

The CompTox Chemicals Dashboard - a web-based database and information hub for over five thousand per- & polyfluoroalkyl chemical substances Antony Williams, Chris Grulke, Grace Patlewicz and Ann Richard

U.S. Environmental Protection Agency, Office of Research and Development, Center for Computational Toxicology and Exposure, Research Triangle Park, NC

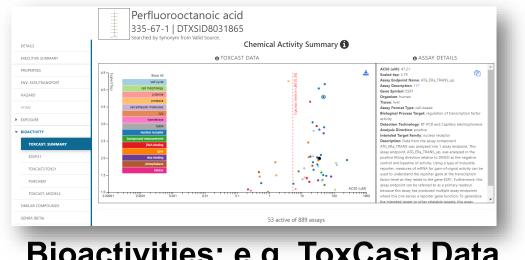
Problem Definition and Goals

Problem: There are many sources of PFAS data online to support computational toxicology. However, curated datasets for the thousands of known PFAS chemicals are not available in structured formats,

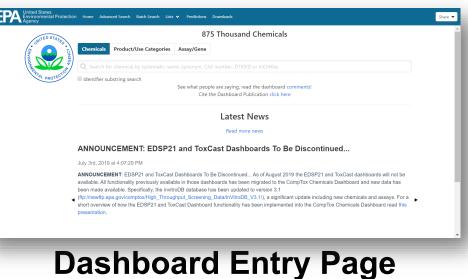
Goals: Deliver online access to hundreds of thousands of chemicals of interest to environmental science and computational toxicology. Provide lists of PFAS substances via a simple to use web-based interface. Deliver application to support diverse types of data including experimental and predicted physicochemical properties, in vivo hazard data and in vitro toxicity and toxicokinetic data. Make the data available as downloadable data for reuse and repurposing in other databases.

Abstract

EPA's Chemicals CompTox Dashboard The (https://comptox.epa.gov/dashboard) is a publicly accessible website providing access to data for ~875,000 chemical substances, the majority of these represented as chemical structures. The web application delivers a wide array of computed and measured physicochemical properties, in vitro high-throughput screening data and in vivo toxicity data, product use information extracted from safety data sheets, and integrated chemical linkages to a growing list of literature, toxicology, and analytical chemistry websites. The application provides access to segregated lists of chemicals that are of specific interest to relevant stakeholders, including Per- & Polyfluoroalkyl Substances (PFAS) containing thousands of chemicals. A procured testing library of hundreds of PFAS chemicals annotated into chemical categories has also been integrated into the dashboard with a number of resulting benefits: a searchable database of chemical properties, with hazard and exposure predictions, and links to the open literature. Several specific search types have been developed to directly support the mass spectrometry non-targeted screening community, enabling cohesive workflows to support data generation for the detection and assessment of environmental exposures to chemicals contained within the database. This presentation will provide an overview of the dashboard, the ongoing expansion of the PFAS chemical library, with associated categorization, and new physicochemical property and environmental fate and transport QSAR prediction models developed for these chemicals. This abstract does not necessarily represent the views or



The CompTox Chemicals Dashboard



Where possible, links are related Wikipedia provided to articles. Structure file formats are available for download to the desktop (SMILES and molfile) executive summary an and report regarding chemical toxicity is provided.

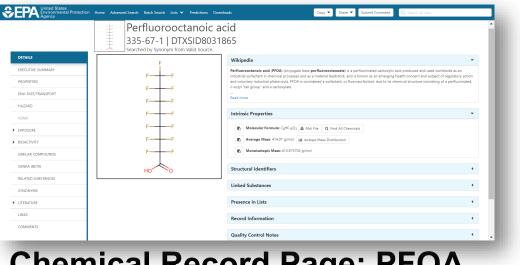
RY	Summary V								
				Summary	/				
DRT	🛓 Download 🔻 Colum	Download Columns							
	Property \$	Experimental average 🕈	Predicted average \$	Experimental median +	Predicted median \$	Experimental range 🗘	Predicted range \$	Unit	
	LogP: Octanol-Water	3.60 (1)	5.51		5.57	3.60	2.95 to 7.75		
	Melting Point	57.0 (14)	34.6	56.5	40.6	54.3 to 59.5	-8.69 to 65.7	°C	
	Boiling Point	189 (9)	192	189	190	188 to 191	188 to 204	°C	
	Water Solubility	1.56e-2 (4)	1.01e-2	1.56e-2	6.38e-5	8.21e-3 to 2.29e-2	6.27e-8 to 4.01e-2	mol/L	
DS	Vapor Pressure	2.23 (5)	0.245	0.525	0.307	1.70e-2 to 10.0	2.24e-2 to 0.345	mmHg	
	Flash Point		68.0		68.0		62.1 to 73.9	°C	
	Surface Tension		16.8				16.8	dyn/cm	
ES	Index of Refraction		1.29				1.29		
	Molar Refractivity		42.9				42.9	cm^3	
	Polarizability		17.0				17.0	A^3	
	Density	1.80 (1)	1.72		1.72	1.80	1.70 to 1.75	g/cm^3	
	Molar Volume		237				237	cm^3	
	Thermal Conductivity		65.3				65.3	mW/(m*K)	
	Henry's Law		2.02e-10				2.02e-10	atm-m3/mole	
	LogKoa: Octanol-Air		4.16				4.16		
	pKa Acidic Apparent	3.15 (2)		3.15		2.50 to 3.80			

Chemical Properties Panel

The Hazard tab provides access to data assembled from a series of public resources including EPA data (i.e. IRIS and PPRTV reports, ToxRef DB). Data can be downloaded as TSV and Excel files.

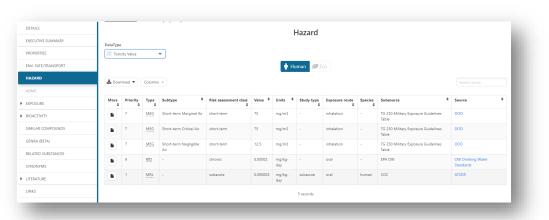
Bioactivities: e.g. ToxCast Data

The the landing page Of dashboard is a simple text entry allowing type-ahead а box search for systematic, trade and CAS trivial Registry names, InChI chemical Numbers and identifiers.



Chemical Record Page: PFOA

chemical records with structures experimental and predicted physicochemical (logP, water solubility etc.) and fate and transport properties are provided. These include OPERA models reported by Mansouri et al. [1]



Toxicity Values Panel

ToxCast Bioactivity data measured over the past decade are under the Bioassay Tab. Data can be downloaded as Excel files. New in vitro data are being generated on a library of ~150 PFAS in collaboration with NTP.

Accessing PFAS Chemical Lists

The dashboard provides access to ~20 individual PFAS chemical lists. These include the list of chemicals that are being studied in a number of *in vitro* screens, a growing list of chemicals that are included in our physical sample library, a growing list of Markush representations of PFAS categories, and a list based on structural filters.

🛓 Download 🔻	Columns ~
List Acronym 🗘	List Name
EPAPFAS7551	PFAS[EPA: List ((Set 1)
EPAPFAS7552	PFAS EPA: List ((Set 2)
EPAPFASCAT	PFAS[EPA Struc Categories
EPAPFASDW	PFAS EPA: New Drinking Water
EPAPFASDW537	PFASJEPAJWATI Method 537.1
EPAPFASDWTREAT	PFASJEPAJWATI Treatment Tech
EPAPFASINSOL	PFAS[EPA: Cher Insoluble in DM
EPAPFASINV	PFASJEPA: ToxC Inventory
EPAPFASINVIVO	PFASJEPA: In Vi
EPAPFASLITSEARCH	PFAS[EPA: Liter Completed:

A list of Markush Representations associated with the selection of chemicals for in vitro toxicity and toxicokinetic screening is also available [2,3].

- dashboard.

References

Acknowledgements

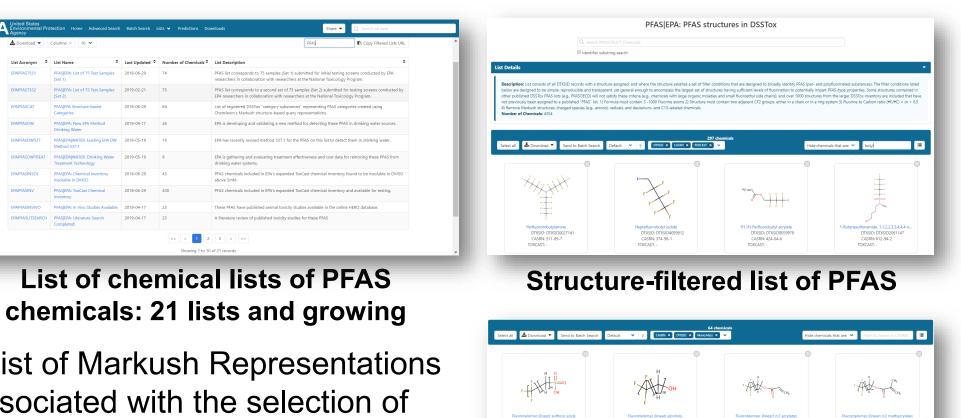
Innovative Research for a Sustainable Future

SETAC 2019 Toronto, CAN November 3-7, 2019



ORCID: 0000-0002-2668-4821

Antony Williams I williams.antony@epa.gov I 919-541-1033



Structure-intered list of PFA5										
Al 🕹 Download 🔻 Send to Batch Search Default 👻 🕴 CXXN x (1700) 1: MonAllia X V Hide chemicals that are: 🆤 Cher by Name or CASRI 🔳										
Fucrotefomer (finea) sufficie acds CASHN: NGCA5 J25258 DDSISL: DISJOS/DB32558		AHH-G-G-Creb Fluorotelomer (Invest) n/2 acylates CASIN: NOCAS 595582 DTXID: DTXID:10955822	$(\mathcal{A}_{n}^{\mu})_{n} \subset \mathcal{A}_{n}^{\mu}$ Functelower (inex) n.2 methacylates CASIN: NOCAS, 593553 DISIDE DISIDE095433							
Mono Mase 0 HO H_{H} F_{F} H_{H} OH	Mono Mare 0	Mono Mass 0	Monto Marce 0							
Fluorotelomer symmetric diols CASRN: NOCAS_093584 DTXSID-DTXSID90693584 Mono.Mass: 0	Fluorotelomer (Incer) amines (accondary) CASRN: NOCAS,893585 DTXSID: DTXSID:50893585 Mono.Mass: 0	F Fluorotelomer (linear) carboxylic acids CASRH: NOCAS, 893586 DTSID: DTSID: DTSID: 10893586 Mono.Mass: 0	Fluorotelomer (linear) phosphate esters _ CASRN: NOCAS_893588 DTXSID: DTXSID30893588 Mono.Mass: 0							

Future Work

• In vitro toxicity and toxicokinetic measurements are underway for ~150 PFAS [3]. These will be released in the future on the

Experimental property data are being harvested from literature and online resources to include into the dashboard and OPERA models. • Chemical categorization efforts continue in order to be encompassing of more of the PFAS library.

Mansouri et al. OPERA models for predicting physchem properties and environmental fate endpoints, *J. ChemInf.* **10**, 10 (2018) PFAS Categories list on the CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard/chemical lists/EPAPFASCAT Patlewicz et al. A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing. Environ Health Perspect. 2019 Jan;127(1):14501.

The authors thank the chemical curation team for their rigorous work and the software development team for the development of the dashboard.