

PROCEDURES FOR ENCODING TOXICITY DATA PUBLISHED IN THE OPEN
LITERATURE FOR USE IN ECOLOGICAL RISK ASSESSMENTS

U.S. Environmental Protection Agency (EPA) Office of
Pollution Prevention and Toxics Risk Assessment Division
(OPPT RAD)

OPPT RAD Chemical Reports

Prepared for:

U.S. Environmental Protection Agency (EPA)

Office of Research and Development (ORD)

National Health and Environmental Effects Research Laboratory (NHEERL)

Mid-Continent Ecology Division (MED)

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TDD 2-8 ECOTOX Application Development and Support

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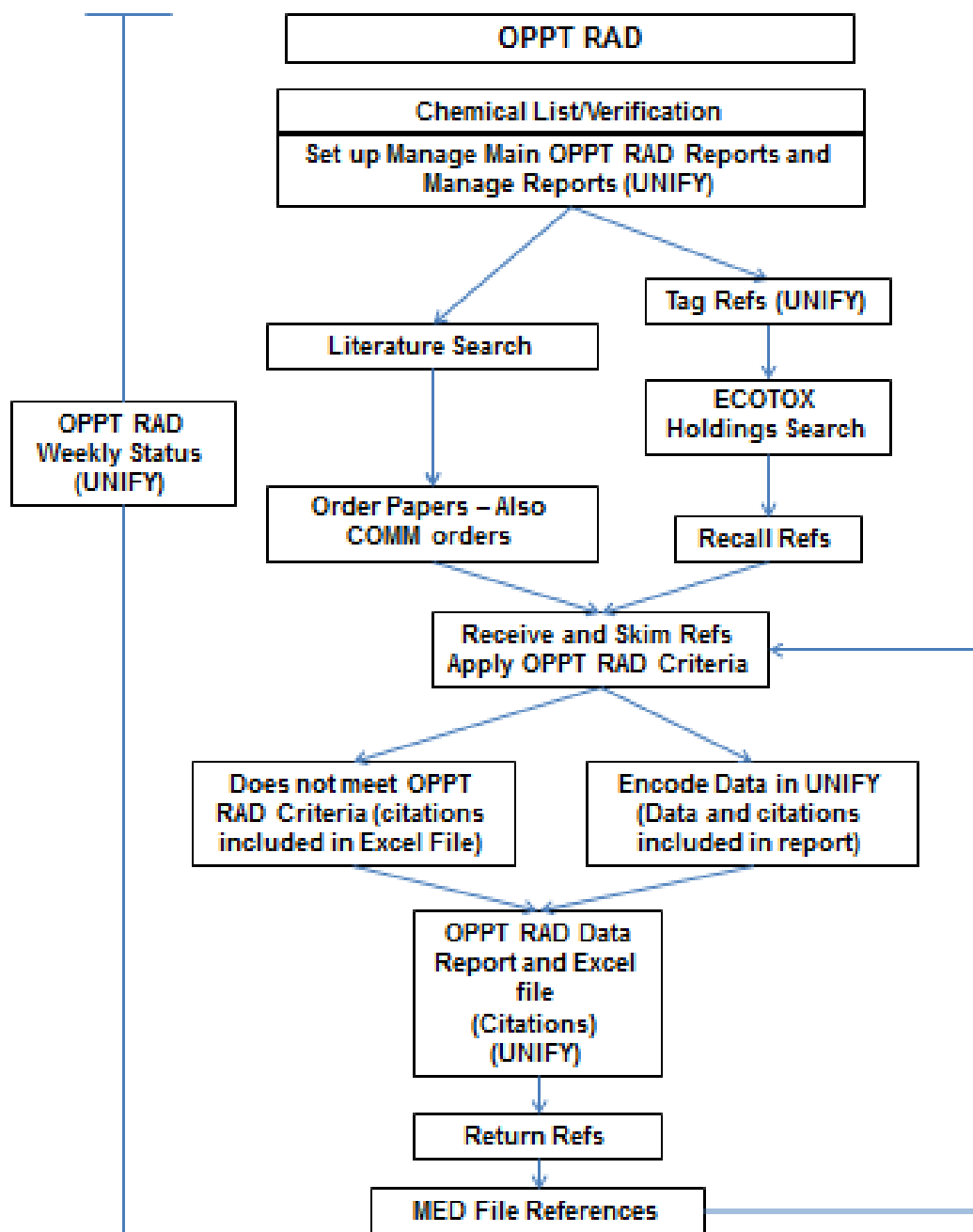
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OVERVIEW

This Standard Operating Procedure (SOP) documents the procedure for U.S. EPA Office of Pollution Prevention and Toxics Risk Assessment Division (OPPT RAD) toxicological reporting processing for chemicals identified in Mid-Continent Ecology Division (MED) Work Requests.

The tasks described in this SOP are intended to track OPPT RAD tasks and reports within the UNIFY Application (UNIFY) and create final data and citation files for EPA OPPT RAD (See Figure 1).













Figure 1. OPPT RAD Workflow




SETTING UP CHEMICAL TRACKING AND REPORTS

The chemical verification process is documented in the OPPT RAD Acquisition_Chemical_Criteria.doc SOP, located on Contractor site. The OPPT RAD chemicals are set up and tracked within the UNIFY report system through four screens; Manage Main OPPT RAD Reports, Manage OPPT RAD Reports, Tagging References and OPPT RAD Reports. All screens use the following Icons/Graphics.


Navigation Icon/Graphics

ICON	Description	Usage
	Magnifying glass	Print View
	Pencil	Edit View
	Page with 'X'	Delete
	Plus Sign/Add Button	Add
	Right Arrow	Hover over to display complete text
	Page with Check	Verified or Activate
	Invoke index to display	Match typed in text to valid index
	Circle with Slash	Reject for Verification
	Binoculars	Search
	Printer	Print Command
	Excel Sheet	Download to Excel
	Circle Arrow	Return to search screen

ICON	Description	Usage
	RIS Export	Exports citations in RIS delimited form for transfer to Excel

Manage Main OPPT RAD Reports

Manage Main OPPT RAD /Skim by Chemical Reports	Sets up new chemicals, title string search and rejected citation batch and history of OPPT RAD reports for the chemical.
---	--

This screen establishes the main chemical and search terms for OPPT RAD reports. After a list of priority chemicals is received from EPA and chemical verification process has been completed, the OPPT RAD reports are set up in UNIFY to track OPPT RAD publications and data status. Select the Add New button () to start a new OPPT RAD Report. Enter the following data fields and click on the “Submit” button.

Report Name: Insert the primary chemical name for the report, e.g. Carbon Tetrachloride. Additional chemical and degradate names/codes are added in the Manage OPPT RAD Report screen.

Title String Search: Insert all chemical names and synonyms of primary and related chemicals in a pipe (|) delimited format, (chemical name | chemical name). Chemical names can be found in the Chemical Report document (e.g. N:\CSRA info\Database (offsite) Work Orders\SMACVCS3 Feb 2017 - Jan 2018\WO011 OPPT RAD\01 Methylene Chloride\Methylene Chloride Chemical Report Memo.docx).

NOT Title String Search: Insert all chemical names and synonyms of primary and related chemicals that cause false results in a pipe (|) delimited format, (chemical name | chemical name).

Reject Batch Name: Select the custom file name as set up in Manage Batches (see the following document located on the Contractor site: ECOTOXLitAcquisition.docx).

Expand/Collapse: Displays/hides all of the reports for that chemical.

SEARCH REPORT GROUPS

Name

☒ Starts With
☐ Contains
☐ Exact
☐ Match Case

COC

- 1,4-Dioxane
- 123BPP
- 124T
- 128PP
- 12DPA
- 12DPE

clear

Reject Batch ID
--SELECT--

Clear Search

Search Results - 2 records

► = The data in this field has been truncated for display. Mouse over the icon to view the entire value.

Page 1 of 1 pages (2 total records)

Report Name	Title String Search	NOT Title String Search	Reject Batch
1,4-Dioxane	1,4-Dioxane p-Dioxane 1,4-Diethylene dioxide 1,4-D		OPPT-RAD 1,4-Dioxane Rejects

Report Group	Report Name	Chemical Groups	Delivery Date
OPPT-RAD 2017	1,4-Dioxane	1 4-Dioxane (01/01/1900-05/31/2017)	

Manage OPPT RAD Reports

Manage OPPT RAD/Skim by Chemical Reports

Sets up due date for current OPPT RAD Report and lists chemicals within the report.

This screen sets up the OPPT RAD Report group for the specific chemicals. These are set up by monthly due dates. These fields can be added, edited and removed.

OPPT RAD Report Group: Name and due date. To add a new OPPT RAD Report group, check the Add New button (), enter the name and due date and select Submit. To edit or delete, highlight the OPPT RAD Report group, select the edit or delete icon.

Reports in Selected Group: Add chemical report names from dropdown and mark in checkbox if this report is a “Refresh” or not (if not checked, this is the first time the chemical has been requested for OPPT RAD project).

Chemicals in Selected Report: Insert primary and related chemicals to be included in the report and the report start and end dates for each chemical. If the report is a new report the Start date is 01/01/1900. If the report is a “Refresh”, the Start date will be the day after the last day of the previous OPPT RAD Report for that chemical. The Report end dates can be found in the Chemical Report document (e.g. N:\CSRA info\Database (offsite) Work Orders\SMACVCS3 Feb 2017 - Jan 2018\WO011 OPPT RAD\01 Methylene Chloride\Methylene Chloride Chemical Report Memo.docx).

Manage Project Reports

SEARCH REPORT GROUPS Collapse Pane

Name

☒ Starts With
☐ Contains
☐ Exact
☐ Match Case

COC

- 1,4-Dioxane
- 123BPP
- 124T
- 12BPP
- 12DPA
- 12DPE

Due Date
From
Through

☐ Include Delivered Reports
☒ Project Reports

Clear **Search**

Project Report Groups:

(Click to View Reports In Group)

- April 7, 2017 (04/07/2017)
- March 31, 2017 (03/31/2017)
- February 15, 2017 (02/15/2017)
- GLRI USGS DEET (01/31/2017)
- GLRI USGS Isophorone (01/31/2017)
- GLRI USGS Carbamazepine (01/31/2017)
- GLRI USGS Diethyl phthalate (01/31/2017)
- GLRI USGS Bisphenol A (01/31/2017)
- OW Selenium 2016 (01/31/2017)
- GLRI USGS Glyphosate (01/31/2017)
- January 31, 2017 (01/31/2017)
- GLRI USGS 4-Nonylphenol (01/31/2017)
- GLRI USGS Benzophenone (01/31/2017)
- GLRI USGS Pentachlorophenol (01/31/2017)
- Test (01/31/2017)
- GLRI USGS Bis(2-ethylhexyl) phthalate (01/31/2017)
- OPPTS-RAD 2017 (01/31/2017)**
- GLRI USGS Triphenyl phosphate (01/31/2017)

Reports in Selected Group:

(Click to View COGs In Report)

- EFED 1,4-Dioxane
- EFED 1-Bromopropane
- EFED Asbestos
- EFED Carbon Tetrachloride
- EFED Cyclic Aliphatic Bromides Cluster**
- EFED Methylene chloride
- EFED N-methylpyrrolidone
- EFED Pigment Violet 29
- EFED Tetrachloroethylene
- EFED Trichloroethylene
- EFED xxxxxx

COGs in Selected Report:

HBC D (01/01/1900 - 05/31/2017)

Tag Refs

Tag Refs	Searches chemical names within the publication title field and citations lacking the Chemical Group code are displayed to be rectified. Tag potentially applicable citations with the chemical code for the report or reject.
-----------------	---

This screen is used for the literature acquisition process to identify and mark references from the chemical searches. See the following SOP located on the Contractor Site: OPPT RAD Acquisition_Chemical_Criteria.docx for ordering and recall details. This section has been included for tracking of recalled and ordered papers.

The UNIFY Application is designed to automatically locate potentially applicable citations by using the search terms/codes established in the Manage Main OPPT RAD Reports feature in UNIFY. Once the citations are found during the Tag References search and marked for the chemical, the citations are tracked via the OPPT RAD report

screen.

Tag References

SEARCH REPORT GROUPS Collapse Pane

Name:

☒ Starts With
☐ Contains
☐ Exact
☐ Match Case

COC:
 1,4-Dioxane
 1236PP
 124T
 126PP
 12DPA
 12DPE

Due Date:
 From:
 Through:
☐ Include Delivered Reports
☒ Project Reports

Project Report Groups:

- GLRI USGS 4-Nonylphenol (c
- GLRI USGS Benzophenone (c
- GLRI USGS Pentachlorophe
- Test (01/31/2017)
- GLRI USGS Bis(2-ethylhexyl)
- OPPTS-RAD 2017 (01/31/201
- GLRI USGS Triphenyl phosph
- January 20, 2017 (01/20/201
- January 18, 2017 (01/18/201
- January 13, 2017 (01/13/201

Reports in Selected Group:

	Last Run	Report Name	COC	Title String	NOT Title String	Batch to Exclude
view results	04/24/2017 at 01:10 PM	1,4-Dioxane	1 4-Dioxane (01/01/1900-05/31/2017)	1,4-Dioxane p-Dioxane 1,4-Diethylene dioxide 1,4-D [X]		OPPT-RAD 1,4-Dioxane Rejects (0)
view results	04/21/2017 at 08:36 AM	1-Bromopropane	1BP (01/01/1900-05/31/2017)	1-Bromopropane 1-Propyl bromide 3-Bromopropane Abz [X]		OPPT-RAD 1-Bromopropane Rejects (10)
view results	04/18/2017 at 08:55 PM	Asbestos	Asbestos (01/01/1900-05/31/2017)	Asbestos 4T04 7N05 7R-F9 7RF10 AT 7-1 BK 6-20 BP 3 [X]	Mountain cork Mountain leather Mountain wood	OPPT-RAD Asbestos rejects (1)

*NOTE: All References that match on Title String search (excluding NOT Title string search matches) are displayed here regardless of whether they have been tagged or not.

Carbon Tetrachloride (Last Run: 04/25/2017 at 05:28 PM) - 1 records

-- SELECT COC --

Select: All, None

You Selected Item(s)

	Order ID	Author	Title	Source	Year	Status	Data Status	EFED Status	Chemical Groups	Species Groups	Reject Batch
<input type="checkbox"/>	220013	Ugazio, G., Burdino, E., Dacasto, M., Bosio [X]	Induction of Hepatic Drug Metabolizing Enzymes and Interaction with Carbon Tetrachloride in Rats After a Single Oral Exposure to Atrazine	Toxicol. Lett.	1993 69 279 288	Filed at EPA	REMOVED - PARTIALLY CODED	LITE EVAL CODED (ATZ)	ATZ, CCL4	RODE	

Page 1 of 1 pages (1 total records)

OPPT RAD Reports

OPPT RAD/Skim by Chemical Reports

Generates the current status of a report, exports RIS files for each category, views with Excel format and delivers the final files.

This screen generates automated counts for each chemical in a report.

Generate Project Reports

SEARCH REPORT GROUPS Collapse Pane

Name

☒ Starts With
☐ Contains
☐ Exact
☐ Match Case

COC

- 1,4-Dioxane
- 123BPP
- 124T
- 12BP P
- 12DP A
- 12DP E

Due Date
From
Through

☐ Include Delivered Reports
☒ Project Reports

[Clear](#) [Search](#)

Search Results

Expand All	Report Group	Due Date
Expand	EFED 2017	01/31/2018
Expand	ORD MED	01/30/2018
Expand	July 2017	07/18/2017
Expand	Fluoribazole-sodium	07/07/2017
Expand	MCPA/MCPB	06/30/2017
Expand	OW Aluminum 2017	06/25/2017
Expand	June 21, 2017	06/21/2017
Expand	May 26, 2017	06/26/2017

Checking the Status of OPPT RAD Report

The status of the OPPT RAD Report categories should be confirmed on a periodic basis towards the end of the project as part of the two week and one week reports. The OPPT RAD Status Report, a weekly summary of prioritized chemicals is available, however a check on the status of these categories by looking at the actual reports provides a better understanding of the entire process. The Matched on Title, the On-Order, the Unknown and the Reject categories are also checked to ensure all citations are processed accordingly throughout the length of the project.

Just prior to the completion of the project, the lead reviewer should do a quick check of all categories to ensure that all citations are processed.

Weekly Summary

On a weekly basis (every Monday) the OPPT RAD Status Report, a weekly summary of prioritized chemicals, is emailed to OPPT RAD. A file, OPPT RAD Status.xlsx, presents the status of all papers for each chemical and is located on the Contractor site.

	Codes	Total	On-Order, Copy Request or Request from MED Files	Need to apply criteria	To Review	Non- Applicable or did not pass criteria	Reviewed	Date Coding completed
1,4-Dioxane	1,4-Dioxane	610	3	3	31	540	33	

		Last Run	Report Name	Codes	On Order/Recall	Received, Not Addressed	Target Species	N/A (Excluded)	Not Acceptable	Reviewed (Acceptable)		
Deliver	Run	05/01/2017 at 07:10 PM	1,4-Dioxane	1 4-Dioxane (01/01/1900-05/31/2017)							EFED Report Old Lite Eval Report	View

1. Expand the OPPT RAD Report and select View to access the counts for each category.

Chemical	Codes	Total*	Matched on Title, not yet Rejected or Tagged	Unknown	Previously Delivered	Rejected	On Order	On Recall	Need to apply criteria	Non-Target Species to Review	Target Species	N/A (Excluded)	Not Acceptable	Reviewed (Acceptable)	Delivery Date
Carbon Tetrachloride	CCL4 (01/01/1900-05/31/2017)	610	2	0	0	7	2	1	3	31	0	334	206	33	

2. The columns that are transferred to the OPPT RAD Status Table.xlsx include:

- Total (auto generated on spreadsheet for QA).
- On Order + On Recall = On-Order, Copy Request or Request from MED Files on spreadsheet.
- Need to apply criteria = Need to apply criteria on spreadsheet.
- N/A (Excluded) + Not Acceptable = Non-Applicable or did not pass criteria on spreadsheet.
- Reviewed (Acceptable) = Reviewed on spreadsheet.

The following are the codes to use in counting the status:

Column Heading	Code / Notes
Chemical of Concern and Delivery Date	This is filled in when entering the chemical into the table (chemical verification staff add this information)
Total	Total number of publications processed (auto sum of all other fields in this row)
On-Order, Copy Request or Request from MED Files	Number of citations on order/called from MED Files (OL, Copy, COMM, Auth, RECALL)
Need to Apply Criteria	Total number of publications to skim
To Review	Number of citations that meet the criteria for OPPT RAD Review
Non-Applicable or NO (did not pass criteria)	Number of citations did not meet OPPT RAD or ECOTOX criteria (NO, Non-applicable or Archive)

3. When chemicals are completed (report is sent to OPPT RAD), the table row is moved to the bottom of the "Completed Chemicals" spreadsheet.

Quality Assurance Procedure for Completion of OPPT RAD Chemicals

1. At report set-up, quality assurance and data updates are conducted for specific data fields that affect calculations and display of records in the OPPT RAD reports. These

data fields include, Chemical Grade, Chemical Formulation, Percent Purity, Concentration Type, Chemical Analysis Method, Concentration Units Author Reported (for Oral exposure types), Exposure Types and Oral exposures types, see Appendix D - OPPT RAD REPORT INITIAL DATA QA

2. Two to three weeks prior to the due date, provide EPA with citations for publications still on order each time a Weekly Status is provided. Internally, track down any publications needing to be skimmed or reviewed and make sure they are processed right away.

3. One week prior to the deadline, make sure all OK papers have been reviewed. This will allow enough time for QA of the individual publications as well as QA of the Excel report and the accompanying Excel files.

Once the steps above are done, the process of quality assuring the data can begin.

- a. In UNIFY, go to References and select OPPT RAD Reports. Expand Report Group. Go to the OPPT RAD Report for chemical. A new window will open up for generating the report. Choose Excel from the Report Type dropdown and select Generate Report. A file download window will open up asking to open or save the Excel file. Choose open.

An Excel window will open asking to verify the file is from a trusted source and choose yes. Data fields included in the OPPT RAD report are found in Appendix B.

- b. With the Excel file open, make sure that the chemical names are reported correctly. Go through each field to ensure there are no blank fields. If there is a blank field, investigate and ensure there was in fact no data to report and update the record as needed.

Scroll to the bottom of the sheet. Make sure that there is no error message here. If there is an error message, report this to the programming staff.

- c. Either sort by the Phylum field or scroll down and make sure there is a phylum listed for all records. If there is a record(s) without one, investigate this record.
- d. Either sort by the Endpoint field or scroll down and make sure there is an Endpoint listed for every record. If there is a record without an Endpoint, investigate the record.
- e. Scroll down and make sure the habitat matches the species. For example, if the habitat is Aquatic and the species is Duck, this should be corrected.
- f. Sort the Conc Unit Orig field and check to make sure that there is an A Conc type for those units that contain AI (active ingredient).
- g. Make sure the conversions look correct in the following fields:
 - Dur Orig/Dur Unit Orig - conversion to - Dur Preferred/Dur Unit Preferred
(The preferred unit is d (days)).

- Conc #1 Author Reported/ Conc Units Author Reported - conversion to - Conc #1 Purity Adjusted (this is converted according to the entry in the Purity field). NOTE: If the Conc Type is A or NR, the purity conversion will not take place.
- Conc #1 Purity Adjusted - conversion to - Conc #1 Purity Adjusted in Preferred Unit (If any of these conversions seem incorrect, alert the programming staff). The Preferred Units are as follows based on taxa:
 - (1) All aquatic organisms: ai mg/L
 - (2) All terrestrial vertebrates: ai mg/kg bw, ai mg/kg(food), ai lb/A
 - (3) Terrestrial plants: ai lb/A
 - (4) Terrestrial invertebrates: ai mg/kg bw ai mg/kg(food) mg/kg-soil, ai lb/A, ai ug//bee (honey bees and other bees).
- Scroll through all the records and make sure none look out of the ordinary and that there are no blank fields in the report. If there are blank fields, this needs to be investigated to ensure that, in fact, no data was coded.
- When all data looks correct, highlight and copy the Ref# column.
- Insert a worksheet and paste the column.
- Put the cursor in the header box (Ref#) and sort in ascending order.
- Highlight the entire column and choose "Data" "Filter" "Advanced filter" and click in the "Unique records only" check box. Choose "OK".
- Select just the unique reference numbers (not the entire column) then choose copy.
- Create a new worksheet and paste the info in the new sheet. Create one column header labeled "OPPT RAD Reviewed" designating the column that contains the Ecoref#'s generated from Reviewed data and one header labeled "UNIFY" designating the column that contains the Ecoref#'s generated from UNIFY. This worksheet will be used to compare the lists of Ecoref# numbers that were from Reviewed data to the Ecoref#'s UNIFY lists as being "Reviewed (Acceptable)" for the chemical.
- In UNIFY, with the Report Group expanded, and in the current UNIFY Report, select "View". A UNIFY Production window will appear. On the far right select the numbered box for "Reviewed (Acceptable)". A File Download window will appear asking whether you want to open or save file, select Open.
- A Microsoft Office Excel window will open asking to verify the file is from a trusted source, choose "Yes".
- Place the cursor in the header box "ECOREF_NUMBER" and sort in ascending order. Highlight the Ecoref#'s under the header and copy and paste into the new OPPT RAD reviewed worksheet created previously under the "UNIFY" header.

- Compare the two columns of ECOREF numbers.
 - If they are exactly the same then all references are OK.
 - If there are ECOREF numbers missing from the OPPT RAD reviewed list, they are most likely involved in the species verification process and the Species Report Table was not updated. If that step was done, check the reviewed records in UNIFY and make sure that they are not in a “general species category” such as Aquatic Community which would not produce a Phylum. These records will need to be looked at and a more specific species assigned.
 - If there are ECOREF numbers missing from the UNIFY list, the status in Field 17 could be incorrect. Investigate this issue by finding the paper and/or looking for data in UNIFY for the ECOREF#. Change Field 17 if necessary
 - Print out the references list to attach to the completion documentation.
- h. Use the Plotting application (pivot table) located on Contractor site as Data Plot Template.xls to determine outliers as one more Quality Assurance step.
- First, in UNIFY OPPT RAD Reports, open the OPPT RAD Report as an Excel file as before and rename the worksheet “dynamic”. Save file as in the following example: dynamic Carbon Tetrachloride plotting.xls.
 - Open Data Plot Template.xls. A security warning appears above the spreadsheet indicating Macros have been disabled. Select Options Next to Update Security Warning. A Microsoft Office Security Options Security Alert pops up. Select enable this content.
 - Select Import & Plot Data and Re-save the file on Contractor site using the same name as before (e.g. dynamic Carbon Tetrachloride plotting.xls); a Microsoft pop-up appears indicating the file already exists. Do you want to replace the existing file? Select yes.
 - From the plot, look for any outlier data points and investigate as needed. You can view the sorted data and plot again based on limits based on Effect, Concentration, Duration, ConcType, Endpoint, Exp Type, Exp Route, Species Group and Conc Unit to determine trends and possible other outliers. As an example, limit based on species group. From the drop-down, select Aves then plot. A Microsoft pop up appears indicating a formula contains one or more invalid references, select OK. View plots and check for outliers. Repeat with other species groups etc. as needed. Save the file upon closing.

When all of the steps above have been completed, and all of the data are acceptable, the Excel files can be created; and data can be released to OPPT RAD.

A data visualization report using the quality assurance plot is also created and forwarded to OPPT RAD. A report template is located in the OPPT RAD report folder at the contractor’s location.

Excel Files Forwarded to OPPT RAD

When all articles have been reviewed for an OPPT RAD chemical, Excel files are created containing all pertinent citations acquired for the chemical. This section describes the naming convention of the Excel files sent to OPPT RAD and how to generate the files.

OPPT RAD Excel File Naming Convention and Content- The following files are forwarded to OPPT RAD using the same naming convention for each chemical:

- “Chemical name” **acceptable date** (e.g., 1,4-Dioxane acceptable May 2017)- This file includes citations for all papers that were identified as acceptable to the ECOTOX Knowledgebase effort and passed OPPT RAD acceptance criteria. These publications were reviewed and data entered into the system.
- “Chemical name” **not acceptable date** (e.g., 1,4-Dioxane not acceptable May 2017)-This file includes citations for all papers that were identified as acceptable to the ECOTOX Knowledgebase effort but did not pass OPPT RAD acceptance criteria. The data from these publications is not included in the OPPT RAD reports.
- “Chemical name” **excluded date** (e.g., 1,4-Dioxane excluded May 2017)-This file include citations of papers that were identified as not acceptable or archived for the ECOTOX Knowledgebase effort either by rejecting the paper once acquired or rejecting the citation during a literature search (i.e. without acquisition of the paper).
- “Chemical name” **on order date** (e.g., 1,4-Dioxane on order May 2017)-This file includes citations of papers that were identified as acceptable to the ECOTOX Knowledgebase effort during the literature acquisition IDing process. The publications have been ordered but have not been received prior to the OPPT RAD coding deadline.

The data from the UNIFY bibliographic files is transferred into the following Excel fields:

Excel Header (Column Title)	Notes
A (BIB_REF_ID_FK)	Reference ID Number
B (AUTHOR2)	Author(s)
C (TITLE)	Publication Title
D (PUBLICATION_YEAR)	Year Published
E (START_PAGE)	Number of the first page
F (END_PAGE)	Number of the last page
G (TOTAL_PAGES)	Total number of pages
H (DISPLAY_SOURCE)	Publication Information

Excel Header (Column Title)	Notes
I (VOLUME)	Journal Volume
J (ISSUE)	Journal Issue
K (ECOREF_NUMBER)	ECOTOX reference ID number
L (CHEMICAL_GROUPS)	Chemicals of Concern identified in the publication
M (SPECIES_GROUPS)	Species groups (e.g. AVIAN, DOMA, FISH, etc...)

Generating Excel Files

The files are exported from UNIFY References and the OPPT RAD Literature Search files, imported into Excel, formatted and quality assured prior to forwarding to OPPT RAD.

As a tool for QA and reference for generating accurate counts, print and attach a hard copy of the chemical report counts to the back of the OPPT RAD Excel File Checklist. See example below.

Chemical	Codes	Total*	Matched on Title, not yet Rejected or Tagged	Unknown	Previously Delivered	Rejected	On Order	On Recall	Need to apply criteria	Non-Target Species to Review	Target Species	N/A (Excluded)	Not Acceptable	Reviewed (Acceptable)	Delivery Date
Carbon Tetrachloride	CCL4 (01/01/1900-05/31/2017)	610	2	0	0	7	2	1	3	31	0	334	206	33	

OPPT RAD Excel File Checklist**Acceptable** (showing correct data fields)

Number from Report	Number from Excel File	Data Fields Modified	Check	Sent
file name (name acceptable date): acceptable				

Not Acceptable (showing correct data fields)

Number from Report	Number from Excel File	Data Fields Modified	Check	Sent
file name (name not acceptable date) not acceptable				

On Order (showing correct data fields)

Number from Report	Number from Excel File	Data Fields Modified	Check	Sent
file name (name on order date): on order				

Excluded (showing correct data fields)




Number from Report	Number from Excel File	Data Fields Modified	Check	Sent
file name (name on order date): on order				

Sum of Not
Acceptable and
Excluded

Sum of Not
Acceptable and
Excluded

Total

Each document generated in this way should have a heading. See example below.
Delete the .rtf file.

-  OPPT RAD Methylene Chloride Acceptable April 2017.xlsx
-  OPPT RAD Methylene Chloride Excluded April 2017.xlsx
-  OPPT RAD Methylene Chloride Not Acceptable April 2017.xlsx

For each file type (e.g. Acceptable, Not Acceptable, Excluded), remove the underscore in the column headers (e.g. ECOREF_NUMBER should be ECOREF NUMBER). The entire Excel spreadsheet must be formatted to wrap text so that there is no hanging text in any of the cells. Format the row height and column width to the smallest possible.

The file and sort order for the various file types are as follows:

Acceptable: Sort order is by Species Group.

Excel File Column	UNIFY Provided Column Title
A	ECOREF NUMBER (ECOTOX reference ID number)
B	ID (Reference ID Number)
C	AUTHOR
D	TITLE
E	PUBLICATION YEAR
F	START PAGE
G	END PAGE
H	TOTAL PAGES
I	SOURCE (Publication Information); original UNIFY title is DISPLAY_SOURCE
J	VOLUME
K	ISSUE
L	CHEMICAL GROUP CODE
M	SPECIES GROUPS

Excluded: Sort order is by Keywords.

Excel File Column	UNIFY Provided Column Title
A	ID (Reference ID Number)
B	AUTHOR
C	TITLE
D	PUBLICATION YEAR
E	START PAGE
F	END PAGE
G	TOTAL PAGES
H	SOURCE (Publication Information) original UNIFY title is DISPLAY_SOURCE
I	KEYWORDS (ECOTOX rejection criteria)
J	VOLUME
K	ISSUE
L	CHEMICAL GROUP CODE
M	SPECIES GROUPS

Not Acceptable: Sort order is by Acceptability Criteria

NOTE: While reviewing the information in the Not Acceptable file, look for NO EXP TYPE in the Acceptability Criteria. Search for the publication, using the ECOREF number, and check for INJECT exposure route. INJECT studies are acceptable for OPPT RAD and will need to be manually moved into the Acceptable file.

Excel File Column	UNIFY Provided Column Title
A	ECOREF NUMBER (ECOTOX reference ID number)
B	ID (Reference ID Number)

Excel File Column	UNIFY Provided Column Title
C	AUTHOR
D	TITLE
E	PUBLICATION YEAR
F	START PAGE
G	END PAGE
H	TOTAL PAGES
I	SOURCE (Publication Information) original UNIFY title is DISPLAY_SOURCE
J	VOLUME
K	ISSUE
L	ACCEPTABILITY CRITERIA
M	CHEMICAL GROUP CODE
N	SPECIES GROUPS

When creating Excel files for deliverables, please make sure to send to the QAer to look over. The best practice so far is:

- Create Excel files
- QA Excel files
- Save QAed files in the 'Files for EPA' folder in the working directory
- Send email stating all files are created and QAed and are ready for delivery to EPA

Quality Assurance of OPPT RAD Reports and Excel Files

Once the chemical report file and the Excel files have been created, another staff member performs quality assurance checks on each of the files created. This person must be familiar with the steps in creating the report and Excel files.

The chemical report is spot checked for any anomalies. If any anomalies are found, they are reported to the staff member who created the file.

Each Excel file is checked for the correct number of publications from each category in

the report group. For example, the number of publications in the Acceptable Excel file should match the number in the Acceptable report in UNIFY. If any questions arise or errors are found, it is reported to the staff member that created the files to rectify.

In addition, as a tool for QA and reference for generating accurate counts, the printed hard copy of the chemical report counts is checked and matched with the OPPT RAD Excel File Checklist.

The numbers that are found on the checklist need to be quality assured with the OPPT RAD Weekly Status report (added by the staff creating the Excel files) as these are the final numbers for the deliverable.

Once all files are quality assured they are forwarded to OPPT RAD.

Sending OPPT RAD Completed Files (Chemical Report and Excel)

Once the chemical report file and the Excel files have been created and quality assured, they are forwarded to the OPPT RAD staff by email with attachments (See example below). A copy of the email without attachments is forwarded to the Contract staff member who is responsible for updating project status tables and the Contract project manager.

Example Email:

Subject: 1,4-Dioxane (14-Dioxane) May 2017 Report and Citation files

The data for the 1,4-Dioxane May 2017 report is available in the attached Excel spreadsheet. Filters are available to sort the data in each field. CSRA would like to note that if data existed in ECOTOX for domesticated mammals and rodents, it was included in the 1,4-Dioxane May 2017 report.

CSRA has included a 1,4-Dioxane May 2017 Report Summary and Data Plot generated from our in-house data array plotting routine; we use this application for QA on our end.

CSRA has also included the OPPT RAD 1,4-Dioxane May 2017 citation files (i.e. Acceptable, Not Acceptable, and Excluded) in an Excel spreadsheet format.

CSRA has also attached the final documentation for the Chemical Search (OPPT RAD 1,4-Dioxane May 2017 Chemical Report Memo.docx) and Literature Search (OPPT RAD 1,4-Dioxane May 2017 Literature Search Memo.docx) strategies.

Please let us know if you have any questions or concerns regarding the data or the citation files.

Large files in Zip format

If the files are large, convert them to a zip file format. In the mail message, click on the Attach File Icon, find and highlight the files you are sending and right click. From the right click menu, select WinZip and choose: Add to "file name". Go to My Computer and

find the zip file created (ex. 1,4-Dioxane May 2017_Excel files.zip). Right click and say yes to security risk comment. Choose "rename" and change the file extension to .zpt (ex. 1,4-Dioxane May 2017 _Excel files.zpt). Confirm the change. Go back to the email and attach the file to the message.

APPENDIX A: OPPT RAD REPORT FIELDS

Excel Column Designator	Field Name	Description
A	CAS Number	Chemical Abstracts Service (CAS) registry number of chemical tested
B	Chemical Name	Name associated with the chemical tested
C	Is Chemical Also Tested as a Mixture (YES/NO)	Is the tested chemical also tested as a Mixture
D	Chemical Grade	Chemical grade
E	Chemical Formulation	Chemical formulation
F	% Purity	Purity of the test chemical
G	Chemical Analysis Method	Reports if chemical analysis is measured or unmeasured
H	Species Number	Internal Number assigned by ECOTOX/OPPT RAD to species tested
I	Age	Species age
J	Age Unit	Species age unit
K	Lifestage	Species lifestage
L	Organism Initial Weight (unit)	Initial weight of organism
M	Phylum	Phylum of species tested, auto-populated based on taxonomy/species number

Excel Column Designator	Field Name	Description
N	Class	Class of species tested, auto-populated based on taxonomy/species number
O	Order	Order of species tested, auto-populated based on taxonomy/species number
P	Family	Family of species tested, auto-populated based on taxonomy/species number
Q	Genus	Genus of species tested, auto-populated based on taxonomy/species number
R	Species	Species of species tested, auto-populated based on taxonomy/species number
S	Common Name	Common name of species tested
T	Plant/Animal	Denotes if the test species is a plant or animal, auto-populated based on taxonomy
U	Habitat	Denotes if the test is conducted on aquatic or terrestrial species
V	Test Loc	Test Location (Lab/Field)
W	Media	The type of Exposure Media
X	Exp Type	Method of chemical delivery in the experiment
Y	Exposure Route Groups	ECOTOX Exposure Route Groups
Z	Doses and unit	Tested doses and units
AA	Number of Conc	Number of concentrations tested
AB	Only Conc Tested	Only one concentration tested

Excel Column Designator	Field Name	Description
AC	Test ID	ECOTOX Location/Result Number for records imported into the OPPT RAD system
AD	Endpoint 1 Result ID	Result Identification (corresponds to Endpoint 1)
AE	Endpoint 2 Result ID	Result Identification (corresponds to Endpoint 2)
AF	Effect Group	ECOTOX/OPPT RAD Effect Group Code
AG	Effect	ECOTOX/OPPT RAD Effect Code
AH	Meas Desc	ECOTOX Measurement Description
AI	Meas	ECOTOX/OPPT RAD Measurement Code
AJ	Endpt1	Endpoint 1 - The quantification of an observed effect obtained through statistics or other means of calculation for the express purpose of comparing equivalent effects (e.g., LC50). ECOTOX Appendix T identifies and defines the ECOTOX/OPPT RAD endpoint codes.
AK	Endpt2	Endpoint 2 (see above) - this is the companion endpoint, i.e. LOAEL if applicable
AL	Response Site	Response site
AM	Effect Percent (Endpoint 1)	Effect percent of response (corresponds to Endpoint 1)
AN	Effect Percent (Endpoint 2)	Effect percent of response (corresponds to Endpoint 2)
AO	Trend (Endpoint 1)	Trend of the response (corresponds to Endpoint 1)
AP	Trend (Endpoint 2)	Trend of the response (corresponds to Endpoint 1)

Excel Column Designator	Field Name	Description
AQ	Endpoint 1 Final Weight (unit)	Final weight of organism and unit (corresponds to Endpoint 1)
AR	Endpoint 2 Final Weight (unit)	Final weight of organism and unit (corresponds to Endpoint 2)
AS	Dur Mean Orig Op	Mean Duration operator as reported by the author
AT	Dur Mean Orig	Mean Duration as reported by the author
AU	Dur Min Orig Op	Mean Duration operator as reported by the author
AV	Dur Min Orig	Mean Duration as reported by the author
AW	Dur Max Orig Op	Mean Duration operator as reported by the author
AX	Dur Max Orig	Mean Duration as reported by the author
AY	Dur Unit Orig	Duration Unit as reported by author
AZ	Dur Preferred Mean Op	Mean Preferred Duration value operator
BA	Dur Preferred Mean	Mean Duration converted electronically to days, when possible. If not possible, Duration Original (Author reported duration) is retained.
BB	Dur Preferred Min Op	Min Preferred Duration value operator
BC	Dur Preferred Min	Min Duration converted electronically to days, when possible. If not possible, Duration Original (Author reported duration) is retained.
BD	Dur Preferred Max Op	Max Preferred Duration value operator
BE	Dur Preferred Max	Max Duration converted electronically to days, when possible. If not possible, Duration Original (Author reported duration) is retained.

Excel Column Designator	Field Name	Description
BF	Dur Unit Preferred	Preferred Duration Unit
BG	Conc Type	Concentration Type denotes the type of chemical used
BH	Conc #1 Ion	Denotes the ion for the concentration, if reported
BI	Conc #1 Author Reported Mean Op	Mean Concentration Value 1 (corresponds to Endpoint 1) as reported by author operator
BJ	Conc #1 Author Reported Mean	Mean Concentration Value 1 (corresponds to Endpoint 1) as reported by author
BK	Conc #1 Author Reported Min Op	Min Concentration Value 1 (corresponds to Endpoint 1) as reported by author operator
BLH	Conc #1 Author Reported Min	Min Concentration Value 1 (corresponds to Endpoint 1) as reported by author
BM	Conc #1 Author Reported Max Op	Max Concentration Value 1 (corresponds to Endpoint 1) as reported by author operator
BN	Conc #1 Author Reported Max	Max Concentration Value 1 (corresponds to Endpoint 1) as reported by author
BO	Conc Units Author Reported	Concentration Unit 1 (corresponds to Endpoint 1) as reported by author
BP	Conc #1 Purity Adjusted Mean Op	Mean Concentration Value 1 (Purity Adjusted) operator

Excel Column Designator	Field Name	Description
BQ	Conc #1 Purity Adjusted Mean	Mean Concentration converted electronically based on the purity and/or molecular weight of the compound. If not reported, no conversion. If the concentration is measured or based on active ingredient no conversion.
BR	Conc #1 Purity Adjusted Min Op	Min Concentration Value 1 (Purity Adjusted) operator
BS	Conc #1 Purity Adjusted Min	Min Concentration converted electronically based on the purity and/or molecular weight of the compound. If not reported, no conversion. If the concentration is measured or based on active ingredient no conversion.
BT	Conc #1 Purity Adjusted Max Op	Max Concentration Value 1 (Purity Adjusted) operator
BU	Conc #1 Purity Adjusted Max	Max Concentration converted electronically based on the purity and/or molecular weight of the compound. If not reported, no conversion. If the concentration is measured or based on active ingredient no conversion.
BV	Conc #1 Purity Adjusted in Preferred Unit Mean Op	Mean Concentration Value 1 (Purity Adjusted) converted to a standard unit operator
BW	Conc #1 Purity Adjusted in Preferred Unit Mean	Mean Concentration Value 1 (Purity Adjusted) converted to a standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, Concentration Value Purity Adjusted is retained
BX	Conc #1 Purity Adjusted in Preferred Unit Min Op	Min Concentration Value 1 (Purity Adjusted) converted to a standard unit operator

Excel Column Designator	Field Name	Description
BY	Conc #1 Purity Adjusted in Preferred Unit Min	Min Concentration Value 1 (Purity Adjusted) converted to a standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, Concentration Value Purity Adjusted is retained
BZ	Conc #1 Purity Adjusted in Preferred Unit Max Op	Max Concentration Value 1 (Purity Adjusted) converted to a standard unit operator
CA	Conc #1 Purity Adjusted in Preferred Unit Max	Max Concentration Value 1 (Purity Adjusted) converted to a standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, Concentration Value Purity Adjusted is retained
CB	Conc#2 Ion	Denotes the ion for the concentration, if reported
CC	Conc #2 Author Reported Mean Op	Mean Concentration Value 1 (corresponds to Endpoint 1) as reported by author operator
CD	Conc #2 Author Reported Mean	Mean Concentration Value 1 (corresponds to Endpoint 1) as reported by author
CE	Conc #2 Author Reported Min Op	Min Concentration Value 1 (corresponds to Endpoint 1) as reported by author operator
CF	Conc #2 Author Reported Min	Min Concentration Value 1 (corresponds to Endpoint 1) as reported by author
CG	Conc #2 Author Reported Max Op	Max Concentration Value 1 (corresponds to Endpoint 1) as reported by author operator

Excel Column Designator	Field Name	Description
CH	Conc #2 Author Reported Max	Max Concentration Value 1 (corresponds to Endpoint 1) as reported by author
CI	Conc #2 Purity Adjusted Mean Op	Mean Concentration Value 1 (Purity Adjusted) operator
CJ	Conc #2 Purity Adjusted Mean	Mean Concentration converted electronically based on the purity and/or molecular weight of the compound. If not reported, no conversion. If the concentration is measured or based on active ingredient no conversion.
CK	Conc #2 Purity Adjusted Min Op	Min Concentration Value 1 (Purity Adjusted) operator
CL	Conc #2 Purity Adjusted Min	Min Concentration converted electronically based on the purity and/or molecular weight of the compound. If not reported, no conversion. If the concentration is measured or based on active ingredient no conversion.
CM	Conc #2 Purity Adjusted Max Op	Max Concentration Value 1 (Purity Adjusted) operator
CN	Conc #2 Purity Adjusted Max	Max Concentration converted electronically based on the purity and/or molecular weight of the compound. If not reported, no conversion. If the concentration is measured or based on active ingredient no conversion.
CO	Conc #2 Purity Adjusted in Preferred Unit Mean Op	Mean Concentration Value 1 (Purity Adjusted) converted to a standard unit operator
CP	Conc #2 Purity Adjusted in Preferred Unit Mean	Mean Concentration Value 1 (Purity Adjusted) converted to a standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, Concentration Value Purity Adjusted is retained

Excel Column Designator	Field Name	Description
CQ	Conc #2 Purity Adjusted in Preferred Unit Min Op	Min Concentration Value 1 (Purity Adjusted) converted to a standard unit operator
CR	Conc #2 Purity Adjusted in Preferred Unit Min	Min Concentration Value 1 (Purity Adjusted) converted to a standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, Concentration Value Purity Adjusted is retained
CQ	Conc #2 Purity Adjusted in Preferred Unit Max Op	Max Concentration Value 1 (Purity Adjusted) converted to a standard unit operator
CS	Conc #2 Purity Adjusted in Preferred Unit Max	Max Concentration Value 1 (Purity Adjusted) converted to a standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, Concentration Value Purity Adjusted is retained
CT	Conc Units Preferred	Standard unit (All aquatic organisms: mg a.i./L; All terrestrial vertebrates: mg a.i./kg-bw, mg a.i./kg(food), lb a.i./A; Terrestrial plants: lb a.i./A; Terrestrial invertebrates: mg a.i./kg-bw, mg a.i./kg(food), mg/kg-soil, lb a.i./A, ug a.i./bee (honey bees and other bees)) when possible. If not possible, original units are retained
CU	pH	pH
CV	Hardness	Hardness value for the test system
CW	Hardness Unit	Hardness Unit
CX	Organic Matter Value	Organic Matter value for the test system

Excel Column Designator	Field Name	Description
CY	Organic Matter Unit	Organic Matter Unit
CZ	Organic Matter Type	The type of Organic Matter in the test system
DA	Ref #	Internal Reference Number assigned by ECOTOX/OPPT RAD to Reference
DB	Author	Author of the Reference
DC	Title	Title of the Reference
DE	Source	Citation of the Reference
DF	Publication Year	Publication year of the Reference
DG	Comments	Additional comments made during the review of the paper into the OPPT RAD system. These include chemical, species, experimental design, and other effects that do not have an explicit data field in the OPPT RAD system.

APPENDIX B: ECOTOX REPORT LOGIC STANDARDIZED CONCENTRATIONS

Purity and Ion adjustments

Purity

Adjustments by the Purity are made for the following conditions.

- a. Chemical Analysis Method is not Measured (U or NR)
- b. Concentration Type is not 'A' = active part (F, T, D, L, or U)
- c. Ion code is NR

The author reported concentration is multiplied by the purity percentage. If 'NR' is entered, the purity is assumed to be 100%. For example, the purity is 65%. If the concentration was 100 ug/g, the purity adjusted concentration would be 65 ug/g.

Ion

Adjustment for Ion is made if Ion code is NR.

The author reported concentration is multiplied by the Ion percent of the total compound, e.g. Hg is 80% of methylmercury chloride. If the concentration was 100 ug/g, the ion adjusted concentration would be 80 ug/g. If this concentration is in a molar unit, the concentration is adjusted for the ion molar weight, not the tested compound molar weight.

Note that ions could have a double adjustment first for Purity, then for Ion. For example, Caspan (a methylmercury chloride product) has a purity of 65%. If the concentration was 100 ug/g, the purity adjusted concentration would be 65 ug/g. Then adjusting for the bromine ion, 80% of the total compound, the final adjusted concentration would be 51.9 ug/g.

Conversions by Species Group and Exposure Type

Conversions for Aquatic taxa – ECOTOX standard unit is AI mg/L

Lab and Field Exposures

Exposure Type	Conversion
Water (AQUA)	<ul style="list-style-type: none"> Converts to AI mg/L.

Exposure Type	Conversion
Oral, Gavage, Injection (OR, GV, I)	<ul style="list-style-type: none"> Converts to AI mg/kg bdwt <ul style="list-style-type: none"> If unit contains food, fd, or diet, it converts to AI mg/kg food.
Diet (D, DT, or FD)	<ul style="list-style-type: none"> Converts to AI mg/kg food. <ul style="list-style-type: none"> If unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Drinking Water (DR)	<ul style="list-style-type: none"> Convert to AI mg/L. <ul style="list-style-type: none"> If unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Choice, Gestation, Topical, or Lactation (C, CH, GE, LC, or TOP)	<ul style="list-style-type: none"> No conversion.

For molar units, converts to AI mg/L.

Conversions for Terrestrial Plants – ECOTOX standard unit is AI lb/acre

Converts to AI lb/acre. If the units cannot be converted to AI lb/acre, leave the units as reported by the author.

Conversions for Terrestrial Vertebrates – ECOTOX standard units are AI mg/kg bdwt, AI mg/kg food, or AI lb/acre

Lab and Field Exposures

Exposure Type	Conversion
Oral, Gavage, or Injection (OR, GV, INJECT)	<ul style="list-style-type: none"> Converts to AI mg/kg bdwt. <ul style="list-style-type: none"> If unit contains food, fd, or diet, then converts to mg/kg food.
Diet (DT or FD)	<ul style="list-style-type: none"> Converts to AI mg/kg food. <ul style="list-style-type: none"> If the unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Drinking Water (DR)	<ul style="list-style-type: none"> Converts to AI mg/L. <ul style="list-style-type: none"> If unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Choice, Topical, or Environmental (CH, LC, GE, TOP, ENV)	<ul style="list-style-type: none"> No conversion.

No conversion for molar units.

Conversions for Field Exposures (Field N, Field A, Field U)

Converts to AI lb/acre. There is no conversion if the units cannot be converted to AI lb/acre.

Conversions for Terrestrial Invertebrates – ECOTOX standard units AI mg/kg bdwt, AI mg/kg food, AI mg/kg soil, or AI lb/acre

Lab and Field Exposures

Exposure Type	Conversion
Oral, Gavage, or Injection (OR, GV, INJECT)	<ul style="list-style-type: none"> Converts to AI mg/kg bdwt. <ul style="list-style-type: none"> If unit contains food, fd, or diet, then converts to mg/kg food.
Diet (DT or FD)	<ul style="list-style-type: none"> Converts to AI mg/kg food. <ul style="list-style-type: none"> If the unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Drinking Water (DR)	<ul style="list-style-type: none"> Converts to AI mg/L. <ul style="list-style-type: none"> If unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Choice, Topical, or Environmental (CH, LC, GE, TOP, ENV)	<ul style="list-style-type: none"> If unit contains soil, media, recalculated to mg/kg soil. <ul style="list-style-type: none"> If not, no conversion.

No conversion to molar units.

Conversions for Field Exposures (Field N, Field A, Field U)

Convert to AI lb/acre. There is no conversion if the units cannot be converted to AI lb/acre.

Conversions for Hymenoptera – ECOTOX standard units are AI ug/org or AI ug/g bdwt

Lab and Field Exposures

Exposure Type	Conversion
Diet (DT or FD)	<ul style="list-style-type: none"> Converts to AI ug/fd. <ul style="list-style-type: none"> If unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt. If unit contains /org or /bee, converts to ug/org.
Drinking Water (DR)	<ul style="list-style-type: none"> Convert to AI mg/kg food. <ul style="list-style-type: none"> If the unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt.
Drinking Water (DR)	<ul style="list-style-type: none"> Converts to AI mg/L. <ul style="list-style-type: none"> If unit contains bdwt, bw, body wt, bwt, recalculated to mg/kg bdwt. If unit contains org or bee, converts to ug/g org.
Choice, Topical, or Environmental (CH, LC, GE, TOP, ENV)	<ul style="list-style-type: none"> No conversion.
Topical (TOP)	<ul style="list-style-type: none"> Converts to ug/g org.

No conversion for molar units.

Conversions for Field Exposures – (Field N, Field A, Field U)

Convert units, if it can be converted, to AI lb/acre. There is no conversion if the units cannot be converted to AI lb/acre.

Conversions for Terrestrial Fungi – no standard units

Conversions for Field Exposures – (Field N, Field A, Field U)

Convert units, if it can be converted, to AI lb/acre. There is no conversion if the units cannot be converted to AI lb/acre.

APPENDIX C: OPPT RAD REPORT INITIAL DATA QA

1. Choose upcoming chemical (typically ~3mo from due date).
2. Create New Report in UNIFY
 - a. Manage OPPT RAD/Skim by Chemical Reports tab.
 - i. Create new report by selecting the green plus area within the 'Reports in Selected Group' tab.
 - ii. Choose your chemical of interest and select the OPPT RAD checkbox. Leave the Refresh box unchecked to eliminate confusion with the existing report.
 - iii. Select all Chemical Group Codes in report group. This information can be found in the ECOTOX Schedule for OPPT RAD Pesticides.docx. Use the Start Date 01/01/1900. The End Date will be the date the chemical is due.
 - iv. Select submit. The report is now created.

The image displays three sequential screenshots from the UNIFY software interface, illustrating the process of creating a new report.

Left Screenshot: Shows the 'Project Report Groups' list. The 'OPPTS-RAD 2017 (01/31/2017)' group is selected and highlighted in blue.

Middle Screenshot: Shows the 'Main Report' configuration dialog. The 'Main Report' dropdown is set to '1,4-Dioxane'. The 'Refresh' and 'EFED' checkboxes are unchecked. The 'submit' button is visible at the bottom.

Right Screenshot: Shows the 'COC' configuration dialog. The 'COC' dropdown is set to '1,4-Dioxane'. The 'Start Date' is set to '01/01/1900' and the 'End Date' is set to '05/31/2017'. The 'submit' button is visible at the bottom.

3. Choose the **OPPT RAD/Skim by Chemical Reports** tab in the UNIFY side bar.
 - a. Expand the pane that your newly created report has been placed.
 - b. Run your newly created report.
 - c. Notice the Report Name as well as the code dates. Choose the report that matches the information set up in step 2.
 - i. Running the report ensures that references associated with the selected Chemical Group Codes are accounted for and displayed in the Excel file we will generate in the next step.

		Last Run	Report Name	Codes	On Order/Recall	Received, Not Addressed	Target Species	N/A (Excluded)	Not Acceptable	Reviewed (Acceptable)		
Deliver	Run	04/24/2017 at 01:10 P.M.	1,4-Dioxane	1 4-Dioxane (01/01/1900-05/31/2017)							Project Report	View
Deliver	Run	04/21/2017 at 08:36 A.M.	1-Bromopropane	1B P (01/01/1900-05/31/2017)							Project Report	View

4. Select OPPT RAD Report.

- All CAS #'s associated with the selected Chemical Group Codes will be displayed. If any rows are displayed that do not have a chemical name assigned they should be forwarded to chemical verification staff for assignment before generating the report. UNIFY will not allow a user to generate a report until all errors are resolved.
- Once all Chemical Group Codes have names, select the report type
 - OPPT RAD Full Summary Report for Non-Metal toxicants
 - OPPT RAD Full Summary Report (Multiple Conc Types and Temperatures) for Metals.
- Choose Excel as a Report Type and select Generate Report.
- Save the newly generated file in the folder corresponding to the contract, chemical, and report date.

In this case:

- N:\CSRA info\Database (offsite) Work Orders\SMACVCS3 2016 - Jan 2017\OPPT RAD\OPPT RAD Reports\May 2017\1,4-Dioxane\1,4-Dioxane Report QA

1,4-Dioxane - OPPT S-RAD 2017

The following table represents the CAS Numbers and their corresponding Chemical Names and date ranges for this EFED Report. If more than one Chemical Name is present for any CAS Number, please select the CAS Number you would like to display on the report.

CAS Number	Chemical Name	Ion Molecular Weights	Start Date	End Date
123911	<input checked="" type="checkbox"/> 1,4-Dioxane	N/A	01/01/1900	05/31/2017

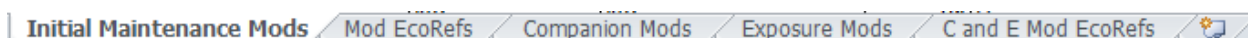
☒ Project Full Summary Report
☐ Project Full Summary Report (Multiple Conc Types and Temperature)
☐ Project Full Summary (OW/TRV Report Excel Format)
☐ Project Full Summary (Include Injection Data)

Report Type

5. Initial QA Concerns

- QA is concerned with updating coding completed prior to Unify. QA is focused on the following data fields (elimination of the Code 'NC' and coding agreement between data fields)
 - Chemical Grade
 - Chemical Formulation
 - % Purity

- iv. Conc Type
- v. Chemical Analysis Method
- vi. Conc Units Author Reported
- vii. Diet and Oral exposures assigned (for conversion)
- viii. NC exposure types
- b. Ensure all of the above columns are in agreement with one another based on current coding paradigm, e.g. Conc Type = A if Grade is T (technical).
 - i. Request an update to all NC and blank cells.
 Note: Purity reported as 100% in the spreadsheet can result from NR or NC in UNIFY as well as 100% actually being reported.
 - ii. Create a new tab titled 'Mod EcoRefs' and populate it with changes to be made. Forward the spreadsheet to Mod staff for updating.



- c. Assign companion endpoints.
 - i. Use the comment 'Only Conc Tested', Test ID, and Result ID to identify potential records from assigning companion endpoints.
- 6. Send email with records to be processed

E-mail Format Example:

SUBJECT: OPPT RAD Purity/Formulation/Grade Mods -- 1,4-Dioxane -WO011

Here are the steps to take for updating the 1,4-Dioxane records. N:\CSRA info\Database (offsite) Work Orders\SMAVCS3 2016 - Jan 2017\OPPT RAD\OPPT RAD Reports\May 2017\1,4-Dioxane \1,4-Dioxane Report QA\1,4-Dioxane Report QA.xls.

The records that need modifications are on the NC mods tab. Please modify the following fields in Unify for all chemicals, Chemical Grade, Purity, Formulation and Radiolabel.

1. Locate the pdf.
2. Open unify and search for the reference number
3. Open the Excel file to see if all or part of the records need to be modified.
4. Print the Coding sheets for the records to be modified.
5. Note the location of the paper (e.g. filed at EPA) so the paper can be returned to the correct status.

6. Check the paper out to you in Data Maintenance status.
7. Locate the chemical information in the paper
 - a. Grades usually use the term grade, e.g. Pharmaceutical Grade, but it is common to see Technical and Analytical without the term grade These codes are located in Appendix B of the ECOTOX Code Appendix at N:\ECOTOX SOPs\REVIEW\ECOTOX Appendices\ECOTOX CODES APPENDIX_draft.docx
****If you find a chemical grade, Also updated the concentration type to A (unless only T,D,L conc types allowed) on the Test Information Tab.
 - b. Formulations are letter codes that follow a chemical name or may be described in the text. These codes are located in Appendix C of the ECOTOX Code Appendix at N:\ECOTOX SOPs\REVIEW\ECOTOX Appendices\ECOTOX CODES APPENDIX_draft.docx
 - c. Update the Purity field if a percent is noted or if there is a number followed by WP for the chemical name.
 - d. Radiolabel is rare, so these will usually be NR. The common radiolabel codes used in text are located in Appendix D of the ECOTOX Code Appendix at N:\ECOTOX SOPs\REVIEW\ECOTOX Appendices\ECOTOX CODES APPENDIX_draft.docx
8. Print and highlight the front page and page(s) where you located the information
9. Mark up coding sheet with changes
10. Make edits in Unity on the Chemical Information Tab, be sure to save.

Thanks.

Subject: OPPT RAD 1,4-Dioxane -WO011- Concentration Type Mods

Please find the following spreadsheet: 1,4-Dioxane QA.xlsx
N:\CSRA info\Database (offsite) Work Orders\SMAVCS3 2016 - Jan 2017\OPPT RAD\OPPT RAD Reports\May 2017\1,4-Dioxane \1,4-Dioxane Report QA\1,4-Dioxane Report QA.xls.

The records that need modifications are on the 'Initial Maintenance Mods' tab. Please modify the following field in Unify: Conc Type (highlighted in red in the spreadsheet).

Here are the steps to take for updating the 1,4-Dioxane records.

1. Locate the pdf.
2. Open unify and search for the reference number

3. Open the Excel file to see if all or part of the records need to be modified.
4. Print the Coding sheets for the records to be modified.
5. Note the location of the paper (e.g. Filed at EPA) so the paper can be returned to the correct status.
6. Check the paper out to you in Data Maintenance status.
7. Locate the chemical information in the paper.

****Rules summarized from the ECOTOX CODES APPENDIX.docx****

-If the chemical grade anything other than NR the conc type should be 'A'. If the chemical purity is ≥ 80 the conc type should be 'A'. If the formulation is CP, CRP, or PF the conc type should be 'A'. If none of these conditions is met, code the conc type as 'F'.

8. Print and highlight the front page and page(s) where you located the information
9. Mark up coding sheet with changes
10. Make edits in Unity on the Chemical Information Tab, be sure to save.

Email for companion endpoints and updated exposure type.

The 1,4-Dioxane Report QA spreadsheet (N:\CSRA Info\Database (offsite) Work Orders\SMACVCS3 Feb 2017 – Jan 2018\WO011 OPPT RAD\06 1,4-Dioxane\1,4-Dioxane Report QA) is ready for QA. Twelve references have been updated with the correct exposure type.

Result summary printouts and PDFs have been placed in your inbox.

7. QA changes
8. Update documentation
9. Associated documentation:
 - a. N:\CSRA info\Database (offsite) Work Orders\SMACVCS3 2016 - Jan 2017\OPPT RAD\OPPT RAD Dose Conversion Logic

Example OPPT RAD Report

(Double click within the table to scroll and view entire report in *xlsx format)

CAS Number	Chemical Name	Is Chemical Also Tested as a Mixture (YES/NO)	Chemical Grade	Chemical Formulation	% Purity	Chemical Analysis Method
134237528	gamma-Hexabromocyclododecane	NC	NR	NR	100	M
134237528	gamma-Hexabromocyclododecane	NC	NR	NR	100	M
134237528	gamma-Hexabromocyclododecane	NC	NR	NR	100	M
134237528	gamma-Hexabromocyclododecane	NO	NR	PRE	100	M
134237528	gamma-Hexabromocyclododecane	NO	NR	PRE	100	M

RELATED SOPS

Documentation related to OPPT RAD

- ECOTOX Chemical Verification and Entry Procedure
- ECOTOX Literature Acquisition and Paper Processing
- ECOTOX Literature Searches, Citation Identification and Skimming
- OPPT RAD Chemical Verification, Literature Searching and Application of OPPT RAD Criteria
- OPPT RAD Coding Guidelines
- Supplemental ECOTOX Guidance_01-21-10.doc
- UNIFY Data Fields and Codes