

Update on Identification and Curation of Ecological Toxicity Data for PFAS with the ECOTOXicology Knowledgebase Protocols

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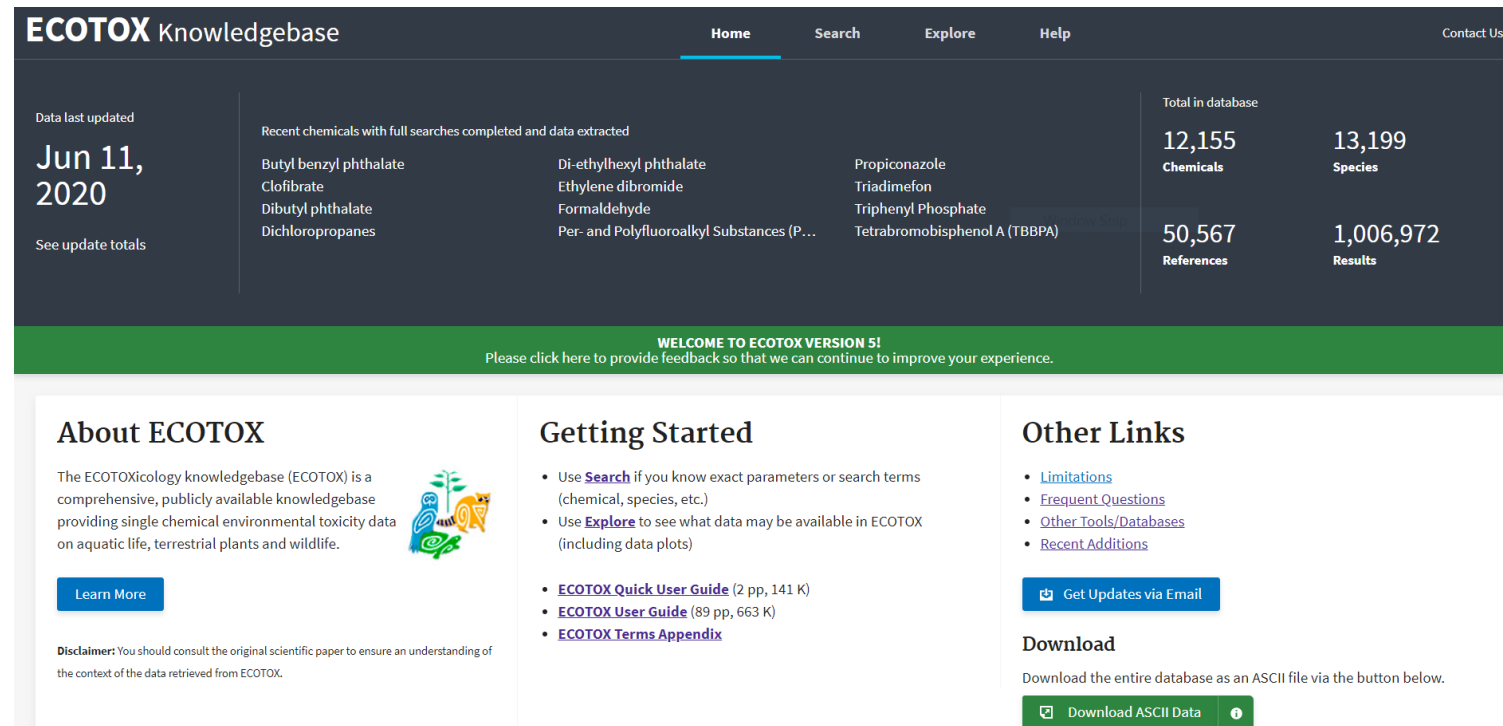
www.epa.gov/ecotox

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
- Recently updated
 - Interactive queries by chemical, species, effect or endpoint
 - Data added quarterly
- 30+ year history
 - Originated in the early 1980s, maintained by EPA ORD
- Current user statistics
 - 8,000 distinct hosts search the Knowledgebase each month

www.epa.gov/ecotox

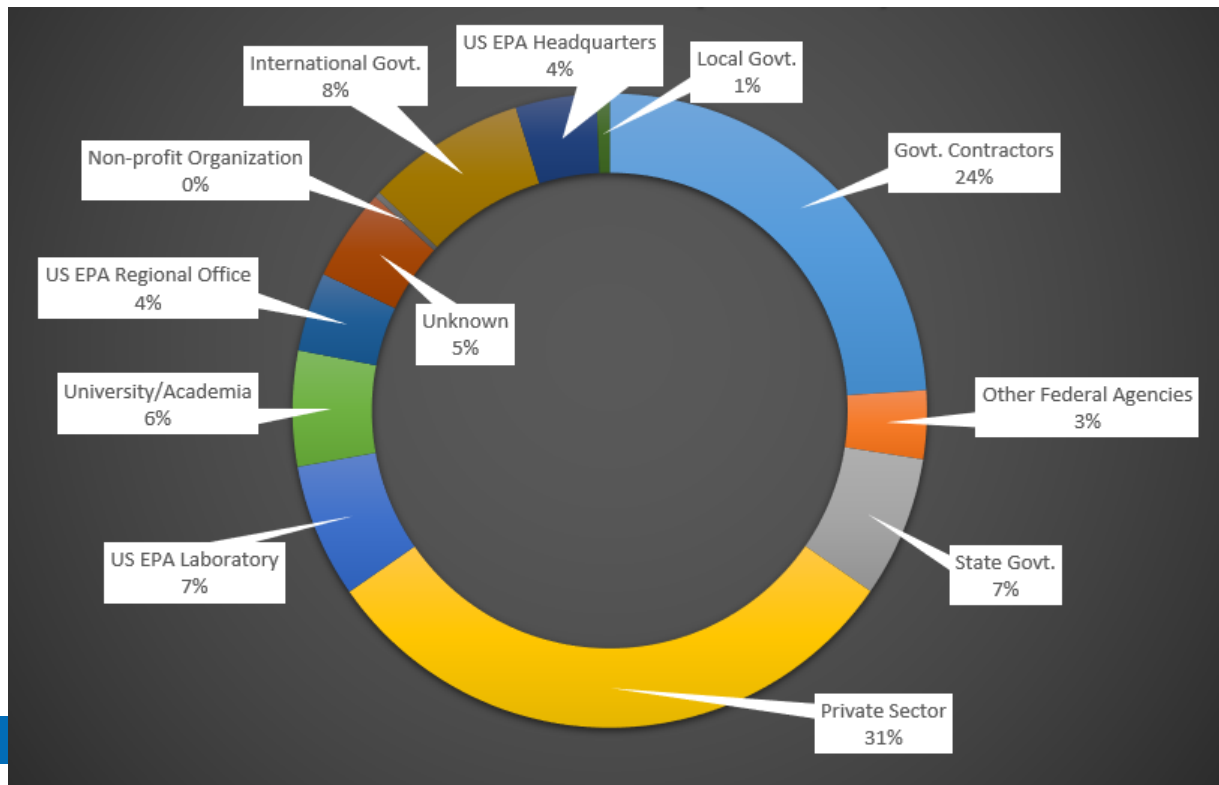


The screenshot shows the ECOTOX Knowledgebase homepage. At the top, there's a navigation bar with links for Home, Search, Explore, Help, and Contact Us. Below this, a dark blue header section displays key statistics: 'Data last updated Jun 11, 2020', 'Recent chemicals with full searches completed and data extracted' (listing Butyl benzyl phthalate, Clofibrate, Dibutyl phthalate, Dichloropropanes, Di-ethylhexyl phthalate, Ethylene dibromide, Formaldehyde, Per- and Polyfluoroalkyl Substances (P...), Propiconazole, Triadimefon, Triphenyl Phosphate, and Tetrabromobisphenol A (TBBPA)), and 'Total in database' (12,155 Chemicals, 13,199 Species, 50,567 References, 1,006,972 Results). A green banner below the header reads 'WELCOME TO ECOTOX VERSION 5!' and 'Please click here to provide feedback so that we can continue to improve your experience.' The main content area is divided into three columns: 'About ECOTOX' (describing the database and providing a 'Learn More' button), 'Getting Started' (listing links for Search, Explore, ECOTOX Quick User Guide, ECOTOX User Guide, and ECOTOX Terms Appendix), and 'Other Links' (listing Limitations, Frequent Questions, Other Tools/Databases, and Recent Additions). A 'Download' section at the bottom right offers a button to 'Download ASCII Data'.

Applications and Users of ECOTOX

ECOTOX Knowledgebase

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



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

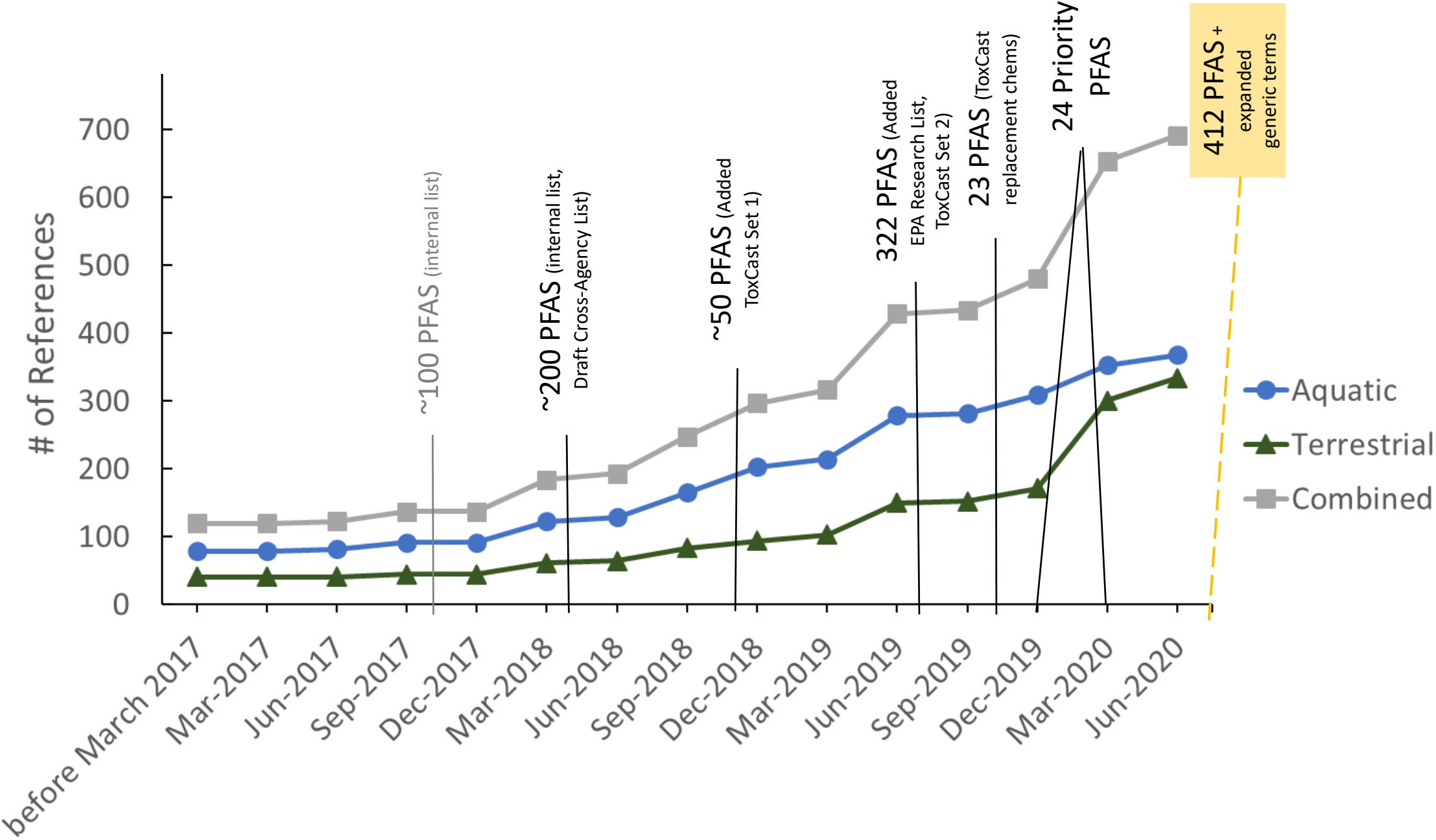
Species Sensitivity Distributions (e.g., US EPA's WebICE, NOAA's CAFÉ)
PNECs and threshold values (e.g., EcoTTC)
QSAR (e.g., ECOSAR, TEST, OECD QSAR Toolbox)
BCF modeling and validation
Adverse Outcome Pathway (AOP) development

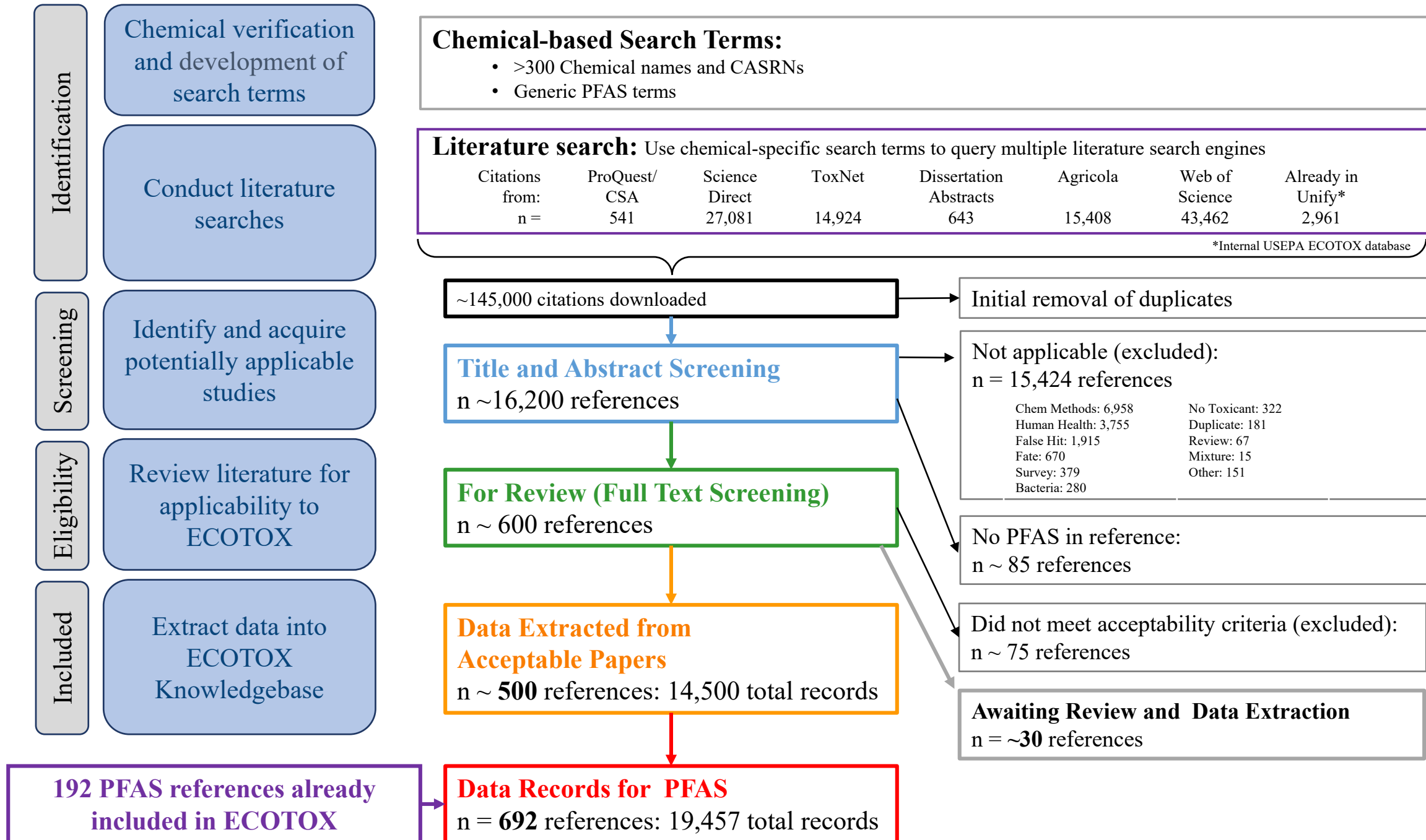
Per- and polyfluoroalkyl substances (PFAS) toxicity data for ecological risk assessment and management

- Providing data to researchers, EPA ERA Forum, DoD Tri-Services ERA Work Group, and others
- ECOTOX comprehensive literature search and systematic review process completed for **>300 PFAS** (April 2018 - present)
- Ecological toxicity data from **692 references**:
 - **130 PFAS**
 - **459 Biological species**
 - Diversity in effects



PFAS references in ECOTOX Knowledgebase





Challenges with PFAS references

Environmental Pollution 256 (2020) 113550

Chemicals Product/Use Categories Assay/Gene

Q Potassium perfluorohexane-1-sulfonate

No results found

High
perf

Subham D

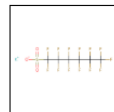
^a Department of E
^b Environmental T
^c Department of C

ARTICLE

Article history:
Received 14 Sep
Received in revised
27 October 2019
Accepted 30 Oct
Available online 3

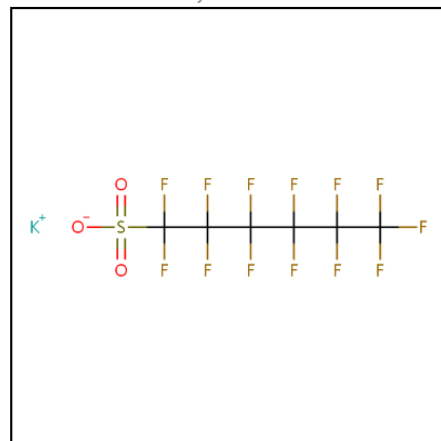
Keywords:
PFAS
Perfluorooctanesu
Embryonic develo
Zebrafish
Hepatotoxicity

DETAILS
EXECUTIVE SUMMARY
PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ADME
EXPOSURE
BIOACTIVITY
SIMILAR COMPOUNDS
GENRA (BETA)
RELATED SUBSTANCES



Potassium perfluorohexanesu
3871-99-6 | DTXSID3037709

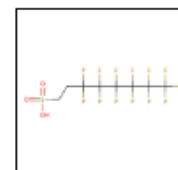
Searched by DSSTox Substance Id.



resulted in a decrease in liver area and increase in yolk sac neutral lipids show that early exposure to PFOSA adversely impacts embryogenesis, as lipid transport and liver development.

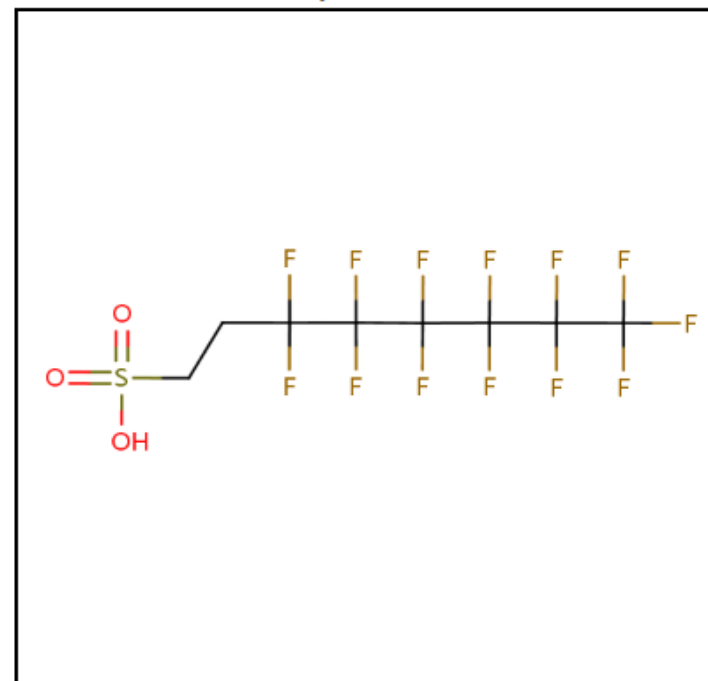
© 2019 |

Home Advanced Search Batch Search Lists Predictions Downloads



6:2 Fluorotelomer sulfonic acid
27619-97-2 | DTXSID6067331

Searched by DSSTox Substance Id.



Quality Control Notes

No Quality Control notes.

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

1H,1H,2H,2H-Perfluorooctanesulfonic acid ---
in paper; had incorrect CAS number
associated with it in Supplemental table;
called another name in Dashboard

Per- and polyfluoroalkyl substances (PFAS) toxicity data for ecological risk assessment and management



ECOTOX Knowledgebase

[Home](#)[Search](#)[Explore](#)[Help](#)[Contact Us](#)

Data last updated


**Jun 11,
2020**

[See update totals](#)

Recent chemicals with full searches completed and data extracted

Butyl benzyl phthalate
Clofibrate
Dibutyl phthalate
Dichloropropanes

Di-ethylhexyl phthalate
Ethylene dibromide
Formaldehyde

 [Per- and Polyfluoroalkyl Substances \(P...](#)

Propiconazole
Triadimefon
Triphenyl Phosphate
Tetrabromobisphenol A (TBBPA)

[Click to Explore Per- and Polyfluoroalkyl Substances \(PFAS\)](#)

Total in database

12,155
Chemicals

13,199
Species

50,567
References

1,006,972
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](#)


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

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](#) (89 pp, 663 K)
- [ECOTOX Terms Appendix](#)


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](#)



☒ Aquatic☒ Terrestrial

Query Filters

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

Chemicals (130)

All



Species Group (14)

All



Class (38)

All



Order (112)

All



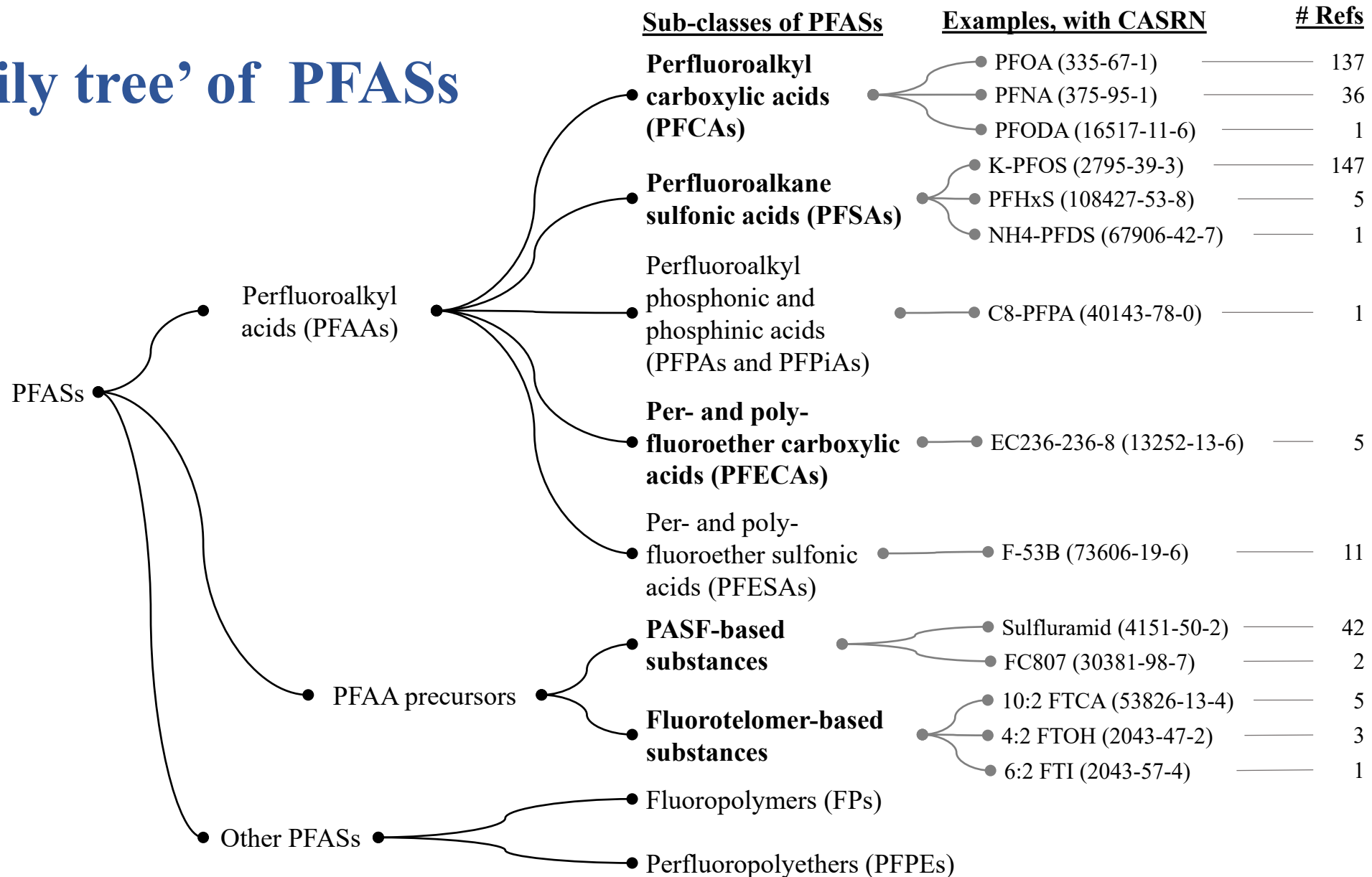
Family (207)

All



CAS NO.	CHEMICAL NAME	SPECIES NAME	COMMO...	EFFECT	MEASUR...	ENDPOINT	DUR (STD)	CONC. T...	CONC. M... ^	CONC. U...	PUB. YEAR	REFERE...
<i>type to filter.</i>
53826134	10:2 FTCA	Elodea canadensis	Waterweed	Growth	Weight	EC10	42	Formulation	1.6E-013	Al mg/L	2008	McGregor,E.B. Microc... Google Scholar EXIT
86479063	Hexaflumuron	Culex quinquefasciatus	Southern House Mosquito	Development	Emergence	ET50	7.13	Formulation	5.04E-010	Al mg/L	1993	Vasuki,V. Sublethal ... Google Scholar EXIT
86479063	Hexaflumuron	Culex quinquefasciatus	Southern House Mosquito	Development	Emergence	ET50	8.38	Formulation	5.04E-010	Al mg/L	1993	Vasuki,V. Sublethal ... Google Scholar EXIT
86479063	Hexaflumuron	Anopheles stephensi	Mosquito	Development	Emergence	ET50	7	Formulation	1.85E-009	Al mg/L	1993	Vasuki,V. Sublethal ... Google Scholar EXIT
86479063	Hexaflumuron	Anopheles stephensi	Mosquito	Development	Emergence	ET50	8	Formulation	1.85E-009	Al mg/L	1993	Vasuki,V. Sublethal ... Google Scholar EXIT
86479063	Hexaflumuron	Culex quinquefasciatus	Southern House Mosquito	Development	Emergence	ET50	5.75	Formulation	2.28E-009	Al mg/L	1993	Vasuki,V. Sublethal ... Google

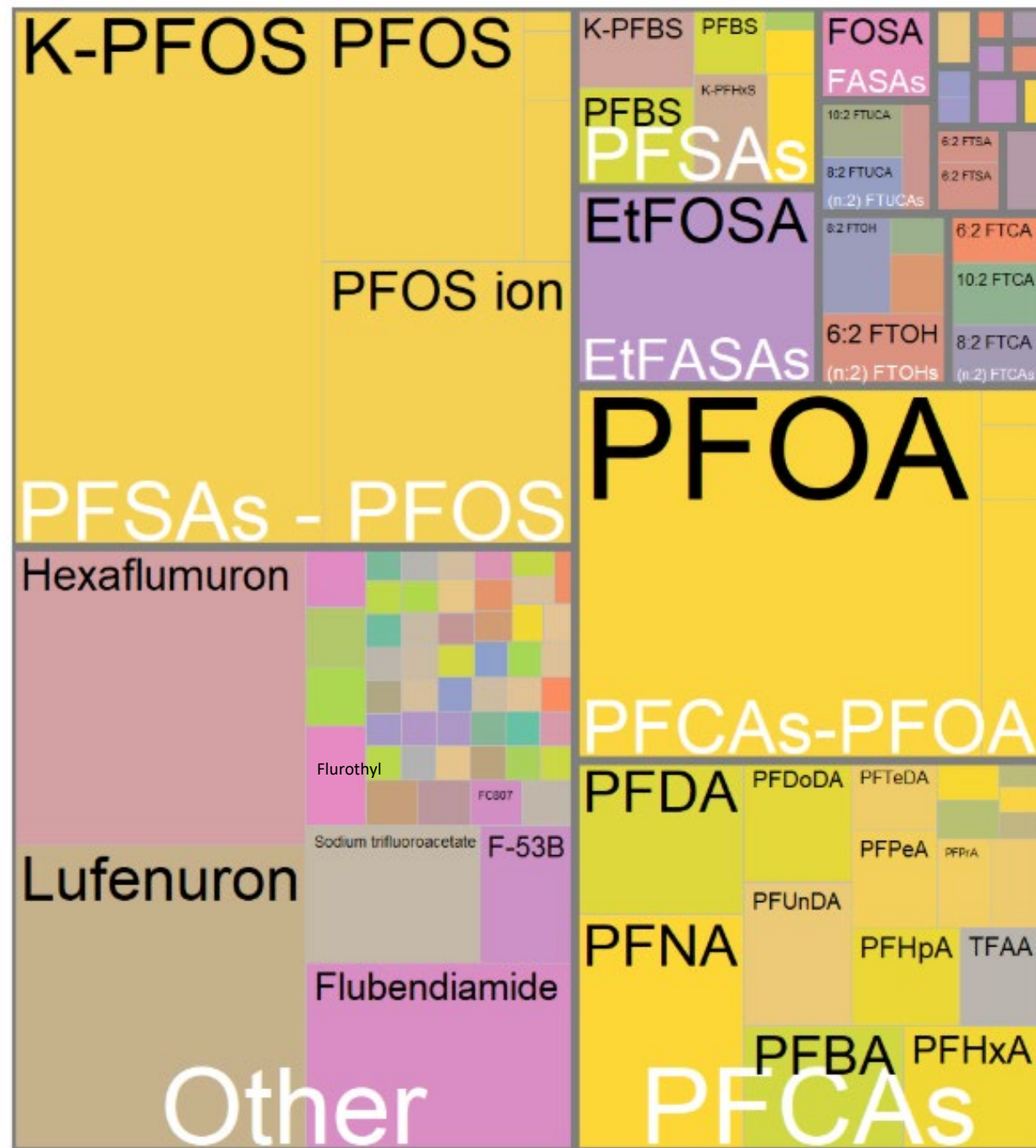
'Family tree' of PFASs



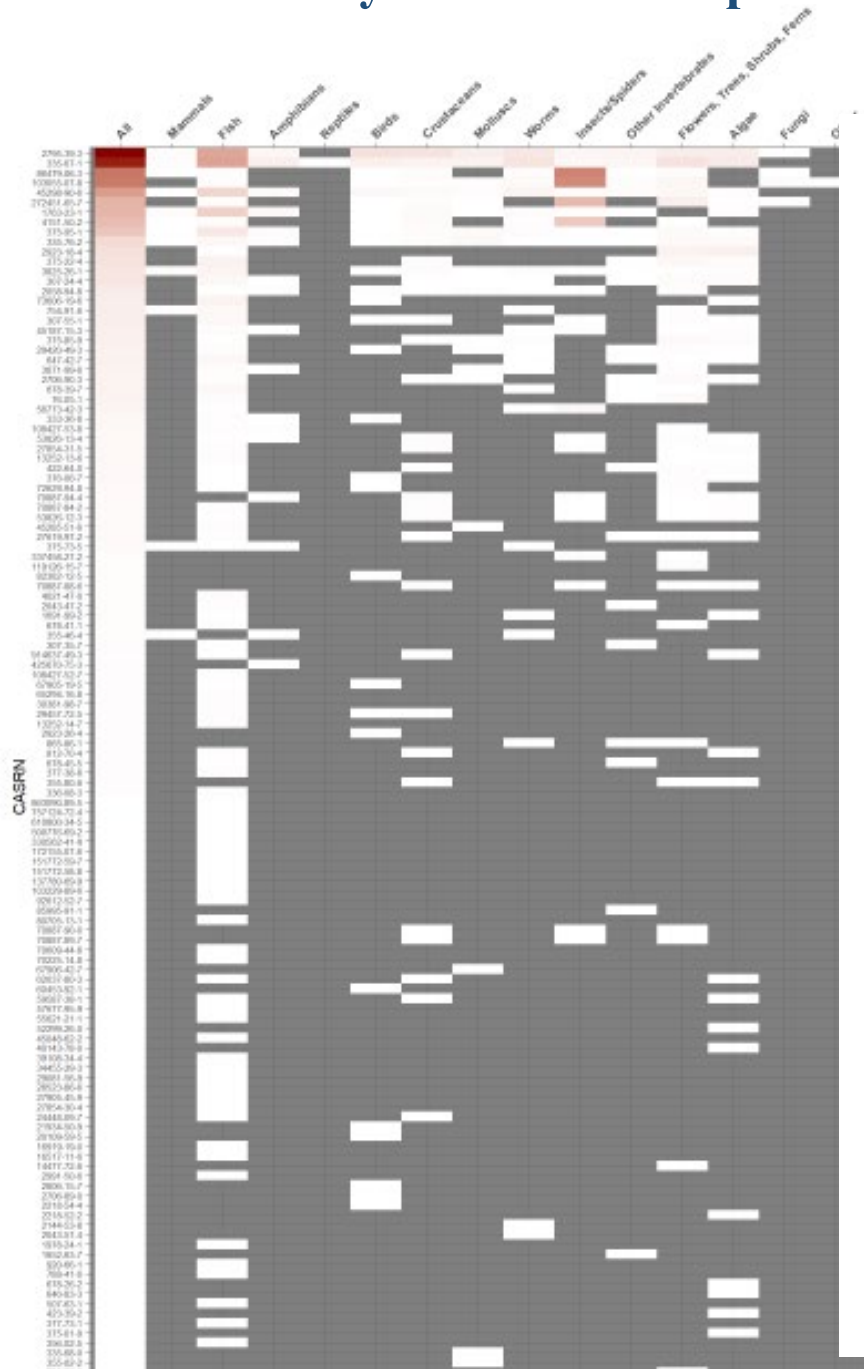
692 Publications

130 PFAS with Ecological Toxicity Data

- Box size represents # of references for each chemical



References by CASRN and Species Group

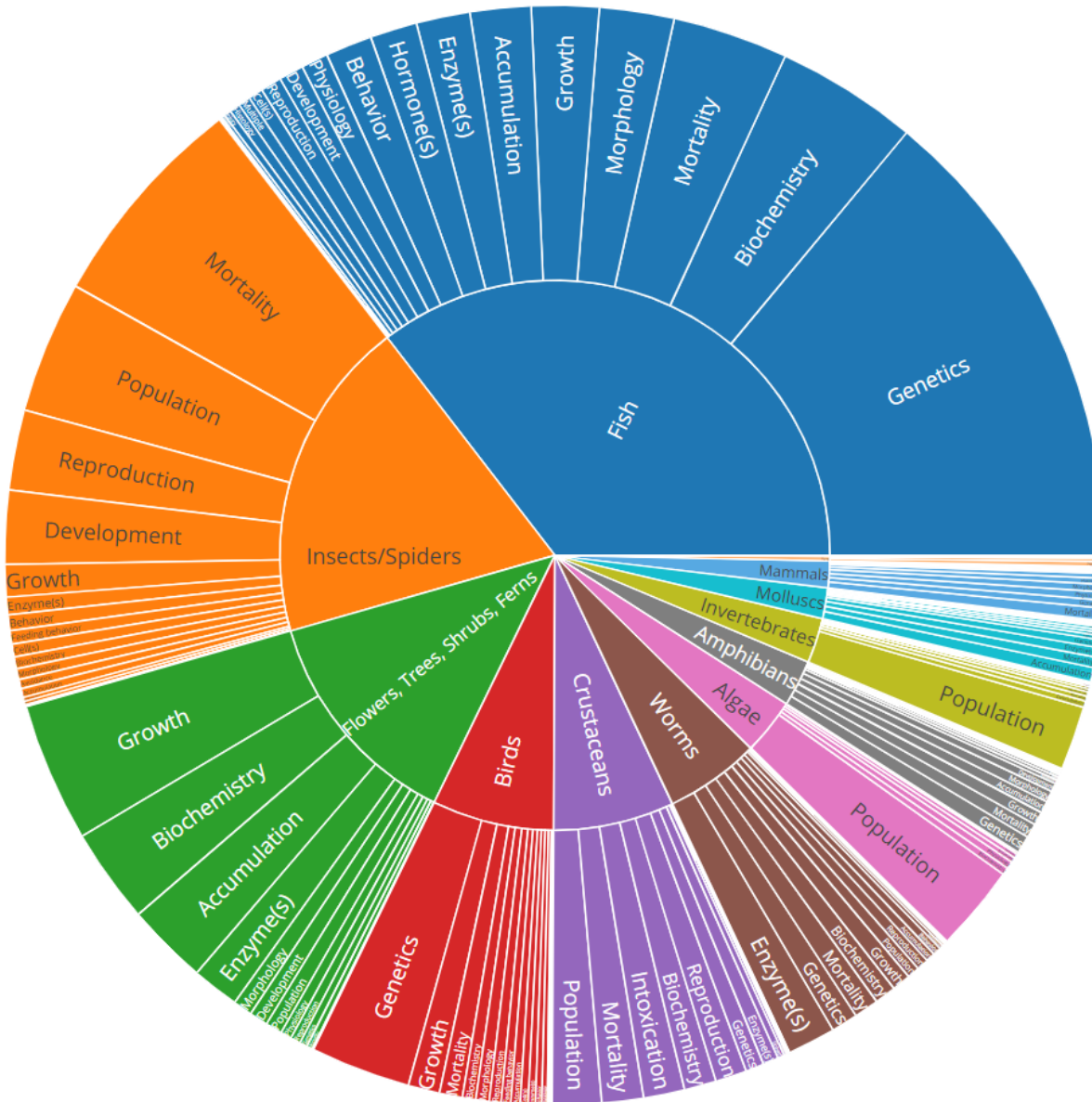


Top 20 Chemicals

	All	Mammals	Fish	Amphibians	Reptiles	Birds	Crustaceans	Molluscs	Worms	Insects/Spiders	Other Invertebrates	Flowers, Trees, Shrubs, Ferns	Algae	Fungi	Other
K-PFOS	147	3	56	6		19	18	11	15	6	7	12	12	1	
PFOA	137	2	58	10	1	10	8	8	17	5	6	18	13		
Hexaflumuron	85	1	2			1	3		3	77	1	3		1	
Lufenuron	83		2			1	2	2	4	73	3	6		3	1
PFOS ion	61	1	26	4		5	4	3	7	2	3	5	2		
Flubendiamide	47		2			1	2	1		44		10	1	2	
PFOS	46	3	29	5		1	4	1	3	2	1		2		
EIFOSA	42	1	3			1	4		2	34		1			
PFNA	36	1	15	3		1	3	4	3	1	1	4	2		
PFDA	23	1	5	2		1	3	5	1	1	1	4	4		
Sodium trifluoroacetate	19		1									8	10		
PFBA	18		9				3				1	5	3		
NH4-PFOA	16	2	7			1	3	1	3	1	1	1	2		
PFHxA	16		5	1			1	1	1		1	3	3		
PFUnDA	13		1	2		3	1	2	1	1		2			
F-53B	11		8			1							2		
FOSA	11	2	5						3			2			
PFDaDA	11		5			1	1			1		2	1		
PFBS	10		3	1					1	2		1	2		
PFHpA	10		1				1	1	2			4	3		



Diversity in Types of Effects



PFAS records for Fish

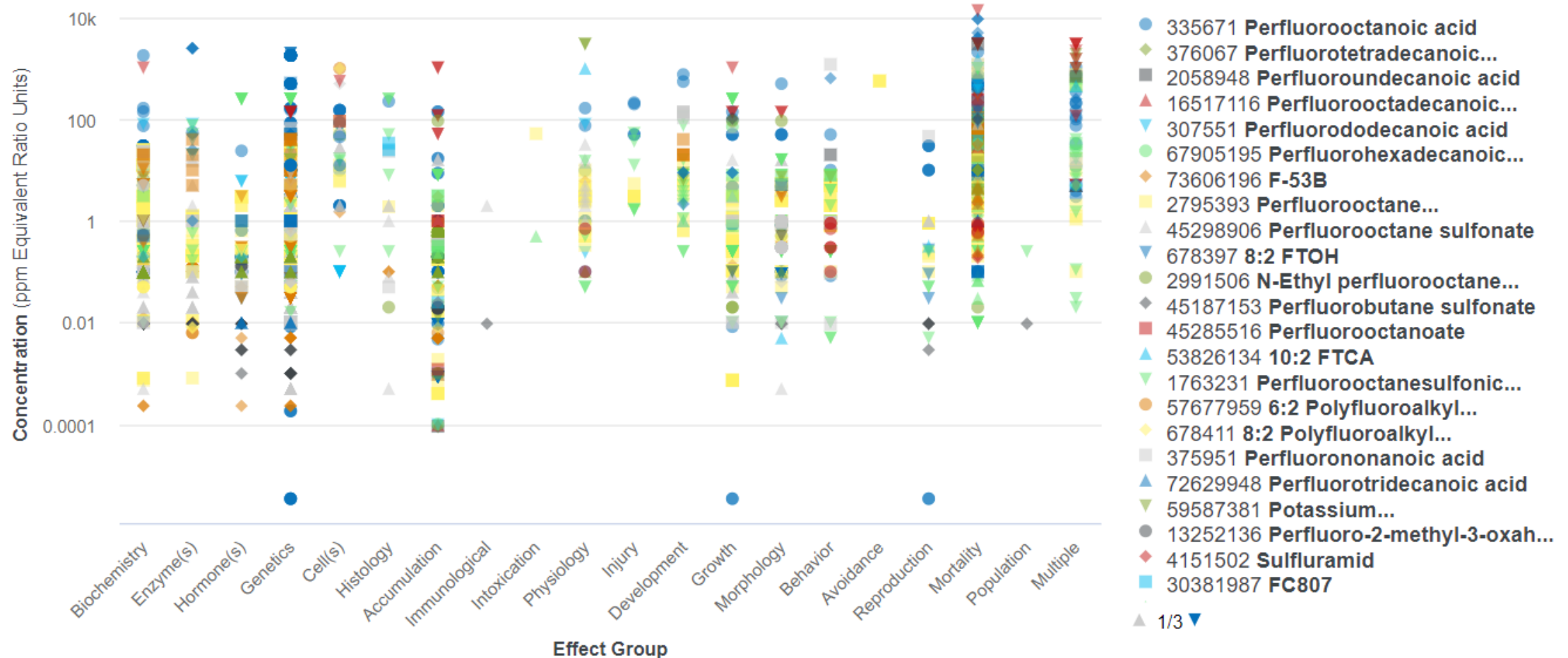
	Effect	# Records
Cellular Responses	Genetics	2,710
	Biochemistry	809
	Enzyme(s)	306
	Hormone(s)	268
	Cell(s)	82
Organ Responses	Histology	61
	Accumulation	349
	Immunological	3
	Physiology	154
Organism Responses	Injury	40
	Intoxication	4
	Development	142
	Growth	383
	Morphology	426
	Behavior	266
	Avoidance	19
	Feeding behavior	4
	Reproduction	120
	Mortality	659
	Genetics	
Population Responses	Population	7
	Other	
Other	Multiple	70
	Total	6,882

Reproduction

Fecundity
Fertility
Fertilization
Gamete production
Hatch
Mean spawns per female
Motility
Number spawning
Pregnant, Parturient or Gravid
Progeny counts/numbers
Spawning frequency
Sperm cell counts
Time to spawn
Velocity
Viability

Diversity in Types of Effects

Data for effects of 91 PFAS in fish shown by exposure concentration and effect type.



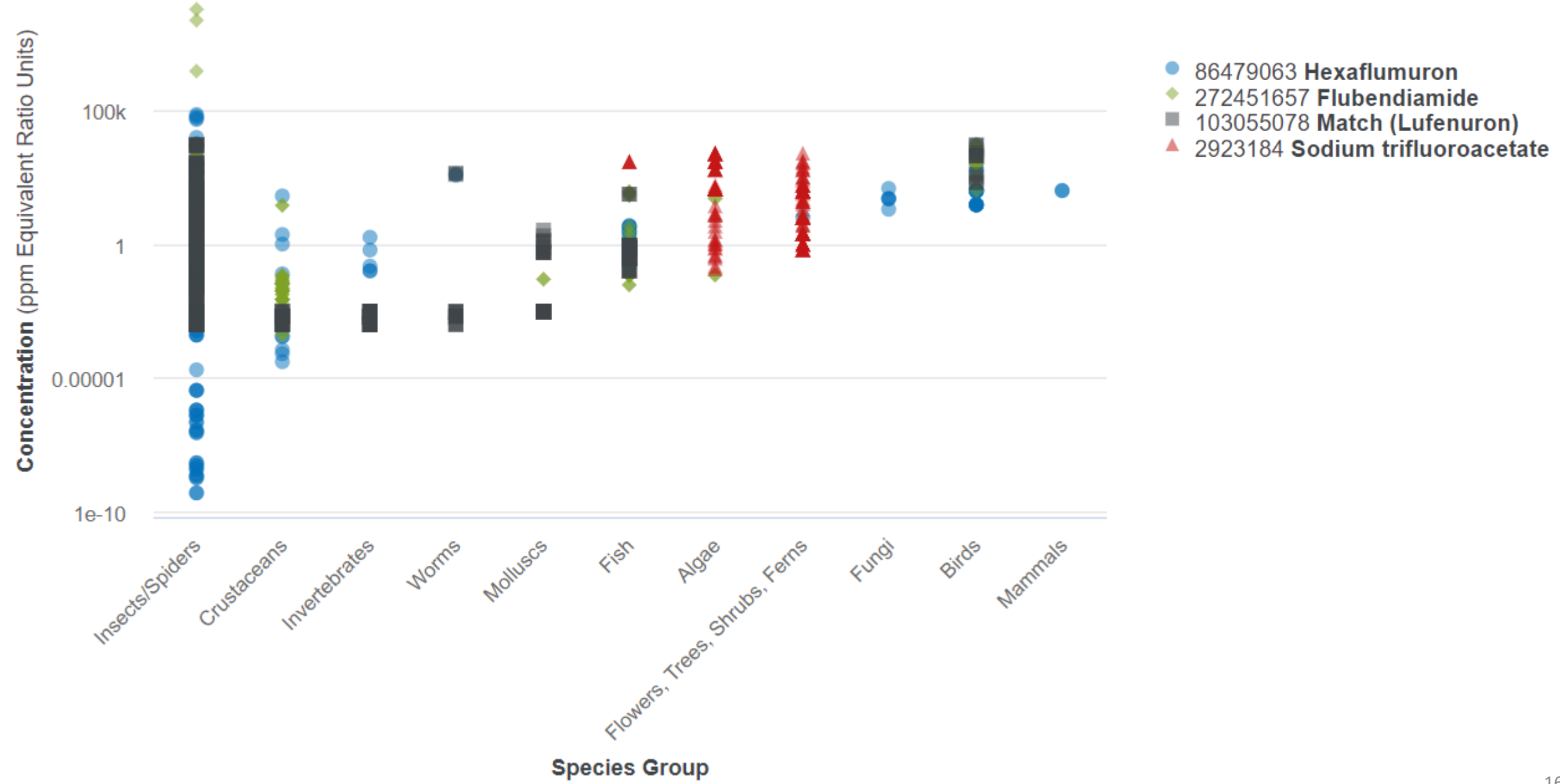
(Endpoints include BAF/BCF, LCXX, LDXX, ECXX, ICXX, LOEC/LOER, MATC/ChV, and lethality; NOEC/NOEL/NOER data excluded from figure)

Recent additions: Chemicals with most references added in past year

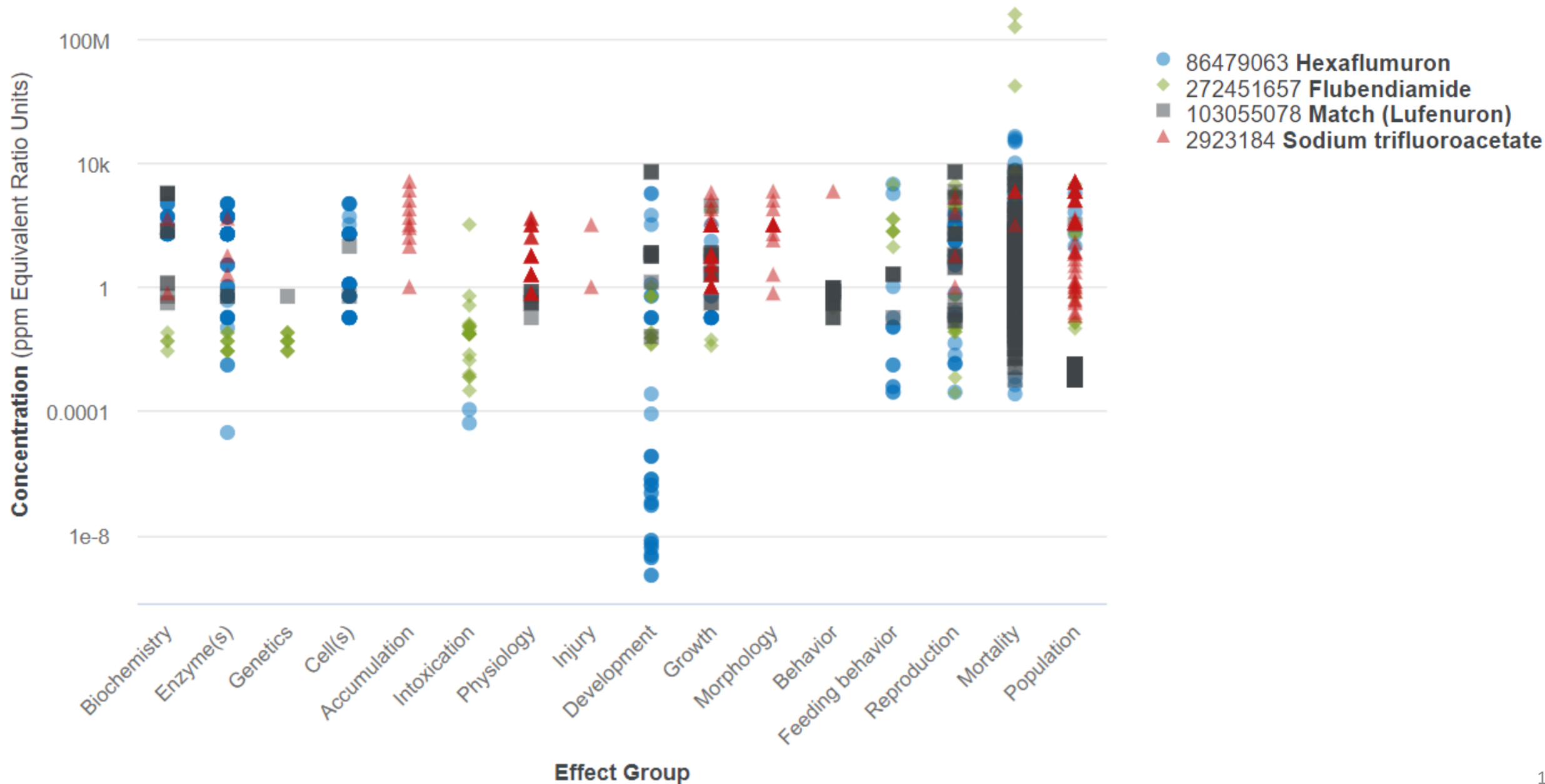
Name	CASRN	# of References	
		Total	New since Sept 2019
K-PFOS	2795-39-3	147	32
PFOS ion	45298-90-6	61	14
PFOS	1763-23-1	46	9
PFOA	335-67-1	137	24
Sodium trifluoroacetate	2923-18-4	20	16
Hexaflumuron	86479-06-3	85	85
Lufenuron	103055-07-8	83	83
Flubendiamide	272451-65-7	47	47

*45 additional chemicals with all references and records added since Sept 2019

Examples of new data: multiple species



Examples of new data: diversity of effects



Continuing literature searches for PFAS

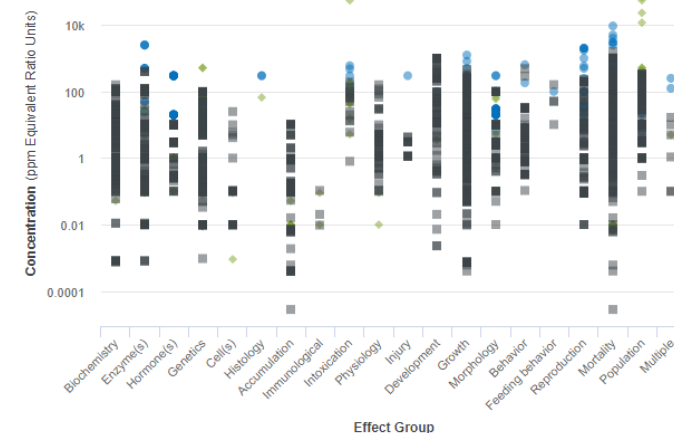
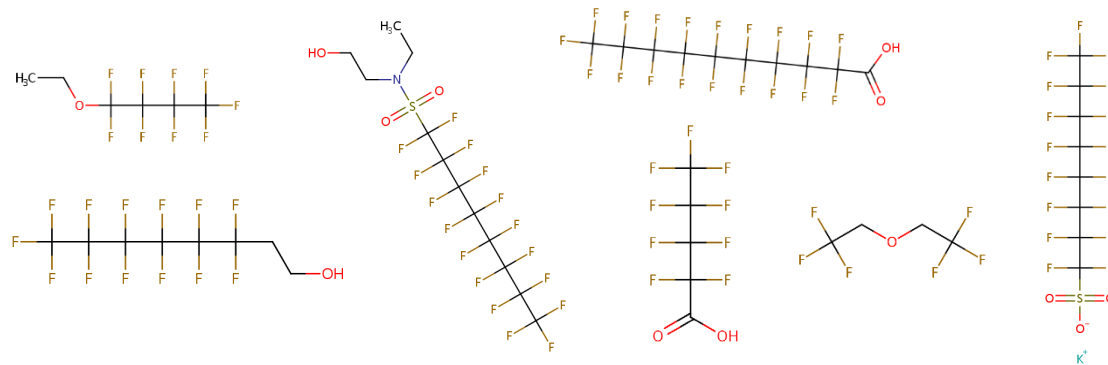
Updated list of >400 unique
CASRN and associated
chemical names

Conduct literature searches

Identify and acquire
potentially applicable studies

Review literature for
applicability to ECOTOX

Extract data and code into
ECOTOX Knowledgebase

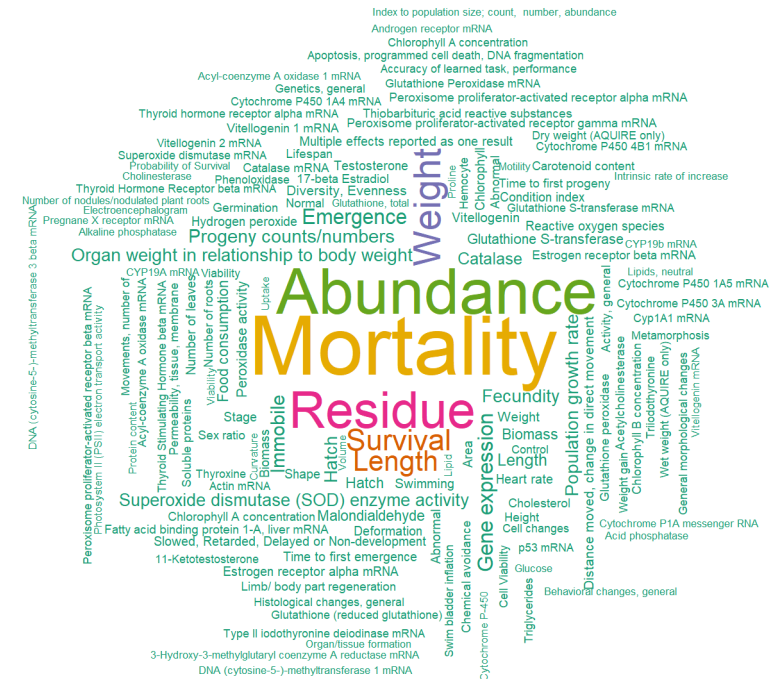
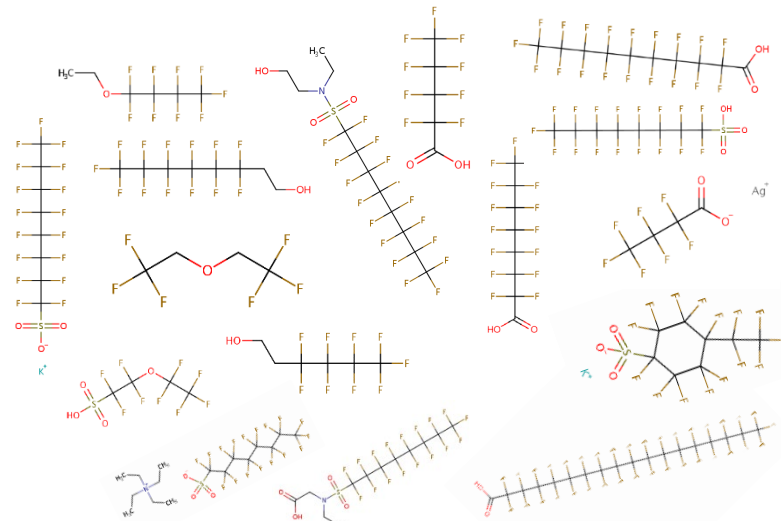


Ecological toxicity data for PFAS

459 Biological Species

130 PFAS

Measurements of 1,225 Effects



Data Inventory \rightarrow Summary/Synthesis

ECOTOX Knowledgebase

[Home](#)[Search](#)[Explore](#)[Help](#)[Contact Us](#)

Data last updated

Jun 11,
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[See update totals](#)

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Di-ethylhexyl phthalate

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Formaldehyde

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Triadimefon

Triphenyl Phosphate

Tetrabromobisphenol A (TBBPA)

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12,155

Chemicals

13,199

Species

50,567

References

1,006,972


Results

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. If you or your team would like training on how to use and find information in ECOTOX, please indicate that in the Feedback box below.

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.

*** Demonstrations and training available**

 [Get Updates via Email](#)

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Fax: 218-529-5003

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Mailing address:

ECOTOX Support

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Duluth, MN 55804

Thank you!

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