

# ECOTOXicology Knowledgebase

*Jennifer Olker, PhD*

*Postdoctoral researcher, Great Lakes Toxicology and Ecology Division*

*US EPA ORD Center for Computational Toxicology and Exposure*

Project Team:

*Colleen Elonen, ECOTOX coordinator*

*Jennifer Olker*

*Dale Hoff*

*Carlie LaLone*

*GDIT contract staff*

*SEE staff*



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

- From comprehensive search and review of open and grey literature
  - Data extracted from acceptable studies, with up to 250 fields
  - Updated quarterly
- 30+ year history: originated in the early 1980s, maintained by EPA ORD
- Major updates 2018-2019
  - Recent and upcoming new functionality and interoperability

The screenshot shows the ECOTOX Knowledgebase website. At the top is a navigation bar with links: Home, Search, Explore, Help, and Contact Us. Below the navigation bar, there's a section titled "Recent chemicals with full searches and coding completed" which lists chemicals like Acetochlor, Dichlorobenzenes, trans-1,2-Dichloroethylene, 1,2-Dichloropropane, Dicyclohexyl phthalate, Forchlorfenuron, Glyphosate, HCHB, Metaldehyde, Phthalic anhydride, Picloram, Propazine, Prothioconazole, Simazine, Topramezone, and Uranium. To the right of this list, there's a table showing the total number of chemicals (11,756) and species (12,906) in the database, and the number of references (49,153) and results (952,634). Below this, a green banner welcomes users to ECOTOX version 5 and provides a link for feedback. The main content area is divided into three columns: "About ECOTOX" (describing the database and providing a "Learn More" link), "Getting Started" (providing links to search, explore, and user guides), and "Other Links" (providing links to limitations, frequent questions, other tools/databases, and recent additions). A "Download" section offers a button to download the entire database as an ASCII file. At the bottom, a blue banner highlights "New Additions!".

**ECOTOX Knowledgebase**

Home Search Explore Help Contact Us

Data last updated  
**Sept 12, 2019**  
See update totals

Recent chemicals with full searches and coding completed

Acetochlor	Glyphosate	Prothioconazole
Dichlorobenzenes	HCHB	Simazine
trans-1,2-Dichloroethylene	Metaldehyde	Topramezone
1,2-Dichloropropane	Phthalic anhydride	Uranium
Dicyclohexyl phthalate	Picloram	
Forchlorfenuron	Propazine	

Total in database

<b>11,756</b> Chemicals	<b>12,906</b> Species
<b>49,153</b> References	<b>952,634</b> Results

**WELCOME TO ECOTOX VERSION 5!**  
Please click here to provide feedback so that we can continue to improve your experience.

**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](#)

**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, 141 K)
- [ECOTOX User Guide](#) (84 pp, 1120 K)
- [ECOTOX Code Appendix \(PDF\)](#) (765 pp, 6447 K, [About PDF](#))

**Other Links**

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

[Get Updates via Email](#)

**Download**

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

[Download ASCII Data](#)

**New Additions!**

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

# ECOTOX Pipeline: Systematic Review/Data Curation

Identification

Chemical verification  
and development of  
search terms

Conduct literature  
searches

Screening

Identify and acquire  
potentially applicable  
studies

Eligibility

Review literature for  
applicability to  
ECOTOX

Included

Extract data and code  
into ECOTOX  
Knowledgebase

## 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/ CSA	Science Direct	ToxNet	Dissertation Abstracts	Agricola	Current Contents (WoS)	Already in Unify*
n =	5,631	11,178	317	234	4,861	15,347	333

\*Internal USEPA ECOTOX database

~37,000 citations downloaded

Initial removal of duplicates

**Title and Abstract Screening**  
n = 8,653 references

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	

**For Review (Full Text Screening)**  
n = 388 references

No PFAS in reference: n = 85 references

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

Awaiting Review and Data Extraction  
n = 1 references

**Data Extracted from Acceptable  
Papers**  
n = 245 references with  
7,496 total records

## ECOTOX Knowledgebase

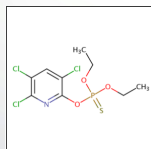
*Chemical  
environmental  
toxicity data for  
aquatic life,  
terrestrial plants  
and wildlife*



**Interoperability with databases/tools**

DTXSID/CASRN

Chemicals  
Dashboard



Species ID; Protein ID

SeqAPASS



Integrated ontology

Adverse  
Outcome  
Pathway  
Wiki

Reference ID

HERO  
(Health &  
Environmental  
Research  
Online)

### 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

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

### Mailing address:

ECOTOX Support

Mid-Continent Ecology Division

6201 Congdon Boulevard

Duluth, MN 55804

Parameters



Aquatic

Terrestrial

All Chemicals



< Chemicals

All Effects



All Endpoints



☒ Contains ☐ Exact Match

All Species



Enter each chemical name and/or CAS registry number on separate lines.

See [EPA Chemistry Dashboard](#).

Customize Output Fields

OX Knowledgebase if you know the



United States  
Environmental Protection  
Agency

[Home](#)

[Advanced Search](#)

[Batch Search](#)

[Lists](#)

[Predictions](#)

[Downloads](#)

Share

## 875 Thousand Chemicals



Chemicals

Product/Use Categories

Assay/Gene

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)

Cite the Dashboard Publication [click here](#)

☒ Chromium

☒ Cobalt

☒ Copper

☒ Iron

### Organic Compounds

☒ Conazoles

☒ DDT and Metabolites

☒ Selenium

☒ Vanadium

☒ Zinc

☒ Per- and Polyfluoroalkyl  
Substances (PFAS)

☒ Phthalate Esters

## Parameters


[Aquatic](#)
[Terrestrial](#)
[All Chemicals](#)

[All Effects](#)

[All Endpoints](#)

[All Species](#)

[All Test Conditions](#)

[All Publication Options](#)


## < Publication Options

### Publication Years



to


 Author(s): *All*

 Ref Num(s): *All*


*Enter each author and/or reference number on separate lines.*

### ☒ Any Independently Compiled Data

- ☒ EPA: Fathead Minnow Acute Toxicity Database (MED-Duluth)
- ☒ EPA: Office of Pesticides Program Database
- ☒ Dutch Dataset
- ☒ French Dataset
- ☒ German Dataset
- ☒ Russian Dataset
- ☒ USGS Acute Toxicity Database

### ☒ Any Recent Modifications/Additions

- ☒ Data Updated Sept. 12th, 2019
- ☒ Data Updated June 13th, 2019

[Customize Output Fields](#)

ECOTOX Knowledgebase if you know the

ve data that can be refined by limiting  
not limited to: Chemical, Species,  
ected your search options, you are able  
preadsheet or delimited text format.

Parameters



Aquatic

Terrestrial

Chemicals



Groups

- Per- and Polyfluoroalkyl Substances (PFAS)

All Effects



All Endpoints



All Species



All Test Conditions



All Publication Options



Reset All

Update Search

Chemicals

Reset

Name(s) or CAS number(s)



Contains



Exact Match

Enter each chemical name and/or CAS registry number on separate lines.

See [EPA Chemistry Dashboard](#).

Any Chemical Group

Metal or Organometal Compounds

- |                                    |                                    |
|------------------------------------|------------------------------------|
| <input type="checkbox"/> Aluminum  | <input type="checkbox"/> Lead      |
| <input type="checkbox"/> Antimony  | <input type="checkbox"/> Manganese |
| <input type="checkbox"/> Arsenic   | <input type="checkbox"/> Mercury   |
| <input type="checkbox"/> Barium    | <input type="checkbox"/> Nickel    |
| <input type="checkbox"/> Beryllium | <input type="checkbox"/> Silver    |
| <input type="checkbox"/> Cadmium   | <input type="checkbox"/> Organotin |
| <input type="checkbox"/> Chromium  | <input type="checkbox"/> Selenium  |
| <input type="checkbox"/> Cobalt    | <input type="checkbox"/> Vanadium  |
| <input type="checkbox"/> Copper    | <input type="checkbox"/> Zinc      |
| <input type="checkbox"/> Iron      |                                    |

Organic Compounds

- |  |  |
|--|--|
| <input type="checkbox"/> Conazoles           | <input checked="" type="checkbox"/> Per- and Polyfluoroalkyl Substances (PFAS) |
| <input type="checkbox"/> DDT and Metabolites |  |
| <input type="checkbox"/> Phthalate Esters    |  |

Create your search.

Customize Output Fields

ECOTOX Knowledgebase if you know the

You can also view data that can be refined by limiting your search to specific chemical groups, not limited to: Chemical, Species, Test Conditions. After selecting your search options, you are able to export your results to a spreadsheet or delimited text format.



## 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
<input type="checkbox"/>	Copper	55792	4736	1915	2018
<input type="checkbox"/>	Pharmaceutical Personal Care Products (PPCPs)	34751	2520	1938	2019
<input type="checkbox"/>	Zinc	29407	3131	1915	2019
<input type="checkbox"/>	Cadmium	24554	3200	1915	2018
<input checked="" type="checkbox"/>	Perfluorooctane Sulfonates and Acids (PFOS/PFOA)	13208	430	1953	2019
<input type="checkbox"/>	Mercury	11246	1604	1927	2018
<input type="checkbox"/>	Conazoles	10079	541	1977	2019
<input type="checkbox"/>	Selenium	10039	659	1934	2015
<input type="checkbox"/>	Neonicotinoids	9033	709	1980	2018
<input type="checkbox"/>	Lead	8985	1400	1915	2017
<input type="checkbox"/>	Major Ions	8702	712	1927	2017
<input type="checkbox"/>	Polycyclic Aromatic Hydrocarbons (PAHs)	8319	944	1917	2016

[← Explore](#) | [🔗 Chemicals](#) | [Per- and Polyfluoroalkyl Substances \(PFAS\)](#) ✕☒ 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 (96)

All

Effect Groups (21)

5 Selected

All

Accumulation

Avoidance

Behavior

Biochemistry

Cell(s)

Development

Enzyme(s)

Feeding behavior

Genetics

Growth

Histology

Hormone(s)

All

## 9,525 Plottable Records — 13,208 Total Records (showing first 3,000) ⓘ

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

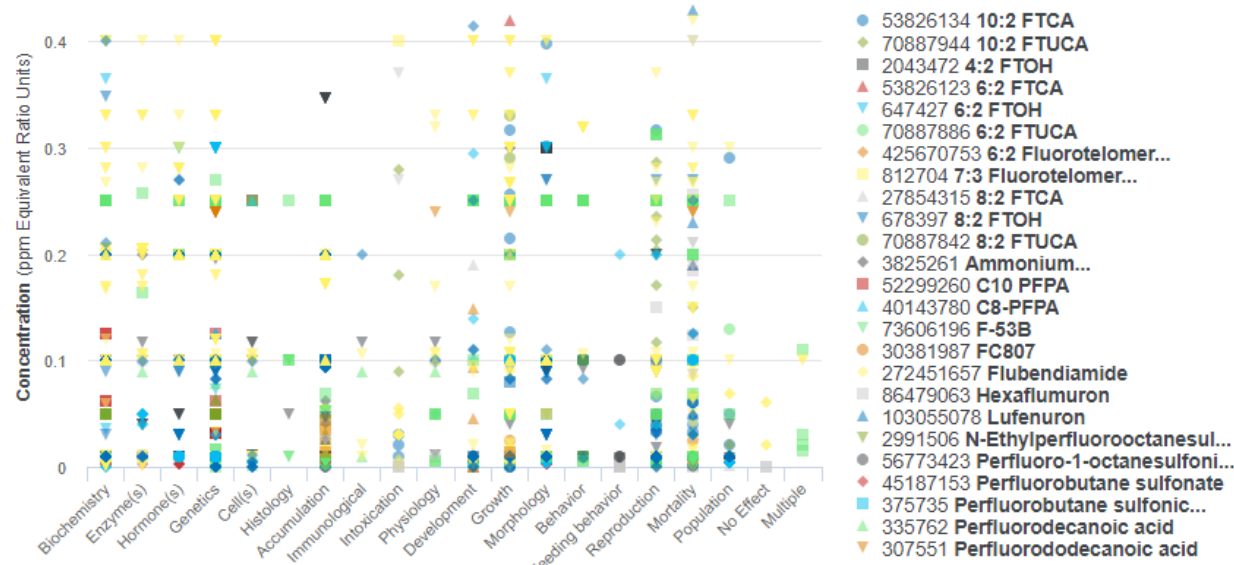
Effect × Chem

Dur × Chem

Dur × Endpt

[Export](#) ▾Y-axis scale: ☒ Linear ☐ Logarithmic

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



☒ 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.

## 2,631 Plottable Records — 2,994 Total Records

### Send Query Filters to Search

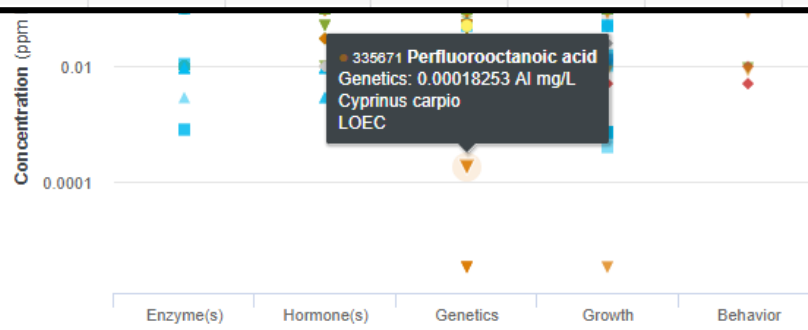
Clicking 'Send to Search' will begin a Search using the selected values from the Query Filters in the left sidebar. Selected values will pre-populate the corresponding parameters on the Search page.

Search will open in a new tab. Selections from Query Filters will pre-populate in the Aquatic search tab unless only Terrestrial is selected as habitat in Explore.

[Cancel](#)
[Send to Search](#)

CAS NO.	CHEMICAL NA...
type to filter.	...
335671	Perfluorooctanoic acid
335671	Perfluorooctanoic acid

Family	(16)
All	▼
Genus	(26)
All	▼



- 56773423 Perfluoro-1-octanesulfoni...
- 45187153 Perfluorobutane sulfonate
- 375224 Perfluorobutanoic acid
- 335762 Perfluorodecanoic acid
- 307551 Perfluorododecanoic acid
- 108427538 Perfluorohexane sulfonate
- 307244 Perfluorohexanoic acid
- 375951 Perfluorononanoic acid
- 45298906 Perfluorooctane sulfonate
- 1763231 Perfluorooctane sulfonic...
- 2795393 Perfluorooctane...
- 45285516 Perfluorooctanoate
- 335671 Perfluorooctanoic acid

Parameters

Aquatic

Terrestrial



Chemicals

+

Groups

- Per- and Polyfluoroalkyl Substances (PFAS)

Effects

+

Groups

- Behavior
- Enzyme
- Genetic
- Growth
- Hormone

All Endpoints

+

Species

+

Groups

- Fish

All Test Conditions

+

All Publication Options

+

× Reset All

View All Applied

129 references

Export CSV

type to find...

Ankley, G.T., D.W. Kuehl, M.D. Kahl, K.M. Jensen, A. Linnam, R.L. Leino, and D.A. Villeneuve. *Reproductive and Developmental Toxicity and Bioconcentration of Perfluorooctanesulfonate in a Partial Life-Cycle Test with the Fathead Minnow (Pimephales promelas)*. Environ. Toxicol. Chem. 24(9): 2318-2324, 2005. ECODEF #81515

[Search Google Scholar](#)

EXIT

Annunziato, K.M., C.E. Jantzen, M.C. Grunske, and K.R. Cooper. *Subtle Morphometric, Behavioral and Gene Expression Effects in Larval Zebrafish Exposed to PFHxA, PFHxS and 6:2 FTOH*. Aquat. Toxicol. 208:128-137, 2019. ECODEF #178562

[Search Google Scholar](#)

EXIT

Arukwe, A., M.V. Cangialosi, R.J. Letcher, B. Fatty Acids and Steroid Hormone Profiles in Sulfonic- or Perfluorooctane Carboxylates

[Search Google Scholar](#)

EXIT

Arukwe, A., and A.S. Mortensen. *Lipid Peroxidation and Oxidative Stress Responses of Salmon Fed a Diet Containing Sulfonic- or Perfluorooctane Carboxylates*. #180548

[Search Google Scholar](#)

EXIT

Ayanda, I.O., M. Yang, Z. Yu, and J. Zha. *Cyotoxicity and Apoptosis Induced by PFOS in Zebrafish (Danio rerio) Embryos*. Knowledge Manag. Aquat. Ecosyst. 4: 1-10, 2019. ECODEF #180548

[Search Google Scholar](#)

EXIT

Bilbao, E., D. Raingeard, O. Diaz de Cerio, M. Ortiz-Zarragoitia, P. Ruiz, U. Izaguirre, A. Orbea, I. Marigomez, M.P. Caj. *Effects of Exposure to Prestige-Like Heavy Fuel Oil and to Perfluorooctane Sulfonate on Conventional Biomarkers and Target Gene Transcription in the*



## Comparative Biochemistry and Physiology Part C: Toxicology & Pharmacology

Volume 154, Issue 4, November 2011, Pages 288-295



# Lipid peroxidation and oxidative stress responses of salmon fed a diet containing perfluorooctane sulfonic- or perfluorooctane carboxylic acids

Augustine Arukwe Anne S. Mortensen

Show more

<https://doi.org/10.1016/j.cbpc.2011.06.012>

Get rights and content

## ECOTOX comprehensive literature search and systematic review process for >300 chemicals (April 2018 – August 2019)

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

### April – Nov 2018

- 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)

Search for 322 chemical names with CASRNs, synonyms, tradenames, etc. with 6 literature search engines:

Citations from:	ProQuest/CSA	Science Direct	ToxNet	Dissertation Abstracts	Agricola	Current Contents (WoS)	Already in Unify*
n =	37,760	25,473	11,158	619	14,107	37,971	1,128

\*Internal USEPA ECOTOX database

~130,000 citations downloaded

Initial removal of duplicates

**Title and Abstract Screening**

n = 15,339 references

Not applicable (excluded): n = 14,693 references

Chem Methods: 6,958  
Human Health: 3,755  
False Hit: 1,915  
Fate: 670  
Survey: 379  
Bacteria: 280

No Toxicant: 322  
Duplicate: 181  
Review: 67  
Mixture: 15  
Other: 151

**For Review (Full Text Screening)**

n = 544 references

No PFAS chemical of interest: n = 112 references

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

**Data Extracted from Acceptable Papers**

n = 252 references with 7,978 total records

**Awaiting Review and Data Extraction**

n = 151 references

**Data Records for 92 PFAS**

n = 437 references with  
13,208 total records

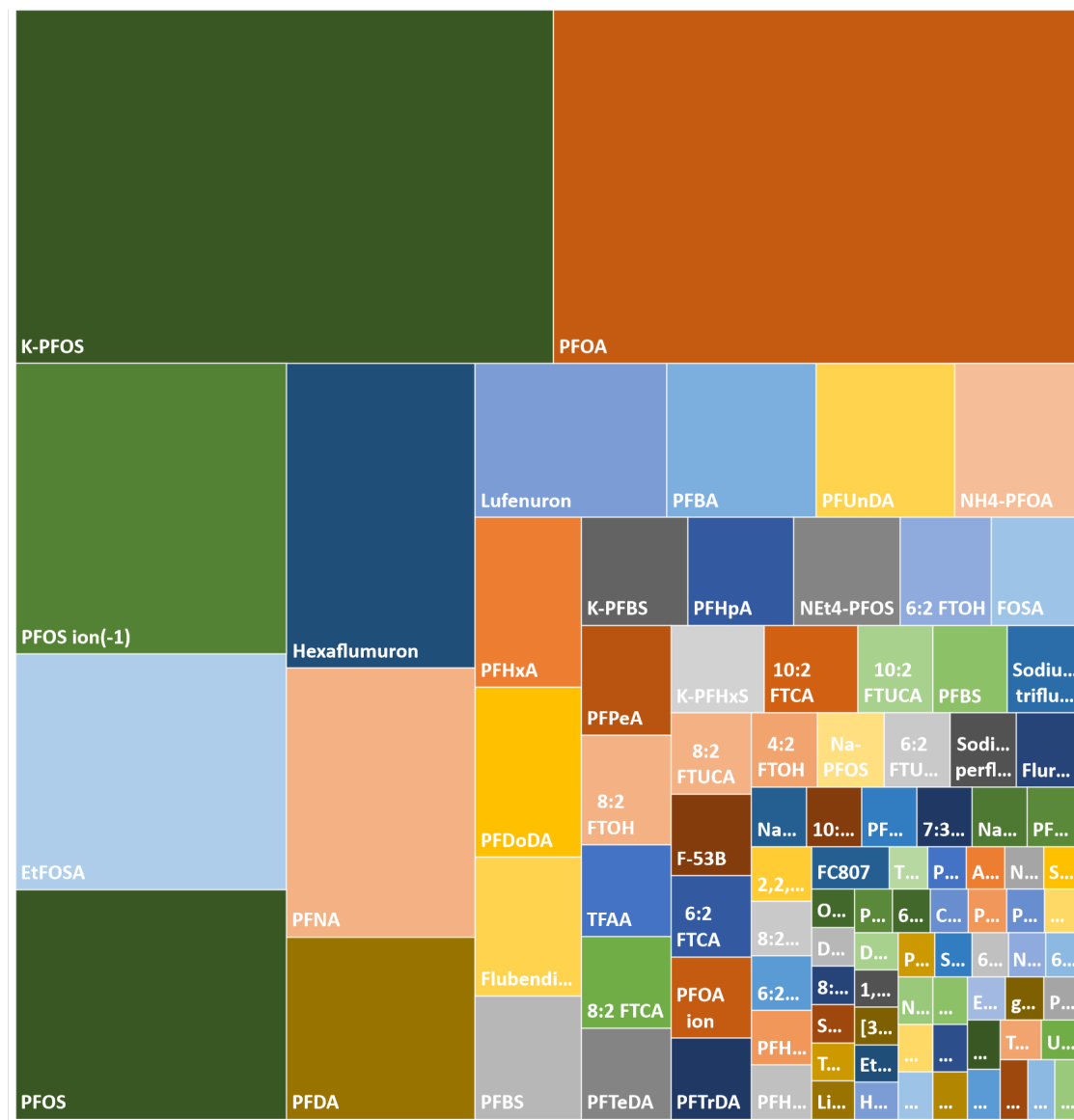
192 PFAS  
references  
already  
included  
in  
ECOTOX

# 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.





# Quarterly Literature Searches for PFAS

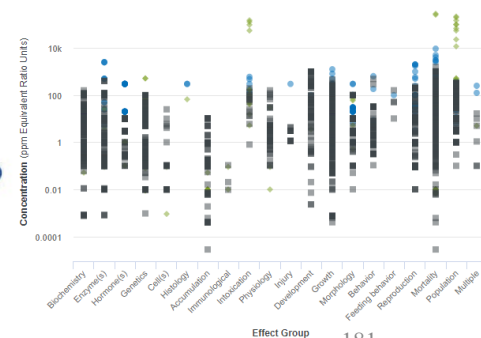
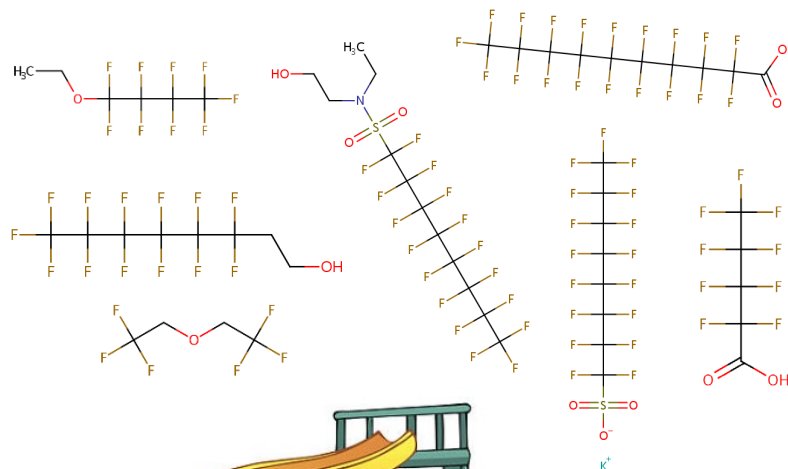
Updated list of >300 unique CASRNs and associated chemical names

Conduct literature searches

Identify and acquire potentially applicable studies

Review literature for applicability to ECOTOX

Extract data and code into ECOTOX Knowledgebase



**Thank you!**

**Questions?**

**Colleen Elonen, Jennifer Olker & Dale Hoff**

US EPA Office of Research and Development  
Center for Computational Toxicology and Exposure  
Great Lakes Toxicology and Ecology Division  
Duluth, MN  
218-529-5000

<http://cfpub.epa.gov/ecotox>

ECOTOX Support: 218-529-5225

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