



United States
Environmental
Protection Agency

Public access to environmental chemistry data via the EPA CompTox Chemistry Dashboard

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Problem Definition and Goals

Problem: There is limited access online to freely available and highly curated data to support environmental science research.

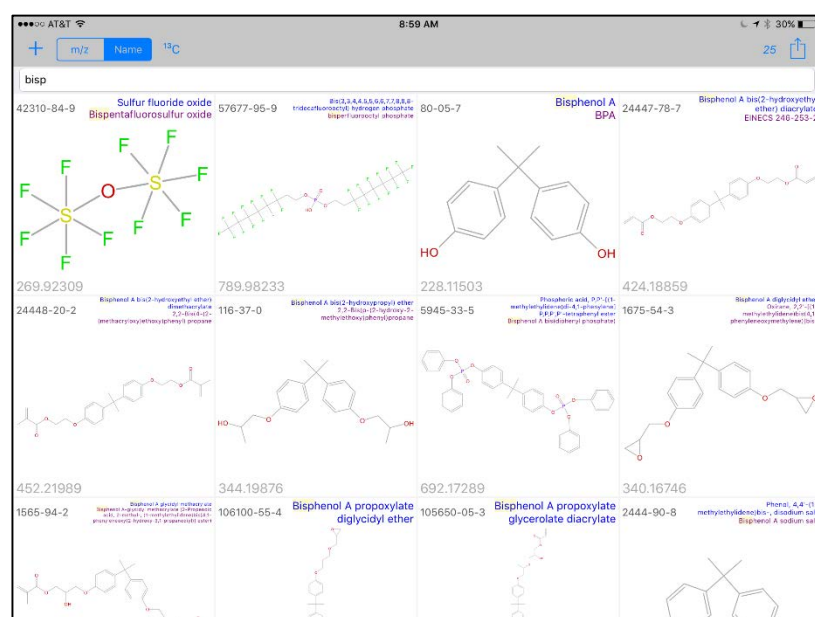
Goals: Provide access to a rich collection of data for ~760,000 chemical substances. Deliver the data via a simple to use web-based interface supporting diverse types of data associated with environmental chemistry, and specifically computational toxicology. Provide support for substances that can be represented as chemical structures as well as for Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB substances). Make the data available as downloadable Open data for repurposing and reuse in other applications.

Abstract

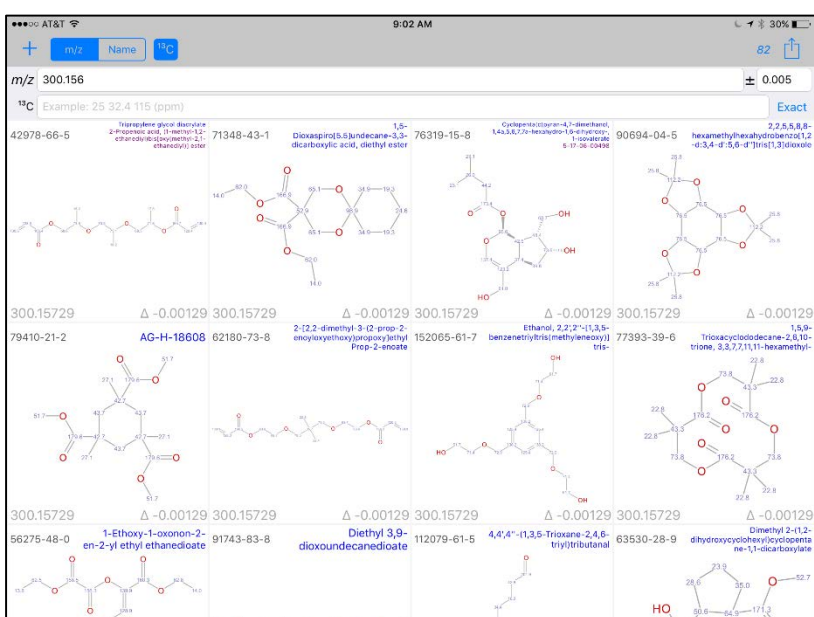
The National Center for Computational Toxicology (NCCT) has assembled and delivered an enormous quantity and diversity of data for the environmental sciences through the CompTox Chemistry Dashboard. These data include high-throughput *in vitro* screening data, *in vivo* and functional use data, exposure models and chemical databases with associated properties.

The web application provides access to data associated with ~760,000 chemical substances and the data can be used to inform fate, exposure, hazard and risk assessment. Much of the data are downloadable and fully open for reuse, therefore allowing for integration into third party applications and databases.

Recently a mobile application was developed for the iOS platform (i.e. iPhone and iPad) that contains hundreds of thousands of chemicals for searching [1].

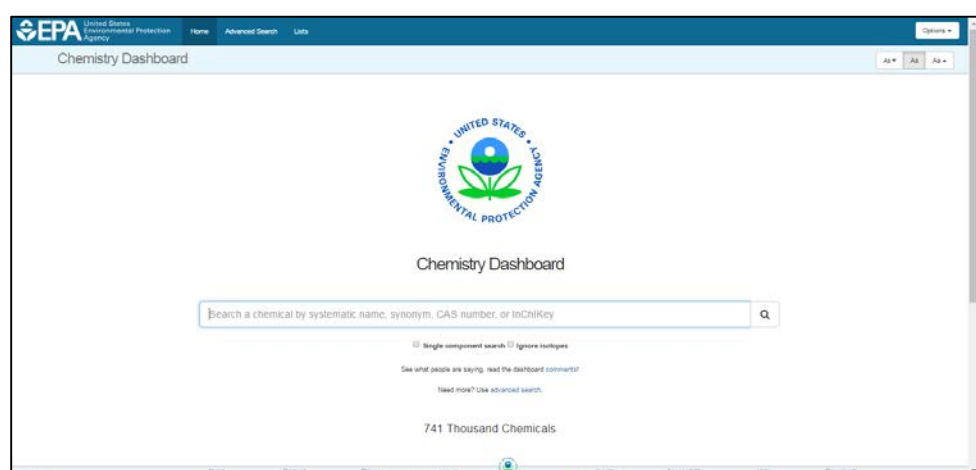


The Open data associated with the dashboard was reformatted for use in both iPhone and iPad applications.



This poster will provide an overview of the dashboard and its capabilities for delivering data to the environmental chemistry community.

The CompTox Chemistry Dashboard



Dashboard Entry Page

Where possible, links are provided to related Wikipedia articles. An associated mol file is available for download to the desktop, and a summary report containing record data can be provided as a PDF file.

Chemical Properties	Summary	Chemical Data	Doc Path/Transport	Toxicity Values	Exposure	Biocatalysis	Similar Molecules	Comments
Summary	LogP Octanol:Water	Experimental	Average	Median	Range			
Water Solubility	Experimental	2.7E-14	2.7E-14	2.7E-14	2.7E-14			
Density	Download as: TSV Excel SDF							
Melting Point	Source	Result	Calculation Details	QM07				
Boiling Point	Source	Result	Calculation Details	QM07				
Surface Tension	Source	Result	Calculation Details	QM07				
Vapor Pressure	Source	Result	Calculation Details	QM07				
LogP Octanol:Water	Source	Result	Calculation Details	QM07				
Henry's Law	Source	Result	Calculation Details	QM07				
Index of Refraction	Source	Result	Calculation Details	QM07				
Molar Refractivity	Source	Result	Calculation Details	QM07				
Yield Based Exposure	Source	Result	Calculation Details	QM07				

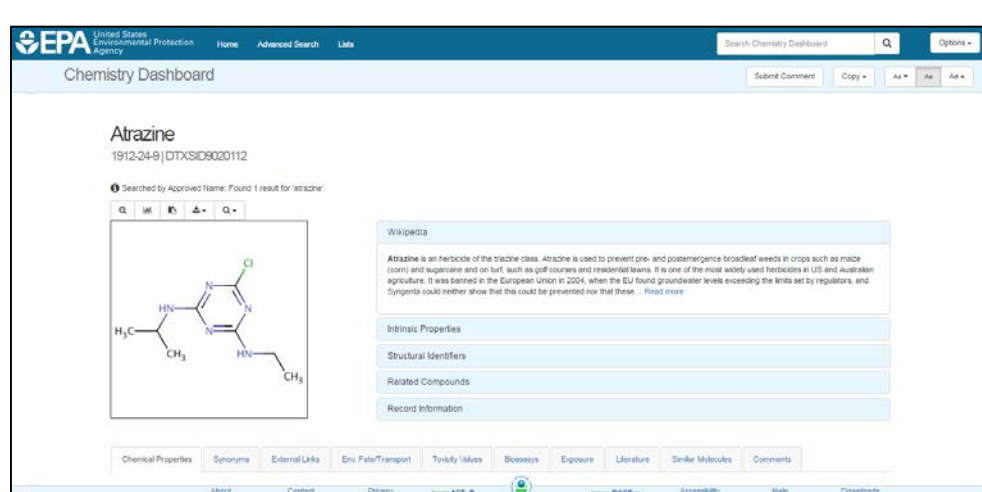
Chemical Properties Panel

The Toxicity Values 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.

Chemical Properties	Doc Path/Transport	Summary	Chemical Data	Doc Path/Transport	Toxicity Values	Exposure	Biocatalysis	Similar Molecules	Comments
Summary	LogP Octanol:Water	Experimental	Average	Median	Range				
Water Solubility	Experimental	2.7E-14	2.7E-14	2.7E-14	2.7E-14				
Density	Download as: TSV Excel SDF								
Melting Point	Source	Result	Calculation Details	QM07					
Boiling Point	Source	Result	Calculation Details	QM07					
Surface Tension	Source	Result	Calculation Details	QM07					
Vapor Pressure	Source	Result	Calculation Details	QM07					
LogP Octanol:Water	Source	Result	Calculation Details	QM07					
Henry's Law	Source	Result	Calculation Details	QM07					
Index of Refraction	Source	Result	Calculation Details	QM07					
Molar Refractivity	Source	Result	Calculation Details	QM07					
Yield Based Exposure	Source	Result	Calculation Details	QM07					

Literature: Pubmed Abstract Sifter

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 InChIs.



Chemical Record Page: Atrazine

For records with chemical structure representations, various inherent properties (e.g. formula and mass) and predicted physicochemical properties (logP, water solubility etc.) are provided.

Chemical Properties	Doc Path/Transport	Summary	Chemical Data	Doc Path/Transport	Toxicity Values	Exposure	Biocatalysis	Similar Molecules	Comments
Summary	LogP Octanol:Water	Experimental	Average	Median	Range				
Water Solubility	Experimental	2.7E-14	2.7E-14	2.7E-14	2.7E-14				
Density	Download as: TSV Excel SDF								
Melting Point	Source	Result	Calculation Details	QM07					
Boiling Point	Source	Result	Calculation Details	QM07					
Surface Tension	Source	Result	Calculation Details	QM07					
Vapor Pressure	Source	Result	Calculation Details	QM07					
LogP Octanol:Water	Source	Result	Calculation Details	QM07					
Henry's Law	Source	Result	Calculation Details	QM07					
Index of Refraction	Source	Result	Calculation Details	QM07					
Molar Refractivity	Source	Result	Calculation Details	QM07					
Yield Based Exposure	Source	Result	Calculation Details	QM07					

Toxicity Values Panel

Literature searching using integration to a series of online resources can be performed using the CASRN and chemical name. This includes Google Scholar, PubMed and PubChem patents.

Batch Searching

Users of the dashboard may be interested in searching for collections of thousands of chemicals. The batch search allows inputs of CASRNs, chemical names, InChIKeys, DTXSIDs and exact molecular formulae. Data that can be downloaded includes SMILES, Molecular Formula and Mass (to support mass spectrometry analyses) and predicted OPERA saR Application (OPERA) [2] and Toxicity Estimation Software Tool (TEST) [3] predictions. The chemicals and associated data can be downloaded as tab-separated values, Excel or SDF files.

Select Input Type(s)	Enter Identifiers to Search
Chemical Name	123456789
CASRN	123456789
InChIKey	123456789
DTXSID	123456789
Exact Molecular Formula	123456789

DTXSID	PREPARED NAME	SMILES	ADN CHEMICAL	OPERA	TEST	OPERA	ADN
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