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Using open data, open services, and open source software to deliver the EPA CompTox Chemicals Dashboard

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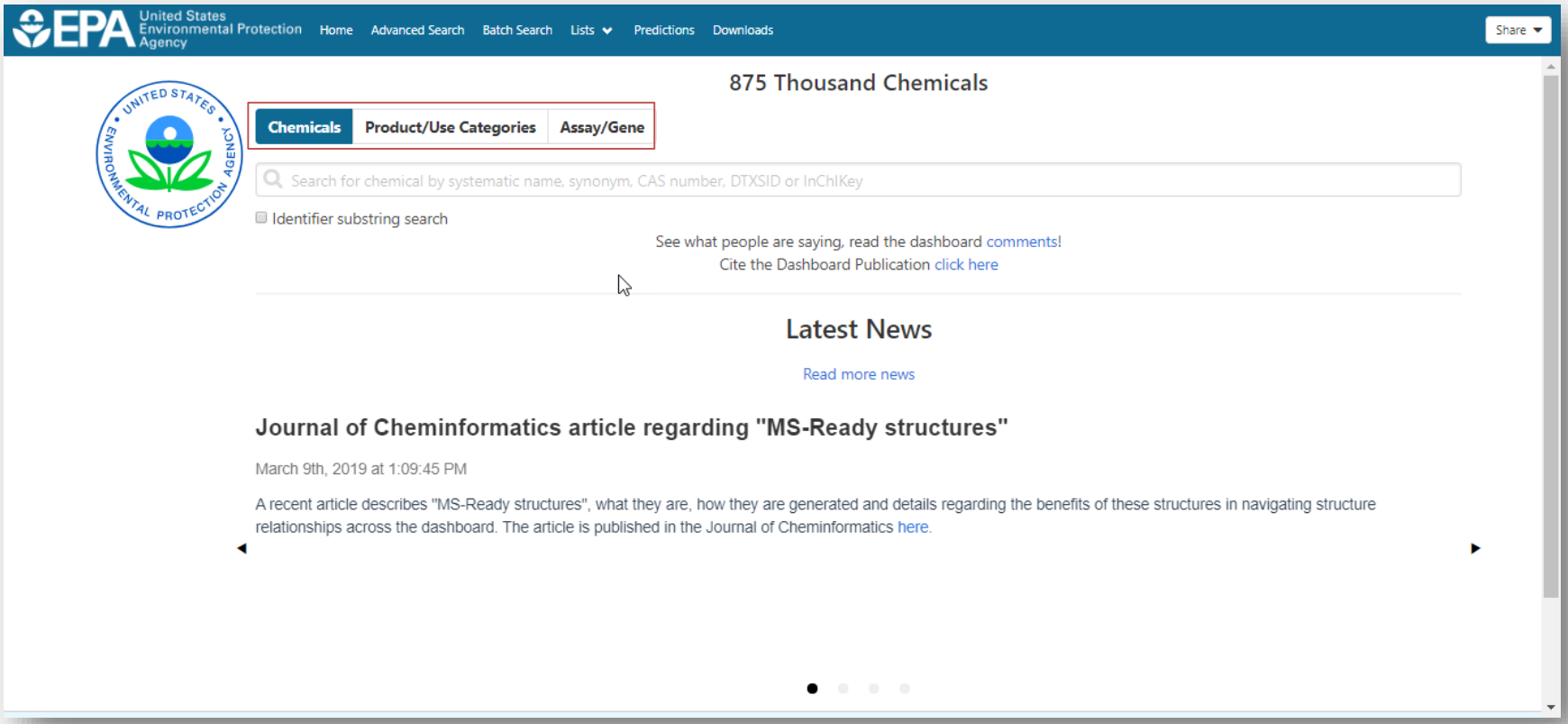
Fall 2019
ACS Fall Meeting, San Diego

CompTox Chemicals Dashboard

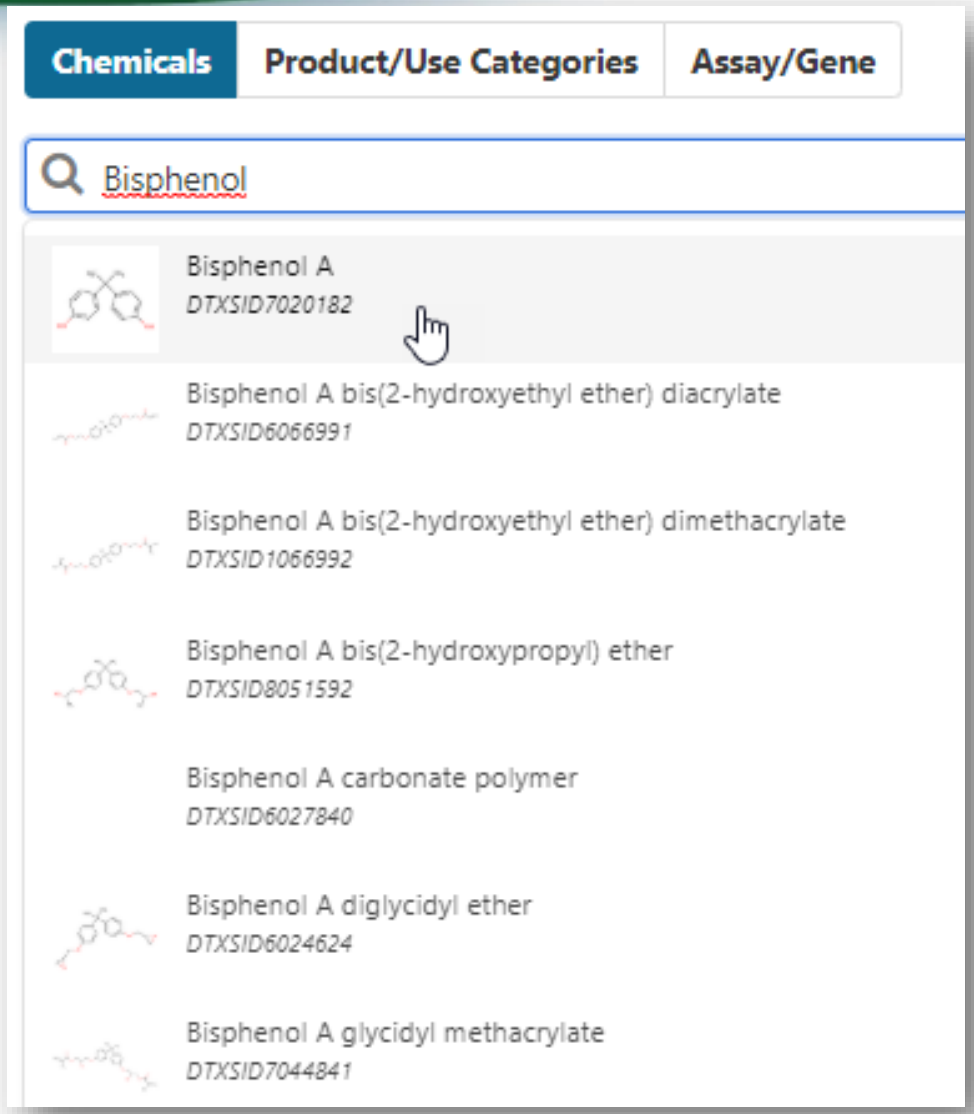
https://comptox.epa.gov/dashboard

EPA United States Environmental Protection Agency

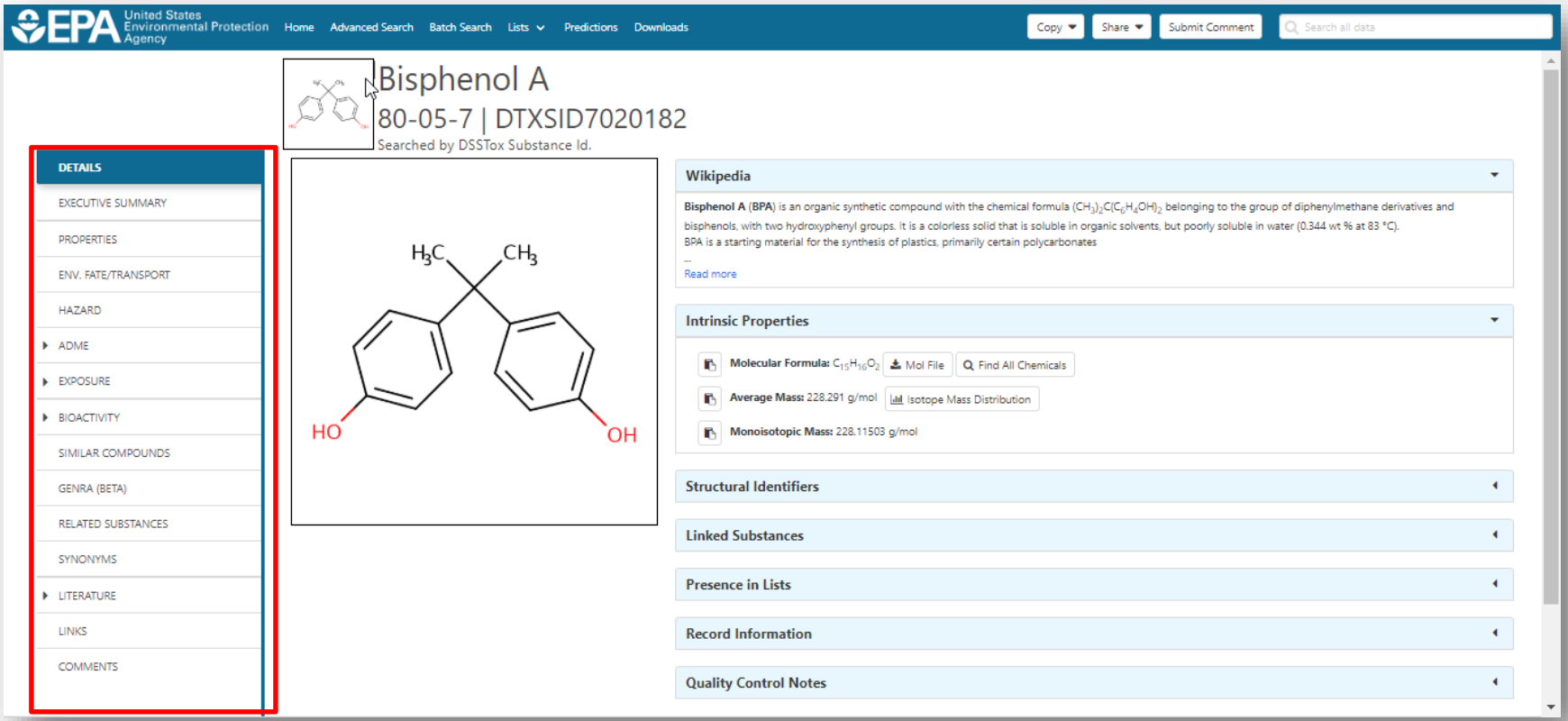
875k Chemical Substances



BASIC Search



Detailed Chemical Pages

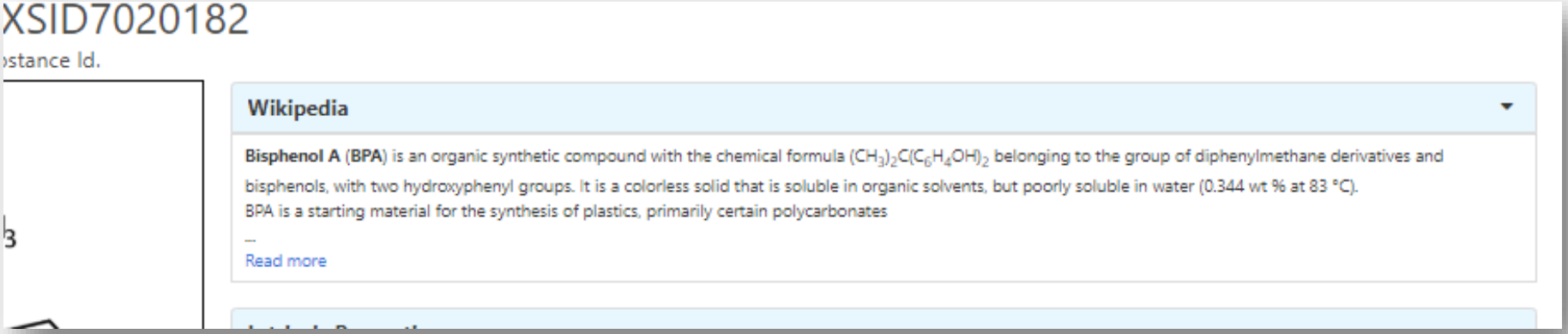


CompTox Chemicals Dashboard

- Total data landscape includes:
  - ~875,000 chemical substances
  - Experimental & predicted physchem property data
  - Experimental Human and Ecological hazard data
  - Bioactivity data for 1000s of chemicals
  - Consumer products containing chemicals
  - “Literature” searches for chemicals using PubMed
  - Real time prediction of physchem/toxicity endpoints

- To make this happen we **CONSUME** open data and open source software
- We also **PRODUCE** open data and both free and open source software
- This presentation is an overview of what we consume and what we produce…

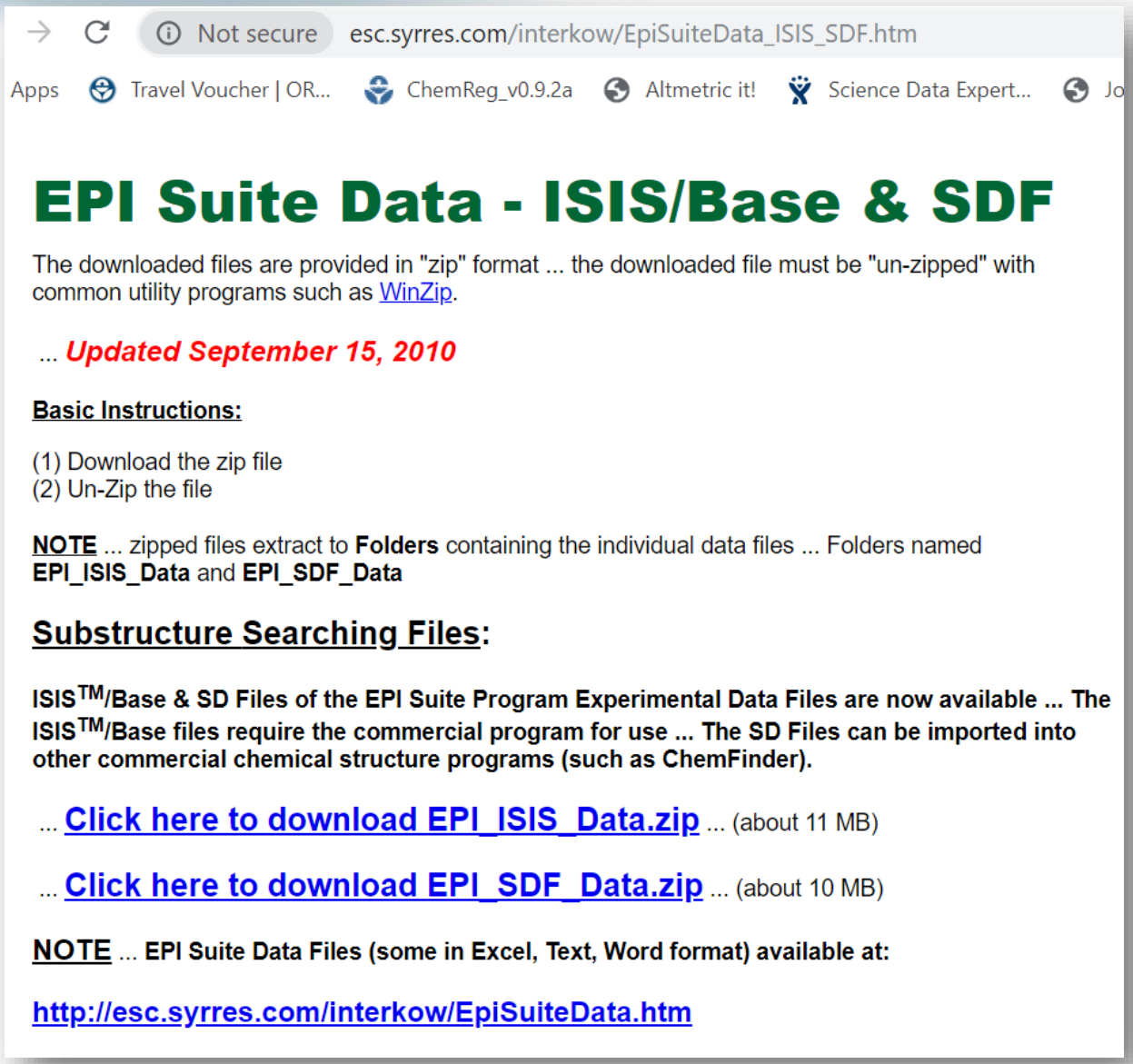
CONSUMER
Integrated Wikipedia Snippet



- Integrated Wikipedia snippet linked out to full article

PhysChem Data and Predictions

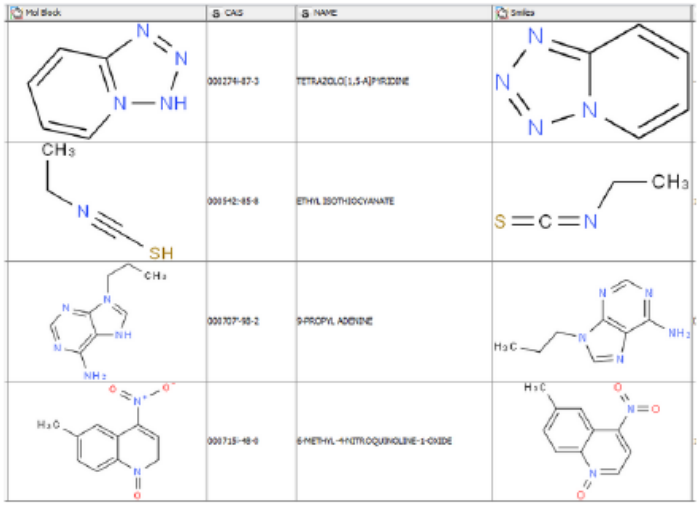
CONSUMER: Available Data
2010 files underlying EPI Suite



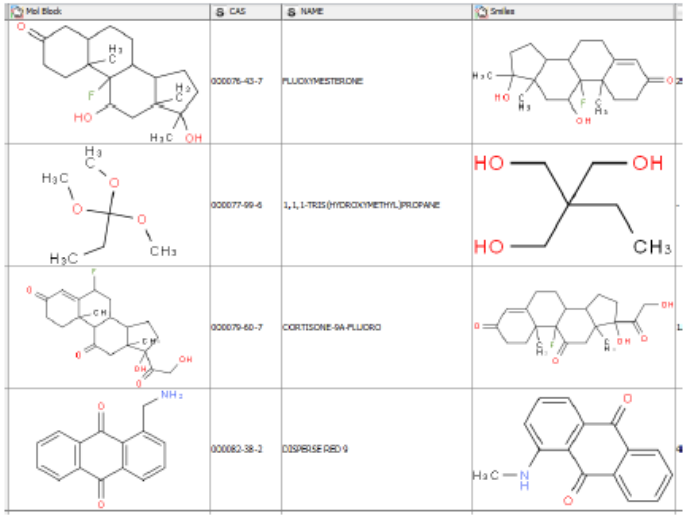
Data required thorough curation

EPA United States Environmental Protection Agency

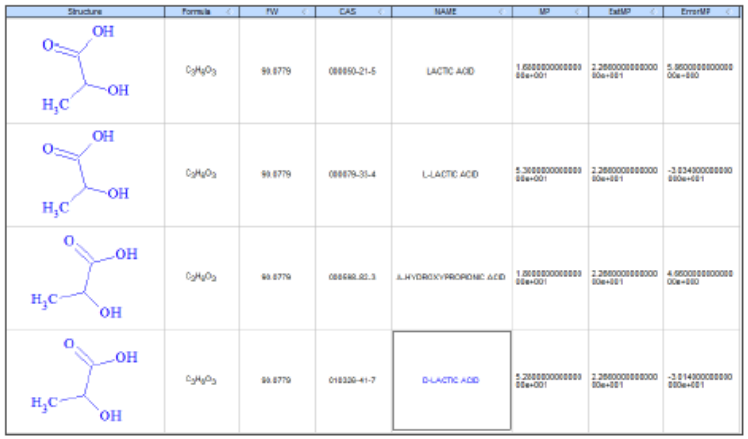
Valence Errors



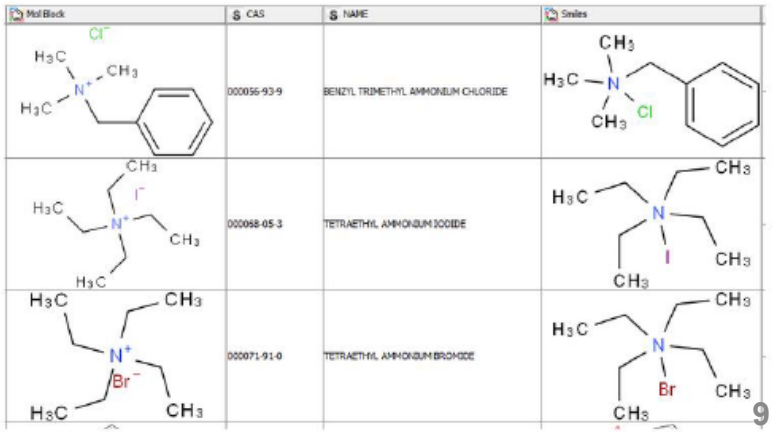
Mismatching structures



Duplicate Structures



Covalent Halogens



CONSUMER
KNIME workflows for curation

EPA United States Environmental Protection Agency

1,363
Views
32
CrossRef citations to date
15
Altmetric

Listen
Articles

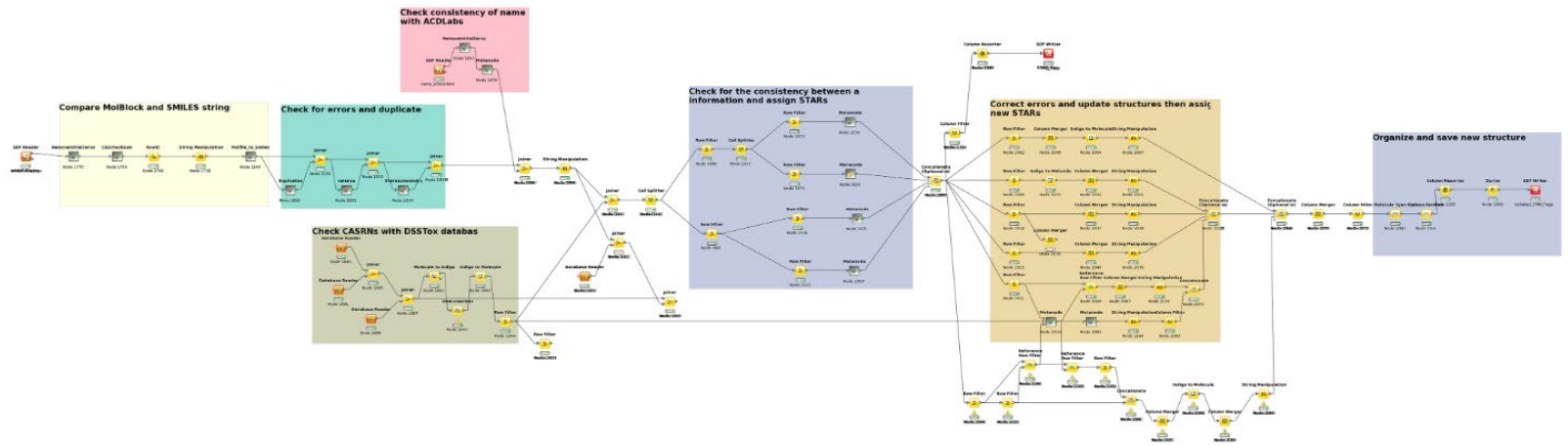
An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling[$]

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams

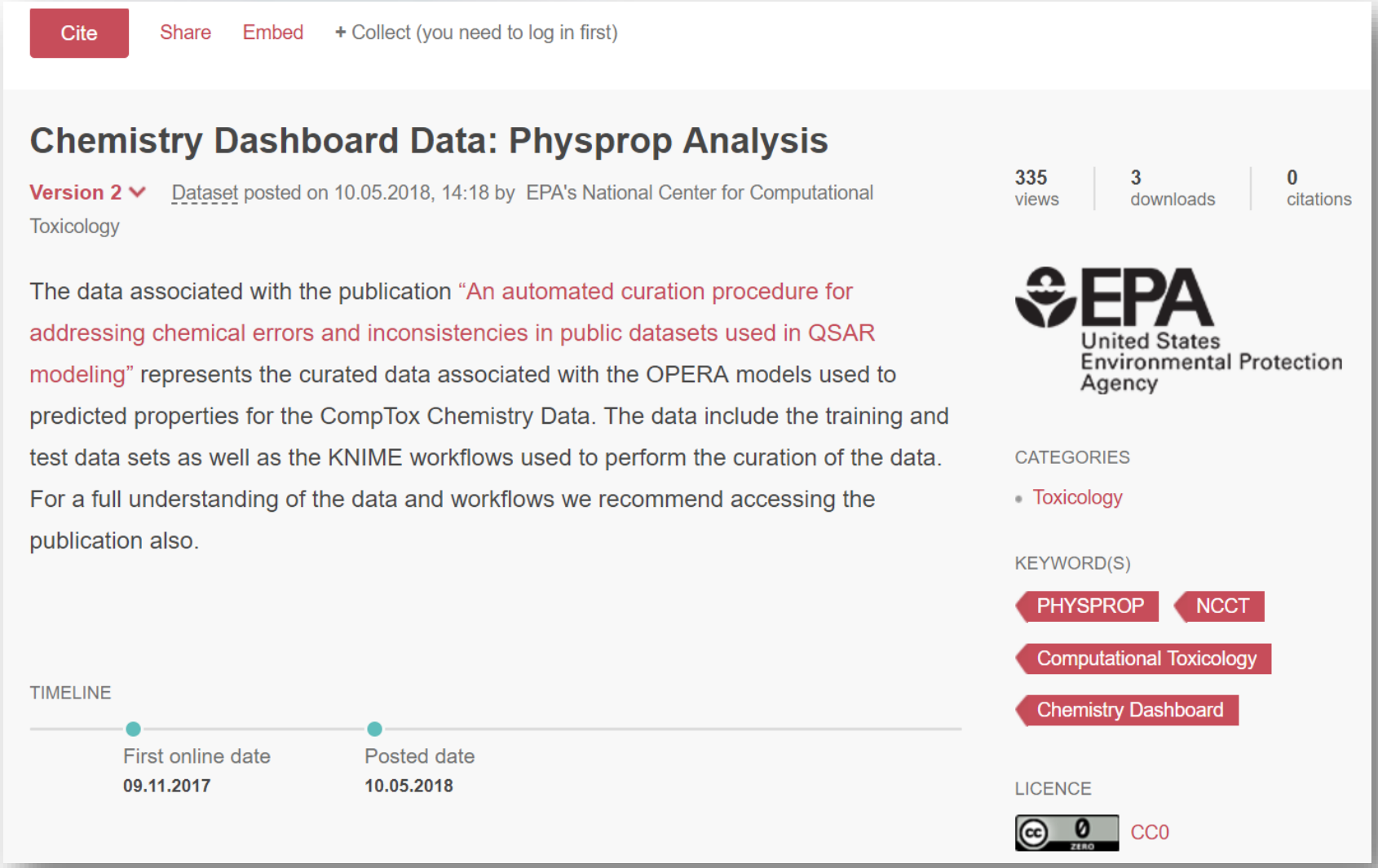
Pages 911-937 | Received 03 Sep 2016, Accepted 24 Oct 2016, Published online: 25 Nov 2016

Figure 8 of 14

Figure 8. The KNIME curation workflow developed based on the log *P* PHYSPROP dataset and generalized for application to other datasets.



PRODUCER
All curated data available



Cite Share Embed + Collect (you need to log in first)

Chemistry Dashboard Data: Physprop Analysis

Version 2 Dataset posted on 10.05.2018, 14:18 by EPA's National Center for Computational Toxicology

335 views | 3 downloads | 0 citations

The data associated with the publication "An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modeling" represents the curated data associated with the OPERA models used to predicted properties for the CompTox Chemistry Data. The data include the training and test data sets as well as the KNIME workflows used to perform the curation of the data. For a full understanding of the data and workflows we recommend accessing the publication also.

EPA United States Environmental Protection Agency

CATEGORIES
- Toxicology

KEYWORD(S)
PHYSPROP NCCT Computational Toxicology Chemistry Dashboard

TIMELINE
First online date 09.11.2017
Posted date 10.05.2018

LICENCE
CC0

PRODUCER
TEST and OPERA Predictions

EPA United States Environmental Protection Agency

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Mansouri *et al. J Cheminform (2018) 10:10*
https://doi.org/10.1186/s13321-018-0263-1

Journal of Cheminformatics

RESEARCH ARTICLE Open Access

OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri[1,2,3*], Chris M. Grulke[1], Richard S. Judson[1] and Antony J. Williams[1]

Predicted

Download Predicted Data

Source	Result	Calculation Details	QMRF
EPISUITE	9.93e-4	Not Available	Not Available
NICEATM	2.16e-4	Not Available	Available
TEST	4.41e-4	TEST Report	Not Available
OPERA	1.42e-4	OPERA Model Report [Inside AD]	Available

Transparency for prediction models

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Predicted

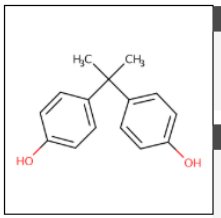
Download Predicted Data

Source	Result	Calculation Details	QMRF
EPISUITE	3.64	Not Available	Not Available
NICEATM	2.40	Not Available	Available
ACD/Labs Consensus	3.63	Not Available	Not Available
ACD/Labs	3.43	Not Available	Not Available
OPERA	3.35	OPERA Model Report [Inside AD]	Available

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182

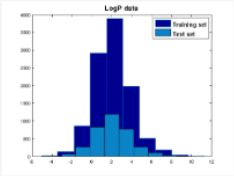


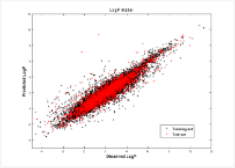
Print PDF

Model Results

Predicted value: 3.35
Global applicability domain: Inside
Local applicability domain index: 0.877
Confidence level: 0.813

Model Performance





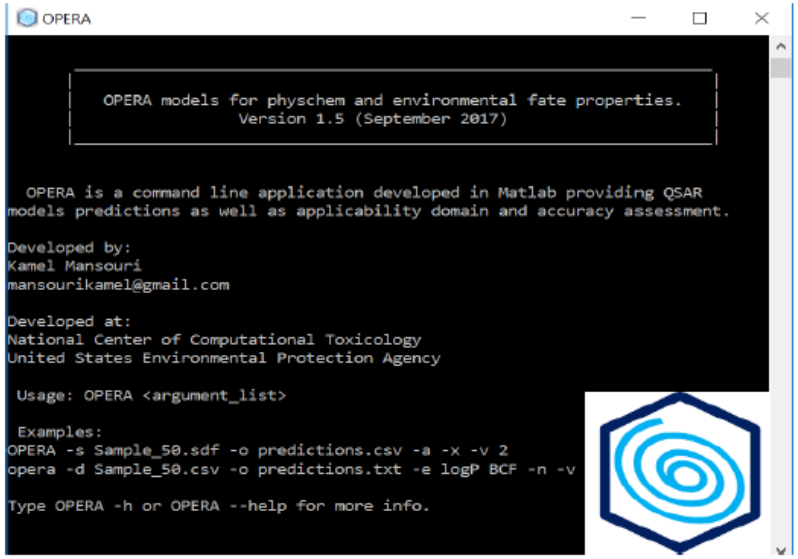
QMRF

Weighted KNN model

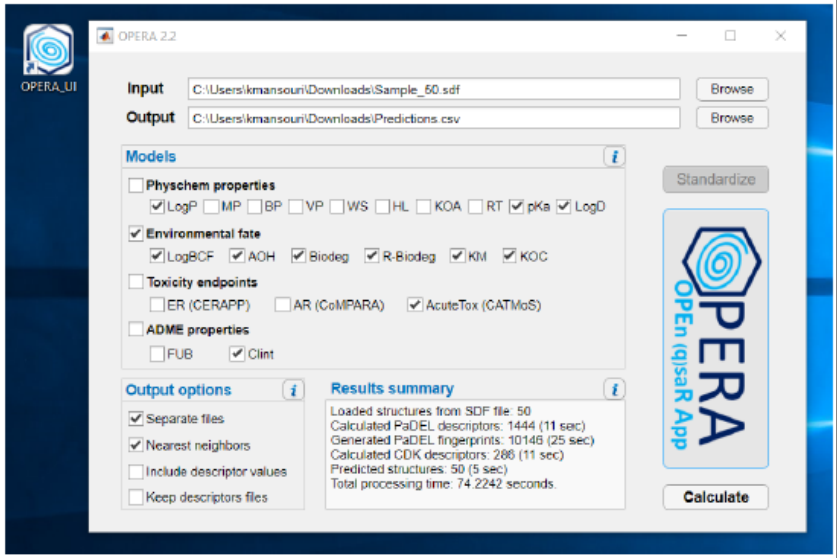
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670	0.860	0.780

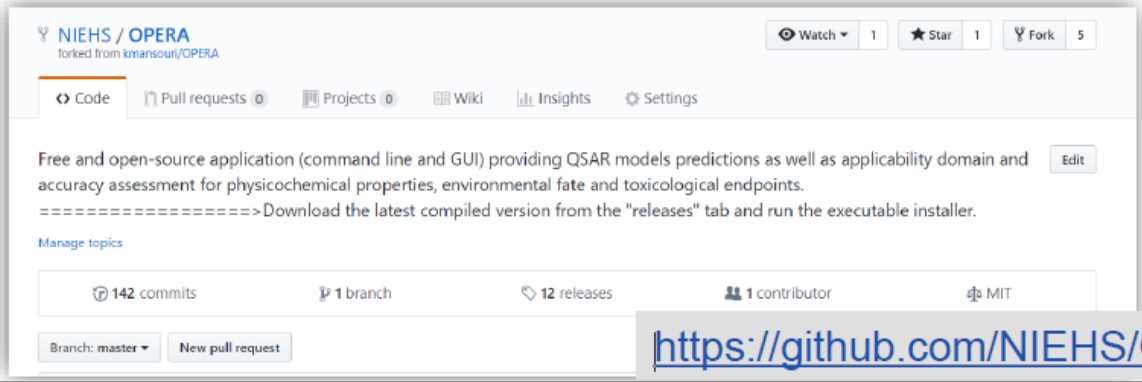
PRODUCER
OPERA Standalone Application

Command line



Graphical User Interface





https://github.com/NIEHS/OPERA

PRODUCER: Open Source
https://github.com/kmansouri/OPERA

README.md

OPERA

OPERA is a free and open-source/open-data suite of QSAR models providing predictions on physicochemical properties, environmental fate and toxcicity endpoints as well as additional information including applicability domain and accuracy assessment. All models were built on curated data and standardized QSAR-ready chemical structures. OPERA is available in command line and user-friendly graphical interface for Windows and Linux operating systems. It can be installed as a standalone desktop application or embedded in a different tool/workflow.

References:

[1] Mansouri K. et al. J Cheminform (2018) https://doi.org/10.1186/s13321-018-0263-1.

[2] Mansouri, K. et al. SAR and QSAR in Env. Res. (2016). https://doi.org/10.1080/1062936X.2016.1253611

[3] Williams A. J. et al. J Cheminform (2017) https://doi.org/10.1186/s13321-017-0247-6

[4] The CompTox Chemistry Dashboard (https://comptox.epa.gov/dashboard)

[5] JRC QSAR Model Database https://qsardb.jrc.ec.europa.eu/qmrf/endpoint

Models:

```
*  Latest version OPERA v2.2:

      + Molecular descriptors:
- PaDEL (2.21) (https://doi.org/10.1002/jcc.21707 )
- CDK (2.0) (https://doi.org/10.1186/s13321-017-0220-4)
```

PRODUCER: Other prediction models
TEST Desktop Software

EPA United States Environmental Protection Agency

Toxicity Estimation Software Tool (TEST)

On this page:

- QSAR Methodologies
- What's New in Version 4.2.1?
- Prior Version History
- System Requirements
- Installation Instructions
- Publications
- Get Email Alerts

The Toxicity Estimation Software Tool (TEST) was developed to allow users to easily estimate the toxicity of chemicals using Quantitative Structure Activity Relationships (QSARs) methodologies. QSARs are mathematical models used to predict measures of toxicity from the physical characteristics of the structure of chemicals (known as molecular descriptors). Simple QSAR models calculate the toxicity of chemicals using a simple linear function of molecular descriptors:

Ask a Technical Expert

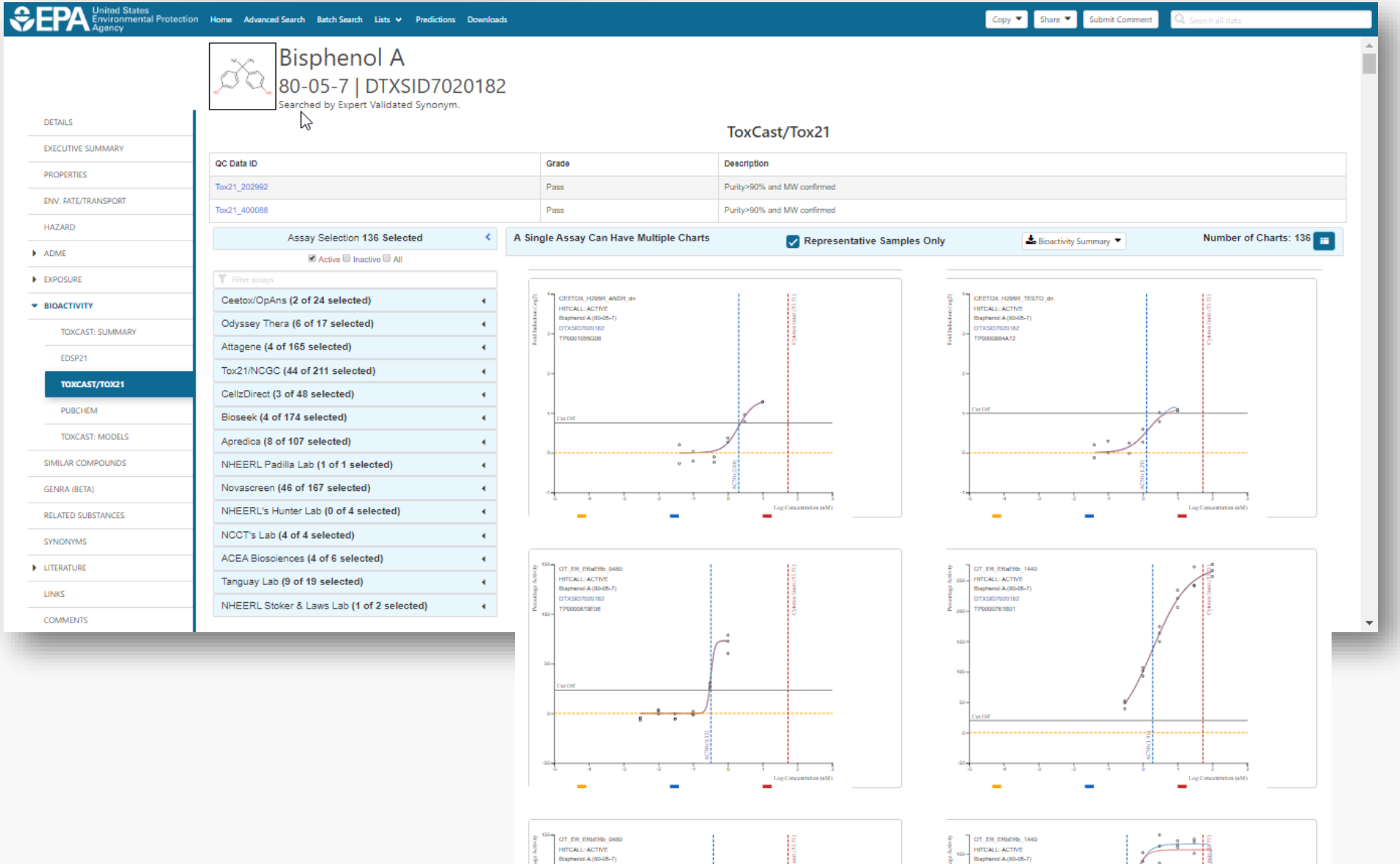
Got a question about our research model? Want to give us feedback? Contact a technical expert about TEST.

Bioactivity Data: Tox21 and Toxcast

PRODUCER

In Vitro Bioassay Screening

EPA United States Environmental Protection Agency



PRODUCER
Bioactivity: Downloadable Data

Exploring ToxCast Data: Downloadable Data

The results after processing through the Pipeline are available on the ToxCast Dashboard, and for most users EPA recommends accessing the data there.

- ToxCast Chemicals
- ToxCast Assays

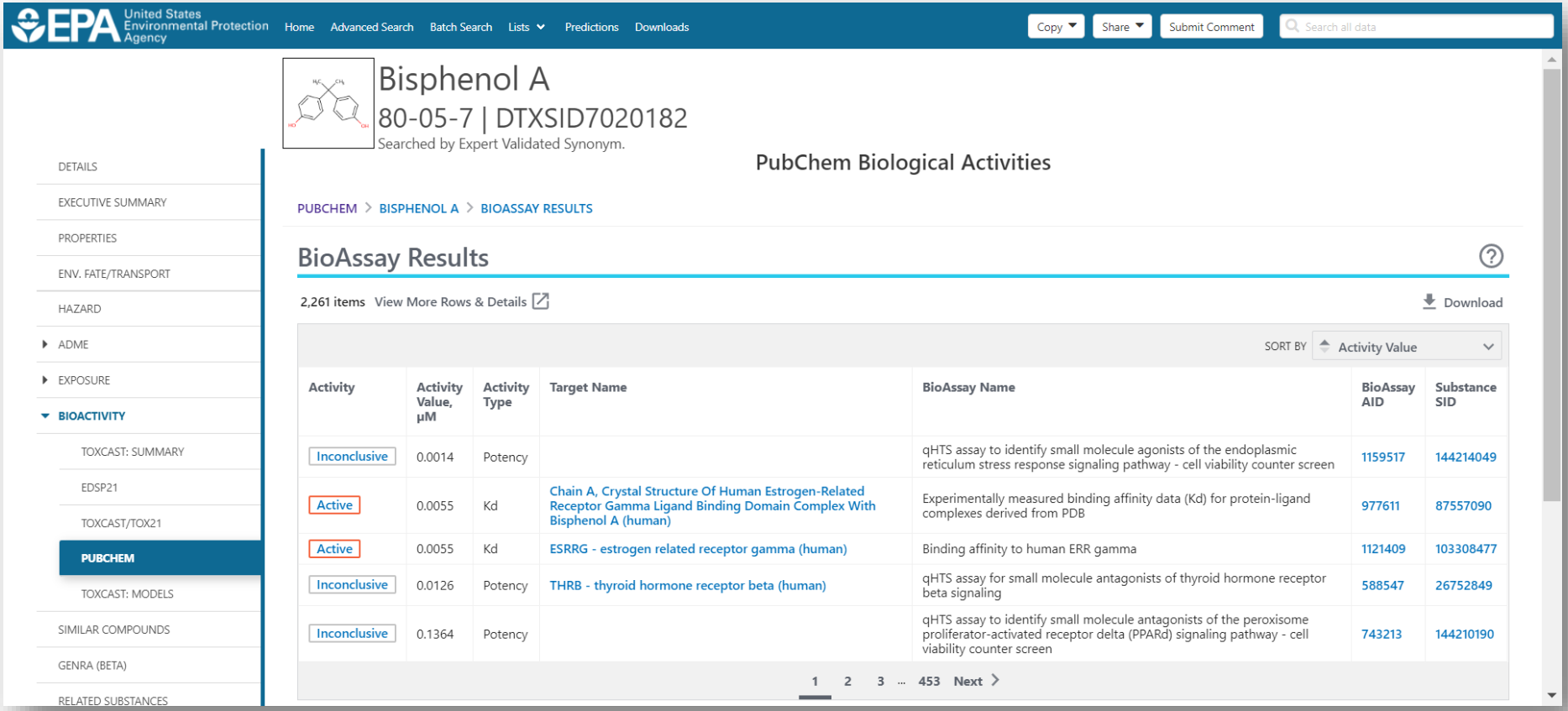
Resources

- Toxicity Forecaster (ToxCast) Fact Sheet
- ToxCast Publications
- ToxCast Citation
- About ToxCast

ToxCast Data and Information

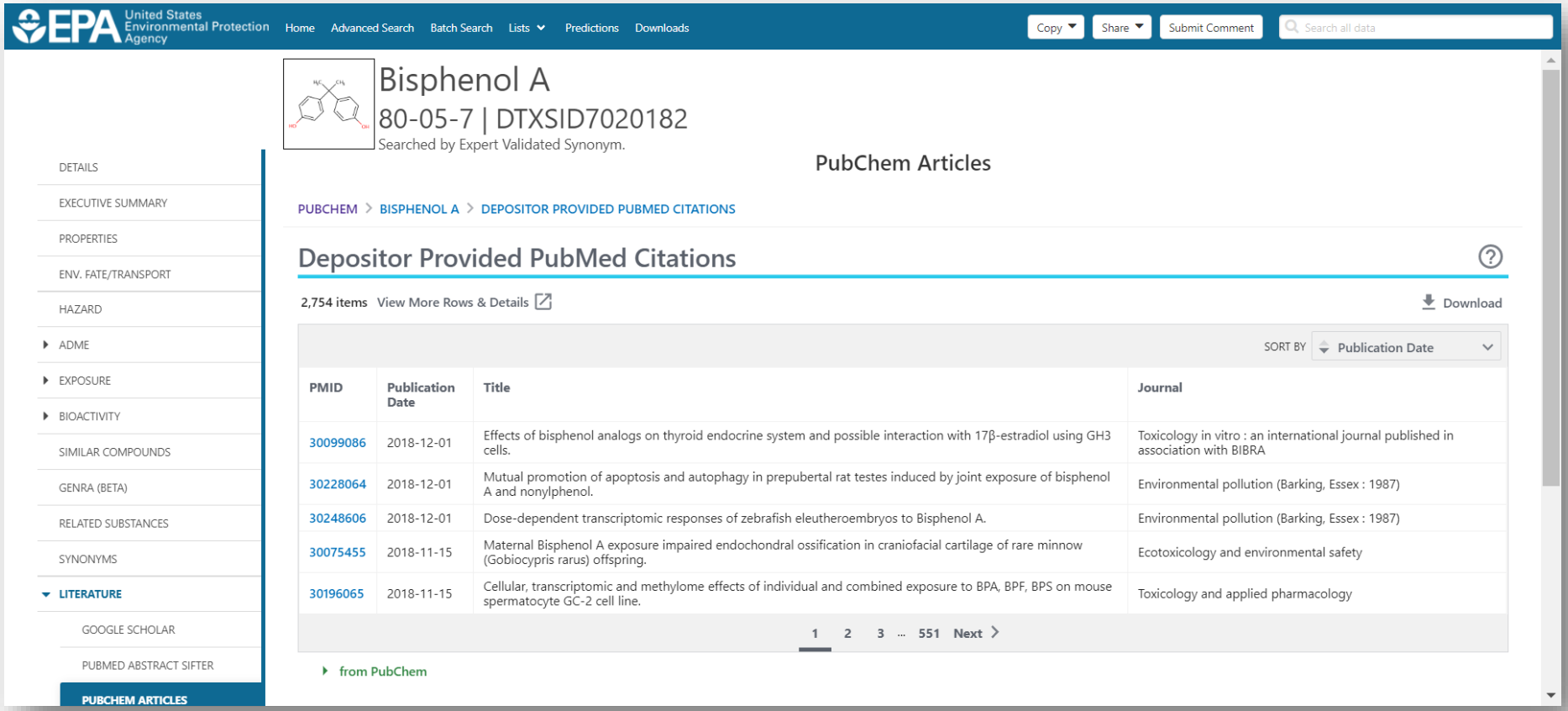
- **ToxCast & Tox21 Summary Files.** Data for a single chemical endpoint pair for thousands of chemicals and assay endpoints for 20 variables such as the activity or hit call, activity concentrations, whether the chemical was tested in a specific assay, etc.
  - Download ToxCast Summary Information
  - Download ReadMe
- **ToxCast & Tox21 Data Spreadsheet.** A spreadsheet of EPA's analysis of the chemicals screened through ToxCast and the Tox21 collaboration which includes EPA's activity calls from the screening of over 1,800 chemicals.
  - Download Data
  - Download ReadMe
- **ToxCast Data Pipeline R Package.** The R computer programming package used to process and model all EPA ToxCast and Tox21 chemical screening data. The files include the R programming package as well as documents that provide overviews of the data analysis pipeline used and the R package. Users will need experience with R to use these files.
  - Download Package
  - TCPL Overview

CONSUMER
PubChem Widgets - Bioactivities

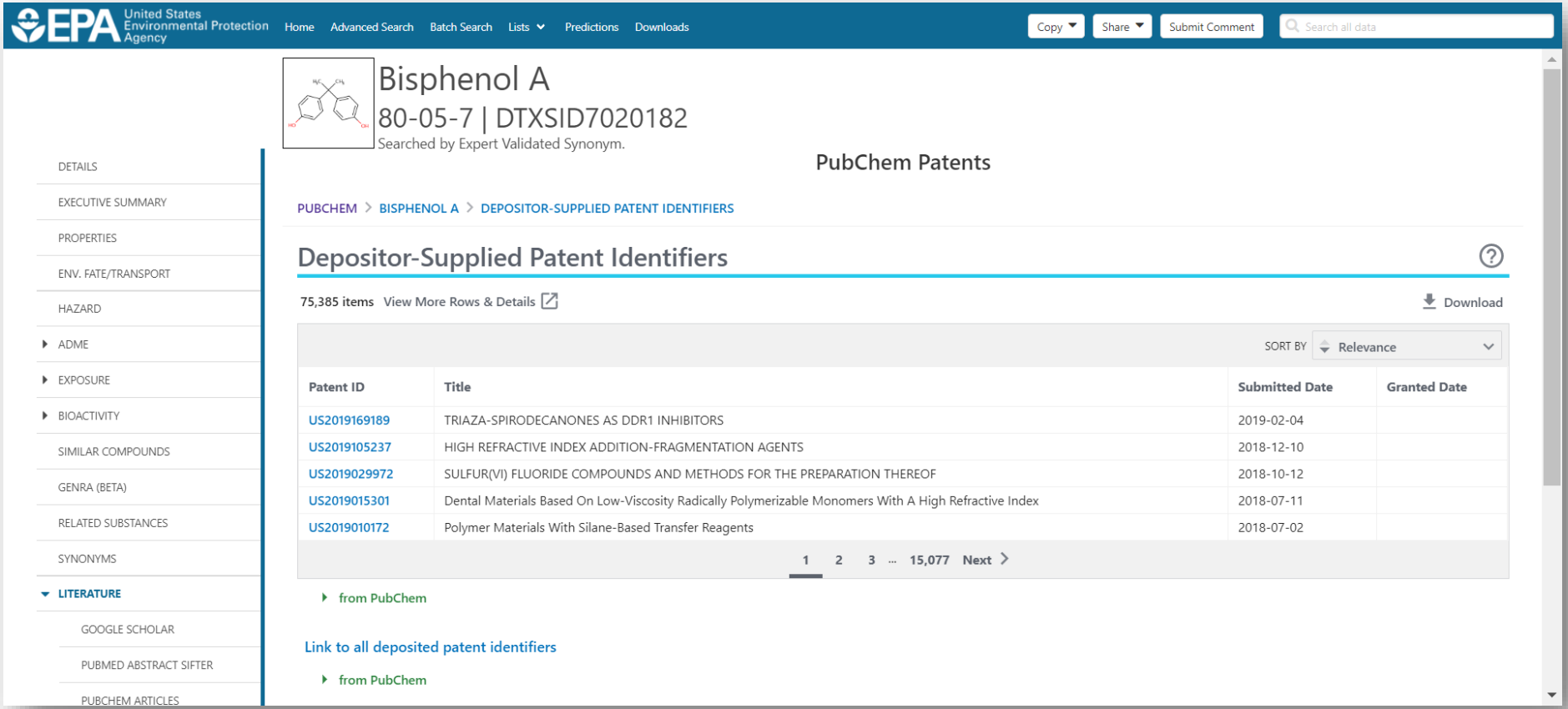


Literature Data

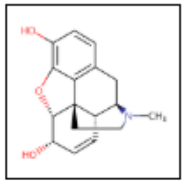
CONSUMER
PubChem Widgets - Articles



CONSUMER
PubChem Widgets – Patents



CONSUMER: Pubmed Services Literature Searching



Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

Abstract Sifter

1) Select PubMed starting point query then 2) click on Retrieve.

Select a Query Term

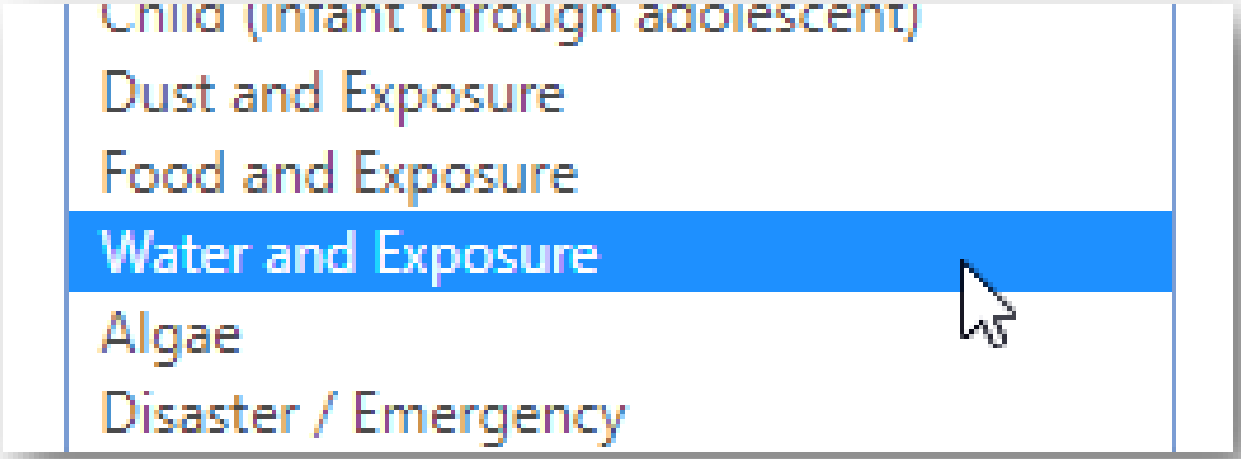
Retrieve Articles

- Select a Query Term
- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Cancer
- Clinical Trials
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure
- Food and Exposure
- Water and Exposure
- Algae
- Disaster / Emergency

Optionally, edit the query before retrieving.

"57-27-2" OR "Morphine"

CONSUMER: Pubmed Services Literature Searching



Optionally, edit the query before retrieving.

("57-27-2" OR "Morphine") AND ((water OR groundwater OR drinking water) AND Environmental Exposure)

CONSUMER: Pubmed Services Literature Searching

EPA United States Environmental Protection Agency

37 of 37 articles loaded...

To find articles quickly, enter terms to sift abstracts.

wastewater | Spectrometry | EPA | Clear Terms

Download / Send to... | Download Sifter for Excel

wastewater	Spectrometry	EPA	Total	PMID	Year	Title	Authors	Journal	Rev
4	2	0	6	29274731	2017	Simultaneous analysis of opioid analgesics and thei...	Krizman-Matasic; Kostanjevecki; Ahel; Terzic	Journal of chromatography. A	
0	1	0	1	25768972	2015	Evaluating external contamination of polybrominate...	Poon; Aleksa; Carnevale; Kapur; Goodyer; Koren	Therapeutic drug monitoring	
0	1	0	1	22544551	2012	Spatial distribution of illicit drugs in surface waters o...	Vazquez-Roig; Andreu; Blasco; Morillas; Picó	Environmental science and pollution research inter...	
1	1	0	2	20801487	2010	Analysis of llicit and illicit drugs in waste, surface an...	Berset; Brenneisen; Mathieu	Chemosphere	
1	1	0	2	17935751	2007	Illicit drugs, a novel group of environmental contami...	Zuccato; Castiglioni; Bagnati; Chiabrando; Grassi; ...	Water research	
2	1	1	4	17607391	2007	Using environmental analytical data to estimate lev...	Bones; Thomas; Paull	Journal of environmental monitoring : JEM	
3	1	2	6	17180984	2006	Simultaneous determination of psychoactive drugs ...	Hummel; Löffler; Fink; Ternes	Environmental science & technology	
6	0	0	6	30583189	2018	Assessment of drugs of abuse in a wastewater trea...	Kumar; Tscharke; O'Brien; Mueller; Wilkins; Padhye	The Science of the total environment	
0	0	3	3	30488421	2018	Effect of enriched environment during adolescence ...	Mohammadian; Najafi; Miladi-Gorji	Developmental psychobiology	
3	0	0	3	29574368	2018	Estimation of the consumption of illicit drugs during ...	Foppe; Hammond-Weinberger; Subedi	The Science of the total environment	
1	0	0	1	28787791	2017	Evaluation of in-sewer transformation of selected illi...	Gao; Banks; Li; Jiang; Lai; Mueller; Thai	The Science of the total environment	
9	0	0	9	28472697	2017	Occurrence and fate of illicit drugs and pharmaceuti...	Causanilles; Ruepert; Ibáñez; Emke; Hernández; d...	The Science of the total environment	
0	0	0	0	28010888	2016	Dose-dependent effects of morphine on lipopolysac...	Mottaz; Schönenberger; Fischer; Eggen; Schirmer; ...	Environmental pollution (Barking, Essex : 1987)	
0	0	0	0	27746311	2016	Effects of voluntary exercise on the viability, prolifer...	Haydari; Safari; Zarbakhsh; Bandegi; Miladi-Gorji	Neuroscience letters	
0	0	0	0	27261879	2016	Genotoxic effects induced by the exposure to an en...	Parolini; Magni; Castiglioni; Binelli	Ecotoxicology and environmental safety	
3	0	0	3	27179320	2016	Temporal trends in drug use in Adelaide, South Aus...	Tscharke; Chen; Gerber; White	The Science of the total environment	

PRODUCER
Abstract Sifter for Excel

Real-Time Predictions

CONSUMER
epam Ketcher

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<epam> | LIFE SCIENCES OPEN SOURCE PRODUCTS RESOURCES DOWNLOADS CONTACT INFO

Home / Ketcher

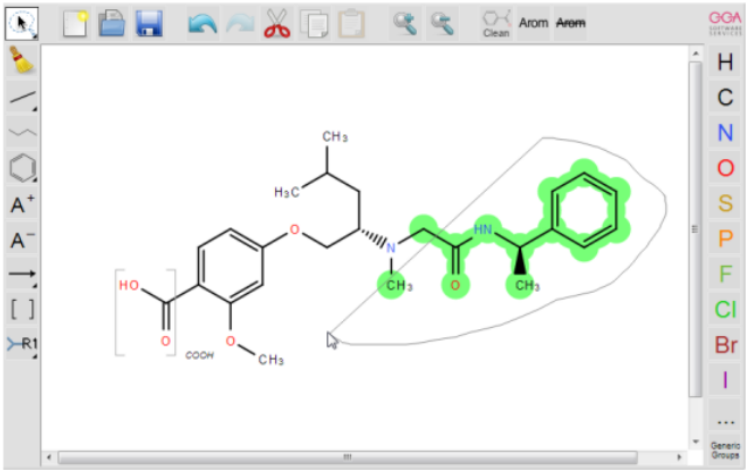
Search

- Overview
- Features
- Supported browsers
- Third-party code
- Ketcher 2.0
- Download
- License
- Feedback
- Commercial Availability

Ketcher

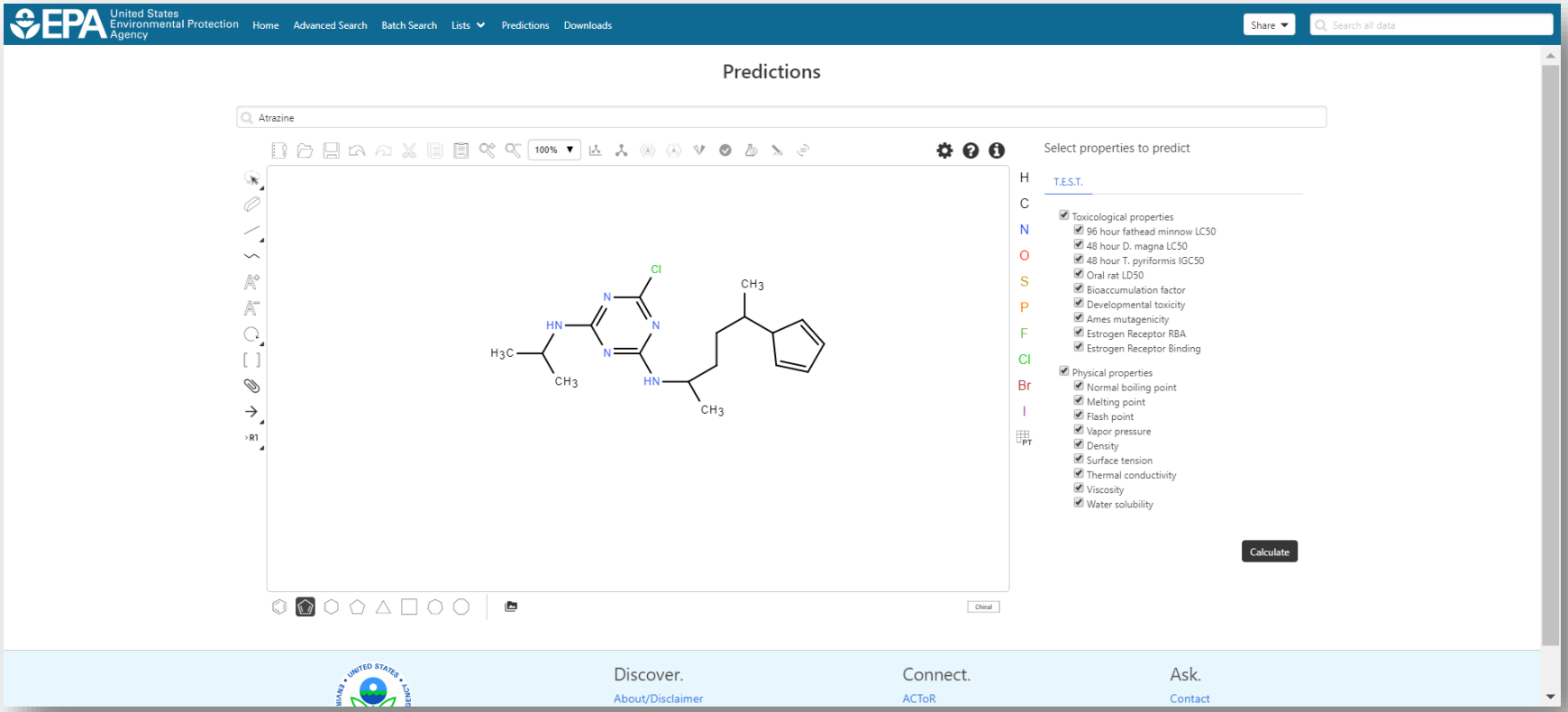
Overview

Ketcher is a web-based chemical structure editor.

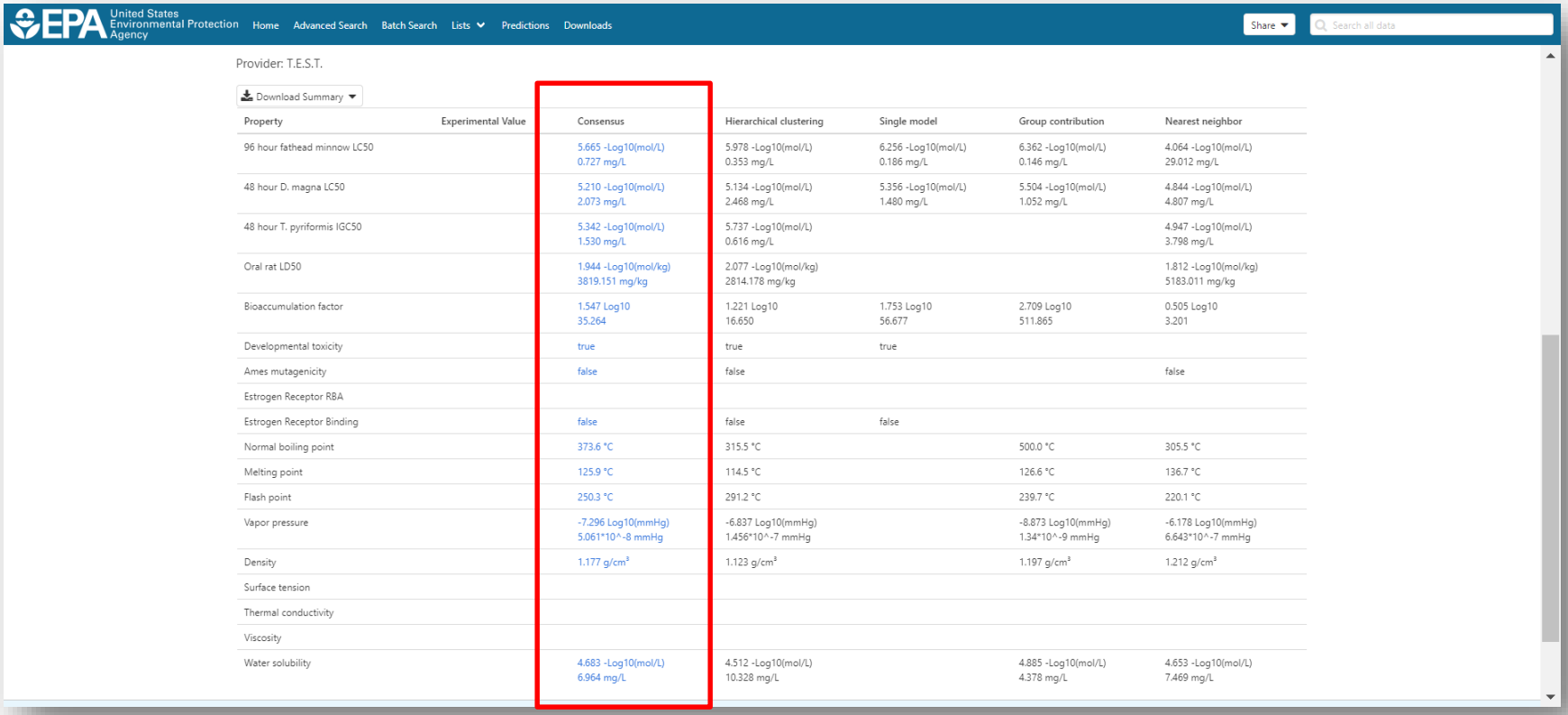


Since Ketcher is written in pure Javascript, it incorporates high performance, good portability and light weight. You will not need any Java or Flash plugins to use it in your browser. Ketcher is completely free and open-source, while also available on a commercial basis.

CONSUMER: Ketcher Drawing TEST Real Time Predictions



Ketcher Drawing
TEST Real Time Predictions



Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		5.665 -Log10(mol/L) 0.727 mg/L	5.978 -Log10(mol/L) 0.353 mg/L	6.256 -Log10(mol/L) 0.186 mg/L	6.362 -Log10(mol/L) 0.146 mg/L	4.064 -Log10(mol/L) 29.012 mg/L
48 hour D. magna LC50		5.210 -Log10(mol/L) 2.073 mg/L	5.134 -Log10(mol/L) 2.468 mg/L	5.356 -Log10(mol/L) 1.480 mg/L	5.504 -Log10(mol/L) 1.052 mg/L	4.844 -Log10(mol/L) 4.807 mg/L
48 hour T. pyriformis IGC50		5.342 -Log10(mol/L) 1.530 mg/L	5.737 -Log10(mol/L) 0.616 mg/L			4.947 -Log10(mol/L) 3.798 mg/L
Oral rat LD50		1.944 -Log10(mol/kg) 3819.151 mg/kg	2.077 -Log10(mol/kg) 2814.178 mg/kg			1.812 -Log10(mol/kg) 5183.011 mg/kg
Bioaccumulation factor		1.547 Log10 35.264	1.221 Log10 16.650	1.753 Log10 56.677	2.709 Log10 511.865	0.505 Log10 3.201
Developmental toxicity		true	true	true		
Ames mutagenicity		false	false			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false		
Normal boiling point		373.6 °C	315.5 °C		500.0 °C	305.5 °C
Melting point		125.9 °C	114.5 °C		126.6 °C	136.7 °C
Flash point		250.3 °C	291.2 °C		239.7 °C	220.1 °C
Vapor pressure		-7.296 Log10(mmHg) 5.061*10^-8 mmHg	-6.837 Log10(mmHg) 1.456*10^-7 mmHg		-8.873 Log10(mmHg) 1.34*10^-9 mmHg	-6.178 Log10(mmHg) 6.643*10^-7 mmHg
Density		1.177 g/cm³	1.123 g/cm³		1.197 g/cm³	1.212 g/cm³
Surface tension						
Thermal conductivity						
Viscosity						
Water solubility		4.683 -Log10(mol/L) 6.964 mg/L	4.512 -Log10(mol/L) 10.328 mg/L		4.885 -Log10(mol/L) 4.378 mg/L	4.653 -Log10(mol/L) 7.469 mg/L

TEST detailed calculation reports

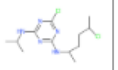
Predicted Vapor pressure at 25°C for ClC=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Vapor pressure at 25°C Log10(mmHg)	N/A	-6.85
Vapor pressure at 25°C mmHg	N/A	1.42E-07

Individual Predictions

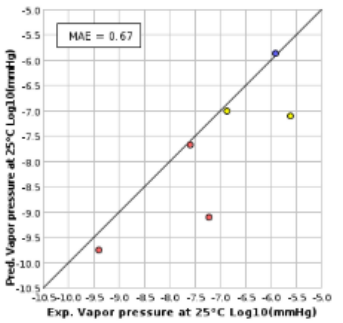
Method	Predicted value Log10(mmHg)
Hierarchical clustering	-6.47
Group contribution	-7.62
Nearest neighbor	-6.46



Predictions for the test chemical and for the most similar chemicals in the external tes

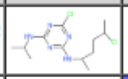
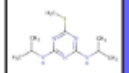
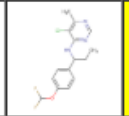
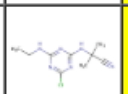
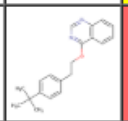
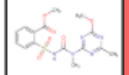
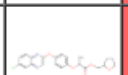
If the predicted value matches the experimental values for similar chemicals in the test set (and the similar che

Prediction results (colors defined in table below)



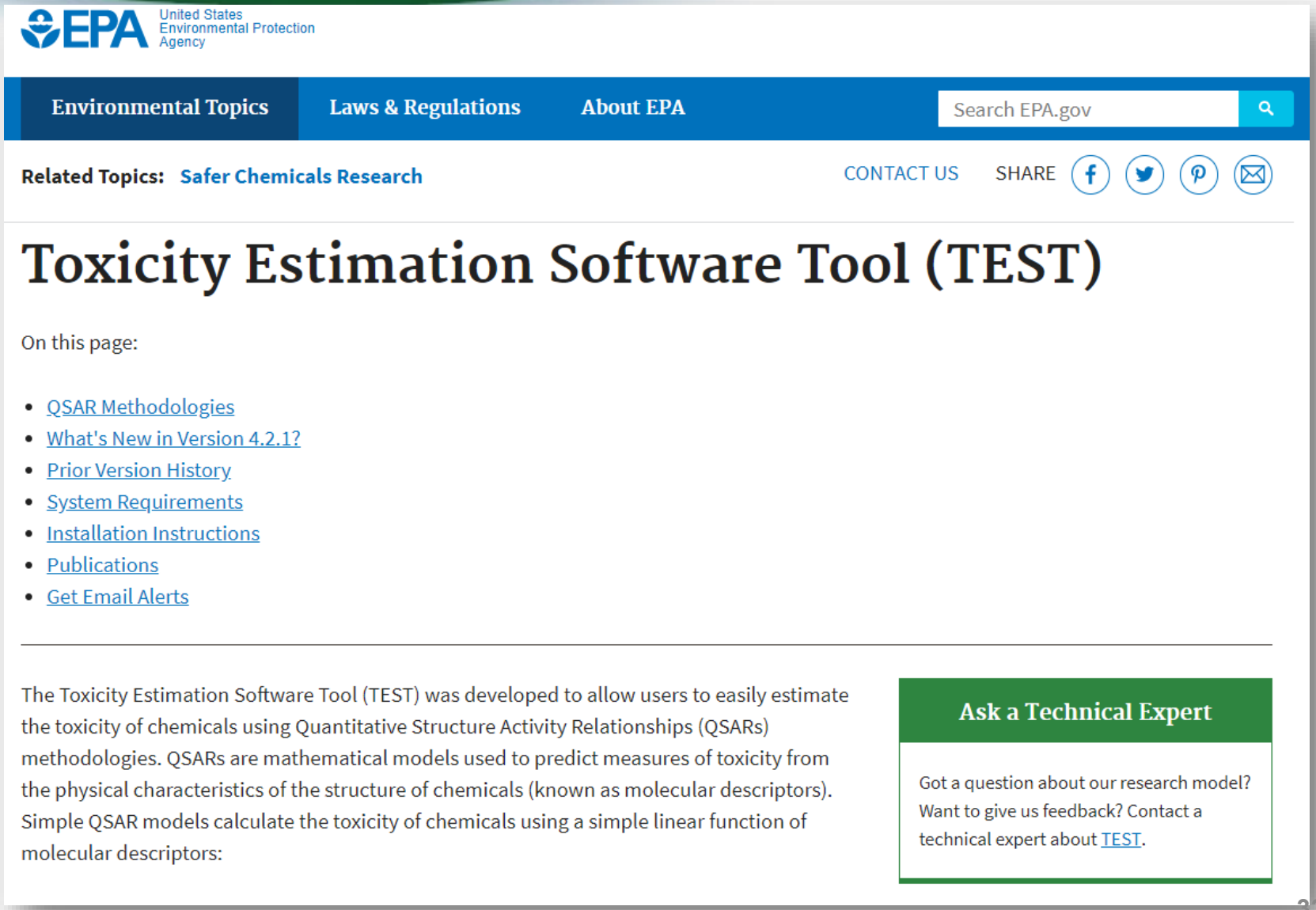
Chemicals	MAE*
Entire set	0.47
Similarity coefficient ≥ 0.5	0.67

*Mean absolute error in Log10(mmHg)

CAS	Structure	Similarity Coefficient	Experimental value Log10(mmHg)	Predicted value Log10(mmHg)
ClC=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C (test chemical)			N/A	-6.85
7287-19-6		0.83	-5.91	-5.86
130339-07-0		0.77	-5.62	-7.11
21725-46-2		0.76	-6.86	-7.01
120928-09-8		0.58	-7.59	-7.67
101200-48-0		0.56	-9.41	-9.76
119738-06-6		0.55	-7.23	-9.11

PRODUCER: TEST Software

https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test



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Related Topics: Safer Chemicals Research

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Toxicity Estimation Software Tool (TEST)

On this page:

- QSAR Methodologies
- What's New in Version 4.2.1?
- Prior Version History
- System Requirements
- Installation Instructions
- Publications
- Get Email Alerts

The Toxicity Estimation Software Tool (TEST) was developed to allow users to easily estimate the toxicity of chemicals using Quantitative Structure Activity Relationships (QSARs) methodologies. QSARs are mathematical models used to predict measures of toxicity from the physical characteristics of the structure of chemicals (known as molecular descriptors). Simple QSAR models calculate the toxicity of chemicals using a simple linear function of molecular descriptors:

Ask a Technical Expert

Got a question about our research model? Want to give us feedback? Contact a technical expert about TEST.

PRODUCER: TEST Web Services

https://www.epa.gov/sites/production/files/2018-08/documents/webtest_users_guide.pdf

EPA United States Environmental Protection Agency

https://comptox.epa.gov/dashboard/web-test/

User's Guide for WebTEST (version 1.0) (Web-services Toxicity Estimation Software Tool)

A Web-Ser
from Mole

5. USING THE WEB SERVICE 43
5.1. Downloading the Web-TEST project 43
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5.9. Docker 50

PRODUCER Web Services

PRODUCER: Web Services https://actorws.epa.gov/actorws/

- Dozens of web services to provide access to data
- Data in UI, JSON and XML format

https://actorws.epa.gov/actorws/dsstox/v02/msready?identifier=80-05-7
https://actorws.epa.gov/actorws/dsstox/v02/msready.json?identifier=80-05-7
https://actorws.epa.gov/actorws/dsstox/v02/msready.xml?identifier=80-05-7

https://actorws.epa.gov/actorws/dsstox/v02/msready?identifier=DTXCID60513
https://actorws.epa.gov/actorws/dsstox/v02/msready.json?identifier=DTXCID60513
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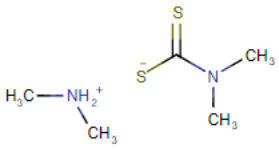
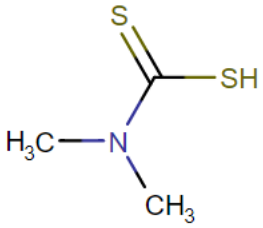
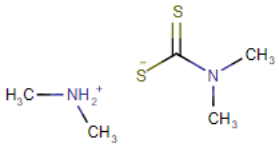
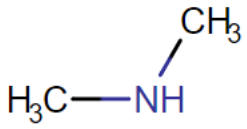
https://actorws.epa.gov/actorws/dsstox/v02/msready.xml?identifier=UVOFGKIRTCCNKG-UHFFFAOYSA-N

PRODUCER
InChIKey to DTXCIDs

EPA United States Environmental Protection Agency

https://actorws.epa.gov/actorws/dsstox/v02/msready?identifier=UVOFGKIRTCCNKG-UHFFFAOYSA-N

Image	DTXCID	Smiles	Image	MsReady DTXCID	MsReady SMILES
	DTXCID60513	C[NH2+]C.CN(C)C([S-])=S		DTXCID0023797	CN(C)C(S)=S
	DTXCID60513	C[NH2+]C.CN(C)C([S-])=S		DTXCID704057	CNC

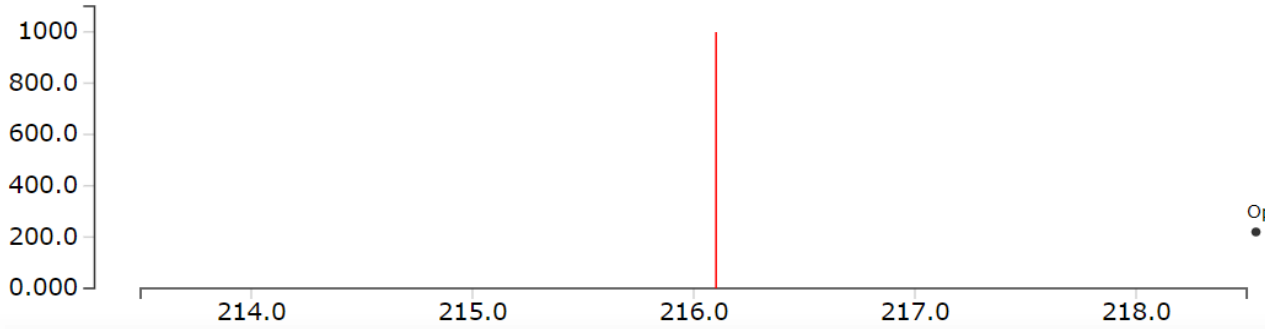
CONSUMER of our services
MassBank mapping to Dashboard

MassBank Record: EA028808

Home | Search | Record Index | Data Privacy | Imprint | MassBank ID: Go

Atrazine; LC-ESI-ITFT; MS2; CE: 15%; R=15000; [M+H]+

Mass Spectrum



Options
● Labels

Chemical Structure

CH$NAME: Atrazine
CH$NAME: 6-chloro-N-ethyl-N'-isopropyl-1,3,5-triazine-2,4-diamine
CH$NAME: 6-chloranyl-N4-ethyl-N2-propan-2-yl-1,3,5-triazine-2,4-diamine
CH$COMPOUND_CLASS: N/A; Environmental Standard
CH$FORMULA: C8H14ClN5
CH$EXACT_MASS: 215.0932
CH$SMILES: c1(nc(nc(n1)Cl)NCC)NC(C)C
CH$IUPAC: InChI=1S/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12,13,14)
CH$LINK: CAS 1912-24-9
CH$LINK: CHEBI 15930
CH$LINK: KEGG C06551
CH$LINK: PUBCHEM CID:2256
CH$LINK: INCHIKEY MXWJVTOOROXGIU-UHFFFAOYSA-N
CH$LINK: CHEMSPIDER 2169
CH$LINK: COMPTOX DTXSID9020112

Open Data Sharing

CONSUMER
NORMAN Suspect List Exchange

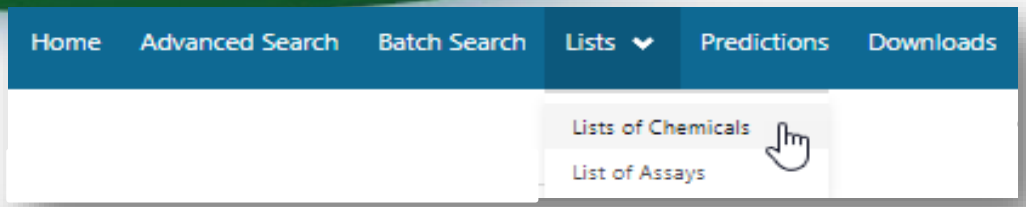
EPA United States Environmental Protection Agency

NORMAN

Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

Wastewater Suspect List based on Swedish Product Data	Wastewater Suspect List **Original File with Mapped DTXSIDs** (12/02/2019)	KEMIWWSUS **InChIKeys** (12/02/2019)	A prioritized list of 1,123 substances relevant for wastewater based on Swedish product registry data, including scores. Provided by Stellan Fischer, KEMI.
Algal toxins list from CompTox	ALGALTOX **XLSX**, **CSV** (14/02/2019) CompTox **ALGALTOX List**	ALGALTOX **InChIKeys** (14/02/2019)	List of algal toxins (generated during blooms) from the CompTox Chemicals Dashboard.
CCL 4 Chemical Candidate List	CCL4 **XLSX**, **CSV** (14/02/2019) CompTox **CCL4 List**	CCL4 **InChIKeys** (14/02/2019)	Contaminants that are not (yet) regulated in the USA but are known or anticipated to occur in public water systems; from CompTox.
Hydrogen Deuterium Exchange (HDX) Standard Set	HDXNOEX **XLSX**, **CSV** (14/02/2019) CompTox **HDXNOEX List** CompTox **HDXEXCH List**	HDXNOEX **InChIKeys** (14/02/2019)	Environmental standard set used to investigate hydrogen deuterium exchange in small molecule HRMS (Ruttkies et al. submitted). **HDXEXCH** list also contains observed deuterated species.
Neurotoxicants Collection from Public Resources	NEUROTOXINS **XLSX**, **CSV** (14/02/2019) CompTox **NEUROTOXINS List**	NEUROTOXINS **InChIKeys** (14/02/2019)	A list of neurotoxicants compiled from public resources, details on CompTox and Schymanski *et al.* (submitted).
Statins Collection from Public Resources	STATINS **XLSX**, **CSV** (14/02/2019) CompTox **STATINS List**	STATINS **InChIKeys** (14/02/2019)	A list of statins (lipid-lowering medications) compiled from public resources, details on CompTox.
Synthetic Cannabinoids and Psychoactive Compounds	SYNTHCANNAB **XLSX**, **CSV** (14/02/2019) CompTox **SYNTHCANNAB List**	SYNTHCANNAB **InChIKeys** (14/02/2019)	A list of synthetic cannabinoids and psychoactive compounds assembled from public resources, from CompTox.

PRODUCER
Curated Chemical Lists

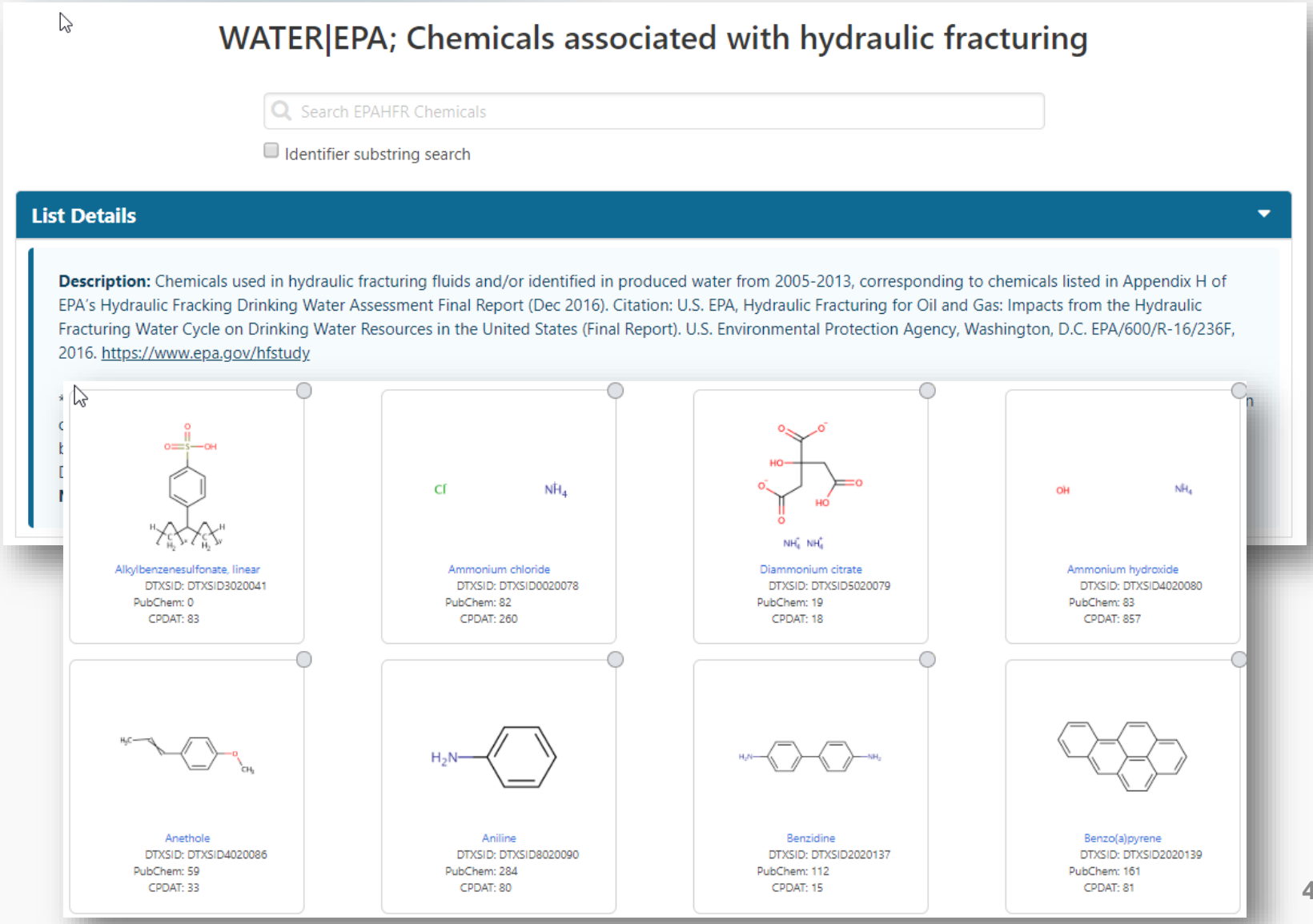


Select List

Download | Columns | PFAS | Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS|EPA: List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFAS75S2	PFAS|EPA: List of 75 Test Samples (Set 2)	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS|EPA Structure-based Categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS|EPA: Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS|EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	PFAS|EPA: Cross-Agency Research List	2017-11-16	199	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.
PFASOECD	PFAS: Listed in OECD Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASTRIER	PFAS Community-Compiled List (Trier et al., 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

PRODUCER
EPAHFR: Hydraulic Fracturing



PRODUCER
Publishing Open Data: CPDat

SCIENTIFIC DATA

Data Descriptor | OPEN ACCESS | Published: 10 July 2018

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products

Kathie L. Dionisio, Katherine Phillips, Paul S. Price, Christopher M. Grulke, Antony Williams, Derya Biryol, Tao Hong & Kristin K. Isaacs

Scientific Data **5**, Article number: 180125 (2018) | Download Citation

Data Citations

1. Williams, A. *Figshare*
http://dx.doi.org/10.23645/epacomptox.5352997 (2017)

…and then reused in PubChem

PubChem Atrazine (Compound)

10.4 Uses

EPA CPDat Chemical and Product Categories

20 items View More

Download

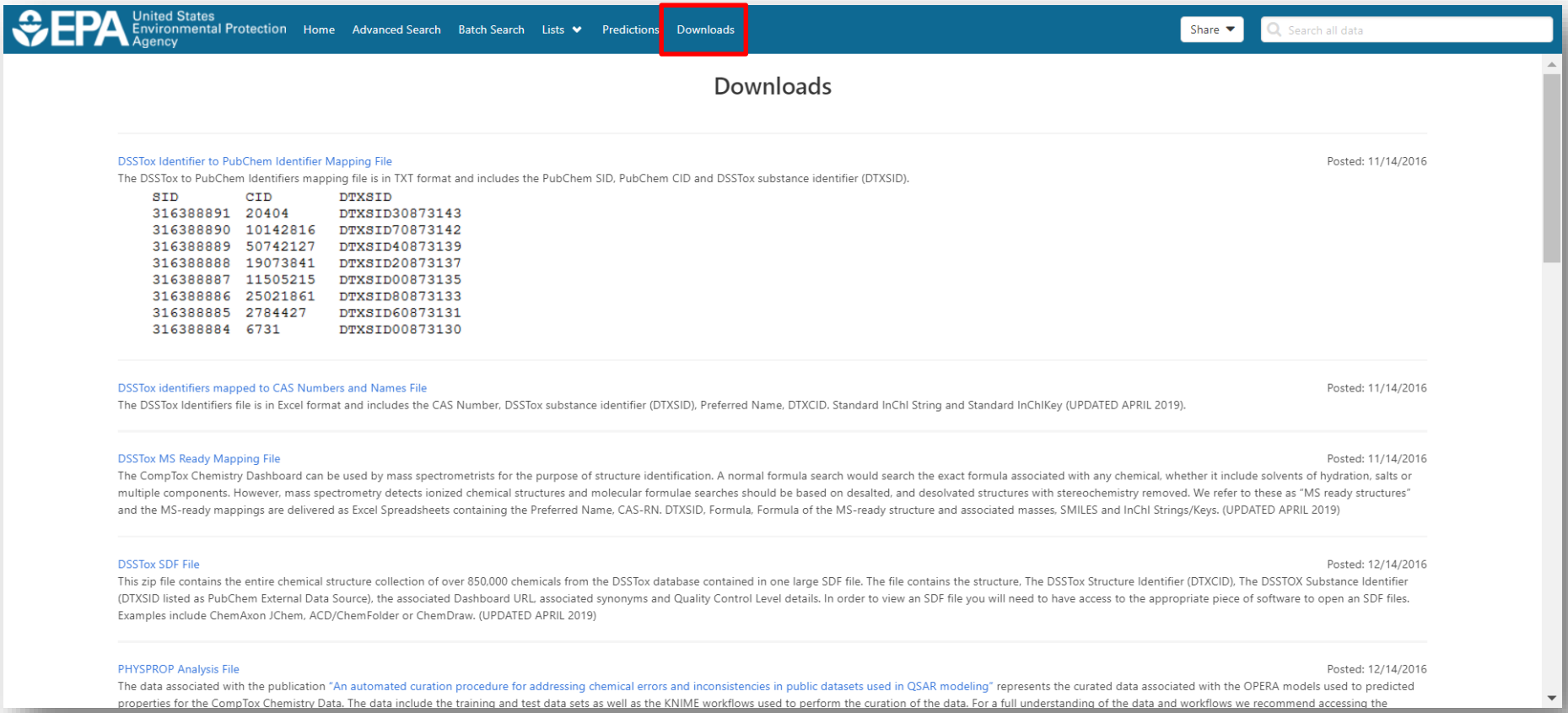
SORT BY Category

Category	Category Description	Categorization Type
Agrochemical, crop	Products used on crops, or related to the growing of crops	CPCat Cassette
Agrochemical, crop, flowers	Related to the growing of flowers as crops	CPCat Cassette
Agrochemical, crop, fruit	Related to fruit crops, or the processing or preserving of fruit	CPCat Cassette
Agrochemical, crop, wheat	Wheat crops	CPCat Cassette
Drinking_water_contaminant, pesticide, detected	Chemicals detected in substances or products (note that these chemicals may be absent from an 'ingredient list' for the product and thus unexpected, but have been detected in product testing studies)	CPCat Cassette

1 2 3 4 Next

from EPA Chemical and Products Database (CPDat)

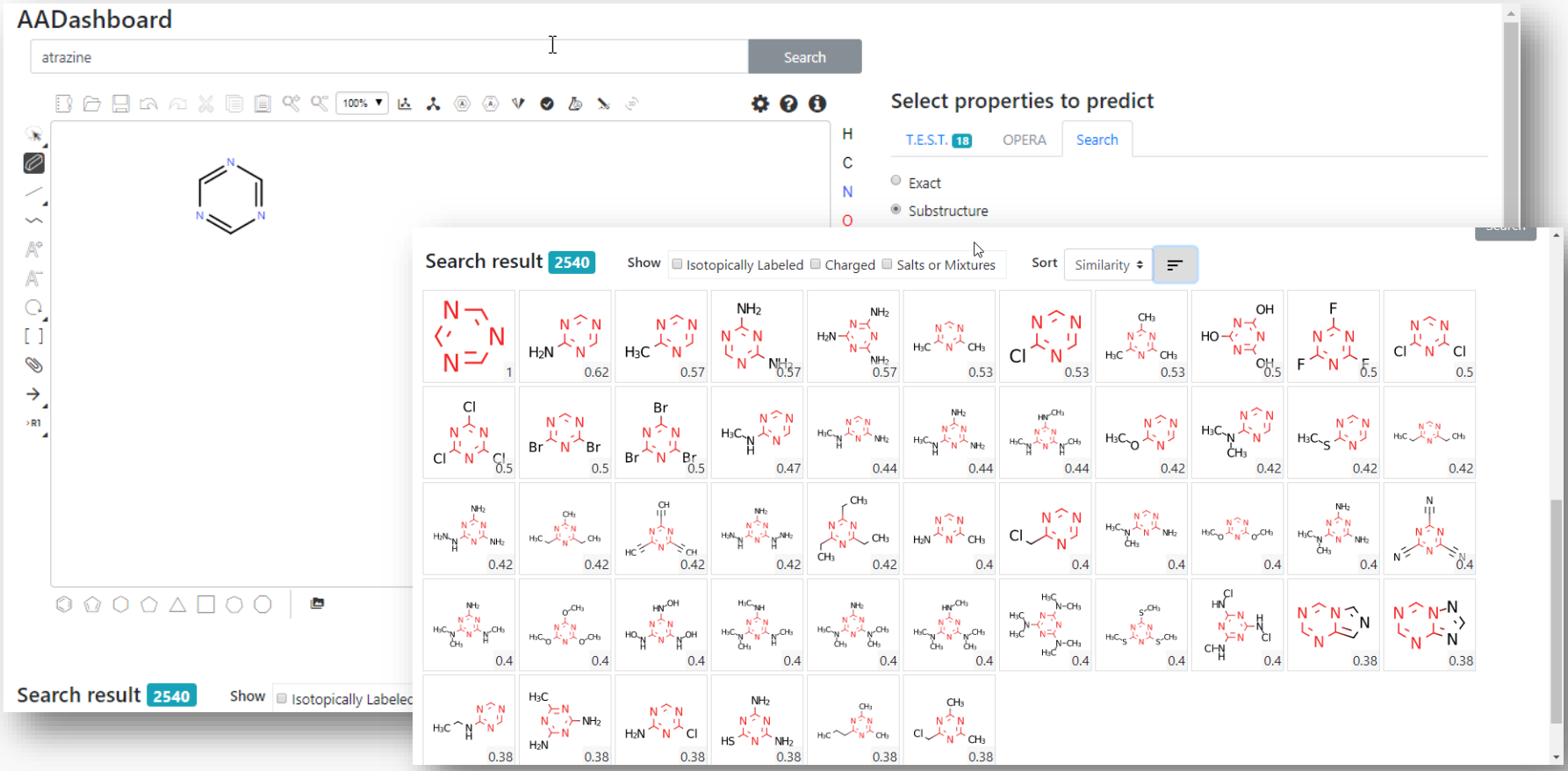
PRODUCER
Downloadable Data



Work in Progress

- Multiple projects in progress that use Open Source software
  - Structure, substructure and similarity searching
  - MS-Ready and QSAR-Ready data preparation
  - WebTEST “Batch” predictions
  - OPERA model predictions
  - Prediction of MS fragmentation patterns and matching to searched experimental spectra
- New services and Full API will be openly available (in future releases)

CONSUMER: Prototype Development
epam Ketcher + Bingo NoSQL



CONSUMER
Epam Bingo NoSQL

EPA United States Environmental Protection Agency

<epam> | LIFE SCIENCES OPEN SOURCE PRODUCTS RESOURCES DOWNLOADS CONTACT INFO Search

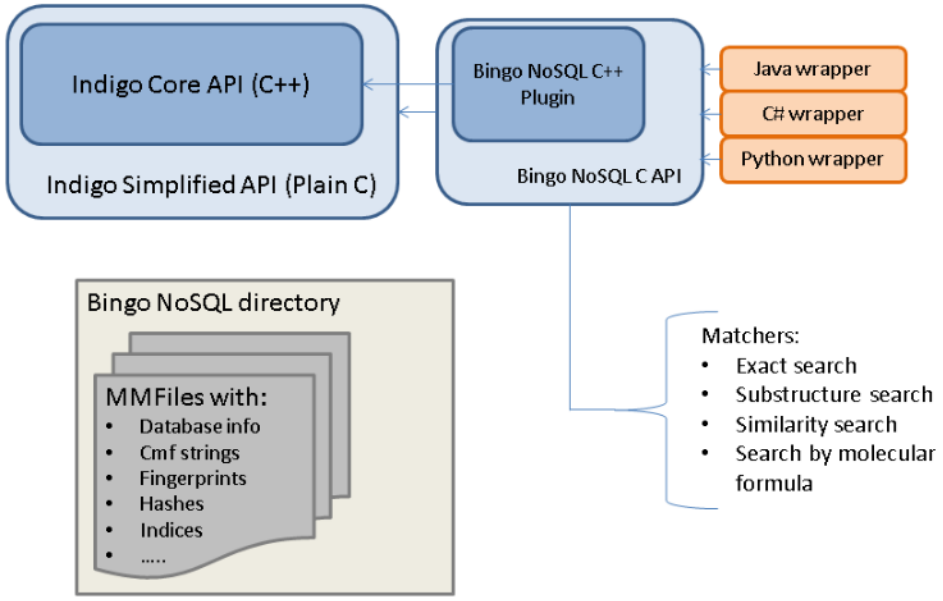
- Overview
- Manuals

Bingo NoSQL

Overview

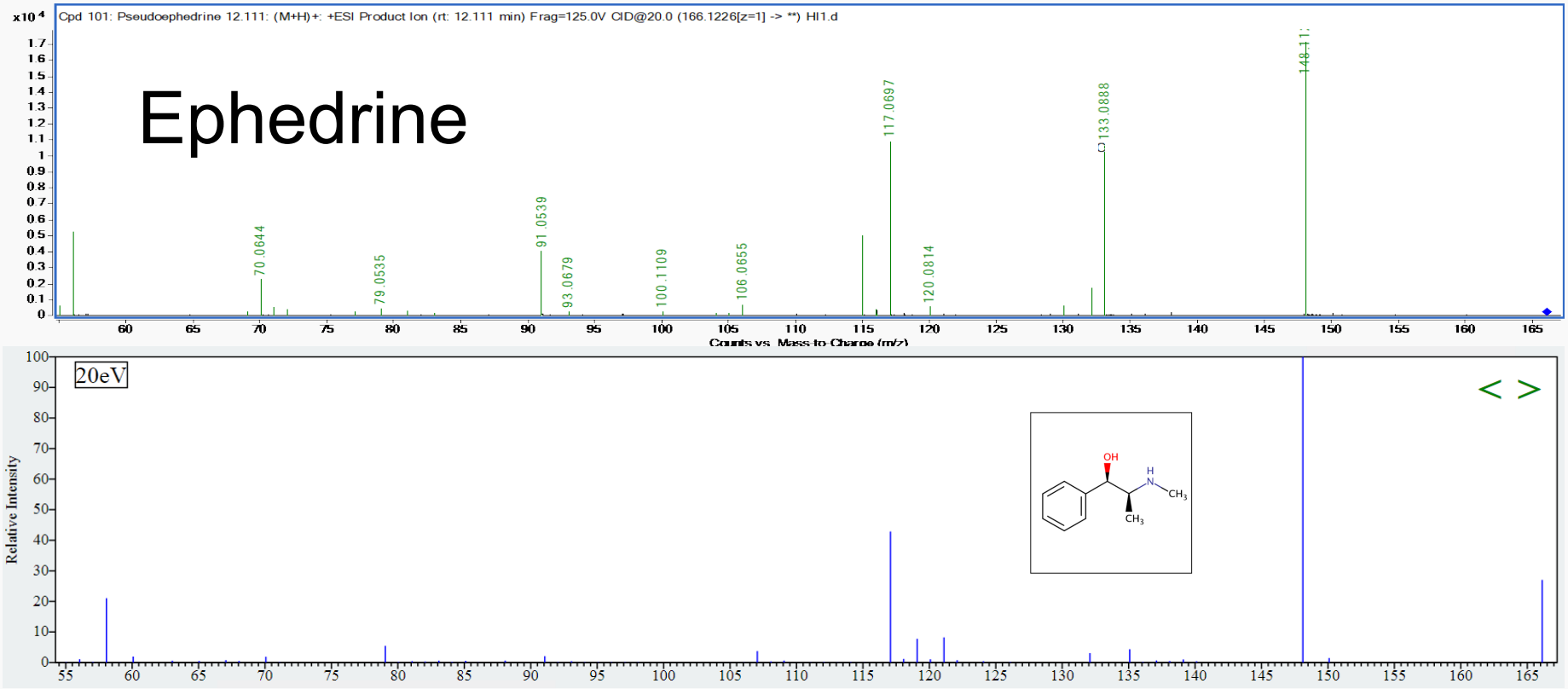
Bingo NoSQL is a Indigo plugin and non-relational database management system for storing chemical information and searching through it. With this plugin you can create databases which will be located on the hard drive of your local machine or some remote server. Bingo NoSQL uses only own and OS functionality for creating and accessing the databases, so there is no need in installing any additional third-party software. For storing chemical structures and other extra information memory-mapped files technology was used. This technology shows better performance than using direct read and write operations, so I/O delays have no significant effect on the Bingo NoSQL speed.

Structure



CONSUMER
CFM-ID Fragmentation Prediction

CFM-ID
Competitive Fragmentation Modeling for Metabolite Identification



PRODUCER
CFM-ID Predicted Library

- Predictions generated and stored for >700,000 structures
- Python code to score experimental vs predicted spectra
- Cosine dot product match score calculation

Data Descriptor | OPEN | Published: 02 August 2019

Linking *in silico* MS/MS spectra with chemistry data to improve identification of unknowns

Andrew D. McEachran, Ilya Balabin, Tommy Cathey, Thomas R. Transue, Hussein Al-Ghoul, Chris Grulke, Jon R. Sobus & Antony J. Williams

Scientific Data **6**, Article number: 141 (2019) | Download Citation

PRODUCER
Published data is on FigShare

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Data Descriptor | OPEN | Published: 02 August 2019

Linking *in silico* MS/MS spectra with chemistry data to improve identification of unknowns

Andrew D. McEachran, Ilya Balabin, Tomm
Grulke, Jon R. Sobus & Antony J. Williams

Scientific Data **6**, Article number: 141 (2019)

CFM-ID Paper Data

Dataset posted on 01.03.2019, 08:38 by EPA's National Center for Computational Toxicology

88 views | 17 downloads | 0 citations

This upload is a zip containing the following files:

Predicted EI-MS Spectra of CompTox Chemicals Dashboard Structures:

Predicted EI-MS spectra of ~700,000 chemical structures from the CompTox Chemicals Dashboard were generated using the CFM-ID model developed by Allen, et al. (https://doi.org/10.1021/acs.analchem.6b01622). These data are provided in .dat ASCII format.

Predicted MS/MS Spectra in ESI-positive mode of CompTox Chemicals Dashboard Structures:

Predicted MS/MS spectra of ~700,000 chemical structures from the CompTox Chemicals Dashboard were generated using the CFM-ID model developed by Allen, et al. (https://doi.org/10.1007/s11306-014-0676-4) in ESI-positive mode. These data are provided in .dat ASCII format.

Predicted MS/MS Spectra in ESI-negative mode of CompTox Chemicals Dashboard Structures:

Predicted MS/MS spectra of ~700,000 chemical structures from the CompTox Chemicals Dashboard were generated using the CFM-ID model developed by Allen, et al. (https://doi.org/10.1007/s11306-014-0676-4) in ESI-negative mode. These data are provided in .dat ASCII format.

EPA United States Environmental Protection Agency

CATEGORIES

- Toxicology

KEYWORD(S)

Computational Toxicology
DSSTox Chemical Database
Chemicals Dashboard
Non-targeted analysis
CFM-ID

LICENCE

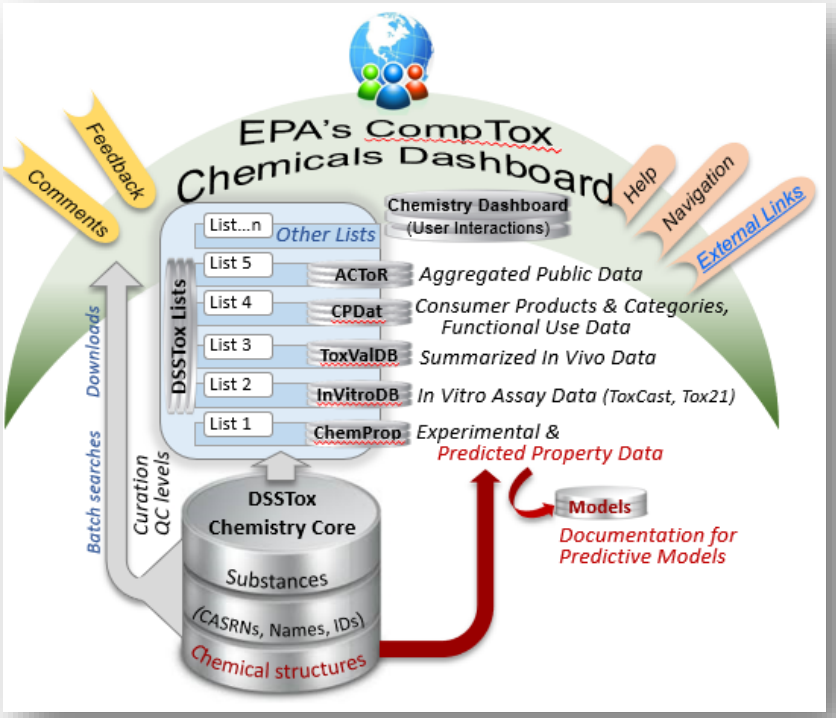
CC0

EXPORT

RefWorks
BibTeX
Ref. manager
Endnote

Conclusion

- Dashboard access to data for ~875,000 chemicals
- Dashboard **CONSUMES** a lot of open source libraries and open data
- We **PRODUCE** open models and data to the community in exchange
- We are committed to an open API to provide more complete data access and real time predictions



Acknowledgements

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- *Todd Martin & Valery Tkachenko, WebTEST*
- *Kathie Dionisio & Kristin Isaacs, CPDat*
- *Thanks to Emma Schymanski, University of Luxembourg, for coordinating all efforts with the NORMAN Network for curation of lists on the Suspect Exchange*

Contact

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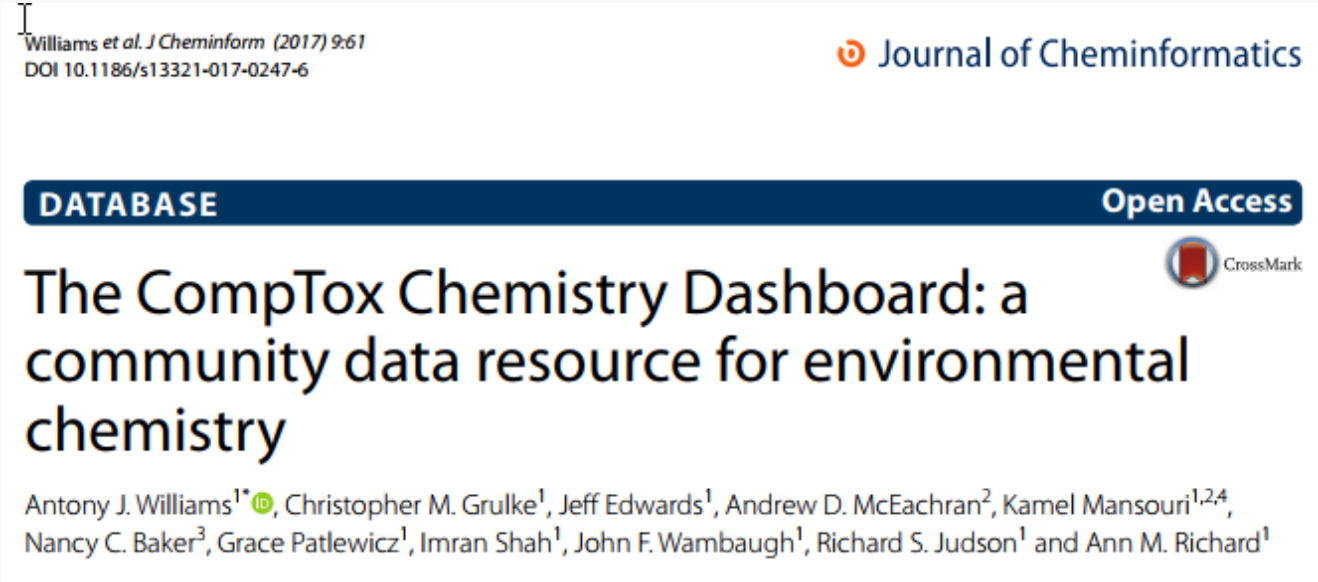
NCCT, US EPA Office of Research and Development,
Williams.Antony@epa.gov
ORCID: https://orcid.org/0000-0002-2668-4821



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The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

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