

ECOTOX

ECOTOXicology Knowledgebase System

ECOTOX Chemical Verification and Entry Procedure

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)

Duluth, Minnesota

By:

CSRA LLC, Duluth, Minnesota

Contract CIO-SP3, HHSN316201200013W

Task Order: EP-G16H-01256, SMAVCS3

TDD 2-8 ECOTOX Application Development and Support

September 2017

ECOTOX Chemical Verification and Entry Procedure

Chemical Module - Table of Contents

Access.....	2
Search.....	2
Navigation	2
Overview	4
Chemicals Excluded in ECOTOX	4
Verification Procedure	5
Minimum Criteria.....	5
Summary and Flowchart of Verification Procedures	5
Verification Sources.....	7
Verification Procedures (Specific Steps)	8
Chemicals submitted through the skimming process	8
Chemicals submitted outside skimming process.....	9
Data fields and Entry into the Unify Chemical Module.....	10
Data Fields	10
Status Section	10
Details Section	10
Alternate Names Section	13
Chemical Information Section (Tabbed)	14
PROPERTIES TAB.....	14
DEGRADATES	15
CHEMICAL GROUPS	16
EPA IDs	18
CONC TYPES.....	18
ION CODES.....	19
REFERENCES.....	20
CHEMICAL USE	20
NOTES.....	21
ATTACHMENTS	21
HISTORICAL CAS	22
EFED.....	23
ARCHIVAL OF UNVERIFIED CHEMICALS.....	23
VERIFICATION QUALITY ASSURANCE.....	25
APPENDIX A: Sources of Verification For Chemical Names And Structures	A-1
APPENDIX B: Chemical Verification Bibliography	B-1
APPENDIX C: Rules to Assist in Chemical Verification Process	C-1
APPENDIX D: STN SEARCH INSTRUCTIONS	D-1
APPENDIX E: SMILES TUTORIAL.....	E-1
APPENDIX F: SMILES Designators	F-1
APPENDIX G: Deleted/Alternate Registry Numbers.....	G-1
APPENDIX H: Valid code creation.....	H-2

ACCESS

The Chemical module can be accessed through the ECOTOX Unify dashboard upon login. To enter, select the Chemical module icon. All users have read access to search for chemicals, view chemicals and view chemical information. To enter, edit or verify records, you must have that role assigned by a data base administrator.







SEARCH

The search function allows users to search by the following data types:







- Chemical/Alternate Name (Starts with, Contains, Exact, and Match Case)
- Molecular Formula (Starts with, Contains, Exact, and Match Case)
- Chemical Abstract Service (CAS) Registry Number
- Dates (Created, Modified and Archived)
- Chemical Group
- Chemical Status (Incomplete, Unverified, Verified, and Deleted/Alternate CAS Number)
- Record Status (Created, Modified, and Archived)
- Record Type (Active, Inactive and Archived)
- Report Type (Excel or HTML)
- Priority References Only (returns only unverified chemical names from priority references)

NAVIGATION

In addition to the search functions, the following icons are used in the navigation of the chemical module:

Icon	Description	Function
	Magnifying glass	Print View
	Binoculars	Search
	Pencil	Edit View
	Page with 'X'	Delete
	Plus Sign/Add Button	Add
	Right Arrow	Hover over to display complete text

ECOTOX Chemical Verification and Entry Procedure

Icon	Description	Function
	Page with Check	Verify
	Circle with Slash	Reject Chemical Verification
	Printer	Print Command
	Excel Sheet	Download to Excel
	Circle Arrow	Return to search screen
	Circle 'i'	Hover over to display modified information

OVERVIEW

The purpose of the chemical files is to integrate a verified chemical, structure and physical properties list into the MED ECOTOXicology Systems software. Chemicals identified through literature review for the ECOTOX databases are verified by ECOTOX staff members and the acquired information is stored in the Chemical Module of Unify, the chemical verification and information data file.

The following documentation details the verification procedures and describes the format of the chemical information data files.

The Chemical Abstracts Services Registry Number (CAS #) is the core of the verification procedure. Each chemical in the database must have a CAS # assigned prior to data entry. The chemical files are linked between ECOTOX software modules by the CAS registry number. The CAS # also provides a link to the Collective Index (CI) name which is stored in the Chemical Module as the Preferred Name (PN). The Chemical Module strives to use the 9th Collective Index Name as its preferred name.

The Chemical Module is accessible to ECOTOX users to assist in linking CAS #s and chemical names to toxicity data. Chemical or physical property data are also stored in the Chemical Module file.

The Chemical Module also provides a link to additional US EPA databases and models (refer to the [SMILES](#) section of this SOP for further information).

Chemicals Excluded in ECOTOX

Any chemical causing an adverse effect is included into the ECOTOX database.

The following are exclusions for the ECOTOX database. For all of the exclusions listed below, an exception for inclusion into ECOTOX will be made as requested by EPA.

- Effluents
- Chemical mixtures (unless a single concentration and CAS number can be provided)
- Water/Soil chemistry effects, e.g. Hardness or pH (unless caused by a single chemical)
- Biological toxicants (venoms, fungal toxins, *Bacillus thuringiensis*, and other plant, animal or microbial extracts or toxins not purified). Essential oils are also Biological toxicants. Exceptions are oils that were previously coded for EFED or those that are commercial products such as Azadirachtin.
- Dietary Chemicals (Nutrients) that are not added in excess (authors state either deficient or sufficient diet)
- Oils (crude or synthetic oils, coal, and petroleum based fuel products or distillates, all of which are mixtures. Note that creosote is OK.)
- Air Pollutants
- Proteins and enzymes
- Clay and diatomaceous earth products

Verification Procedure

Each chemical identified during ECOTOX literature skim and/or review is tracked electronically through the chemical verification process. Each chemical in the data file is verified in one or two chemical name sources (only one source is needed if the source is the Chemical Abstract Services' STN International or the CAS Registry Handbook) and one structure source (Appendices A and B). Chemicals that are not verified through the regular sources are archived. Data associated with unverified chemicals are not entered into ECOTOX.

Minimum Criteria

The minimum criteria for a chemical to be entered into the Chemical Module are a Chemical Abstract Services Registry Number (CAS number) and a preferred name. The Chemical Module Collective Index Name is obtained from either the STN International database or CAS Registry Handbooks available at the MED library, both are indexed by CAS number.

Summary and Flowchart of Verification Procedures

Below are the processes followed to verify chemical information:

- 1) [Search](#) to confirm whether the chemical already exists in the Chemical Module.
- 2) If the chemical name is not in Chemical Module, identify and verify the CAS number, preferred name, synonym(s), chemical and physical property data and structure information.
 - a. Conduct a [STN Search](#) for unverified chemicals
 - i. Located and not trade name, proceed to step 3
 - ii. Located and trade name
 1. Author provides additional information (e.g. another name or molecular formula that confirms the STN match, proceed to step 3.
 2. If the trade name in STN does not match the information that the paper provides, it should be further researched to confirm which source appears to be correct. If STN appears to be incorrect, they should be contacted via email (help@cas.org). The email should contain in detail the discrepancy and chemical product labels and/or MSDS links should be provided along with the paper citation information. STN has fixed discrepancies reported in the past. For example, DCT was reported in the paper as diazinon + captan + thiophanate-methyl. STN listed DCT under diazinon-captan-thiophanate-ethyl. Upon further research, the paper appeared to be correct. STN was notified and updated their records accordingly. If STN's response does not fix the discrepancy then each chemical should be handled on a case by case basis on how to verify/skim/code. If the author does NOT provide additional information to confirm STN match, proceed to step b.

ECOTOX Chemical Verification and Entry Procedure

- b. If chemical information is not found on STN, additional verification sources are checked (the most common and reliable sources are listed below, all additional sources are listed in Appendix A).
 - c. Archive Unverified Chemicals if all sources are investigated and no verification source contains information.
 - 3) Perform Data Entry of Chemical into the Unify Chemical Module.
 - 4) Complete Quality Assurance of Verified Chemical Information.

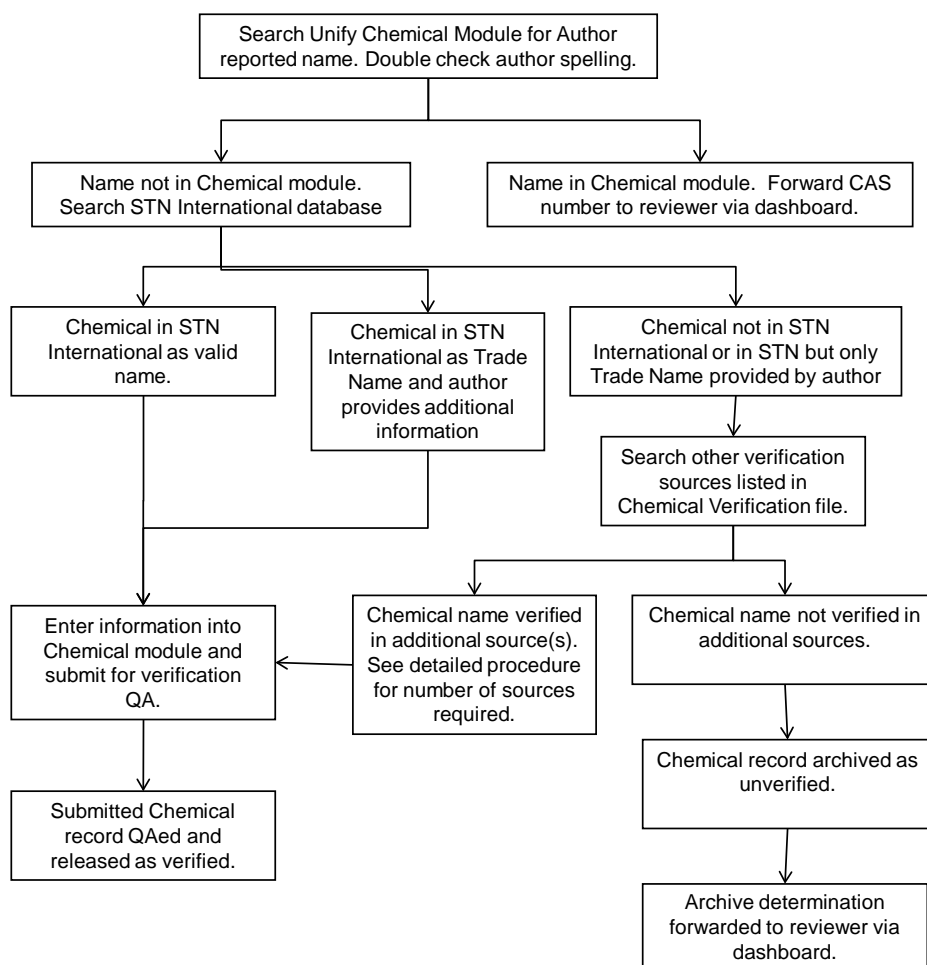


Figure 1. Chemical Verification Flowchart

Verification Sources

Verification sources are used to verify chemical name, synonym CAS number, and structural or physical property information. STN International is the preferred source for chemical verification. The reference number, database location and complete citation of verification publications are listed in Appendices A and B. Appendix C documents additional rules to aid the verification process. The following sources are most commonly used and reliable for verification of chemical name spelling and CAS numbers:

- STN International (ECOREF#1329)
- The U.S. EPA's Chemistry Dashboard (ECOREF#175295)
(<https://comptox.epa.gov/dashboard>)
- ChemBioFinder (www.chembiofinder.com) (ECOREF#58458)
- Sigma-Aldrich on-line catalog (www.sigma-aldrich.com) (ECOREF#58784)
- RTECS (Registry of Toxic Effects of chemical substance, 1983-84 edition, 2 volumes) (ECOREF#13337)
- TSCA (Toxic Substances Control Act Chemical Substance Inventory, 1985 edition, 5 volumes) (ECOREF#13318)
- Dictionary of Chemical Names and Synonyms (1992) (ECOREF#4062)
- The Pesticide Manual 10th edition (1994) (ECOREF#1012)
- The Compendium of Pesticide Common Names website
(<http://www.alanwood.net/pesticides/>) (ECOREF#89844)

VERIFICATION PROCEDURES (SPECIFIC STEPS)

Each chemical identified during ECOTOX skim is tracked through the chemical verification process electronically. All chemicals are searched via STN International database (see Appendix D). Each chemical in the data file is verified in one or two chemical name sources (only one source is needed if the source is the Chemical Abstract Services or STN International reference) and one structure source (Appendices A and B). Chemicals that are not verified through the regular sources will be archived. Data associated with unverified chemicals are not entered into ECOTOX.

If the chemical name from the paper is a trade name, and no other chemical information is given by the author, in addition to STN, the chemical must be verified in an additional source. If the author provides the chemical company that produces the product, CSC will attempt to access the company's web site for additional information about the chemical.

Chemical Degradates, EPA IDs and Use should be researched for prior to starting a New Chemical entry in Unify.

Chemicals submitted through the skimming process

1. Verification staff will retrieve the Incomplete (skim) chemicals to be verified from their dashboard. Prioritized chemicals can be searched by selecting the "Priority References Only" check box in the Search Chemicals screen of the Chemical module or via a custom query searching for upcoming priority chemicals.
2. Select the chemical to be verified by selecting the edit icon.
3. Verify chemical name via the Chemical verification flow chart (Figure 1).
4. If chemical cannot be verified with a CAS number, note "NO 'sources' 'month/year' in the Notes Tab and select the Save Note button. Select the Archive button from the Status section and skip remaining steps listed below. Review the chemical in the paper for additional information. If the author reports the active ingredient associated with the chemical name, instruct the reviewer to code as the active ingredient and note the chemical name in the Chemical Comments data field.
5. If the chemical CAS number is found, add the CAS Number and verification source to the Chemical Name record and click Submit Changes.
 - a. If the CAS number exists in the system, it will ask if this name should become an Alternate Name for the existing CAS Number. Follow prompts to update the record.
 - b. If the CAS Number does not exist in the system, it will ask if you want to be redirected to the Add Chemical screen. Select ok. Add the CAS number to the text box and select submit. Continue to Step 6 and follow additional instructions in Step 10.
6. Update chemical details (e.g., Collective Index name, Molecular Formula, etc.) into the appropriate data fields. Click the Submit Changes button otherwise this information will not be saved.
7. Update chemical Degradates, EPA IDs, Uses, Notes and AR/DR numbers (AR/DR instructions see Appendix G) for the

- chemical.
8. Create a text file containing the information from STN and attach to the record.
 9. Select Submit for Verification from the Status section.
 10. If the original chemical name's CAS Number did not exist in the system, retrieve the original Incomplete (skim) chemical name to be verified from the dashboard in order to link it to the newly created CAS number record. Enter the CAS number and reference. The system will ask if this name should become an Alternate Name for the existing CAS Number. Follow prompts to update the record.
 11. Verify and release Chemical to Unify (see VERIFICATION QUALITY ASSURANCE).
 12. After the chemical has been verified, please go into the Skim module for the particular reference(s) and reskim the paper.

Chemicals submitted outside skimming process

1. If a chemical name is received from an outside source (e.g. upcoming priority chemical) and is not found in the Unify Chemical system complete verification of the chemical name via the Chemical verification flow chart (Figure 1).
2. If a chemical cannot be verified with a CAS number, select Add New Chemical and select Insert Blank CAS Number. Enter the chemical name and note "NO 'sources' 'month/year' " in the Notes Tab and select the Save Note button. If the chemical is an EPA Pesticide Fate Database degradate, designation should also be noted with a comment that 'no papers have been found to be associated with this chemical' in the Notes Tab. Select the Submit for Verification button from the Status section and skip remaining steps listed below.
3. If chemical CAS number is found, search the chemical CAS number.
 - a. If the chemical CAS number is in the Unify system, select the chemical to be verified by selecting the edit icon.
 - b. If the chemical CAS number is not in the Unify system, select Add Chemical from the left hand chemical tab. Add the CAS number to the text box and select submit.
4. Update chemical details (e.g., Collective Index name, Molecular Formula, etc.) into the appropriate data fields, if needed. If any changes have been made, click the Submit Changes button otherwise this information will not be saved.
5. Select the plus sign in the Alternate Names section, add chemical name and reference.
6. Update chemical Degradates, EPA IDs, Uses, Notes and AR/DR numbers (AR/DR instructions see Appendix G) for the chemical.
7. Create a text file containing the information from STN and attach to the record.
8. Select Submit for Verification from the Status section.
9. Verify and release Chemical to Unify (see VERIFICATION QUALITY ASSURANCE).

DATA FIELDS AND ENTRY INTO THE UNIFY CHEMICAL MODULE

Data Fields

The chemical screen is divided into four sections; Status, Details, Alternate Names and Chemical Information. Data fields in each section and their entry/navigation are detailed below.


Status Section

- Record History: The Unify system electronically notes the most recent activity for each record.
- Status: The Unify System tracks the Status, (e.g. Incomplete, Unverified, Verified, or DR/AR) of each chemical electronically.
- Record Type: The Unify system electronically catalogs the chemicals as Active, Inactive, or Archived.
- Record Status: The Unify System tracks the Record Status, (i.e. New, Modified or Deleted) of each chemical electronically.
- Chemical Name - Verified/User: The Unify system provides the verification status of Chemical Name verification and the person who completed the verification.
- Properties - Verified/User: Provides the verification status of Chemical Properties verification and the person who completed the verification.
- SMILES - Verified/User: Provides the verification status of SMILES information verification and the person who completed the verification.

Buttons/Icons

Icon	Description	Function
DR/AR	DR/AR	Selecting this button will cause the chemical to be moved to the Deleted or Alternate Registry number status. If the chemical is changed to this status, the CAS Number needs to be added to the Historical CAS tab of the Chemical Information (tabbed section).
Archive	Archive	Archives the chemical for future verification (See archived chemical processing for further information)
Archive – Under AI	Archive – Under AI	Archives the chemical for future verification (See archived chemical processing for further information) but the chemical will be coded under the Active Ingredient (AI) if reported by the author.

ECOTOX Chemical Verification and Entry Procedure

Icon	Description	Function
Delete	Delete	Deletes the existing chemical from the Chemical Module.
Activate Chemical	Activate Chemical	This selection will reactivate a record that had been changed to a DR/AR, Deleted or Archived status.
Submit For Verification	Submit For Verification	This selection is made once all of the data fields and been entered for a new chemical only. The chemicals set to this status will appear on the Verifier's dashboard for verification processing. Any chemical that has been previously entered and verified and edited will automatically display on the Verifier's dashboard for verification.
	Circle 'i'	This icon reveals the data fields that have been modified for verification

Details Section

- CAS Number: Chemical Abstract Services Registry Number - unique identifier for each chemical. Enter the CAS Registry Number.
- Solvent: Selection box that denote that the chemical is used as a solvent. This selection should be made if the chemical was used as a solvent/carrier for any paper.
- Chemical Structure: 2D depiction of the chemical structure (if SMILES provided)
- CI Name/References: Selection box that denotes the name is a Collective Index name and its associated references. Both references should contain entries unless the verification source is STN International or Chemical Abstract Service Registry Handbooks.
- Chemical Name: The Collective Index name must be obtained from at least one verification source; the CAS Registry Handbook or STN International, the Collective Index name. All associated Alternate Names, CAS Number, Molecular Formula, Structural and Physical property data and the SMILES String are linked electronically to this name in the ECOTOX databases.

The Marked for Delete selection box is for Data Maintenance staff in the event that the Chemical Name is found to be incorrect. If the box is checked, the Chemical Name cannot be selected for skimming/reviewing.


- Tested SMILES (Unique SMILES - Display only)/Reference: SMILES strings are written for chemicals entered into the Ecotoxicology databases. A SMILES string is a linear representation of a chemical structure that is computer

recognizable and can be used to search the chemical in the Ecotoxicology databases. The SMILES String of the compound and its associated reference and page number of the structure image are entered. If a SMILES string cannot be written, a designator is determined (See Appendix F).

SMILES strings are written by the designated personnel using guidelines from one of the following sources:

- Russom, Christine L. 1990. Appendix B. SMILES Tutorial. IN: ASTER Users Manual, ERL-Duluth. (See [Appendix E: SMILES TUTORIAL](#))
- Anderson, E., G.D. Veith, and D. Weininger. 1987. SMILES: A line notation and computerized interpreter for chemical structures. Report No. EPA/600/M-87/021. U.S. Environmental Protection Agency, Environmental Research Laboratory-Duluth, Duluth, MN 55804
- Hunter, R.S., F.D. Culver, and A. Fitzgerald. 1987. SMILES User Manual. A Simplified Molecular Input Line Entry System. Includes extended SMILES for defining fragments. Review Draft, Internal Report, Montana State University, Institute for Biological and Chemical Process Control (IPA), Bozeman, M.T.
- Modeled SMILES (Unique SMILES - Display only)/Reference: The SMILES String used in the modeling software. Usually the same as the Tested SMILES string, but may be entered by removing a disconnected salt or only the active part of the compound.
- Molecular Formula/Reference: Molecular formula identifies each constituent element by its chemical symbol and indicates the number of atoms of each element found in each discrete molecule of that compound, with the associated reference. If the molecular formula cannot be verified the Unspecified check box is selected to denote the formula is unspecified.

Buttons/Icons

Icons	Description	Function
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known. When the reference is retrieved, select the Plus Sign to select the reference and close the search window.
Clear Changes	Clear Changes	Removes all changes made during current session.
Submit Changes button	Submit Changes button	Saves edits made to the Chemical Details section.




Alternate Names Section

- Alternate Chemical Names are obtained from the publication, and entered into the chemical work flow during the skimming process (see ECOTOX Literature Searches, Citation Identification and Skimming SOP). During skimming, a new chemical name will be entered and electronically attached to the reference. The Alternate Name must be verified in two sources unless one is STN International. Alternate Names include synonyms, product IDs, etc. To View/Edit a chemical name, highlight and click the name. To add names select the Plus Sign icon. The Alternate Name view/edit screen contains a Marked for Delete selection box. This is available for Data Maintenance staff in the event that the Alternate Name is found to be incorrect. If the boxed is checked, the Alternate Name cannot be selected for skimming/reviewing.
- In some cases, multiple chemicals will have the same alternate name (this is particularly true for metals but some organics as well). For example, Copper oxide is listed in STN under three CASRN (1344703 (Unspecified), 1317391 (Cu₂O) and 1317380 (CuO)) and Diquat is listed in STN under two CASRN (2764729 (ion) and 85007 (dibromide)). To ensure correct assignment of chemicals in skimming, only the “generic” (or unspecified) name of the compound should be entered into Unify for the generic (or unspecified) CASRN. The generic (or unspecified) name should be omitted from all other CASRNs. The other chemicals would list more specific names such as Copper oxide (Cu₂O) and Diquat dibromide.

If there is no generic or unspecified form of the chemical or if the unspecified form is the Alternate Registry Number, the paper will be skimmed to the generic name under the most common form of the compound using guidelines in this SOP.

Omitting exact duplicate names would create limitations for the public version of ECOTOX in terms of searching for chemicals as only the “generics” would be located in an exact search and more specific names would not. In order that all chemicals within a group can be located in ECOTOX public searches, generic synonyms will be added back to the Chemical file for the public version of ECOTOX by supplying the generic name and CASRN for all versions. A pipe delimited text file is maintained of the CAS Number and Chemical Synonym Names to be added during an ECOTOX update to the chemical file, one combination per line, NO header row. This file is to be stored at the Contractor site (Chemicals_Generic_List.xlsx). This file will be maintained by chemical verification staff and minimal programmer assistance for each update. The list is ongoing as exact duplicates are located and fixed.

Buttons/Icons

Icon	Description	Function
	Plus Sign	Opens the Alternate name entry screen
	Page with X	Deletes the selected Alternate name
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. Alternately, type in the EcoRef Number if known. Search for the reference, select the Plus Sign and the reference number will be transferred.
Cancel	Cancel	Exits the Alternate Name entry screen without committing changes.
Add	Add	Commits the edits to the Alternate name and references.

Chemical Information Section (Tabbed)

PROPERTIES TAB

The format of the entries for most of the following data fields are in the format of mathematical Operator, numeric Value, Units and the associated verification Reference. Enter these data fields as needed. Include verification information into a document that can be attached the chemical for QA. See Appendix A for verification sources of properties.

- **Molecular Weight:** Calculated from the Molecular formula in the Chemical Details section.

The Molecular Weight data field may be over written in some instances. To over write the value, check the Edit box. This opens the data field to editing.

- **TMOA (Toxic Mode of Action):** A common set of physiological and behavioral signs that characterize a type of adverse biological response. Seven major modes of toxic action include: non-polar narcosis, polar narcosis, uncouplers of oxidative phosphorylation, acetylcholinesterase (AChE) inhibitors, irritants, a general group of central nervous system seizure agents, and respiratory blockers (Rand, 1995).


This value is generally calculated from the modeling system (ASTER). In some instances, the TMOA is overridden by selecting and storing the TMOA on the Properties Tabs. This override is directed by EPA.

- **Melting Point:** Melting point is the temperature at which crystals are in equilibrium with the liquid phase at atmospheric pressure. The terms melting point and freezing point are used interchangeably, depending on whether the

substance is being heated or cooled (Hawley, 1981.)

- **Boiling Point:** Boiling point is the temperature at which the vapor pressure of a liquid is equal to the pressure of the atmosphere (Rechsteiner, 1982a). The model used for estimating the boiling point of chemicals is the Meissner method (Rechsteiner 1982a).
- **Vapor Pressure:** Vapor pressure is the pressure in mm of mercury at which a solid is in equilibrium with its own vapor.
- **Vapor Pressure Temperature:** The temperature at which the vapor pressure is reported.
- **Molar Refraction (Henry's Constant):** Molar Refraction (Henry's Constant) is the ratio of chemical concentration in air to concentration in water, when those two phases are in contact and are at equilibrium (Thomas 1982.)
- **Log P:** Log P (the Logarithm of the Octanol-Water partition coefficient) is the equilibrium concentration of solute in a non-polar solvent (octanol) divided by the concentration of the same species in a polar solvent (water; Leo and Weininger, 1984).
- **Water Solubility:** Solubility reflects the maximum amount of chemical that will dissolve in pure water at a given temperature (Lyman, 1982).
- **pKa Value:** pKa is an expression of the strength of an organic acid or base (Perrin et al., 1981). pKa is estimated using an algorithm by Hunter (1988) based on Perrin et al. (1981).
- **LogKoc (Adsorption Coefficient):** The Adsorption Coefficient (Log Koc) is the ratio of soluble fugacity coefficients in the aqueous and organic matter phase (Lyman, 1982b.)

Buttons/Icons

Icon	Description	Function
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. Alternately, type in the EcoRef Number if known. Search for the reference, select the Plus Sign and the reference number will be transferred.
Clear Changes	Clear Changes	Removes all changes made during current session.
Submit This Tab	Submit This Tab	Commits all edits made to the Properties tab.

DEGRADATES

The primary sources of degradate information include:




MED ECOTOXICOLOGY KNOWLEDGEBASE SOPs SEPTEMBER 2017

ECOTOX Chemical Verification and Entry Procedure

- The EPA Pesticide Fate Database (EcoRef # 117876). Web access no longer available. An electronic copy is located on the Contractor site (*PFATE_37_Tables.mdb*).
- Online governmental documents. These can include documents from the U.S. EPA, FAO (Food and Agriculture Organization of the United Nations) and CDPR (California Department of Pesticide Regulation).

To add a degradate, select the Plus Sign icon, perform the chemical search for the degradate. Select the degradate from the retrieved chemicals by adding a reference to the degradate's search result and select the Plus Sign to add and close the Chemical Search screen. If the chemical is not retrieved, the degradate must be verified and added to the Chemical Module prior to selecting the degradate for the Degradate tab.

Buttons/Icons

Icon	Description	Function
	Plus Sign	Opens the Chemical Search screen
	Page with X	Deletes the selected Degradate
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. Alternately, type in the EcoRef Number if known. Search for the reference, select the Plus Sign and the reference number will be transferred.




CHEMICAL GROUPS

The Chemical Group code can be defined by a specific project, e.g. EFED, by chemical element, e.g. As – Arsenic, or by a unique chemical code (e.g. the Chemical Group code for Dieldrin is DLD).

To add a Chemical group, either select the chemical from the Chemical Groups dropdown menu or search for the chemical group by selecting the binocular icon. If the Group has been selected from the dropdown menu, select the Add button to commit the group. If the group was retrieved from the search function, select the Plus Sign icon to add the group and close the search window.

If the Chemical Group code needs to be added, the Binocular icon will link to the code validation file. The code must be added before the group can be selected.

Buttons/Icons


Icon	Description	Function
	Page with X	Deletes the selected Chemical Group
Add	Add	Commits the selection made from the Chemical Group selection box.
	Binocular	Activates the Chemical Groups Validation search page to add or locate the Chemical Group Code(s). Select the Plus Sign to select the code(s) and close the search window.
	Plus Sign	Selects and commits the retrieved Chemical Group Code(s)


Chemical groups can also be added using **Assign Chemicals to Groups** located on the Chemical home page or the navigation links expanded under **Chemicals** within the Unify dashboard. By using this section, multiple chemicals can be added to a chemical group, rather than one chemical at a time.

To add multiple chemicals to a group:

1. Select the group to be added to from the Select Group box (first selection box). When selected, chemicals belonging to the group will appear in the Chemicals in Selected Group box.
2. Search for additional chemicals by selecting the Binoculars icon and perform the search needed to populate the group. Multiple chemicals can be searched as long as they are comma separated.
3. Select retrieved chemicals by clicking the box in the first cell of each record that belongs to the group. If all are to be added, select "All" at the top of the list. "None" will clear all selections.
4. Select **Add Selected Chemicals to Group** to commit the chemicals to the group. The search window will stay open to search for additional chemicals until closed by the user.

Buttons/Icons




Icon	Description	Function
	Page with X	Deletes the selected Chemical from the Group from the Chemicals in Selected Group selection box.

Icon	Description	Function
	Binocular	Activates the Chemical search page to locate chemicals to add to groups.
Add Selected Chemicals to Group	Add Selected Chemicals to Group	Commits the selections from the search retrieval to the Group
All	All	Selects all records retrieved in the chemical search.
None	None	Clears any previous selections in the records retrieved from the chemical search.

EPA IDs

U.S. EPA PC (Pesticide Chemical) Code is a unique chemical code number assigned to a particular pesticide active ingredient or mixture of active ingredients. The primary sources for EPA IDs are the California Department of Pesticide Regulation website (<http://www.cdpr.ca.gov/docs/chemical/monster.htm> or <http://www.cdpr.ca.gov/dprdatabase.htm>) and the Dictionary of Chemical Names and Synonyms CDROM (1998).

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected EPA ID
Add	Add	Commits the entries in EPA ID and Verify ref fields.
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known.
	Plus Sign	Selects the retrieved EcoRef reference and inserts the number into the Verify Ref field.

CONC TYPES

Codes that denote that the concentration is based on the active ingredient or formulation for organic compounds, or as the total, un-ionized or dissolved concentration, for metal, ionic or organo-metallic compounds as a validation source for the Concentration Type data field in the Toxicity Module.




ECOTOX Chemical Verification and Entry Procedure

Metals are defined by the concentration types, total (T), dissolved (D), and labile/free (L); while ammonia or hydrogen sulfide compounds may have total concentrations (T) and/or un-ionized (U) concentrations. Organometals are compounds that contain covalent bonds between carbon atoms and metal atoms and are coded as total (T) concentrations.

Based on the Molecular Formula (or chemical notes for chemicals that have unspecified Molecular Formulas) the Verifier will select the Concentration Type Codes allowable for the chemical from the dropdown list. All approved Concentration Type Codes are shown in the dropdown. If the Molecular Formula is unspecified and there are no notes as to the composition of the compound, the Concentration Types of A and F will be selected by default. In future versions, it is proposed that the system will assign the Concentration Types based on the Molecular Formula and the Verifier will modify them based on the Notes or confirm the Chemical Modules assessment.

EPA must prior approve new Concentration Type codes. Approved codes can be added by selecting the Binocular icon which opens the code validation file in a new window. The code must be added before the Concentration Type can be selected from the dropdown box.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Concentration Type
Add	Add	Commits the selection made from the Concentration Type selection box.
	Binocular	Activates the Concentration Type Validation search page to add an approved Concentration Type Code. Select the Plus Sign to select the Concentration Type and close the search window.
	Plus Sign	Adds new Concentration Type from Concentration Type Validation page.

ION CODES




All constituent elements by chemical symbol are added to Ion Codes as a validation source for the ion data field in the Toxicity Module.

Based on the Molecular Formula (or chemical notes for chemicals that have unspecified Molecular Formulas) the verifier will select the Ion Codes allowable for the chemical from the dropdown list. All approved Ion Codes will show in the dropdown. If the Molecular Formula is unspecified and there are no notes as to the composition of the compound, no Ion codes will be noted. In future versions, it is proposed that the system will assign the Ion Codes based on the Molecular Formula and the verifier will modify them based on the Notes or confirm the Chemical Modules assessment.

If an Ion code needs to be added, the Binocular icon will link to the code validation file.

The code must be added before the Ion Code dropdown can be selected.


Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Ion Code
Add	Add	Commits the selection made from the Ion Code dropdown box.
	Binocular	Activates the Ion Code Validation search page to enter a new Ion Code or select multiple codes. Select the Plus Sign to select each Ion Code and close the search window.
	Plus Sign	Adds new or retrieved Ion Code from Ion Code Validation page.

REFERENCES

This tab will display the Reference Number, Title, Author, Source, Database (AQUIRE and/or TERRETOX) and Publication Year for the verification source for each entry, e.g. Chemical Name, SMILES String, Boiling Point, etc.

Buttons/Icons

Icon	Description	Function
	Page with Arrow	The data in this field has been truncated for display. Mouse over the icon to view the entire value.

CHEMICAL USE

The most common uses for a pesticide active ingredient, e.g. herbicide, are entered.





The primary source of Use information is the PAN

(http://www.pesticideinfo.org/Search_Chemicals.jsp#ChemSearch).

To add a Use either select the use from the Uses dropdown box or search the Uses Validation codes and select the code by clicking the Plus Sign to add and close the Uses screen. If the Use is not retrieved, the Use must be verified and added to the Uses Validation file prior to selecting the degradate for the Degradate tab.

If the Use code needs to be added, the Binocular icon will link to the code validation. The code must be added to the validation file before the Uses can be selected.

Buttons/Icons


Icon	Description	Function
	Page with X	Deletes the selected Use
	Binocular	Activates both the Uses Validation search page and the Reference search page. Locate the Uses code and select the code by clicking the Plus Sign to transfer to the Current Uses field. Locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known. Search for the reference and select the Plus Sign to transfer the reference number to the field.
	Add	Commits the selection made from the Uses selection box.
	Plus Sign	Selects the retrieved Uses Code or Reference.

NOTES

Notes about the chemical entry, e.g. if the same name is used for more than one CAS Number, sources that were checked for verification, or chemical make-up if the molecular formula is contains a 'n' or 'x' (unspecified ratio of ions), etc. are stored.

Enter the text to be saved to the record in the text box.

Buttons/Icons

Icon	Description	Function
	Save Note	Commits the notes that have been added to the chemical.



ATTACHMENTS

An area of the chemical record to upload the verification sources for each chemical entry, this may include a file of the website used for verification.

To add attachments select the Plus Sign to open the file browser. Search for the files to

add. Once located, select the Save Attachment button to commit. A Note area is also available to describe the different attachments, e.g. Boiling Point.



Buttons/Icons

Icon	Description	Function
	Plus Sign	Opens the Browse File window.
Browse	Browse	Opens file explorer window to search for files.
Save Attachment	Save Attachment	Uploads and saves the attachment to the notes entry.
View	View	Opens attachment in Read Only mode.
	Page with X	Deletes the selected attachment

HISTORICAL CAS

- CAS Number/Reference: The Chemical/CAS Number that has been deleted or is an alternate name and its associated reference. The CAS Number can be appended if existing records are stored or Overwritten as needed by selecting one of the two radio buttons.
- Reason: Notes if the Name/CAS number is a Deleted or Alternate number. Select the Reason from the Reason dropdown field.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Historical CAS number selected.
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known. Search for the reference and select the Plus Sign to transfer the reference number.
Add	Add	Commits the edit made from Historical CAS tab.

EFED

This tab allows the selection of the name that should be used in the EFED reports.

ARCHIVAL OF UNVERIFIED CHEMICALS

If the STN search and other sources listed in Appendix A do not provide a CAS number for the chemical name or structure, several additional steps should be taken:

1. Recheck the original paper for accurate spelling and any additional chemical information (active ingredients, formula, synonyms, etc.). Search the bibliography for chemical references. If the author reports the active ingredient associated with the unverified chemical name, instruct the reviewer to code as the active ingredient and note the chemical name in the Chemical Comments data field.
2. Conduct an STN chemical search on the new information found.
3. Check additional verification sources for the new information.
4. If, after an exhaustive search, a CAS number is not found, set the chemical status to Archived. An exhaustive search includes checking printed sources and online sources for the chemical name as well as for probable chemical names (e.g., spelling errors in the chemical name), or contacting the author and/or the chemical manufacturer for more information.
 - a. If the chemical is the only test chemical in the paper, reskim the paper and add the KEYWORD "CAS# UNAVAILABLE and process. (See Reference Module SOP for specific procedures. Process the entire paper as any other deleted reference.)
 - b. If there are other test chemicals, in addition to the Archived chemical(s) in the publication, the verified chemicals will be entered into the system with the following modifications:
 - i. The archived chemical name(s) will be put into the Other Effects field individually if $n \leq 5$ chemicals. If more than five chemicals are unverified, ">n= other chemicals tested" will be put into the Other Effects field. This statement may be modified to include the chemical type if noted in the paper, e.g., "6 surfactants and 4 emulsifiers tested." This information will also be noted on the front of the publication.
 - ii. The total test status will be evaluated and modified if necessary.
 - c. If the chemical name appears to be incorrect or a structurally impossible name, contact the author. If there is no response to the chemical inquiry, forward the chemical name and paper to the EPA Database Manager for final approval for archiving. Archiving will follow the same procedure as outlined above, starting at step # 4.
5. Every two years, the Archived chemicals will be re-searched on STN to ensure that the Chemical Abstract Services has not assigned a CAS number

ECOTOX Chemical Verification and Entry Procedure

to an existing name, or recognized a name as a synonym.

VERIFICATION QUALITY ASSURANCE

Chemicals to be verified upon completion of modifications can be access either through the Quality Assurance Verifier's dashboard or from the link Verify Chemicals on the left column or from the Chemical home page.

From the dashboard:

1. Select the chemical to verify. This will bring the Quality Assurance Verifier to the individual chemical record.
2. QA Verifier will look at the status area to note which areas have been modified; Chemical Name, Properties or SMILES. Specific fields edited are list and can be viewed by hovering the cursor over the "Circle I" icon.
3. QA Verifier will review the notes and attachments to verify the entries/edits made. Each field and tab is looked at and compared to available documentation with special attention to the spelling of chemical names
4. QA Verifier will select the Paper with Check icon to verify the record or reject the edit by selecting the Circle with Line icon for each section as needed. If rejected, a Prompt box will pop-up and the reason for rejection should be added. The chemical and reason for rejection will reappear on the Verification Staff's dashboard for further review and modifications.

Electronic quality assurances have been built into the Chemical module. The QA features eliminate/stop duplicate CAS numbers from being added to the Chemical module or chemical groups. They also ensure that records are in DR/AR status prior to allowing Verification Staff the ability to attach the deleted/alternate CAS Number to the Preferred CAS Number.

APPENDIX A: SOURCES OF VERIFICATION FOR CHEMICAL NAMES AND STRUCTURES

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Agrochemicals Handbook (Royal Society of Chemistry) 1983	5716	Pesticide information, CAS numbers and synonyms	ECOTOX
Aldrich Catalog Handbook 94-95	4292	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Aldrich Catalog Handbook 92-93	4294	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Aldrich Catalog Handbook 83-84	59183	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Aldrich Catalog Handbook 92-93	1009	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Alfa (1990-1991)	7677	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Analysis of PCB Congeners	9451	PCB Congeners CAS only	ECOTOX
ChemBioFinder Web site (www.chembiofinder.com)	58458	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	Online

ECOTOX Chemical Verification and Entry Procedure

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Chemyclopedia-91	1333	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Chemical Information Service (CIS) 1992	3915	Organic and inorganic Compounds by chemical name, has CAS index and structure data	Online system
Chemical Abstracts Services Registry Handbook (numerous volumes)-1965	5713	CAS Numbers and Chemical Module Preferred Collective Index Name	MED Library
Chemistry Dashboard (https://comptox.epa.gov/dashboard)	175295	CAS Numbers, Synonyms, Structures, Properties, Environmental Fate and Transport.	Online
CRC Handbook of Data on Organic Compounds	9825	Organic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	UMD Lib.
Crop Protection Chemicals Reference	1336	Pesticide information, CAS numbers and synonyms	ILL
Dictionary of Chemical Names and Synonyms	4062	Wide assortment of chemical compounds by chemical name and synonym, has CAS index and some structure data	ECOTOX
Dictionary of Organic Chemicals (CDROM)	59184	Organic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	CDROM
Dictionary of Inorganic Chemicals (CDROM)	4295	Inorganic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	CDROM
Dictionary of Organic Chemical -1982	59182	Organic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	ECOTOX

ECOTOX Chemical Verification and Entry Procedure

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network, Version 1.0 (http://www.epa.gov/ncct/dsstox/DSSToxMasterFile.html)	151468	CAS numbers and synonyms, and structure data	Online
Eastman Laboratory Chemicals	8073	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Farm Chemicals Handbook 1994	58206	Pesticide information, CAS numbers and synonyms, some structure data ***Sometimes CAS number presented for a compound is for the main constituent only	MED Lib.
Farm Chemicals Handbook-1992	5327	Pesticide information, CAS numbers and synonyms, some structure data ***Sometimes CAS number presented for a compound is for the main constituent only	ECOTOX
Fluka Chemical Catalog	9826	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Handbook of Chemical Synonyms and Trade Names	2321	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	UMD Lib.
Handbook of Tables for Organic Compound Identification-1967	1008	Organic and inorganic Compounds by chemical name, has some structure and Physical Property data	MED Library

ECOTOX Chemical Verification and Entry Procedure

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Herbicide Handbook of the Weed Society of America	1327	Pesticide information, CAS numbers and synonyms, some structure data ***Sometimes CAS number presented for a compound is for the main constituent only	MED Library
ICN Biomedicals, Inc.	3047	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
National Pesticide Information Retrieval System (http://ppis.ceris.purdue.edu)	156761	Chemical names, synonyms and PC codes	Online
Merck Index, 11th Edition-1989	5728	Mostly organic compounds by chemical name, has some CAS numbers and some structure and Physical Property data	ECOTOX
MSDS Reference for Crop Protection Chemicals	1337	Pesticide information, CAS numbers and synonyms	ILL
OPPT SMILES Verification Source	150908	Structure Data	ECOTOX
Pesticide Index, 5th Edition-1976	5723	Pesticide information, CAS numbers, synonyms and some structure data	ECOTOX
RTECS fiche (January 1990)	58207	Chemical names, synonyms and CAS numbers	ECOTOX
RTECS (Registry of Toxic Effects of chemical substance, 1983-84 ed., 2 vols)	13337	Chemical names, synonyms and CAS numbers	ECOTOX
Sigma	4293	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX

ECOTOX Chemical Verification and Entry Procedure

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Sigma-Aldrich Library of Rare Chemicals-Structure Index	1001	Structure data only, organized by Aldrich product numbers	ECOTOX
STN International (CAS) 1994	1329	***Most complete source of chemical name, synonym and structure information, no physical properties	Online
TCI America	9679	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
The Pesticide Manual 9 th edition, 1991	9824	Pesticide Compounds by chemical name, synonym, product code, has CAS index and some structure and Physical Property data	ECOTOX
The Pesticide Manual 10 th edition, 1994	1012	Pesticide Compounds by chemical name, synonym, product code, has CAS index and some structure and Physical Property data	ECOTOX
Tracor Jitco (A historical commercial source. No longer used.)	58995	Chemical names, synonyms and CAS numbers	Commercial Source
TSCA (Toxic Substances Control Act Chemical Substance Inventory, 1985 ed., 5 vols)	13318	Chemical names, synonyms and CAS numbers	ECOTOX
World Wide Web (misc. web sources) A copy of the verification page is saved to the Attachments tab of the chemical entry. This includes company MSDS sheets or Chemical Labels.	58886	Chemical names, synonyms and CAS numbers	Online

ECOTOX Chemical Verification and Entry Procedure

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
ADDITIONAL SOURCES NOT LISTED IN SOP			
Handbook of Environmental Data on Organic Chemicals – 1977	1002	Organic compounds with chemical name, and has some structure and Physical Property data	MED Library
CRC Handbook of Chemistry and Physics 1982 and 1986	1003	Organic and Inorganic compounds with chemical name, and has some structure and Physical Property data	MED Library
Physical Properties of Compounds (II and III) 1959	1004	Organic and Inorganic compounds with chemical name, and has some structure and Physical Property data	MED Library
The SCS/ARS/CES Pesticide Properties Database for Environmental Decision Making	5739		MED Library
Linear Solvation Energy Relationships. 41. Important Differences Between Aqueous Solubility Relationships for Aliphatic and Aromatic Solutes	1005		
Compendium of Pesticide Common Names (http://www.alanwood.net/pesticides/)	89844	Pesticides listed by common name, CAS #, IUPAC name, and molecular formula. Has some structure information	Online
California Department of Pesticide Regulation (http://www.cdpr.ca.gov/dprdatabase.htm)	89843	Multiple databases containing chemicals, pesticides, companies, products, etc.	Online

ECOTOX Chemical Verification and Entry Procedure

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
PAN Pesticide Database (http://www.pesticideinfo.org/Search_Chemicals.jsp)	89842	Pesticides searchable by name or CAS #. Includes CAS #, Name, synonyms, targets, toxicity data, related chemicals and regulatory information.	Online
US EPA Office of Pesticide Programs Pesticide Fate Database – No web access available. An electronic copy of the data file is located at the Contractor site: PFATE_37_Tables.mdb.	117876	Multiple databases containing chemicals, pesticides, companies, products, etc.	Online
United States National Library of Medicine ChemIDplus Advanced (http://chem.sis.nlm.nih.gov/chemidplus)	117766	Chemical names, synonyms, properties and CAS numbers.	Online

APPENDIX B: CHEMICAL VERIFICATION BIBLIOGRAPHY

- Historical Chemical Verification Sources. (2009) (ECOREF # 117604)

Addison, R. F. and Cote, R. P. - Variation with Chain Length in Acute Toxicity of Alkylhydroxamic Acids to Salmon (*Salmo salar*) Fry. *Lipids* 8(9): 493-497 (1973) (ECOREF # 5377)

Ahlborg, U. G., Hakansson, H., Lindstrom, G., and Rappe, C. - Studies on the Retention of Individual Polychlorinated Dibenzofurans (PCDFs) in the Liver of Different Species. *Chemosphere* 20(7-9): 1235-1240 (1990) (ECOREF # 89416)

Ahmed, A. E., Farooqui, M. Y. H., and Trieff, N. M. - Nitriles. In: M.W.Anders (Ed.), *Bioactivation of Foreign Compounds*. Academic Press, Inc., Orlando, FL : 485-518 (1985) (ECOREF # 145)

Alabaster, J. S. - Survival of Fish in 164 Herbicides, Insecticides, Fungicides, Wetting Agents and Miscellaneous Substances. *Int.Pest Control* 11(2): 29-35 (Author Communication Used) (1969) (ECOREF # 542)

Aldrich Chemical Company Incorporated. - Aldrich Catalog Handbook of Fine Chemicals. Aldrich Chemical Co.Inc., Milwaukee, WI : 1509 p. (1984) (ECOREF # 59183)

Aldrich Chemical Company Incorporated. - Catalog Handbook of Fine Chemicals, 1992-1993. Aldrich Chemical Co.Inc., Milwaukee, WI : -1992 (1992) (ECOREF # 4294)

Aldrich Chemical Company. - Aldrich Structure Index. 1992-1993 Edition. Aldrich Chemical Co.Inc., Milwaukee, WI : 548 (1992) (ECOREF # 1009)

Aldrich Chemical Company, Inc. - Catalog Handbook of Fine Chemicals 1994-1995. Aldrich Chemical Co.Inc., Milwaukee, WI : 2373 p. (1994) (ECOREF # 4292)

Aldrich Chemical Company Inc. - Sigma-Aldrich Brands Home Page. <http://www.sigma-aldrich.com> (2001) (ECOREF # 58784)

Aldrich, Chemical Co. - Sigma-Aldrich Library of Rare Chemicals - Structure Index. Aldrich Chemical Co.Inc., Milwaukee, WI : 1445 p. (1993) (ECOREF # 1001)

America, T. C. I. - Organic Chemicals, Laboratory Organics Fine and Specialty Organics Mfg., 91/92 Catalog. TCI America, Portland, OR : 1405 p. (1991) (ECOREF # 9679)

American Chemical Society. - Chemical Abstracts Services Registry Handbook. Am.Chem.Soc., Columbus, OH (1965) (ECOREF # 5713)

Anonymous. - Introduction of the Recently Registered Pesticides Methyldimlone and Amiprophosmethyl Herbicides. *Shokubutsu Boekisho Chosa Kenkyu Hokoku* (See Res.Bull.Plant Prot.Serv.Jpn.) 32(11): 488-489 (JPN) (1978) (ECOREF # 6756)

Auer, C. M., Nabholz, J. V., and Baetcke, K. P. - Mode of Action and the Assessment of Chemical Hazards in the Presence of Limited Data: Use of Structure-Activity Relationships (SAR) Under TSCA. *Environ.Health Perspect.* 87: 183-197 (1990) (ECOREF # 322)

- Ballesteros, M. L., Bianchi, G. E., Carranza, M., and Bistoni, M. A. - Endosulfan Acute Toxicity and Histomorphological Alterations in *Jenynsia multidentata* (Anablepidae, Cyprinodontiformes). *J.Environ.Sci.Health Part B* 42(4): 351-357 (2007) (ECOREF # 103207)
- Ballschmiter, K. and Zell, M. - Analysis of Polychlorinated Biphenyls (PCB) by Glass Capillary Gas Chromatography. *Fresenius Z.Anal.Chem.* 302: 20-31 (1980) (ECOREF # 9451)
- Benoit-Guyod, J. L., Andre, C., and Clavel, ad K. - Chlorophenols: Degradation and Toxicity (Chlorophenols: Degradation et Toxicite). *J.Fr.Hydrol.* 15(3): 249-266 (FRE) (ENG ABS) (1984) (ECOREF # 4038)
- Bergquist, J., Strandberg, C., Andersson, M., Sterner, O., Pesando, D., and Girard, J. P. - Structure-Activity Relationships for Unsaturated Dialdehydes 8. Comparative Effects of 10 Sesquiterpenoids on the Sea Urchin Gamete Fertilization. *Toxicol.In Vitro* 7(3): 205-212 (1993) (ECOREF # 16764)
- Bernot, R. J., Brueseke, M. A., Evans-White, M. A., and Lamberti, G. A. - Acute and Chronic Toxicity of Imidazolium-Based Ionic Liquids on *Daphnia Magna*. *Environ.Toxicol.Chem.* 24(1): 87-92 (2005) (ECOREF # 80861)
- Bhatnagar, M. C., Laxmi, R., Sharma, V., and Sharma, I. - Toxicity of Valour and Match to Common Carp, *Cyprinus carpio* (Linn.). *J.Ecophysiol.Occup.Health* 3(1/2): 85-92 (2003) (ECOREF # 93481)
- BioByte Corporation. - CLogP Windows DLL Bio-Loom Vers.1.5. ClogP User Guide.BioByte Corp.Claremont, CA 91711 : 29 p. (Available: <http://www.biobyte.com/index.html>) (2005) (ECOREF # 83337)
- Bisiach, M. - Laboratory Algicidal Screening for the Control of Algae in Rice. *Riso* 21: 43-58 (1971) (ECOREF # 58488)
- Bradbury, S. P., Carlson, R. W., Niemi, G. J., and Henry, T. R. - Use of Respiratory-Cardiovascular Responses of Rainbow Trout (*Oncorhynchus mykiss*) in Identifying Acute Toxicity Syndromes in Fish. Part 4. Central Nervous System Seizure Agents. *Environ.Toxicol.Chem.* 10: 115-131 (1991) (ECOREF # 329)
- Bringmann, G. and Kuhn, R. - Limiting Values for the Noxious Effects of Water Pollutant Material to Blue Algae (*Microcystis aeruginosa*) and Green Algae (*Scenedesmus quadricauda*) in Cell Propagation Inhibition Tests (Grenzwerte der Schadwirkung Wassergefahrdender Stoffe Gegen Blaualgen (*Microcystis aeruginosa*) und Grunalgen (*Scenedesmus quadricauda*) im Zellvermehrungshemmtest). *Vom Wasser* 50: 45-60 (GER) (ENG ABS) (ENG TRANSL) (OECDG) (1978) (ECOREF # 19121)
- Brooke, L. T., Call, D. J., Geiger, D. L., and Northcott, C. E. - Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 1. Center for Lake Superior Environmental Stud., Univ.of Wisconsin-Superior, Superior, WI : 414 p. (1984) (ECOREF # 12448)
- Buckingham, J. Ed. - Dictionary of Organic Chemicals. Chapman and Hill, 5th Edition, New York, NY : 5769 p. (1982) (ECOREF # 59182)

- Buckley, J. A., Whitmore, C. M., and Liming, B. D. - Effects of Prolonged Exposure to Ammonia on the Blood and Liver Glycogen of Coho Salmon (*Oncorhynchus kisutch*). *Comp.Biochem.Physiol.C* 63(2): 297-303 (1979) (ECOREF # 5712)
- Budavari, S. - Merck Index, 11th Edition. Merck & Co., Inc., Rahway, NJ (1989) (ECOREF # 5728)
- Buhl, K. J. and Hamilton, S. J. - Acute Toxicity of Fire-Control Chemicals, Nitrogenous Chemicals, and Surfactants to Rainbow Trout. *Trans.Am.Fish.Soc.* 129(2): 408-418 (2000) (ECOREF # 47875)
- Burreau, S., Broman, D., and Orn, U. - Tissue Distribution of 2,2',4,4'-Tetrabromo[14C]Diphenyl Ether ([14C]-PBDE 47) in Pike (*Esox lucius*) After Dietary Exposure - A Time Series Study Using Whole Body Autoradiography. *Chemosphere* 40(9-11): 977-985 (2000) (ECOREF # 47910)
- Byers, R. E. and Carbaugh, D. H. - Vole Population Shifts Related to Rodenticide Usage. *Hortscience* 24(5): 783-785 (1989) (ECOREF # 75463)
- Calumpang, S. M. F., Medina, M. J. B., Tejada, A. W., and Medina, J. R. - Toxicity of Chlorpyrifos, Fenubucarb, Monocrotophos, and Methyl Parathion to Fish and Frogs After a Simulated Overflow of Paddy Water. *Bull.EnvIRON.Contam.Toxicol.* 58(6): 909-914 (1997) (ECOREF # 17983)
- Cambridge Isotope Laboratories. - Cambridge Isotope Laboratories PCB Cogener Listing. Personal Communication, 10/19/94, Cambridge Isotope Laboratories (CIL), Andover, MA : 3 p. (1994) (ECOREF # 1010)
- Campbell, J. B., Woolley, D. E., Vijayan, V. K., and Overmann, S. R. - Morphometric Effects of Postnatal Lead Exposure on Hippocampal Development of the 15-Day-Old Rat. *Brain Res.* 255(4): 595-612 (1982) (ECOREF # 58508)
- Cantone, F. A. and Vandenberg, J. D. - Genetic Transformation and Mutagenesis of the Entomopathogenic Fungus *Paecilomyces fumosoroseus*. *J.Invertebr.Pathol.* 74(3): 281-288 (1999) (ECOREF # 101012)
- Carter, C. C. and Hestand, R. S. - The Effects of Selected Herbicides on Phytoplankton and Sulfur Bacteria Populations. *J.Aquat.Plant Manag.* 15: 47-56 (1977) (ECOREF # 62318)
- Castillo, C. G., Montante, M., Dufour, L., Martinez, M. L., and Jimenez-Capdeville, M. E. - Behavioral Effects of Exposure to Endosulfan and Methyl Parathion in Adult Rats. *Neurotoxicol.Teratol.* 24(6): 797-804 (2002) (ECOREF # 103381)
- Chapman & Hall. - CHCD Dictionary of Organic Compounds on CD-ROM. Chapman and Hall, London, UK (1993) (ECOREF # 59184)
- Chapman & Hall. - CHCD Dictionary of Inorganic Compounds on CD-ROM. Chapman & Hall, London, UK (1993) (ECOREF # 4295)
- Chapman, P. M. and McPherson, C. - Comparative Zinc and Lead Toxicity Tests with Arctic Marine Invertebrates and Implications for Toxicant Discharges. In: E.G.Baddaloo, S.Ramamoorthy and J.W.Moore (Eds.), *Proc.19th Annual Aquatic Toxicity Workshop*, Oct.4-7, 1992, Edmondton, Alberta, Can.Tech.Rep.Fish.Aquat.Sci.No.1942:7-22// Polar

Rec . 29(168): 45-54 (1993) (ECOREF # 4092)

ChemBioFinder.Com. - ChemBioFinder.Com – Scientific Database Gateway.
<http://chembiofinder.cambridgesoft.com> (2001) (ECOREF # 58458)

Chemical and Pharmaceutical, Press. - Crop Protection Chemicals Reference, 8th Ed.
Chemical and Pharmaceutical Press, c/o John Wiley & Sons, Inc., 605 Third Avenue,
New York, NY : 1892 p. (1992) (ECOREF # 1336)

Chemical Information System. - Structure and Nomenclature Search System (SANSS),
Version 7.02. Chemical Information System Inc., Baltimore, MD (1992) (ECOREF #
3915)

Chemical Pharmaceutical Press. - MSDS Reference for Crop Protection Chemicals, 4th
Ed. Chemical and Pharmaceutical Press, c/o John Wiley & Sons, Inc., 605 Third
Avenue, New York, NY : 1414 p. (1992) (ECOREF # 1337)

Clare, A. S., Costlow, J. D., Bedair, H. M., and Lumb, G. - Assessment of Crab Limb
Regeneration as an Assay for Developmental Toxicity. Can.J.Fish.Aquat.Sci. 49: 1268-
1273 (1992) (ECOREF # 13611)

Clements, C., Ralph, S., and Petras, M. - Genotoxicity of Select Herbicides in *Rana*
catesbeiana Tadpoles Using the Alkaline Single-Cell Gel DNA Electrophoresis (Comet)
Assay. Environ.Mol.Mutagen. 29(3): 277-288 (1997) (ECOREF # 20274)

Coats, J. R. - Mechanisms of Toxic Action and Structure-Activity Relationships for
Organochlorine and Synthetic Pyrethroid Insecticides. Environ.Health Perspect. 87:
255-262 (1990) (ECOREF # 9403)

Covey, R. P., Koch, B. L., and Larsen, H. J. - Influence of Vesicular Arbuscular
Mycorrhizae on the Growth of Apple and Corn in Low-Phosphorous Soil.
Phytopathology 71: 712-715 (1981) (ECOREF # 56456)

CRC Press, Inc. - Handbook of Chemical Synonyms and Trade Names. Gardner,W.,
E.I.Cooke and R.W.I.Cooke (Eds.), Handbook of Chemical Synonyms and Trade
Names, CRC Press, Inc., Boca Raton, FL (1978) (ECOREF # 2321)

Damani, L. A. and Crooks, P. A. - Oxidative Metabolism of Heterocyclic Ring Systems.
In: W.B.Jakoby, J.R.Bend, and I.Caldwell (Eds.), Metabolic Basis of
Detoxification. Metabolism of Functional Groups. Academic Press, Inc., New York, NY :
69-89 (1982) (ECOREF # 2005)

Dandy, J. W. T. - Activity Response to Chlorine in the Brook Trout, *Salvelinus fontinalis*
(Mitchill). Can.J.Zool. 50(4): 405-410 (1972) (ECOREF # 9062)

Dawson, D. A., Schultz, T. W., Baker, L. L., and Wilke, T. S. - Comparative
Developmental Toxicity of Acetylenic Alcohols on Embryos and Larvae of *Xenopus*
laevis. In: W.G.Landis and W.H.Van der Schalie (Eds.), Aquatic Toxicology and Risk
Assessment, Vol.13, ASTM STP 1096, Philadelphia, PA : 267-277 (1990) (ECOREF #
5363)

Deneer, J. W., Sinnige, T. L., Seinen, W., and Hermens, J. L. M. - Quantitative
Structure-Activity Relationships for the Toxicity and Bioconcentration Factor of
Nitrobenzene Derivatives Towards the Guppy (*Poecilia reticulata*). Aquat.Toxicol.

10(2/3): 115-129 (OECDG Data File) (1987) (ECOREF # 178)

Department of Pesticide Regulation. - Chemical Ingredient Queries.

<http://www.cdpr.ca.gov/docs/monster/monster.htm> (2003) (ECOREF # 89843)

Dharia, J. R., Gavande, B. M., and Gupta, S. K. - Ecotoxicity Studies of Some Organotin Monomers and Polymers. *Toxicol.Environ.Chem.* 24(3): 149-154 (1989) (ECOREF # 17155)

Diamond, S. A., Newman, M. C., Mulvey, M., and Guttman, S. I. - Allozyme Genotype and Time-to-Death of Mosquitofish, *Gambusia holbrooki*, During Acute Inorganic Mercury Exposure: A Comparison of Populations. *Aquat.Toxicol.* 21: 119-134 (1991) (ECOREF # 5317)

Dreisbach, R. R. - Physical Properties of Compounds (II and III). *Am.Chem.Soc., Adv.in Chem.Ser.No 22* : 491 p. (1959) (ECOREF # 1004)

Eastman Chemical Company. - Laboratory Chemicals. Catalog No.55, Eastman Chemical Co., Rochester, NY : 1195 p. (1993) (ECOREF # 8073)

Eliason, E. A. and Potter, D. A. - Impact of Whole-Canopy and Systemic Insecticidal Treatments on *Callirhytis cornigera* (Hymenoptera: Cynipidae) and Associated Parasitoids on Pin Oak. *J.Econ.Entomol.* 93(1): 165-171 (2000) (ECOREF # 87491)

Fingas, M. F., Kyle, D. A., Laroche, N., Fieldhouse, B., Sergy, G., and Stoodley, G. - The Effectiveness Testing of Oil Spill-Treating Agents. In: P.Lane (Ed.), *The Use of Chemicals in Oil Spill Response*, ASTM STP 1252, Philadelphia, PA : 286-298 (1995) (ECOREF # 19830)

Fisher Scientific. - Handbook of Fine Chemicals, 1995-1996. Fisher Scientific, Pittsburgh, PA : 2004 p. (1995) (ECOREF # 1013)

Fisher, S. W., Lydy, M. J., Barger, J., and Landrum, P. F. - Quantitative Structure-Activity Relationships for Predicting the Toxicity of Pesticides in Aquatic Systems with Sediment. *Environ.Toxicol.Chem.* 12: 1307-1318 (1993) (ECOREF # 7293)

Fisk, A. T., Cymbalisty, C. D., Bergman, A., and Muir, D. C. G. - Dietary Accumulation of C12- and C16-Chlorinated Alkanes by Juvenile Rainbow Trout (*Oncorhynchus mykiss*). *Environ.Toxicol.Chem.* 15(10): 1775-1782 (1996) (ECOREF # 17248)

Fluka Chemical Corporation. - Fluka Chemical Catalog. Fluka Chemical Co., Ronkonkoma, NY : 1512 p. (1993) (ECOREF # 9826)

Franks, N. P. and Lieb, W. R. - Mechanisms of General Anaesthesia. *Environ.Health Perspect.* 87: 199-205 (1990) (ECOREF # 3261)

Fukuto, T. R. - Mechanism of Action of Organophosphorous and Carbamate Insecticides. *Environ.Health Perspect.* 87: 245-254 (1990) (ECOREF # 3577)

Geets, A., Liewes, E. W., and Ollevier, F. - Efficacy of Some Anthelmintics Against the Swimbladder Nematode *Anguillicola crassus* of Eel *Anguilla anguilla* Under Saltwater Conditions. *Dis.Aquat.Org.* 13(2): 123-128 (1992) (ECOREF # 16061)

Geiger, D. L., Northcott, C. E., Call, D. J., and Brooke, L. T. - Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 2. Ctr.for Lake

Superior Environ.Stud., Univ.of Wisconsin-Superior, Superior, WI : 326 p. (1985)
(ECOREF # 12447)

Geiger, D. L., Poirier, S. H., Brooke, L. T., and Call, D. J. - Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*) Volume III. Ctr.for Lake Superior Environ.Stud., Univ.of Wisconsin-Superior, Superior, WI : 328 (1986)
(ECOREF # 12858)

Geiger, D. L., Call, D. J., and Brooke, L. T. - Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*) Volume IV. Ctr.for Lake Superior Environ.Stud., Volume 4, Univ.of Wisconsin-Superior, Superior, WI : 355 (1988)
(ECOREF # 12859)

Geiger, D. L., Brooke, L. T., and Call, D. J. - Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Volume 5. Ctr.for Lake Superior Environ.Stud., Univ.of Wisconsin-Superior, Superior, WI : 332 p. (1990) (ECOREF # 3217)

Gillett, J. W., Chan, T. M., and Terriere, L. C. - Interactions Between DDT Analogs and Microsomal Epoxidase Systems. J.Agric.Food Chem. 14(6): 540-545 (1966) (ECOREF # 58883)

Gillett, J. W. - "No Effect" Level of DDT in Induction of Microsomal Epoxidation. J.Agric.Food Chem. 16(2): 295-297 (1968) (ECOREF # 58885)

Gutsche, C. D. - Carbonyl Compounds. Reactions at the Carbonyl Center. In: C.D.Gutsche and D.J.Pasto (Eds.) Fundamentals of Organic Chemistry, Prentice-Hall Inc., Englewood Cliffs, NJ : 886-887 (1975) (ECOREF # 385)

Hamed, M. S., Ramzi, A., and El Said, S. - Susceptibility Status of Mosquitoes in Egypt to Commonly Used Insectides. J.Egypt.Public Health Assoc. 58(1/2): 160-167 (1983)
(ECOREF # 17815)

Hanafi, A. and Duursma, E. K. - Use of Pesticides in Brackishwater Ponds 2. Effect of Phosvel on Fish and Shrimp. Bull.Shrimp Cult.Res.Cent. 2(1/2): 143-157 (1976)
(ECOREF # 13317)

Hartley, D. and Kidd, H. - Agrochemicals Handbook. Royal Society of Chemistry, The University of Nottingham, Unwin Brothers Limited, Old Woking Surrey, UK (1983)
(ECOREF # 5716)

Hawker, D. W. and Connell, D. W. - Octanol-Water Partition Coefficients of Polychlorinated Biphenyl Congeners. Environ.Sci.Technol. 22(4): 382-387 (1988)
(ECOREF # 58518)

Henderson, R. S. - Marine Microcosm Experiments on Effects of Copper and Tributyltin-Based Antifouling Paint Leachates. Tech.Rep.No.1060, U.S.Naval Ocean Systems Center, San Diego, CA : 51 p. (1988) (ECOREF # 16536)

Herbes, S. E. - Transport and Bioaccumulation of Polycyclic Aromatic Hydrocarbons (PAH) in Aquatic Systems. In: Coal Technology Program Quarterly Progress Report for the Period Ending December 31, 1975, Oak Ridge National Lab., Oak Ridge, TN : 65-71 (1976) (ECOREF # 58457)

- Hermens, J. L. M. - Electrophiles and Acute Toxicity to Fish. Environ.Health Perspect. 87: 219-225 (1990) (ECOREF # 3394)
- Hornung, M. W., Zabel, E. W., and Peterson, R. E. - Toxic Equivalency Factors of Polybrominated Dibenzo-p-Dioxin, Dibenzofuran, Biphenyl, and Polyhalogenated Diphenyl Ether Congeners Based on Rainbow Trout Early Life Stage Mortality. Toxicol.Appl.Pharmacol. 140(2): 227-234 (Author Communication Used) (1996) (ECOREF # 19032)
- Howard, P. H. and Neal, M. - Dictionary of Chemical Names and Synonyms. In: P.H.Howard and M.Neal (Eds.), Dictionary of Chemical Names and Synonyms, Lewis Publ., Chelsea, MI (1992) (also CD 1998) (ECOREF # 4062)
- Huang, G., Bai, Z., Dai, S., and Xie, Q. - Accumulation and Toxic Effect of Organometallic Compounds on Algae. Appl.Organomet.Chem. 7(6): 373-380 (1993) (ECOREF # 4026)
- Hunter, R. S. and Culver, F. D. - QSAR Sysytem User Manual. A Structure-Activity Based Chemical Modeling and Information System. Inst.for Biological and Chemical Process Analysis, Montana State Univ., Bozeman, MT : I1-R5 (1988) (ECOREF # 62963)
- Hurley, S. and Fenton, M. B. - Ineffectiveness of Fenthion, Zinc Phosphide, DDT and Two Ultrasonic Rodent Repellers for Control of Populations of Little Brown Bats (*Myotis lucifugus*). Bull.Environ.Contam.Toxicol. 25: 503-507 (1980) (ECOREF # 35261)
- ICN Biomedicals, Inc. - ICN Catalog. ICN Biomedicals Inc., Irvine, CA : 1951 p. (1992) (ECOREF # 3047)
- Index of Common Names of Pesticides. - Compendium of Pesticide Common Names. <http://www.alanwood.net/pesticides/> (2007) (ECOREF # 89844)
- Jantrarotai, W. - Acute and Subacute Toxicity of Aflatoxin B1 and Cyclopiazonic Acid to Channel Catfish. Ph.D.Thesis, Auburn University, Auburn, AL : 121 p. (Acute Data Publ As 5526) (1990) (ECOREF # 5213)
- Johnson Matthey Alfa Products. - Alfa Catalog, Research Chemicals and Accessories. Johnson Matthey Alfa Products, P.O.Box 8247, Ward Hill, MA : 1120 p. (1990) (ECOREF # 7677)
- Johnson, S. C., Kent, M. L., Whitaker, D. J., and Margolis, J. - Toxicity and Pathological Effects of Orally Administered Ivermectin in Atlantic, Chinook, and Coho Salmon and Steelhead Trout. Dis.Aquat.Org. 17(2): 107-112 (1993) (ECOREF # 17199)
- Jollow, D. J. and Smith, C. - Biochemical Aspects of Toxic Metabolites: Formation, Detoxification and Covalent Binding. In: D.J.Jollow, J.J.Kocsis, R.Snyder, and H.Vainio (Eds.), Biological Reactive Intermediates, Plenum Press, NY : 42-54 (1977) (ECOREF # 3404)
- Kamlet, M. J., Doherty, R. M., Abraham, M. H., Carr, P. W., Doherty, R. F., and Taft, R. W. - Linear Solvation Energy Relationships. 41. Important Differences Between Aqueous Solubility Relationships for Aliphatic and Aromatic Solutes. J.Phys.Chem. 91(7): 1996-2004 (1987) (ECOREF # 1005)

- Kenaga, E. E. - Commercial and Experimental Organic Insecticides. Bull.Entomol.Soc.Am. 6(2): 53-79 (1960) (ECOREF # 90960)
- Keplinger, M. L., Fancher, O. E., Lyman, F. L., and Calandra, J. C. - Toxicologic Studies of Four Fluorescent Whitening Agents. Toxicol.Appl.Pharmacol. 27(3): 494-506 (1974) (ECOREF # 5513)
- Khan, M. Z., Szarek, J., and Markiewicz, K. - Effects of Oral Administration of Toxic Levels of Lead and Selenium upon Concentration of Different Elements in the Liver of Broiler Chicks. J.Vet.Med.A 40: 652-664 (1993) (ECOREF # 58868)
- Kruzynski, G. M. and Birtwell, I. K. - A Predation Bioassay to Quantify the Ecological Significance of Sublethal Responses of Juvenile Chinook Salmon (*Oncorhynchus tshawytscha*) to the Antisapstain Fungicide TCMTB. Can.J.Fish.Aquat.Sci. 51(8): 1780-1790 (1994) (ECOREF # 14446)
- Kuney, J. H. and Mullican, J. M. - Chemcyclopedia. Am.Chem.Soc., Washington, DC : 484 p. (1991) (ECOREF # 1333)
- Lajmanovich, R. C., Cabagna, M., Peltzer, P. M., Stringhini, G. A., and Attademo, A. M. - Micronucleus Induction in Erythrocytes of the *Hyla pulchella* Tadpoles (Amphibia: Hylidae) Exposed to Insecticide Endosulfan. Mutat.Res. 587(1/2): 67-72 (2005) (ECOREF # 86681)
- Lapadula, D. M., Carrington, C. D., and Abou-Donia, M. B. - Induction of Hepatic Microsomal Cytochrome P-450 and Inhibition of Brain, Liver, and Plasma Esterases by an Acute Dose of S,S,S-Tri-N-Butyl Phosphorotrithioate (DEF) in the Adult Hen. Toxicol.Appl.Pharmacol. 73: 300-310 (1984) (ECOREF # 37638)
- Leo, A. and Weininger, D. - Daylight Software Version 3.53 for VAX-11 under VMS 4.6+, CLogP version 3.4. Pomona Medicinal Chemistry Project, Pomona College, Claremont, CA.Distributed by Daylight Chemical Information Systems, Inc., 3951 Claremont St., Irvine, CA 92714 (1988) (ECOREF # 3573)
- Leo, A. and Weininger, D. - Daylight Software CLogP Version 3.15+ for Unix. Pomona Medical Chemistry Project, Pomona College, Claremont, CA.Distributed by Daylight Chemical Information Systems, Inc., 3952 Claremont St., Irving, CA 92714 (1997) (ECOREF # 17934)
- Lewis, R. L. and Sweet, D. V. - Registry of Toxic Effects of Chemical Substances (1983-84 Suppl., Vol. 1 & 2). U.S.Dep.Health Human Serv., Center for Disease Control, Natl.Inst.for Occupational Safety and Health, Cincinnati, OH (1985) (ECOREF # 13337)
- Lewis, R. L. and Sweet, D. V. Eds. - Registry of Toxic Effects of Chemical Substances (Fiche). U.S.Dep.Health Human Serv., Ctr.for Dis.Control, Natl.Inst.for Occup.Saf.and Health, Cincinnati, OH (1990) (ECOREF # 58207)
- Maas, J. L. - Toxicity Research with Thiourea. Laboratory for Ecotoxicology, Institute for Inland Water Management and Waste Water Treatment, Report No.AOCE : 4 p. (DUT) (1990) (ECOREF # 5374)
- Maier, K. J., Nelson, C. R., Bailey, F. C., Klaine, S. J., and Knight, A. W. - Accumulation of Selenium by the Aquatic Biota of a Watershed Treated with Seleniferous Fertilizer.

Bull.Environ.Contam.Toxicol. 60: 409-416 (1998) (ECOREF # 19042)

Maini, P. - Residues of the Algicide Endothal in Water, Soil and Rice, After Paddy Field Applications. Pestic.Sci. 34(1): 45-52 (1992) (ECOREF # 70291)

Mann, R. M. and Bidwell, J. R. - Application of the FETAX Protocol to Assess the Developmental Toxicity of Nonylphenol Ethoxylate to *Xenopus laevis* and Two Australian Frogs. Aquat.Toxicol. 51(1): 19-29 (2000) (ECOREF # 56709)

Mason, R. P. - Redox Cycling of Radical Anion Metabolites of Toxic Chemicals and Drugs and the Marcus Theory of Electron Transfer. Environ.Health Perspect. 87: 237-243 (1990) (ECOREF # 3410)

Mattson, N. S., Egidius, E., and Solbakken, J. E. - Uptake and Elimination of (Methyl-14C) Trichlorfon in Blue Mussel (*Mytilus edulis*) and European Oyster (*Ostrea edulis*)-Impact of Nuegvon Disposal on. Aquaculture 71(1/2): 9-14 (1988) (ECOREF # 9674)

Mayer, F. L. Jr. and Eilersieck, M. R. - Manual of Acute Toxicity: Interpretation and Data Base for 410 Chemicals and 66 Species of Freshwater Animals. Resour.Publ.No.160, U.S.Dep.Interior, Fish Wildl.Serv., Washington, DC : 505 p. (USGS Data File) (1986) (ECOREF # 6797)

McMahon, R. F., Shipman, B. N., and Long, D. P. - Laboratory Efficacies of Nonoxidizing Molluscicides on the Zebra Mussel (*Dreissena polymorpha*) and the Asian Clam (*Corbicula fluminea*). In: T.F.Nalepa and D.W.Schloesser (Eds.), Zebra Mussels - Biology, Impacts, and Control, Lewis Publishers, Boca Raton, FL : 575-598 (1993) (ECOREF # 17514)

Meister, R. T. - Farm Chemicals Handbook. Meister Publishing Co., Willoughby, OH : A4-G28 (1995) (ECOREF # 1014)

Mekenyan, O. - 2D Depiction Applet. Department of Physical Chemistry, Laboratory of Mathematical Chemistry, Bourgas "Prof.As.Zlatarov" University, 8010 Bourgas, Bulgaria (2005) (ECOREF # 83340)

Metcalfe, C. D., Metcalfe, T. L., Cormier, J. A., Huestis, S. Y., and Niimi, A. J. - Early Life-Stage Mortalities of Japanese Medaka (*Oryzias latipes*) Exposed to Polychlorinated Diphenyl Ethers. Environ.Toxicol.Chem. 16(8): 1749-1754 (1997) (ECOREF # 18072)

Mitchell, J. R., Nelson, S. D., Snodgrass, W. R., and Timbrell, J. A. - Metabolic Activation of Hydrazines to Highly Reactive Hepatotoxic Intermediates. In: D.J.Jollow, J.J.Kocsis, R.Snyder, and H.Vainio (Eds.), Biological Reactive Intermediates, Plenum Press, NY : 271-277 (1977) (ECOREF # 3531)

Mulla, M. S., Metcalf, R. L., and Kats, G. - Evaluation of new Mosquito Larvicides, with Notes on Resistant Strains. Mosq.News 24(3): 312-319 (1964) (ECOREF # 4431)

Mulla, M. S., Darwazeh, H. A., and Gillies, P. A. - Evaluation of Aliphatic Amines Against Larvae and Pupae of Mosquitoes. J.Econ.Entomol. 63: 1472-1475 (1970) (ECOREF # 14391)

Murphy, S. D. - Toxic Effects of Pesticides. In: C.D.Klaassen, M.O.Amdur, and J.Doull (Eds.), Casarett & Doull's Toxicology: The Basic Science of Poisons, 3rd Edition, MacMillan Publ.Co., NY : 519-581 (1986) (ECOREF # 3579)

- Nagia, D. K., Kumar, S., Saini, M. L., and Sharma, P. - Persistent Toxicity of Some Insecticides to Mustard Aphid, *Lipaphis erysimi* (Kaltenbach) and Bihar Hairy Caterpillar, *Spilosoma obliqua* (Walker) on Mustard. *Indian J.Plant Prot.* 18(2): 265-269 (1990) (ECOREF # 91432)
- Narain, A. S. and Srivastava, P. N. - Haemato-histological Responses of the Indian Freshwater Catfish, *Heteropneustes fossilis*, to Environmental Pollution by Sewage, Fertilizers and Insect. *Arch.Biol.* 90(2): 141-160 (1979) (ECOREF # 6699)
- Natwick, E. T. and Lopez, M. - New Insecticides for Silverleaf Whitefly, *Bemisia argentifolii* (Homoptera: Aleyrodidae) Control. In: *Proc.Beltwide Cotton Conf.*, Jan.5-9, San Antonio, TX : 1558-1563 (2004) (ECOREF # 76152)
- Norton, S. - Toxic Response of the Central Nervous System. In: C.D.Klaassen, M.O.Amdur, and J.Doull (Eds.), *Casarett and Doull's Toxicology*, Third Edition, MacMillan Publ.Co., New York, NY : 359-386 (1986) (ECOREF # 3532)
- Office of Pesticide Programs. - Pesticide Ecotoxicity Database (Formerly: Environmental Effects Database (EEDB)). Environmental Fate and Effects Division, U.S.EPA, Washington, D.C. (2000) (ECOREF # 344)
- PAN Pesticides Database. - Pesticide Action Network North America. (http://www.pesticideinfo.org/Search_Chemicals.jsp) (2006) (ECOREF # 89842)
- Pearlmutter, N. L. and Lembi, C. A. - The Effect of Copper on the Green Alga *Pithophora oedogonia*. *Weed Sci.* 34(6): 842-849 (1986) (ECOREF # 13312)
- Perrin, D. D, Dempsey, B., and Serjeant, E. P. - pKa Prediction for Organic Acids and Bases. *pKa Prediction for Organic Acids and Bases*, Chapman and Hall, New York, NY : 146 p. (1981) (ECOREF # 84709)
- Rajagopalan, K. V. - Xanthine Oxidase and Aldehyde Oxidase. In: W.B.Jakoby (Ed.), *Enzymatic Basis of Detoxification*, Vol.1, Academic Press, Inc., New York, NY : 295-309 (1980) (ECOREF # 3533)
- Rall, T. W. - Central Nervous System Stimulants. The Methylxanthines. In: A.G.Gilman, L.S.Goodman, T.W.Rall, and F.Murad (Eds.), *Goodman and Gilman's The Pharmacological Basis of Therapeutics*, 7th Edition, MacMillan Publ.Co., New York, NY : 589-603 (1985) (ECOREF # 3534)
- Rappoport, Z. - Handbook of Tables for Organic Compound Identification. The Chemical Rubber Company, Third Edition, Cleveland, OH : 564 p. (1967) (ECOREF # 1008)
- Reddy, M. S. and Rao, K. V. R. - In Vivo Modification of Lipid Metabolism in Response to Phosphamidon, Methyl Parathion and Lindane Exposure in the Penaeid Prawn, *Metapenaeus monoceros*. *Bull.EnvIRON.Contam.Toxicol.* 43(4): 603-610 (1989) (ECOREF # 975)
- Riad, Y., El-Nahas, H. M., El-Kady, E. M., and El-Bardan, A. A. - Aromatic Sulphides, Sulphoxides, and Sulphones as Larvicides for *Culex pipiens molestus* and *Aedes caspius* (Diptera: Culicidae). *J.Econ.Entomol.* 85(6): 2096-2099 (1992) (ECOREF # 13544)

- Rittschof, D., Sasikumar, N., Murlless, D., Clare, A. S., Gerhart, D., and Bonaventura, J. - Mixture Interactions of Lactones and Furans and a Commercial Biocide: Toxicity and Antibarnacle Settlement Activity. In: M.F.Thompson, R.Nagabhushanam, R.Sarojini, and M.Fingerman (Eds.), Recent Developments in Biofouling Control, Oxford & IBH Publ.Co., New Delhi, India : 269-274 (1994) (ECOREF # 16470)
- Riva, M. C., Vilaseca, M., and Crespi, M. - Biodegradability, Toxicity, and Accumulation of Omegachrome Blue B Dye in the Rainbow Trout *Salmo gairdneri*. Bol.Intextar Inst.Text.Coop.Ind. 93: 55-70 (SPA) (ENG ABS) (1988) (ECOREF # 14062)
- Roseth, S., Edvardsson, T., Botten, T. M., Fuglestad, J., Fonnum, F., and Stenersen, J. - Comparison of Acute Toxicity of Process Chemicals Used in the Oil Refinery Industry, Tested with the Diatom *Chaetoceros gracilis*, the Flagellate. Environ.Toxicol.Chem. 15(7): 1211-1217 (1996) (ECOREF # 17223)
- Russom, C. L., Drummond, R. A., and Hoffman, A. D. - Acute Toxicity and Behavioral Effects of Acrylates and Methacrylates to Juvenile Fathead Minnows. Bull.Environ.Contam.Toxicol. 41: 589-596 (1988) (ECOREF # 13120)
- Russom, C. L. - Personal Communication. U.S.EPA, Environmental Research Laboratory-Duluth, Duluth, MN 55804 (1991) (ECOREF # 9003)
- Sarkar, S. K. - Role of Plant Glycocomponents (De-Odorase) on Water Parameters in Fish Ponds. J.Environ.Biol. 20(2): 131-134 (1999) (ECOREF # 20253)
- Sausser, K. R., Liu, J. K., and Wong, T. Y. - Identification of a Copper-Sensitive Ascorbate Peroxidase in the Unicellular Green Alga *Selenastrum capricornutum*. Biometals 10(3): 163-168 (1997) (ECOREF # 19840)
- Schafer, R. and Achazi, R. K. - The Toxicity of Soil Samples Containing TNT and Other Ammunition Derived Compounds in the Enchytraeid and Collembola-Biotest. Environ.Sci.Pollut.Res.Int. 6(4): 213-219 (1999) (ECOREF # 57313)
- Schultz, T. W. and Tichy, M. - Structure-Toxicity Relationships for Unsaturated Alcohols to *Tetrahymena pyriformis*: C5 and C6 Analogs and Primary Propargylic Alcohols. Bull.Environ.Contam.Toxicol. 51(5): 681-688 (1993) (ECOREF # 8080)
- Scott, J. and Redmond, M. S. - Acute Toxicity Tests with Chloropyrifos. Unpublished Data, SAIC, Narragansett, RI : 3 p. (1986) (ECOREF # 4061)
- Sigma, Chemical Company. - Biochemicals Organic Compounds for Research and Diagnostic Reagents. Sigma Chemical Company, St.Louis, MO : 2352 p. (1994) (ECOREF # 4293)
- Sine, C. - Farm Chemicals Handbook. Meister Publications Co., Willoughby, OH (1992) (ECOREF # 5327)
- Sine, C. - Farm Chemicals Handbook. Farm Chemicals Handbook, Meister Publications Co., Willoughby, OH (1994) (ECOREF # 58206)
- Smith, S. B., Savino, J. F., and Blouin, M. A. - Acute Toxicity to *Daphnia pulex* of Six Classes of Chemical Compounds Potentially Hazardous to Great Lakes Aquatic Biota. J.Great Lakes Res.14(4):394-404 / Aquat.Sci.Fish.Abstr. 17(2): 139 (1988) (ECOREF # 3283)

- Song, M. Y., Stark, J. D., and Brown, J. J. - Comparative Toxicity of Four Insecticides, Including Imidacloprid and Tebufenozide, to Four Aquatic Arthropods. *Environ.Toxicol.Chem.* 16(12): 2494-2500 (1997) (ECOREF # 18476)
- Srikanth, S. and Berk, S. G. - Stimulatory Effect of Cooling Tower Biocides on Amoebae. *Appl.Environ.Microbiol.* 59(10): 3245-3249 (1993) (ECOREF # 9293)
- Stark, J. D. - Population-Level Effects of the Neem Insecticide, Neemix, on *Daphnia pulex*. *J.Environ.Sci.Health Part B* 36(4): 457-465 (2001) (ECOREF # 69840)
- STN International. - Registry Searching; CAS On-Line. STN International, Columbus, OH (1994) (ECOREF # 1329)
- Svobodova, Z. and Pecena, M. - Changes in the Red and White Blood Picture of Carp After Acute Exposure to Toxic Substances. *Pr.Vyzk.Ustav Ryb.Hydrobiol.Vodnany* 17: 116-128 (1988) (ECOREF # 3352)
- Syracuse Research Corporation. - BioWin Software Vers 4.0. Syracuse Research Corporation, North Syracuse, NY 13212 (2000) (ECOREF # 83338)
- Syracuse Research Corporation. - KowWin Software Vers. 1.67. Syracuse Research Corporation, North Syracuse, NY 13212 (2000) (ECOREF # 83336)
- Talmage, S. S. - Part I. Alcohol Ethoxylates. In: S.S.Talmage (Ed.), *Environmental and Human Safety of Major Surfactants*, Lewis Publishers, Boca Raton, FL : 3-202 (1994) (ECOREF # 1015)
- Tejada, A. W., Bajet, C. M., Magbauna, M. G., Gambalan, N. B., Araez, L. C., and Magallona, E. D. - Toxicity of Pesticides to Target and Non-Target Fauna of the Lowland Rice Ecosystem. In: B.Widianarko, K.Vink, and N.M.Van Straalen (Eds.), *Environmental Toxicology in South East Asia*, VU Univ.Press, Amsterdam, Netherlands : 89-103 (1994) (ECOREF # 20421)
- Terada, H. - Uncouplers of Oxidative Phosphorylation. *Environ.Health Perspect.* 87: 213-218 (1990) (ECOREF # 3535)
- Tomlin, C. - *The Pesticide Manual*, 10th Edition. The British Crop Protection Council, Farnham, Surrey, U.K.Crop Protection Publications : 1341 p. (1994) (ECOREF # 1012)
- Tonogai, Y., Iwaida, M., Tati, M., Ose, Y., and Sato, T. - Biochemical Decomposition of Coal-Tar Dyes. II. Acute Toxicity of Coal-Tar Dyes and Their Decomposed Products. *J.Toxicol.Sci.* 3(3): 205-214 (1978) (ECOREF # 443)
- Tracor Jitco. - Tracor Jitco (Chemical Research Company, Bethsheda, MD (under contract with USEPA)). Tracor Jitco (Chemical Research Company, Bethsheda, MD - under contract with USEPA) (2001) (ECOREF # 58995)
- Tsuda, T., Kojima, M., Harada, H., Nakajima, A., and Aoki, S. - Acute Toxicity, Accumulation and Excretion of Isoprothiolane and Its Degradation Products in Killifish. *Water Res.* 31(2): 323-327 (1997) (ECOREF # 17959)
- U.S. Environmental Protection Agency. – Chemistry Dashboard. (<https://comptox.epa.gov/dashboard>) – (2017) (ECOREF # 175295) U.S.Environmental Protection Agency Office of Pesticide Programs. - Pesticide Fate Database. Web

ECOTOX Chemical Verification and Entry Procedure

access no longer available - (2009) (ECOREF # 117876) (An electronic copy is located on the Contractor site: PFATE_37_Tables.mdb)

U.S.Environmental Protection Agency. - Toxic Substances Control Act (TSCA) Chemical Substance Inventory. Volumes I-V. TSCA Inventory. U.S.EPA, 1985 Edition, Office of Toxic Substances, Washington, DC (1986) (ECOREF # 13318)

U.S.Environmental Protection Agency. - QSAR System. U.S.EPA, Montana State Univ. (1995) (ECOREF # 58505)

Various. - Miscellaneous Internet Websites for Chemical Verification. CHEMICAL MODULE Chemicals Verification Sources (Various) ECOREF # 58886)

Veith, G. D., Call, D. J., and Brooke, L. T. - Structure-Toxicity Relationships for the Fathead Minnow, *Pimephales promelas*: Narcotic Industrial Chemicals. Can.J.Fish.Aquat.Sci. 40(6): 743-748 (OECDG Data File) (1983) (ECOREF # 15823)

Veith, G. D. and Kosian, P. - Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In: D.Mackay, et al., (Eds.), Physical Behavior of PCBs in the Great Lakes, Ann Arbor Sci.Publ., Ann Arbor, MI : 269-282 (1983) (ECOREF # 7)

Veith, G. D., De Foe, D. L., and Knuth, M. L. - Structure-Activity Relationships for Screening Organic Chemicals for Potential Ecotoxicity Effects. Drug Metab.Rev. 15(7): 1295-1303 (1984) (ECOREF # 3539)

Veith, G. D. and Broderius, S. J. - Structure-Toxicity Relationships for Industrial Chemicals Causing Type (II) Narcosis Syndrome. In: K.L.E.Kaiser (Ed.), QSAR in Environmental Toxicology-II, D.Reidel Publ.Co., Dordrecht, Holland : 385-391 (1987) (ECOREF # 3537)

Veith, G. D. and Broderius, S. J. - Rules for Distinguishing Toxicants that Cause Type I and Type II Narcosis Syndromes. Environ.Health Perspect. 87: 207-211 (1990) (ECOREF # 3536)

Vengris, J. - Annual Weed Control in Alfalfa new Seedlings. Proc.Northeast.Weed Sci.Soc. 31: 99-103 (1977) (ECOREF # 40621)

Verma, Y., Ruparelia, S. G., Hargan, M. C., Venkaiah, K., and Kulkarni, P. K. - Acute Toxicity of Azo - Dyes to Waterflea *Daphnia magna*. Indian J.Environ.Prot. 13(11): 804-807 (1993) (ECOREF # 18209)

Verschueren, K. - Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold Co., New York, NY : 659 p. (OECDG Data File) (1977) (ECOREF # 1002)

Waller, D. L., Rach, J. J., Cope, W. G., Marking, L. L., Fisher, S. W., and Dabrowska, H. - Toxicity of Candidate Molluscicides to Zebra Mussels (*Dreissena polymorpha*) and Selected Nontarget Organisms. J.Gt.Lakes Res. 19(4): 695-702 (1993) (ECOREF # 4175)

Wauchope, R. D., Butler, T. M., Hornsby, A. G., Augustijn-Beckers, P. W. M., and Burt, J. P. - The SCS/ARS/CES Pesticide Properties Database for Environmental Decision-Making. Rev.Environ.Contam.Toxicol. 123: 164 (1992) (ECOREF # 5739)

- Weast, R. C. and Astle, M. J. Eds. - CRC Handbook of Chemistry and Physics. CRC Press, Inc., 63rd Edition, Boca Raton, FL (1982) (ECOREF # 1003)
- Weast, R. C. and Astle, M. J. - CRC Handbook of Data on Organic Compounds. CRC Press Inc, Boca Raton, FL 1-2 (1985) (ECOREF # 9825)
- Weast, R. C. - CRC Handbook of Chemistry and Physics. CRC Press, Inc., 67th Edition, Boca Raton, FL (1986) (ECOREF # 1011)
- Weed Science Society of America. - Herbicide Handbook. Second Edition, W.F.Humphrey Press Inc., Geneva, NY : 368 p. (1970) (ECOREF # 1327)
- Weiner, N. - Norepinephrine, Epinephrine, and the Sympathomimetic Amines. In: A.G.Gilman, L.S.Goodman, T.W.Rall, and F.Murad (Eds.), Goodman and Gilman's The Pharmacological Basis of Therapeutics, 7th Edition, MacMillan Publ.Co., New York, NY : 145-180 (1985) (ECOREF # 3540)
- Werbrouck, S. P. O. and Debergh, P. C. - Imidazole Fungicides and Paclobutrazol Enhance Cytokinin-Induced Adventitious Shoot Proliferation in Araceae. J.Plant Growth Regul. 15(2): 81-85 (1996) (ECOREF # 96404)
- Wheeler, A. E., Zingaro, R. A., Irgolic, K., and Bottino, N. R. - The Effect of Selenate, Selenite, and Sulfate on the Growth of Six Unicellular Marine Algae. J.Exp.Mar.Biol.Ecol. 57: 181-194 (1982) (ECOREF # 58895)
- Winter, J. E. - Long-Term Laboratory Experiments on the Influence of Ferric Hydroxide Flakes on the Filter-Feeding Behaviour, Growth, Iron Content and Mortality in *Mytilus edulis* L. (Experiences de Longue Duree en Laboratoire Concernant l'Influence des Flocons d'Hydroxide Ferrique sur la Filtration de l'eau, la Croissance, la Teneur en fer et la Mortalite de *Mytilus edulis* L.). In: M.Ruivo (Ed.), Marine Pollution and Sea Life, FAO, Fishing News (Books) Ltd., Surrey, England : 392-396 (1972) (ECOREF # 16715)
- Wiswesser, W. J. - Pesticide Index. Entomological Society of America, 5th Edition, College Park, MD : 328 p. (1976) (ECOREF # 5723)
- Worthing, C. R. and Hance, R. J. - The Pesticide Manual, 9th Edition. The British Crop Protection Council, Farnham, Surrey, UK : 1141 p. (1991) (ECOREF # 9824)
- Youn, Y. N., Seo, M. J., Shin, J. G., Jang, C., and Yu, Y. M. - Toxicity of Greenhouse Pesticides to Multicolored Asian Lady Beetles, *Harmonia axyridis* (Coleoptera: Coccinellidae). Biol.Control 28(2): 164-170 (2003) (ECOREF # 72462)
- Zandee, D. I., Holwerda, D. A., and Herwig, H. J. - Accumulation and Effects of Di-n-Butyltin Dichloride in a Freshwater Clam. In: T.D.Lekkas (Ed.), 5th Int.Conf.on Heavy Metals in the Environment, Vol.1, CEP Consultants Ltd., Edinburgh, U.K.:727-729 (1985) / Aquat.Sci.Fish Abstr. 16(10): 16008-1Q16 (1986) (ECOREF # 4478)

APPENDIX C: RULES TO ASSIST IN CHEMICAL VERIFICATION PROCESS

1. Historical names may be interchanged with systematic names.
2. o-,m-,p-, (ortho, meta, and para) descriptors may be replaced with 1,2-, 1,3-, or 1,4-, respectively.
3. N-, O-, P-, and S- are locants for substitution on these atoms.
4. Greek and Latin multiplicative prefixes may be interchanged.

	<u>Greek</u>	<u>Latin</u>
1/2	hemi-	semi-
1	mono-, mon-	uni-
2	di-	bi-
3	tri-	tri-, ter-
4	tetra-, tetr-	quadri-, quadr-, quater-
5	penta-, pent-	quinque-, quinqu-
6	hexa-, hex-	sexi-, sex-
7	hepta-, hept-	septi-, sept-
*8	octa-, octo-,	octi-
*9	nona-, non-,	novi-
*10	deca-, dec-,	deci-
*11	undeca-,	undec-
*12	dodeca-,	dodec-

*Generally, Greek prefixes are used; the exceptions are for nine and eleven, where the Latin prefix is used.

\$ Bi-, ter-, etc., are employed in ring structures. Bis-, tetrakis-, etc., are used for complex functionality, for example the fusion of rings. They multiply the heading functionality (Biscyclohexa-).

5. Formal element names may be interchanged with a form of the common name.

Antimony	Sb	Stibium
*Copper	Cu	Cuprum
Gold	Au	Aurum
*Iron	Fe	Ferrum
*Lead	Pb	Plumbum
Mercury	Hg	Hydrargyrum
Silver	Ag	Argentum
Sodium	Na	Natrium
Tungsten	W	Wolframite
*Tin	Sn	Stannum

*Denotes the most common interchanges

6. Hydrated metal compounds should be assigned CAS numbers of the associated anhydrous compound (e.g., $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ should be assigned the CAS number for CuSO_4). A comment should be made in the chemical characteristics data field reporting the hydrated form used. Sometimes the author reports a common or trade name for a product that is hydrated, (e.g. Borax, $\text{B}_4\text{Na}_2\text{O}_7 \cdot 10\text{H}_2\text{O}$). The paper should be coded to the hydrated CAS number rather than to the anhydrous form as there is no information for review staff that the compound is hydrated. If the paper were to report it as Sodium borate decahydrate (another name for borax), it would be coded to the anhydrous product as per the text for hydrates mentioned above.

The "ph" in sulfur (sulphur) or sulfur derived names will use an "F" instead of "ph."

7. If a CAS number is verified for a racemic mixture (generic) compound and the isomeric forms are unable to be verified, have the review staff code the isomeric forms under the racemic mixture (generic) CAS Number and note the isomeric form in the Chemical Characteristics data field. Archive the unverifiable isomeric forms and track the references associated with the isomeric form.
8. If a CAS number cannot be verified for a compound (e.g. Silvex ester) but the concentration is based on the active ingredient (AI) or acid equivalent (AE) (e.g. Silvex) OR measured concentrations are presented, code as the AI or AE chemical name (e.g. Silvex). Silvex ester would be archived under the "Archive - Under AI".
9. If the paper presents two chemical names for the same compound and one of the names cannot be verified but the other name is verified, code the chemical under the verified name, noting the unverified name in chemical comments (e.g. Paper reports Maneb as Dicotan M22, code as Maneb noting Dicotan M22 in chemical comments).
- 10¹. Phrases with "of" included may be rewritten to omit "of." For example, Alkanolamine salt of 2,4-dichlorophenoxy acetic acid as 2,4-Dichlorophenoxy acetic acid alkanolamine salt.
- 11¹. Non-English names should be translated into English. This can be done through the use of English-non-English chemical dictionaries at the University of Minnesota-Duluth library, reference section.
- 12¹. Names containing letters and numbers should follow these rules:
 - The compound name should be first followed by letters and numbers.
Aliquat 335
Fenthion S2145
 - "Compound" and "Substance" should be omitted.
B713 not Substance B713

ECOTOX Chemical Verification and Entry Procedure

- Company names should be omitted when with letter or number codes.

GC 4072 not General Chemical 4072

AC 84777 not AC 84777 (American Cyanamid)

BAY 5097 not Bayer 5097

- Adjectives describing a compound are not included.

Liquor ammonia as Ammonia

Organic phosphorus as Phosphorus

13. Pay special attention to papers that report three or four letter chemical names (e.g. DNP). DNP exists under multiple CAS numbers. If the paper only provides an acronym (e.g. DNP) and doesn't provide any additional information such as chemical name/structure, the chemical should be archived.
14. Chemical formulations containing a safener should be verified as a single compound. For example, Puma Super contains Fenoxaprop-p-ethyl. Mefenpyr-diethyl is the safener. It was verified under the CAS number for Fenoxaprop-p-ethyl-mefenpyr-diethyl mixture rather than Fenoxaprop-p-ethyl alone. STN categorizes products containing safeners as mixtures (under a single CAS Number) and they should be notified if a discrepancy is found.
15. Compounds that contain the prefix dextrorotatory (d)- or levorotatory (l)- can also be replaced with (+) – or (–) – respectively. For example: d-2-butanol can also be called (+)-2-butanol and l-2-butanol can also be called (–)-2-butanol. (From p. 346-347 of Wade Jr., L.G, Organic Chemistry)
16. If the paper reports a generic compound but does not specify the form used (e.g. Valproate or Ricinoleate can be salts or esters of Valproic acid and Ricinoleic acid respectively), the paper can be skimmed/coded to the acid form (e.g. Paper reports Valproate which could not be verified. It should be skimmed/coded to Valproic acid with a note placed in the Chemical Characteristics data field regarding the use of Valproate). The unverified chemical should be Archived under AI.
17. For toxicity tests with Nanoparticles, the paper may report that it contains a surface coating. For example, "Cadmium selenium (CdSe) quantum dots....coated with mercaptopropionic acid (MPA)..." Coatings are used to improve stability and dispersal of the nanoparticle². However, in some instances, the paper may report it as having a toxic effect. If the paper does not mention a toxic effect of the coating, the chemical will be reviewed as a single chemical with a comment on the coating in the Chemical Characteristics data field. For the example above, CdSe would be reviewed as Cadmium selenide with the comment "Coated with Mercaptopropionic acid". If the paper were to report a toxic coating effect, it should be treated as a mixture and be sent to chemical verification staff if needed (as Cadmium selenide-mercaptopropionic acid mixture).
18. Quantum dots with a core/shell (e.g. CdSe/ZnS) will be verified as mixtures. The

core appears to be the focus of toxicity however “research is still emerging and it appears that toxicity can be caused by whole quantum dots, their degradations products (metallic components), and their coatings.”³ It may be difficult to verify the “generic” mixture but some trade names can be verified (e.g. Lumidot CdSe/ZnS).

19. A bait is a formulation that contains an active ingredient mixed with food or another attractive substance such as a pheromone, (e.g. Golden Malrin fly bait – which contains Methomyl and (Z)-9-tricosene (pheromone)) and would not necessarily be considered mixtures. First, try to locate a CAS number for the formulated product. If a CAS number is located and the paper reports a single concentration, skim/code to the formulated product. If the paper does not report a single concentration, skim/code to the pesticidal active ingredient (e.g. Methomyl). If reviewing, enter the trade name in the Chemical Characteristics data field. The Formulation would be entered as BT (Bait).

If a CAS number for the formulated product cannot be located, the name should be Archived under AI and the paper skimmed/coded to the pesticidal active ingredient. If reviewing, follow the same steps as above.

¹STN International rules paraphrased

²Vasiliev, A.N.,E.A. Gulliver, J.G. Khinast and R.E. Riman. 2009. Highly Dispersible Polymer-Coated Silver Nanoparticles. *Surface & Coatings Technology* 203: 2841-2844.

³Blickley, T.M. 2010. The Toxicological Effects of Engineered Nanoparticles, Quantum Dots, in Estuarine Fish. Ph.D. Thesis, Duke University. 212 p.

APPENDIX D: STN SEARCH INSTRUCTIONS

The following procedure is used to search STN online:

To conduct a search you must obtain a LOGIN ID and PASSWORD from STN International.

1. Open STN and logon by clicking the telephone icon (see STN Access Issues if unable to connect)
2. Capture the session in transcript (filed by month and year). Choose to append to the current month's file if it already exists. If not, open a new file and label it for the current month and year. Click open to start the session
3. Searching by CAS #:
 - A. At the prompt, type "fil lreg" (enter). This opens the learning registry.
 - B. Type "e (CAS #)/rn" (enter). Example: "e 869-29-4/rn"
 - C. In the results, line E3 is what you searched for. The second number is how many results there are for each line.
 - D. If results exist for what you expanded, search for that file by typing "s (line #)" (enter). Example: "s e3" searches for the results in line E3.
 - E. To display the search results, type "dis" (enter).
 - F. The results are displayed. Move immediately on to the next search. The results can be displayed offline later.
4. Searching by chemical name or synonym:
 - A. At the prompt, type "fil lreg" (enter).
 - B. Type "e (chemical name)/cn" (enter). Example: "e chlorophenol/cn"
 - C. Follow steps c-f from above.
5. If searches in the learning registry do not come up with results, search the registry files. This should only be done after first searching the learning registry files. At the prompt, type "fil reg" to open the registry files. All other commands are the same as the learning registry files.
6. To log off STN when all searches are complete:
 - A. Type "dis cost" (enter). This displays the total cost of the session. The cost of all sessions should be recorded in a log.
 - B. At the prompt, type "log off y" (enter). This logs you off from STN online.
7. After logging off, all results can be displayed offline.

ECOTOX Chemical Verification and Entry Procedure

STN Access Issues

The most common reason a connection cannot be made when attempting to logon to STN is due to firewall issues on the CSRA side.

The first step is to confirm with STN that there are not any issues on their end by contacting CAS Customer Center at: 1-800-753-4227 or help@cas.org. If the issue is not with CAS, then a ticket needs to be submitted to the CSRA Service Desk (see the email example below for address, format and carbon copy instructions). In addition to the ticket, there is a Firewall Request Form that needs to be submitted (located on the Contractor site in the ECOTOX SOPs Chemical folder).

****NOTE:** If there are multiple staff members with STN access, only one staff member needs to submit the ticket

For the first tab (Request Overview), only the Required Client Information needs to be filled in:

In the second tab (Firewall Rule Change), the three most pertinent pieces of information that need to be filled in are:

- 1) Source IP Address (this is the IP address of staff computer. Can be found by going to the Start Menu, locate Command Prompt. Enter "ipconfig" and press Enter. The IP address can be found under IPv4 Address).
- 2) Destination IP Address (STNs IP address: 134.243.5.32)
- 3) Port(s) (e.g. TCP/23)

Email example for submitting Firewall Request Tickets

Send ticket to CSGS_Support@csgov.com

Cc: Chancy Humphries (CSRA Network Engineer) and ECOTOX Supervisor (Anne Pilli)

Hello,

I think something in the firewall has changed as I'm unable to access an application that I need in order to do my work.

See attached firewall request form.

Chancy Humphries assisted me with this issue last time (refer to **INC0133551**).

As stated above, I need this application to do my work, so much appreciated if this can be escalated.

Thank you

APPENDIX E: SMILES TUTORIAL

What is SMILES?

SMILES (**S**implified **M**olecular **I**ntput **L**ine **E**ntry **S**ystem) is a chemical notation that allows a user to represent a chemical structure in a way that can be used by the computer. SMILES is an easily learned and flexible notation. The SMILES notation requires that you learn a handful of rules. You do not need to worry about ambiguous representations because the software will automatically reorder your entry into a unique SMILES string when necessary.

SMILES was developed through funding from the U.S. EPA, National Health and Environmental Research Laboratory (NHEERL), Mid-continent Ecology Division (MED-Duluth), to the Medicinal Chemistry Project at Pomona College, Claremont, CA and the Computer Sciences Corporation, Duluth, MN. Several publications discuss SMILES in more detail, including Anderson et al. 1987, Weininger 1988, Weininger et al. 1989, and Hunter et al., 1987.

SMILES has five basic syntax rules which must be observed. If basic rules of chemistry are not followed in SMILES entry, the system will warn the user and ask that the structure be edited or reentered. For example, if the user places too many bonds on an atom, a SMILES warning will appear that the structure is impossible. The rules are described below and some examples are provided. The rules below allow for the representation of a two-dimensional structure of a chemical. For the ASTER and QSAR systems, a two-dimensional depiction is adequate. Other rules are available for chemicals that are structural isomers, but will not be discussed in this basic tutorial.

Rule One: Atoms and Bonds

SMILES supports all elements in the periodic table. An atom is represented using its respective atomic symbol. Upper case letters refer to non-aromatic atoms; lower case letters refer to aromatic atoms. If the atomic symbol has more than one letter the second letter must be lower case.

Bonds are denoted as:

- Single bond
- = Double bond
- # Triple bond
- * Aromatic bond
- . Disconnected structures

Single bonds are the default and therefore need not be entered. For example, 'CC' would mean that there is a non-aromatic carbon attached to another

non-aromatic carbon by a single bond, and the computer would identify the structure as the chemical ethane. It is also assumed that the bond between two lower case atom symbols is aromatic. A blank terminates the SMILES string.

Rule Two: Simple Chains

By combining atomic symbols and bond symbols simple chain structures can be represented. The structures that are entered using SMILES are hydrogen-suppressed, that is to say that the molecules are represented without hydrogens. The SMILES software understands the number of possible connections that an atom can have. If enough bonds are not identified by the user through SMILES notation, the system will automatically assume that the other connections are satisfied by hydrogen bonds. Some examples:

CC	CH ₃ CH ₃	Ethane
C=C	CH ₂ CH ₂	Ethene
CBr	CH ₃ Br	Bromomethane
C#N	C≡N	Hydrocyanic acid
Na.Cl	NaCl	Sodium chloride

The user can explicitly identify the hydrogen bonds, but if one hydrogen bond is identified in the string, the SMILES interpreter will assume that the user has identified **all** hydrogens for that molecule.

HC(H)=C(H)(H) Ethene

Because SMILES allows entry of all elements in the periodic table, and also utilizes hydrogen suppression, the user should be aware of chemicals with two letters that could be misinterpreted by the computer. For example, 'Sc' could be interpreted as a sulfur atom connected to an aromatic carbon by a single bond, or it could be the symbol for scandium. The SMILES interpreter gives priority to the interpretation of a single bond connecting a sulfur atom and an aromatic carbon. To identify scandium the user should enter [Sc].

Rule Three: Branches

A branch from a chain is specified by placing the SMILES symbol(s) for the branch between a parentheses. The string in parentheses is placed directly after the symbol for the atom to which it is connected. If it is connected by a double or triple bond, the bond symbol immediately follows the left parenthesis. Some examples:

CC(O)C 2-Propanol

<chem>CC(=O)C</chem>	2-Propanone
<chem>CC(CC)C</chem>	2-Methylbutane
<chem>CC(C)CC(=O)</chem>	2-Methylbutanal
<chem>c1c(N(=O)=O)cccc1</chem>	Nitrobenzene
<chem>CC(C)(C)CC</chem>	2,2-Dimethylbutane

Rule Four: Rings

SMILES allows a user to identify ring structures by using numbers to identify the opening and closing ring atom. For example, in C1CCCCC1, the first carbon has a number '1' which connects by a single bond with the last carbon which also has a number '1'. The resulting structure is cyclohexane. Chemicals that have multiple rings may be identified by using different numbers for each ring. If a double, single, or aromatic bond is used for the ring closure, the bond symbol is placed before the ring closure number. Some examples:

<chem>C=1CCCCC1</chem>	Cyclohexene
<chem>C*1*C*C*C*C*1</chem>	
or <chem>c1ccccc1</chem>	Benzene
<chem>C1OC1CC</chem>	Ethyloxirane
<chem>c1cc2ccccc2cc1</chem>	Naphthalene

Rule Five: Charged Atoms

Charges on an atom can be used to override the knowledge regarding a valence that is built into SMILES software. The format for identifying a charged atom consists of the atom followed by brackets which enclose the charge on the atom. The number of charges may be explicitly stated ({-1}) or not ({-}). For example:

<chem>CCC(=O)O{-1}</chem>	Ionized form of propanoic acid
or <chem>CCC(=O)O{-}</chem>	
<chem>c1cccn{+1}1CC(=O)O</chem>	1-Carboxymethyl pyridinium

References:

Anderson, E., G.D. Veith, and D. Weininger. 1987. *SMILES: A line notation and computerized interpreter for chemical structures*. Report No. EPA/600/M-87/021. U.S. Environmental Protection Agency, Environmental Research Laboratory-Duluth, Duluth, MN 55804

Hunter, R.S., F.D. Culver, and A. Fitzgerald. 1987. *SMILES User Manual*. A

ECOTOX Chemical Verification and Entry Procedure

Simplified Molecular Input Line Entry System. Includes extended SMILES for defining fragments. Review Draft, Internal Report, Montana State University, Institute for Biological and Chemical Process Control (IPA), Bozeman, MT.

Weininger, D. 1988. SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules. *Journal of Chemical Information and Computer Science* 28: 31-36.

Weininger, D., A. Weininger, and J.L. Weininger. 1989. SMILES. 2. Algorithm for generation of unique SMILES notation. *Journal of Chemical Information and Computer Science* 29: 97-101.

APPENDIX F: SMILES DESIGNATORS

If a SMILES string cannot be written, a designator is determined. The designator is used in the Chemical Module. The designators are:

- PLM--Polymer
- LRG--Too large for existing program (> 60 non-hydrogen atoms or > 120 characters)
- GEN--Generic Chemical (e.g. Cresol)
- CMM--Commercial mixture (PhosFlex 400)
- MXT--Generic mixture (Polyoxyethylene glycols)

APPENDIX G: DELETED/ALTERNATE REGISTRY NUMBERS

If a chemical in Unify is found to be listed under a deleted registered (DR) or alternate registered (AR) CAS number, the following steps should be taken:

- 1) Enter and verify the Preferred CAS Registry number in Unify, if needed.
- 2) Check to see if the Deleted or Alternate Registry number exists in the Chemical Module.
 - a. If the Deleted or Alternate Registry number exists in the Chemical Module, ensure that there are not any references attached to the record. If no references are attached, select the DR/AR button from the Status Section. If references are attached, data maintenance staff needs to be alerted as they are the ones who would update the references to the Preferred Registry number (this is especially important for reviewed papers. Unreviewed papers could be updated by chemical staff). Once all references are updated, select the DR/AR button from the Status Section.
 - b. Once all of the data has been updated in Unify, add the deleted and/or alternate CAS numbers to the Preferred Registry number's Historical CAS tab.
 - c. "AR/DR # XXX-XX-X, all records have been updated to Preferred Registry # XXXXXXXXXX" should be added to the Notes tab of the Preferred Registry number.
 - d. If the Deleted or Alternate Registry number does NOT exist in the Chemical Module, add the deleted and/or alternate CAS numbers to the Preferred Registry number's Historical CAS tab.

APPENDIX H: VALID CODE CREATION

Staff members that are tasked with creation of codes must have Administration privileges to access “Lookup Codes” in Unify. Please review the general procedures outlined in the ECOTOX Valid Code Creation SOP for a better understanding of the code creation process (N:\ECOTOX SOPs\REVIEW\valid codes\ECOTOX Valid Code Creation.doc).

The following codes are created by Chemical Verification staff during the chemical verification process or reviewing process; Chemical Group, Chemical Property Units, Chemical Use, Chemical TMOA (Toxic Mode of Action), Chemical Formulation, Chemical Grade, Ions, and Radiolabel.

Chemical Group

Code file name: Chemical Group Codes (codes made during Chemical Verification)

The Chemical Group code can be defined by a specific project, e.g. EFED, by chemical element, e.g. As – Arsenic, or by a unique chemical code (e.g. the Chemical Group code for Dieldrin is DLD).

Typically, the code created is one that best captures that specific group or COC. For example, if a new COC code is needed, one might use a combination of characters within the chemical name to create a 3 or 4 letter code (e.g. the Chemical Group code for Imidacloprid is IMC).

Chemical Property Units

Code file name: Chemical Property Unit Codes (codes made as needed)

Chemical Properties can be found in the Properties tab within the Chemical Module and consist of Molecular Weight, Melting Point, etc. There is no standard practice for creation of these codes. However, ensure sure that abbreviations used for all parts of the unit code are the same as was used for similar units. A search of the already existing codes for these should be done (for example if adding grams/liter it should be verified as g/L rather than as gm/L in order to be consistent with how Grams and Liters are presented in other Unify data fields).

Chemical TMOA (Toxic Mode of Action)

Code file name: Chemical TMOA Codes (static code list, no new codes)

TMOA codes can be found in the Properties tab within the Chemical Module. They are defined as a common set of physiological and behavioral signs that characterize a type of adverse biological response (e.g. non-polar narcosis). Toxic Mode of Action codes are static and only used in the ASTER application. If/when new TMOAs are developed/approved by EPA, new TMOAs will be added to Unify.

Chemical Use

Code file name: Chemical Use Codes (static code list, no new codes)

It defines the common use(s) for a pesticide active ingredient (e.g. herbicide). The use is added if it can be determined from verification sources. The most common is PAN (http://www.pesticideinfo.org/Search_Chemicals.jsp). STN will also sometimes provide this information. Currently the Chemical Use is a static code list. If/when additional Chemical Uses are located, they will require programmer's assistance in updating the "target Logic" that is contained in Unify to prioritize coding for special projects; typically the code created is one that best captures the chemical use description (e.g. FUMI is the code for Fumigant).

Chemical Formulation

Code file name: Chemical Formulation Codes (codes made as needed during review process)

Chemical Formulation is the way in which the chemical is prepared. These codes are created with two or three characters that best captures the formulation description (e.g. AI is Active Ingredient). A good review of chemical formulation information can be found from the National Association of State Departments of Agriculture at www.nasda.org/File.aspx?id=30509.

Chemical Grade

Code file name: Chemical Grade Codes (codes made as needed during review process)

Chemical Grade reflects the quality of the product. Different industries have different standards for chemical grades depending upon the purpose (for example ACS Grade is a "grade of highest purity and meets or exceeds purity standards set by American Chemical Society (ACS)" - <http://www.sciencecompany.com/Learn-Chemical-Grade-Definitions-from-Highest-to-Lowest-Purity-W53.aspx>

These codes are created with two or three characters that best captures the grade description (e.g. ACS is American Chemical Society Grade).

Ions

Code file name: Ion Codes (codes made as needed during review process)

This code is used when the chemical concentration is based upon an ionic form of a chemical. Typically these codes are used for Metal compounds and are comprised of elemental symbols (e.g. Cd for Cadmium). However, there are occasions where ions may be needed for Organic compounds such as Paraquat or other chemicals that tend to dissociate such as Ammonium. These codes are created using a few characters that

best capture the ion description.

Radiolabel

Code file name: Radio Label Codes (codes made as needed during review process)

This code is used if radiolabeled products are tested. The standard code convention for a nucleus (e.g. ^{12}C) is to use the elemental symbol followed by a dash and then the atomic mass unit. For example, ^{12}C has the code of C-12.