



Using the ECOTOXicology Knowledgebase Protocols for Identification and Evidence Mapping of Ecological Toxicity Data for Per- and Polyfluoroalkyl Substances (PFAS)

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U.S. EPA ORD/CCTE/GLTED
Duluth, MN

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Goals

- Comprehensively and systematically identify, obtain, curate and provide open source PFAS ecotoxicity data for use in research and chemical risk management
- Characterize the extent, distribution, and types of evidence for PFAS ecotoxicity
- Curate data of sufficient quality for end users to determine:
 - Data gaps
 - Susceptible species
 - Target endpoints

Identifying Empirical Evidence: ECOTOX Knowledgebase

www.epa.gov/ecotox

Curated database providing single chemical environmental toxicity data for aquatic life, terrestrial plants and wildlife

- Comprehensive literature searches
- Literature review
- Data extraction

ECOTOX Knowledgebase Home Search Explore Help Contact Us

Data last updated
Sep 15, 2021
See update totals

Recent chemicals with full searches completed and data extracted
Cyanotoxins Per- and Polyfluoroalkyl Substa...


Total in database

12,386 Chemicals	13,621 Species
52,551 References	1,082,981 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.



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)

Other Links

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



ECOTOX Data Curation Pipeline

Chemical verification
and development of
search terms

Conduct literature
searches

Identify and acquire
potentially applicable
studies

Review literature for
applicability to
ECOTOX

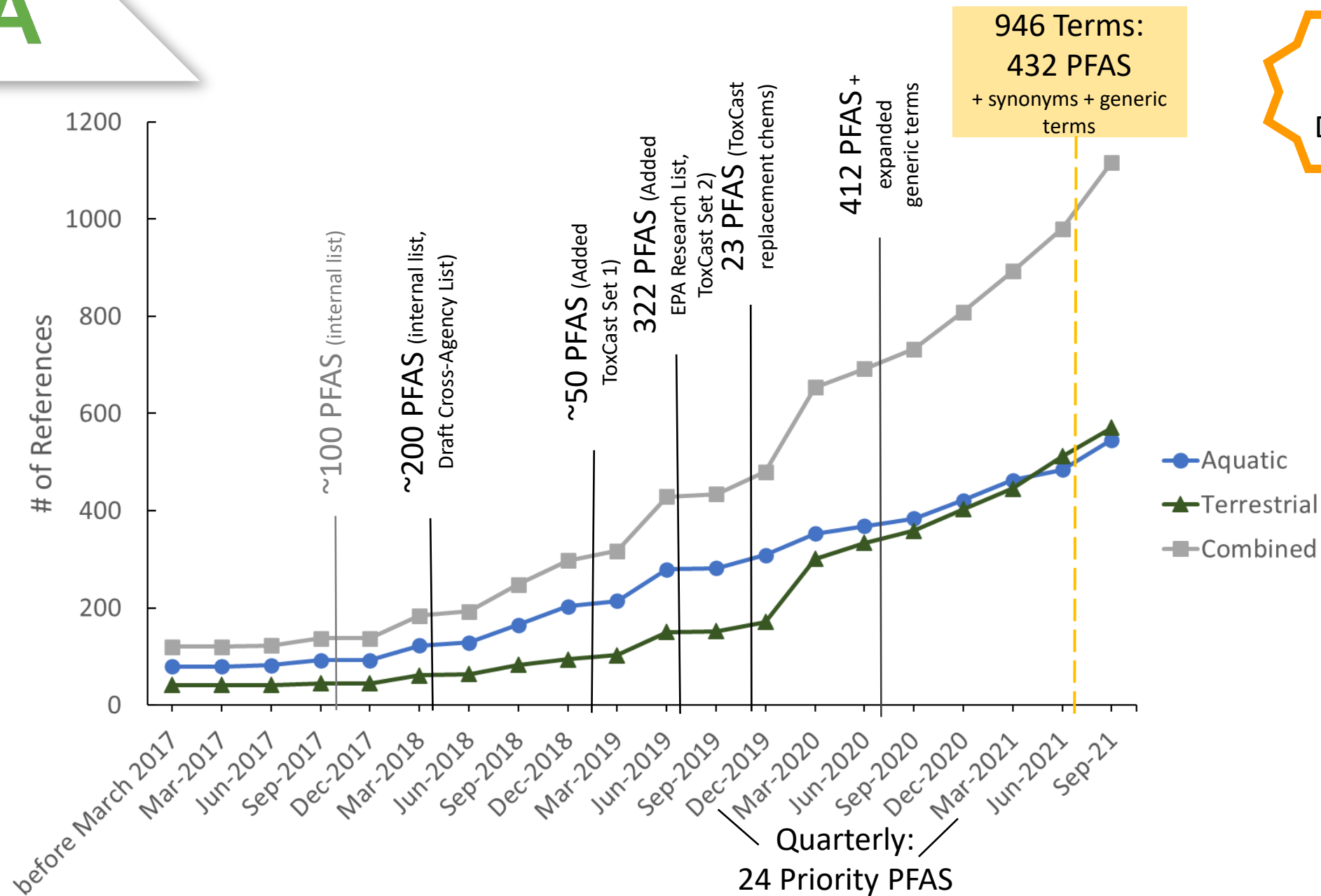
Extract data into
ECOTOX
Knowledgebase

Data Evaluation

See Olker Presentation:
01.01.01



PFAS-specific lit searches, id and data extraction



ECOTOX Pipeline

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 into
ECOTOX
Knowledgebase

Chemical-based Search Terms:

- 400+ Chemicals with CASRNs
- Generic PFAS terms

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

ProQuest

Scopus/Science
Direct

ToxNet/
ToxLine

Dissertation
Abstracts

Agricola
or PubAg

Web of
Science

Already in
Unify*

*Internal USEPA ECOTOX database

~700,000 citations downloaded

Initial removal of duplicates

Title and Abstract Screening
n ~160,000 references

Not applicable (excluded):

- Chem Methods
- Human Health
- Fate
- Survey
- Bacteria
- False Hit
- No Toxicant
- Review
- Mixture
- Other

For Review (Full Text Screening)
n ~ 1,000 references

No PFAS in reference

**Data Extracted from
Acceptable Papers**
n ~ 800 references

Did not meet acceptability criteria (excluded)

Awaiting Review and Data Extraction
n = ~20 references

~200 PFAS references already
included in ECOTOX

Data Records for PFAS
n = 1,117 references: 29,738 records



Incorporation of Advanced Data Analytic Tools

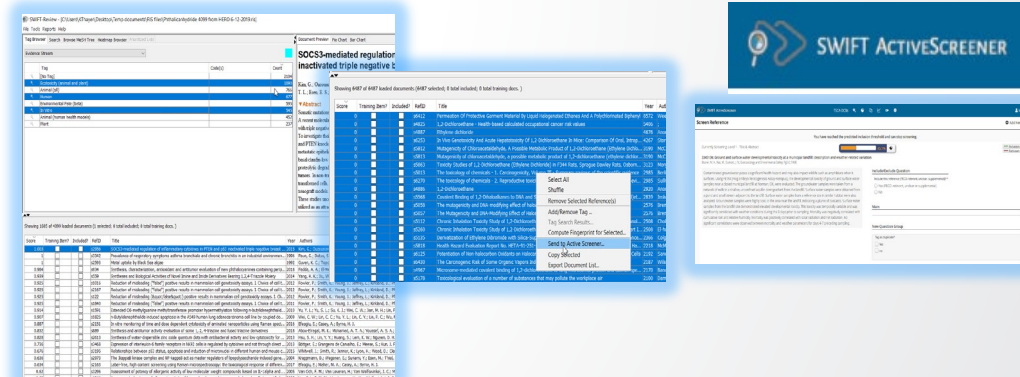
# of Citations	FY18	FY19	FY20	FY21
Downloaded	29,775	98,789	487,497	~800,000*
Reviewed	8,181	7,158	140,966	~80,000*
Added to ECOTOX	111	186	344	384

*July 2021 Final numbers pending (screening still in progress)

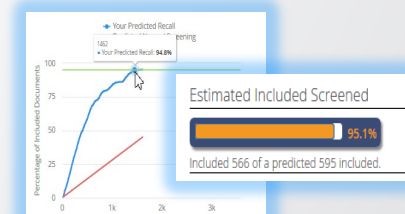
FY20 and FY21:

Implemented use of automated and semi-automated data analytic tools to significantly increase curation efficiencies

Abstract Sifter-plus
for API automated
searches of abstract
services databases



Machine learning AI tools
for rapid Title/Abstract
Screening





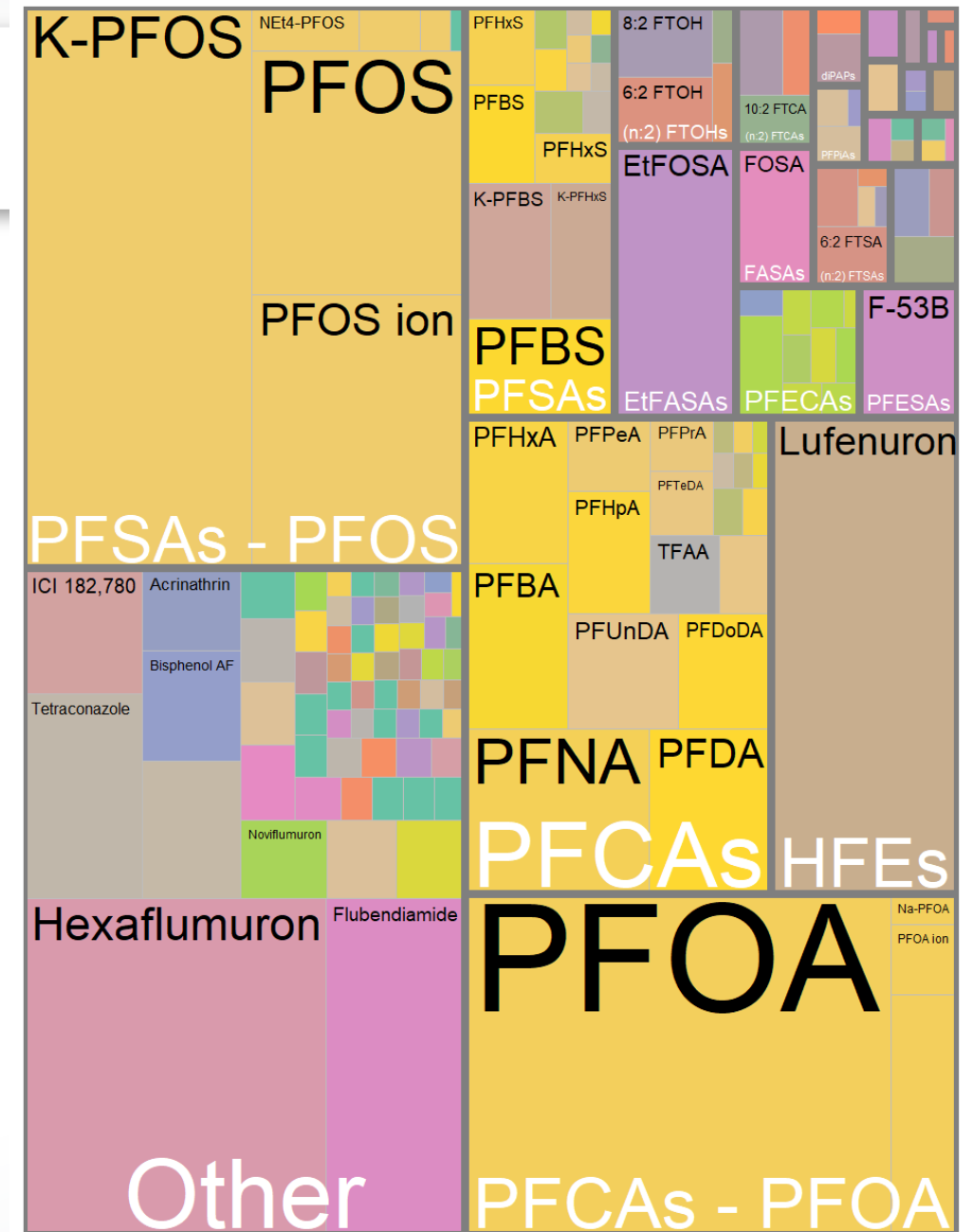
Results

Curation available as of 9/15/2021

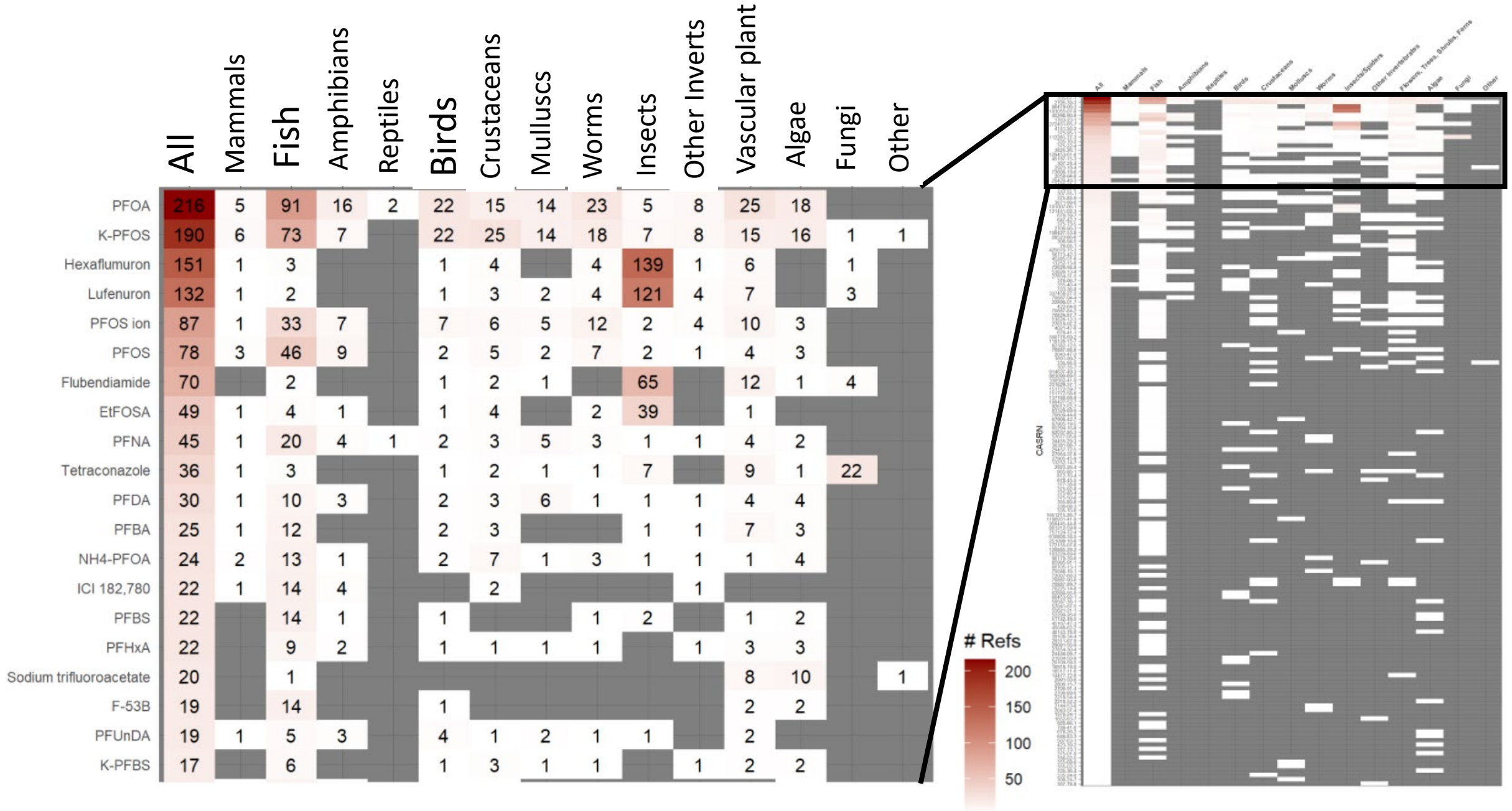
1,117 Publications

159 PFAS with
Ecological Toxicity Data

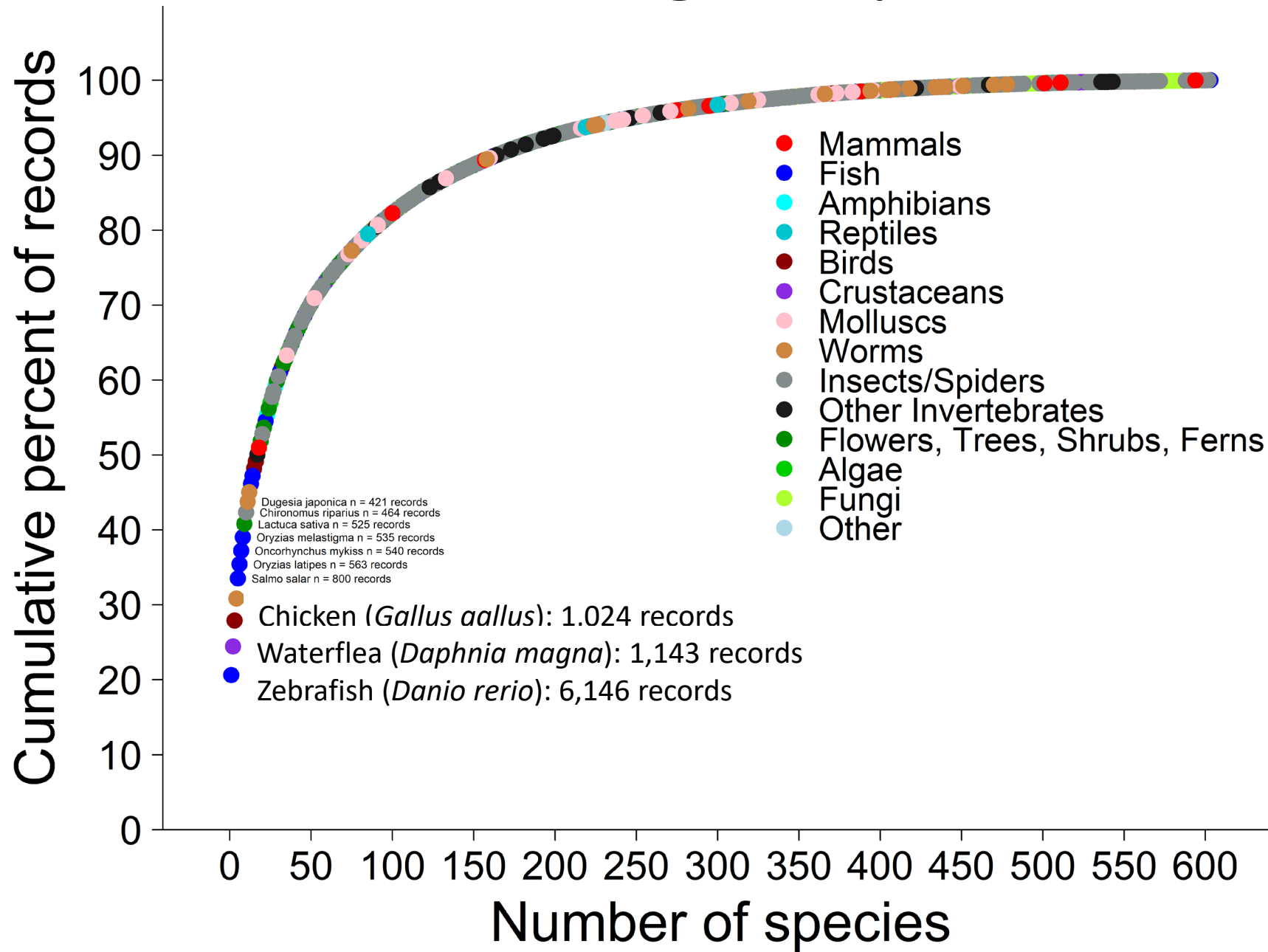
- Box size represents # of references for each chemical



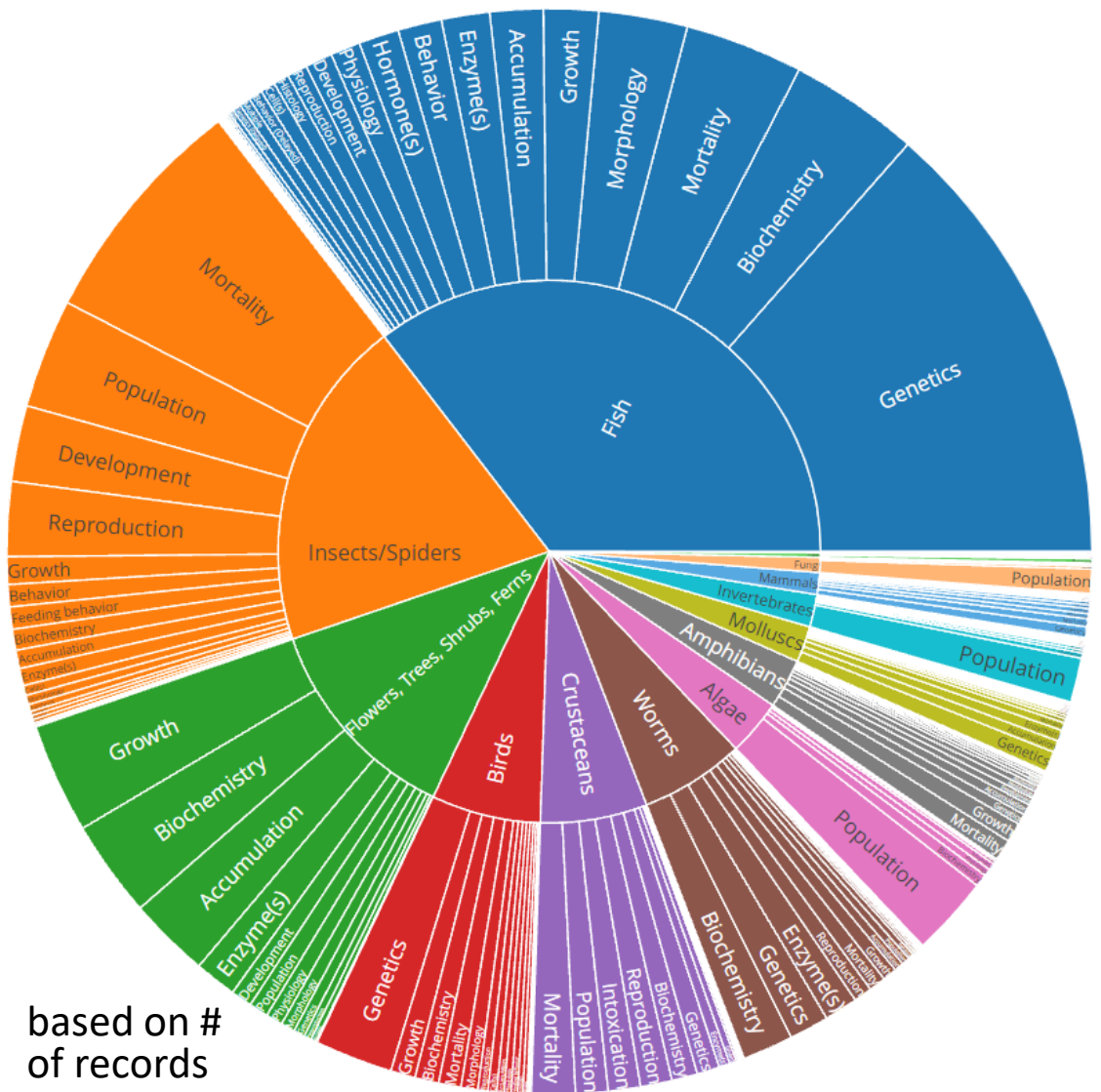
Literature identified for species groups



PFAS Data for >600 Biological Species

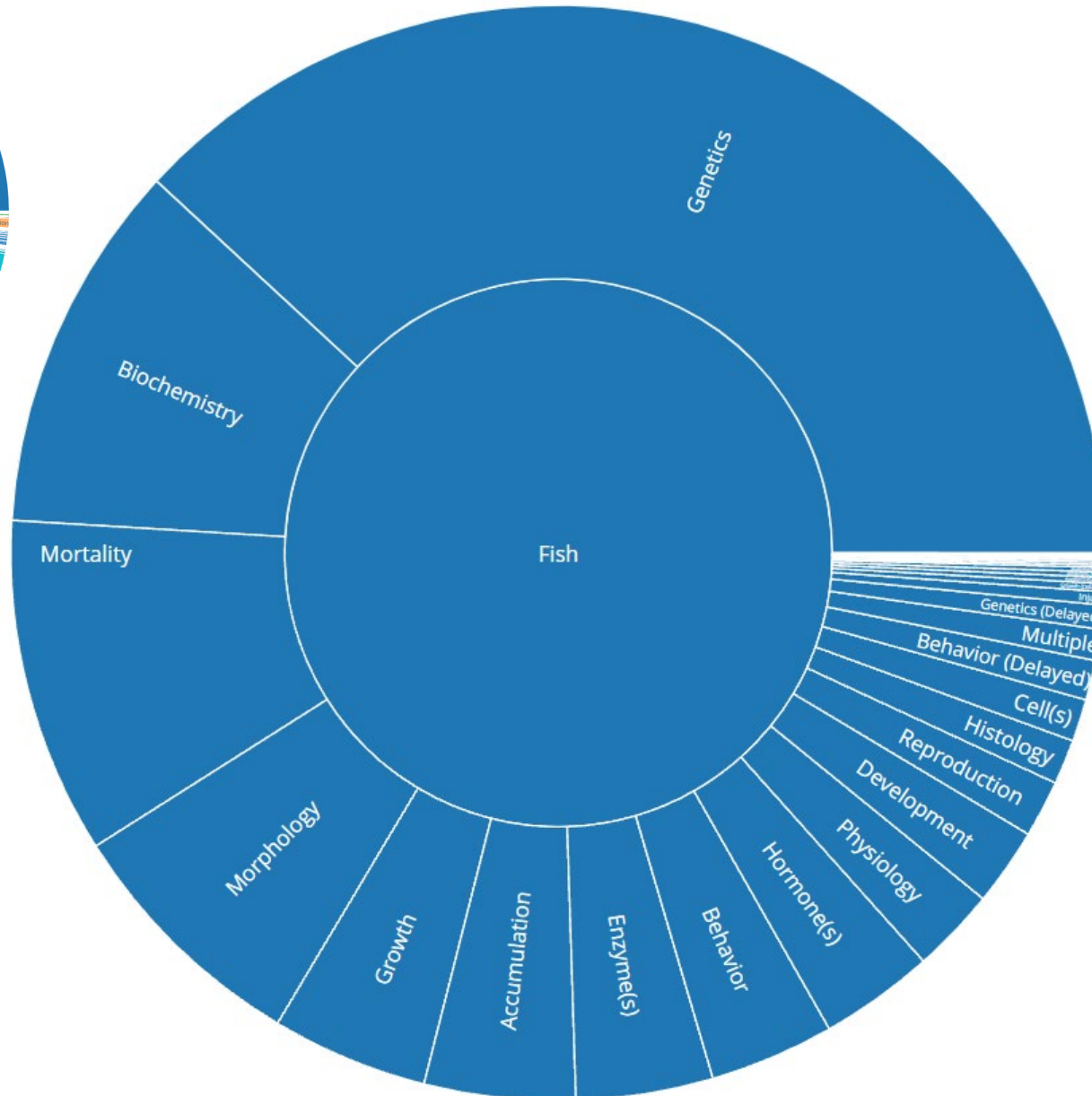
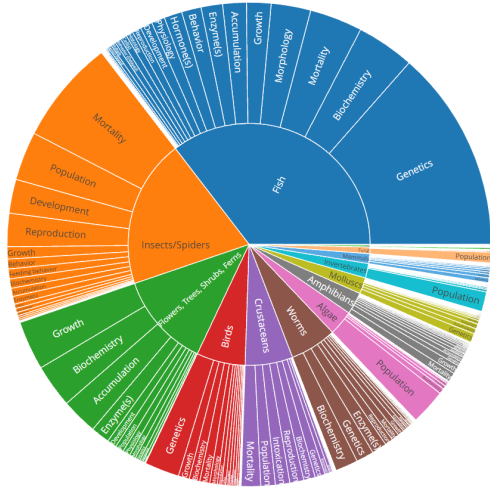


Taxonomic Distribution of PFAS Data



	PFAS data in ECOTOX		
	# of	# of	# of
Group	Compounds	References	Records
All Species	159	1,117	29,797
Fish	115	320	10,560
Insects/Spiders	31	387	5,898
Flowers, Trees, Shrubs, Ferns	53	118	3,792
Birds	41	55	1,940
Crustaceans	43	78	1,900
Worms	32	64	1,857
Algae	46	60	997
Amphibians	24	35	879
Molluscs	23	29	643
Other Invertebrates	26	26	576
Mammals	19	18	389
Fungi	5	31	266
Reptiles	2	3	86
Miscellaneous	3	2	14

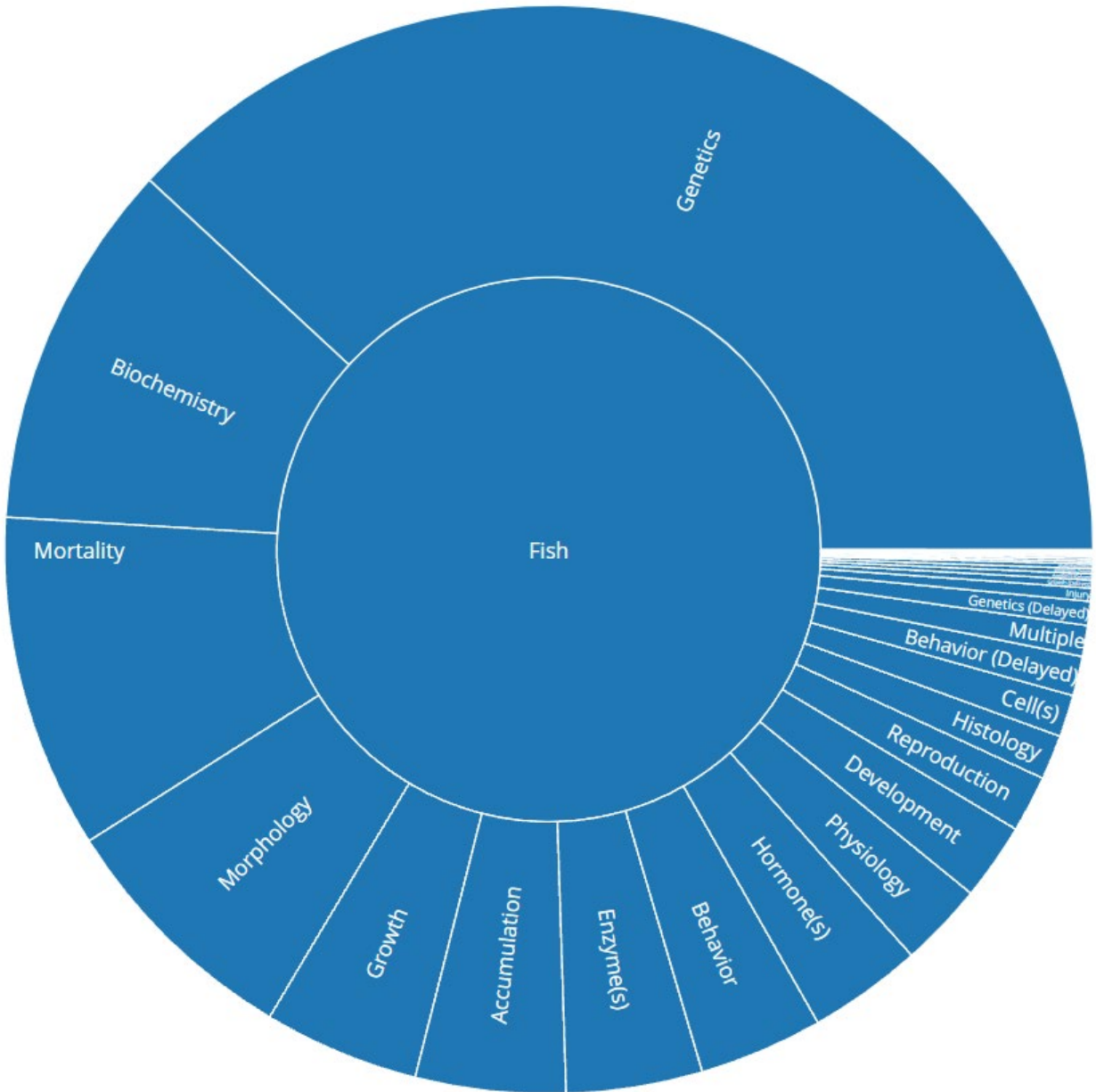
Diversity in Types of Effects



PFAS records for Fish

	Effect	# Records
Celluar Responses	Genetics	4,101
	Biochemistry	1,170
	Enzyme(s)	427
	Hormone(s)	357
	Cell(s)	134
Organ Responses	Histology	142
	Accumulation	475
	Immunological	8
	Physiology	265
Organism Responses	Injury	41
	Intoxication	4
	Development	242
	Growth	513
	Morphology	801
	Behavior	513
	Avoidance	19
	Feeding behavior	8
	Reproduction	181
	Mortality	1,053
	Population Responses	Population
Other	Multiple	97
	Total	10,560

Diversity in Types of Effects



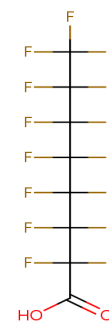
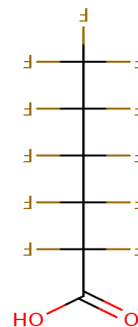
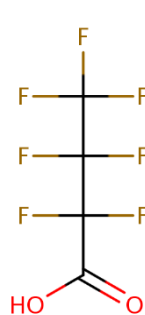
PFAS records for Fish

	Effect	# Records
Cellular Responses	Genetics	4,101
	Biochemistry	1,170
	Enzyme(s)	427
	Hormone(s)	357
	Cell(s)	134
Organ Responses	Histology	142
	Accumulation	475
	Immunological	8
	Physiology	265
Organism Responses	Injury	41
	Intoxication	4
	Development	242
	Growth	513
	Morphology	801
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	Reproduction	181
	Mortality	1,053
Population Responses	Population	7
	Multiple	97
Total		10,560

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



Data Gaps :Perfluorinated Carboxylic Acids



	PFBA		PFHA		PFOA		PFNA		PFDA	
	Acute	Chronic	Acute	Chronic	Acute	Chronic	Acute	Chronic	Acute	Chronic
Molluscs					X	X		X		X
Crustaceans	X			X	X	X	X	X	X	
Fish	X			X	X	X	X	X	X	X
Worms					X	X				
Amphibians					X	X	X		X	
Other										
Invertebrates	X		X		X	X				
Insects/Spiders		X			X	X				
Plants						X				

Acute: <= 96 hour exposure; Mortality; LC50, EC50

Chronic: = > 7 Days; Behavior, Development, Growth, Mortality, Population, Reproduction; all “Endpoints”



Applications

DoD Tri-Services ERA Work Group

- Ecological Screening Values (ESVs) for screening-level ecological risk assessments at DOD federal facilities (*Final Report Sept 2021*)
- Coordination with US EPA OLEM/Superfund, OW, ORD, and Regions

US EPA Office of Water

- Data for PFOS and PFOA aquatic life criteria development
- Data Evaluation Record (DER) generator
 - Objective data directly from ECOTOX
 - Eco-assessors add subjective review observations

US EPA Office of Research and Development

- Hypothesis development
- Reduce redundancy in animal testing

Derivation of PFAS Ecological Screening Values

M. Grippo, J. Hayse, I. Hlohowskyj, and K. Picel

Environmental Science Division

Argonne National Laboratory

FINAL

September 2021

OW DER generator

Data Evaluation Report on the Effects of Potassium perfluorooctanesulfonate on Fish *Danio rerio*

The DER template below has been populated with ECOTOX data coded in UNIFI. Fill in any supplemental information to prepare the DER for the Risk Assessor's evaluation.

Part A: Overview [Collapse](#)

I. Test Information

Chemical

CAS Name: Potassium perfluorooctanesulfonate

CAS Number: 2795393

Purity: 98

[UNIFI purity comments are also displayed if values.]

Storage Conditions: NR

Solubility in Water (units): approximately 500 mg/l

General Notes:

The concentration of PFOS in any experiment was always well below its reported solubility in water (500 mg/L) [26]. [26] Beach SA, Nevstedt A, Cassidy K, Glynn JR 2006.

Ecotoxicological evaluation of perfluorooctanesulfonate (PFOS). Rev Environ Contam Toxicol 186:133-174.

☒ Controlled Experiment (manipulated)

☐ Field Study/Observation (not manipulated)

Primary Reviewer: Acme PBI

QA Reviewer:

Secondary Reviewer:

(At least one reviewer should be from EPA for sensitive taxa)

Date: 10/12/2020

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Environmental
Toxicology and Chemistry

Critical Review | [Open Access](#)

Assessing the Ecological Risks of Per- and Polyfluoroalkyl Substances: Current State-of-the Science and a Proposed Path Forward

Gerald T. Ankley✉, Philippa Cureton, Robert A. Hoke, Magali Houde, Anupama Kumar, Jessy Kurias, Roman Lanno, Chris McCarthy, John Newsted, Christopher J. Salice ... [See all authors](#) ▾

First published: 08 September 2020 | <https://doi.org/10.1002/etc.4869>



Applications-Reuse and Repurpose Lit searches

- Literature Review of PFAS Bioaccumulation Data:
 - Burkhard LP. *Evaluation of published bioconcentration factor (BCF) and bioaccumulation factor (BAF) data for per- and polyfluoroalkyl substances across aquatic species*. Environ Toxicol Chem. 2021 Feb 19. doi: 10.1002/etc.5010.
 - Two additional papers in preparation on Biota-Sediment Accumulation Factors (BSAFs) and food Web modeling
- Initial identification of studies relevant for Sediment Quality Guideline development
 - Began with all references downloaded (775,059)
 - Sediment Toxicity-specific terms identified and employed in Data analytic software for efficient reviews.
 - Resulted in ultimately identifying 25 potentially relevant references
- Sharing References not ecologically relevant but useful for others
 - ECOTOX identifies and rejects Human Health content, but can be used by others

- Extent and distribution of literature of ecological toxicity of PFAS
 - Curated toxicity data for multiple applications
 - Identification of data gaps
- Literature identified for other areas of PFAS research
- Mapping to controlled vocabularies and ontologies will advance synthesis and interpretation
- Limitations:
 - Mixtures currently not included
 - Observational and (most) field data not represented here
 - Limited gene and pathway information for many ecological species



Acknowledgements

Thank you!

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Katie Nehiba*