



# **ECOTOXicology Knowledgebase Workshop**

NAMs Training Workshop

RTP, NC

April 24 – 25, 2024

Jennifer H. Olker

# Agenda

- Welcome and Introductions
- Brief background of ECOTOX
- Demonstration
- Hands-on Activity

The screenshot shows the ECOTOX Knowledgebase website. The header includes navigation links: Home (active), Search, Explore, Help, and Contact Us. The main content area is divided into several sections:

- Data last updated:** Mar 14, 2024. A link to "See update totals" is provided.
- Recent chemicals with full searches completed and data extracted:** A list of chemicals including Arsenic, Phthalates, and Per- and Polyfluoroalkyl Substances (PFAS).
- Total in database:** A table showing the following counts:

Category	Count
Chemicals	12,934
Species	13,915
References	54,475
Results	1,167,326
- About ECOTOX:** A description of the Knowledgebase and a link to "Olker et al. 2022". A "Learn More" button is present.
- Getting Started:** A list of instructions and guides, including "Search", "Explore", "ECOTOX Quick User Guide", "ECOTOX User Guide", and "ECOTOX Terms Appendix".
- Other Links:** A list of links for documentation and resources, including "Frequent Questions", "Limitations", "Other Tools/Databases", "Recent Additions", and "Literature Search Dates".

# Acknowledgements and Contact Info

## Jennifer Olker

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[www.epa.gov/ecotox](http://www.epa.gov/ecotox)

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SpecPro Professional Services (SPS)

Senior Environmental Employment (SEE) staff

**ECOTOX Support:**

**218-529-5225**

[ecotox.support@epa.gov](mailto:ecotox.support@epa.gov)

To cite ECOTOX or read more details: Olker et al. 2022, <https://doi.org/10.1002/etc.5324>

# Background of ECOTOX

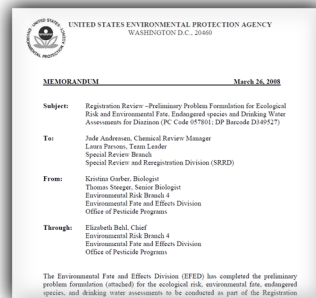
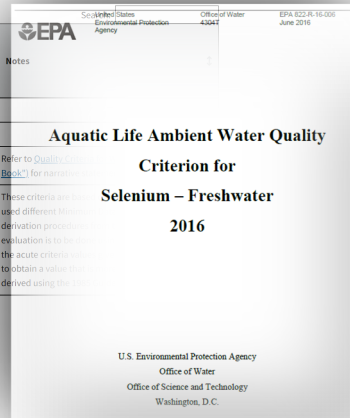
# Background and History

- Ecological risk assessors need cost-effective methods to locate high-quality ecological toxicity data

## Ambient Water Quality Criteria for Aquatic Life (USEPA Office of Water)

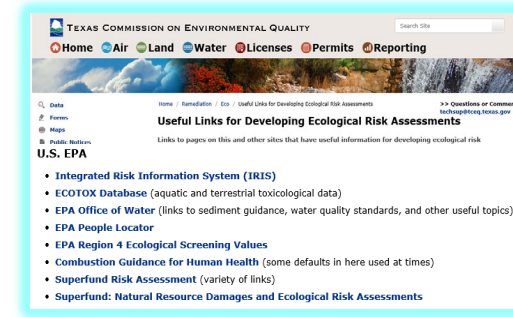
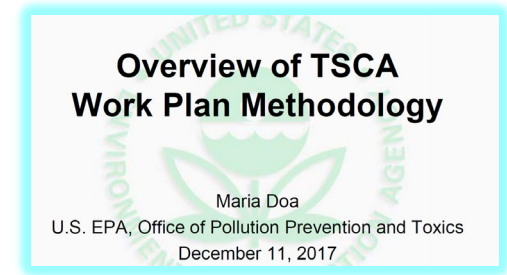
National Recommended Aquatic Life Criteria table

Pollutant (P = Priority Pollutant)	CAS Number	Freshwater CMC <sup>a</sup> (acute) (µg/L)	Freshwater CCC <sup>a</sup> (chronic) (µg/L)	Saltwater CMC <sup>a</sup> (acute) (µg/L)	Saltwater CCC <sup>a</sup> (chronic) (µg/L)	Publication Year	Notes
4,4'-DDT (P)	50293	1.1	0.001	0.13	0.001	1980	
Accrolein (P)	107028	3ug/L	3ug/L	—	—	2009	
Aesthetic Qualities	—	—	—	—	—	1986	
Aldrin (P)	309002	3.0	—	1.3	—	1980	



## Ecological Risk Assessment for chemical registration and re-registration (USEPA Office of Pesticide Programs)

## Ecological hazard data for the Prioritization and Assessment of Chemicals for Toxic Substances Control Act/Lautenberg Act (USEPA Office of Pollution Prevention and Toxics)



## Ecological Site Assessments and in Emergency Response

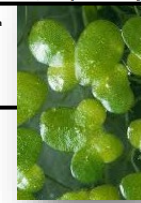
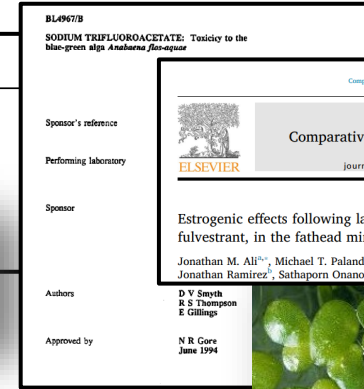
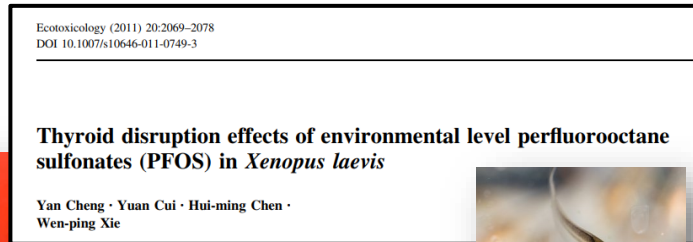
(USEPA Office of Land and Emergency Management - Superfund and Resource Conservation and Recovery Act; Regions and States).

# Background and History

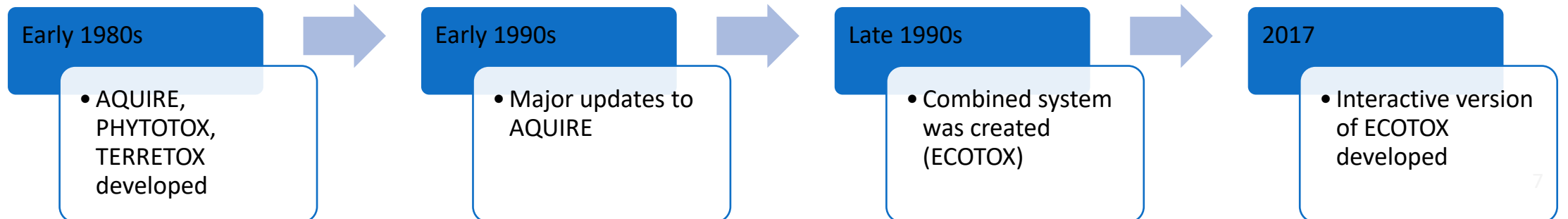
- Ecological risk assessors need cost-effective methods to locate high-quality ecological toxicity data

## MULTIPLE PUBLICATIONS

## DIVERSITY OF SPECIES



- US EPA developed ecological toxicity databases
  - AQUatic toxicity Information Retrieval (AQUIRE) database (Duluth, MN lab)
  - PHYTOTOX (Corvallis, OR lab)
  - TERRETOX (Corvallis, OR lab)



# What is the ECOTOX Knowledgebase?

- From comprehensive search and review of open and grey literature
- Chemical-based literature searches
- Accessible, structured empirical data from *in vivo* toxicity tests
- Updated quarterly to public website
- 30+ year history

The screenshot shows the ECOTOX Knowledgebase website. The header includes navigation links: Home (underlined), Search, Explore, Help, and Contact Us. Below the header is a summary table:

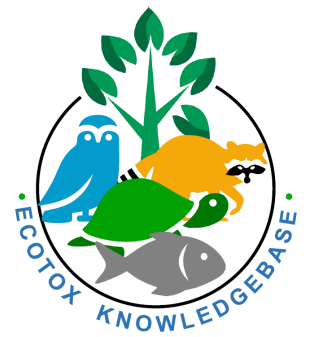
ECOTOX Knowledgebase		Total in database	
Data last updated	Recent chemicals with full searches completed and data extracted	12,934	13,915
Mar 14, 2024	Arsenic Phthalates	<b>Chemicals</b>	<b>Species</b>
See update totals	Per- and Polyfluoroalkyl Substances (PFAS)	54,475	1,167,326
		<b>References</b>	<b>Results</b>

Below the table are three main content sections:

- About ECOTOX**: ECOTOX is a comprehensive Knowledgebase providing single chemical environmental toxicity data on aquatic and terrestrial species. Read more in: [Olker et al. 2022](#). Includes a "Learn More" button and the ECOTOX logo.
- Getting Started**:
  - Use [Search](#) if you know exact parameters or search terms (chemical, species, etc.)
  - Use [Explore](#) to see what data may be available in ECOTOX (including data plots)
  - [ECOTOX Quick User Guide](#) (2 pp, 104 K)
  - [ECOTOX User Guide](#) (100 pp, 735 K)
  - [ECOTOX Terms Appendix](#)
- Other Links**: ECOTOX-related documentation and resources.
  - [Frequent Questions](#)
  - [Limitations](#)
  - [Other Tools/Databases](#)
  - [Recent Additions](#)
  - [Literature Search Dates](#)

[www.epa.gov/ecotox](http://www.epa.gov/ecotox)

# ECOTOX Pipeline



Planning and Identification

Screening

Eligibility

Included

Chemical verification & search term development

Conduct literature searches

Identify & acquire potentially applicable studies

Review literature for applicability

Extract study and toxicity data

Provide toxicity results and study details

## Chemical-based Search Terms\*

- Chemical name and CASRN
- Synonyms, tradenames
- Other relevant forms

## Literature Search

Use chemical-specific search terms to query multiple literature search engines.

\* 40-90 searches conducted per year, not possible to update data for all chemicals each year

## Title/Abstract Screening

- Established applicability (inclusion) criteria
- Documentation of exclusion reason

## Full Text Review

## Data Extraction

- ECOTOX-specific Controlled Vocabularies
  - Test chemical
  - Test organism
  - Study methods and test conditions
  - Toxicity results
- Updated to public website, with downloadable outputs



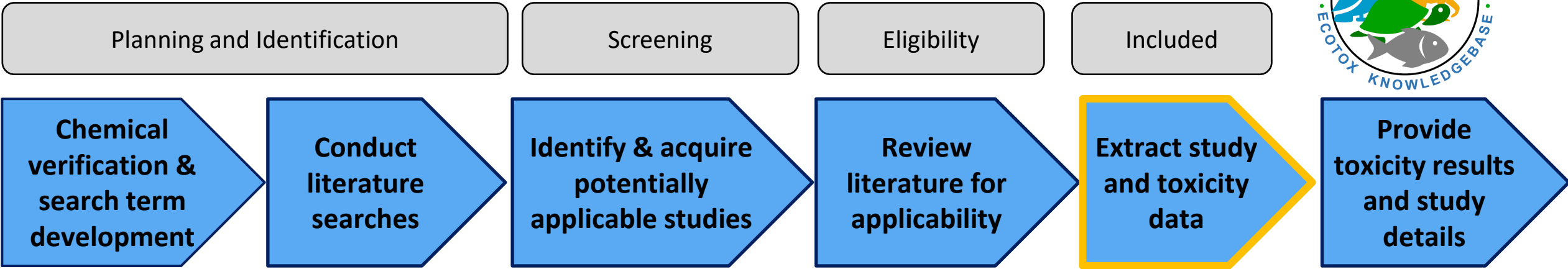
# Inclusion Criteria

Identify and  
acquire potentially  
applicable studies

Review  
literature for  
applicability

Category	Key Area	Data Requirement
<b>P (Population)</b>	Species	<ul style="list-style-type: none"> <li>Taxonomically verifiable, ecologically-relevant organisms (including cells, organs, gametes, embryos, plant cuttings) [NOT bacteria, humans, monkeys, viruses, or yeast]</li> </ul>
<b>E (Exposure)</b>	Chemical	<ul style="list-style-type: none"> <li>Single, verifiable chemical toxicants, administered through an acceptable route</li> </ul>
	Exposure Amount (Concentration)	<ul style="list-style-type: none"> <li>Exposure amount is quantified, either as a concentration in the environment when administered via soil or water, or as a dosage when introduced directly into or on the organism, via injection, orally, or topically</li> </ul>
	Exposure Duration	<ul style="list-style-type: none"> <li>Known duration from the time of initial exposure to the time of measurement</li> </ul>
<b>C (Comparator/ Control)</b>	Control	<ul style="list-style-type: none"> <li>Must have a control treatment</li> </ul>
<b>O (Outcome)</b>	Effect	<ul style="list-style-type: none"> <li>Biological effect measured</li> <li>Effect concurrent with associated chemical exposure</li> </ul>
	Publication Type	<ul style="list-style-type: none"> <li>Primary source of the data [NOT a Review]</li> <li>Study must be a full article in English</li> </ul>

# ECOTOX Pipeline



## Data Extraction

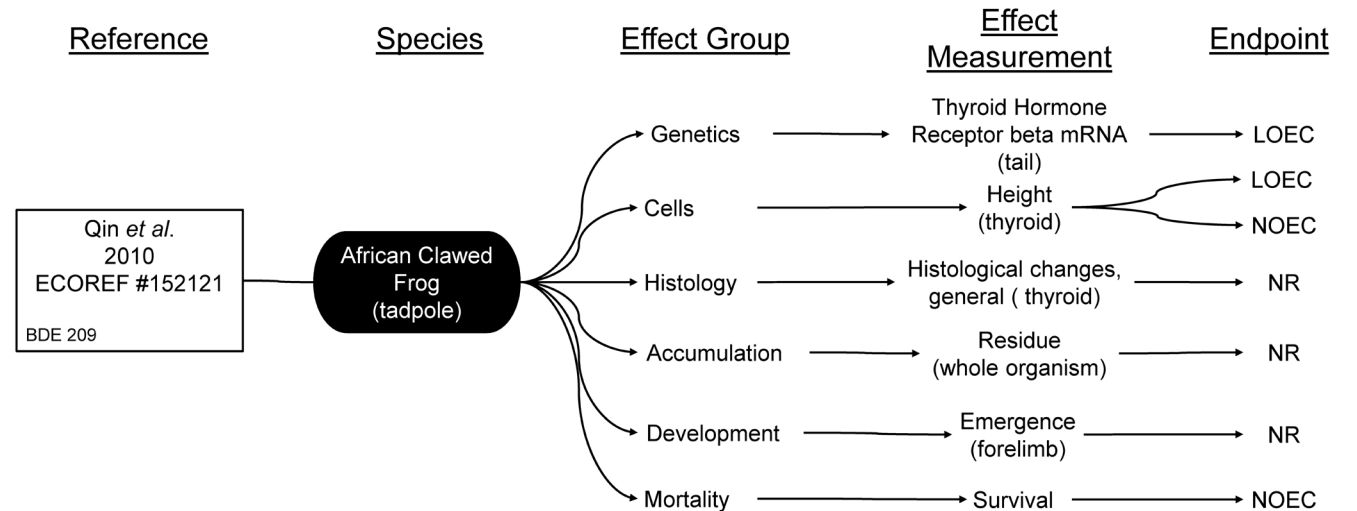
### Example of multiple ECOTOX records from a single study:



Journal of Environmental Sciences  
Volume 22, Issue 5, 2010, Pages 744-751




Thyroid disruption by technical decabromodiphenyl ether (DE-83R) at low concentrations in *Xenopus laevis*



NOEC = No Observed Effect Level LOEC = Lowest Observed Effect Level NR = Not Reported

# ECOTOX Data Fields



Extract study  
and toxicity  
data

Category	ECOTOX data fields (examples)
<b>Chemical</b>	<ul style="list-style-type: none"> <li>• Chemical identifier (CASRN, DTXSID)</li> <li>• Chemical Analysis</li> <li>• Chemical Formulation &amp; Grade</li> <li>• Concentration(s)/Dose(s) tested</li> </ul>
<b>Species</b>	<ul style="list-style-type: none"> <li>• Species identifiers (ITIS TSN, NCBI TaxID, Taxonomy)</li> <li>• Life stage, Age, Sex</li> <li>• Organism Source</li> </ul>
<b>Study Methods &amp; Test Conditions</b>	<ul style="list-style-type: none"> <li>• Experimental design</li> <li>• Control(s)</li> <li>• Test location and method</li> <li>• Exposure type, route, and media</li> <li>• Study and exposure duration</li> <li>• Physical and Chemical Soil and Water Parameters (e.g., pH, Temperature, Dissolved Oxygen)</li> </ul>
<b>Test Results</b>	<ul style="list-style-type: none"> <li>• Specific Effect Measured (with higher-level groups)</li> <li>• Calculated Endpoint</li> <li>• Concentration associated with effect and endpoint</li> <li>• Response site (e.g., whole organism, specific organ or body part)</li> <li>• Statistical significance and level of response</li> </ul>

**\* ECOTOX Data Fields**

<https://cfpub.epa.gov/ecotox/help.cfm?sub=wi-definitions>

**\* ECOTOX Vocabularies:**

<https://cfpub.epa.gov/ecotox/help.cfm?sub=term-appendix>

# Demonstration

# What is the ECOTOXicology Knowledgebase?

## ECOTOX Knowledgebase

Home **Search** Explore Help Contact Us


Data last updated <b>Mar 14, 2024</b> See update totals	Recent chemicals with full searches completed and data extracted Arsenic Per- and Polyfluoroalkyl Substances (PFAS)	Phthalates	Total in database <b>12,934</b> Chemicals	<b>13,915</b> Species
			<b>54,475</b> References	<b>1,167,326</b> Results

### About ECOTOX

ECOTOX is a comprehensive Knowledgebase providing single chemical environmental toxicity data on aquatic and terrestrial species.

Read more in: [Olker et al. 2022](#)

[Learn More](#)



### Getting Started

- Use [Search](#) if you know exact parameters or search terms (chemical, species, etc.)
- Use [Explore](#) to see what data may be available in ECOTOX (including data plots)
- [ECOTOX Quick User Guide](#) (2 pp, 104 K)
- [ECOTOX User Guide](#) (100 pp, 735 K)
- [ECOTOX Terms Appendix](#)

### Other Links

ECOTOX-related documentation and resources.

- [Frequent Questions](#)
- [Limitations](#)
- [Other Tools/Databases](#)
- [Recent Additions](#)
- [Literature Search Dates](#)

# ECOTOXicology Knowledgebase: Explore

Aquatic  Terrestrial

Group Summary

Records

**Plot View**

Send Query Filters to Search ⓘ

### Query Filters

Select one or more ⓘ of each filter to reduce the records.

Chemicals (2)

2 Selected

Species Group (8)

All

Class (12)

All

Order (16)

All

Family (17)

All

Genus (22)

All

Species (31)

All

## 539 Plottable Records — 847 Total Records

Records are **plotted** if they can be converted to **Standardized Concentration Units** ⓘ. Ordered by **Concentration (low-high)**.

**Effect × Chem**

Dur × Chem

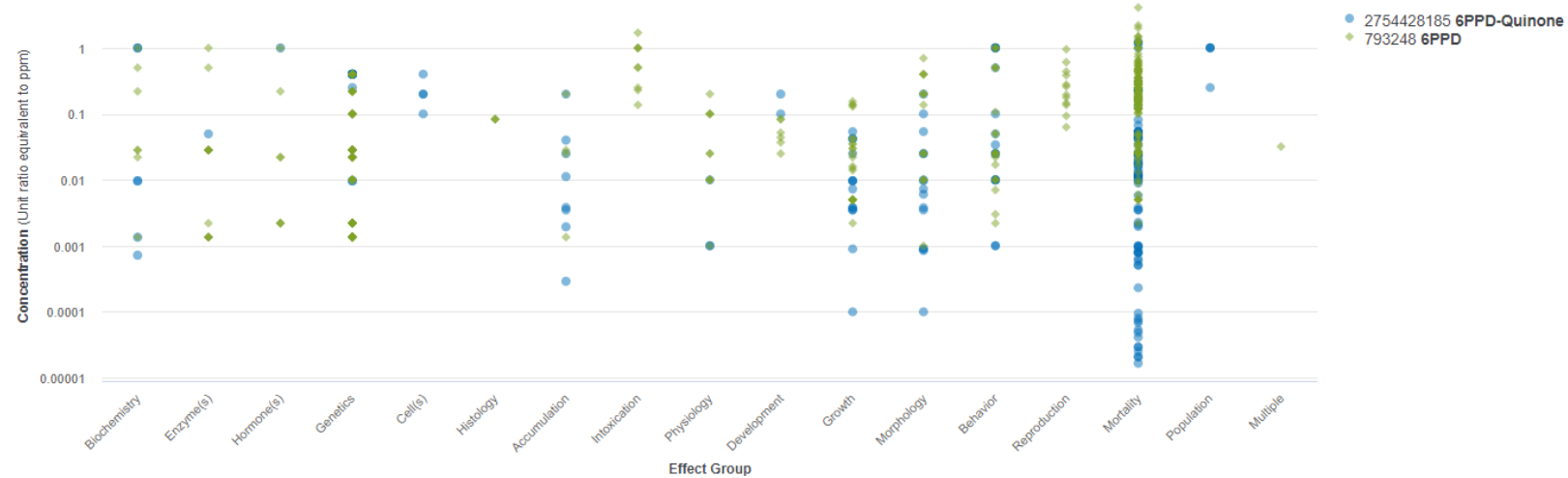
Dur × Endpt

Custom

Export

Y-axis scale:  Linear  Logarithmic

Click and drag to zoom in. Hold down shift key to pan.



Showing all 539 records

# ECOTOXicology Knowledgebase: Search

Parameters



Aquatic

Terrestrial

Customize Output Fields

All Chemicals +

All Effects +

All Endpoints +

All Species +

All Test Conditions +

All Publication Options +

CAS Number	Chemical Name	Chemical Grade	Chemical Analysis	Chemical Purity	Species Scientific Name	Species Common Name	Organism Lifestage	Organism Age	Age Units	Exposure Type	Media Type	Test Location	Number of Doses
2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	>95	Salvelinus leucomaenis	Whitespotted Char	Juvenile	<1	Year(s)	Renewal	Fresh water	Lab	6	
2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	>95	Salvelinus leucomaenis	Whitespotted Char	Juvenile	<1	Year(s)	Renewal	Fresh water	Lab	6	
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2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	>95	Oncorhynchus masou ssp.	Cherry Salmon	Juvenile	<1	Year(s)	Renewal	Fresh water	Lab	2	
2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	>95	Oncorhynchus masou ssp.	Cherry Salmon	Juvenile	<1	Year(s)	Renewal	Fresh water	Lab	2	
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2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Unmeasured	>95	Salvelinus leucomaenis	Whitespotted Char	Juvenile	<1	Year(s)	Static	Fresh water	Lab	3	
2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	>95	Salvelinus leucomaenis	Whitespotted Char	Juvenile	<1	Year(s)	Renewal	Fresh water	Lab	6	
2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Unmeasured	>95	Salvelinus curilus	Southern Dolly Varden	Juvenile	<1	Year(s)	Static	Fresh water	Lab	3	
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2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	NR	Salvelinus alpinus	Arctic Char	Juvenile	~3	Year(s)	Renewal	Fresh water	Lab	2	
2754428185	2-[(1,3-Dimethylbutyl)amino]-5-(phenylamino)2,5-cyclohexanedione	Measured	>95	Oncorhynchus masou ssp.	Cherry Salmon	Juvenile	<1	Year(s)	Renewal	Fresh water	Lab	2	
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# ECOTOXicology Knowledgebase: Help

## Starting Out

### Web Site Information

About ECOTOX

Disclaimer & Limitations

Recent Additions

Navigating this Web Site

Frequent Questions

## How do I...

Learn Basics

Select Search Parameters

Select Report Format/Sort Order

Navigate/View Reports

## Welcome to the U.S. EPA ECOTOX Web site!

The ECOTOXicology Knowledgebase (ECOTOX) is a source for locating single chemical toxicity data for aquatic life, terrestrial plants and wildlife. ECOTOX was created and is maintained by the U.S.EPA's [Center for Computational Toxicology and Exposure's \(CCTE's\) Great Lakes Toxicology Ecology Division \(GLTED\)](#).

ECOTOX integrates three previously independent databases - AQUIRE, PHYTOTOX, and TERRETOX - into a unique system which includes toxicity data derived predominately from the peer-reviewed literature, for aquatic life, terrestrial plants, and terrestrial wildlife, respectively.

You should review the [limitations](#) of ECOTOX data retrieval for an understanding of system and minimum data requirements prior to performing searches on this site.

**You should consult the original scientific paper to ensure an understanding of the context of the data retrieved from ECOTOX.**

### ECOTOX Documentation

- [ECOTOX User Guide](#) (100 pp, 735 K)
- [ECOTOX Quick User Guide](#) (2 pp, 104 K)



# ECOTOXicology Knowledgebase: Search Planner

Table of Contents

Web Site Information

Starting Out

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[Search Planner \(PDF\)](#) (5 pp, 133 K, [About PDF](#))

## Taxonomic Searching

Within ECOTOX you may conduct a search by entering the Species Name or number(s), Genus/Species Name(s), or Common Name or Other Taxonomic Name(s). The Contains and Exact Match radio buttons allow for partial or exact name matches. You can also search by Species Group. All data records within ECOTOX include a Scientific name for the test species. All names and predefined groups have been verified in [reliable taxonomic sources](#).

The ECOTOX species file includes historical synonyms for the species. If a search is conducted using a species name that is noted as a taxonomic synonym in our system, ECOTOX will present the results using the currently acceptable genus and species name.

### Taxonomic Entry

**Species Number:** All species in ECOTOX have been assigned a unique number. You can include numbers and text information (either Scientific or common names) in one search. Species numbers are always searched as an exact match.

### Example Taxonomic Search

The example below is the correct method of entering query text. You can enter a mix of numbers and species terms. Number will always be treated as exact matches by the ECOTOX query.

Example Genus/Species Name Query

## ECOTOX SEARCH PLANNING FORM

Use this form to help plan your searches or to document searches for yourself or others to perform.

### Chemicals

Chemical Names	CAS Numbers	Predefined Groups	
		<b>Metal Compounds</b>	<b>Organic Compounds</b>
		Aluminum	Conazoles
		Antimony	Cyanotoxins
		Arsenic	DDT and metabolites
		Barium	Dibenzofurans
		Beryllium	Explosives
		Cadmium	Glycol Ethers
		Chromium	Major Ions
		Cobalt	Neonicotinoids
		Copper	Nitrosamines
		Iron	Perchlorates
		Lead	Phthalate Esters
		Manganese	Polyaromatic Hydrocarbons (PAH)
		Mercury	Polychlorinated Biphenyls (PCB)
		Nickel	Polybrominated Diphenyl Ethers (PBDE)
		Organotin	Pharmaceutical Personal Care (PPCP)
		Selenium	Strobins
		Silver	
		Vanadium	Per- and Polyfluoroalkyl Substances (PFAS)
		Zinc	

### Species

Scientific Names/ Taxonomic Levels	Common Names	Species ECOTOX Numbers or NCBI TaxIDs	Predefined Taxonomic Groups
			<b>All Animals</b> Amphibians Insects/Spiders Molluscs Birds Other Invertebrates Reptiles Crustaceans Mammals Worms Fish
			<b>All Plants</b> Algae Moss/Hornworts, Fungi, Flowers, Trees, Shrubs, Ferns
			<b>Special Interest</b> Standard Test Species US Threatened/Endangered Species US Exotic/Nuisance

# Demo of ECOTOX: [www.epa.gov/ecotox](http://www.epa.gov/ecotox)

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Mar 14, 2024

[See update totals](#)

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ECOTOX is a comprehensive Knowledgebase providing single chemical environmental toxicity data on aquatic and terrestrial species.

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- [Literature Search Dates](#)

# Example 1

**Use the ECOTOX Knowledgebase to identify and explore records available for specific chemicals, species groups, and other search refinements**

## Example 1 - Chemical List

Category	Compound(s)	Full Chemical Name	CAS Registry Number(s)
Pesticide/ Herbicide	Atrazine	6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine	1912-24-9
Pesticide/ Herbicide	Roundup	N-(Phosphonomethyl)glycine compd. with 2-propanamine (1:1)	38641-94-0
Pesticide/ Herbicide	Chlorpyrifos	Phosphorothioic acid, O,O-Diethyl O-(3,5,6-trichloro-2-pyridinyl) ester	2921-88-2
Metal	Cadmium	-	7440-43-9, 10108-64-2, plus 11 others in the Cadmium group
Metal	Lead	-	7439-92-1, 7758-95-4, 301-04-2, 10099-74-8, plus 9 others in the Lead group
Metal	Selenium	-	35 unique compounds in the Selenium group
Pharmaceutical/Personal Care Product	17 $\alpha$ -Ethinylestradiol	(17 $\alpha$ )-19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol	57-63-6
Pharmaceutical/Personal Care Product	Clofibrate/ Clofibric Acid	2-(4-Chlorophenoxy)-2-methylpropanoic acid, Ethyl ester; 2-(4-Chlorophenoxy)-2-methylpropanoic acid	637-07-0, 882-09-7
Pharmaceutical/Personal Care Product	DEET	N, N-Diethyl-meta-toluamide or diethyltoluamide	134-62-3

## Example 1 - Species Groups

<b>Vertebrates</b>	<b>Invertebrates</b>	<b>Plants and Other</b>
Fish	Insects/Spiders	Flowers, Trees, Shrubs, Ferns
Mammals	Worms	Algae
Birds	Molluscs	Fungi
Amphibian	Crustaceans	Moss, Hornworts
Reptiles	Other Invertebrates	Miscellaneous (Communities, Higher Taxonomic Level)

## Example 2

**With a recent publication as an initial reference, use ECOTOX Knowledgebase to provide biological relevance to the chemicals and concentrations detected in surface water samples with effects data from aquatic toxicity studies.**

# Example 2

## Goal

With a recent publication as an initial reference, use ECOTOX to provide biological relevance to the chemicals and concentrations detected in surface water samples with effects data from aquatic toxicity studies.

## Scenario—Part 1

As a part of your work, you need to determine the scope of aquatic toxicity data available for the 11 chemicals that were detected in more than 25 of the surface water samples collected from the St. Louis River, St. Louis Bay, and Superior Bay sites in Minnesota and Wisconsin in 2010 (Christensen et al. 2012) by using the chemical identifiers provided (CAS Registry Numbers [CASRNs]) and comparing measured concentrations to concentrations producing potential effects. [Christensen et al. 2012, https://pubs.usgs.gov/sir/2012/5184/](https://pubs.usgs.gov/sir/2012/5184/): This worksheet can be completed by reading the abstract for this report and using the below information.

### CAS Registry Numbers for the 11 chemicals detected in more than 25% of the samples from Christensen et al. 2012, Figure 4.

58-08-2	298-46-4
78-51-3	206-44-0
119-61-9	129-00-0
134-62-3	1222-05-5
53-16-7	486-56-6
57-88-5	

## Scenario—Part 2

After seeing the available ECOTOX data, you realize you want to focus on reviewing available literature on mortality effects in short-term studies in fish for the list of 11 chemicals measured at these sites.