Problem

Environmental chemistry community is required for data aggregation, structure-based indexing, read-across, and development of QSAR prediction models. However, structural information is often unavailable for classes of chemicals of current and emerging interest. A prime example is that of PFAS

Chemicals Dashboard

The CompTox Chemicals Dashboard provides an intuitive web-based interface for navigating various types of data associated with a list of ~875,000 DSSTox chemical substances. Data include, where available, experimental and predicted property data (including OPERA QSAR models), hazard data (from the underlying EPA ToxVal database), exposure data (including product and use categories, and exposure predictions) and in vitro bioactivity data associated with ToxCast and Tox21 toxicity testing. Other modules include a literature module that accesses PubMed for abstracts1, a Generalized Read-Across (GenRA) module2, and a batch-search capability for searching up to thousands of chemical names, CASRN or other chemical identifiers (IChI Strings or Keys). The screenshots below illustrate some capabilities across PFAS space.

Source Data and Downloadable Forms

PFAS lists consisting of names and CAS Registry Numbers (CASRN) were assembled from various public and EPA sources, including: the Swedish Chemicals Agency report on Per- and Polyfluoroalkyl Substances (PFAS)3, the OECD Comprehensive Global Database of PFAS4, and commercially available databases such as the EPAPFASINV chemical inventory5.

A list of registered PFAS “category substances” was created using Markush structure-based query representations. These categories can be broad and inclusive of more specific categories, or can represent a unique category not overlapping with other registered categories. This approach offers an objective, transparent and reproducible structure-based means of defining categories.

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References

5. Baker Thillainadarajah and Brian Meyer, for expert review and structure-annotation of the PFAS chemical lists compiled for this work.

This poster does not necessarily reflect EPA policy. Views of trade names or commercial products does not constitute endorsement or recommendation for use.