The CompTox Chemicals Dashboard - a web-based database and information hub for over five thousand per- & polyfluoroalkyl chemical substances

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Problem Definition and Goals

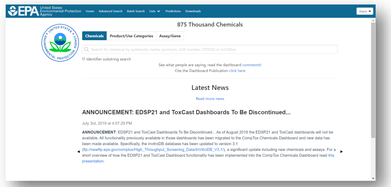
Problem: There are many sources of PFAS data online to support computational toxicology. However, curated datasets for the thousands of known PFAS chemicals are not available in structured formats,

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

The EPA's CompTox Chemicals Dashboard (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 policies of the U.S. Environmental Protection Agency.

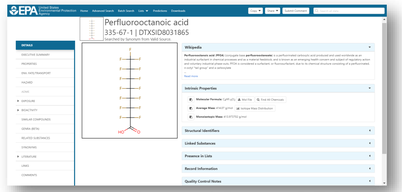
The CompTox Chemicals Dashboard



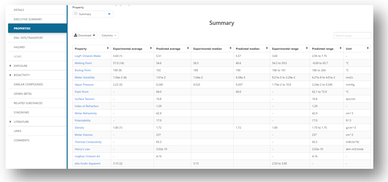
Dashboard Entry Page

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

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



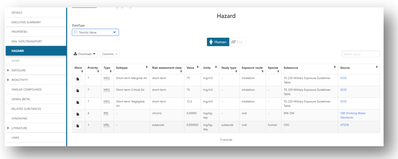
Chemical Record Page: PFOA



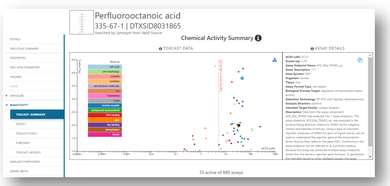
Chemical Properties Panel

For records with chemical 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]

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.



Toxicity Values Panel

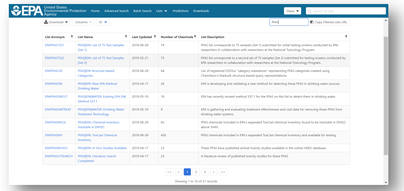


Bioactivities: e.g. ToxCast Data

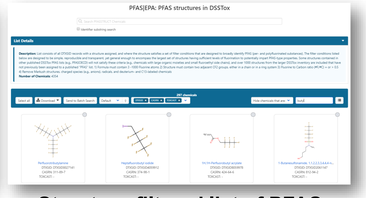
ToxCast Bioactivity data measured over the past decade are under the Bioassay Tab. Data can be downloaded as Excel files. New *in vitro* data are being generated on a library of ~150 PFAS in collaboration with NTP.

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.



List of chemical lists of PFAS chemicals: 21 lists and growing



Structure-filtered list of PFAS

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

Future Work

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

References

1. Mansouri *et al.* OPERA models for predicting physchem properties and environmental fate endpoints, *J. ChemInf.* **10**, 10 (2018)
2. PFAS Categories list on the CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard/chemical_lists/EPAPFASCAT
3. 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.

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