

ECOTOXicology Knowledgebase

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Project Team:
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Jennifer Olker
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GDIT and BTS contract staff
SEE staff



www.epa.gov/ecotox



What is the ECOTOX Knowledgebase?

Publicly available, curated database providing toxicity data from single-chemical exposure studies to aquatic life, terrestrial plants, and wildlife



- Curated data from >49,000 publications
- From comprehensive search and review of open and grey literature
 - Data extracted from acceptable studies, with up to 250 fields
 - Updated quarterly

The impact of the Cyanamid Canada Co. discharges to benthic invertebrates in the Welland River in Niagara Falls, Canada MIKE DICKMAN and ORAZYNA RYGIEL

Biological Sciences Department, Brock University, St. Catharines, Ontario, Canada L253AJ Received 15 July 1992; accepted 6 December 1992

abould be declared an Area of Concern (AOC). This IC recommendation was satisfied by tad of againstense of the Green Lakes Water (Jossil) Againstense in done to define as AOC, it is againstense of the Green Lakes Water (Jossil) Againstense in done to define as AOC, it is project that permit uses that sever previously impaired. To this cost we attempted to determine selection on the confirment of 3 triots to its next the Capasation Canada (Concision) Co. were contempted as device that would result in the impairment of the animal tous which about the The Capasation Canada (Canada) Canada (Canada (Canada (Canada (Canada)) Canada (Canada (Canada)) Canada (Canada (Canada)) Canada (Canada (Canada)) Canada (Canada) Canada (Canada)

The Cyanamid Canada (Cherical) Co. discharges armenta wates, cyanide, mentic and variety of heavy natical into internetive spirms which distansied behaviour for Medianal River and the major Consulan Terbusty to the Nagara River. This persons of the Widnast River are the transport of the Widnast River are the Nagara River. This persons of the Widnast River are the Nagara River. The Property of the Widnast River are the 18th of the Nagara River. The Nagara River are the Nagara River and Property of Nagara (Nagara River and Nagara River) and Property of Nagara River and Nagara Riv

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- 30+ year history: originated in the early 1980s, maintained by EPA ORD
- Supported by ORD's Chemical Safety for Sustainability (CSS) and Safe and Healthy Communities (SHC) research action plans

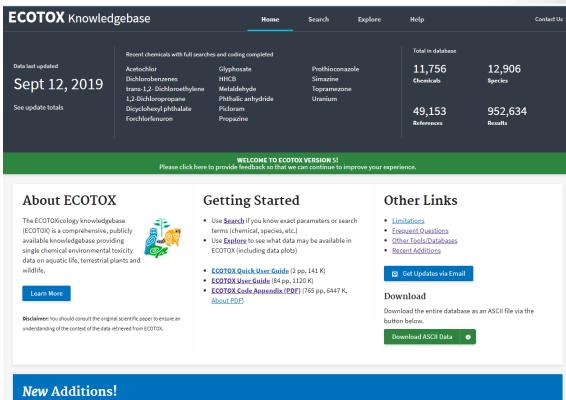






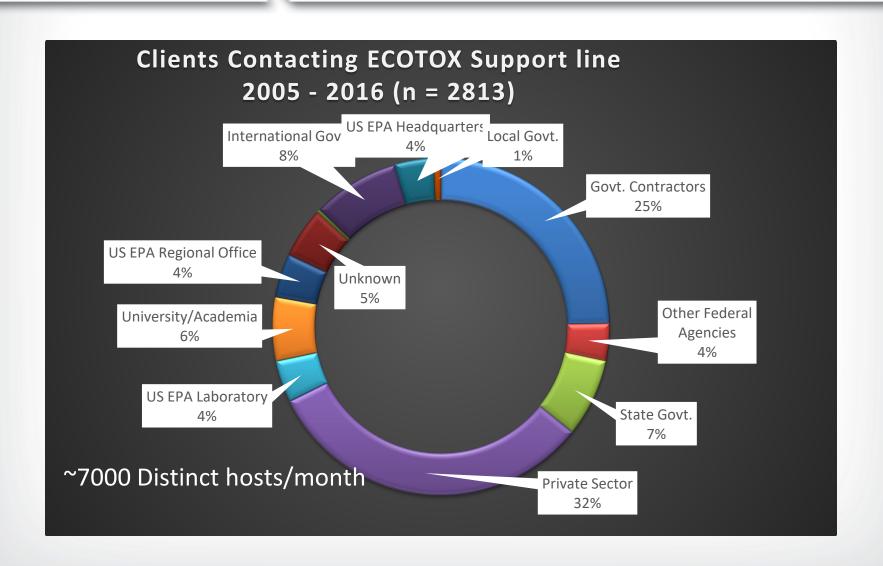
What is the ECOTOX Knowledgebase?

- Publicly available at <u>www.epa.gov/ecotox</u>
 - Interactive queries by chemical, species, effect or endpoint
 - Updated quarterly
- Major updates 2018-2019
 - New User Interface
 - New functionality
 - Interoperability with other databases and tools

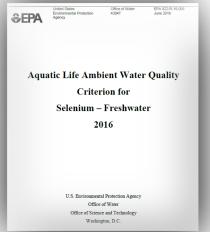




Who uses the ECOTOX Knowledgebase?



Program Offices & Regions Applications: use in environmental decision making



Used for every Ambient Water Quality Criteria for Aquatic Life since 1985.

Used for every Ecological Risk Assessment for Office of Pesticides for chemical registration and re-registration (FY19 – 30 chemicals).

Used by OLEM (Superfund and RCRA), HQ, Regions and States for site assessments and in emergency response

Providing ecological hazard data for the prioritization and assessment of chemicals for TSCA/Lautenberg Act





Superfund: Natural Resource Damages and Ecological Risk Assessments



Maria Doa

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



Providing ecological toxicity data for PFAS to researchers, EPA ERA Forum, DoD Tri-Services ERA Work Group, and others

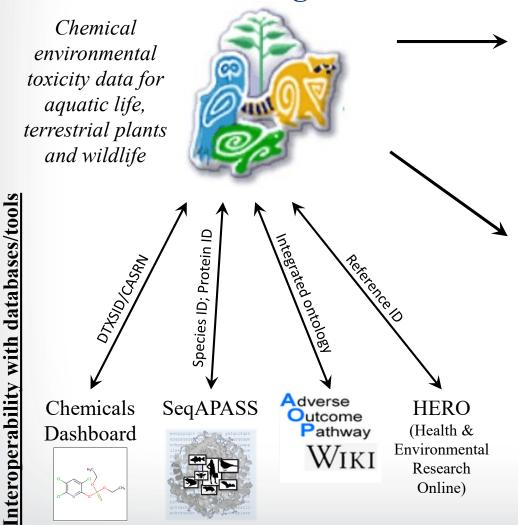
Ecological Hazard

Ecological hazard data are extracted from the EPA ToxValDB 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-actue, 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

ECOTOX Knowledgebase



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 (e.g., US EPA's WebICE, NOAA's CAFÉ)
PNECs and threshold values (e.g., EcoTTC)
QSAR (e.g., ECOSAR, TEST, OECD QSAR
Toolbox)
BCF modeling and validation

Adverse Outcome Pathway (AOP) development

ECOTOX Pipeline: Systematic Review/Data Curation

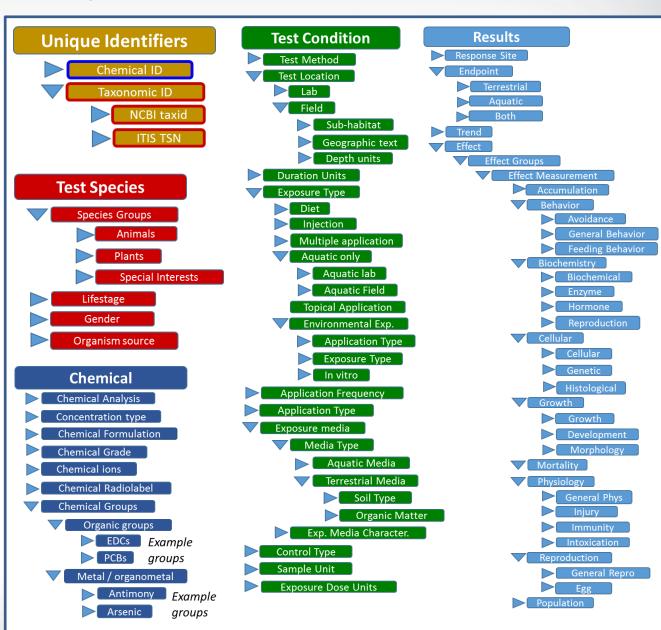
Chemical verification and development of search terms

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to ECOTOX

Extract data and code into ECOTOX
Knowledgebase



Included

Identification

Screening

Eligibility

Identification

Screening

Eligibility

Included

Chemical verification and development of

search terms

Conduct literature searches

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Review literature for applicability to ECOTOX

Data extraction

Study quality evaluation

Chemical-based Search Terms:

- Chemical name and CASRN
- Synonyms, tradenames
- Other relevant forms (metabolites, degradants, parent compound, related chemicals)

Sources include:

- STN
- Pesticide Action Network (PAN)
- EPA's Pesticide Fate Database (PFATE)
- EPA's Chemistry Dashboard.

Literature search: Use chemical-specific search terms to query multiple literature search engines

Citations from: ProQuest/ Science ToxNet Dissertation Agricola Current Contents Already in **CSA** Direct Abstracts (WoS) Unify* 5,631 11.178 317 234 4.861 15,347 333 n =

*Internal USEPA ECOTOX database

~37,000 citations downloaded

Title and Abstract Screening

n = 8,653 references

For Review (Full Text Screening)

n = 388 references

Data Extracted from Acceptable Papers

n = 245 references with 7,496 total records

Data from High Quality Studies

 $n = \underline{\hspace{1cm}}$ references

Initial removal of duplicates

Not applicable (excluded):

n = 8,265 references

Chem Methods: 3,462 No Toxicant: 221 Human Health: 1,797 Duplicate: 153 False Hit: 1,333 Review: 50

Fate: 510 Mixture: 12 Survey: 287 Other: 121

Bacteria: 233

No PFAS in reference: n = 85 references

Did not meet acceptability criteria (excluded): n = 142 references

n = 142 references

Awaiting Review and Data Extraction

n = 1 references

Screening

Eligibility

Included

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to ECOTOX

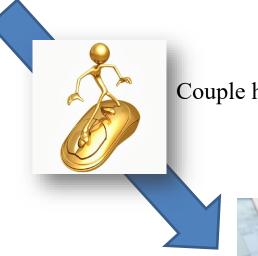
Data extraction

Study quality evaluation

Identify, Test, and QA Search Terms

Search various sources for chemical terms, Synonyms, verify CAS, eliminate poor search terms

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") AND NOT key(human* or child pupat* OR infant* OR homind* OR woman OR pupat* OR patient* OR OSHA OR chromatograph* OR Specific OR pediatric*)



Couple hour process

Enter chemical terms into template for abstracting databases



ECOTOX Literature Searches

Chemical verification and development of search terms

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to **ECOTOX**

Data extraction

Study quality evaluation

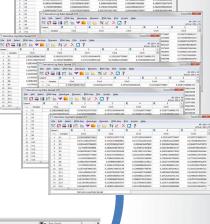
Chemical specific searches (using terms from chemical verification step) OR

> Monthly electronic searches of 11 highly relevant journals

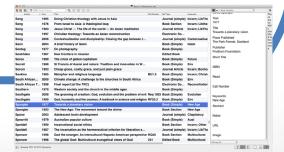


Search Engines

- Science Direct
- **AGRICOLA**
- **TOXNET**
- **ProQuest ESPM**
- **ProQuest Dissertation Abstracts**
- Web of Science/ **Current Contents**



In 2018: $\sim 88,565$ references manually skimmed for applicability



Collate data and remove duplicates

Screening

Eligibility

Included

Chemical verification and development of search terms

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to **ECOTOX**

Data extraction

Study quality evaluation

Skimming for Applicability: Title and Abstract



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

Sulfur Dust Ban: A Novel Technique for Ectoparasite Control in Poultry Systems. Murillo AC(1), Mullens BA(2),

Author information:
(1)Department of Entomology, University of california, Riversida, cA 22521
(1)Department of Entomology, university of california, Riversida, cA 22521
(2)Department of Entomology, Christopher (2)Department of Entomology, Ch

bradley. Millensburr. edu).

Arnial welfar-edriven legislation and concumer demand are changing how laying chickens are housed, thus creating challenges for ectoparastee control. Hers housed in suspended wire cages (battery cages) are usually treated with high-pressure pecticides. This application type is difficult in enriched-cage or enriched-cage or cage-free systems. In this study, we tested the efficacy of sulfur dust deployed in "dust bags for control against the northern fowl mite (Corrithorsous sylviarum), which causes host stress, decreased eagy production, cages or were clipped to the inside front of cages, we also tested be efficacy of the control against the northern fowl mite cages or were clipped to the inside front of cages, we also tested be eggently and the control in cages or were clipped to the inside front of cages, we also tested to only the control of the cages or were clipped to the inside front of cages, we also tested to only the control of the cages or were clipped to the inside front of cages, we also tested to only the control of the cages or were clipped to the inside front of cages, we also tested to only the cage of the ca

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DOI: 10.1093/jee/tow146



Send applicable reference list for acquisition

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Screening

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Study quality evaluation

Skimming for Applicability: Full text





The impact of the Cyanamid Canada Co. discharges to benthic invertebrates in the Welland River in Niagara Falls, Canada

MIKE DICKMAN and GRAZYNA RYGIEL

In 1986, the International Joint Commission (IJC) recommended that the Niagara River watershed In 1986, the International Joint Commission (IU.) recommendors must use resigns knew searches should be declared an Area of Concern (AGC). This ID: Creommendation was ruitfied by the 4 signatories of the Great Lakes Water Quality Agreement. In order to delits an AGC, the concessary to locate any areas of impairment within the waterhead and carry out remediation to the contraction of the

artiety of heavy metals into treatment systems which ultimately discharge to the Welland River, variety of heavy metals into treatment systems which ultimately discharge to the Welland River, the major Canadian tributary to the Niagara River. This portion of the Welland River near the factory was designated a Provincially significant (Class one) wetands by the Ontario Ministry of Natural Resources. In 1986, the mean discharge to a creek from Cyanamid Canada Co. was 27,342

g, sludge worms constituted 68% of all the organisms collected). The lowest chironomid is were observed at stations 1, 2, and 4, which were the only stations situated close to init's discharge pipes. The absence, of clams and mayfiles which burrow to greater depths han do chironomids and sludge worms, probably reflects the inability of the deeper dwel

unversity and the elevated interly flicital confirmations in the estimation seek continuous week continuous week continuous week continuous week and displayed the highest frequency of chironomid mentum deformities. Stations I and 2 were located near a pipe which was one of Cyanamid Canada Company's maj discharge point sources to the Welland River until a court order in 1980 otopoed the company fro discharging toxic material to the Welland River via that pipe. Elevated levels of cobalt (10 times) above background), molvbdenum (6 times above background), nickel (8 times above back come to acagounny, insolvancium to unites acove to acagounny, insche (o unites acove to acagounny, insolvancium) control contr Among the 1.275 chironomids taken from the seven Cyanamid Canada stations, the grea e pollution tolerant taxa. The low biotic diversity and the presence of co

0963-9292 © 1993 Chapman & Hall



Moves on to be curated into ECOTOX.

Sept 2018 – Sept 2019 ~1,089 References added to the public website





ECOTOX Applicability Criteria

Paper must meet these criteria

- Single chemical exposure
- Ecologically-relevant species
- Must be able to verify CAS registry numbers
- Must be able to verify taxonomic information for test species
- Exposure to live organism, viable tissue or cells
- Report concurrent exposure concentration, dose or application rate
- Report duration of exposure
- Must have a control treatment
- Primary source of the data
- Study must be a full article in English

The following studies are excluded

- Air pollution studies related to CO2 and ozone
- Studies on humans, monkeys, bacteria, viruses and yeast
- Review and summary articles
- Terrestrial studies with an inhalation route of exposure
- Non-English publications and abstracts

Review literature for applicability to ECOTOX







ECOTOX Applicability Criteria

All <u>Excluded</u> and <u>Non-Applicable</u> 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, CO2)
- 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

ECOTOX Data Extraction

Chemical verification and development of search terms

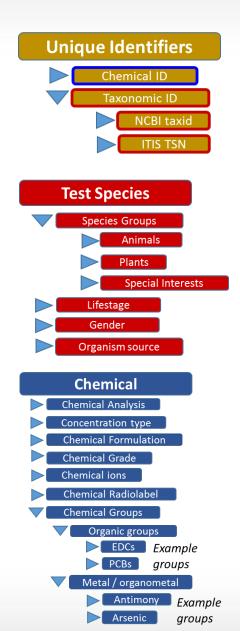
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Review literature for applicability to ECOTOX

Data extraction

Study quality evaluation





Identification

Screening

Eligibility

Study Quality Evaluation

Chemical verification and development of search terms

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Data extraction

Study quality evaluation

• Many fields in ECOTOX can inform study evaluation

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

Study Quality Evaluation

Chemical verification and development of search terms

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to ECOTOX

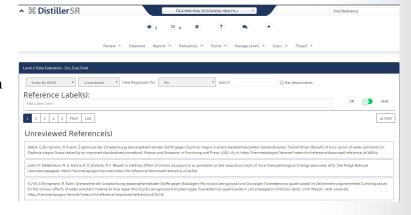
Data extraction

Study quality evaluation

- Identification of studies vetted for regulatory use
- Working towards a unified method for study quality evaluation
 - Pilot data quality evaluation with TSCA (environmental data for first 10 priority chemicals)

Criteria Domains:

- Test Substance
- Test Design
- o Exposure Characterization
- Test Organisms
- Outcome Assessment
- Confounding/ Variable Control
- Data Presentation and Analysis
- Initial discussions with Office of Water on Data Evaluation Reports (DERs)



DERs Include:

- Test Substance
- Exposure Pathway
- Protocols Followed
- Study Design and Methods
- Test Organism
- Study Parameters
- Test Conditions
- Acceptable Control
- Observations
- Statistical Verification

Application of ECOTOX:

PFAS toxicity data for ecological risk assessment and management

Per- and polyfluoroalkyl substances (PFAS)



There are no ecological receptor-based benchmarks or criteria.

Numerous PFAS

- Environmental occurrence
- In active commerce (602 in TSCA Inventory)
- Recently 'discovered' or synthesized
- Manufacturing process data
- ECOTOX comprehensive literature search and systematic review process for >300 chemicals (April 2018 August 2019)

RISK

Terms for Literature Search

List	# of Chemicals (August 2019)
PFAS list internal to ECOTOX	69
EPA Cross-Agency List – Chemistry Dashboard	199
EPA Set 1 List of 75 Test Samples – Chemistry Dashboard	74
Additional chemicals found in literature from 1st search	7
EPA Research List – Chemistry Dashboard	165
EPA Set 2 List of 75 Test Samples – Chemistry Dashboard	75

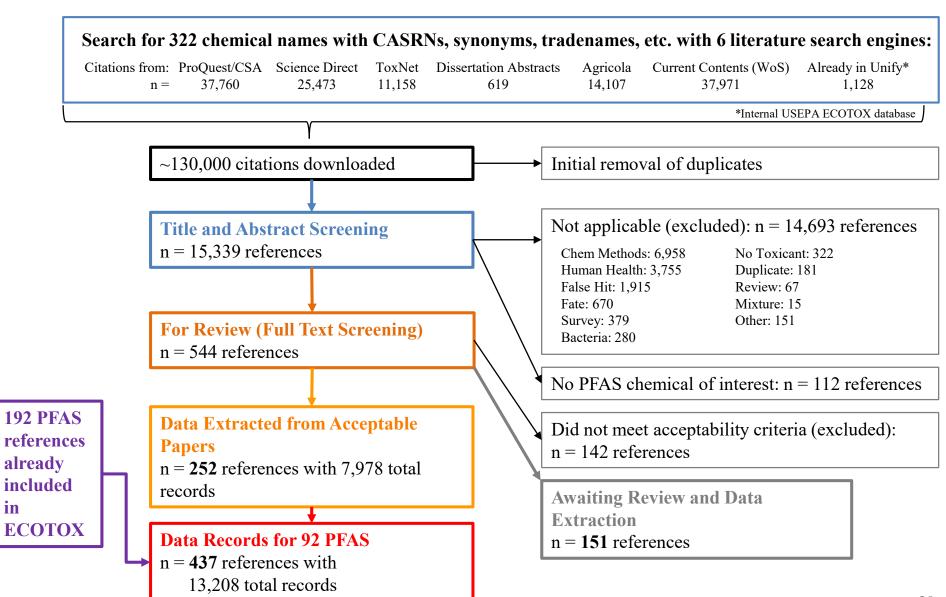
<u>April – Nov 2018</u>

- 254 chemical names with associated CASRNs (if applicable)
- General PFAS search terms (e.g., Dodecafluoro, Fluorotelomer, Nonafluoro, Pentafluoropropanoic, Perfluorobutanesulfon, Perfluoroheptanoate, Perfluorohexanoate, Perfluoropentyl)

July – August 2019

- 322 chemical names with associated CASRNs (if applicable)
- General PFAS search terms

Literature Search and Study Selection (2018-2019)



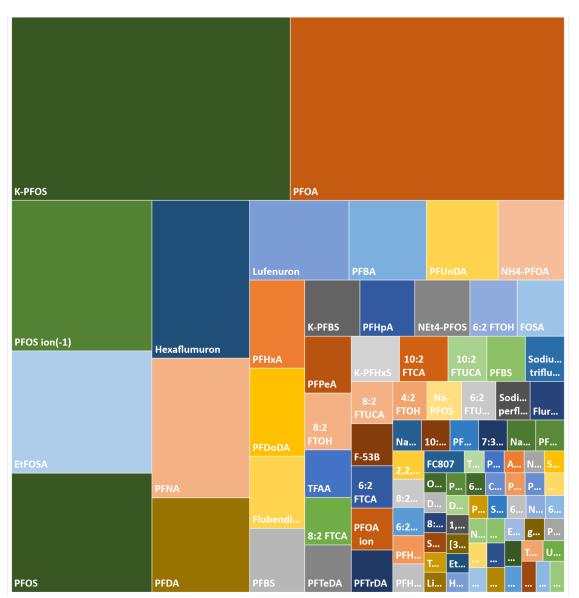
in

PFOS and **PFOA** with Most References

As of September 2019 update, curated data from 437 publications for:

- 96 fluorinated chemicals
- 264 species
- 889 effect measurements

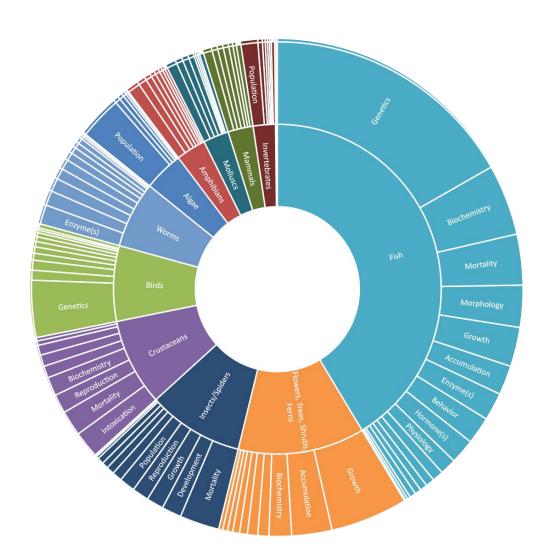
With a total of 13,208 records



Box size represents # references that include relevant and acceptable ecological toxicity data

Diversity in Types of Effects Measured

Distribution of data records in ECOTOX for PFAS, by species and general type of effect.



Search

Contact Us About the ECOTOX Knowledgebase

EPA welcomes your comments on this version of ECOTOX. We are specifically interested in feedback from users about the new functionality and usability. What, if any, issues did you experience? Please be as specific as possible in your comments

For technical questions about the scientific information and data interpretation, you may use the comment form below, or the contact information in the right-side bar, to contact the ECOTOX Support Staff

Please help us answer your request by including a correct e-mail address. If you are referring to a specific page within the ECOTOX web site, please include a URL or title for the page. Your Name First Last Your Organization (Optional) Select an option Name of Organization Your E-mail Address email@example.com

Get Updates via Email

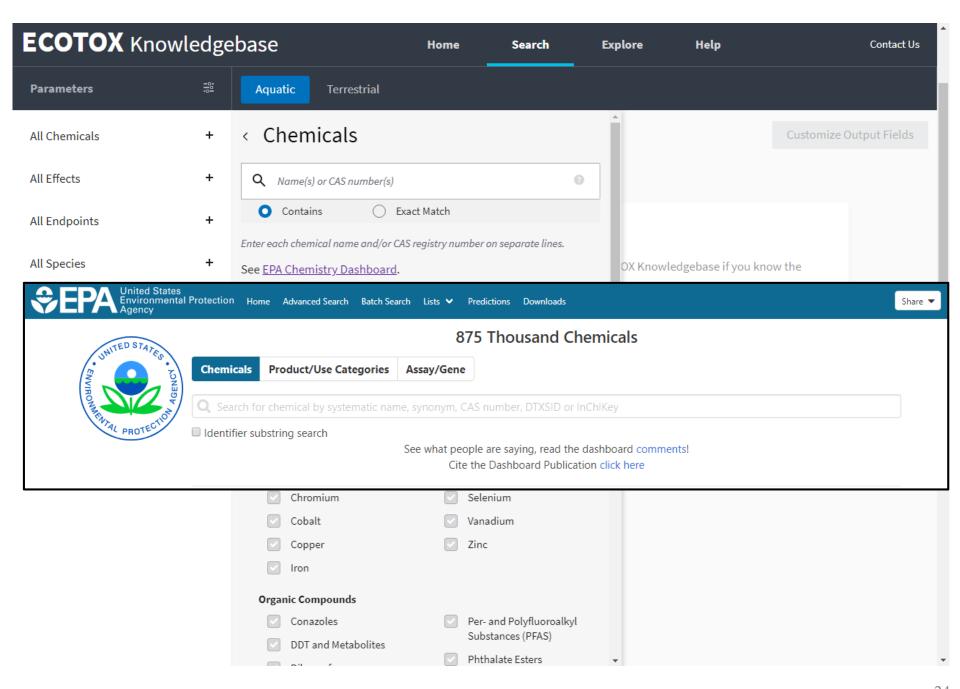
Telephone: 218-529-5225

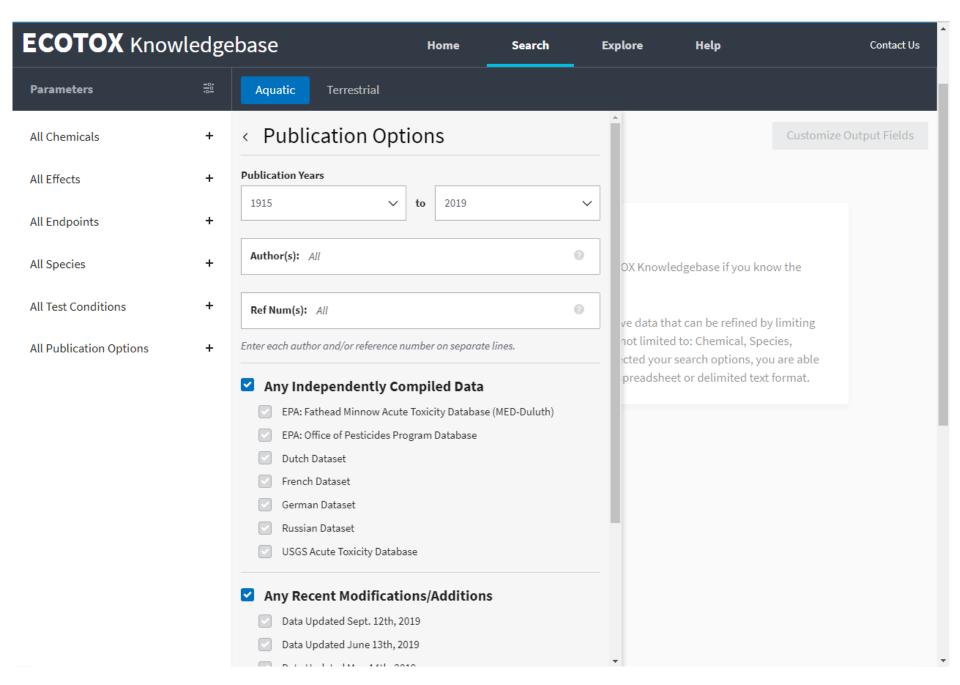
Fax: 218-529-5003

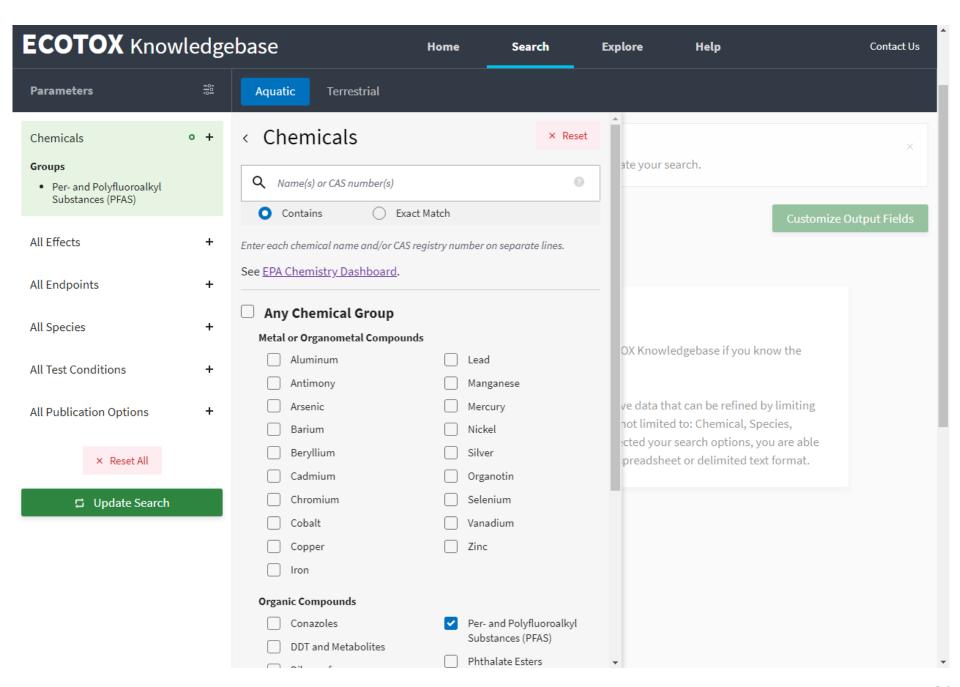
E-mail: ecotox.support@epa.gov

Mailing address:

ECOTOX Support Mid-Continent Ecology Division 6201 Congdon Boulevard Duluth, MN 55804









Custom Group

Create a custom chemical group by browsing available chemicals or entering a list of CAS numbers.

Create Custom Group...

Defined Groups

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



- 16 Organic Compounds
- 19 Metals or Organometal Comp...

35 Chemical Groups

Chemical groups are solely intended for the purposes of searching multiple chemicals efficiently and do not reflect the view(s) or the policy(cies) of the U.S. Environmental Protection Agency.

Some of the Chemical groups are currently being re-evaluated. They will be refreshed and restored in future ECOTOX updates.

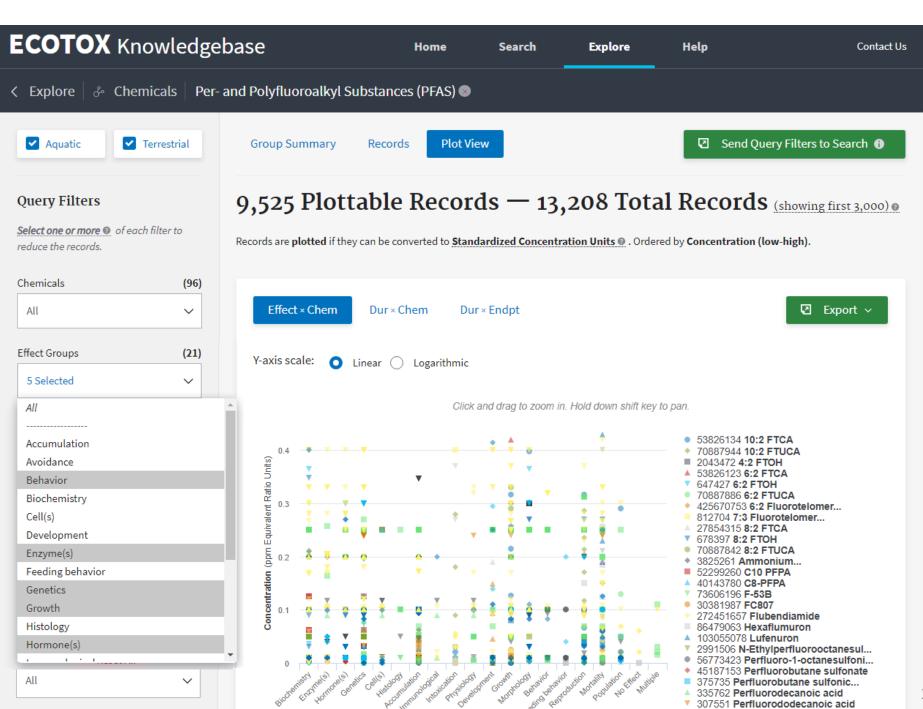
Select one or more groups then click "Explore Data" to continue.

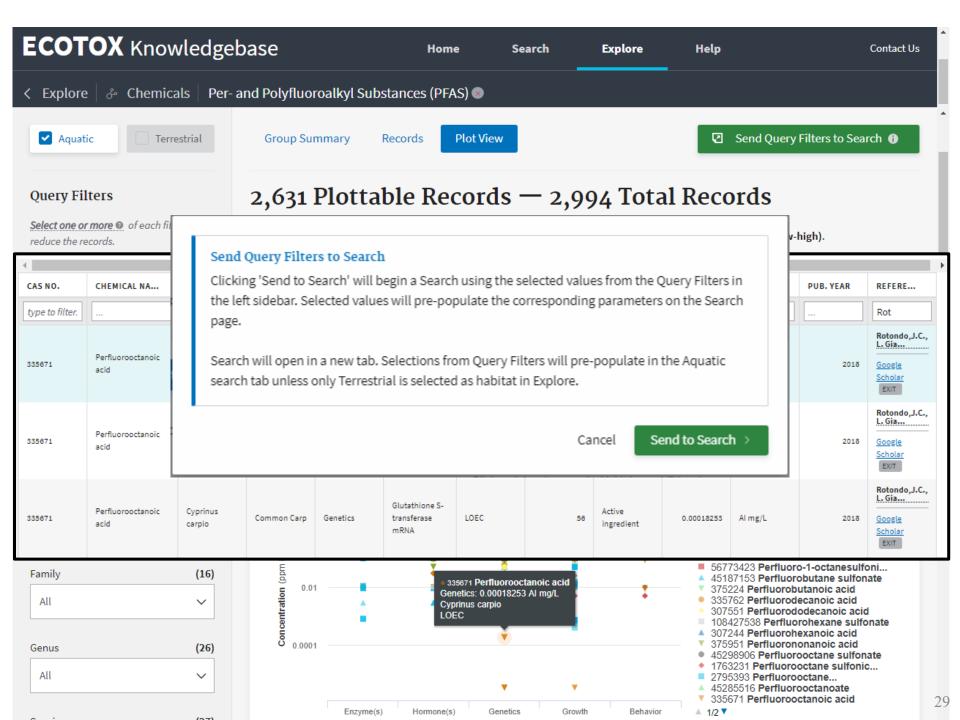
× Reset All

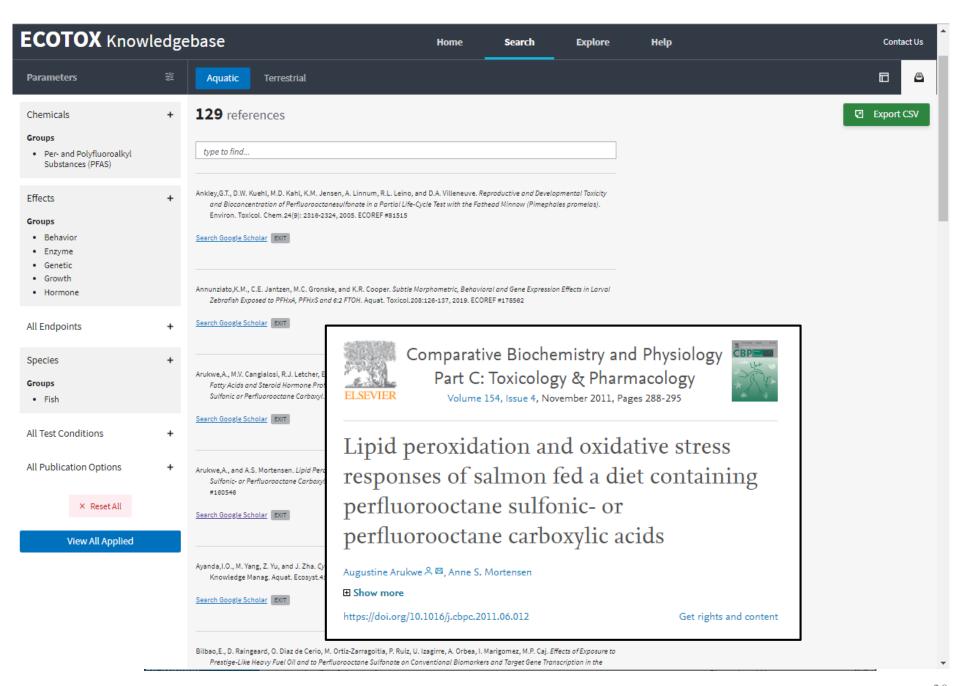
Export CSV

Explore Data

~	CHEMICAL GROUP	RECORDS ~	PUBLICATIO	YEAR MIN	YEAR MAX
	Copper	55792	4736	1915	2018
	Pharmaceutical Personal Care Products (PPCPs)	34751	2520	1938	2019
	Zinc	29407	3131	1915	2019
	Cadmium	24554	3200	1915	2018
~	Perfluorooctane Sulfonates and Acids (PFOS/PFOA)	13208	430	1953	2019
	Mercury	11246	1604	1927	2018
	Conazoles	10079	541	1977	2019
	Selenium	10039	659	1934	2015
	Neonicotinoids	9033	709	1980	2018
	Lead	8985	1400	1915	2017
	Major lons	8702	712	1927	2017
	Polyaromatic Hydrocarbons (PAHs)	8319	944	1917	2016







Quarterly Literature Searches for PFAS

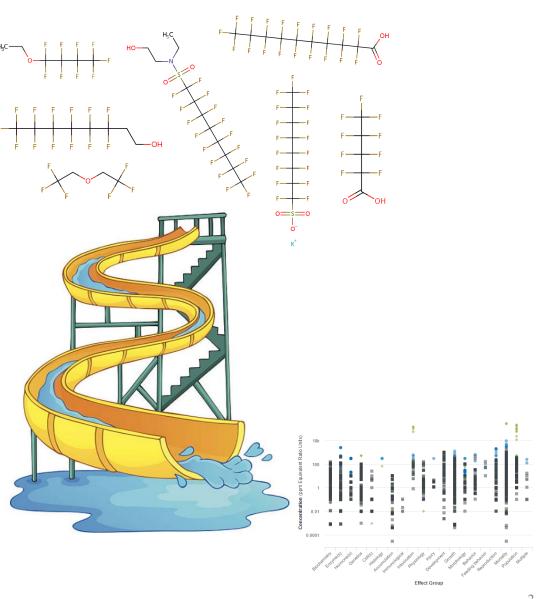
Updated list of >300 unique CASRNs and associated chemical names

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to ECOTOX

Extract data and code into ECOTOX Knowledgebase



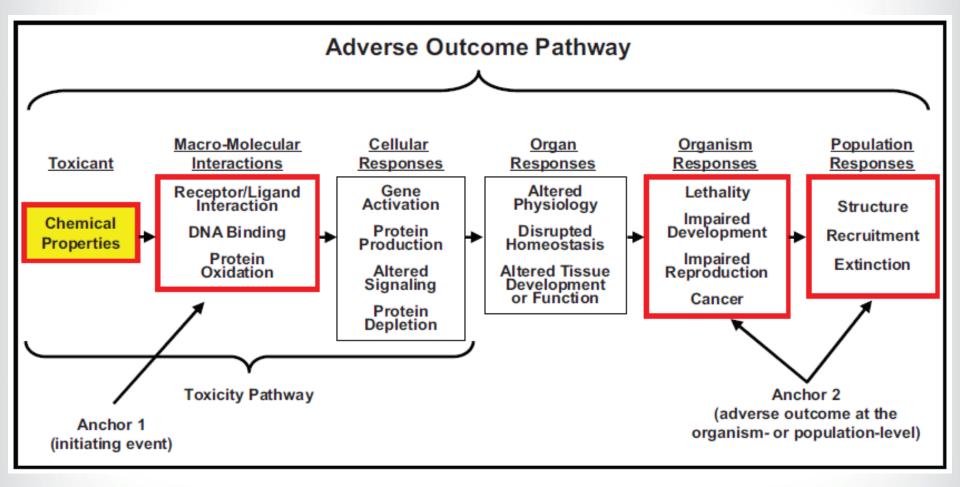
Application of ECOTOX:

Chemicals in Deconstruction Materials*

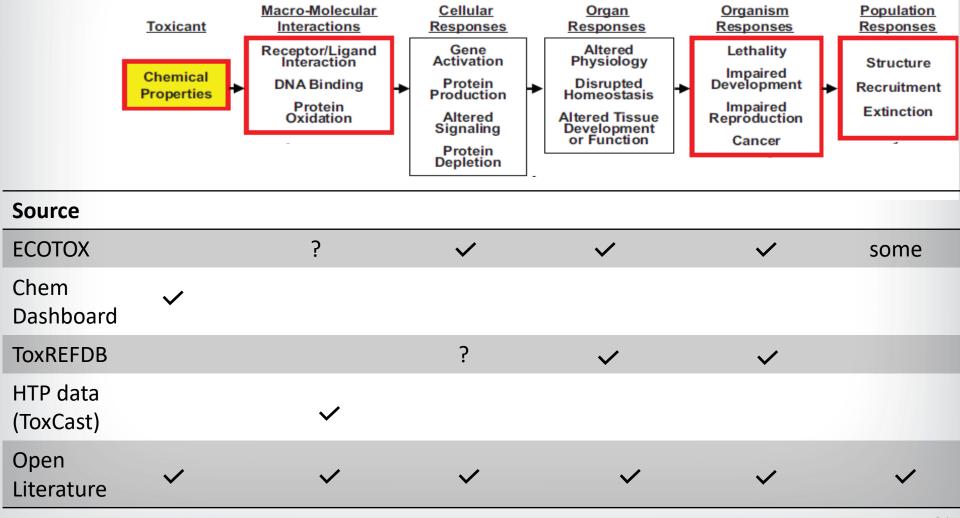
Chemical	Number of Articles
Arsenic	25
Chromium	24
Copper	24
Lead	20
Zinc	19
Nickel	17
Cadmium	17
Mercury	15
Sulfate	11
Selenium	10
Barium	10
Molybdenum	9
Calcium	9
Antimony	8
Chloride	8
Iron	8
Sodium	7
Aluminium	5
Magnesium	5
Potassium	5
Cobalt	4
Hydrogen sulfide	4
Manganese	3
Silicon	3
Sulfite	2
Phosphorus	2
Vanadium	2
Carbon	2
Sulfur	2
Boron	2
Ammonia	2
Cyanide	2
Thioarsenic	2
Carbon dioxide	1
Dimethoxy chloroamphetamine	1
Lithium	1
Strontium	1
Hydrogen	1
Nitrogen	1
Ethanol	1
Polychlorinated dibenzo-p-dioxins	1
Dibenzofurans	1
Biphenyls	1
Chlorobenzenes	1
Chlorophenols	1
Polycyclic aromatic hydrocarbons	1
Uranium	
Chlorine	1
Fluorine	1
Titanium	1
T ttanium	1

Chemical	Number of	ECOTOX Knowledgebase			
Chemicai	Articles	# CASRNs	# of Refs	# of Records	
Arsenic	25	24	524	5,025	
Chromium	24	17	998	7,956	
Copper	24	20	4,736	55,792	
Lead	20	13	1,400	8,985	
Zinc	19	30	3,131	29,407	
Nickel	17	23	598	4,290	
Cadmium	17	13	3,200	24,554	
Mercury	15	59	1,604	11,246	
Sulfate	11				
Selenium	10	35	659	10,039	
Barium	10	11	91	409	
Polycyclic					
aromatic	1	27	944	8,319	
hydrocarbons					

Application of ECOTOX (and other tools/databases): Chemicals in Deconstruction Materials*



<u>Application of ECOTOX (and other tools/databases)</u>: Chemicals in Deconstruction Materials*

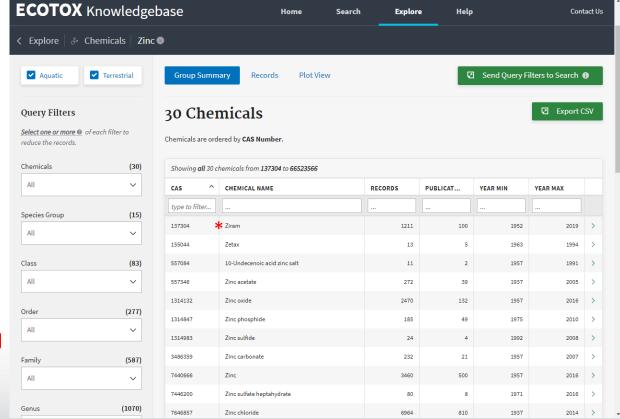


Application of ECOTOX:

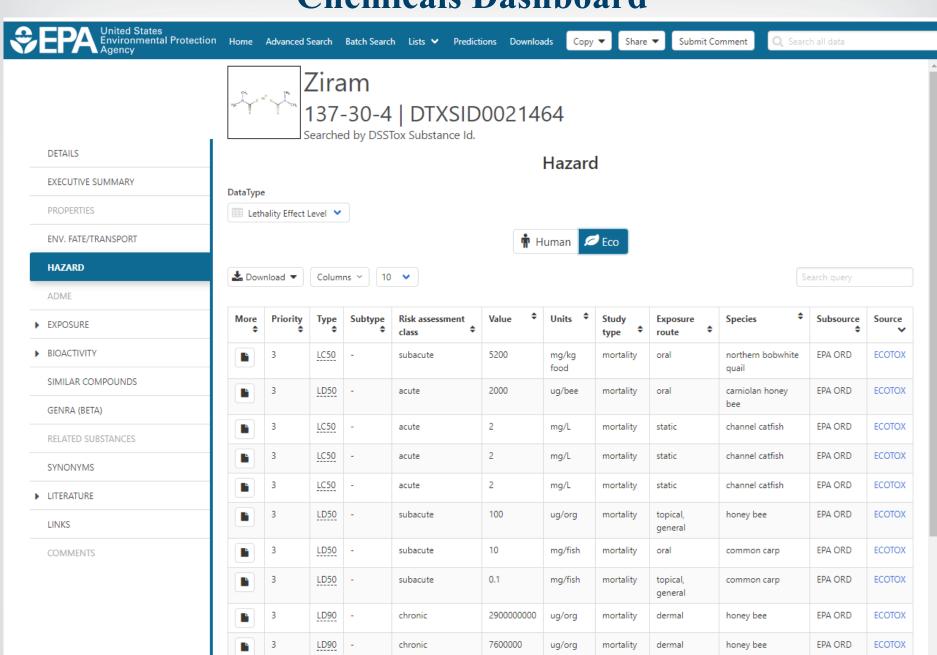
Chemicals in Deconstruction Materials*

П	Chemical	Number of Articles
I	Arsenic	25
IJ	Chromium	24
IJ	Copper	24
I	Lead	20
I	Zinc	19
Ш	Nickel	17
I	Cadmium	17
I	Mercury	15
I	Sulfate	11
I	Selenium	10
Ц	Barium	10
٦	Molybdenum	9
ı	Calcium	9
ı	Antimony	8
j	Chloride	8
ı	Iron	8
j	Sodium	7
ı	Aluminium	5
j	Magnesium	5
j	Potassium	5
j	Cobalt	4
j	Hydrogen sulfide	4
j	Manganese	3
j	Silicon	3
j	Sulfite	2
j	Phosphorus	2
j	Vanadium	2
j	Carbon	2
ı	Sulfur	2
ı	Boron	2
İ	Ammonia	2
İ	Cyanide	2
j	Thioarsenic	2
j	Carbon dioxide	1
j	Dimethoxy chloroamphetamine	1
j	Lithium	1
j	Strontium	1
ı	Hydrogen	1
ı	Nitrogen	1
ı	Ethanol	1
ł	Polychlorinated dibenzo-p-dioxins	1
1	Dibenzofurans	1
ł	Biphenyls	1
1	Chlorobenzenes	1
1	Chlorophenols	1
d	Polycyclic aromatic hydrocarbons	1
Ц	Uranium	·
1	Chlorine	1
1	Fluorine	1
	Titanium	1
41	1 Italiiuiii	1

C1 1	Number of	ECOTOX Knowledgebase			
Chemical	Articles	# CASRNs	# of Refs	# of Records	
Arsenic	25	24	524	5,025	
Chromium	24	17	998	7,956	
Copper	24	20	4,736	55,792	
Lead	20	13	1,400	8,985	
* Zinc	19	30	3,131	29,407	



Chemicals Dashboard



Chemicals Dashboard



DETAILS

PROPERTIES

HAZARD

ADME

▶ EXPOSURE

▶ BIOACTIVITY

GENRA (BETA)

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

EXECUTIVE SUMMARY

ENV. FATE/TRANSPORT

SIMILAR COMPOUNDS

RELATED SUBSTANCES

Advanced Search Batch Search Lists ♥ Predictions Downloads

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Searched by DSSTox Substance Id.

General

- EPA Substance Registry
- Household Products Database
- PubChem
- Chemspider
- @ CPCat
- DrugBank
- W Wikipedia
- Q MSDS Lookup
- Chemble
- Q Chemical Vendors
- ToxPlanet
- ACS Reagent Chemicals
- ChemHat: Hazards and Alternatives Toolbox
- Wolfram Alpha
- ECHA Infocard
- ChemAgora
- ChEBI
- NIST Chemistry Webbook
- Wikidata
- **WEBWISER**
- PubChem Safety Sheet
- MIOSH Chemical Safety Cards
- ECHA Brief Profile
- Consumer Product

Toxicology

- ACToR
- OH, DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Toy
- HSDR.
- ⊕ ToxCast Dashboard 2
- LactMed
- ☑ ATSDR Toxic Substances Portal
- ACTOR PDF Report
- Toxics Release Inventory
- CREST
- National Air Toxics Assessment
- Superfund Chemical Data
- В ЕСОТОХ
- NIOSH IDLH Values
- International Toxicity Estimates for Risk

Publications

- Toxline
- G Google Books
- Google Scholar
- G Google Patents
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- NIOSH Skin Notation Profiles
- MIOSH Pocket Guide
- RSC Publications
- BioCaddie DataMed
- 2 Springer Materials
- Federal Register
- Regulations.gov
- Bielefeld Academic Search
- CORE Literature Search

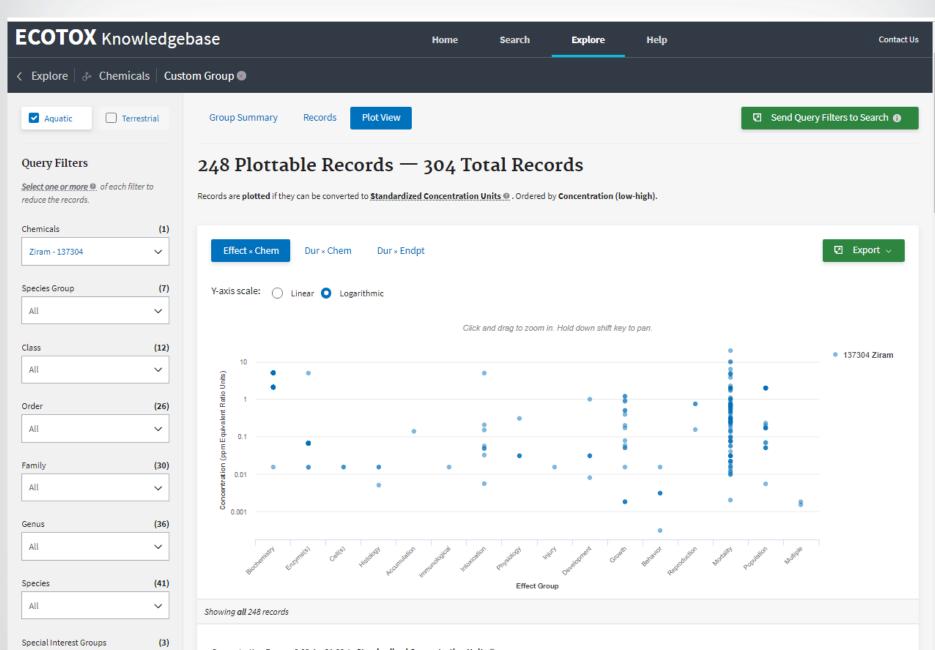
Analytical

- RSC Analytical Abstracts
- △ Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum
- MassBank
- A NEMI: National Environmental Methods Index
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values

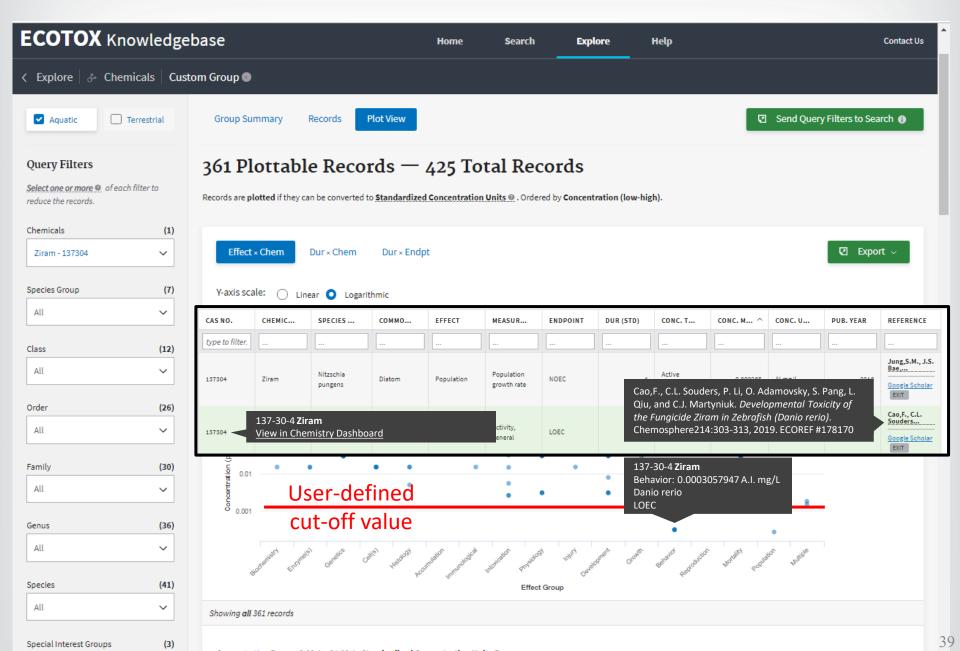
Prediction

- 2D NMR HSOC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- **€** LSERD

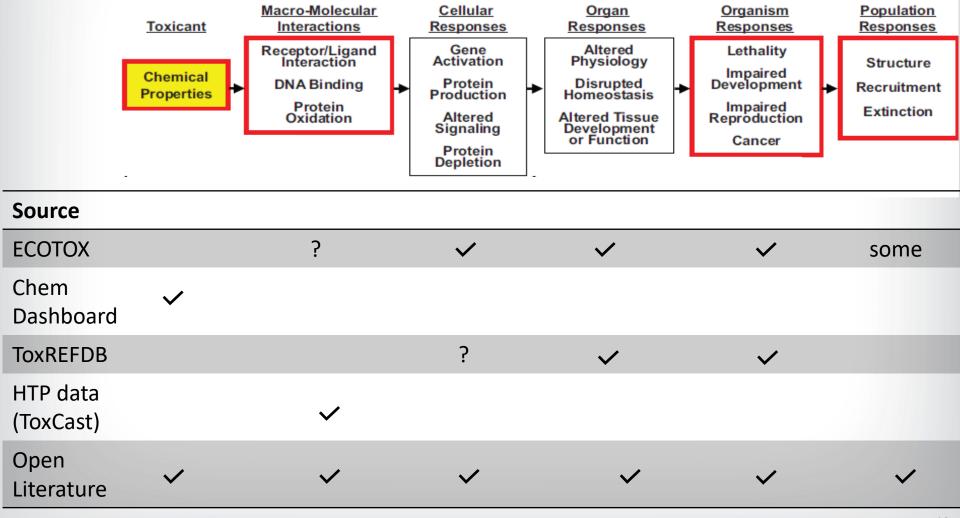
ECOTOX



ECOTOX



<u>Application of ECOTOX (and other tools/databases)</u>: Chemicals in Deconstruction Materials*



Thank you!

Questions?

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http://cfpub.epa.gov/ecotox

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