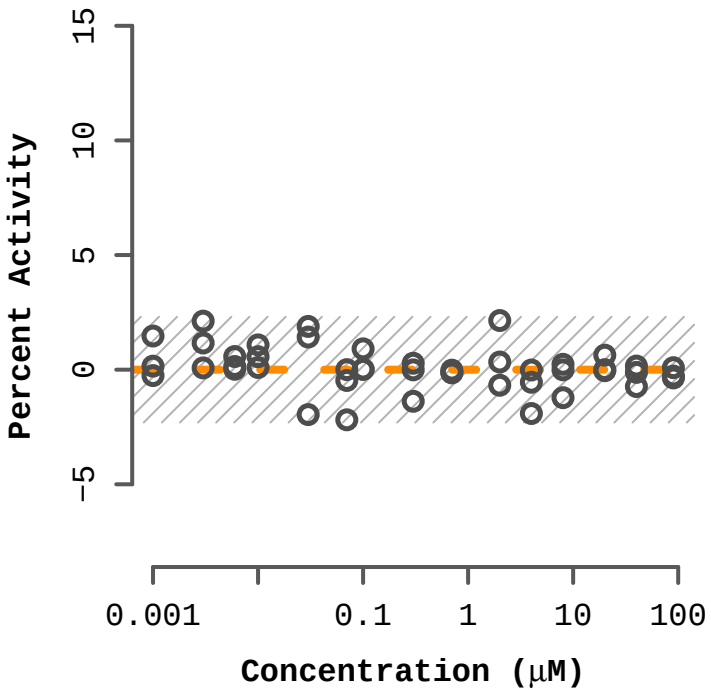
NAME: Orange terpenes
CHID: 47730 **CASRN:** 8028-48-6
SPID(S): Tox21_302597
M4ID: 12476536

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

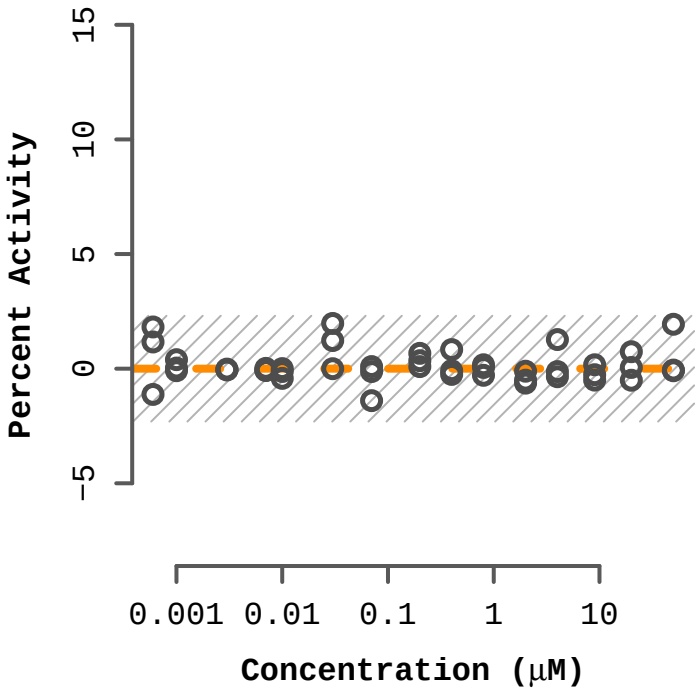
NAME: Dibenzothiophene
CHID: 47741 **CASRN:** 132-65-0
SPID(S): Tox21_303415
M4ID: 12475724

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

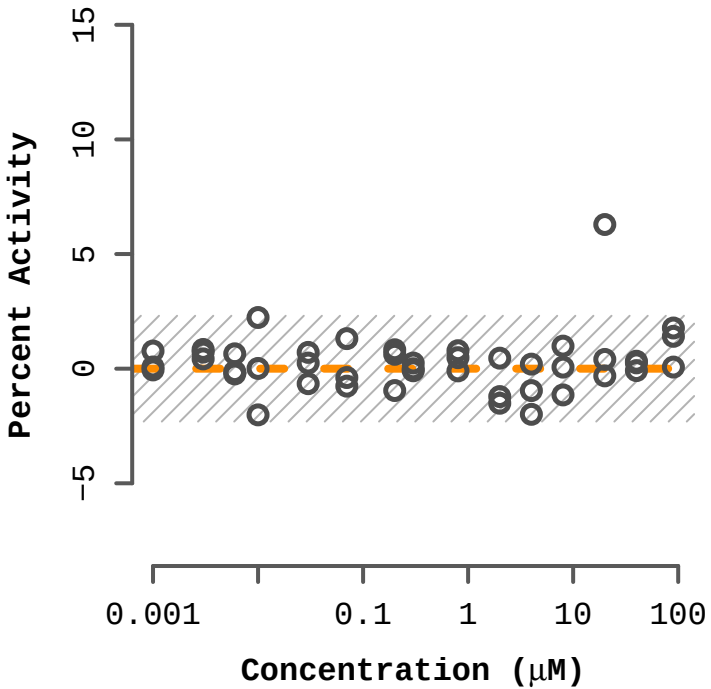
NAME: Dibenzothiophene
CHID: 47741 **CASRN:** 132-65-0
SPID(S): Tox21_111308_1
M4ID: 12483777

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

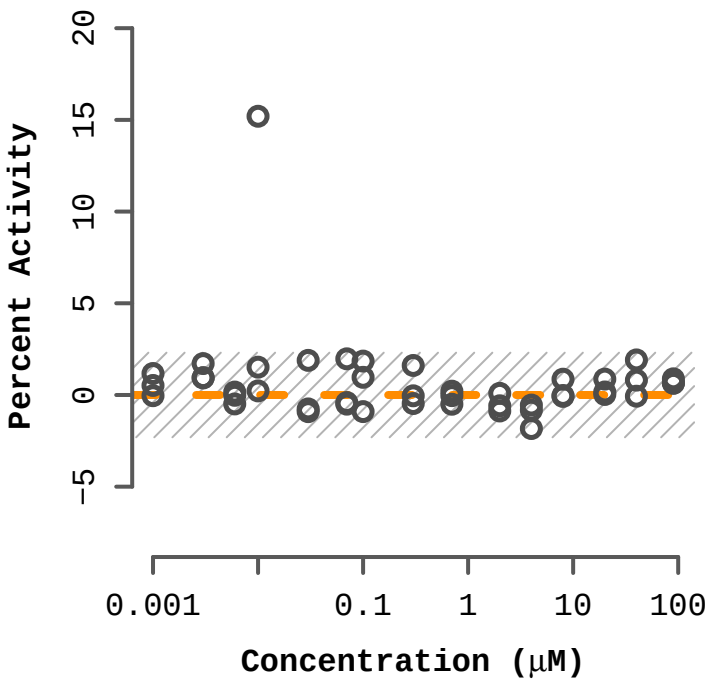
NAME: 2-Fluorobiphenyl
CHID: 47744 **CASRN:** 321-60-8
SPID(S): Tox21_202912
M4ID: 12479340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.13 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

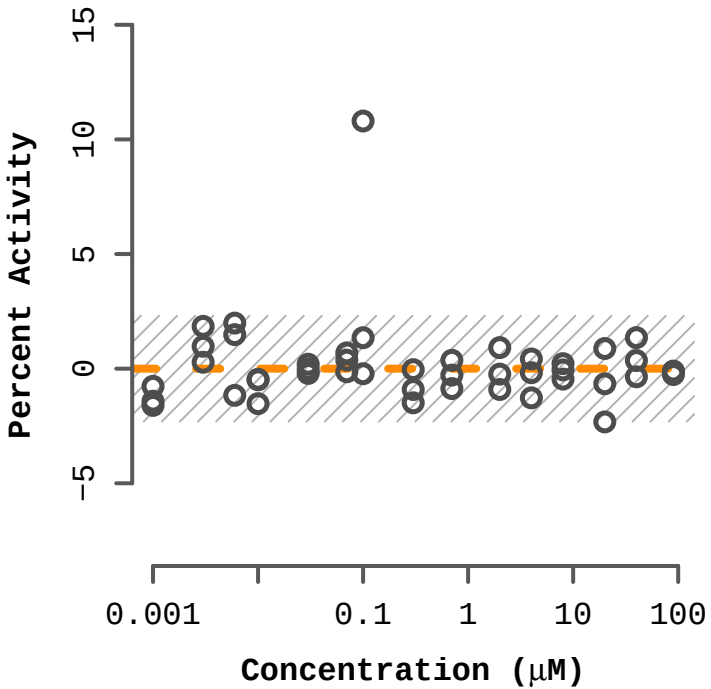
NAME: 2-Fluorophenol
CHID: 47745 CASRN: 367-12-4
SPID(S): Tox21_202915
M4ID: 12479337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.58	NA	NA
PROB:	1	NA	NA
RMSE:	2.45	NA	NA

MAX_MEAN: 5.65 MAX_MED: 1.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

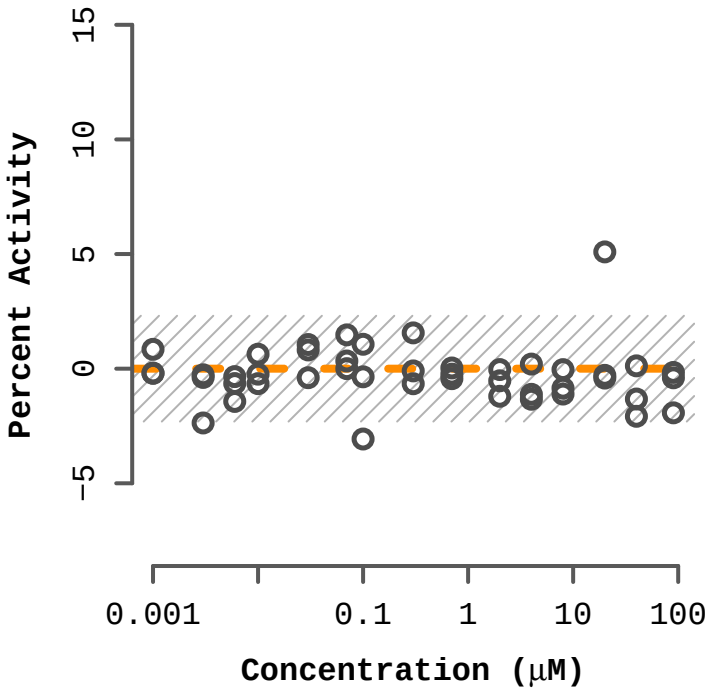
NAME: Methylcyclohexane
CHID: 47749 **CASRN:** 108-87-2
SPID(S): Tox21_303867
M4ID: 12475321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 3.98 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

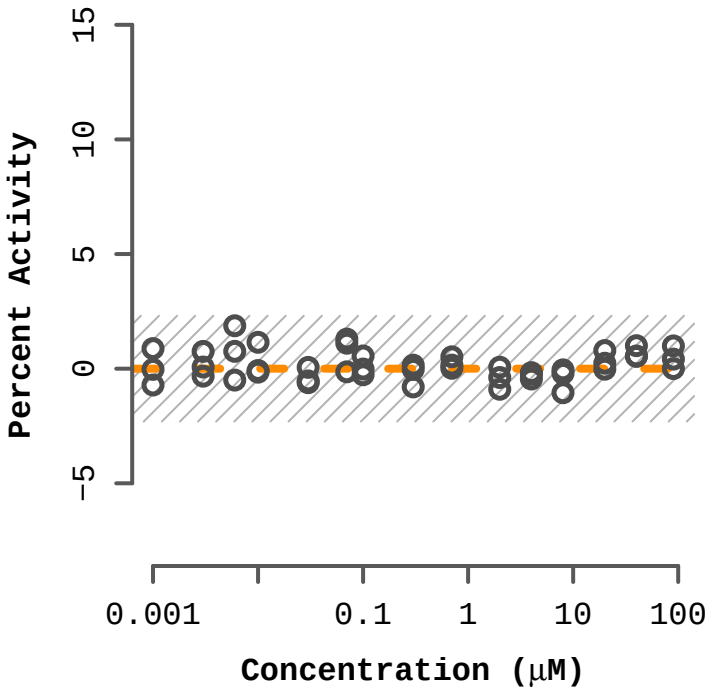
NAME: Tetrahydrothiophene
CHID: 47760 **CASRN:** 110-01-0
SPID(S): Tox21_304026
M4ID: 12475162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 0.818 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

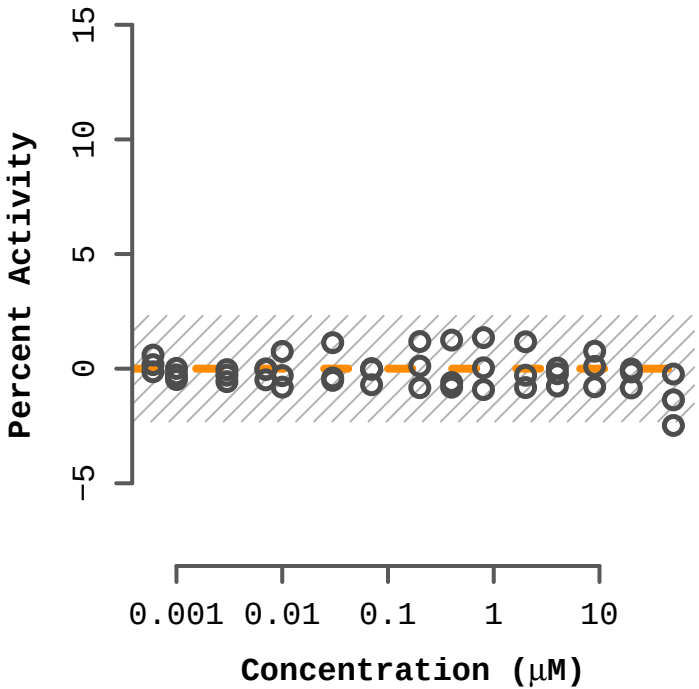
NAME: 1,2,3-Trimethylbenzene
CHID: 47769 **CASRN:** 526-73-8
SPID(S): Tox21_303868
M4ID: 12475320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.756 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

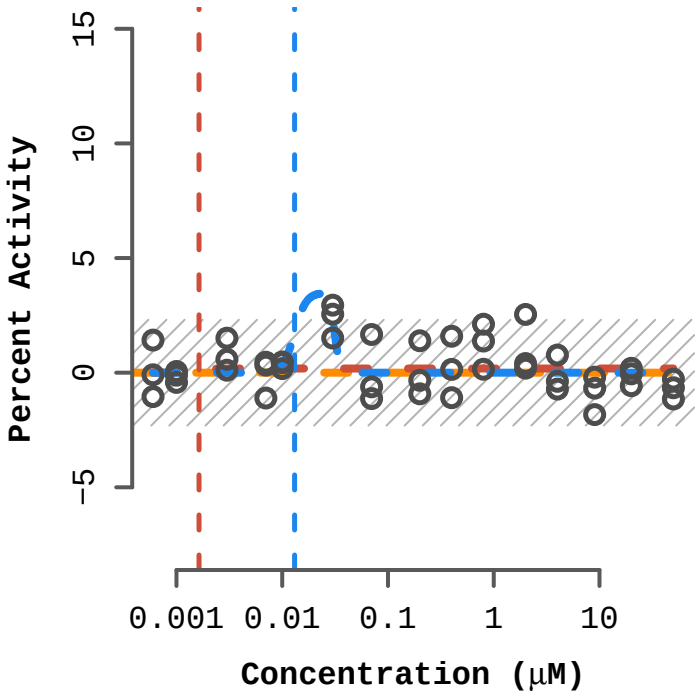
NAME: Diphenylpyraline hydrochloride
CHID: 47772 **CASRN:** 132-18-3
SPID(S): Tox21_110419_1
M4ID: 12484375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.214 **MAX_MED:** 0.181 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclizine hydrochloride
CHID: 47773 **CASRN:** 303-25-3
SPID(S): Tox21_110433_1
M4ID: 12484361

HILL MODEL (in red):

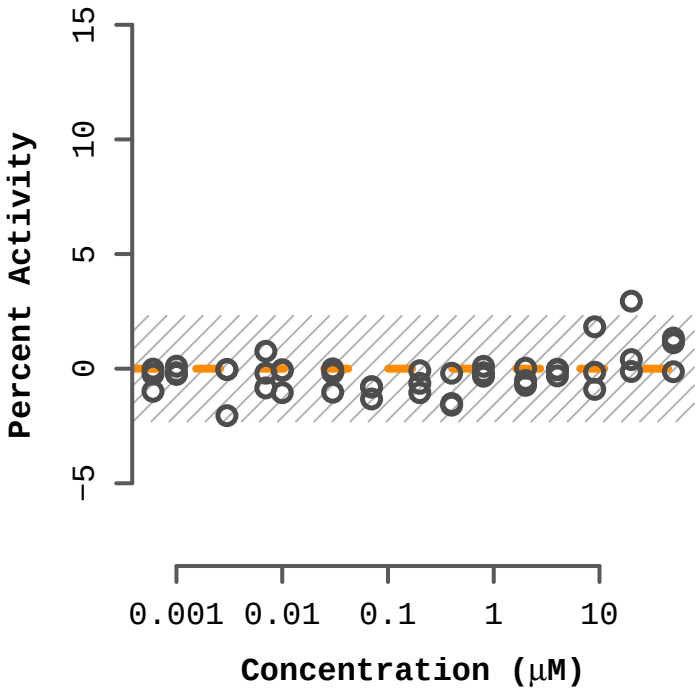
	tp	ga	gw
val:	0.181	−2.79	8
sd:	0.176	0.776	25.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.49	−1.88	8	−1.5	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	140.53	145.44	135.22
PROB:	0.07	0.01	0.93
RMSE:	1.12	1.09	0.94

MAX_MEAN: 2.34 **MAX_MED:** 2.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

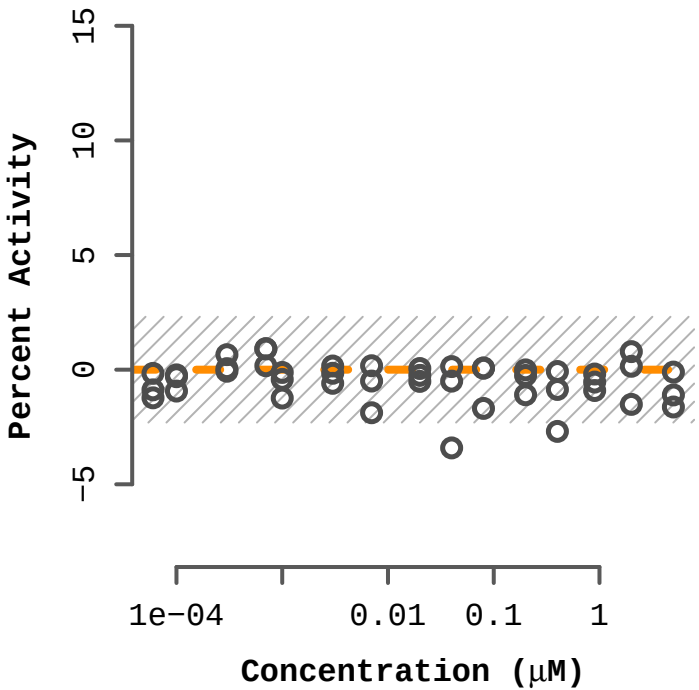
NAME: Trimethobenzamide hydrochloride
CHID: 47774 **CASRN:** 554-92-7
SPID(S): Tox21_110465_1
M4ID: 12484335

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

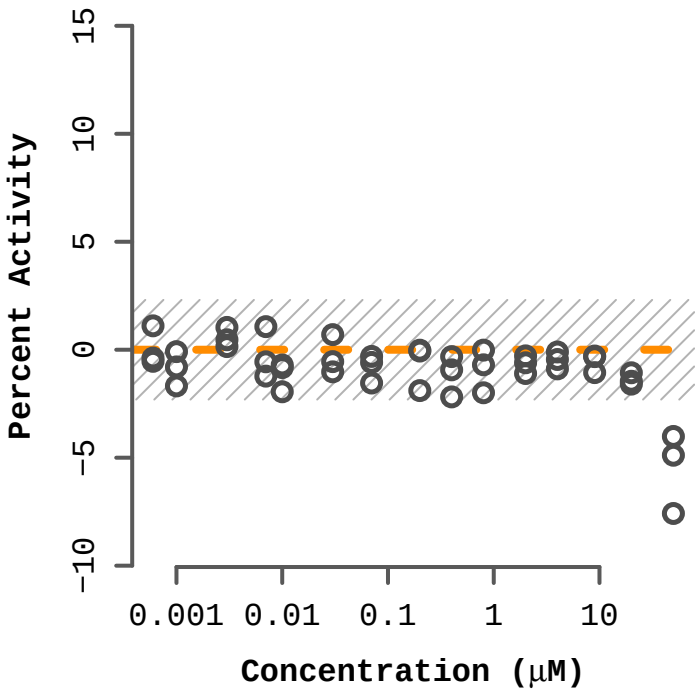
NAME: Debrisoquin sulfate
CHID: 47775 **CASRN:** 581-88-4
SPID(S): Tox21_110468_1
M4ID: 12484332

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.666 **MAX_MED:** 0.906 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

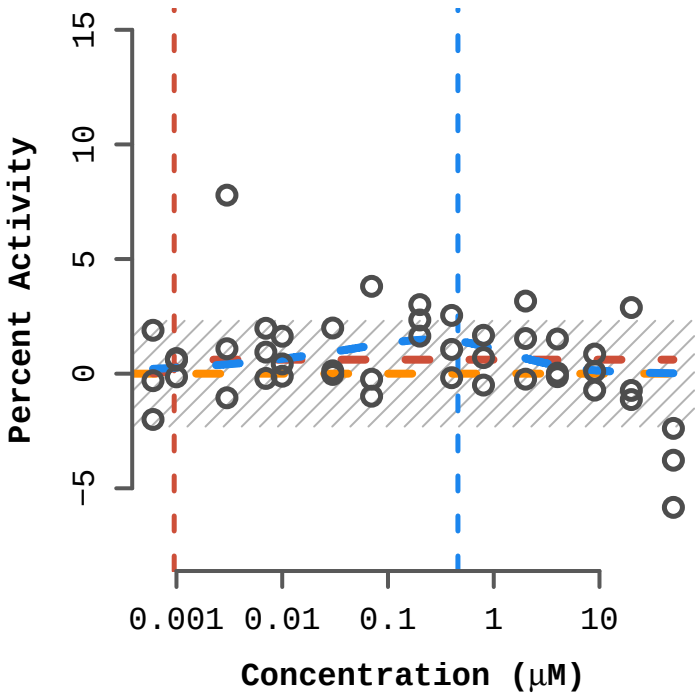
NAME: Proguanil hydrochloride
CHID: 47776 **CASRN:** 637-32-1
SPID(S): Tox21_110476_1
M4ID: 12484327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.76	NA	NA

MAX_MEAN: 0.549 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pramoxine hydrochloride
CHID: 47777 **CASRN:** 637-58-1
SPID(S): Tox21_110477_1
M4ID: 12484326

HILL MODEL (in red):

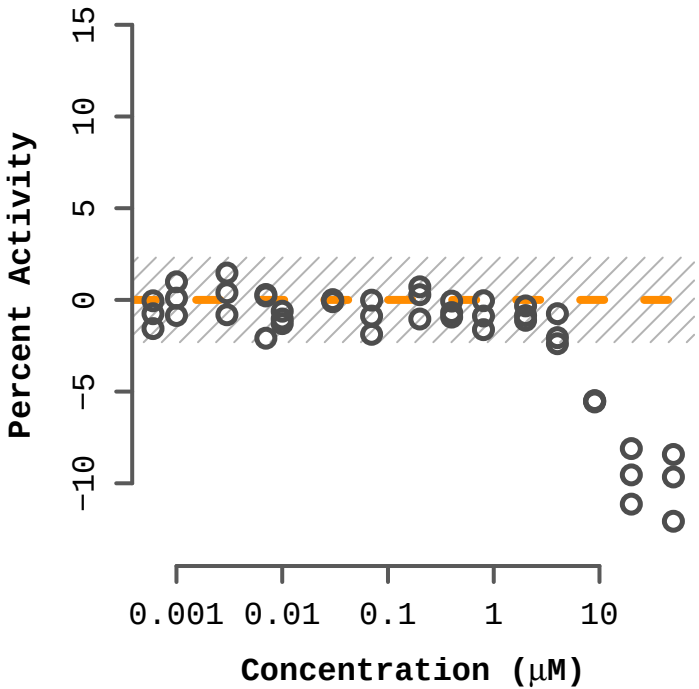
	tp	ga	gw
val:	0.611	−3.02	8
sd:	0.269	0.268	35.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.21	−0.338	0.444	−0.0884	1.27
sd:	55	17.8	0.695	3.95	0.88

	CNST	HILL	GNLS
AIC:	191.33	192.15	190.17
PROB:	0.29	0.19	0.52
RMSE:	2.15	2.06	1.95

MAX_MEAN: 2.61 **MAX_MED:** 2.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

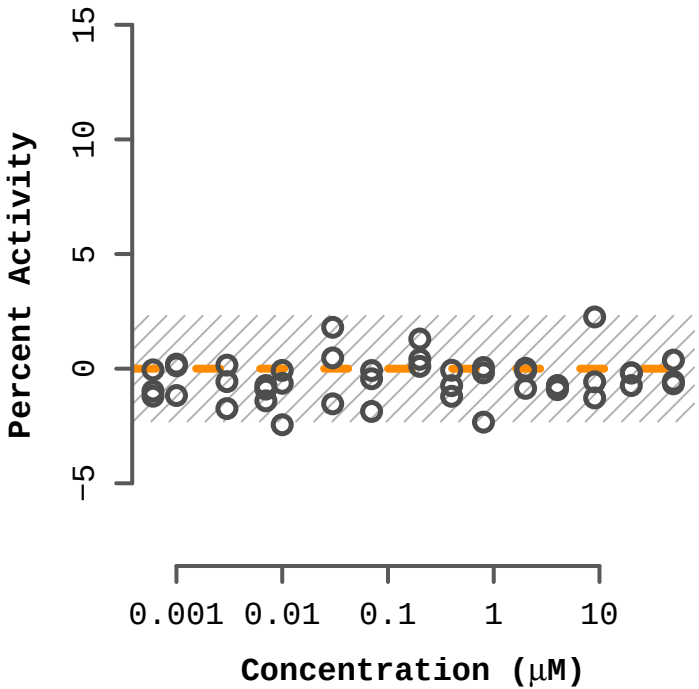
NAME: Ethaverine hydrochloride
CHID: 47779 **CASRN:** 985-13-7
SPID(S): Tox21_110492_1
M4ID: 12484316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.9	NA	NA
PROB:	1	NA	NA
RMSE:	4	NA	NA

MAX_MEAN: 0.351 **MAX_MED:** 0.392 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

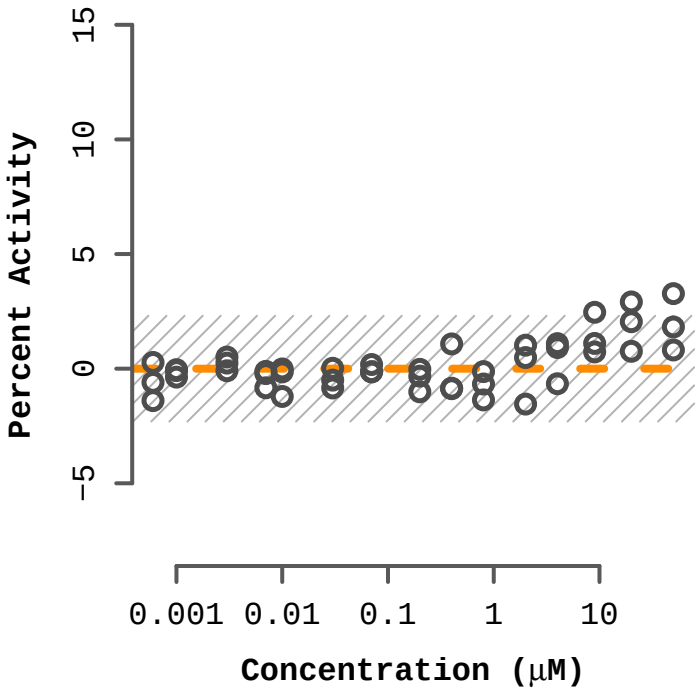
NAME: Mephentermine hemisulfate
CHID: 47780 **CASRN:** 1212-72-2
SPID(S): Tox21_110501_1
M4ID: 12484310

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.96	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.603 **MAX_MED:** 0.471 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

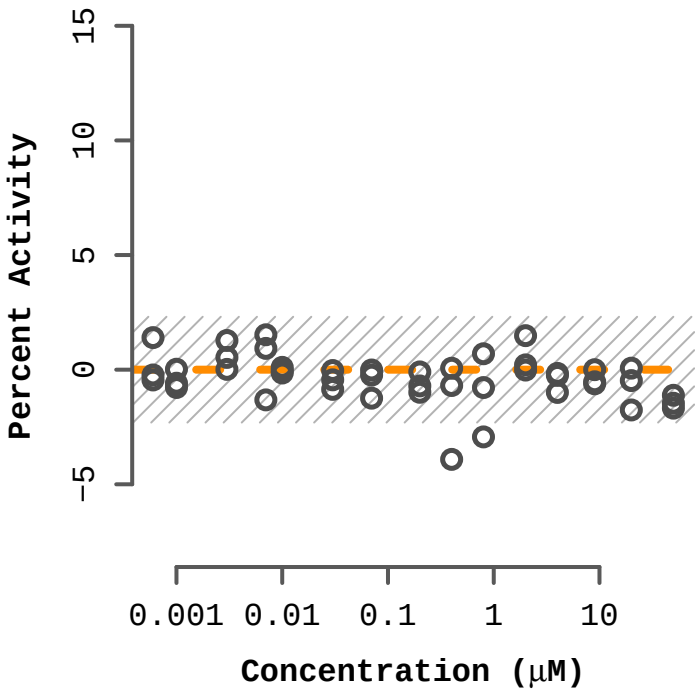
NAME: Tranylcypromine hydrochloride
CHID: 47781 CASRN: 1986-47-6
SPID(S): Tox21_110514_1
M4ID: 12484303

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

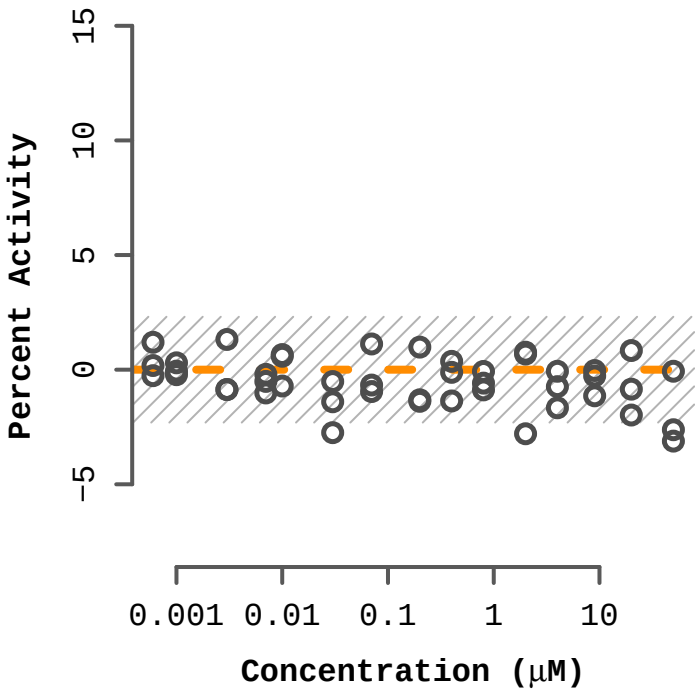
NAME: Antazoline hydrochloride
CHID: 47782 **CASRN:** 2508-72-7
SPID(S): Tox21_110524_1
M4ID: 12484295

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 0.608 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

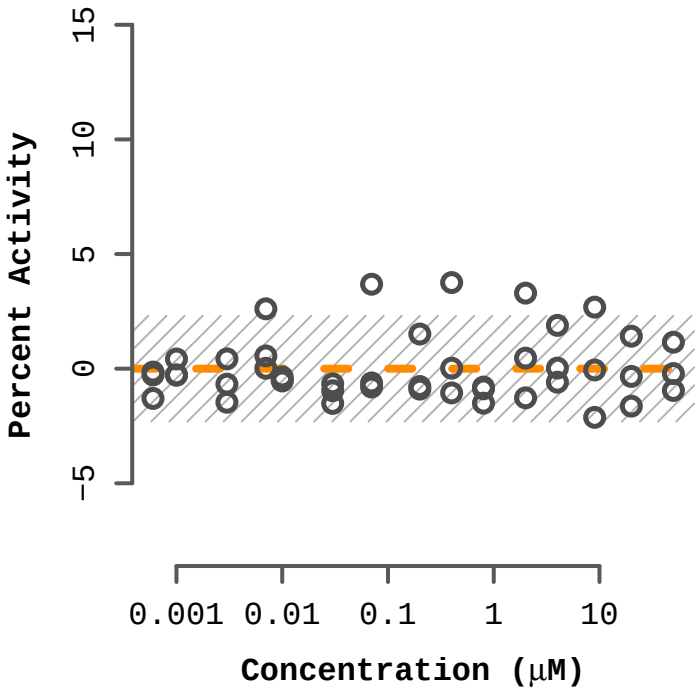
NAME: Acetopromazine maleate
CHID: 47783 **CASRN:** 3598-37-6
SPID(S): Tox21_110536_1
M4ID: 12484284

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.373 **MAX_MED:** 0.682 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

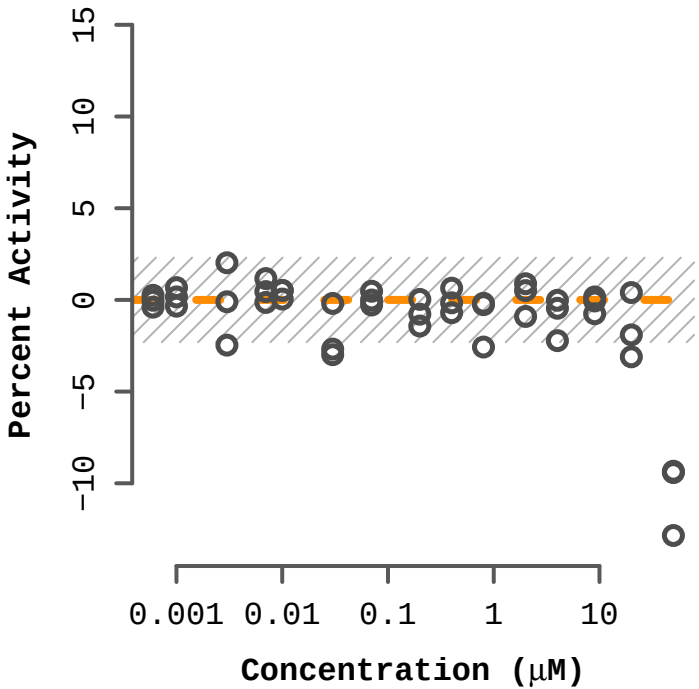
NAME: Flavoxate hydrochloride
CHID: 47784 **CASRN:** 3717-88-2
SPID(S): Tox21_110537_1
M4ID: 12484283

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.557 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

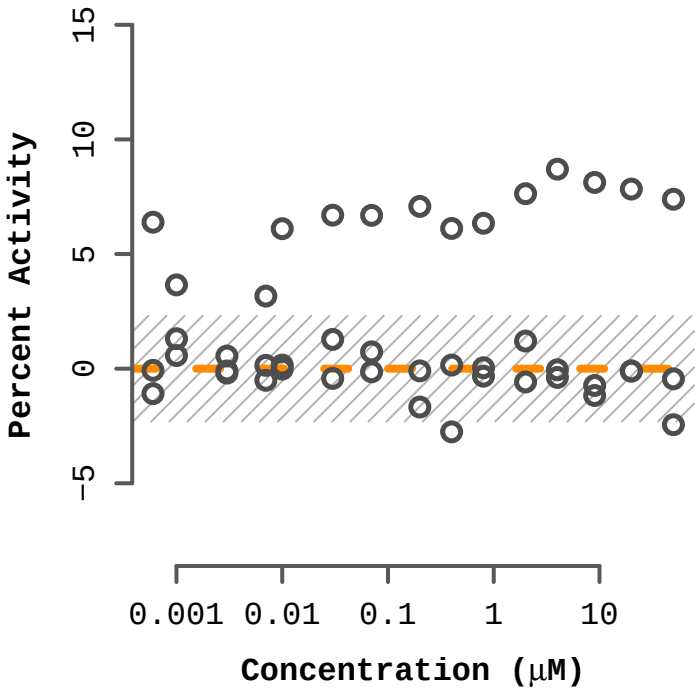
NAME: Clemastine fumarate
CHID: 47785 **CASRN:** 14976-57-9
SPID(S): Tox21_110574_1
M4ID: 12484257

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.44	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 0.495 **MAX_MED:** 0.518 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

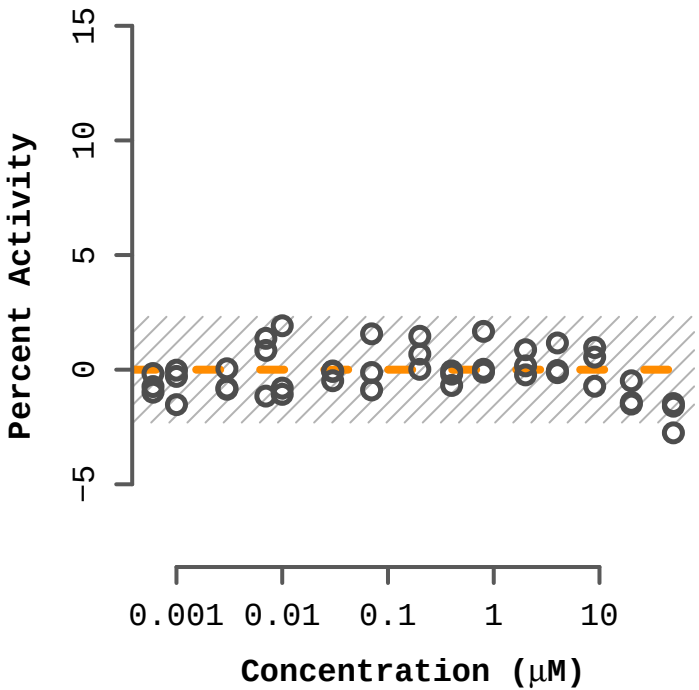
NAME: Moricizine hydrochloride
CHID: 47786 **CASRN:** 29560-58-5
SPID(S): Tox21_110622_1
M4ID: 12484224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	247.35	NA	NA
PROB:	1	NA	NA
RMSE:	3.84	NA	NA

MAX_MEAN: 2.76 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

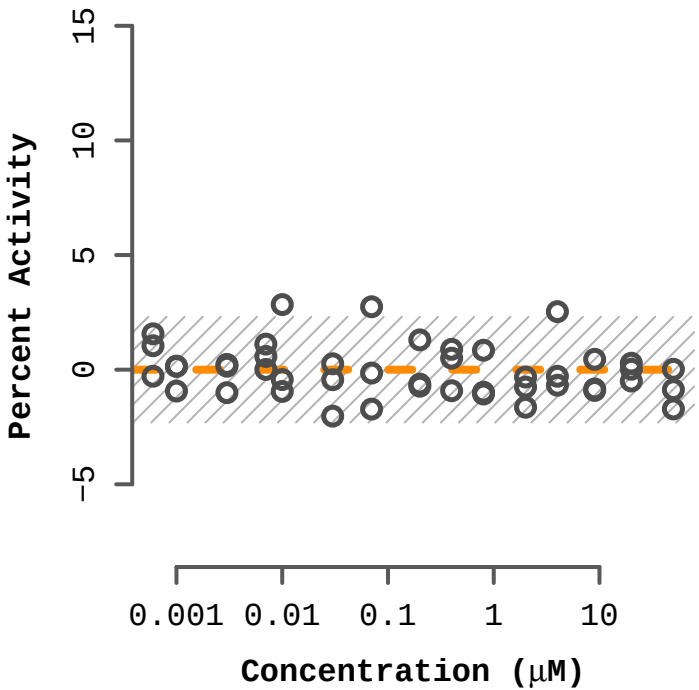
NAME: Clebopride maleate
CHID: 47787 **CASRN:** 84370-95-6
SPID(S): Tox21_110706_1
M4ID: 12484162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.19	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.841 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

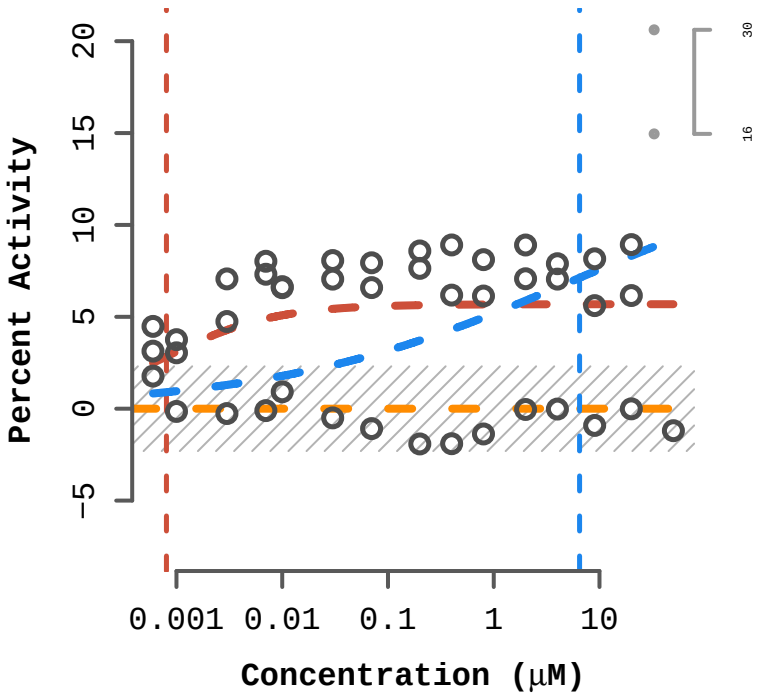
NAME: Ciprofloxacin hydrochloride
CHID: 47788 **CASRN:** 93107-08-5
SPID(S): Tox21_110712_1
M4ID: 12484156

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.775 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Betazole hydrochloride
CHID: 47789 CASRN: 138-92-1
SPID(S): Tox21_110729_1
M4ID: 12484145 BRK

HILL MODEL (in red):

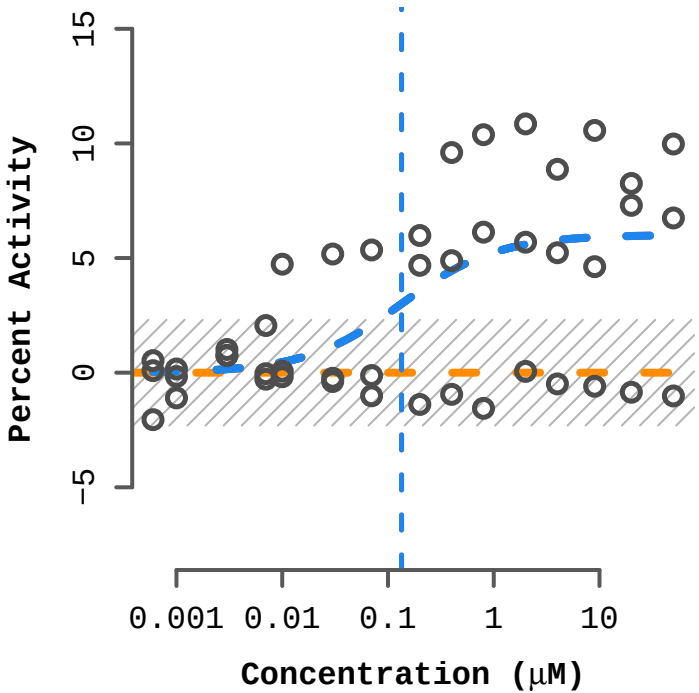
	tp	ga	gw
val:	5.69	−3.09	0.846
sd:	0.935	0.531	1.02

GAIN-LOSS MODEL (in blue):

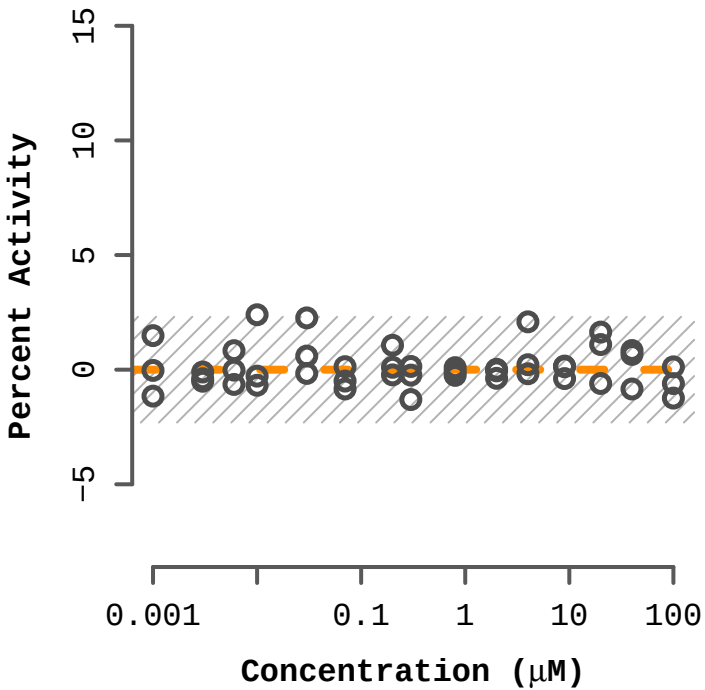
	tp	ga	gw	la	lw
val:	14.2	0.812	0.3	2.99	6.69
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	306.89	276.14	289.75
PROB:	0	1	0
RMSE:	7.51	5.42	5.45

MAX_MEAN: 14.9 **MAX_MED:** 15.7 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Phenyltoloxamine citrate
CHID:    47790   CASRN: 1176-08-5
SPID(S): Tox21_110862_1
M4ID:    12484060

HILL MODEL (in red):
      tp       ga       gw
val:  6.01     -0.872   0.959
sd:   1.29     0.421    0.973

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.01     -0.872   0.959    2.95     6.14
sd:   1.29     0.421    0.973    1940     9460

      CNST        HILL        GNLS
AIC:  272.11      248.95      252.95
PROB: 0           0.88        0.12
RMSE: 4.89        3.43        3.43

MAX_MEAN: 5.53      MAX_MED: 7.3       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

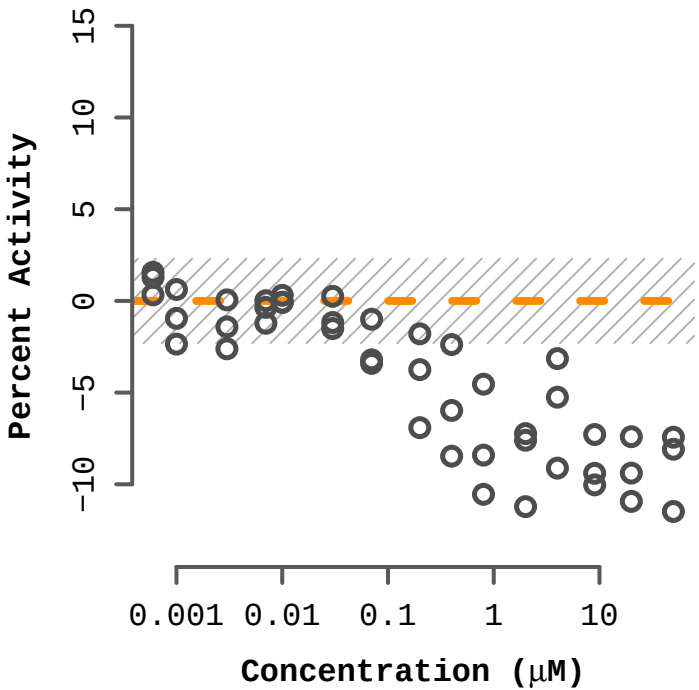
NAME: Formalin
CHID: 47796 **CASRN:** NOCAS_47796
SPID(S): Tox21_302438
M4ID: 12476695

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.898 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

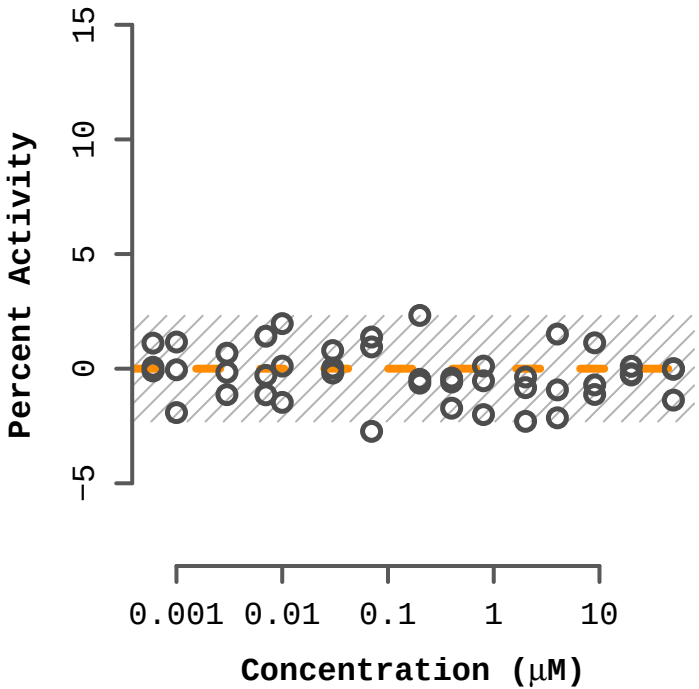
NAME: Idarubicin hydrochloride
CHID: 47797 **CASRN:** 57852-57-0
SPID(S): Tox21_111236_1
M4ID: 12483823

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.19	NA	NA
PROB:	1	NA	NA
RMSE:	5.85	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

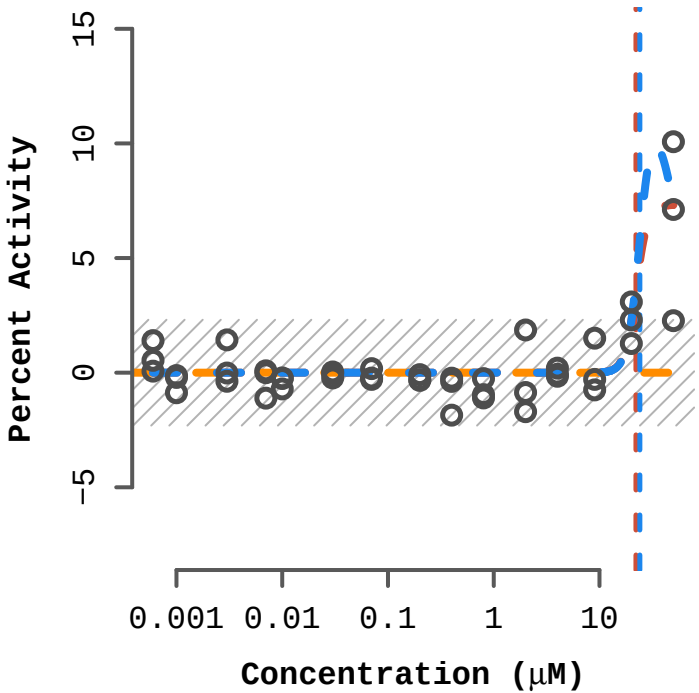
NAME: 3-(Octadecyloxy)-1,2-propanediol
CHID: 47799 **CASRN:** 544-62-7
SPID(S): Tox21_111515_1
M4ID: 12483641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 0.411 **MAX_MED:** 0.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Alendronate sodium
CHID: 47801 CASRN: 121268-17-5
SPID(S): Tox21_111553_1
M4ID: 12483622

HILL MODEL (in red):

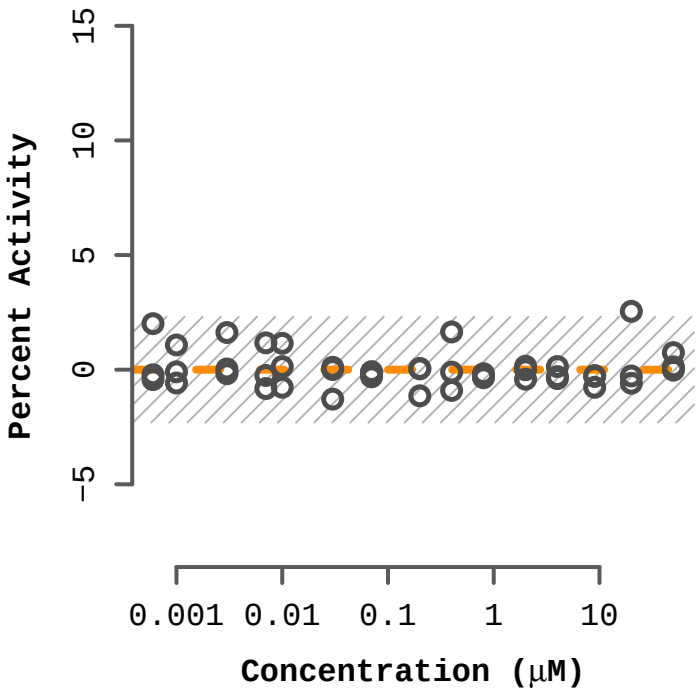
	tp	ga	gw
val:	7.33	1.34	8
sd:	0.702	0.0937	16.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.1	1.38	7.78	1.75	3.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	158.89	130.44	134.44
PROB:	0	0.88	0.12
RMSE:	2.09	1.14	1.14

MAX_MEAN: 6.49 **MAX_MED:** 7.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

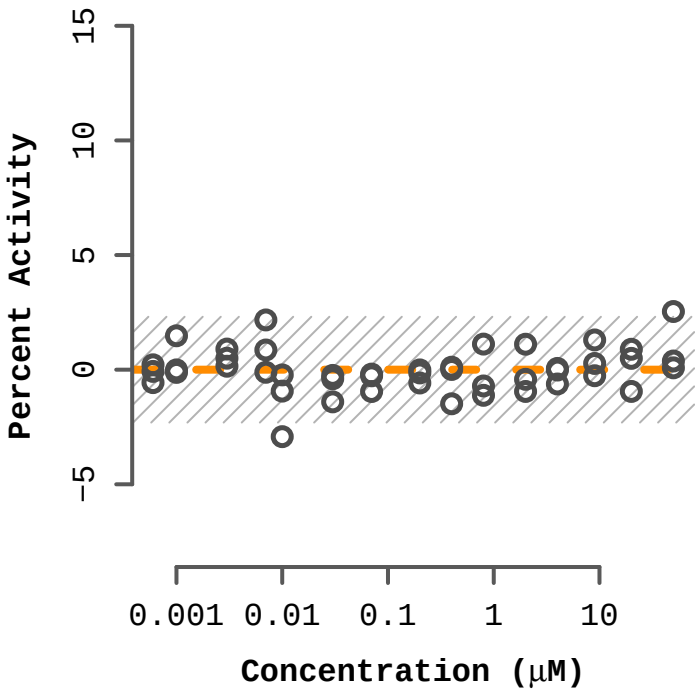
NAME: Lincomycin hydrochloride
CHID: 47803 **CASRN:** 859-18-7
SPID(S): Tox21_111575_1
M4ID: 12483609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.56 **MAX_MED:** 0.136 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

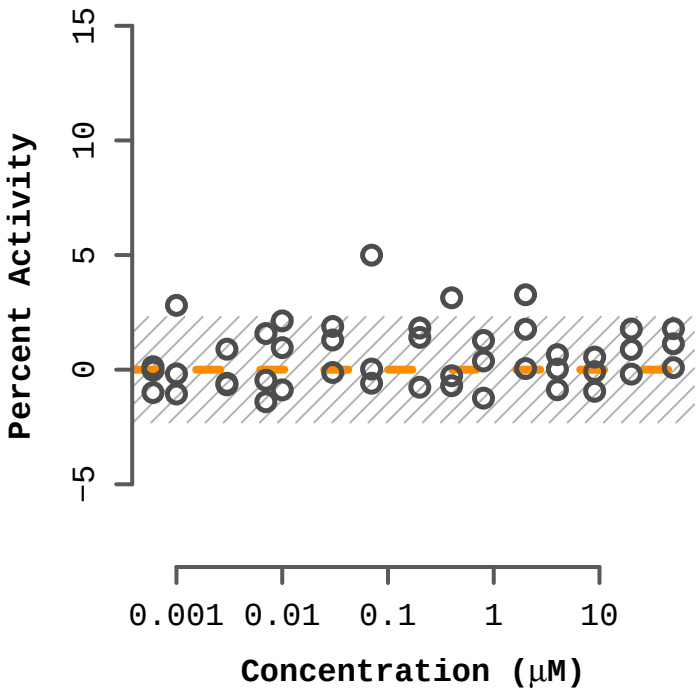
NAME: Benzathine penicillin G
CHID: 47804 **CASRN:** 1538-09-6
SPID(S): Tox21_111587_1
M4ID: 12483603

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1 **MAX_MED:** 0.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

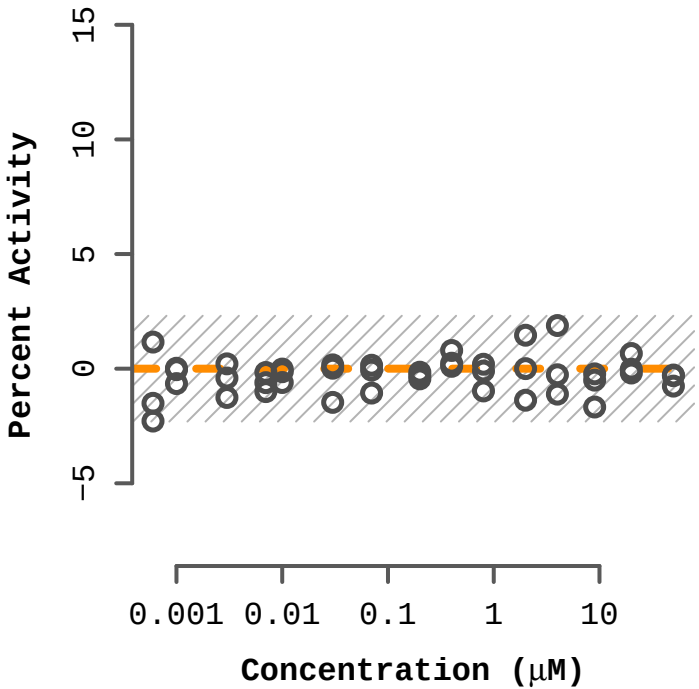
NAME: Norepinephrine bitartrate
CHID: 47806 **CASRN:** 69815-49-2
SPID(S): Tox21_111640_1
M4ID: 12483567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.47	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

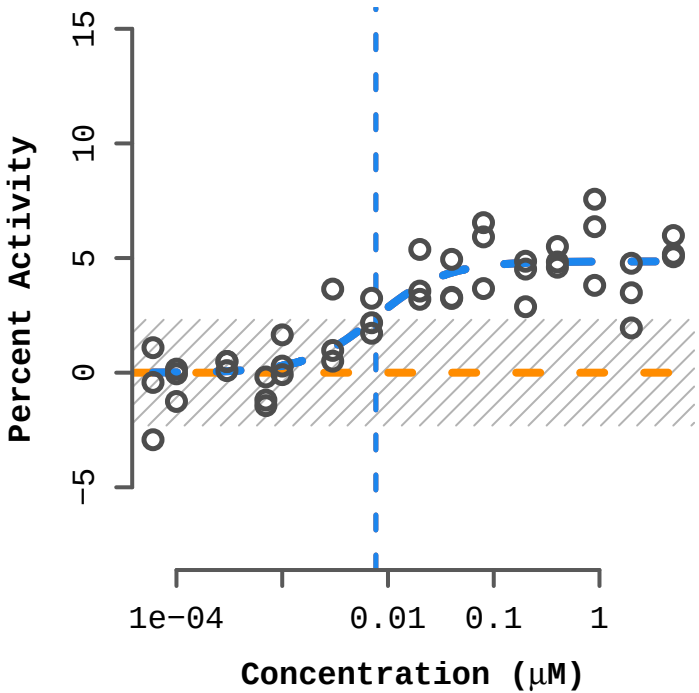
NAME: Clobutinol hydrochloride
CHID: 47807 **CASRN:** 1215-83-4
SPID(S): Tox21_111667_1
M4ID: 12483546

HILL MODEL: Not applicable.

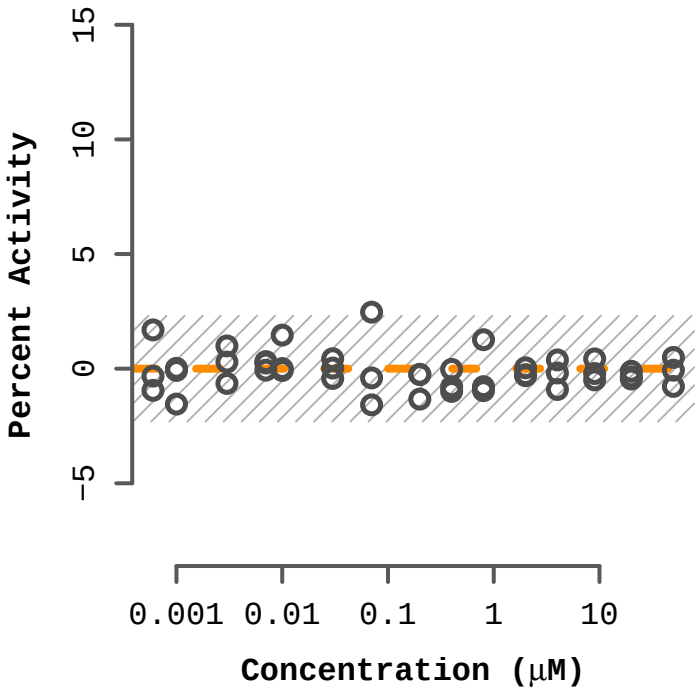
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.379 **MAX_MED:** 0.24 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hydroxychloroquine sulfate
CHID:    47811   CASRN: 747-36-4
SPID(S): Tox21_111707_1
M4ID:    12483525

HILL MODEL (in red):
      tp       ga       gw
val:  4.85     -2.11    1.33
sd:   0.308    0.134    0.423

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.85     -2.11    1.33     2.04     7.22
sd:   0.308    0.134    0.423    4520     24500

      CNST        HILL        GNLS
AIC:  252.23      152.81      156.81
PROB: 0           0.88        0.12
RMSE: 3.67        1.21        1.21

MAX_MEAN: 5.92      MAX_MED: 6.37      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

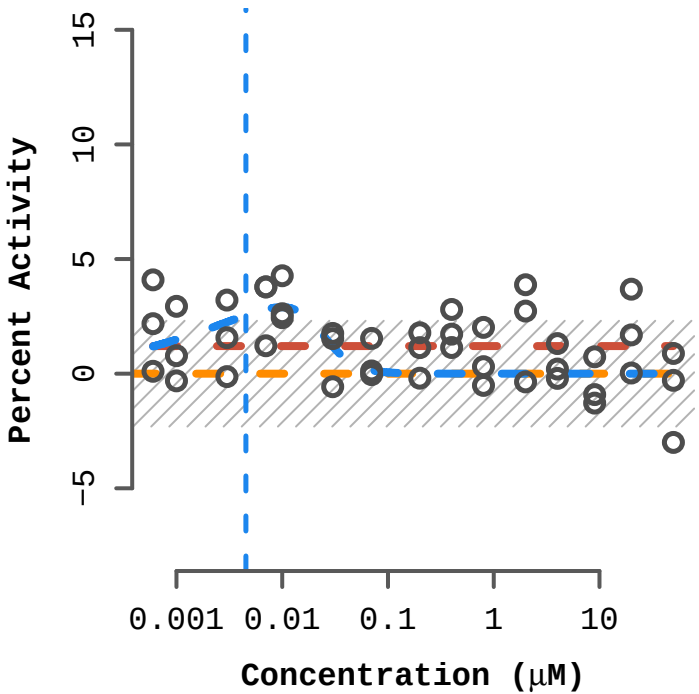
NAME: Rimantadine hydrochloride
CHID: 47813 **CASRN:** 1501-84-4
SPID(S): Tox21_111712_1
M4ID: 12483523

HILL MODEL: Not applicable.

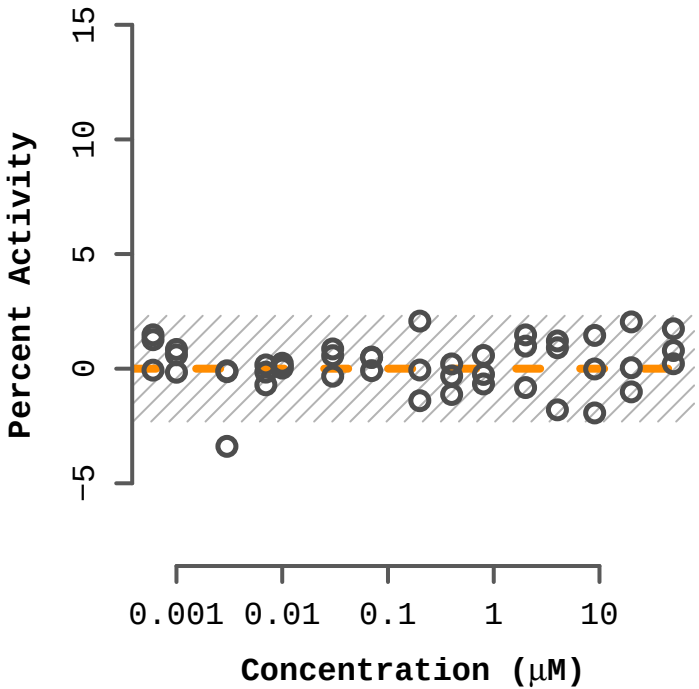
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.465 **MAX_MED:** 0.289 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Chlorphentermine hydrochloride
CHID:    47815   CASRN: 151-06-4
SPID(S): Tox21_111804_1
M4ID:    12483470

HILL MODEL (in red):
      tp       ga       gw
val:  1.2      -4.53    5.67
sd:   0.252    1170     5070

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.13     -2.34    0.593    -1.64    2.95
sd:   5.86     1.65     0.58     0.236    5.31

      CNST        HILL        GNLS
AIC:  197.12      182.83      181.95
PROB: 0           0.39        0.61
RMSE: 2.04        1.62        1.57

MAX_MEAN: 3.11      MAX_MED: 3.79      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

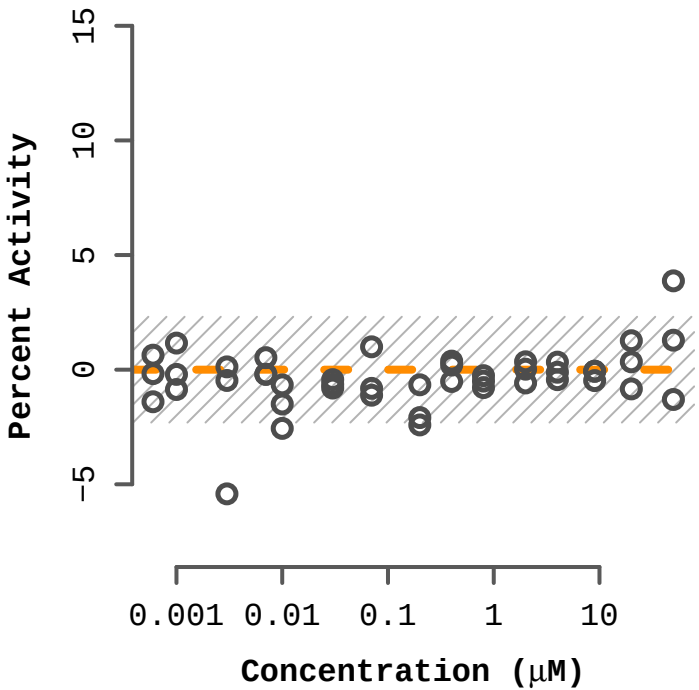
NAME: Trimetrexate trihydrochloride
CHID: 47817 **CASRN:** NOCAS_47817
SPID(S): Tox21_111995_1
M4ID: 12483384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.917 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

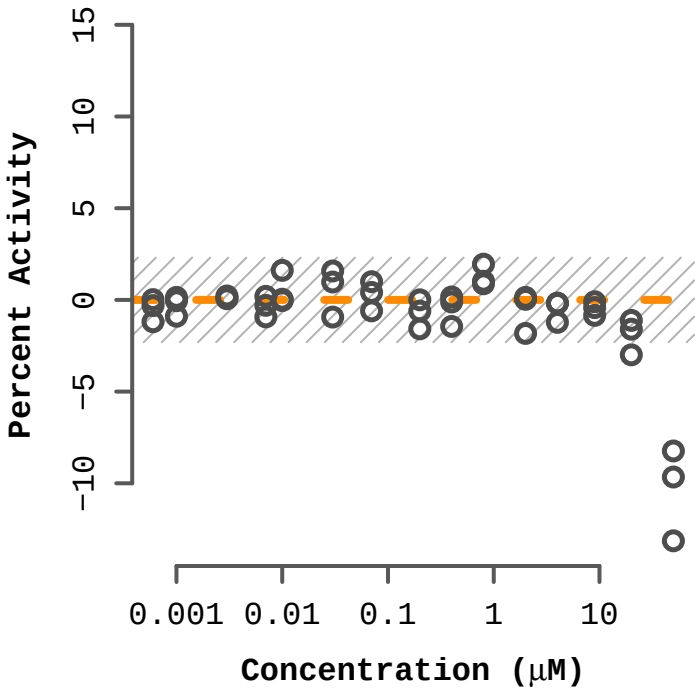
NAME: Dexbrompheniramine maleate
CHID: 47818 **CASRN:** 2391-03-9
SPID(S): Tox21_112000_1
M4ID: 12483380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

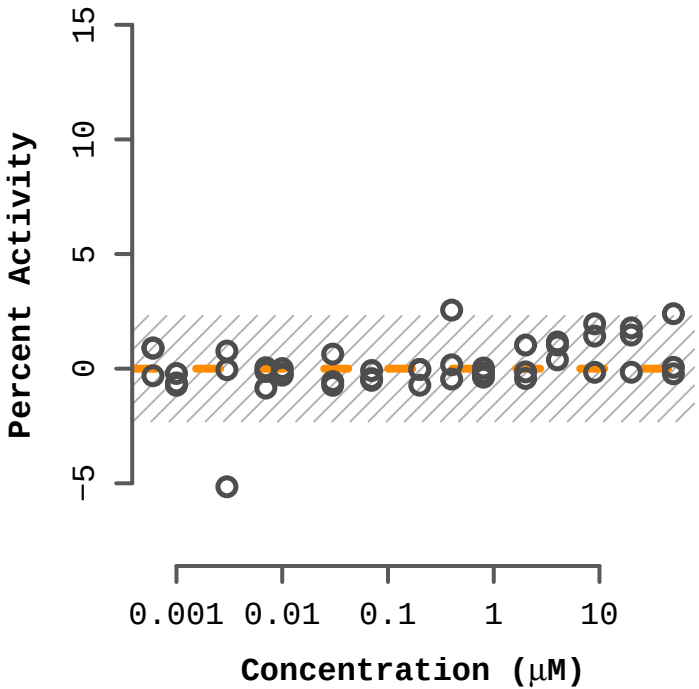
NAME: Mefloquine hydrochloride
CHID: 47819 **CASRN:** 51773-92-3
SPID(S): Tox21_111999_1
M4ID: 12483381

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.95	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

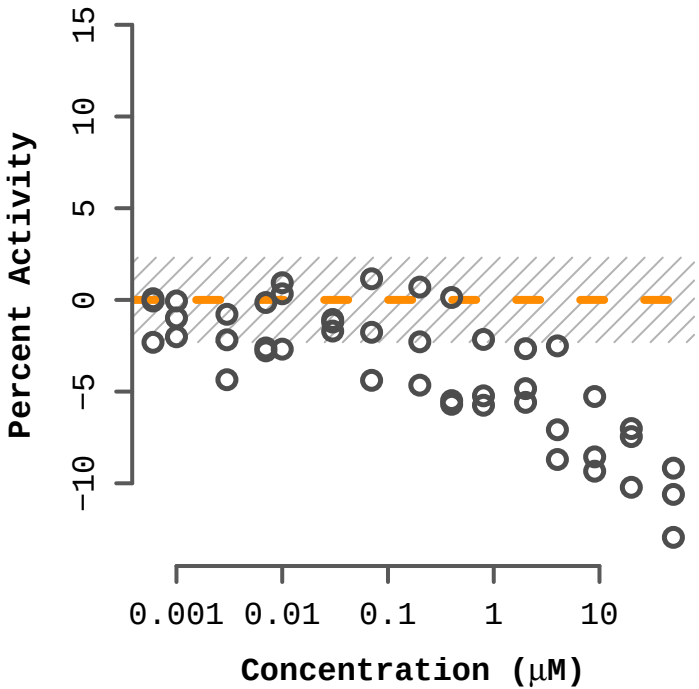
NAME: Phenmetrazine hydrochloride
CHID: 47822 **CASRN:** 1707-14-8
SPID(S): Tox21_112166_1
M4ID: 12483269

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

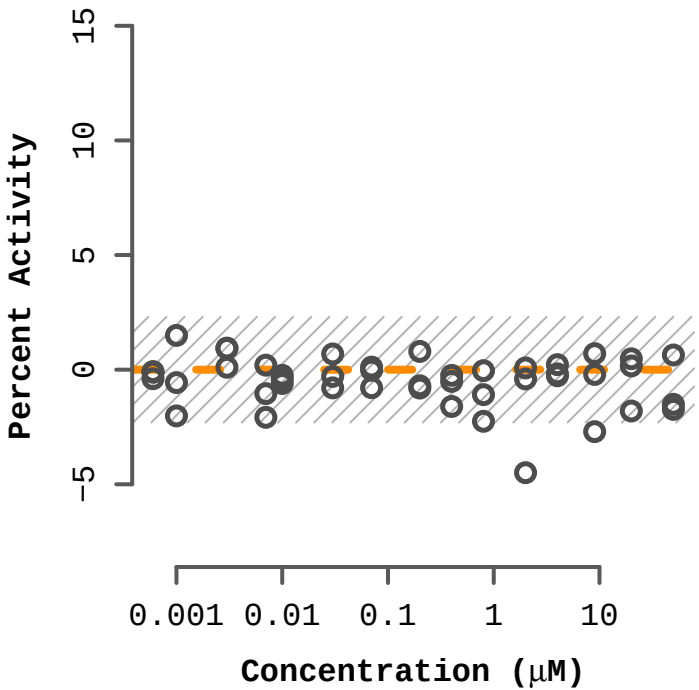
NAME: Vinorelbine tartrate
CHID: 47825 **CASRN:** 125317-39-7
SPID(S): Tox21_112271_1
M4ID: 12483188

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	278.99	NA	NA
PROB:	1	NA	NA
RMSE:	5.16	NA	NA

MAX_MEAN: −0.47 **MAX_MED:** 0.335 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

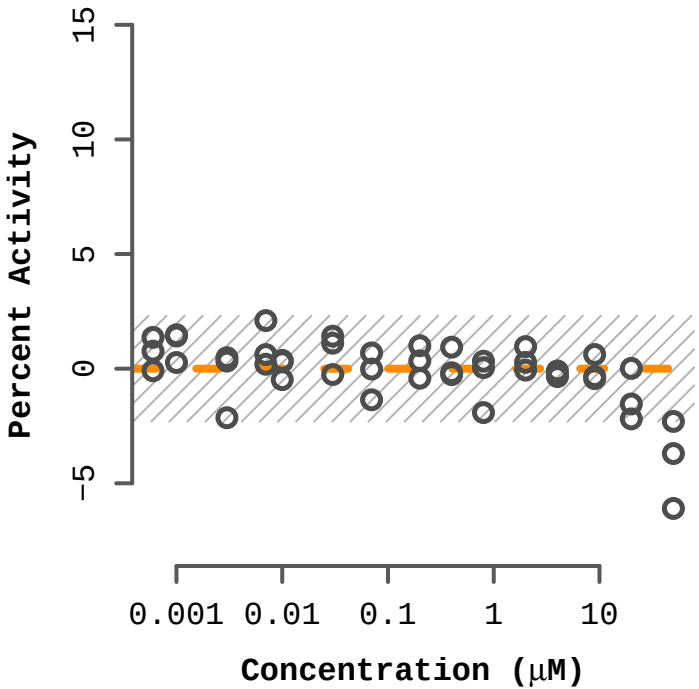
NAME: Carbinoxamine maleate
CHID: 47828 **CASRN:** 3505-38-2
SPID(S): Tox21_112336_1
M4ID: 12483152

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.659 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

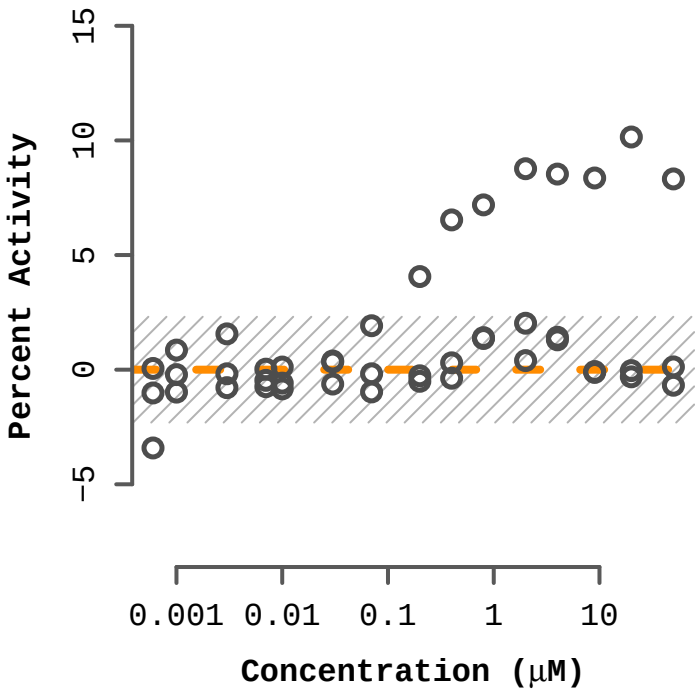
NAME: Lofepramine hydrochloride
CHID: 47833 **CASRN:** 26786-32-3
SPID(S): Tox21_112414_1
M4ID: 12483110

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

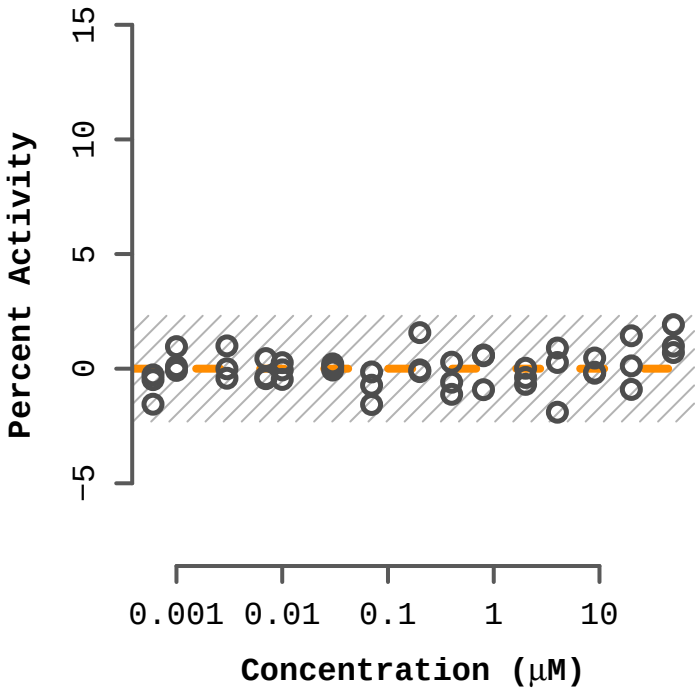
NAME: Caramiphen edisylate
CHID: 47835 **CASRN:** 125-86-0
SPID(S): Tox21_112430_1
M4ID: 12483106

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	223.55	NA	NA
PROB:	1	NA	NA
RMSE:	3.47	NA	NA

MAX_MEAN: 3.75 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

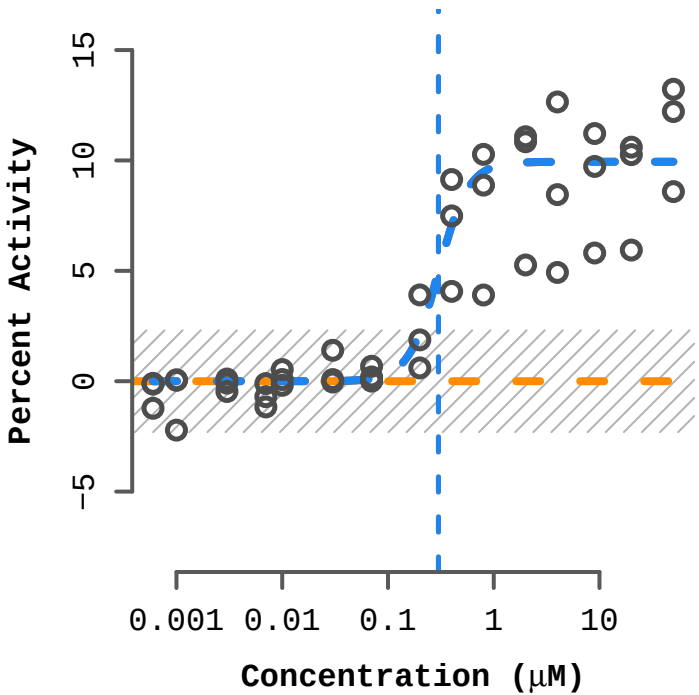
NAME: Doxapram hydrochloride
CHID: 47837 **CASRN:** 113-07-5
SPID(S): Tox21_112463_1
M4ID: 12483086

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 0.983 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethylpropion hydrochloride
CHID: 47838 CASRN: 134-80-5
SPID(S): Tox21_112479_1
M4ID: 12483076

HILL MODEL (in red):

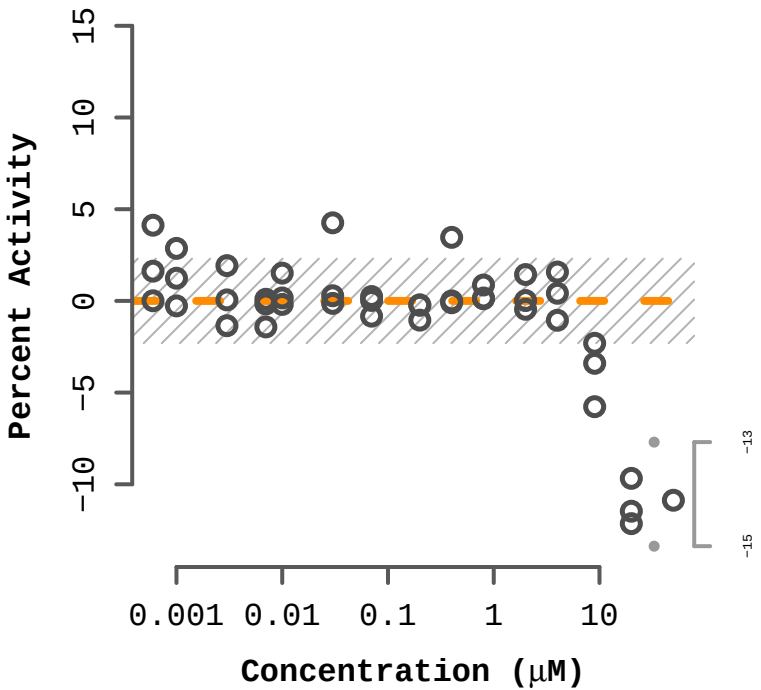
	tp	ga	gw
val:	9.94	−0.523	3.08
sd:	0.542	0.062	1.28

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.94	−0.523	3.08	3.69	4.04
sd:	0.542	0.062	1.28	1050	2130

	CNST	HILL	GNLS
AIC:	297.63	190.63	194.63
PROB:	0	0.88	0.12
RMSE:	6.35	1.96	1.96

MAX_MEAN: 11.3 **MAX_MED:** 12.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

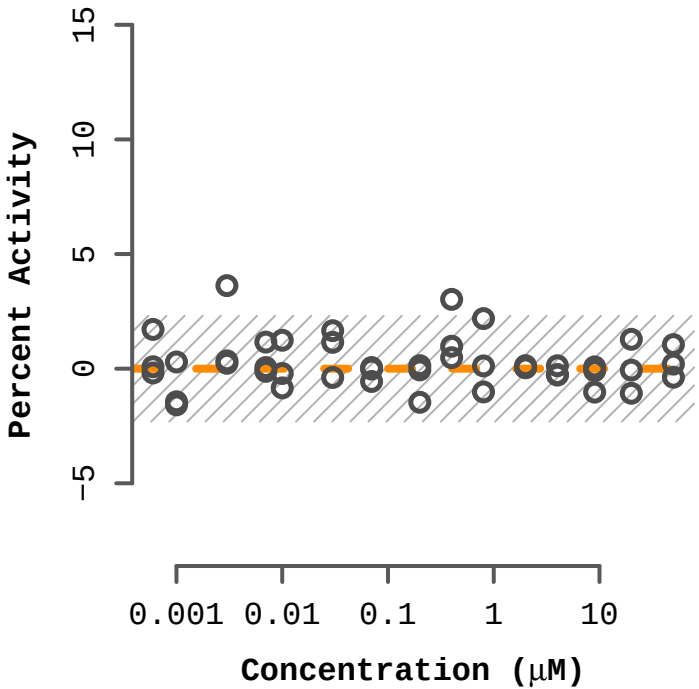
NAME: Sorafenib tosylate
CHID: 47839 **CASRN:** 475207-59-1
SPID(S): Tox21_112489_1
M4ID: 12483074 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	249.77	NA	NA
PROB:	1	NA	NA
RMSE:	4.74	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

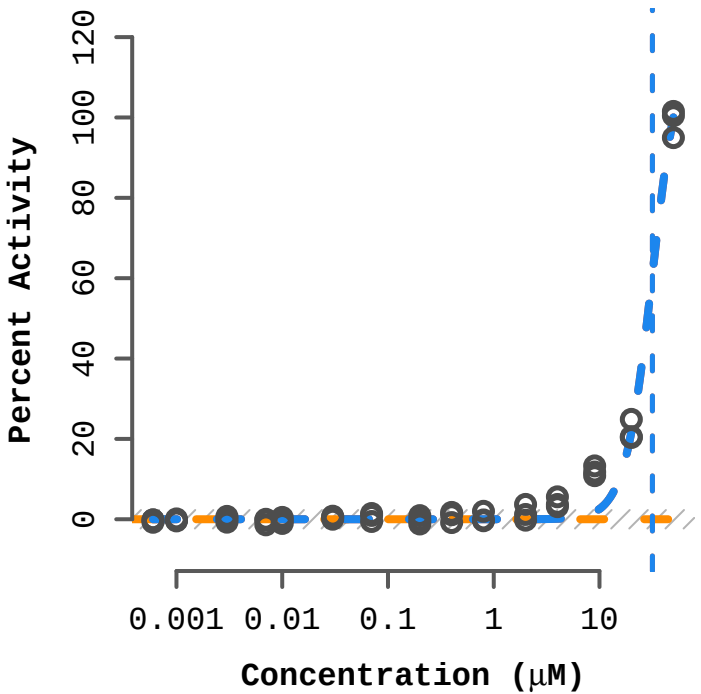
NAME: Rivastigmine tartrate
CHID: 47840 **CASRN:** 129101-54-8
SPID(S): Tox21_112528_1
M4ID: 12483046

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tosufloxacin toluenesulfonic acid
CHID: 47842 CASRN: 115964-29-9
SPID(S): Tox21_112533_1
M4ID: 12483042

HILL MODEL (in red):

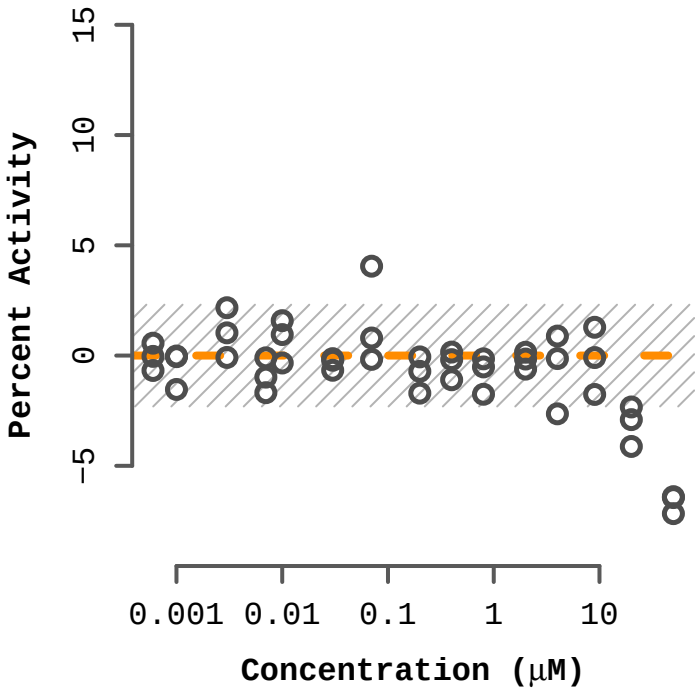
	tp	ga	gw
val:	122	1.5	3.33
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	122	1.5	3.33	2.27	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	346.57	214.84	218.84
PROB:	0	0.88	0.12
RMSE:	26.42	3.13	3.13

MAX_MEAN: 99 MAX_MED: 100 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

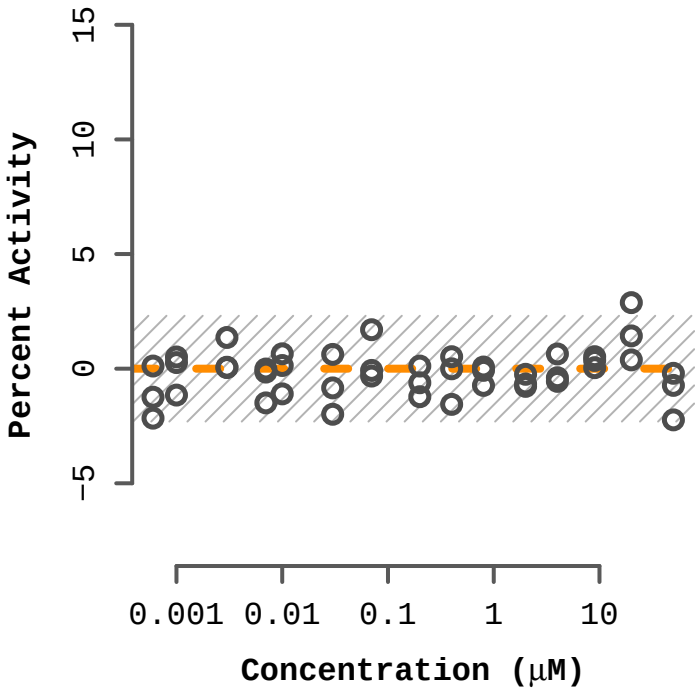
NAME: Diphenoxylate hydrochloride
CHID: 47843 **CASRN:** 3810-80-8
SPID(S): Tox21_112593_1
M4ID: 12483014

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.15	NA	NA
PROB:	1	NA	NA
RMSE:	2.21	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

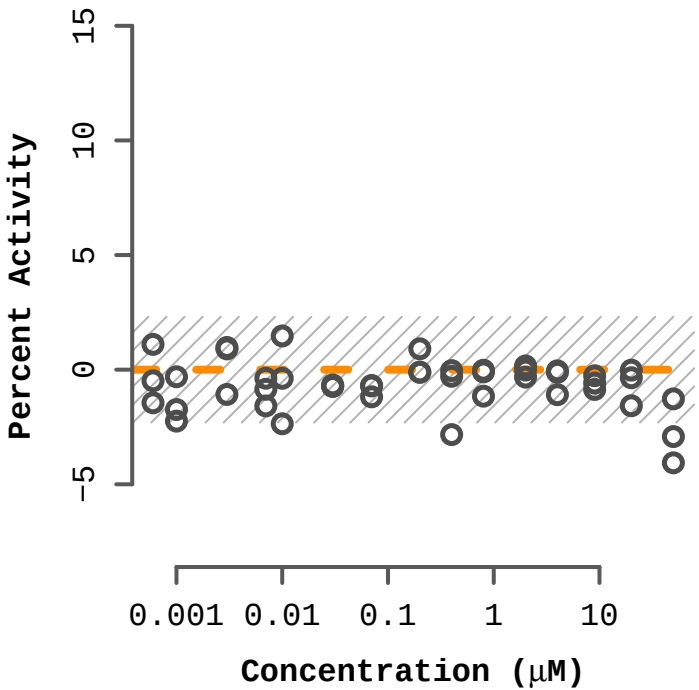
NAME: Eperisone hydrochloride
CHID: 47844 **CASRN:** 56839-43-1
SPID(S): Tox21_112599_1
M4ID: 12483013

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.58	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

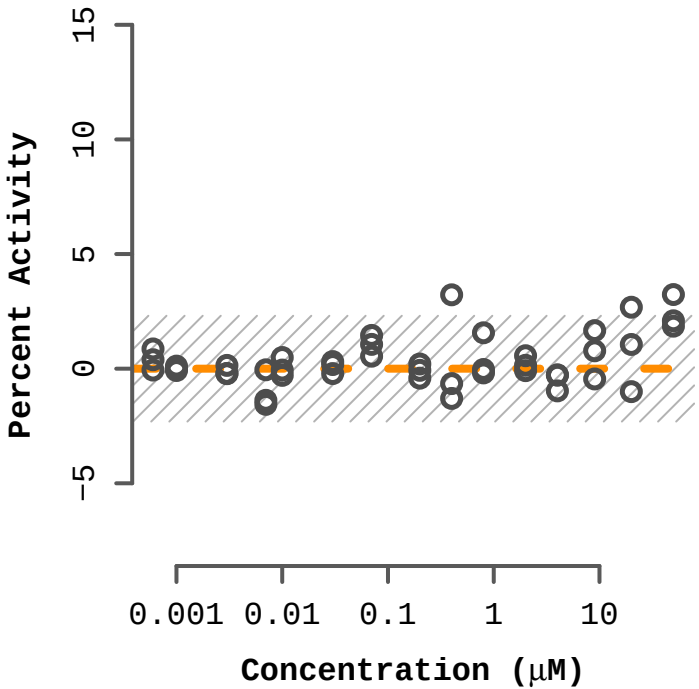
NAME: Midazolam hydrochloride
CHID: 47846 **CASRN:** 59467-96-8
SPID(S): Tox21_112613_1
M4ID: 12483008

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.266 **MAX_MED:** 0.907 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

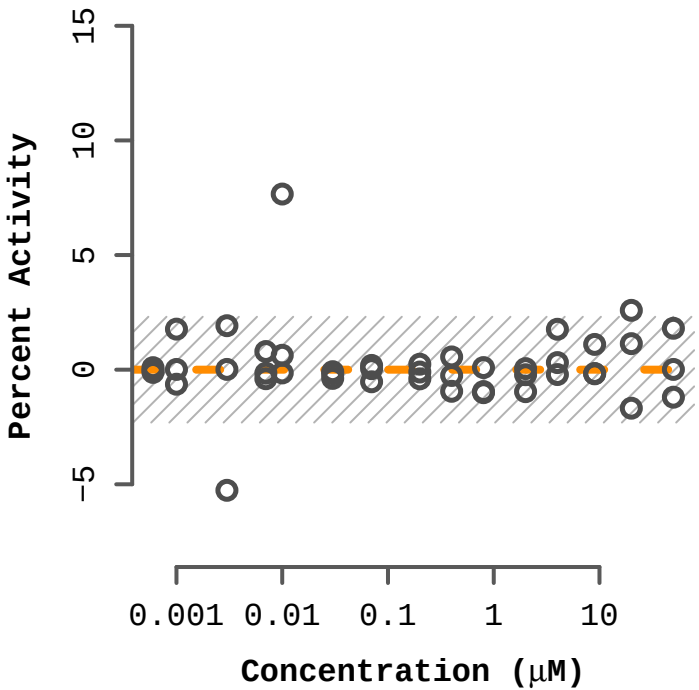
NAME: Rasagiline mesylate
CHID: 47848 **CASRN:** 161735-79-1
SPID(S): Tox21_112635_1
M4ID: 12483001

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 2.39 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

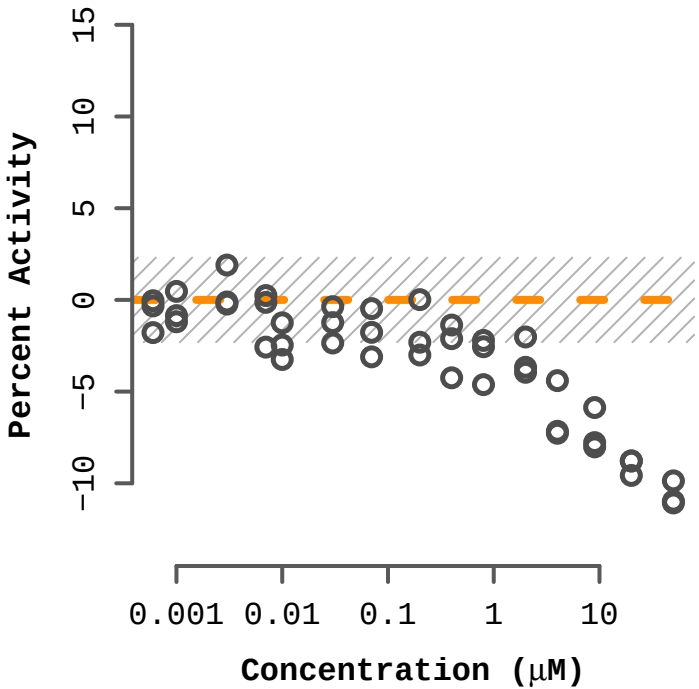
NAME: Gemcitabine hydrochloride
CHID: 47849 **CASRN:** 122111-03-9
SPID(S): Tox21_112644_1
M4ID: 12482997

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.88	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.72 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

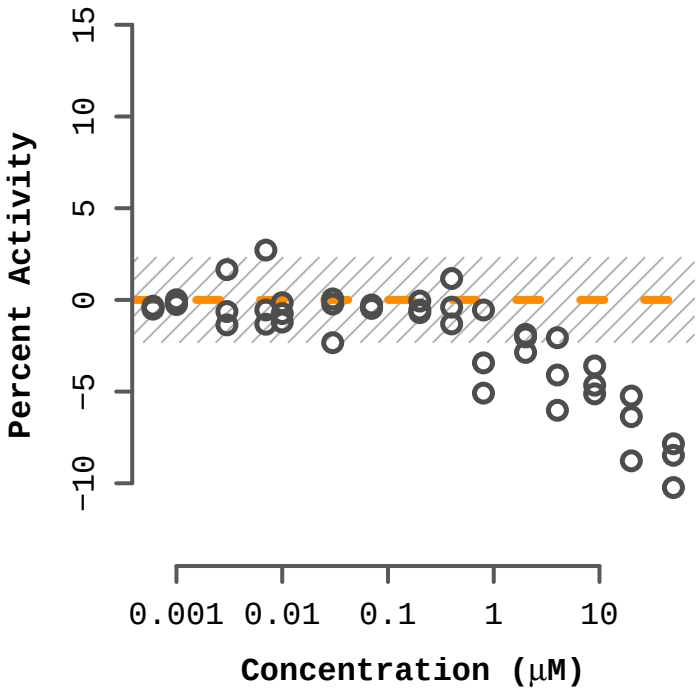
NAME: Vinblastine sulfate
CHID: 47853 **CASRN:** 18556-44-0
SPID(S): Tox21_112735_1
M4ID: 12482972

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270	NA	NA
PROB:	1	NA	NA
RMSE:	4.78	NA	NA

MAX_MEAN: 0.521 **MAX_MED:** −0.112 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

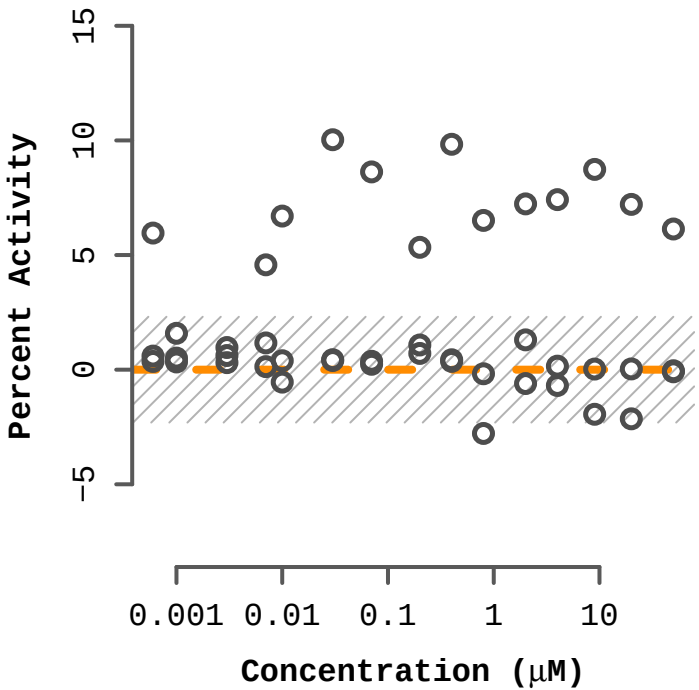
NAME: Vinblastine sulfate
CHID: 47853 **CASRN:** 18556-44-0
SPID(S): Tox21_111498_1
M4ID: 12483650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	239.51	NA	NA
PROB:	1	NA	NA
RMSE:	3.6	NA	NA

MAX_MEAN: 0.282 **MAX_MED:** −0.102 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

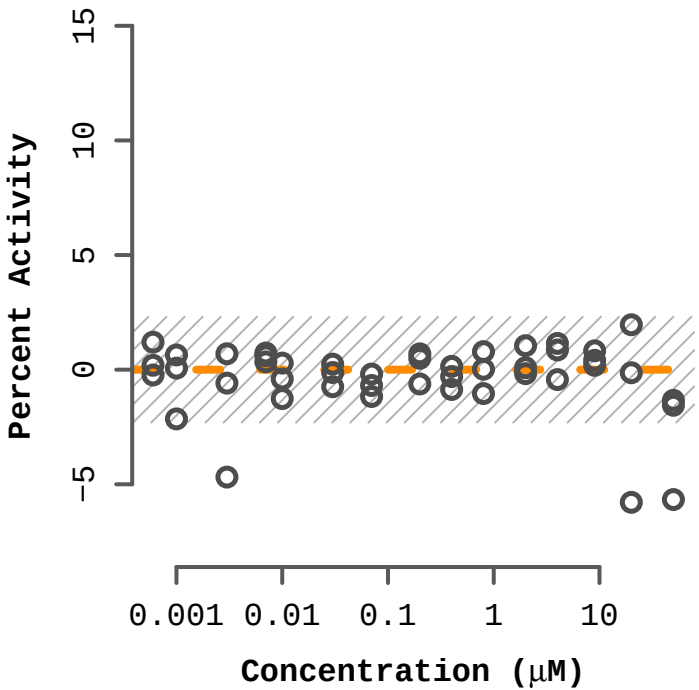
NAME: Biperiden hydrochloride
CHID: 47856 **CASRN:** 1235-82-1
SPID(S): Tox21_112785_1
M4ID: 12482953

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	250.66	NA	NA
PROB:	1	NA	NA
RMSE:	4.07	NA	NA

MAX_MEAN: 3.62 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

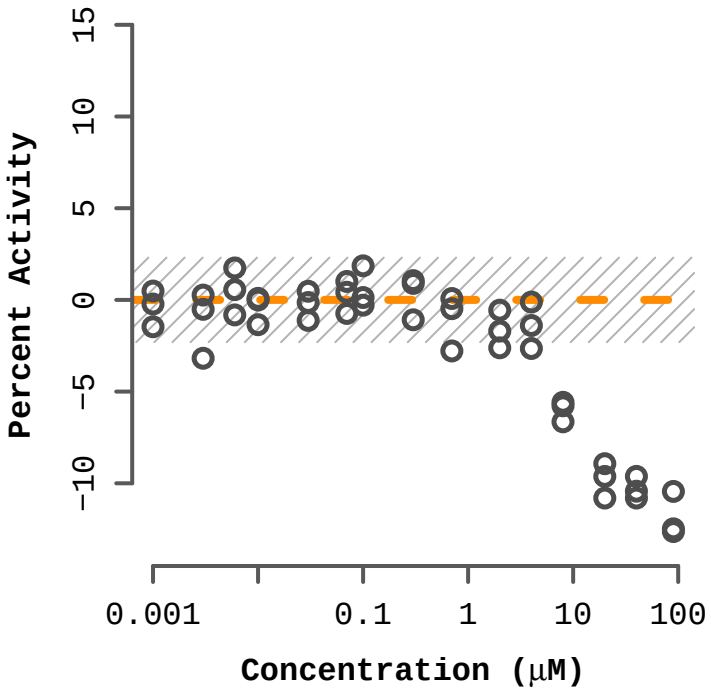
NAME: Gallopamil hydrochloride
CHID: 47858 **CASRN:** 16662-46-7
SPID(S): Tox21_110196_1
M4ID: 12484563

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 0.559 **MAX_MED:** 0.861 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

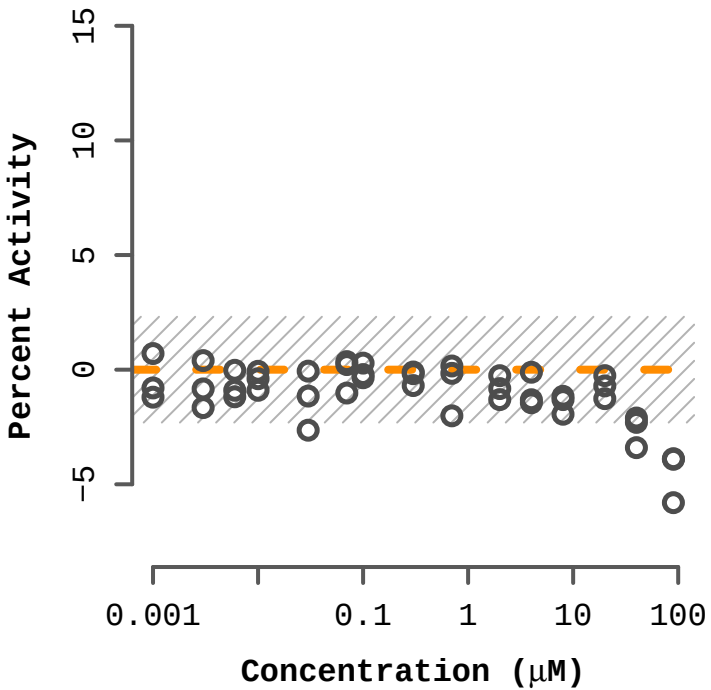
NAME: Palmatine chloride hydrate
CHID: 47869 **CASRN:** 171869-95-7
SPID(S): Tox21_200059
M4ID: 12482193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	270.23	NA	NA
PROB:	1	NA	NA
RMSE:	5.15	NA	NA

MAX_MEAN: 0.568 **MAX_MED:** 0.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

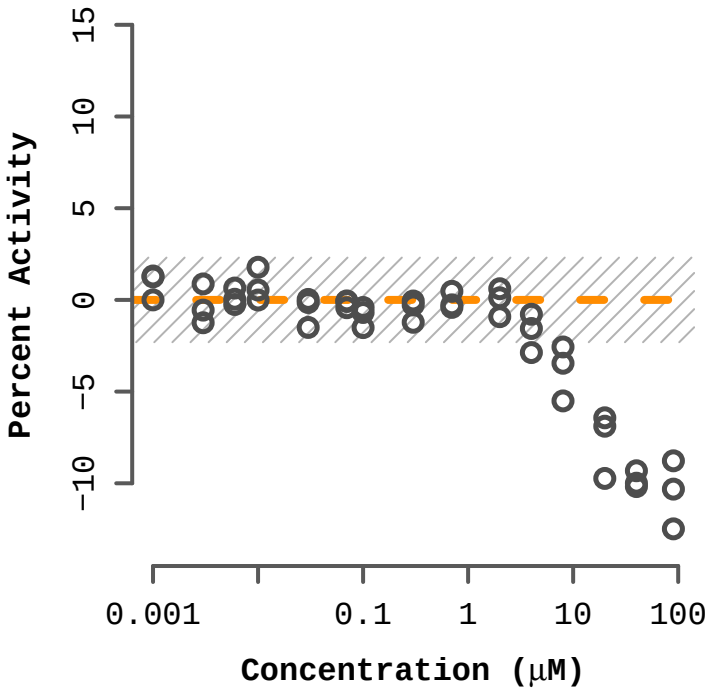
NAME: Tributylmethylphosphonium methyl sulfate
CHID: 47870 CASRN: 69056-62-8
SPID(S): Tox21_200084
M4ID: 12482168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: −0.0914 MAX_MED: 0.223 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

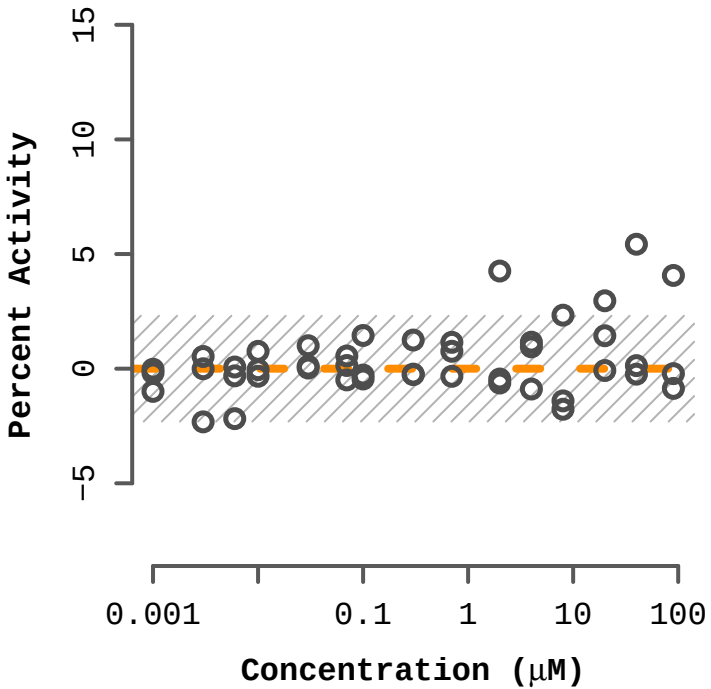
NAME: 1-Hexyl-3-methylimidazolium trifluoromethanesu
CHID: 47871 **CASRN:** 460345-16-8
SPID(S): Tox21_200101
M4ID: 12482151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	252.37	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: 0.855 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

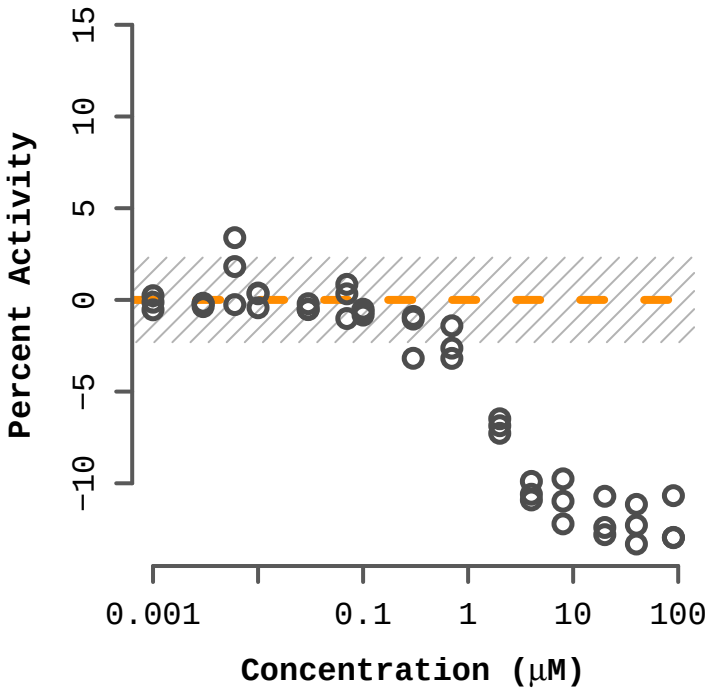
NAME: 1-(2-Hydroxyethyl)-3-methylimidazolium chlorid
CHID: 47872 CASRN: 61755-34-8
SPID(S): Tox21_200118
M4ID: 12482134

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 1.78 MAX_MED: 1.44 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

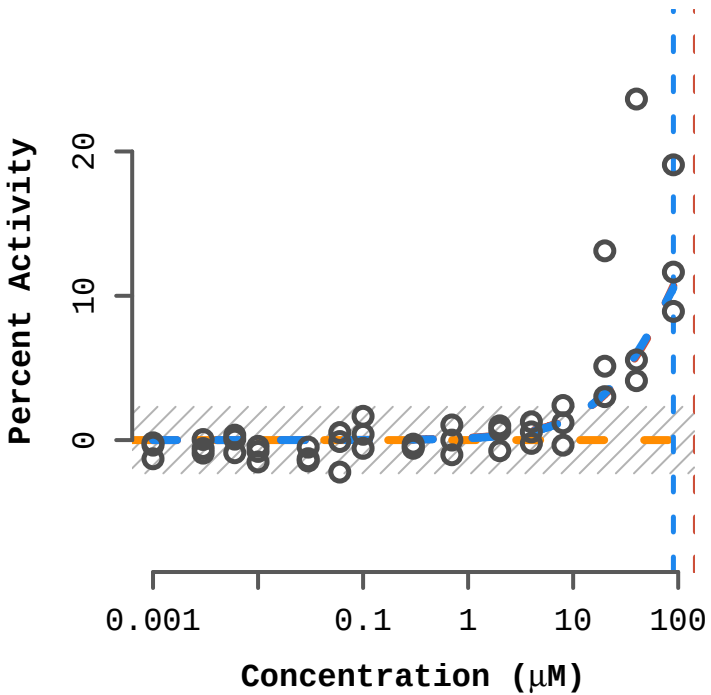
NAME: 1-Methyl-3-octylimidazolium chloride
CHID: 47873 **CASRN:** 64697-40-1
SPID(S): Tox21_200135
M4ID: 12482117

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	306.54	NA	NA
PROB:	1	NA	NA
RMSE:	7.03	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl triclosan
CHID: 47874 CASRN: 4640-01-1
SPID(S): Tox21_200199
M4ID: 12482053

HILL MODEL (in red):

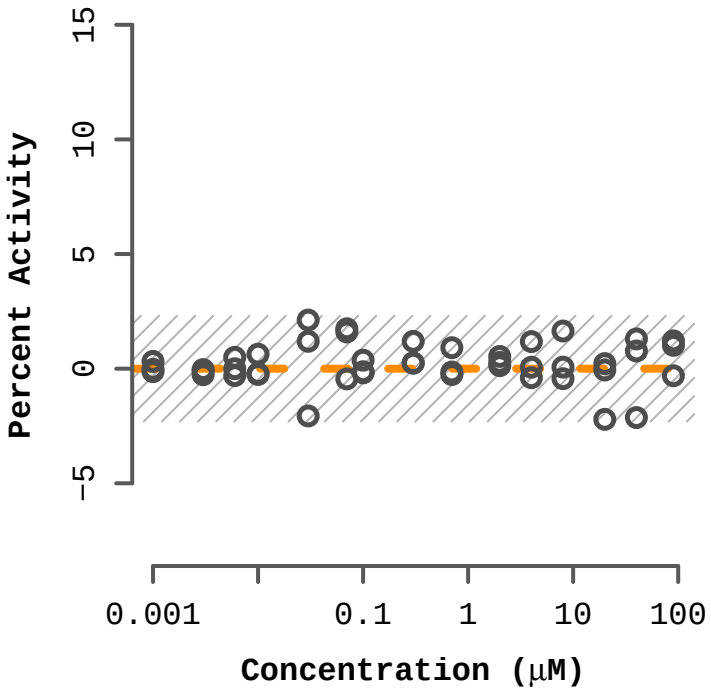
	tp	ga	gw
val:	28.4	2.16	1.04
sd:	28.3	0.683	0.272

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	21.1	1.95	1.14	3.2	8.75
sd:	14.8	0.491	0.296	23300	164000

	CNST	HILL	GNLS
AIC:	244.49	188.77	193.02
PROB:	0	0.89	0.11
RMSE:	5.63	3.42	3.41

MAX_MEAN: 13.2 **MAX_MED:** 11.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

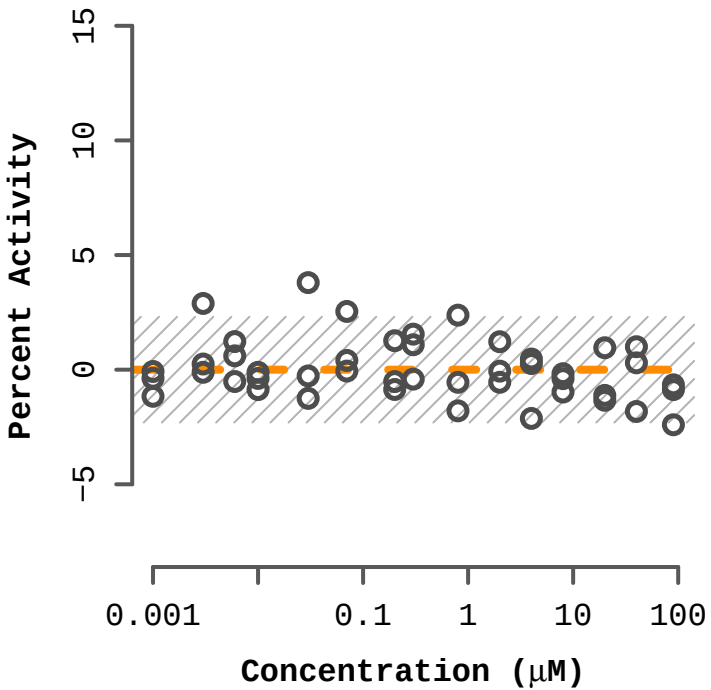
NAME: 1-Ethylpyridinium hexafluorophosphate
CHID: 47875 **CASRN:** 103173-73-5
SPID(S): Tox21_200223
M4ID: 12482029

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.967 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

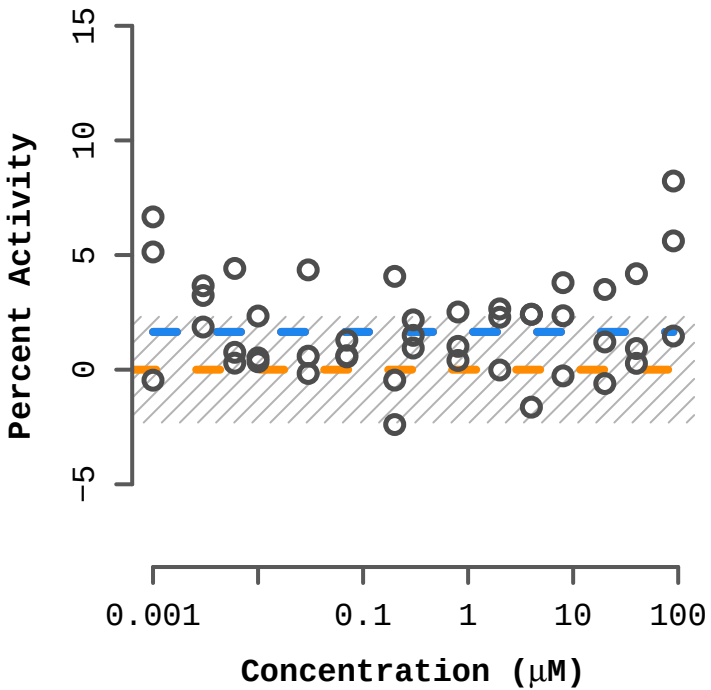
NAME: (−)−Enterodiol
CHID: 47876 CASRN: 80226−00−2
SPID(S): Tox21_200247
M4ID: 12482005

HILL MODEL: Not applicable.

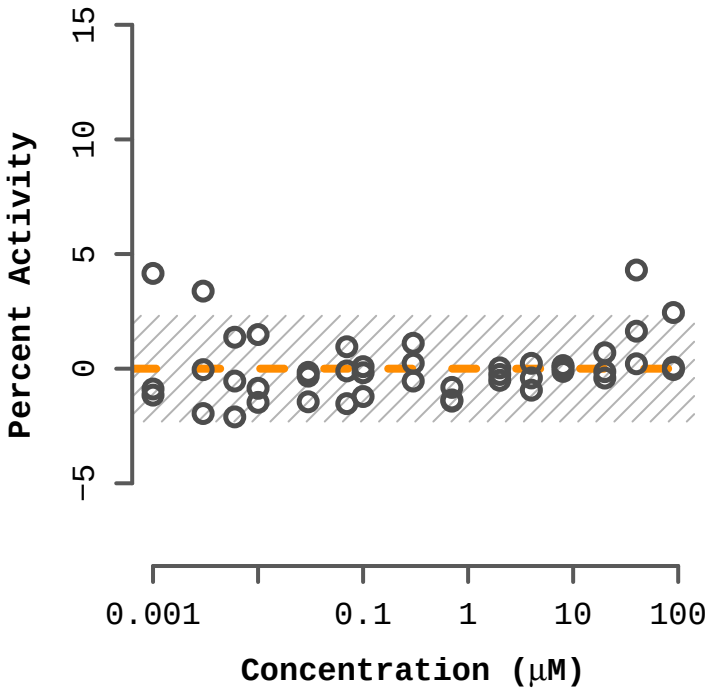
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.01 MAX_MED: 1.09 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Ethyl-1-methylpyrrolidinium hexafluorophospha
CHID:    47877   CASRN: 121057-90-7
SPID(S): Tox21_200261
M4ID:    12481991

HILL MODEL (in red):
      tp       ga       gw
val:  1.65     -4.66    4.5
sd:   0.307    1380     3720

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.65     -4.43    4.93     2.98     10.4
sd:   0.307    772      2650     19600    199000

      CNST        HILL        GNLS
AIC:  223.62      204.48      208.48
PROB: 0           0.88        0.12
RMSE: 2.85        2.15        2.15

MAX_MEAN: 5.11      MAX_MED: 5.62      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

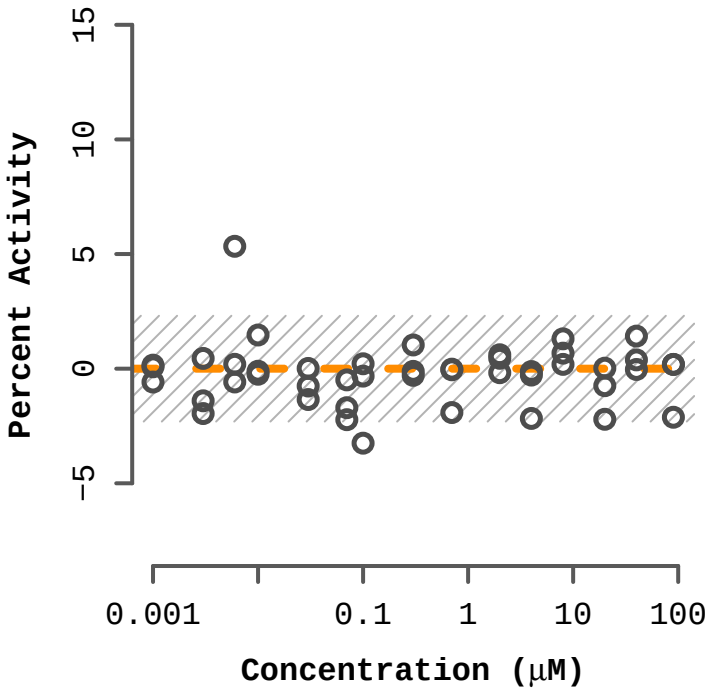
NAME: Hydrastinine hydrochloride
CHID: 47878 **CASRN:** 4884-68-8
SPID(S): Tox21_200396
M4ID: 12481856

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

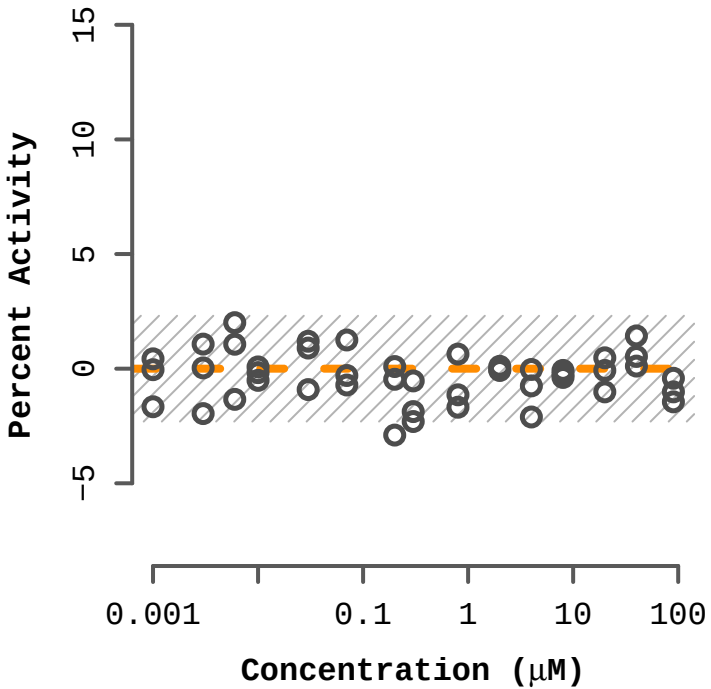
NAME: 2-Hydroxybenzophenone
CHID: 47879 CASRN: 117-99-7
SPID(S): Tox21_303440
M4ID: 12475700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.65 MAX_MED: 0.678 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

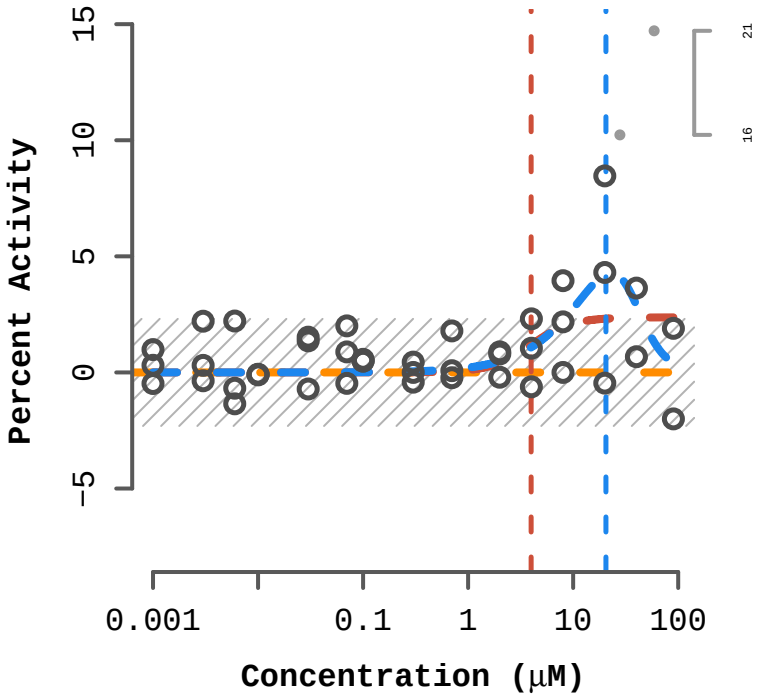
NAME: 2-Hydroxybenzophenone
CHID: 47879 **CASRN:** 117-99-7
SPID(S): Tox21_200541
M4ID: 12481711

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.693 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Hydroxybenzophenone
CHID: 47880 CASRN: 13020-57-0
SPID(S): Tox21_200542
M4ID: 12481710 BRK

HILL MODEL (in red):

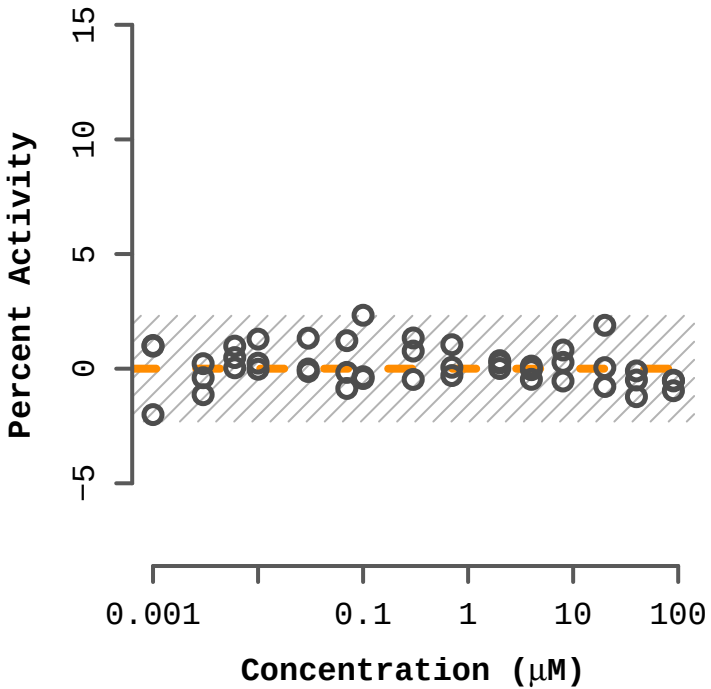
	tp	ga	gw
val:	2.37	0.6	2.25
sd:	0.851	0.271	2.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.74	1.31	1.27	1.56	3.31
sd:	24.5	1.48	1.25	0.319	5.26

	CNST	HILL	GNLS
AIC:	212.13	206.13	206.61
PROB:	0.03	0.54	0.43
RMSE:	4.33	3.74	3.86

MAX_MEAN: 6.92 MAX_MED: 4.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

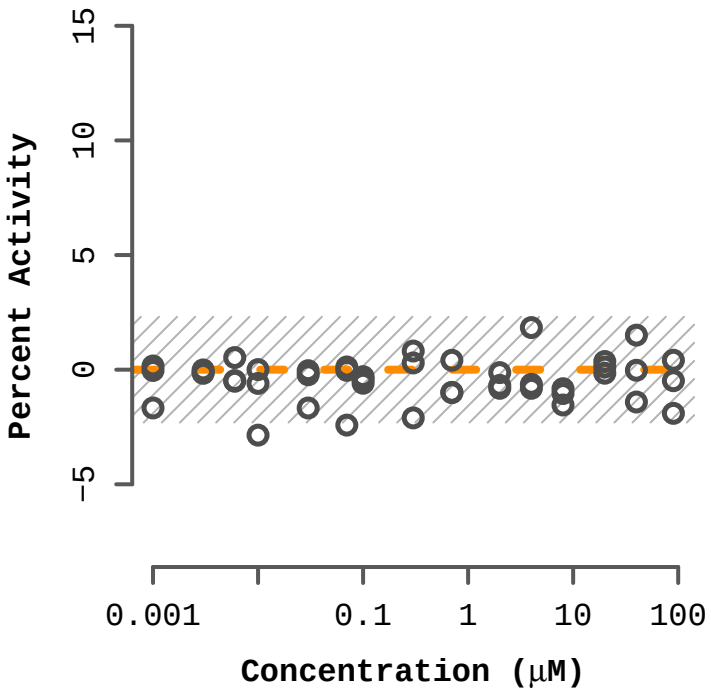
NAME: 2-Hydroxy-5-methylbenzophenone
CHID: 47881 **CASRN:** 1470-57-1
SPID(S): Tox21_200544
M4ID: 12481708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.547 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

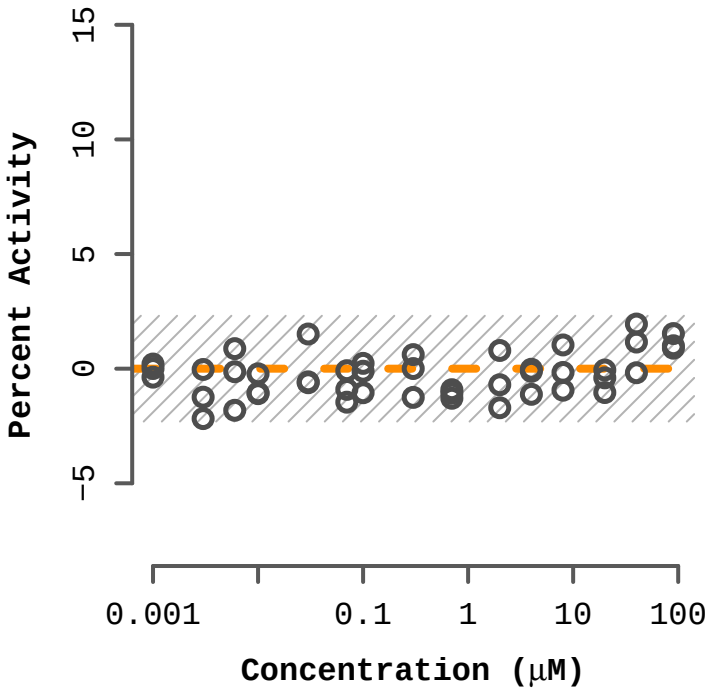
NAME: Phenylparaben
CHID: 47882 **CASRN:** 17696-62-7
SPID(S): Tox21_303589
M4ID: 12475556

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.129 **MAX_MED:** 0.294 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

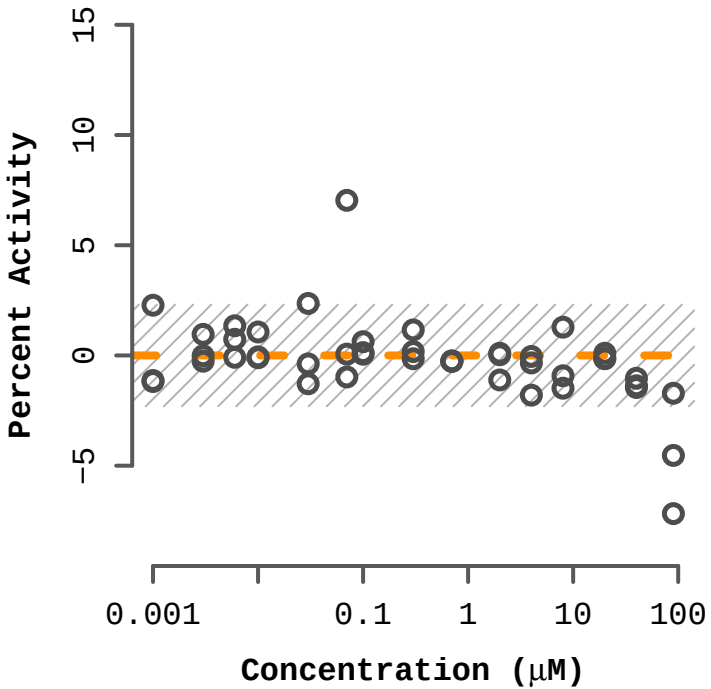
NAME: Phenylparaben
CHID: 47882 **CASRN:** 17696-62-7
SPID(S): Tox21_200545
M4ID: 12481707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

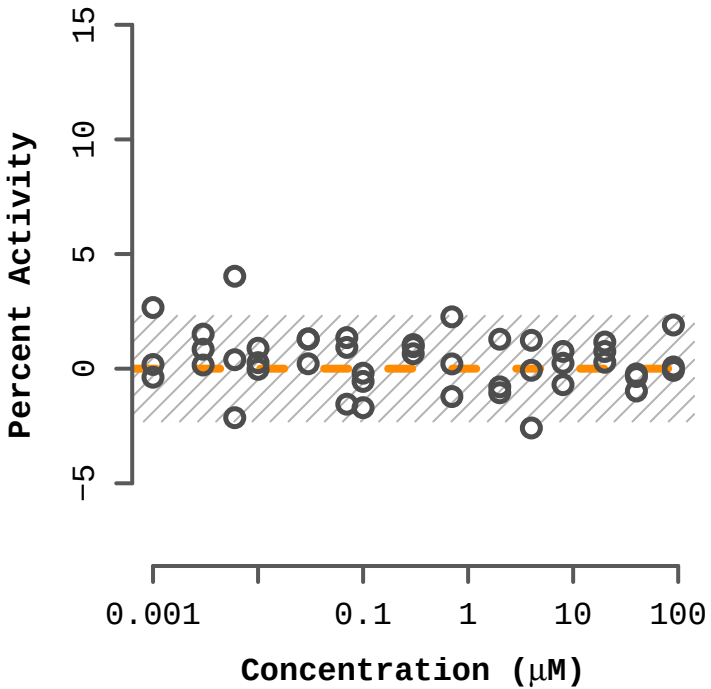
NAME: Dodecylparaben
CHID: 47883 **CASRN:** 2664-60-0
SPID(S): Tox21_200546
M4ID: 12481706

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 2.04 **MAX_MED:** 0.735 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

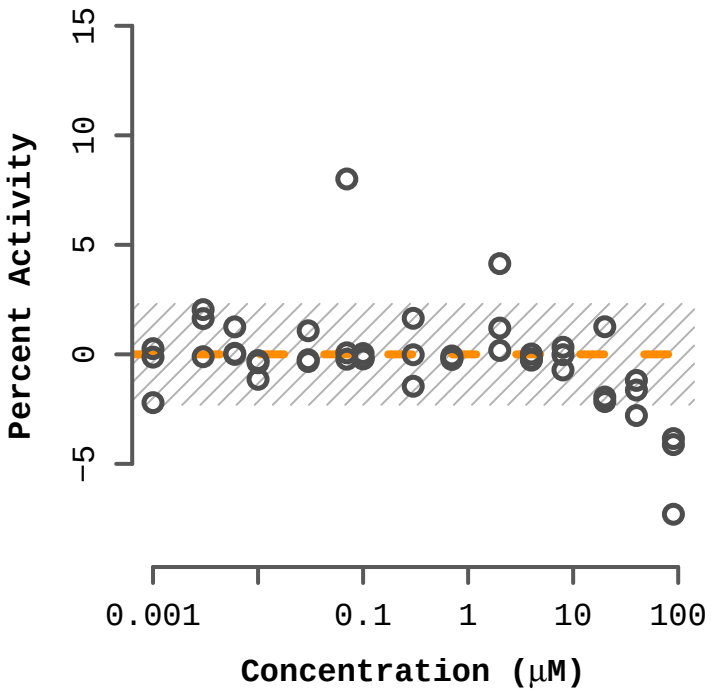
NAME: 1-Ethyl-3-methylimidazolium thiocyanate
CHID: 47884 **CASRN:** 331717-63-6
SPID(S): Tox21_200547
M4ID: 12481705

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.936 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

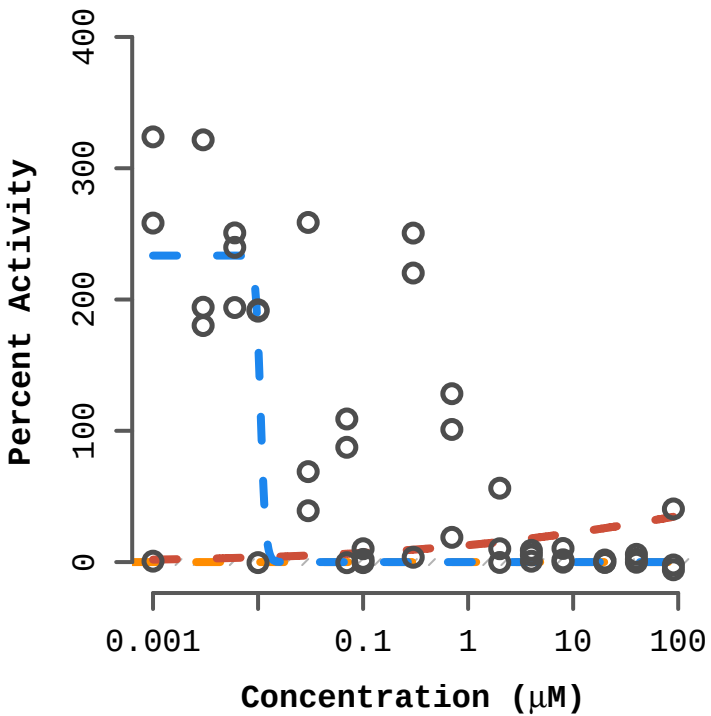
NAME: Nonylparaben
CHID: 47885 **CASRN:** 38713-56-3
SPID(S): Tox21_200548
M4ID: 12481704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.6	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 2.62 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4-Dimethoxy-4'-hydroxy benzophenone
CHID: 47886 CASRN: 41351-30-8
SPID(S): Tox21_200549
M4ID: 12481703

HILL MODEL (in red):

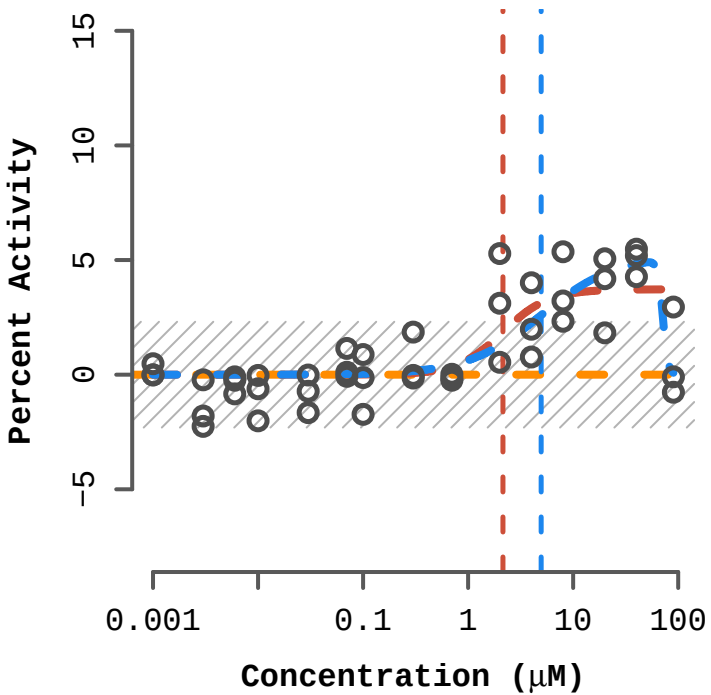
	tp	ga	gw
val:	83.2	2.45	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	233	-4.85	8	-1.98	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	567.75	572.24	527.23
PROB:	0	0	1
RMSE:	134.42	132.13	87.36

MAX_MEAN: 232 MAX_MED: 258 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentylparaben
CHID: 47887 **CASRN:** 6521-29-5
SPID(S): Tox21_200551
M4ID: 12481701

HILL MODEL (in red):

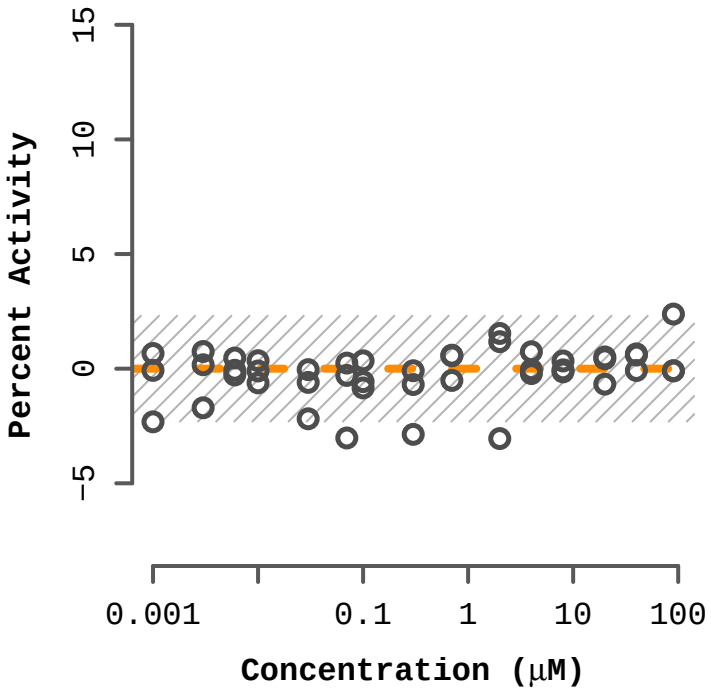
	tp	ga	gw
val:	3.72	0.332	2
sd:	0.698	0.301	1.37

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.19	0.695	1.24	1.85	17.8
sd:	1.03	0.258	0.524	0.351	57.4

	CNST	HILL	GNLS
AIC:	206.48	169.48	159.34
PROB:	0	0.01	0.99
RMSE:	2.4	1.49	1.28

MAX_MEAN: 4.98 **MAX_MED:** 5.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

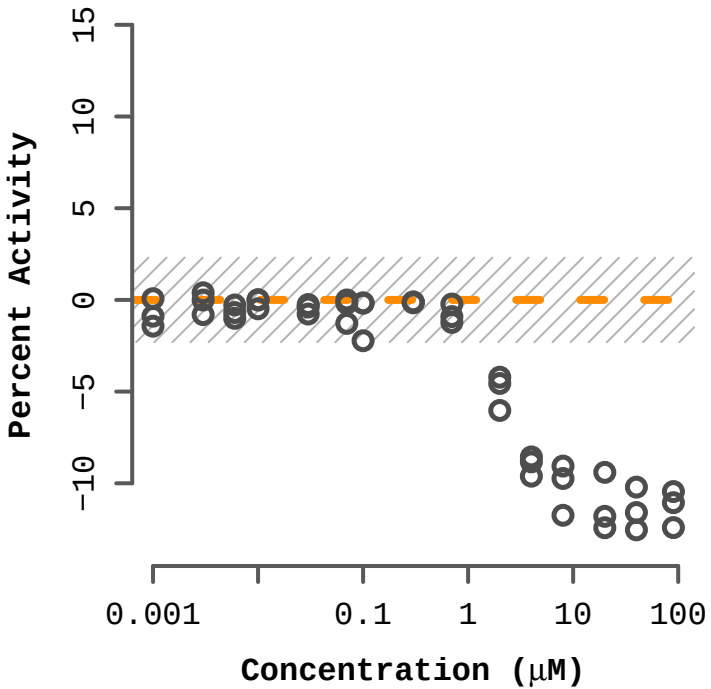
NAME: Triethylsulfonium bis(trifluoromethanesulfonyl
CHID: 47888 **CASRN:** 321746-49-0
SPID(S): Tox21_200552
M4ID: 12481700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.733 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

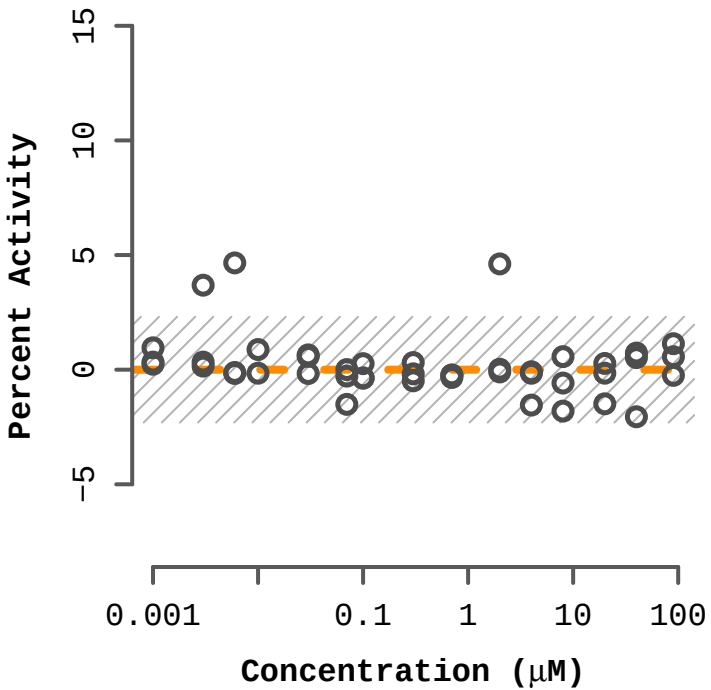
NAME: 1-Ethyl-3-methylimidazolium diethylphosphate
CHID: 47889 **CASRN:** 848641-69-0
SPID(S): Tox21_202638
M4ID: 12479614

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	295.76	NA	NA
PROB:	1	NA	NA
RMSE:	6.34	NA	NA

MAX_MEAN: −0.131 **MAX_MED:** −0.00631 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

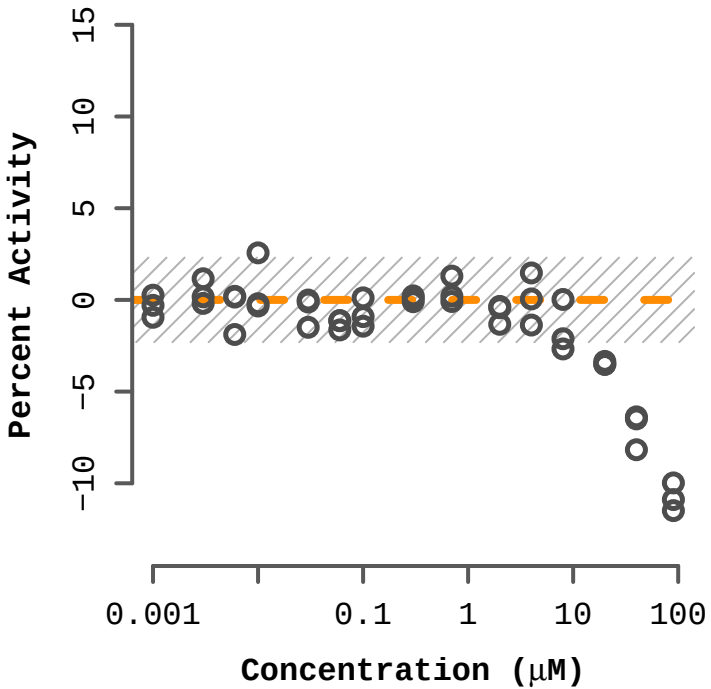
NAME: 1-Ethyl-3-methylimidazolium diethylphosphate
CHID: 47889 **CASRN:** 848641-69-0
SPID(S): Tox21_200553
M4ID: 12481699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 0.584 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

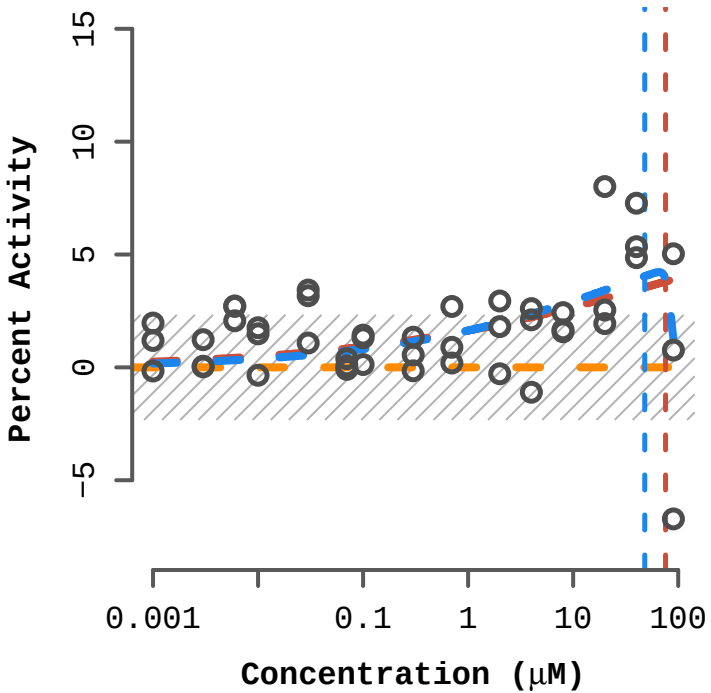
NAME: 3,3'−Dimethylbisphenol A
CHID: 47890 **CASRN:** 79−97−0
SPID(S): Tox21_200554
M4ID: 12481698

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.58	NA	NA

MAX_MEAN: 0.677 **MAX_MED:** 0.202 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bisphenol E
CHID: 47891 CASRN: 2081-08-5
SPID(S): Tox21_304007
M4ID: 12475181

HILL MODEL (in red):

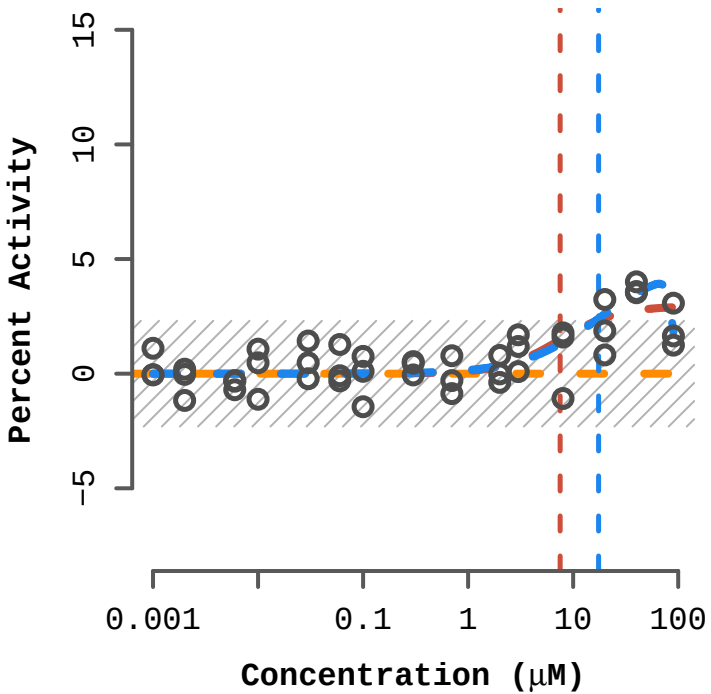
	tp	ga	gw
val:	7.61	1.88	0.3
sd:	8.67	2.75	0.179

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.08	1.68	0.355	1.93	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	219.53	192.9	194.79
PROB:	0	0.72	0.28
RMSE:	2.81	2.28	2.03

MAX_MEAN: 5.83 MAX_MED: 5.35 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bisphenol E
CHID: 47891 CASRN: 2081-08-5
SPID(S): Tox21_200555
M4ID: 12481697

HILL MODEL (in red):

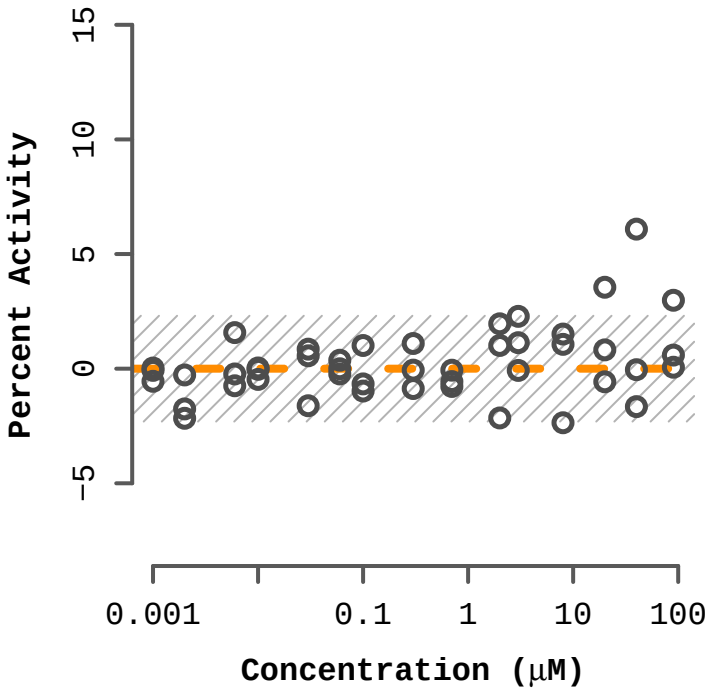
	tp	ga	gw
val:	2.95	0.876	1.59
sd:	0.546	0.193	0.667

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.81	1.24	1.18	1.95	14.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	160.65	126.23	121.93
PROB:	0	0.1	0.9
RMSE:	1.46	0.88	0.82

MAX_MEAN: 3.71 MAX_MED: 3.59 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

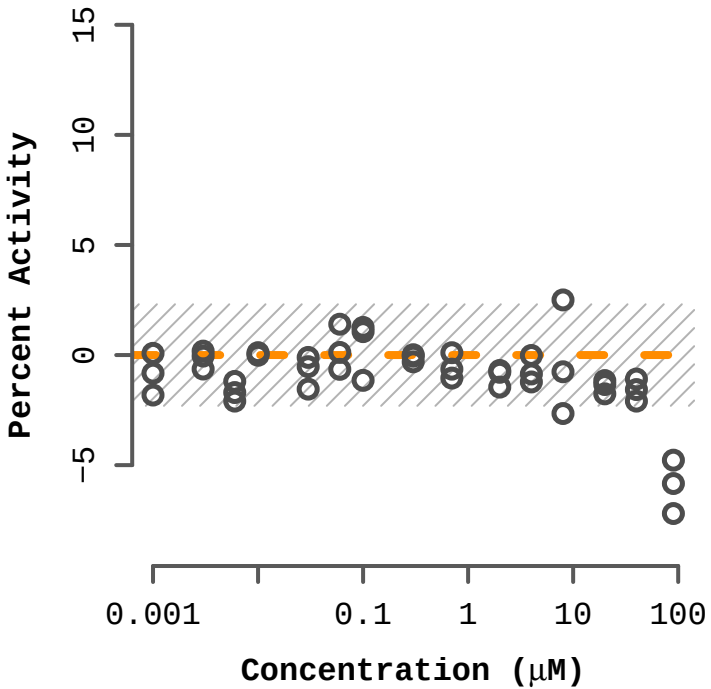
NAME: 2,2−Diphenylpropane
CHID: 47892 **CASRN:** 778−22−3
SPID(S): Tox21_200556
M4ID: 12481696

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.55	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−Octahydro−1H−4,7−methanoindene−5,5−diyldi

CHID: 47893 **CASRN:** 1943−97−1

SPID(S): Tox21_200559

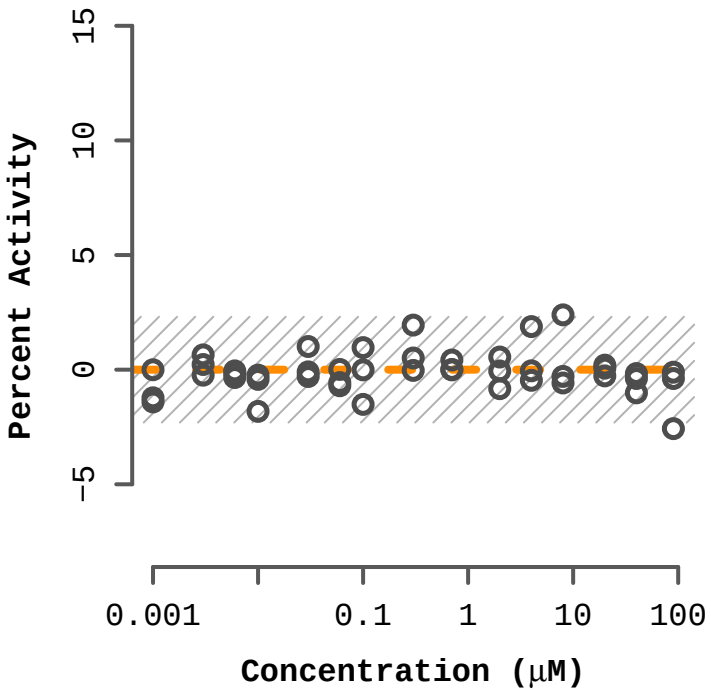
M4ID: 12481693

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.92	NA	NA

MAX_MEAN: 0.391 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

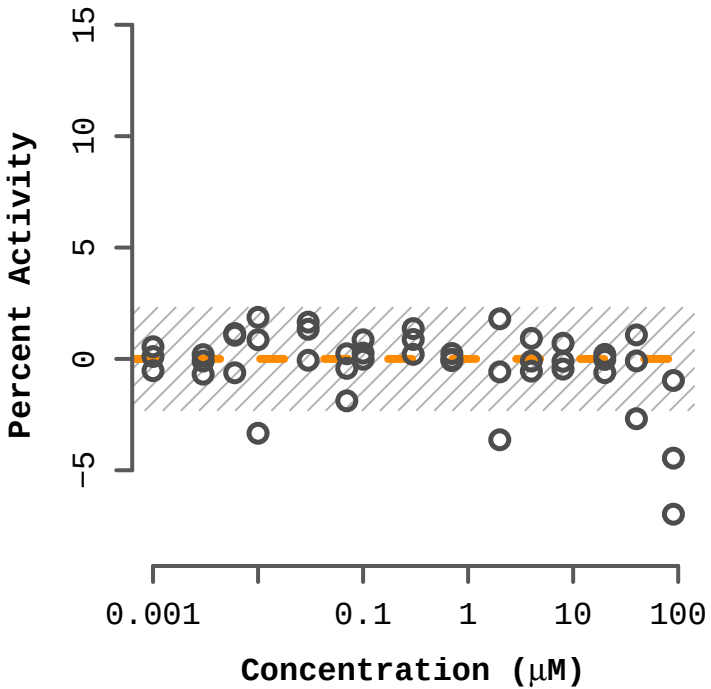
NAME: (5-Chloro-2-hydroxyphenyl)phenylmethanone
CHID: 47894 **CASRN:** 85-19-8
SPID(S): Tox21_200560
M4ID: 12481692

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.808 **MAX_MED:** 0.509 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

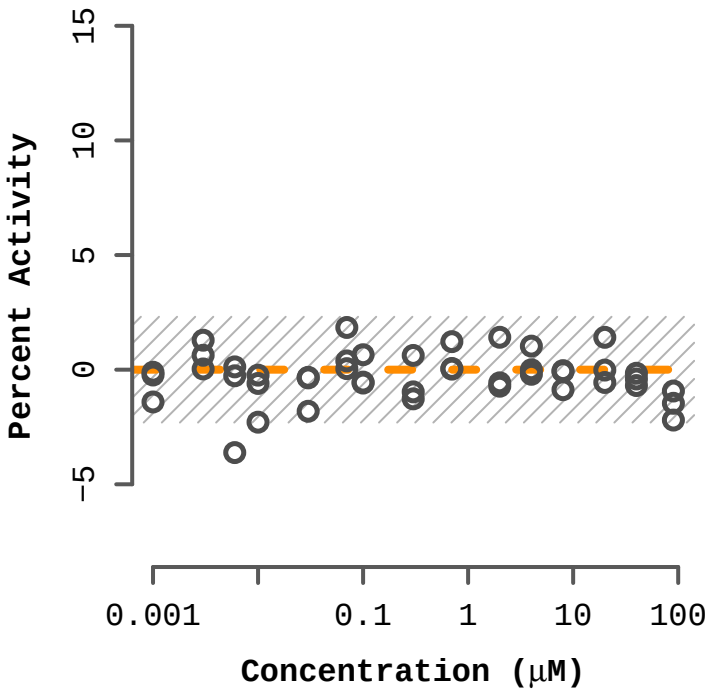
NAME: Menthyl anthranilate
CHID: 47895 **CASRN:** 134-09-8
SPID(S): Tox21_200561
M4ID: 12481691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 0.976 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

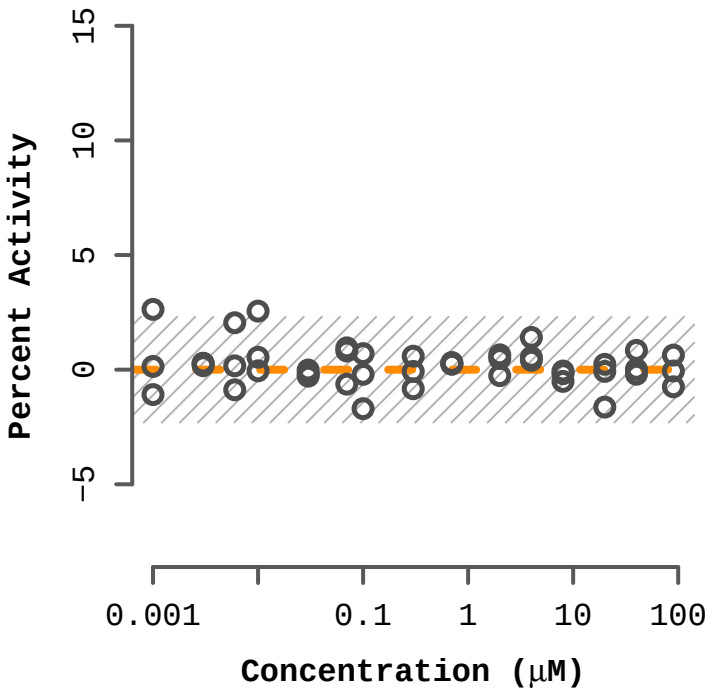
NAME: Enzacamene
CHID: 47896 **CASRN:** 36861-47-9
SPID(S): Tox21_200562
M4ID: 12481690

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.758 **MAX_MED:** 0.629 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

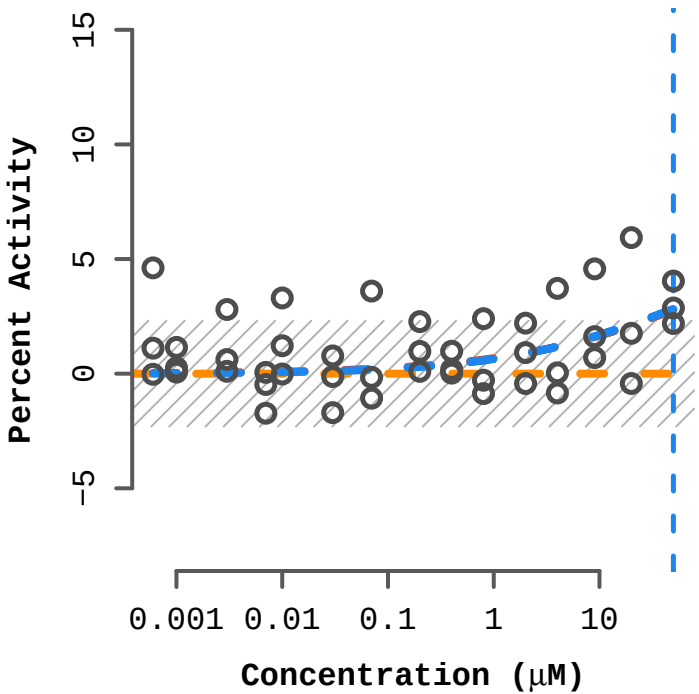
NAME: D-Tagatose
CHID: 47897 CASRN: 87-81-0
SPID(S): Tox21_200563
M4ID: 12481689

HILL MODEL: Not applicable.

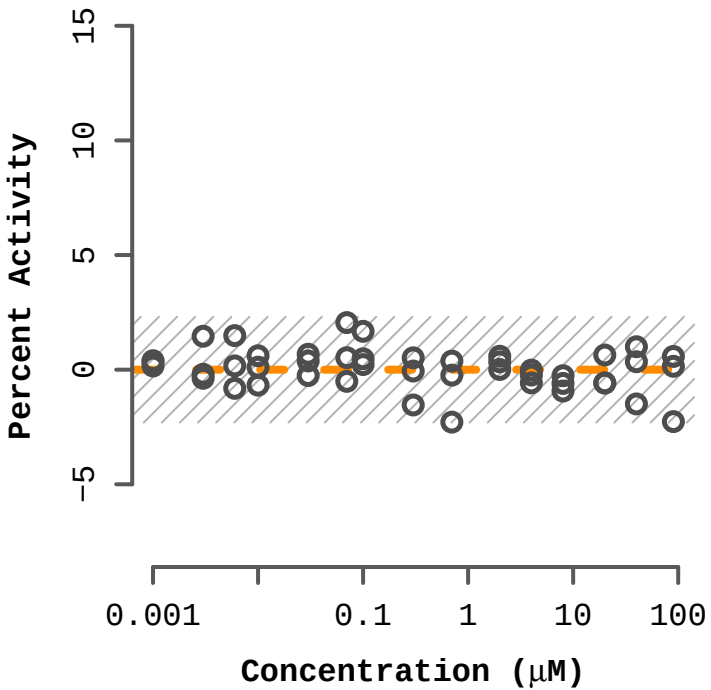
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.02 MAX_MED: 0.818 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    D-Tagatose
CHID:    47897   CASRN: 87-81-0
SPID(S): Tox21_113373_1
M4ID:    12482669

HILL MODEL (in red):
      tp       ga       gw
val:  7.12     2.11     0.466
sd:   10.2     2.39     0.336

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.64     1.7      0.526    3.7      2.97
sd:   7.99     2.22     0.412    371      558

      CNST        HILL        GNLS
AIC:  192.25      179.8       183.91
PROB: 0           0.89        0.11
RMSE: 2.06        1.65        1.65

MAX_MEAN: 3.03      MAX_MED: 2.87      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

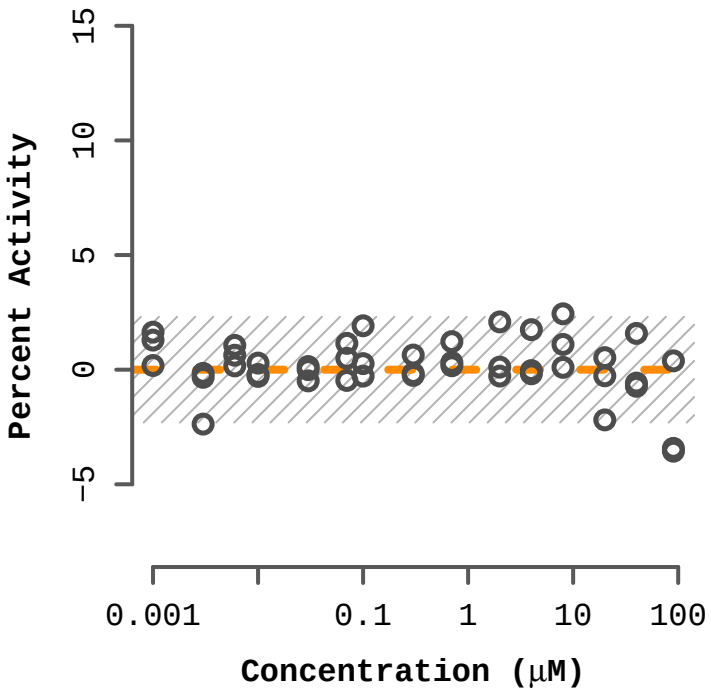
NAME: Rebaudioside A
CHID: 47898 **CASRN:** 58543-16-1
SPID(S): Tox21_200565
M4ID: 12481687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.791 **MAX_MED:** 0.523 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

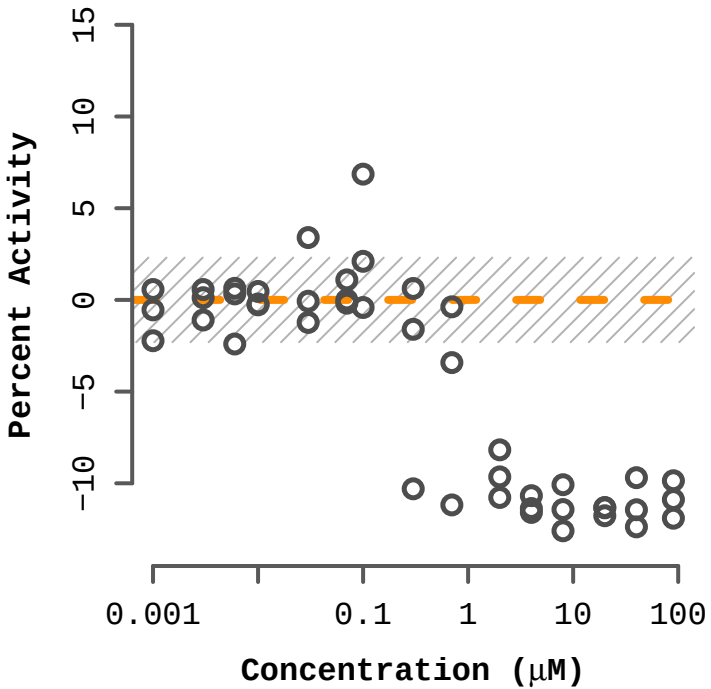
NAME: Triisobutylmethylphosphonium tosylate
CHID: 47899 **CASRN:** 344774-05-6
SPID(S): Tox21_200575
M4ID: 12481677

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

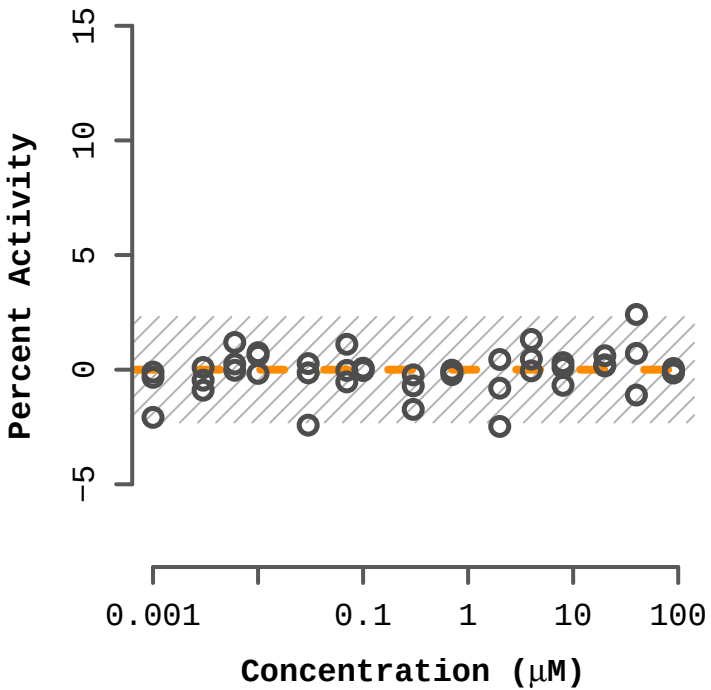
NAME: Tetraoctylphosphonium bromide
CHID: 47900 **CASRN:** 23906-97-0
SPID(S): Tox21_200576
M4ID: 12481676

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	314.76	NA	NA
PROB:	1	NA	NA
RMSE:	7.45	NA	NA

MAX_MEAN: 2.85 **MAX_MED:** 2.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

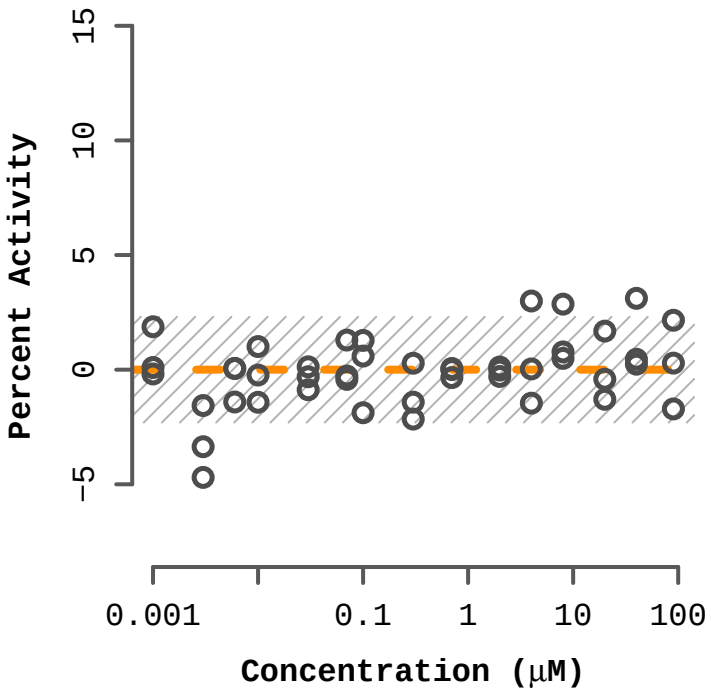
NAME: Ethylammonium nitrate
CHID: 47901 **CASRN:** 22113-86-6
SPID(S): Tox21_200578
M4ID: 12481674

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.712 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

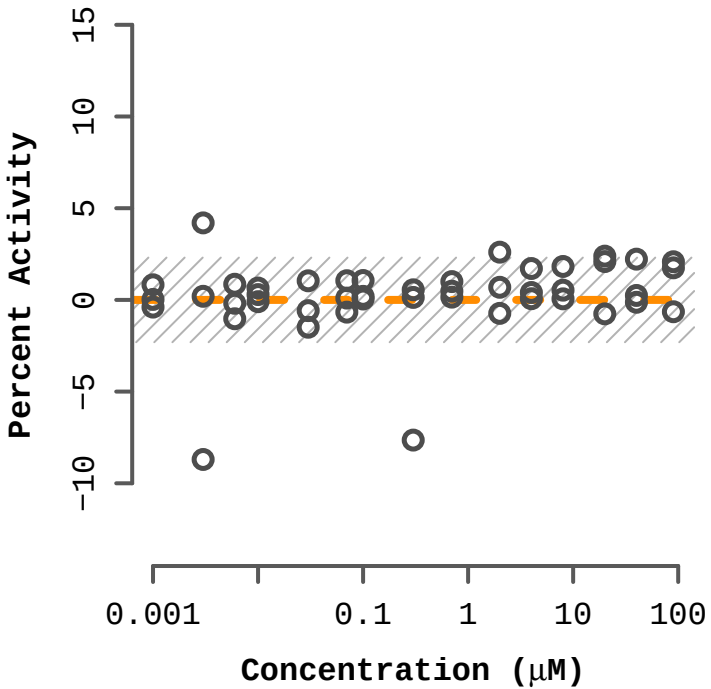
NAME: 2-Hydroxyethylammonium formate
CHID: 47902 **CASRN:** 53226-35-0
SPID(S): Tox21_200579
M4ID: 12481673

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 0.776 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

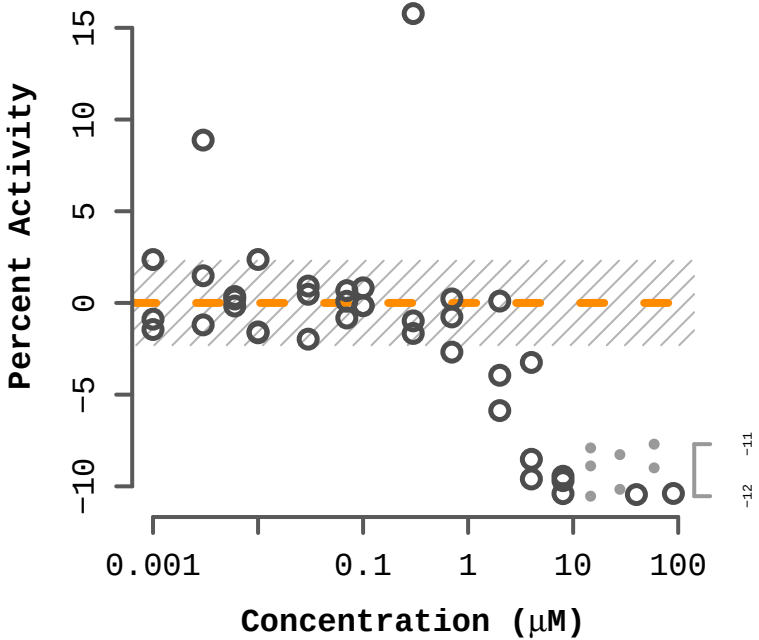
NAME: Dimethylammonium nitrate
CHID: 47903 **CASRN:** 30781-73-8
SPID(S): Tox21_200580
M4ID: 12481672

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.11	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

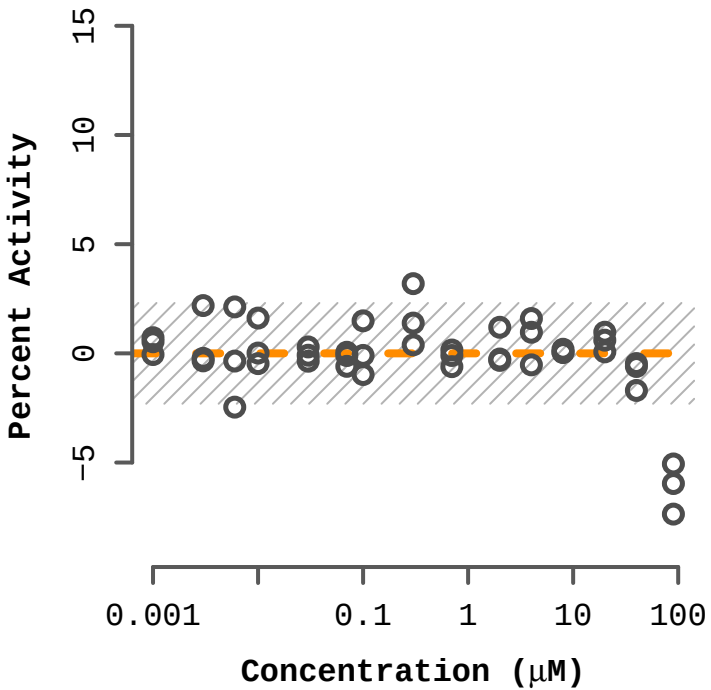
NAME: Methyltrioctylammonium trifluoromethanesulfonat
CHID: 47904 CASRN: 121107-18-4
SPID(S): Tox21_200581
M4ID: 12481671 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.86	NA	NA
PROB:	1	NA	NA
RMSE:	6.63	NA	NA

MAX_MEAN: 4.38 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

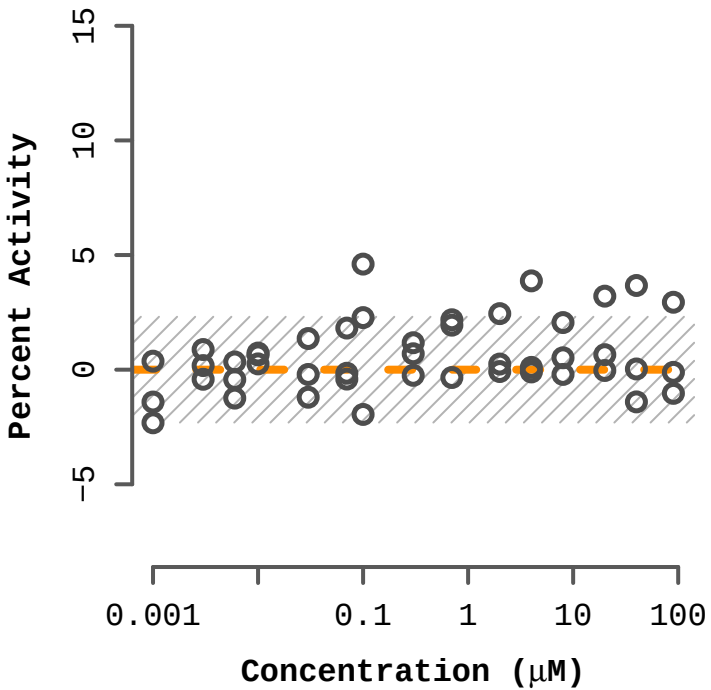
NAME: Tributylmethylammonium bis(trifluoromethylsulf
CHID: 47905 **CASRN:** 405514-94-5
SPID(S): Tox21_200582
M4ID: 12481670

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

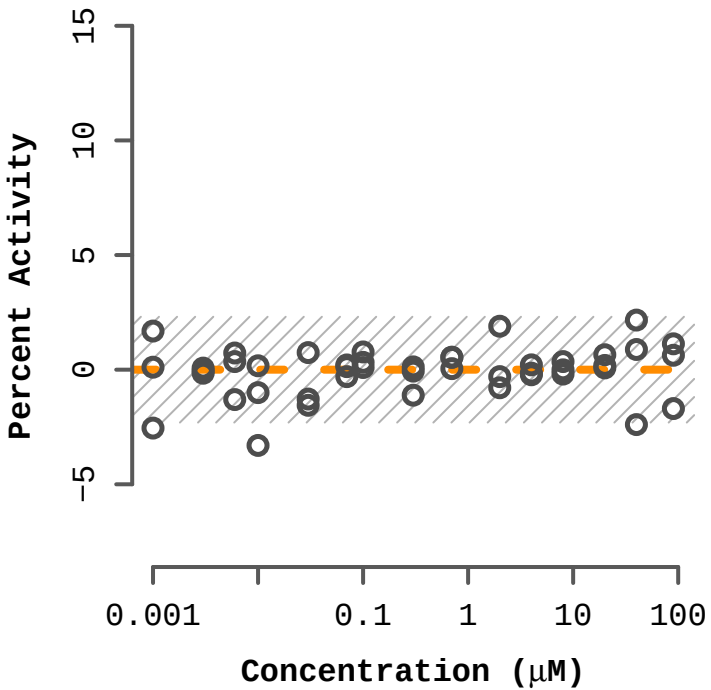
NAME: 1-Butyl-2,3-dimethylimidazolium chloride
CHID: 47906 **CASRN:** 98892-75-2
SPID(S): Tox21_200583
M4ID: 12481669

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

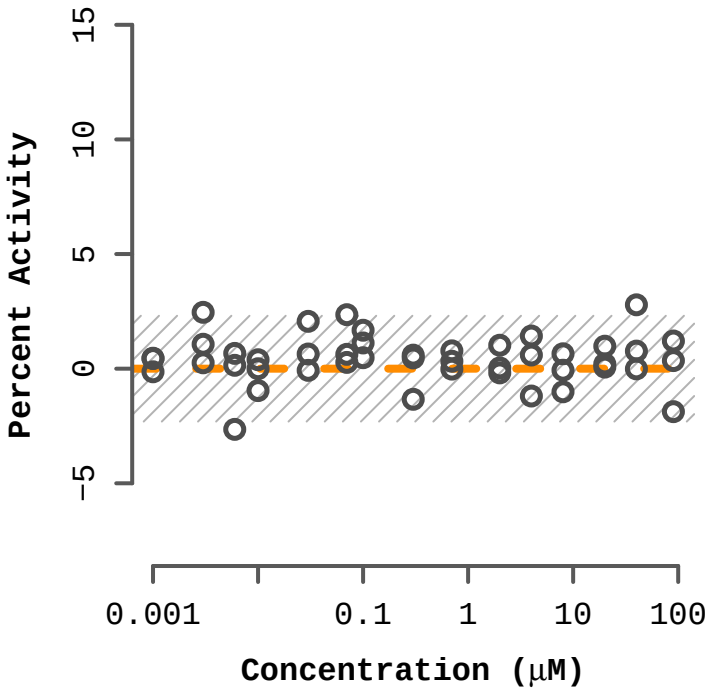
NAME: 1-Butyl-2,3-dimethylimidazolium hexafluorophos
CHID: 47907 **CASRN:** 227617-70-1
SPID(S): Tox21_200584
M4ID: 12481668

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.397 **MAX_MED:** 0.882 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

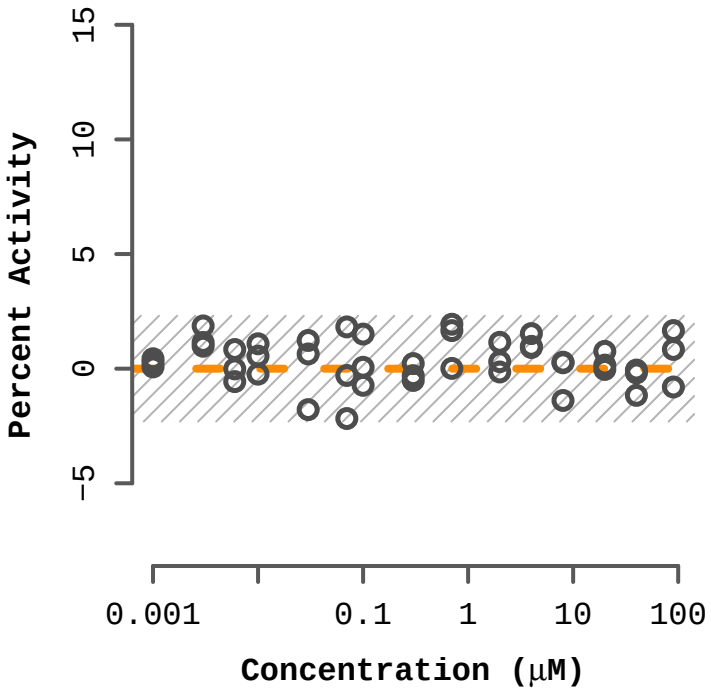
NAME: 1-Butyl-2,3-dimethylimidazolium iodide
CHID: 47908 **CASRN:** 108203-70-9
SPID(S): Tox21_200585
M4ID: 12481667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

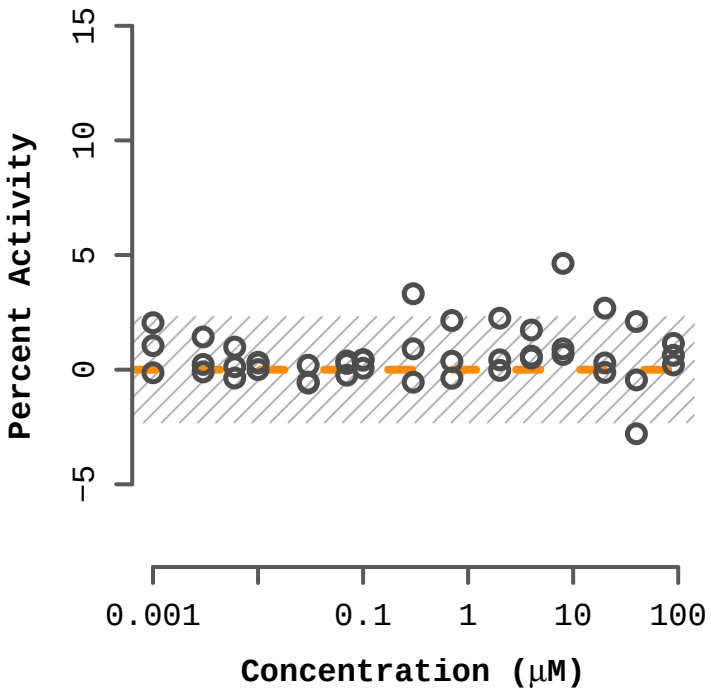
NAME: 1-Butyl-2,3-dimethylimidazolium tetrafluorobora
CHID: 47909 **CASRN:** 402846-78-0
SPID(S): Tox21_200586
M4ID: 12481666

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.5	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

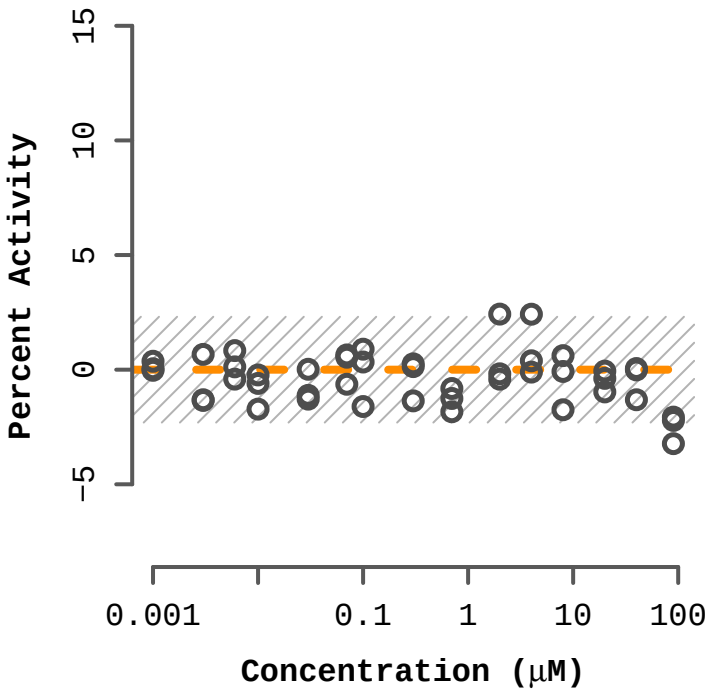
NAME: 1-Butyl-3-methylimidazolium dicyanamide
CHID: 47910 **CASRN:** 448245-52-1
SPID(S): Tox21_200587
M4ID: 12481665

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.07 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylimidazolium hexafluorophosphat

CHID: 47911 **CASRN:** 174501-64-5

SPID(S): Tox21_200588

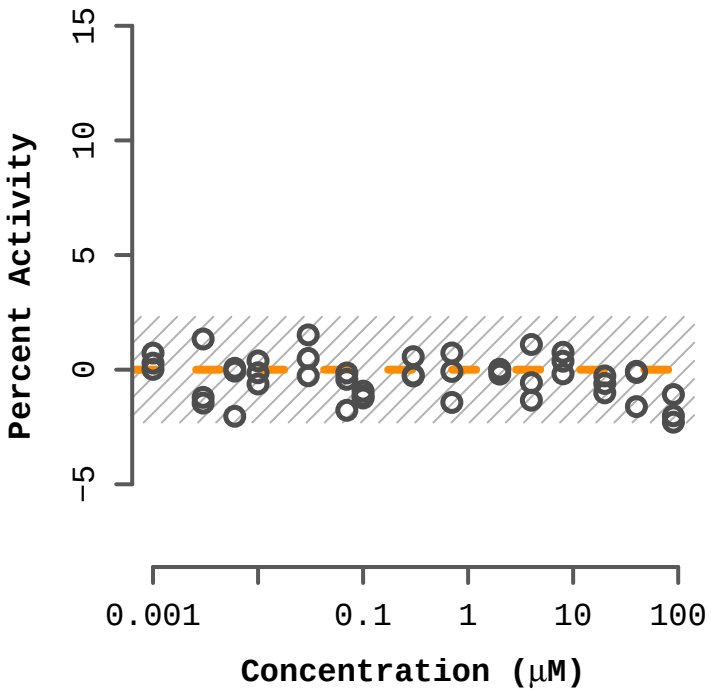
M4ID: 12481664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.544 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

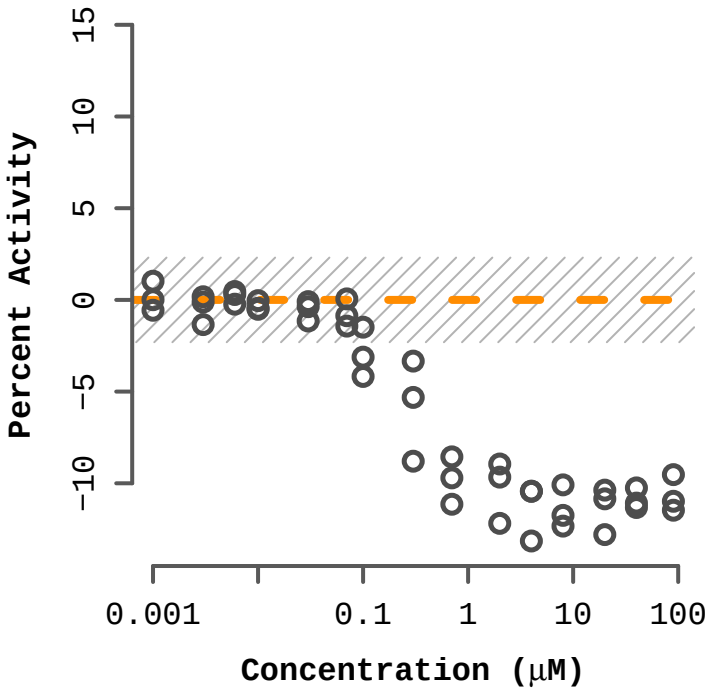
NAME: 1-Butyl-3-methylimidazolium methanesulfonate
CHID: 47912 **CASRN:** 342789-81-5
SPID(S): Tox21_200589
M4ID: 12481663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.582 **MAX_MED:** 0.493 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

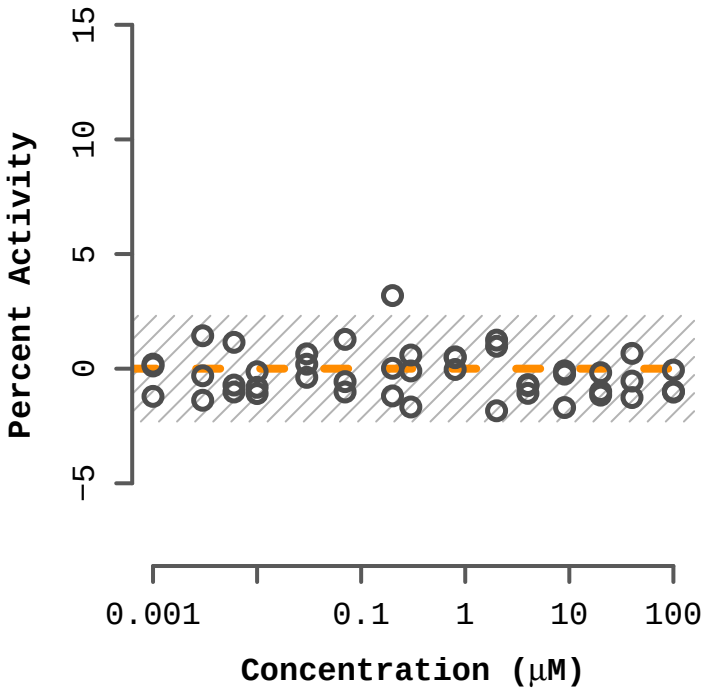
NAME: 1-Decyl-3-methylimidazolium bis(trifluoromethy
CHID: 47913 **CASRN:** 433337-23-6
SPID(S): Tox21_200590
M4ID: 12481662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	318.03	NA	NA
PROB:	1	NA	NA
RMSE:	7.66	NA	NA

MAX_MEAN: 0.174 **MAX_MED:** 0.296 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

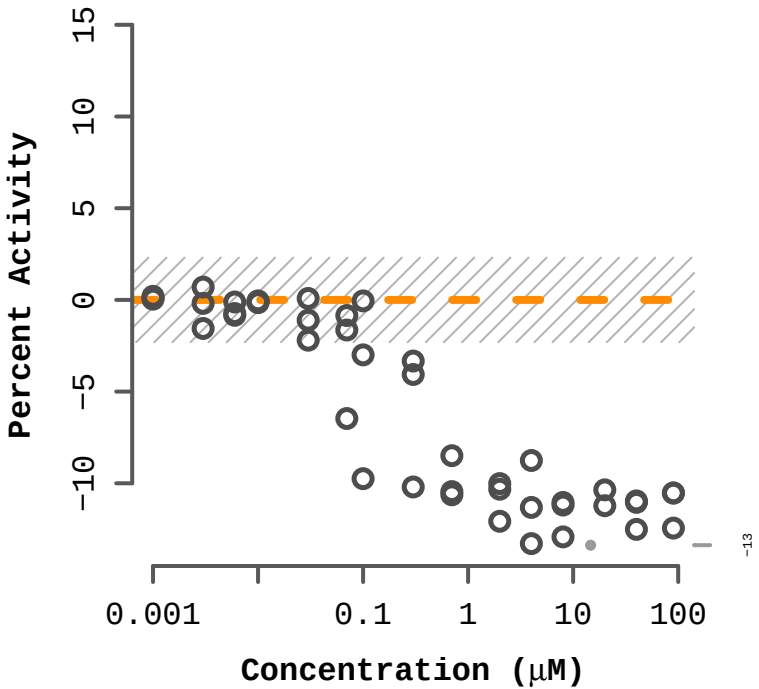
NAME: 1-Butyl-3-methylimidazolium thiocyanate
CHID: 47914 **CASRN:** 344790-87-0
SPID(S): Tox21_200591
M4ID: 12481661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.979 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

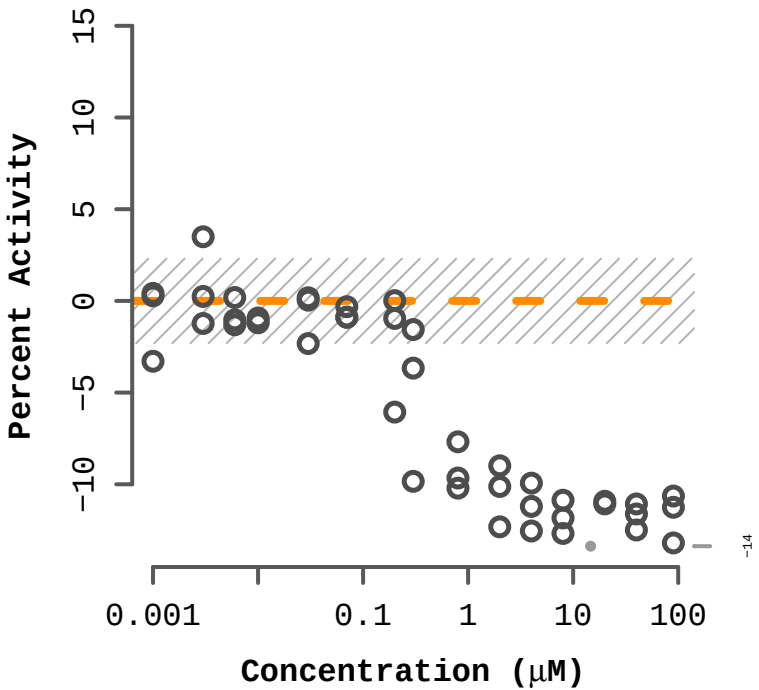
NAME: 1-Decyl-3-methylimidazolium tetrafluoroborate
CHID: 47915 **CASRN:** 244193-56-4
SPID(S): Tox21_200592
M4ID: 12481660 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	323.19	NA	NA
PROB:	1	NA	NA
RMSE:	8.06	NA	NA

MAX_MEAN: 0.118 **MAX_MED:** 0.111 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

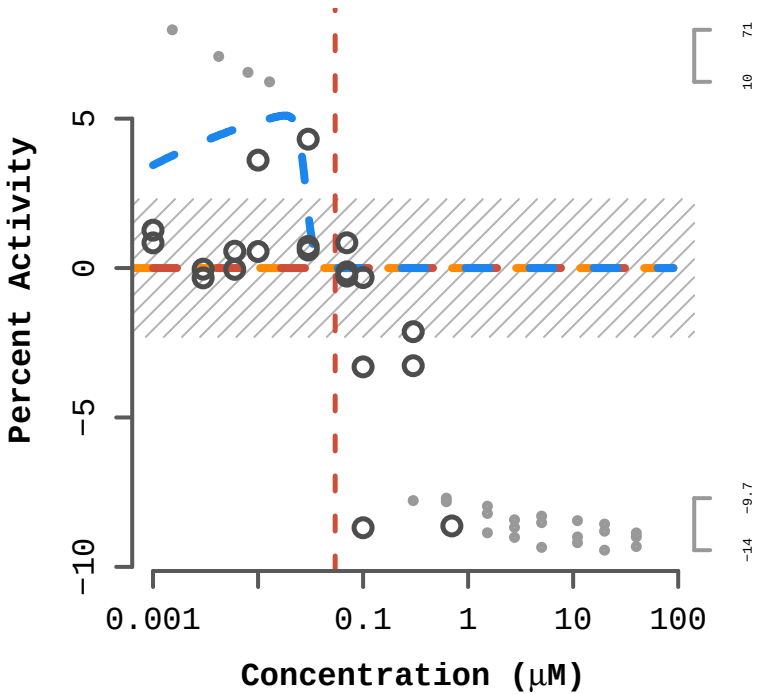
NAME: 1-Decyl-3-methylimidazolium trifluoromethanesu
CHID: 47916 CASRN: 412009-62-2
SPID(S): Tox21_200593
M4ID: 12481659 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	321.25	NA	NA
PROB:	1	NA	NA
RMSE:	7.93	NA	NA

MAX_MEAN: 0.839 MAX_MED: 0.276 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Dodecyl-3-methylimidazolium bis(trifluorometl
CHID: 47917 CASRN: 404001-48-5
SPID(S): Tox21_200594
M4ID: 12481658 BRK

HILL MODEL (in red):

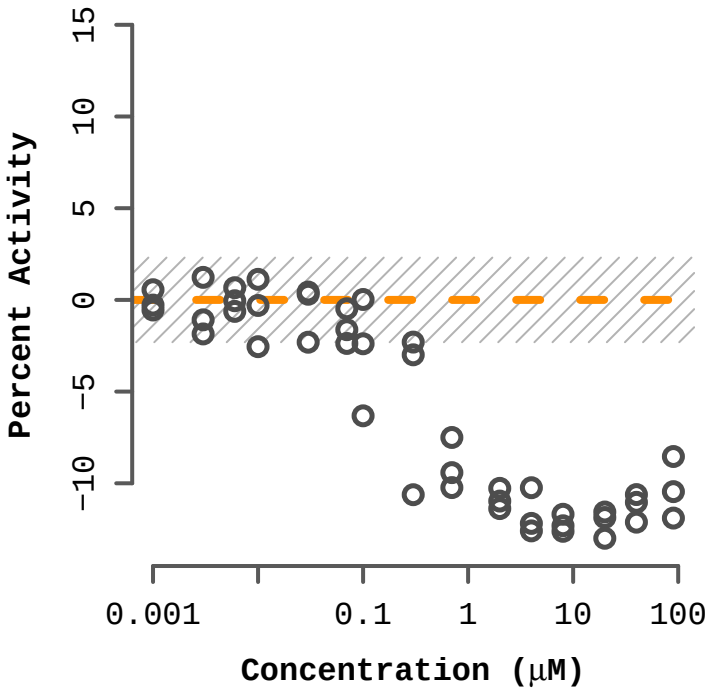
	tp	ga	gw
val:	8.59e-10	-1.27	1.72
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.94	-3.26	0.532	-1.55	11.1
sd:	63.7	13.5	14.9	0.885	411

	CNST	HILL	GNLS
AIC:	357.79	363.79	365.44
PROB:	0.93	0.05	0.02
RMSE:	15.21	15.21	14.49

MAX_MEAN: 24.4 MAX_MED: 3.61 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

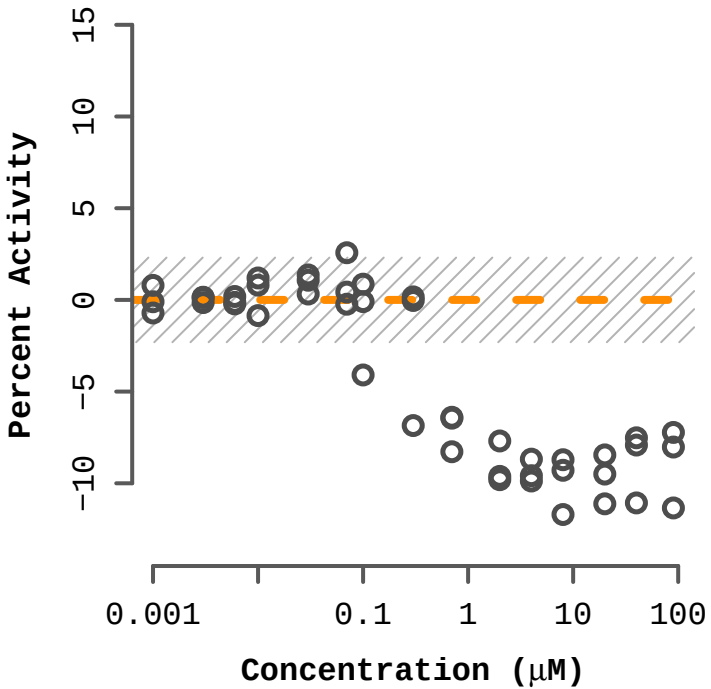
NAME: 1-Dodecyl-3-methylimidazolium chloride
CHID: 47918 **CASRN:** 114569-84-5
SPID(S): Tox21_200595
M4ID: 12481657

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	321.01	NA	NA
PROB:	1	NA	NA
RMSE:	7.91	NA	NA

MAX_MEAN: −1.45e-05 **MAX_MED:** 0.309 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

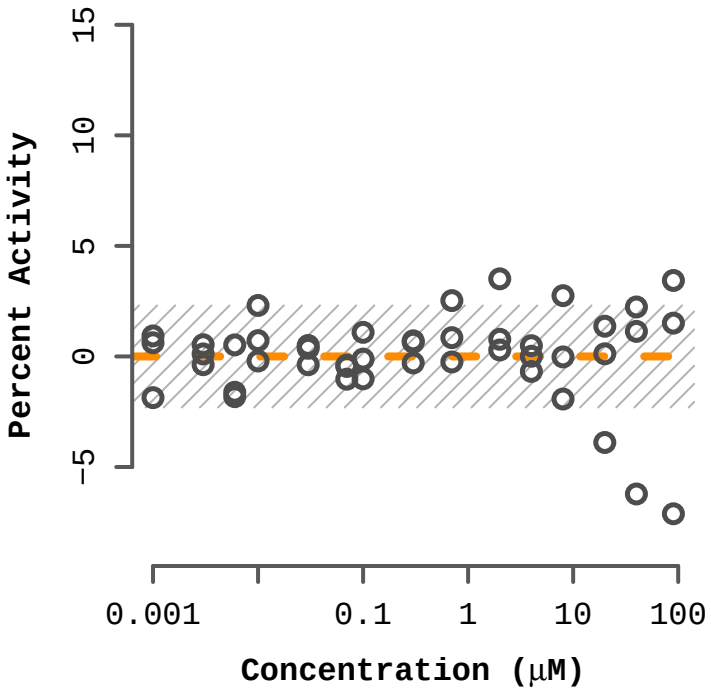
NAME: 1-Dodecyl-3-methylimidazolium hexafluorophospha
CHID: 47919 CASRN: 219947-93-0
SPID(S): Tox21_200596
M4ID: 12481656

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	300.28	NA	NA
PROB:	1	NA	NA
RMSE:	6.35	NA	NA

MAX_MEAN: 0.923 MAX_MED: 1.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

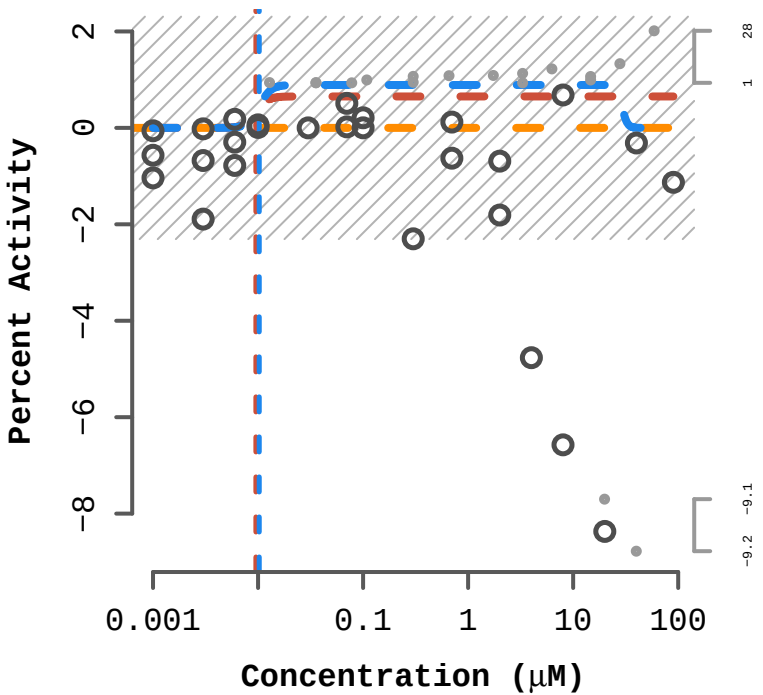
NAME: Butyltrimethylammonium bis(trifluoromethylsulf
CHID: 47920 **CASRN:** 258273-75-5
SPID(S): Tox21_200597
M4ID: 12481655

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Ethyl-3-methylimidazolium hexafluorophosphat

CHID: 47921 **CASRN:** 155371-19-0

SPID(S): Tox21_200598

M4ID: 12481654 **BRK**

HILL MODEL (in red):

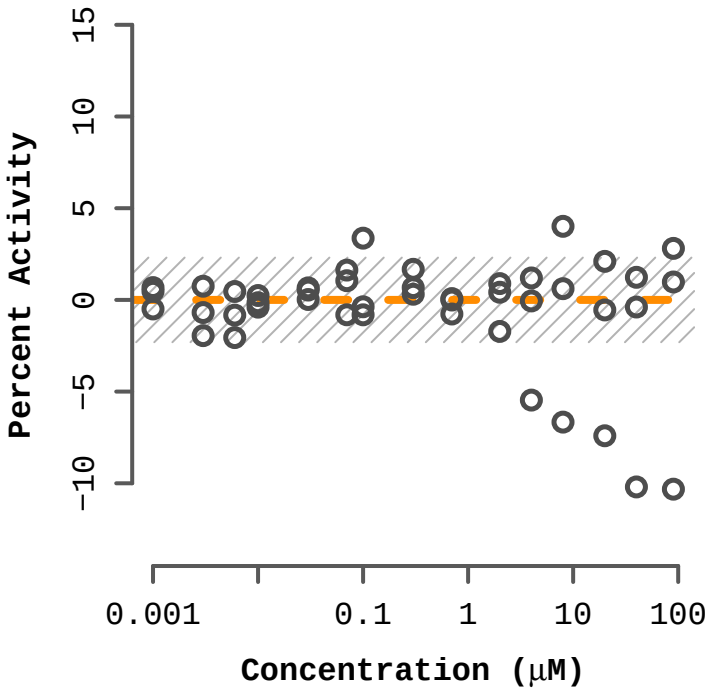
	tp	ga	gw
val:	0.651	−2.02	8
sd:	0.573	0.455	41.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.889	−1.99	8	1.47	17.7
sd:	0.589	0.37	45.2	0.949	111

	CNST	HILL	GNLS
AIC:	259.28	263.95	267
PROB:	0.89	0.09	0.02
RMSE:	5.71	5.63	5.68

MAX_MEAN: 6.03 **MAX_MED:** 2.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

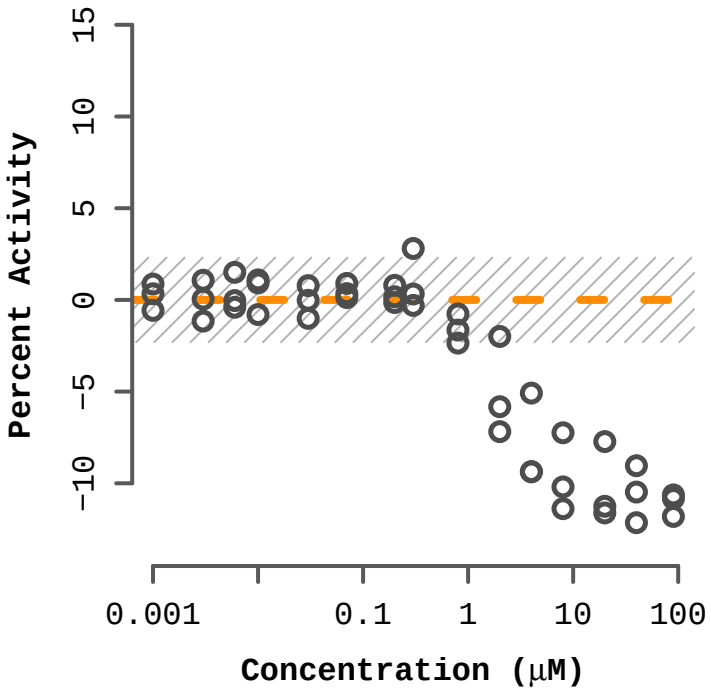
NAME: Choline bis(trifluoromethylsulfonyl)imde
CHID: 47922 **CASRN:** 827027-25-8
SPID(S): Tox21_200599
M4ID: 12481653

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.31	NA	NA
PROB:	1	NA	NA
RMSE:	3.01	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

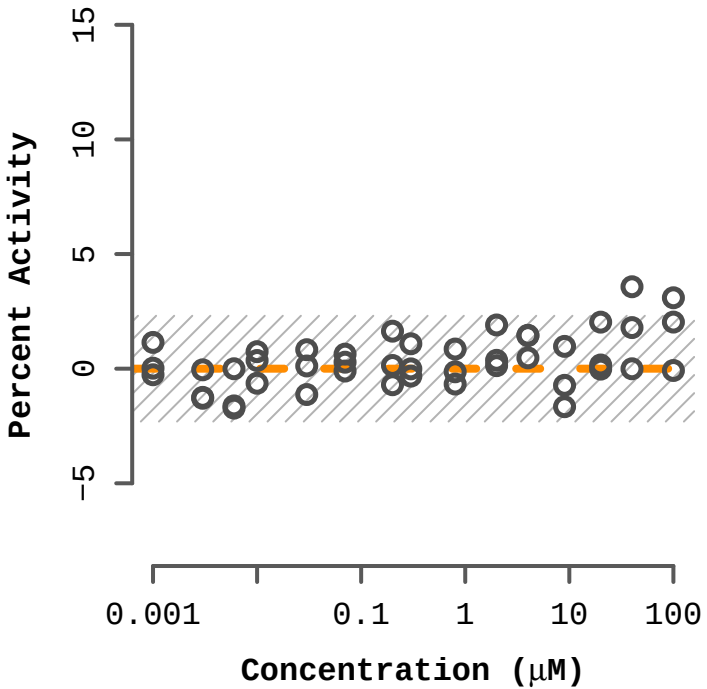
NAME: 1-Hexadecyl-3-methylimidazolium chloride
CHID: 47923 **CASRN:** 61546-01-8
SPID(S): Tox21_200600
M4ID: 12481652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	291.12	NA	NA
PROB:	1	NA	NA
RMSE:	6.03	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

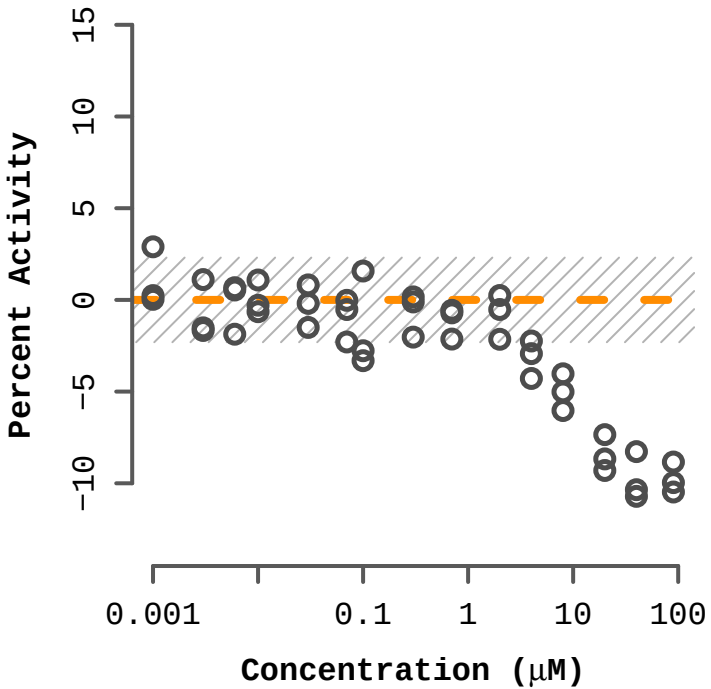
NAME: Methylammonium nitrate
CHID: 47924 **CASRN:** 22113-87-7
SPID(S): Tox21_200601
M4ID: 12481651

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

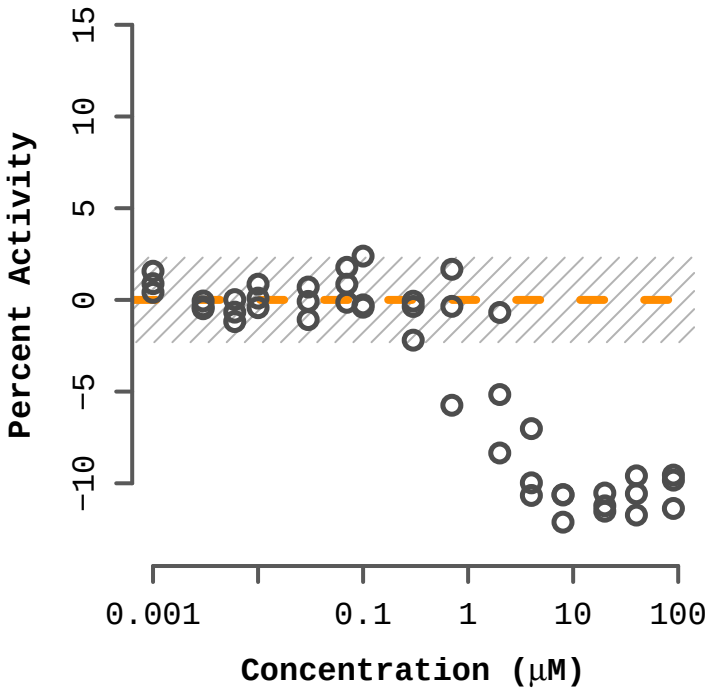
NAME: 1-Hexyl-3-methylimidazolium bromide
CHID: 47925 **CASRN:** 85100-78-3
SPID(S): Tox21_200602
M4ID: 12481650

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	264.05	NA	NA
PROB:	1	NA	NA
RMSE:	4.64	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.541 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

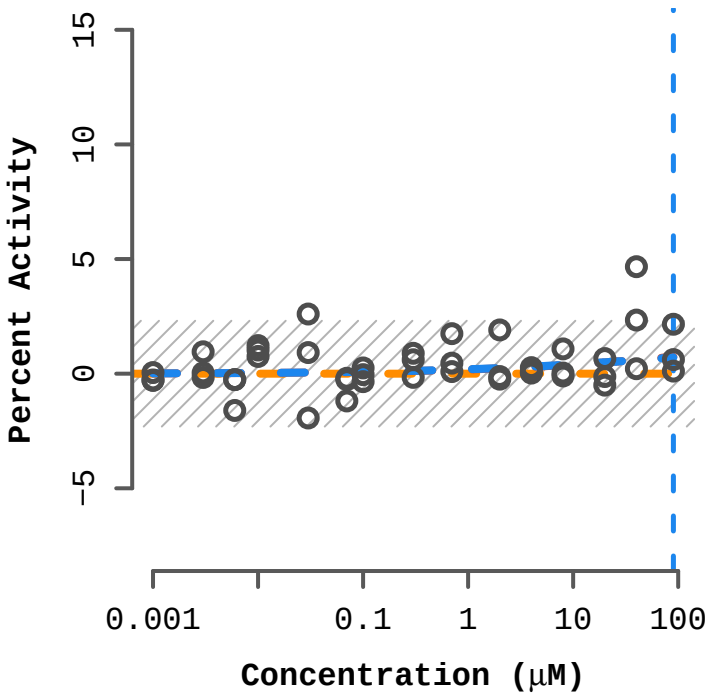
NAME: Methyltrioctylammonium bis(trifluoromethylsulf
CHID: 47926 **CASRN:** 375395-33-8
SPID(S): Tox21_200603
M4ID: 12481649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	297.13	NA	NA
PROB:	1	NA	NA
RMSE:	6.36	NA	NA

MAX_MEAN: 0.956 **MAX_MED:** 0.889 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Propylammonium nitrate
CHID: 47927 **CASRN:** 22113-88-8
SPID(S): Tox21_200604
M4ID: 12481648

HILL MODEL (in red):

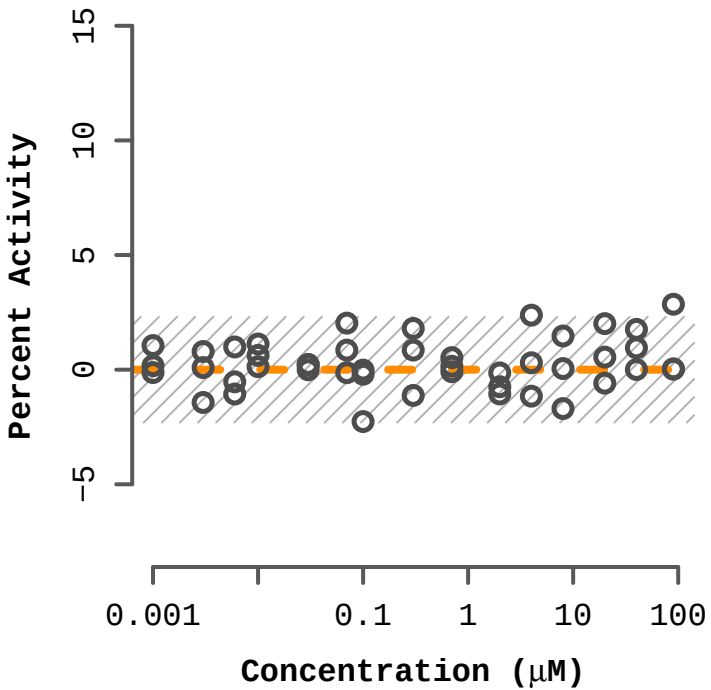
	tp	ga	gw
val:	1.91	2.45	0.398
sd:	6.14	5.05	0.459

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.41	1.95	0.41	3.87	3.42
sd:	3.94	4.49	0.481	1290	2220

	CNST	HILL	GNLS
AIC:	133.05	133.34	137.4
PROB:	0.51	0.44	0.06
RMSE:	1.18	1.07	1.07

MAX_MEAN: 2.41 **MAX_MED:** 2.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

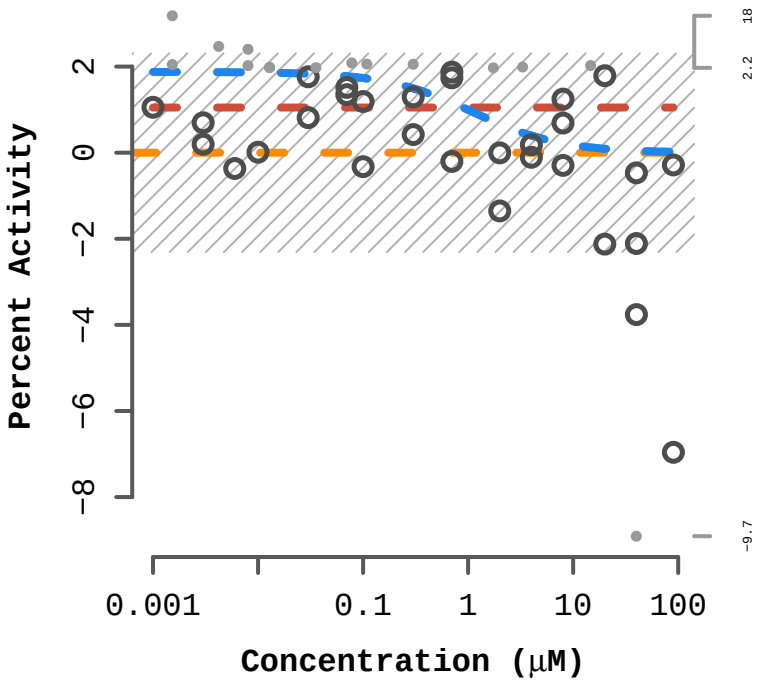
NAME: 1-Allyl-3-methylimidazolium chloride
CHID: 47928 **CASRN:** 65039-10-3
SPID(S): Tox21_200605
M4ID: 12481647

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Benzyl-3-methylimidazolium chloride
CHID: 47929 **CASRN:** 36443-80-8
SPID(S): Tox21_200606
M4ID: 12481646 **BRK**

HILL MODEL (in red):

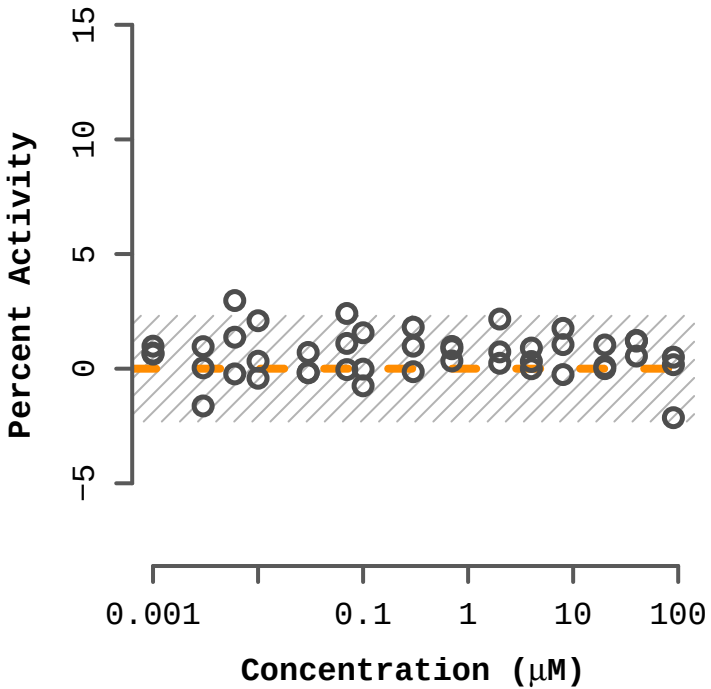
	tp	ga	gw
val:	1.05	−4.99	3.47
sd:	0.327	1070	1860

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.88	−4.46	4.93	0.0486	1.03
sd:	0.544	1090	3680	0.71	1.04

	CNST	HILL	GNLS
AIC:	235.86	232.98	228.06
PROB:	0.02	0.08	0.9
RMSE:	4.05	3.87	3.55

MAX_MEAN: 7.39 **MAX_MED:** 3.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

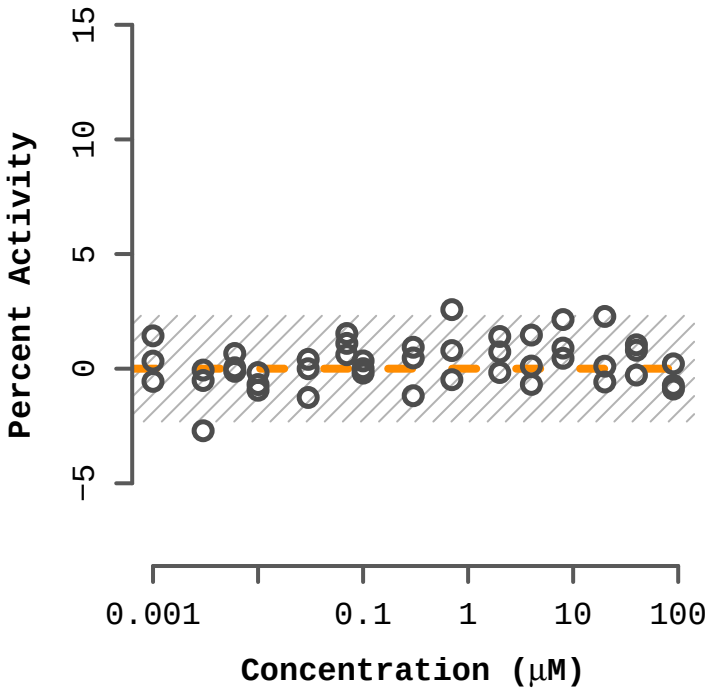
NAME: 1-Butyl-2,3-dimethylimidazolium bis(trifluorom
CHID: 47930 CASRN: 350493-08-2
SPID(S): Tox21_200607
M4ID: 12481645

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.37 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

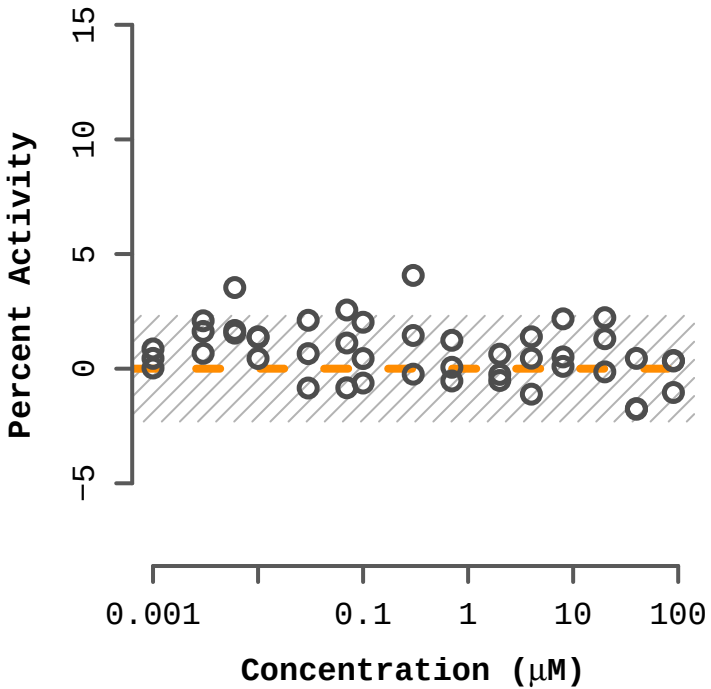
NAME: 1-Butyl-2,3-dimethylimidazolium bromide
CHID: 47931 **CASRN:** 475575-45-2
SPID(S): Tox21_200608
M4ID: 12481644

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

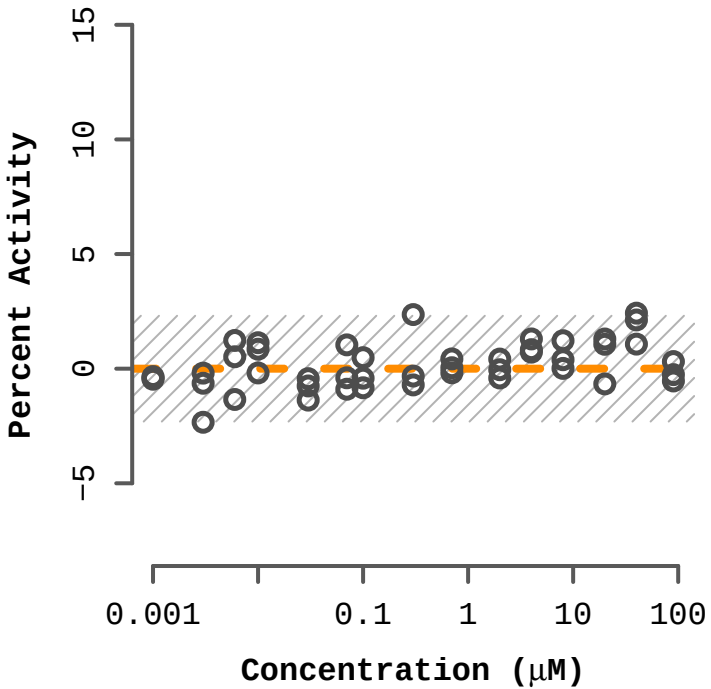
NAME: 1-Butylpyridinium hexafluorophosphate
CHID: 47932 **CASRN:** 186088-50-6
SPID(S): Tox21_200609
M4ID: 12481643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.25 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

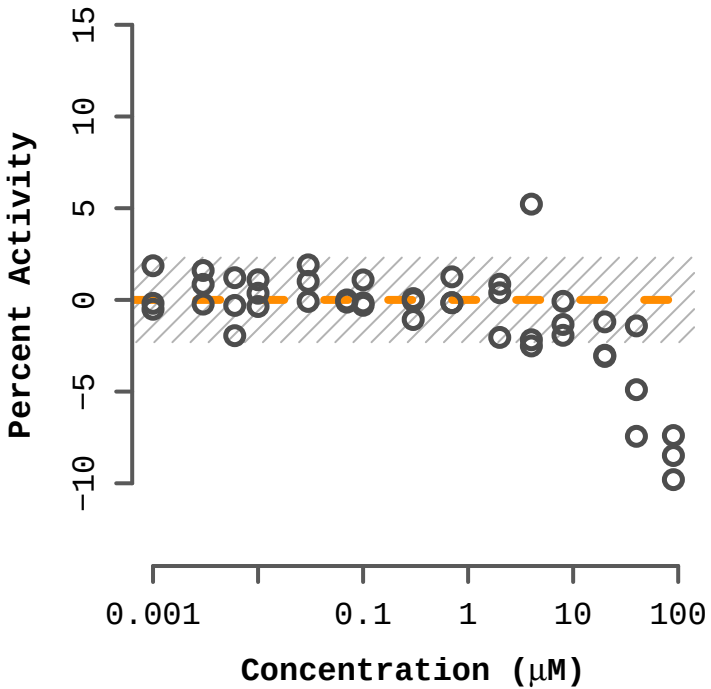
NAME: 1-Butylpyridinium bromide
CHID: 47933 **CASRN:** 874-80-6
SPID(S): Tox21_200610
M4ID: 12481642

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.87 **MAX_MED:** 2.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

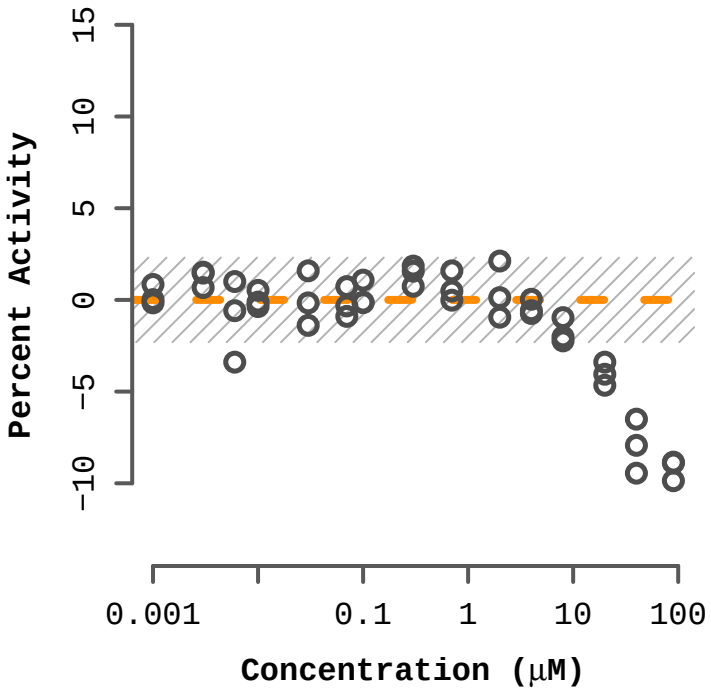
NAME: 1-Hexylpyridinium bromide
CHID: 47934 **CASRN:** 74440-81-6
SPID(S): Tox21_200611
M4ID: 12481641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.37	NA	NA
PROB:	1	NA	NA
RMSE:	2.96	NA	NA

MAX_MEAN: 0.947 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

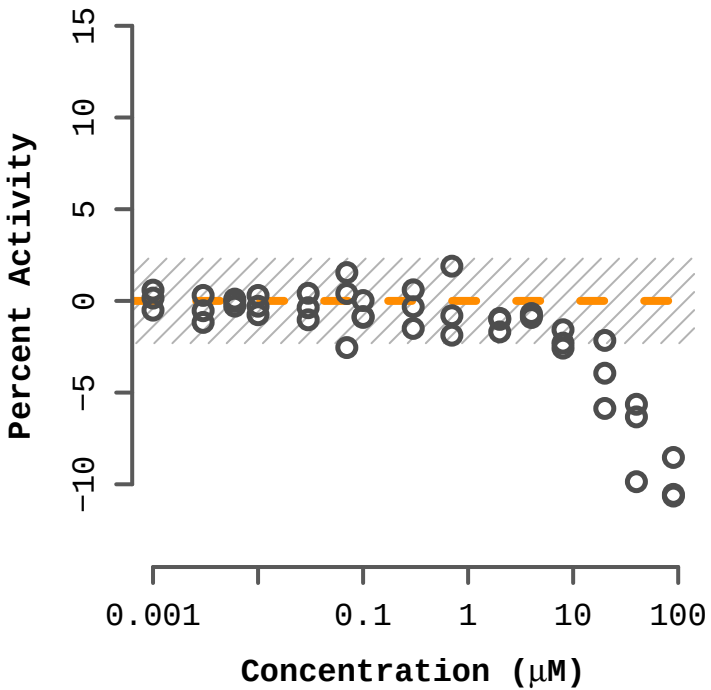
NAME: 1-Hexylpyridinium chloride
CHID: 47935 **CASRN:** 6220-15-1
SPID(S): Tox21_200612
M4ID: 12481640

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	228.82	NA	NA
PROB:	1	NA	NA
RMSE:	3.5	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

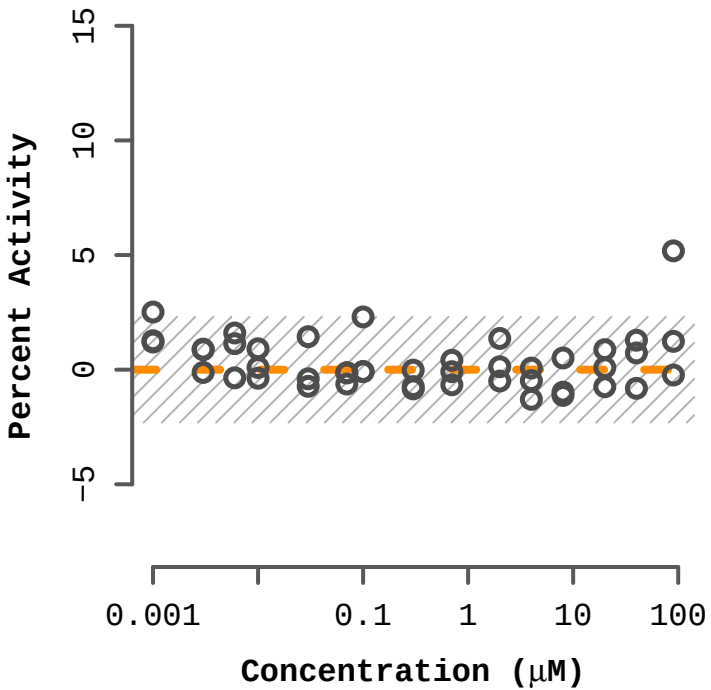
NAME: 1-Hexylpyridinium hexafluorophosphate
CHID: 47936 **CASRN:** 797789-00-5
SPID(S): Tox21_200613
M4ID: 12481639

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.02	NA	NA
PROB:	1	NA	NA
RMSE:	3.55	NA	NA

MAX_MEAN: 0.0807 **MAX_MED:** 0.405 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

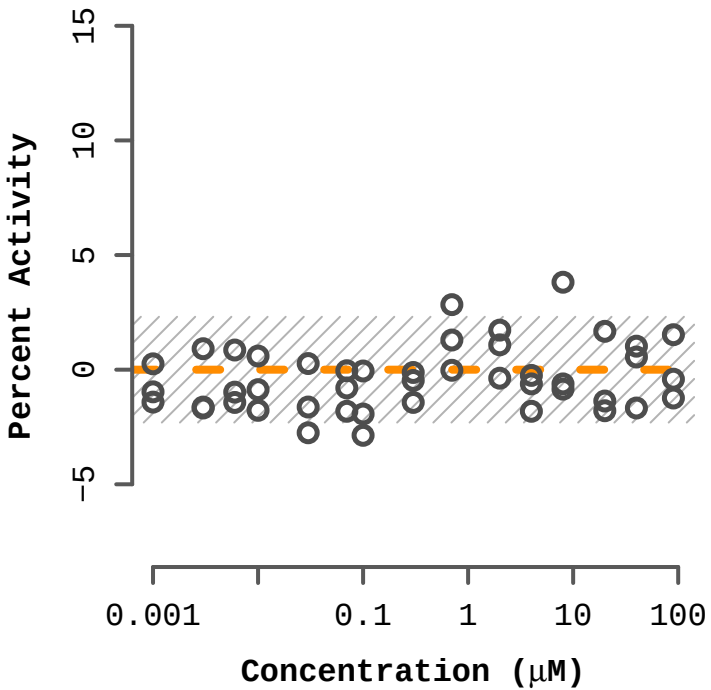
NAME: 1-Butyl-1-methylpyrrolidinium hexafluorophospha
CHID: 47937 **CASRN:** 330671-29-9
SPID(S): Tox21_200614
M4ID: 12481638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

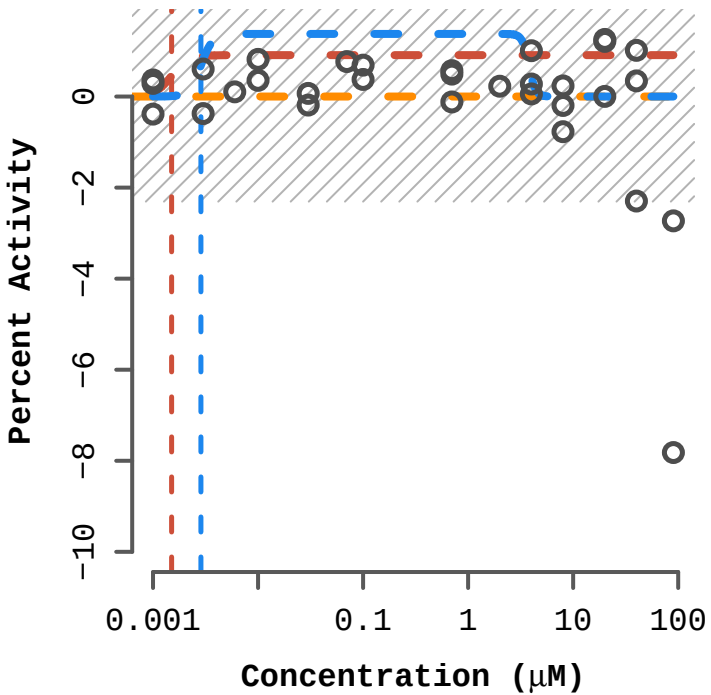
NAME: 1-Butyl-1-methylpyrrolidinium iodide
CHID: 47938 **CASRN:** 56511-17-2
SPID(S): Tox21_200615
M4ID: 12481637

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-1-methylpyrrolidinium dicyanamide
CHID: 47939 **CASRN:** 370865-80-8
SPID(S): Tox21_200616
M4ID: 12481636

HILL MODEL (in red):

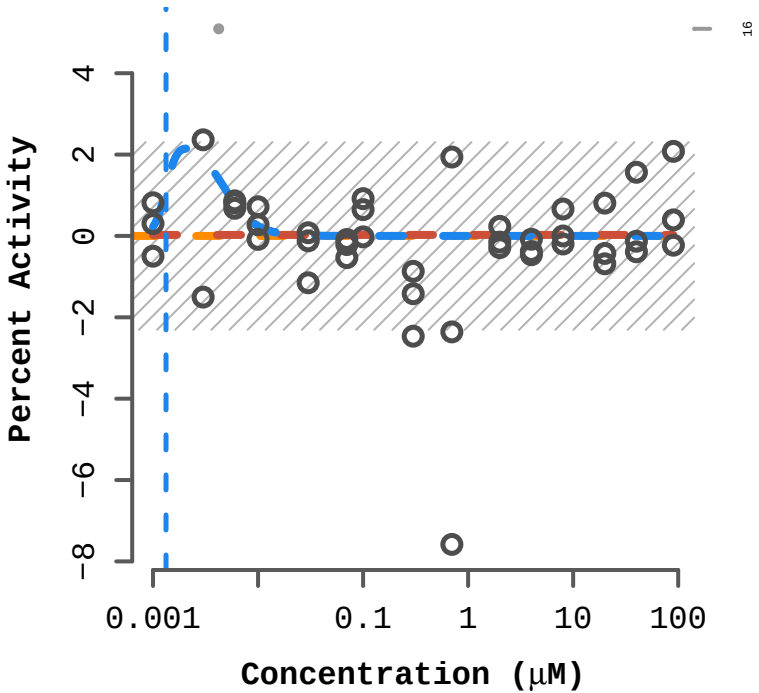
	tp	ga	gw
val:	0.91	−2.82	5.37
sd:	0.23	1	25.5

GAIN-LOSS MODEL (in blue):

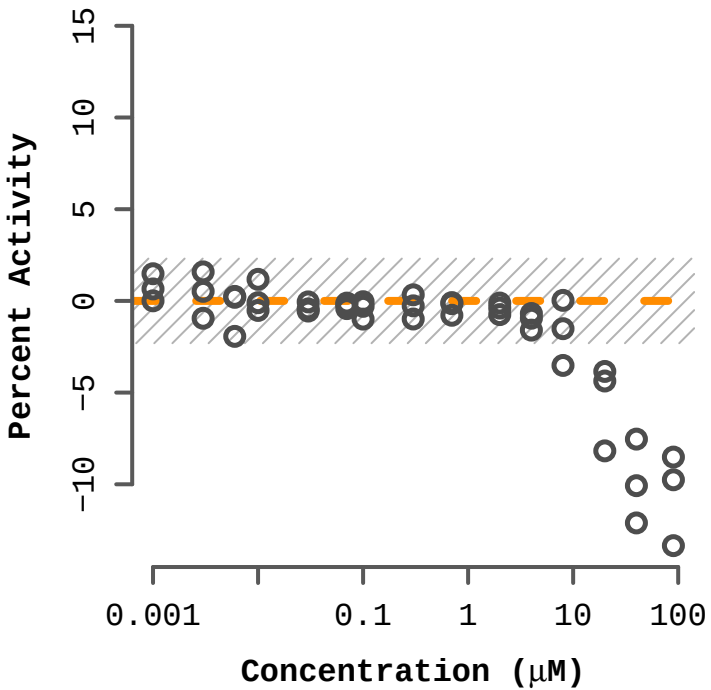
	tp	ga	gw	la	lw
val:	1.38	−2.54	7.74	0.578	14
sd:	0.295	0.175	23.8	0.213	116

	CNST	HILL	GNLS
AIC:	189.4	180.67	178.2
PROB:	0	0.22	0.77
RMSE:	2.08	1.93	1.74

MAX_MEAN: 2.22 **MAX_MED:** 2.91 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Ethyl-1-methylpyrrolidinium bis(trifluorometl
CHID:    47940   CASRN: 223436-99-5
SPID(S): Tox21_200625
M4ID:    12481627  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  0.0255   -4.44    4.02
sd:   0.149    1620     4510

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.41     -2.88    7.92     -2.33    2.91
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  162.48      168.45      167.68
PROB: 0.89        0.04        0.07
RMSE: 2.81        2.8         2.58

MAX_MEAN: 5.61      MAX_MED: 2.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

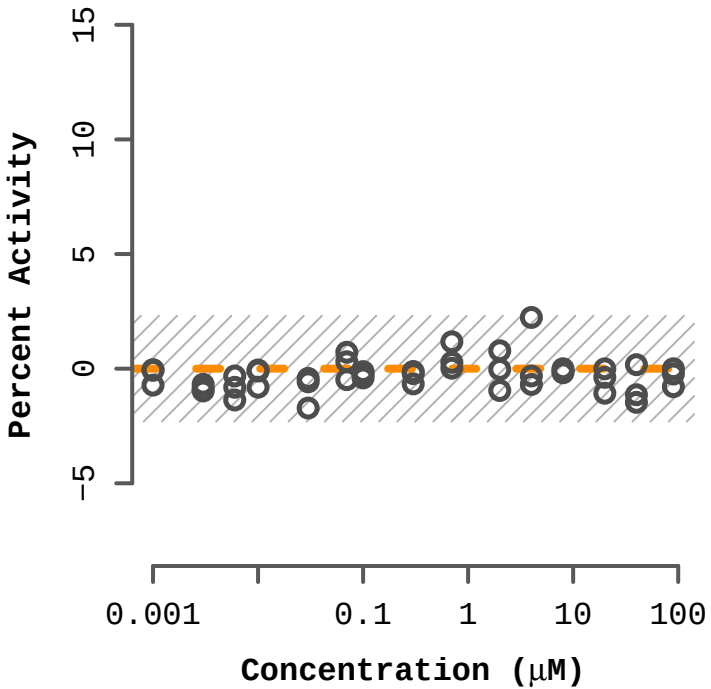
NAME: 1-Ethyl-1-methylpyrrolidinium iodide
CHID: 47941 **CASRN:** 4186-68-9
SPID(S): Tox21_200626
M4ID: 12481626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.26	NA	NA
PROB:	1	NA	NA
RMSE:	4.18	NA	NA

MAX_MEAN: 0.714 **MAX_MED:** 0.654 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

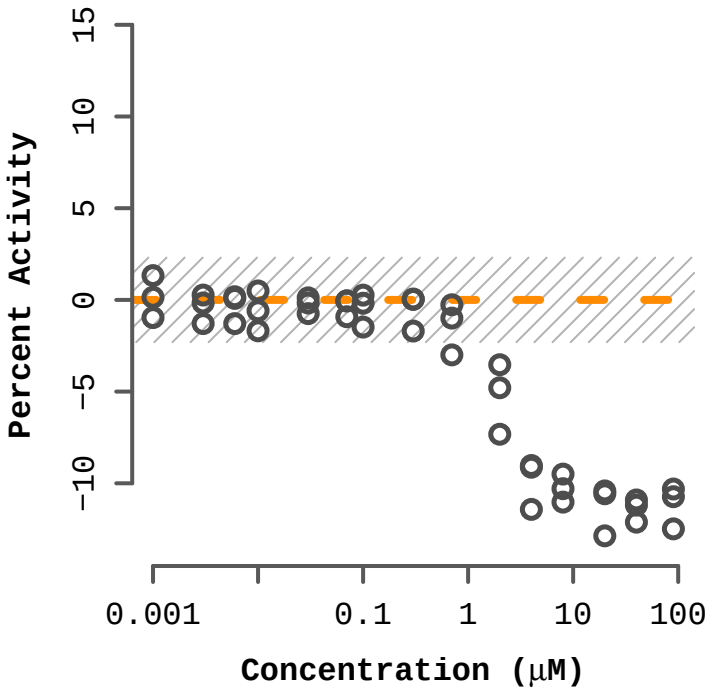
NAME: 1-Methyl-1-propylpyrrolidinium bis(trifluorome
CHID: 47942 CASRN: 223437-05-6
SPID(S): Tox21_200630
M4ID: 12481622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.491 MAX_MED: 0.304 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

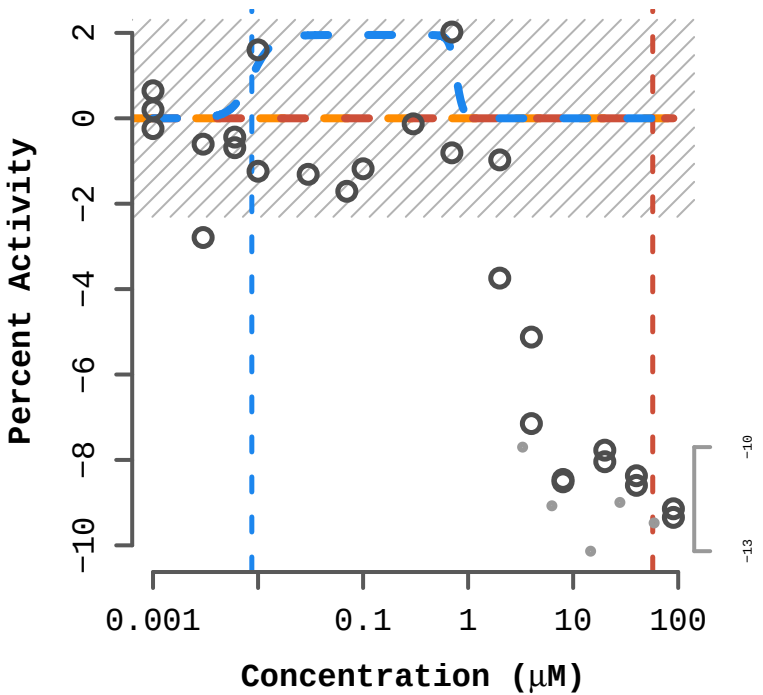
NAME: 1-Methyl-3-octylimidazolium tetrafluoroborate
CHID: 47943 **CASRN:** 244193-52-0
SPID(S): Tox21_200695
M4ID: 12481557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	298.1	NA	NA
PROB:	1	NA	NA
RMSE:	6.47	NA	NA

MAX_MEAN: 0.171 **MAX_MED:** 0.146 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trihexyltetradecylphosphonium chloride
CHID: 47944 CASRN: 258864-54-9
SPID(S): Tox21_200697
M4ID: 12481555 BRK

HILL MODEL (in red):

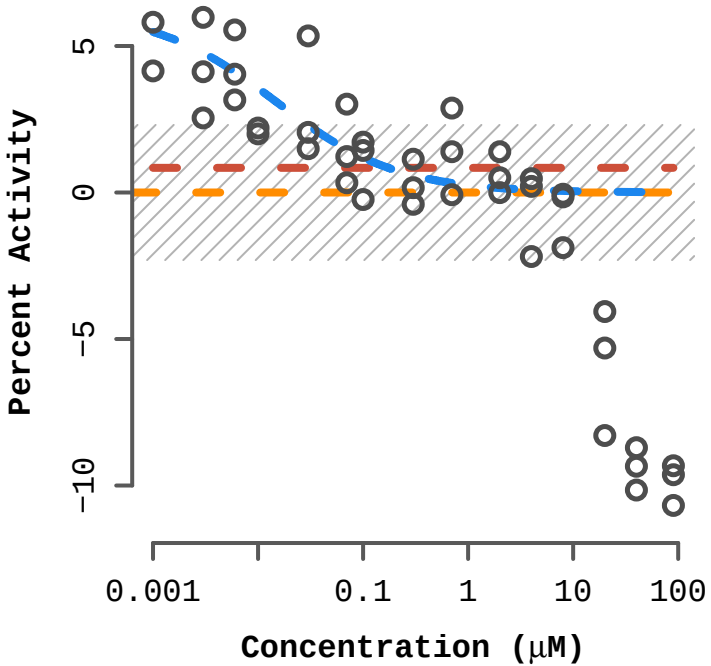
	tp	ga	gw
val:	1.28e-09	1.76	0.581
sd:	4.08e-05	9940	19600

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.95	-2.06	4.45	-0.113	13.2
sd:	1.28	0.495	22.5	3.44	1080

	CNST	HILL	GNLS
AIC:	289.83	295.83	296.94
PROB:	0.93	0.05	0.03
RMSE:	5.81	5.81	5.71

MAX_MEAN: 2.62 MAX_MED: 3.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tetrabutylphosphonium bromide
CHID: 47945 CASRN: 3115-68-2
SPID(S): Tox21_200701
M4ID: 12481551

HILL MODEL (in red):

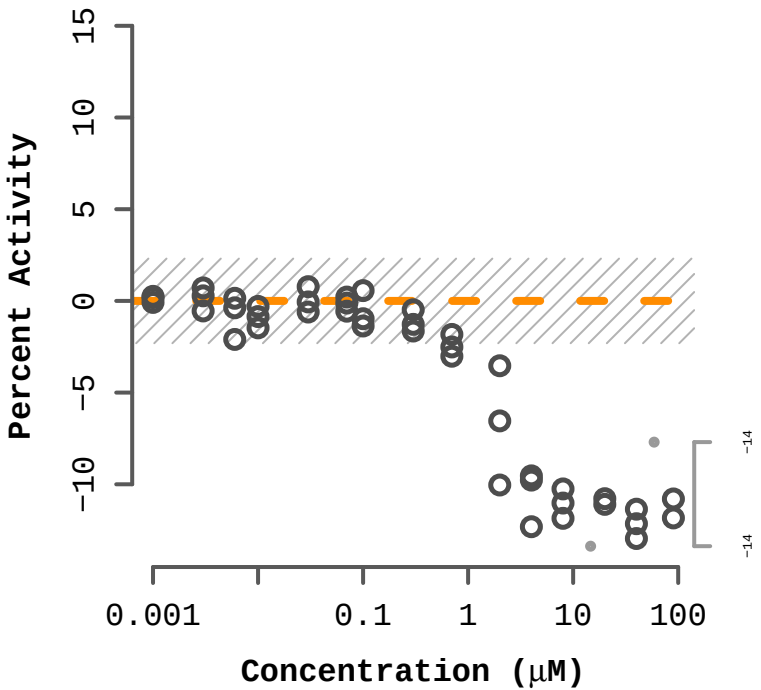
	tp	ga	gw
val:	0.842	−4.56	4.77
sd:	0.624	1620	4930

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.2	−3.95	7.79	−1.83	0.753
sd:	2.92	841	6870	0.778	0.439

	CNST	HILL	GNLS
AIC:	271.11	275.44	254.24
PROB:	0	0	1
RMSE:	4.77	4.85	4.06

MAX_MEAN: 5.84 **MAX_MED:** 5.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

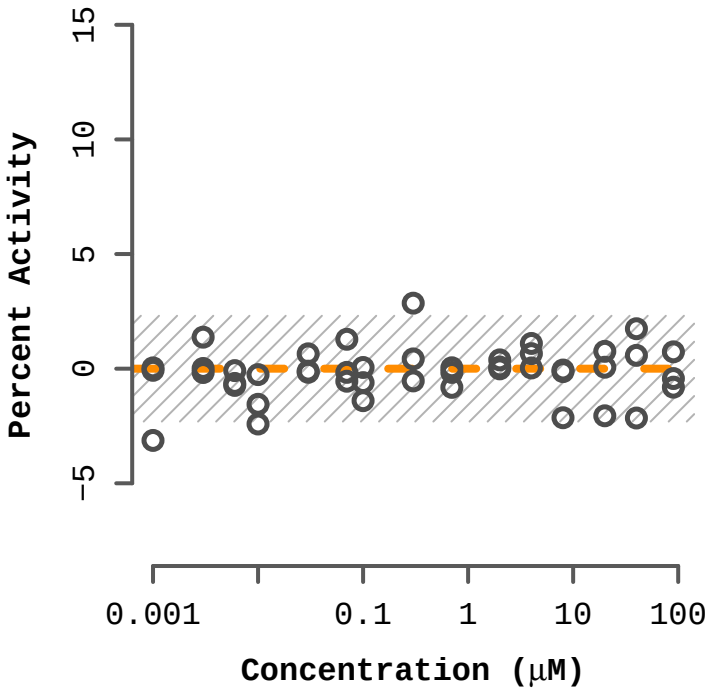
NAME: 1-Methyl-3-octylimidazolium trifluoromethanesu
CHID: 47946 **CASRN:** 403842-84-2
SPID(S): Tox21_200708
M4ID: 12481544 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	305.7	NA	NA
PROB:	1	NA	NA
RMSE:	7	NA	NA

MAX_MEAN: 0.147 **MAX_MED:** 0.278 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

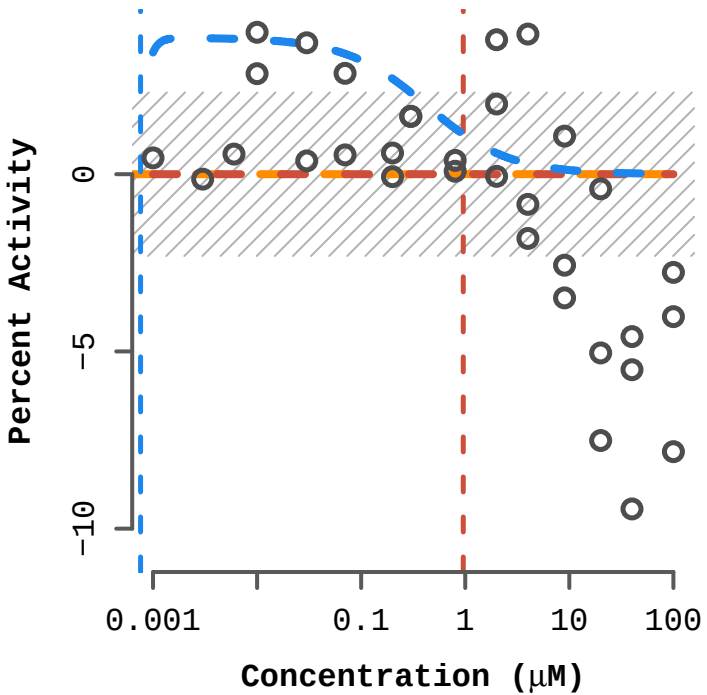
NAME: 1-Methyl-3-propylimidazolium bis(trifluorometh
CHID: 47947 **CASRN:** 216299-72-8
SPID(S): Tox21_200717
M4ID: 12481535

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Hexyl-3-methylimidazolium chloride
CHID: 47948 CASRN: 171058-17-6
SPID(S): Tox21_200718
M4ID: 12481534

HILL MODEL (in red):

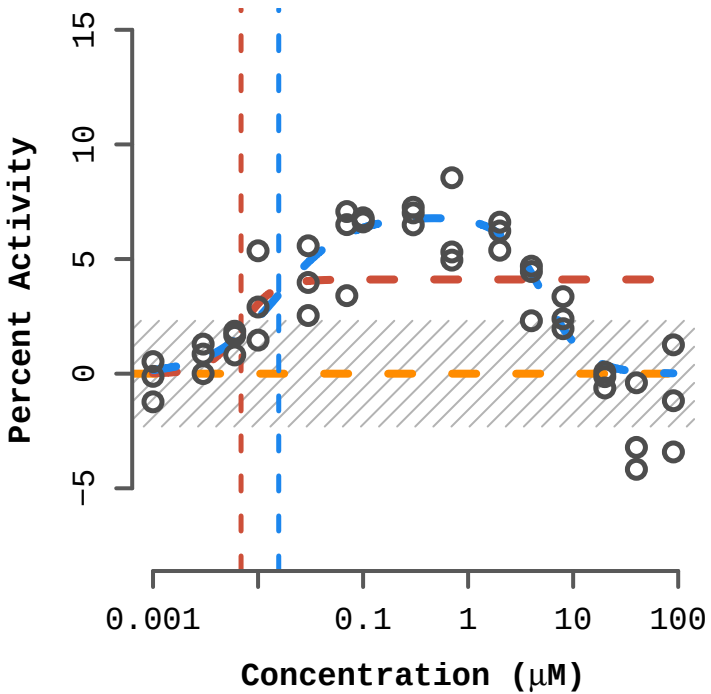
	tp	ga	gw
val:	6.9e-10	-0.0191	1.14
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

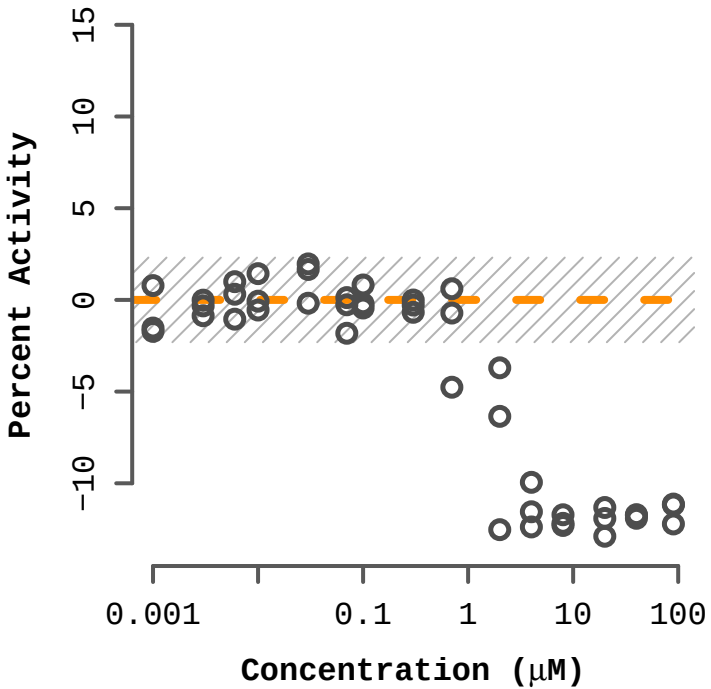
	tp	ga	gw	la	lw
val:	3.85	-3.12	7.68	-0.367	1.11
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	263.55	269.55	250.18
PROB:	0	0	1
RMSE:	4.19	4.19	3.37

MAX_MEAN: 4.03 MAX_MED: 5.85 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Hexyl-3-methylimidazolium hexafluorophosphat
CHID:    47949   CASRN: 304680-35-1
SPID(S): Tox21_200735
M4ID:    12481517

HILL MODEL (in red):
      tp       ga       gw
val:  4.11     -2.16    2.82
sd:   0.561    0.161    2.86

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.89     -1.8     1.35     0.717    2.11
sd:   0.53     0.126    0.314    0.077    0.508

      CNST        HILL        GNLS
AIC:  266.5       234.63      166.37
PROB: 0           0           1
RMSE: 4.31        3.03        1.42

MAX_MEAN: 6.92      MAX_MED: 7.02      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

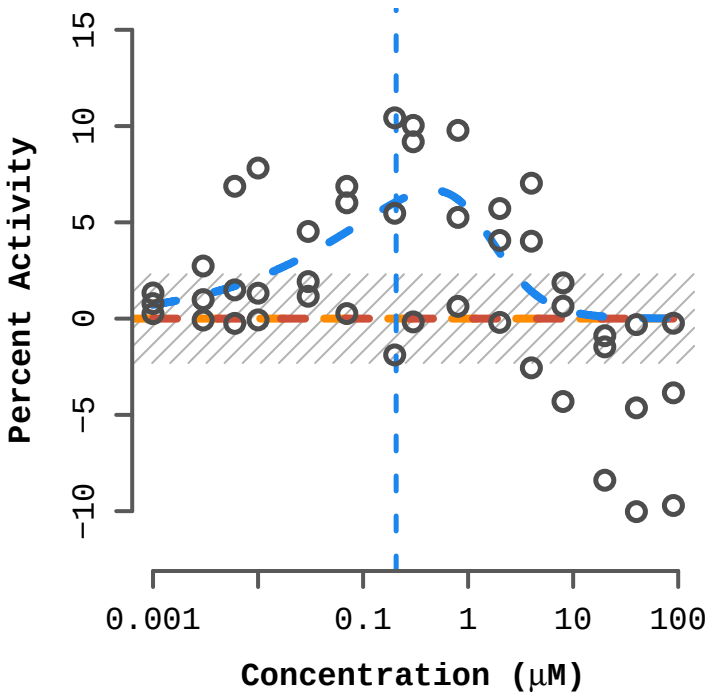
NAME: Trihexyltetradecylphosphonium hexafluorophospha
CHID: 47950 **CASRN:** 374683-44-0
SPID(S): Tox21_200750
M4ID: 12481502

HILL MODEL: Not applicable.

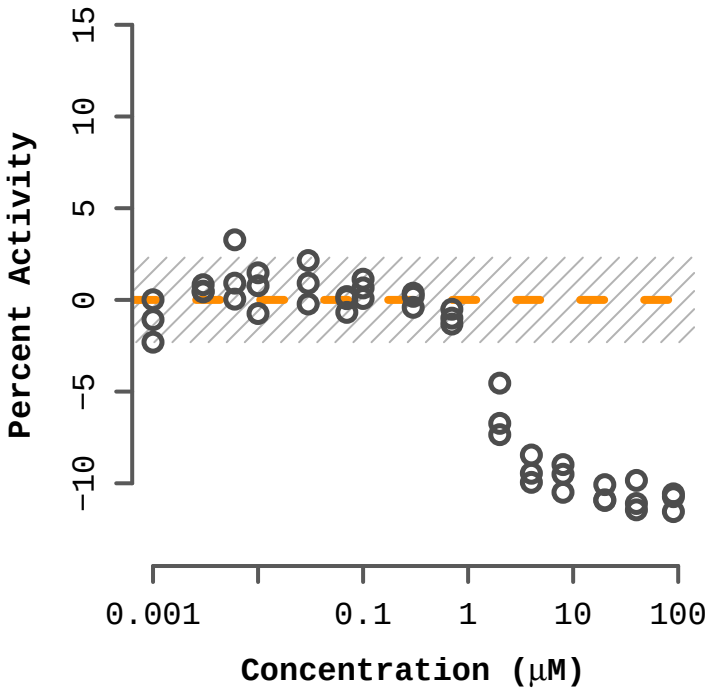
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	308.64	NA	NA
PROB:	1	NA	NA
RMSE:	7.2	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.66 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Hexyl-3-methylimidazolium iodide
CHID:    47951   CASRN: 178631-05-5
SPID(S): Tox21_200752
M4ID:    12481500

HILL MODEL (in red):
      tp        ga        gw
val:  1.98e-06  2.36      6.71
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  12.5      -0.685    0.524     0.155     1.78
sd:   31.5      3.78      0.54      0.688     1.12

      CNST          HILL          GNLS
AIC:  276.49        282.49        263.52
PROB: 0             0             1
RMSE: 5.02          5.02          3.95

MAX_MEAN: 6.35      MAX_MED: 9.19      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

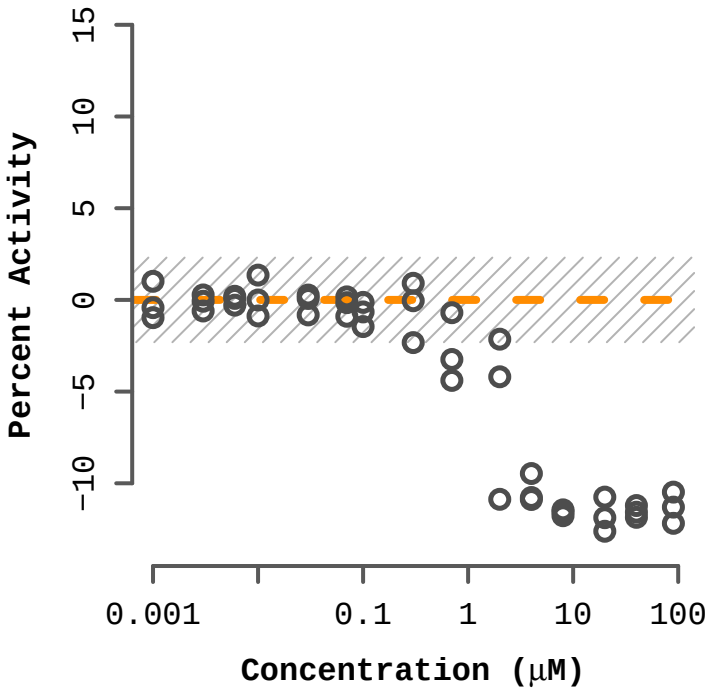
NAME: 1-Methyl-3-octylimidazolium hexafluorophosphat
CHID: 47952 **CASRN:** 304680-36-2
SPID(S): Tox21_200768
M4ID: 12481484

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	295.66	NA	NA
PROB:	1	NA	NA
RMSE:	6.23	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 0.915 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

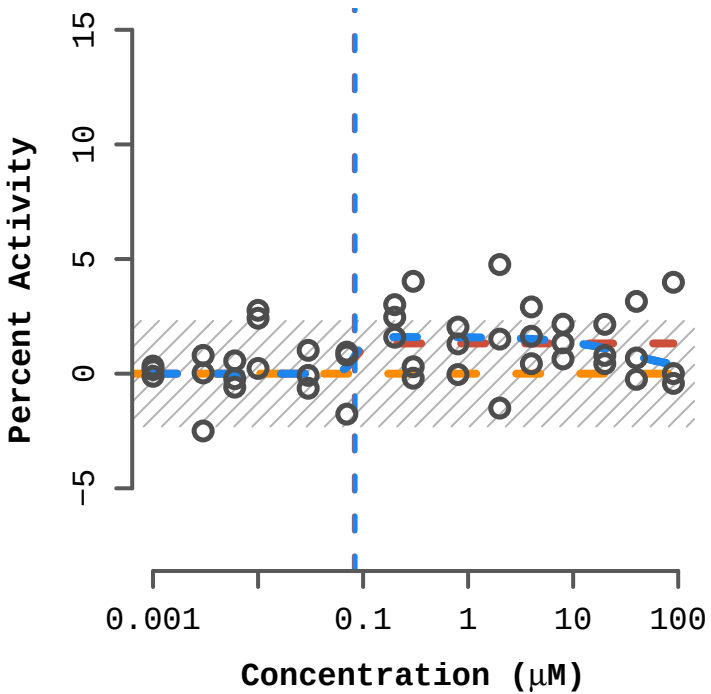
NAME: Trihexyltetradecylphosphonium bromide
CHID: 47953 **CASRN:** 654057-97-3
SPID(S): Tox21_200809
M4ID: 12481443

HILL MODEL: Not applicable.

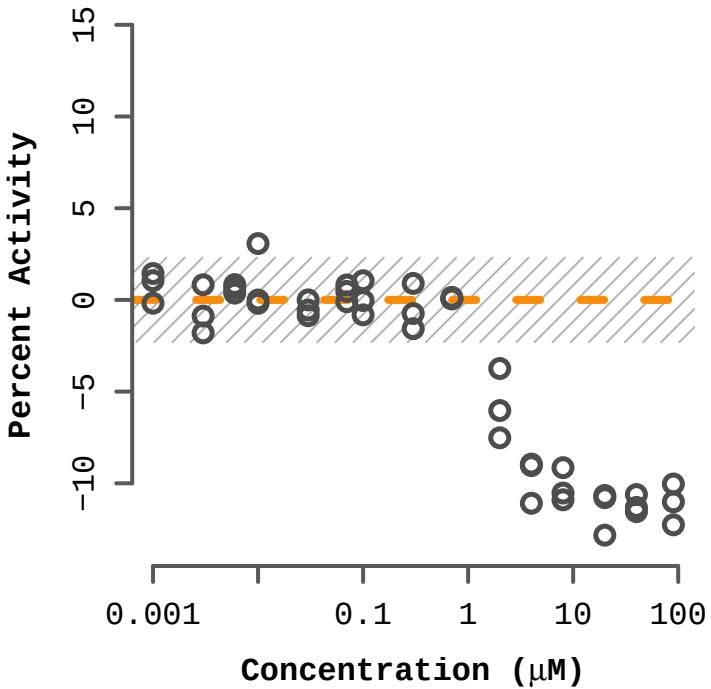
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.87	NA	NA
PROB:	1	NA	NA
RMSE:	6.86	NA	NA

MAX_MEAN: 0.159 **MAX_MED:** 0.0827 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diethylmethylsulfonium bis(trifluoromethylsulf
CHID:    47954   CASRN: 792188-85-3
SPID(S): Tox21_200825
M4ID:    12481427

HILL MODEL (in red):
      tp       ga       gw
val:  1.32     -1.08    8
sd:   0.28     0.241    20.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.6      -1.08    8        1.57     1.28
sd:   0.481    0.228    18.7     0.476    2.17

      CNST        HILL        GNLS
AIC:  182.17      168.04      170.07
PROB: 0           0.73        0.27
RMSE: 1.79        1.41        1.42

MAX_MEAN: 2.36      MAX_MED: 2.46      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

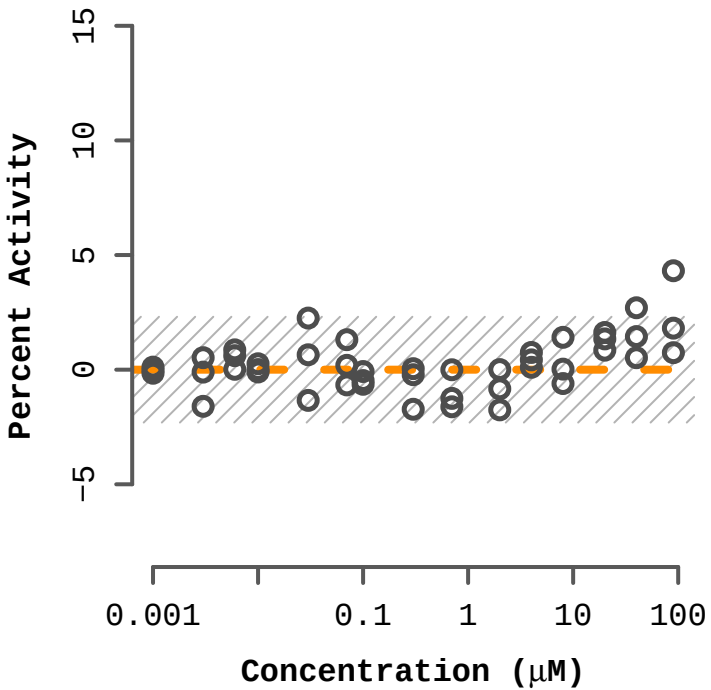
NAME: 1-Methyl-3-octylimidazolium bis(trifluoromethy
CHID: 47955 **CASRN:** 178631-04-4
SPID(S): Tox21_200842
M4ID: 12481410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	298.15	NA	NA
PROB:	1	NA	NA
RMSE:	6.45	NA	NA

MAX_MEAN: 0.962 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

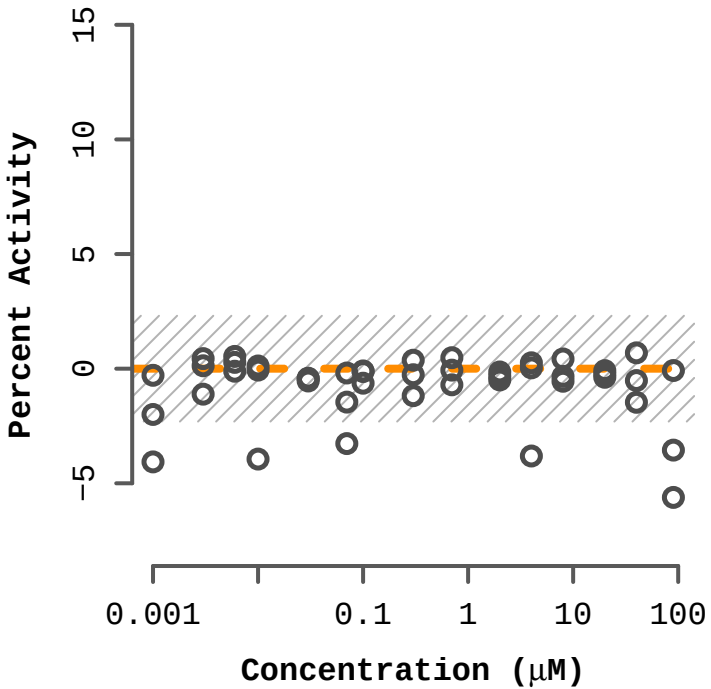
NAME: 2,3,4,4'−Tetrahydroxybenzophenone
CHID: 47956 CASRN: 31127−54−5
SPID(S): Tox21_200892
M4ID: 12481360

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 2.29 MAX_MED: 1.81 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

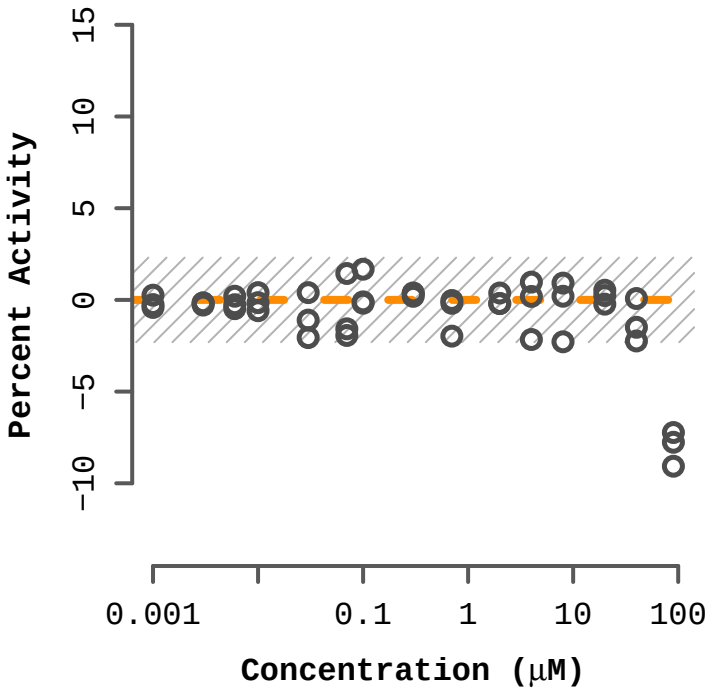
NAME: Octylparaben
CHID: 47957 **CASRN:** 1219-38-1
SPID(S): Tox21_303430
M4ID: 12475709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 0.234 **MAX_MED:** 0.275 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

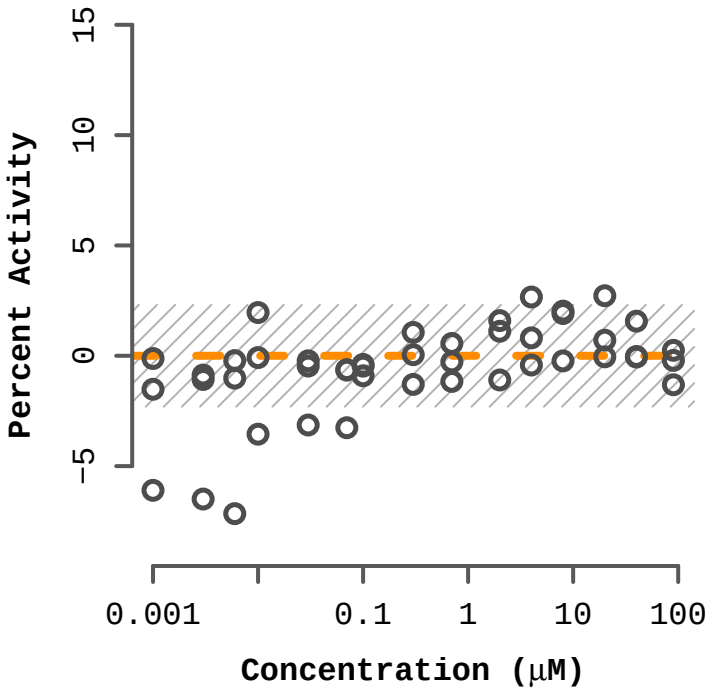
NAME: Octylparaben
CHID: 47957 **CASRN:** 1219-38-1
SPID(S): Tox21_200908
M4ID: 12481344

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.85	NA	NA
PROB:	1	NA	NA
RMSE:	2.29	NA	NA

MAX_MEAN: 0.464 **MAX_MED:** 0.337 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

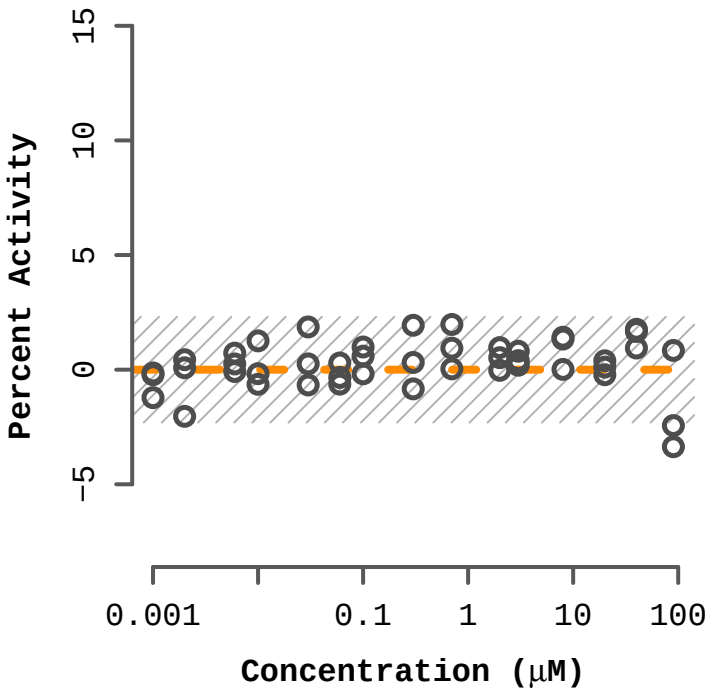
NAME: 2,4-Dichlorobenzotrifluoride
CHID: 47959 **CASRN:** 320-60-5
SPID(S): Tox21_200946
M4ID: 12481306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.17	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

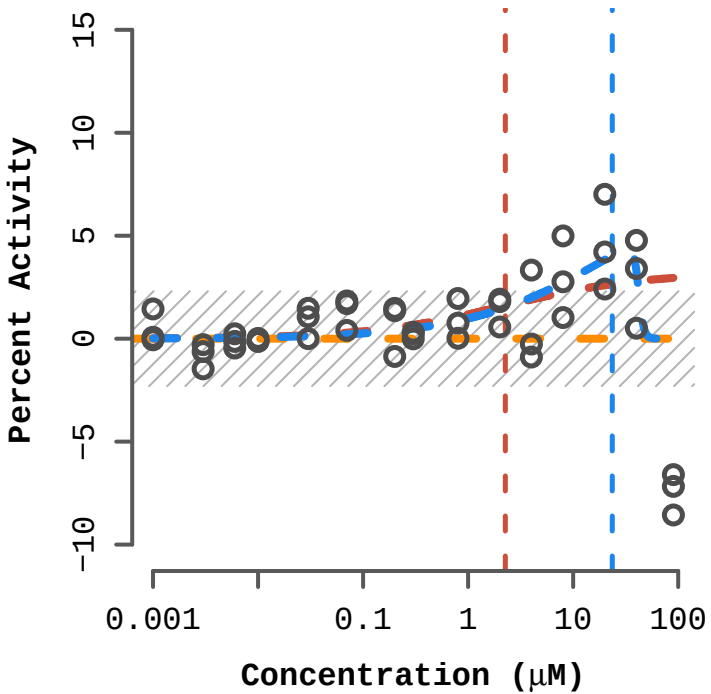
NAME: 4,4'−Thiodiphenol
CHID: 47960 **CASRN:** 2664−63−3
SPID(S): Tox21_200973
M4ID: 12481279

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydroxy-4'-chlorobenzophenone
CHID: 47961 **CASRN:** 42019-78-3
SPID(S): Tox21_200974
M4ID: 12481278

HILL MODEL (in red):

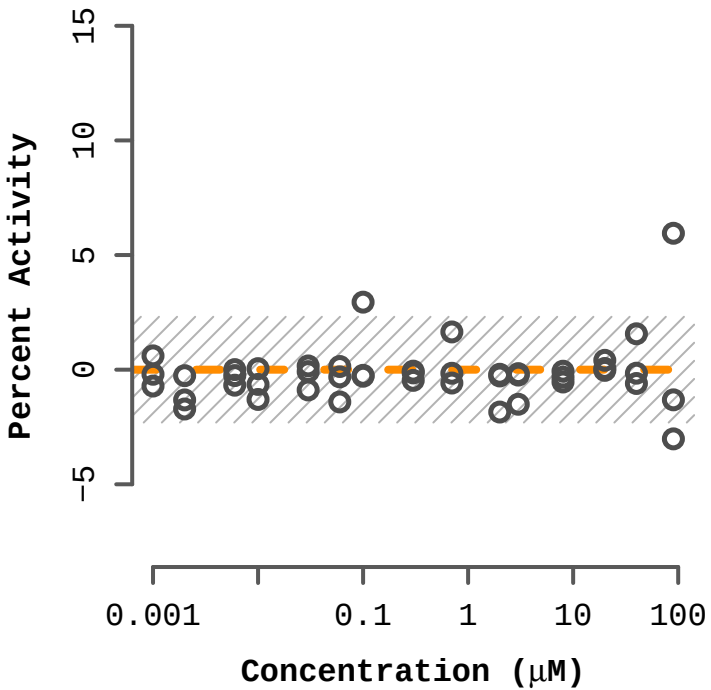
	tp	ga	gw
val:	3.21	0.354	0.665
sd:	1.39	0.685	0.471

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.09	1.37	0.627	1.62	17.9
sd:	9.22	1.35	0.302	0.0457	42.5

	CNST	HILL	GNLS
AIC:	212.91	201.96	194.01
PROB:	0	0.02	0.98
RMSE:	2.8	2.99	2.28

MAX_MEAN: 4.55 **MAX_MED:** 4.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

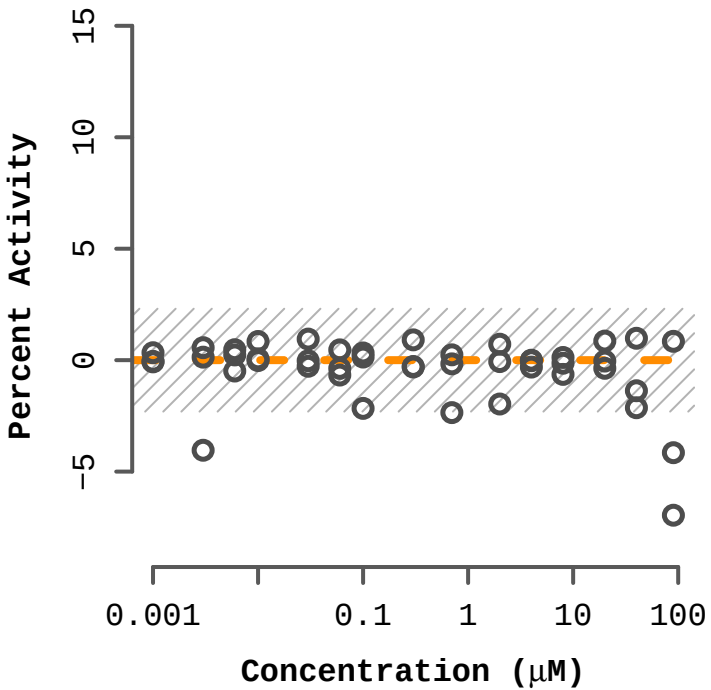
NAME: 4-Benzylphenol
CHID: 47962 **CASRN:** 101-53-1
SPID(S): Tox21_201009
M4ID: 12481243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.805 **MAX_MED:** 0.0535 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

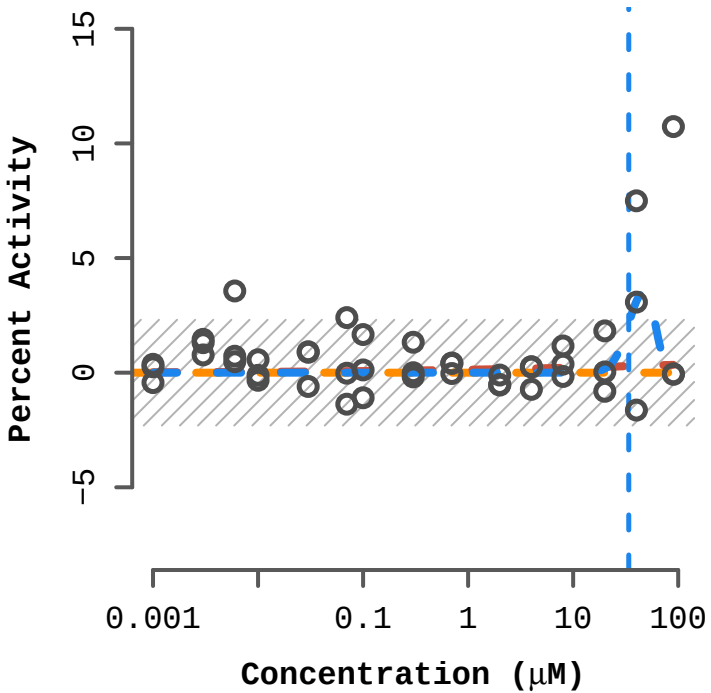
NAME: Bisphenol Z
CHID: 47963 **CASRN:** 843-55-0
SPID(S): Tox21_201017
M4ID: 12481235

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 0.295 **MAX_MED:** 0.236 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Ethyl-3-methylimidazolium dicyanamide
CHID: 47964 CASRN: 370865-89-7
SPID(S): Tox21_201024
M4ID: 12481228

HILL MODEL (in red):

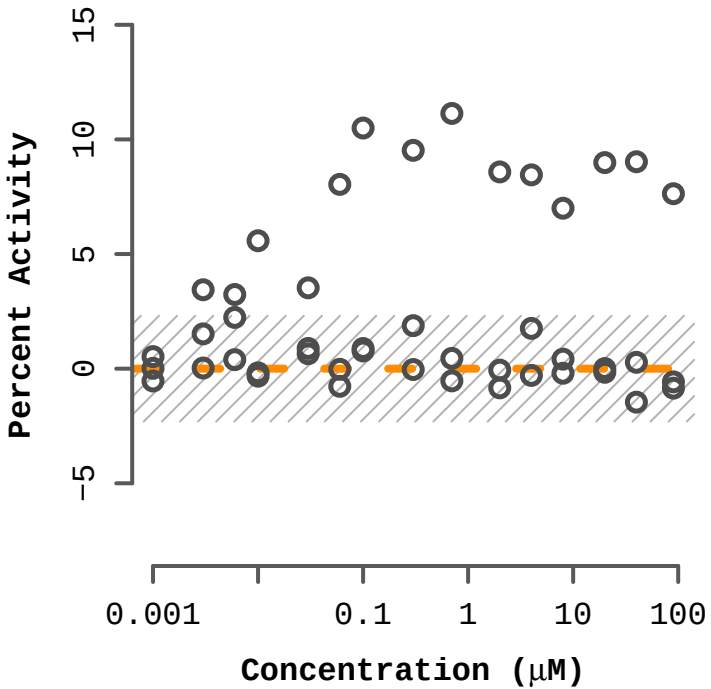
	tp	ga	gw
val:	0.815	2.42	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.33	1.53	5.96	1.78	9.82
sd:	64.2	3.28	61.2	1.84	104

	CNST	HILL	GNLS
AIC:	164.79	169.92	170.42
PROB:	0.88	0.07	0.05
RMSE:	2.24	2.17	2.09

MAX_MEAN: 3.54 MAX_MED: 3.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

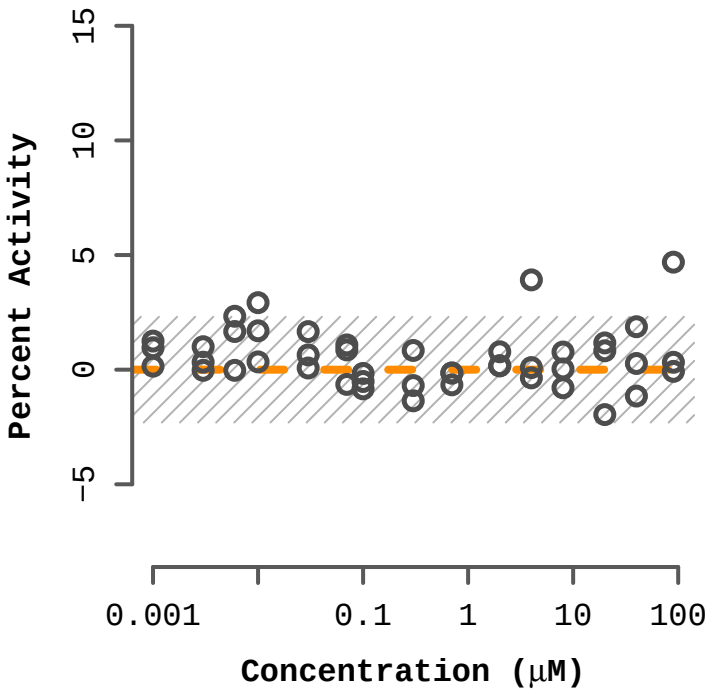
NAME: 1−Ethyl−3−methylimidazolium trifluoromethanesu
CHID: 47965 **CASRN:** 145022−44−2
SPID(S): Tox21_201039
M4ID: 12481213

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	257.23	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: 4.05 **MAX_MED:** 2.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

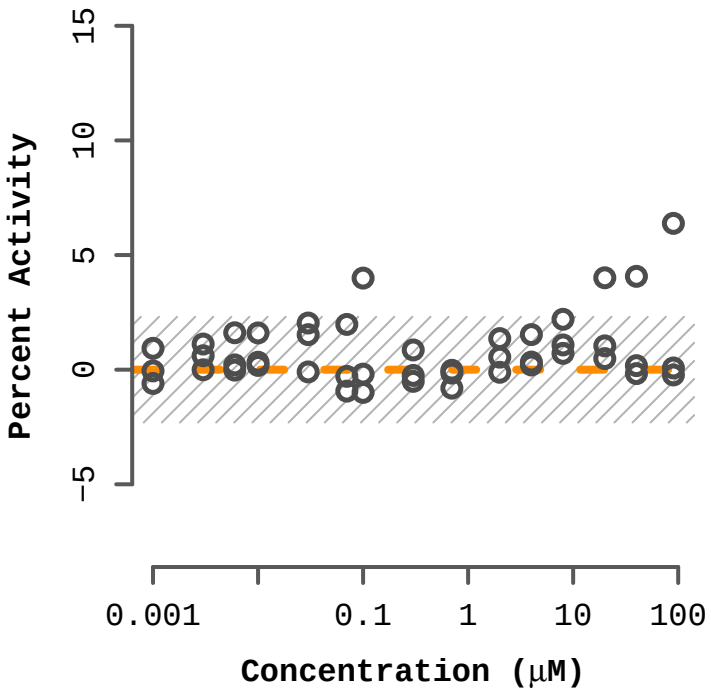
NAME: Dinonyl phthalate
CHID: 47966 **CASRN:** 84-76-4
SPID(S): Tox21_201040
M4ID: 12481212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 1.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

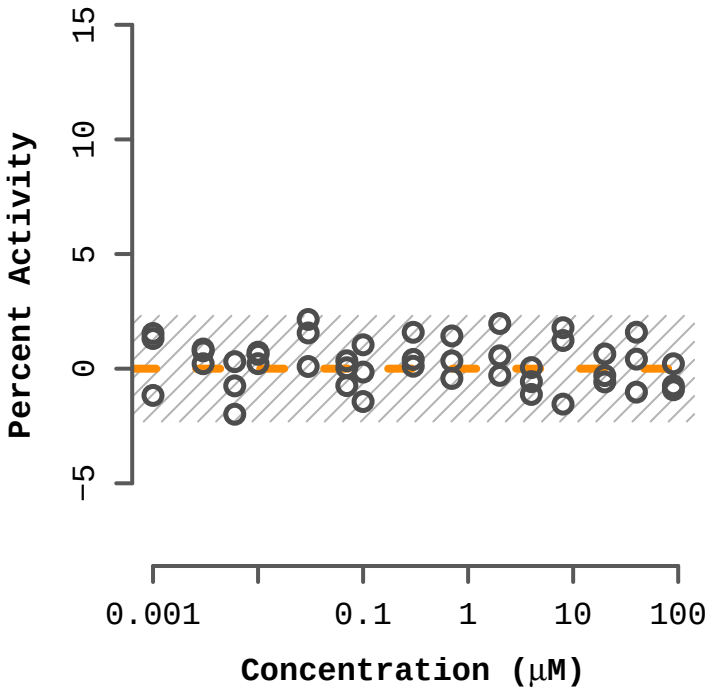
NAME: 1-Ethyl-3-methylimidazolium bis(trifluorometha
CHID: 47967 **CASRN:** 174899-82-2
SPID(S): Tox21_201061
M4ID: 12481191

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 2.08 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

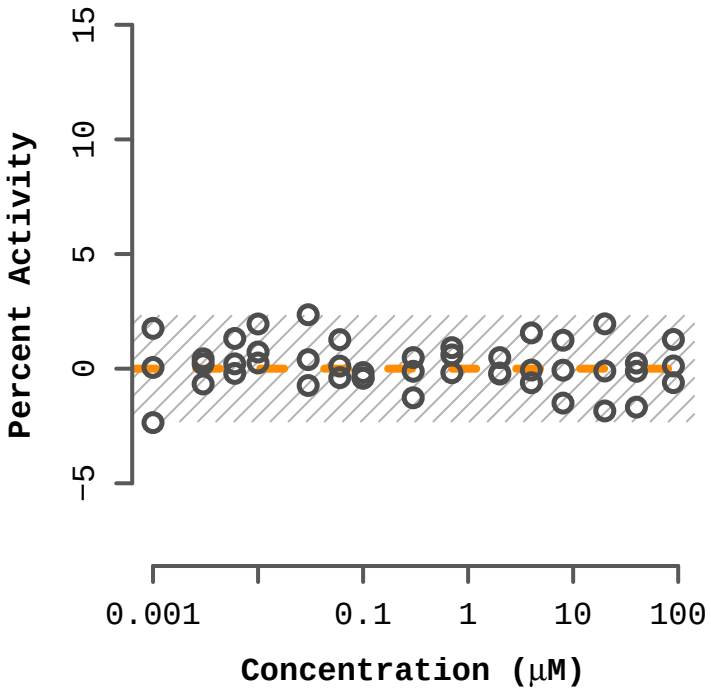
NAME: 1-Butyl-1-methylpyrrolidinium bis(trifluoromethl
CHID: 47968 CASRN: 223437-11-4
SPID(S): Tox21_201083
M4ID: 12481169

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.27 MAX_MED: 1.56 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

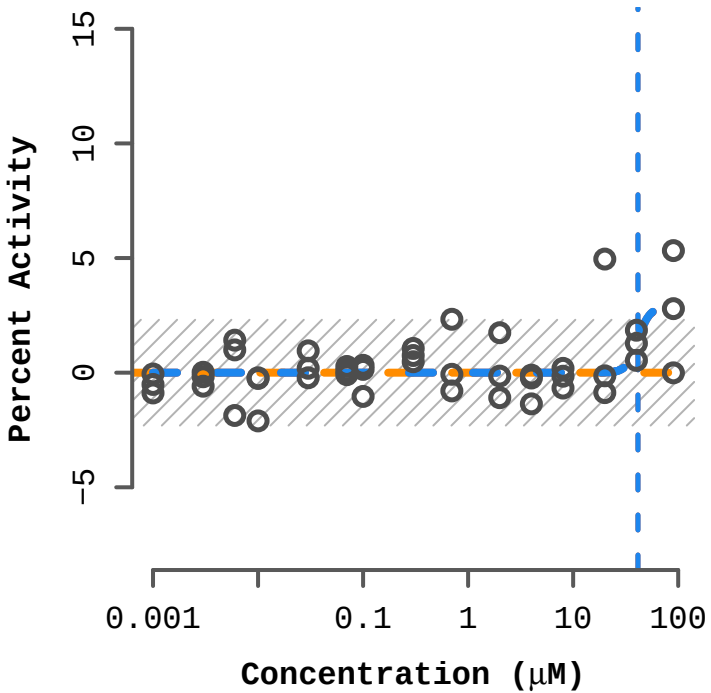
NAME: Trolamine salicylate
CHID: 47969 **CASRN:** 2174-16-5
SPID(S): Tox21_201084
M4ID: 12481168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.977 **MAX_MED:** 0.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,3-Dimethylimidazolium dimethyl phosphate
CHID: 47970 CASRN: 654058-04-5
SPID(S): Tox21_201100
M4ID: 12481152

HILL MODEL (in red):

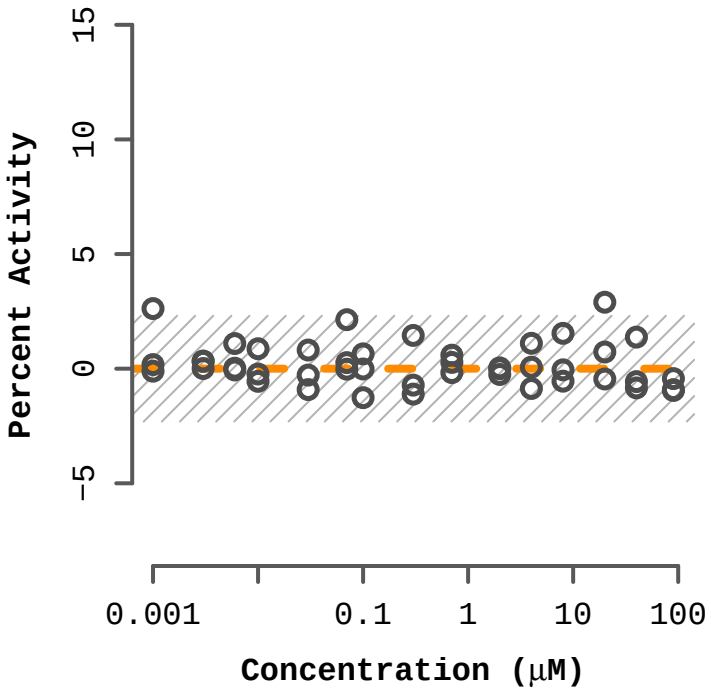
	tp	ga	gw
val:	2.85	1.62	8
sd:	0.829	0.0601	18.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.86	1.62	8	3.91	1.11
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	149.69	144.28	148.28
PROB:	0.06	0.83	0.11
RMSE:	1.46	1.25	1.25

MAX_MEAN: 2.71 MAX_MED: 2.79 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

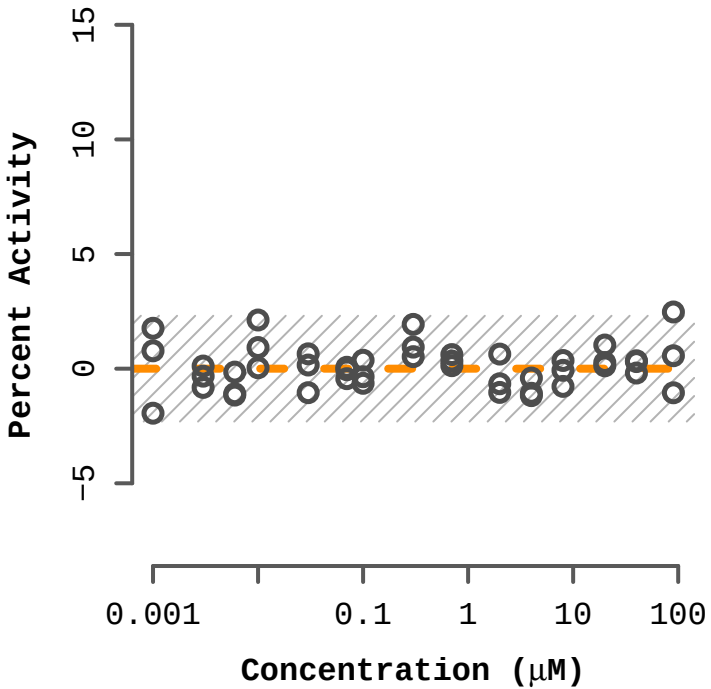
NAME: 1-Butyl-3-methylimidazolium hydrogensulfate
CHID: 47971 **CASRN:** 262297-13-2
SPID(S): Tox21_201105
M4ID: 12481147

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.728 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

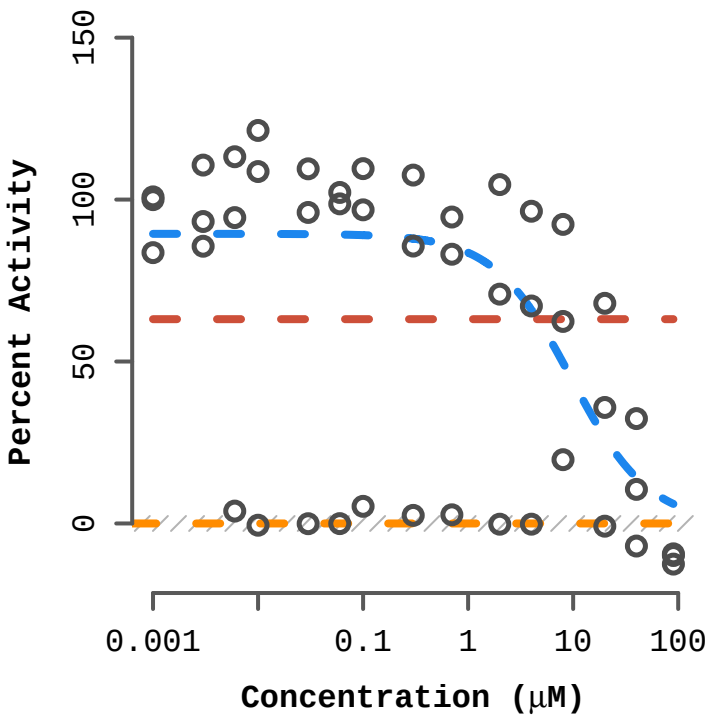
NAME: Trehalose dihydrate
CHID: 47972 **CASRN:** 6138-23-4
SPID(S): Tox21_201106
M4ID: 12481146

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'-Propane-2,2-diylbis(2,6-dimethylphenol)
CHID: 47973 CASRN: 5613-46-7
SPID(S): Tox21_201210
M4ID: 12481042

HILL MODEL (in red):

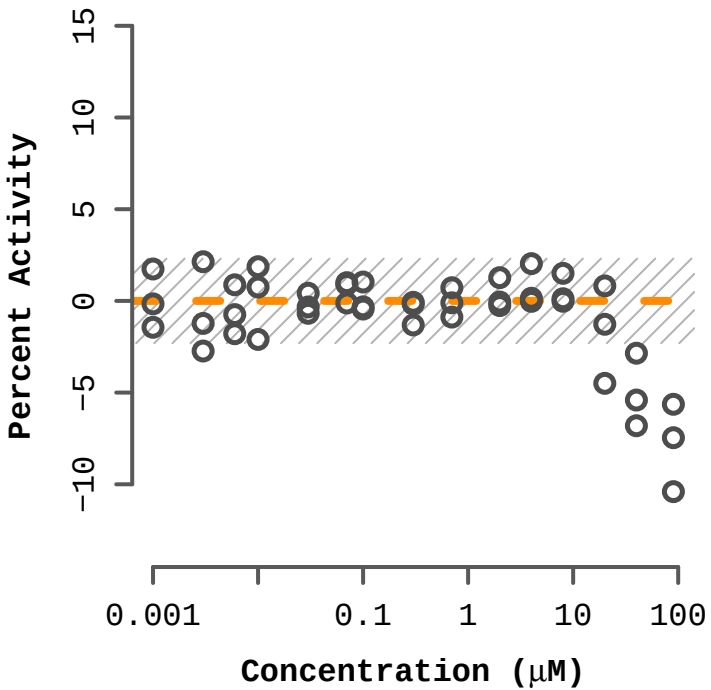
	tp	ga	gw
val:	63.1	-4.99	3.86
sd:	8.34	1250	2420

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	89.4	-4.36	4.88	0.984	1.18
sd:	8.06	375	1340	0.28	0.714

	CNST	HILL	GNLS
AIC:	524.69	490.12	471.1
PROB:	0	0	1
RMSE:	74.74	46.83	41.13

MAX_MEAN: 96.5 MAX_MED: 109 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

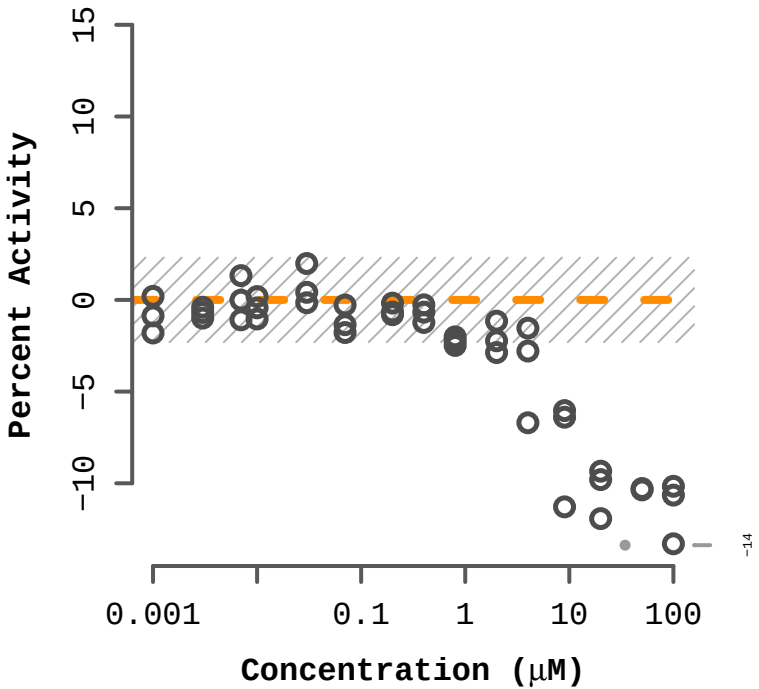
NAME: 2,3',4,4'−Tetrahydroxybenzophenone
CHID: 47974 **CASRN:** 61445−50−9
SPID(S): Tox21_202376
M4ID: 12479876

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	205.61	NA	NA
PROB:	1	NA	NA
RMSE:	2.78	NA	NA

MAX_MEAN: 0.719 **MAX_MED:** 0.901 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

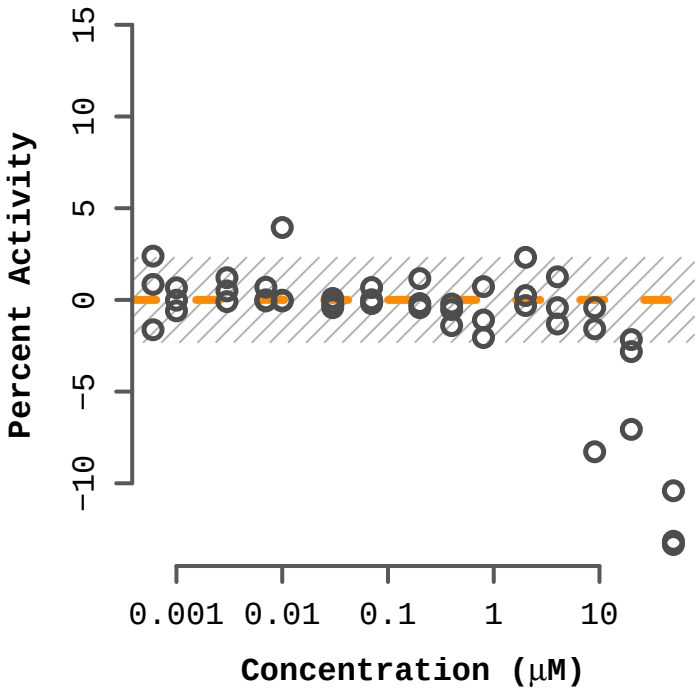
NAME: Benzyl-C8-18-alkyldimethylammonium chlorides
CHID: 48122 **CASRN:** 63449-41-2
SPID(S): Tox21_301833
M4ID: 12477300 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	280.59	NA	NA
PROB:	1	NA	NA
RMSE:	5.66	NA	NA

MAX_MEAN: 0.749 **MAX_MED:** 0.414 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

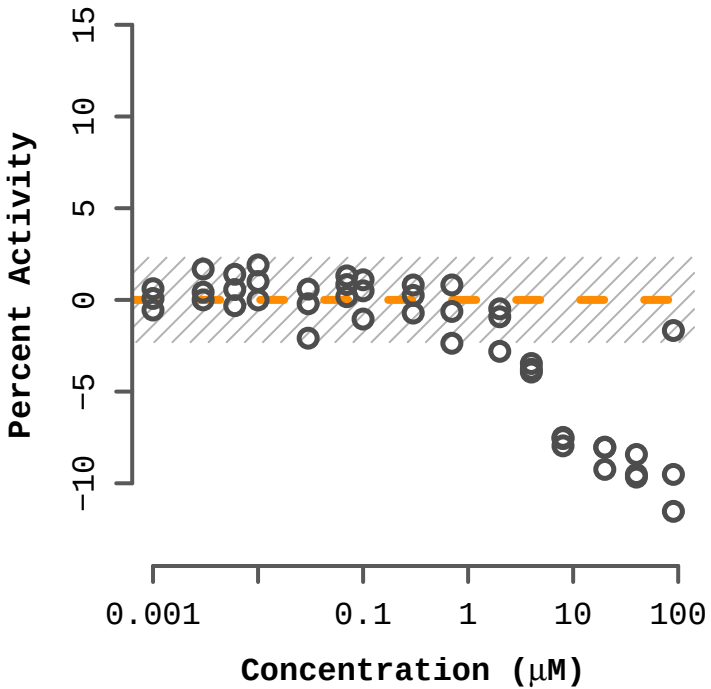
NAME: Rimcazole dihydrochloride
CHID: 48161 **CASRN:** 75859-03-9
SPID(S): Tox21_110953_1
M4ID: 12483988

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.77	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 0.847 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

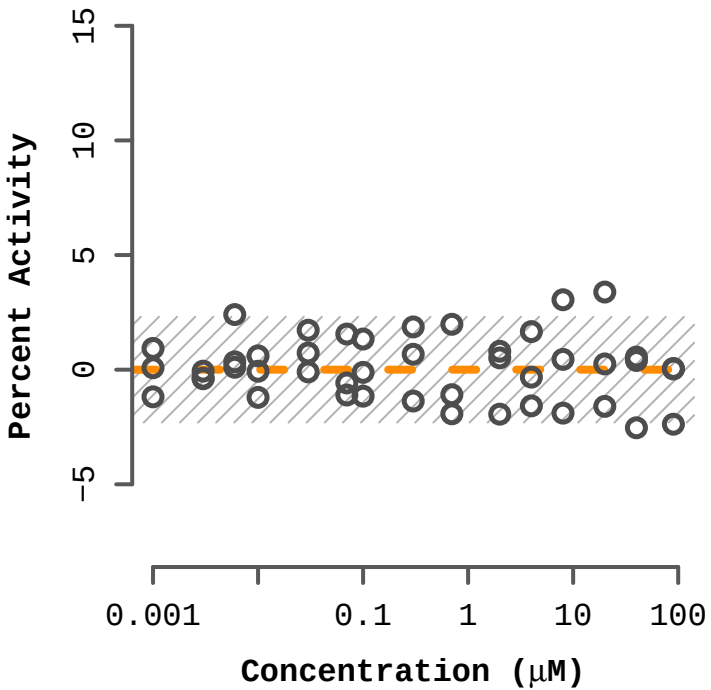
NAME: 3,9-Epoxy-3H-azirino[2,3-c][1]benzazocine-5-ca
CHID: 48166 CASRN: NOCAS_48166
SPID(S): Tox21_303340
M4ID: 12475793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	262.31	NA	NA
PROB:	1	NA	NA
RMSE:	4.6	NA	NA

MAX_MEAN: 0.971 MAX_MED: 1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

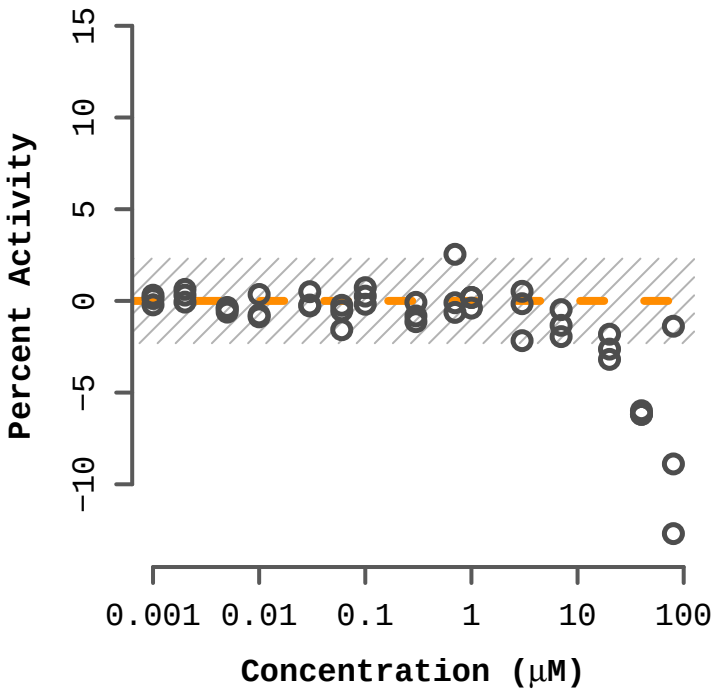
NAME: FR900409
CHID: 48167 **CASRN:** 138472-01-2
SPID(S): Tox21_303605
M4ID: 12475540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.952 **MAX_MED:** 0.731 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

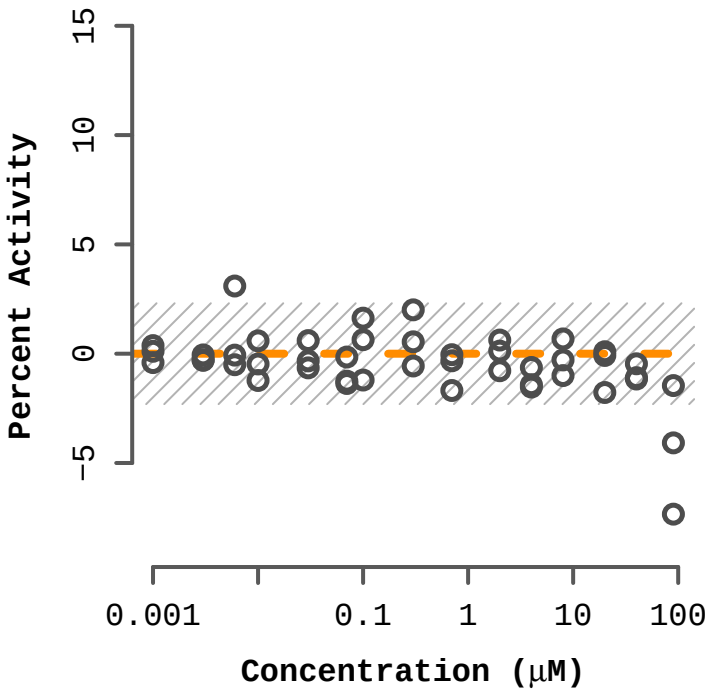
NAME: Fabesetron hydrochloride
CHID: 48168 **CASRN:** 129299-90-7
SPID(S): Tox21_303504
M4ID: 12475638

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.99	NA	NA

MAX_MEAN: 0.606 **MAX_MED:** 0.318 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

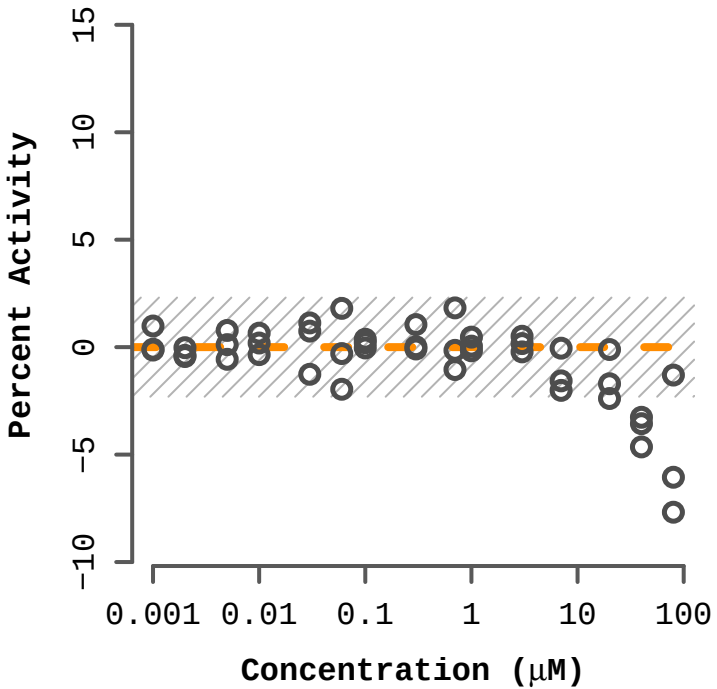
NAME: FR150011
CHID: 48170 **CASRN:** 149413-74-1
SPID(S): Tox21_303474
M4ID: 12475666

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 0.844 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

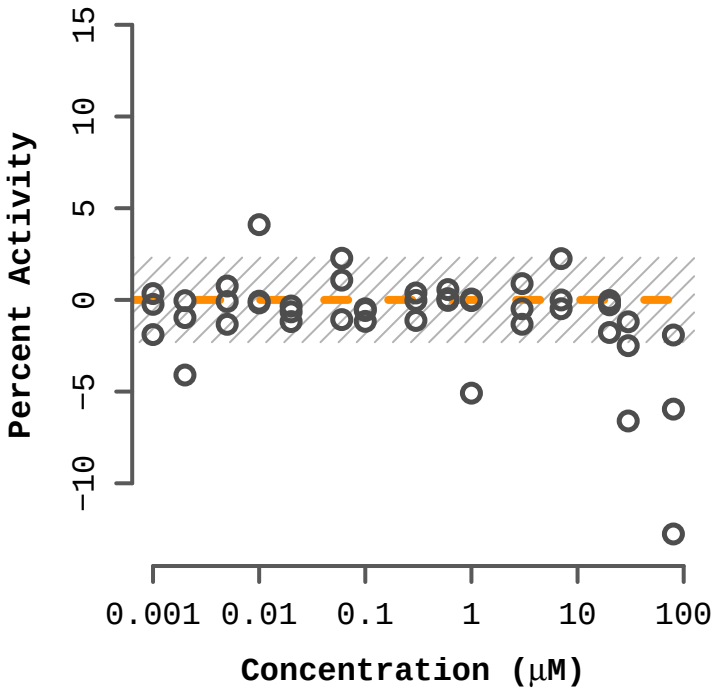
NAME: FR145237
CHID: 48171 **CASRN:** 146011-65-6
SPID(S): Tox21_303375
M4ID: 12475761

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 0.33 **MAX_MED:** 0.746 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

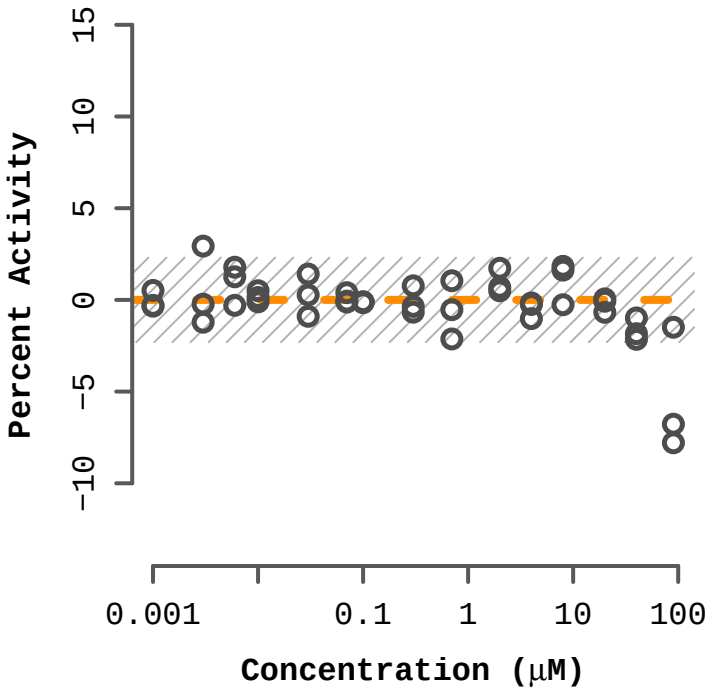
NAME: PharmaGSID_48172
CHID: 48172 **CASRN:** NOCAS_48172
SPID(S): Tox21_303499
M4ID: 12475643

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	195.45	NA	NA
PROB:	1	NA	NA
RMSE:	2.77	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

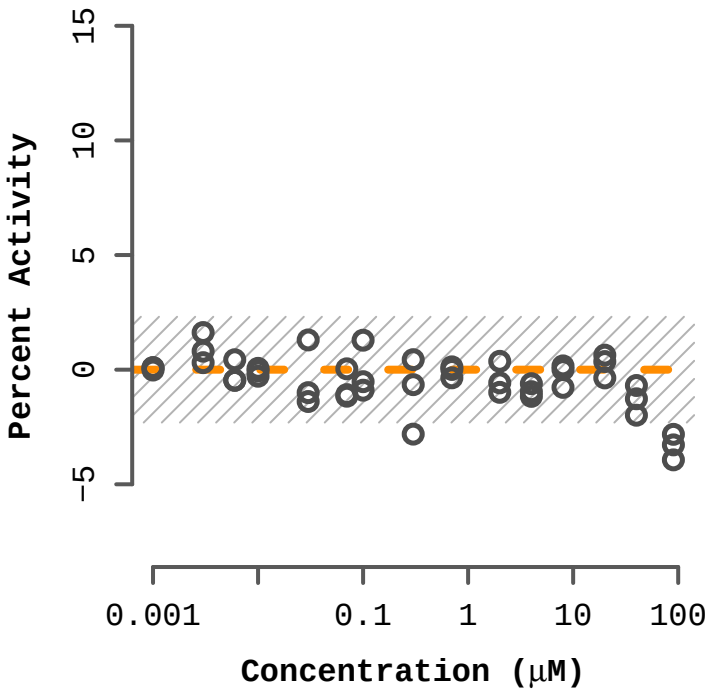
NAME: FR167356
CHID: 48174 **CASRN:** 174185-16-1
SPID(S): Tox21_303349
M4ID: 12475784

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

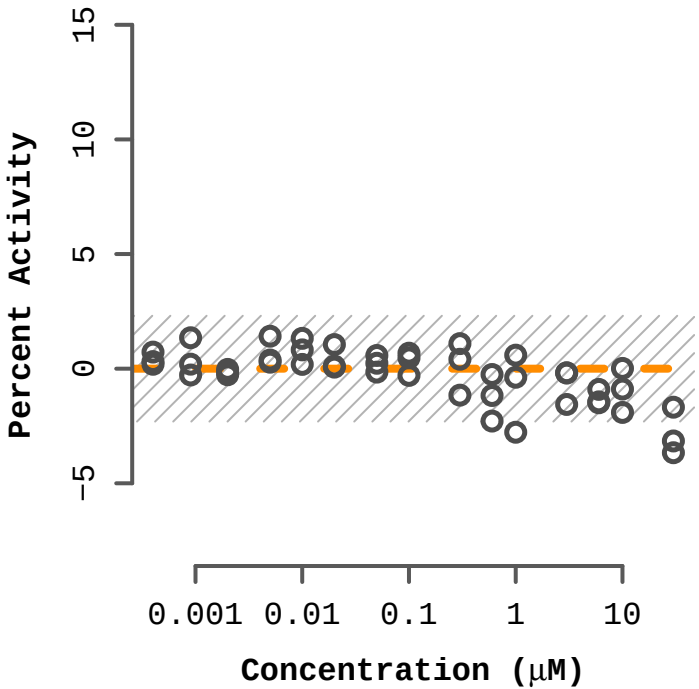
NAME: FR140423
CHID: 48175 CASRN: 151506-44-4
SPID(S): Tox21_303416
M4ID: 12475723

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.912 MAX_MED: 0.807 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

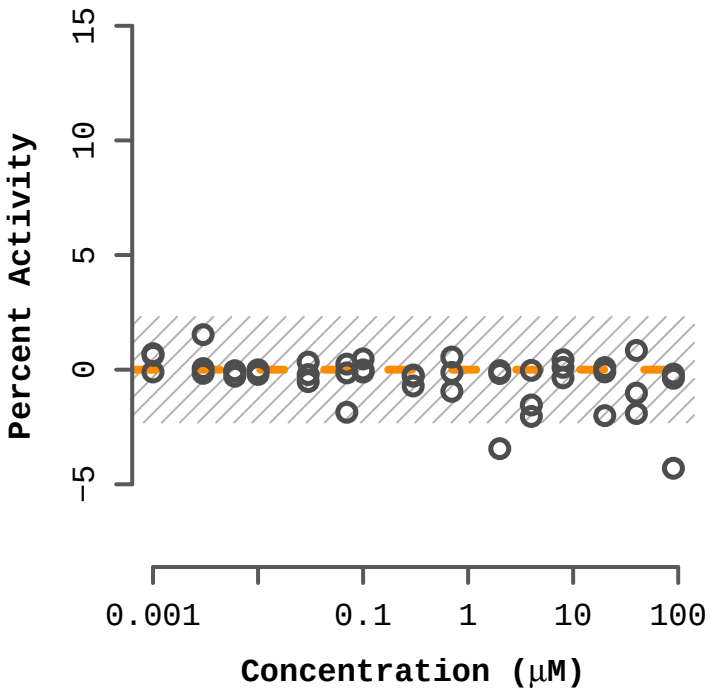
NAME: YM218
CHID: 48176 **CASRN:** NOCAS_48176
SPID(S): Tox21_303441
M4ID: 12475699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.778 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

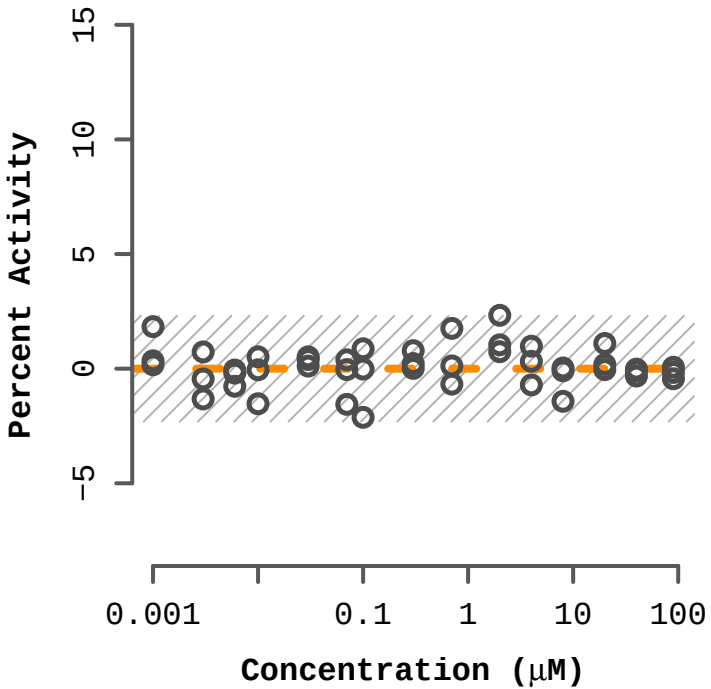
NAME: FR130739
CHID: 48178 **CASRN:** 136042-19-8
SPID(S): Tox21_303554
M4ID: 12475591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.474 **MAX_MED:** 0.627 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

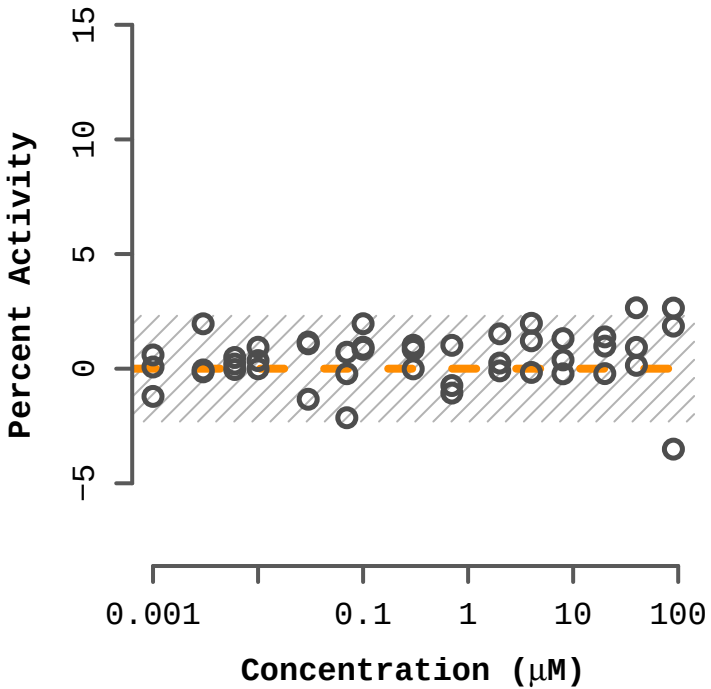
NAME: 4-Propylaniline
CHID: 48180 **CASRN:** 2696-84-6
SPID(S): Tox21_303437
M4ID: 12475703

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

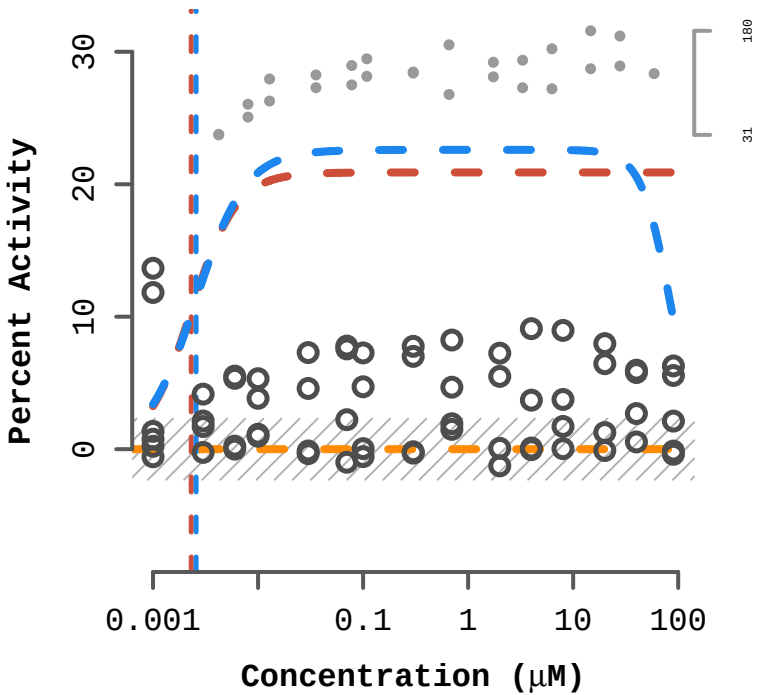
NAME: 4-tert-Butylaniline
CHID: 48181 **CASRN:** 769-92-6
SPID(S): Tox21_303353
M4ID: 12475780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclohexylphenylketone
CHID: 48182 CASRN: 712-50-5
SPID(S): Tox21_303653
M4ID: 12475495 BRK

HILL MODEL (in red):

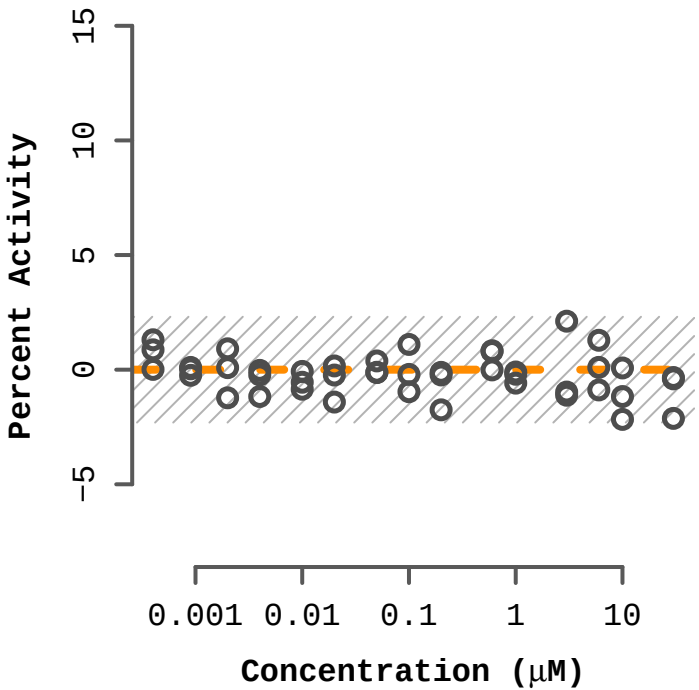
	tp	ga	gw
val:	20.9	-2.64	2.02
sd:	6.03	0.594	3.91

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.6	-2.59	1.84	1.92	3.17
sd:	7.06	0.549	3.54	0.385	14.8

	CNST	HILL	GNLS
AIC:	985.93	972.85	976.27
PROB:	0	0.85	0.15
RMSE:	63.67	54.65	54.35

MAX_MEAN: 52.5 MAX_MED: 7.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

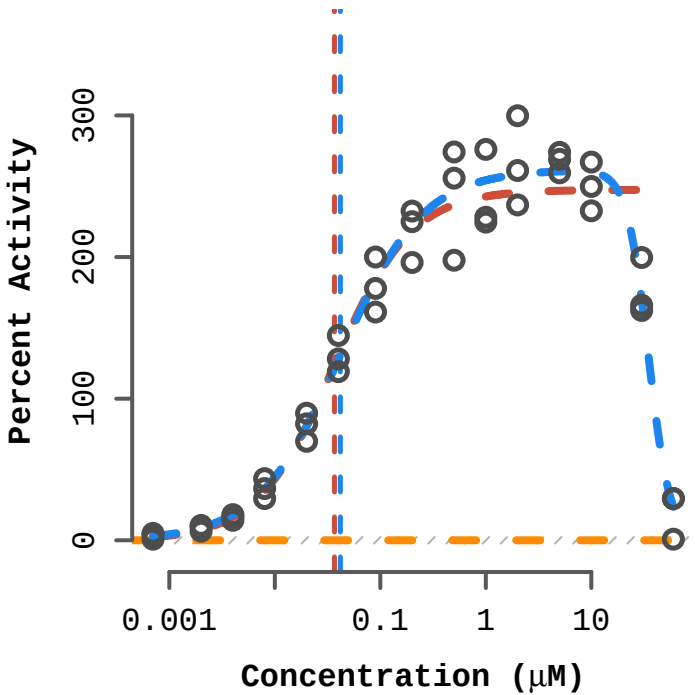
NAME: Enterolactone
CHID: 48183 **CASRN:** 78473-71-9
SPID(S): Tox21_303555
M4ID: 12475590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.73 **MAX_MED:** 0.868 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Melengestrol acetate
CHID: 48184 CASRN: 2919-66-6
SPID(S): Tox21_303411
M4ID: 12475728

HILL MODEL (in red):

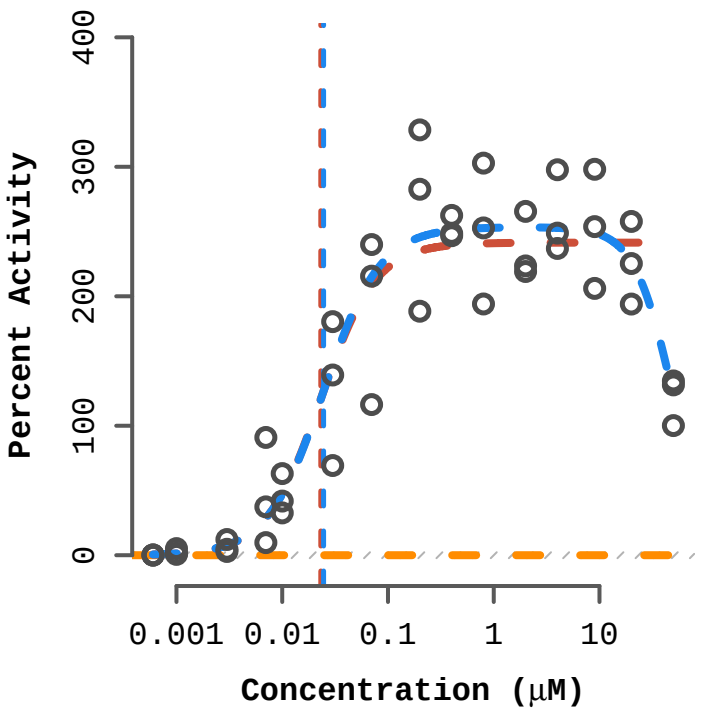
	tp	ga	gw
val:	247	-1.43	1.19
sd:	8.12	0.0558	0.145

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	262	-1.38	1.1	1.54	4.23
sd:	5.49	0.0371	0.08	0.0154	0.626

	CNST	HILL	GNLS
AIC:	601.11	468.78	390.43
PROB:	0	0	1
RMSE:	175.62	64.03	16.61

MAX_MEAN: 268 MAX_MED: 269 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Melengestrol acetate
CHID: 48184 CASRN: 2919-66-6
SPID(S): Tox21_111887_1
M4ID: 12483434

HILL MODEL (in red):

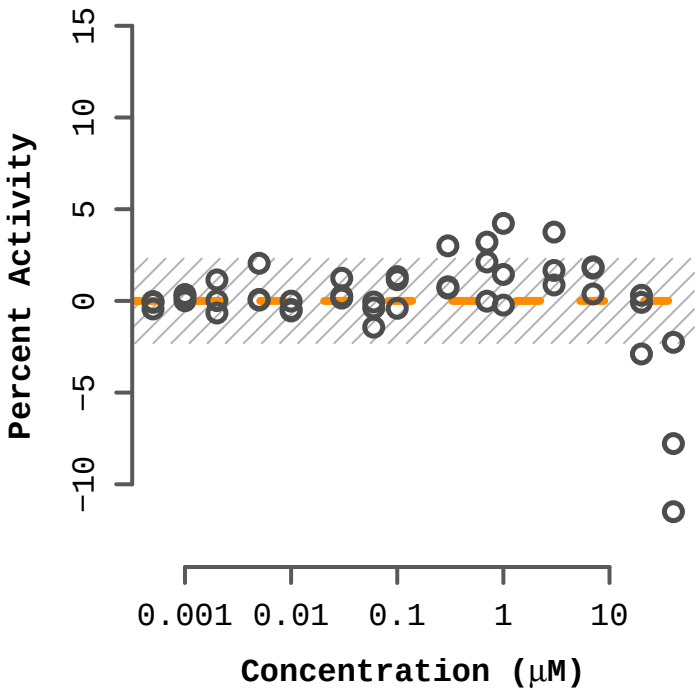
	tp	ga	gw
val:	241	-1.64	1.68
sd:	8.79	0.0789	0.339

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	253	-1.61	1.64	1.69	2.38
sd:	8.41	0.0649	0.272	0.0424	0.862

	CNST	HILL	GNLS
AIC:	606.93	475.85	452.91
PROB:	0	0	1
RMSE:	186.83	46.44	33.85

MAX_MEAN: 267 **MAX_MED:** 283 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

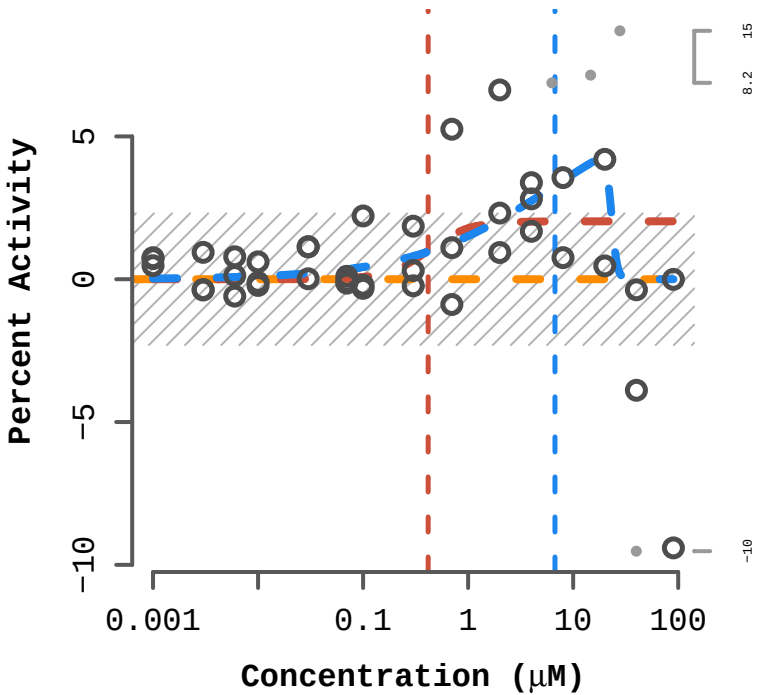
NAME: Apomorphine hydrochloride hydrate
CHID: 48185 **CASRN:** 41372-20-7
SPID(S): Tox21_303480
M4ID: 12475661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Apomorphine hydrochloride hydrate
CHID: 48185 CASRN: 41372-20-7
SPID(S): Tox21_202832
M4ID: 12479420 BRK

HILL MODEL (in red):

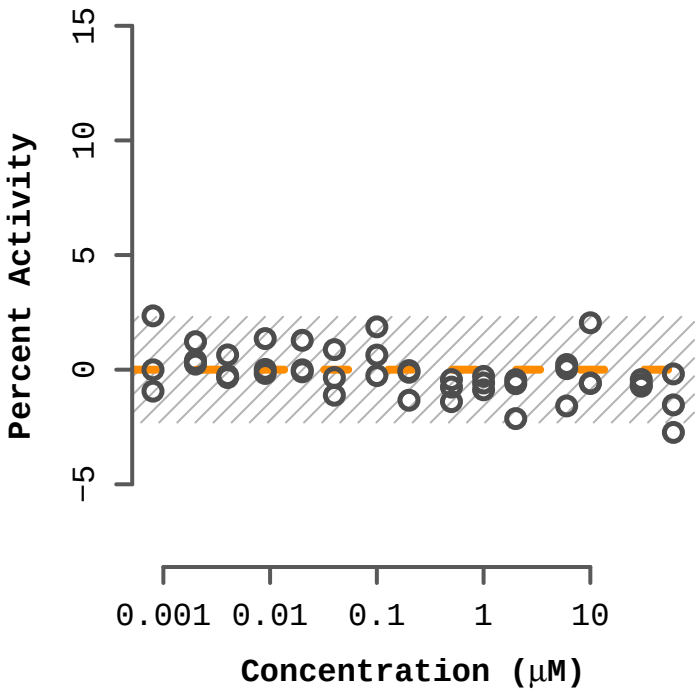
	tp	ga	gw
val:	2.03	−0.38	2.25
sd:	0.645	0.429	3.44

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.55	0.827	0.633	1.36	16.6
sd:	24.3	4.87	1.03	0.524	93.5

	CNST	HILL	GNLS
AIC:	237.5	232.72	224.78
PROB:	0	0.02	0.98
RMSE:	4.08	3.85	3.57

MAX_MEAN: 4.65 MAX_MED: 4.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

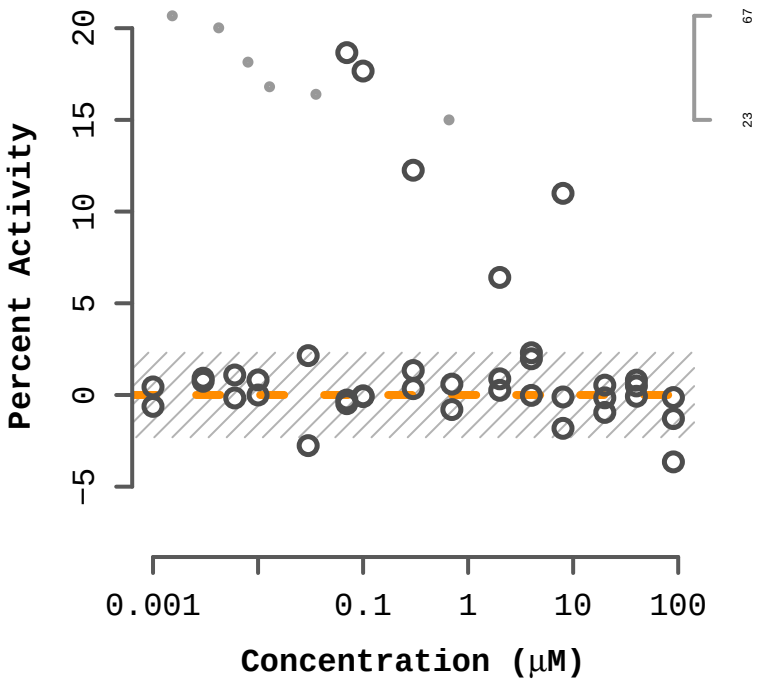
NAME: Tetrac
CHID: 48186 CASRN: 67-30-1
SPID(S): Tox21_303492
M4ID: 12475649

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.751 **MAX_MED:** 0.639 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

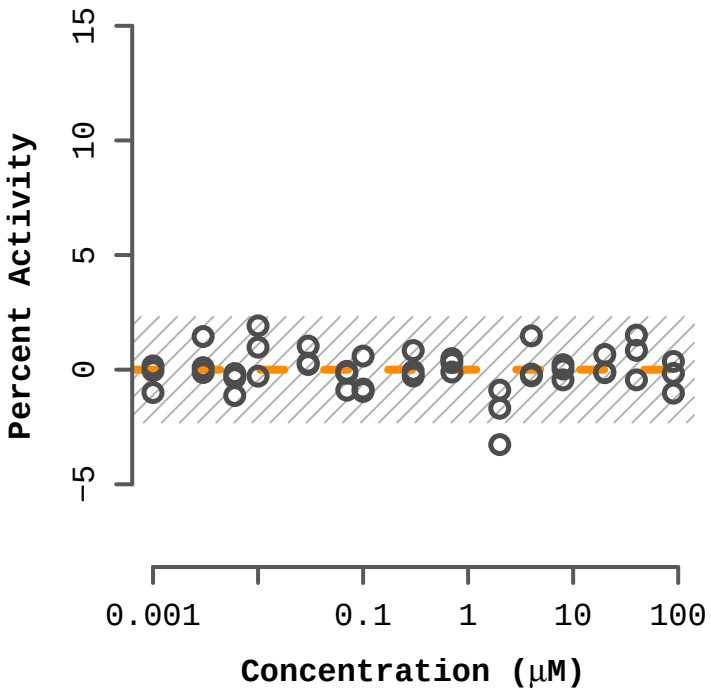
NAME: 1-Methoxy-4-tert-pentylcyclohexane
CHID: 48187 **CASRN:** 199584-38-8
SPID(S): Tox21_303386
M4ID: 12475752 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	351.2	NA	NA
PROB:	1	NA	NA
RMSE:	18.1	NA	NA

MAX_MEAN: 22.3 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

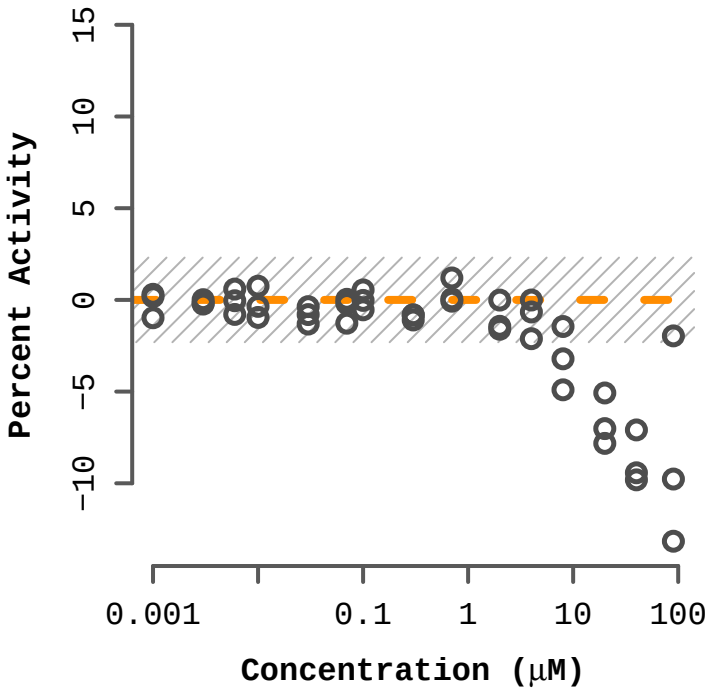
NAME: 4-Thiocresol
CHID: 48188 **CASRN:** 106-45-6
SPID(S): Tox21_303614
M4ID: 12475531

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.871 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

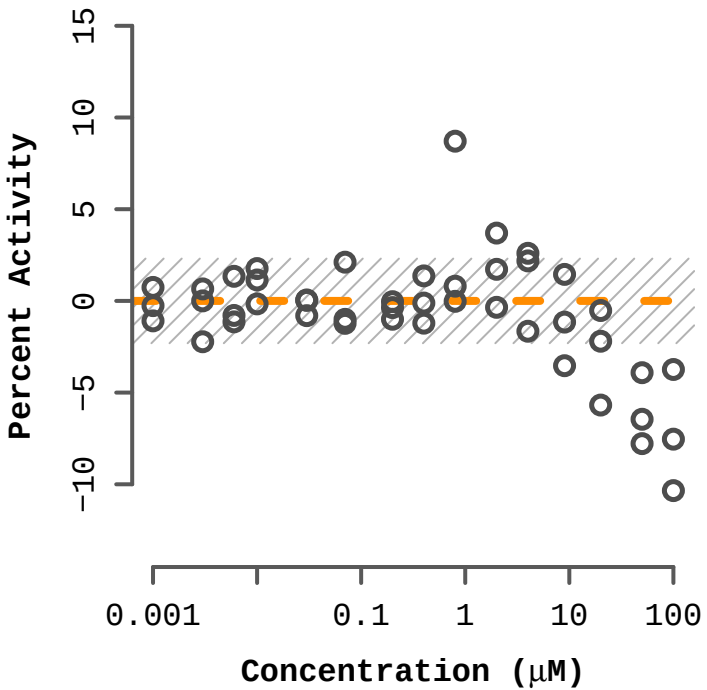
NAME: Dodecyl gallate
CHID: 48189 **CASRN:** 1166-52-5
SPID(S): Tox21_303487
M4ID: 12475654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	235.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.95	NA	NA

MAX_MEAN: 0.397 **MAX_MED:** 0.179 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

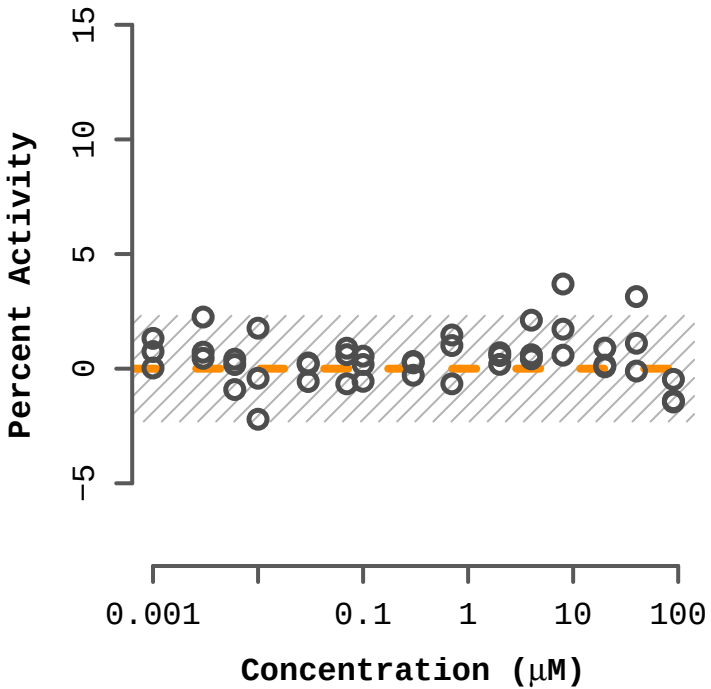
NAME: Dodecyl gallate
CHID: 48189 **CASRN:** 1166-52-5
SPID(S): Tox21_202724
M4ID: 12479528

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.65	NA	NA
PROB:	1	NA	NA
RMSE:	3.28	NA	NA

MAX_MEAN: 3.16 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

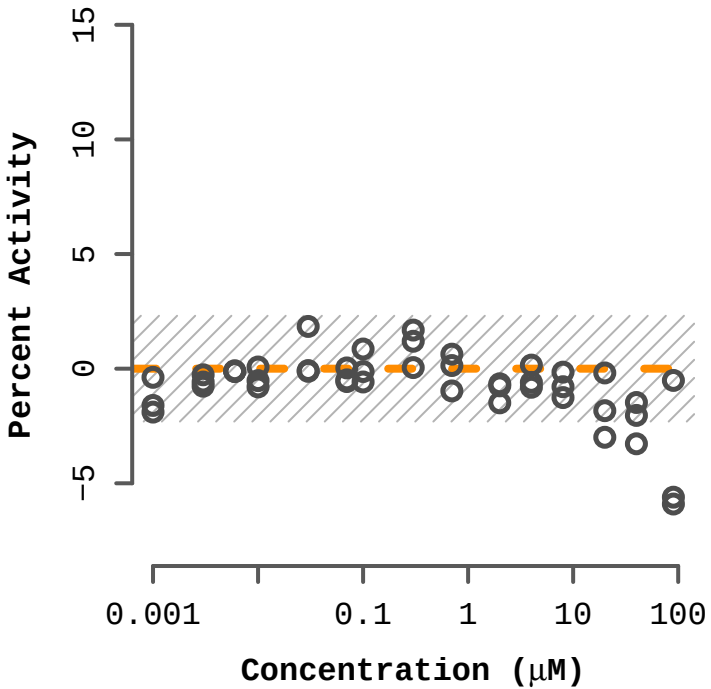
NAME: Methyl abietate
CHID: 48190 CASRN: 127-25-3
SPID(S): Tox21_303509
M4ID: 12475633

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 2 MAX_MED: 1.72 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

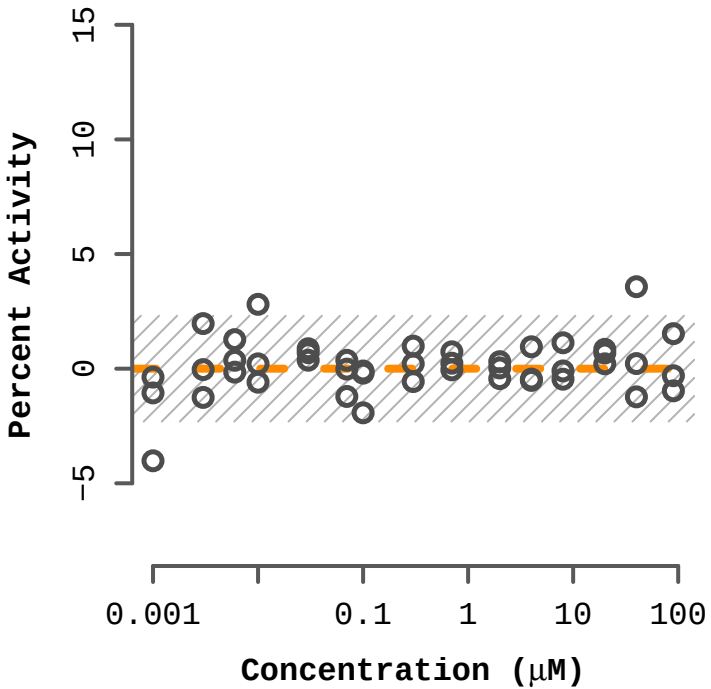
NAME: 4,4'−Methylenebis(2,6−diethylaniline)
CHID: 48191 **CASRN:** 13680−35−8
SPID(S): Tox21_303549
M4ID: 12475596

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 0.977 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

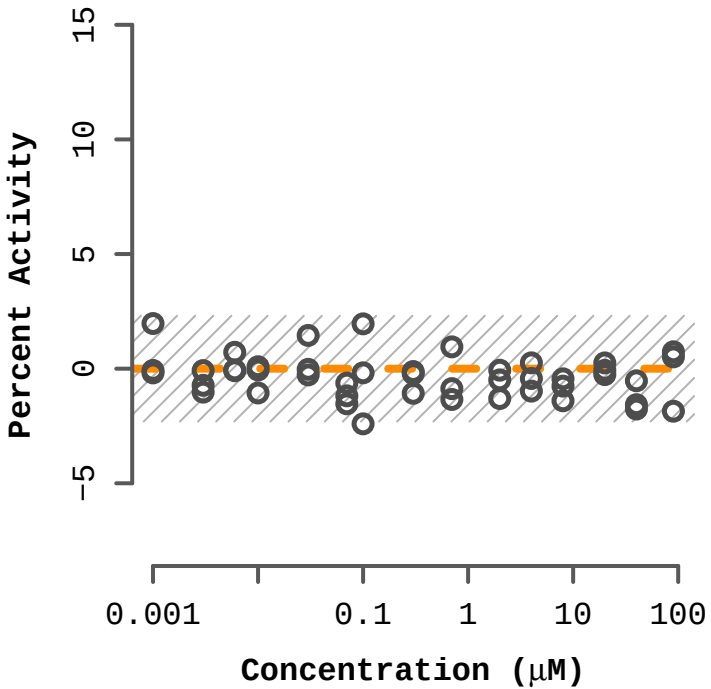
NAME: 4-Butylchlorobenzene
CHID: 48192 **CASRN:** 15499-27-1
SPID(S): Tox21_303435
M4ID: 12475704

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 0.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

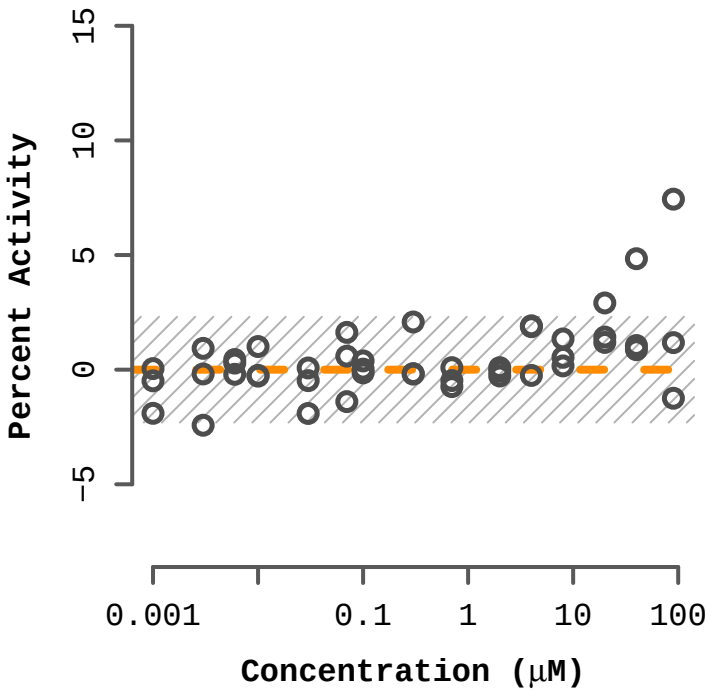
NAME: 4,4'-Di-tert-butylbiphenyl
CHID: 48193 **CASRN:** 1625-91-8
SPID(S): Tox21_303561
M4ID: 12475584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.57 **MAX_MED:** 0.517 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

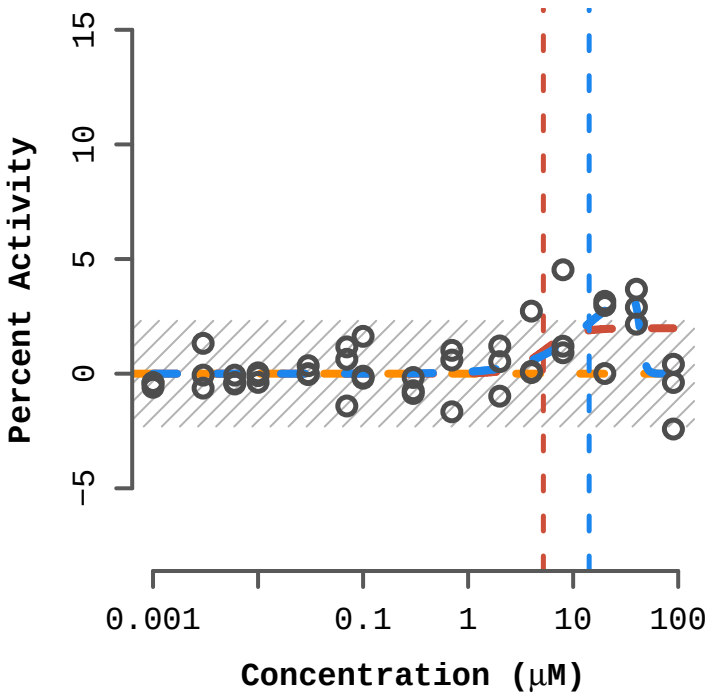
NAME: Heptanophenone
CHID: 48194 **CASRN:** 1671-75-6
SPID(S): Tox21_303543
M4ID: 12475601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 2.46 **MAX_MED:** 1.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(Hexyloxy)phenol
CHID: 48195 **CASRN:** 18979-55-0
SPID(S): Tox21_303471
M4ID: 12475669

HILL MODEL (in red):

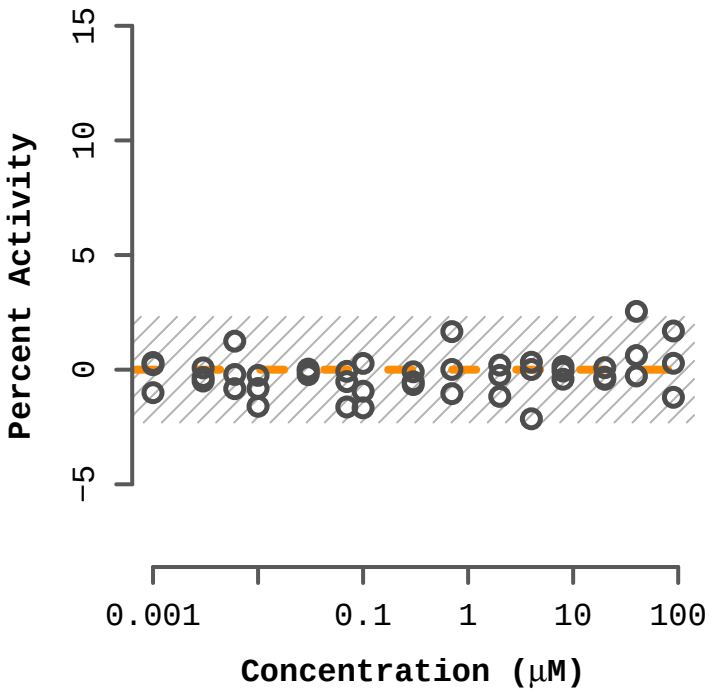
	tp	ga	gw
val:	1.98	0.716	3.01
sd:	0.578	0.223	2.84

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.4	1.15	1.49	1.64	17.2
sd:	8.01	1.18	1.95	0.0753	46.9

	CNST	HILL	GNLS
AIC:	160.1	151.19	137.65
PROB:	0	0	1
RMSE:	1.49	1.25	1.04

MAX_MEAN: 2.91 **MAX_MED:** 2.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

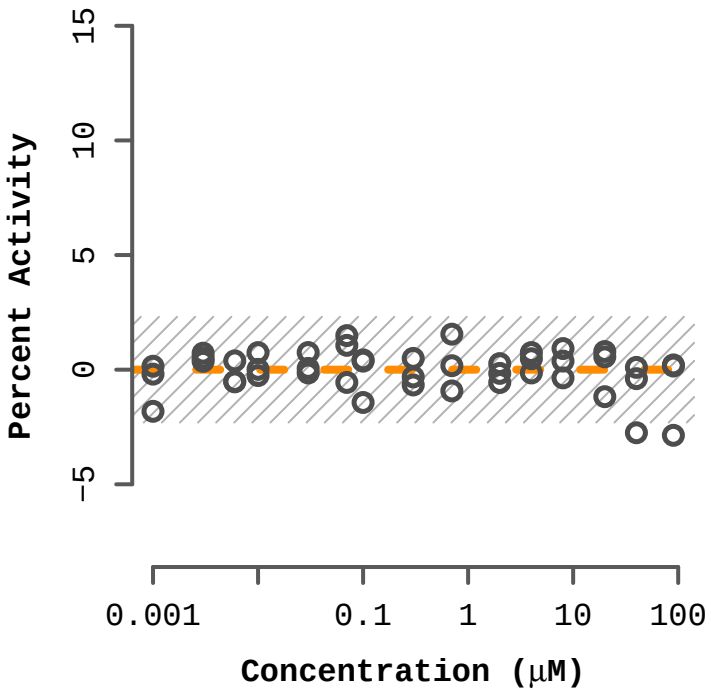
NAME: 4-tert-Butylbenzenethiol
CHID: 48196 **CASRN:** 2396-68-1
SPID(S): Tox21_303557
M4ID: 12475588

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.963 **MAX_MED:** 0.618 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

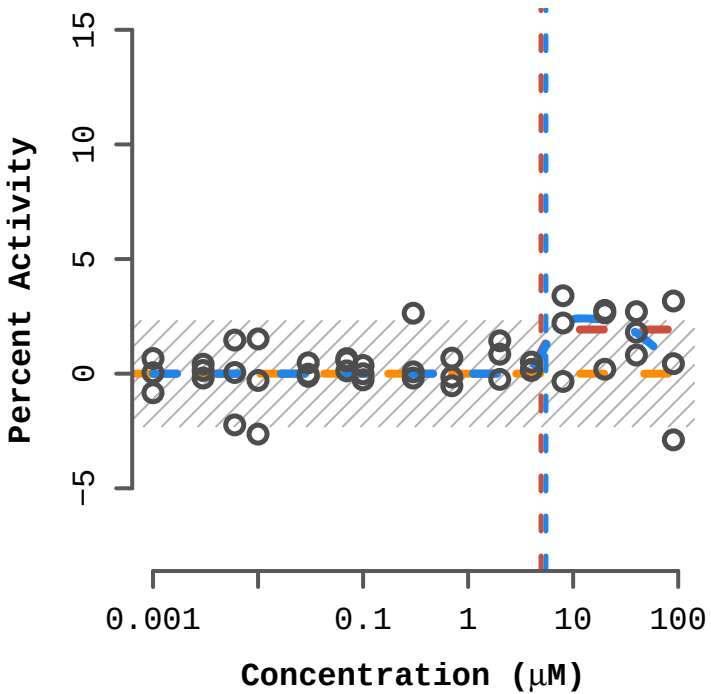
NAME: 4-Propylcyclohexanone
CHID: 48198 **CASRN:** 40649-36-3
SPID(S): Tox21_303343
M4ID: 12475790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.665 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Butyloxyaniline
CHID: 48199 **CASRN:** 4344-55-2
SPID(S): Tox21_303357
M4ID: 12475777

HILL MODEL (in red):

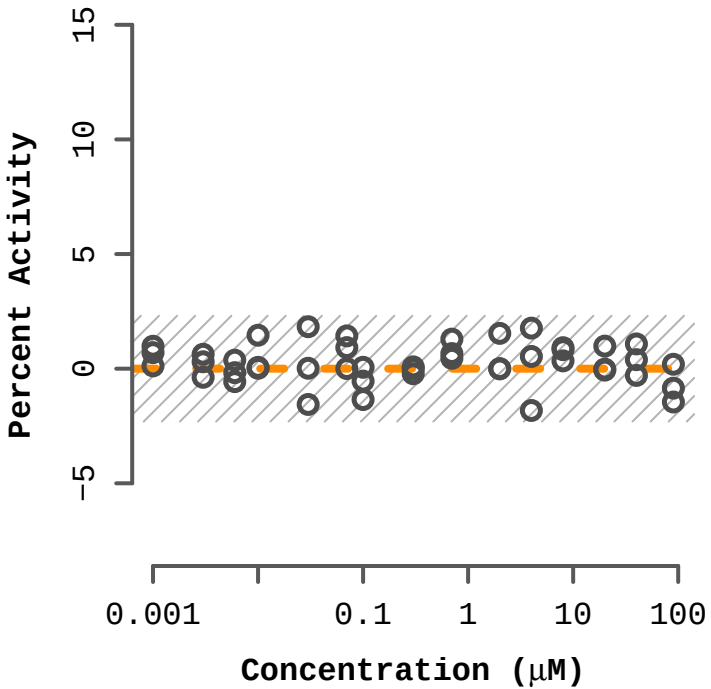
	tp	ga	gw
val:	1.93	0.694	8
sd:	0.393	0.125	10

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.46	0.74	6.31	1.75	2.75
sd:	1.02	0.195	8.59	0.233	3.53

	CNST	HILL	GNLS
AIC:	158.78	146.57	148.04
PROB:	0	0.68	0.32
RMSE:	1.42	1.25	1.18

MAX_MEAN: 1.87 **MAX_MED:** 2.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

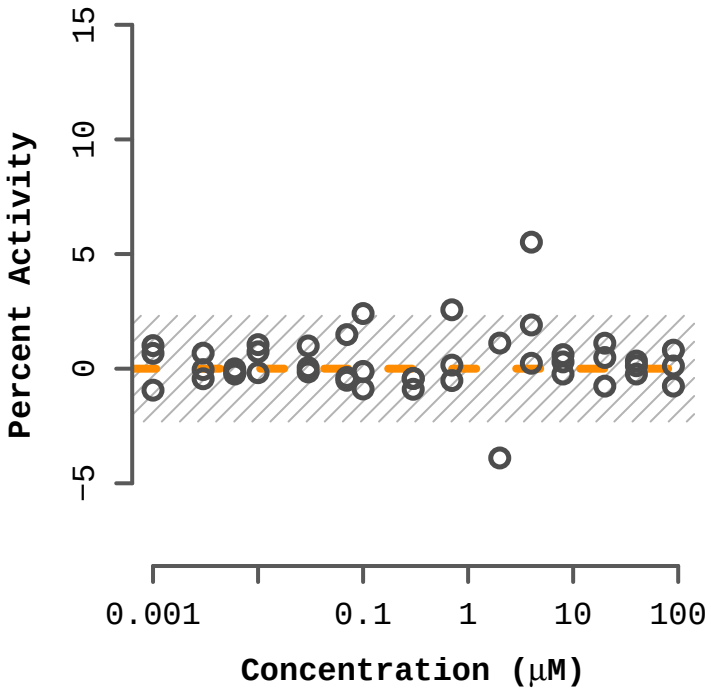
NAME: 2,4,6-Trimethylbenzoic acid
CHID: 48200 **CASRN:** 480-63-7
SPID(S): Tox21_303453
M4ID: 12475687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.801 **MAX_MED:** 0.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

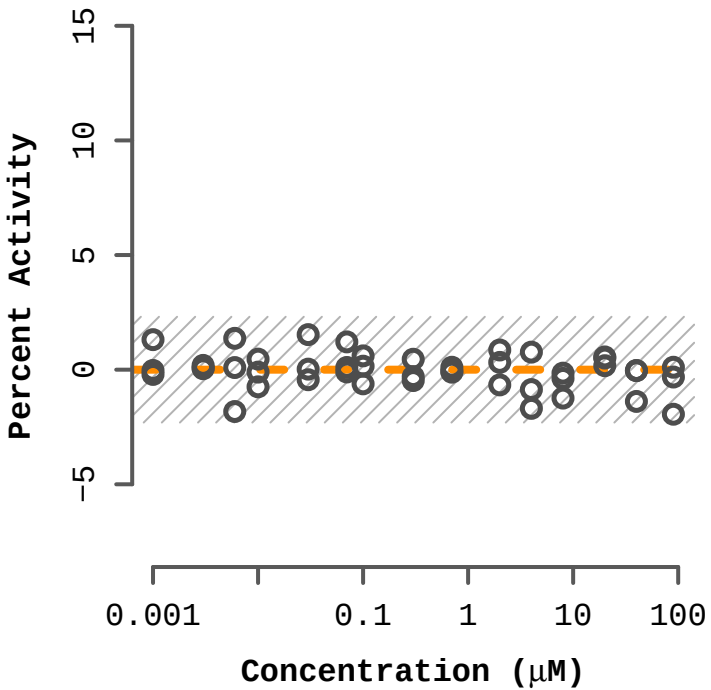
NAME: Cyclobutyl phenyl ketone
CHID: 48201 CASRN: 5407-98-7
SPID(S): Tox21_303524
M4ID: 12475619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 2.55 MAX_MED: 1.91 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

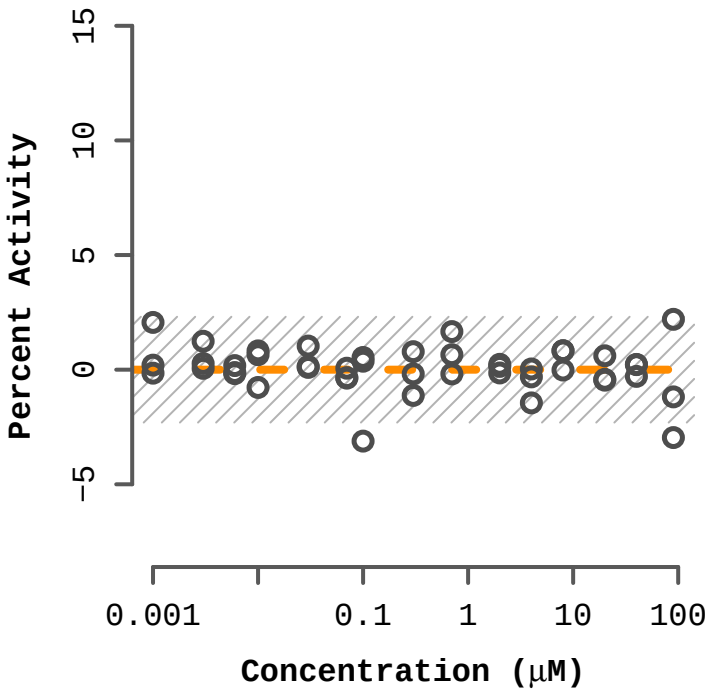
NAME: Isopropyl phenyl ketone
CHID: 48202 CASRN: 611-70-1
SPID(S): Tox21_303431
M4ID: 12475708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.413 MAX_MED: 0.508 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

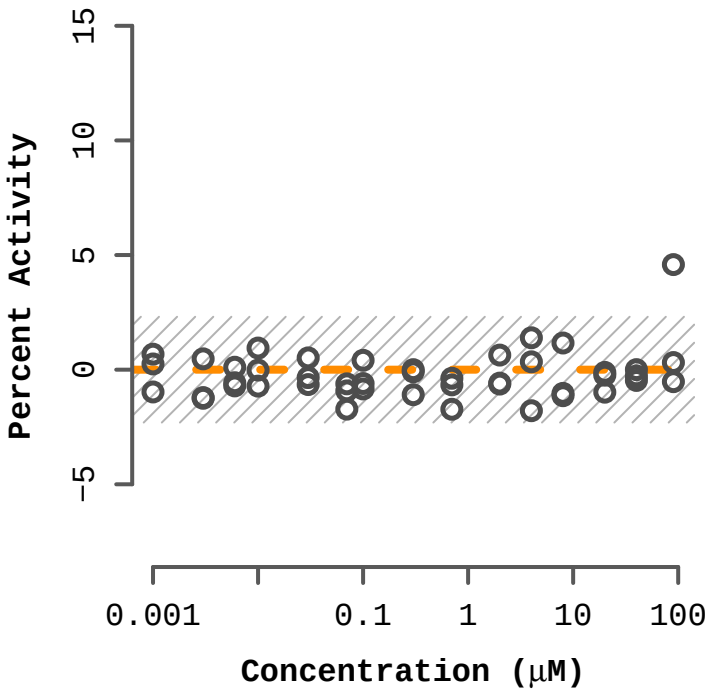
NAME: Ethyl 4-chlorophenyl ketone
CHID: 48203 CASRN: 6285-05-8
SPID(S): Tox21_303381
M4ID: 12475757

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.712 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

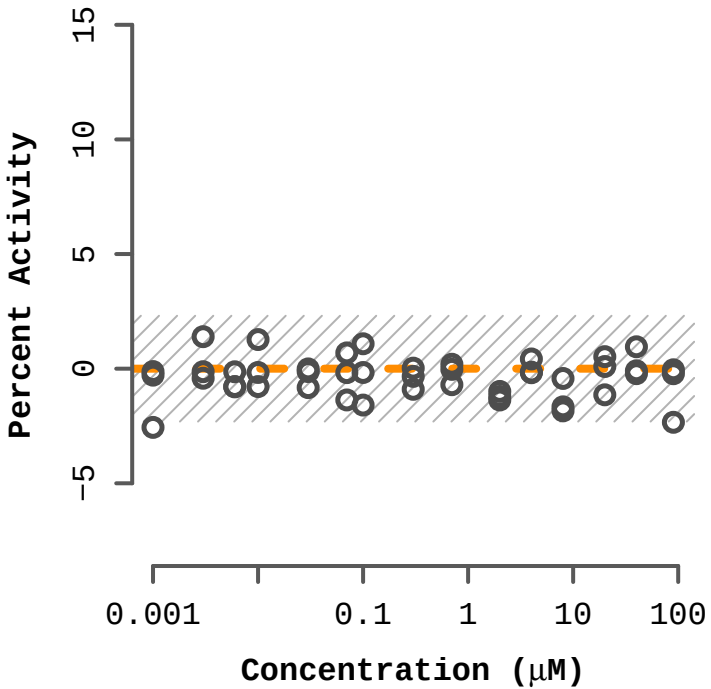
NAME: 4-Butylcyclohexanol
CHID: 48204 **CASRN:** 70568-60-4
SPID(S): Tox21_303529
M4ID: 12475614

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 0.344 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

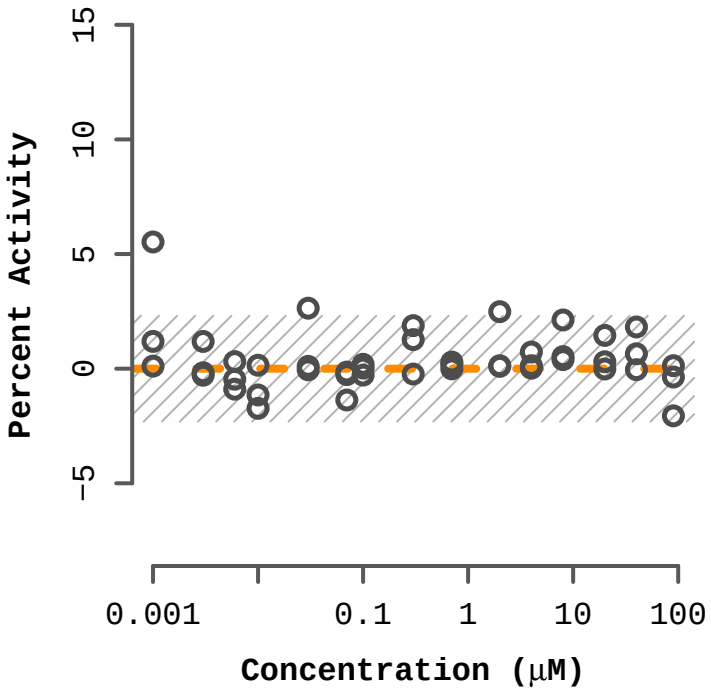
NAME: 4-Chloropentylbenzene
CHID: 48206 **CASRN:** 79098-20-7
SPID(S): Tox21_303473
M4ID: 12475667

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.284 **MAX_MED:** 0.0961 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

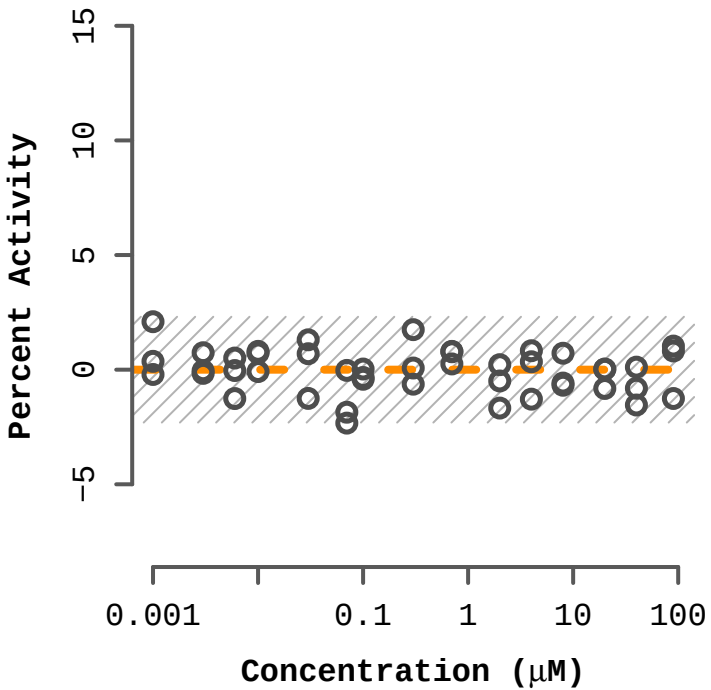
NAME: Diphenyl phosphate
CHID: 48207 **CASRN:** 838-85-7
SPID(S): Tox21_303401
M4ID: 12475738

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

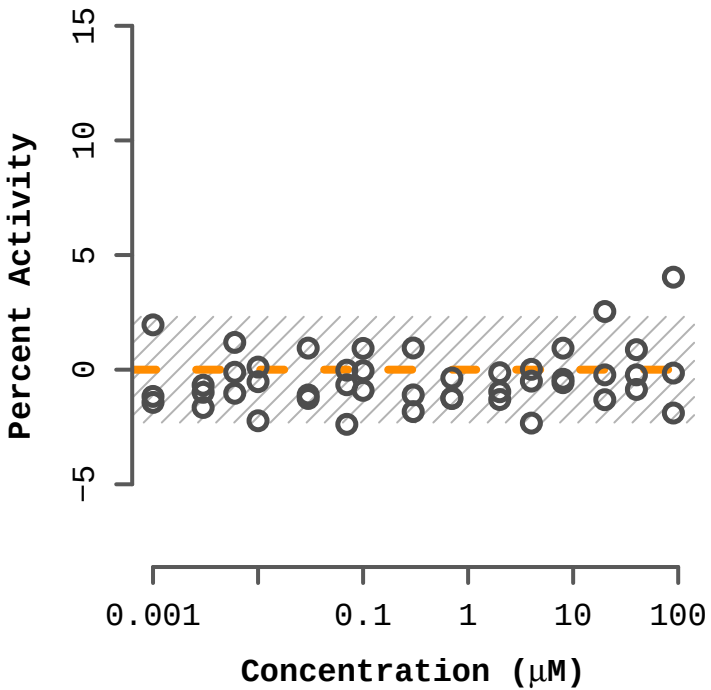
NAME: Methyl 2-methylbenzoate
CHID: 48208 **CASRN:** 89-71-4
SPID(S): Tox21_303461
M4ID: 12475679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.75 **MAX_MED:** 0.817 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

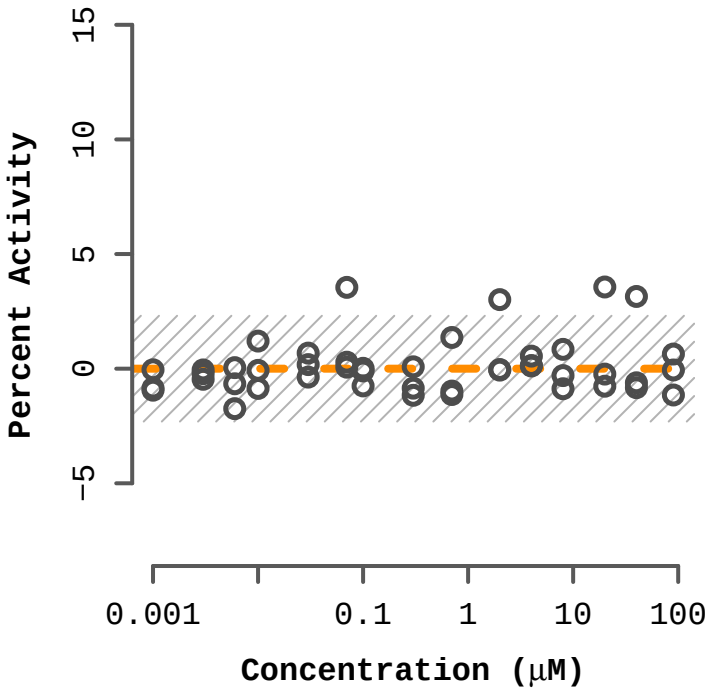
NAME: tert-Butyl phenyl ketone
CHID: 48209 **CASRN:** 938-16-9
SPID(S): Tox21_303564
M4ID: 12475581

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 0.666 **MAX_MED:** −0.046 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

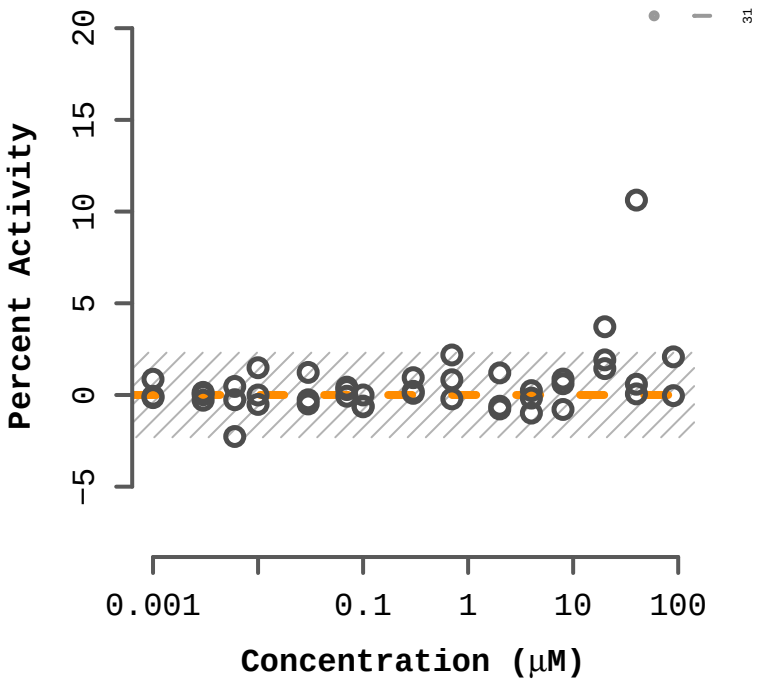
NAME: Phenyl benzoate
CHID: 48210 **CASRN:** 93-99-2
SPID(S): Tox21_303595
M4ID: 12475550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 0.284 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

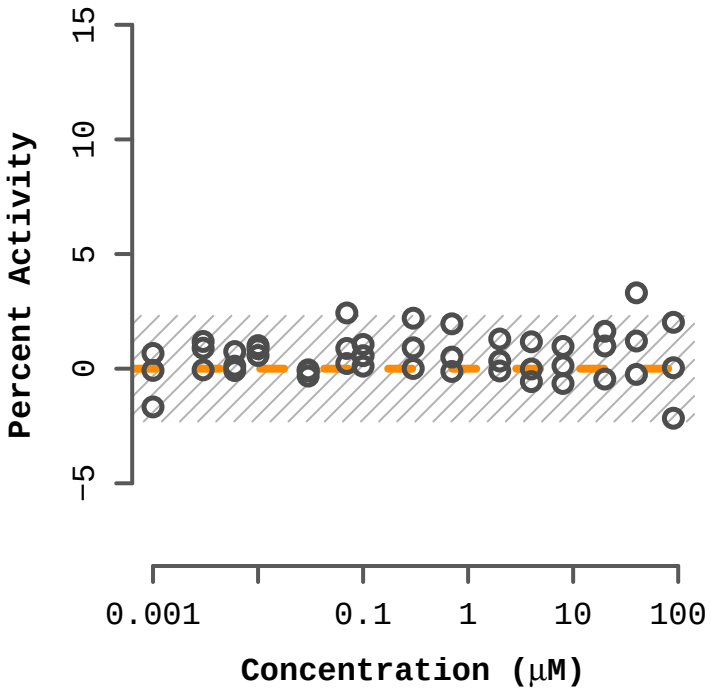
NAME: Phenyl benzoate
CHID: 48210 CASRN: 93-99-2
SPID(S): Tox21_202880
M4ID: 12479372 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.92	NA	NA
PROB:	1	NA	NA
RMSE:	5.06	NA	NA

MAX_MEAN: 11.2 MAX_MED: 2.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

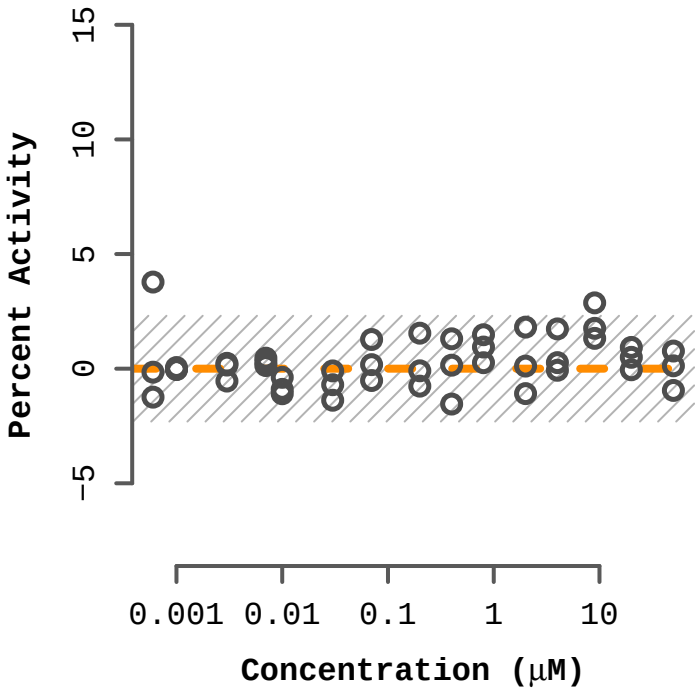
NAME: Ethyl 4-methylbenzoate
CHID: 48211 **CASRN:** 94-08-6
SPID(S): Tox21_303476
M4ID: 12475664

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

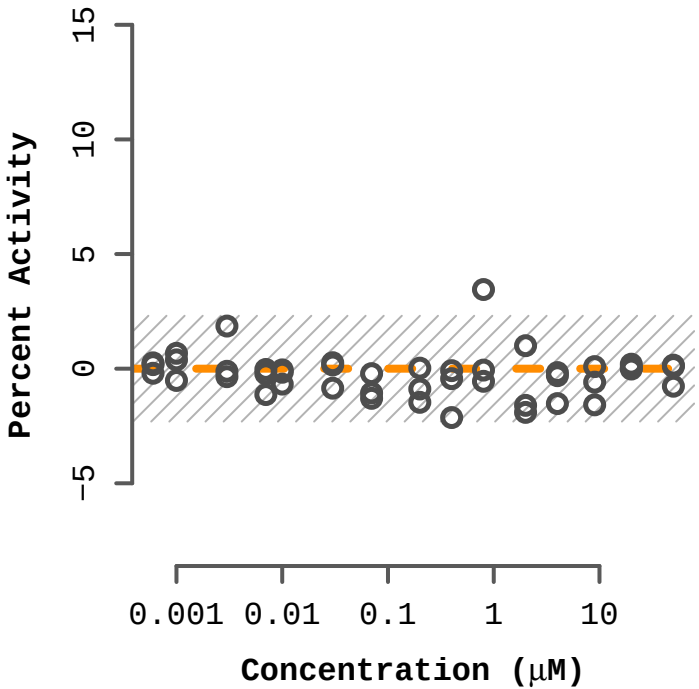
NAME: Ropivacaine hydrochloride
CHID: 48379 **CASRN:** 98717-15-8
SPID(S): Tox21_112221_1
M4ID: 12483224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.99 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

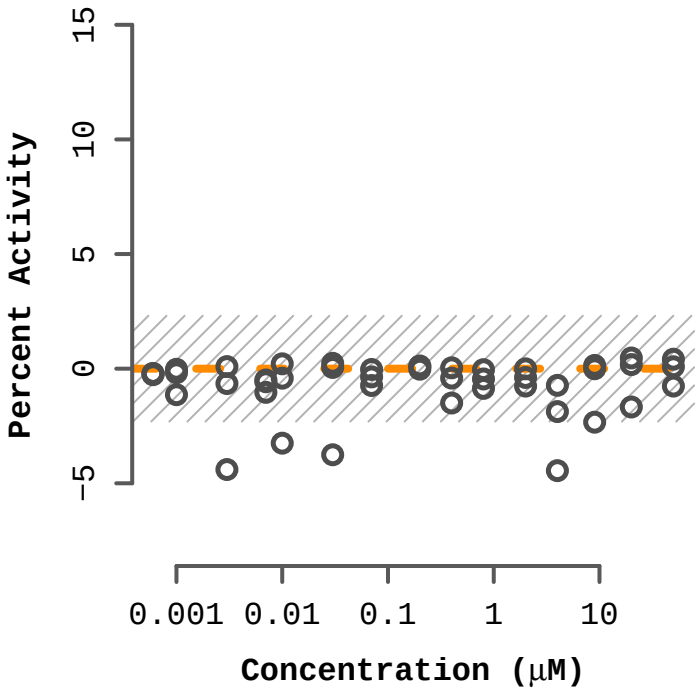
NAME: 2,3-Dihydroxypropyl octanoate
CHID: 48383 **CASRN:** 502-54-5
SPID(S): Tox21_112338_1
M4ID: 12483151

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.948 **MAX_MED:** 0.386 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

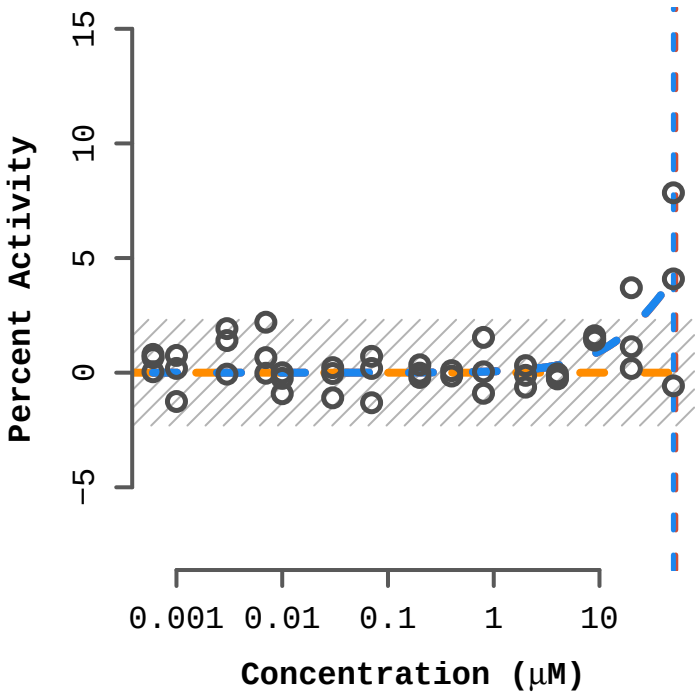
NAME: Dibenzepin hydrochloride
CHID: 48421 **CASRN:** 315-80-0
SPID(S): Tox21_111784_1
M4ID: 12483484

HILL MODEL: Not applicable.

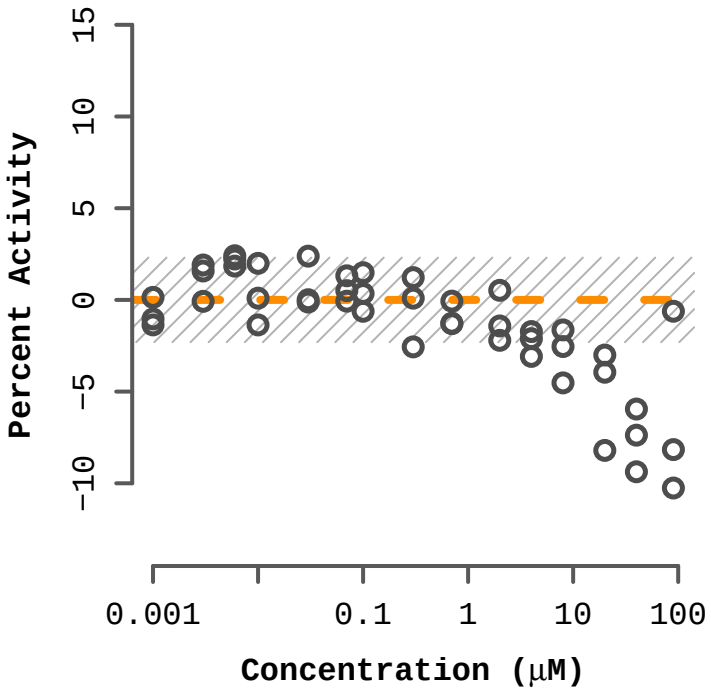
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.38	NA	NA

MAX_MEAN: 0.0654 **MAX_MED:** 0.181 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Sarafloxacin
CHID:    48494   CASRN: 98105-99-8
SPID(S): Tox21_303838
M4ID:    12475350

HILL MODEL (in red):
      tp       ga       gw
val:  8.46     1.72     1.26
sd:   21.3     1.64     0.952

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.18     1.7      1.27     3.66     3.09
sd:   19       1.53     0.937    555      919

      CNST        HILL        GNLS
AIC:  148.17      140.37      144.37
PROB: 0.02        0.87        0.12
RMSE: 1.67        1.24        1.24

MAX_MEAN: 3.79      MAX_MED: 4.09      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

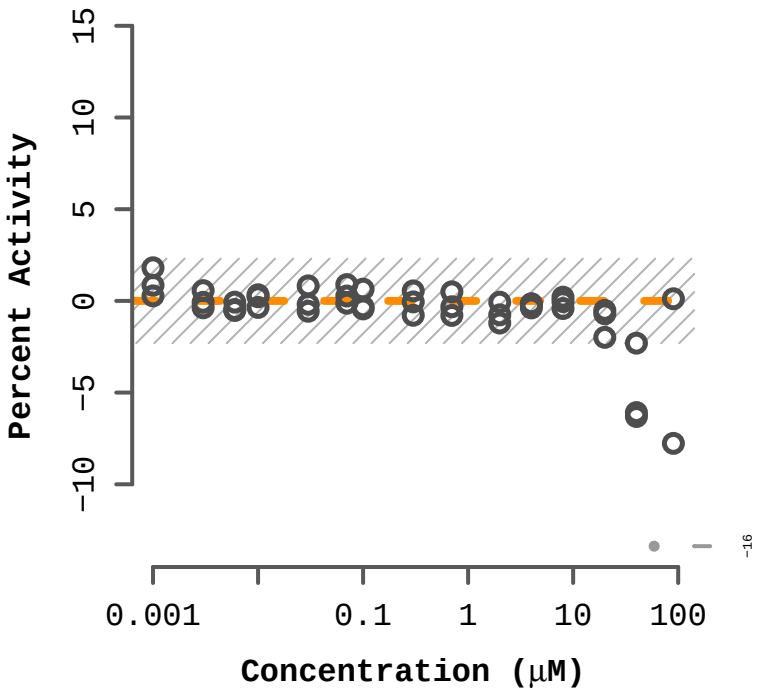
NAME: PharmaGSID_48505
CHID: 48505 CASRN: NOCAS_48505
SPID(S): Tox21_303517
M4ID: 12475625

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	233.88	NA	NA
PROB:	1	NA	NA
RMSE:	3.48	NA	NA

MAX_MEAN: 2.16 MAX_MED: 2.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

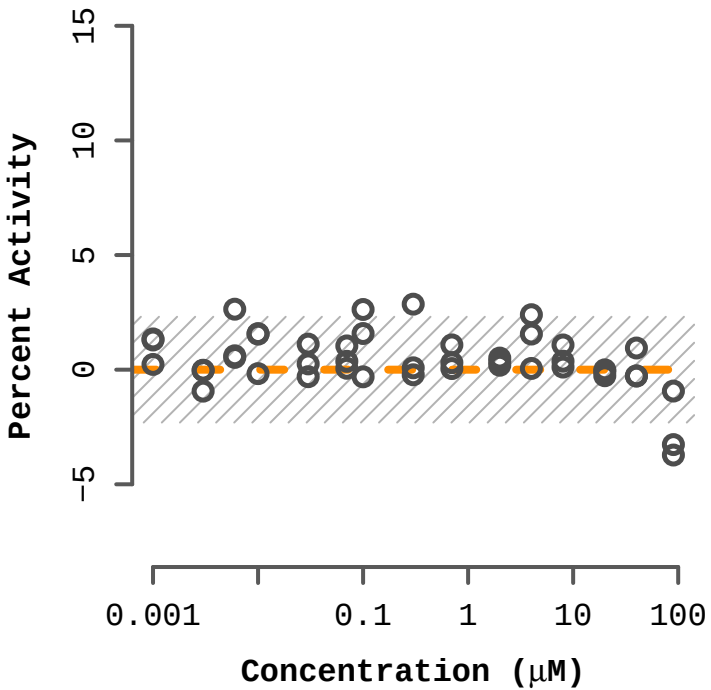
NAME: PharmaGSID_48506
CHID: 48506 CASRN: 588941-45-1
SPID(S): Tox21_303352
M4ID: 12475781 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.6	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 0.978 **MAX_MED:** 0.852 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

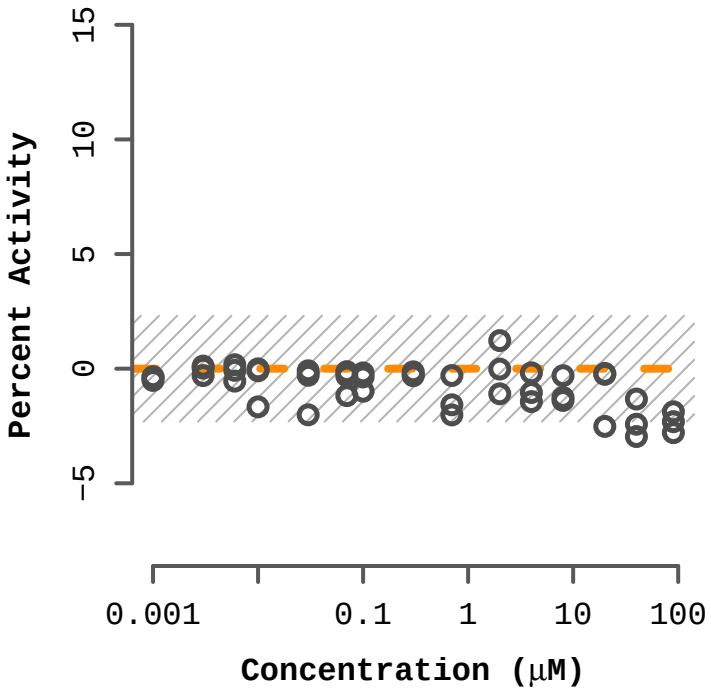
NAME: PharmaGSID_48507
CHID: 48507 **CASRN:** NOCAS_48507
SPID(S): Tox21_303344
M4ID: 12475789

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

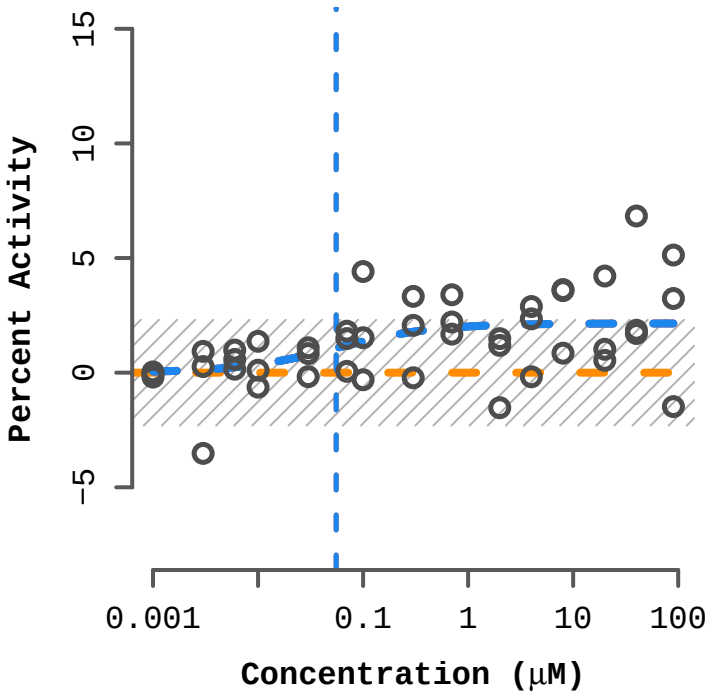
NAME: PharmaGSID_48509
CHID: 48509 **CASRN:** NOCAS_48509
SPID(S): Tox21_303585
M4ID: 12475560

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.0382 **MAX_MED:** 0.0258 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PharmaGSID_48510
CHID: 48510 CASRN: 460081-99-6
SPID(S): Tox21_303410
M4ID: 12475729

HILL MODEL (in red):

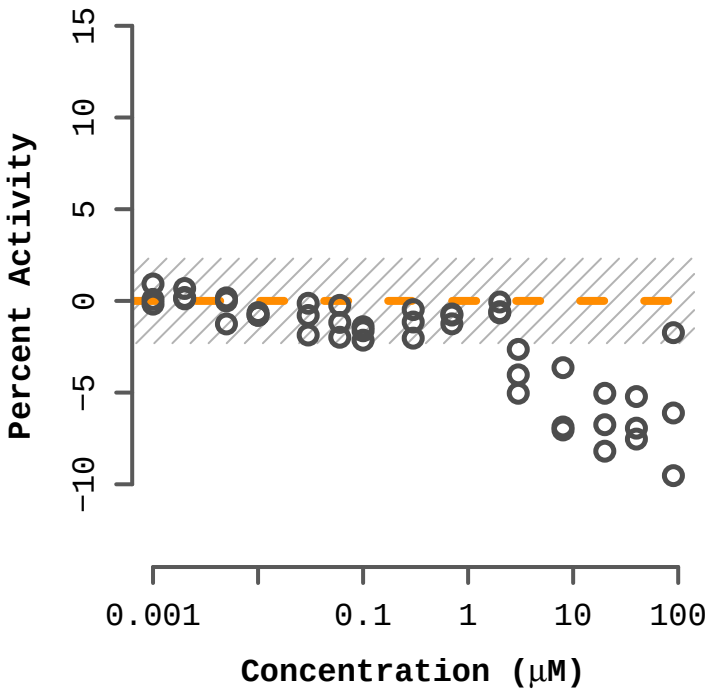
	tp	ga	gw
val:	2.15	−1.26	0.936
sd:	0.47	0.461	0.992

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.15	−1.26	0.936	3.91	3.99
sd:	0.47	0.461	0.992	2010	4090

	CNST	HILL	GNLS
AIC:	204.17	176.95	180.95
PROB:	0	0.88	0.12
RMSE:	2.3	1.63	1.63

MAX_MEAN: 3.47 MAX_MED: 3.58 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

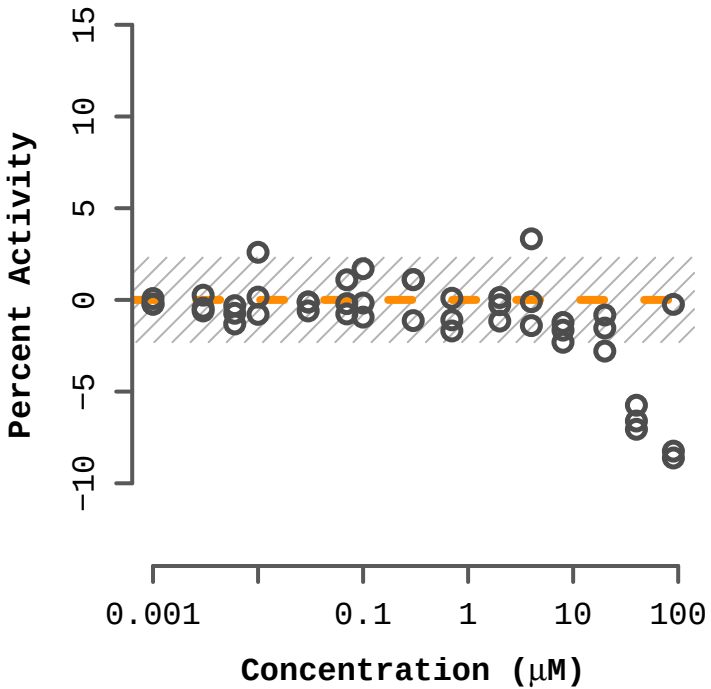
NAME: PharmaGSID_48511
CHID: 48511 **CASRN:** 1062243-51-9
SPID(S): Tox21_303518
M4ID: 12475624

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	241.98	NA	NA
PROB:	1	NA	NA
RMSE:	3.63	NA	NA

MAX_MEAN: 0.326 **MAX_MED:** 0.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

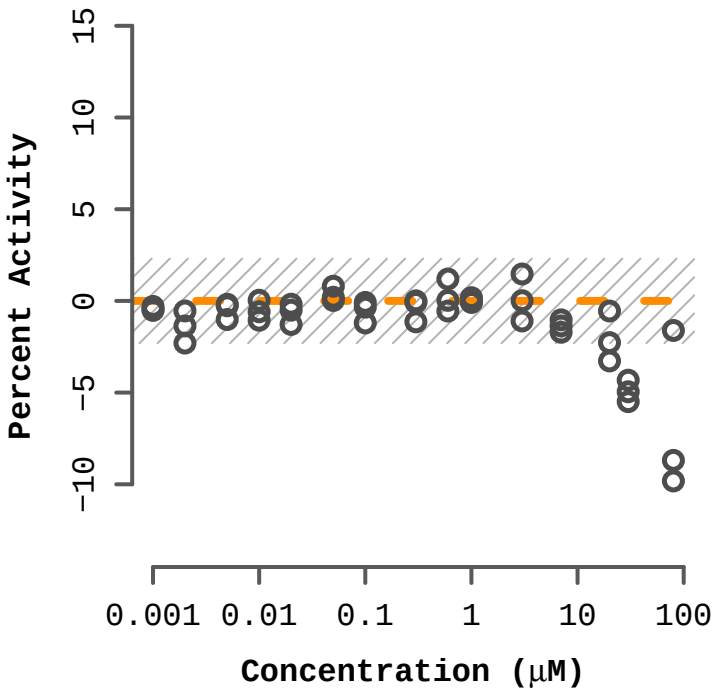
NAME: Ro 23-7637
CHID: 48512 **CASRN:** 107071-66-9
SPID(S): Tox21_303576
M4ID: 12475569

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	201.05	NA	NA
PROB:	1	NA	NA
RMSE:	2.7	NA	NA

MAX_MEAN: 0.655 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

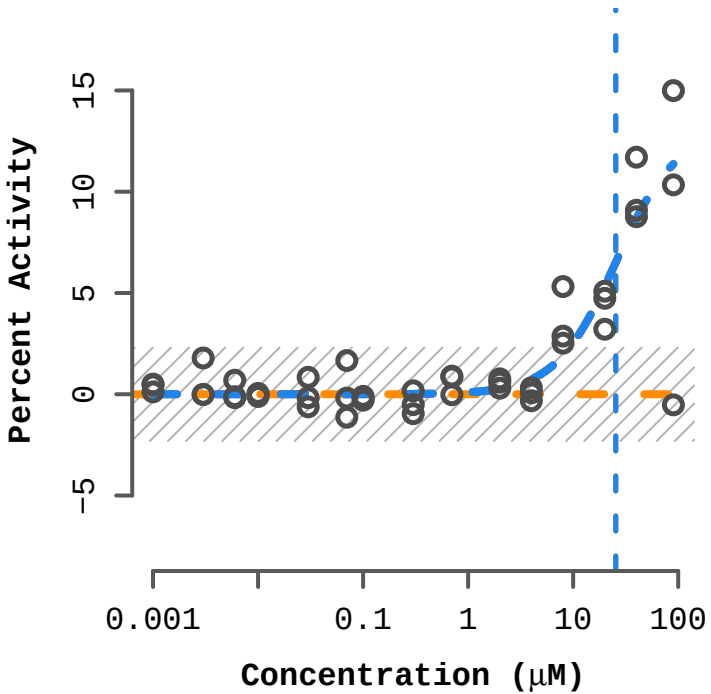
NAME: PharmaGSID_48513
CHID: 48513 **CASRN:** 825643-57-0
SPID(S): Tox21_303601
M4ID: 12475544

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	189.5	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 0.342 **MAX_MED:** 0.201 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PharmaGSID_48514
CHID: 48514 CASRN: NOCAS_48514
SPID(S): Tox21_303405
M4ID: 12475734

HILL MODEL (in red):

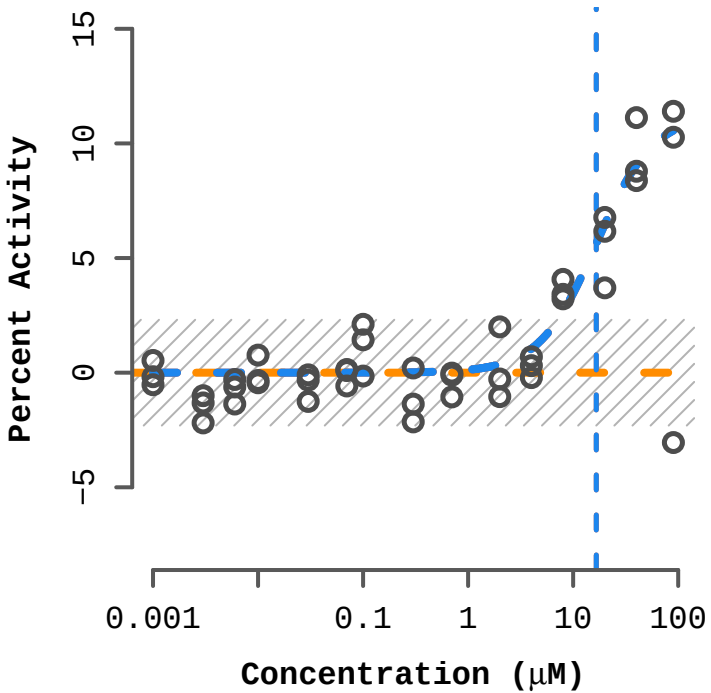
	tp	ga	gw
val:	13	1.41	1.52
sd:	2.56	0.131	0.322

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	13	1.41	1.52	3.23	10.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	229.32	153.66	157.66
PROB:	0	0.88	0.12
RMSE:	4.07	2.09	2.09

MAX_MEAN: 9.85 MAX_MED: 10.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PharmaGSID_48516
CHID: 48516 CASRN: NOCAS_48516
SPID(S): Tox21_303538
M4ID: 12475606

HILL MODEL (in red):

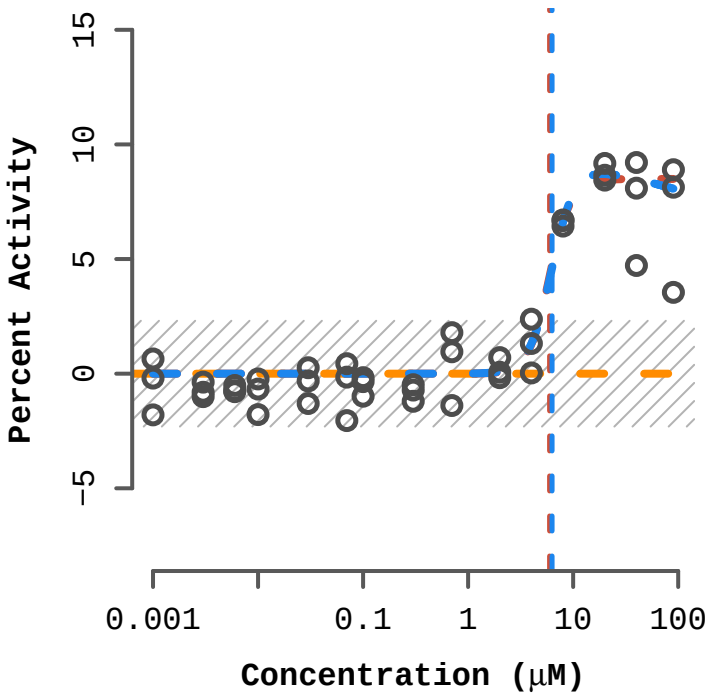
	tp	ga	gw
val:	11.3	1.22	1.6
sd:	1.11	0.0904	0.292

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.3	1.22	1.6	3.29	5.87
sd:	1.11	0.0904	0.292	1210	5330

	CNST	HILL	GNLS
AIC:	238.24	163.24	167.24
PROB:	0	0.88	0.12
RMSE:	3.9	2.29	2.29

MAX_MEAN: 9.43 MAX_MED: 10.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PharmaGSID_48518
CHID: 48518 CASRN: NOCAS_48518
SPID(S): Tox21_303586
M4ID: 12475559

HILL MODEL (in red):

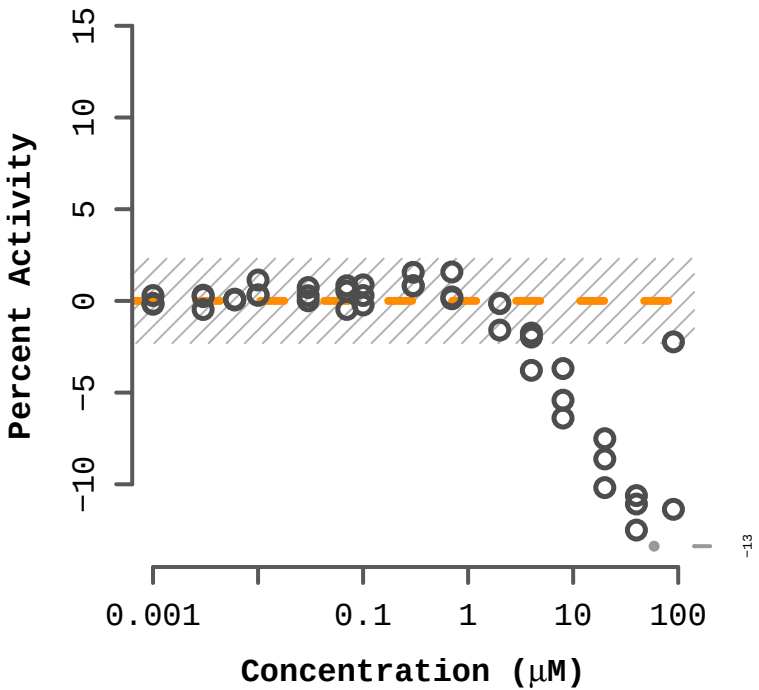
	tp	ga	gw
val:	8.49	0.776	4.31
sd:	0.316	0.031	0.904

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.4	0.799	4	3.73	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	248.04	142.76	146.08
PROB:	0	0.84	0.16
RMSE:	4.02	1.24	1.21

MAX_MEAN: 8.76 MAX_MED: 8.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

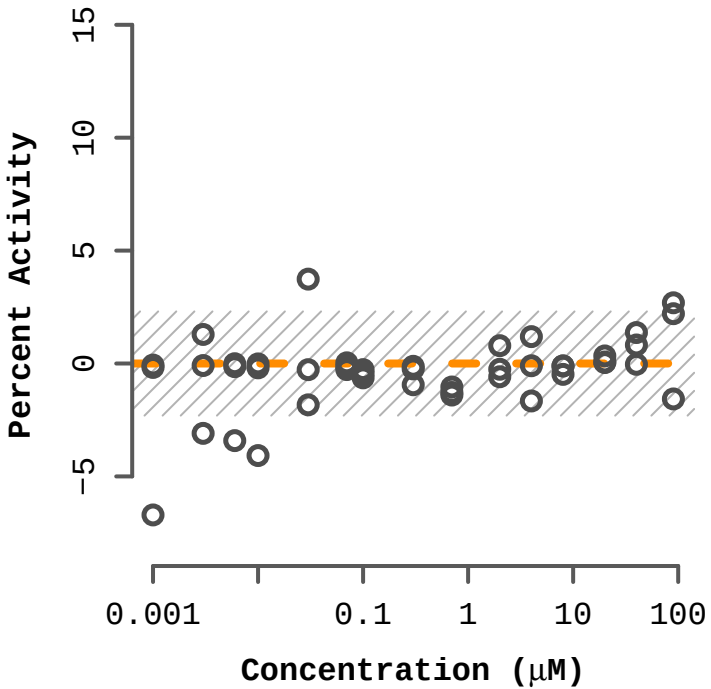
NAME: PharmaGSID_48519
CHID: 48519 CASRN: 686756-87-6
SPID(S): Tox21_303407
M4ID: 12475732 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.64	NA	NA
PROB:	1	NA	NA
RMSE:	4.85	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 0.833 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

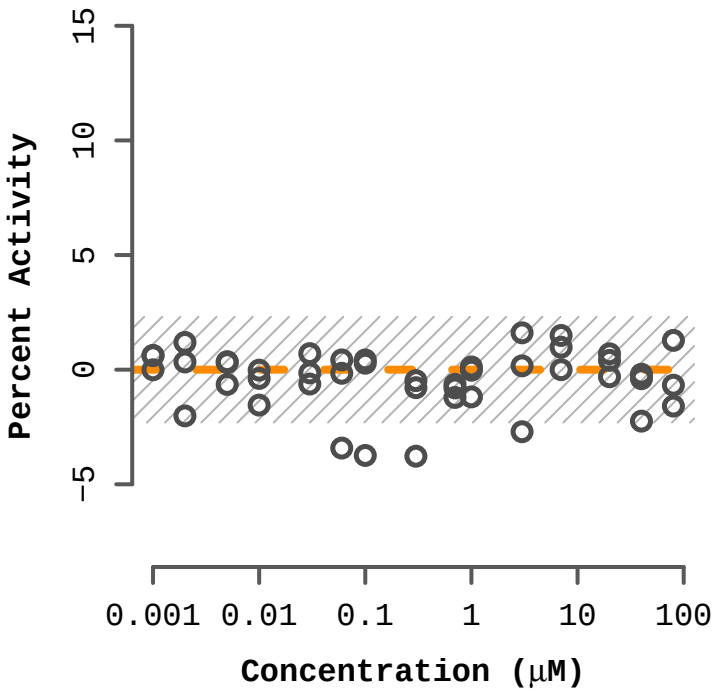
NAME: Piragliatin
CHID: 48520 CASRN: 625114-41-2
SPID(S): Tox21_303593
M4ID: 12475552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.71	NA	NA

MAX_MEAN: 1.11 MAX_MED: 2.21 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

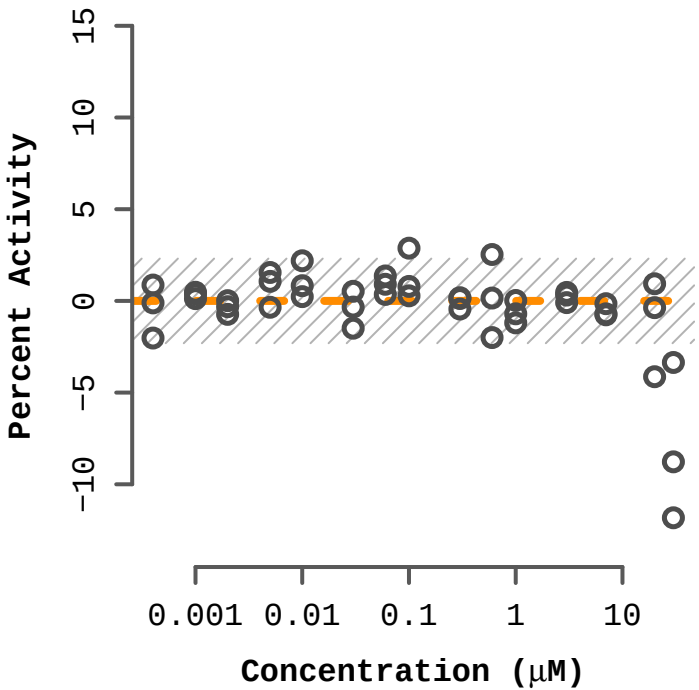
NAME: PharmaGSID_48521
CHID: 48521 **CASRN:** 1191914-21-2
SPID(S): Tox21_303454
M4ID: 12475686

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.825 **MAX_MED:** 0.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

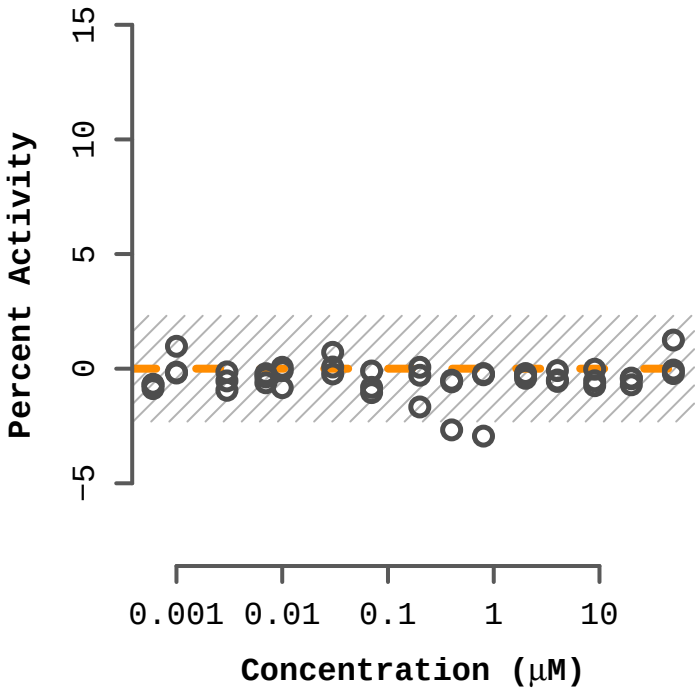
NAME: HMR1171 trifluoroacetate (1:1)
CHID: 48522 **CASRN:** NOCAS_48522
SPID(S): Tox21_303378
M4ID: 12475759

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.82	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

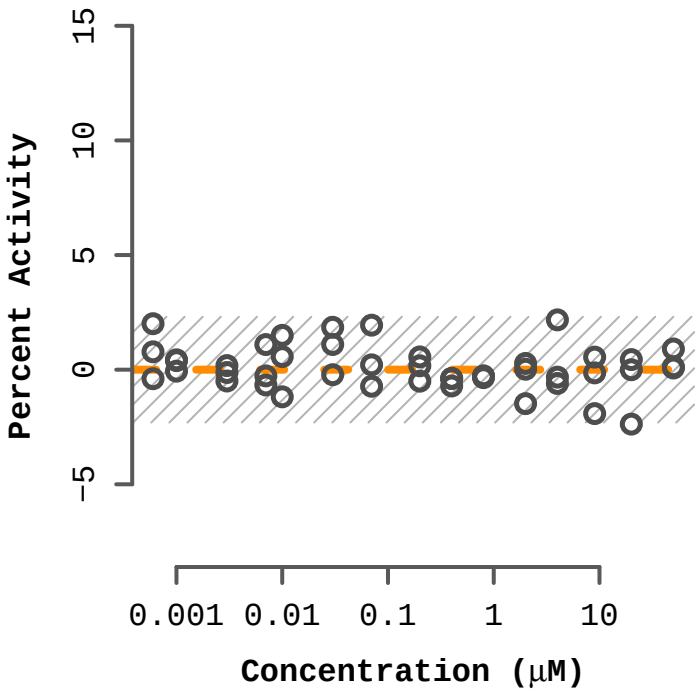
NAME: Sulfonmethane
CHID: 48574 **CASRN:** 115-24-2
SPID(S): Tox21_112150_1
M4ID: 12483281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.326 **MAX_MED:** 0.0736 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

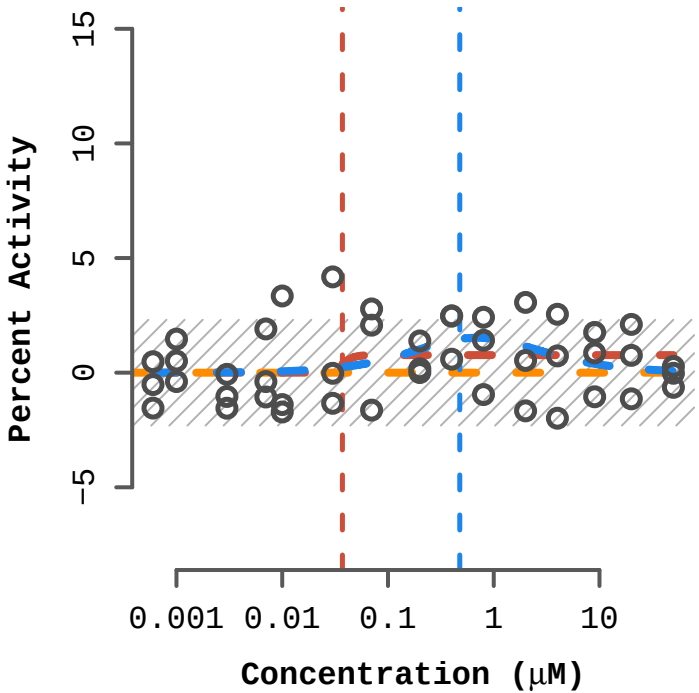
NAME: Alacepril
CHID: 48576 CASRN: 74258-86-9
SPID(S): Tox21_112904
M4ID: 12482882

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.91 MAX_MED: 1.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Saxagliptin
CHID: 48580 CASRN: 361442-04-8
SPID(S): Tox21_112908
M4ID: 12482881

HILL MODEL (in red):

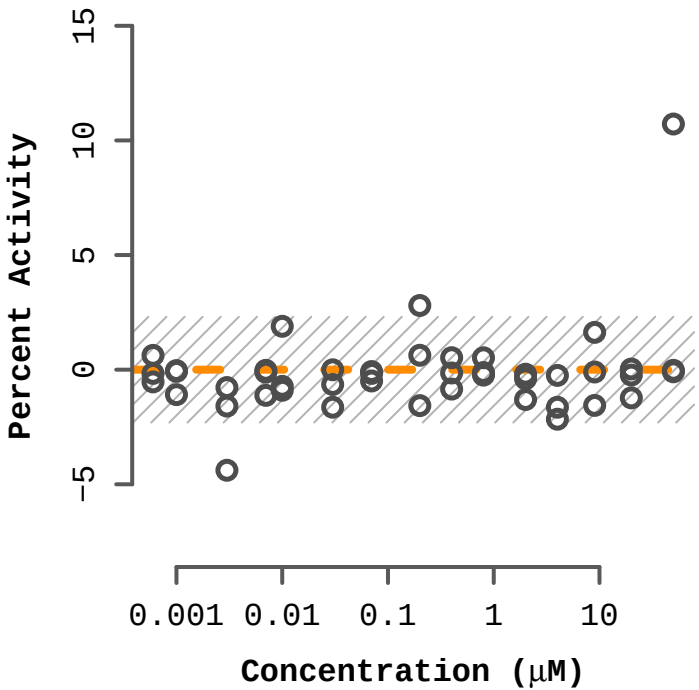
	tp	ga	gw
val:	0.767	−1.43	8
sd:	0.315	0.448	23.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.59	−0.321	1.11	−0.0712	0.992
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	178.43	178.79	181.28
PROB:	0.48	0.4	0.12
RMSE:	1.65	1.55	1.53

MAX_MEAN: 1.85 MAX_MED: 2.47 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

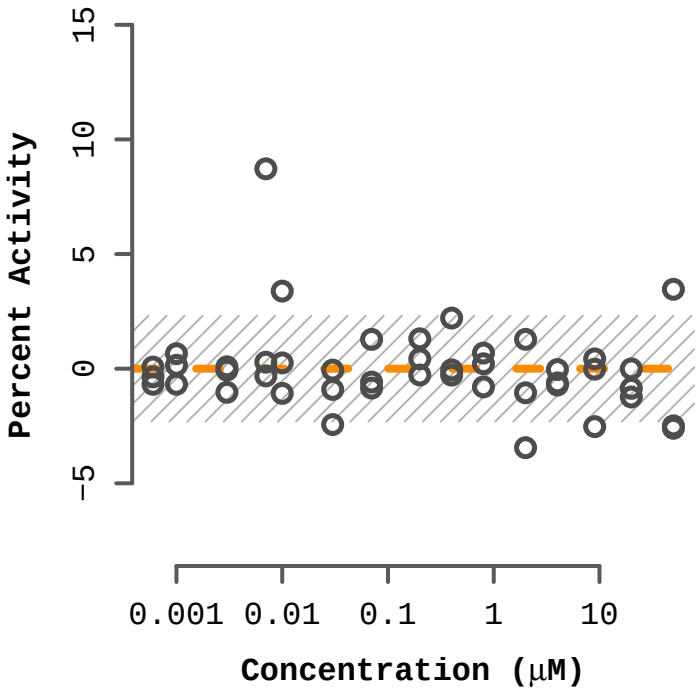
NAME: Tigecycline
CHID: 48581 **CASRN:** 220620-09-7
SPID(S): Tox21_112910
M4ID: 12482880

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 3.53 **MAX_MED:** 0.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

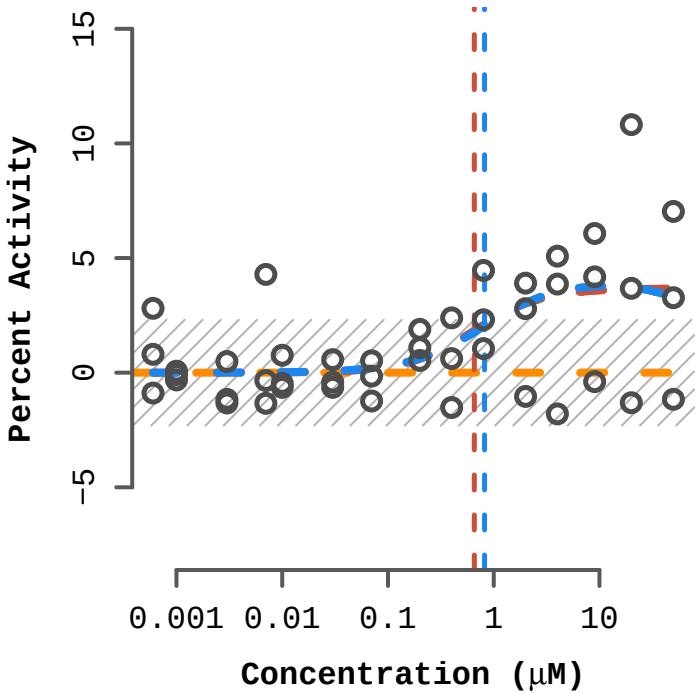
NAME: Cefcapene pivoxil hydrochloride
CHID: 48582 **CASRN:** 147816-23-7
SPID(S): Tox21_113259
M4ID: 12482763

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.88	NA	NA

MAX_MEAN: 2.9 **MAX_MED:** 0.432 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cefcapene pivoxil hydrochloride
CHID: 48582 CASRN: 147816-23-7
SPID(S): Tox21_112911
M4ID: 12482879

HILL MODEL (in red):

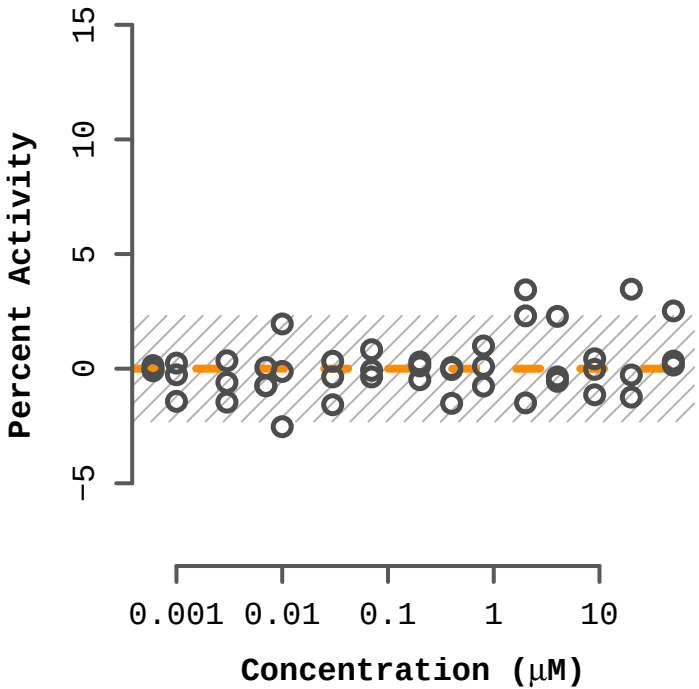
	tp	ga	gw
val:	3.68	−0.184	1.37
sd:	0.89	0.321	0.897

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.08	−0.087	1.22	2.23	1.2
sd:	2.89	0.669	0.994	2.56	6.73

	CNST	HILL	GNLS
AIC:	219.89	203.82	207.73
PROB:	0	0.88	0.12
RMSE:	2.96	2.29	2.29

MAX_MEAN: 4.4 **MAX_MED:** 4.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

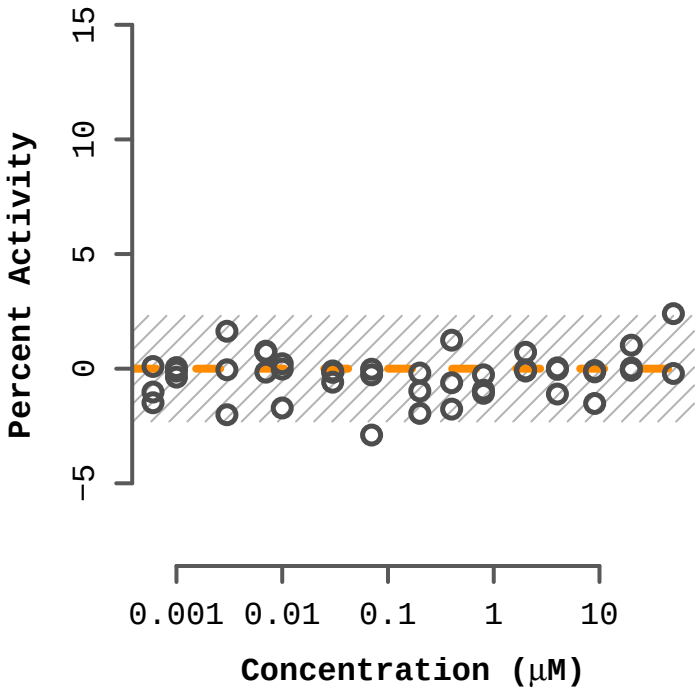
NAME: Cefetamet pivoxil HCl
CHID: 48590 CASRN: 111696-23-2
SPID(S): Tox21_112919
M4ID: 12482878

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

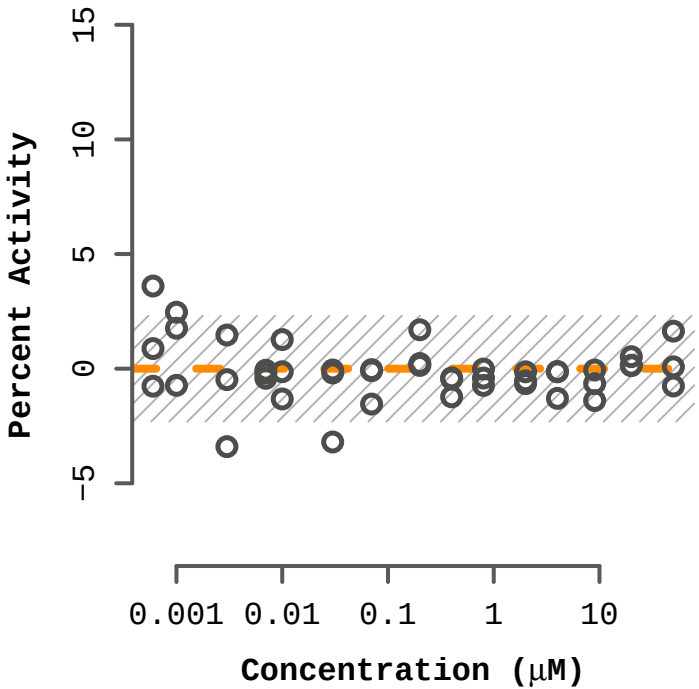
NAME: Cefminox sodium
CHID: 48591 CASRN: 75498-96-3
SPID(S): Tox21_112920
M4ID: 12482877

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

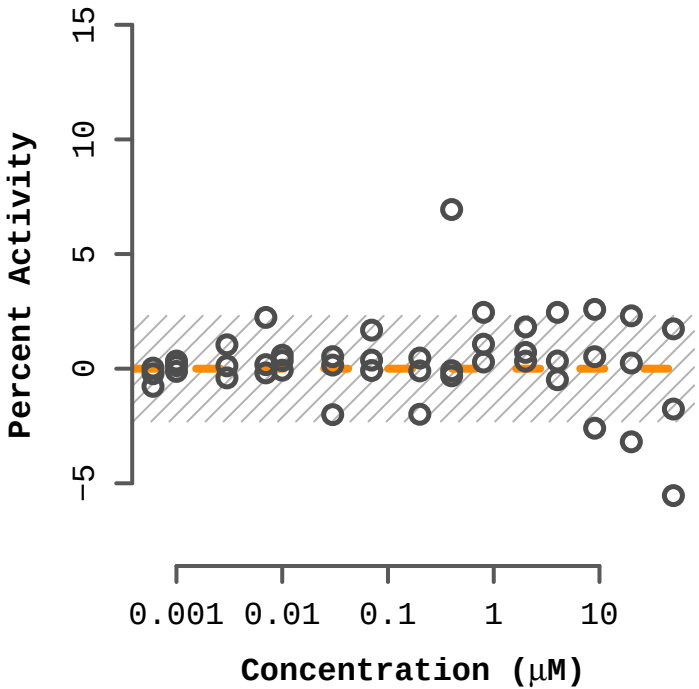
NAME: Cefozopran hydrochloride
CHID: 48592 **CASRN:** 113981-44-5
SPID(S): Tox21_112921
M4ID: 12482876

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

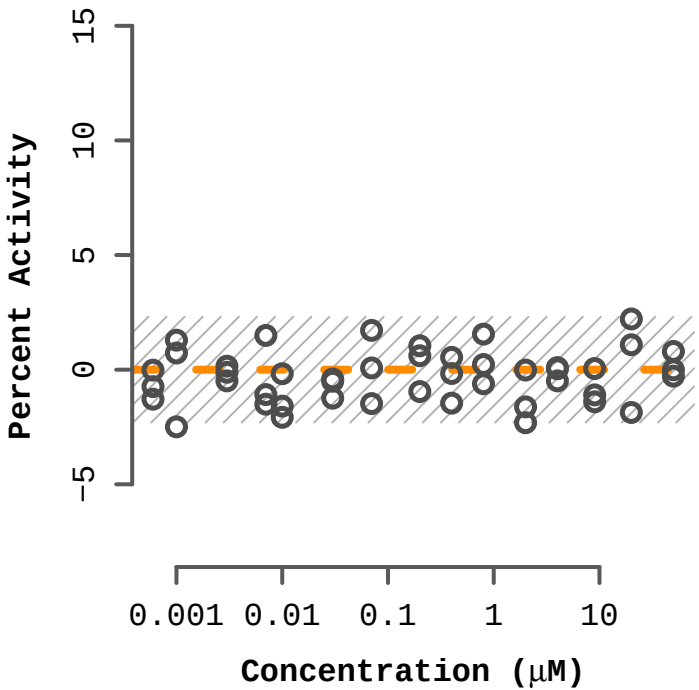
NAME: Deferasirox
CHID: 48596 **CASRN:** 201530-41-8
SPID(S): Tox21_112926_1
M4ID: 12482875

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 2.18 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

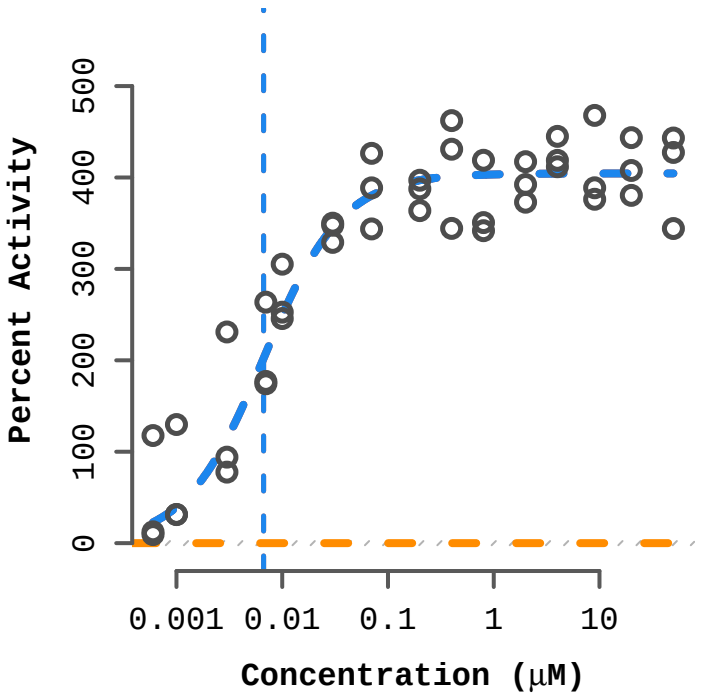
NAME: Delapril hydrochloride
CHID: 48597 CASRN: 83435-67-0
SPID(S): Tox21_112927
M4ID: 12482874

HILL MODEL: Not applicable.

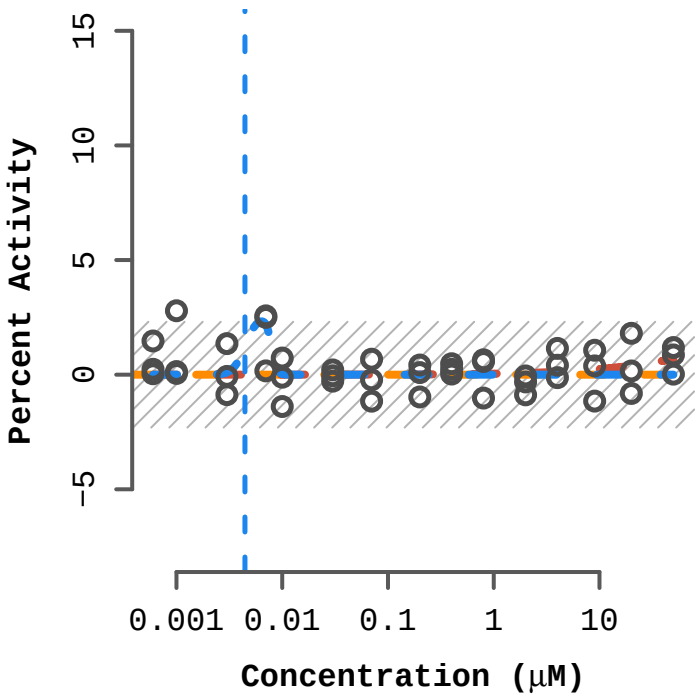
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.478 **MAX_MED:** 1.09 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diflucortolone valerate
CHID:    48598   CASRN: 59198-70-8
SPID(S): Tox21_112929_1
M4ID:    12482872

HILL MODEL (in red):
      tp       ga       gw
val:  404      -2.18    1.17
sd:   8.41     0.0556   0.17

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  404      -2.18    1.17     3.7      4.16
sd:   8.41     0.0556   0.17     1710     3560

      CNST        HILL        GNLS
AIC:  662.94      471.21      475.21
PROB: 0           0.88        0.12
RMSE: 338.42      41.36       41.36

MAX_MEAN: 425       MAX_MED: 431       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Flurbiprofen axetil
CHID: 48600 CASRN: 91503-79-6
SPID(S): Tox21_113023_1
M4ID: 12482838

HILL MODEL (in red):

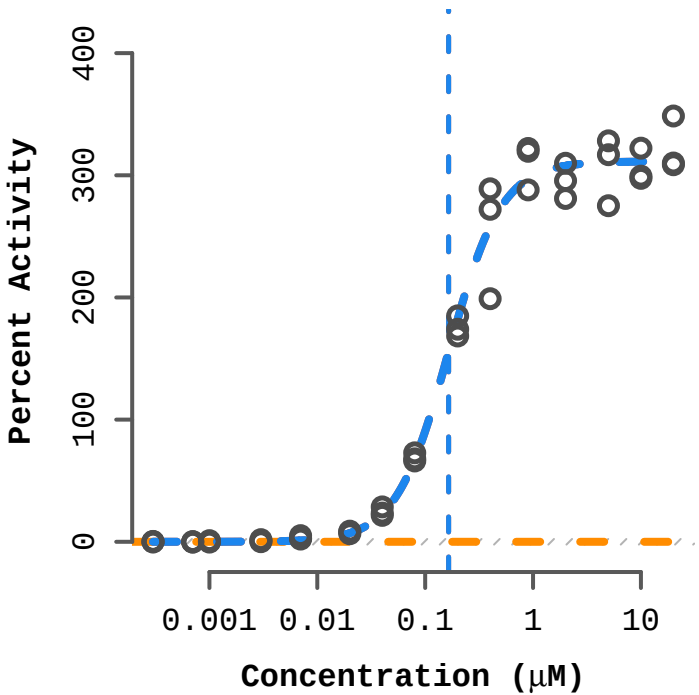
	tp	ga	gw
val:	2.43	2.2	0.797
sd:	23.3	8.03	1.61

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.5	−2.35	8	−2.1	18
sd:	1.7	0.345	15.3	0.105	23.1

	CNST	HILL	GNLS
AIC:	126.18	129.19	128.01
PROB:	0.62	0.14	0.25
RMSE:	0.99	0.97	0.89

MAX_MEAN: 1.74 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone buteprate
CHID: 48603 CASRN: 72590-77-3
SPID(S): Tox21_112938
M4ID: 12482870

HILL MODEL (in red):

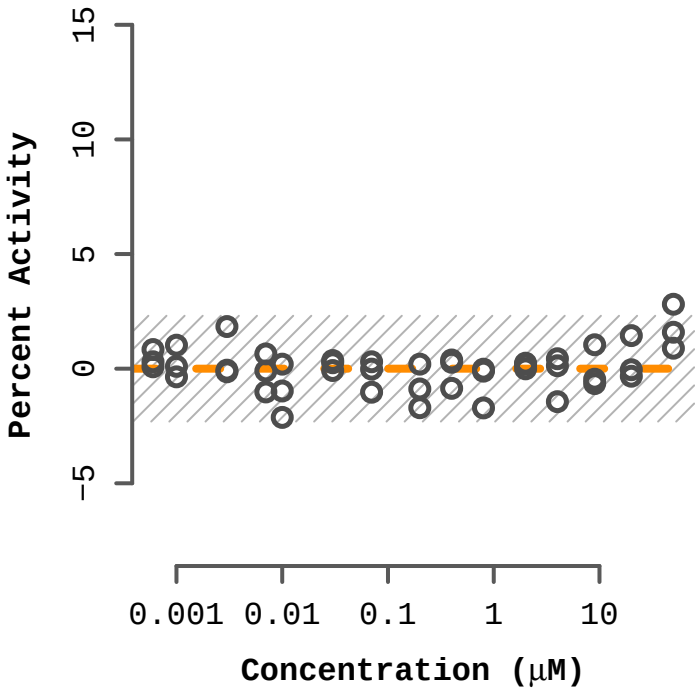
	tp	ga	gw
val:	311	-0.783	1.78
sd:	3.78	0.0171	0.101

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	311	-0.783	1.78	1.76	17.7
sd:	3.78	0.0171	0.101	238	9110

	CNST	HILL	GNLS
AIC:	608.33	365.12	369.12
PROB:	0	0.88	0.12
RMSE:	196.44	15.3	15.3

MAX_MEAN: 322 MAX_MED: 320 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

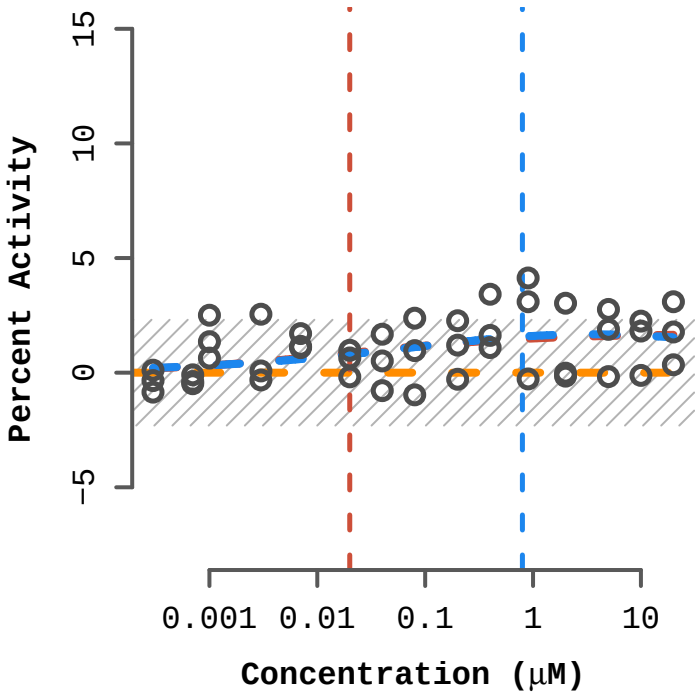
NAME: Landiolol hydrochloride
CHID: 48605 **CASRN:** 144481-98-1
SPID(S): Tox21_113021_1
M4ID: 12482839

HILL MODEL: Not applicable.

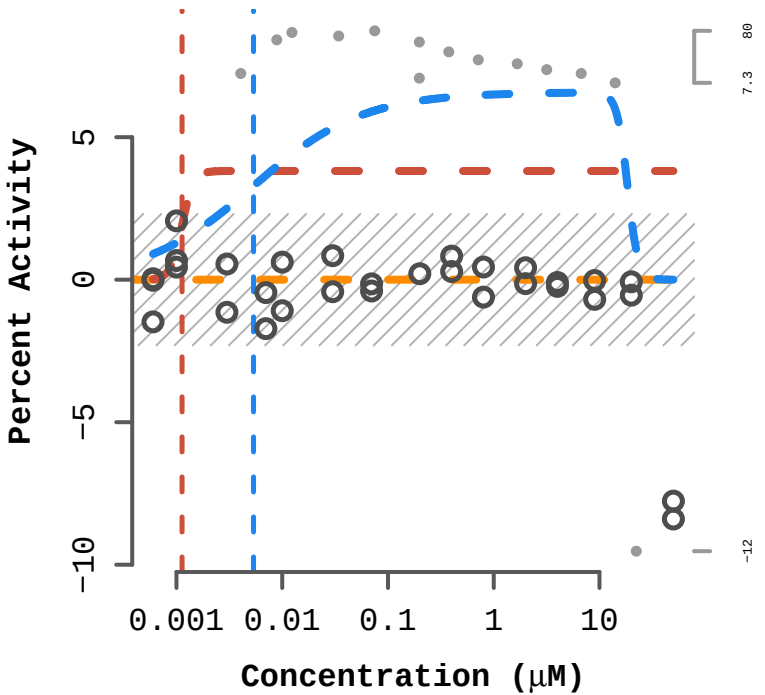
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.76 **MAX_MED:** 1.59 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Lobenzarit sodium
CHID:    48606   CASRN: 64808-48-6
SPID(S): Tox21_112941
M4ID:    12482869

HILL MODEL (in red):
      tp       ga       gw
val:  1.7      -1.7     0.499
sd:   0.562    0.991    0.358

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.95     -0.0985  0.39     0.704    0.3
sd:   26.1     8.12     0.538    10.2     1.23

      CNST        HILL        GNLS
AIC:  177.63      157.69      161.7
PROB: 0           0.88        0.12
RMSE: 1.67        1.21        1.21

MAX_MEAN: 2.32      MAX_MED: 3.1       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Luliconazole
CHID: 48607 CASRN: 187164-19-8
SPID(S): Tox21_112974_1
M4ID: 12482860 BRK

HILL MODEL (in red):

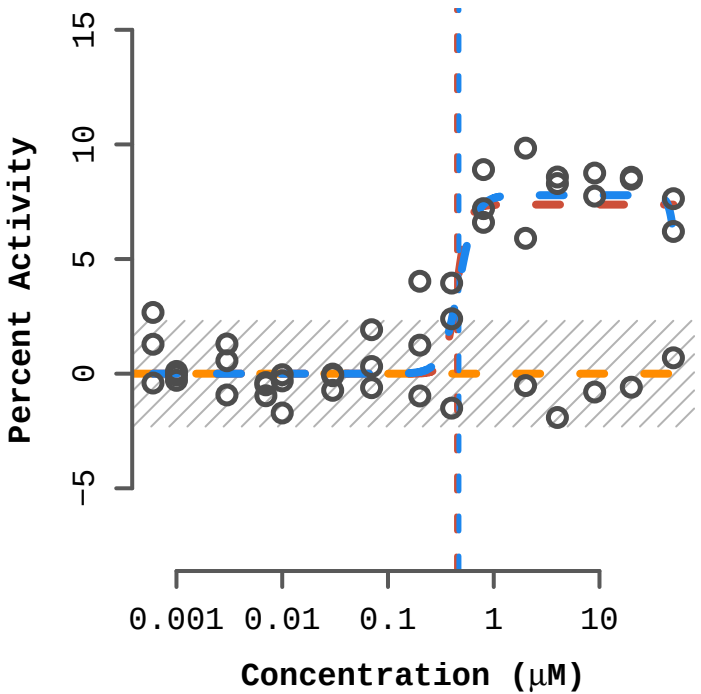
	tp	ga	gw
val:	3.81	−2.95	8
sd:	2.46	0.704	80.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.58	−2.27	0.84	1.26	8.67
sd:	4.21	1.69	1.75	1	210

	CNST	HILL	GNLS
AIC:	405.83	408.24	409.85
PROB:	0.7	0.21	0.09
RMSE:	27.26	25.77	25.12

MAX_MEAN: 26.4 MAX_MED: 13.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lysozyme hydrochloride
CHID: 48608 CASRN: 9066-59-5
SPID(S): Tox21_112943
M4ID: 12482868

HILL MODEL (in red):

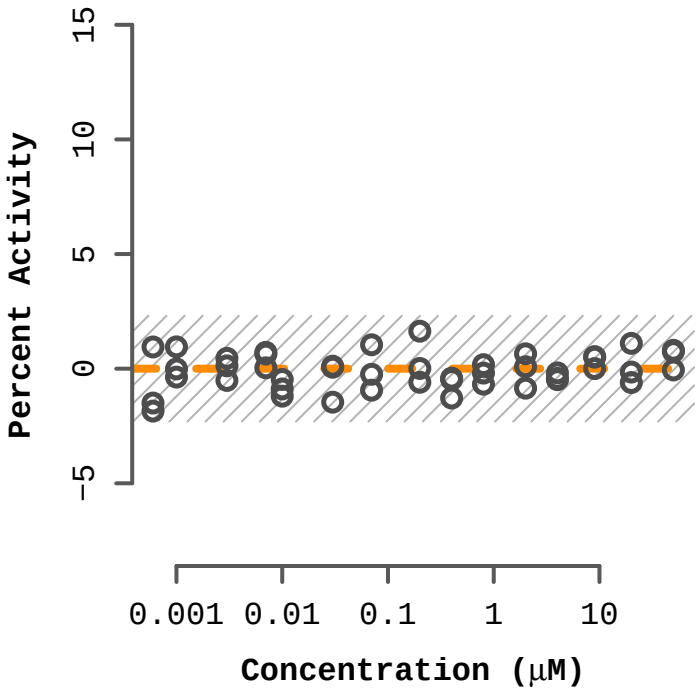
	tp	ga	gw
val:	7.37	−0.352	8
sd:	0.547	0.0902	15.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.79	−0.329	5.39	1.74	12.9
sd:	0.62	0.0646	4.54	0.0784	23.2

	CNST	HILL	GNLS
AIC:	262.58	216.67	219
PROB:	0	0.76	0.24
RMSE:	4.46	2.98	3.01

MAX_MEAN: 7.57 **MAX_MED:** 8.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

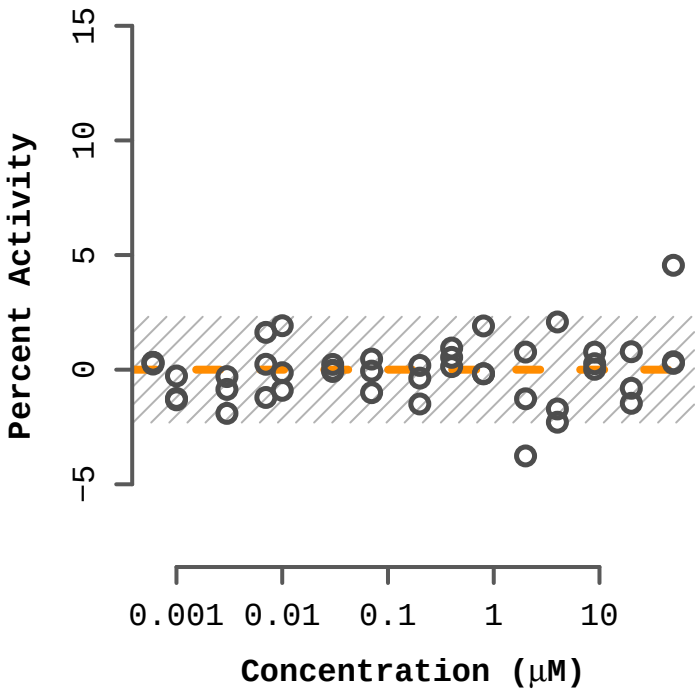
NAME: Dipotassium glycerophosphate
CHID: 48616 **CASRN:** 927-19-5
SPID(S): Tox21_112951
M4ID: 12482867

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.498 **MAX_MED:** 0.744 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

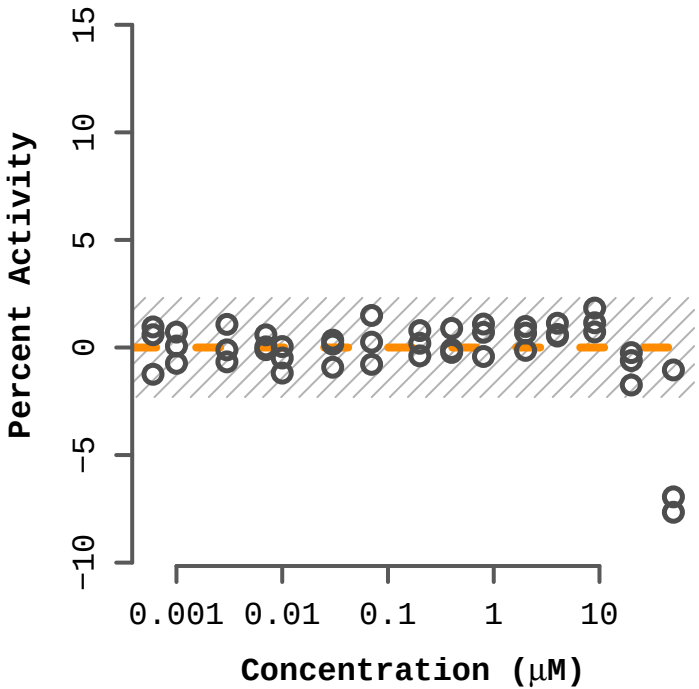
NAME: Sulbenicillin disodium
CHID: 48618 **CASRN:** 28002-18-8
SPID(S): Tox21_112956
M4ID: 12482865

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 0.539 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

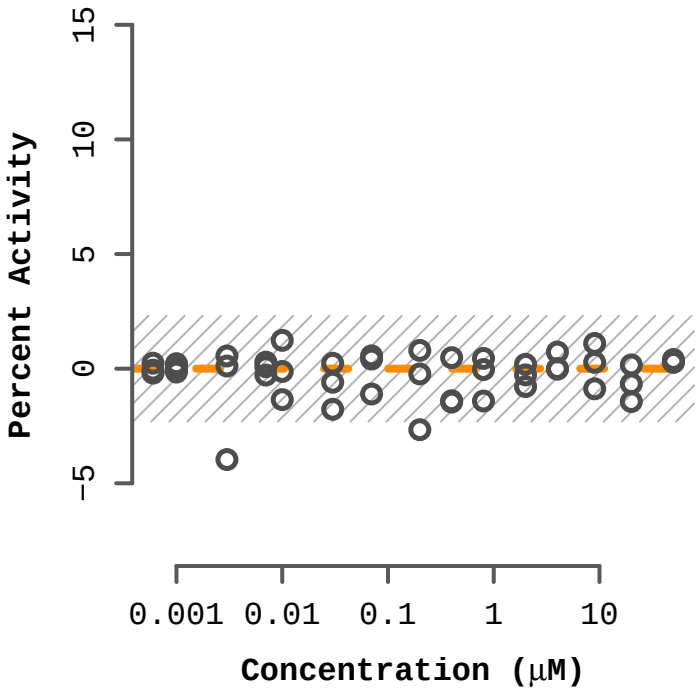
NAME: Temoporfin
CHID: 48619 **CASRN:** 122341-38-2
SPID(S): Tox21_113297
M4ID: 12482728

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

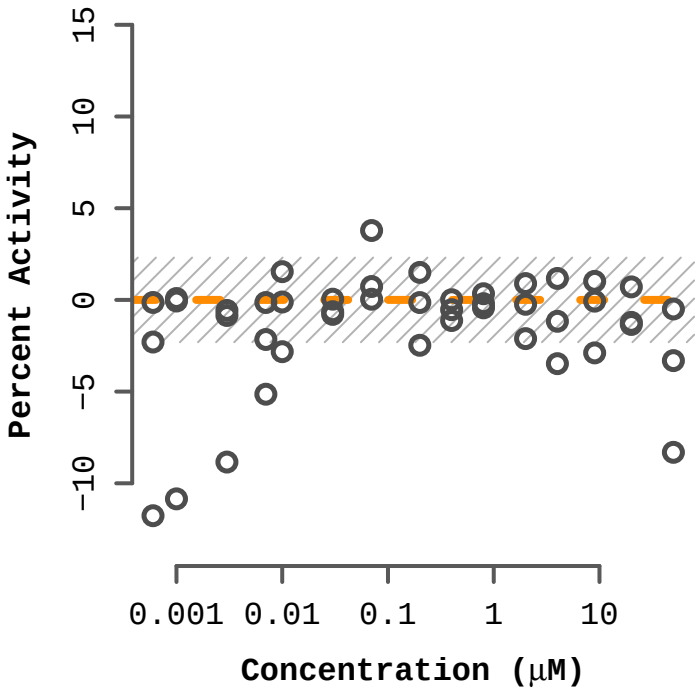
NAME: Teprenone
CHID: 48620 CASRN: 6809-52-5
SPID(S): Tox21_112960
M4ID: 12482864

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.48	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.324 **MAX_MED:** 0.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

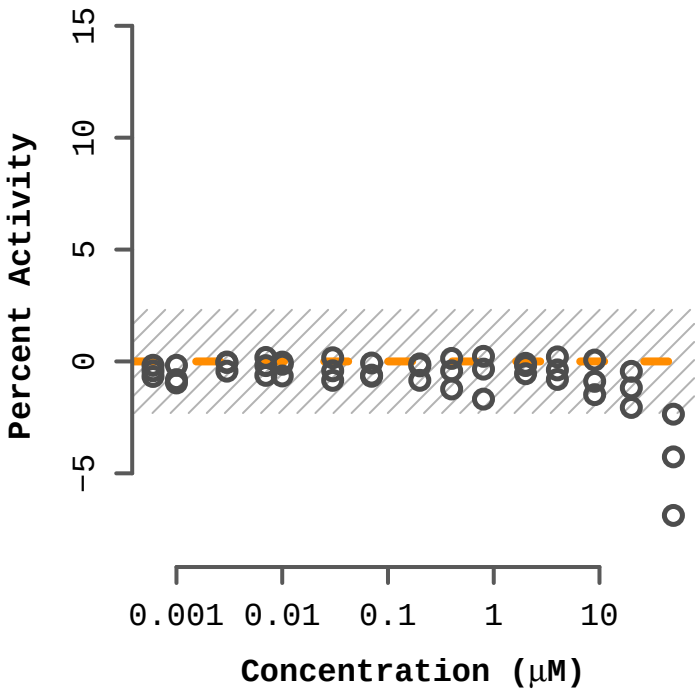
NAME: Tocophersolan
CHID: 48623 **CASRN:** 9002-96-4
SPID(S): Tox21_112964
M4ID: 12482862

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	219.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.41	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 0.732 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

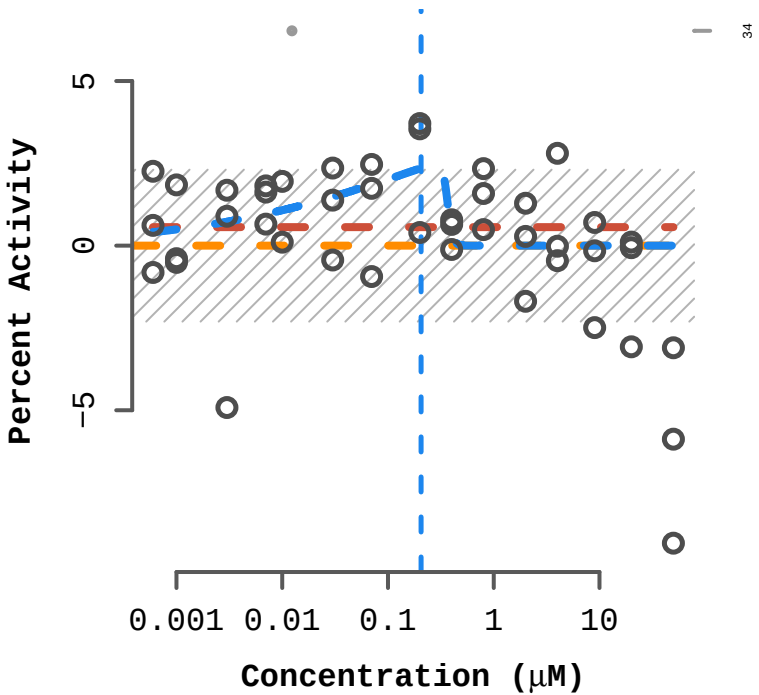
NAME: Ritonavir
CHID: 48627 **CASRN:** 155213-67-5
SPID(S): Tox21_112969_1
M4ID: 12482861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: −0.166 **MAX_MED:** −0.0431 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: l-Oxyfedrine hydrochloride
CHID: 48632 CASRN: 16777-42-7
SPID(S): Tox21_112976_1
M4ID: 12482858 BRK

HILL MODEL (in red):

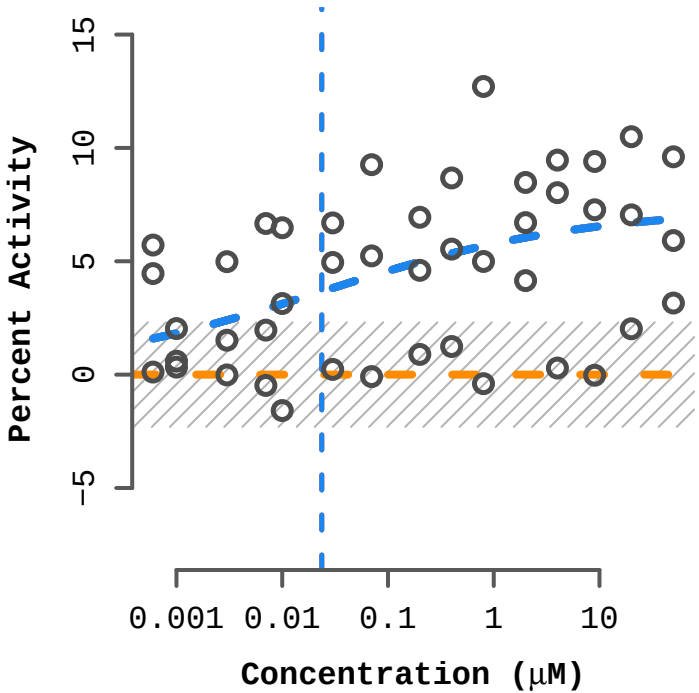
	tp	ga	gw
val:	0.562	−4.95	3.04
sd:	0.292	2150	5600

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.71	−0.687	0.403	−0.437	17.9
sd:	12.2	4.94	0.409	0.643	294

	CNST	HILL	GNLS
AIC:	223.27	225.9	222.57
PROB:	0.37	0.1	0.53
RMSE:	5.56	5.5	5.36

MAX_MEAN: 11.9 MAX_MED: 3.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tirofiban hydrochloride monohydrate
CHID: 48635 CASRN: 150915-40-5
SPID(S): Tox21_112980_1
M4ID: 12482857

HILL MODEL (in red):

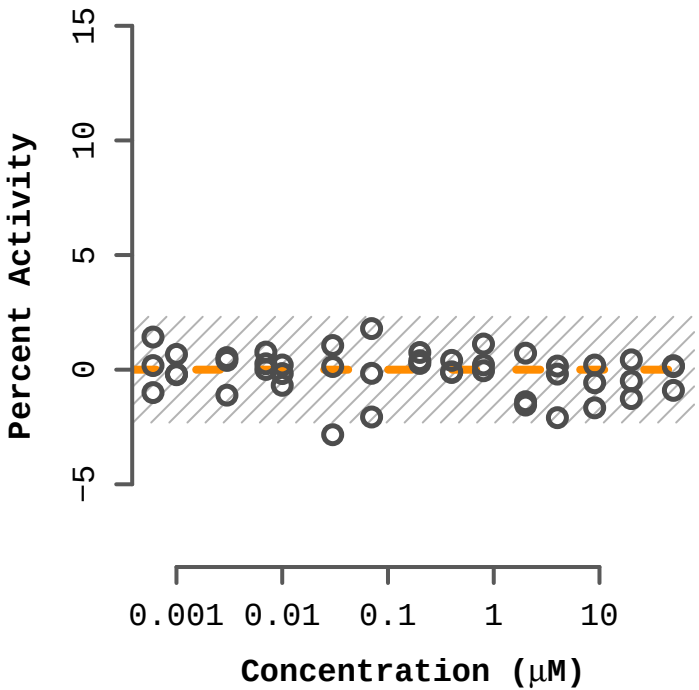
	tp	ga	gw
val:	7.33	−1.63	0.349
sd:	2.35	1.11	0.259

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.33	−1.63	0.349	3.67	5.86
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	291.17	246.79	250.79
PROB:	0	0.88	0.12
RMSE:	5.71	3.25	3.25

MAX_MEAN: 6.52 **MAX_MED:** 8.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

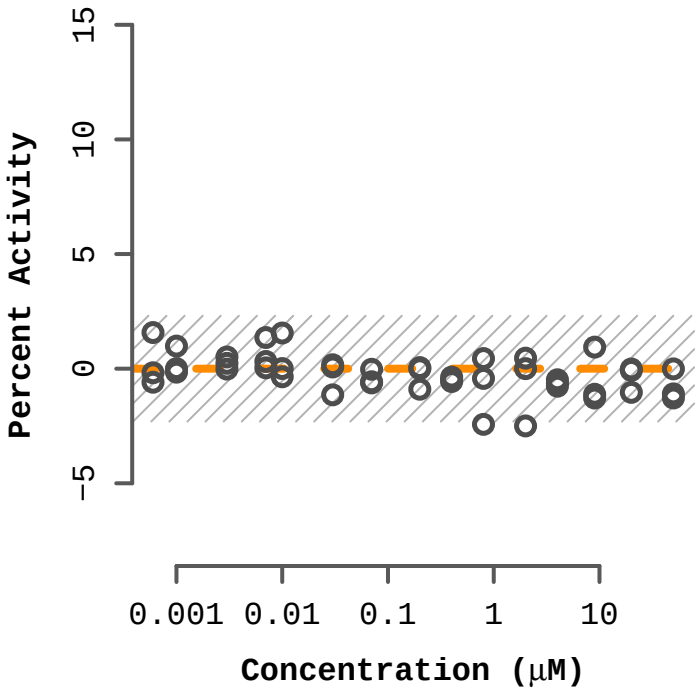
NAME: Gefarnate
CHID: 48636 **CASRN:** 51-77-4
SPID(S): Tox21_112983_1
M4ID: 12482855

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.473 **MAX_MED:** 0.405 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

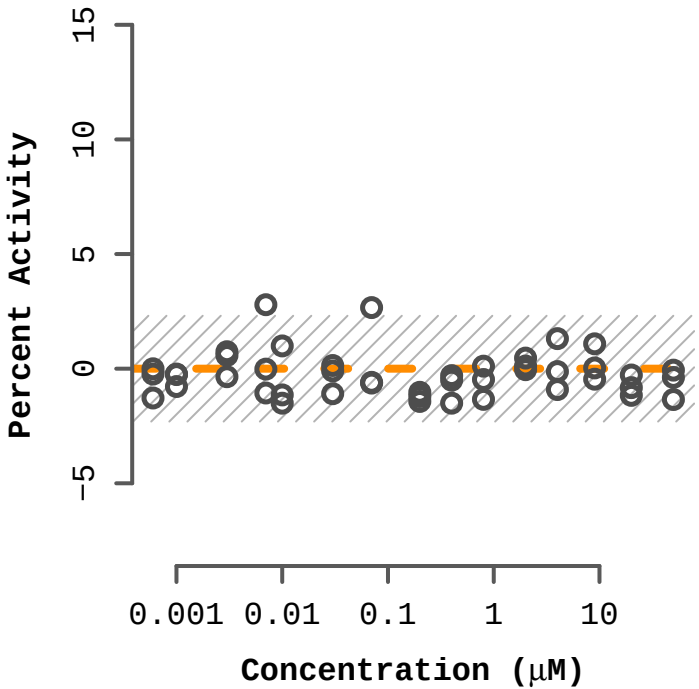
NAME: Nizofenone
CHID: 48637 **CASRN:** 54533-86-7
SPID(S): Tox21_112984_1
M4ID: 12482854

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.571 **MAX_MED:** 0.316 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

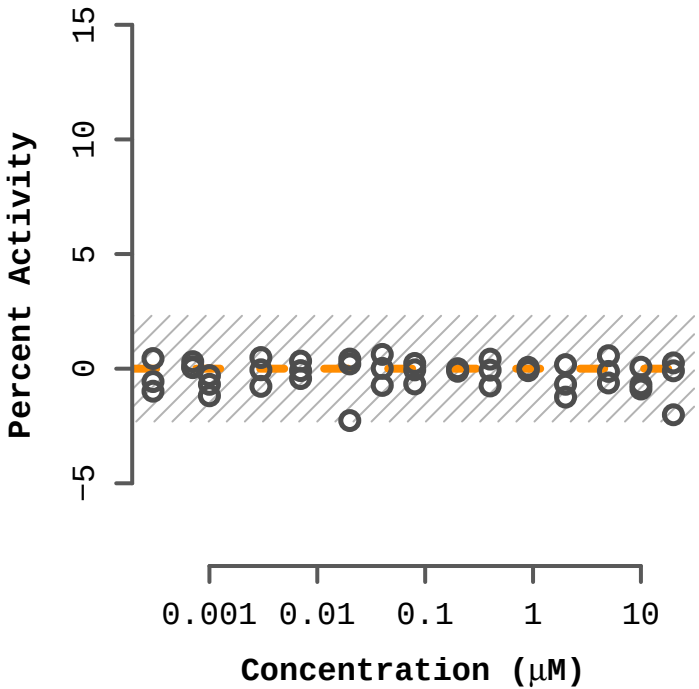
NAME: Nepafenac
CHID: 48638 **CASRN:** 78281-72-8
SPID(S): Tox21_112985_1
M4ID: 12482853

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.572 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

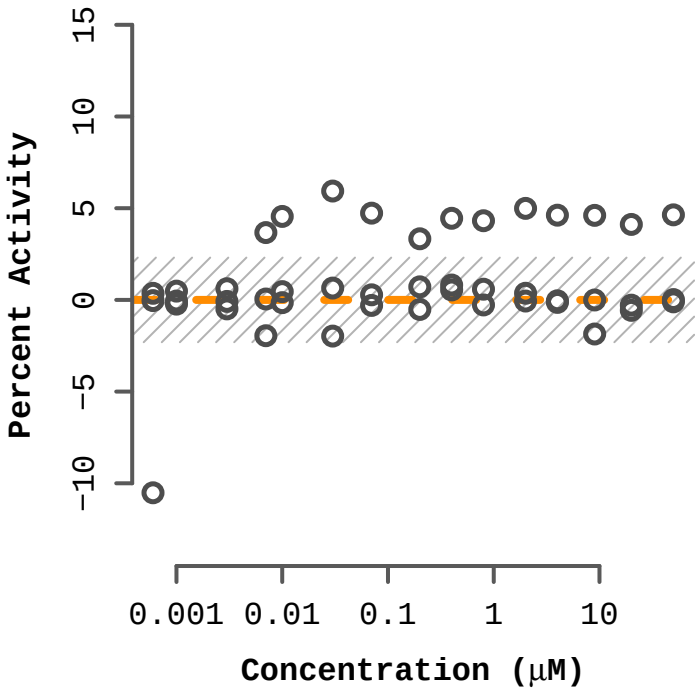
NAME: Garenoxacin mesylate hydrate
CHID: 48644 **CASRN:** 223652-90-2
SPID(S): Tox21_112995_1
M4ID: 12482852

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.148 **MAX_MED:** 0.209 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

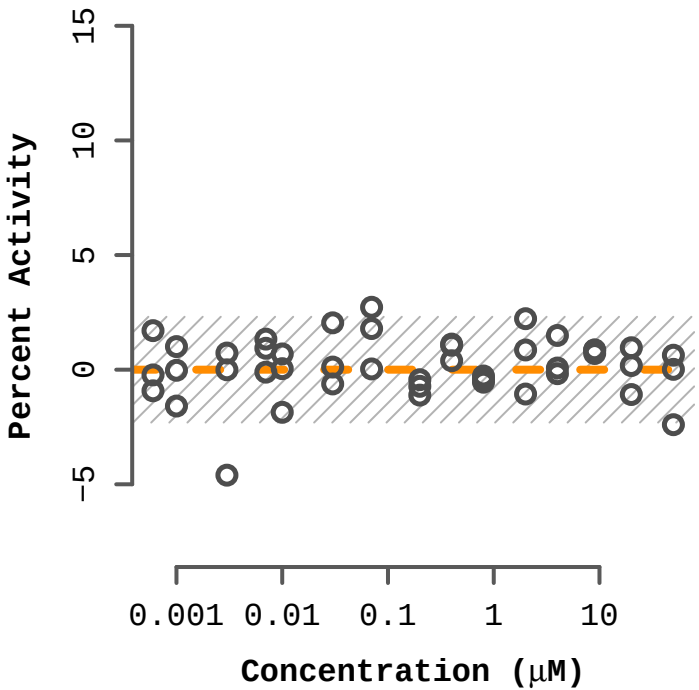
NAME: Gadodiamide hydrate
CHID: 48647 **CASRN:** 122795-43-1
SPID(S): Tox21_113000_1
M4ID: 12482851

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	216.24	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 1.94 **MAX_MED:** 0.813 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

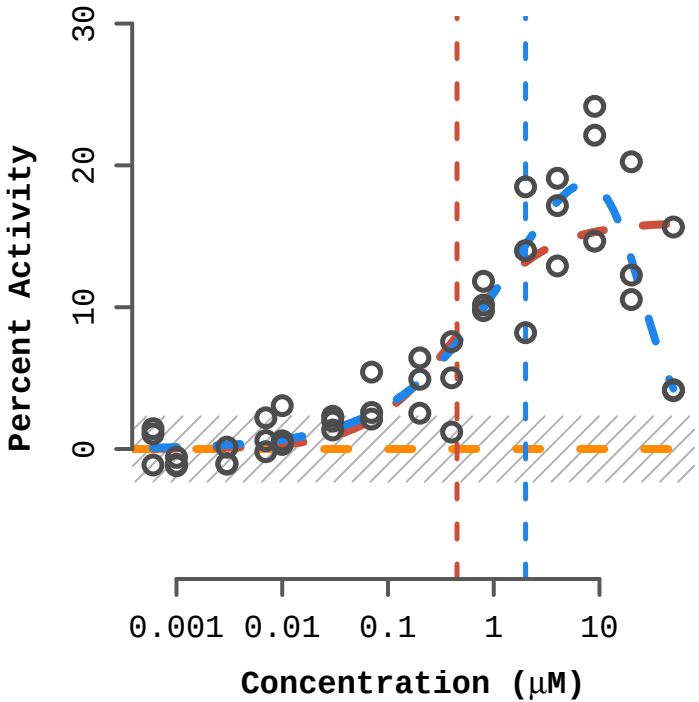
NAME: Aranidipine
CHID: 48649 **CASRN:** 86780-90-7
SPID(S): Tox21_113003_1
M4ID: 12482850

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Febuxostat
CHID: 48650 CASRN: 144060-53-7
SPID(S): Tox21_113004_1
M4ID: 12482849

HILL MODEL (in red):

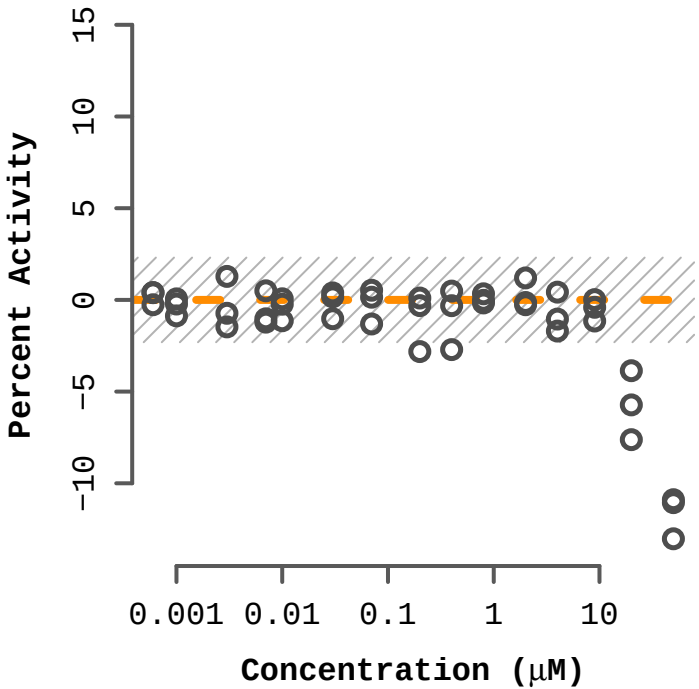
	tp	ga	gw
val:	16	-0.347	1.03
sd:	1.48	0.127	0.265

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	29	0.301	0.708	1.35	2.02
sd:	9.67	0.411	0.141	0.104	0.482

	CNST	HILL	GNLS
AIC:	333.02	245.05	227.93
PROB:	0	0	1
RMSE:	9.71	3.76	3

MAX_MEAN: 20.3 MAX_MED: 22.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

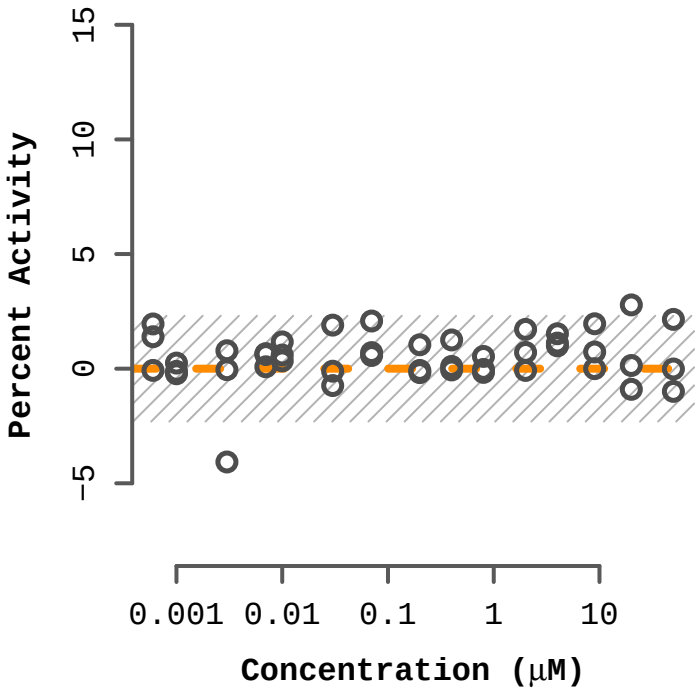
NAME: Dronedarone
CHID: 48653 **CASRN:** 141626-36-0
SPID(S): Tox21_113008_1
M4ID: 12482847

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	206.86	NA	NA
PROB:	1	NA	NA
RMSE:	3.5	NA	NA

MAX_MEAN: 0.266 **MAX_MED:** 0.396 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

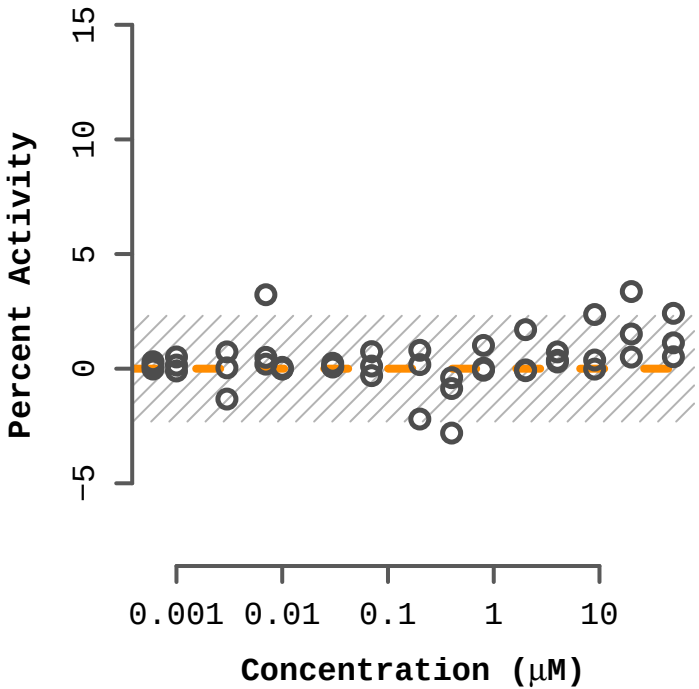
NAME: Flutropium bromide
CHID: 48655 CASRN: 63516-07-4
SPID(S): Tox21_113011_1
M4ID: 12482845

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.21 MAX_MED: 1.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

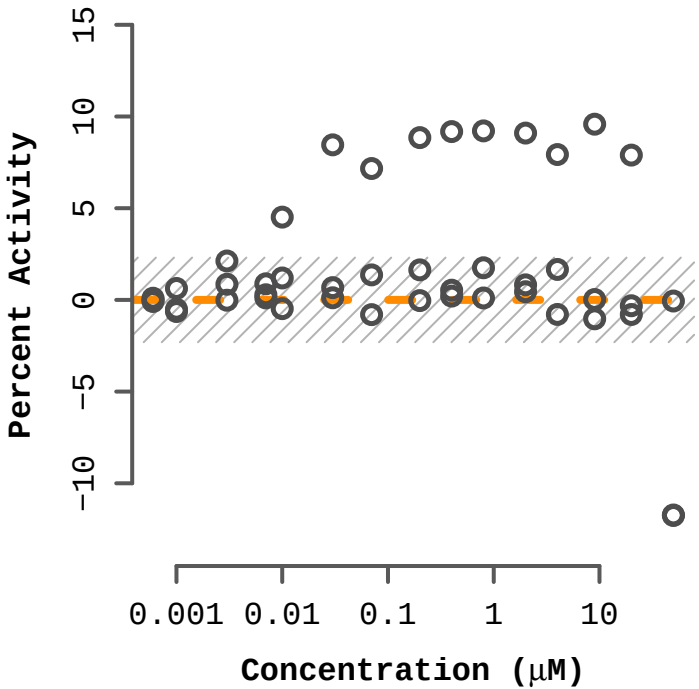
NAME: Vicriviroc maleate
CHID: 48656 **CASRN:** 599179-03-0
SPID(S): Tox21_113012_1
M4ID: 12482844

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

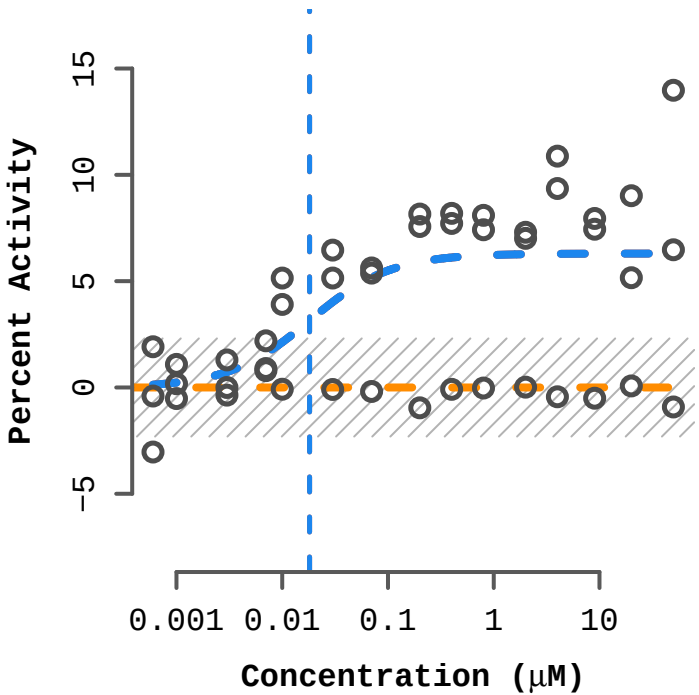
NAME: Bazedoxifene acetate
CHID: 48657 **CASRN:** 198481-33-3
SPID(S): Tox21_113013_1
M4ID: 12482843

HILL MODEL: Not applicable.

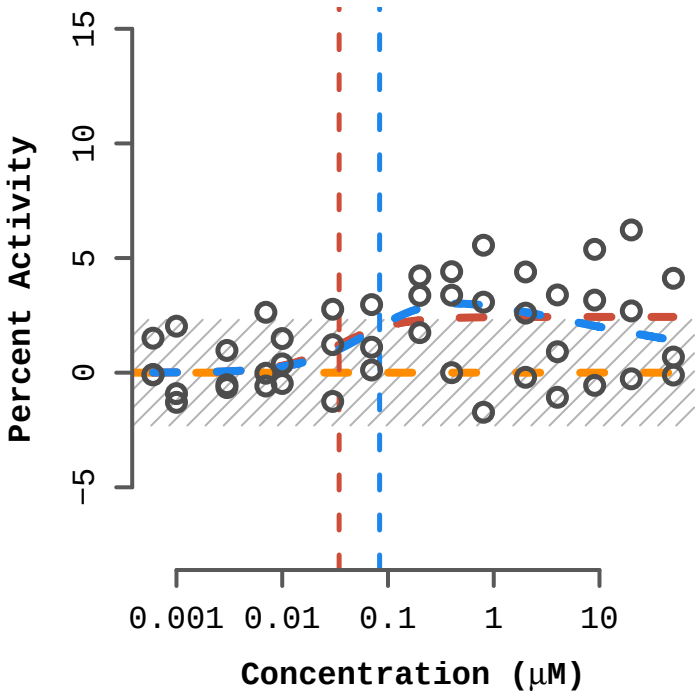
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	260.39	NA	NA
PROB:	1	NA	NA
RMSE:	4.69	NA	NA

MAX_MEAN: 3.69 **MAX_MED:** 1.75 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Lorcaserin
CHID:    48659   CASRN: 616202-92-7
SPID(S): Tox21_113018_1
M4ID:    12482842

HILL MODEL (in red):
      tp       ga       gw
val:  6.3      -1.74    1.13
sd:   0.931    0.34     0.677

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.3      -1.74    1.13     3.04     5.31
sd:   0.931    0.34     0.676    2590     10600

      CNST        HILL        GNLS
AIC:  284.76      249.48      253.48
PROB: 0           0.88        0.12
RMSE: 5.45        3.52        3.52

MAX_MEAN: 6.6       MAX_MED: 9.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Raltegravir
CHID: 48660 CASRN: 518048-05-0
SPID(S): Tox21_113019_1
M4ID: 12482841

HILL MODEL (in red):

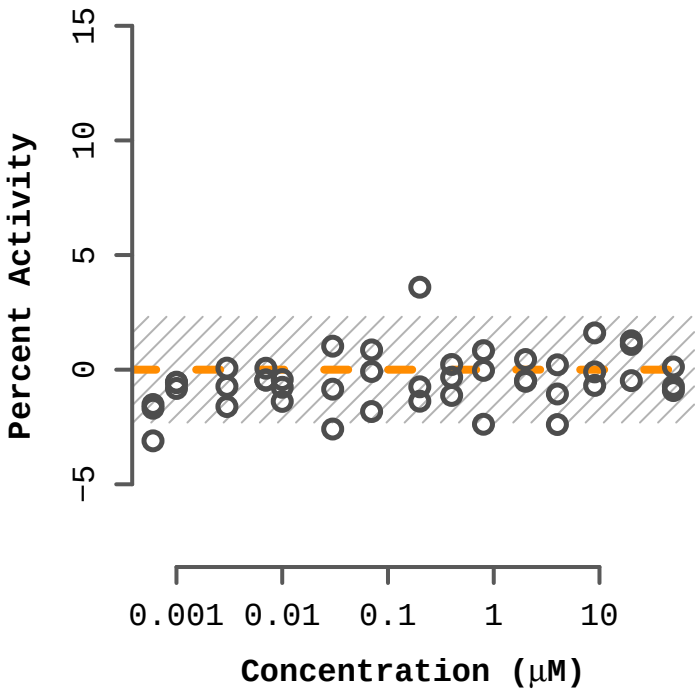
	tp	ga	gw
val:	2.43	−1.46	1.58
sd:	0.487	0.428	1.31

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.86	−1.08	1.33	0.0527	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	214.89	195.45	197.89
PROB:	0	0.77	0.23
RMSE:	2.54	1.85	1.86

MAX_MEAN: 3.11 **MAX_MED:** 3.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

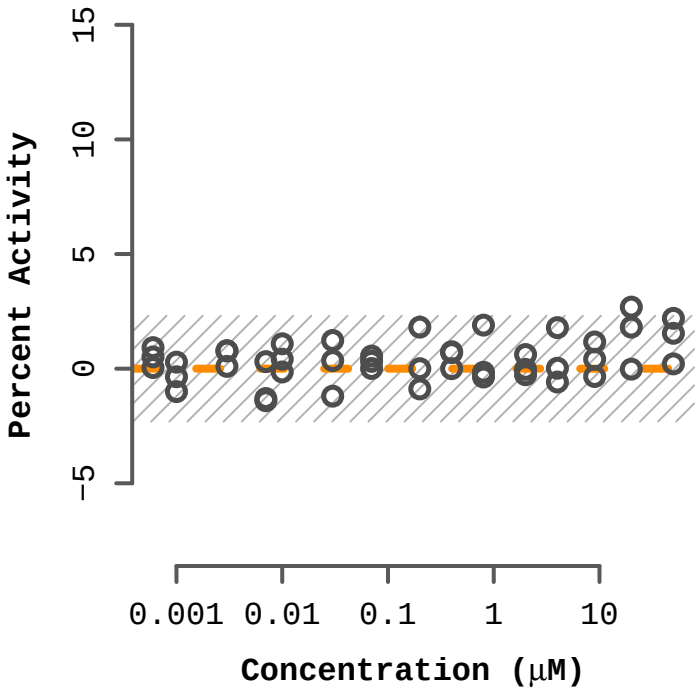
NAME: Detomidine hydrochloride
CHID: 48661 **CASRN:** 90038-01-0
SPID(S): Tox21_113020_1
M4ID: 12482840

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.629 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

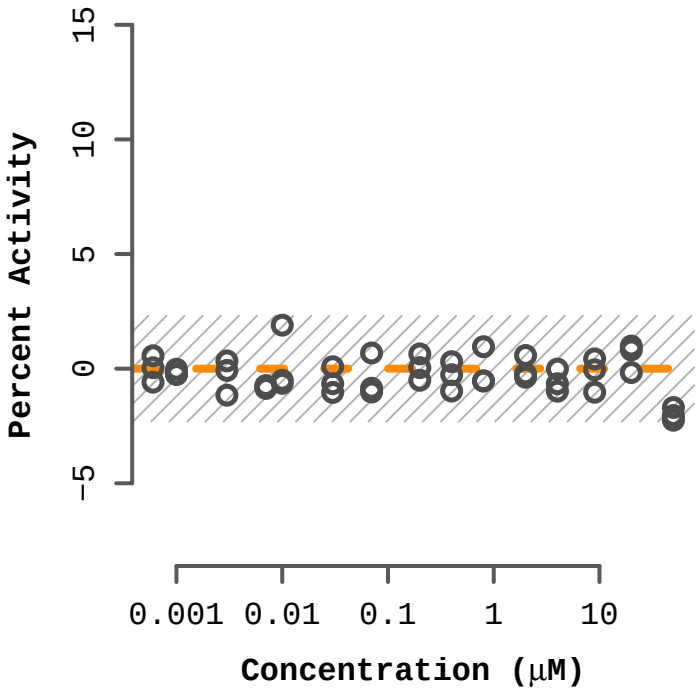
NAME: Gadoteridol
CHID: 48662 CASRN: 120066-54-8
SPID(S): Tox21_113025_1
M4ID: 12482837

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

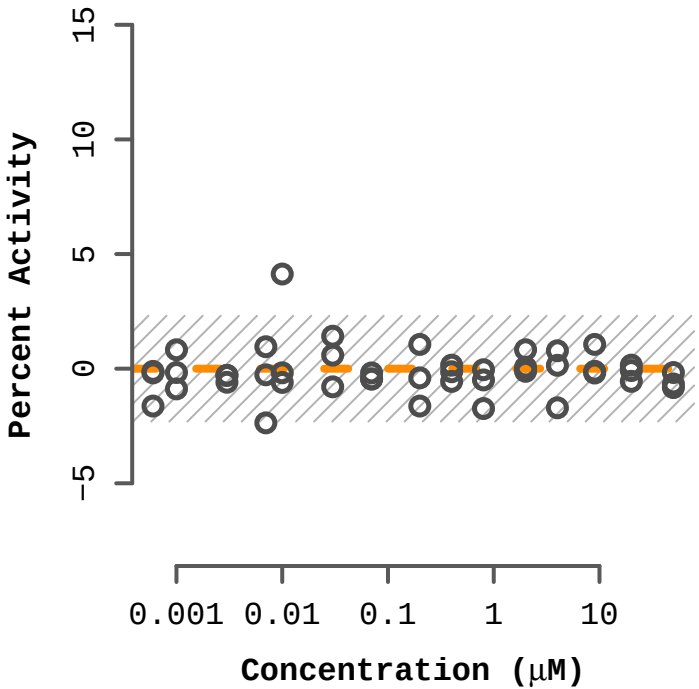
NAME: Dopexamine
CHID: 48666 **CASRN:** 86197-47-9
SPID(S): Tox21_113031_1
M4ID: 12482836

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.547 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

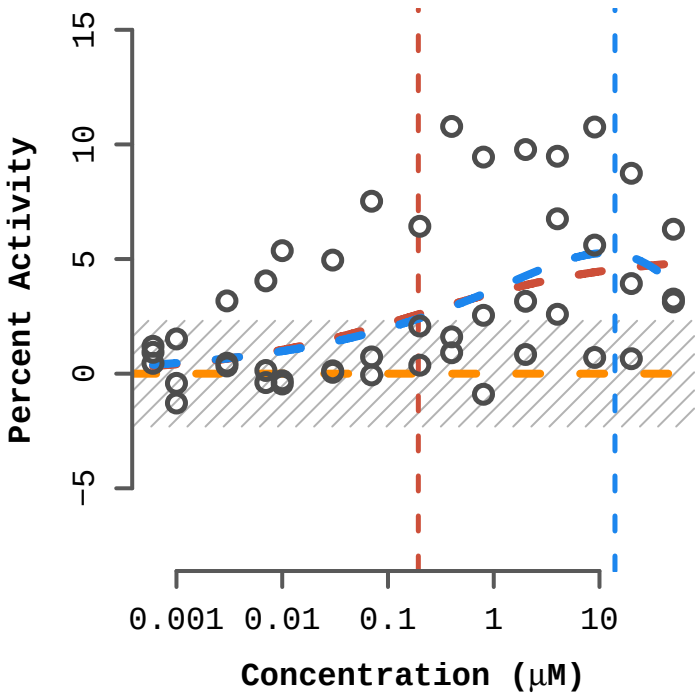
NAME: Dapiprazole hydrochloride
CHID: 48669 **CASRN:** 72822-13-0
SPID(S): Tox21_113035_1
M4ID: 12482835

HILL MODEL: Not applicable.

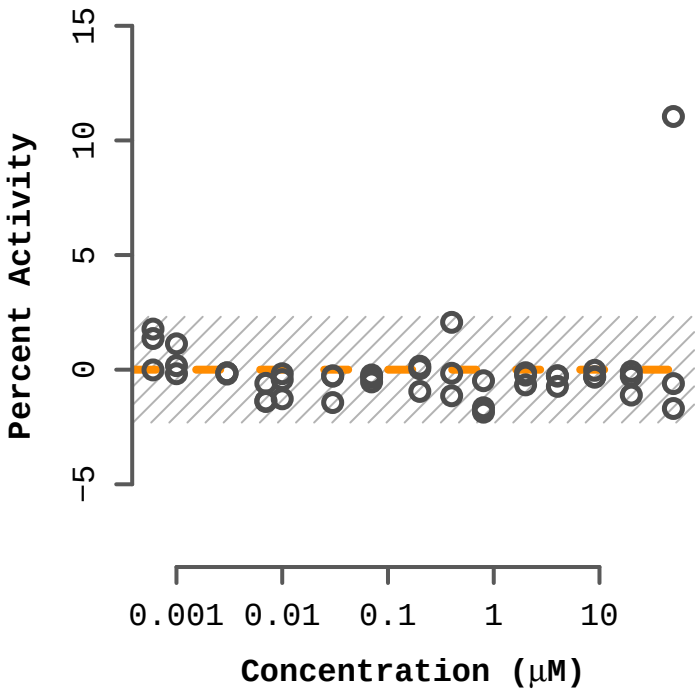
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 0.591 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Chrysarobin
CHID:    48671   CASRN: 491-59-8
SPID(S): Tox21_113041_1
M4ID:    12482834

HILL MODEL (in red):
      tp       ga       gw
val:  5.17     -0.713   0.465
sd:   1.79     0.989    0.325

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.9     1.15     0.345    1.7      1.13
sd:   22.5     3.61     0.219    0.623    1.35

      CNST        HILL        GNLS
AIC:  265.29      237.84      240.9
PROB: 0           0.82        0.18
RMSE: 4.61        3.06        3.02

MAX_MEAN: 6.28      MAX_MED: 6.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

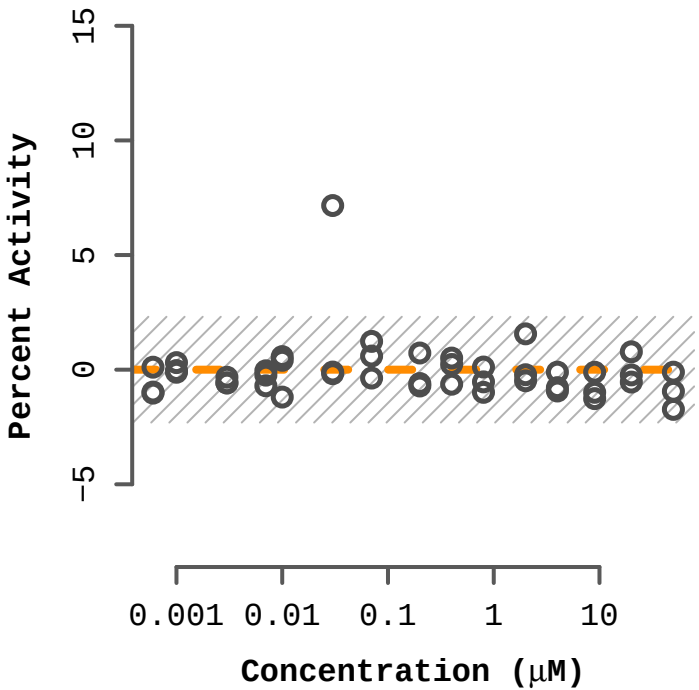
NAME: Thioglycolic acid anilide
CHID: 48672 **CASRN:** 4822-44-0
SPID(S): Tox21_113043_1
M4ID: 12482832

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 2.92 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

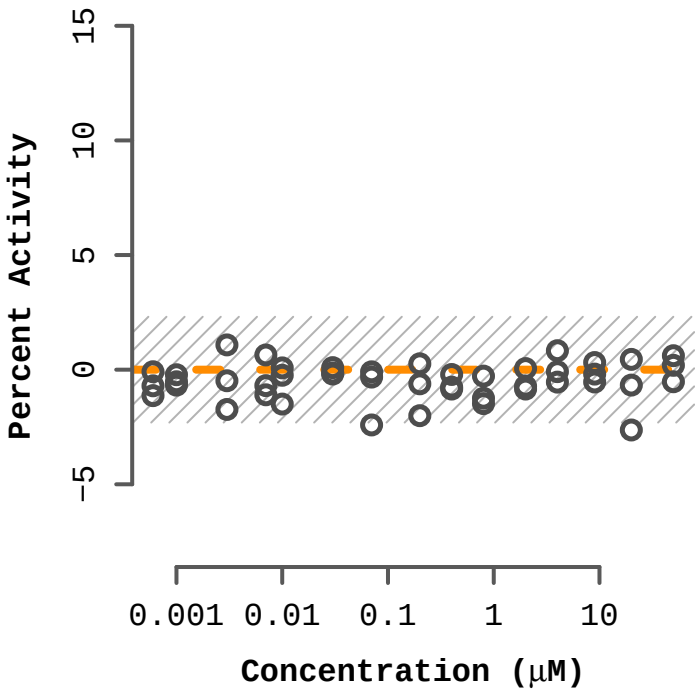
NAME: Propamidine
CHID: 48674 **CASRN:** 104-32-5
SPID(S): Tox21_113051
M4ID: 12482826

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 2.29 **MAX_MED:** 0.596 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

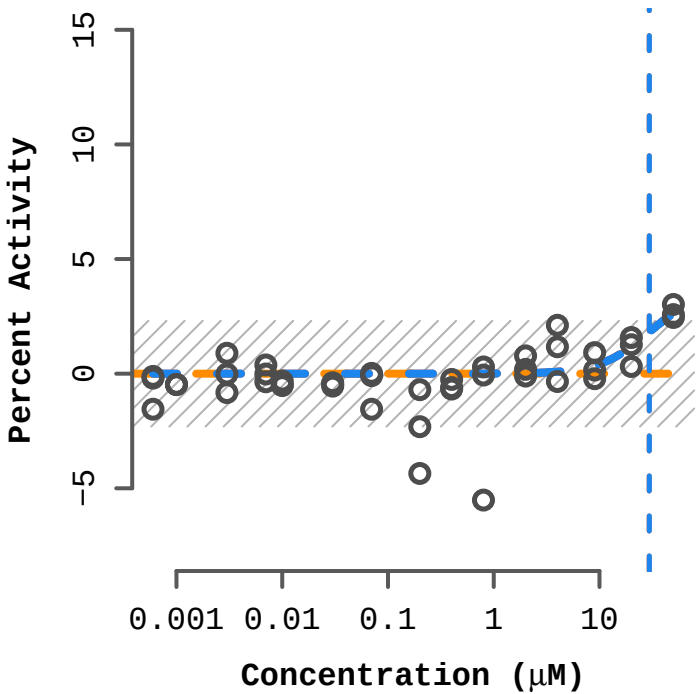
NAME: Binospirone mesylate
CHID: 48676 **CASRN:** 124756-23-6
SPID(S): Tox21_113054_1
M4ID: 12482825

HILL MODEL: Not applicable.

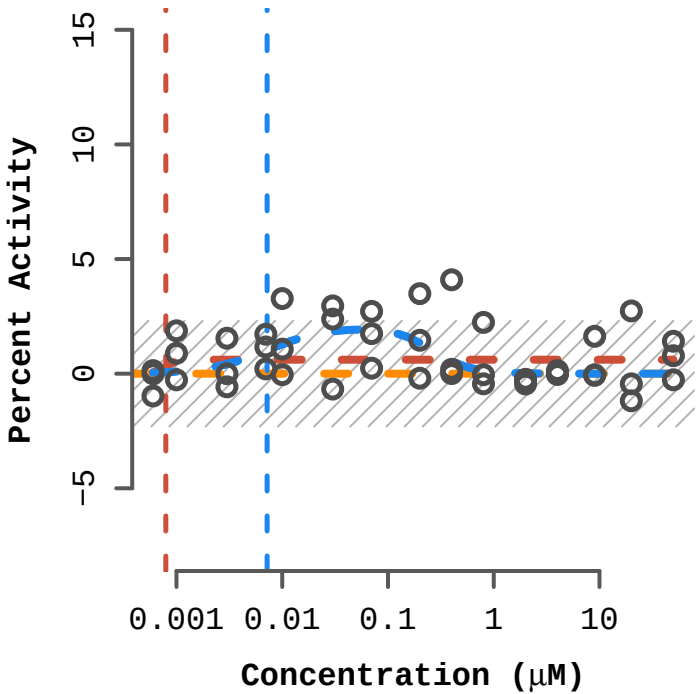
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

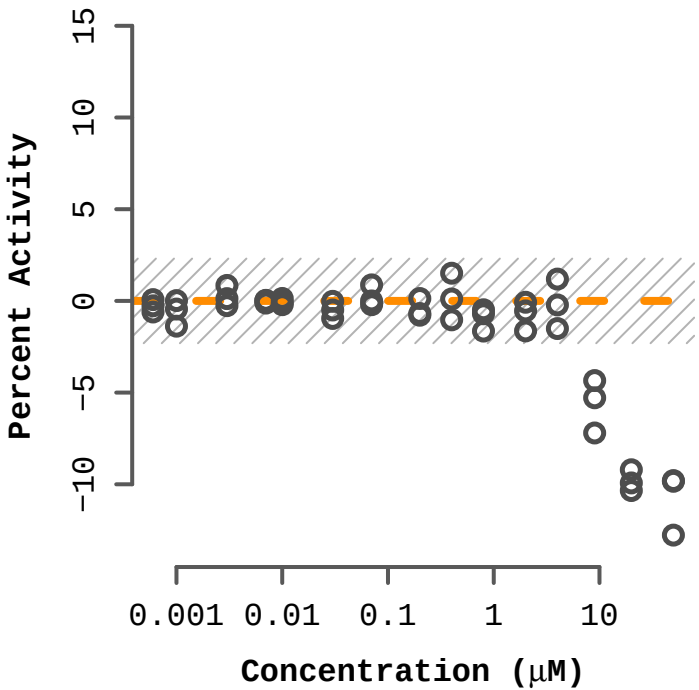
MAX_MEAN: 0.0921 **MAX_MED:** 0.191 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Spiradoline
CHID:    48679   CASRN: 87151-85-7
SPID(S): Tox21_113060_1
M4ID:    12482824

HILL MODEL (in red):
      tp       ga       gw
val:  3.62     1.47     1.86
sd:   2.36     0.374    1.55

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.62     1.47     1.87     3.21     4.77
sd:   2.37     0.375    1.58     1100     3470

      CNST        HILL        GNLS
AIC:  151.07      130.04      134.04
PROB: 0           0.88        0.12
RMSE: 1.48        1.27        1.27

MAX_MEAN: 2.68      MAX_MED: 2.58      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3,5-Diiodo-L-tyrosine
CHID:    48680   CASRN: 300-39-0
SPID(S): Tox21_113061_1
M4ID:    12482823

HILL MODEL (in red):
      tp       ga       gw
val:  0.609    -3.1     8
sd:   0.209    0.18     12.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.05     -2.14    1.56     -0.581   2.38
sd:   1.08     0.386    2.35     0.391    3.75

      CNST        HILL        GNLS
AIC:  163.41      160.11      155.02
PROB: 0.01        0.07        0.91
RMSE: 1.5         1.29        1.2

MAX_MEAN: 1.58      MAX_MED: 2.38      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

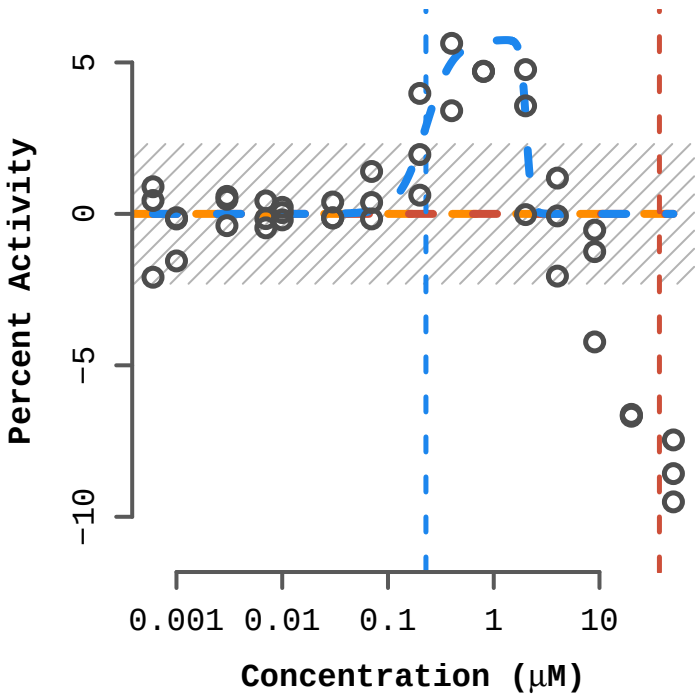
NAME: Cloflucarban
CHID: 48684 **CASRN:** 369-77-7
SPID(S): Tox21_113070_1
M4ID: 12482822

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.98	NA	NA
PROB:	1	NA	NA
RMSE:	4.12	NA	NA

MAX_MEAN: 0.238 **MAX_MED:** 0.127 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: PP242
CHID: 48685 CASRN: 1092351-67-1
SPID(S): Tox21_113072_1
M4ID: 12482820

HILL MODEL (in red):

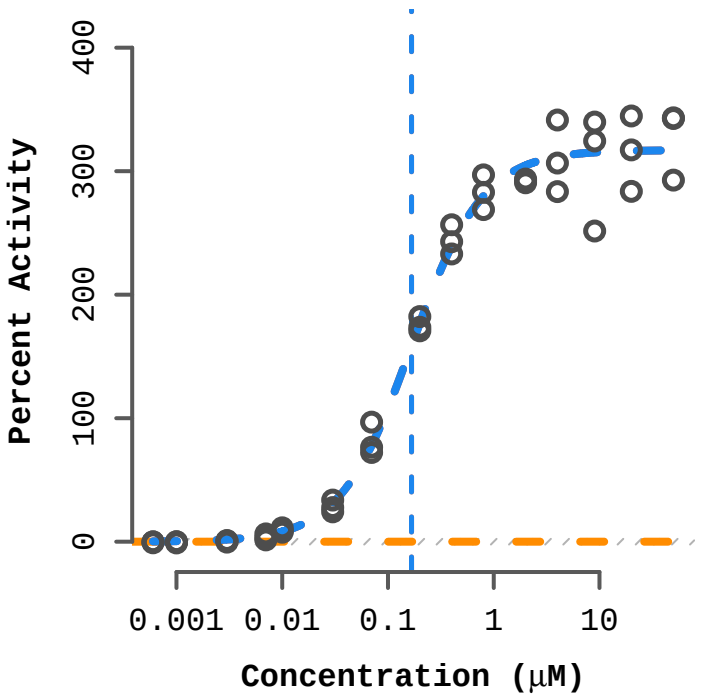
	tp	ga	gw
val:	4.42e-09	1.57	1.68
sd:	5.91e-05	2120	38900

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.76	−0.641	3.39	0.307	16.7
sd:	1.49	0.119	4.53	0.133	372

	CNST	HILL	GNLS
AIC:	246.27	252.27	224.13
PROB:	0	0	1
RMSE:	3.76	3.76	3.05

MAX_MEAN: 5.84 MAX_MED: 5.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone acetate
CHID: 48686 **CASRN:** 50-03-3
SPID(S): Tox21_113074_1
M4ID: 12482818

HILL MODEL (in red):

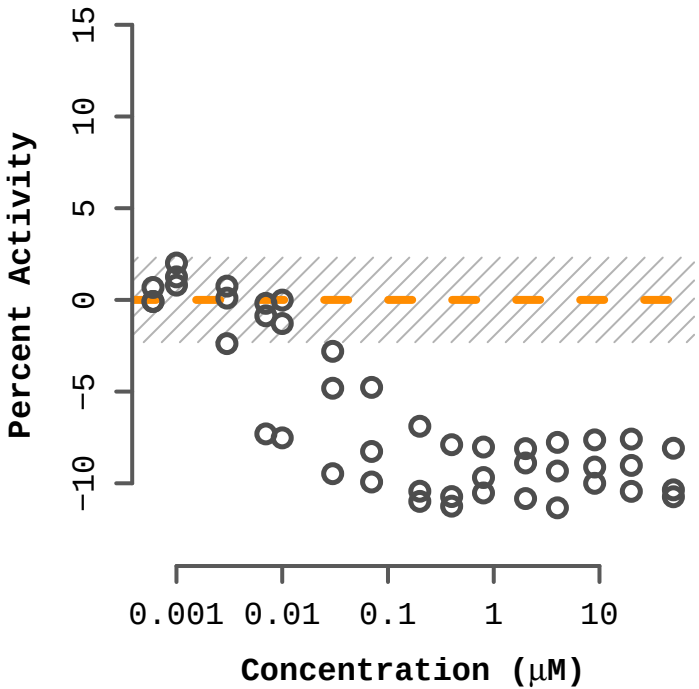
	tp	ga	gw
val:	317	−0.777	1.29
sd:	6.58	0.0261	0.0769

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	317	−0.777	1.29	2.78	8.14
sd:	6.58	0.0261	0.0769	725	5450

	CNST	HILL	GNLS
AIC:	616.23	377.51	381.51
PROB:	0	0.88	0.12
RMSE:	210.17	16.39	16.39

MAX_MEAN: 326 **MAX_MED:** 343 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

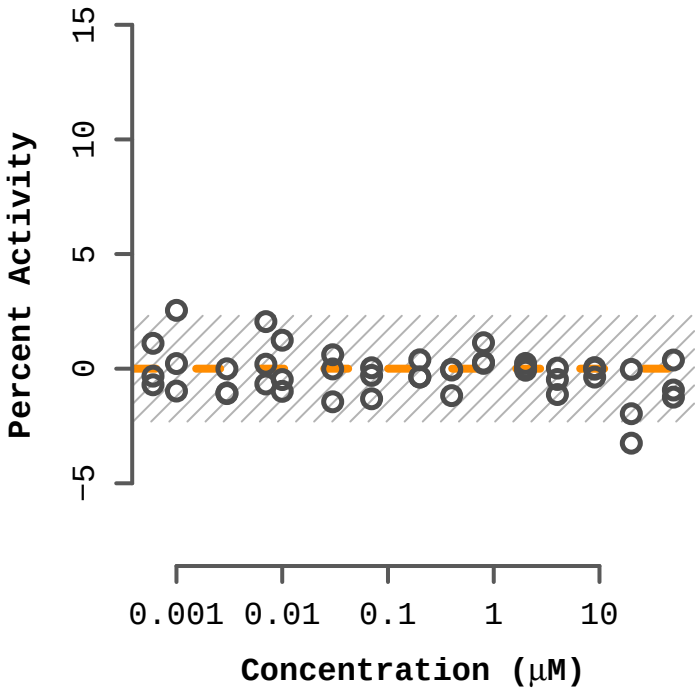
NAME: Carfilzomib
CHID: 48690 CASRN: 868540-17-4
SPID(S): Tox21_113079_1
M4ID: 12482817

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	319.95	NA	NA
PROB:	1	NA	NA
RMSE:	7.6	NA	NA

MAX_MEAN: 1.36 MAX_MED: 1.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

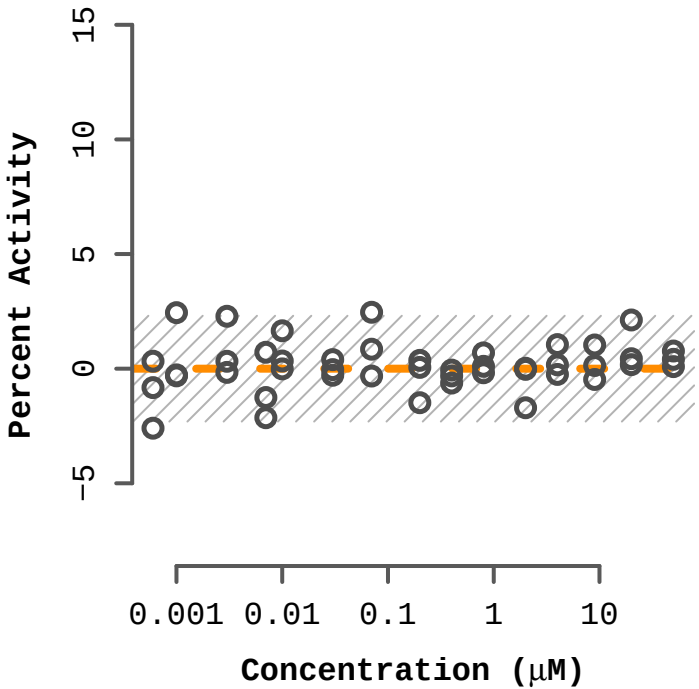
NAME: Atazanavir
CHID: 48691 **CASRN:** 198904-31-3
SPID(S): Tox21_113081_1
M4ID: 12482815

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.96	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.598 **MAX_MED:** 0.288 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

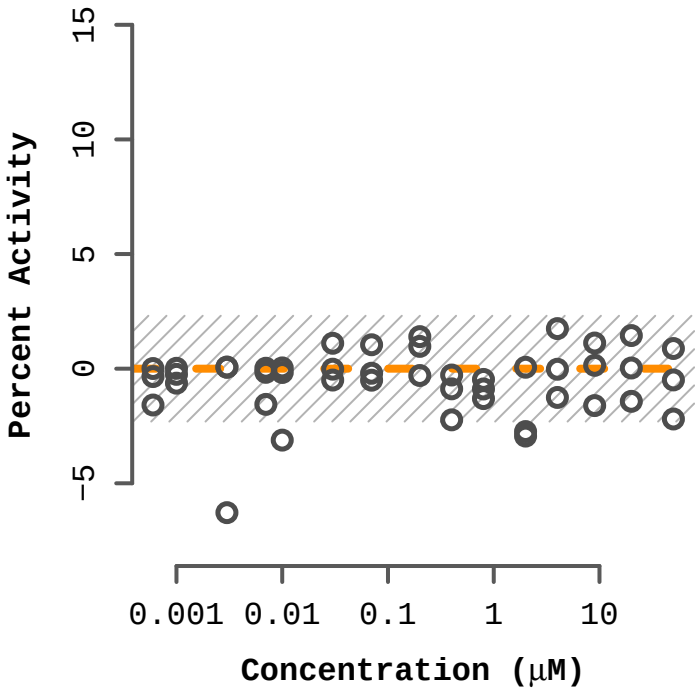
NAME: Pivoxil Sulbactam
CHID: 48692 **CASRN:** 69388-79-0
SPID(S): Tox21_113082_1
M4ID: 12482814

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.998 **MAX_MED:** 0.851 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

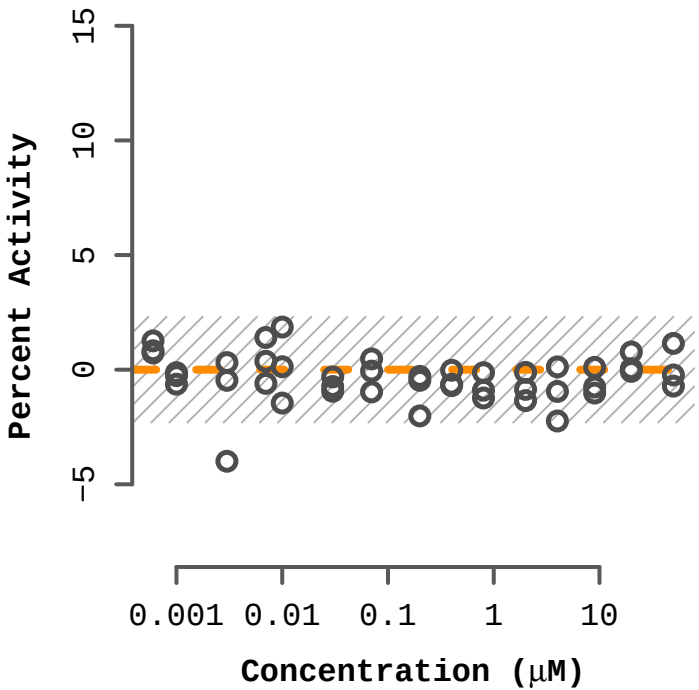
NAME: Nifenalol
CHID: 48693 **CASRN:** 7413-36-7
SPID(S): Tox21_113084_1
M4ID: 12482813

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.692 **MAX_MED:** 0.973 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

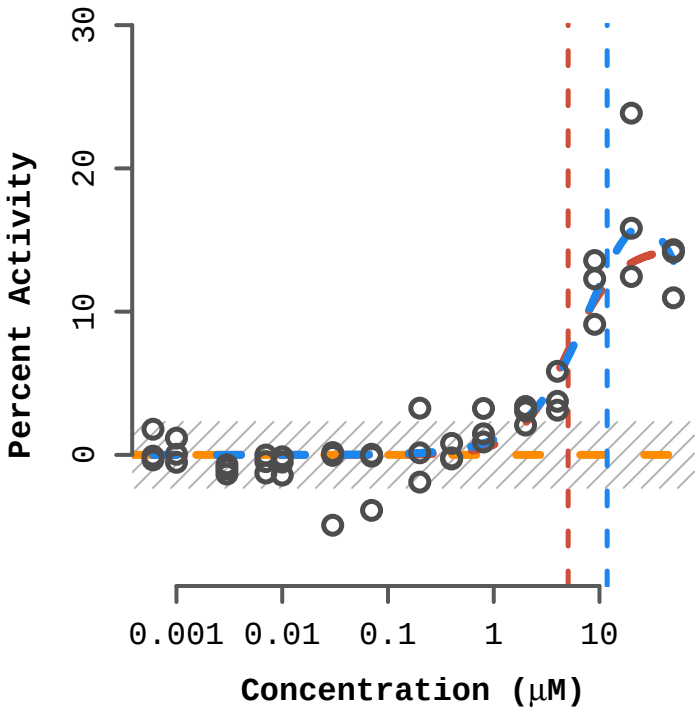
NAME: Fenamol
CHID: 48694 **CASRN:** 5467-78-7
SPID(S): Tox21_113085_1
M4ID: 12482812

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.938 **MAX_MED:** 0.827 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fanetizole
CHID: 48695 CASRN: 79069-94-6
SPID(S): Tox21_113086_1
M4ID: 12482811

HILL MODEL (in red):

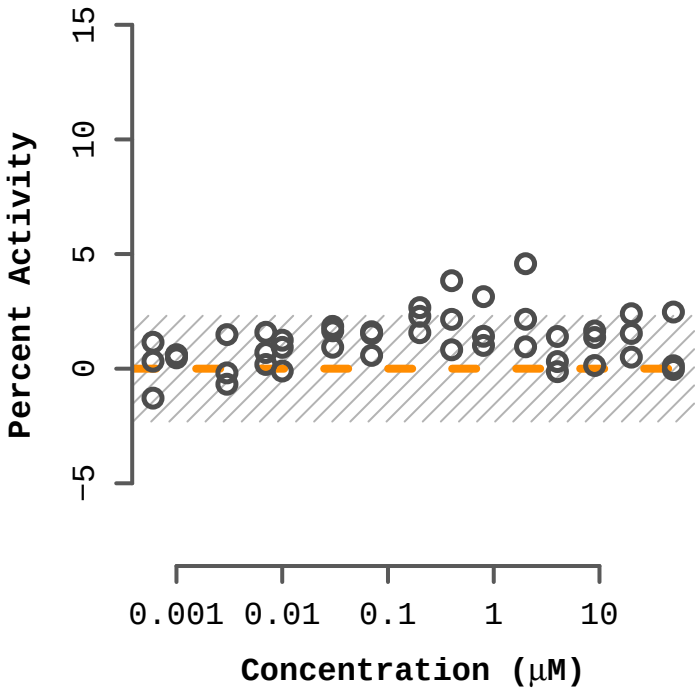
	tp	ga	gw
val:	14.5	0.704	1.83
sd:	0.859	0.0636	0.46

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	28.6	1.07	1.32	1.75	1.45
sd:	28.7	0.468	0.368	0.489	1.56

	CNST	HILL	GNLS
AIC:	288.44	190.36	189.41
PROB:	0	0.38	0.62
RMSE:	6.8	2.25	2

MAX_MEAN: 17.4 MAX_MED: 15.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

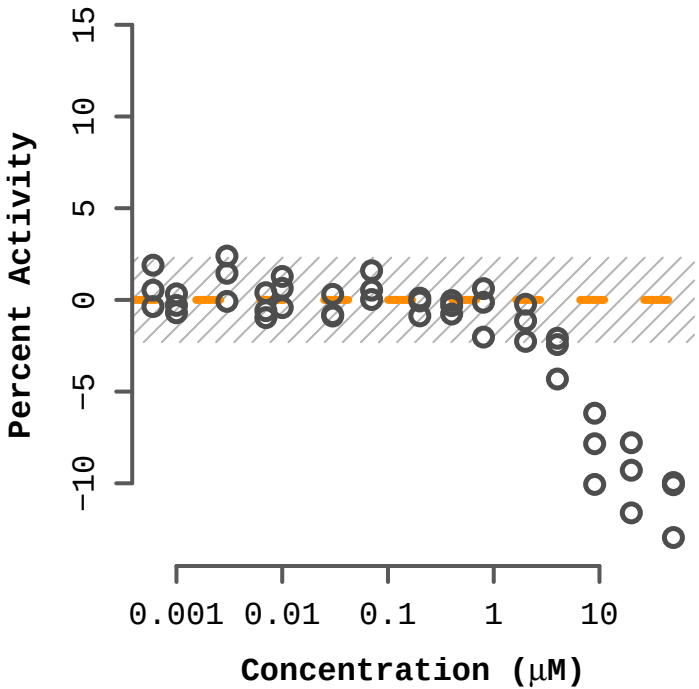
NAME: Sulfaethoxypyridazine
CHID: 48696 **CASRN:** 963-14-4
SPID(S): Tox21_113089
M4ID: 12482809

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 2.56 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

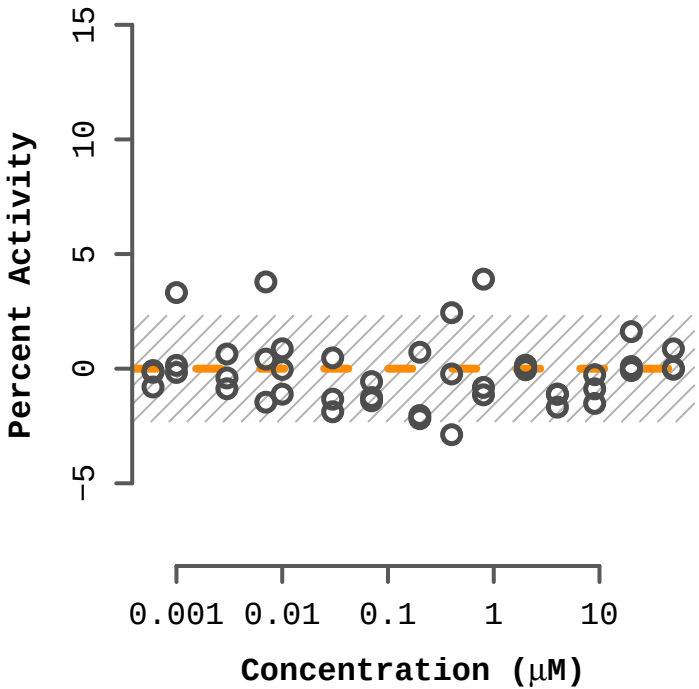
NAME: Benzyldodecyldimethylammonium bromide
CHID: 48698 **CASRN:** 7281-04-1
SPID(S): Tox21_113091_1
M4ID: 12482808

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.73	NA	NA
PROB:	1	NA	NA
RMSE:	4.5	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

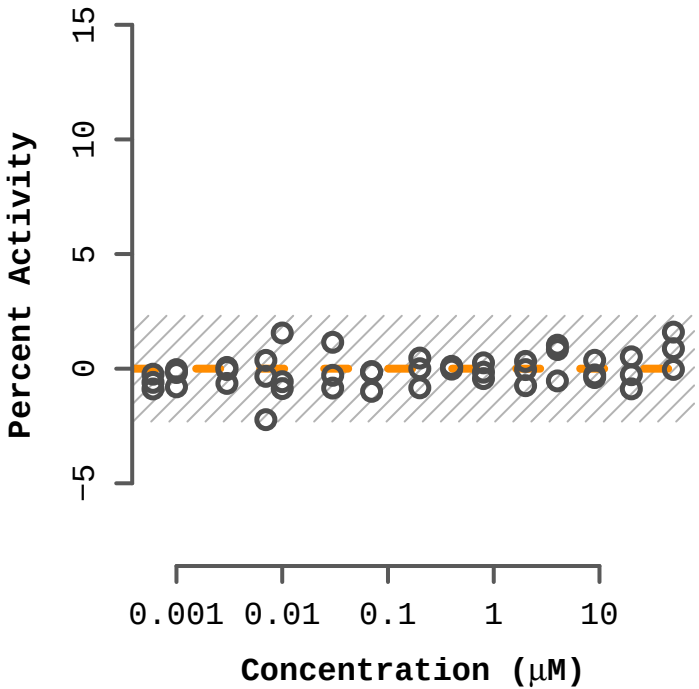
NAME: L−(−)−Sorbose
CHID: 48704 CASRN: 87−79−6
SPID(S): Tox21_113100_1
M4ID: 12482807

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.419 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

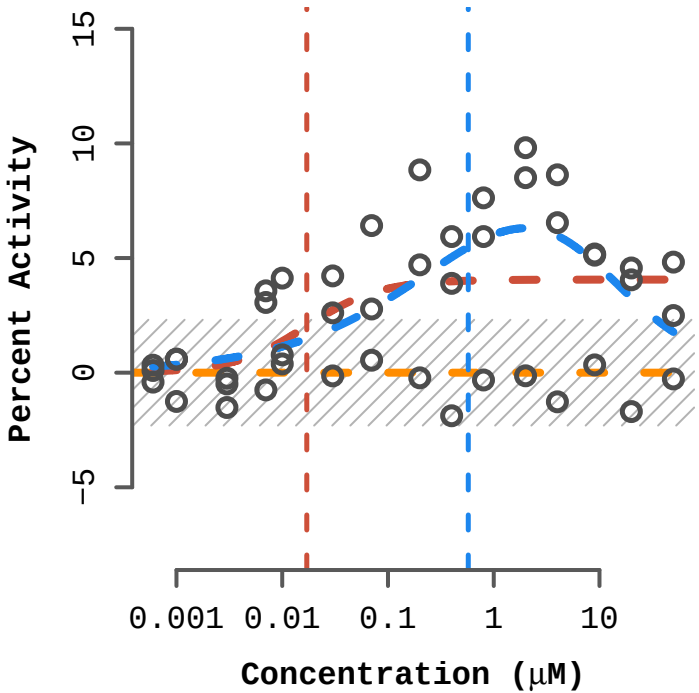
NAME: trans−Aconitic acid
CHID: 48706 **CASRN:** 4023−65−8
SPID(S): Tox21_113103_1
M4ID: 12482806

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.813 **MAX_MED:** 0.875 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Adrenone
CHID: 48710 CASRN: 99-45-6
SPID(S): Tox21_113112_1
M4ID: 12482802

HILL MODEL (in red):

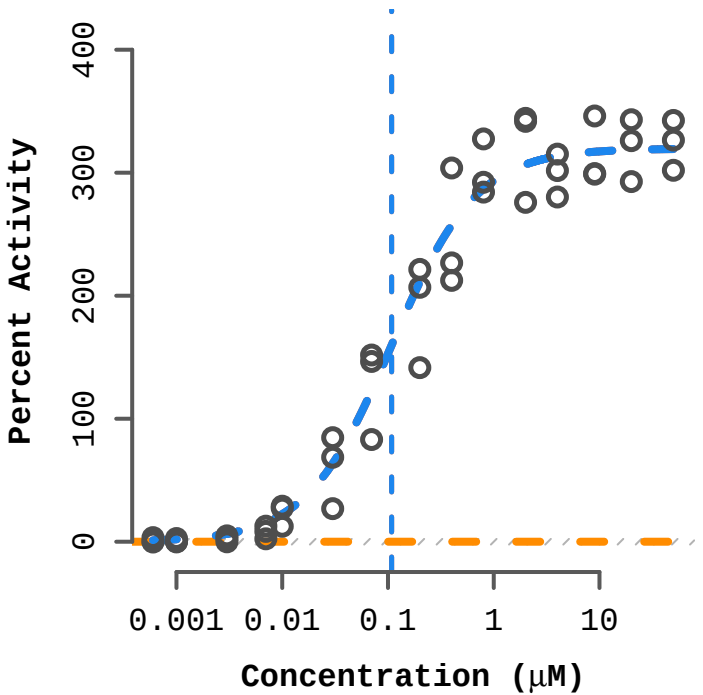
	tp	ga	gw
val:	4.06	−1.77	1.26
sd:	0.759	0.414	0.867

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.8	−0.241	0.551	0.95	0.946
sd:	18.9	2.27	0.318	0.923	0.62

	CNST	HILL	GNLS
AIC:	259.05	233.98	234.08
PROB:	0	0.51	0.49
RMSE:	4.16	2.88	2.88

MAX_MEAN: 6.06 MAX_MED: 8.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Triamcinolone diacetate
CHID: 48713 CASRN: 67-78-7
SPID(S): Tox21_113119_1
M4ID: 12482801

HILL MODEL (in red):

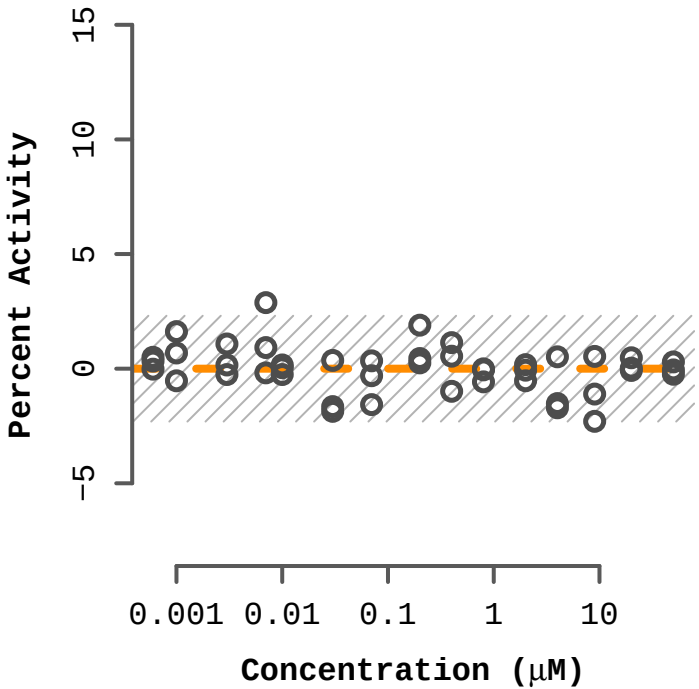
	tp	ga	gw
val:	320	-0.965	1.08
sd:	7.16	0.0603	0.103

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	320	-0.965	1.08	3.64	16.1
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	620.15	421.52	425.52
PROB:	0	0.88	0.12
RMSE:	218.29	23.83	23.83

MAX_MEAN: 324 **MAX_MED:** 342 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

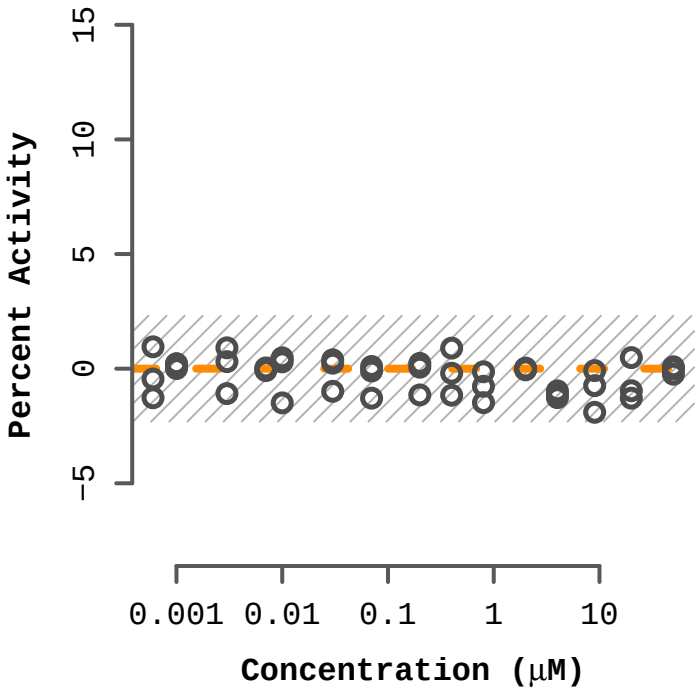
NAME: Fexofenadine hydrochloride
CHID: 48716 **CASRN:** 153439-40-8
SPID(S): Tox21_113125_1
M4ID: 12482798

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.922 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

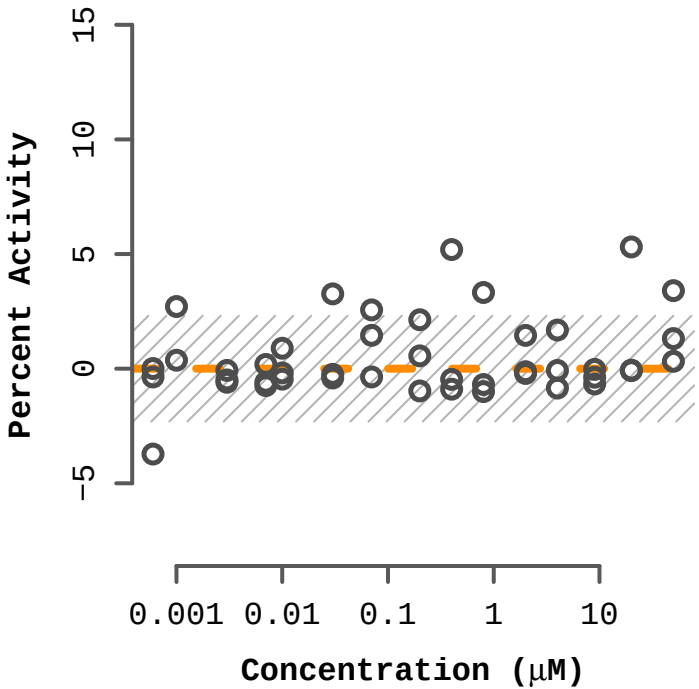
NAME: Ioxilan
CHID: 48717 **CASRN:** 107793-72-6
SPID(S): Tox21_113127_1
M4ID: 12482796

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.143 **MAX_MED:** 0.309 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

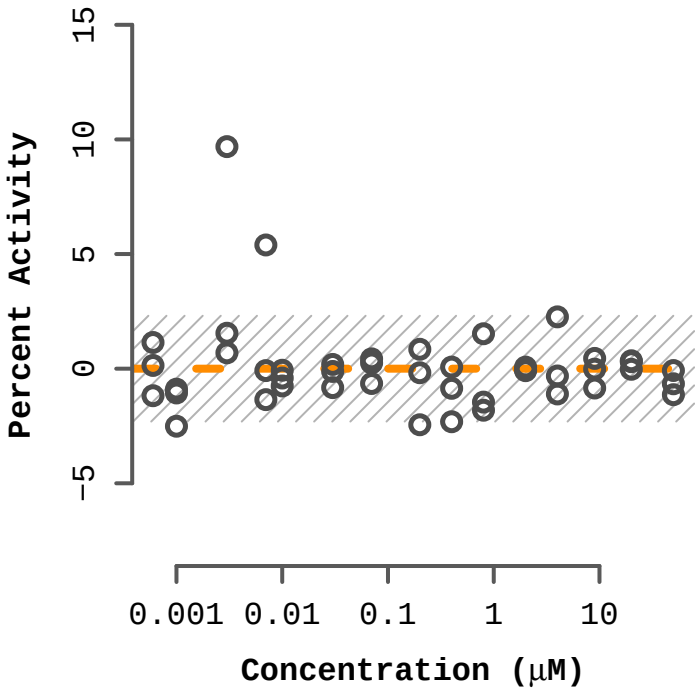
NAME: Bamifylline Hydrochloride
CHID: 48721 CASRN: 20684-06-4
SPID(S): Tox21_113133_1
M4ID: 12482795

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 1.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

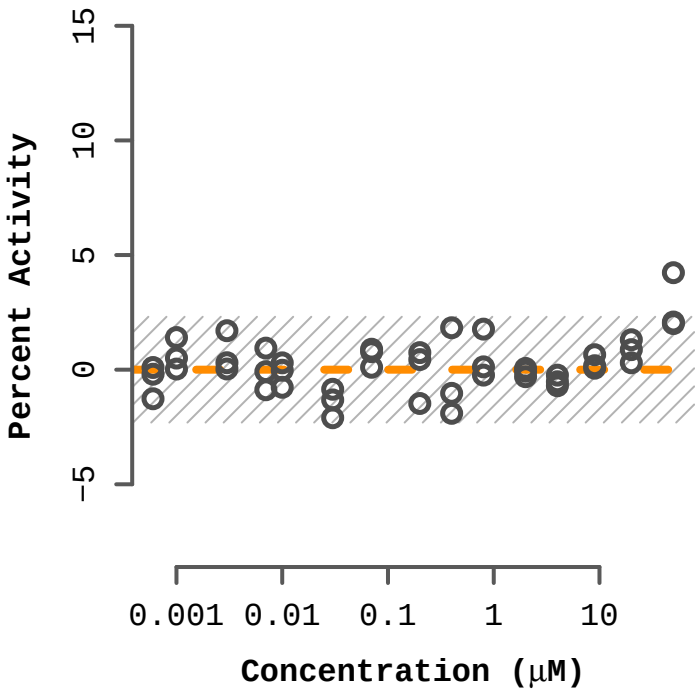
NAME: Nicomolol
CHID: 48722 CASRN: 27959-26-8
SPID(S): Tox21_113136_1
M4ID: 12482793

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 3.98 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

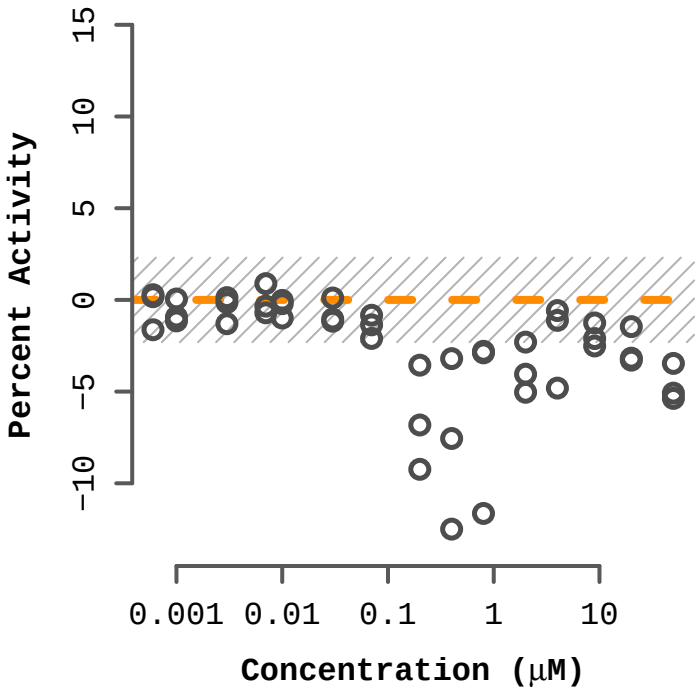
NAME: Cadralazine
CHID: 48725 CASRN: 64241-34-5
SPID(S): Tox21_113146_1
M4ID: 12482790

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 2.77 MAX_MED: 2.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

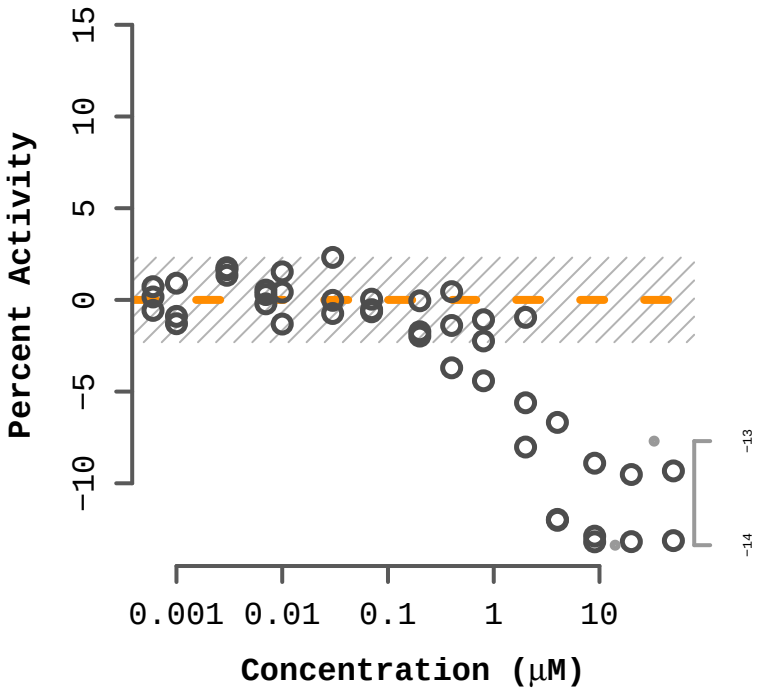
NAME: Dicyclopentamethylenethiuram disulfide
CHID: 48727 **CASRN:** 94-37-1
SPID(S): Tox21_113156_1
M4ID: 12482787

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	246.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.98	NA	NA

MAX_MEAN: −0.0506 **MAX_MED:** 0.175 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

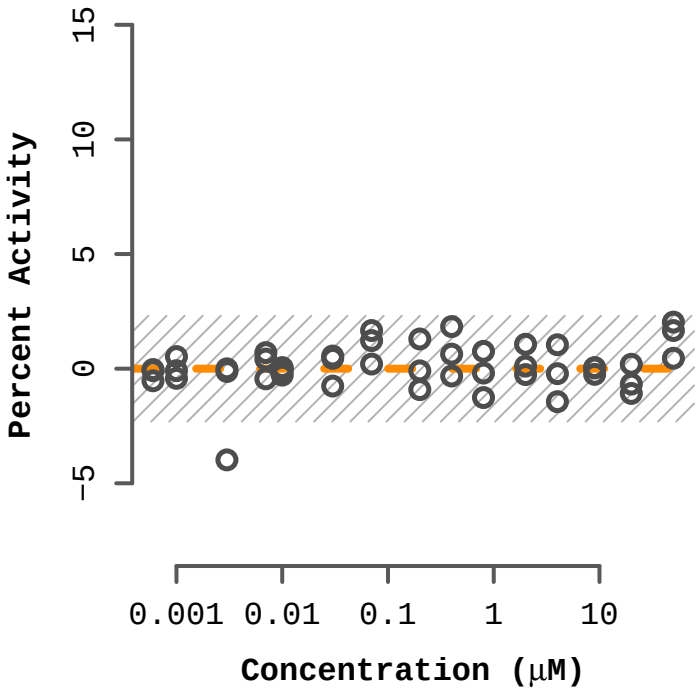
NAME: Toluidine blue
CHID: 48728 **CASRN:** 92-31-9
SPID(S): Tox21_113159_1
M4ID: 12482786 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.47	NA	NA
PROB:	1	NA	NA
RMSE:	6.37	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

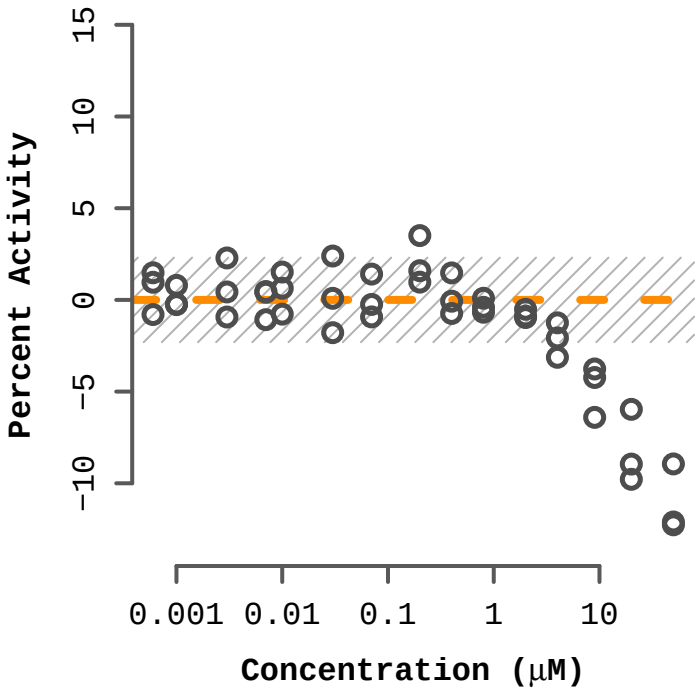
NAME: Acitazanolast
CHID: 48732 **CASRN:** 114607-46-4
SPID(S): Tox21_113173_1
M4ID: 12482782

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.14	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.38 **MAX_MED:** 1.67 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

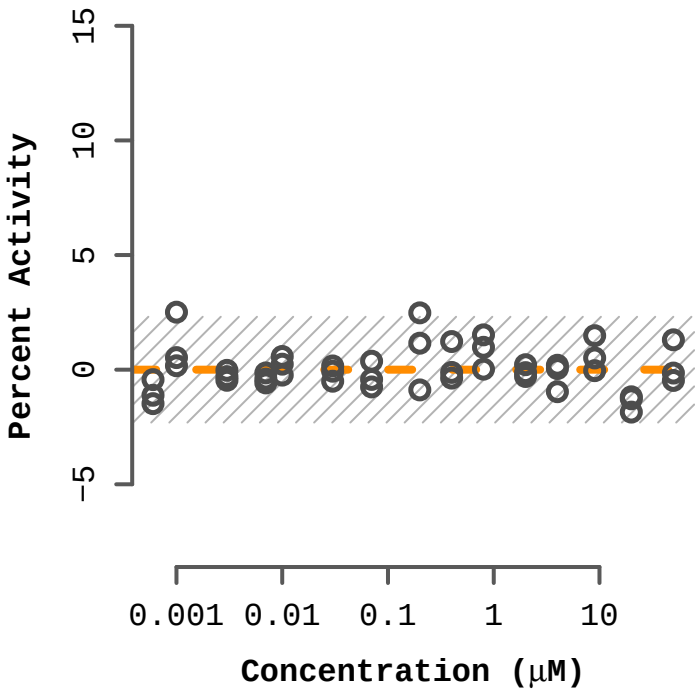
NAME: Pazopanib
CHID: 48733 CASRN: 444731-52-6
SPID(S): Tox21_113174_1
M4ID: 12482781

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	239.67	NA	NA
PROB:	1	NA	NA
RMSE:	4.02	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

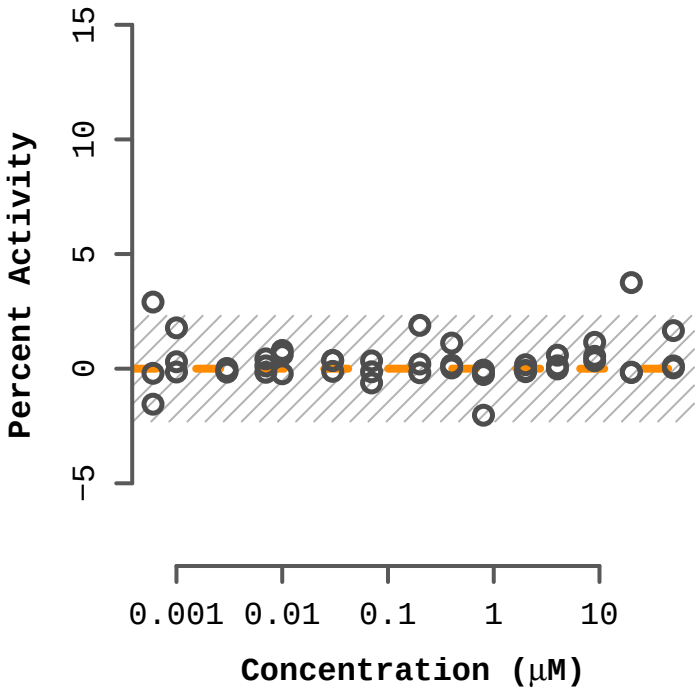
NAME: Erdosteine
CHID: 48735 **CASRN:** 84611-23-4
SPID(S): Tox21_113176_1
M4ID: 12482780

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

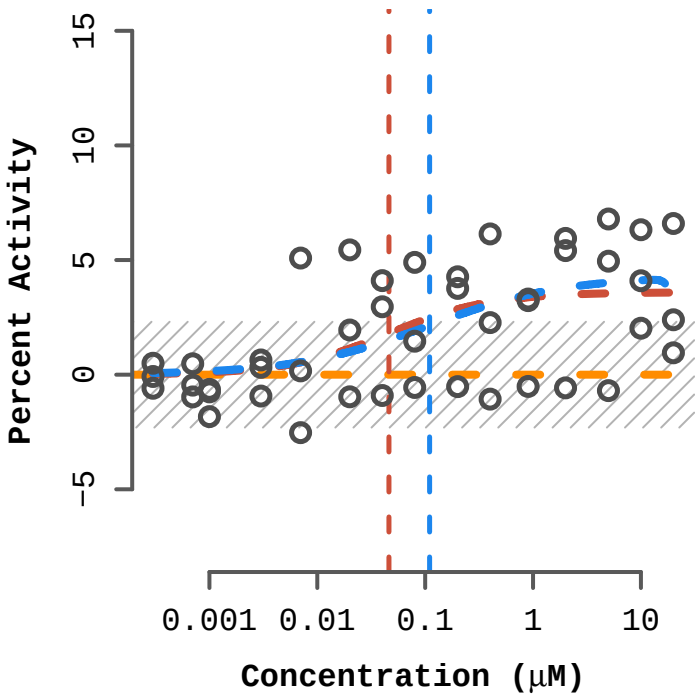
NAME: Imperatorin
CHID: 48737 **CASRN:** 482-44-0
SPID(S): Tox21_113179_1
M4ID: 12482779

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.617 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bekanamycin sulfate
CHID: 48739 CASRN: 29701-07-3
SPID(S): Tox21_113188_1
M4ID: 12482777

HILL MODEL (in red):

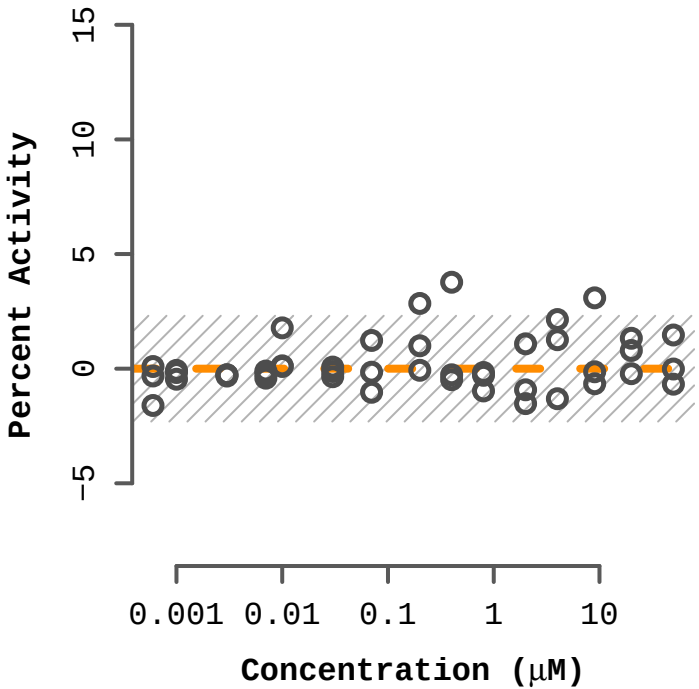
	tp	ga	gw
val:	3.59	−1.34	0.923
sd:	1.08	0.81	0.822

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.29	−0.959	0.699	1.33	12.9
sd:	1.81	1.01	0.492	0.292	153

	CNST	HILL	GNLS
AIC:	237.53	214.1	217.64
PROB:	0	0.85	0.15
RMSE:	3.24	2.28	2.29

MAX_MEAN: 4.15 MAX_MED: 5.41 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

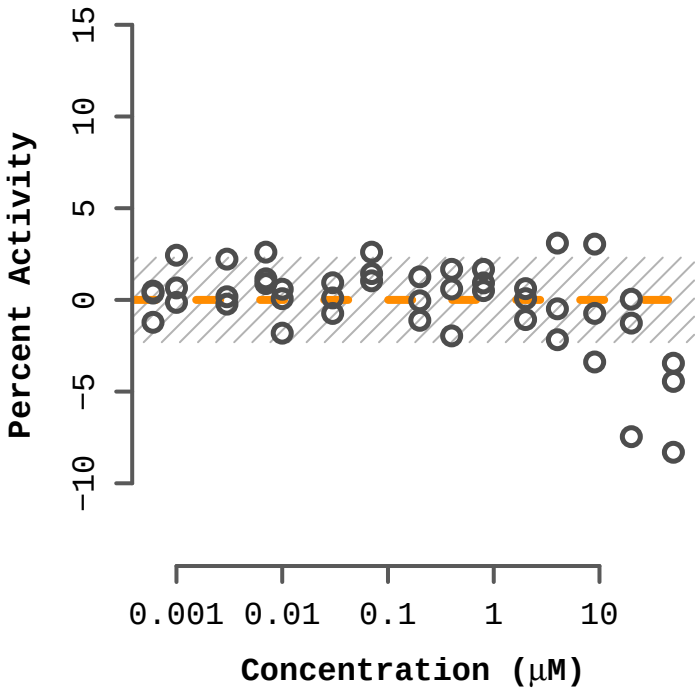
NAME: Mucic acid
CHID: 48740 **CASRN:** 526-99-8
SPID(S): Tox21_113190_1
M4ID: 12482775

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

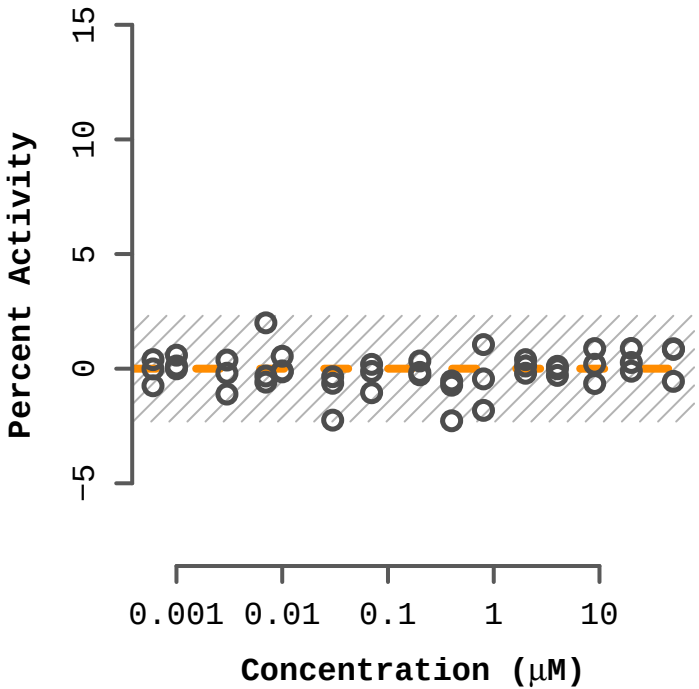
NAME: Trichlomethine
CHID: 48744 **CASRN:** 555-77-1
SPID(S): Tox21_113198_1
M4ID: 12482774

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	196.36	NA	NA
PROB:	1	NA	NA
RMSE:	2.34	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

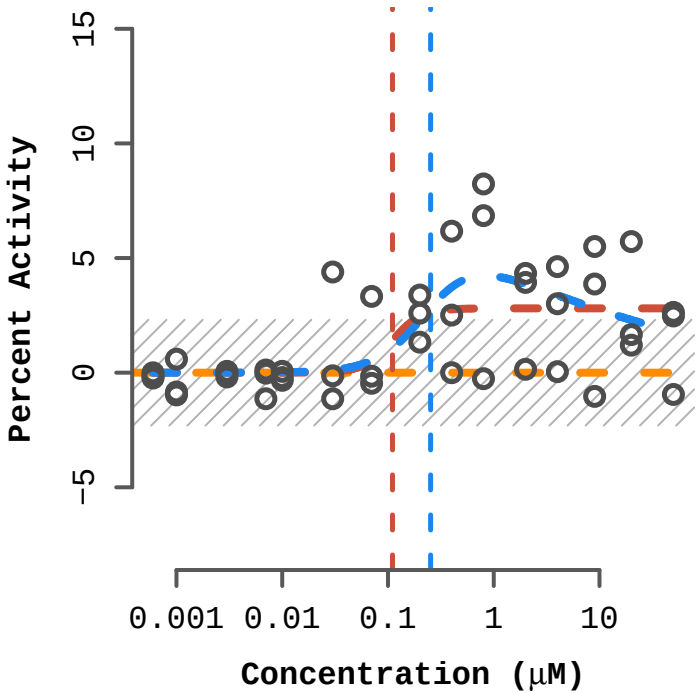
NAME: Oberadilol
CHID: 48745 **CASRN:** 114856-44-9
SPID(S): Tox21_113202
M4ID: 12482773

HILL MODEL: Not applicable.

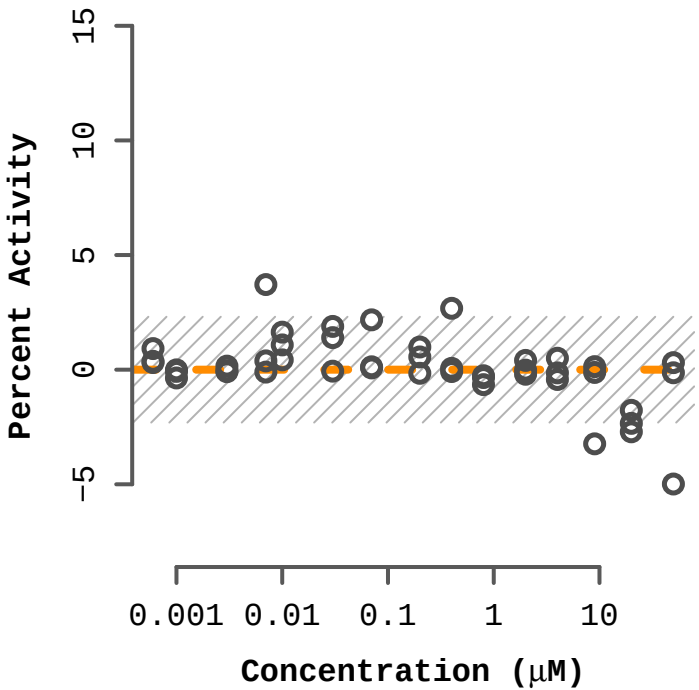
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.387 **MAX_MED:** 0.84 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ataciguat
CHID:    48746   CASRN: 254877-67-3
SPID(S): Tox21_113203_1
M4ID:    12482772

HILL MODEL (in red):
      tp       ga       gw
val:  2.81     -0.957   3.22
sd:   0.522    0.27     3.66

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.88     -0.597   1.92     -0.223   0.34
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  221.83      197.18      198.66
PROB: 0           0.68        0.32
RMSE: 2.89        2.01        1.95

MAX_MEAN: 4.94      MAX_MED: 6.85      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

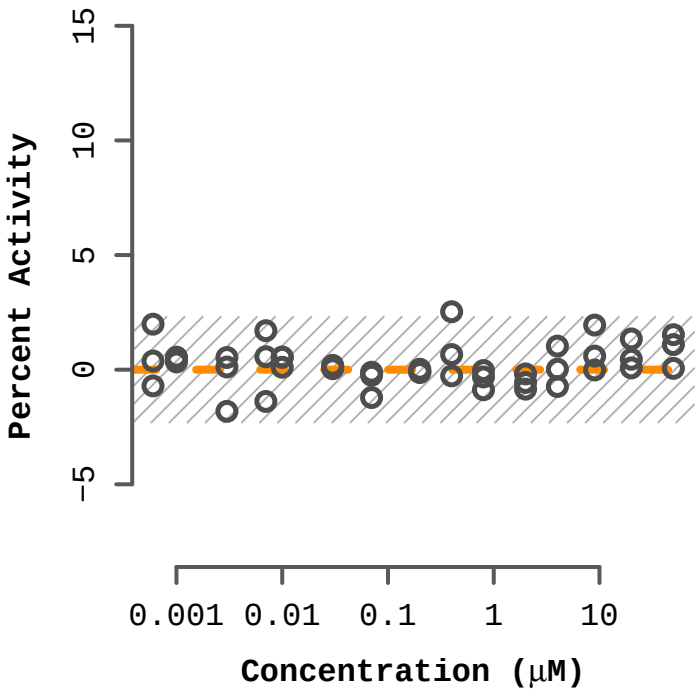
NAME: Tesaglitazar
CHID: 48773 **CASRN:** 251565-85-2
SPID(S): Tox21_113248_1
M4ID: 12482771

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

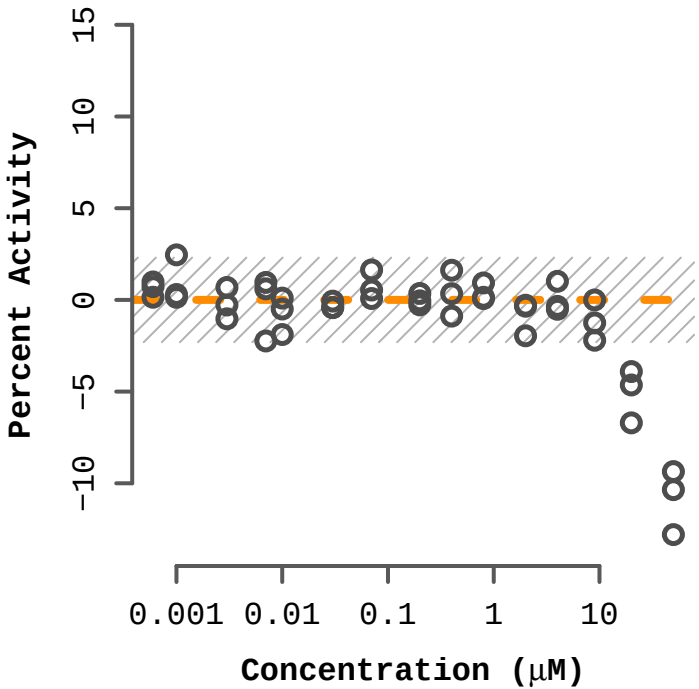
NAME: Iomazenil
CHID: 48774 **CASRN:** 127985-21-1
SPID(S): Tox21_113249
M4ID: 12482770

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.07	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.973 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

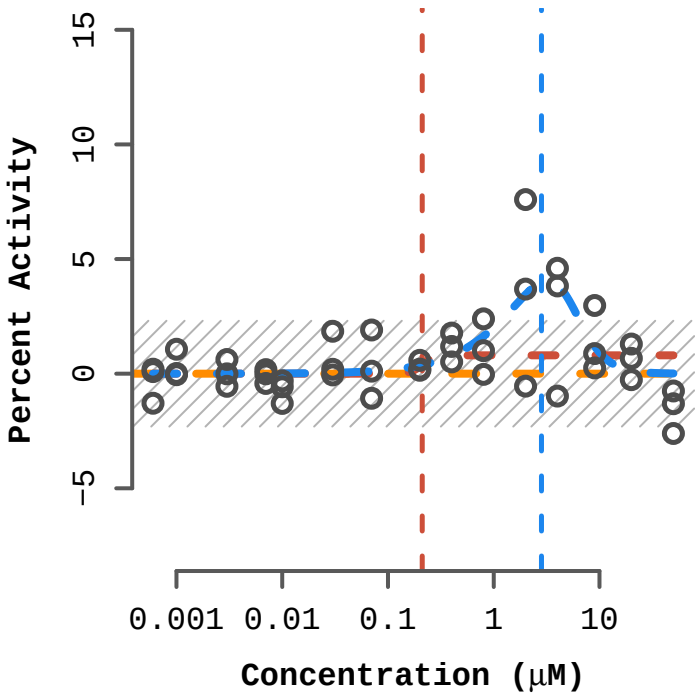
NAME: Zanapezil fumerate
CHID: 48776 **CASRN:** 263248-42-6
SPID(S): Tox21_113251
M4ID: 12482769

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.24	NA	NA
PROB:	1	NA	NA
RMSE:	3.26	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.726 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Depolipon
CHID: 48777 CASRN: 16488-48-5
SPID(S): Tox21_113252
M4ID: 12482768

HILL MODEL (in red):

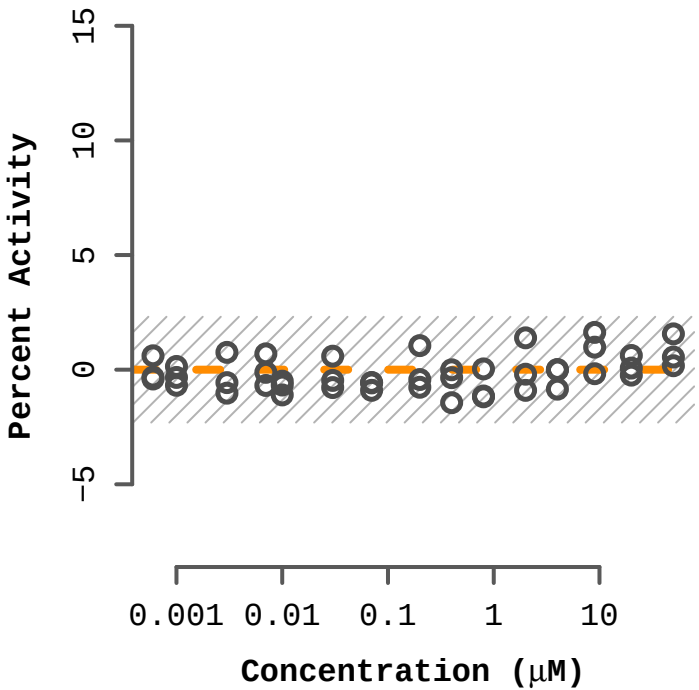
	tp	ga	gw
val:	0.8	−0.676	8
sd:	0.331	0.16	21.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.12	0.452	1.2	0.724	3.09
sd:	11.9	0.778	0.577	0.218	1.56

	CNST	HILL	GNLS
AIC:	170.68	170.39	158.95
PROB:	0	0	0.99
RMSE:	1.86	1.68	1.42

MAX_MEAN: 3.58 MAX_MED: 3.83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

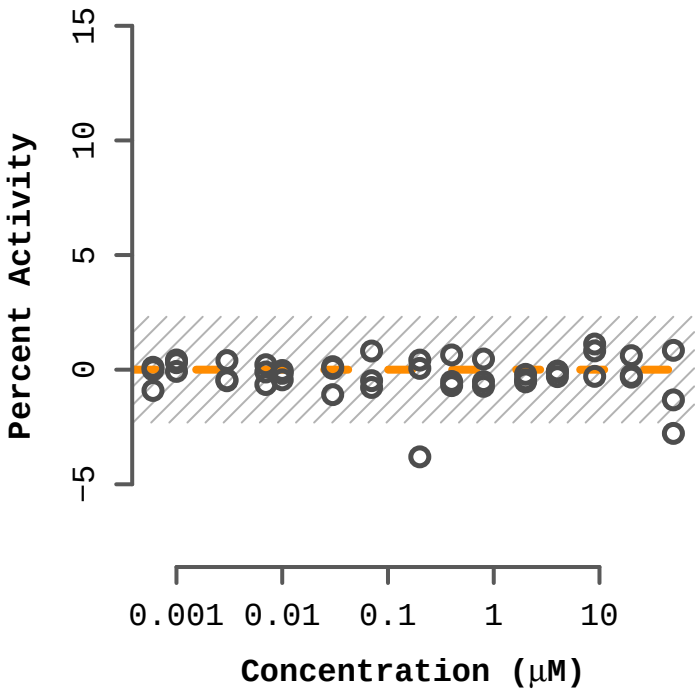
NAME: Phenyl 11-iodo-10-undecynoate
CHID: 48778 **CASRN:** 2020-25-9
SPID(S): Tox21_113254
M4ID: 12482767

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.812 **MAX_MED:** 0.984 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

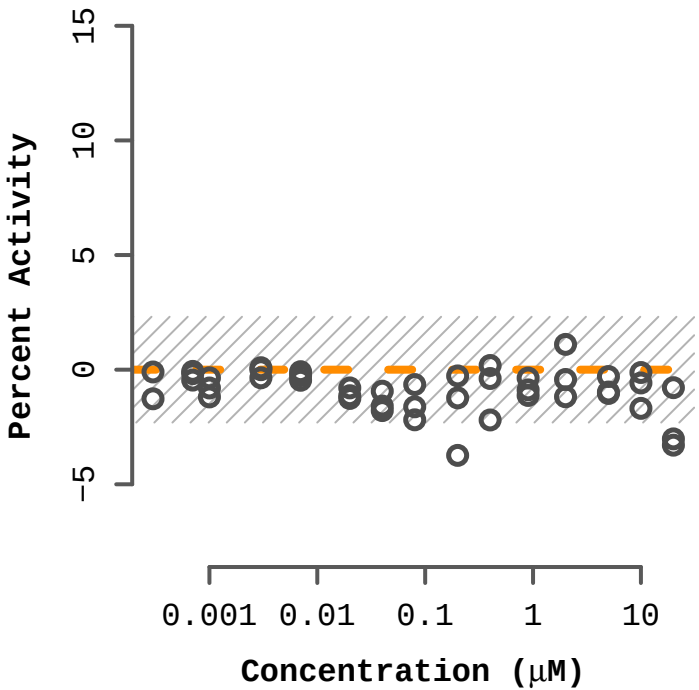
NAME: Tolvaptan
CHID: 48780 CASRN: 150683-30-0
SPID(S): Tox21_113256
M4ID: 12482766

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.551 **MAX_MED:** 0.822 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

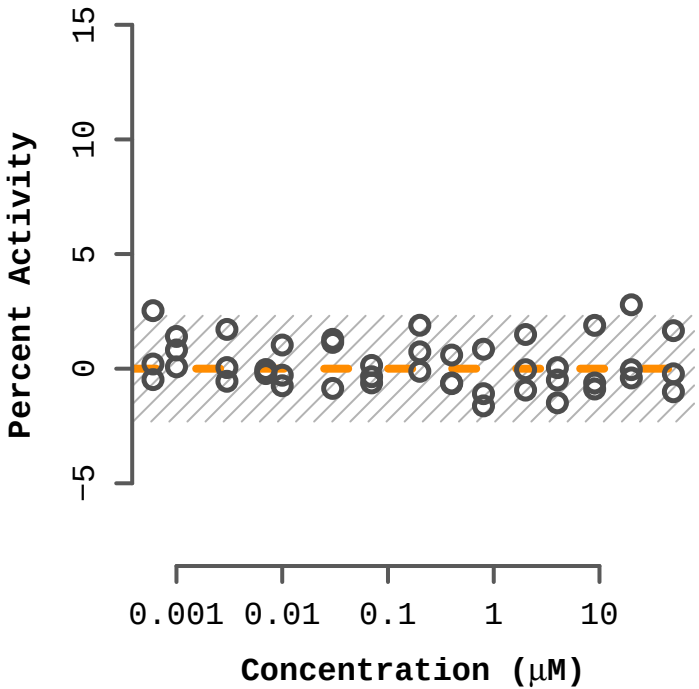
NAME: Anacolin
CHID: 48781 CASRN: 21216-78-4
SPID(S): Tox21_113257
M4ID: 12482765

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: −0.0881 MAX_MED: 0.000521 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

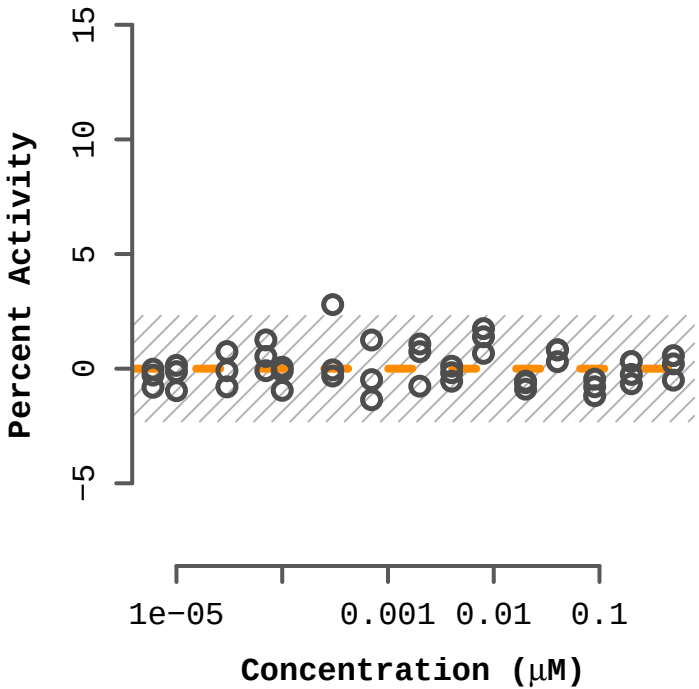
NAME: Biliscopin
CHID: 48782 CASRN: 51022-74-3
SPID(S): Tox21_113258
M4ID: 12482764

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.839 MAX_MED: 1.15 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

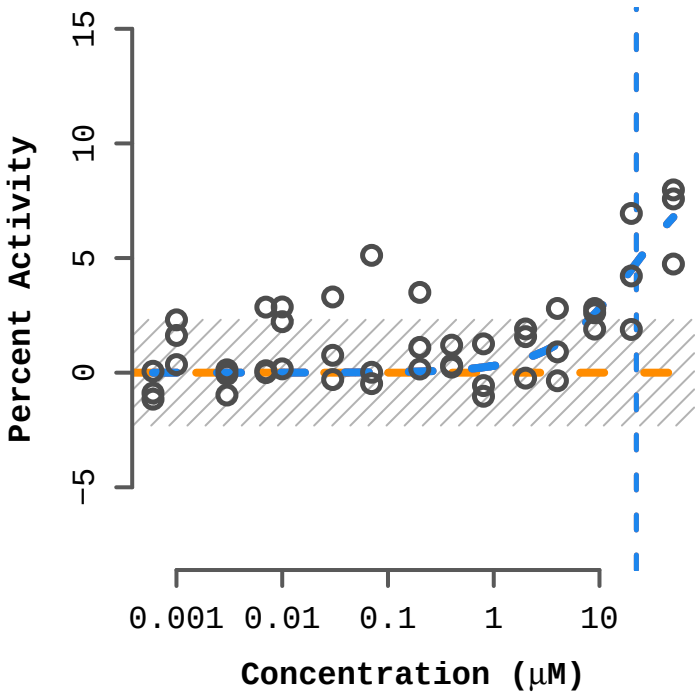
NAME: Bimosiamose
CHID: 48783 **CASRN:** 187269-40-5
SPID(S): Tox21_113260
M4ID: 12482762

HILL MODEL: Not applicable.

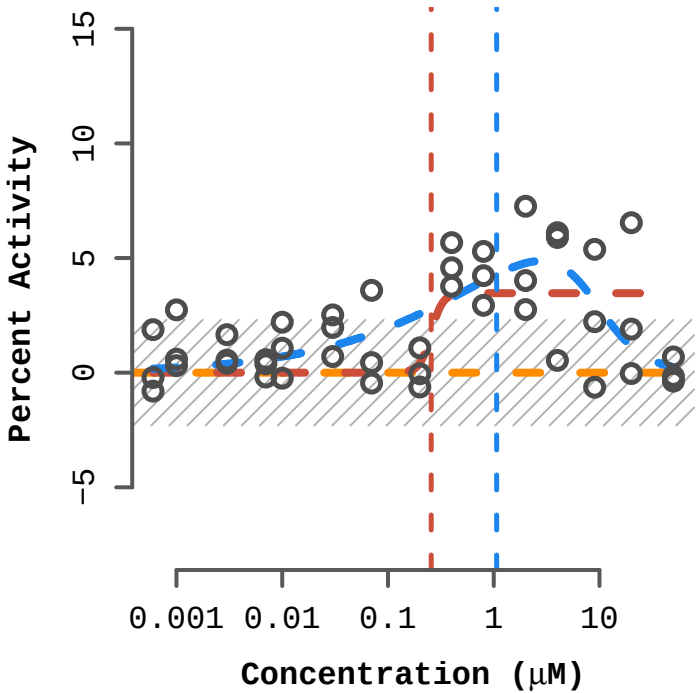
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

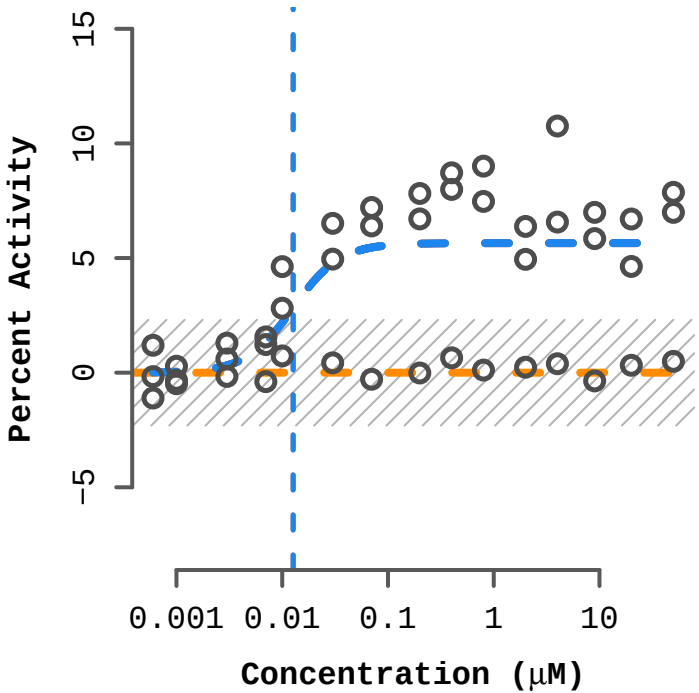
MAX_MEAN: 1.27 **MAX_MED:** 1.39 **BMAD:** 0.769



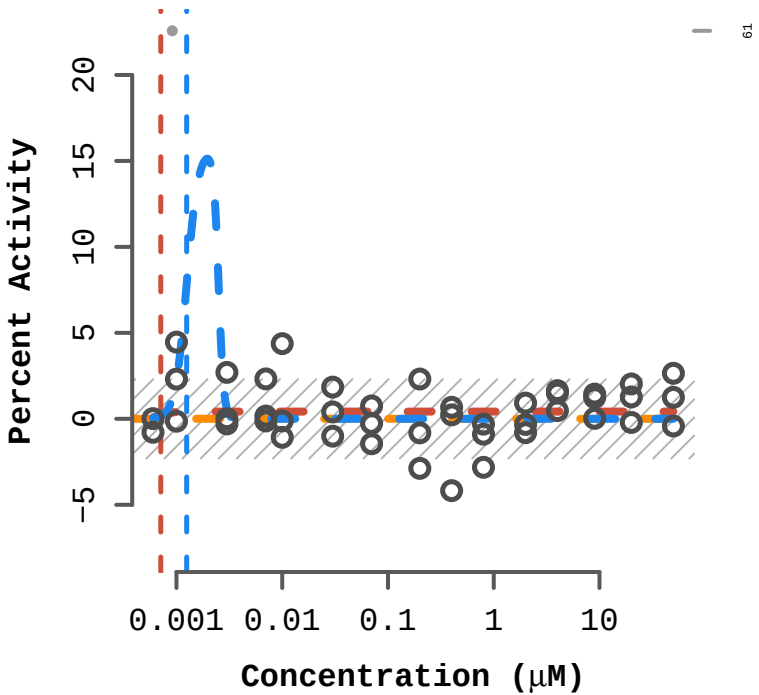

```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pranazepide
CHID:    48785   CASRN: 150408-73-4
SPID(S): Tox21_113262
M4ID:    12482761

HILL MODEL (in red):
      tp       ga       gw
val:  9.57     1.35     1.1
sd:   4.07     0.388    0.494

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.57     1.35     1.11     2.6      9.02
sd:   4.08     0.389    0.496    1040     10300

      CNST        HILL        GNLS
AIC:  214.08      175.65      179.65
PROB: 0           0.88        0.12
RMSE: 2.73        1.61        1.61

MAX_MEAN: 6.77      MAX_MED: 7.58      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    N-[(3R)-1-(2-Fluorophenyl)-4-oxo-3,4,6,7-tetral
CHID:    48786   CASRN: 167820-10-2
SPID(S): Tox21_113263
M4ID:    12482760

HILL MODEL (in red):
      tp       ga       gw
val:  3.47     -0.591   8
sd:   0.544    0.0889   4.98

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.71     0.0276   0.522    0.931    1.94
sd:   5.99     1.1      0.226    0.226    0.986

      CNST        HILL        GNLS
AIC:  227.23      200.88      190.58
PROB: 0           0.01        0.99
RMSE: 2.98        1.99        1.78

MAX_MEAN: 4.68      MAX_MED: 5.9       BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Egualen sodium
CHID:    48787   CASRN: 97683-31-3
SPID(S): Tox21_113264
M4ID:    12482759

HILL MODEL (in red):
      tp       ga       gw
val:  5.65     -1.9     1.96
sd:   0.673    0.209    1.52

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.65     -1.9     1.96     3.17     5.25
sd:   0.673    0.209    1.52     1840     6640

      CNST        HILL        GNLS
AIC:  275.29      232.96      236.96
PROB: 0           0.88        0.12
RMSE: 4.87        2.92        2.92

MAX_MEAN: 5.91      MAX_MED: 8         BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Betiatide
CHID: 48788 CASRN: 103725-47-9
SPID(S): Tox21_113265
M4ID: 12482758 BRK

HILL MODEL (in red):

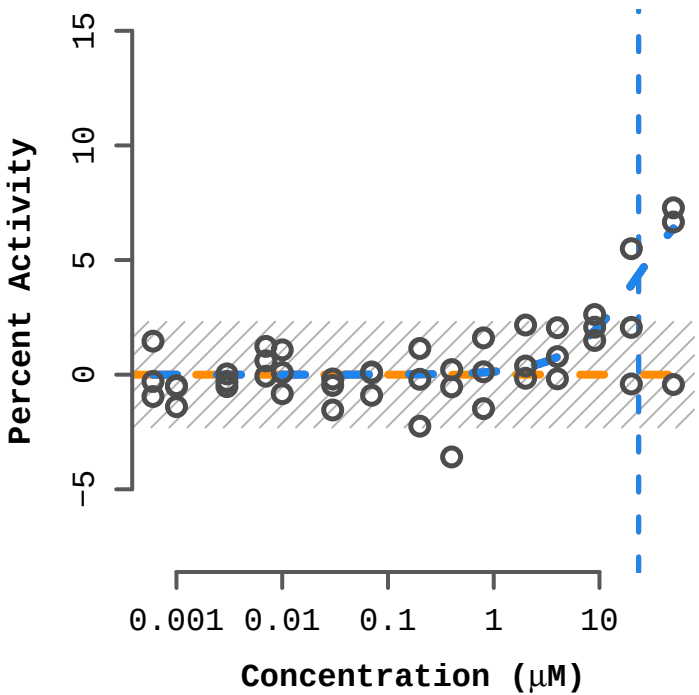
	tp	ga	gw
val:	0.42	−3.15	8
sd:	0.256	0.259	17.4

GAIN-LOSS MODEL (in blue):

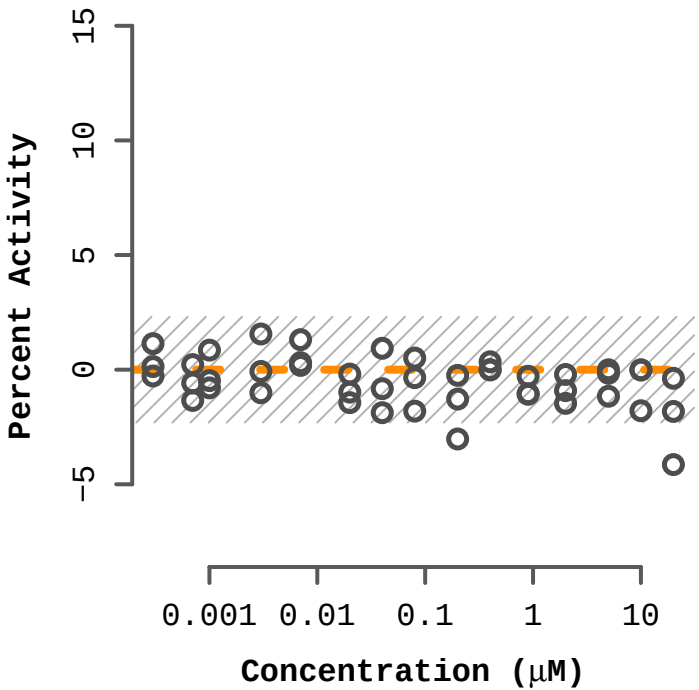
	tp	ga	gw	la	lw
val:	15.7	−2.9	8	−2.6	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	207.62	210.88	213.52
PROB:	0.8	0.16	0.04
RMSE:	9.2	9.18	9.18

MAX_MEAN: 20 MAX_MED: 2.31 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Acetylpheneturide
CHID:    48789   CASRN: 13402-08-9
SPID(S): Tox21_113266
M4ID:    12482757

HILL MODEL (in red):
      tp       ga       gw
val:  8.73     1.37     1.32
sd:   3.07     0.299    0.437

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.73     1.37     1.32     2.96     6.27
sd:   3.07     0.299    0.437    914      4560

      CNST        HILL        GNLS
AIC:  180.06      162.98      166.98
PROB: 0           0.88        0.12
RMSE: 2.07        1.61        1.61

MAX_MEAN: 4.5       MAX_MED: 6.66      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

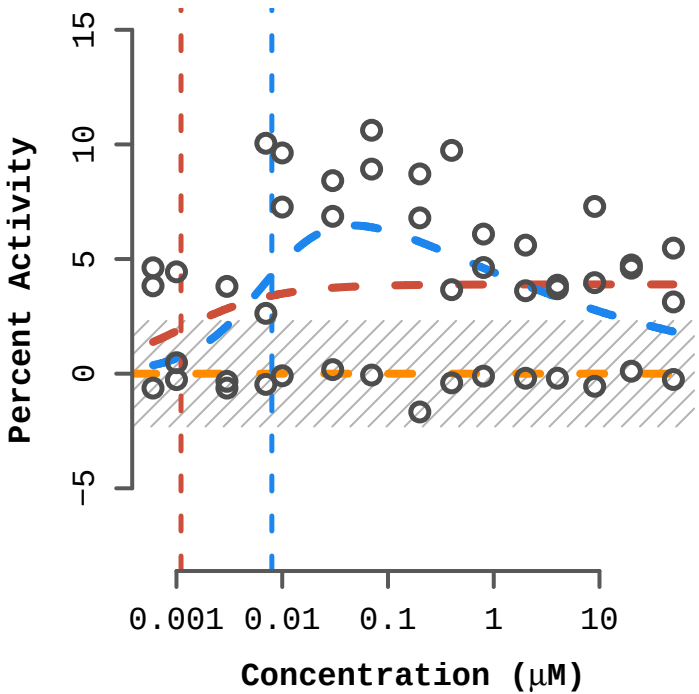
NAME: Blonanserin
CHID: 48790 **CASRN:** 132810-10-7
SPID(S): Tox21_113267
M4ID: 12482756

HILL MODEL: Not applicable.

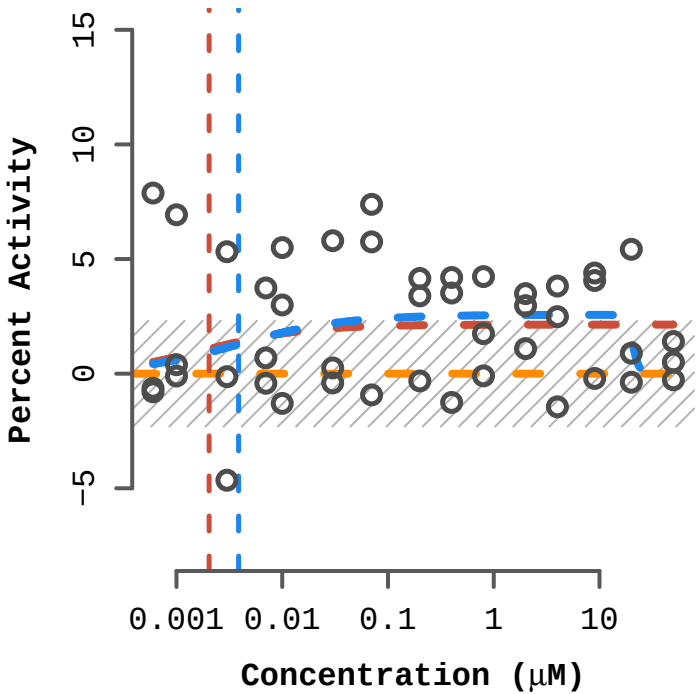
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

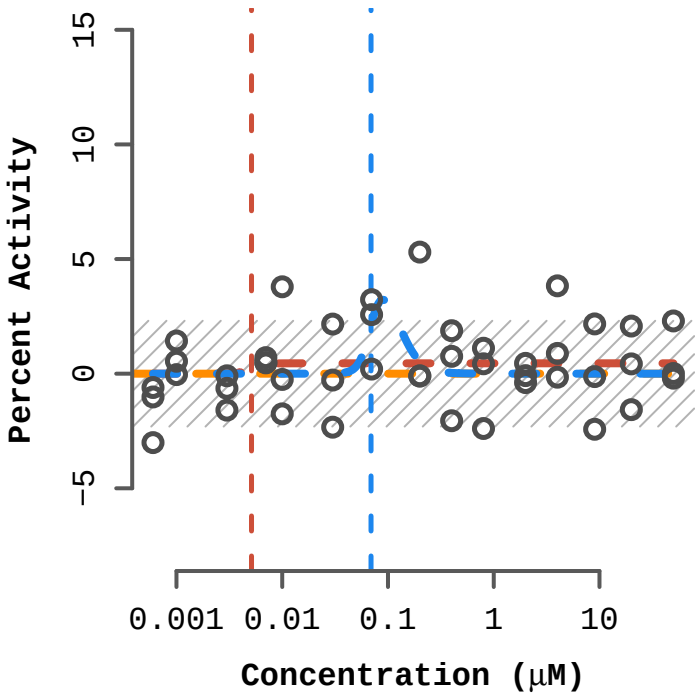
MAX_MEAN: 0.601 **MAX_MED:** 0.306 **BMAD:** 0.769



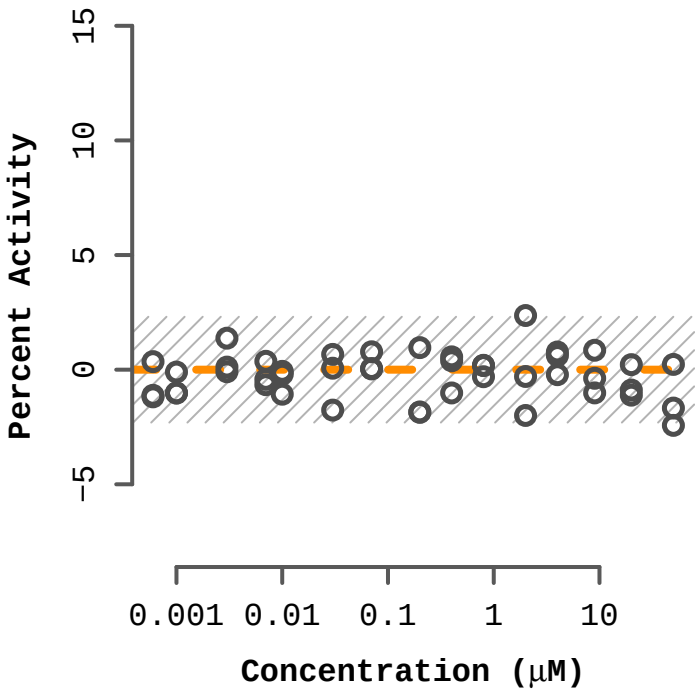

```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Troxacitabine
CHID:    48791   CASRN: 145918-75-8
SPID(S): Tox21_113268
M4ID:    12482755

HILL MODEL (in red):
      tp       ga       gw
val:  3.89     -2.96    0.979
sd:   0.709    0.75     0.863

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.1     -2.1     1.27     -0.79    0.3
sd:   24.8     0.6      1.92     5.56     0.326

      CNST        HILL        GNLS
AIC:  278.92      254.93      255.65
PROB: 0           0.59        0.41
RMSE: 5.06        3.51        3.42

MAX_MEAN: 6.49      MAX_MED: 8.92      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    {4-[4-(Acetylamino)-2-oxopyrimidin-1(2H)-yl]-1,
CHID:    48792   CASRN: NOCAS_48792
SPID(S): Tox21_113269
M4ID:    12482754

HILL MODEL (in red):
      tp       ga       gw
val:  2.14     -2.69    0.955
sd:   0.535    1.05     1.2

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.57     -2.41    0.871    1.31     14
sd:   0.628    0.832    1.21     0.299    324

      CNST        HILL        GNLS
AIC:  243.55      232.11      234.16
PROB: 0           0.73        0.26
RMSE: 3.45        2.82        2.8

MAX_MEAN: 4.07      MAX_MED: 5.75      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Dicethiamine hydrochloride
CHID:    48793   CASRN: 616-96-6
SPID(S): Tox21_113270
M4ID:    12482753

HILL MODEL (in red):
      tp       ga       gw
val:  0.452    -2.29    8
sd:   0.277    0.444    19.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.61     -1.16    8        -0.91    4.13
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  181.07      184.34      185.96
PROB: 0.78        0.15        0.07
RMSE: 1.79        1.71        1.68

MAX_MEAN: 2         MAX_MED: 2.58      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

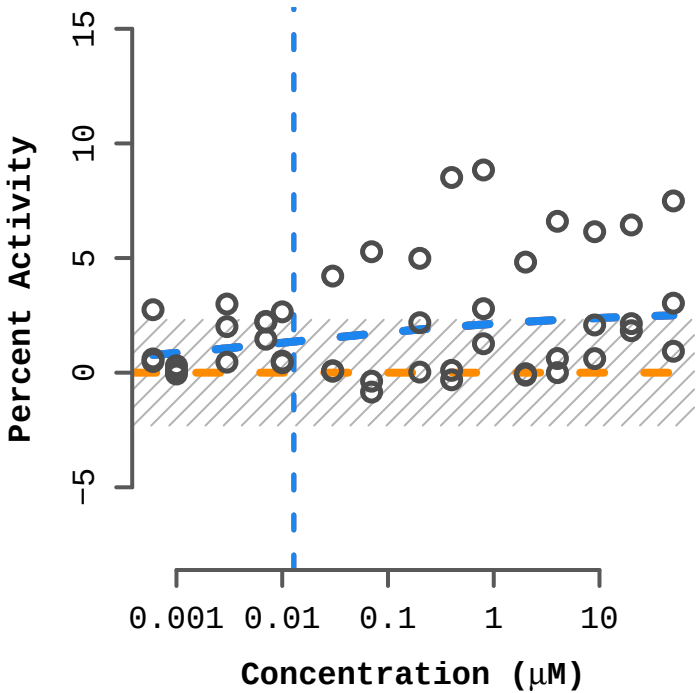
NAME: Cloforex
CHID: 48794 **CASRN:** 14261-75-7
SPID(S): Tox21_113271
M4ID: 12482752

HILL MODEL: Not applicable.

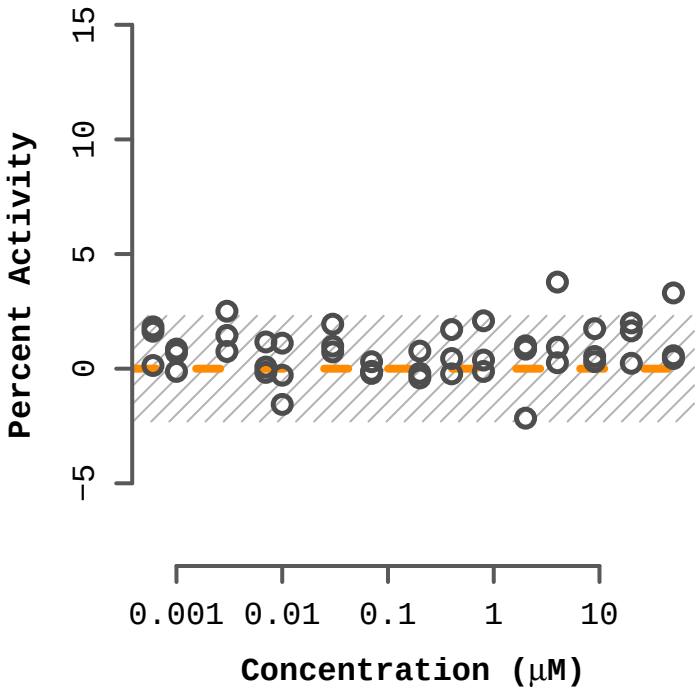
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.467 **MAX_MED:** 0.618 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pelubiprofen
CHID:    48795   CASRN: 69956-77-0
SPID(S): Tox21_113272
M4ID:    12482751

HILL MODEL (in red):
      tp       ga       gw
val:  2.71     -1.89    0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.71     -1.89    0.3      3.69     5.28
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  234.35      215.43      219.43
PROB: 0           0.88        0.12
RMSE: 3.34        2.44        2.44

MAX_MEAN: 4.3       MAX_MED: 3.03      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

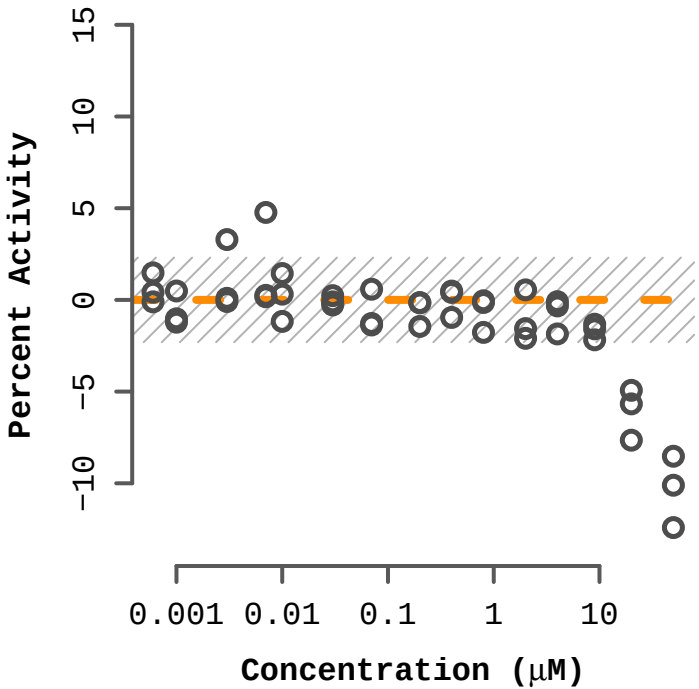
NAME: Risarestat
CHID: 48796 **CASRN:** 79714-31-1
SPID(S): Tox21_113273
M4ID: 12482750

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

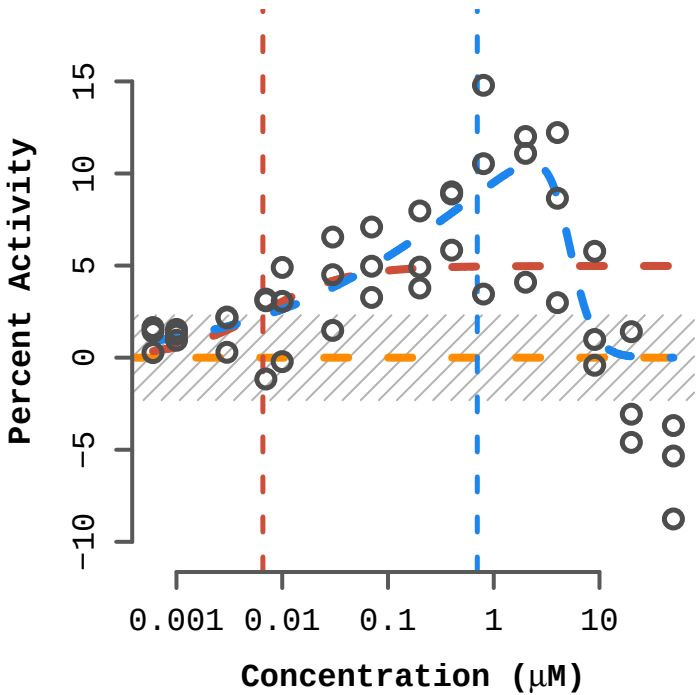
NAME: Diponium bromide
CHID: 48797 CASRN: 2001-81-2
SPID(S): Tox21_113274
M4ID: 12482749

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	217.97	NA	NA
PROB:	1	NA	NA
RMSE:	3.39	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 0.421 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Minopafant
CHID: 48798 CASRN: 128420-61-1
SPID(S): Tox21_113275
M4ID: 12482748

HILL MODEL (in red):

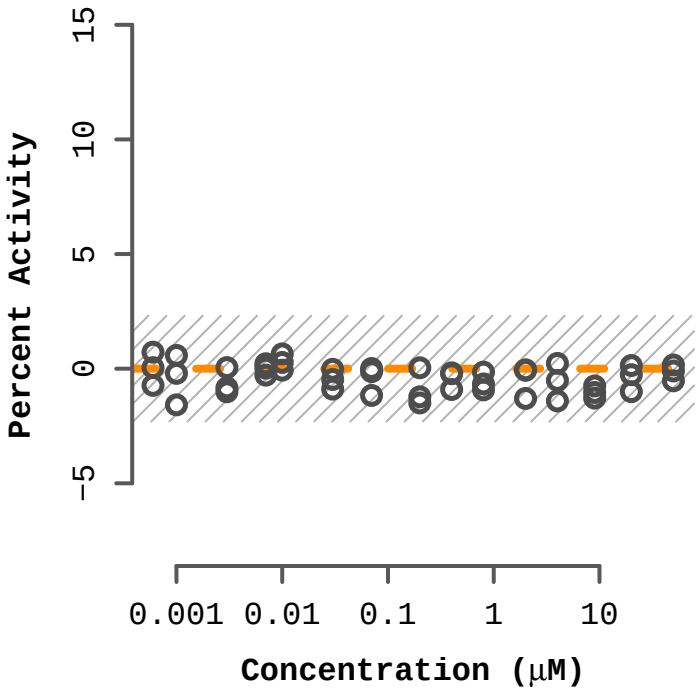
	tp	ga	gw
val:	4.98	−2.18	1.08
sd:	0.965	0.442	0.737

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	17.7	−0.156	0.413	0.713	3.89
sd:	13.4	1.56	0.163	0.116	1.83

	CNST	HILL	GNLS
AIC:	291.46	270.84	236.84
PROB:	0	0	1
RMSE:	5.9	4.65	2.99

MAX_MEAN: 9.59 MAX_MED: 11.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

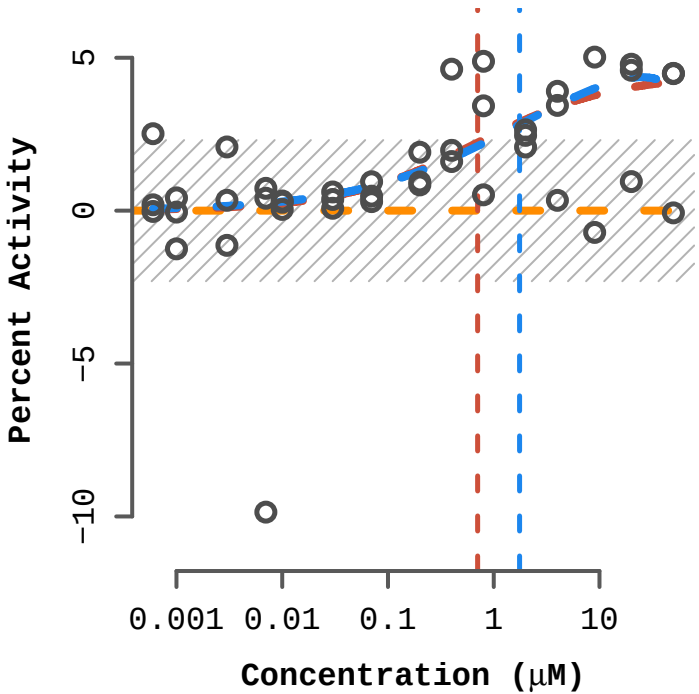
NAME: Emiglitate
CHID: 48799 CASRN: 80879-63-6
SPID(S): Tox21_113276
M4ID: 12482747

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.48	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.286 **MAX_MED:** 0.273 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Etomidoline
CHID: 48800 **CASRN:** 21590-92-1
SPID(S): Tox21_113277
M4ID: 12482746

HILL MODEL (in red):

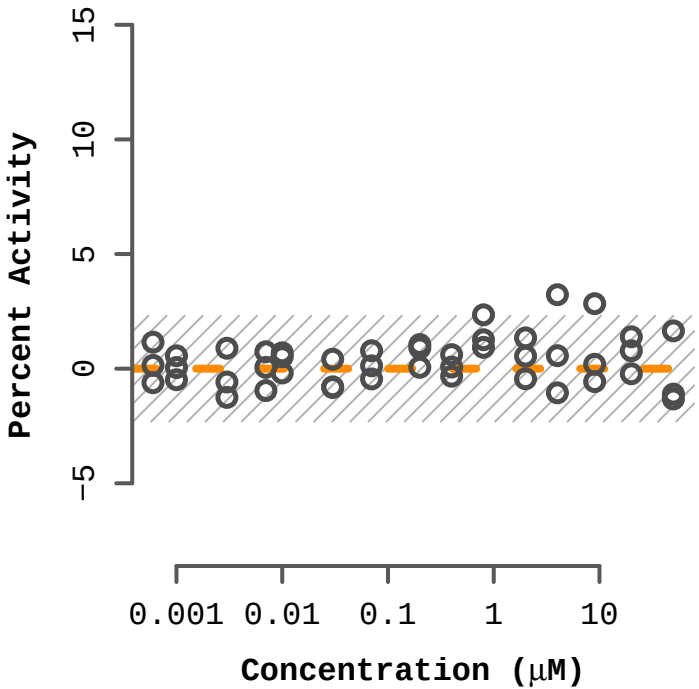
	tp	ga	gw
val:	4.45	−0.152	0.673
sd:	0.977	0.448	0.272

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.63	0.244	0.56	2.02	2.06
sd:	4.85	1.48	0.332	0.789	6.65

	CNST	HILL	GNLS
AIC:	221.46	180.9	184.65
PROB:	0	0.87	0.13
RMSE:	2.92	2.14	2.15

MAX_MEAN: 3.69 **MAX_MED:** 5.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

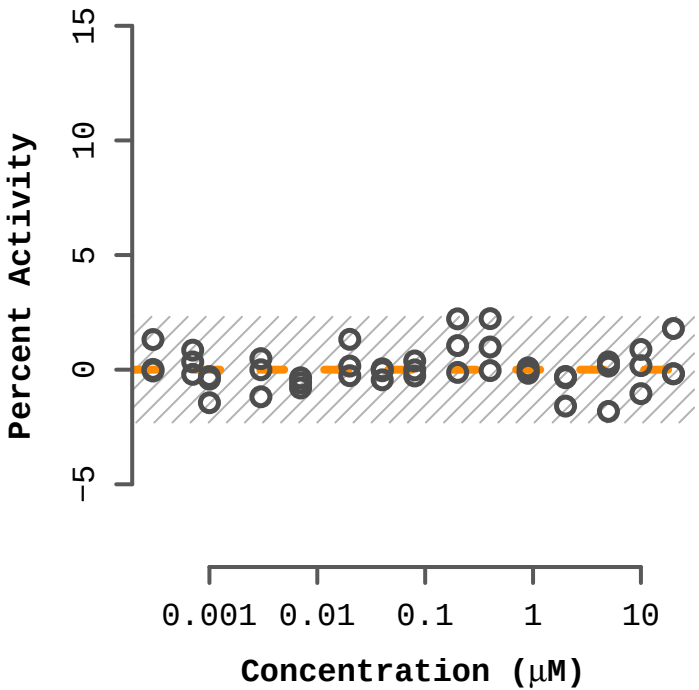
NAME: Fezatione
CHID: 48801 **CASRN:** 15387-18-5
SPID(S): Tox21_113278
M4ID: 12482745

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

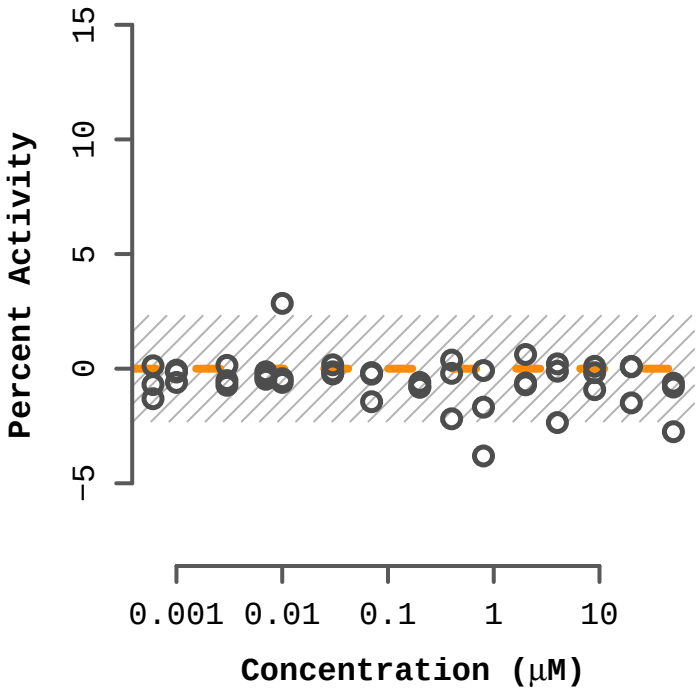
NAME: Pibutidine
CHID: 48802 CASRN: 103922-33-4
SPID(S): Tox21_113279
M4ID: 12482744

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

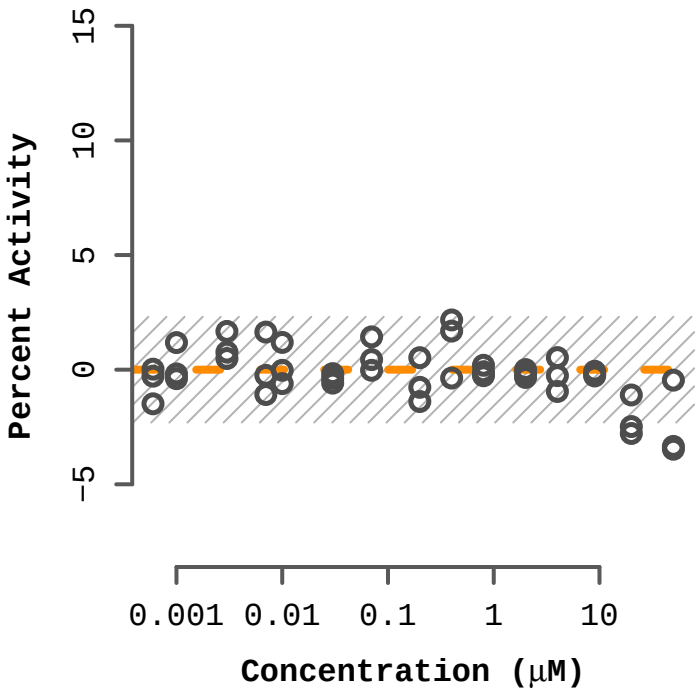
NAME: Itasetron
CHID: 48803 **CASRN:** 123258-84-4
SPID(S): Tox21_113280
M4ID: 12482743

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 0.605 **MAX_MED:** 0.0831 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

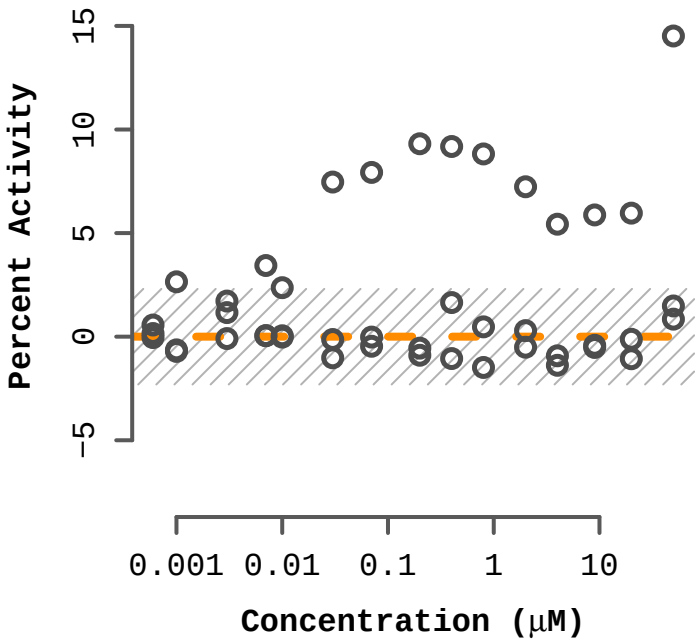
NAME: Pamicogrel
CHID: 48804 CASRN: 101001-34-7
SPID(S): Tox21_113281
M4ID: 12482742

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.16 MAX_MED: 1.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

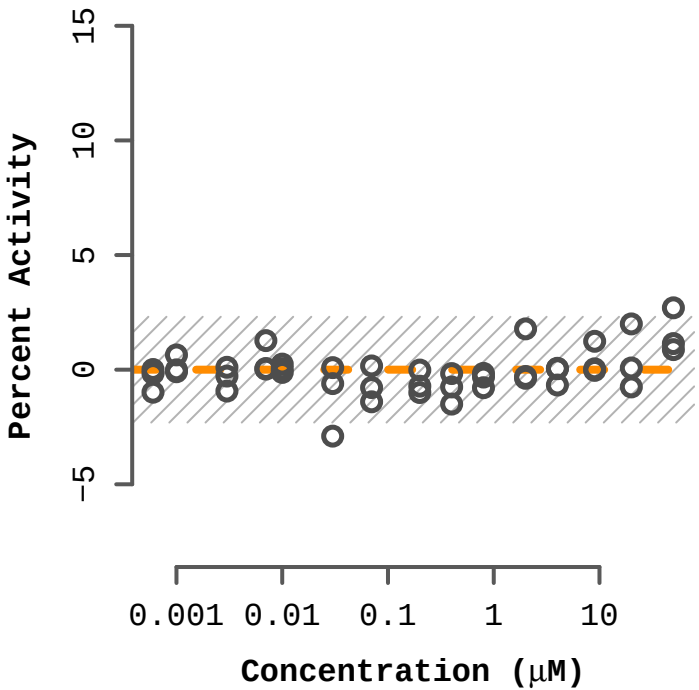
NAME: Esonarimod
CHID: 48805 CASRN: 101973-77-7
SPID(S): Tox21_113282
M4ID: 12482741

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	244.59	NA	NA
PROB:	1	NA	NA
RMSE:	4.15	NA	NA

MAX_MEAN: 5.62 **MAX_MED:** 1.65 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

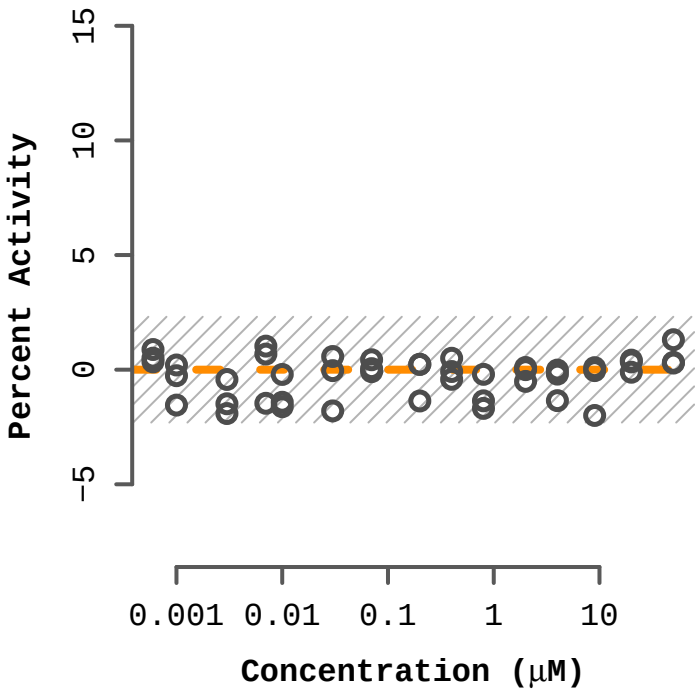
NAME: Dalcotidine
CHID: 48806 **CASRN:** 120958-90-9
SPID(S): Tox21_113283
M4ID: 12482740

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.57	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

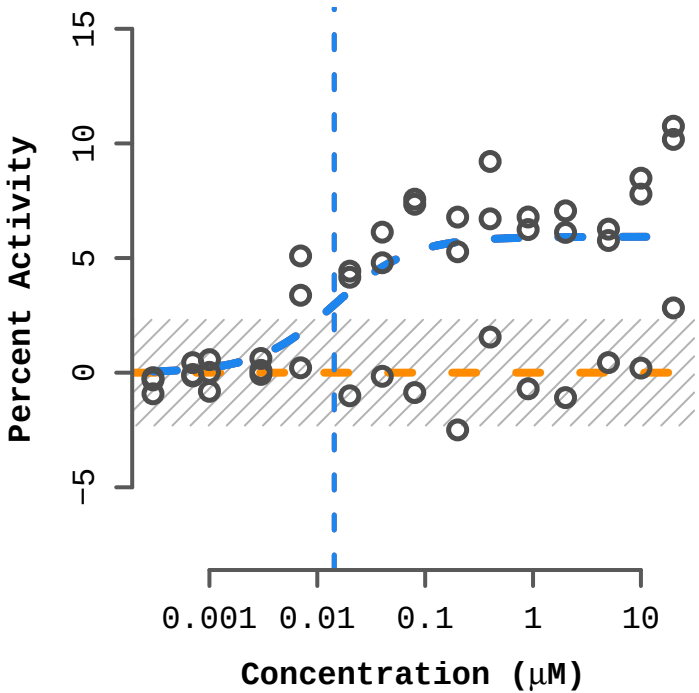
NAME: Alilusem potassium
CHID: 48807 CASRN: 114417-20-8
SPID(S): Tox21_113284
M4ID: 12482739

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.681 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mebanazine
CHID: 48808 CASRN: 3979-76-8
SPID(S): Tox21_113285
M4ID: 12482738

HILL MODEL (in red):

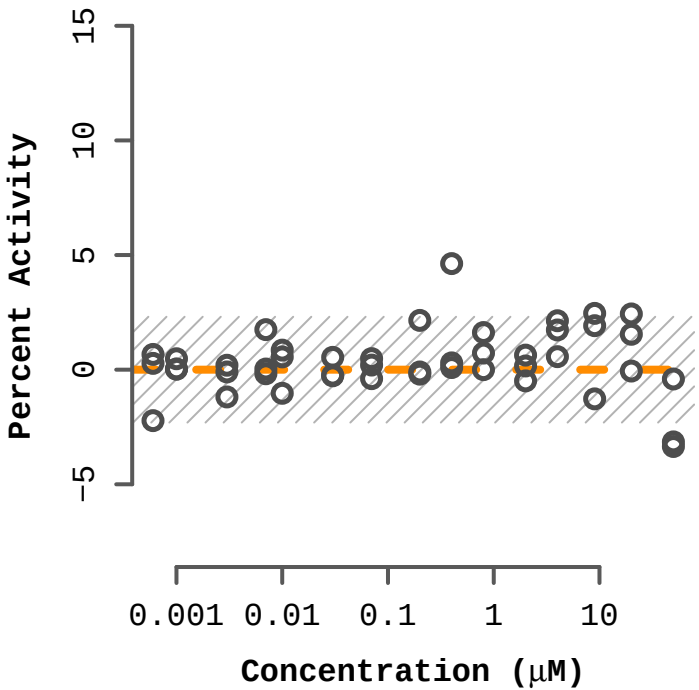
	tp	ga	gw
val:	5.93	−1.84	1.22
sd:	0.75	0.283	0.63

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.93	−1.84	1.22	2.01	12.2
sd:	0.75	0.283	0.63	1320	22600

	CNST	HILL	GNLS
AIC:	275.16	235.3	239.3
PROB:	0	0.88	0.12
RMSE:	4.88	3.1	3.1

MAX_MEAN: 7.92 **MAX_MED:** 10.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

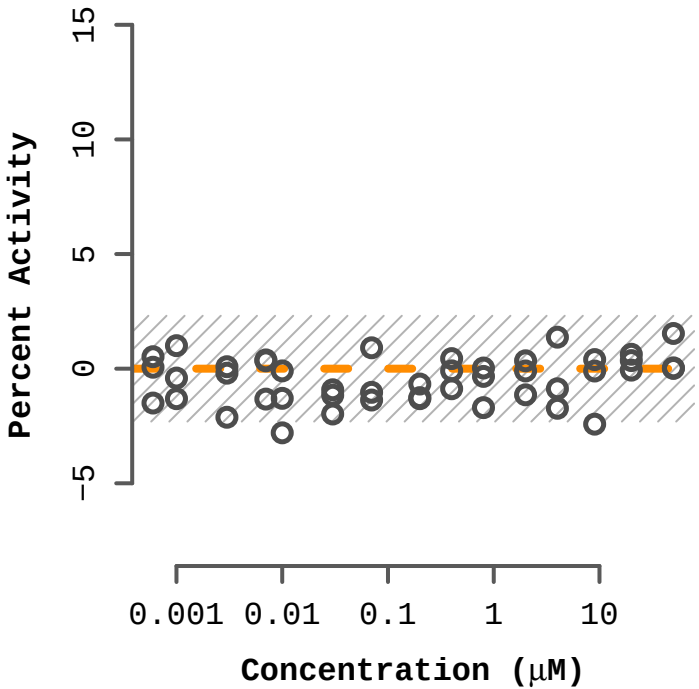
NAME: Melinamide
CHID: 48809 **CASRN:** 14417-88-0
SPID(S): Tox21_113286
M4ID: 12482737

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

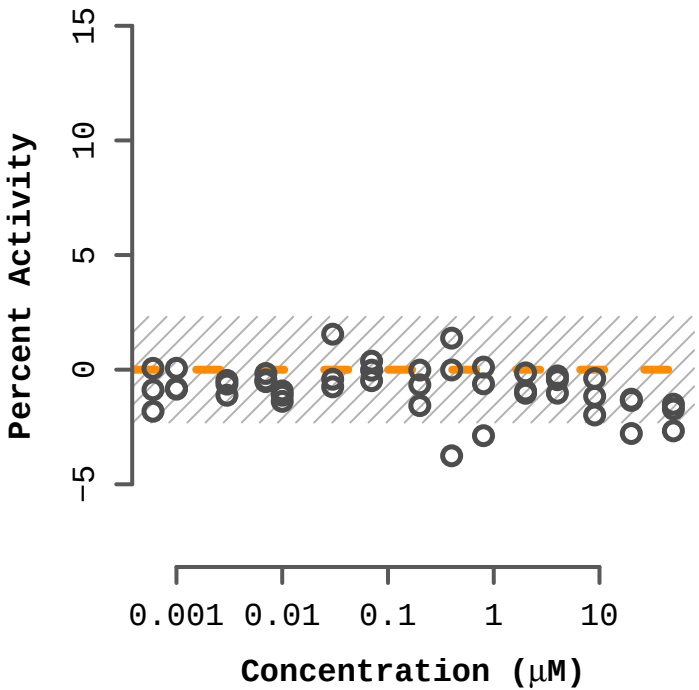
NAME: Meluadrine
CHID: 48810 **CASRN:** 134865-33-1
SPID(S): Tox21_113287
M4ID: 12482736

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.356 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

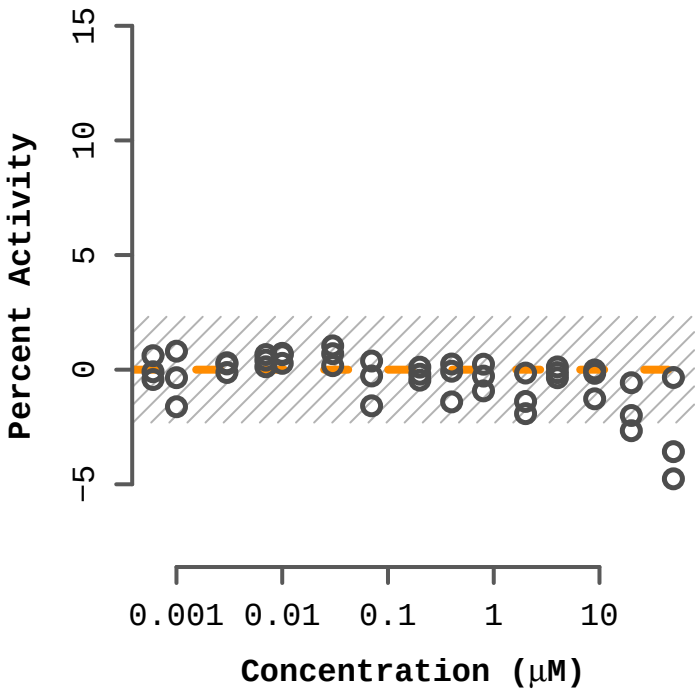
NAME: Monatepil
CHID: 48811 CASRN: 103377-41-9
SPID(S): Tox21_113288
M4ID: 12482735

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.129 MAX_MED: −0.0108 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

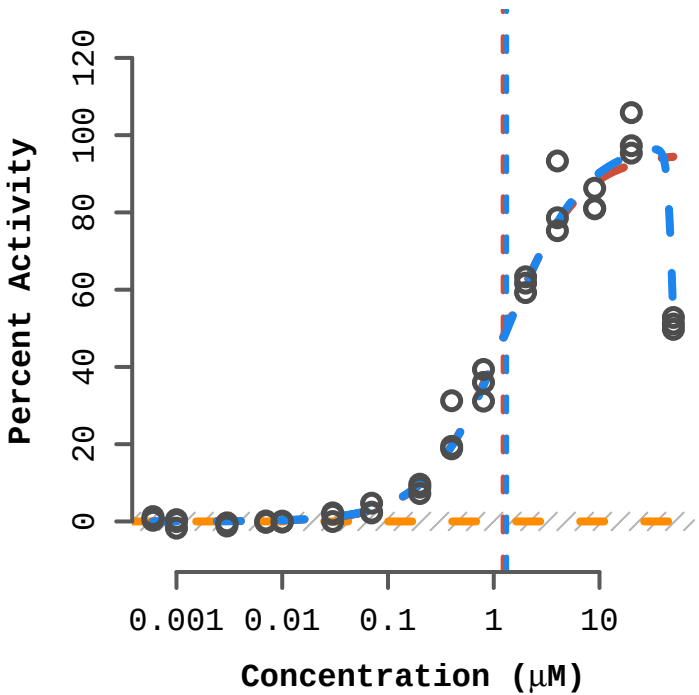
NAME: Lemildipine
CHID: 48812 **CASRN:** 94739-29-4
SPID(S): Tox21_113289
M4ID: 12482734

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.639 **MAX_MED:** 0.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxendolone
CHID: 48814 **CASRN:** 33765-68-3
SPID(S): Tox21_113291
M4ID: 12482733

HILL MODEL (in red):

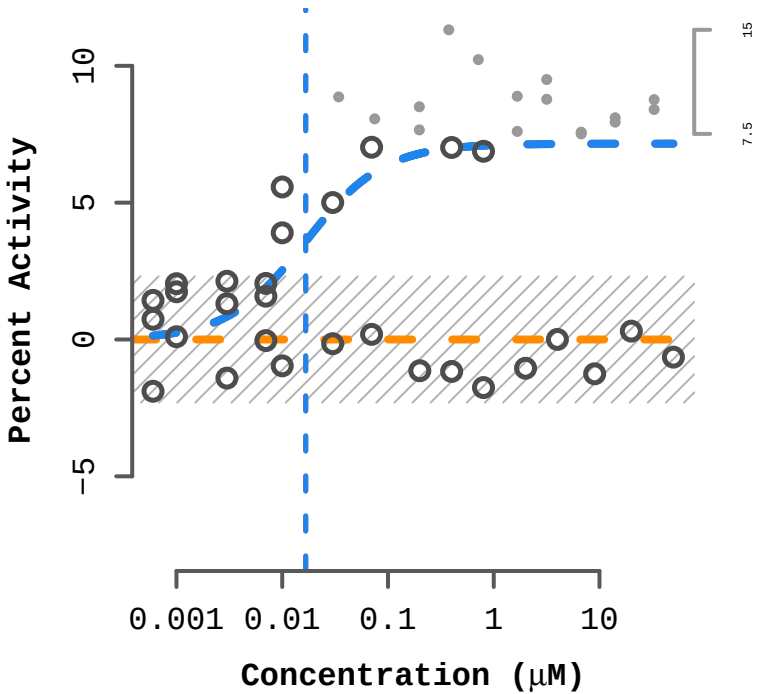
	tp	ga	gw
val:	95.5	0.0892	1.21
sd:	3.77	0.0421	0.0796

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	98.7	0.122	1.17	1.7	15.6
sd:	2.13	0.0253	0.0474	0.00277	9.09

	CNST	HILL	GNLS
AIC:	473.32	302.63	238.51
PROB:	0	0	1
RMSE:	46.16	11.91	4.06

MAX_MEAN: 99.5 **MAX_MED:** 97.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Penflutizide
CHID: 48815 **CASRN:** 1766-91-2
SPID(S): Tox21_113292
M4ID: 12482732 **BRK**

HILL MODEL (in red):

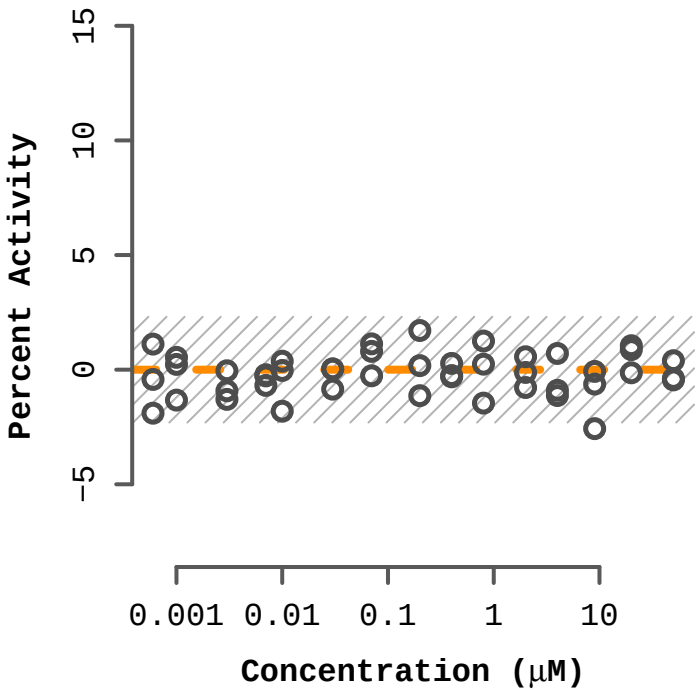
	tp	ga	gw
val:	7.16	−1.78	1.18
sd:	1.06	0.33	0.975

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.16	−1.78	1.18	2.73	7.76
sd:	1.06	0.33	0.975	1880	14100

	CNST	HILL	GNLS
AIC:	299.42	267.24	271.24
PROB:	0	0.88	0.12
RMSE:	6.4	4.26	4.26

MAX_MEAN: 7.23 **MAX_MED:** 10.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

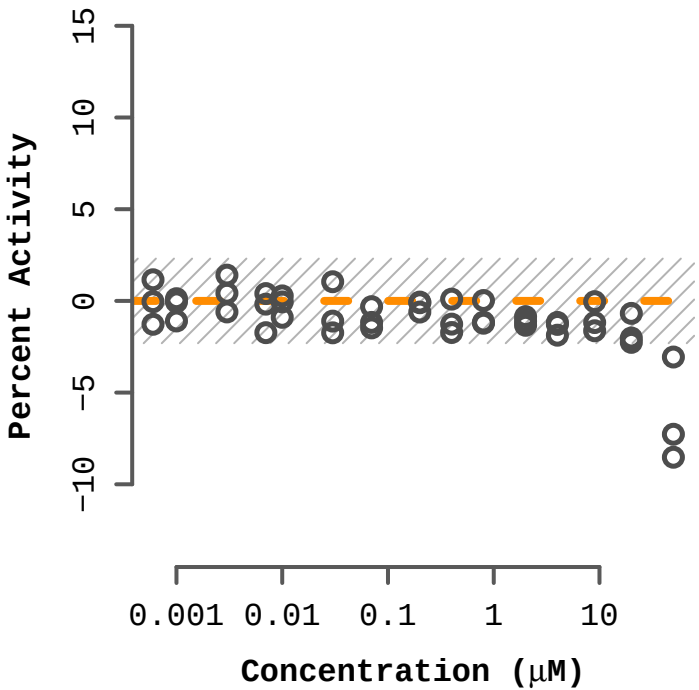
NAME: Doranidazole
CHID: 48817 CASRN: 149838-23-3
SPID(S): Tox21_113294
M4ID: 12482731

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.597 **MAX_MED:** 0.877 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

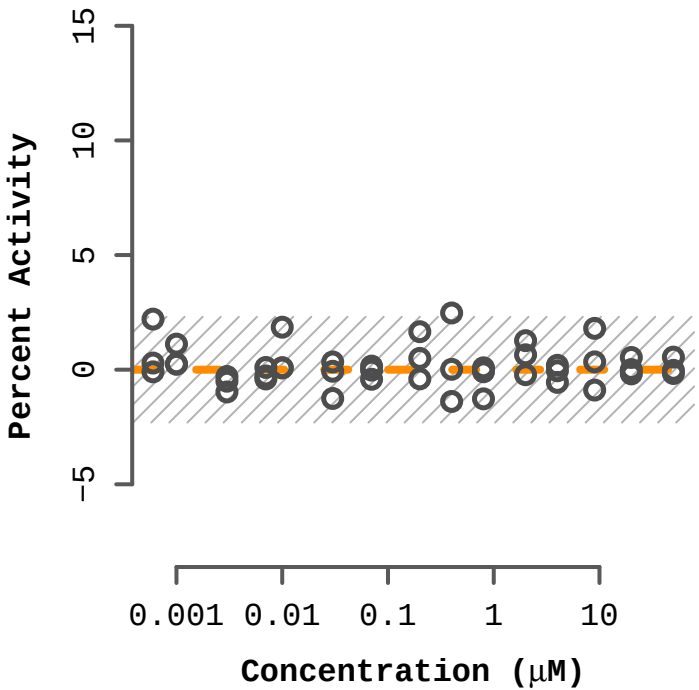
NAME: Tolindate
CHID: 48818 **CASRN:** 27877-51-6
SPID(S): Tox21_113298
M4ID: 12482727

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.59	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 0.41 **MAX_MED:** 0.421 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

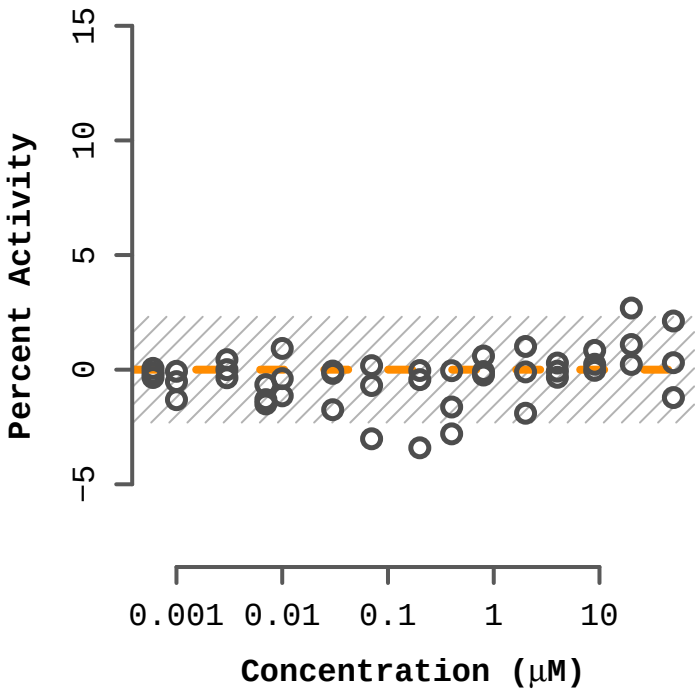
NAME: Acreozast
CHID: 48819 **CASRN:** 123548-56-1
SPID(S): Tox21_113299
M4ID: 12482726

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.7	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.802 **MAX_MED:** 0.652 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

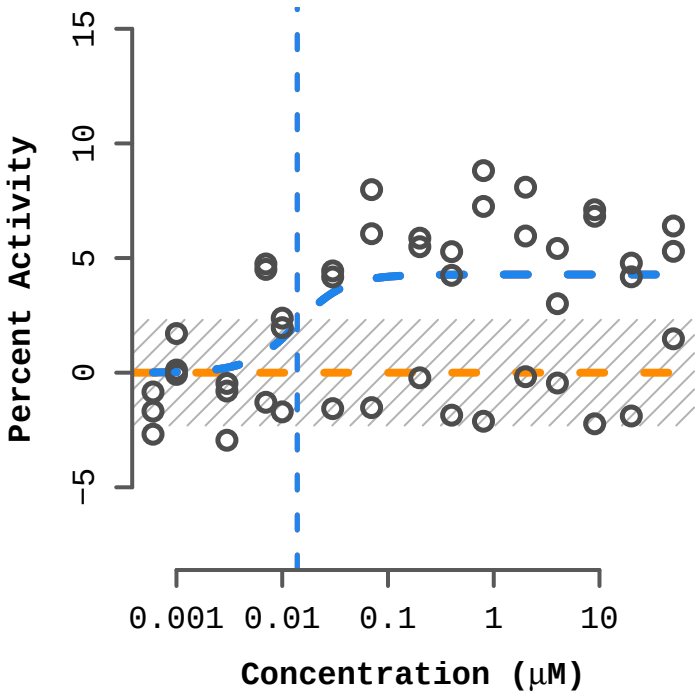
NAME: Zelandopam
CHID: 48820 **CASRN:** 139233-53-7
SPID(S): Tox21_113301
M4ID: 12482724

HILL MODEL: Not applicable.

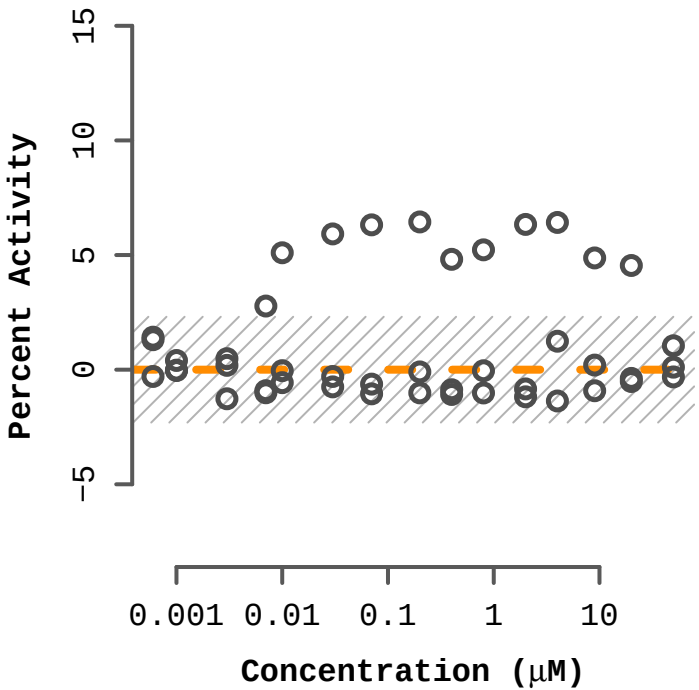
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.1 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cefteram
CHID:    48821   CASRN: 82547-58-8
SPID(S): Tox21_113302
M4ID:    12482723

HILL MODEL (in red):
      tp       ga       gw
val:  4.28     -1.86    1.91
sd:   0.713    0.345    1.49

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.28     -1.86    1.91     3.04     5.37
sd:   0.713    0.345    1.49     1470     5910

      CNST        HILL        GNLS
AIC:  265.59      243.04      247.04
PROB: 0           0.88        0.12
RMSE: 4.29        3.16        3.16

MAX_MEAN: 4.65      MAX_MED: 7.25      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

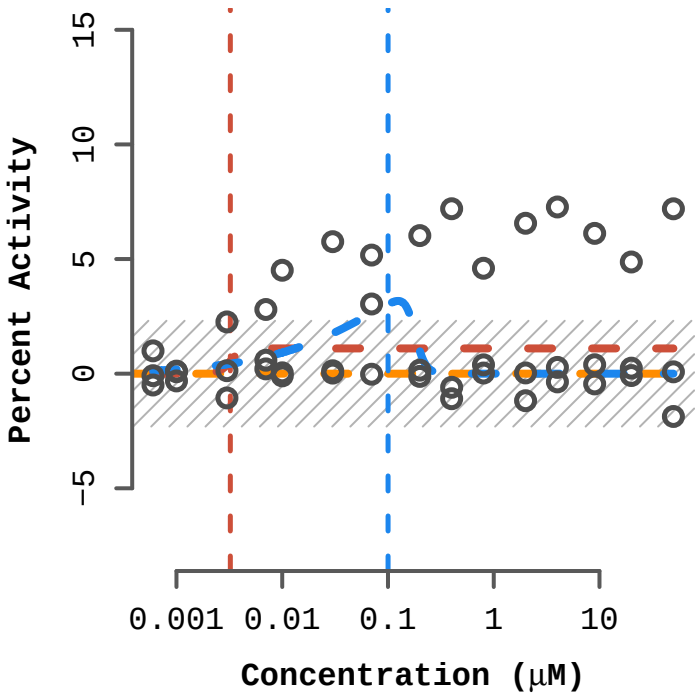
NAME: Glyclopyramide
CHID: 48822 **CASRN:** 631-27-6
SPID(S): Tox21_113303
M4ID: 12482722

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.78	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Rapacuronium bromide
CHID: 48823 CASRN: 156137-99-4
SPID(S): Tox21_113304
M4ID: 12482721

HILL MODEL (in red):

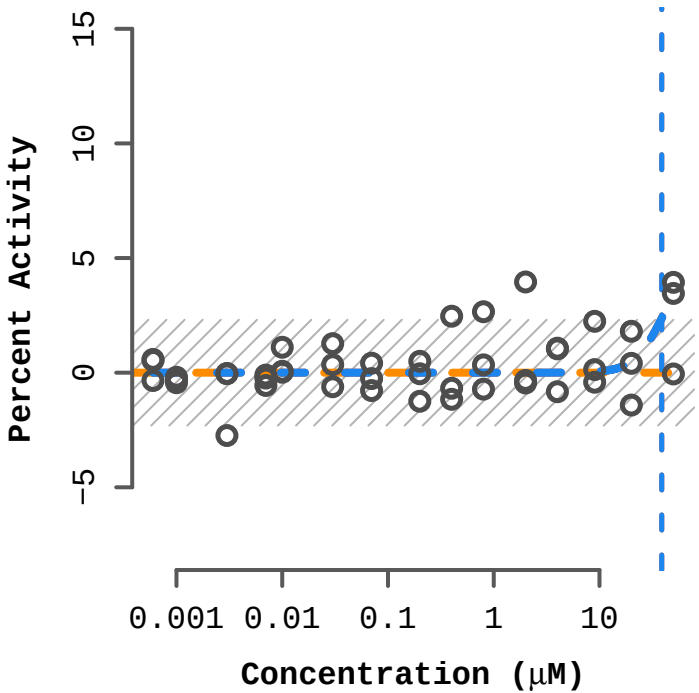
	tp	ga	gw
val:	1.1	−2.49	8
sd:	0.466	0.535	122

GAIN-LOSS MODEL (in blue):

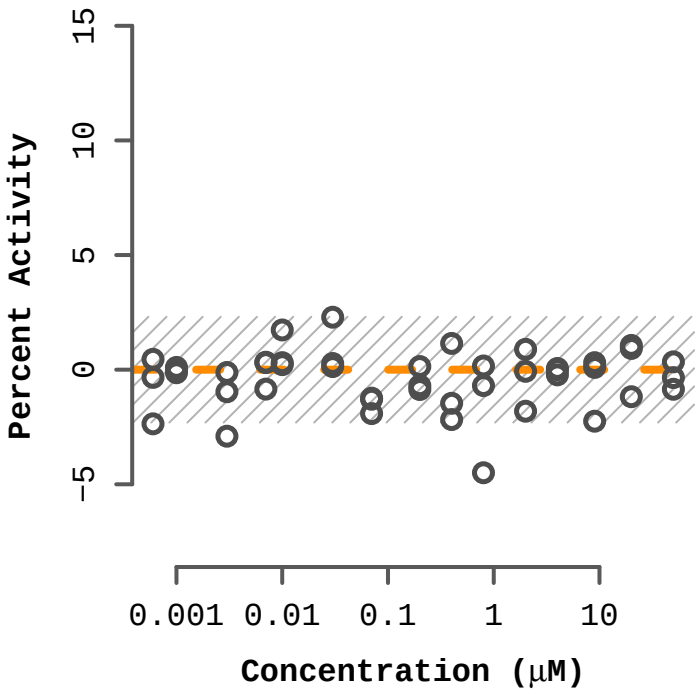
	tp	ga	gw	la	lw
val:	6.1	−0.999	0.75	−0.749	9.05
sd:	25.9	4.26	0.952	0.697	123

	CNST	HILL	GNLS
AIC:	224.94	223.88	228.57
PROB:	0.35	0.59	0.06
RMSE:	3.09	2.68	2.9

MAX_MEAN: 2.73 MAX_MED: 3.04 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Propanidid
CHID:    48825   CASRN: 1421-14-3
SPID(S): Tox21_113307
M4ID:    12482719

HILL MODEL (in red):
      tp       ga       gw
val:  4.75     1.59     3.28
sd:   12.9     0.931    8.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.75     1.59     3.28     3.65     3.47
sd:   13       0.935    8.13     2510     4500

      CNST        HILL        GNLS
AIC:  152.04      149.2       153.2
PROB: 0.18        0.73        0.1
RMSE: 1.39        1.26        1.26

MAX_MEAN: 2.45      MAX_MED: 3.46      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

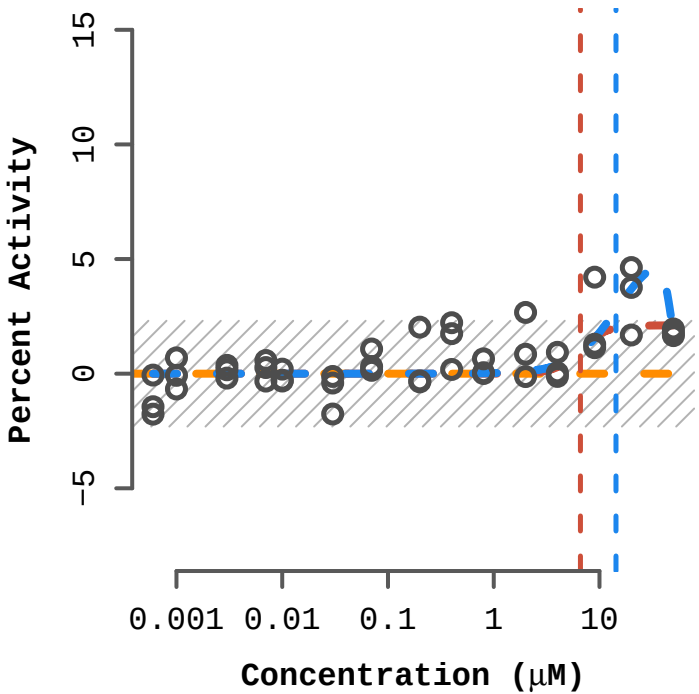
NAME: Nitrefazole
CHID: 48826 **CASRN:** 21721-92-6
SPID(S): Tox21_113308
M4ID: 12482718

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.899 **MAX_MED:** 0.927 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clometacine
CHID: 48827 CASRN: 25803-14-9
SPID(S): Tox21_113309
M4ID: 12482717

HILL MODEL (in red):

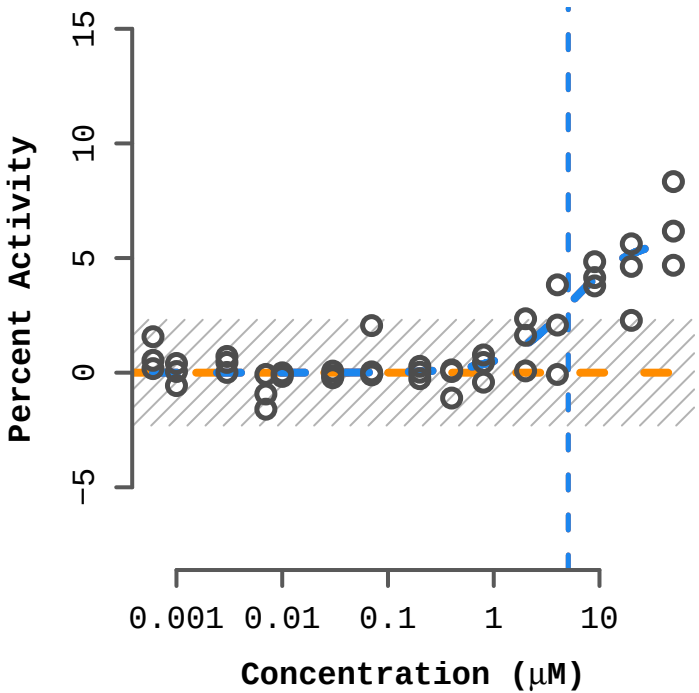
	tp	ga	gw
val:	2.11	0.82	3.64
sd:	0.367	0.147	2.96

GAIN-LOSS MODEL (in blue):

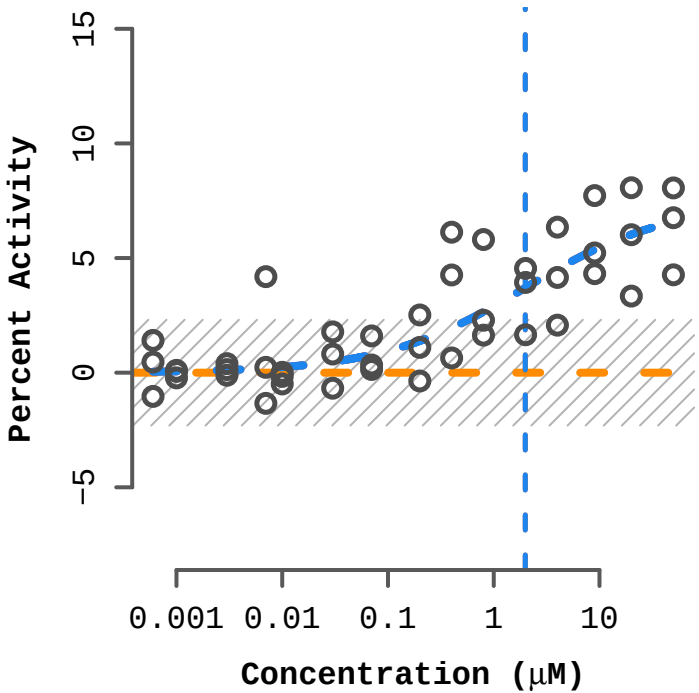
	tp	ga	gw	la	lw
val:	5.56	1.16	2.05	1.67	10.7
sd:	6.4	0.564	2.21	0.0319	16.1

	CNST	HILL	GNLS
AIC:	160.11	134.95	133.05
PROB:	0	0.28	0.72
RMSE:	1.51	1.05	1

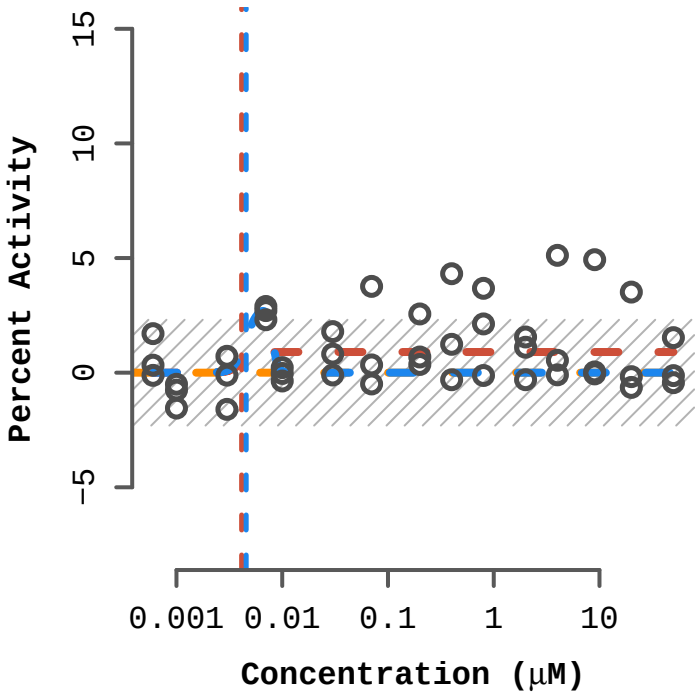
MAX_MEAN: 3.36 **MAX_MED:** 3.76 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pifoxime
CHID:    48828   CASRN: 31224-92-7
SPID(S): Tox21_113310
M4ID:    12482716

HILL MODEL (in red):
      tp       ga       gw
val:  5.88     0.705    1.45
sd:   0.812    0.138    0.391

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.88     0.705    1.45     3.13     5.67
sd:   0.812    0.138    0.391    1220     4830

      CNST        HILL        GNLS
AIC:  201.97      126.43      130.43
PROB: 0           0.88        0.12
RMSE: 2.51        0.98        0.98

MAX_MEAN: 6.4       MAX_MED: 6.18      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4'-Piperidinylcarbonylmethoxyacetophenone
CHID:    48829   CASRN: 31188-99-5
SPID(S): Tox21_113311
M4ID:    12482715

HILL MODEL (in red):
      tp       ga       gw
val:  7.4      0.298    0.64
sd:   1.76     0.451    0.209

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.4      0.298    0.64     3.44     4.42
sd:   1.76     0.451    0.209    3140     8000

      CNST        HILL        GNLS
AIC:  245.48      173.82      177.82
PROB: 0           0.88        0.12
RMSE: 3.6         1.54        1.54

MAX_MEAN: 6.36      MAX_MED: 6.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fenclofenac
CHID: 48830 CASRN: 34645-84-6
SPID(S): Tox21_113312
M4ID: 12482714

HILL MODEL (in red):

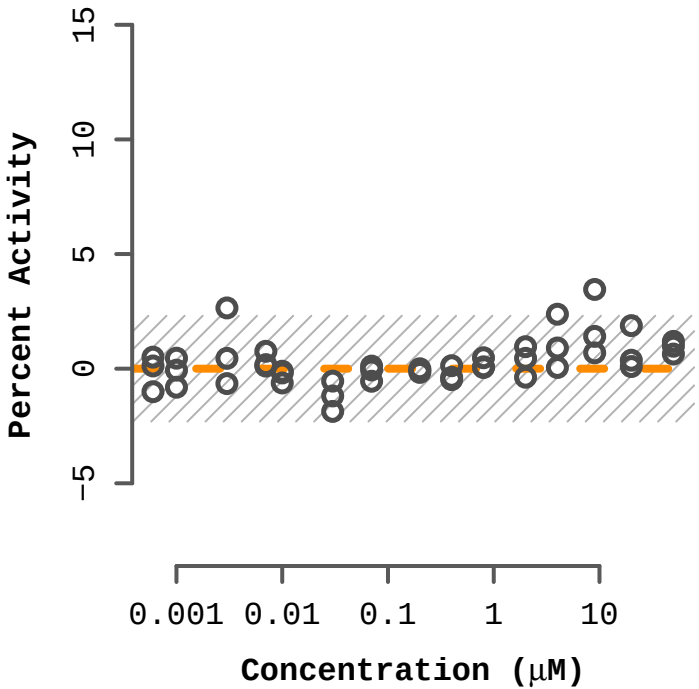
	tp	ga	gw
val:	0.902	−2.38	8
sd:	0.27	0.214	9.36

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.9	−2.34	8	−2.09	18
sd:	2.1	0.277	11.3	0.197	24.3

	CNST	HILL	GNLS
AIC:	183.83	177.59	182.73
PROB:	0.04	0.89	0.07
RMSE:	1.91	1.58	1.79

MAX_MEAN: 2.64 **MAX_MED:** 2.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

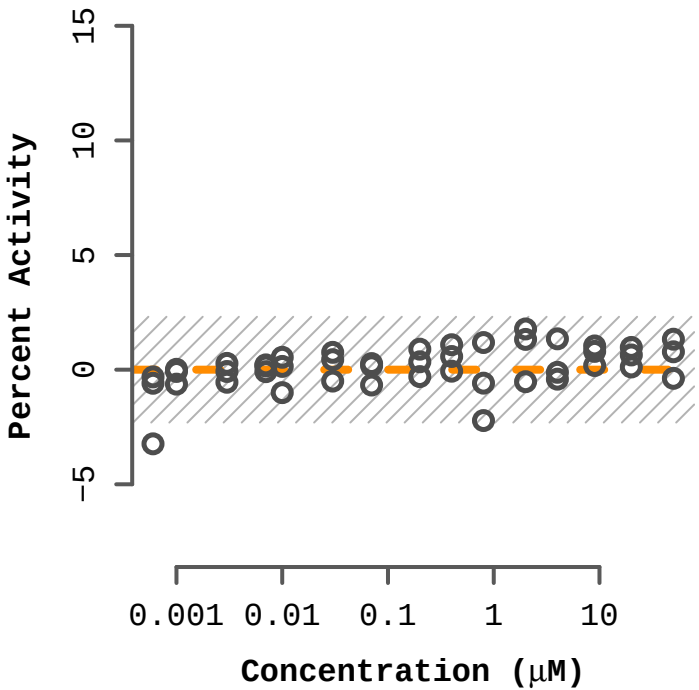
NAME: Amineptine
CHID: 48831 CASRN: 57574-09-1
SPID(S): Tox21_113313
M4ID: 12482713

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

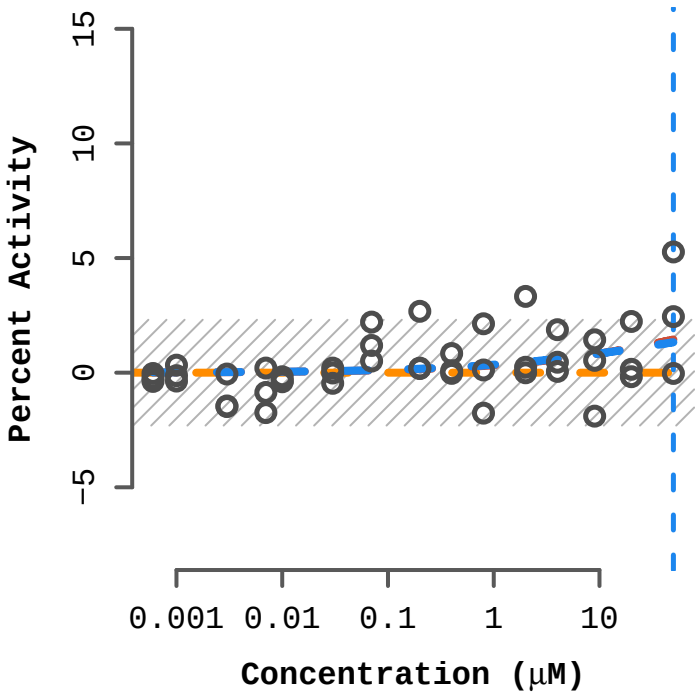
NAME: Flosequinan
CHID: 48833 **CASRN:** 76568-02-0
SPID(S): Tox21_113315
M4ID: 12482712

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.859 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tolrestat
CHID: 48834 CASRN: 75820-08-5
SPID(S): Tox21_113316
M4ID: 12482711

HILL MODEL (in red):

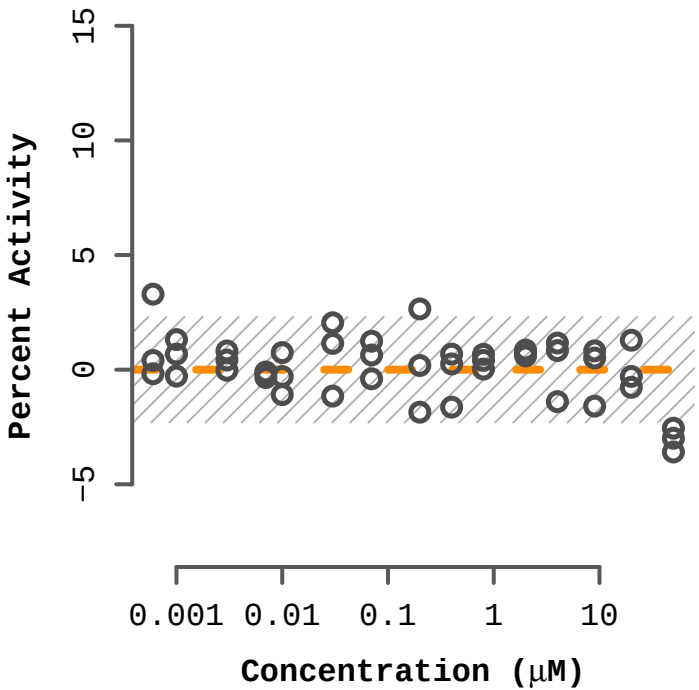
	tp	ga	gw
val:	3.96	2.2	0.478
sd:	22.6	6.7	0.298

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.65	1.7	0.483	2.15	18
sd:	41.9	21.1	0.452	575	22700

	CNST	HILL	GNLS
AIC:	152.67	151.5	155.57
PROB:	0.33	0.59	0.08
RMSE:	1.42	1.24	1.25

MAX_MEAN: 2.56 **MAX_MED:** 2.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

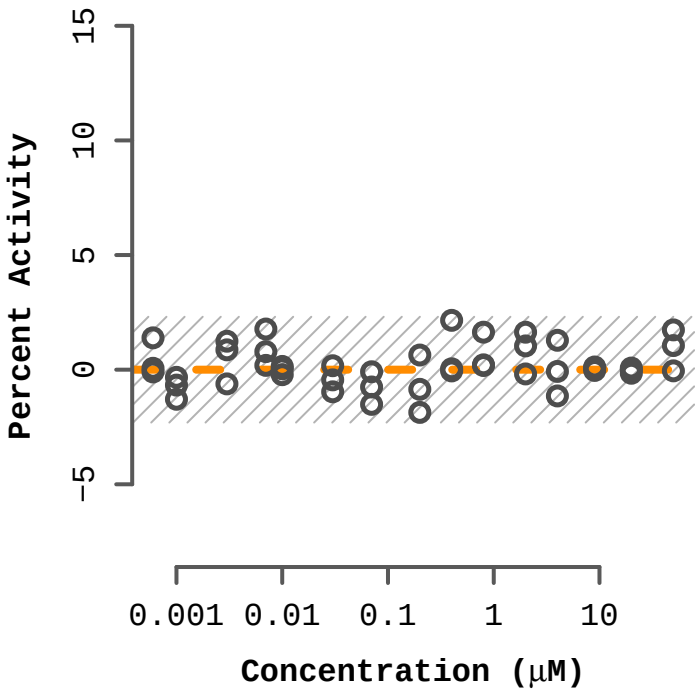
NAME: Thenalidine
CHID: 48835 **CASRN:** 86-12-4
SPID(S): Tox21_113317
M4ID: 12482710

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.17 **MAX_MED:** 1.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

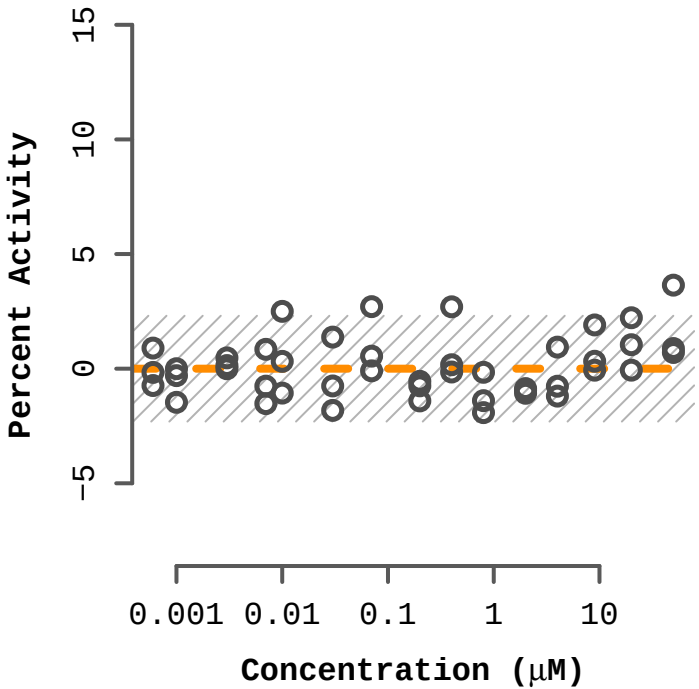
NAME: Tandospirone
CHID: 48836 **CASRN:** 87760-53-0
SPID(S): Tox21_113318
M4ID: 12482709

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.917 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

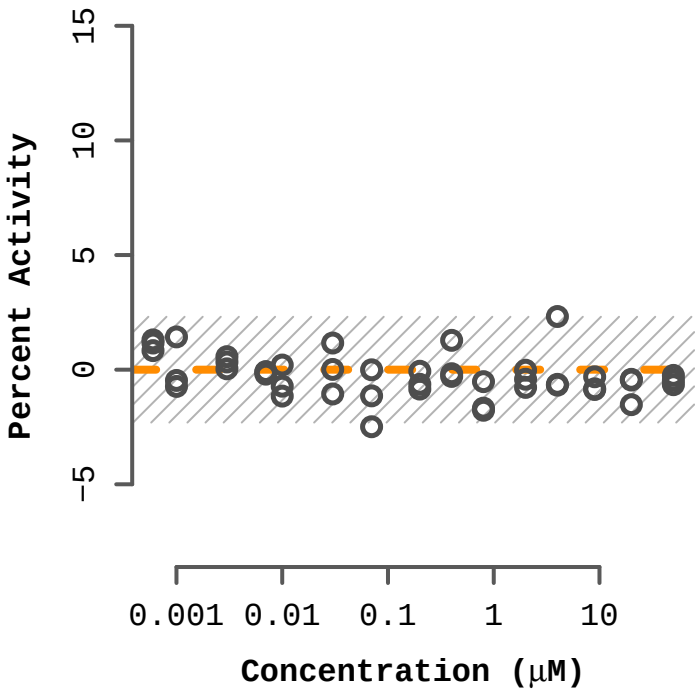
NAME: Phenoxypropazine
CHID: 48837 **CASRN:** 3818-37-9
SPID(S): Tox21_113319
M4ID: 12482708

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

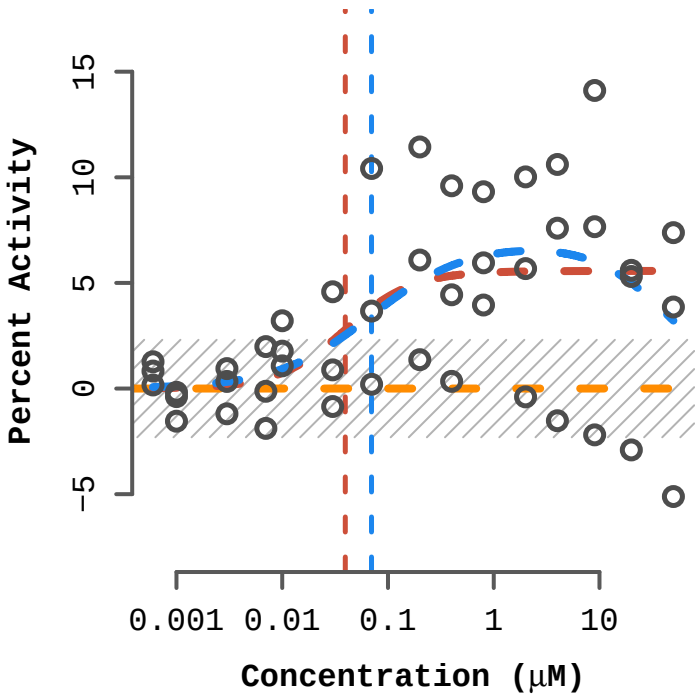
NAME: Amoproxan
CHID: 48838 CASRN: 22661-76-3
SPID(S): Tox21_113320
M4ID: 12482707

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bisoxatin acetate
CHID: 48839 CASRN: 14008-48-1
SPID(S): Tox21_113321
M4ID: 12482706

HILL MODEL (in red):

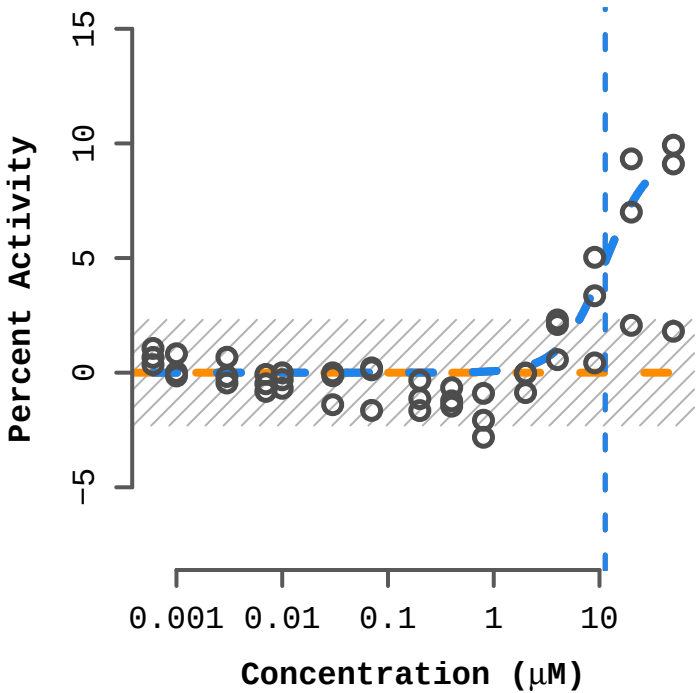
	tp	ga	gw
val:	5.57	−1.4	1.36
sd:	0.897	0.34	1.01

GAIN-LOSS MODEL (in blue):

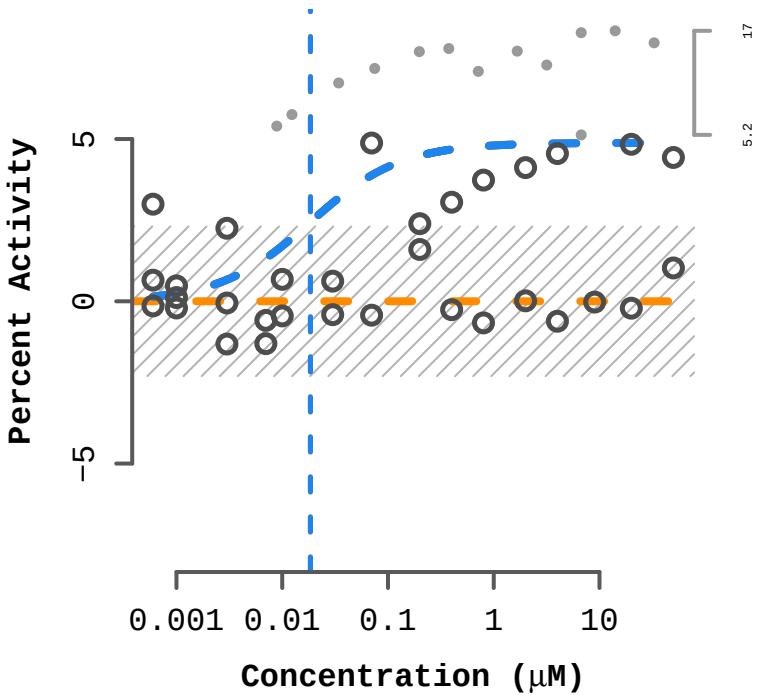
	tp	ga	gw	la	lw
val:	6.93	−1.16	0.965	1.65	1.22
sd:	2.63	0.646	0.828	0.543	1.63

	CNST	HILL	GNLS
AIC:	282.1	255.89	258.36
PROB:	0	0.77	0.23
RMSE:	5.43	3.88	3.78

MAX_MEAN: 6.53 MAX_MED: 7.66 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Safrazine hydrochloride
CHID:    48840   CASRN: 7296-30-2
SPID(S): Tox21_113323
M4ID:    12482704

HILL MODEL (in red):
      tp       ga       gw
val:  9.65     1.05     2.04
sd:   0.996    0.0941   0.514

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.65     1.05     2.04     2.96     5.39
sd:   0.996    0.0941   0.514    937      4000

      CNST        HILL        GNLS
AIC:  205.58      166.31      170.31
PROB: 0           0.88        0.12
RMSE: 2.99        1.74        1.74

MAX_MEAN: 6.95      MAX_MED: 9.11      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (2R)−2−Propyloctanoic acid
CHID: 48841 CASRN: 185517−21−9
SPID(S): Tox21_113324
M4ID: 12482703 BRK

HILL MODEL (in red):

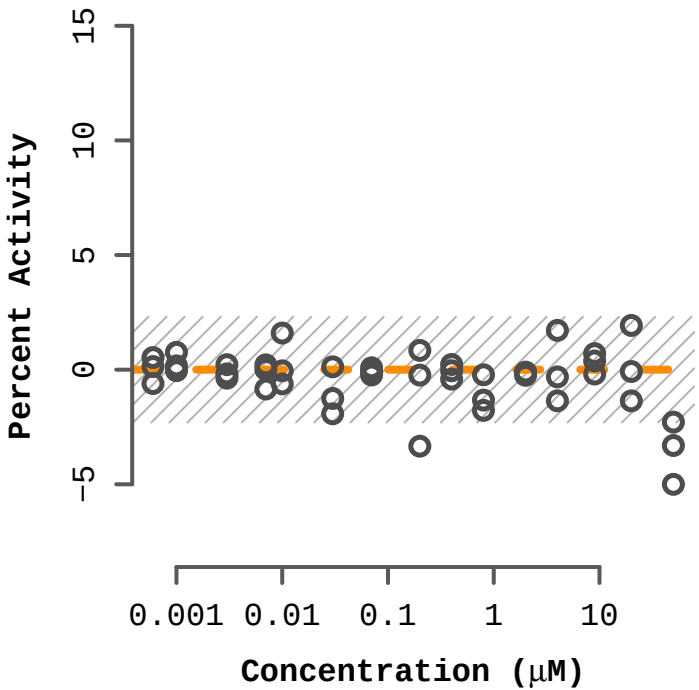
	tp	ga	gw
val:	4.88	−1.73	1.02
sd:	1.48	0.731	1.78

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.88	−1.73	1.02	3.17	4.06
sd:	1.48	0.731	1.78	687	1880

	CNST	HILL	GNLS
AIC:	301.88	286.44	290.44
PROB:	0	0.88	0.12
RMSE:	7.14	5.27	5.27

MAX_MEAN: 7.22 MAX_MED: 5.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

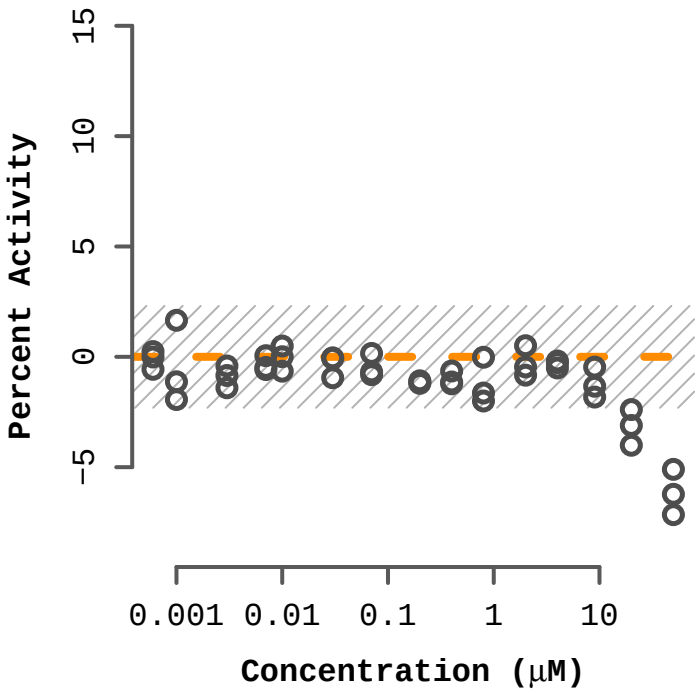
NAME: Proglumetacin
CHID: 48842 CASRN: 57132-53-3
SPID(S): Tox21_113325
M4ID: 12482702

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.31 **MAX_MED:** 0.382 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

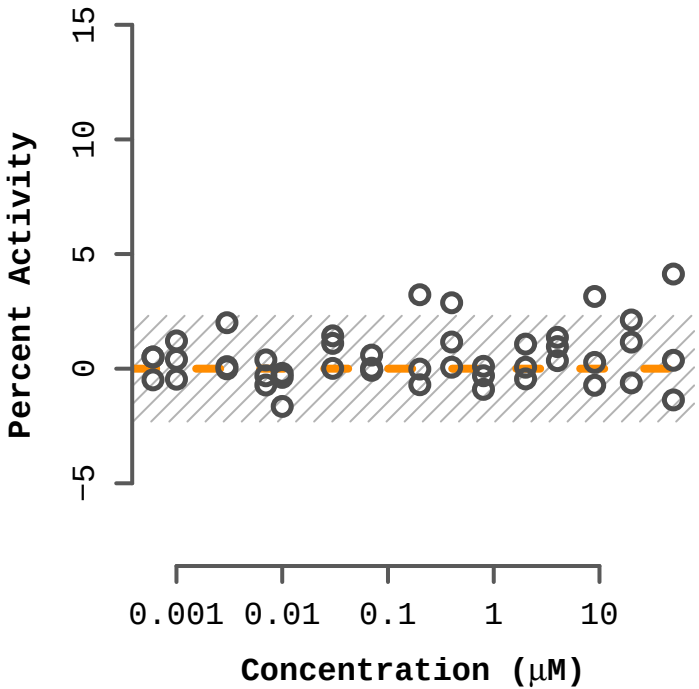
NAME: Ethyl 4-nitrophenyl ethylphosphonate
CHID: 48843 CASRN: 546-71-4
SPID(S): Tox21_113326
M4ID: 12482701

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.78	NA	NA
PROB:	1	NA	NA
RMSE:	2.01	NA	NA

MAX_MEAN: −0.0507 **MAX_MED:** 0.00631 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

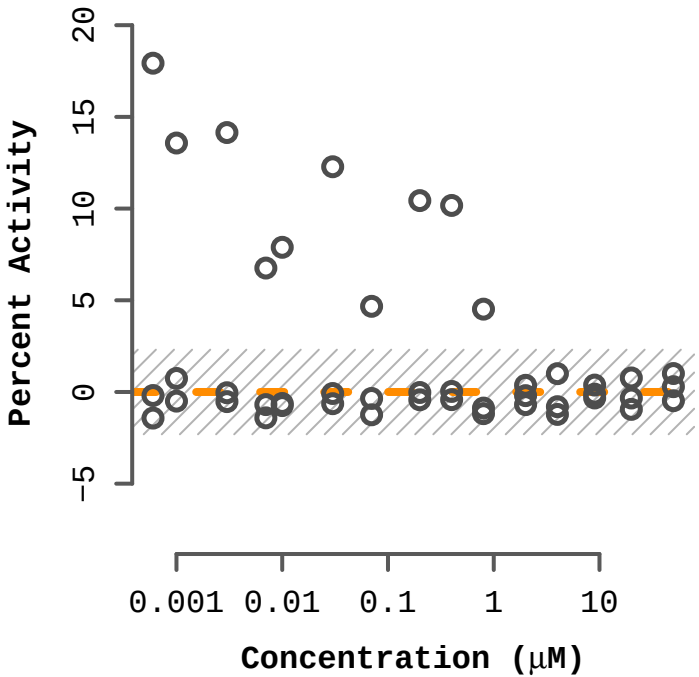
NAME: Mefruside
CHID: 48844 CASRN: 7195-27-9
SPID(S): Tox21_113327
M4ID: 12482700

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.37 MAX_MED: 1.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

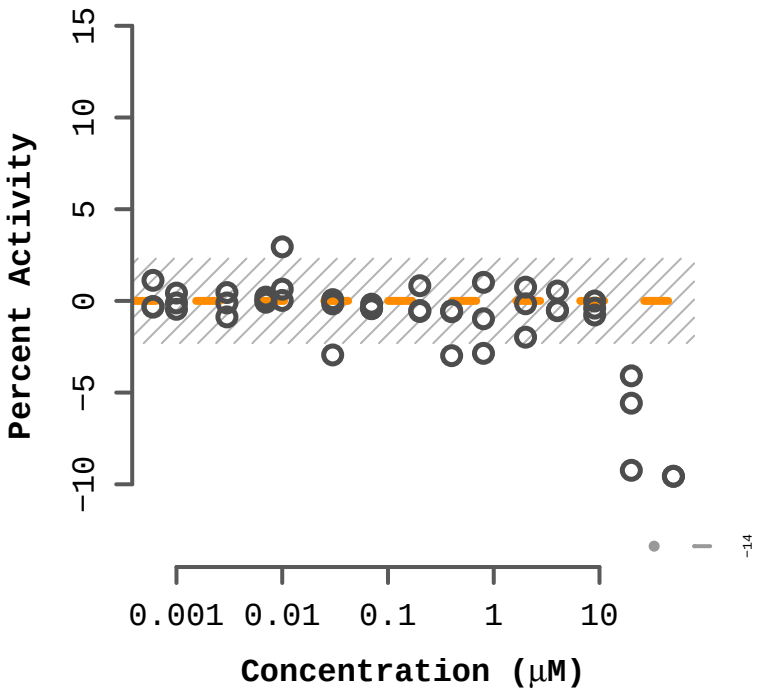
NAME: Flomoxef
CHID: 48845 CASRN: 99665-00-6
SPID(S): Tox21_113328
M4ID: 12482699

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.13	NA	NA
PROB:	1	NA	NA
RMSE:	5.24	NA	NA

MAX_MEAN: 5.44 MAX_MED: 0.738 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

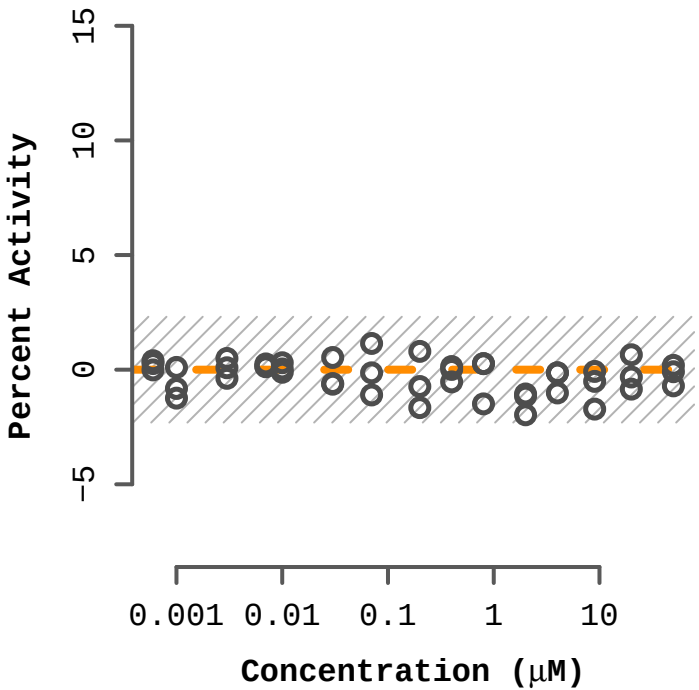
NAME: Mosapramine
CHID: 48846 **CASRN:** 89419-40-9
SPID(S): Tox21_113329
M4ID: 12482698 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.21	NA	NA
PROB:	1	NA	NA
RMSE:	3.54	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.642 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

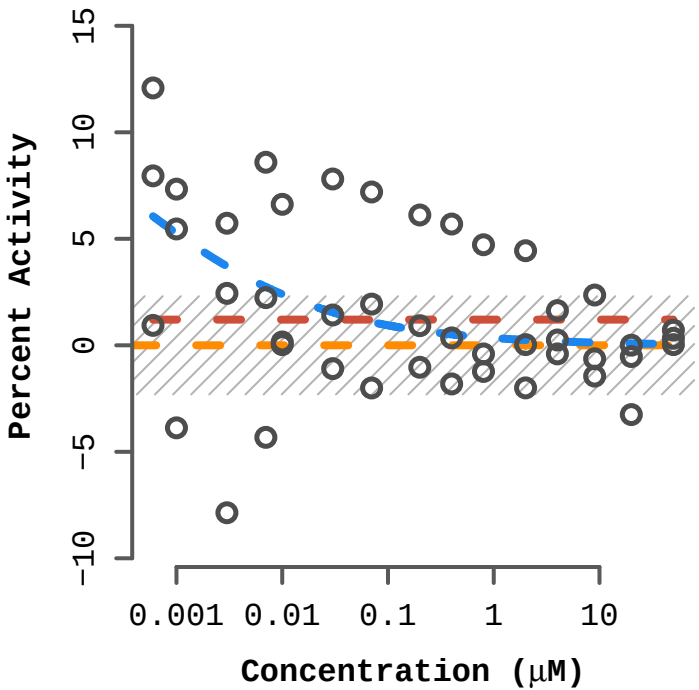
NAME: Sitafloxacin
CHID: 48847 **CASRN:** 127254-12-0
SPID(S): Tox21_113330
M4ID: 12482697

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 0.217 **MAX_MED:** 0.268 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Aceglatone
CHID: 48848 CASRN: 642-83-1
SPID(S): Tox21_113332
M4ID: 12482695

HILL MODEL (in red):

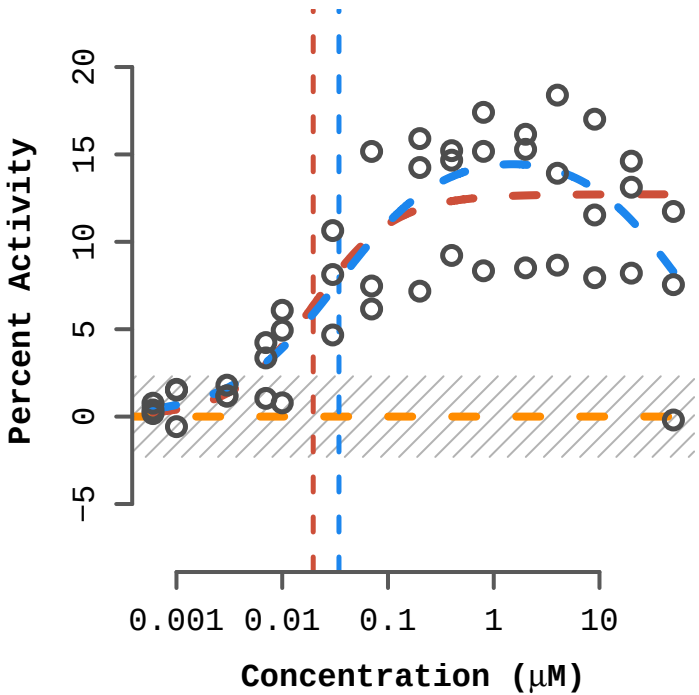
	tp	ga	gw
val:	1.21	−5.08	3.95
sd:	0.574	1590	3360

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.5	−4.53	6.27	−3.54	0.457
sd:	19.1	2140	10200	2.03	0.282

	CNST	HILL	GNLS
AIC:	259.35	260.75	256.14
PROB:	0.15	0.08	0.77
RMSE:	4.27	3.97	3.75

MAX_MEAN: 6.99 **MAX_MED:** 7.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Difeterol
CHID: 48849 CASRN: 14587-50-9
SPID(S): Tox21_113333
M4ID: 12482694

HILL MODEL (in red):

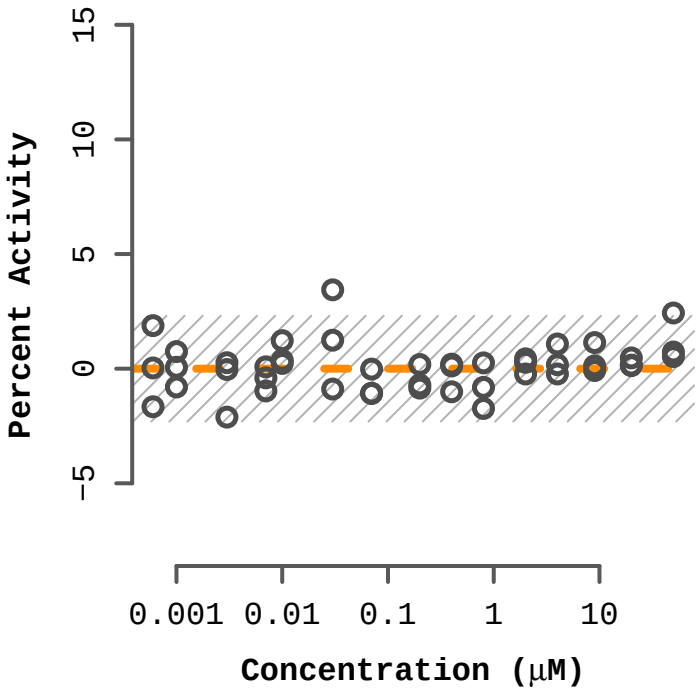
	tp	ga	gw
val:	12.7	−1.71	1.14
sd:	0.893	0.153	0.335

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.5	−1.46	0.876	1.77	0.92
sd:	3.82	0.362	0.321	0.277	1.15

	CNST	HILL	GNLS
AIC:	343.43	247.72	244.62
PROB:	0	0.18	0.82
RMSE:	10.09	3.51	3.14

MAX_MEAN: 13.7 MAX_MED: 15.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

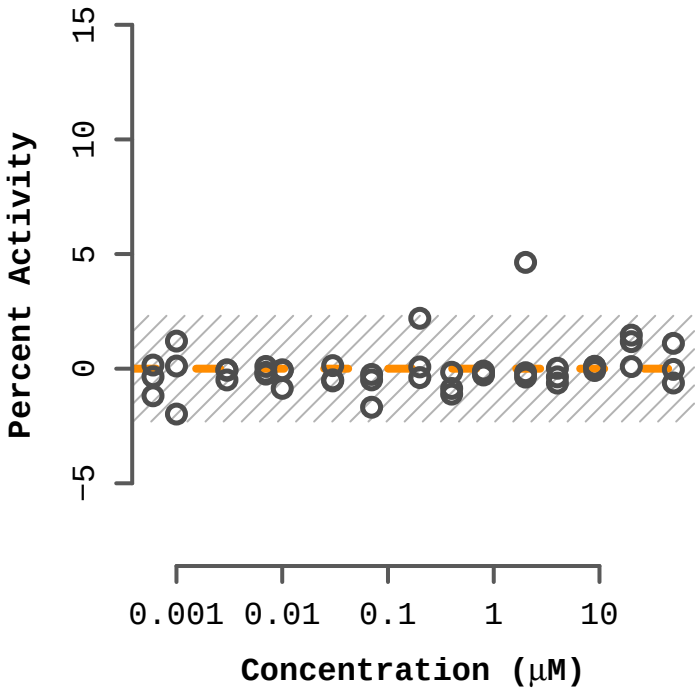
NAME: Sulcaine
CHID: 48850 CASRN: 41653-21-8
SPID(S): Tox21_113334
M4ID: 12482693

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

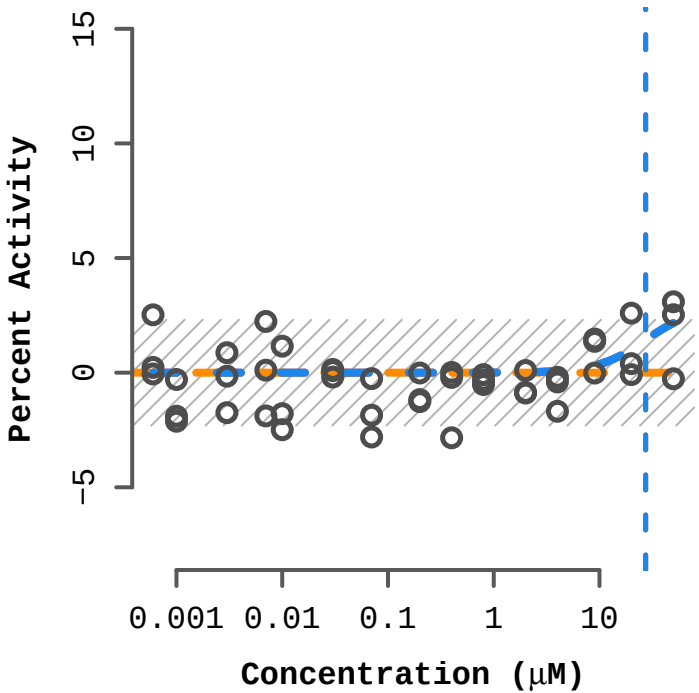
NAME: N,N−Dimethyl−2−(2−phenylacetamido)acetamide
CHID: 48851 **CASRN:** 25439−20−7
SPID(S): Tox21_113335
M4ID: 12482692

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Mepranoprofen arbamel
CHID: 48852 CASRN: 118635-52-2
SPID(S): Tox21_113336
M4ID: 12482690

HILL MODEL (in red):

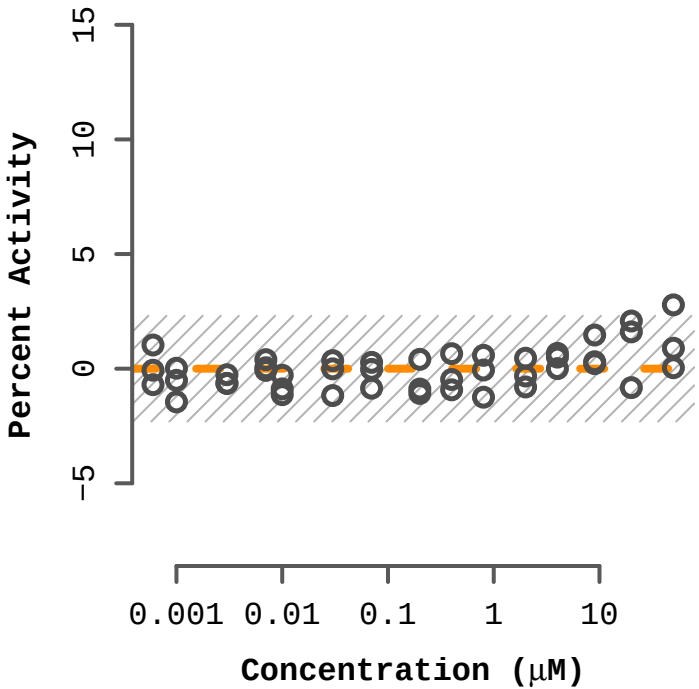
	tp	ga	gw
val:	2.85	1.44	1.9
sd:	3.42	0.753	1.71

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.85	1.44	1.9	3.38	3.43
sd:	3.43	0.753	1.71	713	1510

	CNST	HILL	GNLS
AIC:	163.88	163.47	167.47
PROB:	0.42	0.51	0.07
RMSE:	1.43	1.33	1.33

MAX_MEAN: 1.79 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

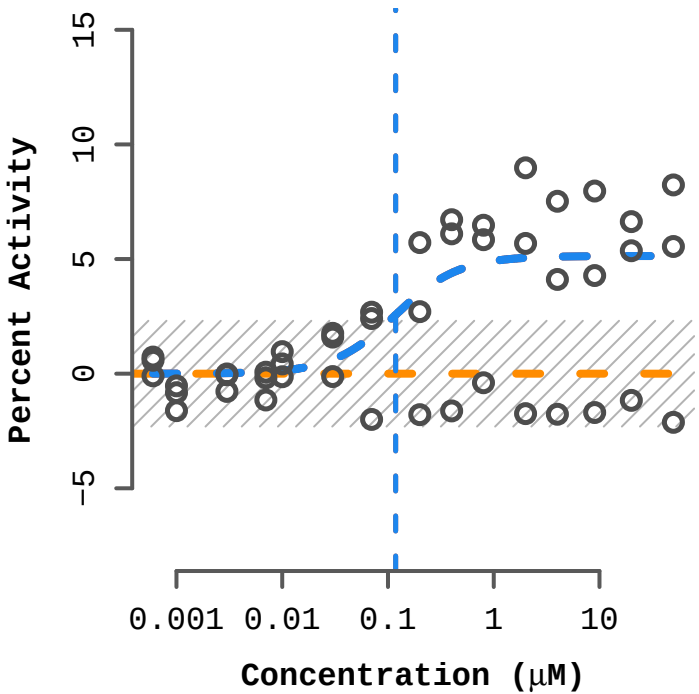
NAME: Mepranoprofen arbamel
CHID: 48852 CASRN: 118635-52-2
SPID(S): Tox21_113336_1
M4ID: 12482691

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Alloclamide
CHID: 48853 CASRN: 5486-77-1
SPID(S): Tox21_113338
M4ID: 12482689

HILL MODEL (in red):

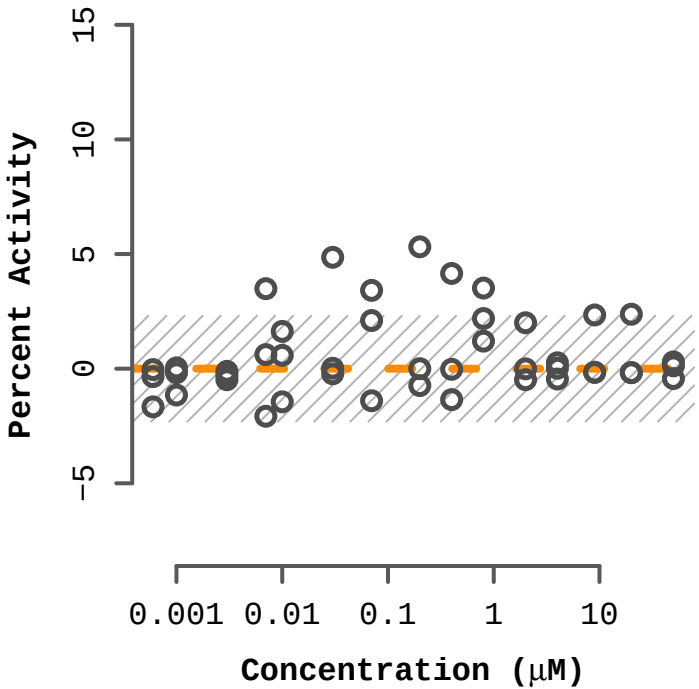
	tp	ga	gw
val:	5.13	−0.927	1.46
sd:	0.787	0.279	0.893

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.13	−0.927	1.46	2.39	11.9
sd:	0.787	0.279	0.893	1510	25900

	CNST	HILL	GNLS
AIC:	253.03	230.72	234.72
PROB:	0	0.88	0.12
RMSE:	3.91	3.02	3.02

MAX_MEAN: 4.31 MAX_MED: 6.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

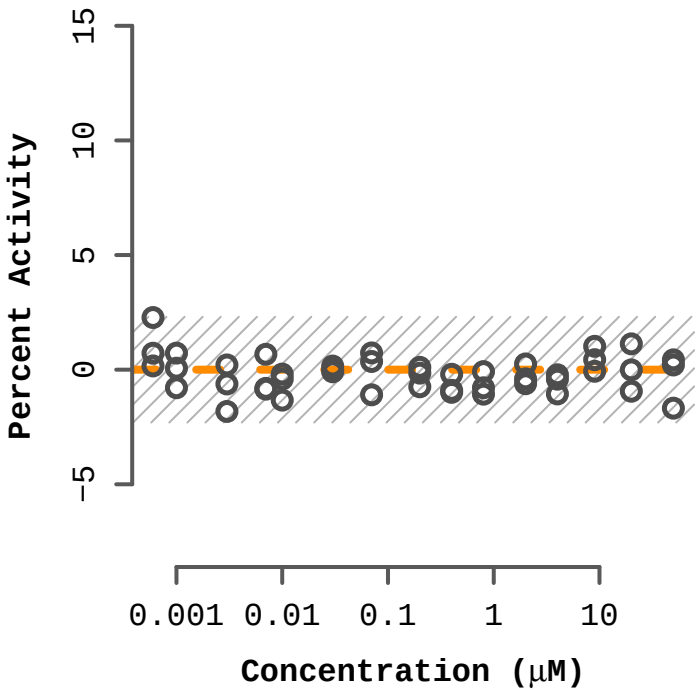
NAME: Bucolome
CHID: 48854 CASRN: 841-73-6
SPID(S): Tox21_113339
M4ID: 12482688

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 2.3 MAX_MED: 2.19 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

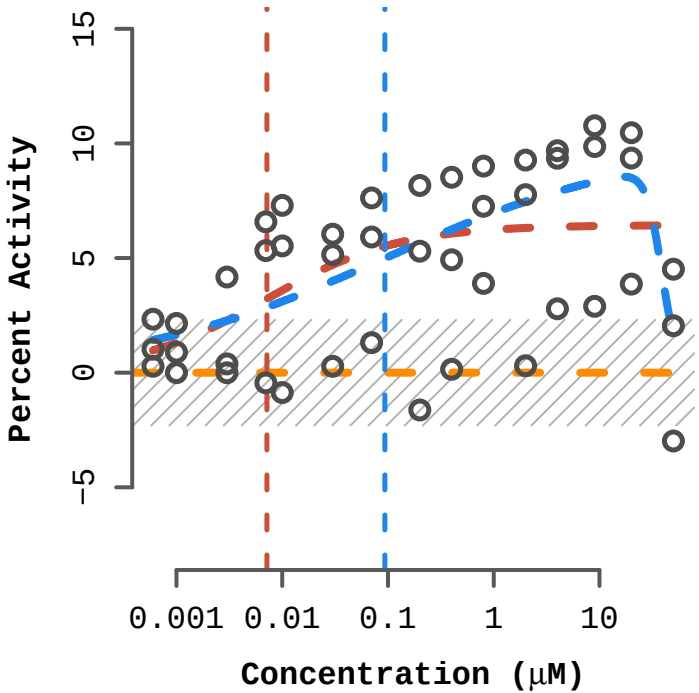
NAME: Fasoracetam
CHID: 48855 **CASRN:** 110958-19-5
SPID(S): Tox21_113340
M4ID: 12482687

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.719 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lanperisone hydrochloride
CHID: 48856 CASRN: 116287-13-9
SPID(S): Tox21_113341
M4ID: 12482686

HILL MODEL (in red):

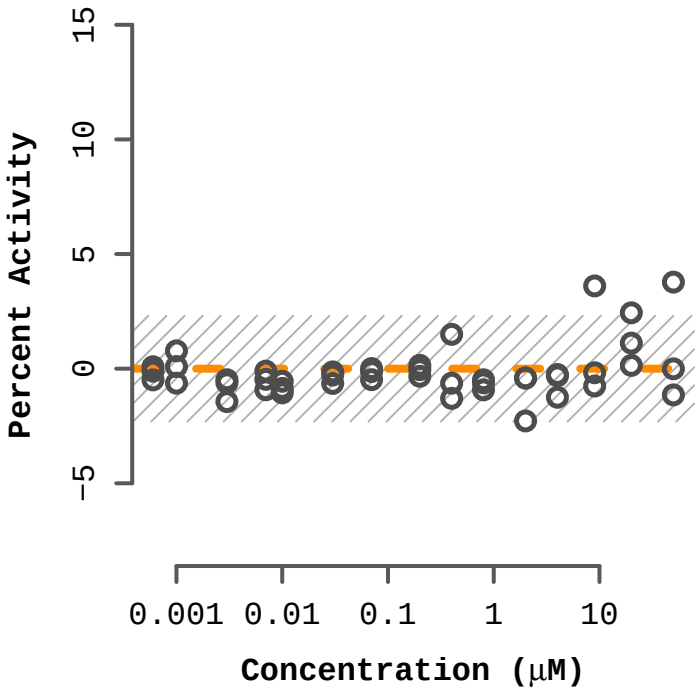
	tp	ga	gw
val:	6.44	−2.14	0.696
sd:	1.12	0.499	0.461

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.98	−1.03	0.355	1.59	5.76
sd:	6.04	1.88	0.254	0.339	15.8

	CNST	HILL	GNLS
AIC:	292.28	248.29	244.01
PROB:	0	0.11	0.89
RMSE:	5.75	3.37	3.08

MAX_MEAN: 7.9 MAX_MED: 9.86 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

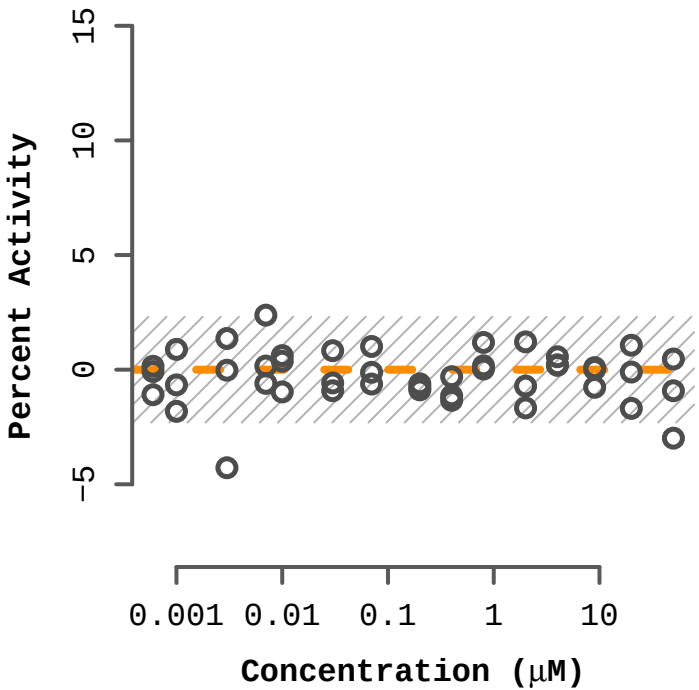
NAME: Pyrantel tartrate
CHID: 48858 **CASRN:** 33401-94-4
SPID(S): Tox21_113347_1
M4ID: 12482682

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

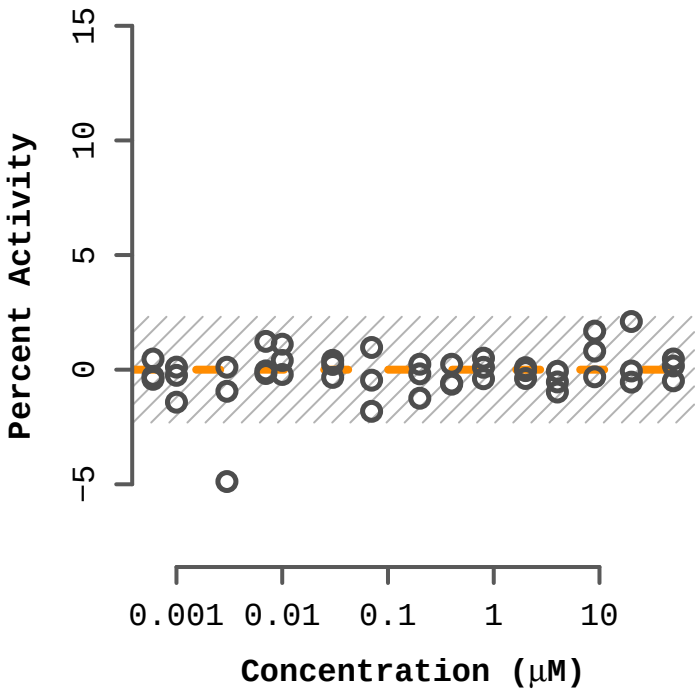
NAME: Chloropyramine hydrochloride
CHID: 48859 **CASRN:** 6170-42-9
SPID(S): Tox21_113349_1
M4ID: 12482680

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.648 **MAX_MED:** 0.372 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

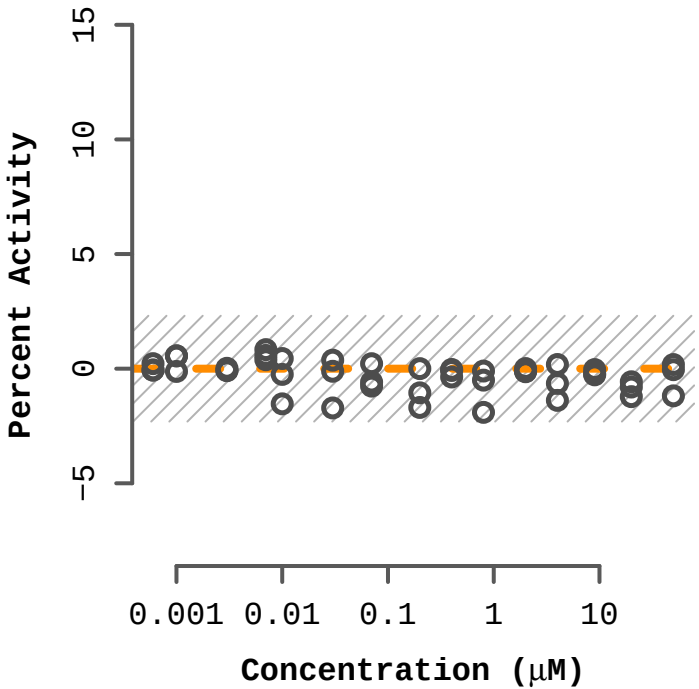
NAME: Ampyrone
CHID: 48860 CASRN: 83-07-8
SPID(S): Tox21_113352_1
M4ID: 12482679

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.729 **MAX_MED:** 0.811 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

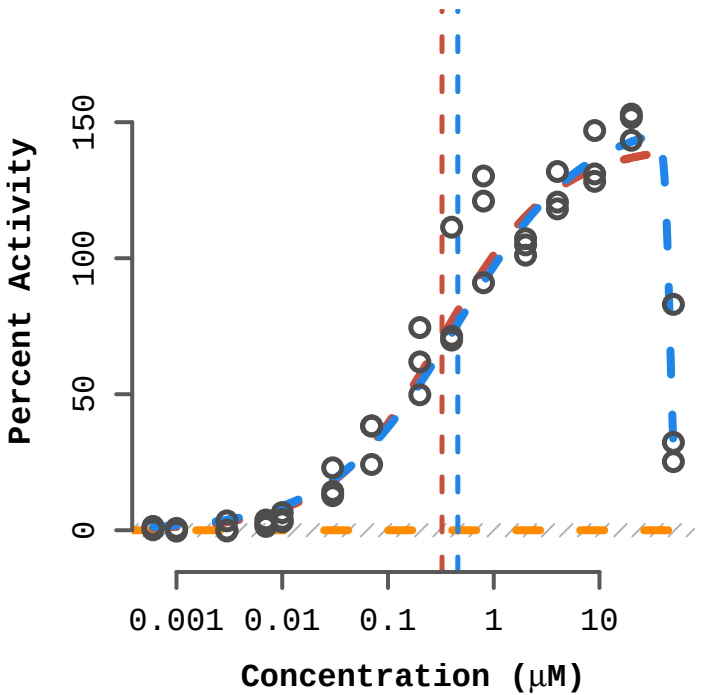
NAME: Lactobionic acid
CHID: 48861 **CASRN:** 96-82-2
SPID(S): Tox21_113353_1
M4ID: 12482678

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.601 **MAX_MED:** 0.578 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Altrenogest
CHID: 48863 CASRN: 850-52-2
SPID(S): Tox21_113356_1
M4ID: 12482677

HILL MODEL (in red):

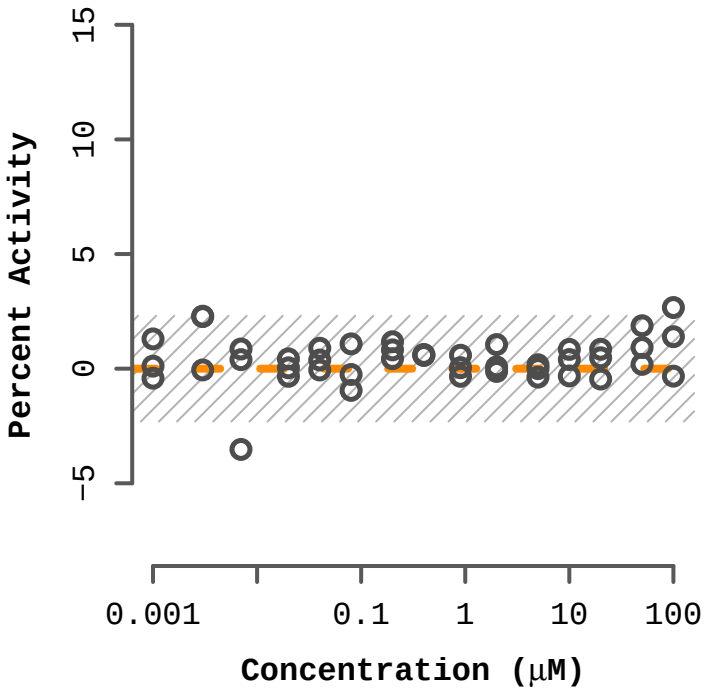
	tp	ga	gw
val:	142	-0.489	0.813
sd:	8.4	0.126	0.108

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	152	-0.339	0.727	1.67	17.4
sd:	7.39	0.0998	0.066	0.00743	3.27

	CNST	HILL	GNLS
AIC:	527.25	389.2	353.21
PROB:	0	0	1
RMSE:	80.01	26.97	13.63

MAX_MEAN: 149 MAX_MED: 152 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

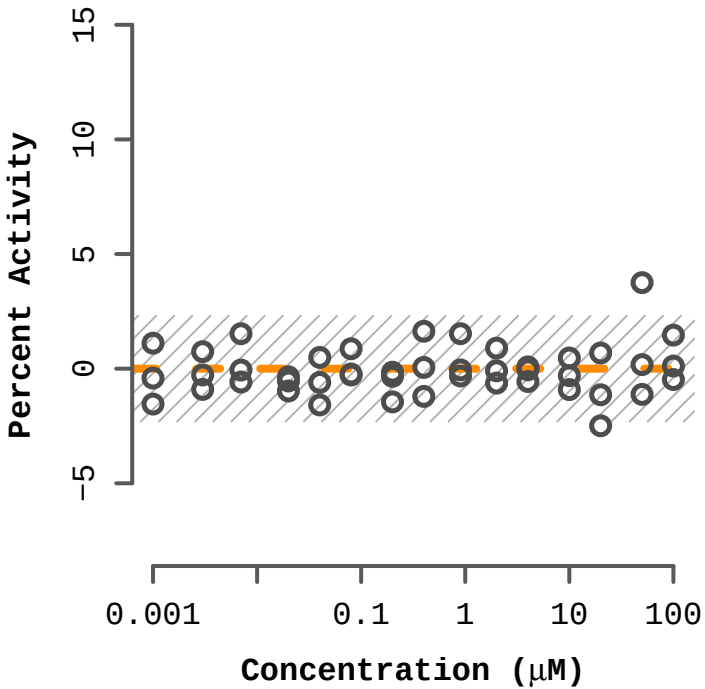
NAME: (S)−(−)−Cathinone hydrochloride
CHID: 48866 **CASRN:** 72739−14−1
SPID(S): Tox21_112816
M4ID: 12482942

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.5 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

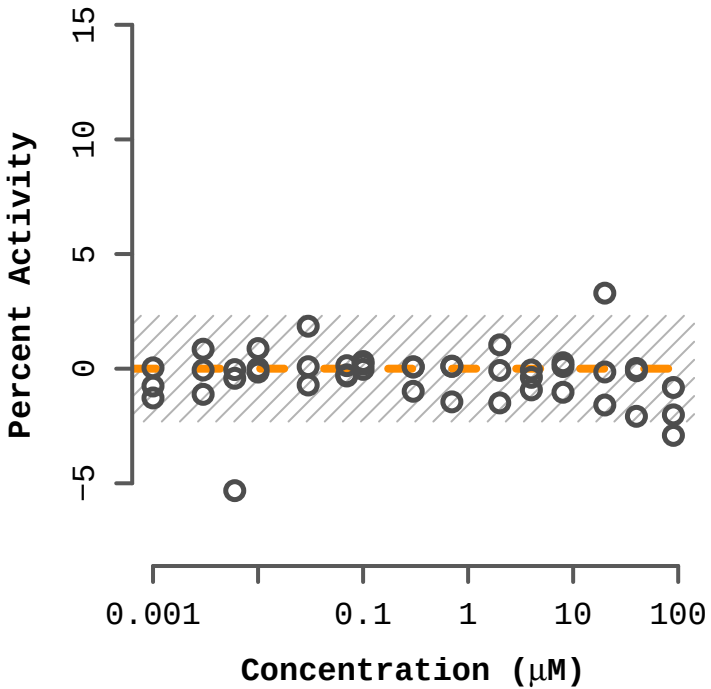
NAME: (S)−(+)−N−Ethylamphetamine hydrochloride
CHID: 48868 CASRN: 26194−77−4
SPID(S): Tox21_112858
M4ID: 12482918

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.937 **MAX_MED:** 0.178 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

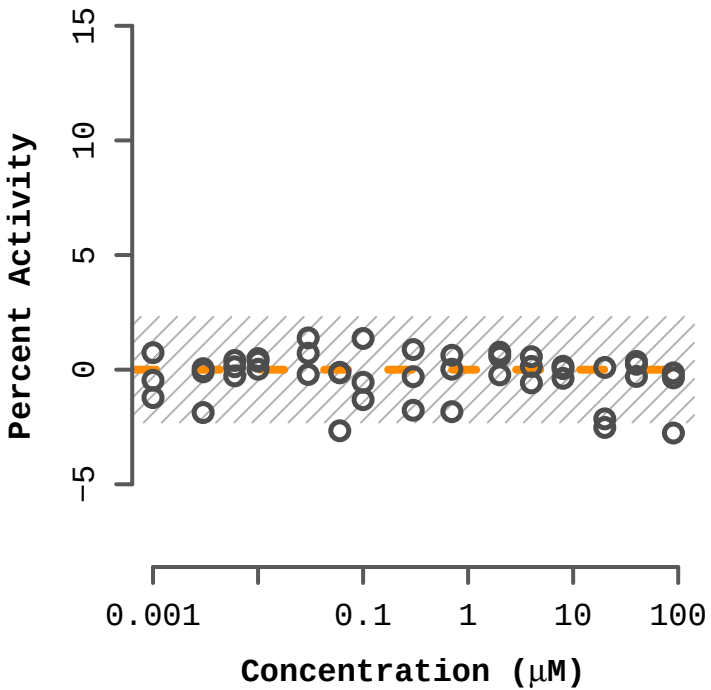
NAME: Fenethylline hydrochloride
CHID: 48869 CASRN: 1892-80-4
SPID(S): Tox21_112896
M4ID: 12482889

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 0.523 **MAX_MED:** 0.195 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxaz

CHID: 48870 **CASRN:** 29493-77-4

SPID(S): Tox21_112818

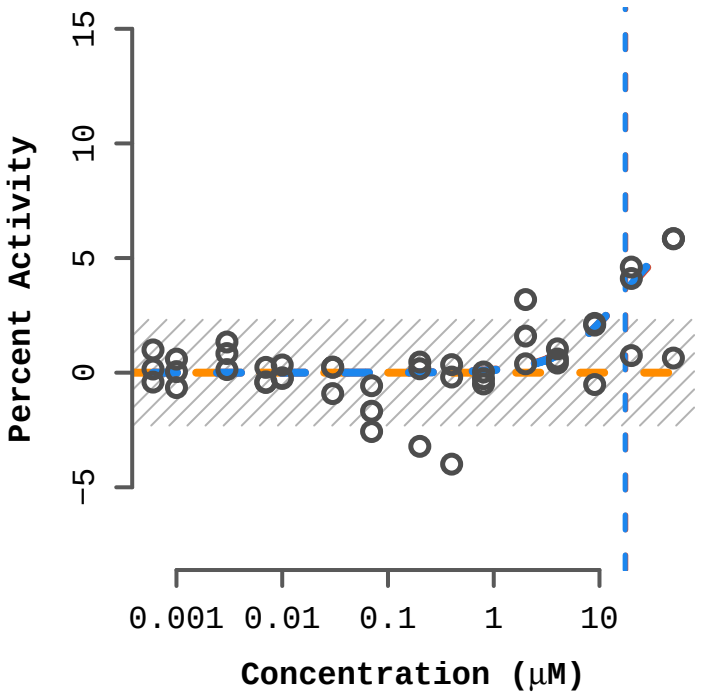
M4ID: 12482941

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.633 **MAX_MED:** 0.719 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexfenfluramine hydrochloride
CHID: 48871 CASRN: 3239-45-0
SPID(S): Tox21_112864_1
M4ID: 12482914

HILL MODEL (in red):

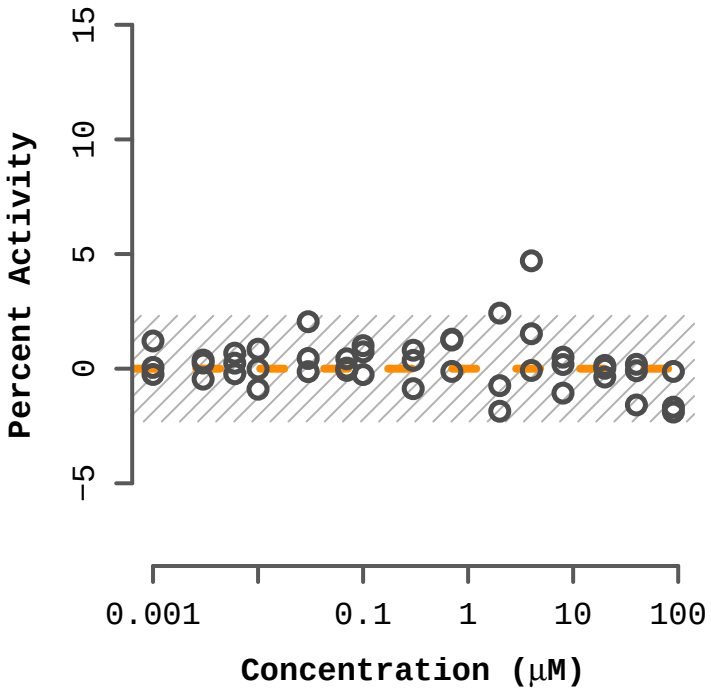
	tp	ga	gw
val:	6.98	1.25	1.39
sd:	2.1	0.26	0.564

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.02	1.24	1.43	1.86	9.83
sd:	5.37	0.456	0.617	1.06	60.9

	CNST	HILL	GNLS
AIC:	179.05	154.06	158.03
PROB:	0	0.88	0.12
RMSE:	1.97	1.45	1.45

MAX_MEAN: 4.11 **MAX_MED:** 5.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

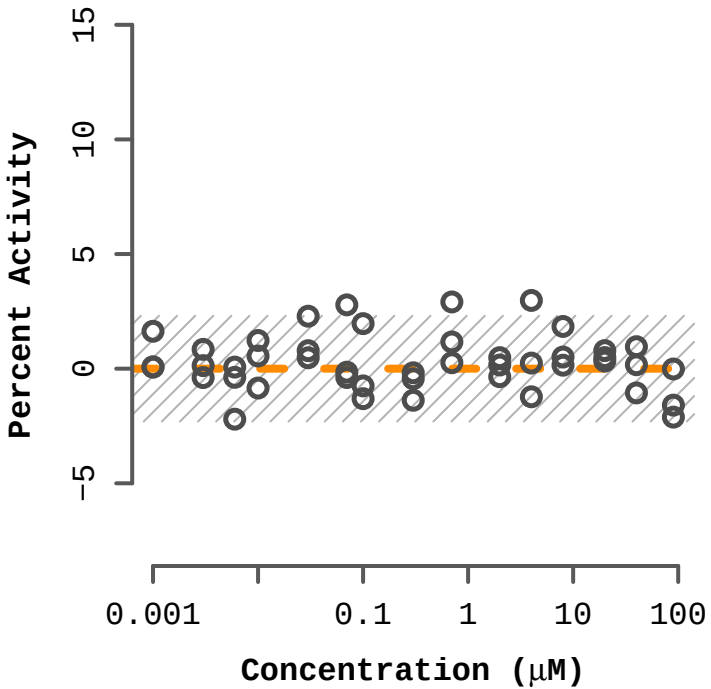
NAME: (−)−Fenfluramine hydrochloride
CHID: 48872 **CASRN:** 3616−78−2
SPID(S): Tox21_112865
M4ID: 12482913

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 2.05 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

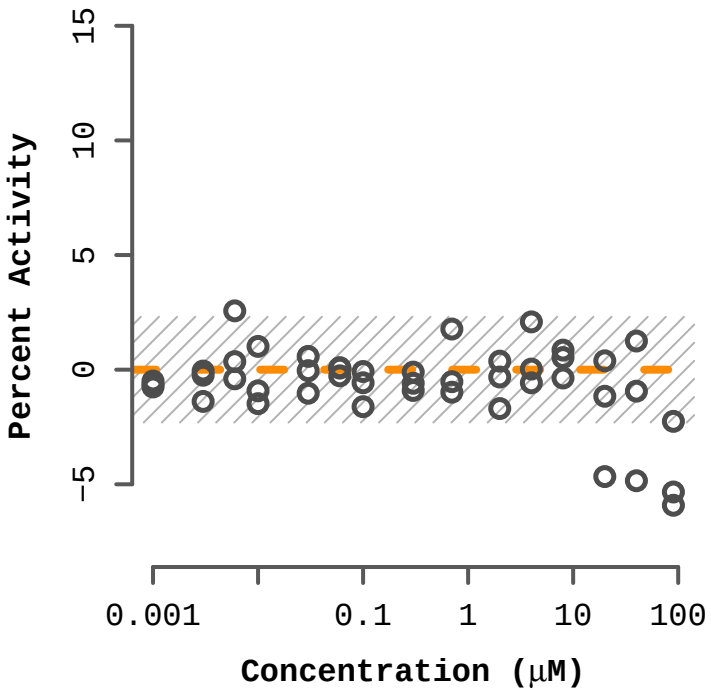
NAME: S−(−)−Secobarbital
CHID: 48873 **CASRN:** 20224−45−7
SPID(S): Tox21_112867
M4ID: 12482911

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

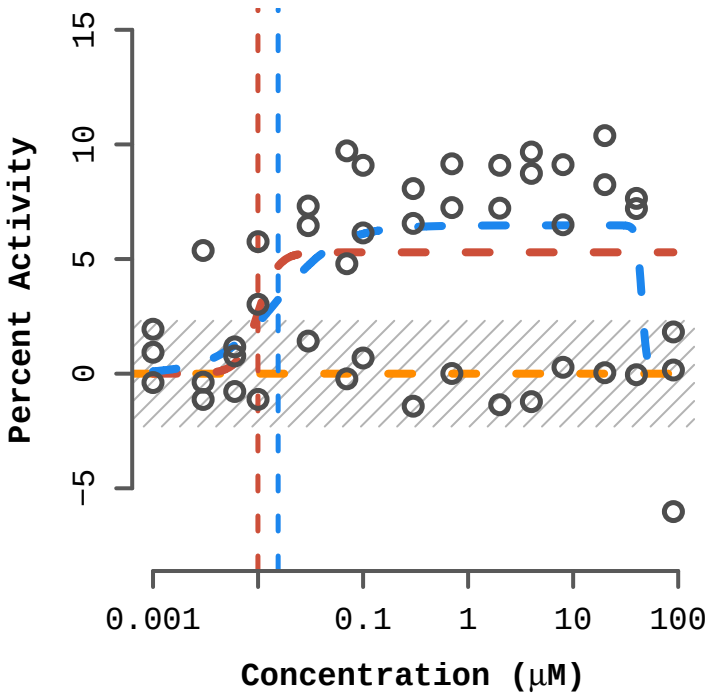
NAME: Mecloqualone
CHID: 48875 CASRN: 340-57-8
SPID(S): Tox21_112870
M4ID: 12482910

HILL MODEL: Not applicable.

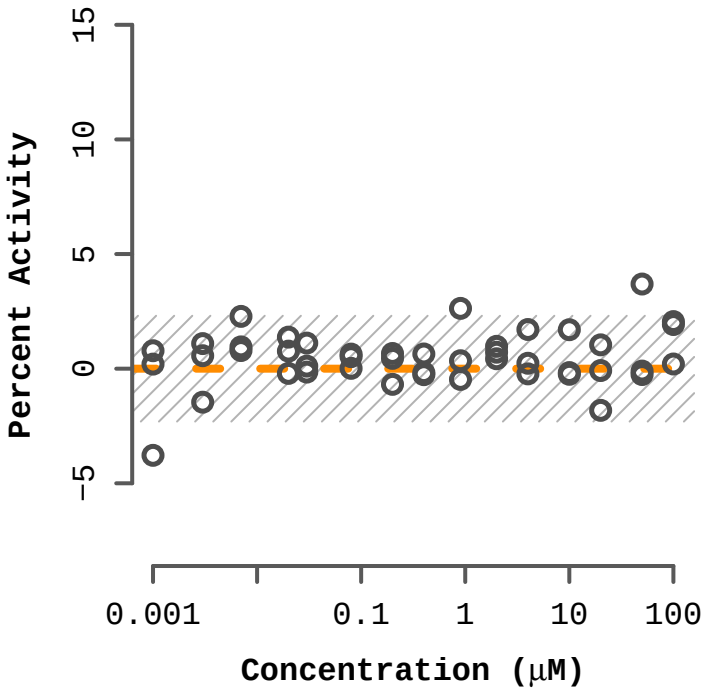
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.83	NA	NA

MAX_MEAN: 0.841 MAX_MED: 0.529 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ibogaine hydrochloride
CHID:    48877   CASRN: 36415-61-9
SPID(S): Tox21_112897
M4ID:    12482888

HILL MODEL (in red):
      tp       ga       gw
val:  5.29     -2       4.6
sd:   0.824    0.16     10.4

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.47     -1.81    1.51     1.65     17.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  289.8       263.87      259.69
PROB: 0           0.11        0.89
RMSE: 5.62        3.98        3.69

MAX_MEAN: 6.23      MAX_MED: 8.74      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

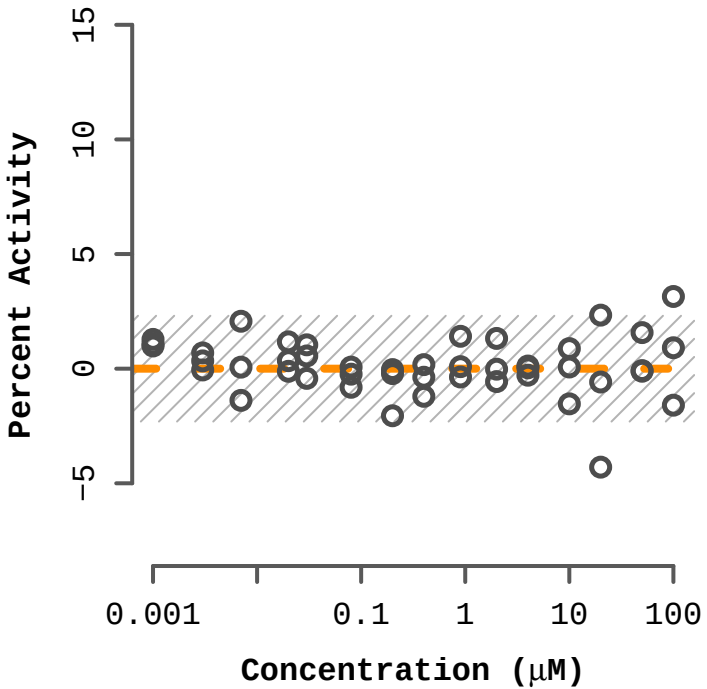
NAME: Mescaline hydrochloride
CHID: 48879 **CASRN:** 832-92-8
SPID(S): Tox21_112822
M4ID: 12482940

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.53	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 1.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

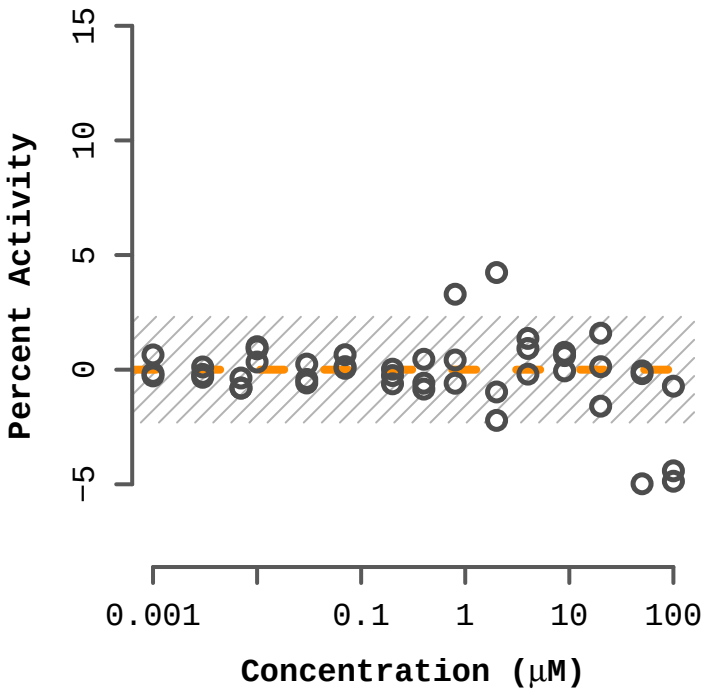
NAME: 3,4,5−Trimethoxyamphetamine hydrochloride
CHID: 48880 CASRN: 5688−80−2
SPID(S): Tox21_112823
M4ID: 12482939

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: R−(−)−2,5−Dimethoxy−4−bromoamphetamine hydroch

CHID: 48882 **CASRN:** 50505−92−5

SPID(S): Tox21_112874

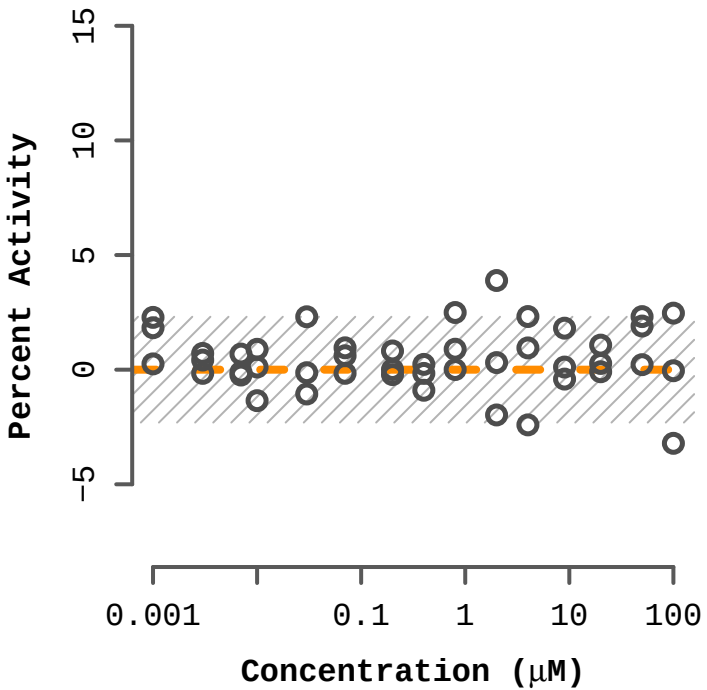
M4ID: 12482908

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

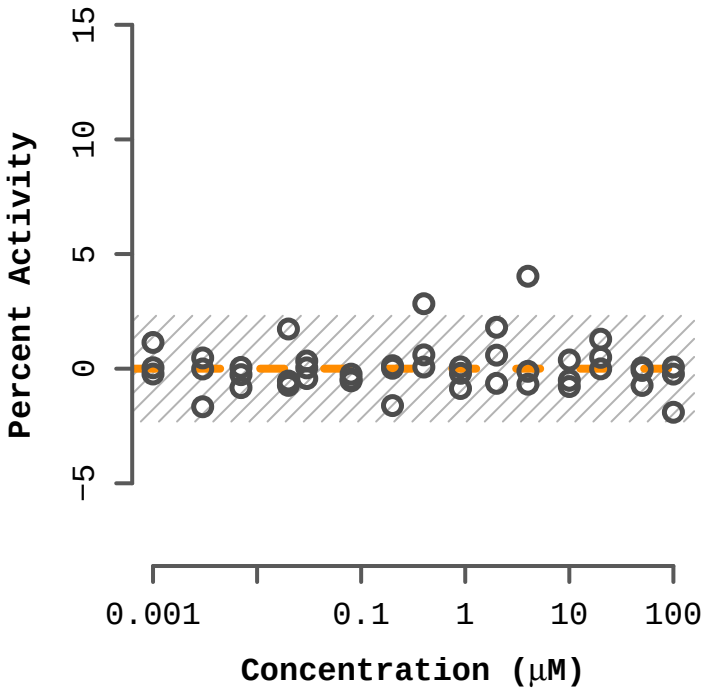
NAME: 4-Bromo-2,5-dimethoxyamphetamine hydrochloride
CHID: 48883 **CASRN:** 29705-96-2
SPID(S): Tox21_112875
M4ID: 12482907

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 1.48 **MAX_MED:** 1.9 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

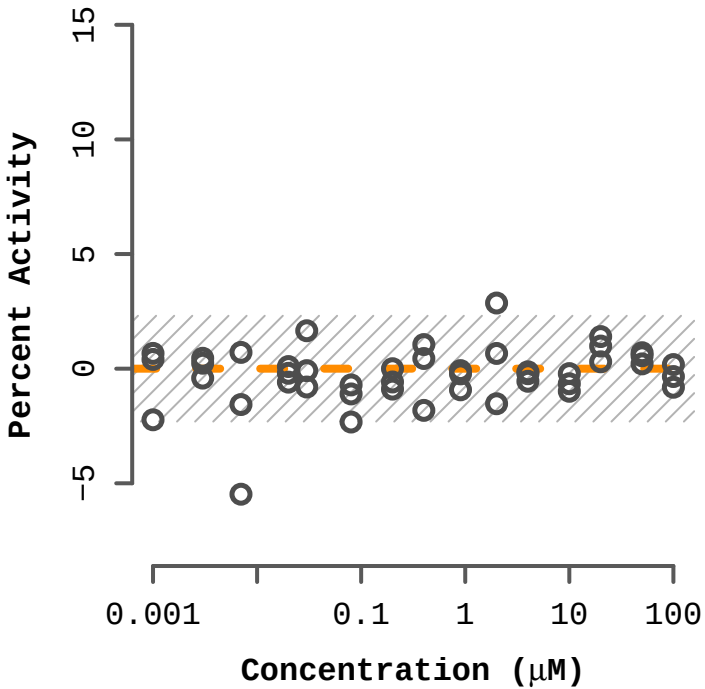
NAME: R−(−)−2,5−Dimethoxy−4−methylamphetamine hydrocl
CHID: 48884 CASRN: 50505−88−9
SPID(S): Tox21_112848
M4ID: 12482921

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.17 MAX_MED: 0.604 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

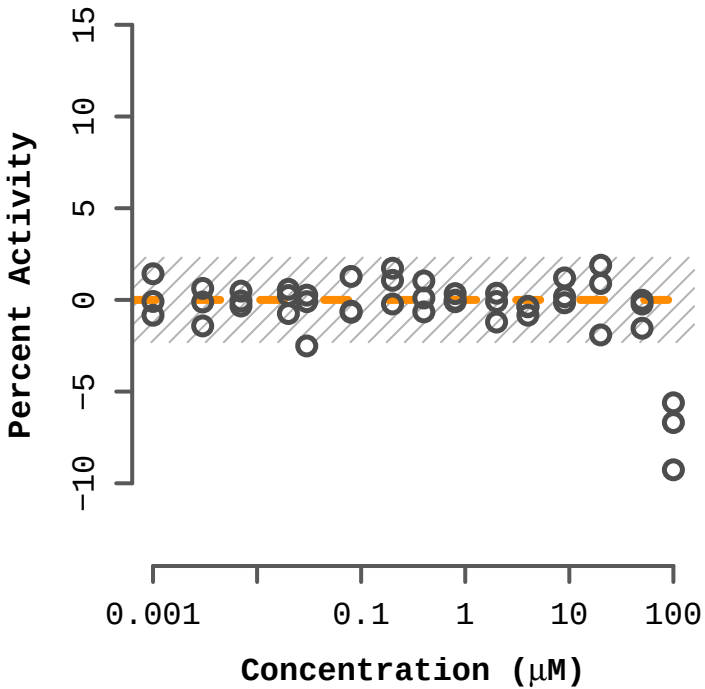
NAME: 2,5-Dimethoxyamphetamine hydrochloride
CHID: 48886 **CASRN:** 24973-25-9
SPID(S): Tox21_112850
M4ID: 12482920

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.897 **MAX_MED:** 0.988 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (+)−2,5−Dimethoxy−4−ethylamphetamine hydrochlo

CHID: 48888 **CASRN:** 50505−91−4

SPID(S): Tox21_112840

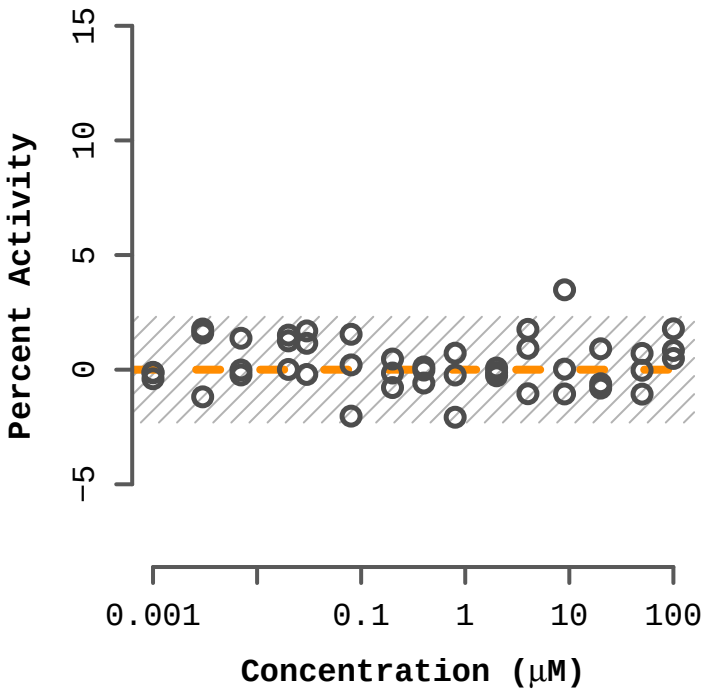
M4ID: 12482928

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.1	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

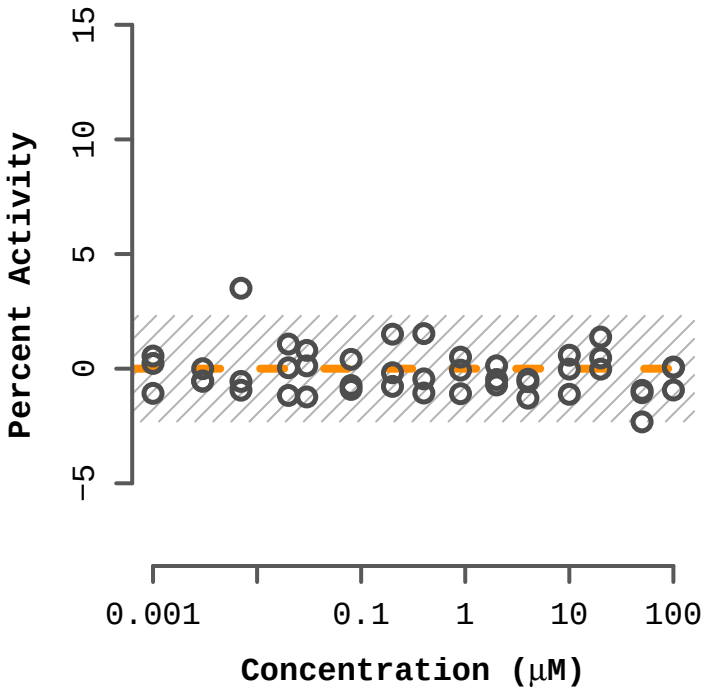
NAME: 1-(7-Methoxy-1,3-benzodioxol-5-yl)propan-2-ami
CHID: 48890 **CASRN:** 60676-84-8
SPID(S): Tox21_112842
M4ID: 12482927

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

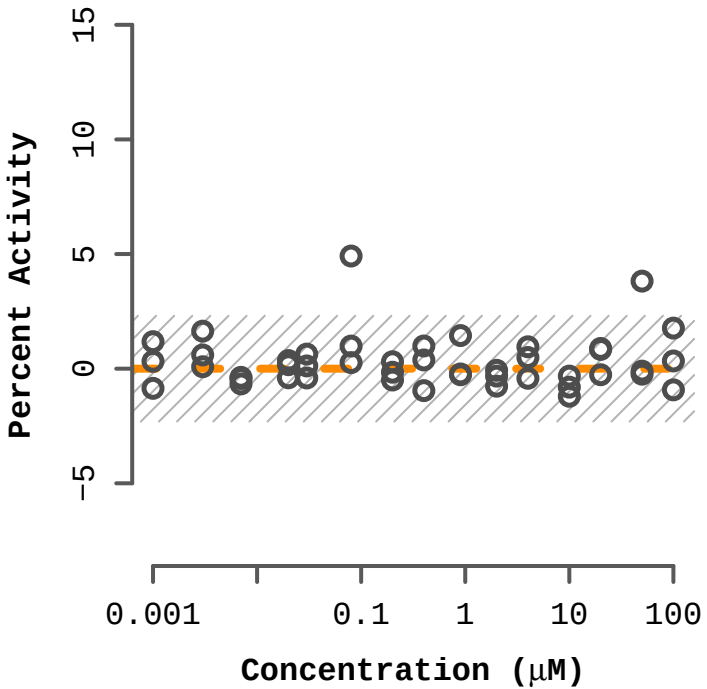
NAME: 1-(1,3-Benzodioxol-5-yl)-N-hydroxypropan-2-ami
CHID: 48891 **CASRN:** 74341-83-6
SPID(S): Tox21_112852
M4ID: 12482919

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.89	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.673 **MAX_MED:** 0.471 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

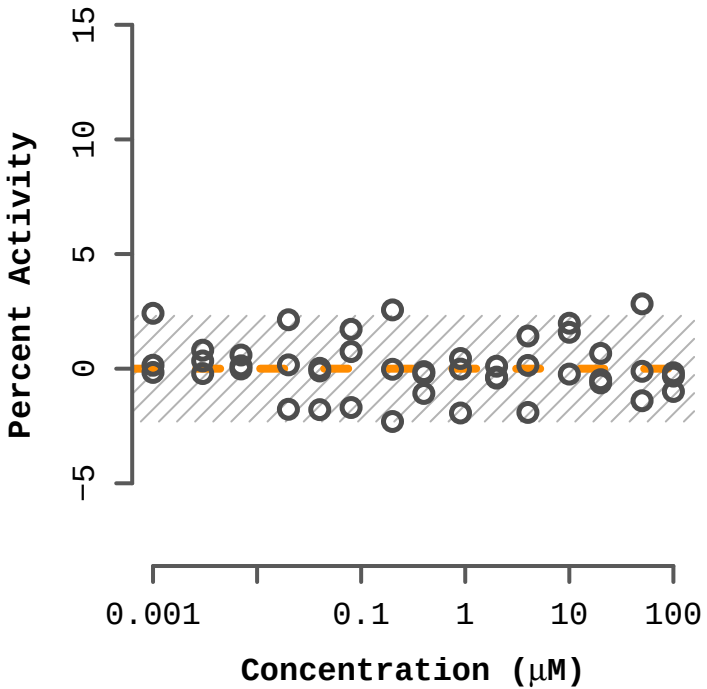
NAME: 1-(1,3-Benzodioxol-5-yl)-N-ethylpropan-2-amine
CHID: 48892 **CASRN:** 74341-78-9
SPID(S): Tox21_112888
M4ID: 12482897

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 0.988 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

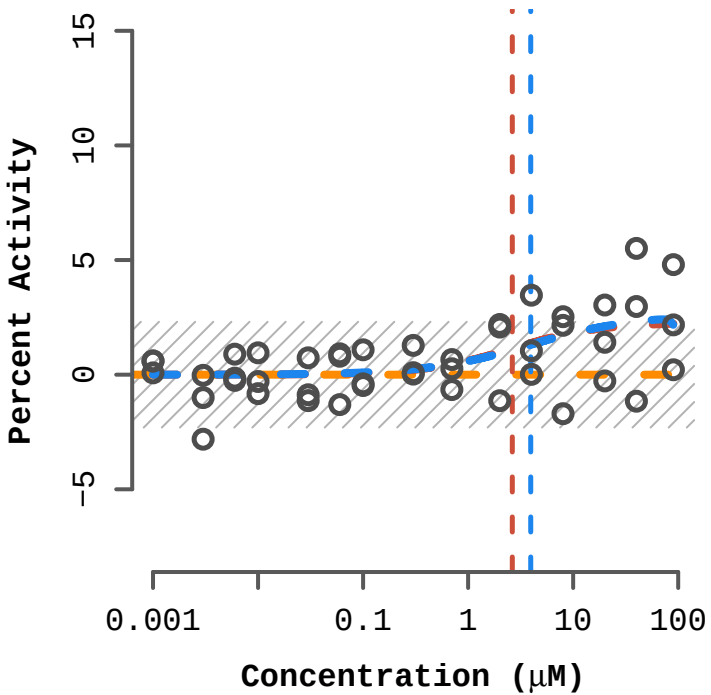
NAME: 1-(1,3-Benzodioxol-5-yl)-N-methylpropan-2-amine
CHID: 48893 **CASRN:** 64057-70-1
SPID(S): Tox21_112889
M4ID: 12482896

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bufotenine
CHID: 48894 CASRN: 487-93-4
SPID(S): Tox21_112890
M4ID: 12482895

HILL MODEL (in red):

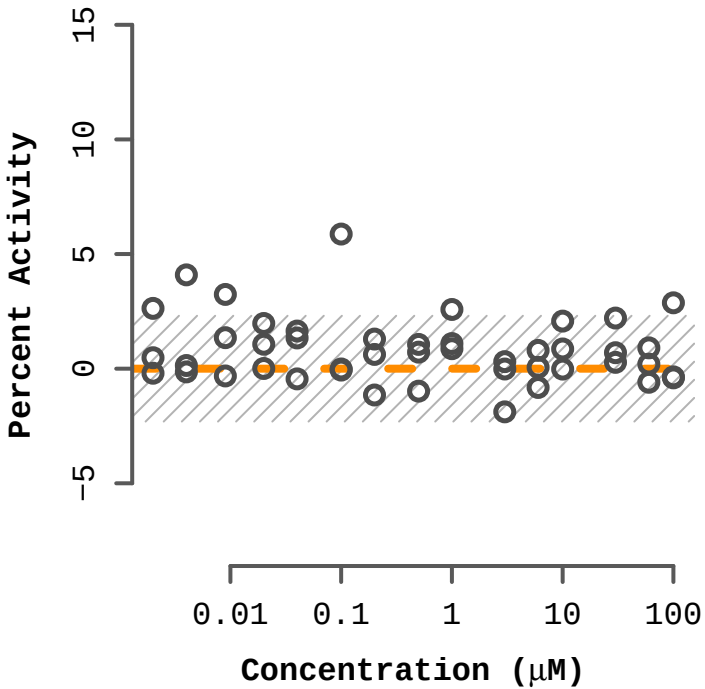
	tp	ga	gw
val:	2.28	0.421	1.05
sd:	1.11	0.736	1.08

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.61	0.596	0.892	2.02	14
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	176.51	165.58	169.56
PROB:	0	0.88	0.12
RMSE:	1.76	1.4	1.4

MAX_MEAN: 2.44 **MAX_MED:** 2.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

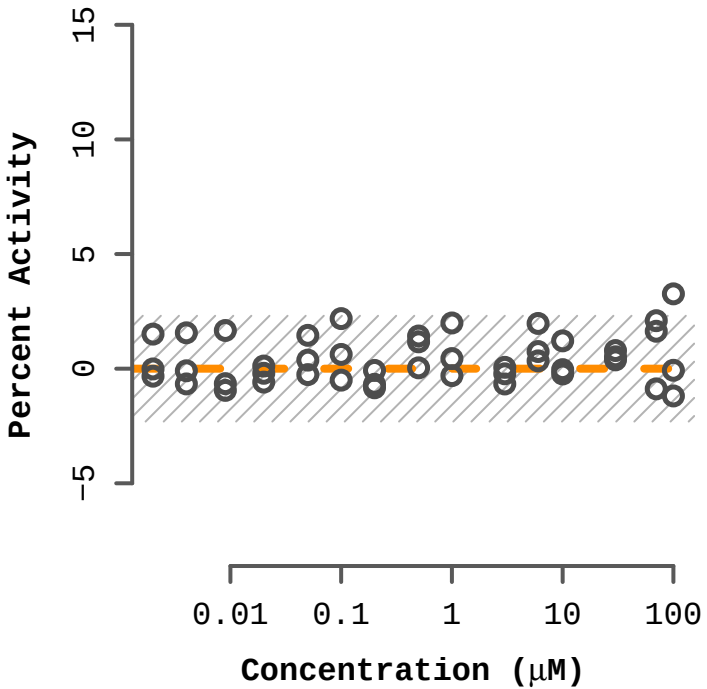
NAME: N,N−Diethyltryptamine fumarate
CHID: 48895 **CASRN:** NOCAS_48895
SPID(S): Tox21_112891
M4ID: 12482894

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.64	NA	NA

MAX_MEAN: 1.93 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

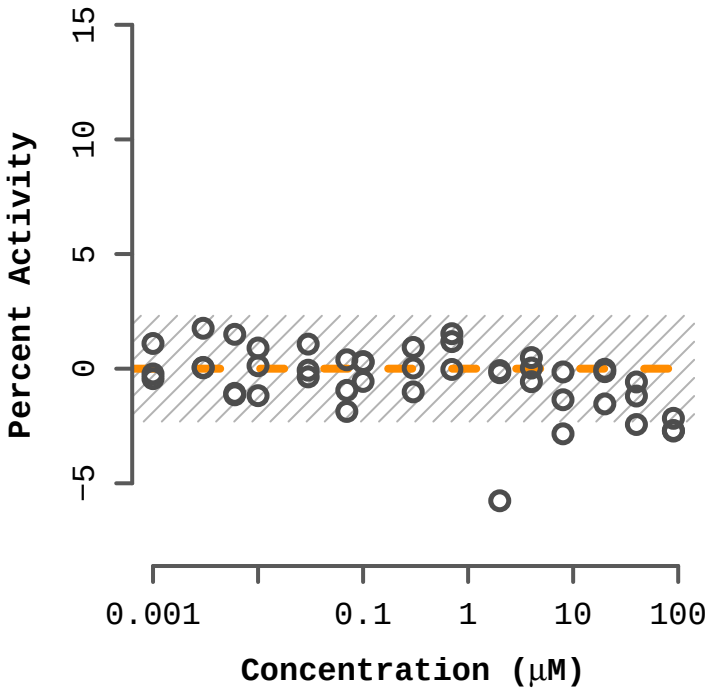
NAME: N,N−Dimethyltryptamine fumarate
CHID: 48896 CASRN: 68677−26−9
SPID(S): Tox21_112892
M4ID: 12482893

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

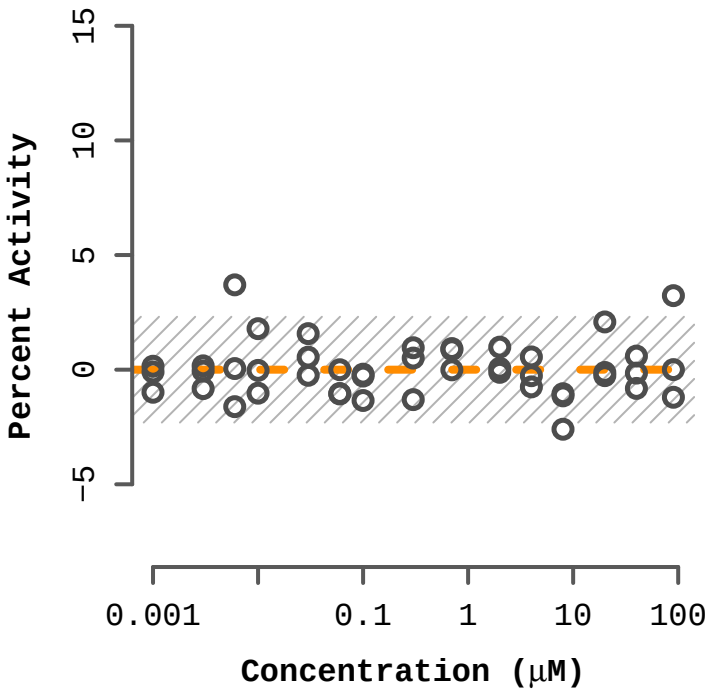
NAME: N,N−Dipropyltryptamine hydrochloride
CHID: 48897 **CASRN:** 7558−73−8
SPID(S): Tox21_112893
M4ID: 12482892

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.892 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

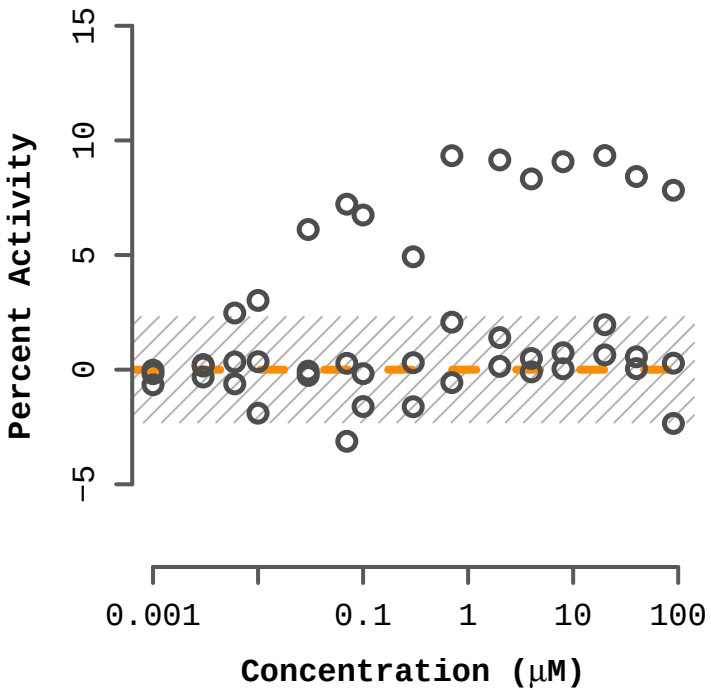
NAME: Psilocybin
CHID: 48898 **CASRN:** 520-52-5
SPID(S): Tox21_112898
M4ID: 12482887

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.713 **MAX_MED:** 0.873 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

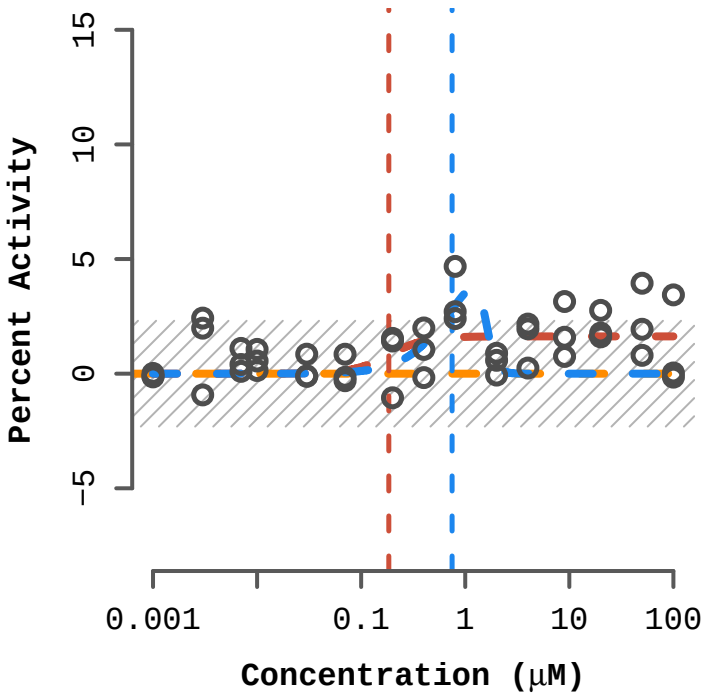
NAME: Psilocin
CHID: 48899 **CASRN:** 520-53-6
SPID(S): Tox21_112894
M4ID: 12482891

HILL MODEL: Not applicable.

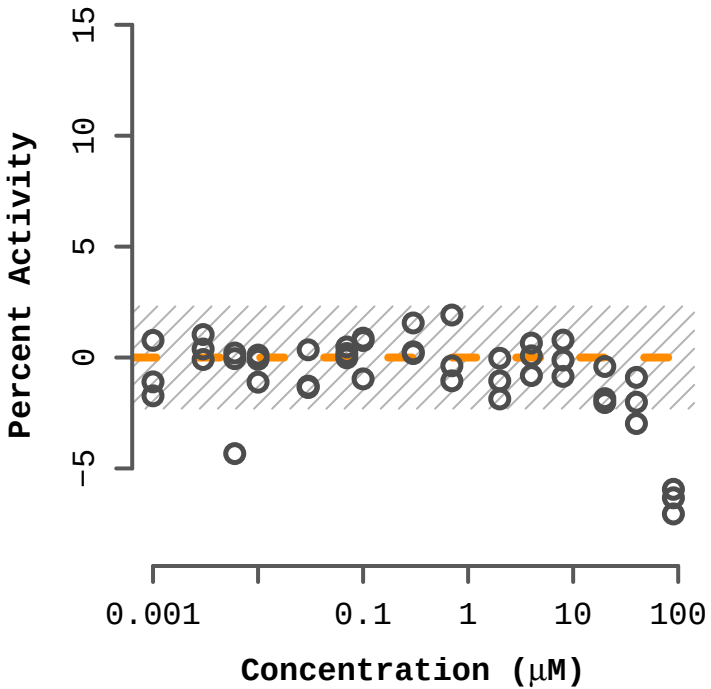
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	250.14	NA	NA
PROB:	1	NA	NA
RMSE:	4.09	NA	NA

MAX_MEAN: 3.98 **MAX_MED:** 2.07 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    5-Methoxy-N,N-diisopropyltryptamine hydrochlor
CHID:    48900   CASRN: 2426-63-3
SPID(S): Tox21_112880
M4ID:    12482903

HILL MODEL (in red):
      tp       ga       gw
val:  1.63     -0.734   2.5
sd:   0.273    0.296    2.78

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.62     -0.127   1.92     0.199    9.41
sd:   6.9      0.571    2.05     0.817    76.6

      CNST        HILL        GNLS
AIC:  176.91      150.47      171.24
PROB: 0           1           0
RMSE: 1.69        1.16        1.44

MAX_MEAN: 3.26      MAX_MED: 2.7       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

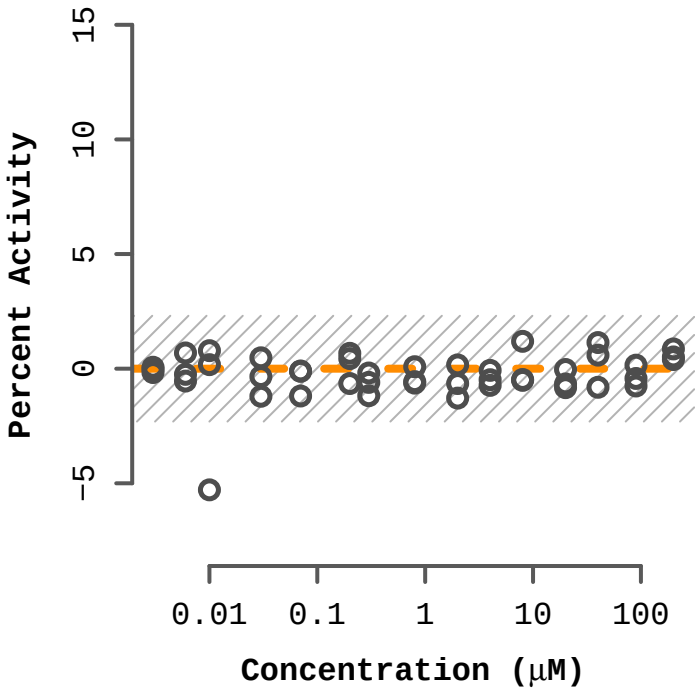
NAME: 1-Phenylcyclohexylamine hydrochloride
CHID: 48901 **CASRN:** 1934-71-0
SPID(S): Tox21_112881
M4ID: 12482902

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 0.665 **MAX_MED:** 0.769 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

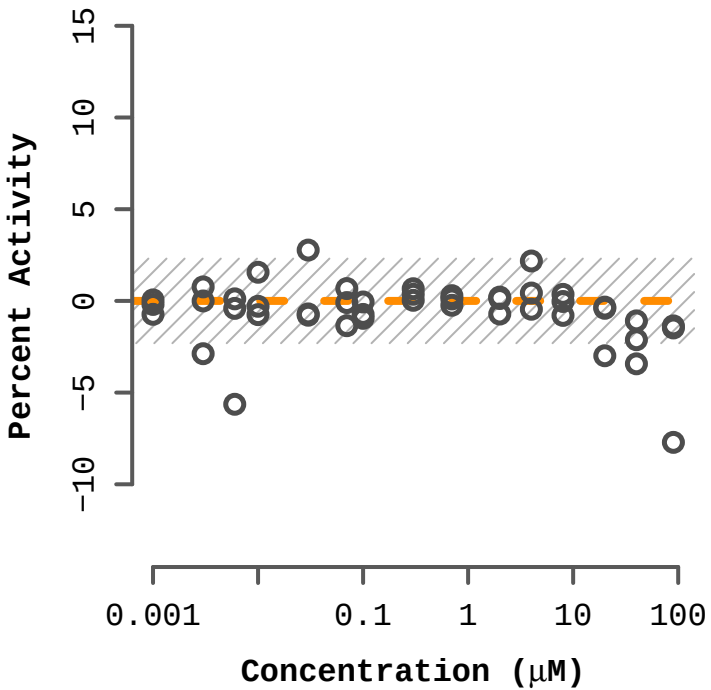
NAME: 1-Benzylpiperazine difumarate
CHID: 48902 **CASRN:** 106133-22-6
SPID(S): Tox21_112882
M4ID: 12482901

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.592 **MAX_MED:** 0.593 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

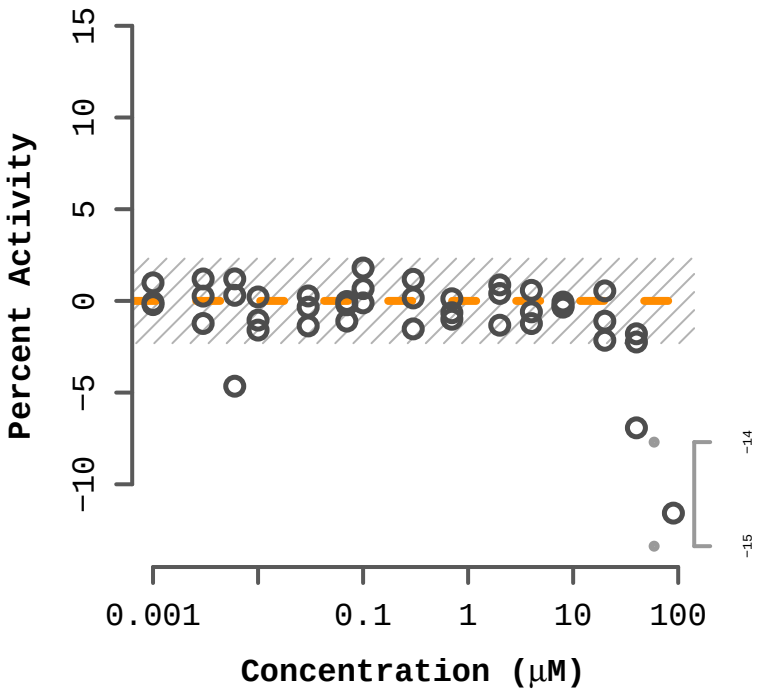
NAME: Codeine hydrochloride
CHID: 48904 **CASRN:** 1422-07-7
SPID(S): Tox21_112884
M4ID: 12482900

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 0.719 **MAX_MED:** 0.431 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

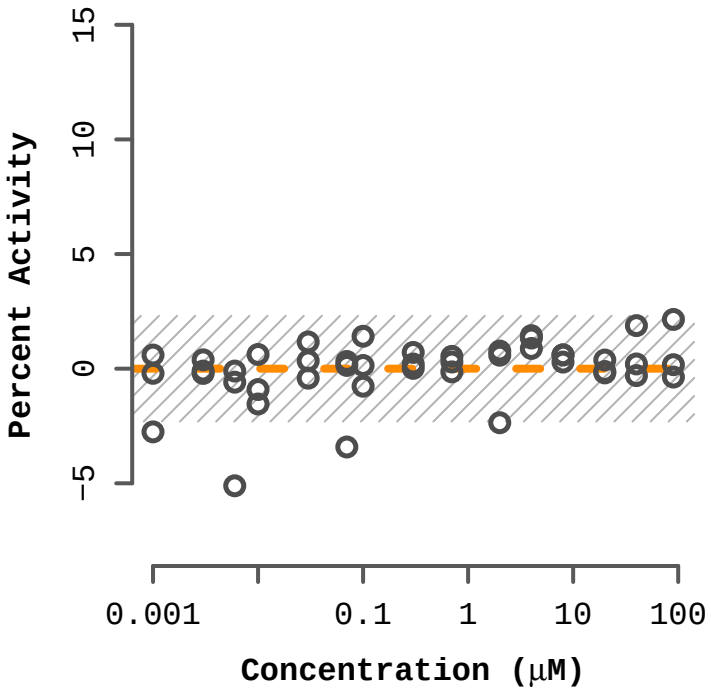
NAME: Buprenorphine hydrochloride
CHID: 48905 **CASRN:** 53152-21-9
SPID(S): Tox21_112899
M4ID: 12482886 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207.28	NA	NA
PROB:	1	NA	NA
RMSE:	3.85	NA	NA

MAX_MEAN: 0.786 **MAX_MED:** 0.671 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

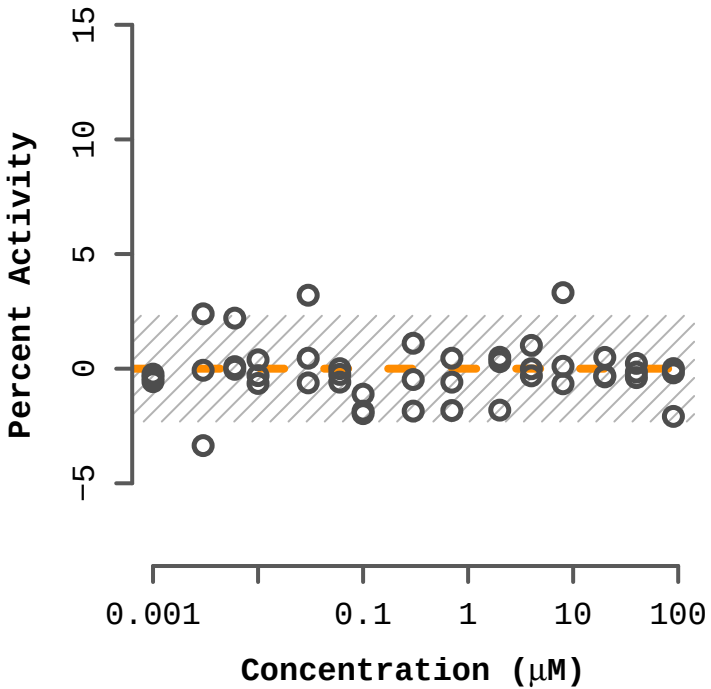
NAME: Dihydroisocodeine
CHID: 48907 CASRN: 795-38-0
SPID(S): Tox21_112885
M4ID: 12482899

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

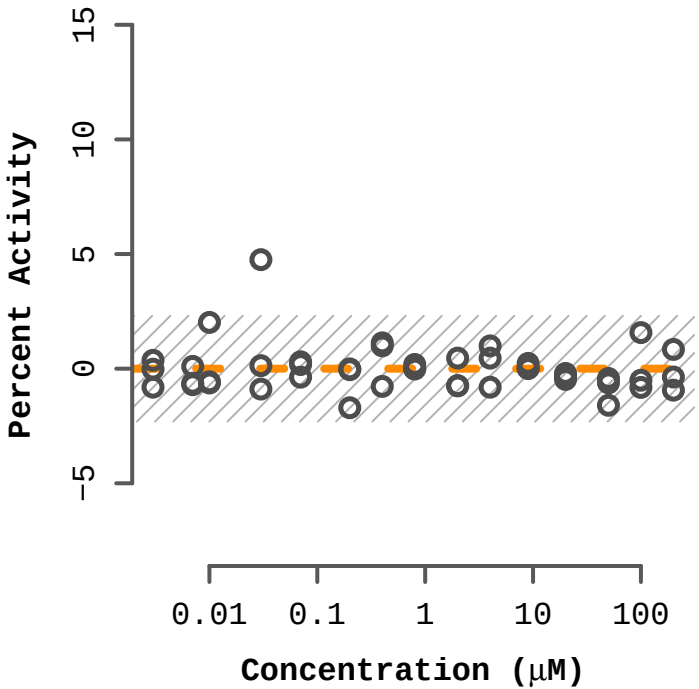
NAME: Dihydromorphine
CHID: 48908 CASRN: 509-60-4
SPID(S): Tox21_112886
M4ID: 12482898

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.02 MAX_MED: 0.457 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

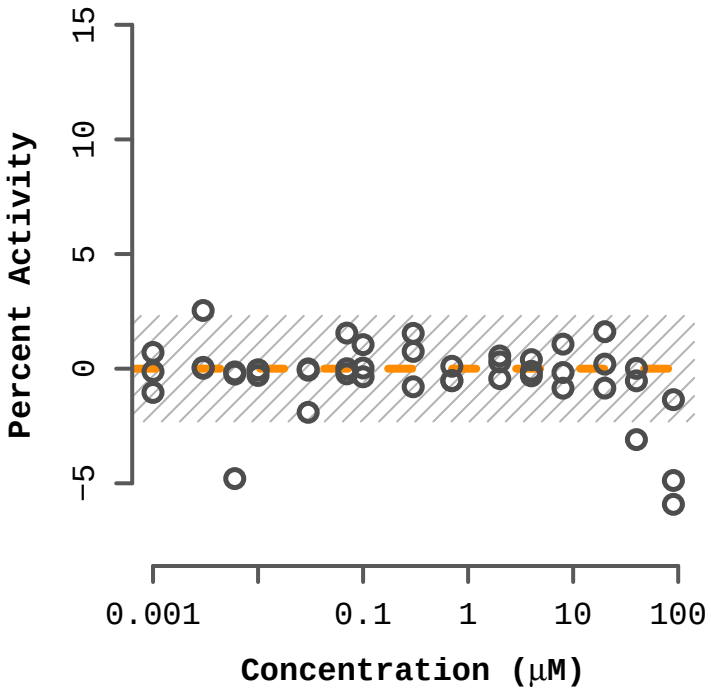
NAME: (+)−Metazocine fumarate (2:1)
CHID: 48910 CASRN: 133005−40−0
SPID(S): Tox21_112826
M4ID: 12482938

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.997 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

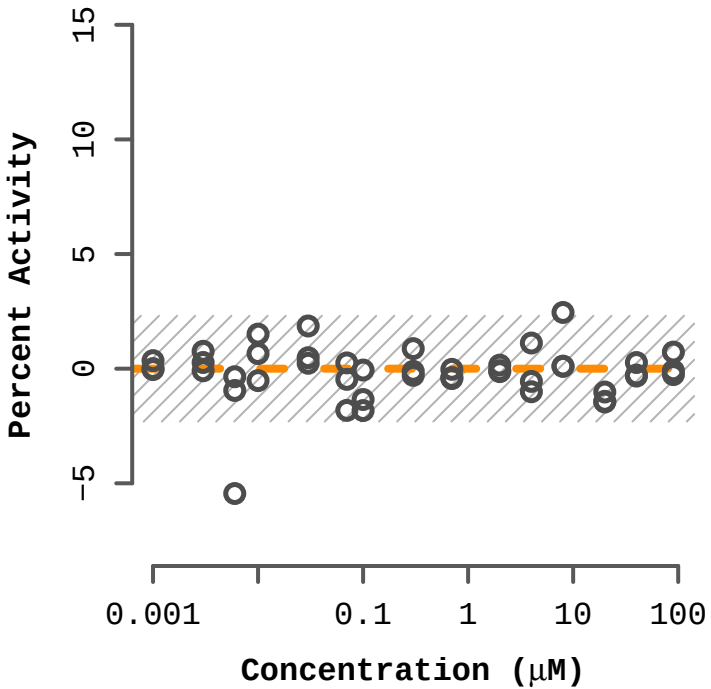
NAME: Premethadone
CHID: 48912 **CASRN:** 125-79-1
SPID(S): Tox21_112859
M4ID: 12482917

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 0.872 **MAX_MED:** 0.754 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

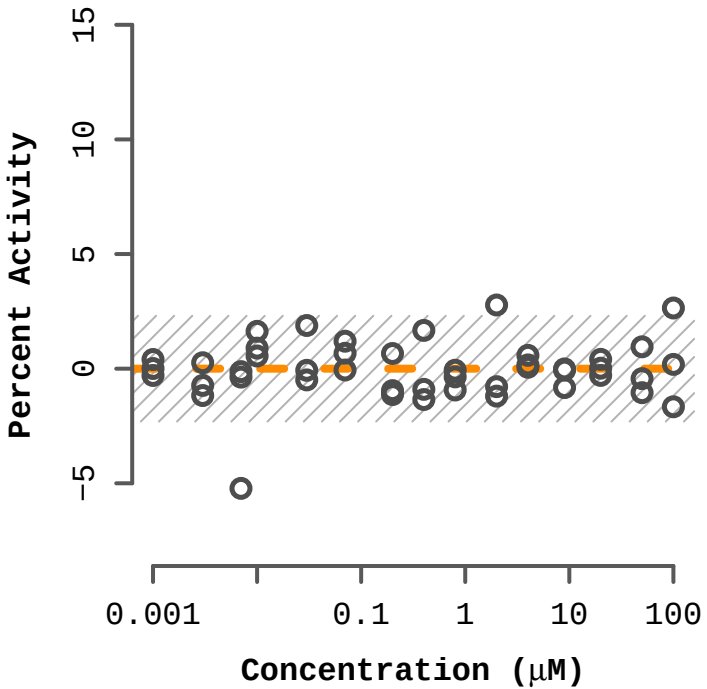
NAME: Morphine sulfate pentahydrate
CHID: 48914 CASRN: 6211-15-0
SPID(S): Tox21_112861
M4ID: 12482916

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 0.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

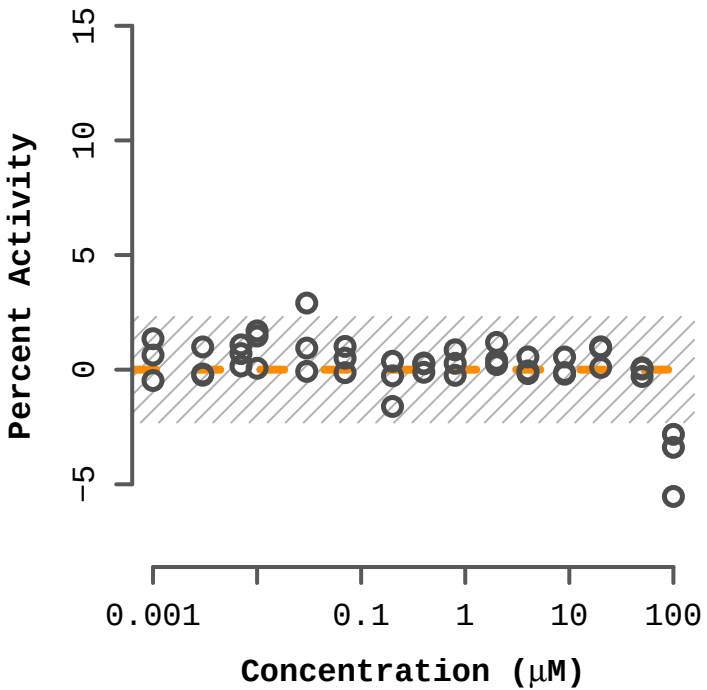
NAME: N-Normorphine hydrochloride
CHID: 48915 **CASRN:** 3372-02-9
SPID(S): Tox21_112862
M4ID: 12482915

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.01	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.897 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

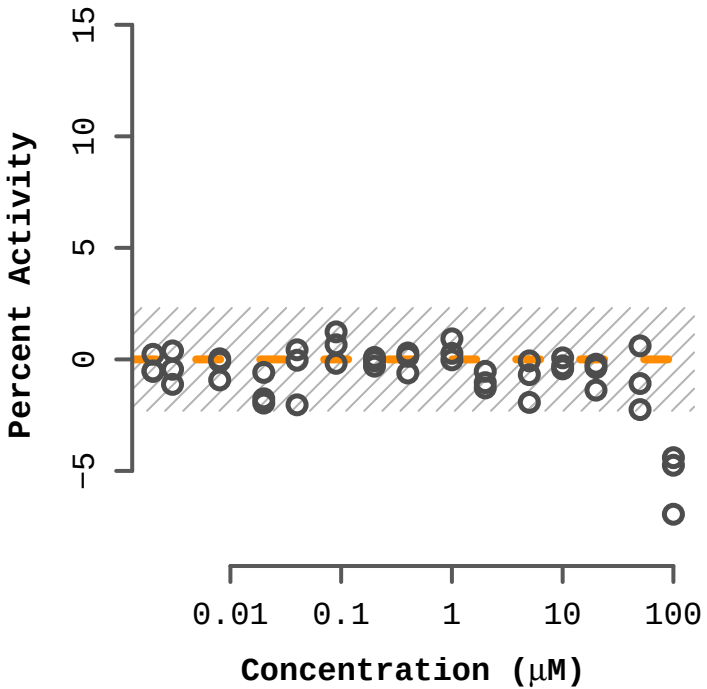
NAME: (−)−alpha−Methadol hydrochloride
CHID: 48916 **CASRN:** 53757−34−9
SPID(S): Tox21_112827
M4ID: 12482937

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

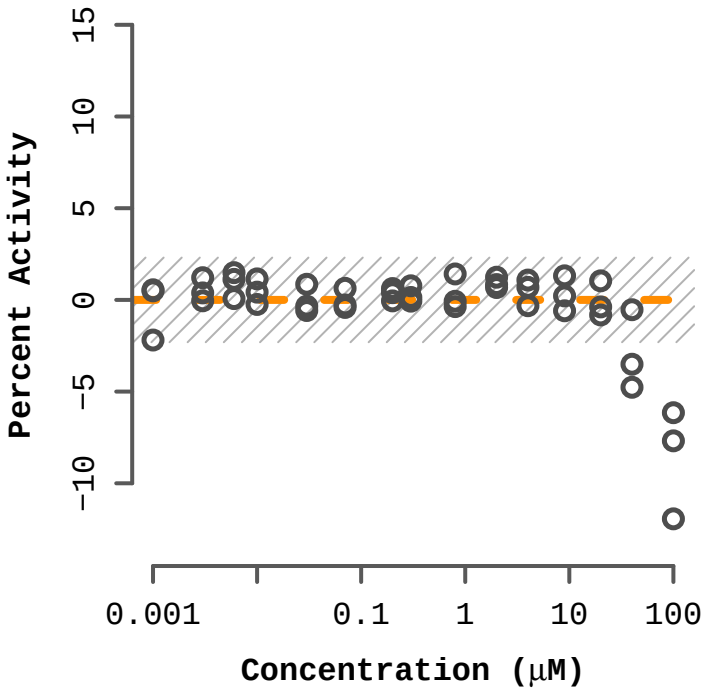
NAME: Dextromoramide tartrate
CHID: 48918 **CASRN:** 2922-44-3
SPID(S): Tox21_112829
M4ID: 12482936

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 0.572 **MAX_MED:** 0.658 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

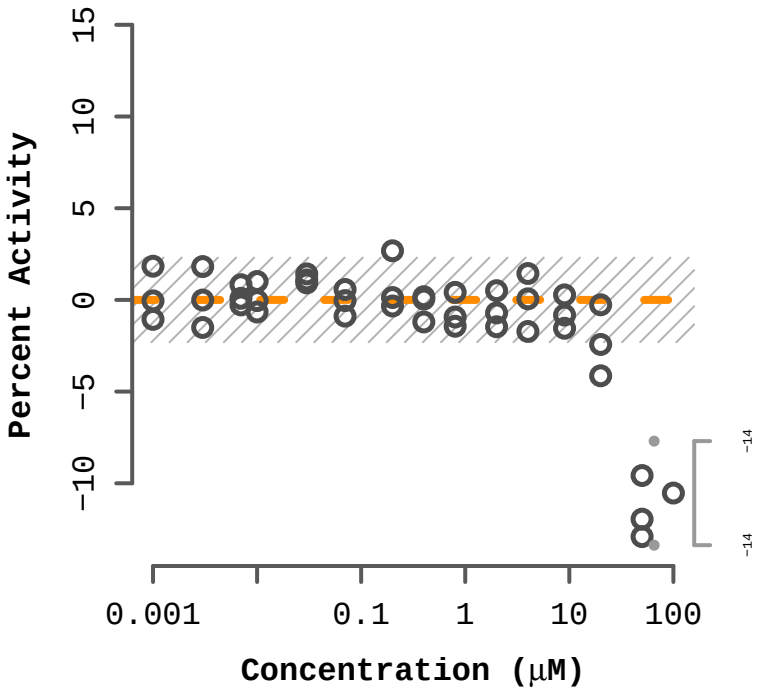
NAME: Etonitazene
CHID: 48919 **CASRN:** 911-65-9
SPID(S): Tox21_112830
M4ID: 12482935

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.58	NA	NA

MAX_MEAN: 0.918 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

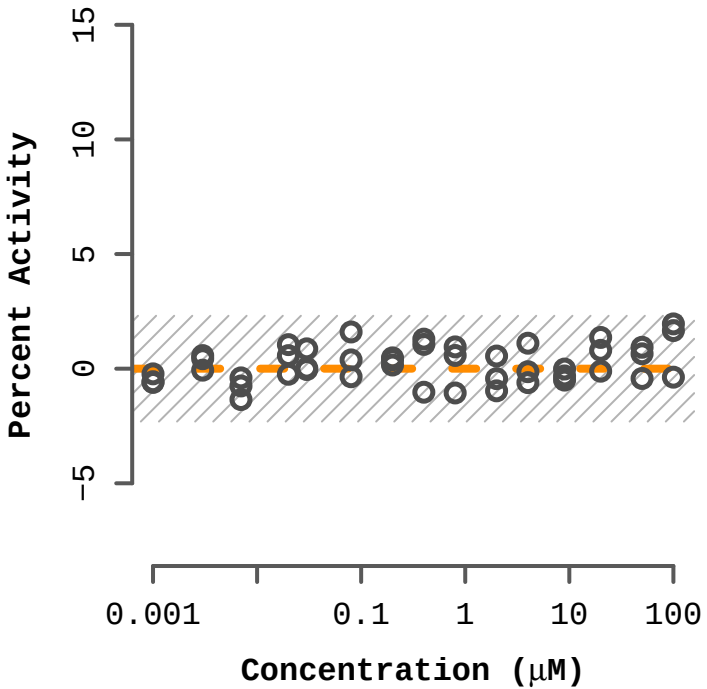
NAME: L-alpha-Acetyl-N-normethadol hydrochloride
CHID: 48920 **CASRN:** 55096-75-8
SPID(S): Tox21_112831
M4ID: 12482934 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	238.63	NA	NA
PROB:	1	NA	NA
RMSE:	4.65	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

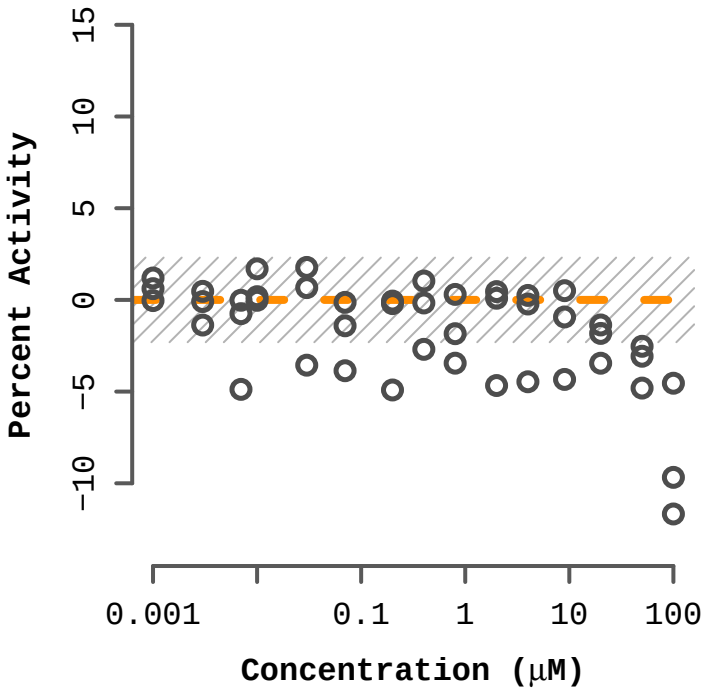
NAME: 1-Methyl-4-phenyl-4-propionoxypiperidine hydroc
CHID: 48921 CASRN: 4968-48-3
SPID(S): Tox21_112832
M4ID: 12482933

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.66 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

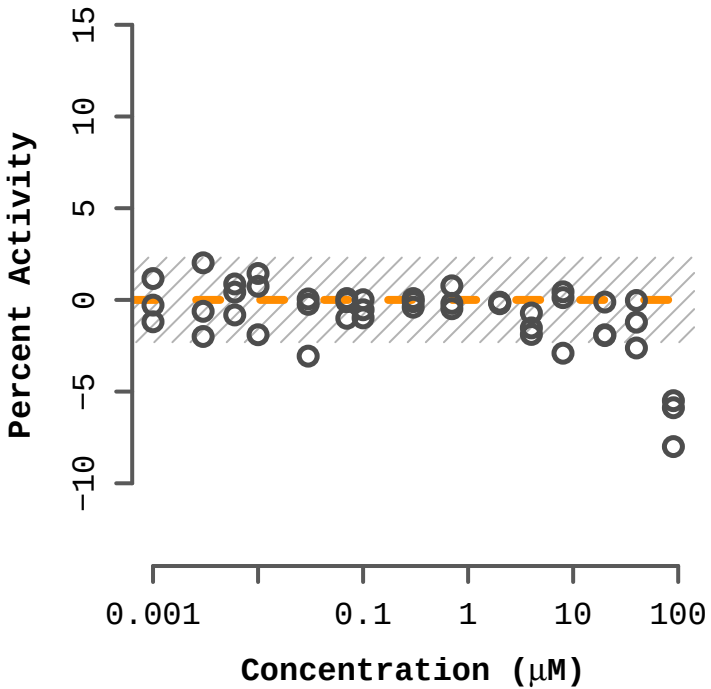
NAME: 1-(2-Phenylethyl)-4-phenyl-4-acetoxypiperidine
CHID: 48922 **CASRN:** 64-52-8
SPID(S): Tox21_112833
M4ID: 12482932

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	227.86	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 0.619 **MAX_MED:** 0.672 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

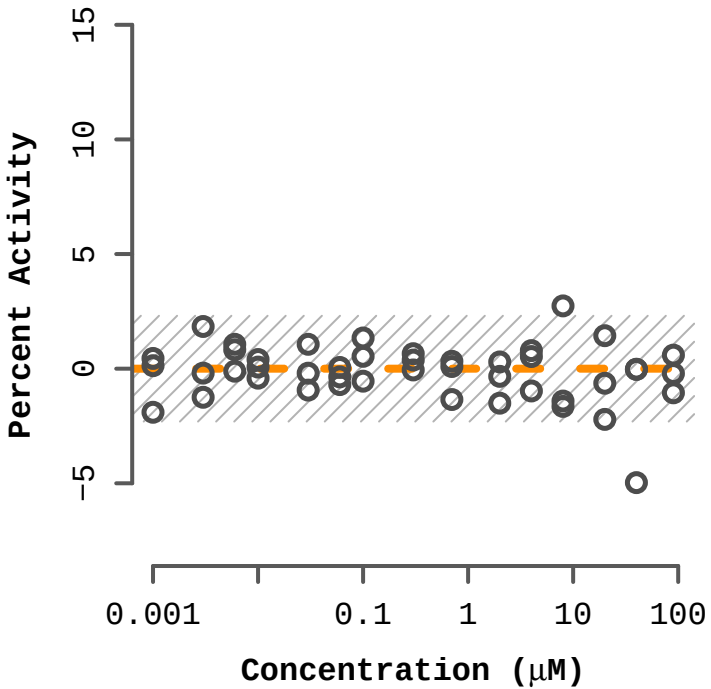
NAME: (−)−Pentazocine succinate
CHID: 48924 **CASRN:** 124819−25−6
SPID(S): Tox21_112877
M4ID: 12482906

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.52	NA	NA
PROB:	1	NA	NA
RMSE:	2.06	NA	NA

MAX_MEAN: 0.159 **MAX_MED:** 0.742 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

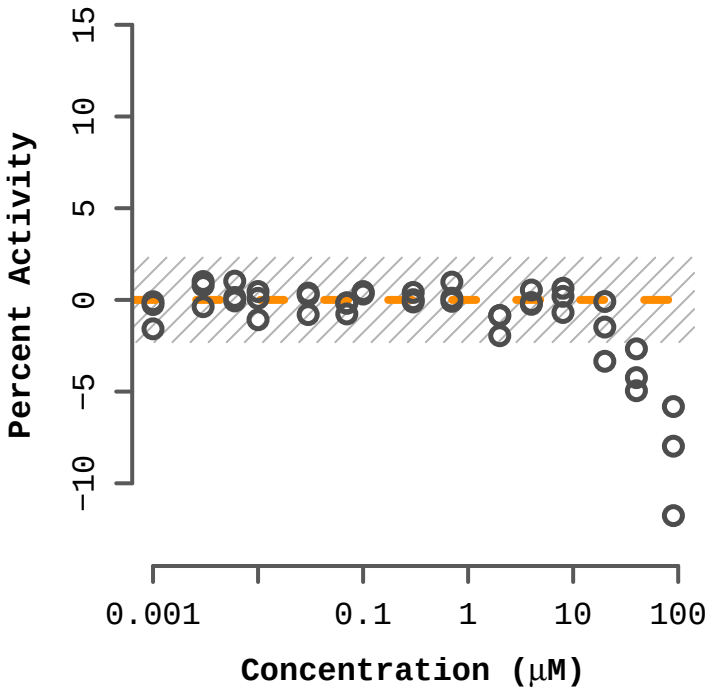
NAME: Alfentanil hydrochloride
CHID: 48927 CASRN: 69049-06-5
SPID(S): Tox21_112878
M4ID: 12482905

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.595 MAX_MED: 0.829 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

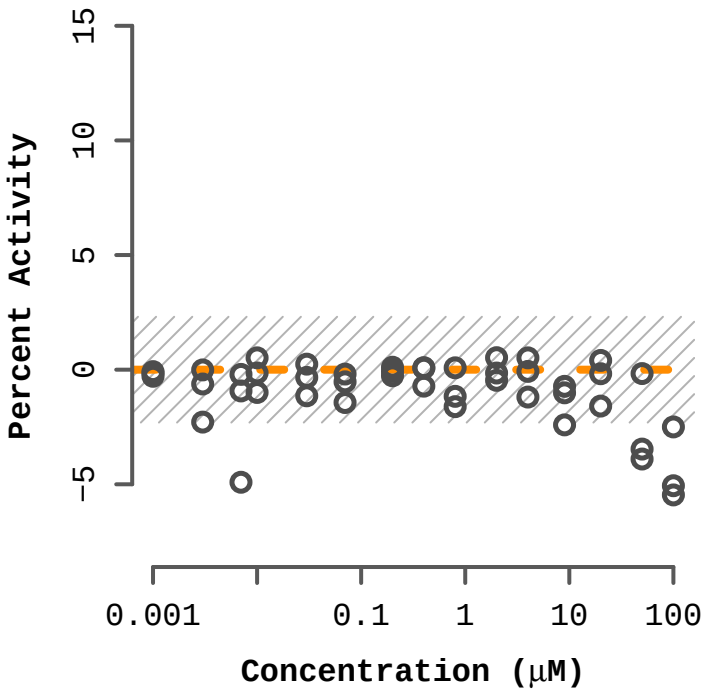
NAME: Sufentanil citrate
CHID: 48928 CASRN: 60561-17-3
SPID(S): Tox21_112879
M4ID: 12482904

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.17	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 0.475 **MAX_MED:** 0.788 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

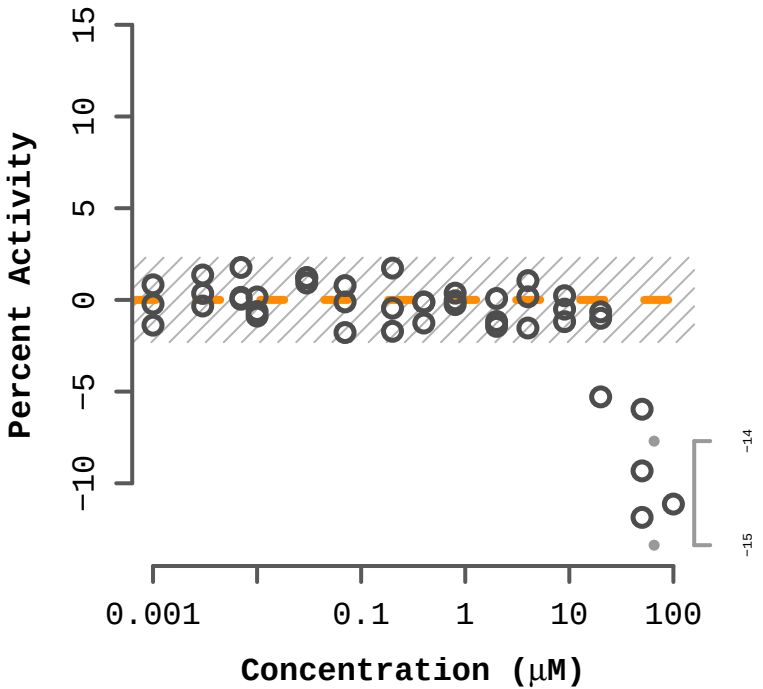
NAME: N-(4-Fluorophenyl)-N-[1-(2-phenylethyl)-4-piper
CHID: 48929 CASRN: 90736-23-5
SPID(S): Tox21_112836
M4ID: 12482931

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	167.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: -0.0281 MAX_MED: 0.0665 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

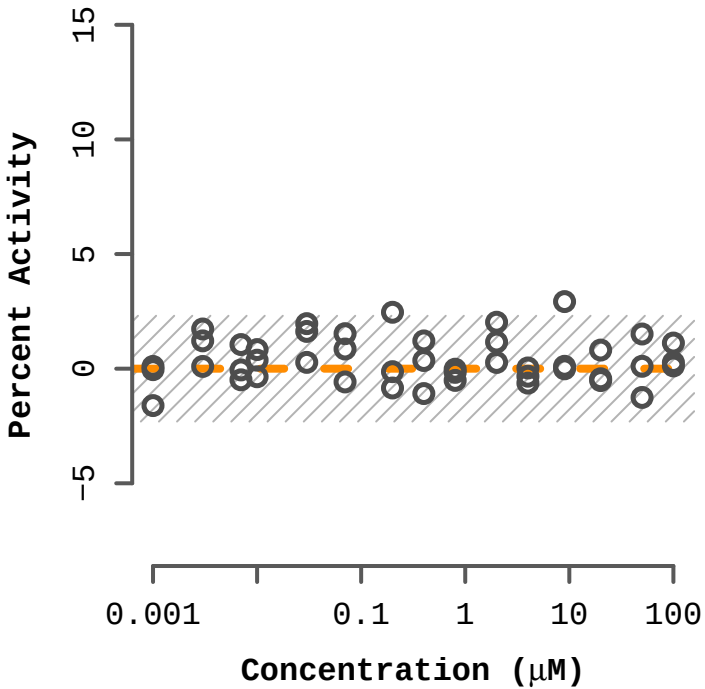
NAME: dl-cis-3-Methylfentanyl hydrochloride
CHID: 48930 **CASRN:** 78995-18-3
SPID(S): Tox21_112837
M4ID: 12482930 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	230.09	NA	NA
PROB:	1	NA	NA
RMSE:	4.37	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

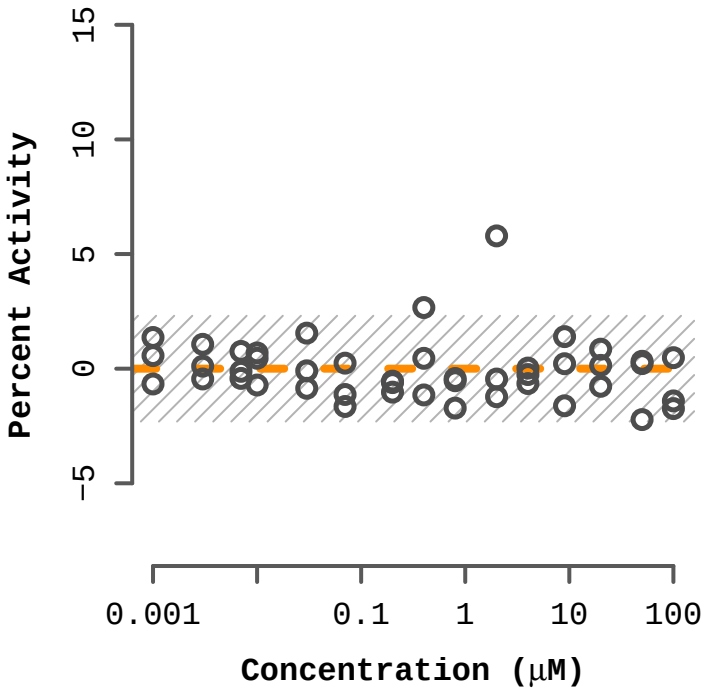
NAME: alpha-Methylfentanyl hydrochloride
CHID: 48932 **CASRN:** 1443-44-3
SPID(S): Tox21_112900
M4ID: 12482885

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

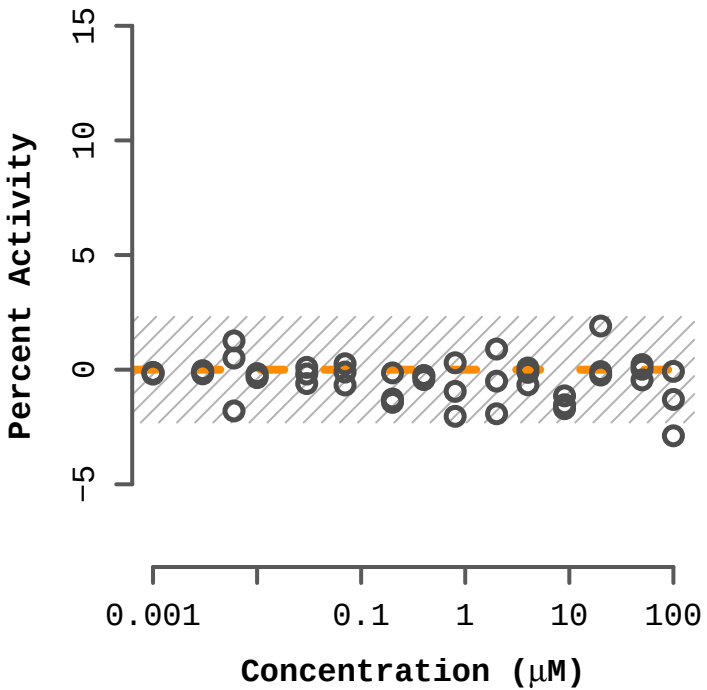
NAME: N−(1−Benzyl−4−piperidyl)−N−phenylpropanamide hy
CHID: 48933 CASRN: 5156−58−1
SPID(S): Tox21_112839
M4ID: 12482929

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.37 MAX_MED: 0.572 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-[1-(2-Hydroxy-2-phenylethyl)-4-piperidyl]-N-

CHID: 48934 **CASRN:** 1473-95-6

SPID(S): Tox21_112843

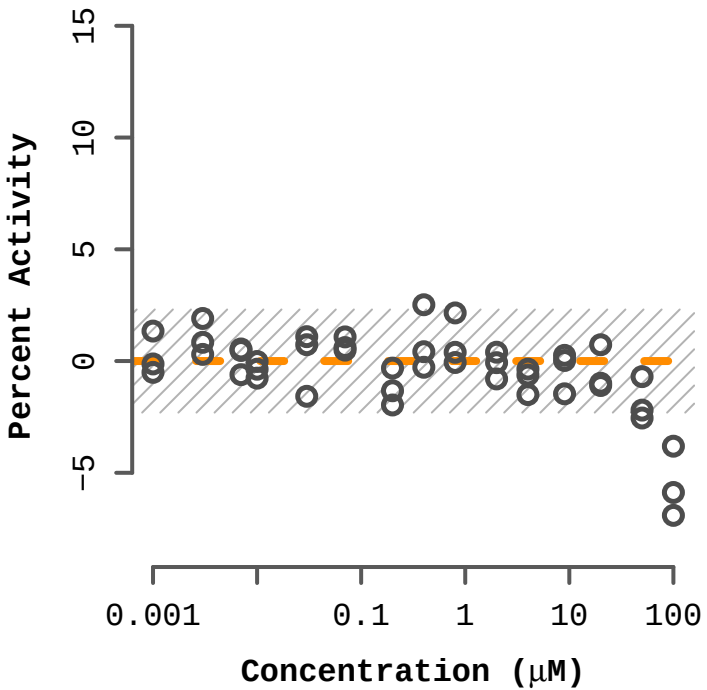
M4ID: 12482926

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.88	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.529 **MAX_MED:** 0.506 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-[1-[1-Methyl-2-(2-thienyl)ethyl]-4-piperidyl

CHID: 48935 **CASRN:** 117332-94-2

SPID(S): Tox21_112844

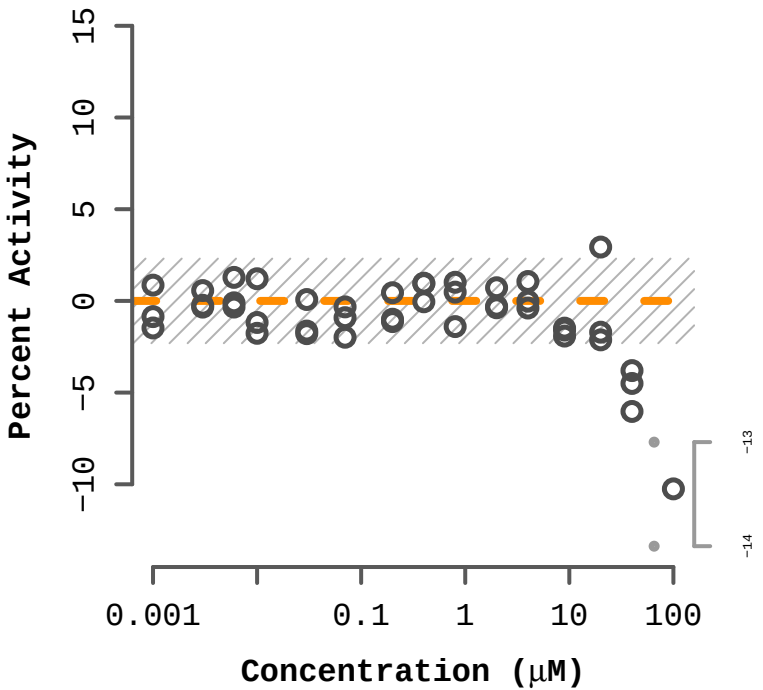
M4ID: 12482925

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

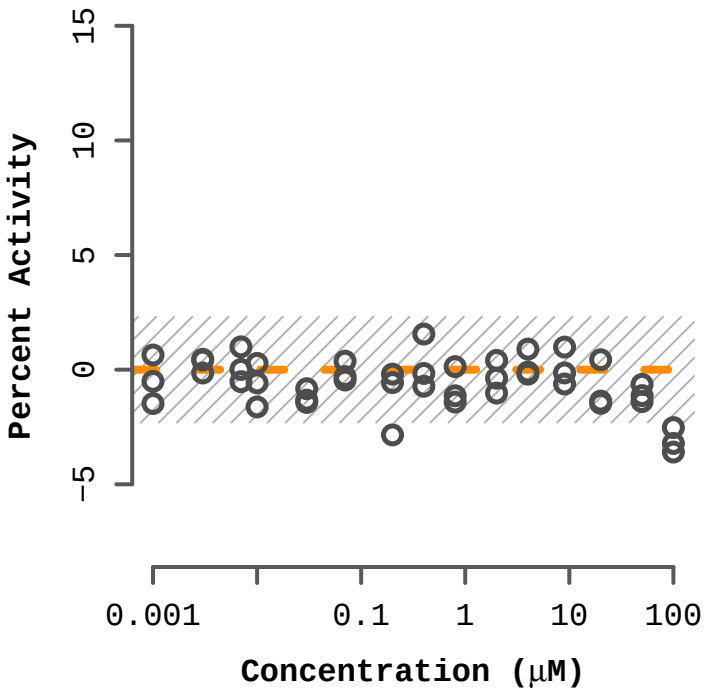
NAME: cis-N-[1-[2-(2-Thienyl)ethyl]-3-methyl-4-piper
CHID: 48936 **CASRN:** 131690-45-4
SPID(S): Tox21_112845
M4ID: 12482924 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.68	NA	NA
PROB:	1	NA	NA
RMSE:	3.66	NA	NA

MAX_MEAN: 0.622 **MAX_MED:** 0.945 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Phenyl-N-[1-(2-thienyl)methyl-4-piperidyl]pr

CHID: 48937 **CASRN:** 117332-93-1

SPID(S): Tox21_112846

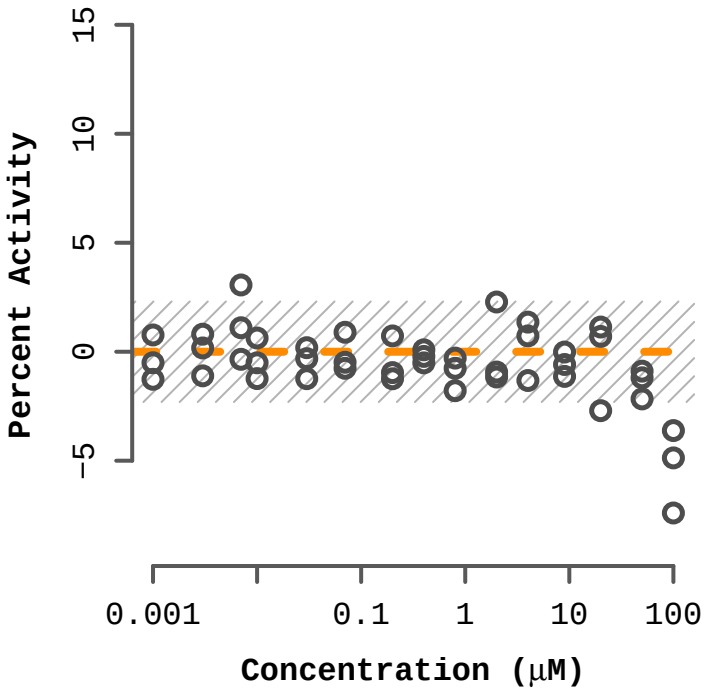
M4ID: 12482923

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.245 **MAX_MED:** 0.421 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

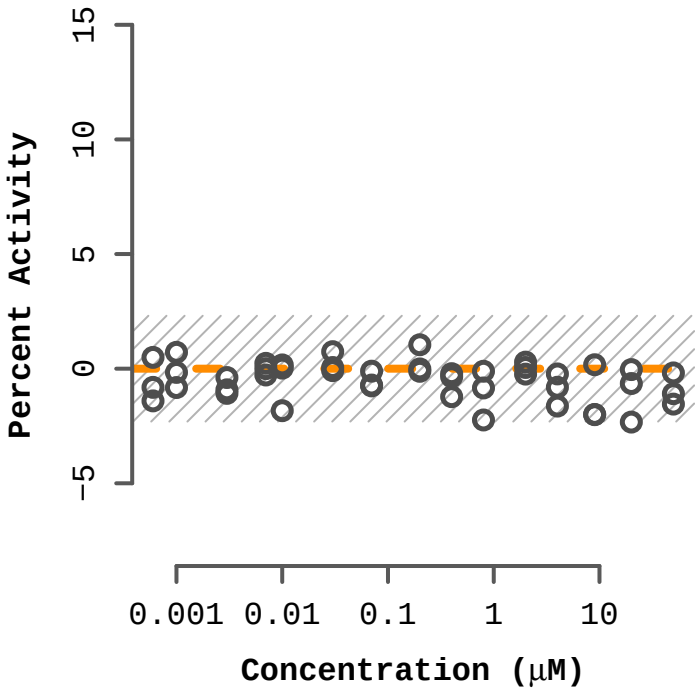
NAME: N-Phenyl-N-[1-[2-(2-thienyl)ethyl]-4-piperidyl
CHID: 48938 **CASRN:** 79278-88-9
SPID(S): Tox21_112847
M4ID: 12482922

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

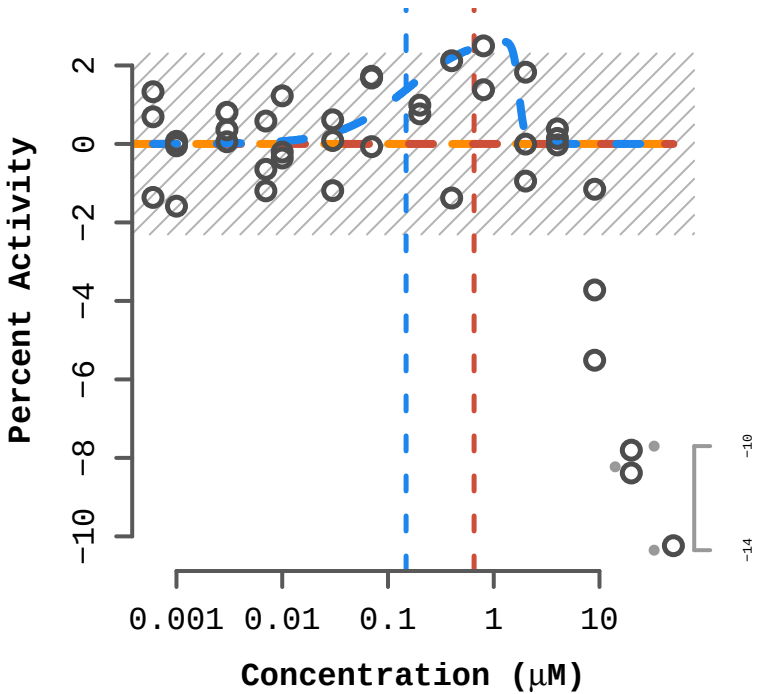
NAME: Varenicline dihydrochloride
CHID: 48941 **CASRN:** 230615-23-3
SPID(S): Tox21_112901_1
M4ID: 12482884

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.308 **MAX_MED:** 0.0537 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Canertinib
CHID: 48943 CASRN: 267243-28-7
SPID(S): Tox21_113361
M4ID: 12482675 BRK

HILL MODEL (in red):

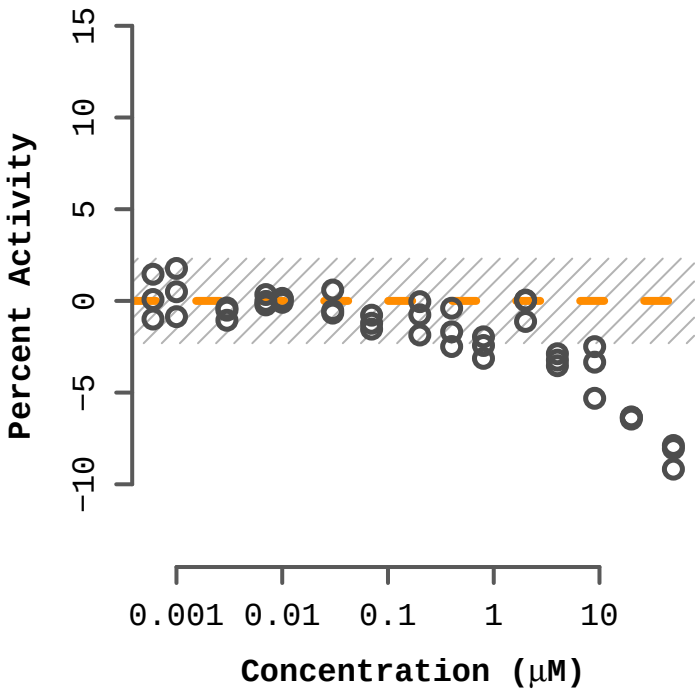
	tp	ga	gw
val:	5.33e-10	-0.186	2.06
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.77	-0.829	1.36	0.237	15.5
sd:	2.48	0.949	1.94	4.72	1150

	CNST	HILL	GNLS
AIC:	242.53	248.53	244.08
PROB:	0.66	0.03	0.3
RMSE:	4.2	4.2	4.09

MAX_MEAN: 2.66 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

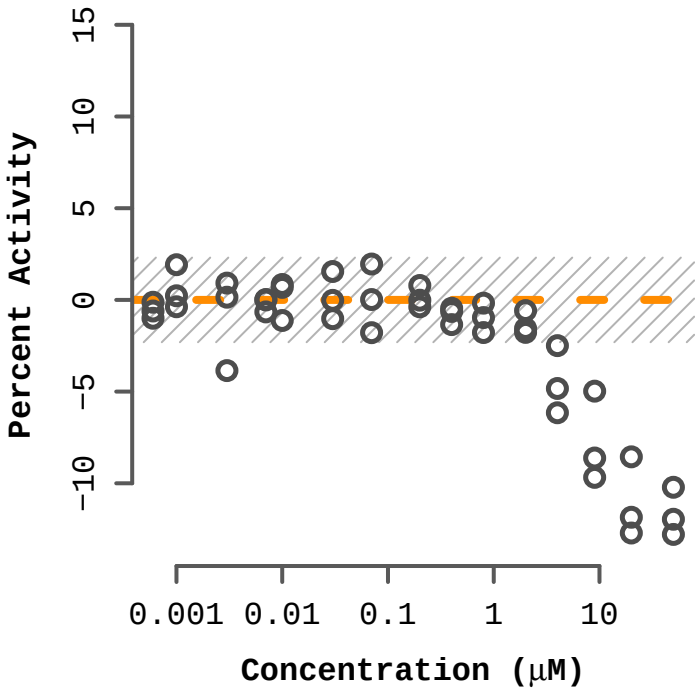
NAME: Selumetinib
CHID: 48944 CASRN: 606143-52-6
SPID(S): Tox21_113362_1
M4ID: 12482674

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.86	NA	NA
PROB:	1	NA	NA
RMSE:	3.19	NA	NA

MAX_MEAN: 0.471 **MAX_MED:** 0.501 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

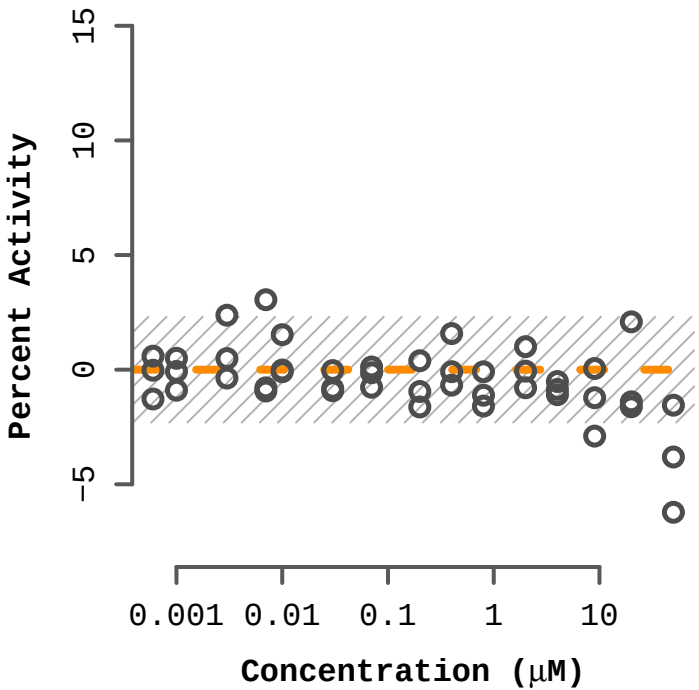
NAME: C.I. 1040
CHID: 48945 **CASRN:** 212631-79-3
SPID(S): Tox21_113363_1
M4ID: 12482673

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	262.06	NA	NA
PROB:	1	NA	NA
RMSE:	4.93	NA	NA

MAX_MEAN: 0.592 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

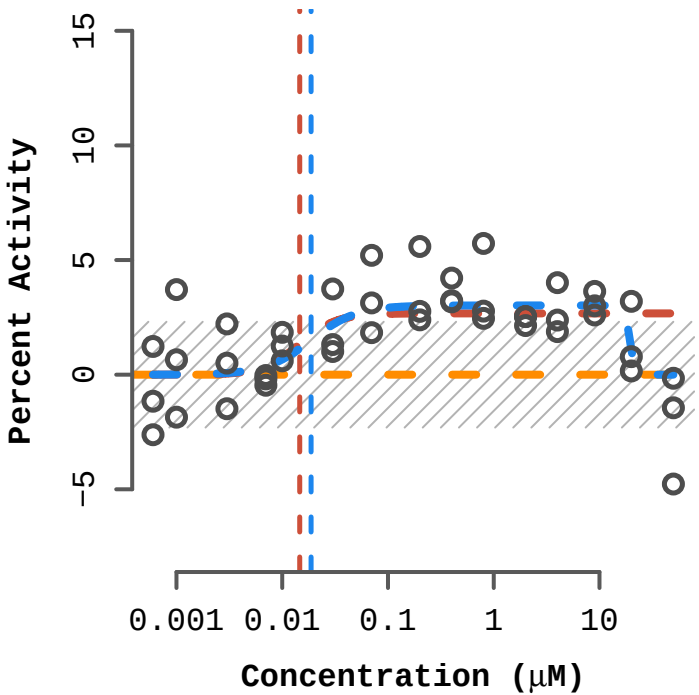
NAME: Tandutinib
CHID: 48947 CASRN: 387867-13-2
SPID(S): Tox21_113366_1
M4ID: 12482672

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.58	NA	NA

MAX_MEAN: 0.832 **MAX_MED:** 0.485 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: MK−2206
CHID: 48948 CASRN: 1032350−13−2
SPID(S): Tox21_113368_1
M4ID: 12482670

HILL MODEL (in red):

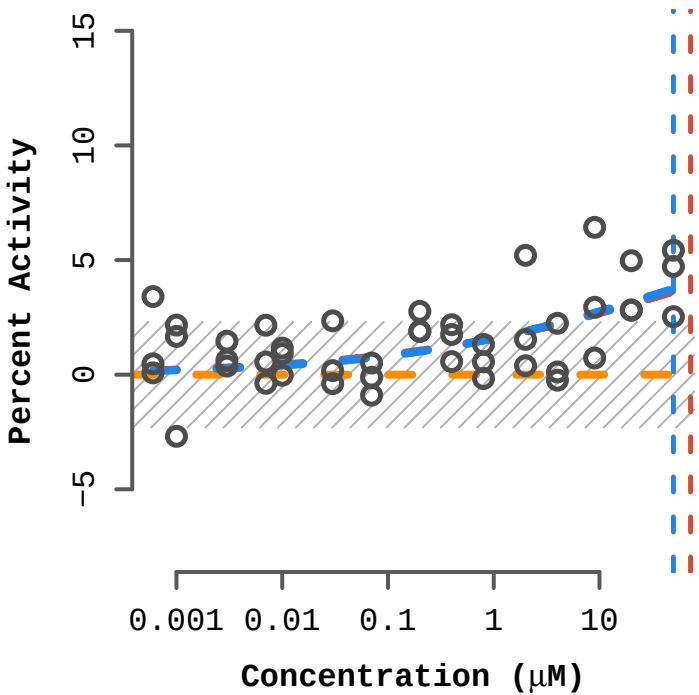
	tp	ga	gw
val:	2.67	−1.83	2.5
sd:	0.306	0.281	2.24

GAIN−LOSS MODEL (in blue):

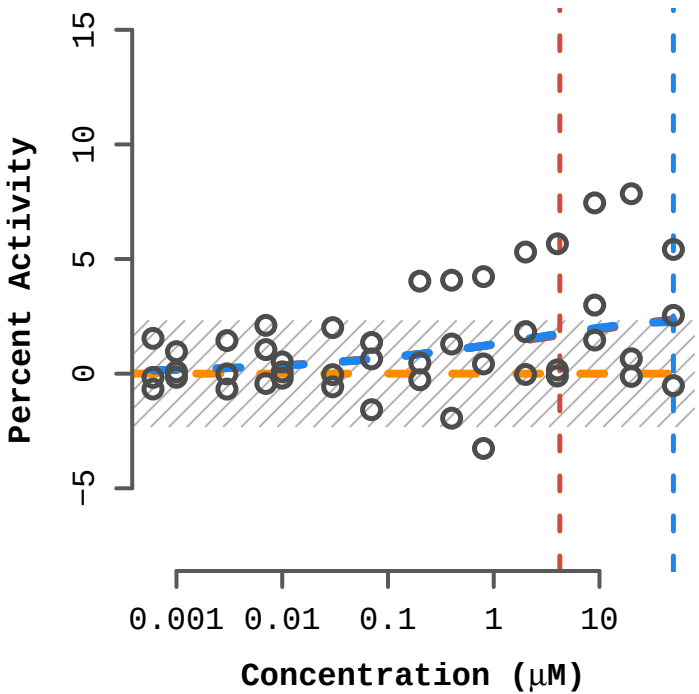
	tp	ga	gw	la	lw
val:	3.02	−1.73	2.02	1.29	16.9
sd:	0.281	0.209	1.04	0.0861	104

	CNST	HILL	GNLS
AIC:	225.32	186.46	172.97
PROB:	0	0	1
RMSE:	2.73	1.91	1.49

MAX_MEAN: 3.65 MAX_MED: 3.23 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Gonadorelin hydrochloride
CHID:    48954   CASRN: 51952-41-1
SPID(S): Tox21_113381_1
M4ID:    12482668

HILL MODEL (in red):
      tp       ga       gw
val:  7.71     1.86     0.315
sd:   4.89     1.53     0.121

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.5      1.7      0.337    3.57     12.5
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  206.38      173.05      177.15
PROB: 0           0.89        0.11
RMSE: 2.37        1.49        1.49

MAX_MEAN: 4.23      MAX_MED: 4.72      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Doramapimod
CHID: 48957 **CASRN:** 285983-48-4
SPID(S): Tox21_113386_1
M4ID: 12482666

HILL MODEL (in red):

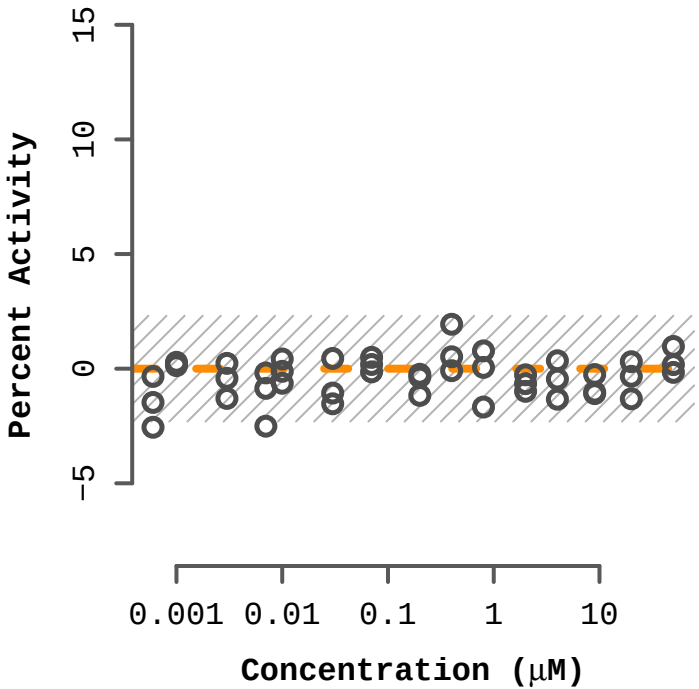
	tp	ga	gw
val:	3.37	0.625	0.351
sd:	6.35	5.16	0.491

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.12	1.7	0.328	2.42	0.615
sd:	61.7	18.5	0.517	9.51	3.38

	CNST	HILL	GNLS
AIC:	210.16	203.04	207.01
PROB:	0.02	0.86	0.12
RMSE:	2.66	2.15	2.14

MAX_MEAN: 3.97 **MAX_MED:** 2.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

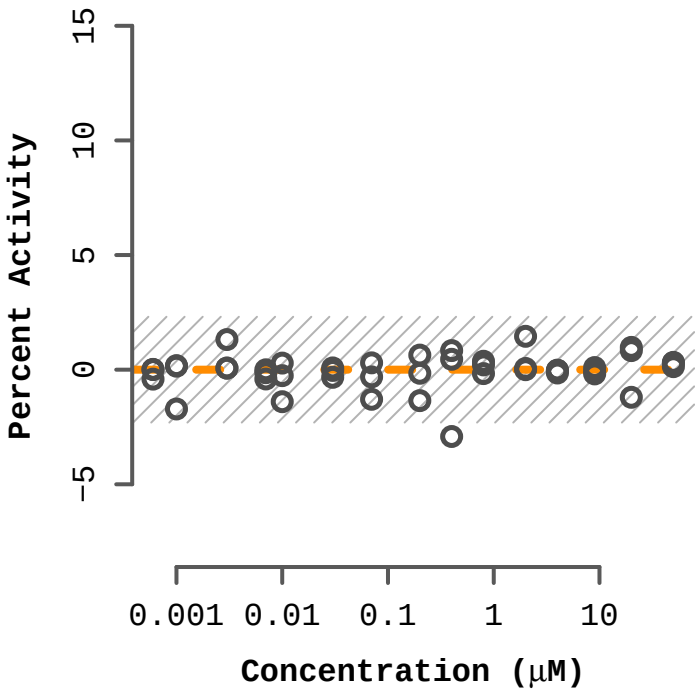
NAME: Nalpha-Acetyl-L-glutamine
CHID: 48959 **CASRN:** 2490-97-3
SPID(S): Tox21_113393_1
M4ID: 12482663

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.79 **MAX_MED:** 0.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

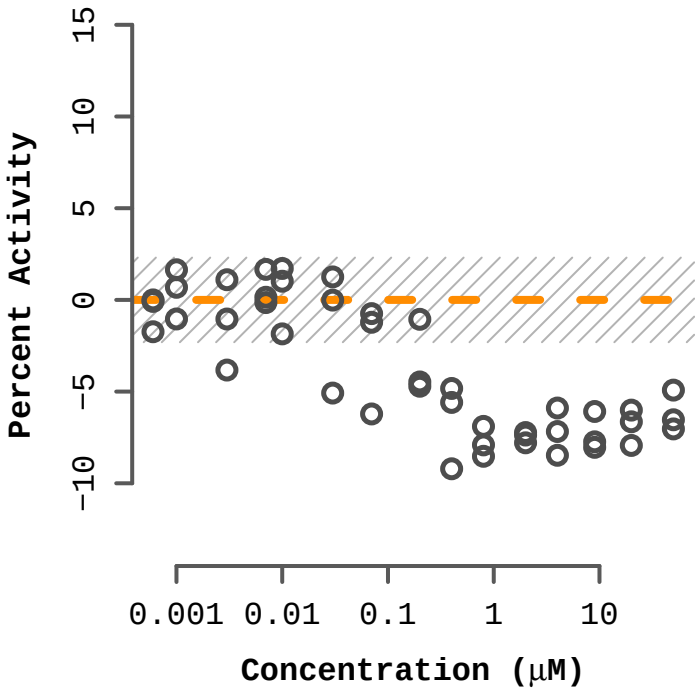
NAME: Diatrizoic acid dihydrate
CHID: 48960 CASRN: 50978-11-5
SPID(S): Tox21_113395_1
M4ID: 12482662

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.504 **MAX_MED:** 0.833 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

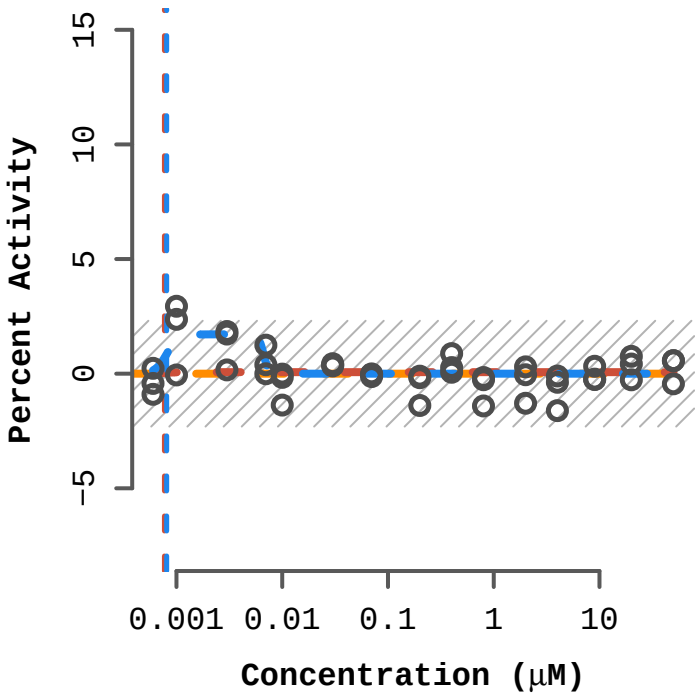
NAME: Flavopiridol hydrochloride
CHID: 48961 **CASRN:** 131740-09-5
SPID(S): Tox21_113396_1
M4ID: 12482661

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	283.95	NA	NA
PROB:	1	NA	NA
RMSE:	5.19	NA	NA

MAX_MEAN: 0.556 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Piperacillin sodium salt
CHID: 48965 CASRN: 59703-84-3
SPID(S): Tox21_113405_1
M4ID: 12482659

HILL MODEL (in red):

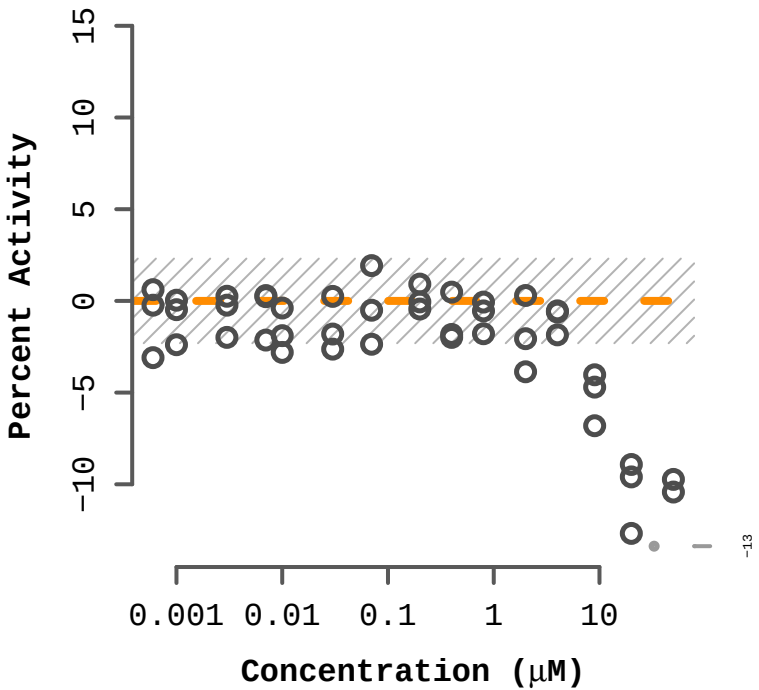
	tp	ga	gw
val:	0.0664	−3.11	8
sd:	0.114	0.324	24.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.72	−3.09	8	−2.18	18
sd:	0.399	0.0652	4.78	0.0309	22.3

	CNST	HILL	GNLS
AIC:	113.9	119.52	109.96
PROB:	0.12	0.01	0.87
RMSE:	0.91	0.9	0.73

MAX_MEAN: 1.75 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

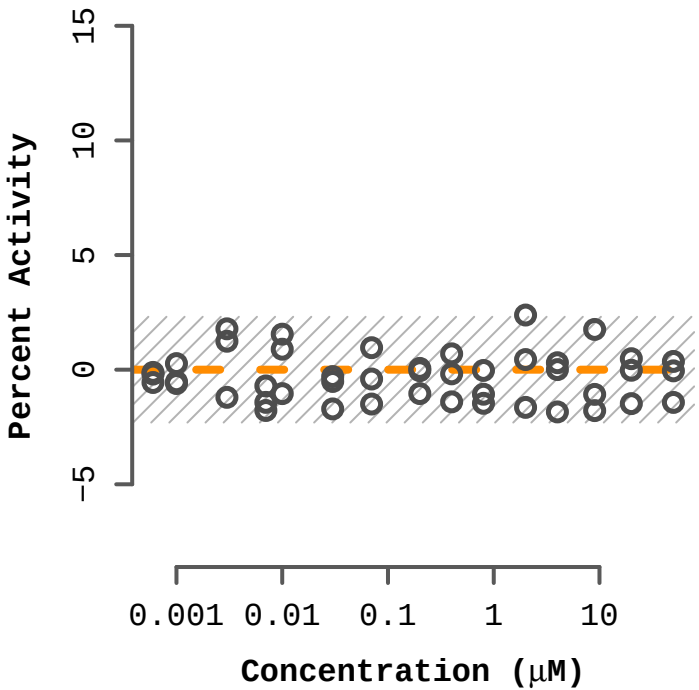
NAME: Sertindole
CHID: 48967 **CASRN:** 106516-24-9
SPID(S): Tox21_113421_1
M4ID: 12482655 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	251.46	NA	NA
PROB:	1	NA	NA
RMSE:	4.45	NA	NA

MAX_MEAN: 0.141 **MAX_MED:** 0.231 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

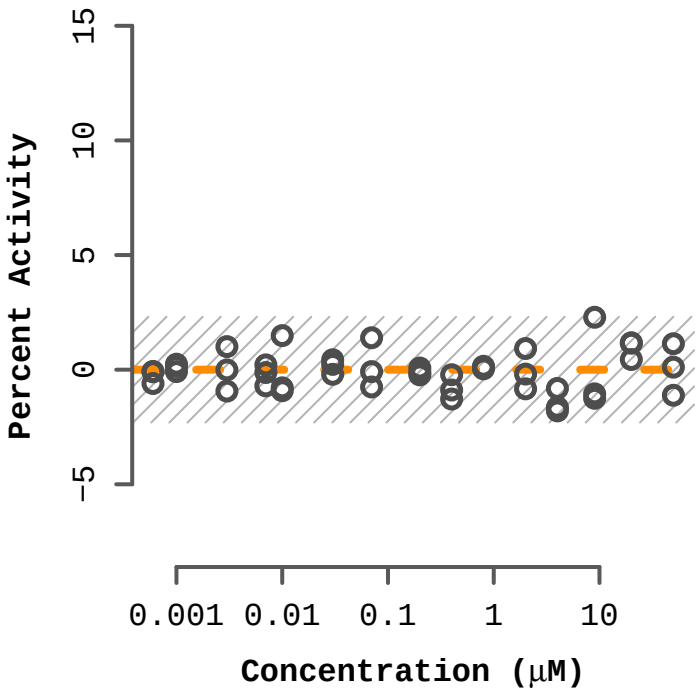
NAME: Apafant
CHID: 48974 **CASRN:** 105219-56-5
SPID(S): Tox21_113594_1
M4ID: 12482590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.607 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

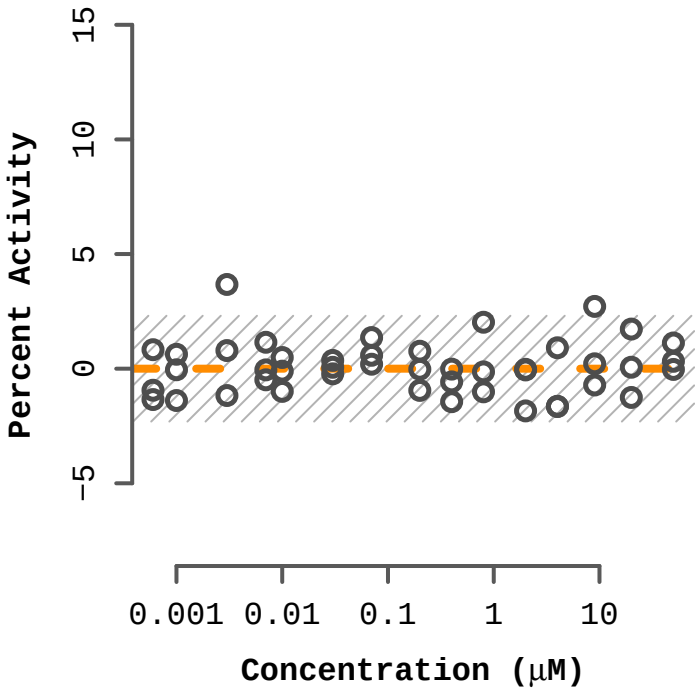
NAME: Enalapril acid
CHID: 48975 CASRN: 76420-72-9
SPID(S): Tox21_113430_1
M4ID: 12482654

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.926 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

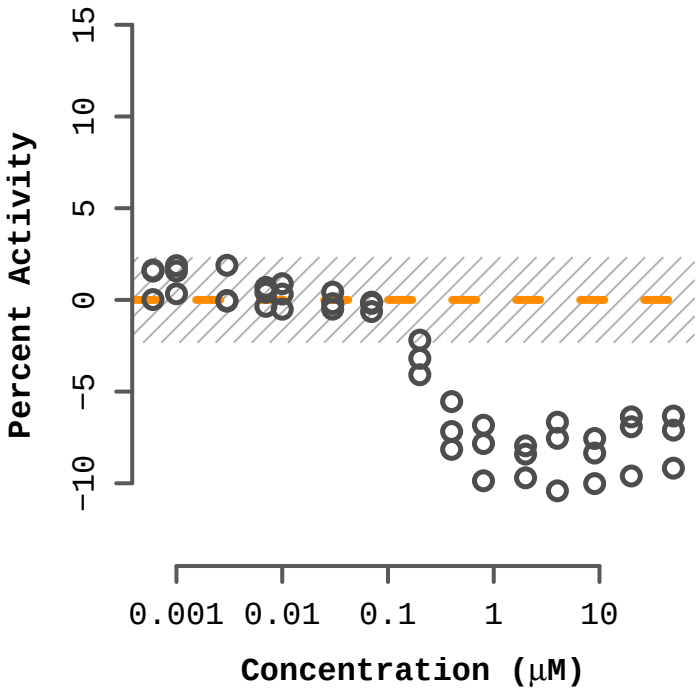
NAME: Acetylcholine chloride
CHID: 48978 **CASRN:** 60-31-1
SPID(S): Tox21_113435_1
M4ID: 12482653

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 0.792 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

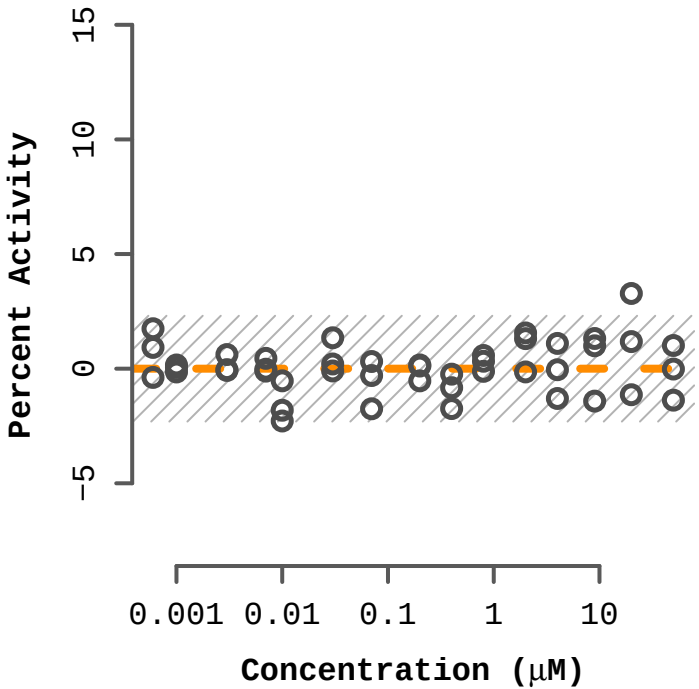
NAME: Maduramicin ammonium
CHID: 48983 **CASRN:** 84878-61-5
SPID(S): Tox21_113443_1
M4ID: 12482652

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.33	NA	NA
PROB:	1	NA	NA
RMSE:	5.62	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

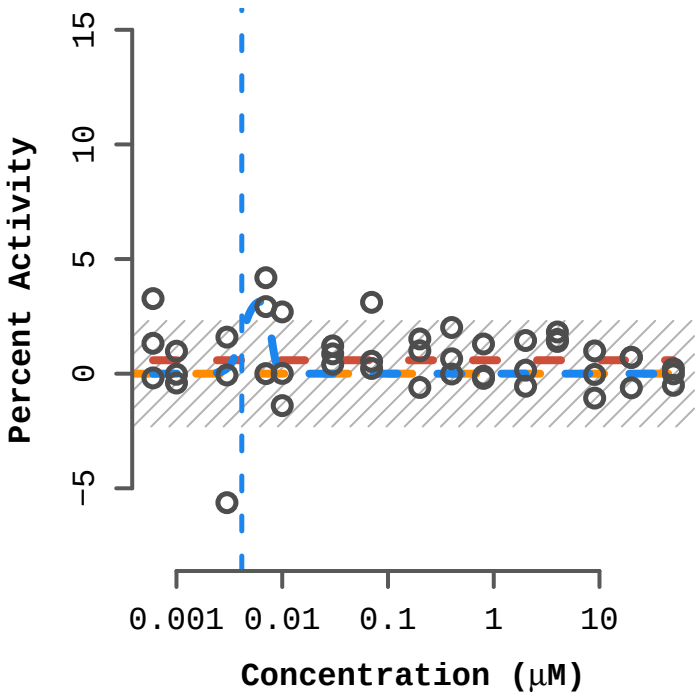
NAME: Dichloro(ethylenediamine)platinum(II)
CHID: 48988 **CASRN:** 14096-51-6
SPID(S): Tox21_113466_1
M4ID: 12482641

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentagastrin
CHID: 48992 **CASRN:** 5534-95-2
SPID(S): Tox21_113479_1
M4ID: 12482637

HILL MODEL (in red):

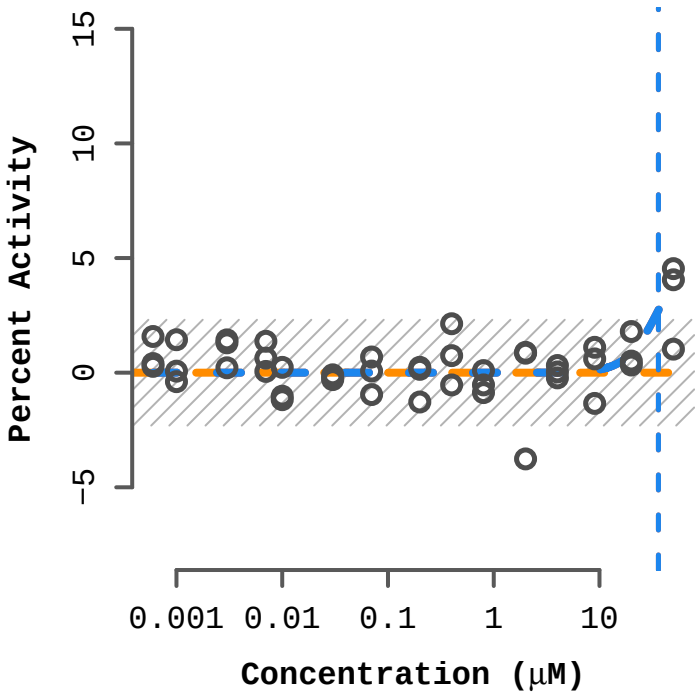
	tp	ga	gw
val:	0.586	−5.21	3.28
sd:	0.179	909	1550

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.33	−2.38	8	−2.1	16.5
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	166.87	162.58	170.53
PROB:	0.1	0.88	0.02
RMSE:	1.63	1.51	1.53

MAX_MEAN: 2.37 **MAX_MED:** 2.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5,7-Dichloro-8-hydroxy-2-methylquinoline
CHID: 48998 CASRN: 72-80-0
SPID(S): Tox21_113490_1
M4ID: 12482633

HILL MODEL (in red):

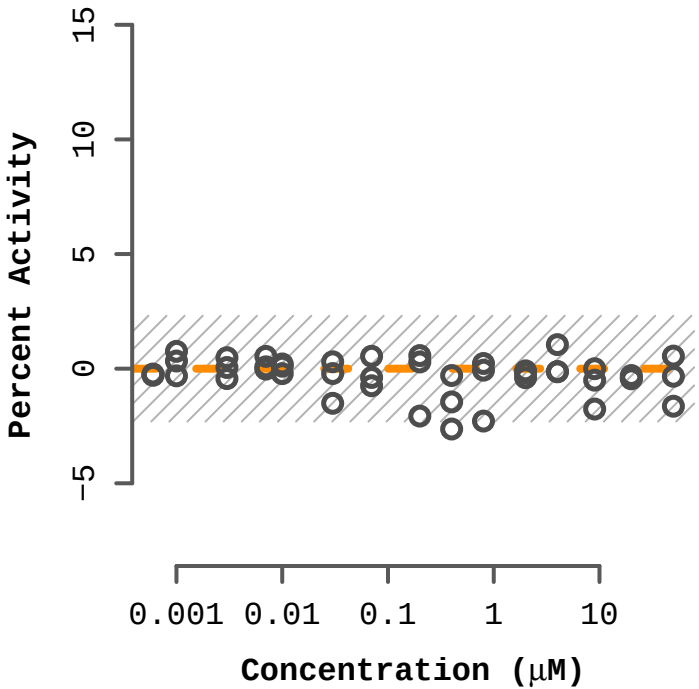
	tp	ga	gw
val:	5.45	1.56	2.85
sd:	7.67	0.571	3.86

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.45	1.56	2.85	3.39	3.93
sd:	7.55	0.563	3.81	1240	2910

	CNST	HILL	GNLS
AIC:	148.36	137.63	141.63
PROB:	0	0.88	0.12
RMSE:	1.37	1.08	1.08

MAX_MEAN: 3.21 **MAX_MED:** 4.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

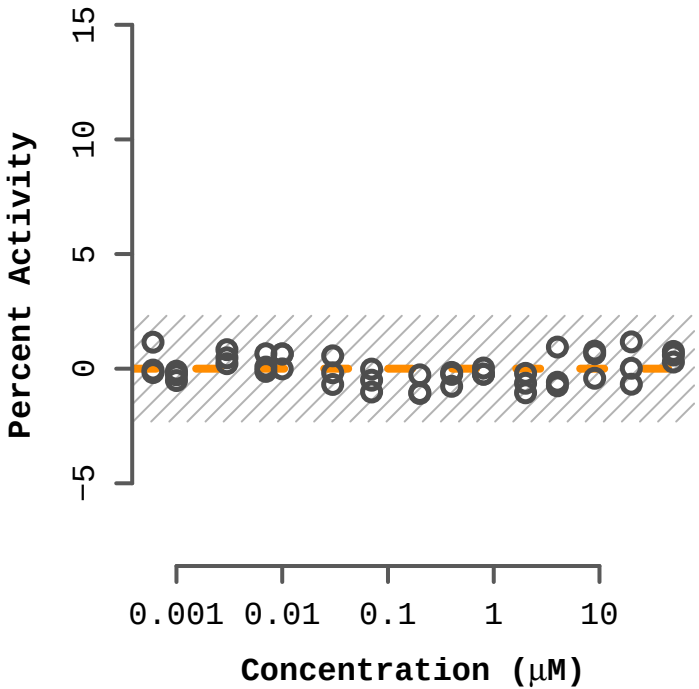
NAME: Diloxanide furoate
CHID: 48999 **CASRN:** 3736-81-0
SPID(S): Tox21_113492_1
M4ID: 12482631

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.265 **MAX_MED:** 0.335 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

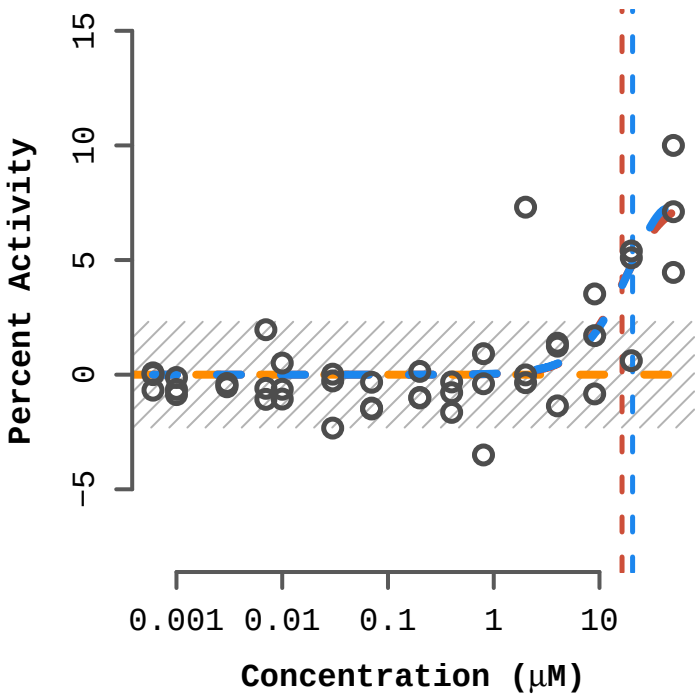
NAME: Dicloxacillin sodium salt monohydrate
CHID: 49002 **CASRN:** 13412-64-1
SPID(S): Tox21_113495_1
M4ID: 12482630

HILL MODEL: Not applicable.

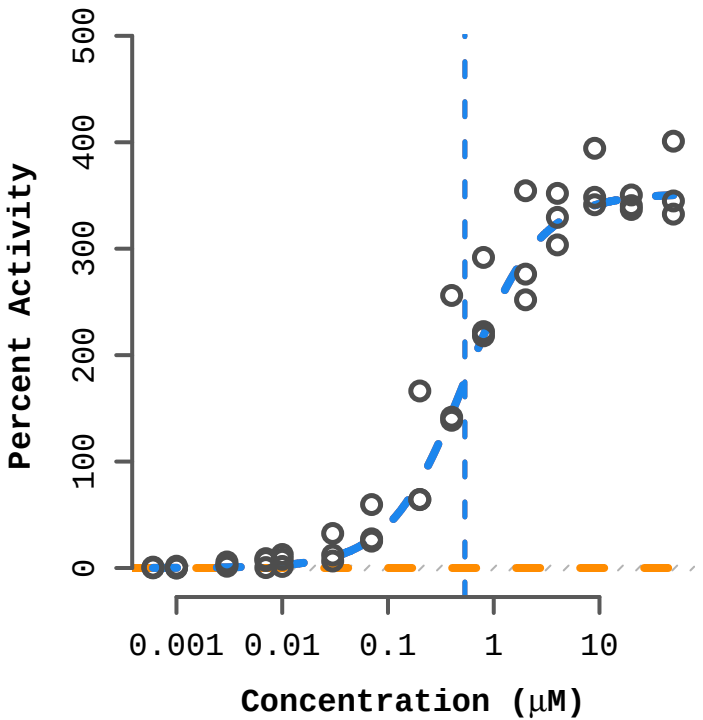
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.61	NA	NA

MAX_MEAN: 0.547 **MAX_MED:** 0.653 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Esmolol hydrochloride
CHID:    49003   CASRN: 81161-17-3
SPID(S): Tox21_113496_1
M4ID:    12482629

HILL MODEL (in red):
      tp       ga       gw
val:  7.89     1.21     1.97
sd:   2.13     0.169    0.952

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.75     1.31     1.8      1.85     5.36
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  204.25      173.96      177.95
PROB: 0           0.88        0.12
RMSE: 2.74        1.75        1.75

MAX_MEAN: 7.19      MAX_MED: 7.11      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortisone 21-hemisuccinate sodium salt
CHID: 49006 CASRN: 125-04-2
SPID(S): Tox21_113501_1
M4ID: 12482628

HILL MODEL (in red):

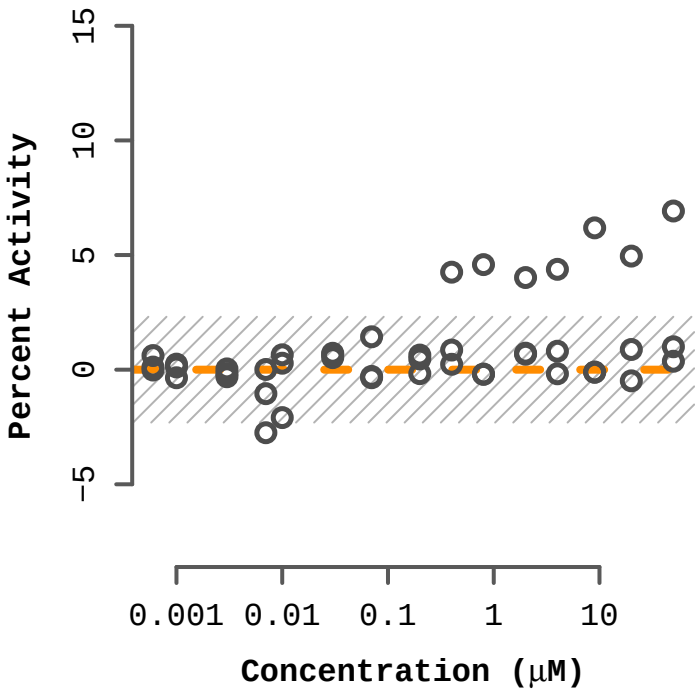
	tp	ga	gw
val:	352	-0.273	1.22
sd:	6.86	0.0331	0.124

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	352	-0.273	1.22	3.6	12.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	615.6	421.75	425.75
PROB:	0	0.88	0.12
RMSE:	213.73	29.92	29.92

MAX_MEAN: 361 **MAX_MED:** 348 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

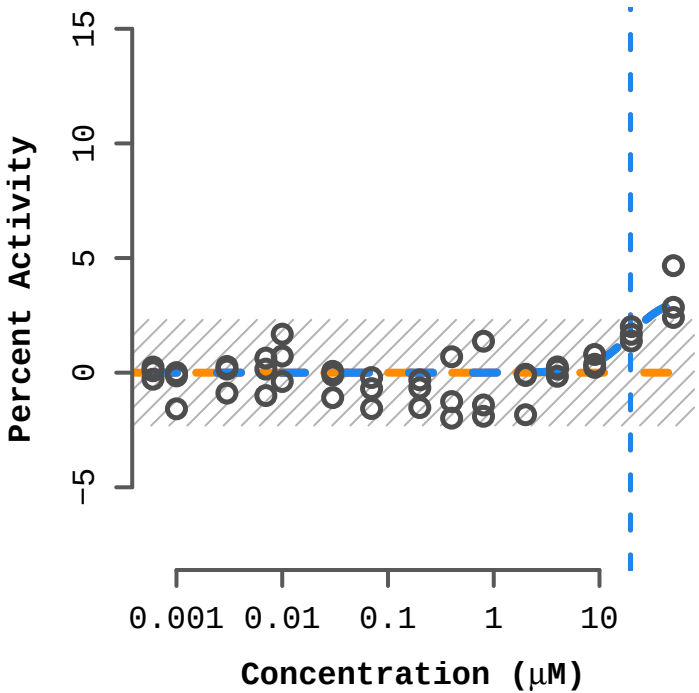
NAME: Ibudilast
CHID: 49007 CASRN: 50847-11-5
SPID(S): Tox21_113503_1
M4ID: 12482626

HILL MODEL: Not applicable.

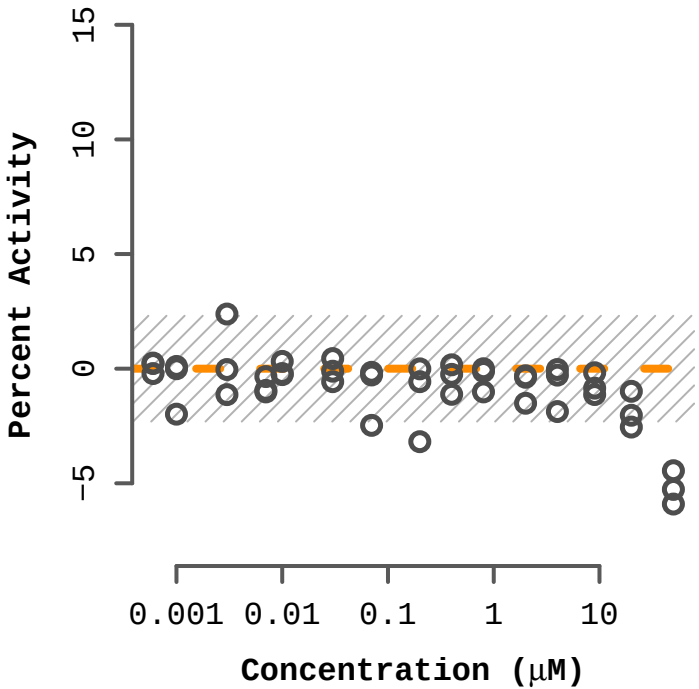
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	180.81	NA	NA
PROB:	1	NA	NA
RMSE:	2.15	NA	NA

MAX_MEAN: 2.76 **MAX_MED:** 1 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Prochlorperazine dimaleate
CHID:    49015   CASRN: 84-02-6
SPID(S): Tox21_113522_1
M4ID:    12482621

HILL MODEL (in red):
      tp       ga       gw
val:  3.32     1.29     2.44
sd:   0.952    0.15     1.33

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.32     1.29     2.44     2.86     5.74
sd:   0.952    0.15     1.33     1780     8880

      CNST        HILL        GNLS
AIC:  150.67      125.72      129.72
PROB: 0           0.88        0.12
RMSE: 1.31        0.89        0.89

MAX_MEAN: 3.31      MAX_MED: 2.85      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

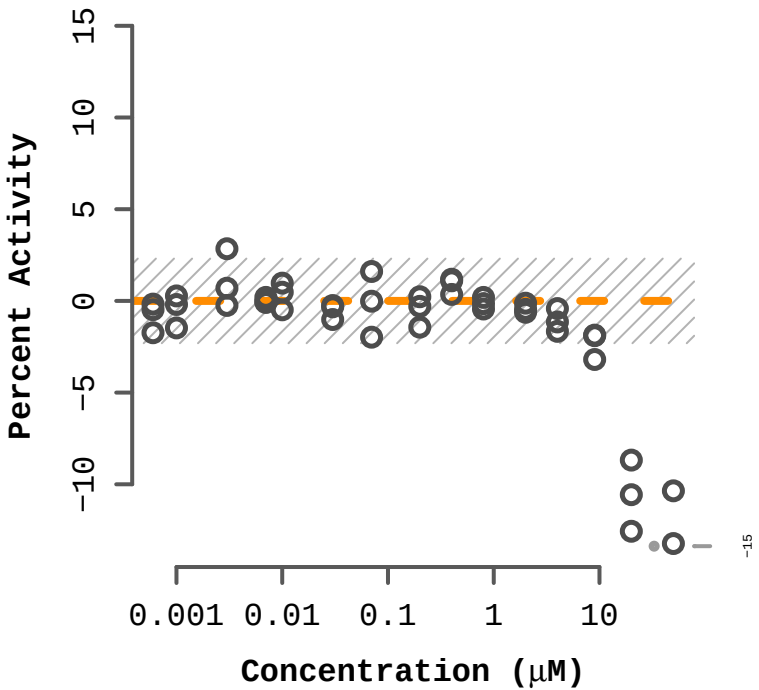
NAME: Dimethyl chloromalonate
CHID: 49018 CASRN: 28868-76-0
SPID(S): Tox21_113538_1
M4ID: 12482616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 0.407 **MAX_MED:** 0.226 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

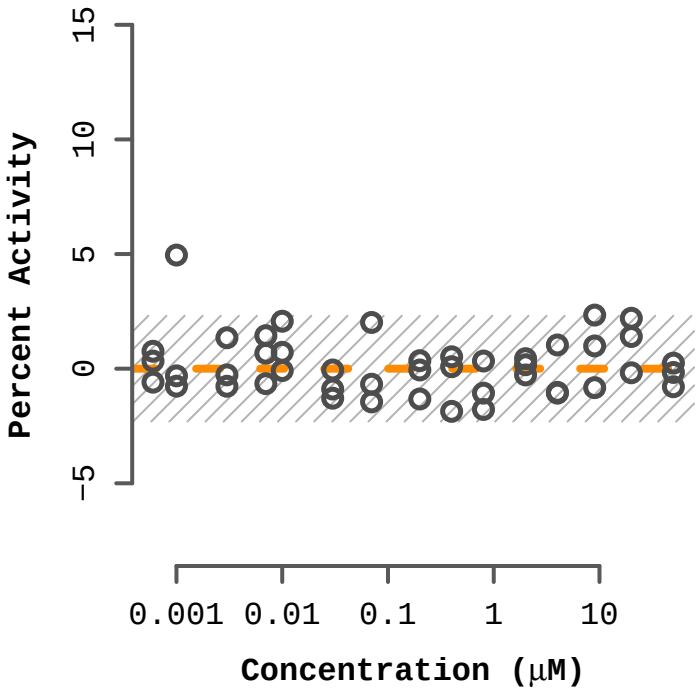
NAME: Penfluridol
CHID: 49021 **CASRN:** 26864-56-2
SPID(S): Tox21_113546_1
M4ID: 12482614 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	232.26	NA	NA
PROB:	1	NA	NA
RMSE:	4.46	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

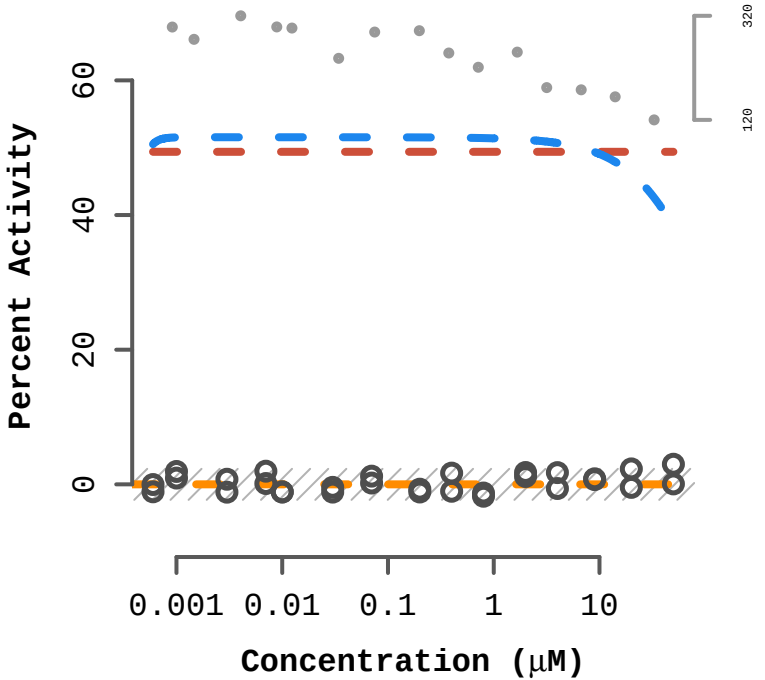
NAME: Proparacaine hydrochloride
CHID: 49022 **CASRN:** 5875-06-9
SPID(S): Tox21_113547_1
M4ID: 12482613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Thiosalicylic acid
CHID: 49032 CASRN: 147-93-3
SPID(S): Tox21_113560_1
M4ID: 12482611 BRK

HILL MODEL (in red):

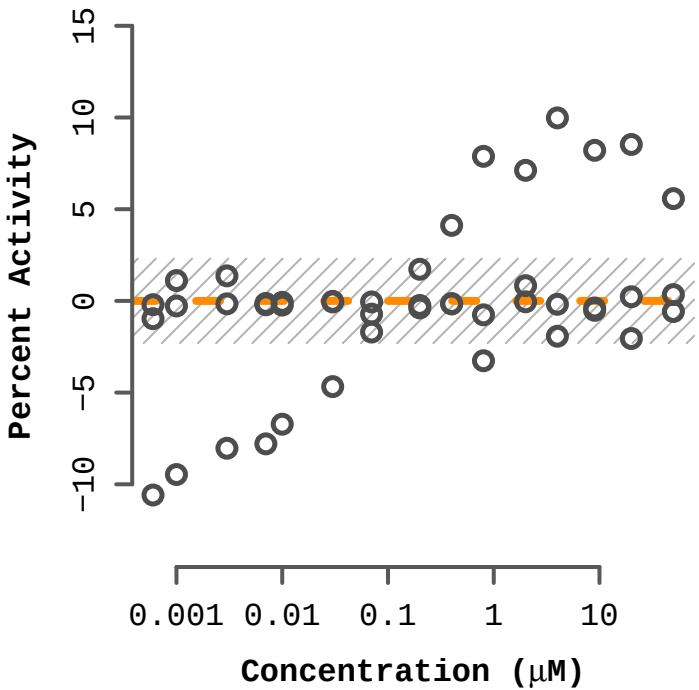
	tp	ga	gw
val:	49.4	-4.74	3.87
sd:	18.6	2220	5330

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	51.6	-3.46	7.21	2.08	1.2
sd:	24.6	10.7	310	4.8	12.3

	CNST	HILL	GNLS
AIC:	615.97	569.96	573.91
PROB:	0	0.88	0.12
RMSE:	144.67	123.75	123.26

MAX_MEAN: 106 MAX_MED: 2.99 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

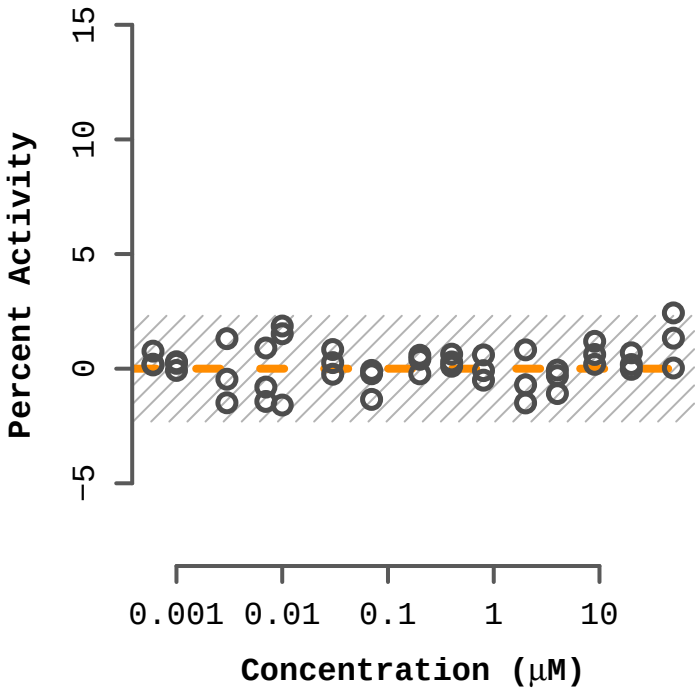
NAME: Salidroside
CHID: 49034 **CASRN:** 10338-51-9
SPID(S): Tox21_113565_1
M4ID: 12482609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	254.82	NA	NA
PROB:	1	NA	NA
RMSE:	4.29	NA	NA

MAX_MEAN: 2.64 **MAX_MED:** 0.834 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

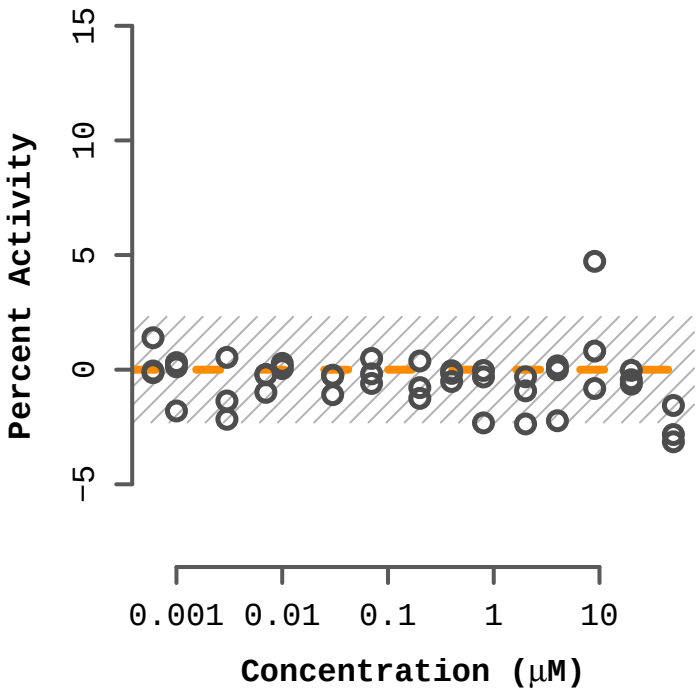
NAME: Lumiracoxib
CHID: 49035 **CASRN:** 220991-20-8
SPID(S): Tox21_113566_1
M4ID: 12482608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

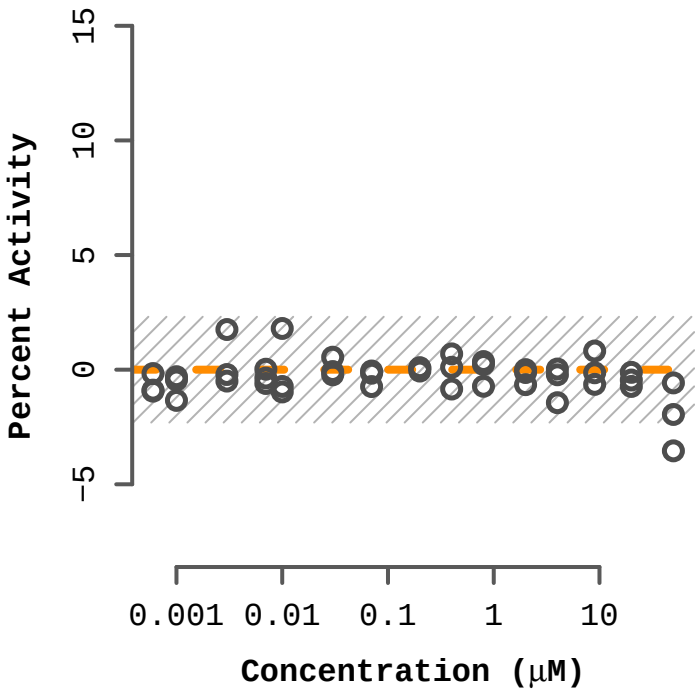
NAME: Dexchlorpheniramine hydrochloride
CHID: 49036 CASRN: 56343-98-7
SPID(S): Tox21_113570_1
M4ID: 12482605

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 0.812 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

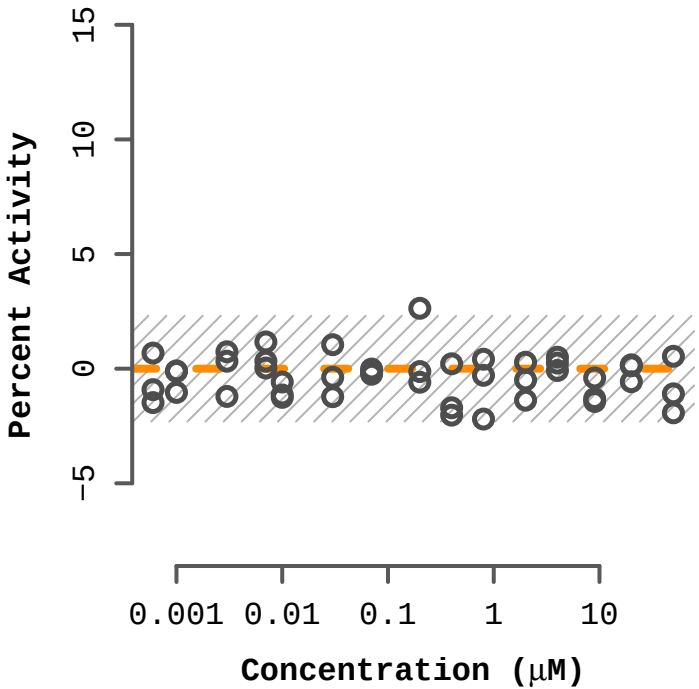
NAME: Zamifenacin fumarate
CHID: 49037 **CASRN:** 127308-98-9
SPID(S): Tox21_113572_1
M4ID: 12482603

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.97	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.349 **MAX_MED:** 0.227 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

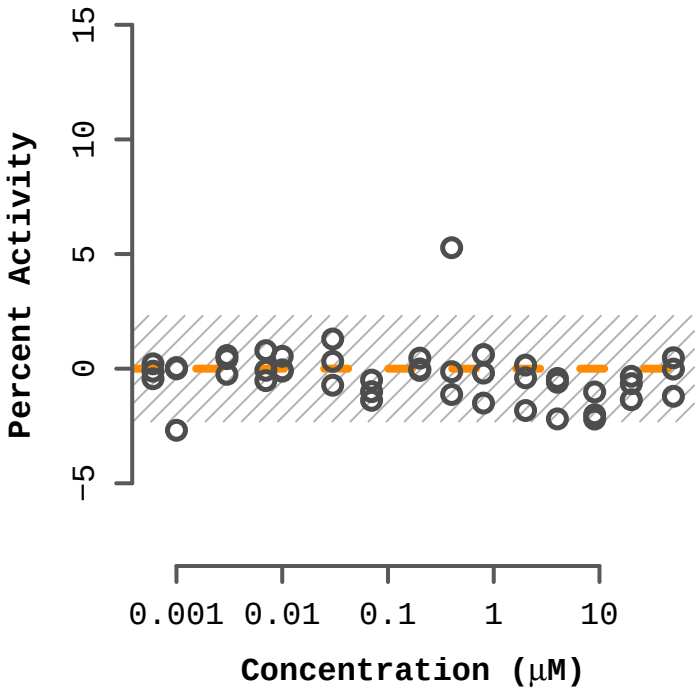
NAME: 2,4-Diamino-6-hydroxypyrimidine
CHID: 49038 **CASRN:** 56-06-4
SPID(S): Tox21_113576_1
M4ID: 12482601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.64 **MAX_MED:** 0.329 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

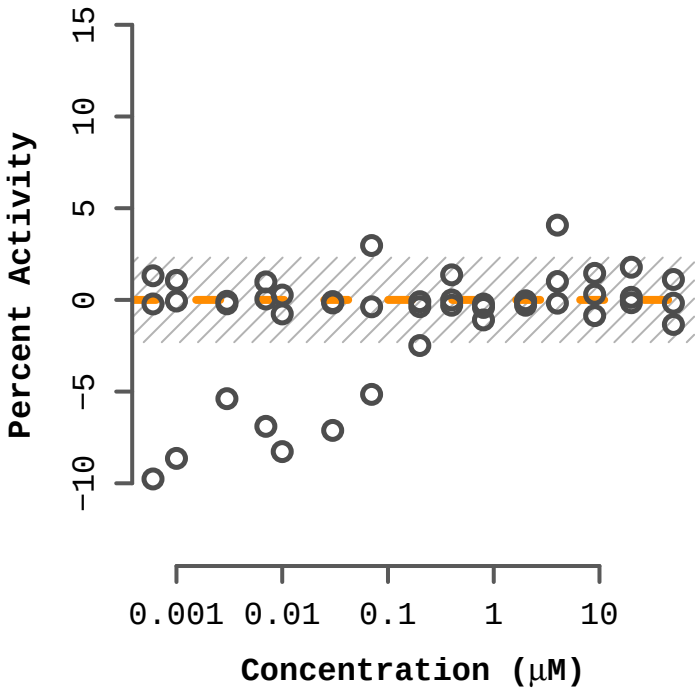
NAME: 3-Morpholinosydnonimine hydrochloride
CHID: 49039 **CASRN:** 16142-27-1
SPID(S): Tox21_113577_1
M4ID: 12482600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 0.438 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

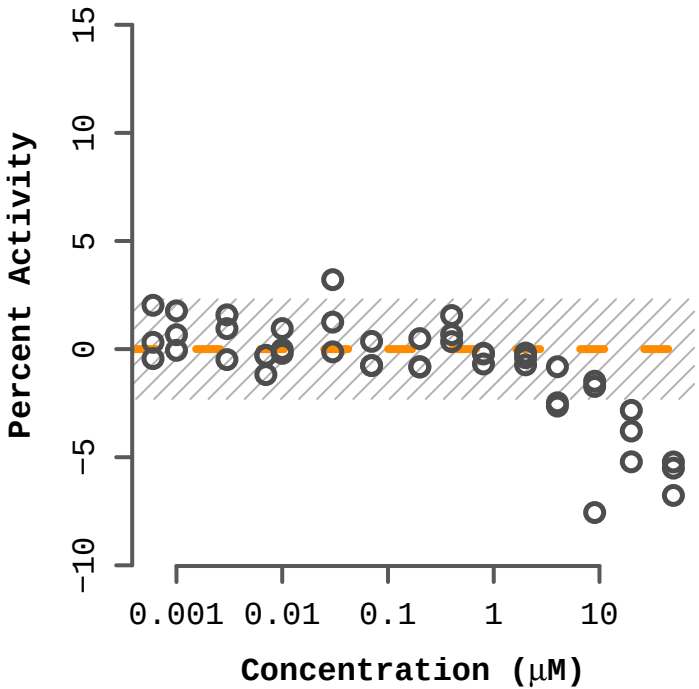
NAME: (S)−(+)−Dimethindene maleate
CHID: 49040 **CASRN:** 1217457−81−2
SPID(S): Tox21_113582_1
M4ID: 12482597

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	214.36	NA	NA
PROB:	1	NA	NA
RMSE:	3.13	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

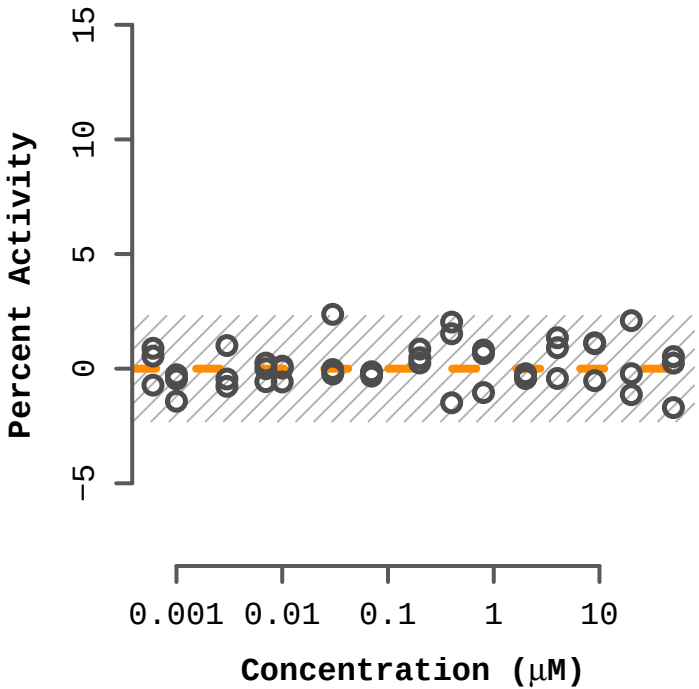
NAME: SDZ 21009
CHID: 49041 CASRN: 39731-05-0
SPID(S): Tox21_113583_1
M4ID: 12482596

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.64	NA	NA
PROB:	1	NA	NA
RMSE:	2.41	NA	NA

MAX_MEAN: 1.45 MAX_MED: 1.25 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

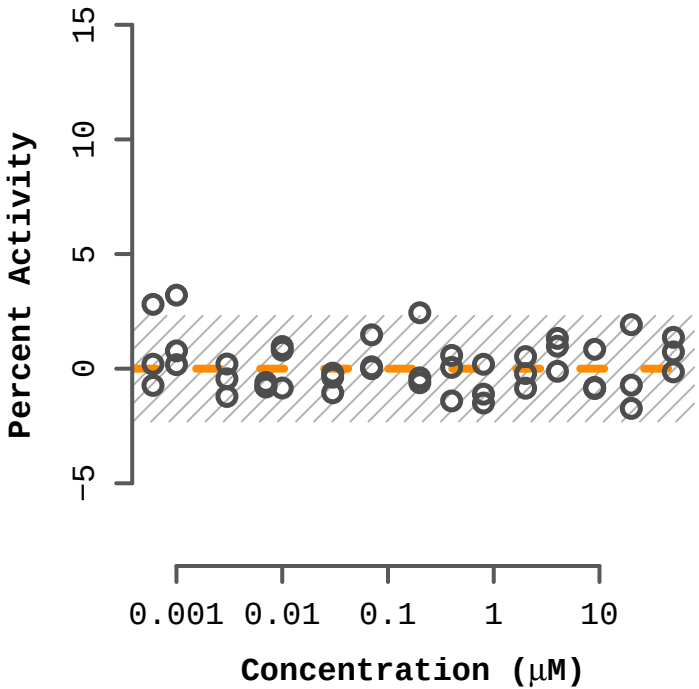
NAME: ZD 2079
CHID: 49042 CASRN: 178600-17-4
SPID(S): Tox21_113587_1
M4ID: 12482595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.701 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

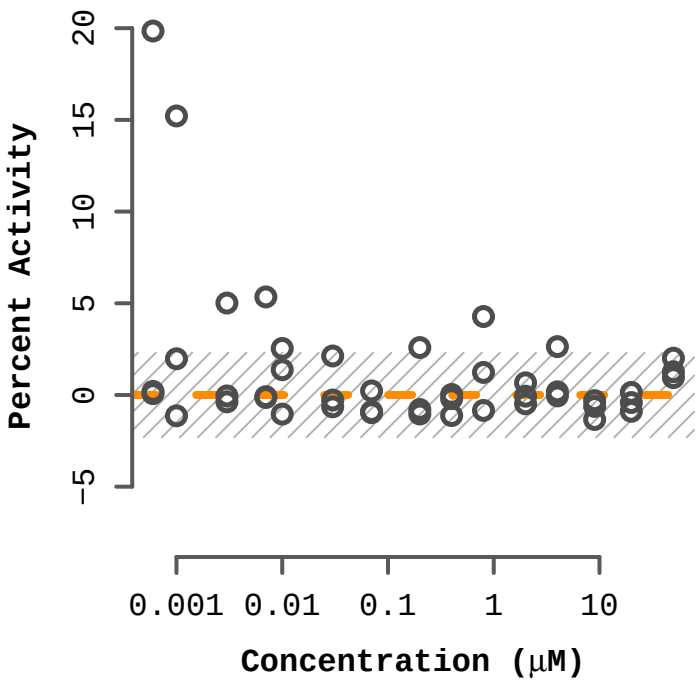
NAME: N-Acetyl sulfamethoxazole
CHID: 49044 **CASRN:** 21312-10-7
SPID(S): Tox21_113591_1
M4ID: 12482593

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

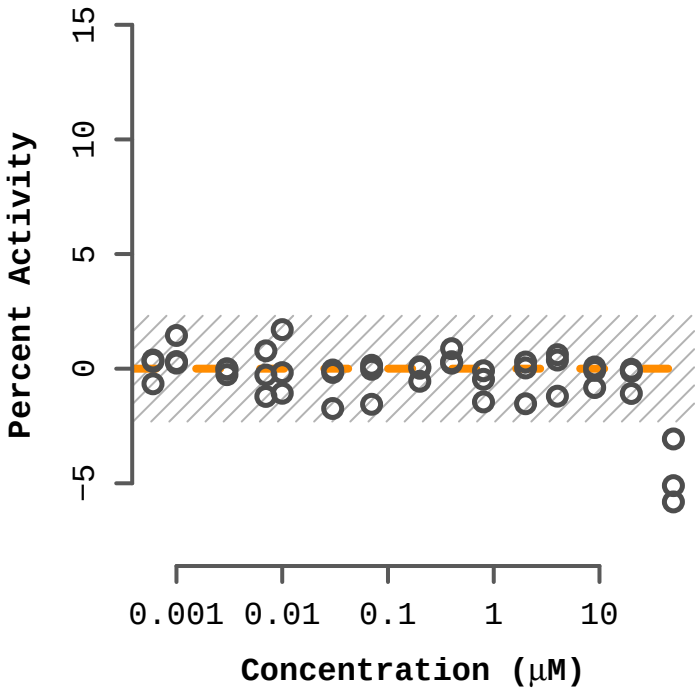
NAME: Aliskiren hydrochloride
CHID: 49045 CASRN: 173399-03-6
SPID(S): Tox21_113592_1
M4ID: 12482592

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.76	NA	NA
PROB:	1	NA	NA
RMSE:	4.08	NA	NA

MAX_MEAN: 6.71 MAX_MED: 1.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

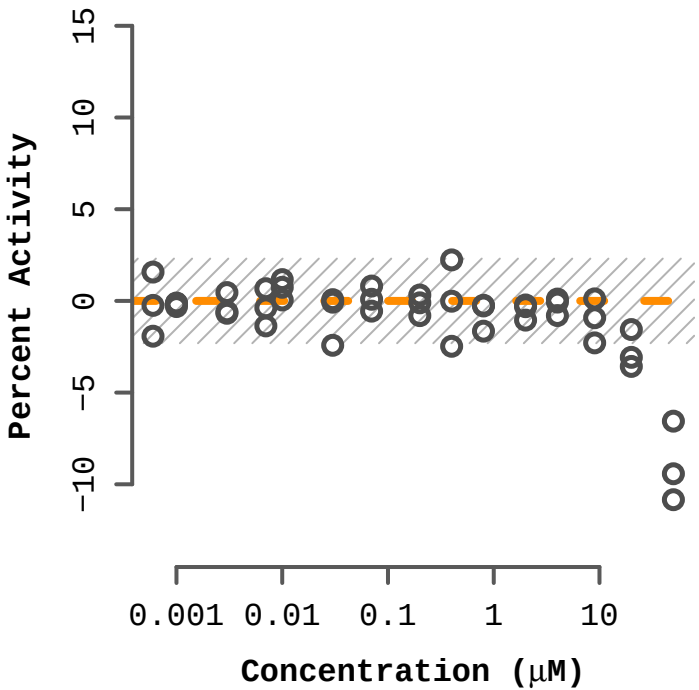
NAME: Alpidem
CHID: 49046 **CASRN:** 82626-01-5
SPID(S): Tox21_113593_1
M4ID: 12482591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 0.669 **MAX_MED:** 0.378 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

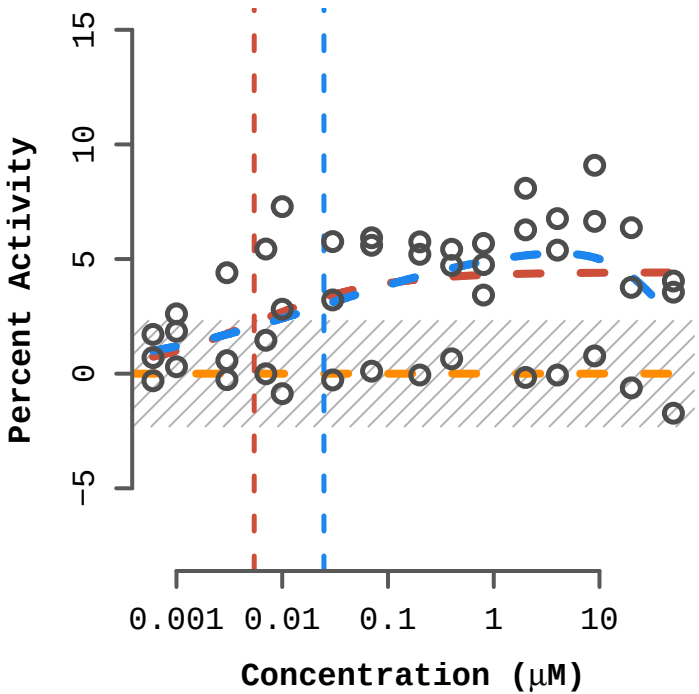
NAME: Aprepitant
CHID: 49047 **CASRN:** 170729-80-3
SPID(S): Tox21_113595_1
M4ID: 12482589

HILL MODEL: Not applicable.

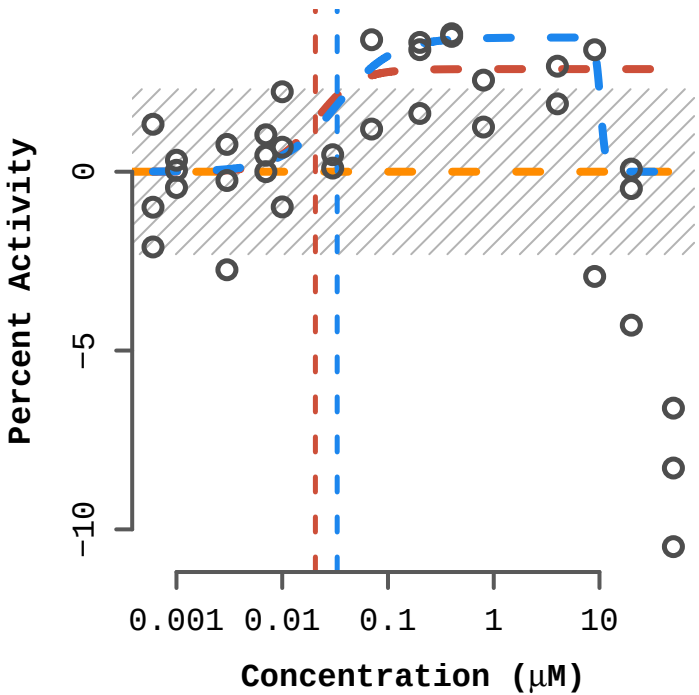
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 0.654 **MAX_MED:** 0.743 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Asenapine
CHID:    49048   CASRN: 65576-45-6
SPID(S): Tox21_113596_1
M4ID:    12482588

HILL MODEL (in red):
      tp       ga       gw
val:  4.42     -2.27    0.726
sd:   0.678    0.478    0.454

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.99     -1.61    0.433    1.6      1.56
sd:   3.52     1.62     0.418    0.384    1.72

      CNST        HILL        GNLS
AIC:  264.54      227.96      229.47
PROB: 0           0.68        0.32
RMSE: 4.24        2.67        2.6

MAX_MEAN: 5.5       MAX_MED: 6.65      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Axitinib
CHID: 49049 CASRN: 319460-85-0
SPID(S): Tox21_113597_1
M4ID: 12482587

HILL MODEL (in red):

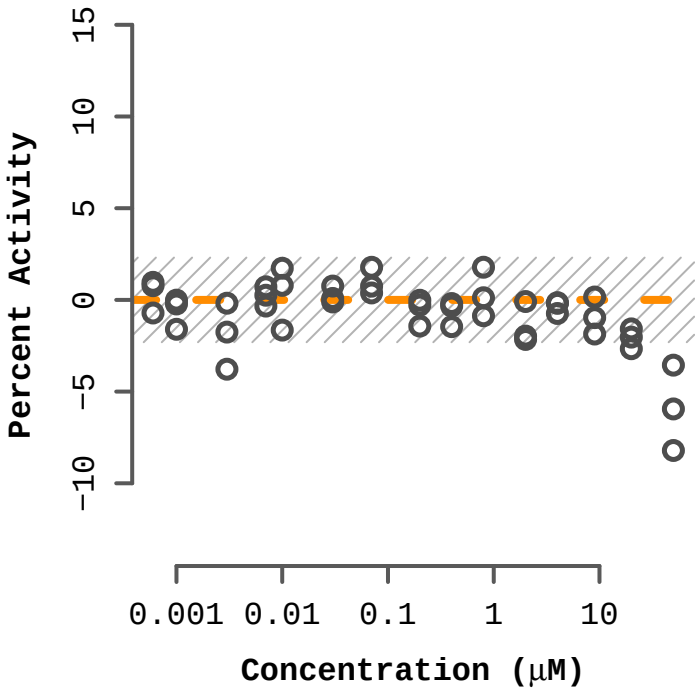
	tp	ga	gw
val:	2.87	−1.69	2.23
sd:	0.547	0.416	1.97

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.75	−1.48	1.66	1.01	17.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	251.99	238.72	224.26
PROB:	0	0	1
RMSE:	3.87	3.73	2.96

MAX_MEAN: 5.11 **MAX_MED:** 5.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

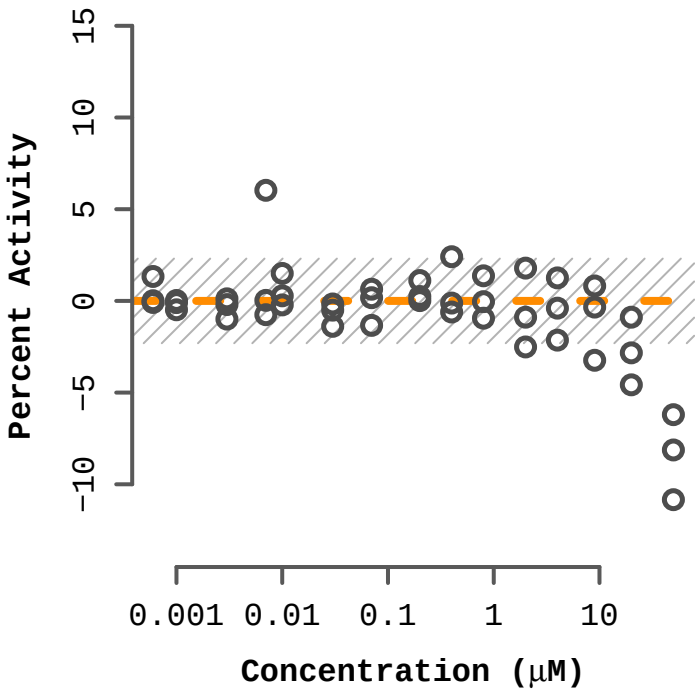
NAME: rac Benidipine hydrochloride
CHID: 49050 **CASRN:** 91599-74-5
SPID(S): Tox21_113598
M4ID: 12482586

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.04	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 0.971 **MAX_MED:** 0.794 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

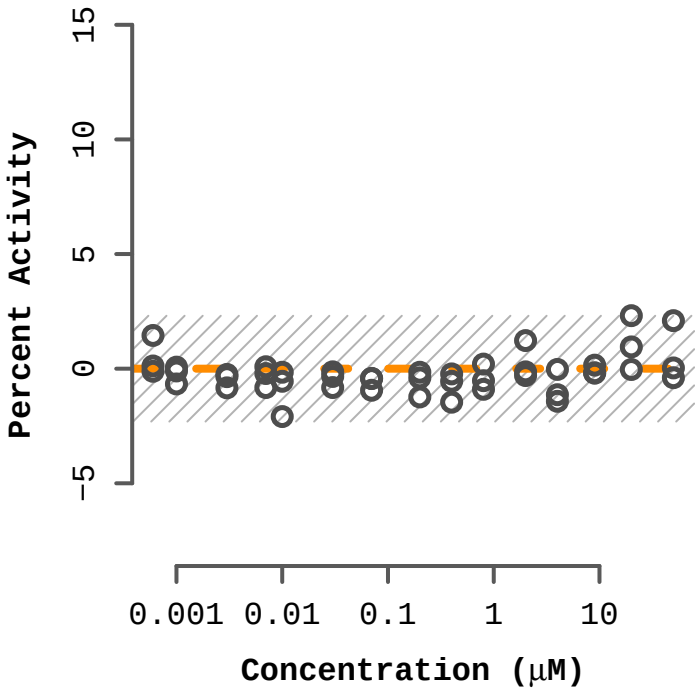
NAME: Bosutinib methanoate
CHID: 49051 **CASRN:** 918639-10-8
SPID(S): Tox21_113600_1
M4ID: 12482585

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.73	NA	NA

MAX_MEAN: 1.77 **MAX_MED:** 0.278 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

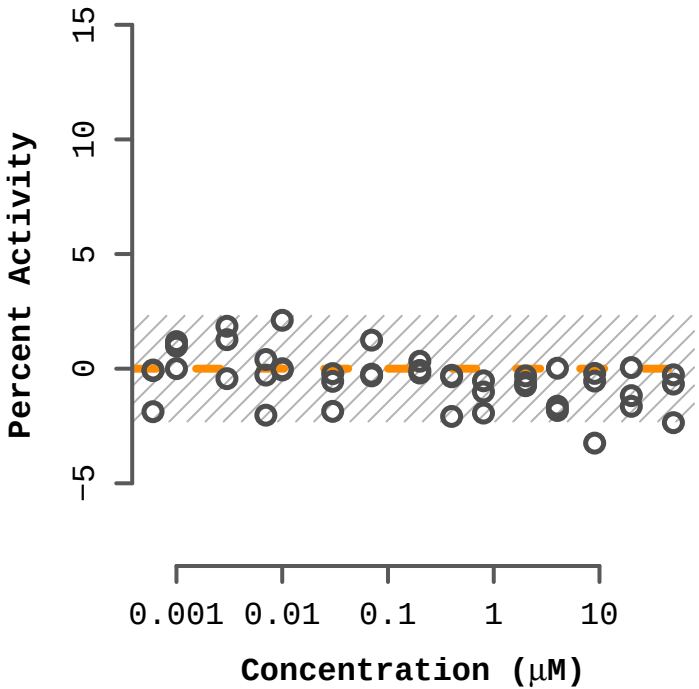
NAME: Cetirizine amide dihydrochloride
CHID: 49052 **CASRN:** 200707-85-3
SPID(S): Tox21_113602_1
M4ID: 12482584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.951 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

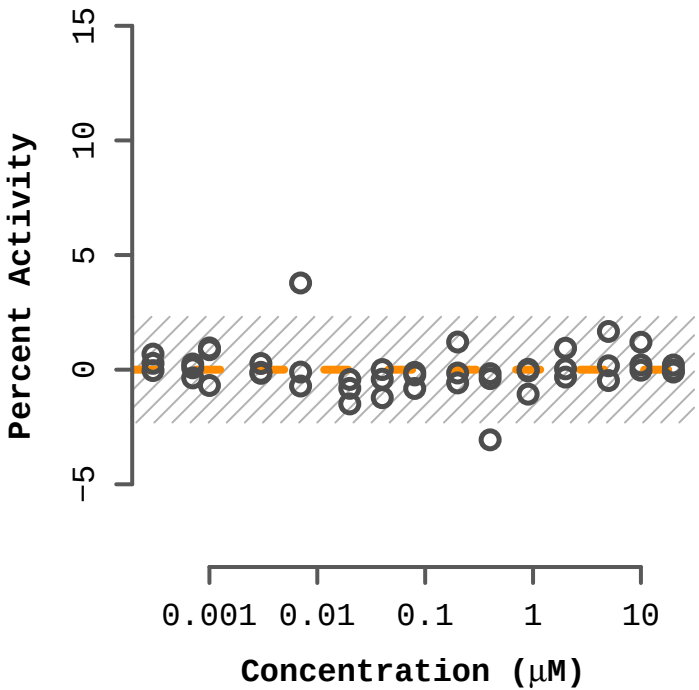
NAME: Dimethyl(2-phenoxyethyl)-2-thenylammonium iodi
CHID: 49055 **CASRN:** 109732-56-1
SPID(S): Tox21_113605
M4ID: 12482583

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.895 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

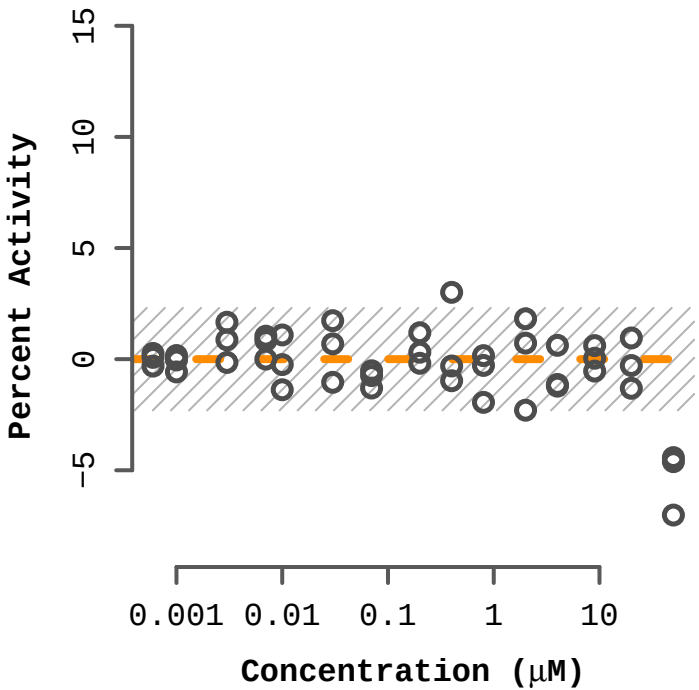
NAME: Paliperidone
CHID: 49059 **CASRN:** 144598-75-4
SPID(S): Tox21_113609_1
M4ID: 12482582

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.989 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

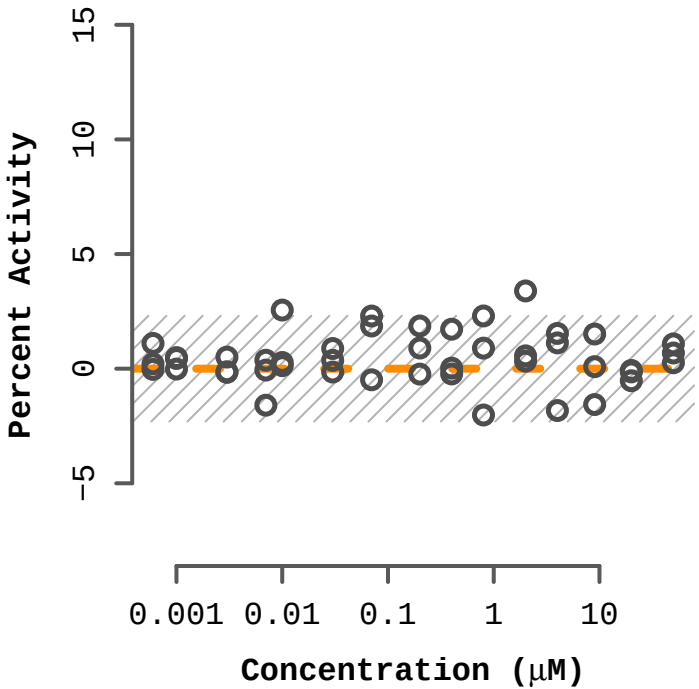
NAME: Iloperidone
CHID: 49060 CASRN: 133454-47-4
SPID(S): Tox21_113610_1
M4ID: 12482581

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	165.09	NA	NA
PROB:	1	NA	NA
RMSE:	1.75	NA	NA

MAX_MEAN: 0.796 **MAX_MED:** 0.872 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

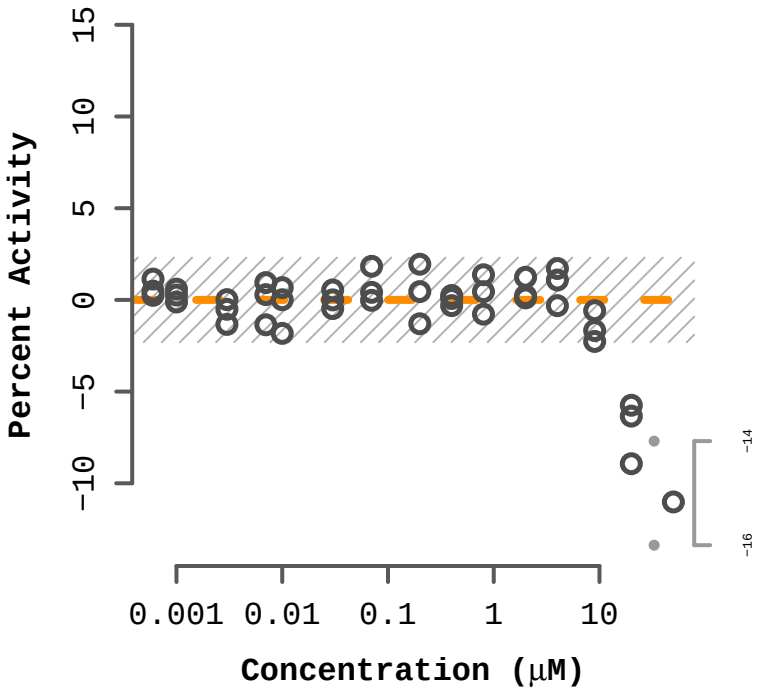
NAME: Naratriptan hydrochloride
CHID: 49064 **CASRN:** 143388-64-1
SPID(S): Tox21_113617_1
M4ID: 12482578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

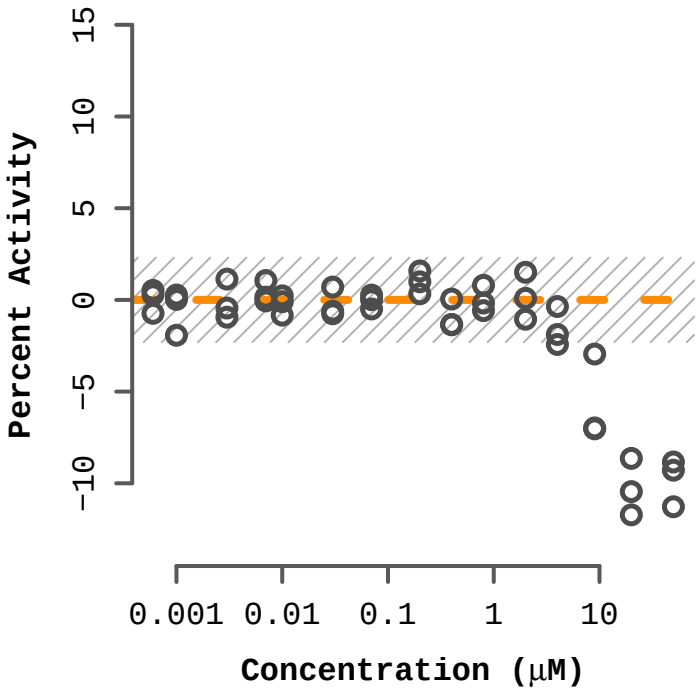
NAME: rac Nebivolol hydrochloride
CHID: 49065 **CASRN:** 169293-50-9
SPID(S): Tox21_113618_1
M4ID: 12482577 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.31	NA	NA
PROB:	1	NA	NA
RMSE:	4.1	NA	NA

MAX_MEAN: 0.828 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

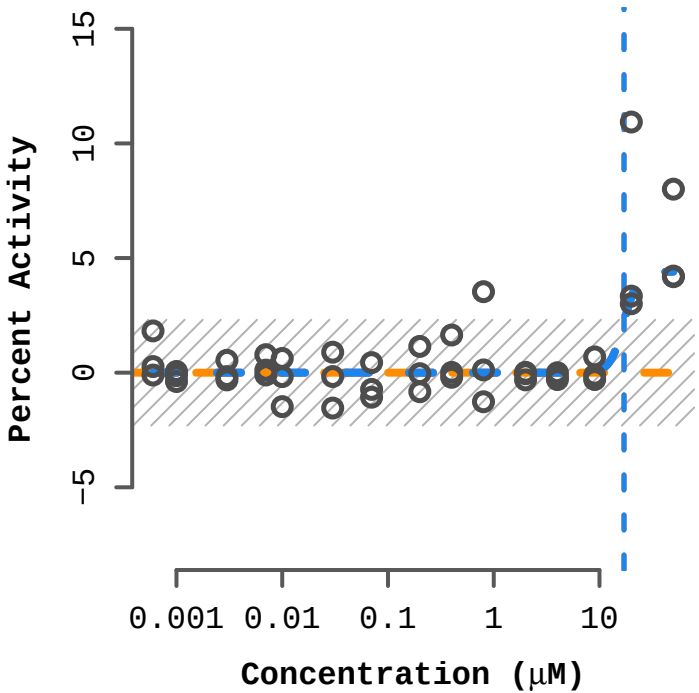
NAME: Posaconazole
CHID: 49066 **CASRN:** 171228-49-2
SPID(S): Tox21_113620_1
M4ID: 12482576

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	237.36	NA	NA
PROB:	1	NA	NA
RMSE:	4.09	NA	NA

MAX_MEAN: 0.968 **MAX_MED:** 0.989 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prasugrel hydrochloride
CHID: 49067 **CASRN:** 389574-19-0
SPID(S): Tox21_113621_1
M4ID: 12482575

HILL MODEL (in red):

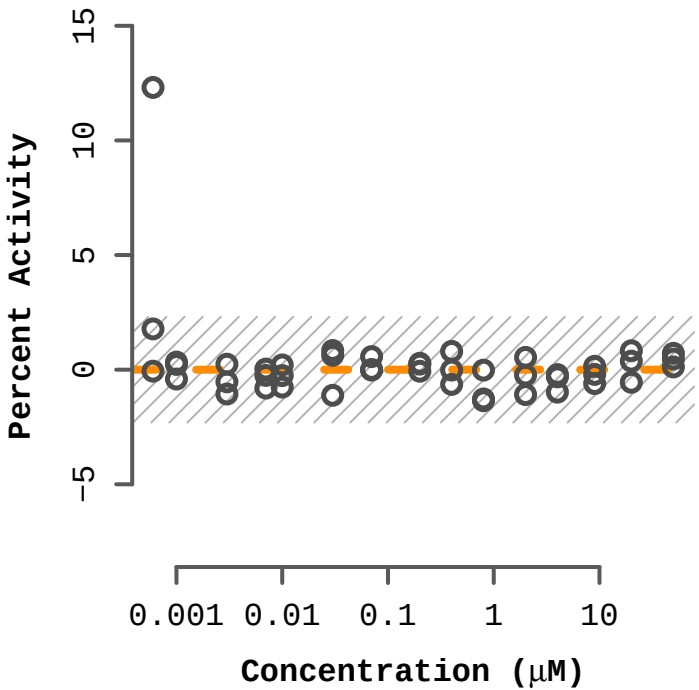
	tp	ga	gw
val:	4.41	1.23	6.72
sd:	0.436	0.0883	8.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.41	1.23	6.72	3.27	3.29
sd:	0.556	0.0897	8.1	3680	7790

	CNST	HILL	GNLS
AIC:	178.31	137.38	141.38
PROB:	0	0.88	0.12
RMSE:	2.45	1.52	1.52

MAX_MEAN: 5.76 **MAX_MED:** 4.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

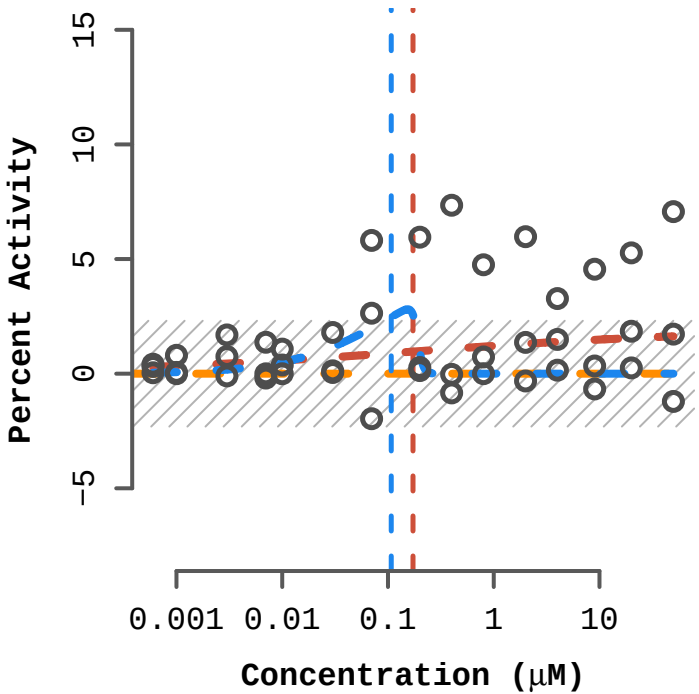
NAME: Stiripentol
CHID: 49068 **CASRN:** 49763-96-4
SPID(S): Tox21_113622
M4ID: 12482574

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.94	NA	NA

MAX_MEAN: 4.68 **MAX_MED:** 1.78 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sucrose octasulfate, sodium salt
CHID: 49069 CASRN: 74135-10-7
SPID(S): Tox21_113624
M4ID: 12482573

HILL MODEL (in red):

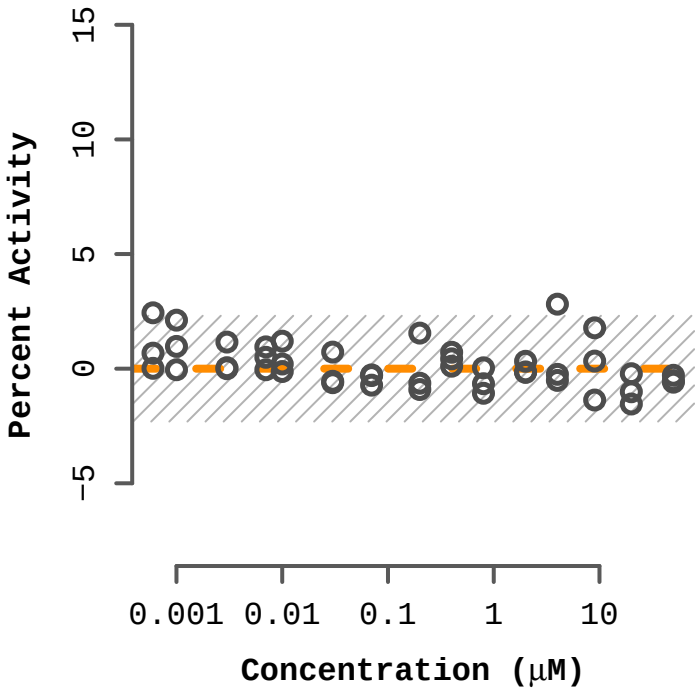
	tp	ga	gw
val:	1.93	−0.764	0.3
sd:	3.3	6.26	0.621

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.94	−0.969	0.918	−0.719	17.5
sd:	32.3	3.01	2.69	0.257	223

	CNST	HILL	GNLS
AIC:	209.54	203.02	215.59
PROB:	0.04	0.96	0
RMSE:	2.69	2.24	2.58

MAX_MEAN: 2.53 **MAX_MED:** 2.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

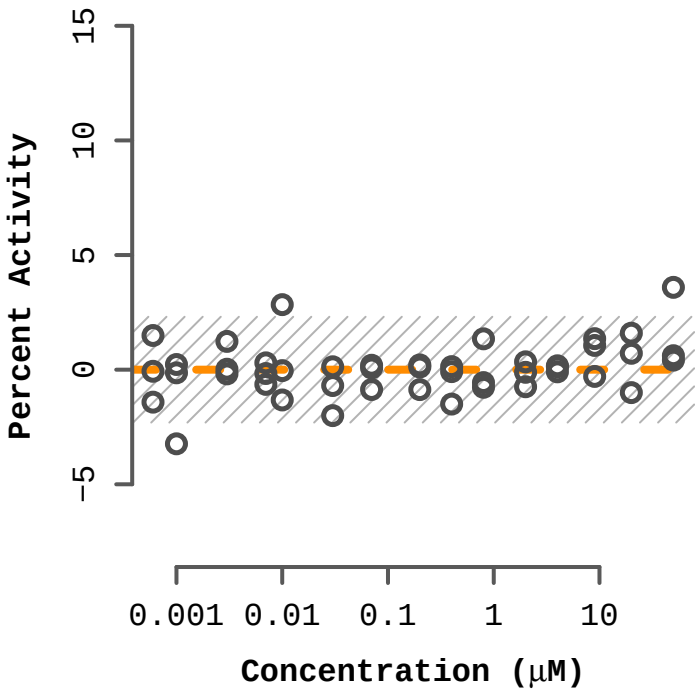
NAME: Zaltoprofen
CHID: 49076 CASRN: 74711-43-6
SPID(S): Tox21_113634_1
M4ID: 12482571

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.973 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

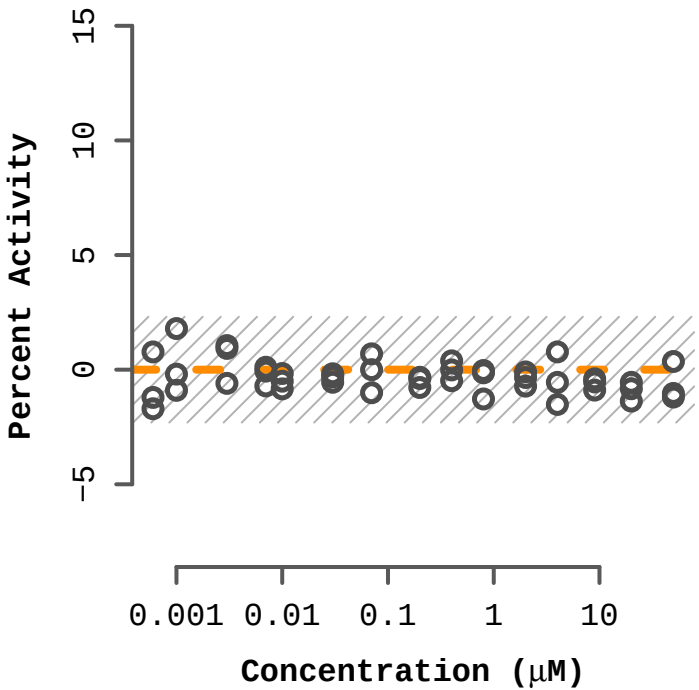
NAME: Sulindac sulfide
CHID: 49078 CASRN: 49627-27-2
SPID(S): Tox21_113636_1
M4ID: 12482570

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.54 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

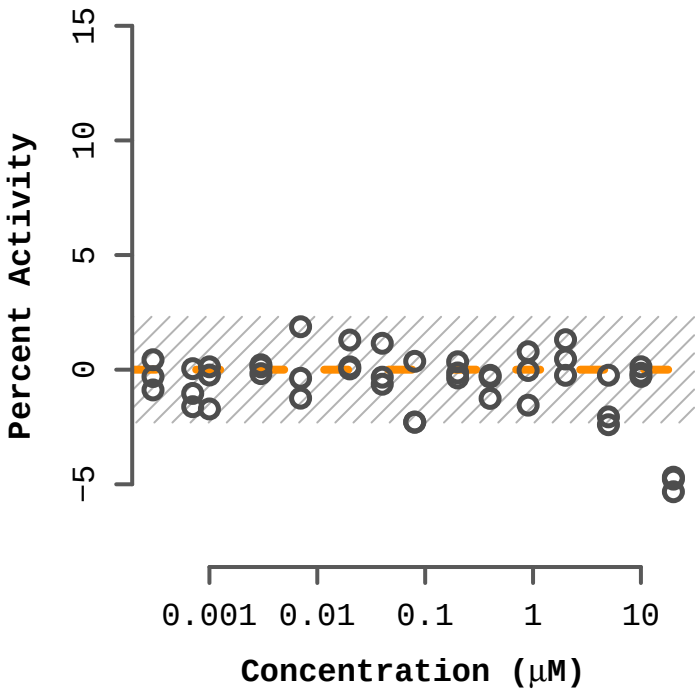
NAME: Lidamidine
CHID: 49080 **CASRN:** 66871-56-5
SPID(S): Tox21_113641_1
M4ID: 12482568

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.462 **MAX_MED:** 0.928 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

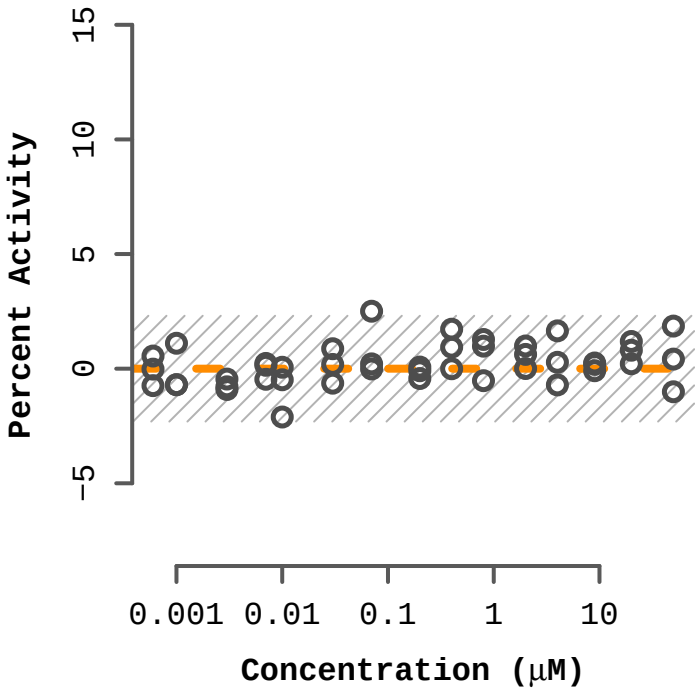
NAME: Prazosin
CHID: 49082 CASRN: 19216-56-9
SPID(S): Tox21_113646_1
M4ID: 12482565

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 0.51 **MAX_MED:** 0.466 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

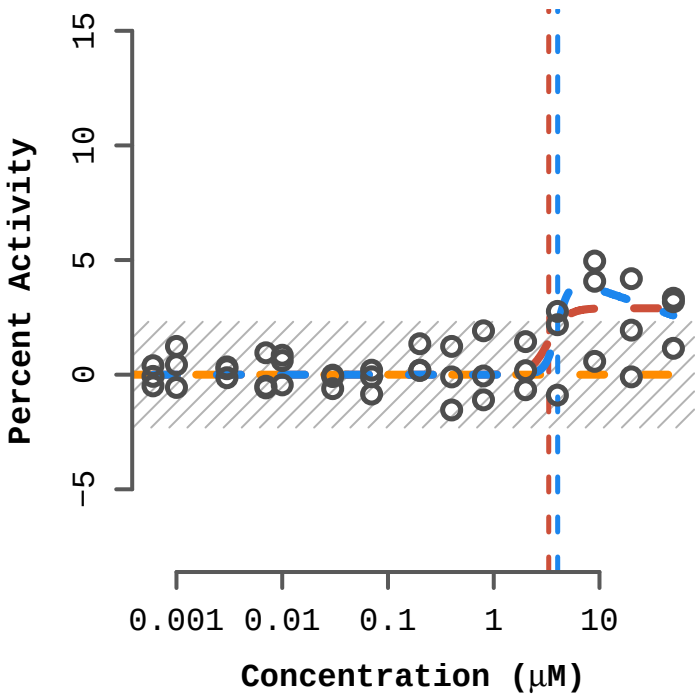
NAME: Anilinium nitrate
CHID: 49083 **CASRN:** 542-15-4
SPID(S): Tox21_113647_1
M4ID: 12482564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.983 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Atipamezole
CHID: 49135 **CASRN:** 104054-27-5
SPID(S): Tox21_113005_1
M4ID: 12482848

HILL MODEL (in red):

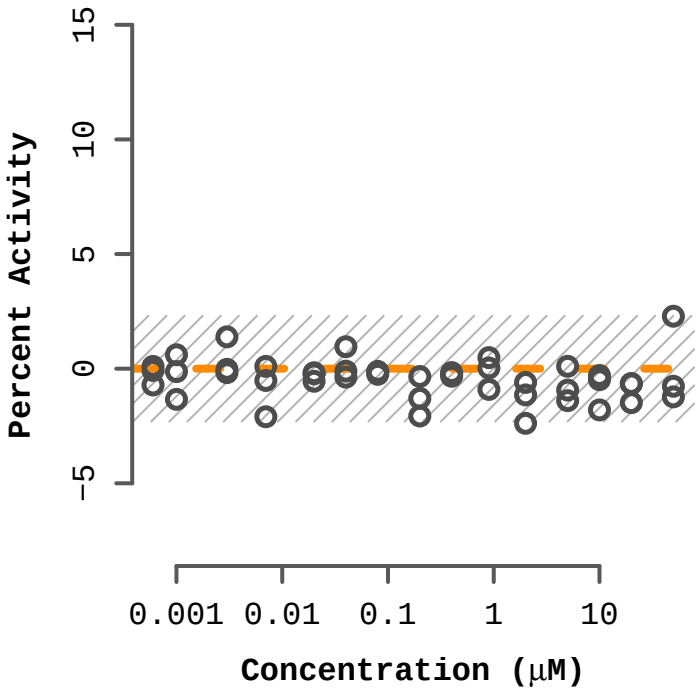
	tp	ga	gw
val:	2.9	0.52	5.07
sd:	0.515	0.114	4.27

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.95	0.605	7.94	1.46	0.474
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	165.46	142.91	145.81
PROB:	0	0.81	0.19
RMSE:	1.62	1.1	1.13

MAX_MEAN: 3.2 **MAX_MED:** 4.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

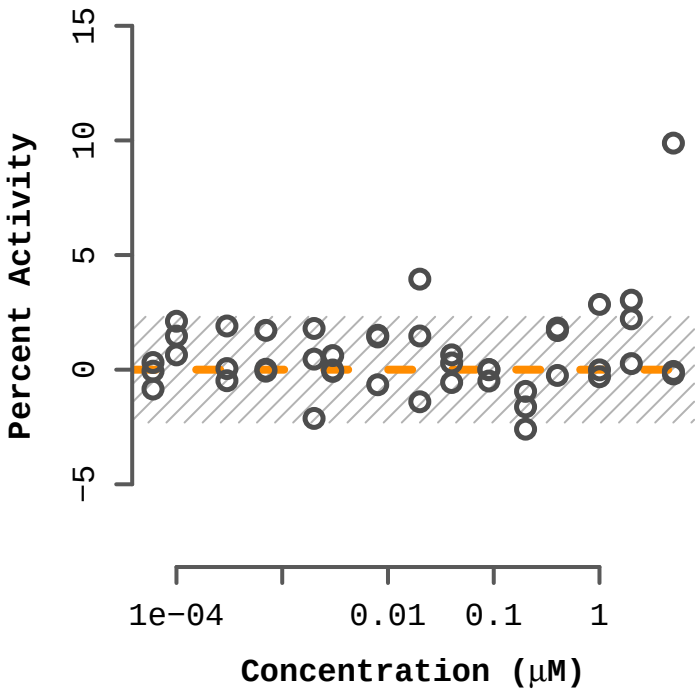
NAME: Barium nitrate
CHID: 49200 CASRN: 10022-31-8
SPID(S): Tox21_202714
M4ID: 12479538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.397 **MAX_MED:** 0.0317 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

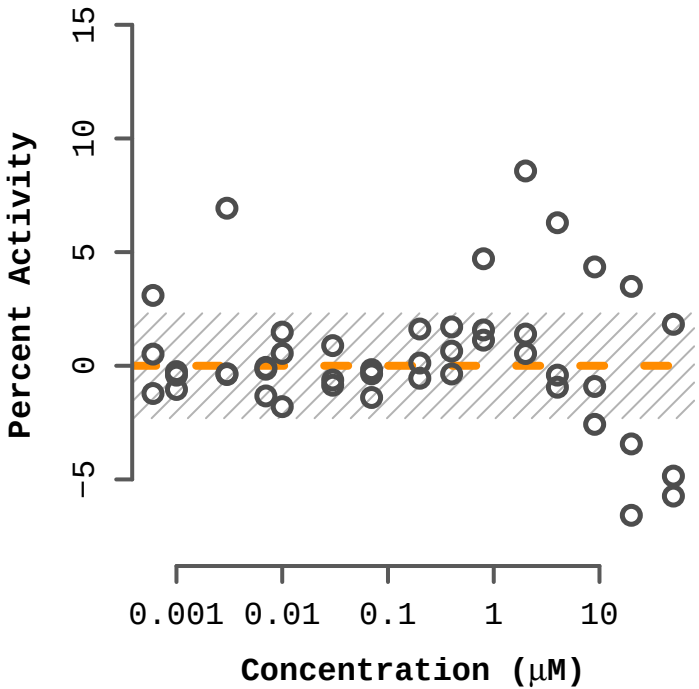
NAME: Lithium sulfate
CHID: 49201 **CASRN:** 10377-48-7
SPID(S): Tox21_202799
M4ID: 12479453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.25	NA	NA
PROB:	1	NA	NA
RMSE:	2.03	NA	NA

MAX_MEAN: 3.21 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

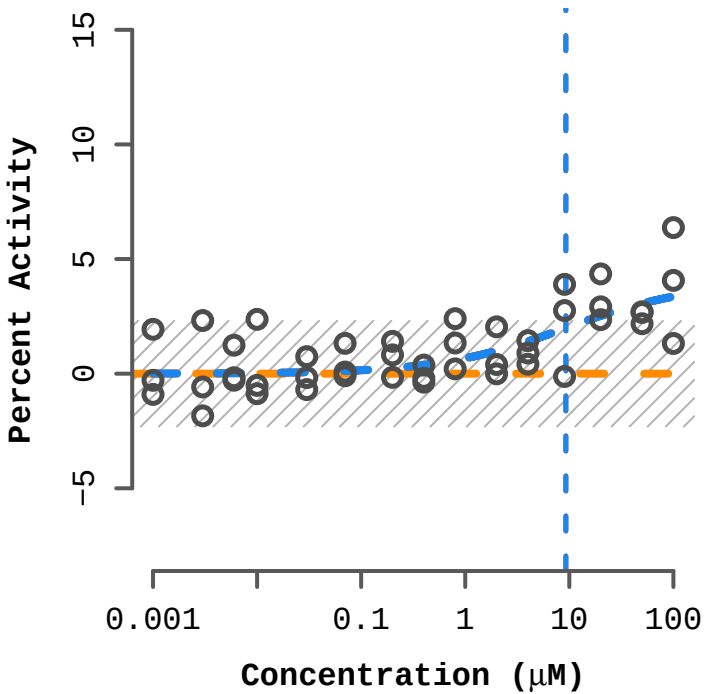
NAME: 10-Chloro-9-anthraldehyde
CHID: 49202 **CASRN:** 10527-16-9
SPID(S): Tox21_202962
M4ID: 12479290

HILL MODEL: Not applicable.

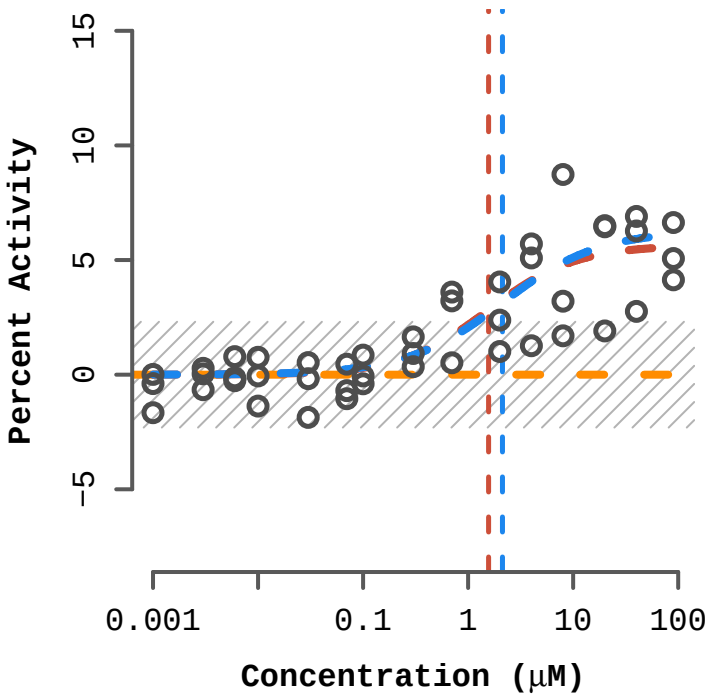
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.53	NA	NA
PROB:	1	NA	NA
RMSE:	2.89	NA	NA

MAX_MEAN: 3.5 **MAX_MED:** 1.58 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Bromopentane
CHID:    49203   CASRN: 110-53-2
SPID(S): Tox21_202717
M4ID:    12479535

HILL MODEL (in red):
      tp       ga       gw
val:  3.98     0.967    0.715
sd:   2.36     0.922    0.542

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.98     0.967    0.715    3.4      5.89
sd:   2.36     0.922    0.542    2060     8750

      CNST        HILL        GNLS
AIC:  188.99      151.91      155.91
PROB: 0           0.88        0.12
RMSE: 1.98        1.17        1.17

MAX_MEAN: 3.92      MAX_MED: 4.07      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-2-methylpyridinium chloride
CHID: 49204 CASRN: 112400-85-8
SPID(S): Tox21_202676
M4ID: 12479576

HILL MODEL (in red):

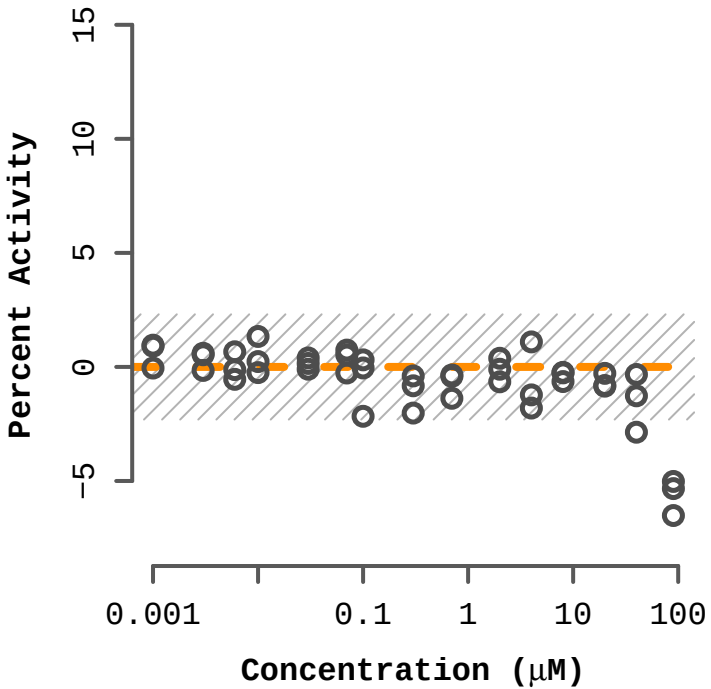
	tp	ga	gw
val:	5.64	0.195	1.05
sd:	0.702	0.245	0.334

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.28	0.327	0.952	2.03	10.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	233.94	169.87	173.33
PROB:	0	0.85	0.15
RMSE:	3.27	1.46	1.47

MAX_MEAN: 5.31 MAX_MED: 6.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

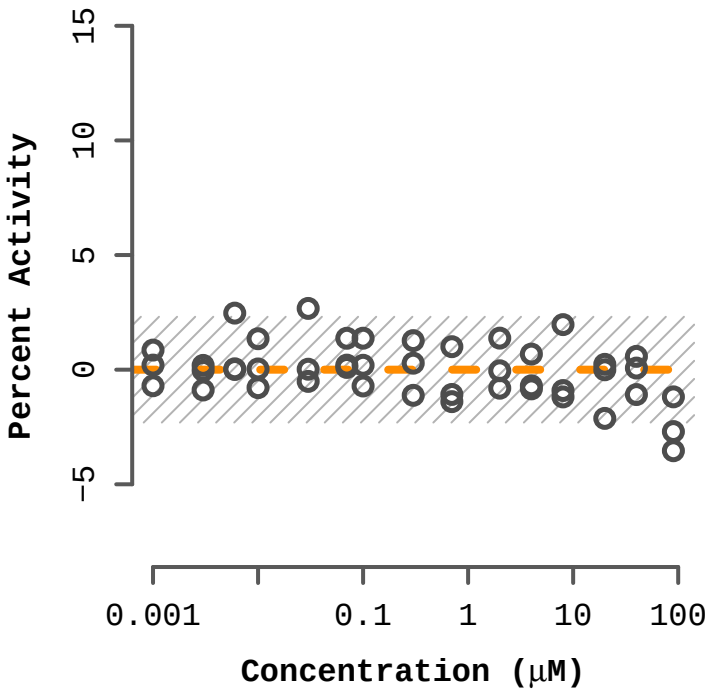
NAME: 1-Butyl-4-methylpyridinium chloride
CHID: 49205 **CASRN:** 112400-86-9
SPID(S): Tox21_202685
M4ID: 12479567

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.44	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 0.605 **MAX_MED:** 0.909 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

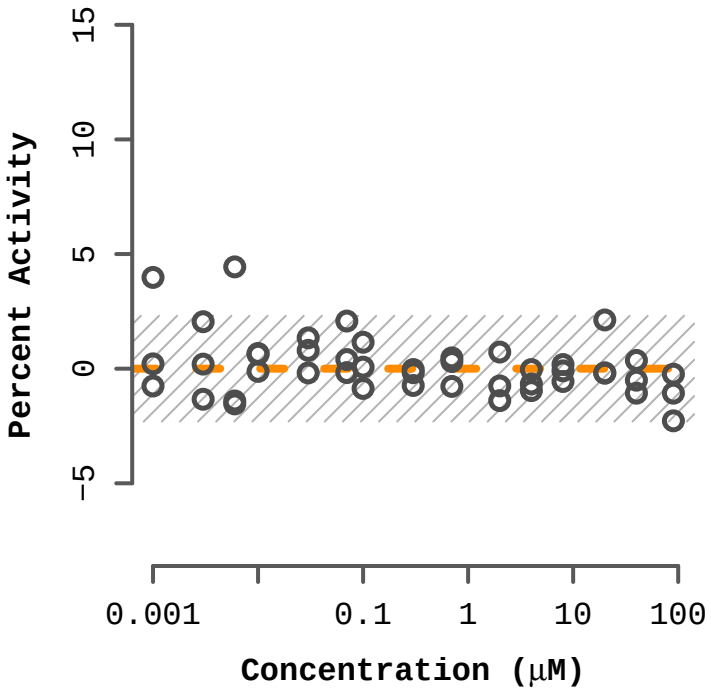
NAME: 1-Ethyl-1-methylpyrrolidinium tetrafluoroborat
CHID: 49206 **CASRN:** 117947-85-0
SPID(S): Tox21_202704
M4ID: 12479548

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.11	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.839 **MAX_MED:** 0.284 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

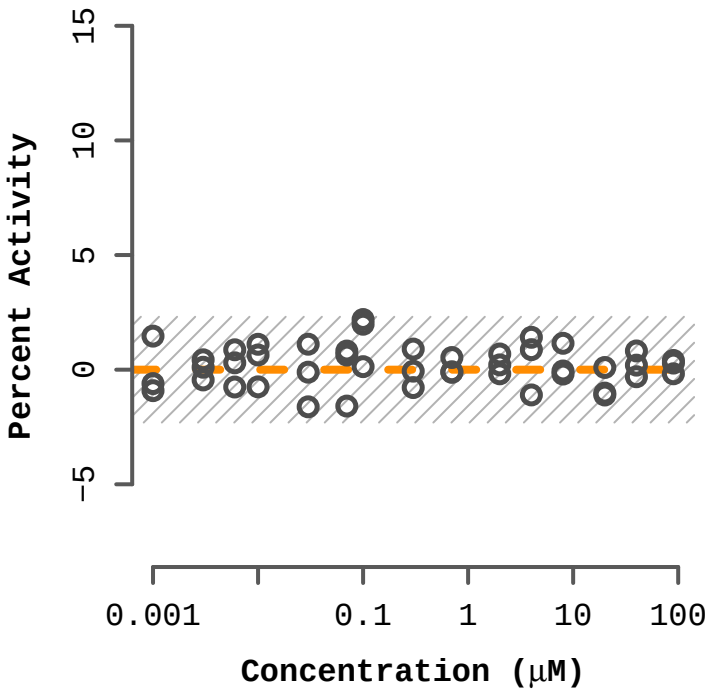
NAME: 1-Methyl-3-propylimidazolium iodide
CHID: 49207 **CASRN:** 119171-18-5
SPID(S): Tox21_202654
M4ID: 12479598

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

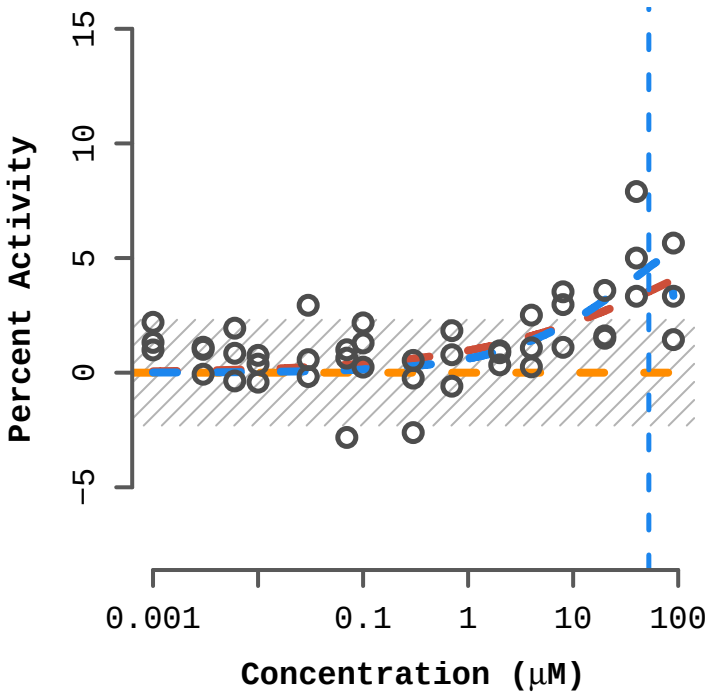
NAME: 2-Methylbenzothiazole
CHID: 49208 **CASRN:** 120-75-2
SPID(S): Tox21_202975
M4ID: 12479277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9-Cyanoanthracene
CHID: 49209 CASRN: 1210-12-4
SPID(S): Tox21_202963
M4ID: 12479289

HILL MODEL (in red):

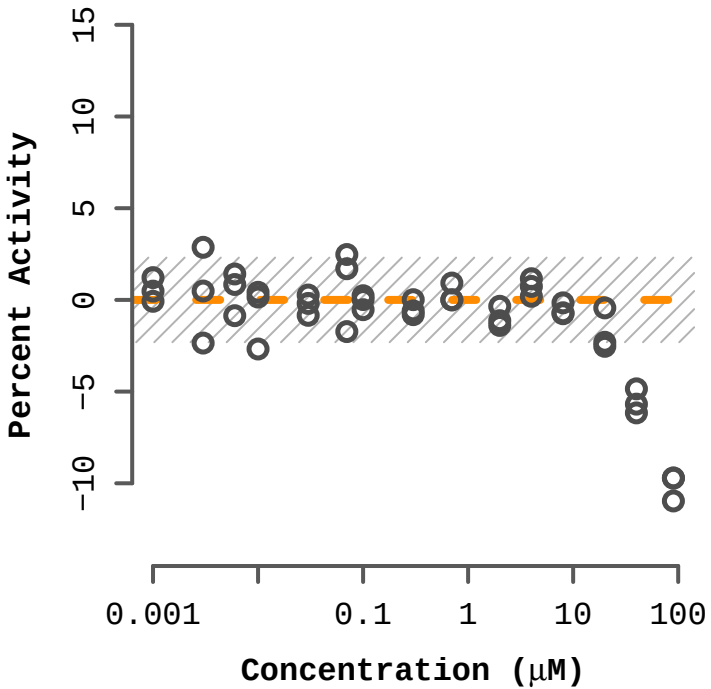
	tp	ga	gw
val:	9.48	2.26	0.418
sd:	12.6	2.64	0.299

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.2	1.72	0.667	1.97	13.1
sd:	11	1.38	0.346	0.0431	36.3

	CNST	HILL	GNLS
AIC:	202.02	167.94	170.56
PROB:	0	0.79	0.21
RMSE:	2.33	1.46	1.39

MAX_MEAN: 5.41 MAX_MED: 5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

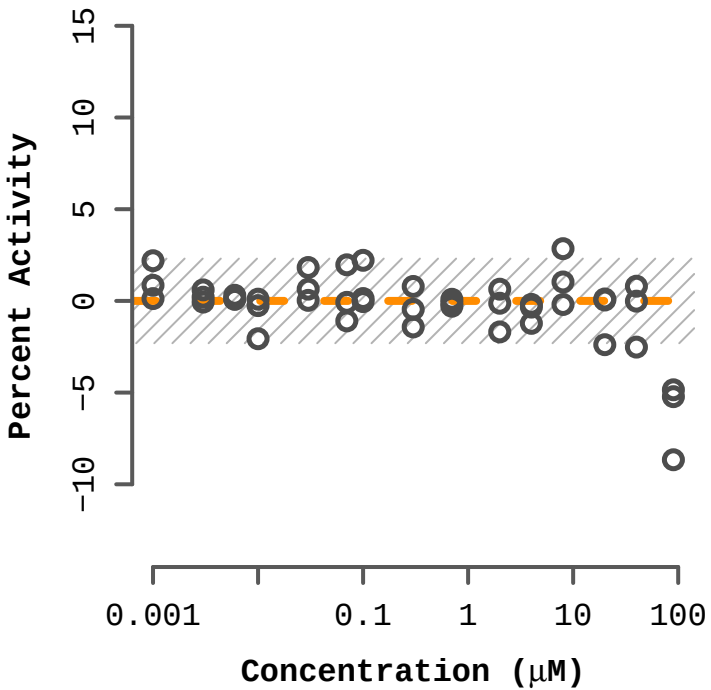
NAME: 2-Propenal,3,3-diphenyl-
CHID: 49210 CASRN: 1210-39-5
SPID(S): Tox21_202800
M4ID: 12479452

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	213.51	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 0.817 MAX_MED: 1.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

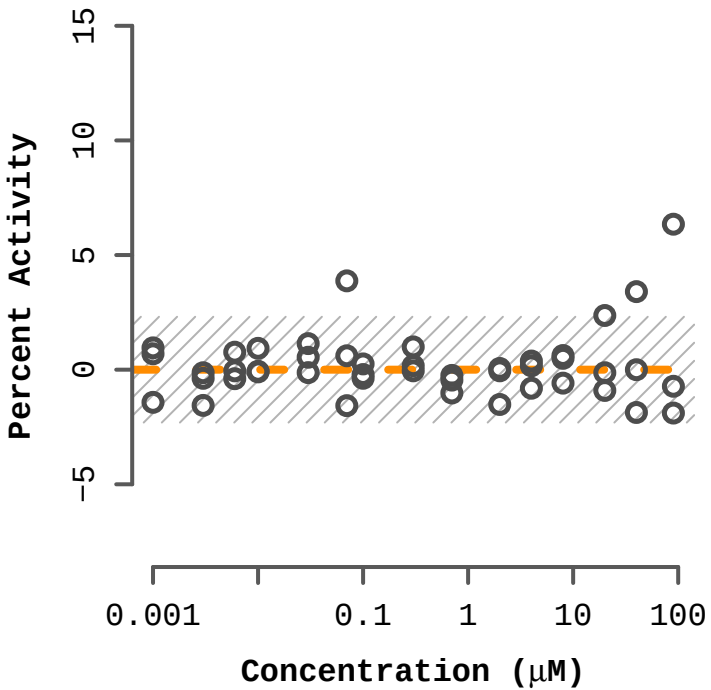
NAME: 4-Nitrochalcone
CHID: 49211 **CASRN:** 1222-98-6
SPID(S): Tox21_202976
M4ID: 12479276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.19	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

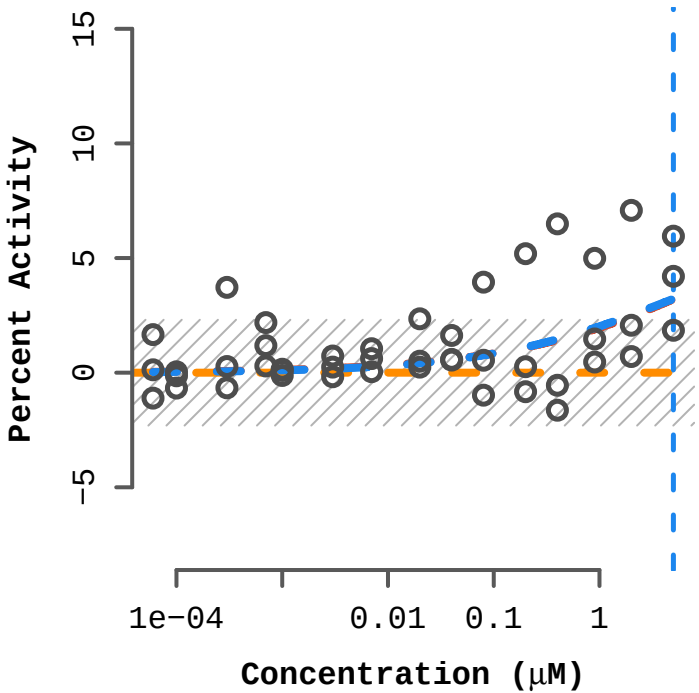
NAME: 1-Butyl-3-methylpyridinium chloride
CHID: 49212 **CASRN:** 125652-55-3
SPID(S): Tox21_202681
M4ID: 12479571

HILL MODEL: Not applicable.

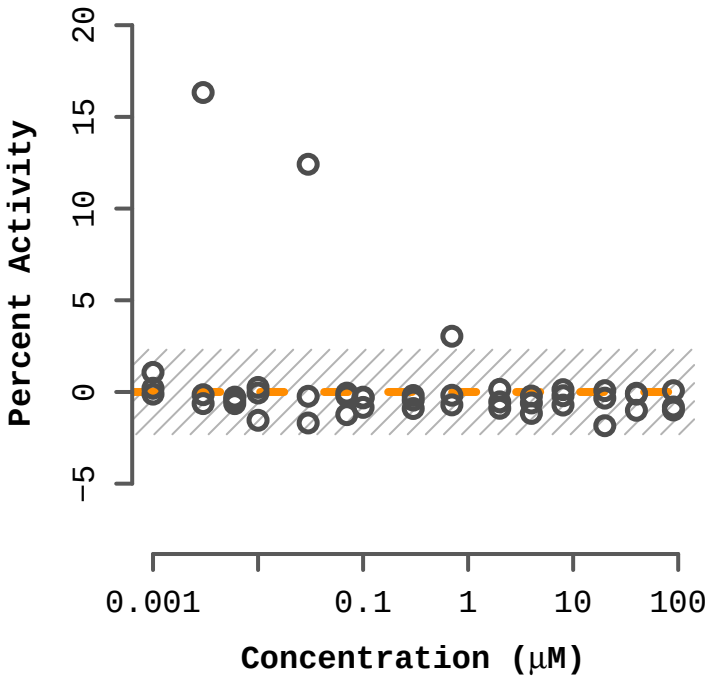
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 0.694 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Chloroanthraquinone
CHID:    49213   CASRN: 131-09-9
SPID(S): Tox21_202964
M4ID:    12479288

HILL MODEL (in red):
      tp       ga       gw
val:  8.5      1.2      0.436
sd:   9.35     1.69     0.282

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.45     0.699    0.487    1.89     7.13
sd:   9.11     1.87     0.359    2130     12800

      CNST        HILL        GNLS
AIC:  199.87      186.27      190.59
PROB: 0           0.9         0.1
RMSE: 2.43        1.83        1.83

MAX_MEAN: 4         MAX_MED: 4.2       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

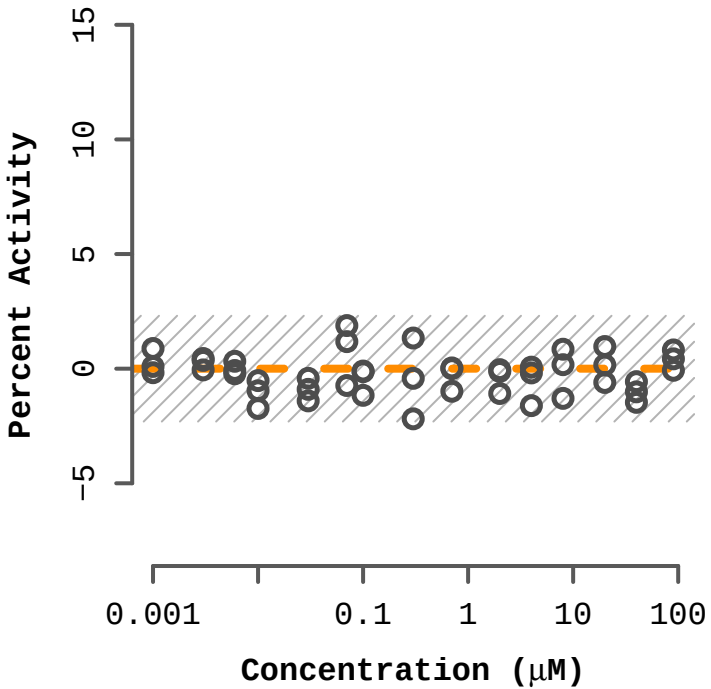
NAME: 1-Butyl-2-methylpyridinium iodide
CHID: 49214 CASRN: 13311-31-4
SPID(S): Tox21_202680
M4ID: 12479572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.86	NA	NA
PROB:	1	NA	NA
RMSE:	3.17	NA	NA

MAX_MEAN: 5.18 MAX_MED: 0.207 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

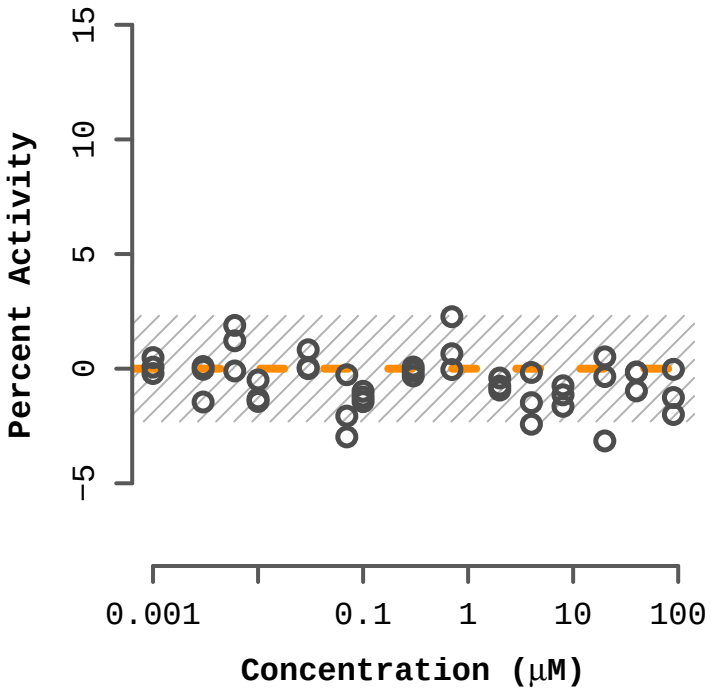
NAME: 5-Methyl-2,3-hexanedione
CHID: 49215 **CASRN:** 13706-86-0
SPID(S): Tox21_202802
M4ID: 12479450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.777 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

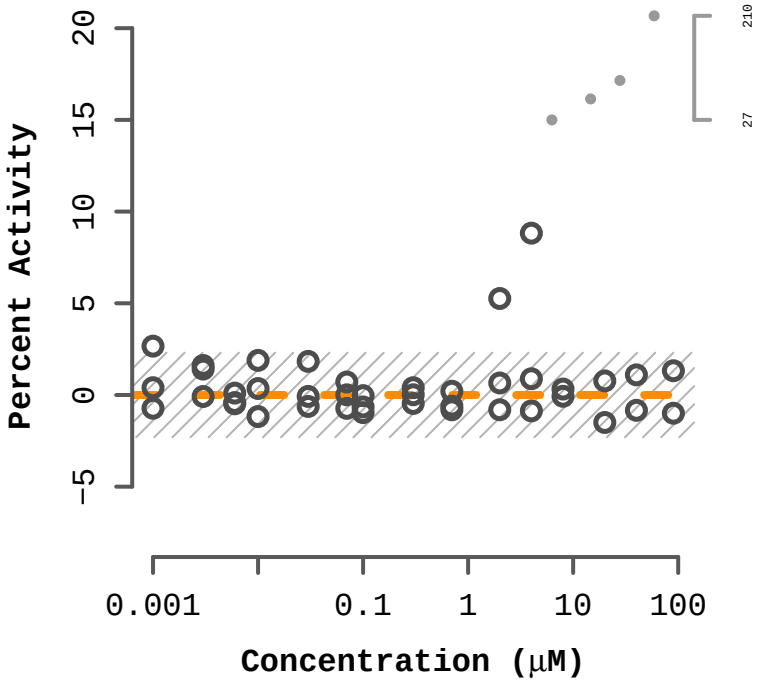
NAME: Ammonium tetrachloroplatinate(II)
CHID: 49216 CASRN: 13820-41-2
SPID(S): Tox21_202803
M4ID: 12479449

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.67	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

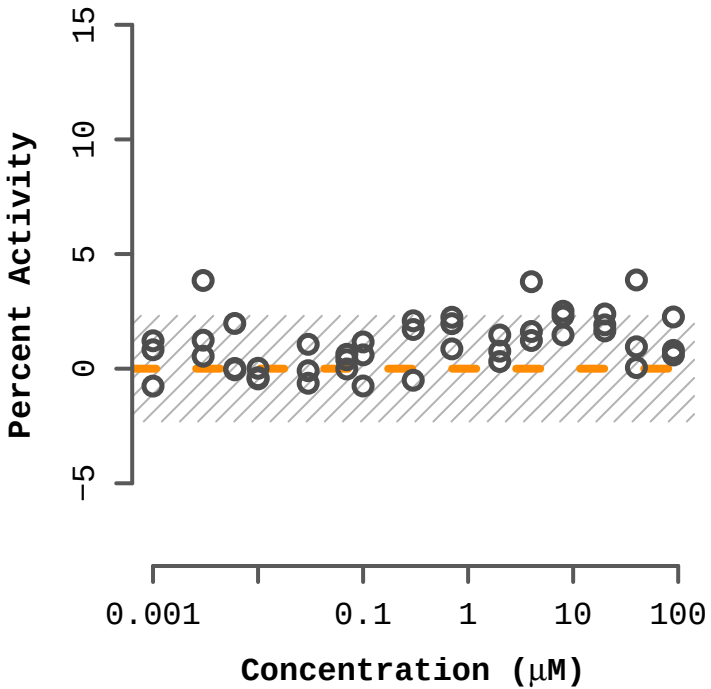
NAME: 1-Ethyl-3-methylimidazolium nitrate
CHID: 49217 **CASRN:** 143314-14-1
SPID(S): Tox21_202798
M4ID: 12479454 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.95	NA	NA
PROB:	1	NA	NA
RMSE:	36.73	NA	NA

MAX_MEAN: 71.6 **MAX_MED:** 1.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

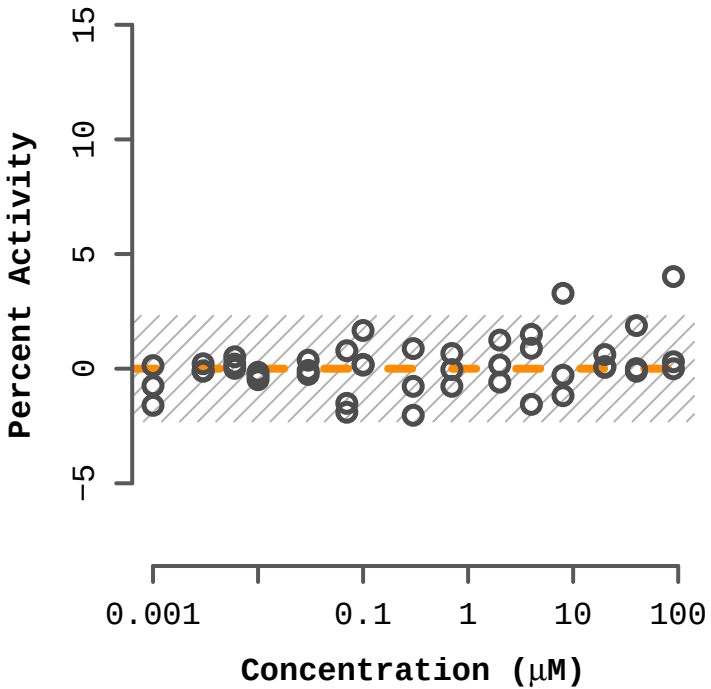
NAME: 1-Ethyl-3-methylimidazolium tetrafluoroborate
CHID: 49218 **CASRN:** 143314-16-3
SPID(S): Tox21_202644
M4ID: 12479608

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

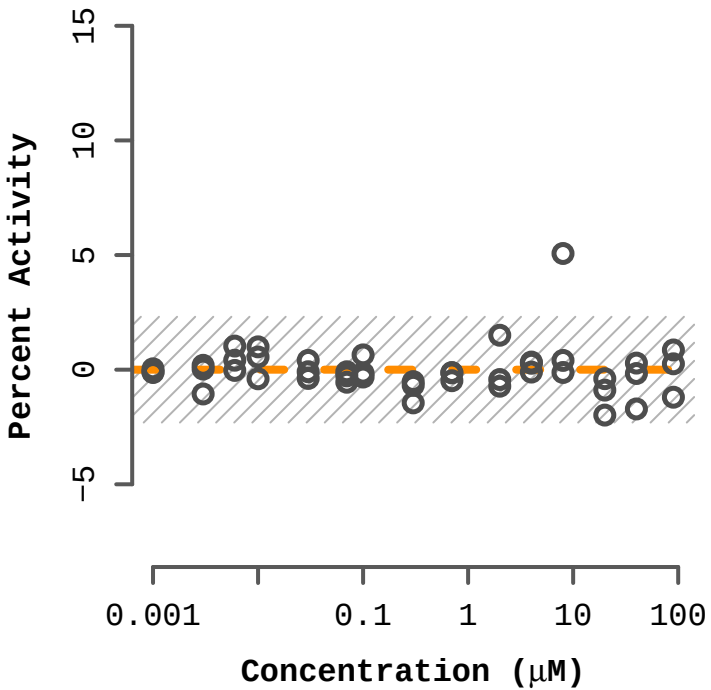
NAME: 1-Ethyl-3-methylimidazolium methanesulfonate
CHID: 49219 **CASRN:** 145022-45-3
SPID(S): Tox21_202640
M4ID: 12479612

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 0.892 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

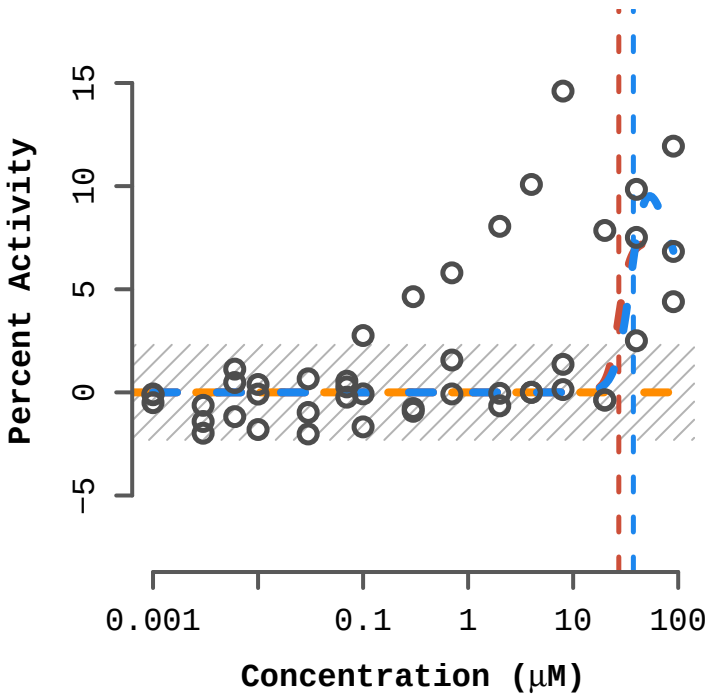
NAME: Pyrimidine−2−thiol
CHID: 49220 **CASRN:** 1450−85−7
SPID(S): Tox21_202805
M4ID: 12479447

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.78 **MAX_MED:** 0.554 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9-Anthracenemethanol
CHID: 49221 CASRN: 1468-95-7
SPID(S): Tox21_202965
M4ID: 12479287

HILL MODEL (in red):

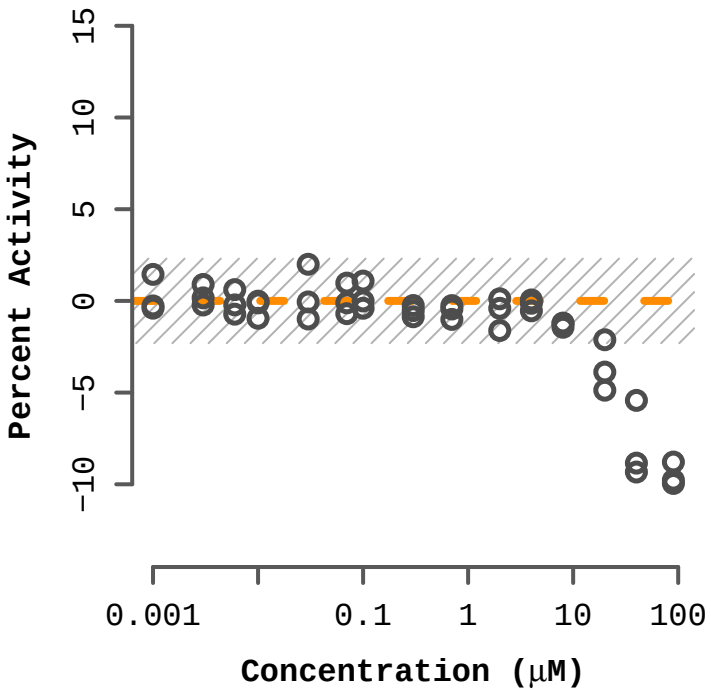
	tp	ga	gw
val:	7.3	1.43	8
sd:	1.3	0.114	6.37

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.6	1.57	5.82	1.87	1.81
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	251.37	230.22	234.02
PROB:	0	0.87	0.13
RMSE:	4.47	3.6	3.62

MAX_MEAN: 7.72 MAX_MED: 7.52 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

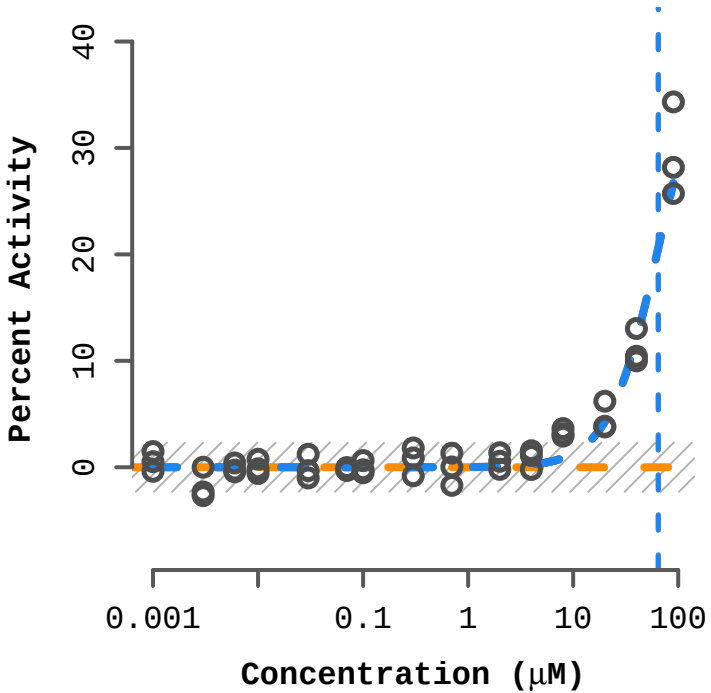
NAME: N-Dodecyl-N,N-dimethyl-3-ammonio-1-propanesulf
CHID: 49222 CASRN: 14933-08-5
SPID(S): Tox21_202807
M4ID: 12479445

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	218.37	NA	NA
PROB:	1	NA	NA
RMSE:	3.44	NA	NA

MAX_MEAN: 0.32 MAX_MED: 0.168 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminofluorene
CHID: 49223 CASRN: 153-78-6
SPID(S): Tox21_202971
M4ID: 12479281

HILL MODEL (in red):

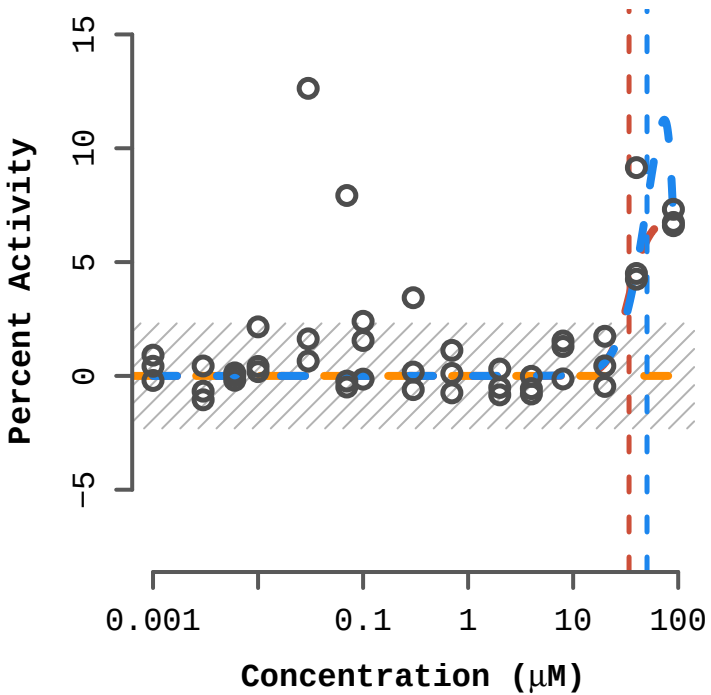
	tp	ga	gw
val:	41.2	1.81	1.84
sd:	11	0.143	0.392

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	41.2	1.81	1.84	3.2	7.47
sd:	11	0.143	0.393	1810	10800

	CNST	HILL	GNLS
AIC:	273.95	168.81	172.81
PROB:	0	0.88	0.12
RMSE:	8.36	1.66	1.66

MAX_MEAN: 29.4 MAX_MED: 28.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9-Bromoanthracene
CHID: 49224 CASRN: 1564-64-3
SPID(S): Tox21_202958
M4ID: 12479294

HILL MODEL (in red):

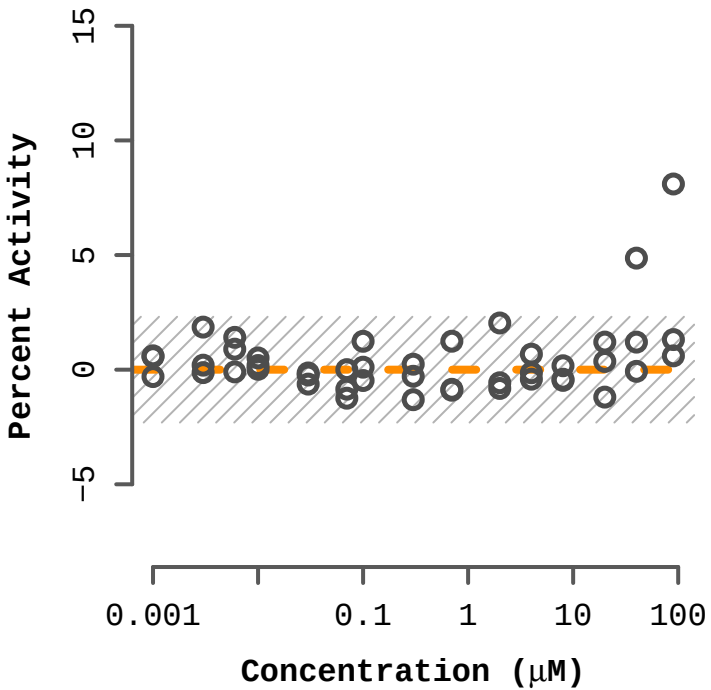
	tp	ga	gw
val:	6.97	1.53	4.57
sd:	0.56	0.0449	2.07

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	15.1	1.7	3.41	1.96	14.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	221.08	174.26	178.2
PROB:	0	0.88	0.12
RMSE:	3.43	2.51	2.51

MAX_MEAN: 6.89 MAX_MED: 6.74 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

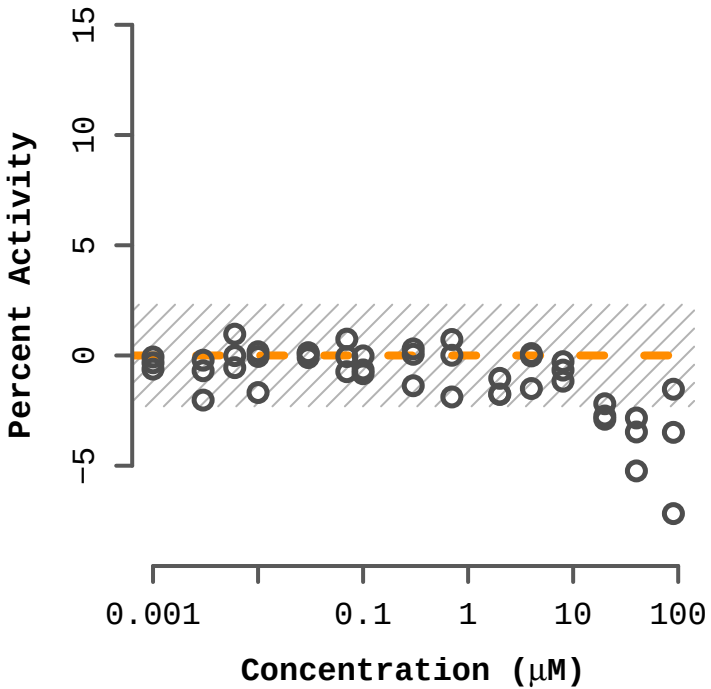
NAME: Oxazolone
CHID: 49225 **CASRN:** 15646-46-5
SPID(S): Tox21_202808
M4ID: 12479444

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.63	NA	NA

MAX_MEAN: 3.34 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

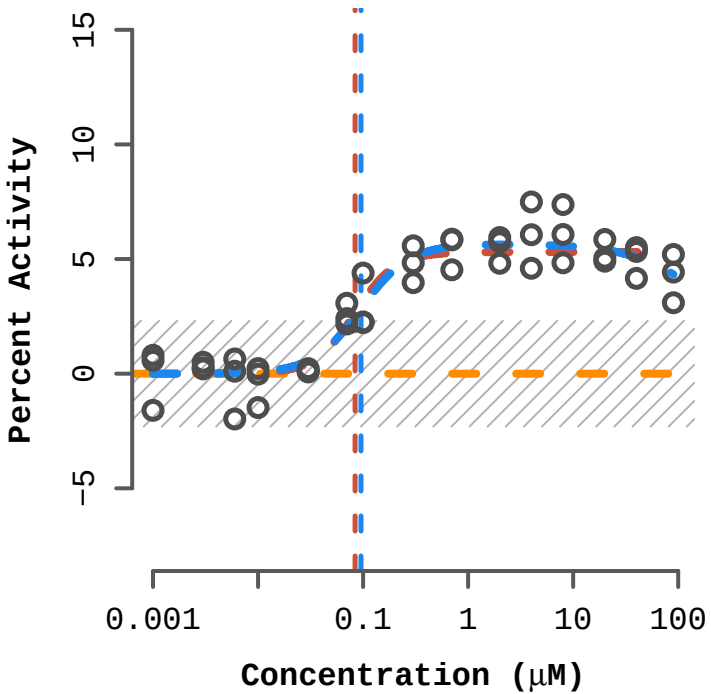
NAME: Tetrabutylthiuram disulfide
CHID: 49226 CASRN: 1634-02-2
SPID(S): Tox21_202809
M4ID: 12479443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.9	NA	NA

MAX_MEAN: 0.138 **MAX_MED:** 0.0834 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,2−Dimethyl−3−propylimidazolium bis(trifluoro
CHID: 49227 CASRN: 169051−76−7
SPID(S): Tox21_202625
M4ID: 12479627

HILL MODEL (in red):

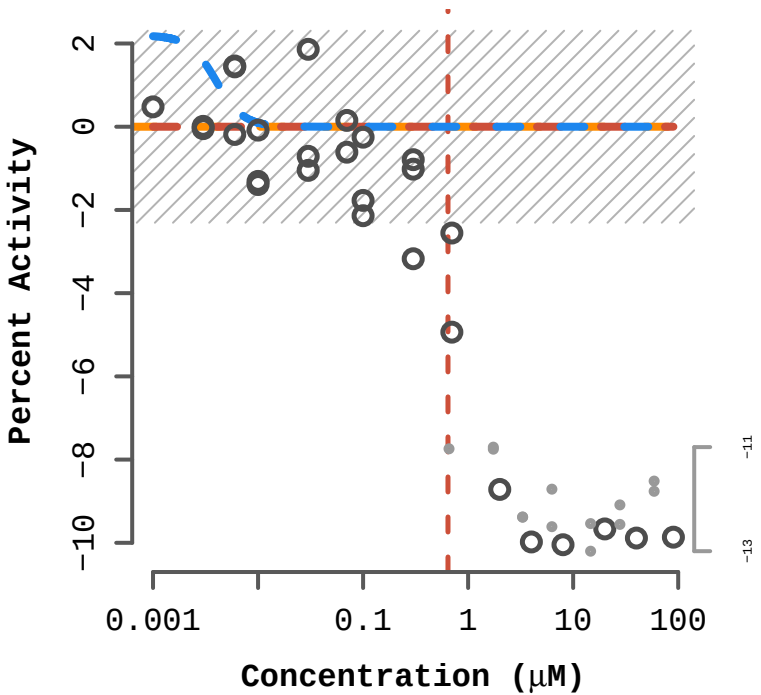
	tp	ga	gw
val:	5.31	−1.08	2.29
sd:	0.192	0.0674	0.697

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.67	−1.02	1.89	2.37	1.22
sd:	0.334	0.0871	0.563	0.395	0.949

	CNST	HILL	GNLS
AIC:	263.13	127.34	126.19
PROB:	0	0.36	0.64
RMSE:	4.1	0.91	0.84

MAX_MEAN: 6.1 MAX_MED: 6.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Decyl-3-methylimidazolium chloride
CHID: 49228 CASRN: 171058-18-7
SPID(S): Tox21_202623
M4ID: 12479629 BRK

HILL MODEL (in red):

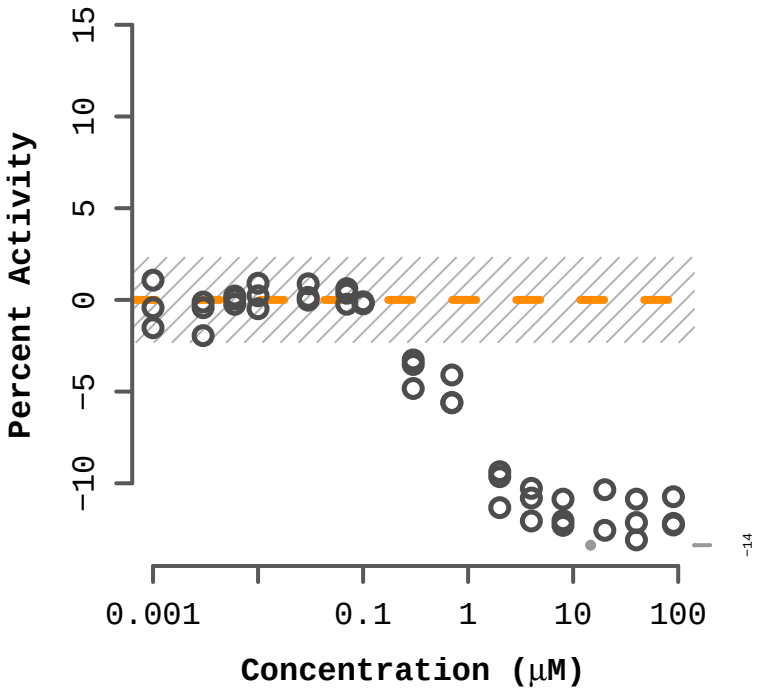
	tp	ga	gw
val:	1.68e-10	-0.192	0.495
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.2	-4.53	3.35	-2.4	3.37
sd:	4.05	1020	2260	1.27	13.1

	CNST	HILL	GNLS
AIC:	316.03	322.03	325.37
PROB:	0.94	0.05	0.01
RMSE:	7.6	7.6	7.57

MAX_MEAN: 2.24 **MAX_MED:** 2.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

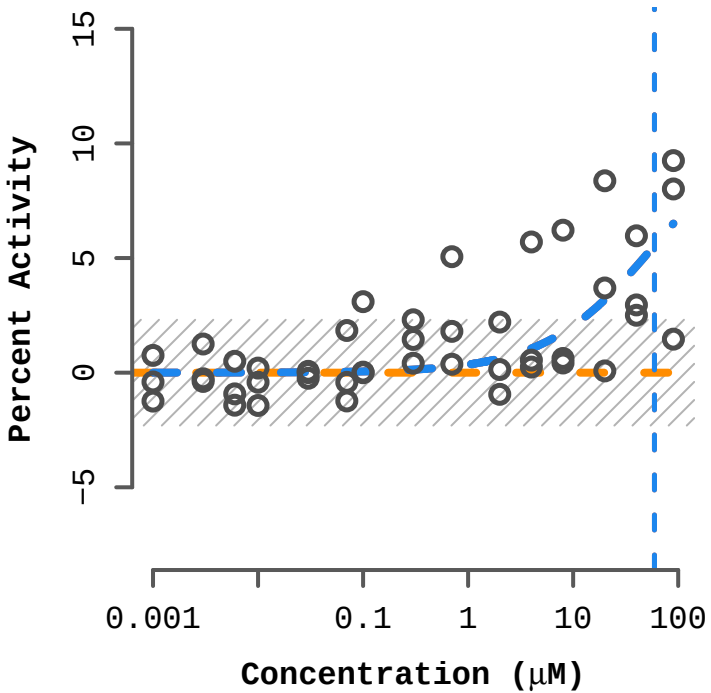
NAME: 1-Methyl-3-tetradecylimidazolium chloride
CHID: 49229 CASRN: 171058-21-2
SPID(S): Tox21_202660
M4ID: 12479592 BRK

HILL MODEL: Not applicable.

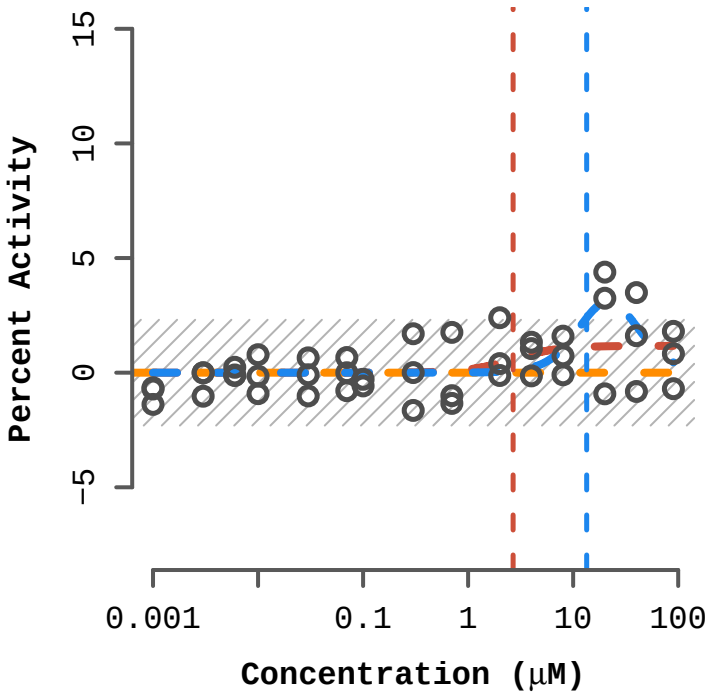
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	314.26	NA	NA
PROB:	1	NA	NA
RMSE:	7.49	NA	NA

MAX_MEAN: 0.337 MAX_MED: 0.366 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Chloroanthracene
CHID:    49230   CASRN: 17135-78-3
SPID(S): Tox21_202960
M4ID:    12479292

HILL MODEL (in red):
      tp       ga       gw
val:  11.1     1.77     0.835
sd:   6.85     0.556    0.541

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  11.1     1.77     0.835    3.95     8.75
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  219.68      196.73      200.73
PROB: 0           0.88        0.12
RMSE: 3.07        2.04        2.04

MAX_MEAN: 6.24      MAX_MED: 8.02      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylimidazolium tetrafluoroborate
CHID: 49231 **CASRN:** 174501-65-6
SPID(S): Tox21_202621
M4ID: 12479631

HILL MODEL (in red):

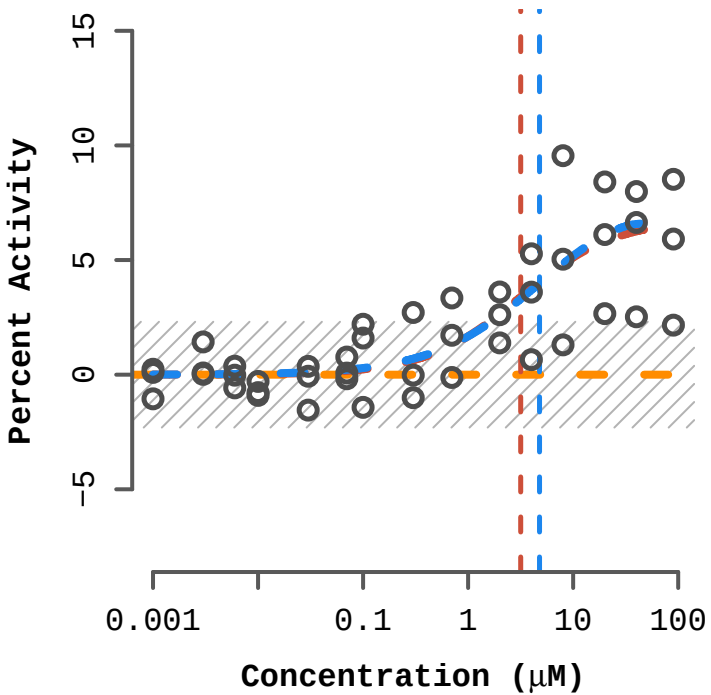
	tp	ga	gw
val:	1.17	0.428	2.03
sd:	0.645	0.584	2.83

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.26	1.13	2.58	1.54	2.46
sd:	4.54	0.374	4.46	0.274	2.74

	CNST	HILL	GNLS
AIC:	150.56	147.37	148.18
PROB:	0.11	0.53	0.36
RMSE:	1.37	1.17	1.18

MAX_MEAN: 2.24 **MAX_MED:** 3.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylimidazolium trifluoromethanesu
CHID: 49232 CASRN: 174899-66-2
SPID(S): Tox21_202619
M4ID: 12479633

HILL MODEL (in red):

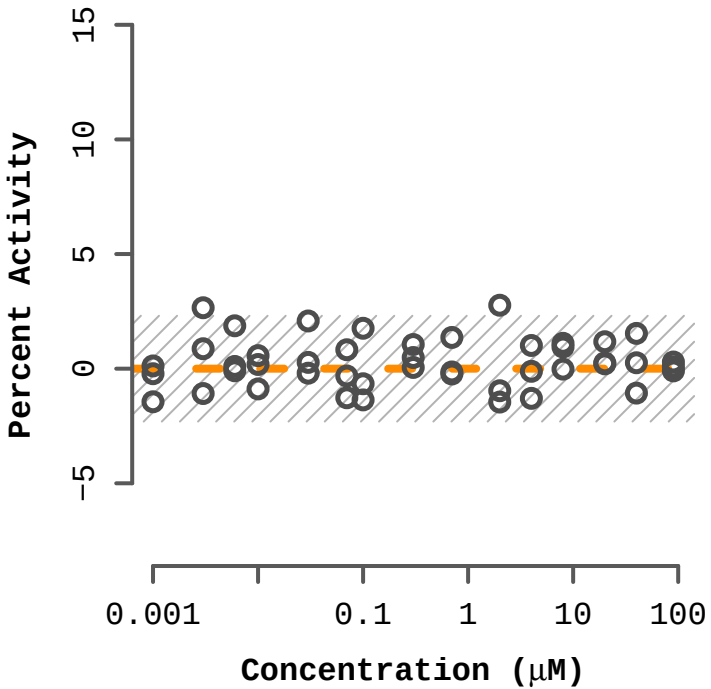
	tp	ga	gw
val:	6.79	0.5	0.967
sd:	1.18	0.251	0.394

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.98	0.68	0.848	2.26	2.08
sd:	6.29	0.85	0.462	1.24	11.6

	CNST	HILL	GNLS
AIC:	238.26	184.08	187.7
PROB:	0	0.86	0.14
RMSE:	3.54	1.75	1.74

MAX_MEAN: 5.73 MAX_MED: 6.64 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

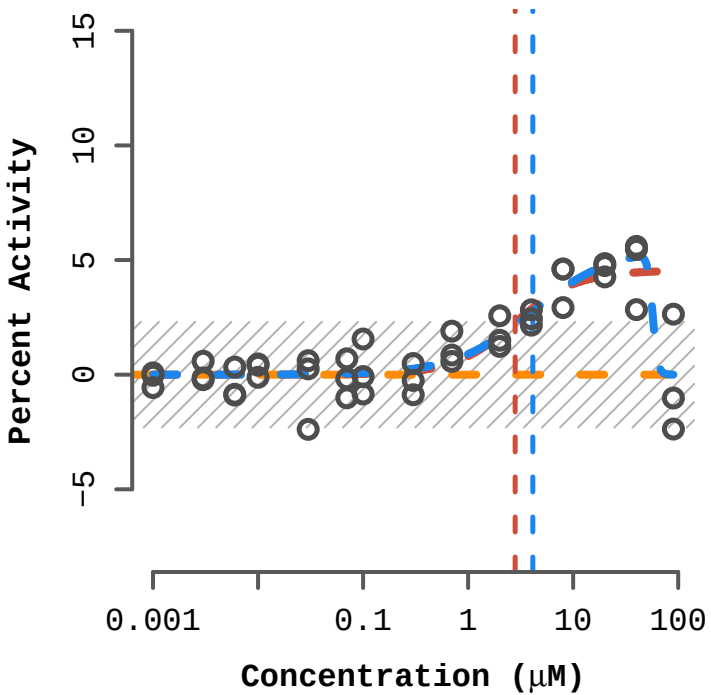
NAME: 1−Ethyl−2,3−dimethylimidazolium trifluorometha
CHID: 49233 **CASRN:** 174899−72−0
SPID(S): Tox21_202637
M4ID: 12479615

HILL MODEL: Not applicable.

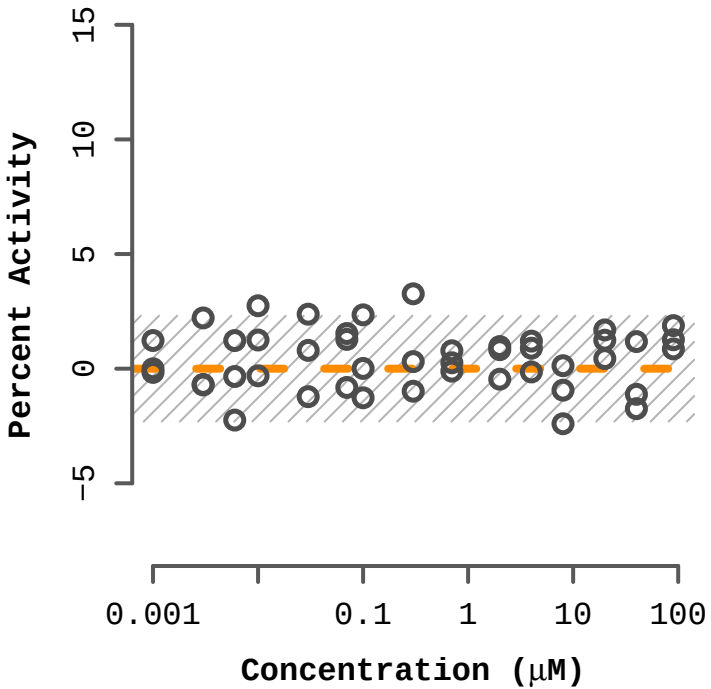
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.816 **MAX_MED:** 0.947 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butyl-3-methylimidazolium bis(trifluoromethy
CHID:    49234   CASRN: 174899-83-3
SPID(S): Tox21_202617
M4ID:    12479635

HILL MODEL (in red):
      tp       ga       gw
val:  4.54     0.448    1.49
sd:   0.539    0.122    0.442

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.53     0.616    1.15     1.76     18
sd:   0.742    0.155    0.333    0.319    32.7

      CNST        HILL        GNLS
AIC:  204.91      147.04      129.76
PROB: 0           0           1
RMSE: 2.34        1.55        0.94

MAX_MEAN: 4.63      MAX_MED: 5.47      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Ethyl-2,3-dimethylimidazolium bis(trifluorom

CHID: 49235 **CASRN:** 174899-90-2

SPID(S): Tox21_202631

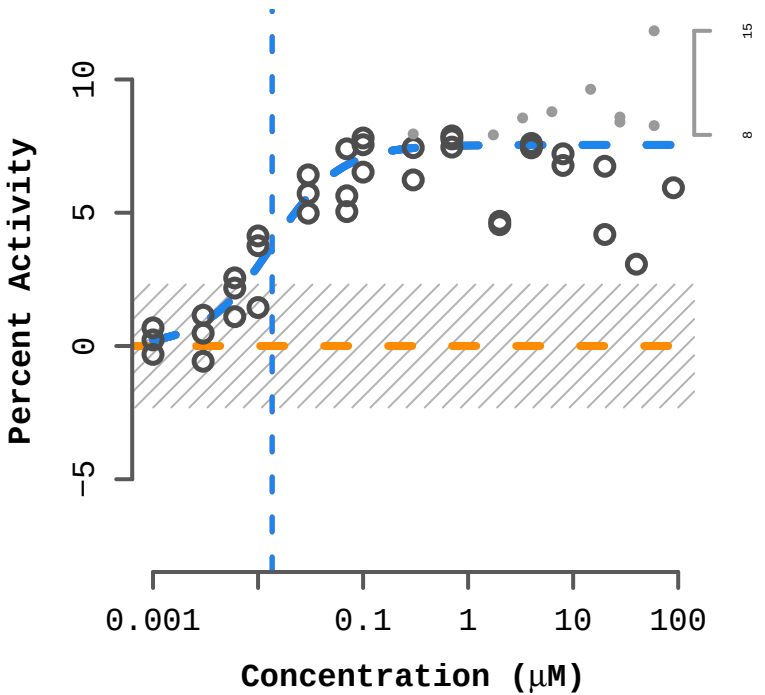
M4ID: 12479621

HILL MODEL: Not applicable.

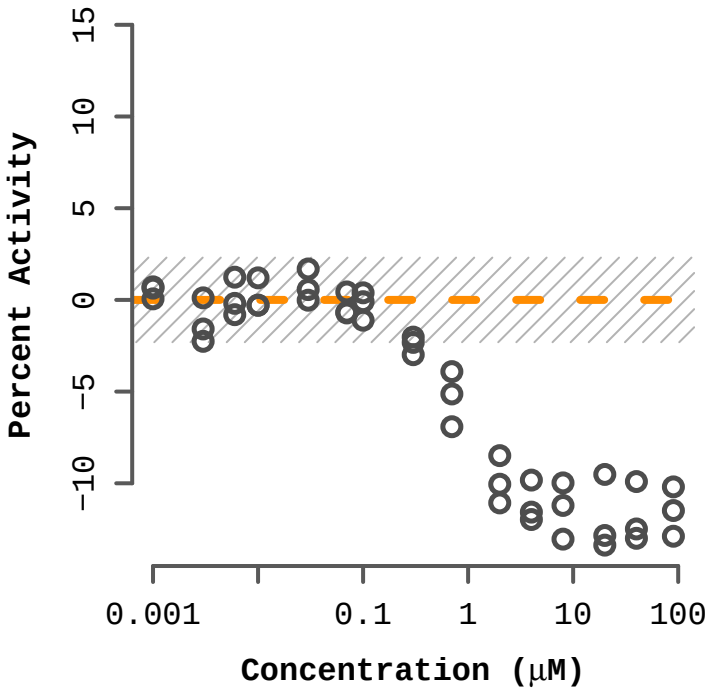
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.34 **MAX_MED:** 1.28 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Methyl-1-propylpiperidinium iodide
CHID:    49236   CASRN: 17874-63-4
SPID(S): Tox21_202671
M4ID:    12479581  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  7.54     -1.87    1.34
sd:   0.322    0.0962   0.31

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.54     -1.87    1.34     3.95     3.67
sd:   0.322    0.0962   0.31     863      1560

      CNST        HILL        GNLS
AIC:  306.44      178.44      182.44
PROB: 0           0.88        0.12
RMSE: 6.6         1.88        1.88

MAX_MEAN: 10        MAX_MED: 8.88      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

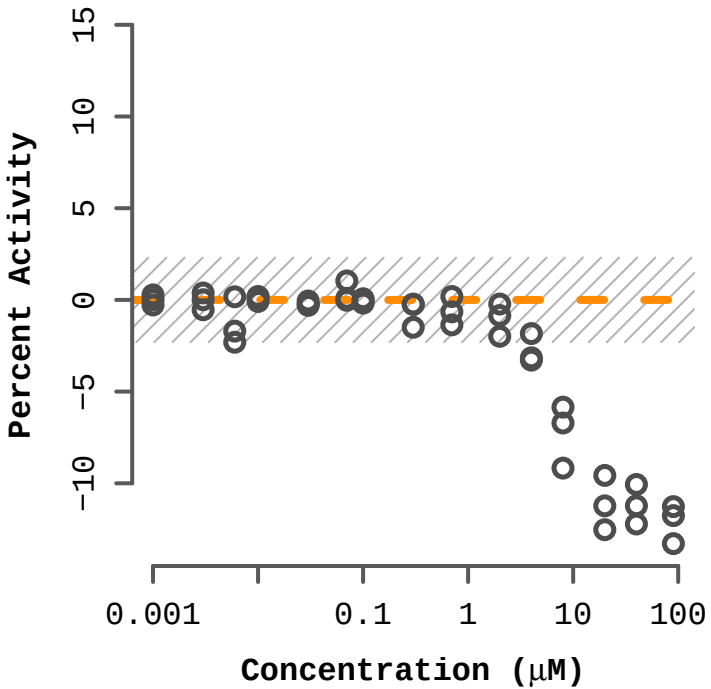
NAME: 1-Decyl-3-methylimidazolium bromide
CHID: 49237 **CASRN:** 188589-32-4
SPID(S): Tox21_202622
M4ID: 12479630

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	312.52	NA	NA
PROB:	1	NA	NA
RMSE:	7.38	NA	NA

MAX_MEAN: 0.746 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

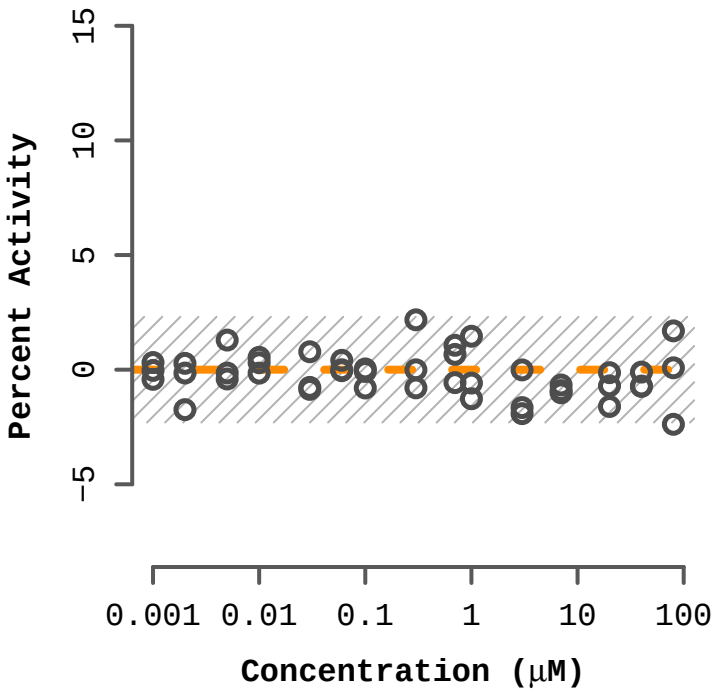
NAME: 1-Ethylpyridinium bromide
CHID: 49238 **CASRN:** 1906-79-2
SPID(S): Tox21_202695
M4ID: 12479557

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	276.58	NA	NA
PROB:	1	NA	NA
RMSE:	5.58	NA	NA

MAX_MEAN: 0.369 **MAX_MED:** 0.131 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

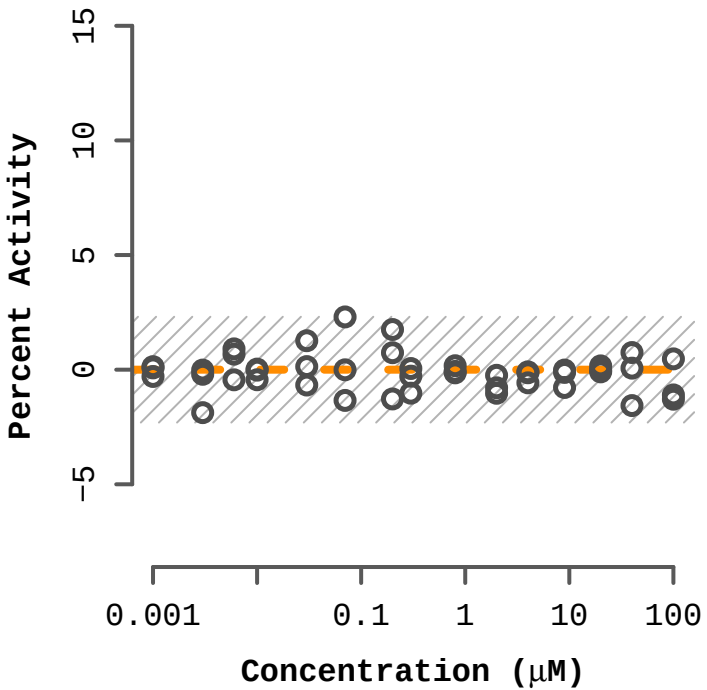
NAME: DL-Glutamic acid monohydrate
CHID: 49239 **CASRN:** 19285-83-7
SPID(S): Tox21_202810
M4ID: 12479442

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.63	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.46 **MAX_MED:** 0.668 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

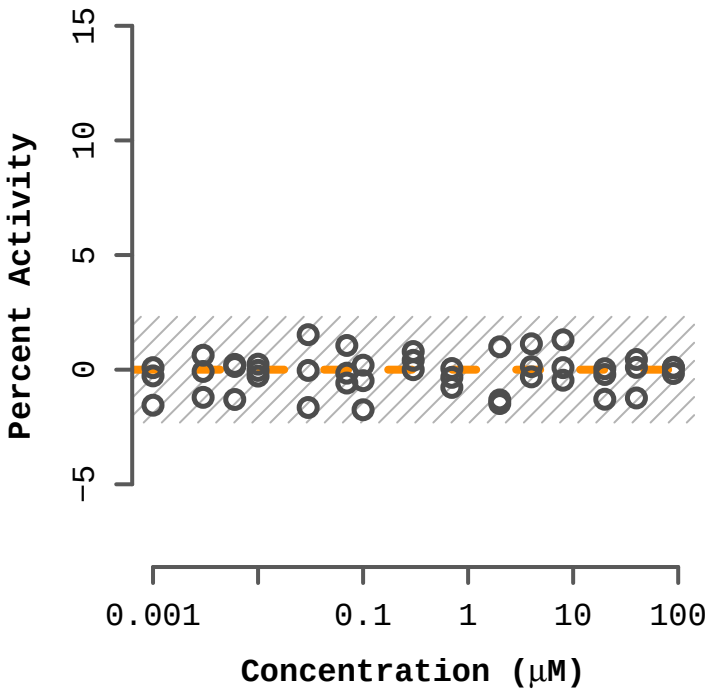
NAME: 6-Chlorohexan-1-ol
CHID: 49240 **CASRN:** 2009-83-8
SPID(S): Tox21_202812
M4ID: 12479440

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.406 **MAX_MED:** 0.741 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

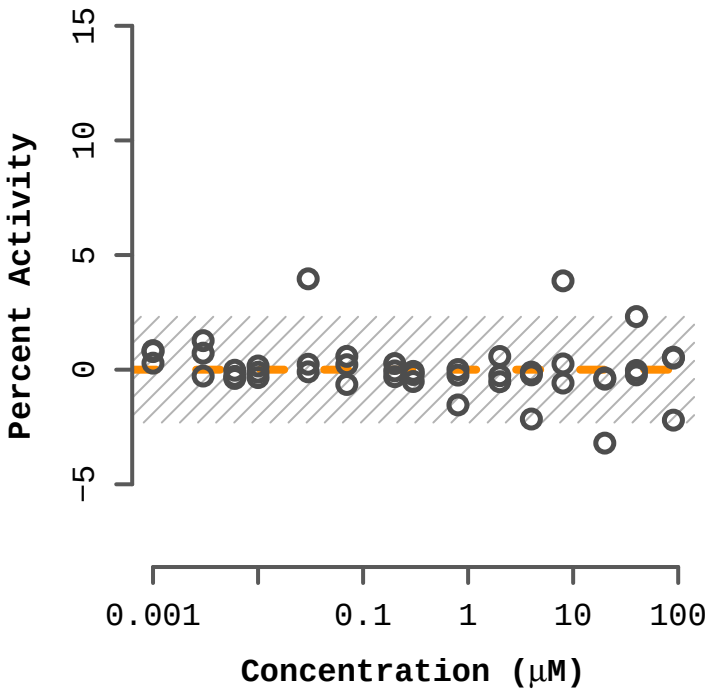
NAME: 1-Butylpyridinium tetrafluoroborate
CHID: 49241 **CASRN:** 203389-28-0
SPID(S): Tox21_202693
M4ID: 12479559

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.401 **MAX_MED:** 0.41 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

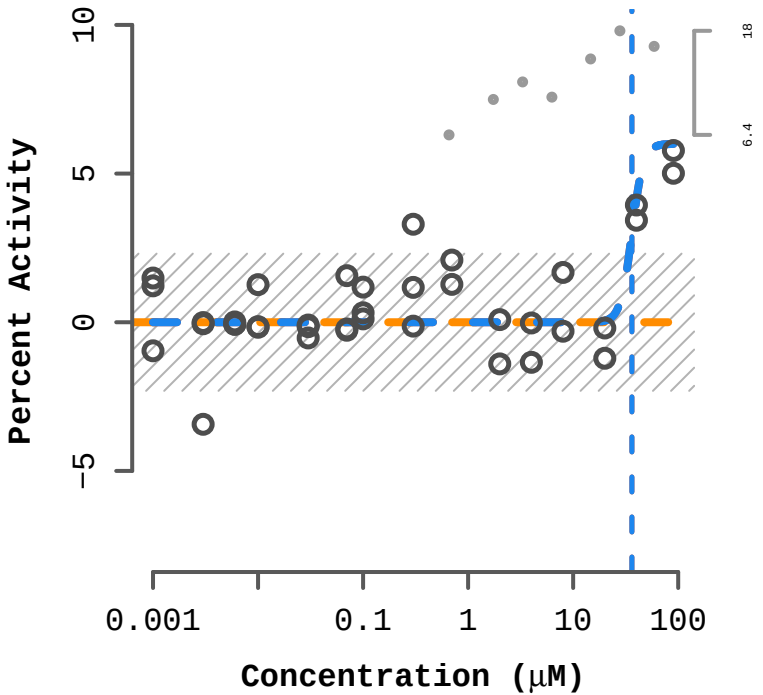
NAME: 1,2-Pyrrolidinedicarboxylicacid,4-fluoro-,1-(1,
CHID: 49242 **CASRN:** 203866-13-1
SPID(S): Tox21_202813
M4ID: 12479439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Acetylphenanthrene
CHID: 49243 CASRN: 2039-76-1
SPID(S): Tox21_202956
M4ID: 12479296 BRK

HILL MODEL (in red):

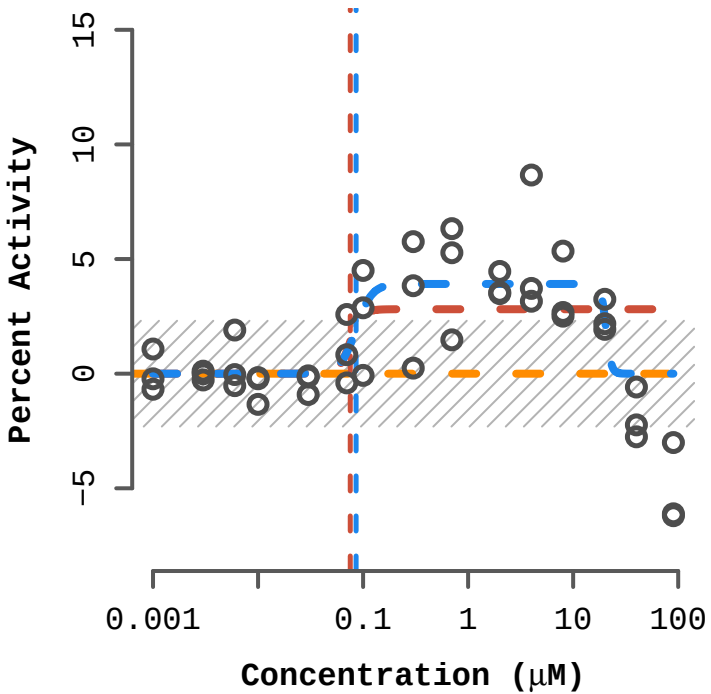
	tp	ga	gw
val:	6	1.56	8
sd:	1.26	0.0885	13.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6	1.56	8	3.68	6.26
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	262.11	247.37	251.37
PROB:	0	0.88	0.12
RMSE:	5.52	4.69	4.69

MAX_MEAN: 9.05 MAX_MED: 5.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyltributylphosphonium diethylphosphate
CHID: 49244 CASRN: 20445-94-7
SPID(S): Tox21_202615
M4ID: 12479637

HILL MODEL (in red):

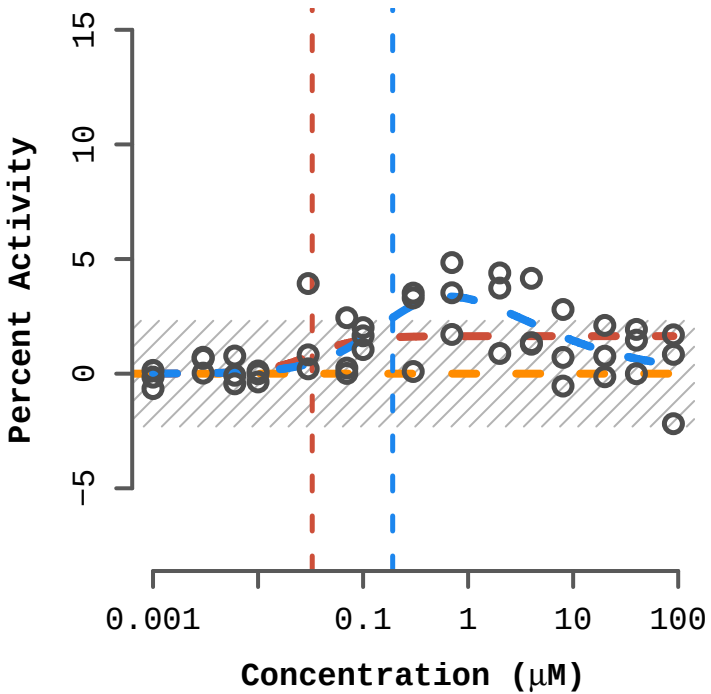
	tp	ga	gw
val:	2.81	−1.12	8
sd:	0.495	0.0931	13.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.91	−1.07	5.78	1.31	18
sd:	0.444	0.0744	4.86	0.0373	54.8

	CNST	HILL	GNLS
AIC:	235.89	219.75	195.26
PROB:	0	0	1
RMSE:	3.21	2.87	2.01

MAX_MEAN: 5.18 **MAX_MED:** 5.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dibenz[a,c]anthracene
CHID: 49245 CASRN: 215-58-7
SPID(S): Tox21_202967
M4ID: 12479285

HILL MODEL (in red):

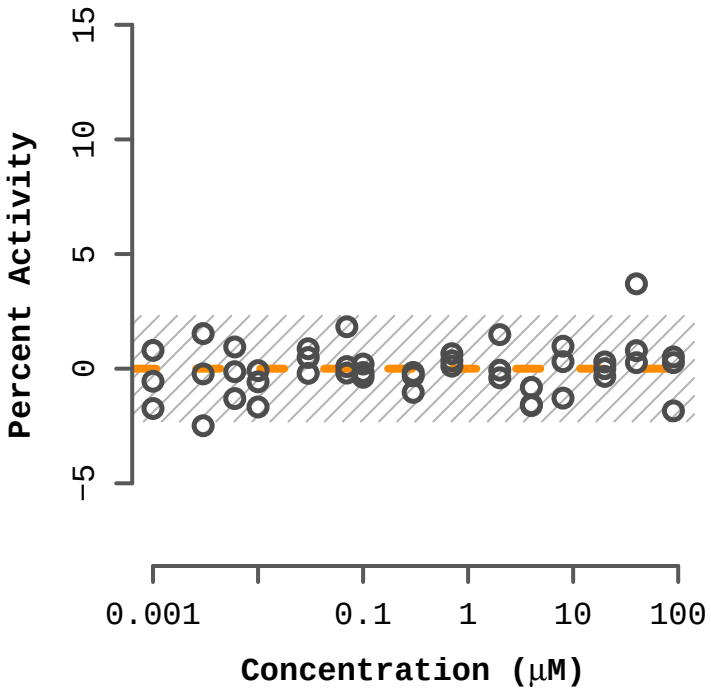
	tp	ga	gw
val:	1.64	−1.48	1.93
sd:	0.298	0.356	1.54

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.82	−0.718	1.34	0.313	0.697
sd:	4.28	0.374	0.677	0.871	0.408

	CNST	HILL	GNLS
AIC:	190.8	164.72	156.55
PROB:	0	0.02	0.98
RMSE:	1.99	1.4	1.21

MAX_MEAN: 3.36 **MAX_MED:** 3.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

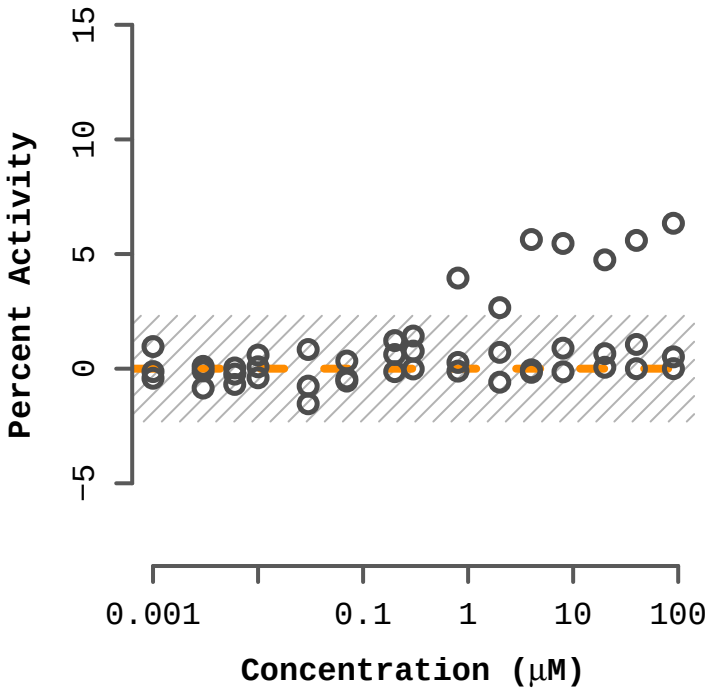
NAME: 1-Methyl-3-propylimidazolium hexafluorophospha
CHID: 49246 **CASRN:** 216300-12-8
SPID(S): Tox21_202659
M4ID: 12479593

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.789 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

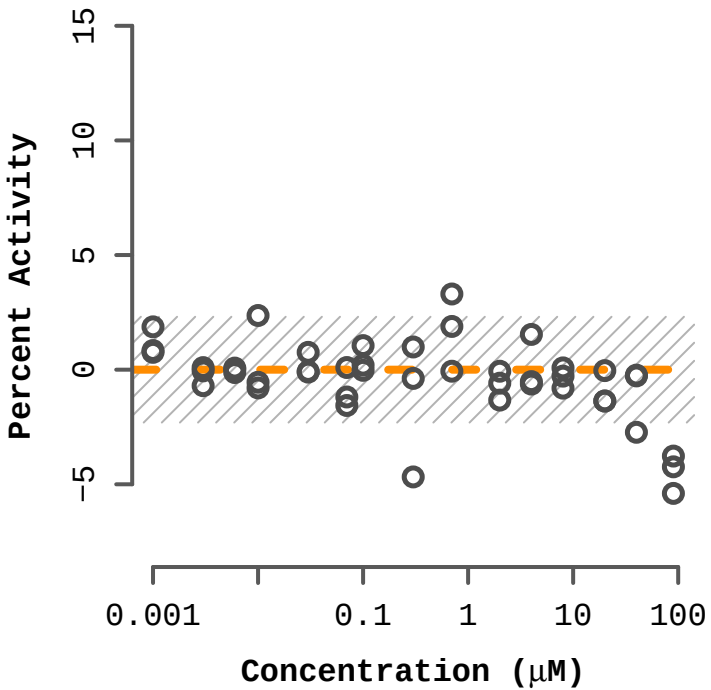
NAME: 1,2-Dimethyl-3-propylimidazolium iodide
CHID: 49247 **CASRN:** 218151-78-1
SPID(S): Tox21_202626
M4ID: 12479626

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	174.2	NA	NA
PROB:	1	NA	NA
RMSE:	2.07	NA	NA

MAX_MEAN: 2.29 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

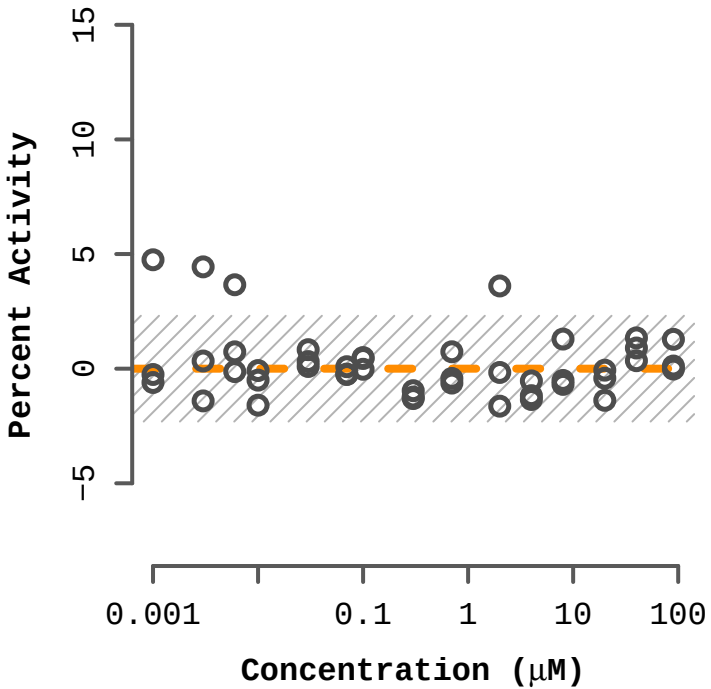
NAME: 1-Methyl-3-tetradecylimidazolium hexafluorophos
CHID: 49248 CASRN: 219947-94-1
SPID(S): Tox21_202661
M4ID: 12479591

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.97	NA	NA
PROB:	1	NA	NA
RMSE:	1.72	NA	NA

MAX_MEAN: 1.71 MAX_MED: 1.89 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1−Hexadecyl−3−methylimidazolium hexafluorophos

CHID: 49249 **CASRN:** 219947−95−2

SPID(S): Tox21_202646

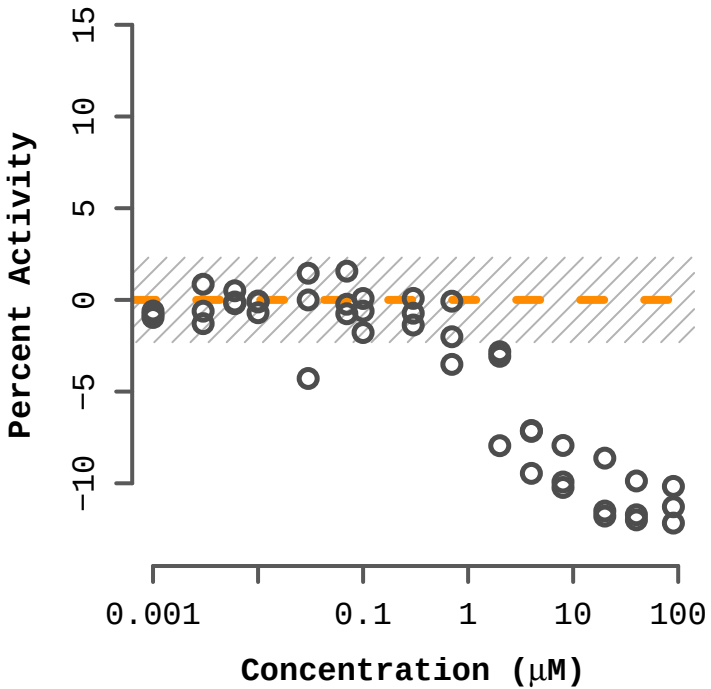
M4ID: 12479606

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.902 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Methyl-3-octadecylimidazolium hexafluorophos

CHID: 49250 **CASRN:** 219947-96-3

SPID(S): Tox21_202652

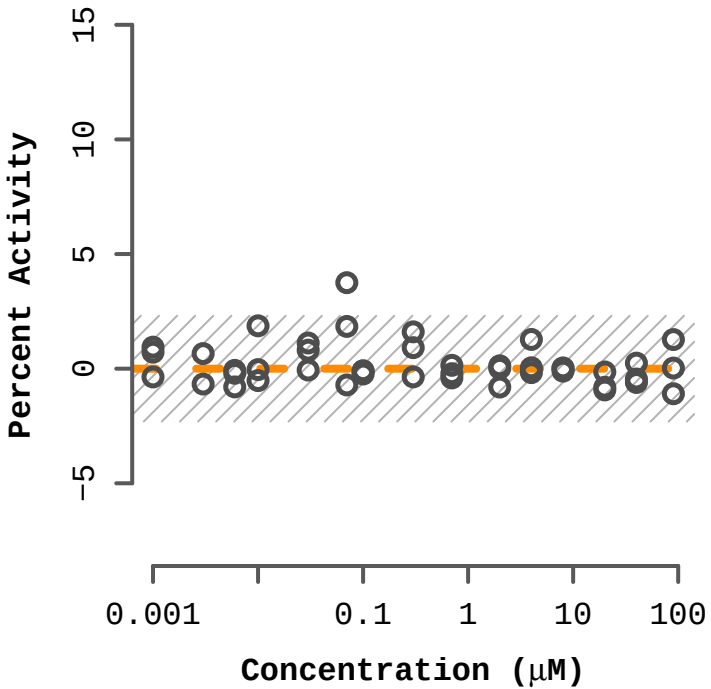
M4ID: 12479600

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	293.19	NA	NA
PROB:	1	NA	NA
RMSE:	6.13	NA	NA

MAX_MEAN: 0.193 **MAX_MED:** −0.00116 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

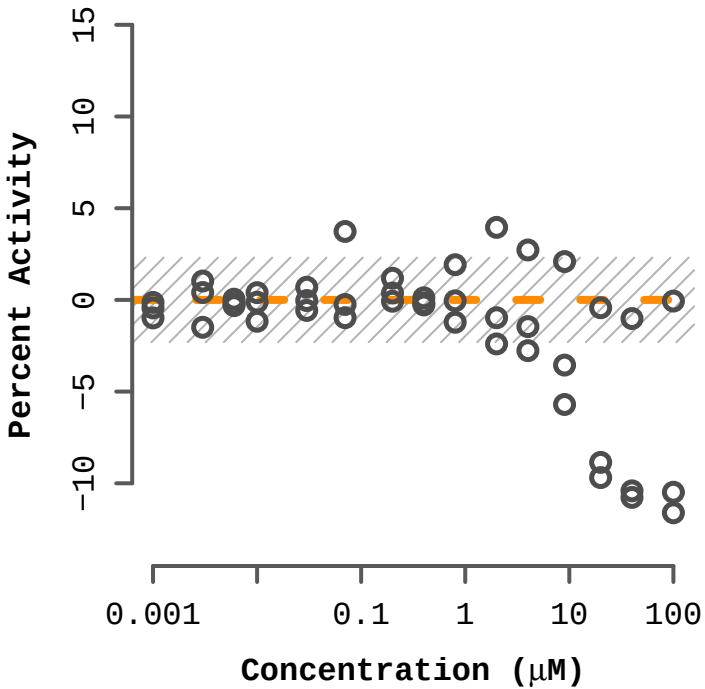
NAME: 1-Methyl-3-propylimidazolium tetrafluoroborate
CHID: 49251 **CASRN:** 244193-48-4
SPID(S): Tox21_202656
M4ID: 12479596

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.51	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.63 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

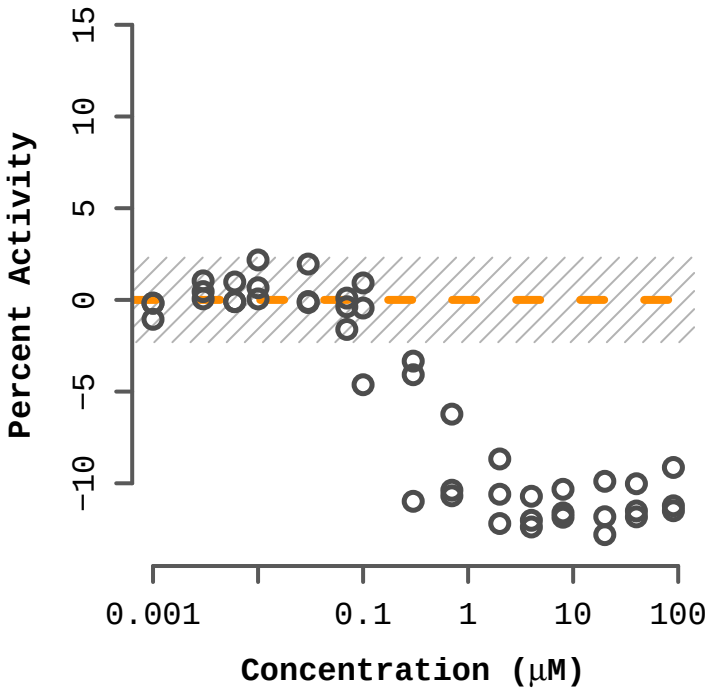
NAME: 1-Hexyl-3-methylimidazolium tetrafluoroborate
CHID: 49252 **CASRN:** 244193-50-8
SPID(S): Tox21_202650
M4ID: 12479602

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	240.63	NA	NA
PROB:	1	NA	NA
RMSE:	4.11	NA	NA

MAX_MEAN: 0.84 **MAX_MED:** 0.405 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

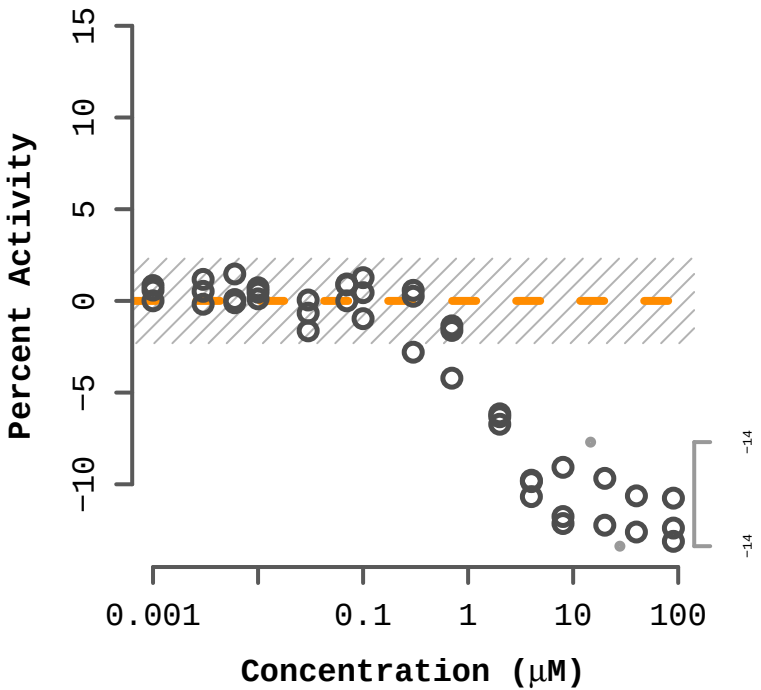
NAME: 1-Dodecyl-3-methylimidazolium tetrafluoroborat
CHID: 49253 **CASRN:** 244193-59-7
SPID(S): Tox21_202629
M4ID: 12479623

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	318.77	NA	NA
PROB:	1	NA	NA
RMSE:	7.74	NA	NA

MAX_MEAN: 0.966 **MAX_MED:** 0.664 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

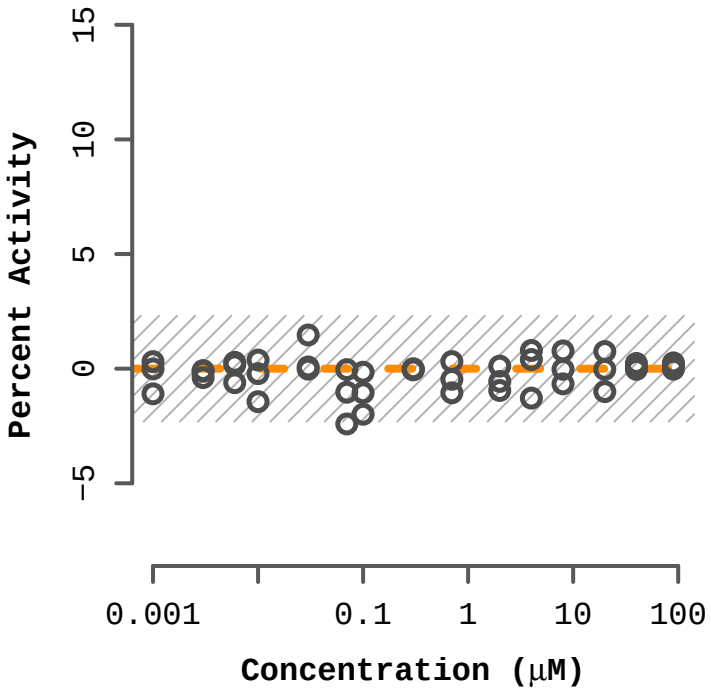
NAME: 1-Hexadecyl-3-methylimidazolium tetrafluorobora
CHID: 49254 CASRN: 244193-64-4
SPID(S): Tox21_202647
M4ID: 12479605 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	305	NA	NA
PROB:	1	NA	NA
RMSE:	6.95	NA	NA

MAX_MEAN: 0.603 MAX_MED: 0.878 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

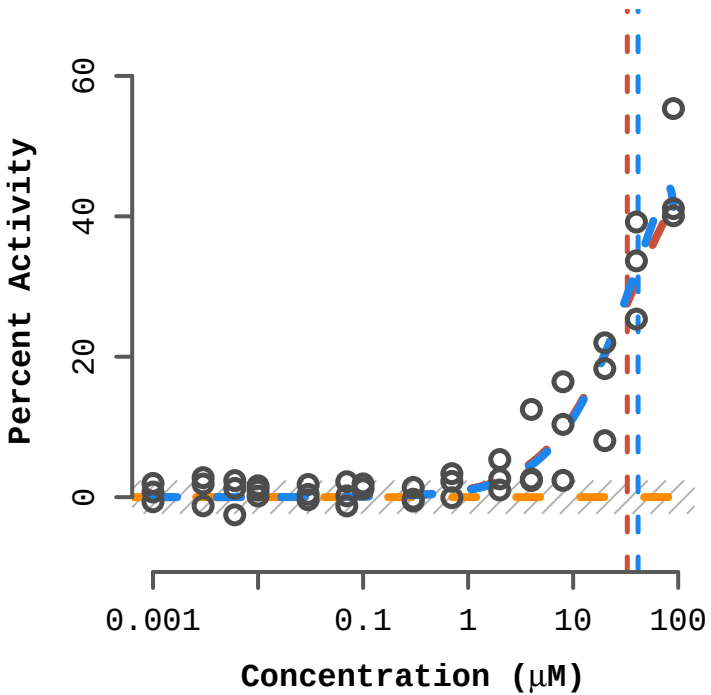
NAME: Nonane,1-chloro-
CHID: 49255 **CASRN:** 2473-01-0
SPID(S): Tox21_202816
M4ID: 12479436

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.509 **MAX_MED:** 0.402 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9-Cyanophenanthrene
CHID: 49256 CASRN: 2510-55-6
SPID(S): Tox21_202906
M4ID: 12479346

HILL MODEL (in red):

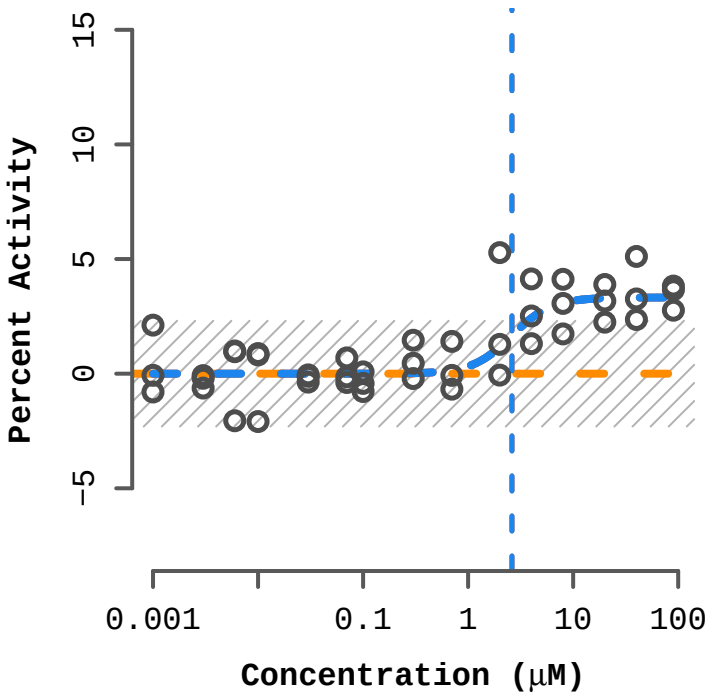
	tp	ga	gw
val:	55.3	1.52	1.11
sd:	11.4	0.21	0.265

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	66.4	1.62	1.11	2	17.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	348.9	241.4	244.37
PROB:	0	0.82	0.18
RMSE:	15.96	3.97	3.99

MAX_MEAN: 45.5 MAX_MED: 41.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylpyridinium iodide
CHID: 49257 CASRN: 258273-67-5
SPID(S): Tox21_202684
M4ID: 12479568

HILL MODEL (in red):

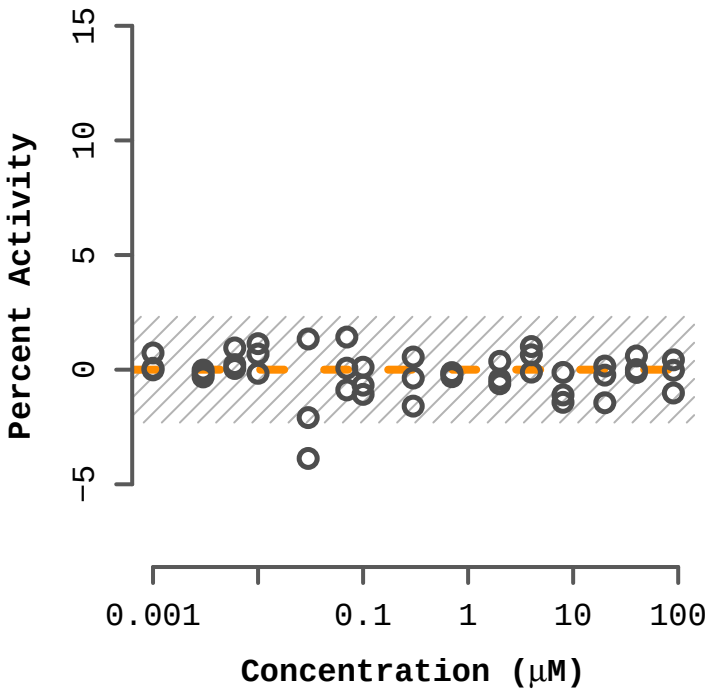
	tp	ga	gw
val:	3.32	0.417	2.32
sd:	0.333	0.133	2.03

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.32	0.417	2.32	3.62	4.37
sd:	0.333	0.133	2.03	927	2430

	CNST	HILL	GNLS
AIC:	200.91	140.66	144.66
PROB:	0	0.88	0.12
RMSE:	2.19	1.11	1.11

MAX_MEAN: 3.58 MAX_MED: 3.66 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

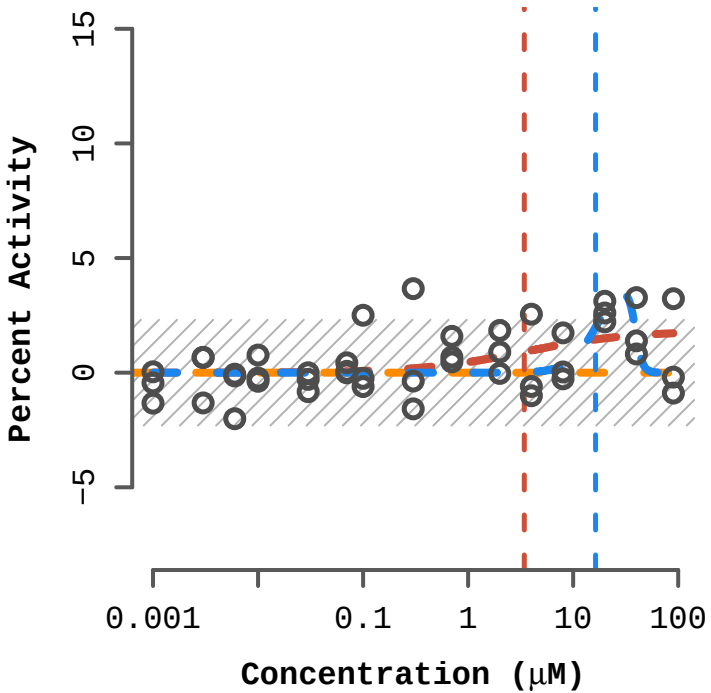
NAME: 1-Butyl-2-methylpyridinium bromide
CHID: 49258 **CASRN:** 26576-84-1
SPID(S): Tox21_202674
M4ID: 12479578

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.555 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylpyridinium bromide
CHID: 49259 **CASRN:** 26576-85-2
SPID(S): Tox21_202679
M4ID: 12479573

HILL MODEL (in red):

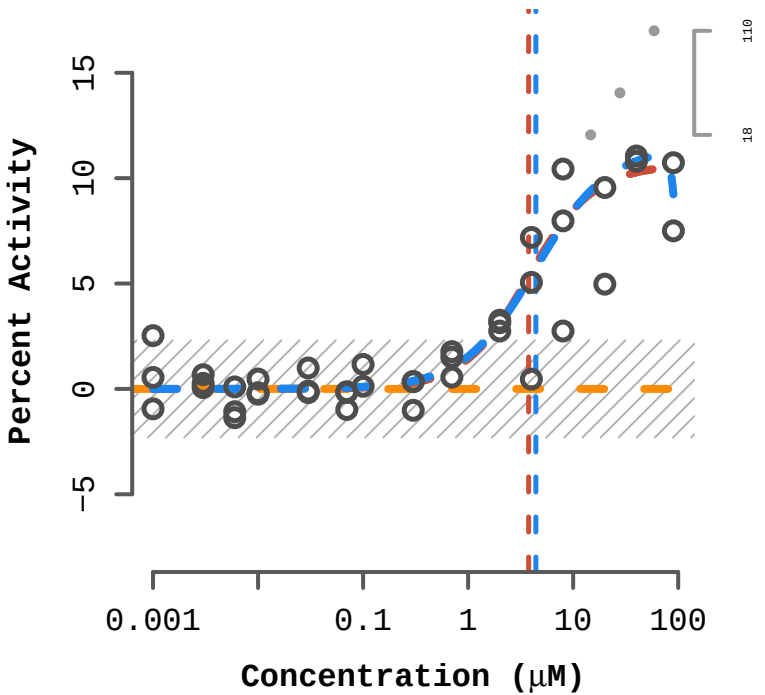
	tp	ga	gw
val:	1.82	0.534	0.879
sd:	0.886	0.785	0.599

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.97	1.21	3.43	1.59	13
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	163.59	156.71	152.55
PROB:	0	0.11	0.89
RMSE:	1.47	1.24	1.21

MAX_MEAN: 2.65 **MAX_MED:** 2.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Aminofluoranthene
CHID: 49260 CASRN: 2693-46-1
SPID(S): Tox21_202908
M4ID: 12479344 BRK

HILL MODEL (in red):

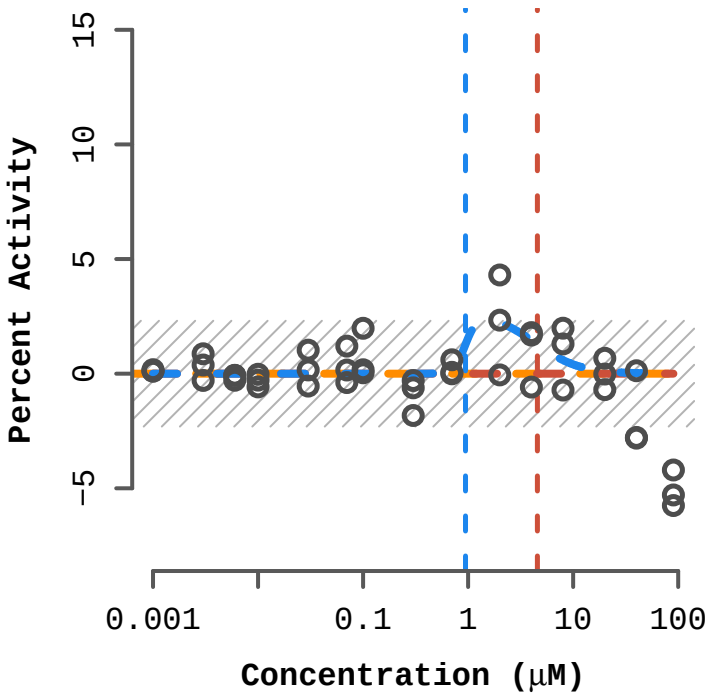
	tp	ga	gw
val:	10.6	0.576	1.41
sd:	0.844	0.101	0.354

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.5	0.645	1.26	2	15
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	306.29	237.56	240.13
PROB:	0	0.78	0.22
RMSE:	18.6	15.92	16.05

MAX_MEAN: 41.4 MAX_MED: 11.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Amino-m-cresol
CHID: 49261 CASRN: 2835-97-4
SPID(S): Tox21_202909
M4ID: 12479343

HILL MODEL (in red):

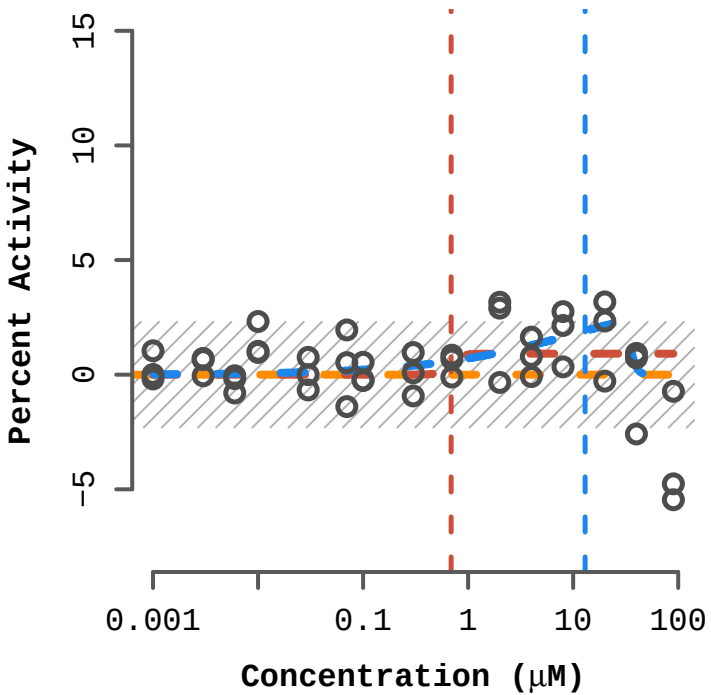
	tp	ga	gw
val:	2.51e-10	0.659	1.63
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.66	-0.025	8	0.642	2.09
sd:	2.71	0.445	25.6	0.582	1.69

	CNST	HILL	GNLS
AIC:	169.48	175.48	170.68
PROB:	0.63	0.03	0.34
RMSE:	1.79	1.79	1.68

MAX_MEAN: 2.2 MAX_MED: 2.34 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Amino-m-cresol
CHID: 49262 CASRN: 2835-99-6
SPID(S): Tox21_202910
M4ID: 12479342

HILL MODEL (in red):

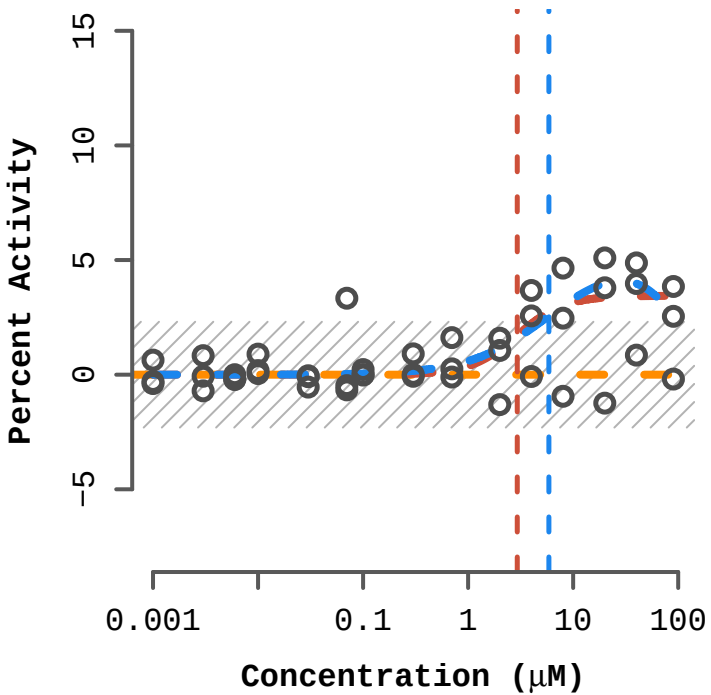
	tp	ga	gw
val:	0.915	-0.162	8
sd:	0.382	0.169	77

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.81	1.11	0.576	1.54	13.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	171.97	171.92	167.44
PROB:	0.09	0.09	0.83
RMSE:	1.71	1.72	1.52

MAX_MEAN: 1.91 MAX_MED: 2.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-2-methylpyridinium tetrafluoroborate
CHID: 49263 CASRN: 286453-46-1
SPID(S): Tox21_202675
M4ID: 12479577

HILL MODEL (in red):

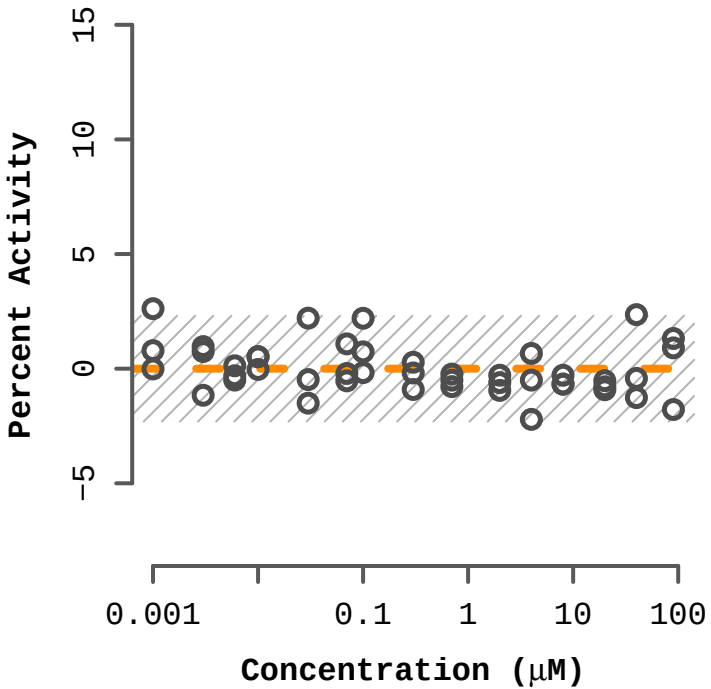
	tp	ga	gw
val:	3.44	0.468	1.95
sd:	0.517	0.157	1.57

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.15	0.769	1.15	1.97	2.09
sd:	5.33	0.88	0.918	0.355	4.32

	CNST	HILL	GNLS
AIC:	184.97	160.21	161.51
PROB:	0	0.66	0.34
RMSE:	1.98	1.47	1.47

MAX_MEAN: 3.24 MAX_MED: 3.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1−Ethyl−2,3−dimethylimidazolium hexafluorophos

CHID: 49264 **CASRN:** 292140−86−4

SPID(S): Tox21_202634

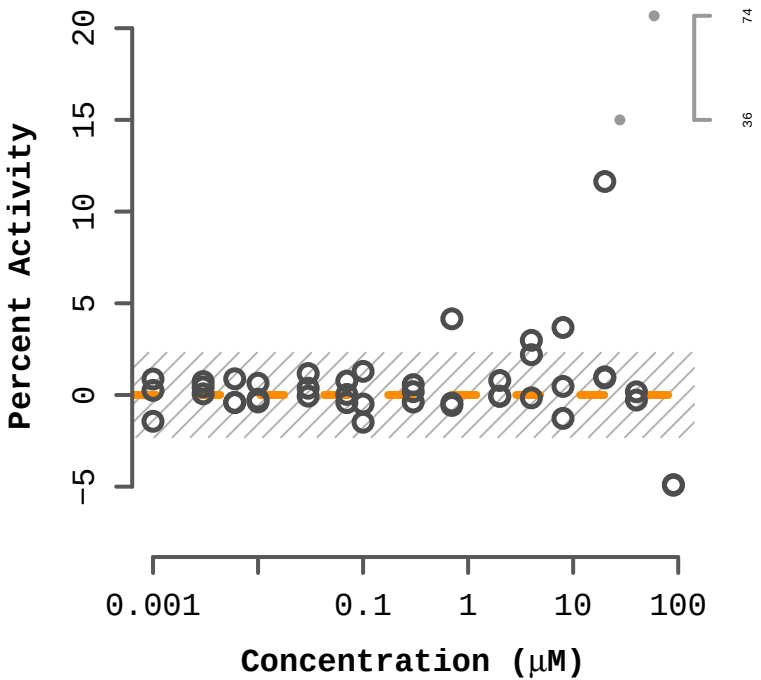
M4ID: 12479618

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.908 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

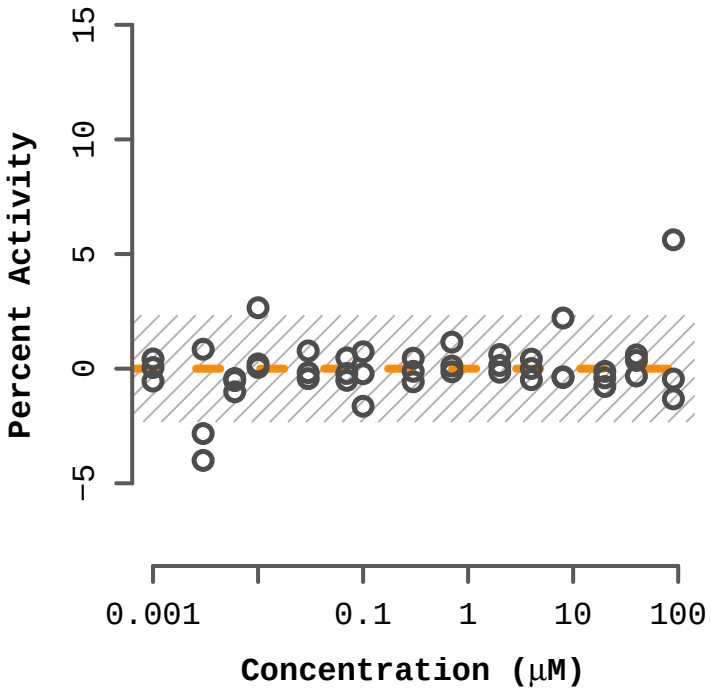
NAME: Benzaldehyde,2-bromo-5-hydroxy-
CHID: 49265 **CASRN:** 2973-80-0
SPID(S): Tox21_202820
M4ID: 12479432 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	234.5	NA	NA
PROB:	1	NA	NA
RMSE:	12.51	NA	NA

MAX_MEAN: 21.5 **MAX_MED:** 2.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

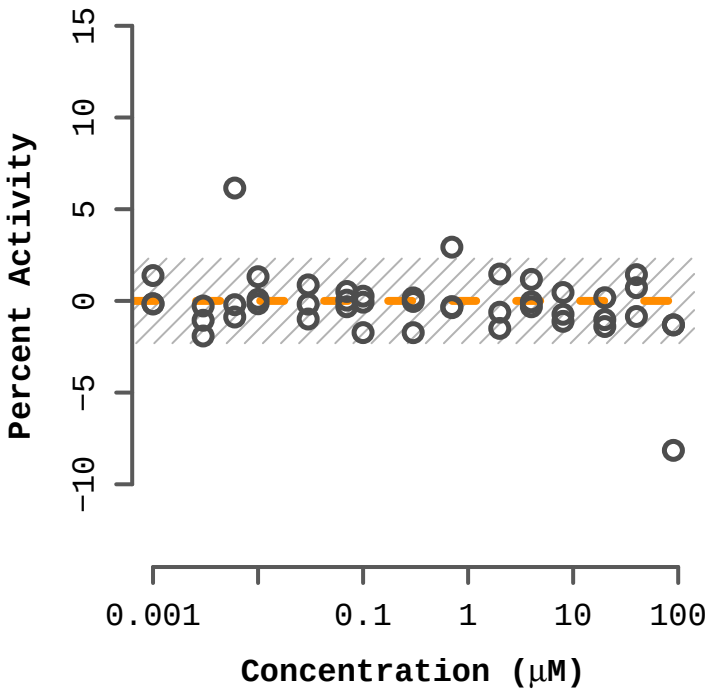
NAME: 1-Ethyl-2,3-dimethylimidazolium tetrafluorobora
CHID: 49266 CASRN: 307492-75-7
SPID(S): Tox21_202636
M4ID: 12479616

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.29 MAX_MED: 0.36 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

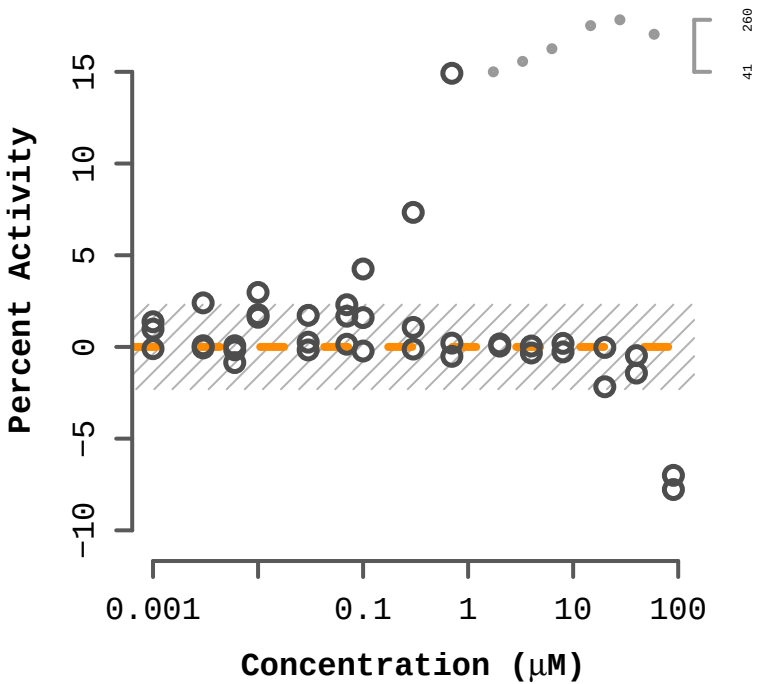
NAME: 1-Butyl-4-methylpyridinium iodide
CHID: 49267 **CASRN:** 32353-64-3
SPID(S): Tox21_202689
M4ID: 12479563

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.82	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 0.723 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

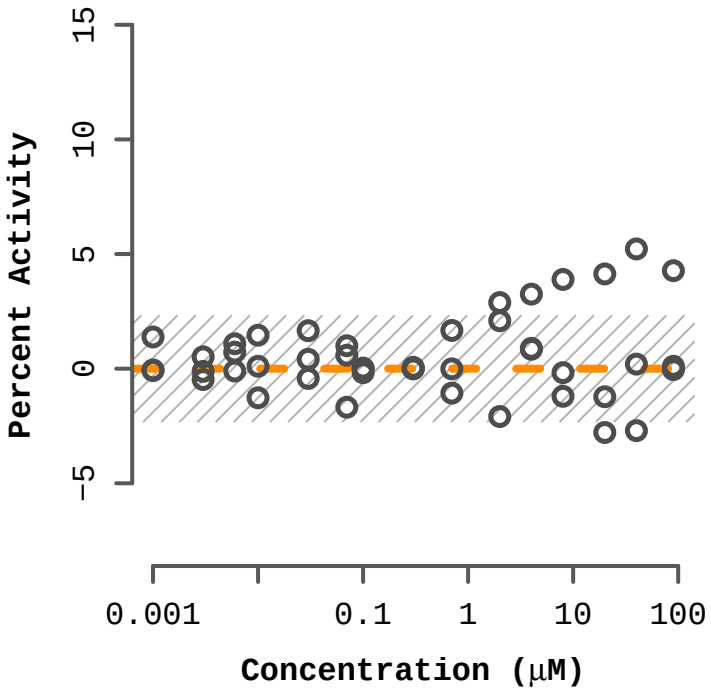
NAME: 4,4,4-Trifluoro-1-phenyl-1,3-butanedione
CHID: 49268 **CASRN:** 326-06-7
SPID(S): Tox21_202821
M4ID: 12479431 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	406.16	NA	NA
PROB:	1	NA	NA
RMSE:	65.16	NA	NA

MAX_MEAN: 85.9 **MAX_MED:** 1.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

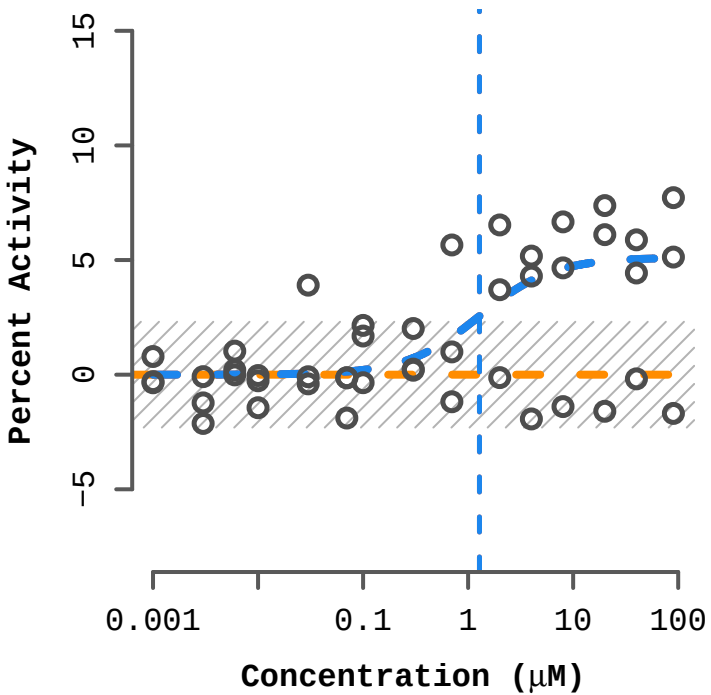
NAME: 1-Methyl-1-propylpyrrolidinium hexfluorophospha
CHID: 49269 CASRN: 327022-58-2
SPID(S): Tox21_202709
M4ID: 12479543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 1.66 MAX_MED: 2.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Ethyl-3-methylimidazolium tosylate
CHID: 49270 CASRN: 328090-25-1
SPID(S): Tox21_202645
M4ID: 12479607

HILL MODEL (in red):

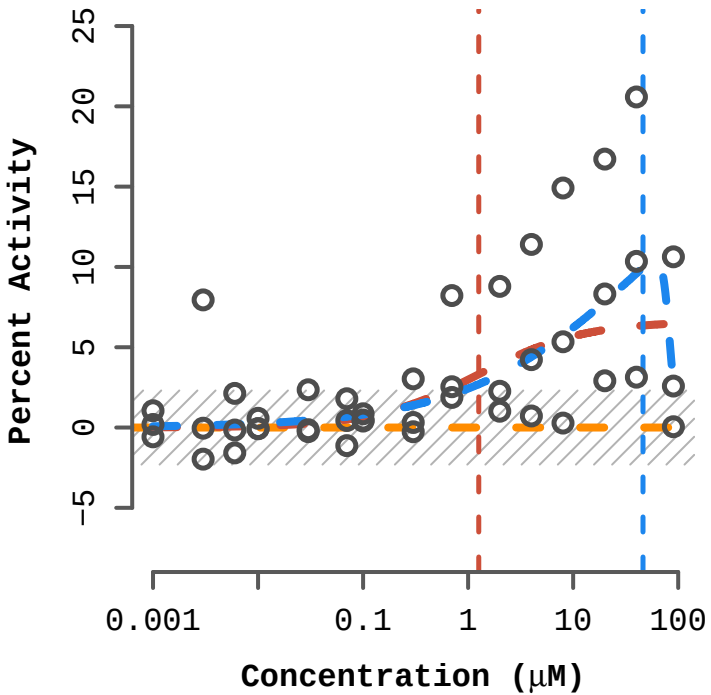
	tp	ga	gw
val:	5.11	0.108	1.24
sd:	0.929	0.309	0.782

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.11	0.108	1.24	3.09	6.76
sd:	0.929	0.309	0.782	1770	10600

	CNST	HILL	GNLS
AIC:	235.73	214.53	218.53
PROB:	0	0.88	0.12
RMSE:	3.29	2.56	2.56

MAX_MEAN: 3.96 MAX_MED: 6.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9,10-Dihydrobenzo[a]pyren-7(8H)-one
CHID: 49271 CASRN: 3331-46-2
SPID(S): Tox21_202913
M4ID: 12479339

HILL MODEL (in red):

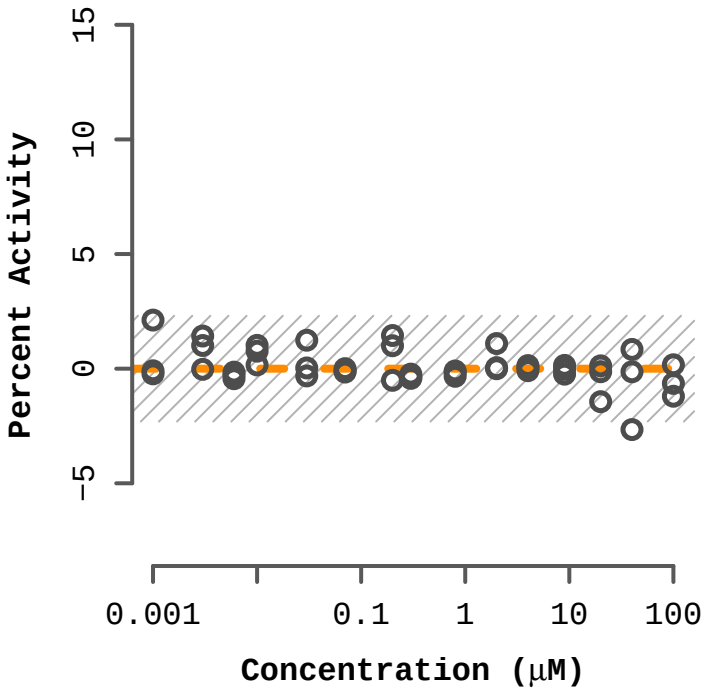
	tp	ga	gw
val:	6.63	0.101	0.868
sd:	2.55	0.61	0.572

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.9	1.66	0.515	1.91	12.8
sd:	35.7	2.69	0.299	0.0744	23.7

	CNST	HILL	GNLS
AIC:	279.38	254.95	255.02
PROB:	0	0.51	0.49
RMSE:	6.1	4.13	3.88

MAX_MEAN: 11.4 MAX_MED: 10.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

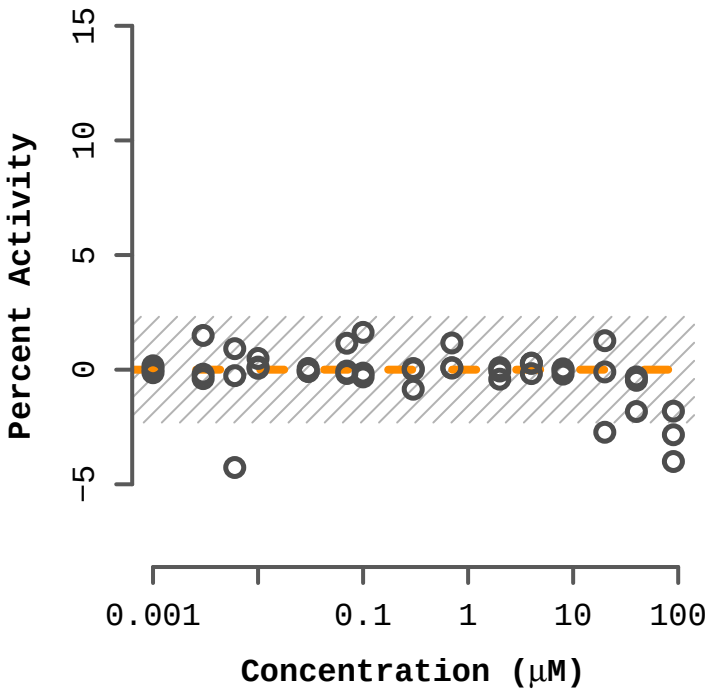
NAME: Methyl trifluoromethanesulfonate
CHID: 49272 CASRN: 333-27-7
SPID(S): Tox21_202914
M4ID: 12479338

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.803 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

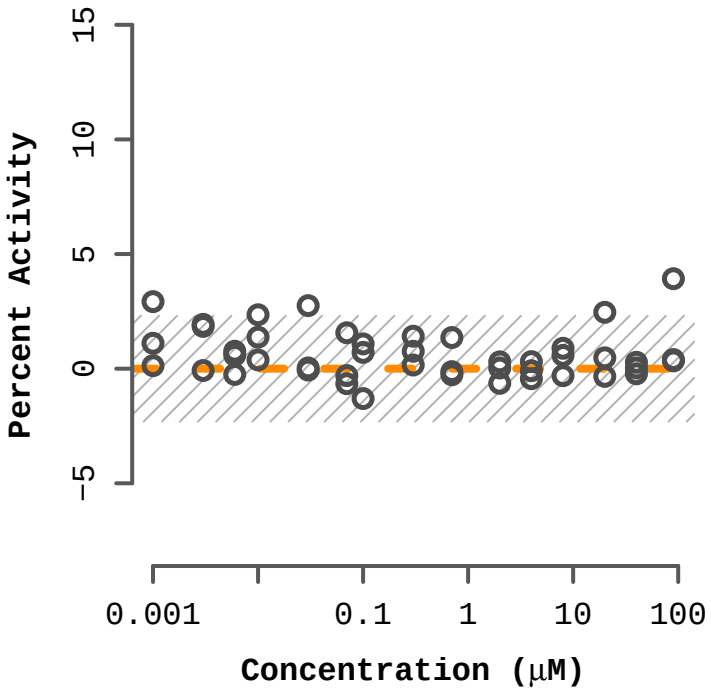
NAME: 12-Bromo-1-dodecanol
CHID: 49273 **CASRN:** 3344-77-2
SPID(S): Tox21_202822
M4ID: 12479430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 0.443 **MAX_MED:** 0.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

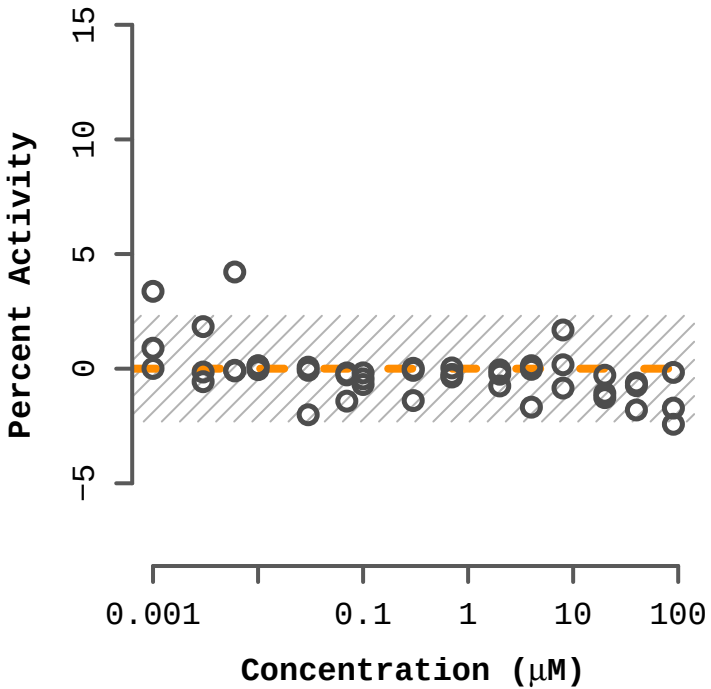
NAME: 1-Ethyl-3-methylimidazolium ethyl sulfate
CHID: 49274 **CASRN:** 342573-75-5
SPID(S): Tox21_202639
M4ID: 12479613

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

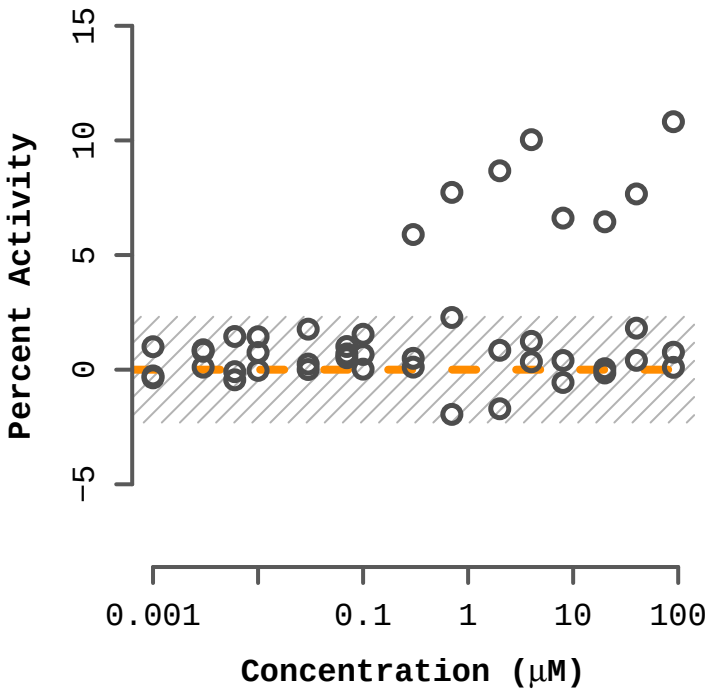
NAME: 1-Butyl-4-methylpyridinium tetrafluoroborate
CHID: 49275 **CASRN:** 343952-33-0
SPID(S): Tox21_202690
M4ID: 12479562

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.43 **MAX_MED:** 0.894 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

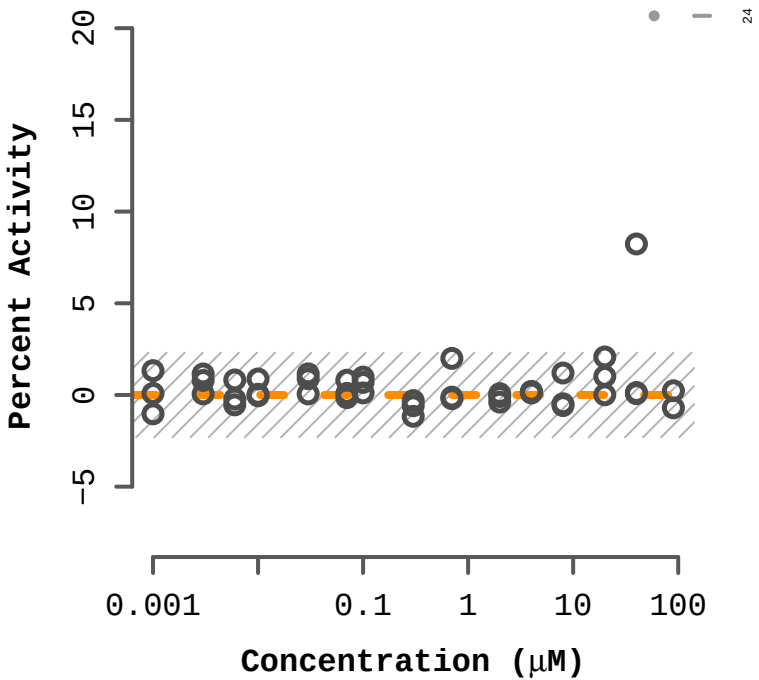
NAME: 1-Butyl-1-methylpyrrolidinium tetrafluoroborat
CHID: 49276 **CASRN:** 345984-11-4
SPID(S): Tox21_202703
M4ID: 12479549

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	225.48	NA	NA
PROB:	1	NA	NA
RMSE:	3.55	NA	NA

MAX_MEAN: 3.89 **MAX_MED:** 2.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

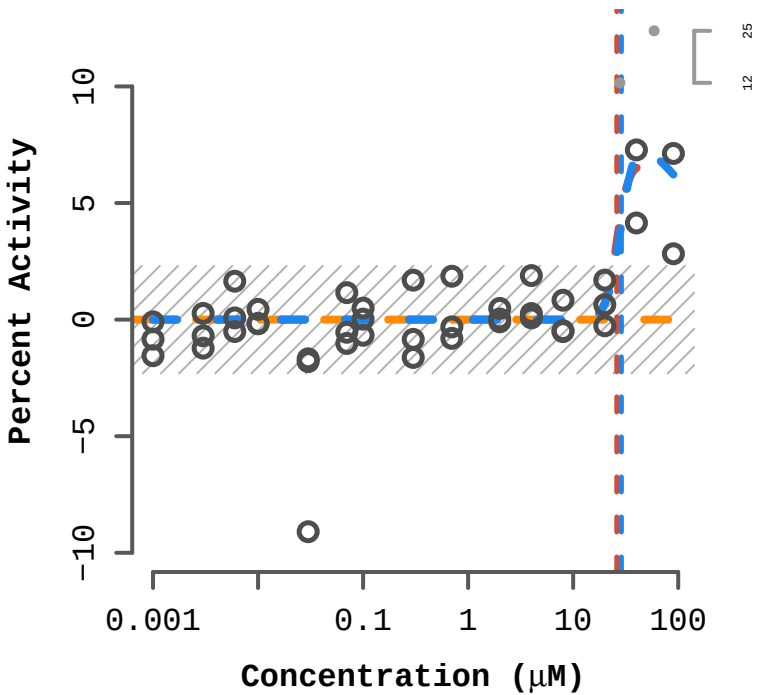
NAME: 3'-Chloropropiophenone
CHID: 49277 CASRN: 34841-35-5
SPID(S): Tox21_202823
M4ID: 12479429 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.8	NA	NA
PROB:	1	NA	NA
RMSE:	3.8	NA	NA

MAX_MEAN: 7.71 MAX_MED: 1.01 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chloro-1-fluoro-4-nitrobenzene
CHID: 49278 CASRN: 350-30-1
SPID(S): Tox21_202824
M4ID: 12479428 BRK

HILL MODEL (in red):

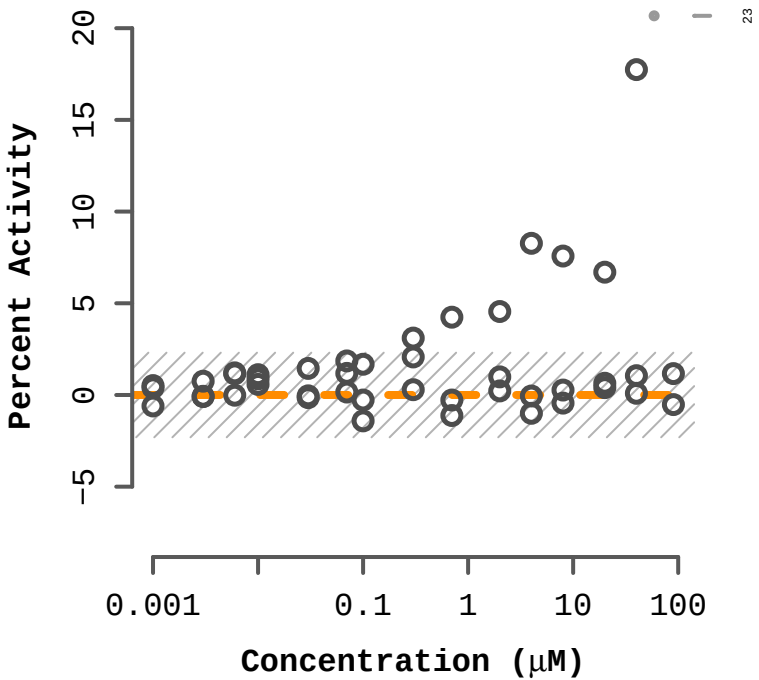
	tp	ga	gw
val:	6.71	1.42	8
sd:	0.936	0.0841	5.38

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.67	1.46	6.75	2.21	0.99
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	219.82	192.61	196.3
PROB:	0	0.86	0.14
RMSE:	4.79	3.37	3.41

MAX_MEAN: 11.7 MAX_MED: 7.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

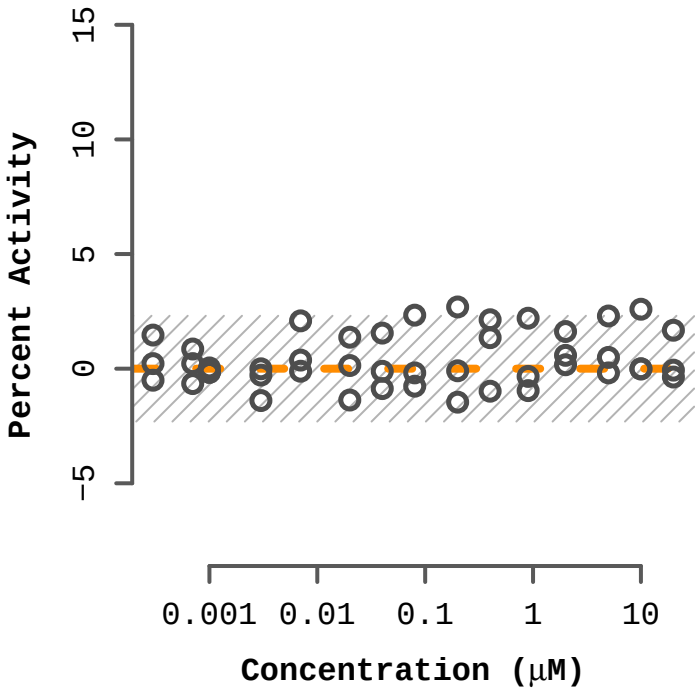
NAME: 1-Ethylpyridinium tetrafluoroborate
CHID: 49279 CASRN: 350-48-1
SPID(S): Tox21_202698
M4ID: 12479554 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	224.97	NA	NA
PROB:	1	NA	NA
RMSE:	4.96	NA	NA

MAX_MEAN: 8 MAX_MED: 2.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

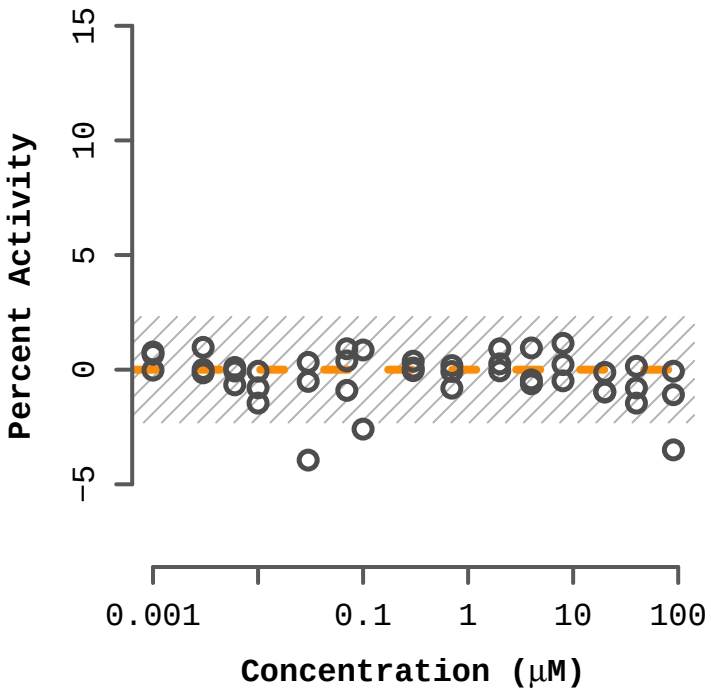
NAME: Heptadecane,1-bromo-
CHID: 49280 **CASRN:** 3508-00-7
SPID(S): Tox21_202825
M4ID: 12479427

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 0.869 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

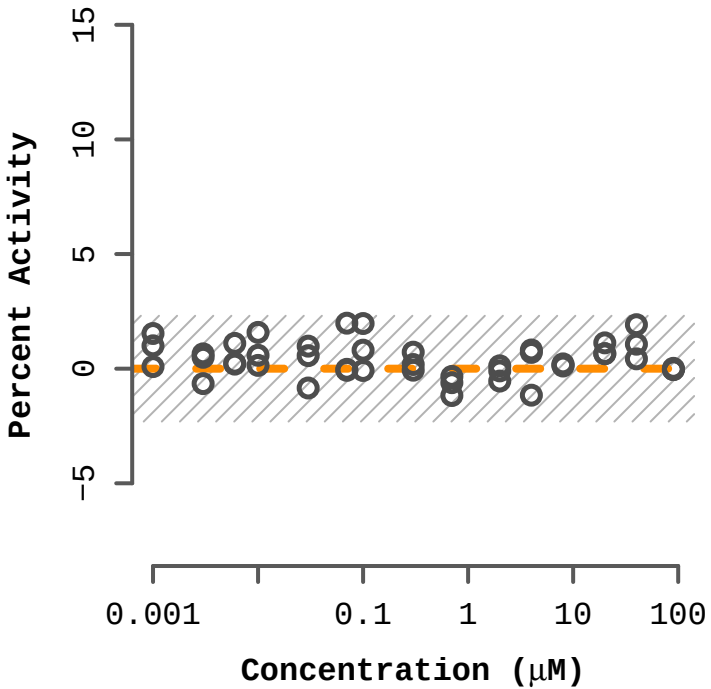
NAME: 1-Ethyl-3-methylimidazolium iodide
CHID: 49281 **CASRN:** 35935-34-3
SPID(S): Tox21_202643
M4ID: 12479609

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.473 **MAX_MED:** 0.666 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

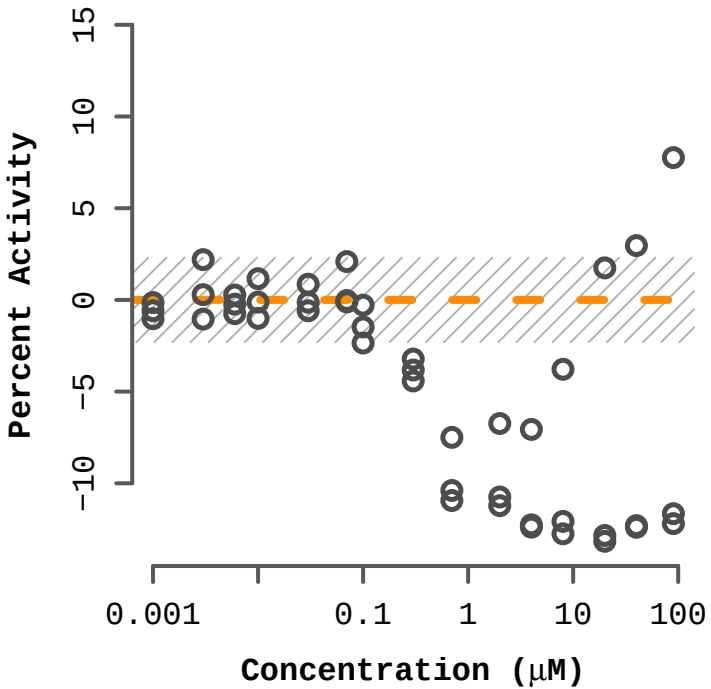
NAME: 1-Butyl-3-methylimidazolium tetrachloroferrate
CHID: 49282 **CASRN:** 359845-21-9
SPID(S): Tox21_202620
M4ID: 12479632

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

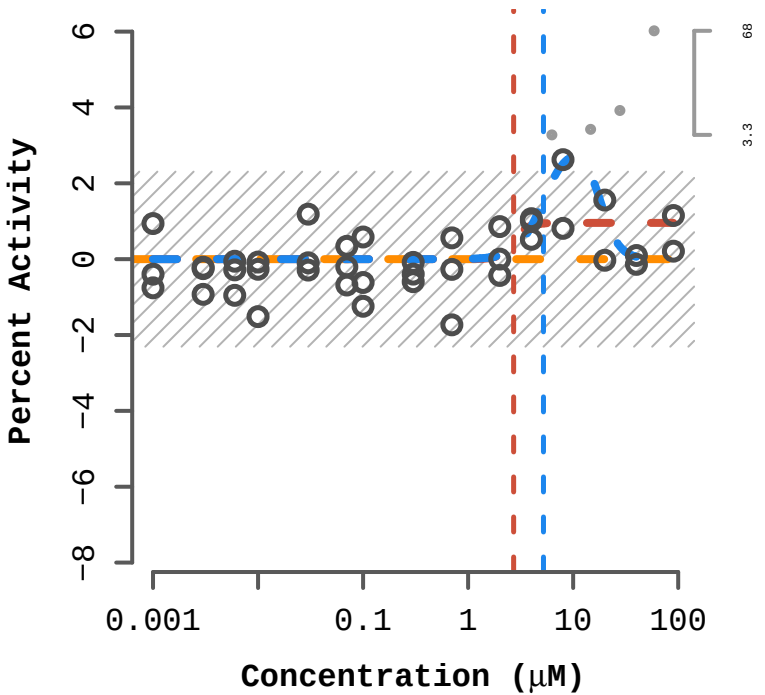
NAME: 1-Decyl-3-methylimidazolium hexafluorophosphat
CHID: 49283 **CASRN:** 362043-46-7
SPID(S): Tox21_202624
M4ID: 12479628

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	309.11	NA	NA
PROB:	1	NA	NA
RMSE:	7.17	NA	NA

MAX_MEAN: 0.649 **MAX_MED:** 0.288 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexanoylchloride,3,5,5-trimethyl-
CHID: 49284 **CASRN:** 36727-29-4
SPID(S): Tox21_202827
M4ID: 12479425 **BRK**

HILL MODEL (in red):

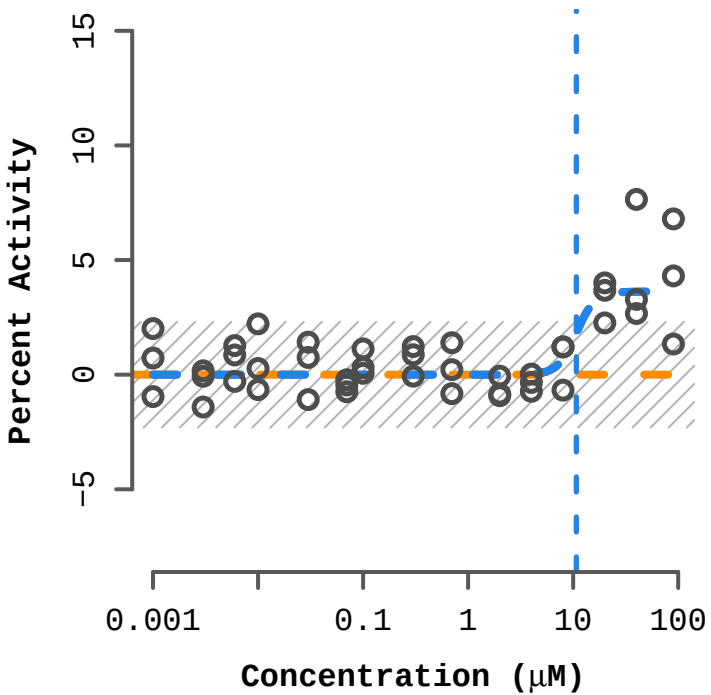
	tp	ga	gw
val:	0.956	0.433	6.5
sd:	0.36	0.315	11.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.12	0.717	3.56	1.26	4.87
sd:	4	0.438	6.49	0.284	15.3

	CNST	HILL	GNLS
AIC:	195.55	190.92	188.77
PROB:	0.02	0.25	0.73
RMSE:	10.6	10.4	10.56

MAX_MEAN: 23.1 **MAX_MED:** 2.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-1-methylpyrrolidinium trifluoromethanes
CHID: 49285 CASRN: 367522-96-1
SPID(S): Tox21_202605
M4ID: 12479647

HILL MODEL (in red):

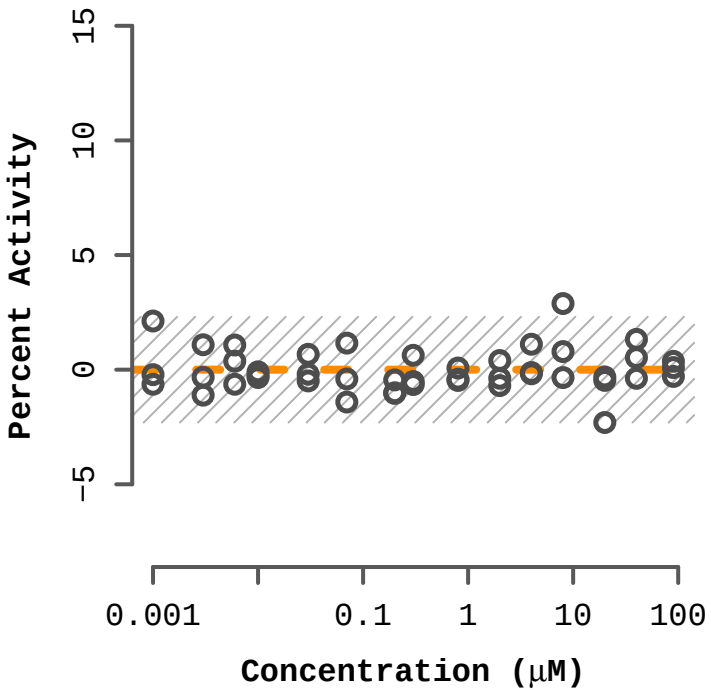
	tp	ga	gw
val:	3.62	1.03	4.94
sd:	0.82	0.268	7.72

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.62	1.03	4.94	3.2	6.67
sd:	0.819	0.268	7.72	1800	9610

	CNST	HILL	GNLS
AIC:	186.61	149.4	153.4
PROB:	0	0.88	0.12
RMSE:	2.16	1.21	1.21

MAX_MEAN: 4.53 MAX_MED: 4.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

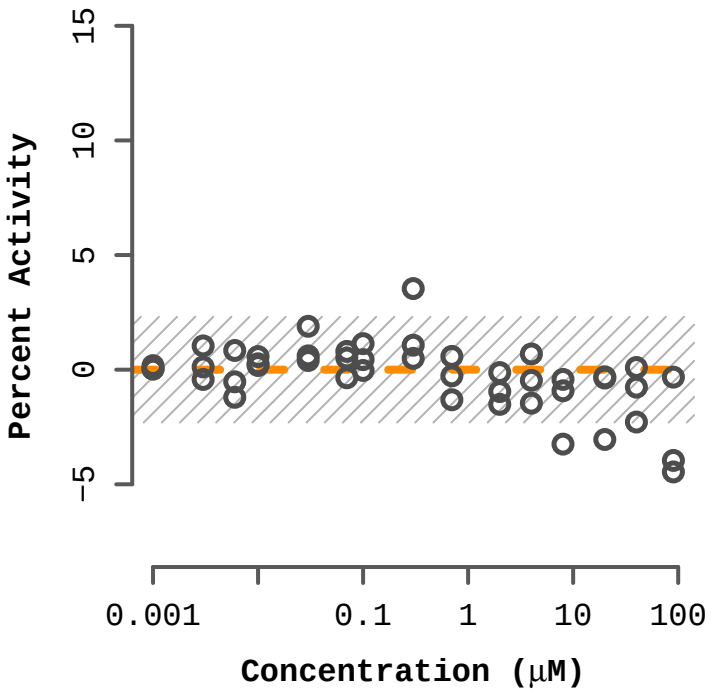
NAME: 1-(2-Hydroxyethyl)-3-methylimidazolium tetrafl
CHID: 49286 CASRN: 374564-83-7
SPID(S): Tox21_202651
M4ID: 12479601

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.11 MAX_MED: 0.791 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

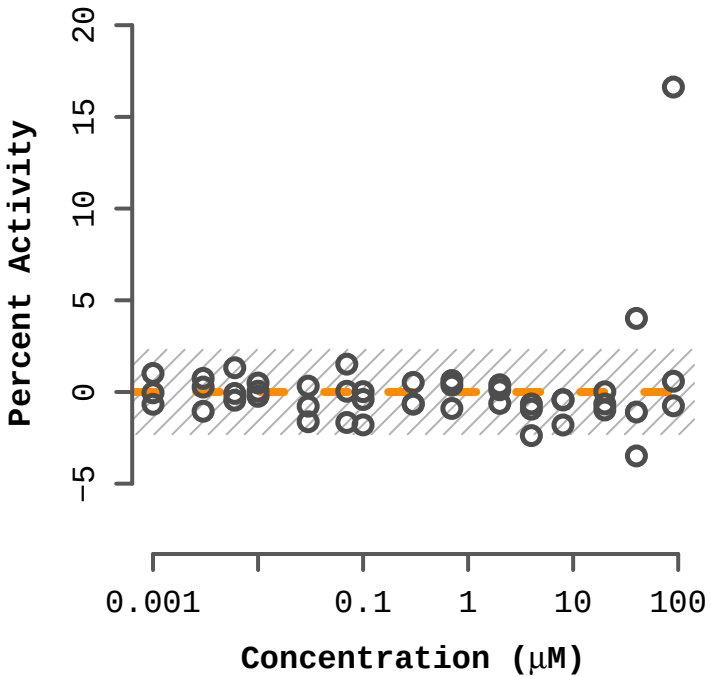
NAME: 2,4,6-Trichloropyrimidine
CHID: 49287 **CASRN:** 3764-01-0
SPID(S): Tox21_202916
M4ID: 12479336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.7 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

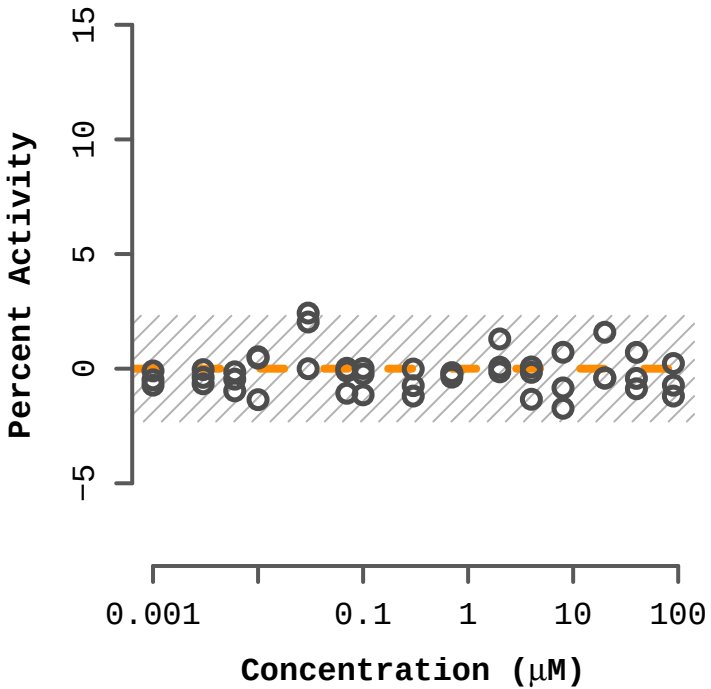
NAME: (S)−(−)−1−Amino−1−phenylpropane
CHID: 49288 CASRN: 3789−59−1
SPID(S): Tox21_202829
M4ID: 12479423

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.74	NA	NA

MAX_MEAN: 5.49 MAX_MED: 0.588 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

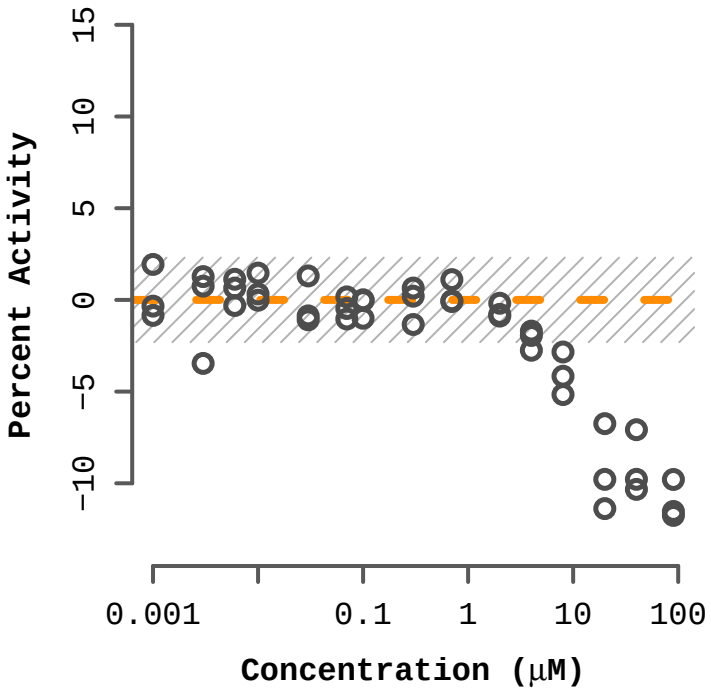
NAME: 1-Butyl-1-methylpiperidinium iodide
CHID: 49289 **CASRN:** 37971-78-1
SPID(S): Tox21_202668
M4ID: 12479584

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.32	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 2.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

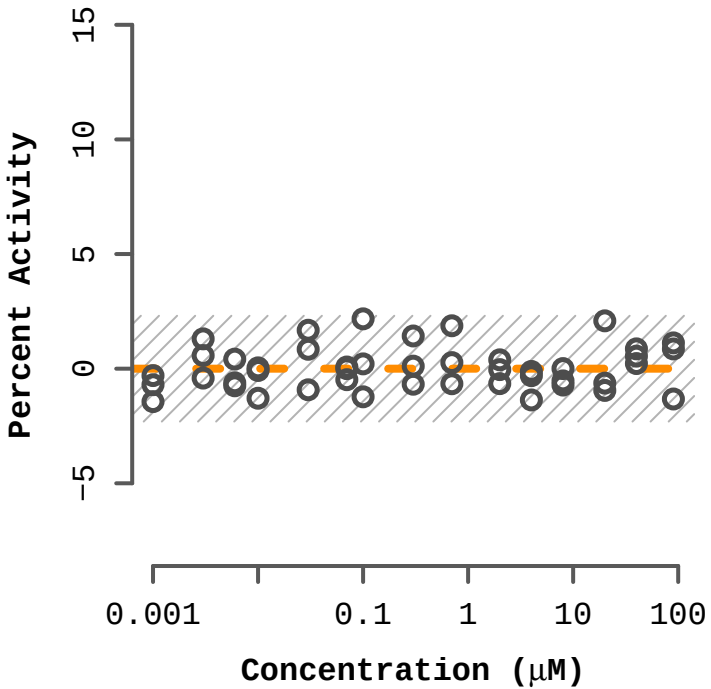
NAME: 1-Hexyl-3-methylimidazolium bis(trifluoromethy
CHID: 49290 **CASRN:** 382150-50-7
SPID(S): Tox21_202649
M4ID: 12479603

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	258.96	NA	NA
PROB:	1	NA	NA
RMSE:	4.69	NA	NA

MAX_MEAN: 0.591 **MAX_MED:** 0.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

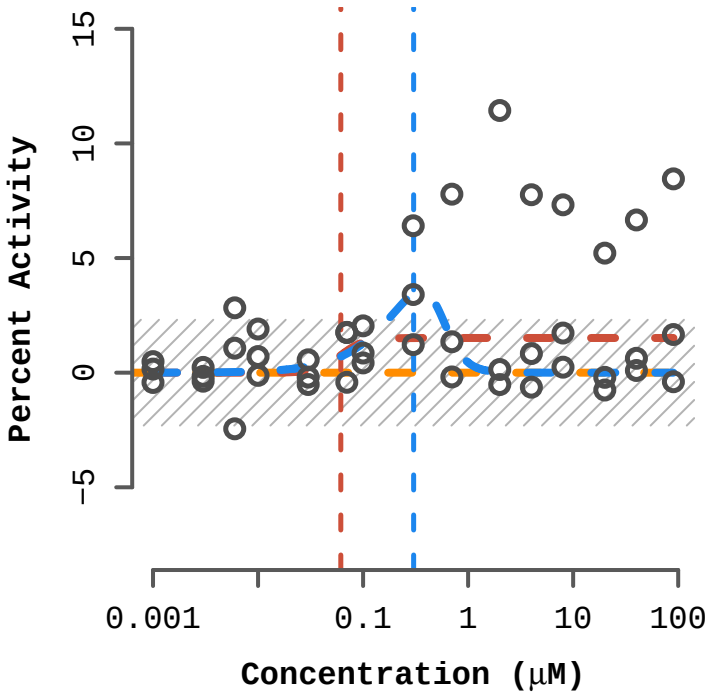
NAME: 1-Ethylpyridinium trifluoromethanesulfonate
CHID: 49291 CASRN: 3878-80-6
SPID(S): Tox21_202696
M4ID: 12479556

HILL MODEL: Not applicable.

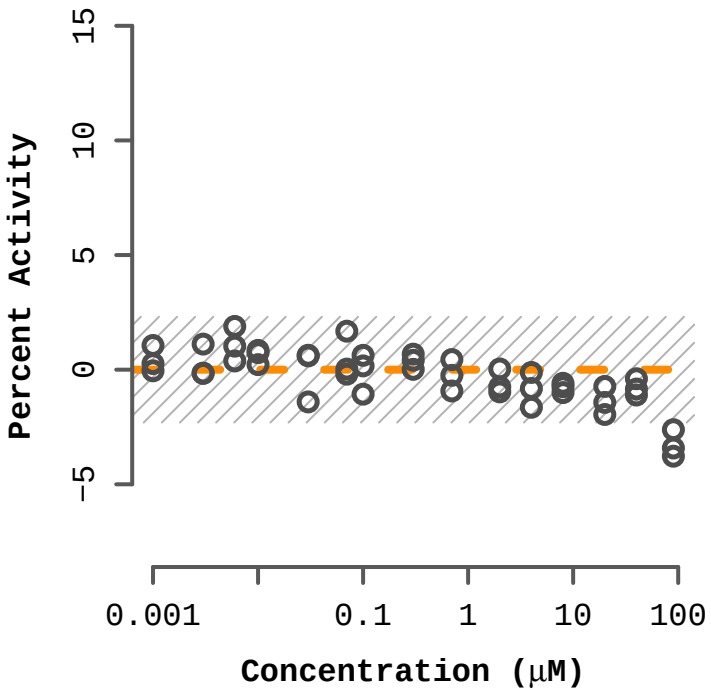
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.546 **MAX_MED:** 0.863 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butylpyridinium trifluoromethanesulfonate
CHID:    49292   CASRN: 390423-43-5
SPID(S): Tox21_202694
M4ID:    12479558

HILL MODEL (in red):
      tp       ga       gw
val:  1.51     -1.21    3.89
sd:   0.576    0.333    8.36

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.53     -0.519   1.42     -0.269   4.19
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  228.16      222.4       227.91
PROB: 0.05        0.89        0.06
RMSE: 3.48        2.91        3.26

MAX_MEAN: 3.69      MAX_MED: 3.41      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

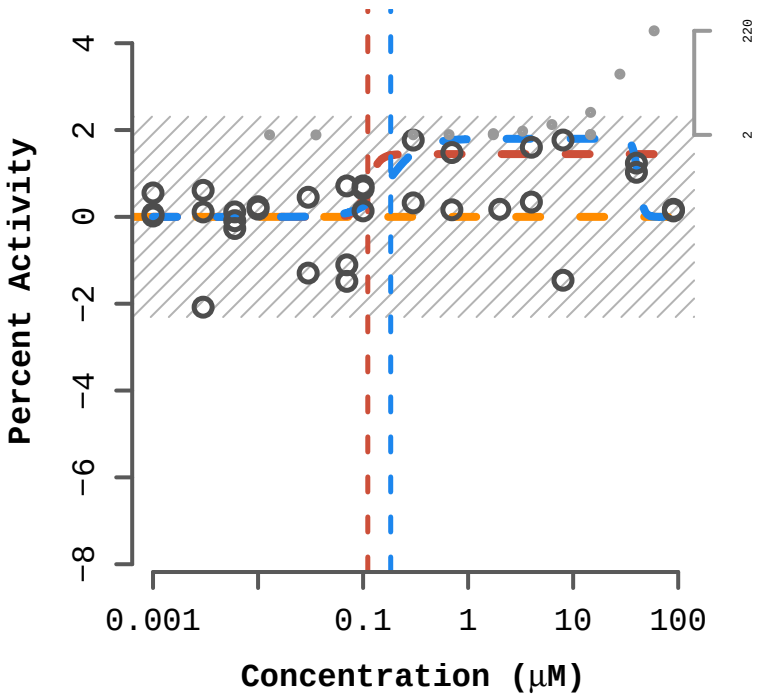
NAME: Pyrimidine,2,4-dichloro-
CHID: 49293 CASRN: 3934-20-1
SPID(S): Tox21_202830
M4ID: 12479422

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.1 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethylpivalate
CHID: 49294 CASRN: 3938-95-2
SPID(S): Tox21_202831
M4ID: 12479421 BRK

HILL MODEL (in red):

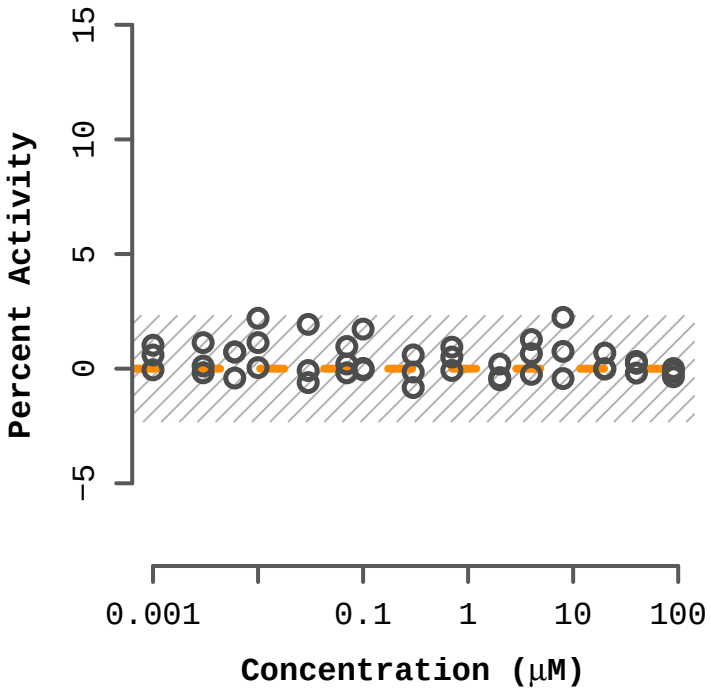
	tp	ga	gw
val:	1.45	−0.955	8
sd:	0.369	0.205	17.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.8	−0.737	3.05	1.62	16.7
sd:	0.541	0.433	4.44	0.0996	105

	CNST	HILL	GNLS
AIC:	302.61	295.58	297.4
PROB:	0.02	0.7	0.28
RMSE:	38.88	38.52	38.7

MAX_MEAN: 73.3 MAX_MED: 2.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

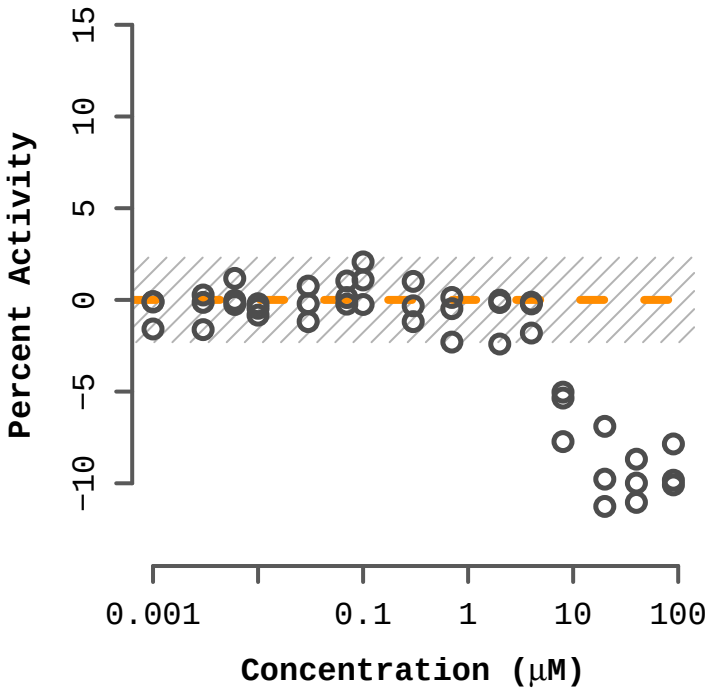
NAME: (E)−3−(2−Furyl)acrolein
CHID: 49295 **CASRN:** 39511−08−5
SPID(S): Tox21_202896
M4ID: 12479356

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.06	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

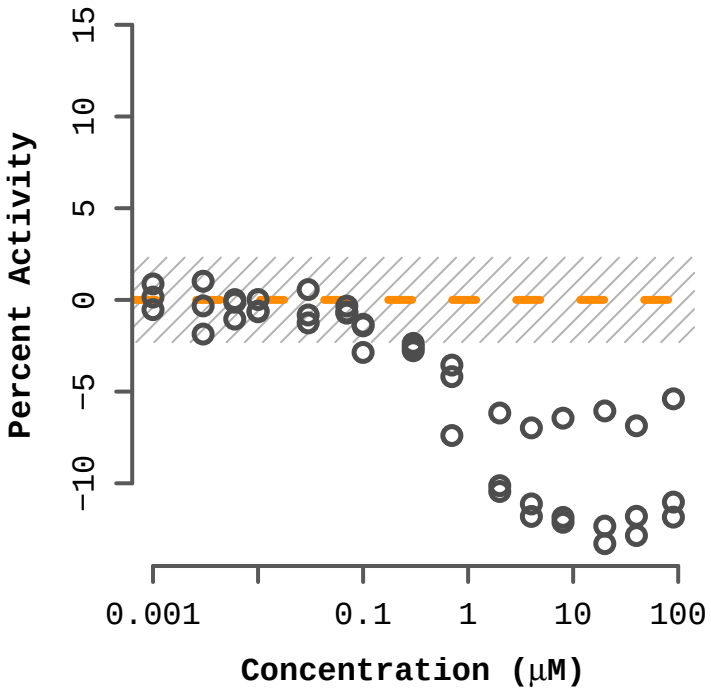
NAME: 1-Butyl-4-methylpyridinium hexafluorophosphate
CHID: 49296 **CASRN:** 401788-99-6
SPID(S): Tox21_202687
M4ID: 12479565

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	260.12	NA	NA
PROB:	1	NA	NA
RMSE:	4.65	NA	NA

MAX_MEAN: 0.972 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

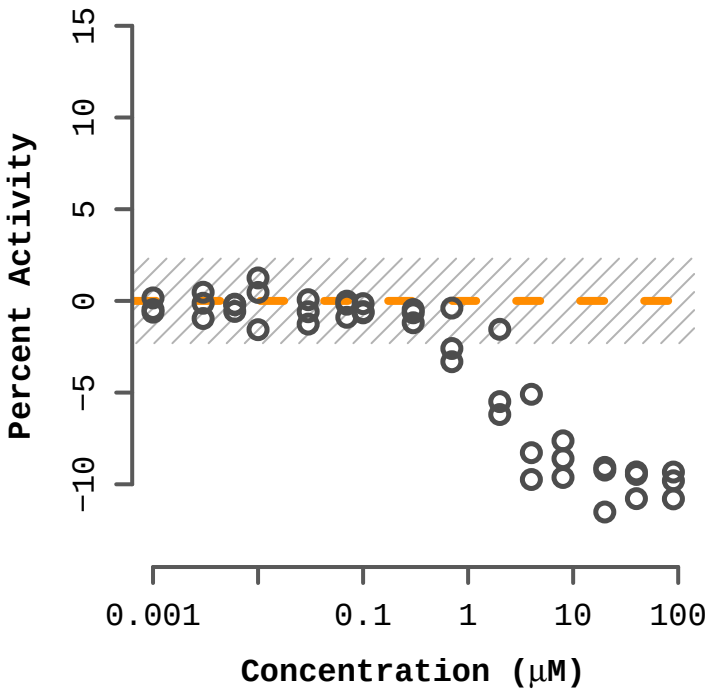
NAME: 1-Methyl-3-tetradecylimidazolium bis(trifluoro
CHID: 49297 **CASRN:** 404001-49-6
SPID(S): Tox21_202658
M4ID: 12479594

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	302.51	NA	NA
PROB:	1	NA	NA
RMSE:	6.71	NA	NA

MAX_MEAN: 0.167 **MAX_MED:** 0.156 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

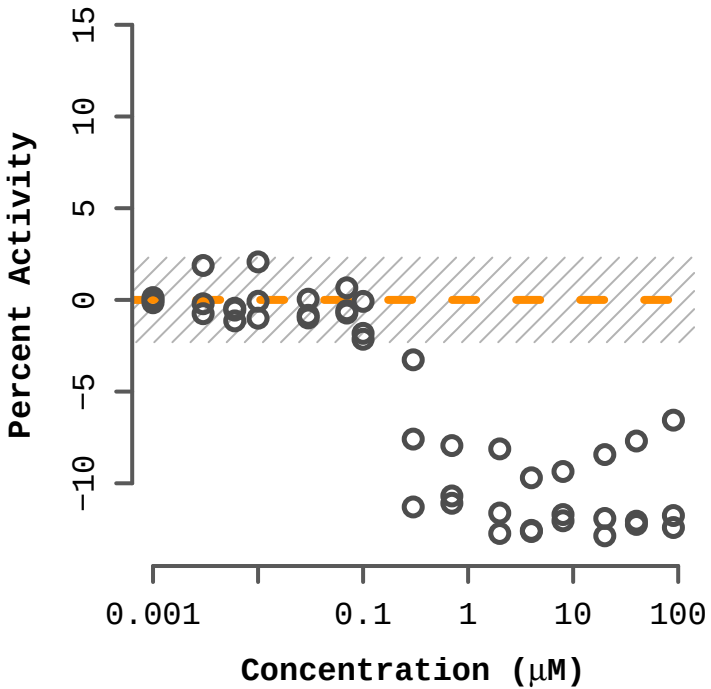
NAME: 1-Hexadecyl-3-methylimidazolium bis(trifluorom
CHID: 49298 **CASRN:** 404001-50-9
SPID(S): Tox21_202648
M4ID: 12479604

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	284.84	NA	NA
PROB:	1	NA	NA
RMSE:	5.59	NA	NA

MAX_MEAN: 0.05 **MAX_MED:** 0.464 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

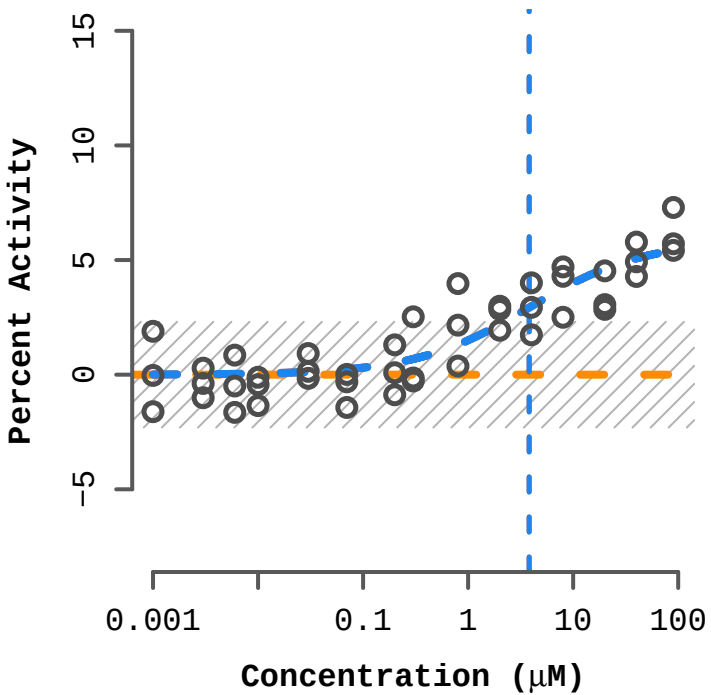
NAME: 1-Dodecyl-3-methylimidazolium trifluoromethanes
CHID: 49299 **CASRN:** 404001-52-1
SPID(S): Tox21_202630
M4ID: 12479622

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	319.11	NA	NA
PROB:	1	NA	NA
RMSE:	7.79	NA	NA

MAX_MEAN: 0.336 **MAX_MED:** −0.00224 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Ethyl-3-methylimidazolium hydrogen sulfate
CHID: 49300 CASRN: 412009-61-1
SPID(S): Tox21_202642
M4ID: 12479610

HILL MODEL (in red):

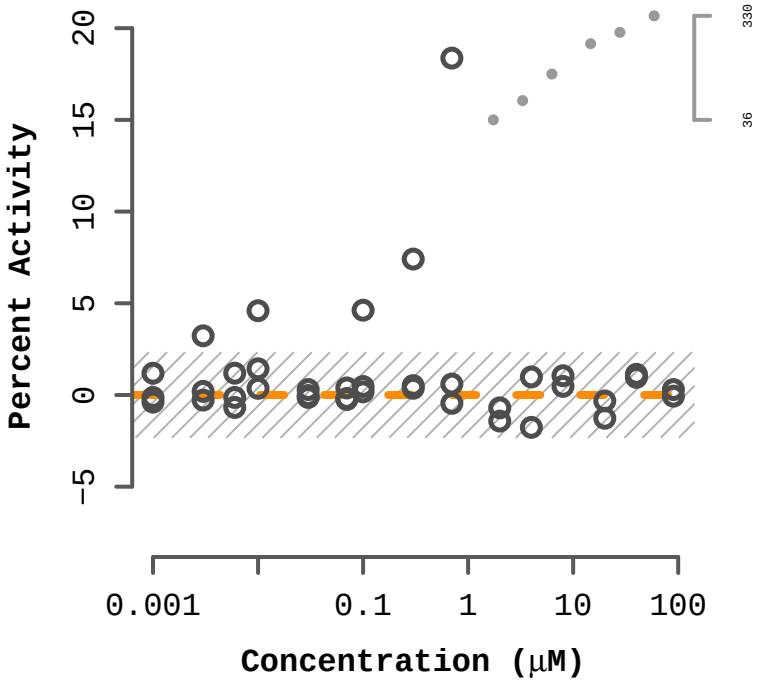
	tp	ga	gw
val:	5.85	0.581	0.795
sd:	1.06	0.326	0.251

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.85	0.581	0.795	3.6	5.78
sd:	1.06	0.326	0.251	4640	16300

	CNST	HILL	GNLS
AIC:	225.83	144.56	148.56
PROB:	0	0.88	0.12
RMSE:	2.87	1.06	1.06

MAX_MEAN: 6.14 MAX_MED: 5.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

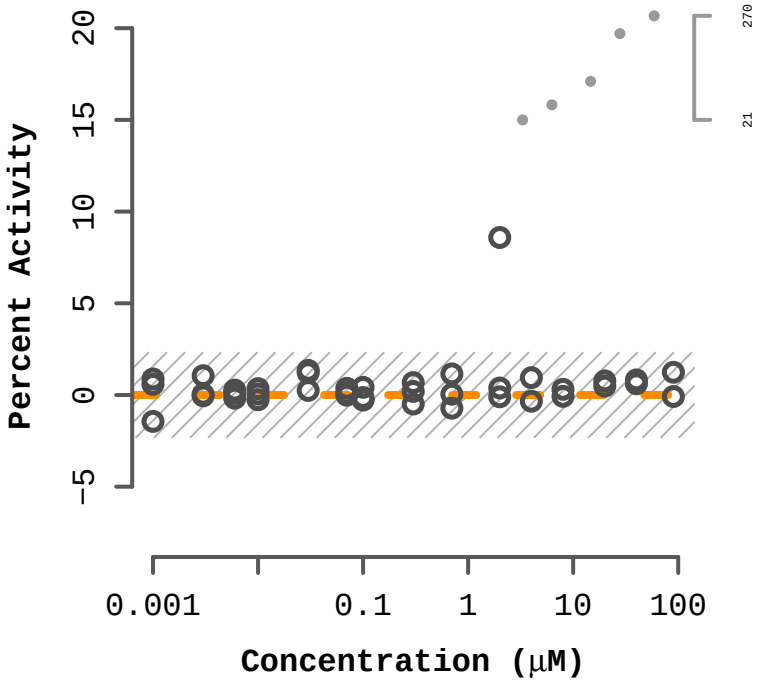
NAME: Nonane,1-iodo-
CHID: 49301 **CASRN:** 4282-42-2
SPID(S): Tox21_202833
M4ID: 12479419 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	408.83	NA	NA
PROB:	1	NA	NA
RMSE:	80.85	NA	NA

MAX_MEAN: 111 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

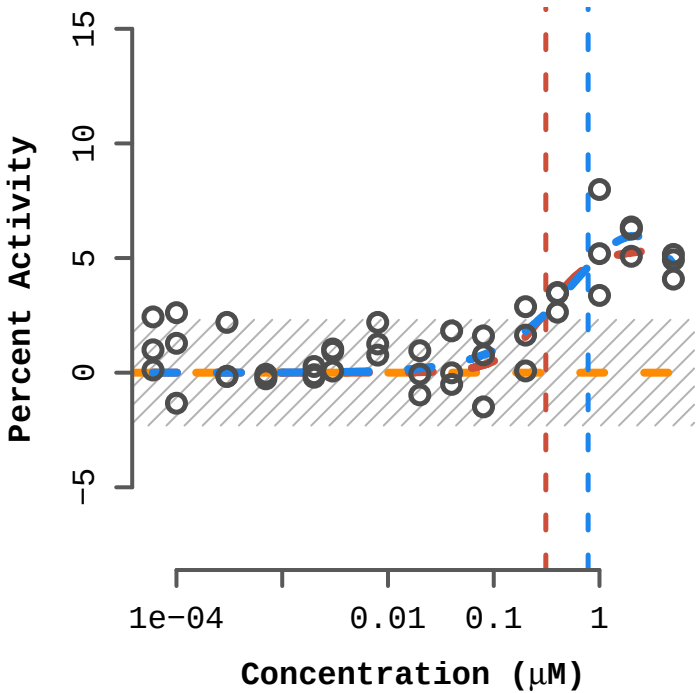
NAME: Dodecane,1-iodo-
CHID: 49302 **CASRN:** 4292-19-7
SPID(S): Tox21_202834
M4ID: 12479418 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	316.35	NA	NA
PROB:	1	NA	NA
RMSE:	55.84	NA	NA

MAX_MEAN: 90 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Dimethylamino−4−nitrostilbene
CHID: 49303 CASRN: 4584−57−0
SPID(S): Tox21_202918
M4ID: 12479334

HILL MODEL (in red):

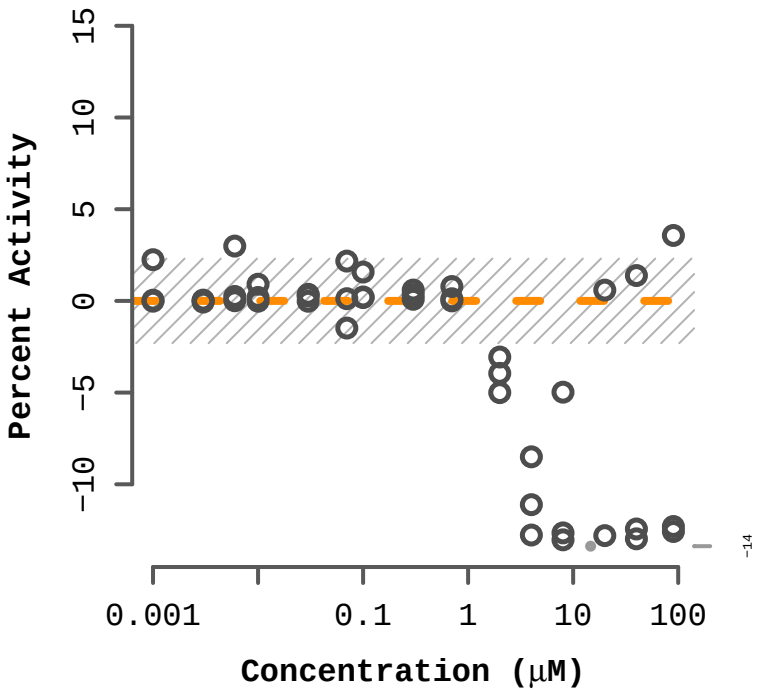
	tp	ga	gw
val:	5.36	−0.508	2
sd:	0.447	0.0875	0.853

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.59	−0.108	1.06	0.767	1.61
sd:	16.3	1.19	0.812	0.649	2.98

	CNST	HILL	GNLS
AIC:	220.75	151	151.42
PROB:	0	0.55	0.45
RMSE:	2.83	1.18	1.15

MAX_MEAN: 5.9 **MAX_MED:** 6.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

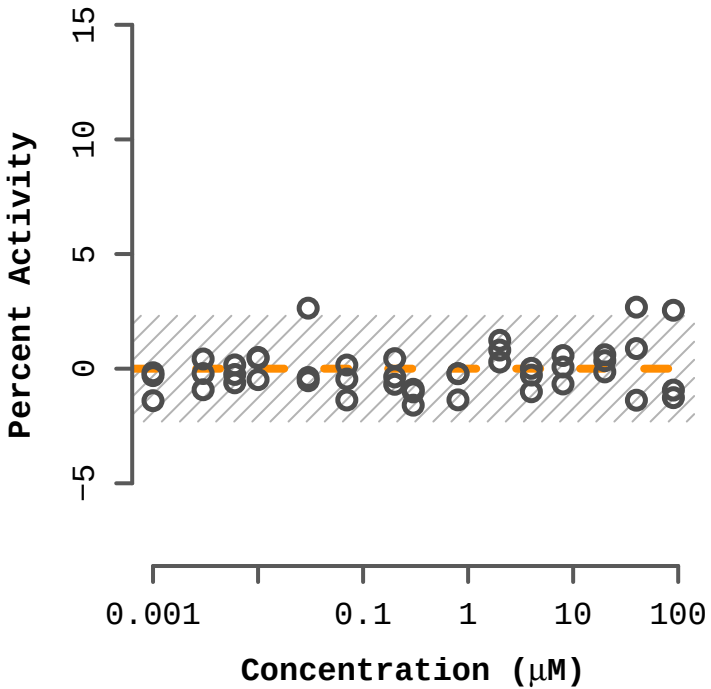
NAME: Trihexyltetradecylphosphonium bis(trifluoromet
CHID: 49304 CASRN: 460092-03-9
SPID(S): Tox21_202614
M4ID: 12479638 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	289.44	NA	NA
PROB:	1	NA	NA
RMSE:	6.31	NA	NA

MAX_MEAN: 1.08 MAX_MED: 0.338 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

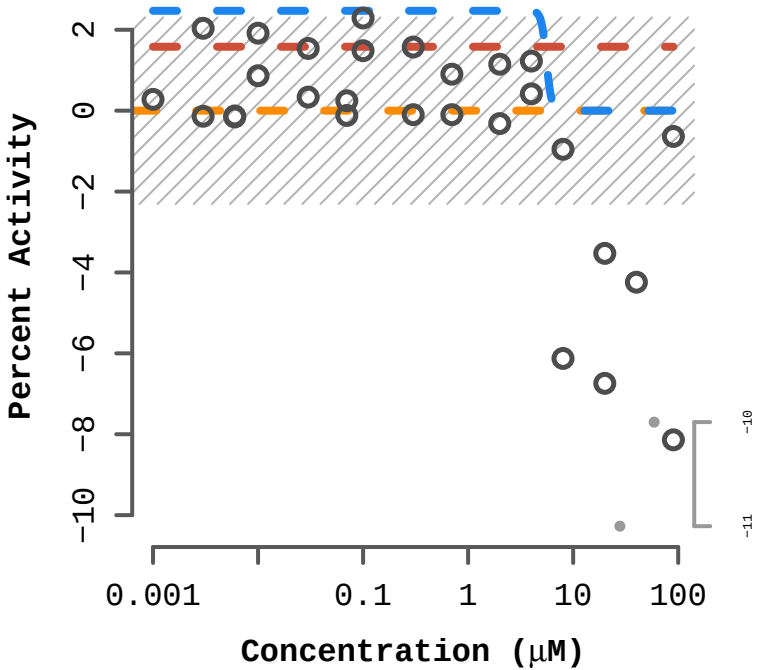
NAME: 1-Hexylpyridinium tetrafluoroborate
CHID: 49305 **CASRN:** 474368-70-2
SPID(S): Tox21_202700
M4ID: 12479552

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,4−Dichlorophthalazine
CHID: 49306 CASRN: 4752−10−7
SPID(S): Tox21_202959
M4ID: 12479293 BRK

HILL MODEL (in red):

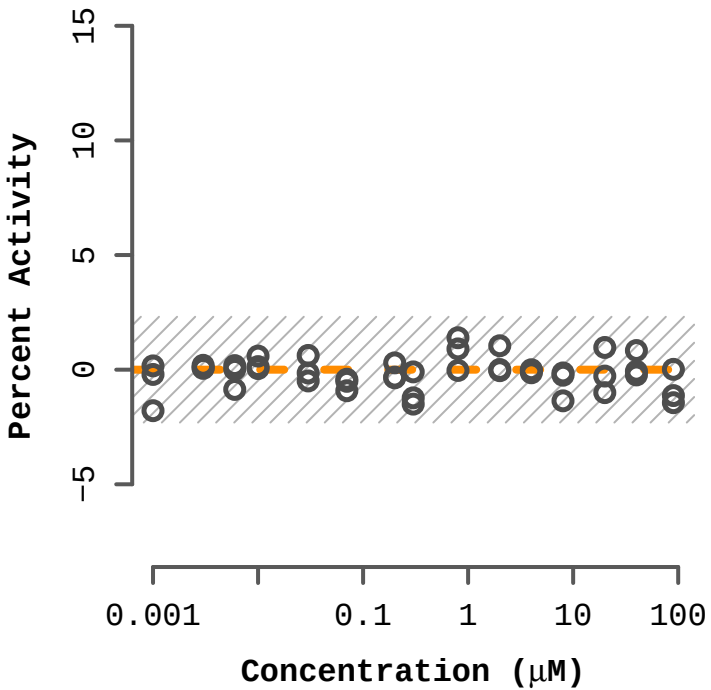
	tp	ga	gw
val:	1.58	−4.72	4.25
sd:	0.721	1600	3960

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.47	−4.58	7.84	0.746	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	286.03	287.36	285.29
PROB:	0.34	0.17	0.49
RMSE:	5.69	5.43	5.02

MAX_MEAN: 5.07 MAX_MED: 6.09 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

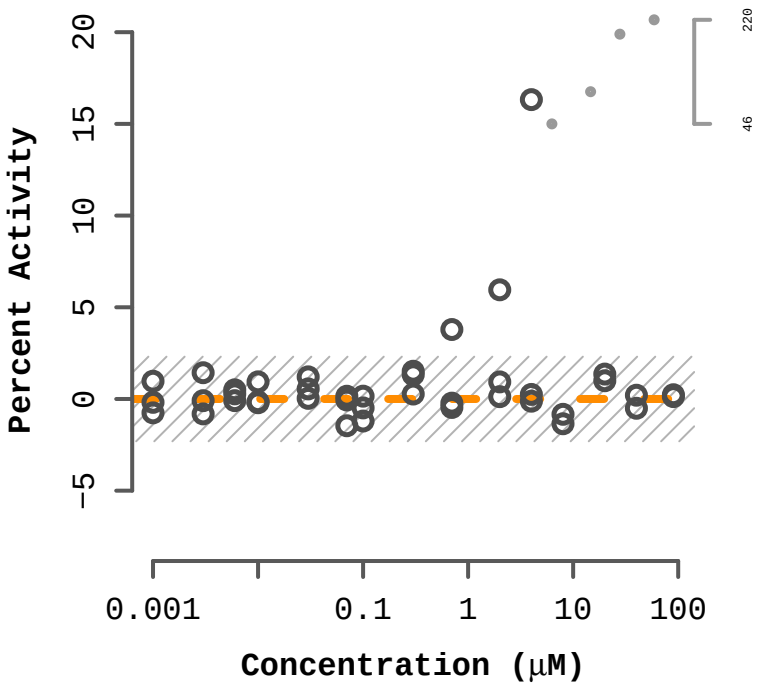
NAME: 9-Fluorenone
CHID: 49307 CASRN: 486-25-9
SPID(S): Tox21_202919
M4ID: 12479333

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.757 MAX_MED: 0.907 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

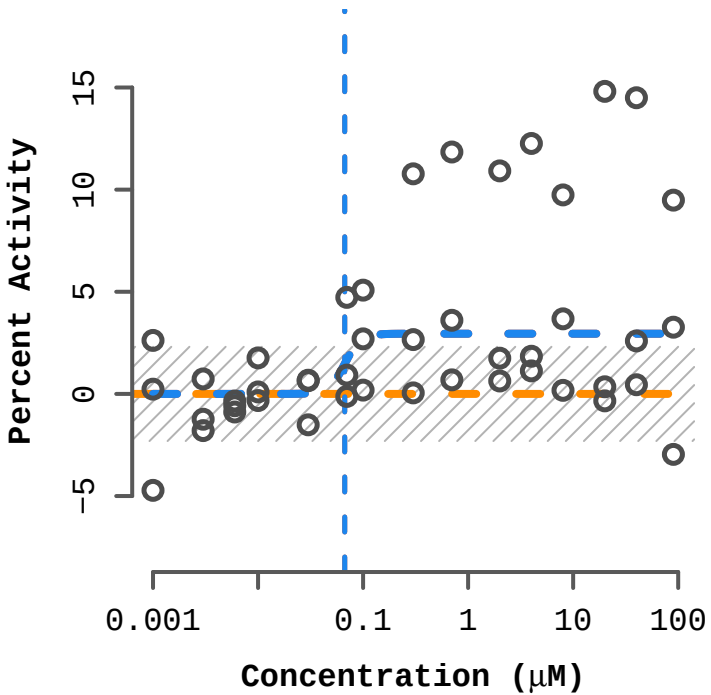
NAME: 2-Methyl-2-butenal
CHID: 49308 **CASRN:** 497-03-0
SPID(S): Tox21_202837
M4ID: 12479415 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	315.52	NA	NA
PROB:	1	NA	NA
RMSE:	47.77	NA	NA

MAX_MEAN: 74.8 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: p-N,N-Dimethylaminophenethanol
CHID: 49309 CASRN: 50438-75-0
SPID(S): Tox21_202921
M4ID: 12479331

HILL MODEL (in red):

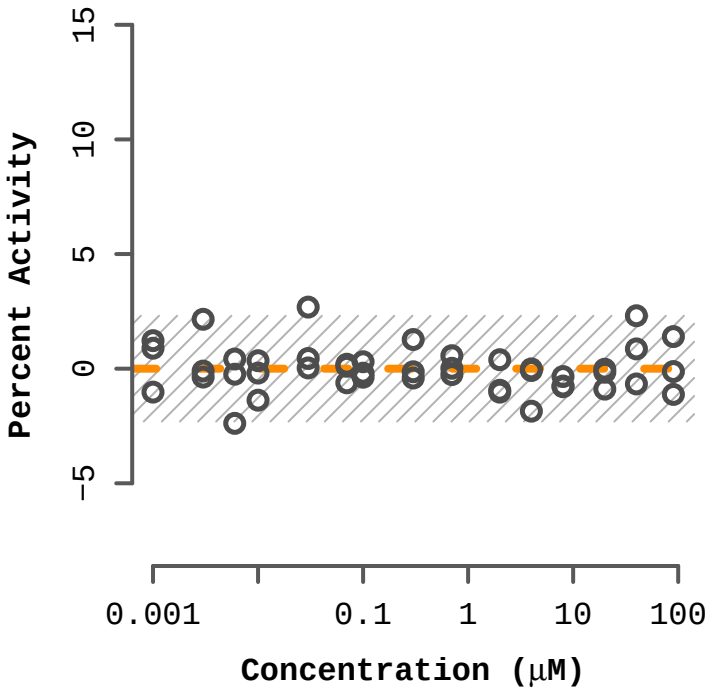
	tp	ga	gw
val:	2.95	-1.17	5.8
sd:	0.854	0.205	19.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.95	-1.17	5.8	2.88	7.51
sd:	0.854	0.205	19.9	1350	11000

	CNST	HILL	GNLS
AIC:	271.35	259.76	263.76
PROB:	0	0.88	0.12
RMSE:	5.39	4.25	4.25

MAX_MEAN: 5.85 MAX_MED: 3.68 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

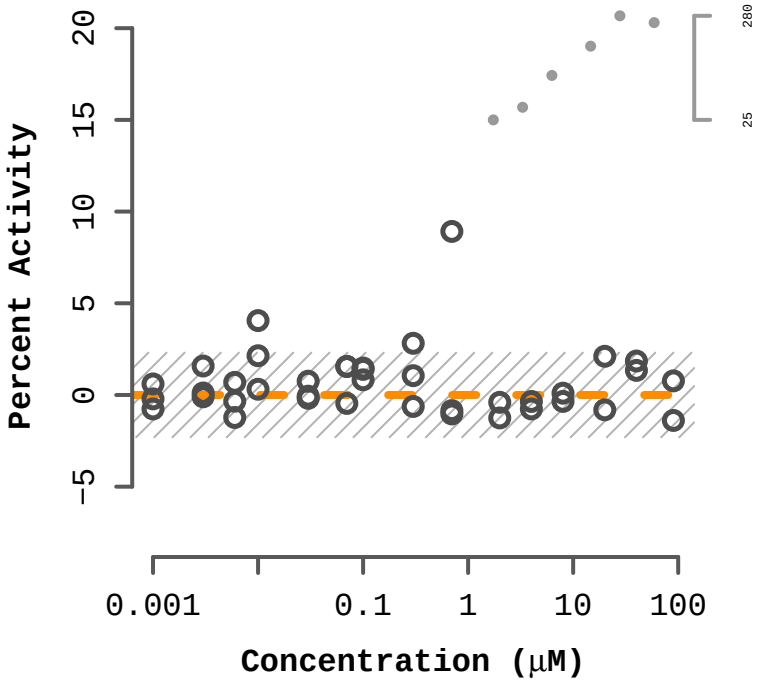
NAME: 1-Ethyl-3-methylimidazolium methyl sulfate
CHID: 49310 **CASRN:** 516474-01-4
SPID(S): Tox21_202641
M4ID: 12479611

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.95	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.893 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

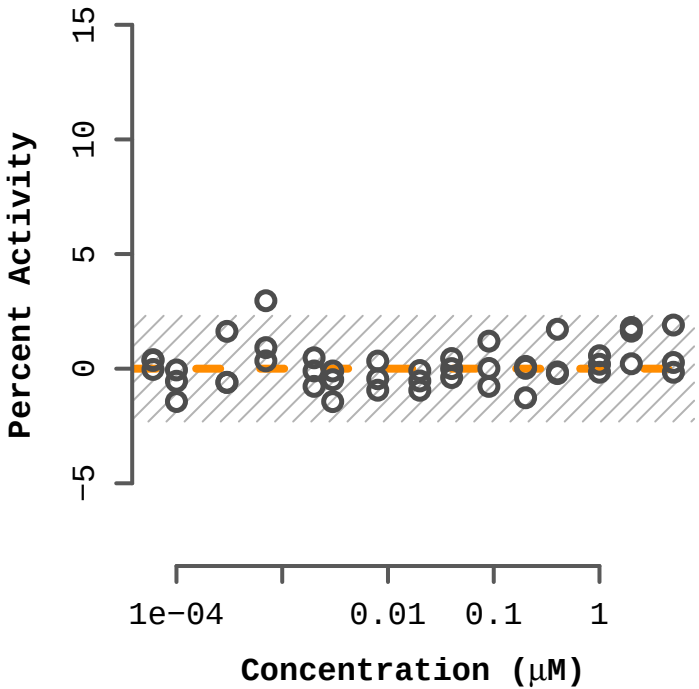
NAME: Benzoicacid,4-iodo-,ethylester
CHID: 49311 **CASRN:** 51934-41-9
SPID(S): Tox21_202840
M4ID: 12479412 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	381.4	NA	NA
PROB:	1	NA	NA
RMSE:	68.39	NA	NA

MAX_MEAN: 94.1 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

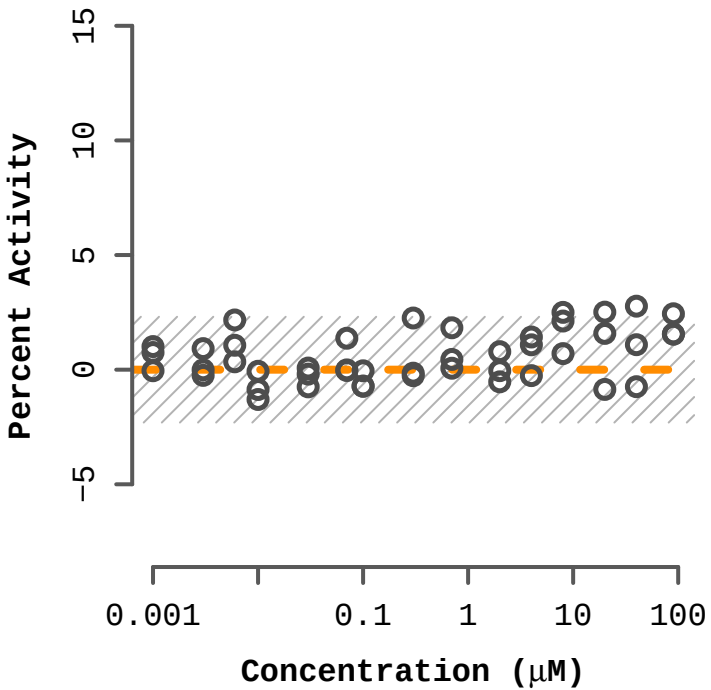
NAME: 9,10-Dibromoanthracene
CHID: 49312 **CASRN:** 523-27-3
SPID(S): Tox21_202923
M4ID: 12479329

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.64 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

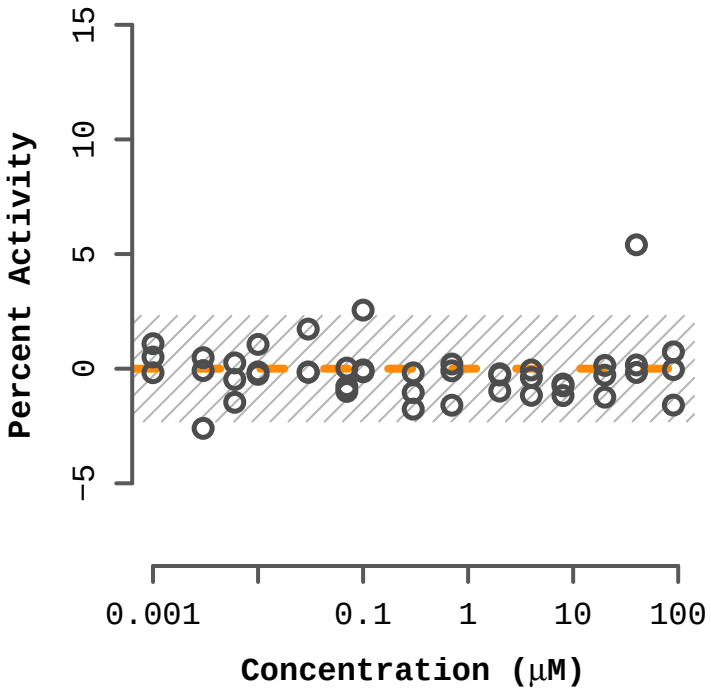
NAME: 4H-3,1-Benzoxazin-4-one,2-methyl-
CHID: 49313 CASRN: 525-76-8
SPID(S): Tox21_202841
M4ID: 12479411

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.85 MAX_MED: 2.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

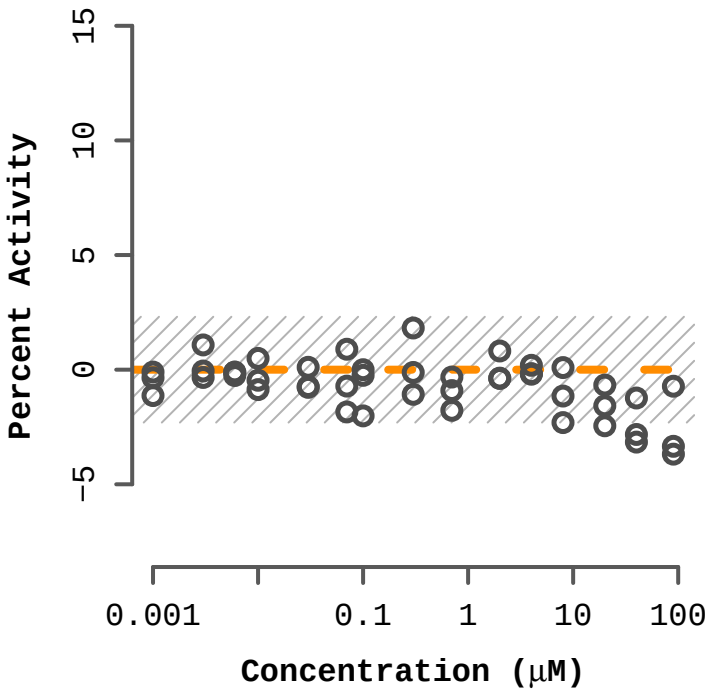
NAME: 1-Methyl-1-propylpyrrolidinium chloride
CHID: 49314 **CASRN:** 528818-82-8
SPID(S): Tox21_202708
M4ID: 12479544

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 0.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

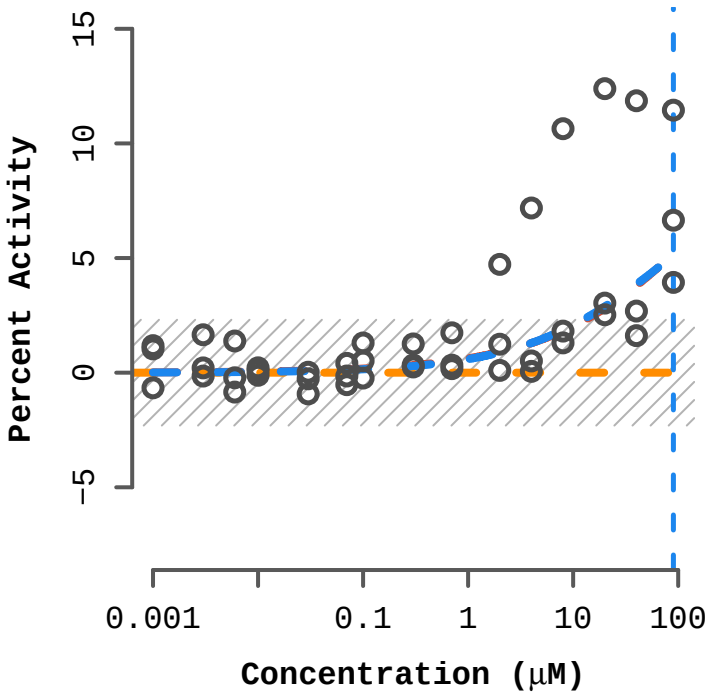
NAME: 1,2−Benzenediamine,N−phenyl−
CHID: 49315 **CASRN:** 534−85−0
SPID(S): Tox21_202842
M4ID: 12479410

HILL MODEL: Not applicable.

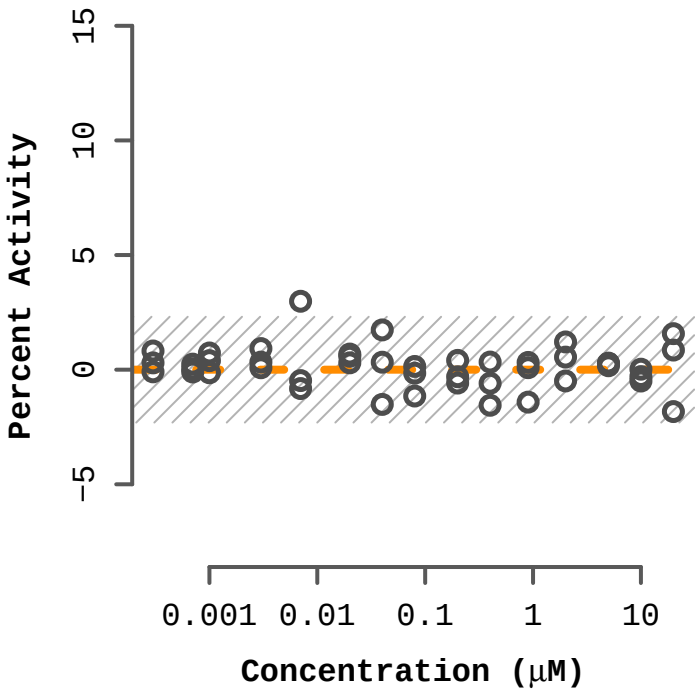
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 0.229 **MAX_MED:** −0.0563 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    5-Nitroindazole
CHID:    49316   CASRN: 5401-94-5
SPID(S): Tox21_202925
M4ID:    12479327

HILL MODEL (in red):
      tp       ga       gw
val:  14.9     2.44     0.558
sd:   16.3     1.34     0.191

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  10.2     1.95     0.621    3.62     4.65
sd:   10.3     1.2      0.23     1050     2950

      CNST        HILL        GNLS
AIC:  232.39      199.44      203.79
PROB: 0           0.9         0.1
RMSE: 4           2.79        2.78

MAX_MEAN: 7.35      MAX_MED: 6.65      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

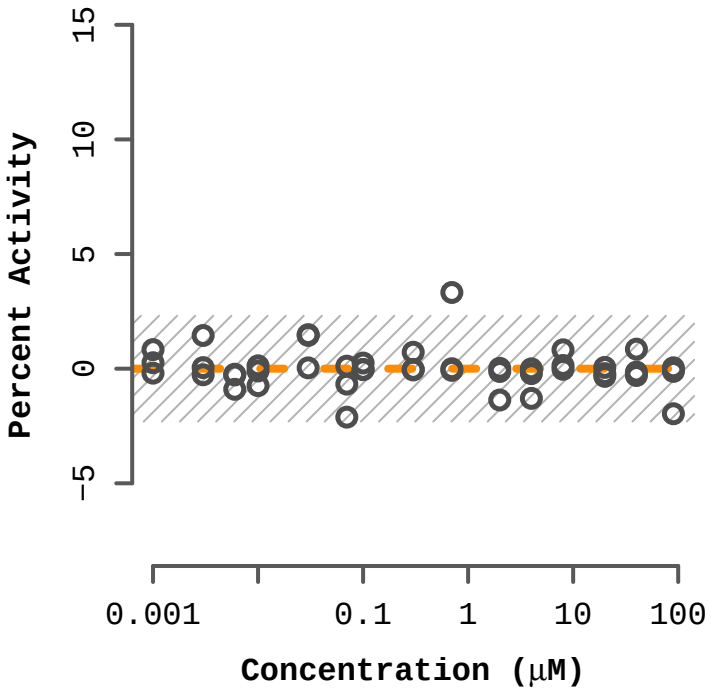
NAME: 1-iodohexadecane
CHID: 49317 **CASRN:** 544-77-4
SPID(S): Tox21_202845
M4ID: 12479407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.91	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.563 **MAX_MED:** 0.857 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

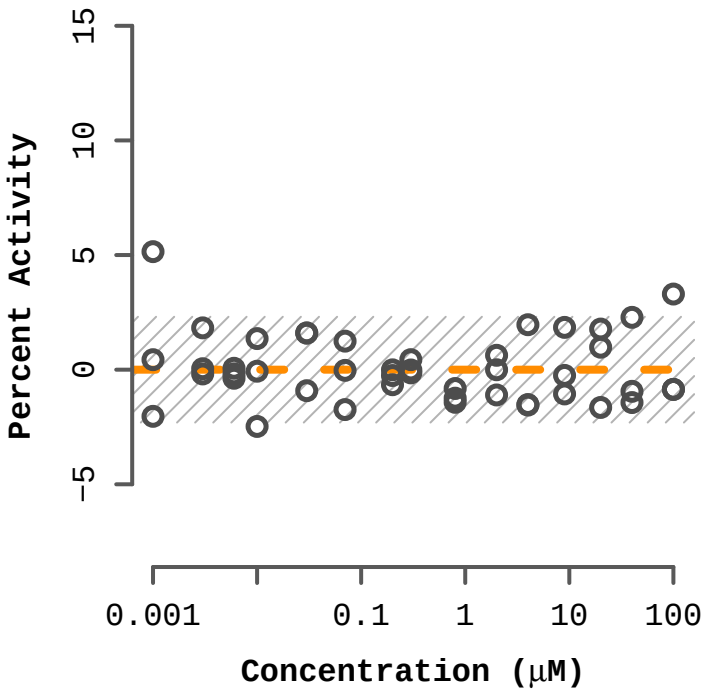
NAME: 9-Methylguanine
CHID: 49318 **CASRN:** 5502-78-3
SPID(S): Tox21_202928
M4ID: 12479324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

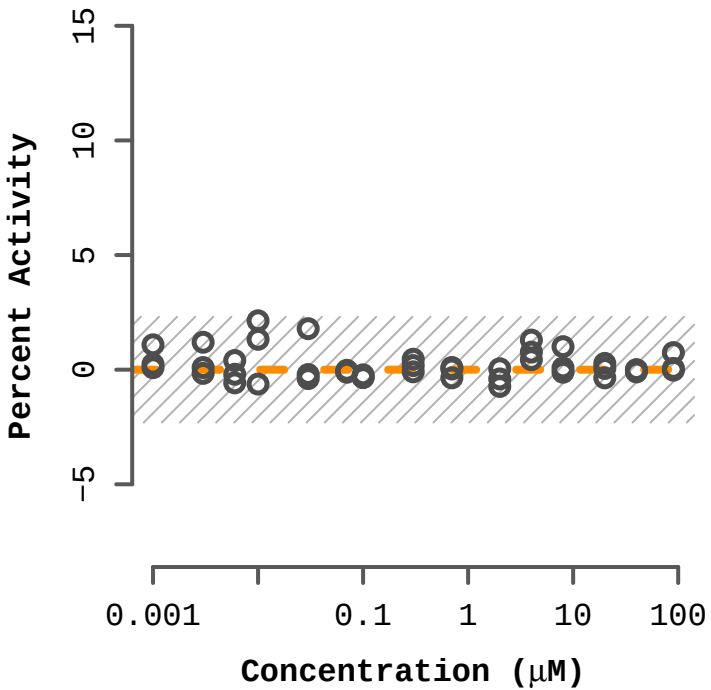
NAME: Pentane,3,3-dimethyl-
CHID: 49319 **CASRN:** 562-49-2
SPID(S): Tox21_202848
M4ID: 12479404

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.51	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

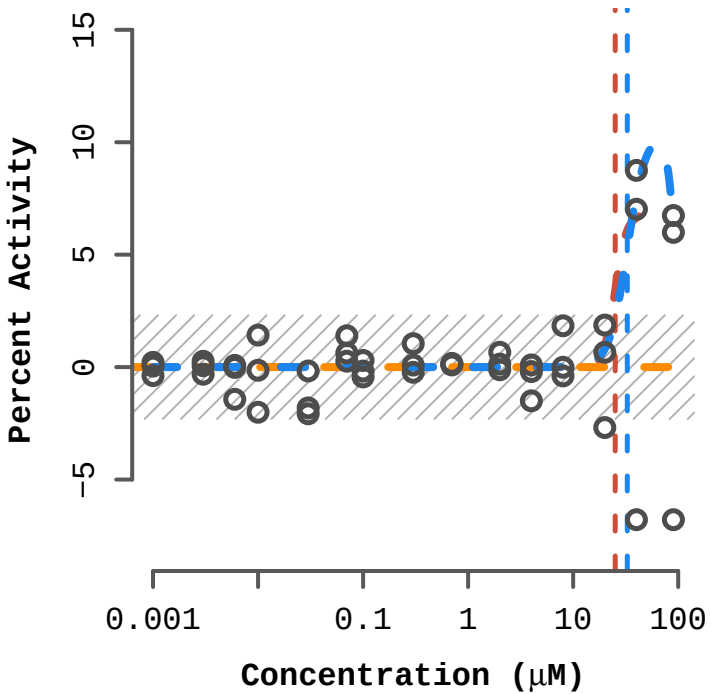
NAME: 1−Methyl−1−propylpyrrolidinium iodide
CHID: 49320 **CASRN:** 56511−19−4
SPID(S): Tox21_202710
M4ID: 12479542

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	82.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.944 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 9−Bromophenanthrene
CHID: 49321 CASRN: 573−17−1
SPID(S): Tox21_202933
M4ID: 12479319

HILL MODEL (in red):

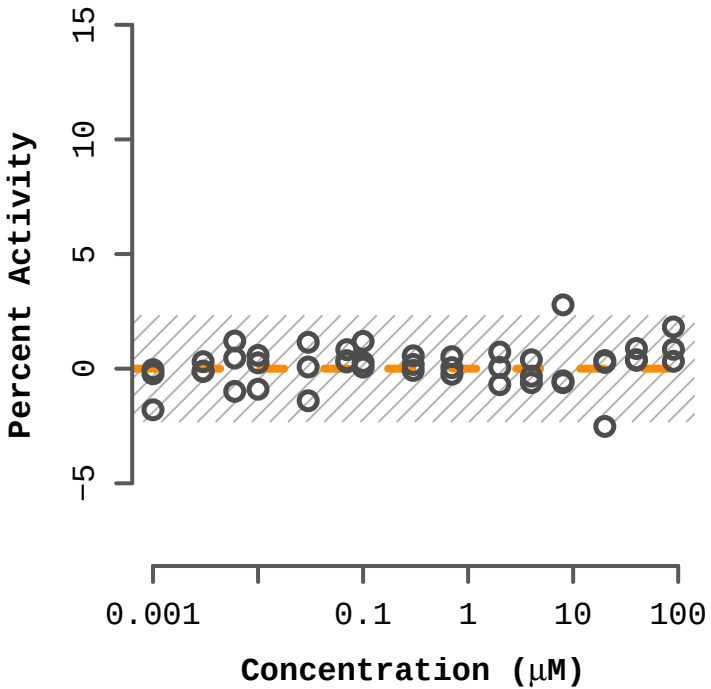
	tp	ga	gw
val:	6.81	1.4	8
sd:	0.502	0.0442	2.89

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.52	5.02	1.97	10.8
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	199.37	171.41	172.43
PROB:	0	0.62	0.38
RMSE:	2.74	3.02	3.06

MAX_MEAN: 3 MAX_MED: 7.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

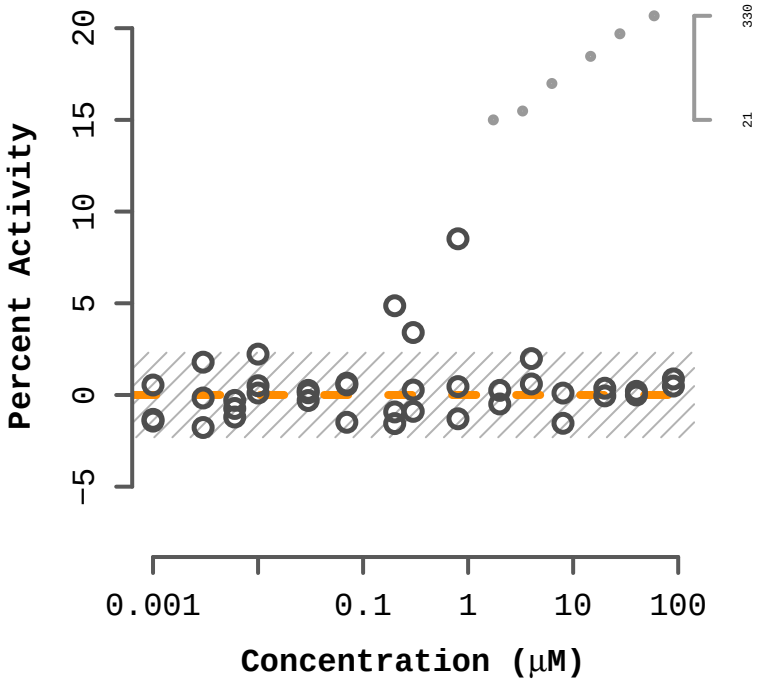
NAME: Benzene,(2-bromoethoxy)-
CHID: 49322 **CASRN:** 589-10-6
SPID(S): Tox21_202849
M4ID: 12479403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 0.996 **MAX_MED:** 0.846 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

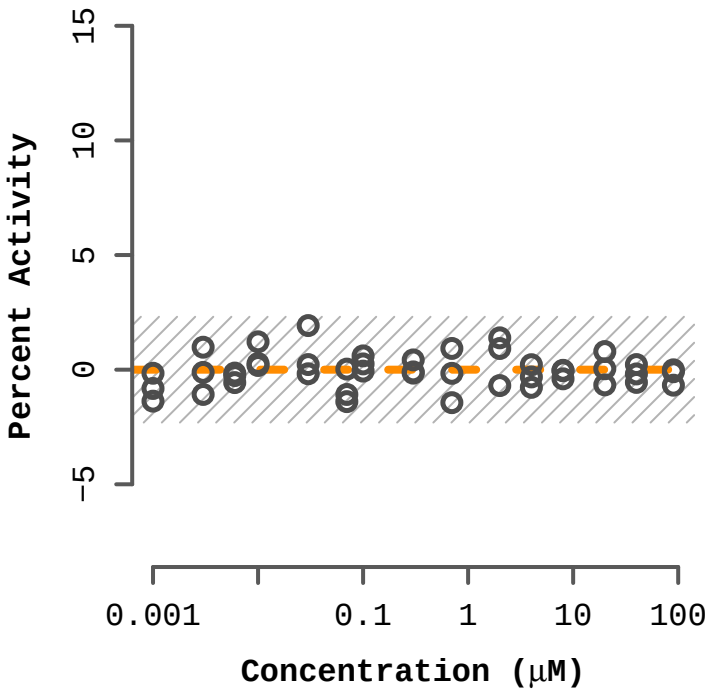
NAME: 1,5-Hexadiene
CHID: 49323 **CASRN:** 592-42-7
SPID(S): Tox21_202852
M4ID: 12479400 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	380.78	NA	NA
PROB:	1	NA	NA
RMSE:	75.21	NA	NA

MAX_MEAN: 112 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

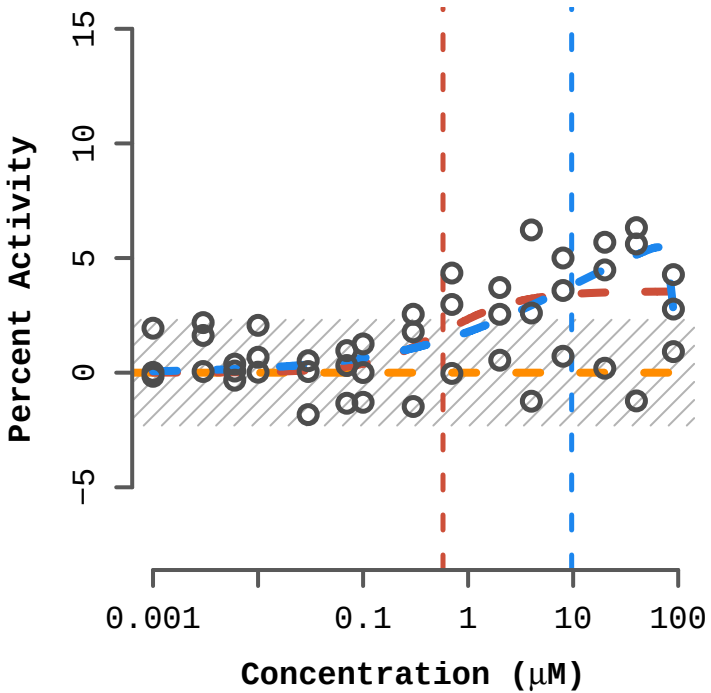
NAME: 2-Benzoxazolinone
CHID: 49324 **CASRN:** 59-49-4
SPID(S): Tox21_202935
M4ID: 12479317

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	100.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.658 **MAX_MED:** 0.925 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylpyridinium tetrafluoroborate
CHID: 49325 CASRN: 597581-48-1
SPID(S): Tox21_202686
M4ID: 12479566

HILL MODEL (in red):

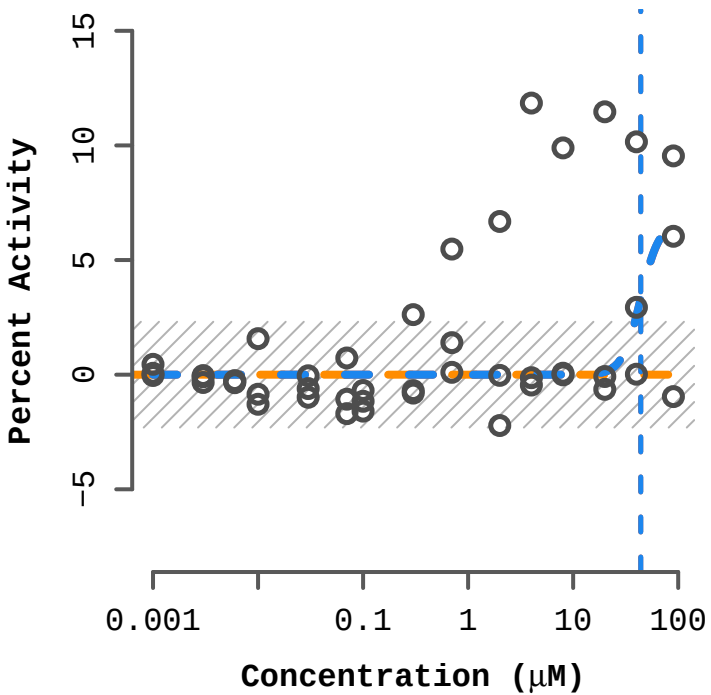
	tp	ga	gw
val:	3.55	-0.239	1.19
sd:	1.03	0.583	1.26

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.6	0.986	0.521	1.95	13.8
sd:	7	1.68	0.329	0.0292	90.6

	CNST	HILL	GNLS
AIC:	218.24	192.26	193.44
PROB:	0	0.64	0.36
RMSE:	2.68	1.84	1.89

MAX_MEAN: 3.57 MAX_MED: 5.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methylpyruvate
CHID: 49326 CASRN: 600-22-6
SPID(S): Tox21_202853
M4ID: 12479399

HILL MODEL (in red):

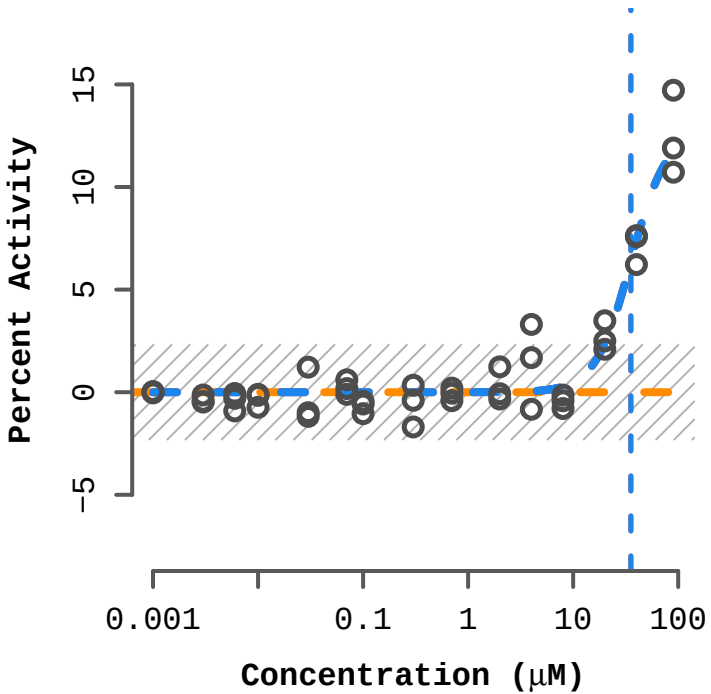
	tp	ga	gw
val:	6.64	1.64	4.97
sd:	2.87	0.2	14.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.66	1.64	4.96	2.14	13.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	233.53	230.05	234.05
PROB:	0.13	0.76	0.1
RMSE:	3.99	3.66	3.66

MAX_MEAN: 4.88 **MAX_MED:** 6.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Hydroxyanthraquinone
CHID: 49327 CASRN: 605-32-3
SPID(S): Tox21_202901
M4ID: 12479351

HILL MODEL (in red):

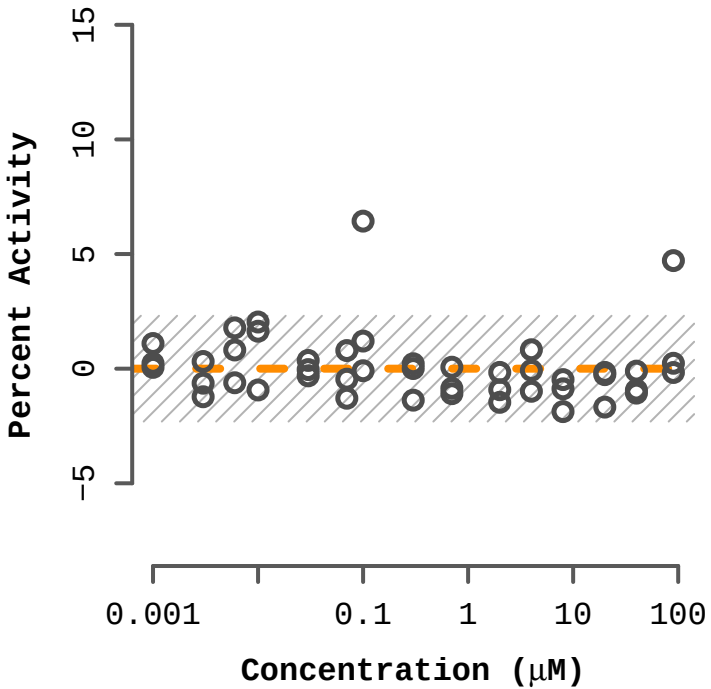
	tp	ga	gw
val:	12.8	1.55	2.57
sd:	1.06	0.0413	0.398

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.8	1.55	2.57	3.74	4.01
sd:	1.06	0.0413	0.398	897	2050

	CNST	HILL	GNLS
AIC:	220.13	124.51	128.51
PROB:	0	0.88	0.12
RMSE:	3.88	0.96	0.96

MAX_MEAN: 12.4 MAX_MED: 11.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

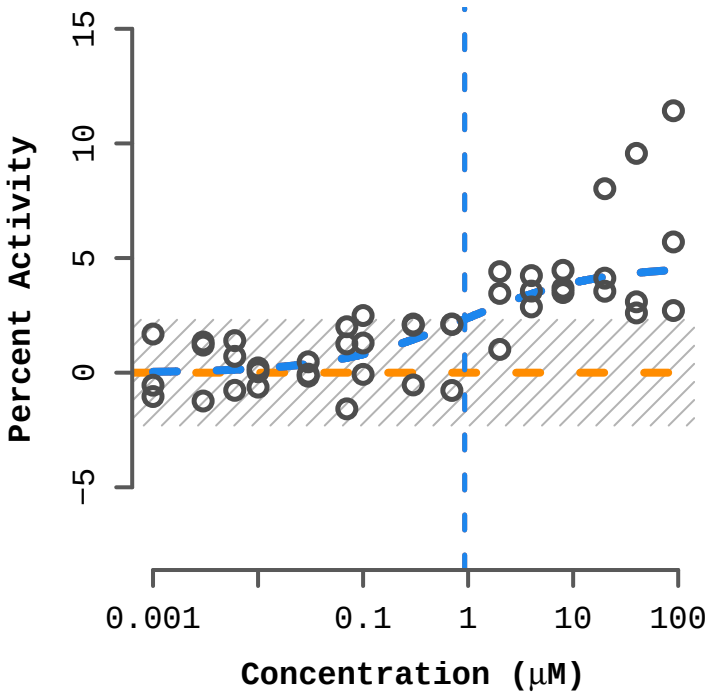
NAME: 1-Methyl-1-propylpyrrolidinium bromide
CHID: 49328 CASRN: 608140-09-6
SPID(S): Tox21_202707
M4ID: 12479545

HILL MODEL: Not applicable.

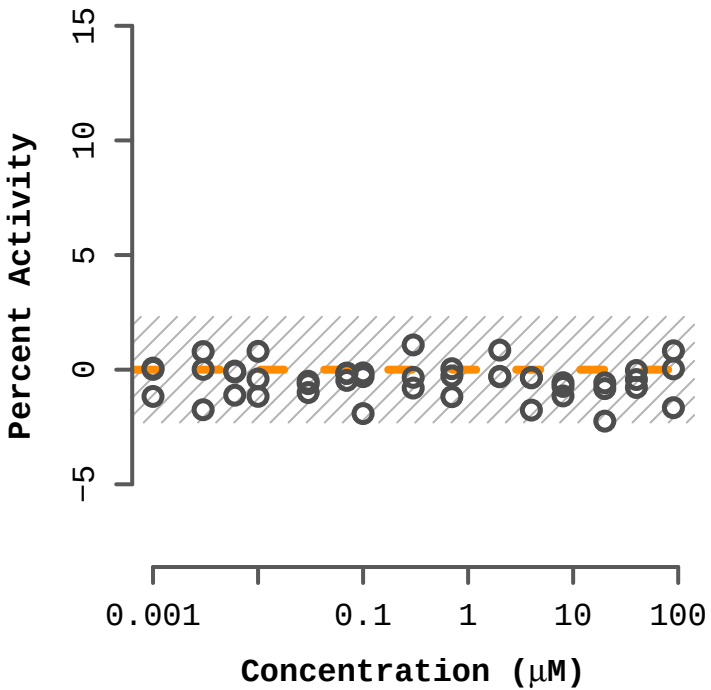
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 2.52 MAX_MED: 1.63 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Methyl-1-propylpiperidinium bis(trifluoromethl
CHID:    49329   CASRN: 608140-12-1
SPID(S): Tox21_202667
M4ID:    12479585

HILL MODEL (in red):
      tp       ga       gw
val:  4.65     -0.033   0.705
sd:   1.07     0.437    0.305

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.65     -0.033   0.705    3.74     4.03
sd:   1.07     0.437    0.305    888      2040

      CNST        HILL        GNLS
AIC:  236.05      176.69      180.69
PROB: 0           0.88        0.12
RMSE: 3.45        1.79        1.79

MAX_MEAN: 6.61      MAX_MED: 5.7       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

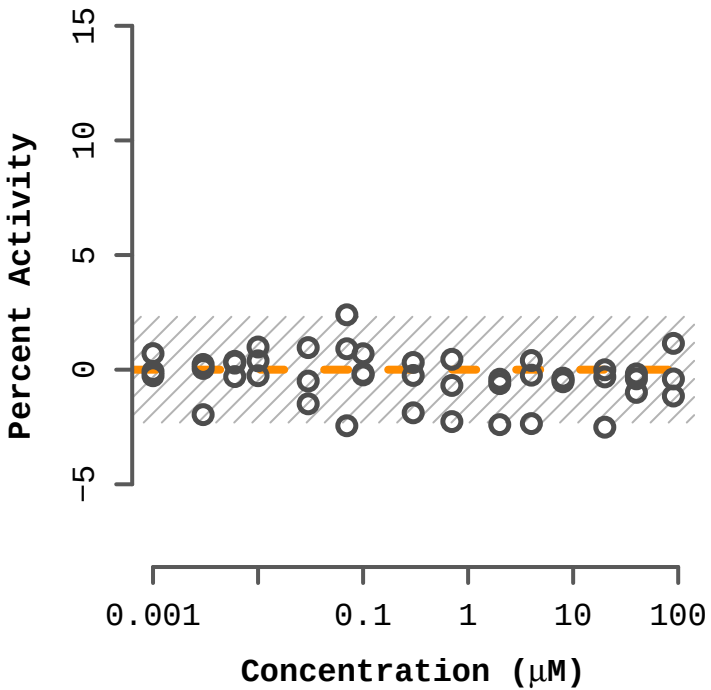
NAME: Ethyl 2-chloroacetoacetate
CHID: 49330 CASRN: 609-15-4
SPID(S): Tox21_202936
M4ID: 12479316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.0858 MAX_MED: 0.0371 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

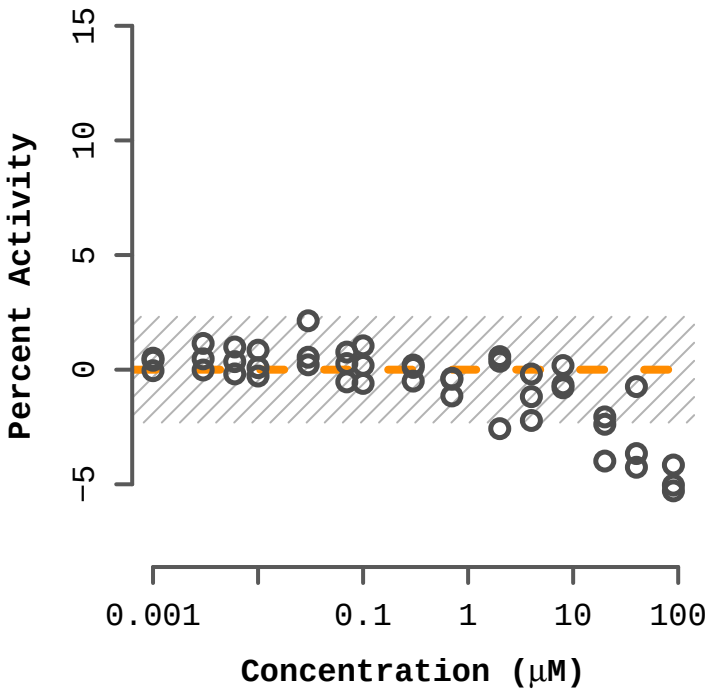
NAME: 5-Nitroisatin
CHID: 49331 **CASRN:** 611-09-6
SPID(S): Tox21_202937
M4ID: 12479315

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.372 **MAX_MED:** 0.913 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

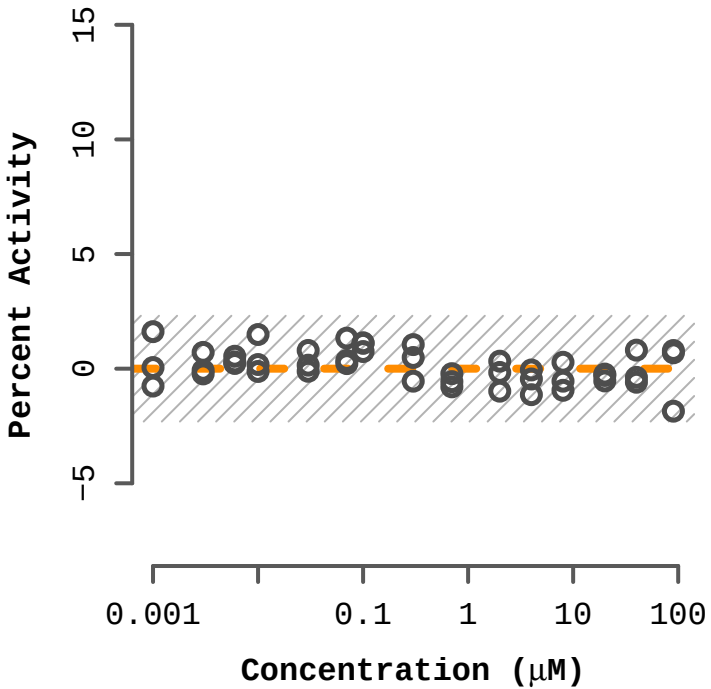
NAME: 1-Methyl-3-octylimidazolium bromide
CHID: 49332 **CASRN:** 61545-99-1
SPID(S): Tox21_202653
M4ID: 12479599

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	176.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.86	NA	NA

MAX_MEAN: 0.964 **MAX_MED:** 0.545 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

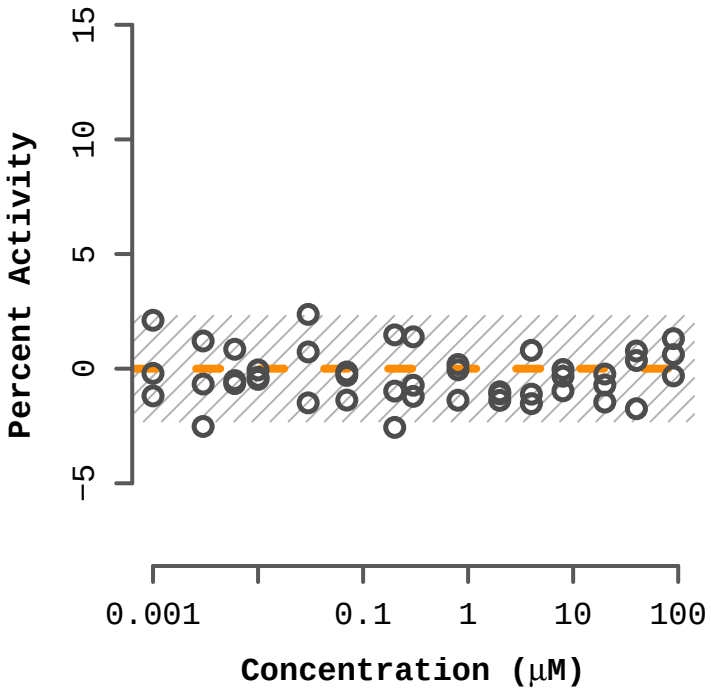
NAME: 1-Dodecyl-3-methylimidazolium bromide
CHID: 49333 CASRN: 61546-00-7
SPID(S): Tox21_202628
M4ID: 12479624

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.996 MAX_MED: 1.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

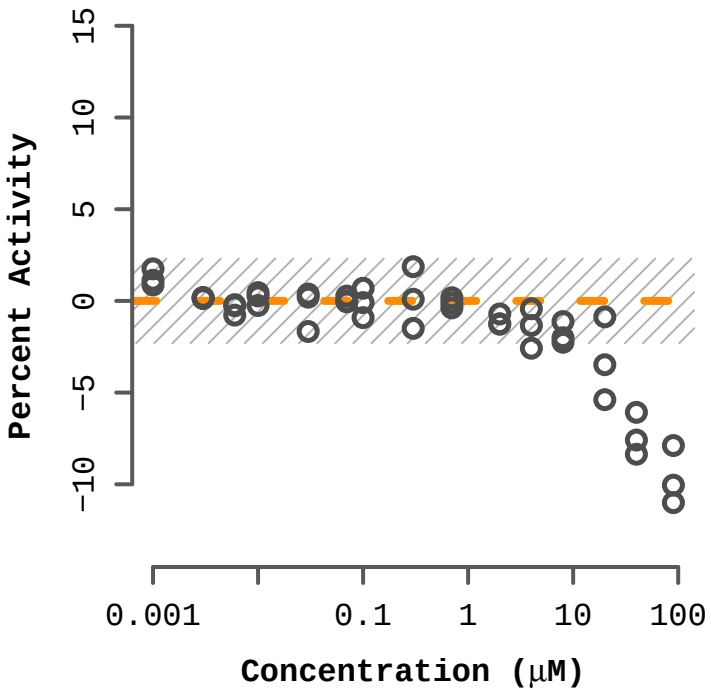
NAME: Propanoic acid,2-hydroxy-,propylester
CHID: 49334 **CASRN:** 616-09-1
SPID(S): Tox21_202856
M4ID: 12479396

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.538 **MAX_MED:** 0.731 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

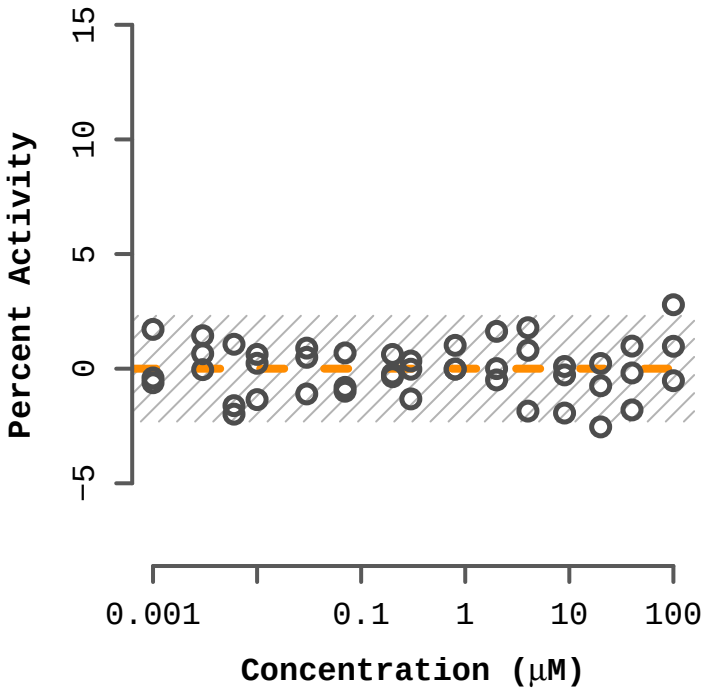
NAME: 1-Hexylpyridinium trifluoromethanesulfonate
CHID: 49335 **CASRN:** 623167-81-7
SPID(S): Tox21_202701
M4ID: 12479551

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	221.83	NA	NA
PROB:	1	NA	NA
RMSE:	3.43	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

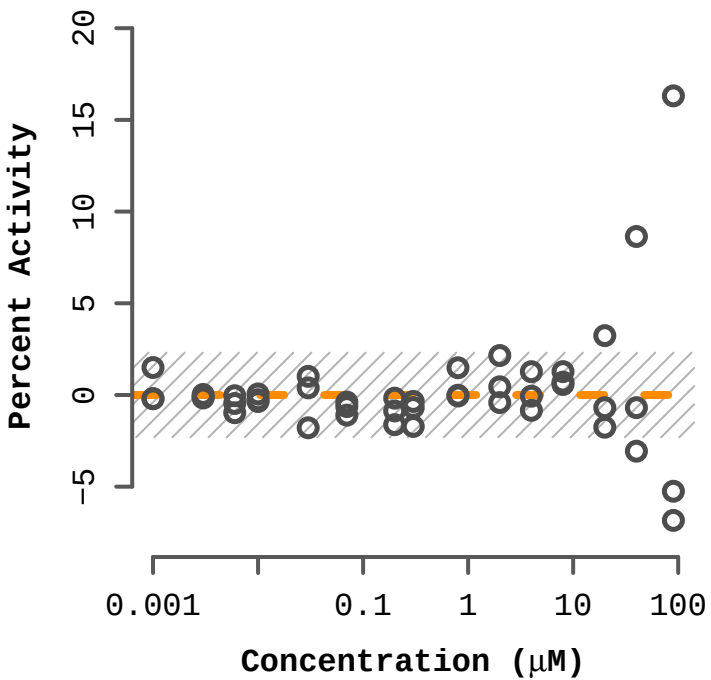
NAME: 1-O-Methylglycerol
CHID: 49336 CASRN: 623-39-2
SPID(S): Tox21_202859
M4ID: 12479393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.977 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

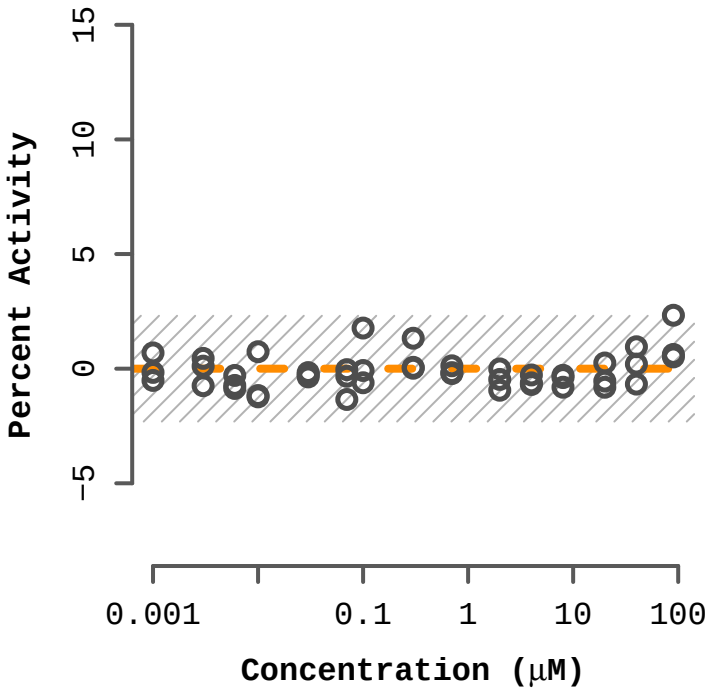
NAME: Acetic acid,mercapto−,ethylester
CHID: 49337 CASRN: 623−51−8
SPID(S): Tox21_202860
M4ID: 12479392

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	193.05	NA	NA
PROB:	1	NA	NA
RMSE:	3.22	NA	NA

MAX_MEAN: 1.63 MAX_MED: 0.699 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

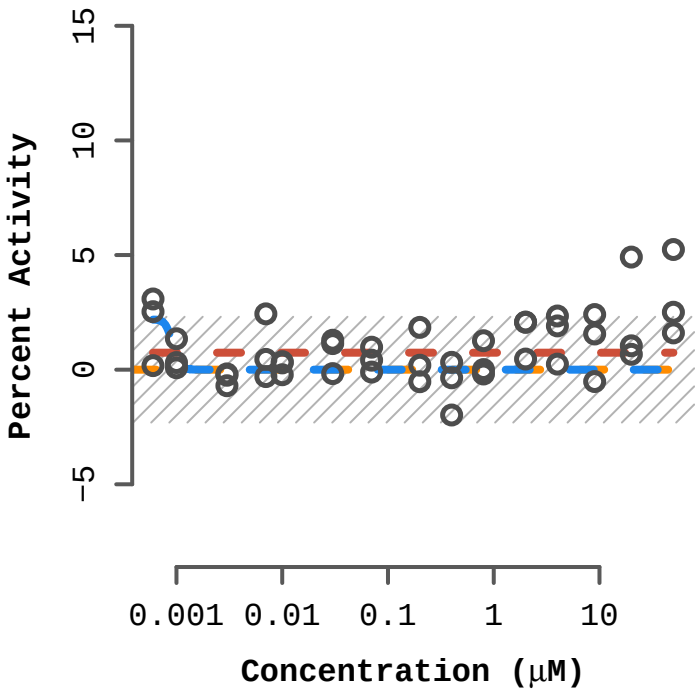
NAME: 1-Butyl-1-methylpiperidinium bis(trifluorometh
CHID: 49338 **CASRN:** 623580-02-9
SPID(S): Tox21_202662
M4ID: 12479590

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.33	NA	NA
PROB:	1	NA	NA
RMSE:	0.75	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.623 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentadecane,1-bromo-
CHID: 49339 **CASRN:** 629-72-1
SPID(S): Tox21_202861
M4ID: 12479391

HILL MODEL (in red):

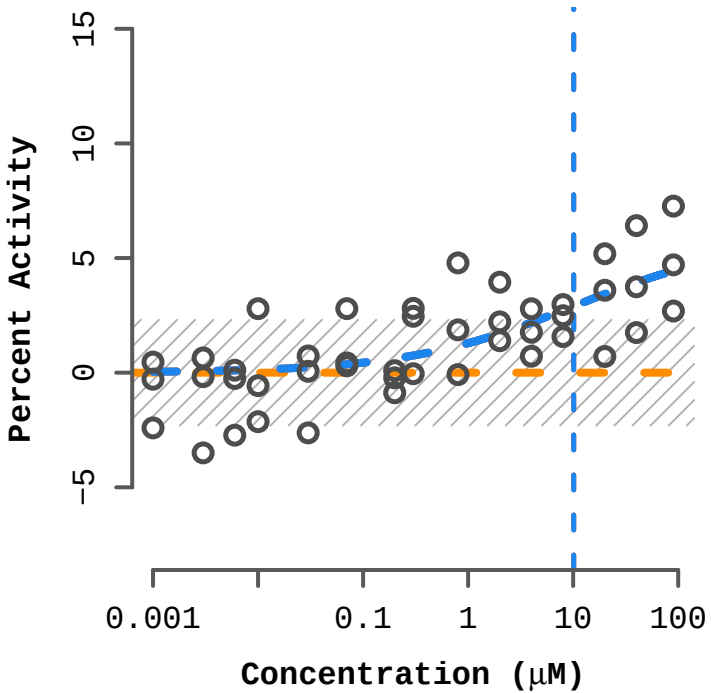
	tp	ga	gw
val:	0.74	-5.2	3.58
sd:	0.193	1120	2040

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.28	-4.01	1.77	-3.04	12.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	172	163.39	175.87
PROB:	0.01	0.98	0
RMSE:	1.68	1.41	1.6

MAX_MEAN: 3.12 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 7-Methylbenzo(a)pyrene
CHID: 49340 CASRN: 63041-77-0
SPID(S): Tox21_202938
M4ID: 12479314

HILL MODEL (in red):

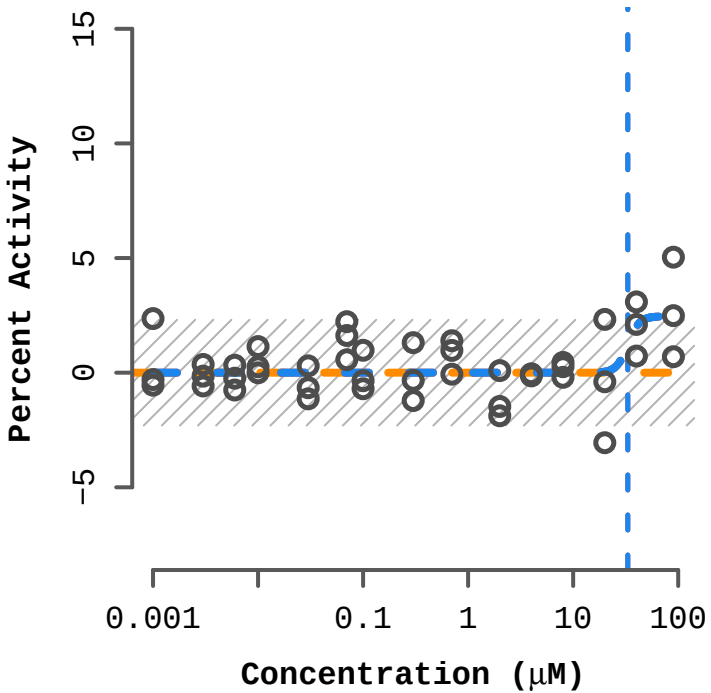
	tp	ga	gw
val:	5.8	1.01	0.543
sd:	3.72	1.17	0.263

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.8	1.01	0.543	3.13	6.66
sd:	3.72	1.17	0.263	1500	8510

	CNST	HILL	GNLS
AIC:	220.29	183.52	187.52
PROB:	0	0.88	0.12
RMSE:	2.7	1.65	1.65

MAX_MEAN: 4.89 MAX_MED: 4.7 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexane,1-iodo-
CHID: 49341 CASRN: 638-45-9
SPID(S): Tox21_202862
M4ID: 12479390

HILL MODEL (in red):

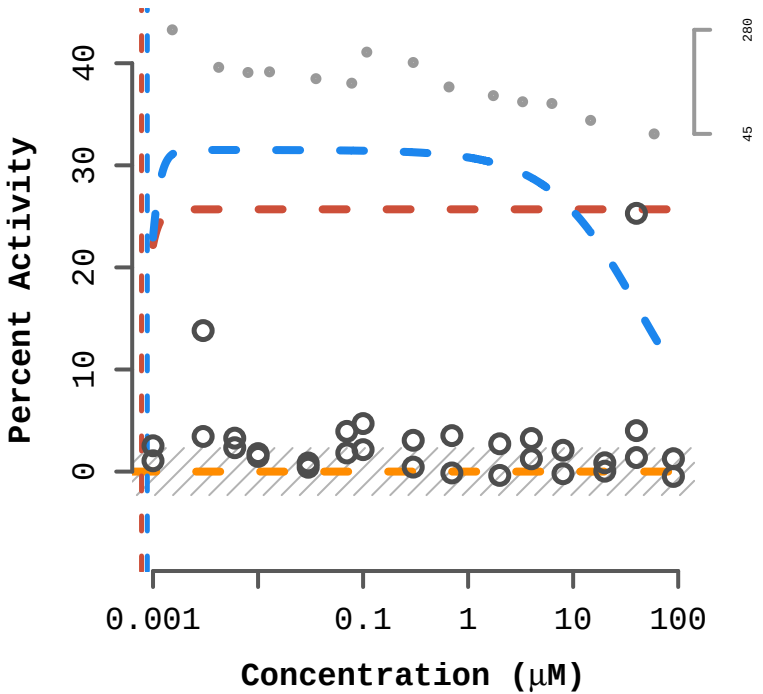
	tp	ga	gw
val:	2.46	1.52	8
sd:	0.818	0.141	10.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.46	1.52	8	3.92	6.27
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	157.26	147.74	151.74
PROB:	0.01	0.87	0.12
RMSE:	1.44	1.15	1.15

MAX_MEAN: 2.74 MAX_MED: 2.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-3-methylimidazolium iodide
CHID: 49342 CASRN: 65039-05-6
SPID(S): Tox21_202618
M4ID: 12479634 BRK

HILL MODEL (in red):

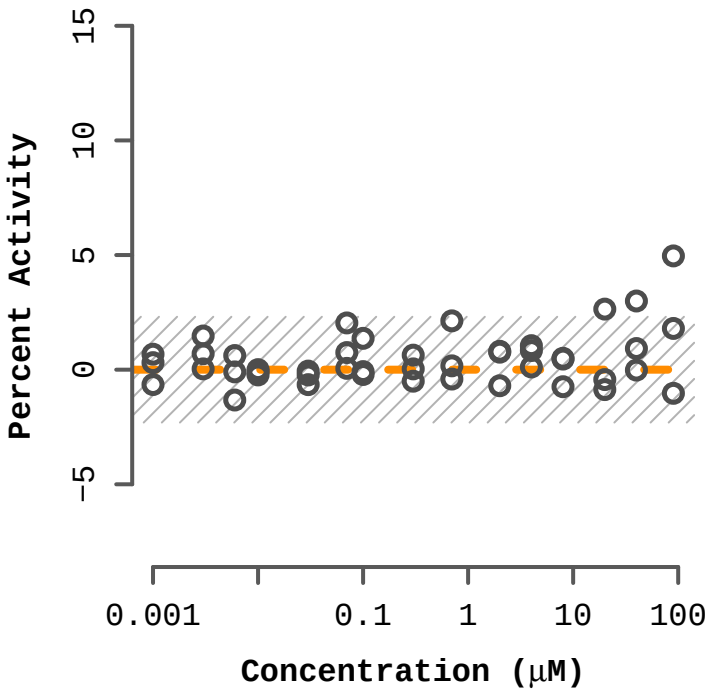
	tp	ga	gw
val:	25.7	-3.11	7.35
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	31.5	-3.05	7.83	1.63	0.995
sd:	15.2	1.15	163	1.18	2.94

	CNST	HILL	GNLS
AIC:	536.48	526.48	529.96
PROB:	0.01	0.85	0.15
RMSE:	94.36	83.4	81.89

MAX_MEAN: 93.3 MAX_MED: 13.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

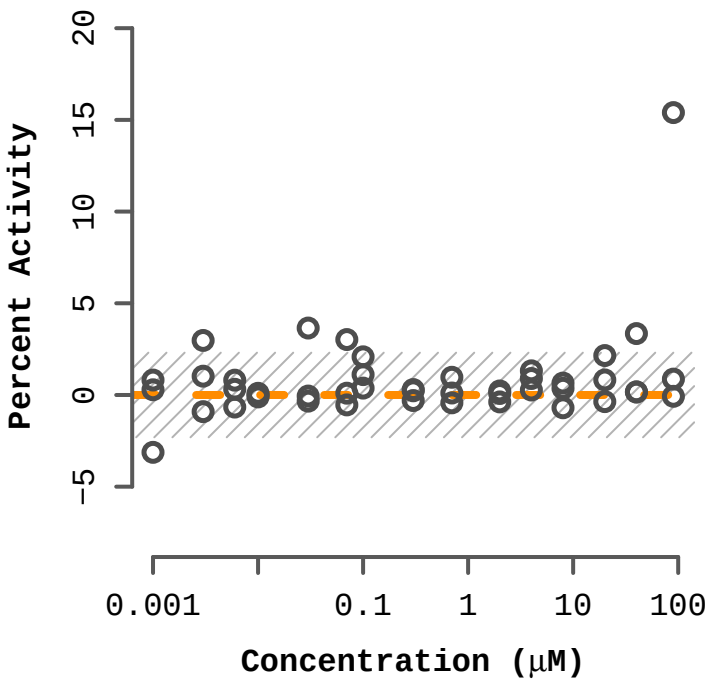
NAME: 1-Ethyl-3-methylmidazolium bromide
CHID: 49343 **CASRN:** 65039-08-9
SPID(S): Tox21_202635
M4ID: 12479617

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

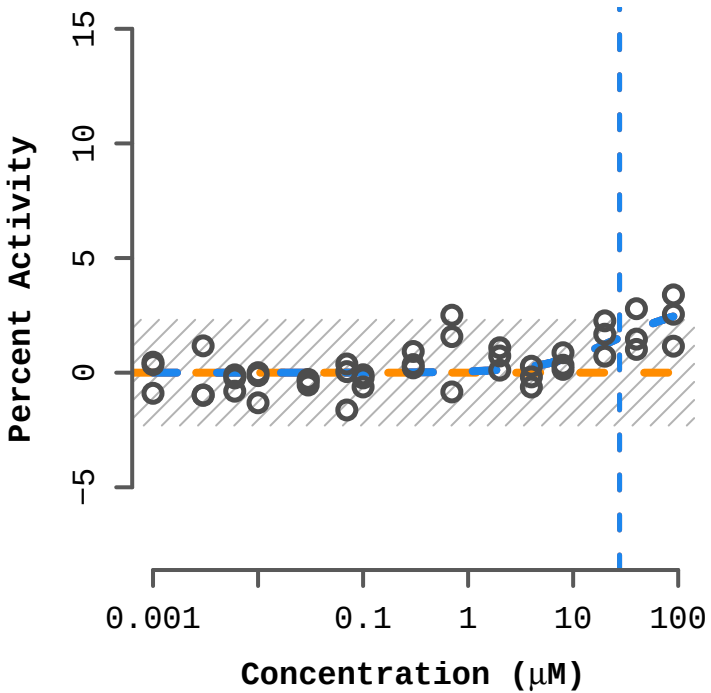
NAME: 3-Chloro-4-fluorobenzoyl chloride
CHID: 49344 CASRN: 65055-17-6
SPID(S): Tox21_202979
M4ID: 12479273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.06	NA	NA
PROB:	1	NA	NA
RMSE:	2.63	NA	NA

MAX_MEAN: 5.4 MAX_MED: 1.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butyl-4-methylpyridinium bromide
CHID: 49345 CASRN: 65350-59-6
SPID(S): Tox21_202683
M4ID: 12479569

HILL MODEL (in red):

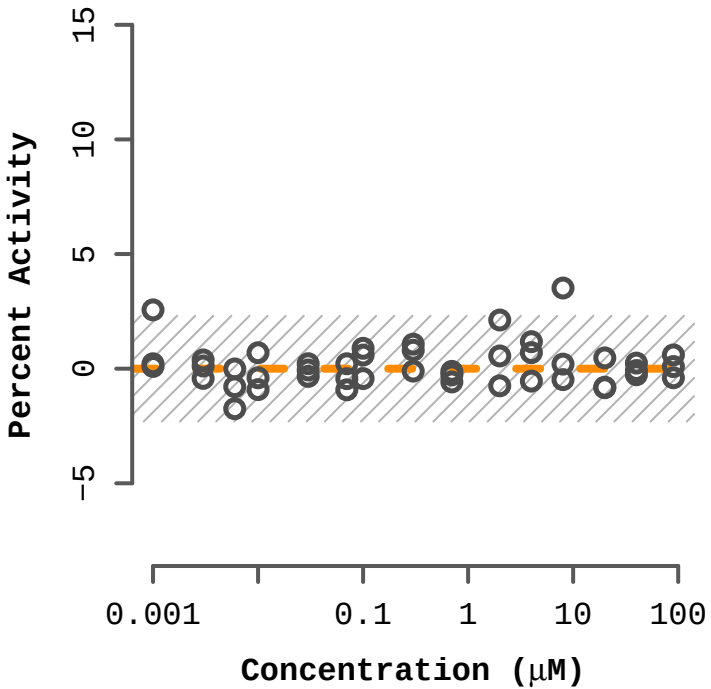
	tp	ga	gw
val:	3.04	1.44	1.2
sd:	4.68	1.44	2.35

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.05	1.44	1.2	3.23	5.93
sd:	4.69	1.44	2.35	2020	9460

	CNST	HILL	GNLS
AIC:	142.99	117.52	121.52
PROB:	0	0.88	0.12
RMSE:	1.18	0.81	0.81

MAX_MEAN: 2.37 MAX_MED: 2.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

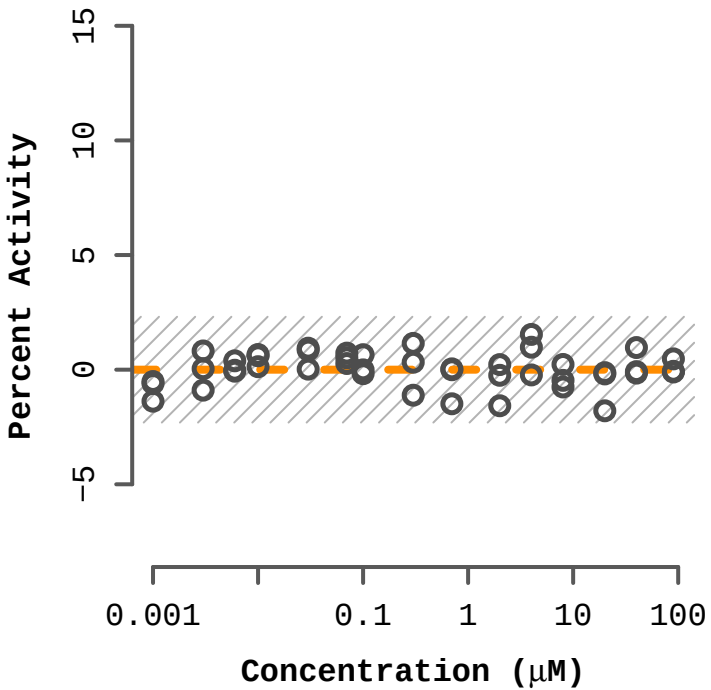
NAME: 2,6-Dichlorobenzenesulfonylchloride
CHID: 49346 **CASRN:** 6579-54-0
SPID(S): Tox21_202863
M4ID: 12479389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.806 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

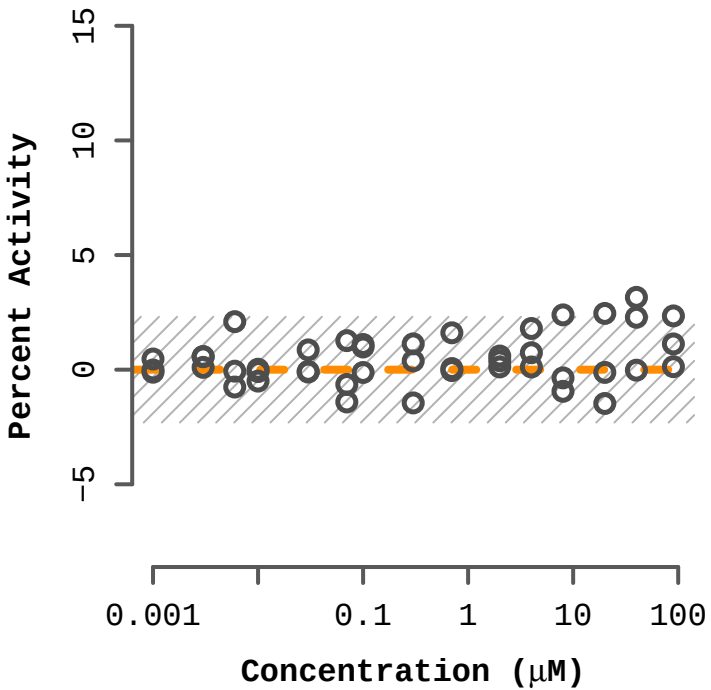
NAME: 1-Ethyl-1-methylpyrrolidinium bromide
CHID: 49347 CASRN: 69227-51-6
SPID(S): Tox21_202705
M4ID: 12479547

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.764 **MAX_MED:** 0.981 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

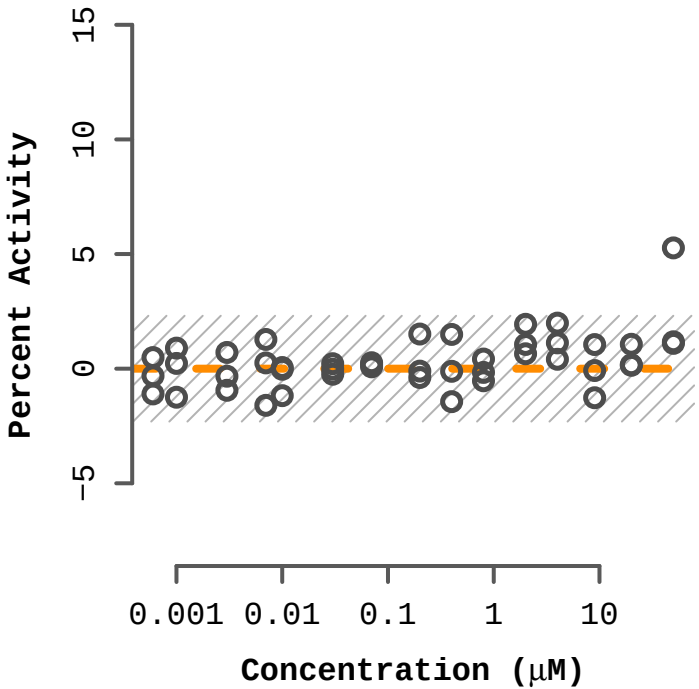
NAME: Nonylbromide
CHID: 49348 **CASRN:** 693-58-3
SPID(S): Tox21_202864
M4ID: 12479388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.81 **MAX_MED:** 2.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

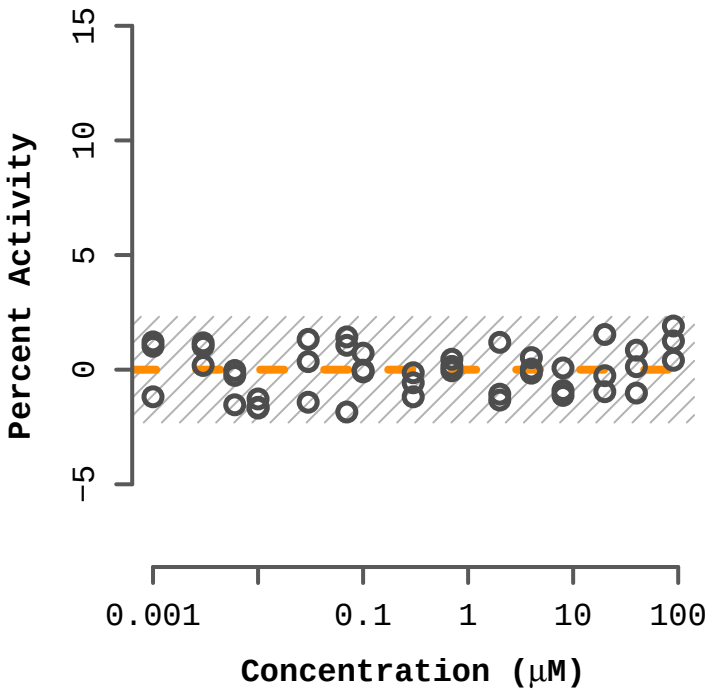
NAME: 1-Bromoundecane
CHID: 49349 **CASRN:** 693-67-4
SPID(S): Tox21_202865
M4ID: 12479387

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 2.52 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

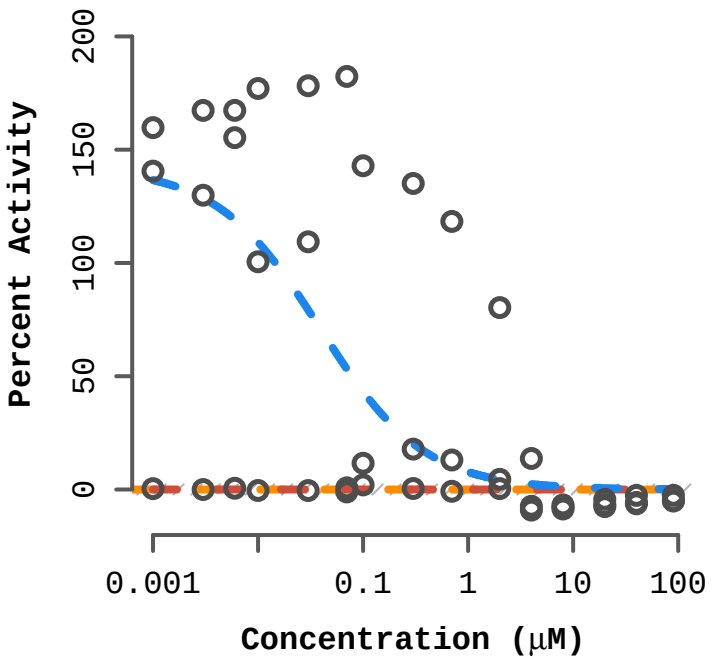
NAME: 1-Bromo-4-chlorobutane
CHID: 49350 **CASRN:** 6940-78-9
SPID(S): Tox21_202866
M4ID: 12479386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Trihexyltetradecylphosphonium dicyanamide
CHID: 49351 CASRN: 701921-71-3
SPID(S): Tox21_202613
M4ID: 12479639

HILL MODEL (in red):

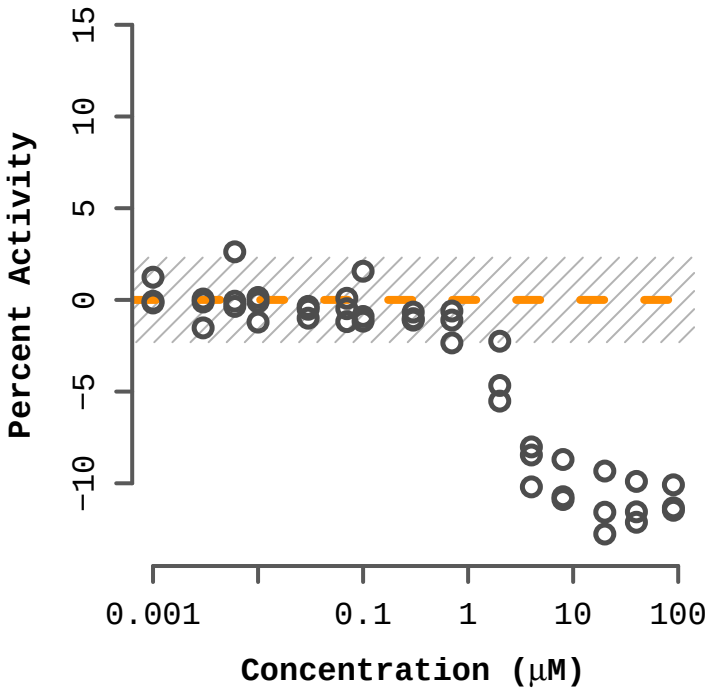
	tp	ga	gw
val:	140	2.45	7.92
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	142	-4.48	7.47	-1.41	0.88
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	525.23	531.23	503.68
PROB:	0	0	1
RMSE:	84.49	84.49	58.81

MAX_MEAN: 108 MAX_MED: 155 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

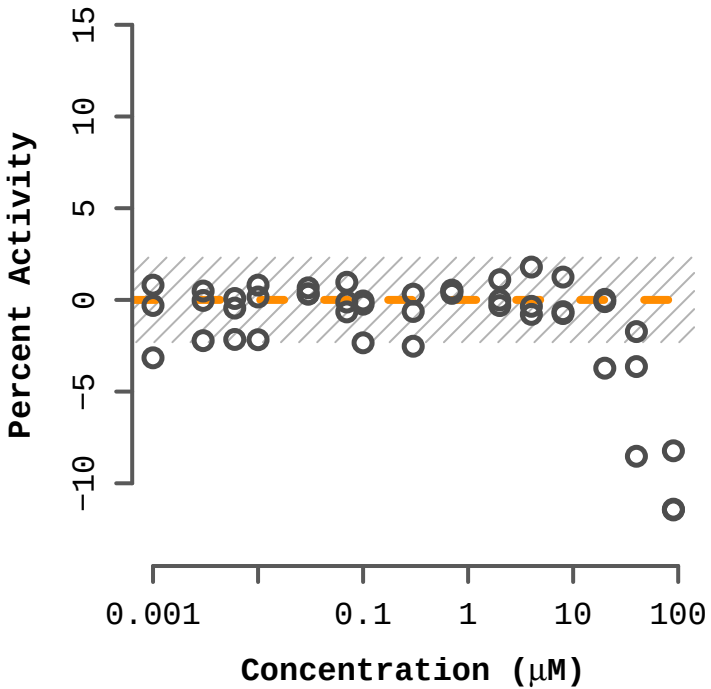
NAME: 1,3-Didecyl-2-methylimidazolium chloride
CHID: 49352 **CASRN:** 70862-65-6
SPID(S): Tox21_202627
M4ID: 12479625

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	294.54	NA	NA
PROB:	1	NA	NA
RMSE:	6.25	NA	NA

MAX_MEAN: 0.734 **MAX_MED:** −0.0681 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

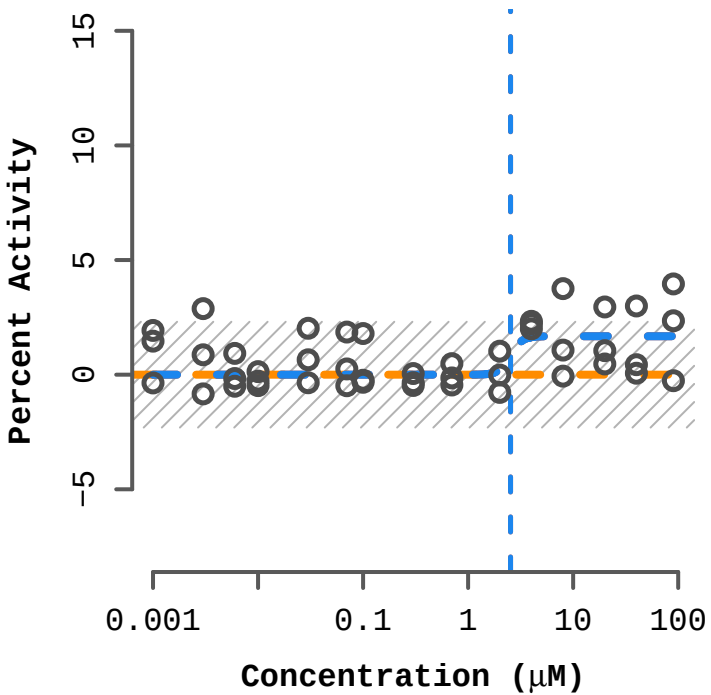
NAME: 1-Hexylpyridinium iodide
CHID: 49353 **CASRN:** 7324-00-7
SPID(S): Tox21_202699
M4ID: 12479553

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	208.28	NA	NA
PROB:	1	NA	NA
RMSE:	3.27	NA	NA

MAX_MEAN: 0.458 **MAX_MED:** 0.481 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 12-BromododecanoicAcid
CHID: 49354 **CASRN:** 73367-80-3
SPID(S): Tox21_202867
M4ID: 12479385

HILL MODEL (in red):

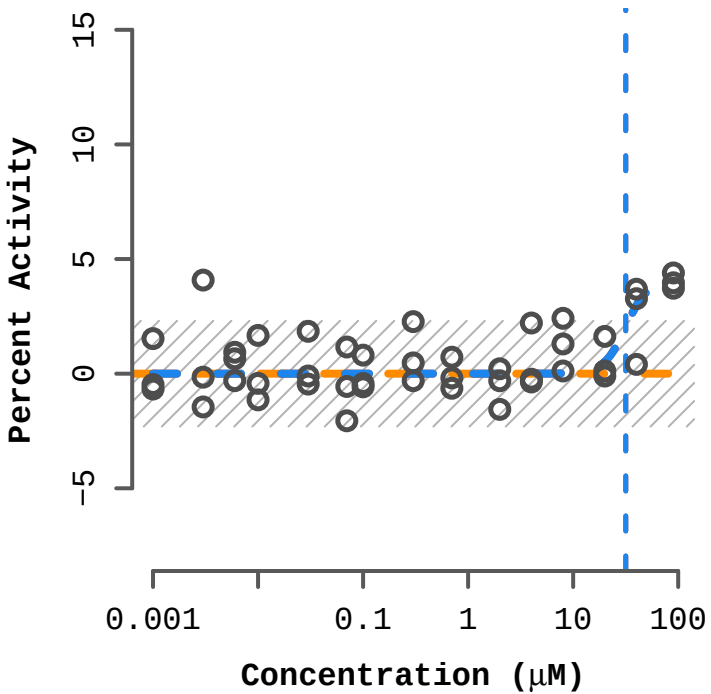
	tp	ga	gw
val:	1.68	0.404	8
sd:	0.366	0.109	6.06

GAIN-LOSS MODEL (in blue):

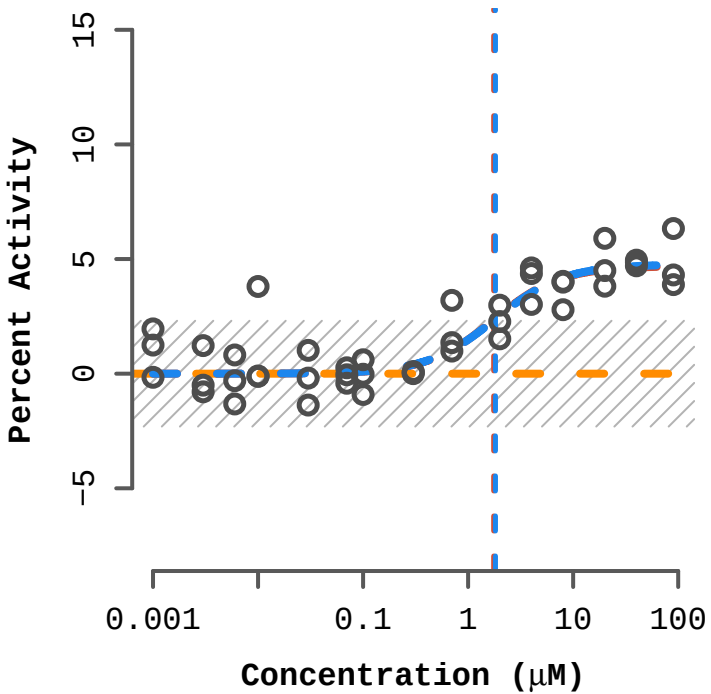
	tp	ga	gw	la	lw
val:	1.68	0.404	8	2.86	10.7
sd:	0.366	0.109	6.06	7170	84300

	CNST	HILL	GNLS
AIC:	164.34	150.18	154.18
PROB:	0	0.88	0.12
RMSE:	1.5	1.14	1.14

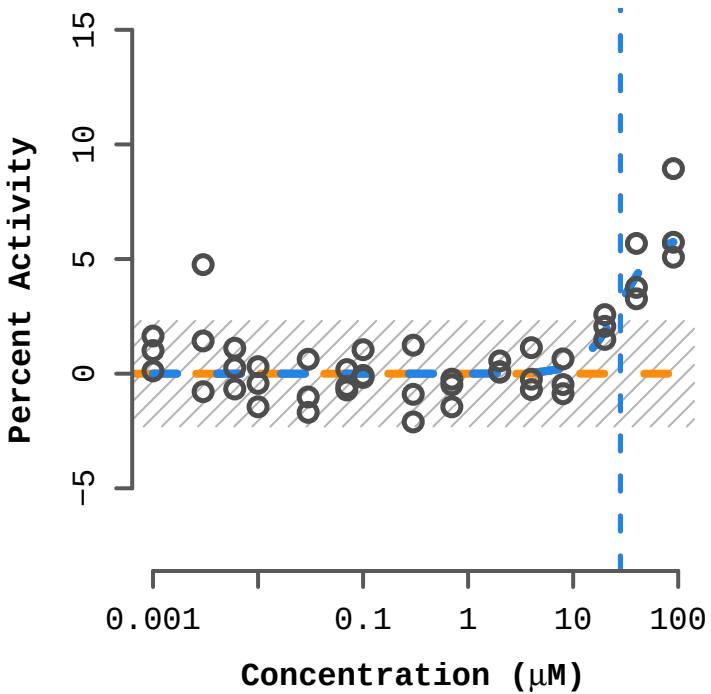
MAX_MEAN: 2.18 **MAX_MED:** 2.35 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Tridecane,1-bromo-
CHID:    49355   CASRN: 765-09-3
SPID(S): Tox21_202870
M4ID:    12479382

HILL MODEL (in red):
      tp       ga       gw
val:  4.09     1.5      4.19
sd:   0.57     0.0841   2.9

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.09     1.5      4.19     3.95     3.84
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  176.62      151.93      155.93
PROB: 0           0.88        0.12
RMSE: 1.74        1.24        1.24

MAX_MEAN: 4.03      MAX_MED: 3.97      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butyl-2,3-dimethylimidazolium trifluorometha
CHID:    49356   CASRN: 765910-73-4
SPID(S): Tox21_202616
M4ID:    12479636

HILL MODEL (in red):
      tp       ga       gw
val:  4.69     0.243    1.37
sd:   0.326    0.115    0.351

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.77     0.26     1.33     2.02     17.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  226.05      130.9       134.75
PROB: 0           0.87        0.13
RMSE: 2.84        1.01        1.01

MAX_MEAN: 4.84      MAX_MED: 4.86      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Acetylfluorene
CHID: 49357 CASRN: 781-73-7
SPID(S): Tox21_202946
M4ID: 12479306

HILL MODEL (in red):

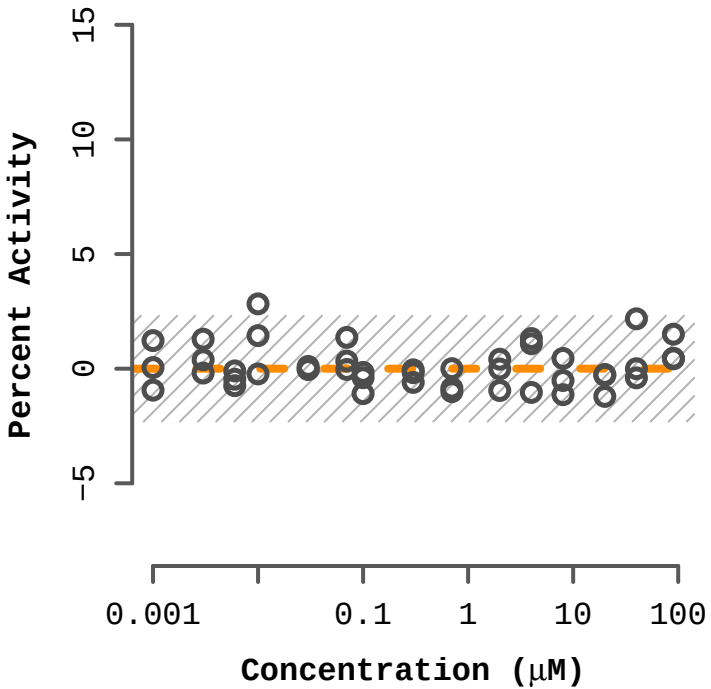
	tp	ga	gw
val:	6.08	1.45	2.45
sd:	1.07	0.112	0.971

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.08	1.45	2.45	3.38	5.35
sd:	1.07	0.112	0.971	1380	5210

	CNST	HILL	GNLS
AIC:	195.82	146.79	150.79
PROB:	0	0.88	0.12
RMSE:	2.41	1.22	1.22

MAX_MEAN: 6.59 MAX_MED: 5.73 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

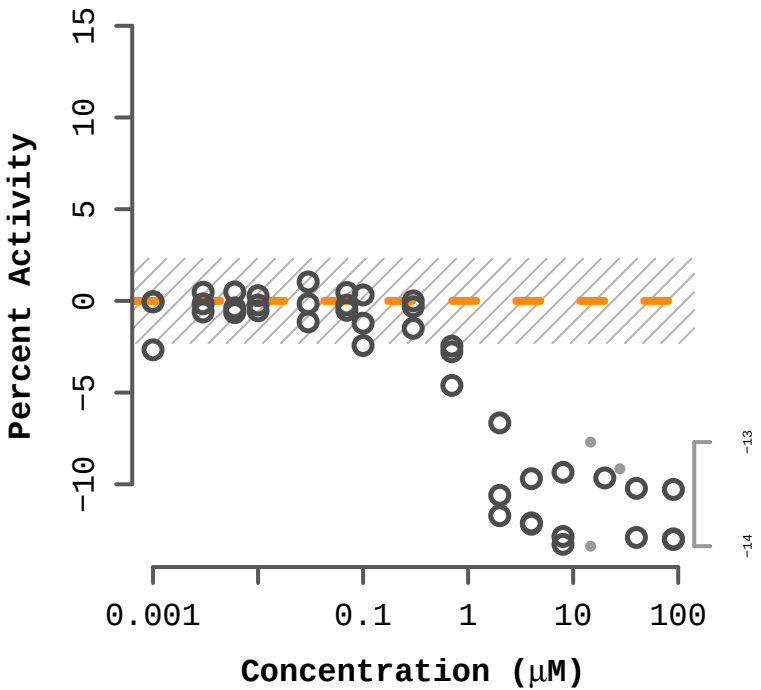
NAME: 1-Methyl-3-propylimidazolium chloride
CHID: 49358 **CASRN:** 79917-89-8
SPID(S): Tox21_202657
M4ID: 12479595

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.2	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

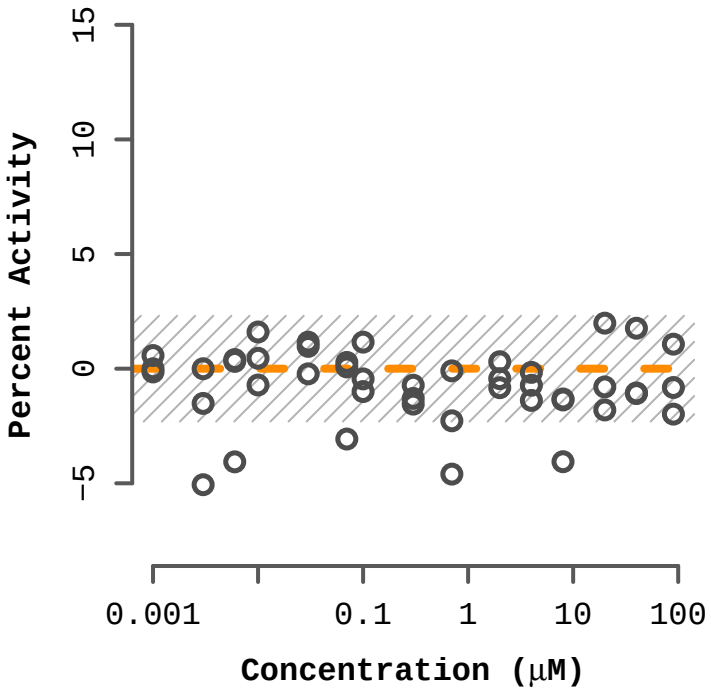
NAME: 1-Dodecyl-3-methylimidazolium iodide
CHID: 49359 **CASRN:** 81995-09-7
SPID(S): Tox21_202632
M4ID: 12479620 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	313.04	NA	NA
PROB:	1	NA	NA
RMSE:	7.53	NA	NA

MAX_MEAN: −0.0863 **MAX_MED:** −0.0544 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

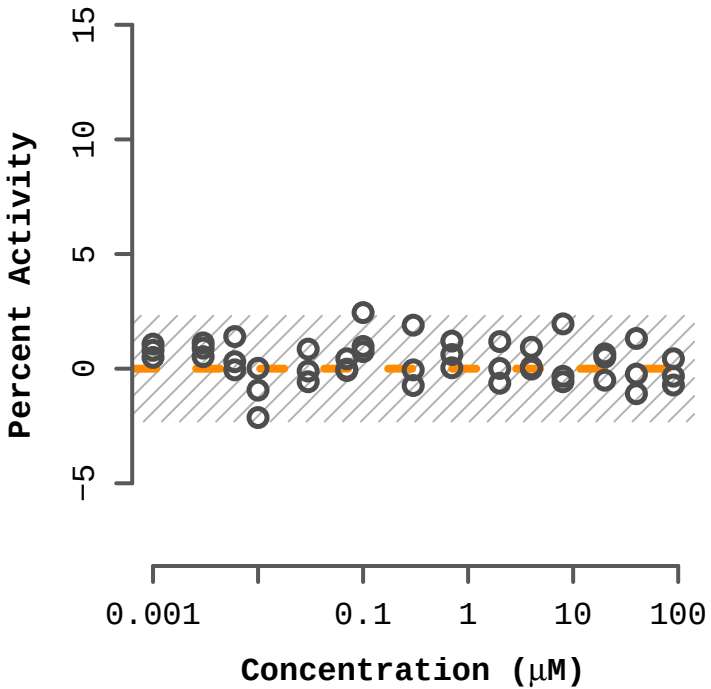
NAME: 1-Butyl-3-methylpyridinium hexafluorophosphate
CHID: 49360 CASRN: 845835-03-2
SPID(S): Tox21_202682
M4ID: 12479570

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	175.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 0.636 MAX_MED: 0.972 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

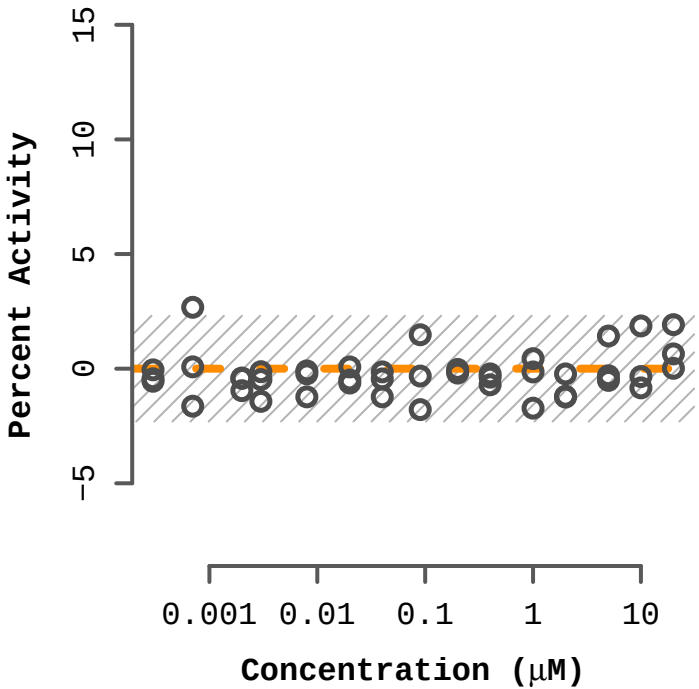
NAME: 1-Methyl-3-propylimidazolium bromide
CHID: 49361 **CASRN:** 85100-76-1
SPID(S): Tox21_202655
M4ID: 12479597

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 0.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

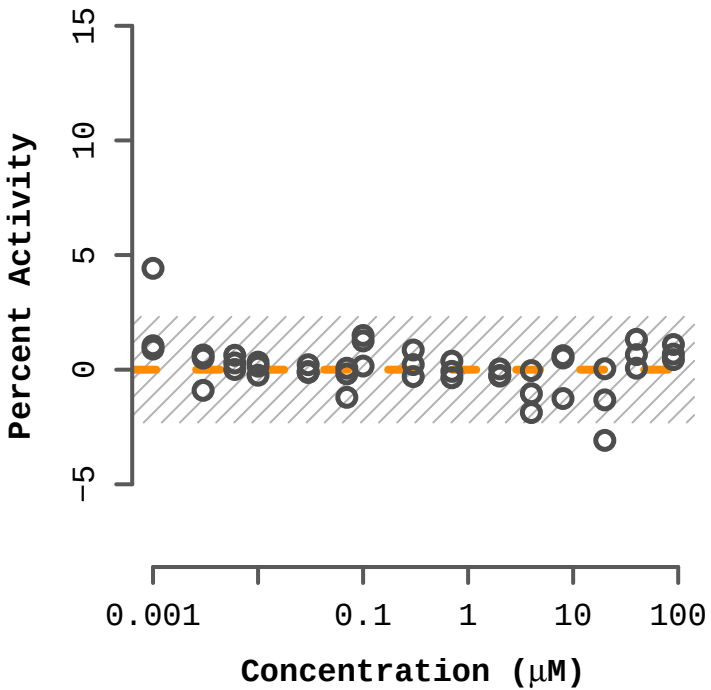
NAME: 1-Butyl-3-methylimidazolium bromide
CHID: 49362 **CASRN:** 85100-77-2
SPID(S): Tox21_202797
M4ID: 12479455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.862 **MAX_MED:** 0.646 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

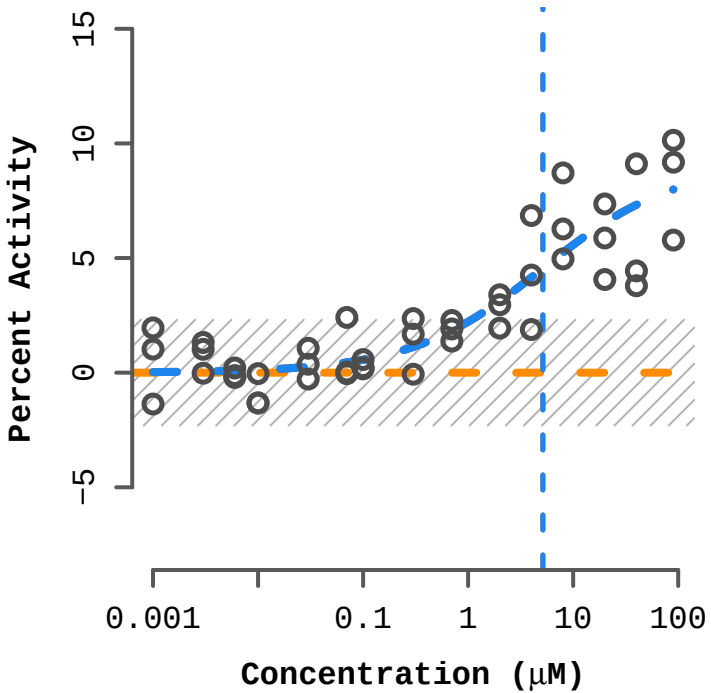
NAME: 1-Butyl-3-methylpyridinium trifluoromethanesul
CHID: 49363 CASRN: 857841-32-8
SPID(S): Tox21_202688
M4ID: 12479564

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.77	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 2.12 MAX_MED: 1.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1−Ethylpyridinium iodide
CHID: 49364 CASRN: 872−90−2
SPID(S): Tox21_202697
M4ID: 12479555

HILL MODEL (in red):

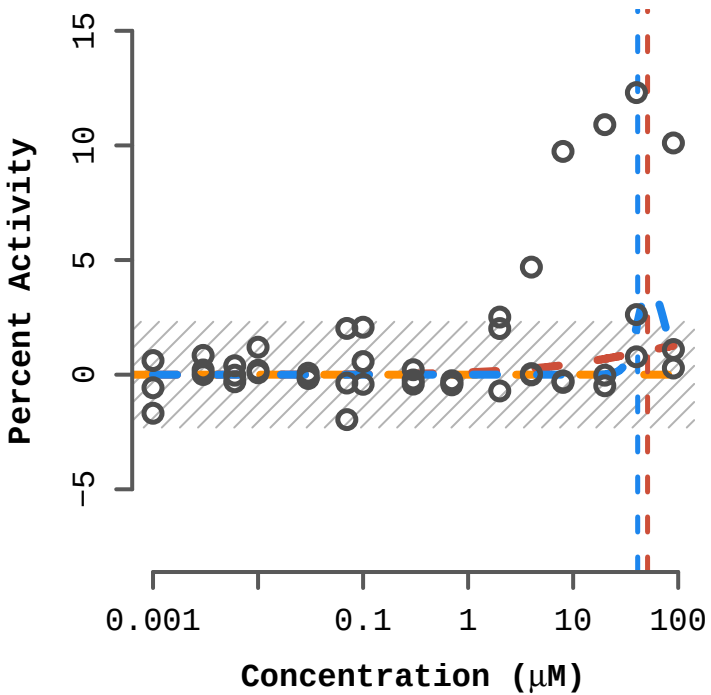
	tp	ga	gw
val:	9.1	0.712	0.69
sd:	3.06	0.521	0.236

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.1	0.712	0.69	3.18	7.08
sd:	3.06	0.521	0.236	1570	9080

	CNST	HILL	GNLS
AIC:	251.8	168.42	172.42
PROB:	0	0.88	0.12
RMSE:	3.99	1.43	1.43

MAX_MEAN: 8.37 MAX_MED: 9.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclohexanone,2-acetyl-
CHID: 49365 CASRN: 874-23-7
SPID(S): Tox21_202874
M4ID: 12479378

HILL MODEL (in red):

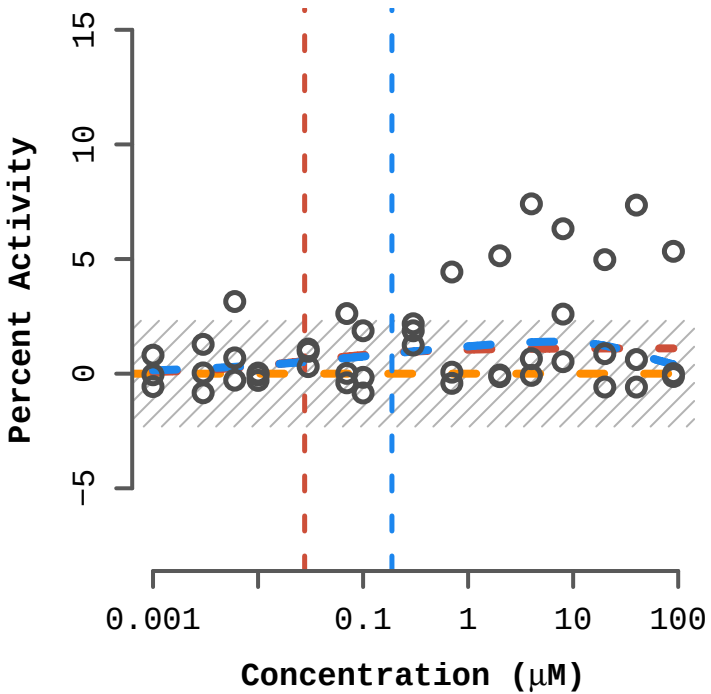
	tp	ga	gw
val:	2.09	1.71	0.751
sd:	7.13	4.2	2.14

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.74	1.61	8	1.86	6.59
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	201.73	203.31	205.1
PROB:	0.61	0.28	0.11
RMSE:	3.43	3.18	3.19

MAX_MEAN: 5.24 MAX_MED: 2.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Butylpyridinium iodide
CHID: 49366 CASRN: 874-81-7
SPID(S): Tox21_202692
M4ID: 12479560

HILL MODEL (in red):

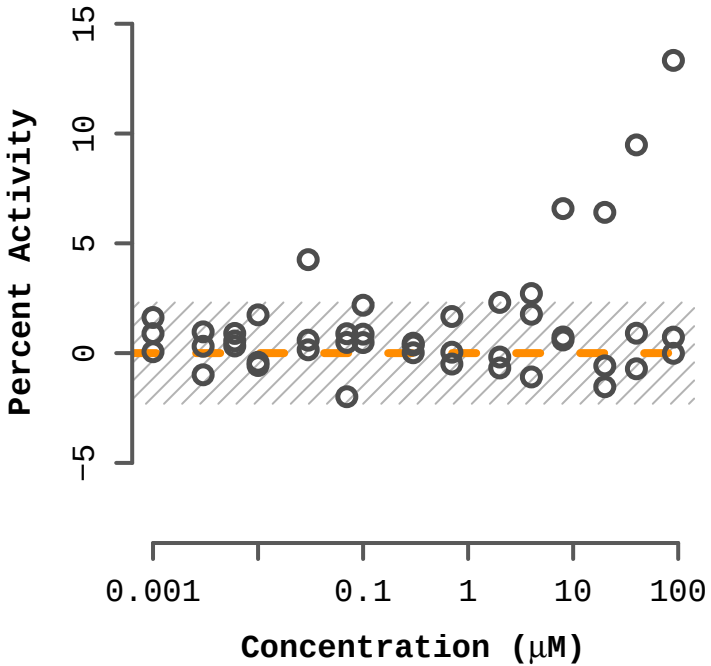
	tp	ga	gw
val:	1.11	−1.56	0.802
sd:	0.496	1.03	1.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.75	−0.725	0.459	1.65	1.58
sd:	4.33	5.85	1.31	1.14	2.82

	CNST	HILL	GNLS
AIC:	201.94	197.8	201.29
PROB:	0.1	0.77	0.13
RMSE:	2.56	2.17	2.16

MAX_MEAN: 3.15 **MAX_MED:** 2.6 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1−Methyl−1−propylpiperidinium tetrafluoroborat

CHID: 49367 **CASRN:** 879866−95−2

SPID(S): Tox21_202672

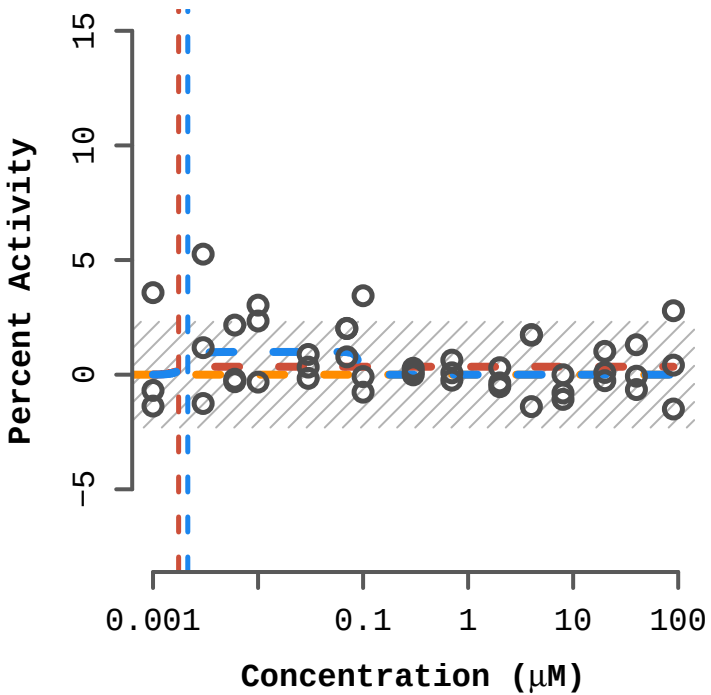
M4ID: 12479580

HILL MODEL: Not applicable.

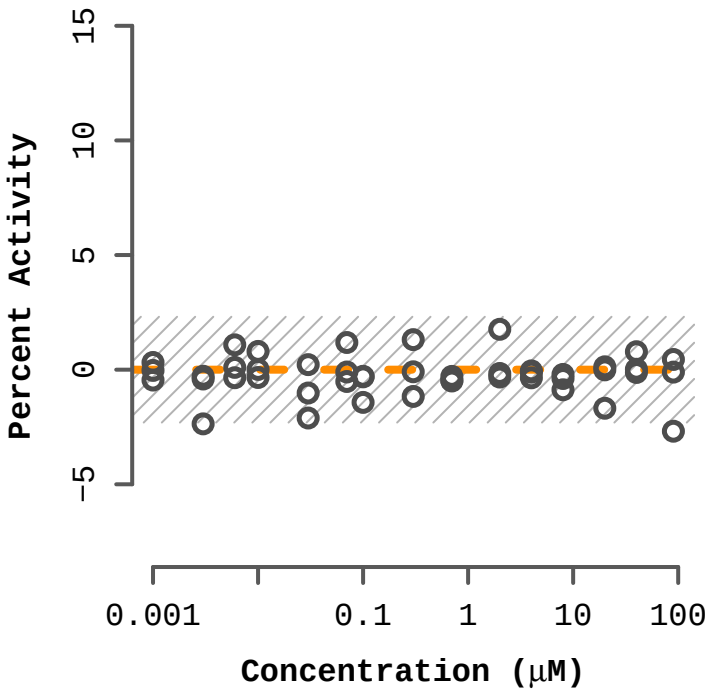
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	198.85	NA	NA
PROB:	1	NA	NA
RMSE:	3.05	NA	NA

MAX_MEAN: 4.69 **MAX_MED:** 1.77 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butyl-4-methylpyridinium trifluoromethanesul
CHID:    49368   CASRN: 882172-79-4
SPID(S): Tox21_202691
M4ID:    12479561

HILL MODEL (in red):
      tp       ga       gw
val:  0.346    -2.76    8
sd:   0.205    0.799    26.8

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  0.991    -2.67    8        -1.04    18
sd:   0.388    0.719    29.6     0.106    29.9

      CNST        HILL        GNLS
AIC:  165.81      168.84      168.6
PROB: 0.68        0.15        0.17
RMSE: 1.58        1.49        1.42

MAX_MEAN: 1.73      MAX_MED: 2.34      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

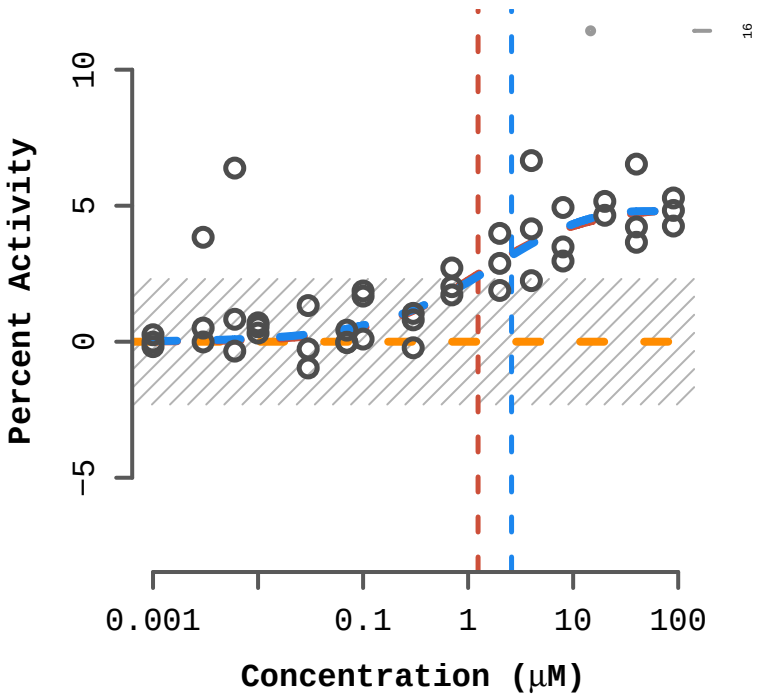
NAME: 1-Butyl-1-methylpiperidinium tetrafluoroborate
CHID: 49369 **CASRN:** 886439-34-5
SPID(S): Tox21_202663
M4ID: 12479589

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.427 **MAX_MED:** 0.102 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Methyl-1-propylpiperidinium bromide
CHID: 49370 CASRN: 88840-42-0
SPID(S): Tox21_202669
M4ID: 12479583 BRK

HILL MODEL (in red):

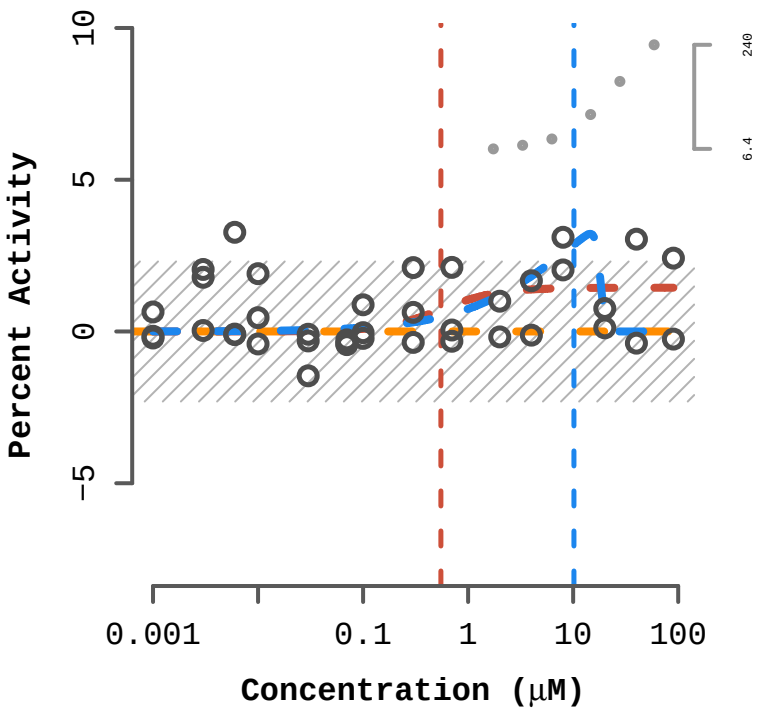
	tp	ga	gw
val:	4.97	0.0946	0.852
sd:	0.531	0.205	0.293

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.24	0.413	0.72	3.23	0.3
sd:	135	5.76	0.762	31.1	13.8

	CNST	HILL	GNLS
AIC:	243.42	163.9	167.76
PROB:	0	0.87	0.13
RMSE:	3.88	2.24	2.22

MAX_MEAN: 8.7 MAX_MED: 5.16 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,4−dinitro Benzenesulfonic acid dihydrate
CHID: 49371 CASRN: 89−02−1
SPID(S): Tox21_202875
M4ID: 12479377 BRK

HILL MODEL (in red):

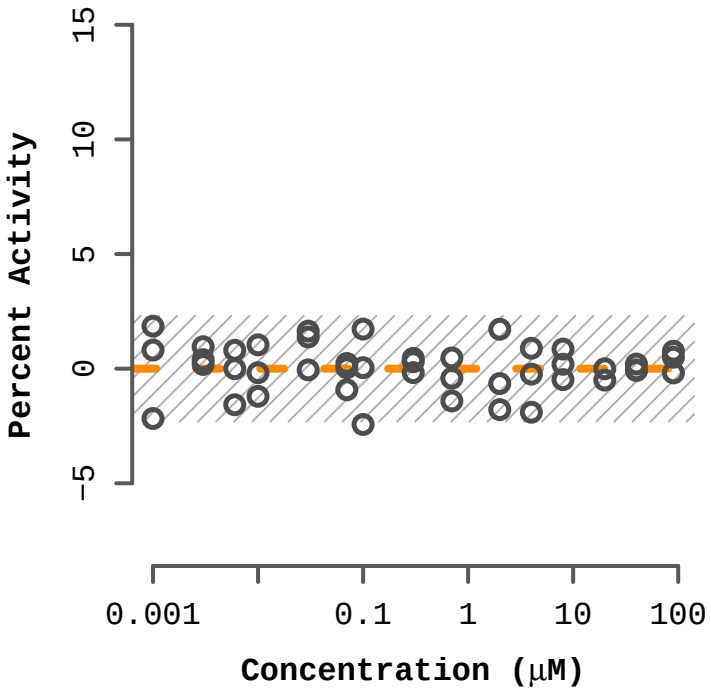
	tp	ga	gw
val:	1.44	−0.259	1.61
sd:	0.626	0.723	1.98

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.73	1.01	0.819	1.26	17.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	318.06	316.76	320.3
PROB:	0.31	0.59	0.1
RMSE:	44.4	44.02	44.32

MAX_MEAN: 79.9 MAX_MED: 3.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

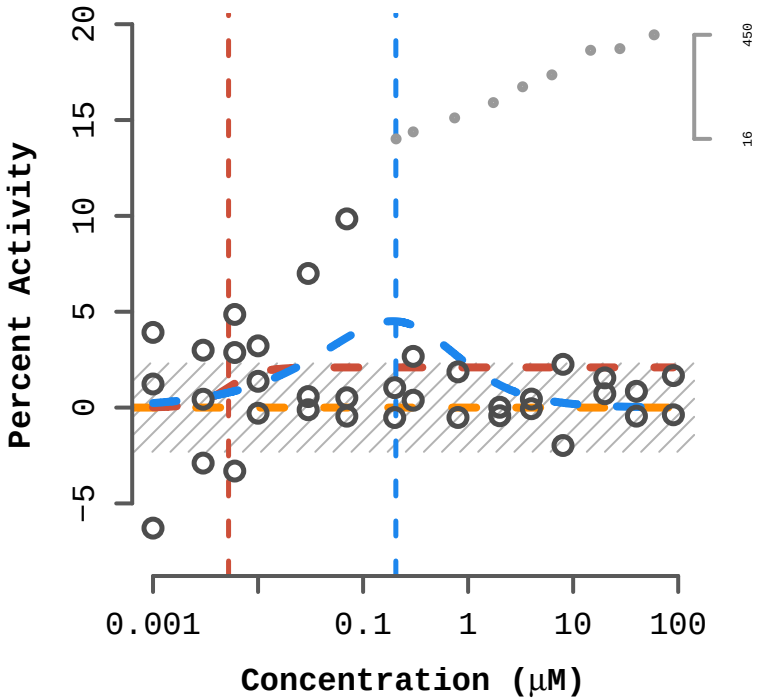
NAME: 1−Ethyl−1−methylpyrrolidinium trifluoromethanes
CHID: 49372 **CASRN:** 893443−18−0
SPID(S): Tox21_202706
M4ID: 12479546

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.991 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: tert-Butyl-3-aminobenzoate
CHID: 49373 **CASRN:** 92146-82-2
SPID(S): Tox21_202904
M4ID: 12479348 **BRK**

HILL MODEL (in red):

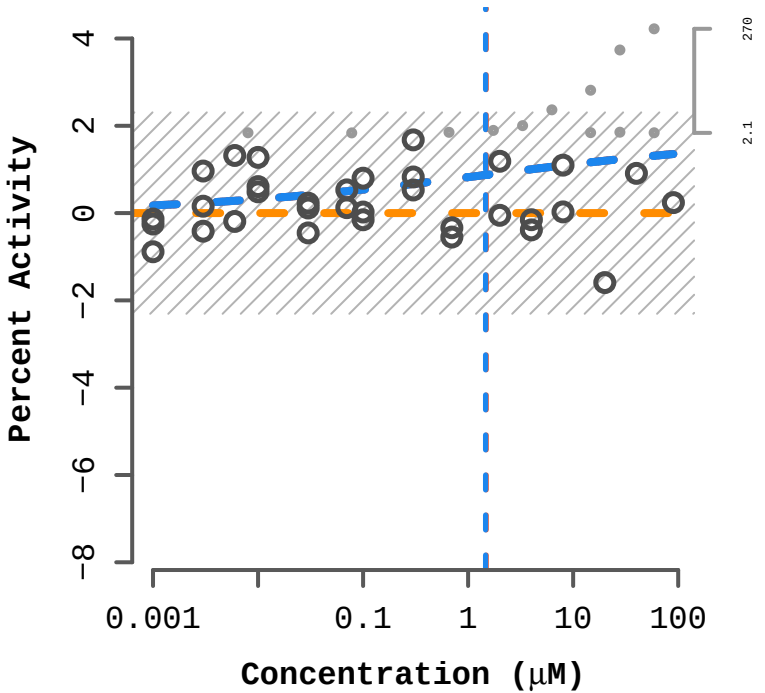
	tp	ga	gw
val:	2.1	−2.28	2.9
sd:	1.83	1.27	19.5

GAIN-LOSS MODEL (in blue):

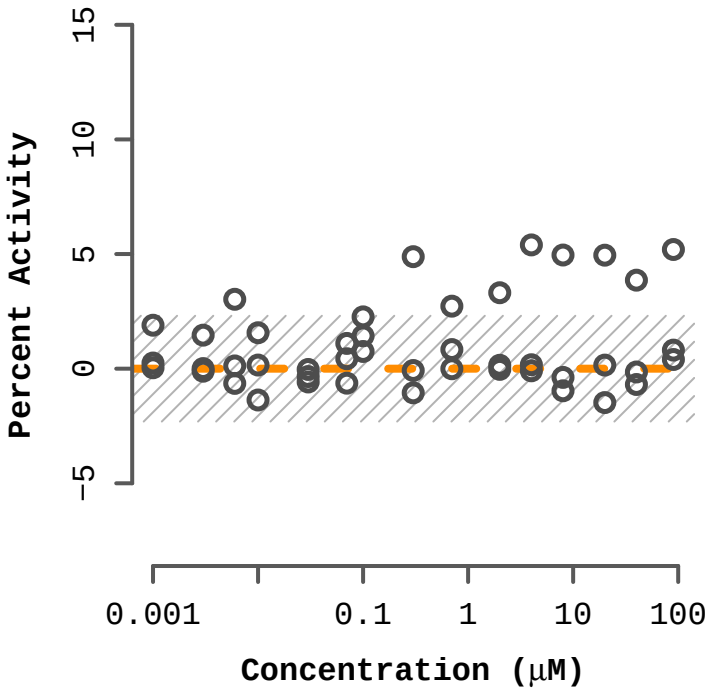
	tp	ga	gw	la	lw
val:	13.3	−0.688	0.756	−0.438	1.26
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	492.74	497	500.44
PROB:	0.88	0.1	0.02
RMSE:	123.53	122.74	123.36

MAX_MEAN: 151 **MAX_MED:** 2.87 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (4R,5S)-(-)-1,5-Dimethyl-4-phenyl-2-imidazolid
CHID:    49374   CASRN: 92841-65-1
SPID(S): Tox21_202878
M4ID:    12479374  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  1.75     0.173    0.3
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.75     0.165    0.3      2.78     8.26
sd:   27.2     52       3.5      2250     22100

      CNST        HILL        GNLS
AIC:  339.16      339.11      343.11
PROB: 0.46        0.47        0.06
RMSE: 55.73       55.38       55.38

MAX_MEAN: 92.1      MAX_MED: 3.88      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

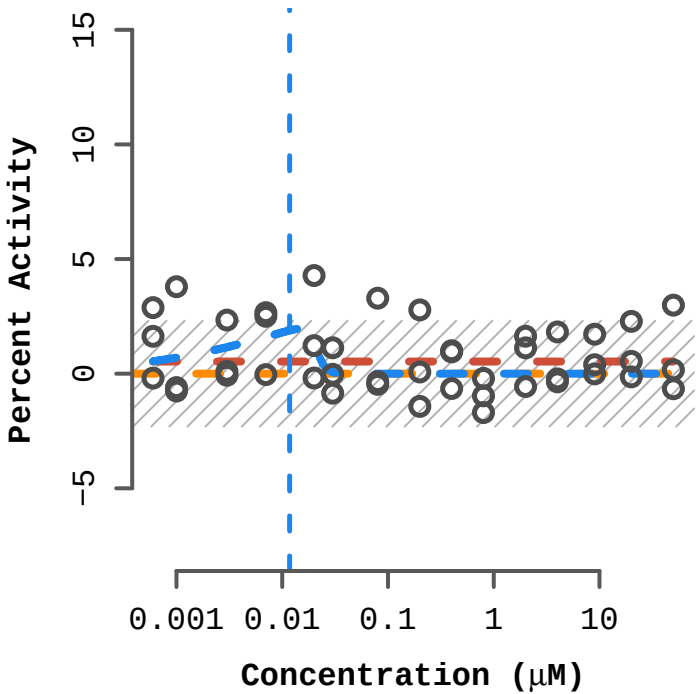
NAME: 1-Butyl-1-methylpyrrolidinium bromide
CHID: 49375 **CASRN:** 93457-69-3
SPID(S): Tox21_202702
M4ID: 12479550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	188.93	NA	NA
PROB:	1	NA	NA
RMSE:	2.1	NA	NA

MAX_MEAN: 2.14 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 7-Methyladenine
CHID: 49376 CASRN: 935-69-3
SPID(S): Tox21_202951
M4ID: 12479301

HILL MODEL (in red):

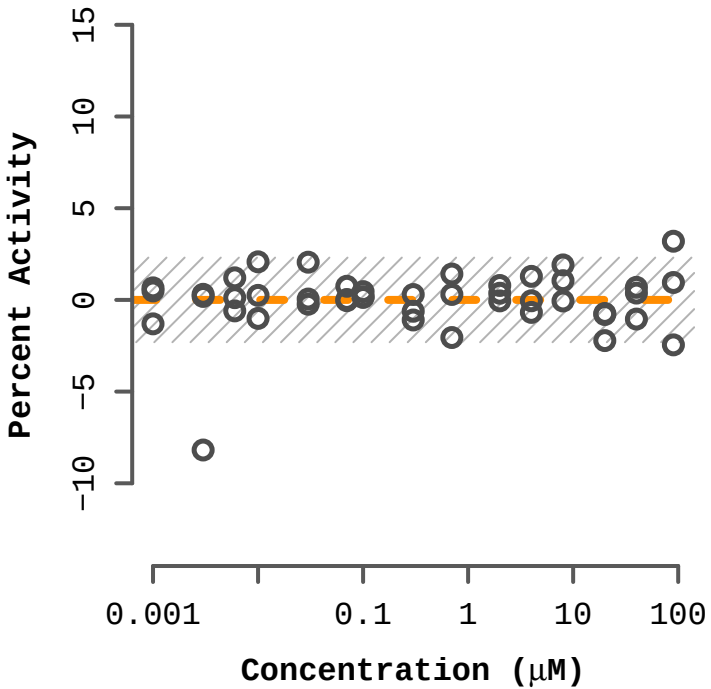
	tp	ga	gw
val:	0.529	−5.18	3.81
sd:	0.228	2400	4720

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.78	−1.93	0.602	−1.68	9.83
sd:	21.9	5.8	1.36	0.308	28.9

	CNST	HILL	GNLS
AIC:	173.4	173.73	176.06
PROB:	0.47	0.4	0.13
RMSE:	1.63	1.47	1.45

MAX_MEAN: 1.77 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

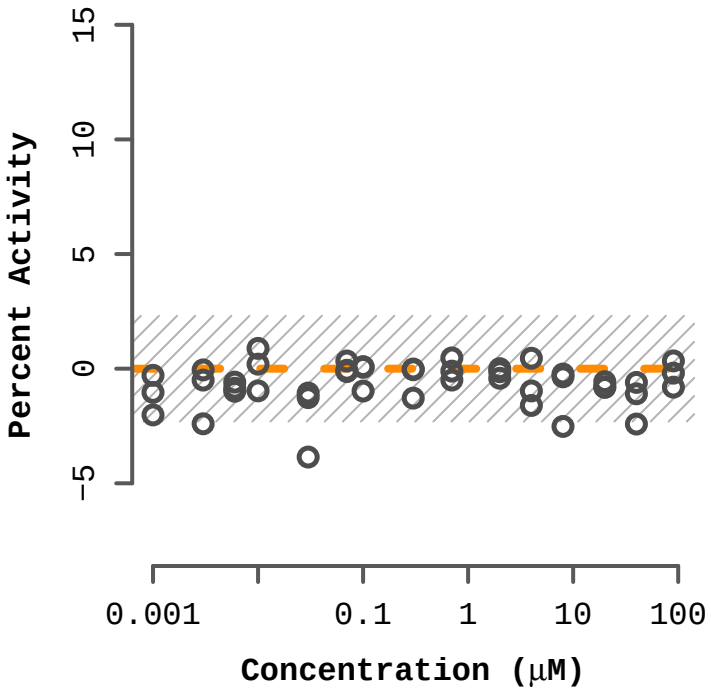
NAME: 1-Methylguanine
CHID: 49377 **CASRN:** 938-85-2
SPID(S): Tox21_202952
M4ID: 12479300

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.65	NA	NA

MAX_MEAN: 0.967 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

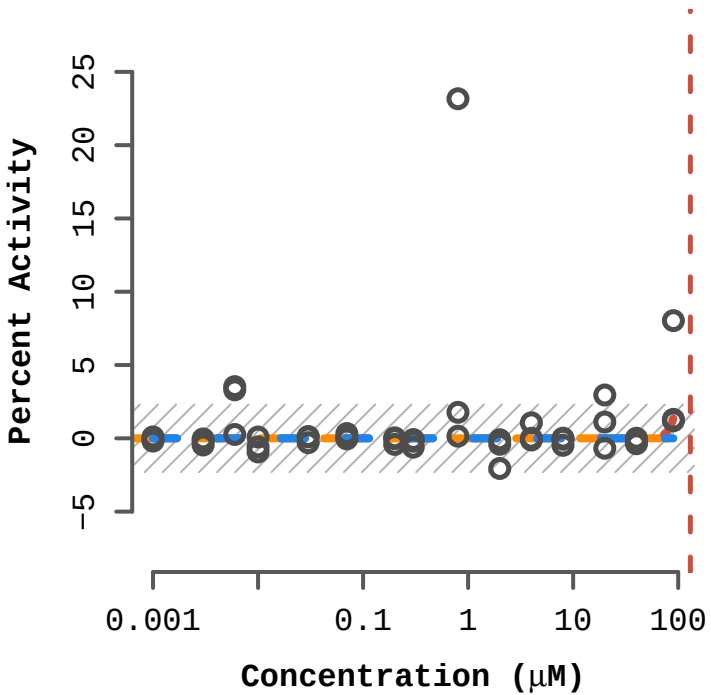
NAME: 1-Butyl-1-methylpiperidinium bromide
CHID: 49378 **CASRN:** 94280-72-5
SPID(S): Tox21_202664
M4ID: 12479588

HILL MODEL: Not applicable.

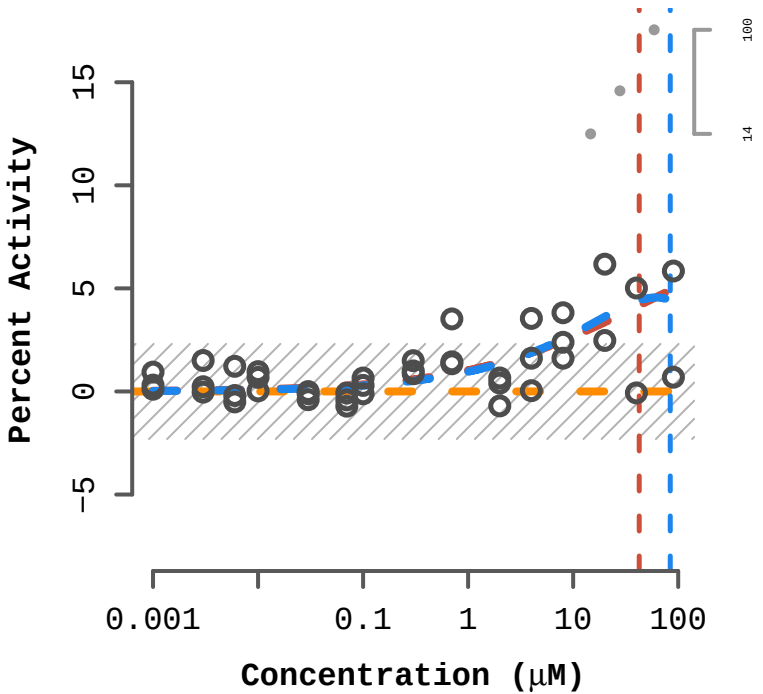
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.83	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.0481 **MAX_MED:** 0.198 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ethyl 4-(2,6-dichloro-5-fluoropyridin-3-yl)-3-(
CHID:    49379   CASRN: 96568-04-6
SPID(S): Tox21_202905
M4ID:    12479347

HILL MODEL (in red):
      tp       ga       gw
val:  27.7     2.12     8
sd:   NaN      NaN      NaN

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.84     -4.92    1.27     -4.64    4.59
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  161         158.61      171
PROB: 0.23        0.77        0
RMSE: 3.8         3.73        3.8

MAX_MEAN: 8.36      MAX_MED: 3.31      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethylbutyraldehyde
CHID: 49380 CASRN: 97-96-1
SPID(S): Tox21_202883
M4ID: 12479369 BRK

HILL MODEL (in red):

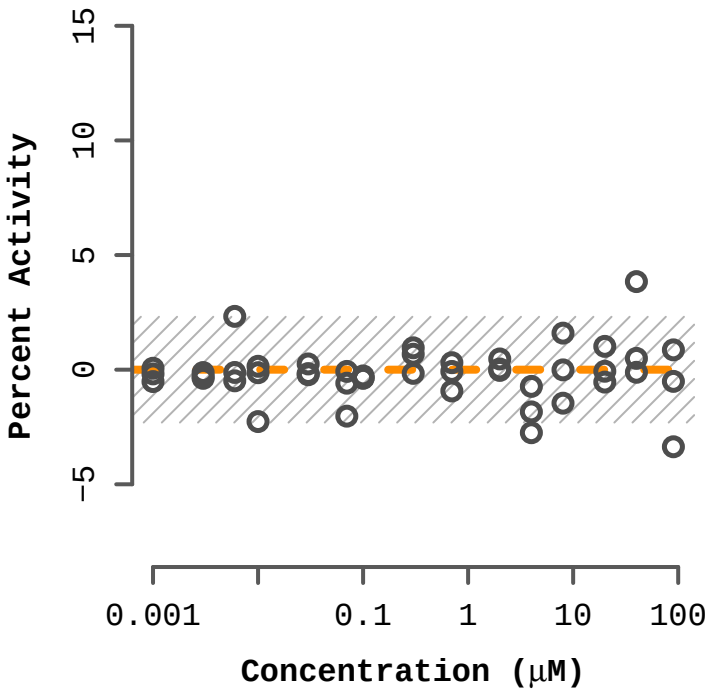
	tp	ga	gw
val:	8.35	1.63	0.524
sd:	9.95	1.96	0.334

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.9	1.92	0.55	2.17	1.85
sd:	27	2.64	0.297	1.09	3.95

	CNST	HILL	GNLS
AIC:	257.82	236.83	240.52
PROB:	0	0.86	0.14
RMSE:	17.09	16.05	16.11

MAX_MEAN: 36 MAX_MED: 6.18 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

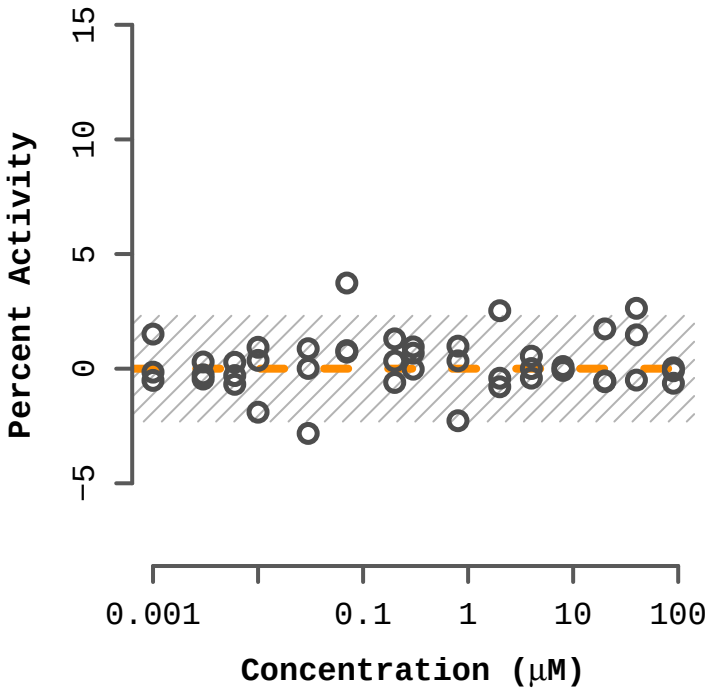
NAME: 1-Ethyl-2,3-dimethylimidazolium bromide
CHID: 49381 **CASRN:** 98892-76-3
SPID(S): Tox21_202633
M4ID: 12479619

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 0.676 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

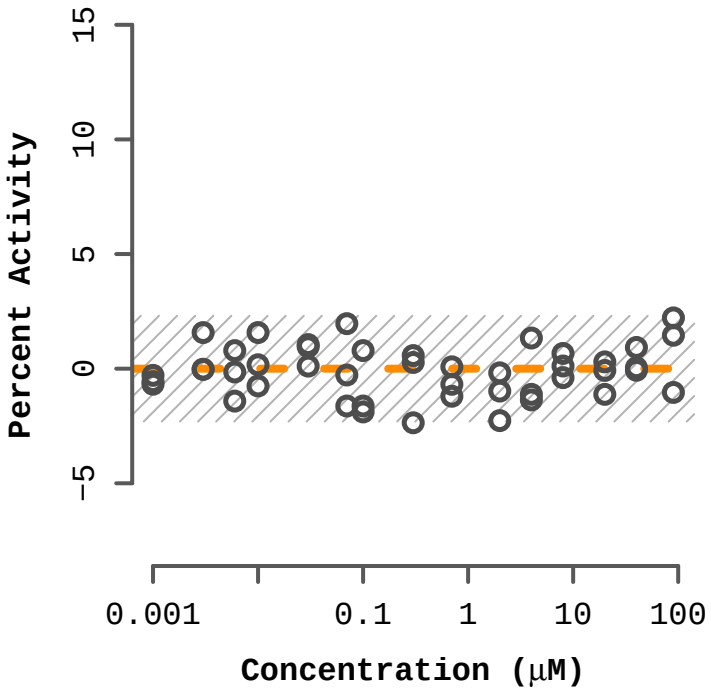
NAME: Triethylgermanium chloride
CHID: 49382 CASRN: 994-28-5
SPID(S): Tox21_202954
M4ID: 12479298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.75 MAX_MED: 1.48 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

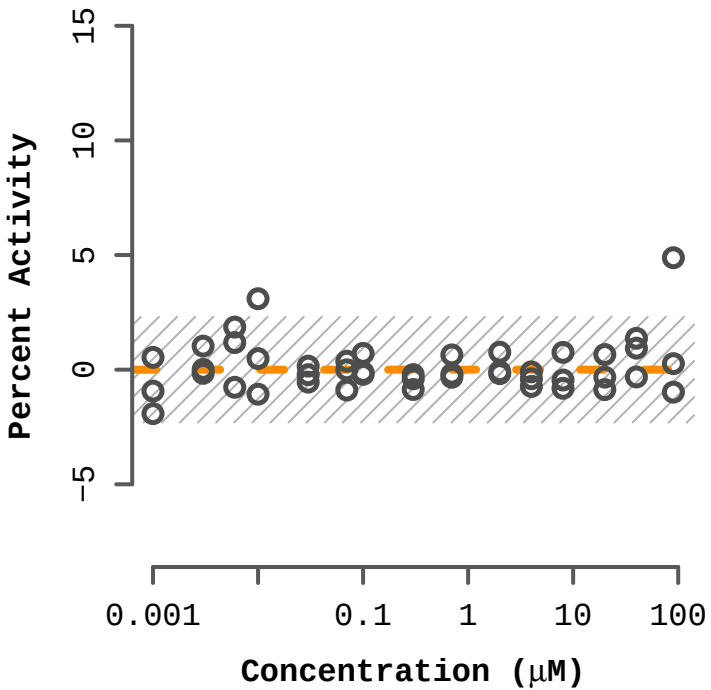
NAME: 3-Nitrobenzaldehyde
CHID: 49383 **CASRN:** 99-61-6
SPID(S): Tox21_202955
M4ID: 12479297

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.88 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

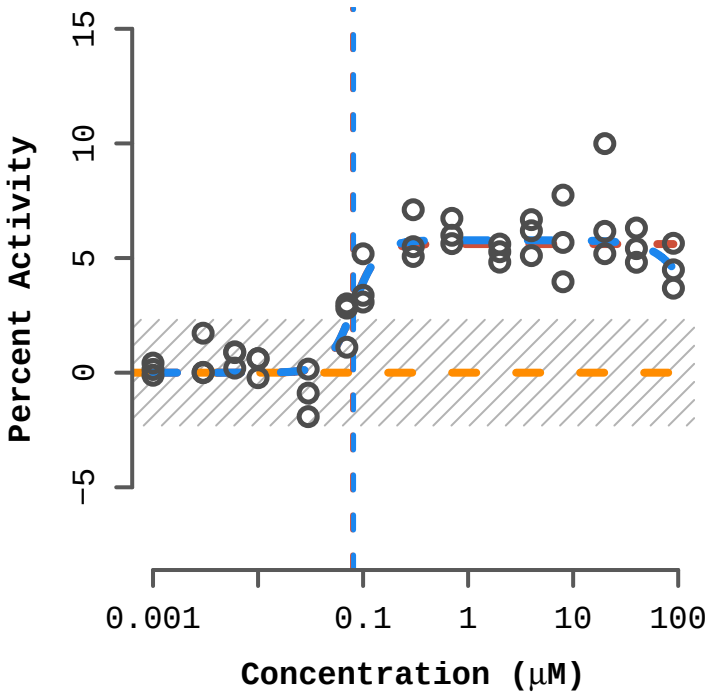
NAME: 1−Butyl−1−methylpiperidinium trifluoromethanesu
CHID: 49384 CASRN: NOCAS_49384
SPID(S): Tox21_202665
M4ID: 12479587

HILL MODEL: Not applicable.

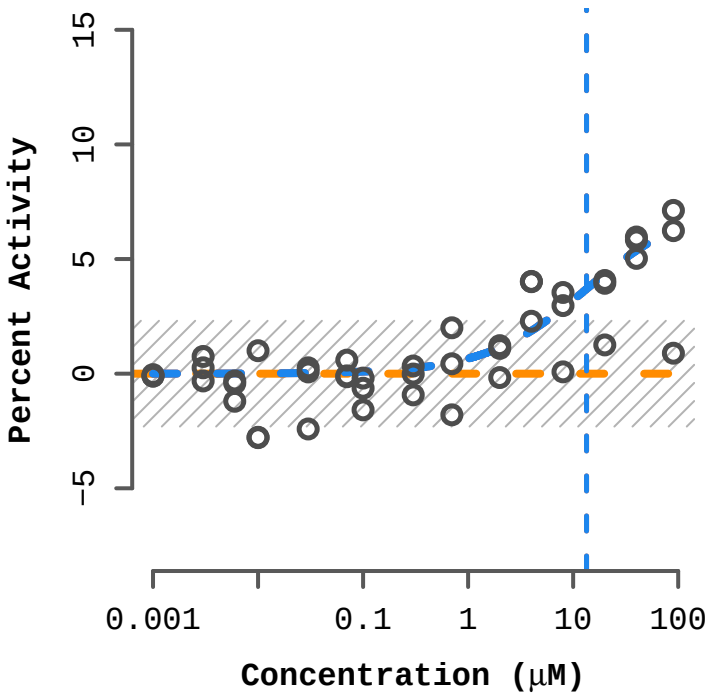
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

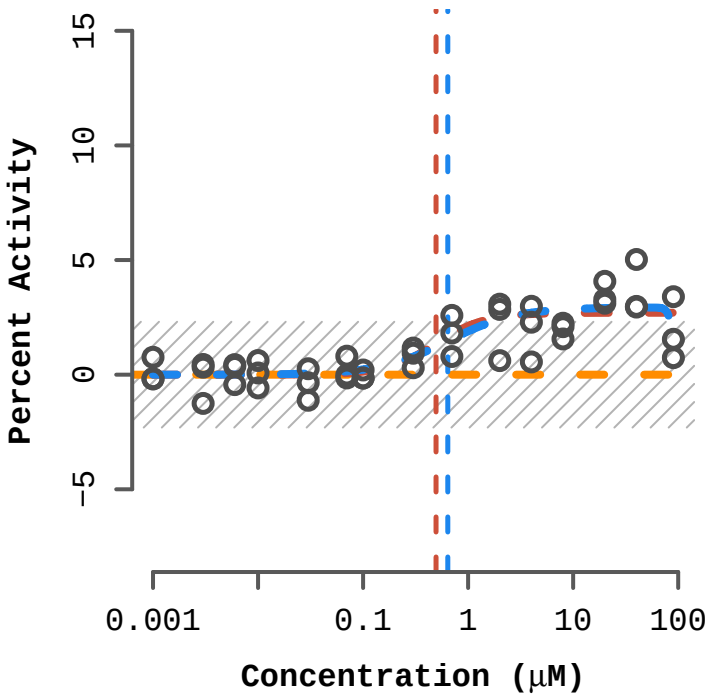
MAX_MEAN: 1.39 **MAX_MED:** 1.18 **BMAD:** 0.769



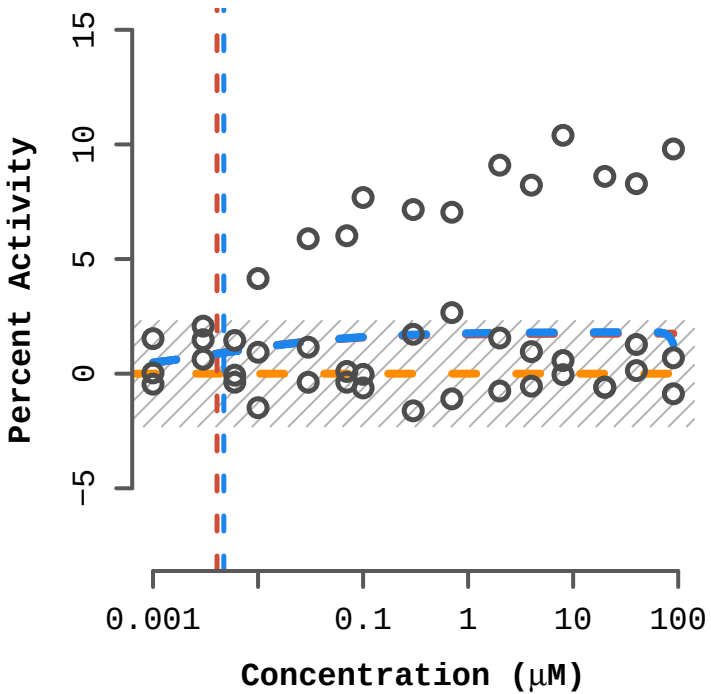

```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butyl-1-methylpiperidinium hexafluorophospha
CHID:    49385   CASRN: NOCAS_49385
SPID(S): Tox21_202666
M4ID:    12479586

HILL MODEL (in red):
      tp       ga       gw
val:  5.61     -1.1     3.81
sd:   0.197    0.0431   1.27

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.78     -1.09    3.63     2.19     2.41
sd:   0.229    0.0436   1.21     0.292    2.72

      CNST        HILL        GNLS
AIC:  271.36      138.48      138.52
PROB: 0           0.51        0.49
RMSE: 4.52        1.11        1.06

MAX_MEAN: 7.12      MAX_MED: 6.19      BMAD: 0.769
```



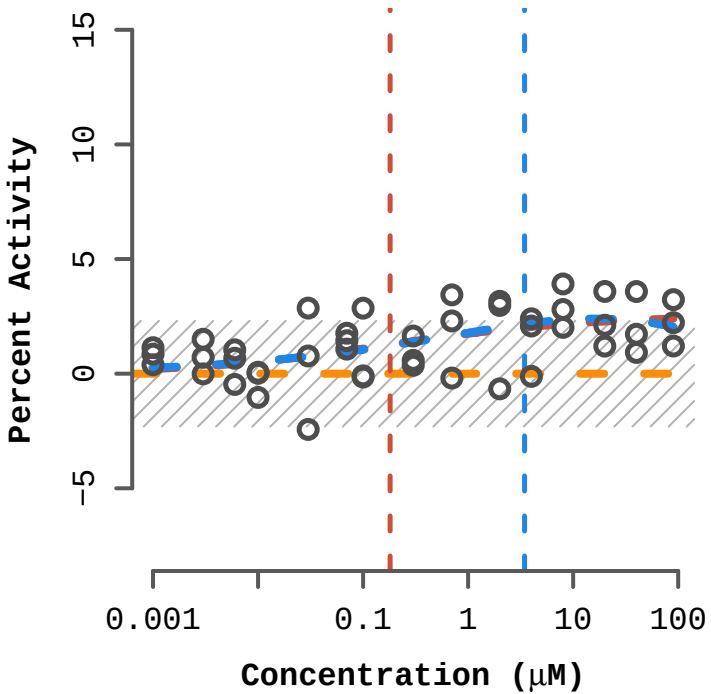

```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Methyl-1-propylpiperidinium hexafluorophospha
CHID:    49386   CASRN: NOCAS_49386
SPID(S): Tox21_202670
M4ID:    12479582

HILL MODEL (in red):
      tp       ga       gw
val:  7.39     1.13     0.895
sd:   1.9      0.343    0.251

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.39     1.13     0.895    3.22     6.05
sd:   1.9      0.343    0.251    1430     6810

      CNST        HILL        GNLS
AIC:  214.06      161.54      165.54
PROB: 0           0.88        0.12
RMSE: 2.66        1.47        1.47

MAX_MEAN: 5.61      MAX_MED: 6.24      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Methyl-1-propylpiperidinium trifluoromethanes
CHID:    49387   CASRN: NOCAS_49387
SPID(S): Tox21_202673
M4ID:    12479579

HILL MODEL (in red):
      tp       ga       gw
val:  2.7      -0.306   1.84
sd:   0.261    0.156    1.08

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.93     -0.193   1.34     1.96     17.6
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  186.03      118.24      118.72
PROB: 0           0.56        0.44
RMSE: 1.87        0.84        0.81

MAX_MEAN: 3.65      MAX_MED: 3.28      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Butyl-2-methylpyridinium trifluoromethanesul
CHID:    49388   CASRN: NOCAS_49388
SPID(S): Tox21_202677
M4ID:    12479575

HILL MODEL (in red):
      tp       ga       gw
val:  1.75     -2.39    0.696
sd:   0.818    1.35     1.36

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.82     -2.33    0.648    1.99     12.5
sd:   0.925    1.4      1.3      0.502    200

      CNST        HILL        GNLS
AIC:  251.99      248.57      252.51
PROB: 0.14        0.76        0.11
RMSE: 4.17        3.53        3.53

MAX_MEAN: 3.64      MAX_MED: 2.66      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1−Butyl−2−methylpyridinium hexafluorophosphate
CHID: 49389 CASRN: NOCAS_49389
SPID(S): Tox21_202678
M4ID: 12479574

HILL MODEL (in red):

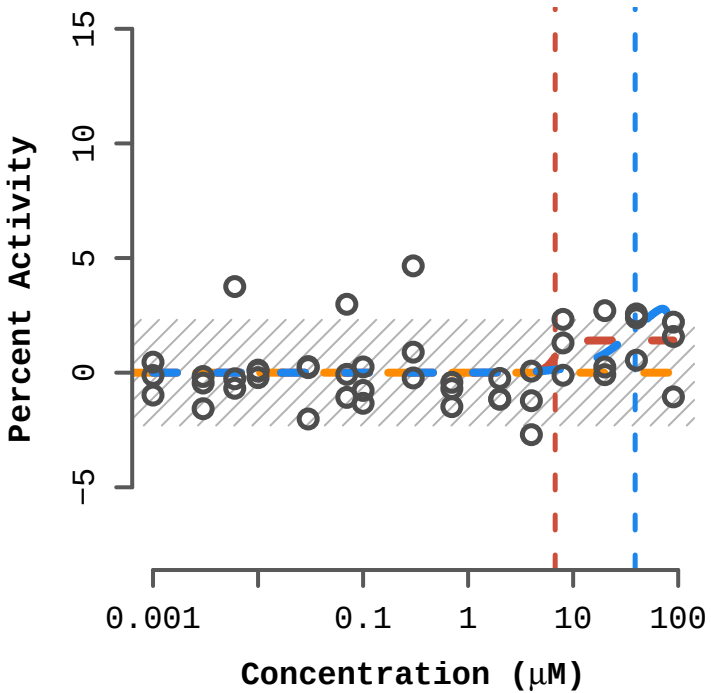
	tp	ga	gw
val:	2.53	−0.743	0.468
sd:	0.655	0.74	0.325

GAIN−LOSS MODEL (in blue):

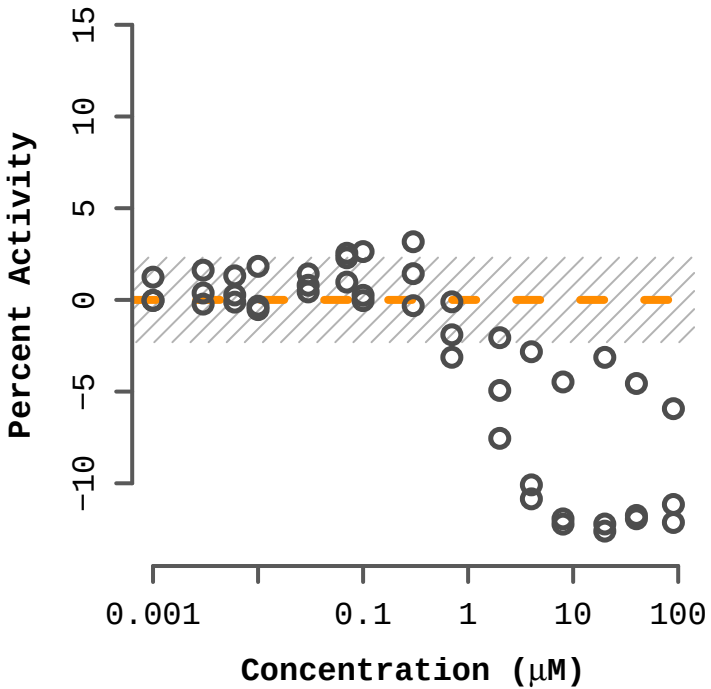
	tp	ga	gw	la	lw
val:	4.7	0.537	0.35	2.15	0.665
sd:	6.92	3.2	0.249	1.3	0.939

	CNST	HILL	GNLS
AIC:	192.91	154.29	157.53
PROB:	0	0.84	0.16
RMSE:	1.92	1.19	1.19

MAX_MEAN: 2.91 **MAX_MED:** 2.98 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Methyl-1-propylpyrrolidinium trifluoromethan
CHID:    49390   CASRN: NOCAS_49390
SPID(S): Tox21_202711
M4ID:    12479541

HILL MODEL (in red):
      tp       ga       gw
val:  1.4      0.829    8
sd:   0.445    0.139    7.99

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.79     1.59     1.89     1.95     16.2
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  166.6       162.42      167.13
PROB: 0.1         0.82        0.08
RMSE: 1.55        1.42        1.43

MAX_MEAN: 1.83      MAX_MED: 2.4       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

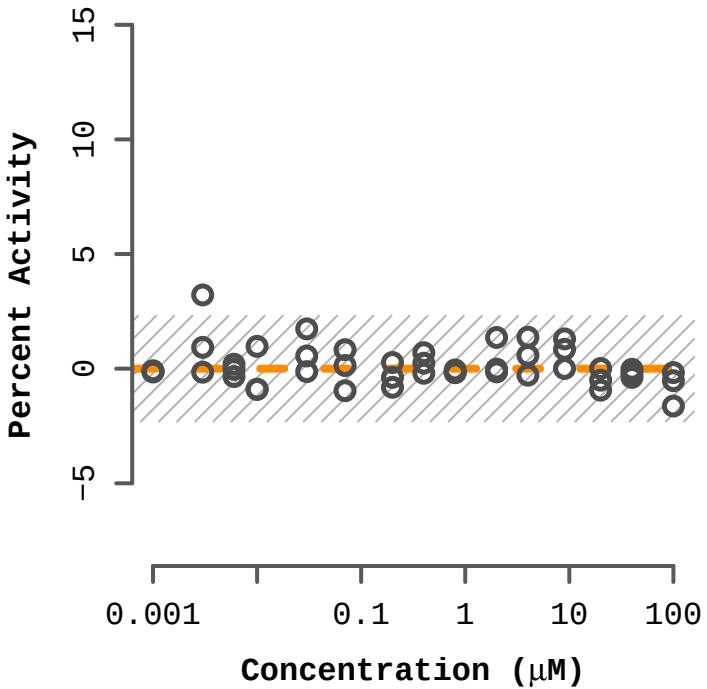
NAME: Tributyltetradecylphosphonium dodecylbenzenesu
CHID: 49391 CASRN: NOCAS_49391
SPID(S): Tox21_202712
M4ID: 12479540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	287.68	NA	NA
PROB:	1	NA	NA
RMSE:	5.98	NA	NA

MAX_MEAN: 1.94 MAX_MED: 2.3 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

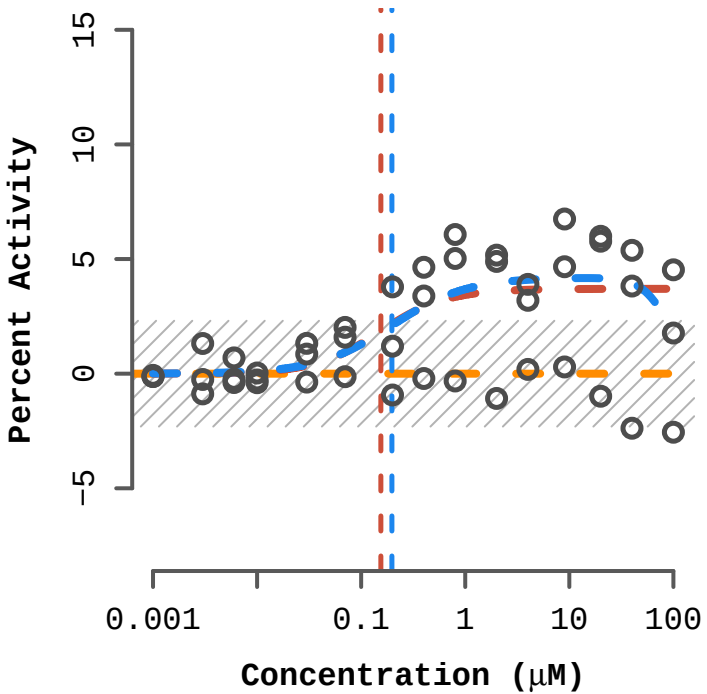
NAME: 4-Nitrobenzylbromide
CHID: 49392 **CASRN:** 100-11-8
SPID(S): Tox21_202713
M4ID: 12479539

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: alpha−Amylcinnamyl alcohol
CHID: 49393 CASRN: 101−85−9
SPID(S): Tox21_202715
M4ID: 12479537

HILL MODEL (in red):

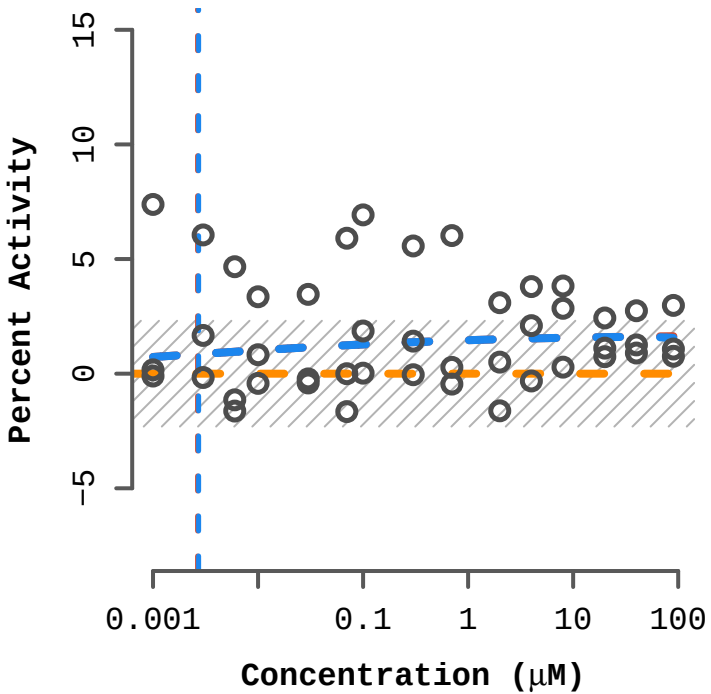
	tp	ga	gw
val:	3.7	−0.811	1.37
sd:	0.611	0.307	0.843

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.2	−0.705	1.21	1.96	3.32
sd:	0.79	0.31	0.805	0.196	4.89

	CNST	HILL	GNLS
AIC:	231.37	207.17	208.99
PROB:	0	0.71	0.29
RMSE:	3.05	2.28	2.23

MAX_MEAN: 3.9 MAX_MED: 5.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (+)Camphorquinone
CHID: 49394 **CASRN:** 10373-78-1
SPID(S): Tox21_202961
M4ID: 12479291

HILL MODEL (in red):

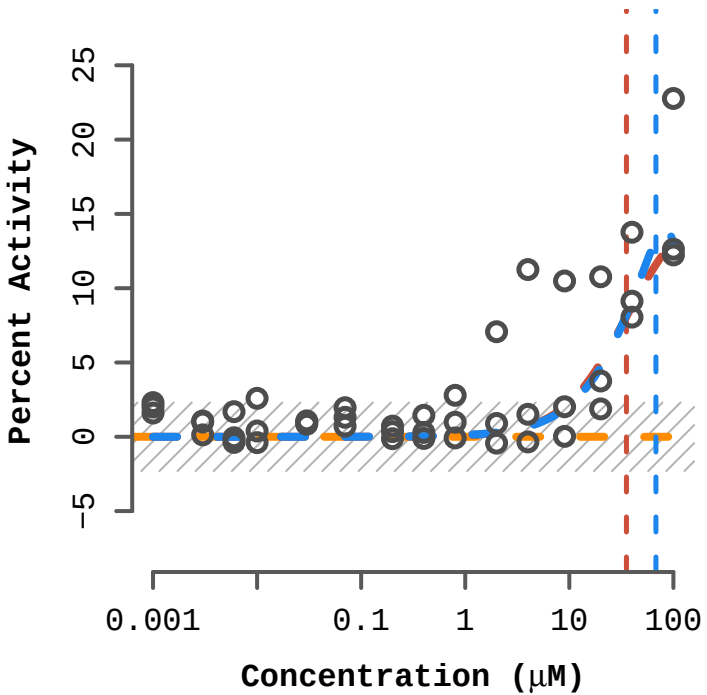
	tp	ga	gw
val:	1.71	−2.58	0.3
sd:	1.28	3.14	0.878

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.71	−2.57	0.3	2.58	2.08
sd:	1.42	3.56	0.768	11.9	39

	CNST	HILL	GNLS
AIC:	224.65	214.78	218.77
PROB:	0.01	0.87	0.12
RMSE:	2.93	2.42	2.42

MAX_MEAN: 2.94 **MAX_MED:** 2.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Pentane,1,5-dibromo-
CHID: 49395 CASRN: 111-24-0
SPID(S): Tox21_202718
M4ID: 12479534

HILL MODEL (in red):

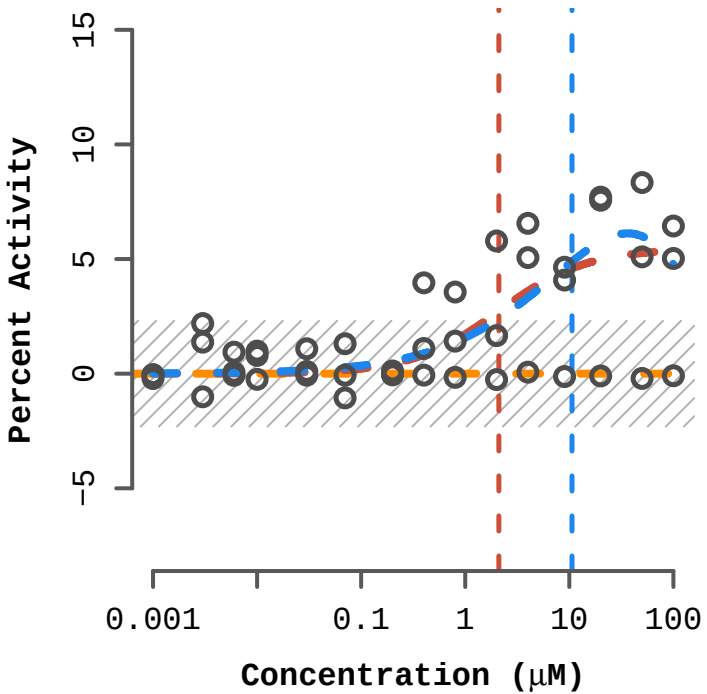
	tp	ga	gw
val:	16.2	1.55	1.42
sd:	8.06	0.366	1.26

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	27.3	1.83	1.29	2.08	6.2
sd:	31.3	0.696	0.778	0.123	13.5

	CNST	HILL	GNLS
AIC:	274.81	220.55	223.81
PROB:	0	0.84	0.16
RMSE:	6.03	3.14	3.15

MAX_MEAN: 15.9 MAX_MED: 12.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dipivaloylmethane
CHID: 49396 CASRN: 1118-71-4
SPID(S): Tox21_202720
M4ID: 12479532

HILL MODEL (in red):

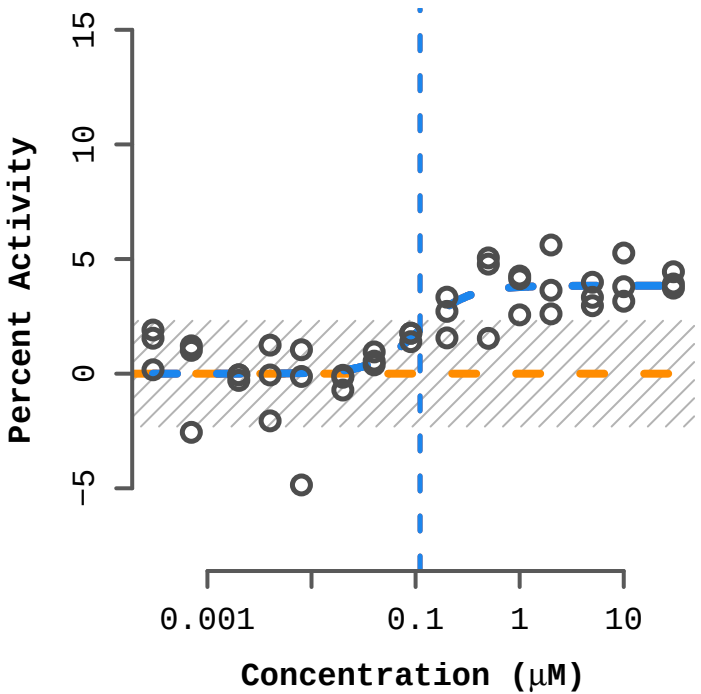
	tp	ga	gw
val:	5.46	0.323	1.04
sd:	1.06	0.337	0.543

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10	1.03	0.712	2.08	1.56
sd:	13.4	1.52	0.418	0.539	2.05

	CNST	HILL	GNLS
AIC:	229.31	201.33	204.47
PROB:	0	0.83	0.17
RMSE:	3.23	2.14	2.17

MAX_MEAN: 5.06 MAX_MED: 7.57 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hexadecane,1-bromo-
CHID: 49397 CASRN: 112-82-3
SPID(S): Tox21_202722
M4ID: 12479530

HILL MODEL (in red):

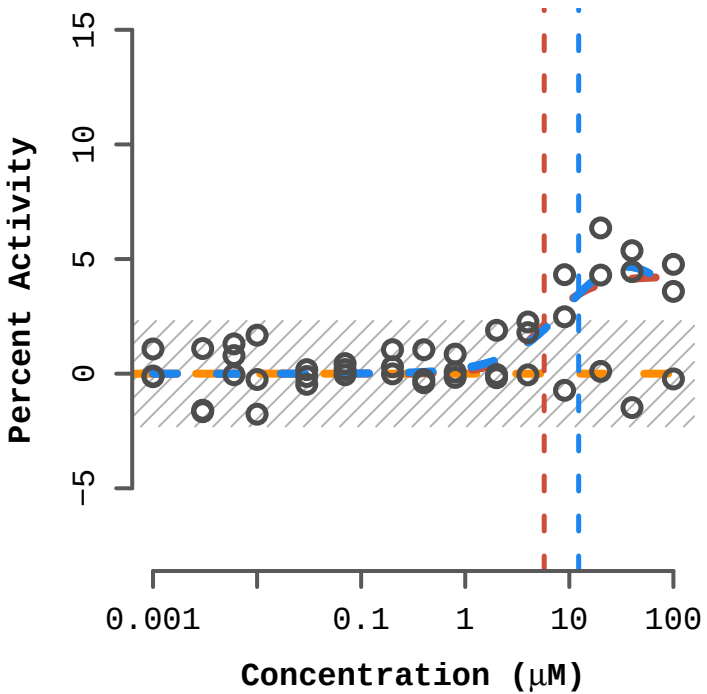
	tp	ga	gw
val:	3.84	−0.957	1.92
sd:	0.247	0.0978	0.629

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.84	−0.957	1.92	3.31	3.67
sd:	0.247	0.0978	0.629	411	822

	CNST	HILL	GNLS
AIC:	227.82	145.83	149.83
PROB:	0	0.88	0.12
RMSE:	2.82	1.22	1.22

MAX_MEAN: 4.07 MAX_MED: 4.78 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,6,6-Trimethylcyclohexa-1,3-dienylmethanal
CHID: 49398 CASRN: 116-26-7
SPID(S): Tox21_202723
M4ID: 12479529

HILL MODEL (in red):

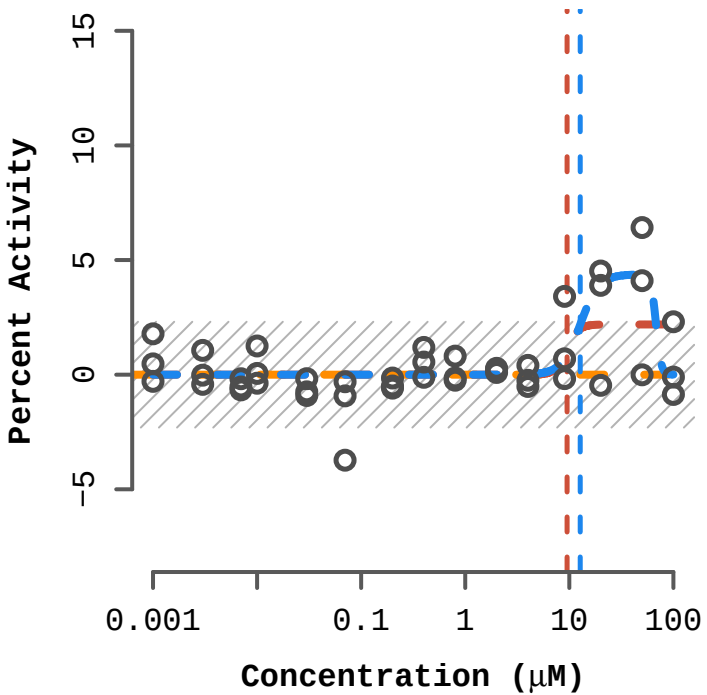
	tp	ga	gw
val:	4.23	0.759	1.98
sd:	0.575	0.148	0.997

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.63	1.09	1.34	2	1.1
sd:	14.9	0.863	0.846	1.41	2.39

	CNST	HILL	GNLS
AIC:	189.32	166.69	169.26
PROB:	0	0.78	0.22
RMSE:	2.12	1.6	1.61

MAX_MEAN: 3.59 MAX_MED: 4.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tropine
CHID: 49399 CASRN: 120-29-6
SPID(S): Tox21_202725
M4ID: 12479527

HILL MODEL (in red):

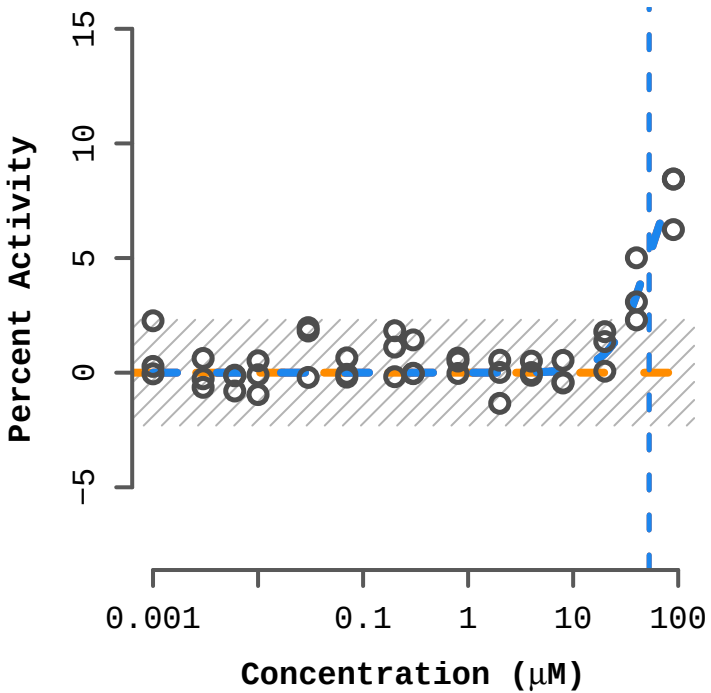
	tp	ga	gw
val:	2.19	0.978	8
sd:	1.18	0.0969	14

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.38	1.1	4.82	1.83	18
sd:	1.18	0.146	3.63	0.752	103

	CNST	HILL	GNLS
AIC:	161.96	162.32	152.82
PROB:	0.01	0.01	0.98
RMSE:	1.76	1.42	1.37

MAX_MEAN: 3.51 **MAX_MED:** 4.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dibenzosuberone
CHID: 49400 CASRN: 1210-35-1
SPID(S): Tox21_202972
M4ID: 12479280

HILL MODEL (in red):

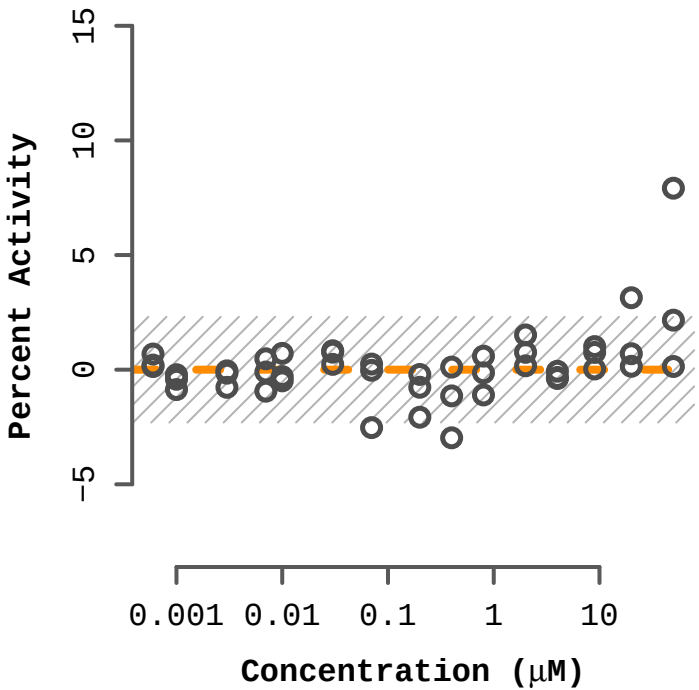
	tp	ga	gw
val:	10.1	1.72	2.48
sd:	2.42	0.118	0.819

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.1	1.72	2.48	3.94	3.27
sd:	2.42	0.118	0.819	377	626

	CNST	HILL	GNLS
AIC:	181.3	123.87	127.87
PROB:	0	0.88	0.12
RMSE:	2.37	0.88	0.88

MAX_MEAN: 7.71 MAX_MED: 8.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

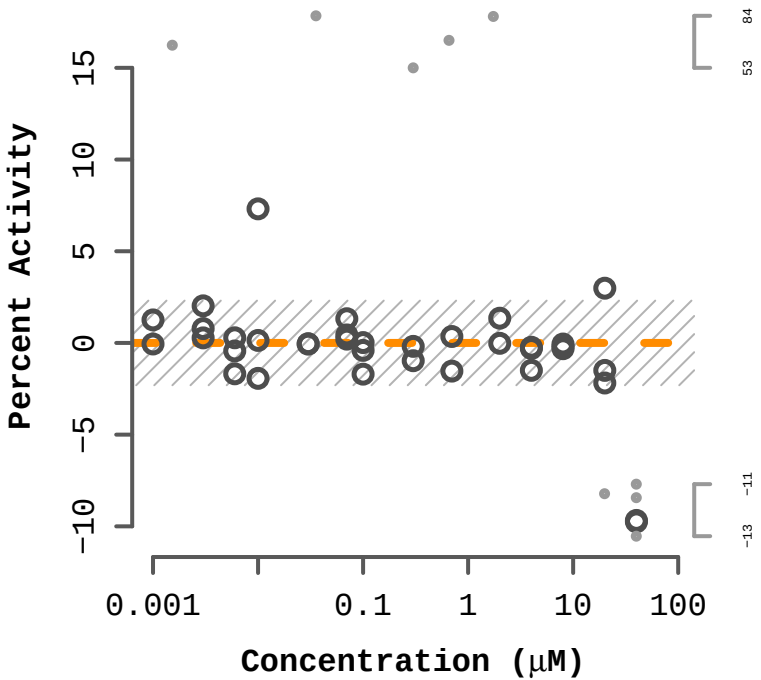
NAME: Dibenzosuberone
CHID: 49400 **CASRN:** 1210-35-1
SPID(S): Tox21_113809
M4ID: 12482410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.57	NA	NA

MAX_MEAN: 3.41 **MAX_MED:** 2.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

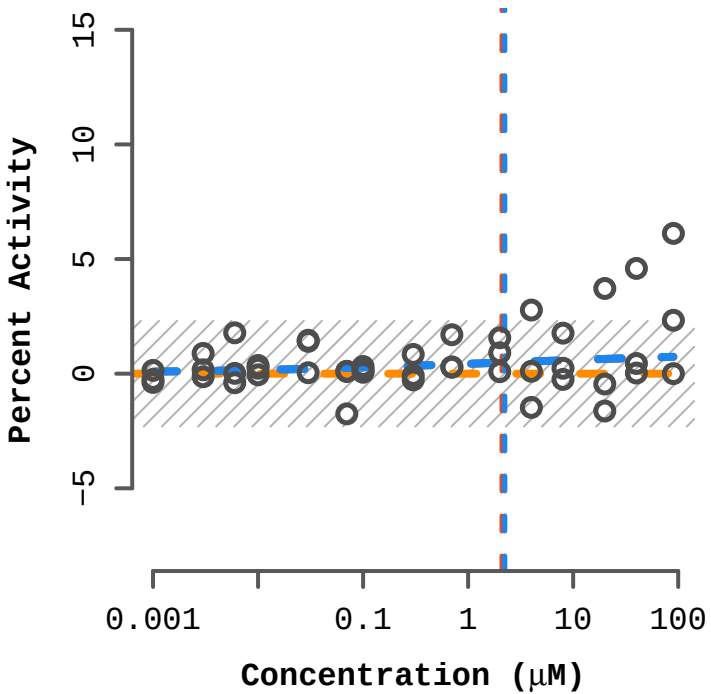
NAME: Thioridazine hydrochloride
CHID: 49401 **CASRN:** 130-61-0
SPID(S): Tox21_202801
M4ID: 12479451 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	361.34	NA	NA
PROB:	1	NA	NA
RMSE:	24.42	NA	NA

MAX_MEAN: 28.3 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zirconyl chloride octahydrate
CHID: 49402 CASRN: 13520-92-8
SPID(S): Tox21_202969
M4ID: 12479283

HILL MODEL (in red):

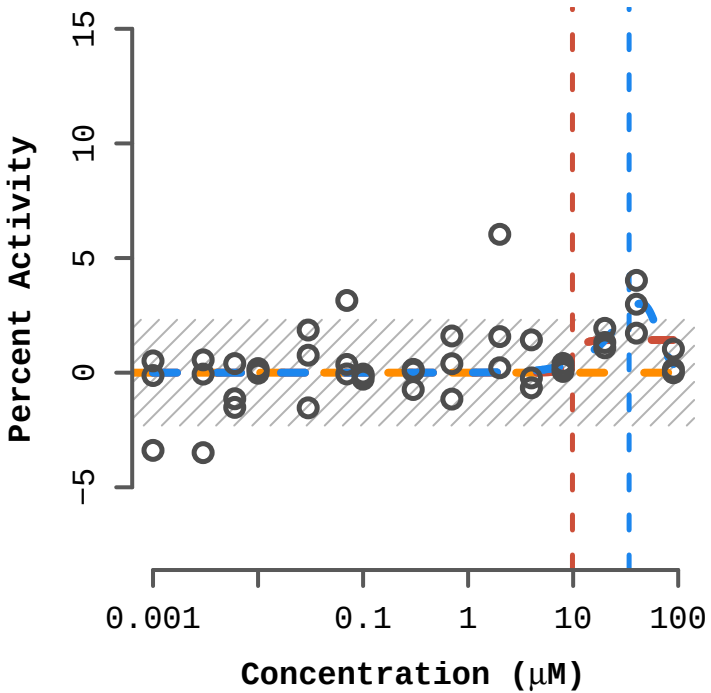
	tp	ga	gw
val:	0.968	0.323	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.977	0.349	0.3	2.74	12.2
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.02	154.94	158.94
PROB:	0.46	0.48	0.06
RMSE:	1.59	1.42	1.42

MAX_MEAN: 2.82 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,3-Trimethylindolenine
CHID: 49403 **CASRN:** 1640-39-7
SPID(S): Tox21_202974
M4ID: 12479278

HILL MODEL (in red):

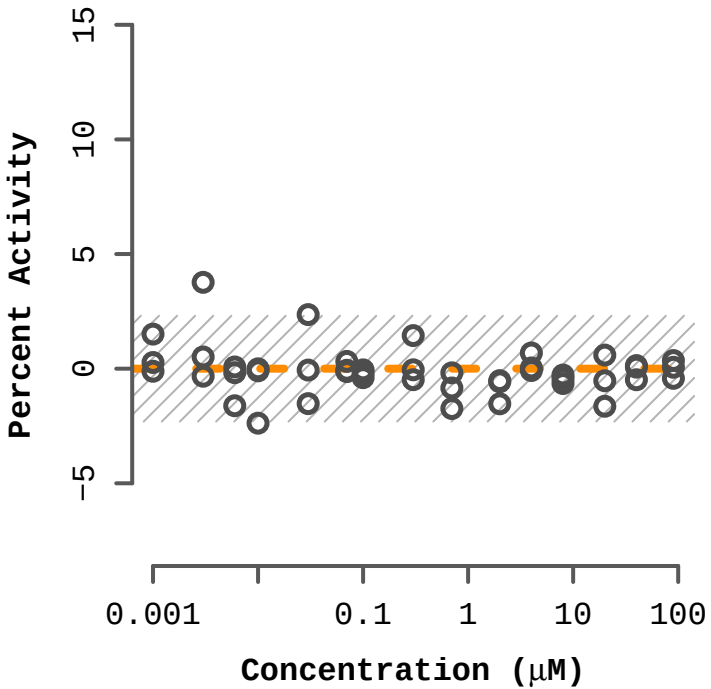
	tp	ga	gw
val:	1.42	0.993	8
sd:	0.395	0.561	48.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.49	1.53	1.97	1.78	6.27
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	167.03	160.45	154.99
PROB:	0	0.06	0.94
RMSE:	1.68	1.52	1.45

MAX_MEAN: 2.91 **MAX_MED:** 2.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

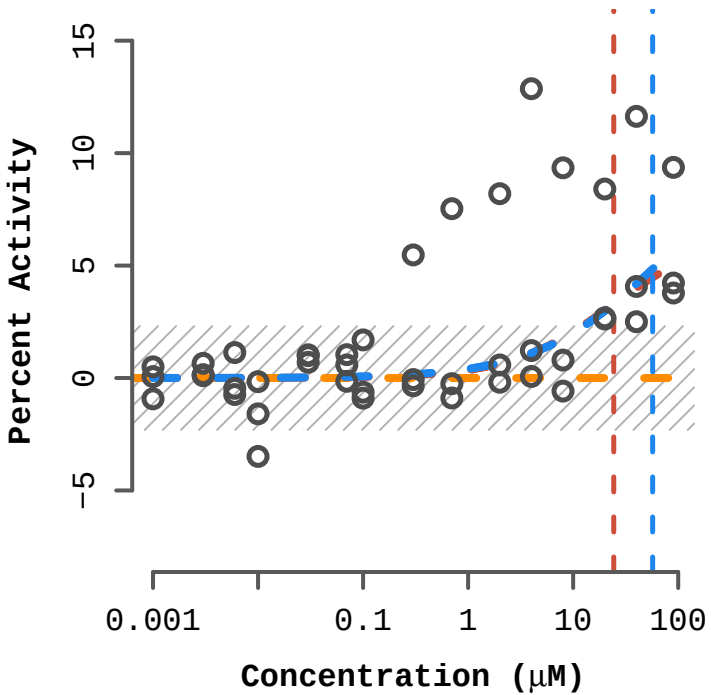
NAME: Cyanamide,cyano−,sodium salt
CHID: 49404 CASRN: 1934−75−4
SPID(S): Tox21_202811
M4ID: 12479441

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.512 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: O6-Methylguanine
CHID: 49405 CASRN: 20535-83-5
SPID(S): Tox21_202966
M4ID: 12479286

HILL MODEL (in red):

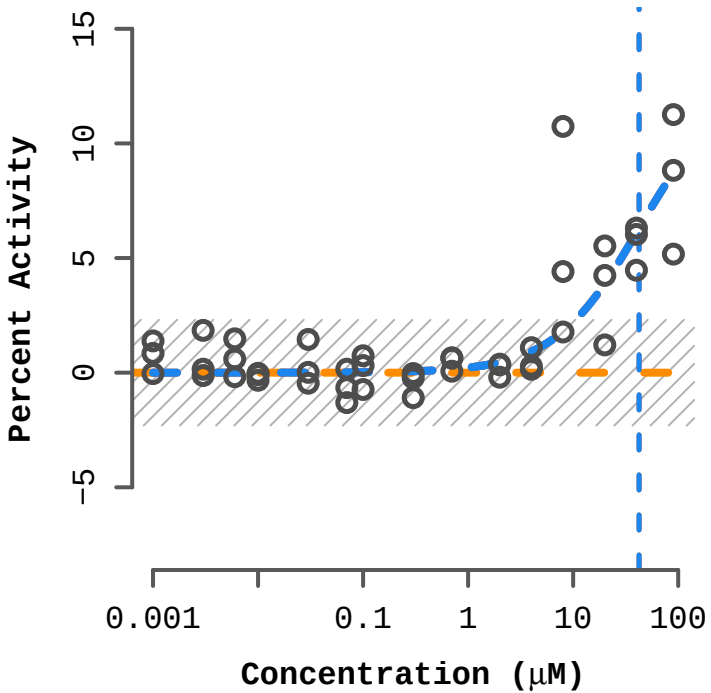
	tp	ga	gw
val:	6.57	1.39	0.887
sd:	7.36	1.28	1.17

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.71	1.76	0.773	2.01	14.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	246.9	224.69	228.6
PROB:	0	0.88	0.12
RMSE:	4.22	3.27	3.26

MAX_MEAN: 6.07 MAX_MED: 4.23 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Benzoic acid,4-(bromomethyl)-,methylester
CHID: 49406 CASRN: 2417-72-3
SPID(S): Tox21_202815
M4ID: 12479437

HILL MODEL (in red):

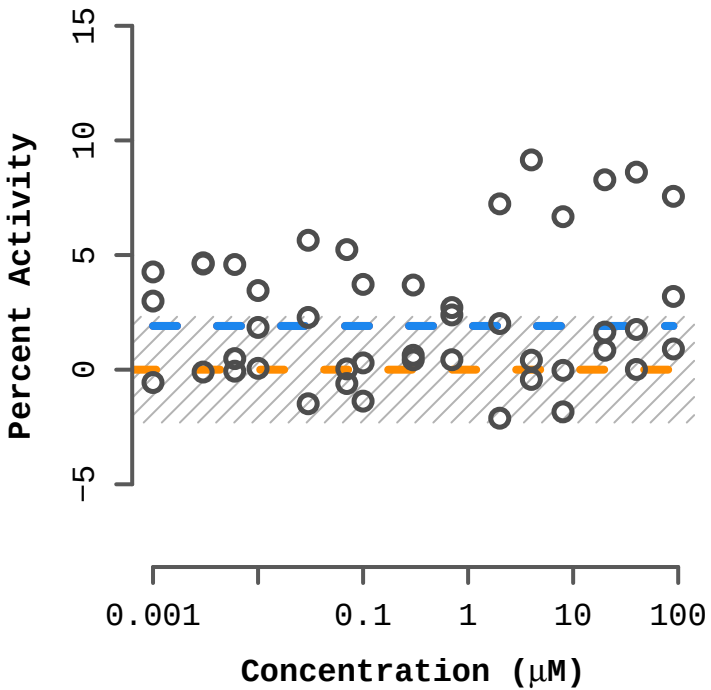
	tp	ga	gw
val:	12.6	1.63	1.08
sd:	5.18	0.362	0.279

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.6	1.63	1.08	3.95	3.69
sd:	5.18	0.362	0.279	956	1800

	CNST	HILL	GNLS
AIC:	223.39	156.38	160.38
PROB:	0	0.88	0.12
RMSE:	3.44	1.74	1.74

MAX_MEAN: 8.42 MAX_MED: 8.83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Phthalazine
CHID: 49407 CASRN: 253-52-1
SPID(S): Tox21_202907
M4ID: 12479345

HILL MODEL (in red):

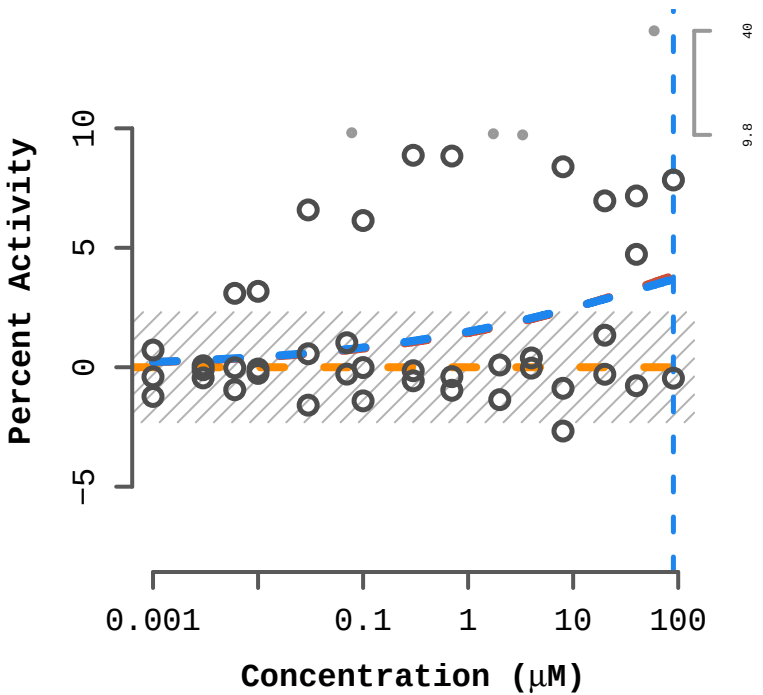
	tp	ga	gw
val:	1.91	−4.99	3.17
sd:	0.445	848	1330

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.91	−4.24	5.68	3.75	3.88
sd:	0.445	1190	5440	948	2040

	CNST	HILL	GNLS
AIC:	247.5	235.5	239.5
PROB:	0	0.88	0.12
RMSE:	3.74	2.96	2.96

MAX_MEAN: 3.89 **MAX_MED:** 4.61 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluorescein 5(6)-isothiocyanate
CHID: 49408 CASRN: 27072-45-3
SPID(S): Tox21_202818
M4ID: 12479434 BRK

HILL MODEL (in red):

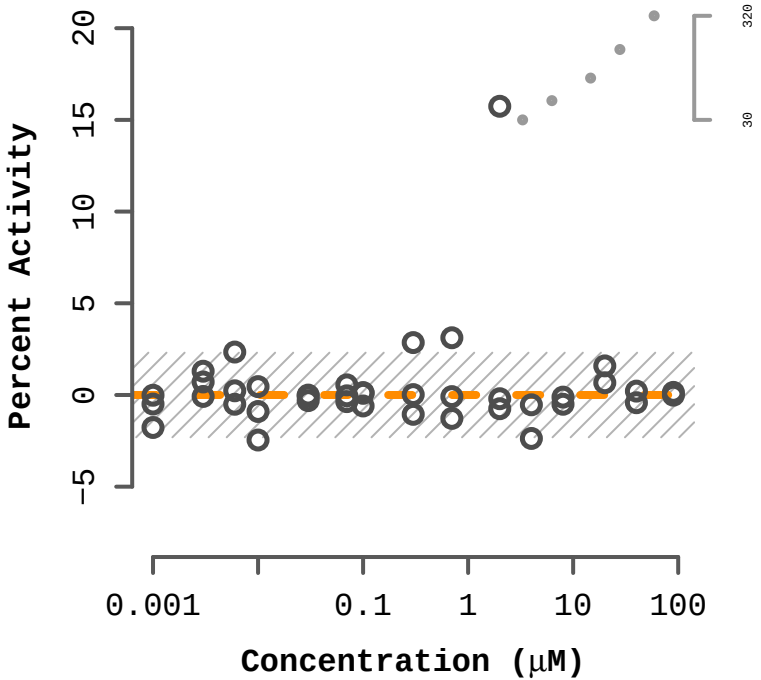
	tp	ga	gw
val:	9.26	2.45	0.3
sd:	31.7	7.26	0.248

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.37	1.95	0.304	3.61	6.48
sd:	21.7	6.68	0.248	128000	507000

	CNST	HILL	GNLS
AIC:	274.5	272.9	276.95
PROB:	0.28	0.63	0.08
RMSE:	7.41	6.62	6.64

MAX_MEAN: 15.9 MAX_MED: 7.84 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

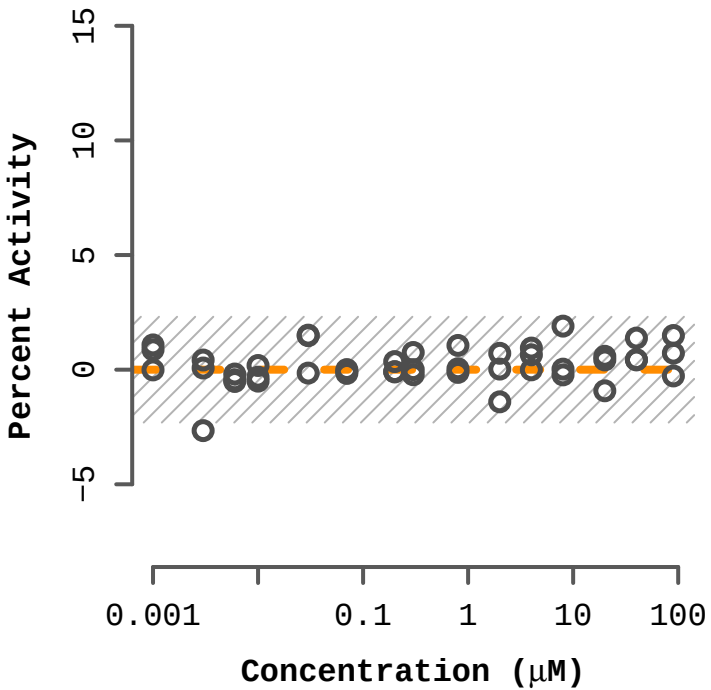
NAME: 3-Cyclobutene-1,2-dione,3,4-dihydroxy-
CHID: 49409 **CASRN:** 2892-51-5
SPID(S): Tox21_202819
M4ID: 12479433 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	350.18	NA	NA
PROB:	1	NA	NA
RMSE:	63.91	NA	NA

MAX_MEAN: 107 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

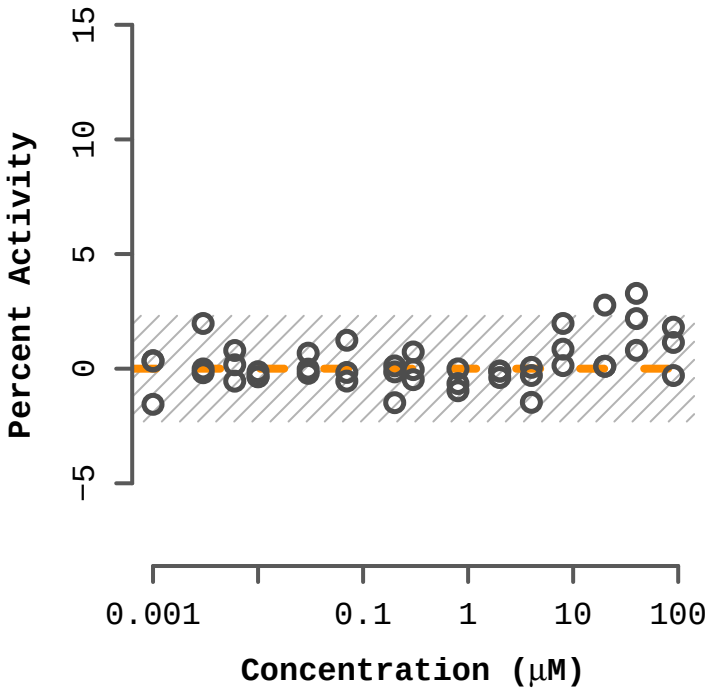
NAME: Pyrazine
CHID: 49410 CASRN: 290-37-9
SPID(S): Tox21_202911
M4ID: 12479341

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.38	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.949 MAX_MED: 1.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

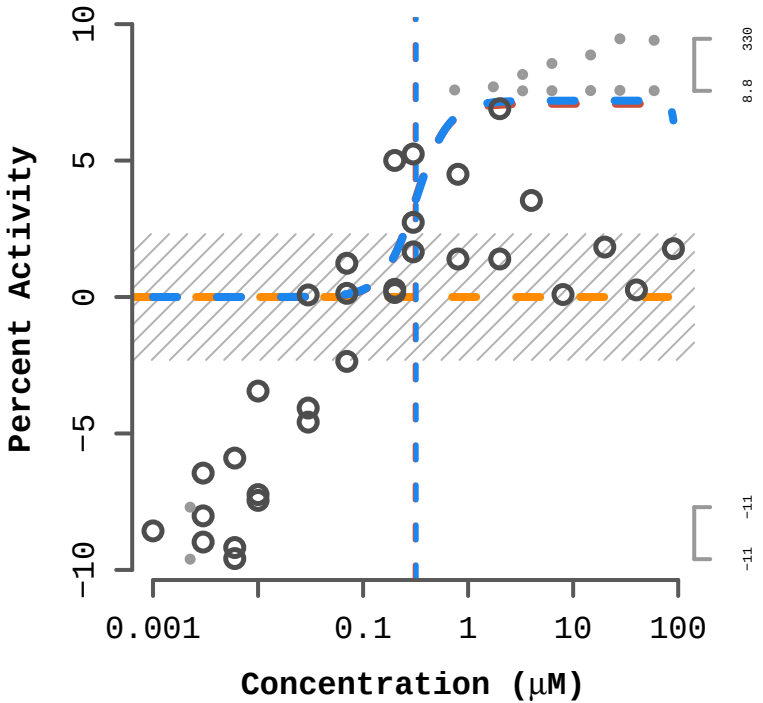
NAME: Ethylene sulfide
CHID: 49411 **CASRN:** 420-12-2
SPID(S): Tox21_202917
M4ID: 12479335

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 2.09 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Hydroxyquinazoline
CHID: 49412 CASRN: 491-36-1
SPID(S): Tox21_202920
M4ID: 12479332 BRK

HILL MODEL (in red):

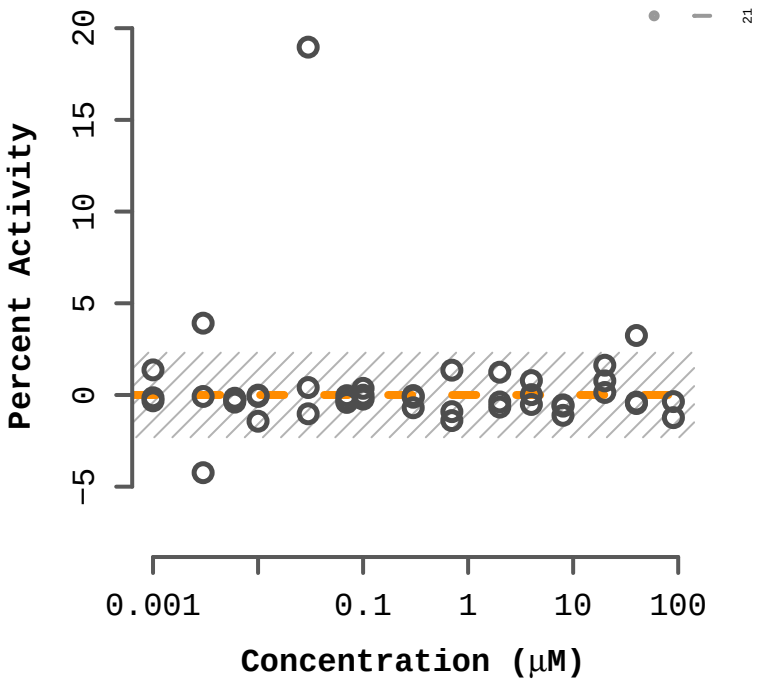
	tp	ga	gw
val:	7.08	−0.504	2.86
sd:	2.45	0.382	6.03

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.2	−0.494	2.78	2.01	18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	442.99	439.78	443.76
PROB:	0.15	0.75	0.1
RMSE:	82.62	80.29	80.31

MAX_MEAN: 113 MAX_MED: 11.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

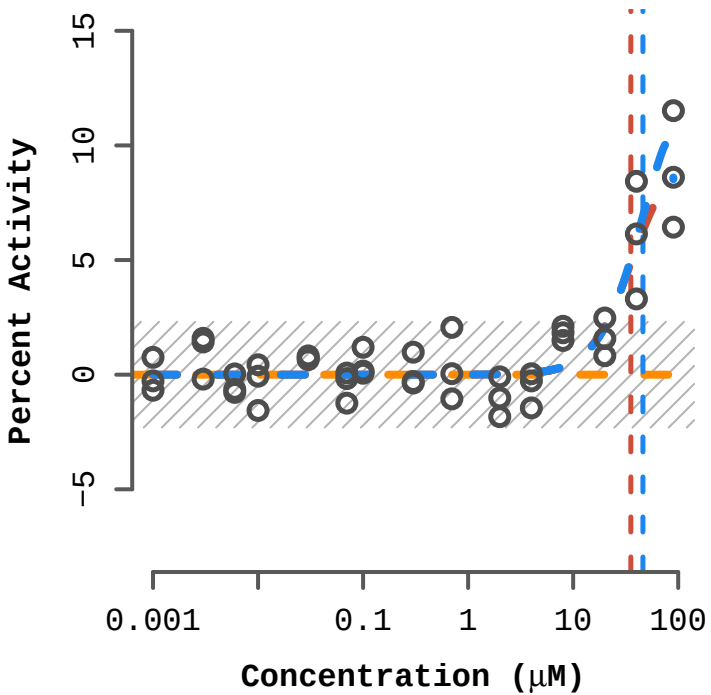
NAME: Ethanedione,di-2-furanyl-
CHID: 49413 CASRN: 492-94-4
SPID(S): Tox21_202835
M4ID: 12479417 BRK

HILL MODEL: Not applicable.

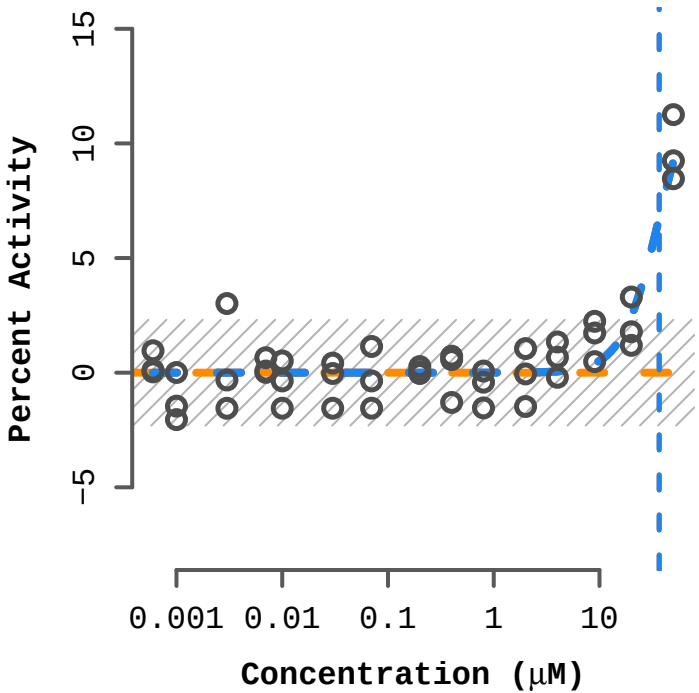
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.69	NA	NA
PROB:	1	NA	NA
RMSE:	4.41	NA	NA

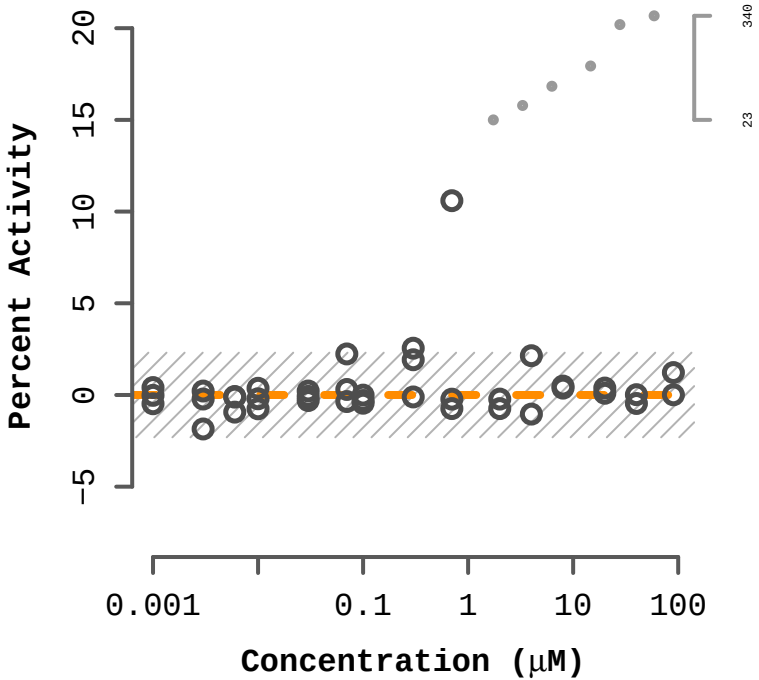
MAX_MEAN: 6.54 MAX_MED: 0.77 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    10,11-Dihydro-5H-dibenz[b,f]azepine
CHID:    49414   CASRN: 494-19-9
SPID(S): Tox21_202836
M4ID:    12479416

HILL MODEL (in red):
      tp       ga       gw
val:  9.77     1.55     2.24
sd:   3.49     0.222    1.94

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.8     1.66     2.09     1.98     18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  205.83      152.47      155.88
PROB: 0           0.85        0.15
RMSE: 3.04        1.18        1.18

MAX_MEAN: 8.86      MAX_MED: 8.61      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    10,11-Dihydro-5H-dibenz[b,f]azepine
CHID:    49414   CASRN: 494-19-9
SPID(S): Tox21_113758
M4ID:    12482457

HILL MODEL (in red):
      tp       ga       gw
val:  13.5     1.56     2.48
sd:   5.64     0.177    1.15

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.5     1.56     2.48     3.41     5.15
sd:   5.65     0.177    1.15     3720     11200

      CNST        HILL        GNLS
AIC:  190.17      143.55      147.55
PROB: 0           0.88        0.12
RMSE: 2.78        1.07        1.07

MAX_MEAN: 9.66      MAX_MED: 9.25      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

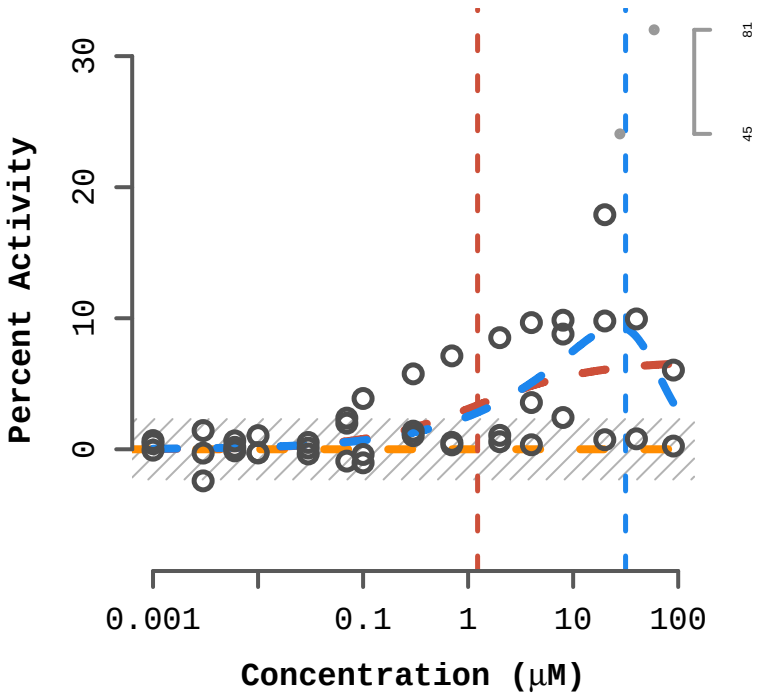
NAME: Epinephrine bitartrate
CHID: 49415 CASRN: 51-42-3
SPID(S): Tox21_202839
M4ID: 12479413 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	378.4	NA	NA
PROB:	1	NA	NA
RMSE:	78.23	NA	NA

MAX_MEAN: 115 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tropolone
CHID: 49416 CASRN: 533-75-5
SPID(S): Tox21_202924
M4ID: 12479328 BRK

HILL MODEL (in red):

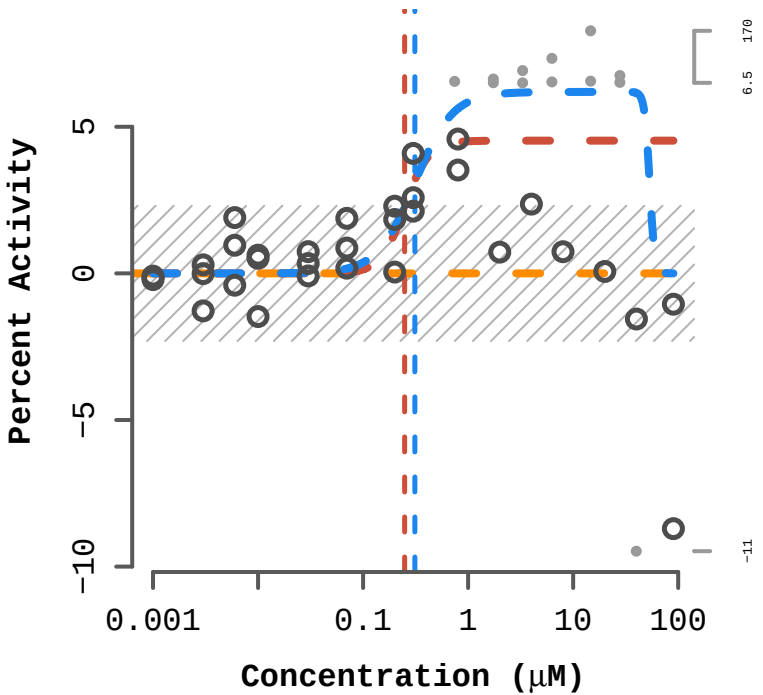
	tp	ga	gw
val:	6.72	0.0903	0.804
sd:	2.25	0.568	0.473

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	22.9	1.5	0.607	1.75	2.49
sd:	49.4	2.43	0.35	0.352	1.85

	CNST	HILL	GNLS
AIC:	302.32	284.01	284.43
PROB:	0	0.55	0.45
RMSE:	14.7	13	13.2

MAX_MEAN: 29.2 MAX_MED: 9.95 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Maleimide
CHID: 49417 CASRN: 541-59-3
SPID(S): Tox21_202926
M4ID: 12479326 BRK

HILL MODEL (in red):

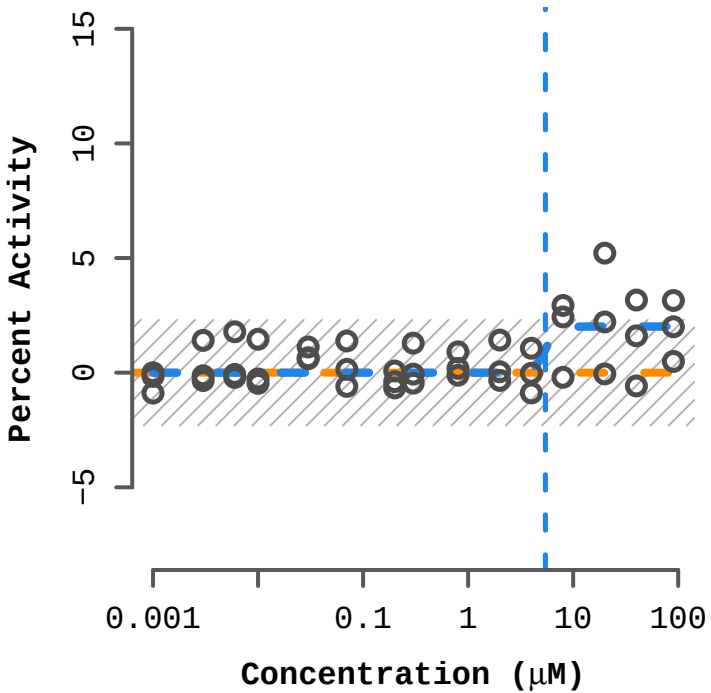
	tp	ga	gw
val:	4.53	−0.605	3.82
sd:	1.42	0.202	6.81

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.19	−0.507	2.42	1.73	18
sd:	1.65	0.223	4.27	0.849	85.8

	CNST	HILL	GNLS
AIC:	347.83	342.26	337.75
PROB:	0.01	0.09	0.9
RMSE:	29.86	28.67	28.16

MAX_MEAN: 60.8 MAX_MED: 11.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-Butylnitrite
CHID: 49418 **CASRN:** 544-16-1
SPID(S): Tox21_202927
M4ID: 12479325

HILL MODEL (in red):

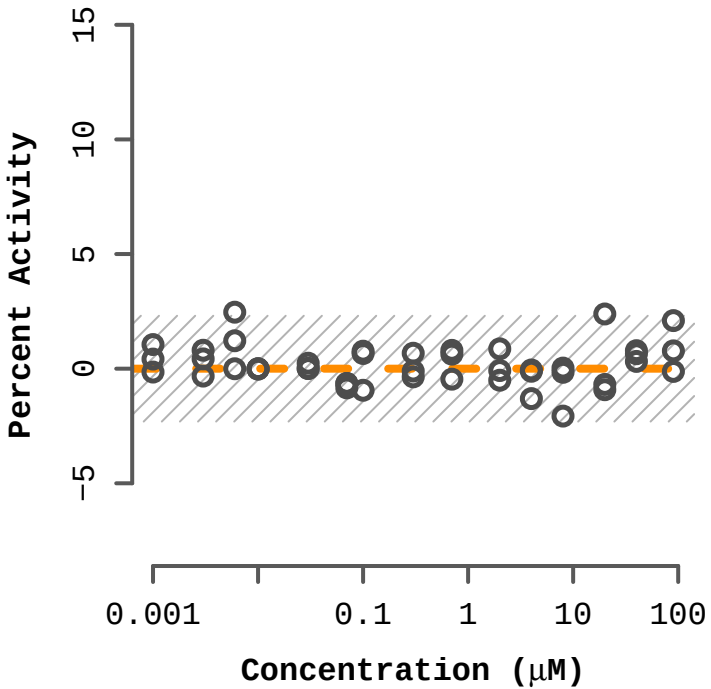
	tp	ga	gw
val:	2.01	0.736	8
sd:	0.384	0.13	7.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.01	0.736	8	3.55	5.08
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	155.4	141.51	145.51
PROB:	0	0.88	0.12
RMSE:	1.45	1.08	1.08

MAX_MEAN: 2.46 **MAX_MED:** 2.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

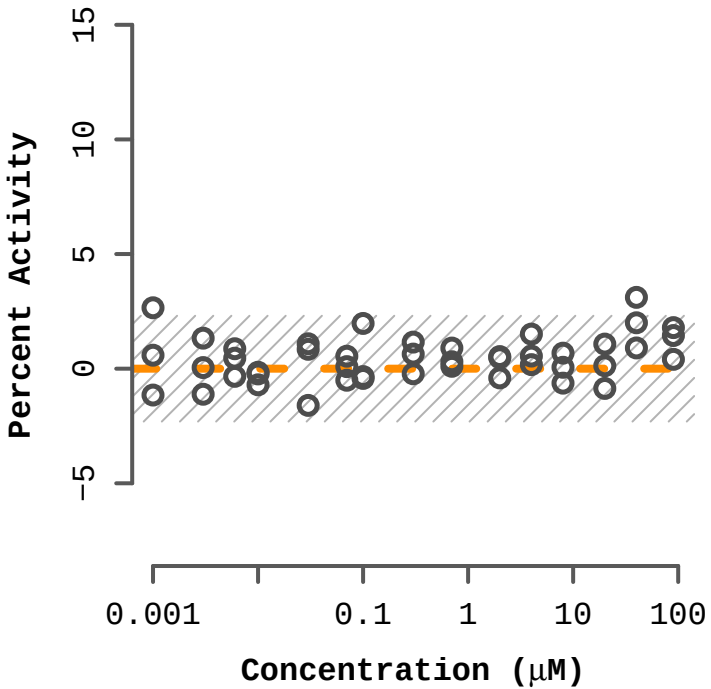
NAME: Atropine sulfate anhydrous (2:1) salt
CHID: 49419 CASRN: 55-48-1
SPID(S): Tox21_202846
M4ID: 12479406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

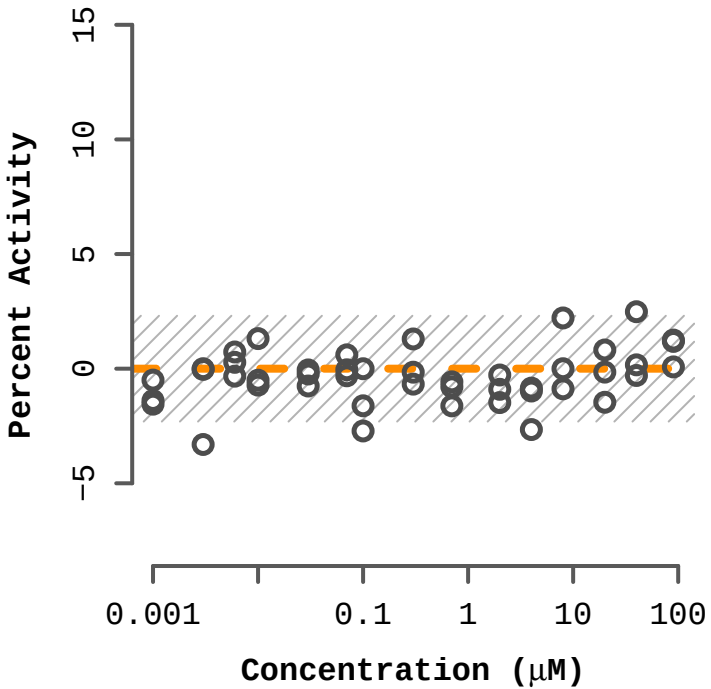
NAME: 2-Amino-4,6-dichloropyrimidine
CHID: 49420 **CASRN:** 56-05-3
SPID(S): Tox21_202931
M4ID: 12479321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 2.01 **MAX_MED:** 2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

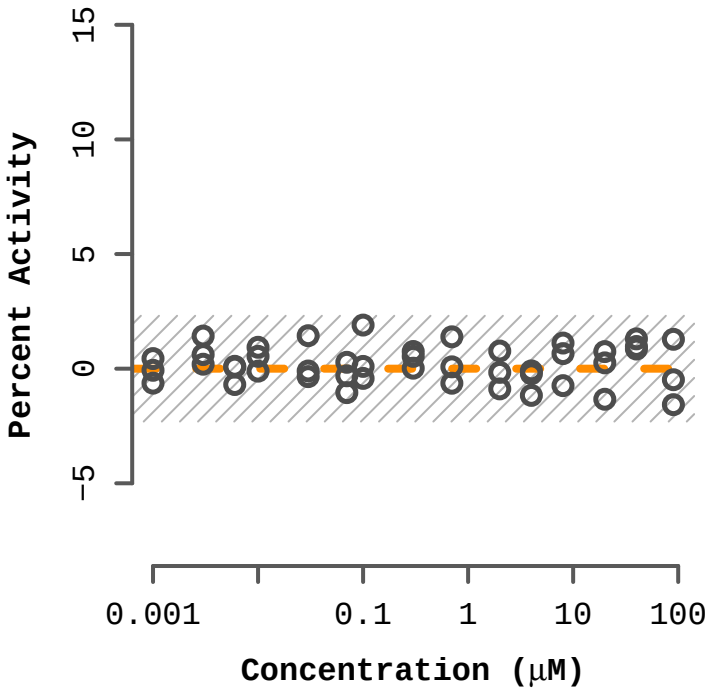
NAME: Betaine monohydrate
CHID: 49421 **CASRN:** 590-47-6
SPID(S): Tox21_202851
M4ID: 12479401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.76	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.839 **MAX_MED:** 1.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

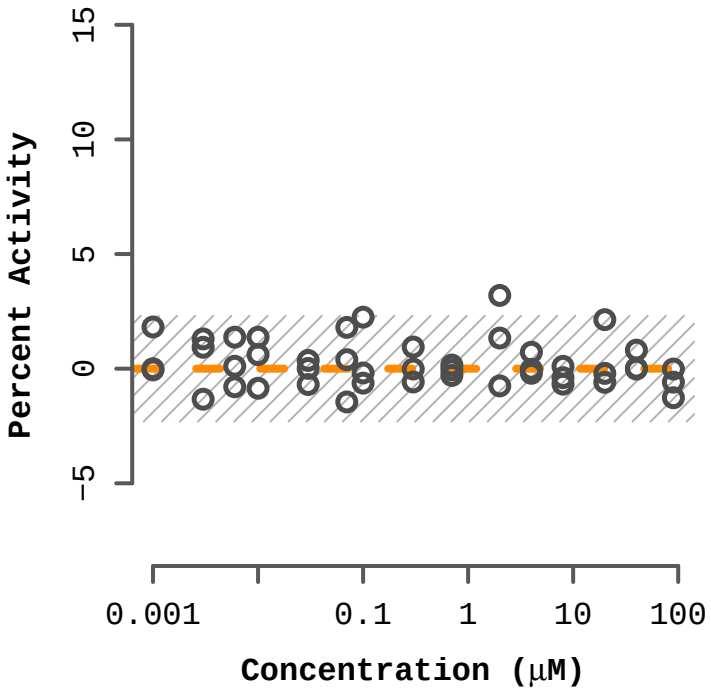
NAME: Procainamide hydrochloride
CHID: 49422 CASRN: 614-39-1
SPID(S): Tox21_202855
M4ID: 12479397

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

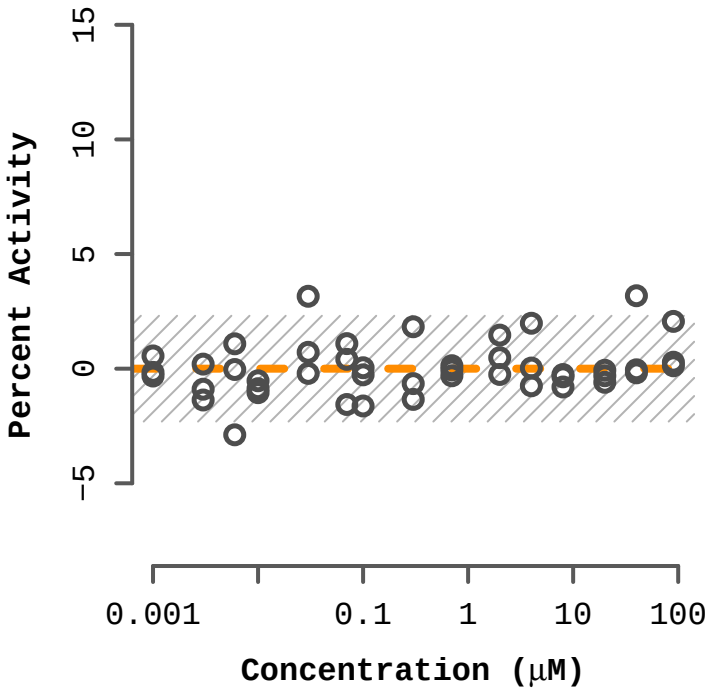
NAME: 3-Hydroxy-4-methoxy-benzaldehyde
CHID: 49423 **CASRN:** 621-59-0
SPID(S): Tox21_202858
M4ID: 12479394

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.46	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

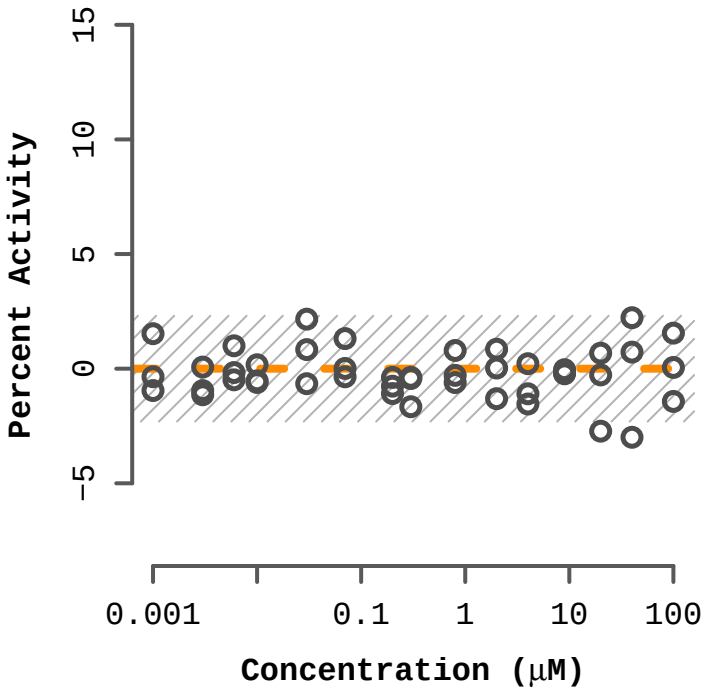
NAME: 1,8−Diazabicyclo[5.4.0]undec−7−ene
CHID: 49424 **CASRN:** 6674−22−2
SPID(S): Tox21_202939
M4ID: 12479313

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 0.716 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

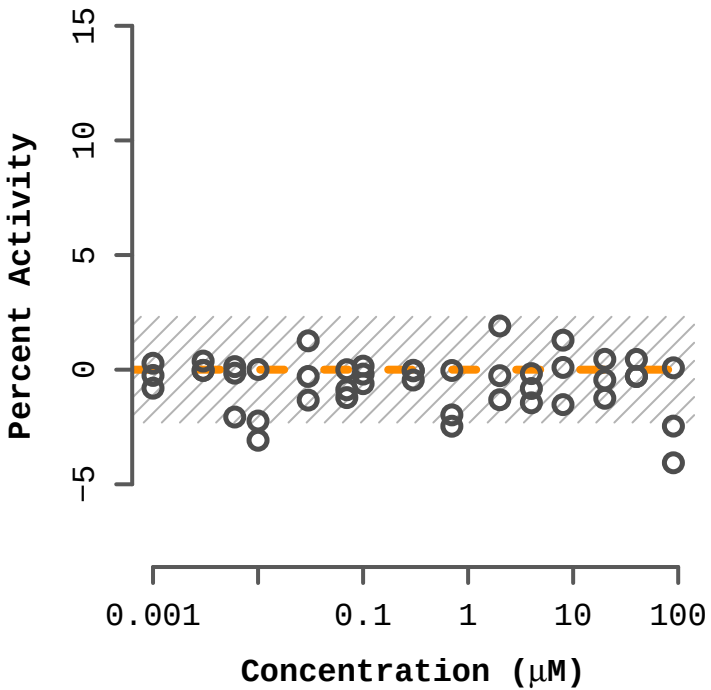
NAME: Tetracyanoethylene
CHID: 49425 **CASRN:** 670-54-2
SPID(S): Tox21_202940
M4ID: 12479312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.834 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

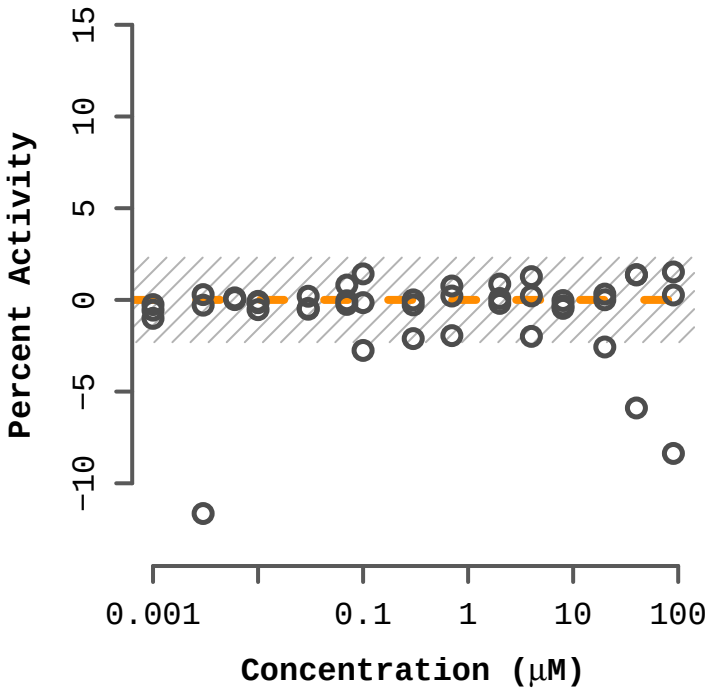
NAME: 2-Bromoacetophenone
CHID: 49426 CASRN: 70-11-1
SPID(S): Tox21_202941
M4ID: 12479311

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.113 MAX_MED: 0.0986 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

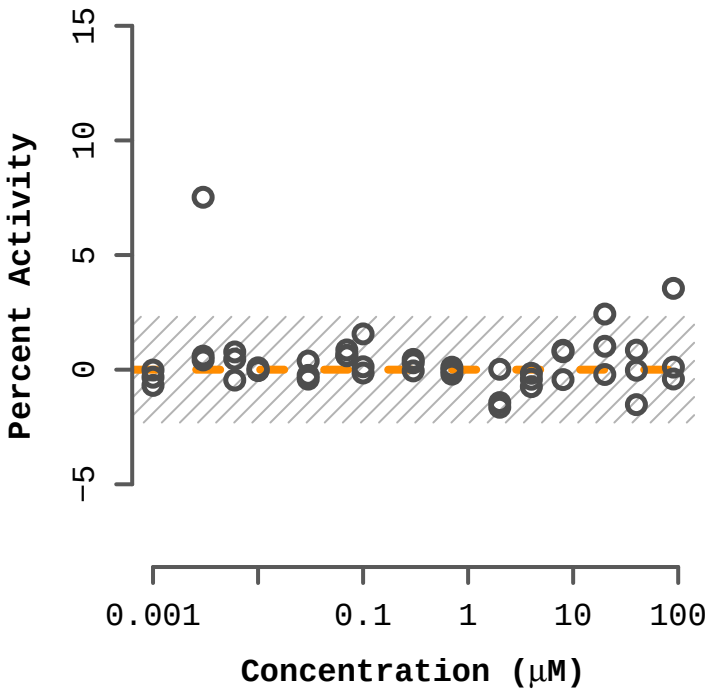
NAME: 9-Anthracenecarboxylic acid
CHID: 49427 **CASRN:** 723-62-6
SPID(S): Tox21_202942
M4ID: 12479310

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.5	NA	NA

MAX_MEAN: 0.253 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

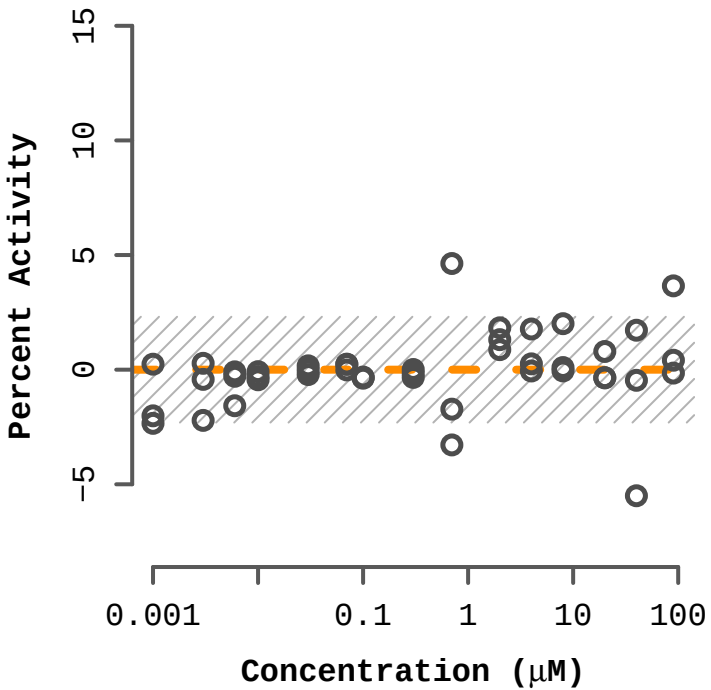
NAME: 3-Indazolinone
CHID: 49428 **CASRN:** 7364-25-2
SPID(S): Tox21_202943
M4ID: 12479309

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.44	NA	NA

MAX_MEAN: 2.85 **MAX_MED:** 1.02 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

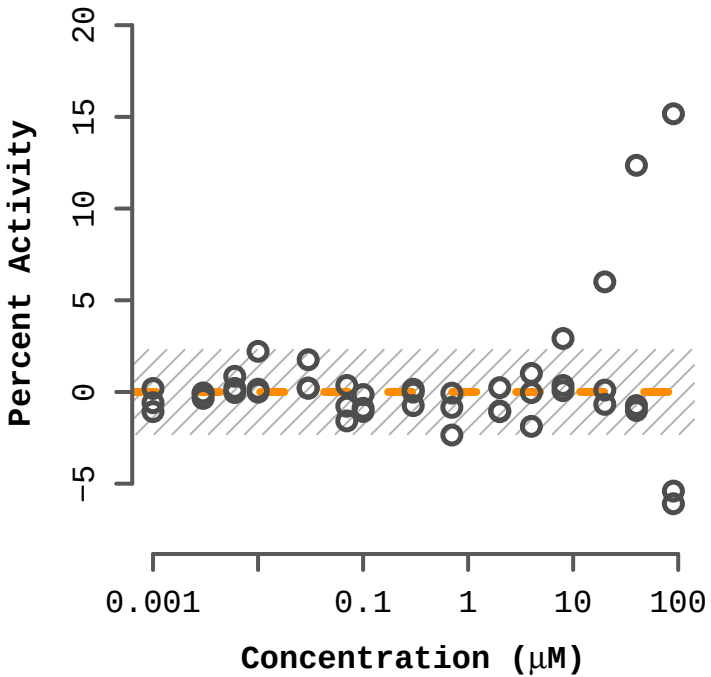
NAME: Acenaphthenequinone
CHID: 49429 CASRN: 82-86-0
SPID(S): Tox21_202947
M4ID: 12479305

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.59	NA	NA

MAX_MEAN: 1.34 MAX_MED: 1.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

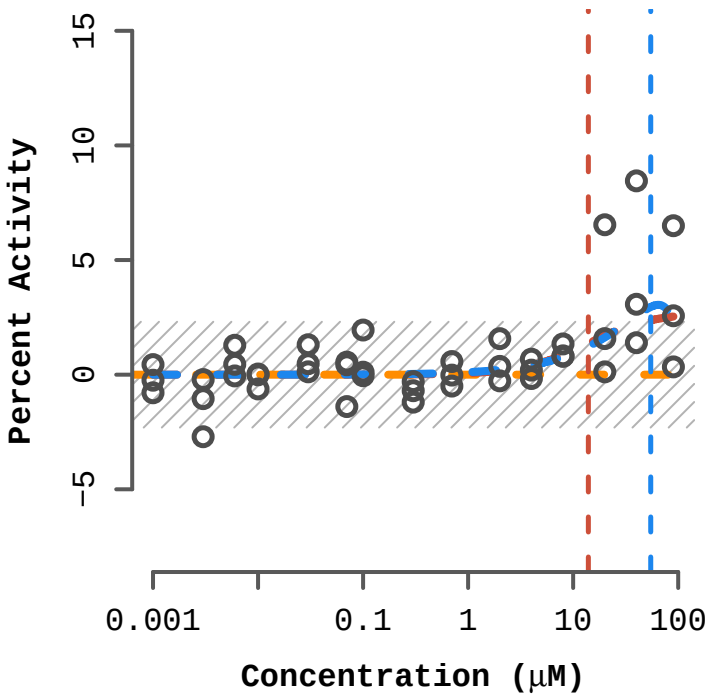
NAME: Lapachol
CHID: 49430 CASRN: 84-79-7
SPID(S): Tox21_202948
M4ID: 12479304

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	197.75	NA	NA
PROB:	1	NA	NA
RMSE:	3.42	NA	NA

MAX_MEAN: 3.54 MAX_MED: 0.357 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Anthrone
CHID: 49431 CASRN: 90-44-8
SPID(S): Tox21_202949
M4ID: 12479303

HILL MODEL (in red):

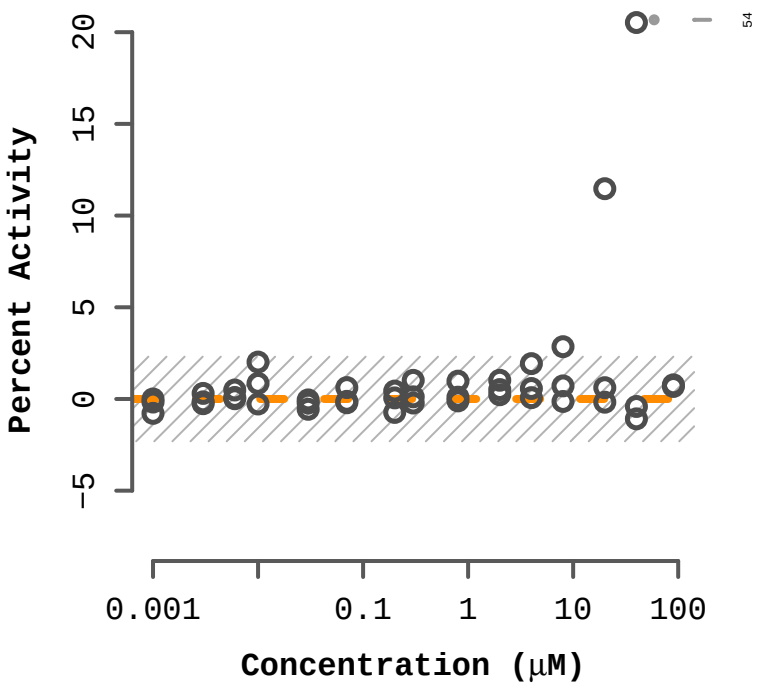
	tp	ga	gw
val:	2.72	1.14	1.4
sd:	1.17	0.404	0.973

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.08	1.74	1	1.99	6.15
sd:	20.1	2.5	0.981	0.297	32.1

	CNST	HILL	GNLS
AIC:	172.46	156.6	160.24
PROB:	0	0.86	0.14
RMSE:	2.14	1.58	1.56

MAX_MEAN: 4.31 MAX_MED: 3.07 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

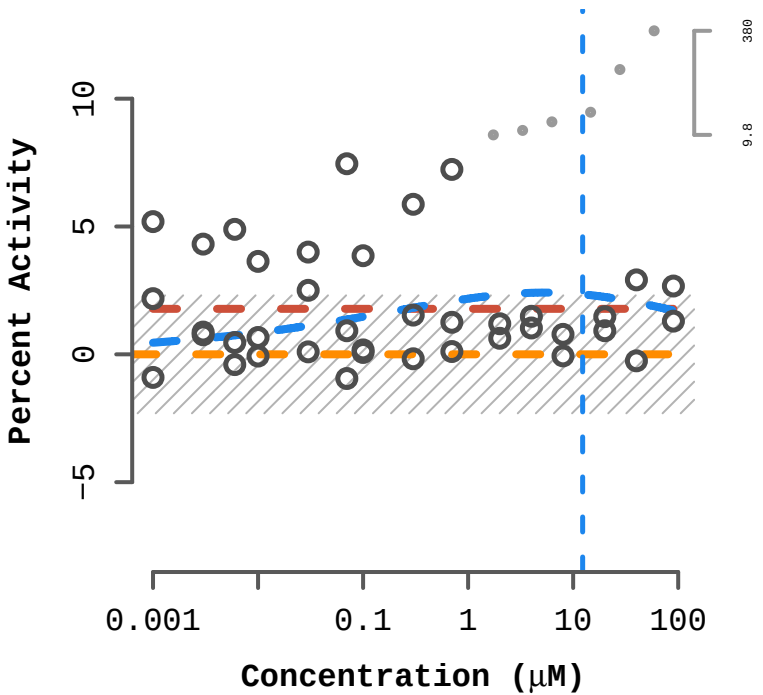
NAME: Quinoxaline
CHID: 49432 CASRN: 91-19-0
SPID(S): Tox21_202950
M4ID: 12479302 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.92	NA	NA
PROB:	1	NA	NA
RMSE:	8.78	NA	NA

MAX_MEAN: 18.4 MAX_MED: 0.852 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Pyrazolidinone,1-phenyl-
CHID: 49433 CASRN: 92-43-3
SPID(S): Tox21_202877
M4ID: 12479375 BRK

HILL MODEL (in red):

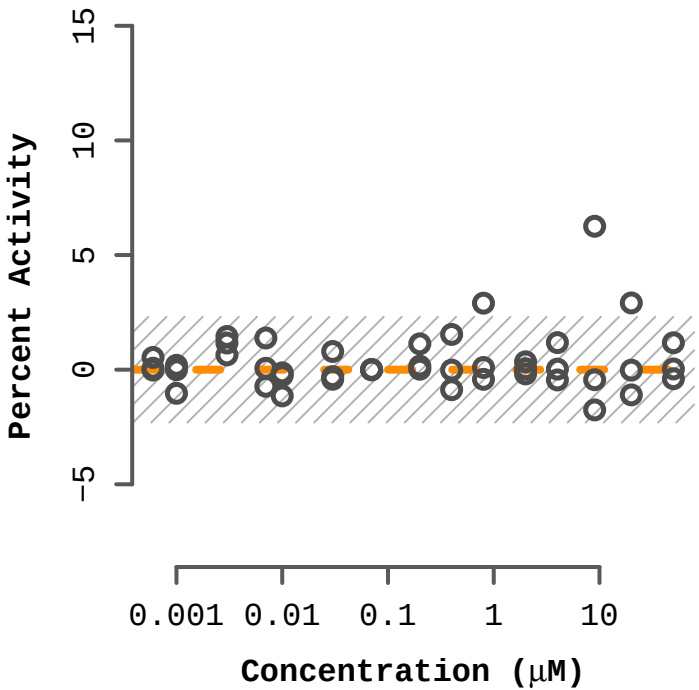
	tp	ga	gw
val:	1.78	-4.82	3.66
sd:	0.516	1740	3490

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.17	1.09	0.3	1.34	0.517
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	367.42	362.32	368.28
PROB:	0.07	0.89	0.04
RMSE:	68.6	68.12	68.08

MAX_MEAN: 127 MAX_MED: 2.91 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

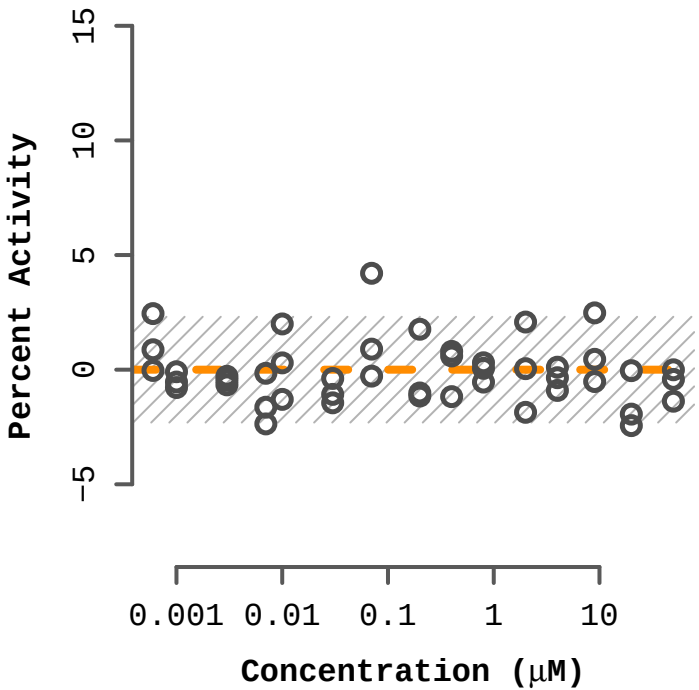
NAME: NTP Mix57 CT1 62-EQP
CHID: 49445 **CASRN:** NOCAS_49445
SPID(S): Tox21_203004
M4ID: 12479248

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

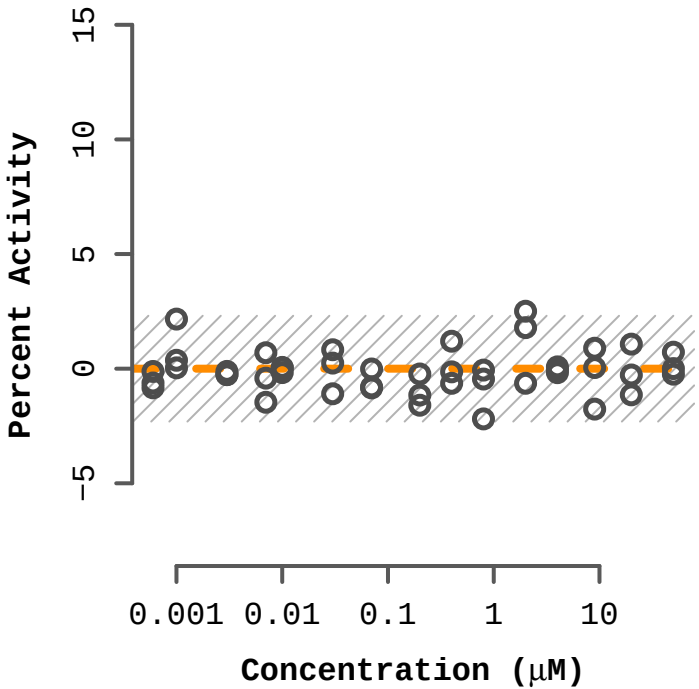
NAME: NTP Mix58 CT1 62-EQP
CHID: 49446 **CASRN:** NOCAS_49446
SPID(S): Tox21_203005
M4ID: 12479247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 0.897 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

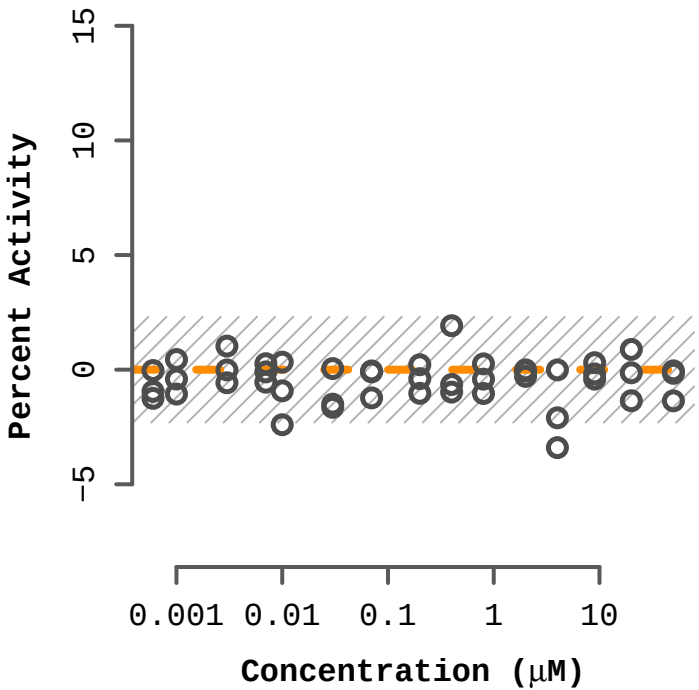
NAME: NTP Mix59 CT1 62-EQP
CHID: 49447 **CASRN:** NOCAS_49447
SPID(S): Tox21_203006
M4ID: 12479246

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

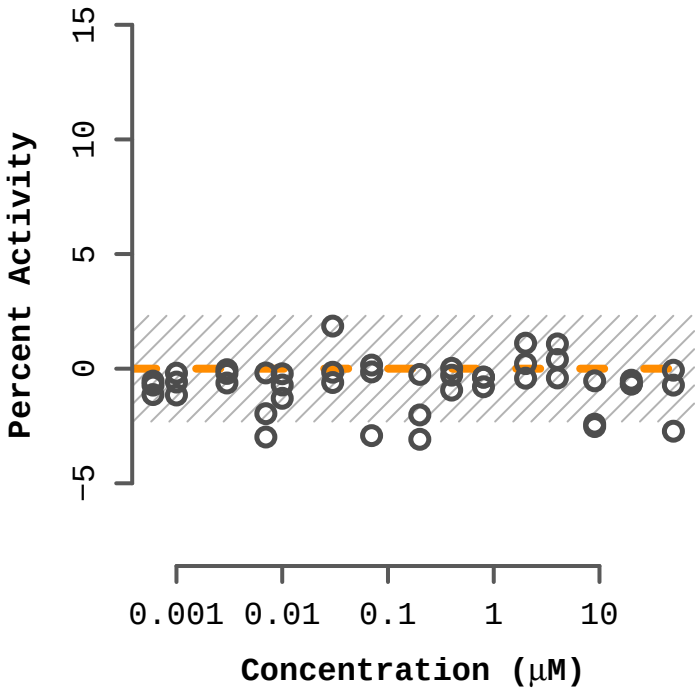
NAME: NTP Mix60 CT1 62-EQP
CHID: 49448 **CASRN:** NOCAS_49448
SPID(S): Tox21_203007
M4ID: 12479245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.151 **MAX_MED:** −0.00882 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

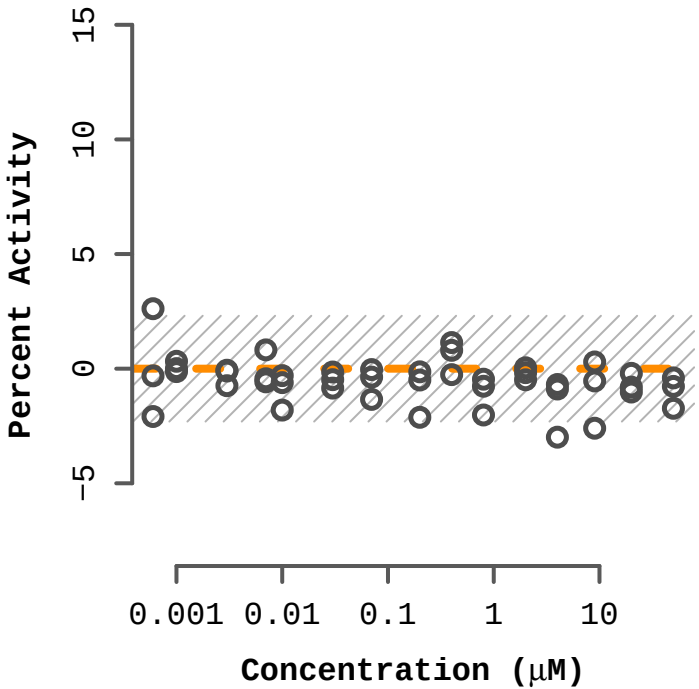
NAME: NTP Mix61 CT1 62-EQP
CHID: 49449 **CASRN:** NOCAS_49449
SPID(S): Tox21_203008
M4ID: 12479244

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 0.368 **MAX_MED:** 0.402 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

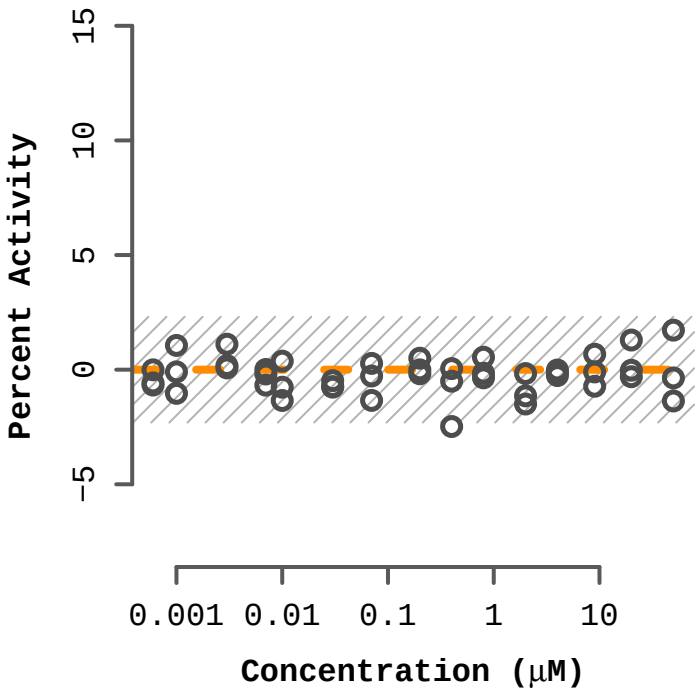
NAME: NTP Mix62 CT1 62-EQP
CHID: 49450 CASRN: NOCAS_49450
SPID(S): Tox21_203009
M4ID: 12479243

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.561 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

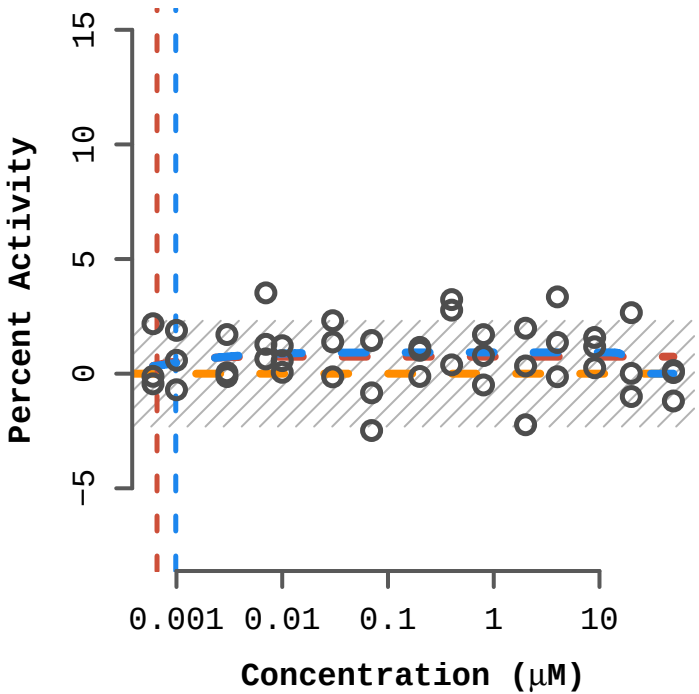
NAME: NTP Mix63 CT1 62-EQP
CHID: 49451 CASRN: NOCAS_49451
SPID(S): Tox21_203010
M4ID: 12479242

HILL MODEL: Not applicable.

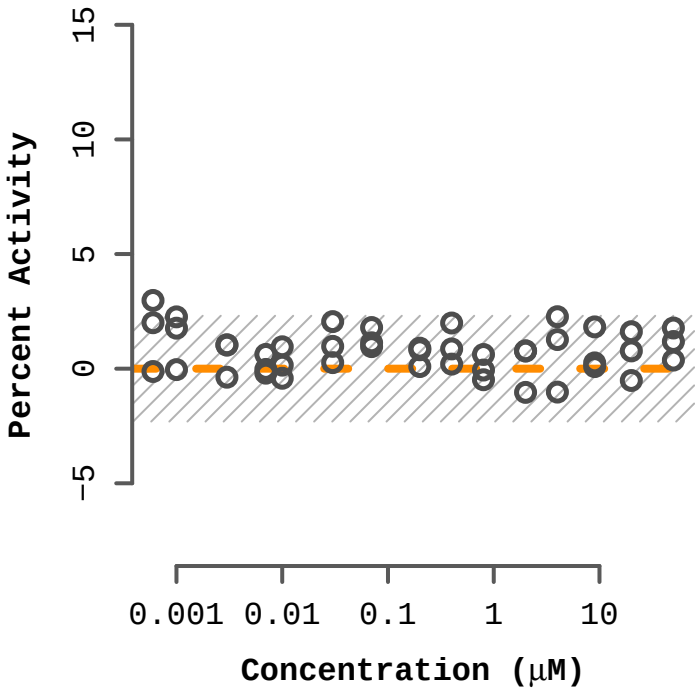
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.93	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.457 **MAX_MED:** 0.181 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix64 CT1 62-EQP
CHID:    49452   CASRN: NOCAS_49452
SPID(S): Tox21_203011
M4ID:    12479241

HILL MODEL (in red):
      tp       ga       gw
val:  0.742    -3.18    2.22
sd:   0.221    0.66     9.29

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  0.928    -3.01    1.24     1.26     18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  169.89      164.02      164.55
PROB: 0.03        0.55        0.42
RMSE: 1.53        1.34        1.31

MAX_MEAN: 2.13      MAX_MED: 2.77      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

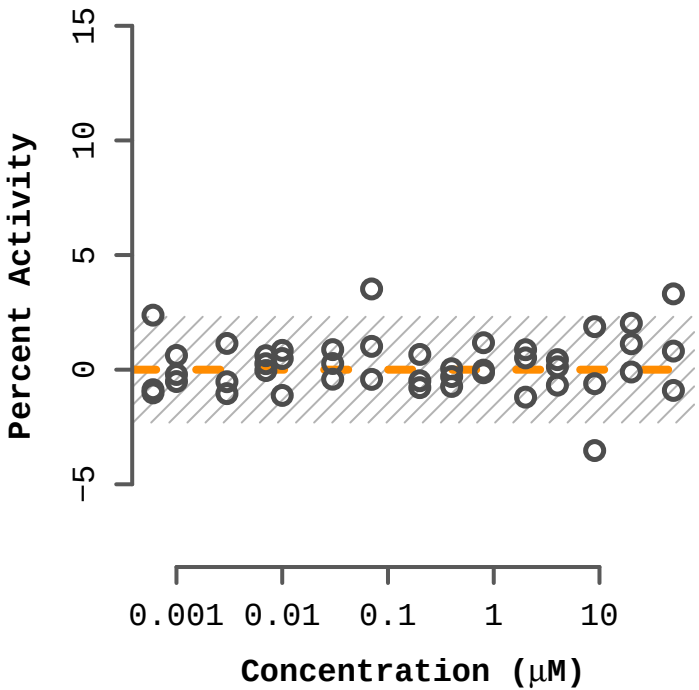
NAME: NTP Mix65 CT1 62-EQP
CHID: 49453 **CASRN:** NOCAS_49453
SPID(S): Tox21_203012
M4ID: 12479240

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

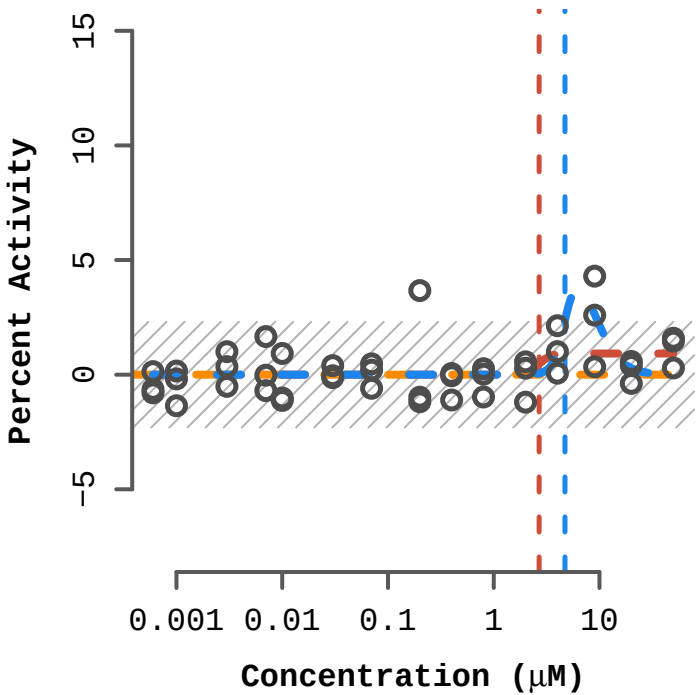
NAME: NTP Mix66 CT1 62-EQP
CHID: 49454 CASRN: NOCAS_49454
SPID(S): Tox21_203013
M4ID: 12479239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix67 CT1 62-EQP
CHID: 49455 CASRN: NOCAS_49455
SPID(S): Tox21_203014
M4ID: 12479238

HILL MODEL (in red):

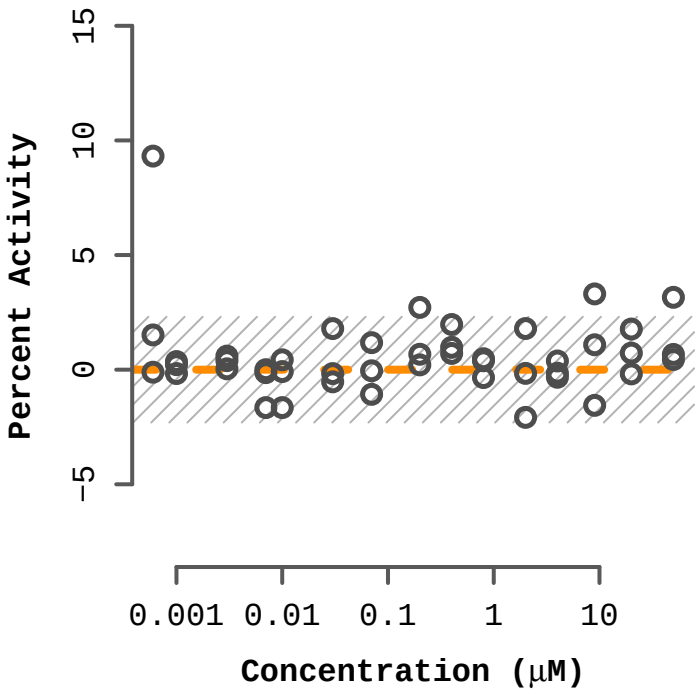
	tp	ga	gw
val:	0.923	0.429	8
sd:	0.301	0.237	12.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.16	0.674	8	0.961	3.63
sd:	20.7	0.525	57	0.988	7.43

	CNST	HILL	GNLS
AIC:	139.72	135.61	138.17
PROB:	0.09	0.71	0.2
RMSE:	1.23	1.07	1.02

MAX_MEAN: 2.41 MAX_MED: 2.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

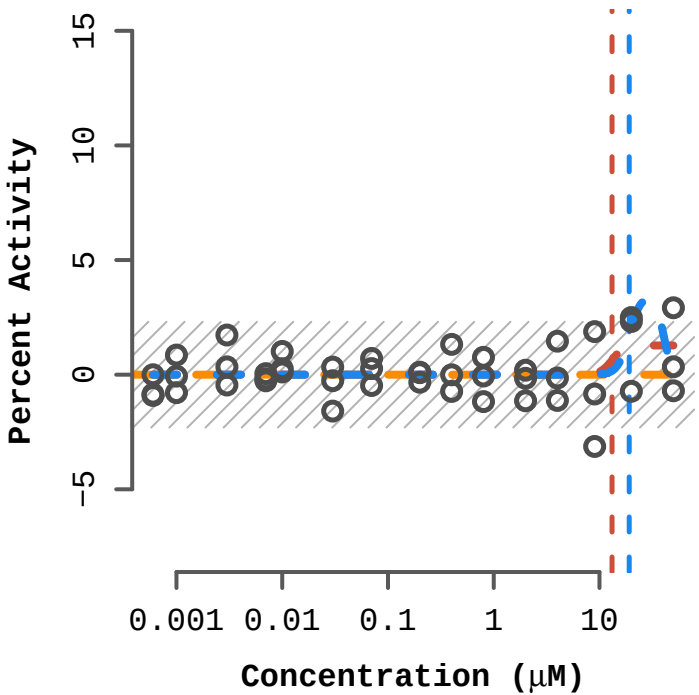
NAME: NTP Mix68 CT1 62-EQP
CHID: 49456 CASRN: NOCAS_49456
SPID(S): Tox21_203015
M4ID: 12479237

HILL MODEL: Not applicable.

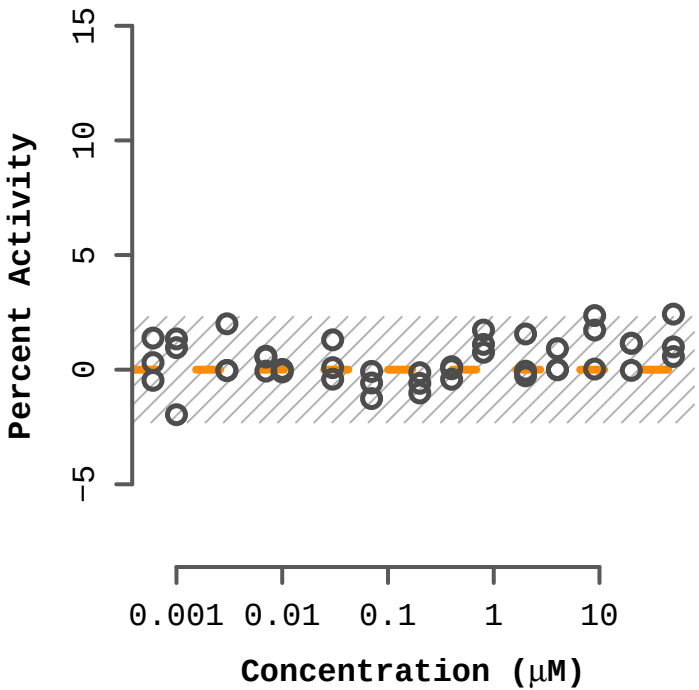
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.84	NA	NA

MAX_MEAN: 3.57 **MAX_MED:** 1.52 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix69 CT1 62-EQP
CHID:    49457   CASRN: NOCAS_49457
SPID(S): Tox21_203016
M4ID:    12479236

HILL MODEL (in red):
      tp       ga       gw
val:  1.27     1.12     8
sd:   0.927    0.167    7.84

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.5      1.28     8        1.6      10.8
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  135.73      139.21      140.06
PROB: 0.77        0.14        0.09
RMSE: 1.11        1.04        1.05

MAX_MEAN: 1.36      MAX_MED: 2.32      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

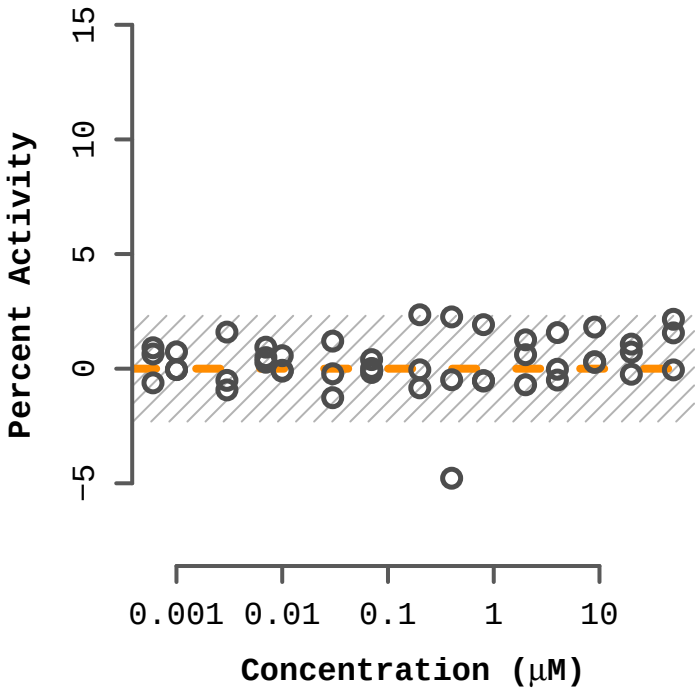
NAME: NTP Mix70 CT1 62-EQP
CHID: 49458 **CASRN:** NOCAS_49458
SPID(S): Tox21_203017
M4ID: 12479235

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.75	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.73 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

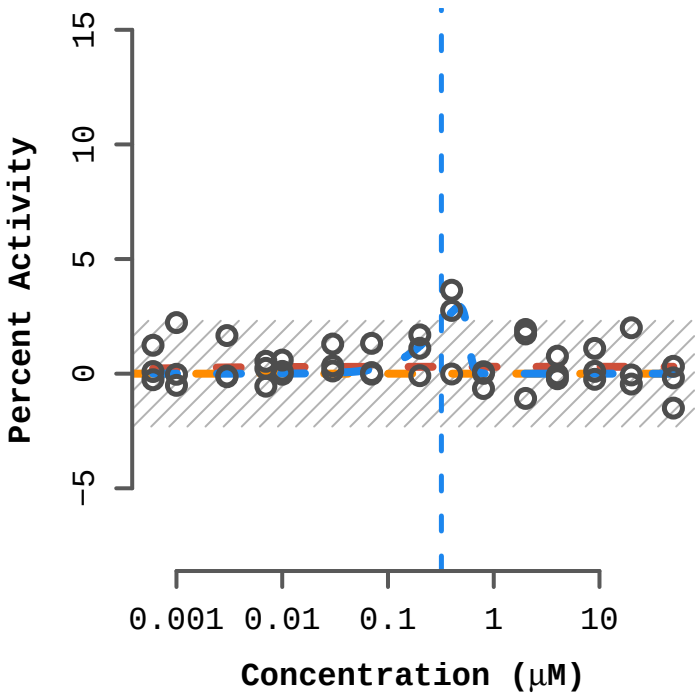
NAME: NTP Mix71 CT1 62-EQP
CHID: 49459 **CASRN:** NOCAS_49459
SPID(S): Tox21_203018
M4ID: 12479234

HILL MODEL: Not applicable.

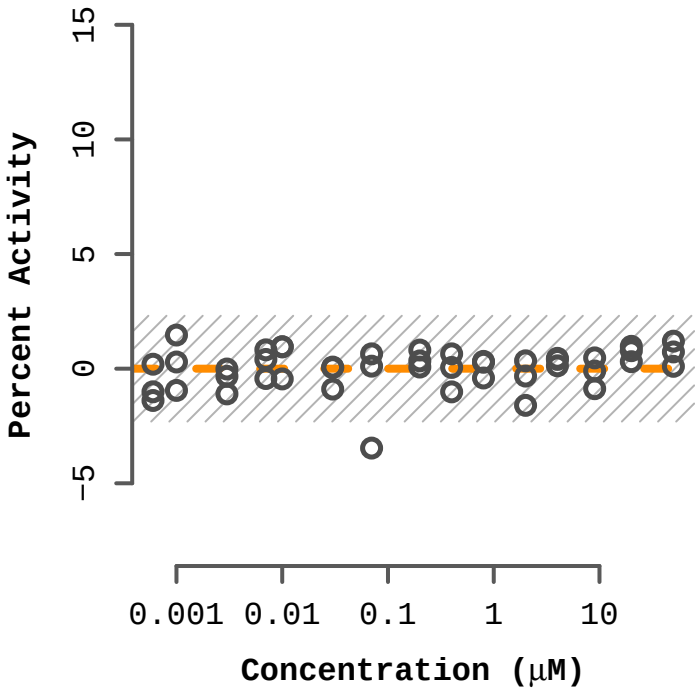
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.56 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix72 CT1 62-EQP
CHID:    49460   CASRN: NOCAS_49460
SPID(S): Tox21_203019
M4ID:    12479233

HILL MODEL (in red):
      tp       ga       gw
val:  0.3      -3.8     0.759
sd:   0.17     5.46     2.74

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.37     -0.495   2.05     -0.245   18
sd:   4.22     0.45     2.79     0.258    31.1

      CNST        HILL        GNLS
AIC:  133.98      135.32      131.9
PROB: 0.23        0.12        0.65
RMSE: 1.12        1.03        0.95

MAX_MEAN: 2.13      MAX_MED: 2.76      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

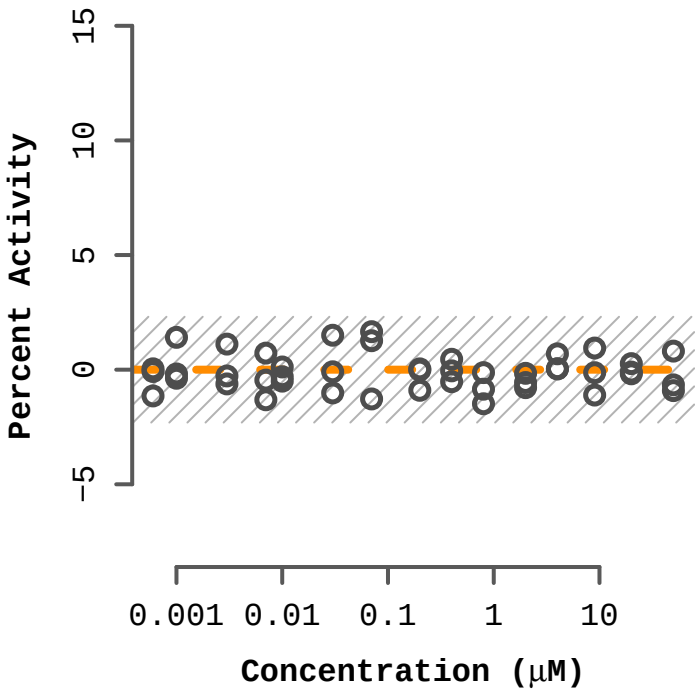
NAME: NTP Mix73 CT1 62-EQP
CHID: 49461 CASRN: NOCAS_49461
SPID(S): Tox21_203020
M4ID: 12479232

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.689 MAX_MED: 0.954 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

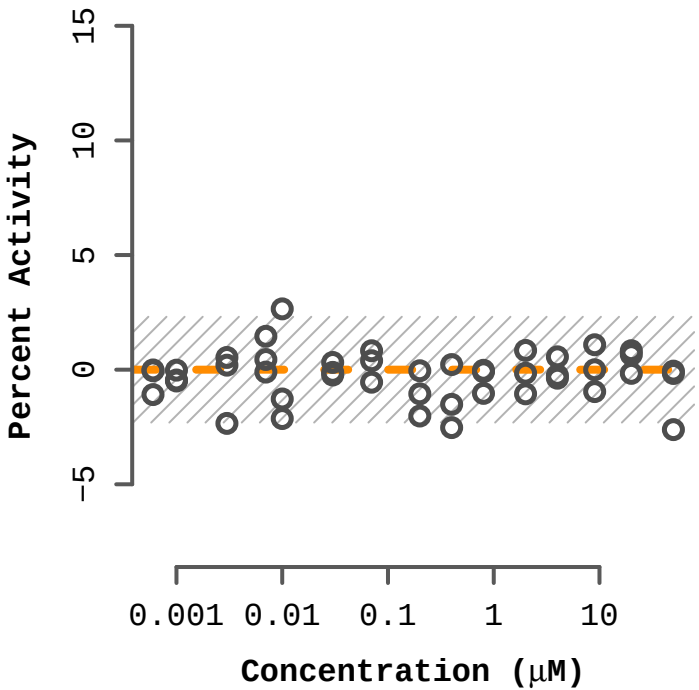
NAME: NTP Mix74 CT1 62-EQP
CHID: 49462 **CASRN:** NOCAS_49462
SPID(S): Tox21_203021
M4ID: 12479231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.55 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

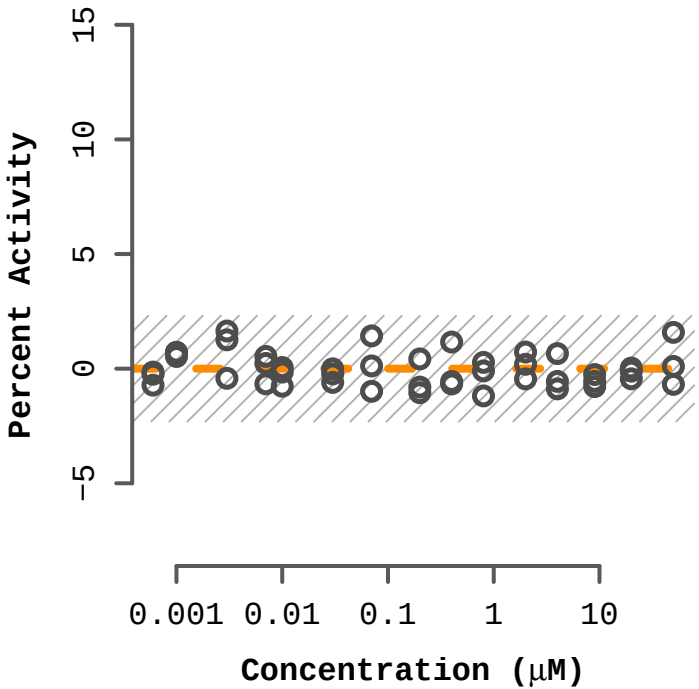
NAME: NTP Mix75 CT1 62-EQP
CHID: 49463 **CASRN:** NOCAS_49463
SPID(S): Tox21_203022
M4ID: 12479230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.599 **MAX_MED:** 0.657 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

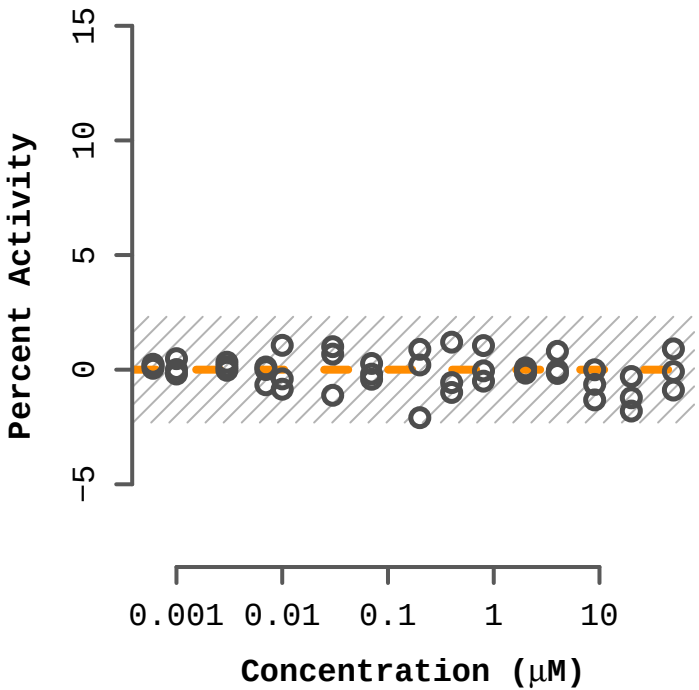
NAME: NTP Mix76 CT1 62-EQP
CHID: 49464 CASRN: NOCAS_49464
SPID(S): Tox21_203023
M4ID: 12479229

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	103.54	NA	NA
PROB:	1	NA	NA
RMSE:	0.72	NA	NA

MAX_MEAN: 0.828 MAX_MED: 1.26 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

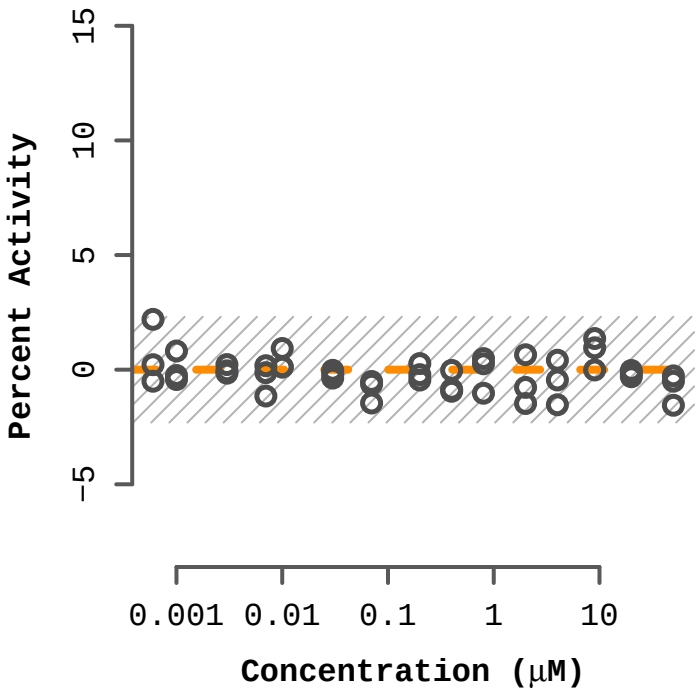
NAME: NTP Mix77 CT1 62-EQP
CHID: 49465 **CASRN:** NOCAS_49465
SPID(S): Tox21_203024
M4ID: 12479228

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.203 **MAX_MED:** 0.679 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

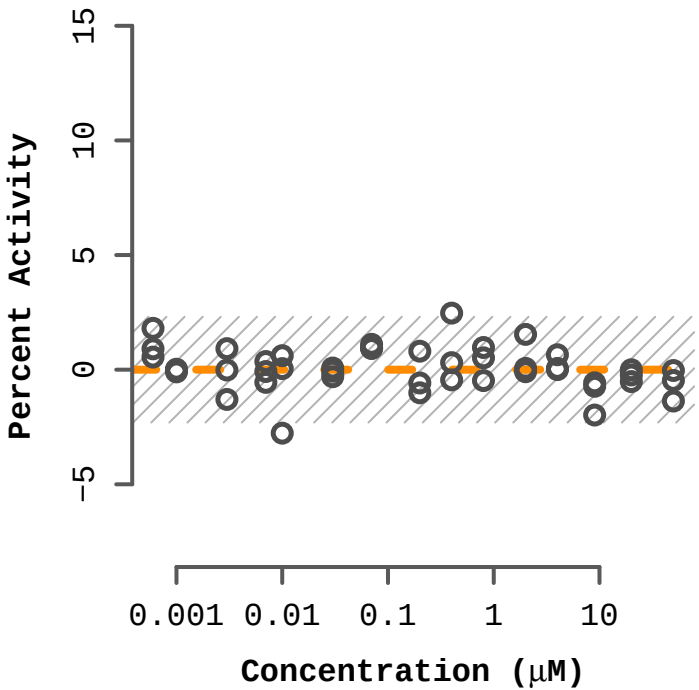
NAME: NTP Mix78 CT1 62-EQP
CHID: 49466 **CASRN:** NOCAS_49466
SPID(S): Tox21_203025
M4ID: 12479227

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.44	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 0.768 **MAX_MED:** 0.956 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

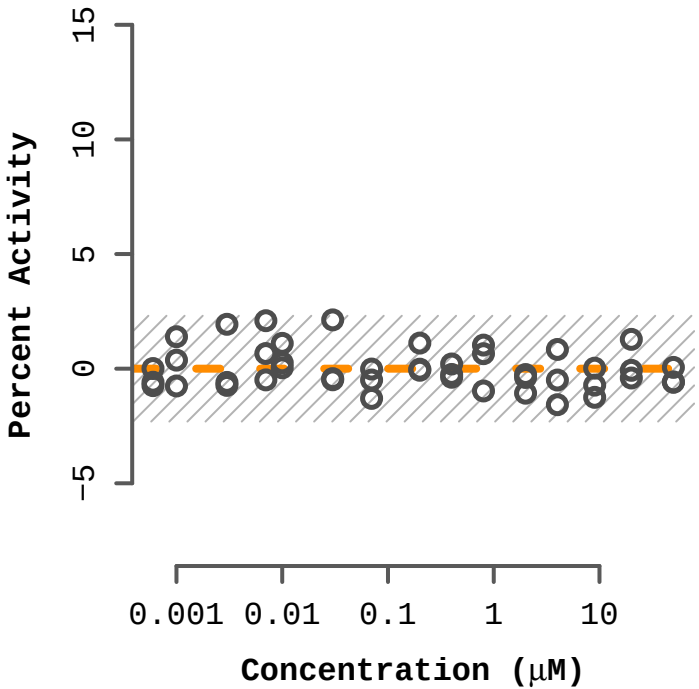
NAME: NTP Mix79 CT1 62-EQP
CHID: 49467 **CASRN:** NOCAS_49467
SPID(S): Tox21_203026
M4ID: 12479226

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.01	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.947 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

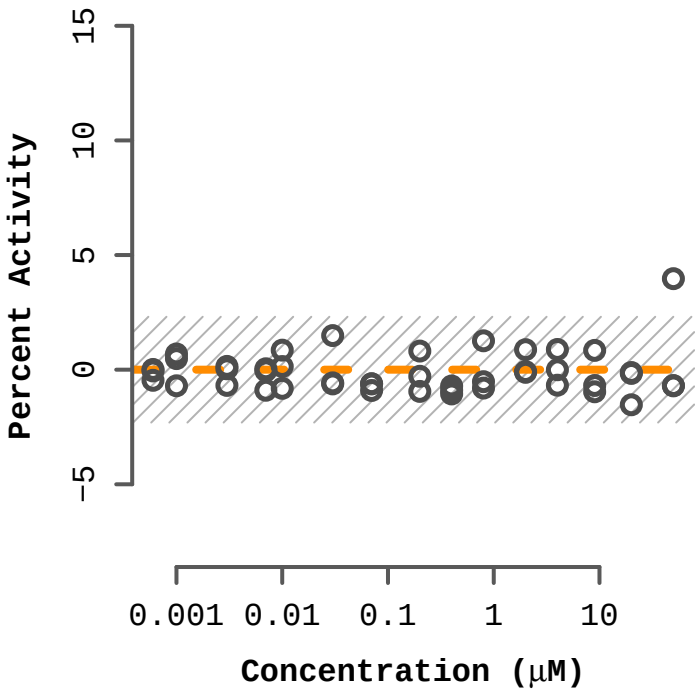
NAME: NTP Mix80 CT1 62-EQP
CHID: 49468 **CASRN:** NOCAS_49468
SPID(S): Tox21_203027
M4ID: 12479225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.756 **MAX_MED:** 0.663 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

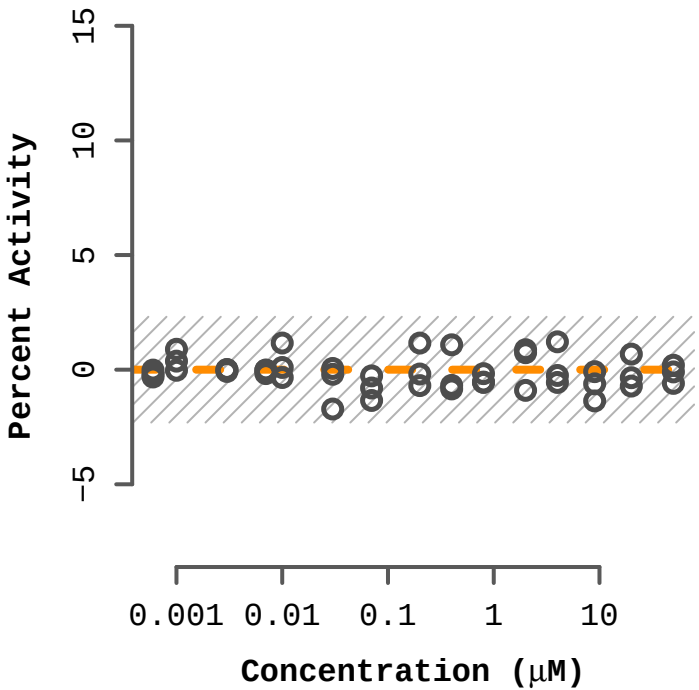
NAME: NTP Mix81 CT1 62-EQP
CHID: 49469 **CASRN:** NOCAS_49469
SPID(S): Tox21_203028
M4ID: 12479224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.31	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 0.858 **MAX_MED:** 0.485 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

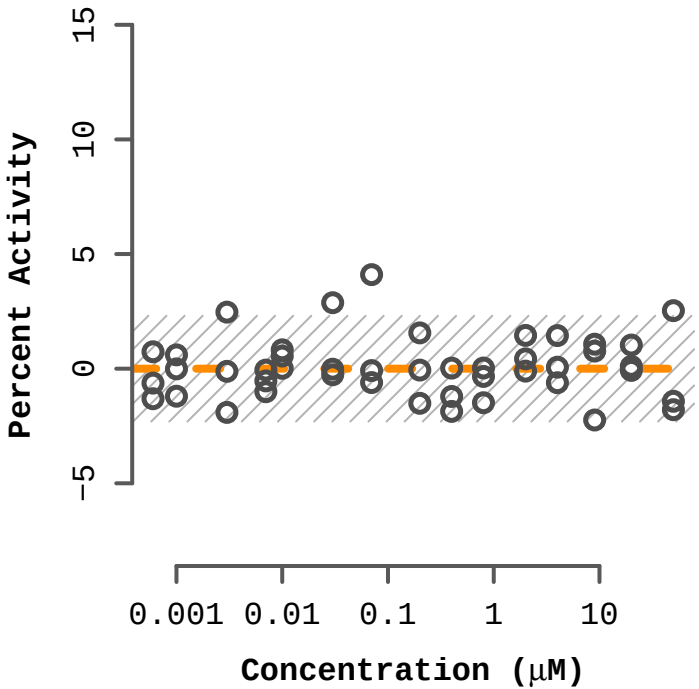
NAME: NTP Mix52 CT1 3-EQP
CHID: 49470 CASRN: NOCAS_49470
SPID(S): Tox21_203029
M4ID: 12479223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	96.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.68	NA	NA

MAX_MEAN: 0.413 **MAX_MED:** 0.742 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

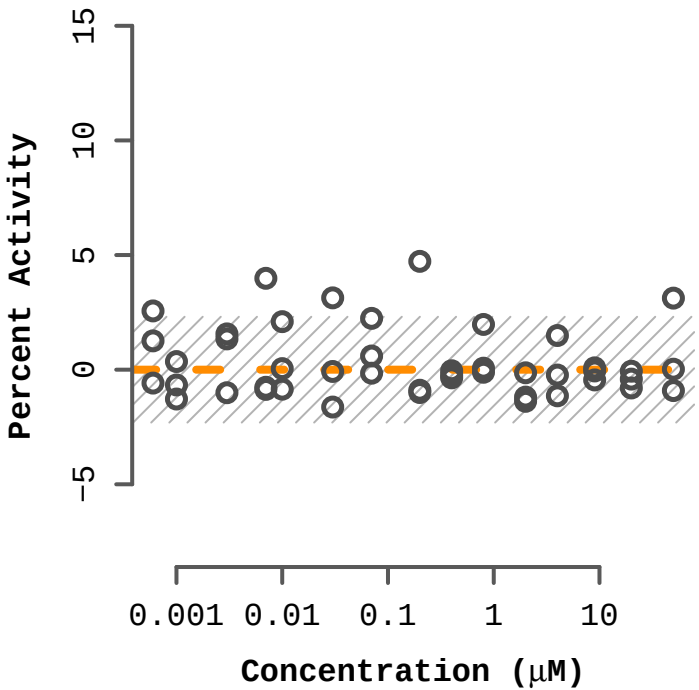
NAME: NTP Mix39 CT1 2-EQP
CHID: 49471 CASRN: NOCAS_49471
SPID(S): Tox21_203030
M4ID: 12479222

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.769 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

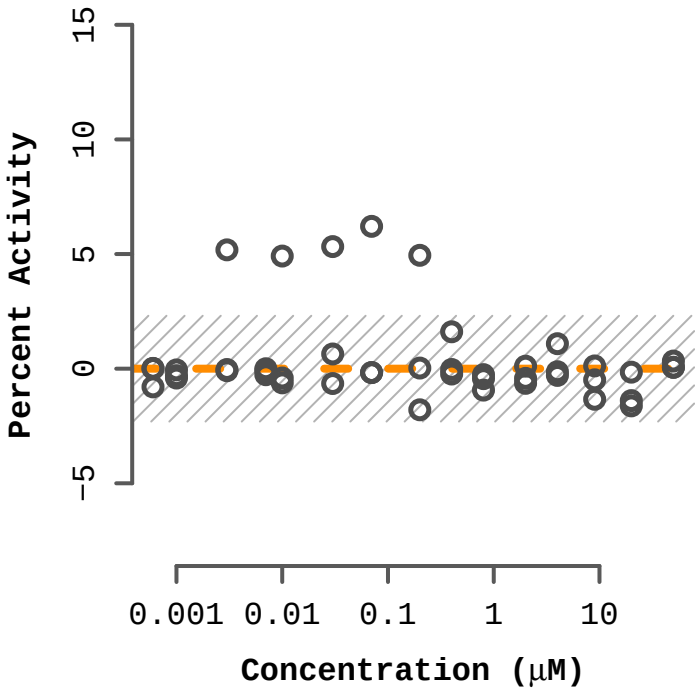
NAME: NTP Mix53 CT1 3-EQP
CHID: 49472 **CASRN:** NOCAS_49472
SPID(S): Tox21_203031
M4ID: 12479221

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.51	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

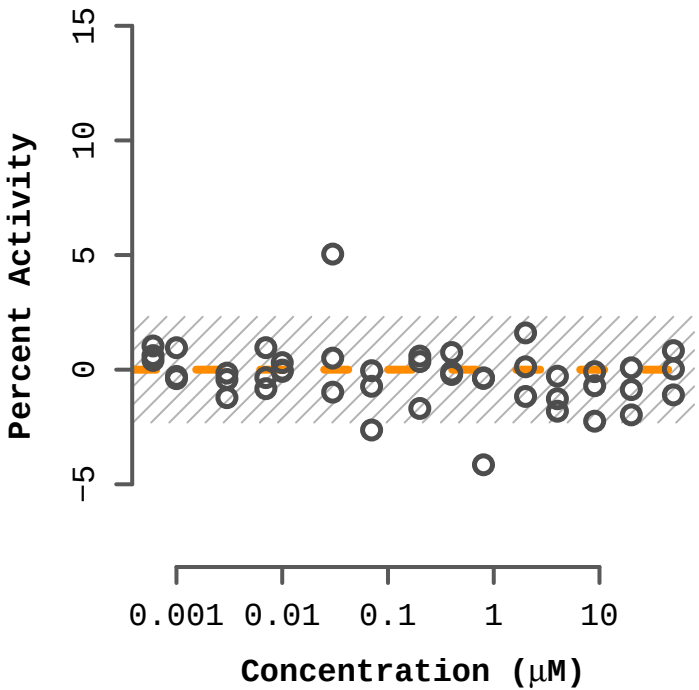
NAME: NTP Mix54 CT1 3-EQP
CHID: 49473 **CASRN:** NOCAS_49473
SPID(S): Tox21_203032
M4ID: 12479220

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	159.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.89	NA	NA

MAX_MEAN: 1.96 **MAX_MED:** 0.643 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

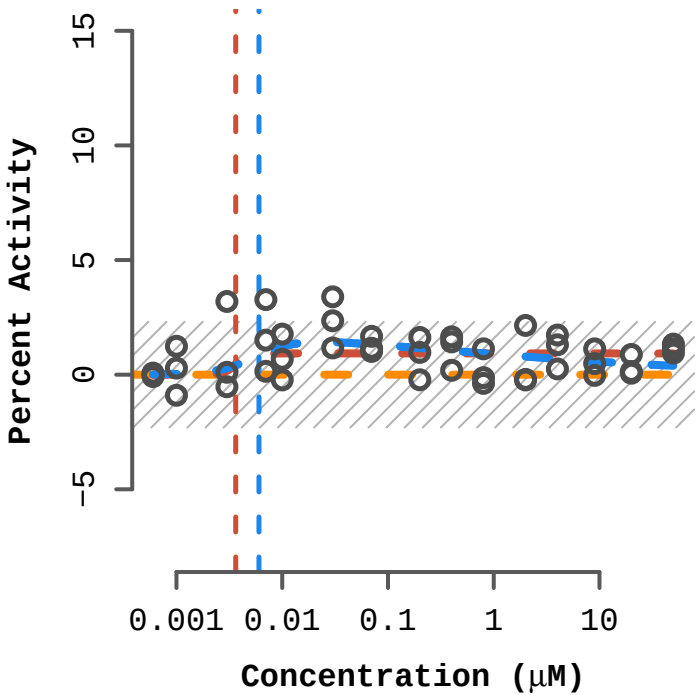
NAME: NTP Mix55 CT1 3-EQP
CHID: 49474 CASRN: NOCAS_49474
SPID(S): Tox21_203033
M4ID: 12479219

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.05	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 0.616 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix56 CT1 3-EQP
CHID: 49475 CASRN: NOCAS_49475
SPID(S): Tox21_203034
M4ID: 12479218

HILL MODEL (in red):

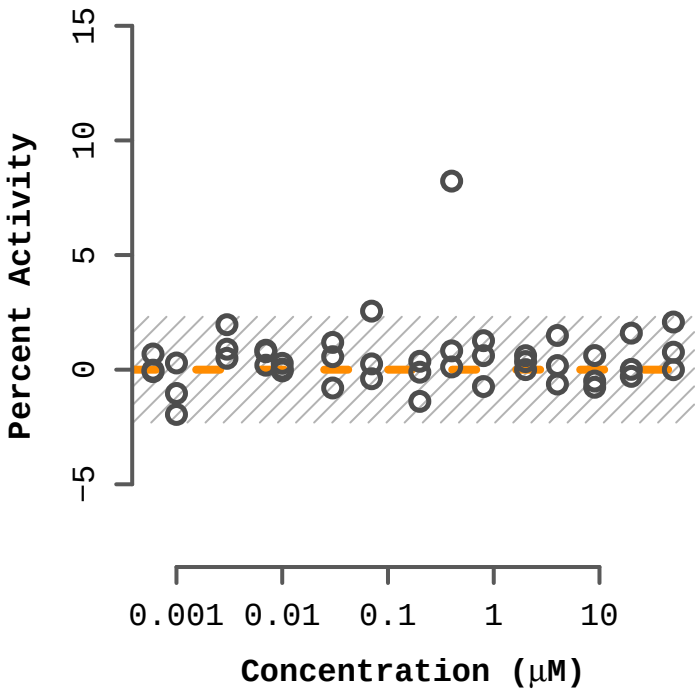
	tp	ga	gw
val:	0.926	−2.44	8
sd:	0.155	0.237	16.5

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.18	−2.22	2.32	−0.515	0.3
sd:	4.71	0.486	2.28	6.43	0.383

	CNST	HILL	GNLS
AIC:	155	132.68	134.43
PROB:	0	0.71	0.29
RMSE:	1.32	0.98	0.95

MAX_MEAN: 2.31 **MAX_MED:** 2.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

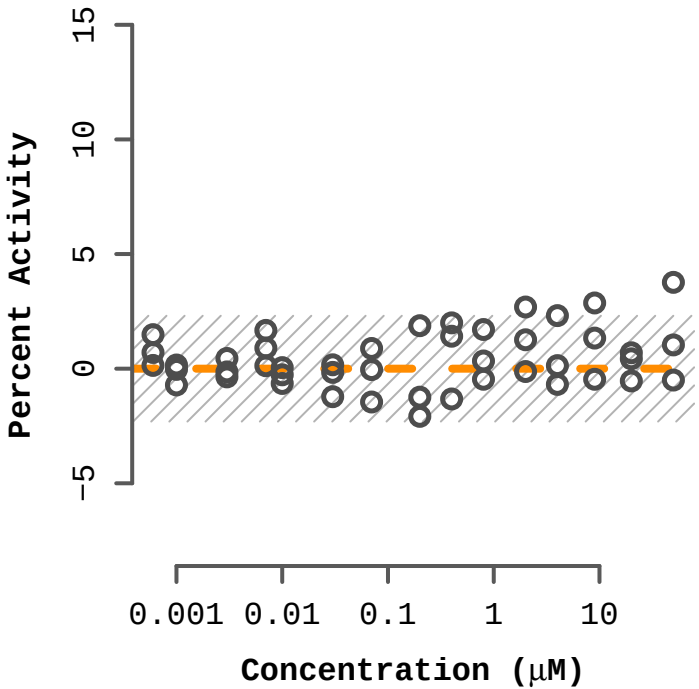
NAME: NTP Mix40 CT1 3-EQP
CHID: 49476 CASRN: NOCAS_49476
SPID(S): Tox21_203035
M4ID: 12479217

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 3.06 **MAX_MED:** 0.895 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

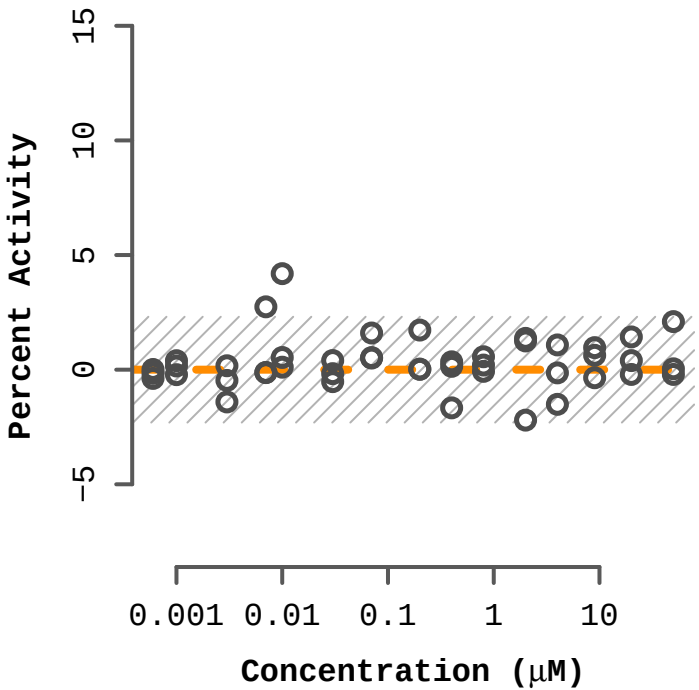
NAME: NTP Mix41 CT1 3-EQP
CHID: 49477 **CASRN:** NOCAS_49477
SPID(S): Tox21_203036
M4ID: 12479216

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

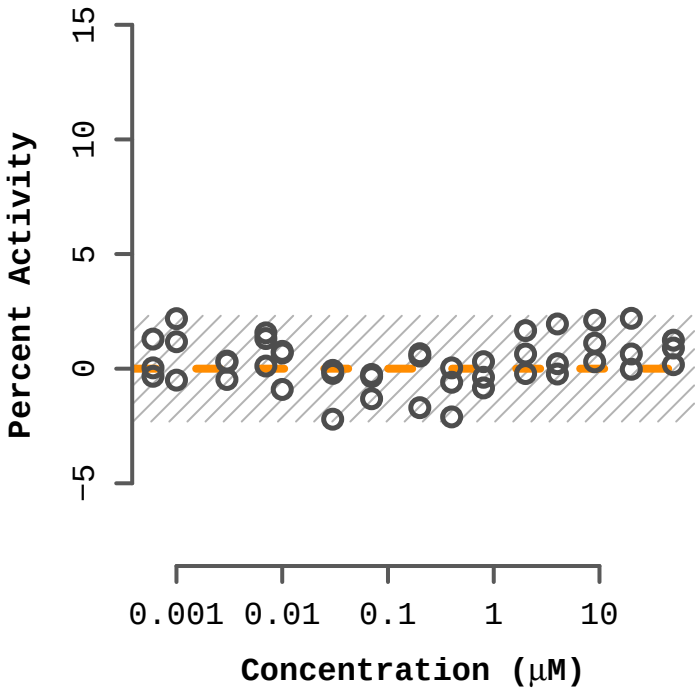
NAME: NTP Mix42 CT1 3-EQP
CHID: 49478 **CASRN:** NOCAS_49478
SPID(S): Tox21_203037
M4ID: 12479215

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

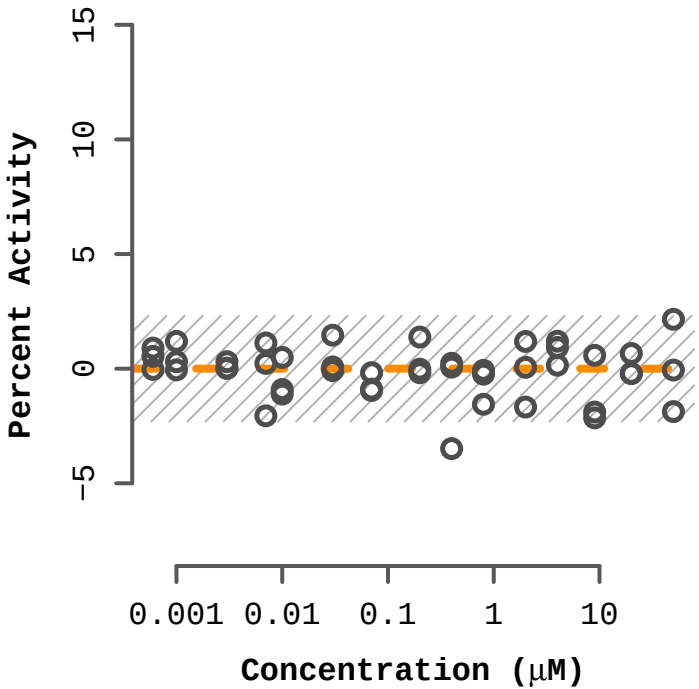
NAME: NTP Mix33 CT1 1-EQP
CHID: 49479 **CASRN:** NOCAS_49479
SPID(S): Tox21_203038
M4ID: 12479214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

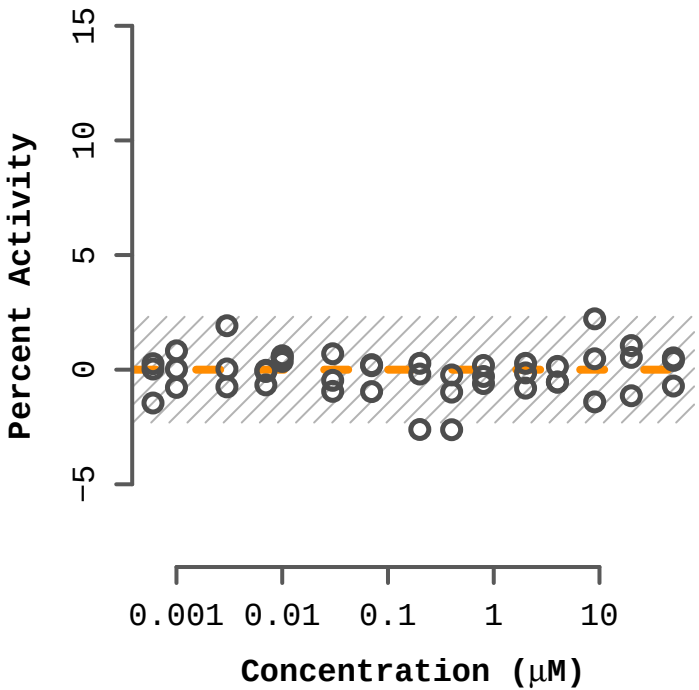
NAME: NTP Mix43 CT1 3-EQP
CHID: 49480 CASRN: NOCAS_49480
SPID(S): Tox21_203039
M4ID: 12479213

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.759 **MAX_MED:** 0.926 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

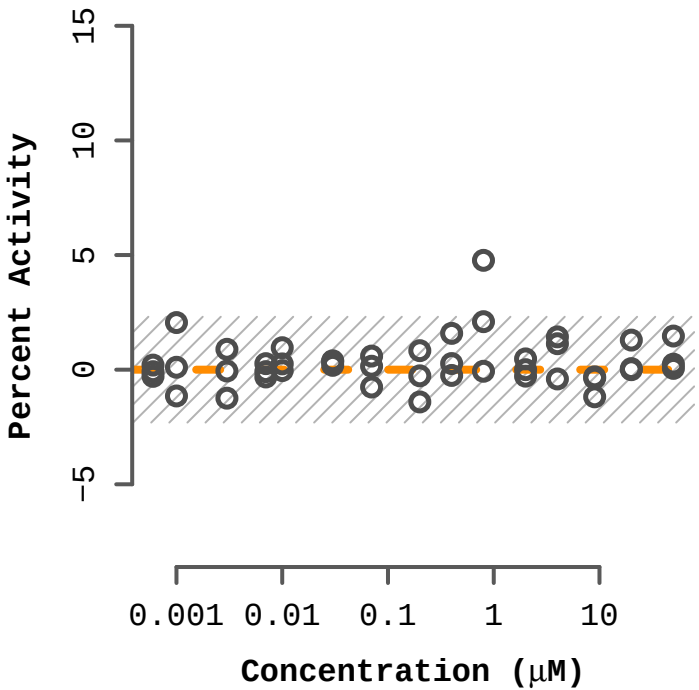
NAME: NTP Mix44 CT1 3-EQP
CHID: 49481 **CASRN:** NOCAS_49481
SPID(S): Tox21_203040
M4ID: 12479212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.507 **MAX_MED:** 0.551 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

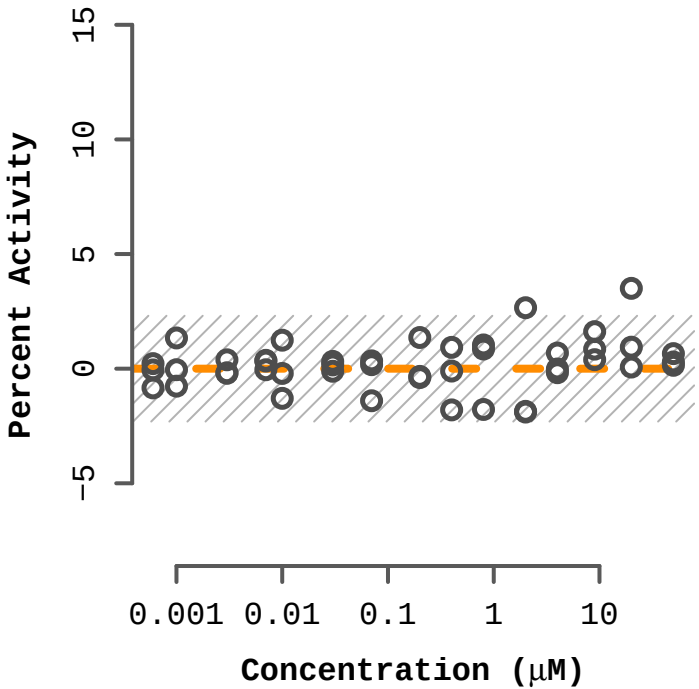
NAME: NTP Mix45 CT1 3-EQP
CHID: 49482 CASRN: NOCAS_49482
SPID(S): Tox21_203041
M4ID: 12479211

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 2.27 MAX_MED: 2.1 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

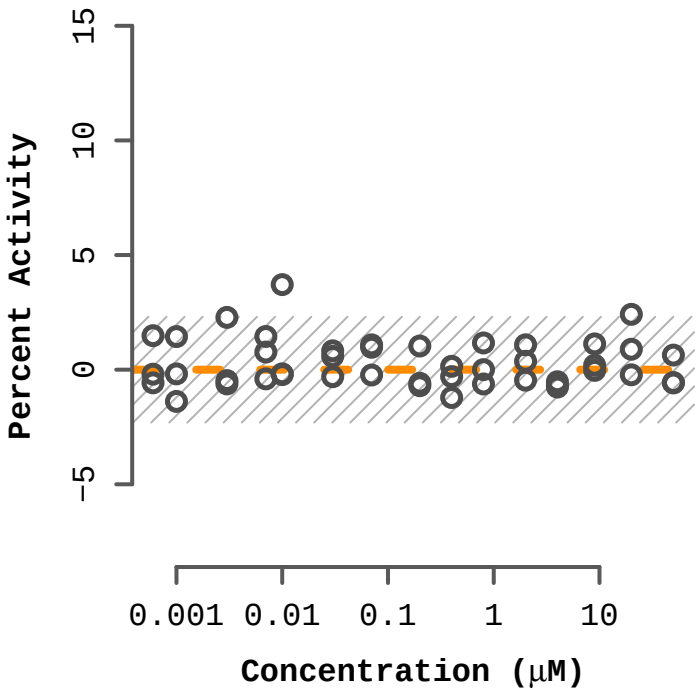
NAME: NTP Mix36 CT1 2−EQP
CHID: 49483 **CASRN:** NOCAS_49483
SPID(S): Tox21_203042
M4ID: 12479210

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

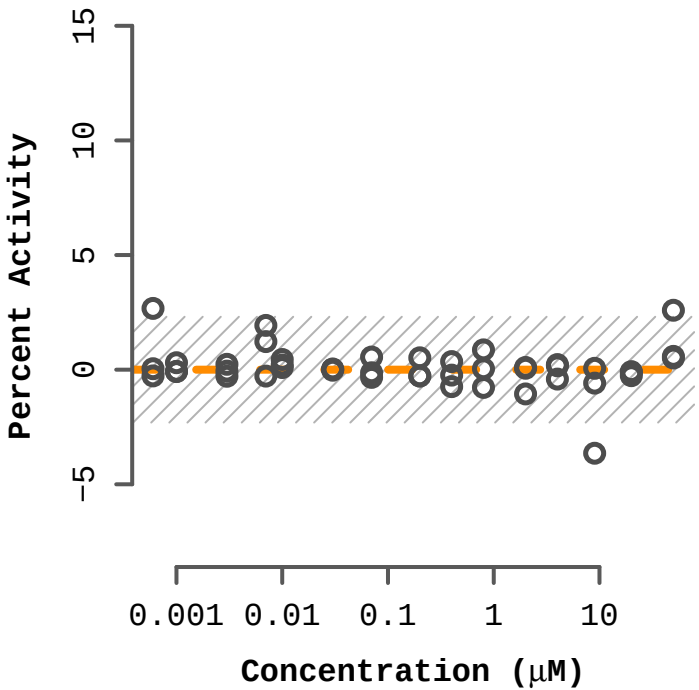
NAME: NTP Mix37 CT1 2-EQP
CHID: 49484 **CASRN:** NOCAS_49484
SPID(S): Tox21_203043
M4ID: 12479209

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

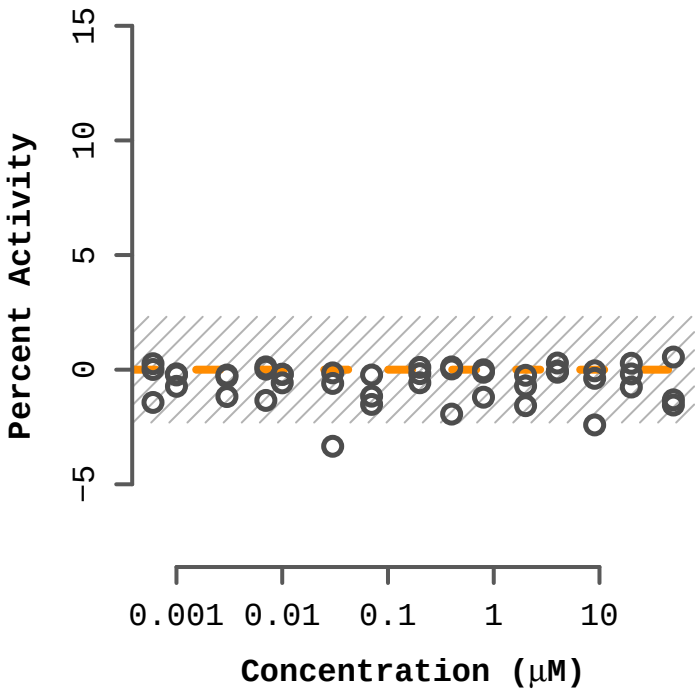
NAME: NTP Mix46 CT1 3-EQP
CHID: 49485 **CASRN:** NOCAS_49485
SPID(S): Tox21_203044
M4ID: 12479208

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.55	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

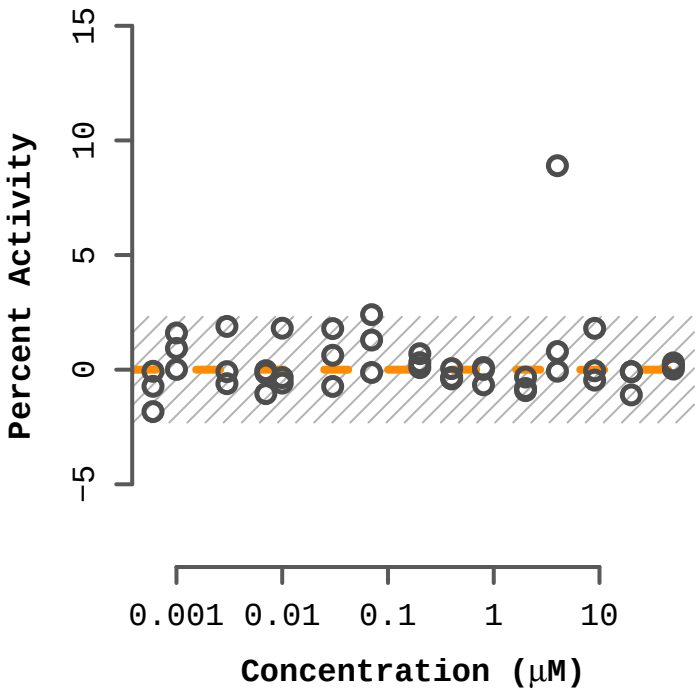
NAME: NTP Mix34 CT1 1−EQP
CHID: 49486 CASRN: NOCAS_49486
SPID(S): Tox21_203045
M4ID: 12479207

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.0414 **MAX_MED:** 0.0328 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

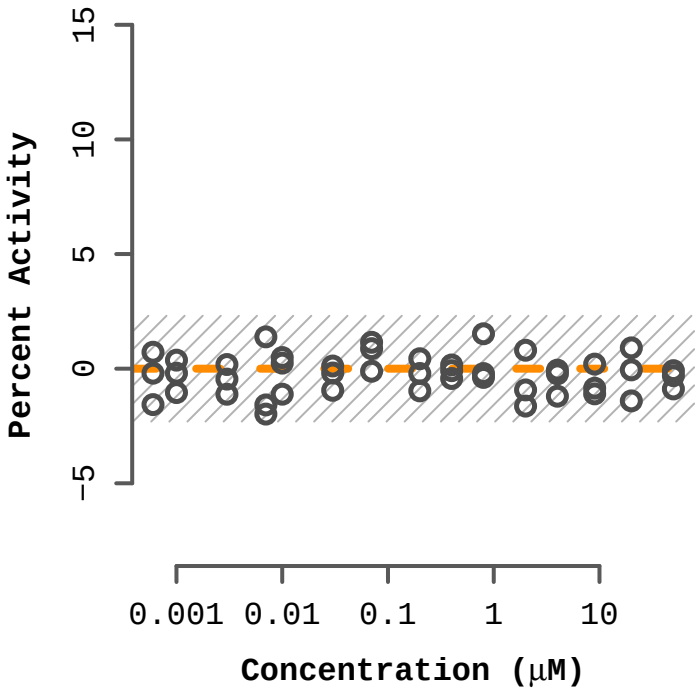
NAME: NTP Mix47 CT1 3-EQP
CHID: 49487 **CASRN:** NOCAS_49487
SPID(S): Tox21_203046
M4ID: 12479206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 3.21 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

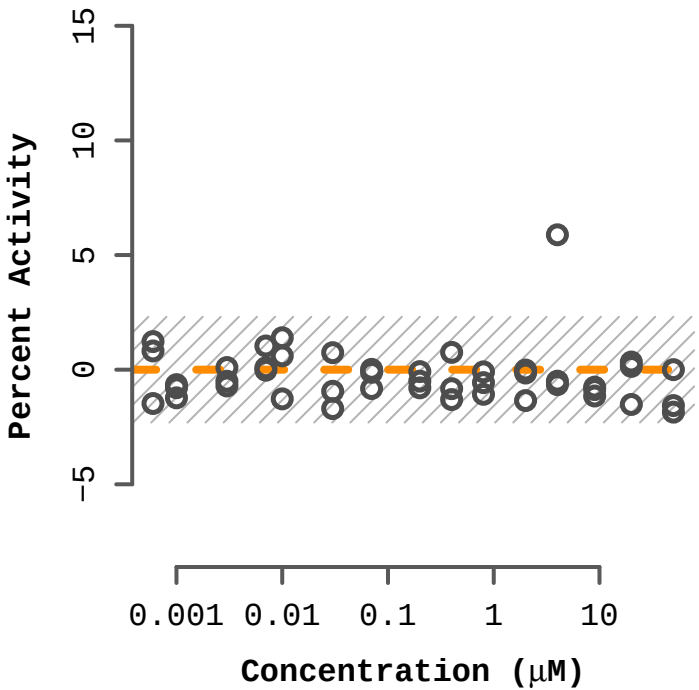
NAME: NTP Mix48 CT1 3-EQP
CHID: 49488 **CASRN:** NOCAS_49488
SPID(S): Tox21_203047
M4ID: 12479205

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.56	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.639 **MAX_MED:** 0.875 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

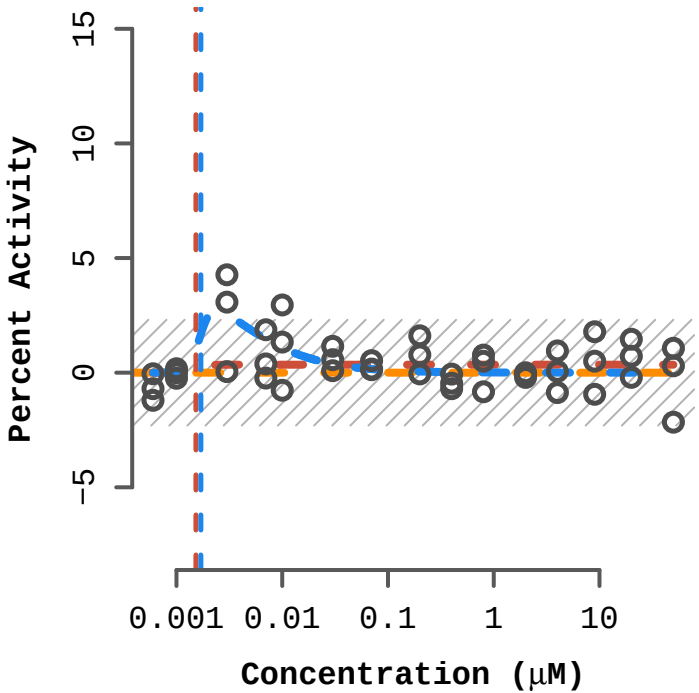
NAME: NTP Mix49 CT1 3-EQP
CHID: 49489 **CASRN:** NOCAS_49489
SPID(S): Tox21_203048
M4ID: 12479204

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.64	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 0.818 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix38 CT1 2−EQP
CHID: 49490 CASRN: NOCAS_49490
SPID(S): Tox21_203049
M4ID: 12479203

HILL MODEL (in red):

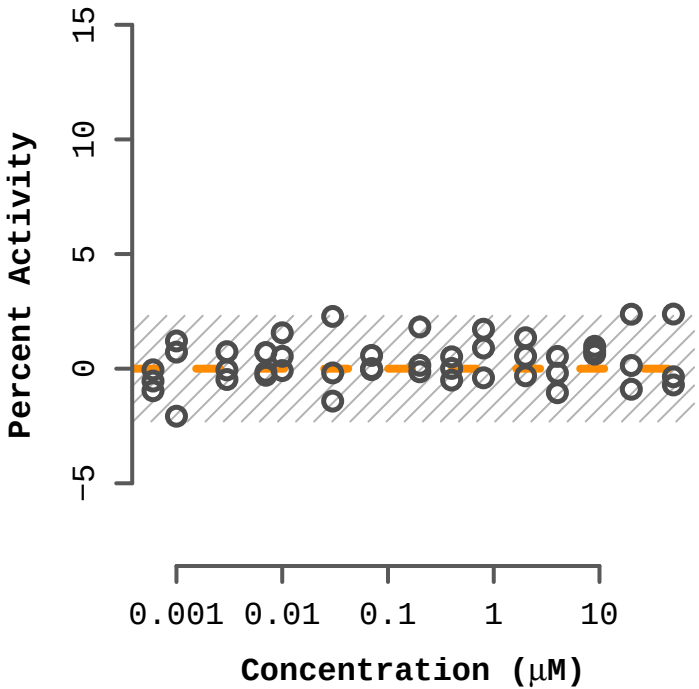
	tp	ga	gw
val:	0.347	−2.82	8
sd:	0.152	0.679	20.7

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.12	−2.77	8	−2.52	1.1
sd:	4.5	0.202	6.4	0.554	0.838

	CNST	HILL	GNLS
AIC:	139.41	140.21	138.66
PROB:	0.32	0.21	0.47
RMSE:	1.22	1.13	0.98

MAX_MEAN: 2.47 MAX_MED: 3.08 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

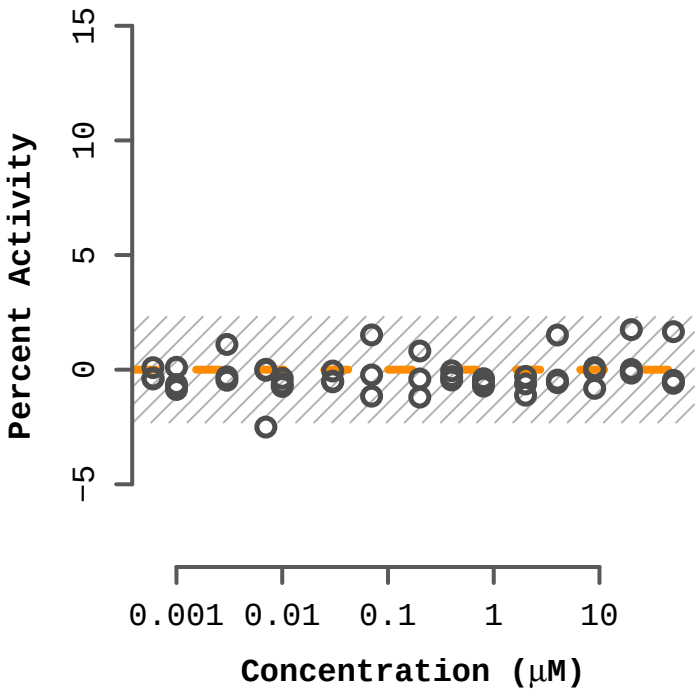
NAME: NTP Mix50 CT1 3-EQP
CHID: 49491 **CASRN:** NOCAS_49491
SPID(S): Tox21_203050
M4ID: 12479202

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.99	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.794 **MAX_MED:** 0.902 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

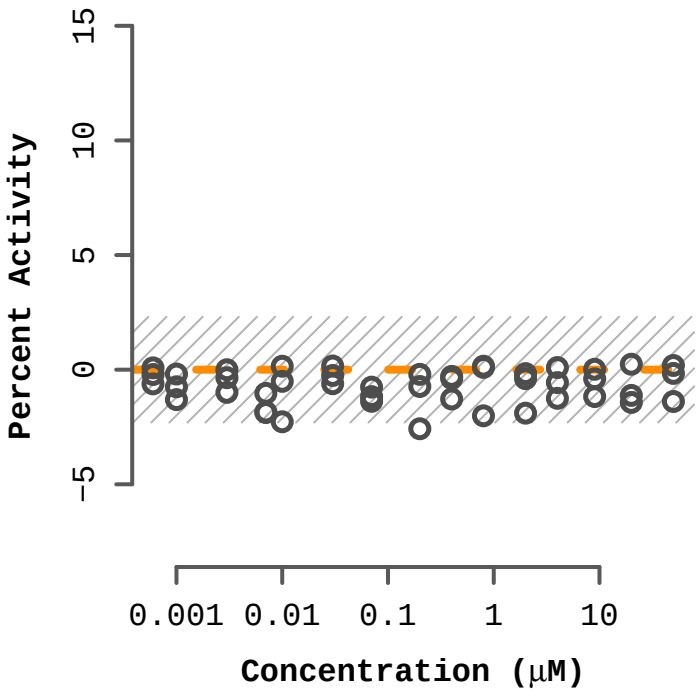
NAME: NTP Mix35 CT1 1−EQP
CHID: 49492 **CASRN:** NOCAS_49492
SPID(S): Tox21_203051
M4ID: 12479201

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.538 **MAX_MED:** 0.0135 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

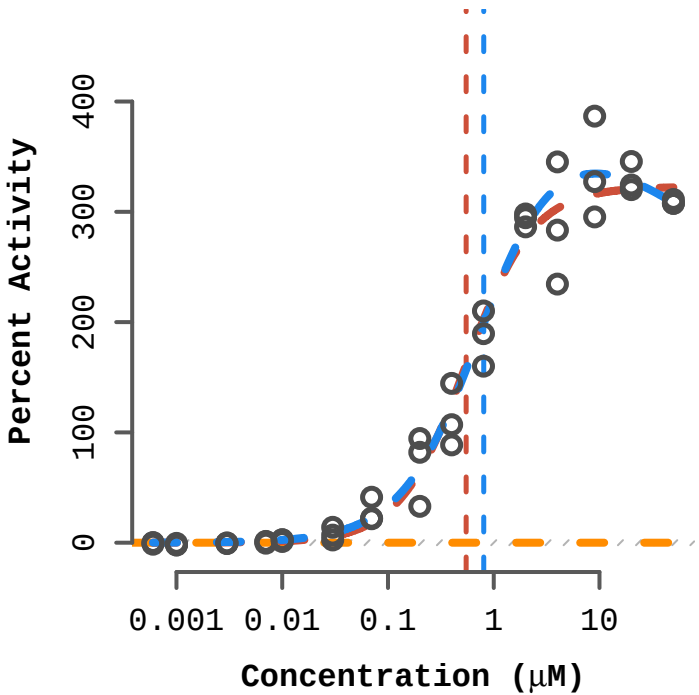
NAME: NTP Mix51 CT1 3-EQP
CHID: 49493 **CASRN:** NOCAS_49493
SPID(S): Tox21_203052
M4ID: 12479200

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.78	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: −0.234 **MAX_MED:** 0.102 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix1 AR1 4-EQP
CHID: 49494 CASRN: NOCAS_49494
SPID(S): Tox21_203053
M4ID: 12479199

HILL MODEL (in red):

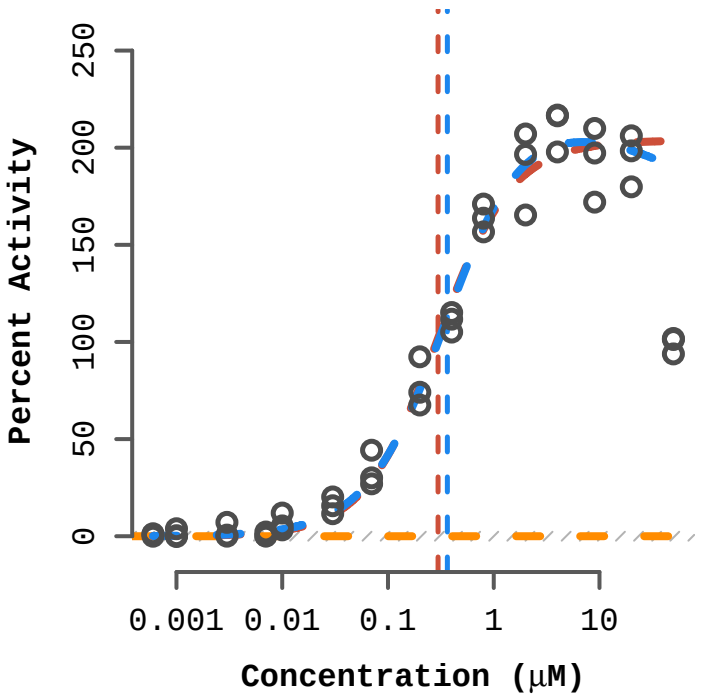
	tp	ga	gw
val:	323	−0.261	1.37
sd:	6.39	0.0422	0.163

GAIN-LOSS MODEL (in blue):

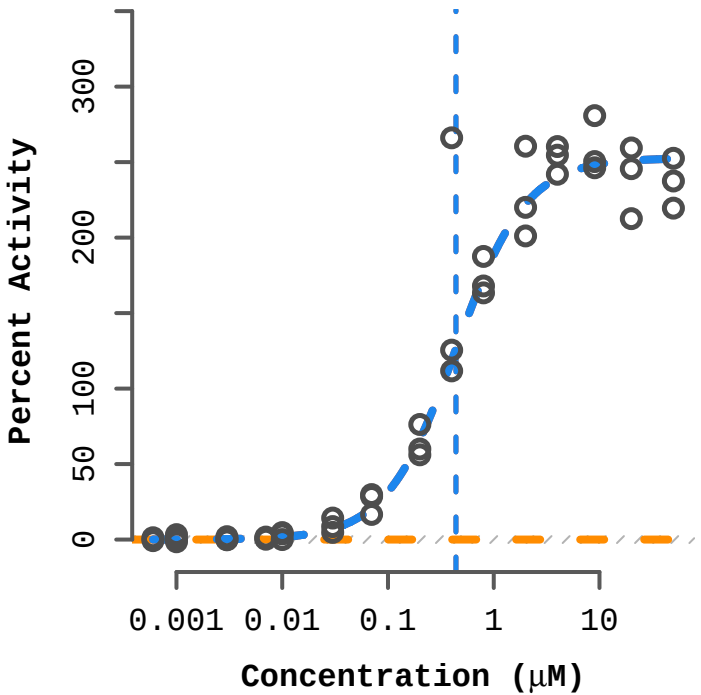
	tp	ga	gw	la	lw
val:	449	−0.0943	1.17	2.87	0.3
sd:	211	0.103	0.107	0.806	0.41

	CNST	HILL	GNLS
AIC:	604.05	404.49	400.25
PROB:	0	0.11	0.89
RMSE:	190.63	21.9	21.53

MAX_MEAN: 337 MAX_MED: 327 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix2 AR1 4-EQP
CHID:    49495   CASRN: NOCAS_49495
SPID(S): Tox21_203054
M4ID:    12479198

HILL MODEL (in red):
      tp       ga       gw
val:  204      -0.526   1.25
sd:   5.05     0.0369   0.108

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  239      -0.438   1.16     3.7      0.301
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  563.15      395.23      389.65
PROB: 0           0.06        0.94
RMSE: 119.14      28.85       25.4

MAX_MEAN: 210       MAX_MED: 216       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix3 AR1 8-EQC
CHID: 49496 CASRN: NOCAS_49496
SPID(S): Tox21_203055
M4ID: 12479197

HILL MODEL (in red):

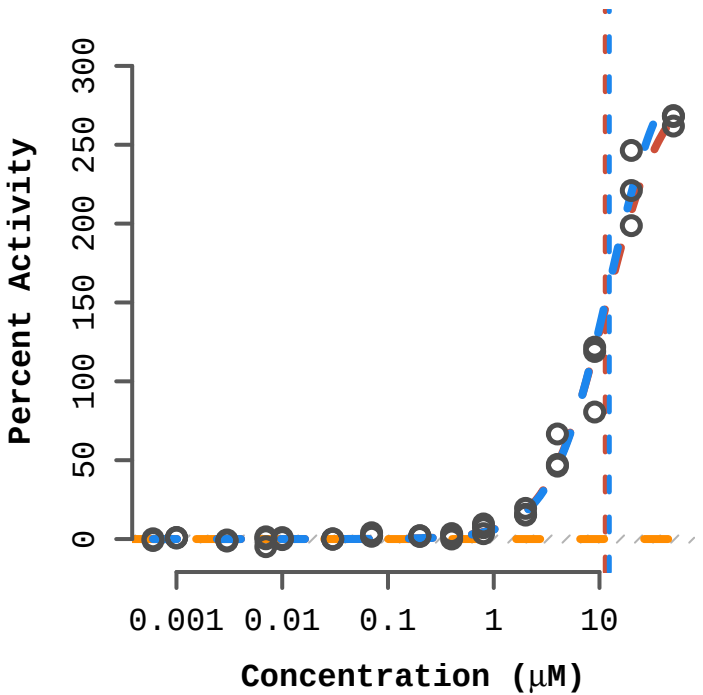
	tp	ga	gw
val:	253	-0.357	1.32
sd:	4.02	0.0269	0.0917

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	253	-0.357	1.32	3.53	15
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	587.48	374.74	378.74
PROB:	0	0.88	0.12
RMSE:	156.02	25.48	25.48

MAX_MEAN: 259 MAX_MED: 255 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix4 AR1 8-EQC
CHID: 49497 CASRN: NOCAS_49497
SPID(S): Tox21_203056
M4ID: 12479196

HILL MODEL (in red):

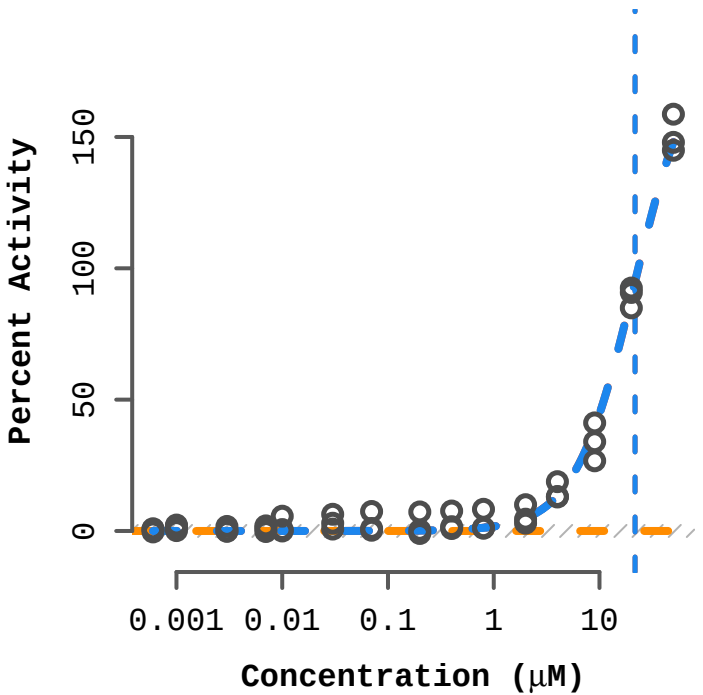
	tp	ga	gw
val:	293	1.05	1.58
sd:	3.19	0.0119	0.0436

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	322	1.09	1.58	1.84	7.49
sd:	4.42	0.00985	0.0299	0.00683	0.491

	CNST	HILL	GNLS
AIC:	505.29	271.93	270.33
PROB:	0	0.31	0.69
RMSE:	96.17	9.32	8.79

MAX_MEAN: 266 MAX_MED: 268 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix5 AR1 8-EQC
CHID: 49498 CASRN: NOCAS_49498
SPID(S): Tox21_203057
M4ID: 12479195

HILL MODEL (in red):

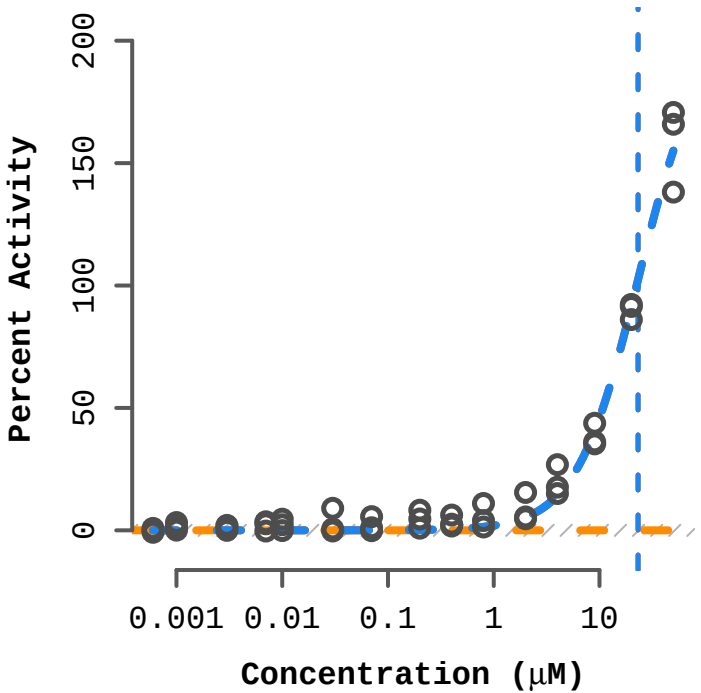
	tp	ga	gw
val:	190	1.34	1.52
sd:	11.5	0.0453	0.109

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	190	1.34	1.53	3.61	1.17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	435.03	253.5	257.47
PROB:	0	0.88	0.12
RMSE:	46.39	3.98	3.99

MAX_MEAN: 151 MAX_MED: 148 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix6 AR1 8-EQC
CHID: 49499 CASRN: NOCAS_49499
SPID(S): Tox21_203058
M4ID: 12479194

HILL MODEL (in red):

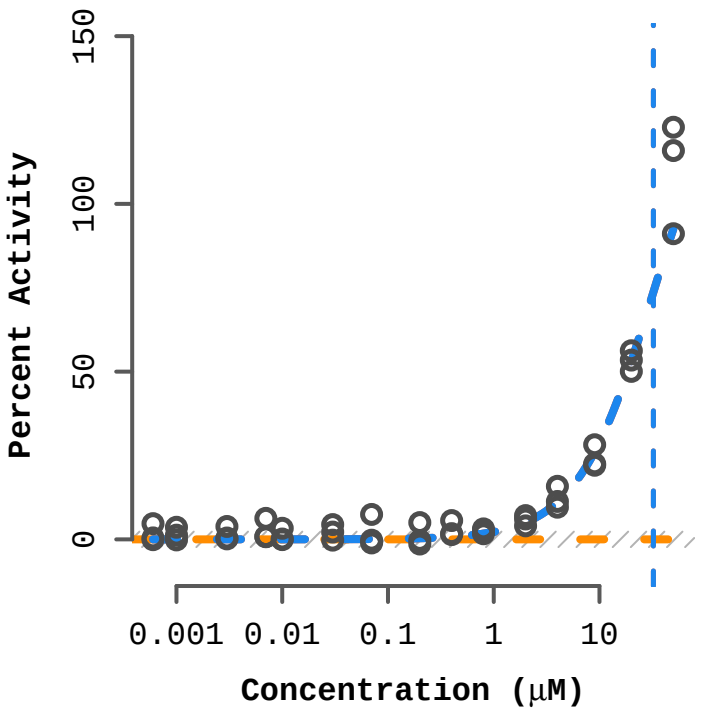
	tp	ga	gw
val:	205	1.36	1.48
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	205	1.36	1.48	2.27	17
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	442.83	283.39	287.39
PROB:	0	0.88	0.12
RMSE:	48.66	5.6	5.6

MAX_MEAN: 158 MAX_MED: 166 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix7 AR1 8-EQC
CHID: 49500 CASRN: NOCAS_49500
SPID(S): Tox21_203059
M4ID: 12479193

HILL MODEL (in red):

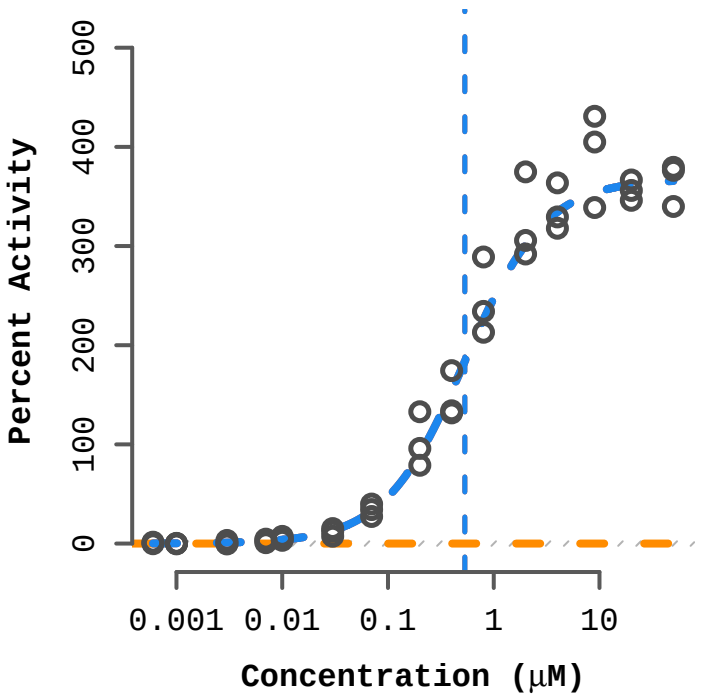
	tp	ga	gw
val:	147	1.51	1.2
sd:	20.1	0.104	0.108

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	147	1.51	1.2	3.5	7.15
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	403.12	258.81	262.81
PROB:	0	0.88	0.12
RMSE:	32.66	6.3	6.3

MAX_MEAN: 110 MAX_MED: 116 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix8 AR1 8-EQC
CHID: 49501 CASRN: NOCAS_49501
SPID(S): Tox21_203060
M4ID: 12479192

HILL MODEL (in red):

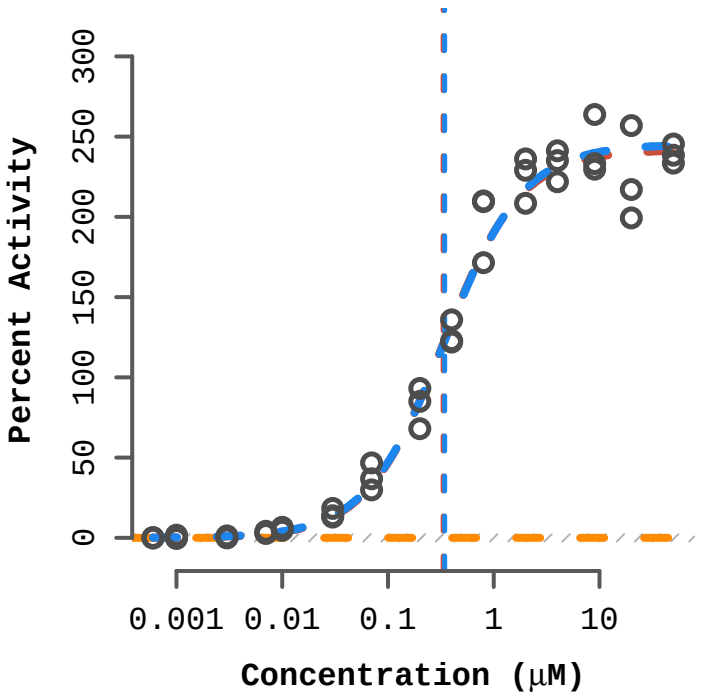
	tp	ga	gw
val:	368	−0.273	1.15
sd:	6.74	0.0349	0.0709

GAIN-LOSS MODEL (in blue):

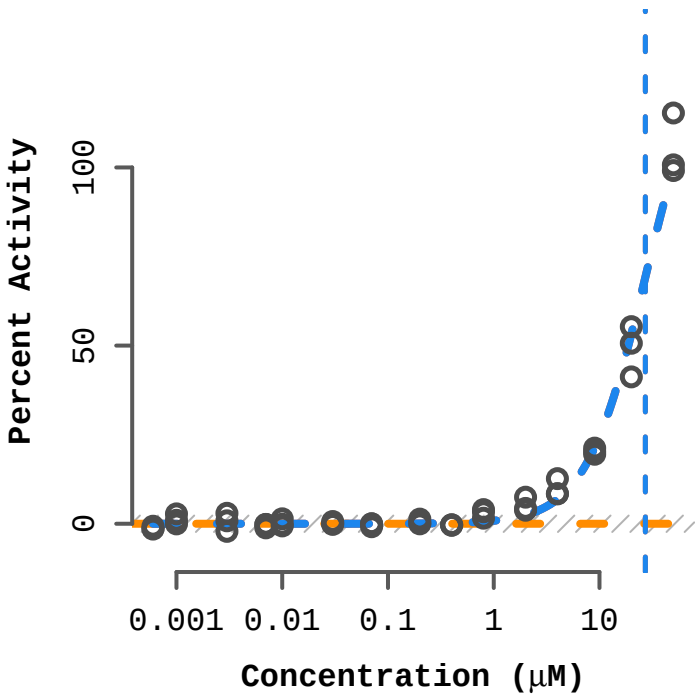
	tp	ga	gw	la	lw
val:	368	−0.273	1.15	3.39	5.31
sd:	6.74	0.0349	0.0709	1710	5390

	CNST	HILL	GNLS
AIC:	618.02	400.22	404.22
PROB:	0	0.88	0.12
RMSE:	220.83	23.28	23.28

MAX_MEAN: 392 **MAX_MED:** 405 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix9 AR1 8-EQC
CHID:    49502   CASRN: NOCAS_49502
SPID(S): Tox21_203061
M4ID:    12479191

HILL MODEL (in red):
      tp       ga       gw
val:  242      -0.478   1.19
sd:   3.77     0.0291   0.0819

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  245      -0.464   1.16     1.79     18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  584.28      354.07      357.56
PROB: 0           0.85        0.15
RMSE: 149.61      12.5        12.65

MAX_MEAN: 242       MAX_MED: 238       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix10 AR1 8-EQC
CHID: 49503 CASRN: NOCAS_49503
SPID(S): Tox21_203062
M4ID: 12479190

HILL MODEL (in red):

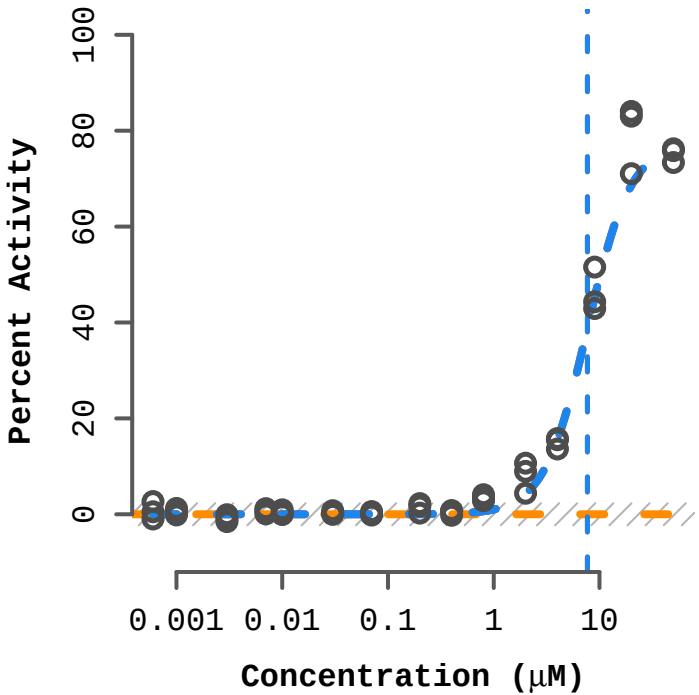
	tp	ga	gw
val:	138	1.43	1.54
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	138	1.43	1.54	2.42	16.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	391.26	213.99	217.99
PROB:	0	0.88	0.12
RMSE:	30.66	3.44	3.44

MAX_MEAN: 105 MAX_MED: 101 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix11 AR1 8-EQP
CHID: 49504 CASRN: NOCAS_49504
SPID(S): Tox21_203063
M4ID: 12479189

HILL MODEL (in red):

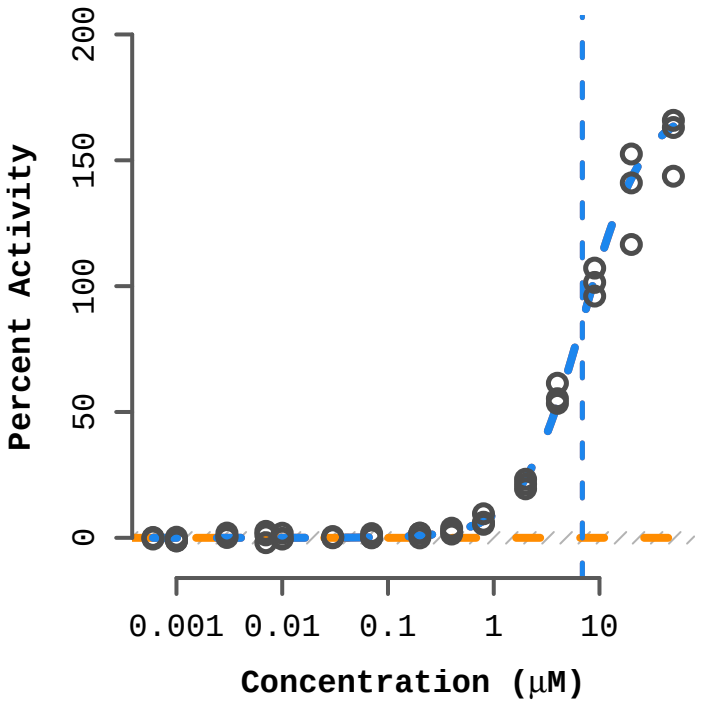
	tp	ga	gw
val:	77.6	0.886	2.12
sd:	1.16	0.016	0.137

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	77.6	0.886	2.12	3.41	14.2
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	417.16	220.37	224.37
PROB:	0	0.88	0.12
RMSE:	31.04	3.73	3.73

MAX_MEAN: 79.4 MAX_MED: 83 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix12 AR1 8-EQC
CHID: 49505 CASRN: NOCAS_49505
SPID(S): Tox21_203064
M4ID: 12479188

HILL MODEL (in red):

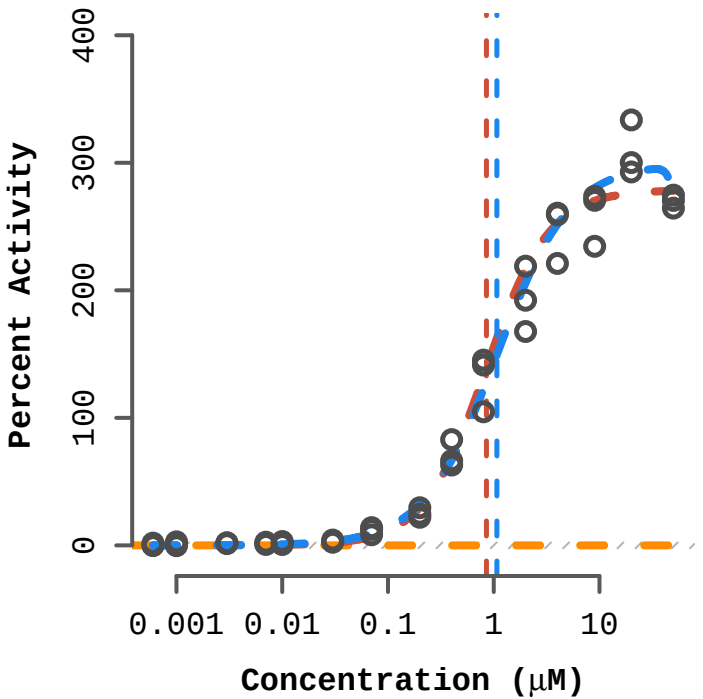
	tp	ga	gw
val:	172	0.838	1.49
sd:	2.45	0.0168	0.0543

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	172	0.838	1.49	2.79	7.96
sd:	2.45	0.0168	0.0543	608	4450

	CNST	HILL	GNLS
AIC:	487.34	243.33	247.33
PROB:	0	0.88	0.12
RMSE:	62.14	5.55	5.55

MAX_MEAN: 158 MAX_MED: 163 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix13 AR1 8-EQC
CHID: 49506 CASRN: NOCAS_49506
SPID(S): Tox21_203065
M4ID: 12479187

HILL MODEL (in red):

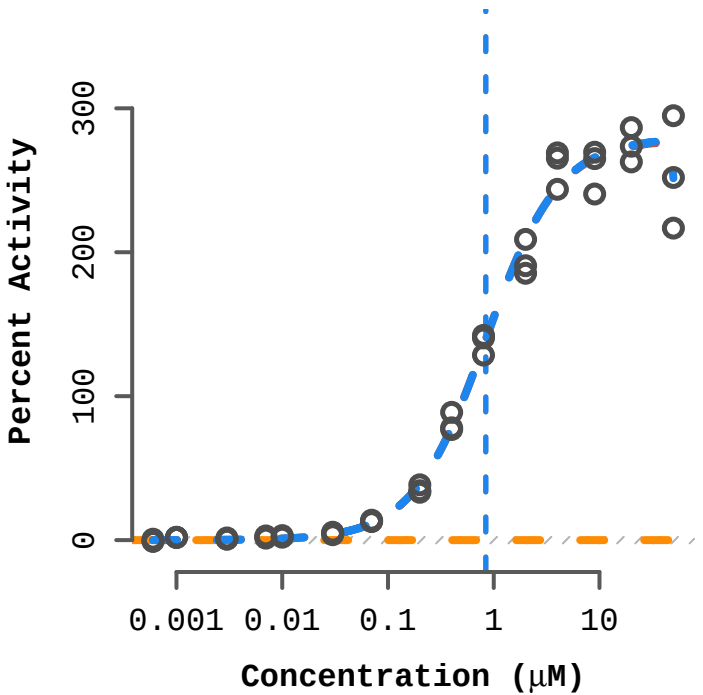
	tp	ga	gw
val:	279	-0.0689	1.47
sd:	4.98	0.0323	0.105

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	299	0.0299	1.26	1.79	11
sd:	9.68	0.0755	0.137	0.0115	2.15

	CNST	HILL	GNLS
AIC:	583.39	365.08	359.63
PROB:	0	0.06	0.94
RMSE:	154.61	15.83	13.86

MAX_MEAN: 309 MAX_MED: 300 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix14 AR1 8-EQC
CHID: 49507 CASRN: NOCAS_49507
SPID(S): Tox21_203066
M4ID: 12479186

HILL MODEL (in red):

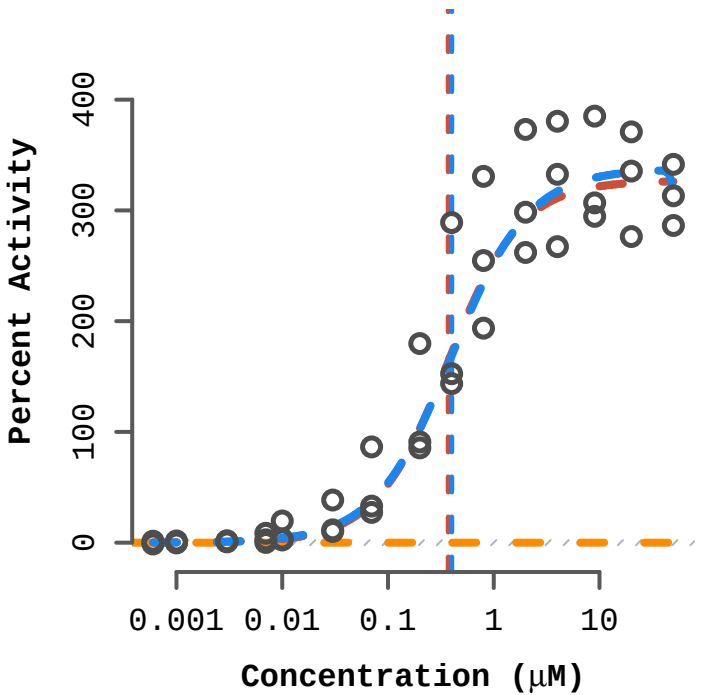
	tp	ga	gw
val:	279	−0.0765	1.26
sd:	4.95	0.0243	0.063

GAIN-LOSS MODEL (in blue):

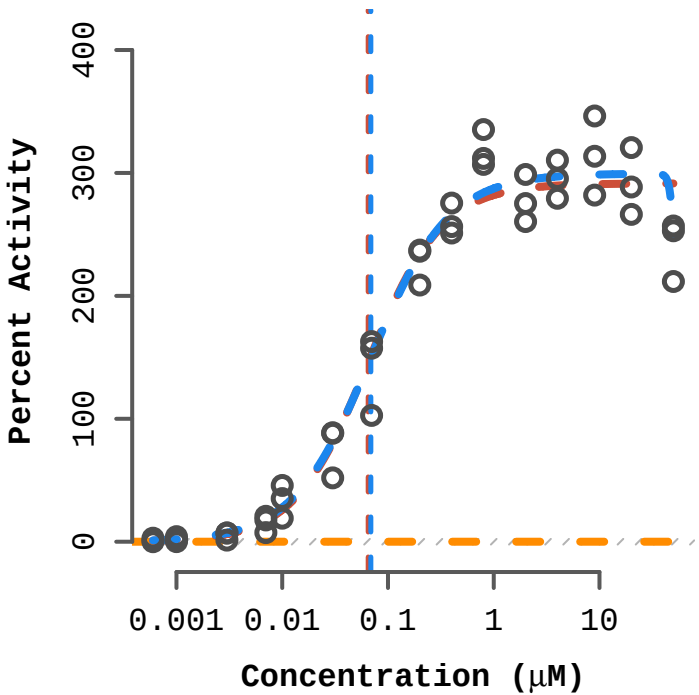
	tp	ga	gw	la	lw
val:	279	−0.0734	1.26	1.75	17.9
sd:	4.23	0.022	0.0562	0.011	2.18

	CNST	HILL	GNLS
AIC:	581.97	342.77	340.4
PROB:	0	0.23	0.77
RMSE:	150.67	13.11	11.79

MAX_MEAN: 274 MAX_MED: 274 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix15 AR1 8-EQC
CHID:    49508   CASRN: NOCAS_49508
SPID(S): Tox21_203067
M4ID:    12479185

HILL MODEL (in red):
      tp       ga       gw
val:  327      -0.43    1.26
sd:   11.4     0.0661   0.195

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  338      -0.397   1.19     1.76     17.9
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  614.22      454.1       457.07
PROB: 0           0.81        0.19
RMSE: 209.52      37.21       36.99

MAX_MEAN: 329       MAX_MED: 336       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix16 AR1 8-EQC
CHID: 49509 CASRN: NOCAS_49509
SPID(S): Tox21_203068
M4ID: 12479184

HILL MODEL (in red):

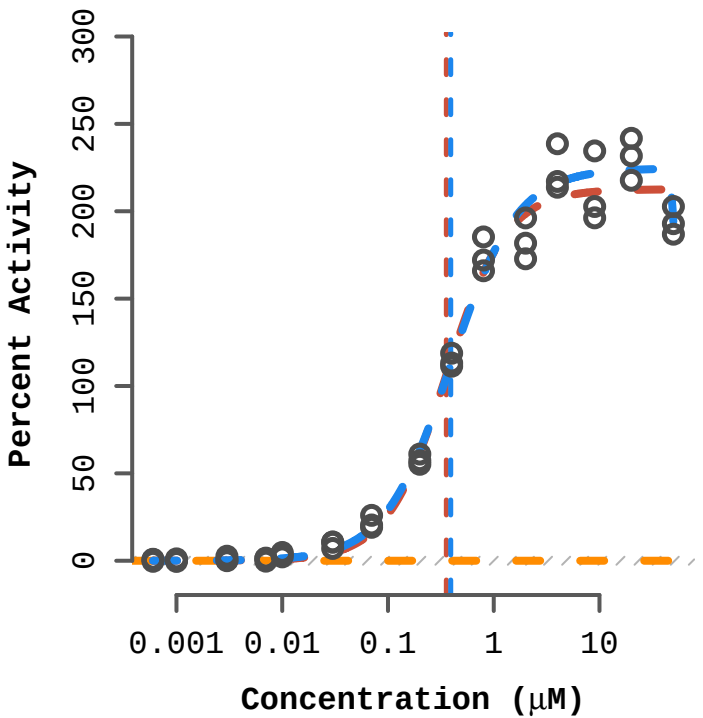
	tp	ga	gw
val:	291	-1.19	1.24
sd:	6.44	0.0425	0.106

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	300	-1.16	1.18	1.74	18
sd:	6.4	0.0401	0.089	0.00879	4.04

	CNST	HILL	GNLS
AIC:	617	415.83	404.12
PROB:	0	0	1
RMSE:	209.41	24.02	19.41

MAX_MEAN: 318 MAX_MED: 314 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix17 AR1 8-EQC
CHID: 49510 CASRN: NOCAS_49510
SPID(S): Tox21_203069
M4ID: 12479183

HILL MODEL (in red):

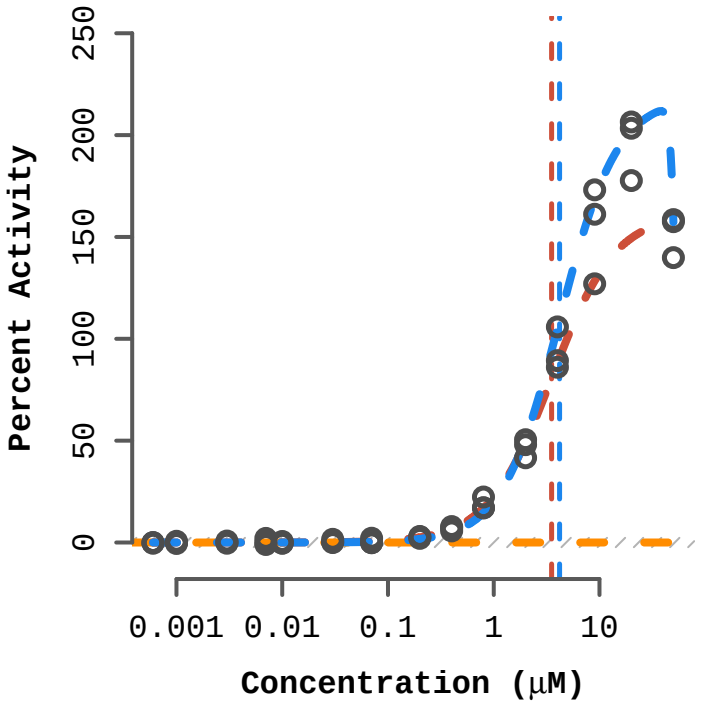
	tp	ga	gw
val:	213	-0.448	1.54
sd:	5.28	0.0238	0.128

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	225	-0.407	1.39	1.74	18
sd:	4.77	0.0225	0.0976	0.00495	2.32

	CNST	HILL	GNLS
AIC:	573.5	350.74	336.83
PROB:	0	0	1
RMSE:	133.44	11.66	10.02

MAX_MEAN: 230 MAX_MED: 232 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix18 AR1 8-EQC
CHID: 49511 CASRN: NOCAS_49511
SPID(S): Tox21_203070
M4ID: 12479182

HILL MODEL (in red):

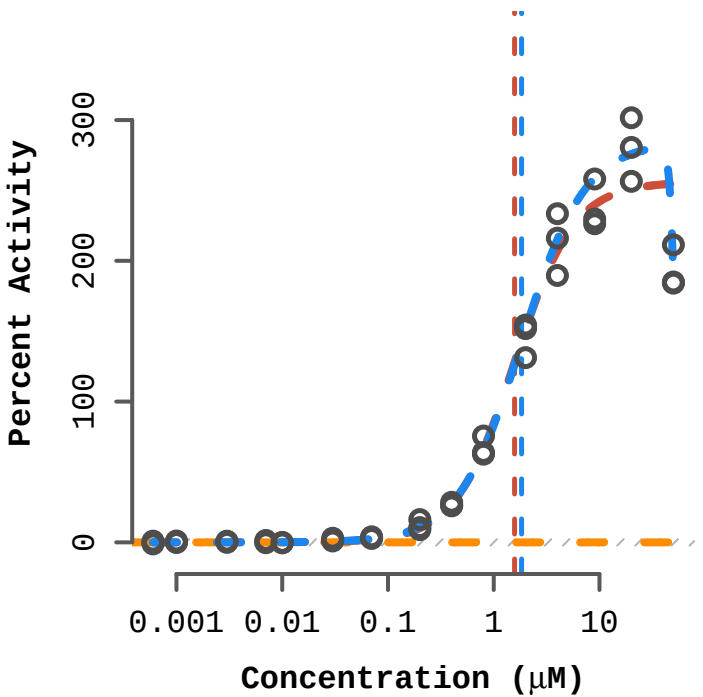
	tp	ga	gw
val:	162	0.547	1.45
sd:	1.9	0.0139	0.0526

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	219	0.623	1.59	1.72	18
sd:	5.27	0.0211	0.0829	0.00289	1.48

	CNST	HILL	GNLS
AIC:	518.01	326.77	294.37
PROB:	0	0	1
RMSE:	80.5	15.5	8.88

MAX_MEAN: 196 MAX_MED: 203 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix19 AR1 8-EQC
CHID: 49512 CASRN: NOCAS_49512
SPID(S): Tox21_203071
M4ID: 12479181

HILL MODEL (in red):

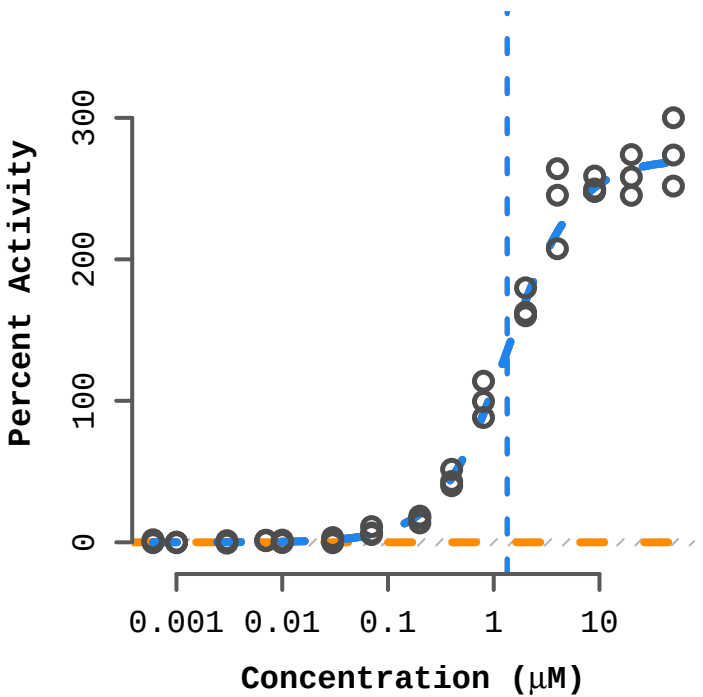
	tp	ga	gw
val:	256	0.197	1.55
sd:	11.1	0.0335	0.102

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	284	0.263	1.45	1.71	17.9
sd:	5.76	0.0186	0.0517	0.00294	1.97

	CNST	HILL	GNLS
AIC:	563.43	372.21	329.63
PROB:	0	0	1
RMSE:	127.95	19.71	10.73

MAX_MEAN: 280 MAX_MED: 281 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix20 AR1 8-EQC
CHID: 49513 CASRN: NOCAS_49513
SPID(S): Tox21_203072
M4ID: 12479180

HILL MODEL (in red):

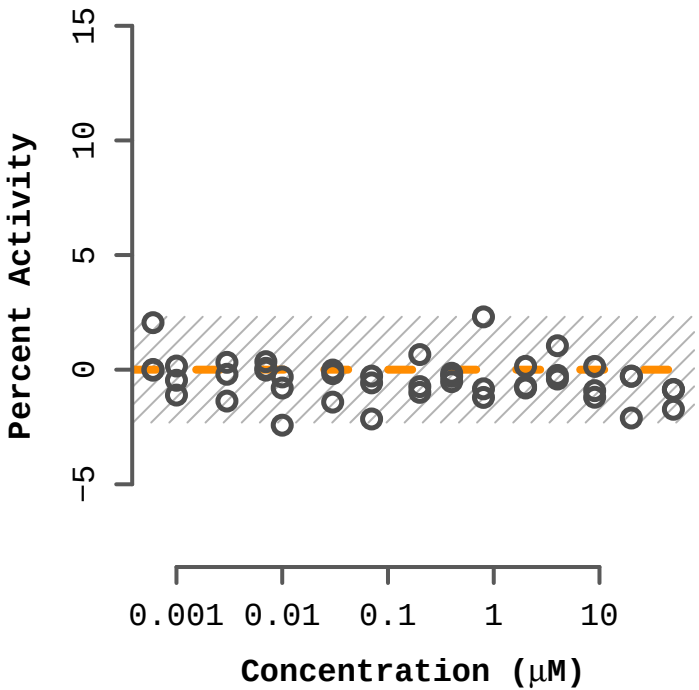
	tp	ga	gw
val:	271	0.128	1.33
sd:	5.48	0.0355	0.0844

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	271	0.128	1.33	3.51	5.79
sd:	5.48	0.0355	0.0844	9570	30600

	CNST	HILL	GNLS
AIC:	575.14	334.43	338.43
PROB:	0	0.88	0.12
RMSE:	142.71	11.28	11.28

MAX_MEAN: 275 MAX_MED: 274 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

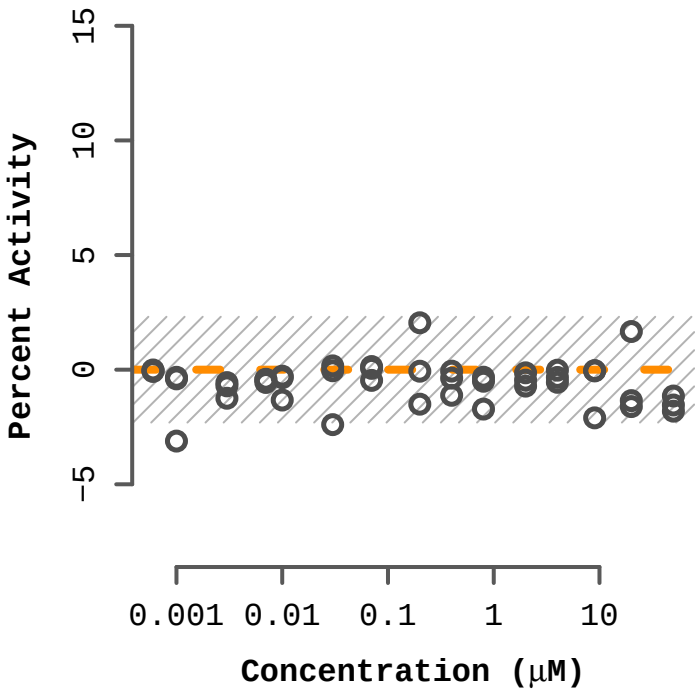
NAME: NTP Mix118 ER1 5-EQP
CHID: 49514 **CASRN:** NOCAS_49514
SPID(S): Tox21_203073
M4ID: 12479179

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.73	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.68 **MAX_MED:** 0.0622 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

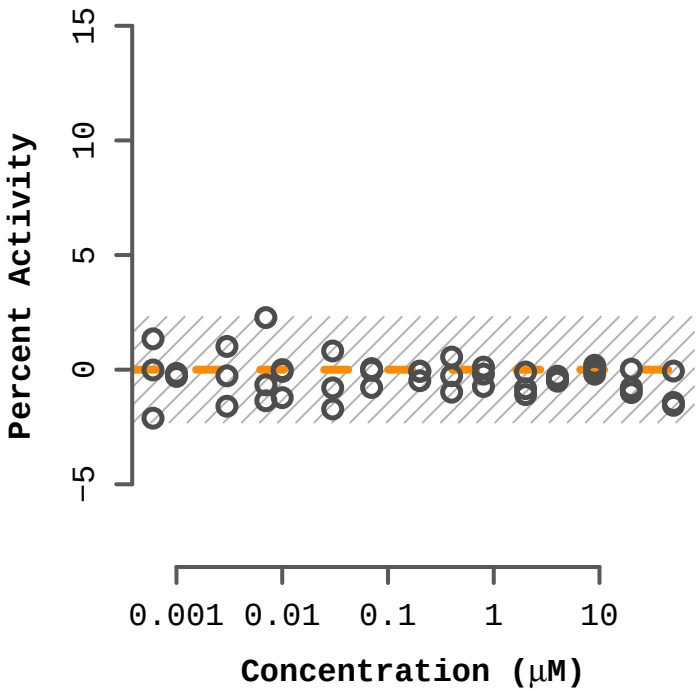
NAME: NTP Mix117 ER1 5-EQP
CHID: 49515 **CASRN:** NOCAS_49515
SPID(S): Tox21_203074
M4ID: 12479178

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.159 **MAX_MED:** 0.058 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

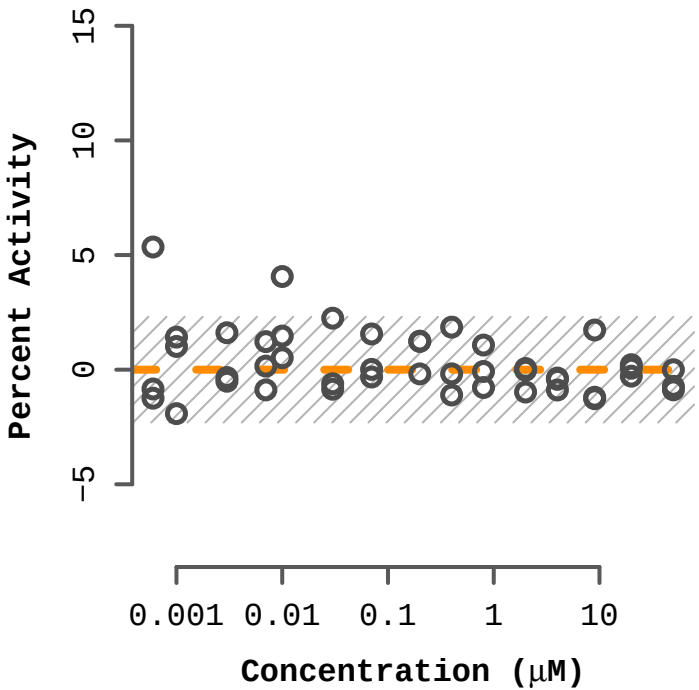
NAME: NTP Mix96 ER1 10-EQP
CHID: 49516 **CASRN:** NOCAS_49516
SPID(S): Tox21_203075
M4ID: 12479177

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.0865 **MAX_MED:** 0.000946 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

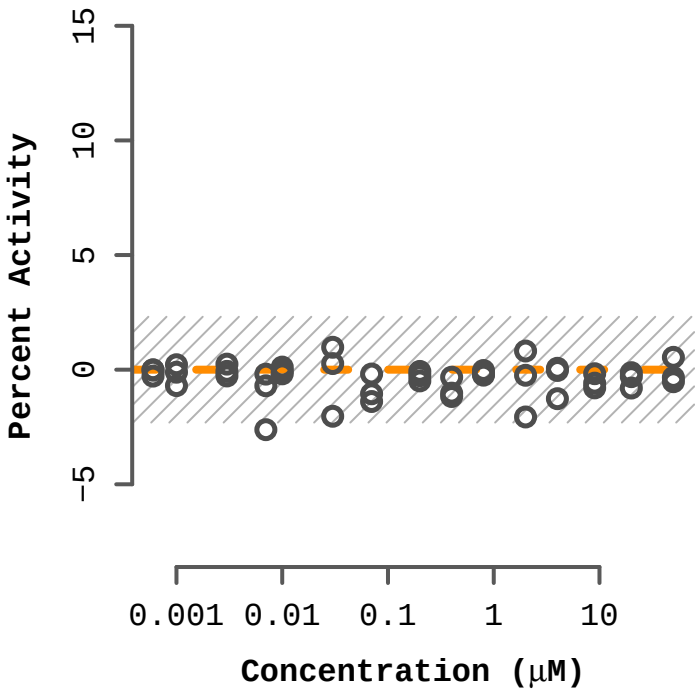
NAME: NTP Mix97 ER1 10-EQC
CHID: 49517 **CASRN:** NOCAS_49517
SPID(S): Tox21_203076
M4ID: 12479176

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.41	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

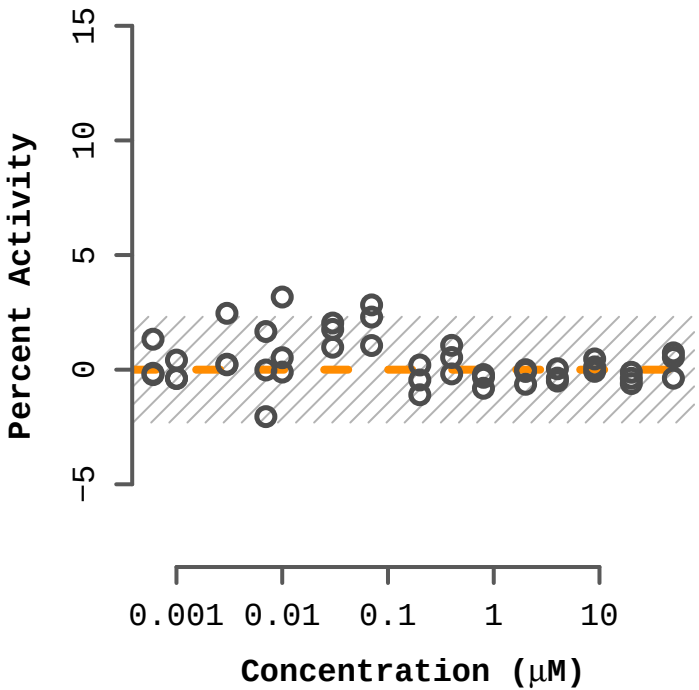
NAME: NTP Mix99 ER1 10−EQC
CHID: 49518 **CASRN:** NOCAS_49518
SPID(S): Tox21_203077
M4ID: 12479175

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.15	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: −0.0343 **MAX_MED:** 0.267 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

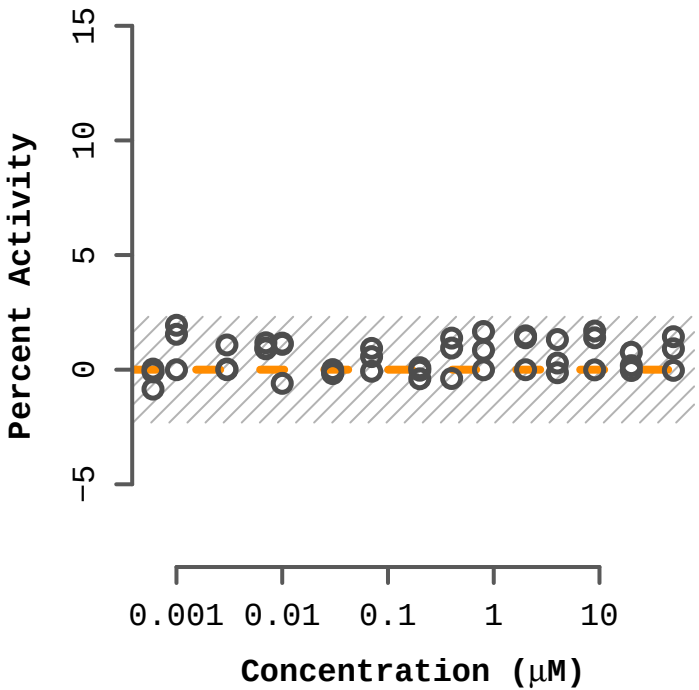
NAME: NTP Mix98 ER1 10-EQC
CHID: 49519 **CASRN:** NOCAS_49519
SPID(S): Tox21_203078
M4ID: 12479174

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 2.06 **MAX_MED:** 2.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

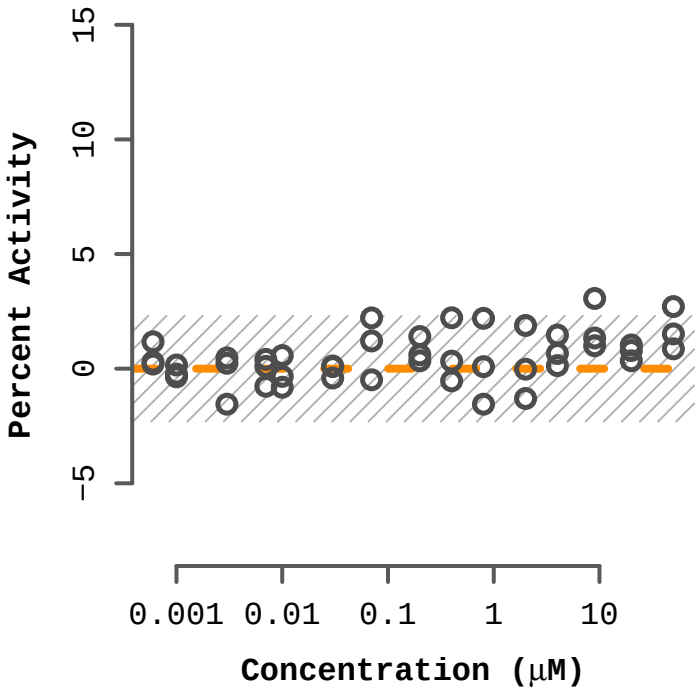
NAME: NTP Mix100 ER1 10-EQC
CHID: 49520 **CASRN:** NOCAS_49520
SPID(S): Tox21_203079
M4ID: 12479173

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.37	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

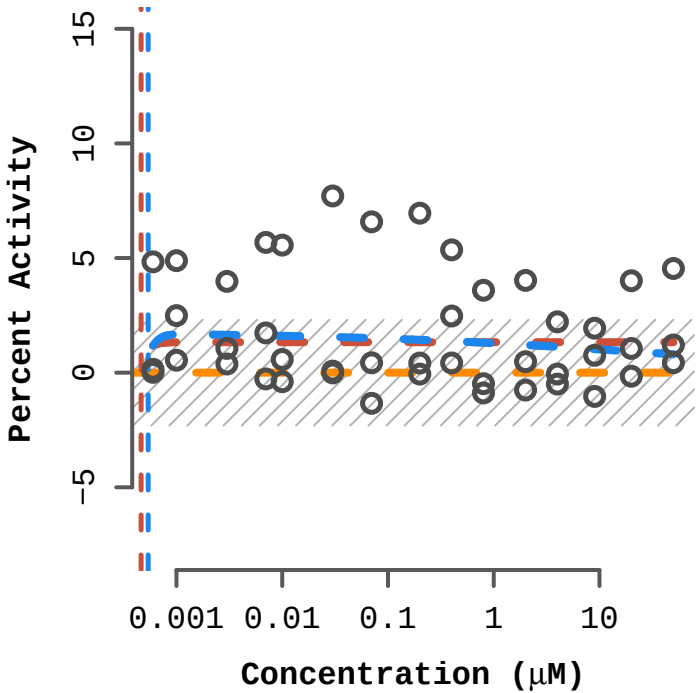
NAME: NTP Mix101 ER1 10-EQC
CHID: 49521 **CASRN:** NOCAS_49521
SPID(S): Tox21_203080
M4ID: 12479172

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.8 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix102 ER1 10-EQC
CHID: 49522 CASRN: NOCAS_49522
SPID(S): Tox21_203081
M4ID: 12479171

HILL MODEL (in red):

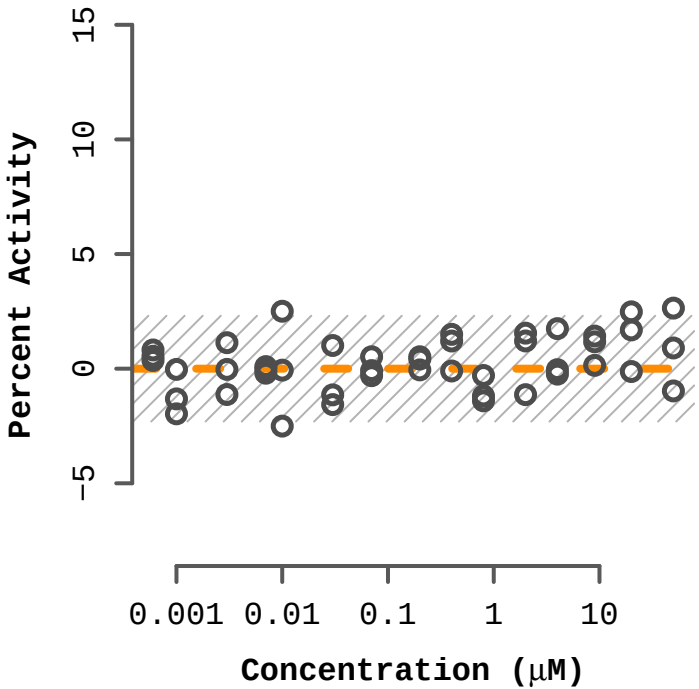
	tp	ga	gw
val:	1.33	−3.33	8
sd:	0.386	1.51	63.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.76	−3.27	8	1.45	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	226.13	218.08	221.8
PROB:	0.02	0.85	0.13
RMSE:	3.01	2.46	2.43

MAX_MEAN: 2.75 MAX_MED: 2.49 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

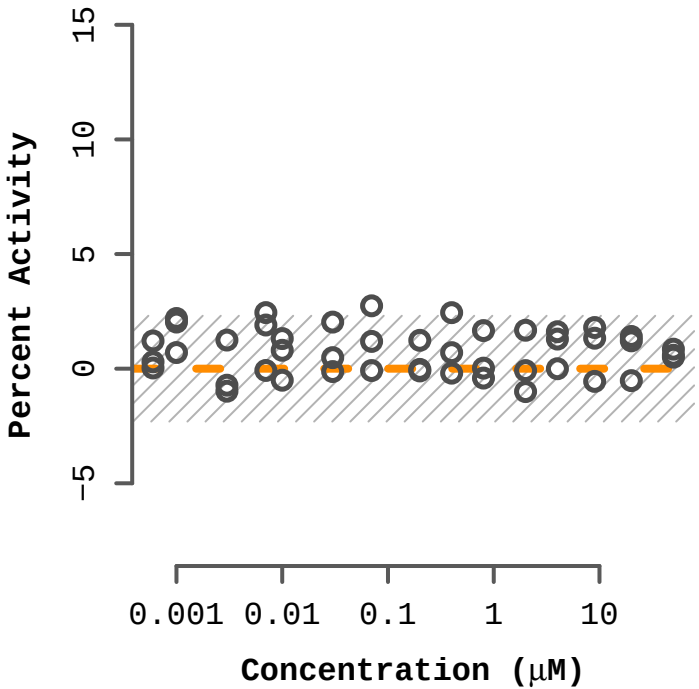
NAME: NTP Mix103 ER1 10-EQC
CHID: 49523 **CASRN:** NOCAS_49523
SPID(S): Tox21_203082
M4ID: 12479170

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.69 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

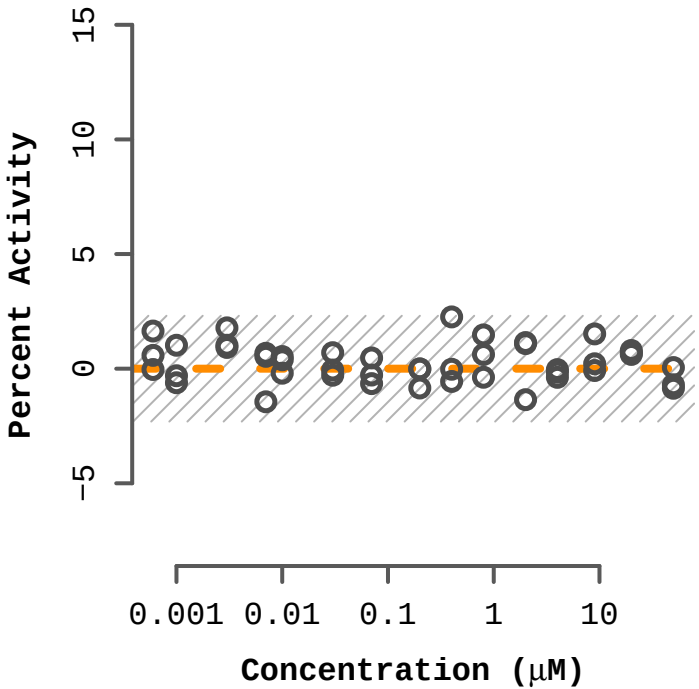
NAME: NTP Mix104 ER1 10−EQC
CHID: 49524 **CASRN:** NOCAS_49524
SPID(S): Tox21_203083
M4ID: 12479169

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

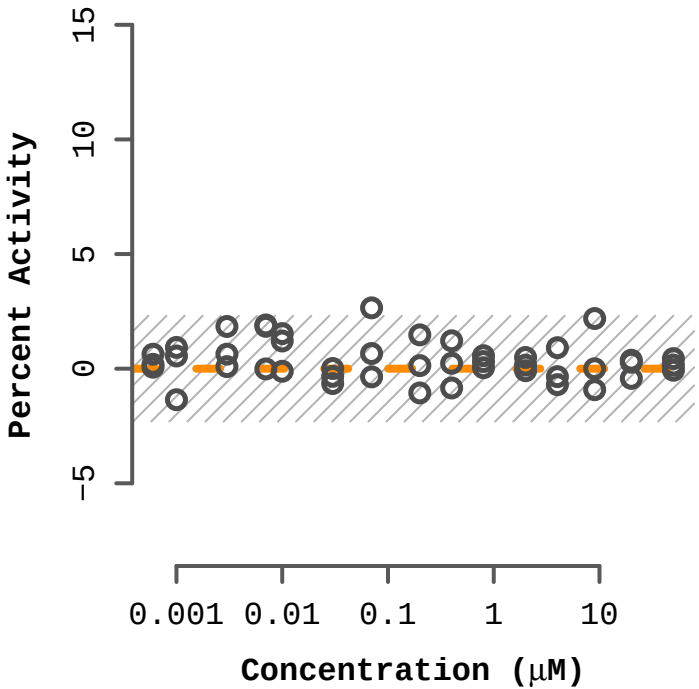
NAME: NTP Mix105 ER1 10-EQC
CHID: 49525 **CASRN:** NOCAS_49525
SPID(S): Tox21_203084
M4ID: 12479168

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.24	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

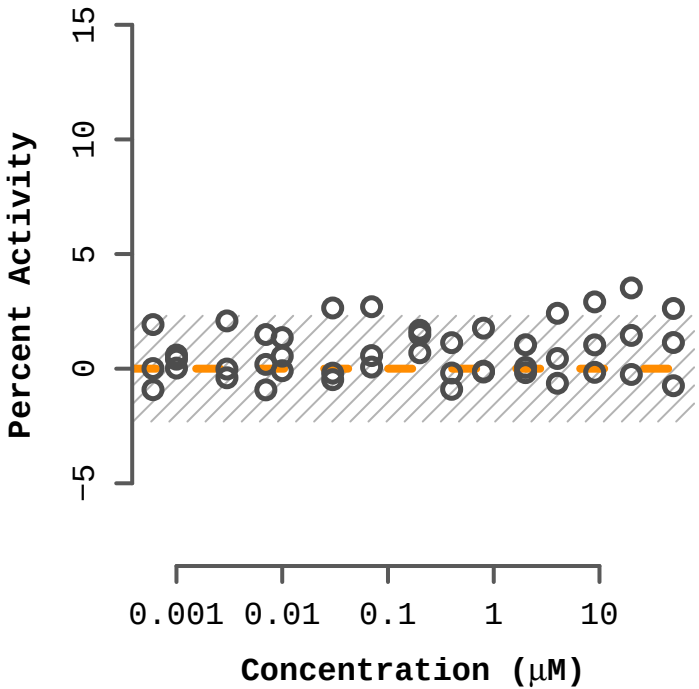
NAME: NTP Mix106 ER1 10−EQC
CHID: 49526 **CASRN:** NOCAS_49526
SPID(S): Tox21_203085
M4ID: 12479167

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

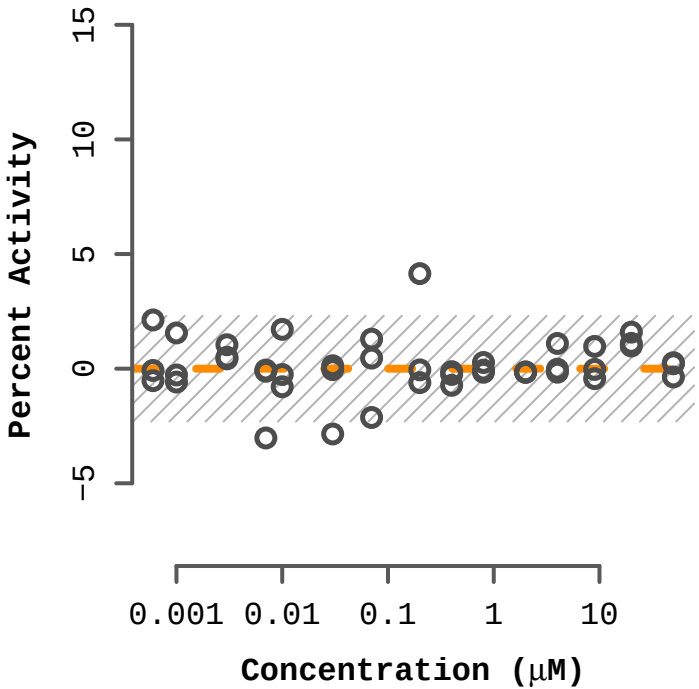
NAME: NTP Mix107 ER1 10-EQC
CHID: 49527 **CASRN:** NOCAS_49527
SPID(S): Tox21_203086
M4ID: 12479166

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.86	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.49 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

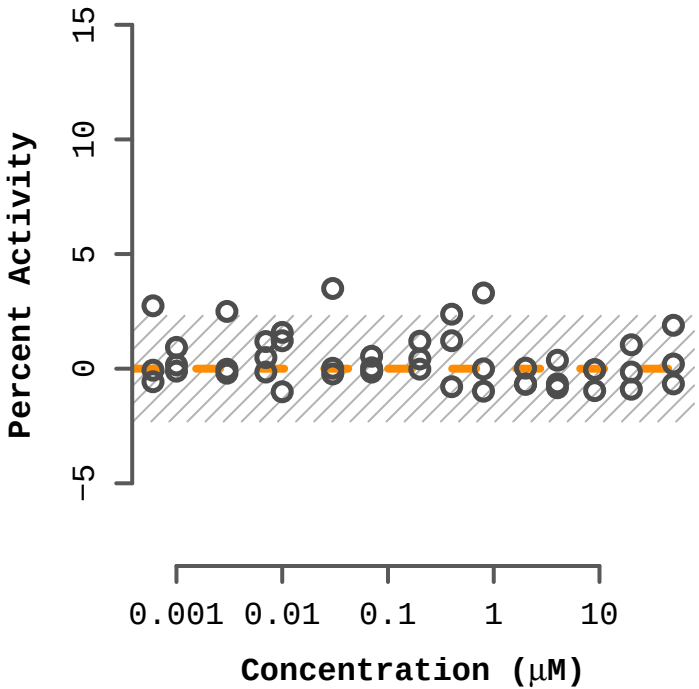
NAME: NTP Mix108 ER1 10-EQC
CHID: 49528 **CASRN:** NOCAS_49528
SPID(S): Tox21_203087
M4ID: 12479165

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

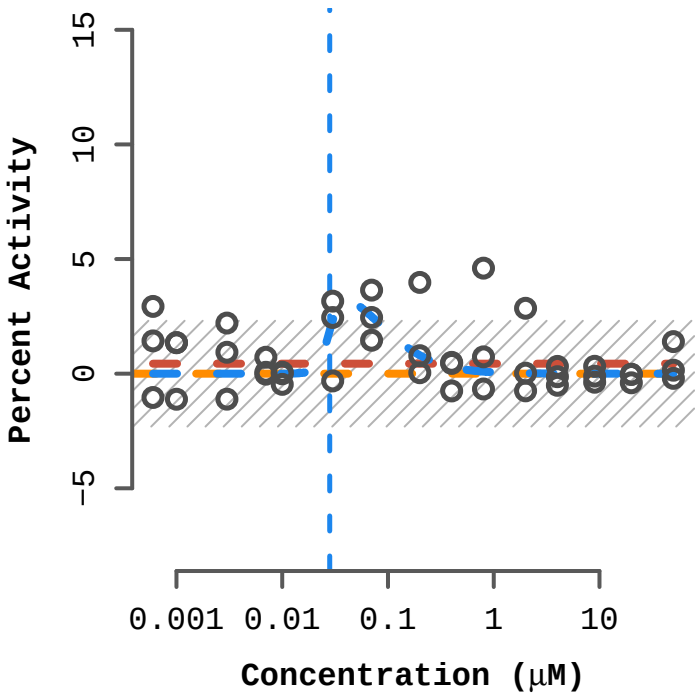
NAME: NTP Mix109 ER1 10−EQC
CHID: 49529 **CASRN:** NOCAS_49529
SPID(S): Tox21_203088
M4ID: 12479164

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix110 ER1 10−EQC
CHID: 49530 CASRN: NOCAS_49530
SPID(S): Tox21_203089
M4ID: 12479163

HILL MODEL (in red):

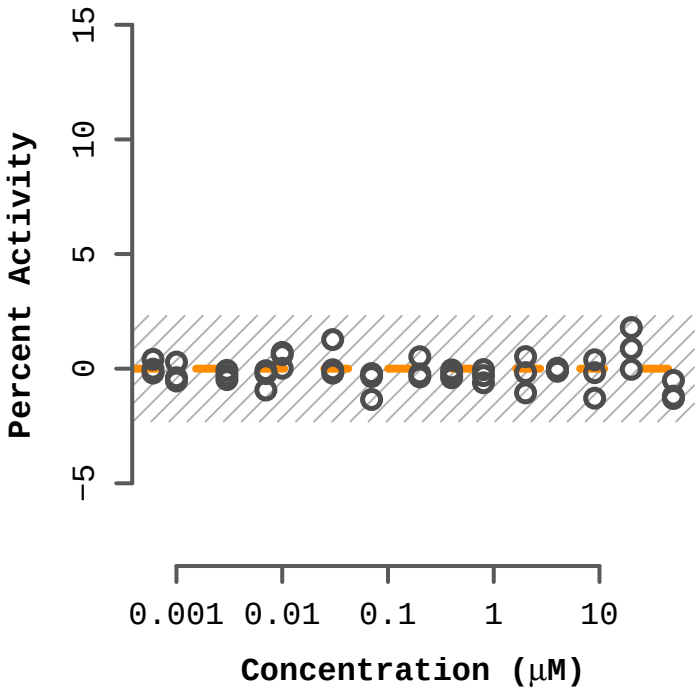
	tp	ga	gw
val:	0.436	−5.22	2.96
sd:	0.196	518	755

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.36	−1.55	8	−1.08	1.7
sd:	29.4	0.49	40	3.74	6.35

	CNST	HILL	GNLS
AIC:	165.79	166.49	157.15
PROB:	0.01	0.01	0.98
RMSE:	1.59	1.44	1.33

MAX_MEAN: 2.52 **MAX_MED:** 2.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

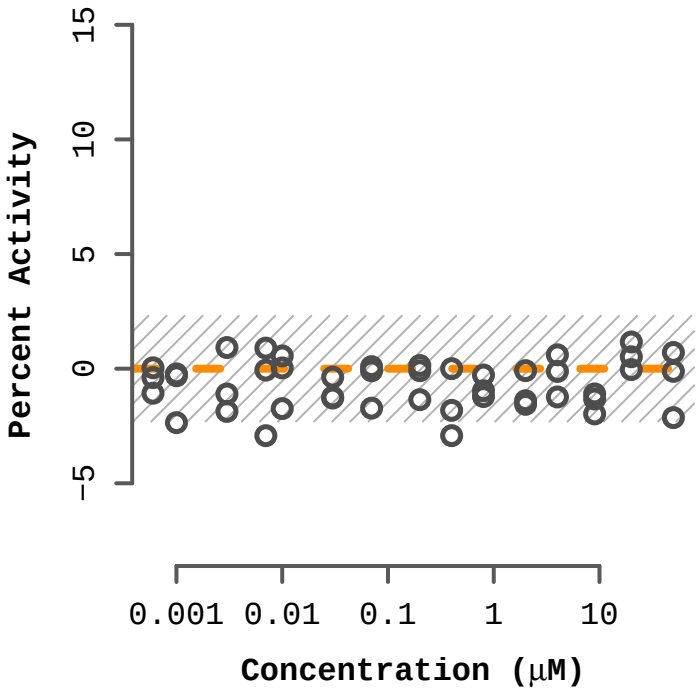
NAME: NTP Mix111 ER1 10-EQC
CHID: 49531 **CASRN:** NOCAS_49531
SPID(S): Tox21_203090
M4ID: 12479162

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	87.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.883 **MAX_MED:** 0.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

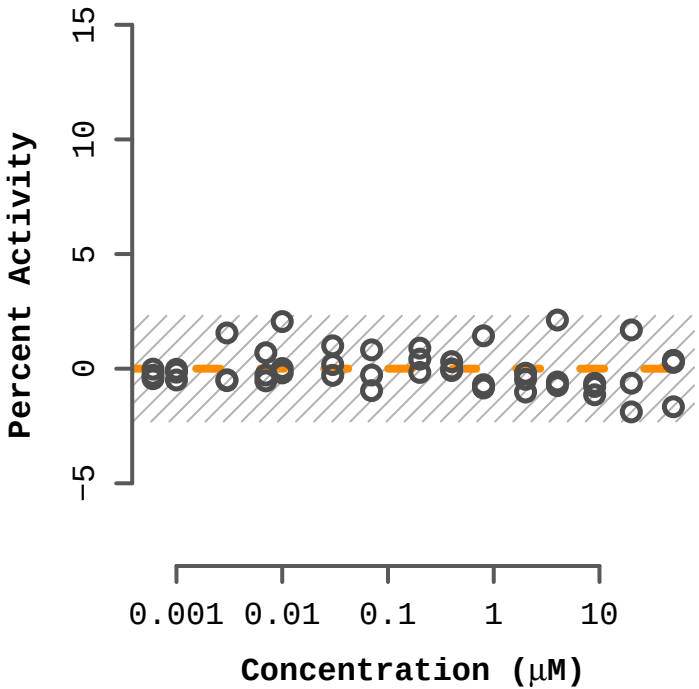
NAME: NTP Mix112 ER1 10-EQC
CHID: 49532 **CASRN:** NOCAS_49532
SPID(S): Tox21_203091
M4ID: 12479161

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.22	NA	NA

MAX_MEAN: 0.55 **MAX_MED:** 0.521 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

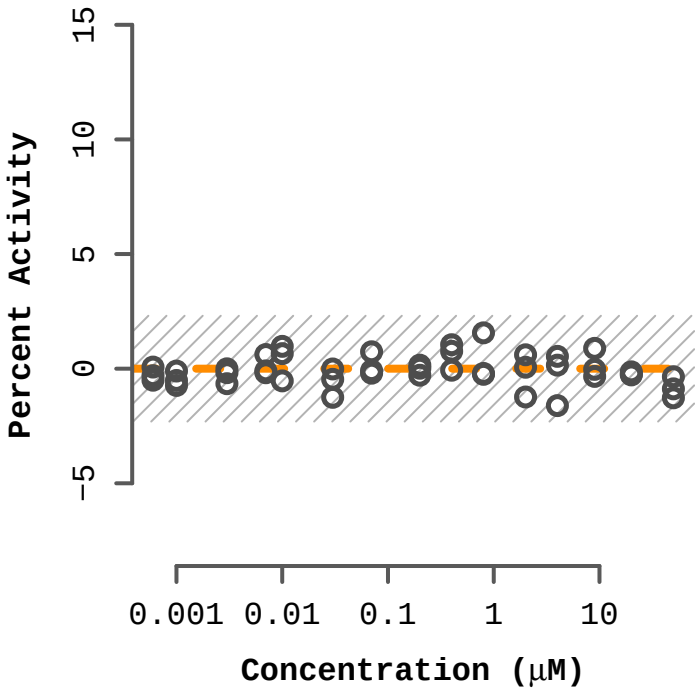
NAME: NTP Mix113 ER1 10-EQC
CHID: 49533 **CASRN:** NOCAS_49533
SPID(S): Tox21_203092
M4ID: 12479160

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.627 **MAX_MED:** 0.418 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

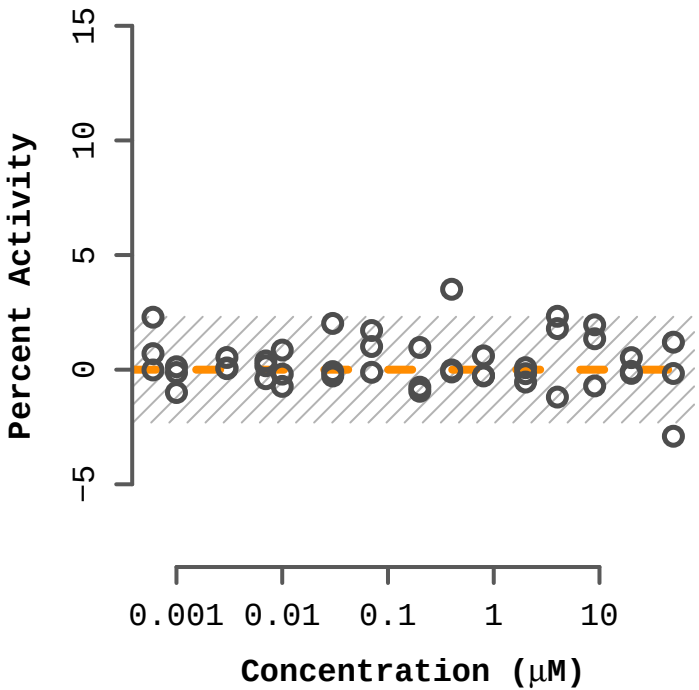
NAME: NTP Mix114 ER1 10-EQC
CHID: 49534 **CASRN:** NOCAS_49534
SPID(S): Tox21_203093
M4ID: 12479159

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.65	NA	NA

MAX_MEAN: 0.581 **MAX_MED:** 0.76 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

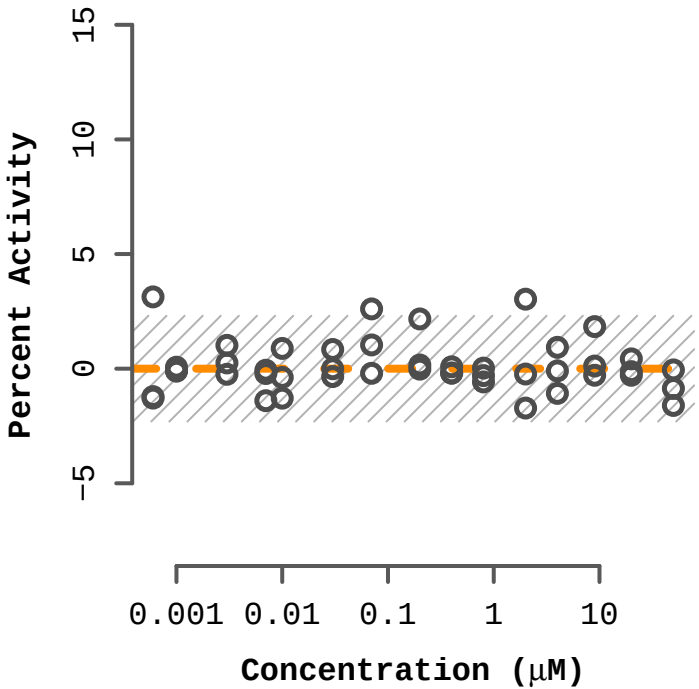
NAME: NTP Mix115 ER1 10-EQC
CHID: 49535 **CASRN:** NOCAS_49535
SPID(S): Tox21_203094
M4ID: 12479158

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 1.79 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

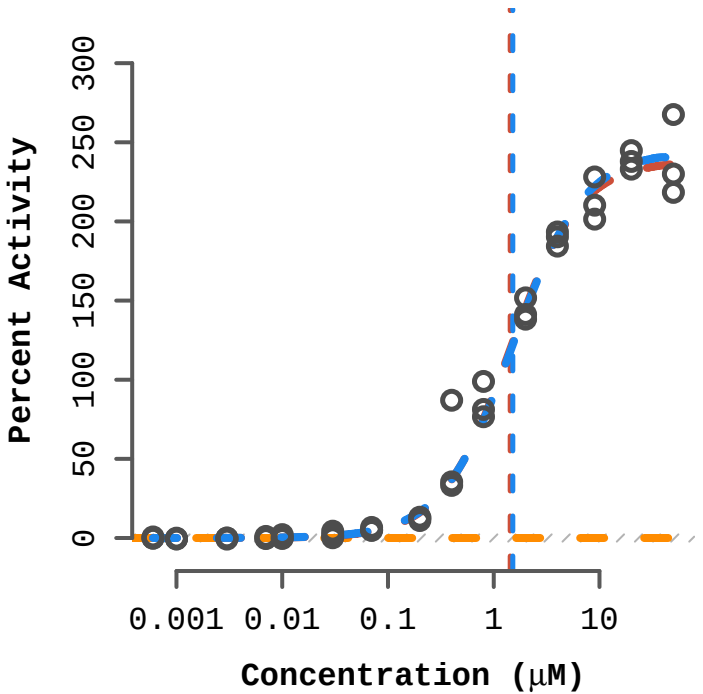
NAME: NTP Mix116 ER1 10-EQC
CHID: 49536 **CASRN:** NOCAS_49536
SPID(S): Tox21_203095
M4ID: 12479157

HILL MODEL: Not applicable.

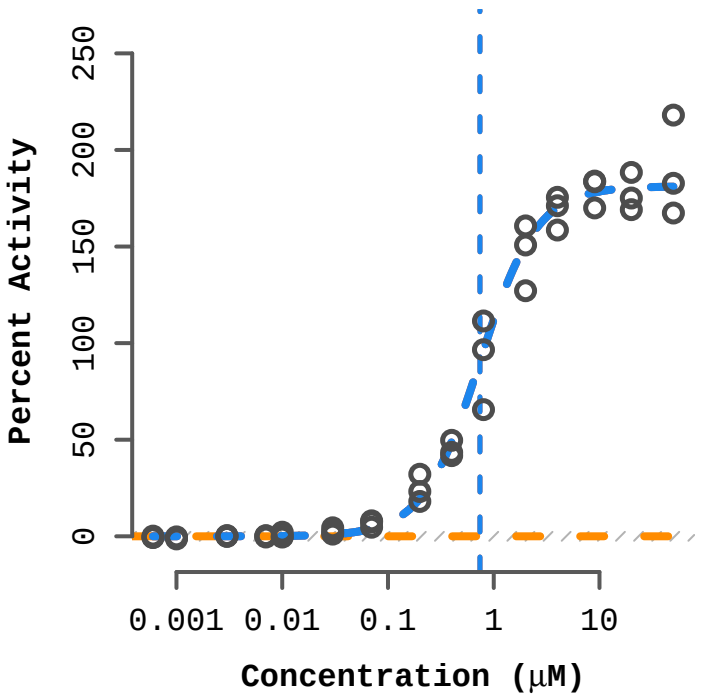
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.04 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix82 ER AR1 18-EQC
CHID:    49537   CASRN: NOCAS_49537
SPID(S): Tox21_203096
M4ID:    12479156

HILL MODEL (in red):
      tp       ga       gw
val:  238      0.156    1.33
sd:   4.91     0.0233   0.0566

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  244      0.18     1.29     1.77     18
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  561.96      319.66      317.79
PROB: 0           0.28        0.72
RMSE: 123.14      10.95       11.36

MAX_MEAN: 239       MAX_MED: 238       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix83 ER AR1 18-EQC
CHID: 49538 CASRN: NOCAS_49538
SPID(S): Tox21_203097
M4ID: 12479155

HILL MODEL (in red):

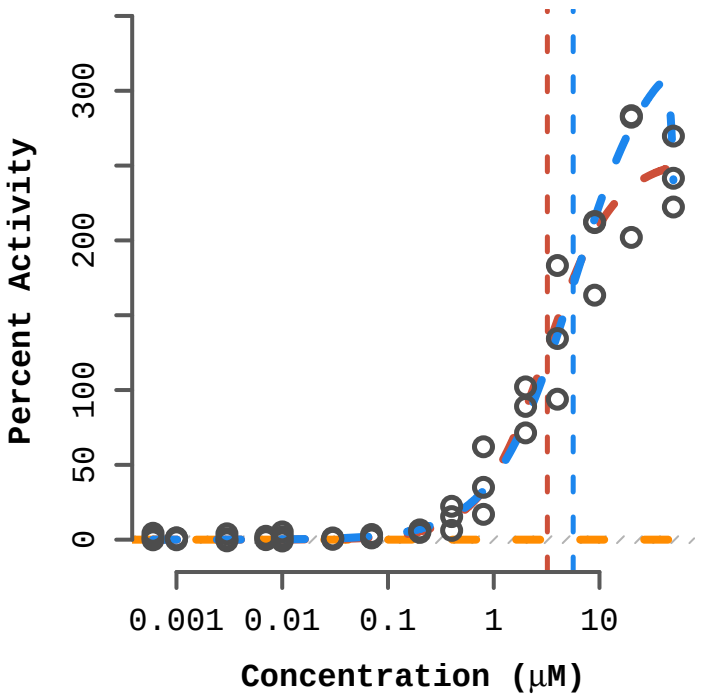
	tp	ga	gw
val:	181	-0.13	1.62
sd:	3.04	0.0233	0.111

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	181	-0.13	1.62	3.17	14.8
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	548.16	320.45	324.45
PROB:	0	0.88	0.12
RMSE:	103.75	9.67	9.67

MAX_MEAN: 189 MAX_MED: 184 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix84 ER AR1 18-EQC
CHID: 49539 **CASRN:** NOCAS_49539
SPID(S): Tox21_203098
M4ID: 12479154

HILL MODEL (in red):

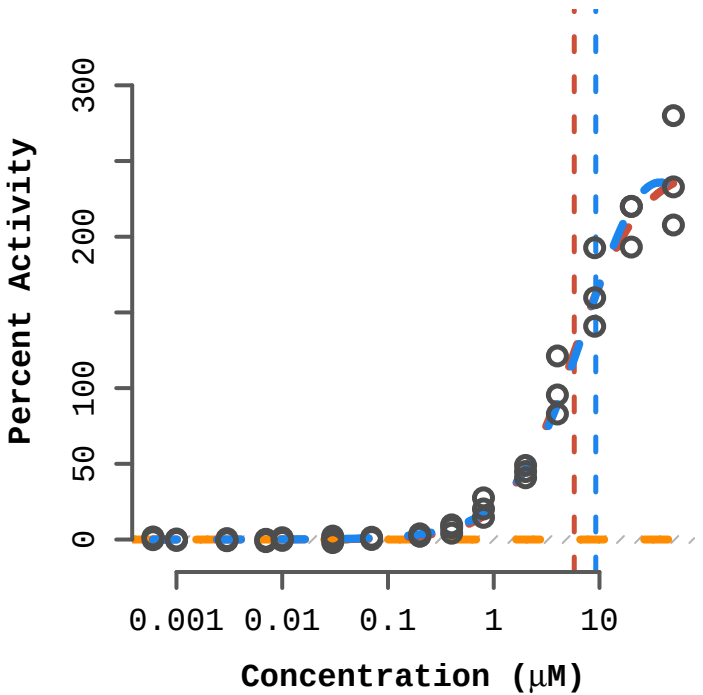
	tp	ga	gw
val:	255	0.507	1.37
sd:	14.7	0.0593	0.142

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	340	0.751	1.15	1.73	17.8
sd:	23.8	0.0673	0.0828	0.00455	3.69

	CNST	HILL	GNLS
AIC:	548.52	382.82	373.26
PROB:	0	0.01	0.99
RMSE:	114.36	18.06	18.47

MAX_MEAN: 256 **MAX_MED:** 282 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix85 ER AR1 18-EQC
CHID: 49540 CASRN: NOCAS_49540
SPID(S): Tox21_203099
M4ID: 12479153

HILL MODEL (in red):

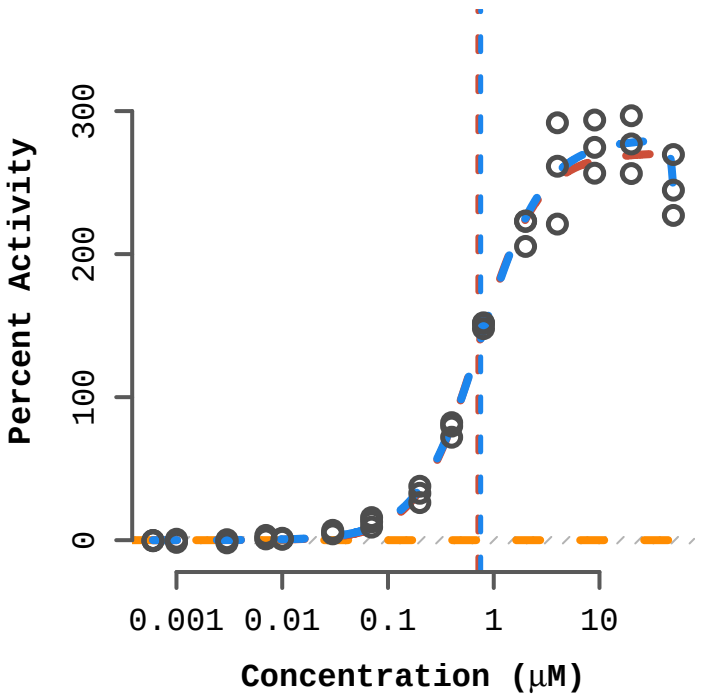
	tp	ga	gw
val:	248	0.761	1.37
sd:	6.63	0.027	0.0731

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	336	0.965	1.19	2.18	1.15
sd:	13.5	0.0251	0.038	0.0619	0.231

	CNST	HILL	GNLS
AIC:	534.29	325.44	320.95
PROB:	0	0.1	0.9
RMSE:	97.85	11.39	11.86

MAX_MEAN: 240 MAX_MED: 233 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix86 ER AR1 18-EQP
CHID: 49541 CASRN: NOCAS_49541
SPID(S): Tox21_203100
M4ID: 12479152

HILL MODEL (in red):

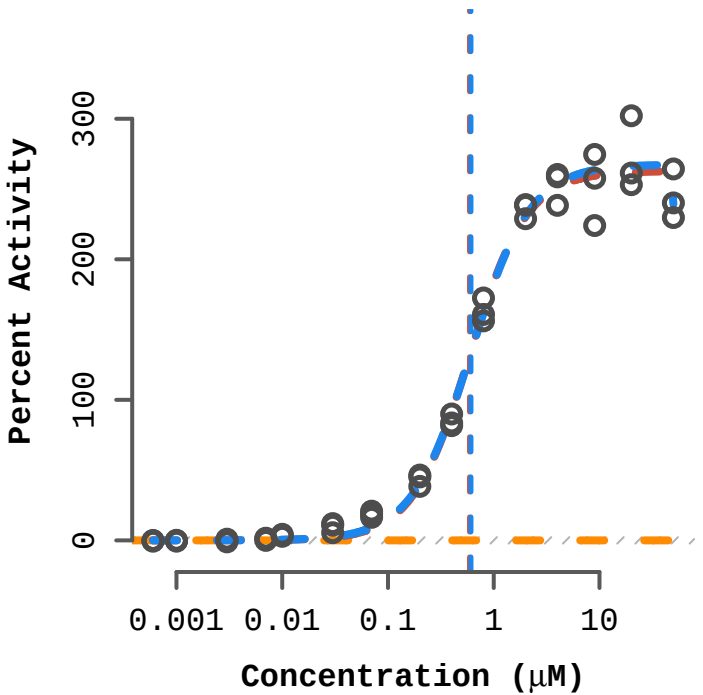
	tp	ga	gw
val:	271	-0.15	1.52
sd:	4.97	0.0175	0.0741

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	280	-0.123	1.44	1.74	18
sd:	4.84	0.018	0.0671	0.00591	2.39

	CNST	HILL	GNLS
AIC:	584.55	349.05	342.29
PROB:	0	0.03	0.97
RMSE:	154.66	13.18	11.33

MAX_MEAN: 277 MAX_MED: 277 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix87 ER AR1 18-EQC
CHID: 49542 CASRN: NOCAS_49542
SPID(S): Tox21_203101
M4ID: 12479151

HILL MODEL (in red):

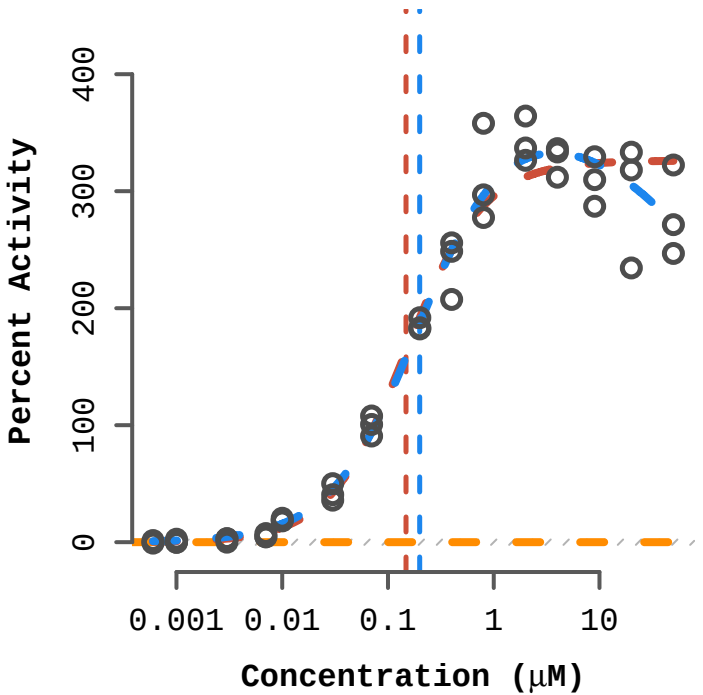
	tp	ga	gw
val:	263	-0.229	1.6
sd:	3.62	0.0167	0.0919

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	268	-0.215	1.55	1.75	17.6
sd:	4.76	0.0185	0.0894	0.00665	2.66

	CNST	HILL	GNLS
AIC:	584.74	343.17	339.21
PROB:	0	0.12	0.88
RMSE:	153.68	11.7	10.76

MAX_MEAN: 272 MAX_MED: 261 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix88 ER AR1 18-EQP
CHID: 49543 CASRN: NOCAS_49543
SPID(S): Tox21_203102
M4ID: 12479150

HILL MODEL (in red):

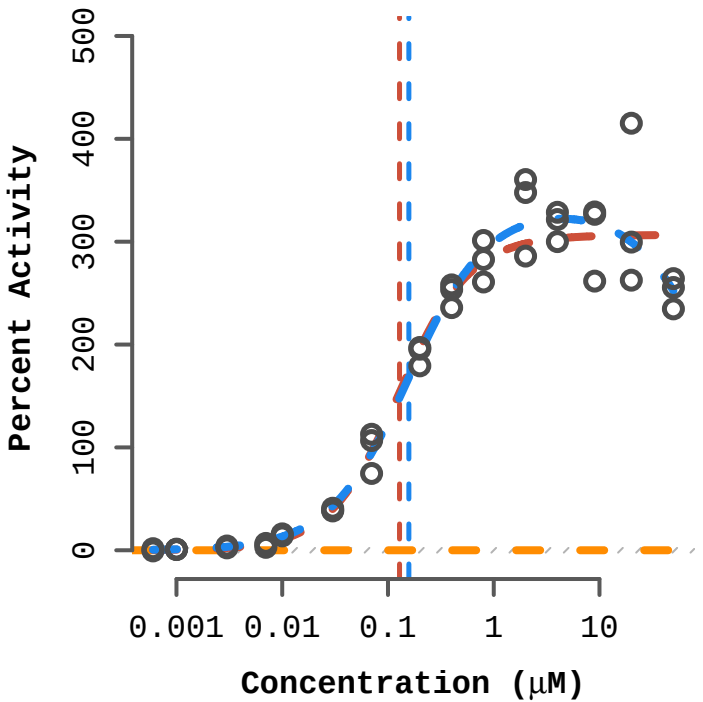
	tp	ga	gw
val:	326	-0.829	1.19
sd:	5.2	0.0264	0.0658

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	380	-0.7	1.05	2.43	0.56
sd:	64.8	0.107	0.0792	0.284	0.488

	CNST	HILL	GNLS
AIC:	618.12	407.14	395.1
PROB:	0	0	1
RMSE:	214.55	26.19	20.66

MAX_MEAN: 343 MAX_MED: 337 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix89 ER AR1 18-EQP
CHID: 49544 CASRN: NOCAS_49544
SPID(S): Tox21_203103
M4ID: 12479149

HILL MODEL (in red):

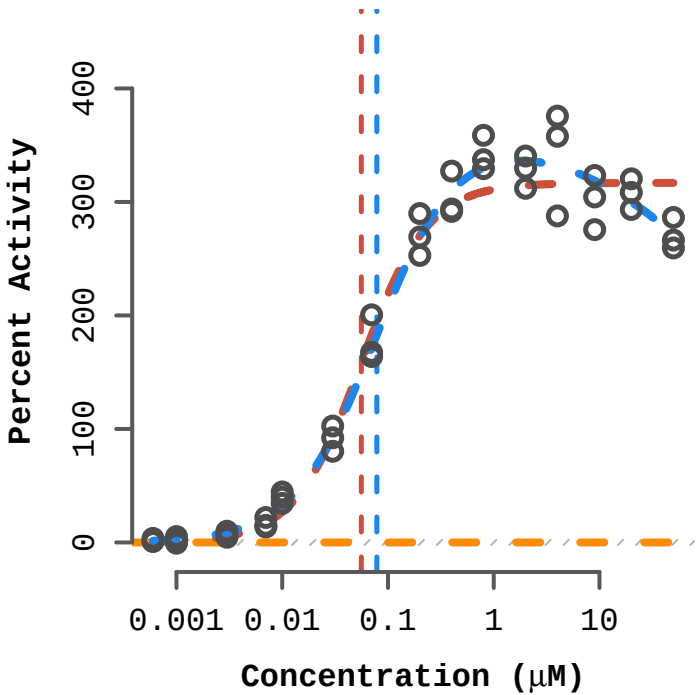
	tp	ga	gw
val:	307	-0.891	1.3
sd:	8.75	0.0399	0.104

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	336	-0.803	1.16	2.13	1.13
sd:	15.6	0.0492	0.0791	0.156	0.499

	CNST	HILL	GNLS
AIC:	616.61	421.98	397.41
PROB:	0	0	1
RMSE:	211.27	28.32	23.77

MAX_MEAN: 331 MAX_MED: 348 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix90 ER AR1 18-EQP
CHID: 49545 CASRN: NOCAS_49545
SPID(S): Tox21_203104
M4ID: 12479148

HILL MODEL (in red):

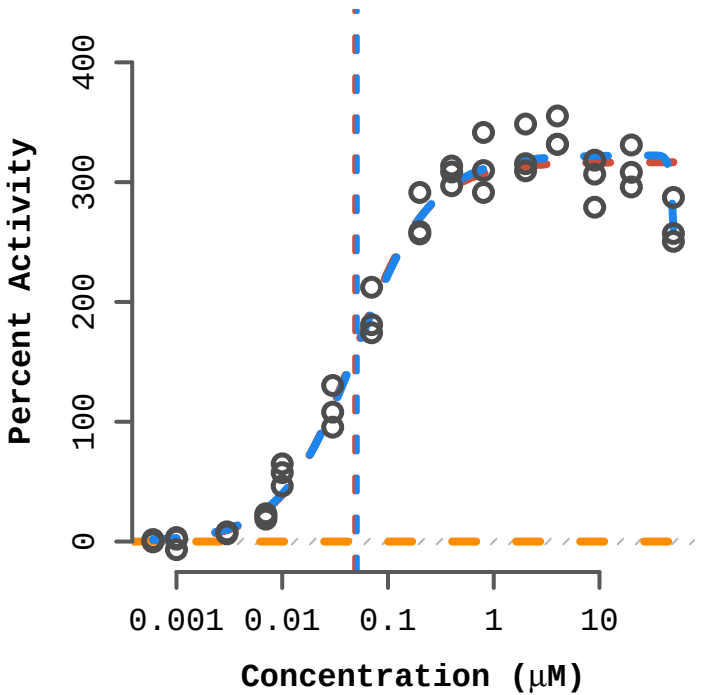
	tp	ga	gw
val:	317	-1.25	1.38
sd:	6.18	0.0354	0.113

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	372	-1.11	1.13	2.59	0.486
sd:	39.9	0.0721	0.0878	0.329	0.31

	CNST	HILL	GNLS
AIC:	626.63	414.42	388
PROB:	0	0	1
RMSE:	232.28	22.8	16.48

MAX_MEAN: 342 MAX_MED: 358 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix91 ER AR1 18-EQP
CHID: 49546 CASRN: NOCAS_49546
SPID(S): Tox21_203105
M4ID: 12479147

HILL MODEL (in red):

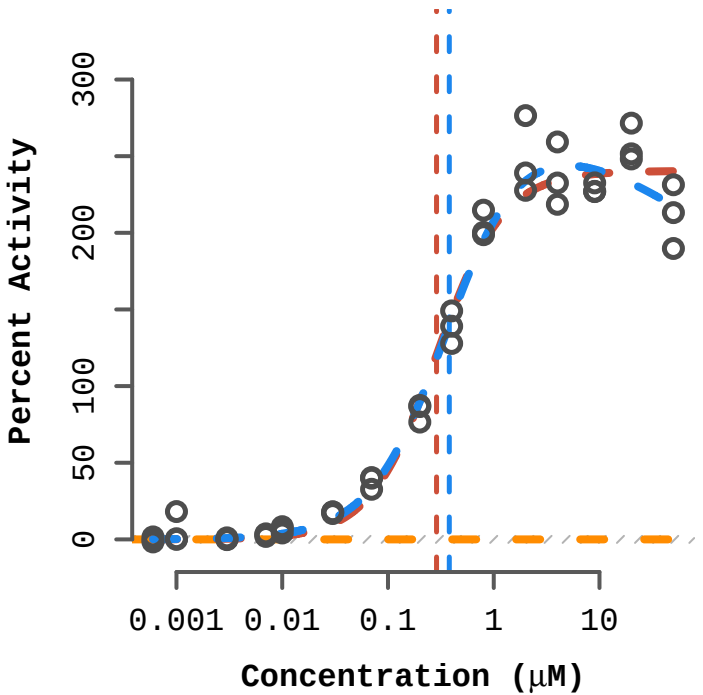
	tp	ga	gw
val:	317	-1.31	1.24
sd:	5.26	0.0372	0.0919

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	322	-1.29	1.2	1.73	17.9
sd:	4.92	0.0347	0.079	0.00564	2.79

	CNST	HILL	GNLS
AIC:	626.31	405.15	390.09
PROB:	0	0	1
RMSE:	230.66	20.95	15.92

MAX_MEAN: 340 MAX_MED: 332 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix92 ER AR1 18-EQP
CHID: 49547 CASRN: NOCAS_49547
SPID(S): Tox21_203106
M4ID: 12479146

HILL MODEL (in red):

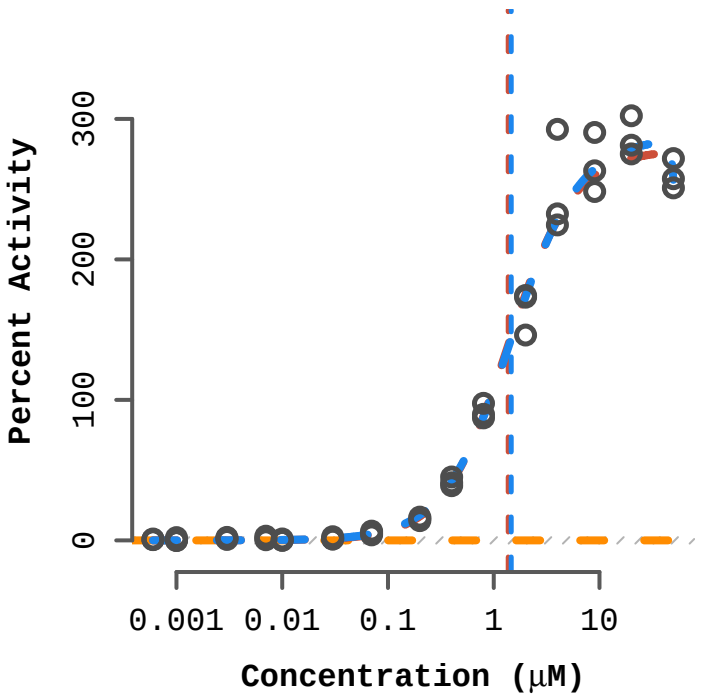
	tp	ga	gw
val:	240	-0.541	1.38
sd:	4.6	0.0266	0.115

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	307	-0.42	1.2	3.01	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	586.46	370.28	365.39
PROB:	0	0.08	0.92
RMSE:	153.17	15.34	13.3

MAX_MEAN: 257 MAX_MED: 252 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix93 ER AR1 18-EQP
CHID: 49548 CASRN: NOCAS_49548
SPID(S): Tox21_203107
M4ID: 12479145

HILL MODEL (in red):

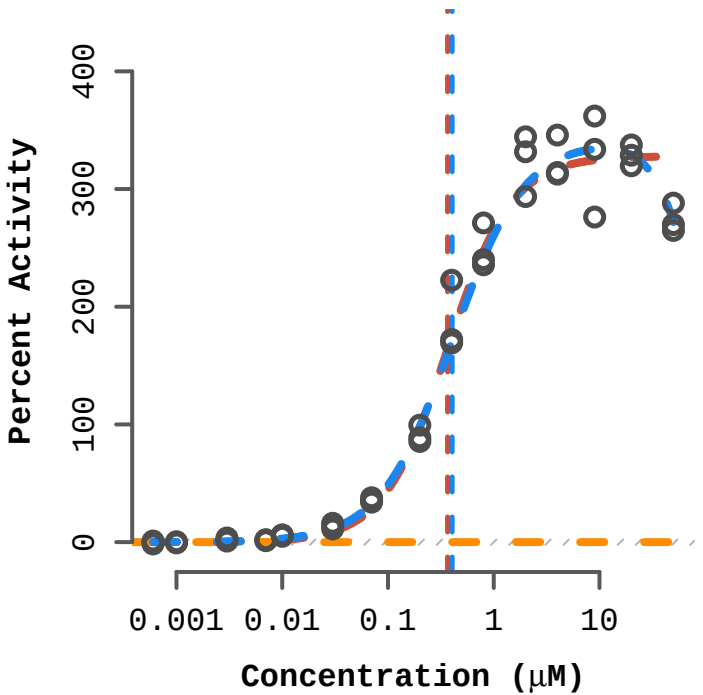
	tp	ga	gw
val:	278	0.137	1.42
sd:	4.13	0.0152	0.0431

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	287	0.165	1.36	1.75	18
sd:	3.25	0.0123	0.0358	0.0043	1.31

	CNST	HILL	GNLS
AIC:	576.93	328.71	313.24
PROB:	0	0	1
RMSE:	146.64	13.61	12.32

MAX_MEAN: 286 MAX_MED: 281 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix94 ER AR1 18-EQP
CHID: 49549 CASRN: NOCAS_49549
SPID(S): Tox21_203108
M4ID: 12479144

HILL MODEL (in red):

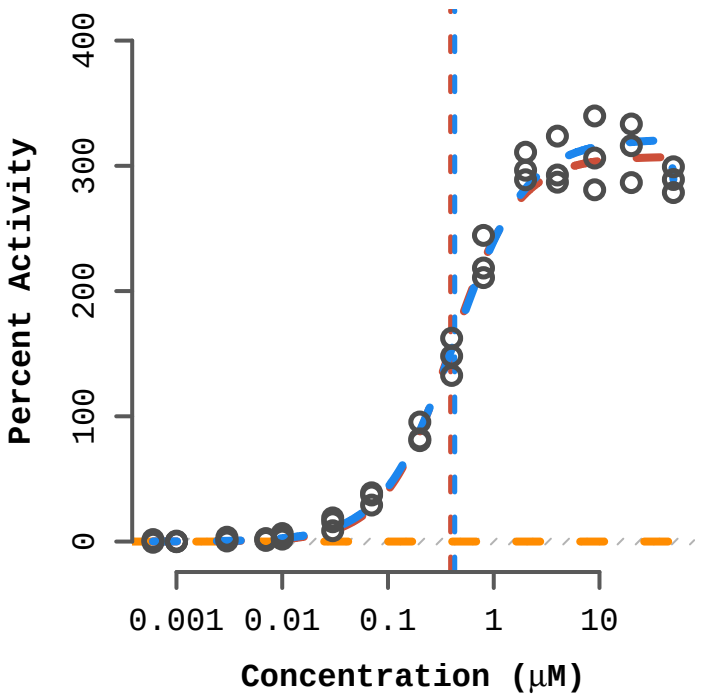
	tp	ga	gw
val:	328	−0.437	1.43
sd:	5.86	0.0251	0.11

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	342	−0.393	1.29	1.96	2.24
sd:	11	0.0292	0.0729	0.112	1.13

	CNST	HILL	GNLS
AIC:	610.69	397.4	369.39
PROB:	0	0	1
RMSE:	201.34	21.17	16.33

MAX_MEAN: 329 MAX_MED: 334 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix95 ER AR1 18-EQP
CHID: 49550 CASRN: NOCAS_49550
SPID(S): Tox21_203109
M4ID: 12479143

HILL MODEL (in red):

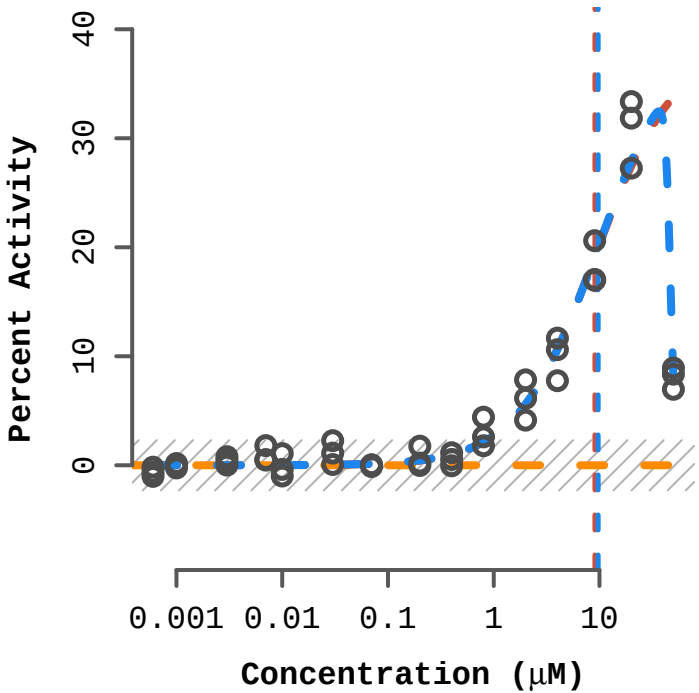
	tp	ga	gw
val:	307	-0.407	1.37
sd:	5.68	0.0246	0.0962

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	321	-0.369	1.28	1.75	18
sd:	6.91	0.0259	0.078	0.00638	2.73

	CNST	HILL	GNLS
AIC:	604.99	369.45	361.66
PROB:	0	0.02	0.98
RMSE:	189.61	13.82	12.37

MAX_MEAN: 312 MAX_MED: 316 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix21 AR2 2-EQP
CHID: 49551 CASRN: NOCAS_49551
SPID(S): Tox21_203110
M4ID: 12479142

HILL MODEL (in red):

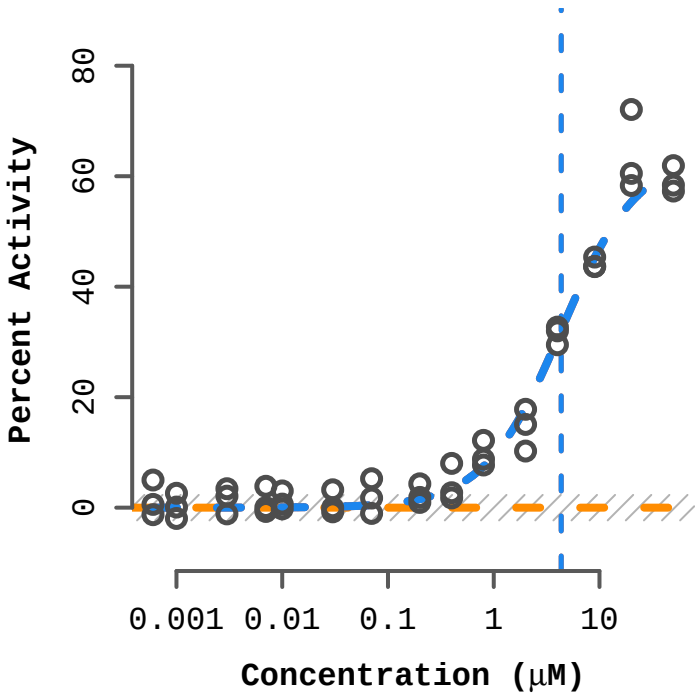
	tp	ga	gw
val:	38.4	0.957	1.17
sd:	6.77	0.149	0.167

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	40	0.987	1.15	1.67	17.7
sd:	5.32	0.116	0.12	0.00369	2.2

	CNST	HILL	GNLS
AIC:	317.31	234.37	166.99
PROB:	0	0	1
RMSE:	10.05	6.81	1.49

MAX_MEAN: 30.8 MAX_MED: 31.8 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix22 AR2 2-EQP
CHID: 49552 CASRN: NOCAS_49552
SPID(S): Tox21_203111
M4ID: 12479141

HILL MODEL (in red):

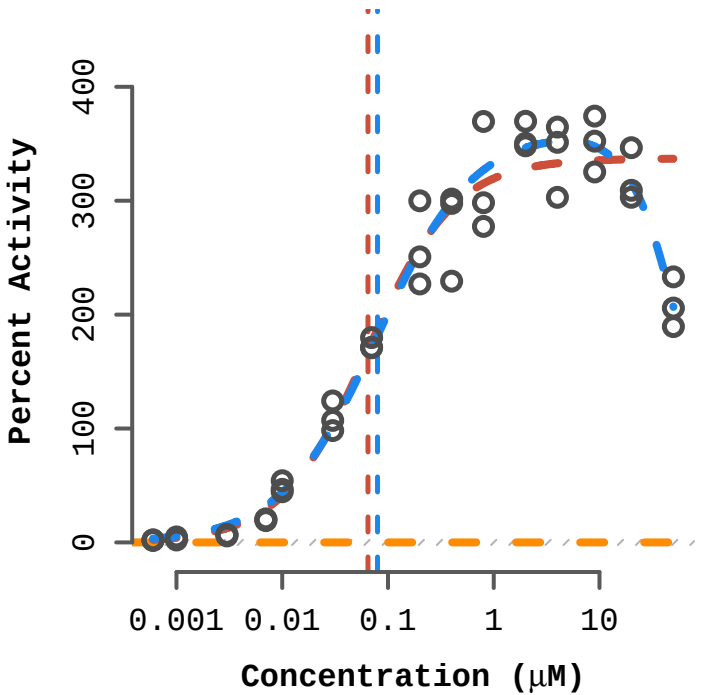
	tp	ga	gw
val:	64.2	0.638	1.2
sd:	2.39	0.0391	0.0987

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	64.2	0.638	1.2	2.81	9.86
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	417.4	237.17	241.17
PROB:	0	0.88	0.12
RMSE:	26.99	3.64	3.64

MAX_MEAN: 63.6 MAX_MED: 60.5 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix23 AR2 2-EQP
CHID: 49553 CASRN: NOCAS_49553
SPID(S): Tox21_203112
M4ID: 12479140

HILL MODEL (in red):

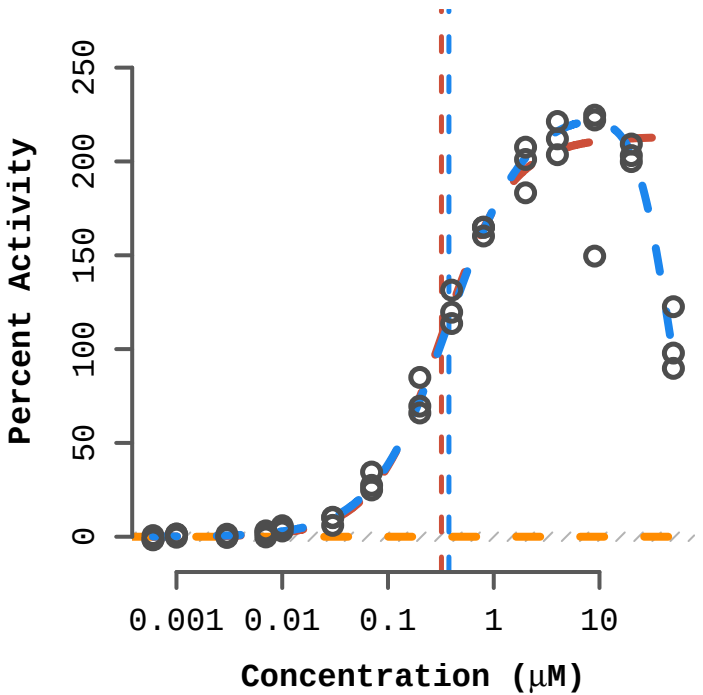
	tp	ga	gw
val:	337	-1.19	1.06
sd:	9.4	0.0504	0.0949

GAIN-LOSS MODEL (in blue):

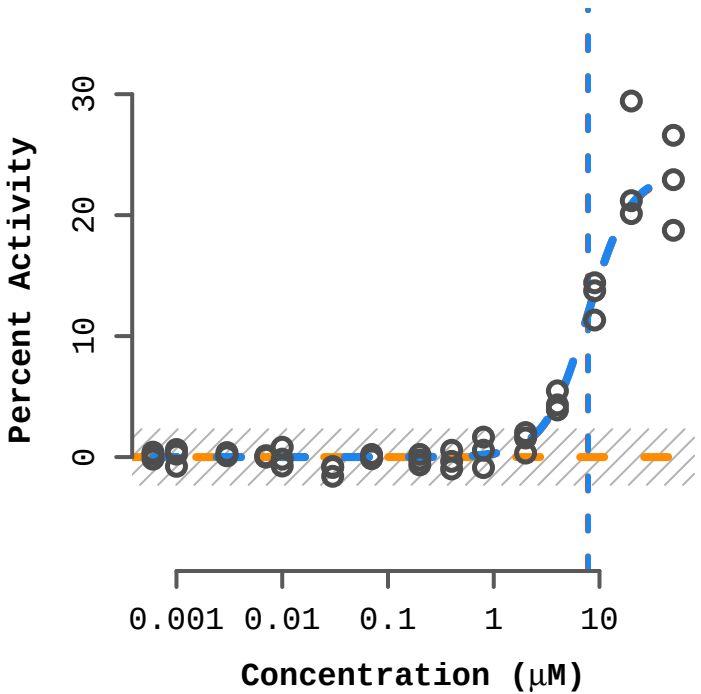
	tp	ga	gw	la	lw
val:	363	-1.1	0.957	1.77	1.82
sd:	10.1	0.0467	0.0666	0.0353	0.377

	CNST	HILL	GNLS
AIC:	625.95	447.99	408.97
PROB:	0	0	1
RMSE:	231.63	39.76	21.44

MAX_MEAN: 356 MAX_MED: 352 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix24 AR2 2-EQP
CHID:    49554   CASRN: NOCAS_49554
SPID(S): Tox21_203113
M4ID:    12479139

HILL MODEL (in red):
      tp       ga       gw
val:  213      -0.494   1.32
sd:   4.22     0.026    0.0792

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  229      -0.424   1.2      1.65     2.74
sd:   3.72     0.0199   0.0465   0.012    0.225

      CNST        HILL        GNLS
AIC:  565.54      381.81      312.39
PROB: 0           0           1
RMSE: 122.61      30.54       12.51

MAX_MEAN: 212       MAX_MED: 222       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix25 AR2 2-EQP
CHID: 49555 CASRN: NOCAS_49555
SPID(S): Tox21_203114
M4ID: 12479138

HILL MODEL (in red):

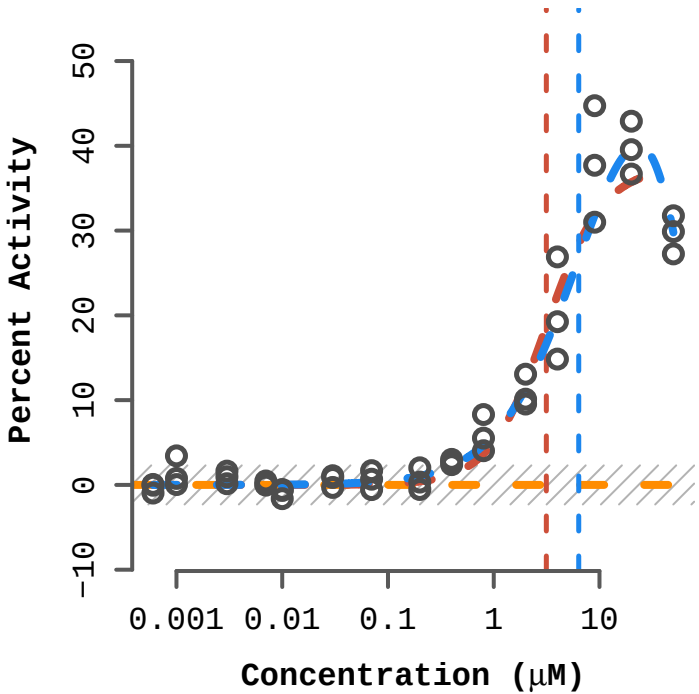
	tp	ga	gw
val:	23.5	0.887	2.16
sd:	0.724	0.0234	0.18

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	24	0.896	2.12	3.7	0.792
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	306.76	144.27	148.24
PROB:	0	0.88	0.12
RMSE:	9.33	1.68	1.67

MAX_MEAN: 23.6 MAX_MED: 22.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix26 AR2 2-EQP
CHID: 49556 **CASRN:** NOCAS_49556
SPID(S): Tox21_203115
M4ID: 12479137

HILL MODEL (in red):

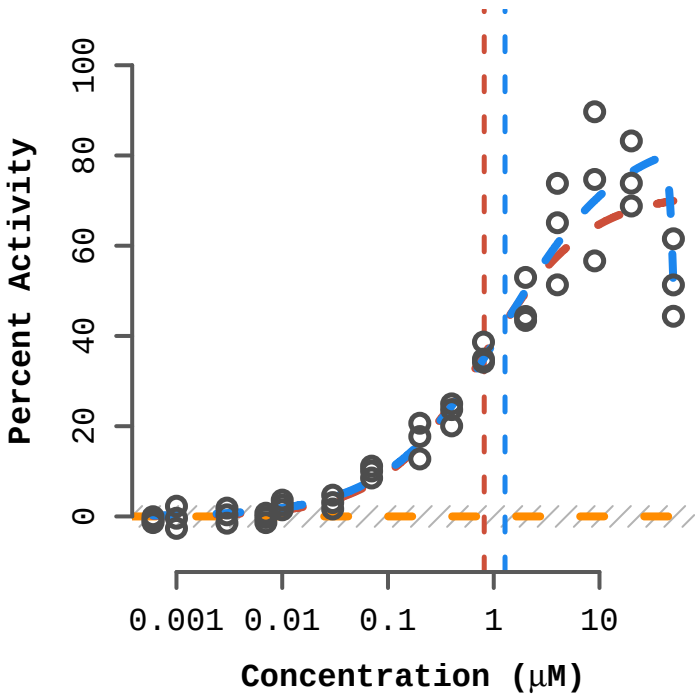
	tp	ga	gw
val:	37.5	0.497	1.63
sd:	3.07	0.0682	0.284

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	53.7	0.804	1.13	1.77	2.58
sd:	10.8	0.156	0.134	0.0414	1.6

	CNST	HILL	GNLS
AIC:	378.04	241.46	210.33
PROB:	0	0	1
RMSE:	17.4	3.67	2.83

MAX_MEAN: 39.7 **MAX_MED:** 39.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix27 AR2 2-EQP
CHID: 49557 CASRN: NOCAS_49557
SPID(S): Tox21_203116
M4ID: 12479136

HILL MODEL (in red):

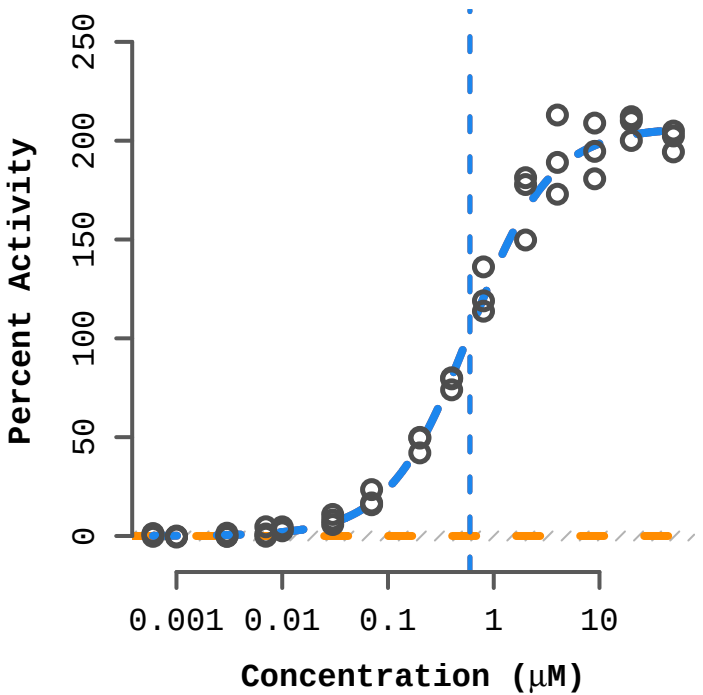
	tp	ga	gw
val:	71.8	−0.0898	0.887
sd:	5.34	0.0932	0.102

GAIN-LOSS MODEL (in blue):

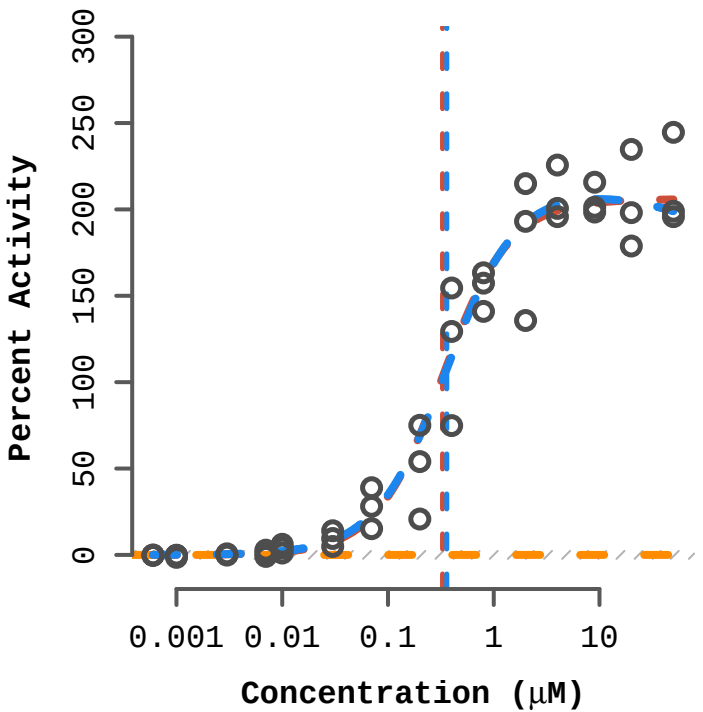
	tp	ga	gw	la	lw
val:	85.2	0.107	0.783	1.71	17.8
sd:	6.57	0.108	0.0783	0.00568	8

	CNST	HILL	GNLS
AIC:	459.59	304.5	283.4
PROB:	0	0	1
RMSE:	38.89	7.79	5.48

MAX_MEAN: 75.3 MAX_MED: 74.7 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix32 AR2 7-EQP
CHID:    49558   CASRN: NOCAS_49558
SPID(S): Tox21_203117
M4ID:    12479135

HILL MODEL (in red):
      tp       ga       gw
val:  207      -0.225   1.13
sd:   2.72     0.0245   0.0668

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  207      -0.225   1.13     2.92     12.5
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  561.9       311.89      315.89
PROB: 0           0.88        0.12
RMSE: 118.7       7.84        7.84

MAX_MEAN: 207       MAX_MED: 210       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix28 AR2 3-EQP
CHID: 49559 CASRN: NOCAS_49559
SPID(S): Tox21_203118
M4ID: 12479134

HILL MODEL (in red):

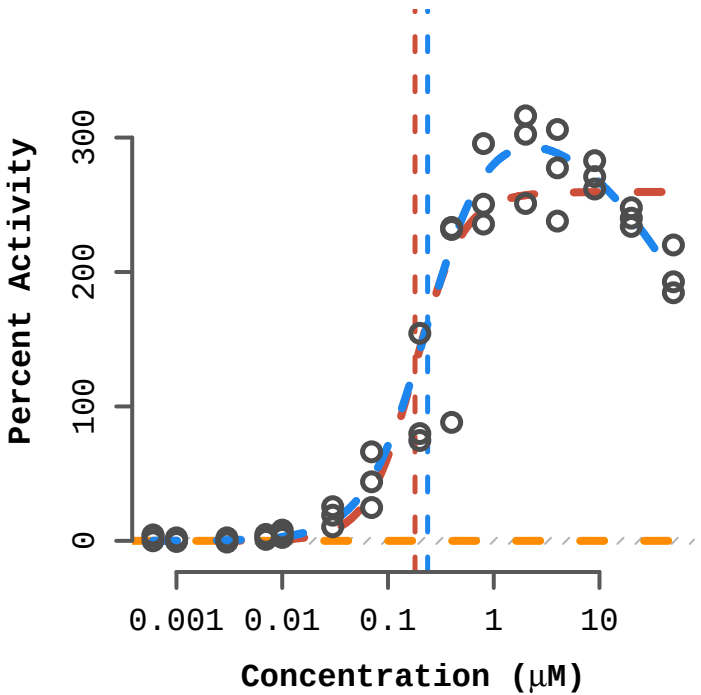
	tp	ga	gw
val:	206	−0.484	1.37
sd:	4.63	0.0471	0.142

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	217	−0.444	1.28	3.7	0.532
sd:	32.6	0.0995	0.171	3.02	1.2

	CNST	HILL	GNLS
AIC:	570.46	384.73	387.72
PROB:	0	0.82	0.18
RMSE:	129.22	17.95	18.16

MAX_MEAN: 213 MAX_MED: 201 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix29 AR2 5-EQP-HF
CHID: 49560 CASRN: NOCAS_49560
SPID(S): Tox21_203119
M4ID: 12479133

HILL MODEL (in red):

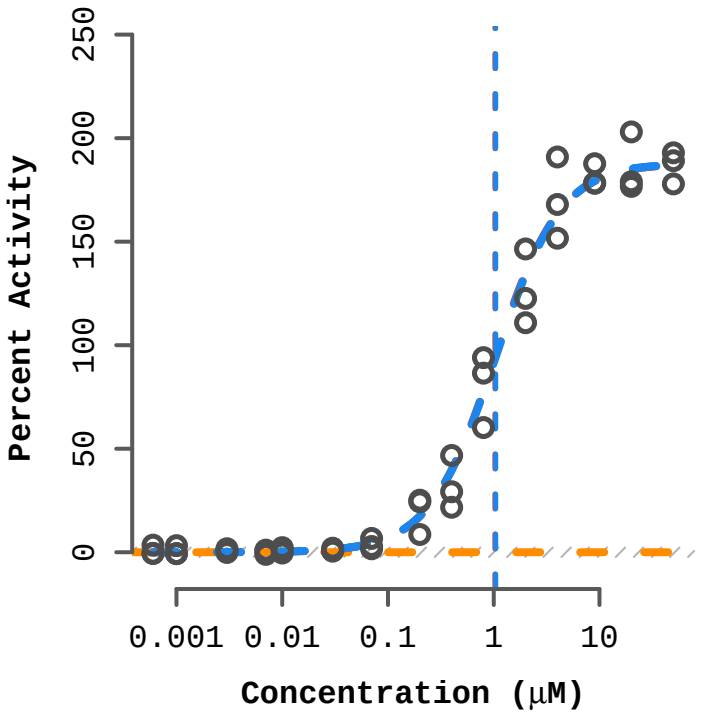
	tp	ga	gw
val:	260	−0.744	1.93
sd:	7.52	0.0639	0.324

GAIN-LOSS MODEL (in blue):

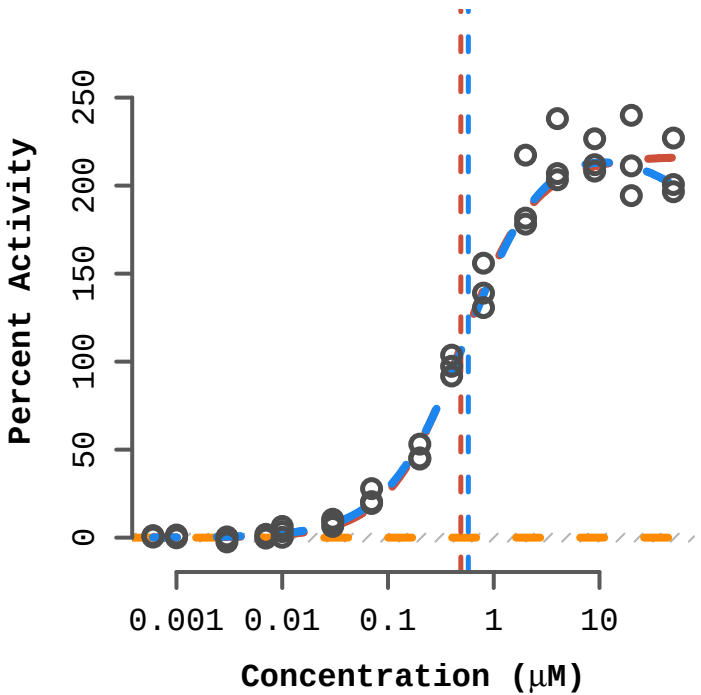
	tp	ga	gw	la	lw
val:	329	−0.625	1.48	1.96	0.672
sd:	48.2	0.0905	0.204	0.139	0.323

	CNST	HILL	GNLS
AIC:	597.96	441.99	414.64
PROB:	0	0	1
RMSE:	174.02	33.86	28.17

MAX_MEAN: 290 MAX_MED: 303 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    NTP Mix31 AR2 7-EQC
CHID:    49561   CASRN: NOCAS_49561
SPID(S): Tox21_203120
M4ID:    12479132

HILL MODEL (in red):
      tp       ga       gw
val:  188      0.0107   1.4
sd:   3.99     0.0707   0.146

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  189      0.0188   1.38     3.7      1.13
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  545.74      330.25      334.25
PROB: 0           0.88        0.12
RMSE: 102.12      9.15        9.12

MAX_MEAN: 187       MAX_MED: 189       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: NTP Mix30 AR2 7-EQP
CHID: 49562 CASRN: NOCAS_49562
SPID(S): Tox21_203121
M4ID: 12479131

HILL MODEL (in red):

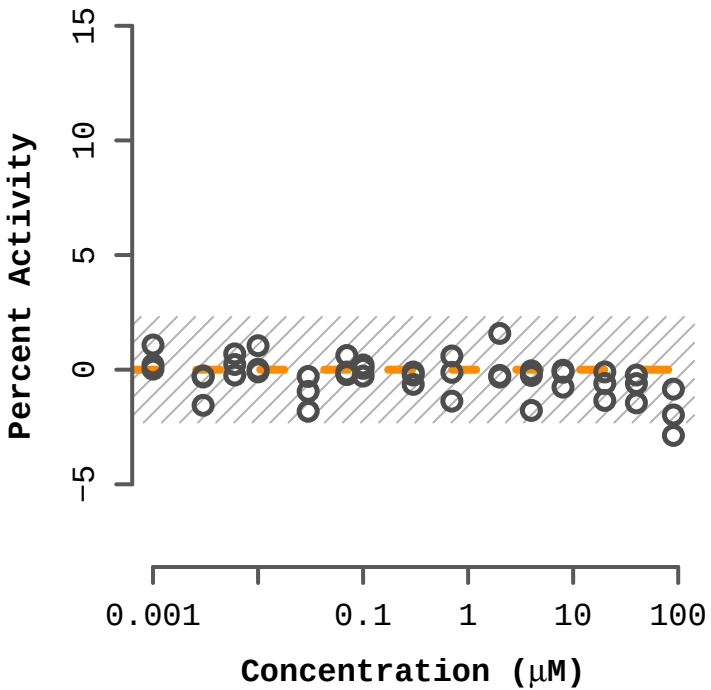
	tp	ga	gw
val:	217	-0.311	1.25
sd:	4.12	0.0265	0.0826

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	237	-0.24	1.14	3.03	0.572
sd:	32.9	0.0736	0.076	1.13	0.751

	CNST	HILL	GNLS
AIC:	570.48	336.89	333.29
PROB:	0	0.14	0.86
RMSE:	130.04	10.8	10.59

MAX_MEAN: 216 MAX_MED: 212 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

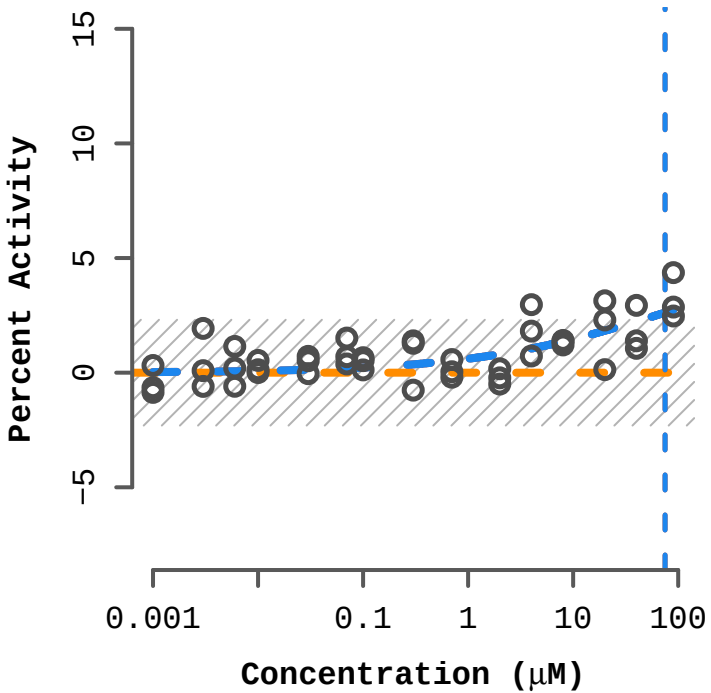
NAME: o-Terphenyl
CHID: 49697 CASRN: 84-15-1
SPID(S): Tox21_303755
M4ID: 12475433

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.99	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.438 MAX_MED: 0.227 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Ethyltoluene
CHID: 50386 CASRN: 620-14-4
SPID(S): Tox21_202857
M4ID: 12479395

HILL MODEL (in red):

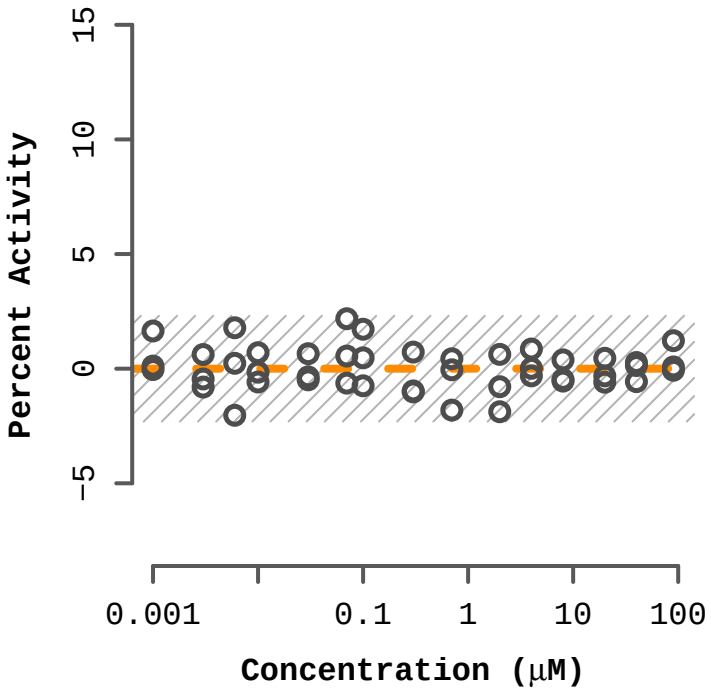
	tp	ga	gw
val:	5.24	1.87	0.471
sd:	3.37	1.16	0.202

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.24	1.87	0.471	2.74	10.5
sd:	3.37	1.16	0.202	814	11000

	CNST	HILL	GNLS
AIC:	160.78	122.33	126.33
PROB:	0	0.88	0.12
RMSE:	1.45	0.84	0.84

MAX_MEAN: 3.23 MAX_MED: 2.86 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

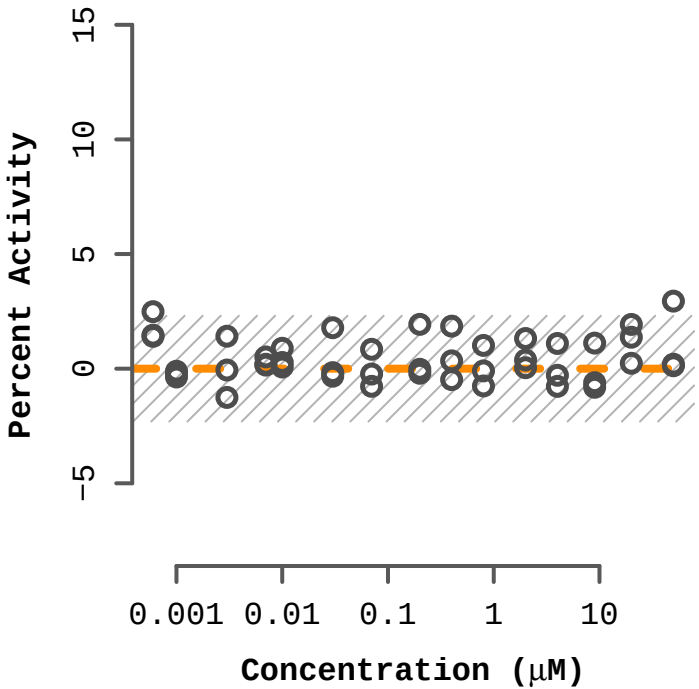
NAME: 1-Ethyl-2-methylbenzene
CHID: 50403 CASRN: 611-14-3
SPID(S): Tox21_303797
M4ID: 12475391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.84	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.701 MAX_MED: 0.551 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

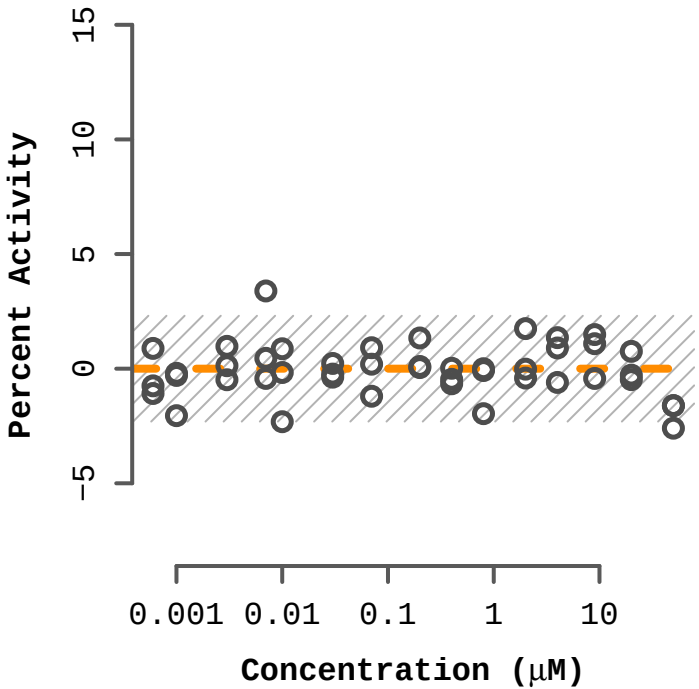
NAME: 1,5-Dicaffeoylquinic acid
CHID: 50423 **CASRN:** 30964-13-7
SPID(S): Tox21_111176_1
M4ID: 12483861

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

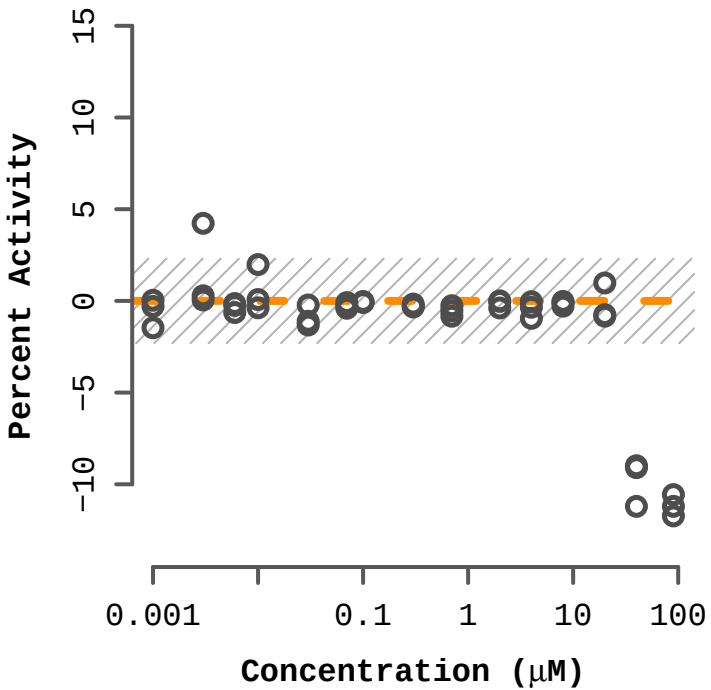
NAME: Tenofovir disoproxil fumarate
CHID: 50426 CASRN: 202138-50-9
SPID(S): Tox21_113627_1
M4ID: 12482572

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.13	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

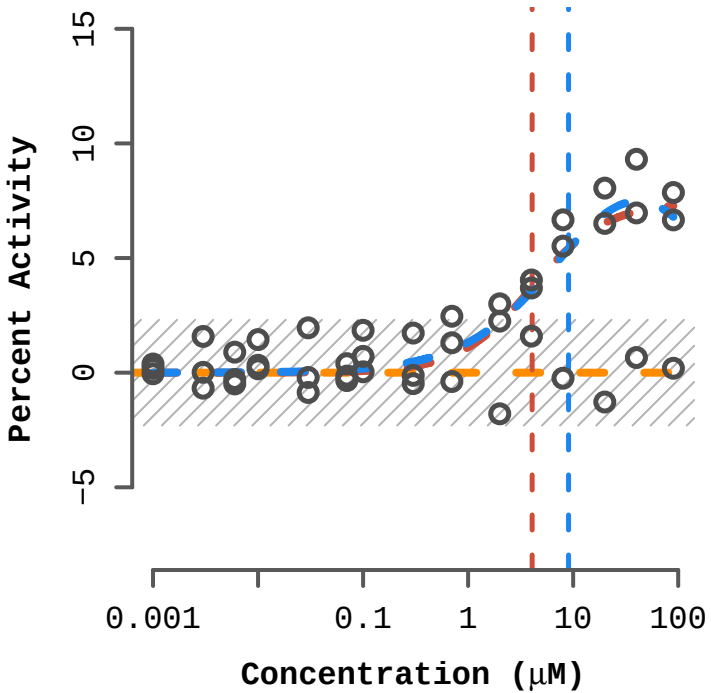
NAME: 1,1-Bis(3-cyclohexyl-4-hydroxyphenyl)cyclohexa
CHID: 51306 CASRN: 4221-68-5
SPID(S): Tox21_303717
M4ID: 12475471

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.18	NA	NA
PROB:	1	NA	NA
RMSE:	3.98	NA	NA

MAX_MEAN: 1.52 MAX_MED: 0.28 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bis(p-methylbenzylidene)sorbitol
CHID: 51381 **CASRN:** 54686-97-4
SPID(S): Tox21_303848
M4ID: 12475340

HILL MODEL (in red):

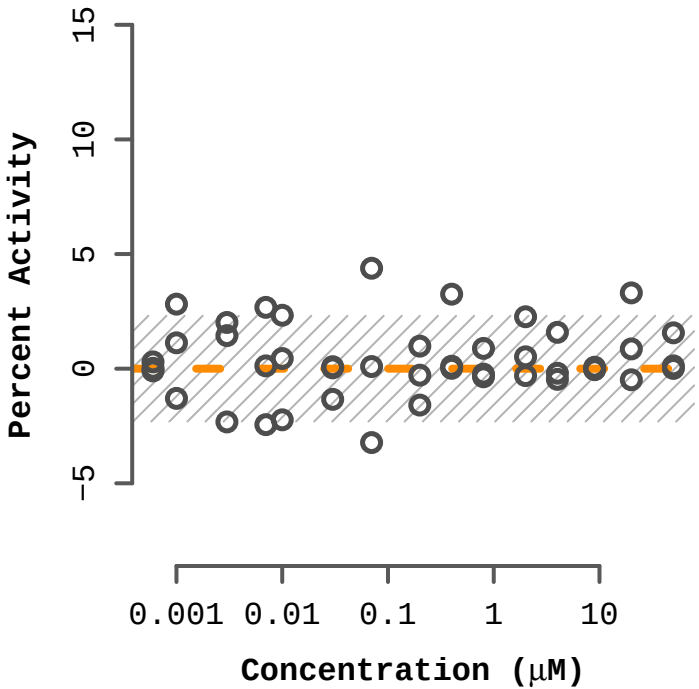
	tp	ga	gw
val:	7.43	0.609	1.24
sd:	0.828	0.133	0.504

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.2	0.956	0.912	2.25	1.12
sd:	11.8	0.83	0.455	0.666	2.34

	CNST	HILL	GNLS
AIC:	229.99	189.45	192.38
PROB:	0	0.81	0.19
RMSE:	3.34	2.28	2.3

MAX_MEAN: 5.65 **MAX_MED:** 6.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

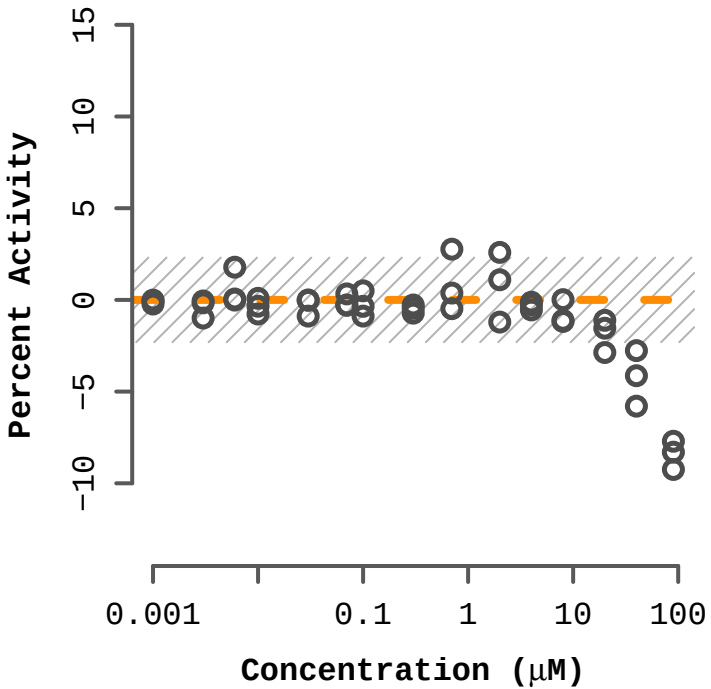
NAME: 1-(2-Methoxyphenyl)piperazine hydrochloride
CHID: 51440 **CASRN:** 5464-78-8
SPID(S): Tox21_111273_1
M4ID: 12483802

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.06	NA	NA
PROB:	1	NA	NA
RMSE:	1.6	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

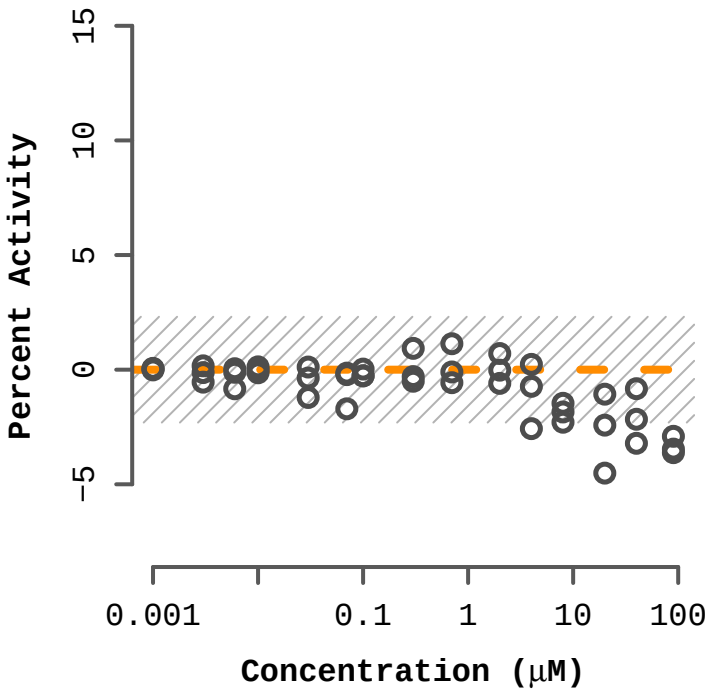
NAME: 4,4'−(1−Phenylethylidene)bisphenol
CHID: 51444 **CASRN:** 1571−75−1
SPID(S): Tox21_303999
M4ID: 12475189

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	192.26	NA	NA
PROB:	1	NA	NA
RMSE:	2.63	NA	NA

MAX_MEAN: 0.889 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

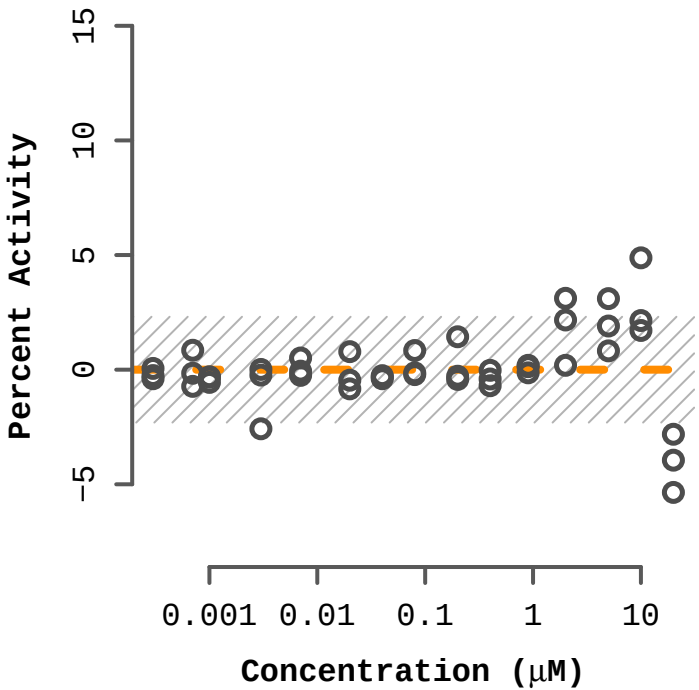
NAME: 6-Aminonicotinamide
CHID: 51446 CASRN: 329-89-5
SPID(S): Tox21_303956
M4ID: 12475232

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	161.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.156 MAX_MED: 0.0383 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

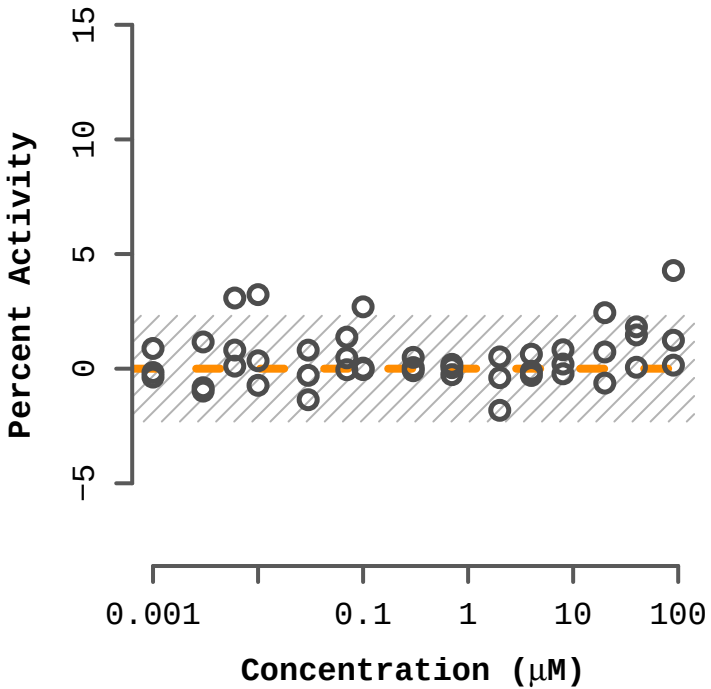
NAME: Tyrphostin
CHID: 51447 **CASRN:** 175178-82-2
SPID(S): Tox21_303781
M4ID: 12475407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	164.74	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: 2.91 **MAX_MED:** 2.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

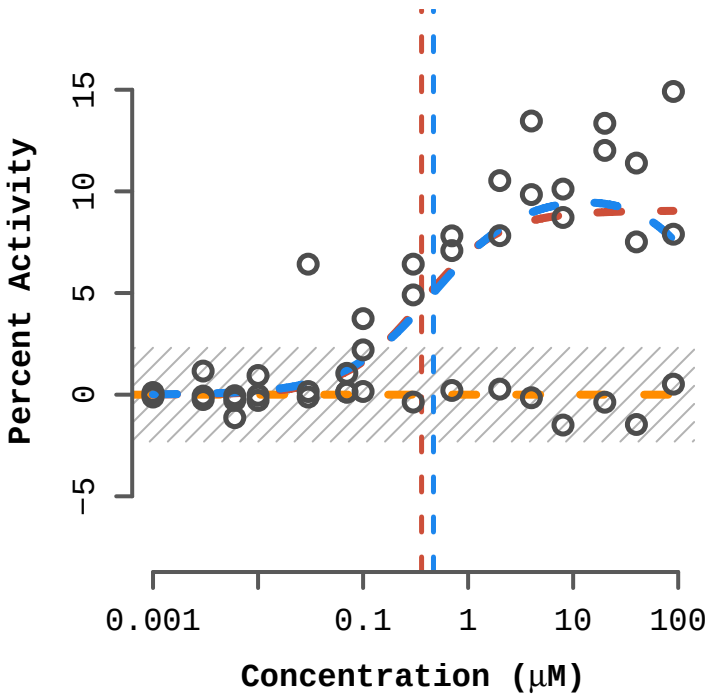
NAME: 3-Methylstyrene
CHID: 51454 **CASRN:** 100-80-1
SPID(S): Tox21_303890
M4ID: 12475298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.47 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tributyl phosphite
CHID: 51474 CASRN: 102-85-2
SPID(S): Tox21_303877
M4ID: 12475311

HILL MODEL (in red):

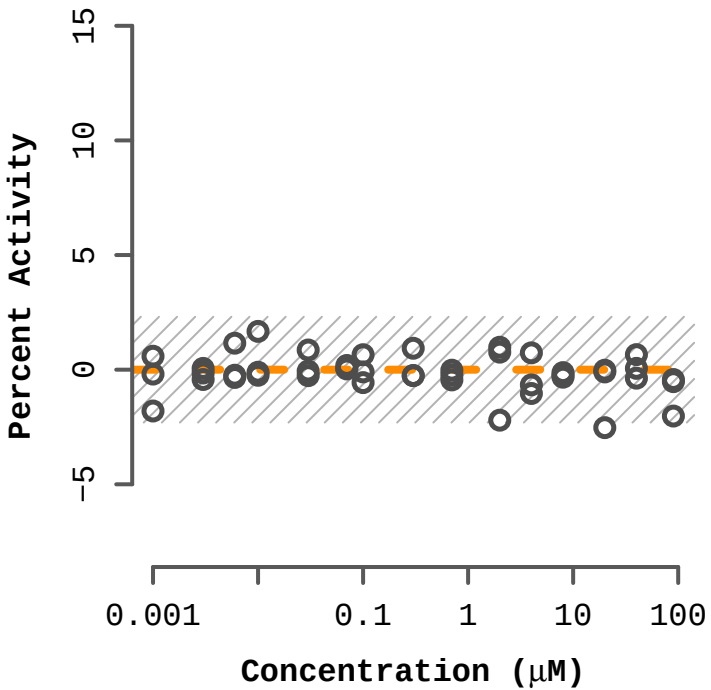
	tp	ga	gw
val:	9.05	−0.443	1.18
sd:	1.25	0.24	0.532

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10	−0.33	1.03	2.35	1.3
sd:	2.93	0.407	0.555	1.05	3.1

	CNST	HILL	GNLS
AIC:	290.12	254.47	258.04
PROB:	0	0.86	0.14
RMSE:	6.09	4.03	4.06

MAX_MEAN: 8.33 MAX_MED: 12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

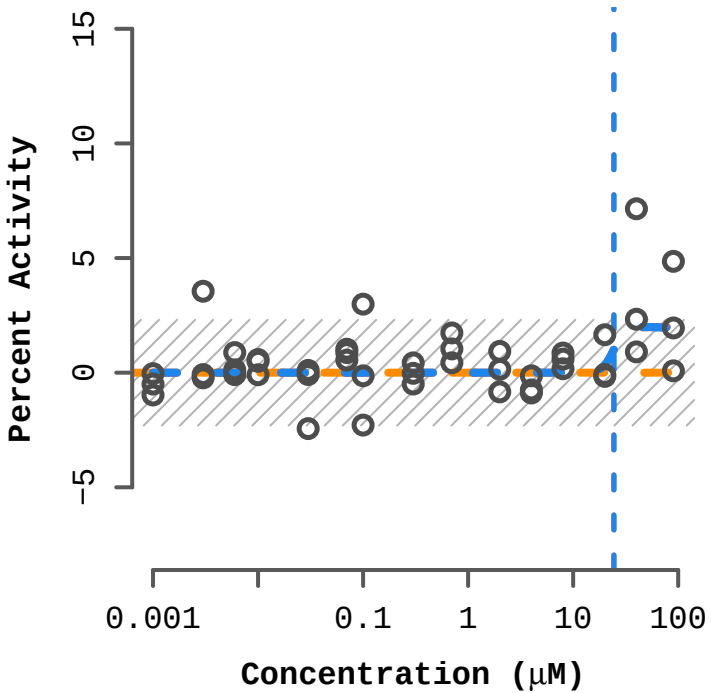
NAME: 4-Methylbenzyl chloride
CHID: 51477 **CASRN:** 104-82-5
SPID(S): Tox21_303978
M4ID: 12475210

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	106.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.439 **MAX_MED:** 0.766 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Diaminopyridine
CHID: 51493 **CASRN:** 452-58-4
SPID(S): Tox21_303818
M4ID: 12475370

HILL MODEL (in red):

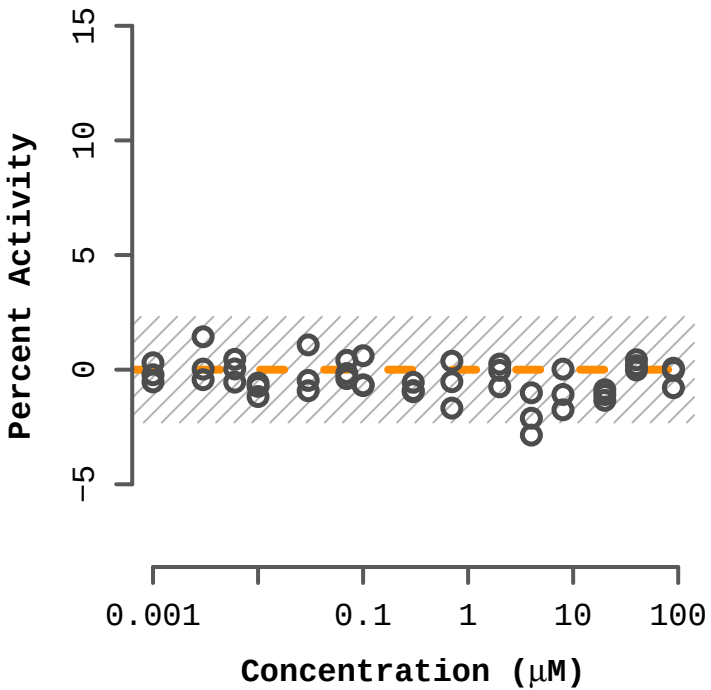
	tp	ga	gw
val:	1.99	1.39	8
sd:	0.615	0.199	17.1

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.42	1.39	8	3.95	0.301
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	160.91	155.07	159.04
PROB:	0.05	0.84	0.12
RMSE:	1.72	1.4	1.4

MAX_MEAN: 3.46 **MAX_MED:** 2.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

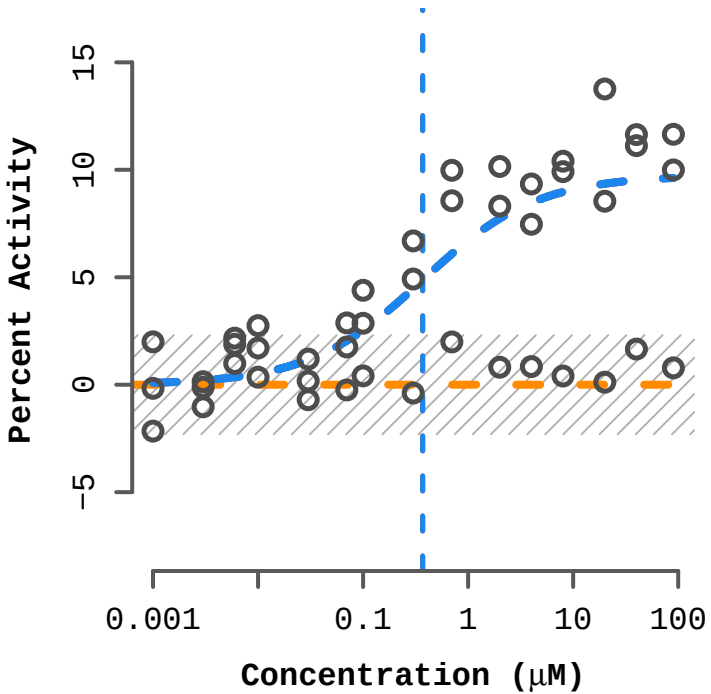
NAME: 2,3-Dihydro-4-methyl-1-phenyl-1H-phosphole 1-ox
CHID: 51497 CASRN: 707-61-9
SPID(S): Tox21_303982
M4ID: 12475206

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.17	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.343 MAX_MED: 0.177 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Vinylpyridine
CHID: 51499 **CASRN:** 100-43-6
SPID(S): Tox21_303844
M4ID: 12475344

HILL MODEL (in red):

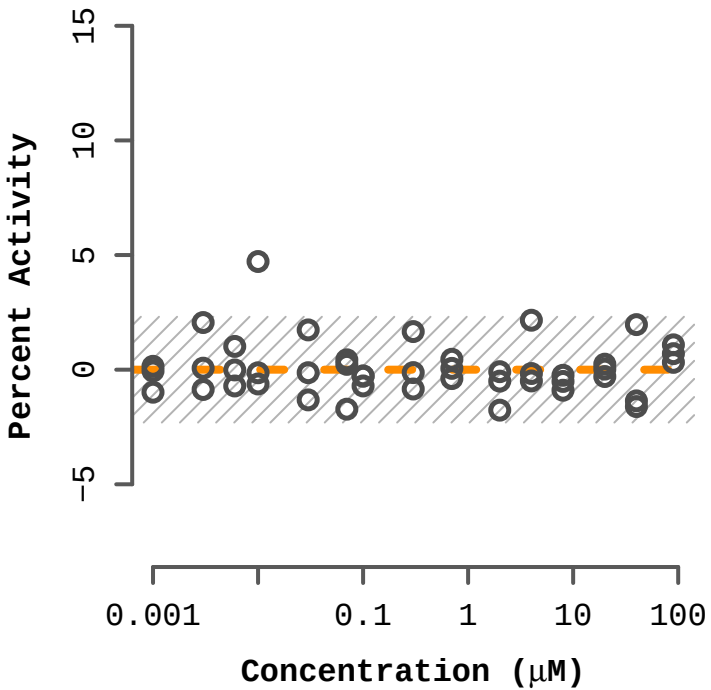
	tp	ga	gw
val:	9.74	−0.433	0.797
sd:	1.55	0.37	0.404

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.74	−0.433	0.797	3.91	5.19
sd:	1.55	0.37	0.403	74700	192000

	CNST	HILL	GNLS
AIC:	290.46	242.76	246.76
PROB:	0	0.88	0.12
RMSE:	5.96	3.51	3.51

MAX_MEAN: 8.14 **MAX_MED:** 11.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

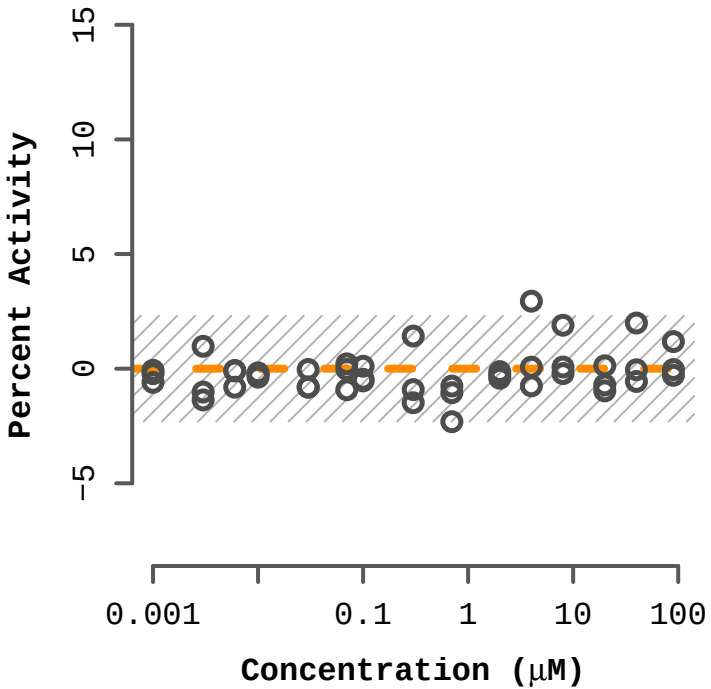
NAME: N,O-bis(Trimethylsilyl)acetamide
CHID: 51525 **CASRN:** 10416-59-8
SPID(S): Tox21_303908
M4ID: 12475280

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.45	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.32 **MAX_MED:** 0.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

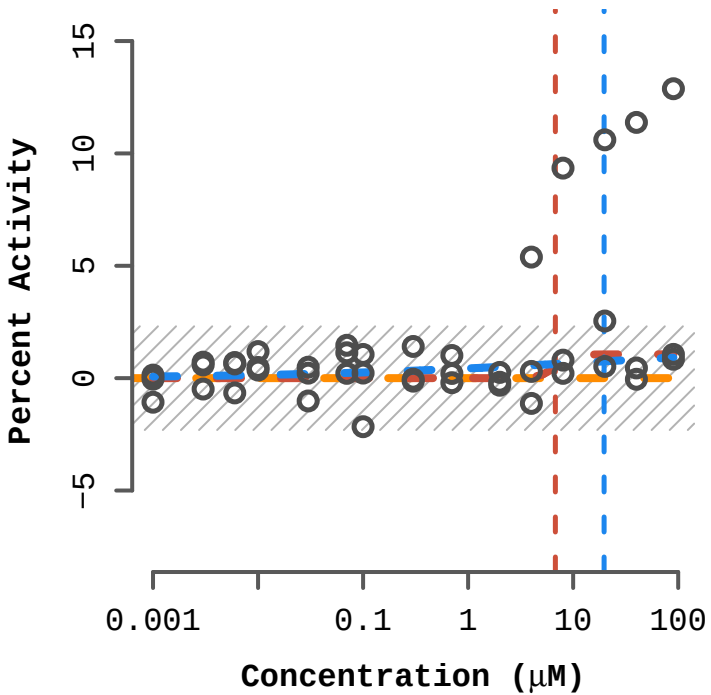
NAME: Decylbenzene
CHID: 51529 **CASRN:** 104-72-3
SPID(S): Tox21_303866
M4ID: 12475322

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.755 **MAX_MED:** 0.0738 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hex-1-yn-3-ol
CHID: 51536 **CASRN:** 105-31-7
SPID(S): Tox21_303791
M4ID: 12475397

HILL MODEL (in red):

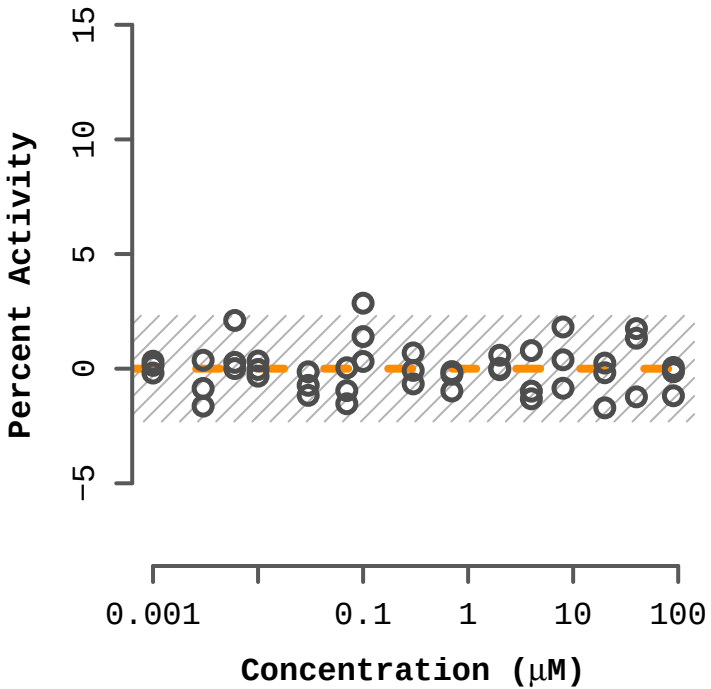
	tp	ga	gw
val:	1.06	0.831	5.88
sd:	0.466	0.407	22.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.49	1.29	0.3	3.95	8.02
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	198.94	198.07	201.82
PROB:	0.36	0.56	0.09
RMSE:	3.51	3.21	3.25

MAX_MEAN: 4.93 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

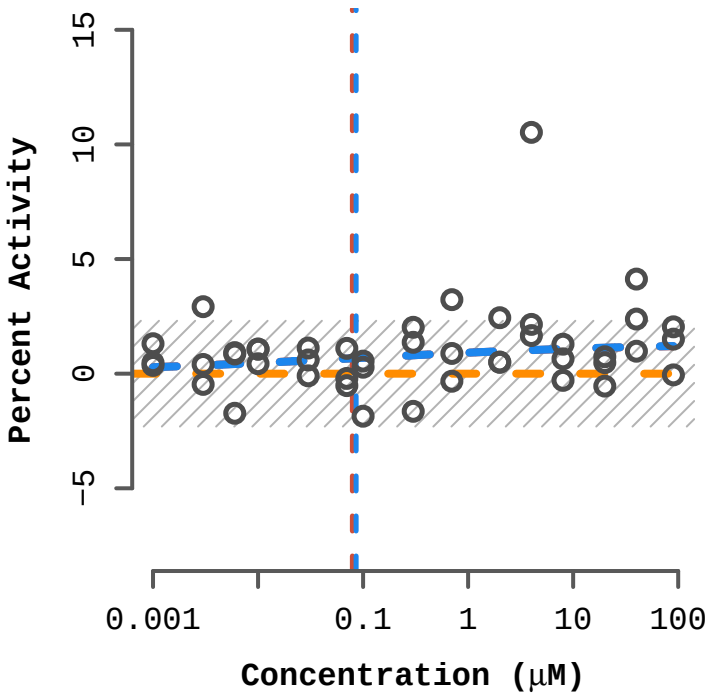
NAME: Geranyl propionate
CHID: 51540 **CASRN:** 105-90-8
SPID(S): Tox21_303994
M4ID: 12475194

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Ethyl octanoate
CHID: 51542 CASRN: 106-32-1
SPID(S): Tox21_303730
M4ID: 12475458

HILL MODEL (in red):

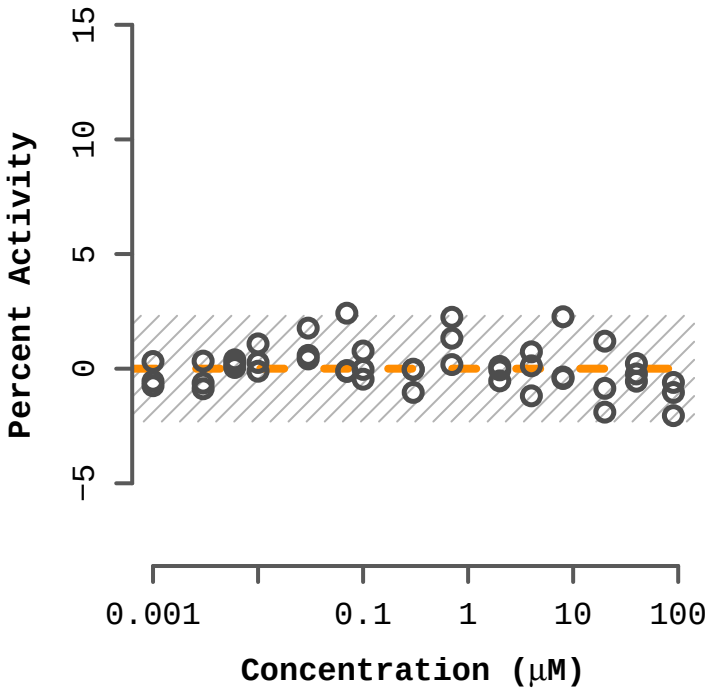
	tp	ga	gw
val:	1.34	−1.1	0.3
sd:	1.3	3.52	0.539

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	1.35	−1.07	0.3	2.93	6.59
sd:	1.52	4.03	0.617	681	4490

	CNST	HILL	GNLS
AIC:	177.53	165.24	169.24
PROB:	0	0.88	0.12
RMSE:	2.12	1.83	1.83

MAX_MEAN: 4.78 **MAX_MED:** 2.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

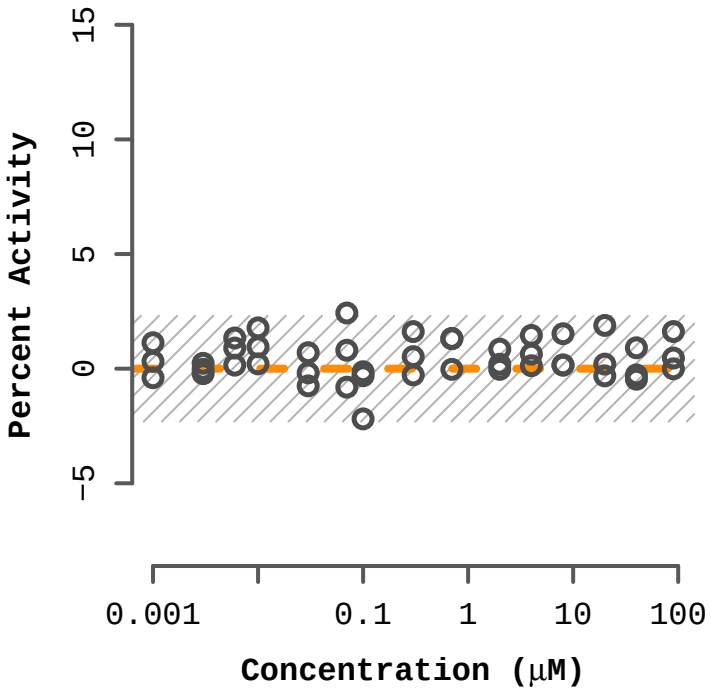
NAME: 1,4-Dimethylpiperazine
CHID: 51544 **CASRN:** 106-58-1
SPID(S): Tox21_303778
M4ID: 12475410

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

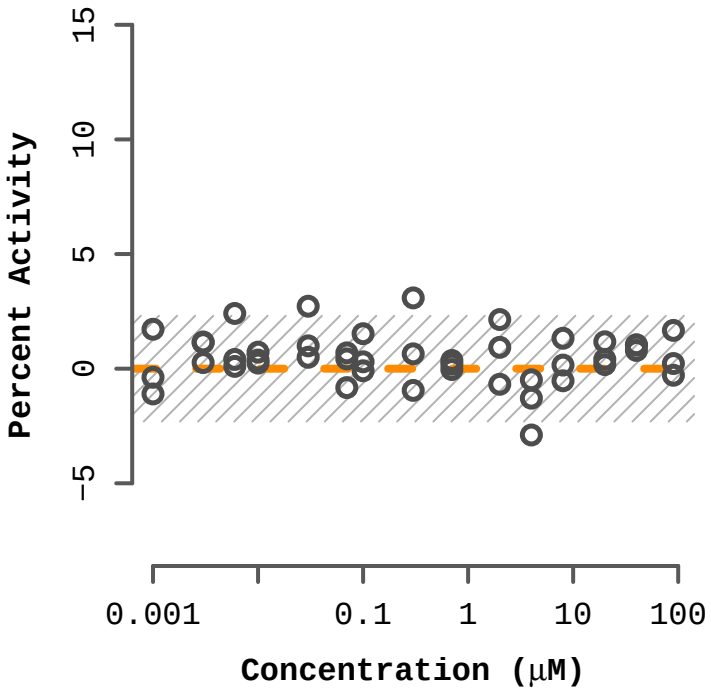
NAME: 2,6-Dimethylpyridine
CHID: 51557 **CASRN:** 108-48-5
SPID(S): Tox21_303862
M4ID: 12475326

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.982 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

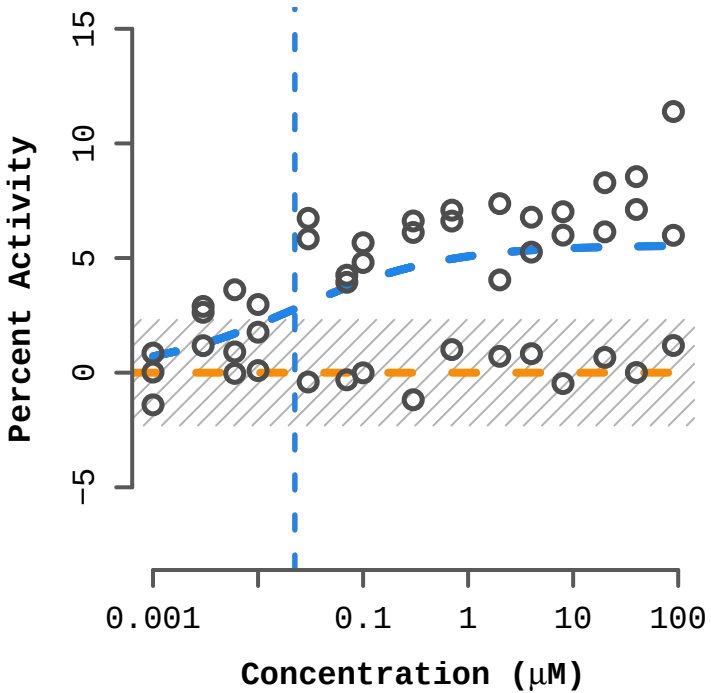
NAME: Hexahydro-1,3,5-trimethyl-1,3,5-triazine
CHID: 51560 **CASRN:** 108-74-7
SPID(S): Tox21_304038
M4ID: 12475150

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.41 **MAX_MED:** 1.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Bromopyridine
CHID: 51564 CASRN: 109-04-6
SPID(S): Tox21_303772
M4ID: 12475416

HILL MODEL (in red):

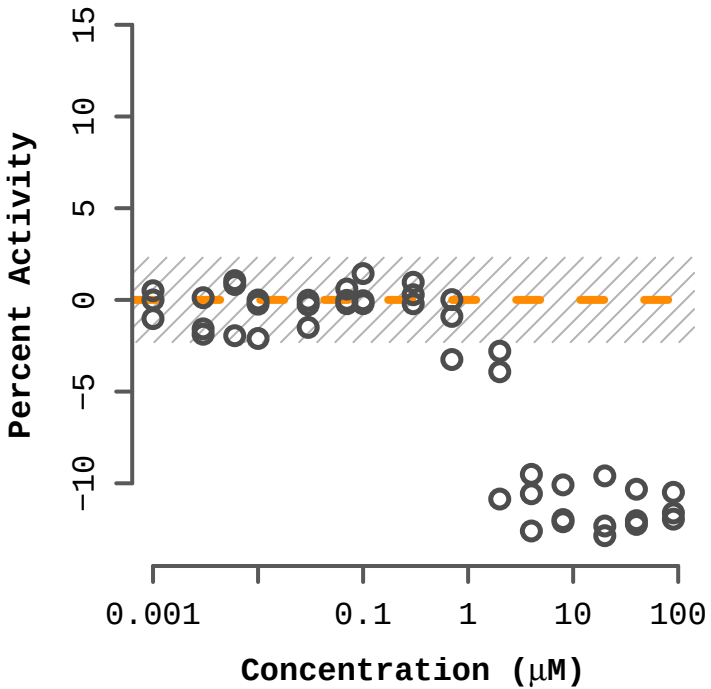
	tp	ga	gw
val:	5.56	−1.65	0.616
sd:	1.07	0.554	0.42

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.56	−1.65	0.616	3.02	7.41
sd:	1.07	0.554	0.42	2160	15000

	CNST	HILL	GNLS
AIC:	274.21	233.52	237.52
PROB:	0	0.88	0.12
RMSE:	4.76	2.86	2.86

MAX_MEAN: 6.19 MAX_MED: 7.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

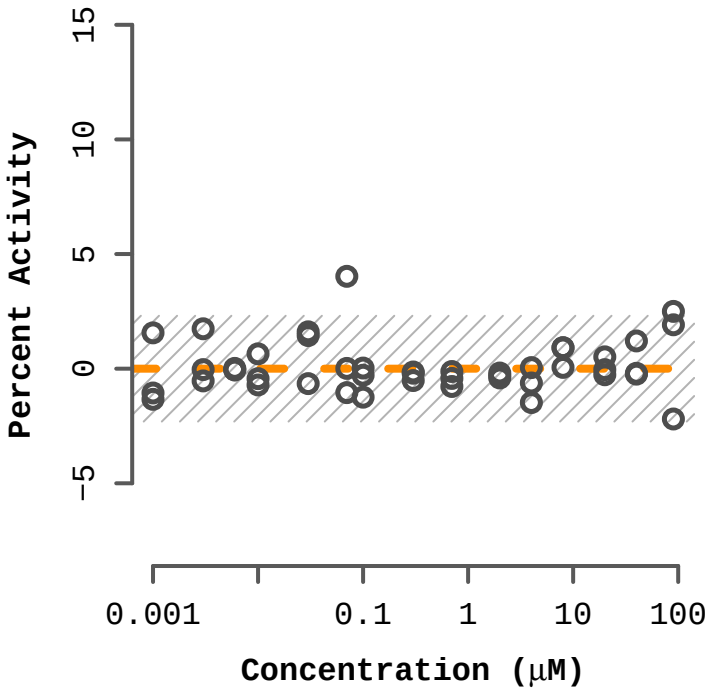
NAME: Benzyltriphenylphosphonium chloride
CHID: 51566 **CASRN:** 1100-88-5
SPID(S): Tox21_303954
M4ID: 12475234

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	303.71	NA	NA
PROB:	1	NA	NA
RMSE:	6.87	NA	NA

MAX_MEAN: 0.397 **MAX_MED:** 0.841 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

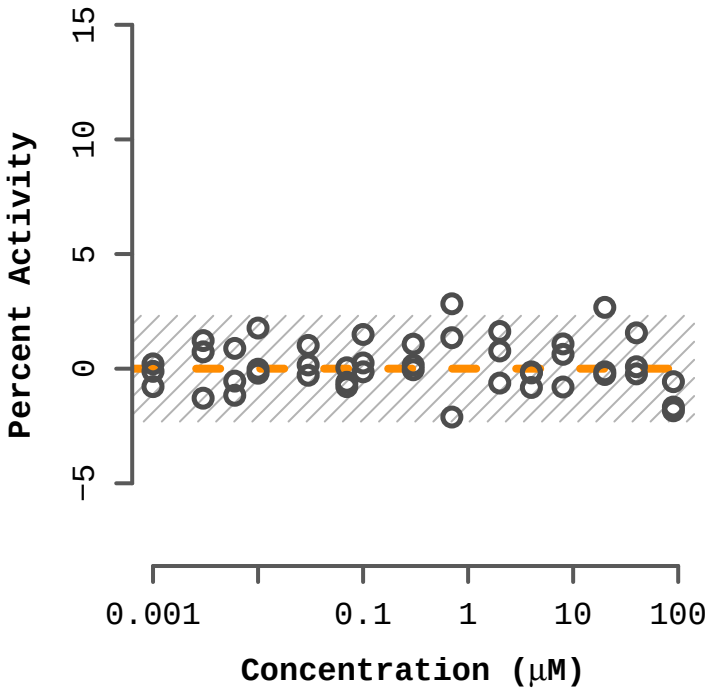
NAME: 2-Chloroethyl vinyl ether
CHID: 51570 **CASRN:** 110-75-8
SPID(S): Tox21_303853
M4ID: 12475335

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.92 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

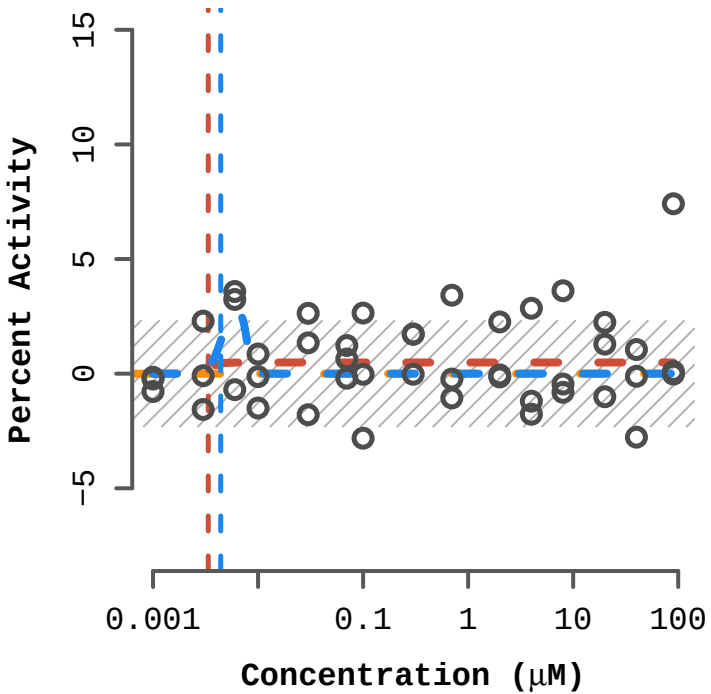
NAME: 1-Hexanethiol
CHID: 51574 **CASRN:** 111-31-9
SPID(S): Tox21_303860
M4ID: 12475328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.57	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 0.762 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butyl vinyl ether
CHID: 51575 **CASRN:** 111-34-2
SPID(S): Tox21_303721
M4ID: 12475467

HILL MODEL (in red):

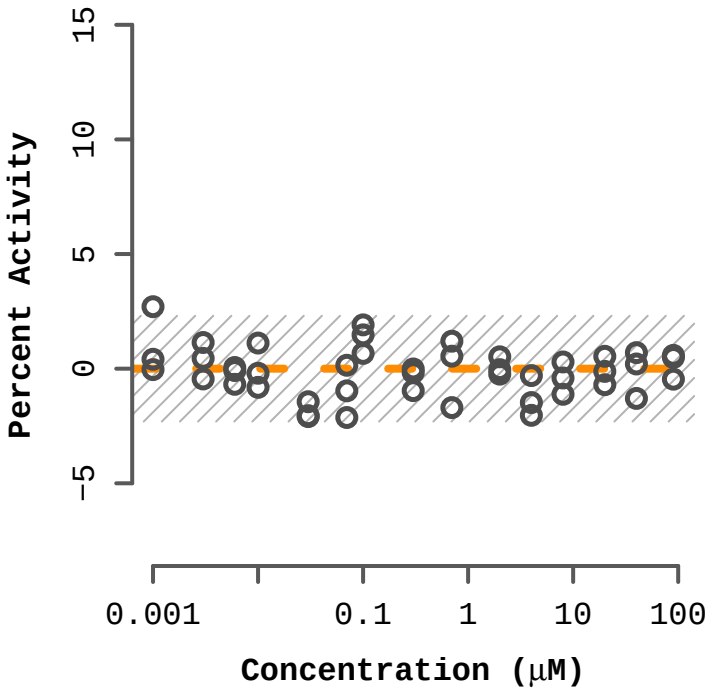
	tp	ga	gw
val:	0.488	−2.47	8
sd:	0.3	0.456	25.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.87	−2.36	8	−2.11	18
sd:	5.09	0.731	30.3	0.287	48.3

	CNST	HILL	GNLS
AIC:	190.43	193.72	196.57
PROB:	0.81	0.16	0.04
RMSE:	2.03	1.94	1.97

MAX_MEAN: 2.5 **MAX_MED:** 3.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

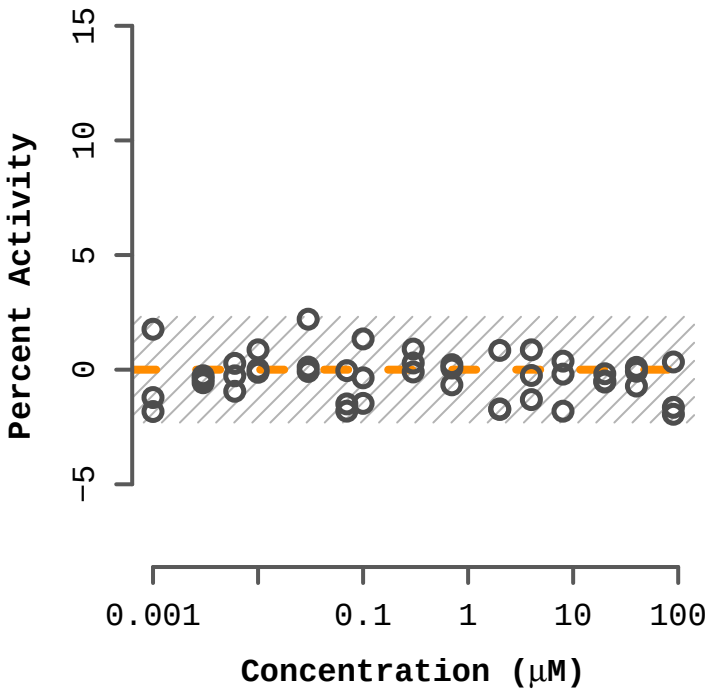
NAME: 6-Methyl-3-hydroxypyridine
CHID: 51580 **CASRN:** 1121-78-4
SPID(S): Tox21_304013
M4ID: 12475175

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.35 **MAX_MED:** 1.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

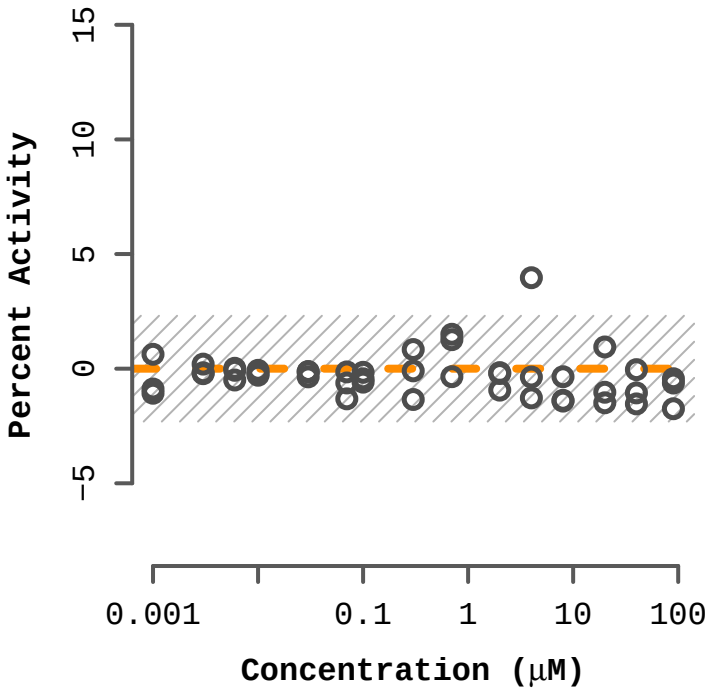
NAME: 1-Bromodecane
CHID: 51581 **CASRN:** 112-29-8
SPID(S): Tox21_303974
M4ID: 12475214

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.748 **MAX_MED:** 0.294 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

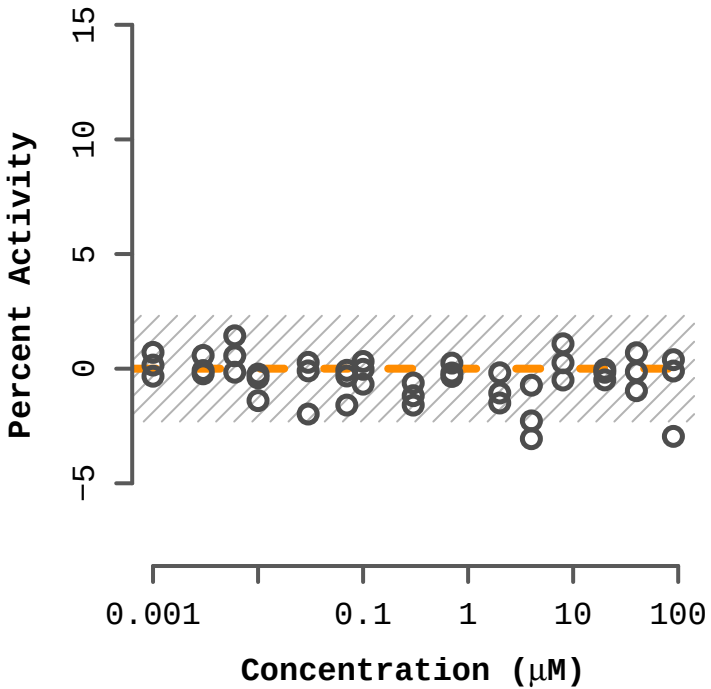
NAME: (−)Carophyllene oxide
CHID: 51586 **CASRN:** 1139-30-6
SPID(S): Tox21_303807
M4ID: 12475381

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.807 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

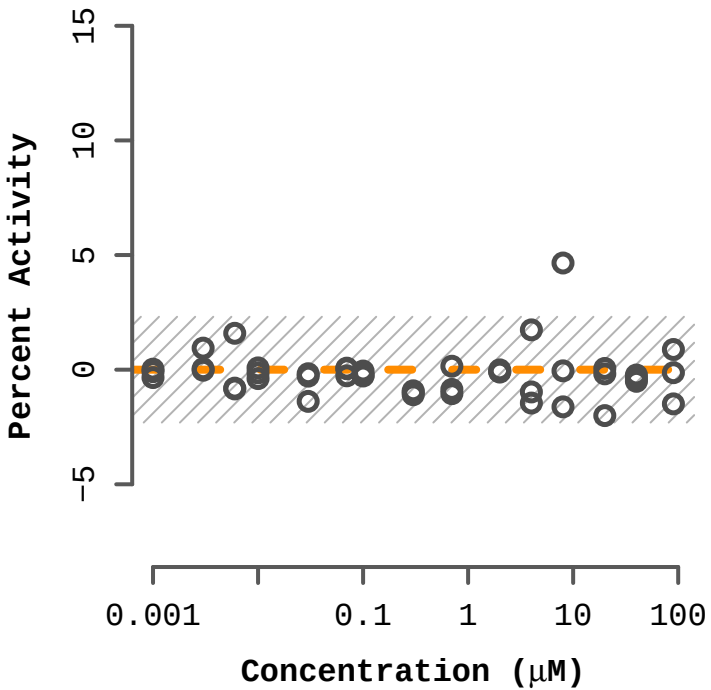
NAME: N,N,3-Trimethylaniline
CHID: 51618 **CASRN:** 121-72-2
SPID(S): Tox21_303992
M4ID: 12475196

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.615 **MAX_MED:** 0.564 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

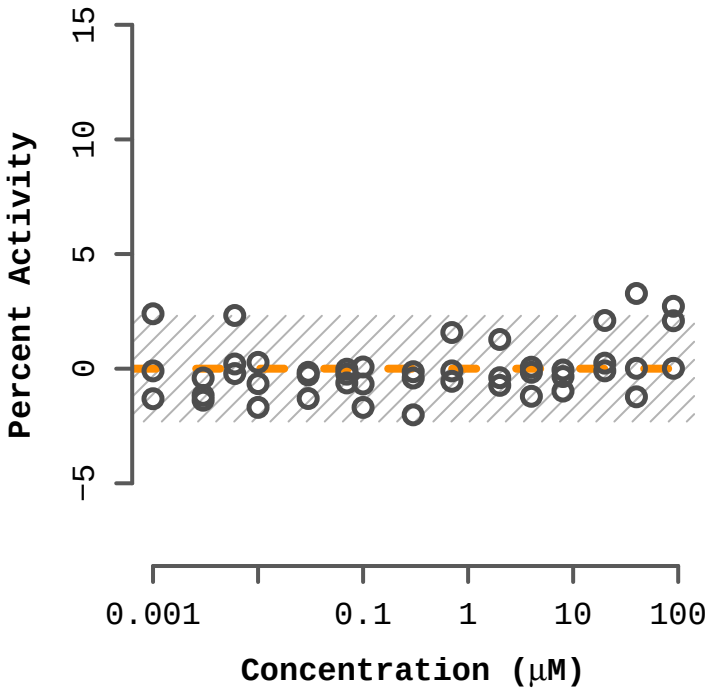
NAME: 4-Chlorobenzoyl chloride
CHID: 51619 **CASRN:** 122-01-0
SPID(S): Tox21_303719
M4ID: 12475469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.995 **MAX_MED:** 0.0431 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

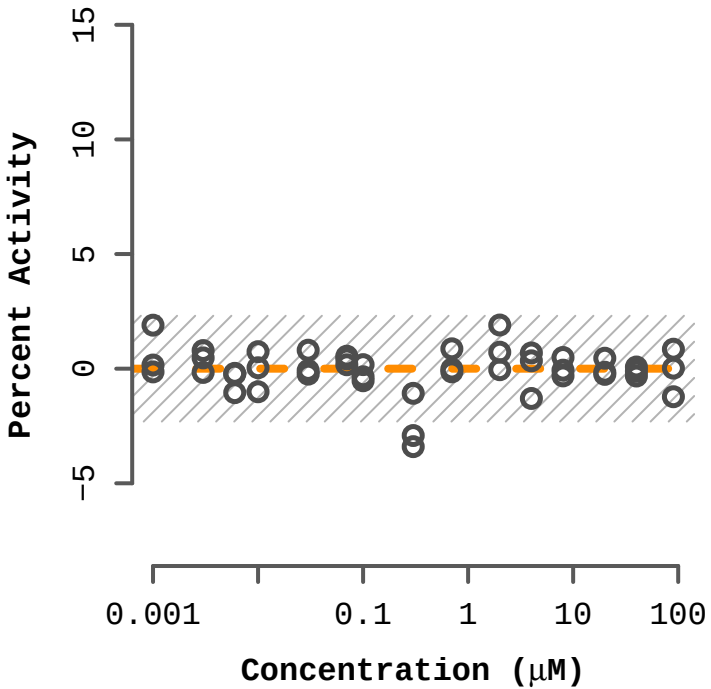
NAME: Succinimide
CHID: 51629 **CASRN:** 123-56-8
SPID(S): Tox21_303851
M4ID: 12475337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	145.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.61 **MAX_MED:** 2.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

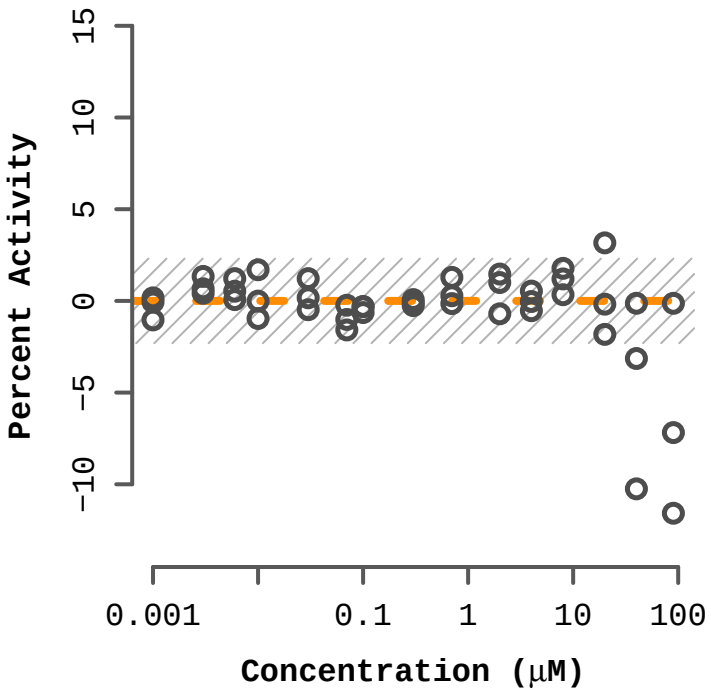
NAME: 1,2−Bis((chlorocarbonyl)oxy)ethane
CHID: 51631 **CASRN:** 124−05−0
SPID(S): Tox21_304040
M4ID: 12475148

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.861 **MAX_MED:** 0.722 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,4'−(Isopropylidenebis(4,1−phenyleneoxy))dian

CHID: 51650 **CASRN:** 13080−86−9

SPID(S): Tox21_303839

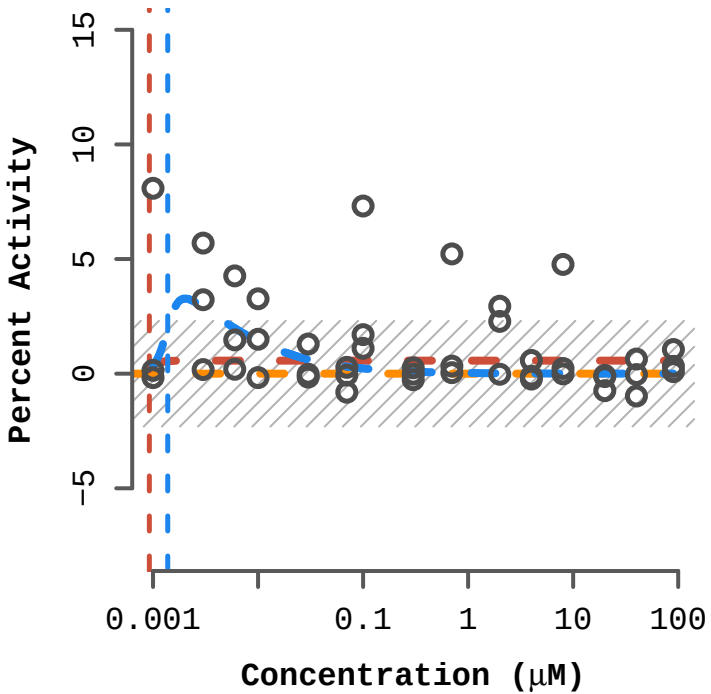
M4ID: 12475349

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.99	NA	NA
PROB:	1	NA	NA
RMSE:	2.75	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-N-Methyl-5-thiotetrazole
CHID: 51662 **CASRN:** 13183-79-4
SPID(S): Tox21_303990
M4ID: 12475198

HILL MODEL (in red):

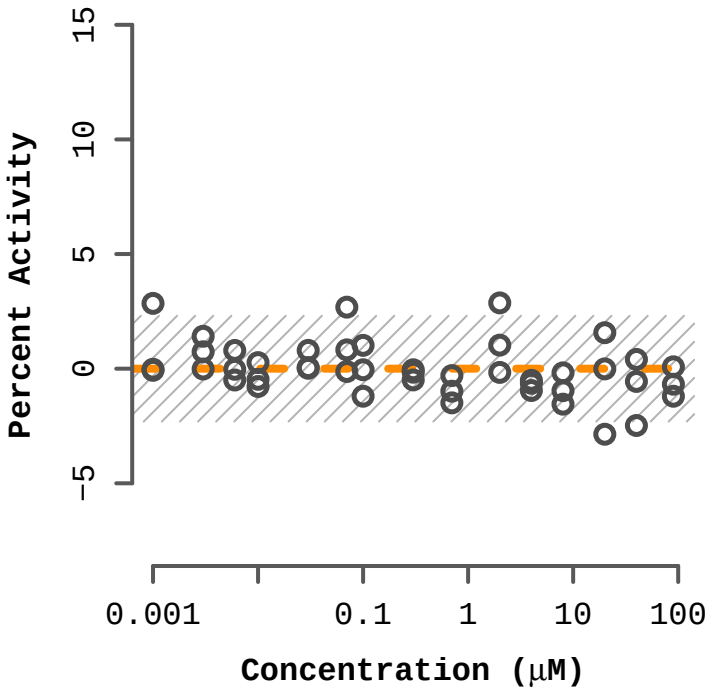
	tp	ga	gw
val:	0.568	−3.03	8
sd:	0.23	0.536	95.4

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.37	−2.86	7.56	−2.61	0.888
sd:	11.8	0.343	17.6	1.61	0.886

	CNST	HILL	GNLS
AIC:	193.74	192.67	190.84
PROB:	0.14	0.25	0.61
RMSE:	2.45	2.23	2.18

MAX_MEAN: 3.38 **MAX_MED:** 3.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

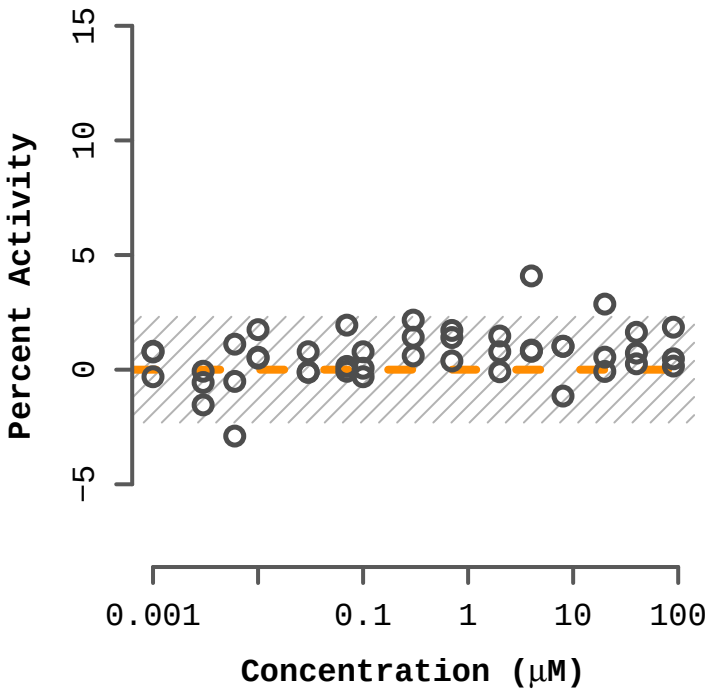
NAME: 4-Chlorobenzophenone
CHID: 51687 CASRN: 134-85-0
SPID(S): Tox21_304009
M4ID: 12475179

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.25 MAX_MED: 1.03 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

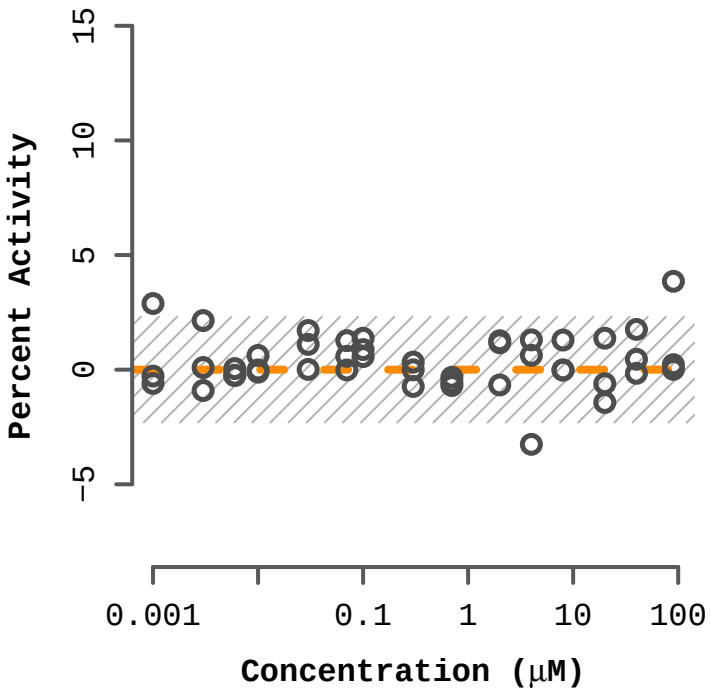
NAME: 2-Methoxybenzaldehyde
CHID: 51690 **CASRN:** 135-02-4
SPID(S): Tox21_303774
M4ID: 12475414

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 1.92 **MAX_MED:** 1.42 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

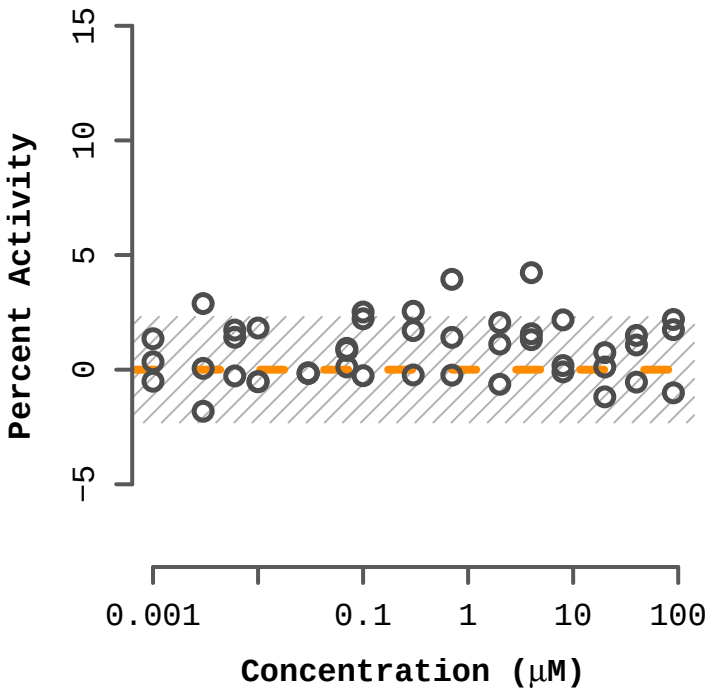
NAME: Europium(III) chloride hexahydrate
CHID: 51695 **CASRN:** 13759-92-7
SPID(S): Tox21_303707
M4ID: 12475481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.17 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

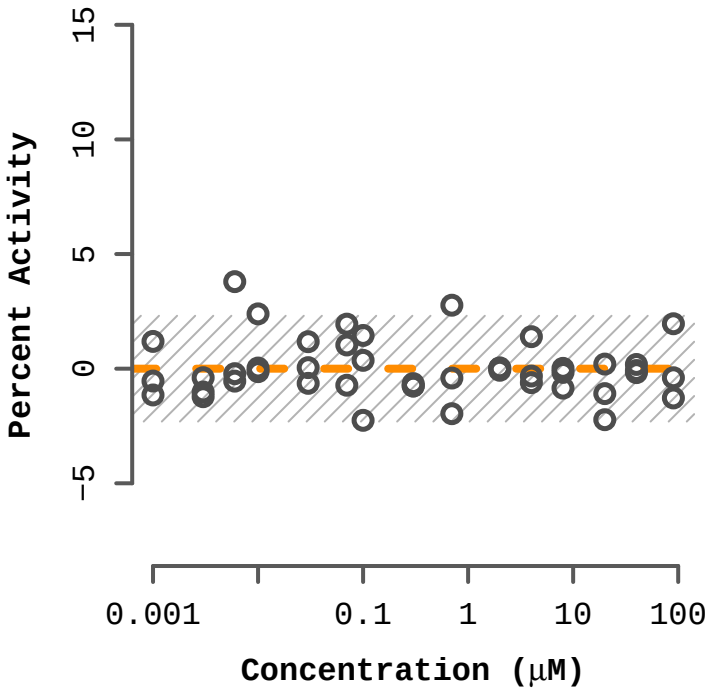
NAME: Aluminum trisacetoacetate
CHID: 51704 CASRN: 13963-57-0
SPID(S): Tox21_303741
M4ID: 12475447

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.37 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

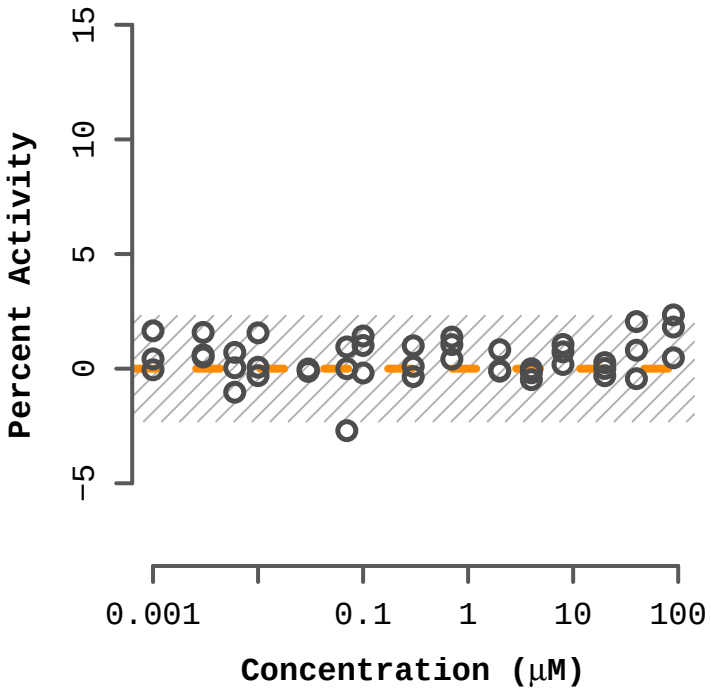
NAME: Iron(III) acetylacetonate
CHID: 51707 **CASRN:** 14024-18-1
SPID(S): Tox21_303809
M4ID: 12475379

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.18	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

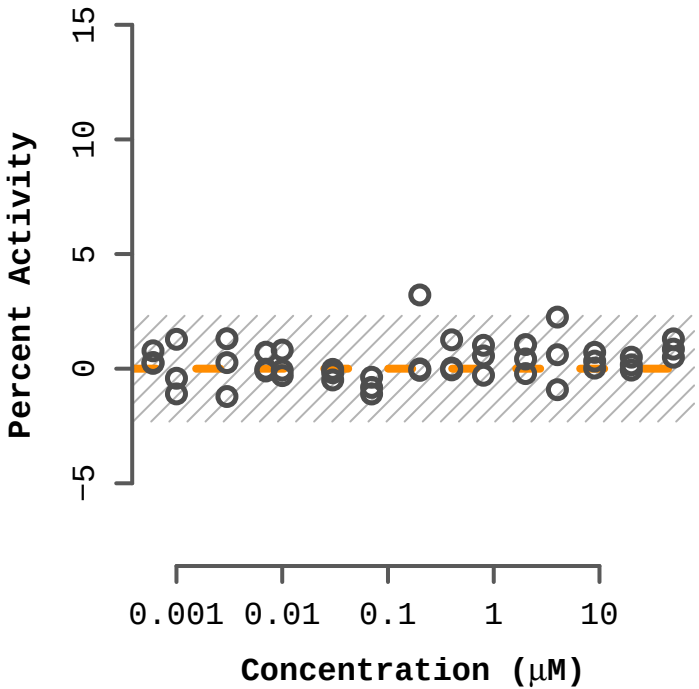
NAME: 4-Chlorophenylacetonitrile
CHID: 51708 **CASRN:** 140-53-4
SPID(S): Tox21_303864
M4ID: 12475324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.55 **MAX_MED:** 1.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

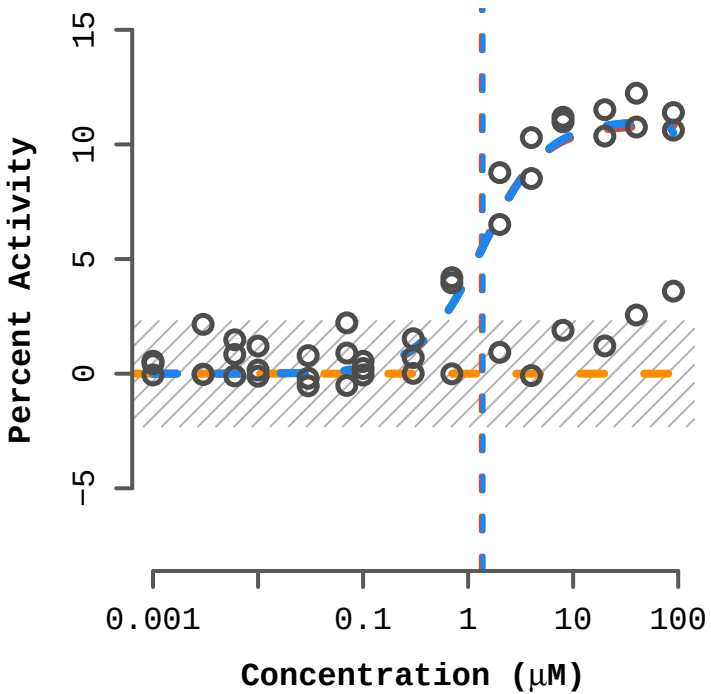
NAME: Methyl 3-aminobut-2-enoate
CHID: 51715 **CASRN:** 14205-39-1
SPID(S): Tox21_113788
M4ID: 12482429

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.79	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 0.854 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Pyridone
CHID: 51716 CASRN: 142-08-5
SPID(S): Tox21_303883
M4ID: 12475305

HILL MODEL (in red):

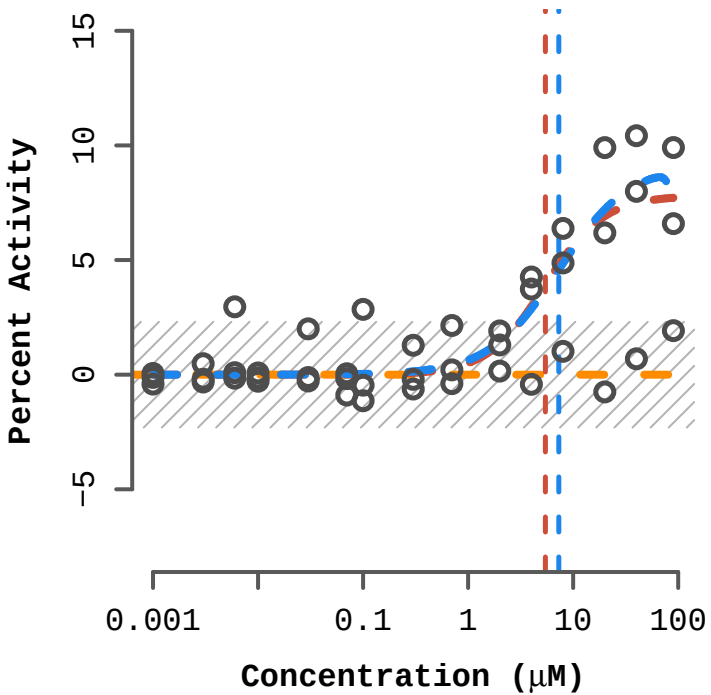
	tp	ga	gw
val:	10.8	0.125	1.49
sd:	0.599	0.0985	0.348

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11	0.143	1.44	2.1	9.08
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	278.72	213.66	217.47
PROB:	0	0.87	0.13
RMSE:	5.52	3.11	3.12

MAX_MEAN: 8.54 MAX_MED: 11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sulfathiazole sodium
CHID: 51724 **CASRN:** 144-74-1
SPID(S): Tox21_303846
M4ID: 12475342

HILL MODEL (in red):

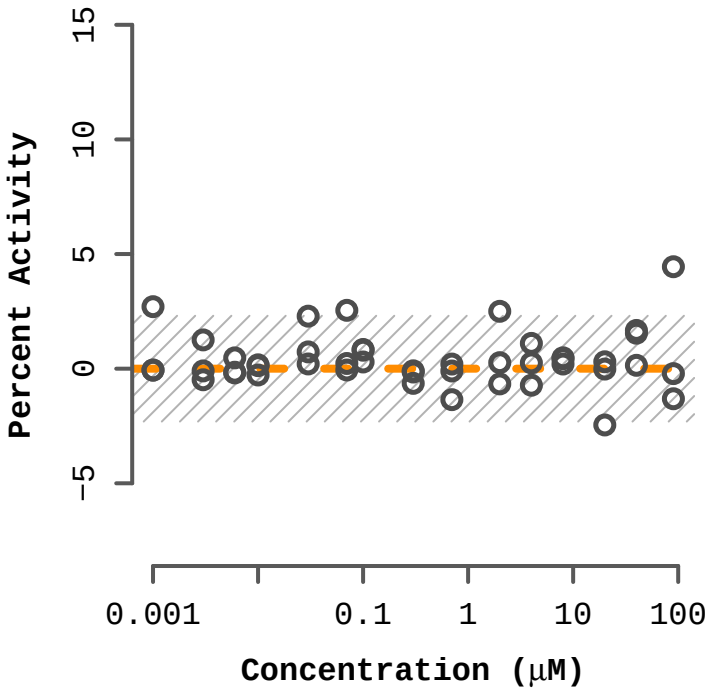
	tp	ga	gw
val:	7.81	0.735	1.57
sd:	1.18	0.152	0.598

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.15	0.863	1.3	1.99	13.2
sd:	2.47	0.277	0.579	0.0433	16.1

	CNST	HILL	GNLS
AIC:	232.59	194.28	197.33
PROB:	0	0.82	0.18
RMSE:	3.62	2.24	2.26

MAX_MEAN: 6.37 **MAX_MED:** 8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

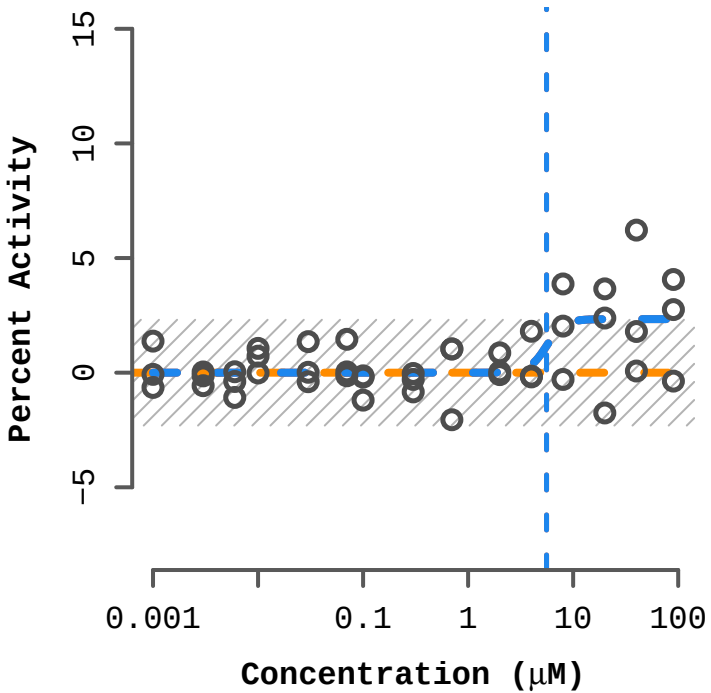
NAME: Indan-5-ol
CHID: 51732 **CASRN:** 1470-94-6
SPID(S): Tox21_303902
M4ID: 12475286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	137.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.23	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.55 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclopropanecarboxaldehyde
CHID: 51736 **CASRN:** 1489-69-6
SPID(S): Tox21_303871
M4ID: 12475317

HILL MODEL (in red):

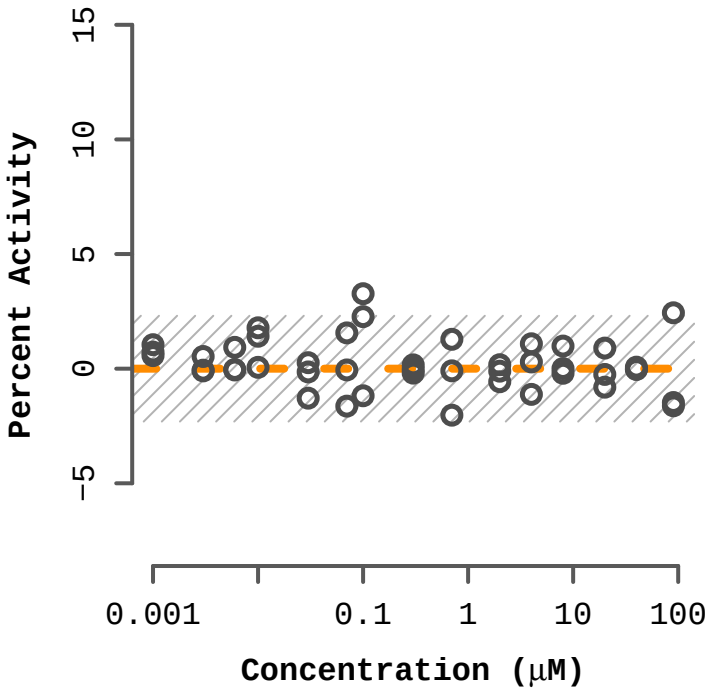
	tp	ga	gw
val:	2.34	0.746	5.24
sd:	0.538	0.173	6.58

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.34	0.746	5.24	3.93	16.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	167.28	156.51	160.51
PROB:	0	0.88	0.12
RMSE:	1.7	1.33	1.33

MAX_MEAN: 2.7 **MAX_MED:** 2.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

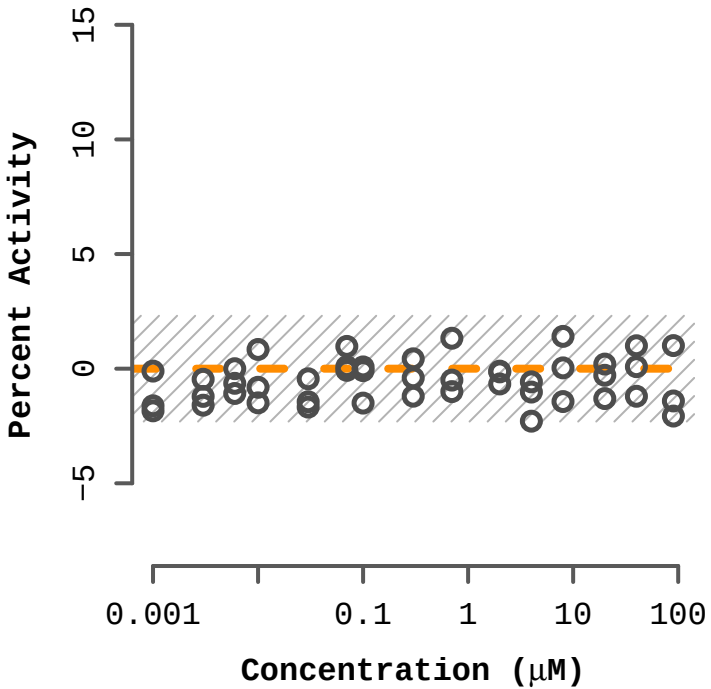
NAME: Dysprosium(III) chloride hexahydrate
CHID: 51738 **CASRN:** 15059-52-6
SPID(S): Tox21_304034
M4ID: 12475154

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

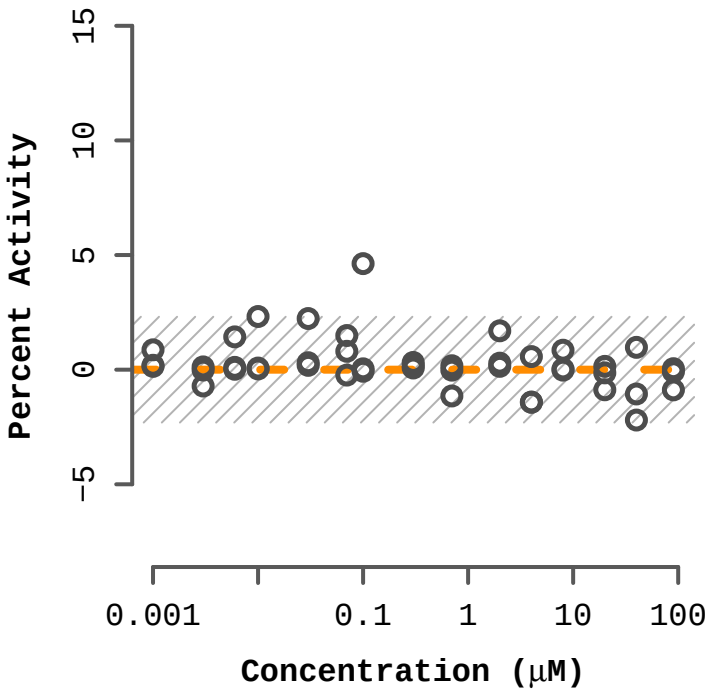
NAME: 6-Methylhept-5-en-2-ol
CHID: 51754 **CASRN:** 1569-60-4
SPID(S): Tox21_303934
M4ID: 12475254

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.331 **MAX_MED:** 0.091 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

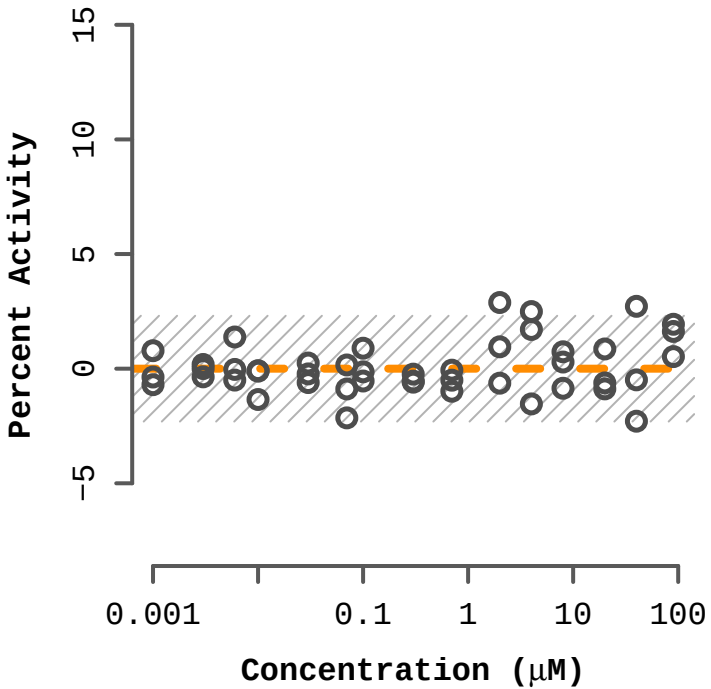
NAME: Diethyl dicarbonate
CHID: 51764 **CASRN:** 1609-47-8
SPID(S): Tox21_303976
M4ID: 12475212

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 0.802 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Methyl-2-(2-methylprop-1-en-1-yl)tetrahydro-2

CHID: 51771 **CASRN:** 16409-43-1

SPID(S): Tox21_303917

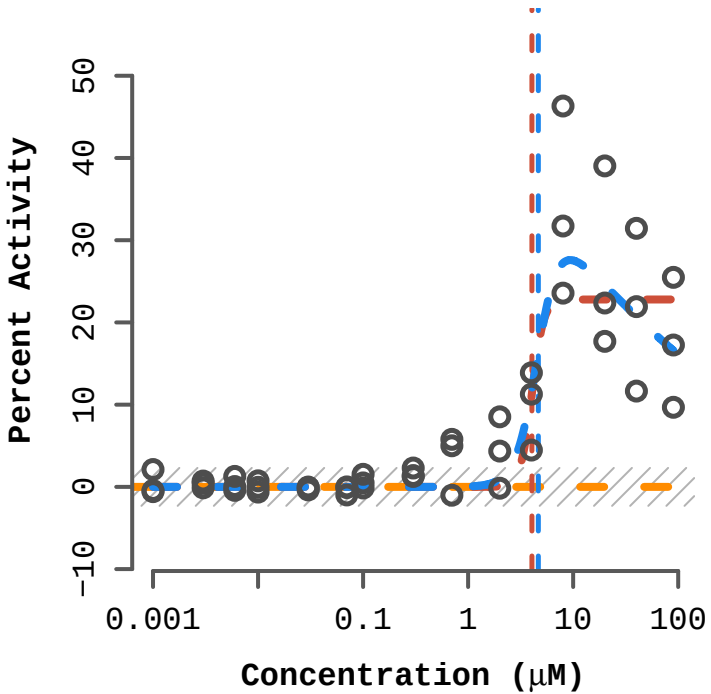
M4ID: 12475271

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 1.71 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Digoxigenin
CHID: 51778 **CASRN:** 1672-46-4
SPID(S): Tox21_303893
M4ID: 12475295

HILL MODEL (in red):

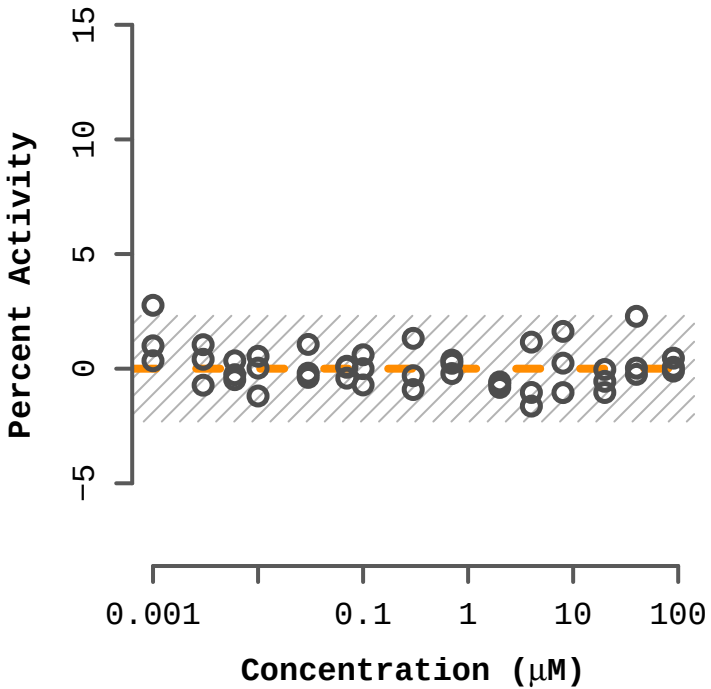
	tp	ga	gw
val:	22.8	0.607	8
sd:	1.59	0.023	17.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	55.6	0.668	4.33	1.06	0.414
sd:	53.2	0.0639	3.62	1.94	0.294

	CNST	HILL	GNLS
AIC:	356.83	275.8	273.05
PROB:	0	0.2	0.8
RMSE:	14.3	5.89	5.15

MAX_MEAN: 33.9 **MAX_MED:** 31.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

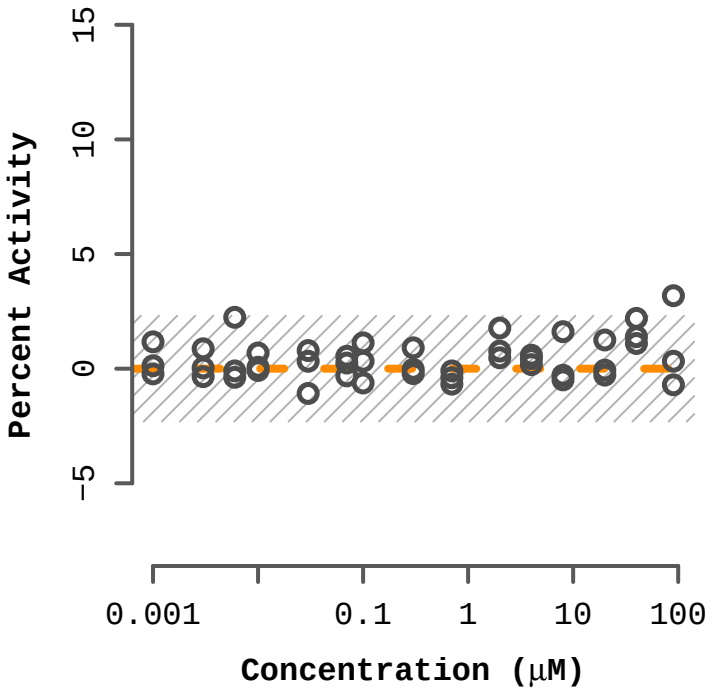
NAME: Ethylcyclohexane
CHID: 51779 **CASRN:** 1678-91-7
SPID(S): Tox21_303745
M4ID: 12475443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

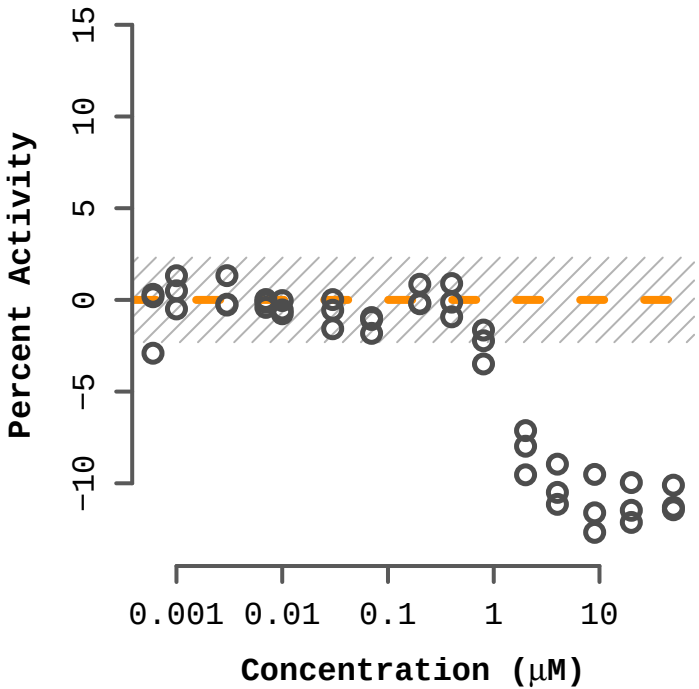
NAME: 3-Hydroxy-2-pyridone
CHID: 51782 **CASRN:** 16867-04-2
SPID(S): Tox21_303751
M4ID: 12475437

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.52	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 1.56 **MAX_MED:** 1.4 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

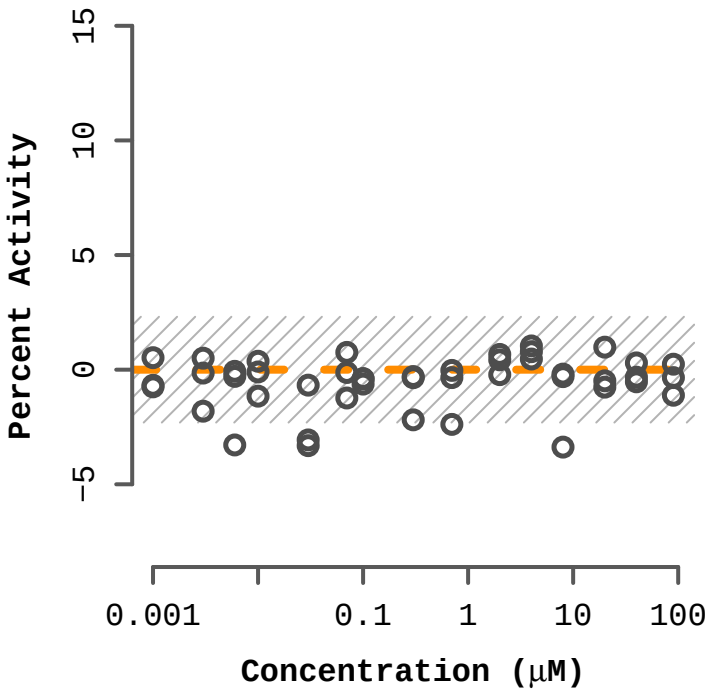
NAME: C.I. Basic Green 4 oxalate (1:x)
CHID: 51808 CASRN: 18015-76-4
SPID(S): Tox21_303916
M4ID: 12475272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	291.48	NA	NA
PROB:	1	NA	NA
RMSE:	6.13	NA	NA

MAX_MEAN: 0.442 **MAX_MED:** 0.497 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

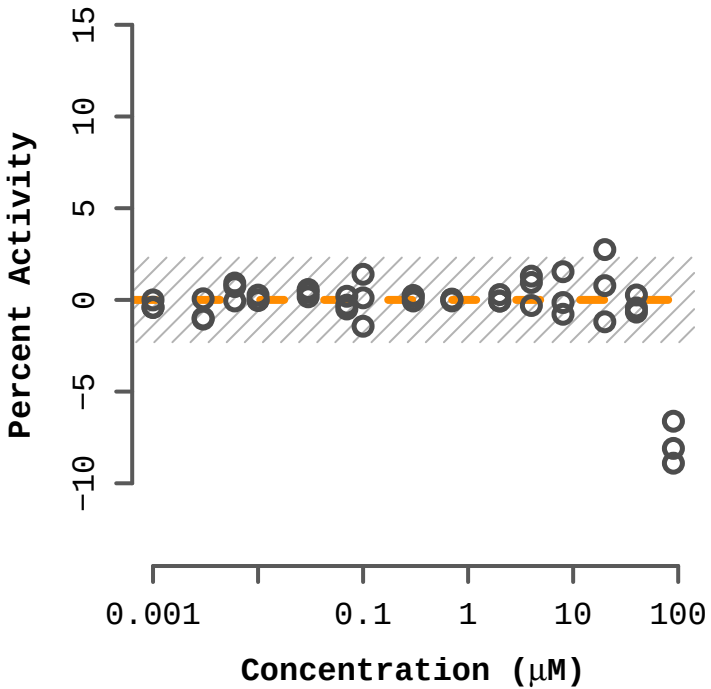
NAME: 2-Aminobenzonitrile
CHID: 51824 **CASRN:** 1885-29-6
SPID(S): Tox21_304036
M4ID: 12475152

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.763 **MAX_MED:** 0.786 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

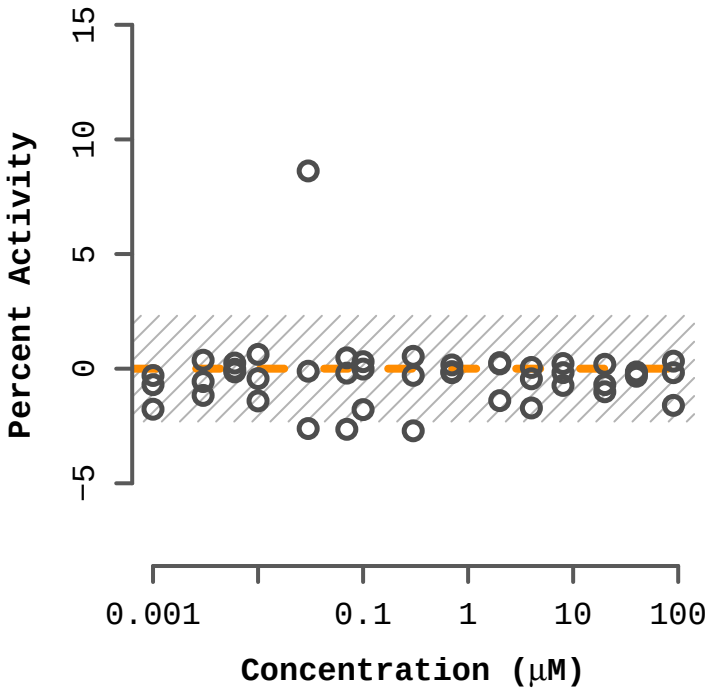
NAME: 2-(4-tert-Butylphenoxy)cyclohexan-1-ol
CHID: 51834 **CASRN:** 1942-71-8
SPID(S): Tox21_303920
M4ID: 12475268

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.39	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 0.778 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

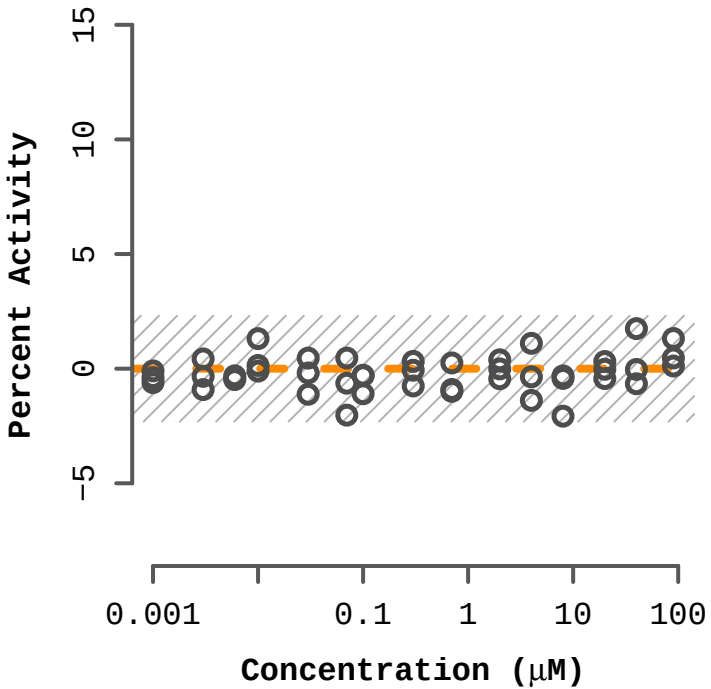
NAME: 3-Mercapto-1-propanol
CHID: 51836 **CASRN:** 19721-22-3
SPID(S): Tox21_303927
M4ID: 12475261

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.62	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 0.209 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

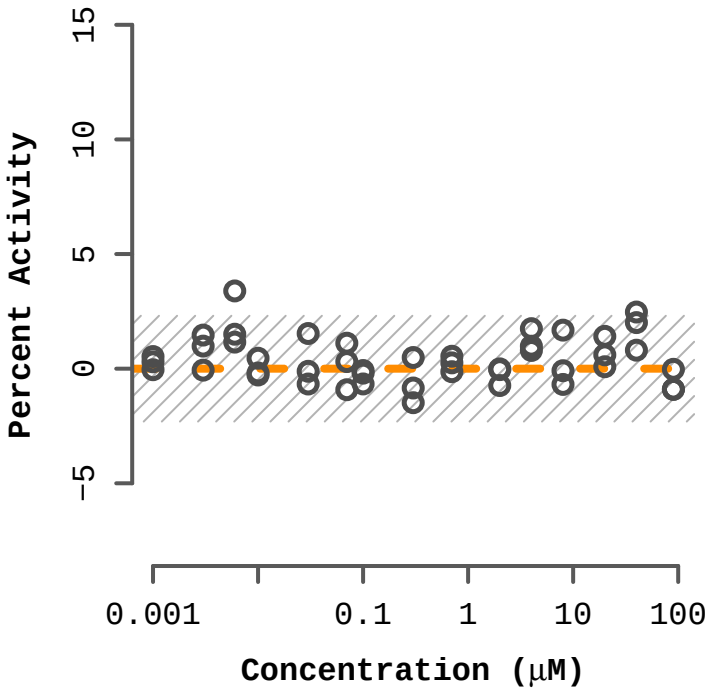
NAME: Scandium chloride hexahydrate
CHID: 51850 **CASRN:** 20662-14-0
SPID(S): Tox21_304021
M4ID: 12475167

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.634 **MAX_MED:** 0.469 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

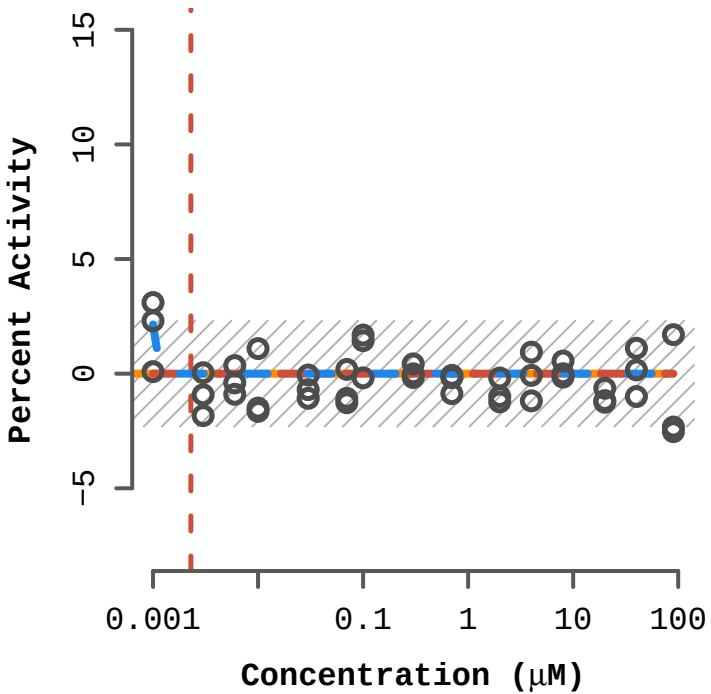
NAME: Allyl carbamate
CHID: 51856 **CASRN:** 2114-11-6
SPID(S): Tox21_303906
M4ID: 12475282

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 2.02 **MAX_MED:** 2.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Chromium(III) acetylacetonate
CHID: 51863 **CASRN:** 21679-31-2
SPID(S): Tox21_303935
M4ID: 12475253

HILL MODEL (in red):

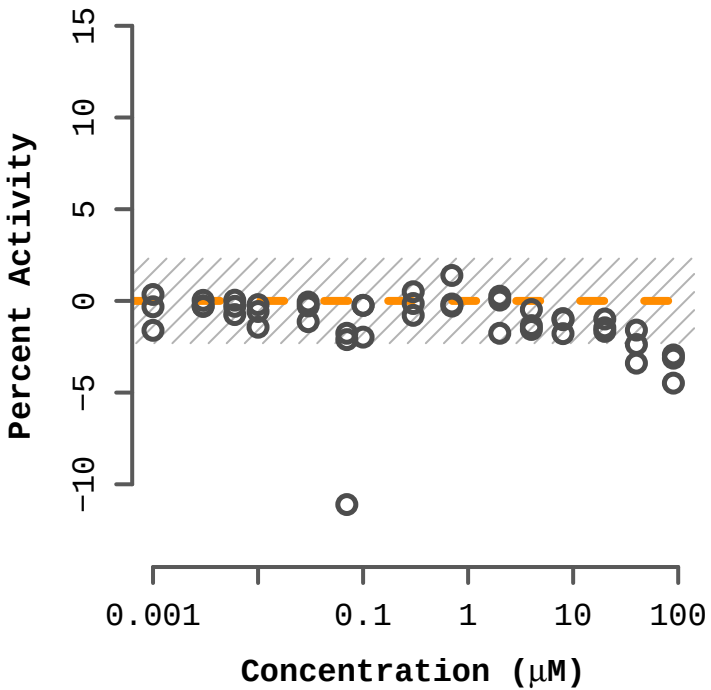
	tp	ga	gw
val:	2.74e-11	-2.64	0.814
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.66	-4.96	1.73	-2.99	14.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	146.34	152.34	150.3
PROB:	0.84	0.04	0.12
RMSE:	1.18	1.18	1.08

MAX_MEAN: 1.83 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

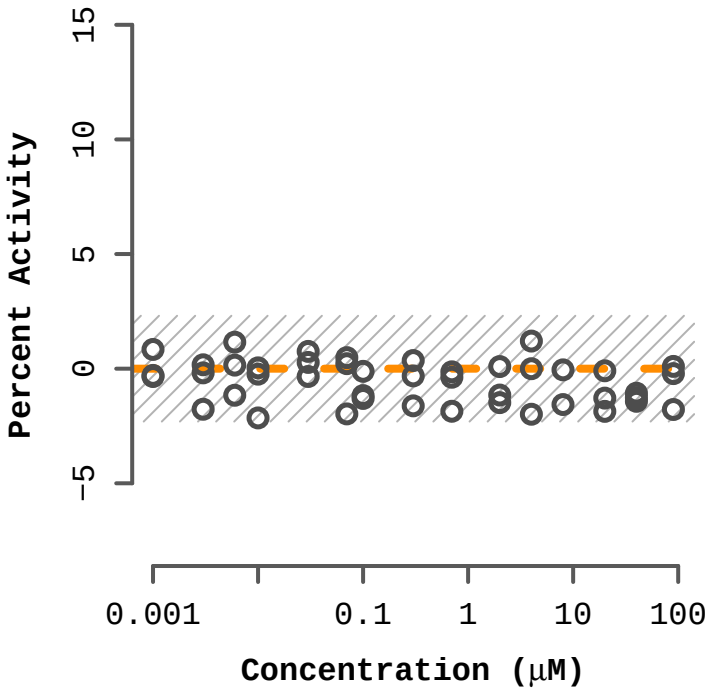
NAME: (E)-beta-Damascone
CHID: 51890 **CASRN:** 23726-91-2
SPID(S): Tox21_304045
M4ID: 12475143

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	179.16	NA	NA
PROB:	1	NA	NA
RMSE:	2.22	NA	NA

MAX_MEAN: 0.313 **MAX_MED:** 0.045 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

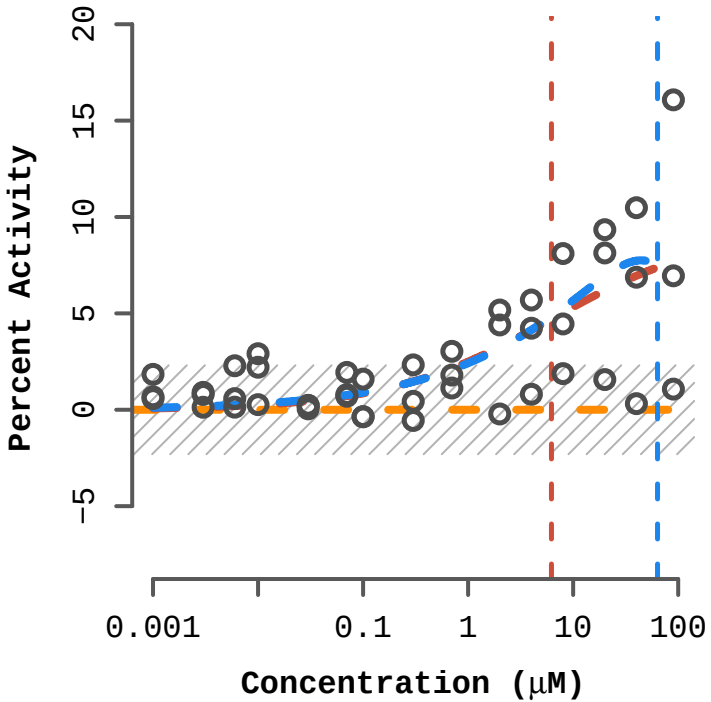
NAME: 2,6-Dichloropyridine
CHID: 51895 **CASRN:** 2402-78-0
SPID(S): Tox21_303965
M4ID: 12475223

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.23 **MAX_MED:** 0.274 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-(Diethylamino)ethyl acrylate
CHID: 51900 CASRN: 2426-54-2
SPID(S): Tox21_303835
M4ID: 12475353

HILL MODEL (in red):

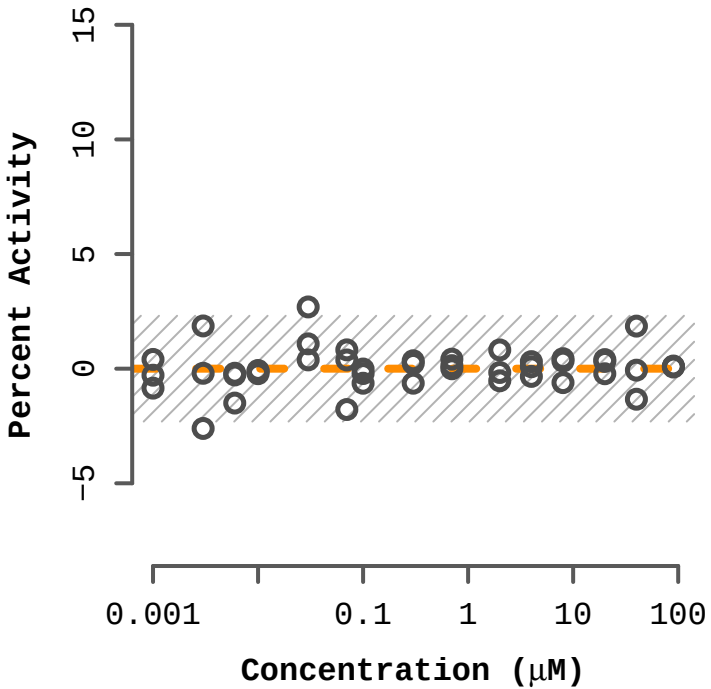
	tp	ga	gw
val:	9.41	0.793	0.558
sd:	4.95	1.02	0.358

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.3	1.8	0.468	2.05	2.11
sd:	25.1	1.97	0.193	0.257	2.78

	CNST	HILL	GNLS
AIC:	251.41	211.81	214.34
PROB:	0	0.78	0.22
RMSE:	4.37	2.54	2.6

MAX_MEAN: 8.03 MAX_MED: 8.14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

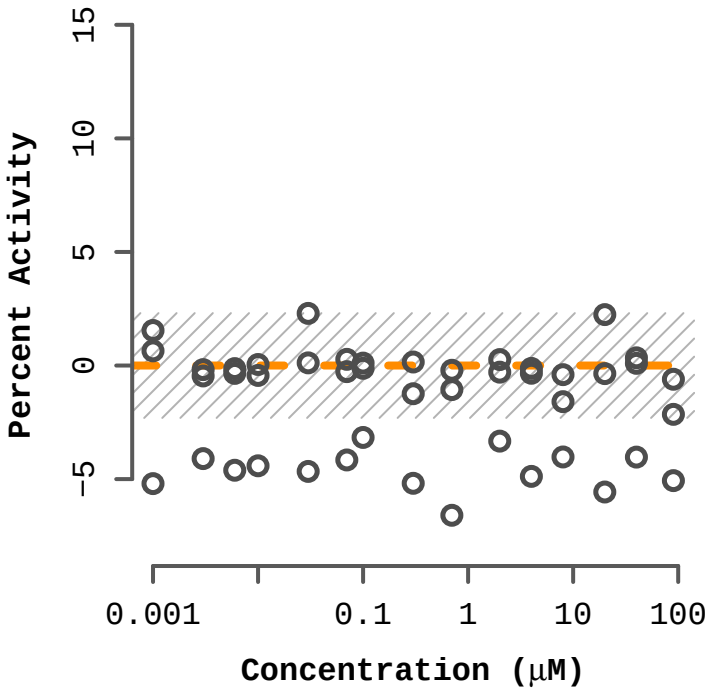
NAME: 2-Isobutyl-3-methoxypyrazine
CHID: 51907 **CASRN:** 24683-00-9
SPID(S): Tox21_303996
M4ID: 12475192

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.08 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

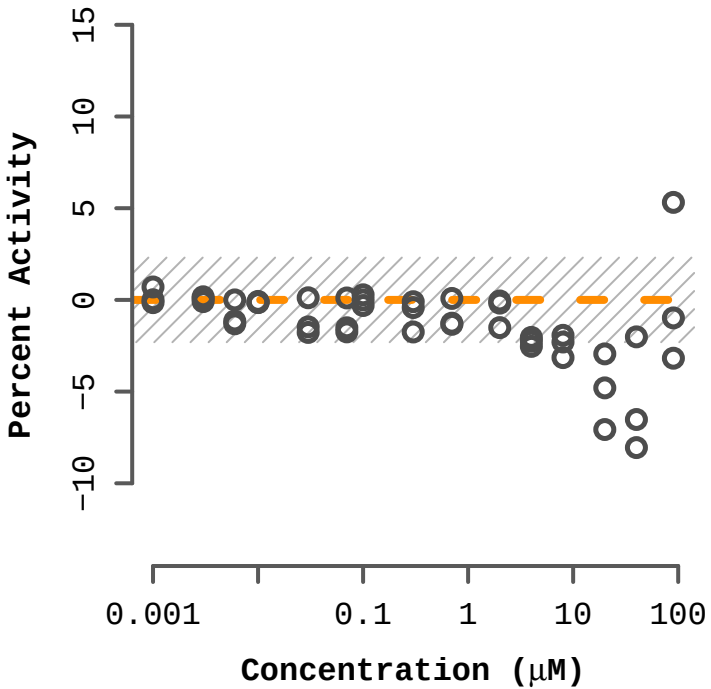
NAME: 1,3-Bis(4-aminophenoxy)benzene
CHID: 51914 **CASRN:** 2479-46-1
SPID(S): Tox21_303941
M4ID: 12475247

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	222.38	NA	NA
PROB:	1	NA	NA
RMSE:	2.8	NA	NA

MAX_MEAN: −0.749 **MAX_MED:** 0.647 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

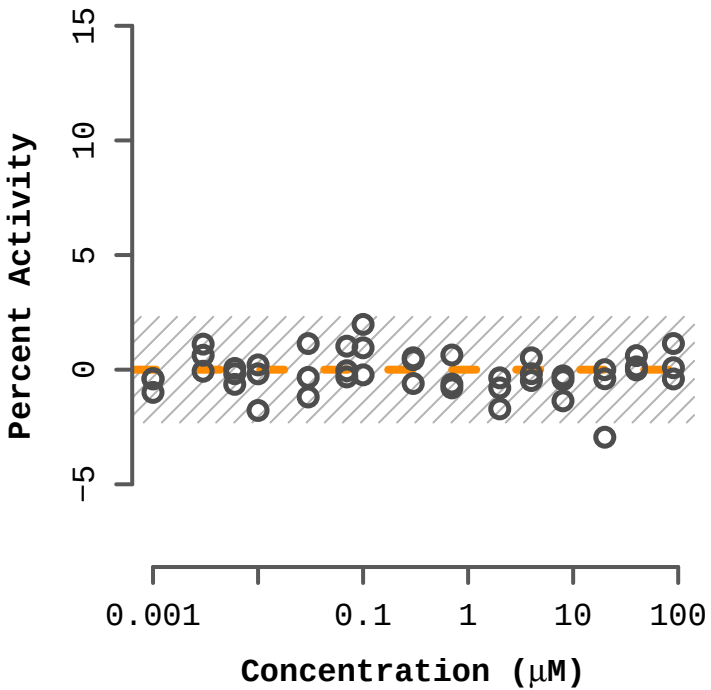
NAME: 2,2-Dichloro-1-phenylethanone
CHID: 51939 **CASRN:** 2648-61-5
SPID(S): Tox21_303816
M4ID: 12475372

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	204.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.54	NA	NA

MAX_MEAN: 0.387 **MAX_MED:** 0.0753 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

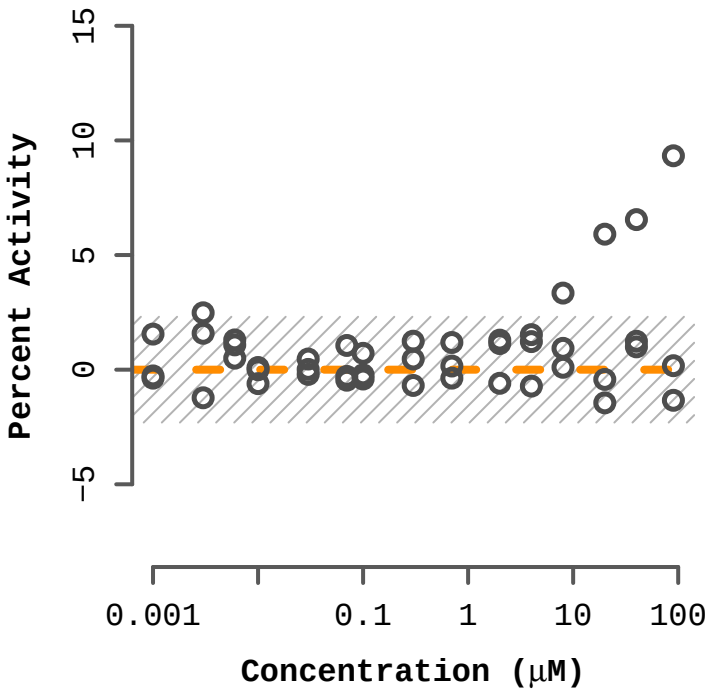
NAME: N,N−Dimethylacrylamide
CHID: 51944 **CASRN:** 2680−03−7
SPID(S): Tox21_303732
M4ID: 12475456

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 0.902 **MAX_MED:** 0.956 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

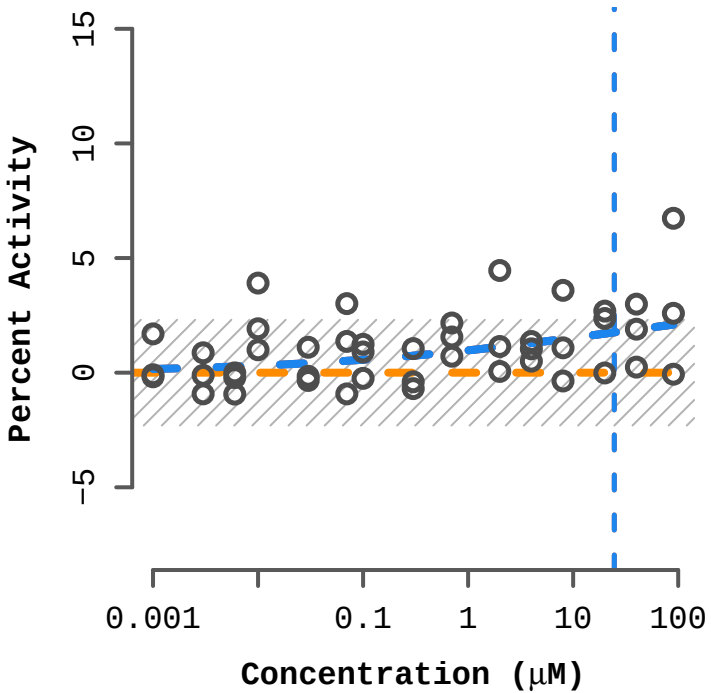
NAME: 3-Methyl-4-(methylthio)phenol
CHID: 51996 **CASRN:** 3120-74-9
SPID(S): Tox21_303747
M4ID: 12475441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	173.94	NA	NA
PROB:	1	NA	NA
RMSE:	2.18	NA	NA

MAX_MEAN: 2.93 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: C.I. Disperse Orange 25
CHID: 51999 CASRN: 31482-56-1
SPID(S): Tox21_303759
M4ID: 12475429

HILL MODEL (in red):

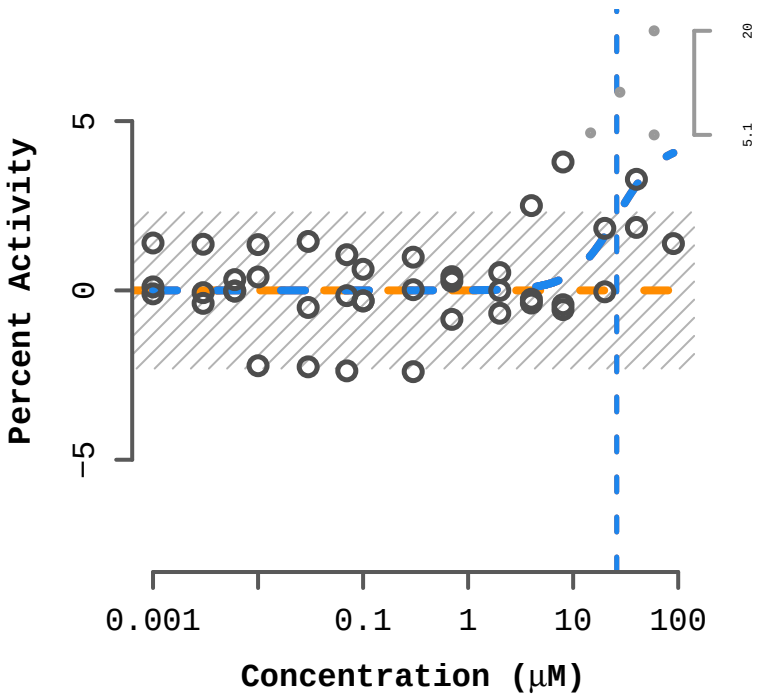
	tp	ga	gw
val:	3.52	1.39	0.3
sd:	9.26	7.45	0.389

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.52	1.39	0.3	3.7	3.94
sd:	9.27	7.46	0.389	1290	2920

	CNST	HILL	GNLS
AIC:	183.31	166.53	170.53
PROB:	0	0.88	0.12
RMSE:	1.92	1.45	1.45

MAX_MEAN: 3.09 **MAX_MED:** 2.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,1,3,3-Tetramethyldisiloxane
CHID: 52010 CASRN: 3277-26-7
SPID(S): Tox21_303833
M4ID: 12475355 BRK

HILL MODEL (in red):

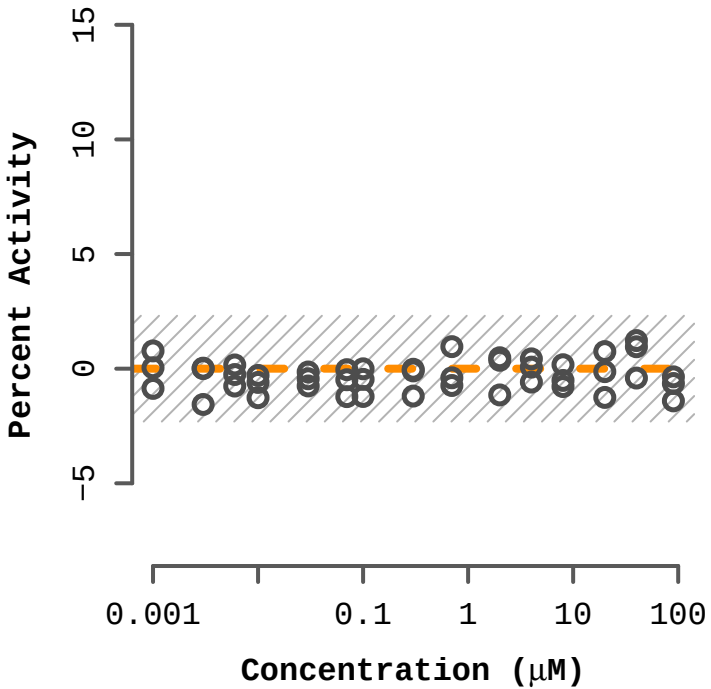
	tp	ga	gw
val:	4.37	1.41	2.06
sd:	2.73	0.379	2.13

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.37	1.41	2.06	2.86	7.95
sd:	2.73	0.379	2.13	1440	12800

	CNST	HILL	GNLS
AIC:	204.99	192.16	196.16
PROB:	0	0.88	0.12
RMSE:	3.79	2.95	2.95

MAX_MEAN: 8.77 MAX_MED: 5.12 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

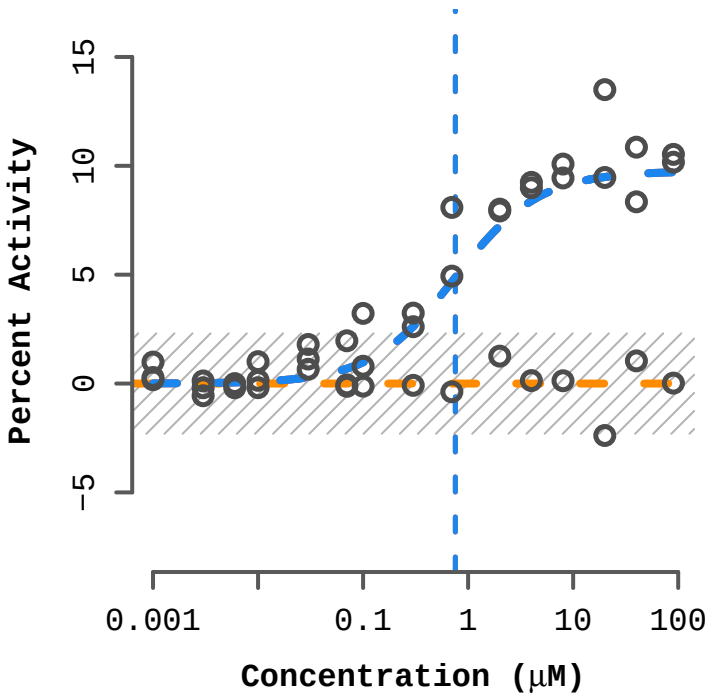
NAME: 4-Fluoro-3-nitroaniline
CHID: 52042 **CASRN:** 364-76-1
SPID(S): Tox21_303736
M4ID: 12475452

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.592 **MAX_MED:** 0.958 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-(2-Chloroethyl)morpholine hydrochloride (1:1
CHID: 52043 CASRN: 3647-69-6
SPID(S): Tox21_303894
M4ID: 12475294

HILL MODEL (in red):

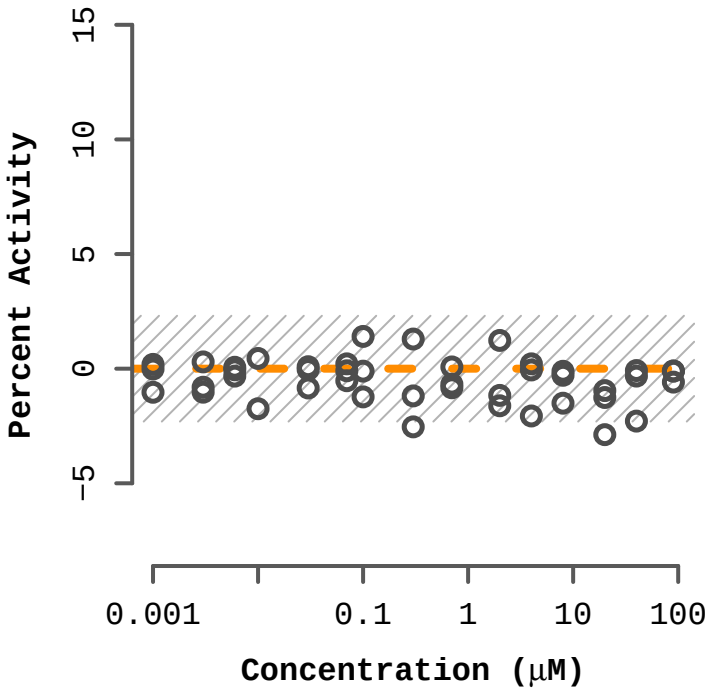
	tp	ga	gw
val:	9.76	-0.122	1.09
sd:	0.839	0.162	0.332

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.76	-0.122	1.09	3.31	4.92
sd:	0.839	0.162	0.332	721	2720

	CNST	HILL	GNLS
AIC:	277.82	230.17	234.17
PROB:	0	0.88	0.12
RMSE:	5.37	3.57	3.57

MAX_MEAN: 6.91 MAX_MED: 10.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

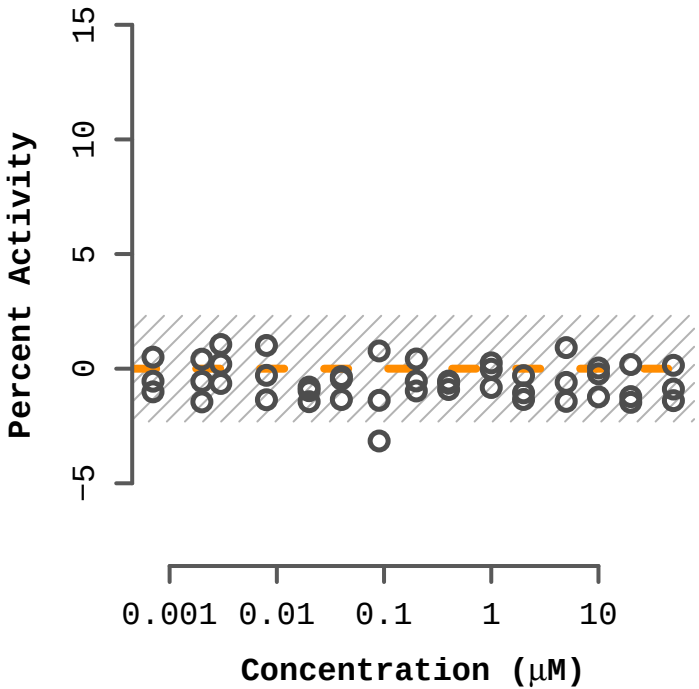
NAME: Methyl 3-methoxypropionate
CHID: 52060 CASRN: 3852-09-3
SPID(S): Tox21_304047
M4ID: 12475141

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.91	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.0238 **MAX_MED:** −0.014 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

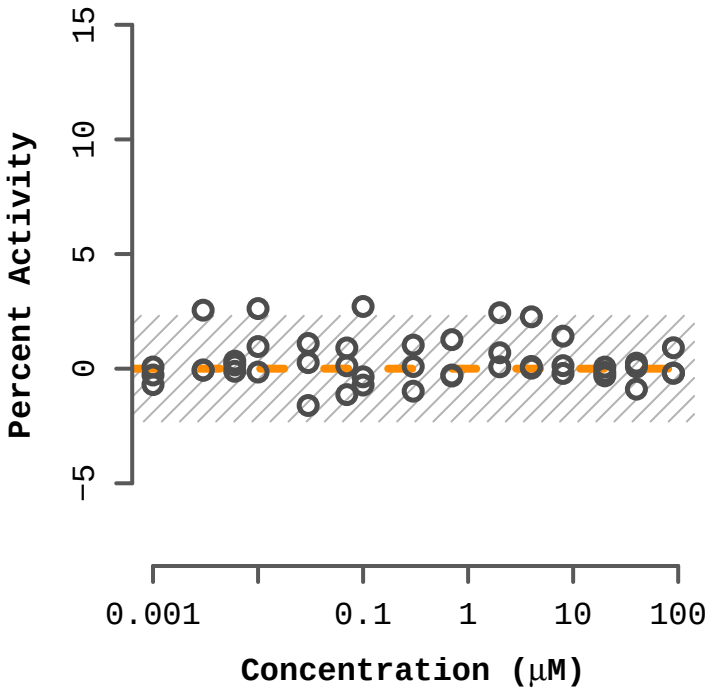
NAME: 2,2,4,4,6,8,8−Heptamethylnonane
CHID: 52101 **CASRN:** 4390−04−9
SPID(S): Tox21_303743
M4ID: 12475445

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.4	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.204 **MAX_MED:** 0.199 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

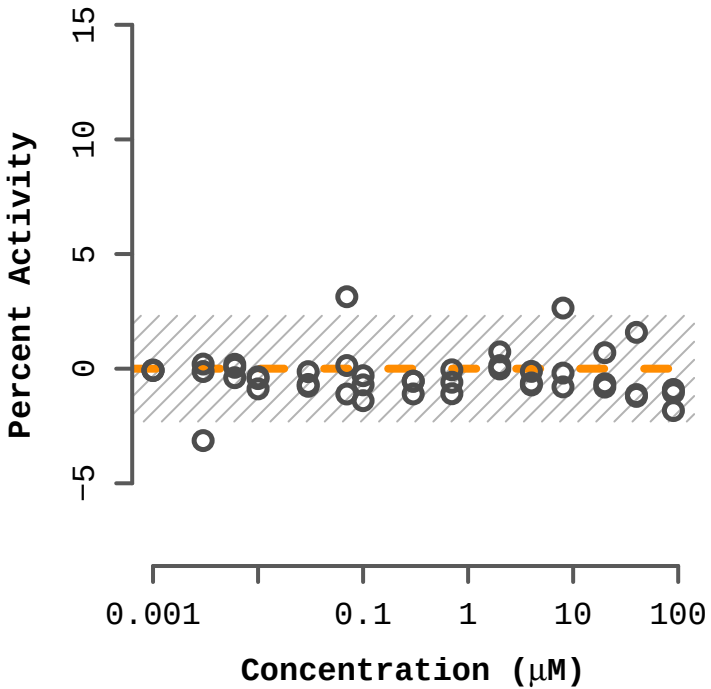
NAME: (2-Chloroethyl)dimethylamine hydrochloride
CHID: 52109 **CASRN:** 4584-46-7
SPID(S): Tox21_303802
M4ID: 12475386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.08	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.967 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

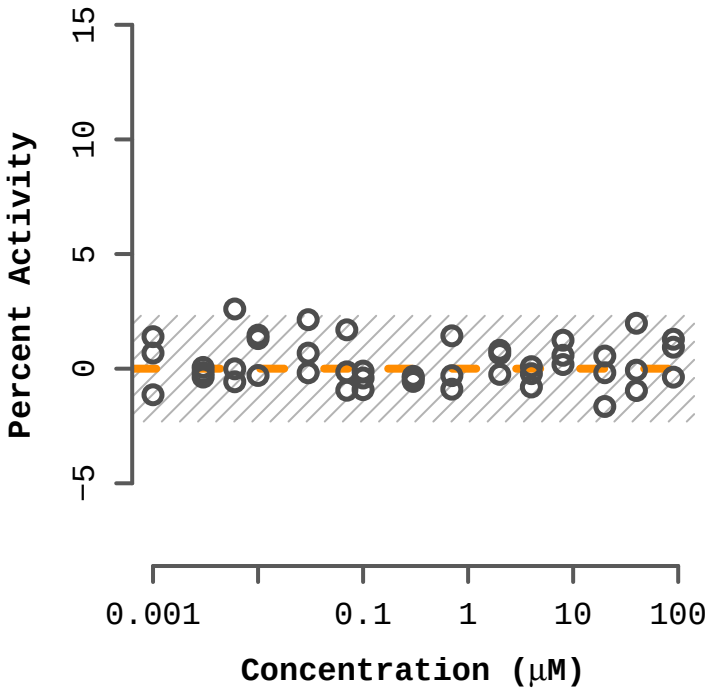
NAME: Diethoxymethane
CHID: 52112 **CASRN:** 462-95-3
SPID(S): Tox21_303824
M4ID: 12475364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.82	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.725 **MAX_MED:** 0.139 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

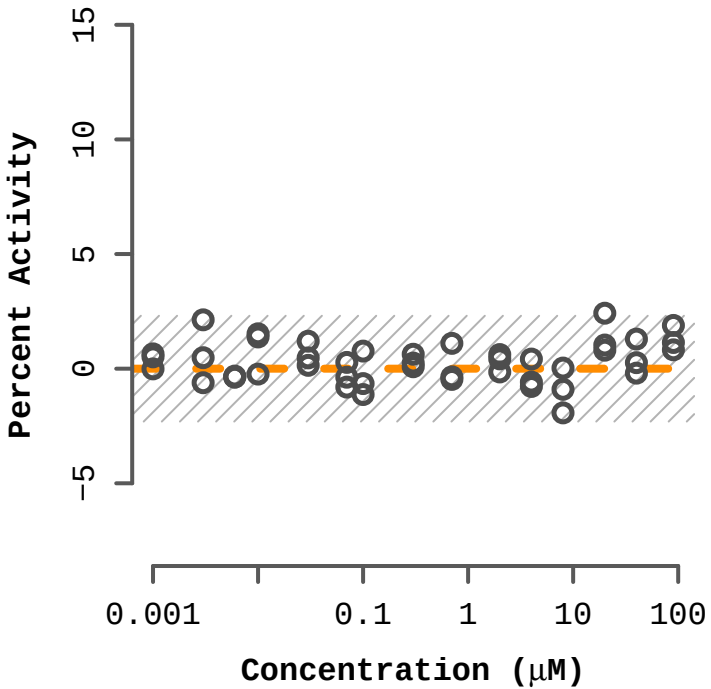
NAME: Borane – morpholine complex
CHID: 52124 **CASRN:** 4856-95-5
SPID(S): Tox21_303932
M4ID: 12475256

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 1.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

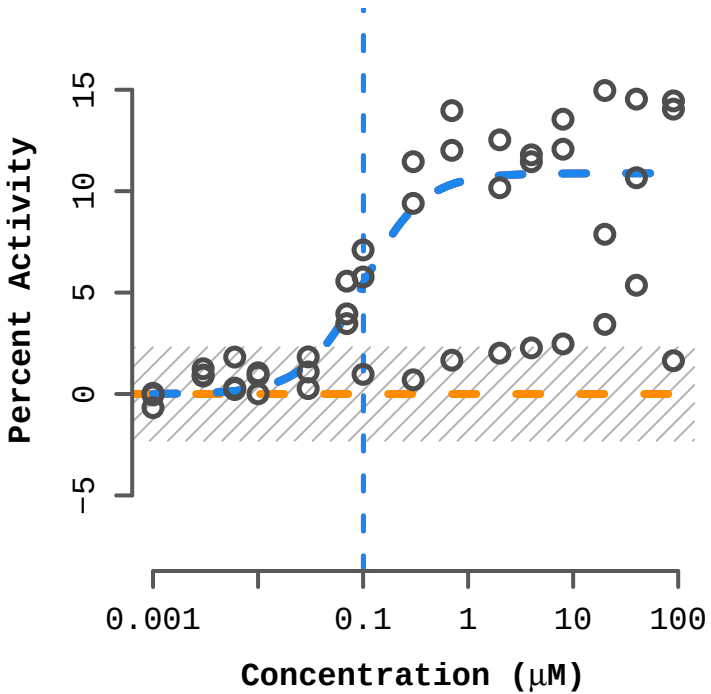
NAME: 2,4,6-Trimethylbenzaldehyde
CHID: 52125 **CASRN:** 487-68-3
SPID(S): Tox21_303703
M4ID: 12475485

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.86	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indan
CHID: 52132 CASRN: 496-11-7
SPID(S): Tox21_303879
M4ID: 12475309

HILL MODEL (in red):

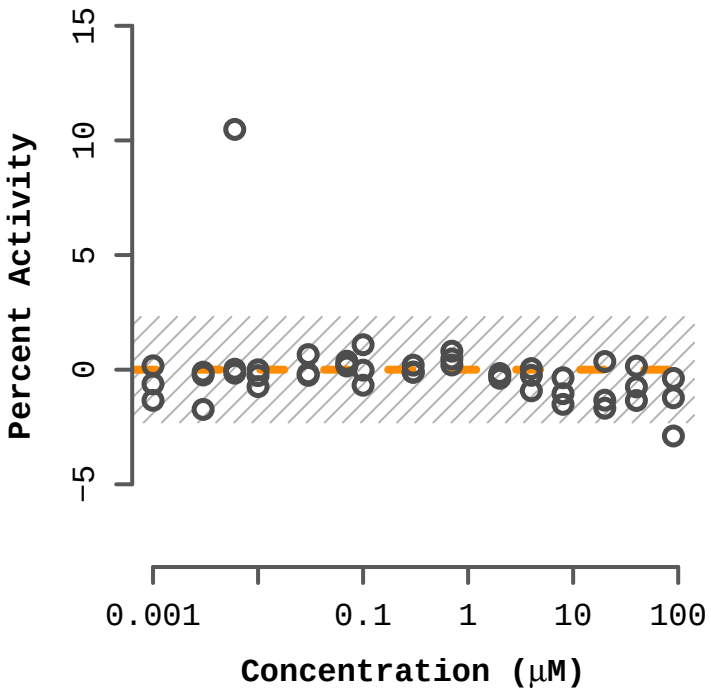
	tp	ga	gw
val:	10.9	−0.997	1.52
sd:	0.977	0.133	0.736

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.9	−0.997	1.52	3.95	13.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	315.16	251.94	255.94
PROB:	0	0.88	0.12
RMSE:	7.68	3.86	3.86

MAX_MEAN: 10.2 MAX_MED: 14 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

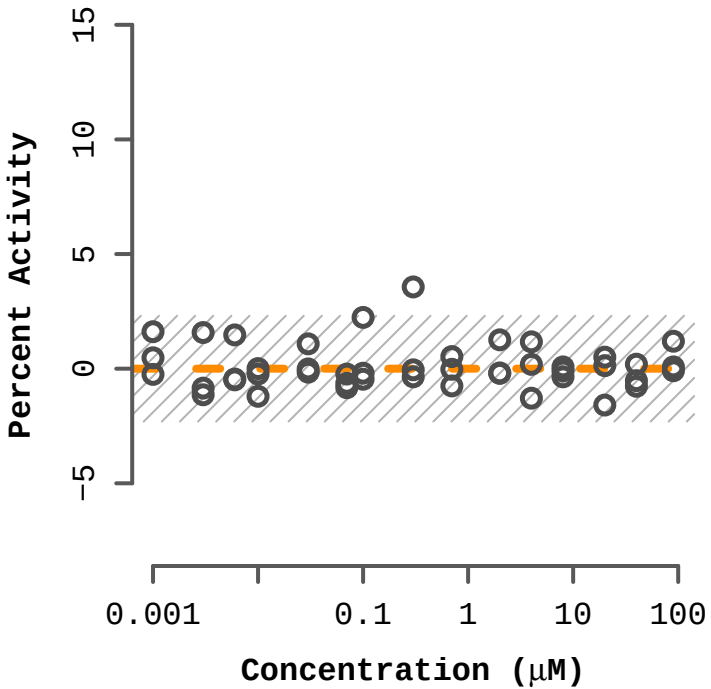
NAME: 4-Iodophenol
CHID: 52186 **CASRN:** 540-38-5
SPID(S): Tox21_303957
M4ID: 12475231

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.77	NA	NA

MAX_MEAN: 3.45 **MAX_MED:** 0.467 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

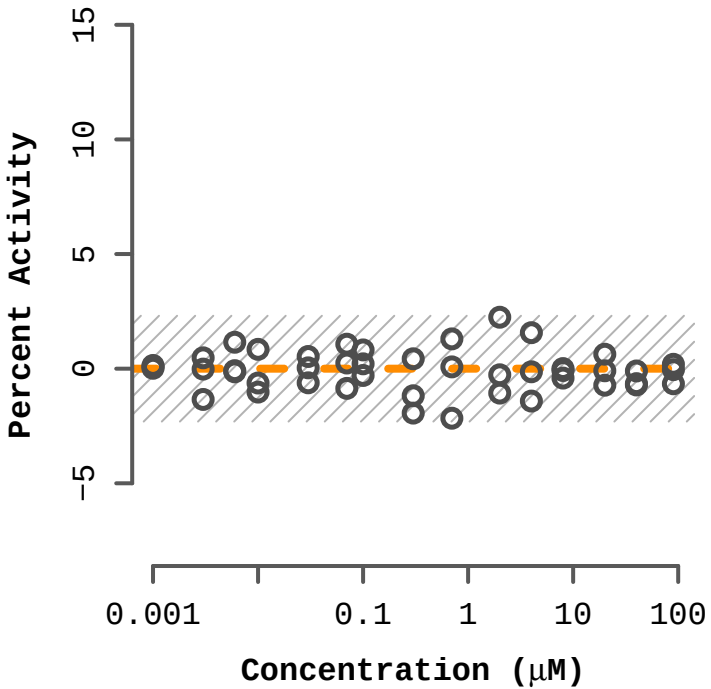
NAME: Isoamyl ether
CHID: 52198 **CASRN:** 544-01-4
SPID(S): Tox21_303780
M4ID: 12475408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.476 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

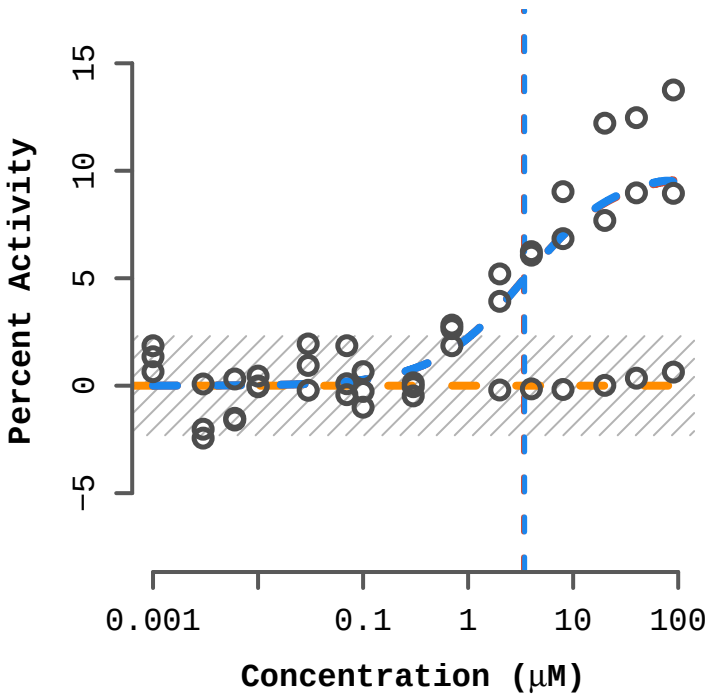
NAME: 2'−Aminoacetophenone
CHID: 52213 **CASRN:** 551−93−9
SPID(S): Tox21_304027
M4ID: 12475161

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.311 **MAX_MED:** 0.248 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: (−)Bronyl acetate
CHID: 52228 CASRN: 5655-61-8
SPID(S): Tox21_303841
M4ID: 12475347

HILL MODEL (in red):

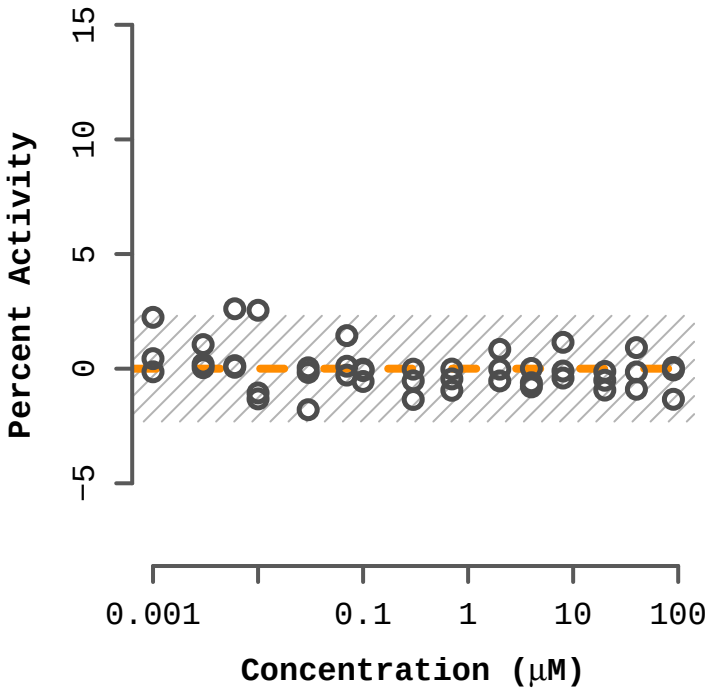
	tp	ga	gw
val:	9.89	0.527	1.02
sd:	1.74	0.246	0.346

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	9.99	0.538	1.01	2.14	9.41
sd:	2.49	0.315	0.383	2.31	115

	CNST	HILL	GNLS
AIC:	259.8	222.49	226.48
PROB:	0	0.88	0.12
RMSE:	4.74	3.03	3.03

MAX_MEAN: 7.78 MAX_MED: 8.97 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

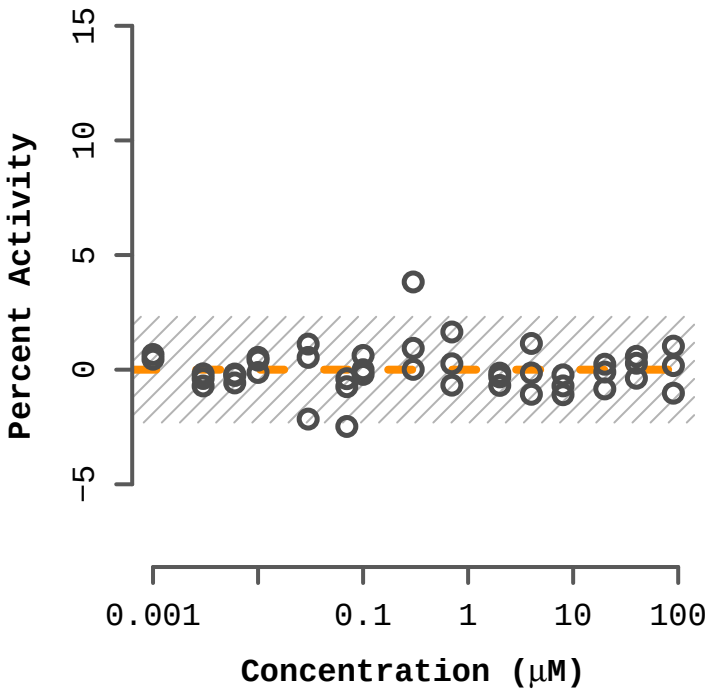
NAME: Isobornyl acrylate
CHID: 52250 **CASRN:** 5888-33-5
SPID(S): Tox21_303930
M4ID: 12475258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.23	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.937 **MAX_MED:** 0.439 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

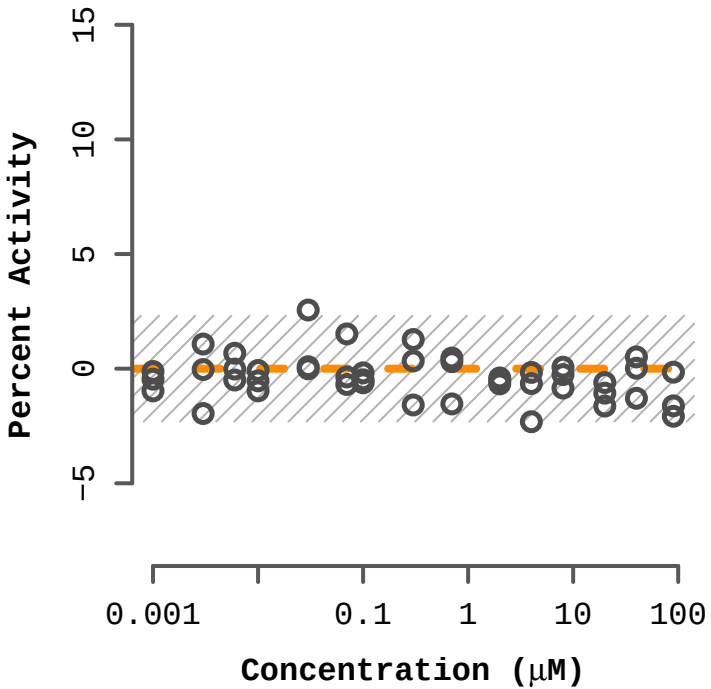
NAME: 3,5-Dimethylpyridine
CHID: 52254 **CASRN:** 591-22-0
SPID(S): Tox21_303943
M4ID: 12475245

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 0.933 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

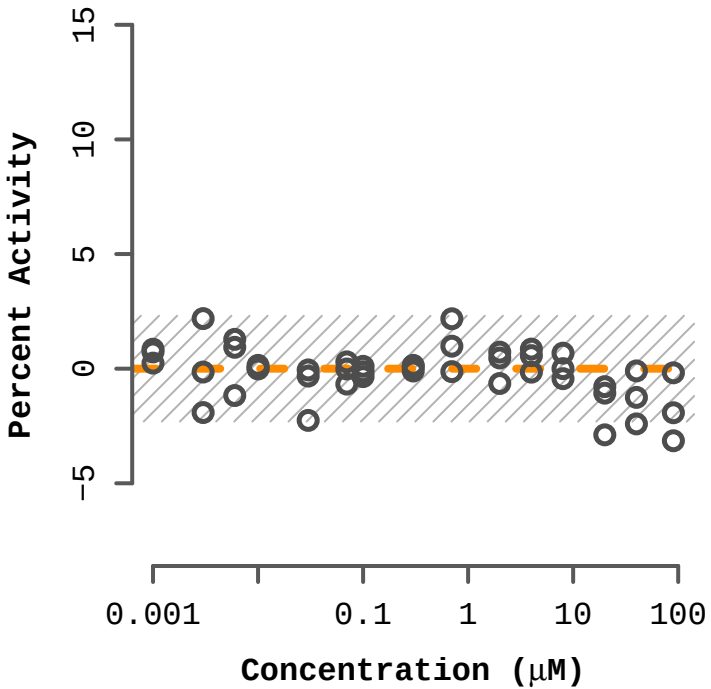
NAME: Glycerol tributyrate
CHID: 52267 **CASRN:** 60-01-5
SPID(S): Tox21_303991
M4ID: 12475197

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.881 **MAX_MED:** 0.341 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

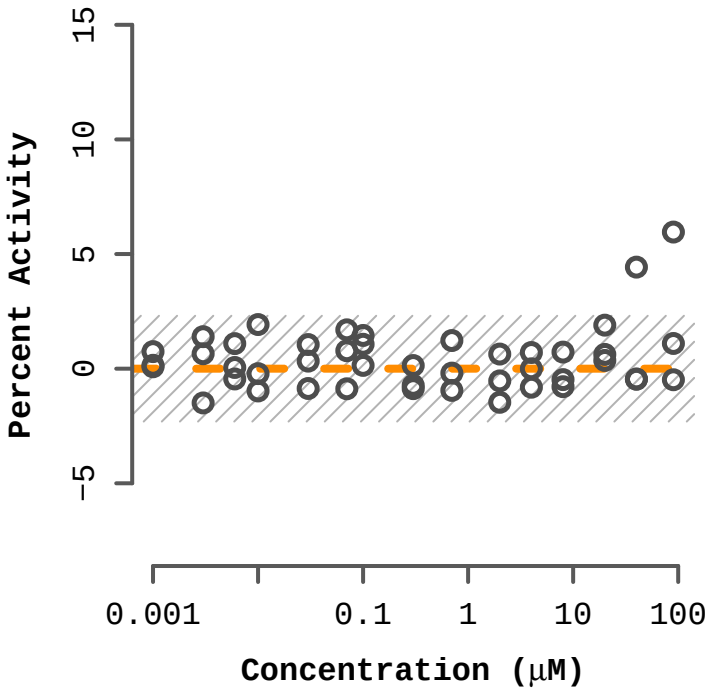
NAME: Triphenylstibine
CHID: 52269 CASRN: 603-36-1
SPID(S): Tox21_304035
M4ID: 12475153

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	138.29	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.01 **MAX_MED:** 0.982 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

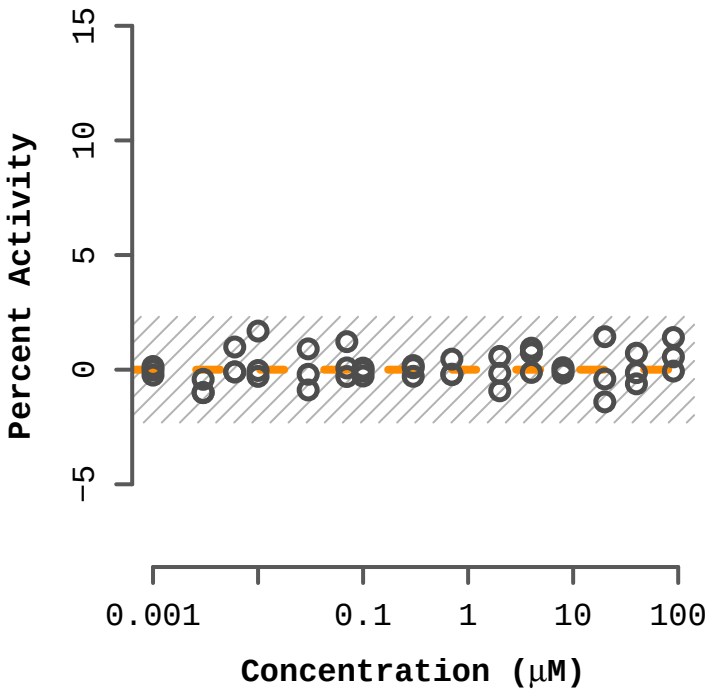
NAME: 2-Chlorobenzamide
CHID: 52278 **CASRN:** 609-66-5
SPID(S): Tox21_303767
M4ID: 12475421

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.42	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 1.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

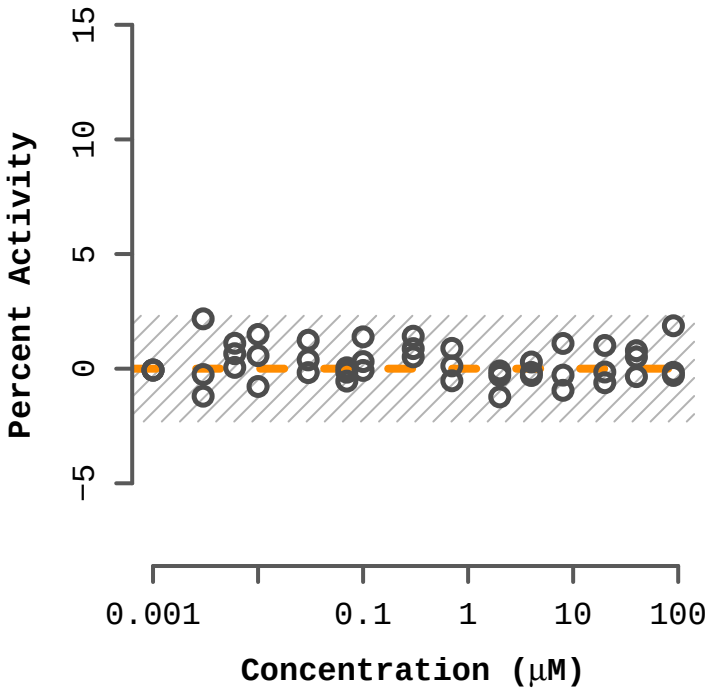
NAME: 1,7-Dimethylxanthine
CHID: 52281 **CASRN:** 611-59-6
SPID(S): Tox21_303803
M4ID: 12475385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	92.75	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 0.635 **MAX_MED:** 0.741 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

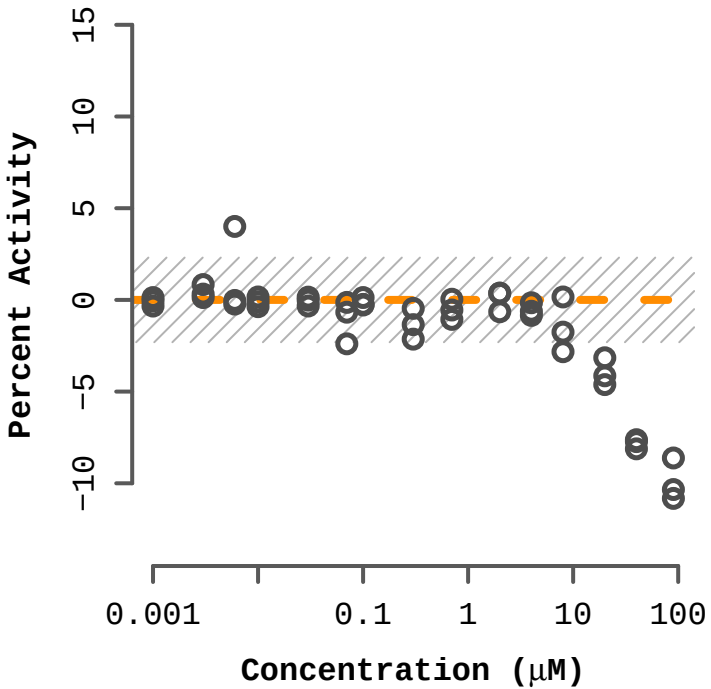
NAME: But-2-en-1-ol
CHID: 52283 CASRN: 6117-91-5
SPID(S): Tox21_303907
M4ID: 12475281

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.02	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.937 MAX_MED: 0.877 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

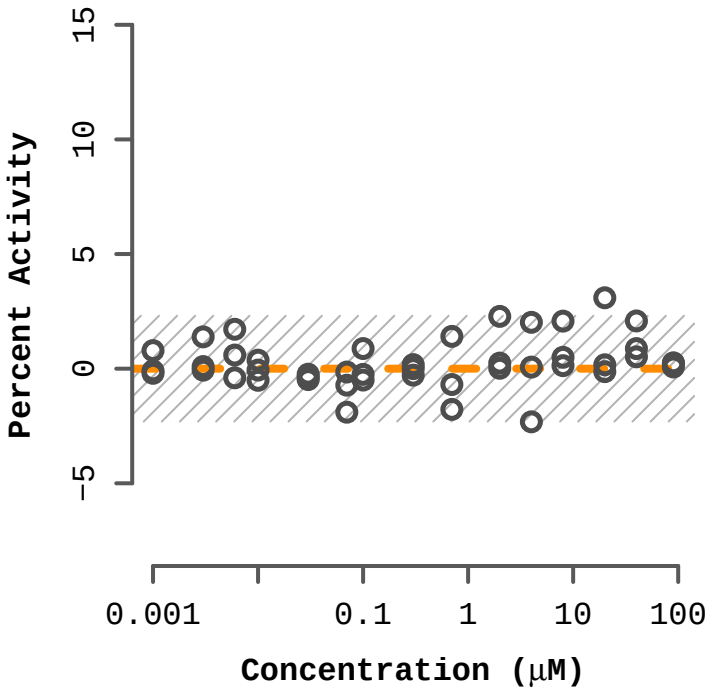
NAME: 1,2-Bis(chloromethyl)benzene
CHID: 52284 **CASRN:** 612-12-4
SPID(S): Tox21_303964
M4ID: 12475224

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	226.97	NA	NA
PROB:	1	NA	NA
RMSE:	3.57	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.368 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

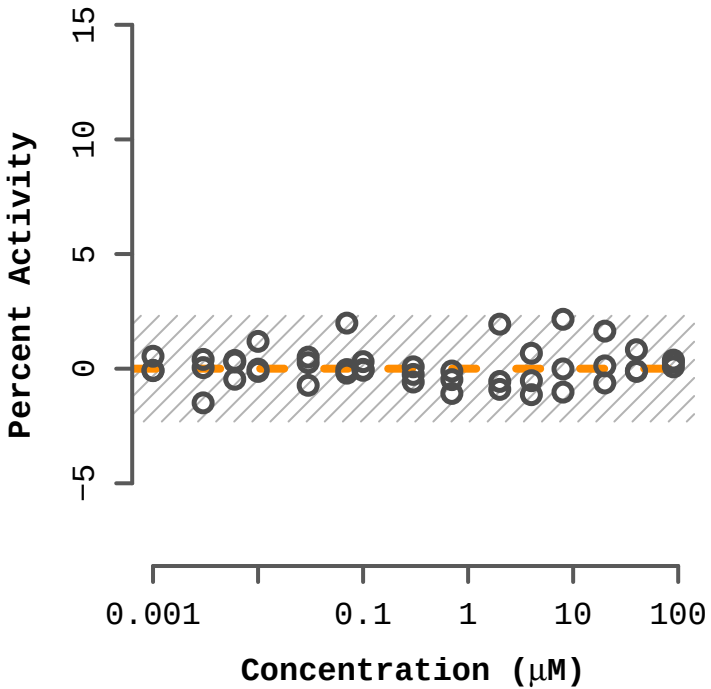
NAME: 1,3-Dihydro-2H-inden-2-one
CHID: 52288 **CASRN:** 615-13-4
SPID(S): Tox21_304008
M4ID: 12475180

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.16 **MAX_MED:** 0.878 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

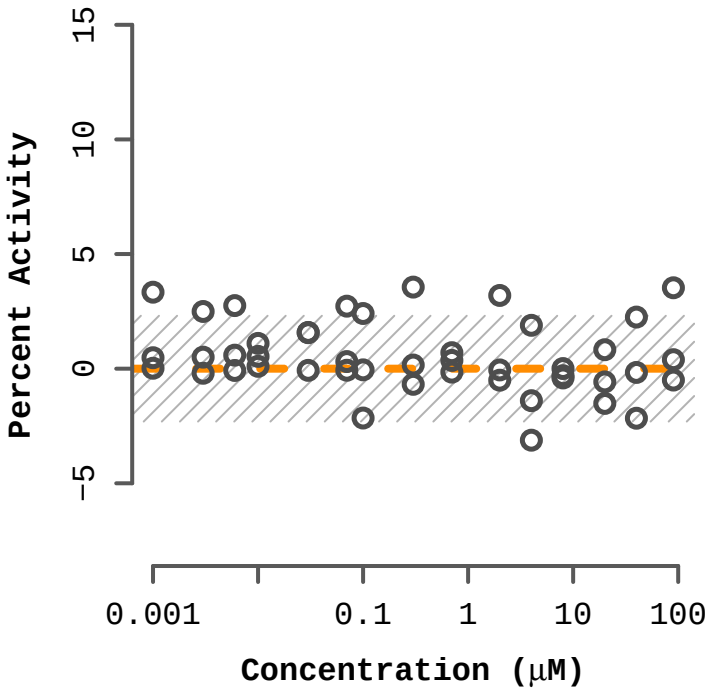
NAME: 2-Chlorobenzothiazole
CHID: 52289 CASRN: 615-20-3
SPID(S): Tox21_303729
M4ID: 12475459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.586 MAX_MED: 0.291 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

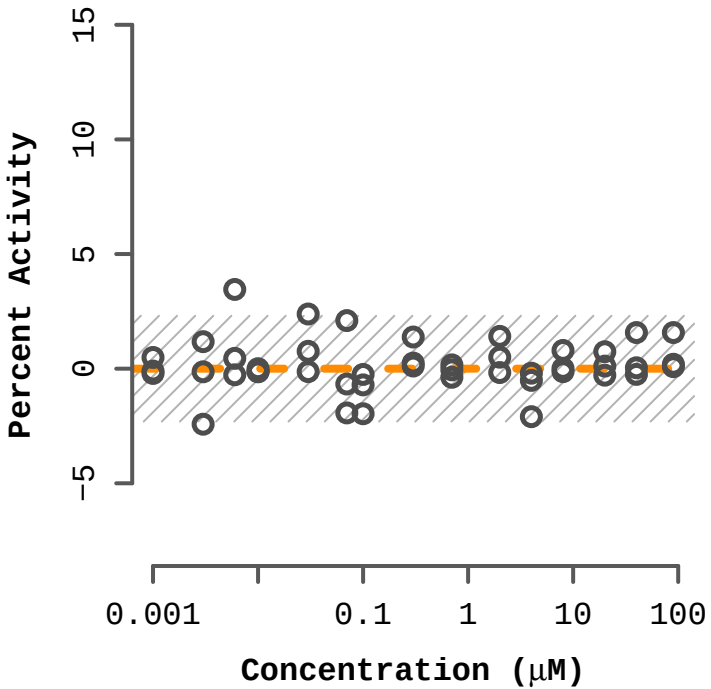
NAME: 1-Methylimidazole
CHID: 52291 **CASRN:** 616-47-7
SPID(S): Tox21_304006
M4ID: 12475182

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 1.28 **MAX_MED:** 1.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

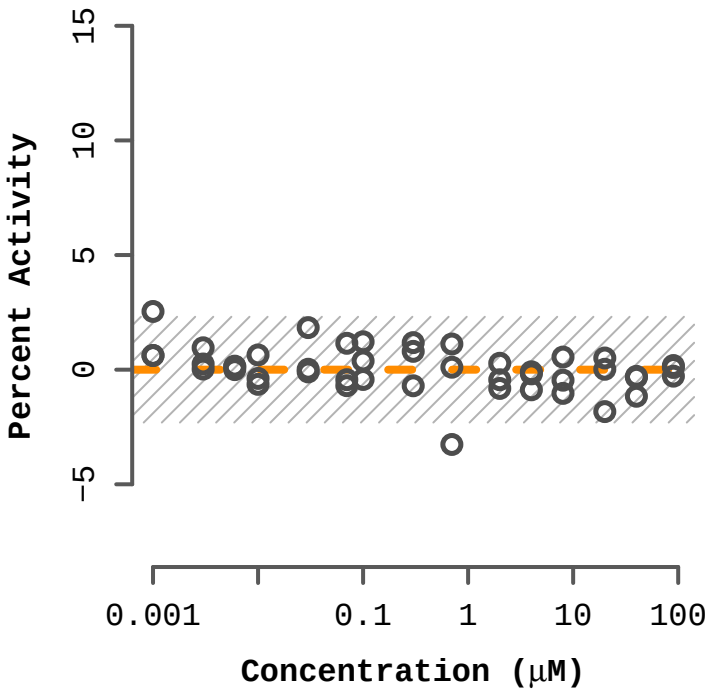
NAME: 2,2−Diethoxyacetophenone
CHID: 52294 **CASRN:** 6175−45−7
SPID(S): Tox21_303796
M4ID: 12475392

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 0.759 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

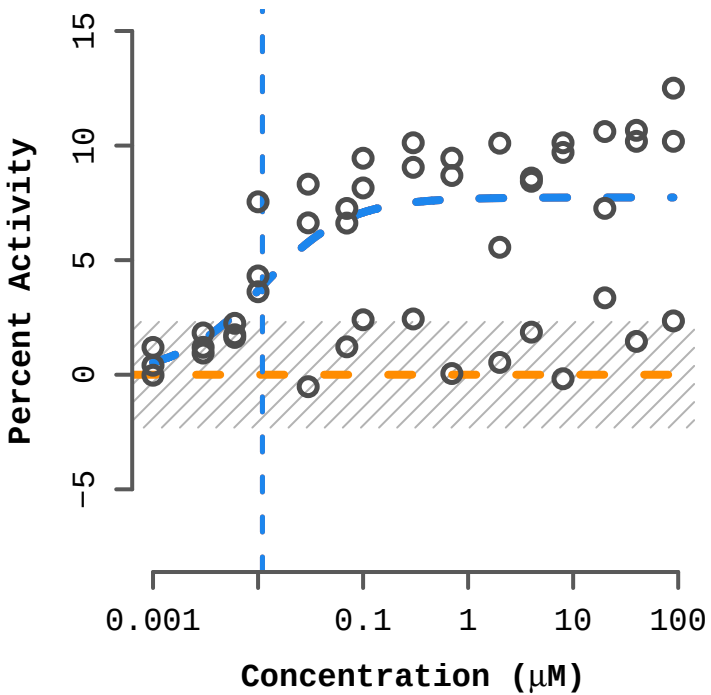
NAME: Furfurylamine
CHID: 52295 **CASRN:** 617-89-0
SPID(S): Tox21_304050
M4ID: 12475138

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 0.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Nitrobenzyl alcohol
CHID: 52298 CASRN: 619-73-8
SPID(S): Tox21_303773
M4ID: 12475415

HILL MODEL (in red):

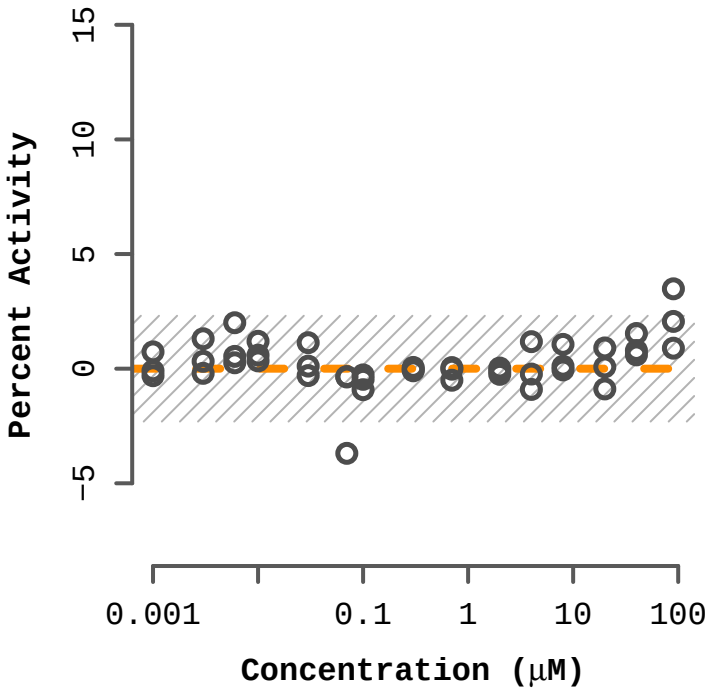
	tp	ga	gw
val:	7.74	-1.96	1.08
sd:	0.914	0.273	0.691

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.74	-1.96	1.08	3.94	12.6
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	305.4	247.78	251.78
PROB:	0	0.88	0.12
RMSE:	6.63	3.44	3.44

MAX_MEAN: 8.35 MAX_MED: 10.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

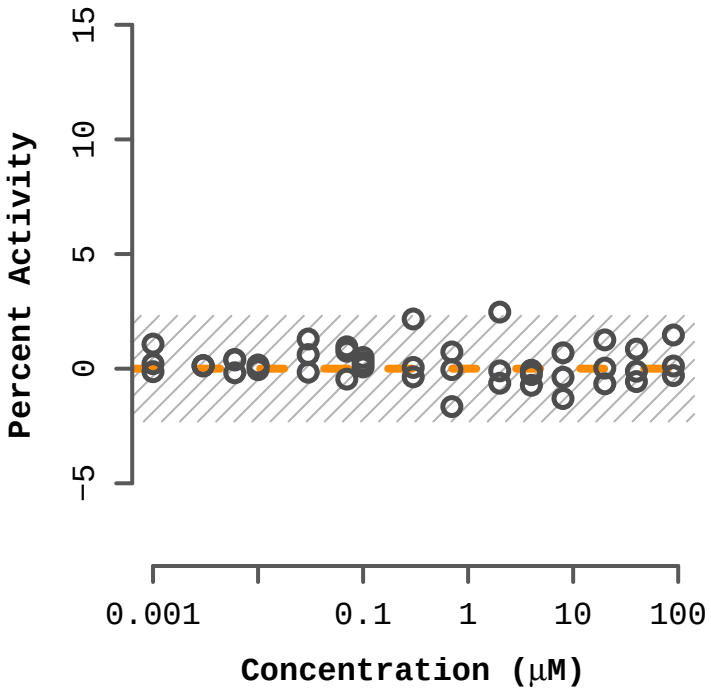
NAME: Cyclohexyl acetate
CHID: 52299 **CASRN:** 622-45-7
SPID(S): Tox21_303723
M4ID: 12475465

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.33	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 2.15 **MAX_MED:** 2.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

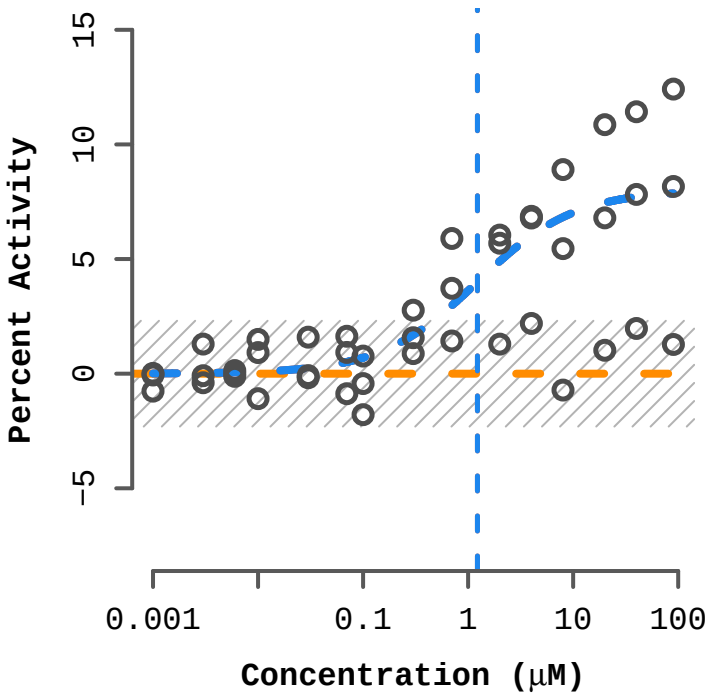
NAME: Ethyl glycinate hydrochloride
CHID: 52300 CASRN: 623-33-6
SPID(S): Tox21_304019
M4ID: 12475169

HILL MODEL: Not applicable.

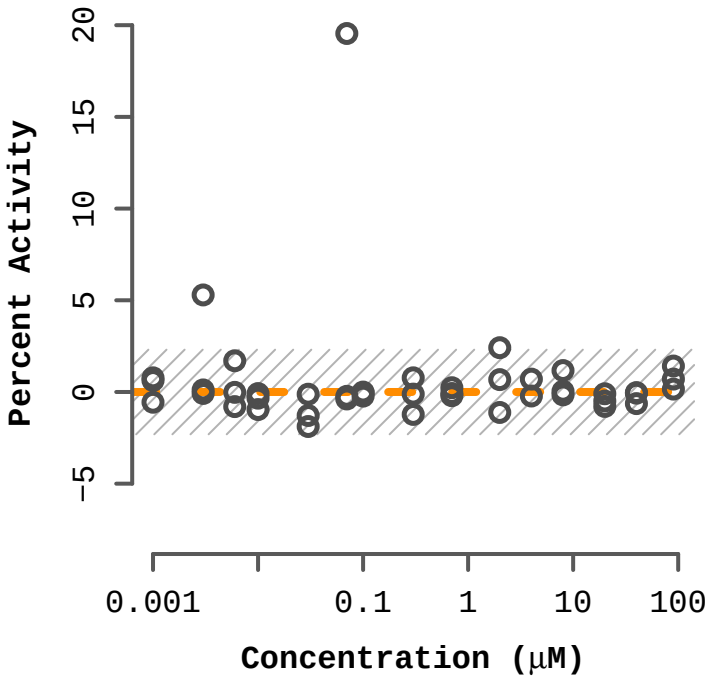
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.623 MAX_MED: 0.763 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Methylpent-2-enal
CHID:    52301   CASRN: 623-36-9
SPID(S): Tox21_303885
M4ID:    12475303

HILL MODEL (in red):
      tp       ga       gw
val:  8.01     0.0888   0.938
sd:   1.47     0.309    0.381

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  8.01     0.0887   0.938    3.02     7.91
sd:   1.47     0.309    0.381    2010     14900

      CNST        HILL        GNLS
AIC:  261.38      211.61      215.61
PROB: 0           0.88        0.12
RMSE: 4.57        2.54        2.54

MAX_MEAN: 7.29      MAX_MED: 8.17      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

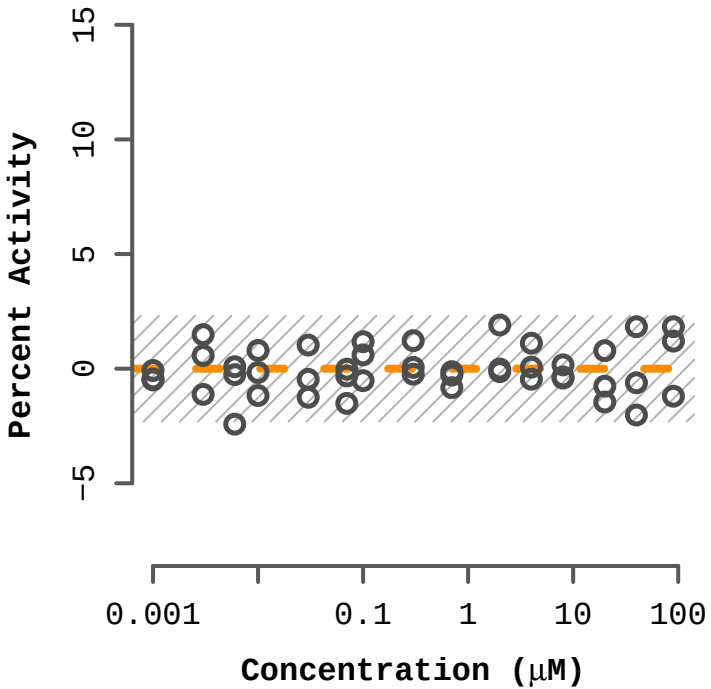
NAME: 1,3,5-Tribromobenzene
CHID: 52307 CASRN: 626-39-1
SPID(S): Tox21_303951
M4ID: 12475237

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.15	NA	NA

MAX_MEAN: 6.31 MAX_MED: 0.706 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

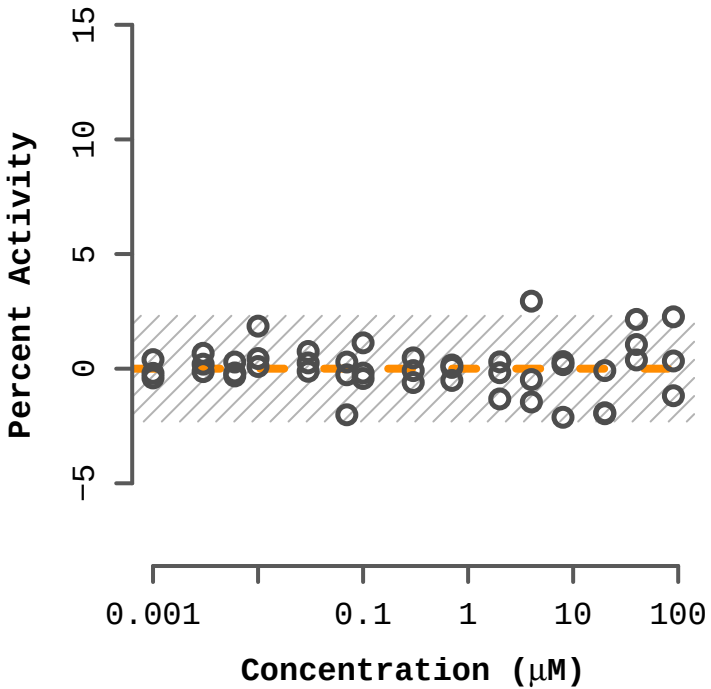
NAME: 6-Methyluracil
CHID: 52308 **CASRN:** 626-48-2
SPID(S): Tox21_304049
M4ID: 12475139

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.96	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.612 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

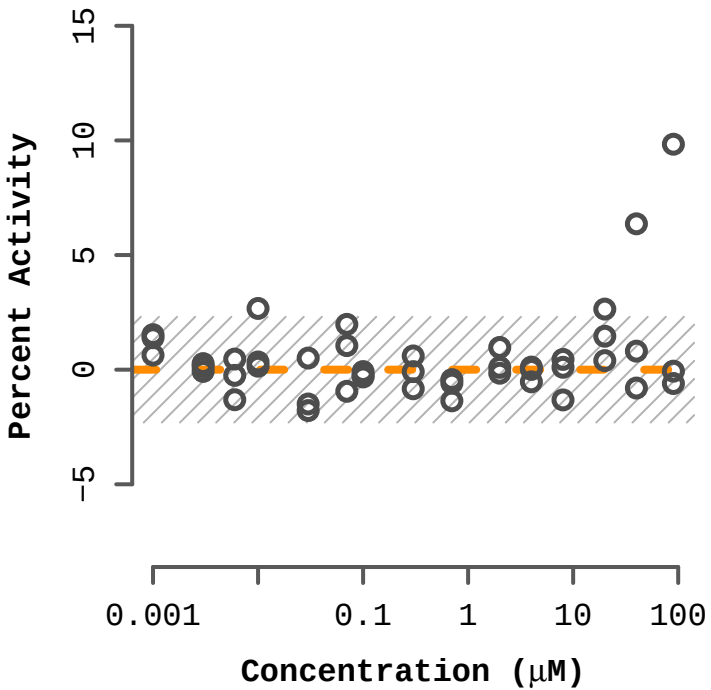
NAME: 3-Chloropyridine
CHID: 52309 **CASRN:** 626-60-8
SPID(S): Tox21_303995
M4ID: 12475193

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

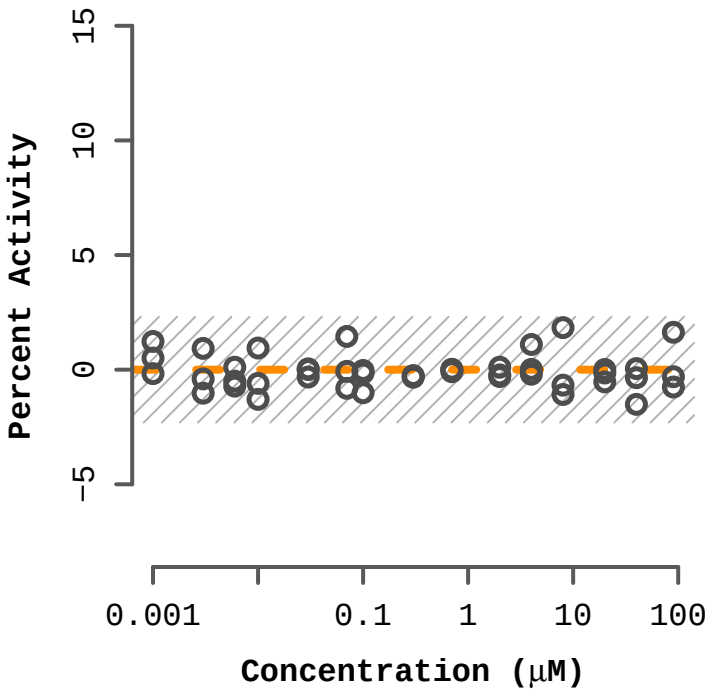
NAME: 4-Pyridinol
CHID: 52310 **CASRN:** 626-64-2
SPID(S): Tox21_303817
M4ID: 12475371

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.27	NA	NA
PROB:	1	NA	NA
RMSE:	2	NA	NA

MAX_MEAN: 3.06 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

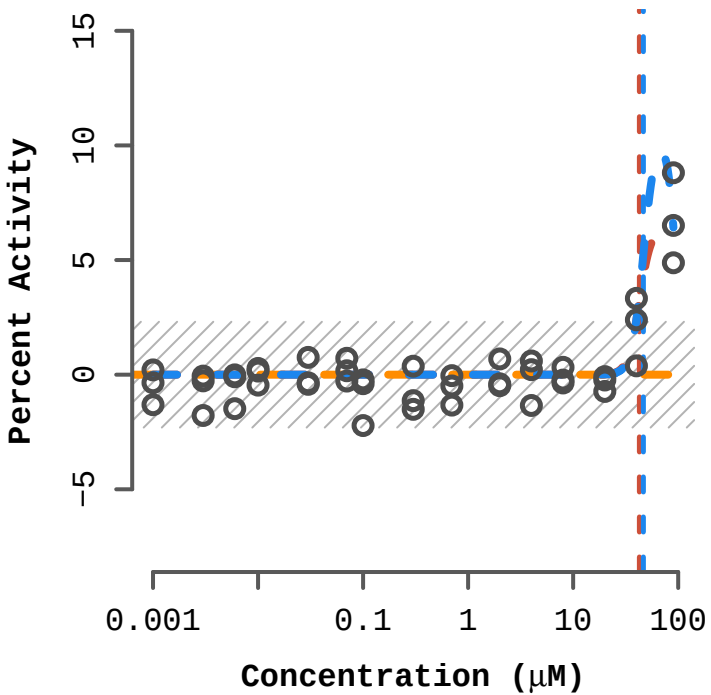
NAME: 1-Ethoxybutane
CHID: 52311 CASRN: 628-81-9
SPID(S): Tox21_303804
M4ID: 12475384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	101.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.73	NA	NA

MAX_MEAN: 0.524 MAX_MED: 0.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Chloro-3-nitroaniline
CHID: 52319 CASRN: 635-22-3
SPID(S): Tox21_303987
M4ID: 12475201

HILL MODEL (in red):

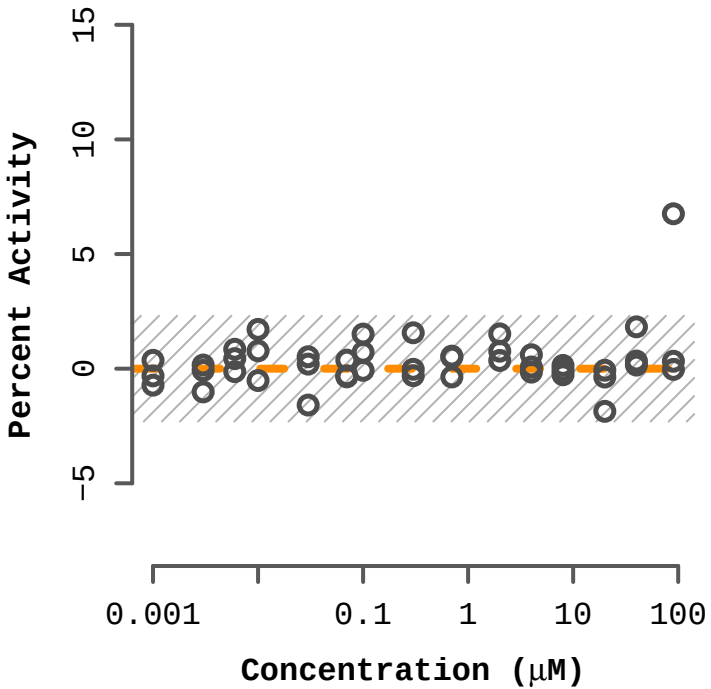
	tp	ga	gw
val:	6.44	1.63	8
sd:	0.678	0.0337	6.71

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.5	1.67	8	1.97	10.9
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	161.93	124.51	128.5
PROB:	0	0.88	0.12
RMSE:	2.03	0.91	0.91

MAX_MEAN: 6.73 MAX_MED: 6.51 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

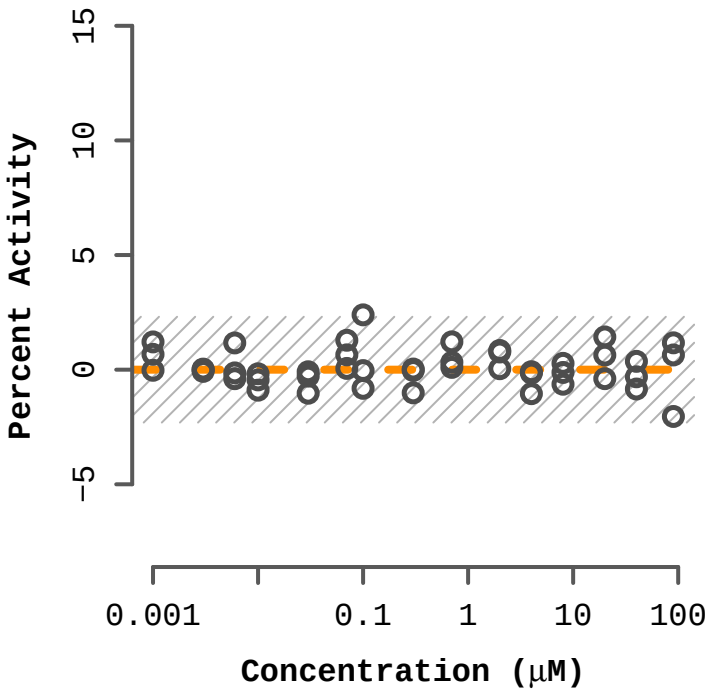
NAME: 2-Isopropylaniline
CHID: 52328 CASRN: 643-28-7
SPID(S): Tox21_303899
M4ID: 12475289

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.55	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 2.35 MAX_MED: 0.778 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

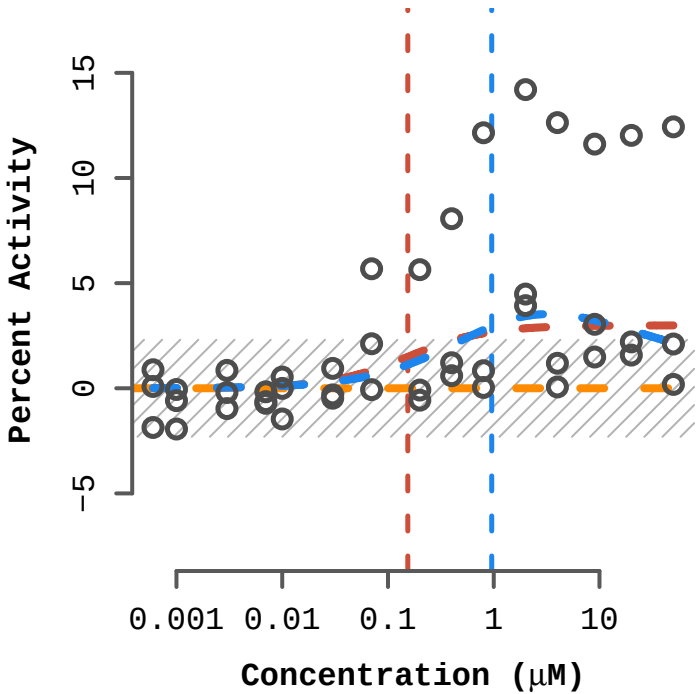
NAME: Thymine
CHID: 52342 CASRN: 65-71-4
SPID(S): Tox21_303929
M4ID: 12475259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.18	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.663 **MAX_MED:** 0.773 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3,5-Trimethylhydroquinone
CHID: 52446 CASRN: 700-13-0
SPID(S): Tox21_113944
M4ID: 12482287

HILL MODEL (in red):

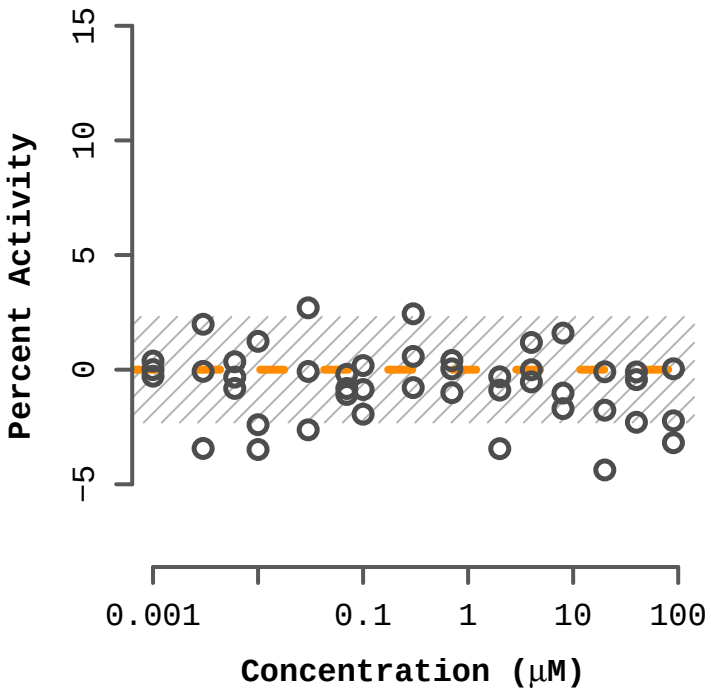
	tp	ga	gw
val:	2.99	−0.813	1.18
sd:	0.971	0.733	0.907

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.6	−0.0191	0.961	0.231	0.395
sd:	124	2.58	1.08	21.7	1.58

	CNST	HILL	GNLS
AIC:	260.66	247.56	251.13
PROB:	0	0.85	0.14
RMSE:	5.07	3.95	3.93

MAX_MEAN: 7.54 **MAX_MED:** 4.48 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

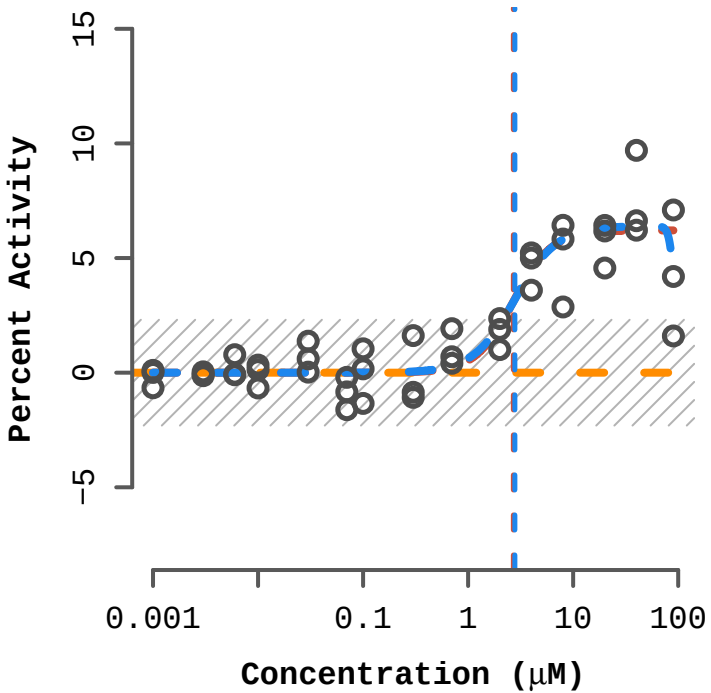
NAME: 1-Chloro-4-phenoxybenzene
CHID: 52447 **CASRN:** 7005-72-3
SPID(S): Tox21_304039
M4ID: 12475149

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.03	NA	NA
PROB:	1	NA	NA
RMSE:	1.69	NA	NA

MAX_MEAN: 0.746 **MAX_MED:** 0.579 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Phenylbenzimidazole
CHID: 52460 CASRN: 716-79-0
SPID(S): Tox21_303711
M4ID: 12475477

HILL MODEL (in red):

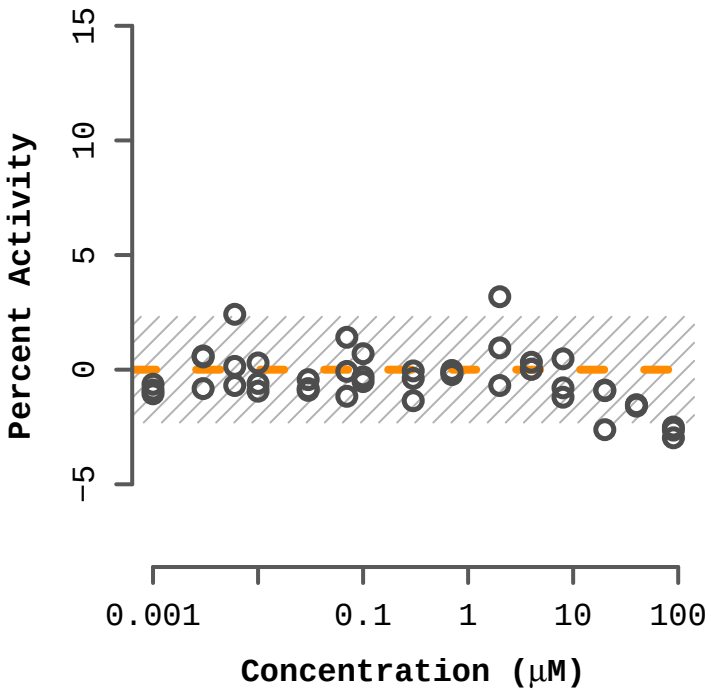
	tp	ga	gw
val:	6.21	0.431	2.39
sd:	0.389	0.0565	0.951

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.4	0.445	2.18	1.97	17.4
sd:	0.417	0.0602	0.845	0.0196	19.8

	CNST	HILL	GNLS
AIC:	236.85	145.62	145.89
PROB:	0	0.53	0.47
RMSE:	3.42	1.25	1.14

MAX_MEAN: 7.52 MAX_MED: 6.63 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

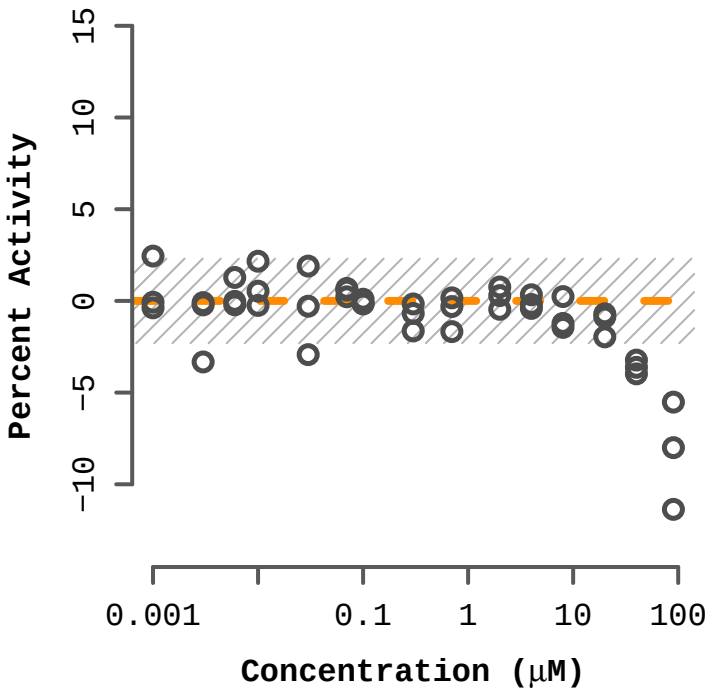
NAME: 2-Amino-5-chlorobenzophenone
CHID: 52463 **CASRN:** 719-59-5
SPID(S): Tox21_304017
M4ID: 12475171

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.26	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 0.952 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

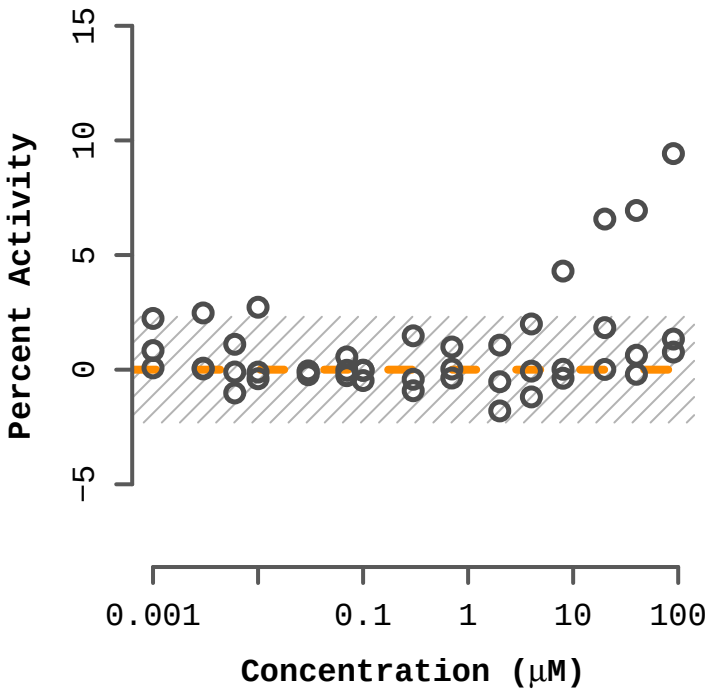
NAME: Diphenyl(2,4,6-trimethylbenzoyl)phosphine oxid
CHID: 52502 CASRN: 75980-60-8
SPID(S): Tox21_303757
M4ID: 12475431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	194.55	NA	NA
PROB:	1	NA	NA
RMSE:	2.65	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 0.589 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

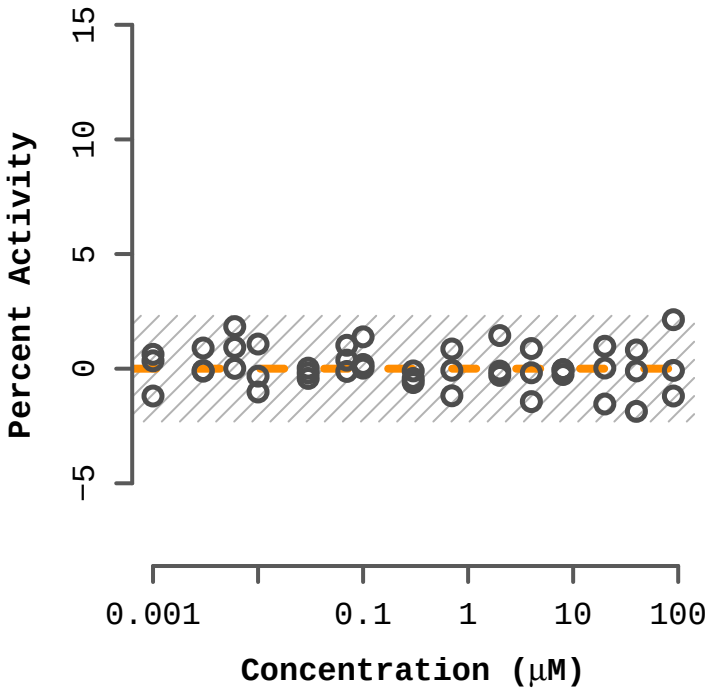
NAME: 2-Methylpent-1-ene
CHID: 52505 **CASRN:** 763-29-1
SPID(S): Tox21_303811
M4ID: 12475377

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.32	NA	NA
PROB:	1	NA	NA
RMSE:	2.32	NA	NA

MAX_MEAN: 3.84 **MAX_MED:** 1.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

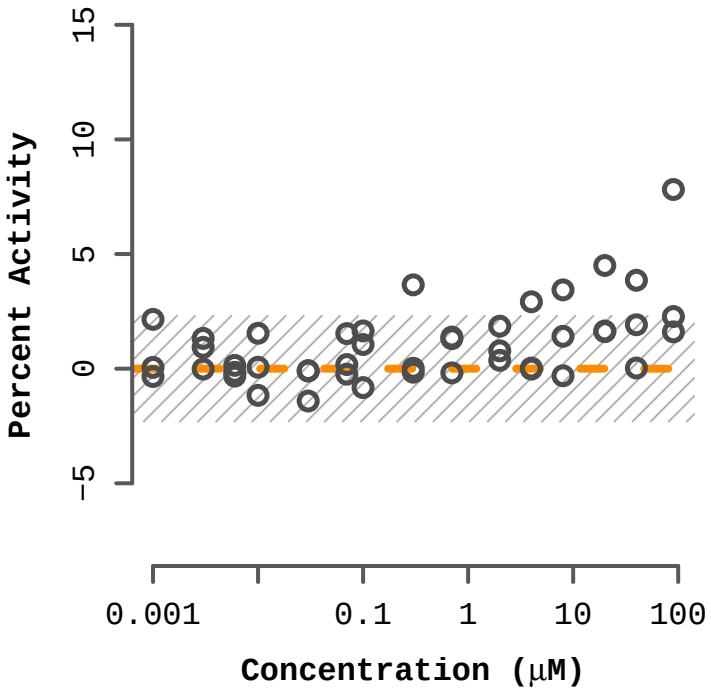
NAME: 3-Methylbut-3-en-1-ol
CHID: 52506 CASRN: 763-32-6
SPID(S): Tox21_303733
M4ID: 12475455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.928 MAX_MED: 0.931 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

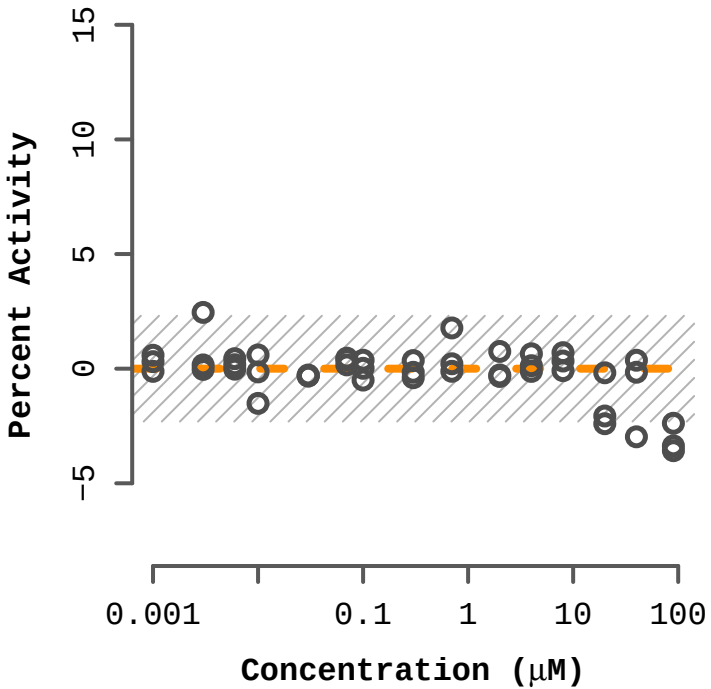
NAME: 4-Hydroxybenzonitrile
CHID: 52509 **CASRN:** 767-00-0
SPID(S): Tox21_303855
M4ID: 12475333

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.85	NA	NA
PROB:	1	NA	NA
RMSE:	1.98	NA	NA

MAX_MEAN: 3.9 **MAX_MED:** 2.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

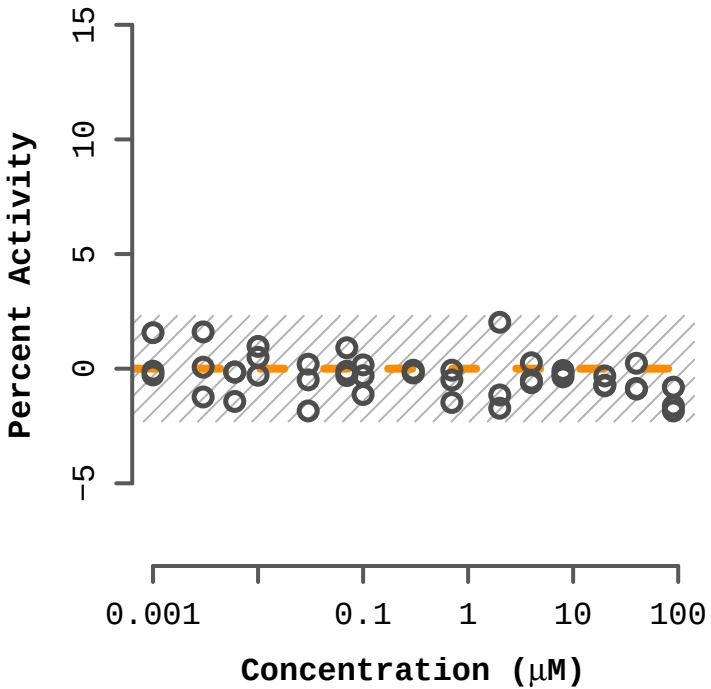
NAME: Trityl chloride
CHID: 52511 **CASRN:** 76-83-5
SPID(S): Tox21_303949
M4ID: 12475239

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 0.863 **MAX_MED:** 0.397 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

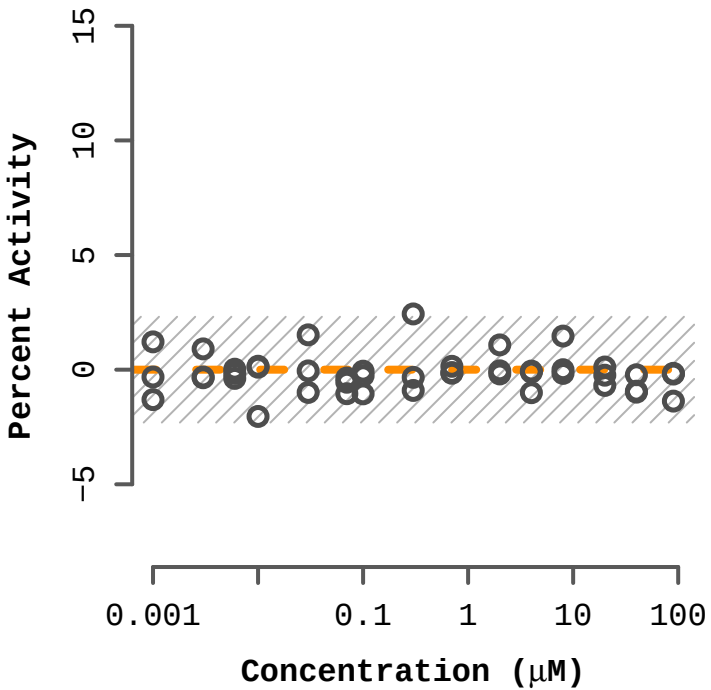
NAME: 2-Methoxy-4-vinylphenol
CHID: 52529 **CASRN:** 7786-61-0
SPID(S): Tox21_304024
M4ID: 12475164

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.62	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.398 **MAX_MED:** 0.497 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

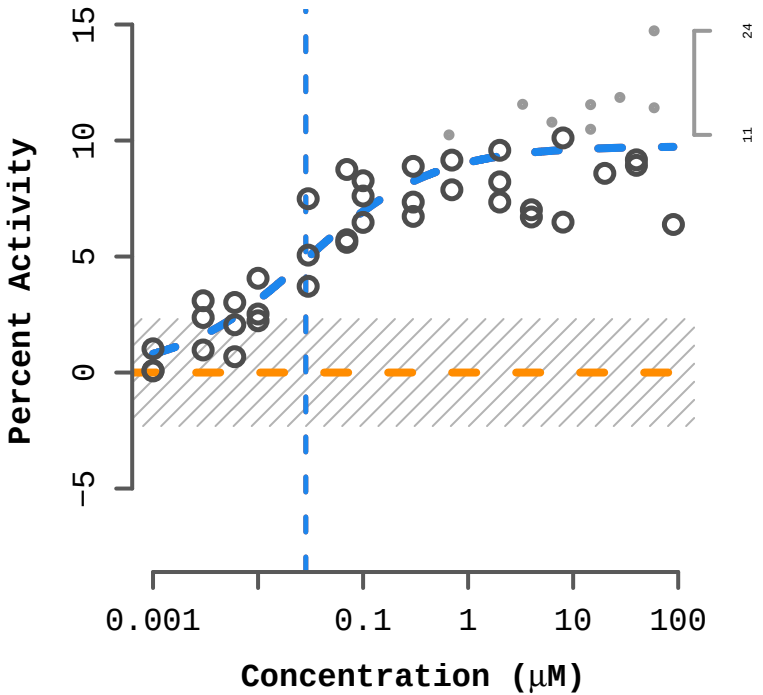
NAME: Dibutyl butylphosphonate
CHID: 52536 **CASRN:** 78-46-6
SPID(S): Tox21_303718
M4ID: 12475470

HILL MODEL: Not applicable.

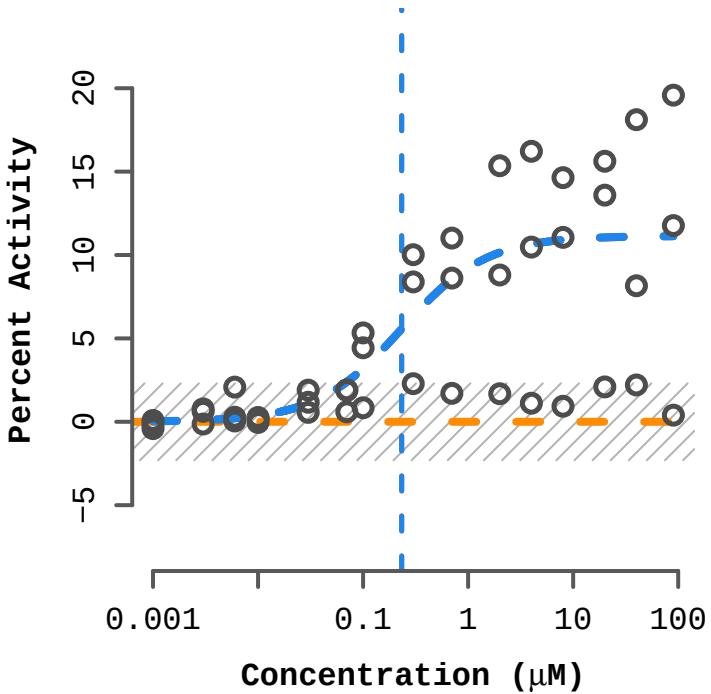
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.435 **MAX_MED:** 0.11 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Diethoxy(dimethyl)silane
CHID:    52538   CASRN: 78-62-6
SPID(S): Tox21_303834
M4ID:    12475354  BRK

HILL MODEL (in red):
      tp       ga       gw
val:  9.76     -1.55    0.719
sd:   0.791    0.185    0.187

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  9.76     -1.55    0.719    2.61     15.7
sd:   0.791    0.185    0.187    3560     84700

      CNST        HILL        GNLS
AIC:  328.15      213.05      217.05
PROB: 0           0.88        0.12
RMSE: 8.65        2.99        2.99

MAX_MEAN: 14.9      MAX_MED: 14.2      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1-Bromo-2-methylpropane
CHID: 52539 CASRN: 78-77-3
SPID(S): Tox21_303878
M4ID: 12475310

HILL MODEL (in red):

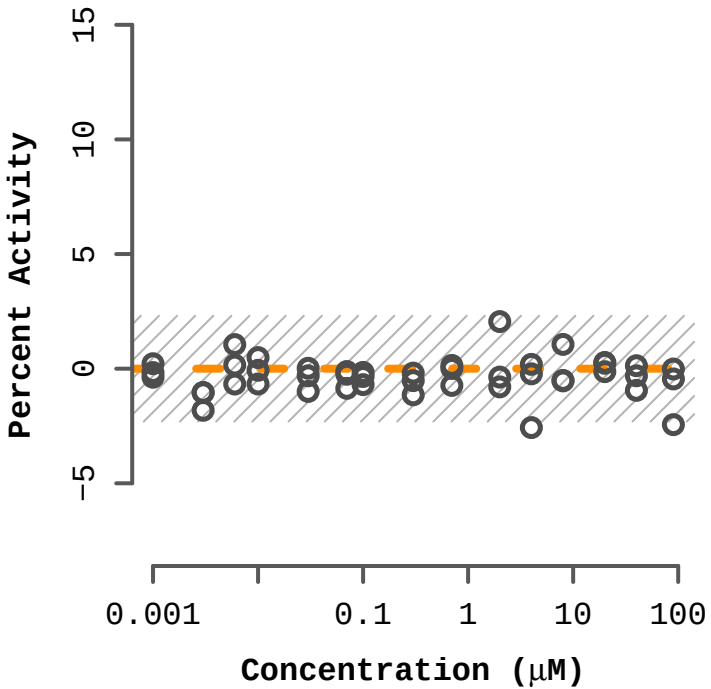
	tp	ga	gw
val:	11.1	−0.633	1.08
sd:	1.75	0.289	0.565

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.1	−0.633	1.08	3.57	6.33
sd:	1.75	0.289	0.565	28000	110000

	CNST	HILL	GNLS
AIC:	313.65	265.91	269.91
PROB:	0	0.88	0.12
RMSE:	7.92	4.41	4.41

MAX_MEAN: 10.6 MAX_MED: 13.6 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

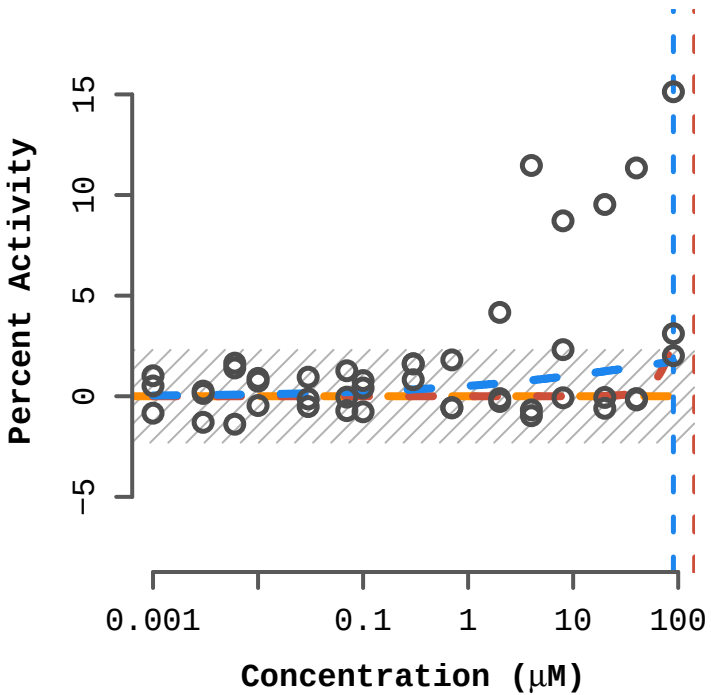
NAME: 2-Methylpropanoyl chloride
CHID: 52542 **CASRN:** 79-30-1
SPID(S): Tox21_303786
M4ID: 12475402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.72	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.299 **MAX_MED:** 0.236 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl toluene-4-sulfonate
CHID: 52550 CASRN: 80-48-8
SPID(S): Tox21_303790
M4ID: 12475398

HILL MODEL (in red):

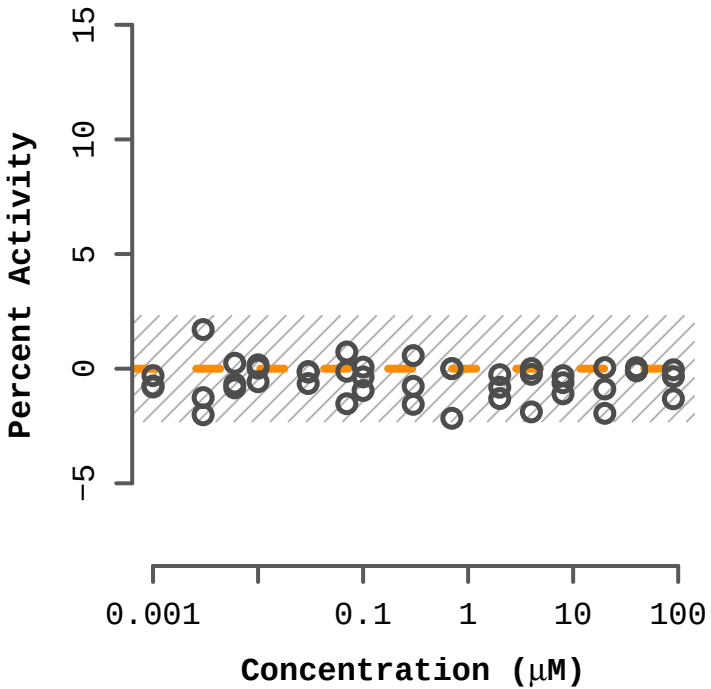
	tp	ga	gw
val:	18.1	2.16	3.56
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.47	1.95	0.389	3.86	5.17
sd:	16.1	7.32	0.527	17800	48500

	CNST	HILL	GNLS
AIC:	221.39	219.95	225.57
PROB:	0.32	0.65	0.04
RMSE:	4	3.73	3.58

MAX_MEAN: 6.75 MAX_MED: 3.11 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

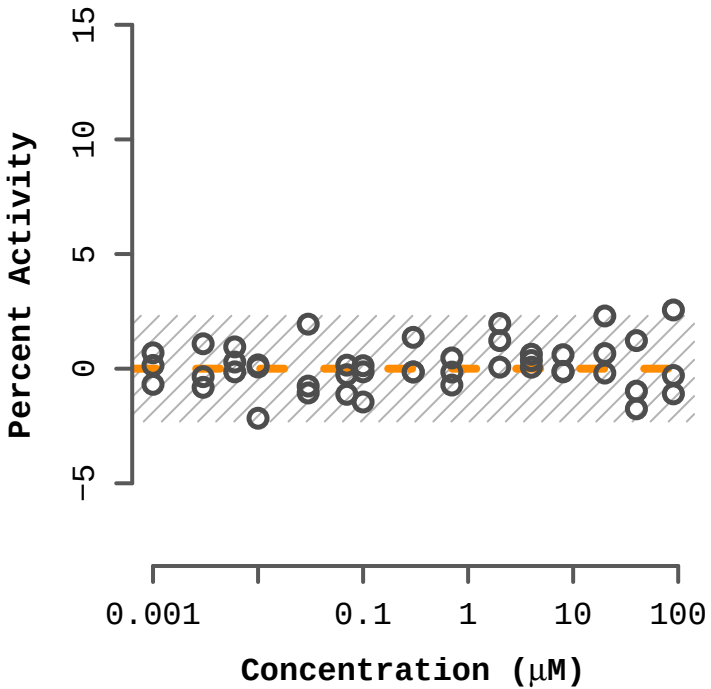
NAME: Naphthalene−1,8:4,5−tetracarboxylic dianhydrid
CHID: 52554 CASRN: 81−30−1
SPID(S): Tox21_304005
M4ID: 12475183

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.92	NA	NA

MAX_MEAN: −0.0441 MAX_MED: 0.0243 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

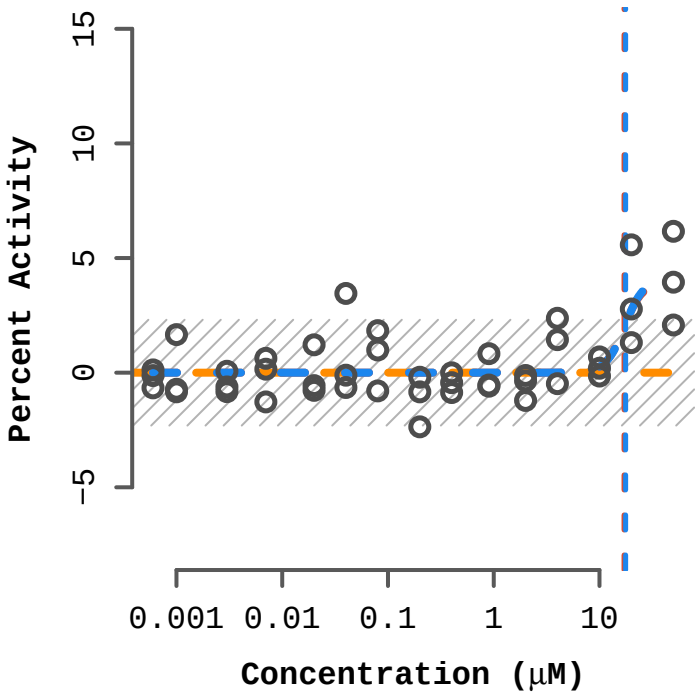
NAME: Bis(2-chloroethyl)amine hydrochloride
CHID: 52567 **CASRN:** 821-48-7
SPID(S): Tox21_303731
M4ID: 12475457

HILL MODEL: Not applicable.

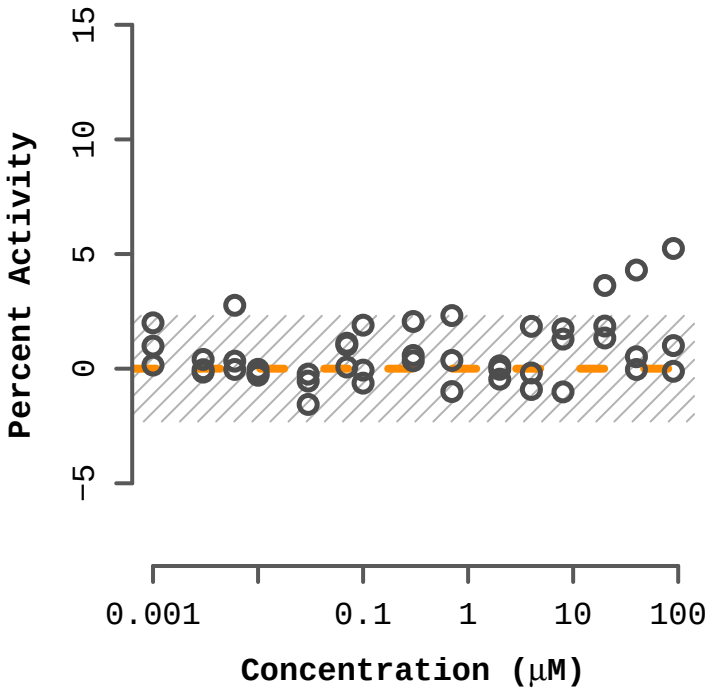
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 1.23 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    1-Chloroanthraquinone
CHID:    52571   CASRN: 82-44-0
SPID(S): Tox21_303937
M4ID:    12475251

HILL MODEL (in red):
      tp       ga       gw
val:  3.95     1.23     4.99
sd:   0.889    0.0926   3.58

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.14     1.25     4.86     3.29     0.331
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  170.92      150.4       154.4
PROB: 0           0.88        0.12
RMSE: 1.79        1.2         1.2

MAX_MEAN: 4.07      MAX_MED: 3.95      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

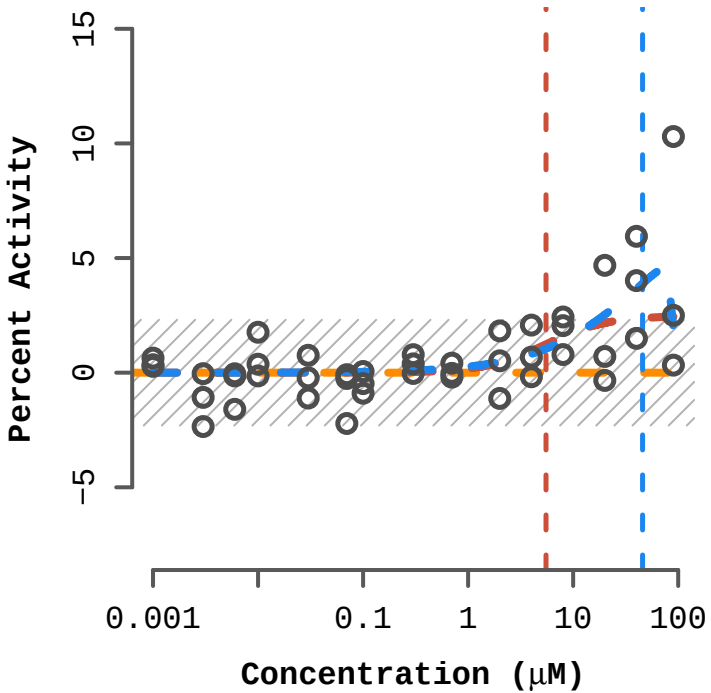
NAME: 2,6-Dibromo-4-nitroaniline
CHID: 52573 **CASRN:** 827-94-1
SPID(S): Tox21_303713
M4ID: 12475475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.56	NA	NA

MAX_MEAN: 2.28 **MAX_MED:** 1.86 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 1,5-Dihydroxynaphthalene
CHID: 52574 CASRN: 83-56-7
SPID(S): Tox21_303746
M4ID: 12475442

HILL MODEL (in red):

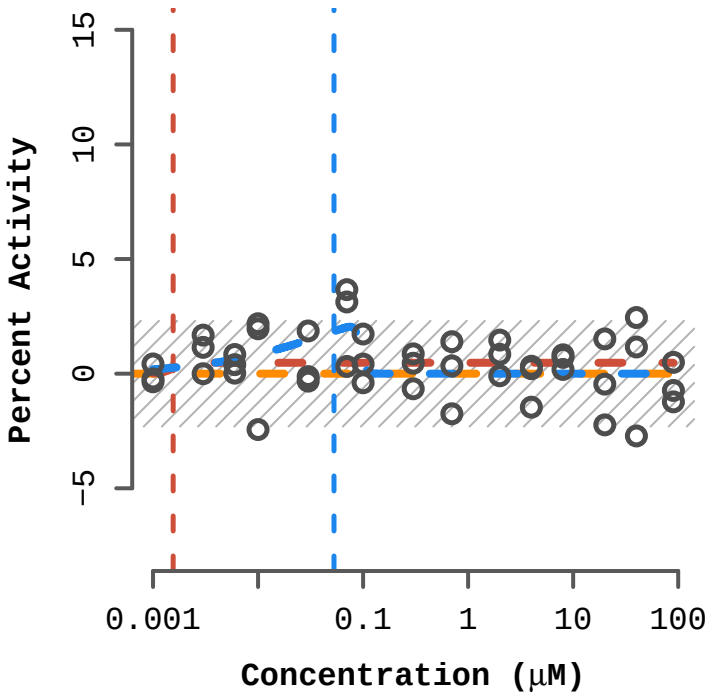
	tp	ga	gw
val:	2.48	0.741	1.51
sd:	0.911	0.342	1.45

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.78	1.66	0.879	1.94	16.7
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	180.52	165.66	168.18
PROB:	0	0.78	0.22
RMSE:	2.27	1.69	1.7

MAX_MEAN: 4.38 MAX_MED: 4.02 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2,3-Dichloro-5,6-dicyano-p-benzoquinone
CHID: 52577 CASRN: 84-58-2
SPID(S): Tox21_304048
M4ID: 12475140

HILL MODEL (in red):

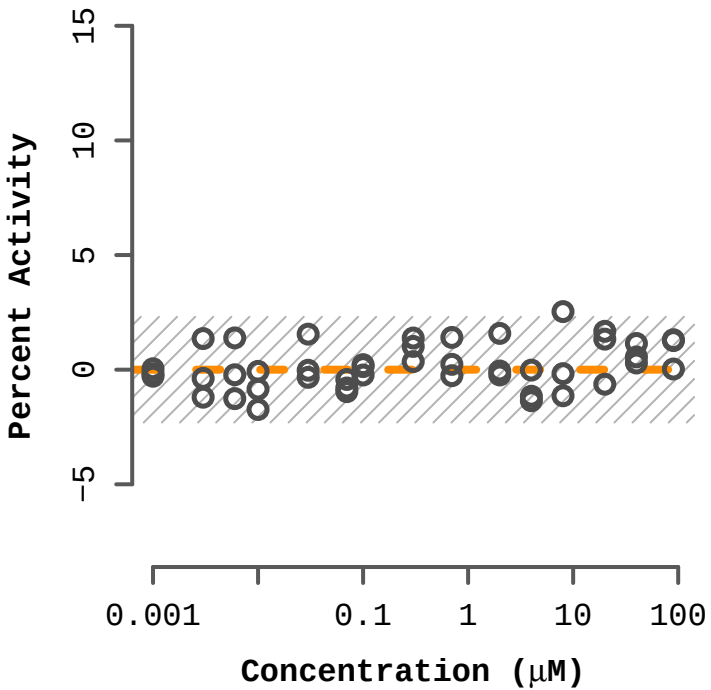
	tp	ga	gw
val:	0.475	−2.81	8
sd:	0.192	0.681	22.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.7	−1.28	0.732	−1.03	18
sd:	9.38	2.51	0.48	0.0587	28.1

	CNST	HILL	GNLS
AIC:	160.81	161.13	162.13
PROB:	0.42	0.36	0.22
RMSE:	1.4	1.33	1.24

MAX_MEAN: 2.37 MAX_MED: 3.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

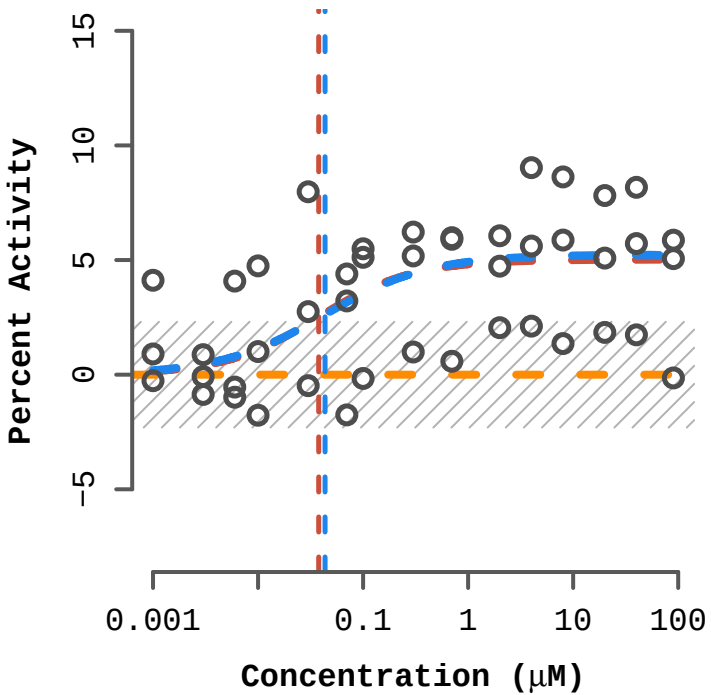
NAME: 9-Ethylcarbazole
CHID: 52585 **CASRN:** 86-28-2
SPID(S): Tox21_303819
M4ID: 12475369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.917 **MAX_MED:** 1.33 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl 2-methylbutyrate
CHID: 52587 CASRN: 868-57-5
SPID(S): Tox21_303742
M4ID: 12475446

HILL MODEL (in red):

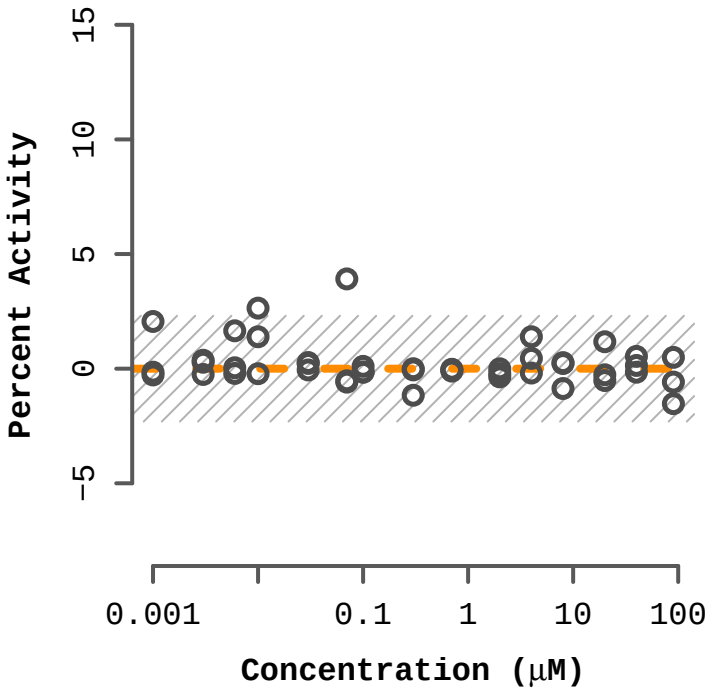
	tp	ga	gw
val:	5.02	−1.42	0.965
sd:	0.689	0.36	0.67

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.24	−1.36	0.87	2	13
sd:	0.869	0.402	0.642	0.287	78.7

	CNST	HILL	GNLS
AIC:	269.77	226.32	230
PROB:	0	0.86	0.14
RMSE:	4.49	2.61	2.59

MAX_MEAN: 5.59 **MAX_MED:** 5.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

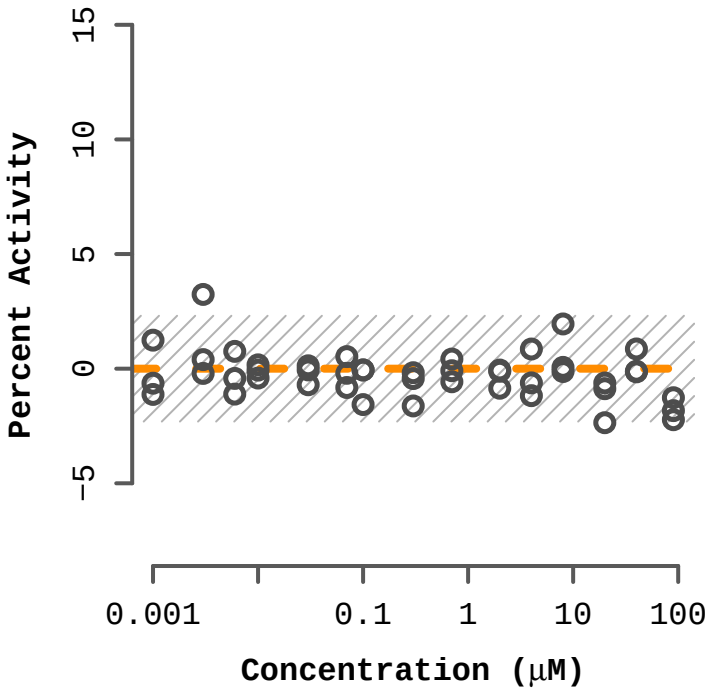
NAME: 4,7-Dichloroquinoline
CHID: 52590 **CASRN:** 86-98-6
SPID(S): Tox21_303863
M4ID: 12475325

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.39 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

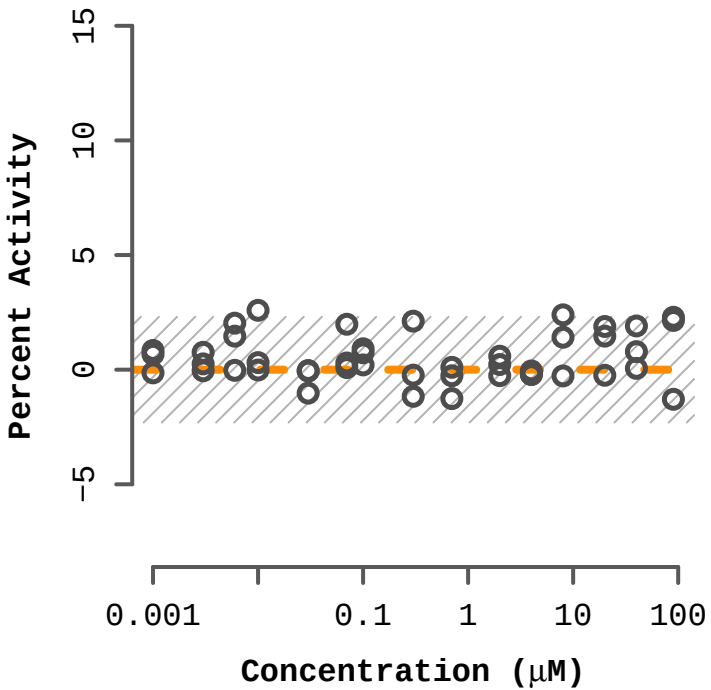
NAME: Diethyl ethoxymethylenemalonate
CHID: 52591 **CASRN:** 87-13-8
SPID(S): Tox21_303975
M4ID: 12475213

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.41	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.398 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

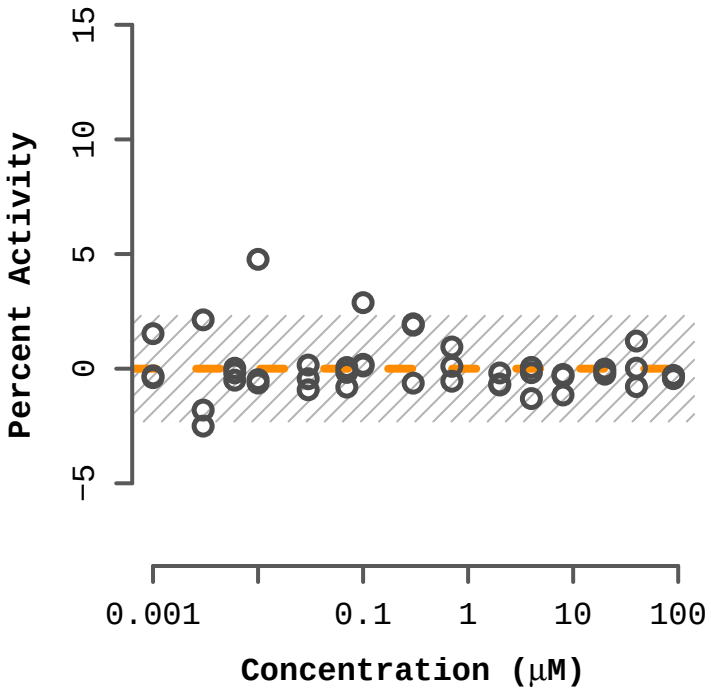
NAME: 2-Chlorobenzonitrile
CHID: 52593 **CASRN:** 873-32-5
SPID(S): Tox21_303775
M4ID: 12475413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 2.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

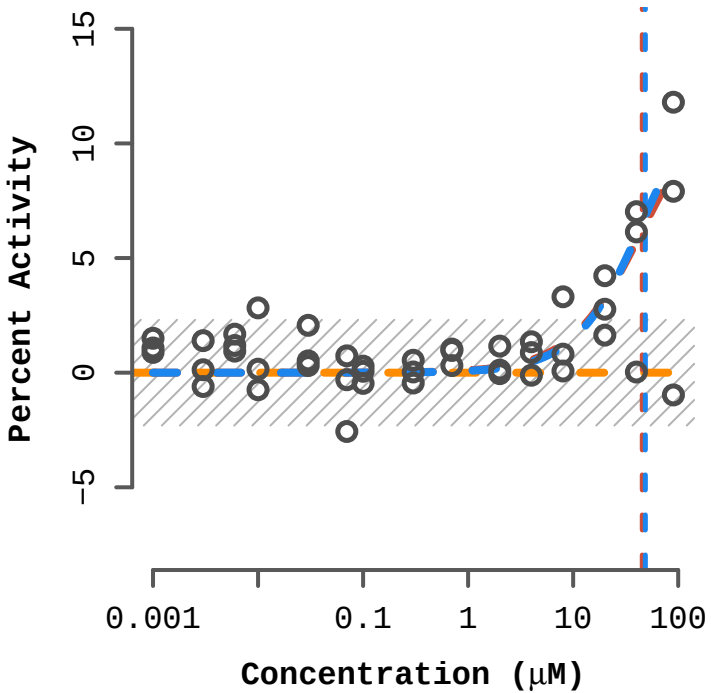
NAME: Phthalide
CHID: 52594 CASRN: 87-41-2
SPID(S): Tox21_303762
M4ID: 12475426

HILL MODEL: Not applicable.

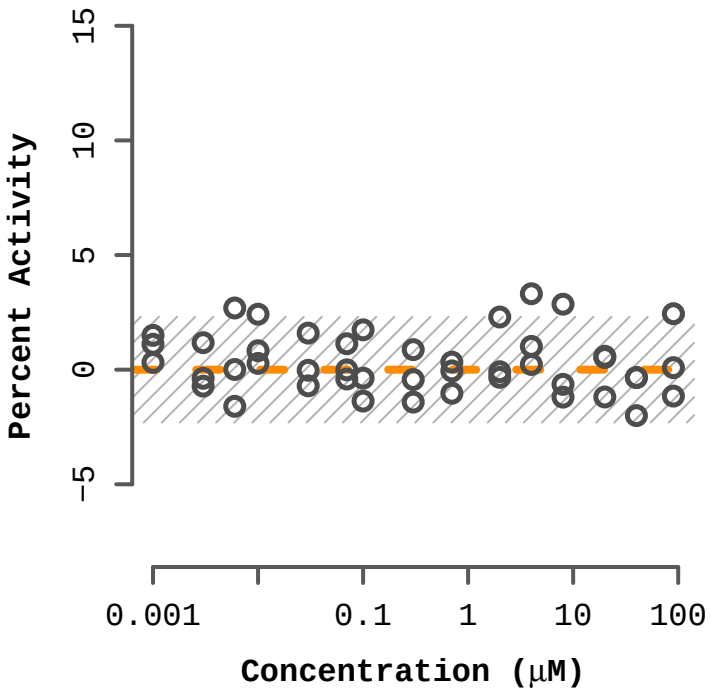
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.35	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.22 MAX_MED: 1.9 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    p-Toluoyl chloride
CHID:    52595   CASRN: 874-60-2
SPID(S): Tox21_303832
M4ID:    12475356

HILL MODEL (in red):
      tp       ga       gw
val:  12.5     1.66     1.26
sd:   7.77     0.479    0.674

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  13.7     1.69     1.33     2.05     9.28
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  201.55      174.48      178.23
PROB: 0           0.87        0.13
RMSE: 2.86        2.03        2.02

MAX_MEAN: 6.25      MAX_MED: 7.91      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

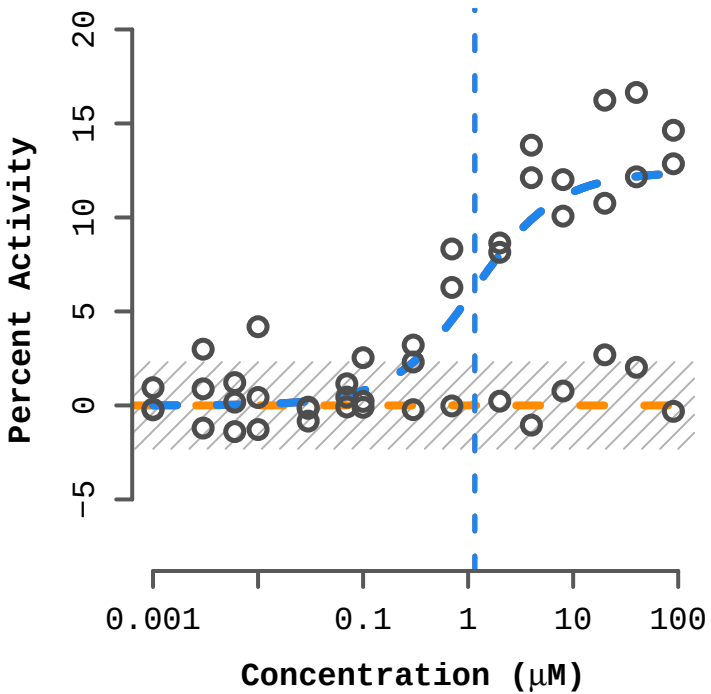
NAME: 4-Anisonitrile
CHID: 52596 **CASRN:** 874-90-8
SPID(S): Tox21_304041
M4ID: 12475147

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.9	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.52 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Diethyl L-tartrate
CHID: 52597 CASRN: 87-91-2
SPID(S): Tox21_303884
M4ID: 12475304

HILL MODEL (in red):

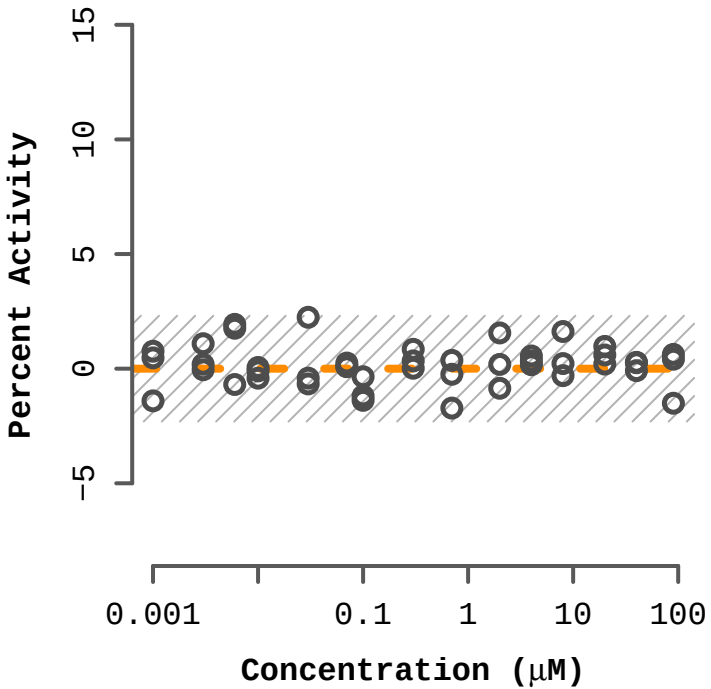
	tp	ga	gw
val:	12.4	0.0637	1.1
sd:	1.49	0.212	0.392

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.4	0.0637	1.1	3.15	6.33
sd:	1.49	0.212	0.392	933	4920

	CNST	HILL	GNLS
AIC:	297.95	252.52	256.52
PROB:	0	0.88	0.12
RMSE:	6.82	4.19	4.19

MAX_MEAN: 10.3 MAX_MED: 12.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

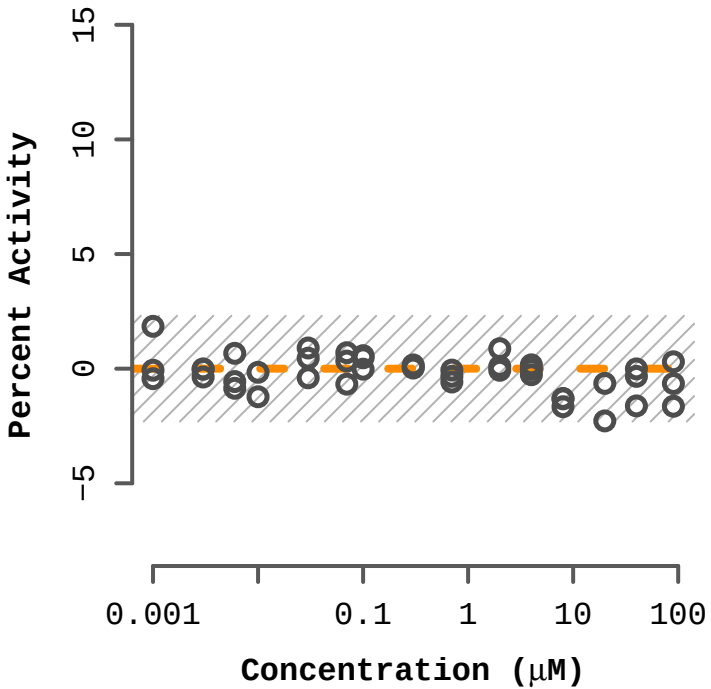
NAME: Diethylcarbamoyl chloride
CHID: 52598 CASRN: 88-10-8
SPID(S): Tox21_303825
M4ID: 12475363

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.76	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

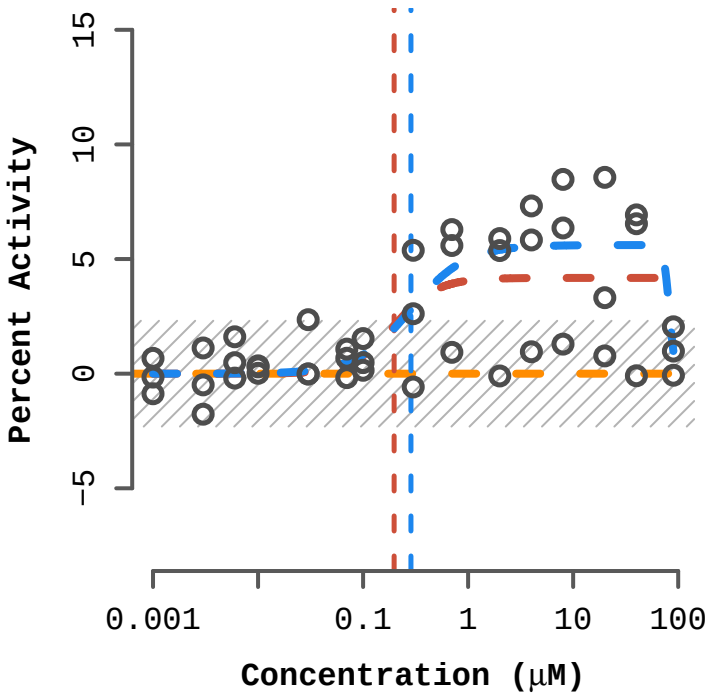
NAME: 1,4-Dichloro-2-nitrobenzene
CHID: 52602 **CASRN:** 89-61-2
SPID(S): Tox21_303735
M4ID: 12475453

HILL MODEL: Not applicable.

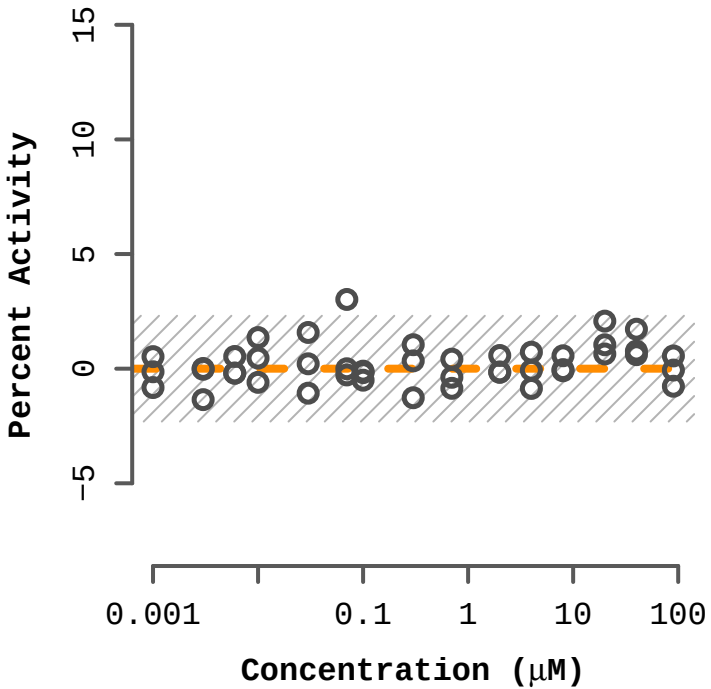
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.449 **MAX_MED:** 0.476 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2,4-Dichlorobenzoyl chloride
CHID:    52603   CASRN: 89-75-8
SPID(S): Tox21_303889
M4ID:    12475299

HILL MODEL (in red):
      tp       ga       gw
val:  4.18     -0.705   2.16
sd:   0.774    0.236    1.49

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.61     -0.544   1.67     1.91     16.6
sd:   0.732    0.196    0.978    0.115    48.5

      CNST        HILL        GNLS
AIC:  240.78      211.77      204.33
PROB: 0           0.02        0.98
RMSE: 3.57        2.23        2.15

MAX_MEAN: 5.37      MAX_MED: 6.54      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

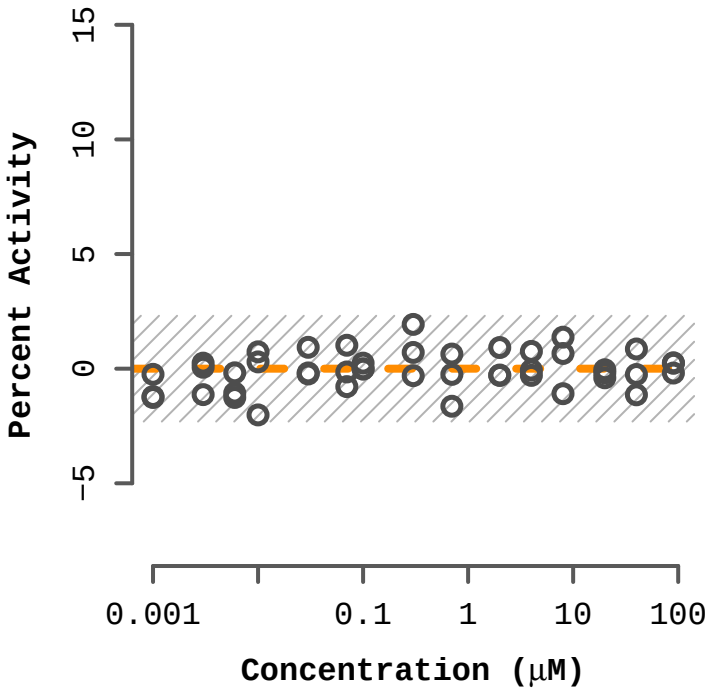
NAME: 2,6-Dimethoxyphenol
CHID: 52607 **CASRN:** 91-10-1
SPID(S): Tox21_303953
M4ID: 12475235

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.22	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

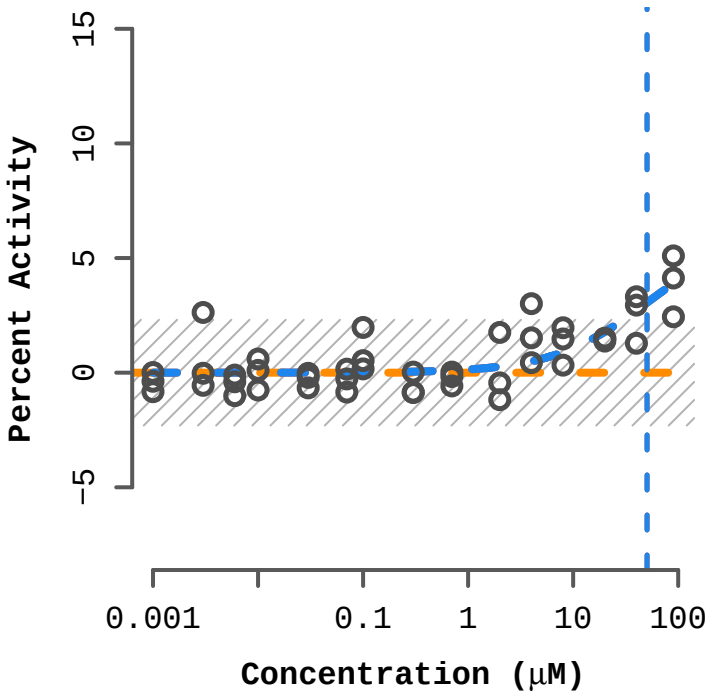
NAME: N,N−Diethyl−m−toluidine
CHID: 52610 CASRN: 91−67−8
SPID(S): Tox21_304015
M4ID: 12475173

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.41	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.78 MAX_MED: 0.71 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4'−Acetylbiphenyl
CHID: 52619 CASRN: 92−91−1
SPID(S): Tox21_303801
M4ID: 12475387

HILL MODEL (in red):

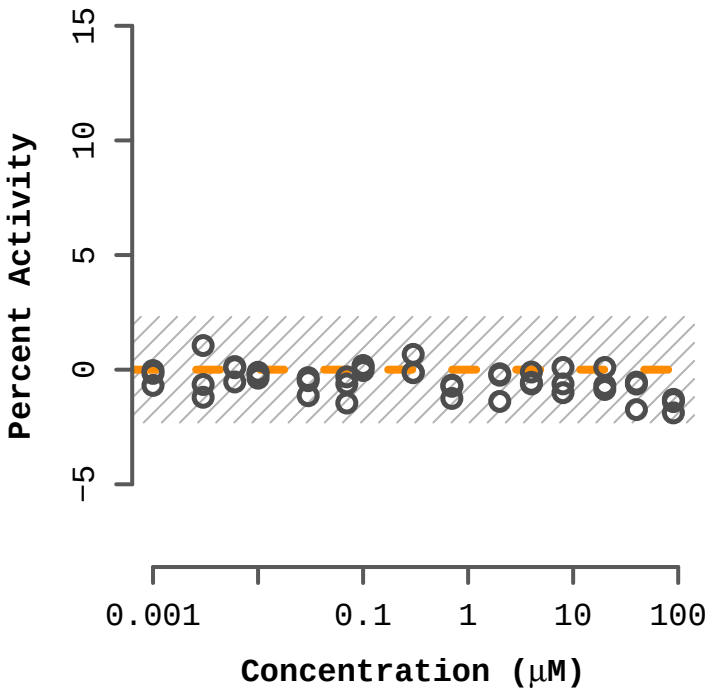
	tp	ga	gw
val:	6.12	1.7	0.958
sd:	3.14	0.469	0.32

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.12	1.7	0.958	3.82	6.05
sd:	3.14	0.469	0.32	73600	240000

	CNST	HILL	GNLS
AIC:	167.69	126.4	130.4
PROB:	0	0.88	0.12
RMSE:	1.61	0.92	0.92

MAX_MEAN: 3.89 MAX_MED: 4.13 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

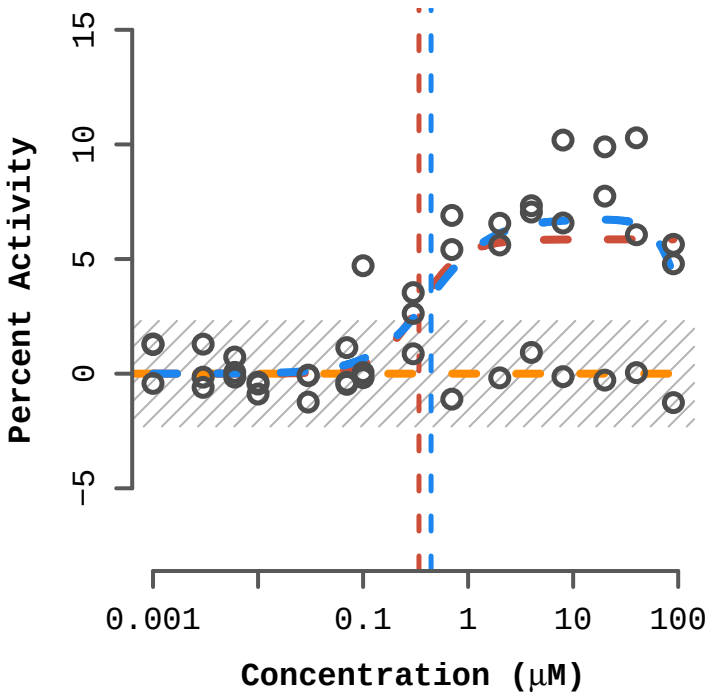
NAME: 2,5-Dimethoxybenzaldehyde
CHID: 52620 **CASRN:** 93-02-7
SPID(S): Tox21_303938
M4ID: 12475250

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.58	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.141 **MAX_MED:** 0.105 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4-Prop-1-enylveratrole
CHID: 52621 CASRN: 93-16-3
SPID(S): Tox21_303830
M4ID: 12475358

HILL MODEL (in red):

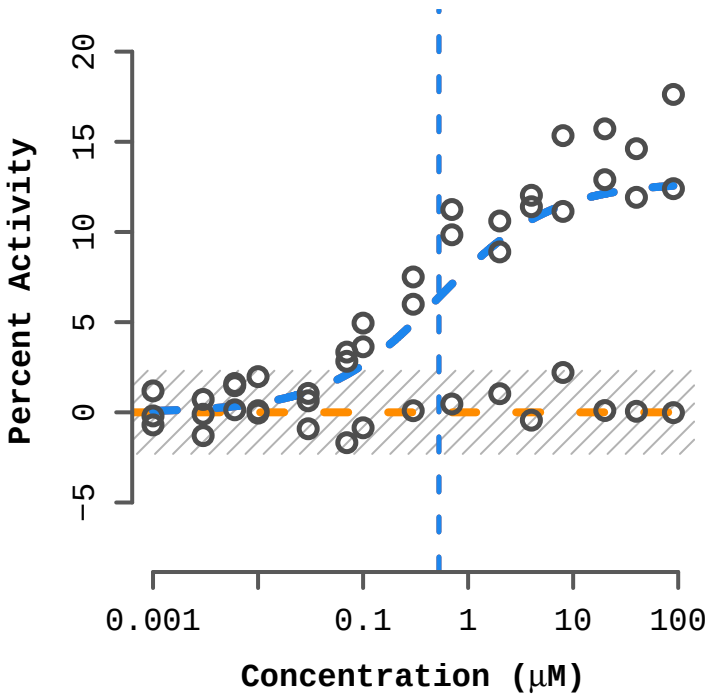
	tp	ga	gw
val:	5.86	−0.468	2.1
sd:	0.721	0.155	1.58

GAIN-LOSS MODEL (in blue):

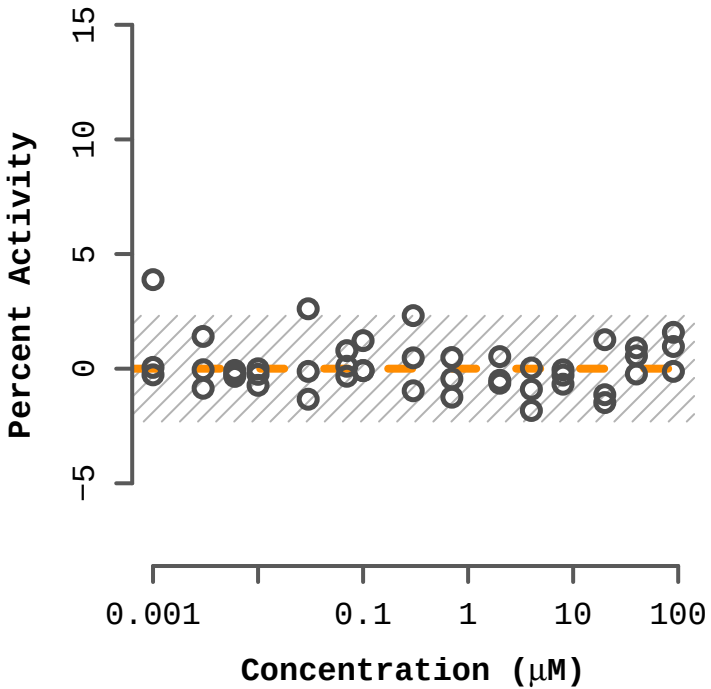
	tp	ga	gw	la	lw
val:	6.76	−0.353	1.5	2.02	3.6
sd:	1.26	0.294	1.12	0.182	8.44

	CNST	HILL	GNLS
AIC:	257.34	223.28	224.95
PROB:	0	0.7	0.3
RMSE:	4.25	2.81	2.79

MAX_MEAN: 5.79 MAX_MED: 7.74 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Hydratropaldehyde
CHID:    52629   CASRN: 93-53-8
SPID(S): Tox21_303843
M4ID:    12475345

HILL MODEL (in red):
      tp       ga       gw
val:  12.8     -0.278   0.808
sd:   1.87     0.331    0.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.8     -0.278   0.808    3.71     5.96
sd:   1.87     0.331    0.3      41000    140000

      CNST        HILL        GNLS
AIC:  308.31      262.69      266.69
PROB: 0           0.88        0.12
RMSE: 7.39        4.59        4.59

MAX_MEAN: 10        MAX_MED: 12.9      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

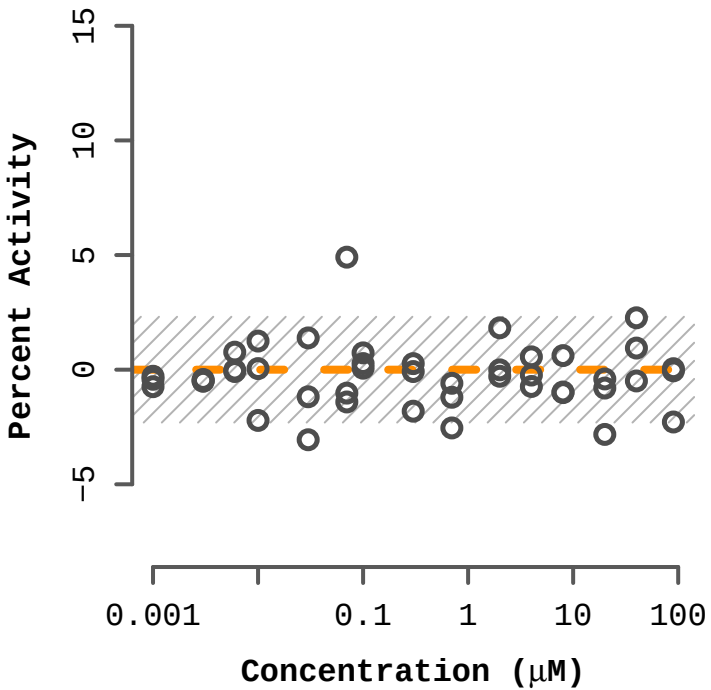
NAME: 2-Bromophenol
CHID: 52641 CASRN: 95-56-7
SPID(S): Tox21_303903
M4ID: 12475285

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.93	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.23 MAX_MED: 0.969 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

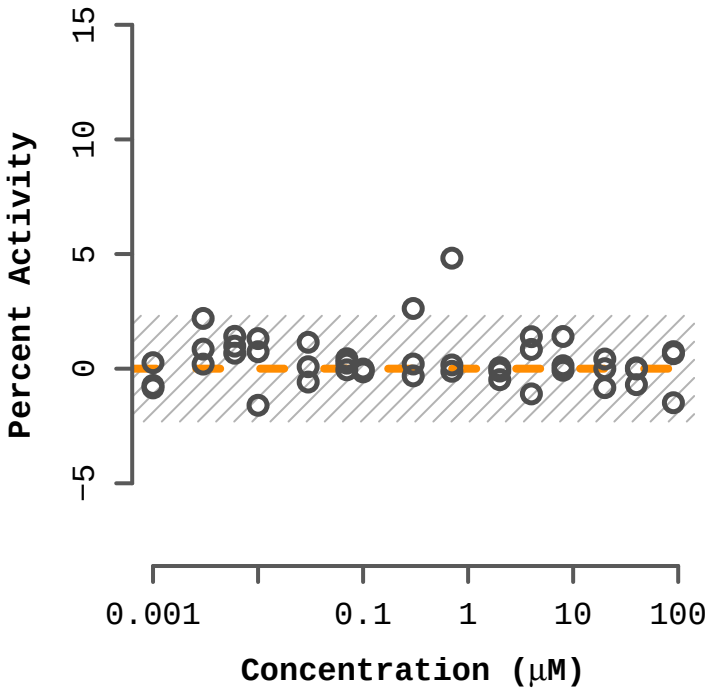
NAME: 1-Methylpyrrole
CHID: 52648 **CASRN:** 96-54-8
SPID(S): Tox21_303918
M4ID: 12475270

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.21	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 0.943 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

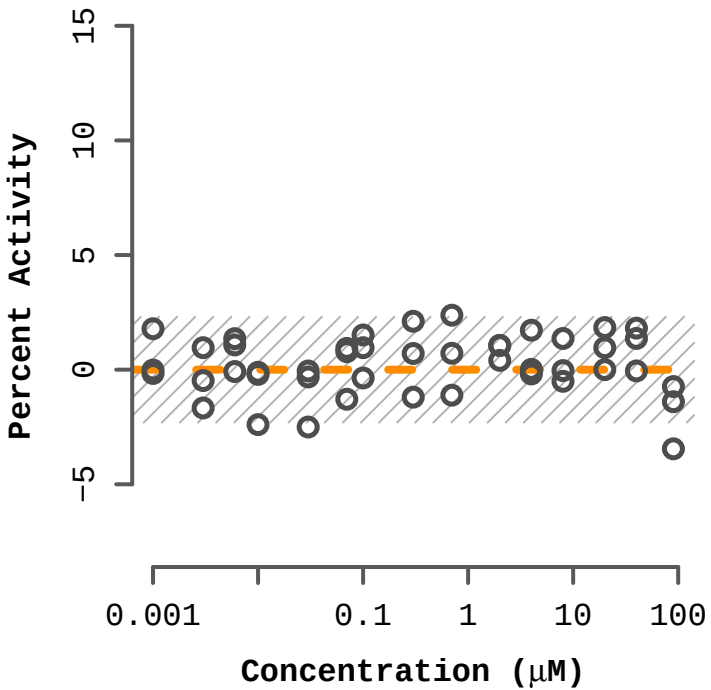
NAME: Citronellyl isobutyrate
CHID: 52652 **CASRN:** 97-89-2
SPID(S): Tox21_303859
M4ID: 12475329

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 0.983 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

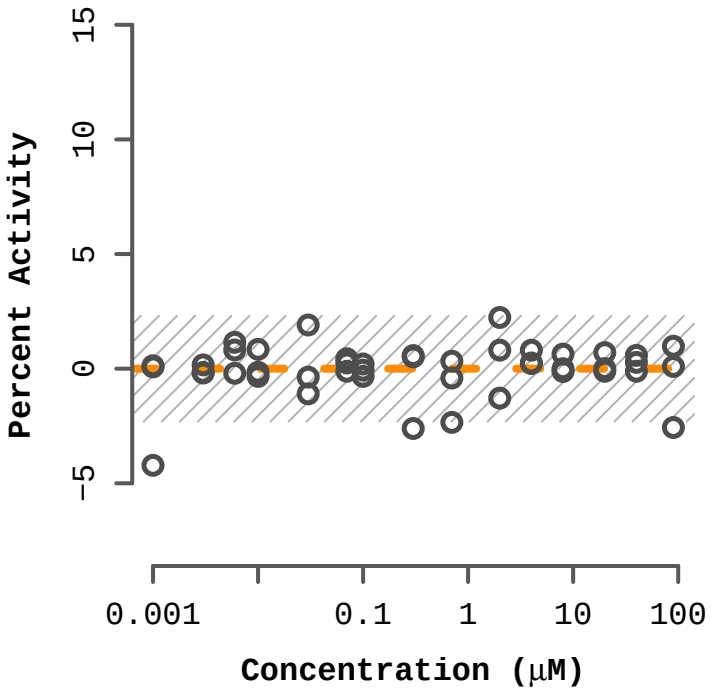
NAME: 2-Furylmethanethiol
CHID: 52654 **CASRN:** 98-02-2
SPID(S): Tox21_303886
M4ID: 12475302

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.8	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

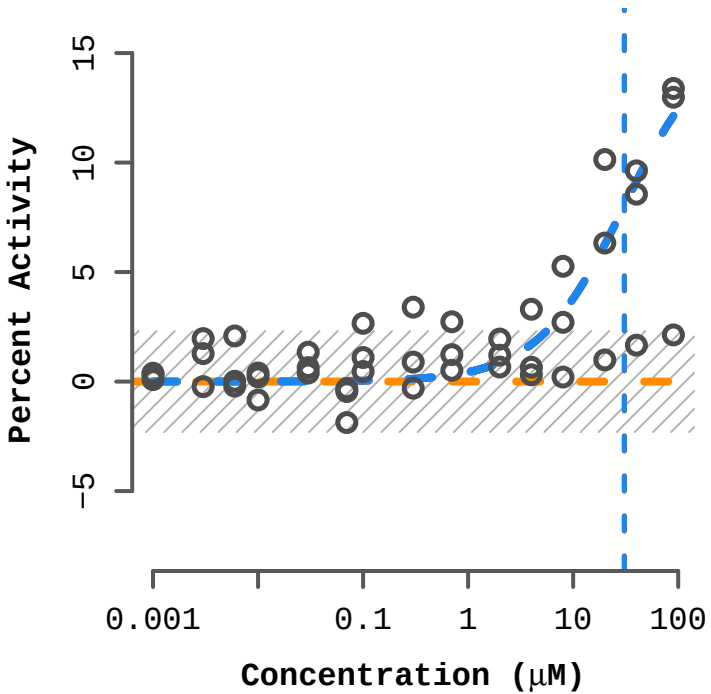
NAME: (L)−alpha−Terpineol
CHID: 52672 **CASRN:** 10482−56−1
SPID(S): Tox21_303728
M4ID: 12475460

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 0.589 **MAX_MED:** 0.816 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 3-Chloro-7-hydroxy-4-methyl-2-benzopyrone
CHID: 52724 **CASRN:** 6174-86-3
SPID(S): Tox21_303840
M4ID: 12475348

HILL MODEL (in red):

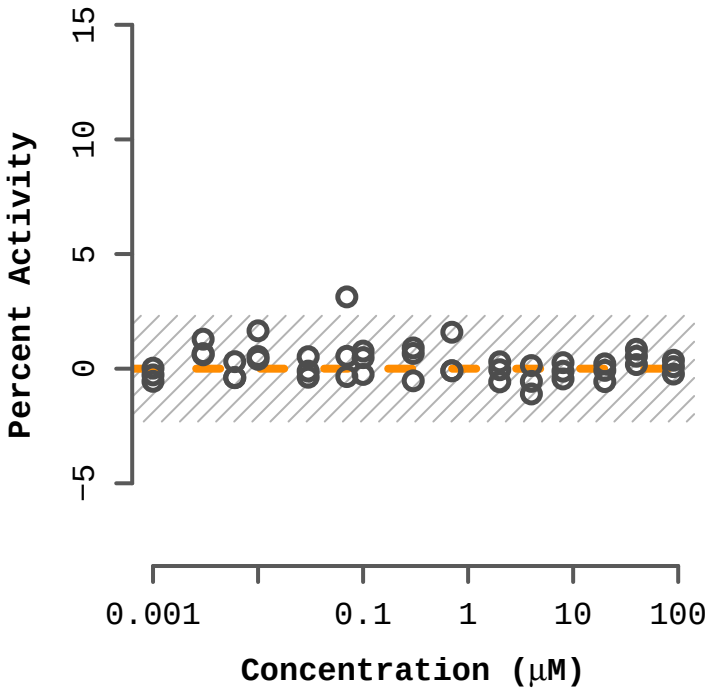
	tp	ga	gw
val:	16.1	1.49	1.05
sd:	3.82	0.231	0.272

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	16.1	1.49	1.05	3.02	8.03
sd:	3.82	0.232	0.272	1020	7720

	CNST	HILL	GNLS
AIC:	238.04	196.23	200.23
PROB:	0	0.88	0.12
RMSE:	4.12	2.43	2.43

MAX_MEAN: 9.5 **MAX_MED:** 13 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

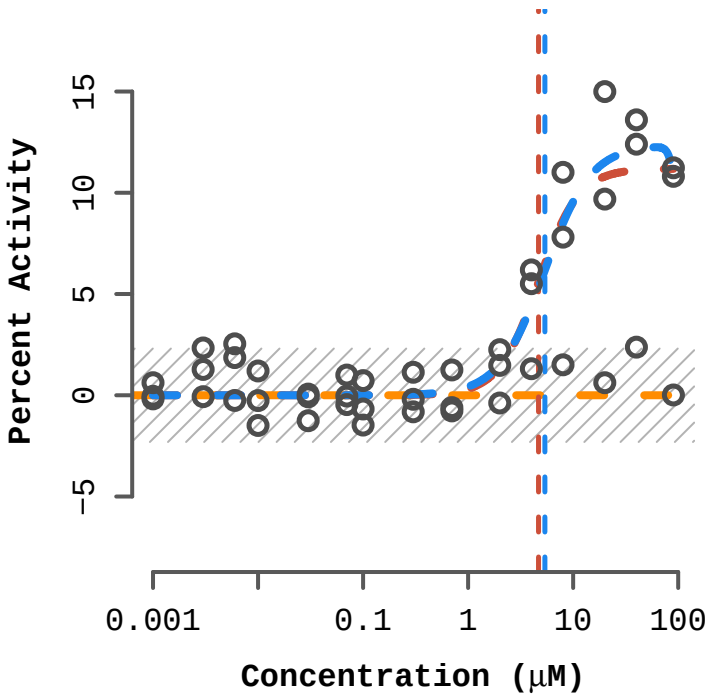
NAME: 1,2-dibromo(phenyl)ethane
CHID: 52735 **CASRN:** 93-52-7
SPID(S): Tox21_303993
M4ID: 12475195

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	95.3	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.665 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 4,6-Dimethyldibenzothiophene
CHID: 52740 CASRN: 1207-12-1
SPID(S): Tox21_303847
M4ID: 12475341

HILL MODEL (in red):

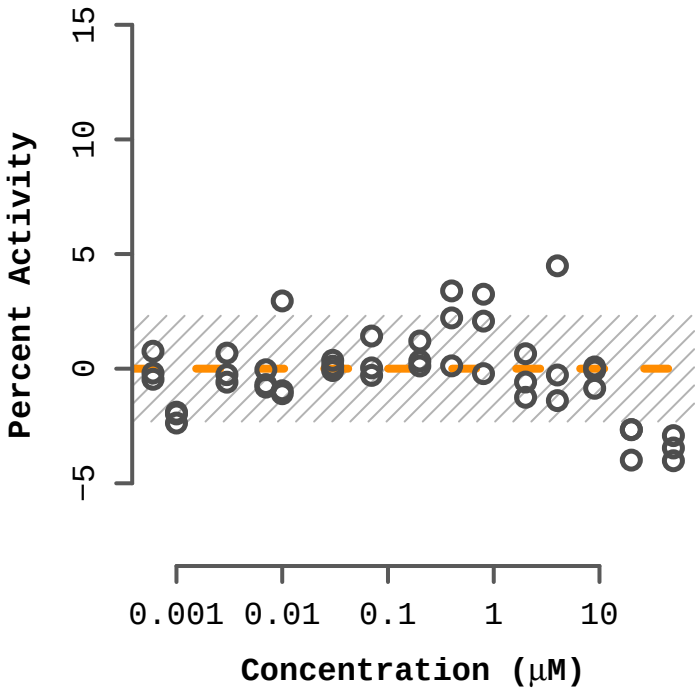
	tp	ga	gw
val:	11.2	0.67	2.29
sd:	0.855	0.085	0.749

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.4	0.731	1.98	2.01	13.3
sd:	1.38	0.111	0.666	0.0506	12.5

	CNST	HILL	GNLS
AIC:	262.83	214.71	217.69
PROB:	0	0.82	0.18
RMSE:	5.17	3.12	3.16

MAX_MEAN: 9.46 MAX_MED: 12.4 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

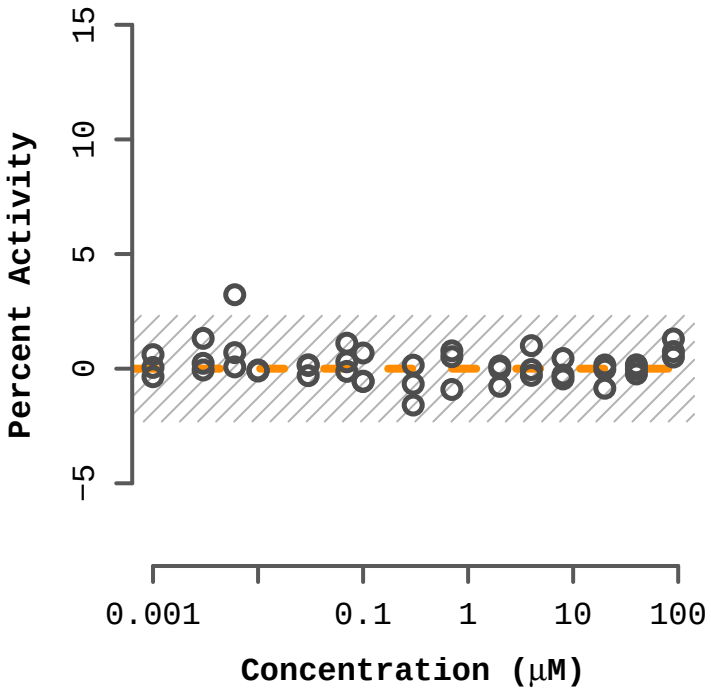
NAME: 2,2',3,4',5,5',6-Heptachloro-1,1'-biphenyl
CHID: 52832 **CASRN:** 52663-68-0
SPID(S): Tox21_303787
M4ID: 12475401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	184.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.85	NA	NA

MAX_MEAN: 1.91 **MAX_MED:** 2.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

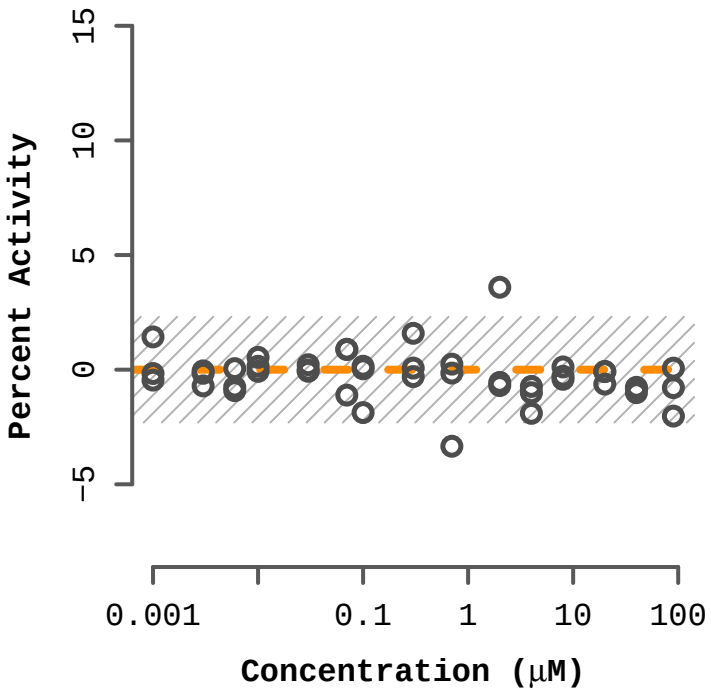
NAME: Arsenobetaine
CHID: 52833 CASRN: 64436-13-1
SPID(S): Tox21_304031
M4ID: 12475157

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	94.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.76	NA	NA

MAX_MEAN: 1.34 MAX_MED: 0.748 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

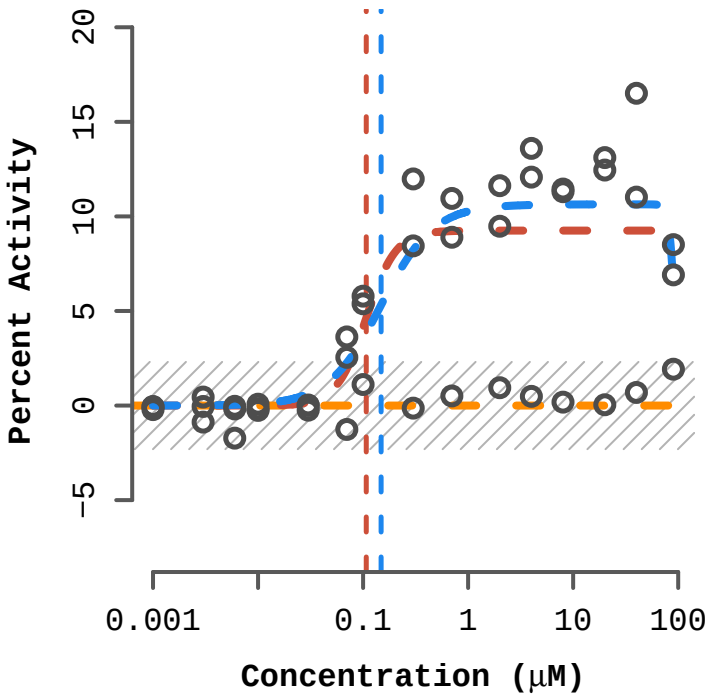
NAME: Alachlor ESA, sodium salt
CHID: 52837 **CASRN:** 140939-15-7
SPID(S): Tox21_303958
M4ID: 12475230

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 0.784 **MAX_MED:** 0.882 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Alachlor sec-oxanilic acid sodium salt
CHID: 52838 CASRN: 140939-17-9
SPID(S): Tox21_303888
M4ID: 12475300

HILL MODEL (in red):

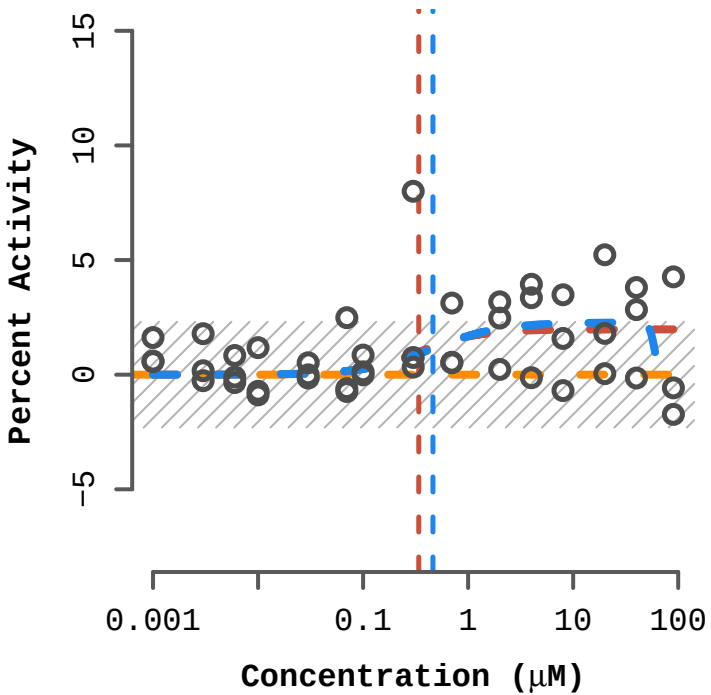
	tp	ga	gw
val:	9.25	−0.97	3.11
sd:	1.01	0.157	3.97

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.6	−0.828	1.74	1.96	16.5
sd:	1.13	0.228	1.16	0.039	65.3

	CNST	HILL	GNLS
AIC:	303.72	259.15	259.08
PROB:	0	0.49	0.51
RMSE:	6.94	4.14	4.24

MAX_MEAN: 9.41 **MAX_MED:** 12.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Metribuzin-DA
CHID: 52839 **CASRN:** 35045-02-4
SPID(S): Tox21_303904
M4ID: 12475284

HILL MODEL (in red):

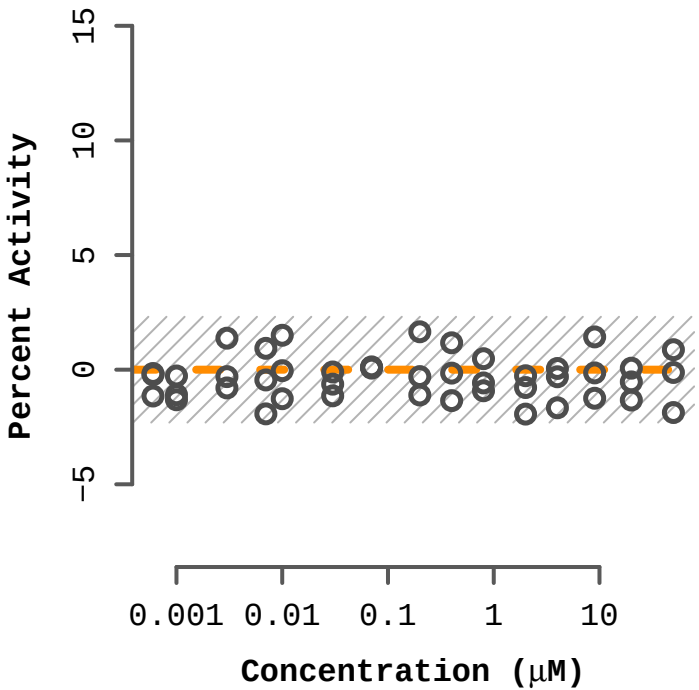
	tp	ga	gw
val:	1.98	−0.47	1.56
sd:	0.537	0.427	1.43

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.28	−0.335	1.36	1.77	18
sd:	0.584	0.396	1.2	0.669	68.4

	CNST	HILL	GNLS
AIC:	195.24	182.9	183.33
PROB:	0	0.55	0.45
RMSE:	2.24	1.8	1.78

MAX_MEAN: 3.03 **MAX_MED:** 3.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

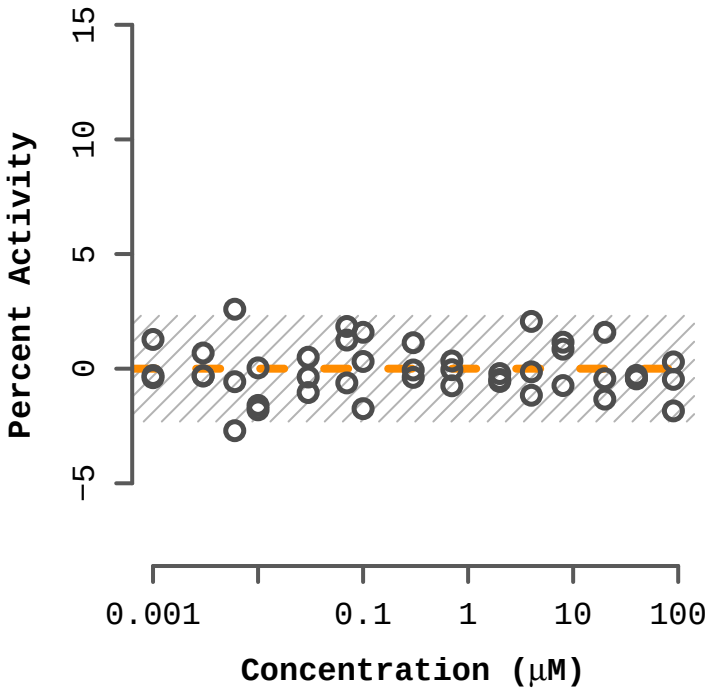
NAME: Ameltolide
CHID: 52860 **CASRN:** 787-93-9
SPID(S): Tox21_113872
M4ID: 12482353

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.0964 **MAX_MED:** 0.0963 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

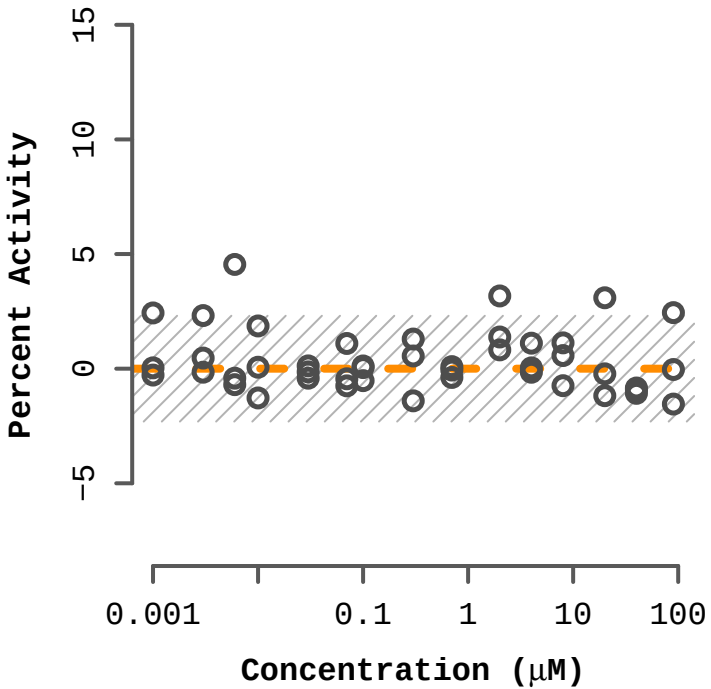
NAME: cis−Permethrin in cyclohexane
CHID: 52866 **CASRN:** NOCAS_52866
SPID(S): Tox21_303933
M4ID: 12475255

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	140.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.824 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

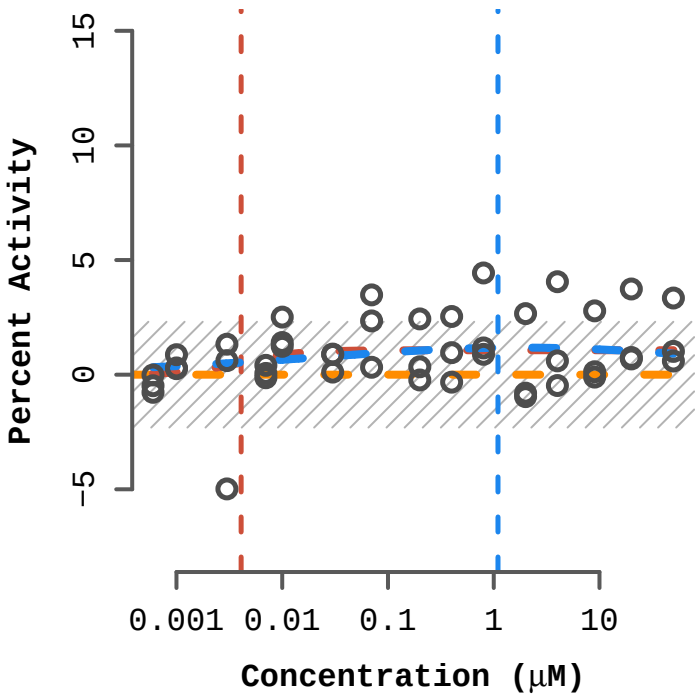
NAME: 1,2,3-Hexanetriol
CHID: 52884 **CASRN:** 90325-47-6
SPID(S): Tox21_303952
M4ID: 12475236

HILL MODEL: Not applicable.

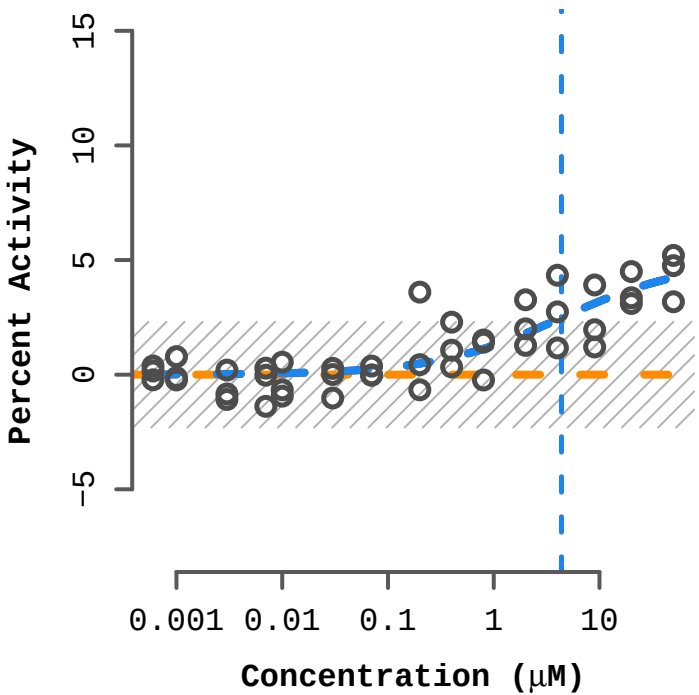
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.36	NA	NA

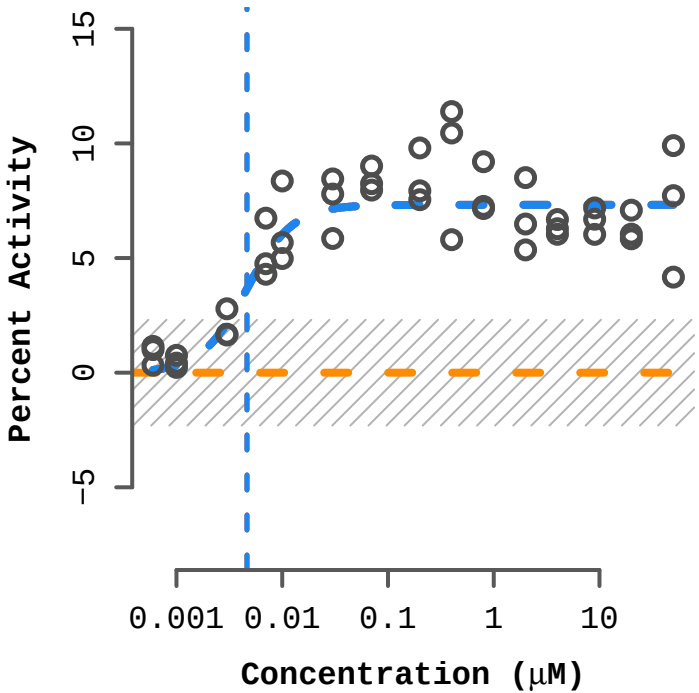
MAX_MEAN: 1.79 **MAX_MED:** 1.38 **BMAD:** 0.769



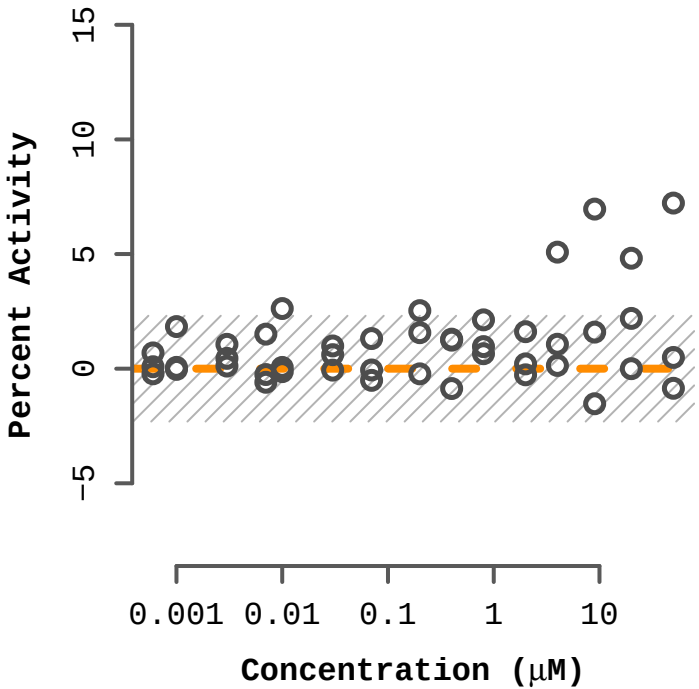

```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Glymidine sodium
CHID:    57601   CASRN: 3459-20-9
SPID(S): Tox21_113714
M4ID:    12482500

HILL MODEL (in red):
      tp       ga       gw
val:  1.07     -2.39    1.6
sd:   0.273    0.618    2.13

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.32     0.0402   0.321    0.29     0.3
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  182.21      169.54      175.04
PROB: 0           0.94        0.06
RMSE: 1.85        1.52        1.55

MAX_MEAN: 2.17      MAX_MED: 2.35      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Lotrafiban
CHID:    57602   CASRN: 171049-14-2
SPID(S): Tox21_113989
M4ID:    12482255

HILL MODEL (in red):
      tp       ga       gw
val:  4.96     0.64     0.721
sd:   1.67     0.571    0.264

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.96     0.64     0.721    3.23     5.27
sd:   1.67     0.571    0.264    1370     4710

      CNST        HILL        GNLS
AIC:  194.72      130.35      134.35
PROB: 0           0.88        0.12
RMSE: 2.1         0.95        0.95

MAX_MEAN: 4.38      MAX_MED: 4.76      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    R-Lotrafiban
CHID:    57603   CASRN: NOCAS_57603
SPID(S): Tox21_113990
M4ID:    12482254

HILL MODEL (in red):
      tp       ga       gw
val:  7.32     -2.33    2
sd:   0.272    0.0667   0.548

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  7.32     -2.33    2        3.4      10.3
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  308.33      168.03      172.03
PROB: 0           0.88        0.12
RMSE: 6.63        1.43        1.43

MAX_MEAN: 9.22      MAX_MED: 10.5      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

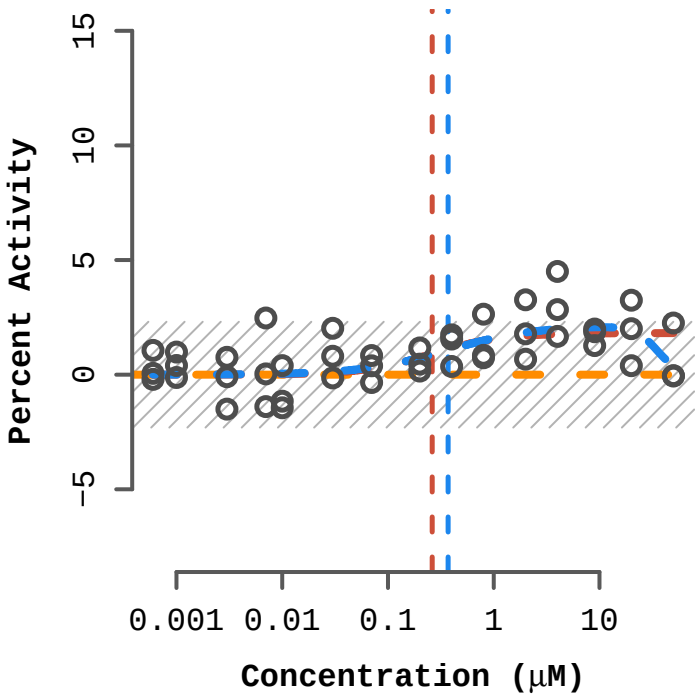
NAME: Aminopentamide sulfate
CHID: 57604 **CASRN:** 20701-77-3
SPID(S): Tox21_113961
M4ID: 12482271

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.36	NA	NA
PROB:	1	NA	NA
RMSE:	2.12	NA	NA

MAX_MEAN: 2.34 **MAX_MED:** 2.19 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Aminoethyldiethylamine
CHID: 57606 **CASRN:** 100-36-7
SPID(S): Tox21_113860
M4ID: 12482363

HILL MODEL (in red):

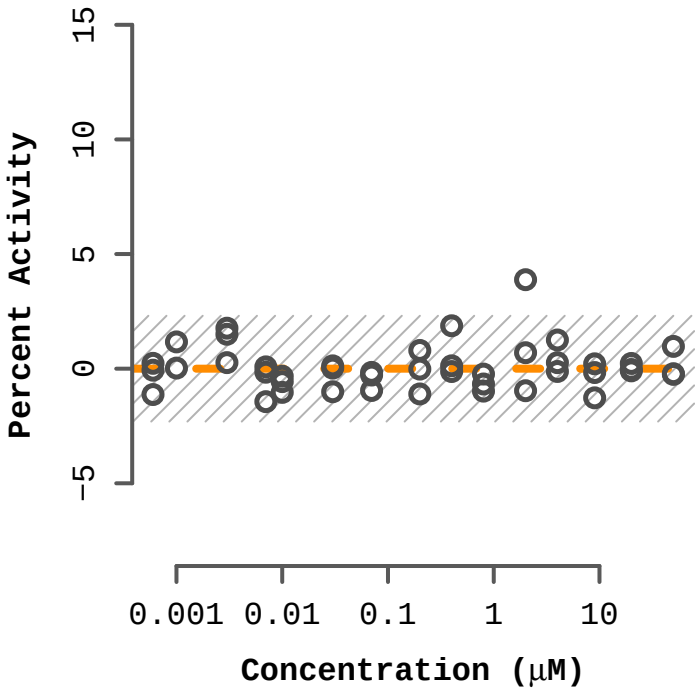
	tp	ga	gw
val:	1.82	−0.582	1.33
sd:	0.306	0.281	0.922

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.14	−0.431	1.07	1.54	4.17
sd:	0.592	0.363	0.741	0.288	7.94

	CNST	HILL	GNLS
AIC:	171.7	141.47	141.15
PROB:	0	0.46	0.54
RMSE:	1.58	1.05	1

MAX_MEAN: 3.01 **MAX_MED:** 2.84 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

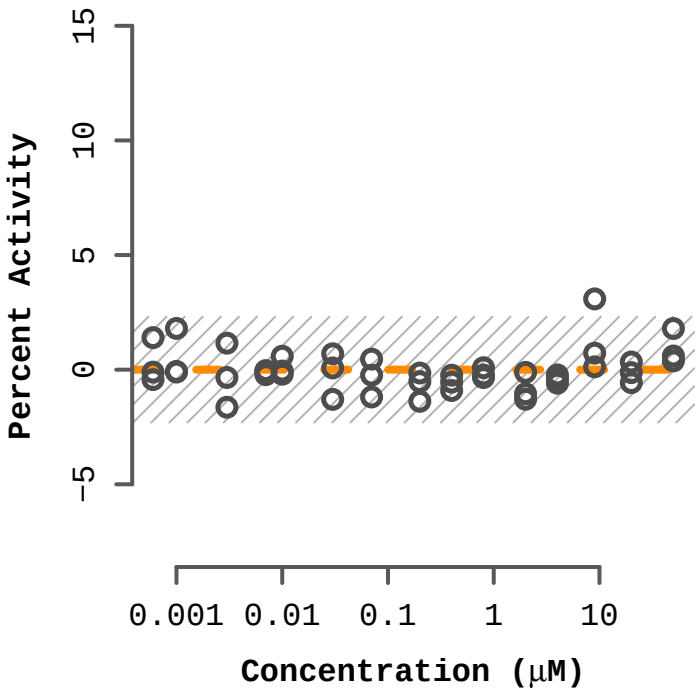
NAME: Quinuclidine
CHID: 57607 **CASRN:** 100-76-5
SPID(S): Tox21_113847
M4ID: 12482375

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.82	NA	NA
PROB:	1	NA	NA
RMSE:	0.97	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

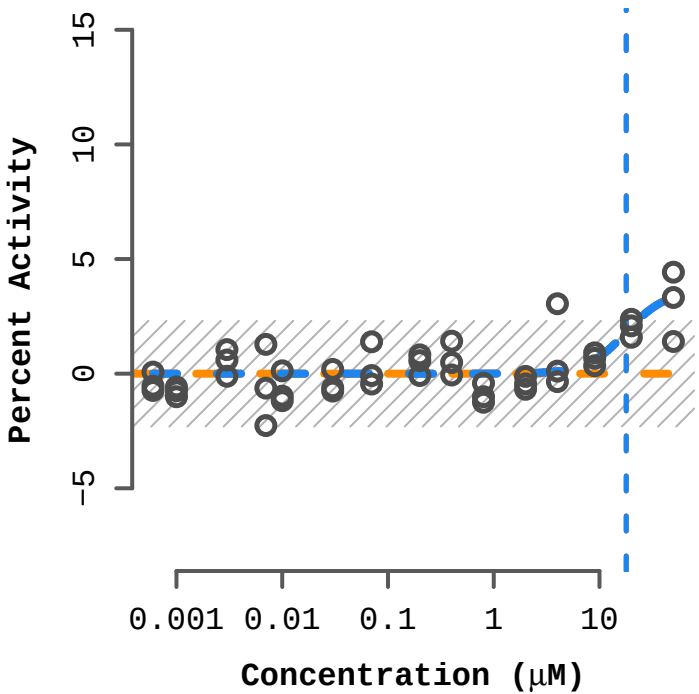
NAME: Fenadiazole
CHID: 57608 **CASRN:** 1008-65-7
SPID(S): Tox21_113759
M4ID: 12482456

HILL MODEL: Not applicable.

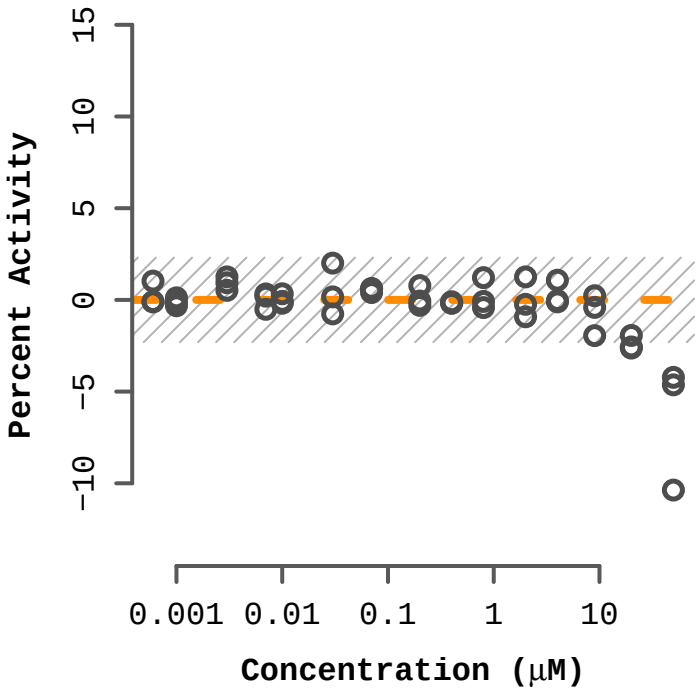
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.29	NA	NA
PROB:	1	NA	NA
RMSE:	0.88	NA	NA

MAX_MEAN: 1.31 **MAX_MED:** 0.721 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Pentifylline
CHID:    57609   CASRN: 1028-33-7
SPID(S): Tox21_113810
M4ID:    12482409

HILL MODEL (in red):
      tp       ga       gw
val:  3.62     1.25     2.35
sd:   1.03     0.149    1.09

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.62     1.25     2.35     3.46     5.46
sd:   1.03     0.149    1.09     43200    135000

      CNST        HILL        GNLS
AIC:  150.41      125.91      129.91
PROB: 0           0.88        0.12
RMSE: 1.33        0.92        0.92

MAX_MEAN: 3.05      MAX_MED: 3.32      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

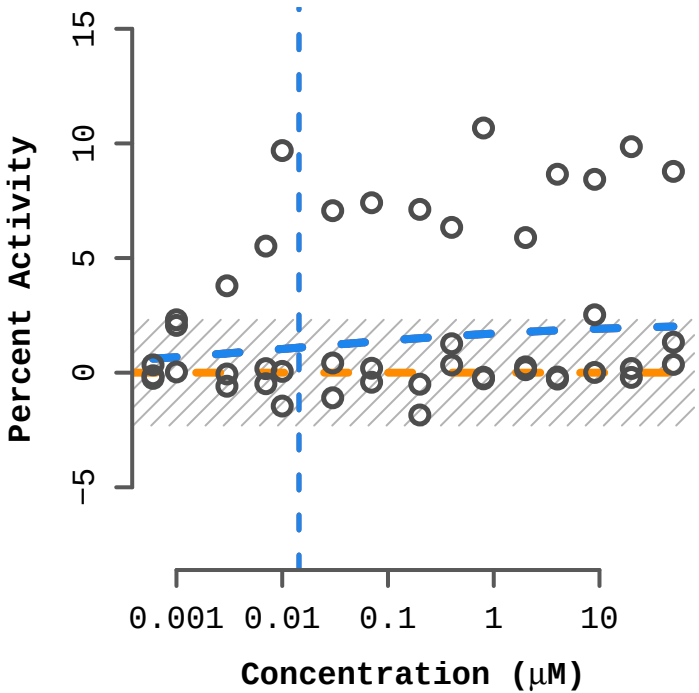
NAME: Tepoxalin
CHID: 57610 **CASRN:** 103475-41-8
SPID(S): Tox21_113717
M4ID: 12482497

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.51	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 0.906 **MAX_MED:** 0.938 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Moexiprilat
CHID: 57611 **CASRN:** 103775-14-0
SPID(S): Tox21_113957
M4ID: 12482274

HILL MODEL (in red):

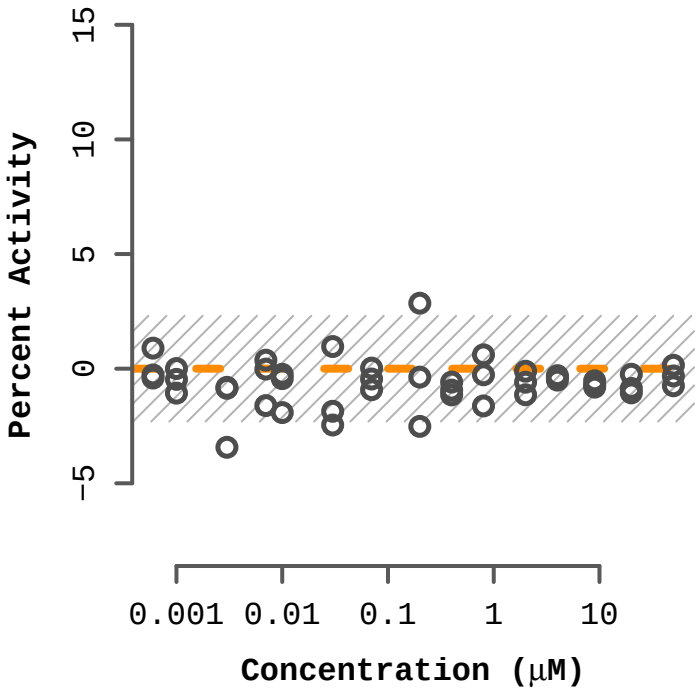
	tp	ga	gw
val:	2.19	−1.84	0.3
sd:	4.74	8.35	1.3

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.19	−1.84	0.3	3.05	4.84
sd:	4.73	8.34	1.3	1110	3970

	CNST	HILL	GNLS
AIC:	254.82	252.2	256.2
PROB:	0.19	0.71	0.1
RMSE:	4.3	3.67	3.67

MAX_MEAN: 3.66 **MAX_MED:** 2.53 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

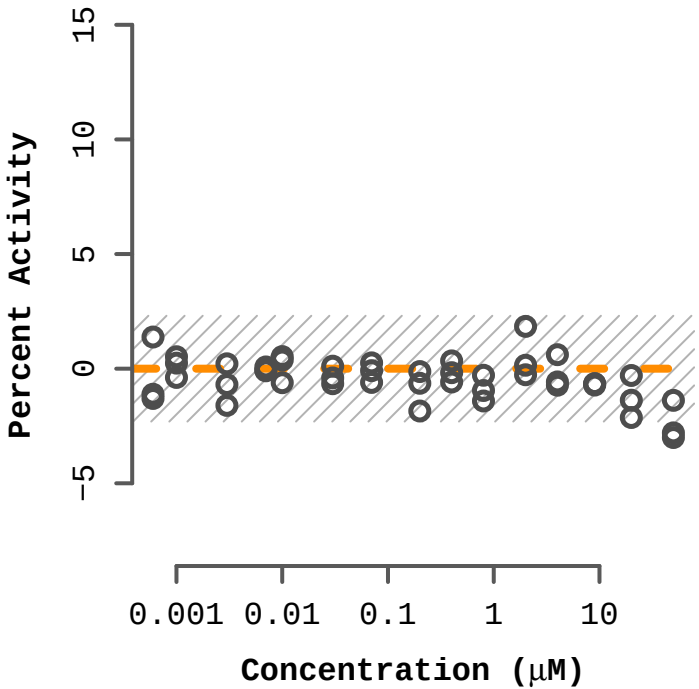
NAME: Benzilonium bromide
CHID: 57612 **CASRN:** 1050-48-2
SPID(S): Tox21_113937
M4ID: 12482294

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.99	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 0.0722 **MAX_MED:** −0.0172 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

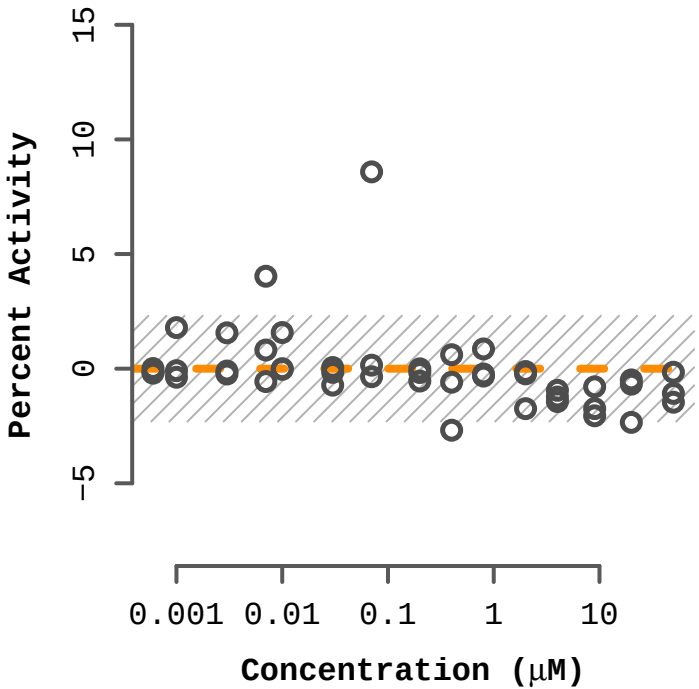
NAME: Moxaverine
CHID: 57613 **CASRN:** 10539-19-2
SPID(S): Tox21_113958
M4ID: 12482273

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.578 **MAX_MED:** 0.38 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

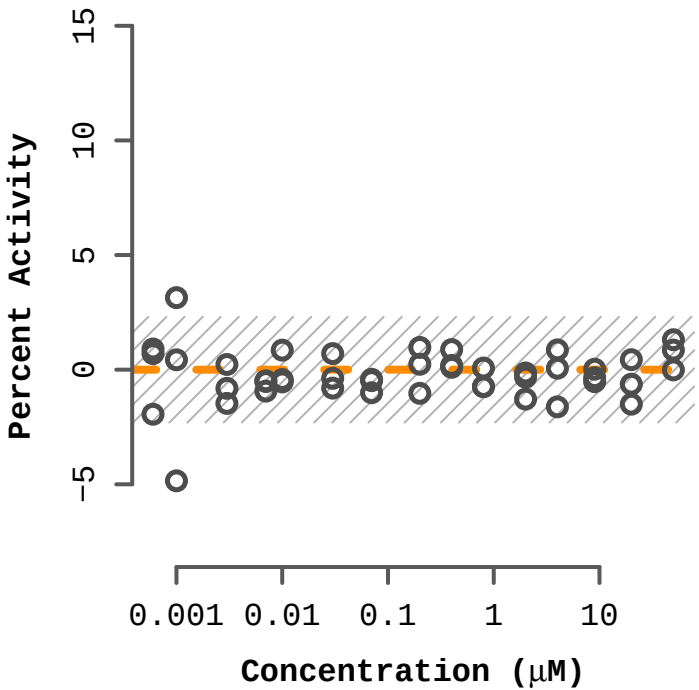
NAME: Exametazime
CHID: 57614 **CASRN:** 105613-48-7
SPID(S): Tox21_113984
M4ID: 12482258

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.73	NA	NA

MAX_MEAN: 2.8 **MAX_MED:** 0.814 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

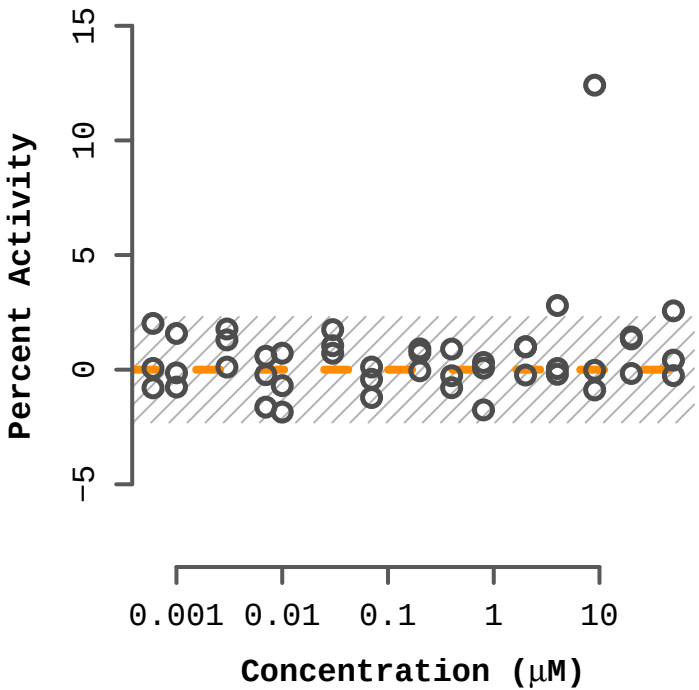
NAME: Loxiglumide
CHID: 57615 **CASRN:** 107097-80-3
SPID(S): Tox21_113968
M4ID: 12482266

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 0.719 **MAX_MED:** 0.856 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

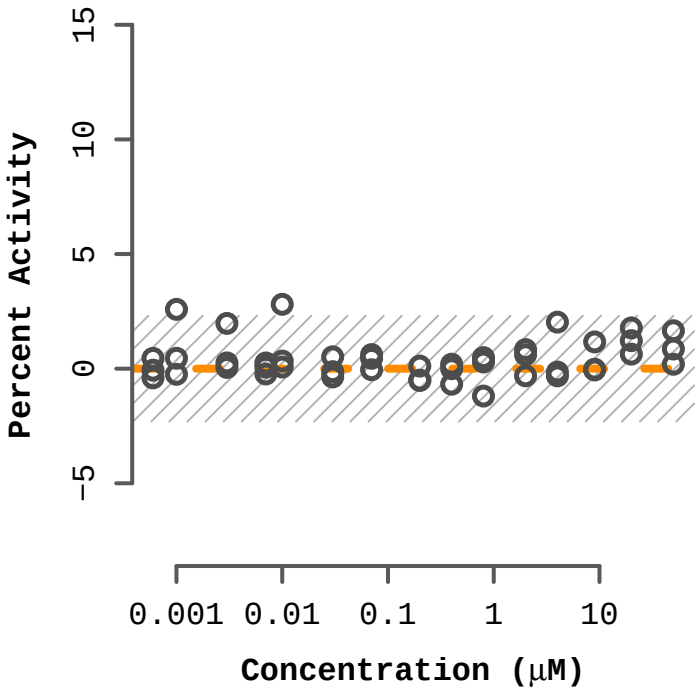
NAME: 3,3−Tetramethyleneglutarimide
CHID: 57616 **CASRN:** 1075−89−4
SPID(S): Tox21_113849
M4ID: 12482373

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.49	NA	NA
PROB:	1	NA	NA
RMSE:	2.15	NA	NA

MAX_MEAN: 3.83 **MAX_MED:** 1.34 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

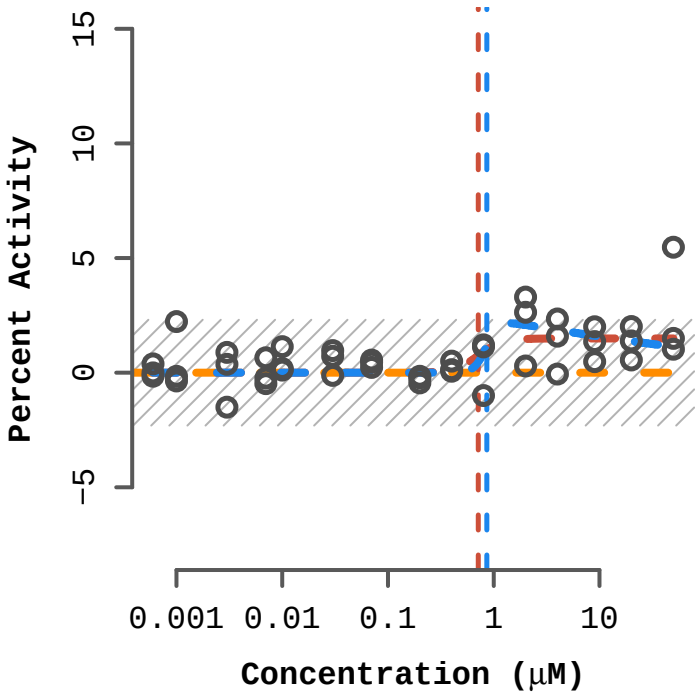
NAME: 6-Methoxy-?1-?tetralone
CHID: 57617 **CASRN:** 1078-19-9
SPID(S): Tox21_113778
M4ID: 12482438

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.89	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Isoniazid pyruvate
CHID: 57618 **CASRN:** 1081-50-1
SPID(S): Tox21_113689
M4ID: 12482525

HILL MODEL (in red):

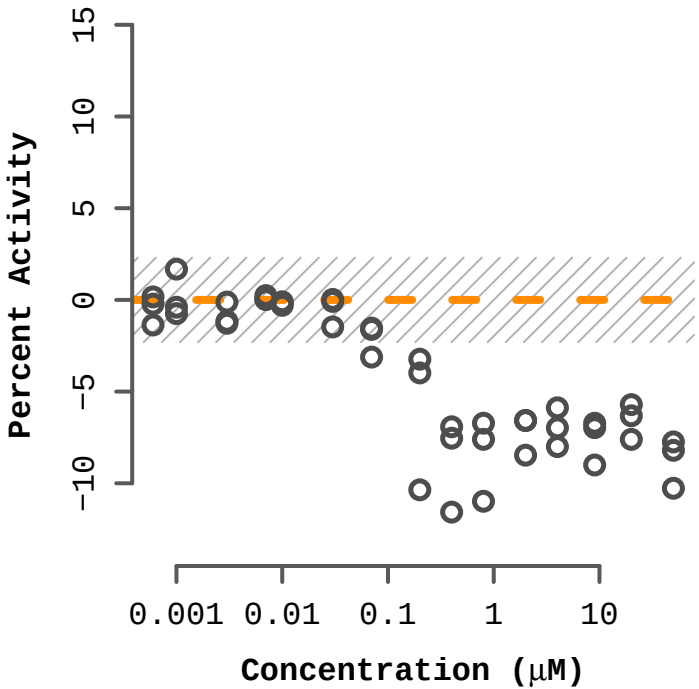
	tp	ga	gw
val:	1.49	−0.146	4
sd:	0.232	0.143	3.29

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.34	−0.0651	7.81	0.187	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	151.33	125.18	128.49
PROB:	0	0.84	0.16
RMSE:	1.4	0.99	1.03

MAX_MEAN: 2.66 **MAX_MED:** 2.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

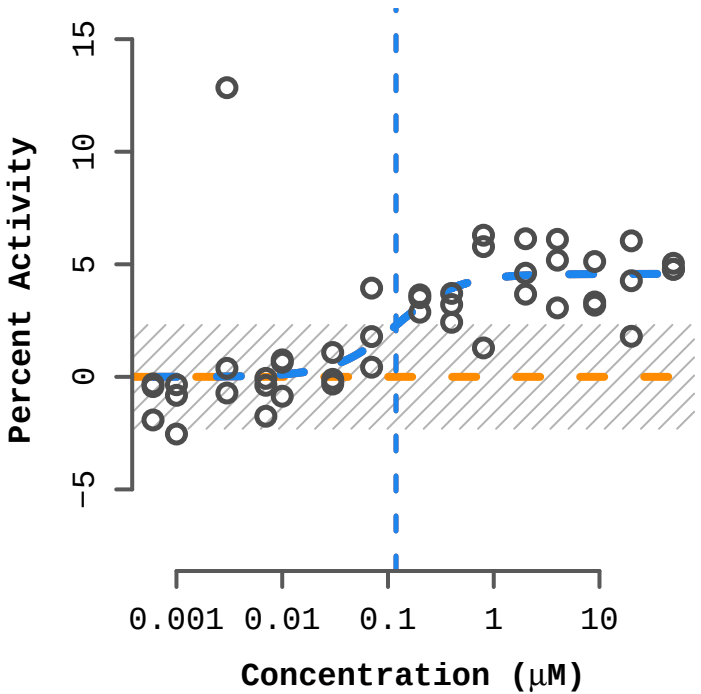
NAME: Nemorubicin
CHID: 57619 **CASRN:** 108852-90-0
SPID(S): Tox21_113985
M4ID: 12482257

HILL MODEL: Not applicable.

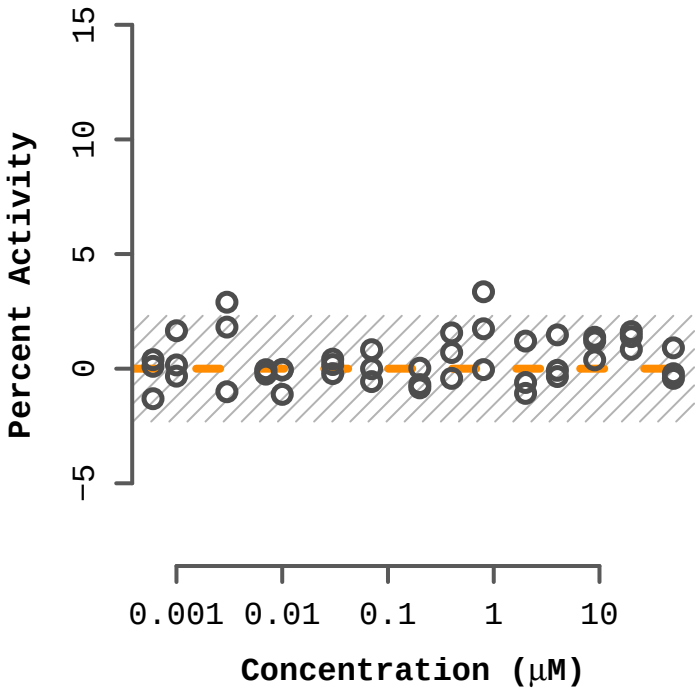
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	290.7	NA	NA
PROB:	1	NA	NA
RMSE:	5.7	NA	NA

MAX_MEAN: 0.179 **MAX_MED:** 0.0369 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Cromoglicate lisetil
CHID:    57620   CASRN: 110816-79-0
SPID(S): Tox21_113952
M4ID:    12482279

HILL MODEL (in red):
      tp       ga       gw
val:  4.57     -0.924   1.51
sd:   0.347    0.145    0.499

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.57     -0.924   1.51     3.09     6.2
sd:   0.347    0.145    0.499    2160     9650

      CNST        HILL        GNLS
AIC:  251.15      173.04      177.04
PROB: 0           0.88        0.12
RMSE: 3.84        2.27        2.27

MAX_MEAN: 4.87      MAX_MED: 5.79      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

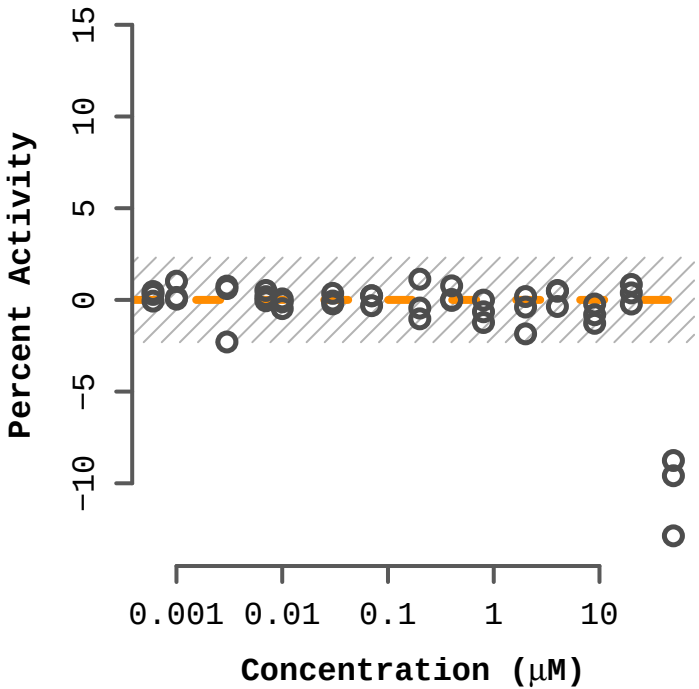
NAME: Ulifloxacin
CHID: 57621 **CASRN:** 112984-60-8
SPID(S): Tox21_113769
M4ID: 12482446

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.1	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

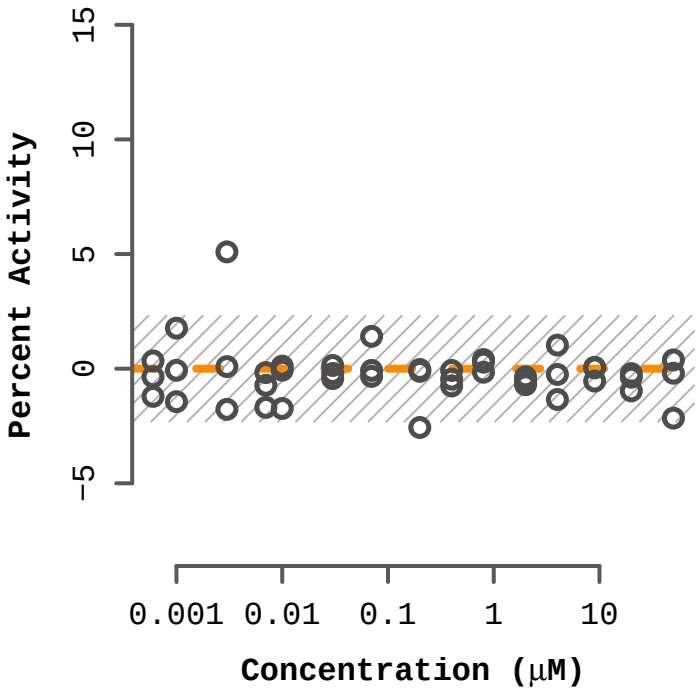
NAME: Etifelmine hydrochloride
CHID: 57622 **CASRN:** 1146-95-8
SPID(S): Tox21_113935
M4ID: 12482296

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.98	NA	NA
PROB:	1	NA	NA
RMSE:	2.81	NA	NA

MAX_MEAN: 0.4 **MAX_MED:** 0.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

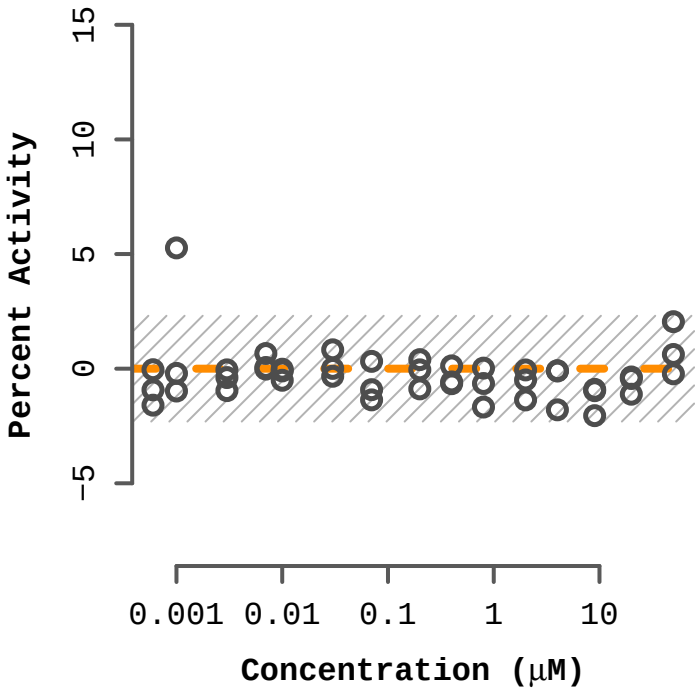
NAME: 4'−Methylbiphenyl−2−carbonitrile
CHID: 57623 **CASRN:** 114772−53−1
SPID(S): Tox21_113764
M4ID: 12482451

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	129.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.287 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

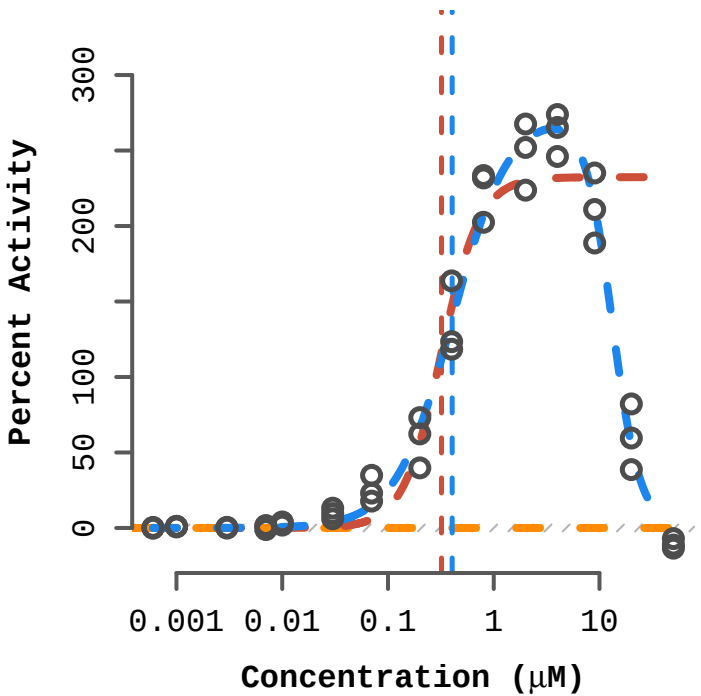
NAME: Metyridine
CHID: 57624 **CASRN:** 114-91-0
SPID(S): Tox21_113813
M4ID: 12482406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.15	NA	NA

MAX_MEAN: 1.36 **MAX_MED:** 0.621 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Prednisolone farnesylate
CHID: 57625 CASRN: 118244-44-3
SPID(S): Tox21_113887
M4ID: 12482339

HILL MODEL (in red):

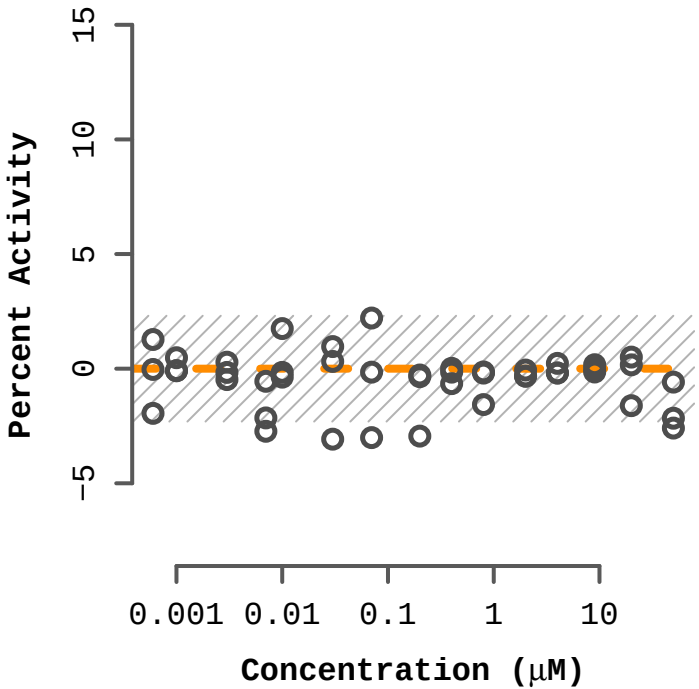
	tp	ga	gw
val:	232	-0.494	2.4
sd:	11.6	0.0477	0.516

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	276	-0.393	1.63	1.12	3.3
sd:	10.5	0.0438	0.219	0.0257	0.389

	CNST	HILL	GNLS
AIC:	565.51	493	373.88
PROB:	0	0	1
RMSE:	129.73	78.79	13.54

MAX_MEAN: 262 MAX_MED: 265 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

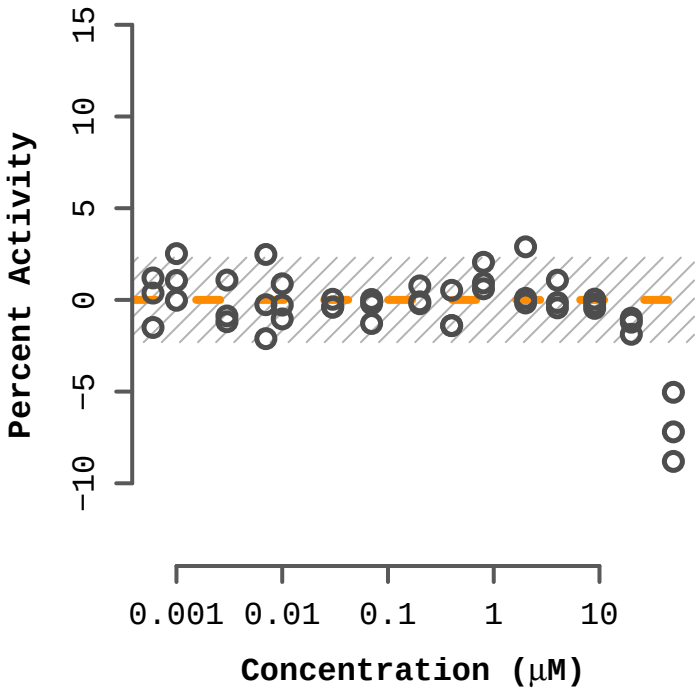
NAME: Ipenoxazone hydrochloride
CHID: 57626 **CASRN:** 118635-68-0
SPID(S): Tox21_113934
M4ID: 12482297

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.32	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.407 **MAX_MED:** 0.317 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

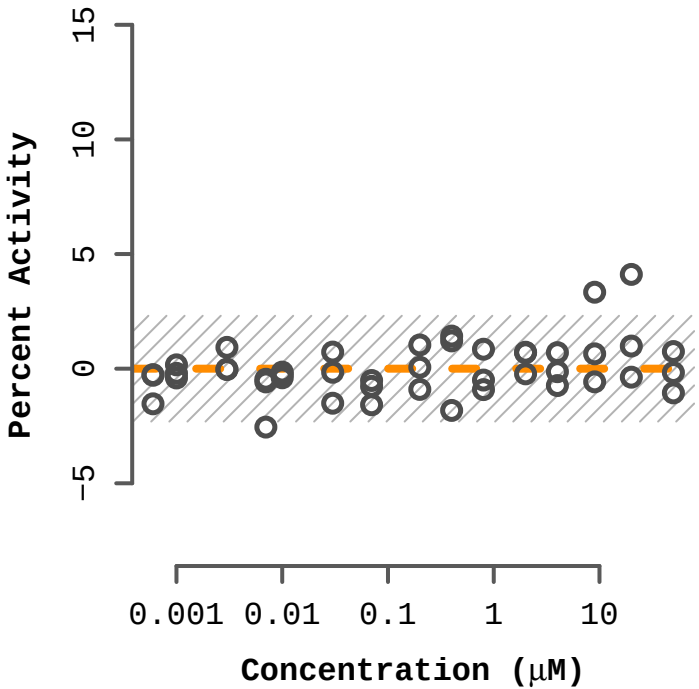
NAME: Dapoxetine
CHID: 57627 **CASRN:** 119356-77-3
SPID(S): Tox21_113784
M4ID: 12482433

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.34	NA	NA
PROB:	1	NA	NA
RMSE:	2.16	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 1.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

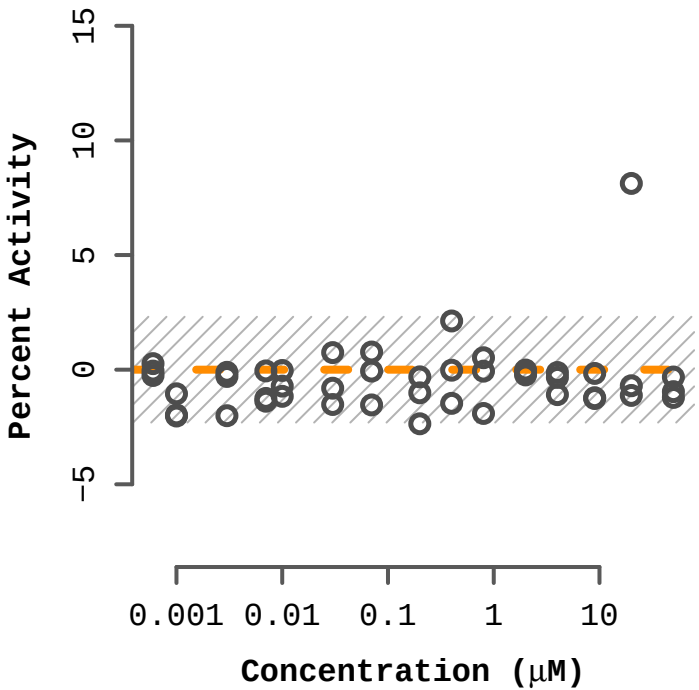
NAME: Dimorpholamine
CHID: 57628 **CASRN:** 119-48-2
SPID(S): Tox21_113692
M4ID: 12482522

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.58 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

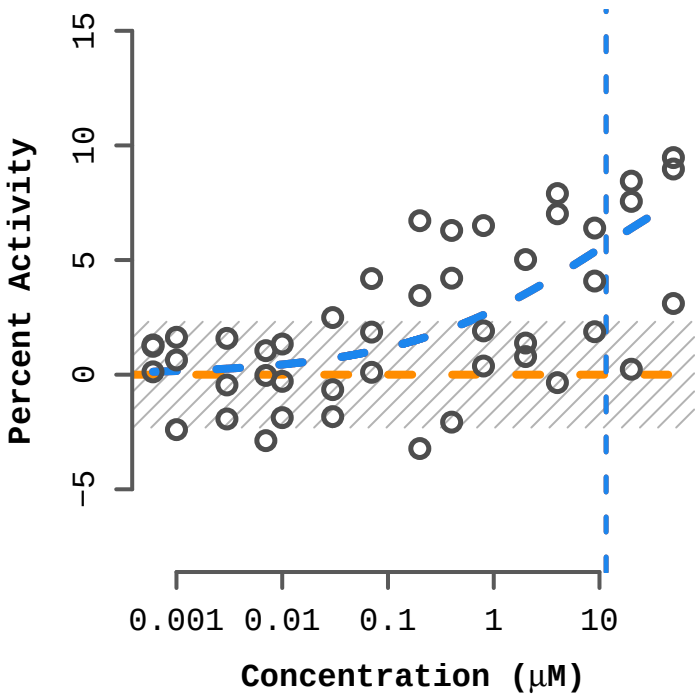
NAME: Goralatide
CHID: 57629 **CASRN:** 120081-14-3
SPID(S): Tox21_113896
M4ID: 12482332

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.61	NA	NA

MAX_MEAN: 2.1 **MAX_MED:** −0.0215 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Zolimidine
CHID: 57630 **CASRN:** 1222-57-7
SPID(S): Tox21_113899
M4ID: 12482329

HILL MODEL (in red):

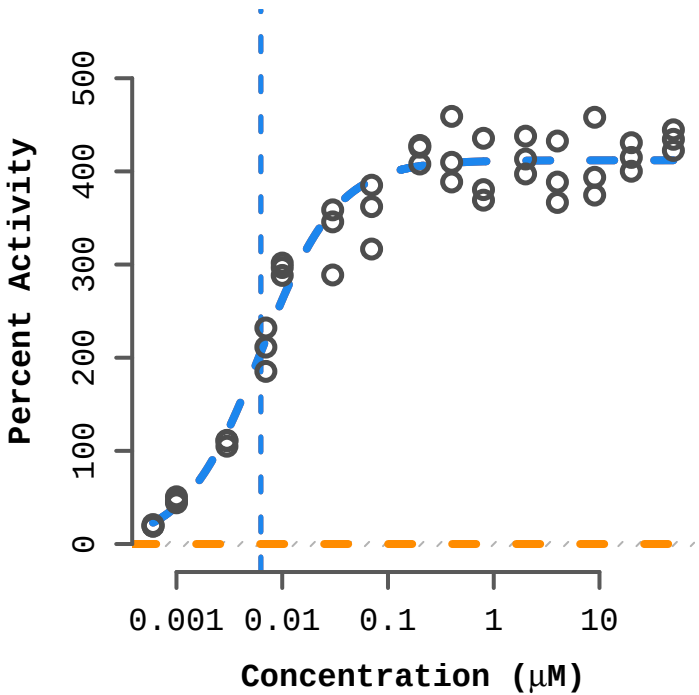
	tp	ga	gw
val:	11.4	1.06	0.454
sd:	8.82	1.56	0.211

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	11.4	1.06	0.454	3.12	5.16
sd:	8.83	1.56	0.211	1010	3650

	CNST	HILL	GNLS
AIC:	256.53	227.24	231.24
PROB:	0	0.88	0.12
RMSE:	4.08	2.64	2.64

MAX_MEAN: 7.18 **MAX_MED:** 8.97 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amelometasone
CHID: 57631 CASRN: 123013-22-9
SPID(S): Tox21_113719
M4ID: 12482495

HILL MODEL (in red):

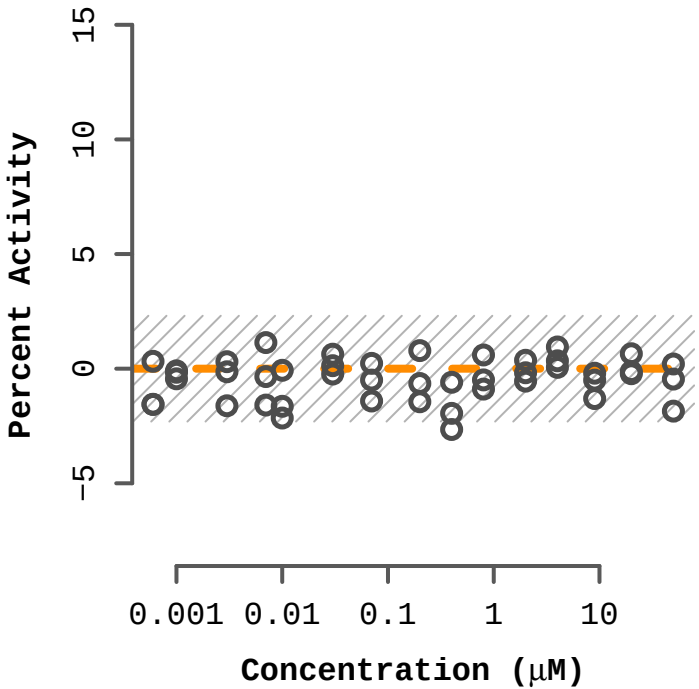
	tp	ga	gw
val:	412	-2.2	1.21
sd:	5.96	0.0369	0.114

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	412	-2.2	1.21	3.27	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	663.81	434.37	438.37
PROB:	0	0.88	0.12
RMSE:	341.99	27.32	27.32

MAX_MEAN: 434 MAX_MED: 434 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

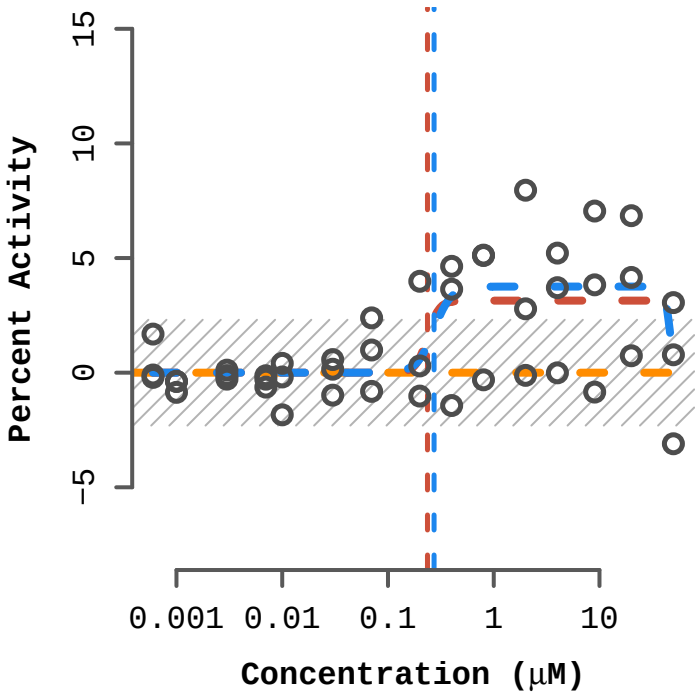
NAME: 1,2,3,5-Tetraacetyl-.-d-ribofuranose
CHID: 57632 **CASRN:** 13035-61-5
SPID(S): Tox21_113750
M4ID: 12482465

HILL MODEL: Not applicable.

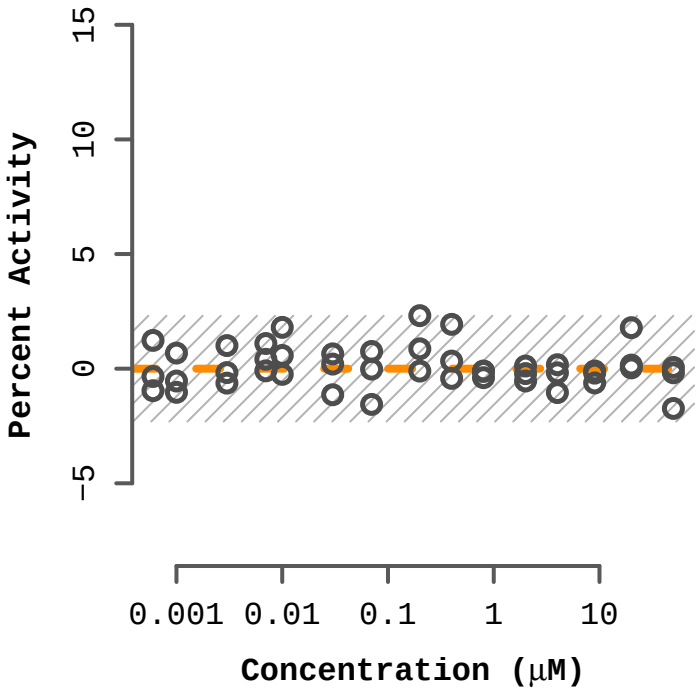
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.3	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.45 **MAX_MED:** 0.344 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Neticonazole
CHID:    57633   CASRN: 130726-68-0
SPID(S): Tox21_113705
M4ID:    12482509

HILL MODEL (in red):
      tp       ga       gw
val:  3.14     -0.626   8
sd:   0.587    0.209    20.5

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.76     -0.564   5.34     1.66     17.5
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  222.87      205.66      205.41
PROB: 0           0.47        0.53
RMSE: 2.92        2.21        2.09

MAX_MEAN: 3.91      MAX_MED: 5.11      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

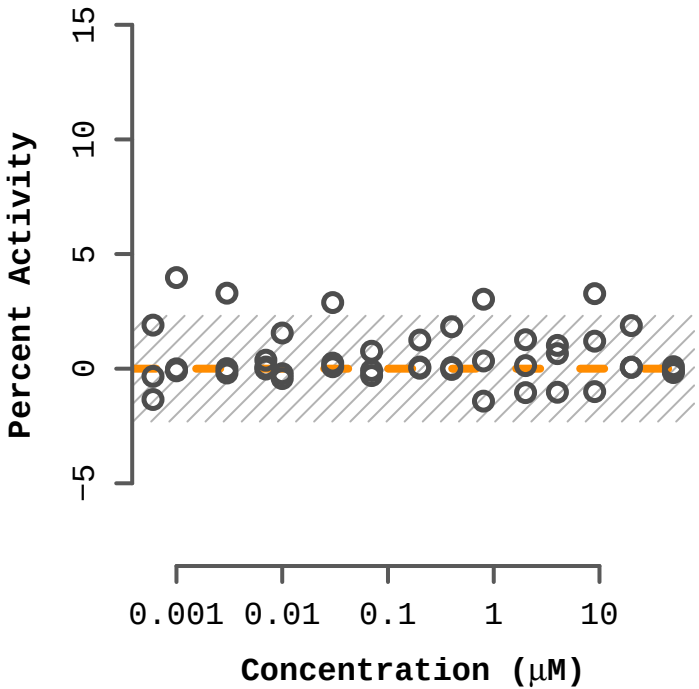
NAME: Phthalofyne
CHID: 57634 **CASRN:** 131-67-9
SPID(S): Tox21_113681
M4ID: 12482533

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.28	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.03 **MAX_MED:** 0.868 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

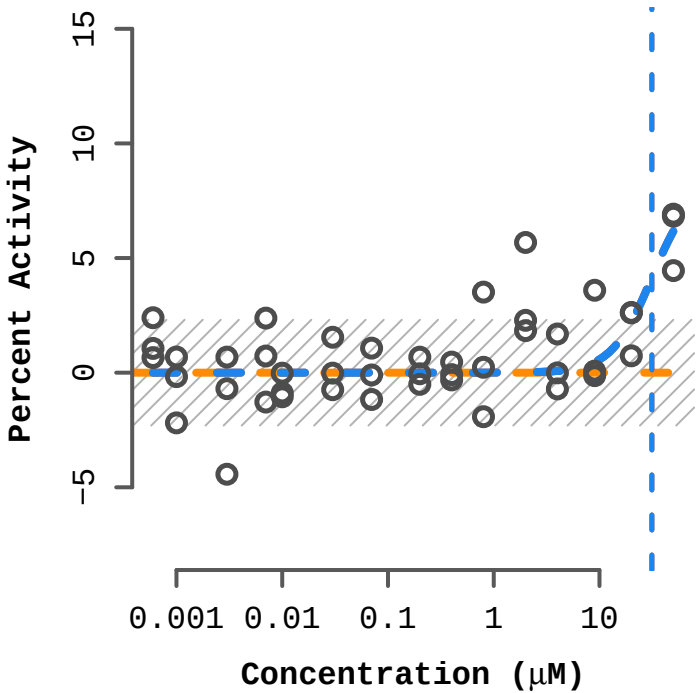
NAME: Nicoboxil
CHID: 57635 **CASRN:** 13912-80-6
SPID(S): Tox21_113682
M4ID: 12482532

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	149.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.35	NA	NA

MAX_MEAN: 1.29 **MAX_MED:** 1.2 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: N-isopropyl-4-formylbenzamide
CHID: 57636 **CASRN:** 13255-50-0
SPID(S): Tox21_113780
M4ID: 12482437

HILL MODEL (in red):

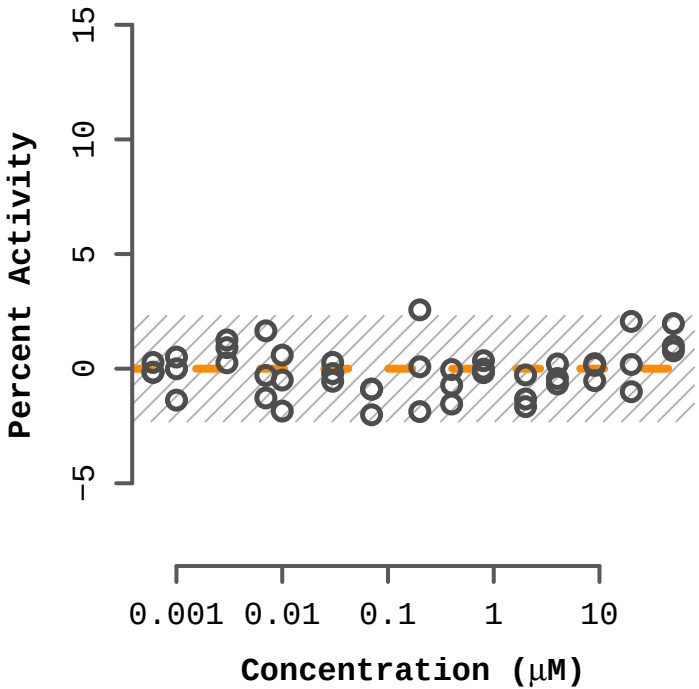
	tp	ga	gw
val:	8.3	1.5	2.27
sd:	6.32	0.377	2.23

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.3	1.5	2.27	2.84	7.62
sd:	6.32	0.377	2.23	4310	28800

	CNST	HILL	GNLS
AIC:	200.25	176.4	180.4
PROB:	0	0.88	0.12
RMSE:	2.36	1.67	1.67

MAX_MEAN: 6.07 **MAX_MED:** 6.82 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

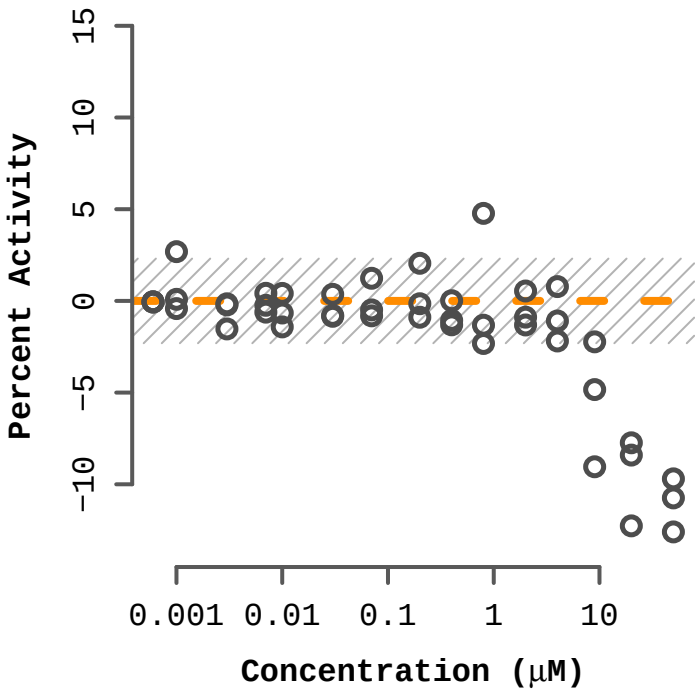
NAME: 3,4,5−Trimethoxyphenylacetonitrile
CHID: 57637 **CASRN:** 13338−63−1
SPID(S): Tox21_113825
M4ID: 12482396

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.25 **MAX_MED:** 0.987 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

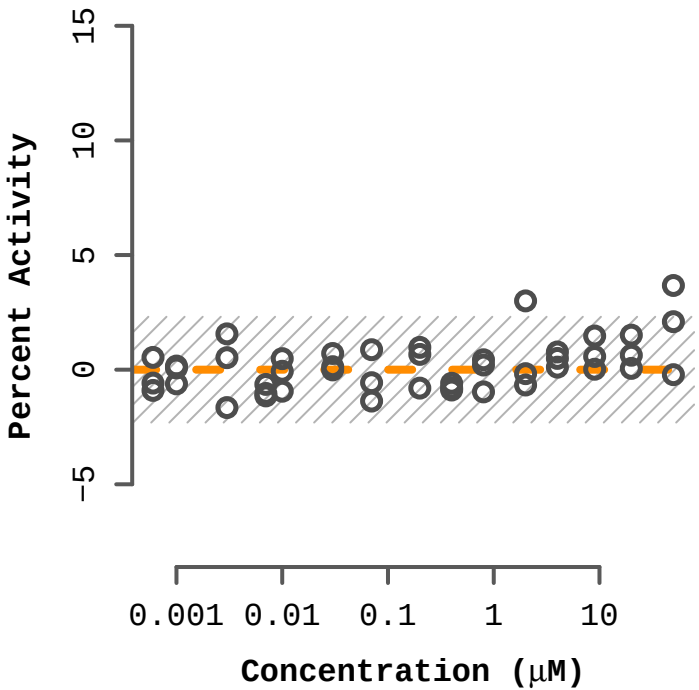
NAME: Nitromersol
CHID: 57638 **CASRN:** 133-58-4
SPID(S): Tox21_113673
M4ID: 12482541

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	243.51	NA	NA
PROB:	1	NA	NA
RMSE:	4.28	NA	NA

MAX_MEAN: 0.786 **MAX_MED:** 0.0877 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

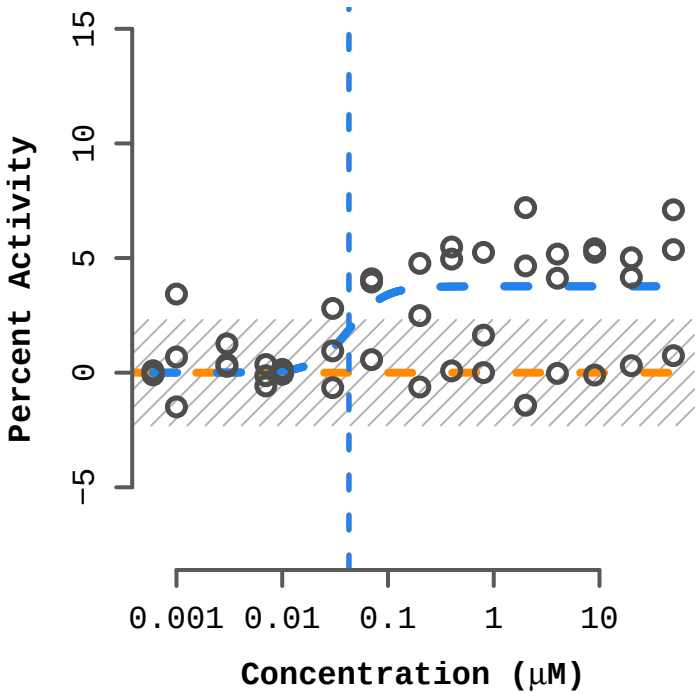
NAME: Odiparcil
CHID: 57639 **CASRN:** 137215-12-4
SPID(S): Tox21_113853
M4ID: 12482370

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.85 **MAX_MED:** 2.1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Octotiamine
CHID: 57640 **CASRN:** 137-86-0
SPID(S): Tox21_113988
M4ID: 12482256

HILL MODEL (in red):

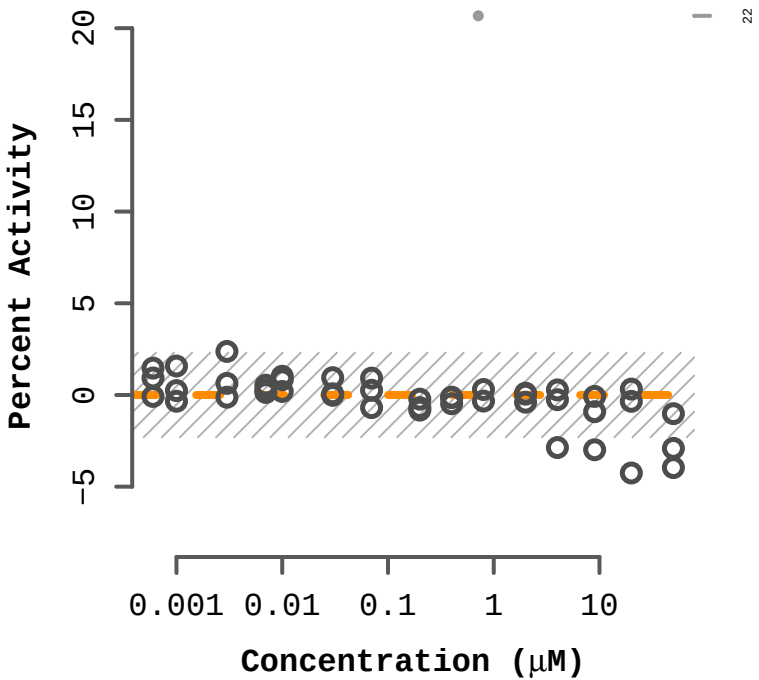
	tp	ga	gw
val:	3.77	−1.37	2.63
sd:	0.6	0.223	4.24

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.77	−1.37	2.63	3.68	6.82
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	236.85	205.2	209.2
PROB:	0	0.88	0.12
RMSE:	3.24	2.13	2.13

MAX_MEAN: 4.41 **MAX_MED:** 5.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

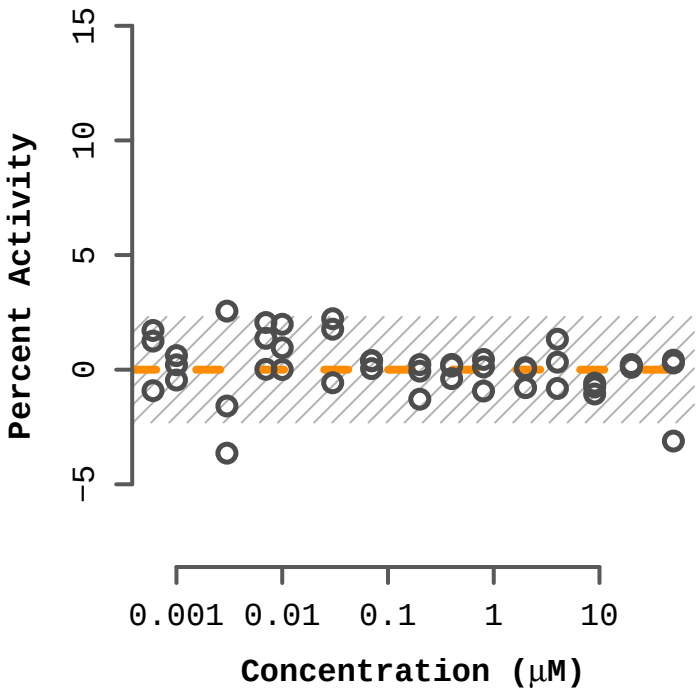
NAME: Mozavaptan
CHID: 57641 **CASRN:** 137975-06-5
SPID(S): Tox21_113926
M4ID: 12482305 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	168.03	NA	NA
PROB:	1	NA	NA
RMSE:	3.59	NA	NA

MAX_MEAN: 7.44 **MAX_MED:** 0.93 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

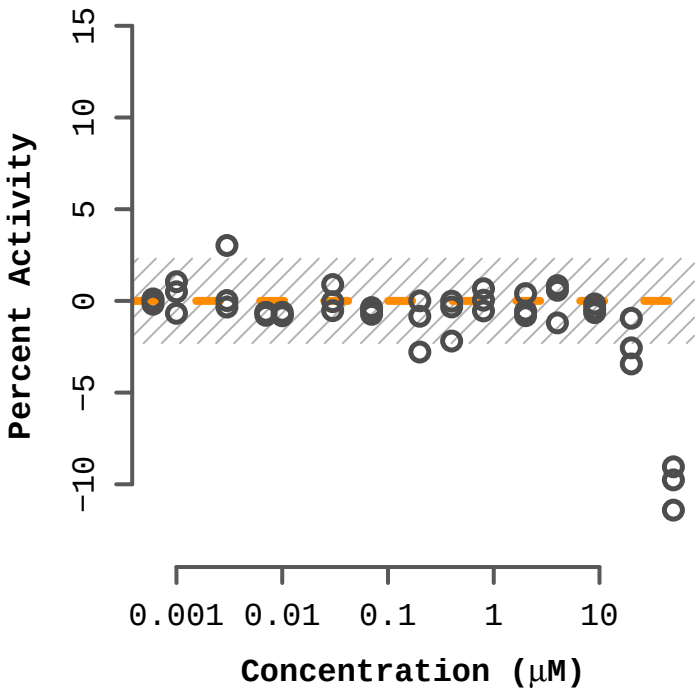
NAME: Agomelatine
CHID: 57642 **CASRN:** 138112-76-2
SPID(S): Tox21_113772
M4ID: 12482443

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.6	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.77 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

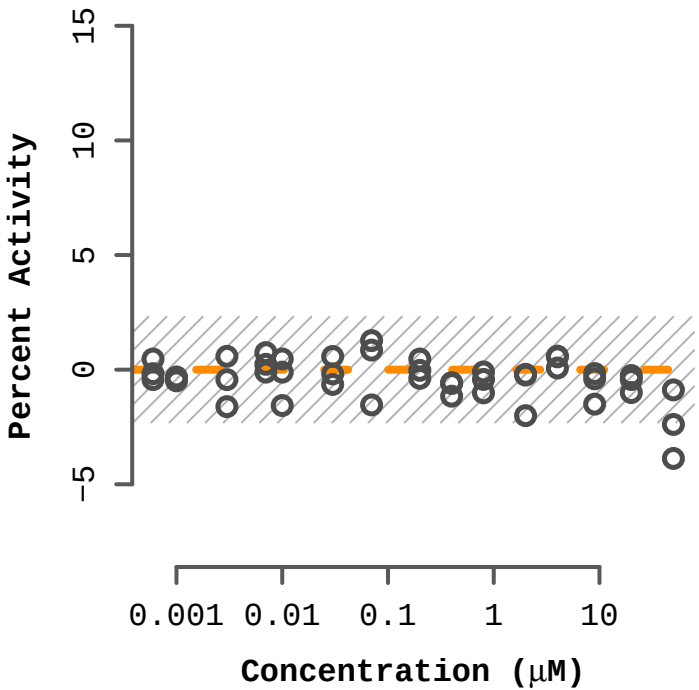
NAME: Cyclomethycaine
CHID: 57643 **CASRN:** 139-62-8
SPID(S): Tox21_113723
M4ID: 12482491

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.97	NA	NA
PROB:	1	NA	NA
RMSE:	2.83	NA	NA

MAX_MEAN: 0.904 **MAX_MED:** 0.58 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

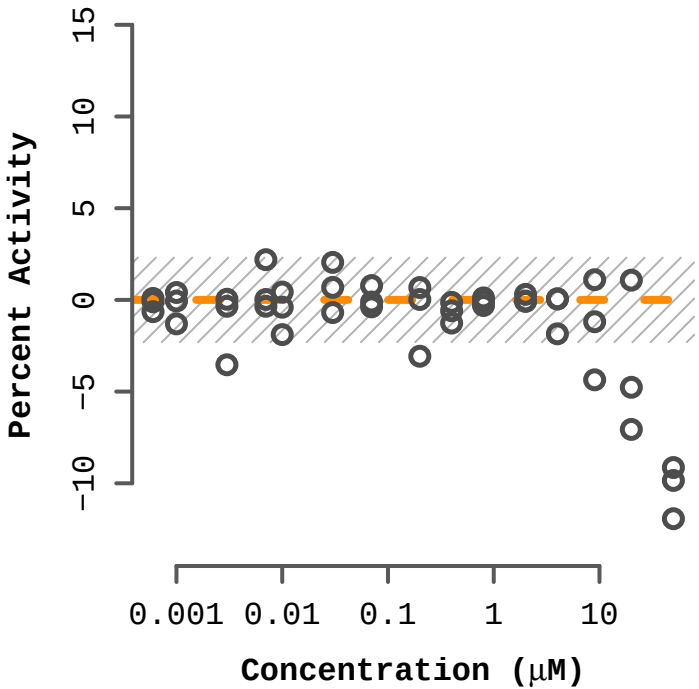
NAME: Darglitazone
CHID: 57644 **CASRN:** 141200-24-0
SPID(S): Tox21_113876
M4ID: 12482349

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 0.41 **MAX_MED:** 0.855 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

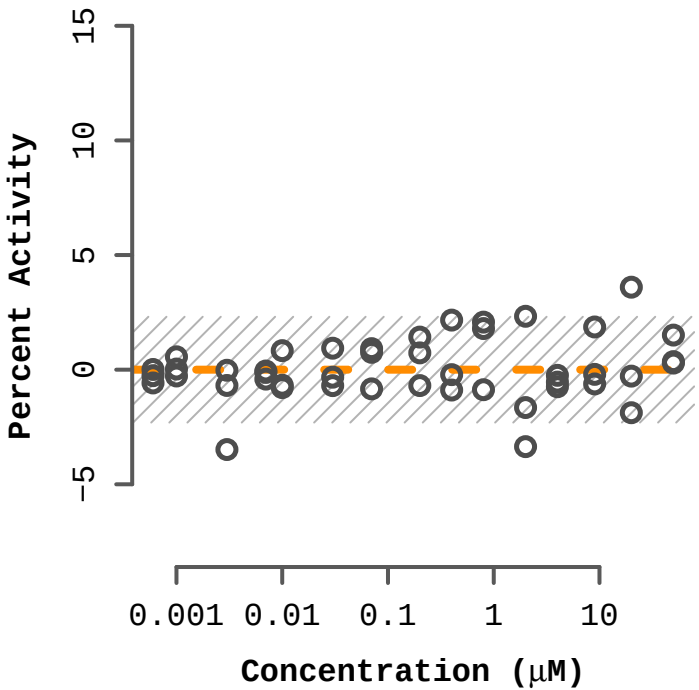
NAME: Methyl 3-amino-5,6-dichloropyrazine-2-carboxyla
CHID: 57645 **CASRN:** 1458-18-0
SPID(S): Tox21_113824
M4ID: 12482397

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	207	NA	NA
PROB:	1	NA	NA
RMSE:	3.21	NA	NA

MAX_MEAN: 0.681 **MAX_MED:** 0.684 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

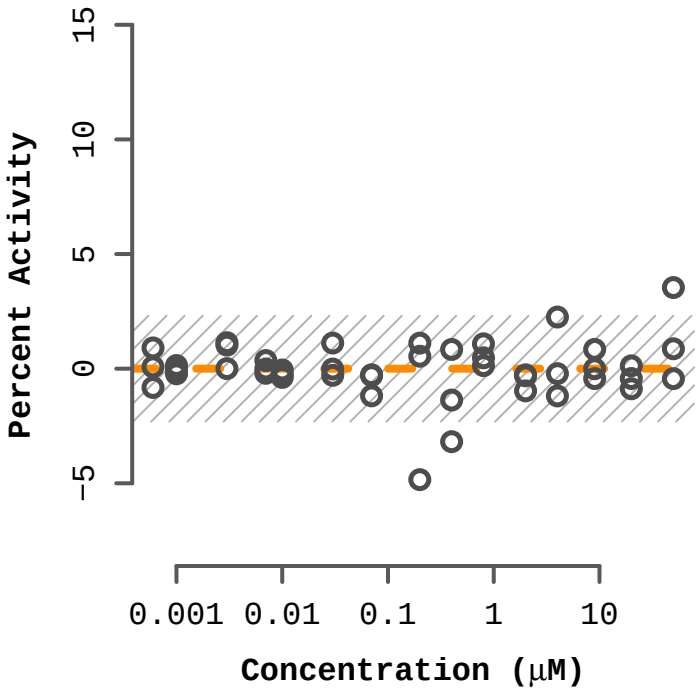
NAME: (4S,6s)-5,6-dihydro-6-methyl-4h-thieno[2,3-b]tl
CHID: 57646 **CASRN:** 147086-81-5
SPID(S): Tox21_113917
M4ID: 12482313

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.98	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 0.999 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

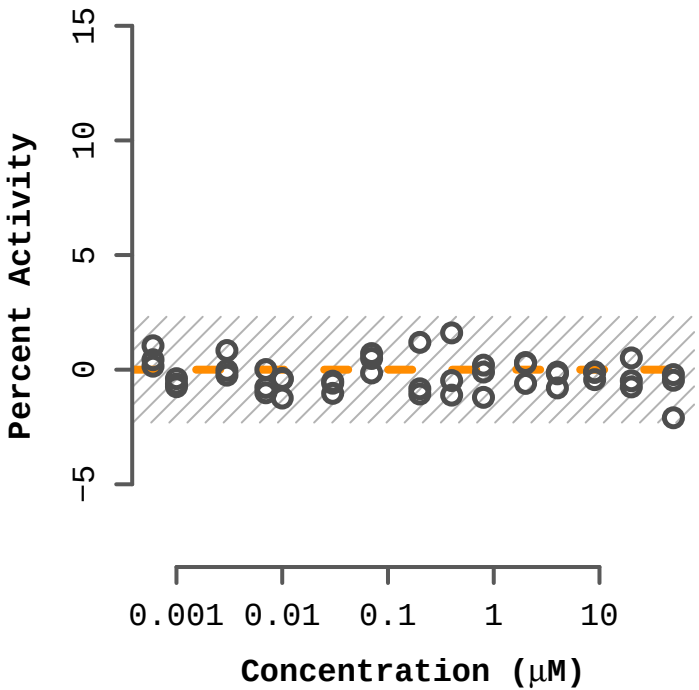
NAME: Cholesolvin
CHID: 57647 **CASRN:** 14929-11-4
SPID(S): Tox21_113699
M4ID: 12482515

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.56	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 1.33 **MAX_MED:** 1.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

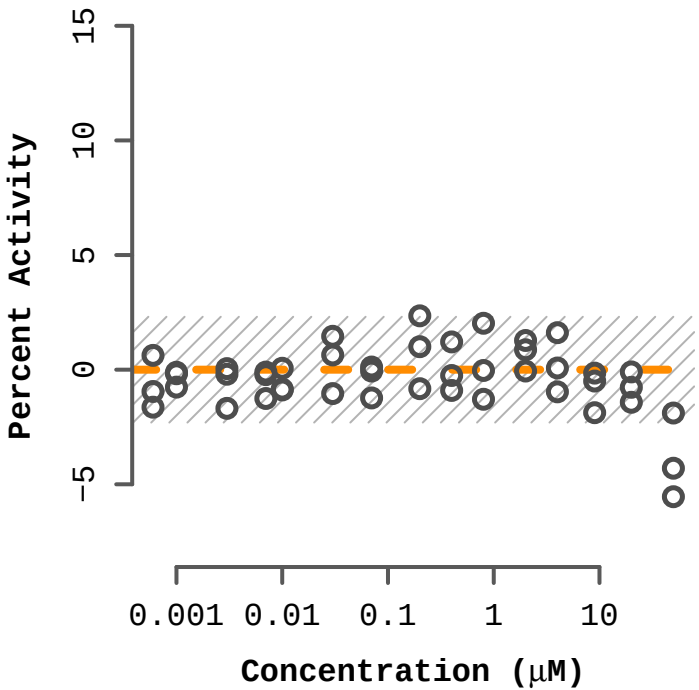
NAME: Tobicillin
CHID: 57648 **CASRN:** 151287-22-8
SPID(S): Tox21_113948
M4ID: 12482283

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	105.6	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.545 **MAX_MED:** 0.489 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

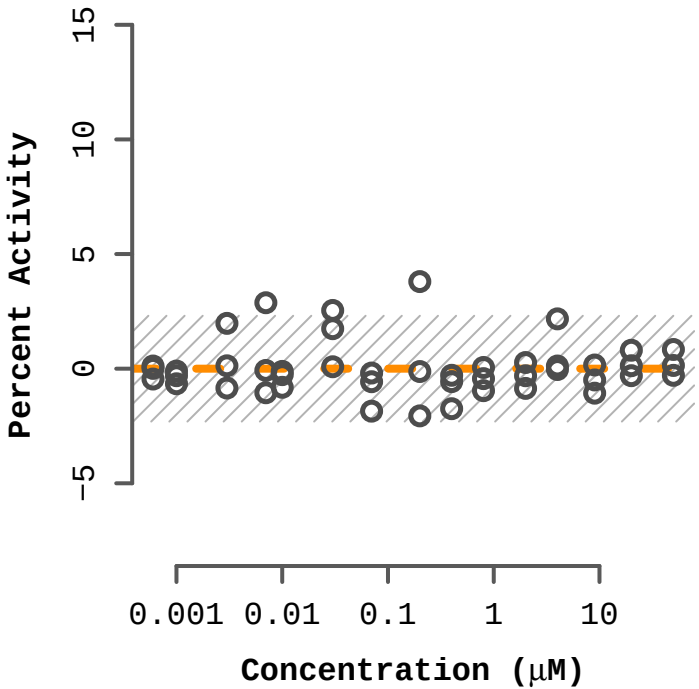
NAME: Pleconaril
CHID: 57649 **CASRN:** 153168-05-9
SPID(S): Tox21_113756
M4ID: 12482459

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

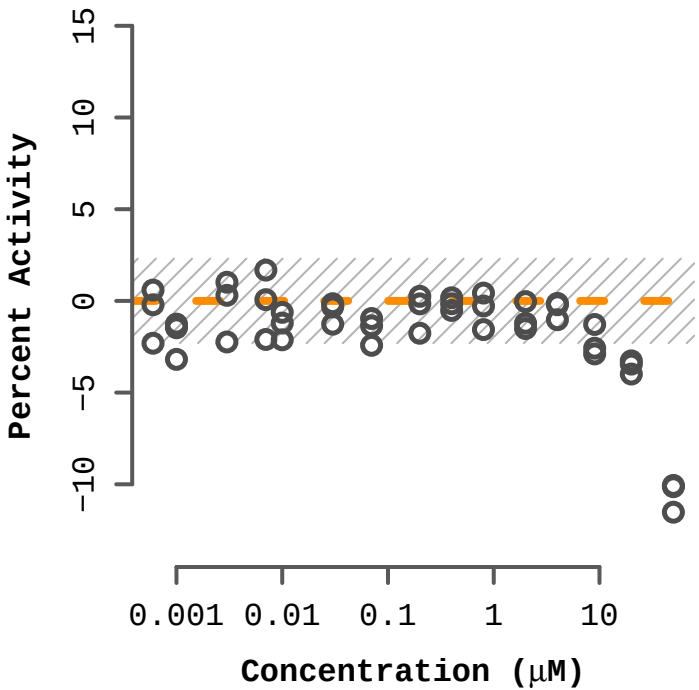
NAME: Metamfepramone
CHID: 57650 **CASRN:** 15351-09-4
SPID(S): Tox21_113894
M4ID: 12482334

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.75	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

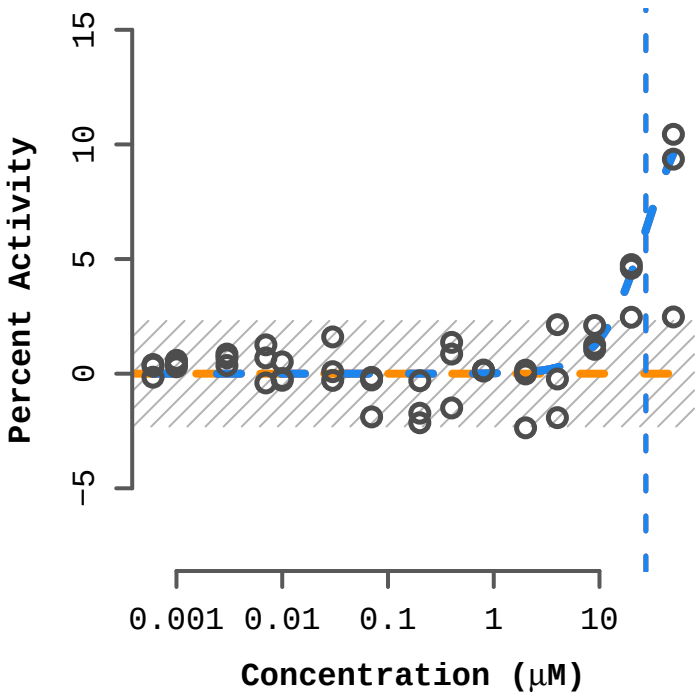
NAME: Simetride
CHID: 57651 **CASRN:** 154-82-5
SPID(S): Tox21_113703
M4ID: 12482511

HILL MODEL: Not applicable.

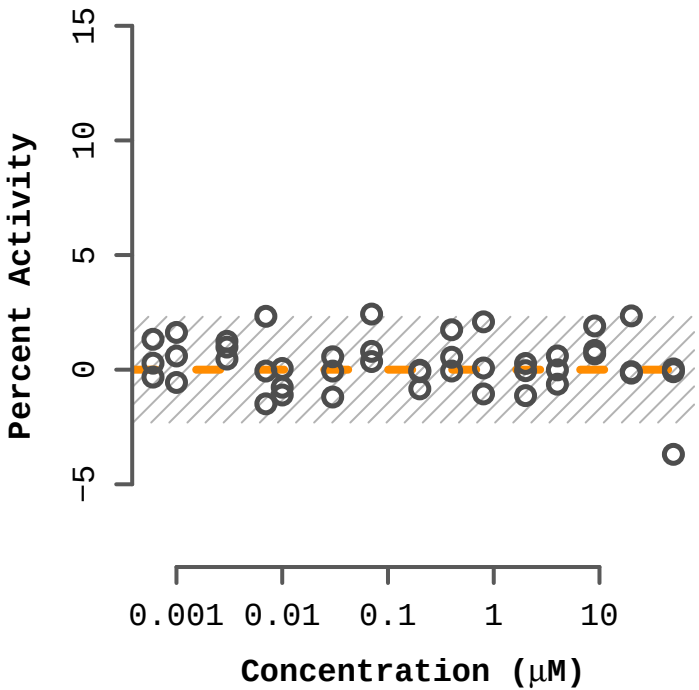
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	212.64	NA	NA
PROB:	1	NA	NA
RMSE:	3.17	NA	NA

MAX_MEAN: −0.117 **MAX_MED:** 0.305 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Istradefylline
CHID:    57652   CASRN: 155270-99-8
SPID(S): Tox21_113855
M4ID:    12482368

HILL MODEL (in red):
      tp       ga       gw
val:  12.5     1.44     1.98
sd:   3.12     0.145    0.569

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  12.5     1.44     1.98     3.61     3.76
sd:   3.13     0.145    0.569    1130     2250

      CNST        HILL        GNLS
AIC:  189.26      147.92      151.92
PROB: 0           0.88        0.12
RMSE: 2.57        1.45        1.45

MAX_MEAN: 7.43      MAX_MED: 9.36      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

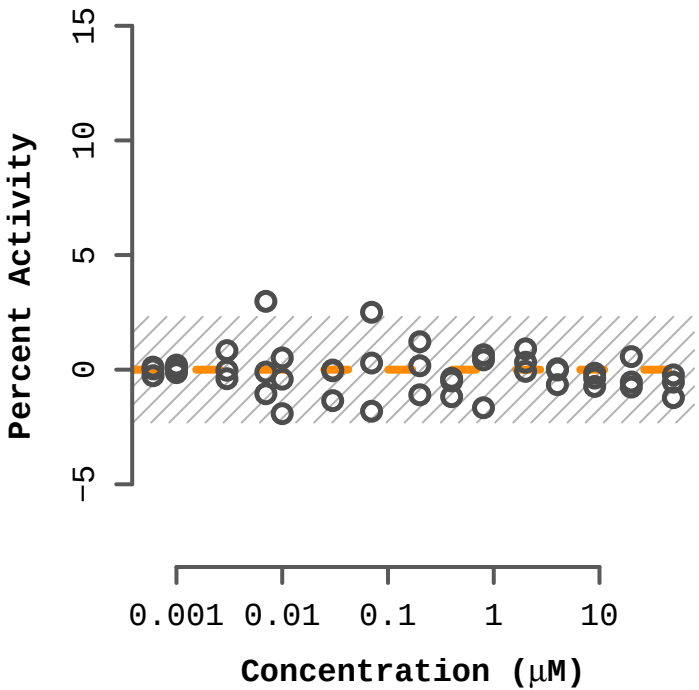
NAME: Nepaprazole
CHID: 57653 **CASRN:** 156601-79-5
SPID(S): Tox21_113728
M4ID: 12482486

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.19 **MAX_MED:** 0.986 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

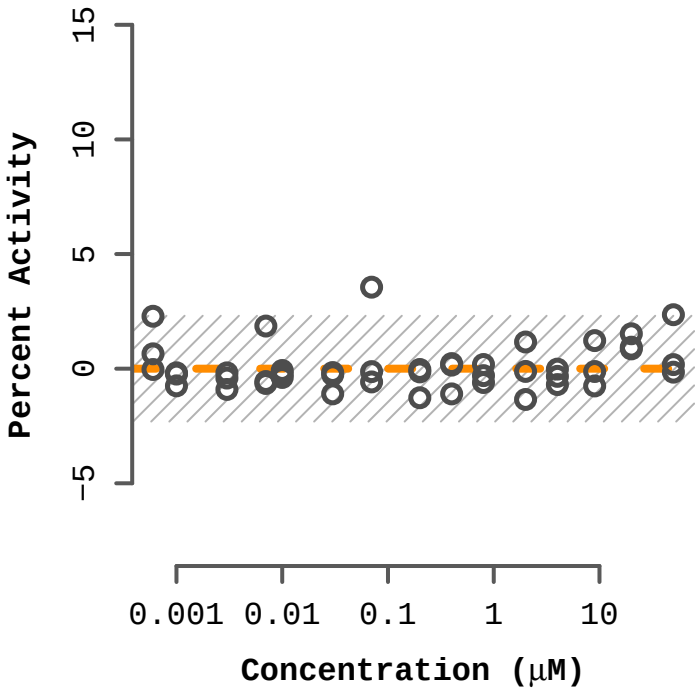
NAME: Embutramide
CHID: 57654 **CASRN:** 15687-14-6
SPID(S): Tox21_113716
M4ID: 12482498

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.61 **MAX_MED:** 0.429 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

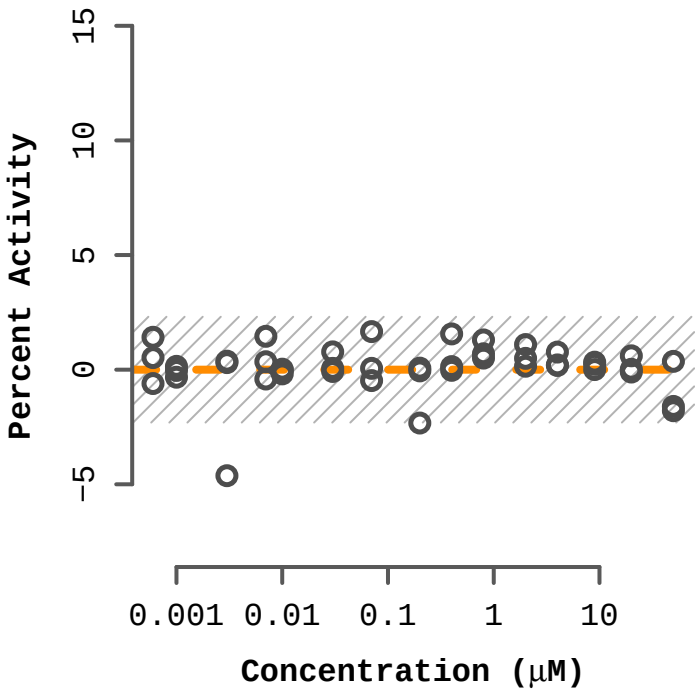
NAME: Alatrofloxacin mesylate
CHID: 57655 **CASRN:** 146961-77-5
SPID(S): Tox21_113889
M4ID: 12482337

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.62	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 0.939 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

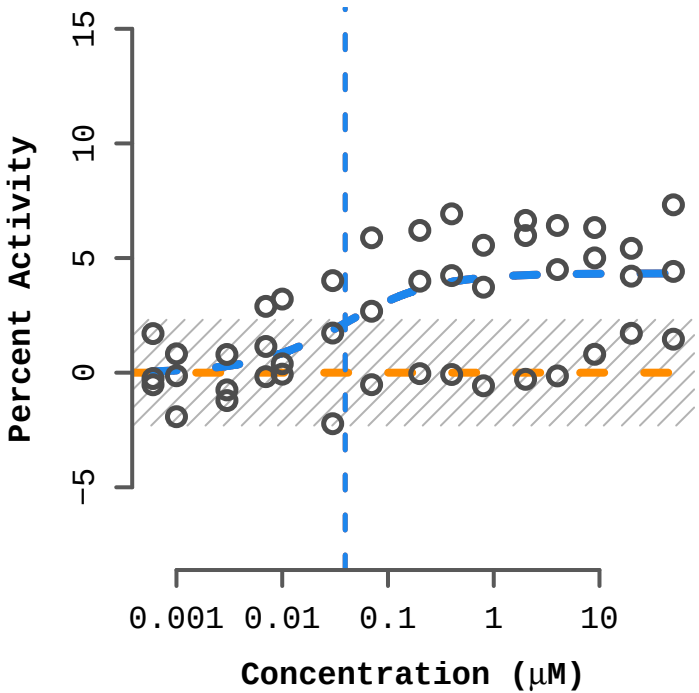
NAME: 2-Bromo-4'-chloro-2'-(2-fluorobenzoyl)acetanil
CHID: 57656 **CASRN:** 1584-62-9
SPID(S): Tox21_113843
M4ID: 12482379

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 0.834 **MAX_MED:** 0.696 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Norfentanyl
CHID: 57657 CASRN: 1609-66-1
SPID(S): Tox21_113943
M4ID: 12482288

HILL MODEL (in red):

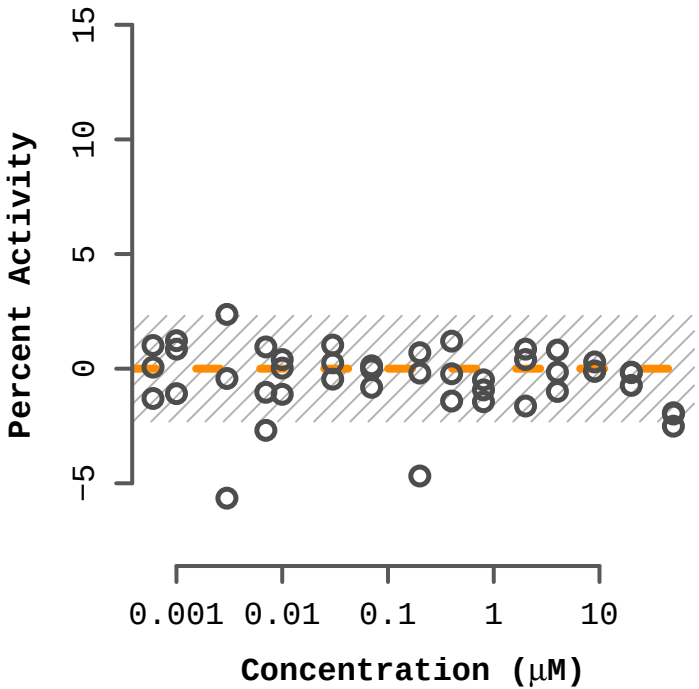
	tp	ga	gw
val:	4.33	−1.4	1.02
sd:	0.643	0.396	0.611

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.33	−1.4	1.02	2.77	6.74
sd:	0.643	0.396	0.611	1850	11800

	CNST	HILL	GNLS
AIC:	249.14	213.09	217.09
PROB:	0	0.88	0.12
RMSE:	3.64	2.27	2.27

MAX_MEAN: 4.4 MAX_MED: 5.98 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

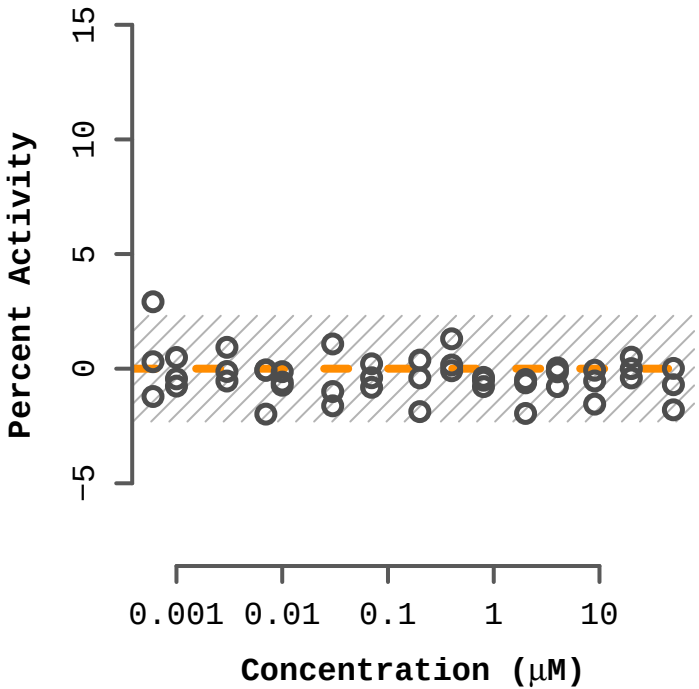
NAME: 3,5-Di-tert-butyl-4-hydroxybenzaldehyde
CHID: 57658 **CASRN:** 1620-98-0
SPID(S): Tox21_113770
M4ID: 12482445

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	158.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.53	NA	NA

MAX_MEAN: 0.33 **MAX_MED:** 0.853 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

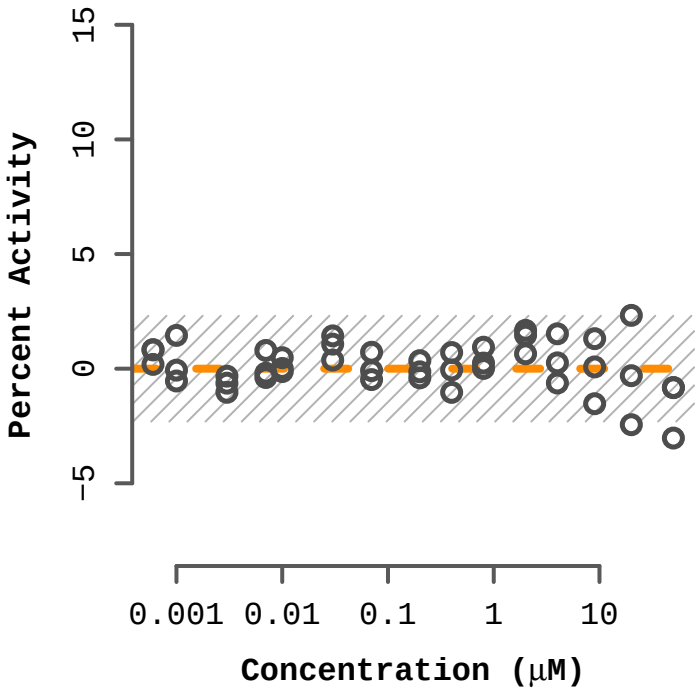
NAME: Clevudine
CHID: 57659 **CASRN:** 163252-36-6
SPID(S): Tox21_113880
M4ID: 12482345

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.8	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.671 **MAX_MED:** 0.305 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

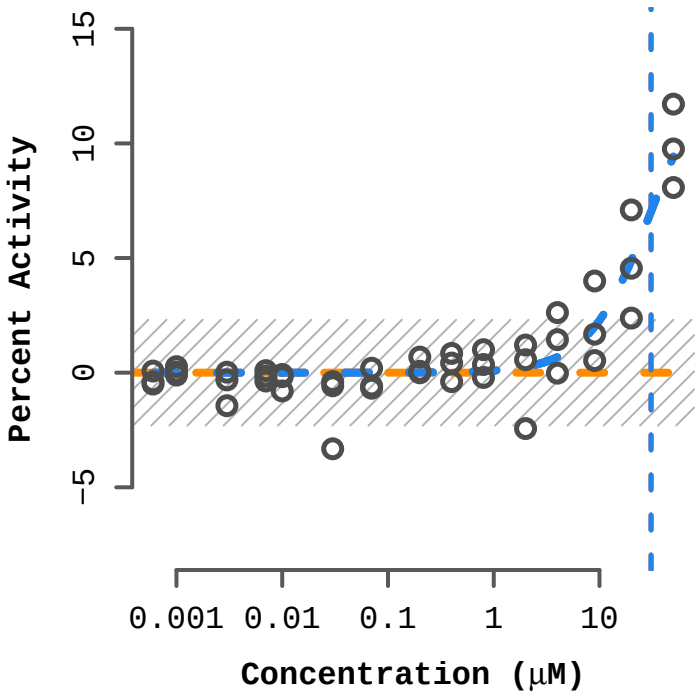
NAME: N-(2-(4-sulfamoyl)phenyl)ethyl-5-chloro-2-meth
CHID: 57660 **CASRN:** 16673-34-0
SPID(S): Tox21_113826
M4ID: 12482395

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.19	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.26 **MAX_MED:** 1.46 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Clevidipine
CHID: 57661 CASRN: 167221-71-8
SPID(S): Tox21_113923
M4ID: 12482308

HILL MODEL (in red):

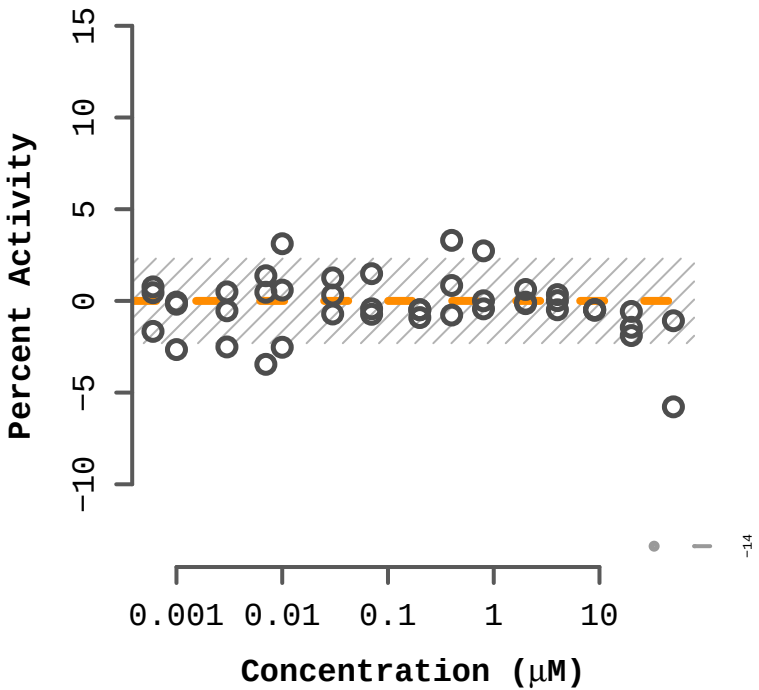
	tp	ga	gw
val:	14.1	1.49	1.46
sd:	4.41	0.216	0.461

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	14.1	1.49	1.46	3.68	4.88
sd:	4.41	0.216	0.461	8990	22200

	CNST	HILL	GNLS
AIC:	202.59	139.85	143.85
PROB:	0	0.88	0.12
RMSE:	3.09	1.12	1.12

MAX_MEAN: 9.85 MAX_MED: 9.76 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

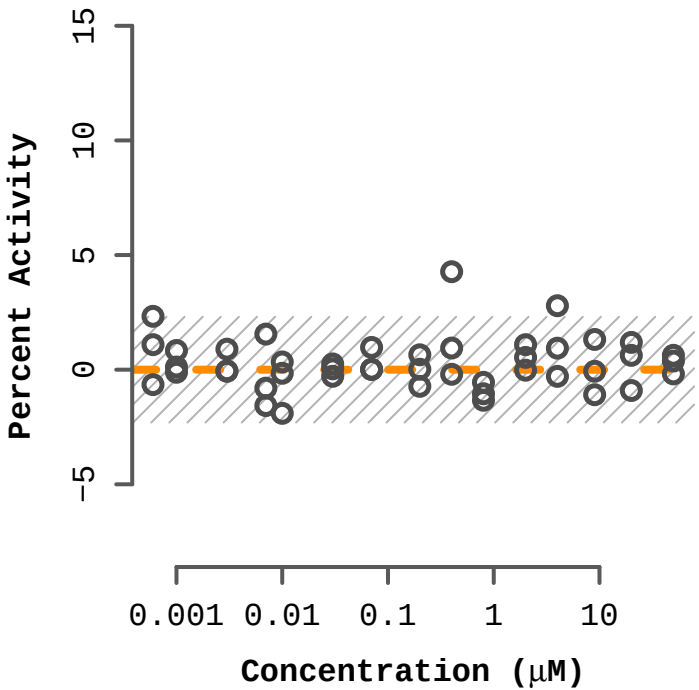
NAME: LY335979 trihydrochloride
CHID: 57662 CASRN: 167465-36-3
SPID(S): Tox21_113964
M4ID: 12482269 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.84	NA	NA
PROB:	1	NA	NA
RMSE:	2.59	NA	NA

MAX_MEAN: 1.13 **MAX_MED:** 0.842 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

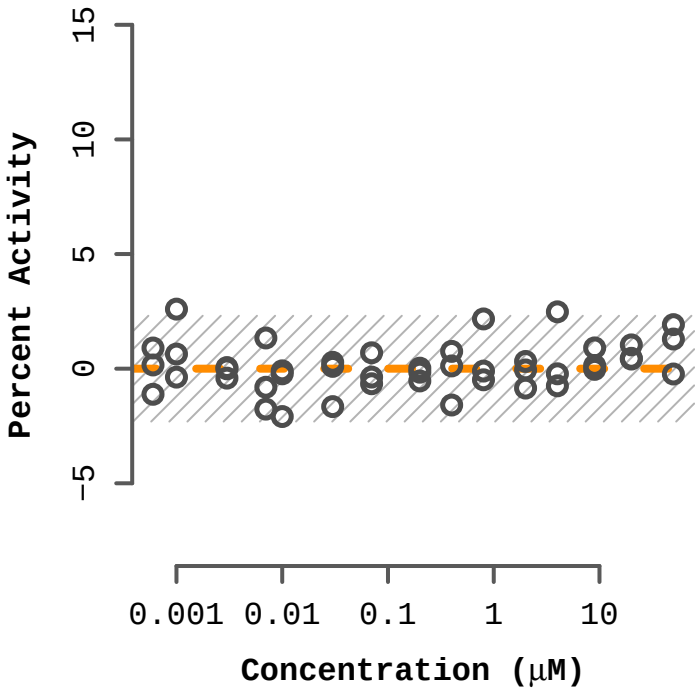
NAME: Pmic chloride
CHID: 57663 **CASRN:** 16883-16-2
SPID(S): Tox21_113795
M4ID: 12482424

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

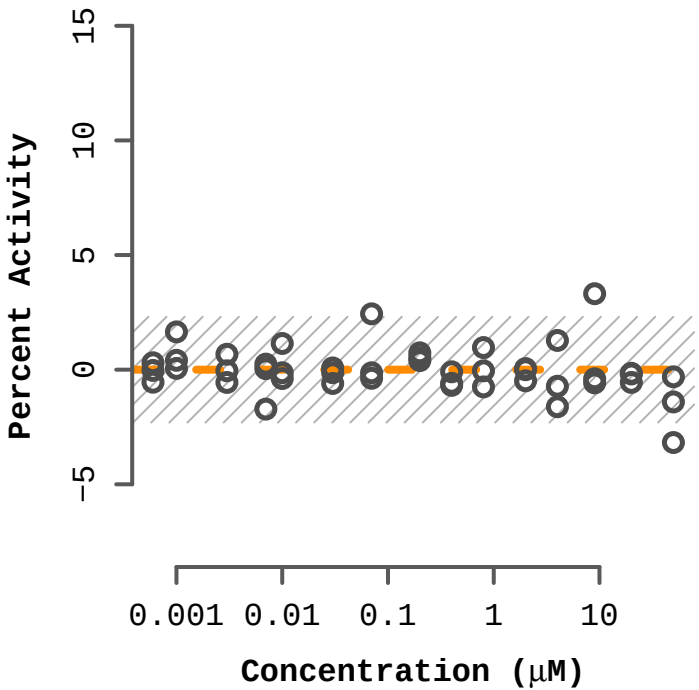
NAME: Darusentan
CHID: 57664 **CASRN:** 171714-84-4
SPID(S): Tox21_113760
M4ID: 12482455

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 0.995 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

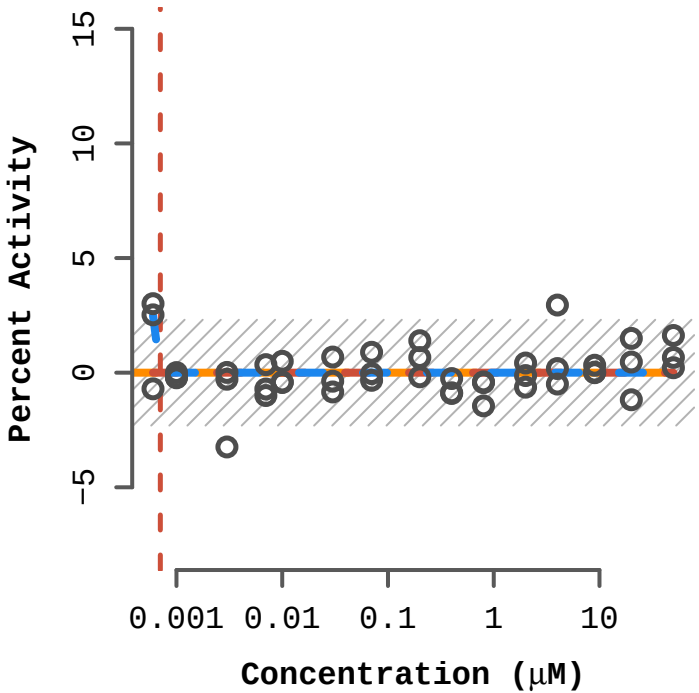
NAME: Mefenorex
CHID: 57665 **CASRN:** 17243-57-1
SPID(S): Tox21_113684
M4ID: 12482530

HILL MODEL: Not applicable.

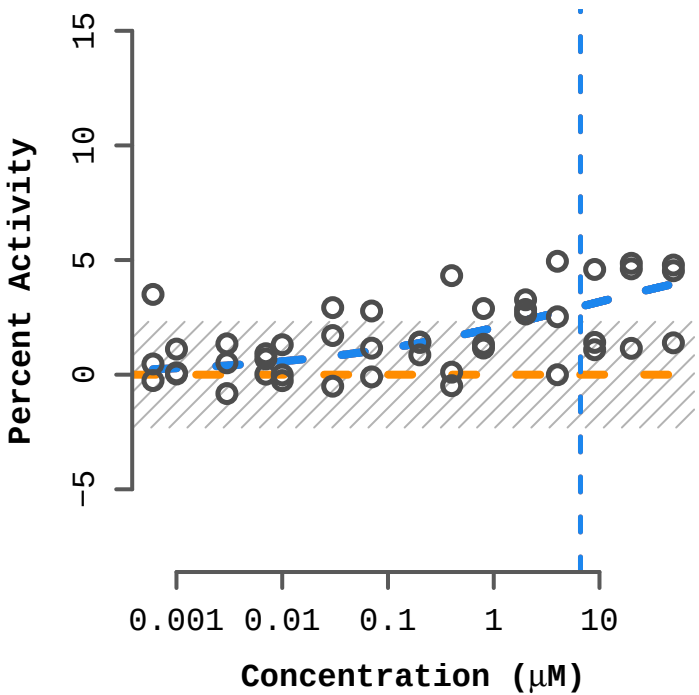
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	122.23	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 0.781 **MAX_MED:** 0.528 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Lacosamide
CHID:    57666   CASRN: 175481-36-4
SPID(S): Tox21_113857
M4ID:    12482366

HILL MODEL (in red):
      tp        ga        gw
val:  6.22e-11  -3.15     1.87
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.61      -4.89     7.97      -3.2      18
sd:   NA        NA        NA        NA        NA

      CNST         HILL         GNLS
AIC:  130.39       136.39       133.27
PROB: 0.78         0.04         0.18
RMSE: 1.1          1.1          1.04

MAX_MEAN: 1.61      MAX_MED: 2.52      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Chlorooxindole
CHID: 57667 **CASRN:** 17630-75-0
SPID(S): Tox21_113839
M4ID: 12482383

HILL MODEL (in red):

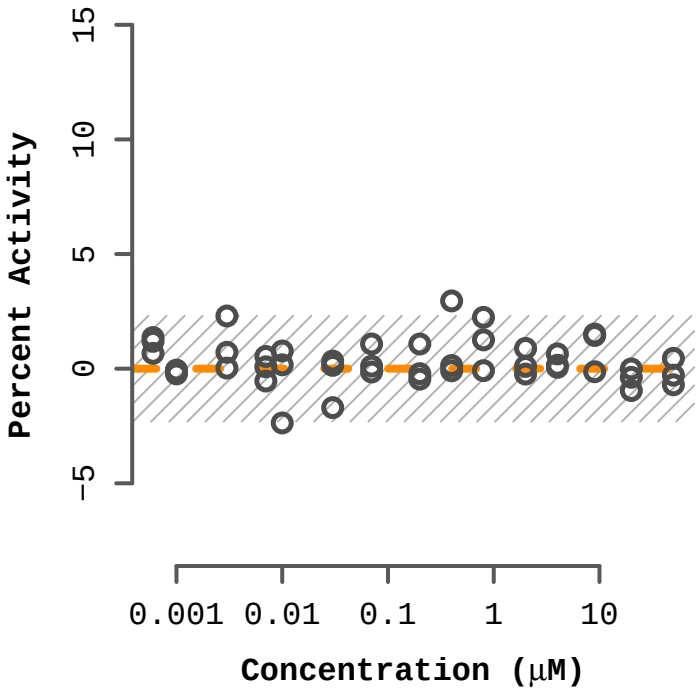
	tp	ga	gw
val:	5.94	0.82	0.341
sd:	3.52	1.58	0.144

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.94	0.82	0.341	2.82	6.94
sd:	3.52	1.58	0.144	1800	11100

	CNST	HILL	GNLS
AIC:	207.49	165.44	169.44
PROB:	0	0.88	0.12
RMSE:	2.35	1.36	1.36

MAX_MEAN: 3.57 **MAX_MED:** 4.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

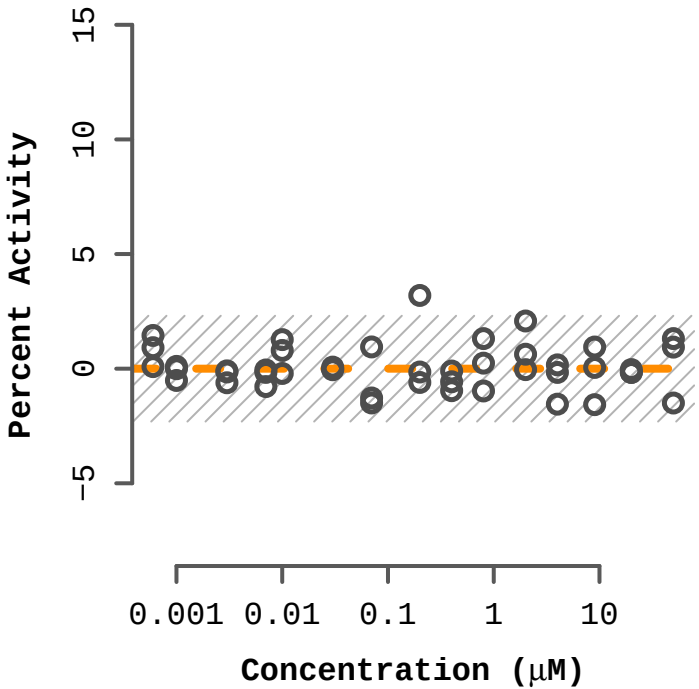
NAME: Iothalamate sodium
CHID: 57668 **CASRN:** 1225-20-3
SPID(S): Tox21_113735
M4ID: 12482479

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.24	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

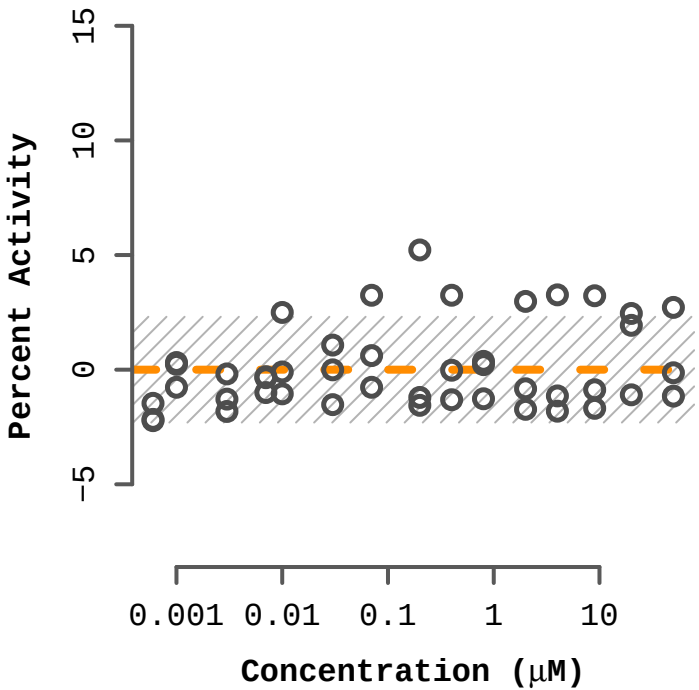
NAME: (4-Carboxybutyl)triphenylphosphonium bromide
CHID: 57669 **CASRN:** 17814-85-6
SPID(S): Tox21_113895
M4ID: 12482333

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.68	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.89 **MAX_MED:** 0.941 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

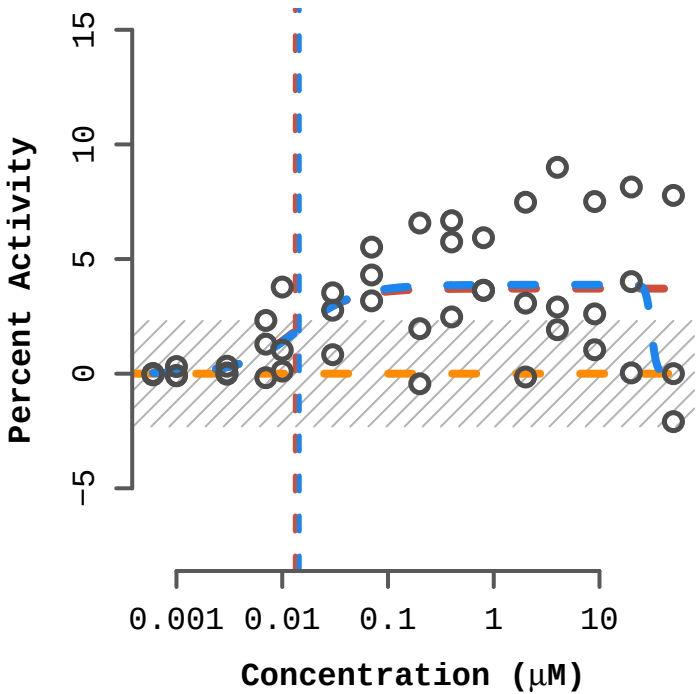
NAME: Prucalopride
CHID: 57670 **CASRN:** 179474-81-8
SPID(S): Tox21_113885
M4ID: 12482340

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.16	NA	NA
PROB:	1	NA	NA
RMSE:	1.81	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.94 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tilmacoxib
CHID: 57671 **CASRN:** 180200-68-4
SPID(S): Tox21_113701
M4ID: 12482513

HILL MODEL (in red):

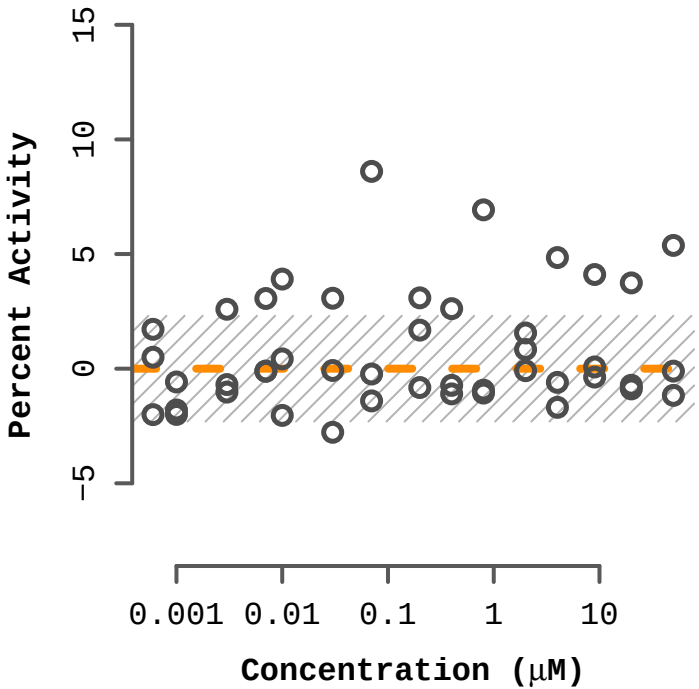
	tp	ga	gw
val:	3.71	−1.88	1.67
sd:	0.554	0.258	1.04

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.88	−1.84	1.59	1.49	17.8
sd:	0.549	0.244	0.892	1.97	176

	CNST	HILL	GNLS
AIC:	251.54	213.53	213.41
PROB:	0	0.48	0.52
RMSE:	3.85	2.36	2.35

MAX_MEAN: 4.97 **MAX_MED:** 5.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

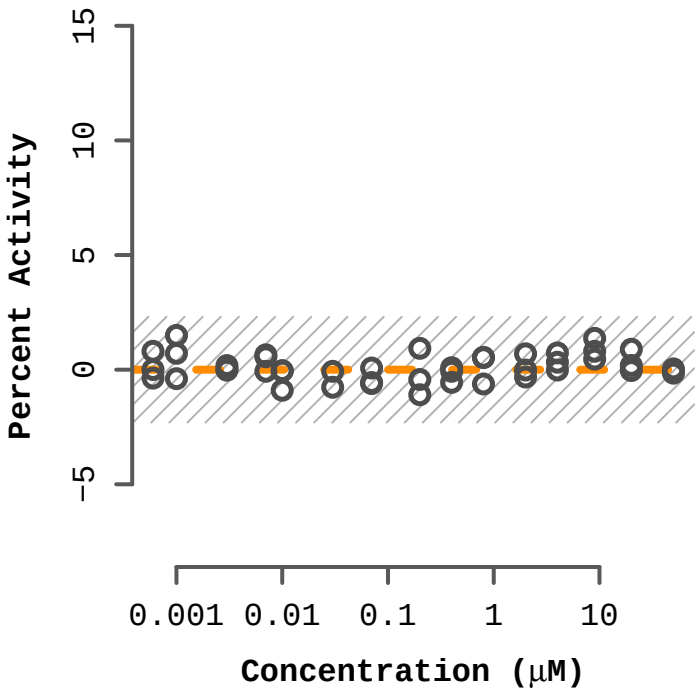
NAME: Pipoxolan hydrochloride
CHID: 57672 **CASRN:** 18174-58-8
SPID(S): Tox21_113956
M4ID: 12482275

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	211.62	NA	NA
PROB:	1	NA	NA
RMSE:	2.62	NA	NA

MAX_MEAN: 2.32 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

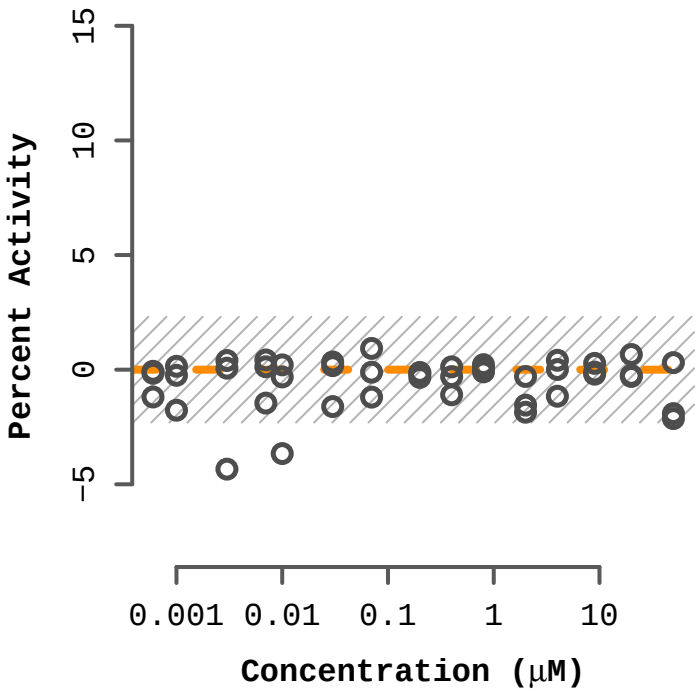
NAME: Sitaxentan
CHID: 57673 **CASRN:** 184036-34-8
SPID(S): Tox21_113725
M4ID: 12482489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	81.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.58	NA	NA

MAX_MEAN: 0.877 **MAX_MED:** 0.803 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

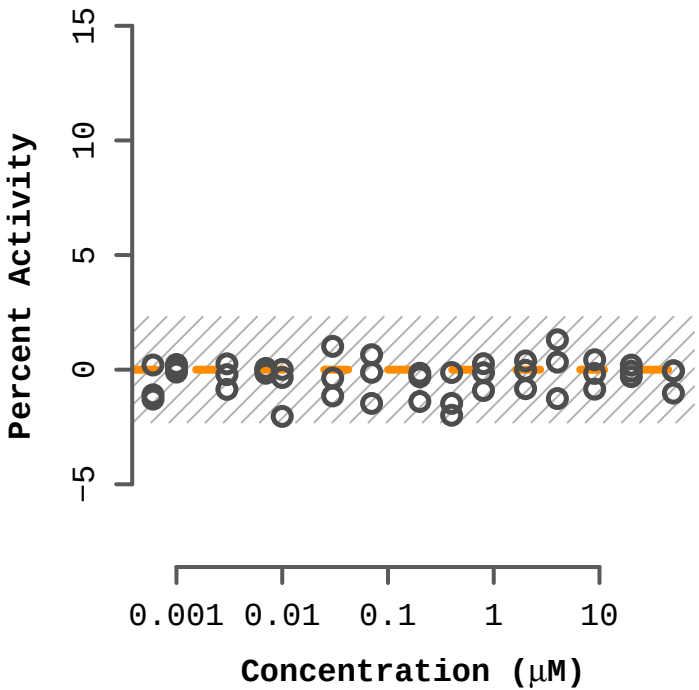
NAME: 3-Trifluoromethylisobutyranilide
CHID: 57674 **CASRN:** 1939-27-1
SPID(S): Tox21_113916
M4ID: 12482314

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.79	NA	NA
PROB:	1	NA	NA
RMSE:	1.18	NA	NA

MAX_MEAN: 0.0635 **MAX_MED:** 0.177 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

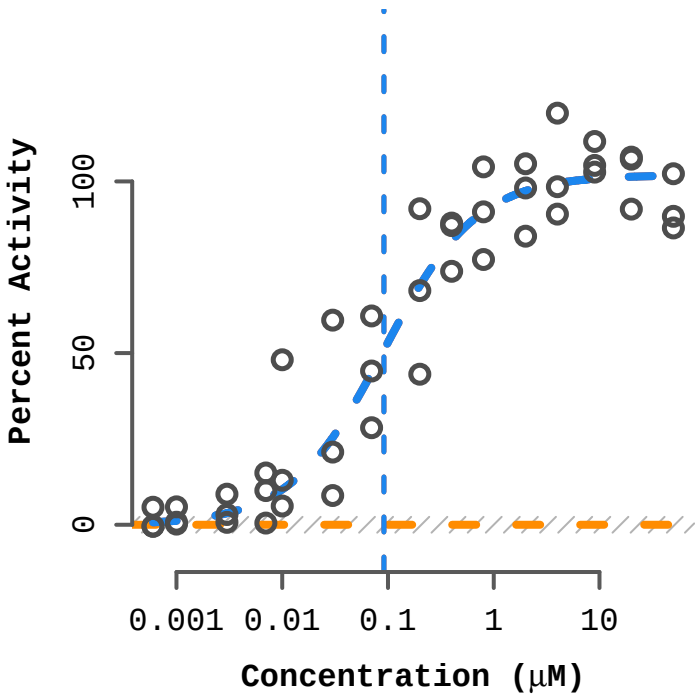
NAME: Variotin
CHID: 57676 CASRN: 19504-77-9
SPID(S): Tox21_113727
M4ID: 12482487

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.126 **MAX_MED:** 0.329 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bolandiol dipropionate
CHID: 57677 CASRN: 1986-53-4
SPID(S): Tox21_113721
M4ID: 12482493

HILL MODEL (in red):

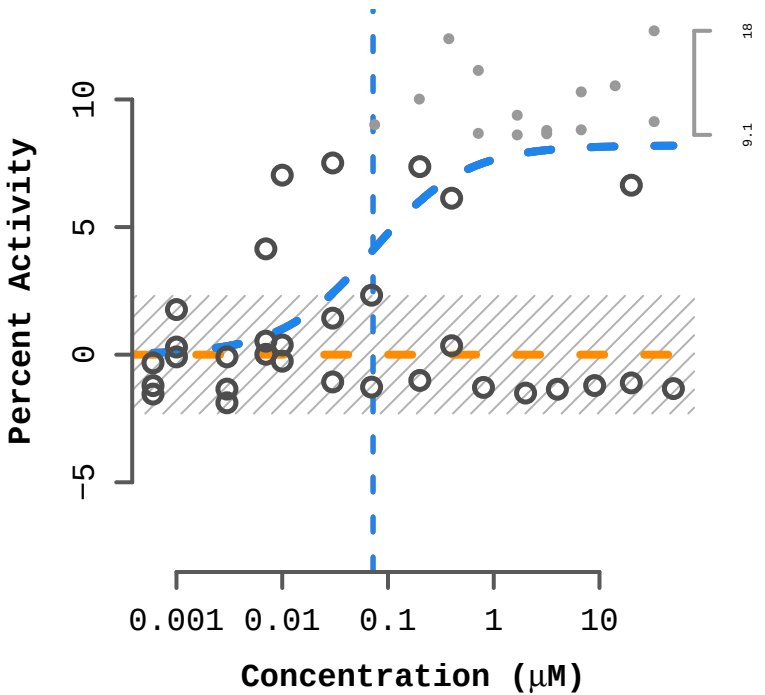
	tp	ga	gw
val:	102	-1.04	0.987
sd:	3.09	0.0846	0.136

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	102	-1.04	0.987	3.1	17.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	519.49	355.95	359.95
PROB:	0	0.88	0.12
RMSE:	70.83	12.2	12.2

MAX_MEAN: 106 **MAX_MED:** 106 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bilastine
CHID: 57678 CASRN: 202189-78-4
SPID(S): Tox21_113905
M4ID: 12482325 BRK

HILL MODEL (in red):

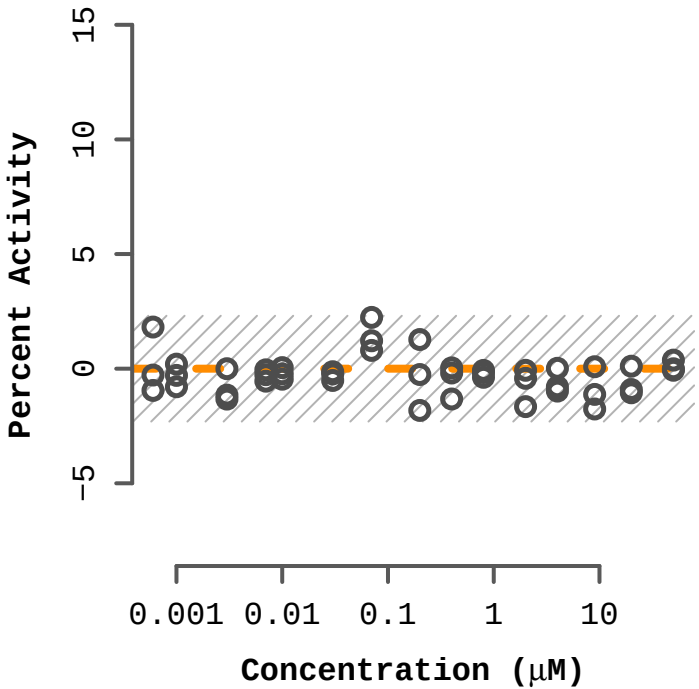
	tp	ga	gw
val:	8.2	−1.14	0.995
sd:	1.58	0.452	0.702

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.2	−1.14	0.995	3.39	18
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	307.08	282.52	286.52
PROB:	0	0.88	0.12
RMSE:	7.19	5.01	5.01

MAX_MEAN: 8.84 MAX_MED: 10.2 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

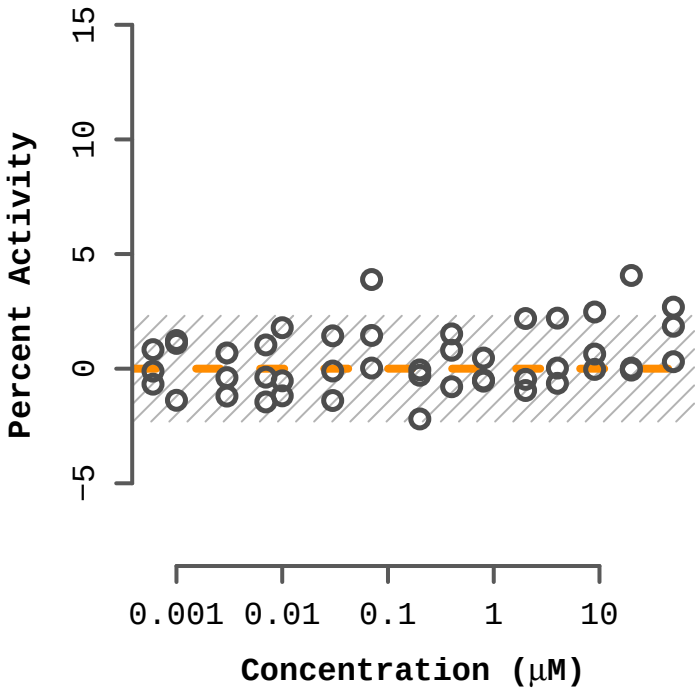
NAME: Benzimidazolone
CHID: 57679 **CASRN:** 20662-53-7
SPID(S): Tox21_113910
M4ID: 12482320

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

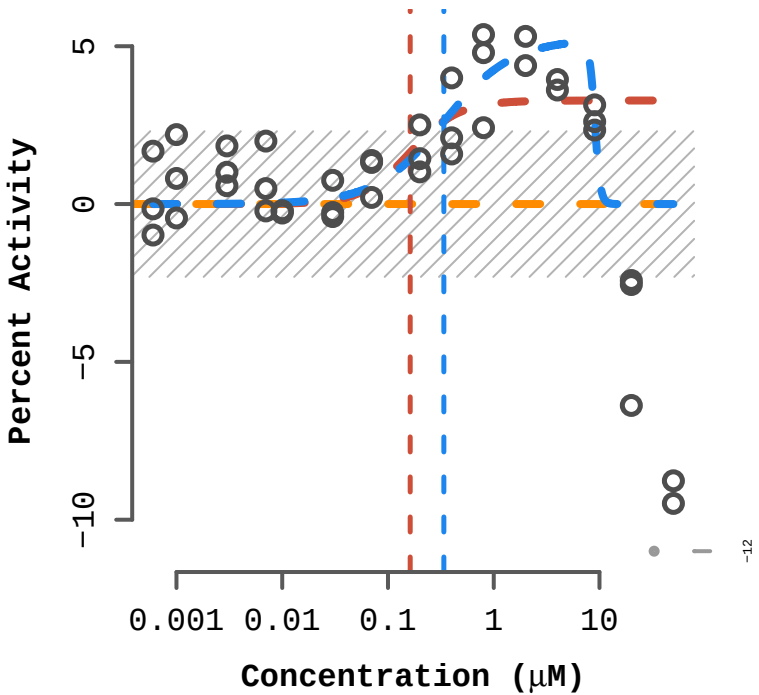
NAME: 5,6-Dimethoxy-1-indanone
CHID: 57680 **CASRN:** 2107-69-9
SPID(S): Tox21_113806
M4ID: 12482413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.54	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dabigatran etexilate
CHID: 57681 CASRN: 211915-06-9
SPID(S): Tox21_113924
M4ID: 12482307 BRK

HILL MODEL (in red):

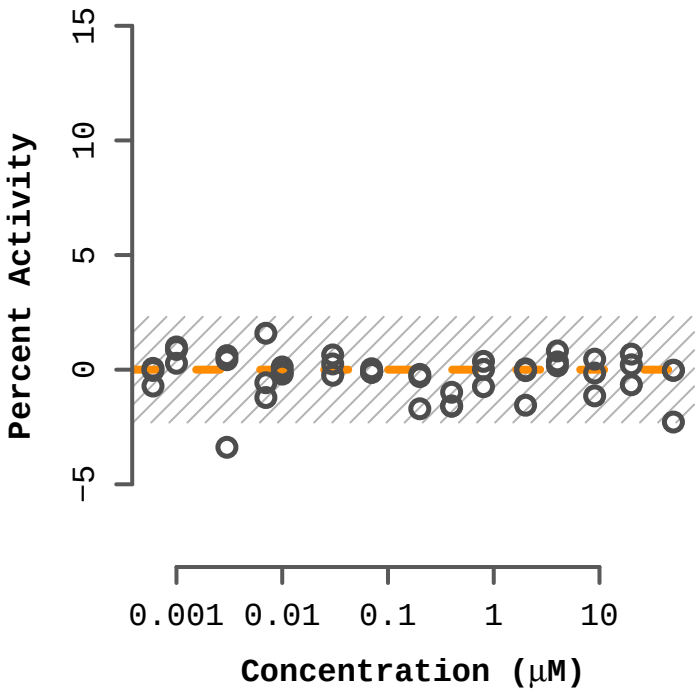
	tp	ga	gw
val:	3.28	−0.79	1.91
sd:	0.599	0.284	1.19

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	5.23	−0.472	1.35	0.957	16.9
sd:	0.892	0.186	0.697	0.0341	237

	CNST	HILL	GNLS
AIC:	245.55	231.63	205.35
PROB:	0	0	1
RMSE:	3.79	4.1	2.98

MAX_MEAN: 5.23 MAX_MED: 5.31 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

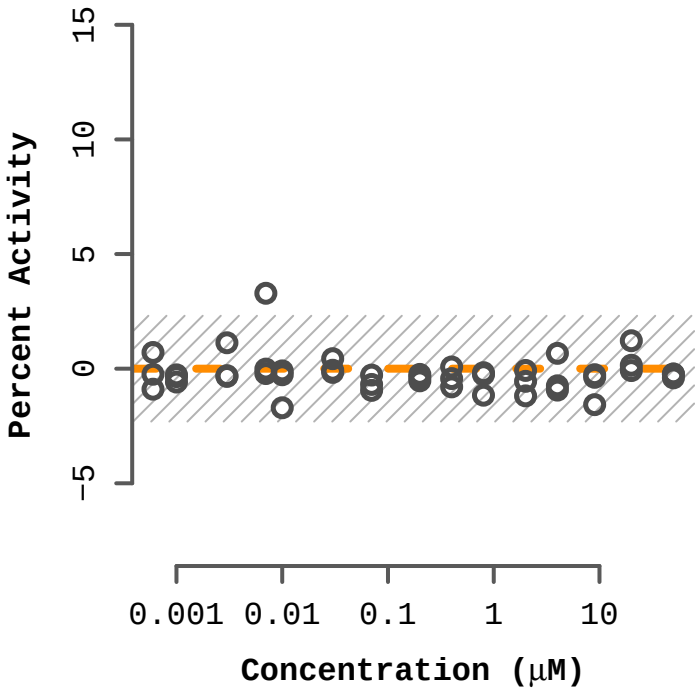
NAME: Dorastine
CHID: 57682 CASRN: 21228-13-7
SPID(S): Tox21_113845
M4ID: 12482377

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	117.43	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.718 **MAX_MED:** 0.883 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

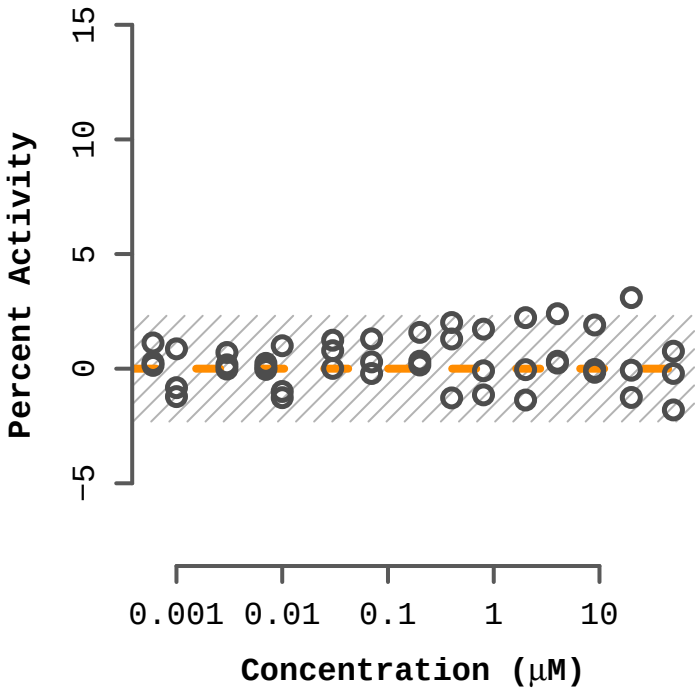
NAME: Chlorexolone
CHID: 57683 **CASRN:** 2127-01-7
SPID(S): Tox21_113742
M4ID: 12482472

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.53	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.15 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

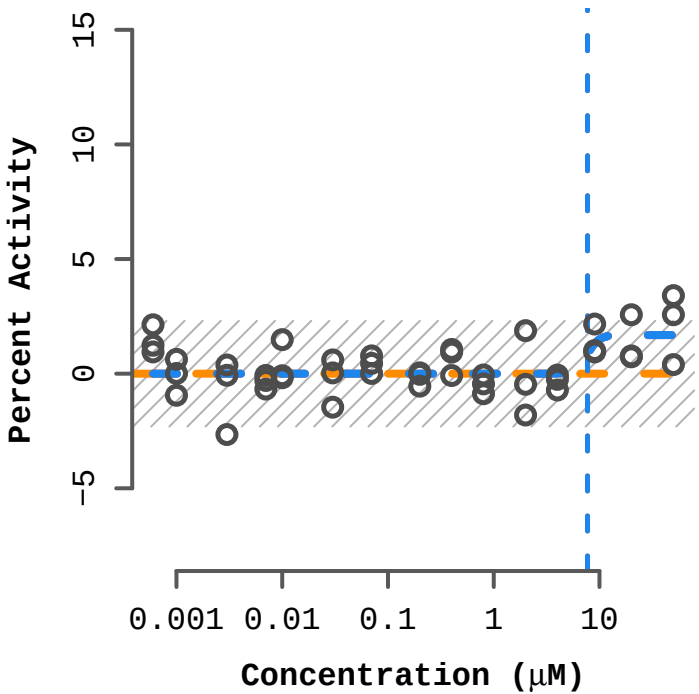
NAME: 2,3,4−Trihydroxybenzaldehyde
CHID: 57684 **CASRN:** 2144−08−3
SPID(S): Tox21_113928
M4ID: 12482303

HILL MODEL: Not applicable.

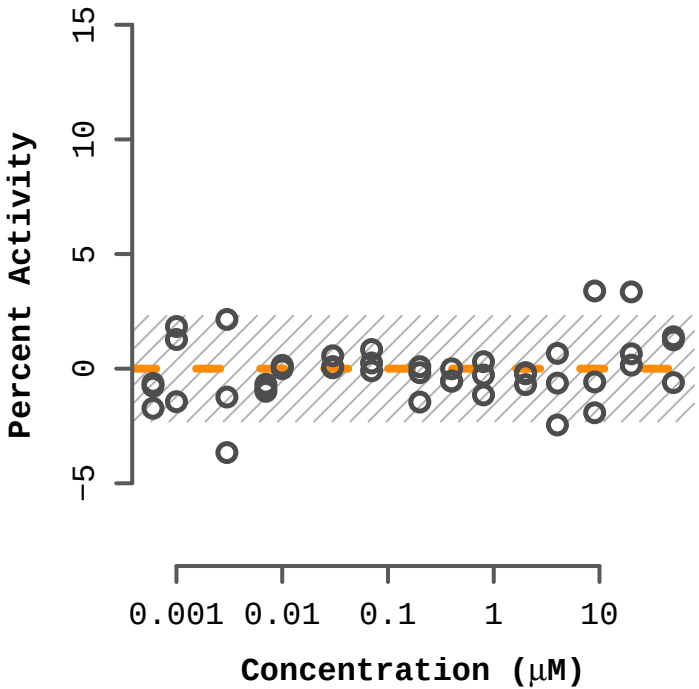
GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 0.99 **MAX_MED:** 1.3 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Brofoxine
CHID:    57685   CASRN: 21440-97-1
SPID(S): Tox21_113781
M4ID:    12482436

HILL MODEL (in red):
      tp       ga       gw
val:  1.68     0.887    8
sd:   0.559    0.124    10.1

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.68     0.887    8        2.73     8.81
sd:   0.559    0.124    10.1     3520     30100

      CNST        HILL        GNLS
AIC:  144.29      132.52      136.52
PROB: 0           0.88        0.12
RMSE: 1.2         0.96        0.96

MAX_MEAN: 2.13      MAX_MED: 2.57      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

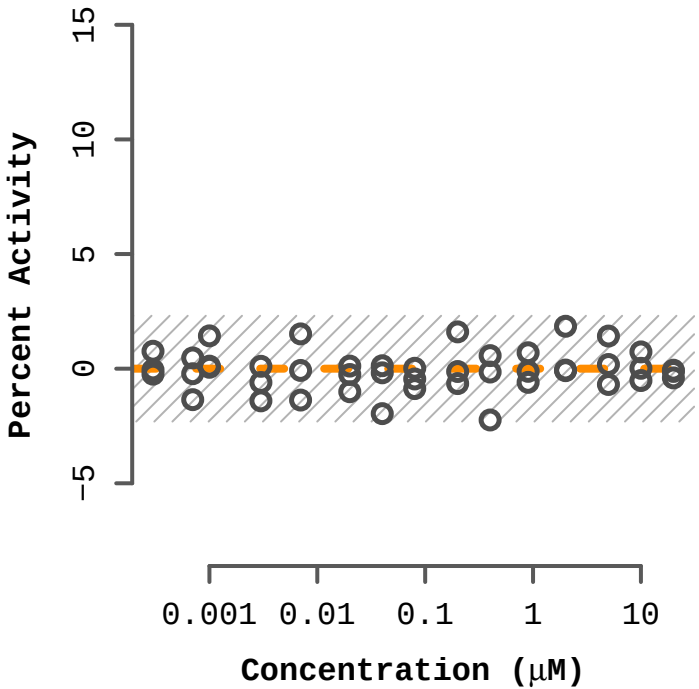
NAME: 1H-Tetrazol-1-acetic acid
CHID: 57686 **CASRN:** 21732-17-2
SPID(S): Tox21_113762
M4ID: 12482453

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.39 **MAX_MED:** 1.27 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

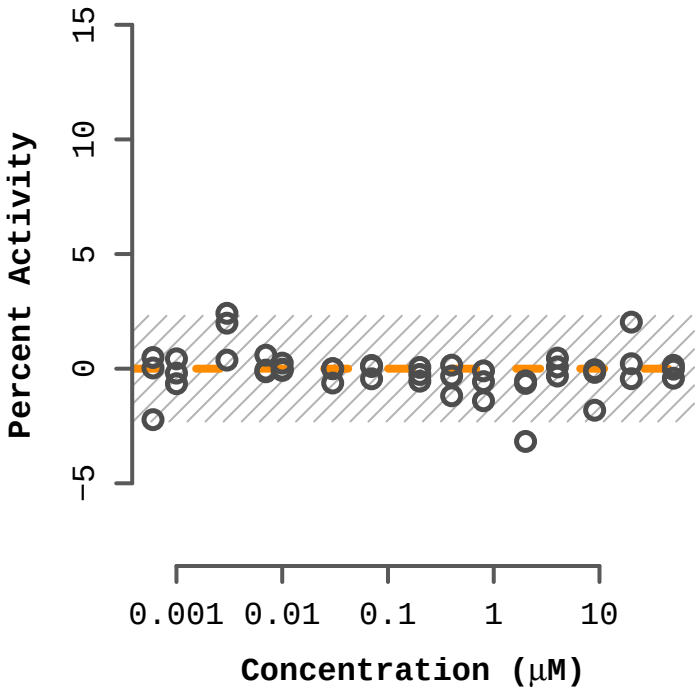
NAME: 7-Aminodeacetoxycephalosporanic acid
CHID: 57687 CASRN: 22252-43-3
SPID(S): Tox21_113804
M4ID: 12482415

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.87	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.569 **MAX_MED:** 0.184 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

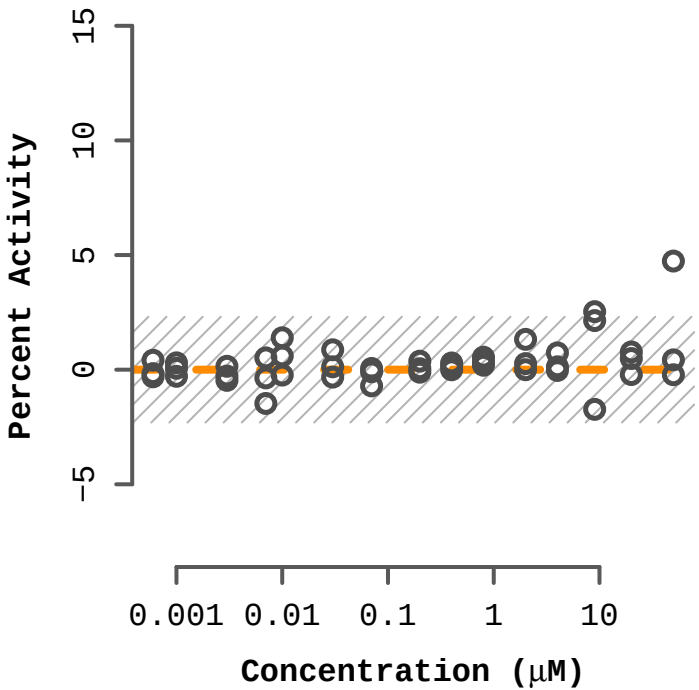
NAME: Bornelone
CHID: 57688 **CASRN:** 2226-11-1
SPID(S): Tox21_113671
M4ID: 12482543

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.74	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 1.59 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

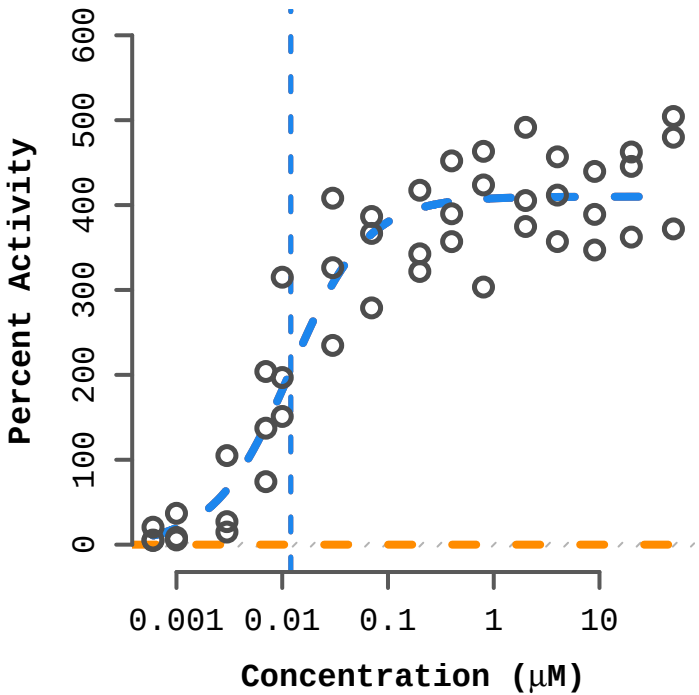
NAME: Estriol tripropionate
CHID: 57689 **CASRN:** 2236-31-9
SPID(S): Tox21_113694
M4ID: 12482520

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.65 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dexamethasone isonicotinate
CHID: 57690 **CASRN:** 2265-64-7
SPID(S): Tox21_113679
M4ID: 12482535

HILL MODEL (in red):

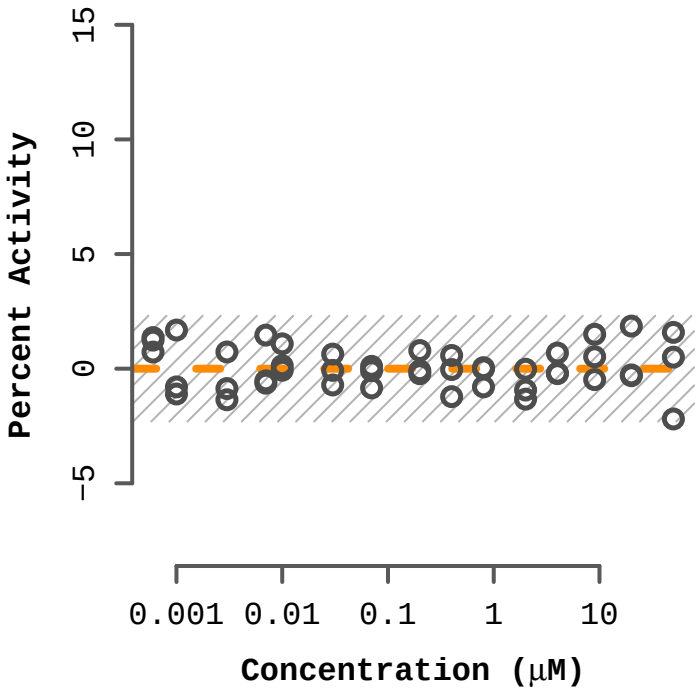
	tp	ga	gw
val:	410	-1.92	1.2
sd:	13.2	0.0881	0.269

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	410	-1.92	1.2	3.19	13.6
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	660.52	495.97	499.97
PROB:	0	0.88	0.12
RMSE:	332.67	52.72	52.72

MAX_MEAN: 452 **MAX_MED:** 480 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

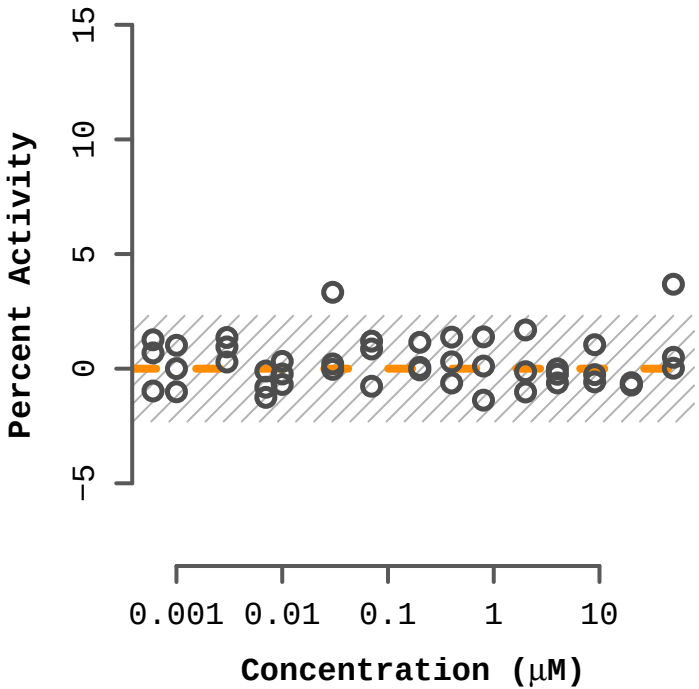
NAME: 1-(4-Chlorobenzenesulfonyl)urea
CHID: 57691 **CASRN:** 22663-37-2
SPID(S): Tox21_113761
M4ID: 12482454

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 1.11 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

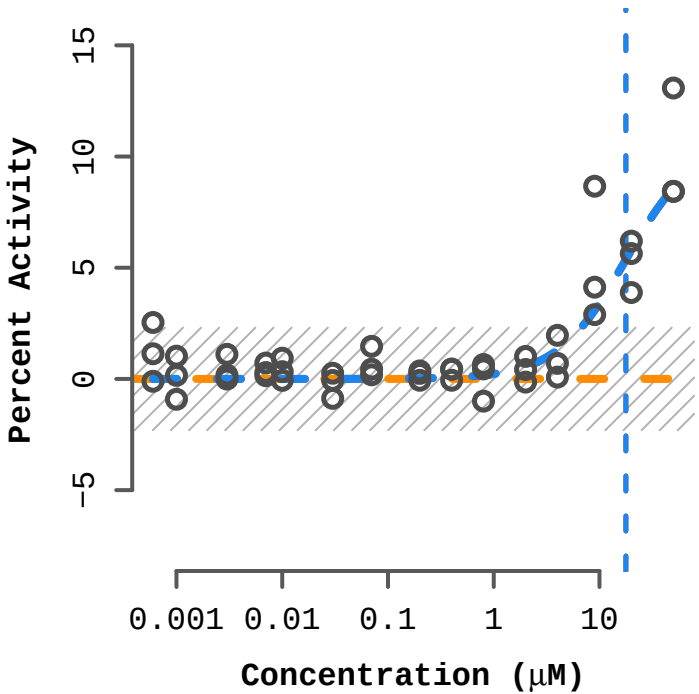
NAME: 2-Acetylbenzo[b]thiophene
CHID: 57692 **CASRN:** 22720-75-8
SPID(S): Tox21_113819
M4ID: 12482402

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.69	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.4 **MAX_MED:** 0.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Enfenamic acid
CHID: 57693 **CASRN:** 23049-93-6
SPID(S): Tox21_113941
M4ID: 12482290

HILL MODEL (in red):

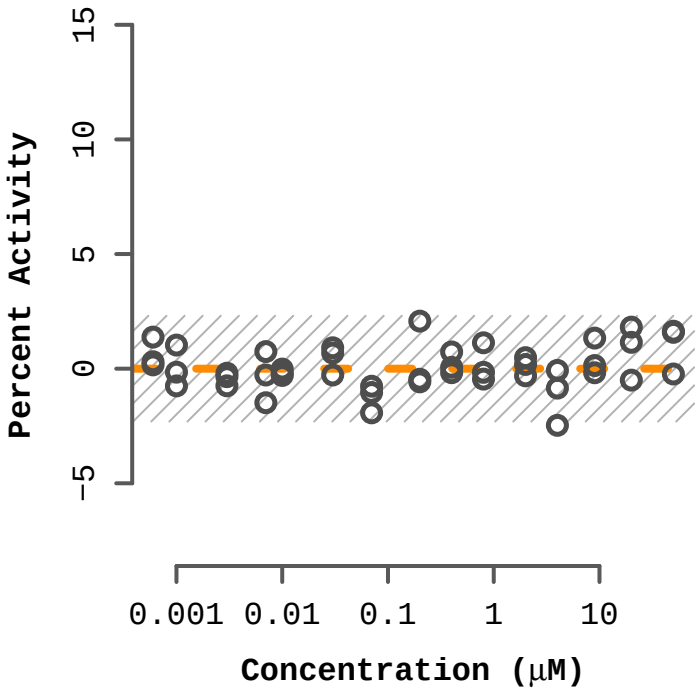
	tp	ga	gw
val:	10.7	1.25	1.33
sd:	2.04	0.165	0.322

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.7	1.25	1.33	3.53	5.26
sd:	2.04	0.165	0.322	11800	34100

	CNST	HILL	GNLS
AIC:	215.63	135.22	139.22
PROB:	0	0.88	0.12
RMSE:	3.41	1.31	1.31

MAX_MEAN: 9.98 **MAX_MED:** 8.44 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

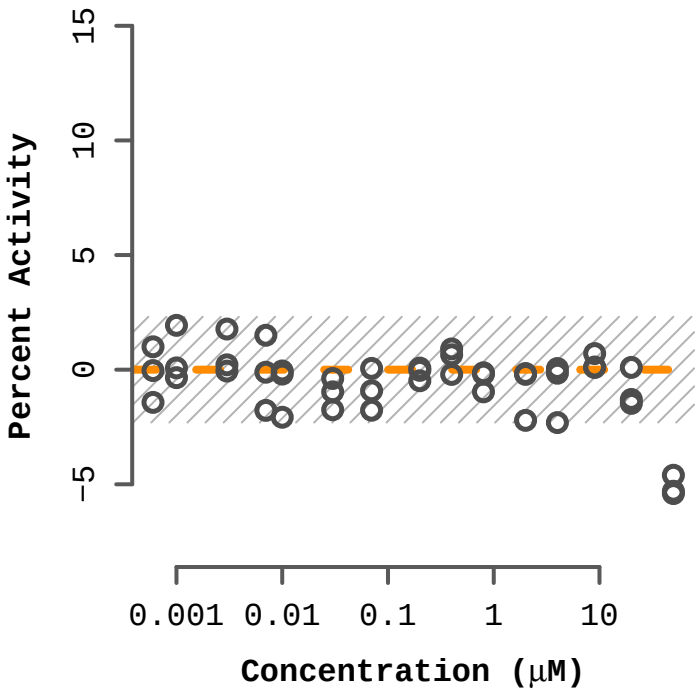
NAME: 4-Amino-2-chloro-6,7-dimethoxyquinazoline
CHID: 57694 **CASRN:** 23680-84-4
SPID(S): Tox21_113801
M4ID: 12482418

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.997 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

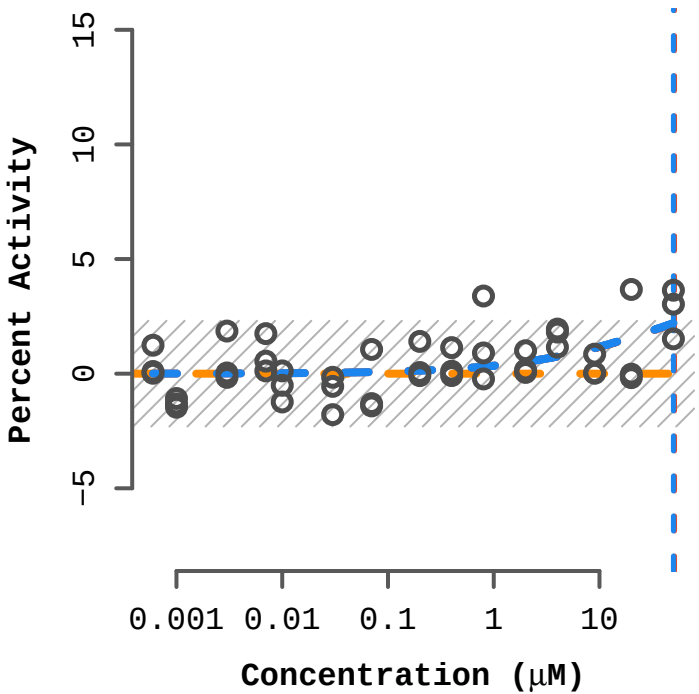
NAME: Floctafenine
CHID: 57695 **CASRN:** 23779-99-9
SPID(S): Tox21_113688
M4ID: 12482526

HILL MODEL: Not applicable.

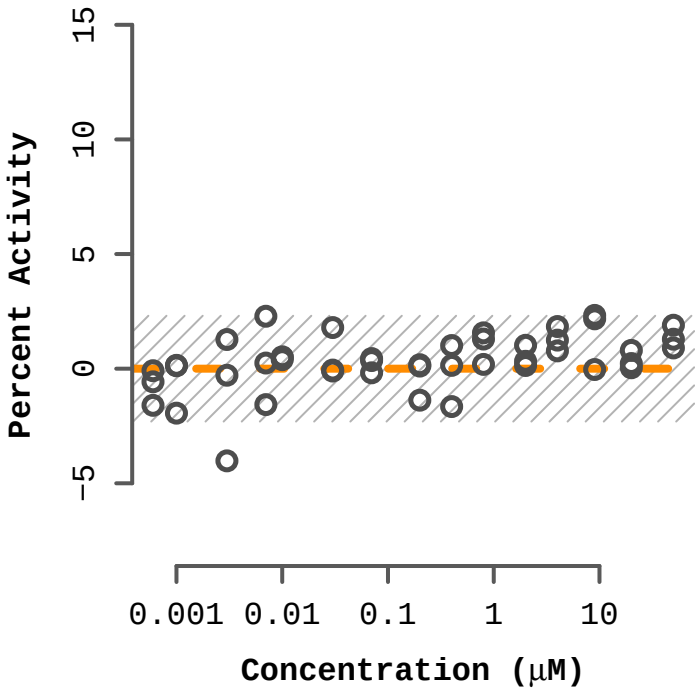
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 0.643 **MAX_MED:** 0.652 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    4-Hydroxyindole
CHID:    57696   CASRN: 2380-94-1
SPID(S): Tox21_113766
M4ID:    12482449

HILL MODEL (in red):
      tp       ga       gw
val:  4.41     1.71     0.624
sd:   4.3      1.15     0.289

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.41     1.7      0.629    3.16     5.31
sd:   4.51     1.2      0.289    1090     3960

      CNST        HILL        GNLS
AIC:  157.62      148.51      152.51
PROB: 0.01        0.87        0.12
RMSE: 1.4         1.11        1.11

MAX_MEAN: 2.73      MAX_MED: 3.03      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

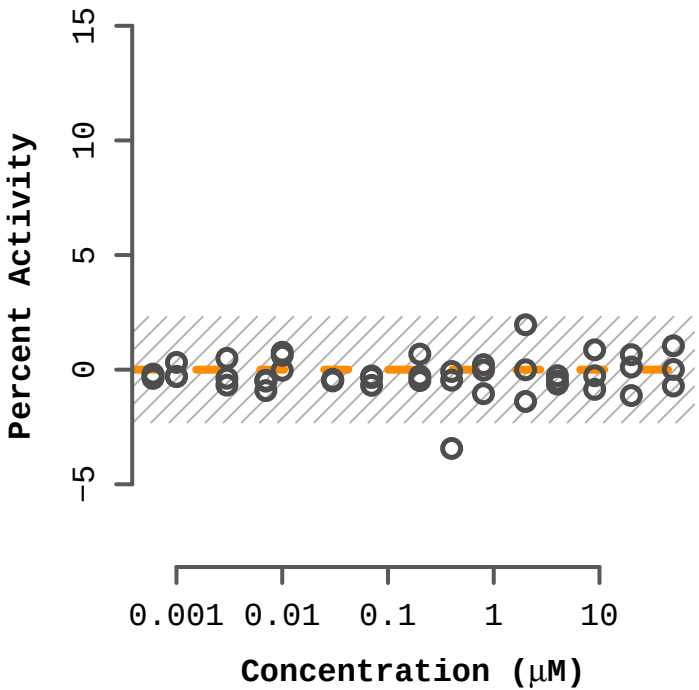
NAME: Estriol benzoate diacetate
CHID: 57697 **CASRN:** 2508-47-6
SPID(S): Tox21_113698
M4ID: 12482516

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.49 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

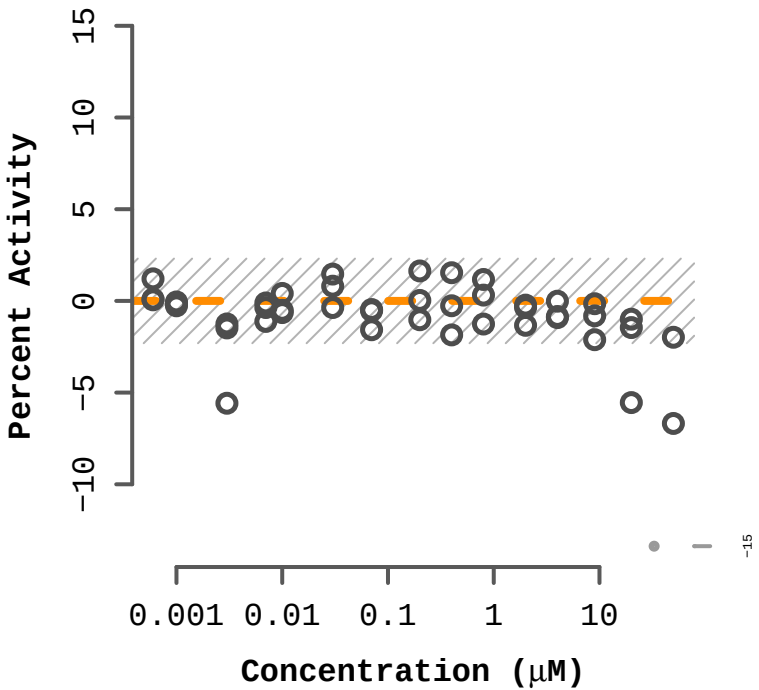
NAME: 1-Ethylpyrrolidin-2-ylmethylamine
CHID: 57698 **CASRN:** 26116-12-1
SPID(S): Tox21_113800
M4ID: 12482419

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	102.66	NA	NA
PROB:	1	NA	NA
RMSE:	0.82	NA	NA

MAX_MEAN: 0.457 **MAX_MED:** 0.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

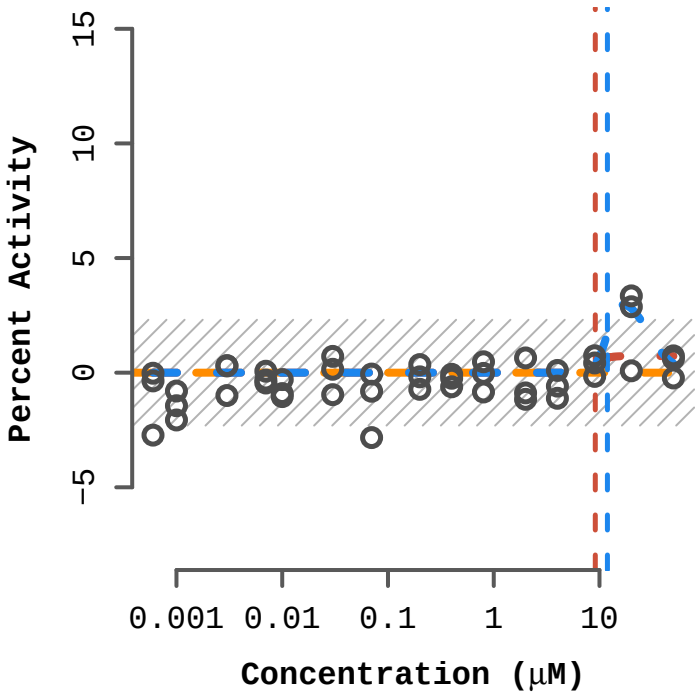
NAME: 1-(Bis(4-fluorophenyl)methyl)piperazine
CHID: 57699 **CASRN:** 27469-60-9
SPID(S): Tox21_113827
M4ID: 12482394 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	185.14	NA	NA
PROB:	1	NA	NA
RMSE:	2.88	NA	NA

MAX_MEAN: 0.636 **MAX_MED:** 0.804 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 5-Hydroxy-1-tetralone
CHID: 57700 **CASRN:** 28315-93-7
SPID(S): Tox21_113911
M4ID: 12482319

HILL MODEL (in red):

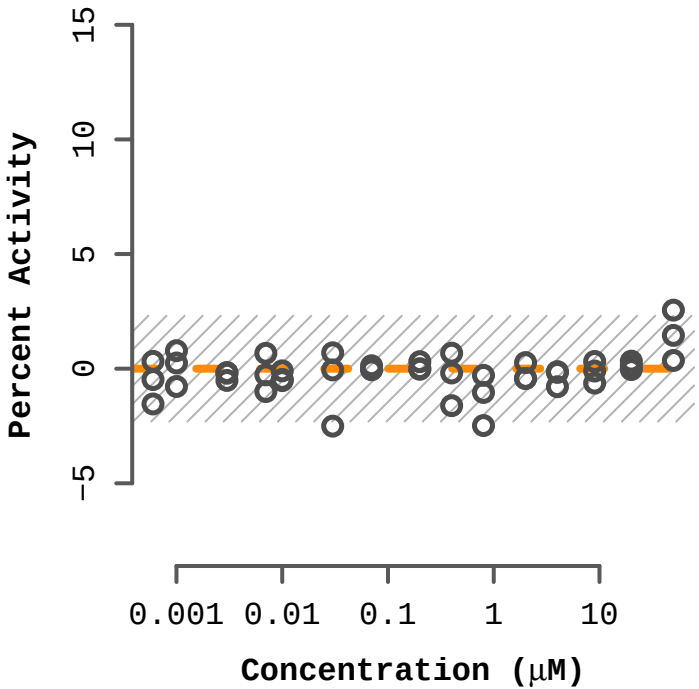
	tp	ga	gw
val:	0.725	0.96	8
sd:	0.417	0.138	17.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.56	1.08	8	1.46	3.77
sd:	170	2.61	30.2	18.6	196

	CNST	HILL	GNLS
AIC:	131.96	133.89	131.36
PROB:	0.37	0.14	0.49
RMSE:	1.11	1.03	0.98

MAX_MEAN: 2.1 **MAX_MED:** 2.88 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

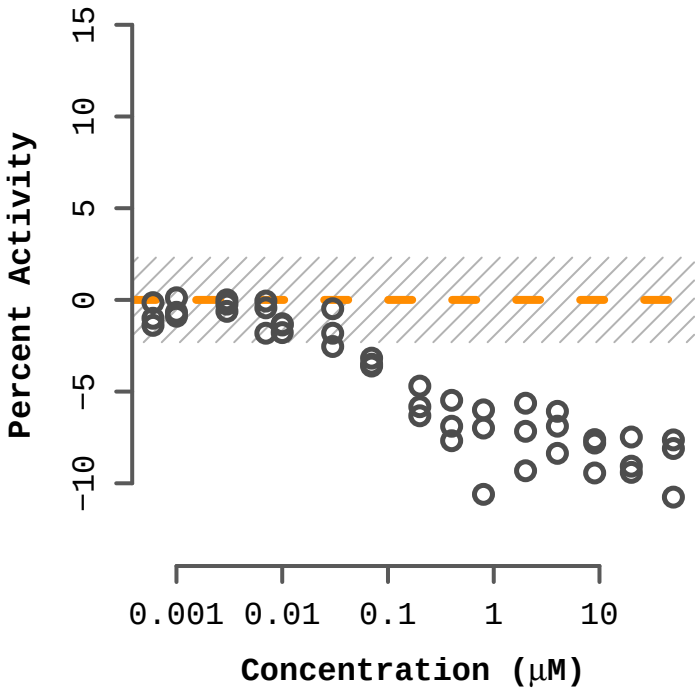
NAME: Arimoclomol
CHID: 57701 CASRN: 289893-25-0
SPID(S): Tox21_113718
M4ID: 12482496

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.83	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 1.46 **MAX_MED:** 1.45 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

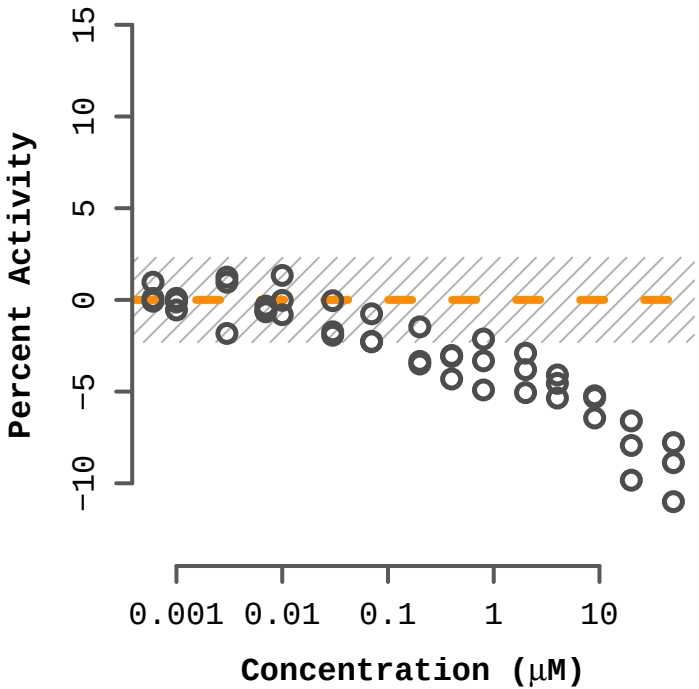
NAME: Gimatecan
CHID: 57702 **CASRN:** 292618-32-7
SPID(S): Tox21_113726
M4ID: 12482488

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	292.63	NA	NA
PROB:	1	NA	NA
RMSE:	5.75	NA	NA

MAX_MEAN: −0.282 **MAX_MED:** −0.228 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

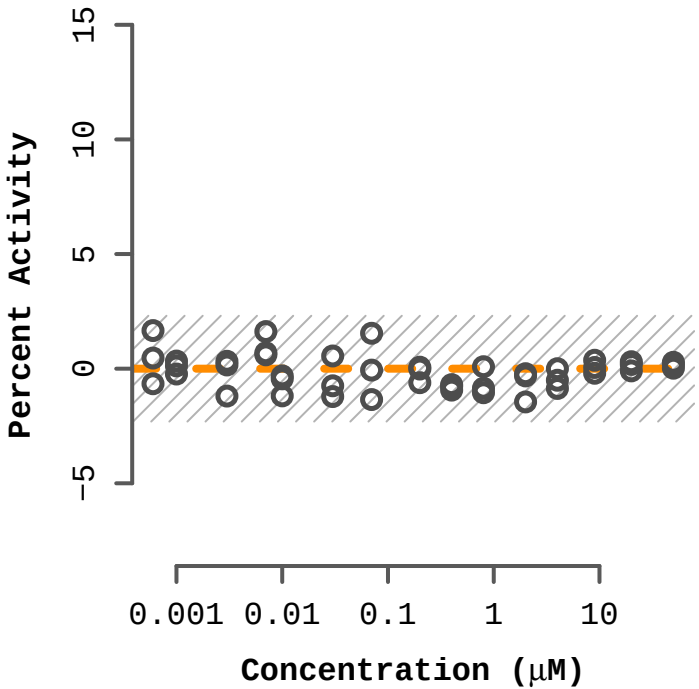
NAME: Almitrine dimethanesulfonate
CHID: 57703 **CASRN:** 29608-49-9
SPID(S): Tox21_113959
M4ID: 12482272

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	259.92	NA	NA
PROB:	1	NA	NA
RMSE:	4.23	NA	NA

MAX_MEAN: 0.327 **MAX_MED:** 0.965 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

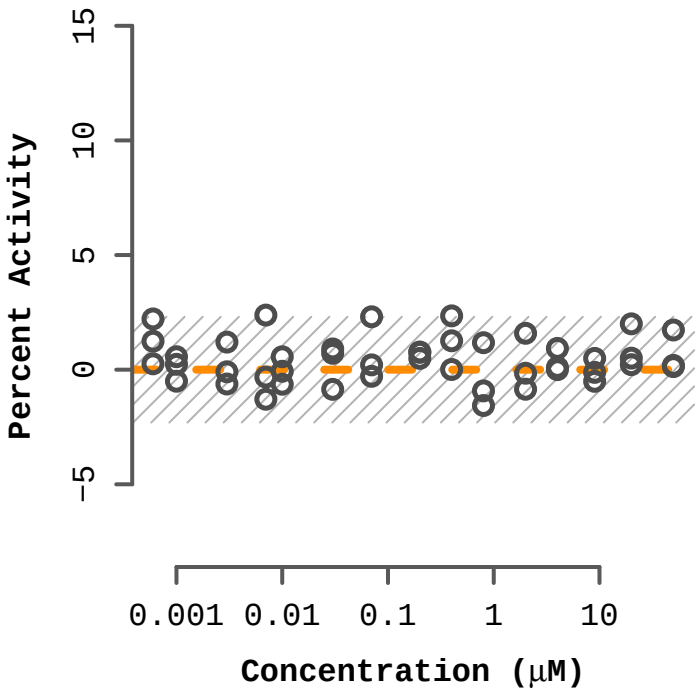
NAME: Ethyl 4-oxo-1-piperidinecarboxylate
CHID: 57704 **CASRN:** 29976-53-2
SPID(S): Tox21_113793
M4ID: 12482426

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.34	NA	NA
PROB:	1	NA	NA
RMSE:	0.74	NA	NA

MAX_MEAN: 0.974 **MAX_MED:** 0.696 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

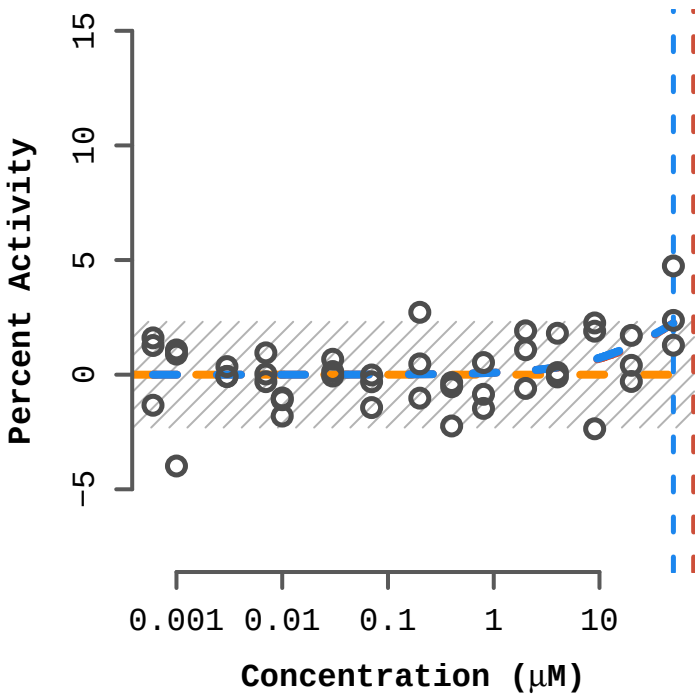
NAME: Medazomide
CHID: 57705 **CASRN:** 300-22-1
SPID(S): Tox21_113915
M4ID: 12482315

HILL MODEL: Not applicable.

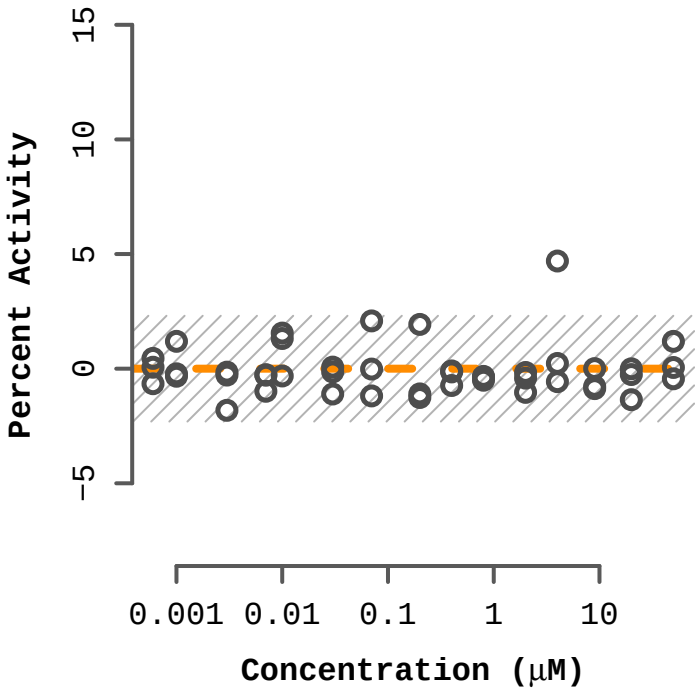
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.36	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.24 **MAX_MED:** 1.26 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Etienic acid
CHID:    57706   CASRN: 302-97-6
SPID(S): Tox21_113782
M4ID:    12482435

HILL MODEL (in red):
      tp       ga       gw
val:  5.69     1.89     0.959
sd:   10.9     1.4      0.636

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.47     1.7      1.01     2.98     6.21
sd:   9.19     1.55     0.651    2010     9770

      CNST        HILL        GNLS
AIC:  167.14      162.74      166.81
PROB: 0.09        0.81        0.11
RMSE: 1.54        1.34        1.35

MAX_MEAN: 2.8       MAX_MED: 2.37      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

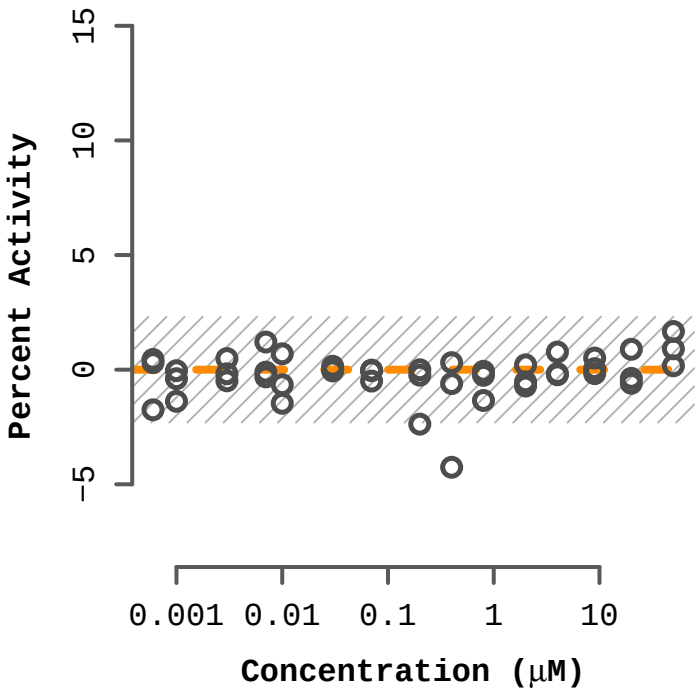
NAME: 3-Bromo-2-methylthiophene
CHID: 57707 **CASRN:** 30319-05-2
SPID(S): Tox21_113850
M4ID: 12482372

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.32 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

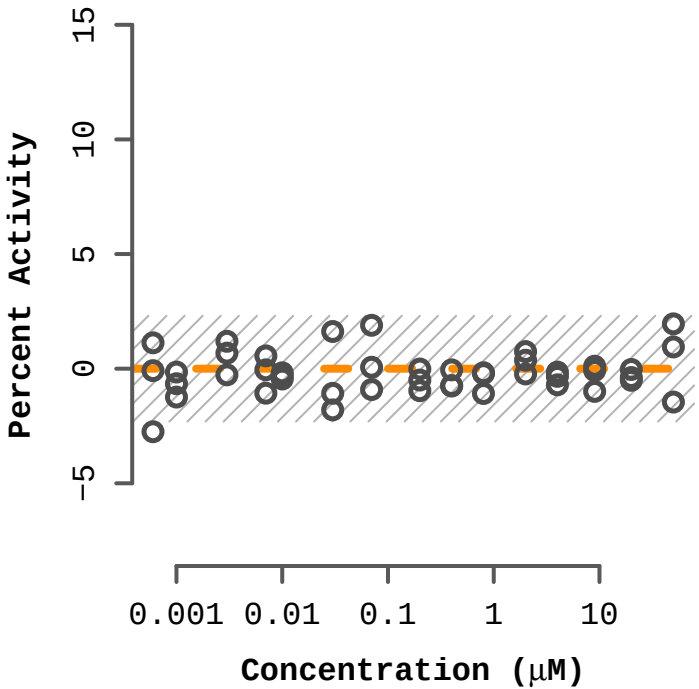
NAME: Fenaclon
CHID: 57708 CASRN: 306-20-7
SPID(S): Tox21_113856
M4ID: 12482367

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.25	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.916 MAX_MED: 0.912 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

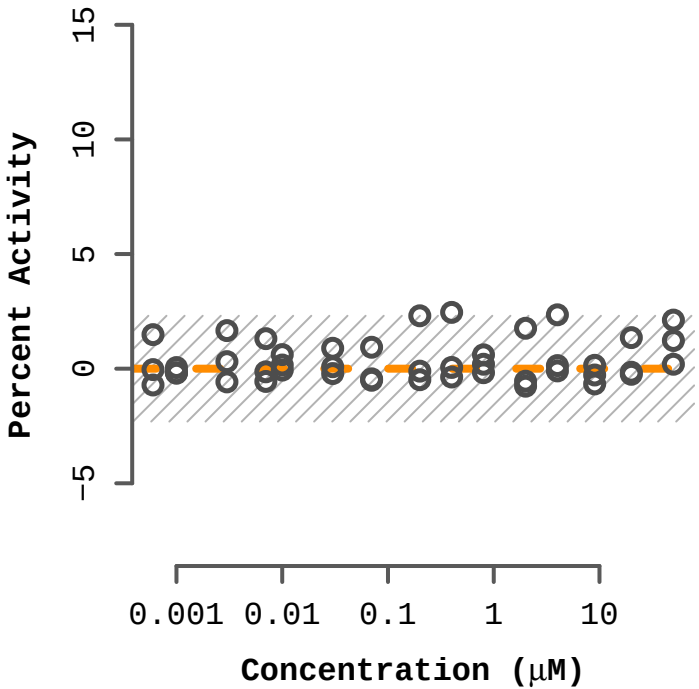
NAME: Tizoprolic acid
CHID: 57709 **CASRN:** 30709-69-4
SPID(S): Tox21_113854
M4ID: 12482369

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.39	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.536 **MAX_MED:** 0.949 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

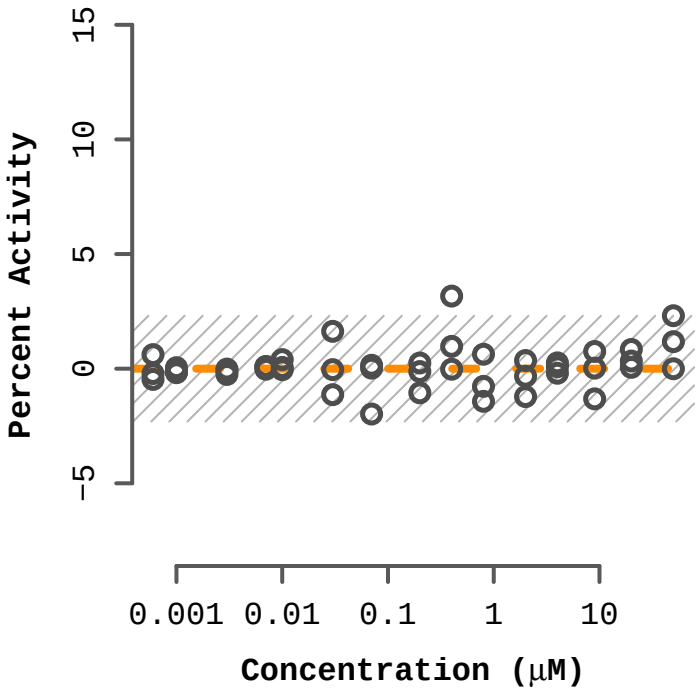
NAME: Iodoxamic Acid
CHID: 57710 **CASRN:** 31127-82-9
SPID(S): Tox21_113933
M4ID: 12482298

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.05	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 1.18 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

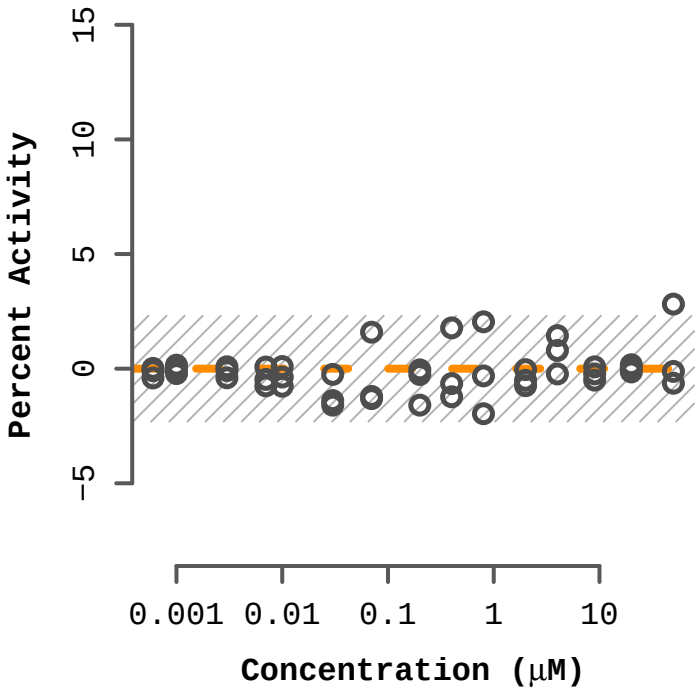
NAME: Iobenzamic acid
CHID: 57711 **CASRN:** 3115-05-7
SPID(S): Tox21_113974
M4ID: 12482264

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	109.45	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 1.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

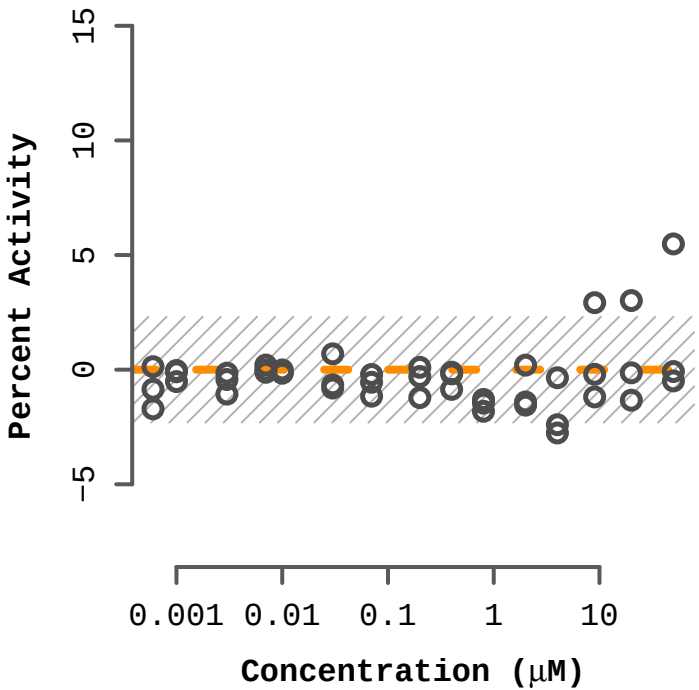
NAME: Lexiscan
CHID: 57712 CASRN: 313348-27-5
SPID(S): Tox21_113668
M4ID: 12482546

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.689 **MAX_MED:** 0.795 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

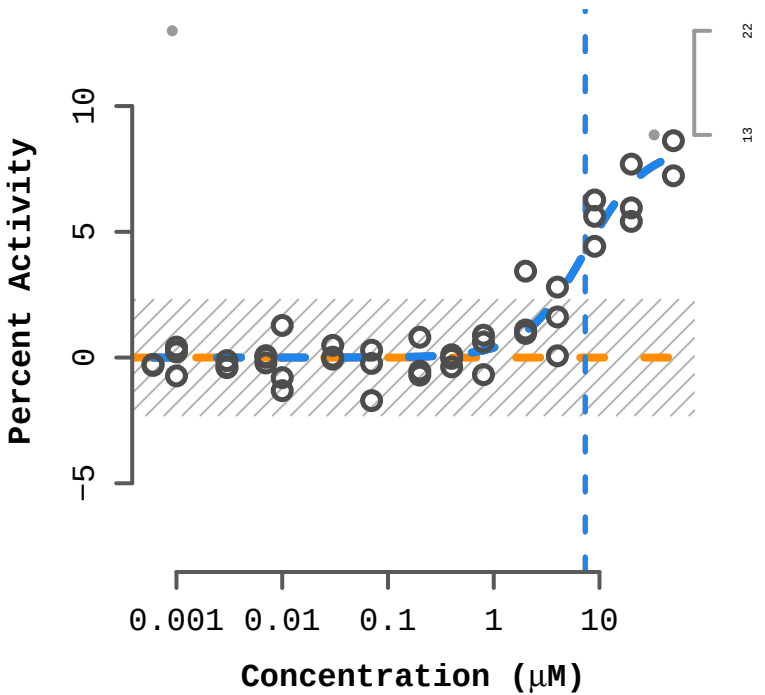
NAME: Cyclobendazole
CHID: 57713 **CASRN:** 31431-43-3
SPID(S): Tox21_113945
M4ID: 12482286

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.89	NA	NA
PROB:	1	NA	NA
RMSE:	1.39	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** −0.0154 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Chlorodibenz(b,f)-1,4-oxazepin-11(10H)-one
CHID: 57714 CASRN: 3158-91-6
SPID(S): Tox21_113919
M4ID: 12482311 BRK

HILL MODEL (in red):

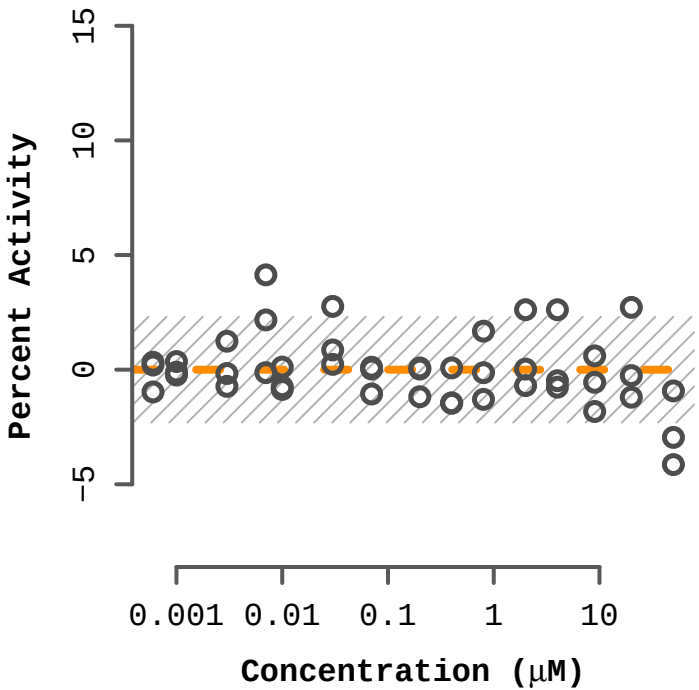
	tp	ga	gw
val:	8.43	0.865	1.51
sd:	1.05	0.118	0.403

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	8.43	0.865	1.51	2.94	6.56
sd:	1.05	0.118	0.403	1000	5280

	CNST	HILL	GNLS
AIC:	242.09	157.63	161.63
PROB:	0	0.88	0.12
RMSE:	4.77	3.45	3.45

MAX_MEAN: 9.65 MAX_MED: 8.62 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

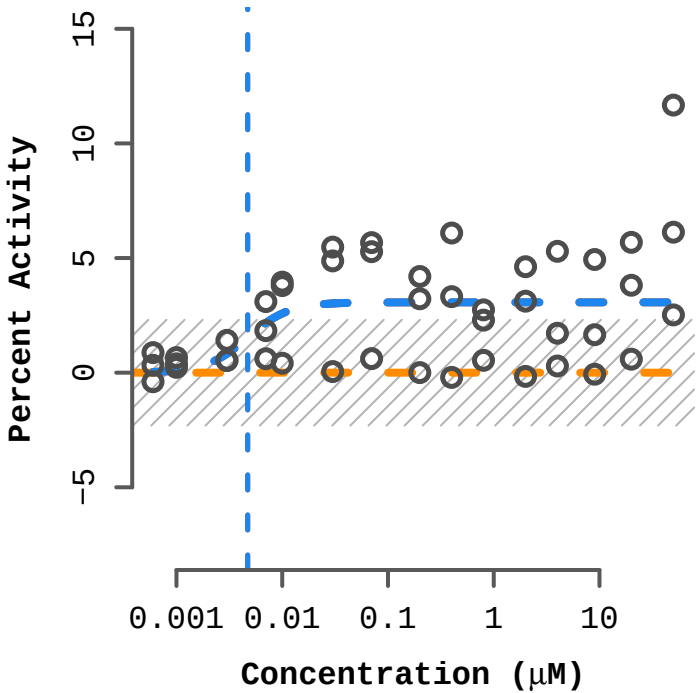
NAME: Mexazolam
CHID: 57715 **CASRN:** 31868-18-5
SPID(S): Tox21_113740
M4ID: 12482474

HILL MODEL: Not applicable.

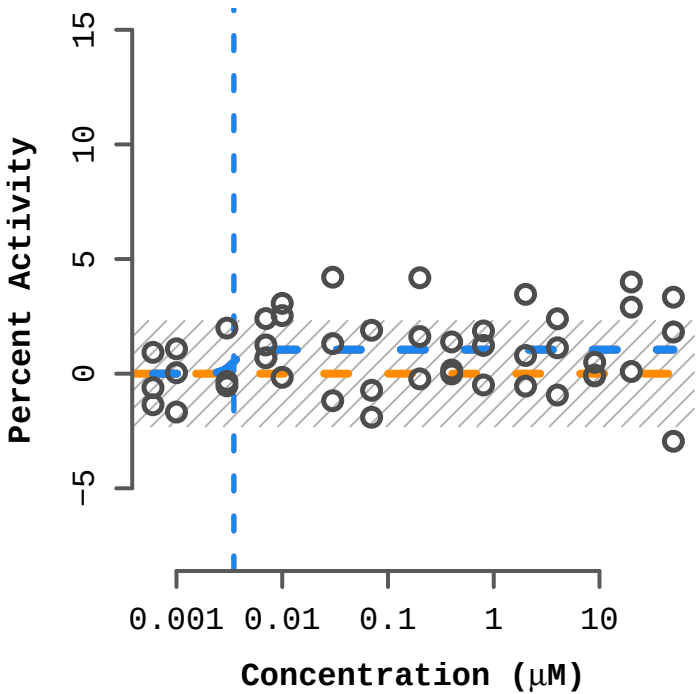
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	162.42	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

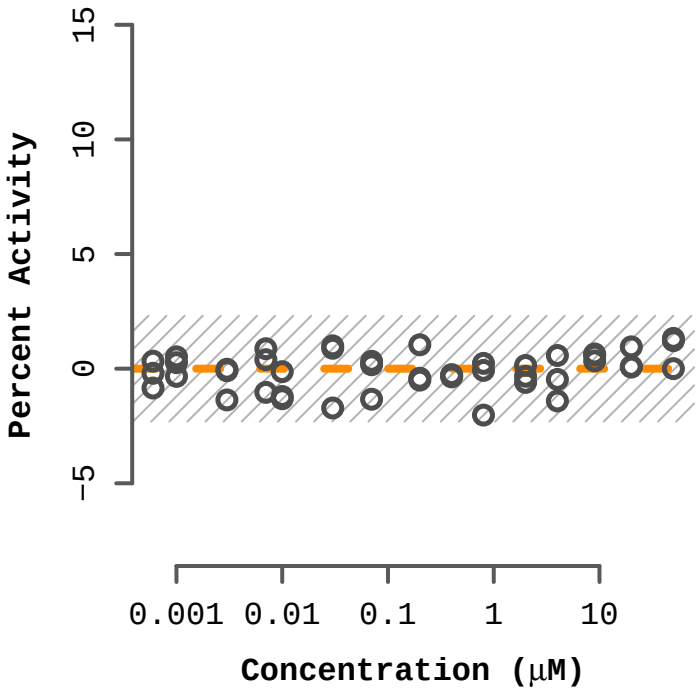
MAX_MEAN: 2.06 **MAX_MED:** 2.17 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Butoctamide semisuccinate
CHID:    57716   CASRN: 32838-28-1
SPID(S): Tox21_113893
M4ID:    12482335

HILL MODEL (in red):
      tp       ga       gw
val:  3.07     -2.33    2.22
sd:   0.437    0.23     2.03

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  3.07     -2.33    2.22     3.22     18
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  243.02      206.11      210.11
PROB: 0           0.88        0.12
RMSE: 3.55        2.25        2.25

MAX_MEAN: 6.77      MAX_MED: 6.13      BMAD: 0.769
```




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    (R,S)-Epinephrine hydrochloride
CHID:    57717   CASRN: 329-63-5
SPID(S): Tox21_113650
M4ID:    12482562

HILL MODEL (in red):
      tp       ga       gw
val:  1.05     -2.46    8
sd:   0.287    0.276    22.3

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  1.05     -2.46    8        3.7      11.1
sd:   NA       NA       NA       NA       NA

      CNST        HILL        GNLS
AIC:  188.92      182.36      186.36
PROB: 0.03        0.85        0.12
RMSE: 1.88        1.61        1.61

MAX_MEAN: 2.33      MAX_MED: 2.9       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

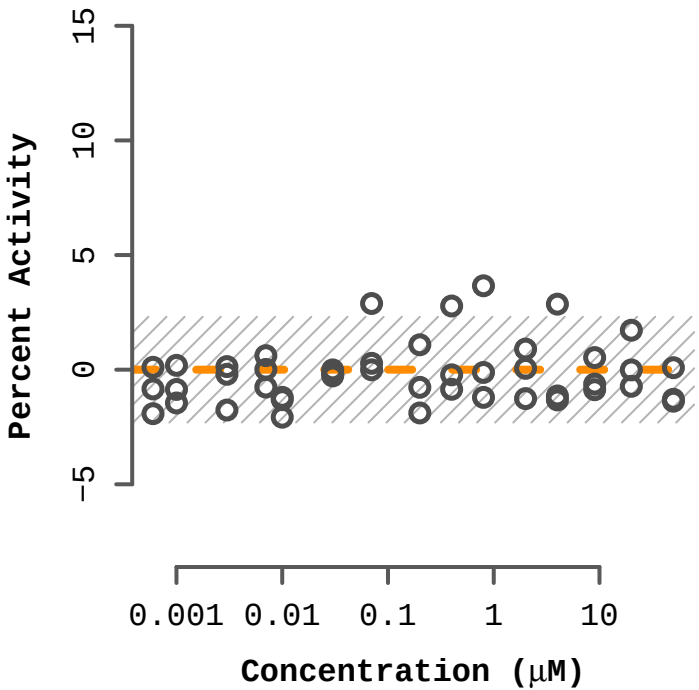
NAME: Methyl 5-sulfamoyl-o-anisate
CHID: 57718 **CASRN:** 33045-52-2
SPID(S): Tox21_113746
M4ID: 12482469

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.14	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 0.849 **MAX_MED:** 1.22 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

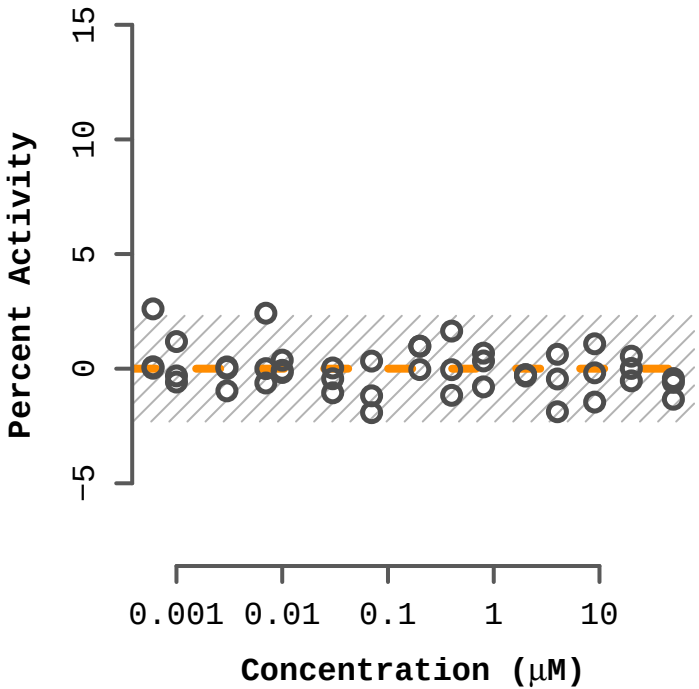
NAME: Muraglitazar
CHID: 57719 **CASRN:** 331741-94-7
SPID(S): Tox21_113946
M4ID: 12482285

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.66	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.279 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

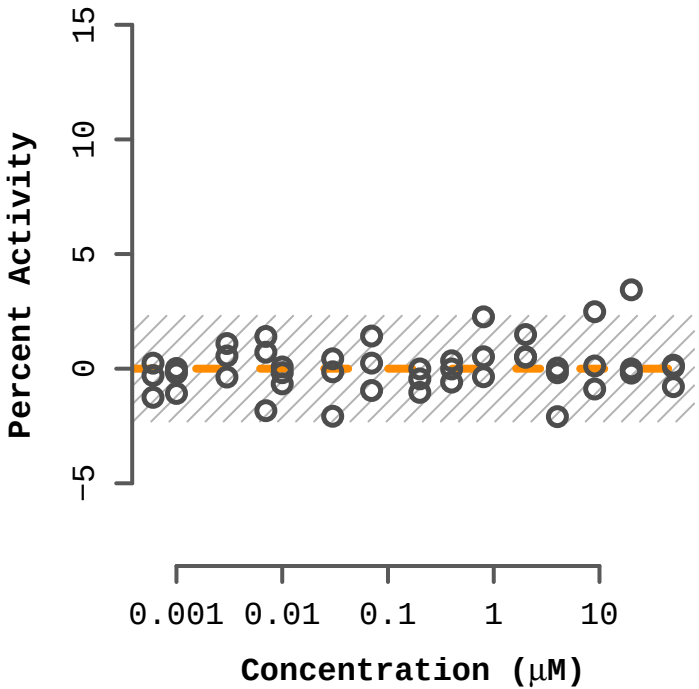
NAME: Methyl 5-chloro-o-anisate
CHID: 57720 **CASRN:** 33924-48-0
SPID(S): Tox21_113805
M4ID: 12482414

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.35	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.905 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

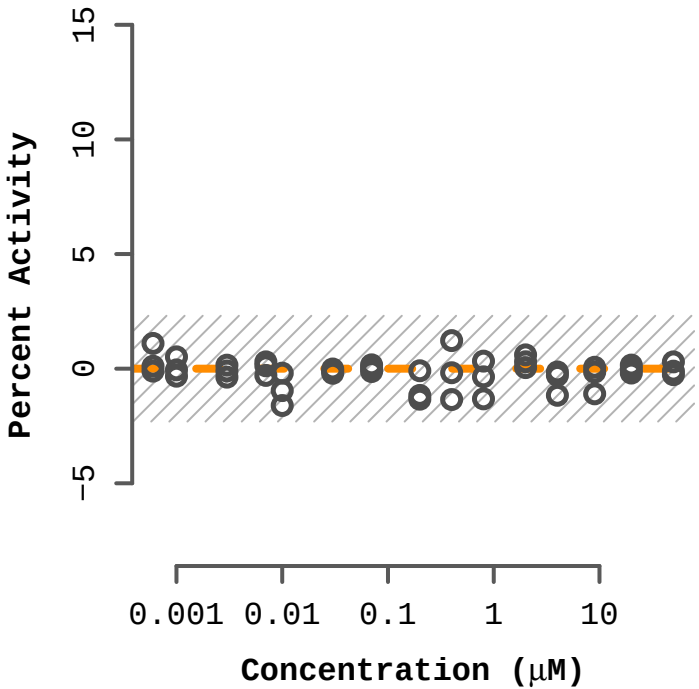
NAME: 6-Methoxy-2-naphthalaldehyde
CHID: 57721 **CASRN:** 3453-33-6
SPID(S): Tox21_113771
M4ID: 12482444

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.08	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.718 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

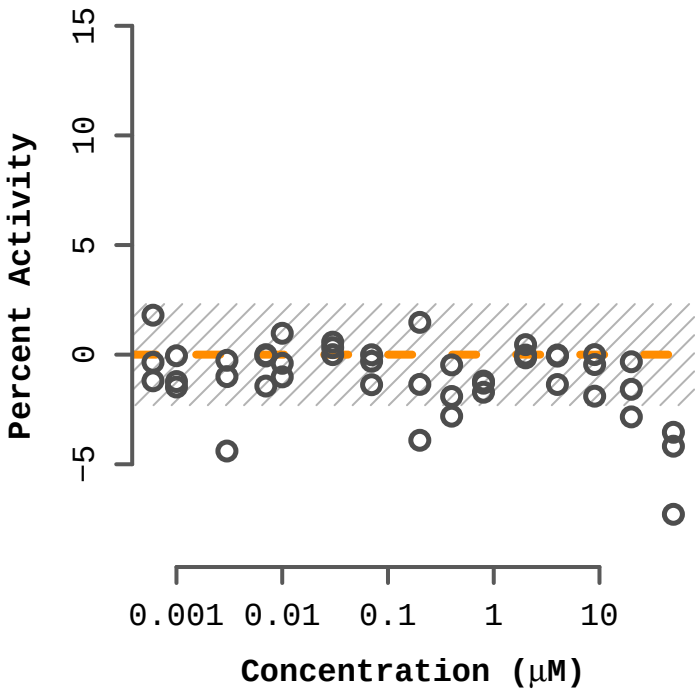
NAME: Viloxazine hydrochloride
CHID: 57722 **CASRN:** 35604-67-2
SPID(S): Tox21_113955
M4ID: 12482276

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	82.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.62	NA	NA

MAX_MEAN: 0.368 **MAX_MED:** 0.303 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

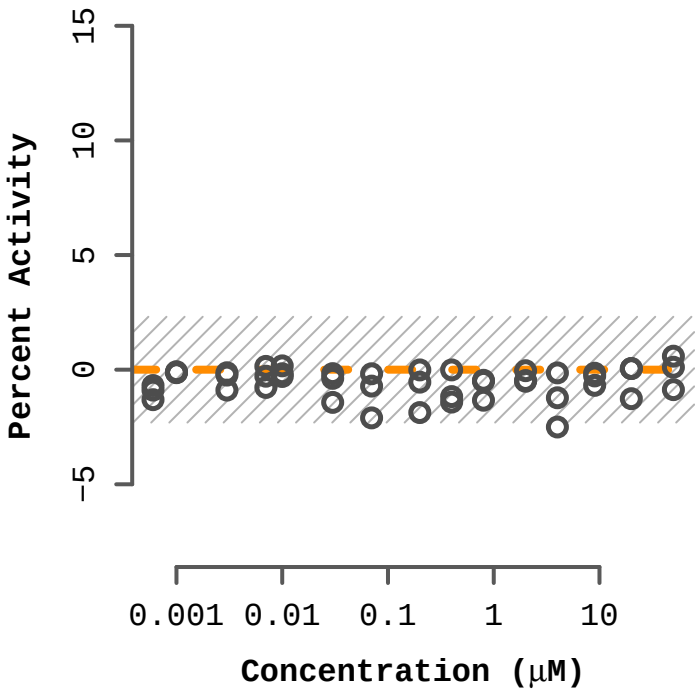
NAME: Rivaroxaban
CHID: 57723 **CASRN:** 366789-02-8
SPID(S): Tox21_113938
M4ID: 12482293

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	181.5	NA	NA
PROB:	1	NA	NA
RMSE:	1.96	NA	NA

MAX_MEAN: 0.298 **MAX_MED:** 0.321 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

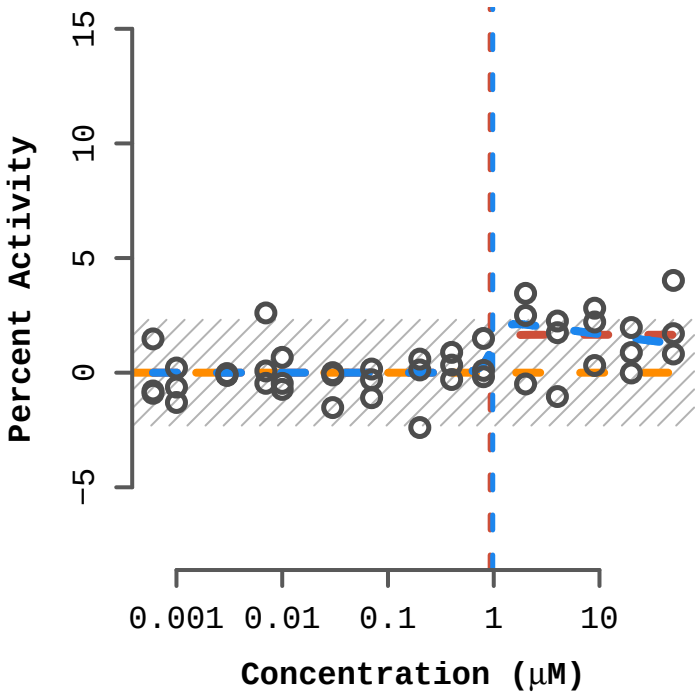
NAME: Tolycaine
CHID: 57724 **CASRN:** 3686-58-6
SPID(S): Tox21_113706
M4ID: 12482508

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.03	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: −0.0576 **MAX_MED:** 0.107 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cyclobutanecarboxylic acid
CHID: 57725 **CASRN:** 3721-95-7
SPID(S): Tox21_113791
M4ID: 12482427

HILL MODEL (in red):

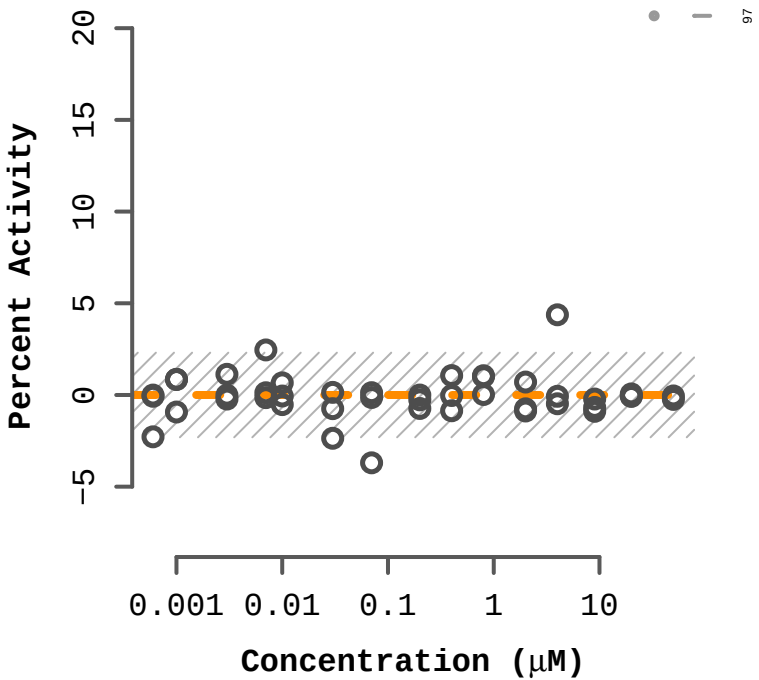
	tp	ga	gw
val:	1.65	−0.0338	8
sd:	0.319	0.182	21.9

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.51	−0.00943	7.99	0.883	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	160.3	145.28	148.71
PROB:	0	0.85	0.15
RMSE:	1.43	1.11	1.14

MAX_MEAN: 2.18 **MAX_MED:** 2.5 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

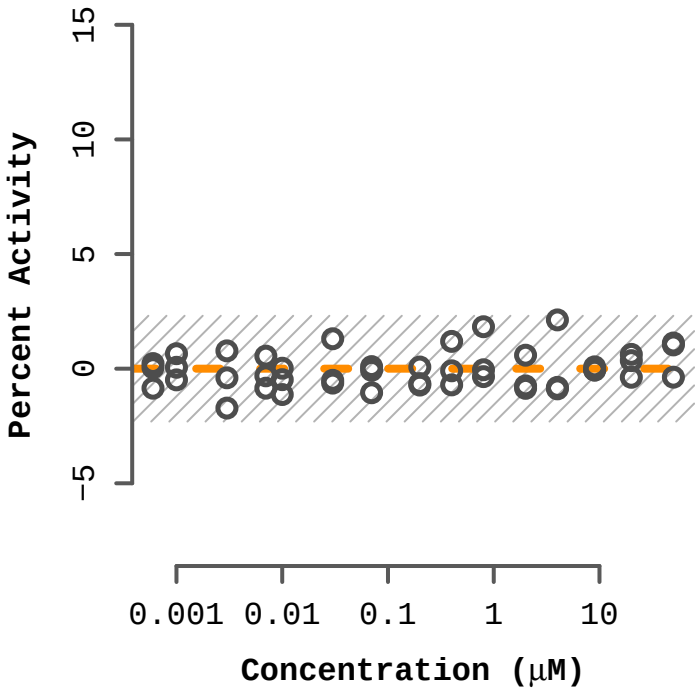
NAME: Phenylacetylglycine dimethylamide
CHID: 57726 CASRN: 3738-06-5
SPID(S): Tox21_113711
M4ID: 12482503 BRK

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.68	NA	NA
PROB:	1	NA	NA
RMSE:	14.54	NA	NA

MAX_MEAN: 32.3 **MAX_MED:** 1 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

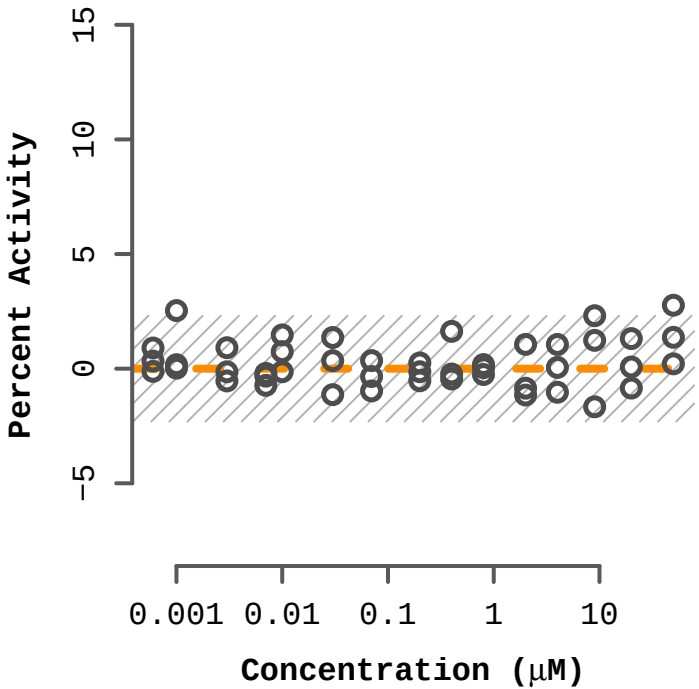
NAME: Furfenorex
CHID: 57727 CASRN: 13445-60-8
SPID(S): Tox21_113981
M4ID: 12482260

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.79	NA	NA

MAX_MEAN: 0.597 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

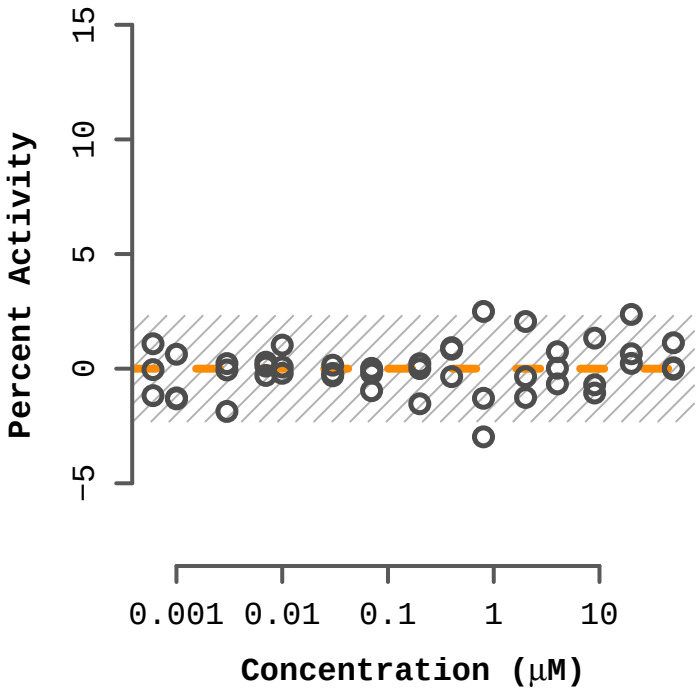
NAME: Fertirelin
CHID: 57728 **CASRN:** 38234-21-8
SPID(S): Tox21_113925
M4ID: 12482306

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.26	NA	NA
PROB:	1	NA	NA
RMSE:	1.02	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

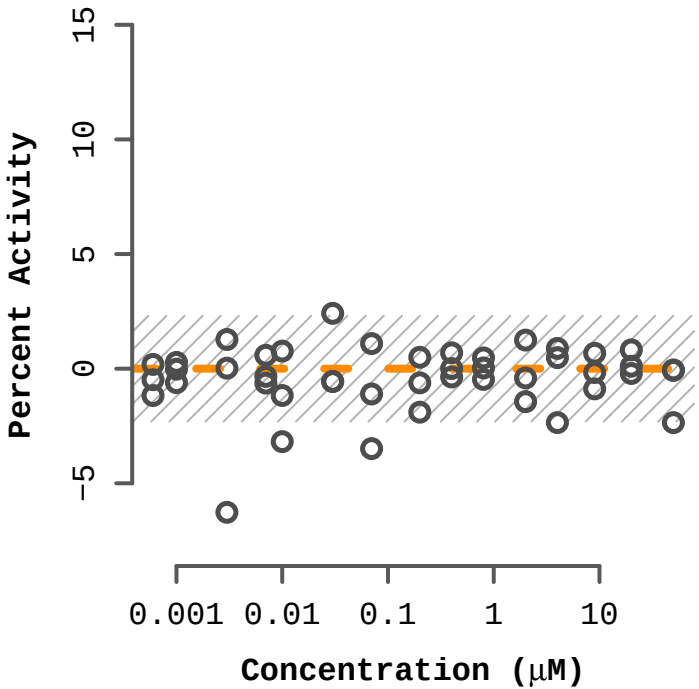
NAME: 4-Chloro-1-(4-fluorophenyl)-1-butanone
CHID: 57729 **CASRN:** 3874-54-2
SPID(S): Tox21_113749
M4ID: 12482466

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.15	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 1.08 **MAX_MED:** 0.85 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

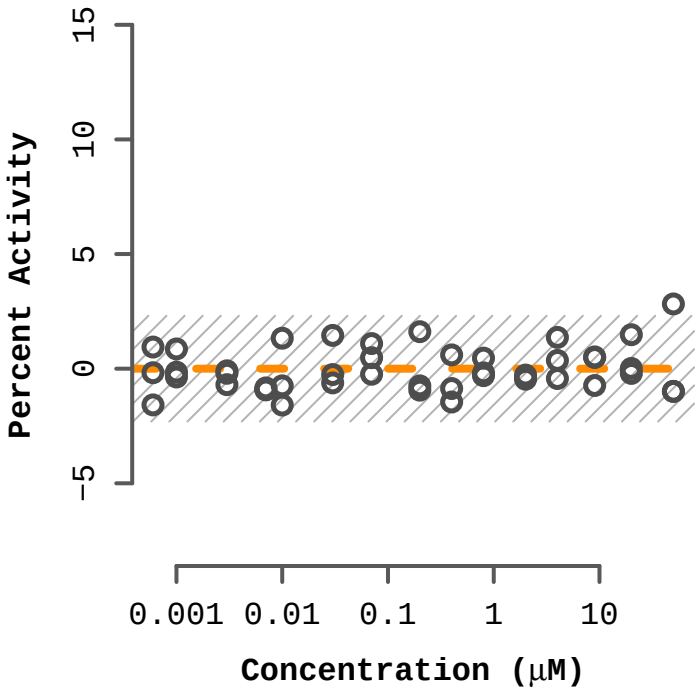
NAME: Promestriene
CHID: 57730 **CASRN:** 39219-28-8
SPID(S): Tox21_113830
M4ID: 12482391

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.52	NA	NA
PROB:	1	NA	NA
RMSE:	1.49	NA	NA

MAX_MEAN: 0.433 **MAX_MED:** 0.483 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

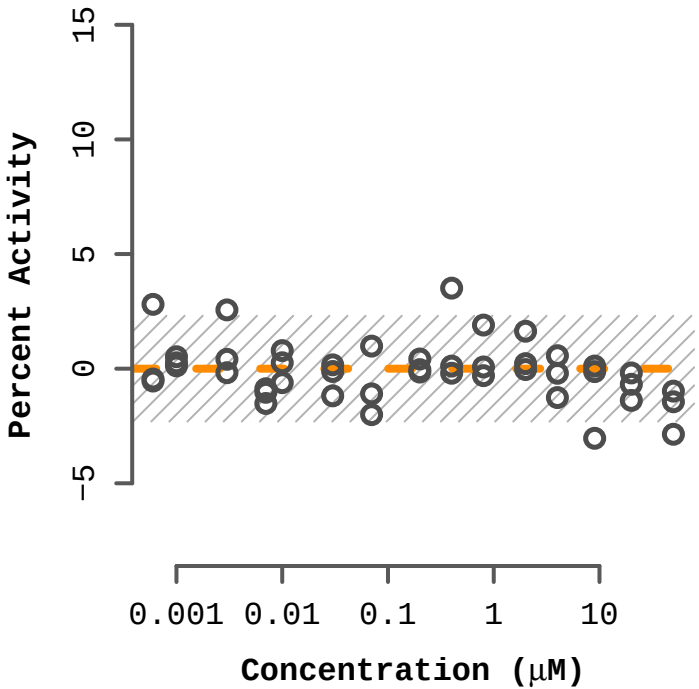
NAME: 3-Trifluoromethyl-4-nitroanilide
CHID: 57731 **CASRN:** 393-11-3
SPID(S): Tox21_113790
M4ID: 12482428

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.16	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.445 **MAX_MED:** 0.488 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

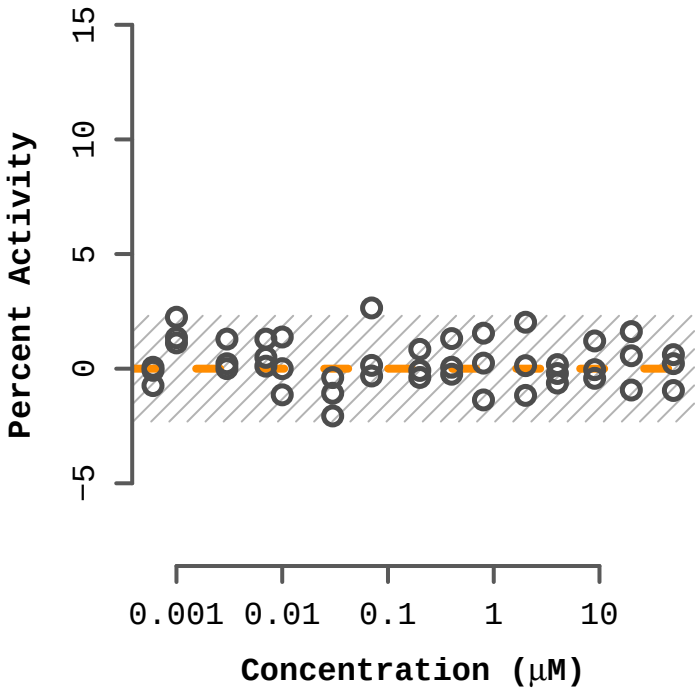
NAME: Ethyl protocatechuate
CHID: 57732 **CASRN:** 3943-89-3
SPID(S): Tox21_113836
M4ID: 12482386

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 0.409 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

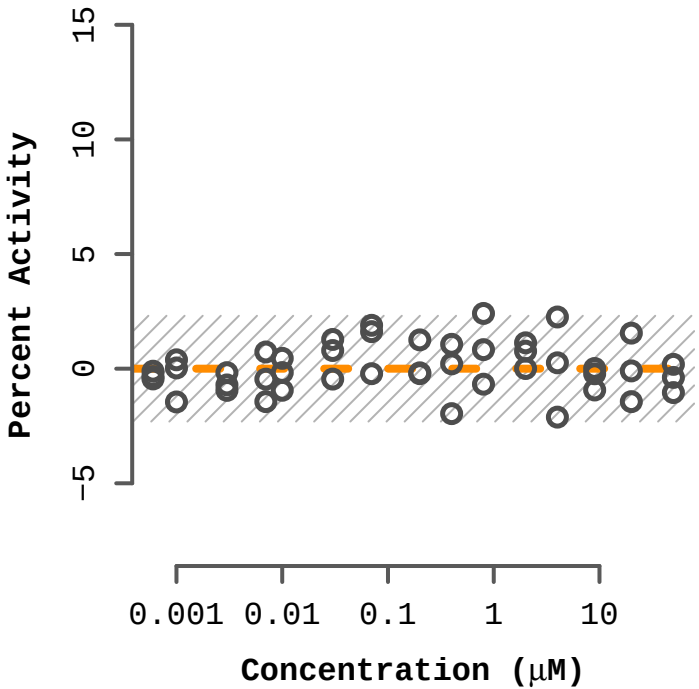
NAME: 4-(4-Chlorophenyl)-4-piperidinol
CHID: 57733 **CASRN:** 39512-49-7
SPID(S): Tox21_113829
M4ID: 12482392

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.03	NA	NA

MAX_MEAN: 1.57 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

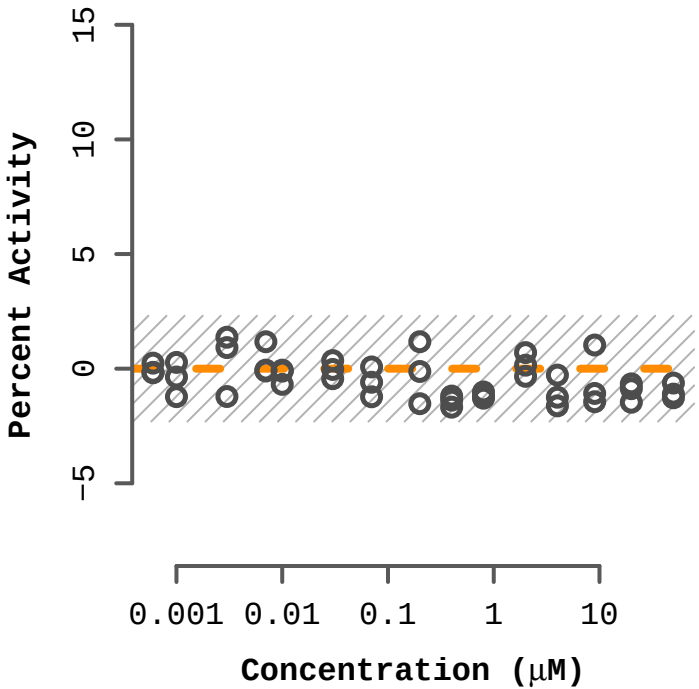
NAME: 1-(2-Chlorophenyl)piperazine
CHID: 57734 **CASRN:** 39512-50-0
SPID(S): Tox21_113875
M4ID: 12482350

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 1.1 **MAX_MED:** 1.62 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

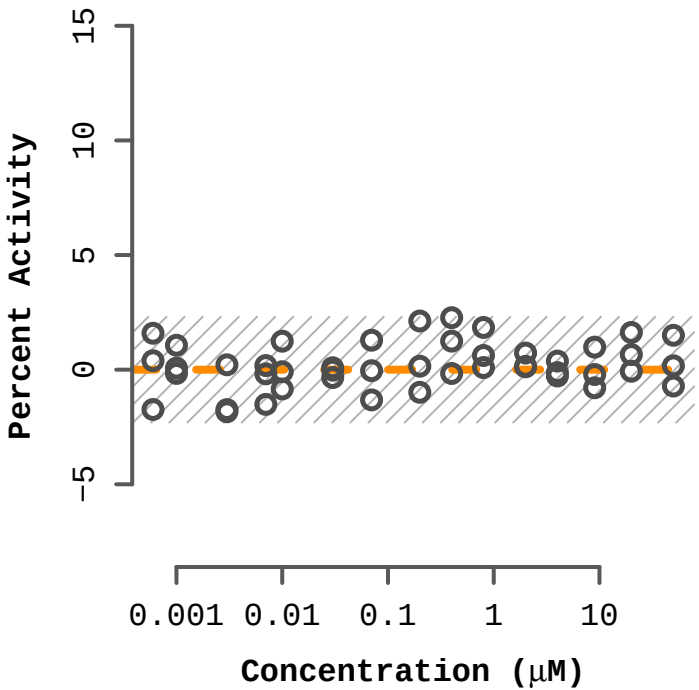
NAME: 1-(2-Furoyl)piperazine
CHID: 57735 **CASRN:** 40172-95-0
SPID(S): Tox21_113787
M4ID: 12482430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	130.5	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.361 **MAX_MED:** 0.922 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

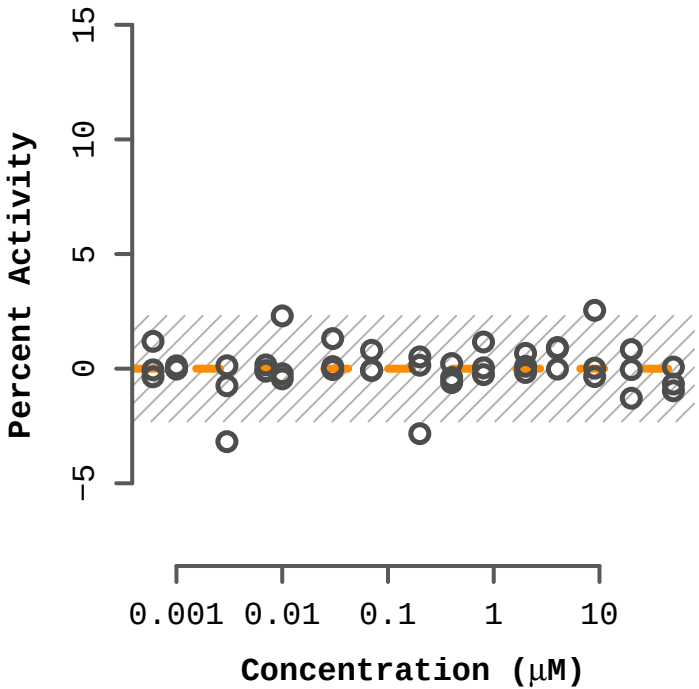
NAME: 5-Acetylsalicylamide
CHID: 57736 **CASRN:** 40187-51-7
SPID(S): Tox21_113835
M4ID: 12482387

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.4	NA	NA
PROB:	1	NA	NA
RMSE:	1.01	NA	NA

MAX_MEAN: 1.12 **MAX_MED:** 1.25 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

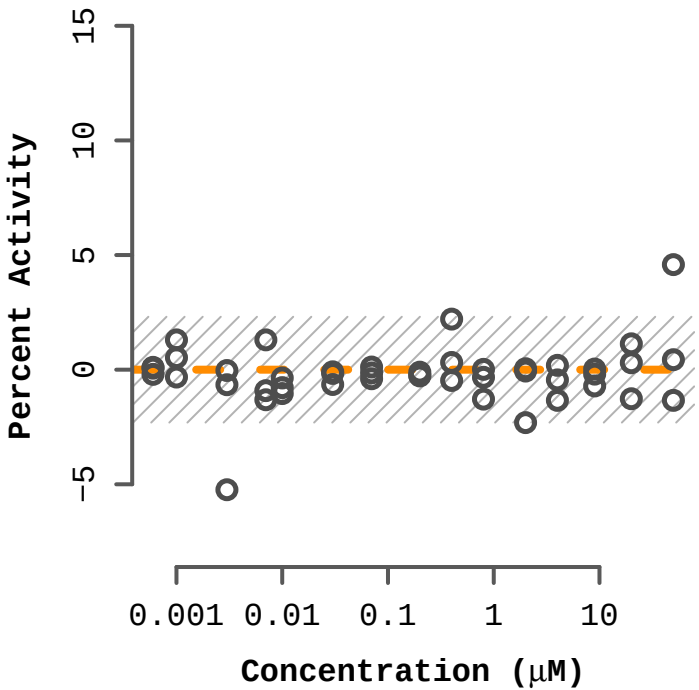
NAME: 3'−Acetyl−4'−hydroxybutyranilide
CHID: 57737 **CASRN:** 40188−45−2
SPID(S): Tox21_113821
M4ID: 12482400

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	115.11	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.742 **MAX_MED:** 0.883 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

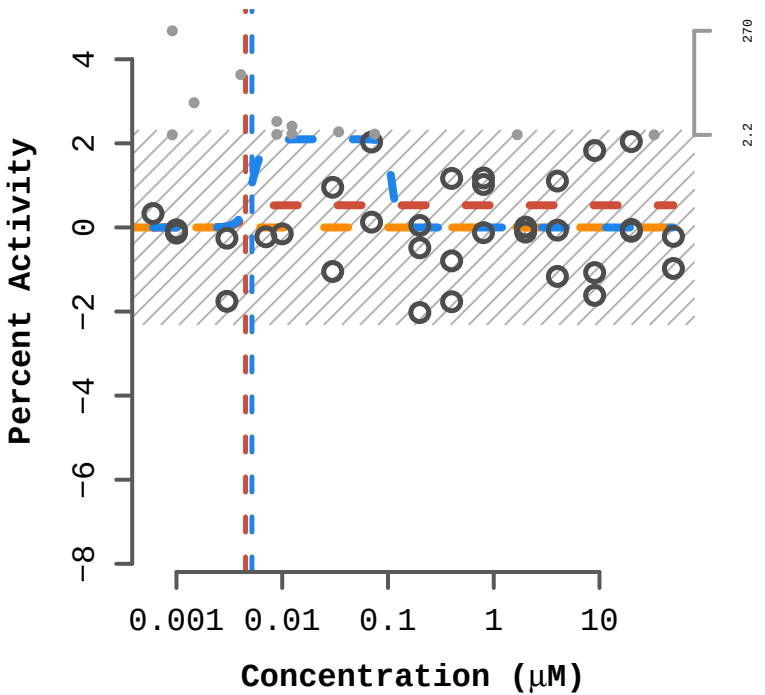
NAME: 4-Phenylpiperidin-4-ol
CHID: 57738 **CASRN:** 40807-61-2
SPID(S): Tox21_113808
M4ID: 12482411

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 0.528 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Methyl 4-acetamido-o-anisate
CHID: 57739 CASRN: 4093-29-2
SPID(S): Tox21_113908
M4ID: 12482322 BRK

HILL MODEL (in red):

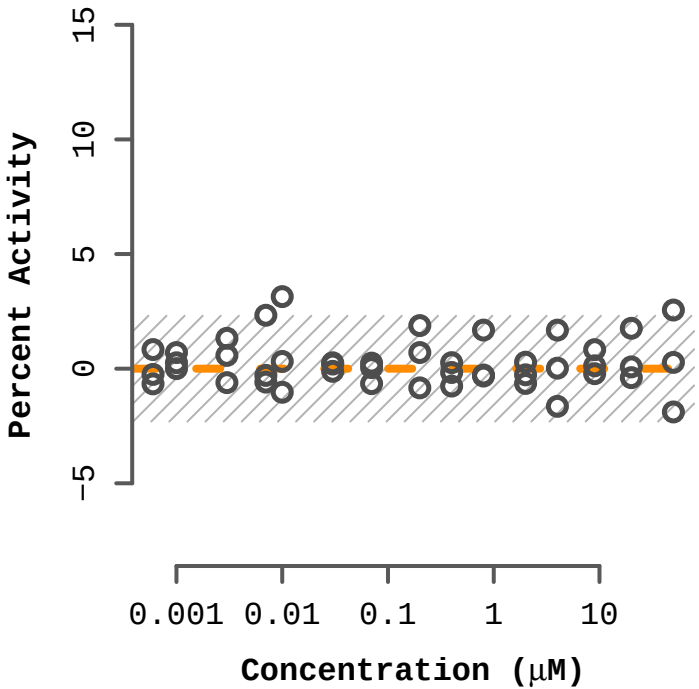
	tp	ga	gw
val:	0.527	−2.35	8
sd:	0.431	0.47	19.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.1	−2.29	8	−0.962	14.7
sd:	0.986	0.337	13.6	2.47	148

	CNST	HILL	GNLS
AIC:	337.82	342.27	342.45
PROB:	0.83	0.09	0.08
RMSE:	49.19	49.17	49.12

MAX_MEAN: 91.6 MAX_MED: 4.45 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

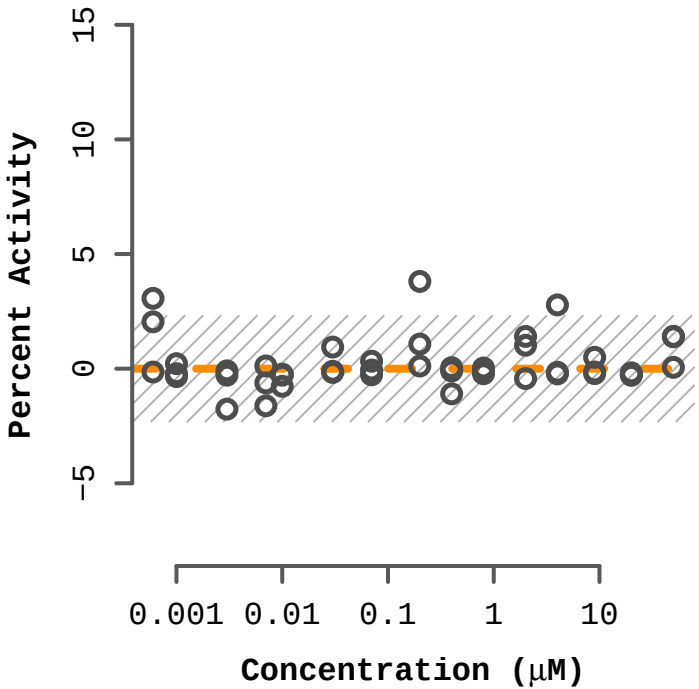
NAME: Methyl 4-acetamido-5-chloro-o-anisate
CHID: 57740 **CASRN:** 4093-31-6
SPID(S): Tox21_113842
M4ID: 12482380

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.07	NA	NA
PROB:	1	NA	NA
RMSE:	1.06	NA	NA

MAX_MEAN: 0.811 **MAX_MED:** 0.706 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

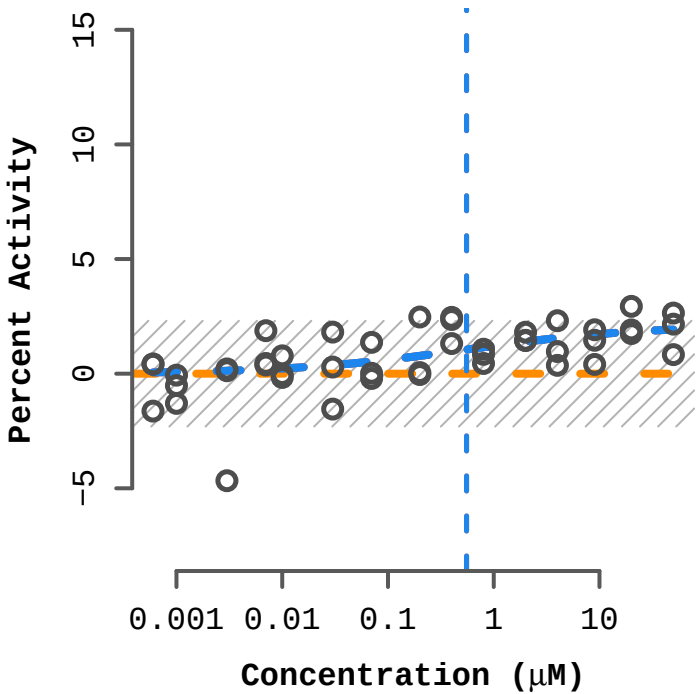
NAME: 7-Ethyltryptophol
CHID: 57741 **CASRN:** 41340-36-7
SPID(S): Tox21_113757
M4ID: 12482458

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 1.67 **MAX_MED:** 2.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Calcium undecylenate
CHID: 57742 **CASRN:** 1322-14-1
SPID(S): Tox21_113736
M4ID: 12482478

HILL MODEL (in red):

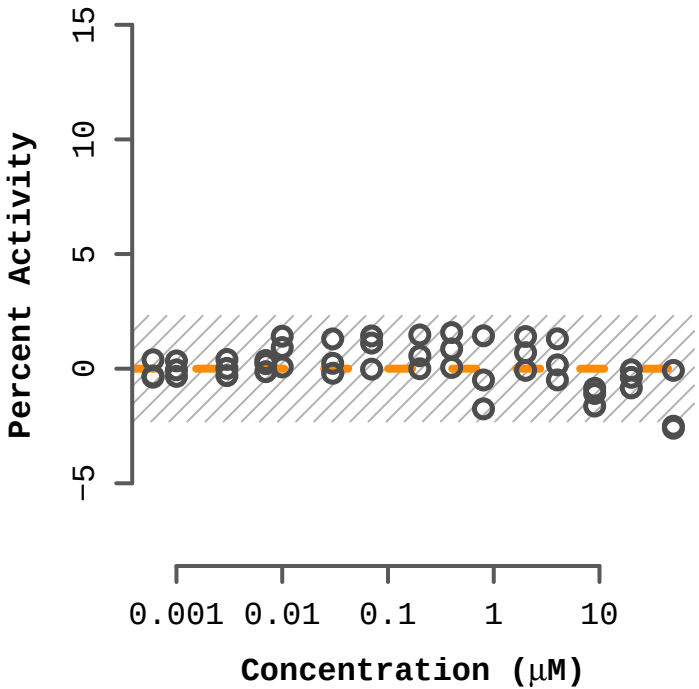
	tp	ga	gw
val:	2.1	−0.257	0.526
sd:	0.85	1	0.325

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.1	−0.257	0.526	2.59	8.82
sd:	0.85	1	0.325	1950	19200

	CNST	HILL	GNLS
AIC:	170.75	135.24	139.24
PROB:	0	0.88	0.12
RMSE:	1.55	1.11	1.11

MAX_MEAN: 2.2 **MAX_MED:** 2.37 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

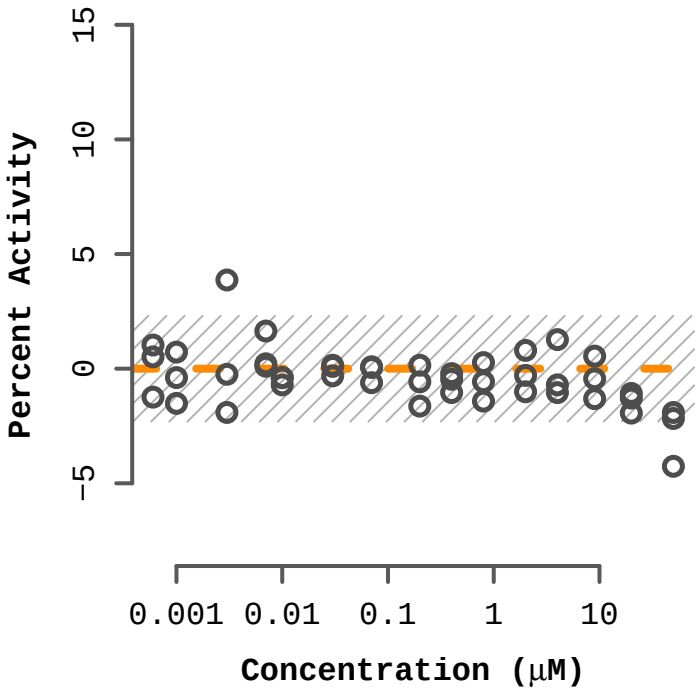
NAME: Mazaticol
CHID: 57743 **CASRN:** 42024-98-6
SPID(S): Tox21_113891
M4ID: 12482336

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	127.42	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.842 **MAX_MED:** 1.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

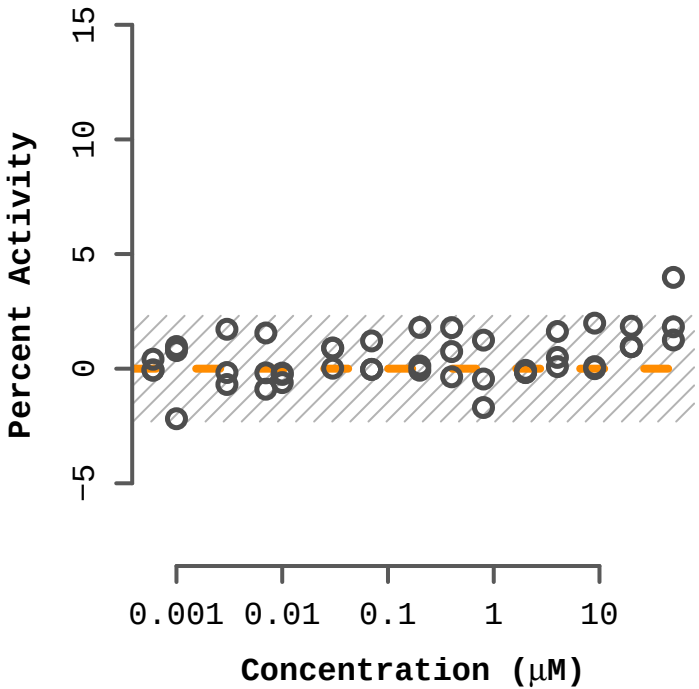
NAME: (2S,3s)-3-hydroxy-2-(4-methoxyphenyl)-2,3-dihy
CHID: 57744 **CASRN:** 42399-49-5
SPID(S): Tox21_113796
M4ID: 12482423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	148.47	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.655 **MAX_MED:** 0.516 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

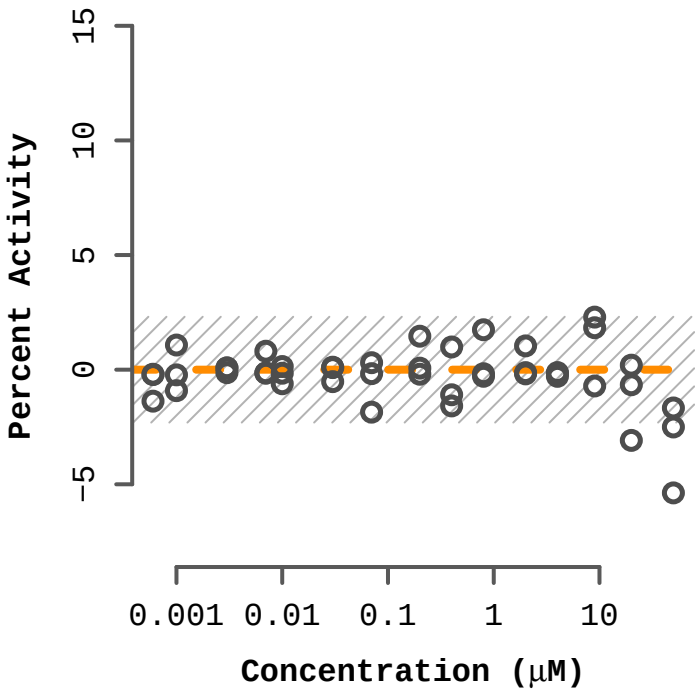
NAME: 4'-Tert-butyl-4-chlorobutyrophenone
CHID: 57745 **CASRN:** 43076-61-5
SPID(S): Tox21_113820
M4ID: 12482401

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 2.35 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

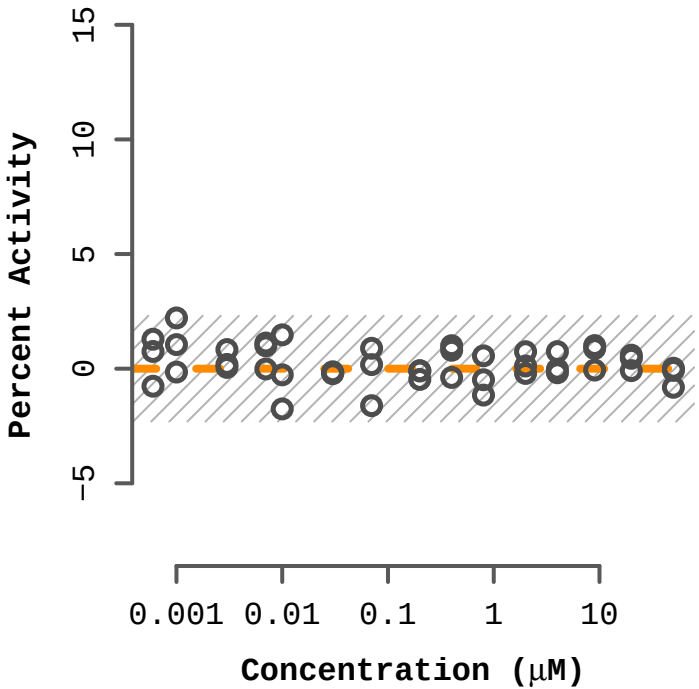
NAME: Fenbutrazate
CHID: 57746 **CASRN:** 4378-36-3
SPID(S): Tox21_113685
M4ID: 12482529

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.31	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

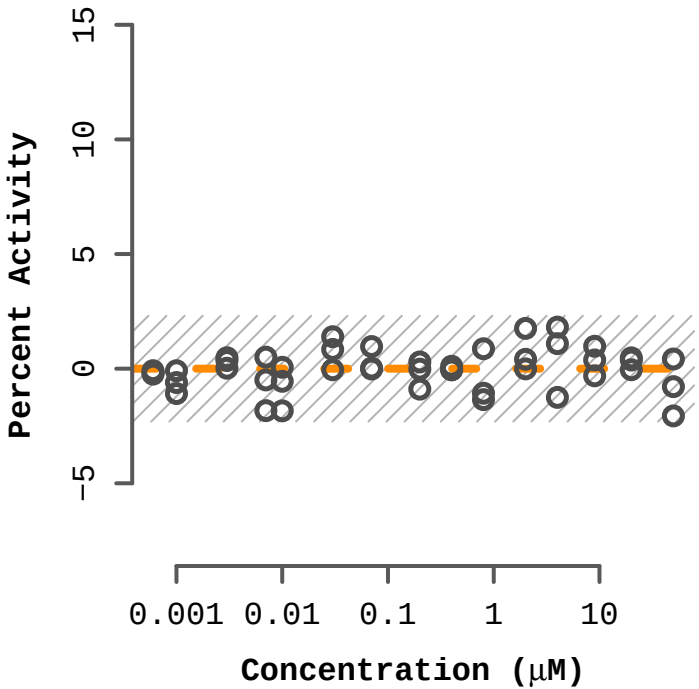
NAME: 3-(2,6-Dichlorophenyl)-5-methylisoxazole-4-carl
CHID: 57747 **CASRN:** 4462-55-9
SPID(S): Tox21_113775
M4ID: 12482441

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	110.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.04 **MAX_MED:** 1.05 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

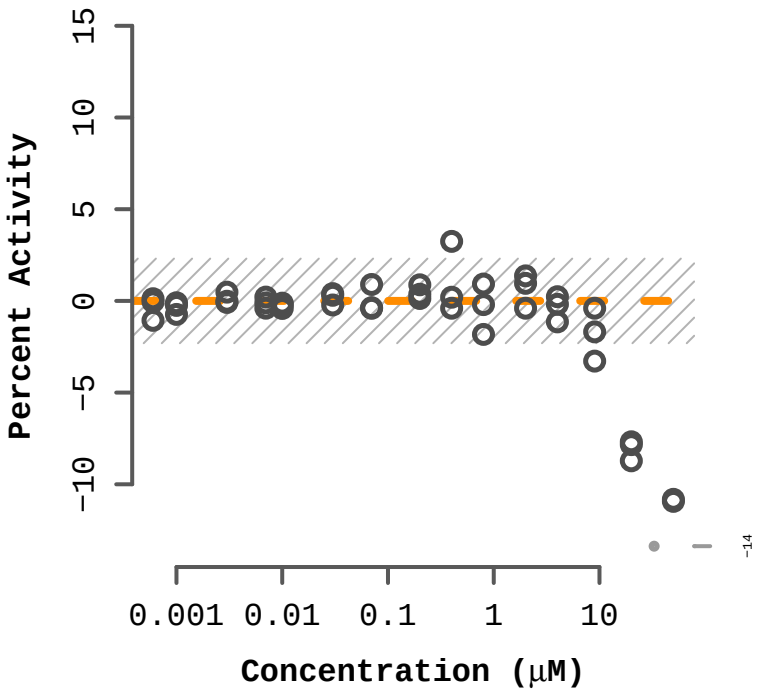
NAME: Normethadone
CHID: 57748 **CASRN:** 467-85-6
SPID(S): Tox21_113687
M4ID: 12482527

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	116.92	NA	NA
PROB:	1	NA	NA
RMSE:	0.86	NA	NA

MAX_MEAN: 0.73 **MAX_MED:** 1.09 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

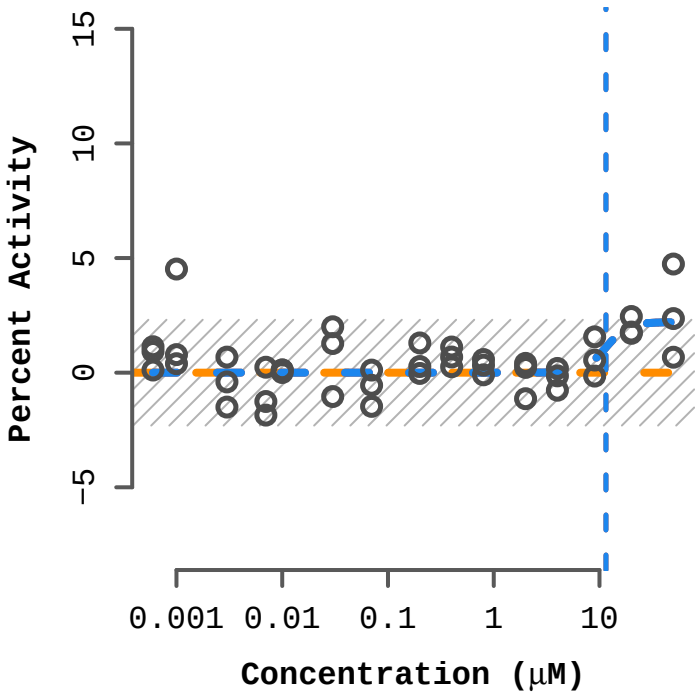
NAME: Clocapramine
CHID: 57749 **CASRN:** 47739-98-0
SPID(S): Tox21_113731
M4ID: 12482483 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	215.71	NA	NA
PROB:	1	NA	NA
RMSE:	3.83	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 0.958 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Oxycinchophen
CHID: 57750 **CASRN:** 485-89-2
SPID(S): Tox21_113947
M4ID: 12482284

HILL MODEL (in red):

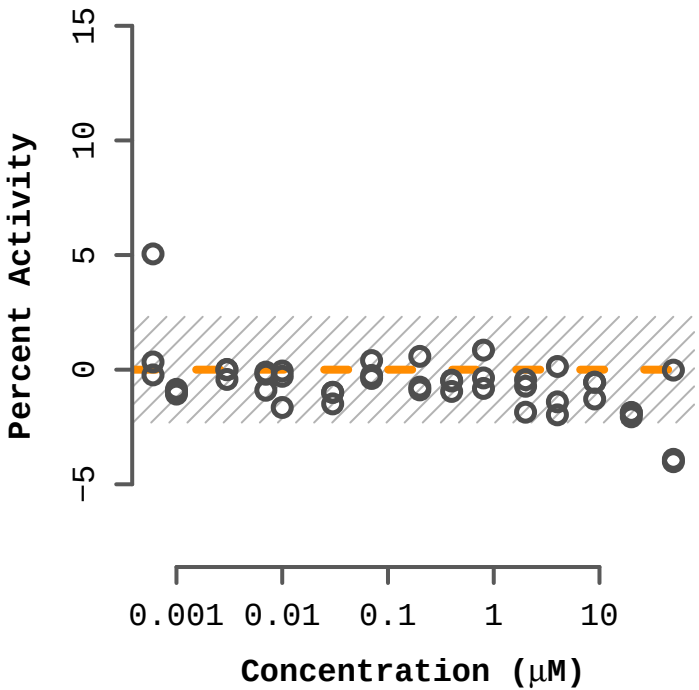
	tp	ga	gw
val:	2.21	1.06	4.19
sd:	0.864	0.24	5.45

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.21	1.06	4.19	2.97	5.65
sd:	0.864	0.24	5.45	1490	6670

	CNST	HILL	GNLS
AIC:	153.54	138.58	142.58
PROB:	0	0.88	0.12
RMSE:	1.41	1.13	1.13

MAX_MEAN: 2.59 **MAX_MED:** 2.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

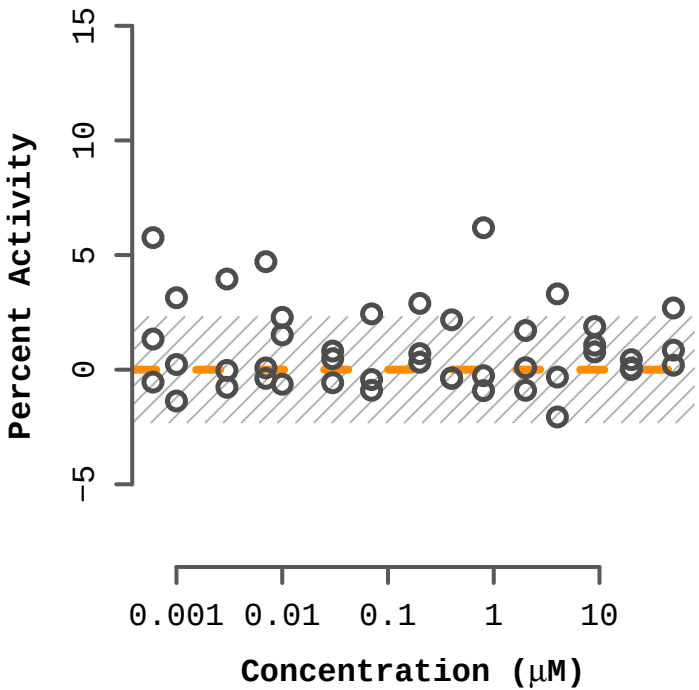
NAME: Bamipine
CHID: 57751 **CASRN:** 4945-47-5
SPID(S): Tox21_113882
M4ID: 12482343

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.24	NA	NA
PROB:	1	NA	NA
RMSE:	1.46	NA	NA

MAX_MEAN: 1.72 **MAX_MED:** 0.338 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

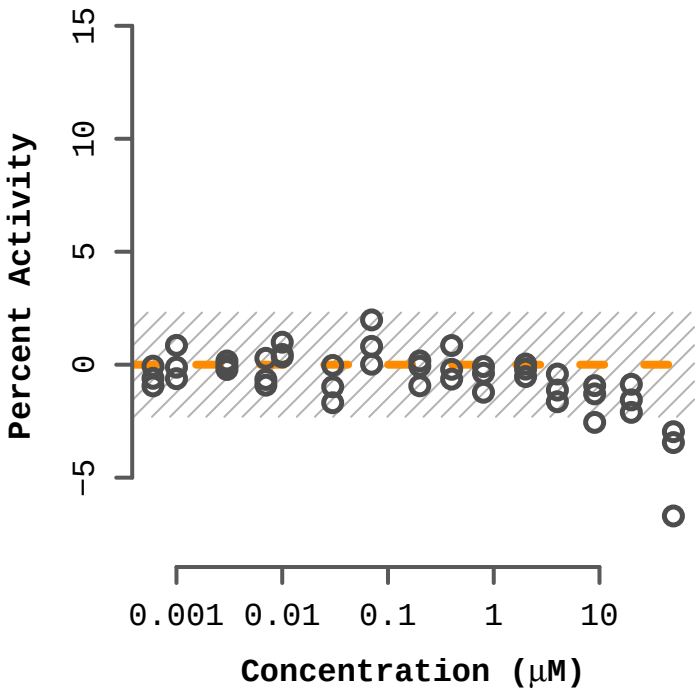
NAME: 7-Chloro-2-methylquinoline
CHID: 57752 **CASRN:** 4965-33-7
SPID(S): Tox21_113767
M4ID: 12482448

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	187.57	NA	NA
PROB:	1	NA	NA
RMSE:	2.04	NA	NA

MAX_MEAN: 2.19 **MAX_MED:** 1.52 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

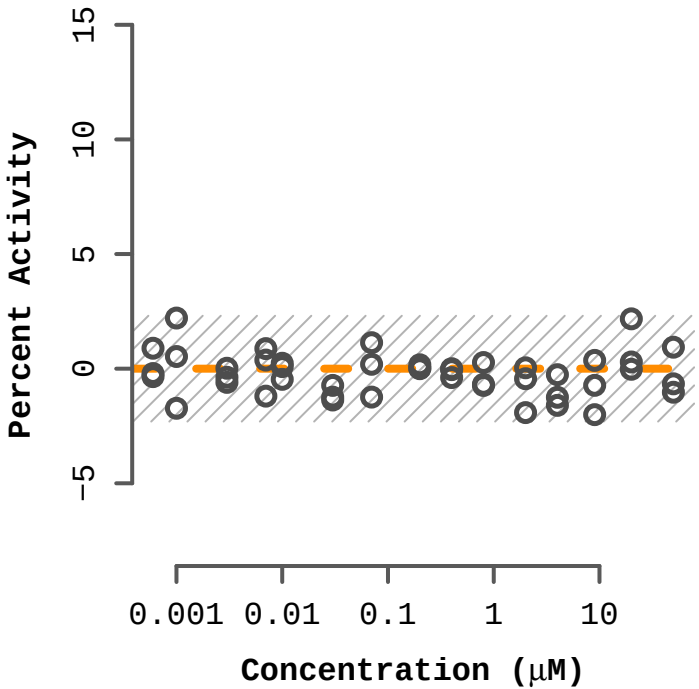
NAME: Eltrombopag
CHID: 57753 **CASRN:** 496775-61-2
SPID(S): Tox21_113965
M4ID: 12482268

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.27	NA	NA
PROB:	1	NA	NA
RMSE:	1.52	NA	NA

MAX_MEAN: 0.939 **MAX_MED:** 0.813 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

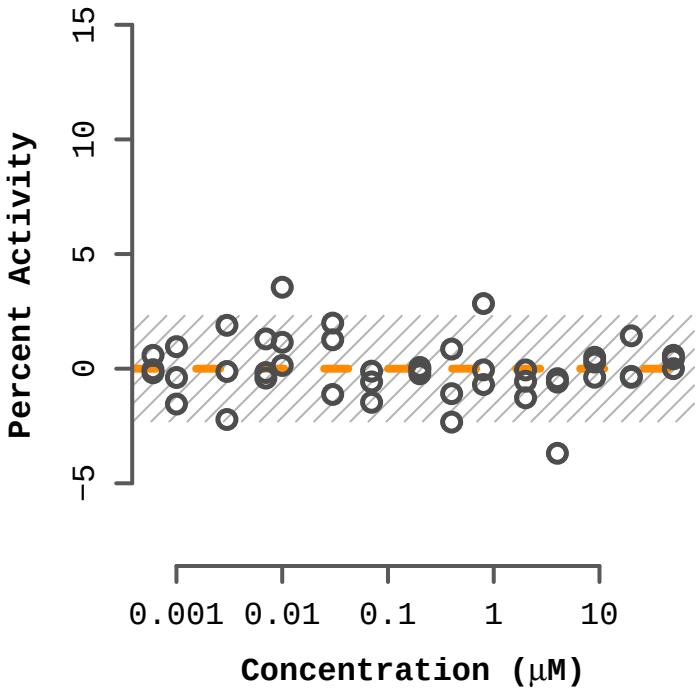
NAME: 6-Hydroxynicotinic acid
CHID: 57754 **CASRN:** 5006-66-6
SPID(S): Tox21_113747
M4ID: 12482468

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.47	NA	NA
PROB:	1	NA	NA
RMSE:	0.94	NA	NA

MAX_MEAN: 0.814 **MAX_MED:** 0.531 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

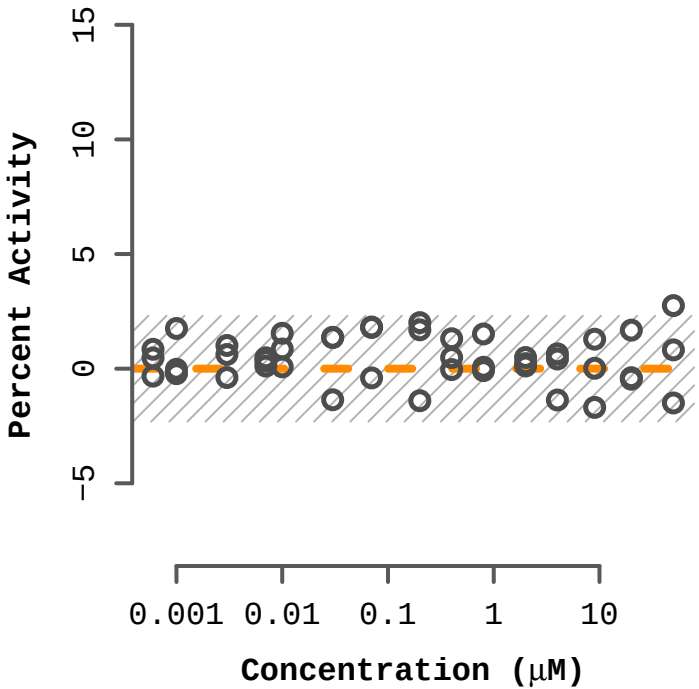
NAME: Beclamide
CHID: 57755 **CASRN:** 501-68-8
SPID(S): Tox21_113912
M4ID: 12482318

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

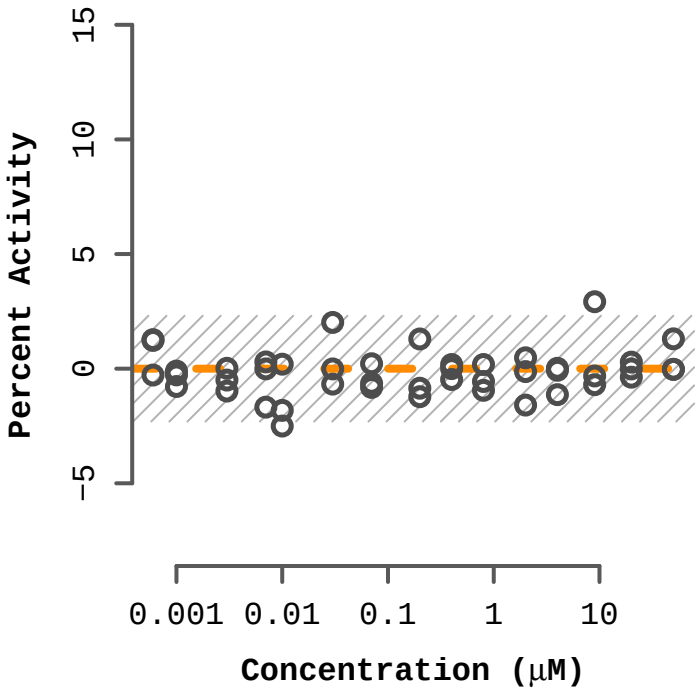
NAME: Octamylamine
CHID: 57756 **CASRN:** 502-59-0
SPID(S): Tox21_113900
M4ID: 12482328

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.07 **MAX_MED:** 1.8 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

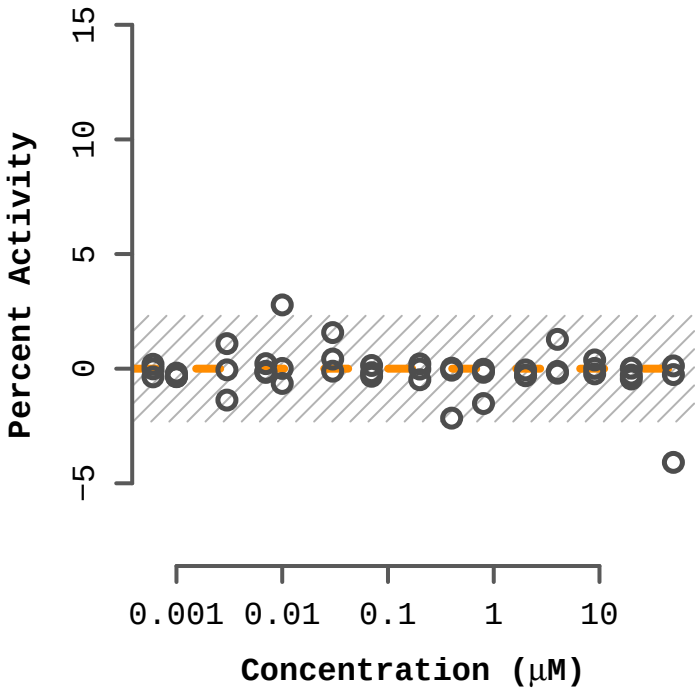
NAME: 3-(2-Chloroethyl)quinazoline-2,4(1H,3H)-dione
CHID: 57757 **CASRN:** 5081-87-8
SPID(S): Tox21_113823
M4ID: 12482398

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.99	NA	NA

MAX_MEAN: 0.741 **MAX_MED:** 1.23 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

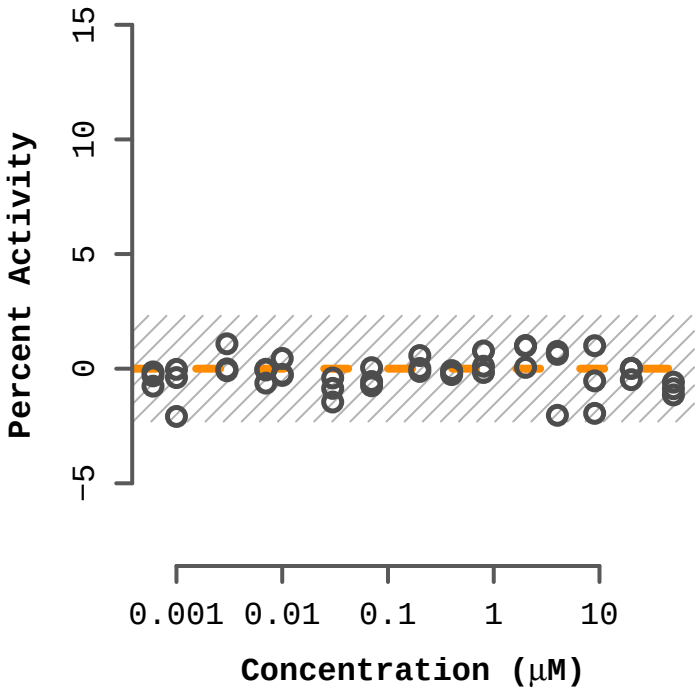
NAME: Tolciclate
CHID: 57758 **CASRN:** 50838-36-3
SPID(S): Tox21_113710
M4ID: 12482504

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	98.21	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.717 **MAX_MED:** 0.421 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

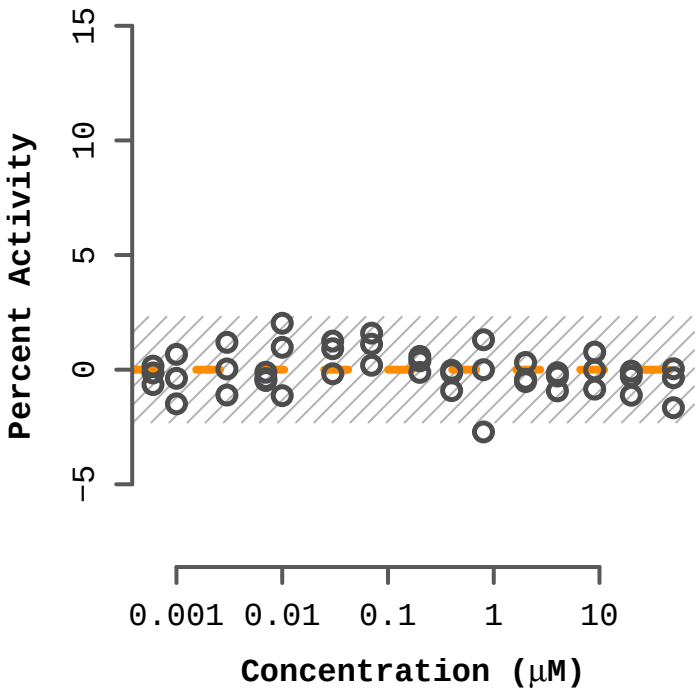
NAME: Dimenoxadol
CHID: 57759 **CASRN:** 509-78-4
SPID(S): Tox21_113866
M4ID: 12482359

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.27	NA	NA
PROB:	1	NA	NA
RMSE:	0.77	NA	NA

MAX_MEAN: 0.684 **MAX_MED:** 0.978 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

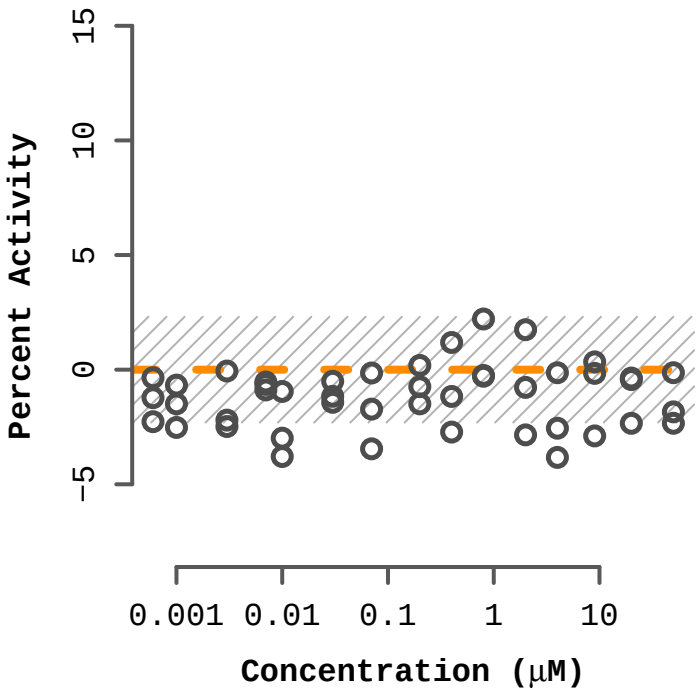
NAME: Ambucetamide
CHID: 57760 **CASRN:** 519-88-0
SPID(S): Tox21_113898
M4ID: 12482330

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.69	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 0.968 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

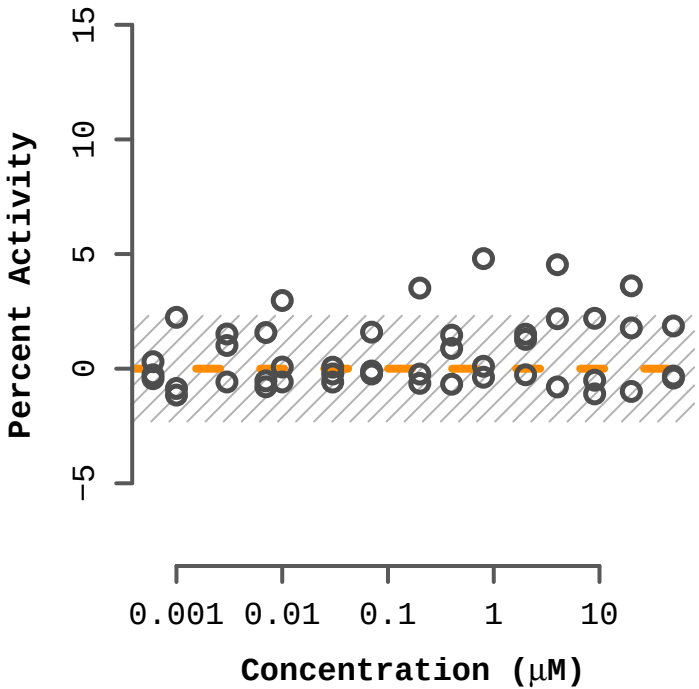
NAME: 1-(3-Chlorophenyl)-4-(3-chloropropyl)piperazine
CHID: 57761 **CASRN:** 52605-52-4
SPID(S): Tox21_113914
M4ID: 12482316

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	186.12	NA	NA
PROB:	1	NA	NA
RMSE:	1.79	NA	NA

MAX_MEAN: 0.558 **MAX_MED:** −0.16 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

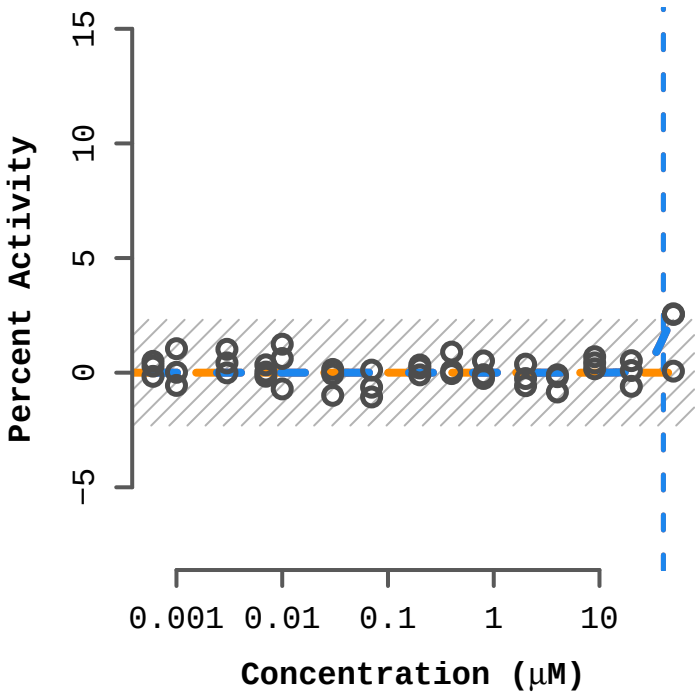
NAME: Glybuthiazol
CHID: 57762 **CASRN:** 535-65-9
SPID(S): Tox21_113930
M4ID: 12482301

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	170.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 1.97 **MAX_MED:** 2.18 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Bufetolol
CHID: 57763 **CASRN:** 53684-49-4
SPID(S): Tox21_113888
M4ID: 12482338

HILL MODEL (in red):

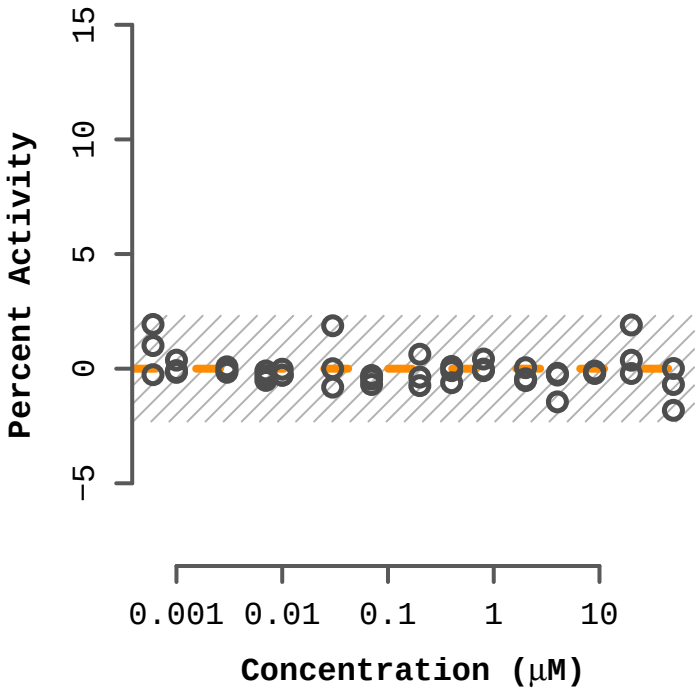
	tp	ga	gw
val:	3.08	1.6	5.72
sd:	17.3	1.47	27.8

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.08	1.6	5.72	3.38	5.01
sd:	16.8	1.43	27.1	37500	112000

	CNST	HILL	GNLS
AIC:	93.53	88.4	92.4
PROB:	0.06	0.82	0.11
RMSE:	0.75	0.62	0.62

MAX_MEAN: 1.73 **MAX_MED:** 2.54 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

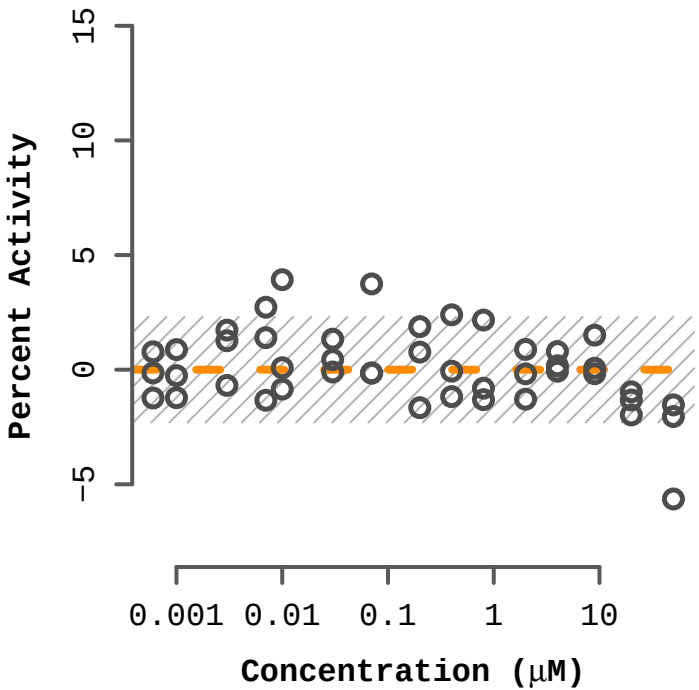
NAME: 5-Chloro-1-(4-piperidyl)-1H-benzimidazol-2(3H)·
CHID: 57764 **CASRN:** 53786-28-0
SPID(S): Tox21_113838
M4ID: 12482384

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	89.36	NA	NA
PROB:	1	NA	NA
RMSE:	0.71	NA	NA

MAX_MEAN: 0.893 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

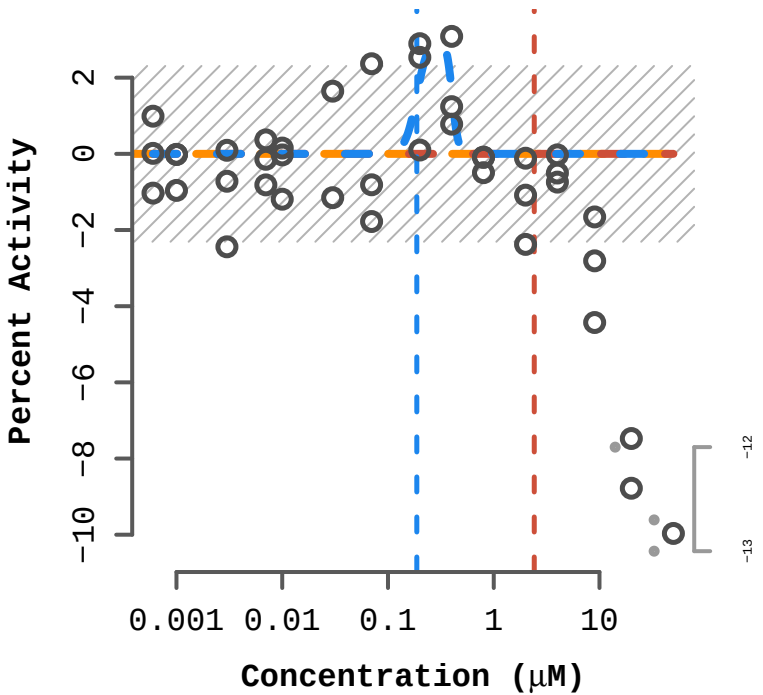
NAME: Ethyl 4-(2-amino-4-chloroanilino)piperidine-1-c
CHID: 57765 **CASRN:** 53786-45-1
SPID(S): Tox21_113929
M4ID: 12482302

HILL MODEL: Not applicable.

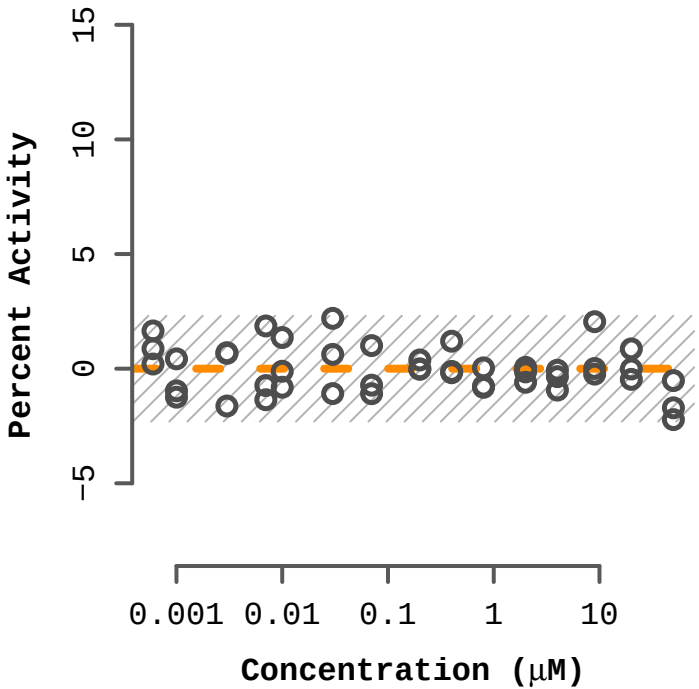
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	172.37	NA	NA
PROB:	1	NA	NA
RMSE:	1.66	NA	NA

MAX_MEAN: 1.15 **MAX_MED:** 1.4 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Ethyl 4-(5-chloro-2,3-dihydro-2-oxo-1h-benzimi
CHID:    57766   CASRN: 53786-46-2
SPID(S): Tox21_113868
M4ID:    12482357  BRK

HILL MODEL (in red):
      tp        ga        gw
val:  9.6e-10   0.383     1.34
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  3.08      -0.727    7.96      -0.393    15.5
sd:   55.3      2.51      74.7      1.08      348

      CNST          HILL          GNLS
AIC:  240.49        246.49        246.13
PROB: 0.9           0.04          0.05
RMSE: 4.21          4.21          4.16

MAX_MEAN: 1.84      MAX_MED: 2.53      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

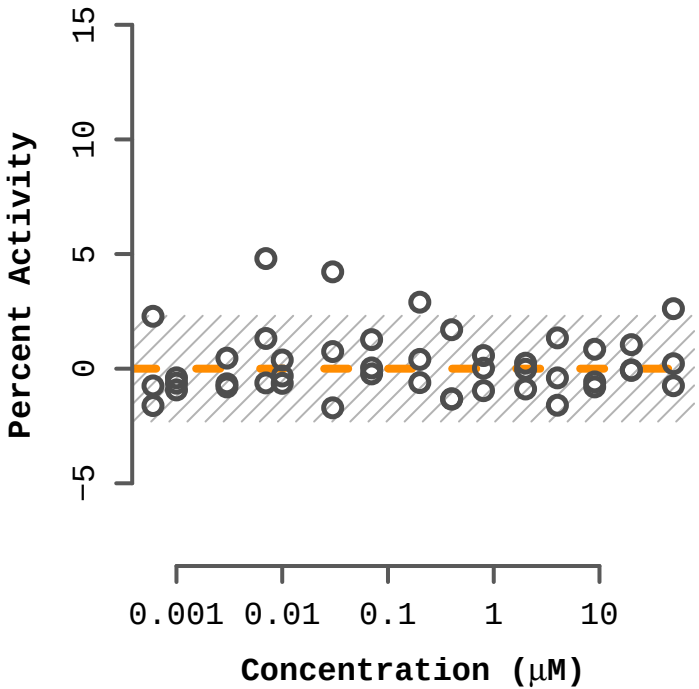
NAME: Lodoxamide
CHID: 57767 **CASRN:** 53882-12-5
SPID(S): Tox21_113669
M4ID: 12482545

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.28	NA	NA
PROB:	1	NA	NA
RMSE:	1	NA	NA

MAX_MEAN: 0.907 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

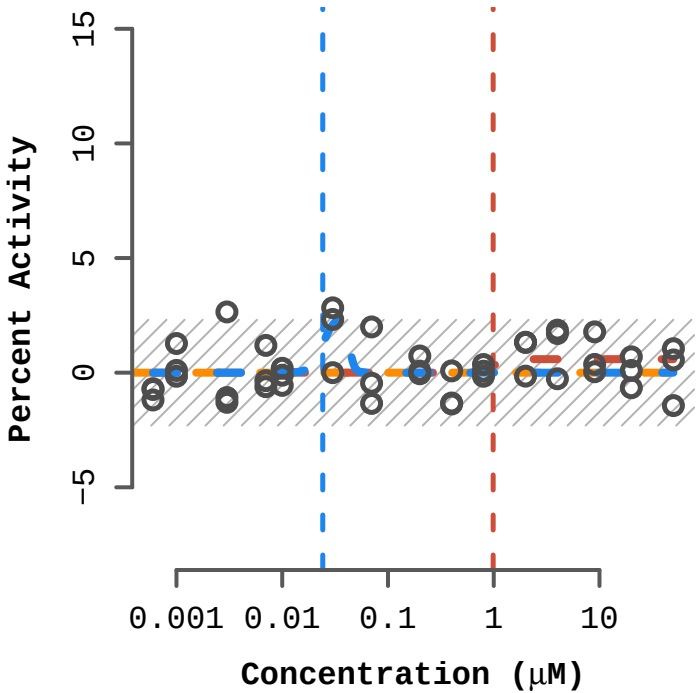
NAME: Albendazole oxide
CHID: 57768 **CASRN:** 54029-12-8
SPID(S): Tox21_113873
M4ID: 12482352

HILL MODEL: Not applicable.

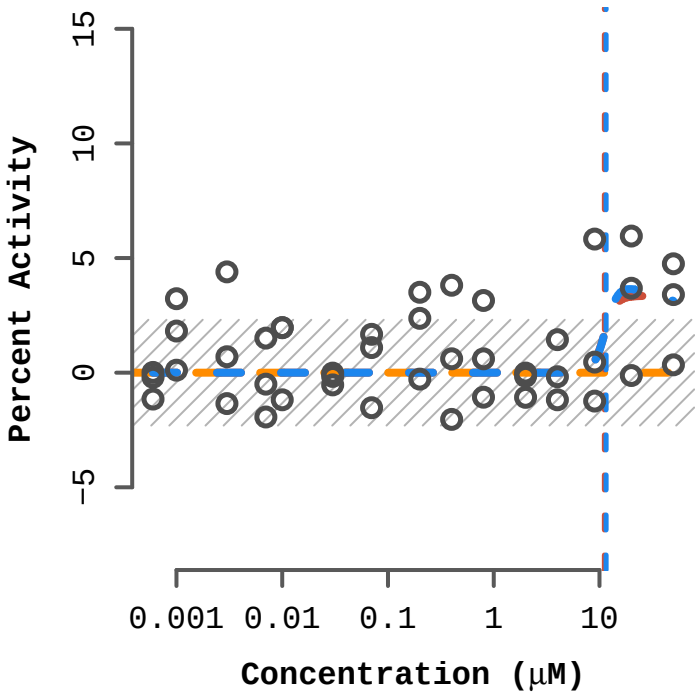
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	155.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.43	NA	NA

MAX_MEAN: 1.83 **MAX_MED:** 1.32 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    3-(Trifluoromethyl)-o-toluidine
CHID:    57769   CASRN: 54396-44-0
SPID(S): Tox21_113763
M4ID:    12482452

HILL MODEL (in red):
      tp       ga       gw
val:  0.59     -0.00531 8
sd:   0.268    0.359    20.7

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.46     -1.62    8        -1.37    18
sd:   8.73     1.1      29.2     2.34     201

      CNST        HILL        GNLS
AIC:  142.32      143.67      146.27
PROB: 0.61        0.31        0.08
RMSE: 1.13        1.09        1.05

MAX_MEAN: 1.72      MAX_MED: 2.32      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Butamisole
CHID: 57770 **CASRN:** 54400-59-8
SPID(S): Tox21_113680
M4ID: 12482534

HILL MODEL (in red):

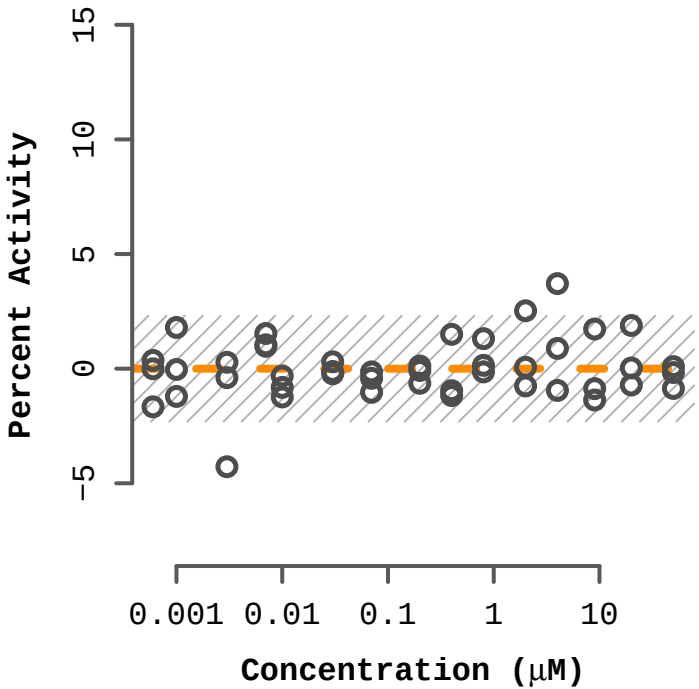
	tp	ga	gw
val:	3.35	1.05	8
sd:	0.889	0.226	17.2

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.55	1.06	7.81	2.17	0.732
sd:	249	4.07	270	27.2	125

	CNST	HILL	GNLS
AIC:	201.85	197.07	200.97
PROB:	0.07	0.81	0.12
RMSE:	2.27	1.96	1.96

MAX_MEAN: 3.17 **MAX_MED:** 3.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

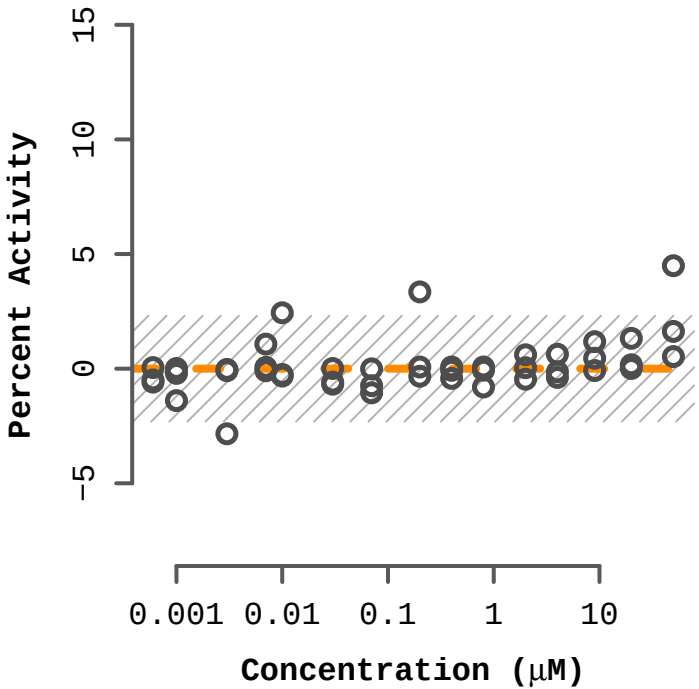
NAME: Ethyl biscoumacetate
CHID: 57771 **CASRN:** 548-00-5
SPID(S): Tox21_113859
M4ID: 12482364

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.02	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 1.22 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

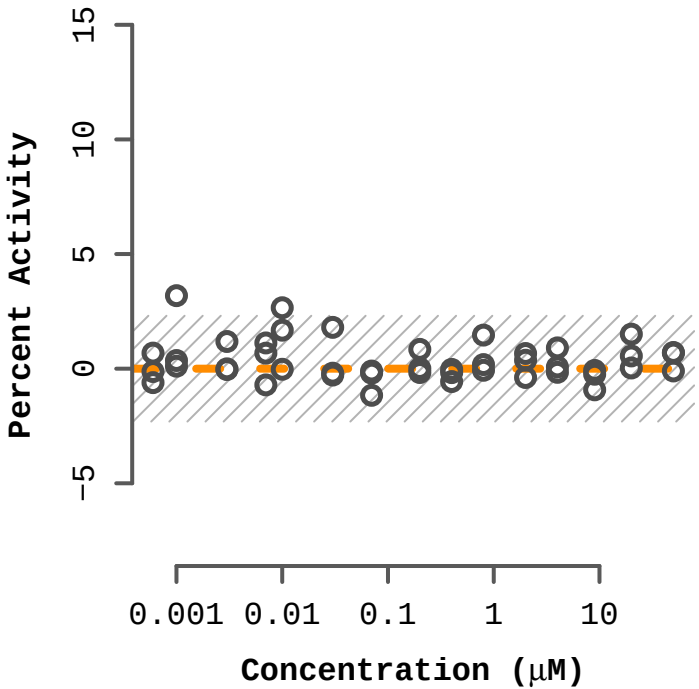
NAME: Isoxepac
CHID: 57772 **CASRN:** 55453-87-7
SPID(S): Tox21_113815
M4ID: 12482404

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 2.22 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

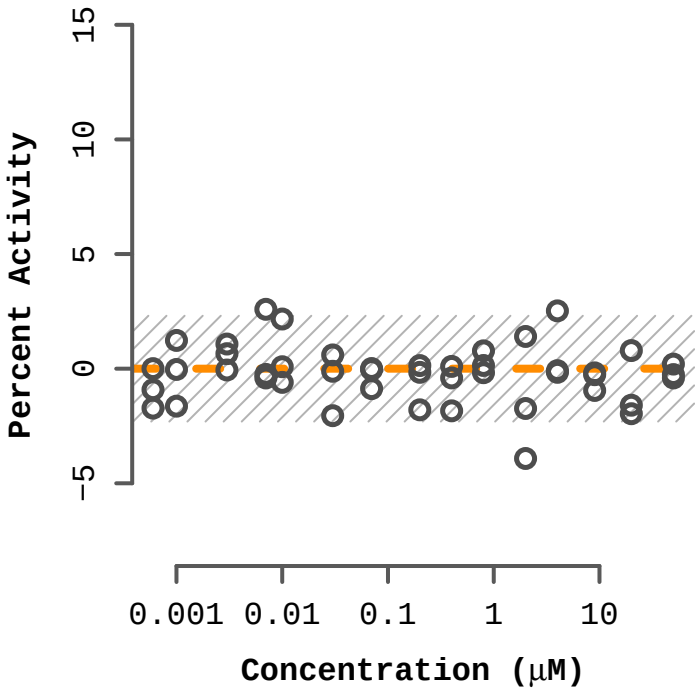
NAME: Arprinocid
CHID: 57773 **CASRN:** 55779-18-5
SPID(S): Tox21_113931
M4ID: 12482300

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.94	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 1.44 **MAX_MED:** 1.68 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

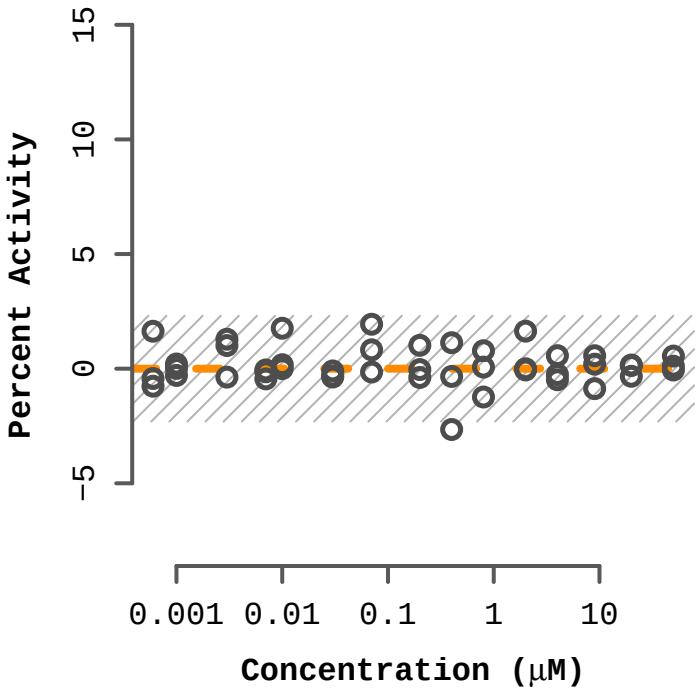
NAME: Isalon
CHID: 57774 **CASRN:** 5579-81-7
SPID(S): Tox21_113724
M4ID: 12482490

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.24	NA	NA

MAX_MEAN: 0.76 **MAX_MED:** 0.656 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

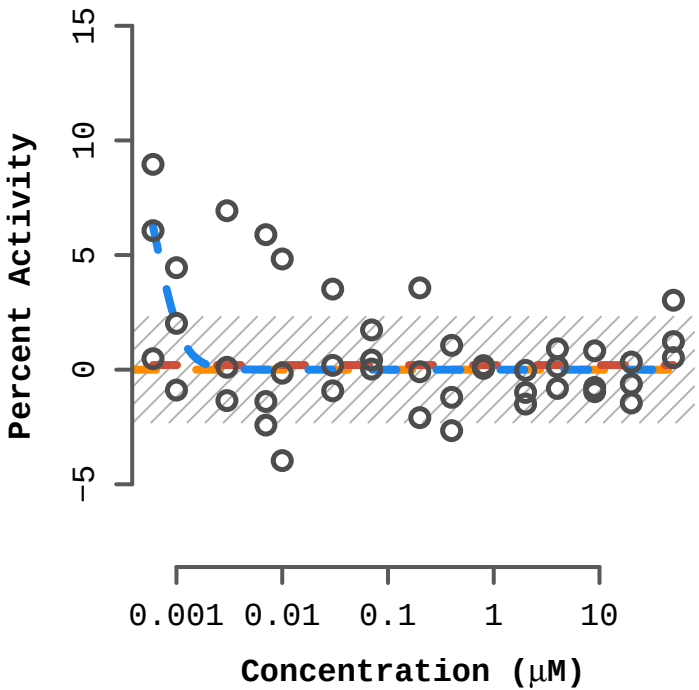
NAME: Cintriamide
CHID: 57775 **CASRN:** 5588-21-6
SPID(S): Tox21_113833
M4ID: 12482389

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.13	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.873 **MAX_MED:** 1.01 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: 2-Ethoxy-5-fluorouracil
CHID: 57776 **CASRN:** 56177-80-1
SPID(S): Tox21_113748
M4ID: 12482467

HILL MODEL (in red):

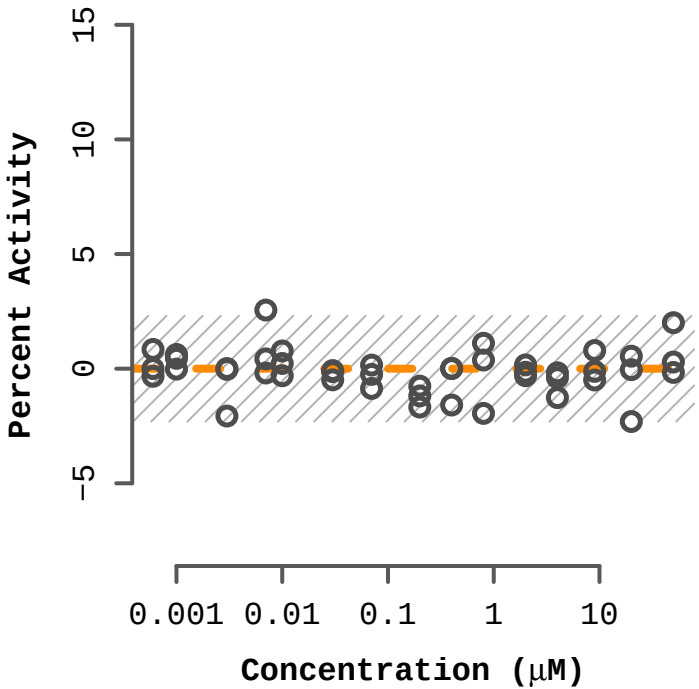
	tp	ga	gw
val:	0.201	−4.96	4.35
sd:	0.321	3520	8730

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	10.7	−5.22	1.21	−3.18	3.58
sd:	23.1	131	83.2	0.549	5.38

	CNST	HILL	GNLS
AIC:	212.4	218	212.16
PROB:	0.46	0.03	0.52
RMSE:	2.74	2.69	2.36

MAX_MEAN: 5.17 **MAX_MED:** 6.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

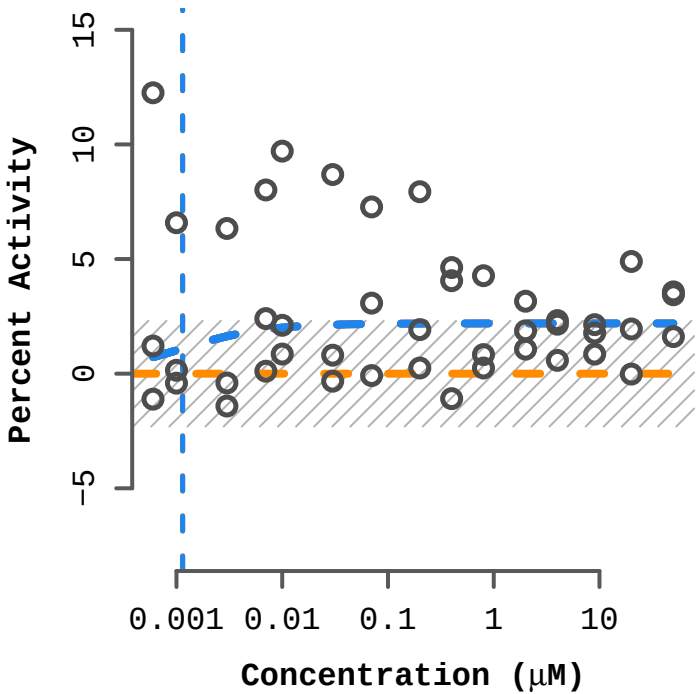
NAME: 1-(4-Fluorophenyl)-4-oxocyclohexanecarbonitril
CHID: 57777 CASRN: 56326-98-8
SPID(S): Tox21_113828
M4ID: 12482393

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	118.61	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.933 **MAX_MED:** 0.453 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Tocanfil
CHID: 57778 **CASRN:** 5634-42-4
SPID(S): Tox21_113936
M4ID: 12482295

HILL MODEL (in red):

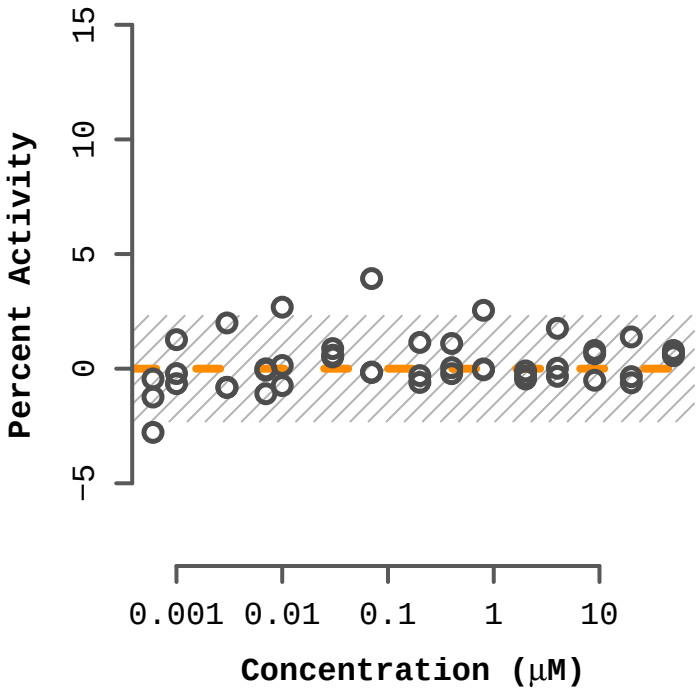
	tp	ga	gw
val:	2.19	−2.94	1.1
sd:	0.454	0.899	1.64

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.19	−2.94	1.1	2.8	7.2
sd:	0.454	0.899	1.64	1710	11200

	CNST	HILL	GNLS
AIC:	252.91	235.4	239.4
PROB:	0	0.88	0.12
RMSE:	4.11	3.27	3.27

MAX_MEAN: 4.23 **MAX_MED:** 4.06 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

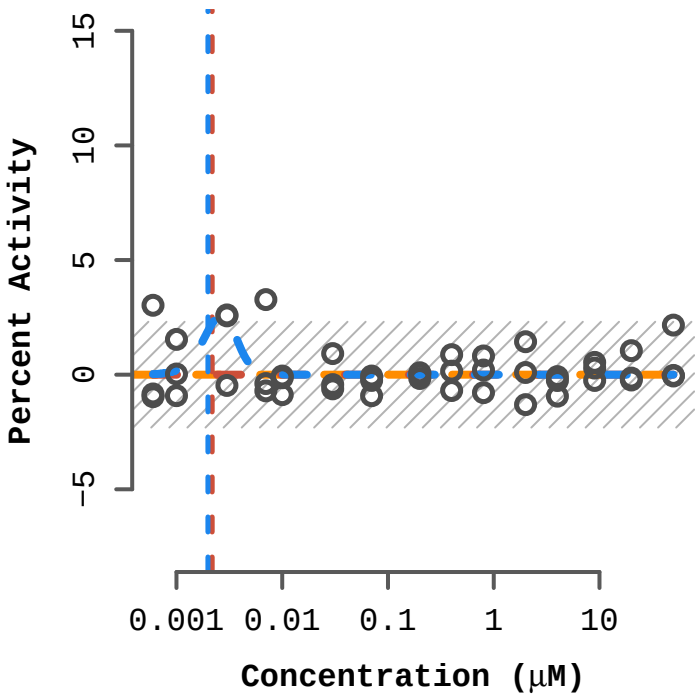
NAME: 2,3-Epoxypropyl 4-(2-methoxyethyl)phenyl ether
CHID: 57779 **CASRN:** 56718-70-8
SPID(S): Tox21_113752
M4ID: 12482463

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.16	NA	NA

MAX_MEAN: 1.21 **MAX_MED:** 0.675 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Fluretofene
CHID: 57780 **CASRN:** 56917-29-4
SPID(S): Tox21_113903
M4ID: 12482326

HILL MODEL (in red):

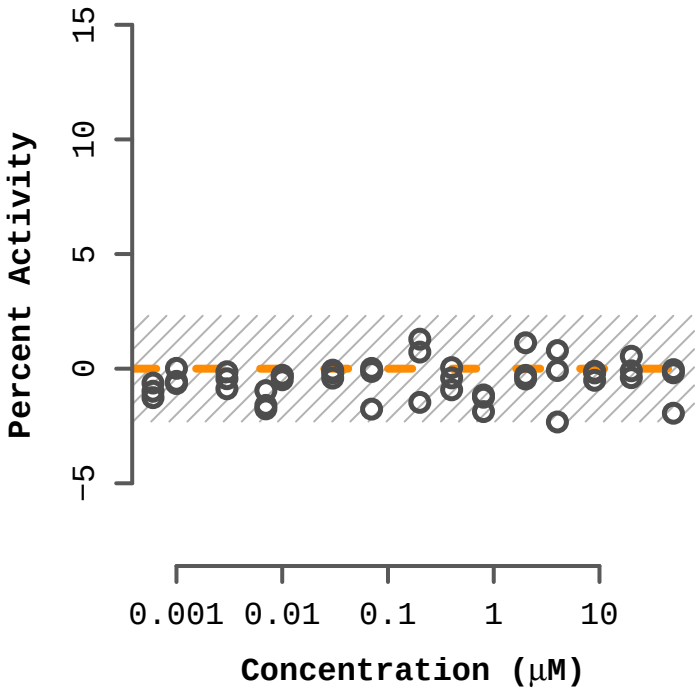
	tp	ga	gw
val:	9.88e-12	-2.66	2.2
sd:	9.97e-06	35500	829000

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	3.93	-2.7	4.32	-2.45	5.94
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	132.87	138.87	136.61
PROB:	0.83	0.04	0.13
RMSE:	1.11	1.11	1.06

MAX_MEAN: 1.57 **MAX_MED:** 2.57 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

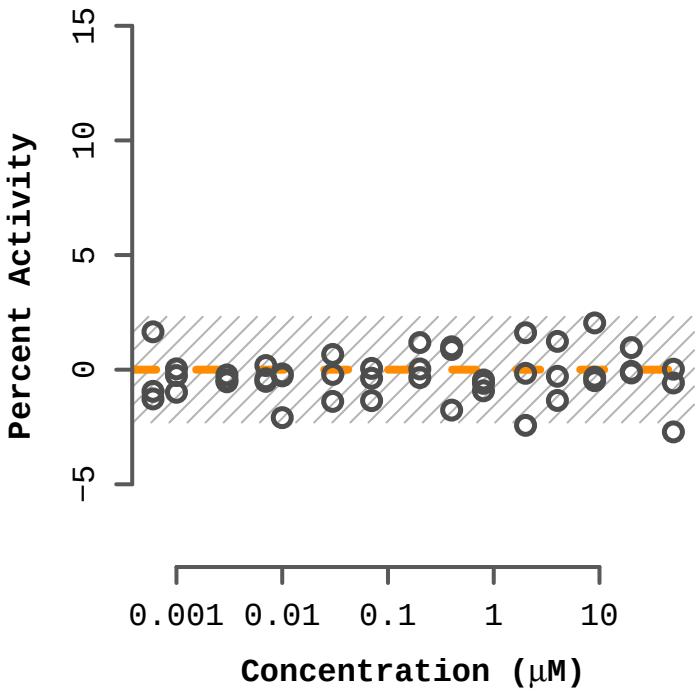
NAME: Glyceryl methacrylate
CHID: 57781 **CASRN:** 5919-74-4
SPID(S): Tox21_113953
M4ID: 12482278

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.09	NA	NA
PROB:	1	NA	NA
RMSE:	0.93	NA	NA

MAX_MEAN: 0.181 **MAX_MED:** 0.725 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

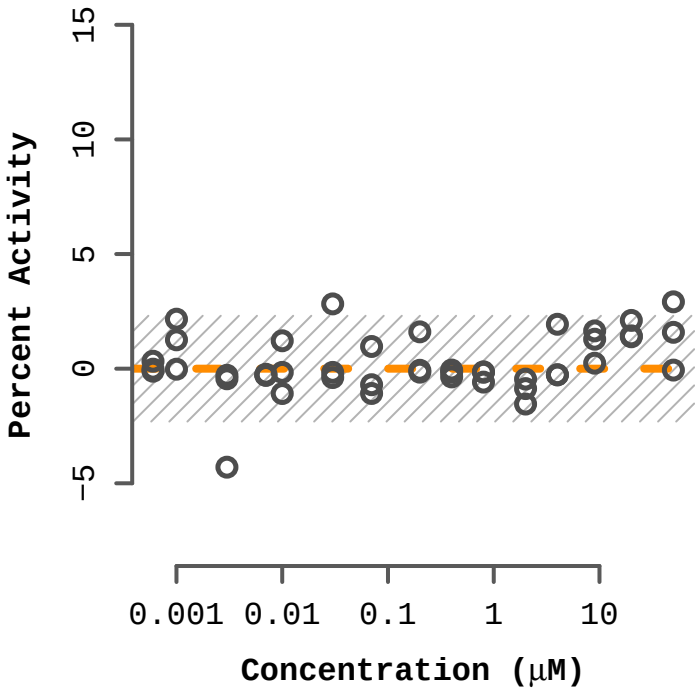
NAME: Sulfaperin
CHID: 57782 **CASRN:** 599-88-2
SPID(S): Tox21_113864
M4ID: 12482361

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.04	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.412 **MAX_MED:** 0.881 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

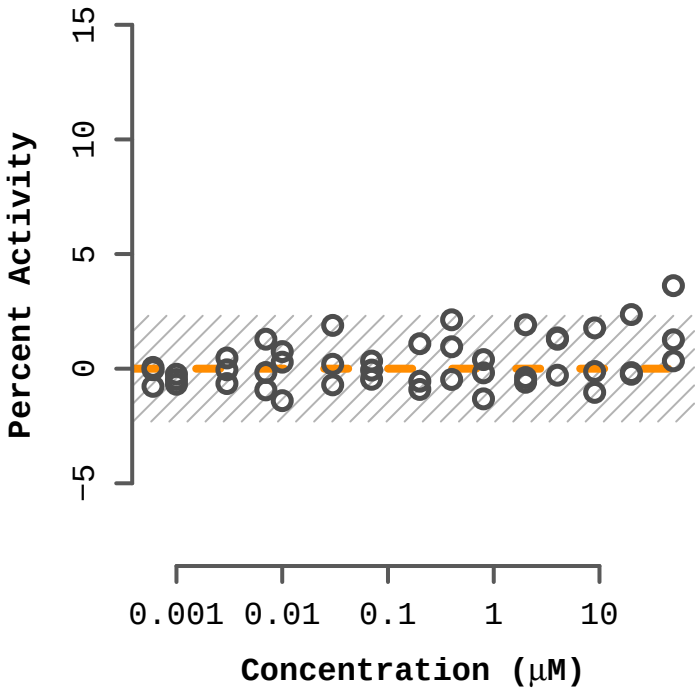
NAME: Diethyl dipropylmalonate
CHID: 57783 **CASRN:** 6065-63-0
SPID(S): Tox21_113799
M4ID: 12482420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.72	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 1.64 **MAX_MED:** 1.59 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

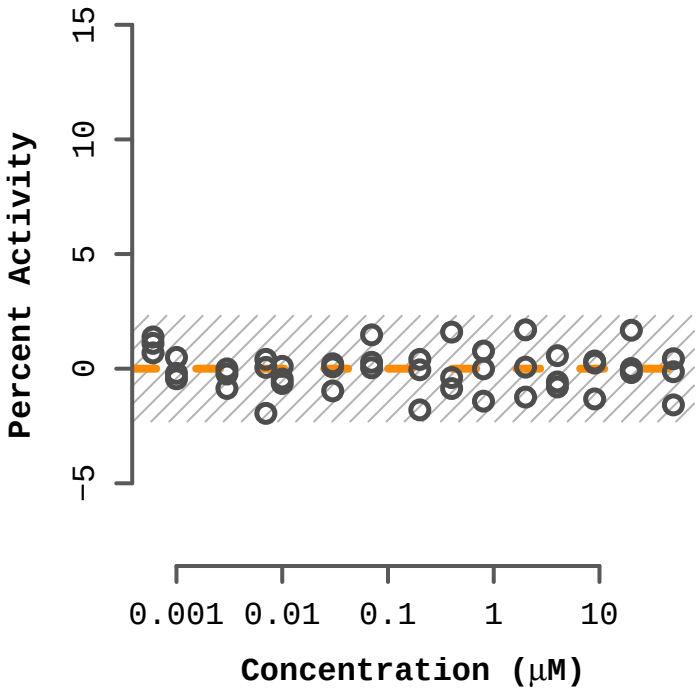
NAME: Cycotiamine
CHID: 57784 **CASRN:** 6092-18-8
SPID(S): Tox21_113932
M4ID: 12482299

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	135.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.09	NA	NA

MAX_MEAN: 1.74 **MAX_MED:** 1.28 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

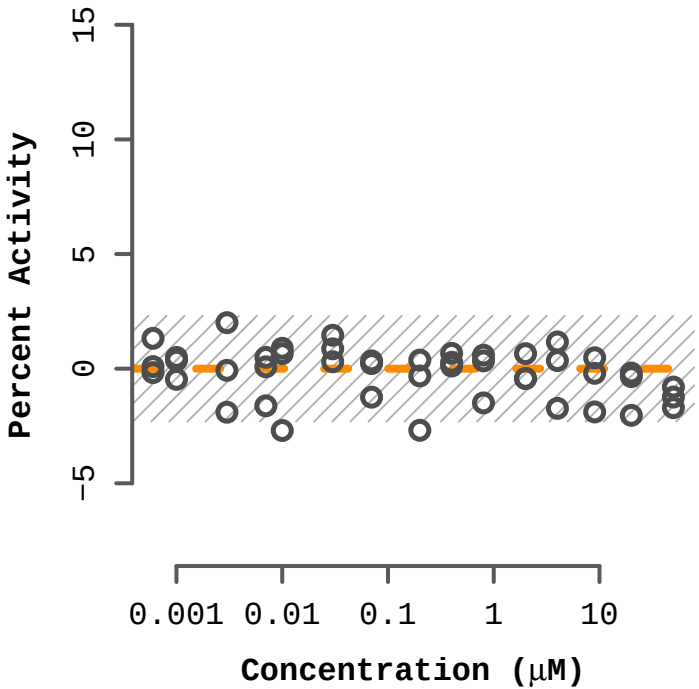
NAME: Ethyl 2-oxopyrrolidin-2-ylacetate
CHID: 57785 **CASRN:** 61516-73-2
SPID(S): Tox21_113837
M4ID: 12482385

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	120.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.89	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 1.11 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

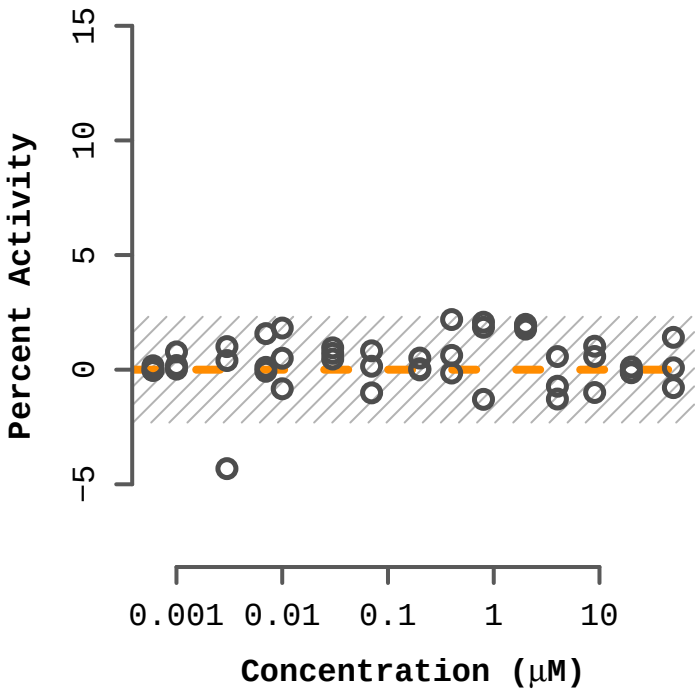
NAME: 1-Chloro-3-(chloromethyl)-benzene
CHID: 57786 **CASRN:** 620-20-2
SPID(S): Tox21_113840
M4ID: 12482382

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	139.7	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 0.877 **MAX_MED:** 0.869 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

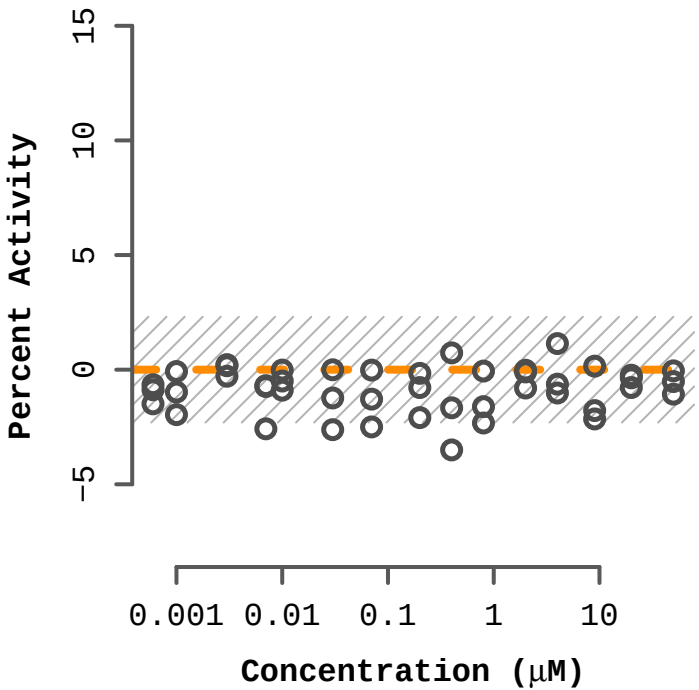
NAME: Methyl 5-(ethylsulfonyl)-o-anisate
CHID: 57787 **CASRN:** 62140-67-4
SPID(S): Tox21_113858
M4ID: 12482365

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.62	NA	NA
PROB:	1	NA	NA
RMSE:	1.19	NA	NA

MAX_MEAN: 1.89 **MAX_MED:** 1.91 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

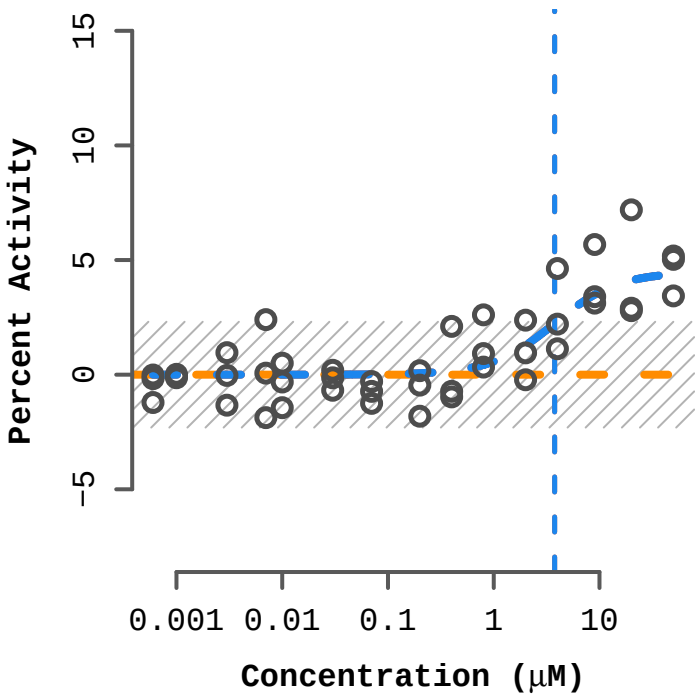
NAME: o-Chlorothiophenol
CHID: 57788 **CASRN:** 6320-03-2
SPID(S): Tox21_113777
M4ID: 12482439

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.34	NA	NA
PROB:	1	NA	NA
RMSE:	1.29	NA	NA

MAX_MEAN: 0.0369 **MAX_MED:** 0.172 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Indobufen
CHID: 57789 **CASRN:** 63610-08-2
SPID(S): Tox21_113871
M4ID: 12482354

HILL MODEL (in red):

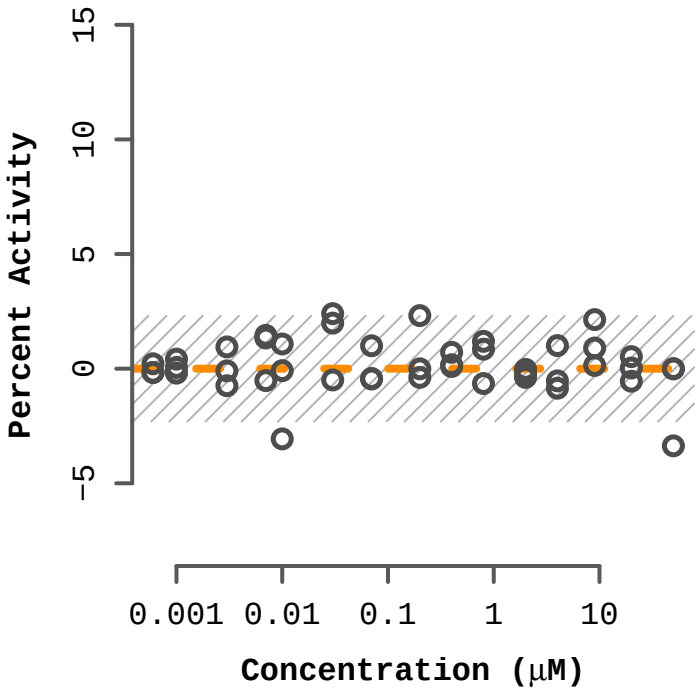
	tp	ga	gw
val:	4.48	0.576	1.45
sd:	0.744	0.192	0.63

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.48	0.576	1.45	2.95	6.54
sd:	0.744	0.192	0.63	1440	7560

	CNST	HILL	GNLS
AIC:	203.75	152.49	156.49
PROB:	0	0.88	0.12
RMSE:	2.38	1.19	1.19

MAX_MEAN: 4.55 **MAX_MED:** 5.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

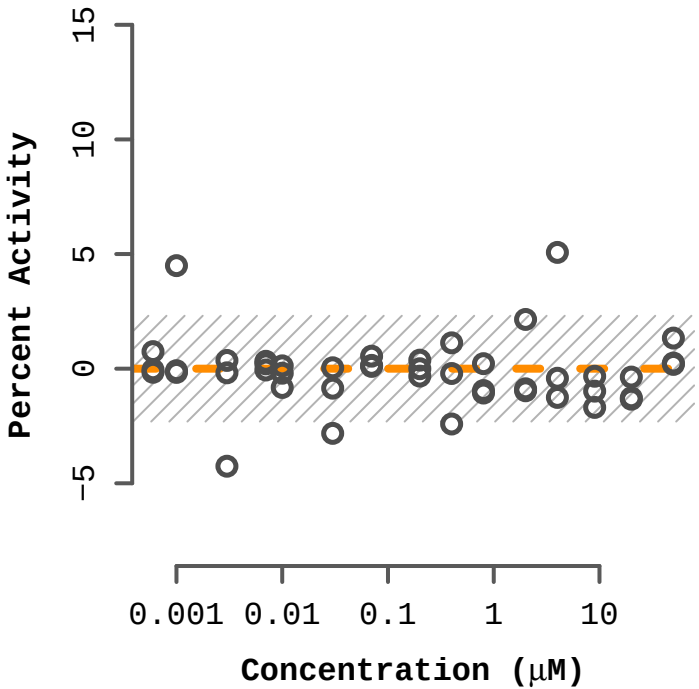
NAME: Thiocyanoacetic acid sodium salt
CHID: 57790 **CASRN:** 63906-52-5
SPID(S): Tox21_113677
M4ID: 12482537

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	133.39	NA	NA
PROB:	1	NA	NA
RMSE:	1.12	NA	NA

MAX_MEAN: 1.3 **MAX_MED:** 1.99 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

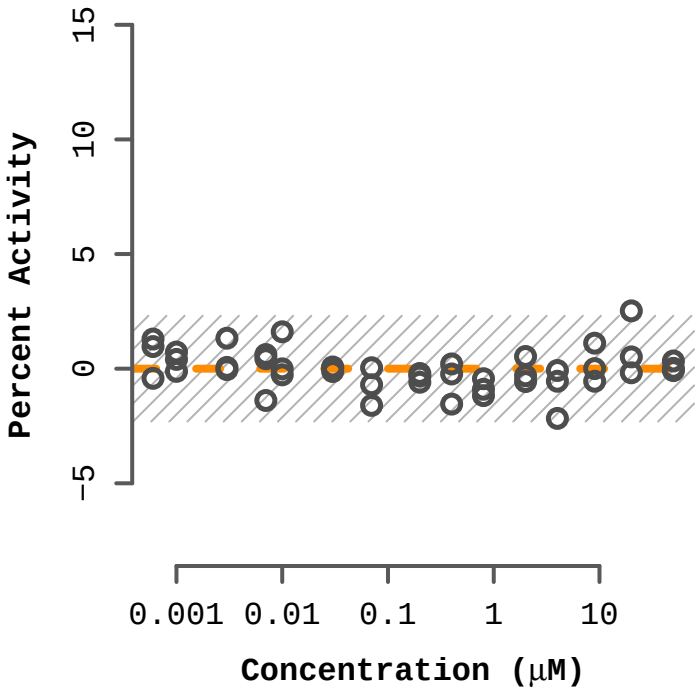
NAME: (2Z)−{2−[(Chloroacetyl)amino]−1,3−thiazol−4−yl
CHID: 57791 **CASRN:** 64486−18−6
SPID(S): Tox21_113869
M4ID: 12482356

HILL MODEL: Not applicable.

GAIN−LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	151.49	NA	NA
PROB:	1	NA	NA
RMSE:	1.5	NA	NA

MAX_MEAN: 1.42 **MAX_MED:** 0.247 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

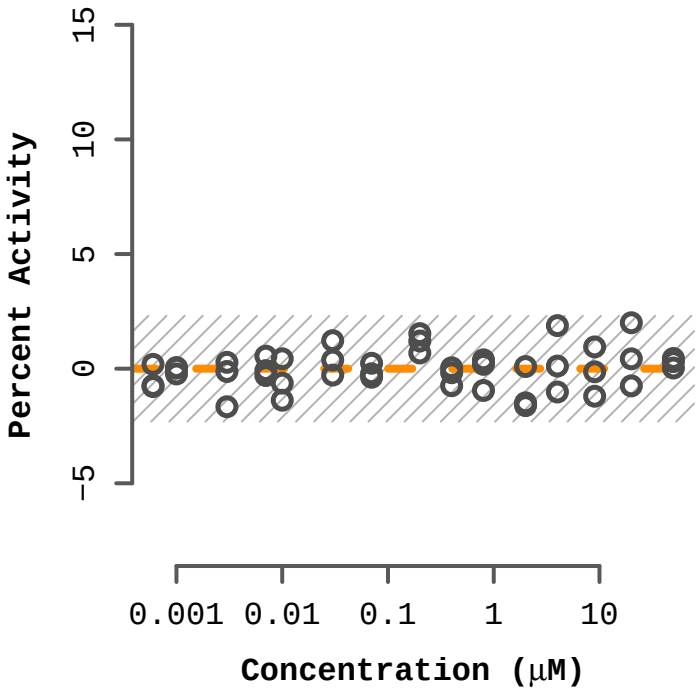
NAME: Ethyl 2-oxo-4-phenylbutyrate
CHID: 57793 **CASRN:** 64920-29-2
SPID(S): Tox21_113802
M4ID: 12482417

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	112.65	NA	NA
PROB:	1	NA	NA
RMSE:	0.85	NA	NA

MAX_MEAN: 0.954 **MAX_MED:** 0.966 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

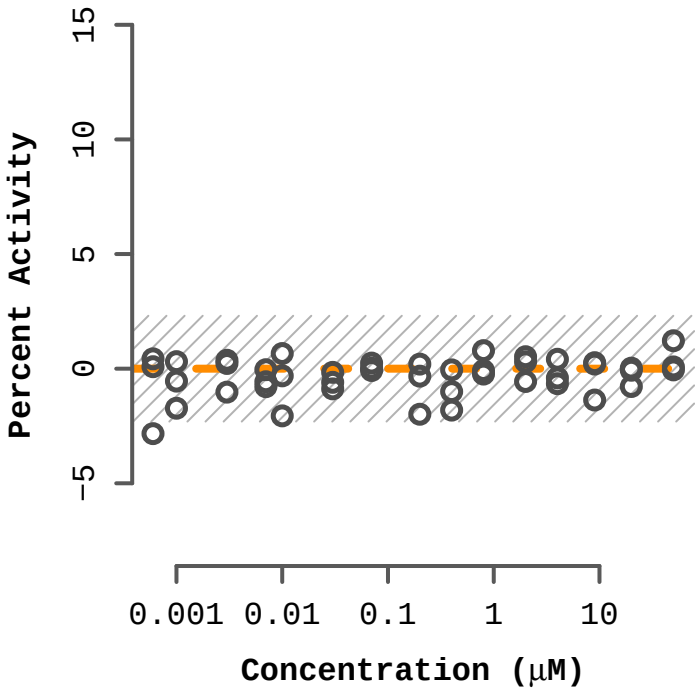
NAME: Ethyl (2-formamido-1,3-thiazol-4-yl)glyoxylate
CHID: 57794 CASRN: 64987-03-7
SPID(S): Tox21_113773
M4ID: 12482442

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	114.64	NA	NA
PROB:	1	NA	NA
RMSE:	0.84	NA	NA

MAX_MEAN: 1.14 **MAX_MED:** 1.21 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

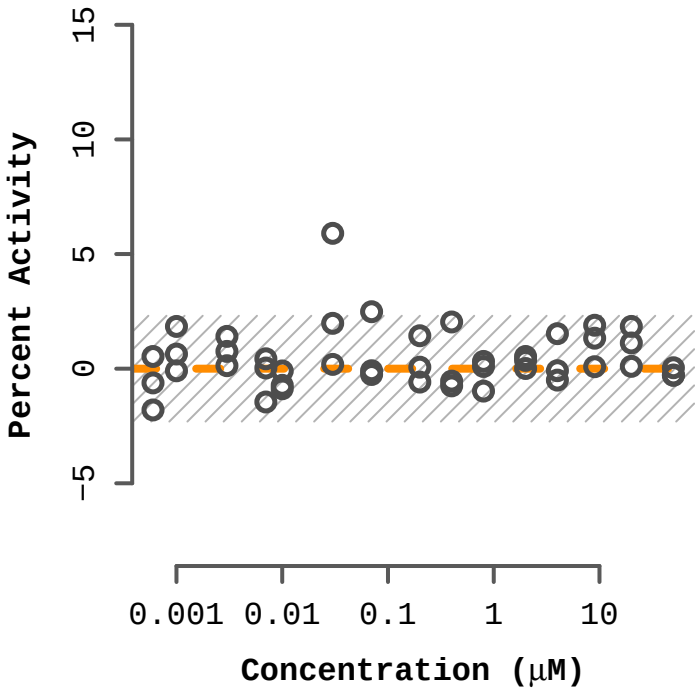
NAME: Nimorazole
CHID: 57795 **CASRN:** 6506-37-2
SPID(S): Tox21_113897
M4ID: 12482331

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.87	NA	NA

MAX_MEAN: 0.416 **MAX_MED:** 0.304 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

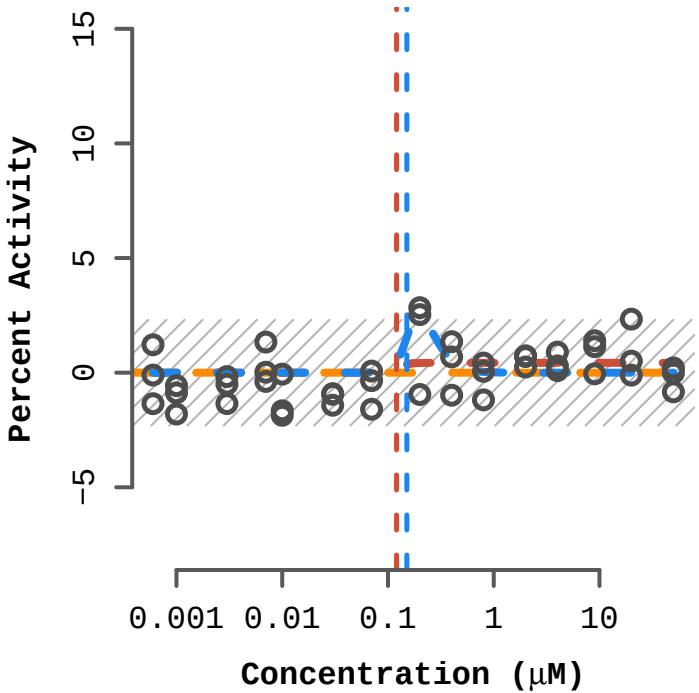
NAME: Acephylline
CHID: 57796 **CASRN:** 652-37-9
SPID(S): Tox21_113765
M4ID: 12482450

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.94	NA	NA
PROB:	1	NA	NA
RMSE:	1.34	NA	NA

MAX_MEAN: 2.69 **MAX_MED:** 1.98 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Lofemizole
CHID: 57797 CASRN: 65571-68-8
SPID(S): Tox21_113877
M4ID: 12482348

HILL MODEL (in red):

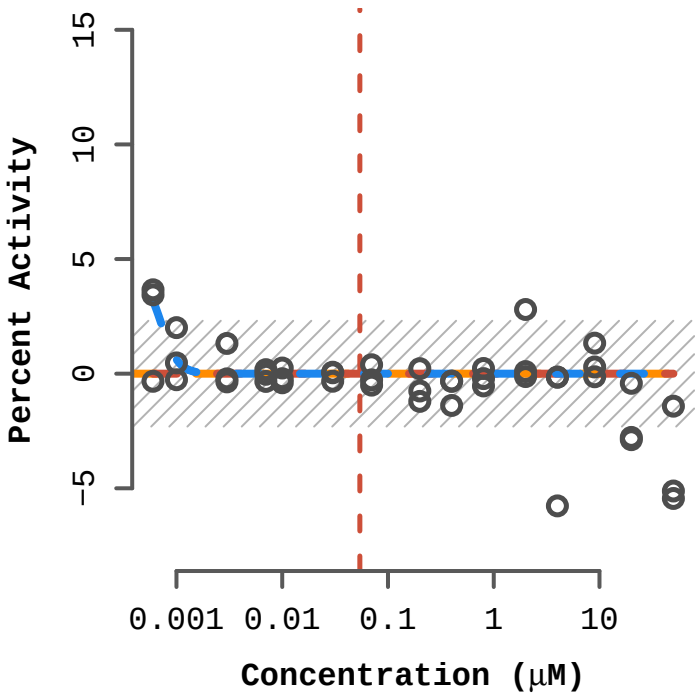
	tp	ga	gw
val:	0.428	−0.919	8
sd:	0.209	0.391	13.7

GAIN-LOSS MODEL (in blue):

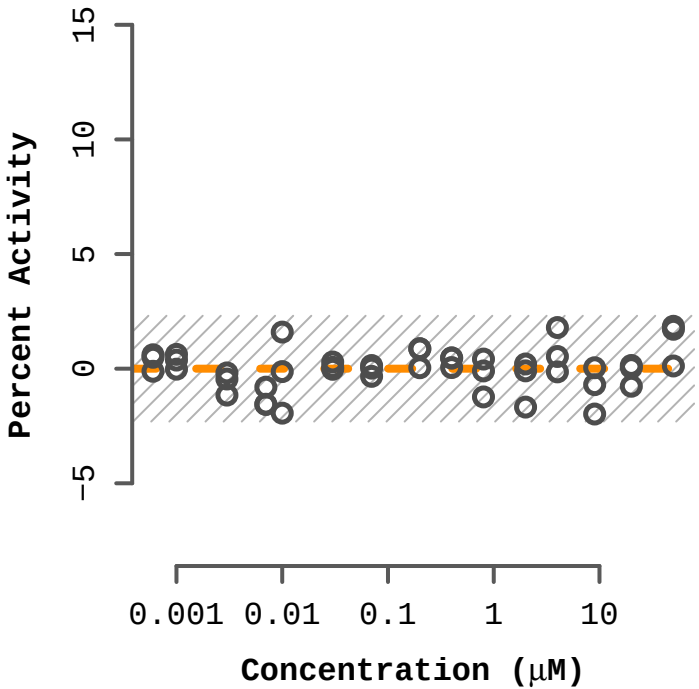
	tp	ga	gw	la	lw
val:	3.4	−0.822	8	−0.572	4.18
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	142.03	143.91	146.26
PROB:	0.66	0.26	0.08
RMSE:	1.12	1.06	1.07

MAX_MEAN: 1.47 **MAX_MED:** 2.54 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Morniflumate
CHID:    57798   CASRN: 65847-85-0
SPID(S): Tox21_113913
M4ID:    12482317

HILL MODEL (in red):
      tp        ga        gw
val:  4.97e-11  -1.27     0.408
sd:   NaN       NaN       NaN

GAIN-LOSS MODEL (in blue):
      tp        ga        gw        la        lw
val:  4.39      -5.22     1.87      -3.14     5.4
sd:   11.9      423       401       0.6       14.3

      CNST         HILL         GNLS
AIC:  169.32       175.32       170.84
PROB: 0.66         0.03         0.31
RMSE: 1.85         1.85         1.76

MAX_MEAN: 2.26      MAX_MED: 3.44      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

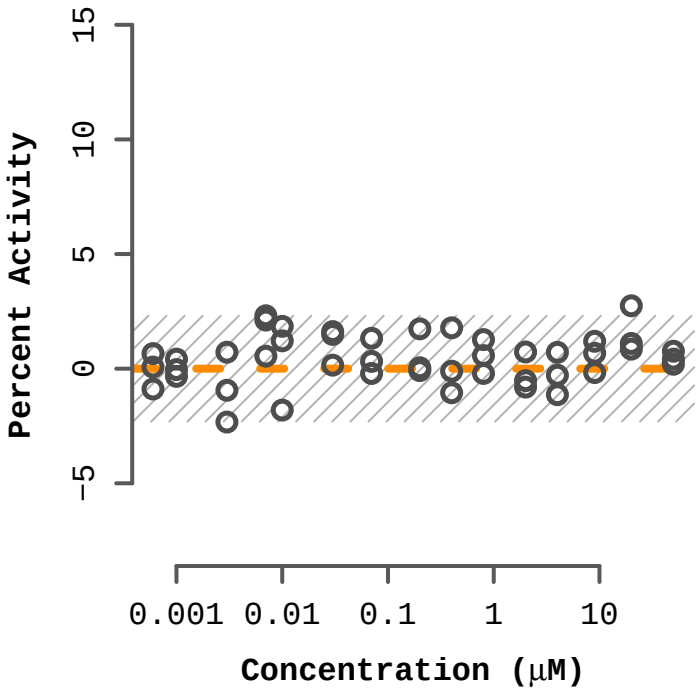
NAME: Epicainide
CHID: 57799 **CASRN:** 66304-03-8
SPID(S): Tox21_113865
M4ID: 12482360

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	119.08	NA	NA
PROB:	1	NA	NA
RMSE:	0.9	NA	NA

MAX_MEAN: 1.23 **MAX_MED:** 1.72 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

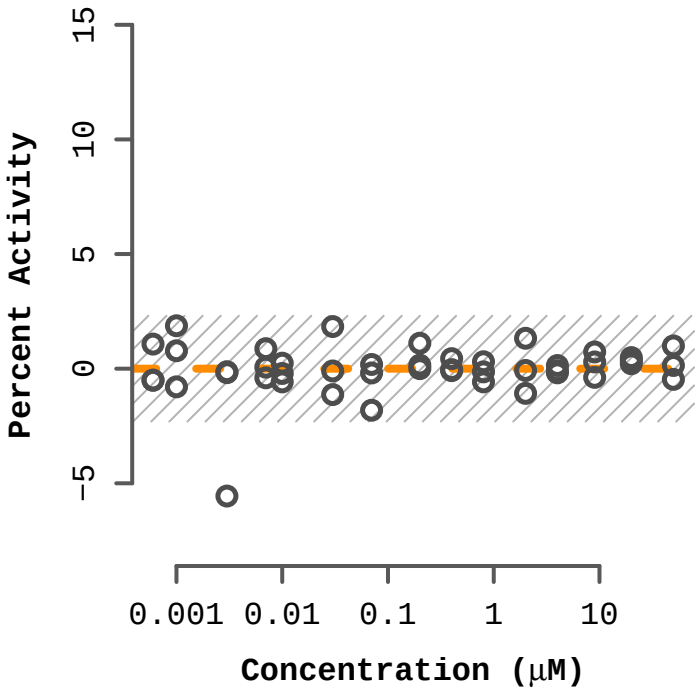
NAME: Propacetamol
CHID: 57800 **CASRN:** 66532-85-2
SPID(S): Tox21_113811
M4ID: 12482408

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	143.95	NA	NA
PROB:	1	NA	NA
RMSE:	1.14	NA	NA

MAX_MEAN: 1.66 **MAX_MED:** 2.12 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

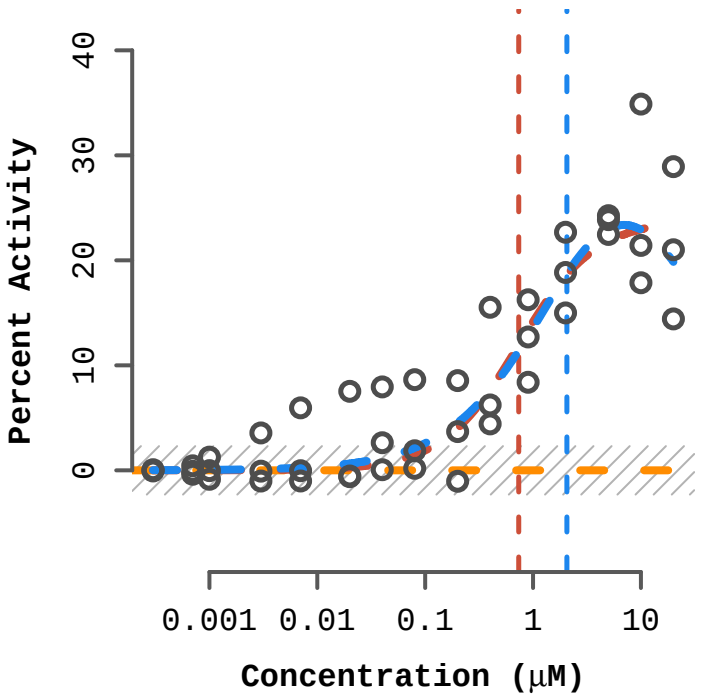
NAME: 2,3-Dimethoxy-5-sulphamoylbenzoic acid
CHID: 57801 **CASRN:** 66644-80-2
SPID(S): Tox21_113783
M4ID: 12482434

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.25	NA	NA
PROB:	1	NA	NA
RMSE:	1.1	NA	NA

MAX_MEAN: 0.622 **MAX_MED:** 0.783 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Daniquidone
CHID: 57802 CASRN: 67199-66-0
SPID(S): Tox21_113867
M4ID: 12482358

HILL MODEL (in red):

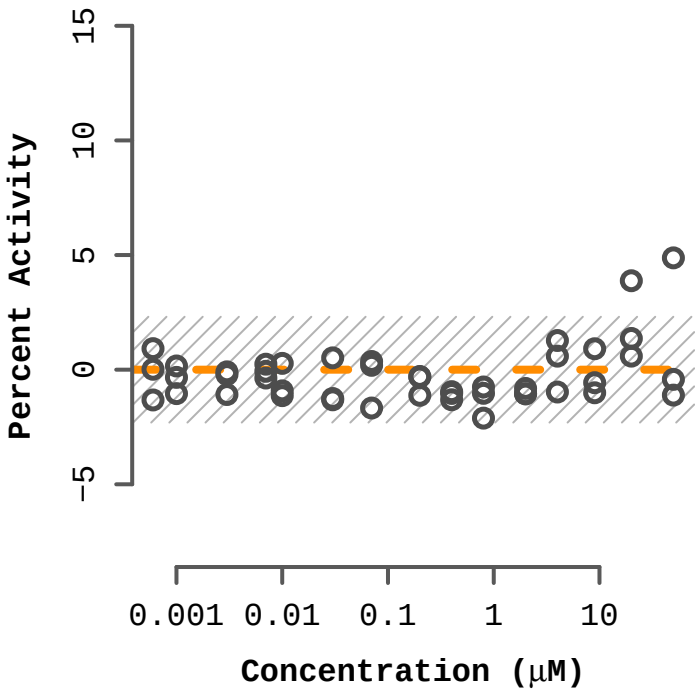
	tp	ga	gw
val:	23.9	-0.133	1.23
sd:	2.25	0.114	0.38

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	41.9	0.314	0.896	1.37	0.882
sd:	33.6	0.588	0.309	0.682	0.772

	CNST	HILL	GNLS
AIC:	357.3	255.91	256.91
PROB:	0	0.62	0.38
RMSE:	12.81	3.94	3.85

MAX_MEAN: 24.7 MAX_MED: 23.9 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

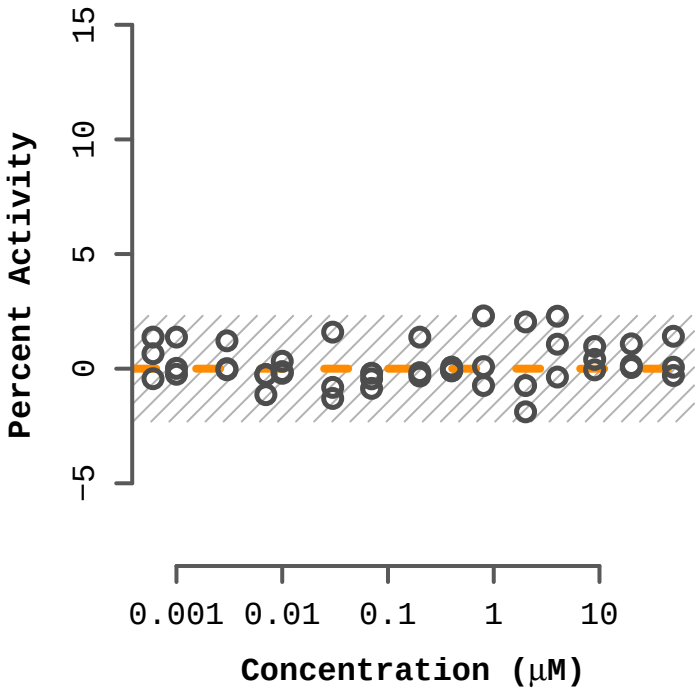
NAME: Enefexine
CHID: 57803 **CASRN:** 67765-04-2
SPID(S): Tox21_113902
M4ID: 12482327

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	146.28	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 1.95 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

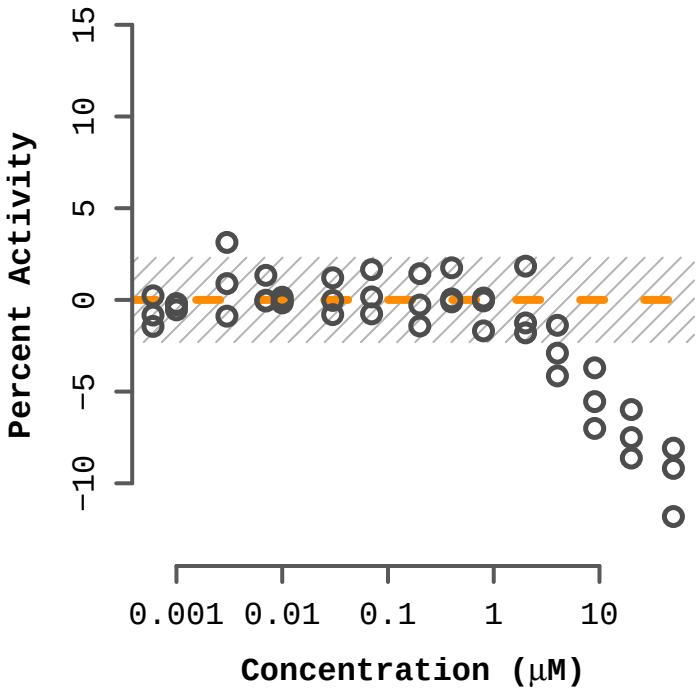
NAME: 4-(4-Acetylpiperazin-4-yl)phenol
CHID: 57804 **CASRN:** 67914-60-7
SPID(S): Tox21_113834
M4ID: 12482388

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	124.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.998 **MAX_MED:** 1.07 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

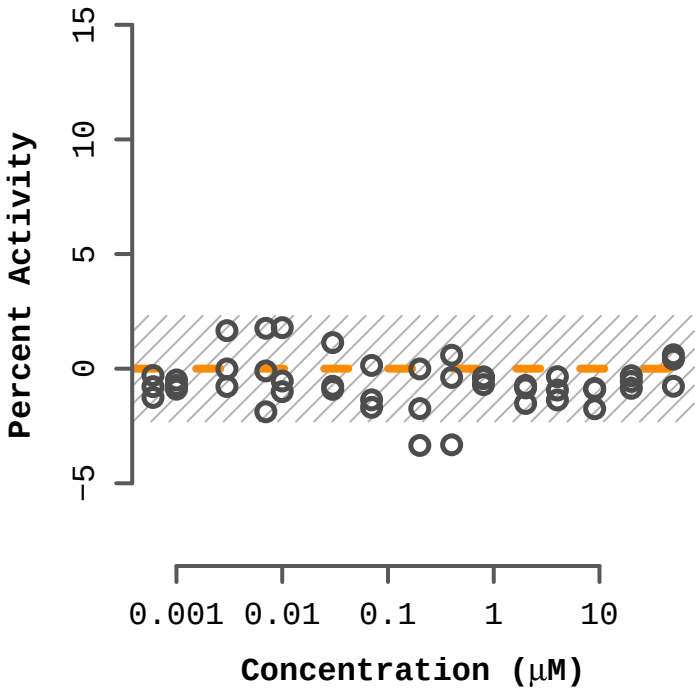
NAME: Isosulfan blue
CHID: 57805 **CASRN:** 68238-36-8
SPID(S): Tox21_113733
M4ID: 12482481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	236.13	NA	NA
PROB:	1	NA	NA
RMSE:	3.7	NA	NA

MAX_MEAN: 1.05 **MAX_MED:** 0.891 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

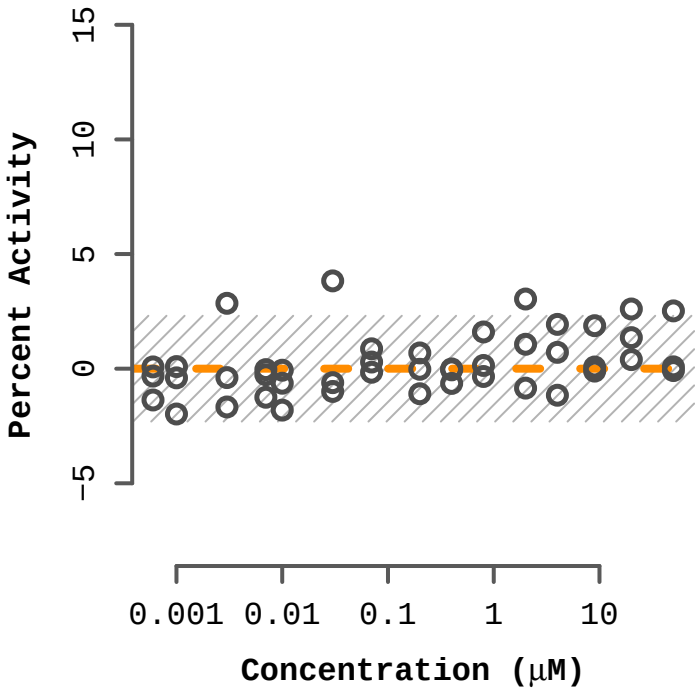
NAME: Enciprazine
CHID: 57806 **CASRN:** 68576-86-3
SPID(S): Tox21_113874
M4ID: 12482351

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	147.65	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.291 **MAX_MED:** 0.417 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

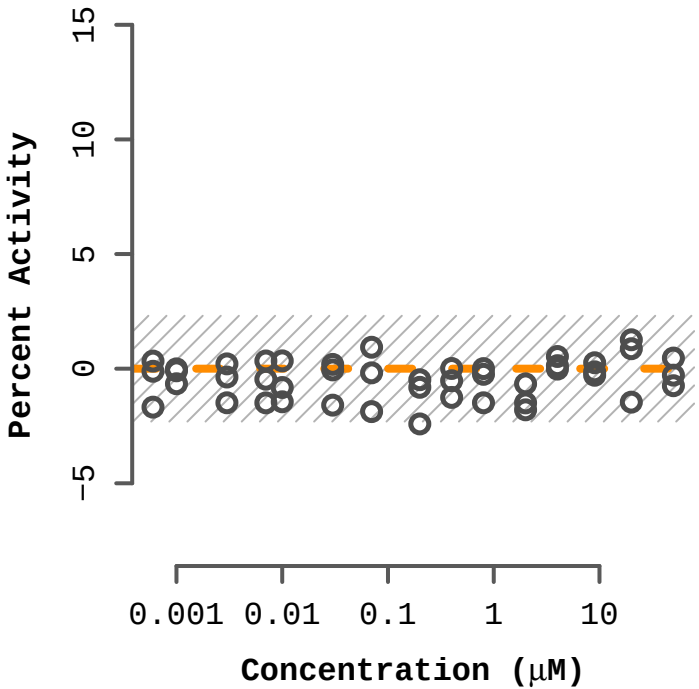
NAME: Fiacitabine
CHID: 57807 **CASRN:** 69123-90-6
SPID(S): Tox21_113954
M4ID: 12482277

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	153.14	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.45 **MAX_MED:** 1.36 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

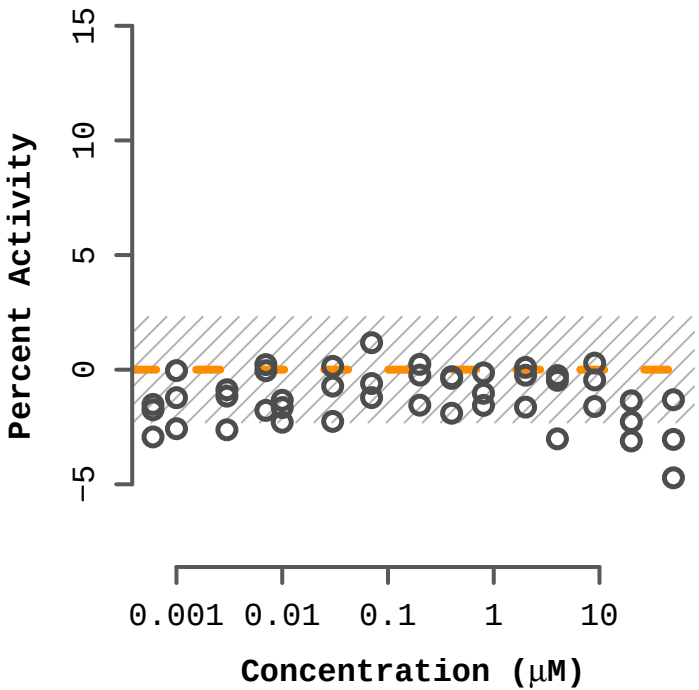
NAME: 4-Methyl-1-piperazinamine
CHID: 57808 **CASRN:** 6928-85-4
SPID(S): Tox21_113841
M4ID: 12482381

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	126.49	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.225 **MAX_MED:** 0.872 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

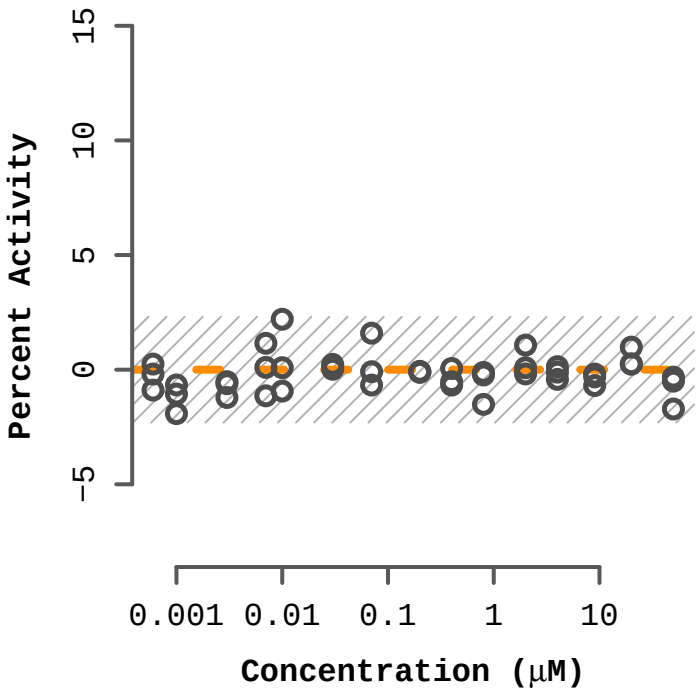
NAME: Ticlatone
CHID: 57809 **CASRN:** 70-10-0
SPID(S): Tox21_113906
M4ID: 12482324

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	178.81	NA	NA
PROB:	1	NA	NA
RMSE:	1.68	NA	NA

MAX_MEAN: −0.214 **MAX_MED:** −0.0455 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

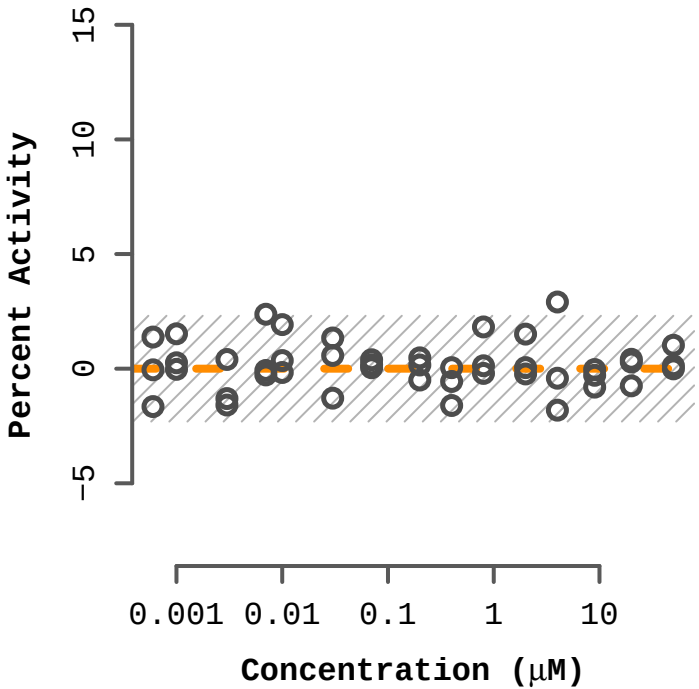
NAME: Propoxate
CHID: 57810 **CASRN:** 7036-58-0
SPID(S): Tox21_113881
M4ID: 12482344

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	108.59	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.494 **MAX_MED:** 0.258 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

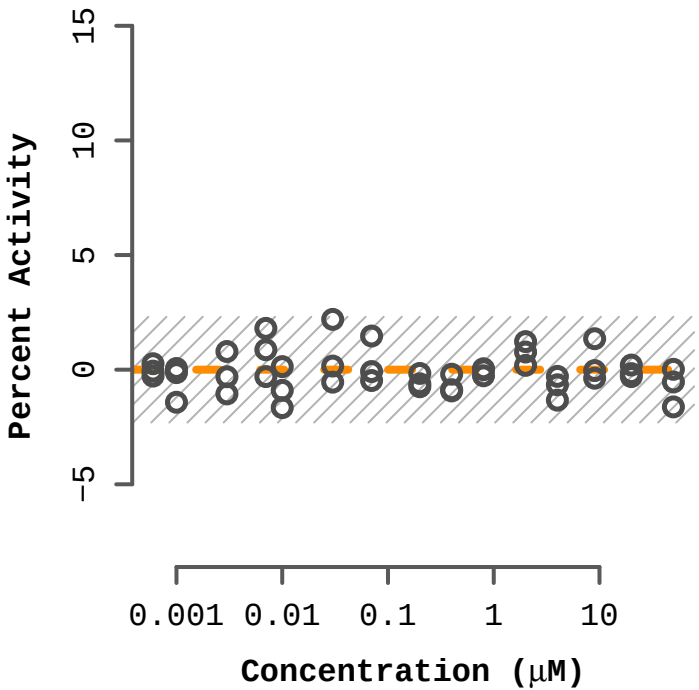
NAME: Glyceryl 1-(2-aminobenzoate)
CHID: 57811 **CASRN:** 71574-35-1
SPID(S): Tox21_113676
M4ID: 12482538

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.84	NA	NA
PROB:	1	NA	NA
RMSE:	1.04	NA	NA

MAX_MEAN: 0.705 **MAX_MED:** 0.577 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

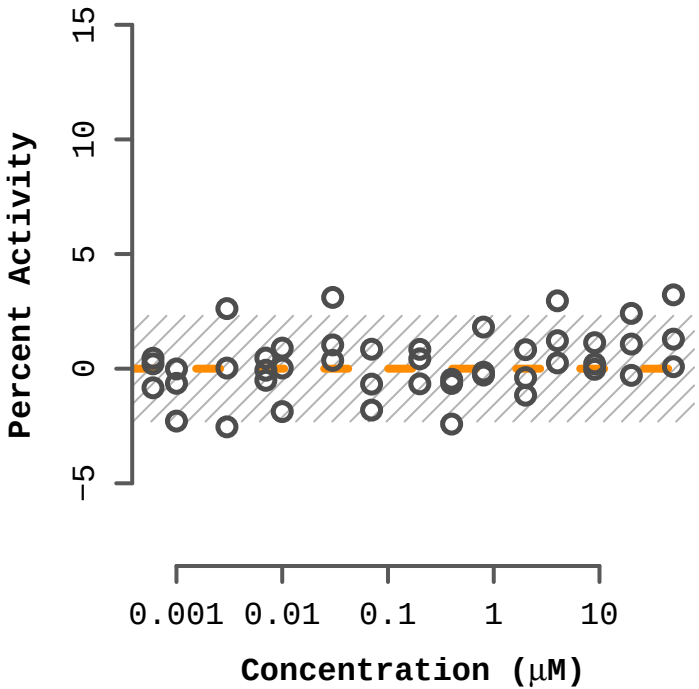
NAME: Fenticonazole
CHID: 57812 **CASRN:** 72479-26-6
SPID(S): Tox21_113832
M4ID: 12482390

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113.46	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.792 **MAX_MED:** 0.871 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

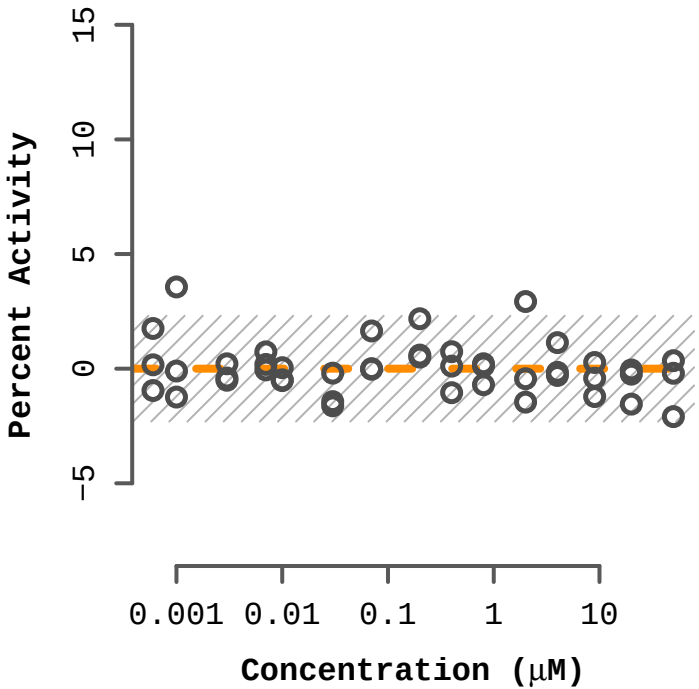
NAME: Imidoline
CHID: 57813 **CASRN:** 7303-78-8
SPID(S): Tox21_113812
M4ID: 12482407

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	157.48	NA	NA
PROB:	1	NA	NA
RMSE:	1.37	NA	NA

MAX_MEAN: 1.53 **MAX_MED:** 1.29 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

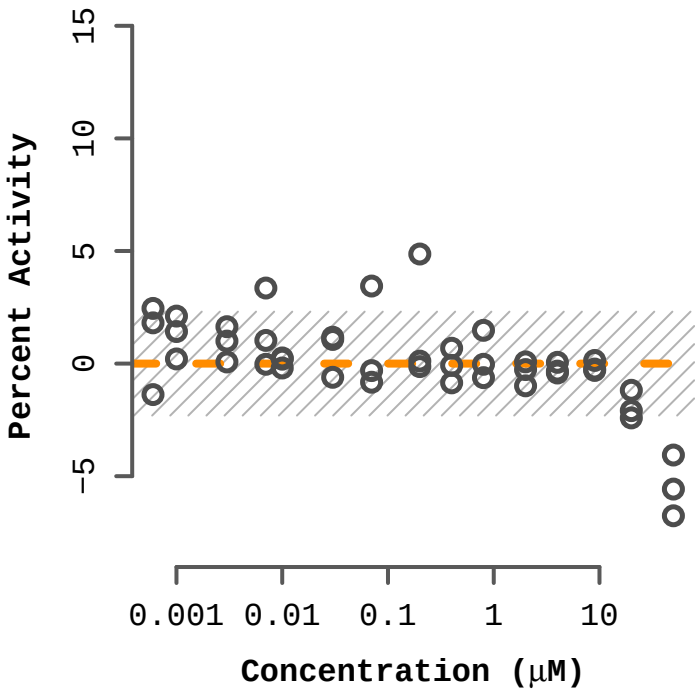
NAME: Eicosapentaenoic acid ethyl ester
CHID: 57814 **CASRN:** 73310-10-8
SPID(S): Tox21_113704
M4ID: 12482510

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.61	NA	NA
PROB:	1	NA	NA
RMSE:	1.11	NA	NA

MAX_MEAN: 1.09 **MAX_MED:** 0.595 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

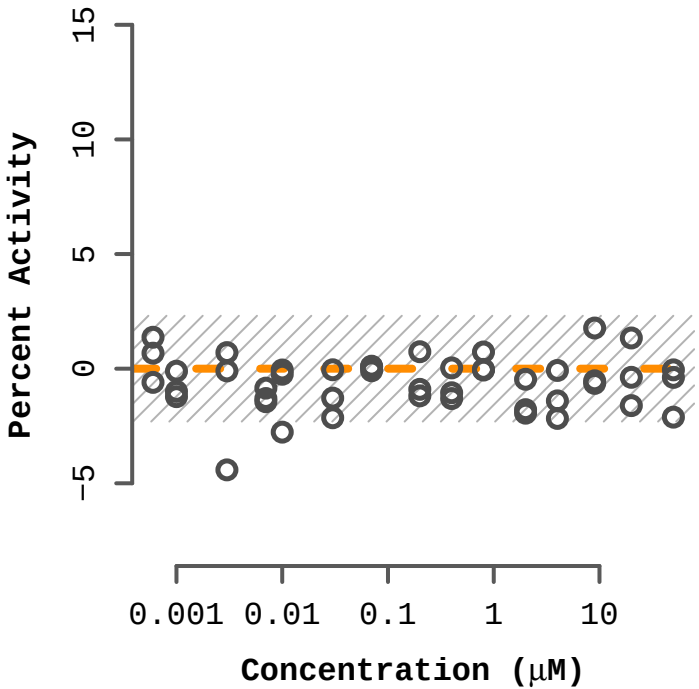
NAME: Rescimetol
CHID: 57815 **CASRN:** 73573-42-9
SPID(S): Tox21_113739
M4ID: 12482475

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	182.54	NA	NA
PROB:	1	NA	NA
RMSE:	2.02	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.81 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

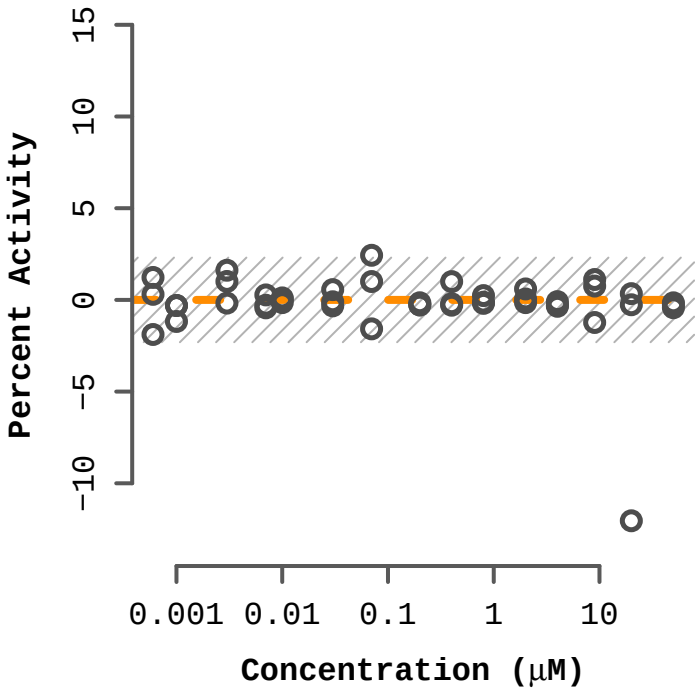
NAME: Omeprazole sulfide
CHID: 57816 **CASRN:** 73590-85-9
SPID(S): Tox21_113939
M4ID: 12482292

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.22	NA	NA
PROB:	1	NA	NA
RMSE:	1.3	NA	NA

MAX_MEAN: 0.484 **MAX_MED:** 0.677 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

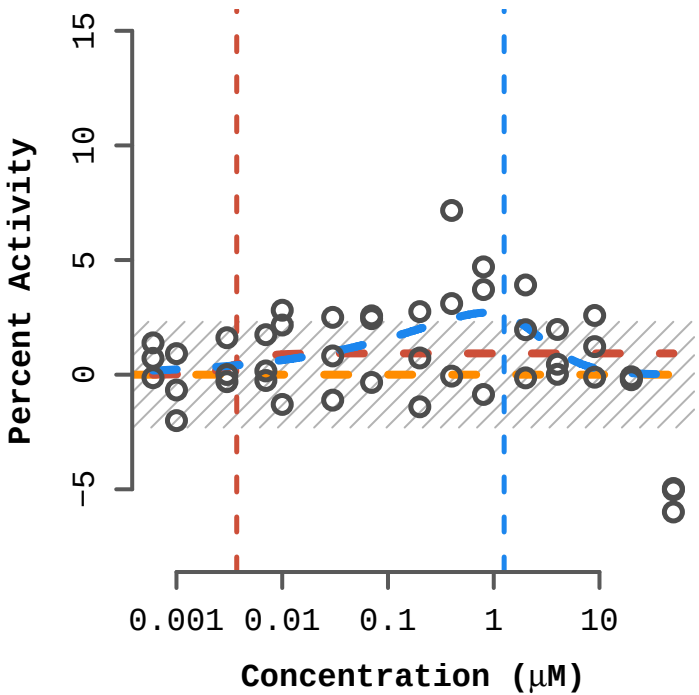
NAME: Tripamide
CHID: 57817 **CASRN:** 73803-48-2
SPID(S): Tox21_113978
M4ID: 12482262

HILL MODEL: Not applicable.

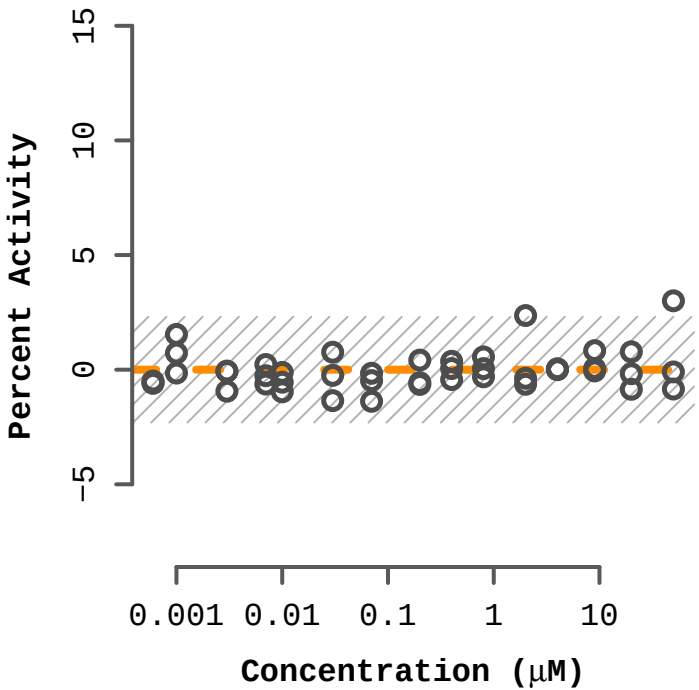
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	123.71	NA	NA
PROB:	1	NA	NA
RMSE:	1.95	NA	NA

MAX_MEAN: 0.818 **MAX_MED:** 1.01 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Omoconazole
CHID:    57818   CASRN: 74512-12-2
SPID(S): Tox21_113697
M4ID:    12482517

HILL MODEL (in red):
      tp       ga       gw
val:  0.928    -2.43    3.08
sd:   0.386    0.684    7.49

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.83     0.0984   0.472    0.348    1.99
sd:   20.4     4.37     0.367    0.459    1.54

      CNST        HILL        GNLS
AIC:  208.63      208.14      204.08
PROB: 0.08        0.11        0.81
RMSE: 2.47        2.37        2.1

MAX_MEAN: 3.4       MAX_MED: 3.71      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

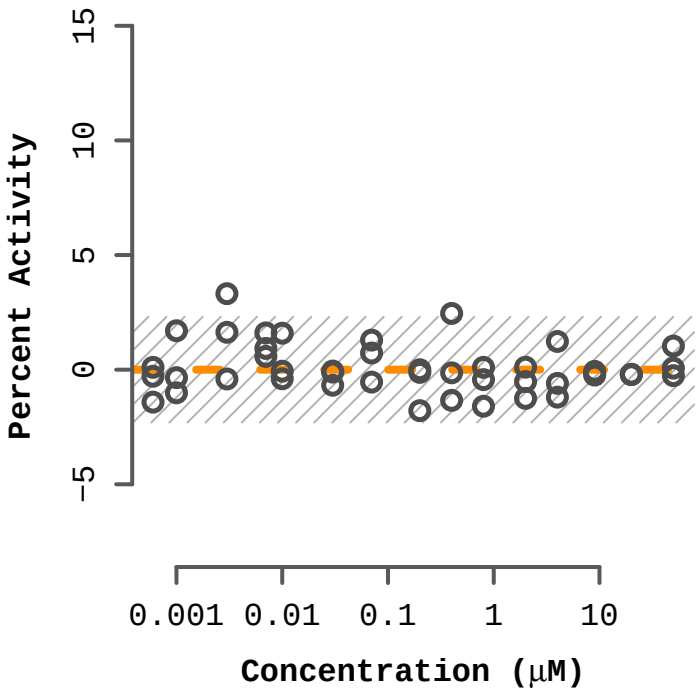
NAME: Indecainide
CHID: 57819 **CASRN:** 74517-78-5
SPID(S): Tox21_113663
M4ID: 12482550

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	104.81	NA	NA
PROB:	1	NA	NA
RMSE:	0.83	NA	NA

MAX_MEAN: 0.706 **MAX_MED:** 0.726 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

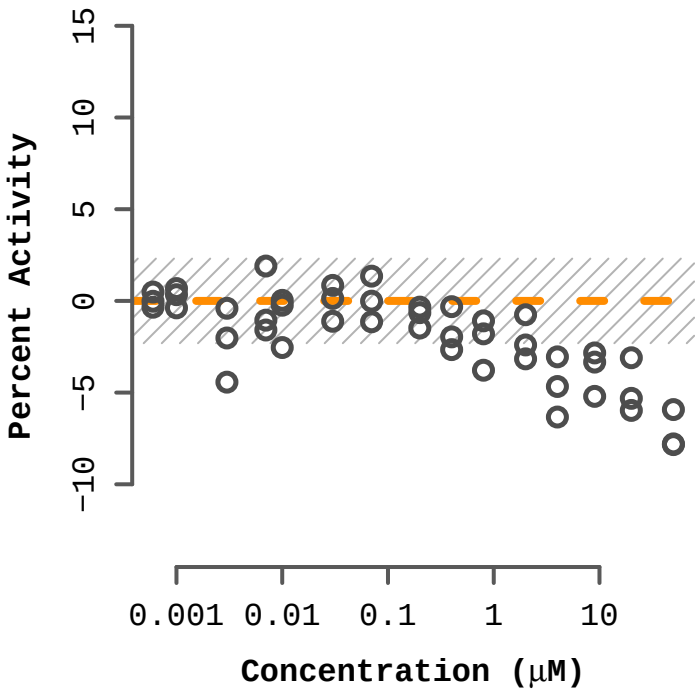
NAME: Docarpamine
CHID: 57820 **CASRN:** 74639-40-0
SPID(S): Tox21_113707
M4ID: 12482507

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.31	NA	NA
PROB:	1	NA	NA
RMSE:	1.05	NA	NA

MAX_MEAN: 1.51 **MAX_MED:** 1.63 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

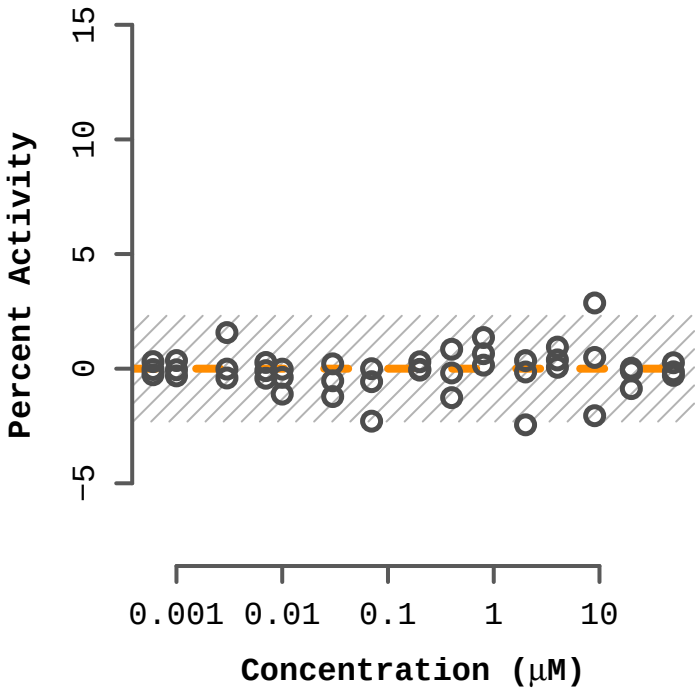
NAME: Artemotil
CHID: 57821 **CASRN:** 75887-54-6
SPID(S): Tox21_113883
M4ID: 12482342

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	231.47	NA	NA
PROB:	1	NA	NA
RMSE:	3.13	NA	NA

MAX_MEAN: 0.213 **MAX_MED:** 0.341 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

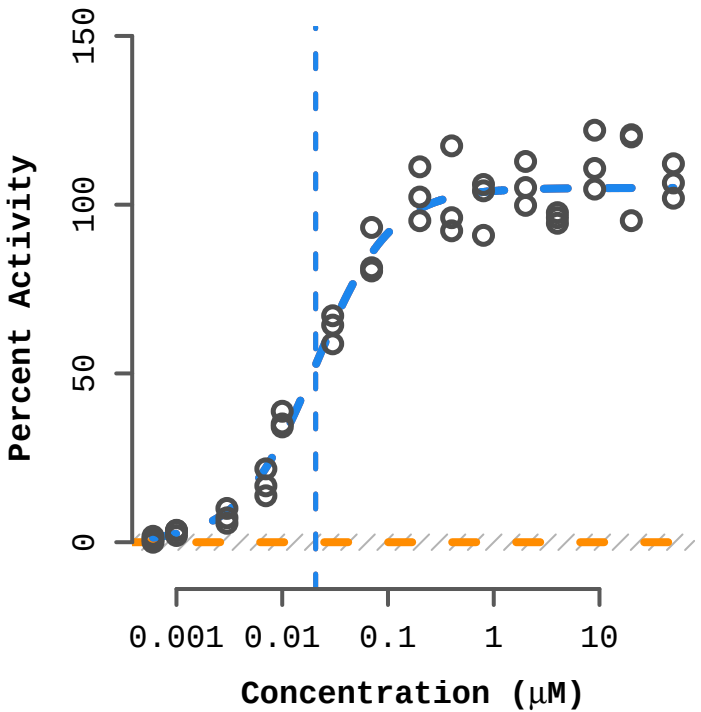
NAME: 4-Bromo-1-(bromomethyl)-2-fluoro-benzene
CHID: 57822 **CASRN:** 76283-09-5
SPID(S): Tox21_113803
M4ID: 12482416

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	111.9	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.723 **MAX_MED:** 0.655 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nandrolone furylpropionate
CHID: 57823 CASRN: 7642-64-0
SPID(S): Tox21_113695
M4ID: 12482519

HILL MODEL (in red):

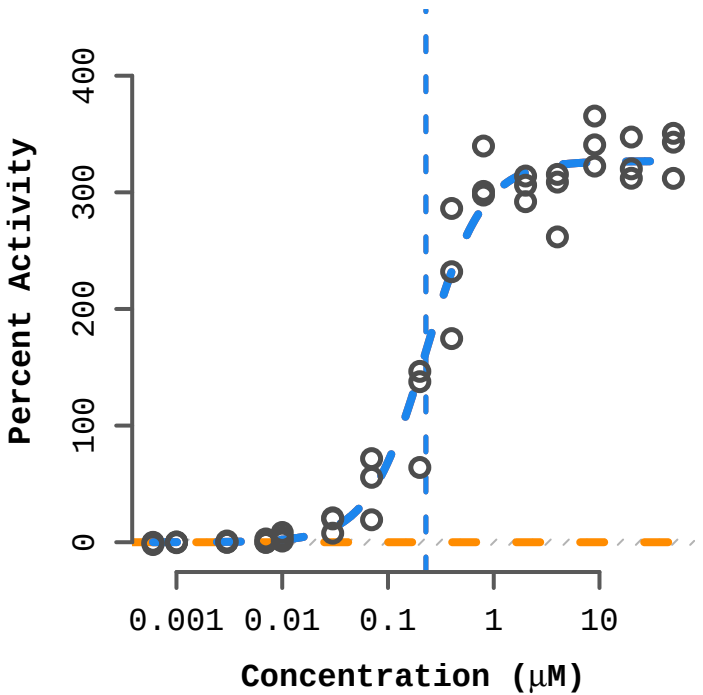
	tp	ga	gw
val:	105	-1.68	1.22
sd:	1.88	0.0376	0.103

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	105	-1.68	1.22	2.7	8.71
sd:	1.88	0.0376	0.103	986	8530

	CNST	HILL	GNLS
AIC:	534.4	315.32	319.32
PROB:	0	0.88	0.12
RMSE:	82.28	7.25	7.25

MAX_MEAN: 112 MAX_MED: 120 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Hydrocortamate
CHID: 57824 CASRN: 76-47-1
SPID(S): Tox21_113659
M4ID: 12482554

HILL MODEL (in red):

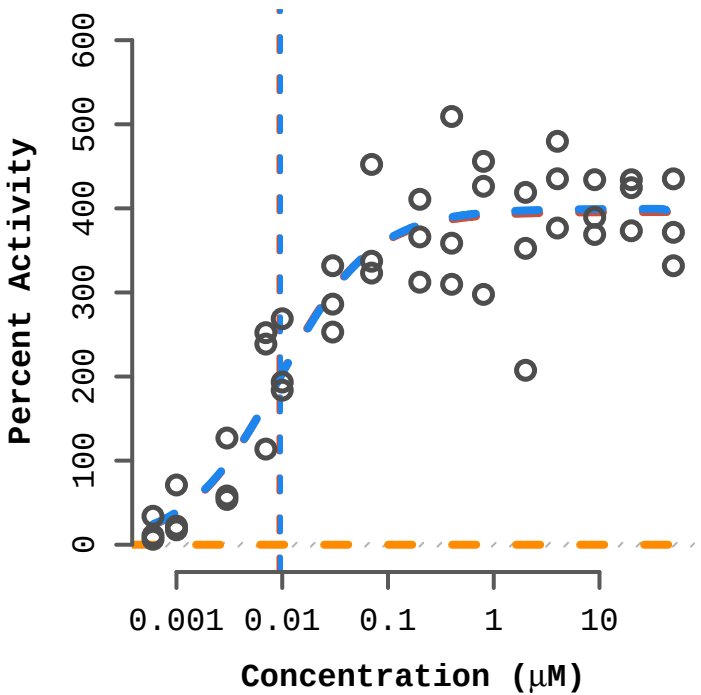
	tp	ga	gw
val:	327	-0.641	1.6
sd:	5.51	0.0289	0.19

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	327	-0.641	1.6	3.7	15
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	617.15	409.01	413.01
PROB:	0	0.88	0.12
RMSE:	214.38	24.08	24.08

MAX_MEAN: 343 MAX_MED: 343 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Resocortol butyrate
CHID: 57825 CASRN: 76738-96-0
SPID(S): Tox21_113951
M4ID: 12482280

HILL MODEL (in red):

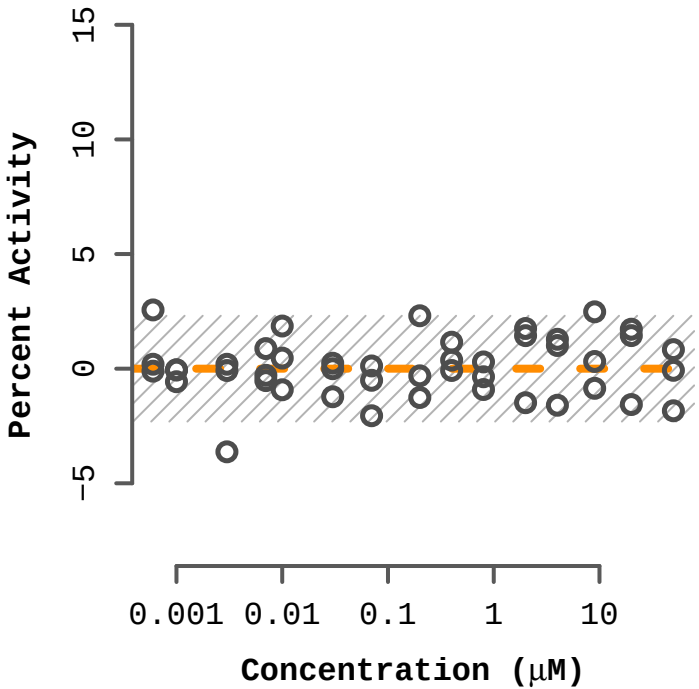
	tp	ga	gw
val:	396	-2.03	1.01
sd:	12.5	0.0876	0.168

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	400	-2.02	0.985	1.77	17.6
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	657.8	496.56	500.08
PROB:	0	0.85	0.15
RMSE:	322.28	55.75	55.75

MAX_MEAN: 431 MAX_MED: 435 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

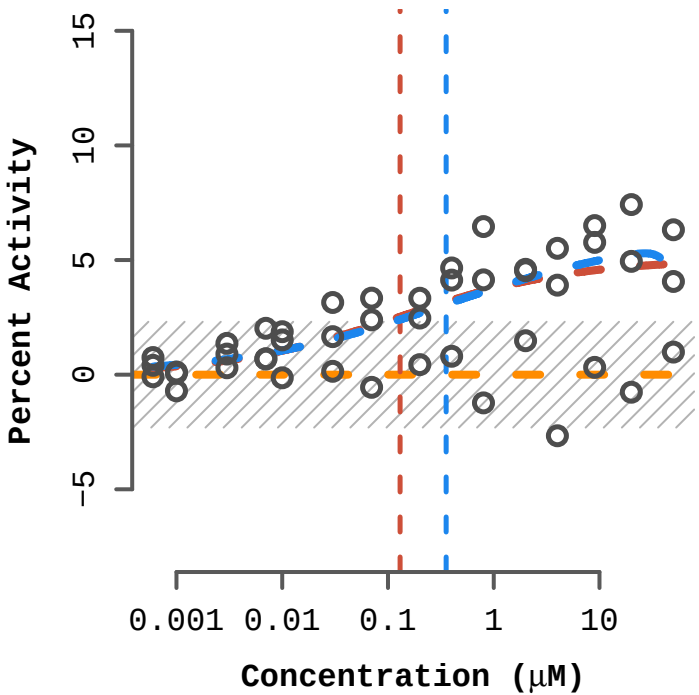
NAME: Dimecrotic acid
CHID: 57826 **CASRN:** 7706-67-4
SPID(S): Tox21_113846
M4ID: 12482376

HILL MODEL: Not applicable.

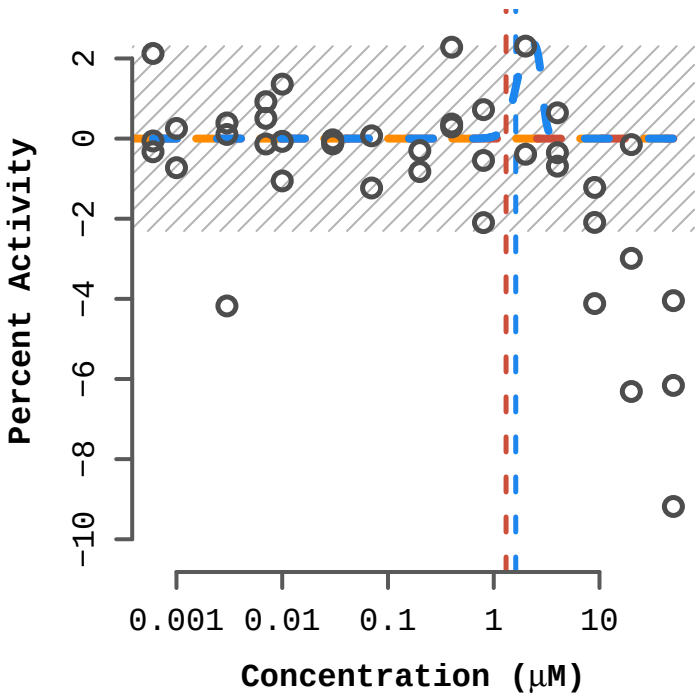
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	152.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.27	NA	NA

MAX_MEAN: 0.884 **MAX_MED:** 1.44 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Bravavir
CHID:    57827   CASRN: 77181-69-2
SPID(S): Tox21_113949
M4ID:    12482282

HILL MODEL (in red):
      tp       ga       gw
val:  5.05     -0.886   0.523
sd:   1.08     0.551    0.204

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  6.14     -0.45    0.44     1.77     5.86
sd:   2.69     1.11     0.207    1.1      87.7

      CNST        HILL        GNLS
AIC:  237.37      196.01      199.21
PROB: 0           0.83        0.17
RMSE: 3.24        2.12        2.14

MAX_MEAN: 4.2       MAX_MED: 5.77      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Riboprine
CHID: 57828 **CASRN:** 7724-76-7
SPID(S): Tox21_113776
M4ID: 12482440

HILL MODEL (in red):

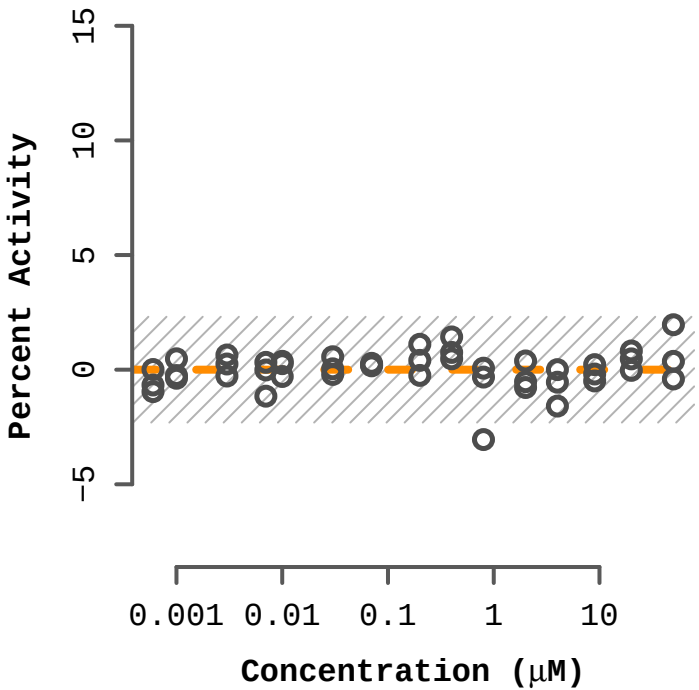
	tp	ga	gw
val:	3.36e-10	0.117	1.72
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.56	0.208	8	0.458	18
sd:	9.3	1.05	24.9	1.18	147

	CNST	HILL	GNLS
AIC:	206.43	212.43	213.54
PROB:	0.93	0.05	0.03
RMSE:	2.59	2.59	2.54

MAX_MEAN: 2.02 **MAX_MED:** 2.31 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

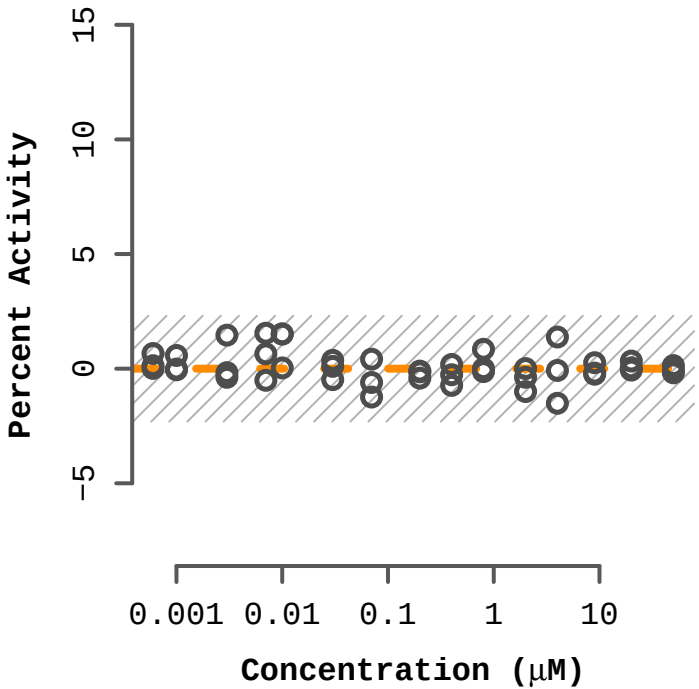
NAME: Ethyl mandelate
CHID: 57829 **CASRN:** 774-40-3
SPID(S): Tox21_113879
M4ID: 12482346

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	97.96	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.887 **MAX_MED:** 0.754 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

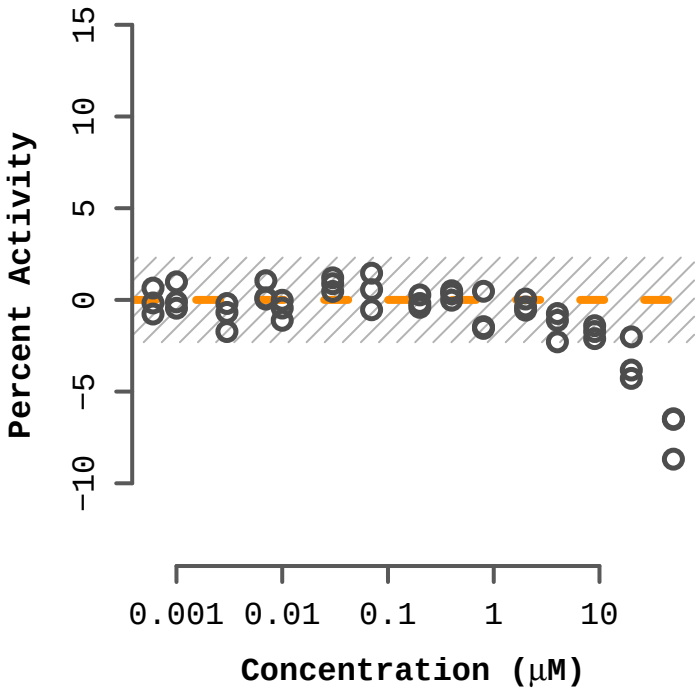
NAME: Isoaminile
CHID: 57830 **CASRN:** 77-51-0
SPID(S): Tox21_113743
M4ID: 12482471

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	90.71	NA	NA
PROB:	1	NA	NA
RMSE:	0.67	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.51 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

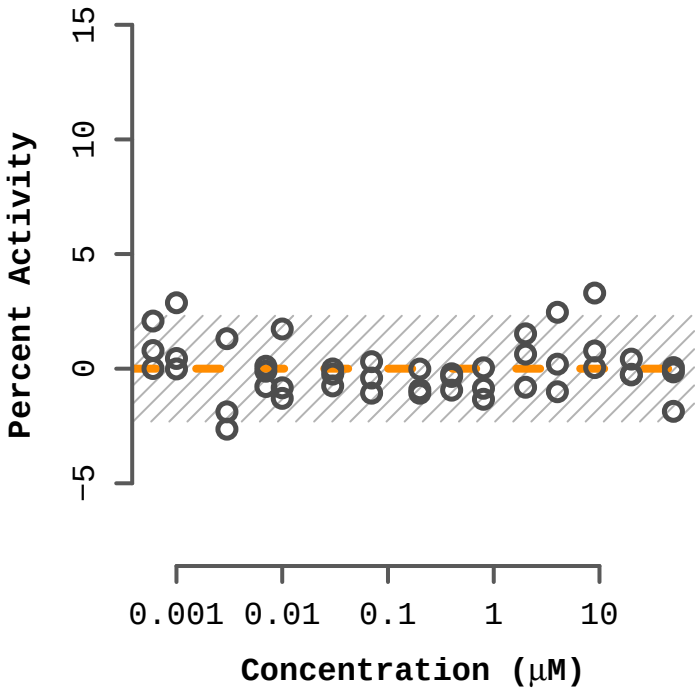
NAME: Methodichlorophen
CHID: 57831 **CASRN:** 7761-45-7
SPID(S): Tox21_113755
M4ID: 12482460

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	183.13	NA	NA
PROB:	1	NA	NA
RMSE:	2.27	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 0.886 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

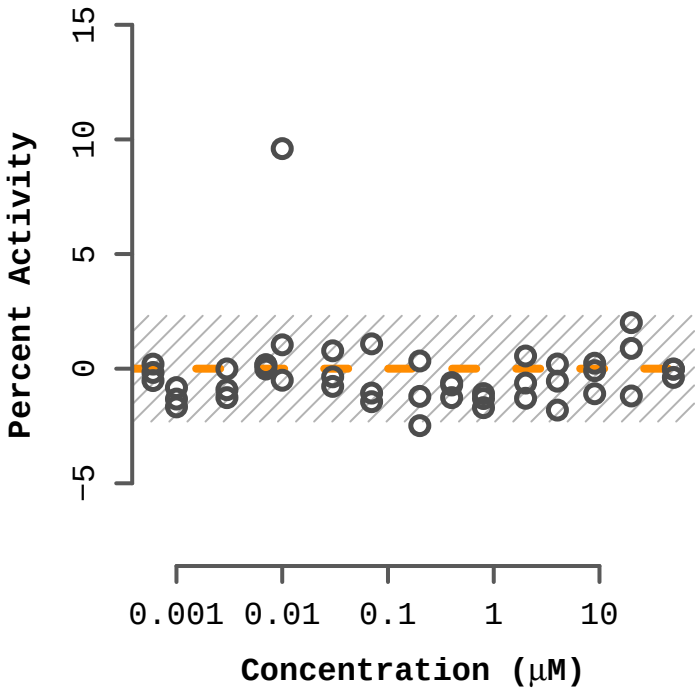
NAME: 2-Amino-5-chloro-2'-fluorobenzophenone
CHID: 57832 **CASRN:** 784-38-3
SPID(S): Tox21_113844
M4ID: 12482378

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	144.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.2	NA	NA

MAX_MEAN: 1.37 **MAX_MED:** 0.794 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

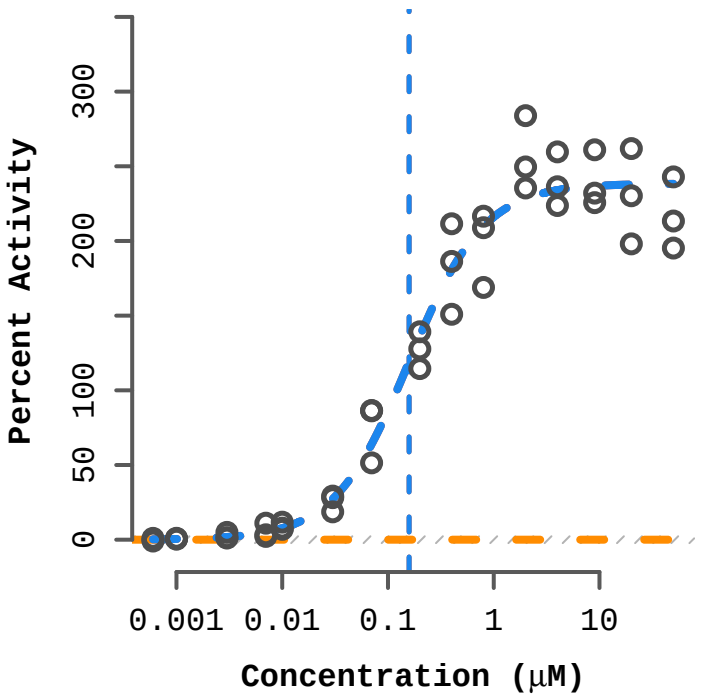
NAME: Ethyl 7-chloro-2-oxoheptanoate
CHID: 57833 **CASRN:** 78834-75-0
SPID(S): Tox21_113807
M4ID: 12482412

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.17	NA	NA
PROB:	1	NA	NA
RMSE:	1.74	NA	NA

MAX_MEAN: 3.38 **MAX_MED:** 1.04 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Dimethisteron
CHID: 57834 CASRN: 79-64-1
SPID(S): Tox21_113973
M4ID: 12482265

HILL MODEL (in red):

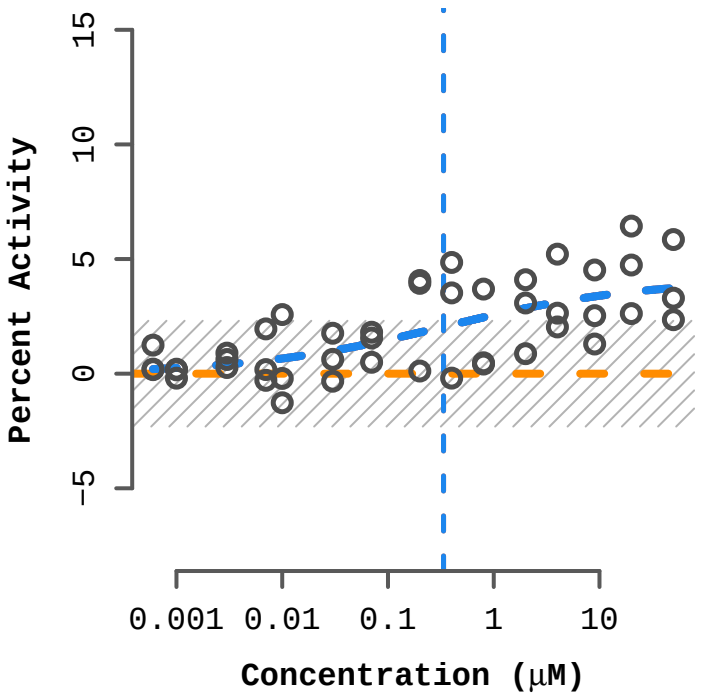
	tp	ga	gw
val:	238	-0.8	1.23
sd:	5.3	0.044	0.107

GAIN-LOSS MODEL (in blue):

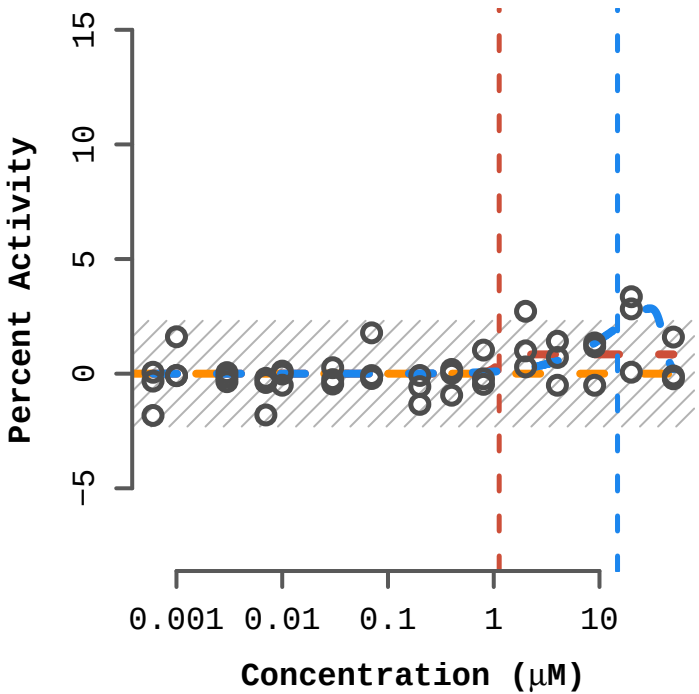
	tp	ga	gw	la	lw
val:	238	-0.8	1.23	2.47	15.1
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	591.01	392.72	396.72
PROB:	0	0.88	0.12
RMSE:	159.04	18.41	18.41

MAX_MEAN: 256 MAX_MED: 250 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    Lenampicillin hydrochloride
CHID:    57835   CASRN: 80734-02-7
SPID(S): Tox21_113720
M4ID:    12482494

HILL MODEL (in red):
      tp       ga       gw
val:  4.09     -0.475   0.469
sd:   1.72     1.2      0.308

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  4.09     -0.475   0.469    3.49     4.96
sd:   NaN      NaN      NaN      NaN      NaN

      CNST        HILL        GNLS
AIC:  219.71      170.85      174.85
PROB: 0           0.88        0.12
RMSE: 2.68        1.4         1.4

MAX_MEAN: 4.6       MAX_MED: 4.74      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Sancycline
CHID: 57836 **CASRN:** 808-26-4
SPID(S): Tox21_113907
M4ID: 12482323

HILL MODEL (in red):

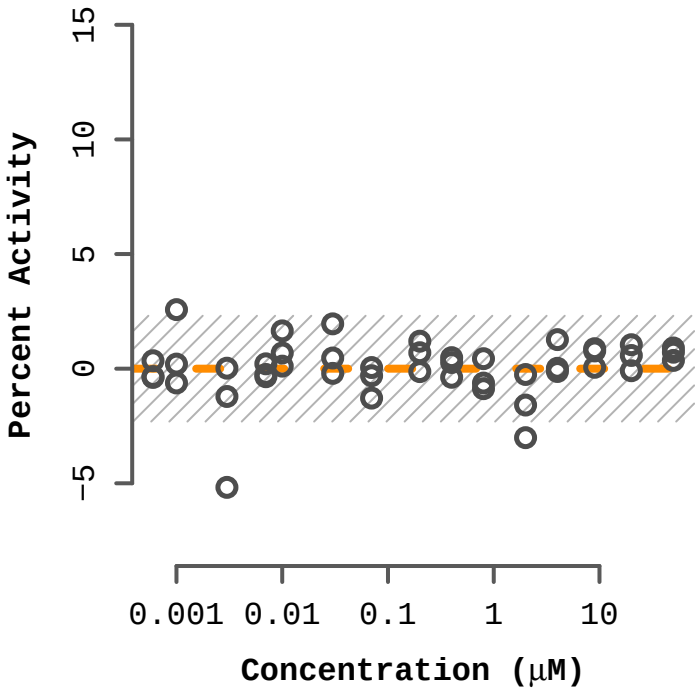
	tp	ga	gw
val:	0.843	0.0515	8
sd:	0.265	0.348	14.6

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.03	1.17	1.4	1.6	12.4
sd:	2.55	0.366	0.766	0.492	60.5

	CNST	HILL	GNLS
AIC:	132.2	128.19	129.01
PROB:	0.07	0.56	0.37
RMSE:	1.1	0.94	0.93

MAX_MEAN: 2.08 **MAX_MED:** 2.83 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

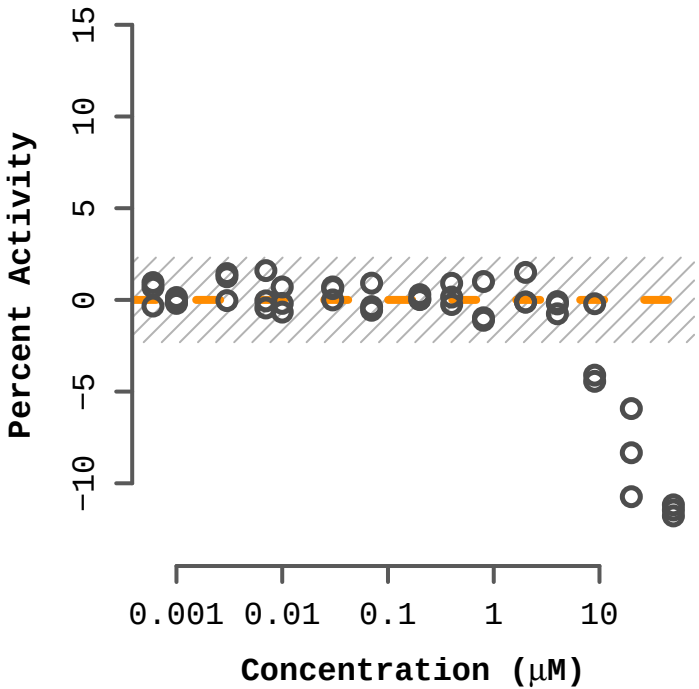
NAME: Sodium 3, 4-dimethylphenyl-glyoxylate
CHID: 57837 **CASRN:** 81632-85-1
SPID(S): Tox21_113674
M4ID: 12482540

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	132.2	NA	NA
PROB:	1	NA	NA
RMSE:	1.21	NA	NA

MAX_MEAN: 0.816 **MAX_MED:** 0.775 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

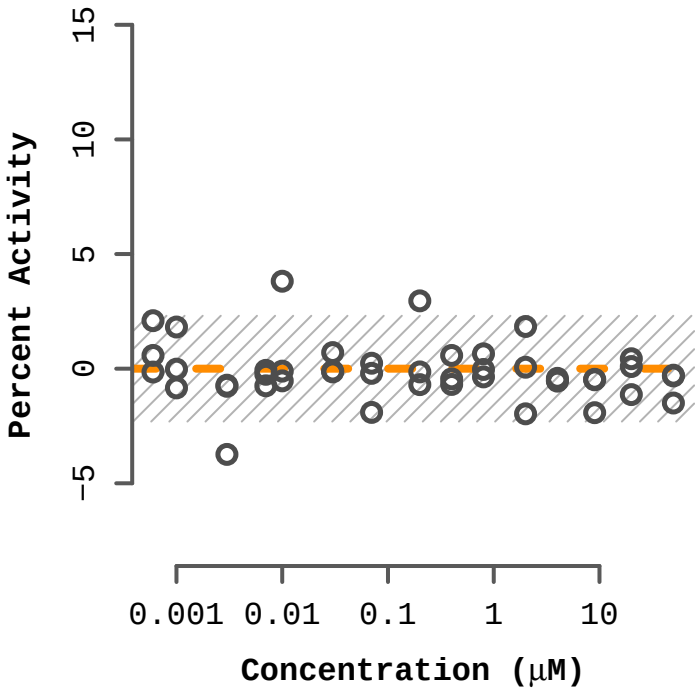
NAME: 1-(4-Fluorobenzyl)-1H-benzimidazol-2-amine
CHID: 57838 **CASRN:** 83783-69-1
SPID(S): Tox21_113754
M4ID: 12482461

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	220.15	NA	NA
PROB:	1	NA	NA
RMSE:	3.86	NA	NA

MAX_MEAN: 0.888 **MAX_MED:** 1.26 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

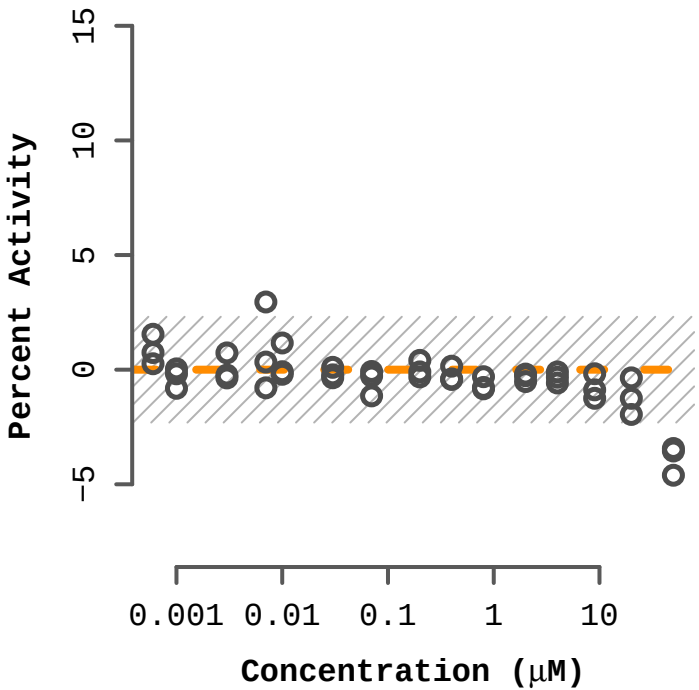
NAME: Ambasilide
CHID: 57839 **CASRN:** 83991-25-7
SPID(S): Tox21_113814
M4ID: 12482405

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	141.68	NA	NA
PROB:	1	NA	NA
RMSE:	1.25	NA	NA

MAX_MEAN: 1.06 **MAX_MED:** 0.579 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

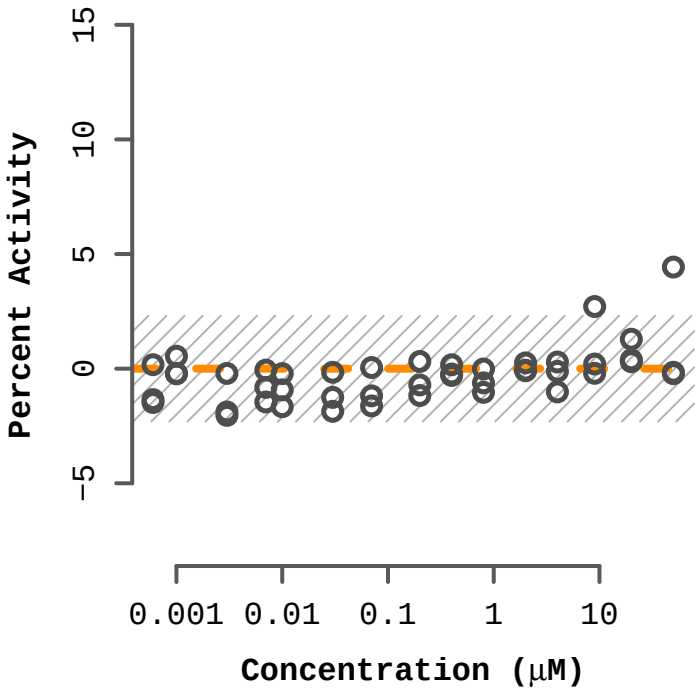
NAME: Dienestrol diacetate
CHID: 57840 **CASRN:** 84-19-5
SPID(S): Tox21_113818
M4ID: 12482403

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	134.92	NA	NA
PROB:	1	NA	NA
RMSE:	1.28	NA	NA

MAX_MEAN: 0.852 **MAX_MED:** 0.75 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

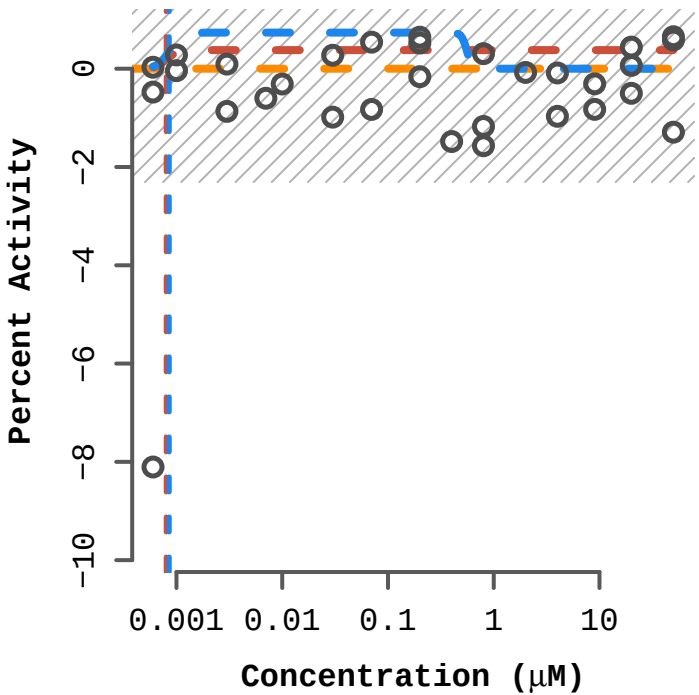
NAME: 4-(2-Piperidinoethoxy)benzoic acid hydrochlori
CHID: 57841 CASRN: 84449-80-9
SPID(S): Tox21_113785
M4ID: 12482432

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	136.58	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.35 MAX_MED: 0.388 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Amidoflumet
CHID: 57842 **CASRN:** 84466-05-7
SPID(S): Tox21_113713
M4ID: 12482501

HILL MODEL (in red):

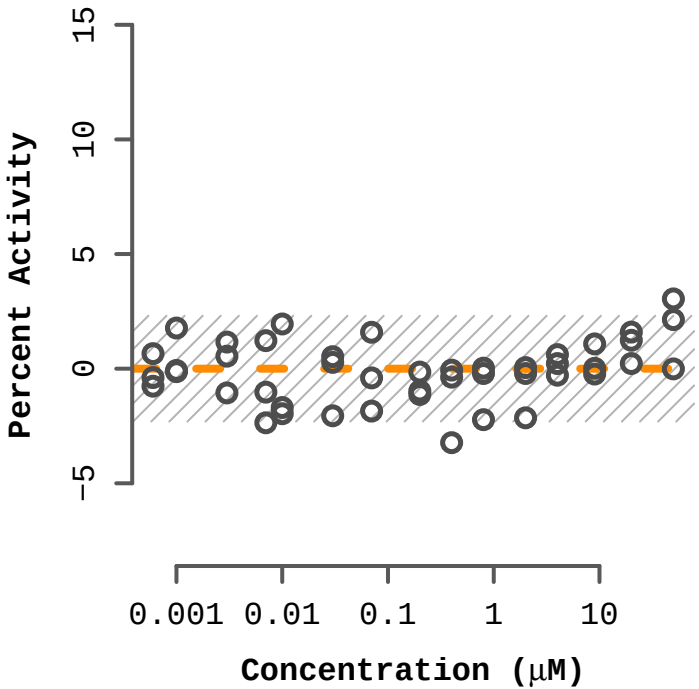
	tp	ga	gw
val:	0.378	−3.1	8
sd:	0.236	0.247	17.7

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.735	−3.07	8	−0.254	17.3
sd:	0.35	0.207	14.3	0.406	46.6

	CNST	HILL	GNLS
AIC:	182.97	186.27	188.12
PROB:	0.79	0.15	0.06
RMSE:	2.08	2	1.94

MAX_MEAN: 2.7 **MAX_MED:** 4.7 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

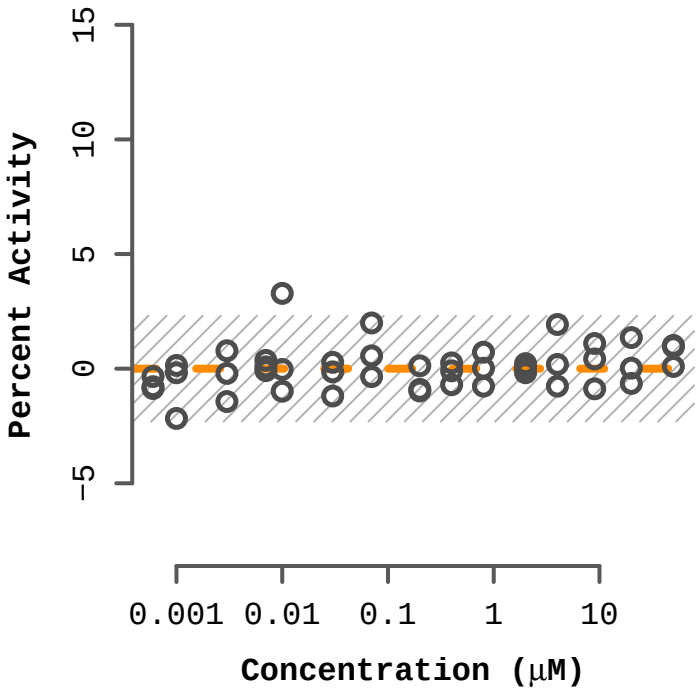
NAME: 4-(4-Chlorophenyl)piperidine-2,6-dione
CHID: 57843 **CASRN:** 84803-46-3
SPID(S): Tox21_113918
M4ID: 12482312

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	156.59	NA	NA
PROB:	1	NA	NA
RMSE:	1.32	NA	NA

MAX_MEAN: 1.73 **MAX_MED:** 2.14 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

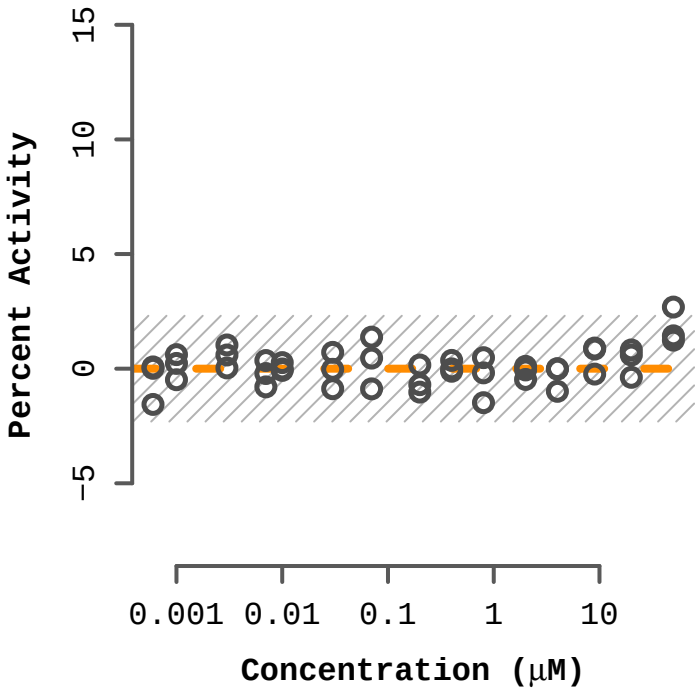
NAME: Indomethacin farnesil
CHID: 57844 **CASRN:** 85801-02-1
SPID(S): Tox21_113722
M4ID: 12482492

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	121.26	NA	NA
PROB:	1	NA	NA
RMSE:	0.95	NA	NA

MAX_MEAN: 0.756 **MAX_MED:** 0.961 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

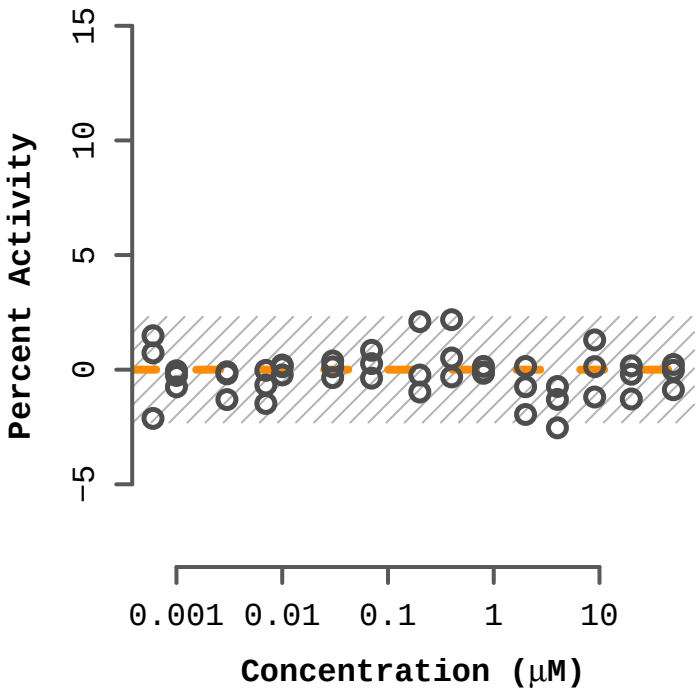
NAME: Methylchromone
CHID: 57845 **CASRN:** 85-90-5
SPID(S): Tox21_113786
M4ID: 12482431

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	107.19	NA	NA
PROB:	1	NA	NA
RMSE:	0.8	NA	NA

MAX_MEAN: 1.79 **MAX_MED:** 1.43 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

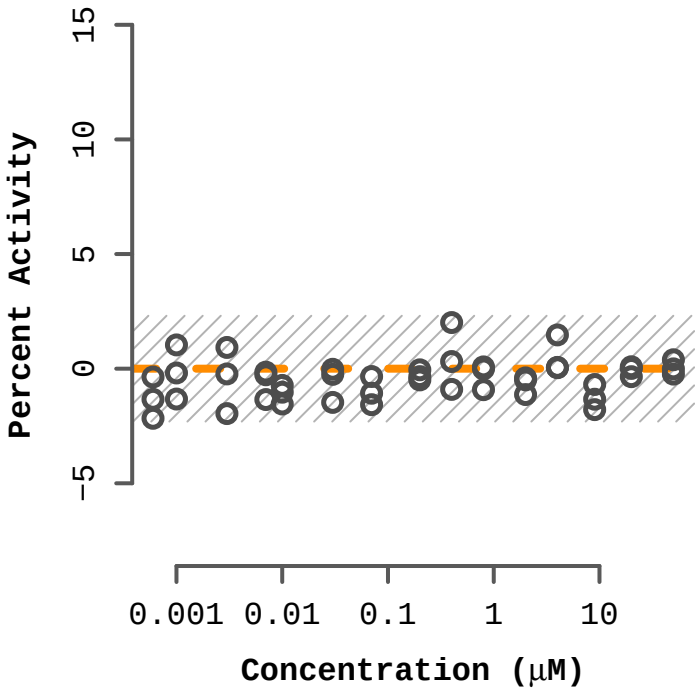
NAME: Fluoroquinolonic acid
CHID: 57846 CASRN: 86393-33-1
SPID(S): Tox21_113798
M4ID: 12482421

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	125.77	NA	NA
PROB:	1	NA	NA
RMSE:	0.98	NA	NA

MAX_MEAN: 0.793 **MAX_MED:** 0.733 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

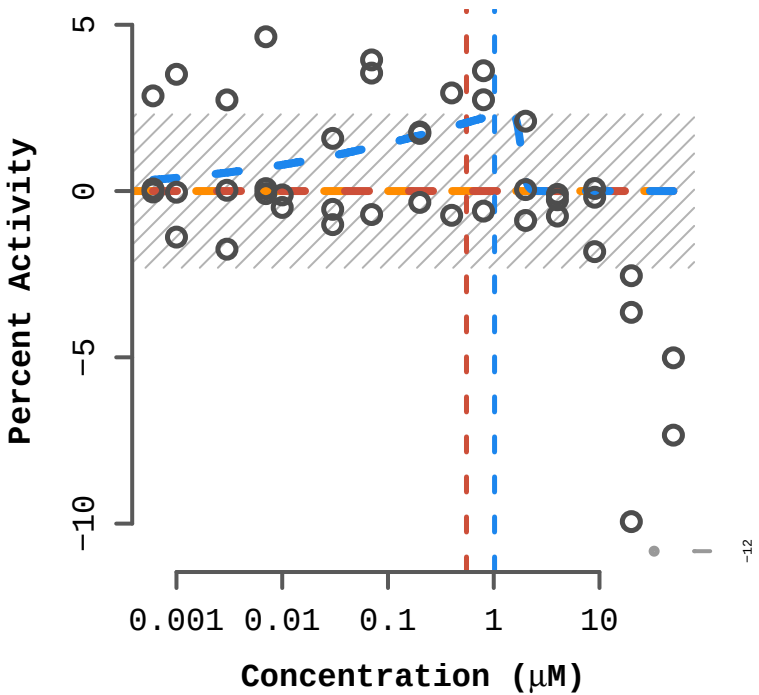
NAME: Ecabet sodium
CHID: 57847 CASRN: 86408-72-2
SPID(S): Tox21_113921
M4ID: 12482310

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	128.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.96	NA	NA

MAX_MEAN: 0.525 **MAX_MED:** 0.313 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Setoperone
CHID: 57848 CASRN: 86487-64-1
SPID(S): Tox21_113942
M4ID: 12482289 BRK

HILL MODEL (in red):

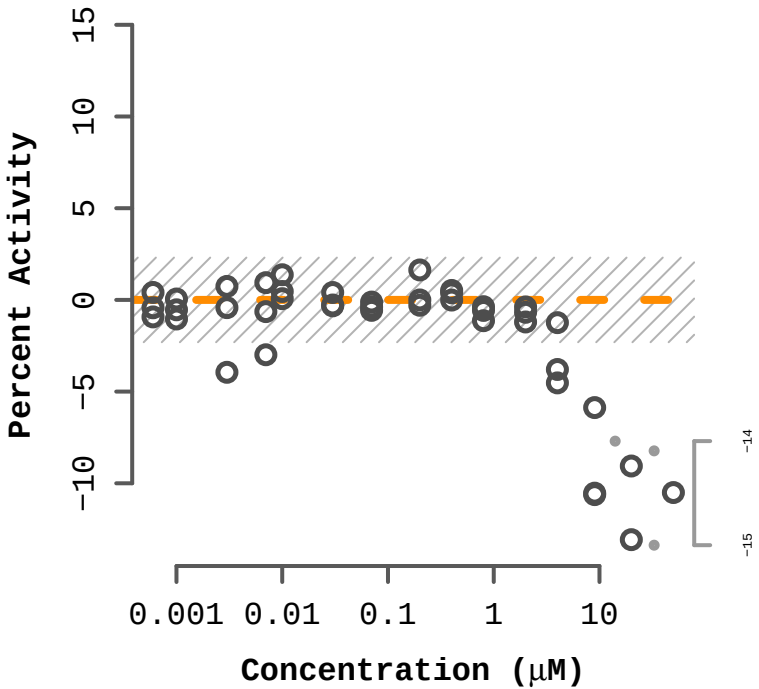
	tp	ga	gw
val:	7.14e-10	-0.258	1.86
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.59	0.00801	0.34	0.258	17.7
sd:	15.3	7.75	0.508	0.882	363

	CNST	HILL	GNLS
AIC:	233.77	239.77	236.38
PROB:	0.76	0.04	0.2
RMSE:	3.51	3.51	3.33

MAX_MEAN: 2.57 MAX_MED: 3.55 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

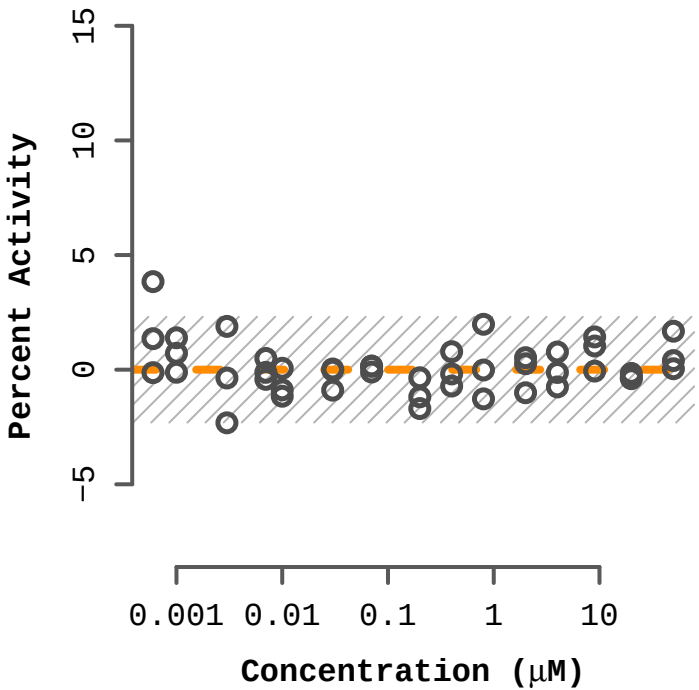
NAME: Buparvaquone
CHID: 57849 **CASRN:** 88426-33-9
SPID(S): Tox21_113753
M4ID: 12482462 **BRK**

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	265.67	NA	NA
PROB:	1	NA	NA
RMSE:	5.42	NA	NA

MAX_MEAN: 0.634 **MAX_MED:** 0.461 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

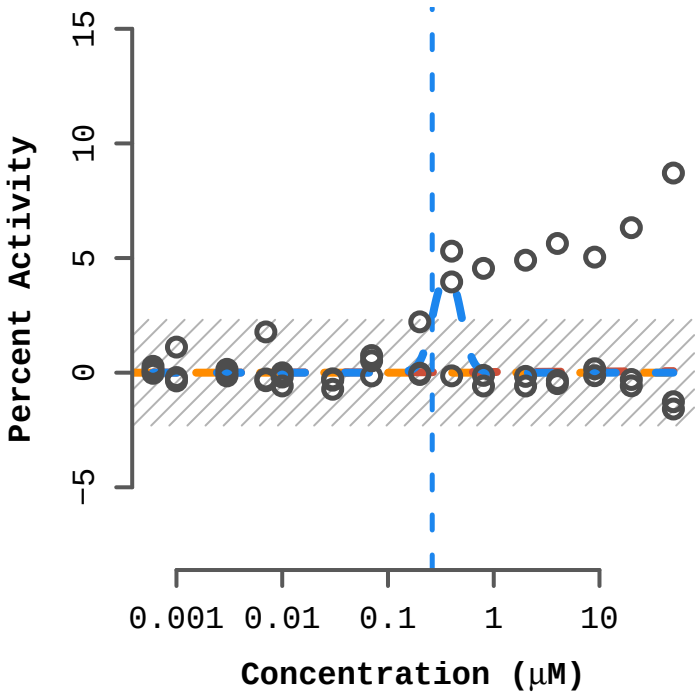
NAME: Imidaprilat
CHID: 57850 **CASRN:** 89371-44-8
SPID(S): Tox21_113982
M4ID: 12482259

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	131.13	NA	NA
PROB:	1	NA	NA
RMSE:	1.07	NA	NA

MAX_MEAN: 1.69 **MAX_MED:** 1.35 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Cinnamedrine
CHID: 57851 **CASRN:** 90-86-8
SPID(S): Tox21_113672
M4ID: 12482542

HILL MODEL (in red):

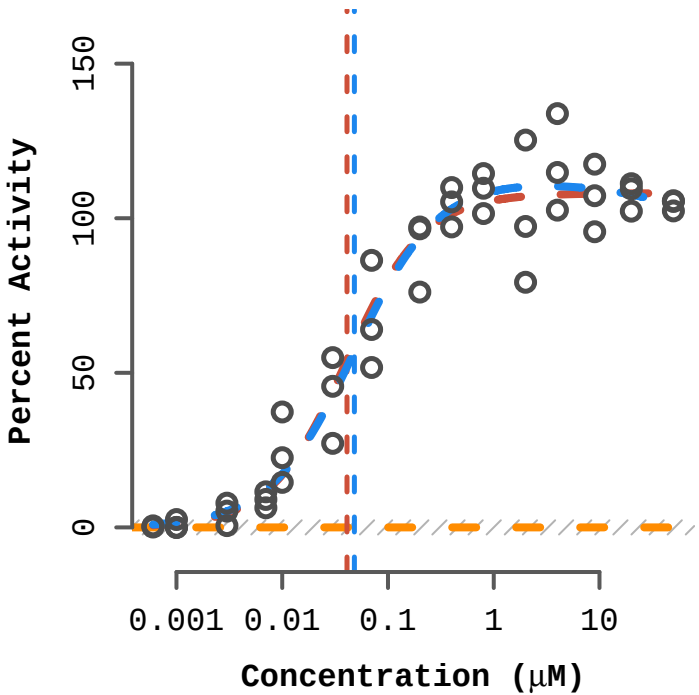
	tp	ga	gw
val:	0.157	2.13	0.3
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	4.82	−0.582	7.99	−0.302	8.58
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	192	197.98	193.66
PROB:	0.67	0.03	0.29
RMSE:	2.49	2.48	2.37

MAX_MEAN: 3.04 **MAX_MED:** 3.96 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nandrolone cyclohexylpropionate
CHID: 57852 CASRN: 912-57-2
SPID(S): Tox21_113696
M4ID: 12482518

HILL MODEL (in red):

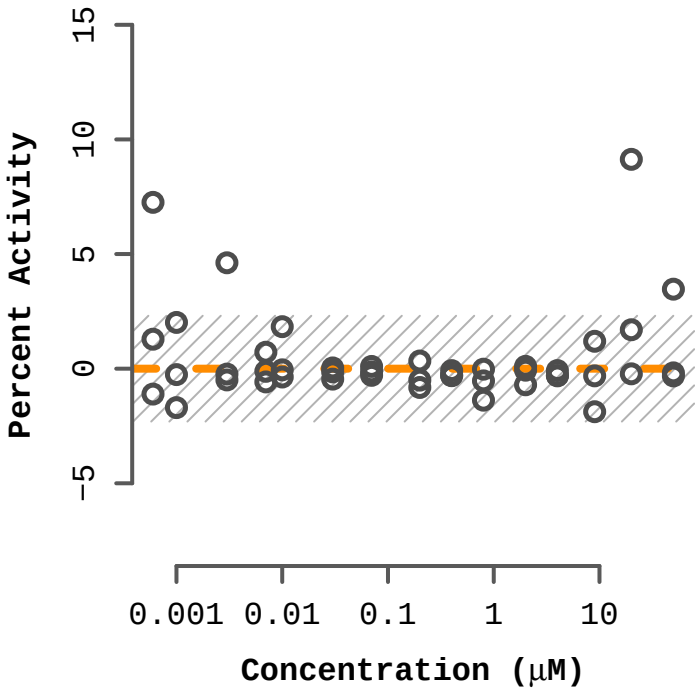
	tp	ga	gw
val:	108	-1.39	1.19
sd:	2.15	0.0615	0.12

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	114	-1.32	1.1	3.7	0.517
sd:	12.1	0.119	0.149	3.49	1.11

	CNST	HILL	GNLS
AIC:	531.4	338.34	340.4
PROB:	0	0.74	0.26
RMSE:	80.32	9.93	9.81

MAX_MEAN: 117 MAX_MED: 115 BMAD: 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

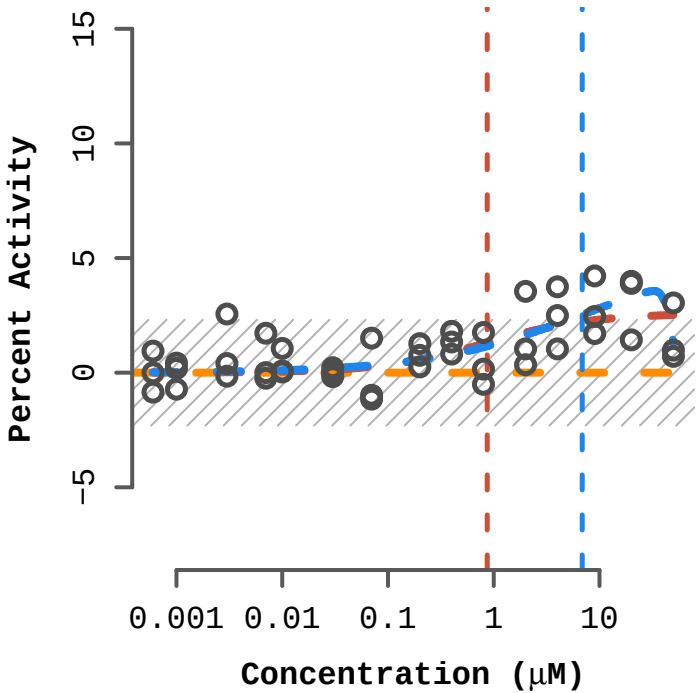
NAME: Ibafloxacine
CHID: 57853 **CASRN:** 91618-36-9
SPID(S): Tox21_113686
M4ID: 12482528

HILL MODEL: Not applicable.

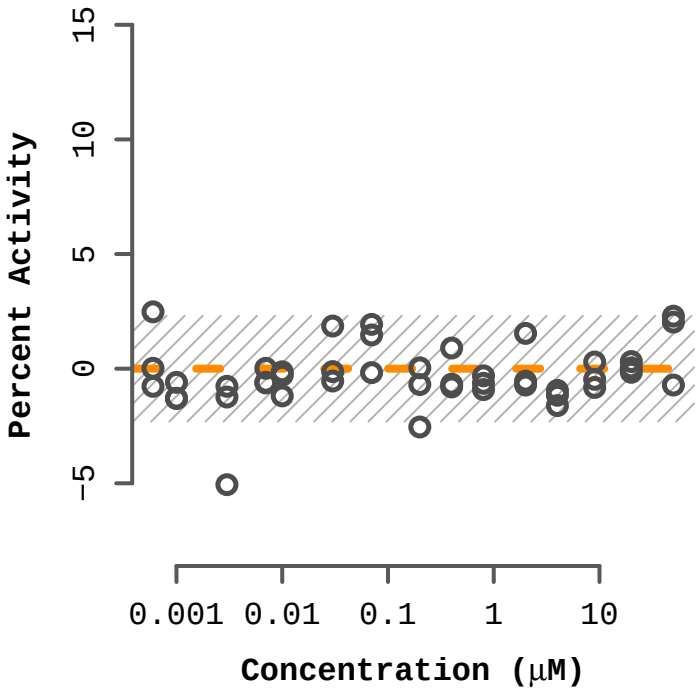
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	160.79	NA	NA
PROB:	1	NA	NA
RMSE:	2.09	NA	NA

MAX_MEAN: 3.54 **MAX_MED:** 1.7 **BMAD:** 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Chlorophenothiazine
CHID:    57854   CASRN: 92-39-7
SPID(S): Tox21_113822
M4ID:    12482399

HILL MODEL (in red):
      tp       ga       gw
val:  2.59     -0.0616  0.868
sd:   0.649    0.411    0.486

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  5.07     0.837    0.589    1.67     11.3
sd:   3.11     0.968    0.261    0.102    44

      CNST       HILL       GNLS
AIC:  177.73     143.69     142.11
PROB: 0          0.31       0.69
RMSE: 1.73       1.05       1

MAX_MEAN: 3.1       MAX_MED: 3.9       BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

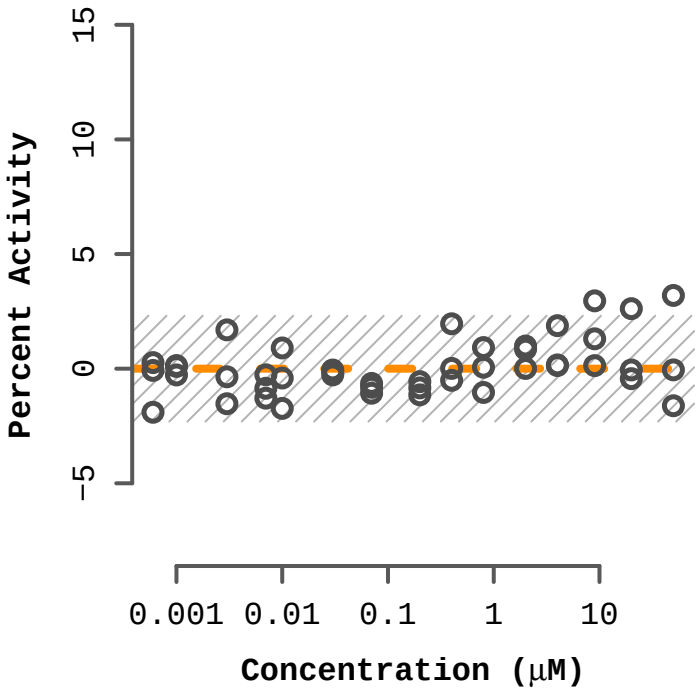
NAME: Phenylpiperazine
CHID: 57855 **CASRN:** 92-54-6
SPID(S): Tox21_113878
M4ID: 12482347

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.3	NA	NA
PROB:	1	NA	NA
RMSE:	1.33	NA	NA

MAX_MEAN: 1.2 **MAX_MED:** 2.03 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

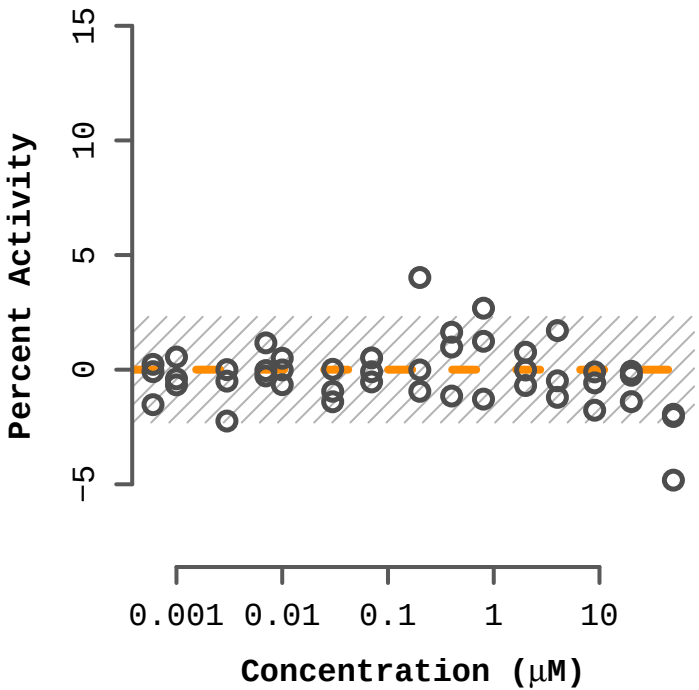
NAME: 1,1-Dimethoxy-2-(2-methoxyethoxy)ethane
CHID: 57856 **CASRN:** 94158-44-8
SPID(S): Tox21_113751
M4ID: 12482464

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	142.73	NA	NA
PROB:	1	NA	NA
RMSE:	1.17	NA	NA

MAX_MEAN: 1.47 **MAX_MED:** 1.3 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

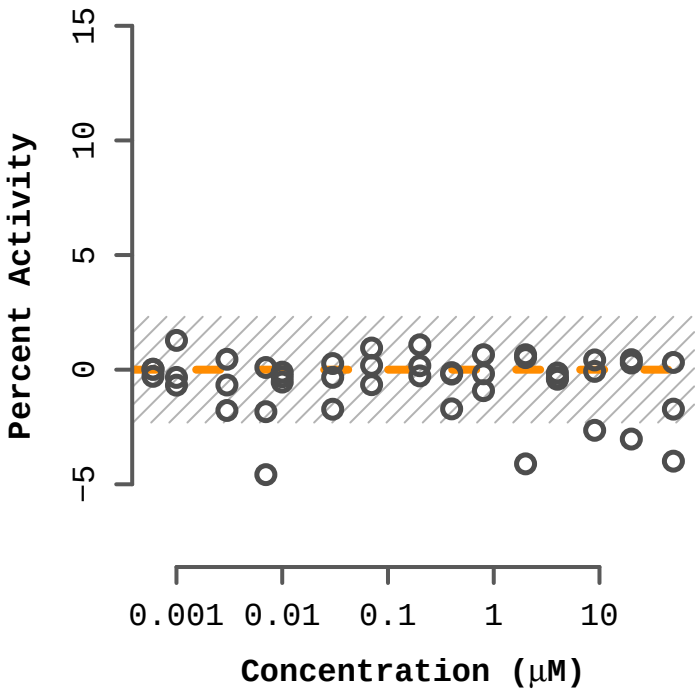
NAME: Dehydropregnenolone acetate
CHID: 57857 CASRN: 979-02-2
SPID(S): Tox21_113909
M4ID: 12482321

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	154.43	NA	NA
PROB:	1	NA	NA
RMSE:	1.4	NA	NA

MAX_MEAN: 1.02 **MAX_MED:** 1.24 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

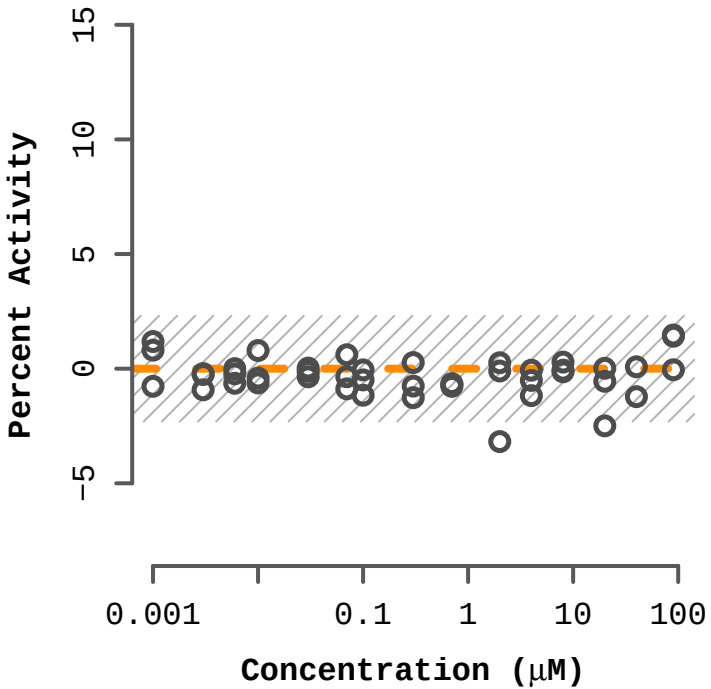
NAME: Epsiprantel
CHID: 57858 **CASRN:** 98123-83-2
SPID(S): Tox21_113678
M4ID: 12482536

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	150.63	NA	NA
PROB:	1	NA	NA
RMSE:	1.45	NA	NA

MAX_MEAN: 0.33 **MAX_MED:** 0.529 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

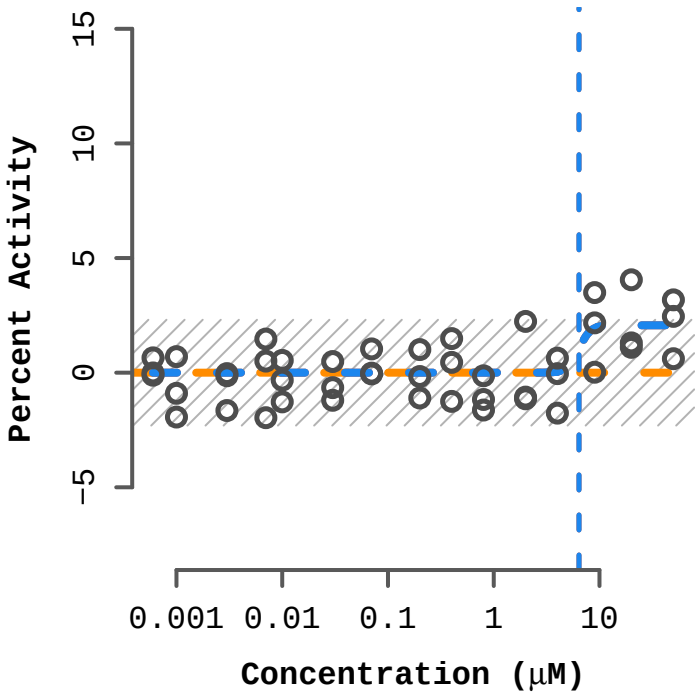
NAME: Anti-OP-18/Stathmin antibody produced in rabbi
CHID: 57890 CASRN: NOCAS_57890
SPID(S): Tox21_303959
M4ID: 12475229

HILL MODEL: Not applicable.

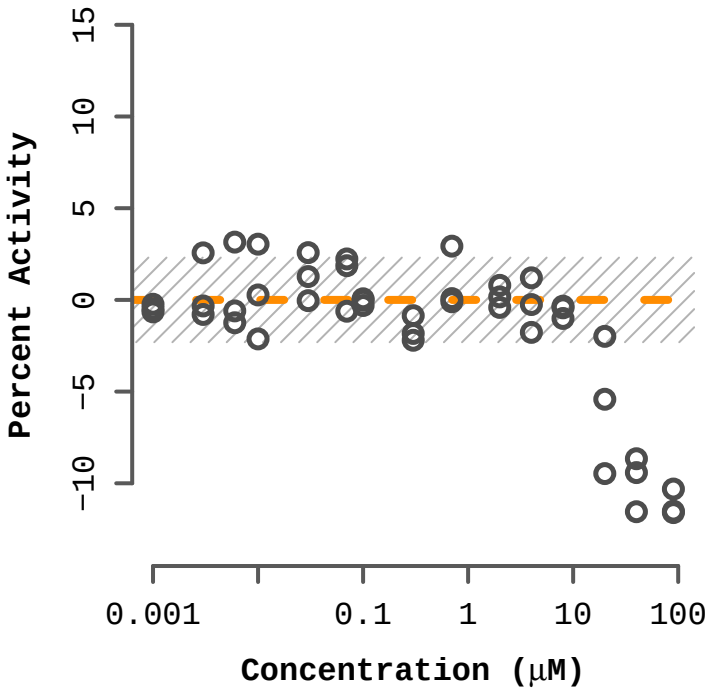
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	113	NA	NA
PROB:	1	NA	NA
RMSE:	0.91	NA	NA

MAX_MEAN: 0.947 MAX_MED: 1.42 BMAD: 0.769




```
ASSAY:   AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME:    2-Amino-4-(trifluoromethyl)benzenethiol hydrocl
CHID:    57898   CASRN: 4274-38-8
SPID(S): Tox21_113922
M4ID:    12482309

HILL MODEL (in red):
      tp       ga       gw
val:  2.07     0.806    8
sd:   0.49     0.196    8.82

GAIN-LOSS MODEL (in blue):
      tp       ga       gw       la       lw
val:  2.07     0.806    8        3.32     4.22
sd:   0.49     0.196    8.82     925      2430

      CNST        HILL        GNLS
AIC:  162.9       151.01      155.01
PROB: 0           0.88        0.12
RMSE: 1.44        1.12        1.12

MAX_MEAN: 2.15      MAX_MED: 2.46      BMAD: 0.769
```



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

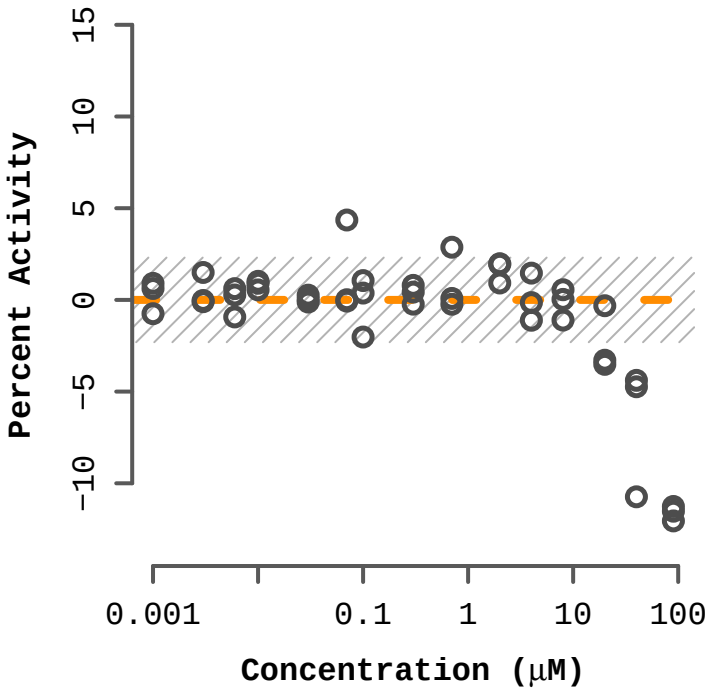
NAME: BisOPP-A
CHID: 58654 CASRN: 24038-68-4
SPID(S): Tox21_303963
M4ID: 12475225

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	248.95	NA	NA
PROB:	1	NA	NA
RMSE:	4.39	NA	NA

MAX_MEAN: 1.27 **MAX_MED:** 1.87 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

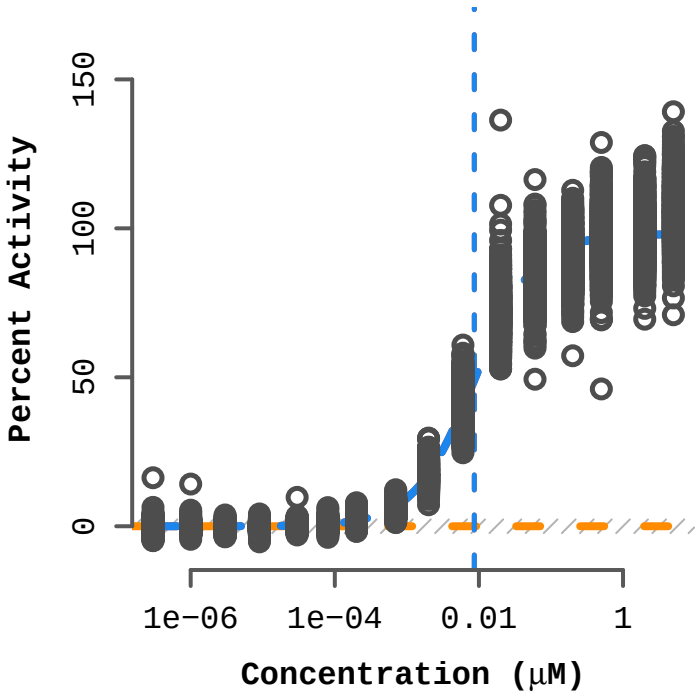
NAME: BPS-MPE4
CHID: 58655 **CASRN:** 63134-33-8
SPID(S): Tox21_304051
M4ID: 12475137

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	223.67	NA	NA
PROB:	1	NA	NA
RMSE:	3.77	NA	NA

MAX_MEAN: 1.62 **MAX_MED:** 1.95 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: R1881 (spid not in DB)
CHID: NA CASRN: NA
SPID(S): R1881
M4ID: 12484716

HILL MODEL (in red):

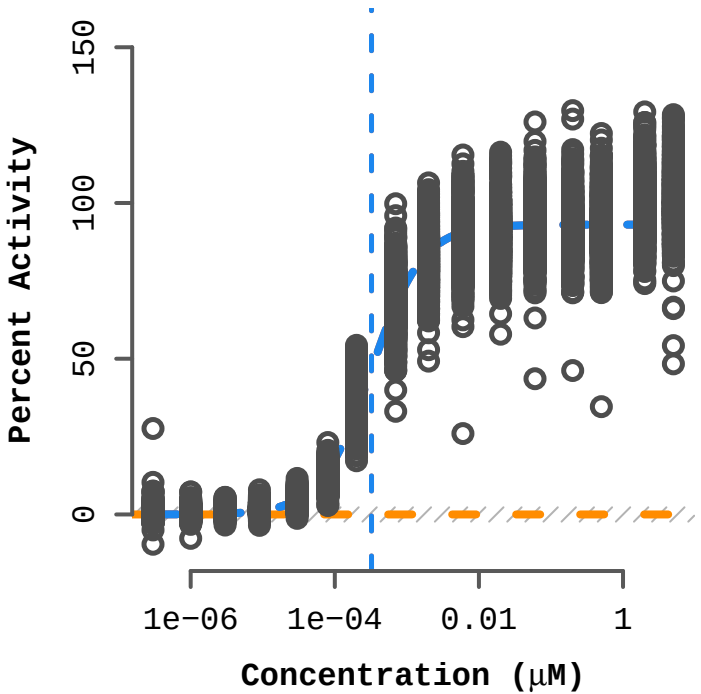
	tp	ga	gw
val:	98.2	−2.06	1.04
sd:	0.134	0.00283	0.00515

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	98.2	−2.06	1.04	1.4	18
sd:	0.134	0.00283	0.00515	1190	30100

	CNST	HILL	GNLS
AIC:	126354.29	69745.51	69749.51
PROB:	0	0.88	0.12
RMSE:	57.48	5.82	5.82

MAX_MEAN: 105 **MAX_MED:** 105 **BMAD:** 0.769



ASSAY: AEID1822 (TOX21_AR_LUC_MDAKB2_Agonist2)

NAME: Nilutamide free R1881 (spid not in DB)
CHID: NA CASRN: NA
SPID(S): Nilutamide free R1881
M4ID: 12484717

HILL MODEL (in red):

	tp	ga	gw
val:	93.1	−3.49	1.23
sd:	0.107	0.00303	0.00822

GAIN−LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	93.1	−3.49	1.23	1.34	15.8
sd:	0.107	0.00303	0.00822	113	2780

	CNST	HILL	GNLS
AIC:	131604.64	76499.71	76503.71
PROB:	0	0.88	0.12
RMSE:	68.25	7.21	7.21

MAX_MEAN: 101 MAX_MED: 100 BMAD: 0.769