

# EPA Center for Computational Toxicology and Exposure ECOTOXicology Knowledgebase Virtual Training

Jennifer H. Olker US EPA Office of Research and Development

May 17, 2022

**Office of Research and Development** 

# **EPA NAMs Pilot Training Program**

United States Environmental Protection Agency

- New Approach Methodologies (NAMs) Training Program is a deliverable in the Agency's Work Plan, first released in 2019 and updated in 2021.
  - First topic: Today's ECOTOX Knowledgebase training
- Goal: Develop, implement and maintain an engaging training program.
  - Interactive case studies to encourage active learning
  - Train the trainer
  - Obtain feedback
- More virtual and in-person trainings are being planned.
- The EPA NAMs training website includes existing training resources, including recordings and guidance documents.



## Agenda



- Welcome and Introductions
- Background of ECOTOX
- Basic Features
- Demonstration
- Case Studies
- Summary

ECOTOX Knowledg	gebase	Home	Search	Explore	Help			Contact Us
Data last updated	Recent chemicals with full search	es completed and data extracted				Total in database 12,485 Chemicals	13,709 Species	
Mar 10, 2022	Acetamiprid Dinotefuran		Sabadilla alkaloids Per- and Polyfluoroalkyl Substances (PFAS)			Gillinguo	openeo	
See update totals			<i>ynae 2</i> an y CC			53,020 References	1,102,544 Results	

#### About ECOTOX

The ECOTOXicology Knowledgebase (ECOTOX) is a comprehensive, publicly available Knowledgebase providing single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife.

#### Learn More

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

#### Getting Started

- Use <u>Search</u> if you know exact parameters or search terms (chemical, species, etc.)
- Use <u>Explore</u> to see what data may be available in ECOTOX (including data plots)
- ECOTOX Quick User Guide (2 pp, 141 K)
- <u>ECOTOX User Guide</u> (95 pp, 672 K)
- ECOTOX Terms Appendix

#### Other Links

- Limitations
- Frequent Questions
- Other Tools/Databases
- <u>Recent Additions</u>
- <u>Literature Search Dates</u>

#### ڬ Get Updates via Email

#### Download

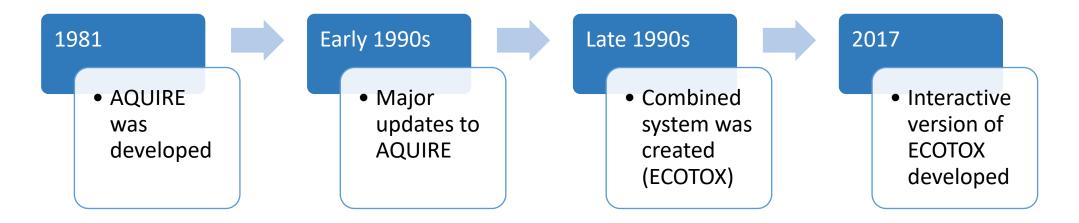
Download the entire database as an ASCII file via the button below.



# **Background of ECOTOX**

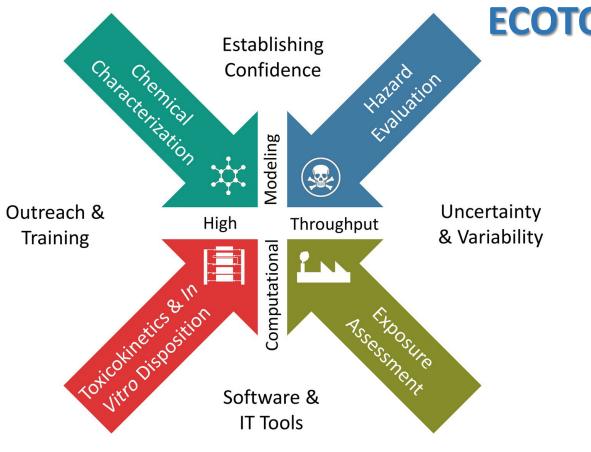
# **History of ECOTOX**





- Developed to meet the need for—
  - Authoritative source of toxicological data
  - Document literature searches of data
  - Development and validation

# **ECOTOX** and the next generation of chemical safety evaluation



# **ECOTOX** Accessible, structured empirical data from *in vivo* toxicity tests

- Chemical risk assessments
- Identify data gaps and guide targeted testing
- Development of computational models
- Support development, evaluation, and adoption of new approach methodologies

vironmental Protection

Environmental Protection

Agency

# What is the ECOTOX Knowledgebase?

- From comprehensive search and review of open and grey literature
- Updated quarterly to public website
- 30+ year history
- 8,000 distinct hosts search the Knowledgebase each month

#### **ECOTOX** Knowledgebase Home Search Explore Help Contact Us Total in database Data last updated 12.485 13,709 Recent chemicals with full searches completed and data extracted Mar 10, 2022 Chemicals Species Acetamiprid Sabadilla alkaloids Dinotefuran Per- and Polyfluoroalkyl Substances (PFAS) See update totals 53.020 1.102.544 References Results

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#### Download

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### www.epa.gov/ecotox



### **EPA Program and Regional Office Applications**





Aquatic Life Ambient Water Quality

Criterion for

Selenium – Freshwater

2016

OHome ≥Air ≥Land ≥Water @Licenses Permits Reporting Q Data Home / Remediation / Eco / Useful Links for Developing Ecological Risk Assessments >> Questions or Comment techsup@tceq.texas.gov Ø Forms Useful Links for Developing Ecological Risk Assessments m Mans Links to pages on this and other sites that have useful information for developing ecological risk Public Notices U.S. EPA Integrated Risk Information System (IRIS) ECOTOX Database (aquatic and terrestrial toxicological data) EPA Office of Water (links to sediment guidance, water guality standards, and other useful topics) • EPA People Locator EPA Region 4 Ecological Screening Values

Search Site

- Combustion Guidance for Human Health (some defaults in here used at times)
- Superfund Risk Assessment (variety of links)

TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

Superfund: Natural Resource Damages and Ecological Risk Assessments

A PROTECTION	WASHINGTON D.C., 20460
MEMORA	NDUM March 26, 2008
Subject:	Registration Review –Preliminary Problem Formulation for Ecologica Risk and Environmental Fate, Endangered species and Drinking Wate Assessments for Diazinon (PC Code 057801; DP Barcode D349527)
То:	Jude Andreasen, Chemical Review Manager Laura Parsons, Team Leader Special Review Branch Special Review and Reregistration Division (SRRD)
From:	Kristina Garber, Biologist Thomas Steeger, Senior Biologist Environmental Risk Branch 4 Environmental Fate and Effects Division Office of Pesticide Programs
Through:	Elizabeth Behl, Chief

Junited STATES ENVIRONMENTAL PROTECTION AGENCY

bugh: Elizabeth Behl, Chief Environmental Risk Branch 4 Environmental Fate and Effects Division Office of Pesticide Programs

The Environmental Fate and Effects Division (EFED) has completed the preliminary problem formulation (attached) for the ecological risk, environmental fate, endangered species, and drinking water assessments to be conducted as part of the Registration

U.S. Environmental Protection Agency Office of Water Office of Science and Technology Washington, D.C.



### Overview of TSCA Work Plan Methodology

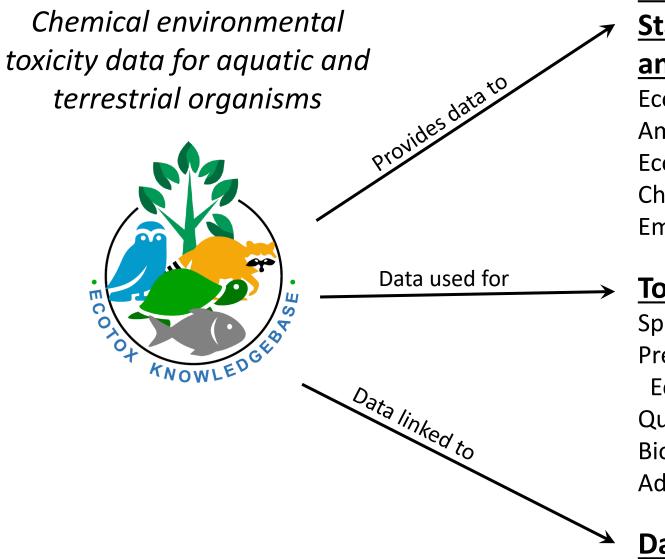
Maria Doa U.S. EPA, Office of Pollution Prevention and Toxics December 11, 2017

#### Ecological Hazard

Ecological hazard data are extracted from the EPA ToxVaIDB database where it had been compiled from the EPA ECOTOX database. Although data are available for a variety of species, only data for aquatic species are used in the current illustration. The data can come from any of the following study types: mortality:acute, mortality:chronic, reproductive:acute, reproductive:chronic, growth:acute, growth:chronic (all from ECOTOX). The types of effect levels are LDxx/LCxx/ECxx/EDxx where xx can range from 1% to 100%, and LOEL/NOEL/LOEC/NOEC. Values must be in units of mg/L. For each chemical, the lowest toxicity value was separately determined for acute and chronic studies, regardless of species. The

# **Applications of ECOTOX**





### **EPA Program Offices and Regions,**

States, Tribes, Other Federal Agencies

### and International Entities

Ecological Risk Assessments Ambient Water Quality Criteria Ecological Screening Values Chemical Prioritization Emergency Response

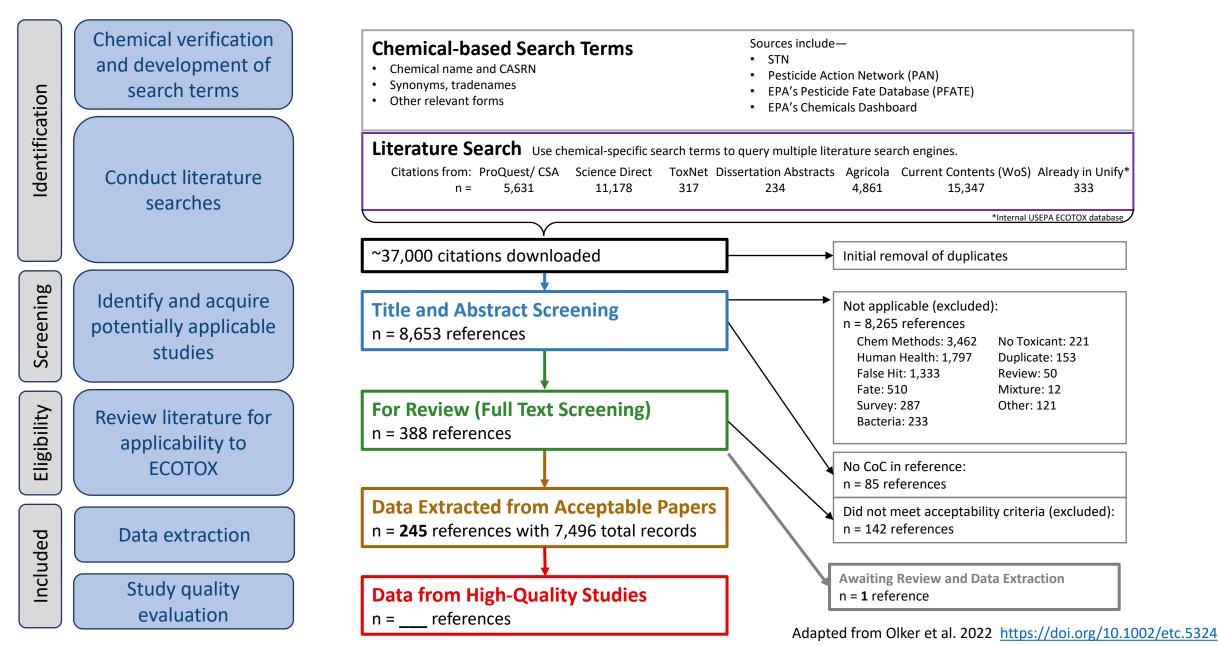
### Tools and Applications

Species Sensitivity Distributions Predicted No-Effect Concentrations and Eco-Thresholds for Toxicological Concern Quantitative Structure–Activity Relationships Bioaccumulation Factor Modeling and Validation Adverse Outcome Pathway Development

### **Databases/Resources**

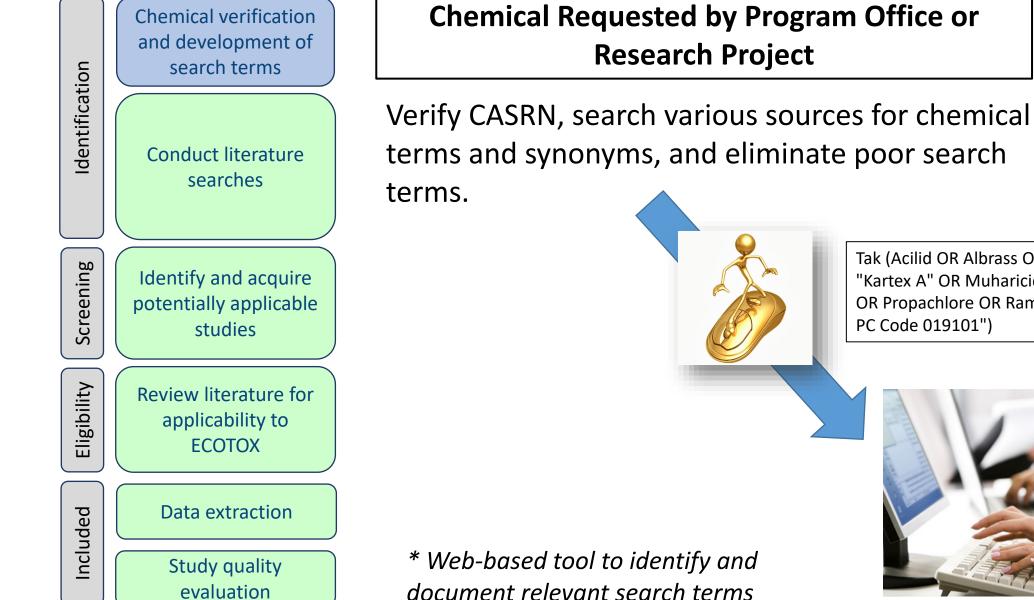
# **ECOTOX Pipeline**





# **Chemical Search Terms: ID, Test and QA**





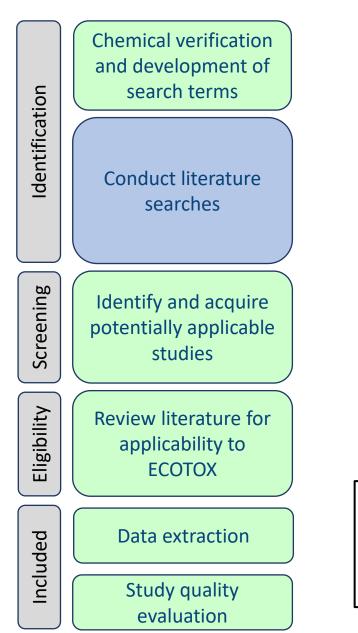
Tak (Acilid OR Albrass OR Bexton OR "CP 31393" OR "Kartex A" OR Muharicid OR Niticid OR Propachlor OR Propachlore OR Ramrod OR Satecid OR "US EPA PC Code 019101")



Enter chemical terms into template for abstracting databases.

### **Literature Searches**

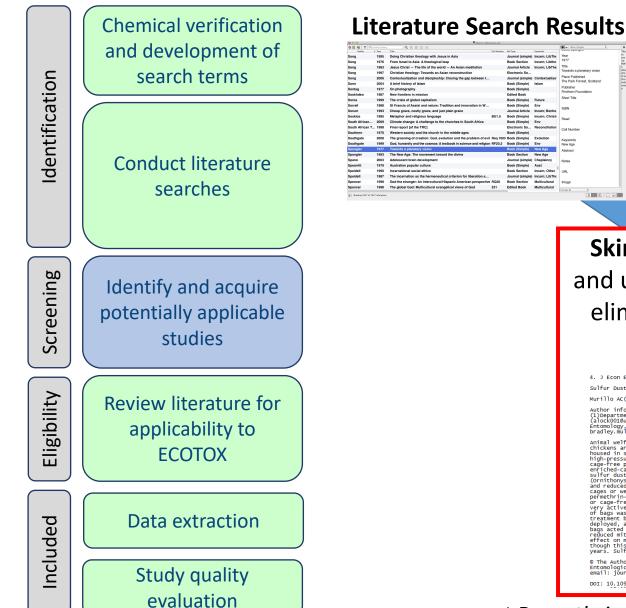




	<b>Sed literature searches</b> In chemical verification step) OR	
	electronic searches nly relevant journals	
<ol> <li>ProQ</li> <li>Web</li> <li>PubA</li> <li>PubN</li> <li>Disse</li> <li>* Semi-0</li> </ol>	us/Science Direct	
100,000–400,000 references screened for applicability each year	Constant and a set of the se	Collate data and remove duplicates.

### **Skimming for Applicability: Title and Abstract**





Skim titles and abstracts and use exclusion criteria to eliminate non-applicable results.

4. J Econ Entomol. 2016 Jul 18. pii: tow146. [Epub ahead of print]

Sulfur Dust Bag: A Novel Technique for Ectoparasite Control in Poultry Systems.

Murillo AC(1), Mullens BA(2)

Author information Automannormatic Entennology, university of California, Riverside, CA 92521 (dlockOOlBurr, edu; bradley.mullenskurr.edu) alockOOlBurr,edu, (2)Department of Entomology, University of California, Riverside, CA 92521 (alockOOlBurr.edu; bradley.mullenskurr.edu).

bradley.multenseur.edu).
Armian weifingrad-tiven legislation and consumer demand are changing how laying chickens are housed, thus creating challenges for accoparasite control. Here some source is suppended where cages (Datery cages) are usually treated with high-pressure pesticides. This application type is difficult in enriched-cage or cage-free production. Alternatives to pesticide sprays are needed in enriched-cage or cage-free systems. In this study, we tested the efficacy of stocked reduction were clipped to the inside the stocked sprays are usually out that the output of the stocked sprays are usually output of the stocked sprays are stocked. The stocked spray are usually treated with output of the stocked spray are usually treated with output of the stocked spray are stocked to be stocked with the stocked spray are stocked to be stocked to be stocked to be stocked the stocked spray are usually output of the stocked spray are stocked to be stocked to be stocked to be stocked for the stocked to be stocked for the stocked to be stocked to be stocked for the stocked to be stocked for the stocked to be sto

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DOI: 10.1093/jee/tow146

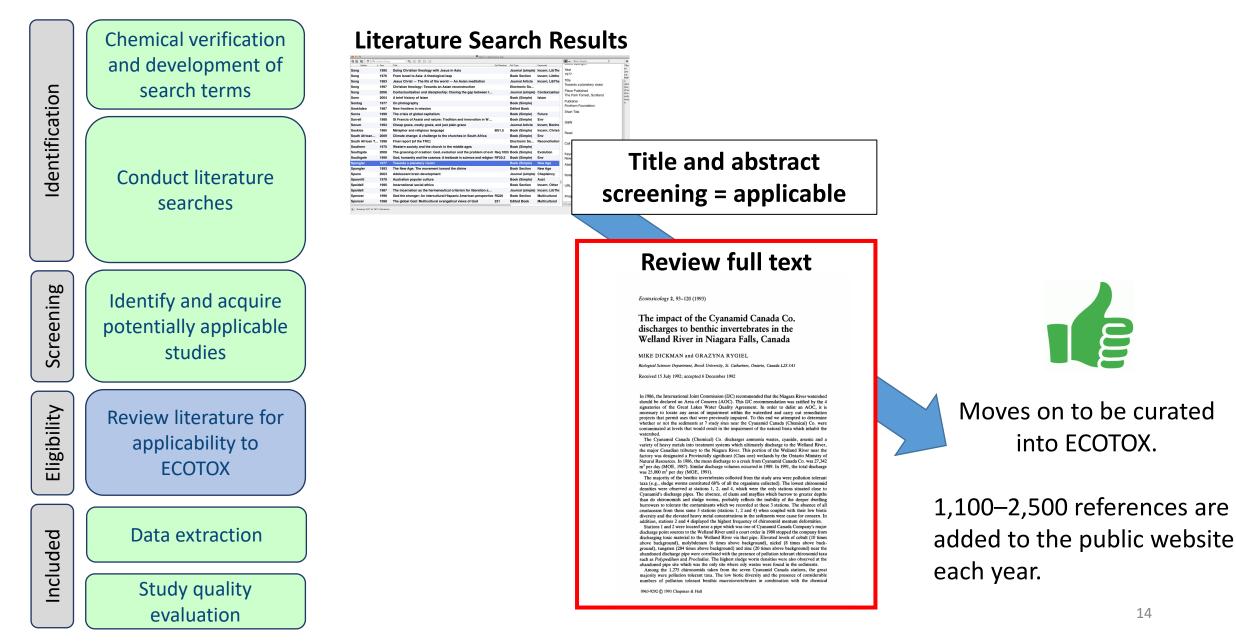
Caladopure Innov & A (F (= − A)) | B (A) | B 890018--

### Send the applicable reference list for acquisition.

\* Recently incorporated filtering and AI tools

## **Review for Applicability: Full text**





# **ECOTOX Applicability Criteria**



	Key Area	Data Requirement
P (Population)	Species	<ul> <li>Taxonomically verifiable, ecologically relevant organisms (including cells, organs, gametes, embryos, plant cuttings) [NOT bacteria, humans, monkeys, viruses or yeast]</li> </ul>
E (Exposure)	Chemical	<ul> <li>Single, verifiable chemical toxicants, administered through an acceptable route</li> </ul>
	Exposure Amount (Concentration)	• 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
	Exposure Duration	<ul> <li>Known duration from the time of initial exposure to the time of measurement</li> </ul>
C (Comparator/ Control)	Control	<ul> <li>Must have a control treatment</li> </ul>
O (Outcome)	Effect	<ul> <li>Biological effect measured</li> <li>Effect concurrent with associated chemical exposure</li> </ul>
	Publication Type	<ul> <li>Primary source of the data [NOT a Review]</li> <li>Study must be a full article in English</li> </ul>

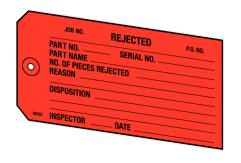
### **Exclusion Documentation**



### All Excluded and Non-Applicable studies are tagged with the reason for rejection.

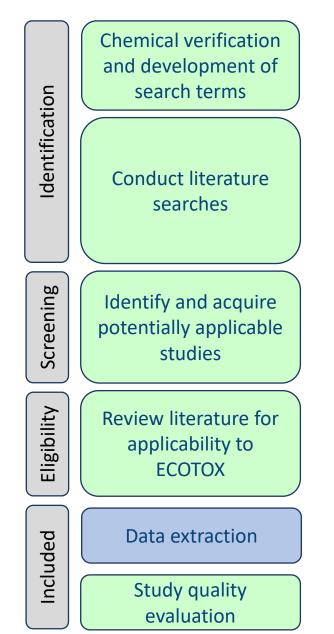
- Abstract published as an abstract
- Bacteria only test organism is a bacteria
- CAS # Unavailable could not verify/locate chemical CAS Registry number
- Chemical method description of chemical analysis procedures
- Fate only report chemical distribution in media
- Human Health data on human subjects of surrogate animal subjects for human health risk assessment
- Incident reports death of animal by poison, but does not provide concentration/duration of exposure
- Method paper only reports methods for conducting a toxicity test or other aspect of an experiment
- Mixture paper reports results from mixture of chemicals; no single-chemical exposure results
- Modeling results of the development of a model; no primary data available

- No Conc the authors report a response in an organism but do not provide conc/dose/app rate
- No Duration duration of exposure is not presented
- No Effect paper does not report observed responses adverse of otherwise
- No Toxicant (ozone, CO<sub>2</sub>)
- Non-English
- Nutrient in situ chemical tested as nutrient
- PUBL AS duplicate data published elsewhere
- Retracted paper retracted by Journal
- Review primary data published elsewhere
- Sediment only sediment concentration presented
- Survey chemical measured in organism, but lack quantification of exposure (dose/duration)
- Virus virus is only test organism
- Yeast yeast is only test organism



### **Data Extraction**

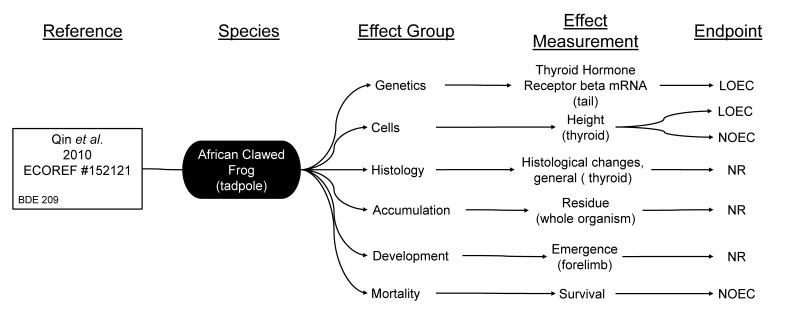






Journal of Environmental Sciences Volume 22, Issue 5, 2010, Pages 744-751

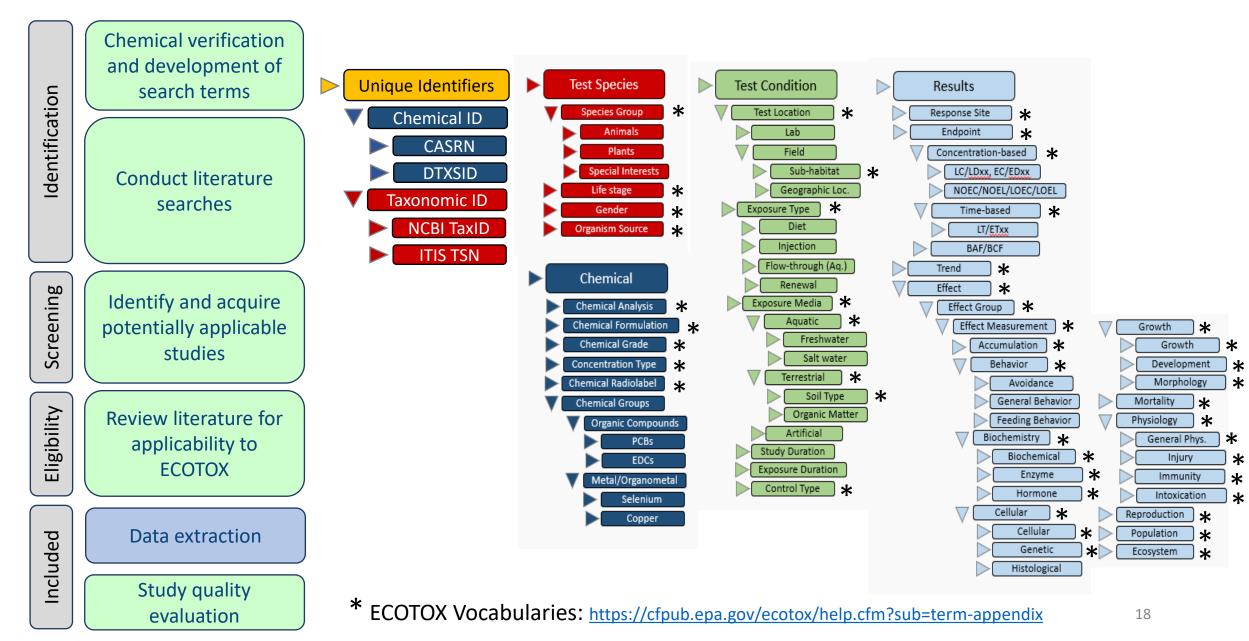
Thyroid disruption by technical decabromodiphenyl ether (DE-83R) at low concentrations in *Xenopus laevis* 



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

### **Data Extraction**





# **Study Quality Evaluation**



Chemical verification and development of search terms Identification **Conduct literature** searches Screening Identify and acquire potentially applicable studies Eligibility Review literature for applicability to **ECOTOX** Data extraction Included Study quality evaluation

Many fields in ECOTOX can inform study evaluation.

Category	Select study evaluation questions with relevant ECOTOX field(s)
Chemical	<ul> <li>Is the test substance identified? Required for inclusion in ECOTOX</li> </ul>
	<ul> <li>Is the purity of the test substance reported? <u>Chemical Purity</u></li> </ul>
	<ul> <li>Were chemical concentrations verified? <u>Chemical Analysis</u> (e.g., nominal versus measured concentrations)</li> </ul>
Species	<ul> <li>Is the species given? Verifiable species (Scientific Name, etc.) required for inclusion in ECOTOX</li> </ul>
	<ul> <li>Are the organisms well described? <u>Organism Source</u>, <u>Lifestage</u>, <u>Age</u>, <u>Gender</u>, <u>Initial</u> and <u>Final Weight</u></li> </ul>
Test Conditions	<ul> <li>Are appropriate controls performed? Control required for inclusion in ECOTOX, type described in Control</li> </ul>
	<ul> <li>Is a guideline method (e.g., OECD) used? <u>Test Method</u></li> </ul>
	<ul> <li>Are the experimental conditions appropriate and acceptable for the test substance and organism? <u>Test Method</u>, <u>Media Type</u>, <u>Test Location</u>, <u>Experimental Design</u>, Physical and Chemical Soil and Water Parameters (e.g., <u>pH</u>, <u>Temperature</u>, <u>Dissolved</u> <u>Oxygen</u>)</li> </ul>
Test Results	<ul> <li>Are the reported effects and endpoints appropriate for the purpose, test substance and organism? <u>Effect Measurement</u>, <u>Endpoint</u></li> </ul>
	<ul> <li>Is the response/effect statistically significant? <u>Statistical</u></li> <li><u>Significance</u>, <u>Significance Level</u></li> </ul>



# **Basic Features**

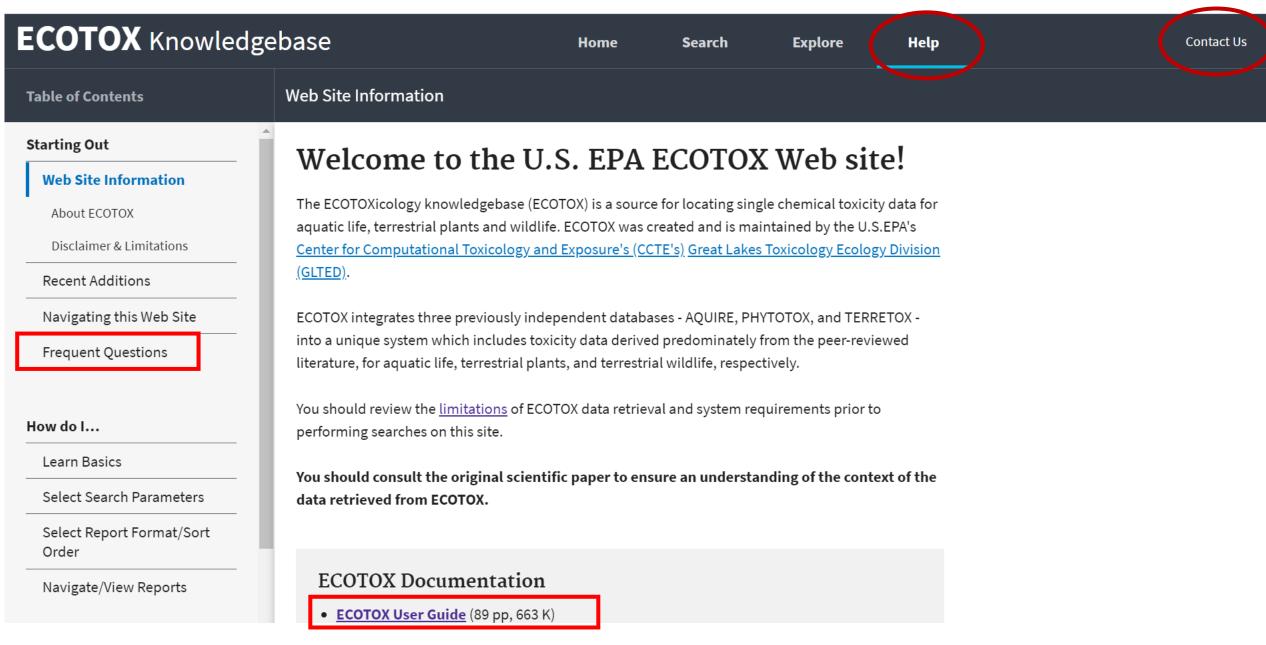
# **Search Planner**



Table of Contents	Select Search Parameters	ECOTOX SEA			
Starting Out		Obse this form to help others to perform.	o plan your sea	rches or to docume	ent searches for yourself or
Web Site Information	<u>Search Planner (PDF)</u> (5 pp, 133 K, <u>About PDF</u> )	Chemical Names	CAS Numbers	Predefined Groups	
web site mornation				Metal Compounds Aluminum	Organic Compounds Conazoles
Recent Additions	Torres and a Constant in a			Antimony Arsenic	Cyanotoxins DDT and metabolites
Navigating this Web Site	Taxonomic Searching			Barium Beryllium	Dibenzofurans Explosives
Hungaring this web site	With a SCOTOY and a stand of the second block of the Constant News and the (a). Constant Scoto is			Cadmium Chromium	Glycol Ethers Major Ions
Frequent Questions	Within ECOTOX you may conduct a search by entering the Species Name or number(s), Genus/Species			Cobalt Copper	Neonicotinoids Nitrosamines
	Name(s), or Common Name or Other Taxonomic Name(s). The Contains and Exact Match radio			Iron Lead	Perchlorates Phthalate Esters
	buttons allow for partial or exact name matches. You can also search by Species Group. All data			Manganese Mercury	Polyaromatic Hydrocarbons (P/ Polychlorinated Biphenyls (PCB
low do I	records within ECOTOX include a Scientific name for the test species. All names and predefined groups			Nickel Organotin	Polybrominated Diphenyl Ethers Pharmaceutical Personal Care
	have been verified in <u>reliable taxonomic sources</u> .			Selenium Silver Vanadium	Strobins Per- and Polyfluoroalkyl Substar
Learn Basics	The ECOTOX species file includes historical synonyms for the species. If a search is conducted using a			Zinc	
Select Search Parameters	species name that is noted as a taxonomic synonym in our system, ECOTOX will present the results	Species		,	
T	using the currently acceptable genus and species name.	Scientific Names/	Common N	Species	Predefined Taxonomi
Taxonomic		Taxonomic Levels	Common Na	Numbers or	r
Chemicals	Taxonomic Entry			NCBI TaxIE	All Animals Amphibians
Test Conditions					Insects/Spiders Molluscs
	Species Number: All species in ECOTOX have been assigned a unique number. You can include				Birds Other Invertebrates
Test Results	numbers and text information (either Scientific or common names) in one search. Species numbers				Reptiles
Publications/Updates	are always searched as an exact match.				Mammals Worms
	Evernle Tevenemic Search				Fish All Plants
Select Report Format/Sort	Example Taxonomic Search				Algae Moss/Hornworts, Fungi,
Order	The example below is the correct method of entering query text. You can enter a mix of numbers and				Flowers, Trees, Shrubs, Fe Special Interest
Navigate/View Reports	species terms. Number will always be treated as exact matches by the ECOTOX query.				Standard Test Species US Threatened/Endangere

# Help and Contact Us







# Demonstration

# **Demo of ECOTOX: www.epa.gov/ecotox**



ECOTOX Knowledg	ebase	Home	Search	Explore	Help			Contact Us
Data last updated Mar 10, 2022	Recent chemicals with full searche		111			Total in database 12,485 Chemicals	13,709 Species	
See update totals	Acetamiprid Dinotefuran	Sabadilla al Per- and Po		bstances (PFAS)		53,020 References	1,102,544 Results	

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### **Other Links**

- <u>Limitations</u>
- Frequent Questions
- Other Tools/Databases
- <u>Recent Additions</u>
- Literature Search Dates

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### **Recent Additions and Literature Search Dates**



### **ECOTOX** Knowledgebase

Data last updated

Mar 10, 2022

See update totals

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Learn More

### Literature Search Dates

#### 801 results

Targeted literature searches are conducted using chemical names, synonyms, and CASRNs in multiple search engines (e.g., Web of Science, Agricola, ToxNet, ProQuest, etc). Chemicals listed below had targeted searches corresponding to the date indicated in the second column. Each search is identified in the table by the requested chemical or chemical group, with some searches including multiple chemicals/CASRNs. Citations from these searches are reviewed. Studies meeting inclusionary criteria added to ECOTOX; toxicity data results may take 6 months or longer to appear on-line. There may be more recent publications in ECOTOX for a chemical due to related chemical literature searches.

	type to find
CHEMICAL	DATE ~
Sabadilla alkaloids	November 2021
<u>Dinotefuran</u>	November 2021
Acetamiprid	November 2021
PFAS	July 2021
Cyanotoxins	June 2021
2-Phenylphenol	December 2020
Chlorflurenol	November 2020

. . . .

		Contact
Total in database		
12,485 Chemicals	13,709 Species	
53,020 References	1,102,544 Results	

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<u>stions</u>

<u>atabases</u>

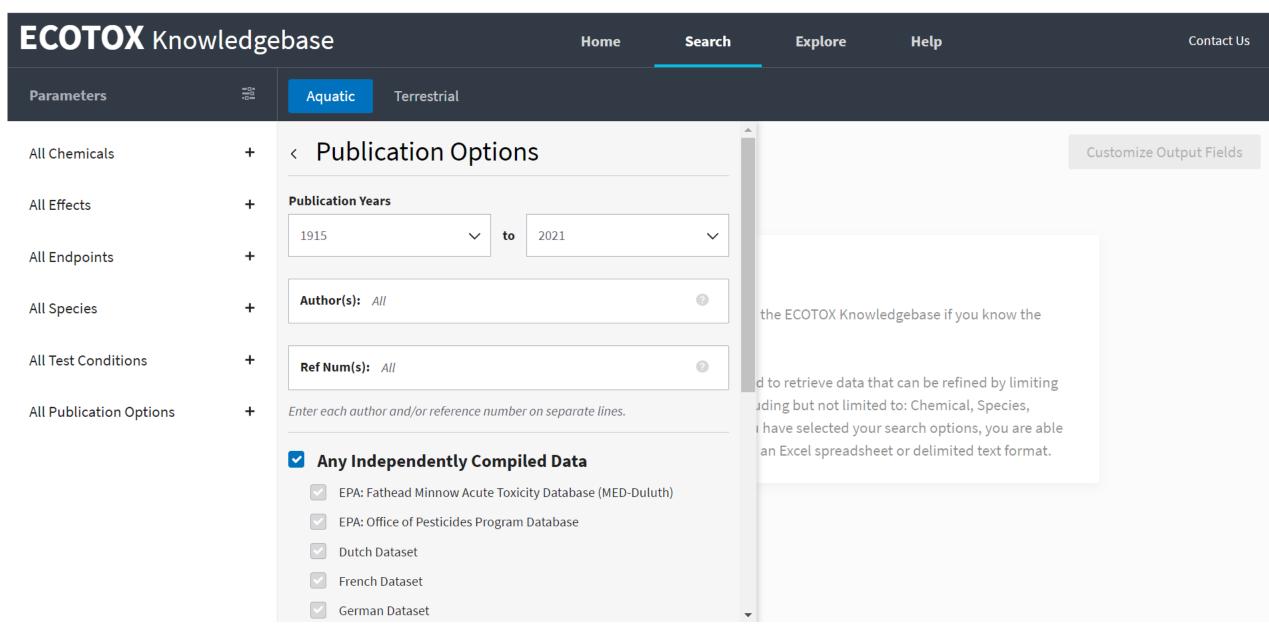
<u>rch Dates</u>

<u>ns</u>

s via Email

## **Search: Exact Parameters or Search Terms**



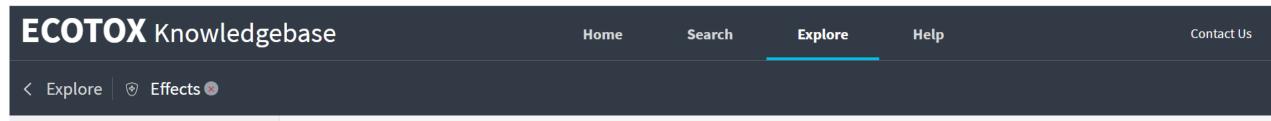


### **Explore:** Interactive Filters and Visualization

23 Effect Groups

Select one or more groups then click "Explore Data" to continue.





#### **Custom Group**

Create a custom effects group by browsing available effect measurements or entering a list of effect and measurement terms.

```
Create Custom Group...
```

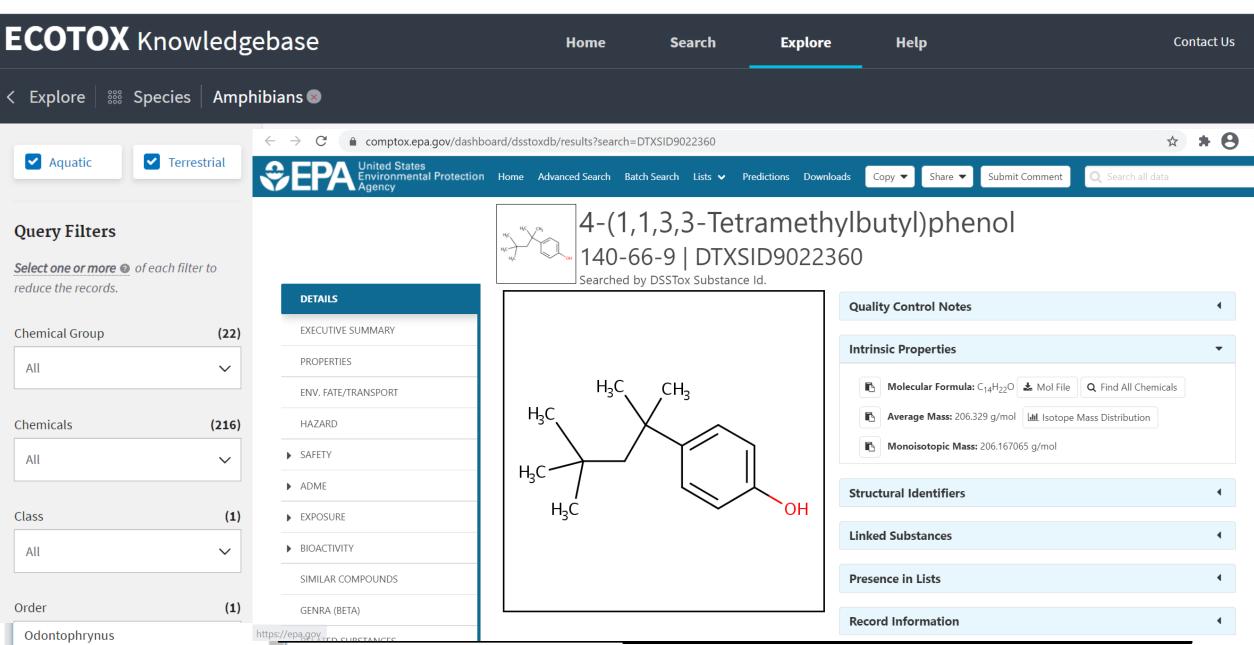
#### **Defined Groups**

**Select one or more** categories from the graph to filter groups in the table.



×R	× Reset All Export CSV						
$\sim$	EFFECT GROUP	RECORDS	PUBLICATIONS	YEAR MIN	YEAR MAX		
	Accumulation	47626	7217	1915	2020		
	Avoidance	4394	579	1947	2020		
	Behavior	18751	2591	1946	2020		
	Biochemistry	76629	9784	1931	2020		
	Cell(s)	12786	2306	1935	2020		
	Development	32771	3904	1925	2020		
	Ecosystem process	743	161	1963	2018		
	Enzyme(s)	47201	6323	1931	2020		
	Feeding behavior	10281	2304	1937	2020		

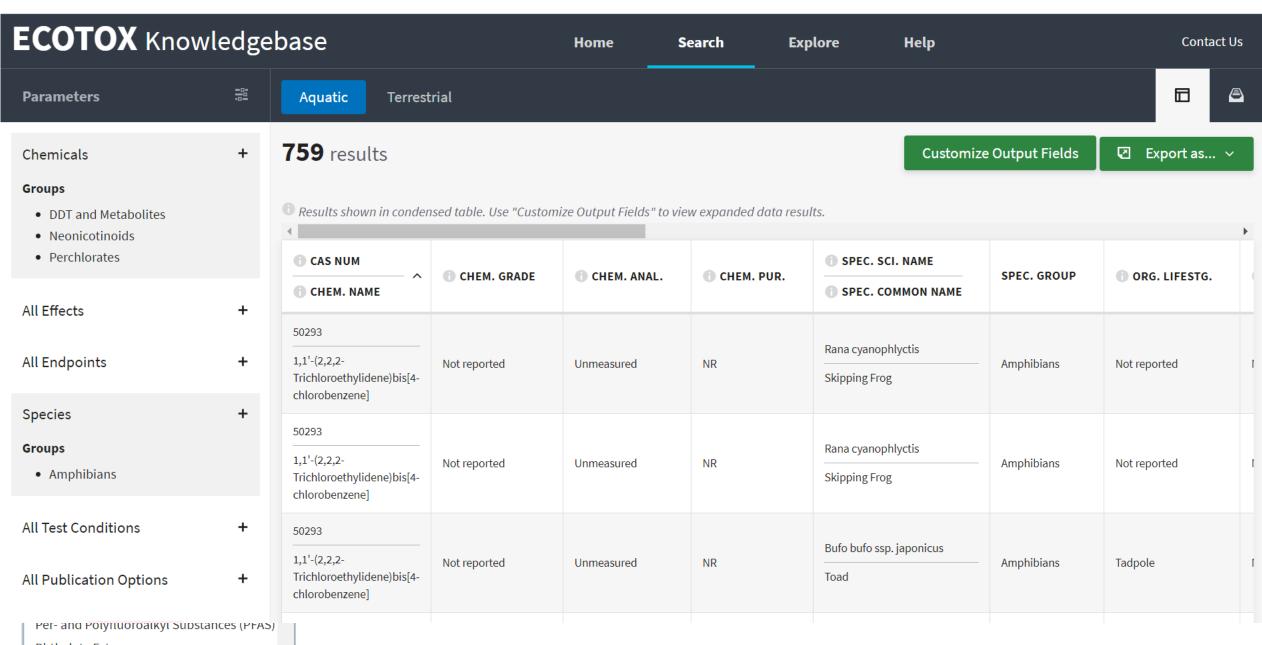
# **Explore by Species: Filter and Visualize**



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# **Explore by Species: Send to Search**

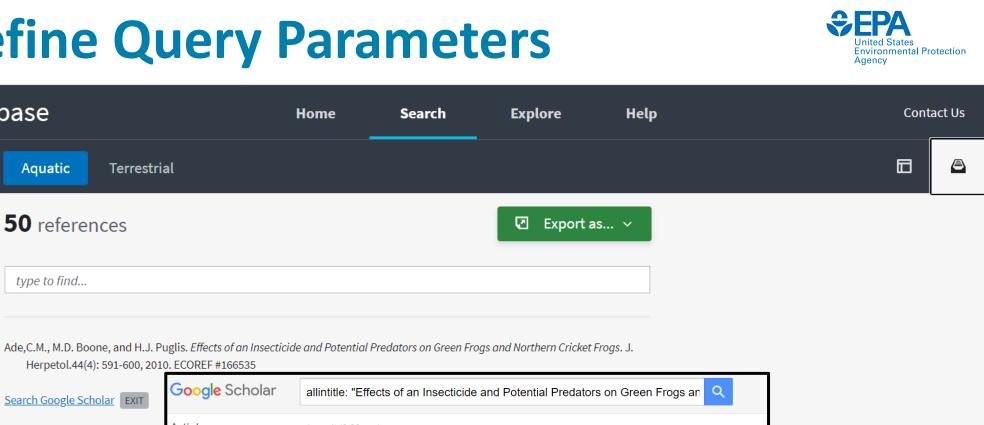


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# **Search: Refine Query Parameters**

Terrestrial



Perchlorates

 DDT and Metabolites Neonicotinoids

**Parameters** 

Chemicals

Groups

**ECOTOX** Knowledgebase

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+

Aquatic

**50** references

type to find ...

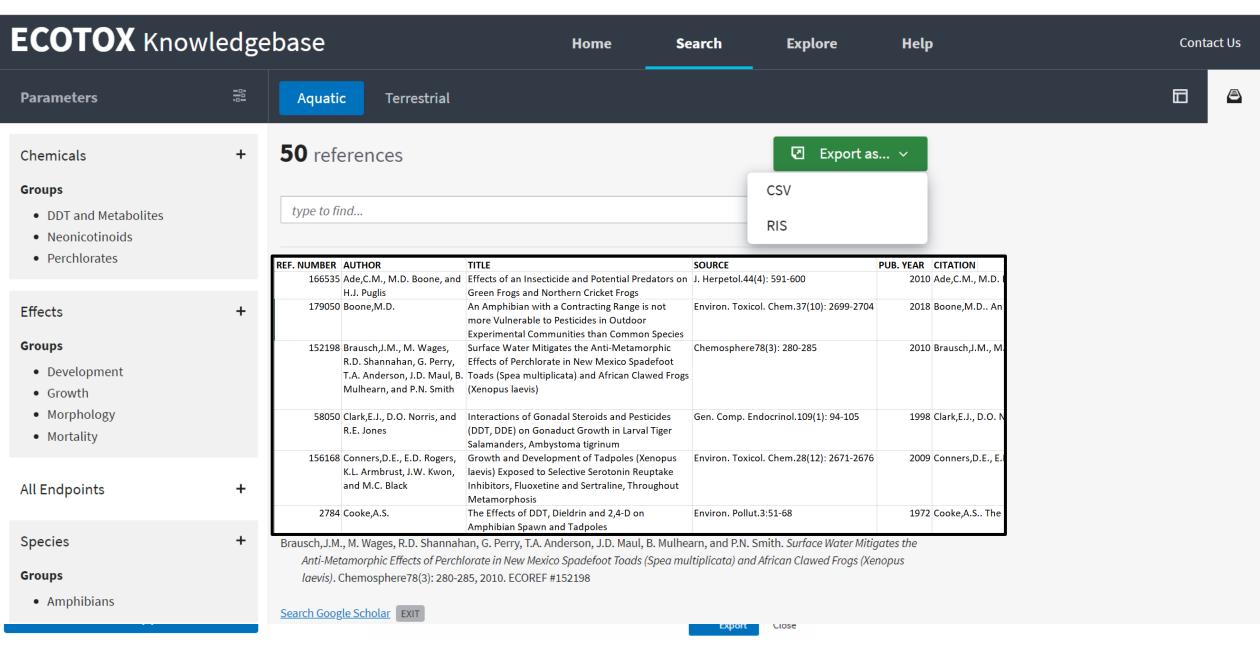
#### Effects

#### Groups

- Development
- Growth
- Morphology
- Mortality
- All Endpoints Species Groups • Amphibians

+	Search Google Scholar EXIT	Google Scholar	allintitle: "Effects of an Insecticide and Potential F	Predators on Green Frogs an	
		Articles	1 result (0.03 sec)		
÷	Boone,M.D <i>An Amphibian with a</i> <i>Common Species</i> . Environ. To <u>Search Google Scholar</u> EXIT	01 0000	Effects of an insecticide and potential predator cricket frogs CM Ade, <u>MD Boone</u> , HJ Puglis - Journal of Herpetology, 20 Worldwide amphibian population declines have occurred in been attributed to a range of factors including introduced sp contamination. Anuran species may differ in their susceptibil history characteristics, leading to different probabilities of de In this experiment, we looked at two anuran species, Northe and Green Frogs (Rana clamitans), reared in mesocosms of 𝔅 𝔅𝔅 Cited by 24 Related articles All 5 versions	Journal of Herpetology, Vol. 44, No. 4, pp. 591-600, 2010 Copyright 2010 Society for the Study of Amphibians and Reptiles Effects of an Insecticide and Potential Northern Cricke	et Frogs
+		Perchlorate in New Mexico Sp	rson, J.D. Maul, B. Mulhearn, and P.N. Smith. Surface V padefoot Toads (Spea multiplicata) and African Clawed 198	ABSTRACT.—Worldwide amphibian population declines h. been attributed to a range of factors including introduced species may differ in their susceptibility to declines based or probabilities of decline and conservation statuses. In this Northern Cricket Frogs ( <i>Acris crepitans</i> ) and Green Frogs ( <i>Ra</i> common invasive or introduced potential predator (Rusty Cr and imidacloprid, a common insecticide. We found that anu Cricket Frog survival was significantly reduced with imidacl Abundance of both amphibian species was reduced in the p study suggests that Cricket Frogs may be especially sensitiv	I species and chemical contamination. Anuran n life-history characteristics, leading to different experiment, we looked at two anuran species, <i>na clamitans</i> ), reared in mesocosms containing a 'ayfish, Bluegill Sunfish, or triploid Grass Carp) rans differed in their sensitivity to these factors. loprid exposure, whereas Green Frogs were not. presence of predators, particularly the fish. Our e to the insecticide imidacloprid, as well as fish

### Search: Export Toxicity Data and References



Environmental Protection

Agency



# Example



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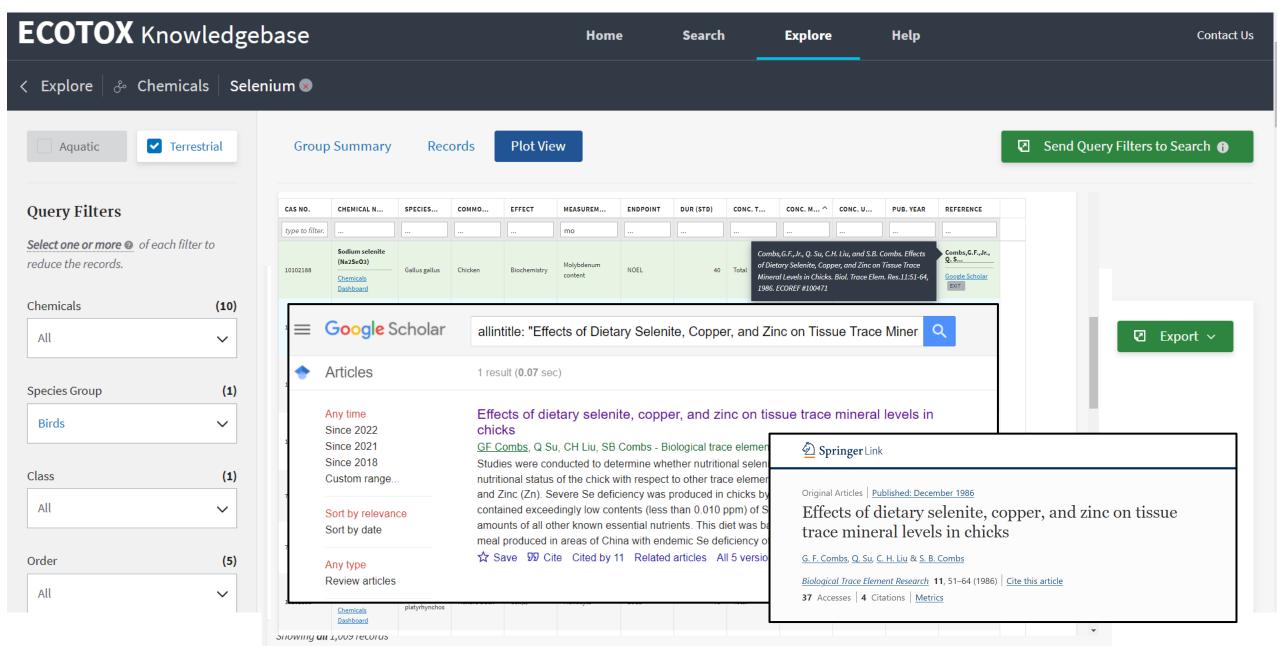


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Animals Amphibians	1313855	Sodium selenide	2	1	1987	1987	>
Birds Crustaceans Fish	1464422	Selenomethionine (Unspecified) 	1075	61	1971	2014	>
Insects/Spiders Other Invertebrates Mammals Molluscs	2697612	Selenocystamine Chemicals Dashboard	6 30867	1 3270	2000	2000	>







Test (	CAS			Reference			
		Chemical Name	Author	Number 💌	Title	• Source •	Publication Year
2156245	1464422	2-Amino-4-(methylseleno)butanoic acid	Heinz,G.H., and M.A. Fitzgerald	58951	Overwinter Survival of Mallards fed Selenium	Arch. Environ. Cont	a 1993
2155067	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, C.M.	58954	Subchronic Hepatotoxicity of Selenomethionine Ingestion in Ma	lle J. Toxicol. Environ.	1991
2164321	1464422	2-Amino-4-(methylseleno)butanoic acid	Heinz,G.H., and D.J. Hoffman	40269	Comparison of the Effects of Seleno-L-Methionine, Seleno-DL-M	AcEnviron. Pollut.91(2	) 1996
2156295	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	58953	Interactive Effects of Selenium, Methionine, and Dietary Protein	ı c Arch. Environ. Cont	a 1992
2156295	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	58953	Interactive Effects of Selenium, Methionine, and Dietary Protein	ı c Arch. Environ. Cont	a 1992
2157062	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., and G.H. Heinz	39729	Embryotoxic and Teratogenic Effects of Selenium in the Diet of	M J. Toxicol. Environ.	1988
2250263	1464422	2-Amino-4-(methylseleno)butanoic acid	Fairbrother, A., and J. Fowles	35152	Subchronic Effects of Sodium Selenite and Selenomethionine on	SArch. Environ. Cont	a 1990
2155067	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, C.M.	58954	Subchronic Hepatotoxicity of Selenomethionine Ingestion in Ma	lle J. Toxicol. Environ.	1991
2157083	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., and G.H. Heinz	39729	Embryotoxic and Teratogenic Effects of Selenium in the Diet of	M J. Toxicol. Environ.	1988
2155941	1464422	2-Amino-4-(methylseleno)butanoic acid	Heinz,G.H., and D.J. Hoffman	58949	Methylmercury Chloride and Selenomethionine Interactions on	Henviron. Toxicol. Ch	( 1998
2155067	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, C.M.	58954	Subchronic Hepatotoxicity of Selenomethionine Ingestion in Ma	lla J. Toxicol. Environ.	1991
2156361	1464422	2-Amino-4-(methylseleno)butanoic acid	Heinz,G.H., D.J. Hoffman, and L.J. LeCaptain	40189	Toxicity of Seleno-L-Methionine, Seleno-DL-Methionine, High Se	ele Arch. Environ. Cont	a 1996
562708	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	39733	Interactive Effects of Boron, Selenium, and Dietary Protein on S	ur Arch. Environ. Cont	a 1991
2156902	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman, D.J., G.H. Heinz, and A.J. Krynitsky	39873	Hepatic Glutathione Metabolism and Lipid Peroxidation in Respo	on J. Toxicol. Environ.	1989
2156245	1464422	2-Amino-4-(methylseleno)butanoic acid	Heinz,G.H., and M.A. Fitzgerald	58951	Overwinter Survival of Mallards fed Selenium	Arch. Environ. Cont	a 1993
2155067	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, C.M.	58954	Subchronic Hepatotoxicity of Selenomethionine Ingestion in Ma	lla J. Toxicol. Environ.	1991
2156902	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, and A.J. Krynitsky	39873	Hepatic Glutathione Metabolism and Lipid Peroxidation in Respo	on J. Toxicol. Environ.	- 1989
2156802	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, J.D. E	50242	Toxicity and Oxidative Stress of Different Forms of Organic Sele	ni Arch. Environ. Cont	a 1996
2156902	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman, D.J., G.H. Heinz, and A.J. Krynitsky	39873	Hepatic Glutathione Metabolism and Lipid Peroxidation in Respo	on J. Toxicol. Environ.	- 1989
562713	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	39733	Interactive Effects of Boron, Selenium, and Dietary Protein on S	ur Arch. Environ. Cont	1991
2155067	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, C.M.	58954	Subchronic Hepatotoxicity of Selenomethionine Ingestion in Ma	lleJ. Toxicol. Environ.	- 1991
2156902	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, and A.J. Krynitsky	39873	Hepatic Glutathione Metabolism and Lipid Peroxidation in Respo	on J. Toxicol. Environ.	- 1989
2156295	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	58953	Interactive Effects of Selenium, Methionine, and Dietary Protein	n <mark>c Arch.</mark> Environ. Cont	a 1992
562710	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	39733	Interactive Effects of Boron, Selenium, and Dietary Protein on S	ur Arch. Environ. Cont	a 1991
562715	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	39733	Interactive Effects of Boron, Selenium, and Dietary Protein on S	ur Arch. Environ. Cont	a 1991
2156879	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, J.D. E	50242	Toxicity and Oxidative Stress of Different Forms of Organic Sele	ni Arch. Environ. Cont	1996
2156044	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., and G.H. Heinz	50244	Effects of Mercury and Selenium on Glutathione Metabolism an	d Environ. Toxicol. Ch	. 1998
2156295	1464422	2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., C.J. Sanderson, L.J. LeCaptain, E	58953	Interactive Effects of Selenium, Methionine, and Dietary Protein		
2156879		2-Amino-4-(methylseleno)butanoic acid	Hoffman,D.J., G.H. Heinz, L.J. LeCaptain, J.D. E	50242	Toxicity and Oxidative Stress of Different Forms of Organic Sele		
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# **Case Studies**

### **Case Studies**



- Breakout groups are assigned based on your familiarity with and level of ECOTOX use.
- Each breakout group has a moderator to help participants and answer questions.
- There is a beginner and advanced case study. Each case study has an associated worksheet to guide the breakout group.
- Use the associated worksheet to complete the case study.
- If you finish early, notify your breakout group moderator. They can provide you other activities to complete.
- After the time is up, we will debrief the case studies.

# **Debrief: Level 1 Case Study**



- In what case example from your work environment would ECOTOX be useful?
- What have you learned about the process and workflow used to find information and papers in ECOTOX?
- What challenges did you encounter, and how did you solve them?

### **Debrief: Level 2 and Additional Case Studies**



- What process did you follow in ECOTOX to explore the information presented in the initial publication?
- What challenges did you encounter? How did you solve them?
- In what case example from your work environment would ECOTOX be useful?



# Summary





- Systematic and transparent procedures to identify and curate ecological toxicity data
- 30+ year history, with major recent updates and evolution in the near future
  - Maintain comprehensive and quality review of toxicity data
  - Enhance ease of data access and clarity
  - Meet the demands for increased pace of chemical assessments
  - Expand to reflect shifts in toxicity testing paradigm
- Curated data are on the public website (<u>www.epa.gov/ecotox</u>), readily available for exploration, querying and export for risk assessments, risk management and research

# **Thank You!**



### **ECOTOXicology Knowledgebase Team**

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Jason Berninger, GLTED

Colleen Elonen, Scientific Computing and Data Curation Division (SCDCD) (previous ECOTOX Coordinator)

Sara Vliet, SCDCD (liaison to ECOTOX)

Contract staff:

General Dynamics Information Technology (GDIT) SpecPro Professional Services (SPS)

Senior Environmental Employment (SEE) staff

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# **Future NAMs Trainings: Potential Topics**



Topic Area	Specific Products, Including Web Applications, Databases, Tools and Workflows
CompTox Chemicals Dashboard	CompTox Chemicals Dashboard: overview, all sub-modules and their functionality tailored to be a chemical specific case study approach that is trainee/user-defined.
Ecotoxicology	ECOTOX Knowledgebase, SeqAPASS
Exposure	CPDat (CPCat, CPCPdb, Ingredient Lists, Functional Use Data, Measured Data), Expocast/SEEM3; SHEDS HT
Databases relevant to toxicity and bioactivity	ToxCast, ToxRefDB, ToxVal, TEST; invitroDB
Toxicokinetics and dosimetry	High-Throughput Toxicokinetics R-Package (HTTK)
Chemical safety proof-of-concept (POC) workflows	Toxic Substances Control Act (TSCA) POC, Bioactivity:Exposure Ratio
Chemistry	GenRA; phys-chem properties (OPERA models); ENTACT; Non-Targeted Analysis (NTA)

For more information: www.epa.gov/chemical-research/new-approach-methods-nams-training

### Contact

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### **ECOTOX Support:**

### 218-529-5225

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