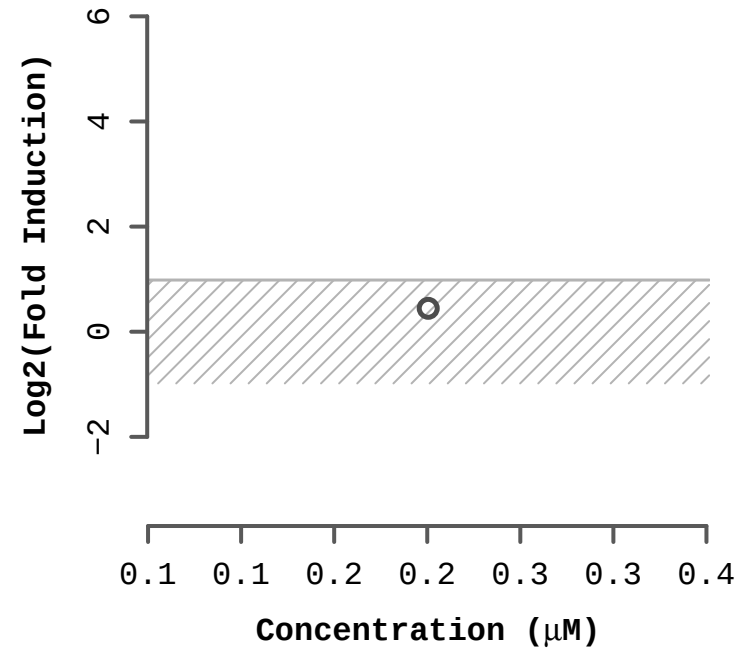




ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Norgestrel (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Norgestrel

M4ID: 18128491

HILL MODEL: Not applicable.

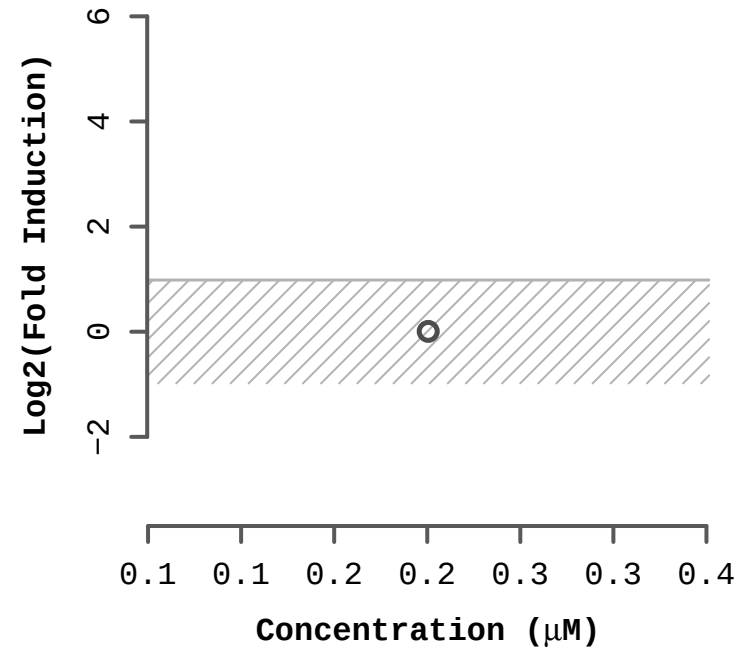
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | NA   | NA   | NA   |
| PROB: | NA   | NA   | NA   |
| RMSE: | NA   | NA   | NA   |

MAX\_MEAN: 0.446 MAX\_MED: 0.446 BMAD: 0.328

COFF: 0.984 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Estradiol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Estradiol

M4ID: 18128492

HILL MODEL: Not applicable.

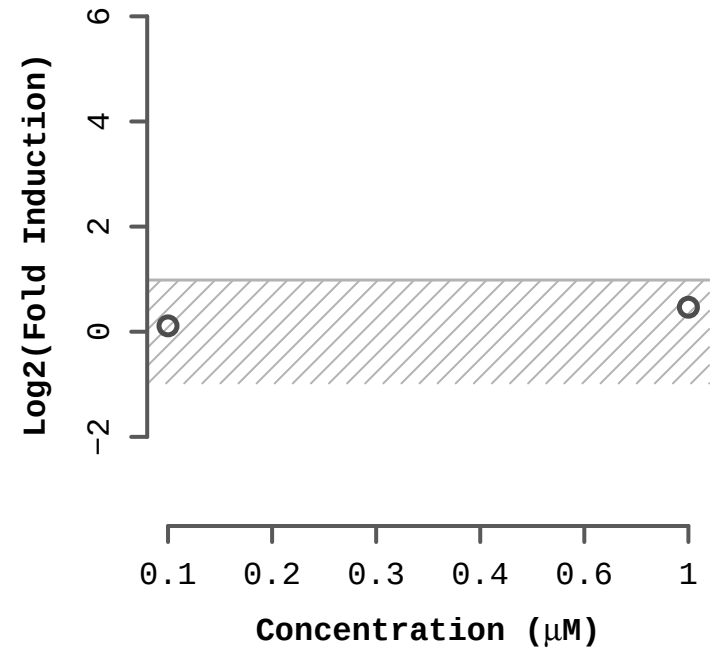
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | NA   | NA   | NA   |
| PROB: | NA   | NA   | NA   |
| RMSE: | NA   | NA   | NA   |

MAX\_MEAN: 0.00699 MAX\_MED: 0.00699 BMAD: 0.328

COFF: 0.984 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 6a-Fluorotestosterone (spid not in DB)

CHID: NA CASRN: NA

SPID(S): 6a-Fluorotestosterone

M4ID: 18128493

HILL MODEL: Not applicable.

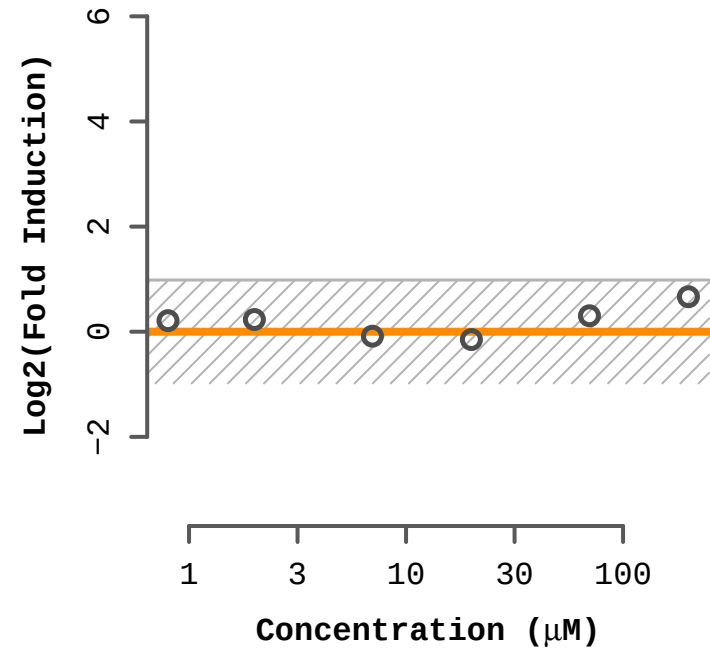
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | NA   | NA   | NA   |
| PROB: | NA   | NA   | NA   |
| RMSE: | NA   | NA   | NA   |

MAX\_MEAN: 0.467 MAX\_MED: 0.467 BMAD: 0.328

COFF: 0.984 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Azinphos-methyl

CHID: 20122 CASRN: 86-50-0

SPID(S): TP0001562D08

M4ID: 18128451

HILL MODEL: Not applicable.

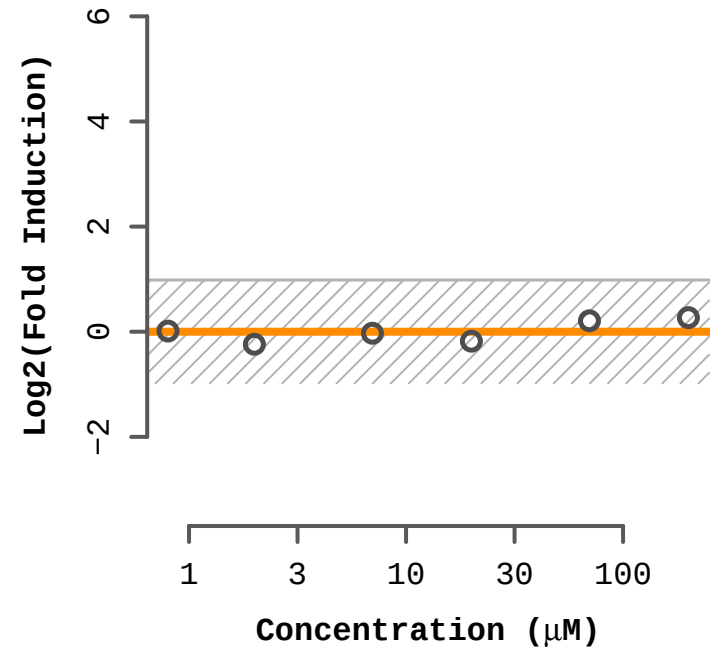
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>6.11</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.33</b> | NA   | NA   |

MAX\_MEAN: 0.666 MAX\_MED: 0.666 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-tert-Butylphenol

CHID: 20221 CASRN: 98-54-4

SPID(S): TP0001562G08

M4ID: 18128418

HILL MODEL: Not applicable.

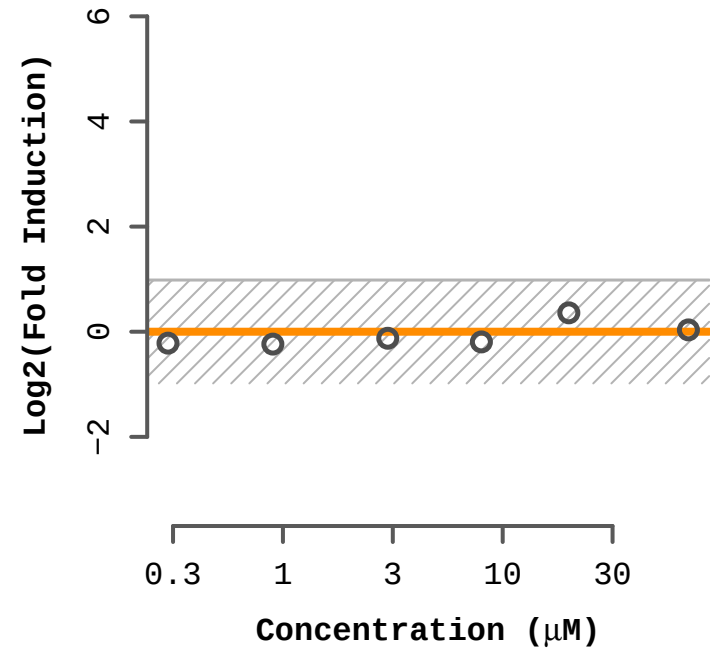
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>-0.2</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.19</b> | NA   | NA   |

MAX\_MEAN: 0.269 MAX\_MED: 0.269 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Chloromethyl methyl ether

CHID: 20307 CASRN: 107-30-2

SPID(S): TP0001562C03

M4ID: 18128467

HILL MODEL: Not applicable.

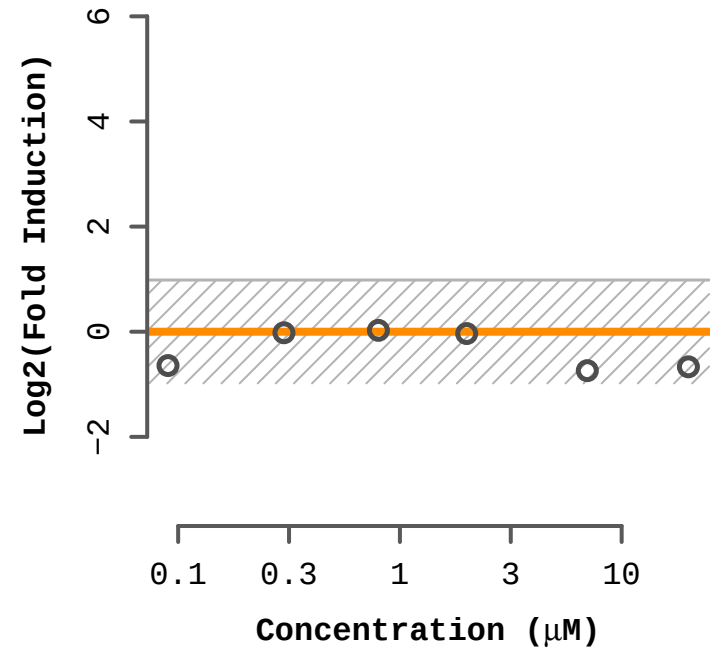
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>1.74</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.22</b> | NA   | NA   |

MAX\_MEAN: 0.36 MAX\_MED: 0.36 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Clomiphene citrate (1:1)

CHID: 20337 CASRN: 50-41-9

SPID(S): TP0001562H07

M4ID: 18128408

HILL MODEL: Not applicable.

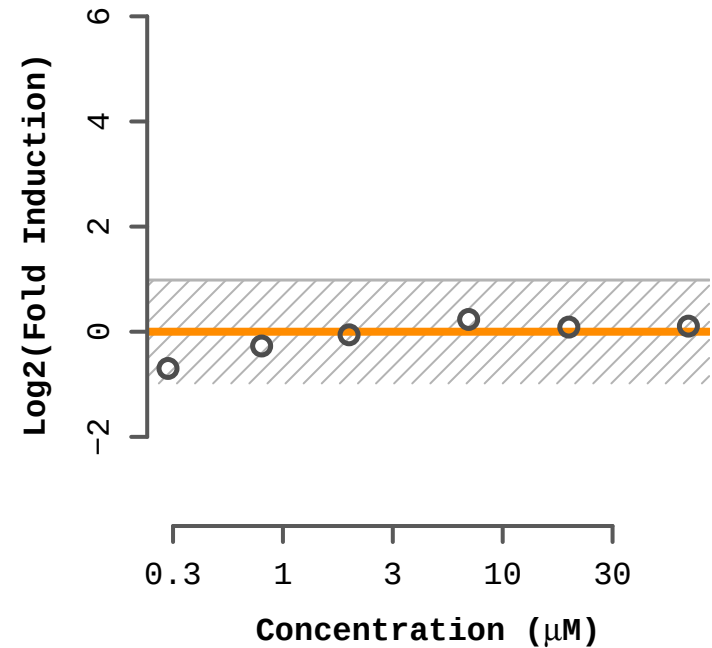
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 11   | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.48 | NA   | NA   |

MAX\_MEAN: 0.0267 MAX\_MED: 0.0267 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: o,p'-DDD

CHID: 20372 CASRN: 53-19-0

SPID(S): TP0001562A03

M4ID: 18128489

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

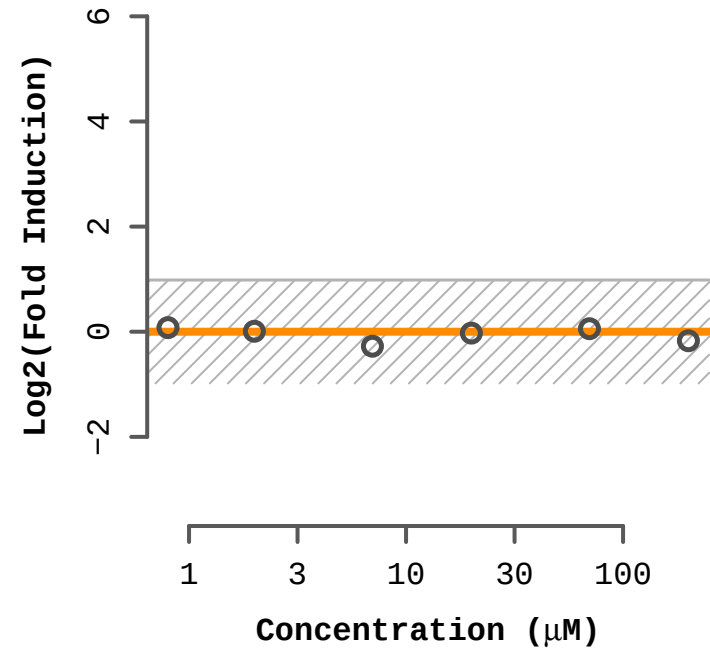
|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>5.26</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.33</b> | NA   | NA   |

MAX\_MEAN: 0.234 MAX\_MED: 0.234 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Dehydroepiandrosterone

CHID: 20379 CASRN: 53-43-0

SPID(S): TP0001562C06

M4ID: 18128464

HILL MODEL: Not applicable.

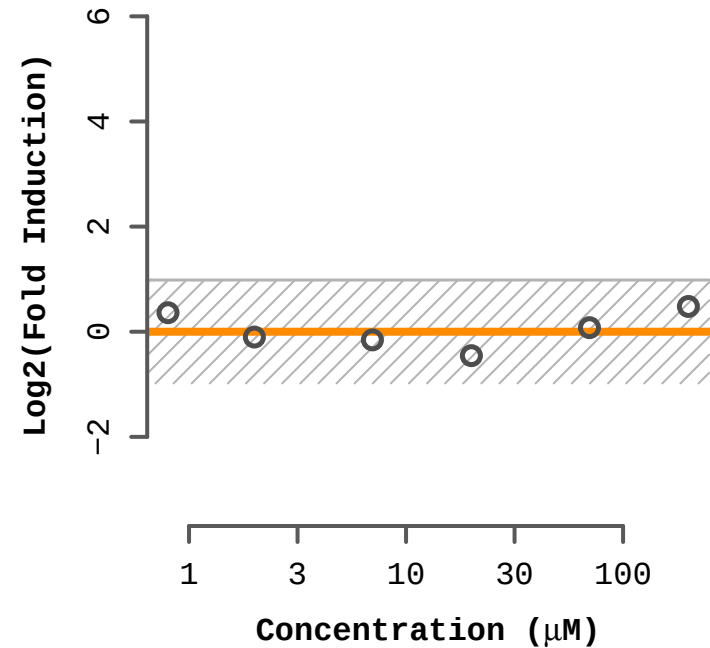
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>-4.63</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.14</b>  | NA   | NA   |

MAX\_MEAN: 0.0788 MAX\_MED: 0.0788 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Diallyl phthalate

CHID: 20392 CASRN: 131-17-9

SPID(S): TP0001562D07

M4ID: 18128452

HILL MODEL: Not applicable.

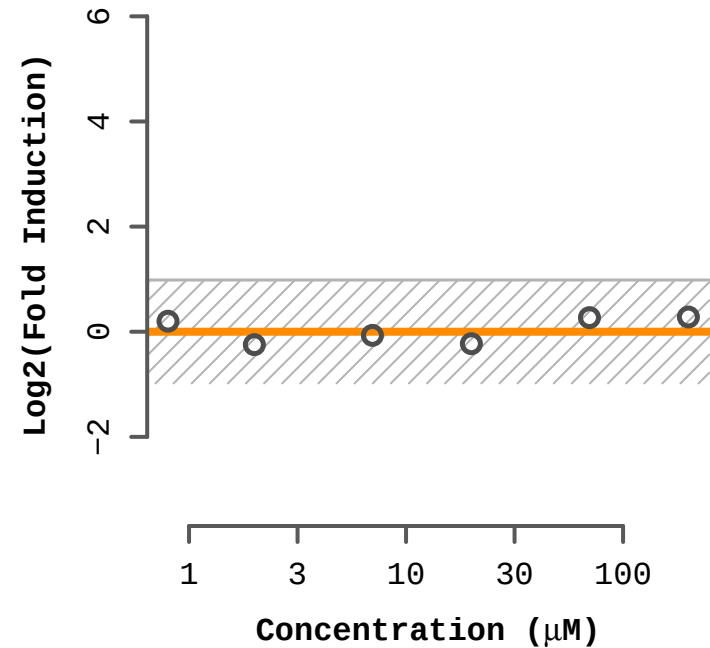
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>6.16</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.32</b> | NA   | NA   |

MAX\_MEAN: 0.481 MAX\_MED: 0.481 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Diuron

CHID: 20446 CASRN: 330-54-1

SPID(S): TP0001562C02

M4ID: 18128468

HILL MODEL: Not applicable.

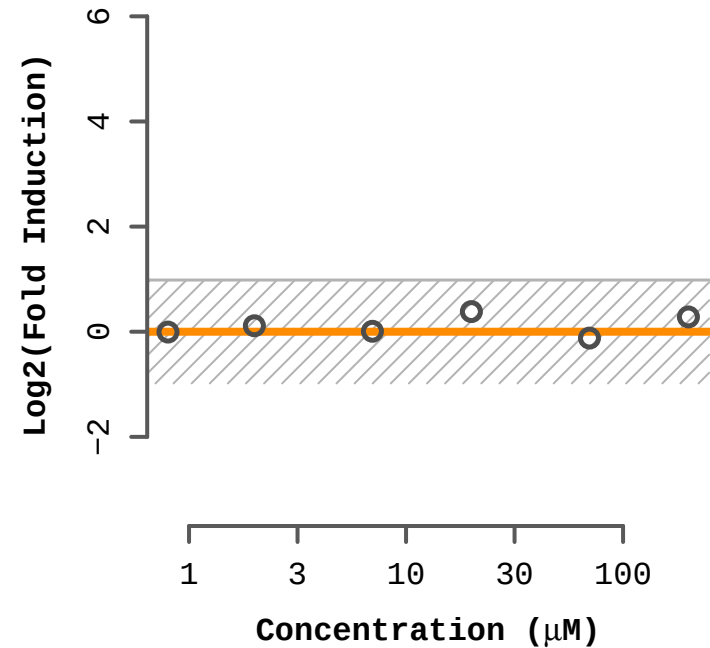
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 2.49 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.23 | NA   | NA   |

MAX\_MEAN: 0.28 MAX\_MED: 0.28 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 3,3'-Dimethylbenzidine dihydrochloride

CHID: 20511 CASRN: 612-82-8

SPID(S): TP0001562E06

M4ID: 18128442

HILL MODEL: Not applicable.

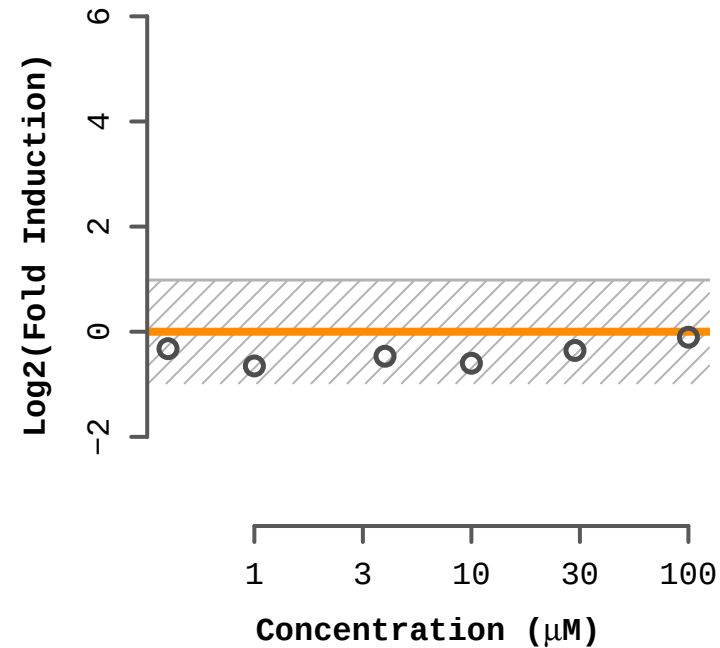
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 0.37 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.21 | NA   | NA   |

MAX\_MEAN: 0.384 MAX\_MED: 0.384 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Fadrozole hydrochloride

CHID: 20618 CASRN: 102676-31-3

SPID(S): TP0001562D03

M4ID: 18128456

HILL MODEL: Not applicable.

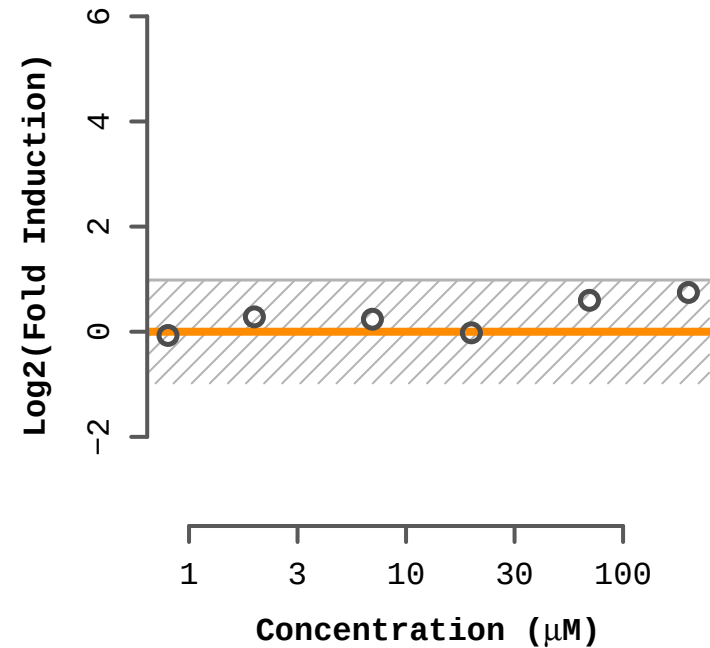
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>10.68</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.45</b>  | NA   | NA   |

MAX\_MEAN: -0.104 MAX\_MED: -0.104 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Kaempferol

CHID: 20768 CASRN: 520-18-3

SPID(S): TP0001562G02

M4ID: 18128424

HILL MODEL: Not applicable.

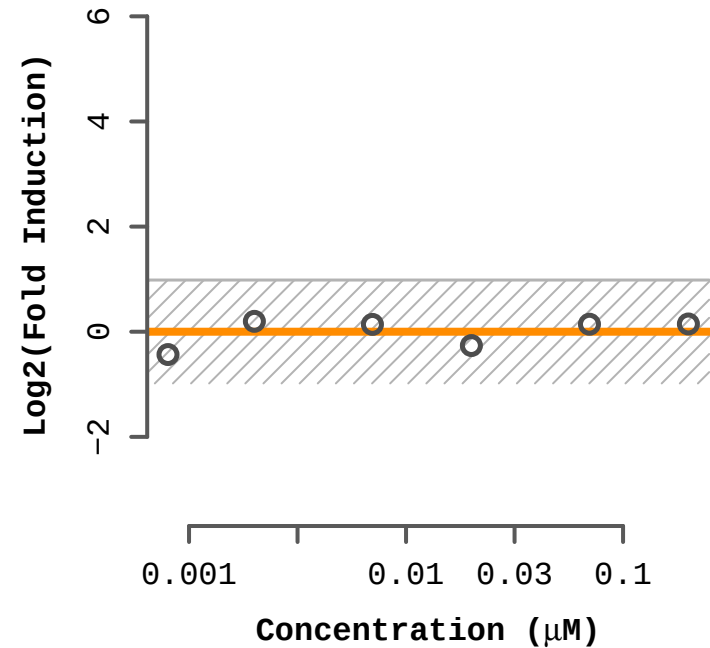
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 9.08 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.42 | NA   | NA   |

MAX\_MEAN: 0.748 MAX\_MED: 0.748 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Mestranol

CHID: 20814 CASRN: 72-33-3

SPID(S): TP0001562H11

M4ID: 18128404

HILL MODEL: Not applicable.

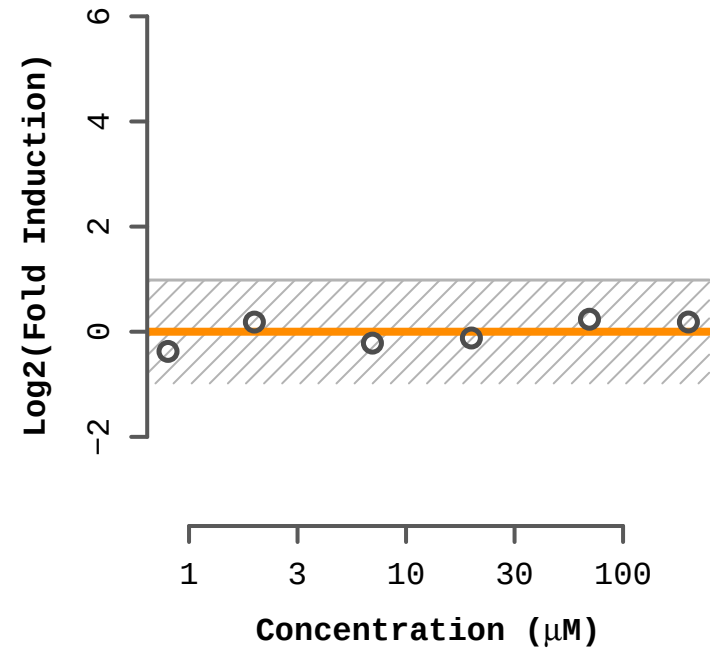
GAIN-LOSS MODEL: Not applicable.

|       |      |      |      |
|-------|------|------|------|
|       | CNST | HILL | GNLS |
| AIC:  | 2.96 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.24 | NA   | NA   |

MAX\_MEAN: 0.198 MAX\_MED: 0.198 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Methyl parathion

CHID: 20855 CASRN: 298-00-0

SPID(S): TP0001562H09

M4ID: 18128406

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

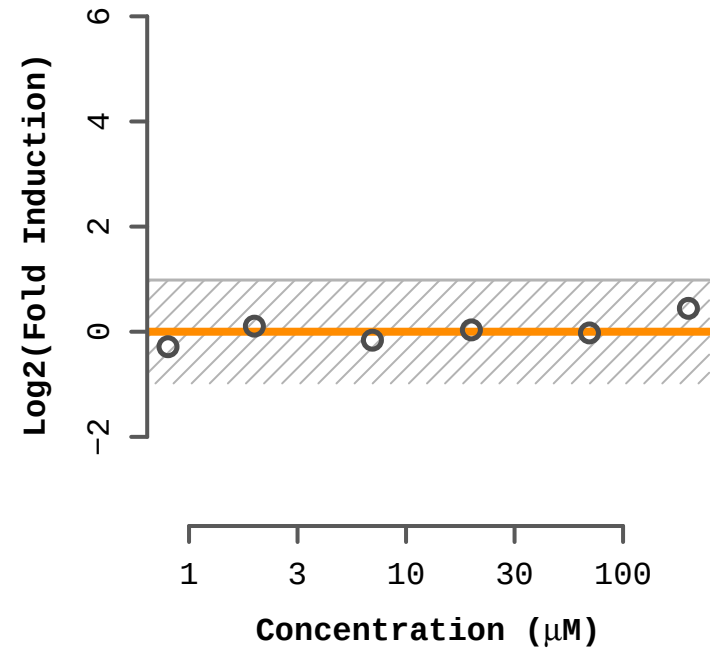
|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>2.67</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.23</b> | NA   | NA   |

MAX\_MEAN: 0.238 MAX\_MED: 0.238 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Nitrofen

CHID: 20970 CASRN: 1836-75-5

SPID(S): TP0001562C10

M4ID: 18128460

HILL MODEL: Not applicable.

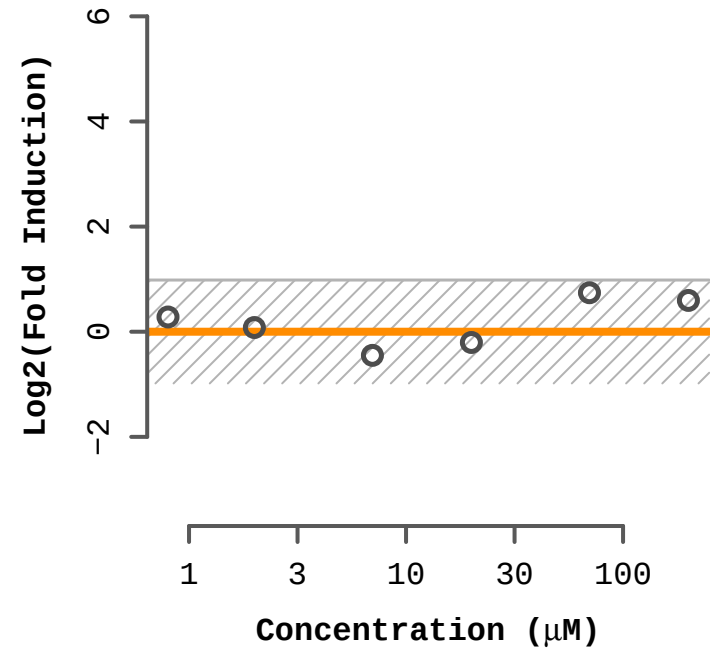
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 1.65 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.23 | NA   | NA   |

MAX\_MEAN: 0.446 MAX\_MED: 0.446 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Phenothiazine

CHID: 21126 CASRN: 92-84-2

SPID(S): TP0001562H08

M4ID: 18128407

HILL MODEL: Not applicable.

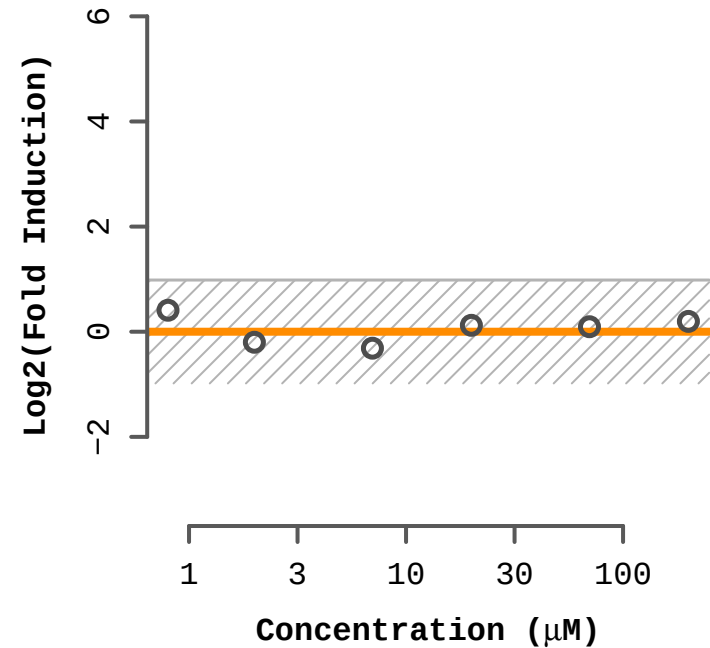
GAIN-LOSS MODEL: Not applicable.

|       |      |      |      |
|-------|------|------|------|
|       | CNST | HILL | GNLS |
| AIC:  | 10.4 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.45 | NA   | NA   |

MAX\_MEAN: 0.743 MAX\_MED: 0.743 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-Phenylphenol

CHID: 21152 CASRN: 92-69-3

SPID(S): TP0001562A05

M4ID: 18128487

HILL MODEL: Not applicable.

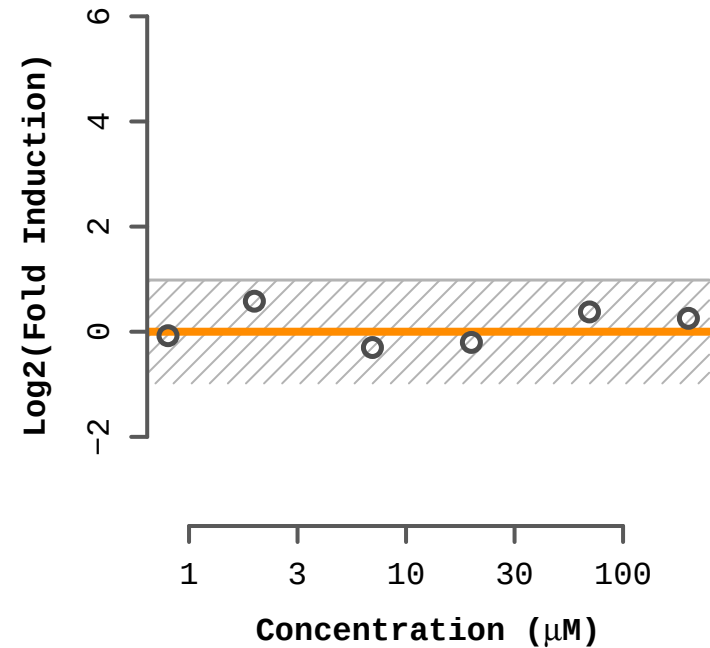
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 3.21 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.25 | NA   | NA   |

MAX\_MEAN: 0.409 MAX\_MED: 0.409 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 6-Propyl-2-thiouracil

CHID: 21209 CASRN: 51-52-5

SPID(S): TP0001562D11

M4ID: 18128448

HILL MODEL: Not applicable.

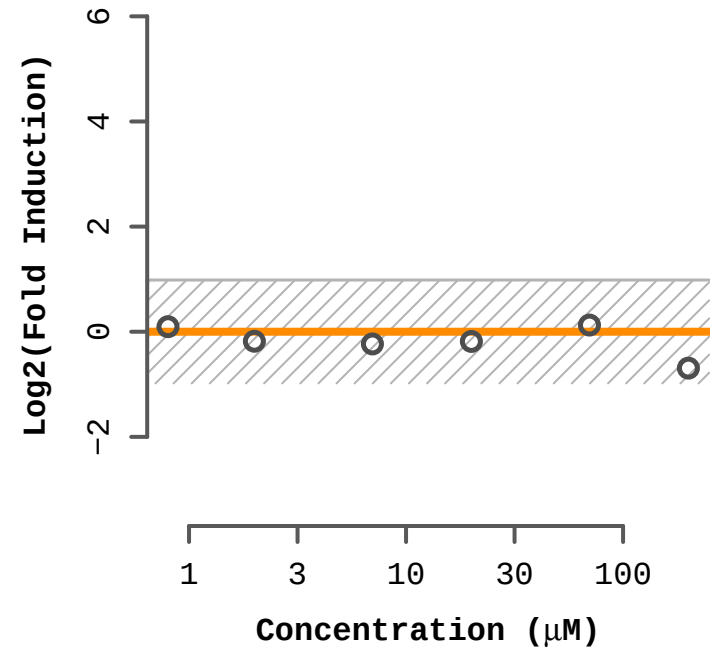
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 6.86 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.34 | NA   | NA   |

MAX\_MEAN: 0.581 MAX\_MED: 0.581 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-(2-Methylbutan-2-yl)phenol

CHID: 21771 CASRN: 80-46-6

SPID(S): TP0001562A06

M4ID: 18128486

HILL MODEL: Not applicable.

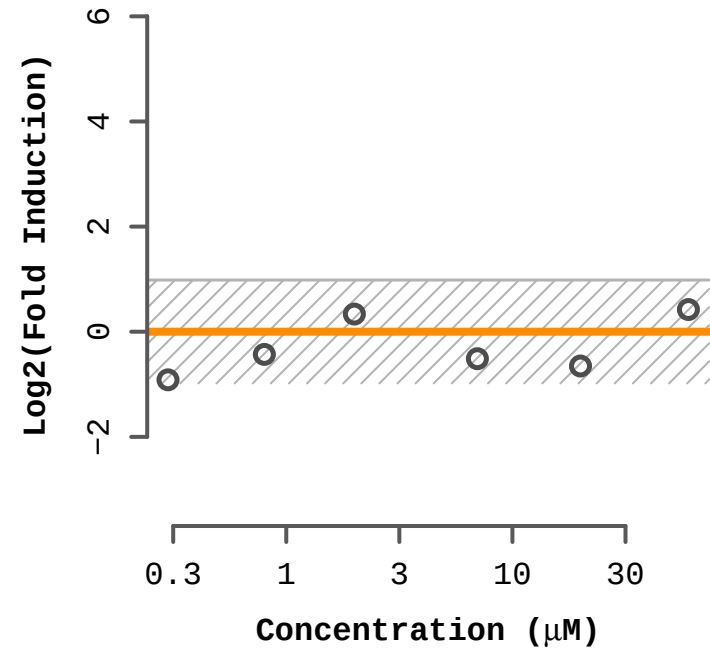
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>5.21</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.32</b> | NA   | NA   |

MAX\_MEAN: 0.128 MAX\_MED: 0.128 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 1-Dodecanamine

CHID: 21984 CASRN: 124-22-1

SPID(S): TP0001562E04

M4ID: 18128444

HILL MODEL: Not applicable.

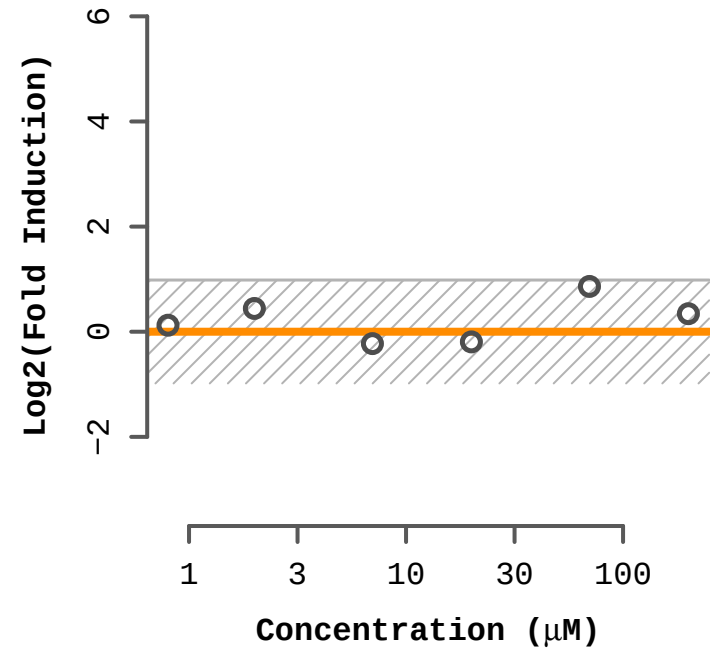
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>13.56</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.58</b>  | NA   | NA   |

MAX\_MEAN: 0.423 MAX\_MED: 0.423 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Propanil

CHID: 22111 CASRN: 709-98-8

SPID(S): TP0001562E08

M4ID: 18128440

HILL MODEL: Not applicable.

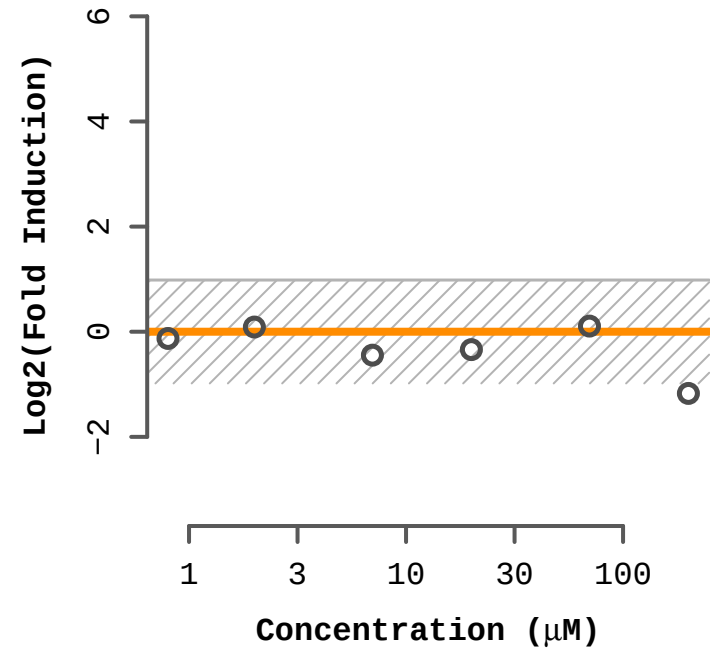
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>9.55</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.44</b> | NA   | NA   |

MAX\_MEAN: 0.862 MAX\_MED: 0.862 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Pentachloropyridine

CHID: 22179 CASRN: 2176-62-7

SPID(S): TP0001562A10

M4ID: 18128482

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

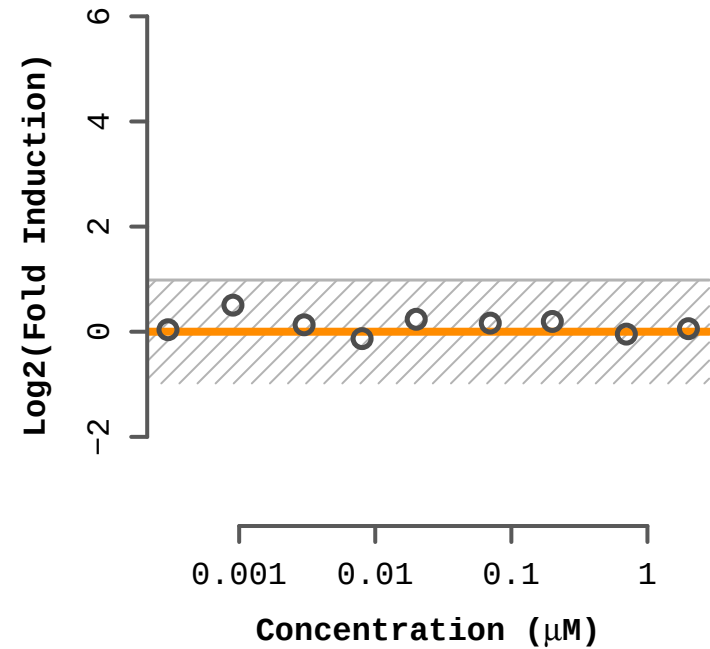
|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>10.94</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.54</b>  | NA   | NA   |

MAX\_MEAN: 0.108 MAX\_MED: 0.108 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Genistein

CHID: 22308 CASRN: 446-72-0

SPID(S): TP0001564B02

M4ID: 18128401

HILL MODEL: Not applicable.

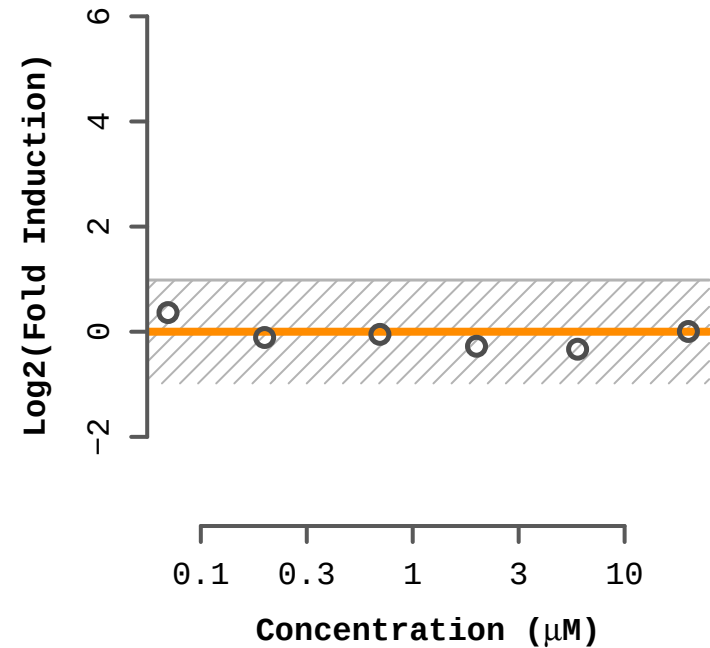
GAIN-LOSS MODEL: Not applicable.

|       | CNST  | HILL | GNLS |
|-------|-------|------|------|
| AIC:  | -0.23 | NA   | NA   |
| PROB: | 1     | NA   | NA   |
| RMSE: | 0.22  | NA   | NA   |

MAX\_MEAN: 0.506 MAX\_MED: 0.506 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Daidzein

CHID: 22310 CASRN: 486-66-8

SPID(S): TP0001562G12

M4ID: 18128414

HILL MODEL: Not applicable.

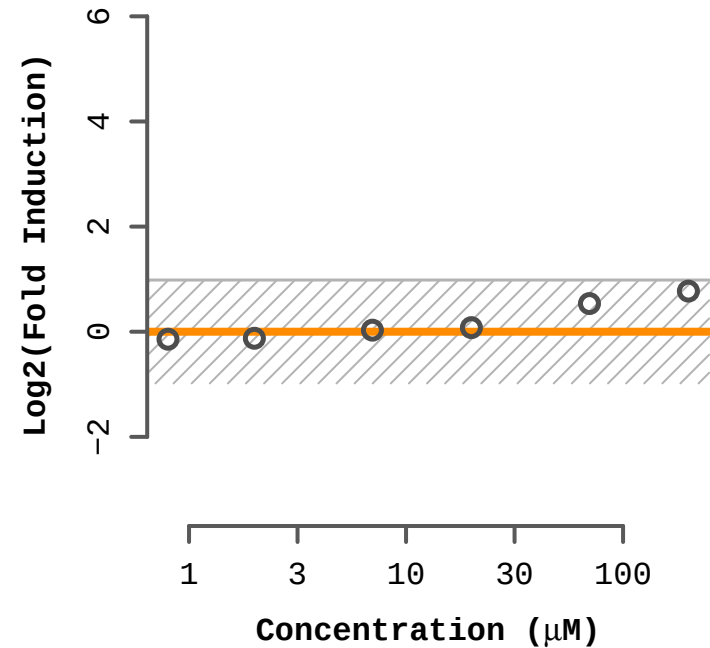
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>2.48</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.24</b> | NA   | NA   |

MAX\_MEAN: 0.365 MAX\_MED: 0.365 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-(Butan-2-yl)phenol

CHID: 22332 CASRN: 99-71-8

SPID(S): TP0001562A09

M4ID: 18128483

HILL MODEL: Not applicable.

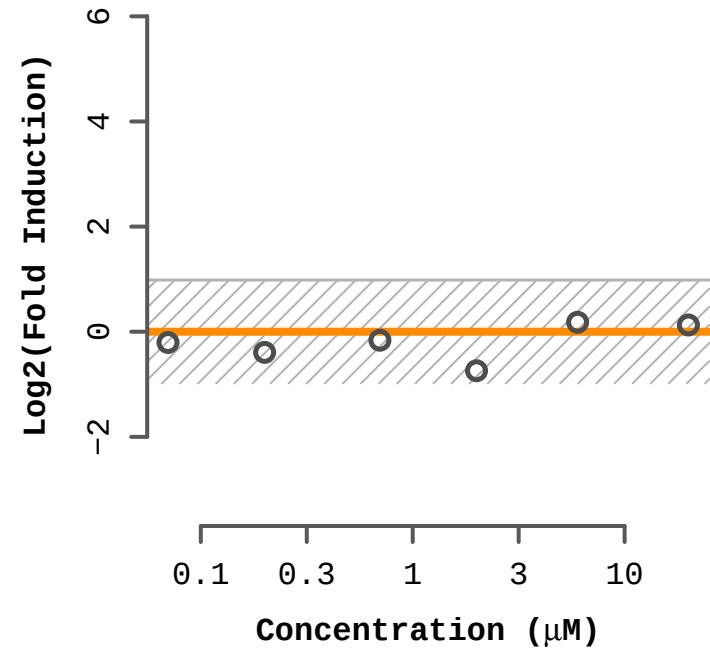
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>7.73</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.39</b> | NA   | NA   |

MAX\_MEAN: 0.773 MAX\_MED: 0.773 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Biochanin A

CHID: 22394 CASRN: 491-80-5

SPID(S): TP0001562H12

M4ID: 18128403

HILL MODEL: Not applicable.

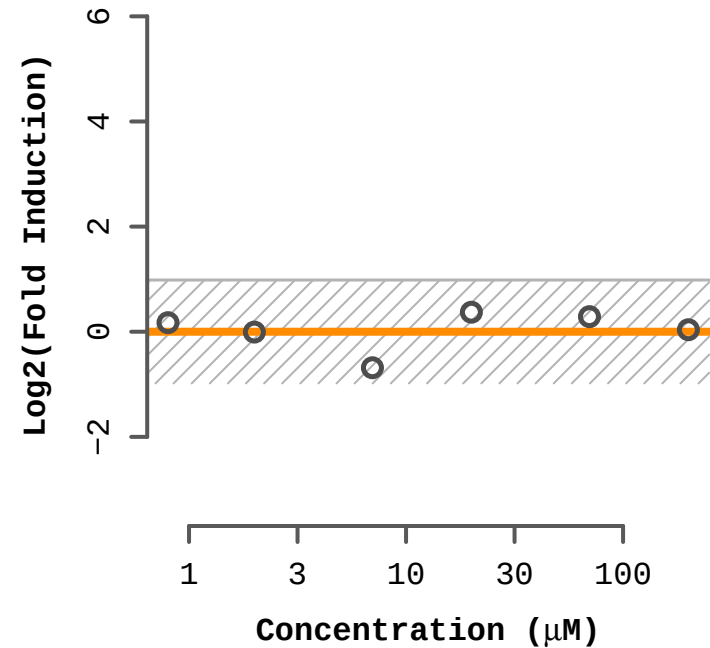
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>7.29</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.37</b> | NA   | NA   |

MAX\_MEAN: 0.18 MAX\_MED: 0.18 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 2-Hydroxy-4-methoxybenzophenone

CHID: 22405 CASRN: 131-57-7

SPID(S): TP0001562G05

M4ID: 18128421

HILL MODEL: Not applicable.

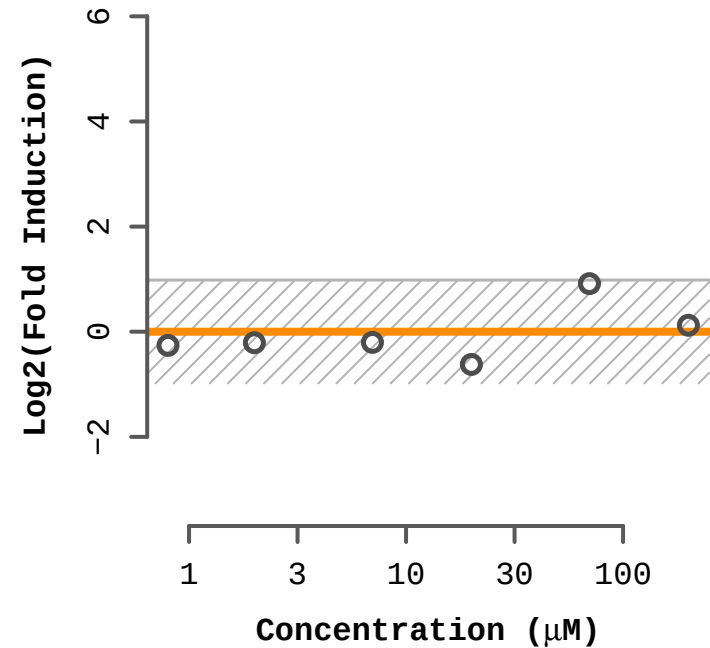
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>6.54</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.35</b> | NA   | NA   |

MAX\_MEAN: 0.372 MAX\_MED: 0.372 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4,4'-Sulfonyldiphenol

CHID: 22409 CASRN: 80-09-1

SPID(S): TP0001562B02

M4ID: 18128479

HILL MODEL: Not applicable.

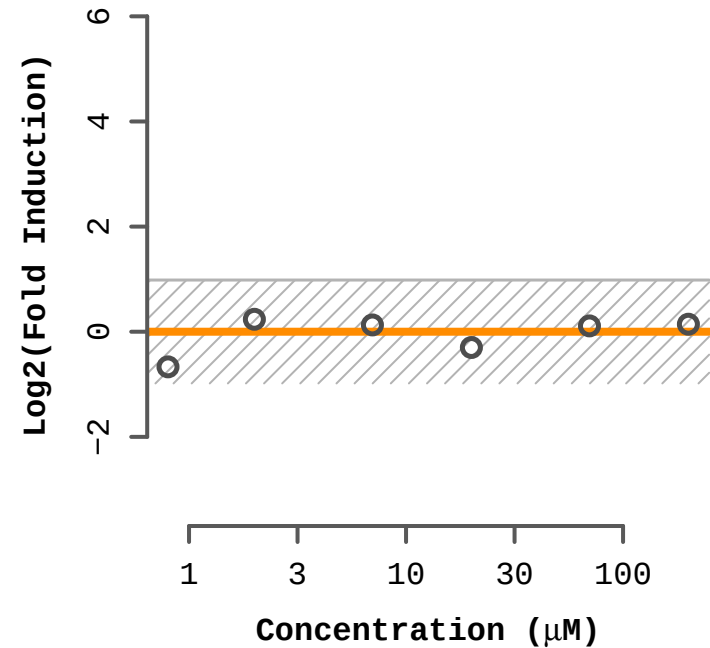
GAIN-LOSS MODEL: Not applicable.

|       |       |      |      |
|-------|-------|------|------|
|       | CNST  | HILL | GNLS |
| AIC:  | 10.58 | NA   | NA   |
| PROB: | 1     | NA   | NA   |
| RMSE: | 0.48  | NA   | NA   |

MAX\_MEAN: 0.916 MAX\_MED: 0.916 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Diphenolic acid

CHID: 22436 CASRN: 126-00-1

SPID(S): TP0001562G04

M4ID: 18128422

HILL MODEL: Not applicable.

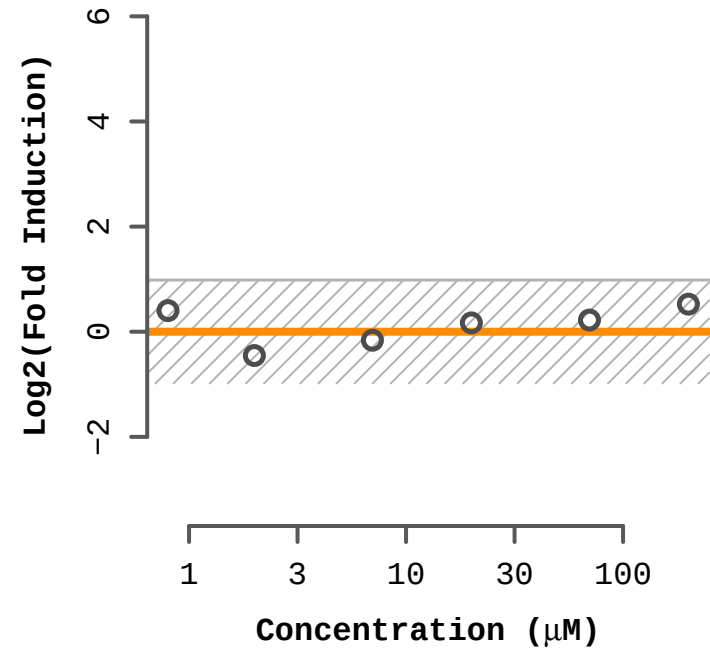
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 5.75 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.33 | NA   | NA   |

MAX\_MEAN: 0.237 MAX\_MED: 0.237 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 2,2'-Bisphenol F

CHID: 22446 CASRN: 2467-02-9

SPID(S): TP0001562G06

M4ID: 18128420

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

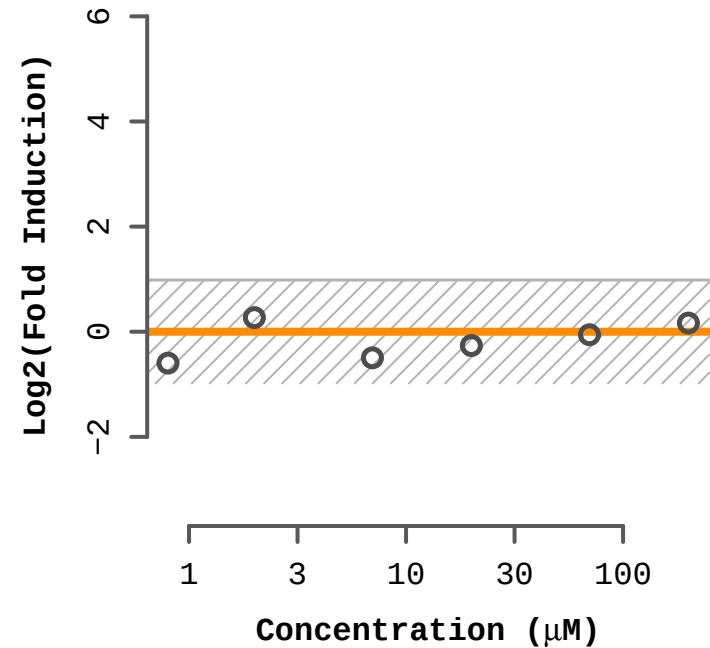
|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 7.58 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.35 | NA   | NA   |

MAX\_MEAN: 0.525 MAX\_MED: 0.525 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: E-Cinnamic acid

CHID: 22489 CASRN: 140-10-3

SPID(S): TP0001562F02

M4ID: 18128435

HILL MODEL: Not applicable.

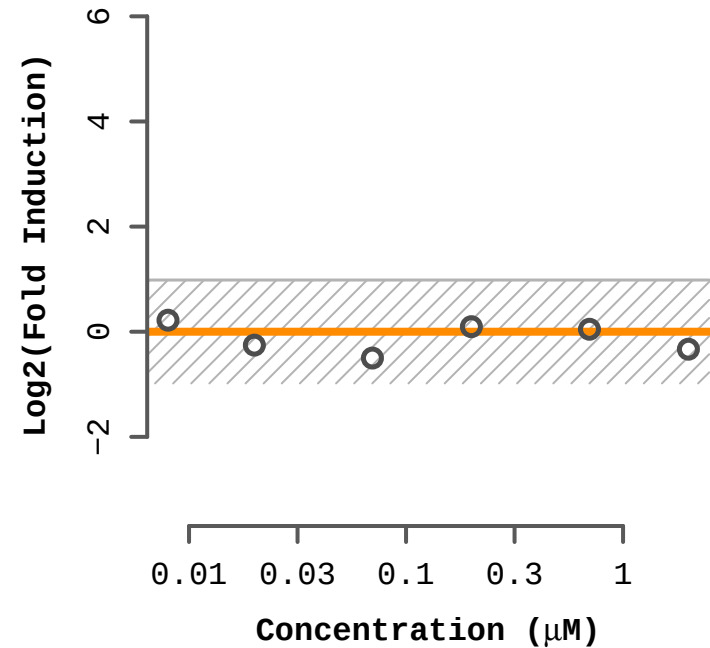
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 7.52 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.36 | NA   | NA   |

MAX\_MEAN: 0.269 MAX\_MED: 0.269 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-Dodecylphenol

CHID: 22508 CASRN: 104-43-8

SPID(S): TP0001562C12

M4ID: 18128458

HILL MODEL: Not applicable.

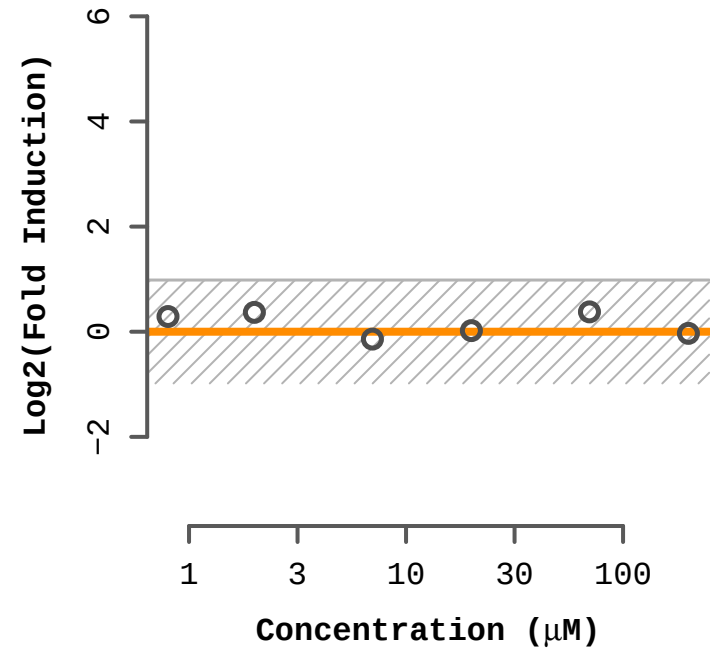
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 4.7  | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.28 | NA   | NA   |

MAX\_MEAN: 0.22 MAX\_MED: 0.22 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 3,3'-Dimethylbenzidine

CHID: 24059 CASRN: 119-93-7

SPID(S): TP0001562E07

M4ID: 18128441

HILL MODEL: Not applicable.

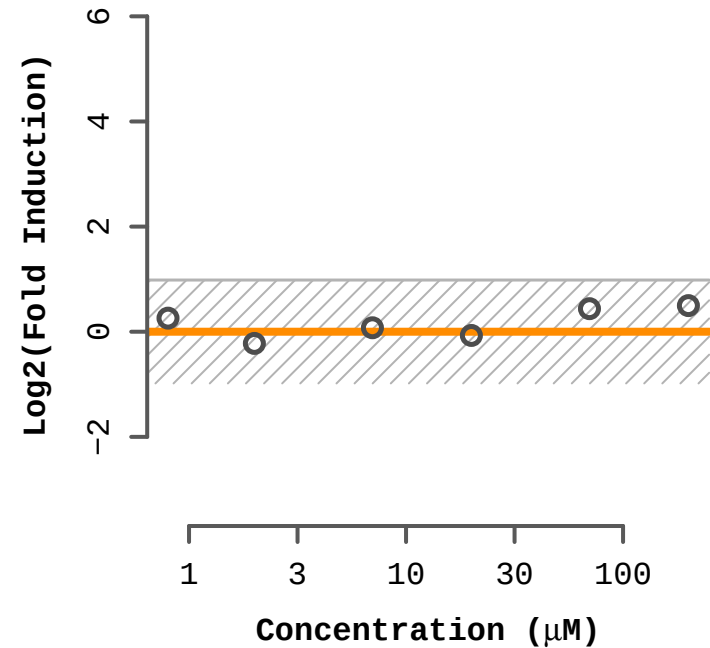
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 3.35 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.25 | NA   | NA   |

MAX\_MEAN: 0.378 MAX\_MED: 0.378 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Fenamiphos

CHID: 24102 CASRN: 22224-92-6

SPID(S): TP0001562B07

M4ID: 18128474

HILL MODEL: Not applicable.

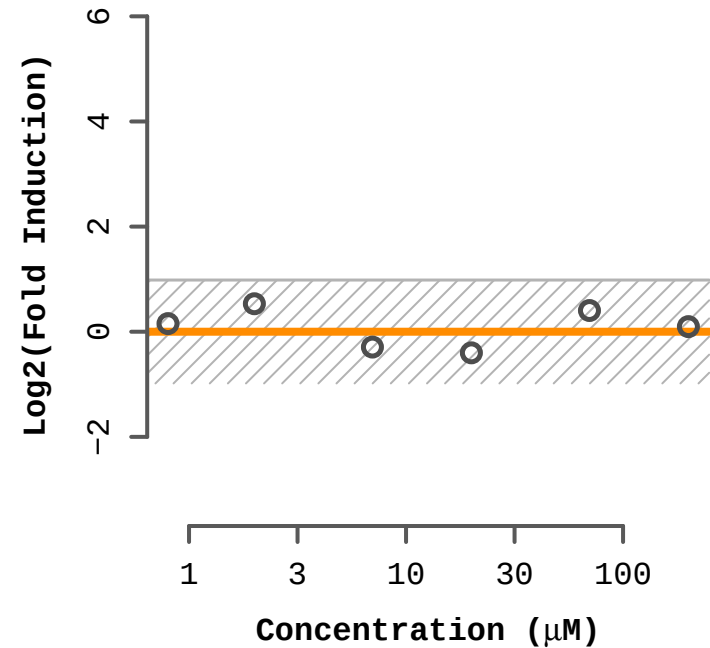
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>5.67</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.31</b> | NA   | NA   |

MAX\_MEAN: 0.498 MAX\_MED: 0.498 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Fluoranthene

CHID: 24104 CASRN: 206-44-0

SPID(S): TP0001562C08

M4ID: 18128462

HILL MODEL: Not applicable.

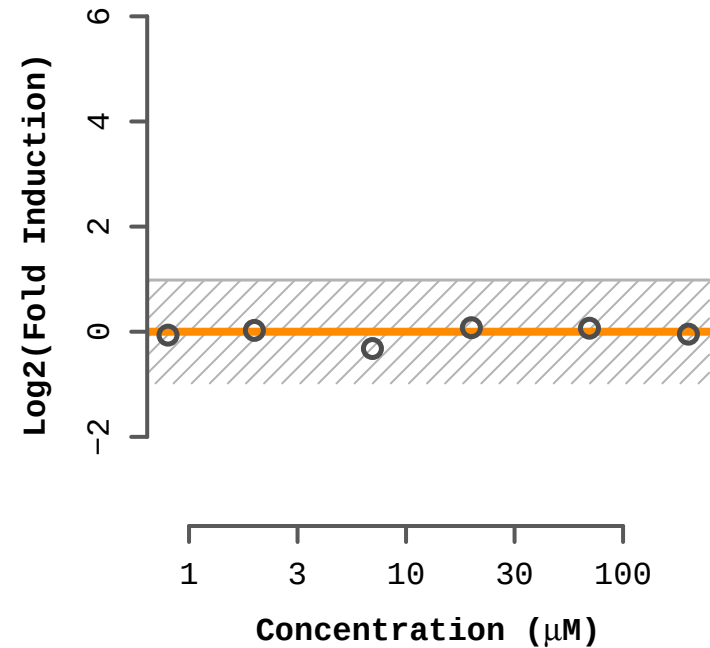
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>7.41</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.35</b> | NA   | NA   |

MAX\_MEAN: 0.533 MAX\_MED: 0.533 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Pendimethalin

CHID: 24245 CASRN: 40487-42-1

SPID(S): TP0001562F08

M4ID: 18128429

HILL MODEL: Not applicable.

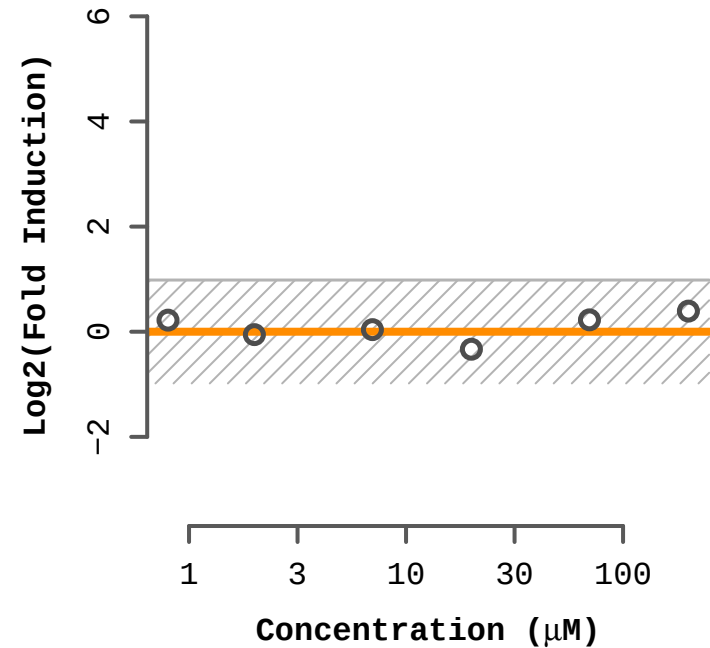
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>-5.51</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.14</b>  | NA   | NA   |

MAX\_MEAN: 0.0778 MAX\_MED: 0.0778 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Phenanthrene

CHID: 24254 CASRN: 85-01-8

SPID(S): TP0001562F09

M4ID: 18128428

HILL MODEL: Not applicable.

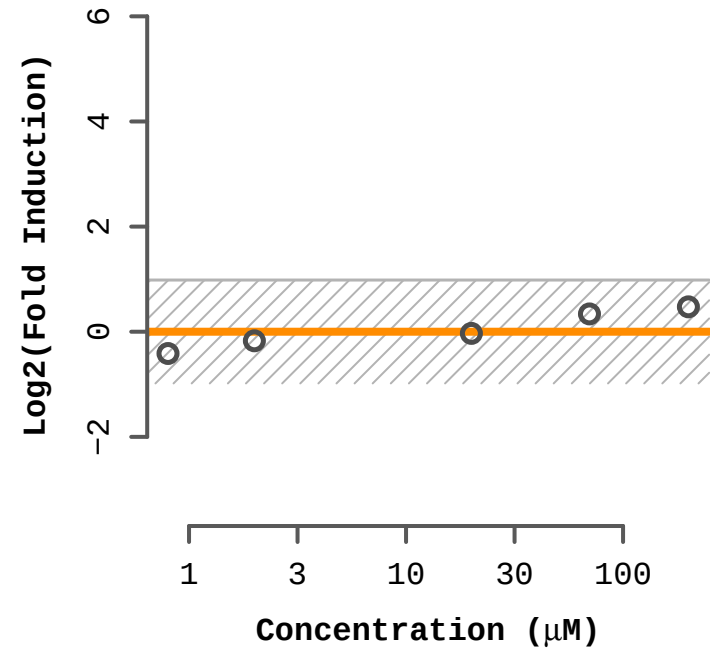
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>3.21</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.25</b> | NA   | NA   |

MAX\_MEAN: 0.393 MAX\_MED: 0.393 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Pyrene

CHID: 24289 CASRN: 129-00-0

SPID(S): TP0001562F07

M4ID: 18128430

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

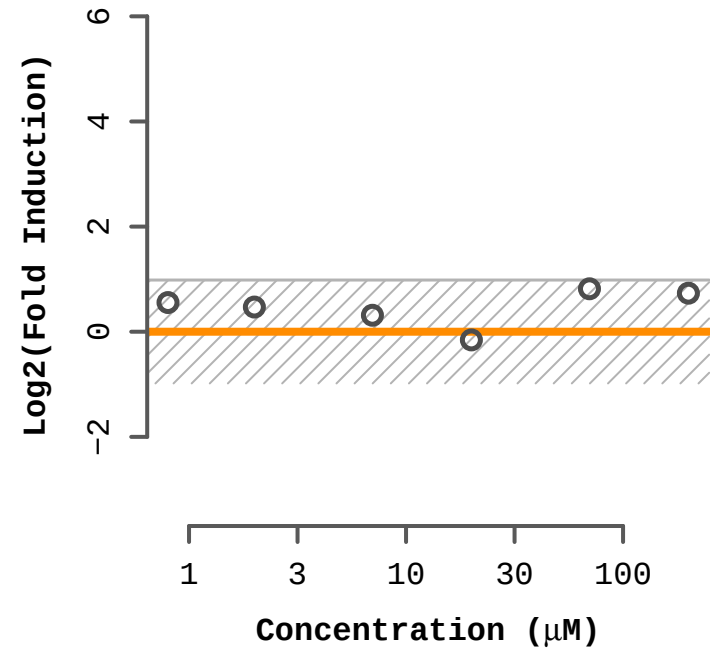
|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>5.93</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.33</b> | NA   | NA   |

MAX\_MEAN: 0.474 MAX\_MED: 0.474 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4,4'-Dichlorodiphenyl sulfone

CHID: 24986 CASRN: 80-07-9

SPID(S): TP0001562A02

M4ID: 18128490

HILL MODEL: Not applicable.

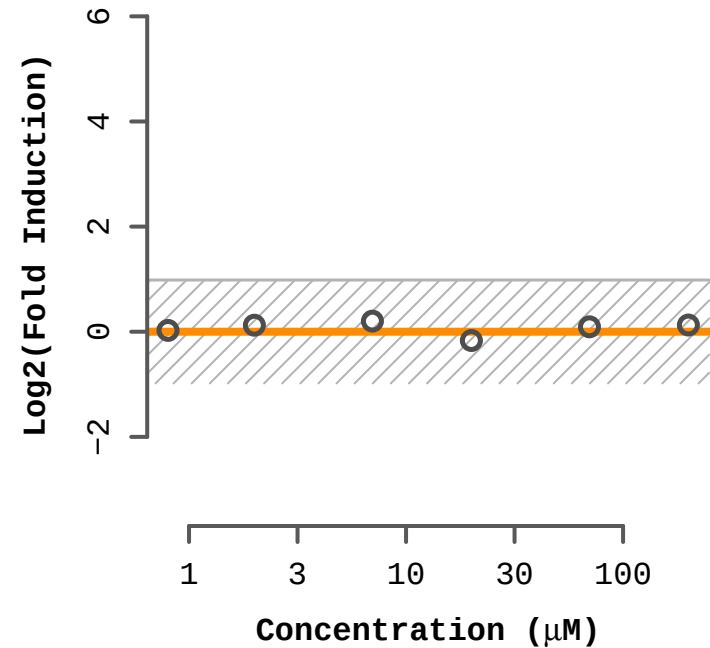
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>13.08</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.56</b>  | NA   | NA   |

MAX\_MEAN: 0.818 MAX\_MED: 0.818 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Tris(2-ethylhexyl) trimellitate

CHID: 26265 CASRN: 3319-31-1

SPID(S): TP0001562B09

M4ID: 18128472

HILL MODEL: Not applicable.

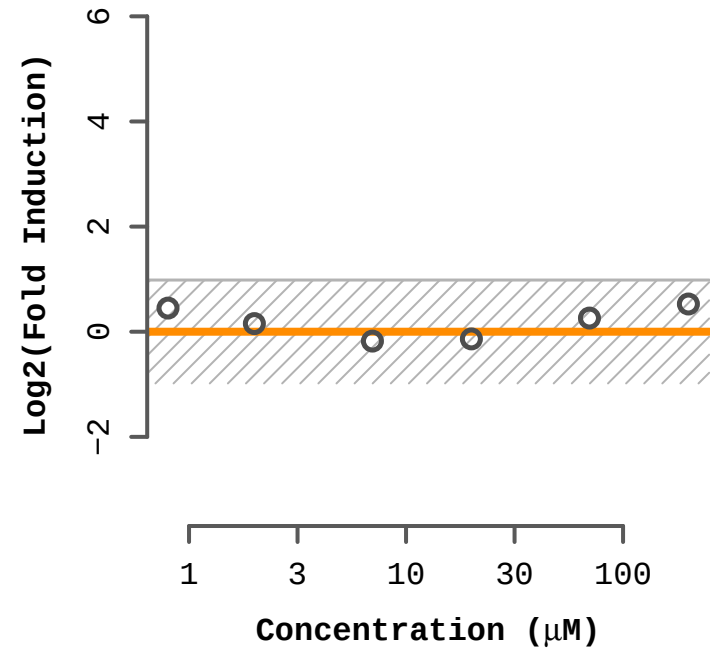
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>-3.83</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.14</b>  | NA   | NA   |

MAX\_MEAN: 0.203 MAX\_MED: 0.203 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Triphenylborane

CHID: 27345 CASRN: 960-71-4

SPID(S): TP0001562H03

M4ID: 18128412

HILL MODEL: Not applicable.

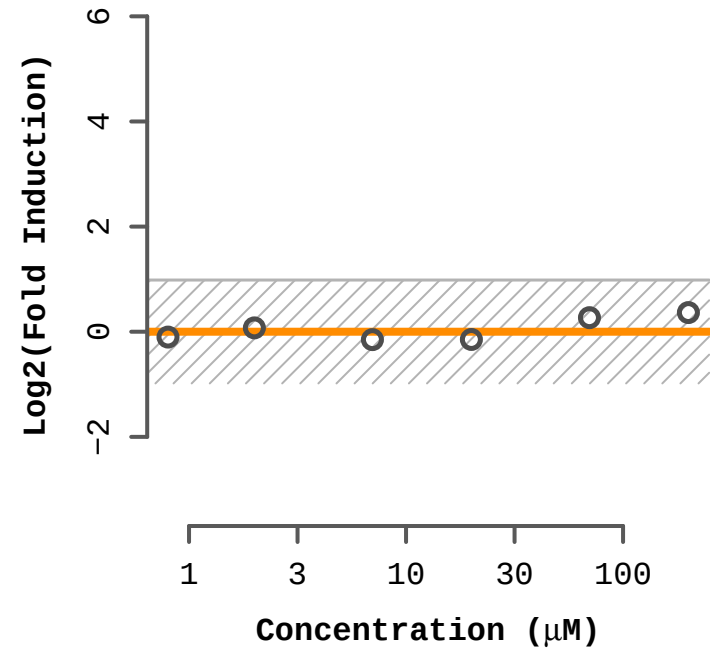
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 6.28 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.32 | NA   | NA   |

MAX\_MEAN: 0.528 MAX\_MED: 0.528 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 3-Phenoxybenzenemethanol

CHID: 27756 CASRN: 13826-35-2

SPID(S): TP0001562D02

M4ID: 18128457

HILL MODEL: Not applicable.

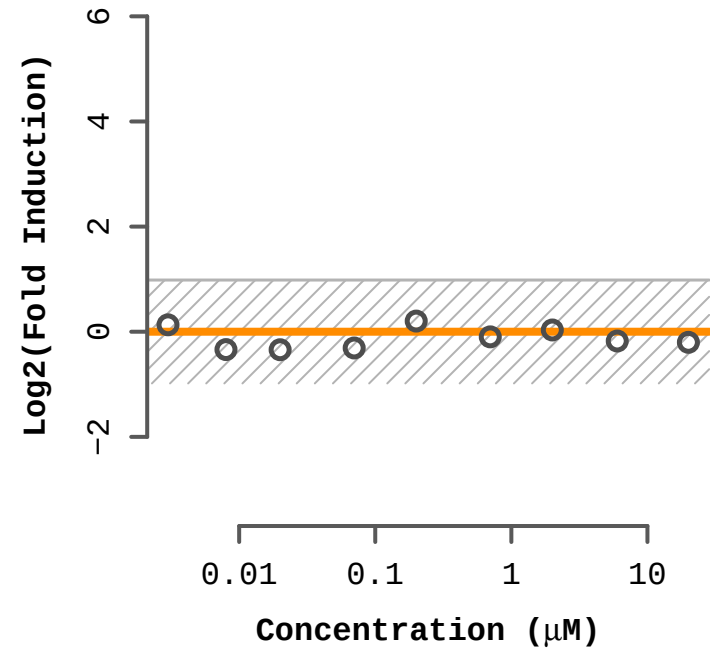
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 1.07 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.21 | NA   | NA   |

MAX\_MEAN: 0.365 MAX\_MED: 0.365 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Dodecylphenol

CHID: 27926 CASRN: 27193-86-8

SPID(S): TP0001564A02

M4ID: 18128402

HILL MODEL: Not applicable.

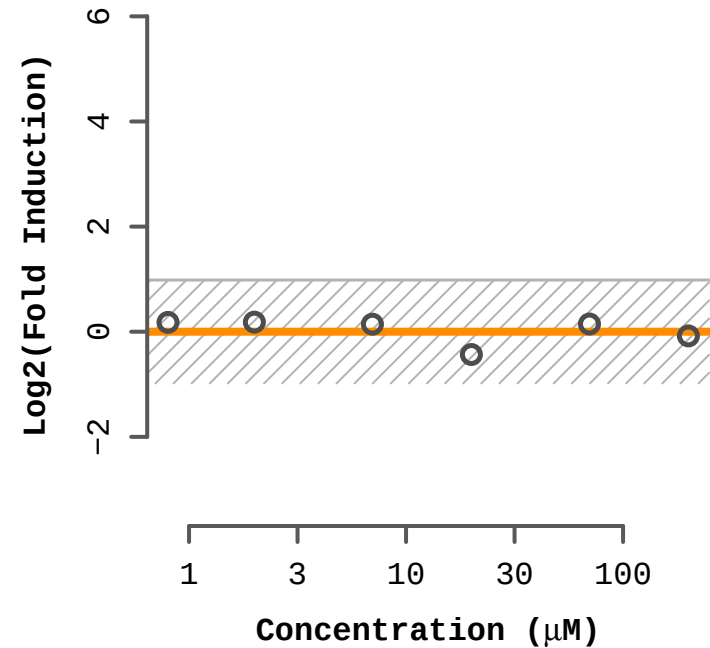
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 2.43 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.23 | NA   | NA   |

MAX\_MEAN: 0.203 MAX\_MED: 0.203 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 1-(Bromomethyl)-3-phenoxybenzene

CHID: 28022 CASRN: 51632-16-7

SPID(S): TP0001562F05

M4ID: 18128432

HILL MODEL: Not applicable.

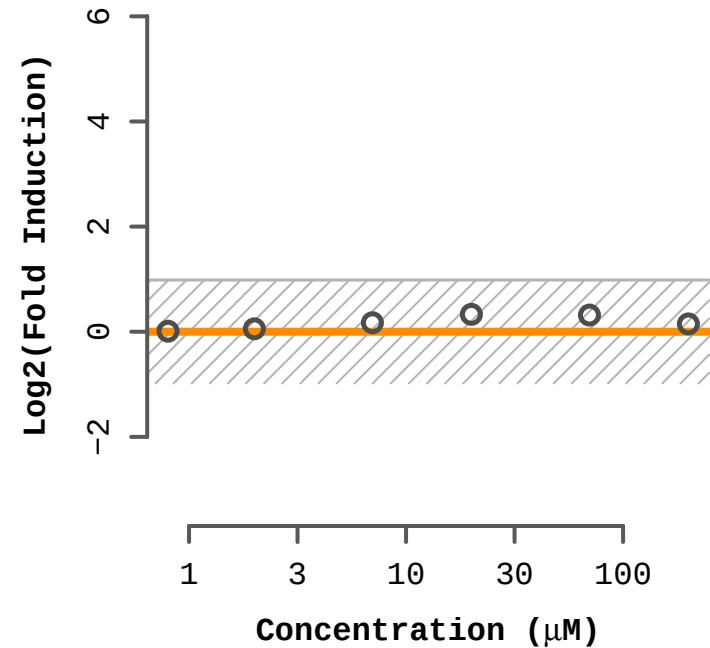
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 1.62 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.22 | NA   | NA   |

MAX\_MEAN: 0.183 MAX\_MED: 0.183 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Triisopropylated phenyl phosphate

CHID: 28880 CASRN: 68937-41-7

SPID(S): TP0001562D04

M4ID: 18128455

HILL MODEL: Not applicable.

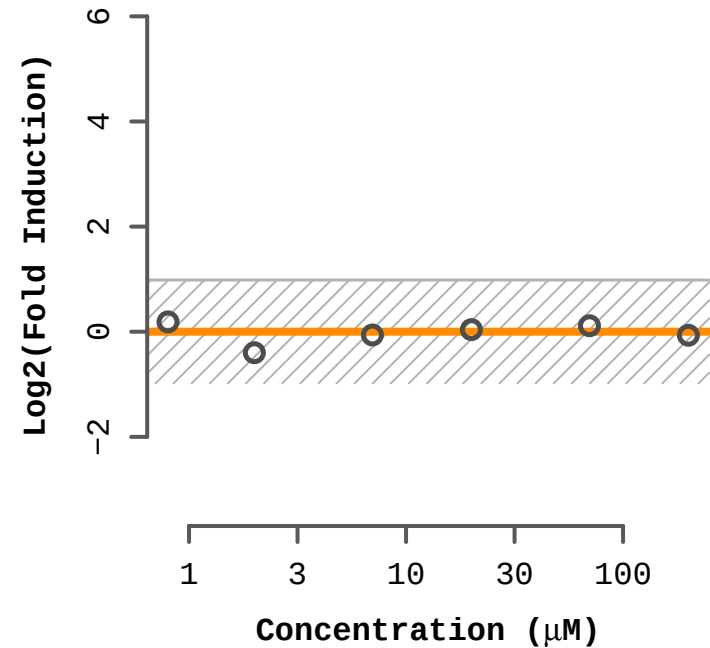
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>1.07</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.21</b> | NA   | NA   |

MAX\_MEAN: 0.331 MAX\_MED: 0.331 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-Methylpent-3-en-2-one

CHID: 29170 CASRN: 141-79-7

SPID(S): TP0001562H02

M4ID: 18128413

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

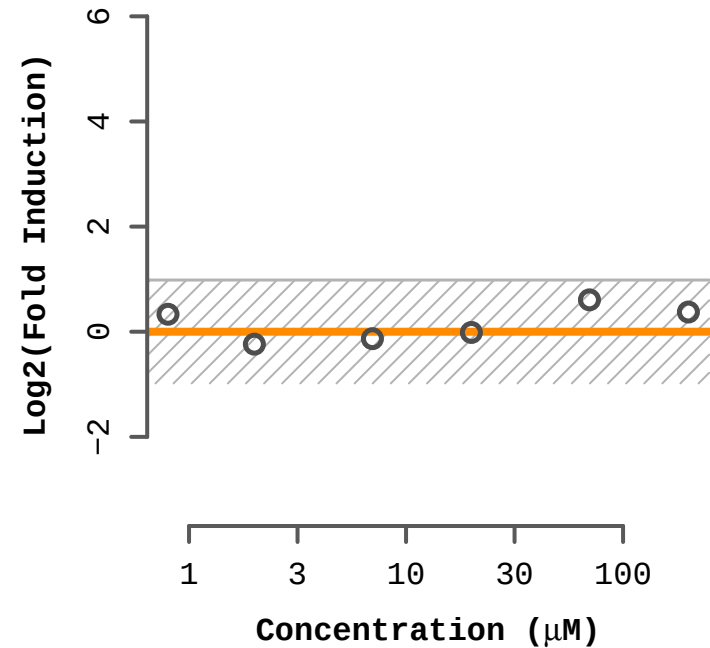
|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>-1.06</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.19</b>  | NA   | NA   |

MAX\_MEAN: 0.187 MAX\_MED: 0.187 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Triethylene glycol dibenzoate

CHID: 29611 CASRN: 120-56-9

SPID(S): TP0001562D06

M4ID: 18128453

HILL MODEL: Not applicable.

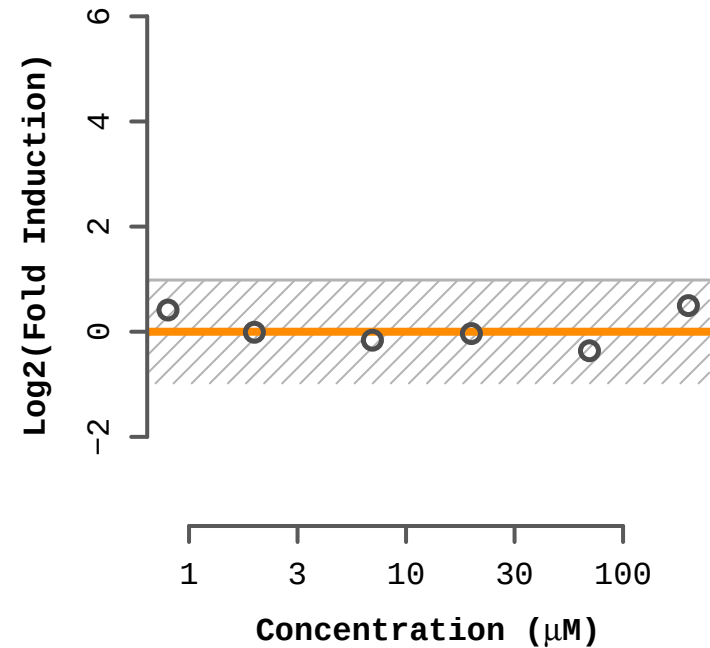
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>6.8</b>  | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.34</b> | NA   | NA   |

MAX\_MEAN: 0.607 MAX\_MED: 0.607 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Tebuconazole

CHID: 32113 CASRN: 107534-96-3

SPID(S): TP0001562G11

M4ID: 18128415

HILL MODEL: Not applicable.

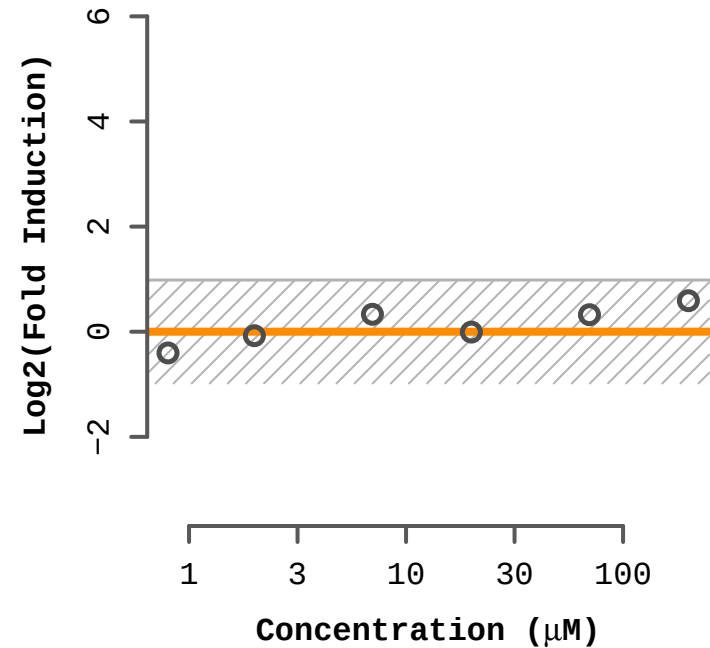
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 5.73 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.31 | NA   | NA   |

MAX\_MEAN: 0.498 MAX\_MED: 0.498 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-Chloro-3,5-dimethylphenol

CHID: 32316 CASRN: 88-04-0

SPID(S): TP0001562A08

M4ID: 18128484

HILL MODEL: Not applicable.

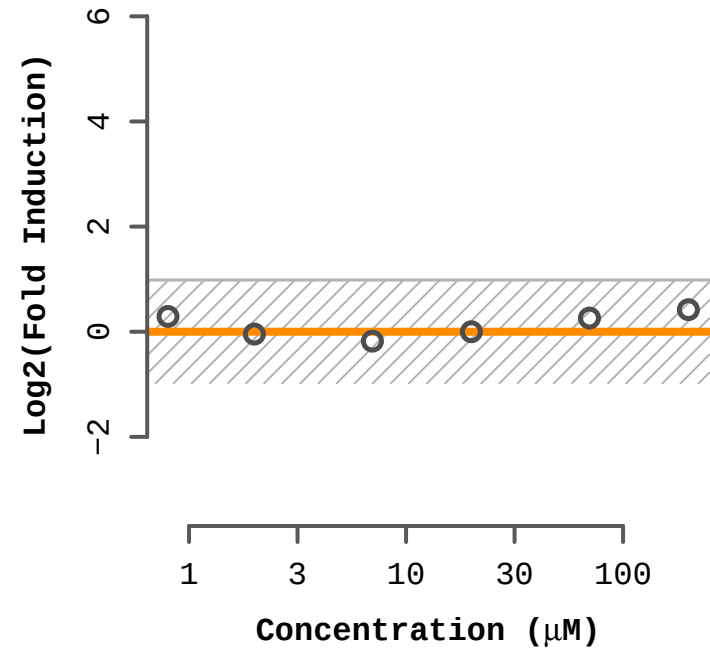
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>7.25</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.35</b> | NA   | NA   |

MAX\_MEAN: 0.591 MAX\_MED: 0.591 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Ethalfluralin

CHID: 32386 CASRN: 55283-68-6

SPID(S): TP0001562C11

M4ID: 18128459

HILL MODEL: Not applicable.

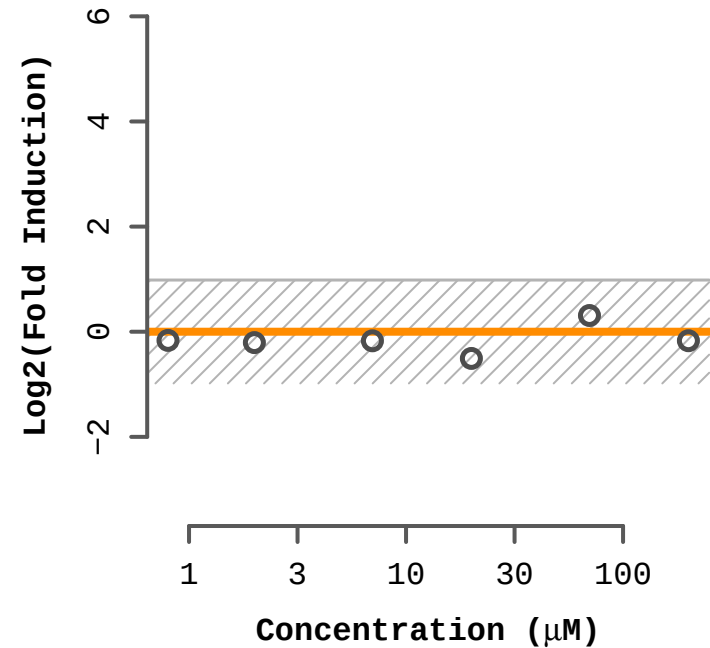
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>2.98</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.25</b> | NA   | NA   |

MAX\_MEAN: 0.421 MAX\_MED: 0.421 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Acibenzolar-S-methyl

CHID: 32519 CASRN: 135158-54-2

SPID(S): TP0001562F10

M4ID: 18128427

HILL MODEL: Not applicable.

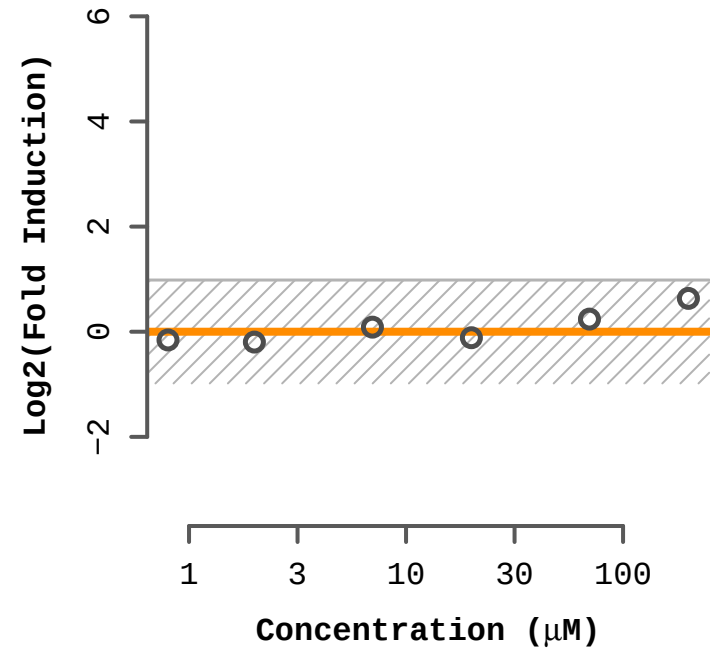
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 4.8  | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.28 | NA   | NA   |

MAX\_MEAN: 0.309 MAX\_MED: 0.309 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Bromuconazole

CHID: 32531 CASRN: 116255-48-2

SPID(S): TP0001562H06

M4ID: 18128409

HILL MODEL: Not applicable.

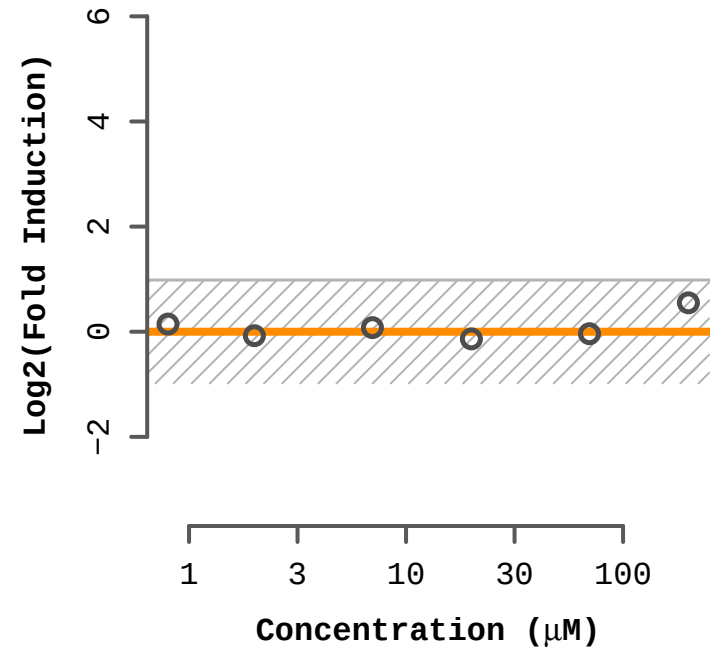
GAIN-LOSS MODEL: Not applicable.

|       |      |      |      |
|-------|------|------|------|
|       | CNST | HILL | GNLS |
| AIC:  | 4.53 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.3  | NA   | NA   |

MAX\_MEAN: 0.635 MAX\_MED: 0.635 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Procymidone

CHID: 33923 CASRN: 32809-16-8

SPID(S): TP0001562F11

M4ID: 18128426

HILL MODEL: Not applicable.

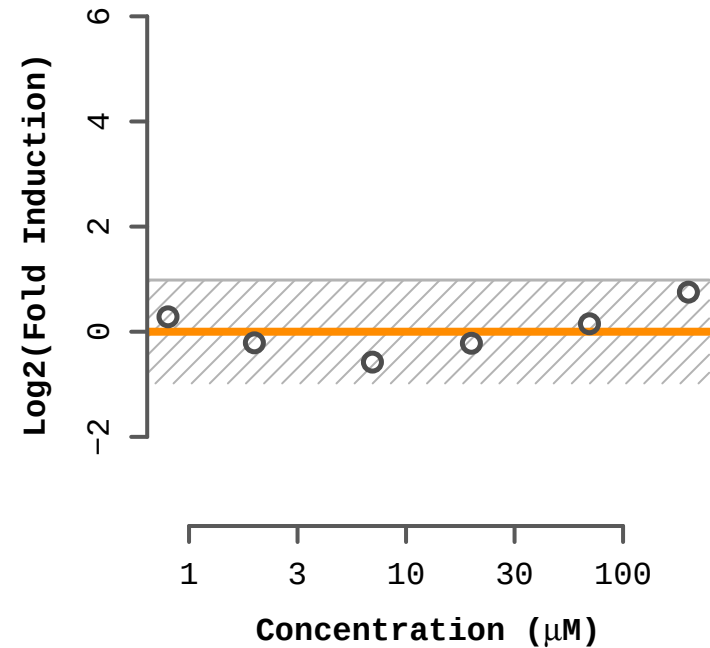
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>1.06</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.24</b> | NA   | NA   |

MAX\_MEAN: 0.551      MAX\_MED: 0.551      BMAD: 0.328

COFF: 0.984    HIT-CALL: 0      FITC: 4      ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Nilutamide

CHID: 34165 CASRN: 63612-50-0

SPID(S): TP0001562D10

M4ID: 18128449

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

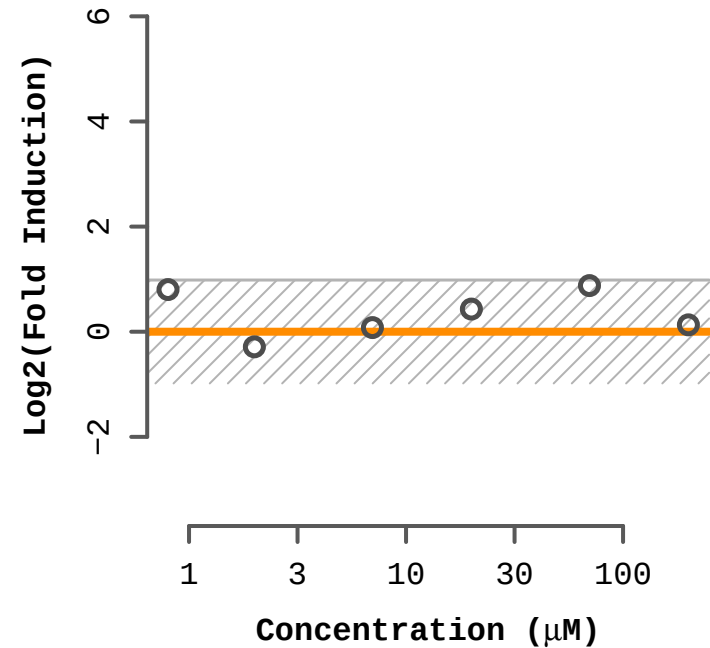
|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 9.48 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.43 | NA   | NA   |

MAX\_MEAN: 0.754 MAX\_MED: 0.754 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Phoxim

CHID: 34324 CASRN: 14816-18-3

SPID(S): TP0001562B03

M4ID: 18128478

HILL MODEL: Not applicable.

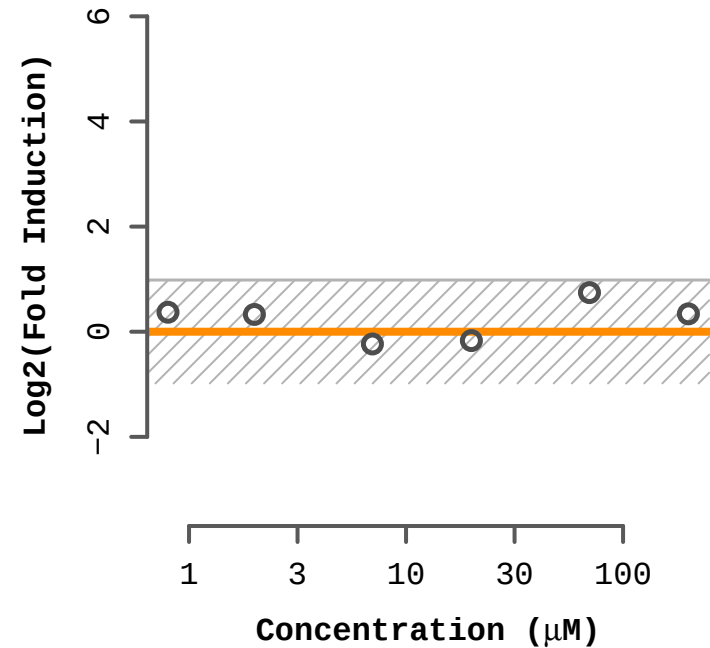
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>12.12</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.53</b>  | NA   | NA   |

MAX\_MEAN: 0.878 MAX\_MED: 0.878 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Dimethomorph

CHID: 34545 CASRN: 110488-70-5

SPID(S): TP0001562C07

M4ID: 18128463

HILL MODEL: Not applicable.

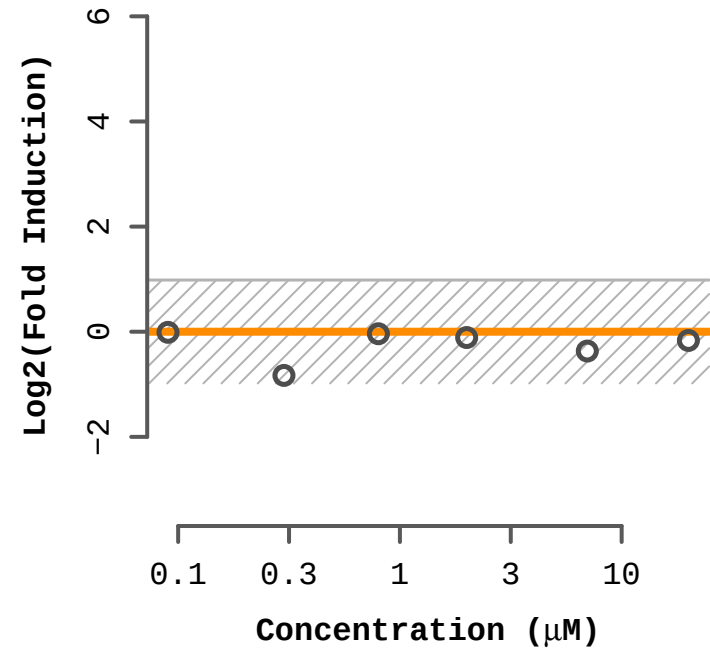
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 9.05 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.41 | NA   | NA   |

MAX\_MEAN: 0.745 MAX\_MED: 0.745 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Ipconazole

CHID: 34674 CASRN: 125225-28-7

SPID(S): TP0001562E02

M4ID: 18128446

HILL MODEL: Not applicable.

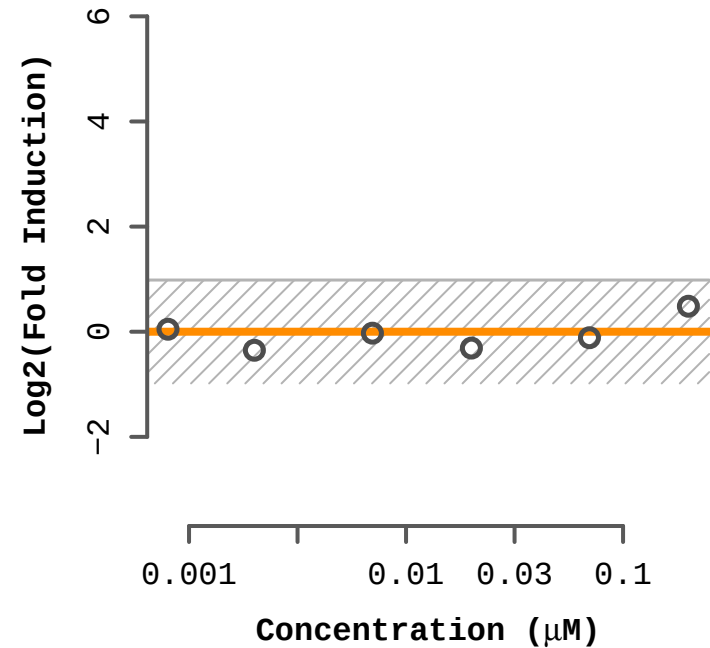
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>6.69</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.38</b> | NA   | NA   |

MAX\_MEAN: -0.0107 MAX\_MED: -0.0107 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Testosterone propionate

CHID: 36515 CASRN: 57-85-2

SPID(S): TP0001562B12

M4ID: 18128469

HILL MODEL: Not applicable.

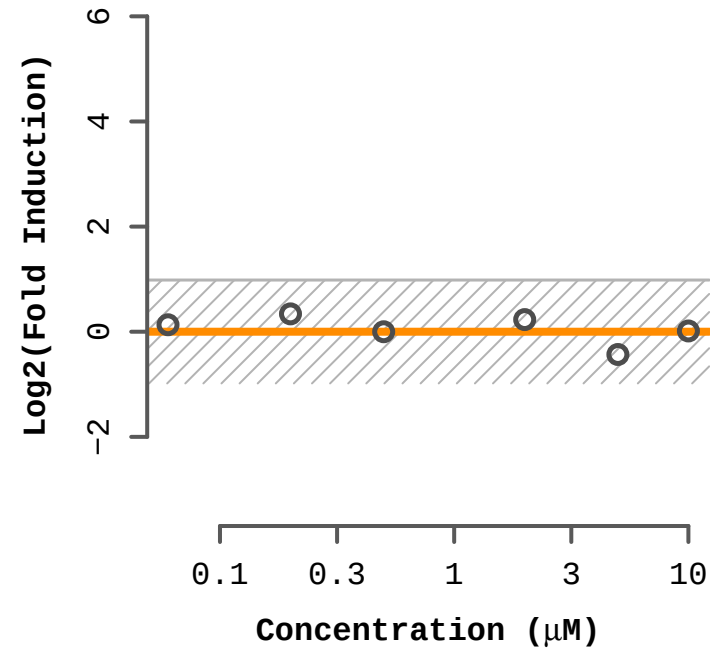
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 4.4  | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.28 | NA   | NA   |

MAX\_MEAN: 0.485      MAX\_MED: 0.485      BMAD: 0.328

COFF: 0.984    HIT-CALL: 0    FITC: 4    ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-Hydroxytamoxifen

CHID: 37094 CASRN: 68392-35-8

SPID(S): TP0001562C09

M4ID: 18128461

HILL MODEL: Not applicable.

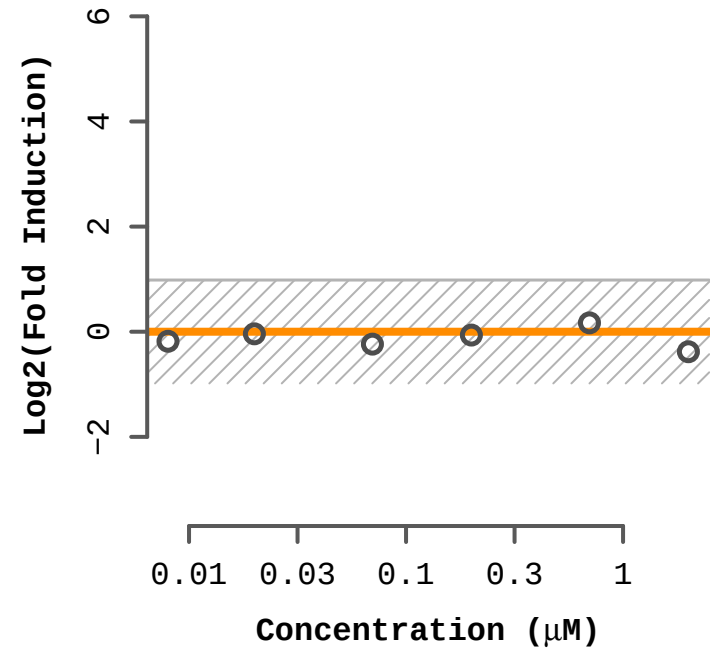
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 2.99 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.25 | NA   | NA   |

MAX\_MEAN: 0.34 MAX\_MED: 0.34 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4,4',4''-Ethane-1,1,1-triyltriphenol

CHID: 37712 CASRN: 27955-94-8

SPID(S): TP0001562D12

M4ID: 18128447

HILL MODEL: Not applicable.

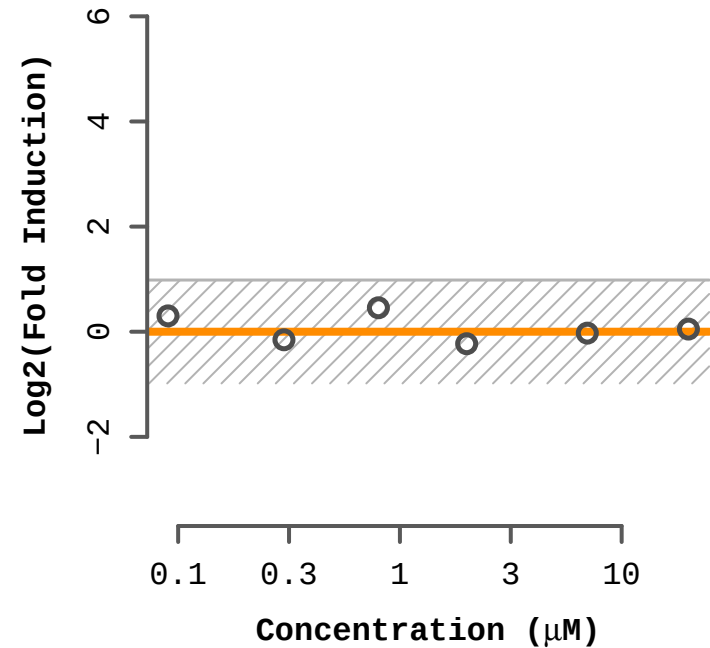
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>1.05</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.21</b> | NA   | NA   |

MAX\_MEAN: 0.169 MAX\_MED: 0.169 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 1-Hydroxypyrene

CHID: 38298 CASRN: 5315-79-7

SPID(S): TP0001562E10

M4ID: 18128438

HILL MODEL: Not applicable.

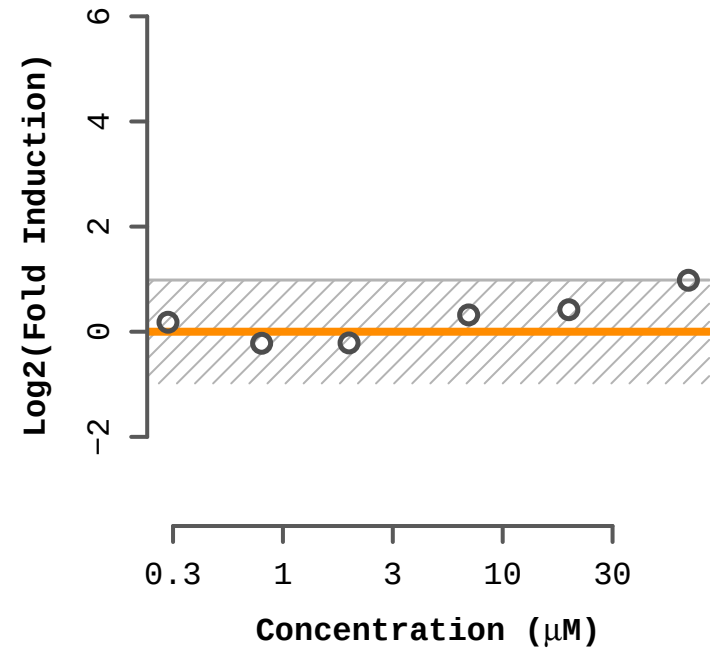
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>3.02</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.25</b> | NA   | NA   |

MAX\_MEAN: 0.457 MAX\_MED: 0.457 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Diniconazole

CHID: 40363 CASRN: 83657-24-3

SPID(S): TP0001562A11

M4ID: 18128481

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

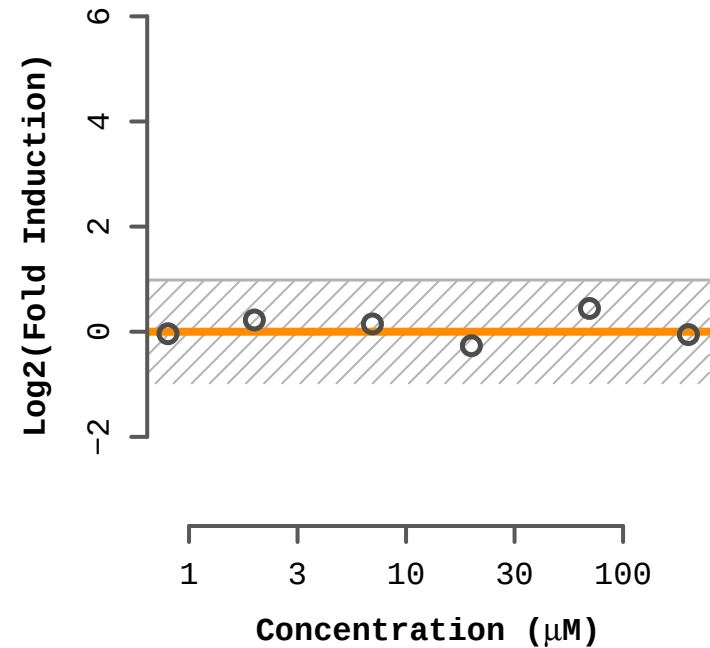
|       | CNST  | HILL | GNLS |
|-------|-------|------|------|
| AIC:  | 10.25 | NA   | NA   |
| PROB: | 1     | NA   | NA   |
| RMSE: | 0.48  | NA   | NA   |

MAX\_MEAN: 0.979 MAX\_MED: 0.979 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 17alpha-Hydroxyprogesterone

CHID: 40747 CASRN: 68-96-2

SPID(S): TP0001562B11

M4ID: 18128470

HILL MODEL: Not applicable.

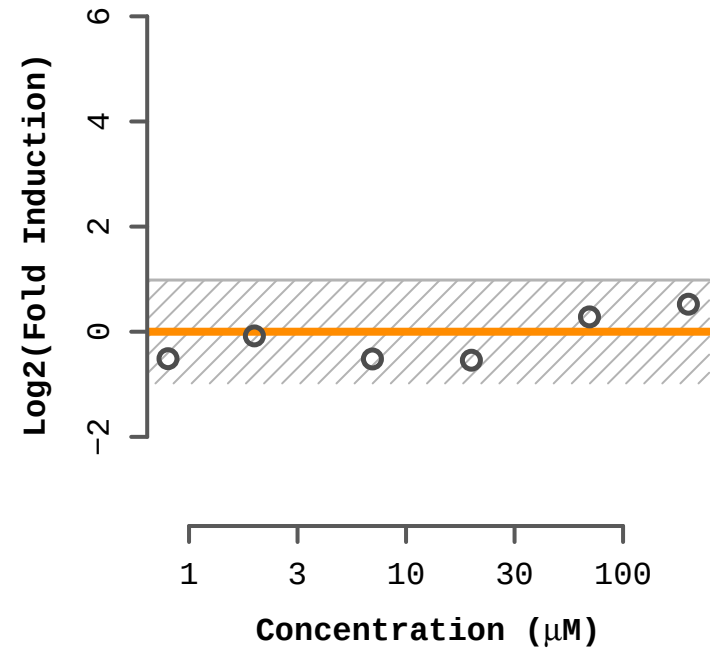
GAIN-LOSS MODEL: Not applicable.

|       |      |      |      |
|-------|------|------|------|
|       | CNST | HILL | GNLS |
| AIC:  | 2.43 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.24 | NA   | NA   |

MAX\_MEAN: 0.443 MAX\_MED: 0.443 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 7-(Dimethylamino)-4-methylcoumarin

CHID: 41422 CASRN: 87-01-4

SPID(S): TP0001562E03

M4ID: 18128445

HILL MODEL: Not applicable.

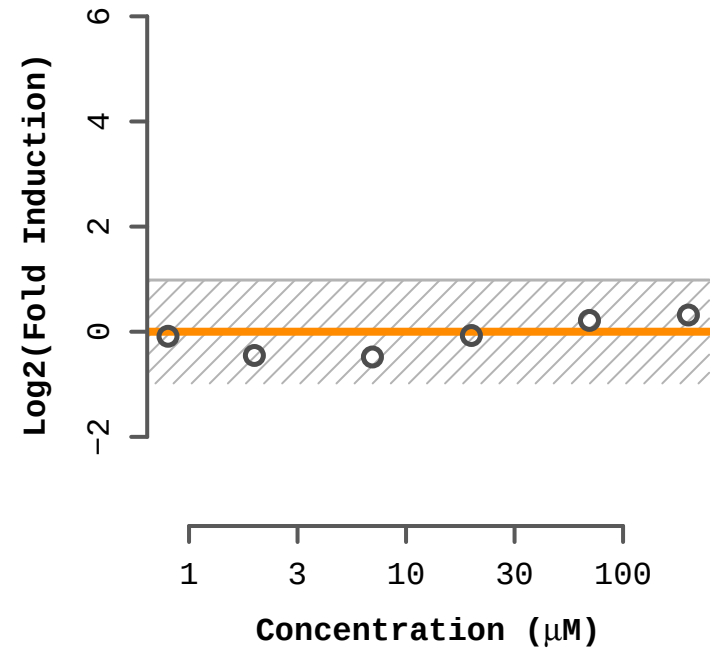
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>10.51</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.44</b>  | NA   | NA   |

MAX\_MEAN: 0.524 MAX\_MED: 0.524 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Diphenyl phosphite

CHID: 41889 CASRN: 4712-55-4

SPID(S): TP0001562F06

M4ID: 18128431

HILL MODEL: Not applicable.

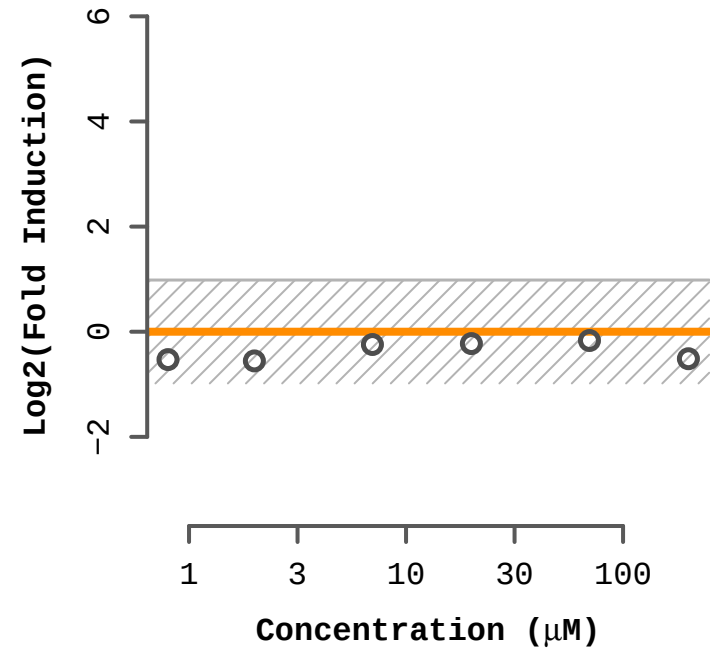
GAIN-LOSS MODEL: Not applicable.

|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 6.04 | NA   | NA   |
| PROB: | 1    | NA   | NA   |
| RMSE: | 0.31 | NA   | NA   |

MAX\_MEAN: 0.318 MAX\_MED: 0.318 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Hydroxyprogesterone caproate

CHID: 43915 CASRN: 630-56-8

SPID(S): TP0001562E05

M4ID: 18128443

HILL MODEL: Not applicable.

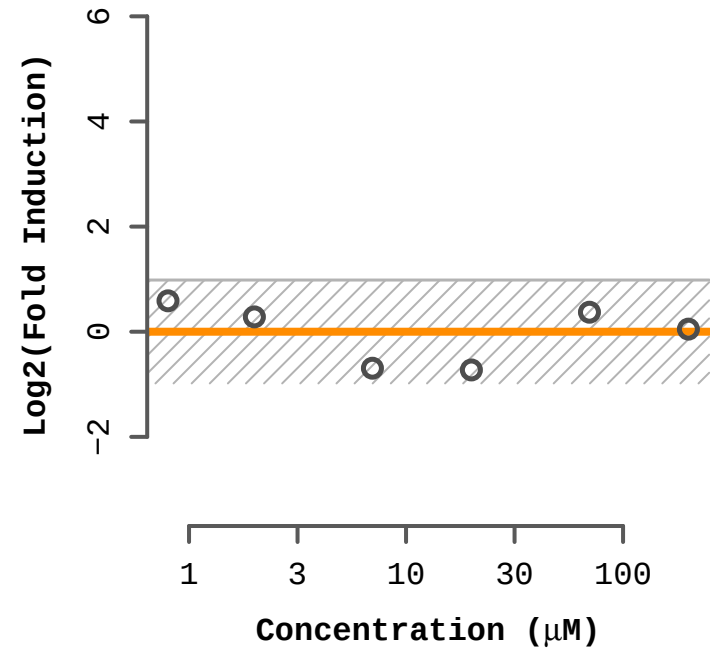
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>9.29</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.41</b> | NA   | NA   |

MAX\_MEAN: -0.167 MAX\_MED: -0.167 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-Butylphenol

CHID: 47425 CASRN: 1638-22-8

SPID(S): TP0001562C04

M4ID: 18128466

HILL MODEL: Not applicable.

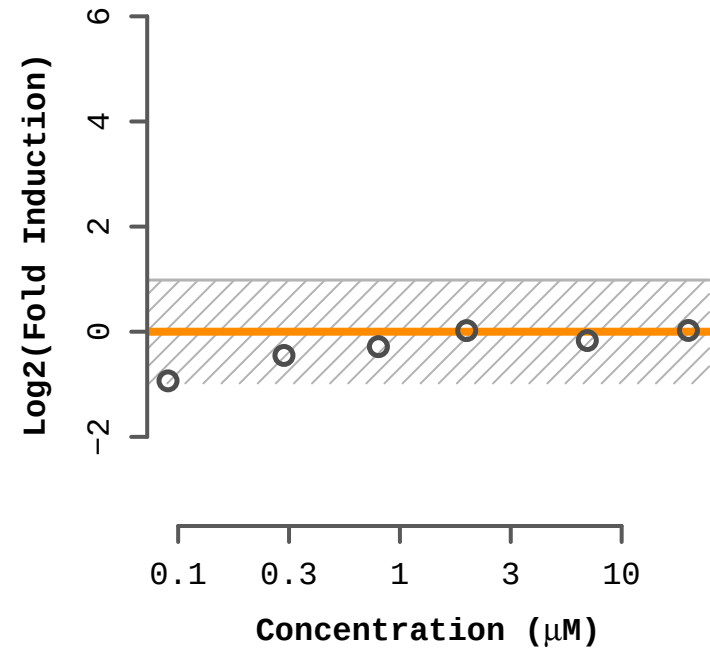
GAIN-LOSS MODEL: Not applicable.

|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>12.05</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.51</b>  | NA   | NA   |

MAX\_MEAN: 0.588 MAX\_MED: 0.588 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Octylparaben

CHID: 47957 CASRN: 1219-38-1

SPID(S): TP0001562H04

M4ID: 18128411

HILL MODEL: Not applicable.

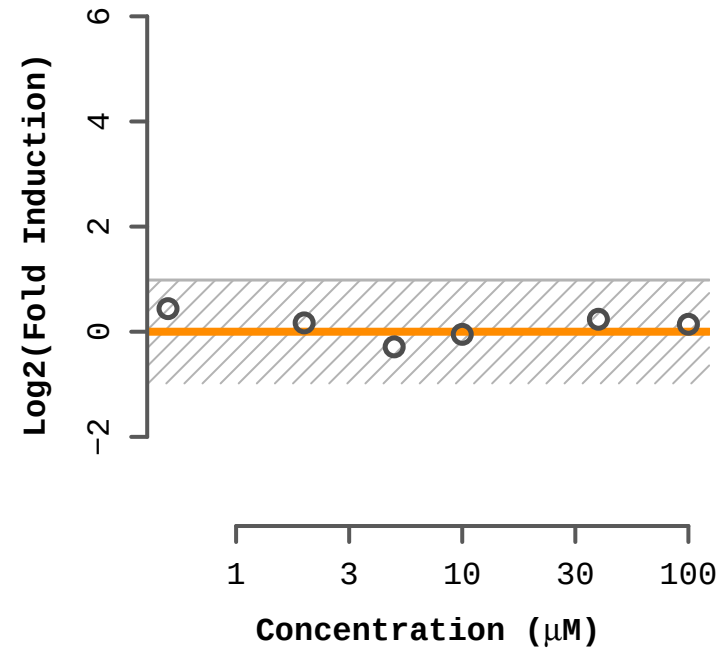
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>9.05</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.44</b> | NA   | NA   |

MAX\_MEAN: 0.0246 MAX\_MED: 0.0246 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Melengestrol acetate

CHID: 48184 CASRN: 2919-66-6

SPID(S): TP0001562B04

M4ID: 18128477

HILL MODEL: Not applicable.

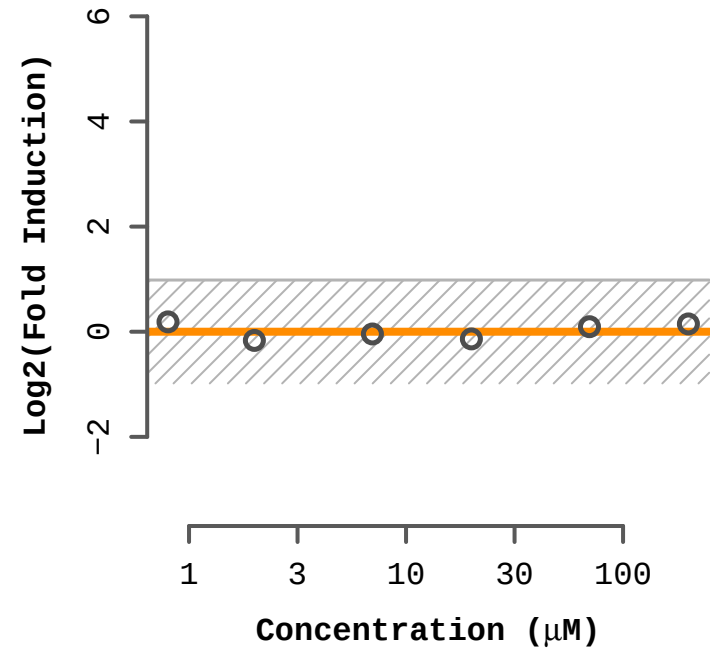
GAIN-LOSS MODEL: Not applicable.

|       |             |      |      |
|-------|-------------|------|------|
|       | <b>CNST</b> | HILL | GNLS |
| AIC:  | <b>3.36</b> | NA   | NA   |
| PROB: | <b>1</b>    | NA   | NA   |
| RMSE: | <b>0.25</b> | NA   | NA   |

MAX\_MEAN: 0.44 MAX\_MED: 0.44 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 4-tert-Butylbenzenethiol

CHID: 48196 CASRN: 2396-68-1

SPID(S): TP0001562G03

M4ID: 18128423

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

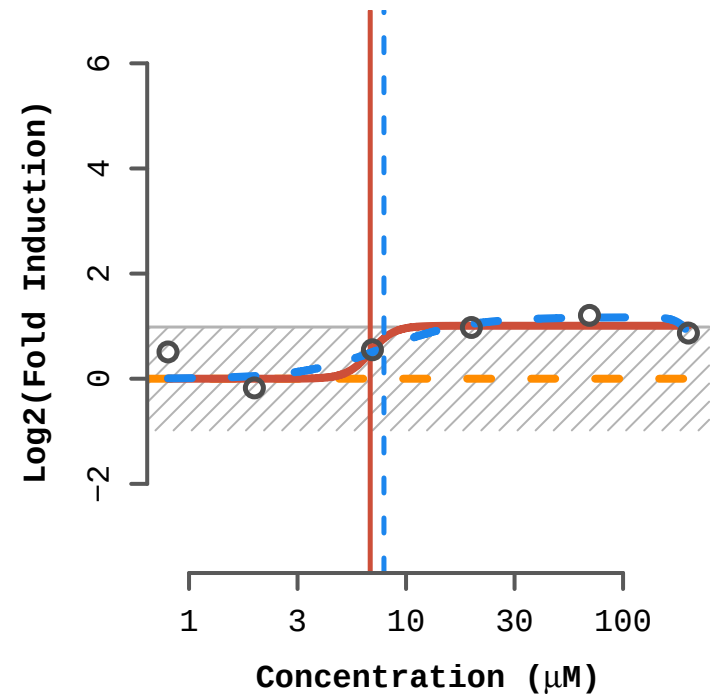
|       |              |      |      |
|-------|--------------|------|------|
|       | <b>CNST</b>  | HILL | GNLS |
| AIC:  | <b>-3.51</b> | NA   | NA   |
| PROB: | <b>1</b>     | NA   | NA   |
| RMSE: | <b>0.14</b>  | NA   | NA   |

MAX\_MEAN: 0.188 MAX\_MED: 0.188 BMAD: 0.328

COFF: 0.984 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Chrysin

CHID: 22396 CASRN: 480-40-0

SPID(S): TP0001562F03

M4ID: 18128434

HILL MODEL (in red):

|      | tp    | ga     | gw   |
|------|-------|--------|------|
| val: | 1.01  | 0.835  | 8    |
| sd:  | 0.115 | 0.0952 | 69.6 |

GAIN-LOSS MODEL (in blue):

|      | tp    | ga    | gw   | la     | lw   |
|------|-------|-------|------|--------|------|
| val: | 1.17  | 0.898 | 2.25 | 2.34   | 12   |
| sd:  | 0.198 | 0.155 | 1.81 | 0.0302 | 10.8 |

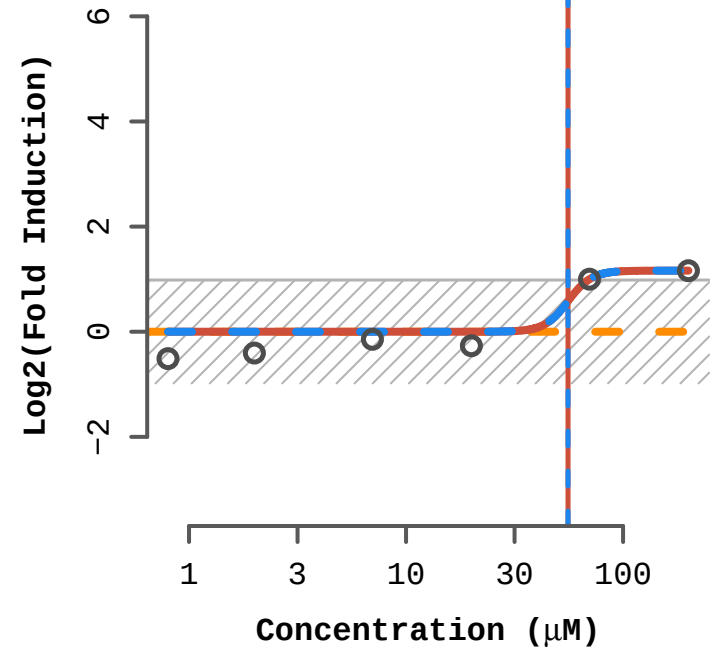
|       | CNST  | HILL | GNLS  |
|-------|-------|------|-------|
| AIC:  | 17.27 | 7.81 | 10.39 |
| PROB: | 0.01  | 0.78 | 0.21  |
| RMSE: | 0.79  | 0.24 | 0.23  |

MAX\_MEAN: 1.21 MAX\_MED: 1.21 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 37 ACTP: 0.99

FLAGS:

7; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Bicalutamide

CHID: 22678 CASRN: 90357-06-5

SPID(S): TP0001562B05

M4ID: 18128476

HILL MODEL (in red):

|      |       |       |      |
|------|-------|-------|------|
|      | tp    | ga    | gw   |
| val: | 1.16  | 1.75  | 8    |
| sd:  | 0.224 | 0.305 | 23.4 |

GAIN-LOSS MODEL (in blue):

|      |      |      |    |     |      |
|------|------|------|----|-----|------|
|      | tp   | ga   | gw | la  | lw   |
| val: | 1.16 | 1.75 | 8  | 4.3 | 13.3 |
| sd:  | NA   | NA   | NA | NA  | NA   |

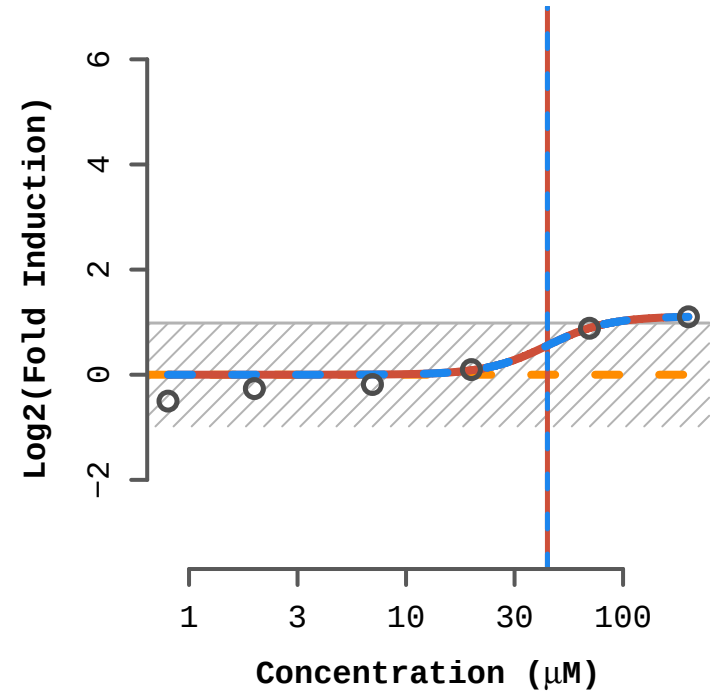
|       |       |       |       |
|-------|-------|-------|-------|
|       | CNST  | HILL  | GNLS  |
| AIC:  | 15.27 | 10.87 | 14.87 |
| PROB: | 0.09  | 0.8   | 0.11  |
| RMSE: | 0.69  | 0.29  | 0.29  |

MAX\_MEAN: 1.16      MAX\_MED: 1.16      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 37    ACTP: 0.91

FLAGS:

11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 2,4,5-Trichlorophenol  
CHID: 24359 CASRN: 95-95-4  
SPID(S): TP0001562D09  
M4ID: 18128450

HILL MODEL (in red):

|      | tp    | ga    | gw   |
|------|-------|-------|------|
| val: | 1.11  | 1.65  | 3.08 |
| sd:  | 0.182 | 0.157 | 1.78 |

GAIN-LOSS MODEL (in blue):

|      | tp    | ga    | gw   | la   | lw   |
|------|-------|-------|------|------|------|
| val: | 1.11  | 1.65  | 3.08 | 3.87 | 4.19 |
| sd:  | 0.182 | 0.157 | 1.78 | 2080 | 5610 |

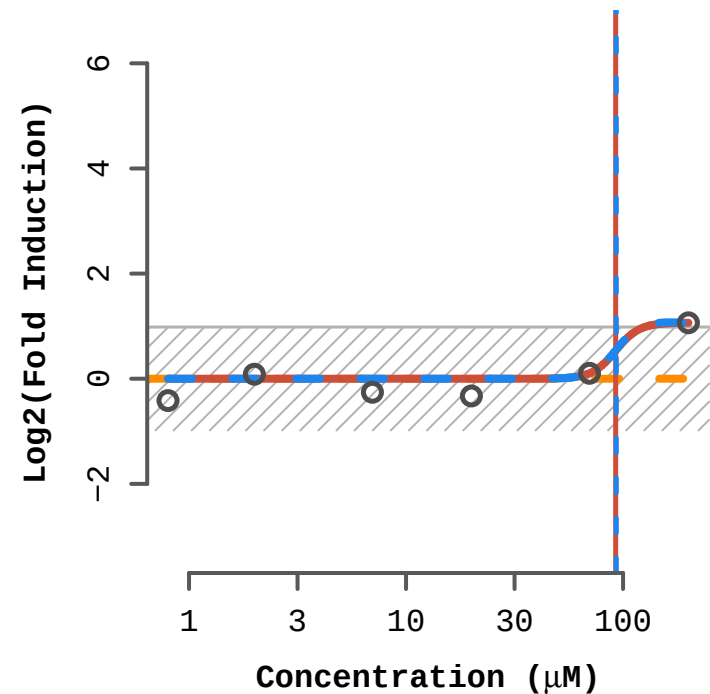
|       | CNST  | HILL | GNLS  |
|-------|-------|------|-------|
| AIC:  | 13.96 | 7.94 | 11.94 |
| PROB: | 0.04  | 0.84 | 0.11  |
| RMSE: | 0.63  | 0.24 | 0.24  |

MAX\_MEAN: 1.1      MAX\_MED: 1.1      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 37    ACTP: 0.96

FLAGS:

6; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Methyl 2,4-dihydroxy-3,6-dimethylbenzoate

CHID: 41653 CASRN: 4707-47-5

SPID(S): TP0001562C05

M4ID: 18128465

HILL MODEL (in red):

|      | tp   | ga   | gw  |
|------|------|------|-----|
| val: | 1.07 | 1.97 | 8   |
| sd:  | NaN  | NaN  | NaN |

GAIN-LOSS MODEL (in blue):

|      | tp   | ga   | gw   | la   | lw   |
|------|------|------|------|------|------|
| val: | 1.13 | 1.97 | 7.99 | 3.02 | 1.74 |
| sd:  | NaN  | NaN  | NaN  | NaN  | NaN  |

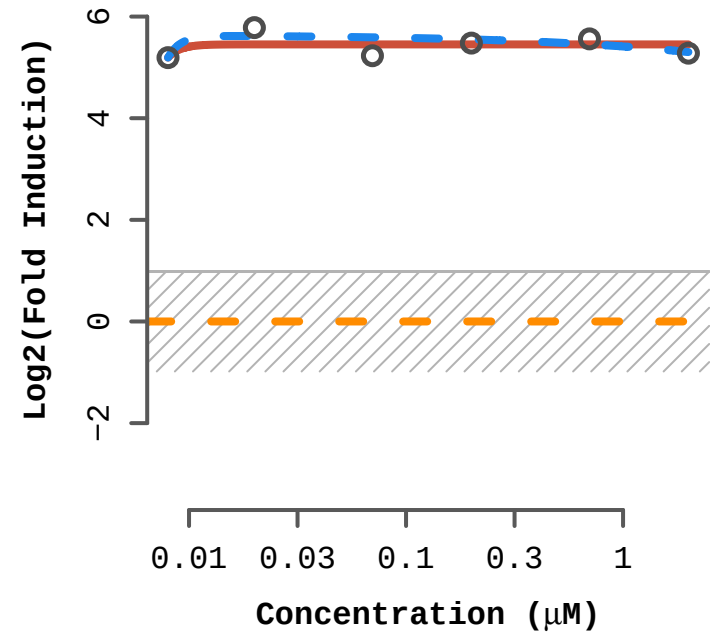
|       | CNST  | HILL | GNLS  |
|-------|-------|------|-------|
| AIC:  | 10.44 | 8.61 | 12.61 |
| PROB: | 0.26  | 0.65 | 0.09  |
| RMSE: | 0.5   | 0.24 | 0.24  |

MAX\_MEAN: 1.06      MAX\_MED: 1.06      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 37    ACTP: 0.74

FLAGS:

6; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Tiratricol

CHID: 45232 CASRN: 51-24-1

SPID(S): TP0001562E12

M4ID: 18128436

HILL MODEL (in red):

|      |      |       |     |
|------|------|-------|-----|
|      | tp   | ga    | gw  |
| val: | 5.45 | -2.26 | 8   |
| sd:  | NaN  | NaN   | NaN |

GAIN-LOSS MODEL (in blue):

|      |      |       |     |     |       |
|------|------|-------|-----|-----|-------|
|      | tp   | ga    | gw  | la  | lw    |
| val: | 5.64 | -2.23 | 8   | 2.3 | 0.598 |
| sd:  | NaN  | NaN   | NaN | NaN | NaN   |

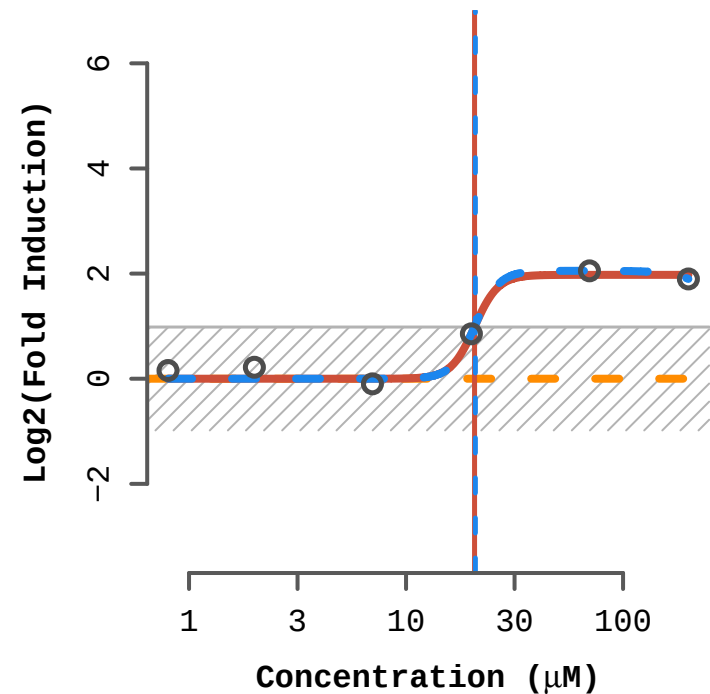
|       |       |      |      |
|-------|-------|------|------|
|       | CNST  | HILL | GNLS |
| AIC:  | 56.06 | 5.24 | 7.58 |
| PROB: | 0     | 0.76 | 0.24 |
| RMSE: | 5.43  | 0.18 | 0.17 |

MAX\_MEAN: 5.78      MAX\_MED: 5.78      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 40    ACTP: 1

FLAGS:

18



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Dicloran

CHID: 20426 CASRN: 99-30-9

SPID(S): TP0001562B08

M4ID: 18128473

HILL MODEL (in red):

|      |        |        |      |
|------|--------|--------|------|
|      | tp     | ga     | gw   |
| val: | 1.98   | 1.32   | 8    |
| sd:  | 0.0837 | 0.0181 | 8.87 |

GAIN-LOSS MODEL (in blue):

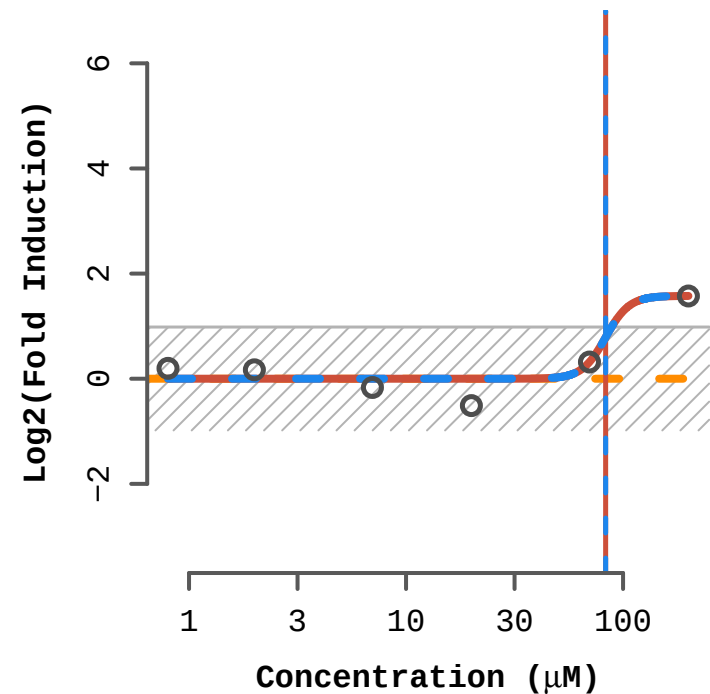
|      |      |      |     |      |      |
|------|------|------|-----|------|------|
|      | tp   | ga   | gw  | la   | lw   |
| val: | 2.05 | 1.32 | 8   | 2.51 | 5.29 |
| sd:  | NaN  | NaN  | NaN | NaN  | NaN  |

|       |       |      |      |
|-------|-------|------|------|
|       | CNST  | HILL | GNLS |
| AIC:  | 21.52 | 0.85 | 3.54 |
| PROB: | 0     | 0.79 | 0.21 |
| RMSE: | 1.2   | 0.13 | 0.12 |

MAX\_MEAN: 2.05      MAX\_MED: 2.05      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 41    ACTP: 1

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 6-Hydroxy-2-naphthyl disulfide

CHID: 25429 CASRN: 6088-51-3

SPID(S): TP0001562A04

M4ID: 18128488

HILL MODEL (in red):

|      |      |       |      |
|------|------|-------|------|
|      | tp   | ga    | gw   |
| val: | 1.58 | 1.92  | 8    |
| sd:  | 0.17 | 0.152 | 16.1 |

GAIN-LOSS MODEL (in blue):

|      |      |      |    |     |      |
|------|------|------|----|-----|------|
|      | tp   | ga   | gw | la  | lw   |
| val: | 1.58 | 1.92 | 8  | 4.3 | 4.36 |
| sd:  | NA   | NA   | NA | NA  | NA   |

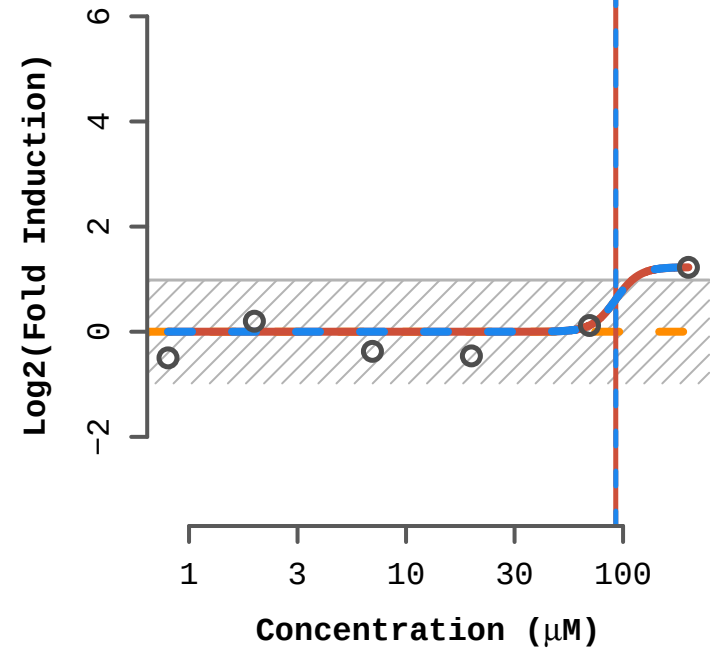
|       |       |      |       |
|-------|-------|------|-------|
|       | CNST  | HILL | GNLS  |
| AIC:  | 13.76 | 7.99 | 11.99 |
| PROB: | 0.05  | 0.84 | 0.11  |
| RMSE: | 0.7   | 0.24 | 0.24  |

MAX\_MEAN: 1.57 MAX\_MED: 1.57 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 41 ACTP: 0.95

FLAGS:

6; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Phenylparaben

CHID: 47882 CASRN: 17696-62-7

SPID(S): TP0001562F04

M4ID: 18128433

HILL MODEL (in red):

|      |      |      |     |
|------|------|------|-----|
|      | tp   | ga   | gw  |
| val: | 1.23 | 1.97 | 8   |
| sd:  | NaN  | NaN  | NaN |

GAIN-LOSS MODEL (in blue):

|      |      |      |     |     |      |
|------|------|------|-----|-----|------|
|      | tp   | ga   | gw  | la  | lw   |
| val: | 1.23 | 1.97 | 8   | 4   | 1.35 |
| sd:  | NaN  | NaN  | NaN | NaN | NaN  |

|       |      |       |       |
|-------|------|-------|-------|
|       | CNST | HILL  | GNLS  |
| AIC:  | 13   | 12.39 | 16.39 |
| PROB: | 0.39 | 0.53  | 0.07  |
| RMSE: | 0.6  | 0.33  | 0.33  |

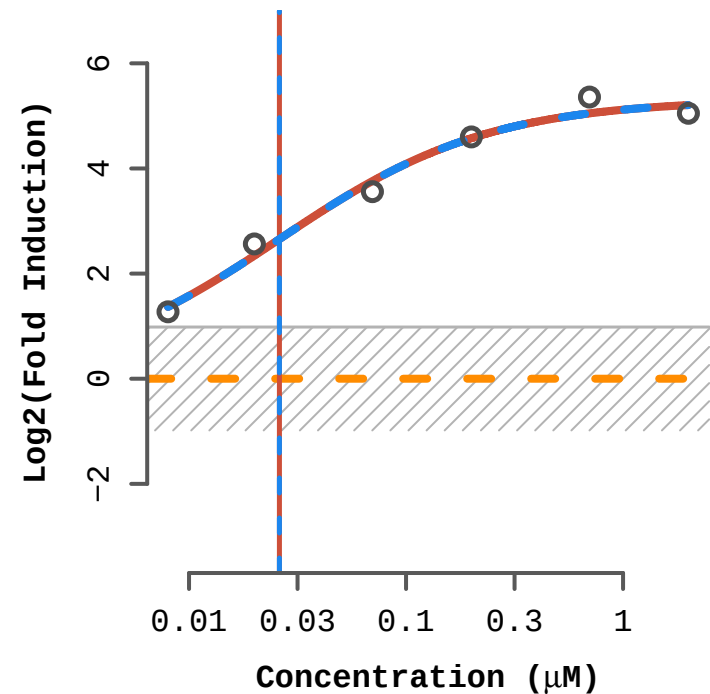
MAX\_MEAN: 1.22      MAX\_MED: 1.22      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 41    ACTP: 0.61

FLAGS:

6; 11; 16





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Tetrac

CHID: 48186 CASRN: 67-30-1

SPID(S): TP0001562F12

M4ID: 18128425

HILL MODEL (in red):

|      |       |        |       |
|------|-------|--------|-------|
|      | tp    | ga     | gw    |
| val: | 5.31  | -1.58  | 0.897 |
| sd:  | 0.248 | 0.0842 | 0.121 |

GAIN-LOSS MODEL (in blue):

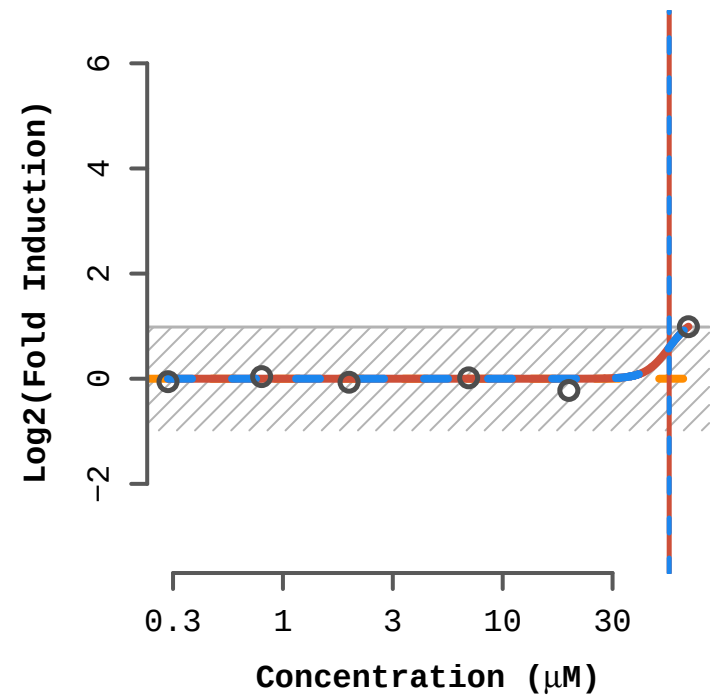
|      |      |       |       |     |      |
|------|------|-------|-------|-----|------|
|      | tp   | ga    | gw    | la  | lw   |
| val: | 5.31 | -1.58 | 0.897 | 2.3 | 8.02 |
| sd:  | NaN  | NaN   | NaN   | NaN | NaN  |

|       |       |      |       |
|-------|-------|------|-------|
|       | CNST  | HILL | GNLS  |
| AIC:  | 36.87 | 6.17 | 10.17 |
| PROB: | 0     | 0.88 | 0.12  |
| RMSE: | 4.01  | 0.19 | 0.19  |

MAX\_MEAN: 5.36      MAX\_MED: 5.36      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 41    ACTP: 1

FLAGS:



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Chlorobenzilate

CHID: 20299 CASRN: 510-15-6

SPID(S): TP0001562G09

M4ID: 18128417

HILL MODEL (in red):

|      |       |        |      |
|------|-------|--------|------|
|      | tp    | ga     | gw   |
| val: | 1.19  | 1.76   | 8    |
| sd:  | 0.987 | 0.0863 | 18.9 |

GAIN-LOSS MODEL (in blue):

|      |      |      |    |      |      |
|------|------|------|----|------|------|
|      | tp   | ga   | gw | la   | lw   |
| val: | 1.19 | 1.76 | 8  | 2.84 | 15.1 |
| sd:  | NA   | NA   | NA | NA   | NA   |

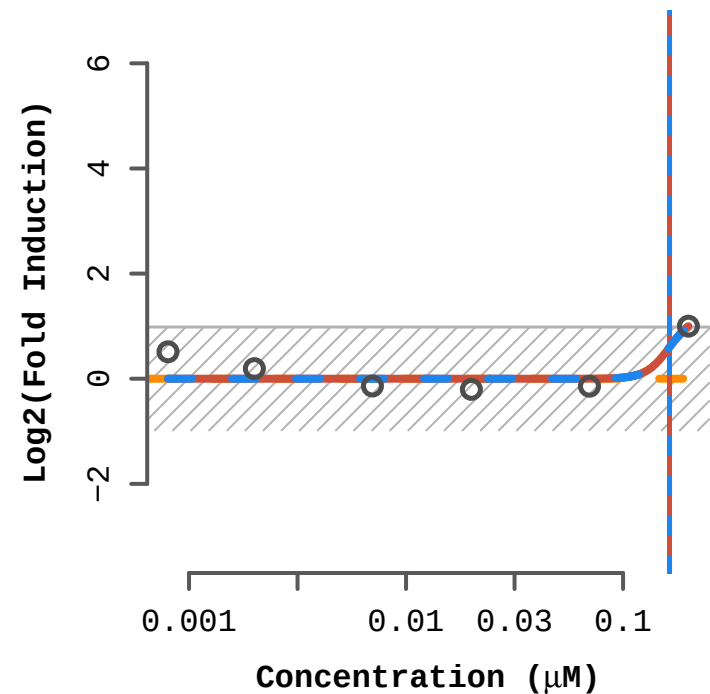
|       |      |       |      |
|-------|------|-------|------|
|       | CNST | HILL  | GNLS |
| AIC:  | 5.9  | -3.64 | 0.36 |
| PROB: | 0.01 | 0.87  | 0.12 |
| RMSE: | 0.42 | 0.1   | 0.1  |

MAX\_MEAN: 0.99      MAX\_MED: 0.99      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 42    ACTP: 0.99

FLAGS:

6; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Zearalenone

CHID: 21460 CASRN: 17924-92-4

SPID(S): TP0001562A12

M4ID: 18128480

HILL MODEL (in red):

|      |      |        |      |
|------|------|--------|------|
|      | tp   | ga     | gw   |
| val: | 1.2  | -0.786 | 8    |
| sd:  | 2.89 | 0.67   | 17.5 |

GAIN-LOSS MODEL (in blue):

|      |      |        |      |       |      |
|------|------|--------|------|-------|------|
|      | tp   | ga     | gw   | la    | lw   |
| val: | 1.2  | -0.786 | 8    | 0.606 | 4.69 |
| sd:  | 2.87 | 0.666  | 17.4 | 1650  | 5910 |

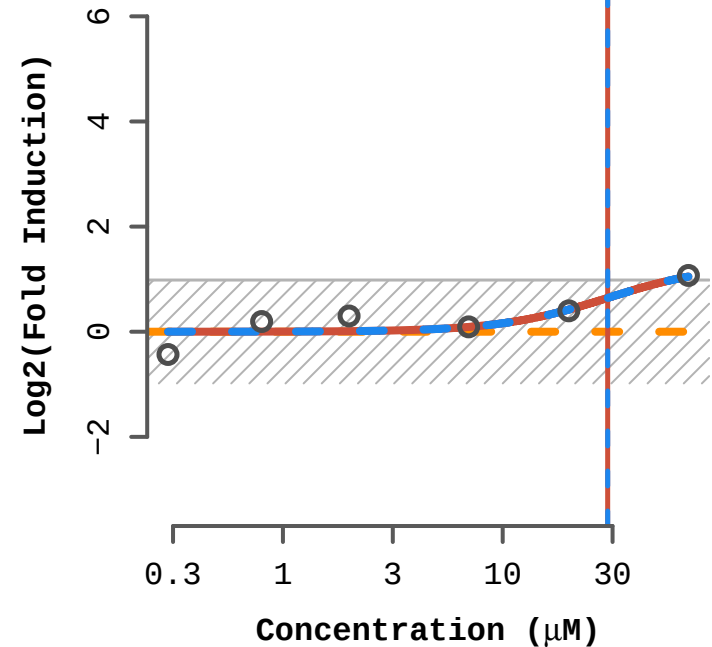
|       |       |      |       |
|-------|-------|------|-------|
|       | CNST  | HILL | GNLS  |
| AIC:  | 10.04 | 8.67 | 12.67 |
| PROB: | 0.31  | 0.61 | 0.08  |
| RMSE: | 0.48  | 0.25 | 0.25  |

MAX\_MEAN: 1 MAX\_MED: 1 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 42 ACTP: 0.69

FLAGS:

6; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 2-Chloro-4-phenylphenol

CHID: 22353 CASRN: 92-04-6

SPID(S): TP0001562H05

M4ID: 18128410

HILL MODEL (in red):

|      |       |       |      |
|------|-------|-------|------|
|      | tp    | ga    | gw   |
| val: | 1.29  | 1.48  | 1.76 |
| sd:  | 0.817 | 0.436 | 2.06 |

GAIN-LOSS MODEL (in blue):

|      |       |       |      |      |      |
|------|-------|-------|------|------|------|
|      | tp    | ga    | gw   | la   | lw   |
| val: | 1.29  | 1.48  | 1.76 | 3.26 | 5.51 |
| sd:  | 0.829 | 0.442 | 2.09 | 2090 | 8120 |

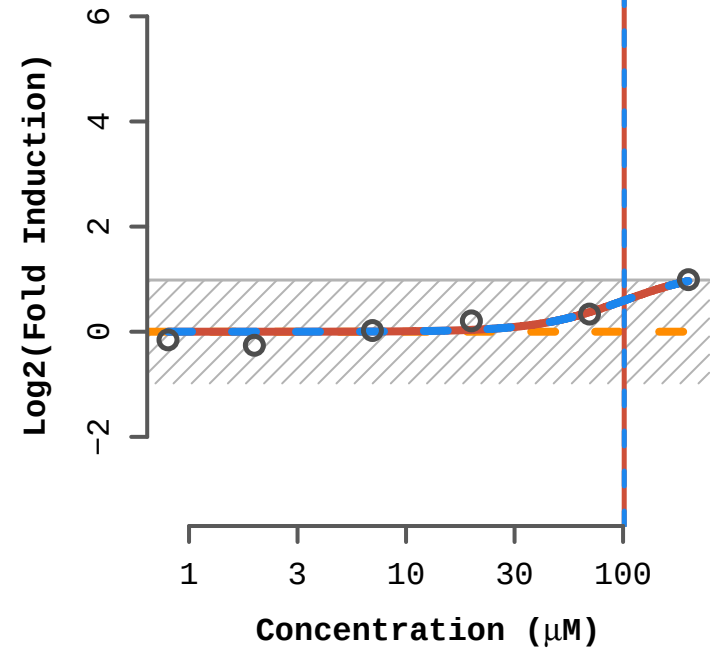
|       |      |      |       |
|-------|------|------|-------|
|       | CNST | HILL | GNLS  |
| AIC:  | 11.3 | 7.45 | 11.45 |
| PROB: | 0.11 | 0.78 | 0.11  |
| RMSE: | 0.52 | 0.23 | 0.23  |

MAX\_MEAN: 1.07 MAX\_MED: 1.07 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 42 ACTP: 0.89

FLAGS:

6; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Propylparaben

CHID: 22527 CASRN: 94-13-3

SPID(S): TP0001562A07

M4ID: 18128485

HILL MODEL (in red):

|      | tp    | ga    | gw   |
|------|-------|-------|------|
| val: | 1.19  | 2.01  | 2.14 |
| sd:  | 0.634 | 0.275 | 2.39 |

GAIN-LOSS MODEL (in blue):

|      | tp    | ga    | gw   | la   | lw    |
|------|-------|-------|------|------|-------|
| val: | 1.19  | 2.01  | 2.15 | 3.31 | 8.08  |
| sd:  | 0.654 | 0.284 | 2.47 | 1290 | 10400 |

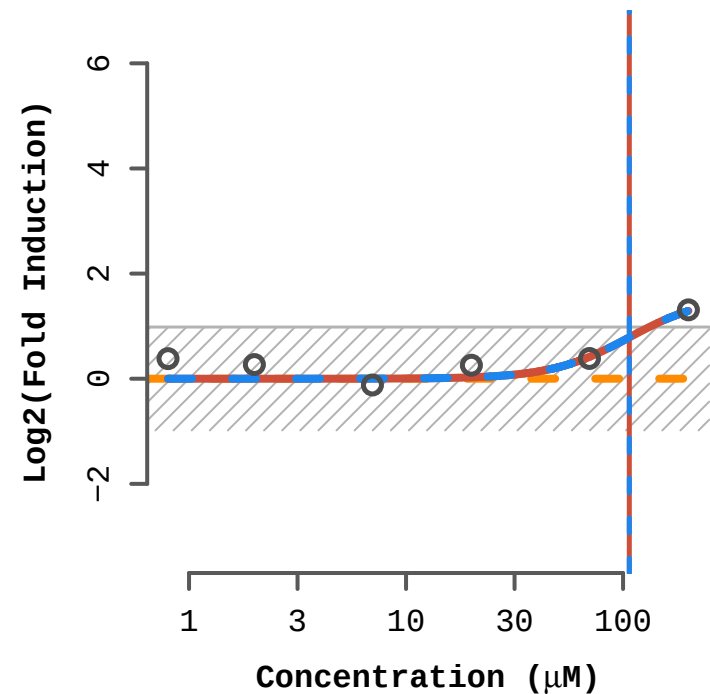
|       | CNST | HILL | GNLS |
|-------|------|------|------|
| AIC:  | 8.97 | 2.13 | 6.13 |
| PROB: | 0.03 | 0.86 | 0.12 |
| RMSE: | 0.45 | 0.14 | 0.14 |

MAX\_MEAN: 0.991      MAX\_MED: 0.991      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 42    ACTP: 0.97

FLAGS:

6; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Fludioxonil

CHID: 32398 CASRN: 131341-86-1

SPID(S): TP0001562E11

M4ID: 18128437

HILL MODEL (in red):

|      | tp   | ga    | gw   |
|------|------|-------|------|
| val: | 1.57 | 2.03  | 2.42 |
| sd:  | 1.24 | 0.406 | 3.62 |

GAIN-LOSS MODEL (in blue):

|      | tp   | ga    | gw   | la   | lw   |
|------|------|-------|------|------|------|
| val: | 1.57 | 2.03  | 2.42 | 4.06 | 4.34 |
| sd:  | 1.24 | 0.406 | 3.62 | 2090 | 5160 |

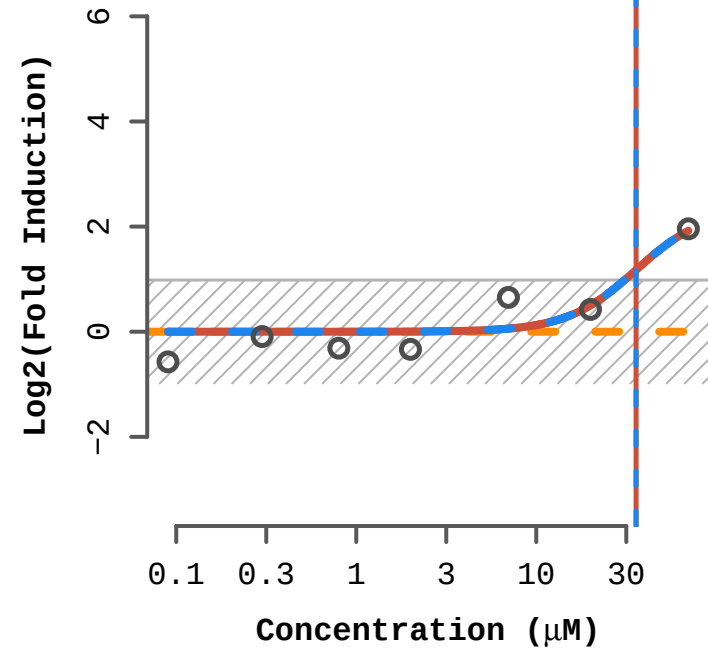
|       | CNST  | HILL | GNLS  |
|-------|-------|------|-------|
| AIC:  | 12.46 | 7.49 | 11.49 |
| PROB: | 0.07  | 0.82 | 0.11  |
| RMSE: | 0.6   | 0.22 | 0.22  |

MAX\_MEAN: 1.31      MAX\_MED: 1.31      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 42    ACTP: 0.93

FLAGS:

6; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 9-Phenanthrol

CHID: 47592 CASRN: 484-17-3

SPID(S): TP0001562B10

M4ID: 18128471

HILL MODEL (in red):

|      |      |       |      |
|------|------|-------|------|
|      | tp   | ga    | gw   |
| val: | 2.35 | 1.55  | 2.24 |
| sd:  | 1.49 | 0.366 | 2.54 |

GAIN-LOSS MODEL (in blue):

|      |      |       |      |      |      |
|------|------|-------|------|------|------|
|      | tp   | ga    | gw   | la   | lw   |
| val: | 2.35 | 1.55  | 2.24 | 3    | 6.79 |
| sd:  | 1.48 | 0.366 | 2.54 | 1660 | 9790 |

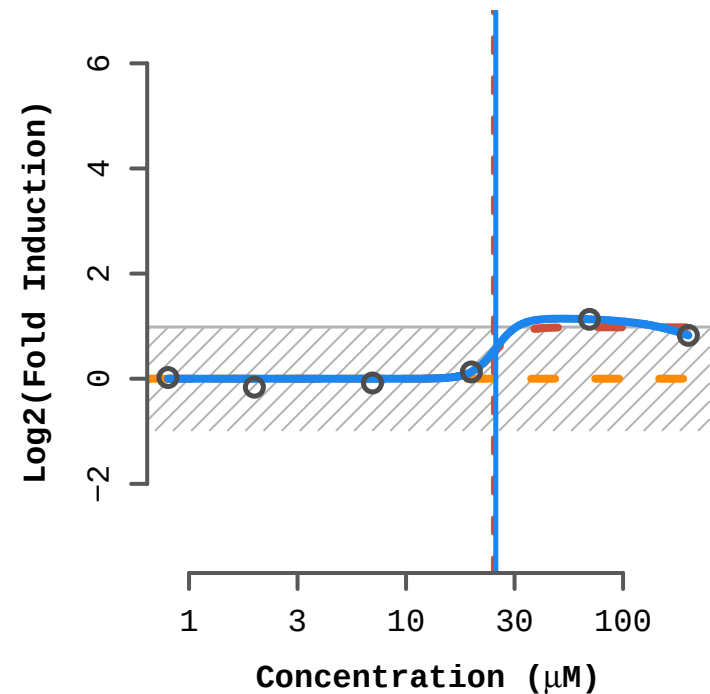
|       |       |       |       |
|-------|-------|-------|-------|
|       | CNST  | HILL  | GNLS  |
| AIC:  | 18.72 | 14.32 | 18.32 |
| PROB: | 0.09  | 0.8   | 0.11  |
| RMSE: | 0.84  | 0.36  | 0.36  |

MAX\_MEAN: 1.96      MAX\_MED: 1.96      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 42    ACTP: 0.91

FLAGS:

6; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 3-Hydroxyfluorene

CHID: 47540 CASRN: 6344-67-8

SPID(S): TP0001562G07

M4ID: 18128419

HILL MODEL (in red):

|      |       |       |      |
|------|-------|-------|------|
|      | tp    | ga    | gw   |
| val: | 0.978 | 1.4   | 8    |
| sd:  | 0.149 | 0.191 | 14.7 |

GAIN-LOSS MODEL (in blue):

|      |       |        |      |        |      |
|------|-------|--------|------|--------|------|
|      | tp    | ga     | gw   | la     | lw   |
| val: | 1.16  | 1.41   | 8    | 2.45   | 2.66 |
| sd:  | 0.101 | 0.0849 | 6.01 | 0.0874 | 2.31 |

|       |       |      |       |
|-------|-------|------|-------|
|       | CNST  | HILL | GNLS  |
| AIC:  | 12.25 | 0.03 | -3.07 |
| PROB: | 0     | 0.18 | 0.82  |
| RMSE: | 0.58  | 0.12 | 0.07  |

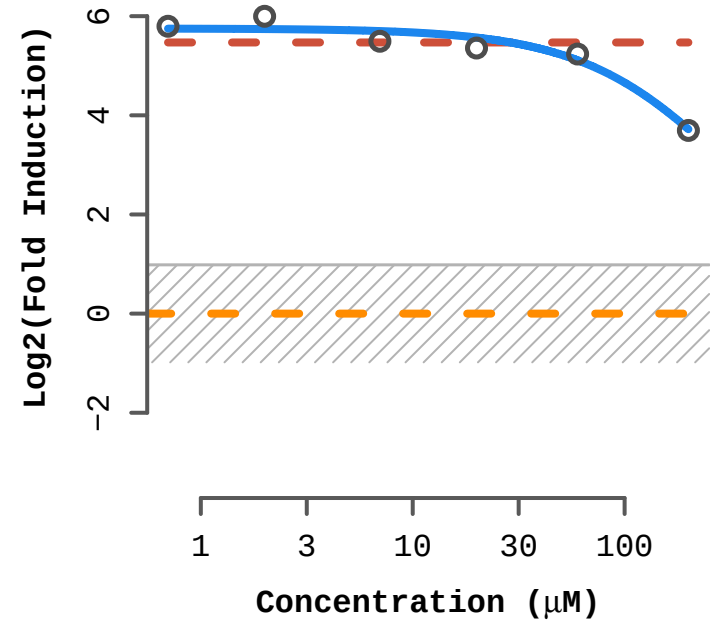
MAX\_MEAN: 1.13      MAX\_MED: 1.13      BMAD: 0.328

COFF: 0.984    HIT-CALL: 1    FITC: 46    ACTP: 1

FLAGS:

7; 11; 16





ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 3,5,3'-Triiodothyronine

CHID: 23216 CASRN: 6893-02-3

SPID(S): TP0001562E09

M4ID: 18128439

HILL MODEL (in red):

|      | tp    | ga    | gw   |
|------|-------|-------|------|
| val: | 5.47  | -1.42 | 6.74 |
| sd:  | 0.222 | 1200  | 6440 |

GAIN-LOSS MODEL (in blue):

|      | tp    | ga    | gw   | la     | lw    |
|------|-------|-------|------|--------|-------|
| val: | 5.75  | -2.15 | 4.37 | 2.52   | 1.22  |
| sd:  | 0.142 | 1930  | 4190 | 0.0755 | 0.381 |

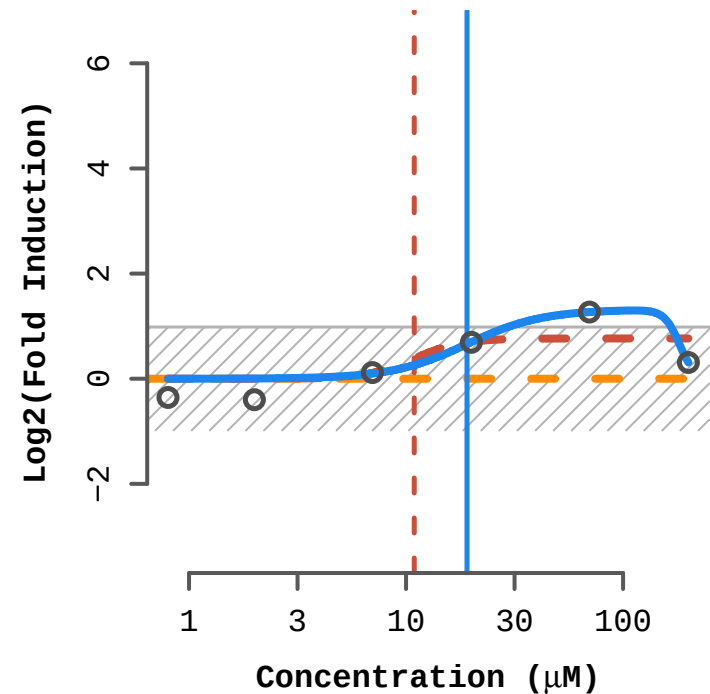
|       | CNST  | HILL  | GNLS |
|-------|-------|-------|------|
| AIC:  | 43.83 | 20.61 | 8.67 |
| PROB: | 0     | 0     | 1    |
| RMSE: | 5.32  | 0.77  | 0.17 |

MAX\_MEAN: 6 MAX\_MED: 6 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 49 ACTP: 1

FLAGS:

16; 18



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: 2,4,6-Triiodophenol  
CHID: 22080 CASRN: 609-23-4  
SPID(S): TP0001562D05  
M4ID: 18128454

HILL MODEL (in red):

|      | tp    | ga   | gw   |
|------|-------|------|------|
| val: | 0.766 | 1.04 | 4.01 |
| sd:  | 0.44  | 0.49 | 7.04 |

GAIN-LOSS MODEL (in blue):

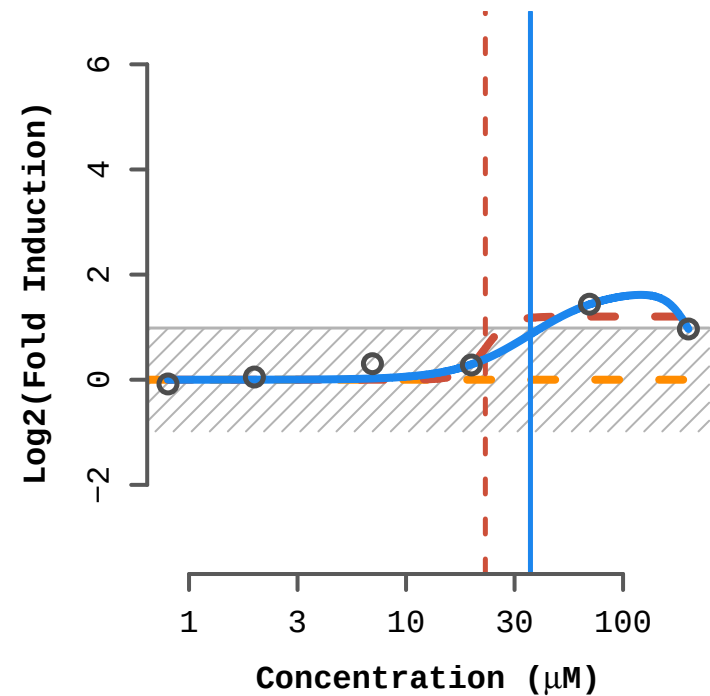
|      | tp    | ga     | gw   | la     | lw   |
|------|-------|--------|------|--------|------|
| val: | 1.32  | 1.28   | 2.51 | 2.26   | 12.4 |
| sd:  | 0.193 | 0.0957 | 1.38 | 0.0296 | 8.68 |

|       | CNST  | HILL  | GNLS  |
|-------|-------|-------|-------|
| AIC:  | 14.04 | 13.54 | 10.57 |
| PROB: | 0.13  | 0.16  | 0.71  |
| RMSE: | 0.64  | 0.35  | 0.22  |

MAX\_MEAN: 1.27 MAX\_MED: 1.27 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 50 ACTP: 0.87

FLAGS:  
7; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Apigenin

CHID: 22391 CASRN: 520-36-5

SPID(S): TP0001562B06

M4ID: 18128475

HILL MODEL (in red):

|      |       |       |      |
|------|-------|-------|------|
|      | tp    | ga    | gw   |
| val: | 1.2   | 1.37  | 8    |
| sd:  | 0.223 | 0.192 | 23.6 |

GAIN-LOSS MODEL (in blue):

|      |      |       |      |        |      |
|------|------|-------|------|--------|------|
|      | tp   | ga    | gw   | la     | lw   |
| val: | 1.72 | 1.57  | 2.54 | 2.32   | 7.6  |
| sd:  | 0.69 | 0.236 | 1.55 | 0.0118 | 22.3 |

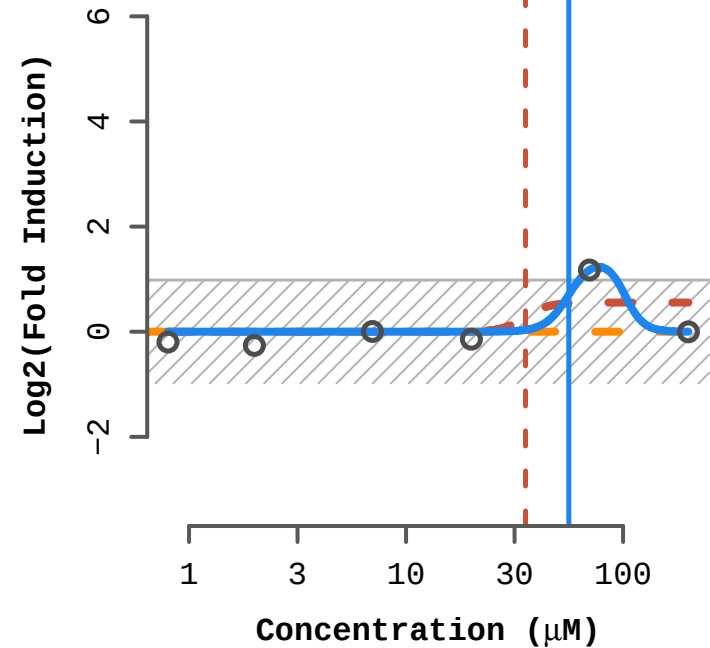
|       |       |      |      |
|-------|-------|------|------|
|       | CNST  | HILL | GNLS |
| AIC:  | 15.16 | 5.78 | 2.03 |
| PROB: | 0     | 0.13 | 0.87 |
| RMSE: | 0.73  | 0.19 | 0.12 |

MAX\_MEAN: 1.44 MAX\_MED: 1.44 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 50 ACTP: 1

FLAGS:

7; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME:  $\alpha$ -Isomethylionone

CHID: 27047 CASRN: 127-51-5

SPID(S): TP0001562H10

M4ID: 18128405

HILL MODEL (in red):

|      |       |       |      |
|------|-------|-------|------|
|      | tp    | ga    | gw   |
| val: | 0.555 | 1.55  | 8    |
| sd:  | 0.996 | 0.395 | 11.9 |

GAIN-LOSS MODEL (in blue):

|      |      |      |     |      |      |
|------|------|------|-----|------|------|
|      | tp   | ga   | gw  | la   | lw   |
| val: | 1.41 | 1.75 | 8   | 2.01 | 10.1 |
| sd:  | NaN  | NaN  | NaN | NaN  | NaN  |

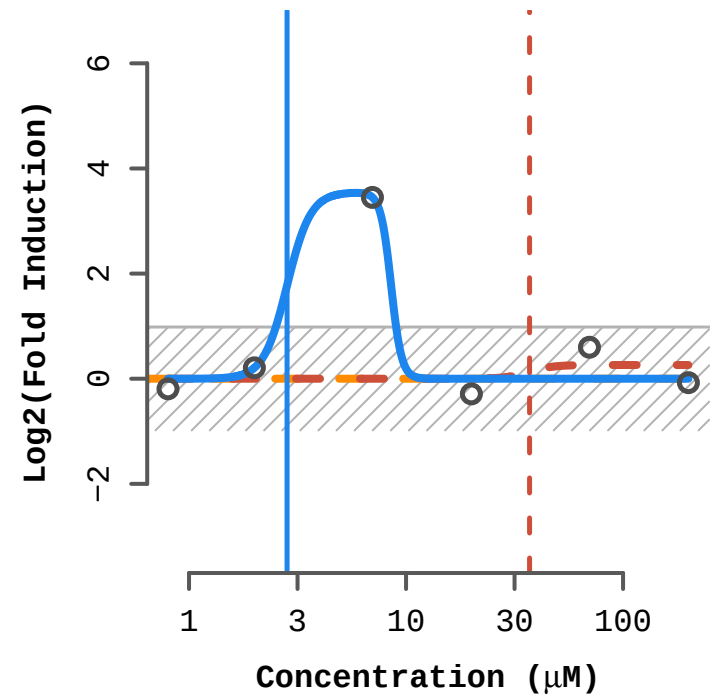
|       |      |       |      |
|-------|------|-------|------|
|       | CNST | HILL  | GNLS |
| AIC:  | 8.78 | 13.71 | 6.26 |
| PROB: | 0.22 | 0.02  | 0.76 |
| RMSE: | 0.5  | 0.37  | 0.14 |

MAX\_MEAN: 1.17 MAX\_MED: 1.17 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 50 ACTP: 0.78

FLAGS:

7; 11; 16



ASSAY: AEID2027 (ATG\_hTRa\_XSP2\_up)

NAME: Flumetralin

CHID: 32553 CASRN: 62924-70-3

SPID(S): TP0001562G10

M4ID: 18128416

HILL MODEL (in red):

|      | tp    | ga   | gw   |
|------|-------|------|------|
| val: | 0.261 | 1.57 | 8    |
| sd:  | 0.406 | 0.86 | 25.4 |

GAIN-LOSS MODEL (in blue):

|      | tp   | ga    | gw  | la    | lw  |
|------|------|-------|-----|-------|-----|
| val: | 3.55 | 0.452 | 8   | 0.931 | 18  |
| sd:  | NaN  | NaN   | NaN | NaN   | NaN |

|       | CNST  | HILL  | GNLS  |
|-------|-------|-------|-------|
| AIC:  | 20.46 | 26.07 | 13.62 |
| PROB: | 0.03  | 0     | 0.97  |
| RMSE: | 1.44  | 1.43  | 0.28  |

MAX\_MEAN: 3.45 MAX\_MED: 3.45 BMAD: 0.328

COFF: 0.984 HIT-CALL: 1 FITC: 50 ACTP: 0.97

FLAGS:

7; 16