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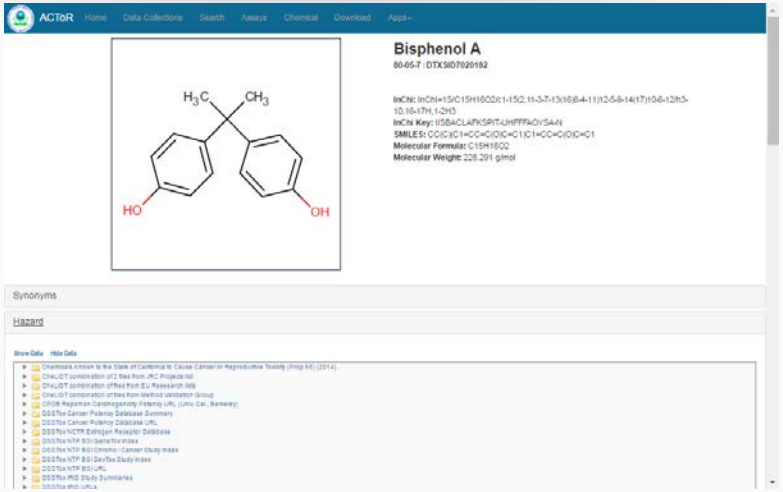
The EPA Comptox Chemistry Dashboard: Two Years in as an Integration Hub for Environmental Toxicology Data

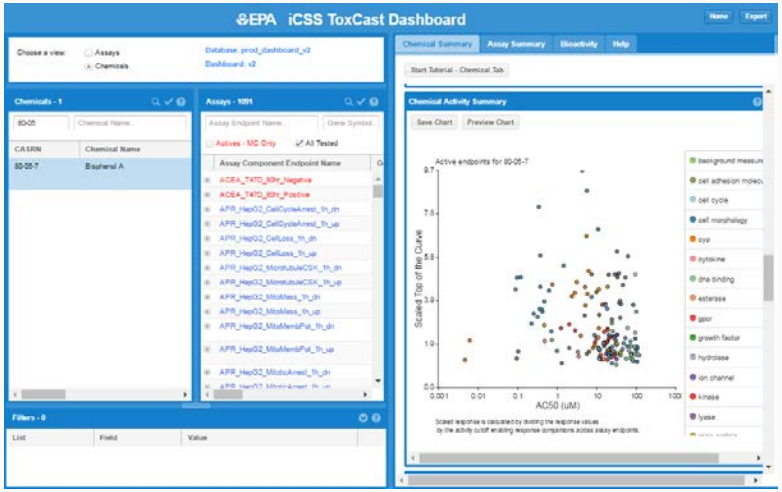
Antony Williams

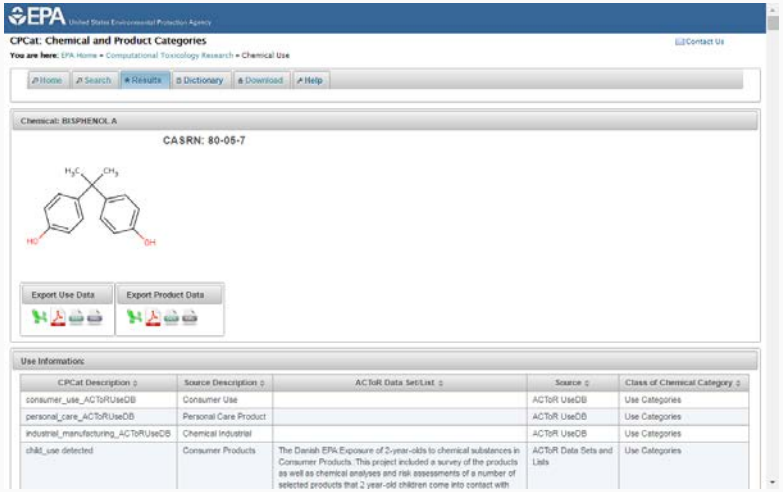
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

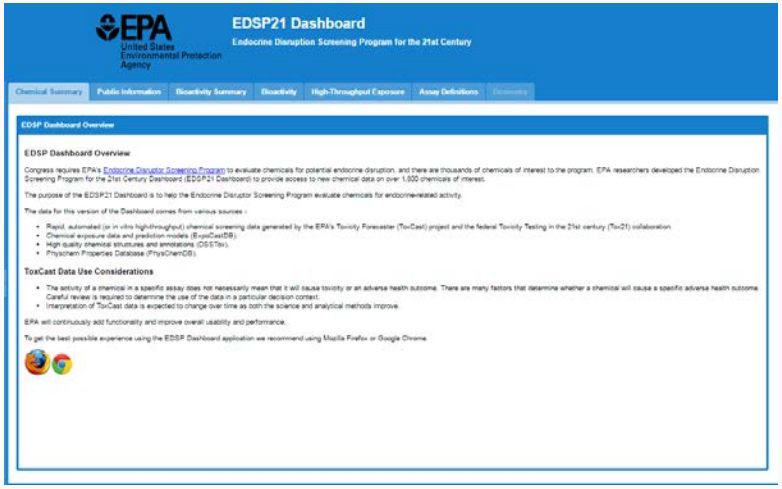
April 30th 2018
NIEHS

Early Dashboard Applications









Earlier Dashboards

- Chemistry data mashed together based on CAS Number/Names
- Chemistry data quality issues
- Multiple applications requiring maintenance

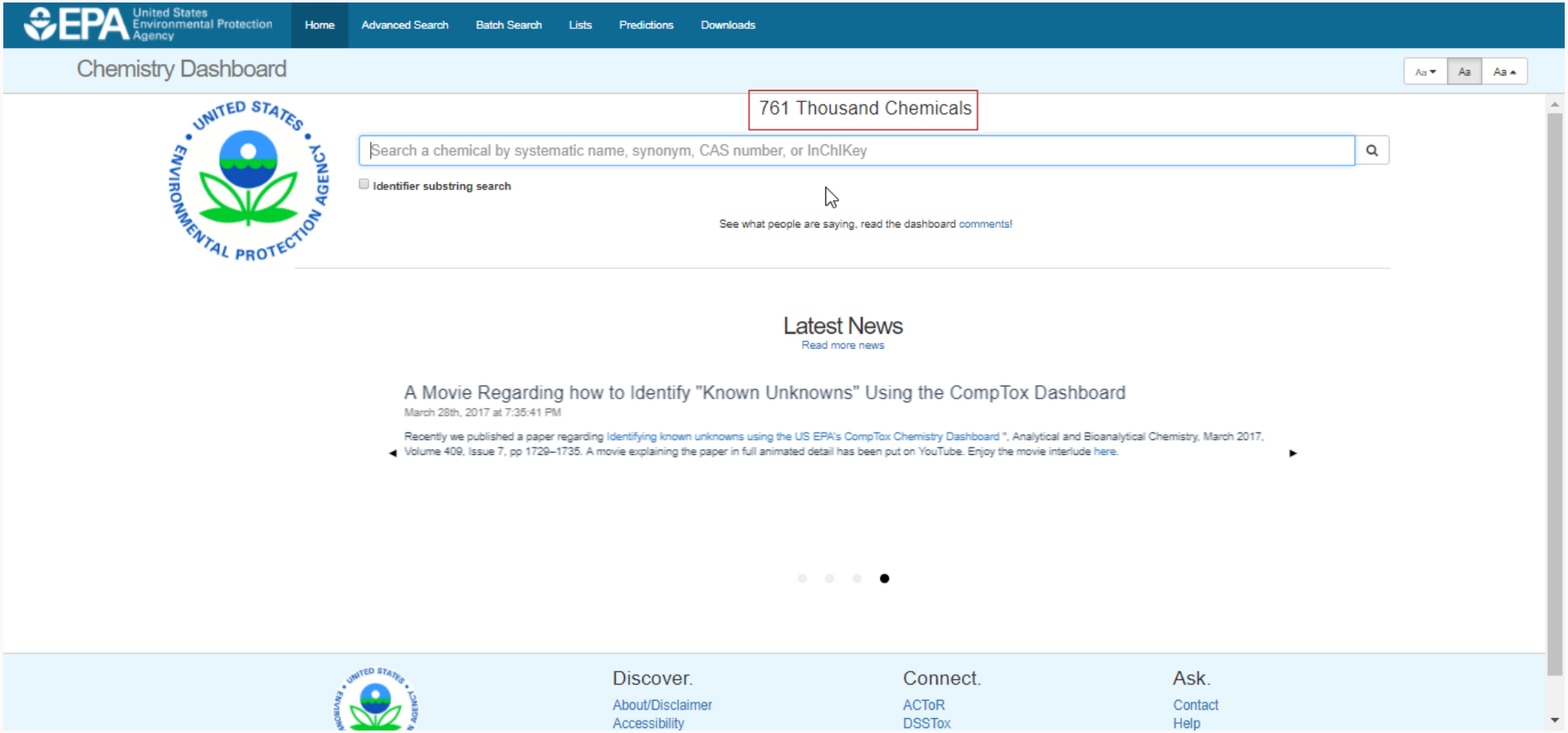
- April 2016 – beta release of the CompTox Chemistry Dashboard as an integration hub

The CompTox Chemistry Dashboard

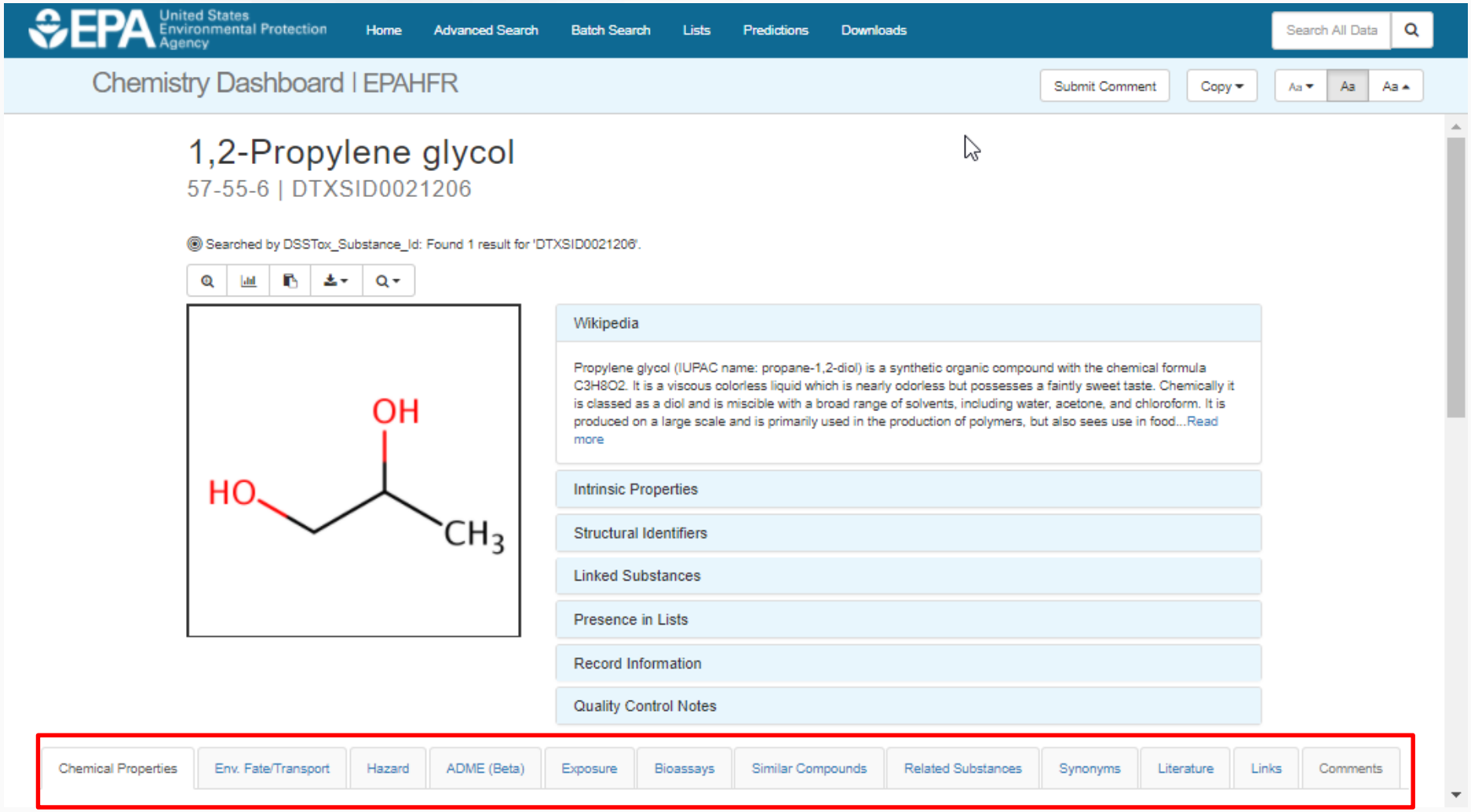
- A **publicly accessible website** delivering access:
  - ~760,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals
  - **DOWNLOADABLE Open Data for reuse and repurposing**

CompTox Chemistry Dashboard

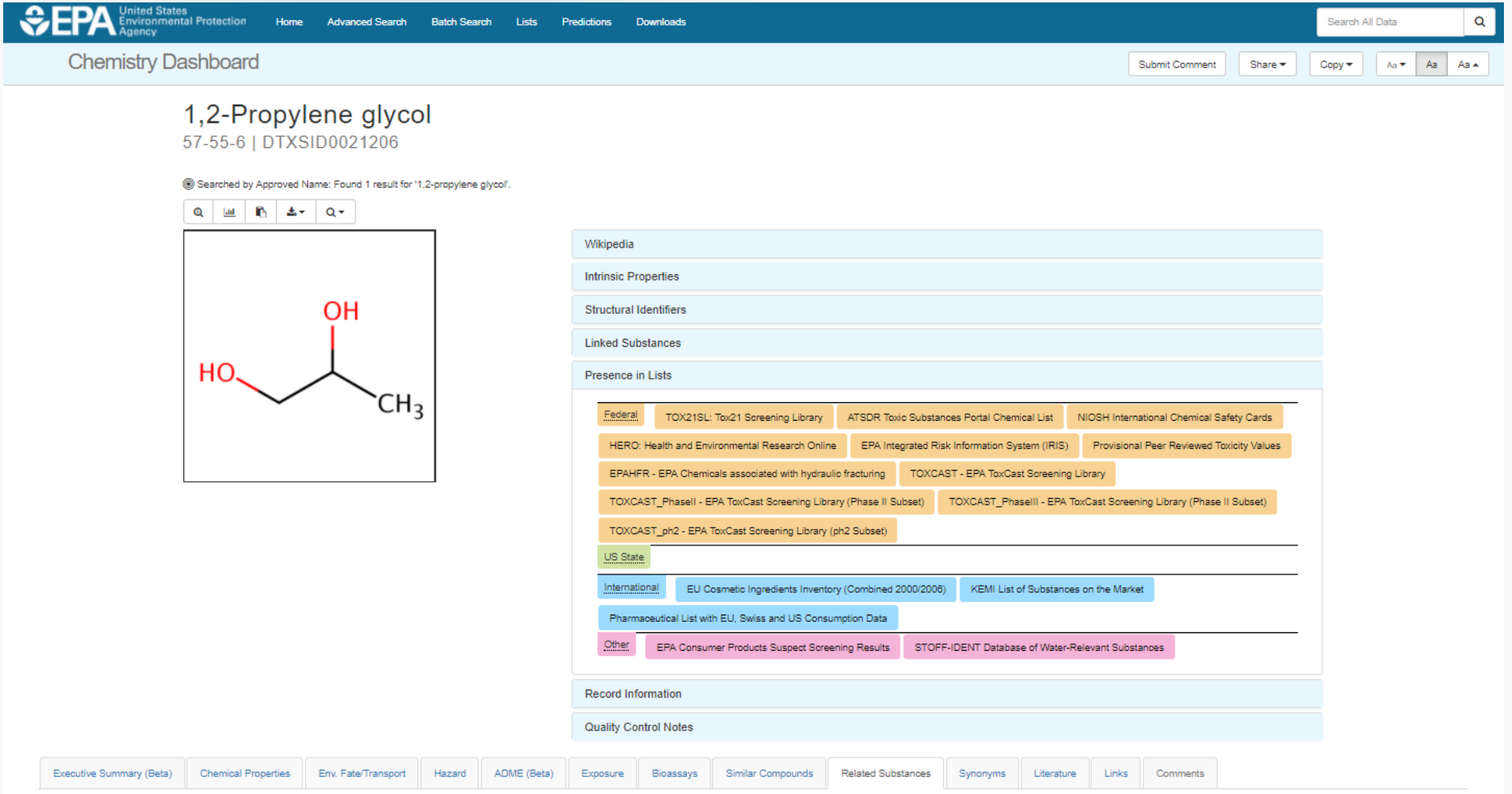
https://comptox.epa.gov/dashboard



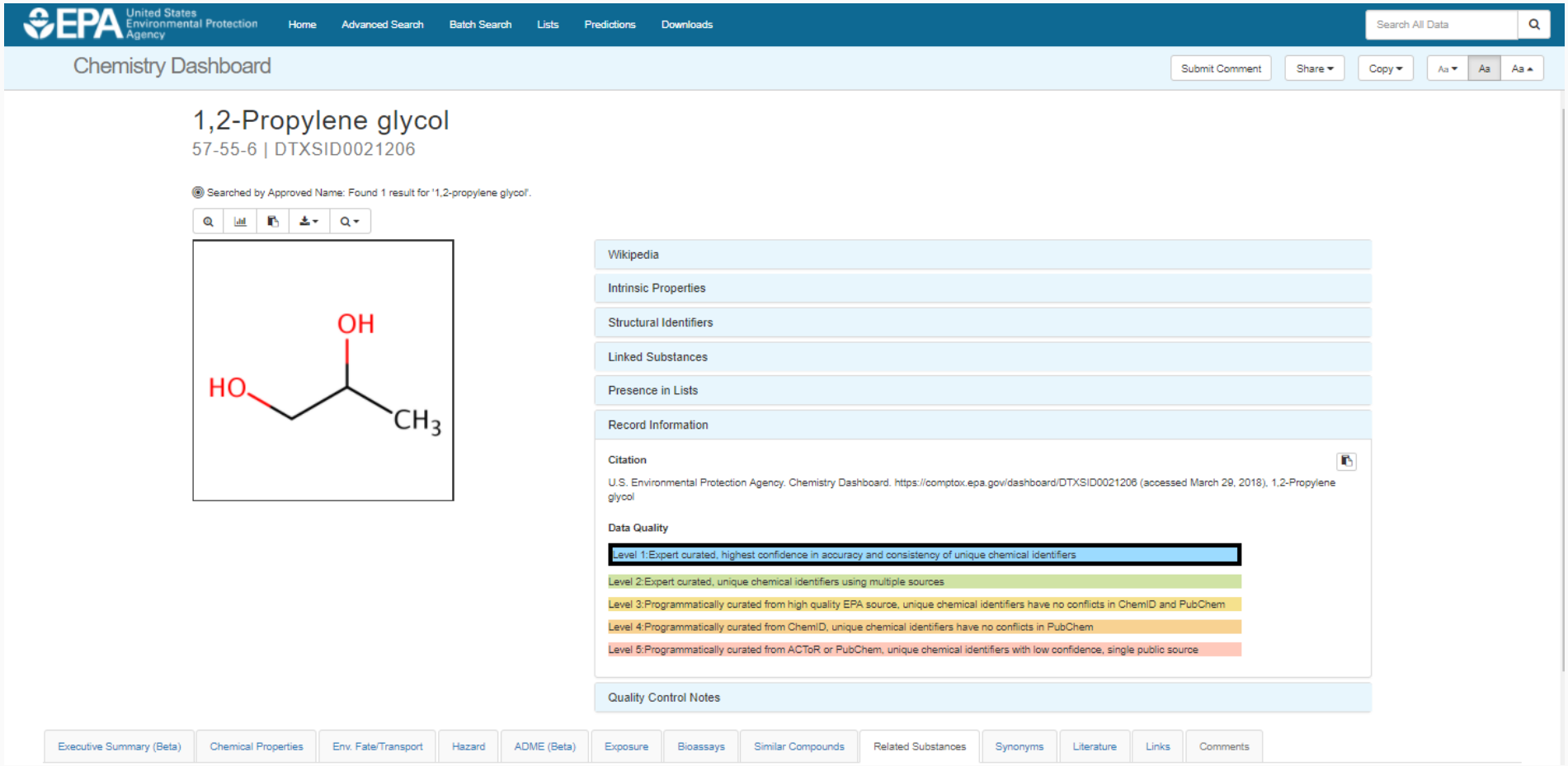
Detailed Chemical Pages



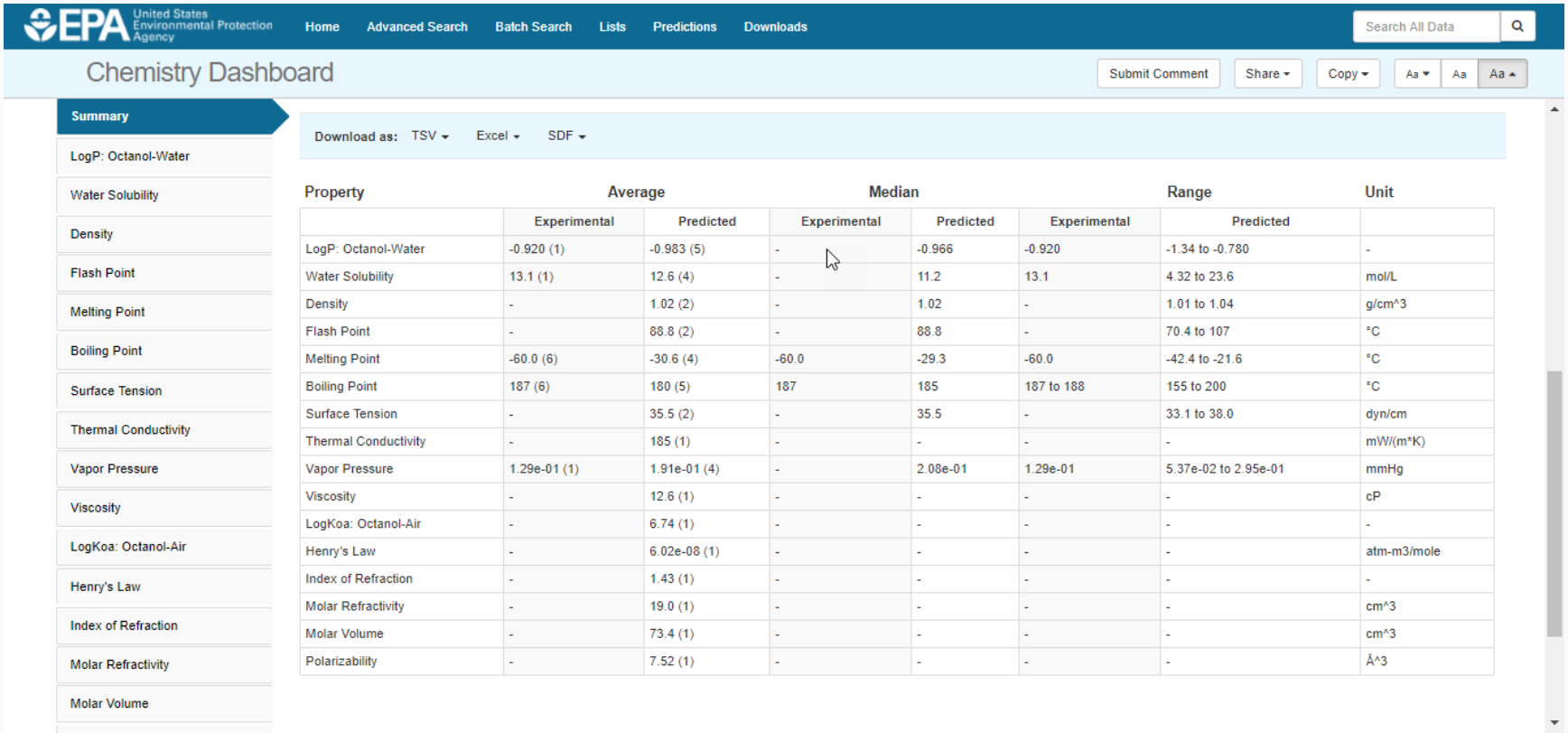
Presence in Lists



Data Quality



Properties, Fate and Transport



Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-0.920 (1)	-0.983 (5)	-	-0.966	-0.920	-1.34 to -0.780	-
Water Solubility	13.1 (1)	12.6 (4)	-	11.2	13.1	4.32 to 23.6	mol/L
Density	-	1.02 (2)	-	1.02	-	1.01 to 1.04	g/cm^3
Flash Point	-	88.8 (2)	-	88.8	-	70.4 to 107	°C
Melting Point	-60.0 (6)	-30.6 (4)	-60.0	-29.3	-60.0	-42.4 to -21.6	°C
Boiling Point	187 (6)	180 (5)	187	185	187 to 188	155 to 200	°C
Surface Tension	-	35.5 (2)	-	35.5	-	33.1 to 38.0	dyn/cm
Thermal Conductivity	-	185 (1)	-	-	-	-	mW/(m*K)
Vapor Pressure	1.29e-01 (1)	1.91e-01 (4)	-	2.08e-01	1.29e-01	5.37e-02 to 2.95e-01	mmHg
Viscosity	-	12.6 (1)	-	-	-	-	cP
LogKoa: Octanol-Air	-	6.74 (1)	-	-	-	-	-
Henry's Law	-	6.02e-08 (1)	-	-	-	-	atm-m3/mole
Index of Refraction	-	1.43 (1)	-	-	-	-	-
Molar Refractivity	-	19.0 (1)	-	-	-	-	cm^3
Molar Volume	-	73.4 (1)	-	-	-	-	cm^3
Polarizability	-	7.52 (1)	-	-	-	-	Å^3

Model Performance Details
(Redesigned display)

EPA United States Environmental Protection Agency

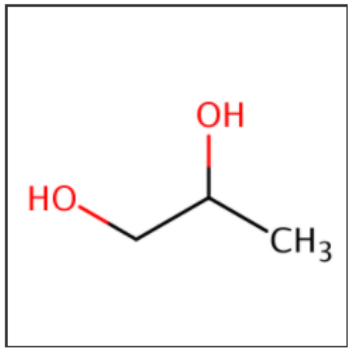
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | 21206

Chemistry Dashboard

OPERA Models: Fish Biotrans. Half-Life (Km)

1,2-Propylene glycol
57-55-6 | DTXSID0021206

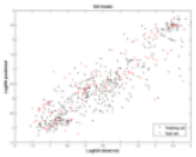
Save PDF

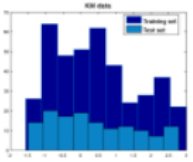


Model Results

Predicted value: 8.30e-02 days
Global applicability domain: Inside
Local applicability domain index: 0.28
Confidence level: 0.71

Model Performance



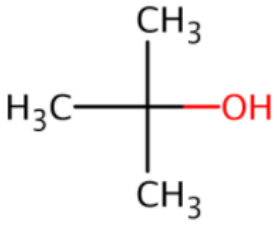


Weighted KNN model

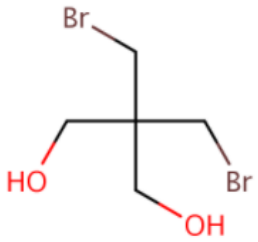
QMRF

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.83	0.49	0.82	0.5	0.73	0.62

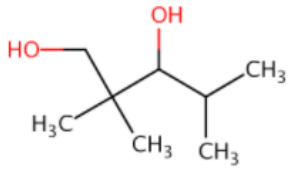
Nearest Neighbors from the Training Set



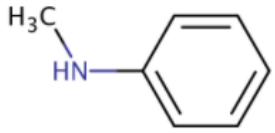
tert-Butyl alcohol
Measured: 7.41e-02
Predicted: 7.66e-02



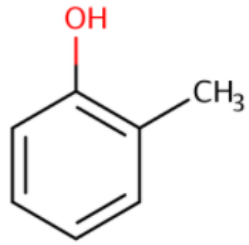
Pentaerythritol dibromide
Measured: 3.98e-02
Predicted: 5.44e-02



2,2,4-Trimethyl-1,3-pentanediol
Measured: 4.57e-02
Predicted: 5.13e-02



N-Methylaniline
Measured: 1.32e-01
Predicted: 1.50e-01



o-Cresol
Measured: 3.02e-01
Predicted: 2.42e-01

OPERA: OPEN Data and OPEN Models

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

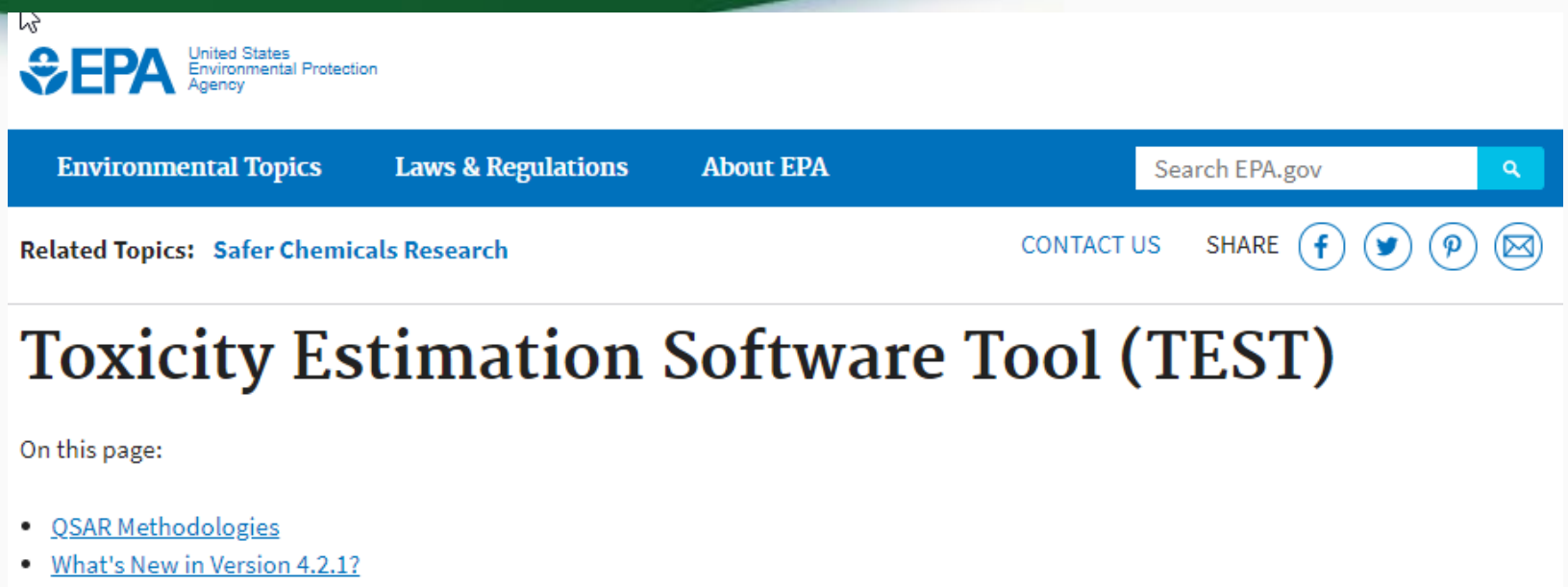
Journal of Cheminformatics

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]

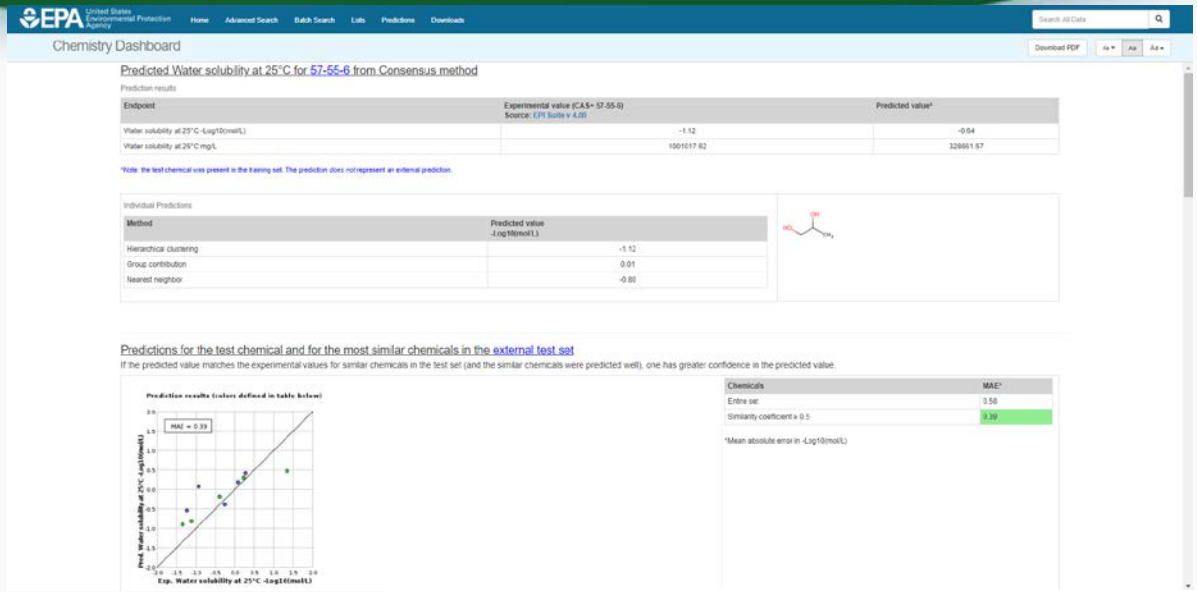
T.E.S.T Models



- Predictions made for the whole database
- Includes detailed calculation reports

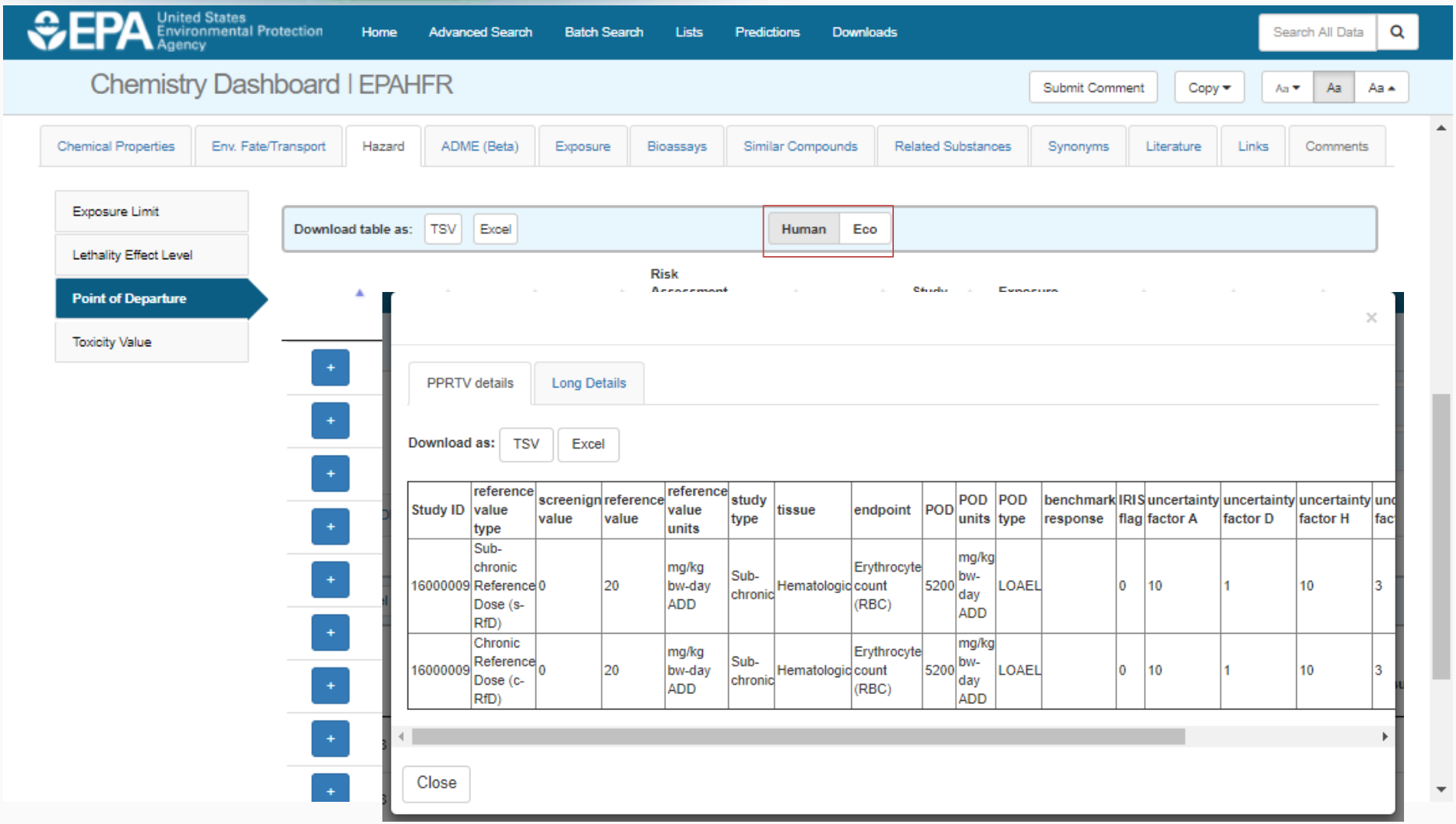
T.E.S.T Calculation Reports

EPA United States Environmental Protection Agency



CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
57-55-6 (test chemical)			-1.12	-0.64
78-92-2		0.96	-0.39	-0.18
64-17-5		0.95	-1.34	-0.91
584-02-1		0.92	0.23	0.30
353-36-6		0.91	1.35	0.48
109-86-4		0.90	-1.12	-0.82
75-52-5		0.90	-0.26	-0.39

Access to Chemical Hazard Data



Study ID	reference value type	screenign value	reference value	reference value units	study type	tissue	endpoint	POD	POD units	POD type	benchmark response	IRIS flag	uncertainty factor A	uncertainty factor D	uncertainty factor H	unc fac
16000009	Sub-chronic Reference Dose (s-RfD)	0	20	mg/kg bw-day ADD	Sub-chronic	Hematologic	Erythrocyte count (RBC)	5200	mg/kg bw-day ADD	LOAEL		0	10	1	10	3
16000009	Chronic Reference Dose (c-RfD)	0	20	mg/kg bw-day ADD	Sub-chronic	Hematologic	Erythrocyte count (RBC)	5200	mg/kg bw-day ADD	LOAEL		0	10	1	10	3

In Vitro Bioassay Screening

ToxCast and Tox21

Detailed Assay Description as PDF (limited number of assays)

NVS_NR_hFXR_Antagonist

Assay Title: NovaScreen Human Farnesoid x Receptor Alpha (FXR) Ligand-Binding Antagonist Screening Assay

1. Assay Descriptions

1.1. Overview

Assay Summary:

High-throughput screening of in vitro chemical-target interactions across a wide variety of compounds through a broad range of biochemical interactions will help describe the chemical-assay bioactivity space for chemicals with limited available information. There exists a large number of environmental chemicals for which there is little information about the potential for bioactivity. The NVS NR human farnesoid x receptor (FXR, NR1H4) agonist assay format allows for an efficient screening of thousands of chemicals for the ability to competitively bind to the ligand-binding domain of a xenobiotic sensing nuclear receptor. This assay was developed to screen the ToxCast chemical library for potential farnesoid x receptor ligand-binding activity using a TR-FRET competitive displacement assay and a known FXR receptor agonist (Chenodeoxycholic Acid, CDCA) as a reference compound. Biochemical high-throughput screening offers preliminary evidence for chemical targets in a cell or tissues which, when combined with information from literature or targeted in vivo studies, can indicate potential pathways for toxicity. This assay was run for a test duration of 1 hour in a 384-well plate.

1.2. Assay Definition

Assay Throughput:

Human FXR ligand-binding domain (LBD) incubated in 384-well microtiter plates for 1 hour prior to measuring ligand dependent binding of cofactor to the receptor using TR-FRET.

Sources of Exposure to Chemicals

- **Product & Use Categories**
- Chemical Weight Fraction
- Chemical Functional Use
- Monitoring Data
- Exposure Predictions
- Production Volume

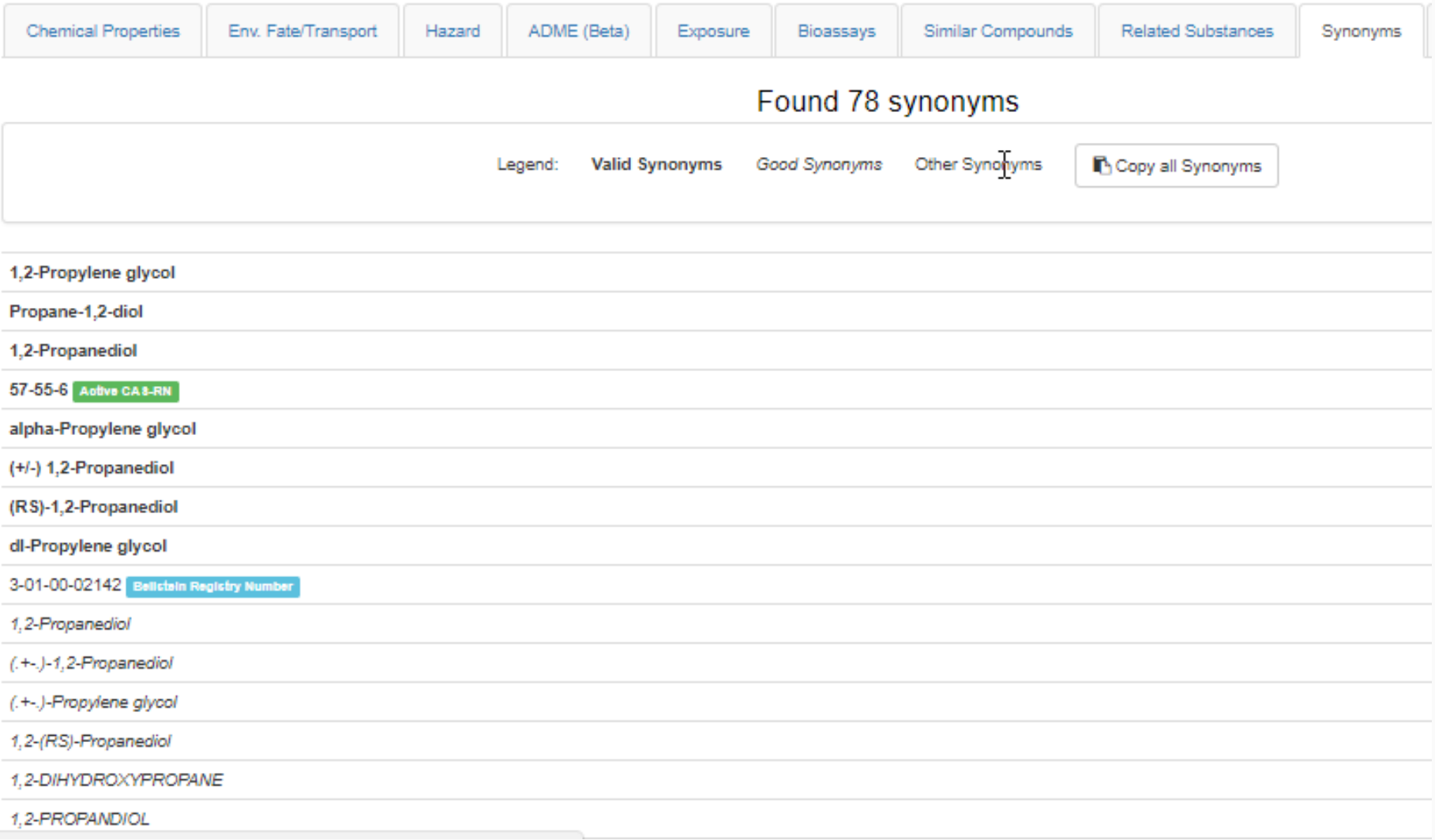
osure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

Product & Use Categories (PUCs)

Categorization type	Number of Unique Products
PUC	288
PUC	206
PUC	117
PUC	107
PUC	107
PUC	101
PUC	101
PUC	90
PUC	89

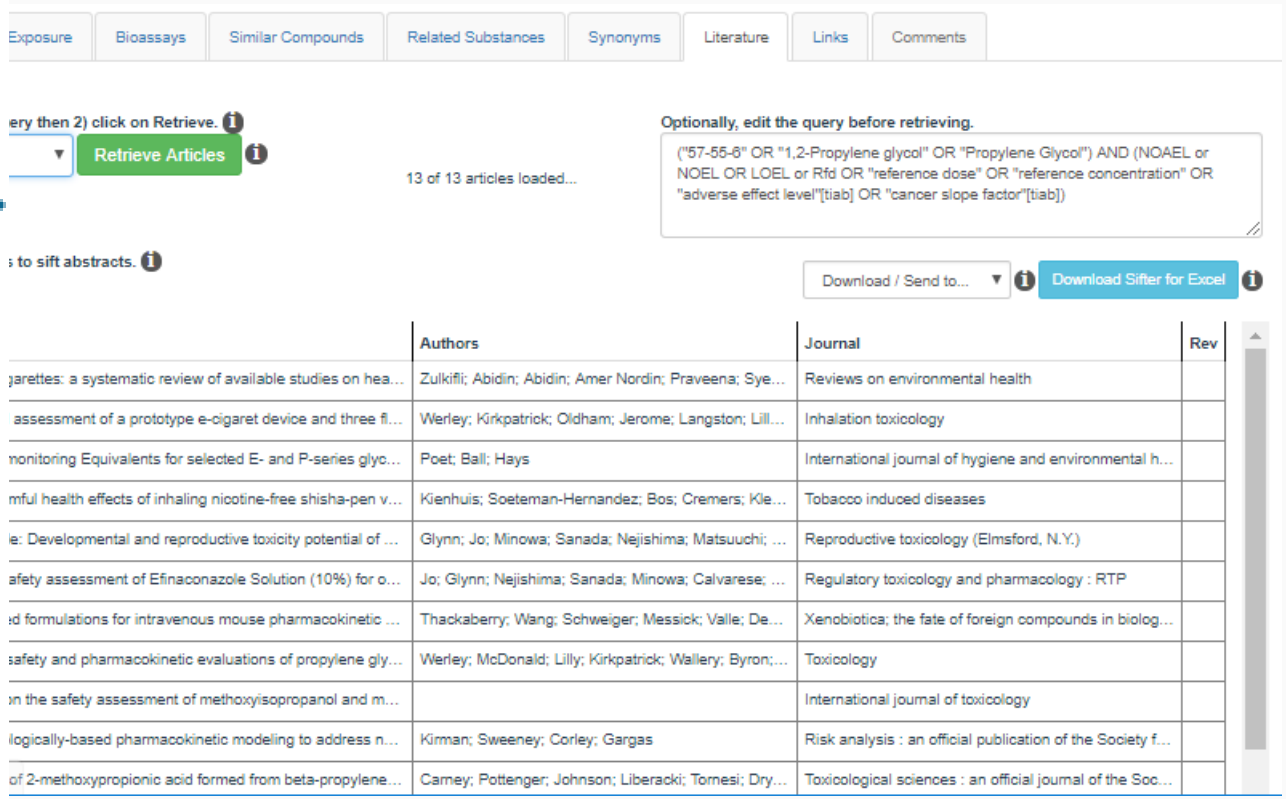
Identifiers to Support Searches

EPA United States Environmental Protection Agency



Literature Searches and Links

- Google Scholar
- **PubMed Abstract Sifter**
- PubChem Articles
- PubChem Patents
- PPRTV
- IRIS



Abstract Sifter for Excel

F1000Research 2017, 6(Chem Inf Sci):2164 Last updated: 06 FEB 2018

Check for updates

SOFTWARE TOOL ARTICLE

Abstract Sifter: a comprehensive front-end system to PubMed [version 1; referees: 2 approved]

Nancy Baker [1], Thomas Knudsen[2], Antony Williams [2]

[1]Leidos, Research Triangle Park, NC, USA
[2]National Center for Computational Toxicology, U.S. Environmental Protection Agency, Research Triangle Park, NC, USA

v1 **First published:** 21 Dec 2017, **6**(Chem Inf Sci):2164 (doi: 10.12688/f1000research.12865.1)
Latest published: 21 Dec 2017, **6**(Chem Inf Sci):2164 (doi: 10.12688/f1000research.12865.1)

Abstract

The Abstract Sifter is a Microsoft Excel based application that enhances existing search capabilities of PubMed. The Abstract Sifter assists researchers to search effectively, triage results, and keep track of articles of interest. The tool implements an innovative "sifter" functionality for relevance ranking, giving the researcher a way to find articles of interest quickly. The tool also gives researchers a view of the literature landscape for a set of entities such as chemicals or genes. The Abstract Sifter is available as a Microsoft Excel macro-enabled workbook application.

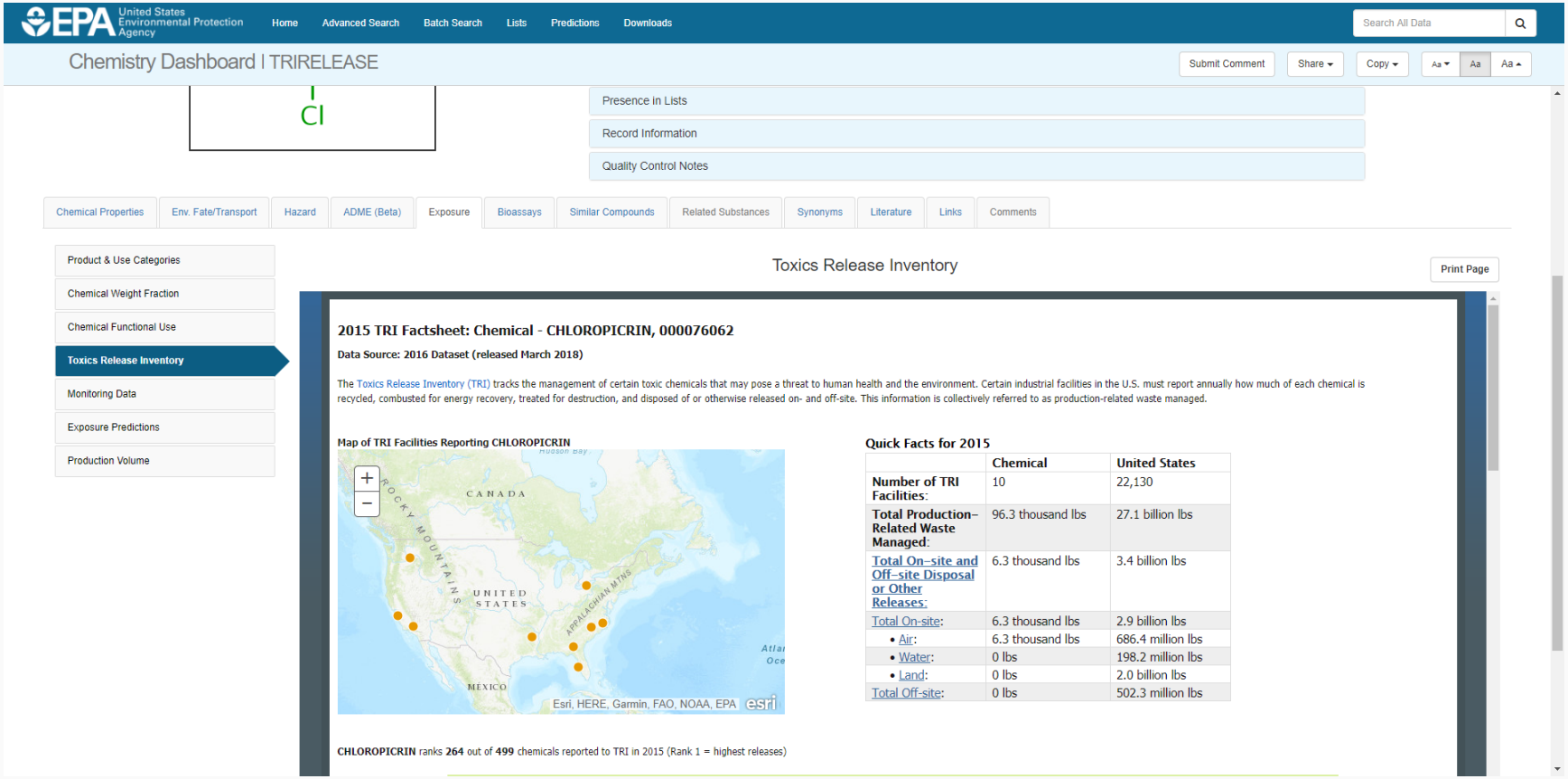
Open Peer Review

Referee Status: ✓ ✓

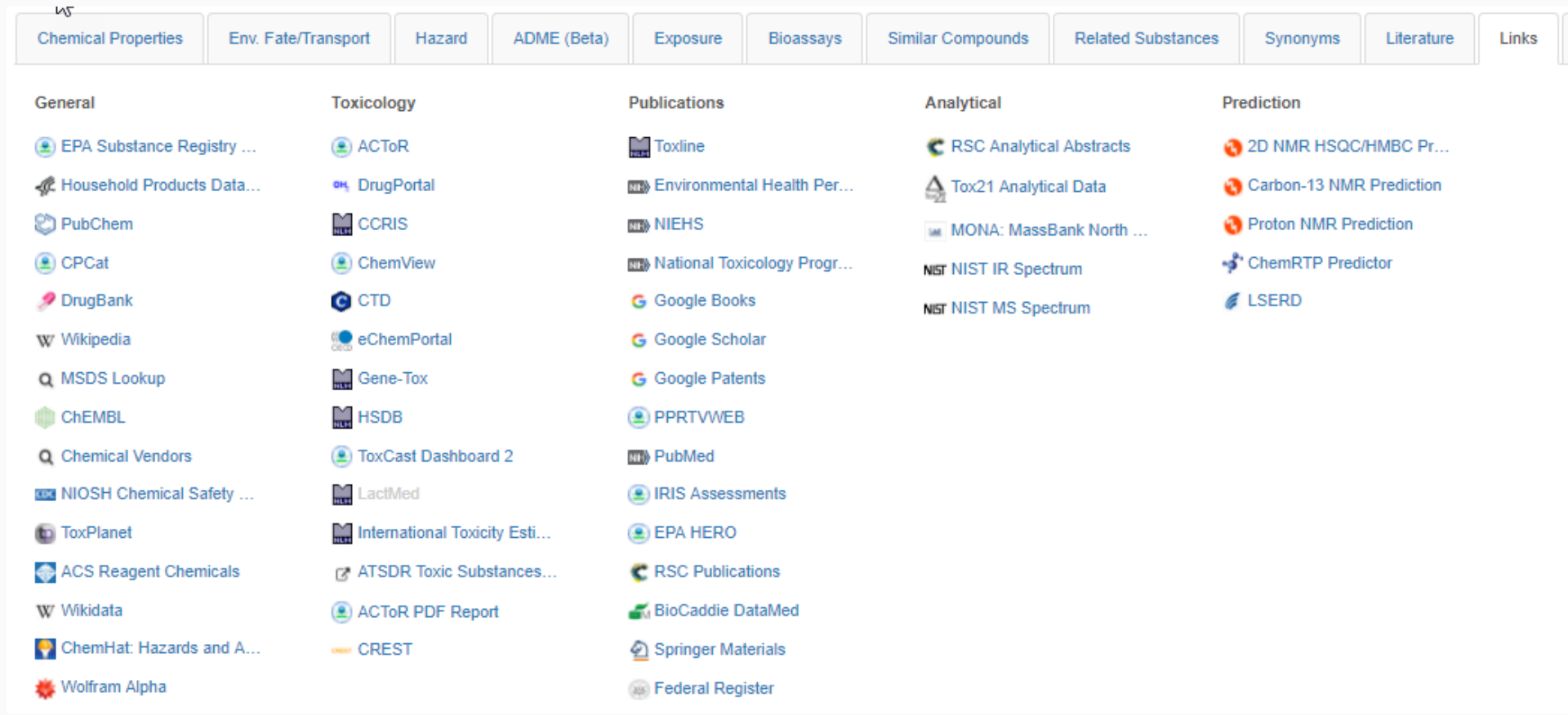
	Invited Referees 1	2
version 1 published 21 Dec 2017	✓ report	✓ report

1 **Paulina Damdimopoulou**, Karolinska Institutet, Sweden

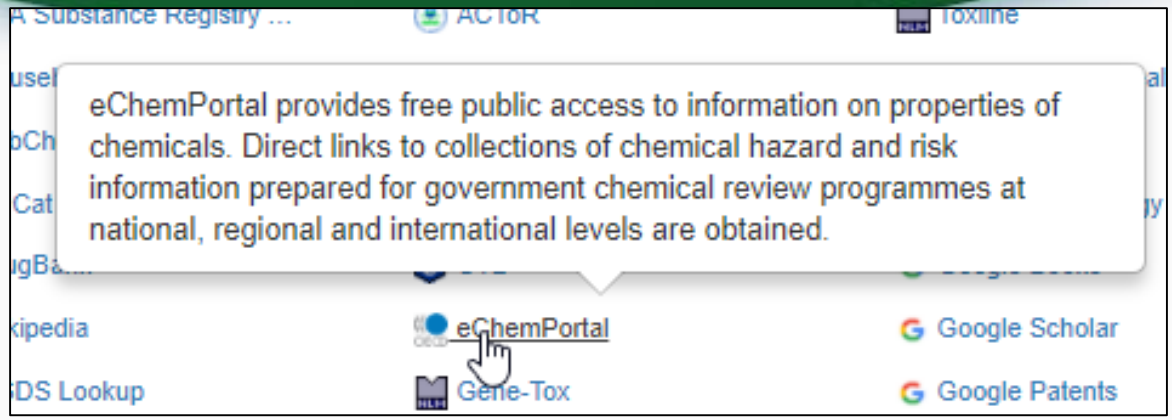
Embedded Toxics Release Inventory

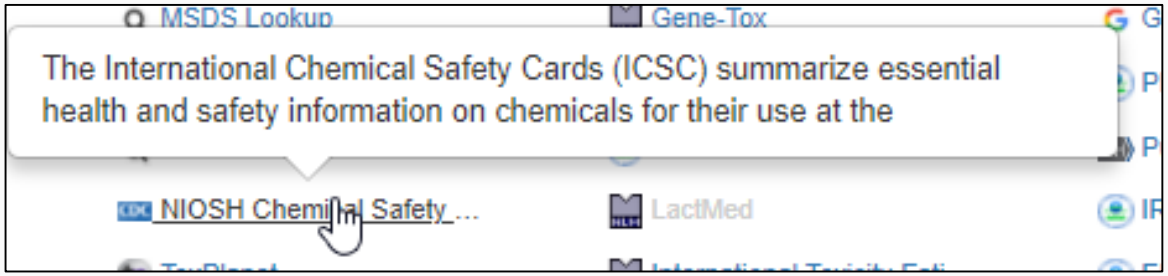


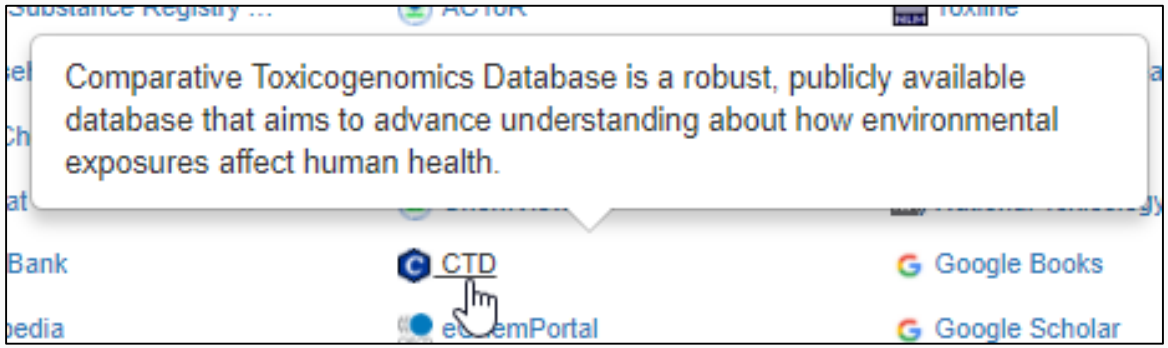
External Links to Data and Services



Integrated Linkouts



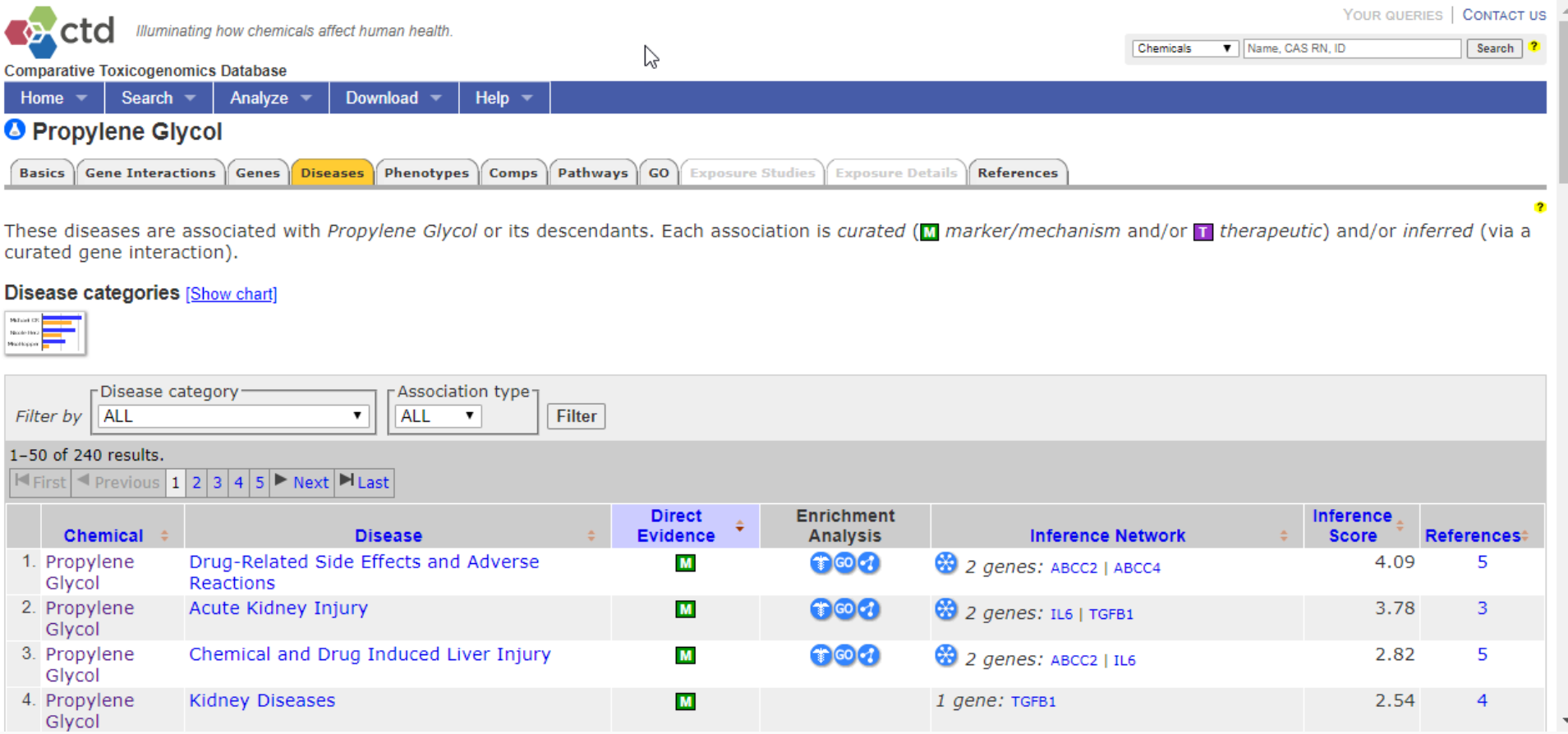




Integrated Linkouts

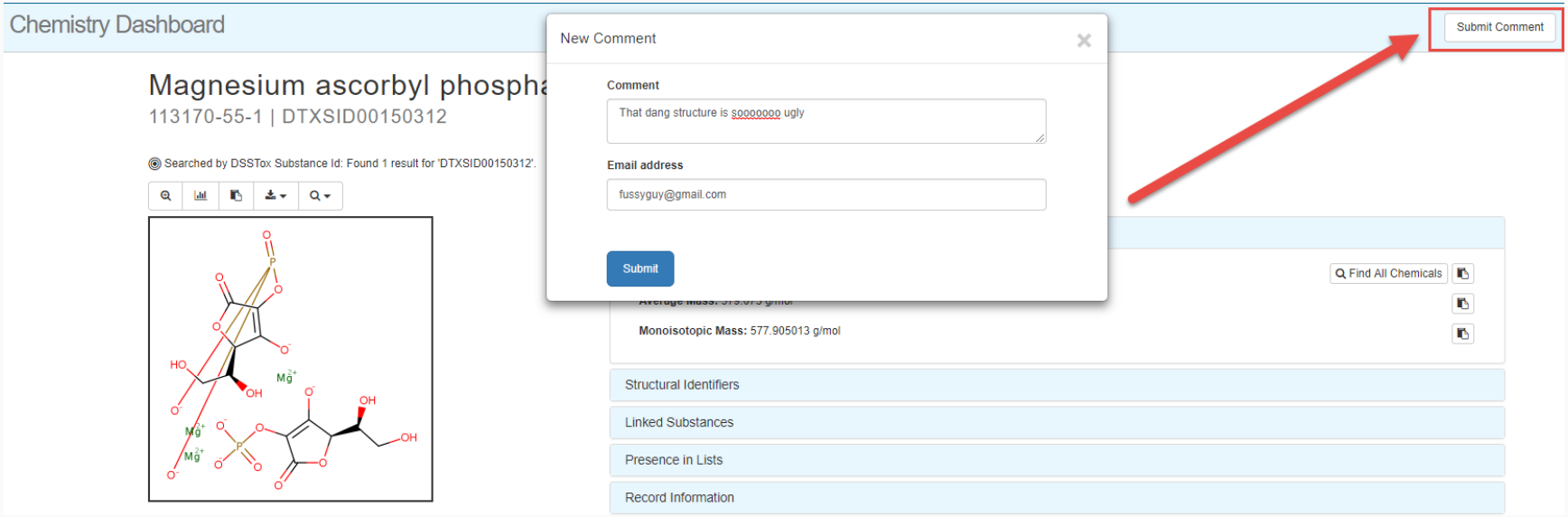
Comparative Toxicogenomics DB

EPA United States Environmental Protection Agency

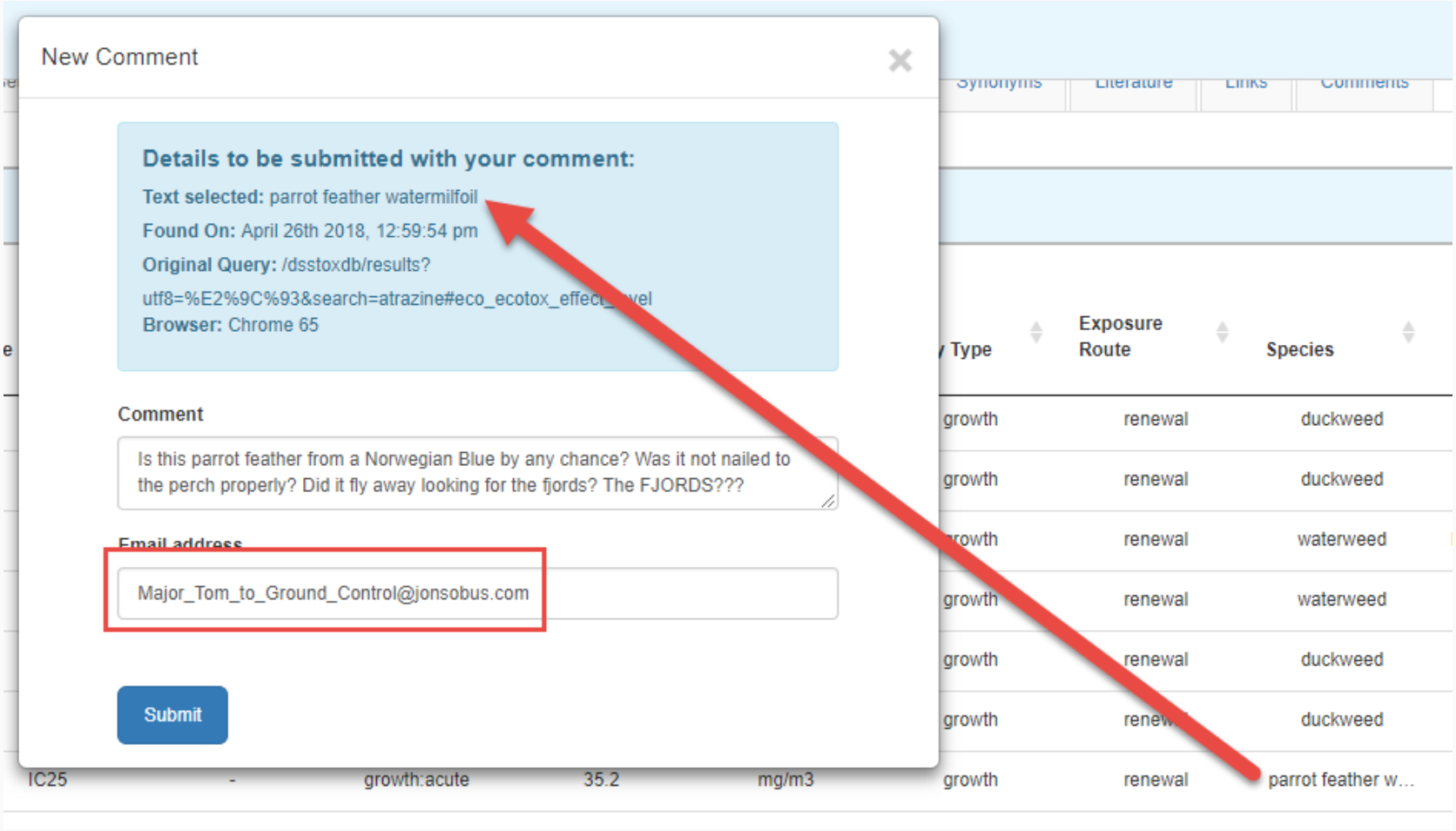


	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M		2 genes: ABCC2 | ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M		2 genes: IL6 | TGFB1	3.78	3
3.	Propylene Glycol	Chemical and Drug Induced Liver Injury	M		2 genes: ABCC2 | IL6	2.82	5
4.	Propylene Glycol	Kidney Diseases	M		1 gene: TGFB1	2.54	4

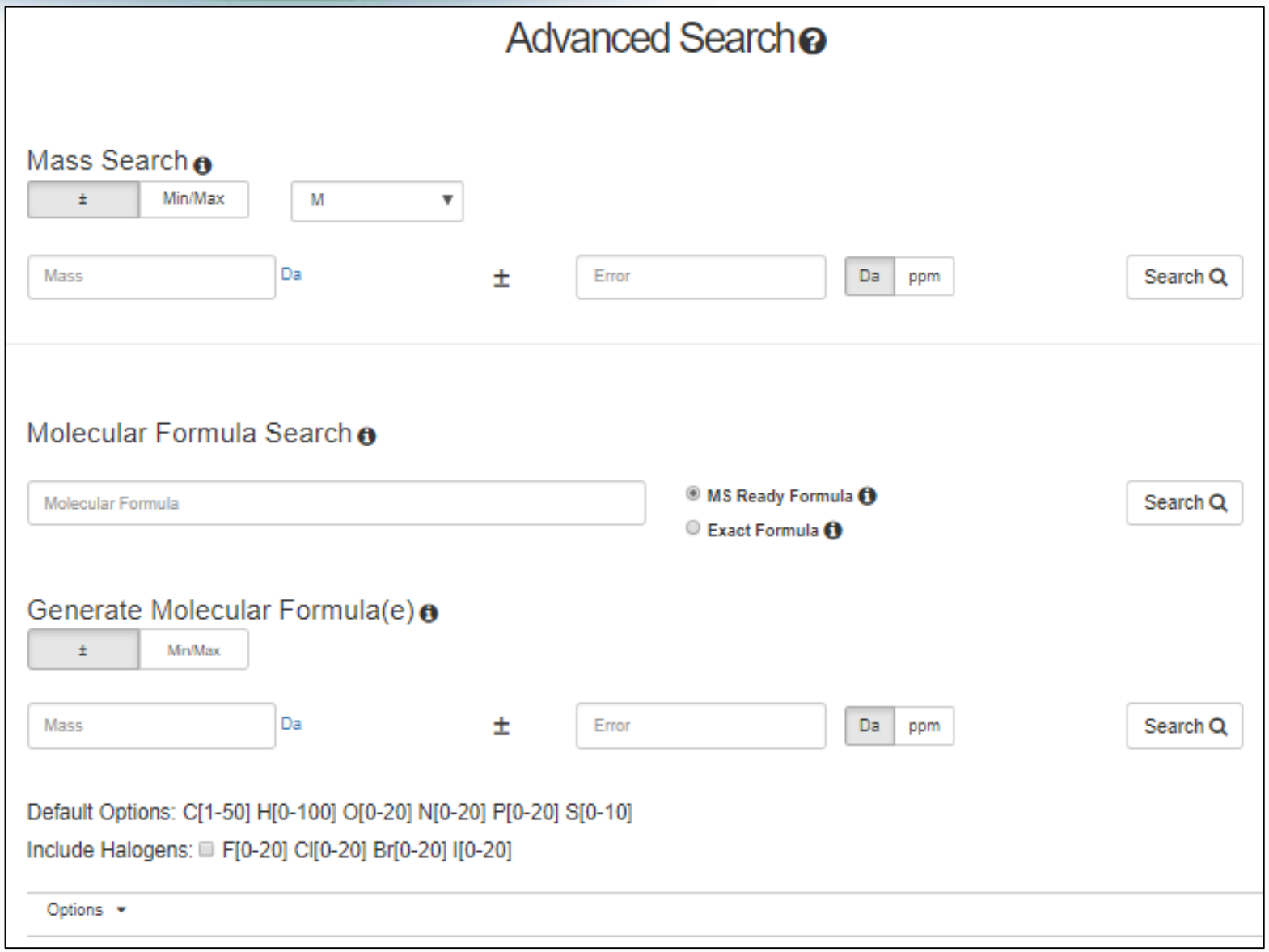
Submit Comments for Review



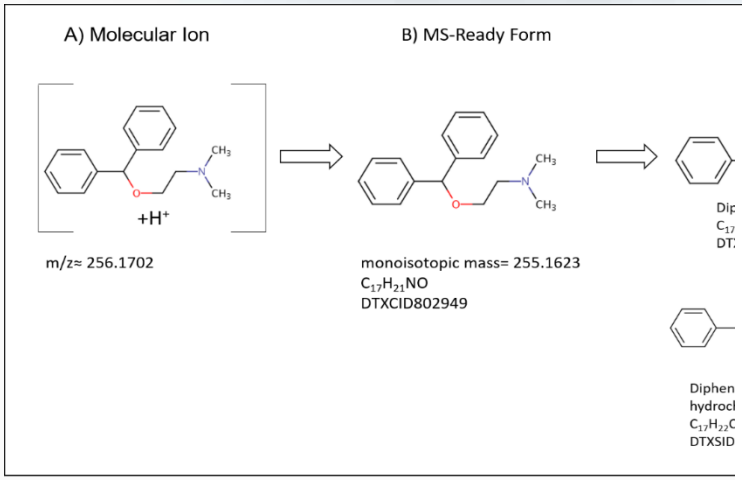
Submit Comments for Review

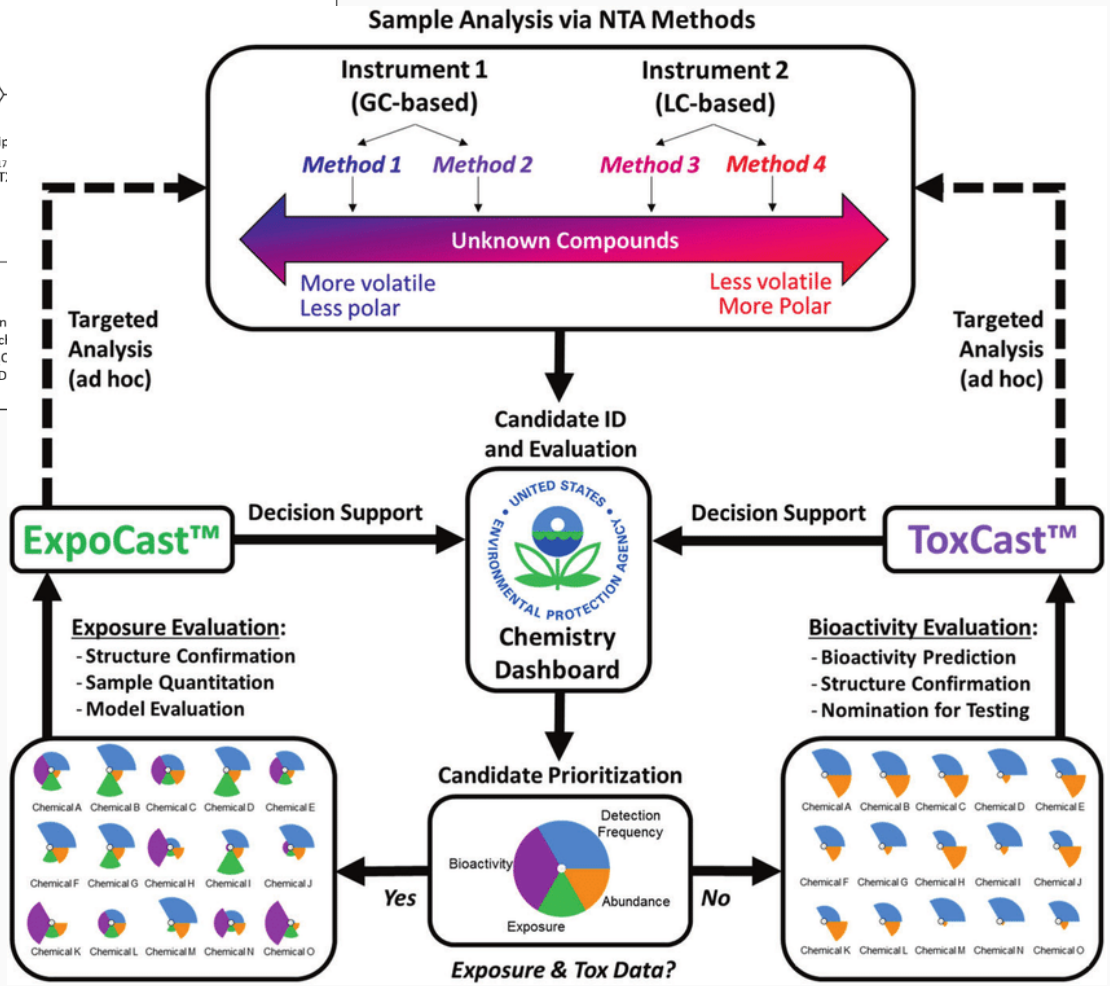


Advanced Searches

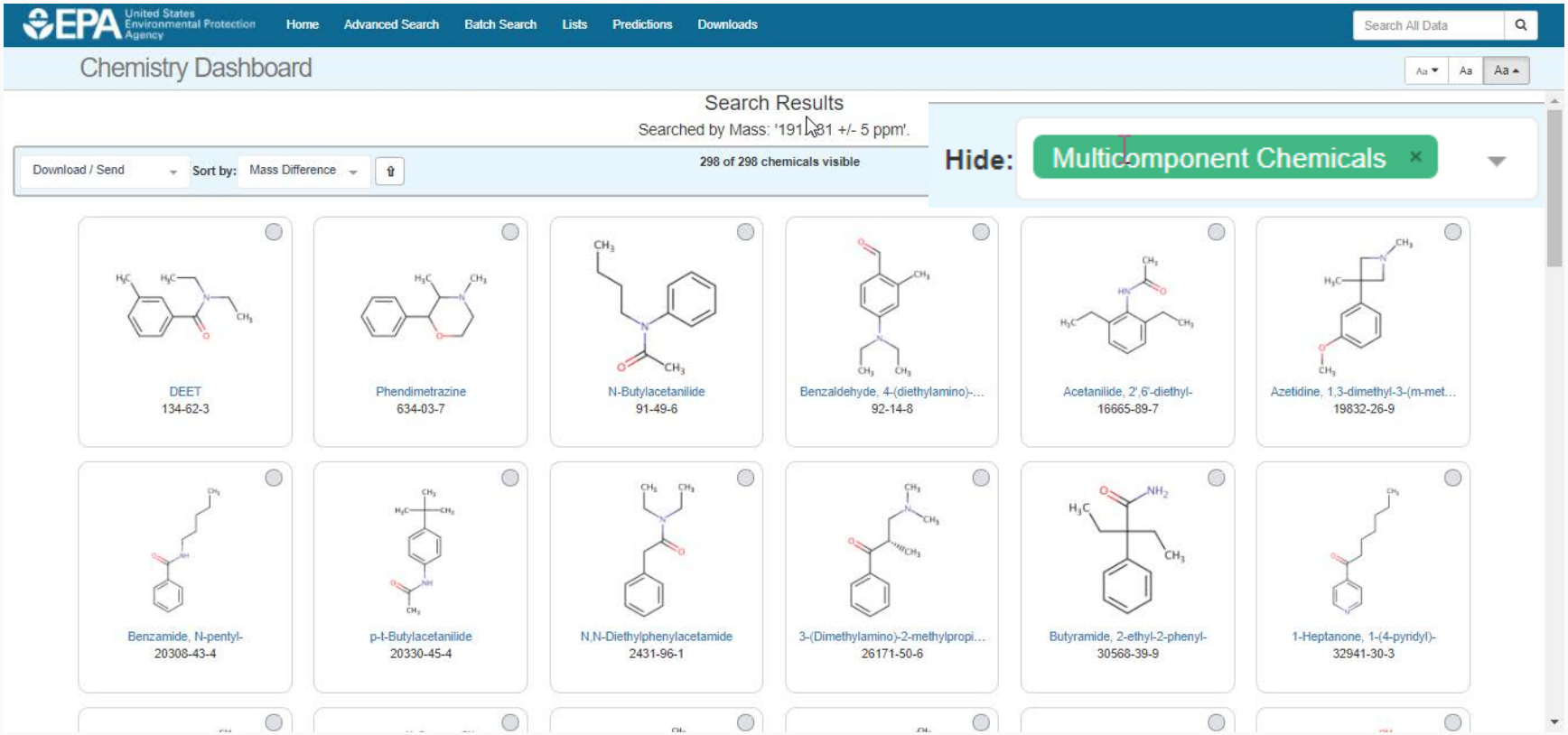


Specific Data-Mappings "MS-Ready Structures"

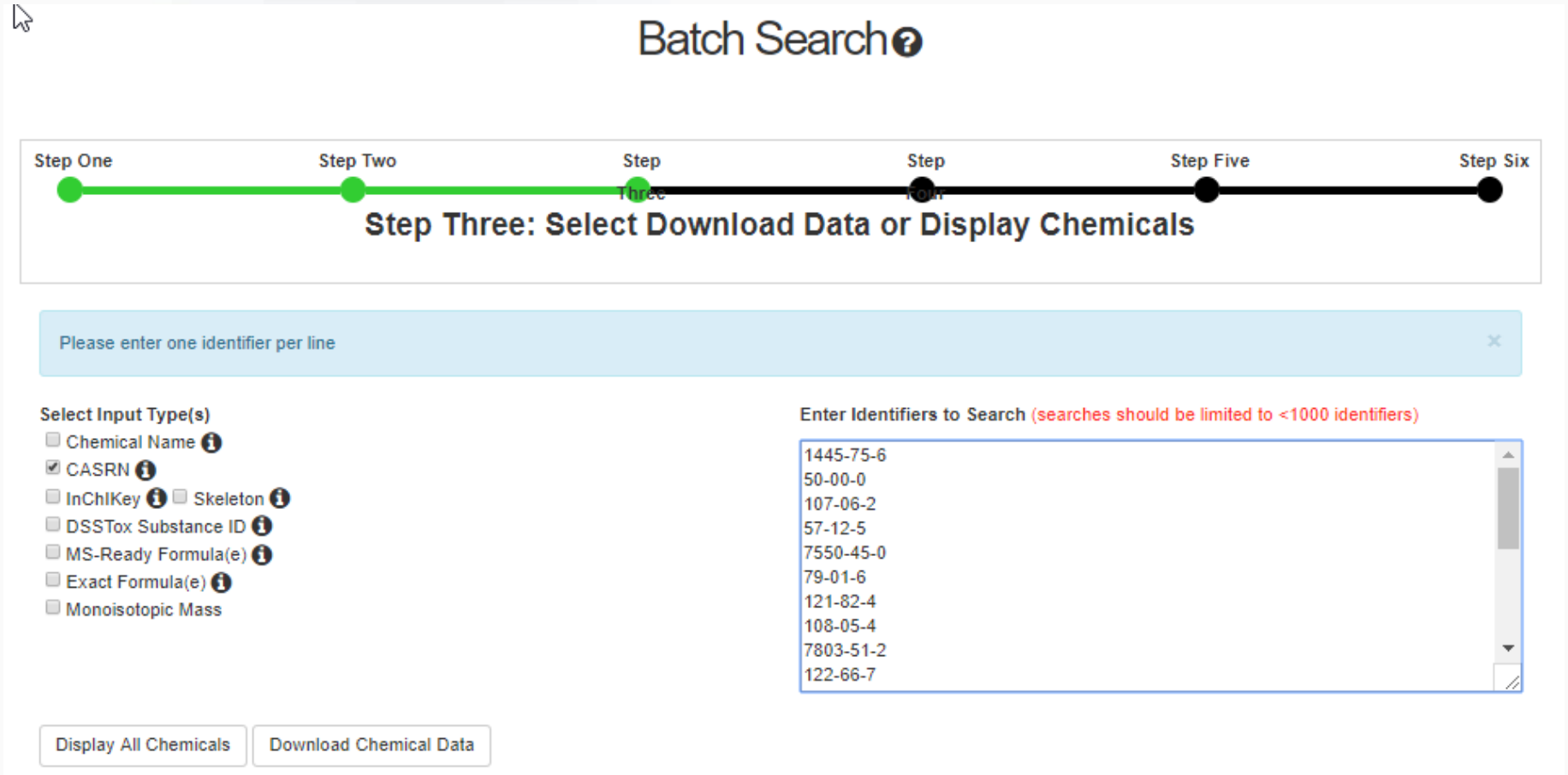




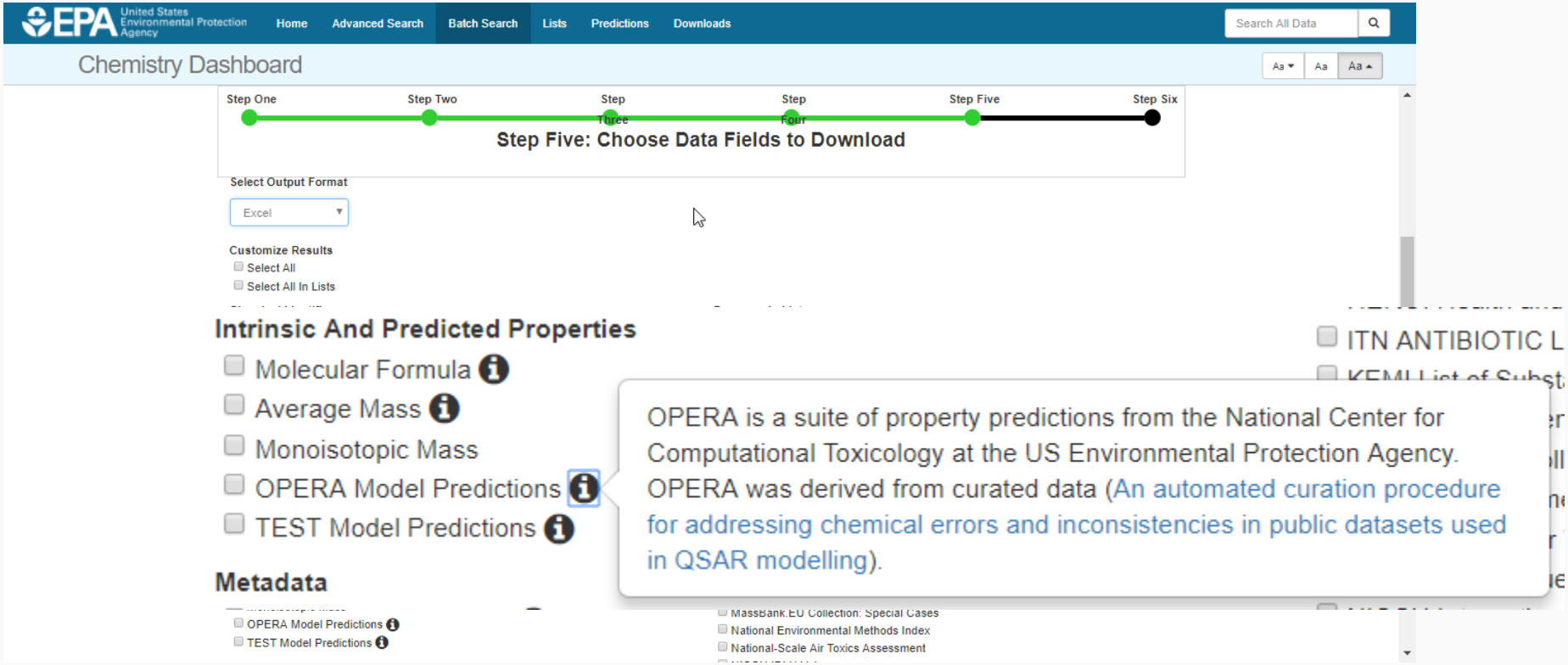
Advanced Searches



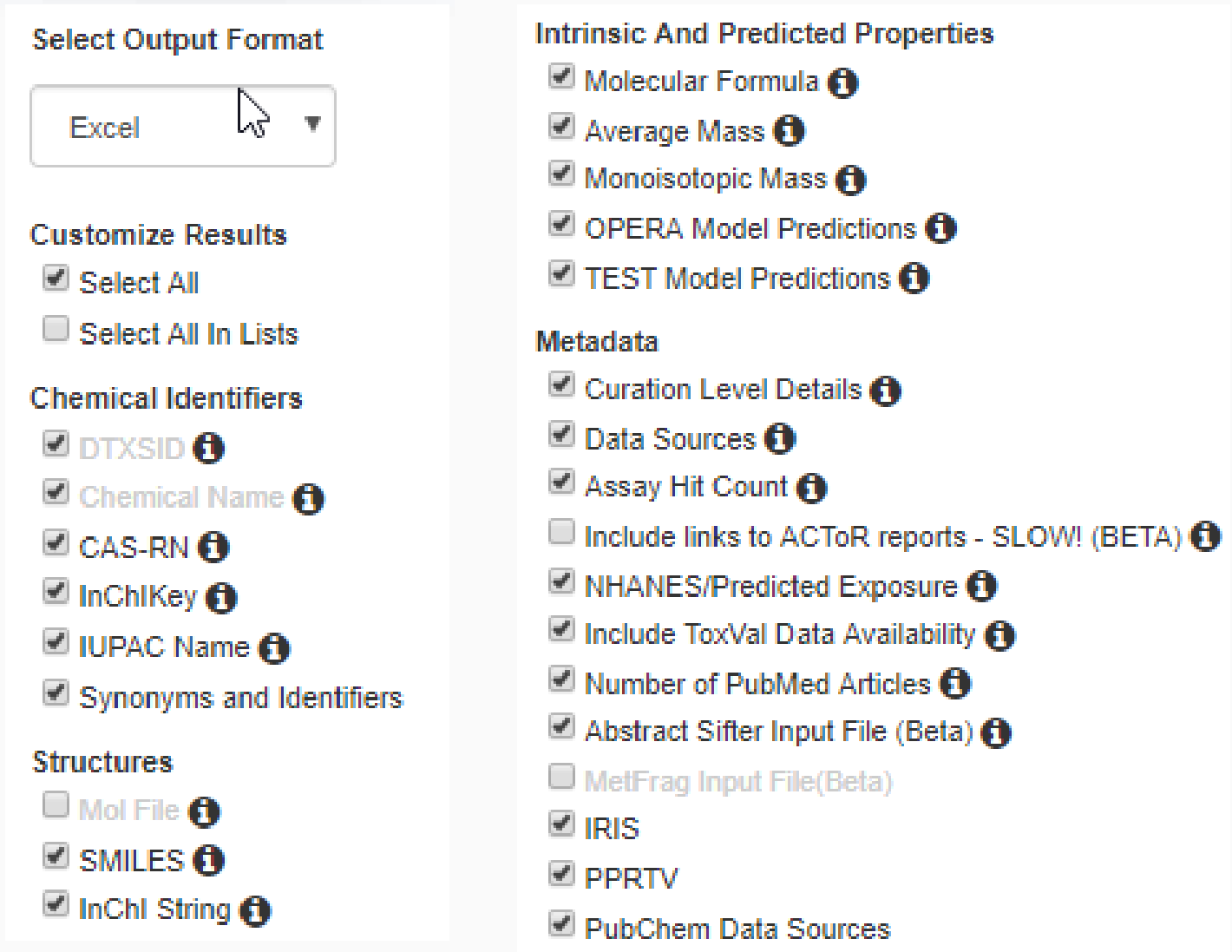
Batch Searches



OPERA and TEST in Batch



Batch Search



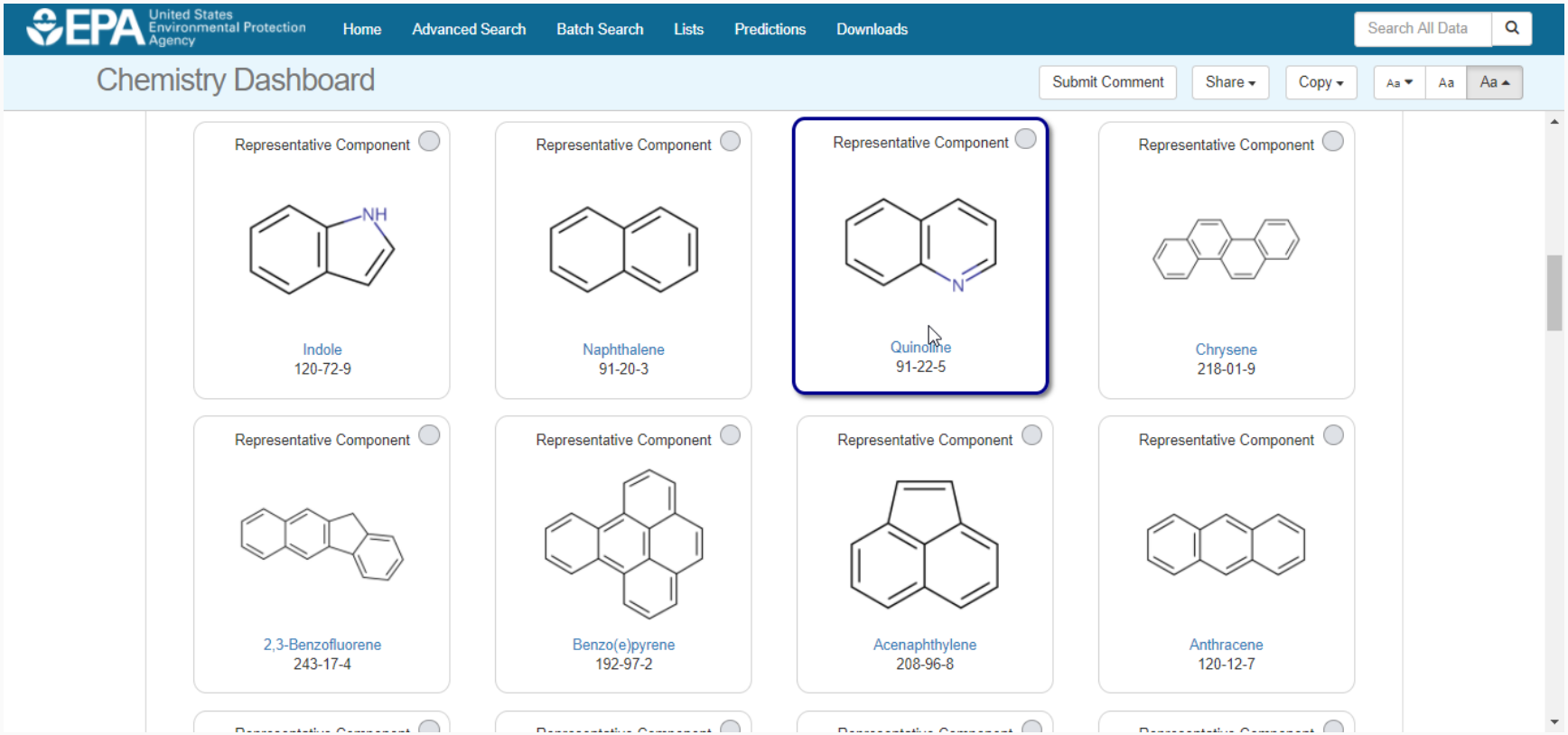
Excel Output

	A	B	C	D	E	F	G	H
1	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	EXPOCAST	EXPOCAST	NHANES	TOXVAL_D
2	1445-75-6	CAS-RN	DTXSID5024051	Diisopropyl methylpho	2.09e-08	Y	-	Y
3	50-00-0	CAS-RN	DTXSID7020637	Formaldehyde	1.32e-06	Y	-	Y
4	107-06-2	CAS-RN	DTXSID6020438	1,2-Dichloroethane	4.9e-06	Y	-	Y
5	57-12-5	CAS-RN	DTXSID6023991	Cyanide	-	-	-	Y
6	7550-45-0	CAS-RN	DTXSID8042476	Titanium tetrachloride	-	-	-	Y
7	79-01-6	CAS-RN	DTXSID0021383	Trichloroethylene	7.27e-06	Y	-	Y
8	121-82-4	CAS-RN	DTXSID9024142	Cyclonite	6.72e-08	Y	-	Y
9	108-05-4	CAS-RN	DTXSID3021431	Vinyl acetate	8.3e-05	Y	-	Y
10	7803-51-2	CAS-RN	DTXSID2021157	Phosphine	-	-	-	Y
11	122-66-7	CAS-RN	DTXSID7020710	1,2-Diphenylhydrazine	1.49e-07	Y	-	Y
12	101-77-9	CAS-RN	DTXSID6022422	4,4'-Methylenedianiline	6.08e-06	Y	-	Y
13	14017-34-6	CAS-RN	DTXSID90161250	Selenium difluoride	-	-	-	-
14	75-44-5	CAS-RN	DTXSID0024260	Phosgene	-	-	-	Y
15	621-64-7	CAS-RN	DTXSID6021032	N-Nitrosodipropylamine	4.55e-07	Y	-	Y
16	75-09-2	CAS-RN	DTXSID0020868	Dichloromethane	2.02e-06	Y	-	Y
17	100-41-4	CAS-RN	DTXSID3020596	Ethylbenzene	8.32e-05	Y	-	Y
18	7440-28-0	CAS-RN	DTXSID2036035	Thallium	-	-	-	Y
19	108-88-3	CAS-RN	DTXSID7021360	Toluene	8.61e-05	Y	-	Y
20	111-44-4	CAS-RN	DTXSID9020168	Bis(2-chloroethyl) ethe	2.82e-07	Y	-	Y
21	7440-42-8	CAS-RN	DTXSID3023922	Boron	-	-	-	Y
22	7440-29-1	CAS-RN	DTXSID6049800	Thorium	-	-	-	Y

Lists and Families

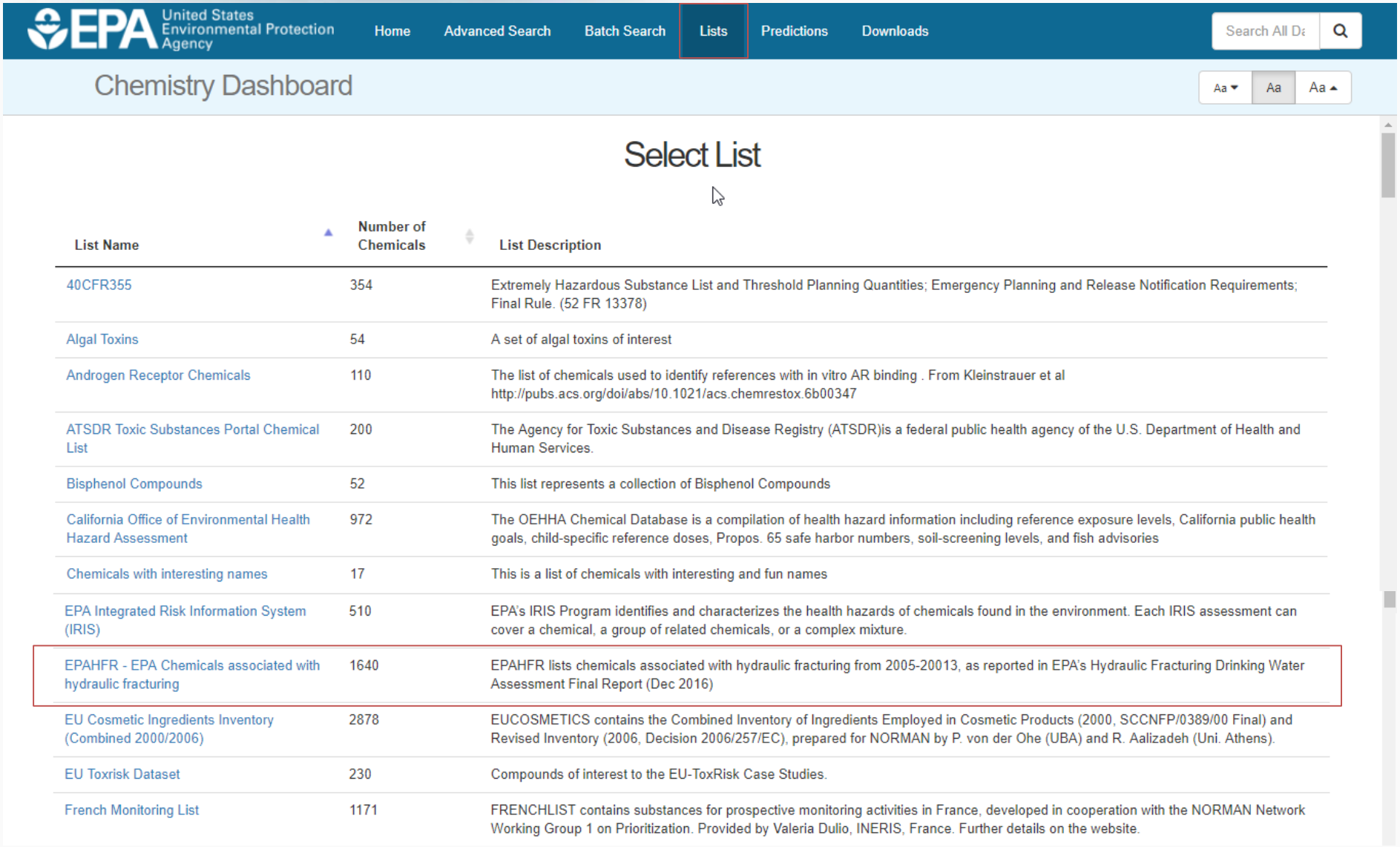
- Growing chemical categories of interest
  - Polychlorinated biphenyls (PCBs)
  - Polybrominated diphenyl ethers (PBDEs)
  - Polyaromatic hydrocarbons (PAHs)

Searching Families of chemicals Polyaromatic Hydrocarbons



A List of Lists of Chemicals

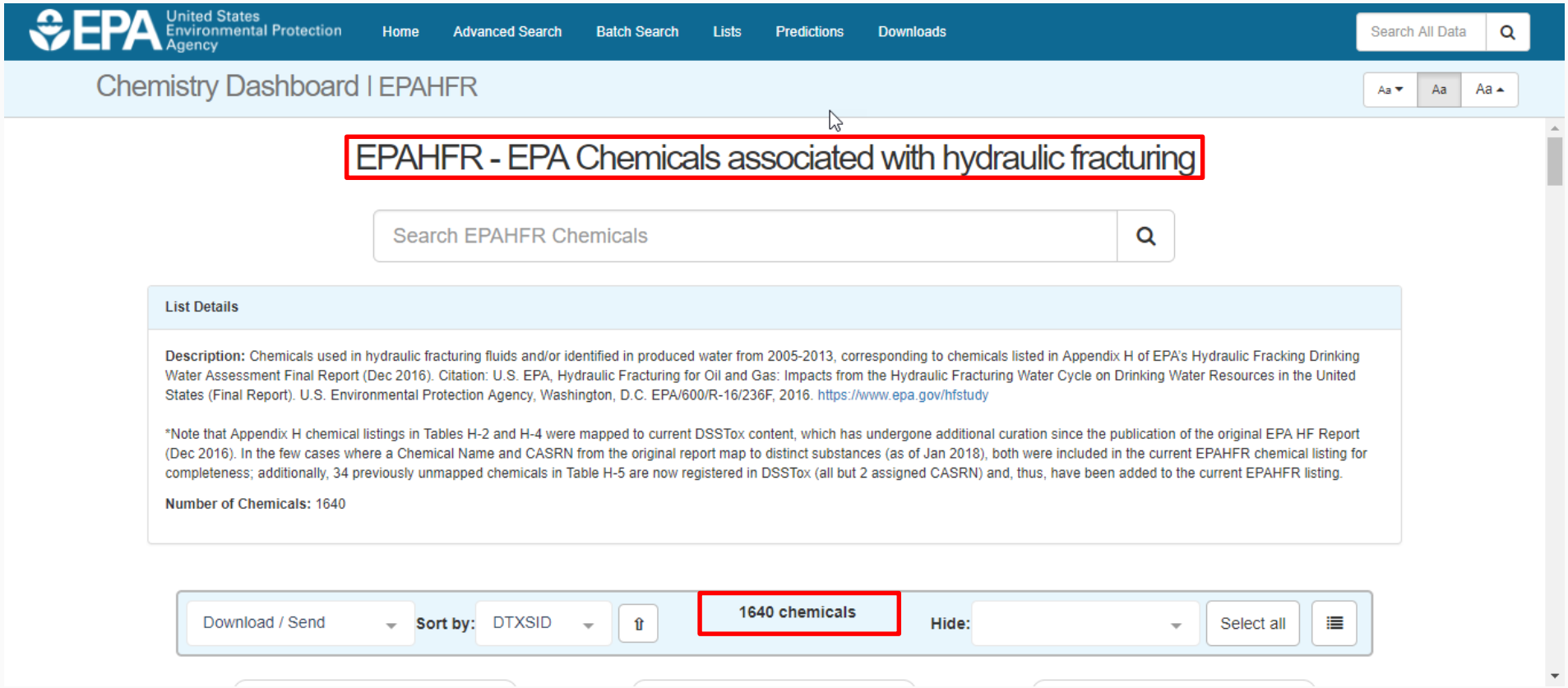
https://comptox.epa.gov/dashboard/chemical_lists



Select List

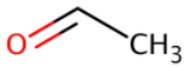
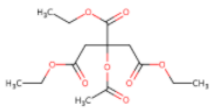
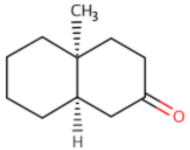
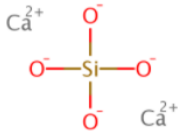
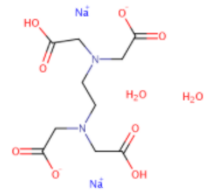
List Name	Number of Chemicals	List Description
40CFR355	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
Algal Toxins	54	A set of algal toxins of interest
Androgen Receptor Chemicals	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstrauer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATSDR Toxic Substances Portal Chemical List	200	The Agency for Toxic Substances and Disease Registry (ATSDR)is a federal public health agency of the U.S. Department of Health and Human Services.
Bisphenol Compounds	52	This list represents a collection of Bisphenol Compounds
California Office of Environmental Health Hazard Assessment	972	The OEHHA Chemical Database is a compilation of health hazard information including reference exposure levels, California public health goals, child-specific reference doses, Propos. 65 safe harbor numbers, soil-screening levels, and fish advisories
Chemicals with interesting names	17	This is a list of chemicals with interesting and fun names
EPA Integrated Risk Information System (IRIS)	510	EPA's IRIS Program identifies and characterizes the health hazards of chemicals found in the environment. Each IRIS assessment can cover a chemical, a group of related chemicals, or a complex mixture.
EPAHFR - EPA Chemicals associated with hydraulic fracturing	1640	EPAHFR lists chemicals associated with hydraulic fracturing from 2005-20013, as reported in EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016)
EU Cosmetic Ingredients Inventory (Combined 2000/2006)	2878	EUCOSMETICS contains the Combined Inventory of Ingredients Employed in Cosmetic Products (2000, SCCNFP/0389/00 Final) and Revised Inventory (2006, Decision 2006/257/EC), prepared for NORMAN by P. von der Ohe (UBA) and R. Aalizadeh (Uni. Athens).
EU Toxrisk Dataset	230	Compounds of interest to the EU-ToxRisk Case Studies.
French Monitoring List	1171	FRENCHLIST contains substances for prospective monitoring activities in France, developed in cooperation with the NORMAN Network Working Group 1 on Prioritization. Provided by Valeria Dulio, INERIS, France. Further details on the website.

The EPA List of Hydraulic Fracturing Chemicals



Many Hydraulic Fracturing Chemicals are “Complex”

EPA United States Environmental Protection Agency

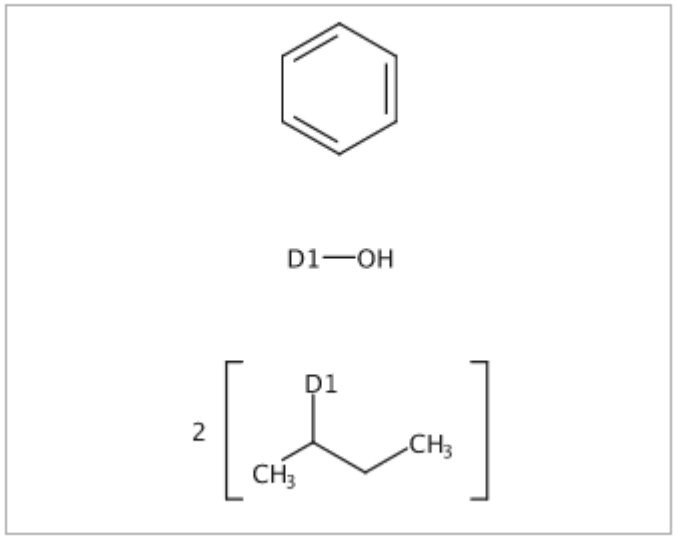
 Acetaldehyde 75-07-0	0 related chemical structures with this substance Amines, dicoco alkyl 61789-76-2	0 related chemical structures with this substance Amines, coco alkyldimethyl 61788-93-0	1 related chemical structure with this substance Cristobalite 14464-46-1	 Copper(I) iodide 7681-65-4
0 related chemical structures with this substance Alcohols, C12-13, ethoxylated 66455-14-9	1 related chemical structure with this substance Alcohols, C12-15, ethoxylated 68131-39-5	0 related chemical structures with this substance Alcohols, C14-15, ethoxylated 68951-67-7	 Iron 7439-89-6	 Acetyltriethyl citrate 77-89-4
 (4aS,8aR)-4a-Methyloctahydronaphthal... 938-06-7	 Dicalcium silicate 10034-77-2	0 related chemical structures with this substance Diethylenetriamine reaction product wit... 68647-57-4	2 related chemical structures with this substance Di-sec-butylphenol 31291-60-8	 Disodium ethylenediaminetetraacetate ... 6381-92-6

Di-sec-butylphenol

CAS Representation

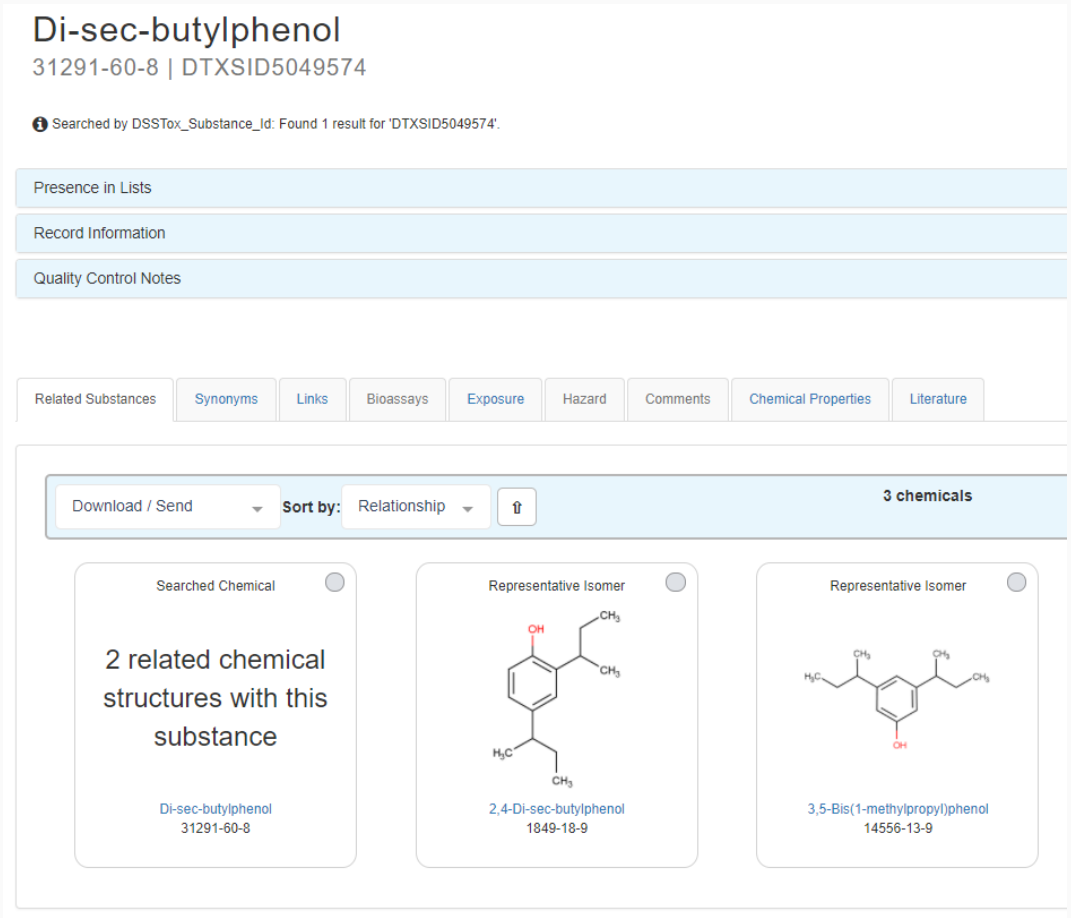
1. 31291-60-8

~31 ~4



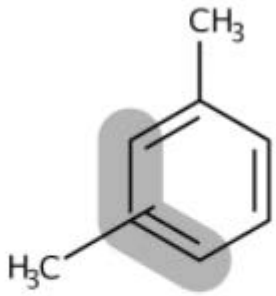
$C_{14}H_{22}O$
Phenol, bis(1-methylpropyl)-

Dashboard Representation

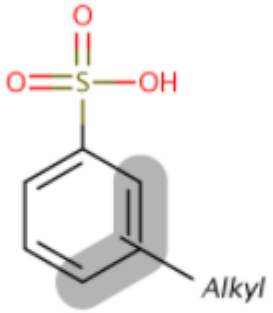


“Markush Structures”

https://en.wikipedia.org/wiki/Markush_structure

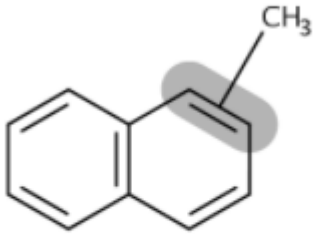


Xylenes
1330-20-7

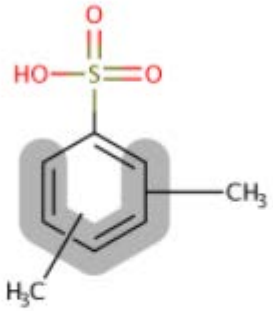


(C10-C16) Alkylbenzenesulfonic acid
68584-22-5

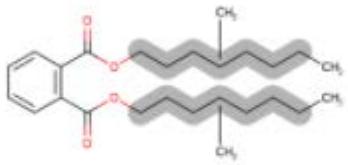
n-Nonylphenol
25154-52-3



Methylnaphthalene
1321-94-4



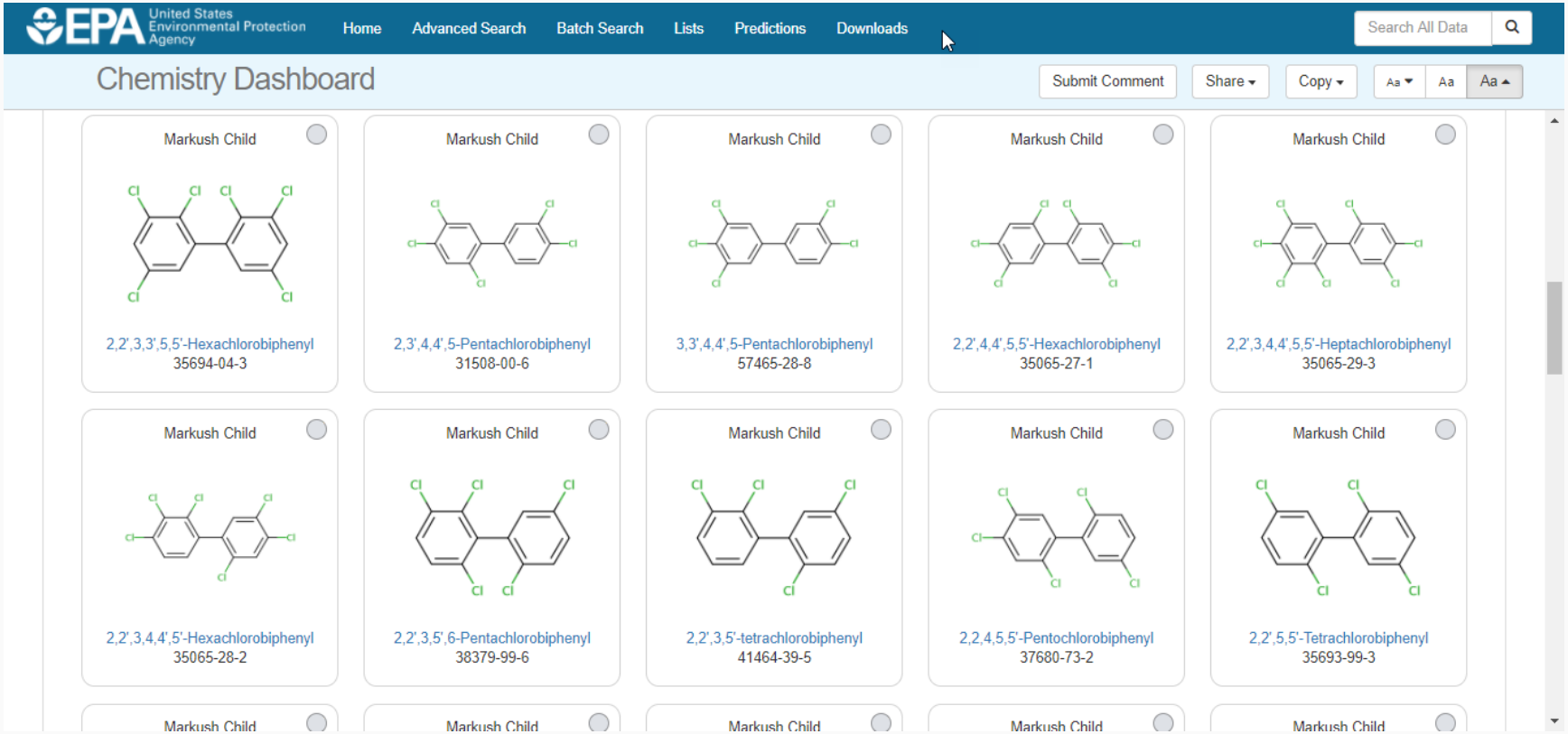
Sodium xylenesulfonate
1300-72-7



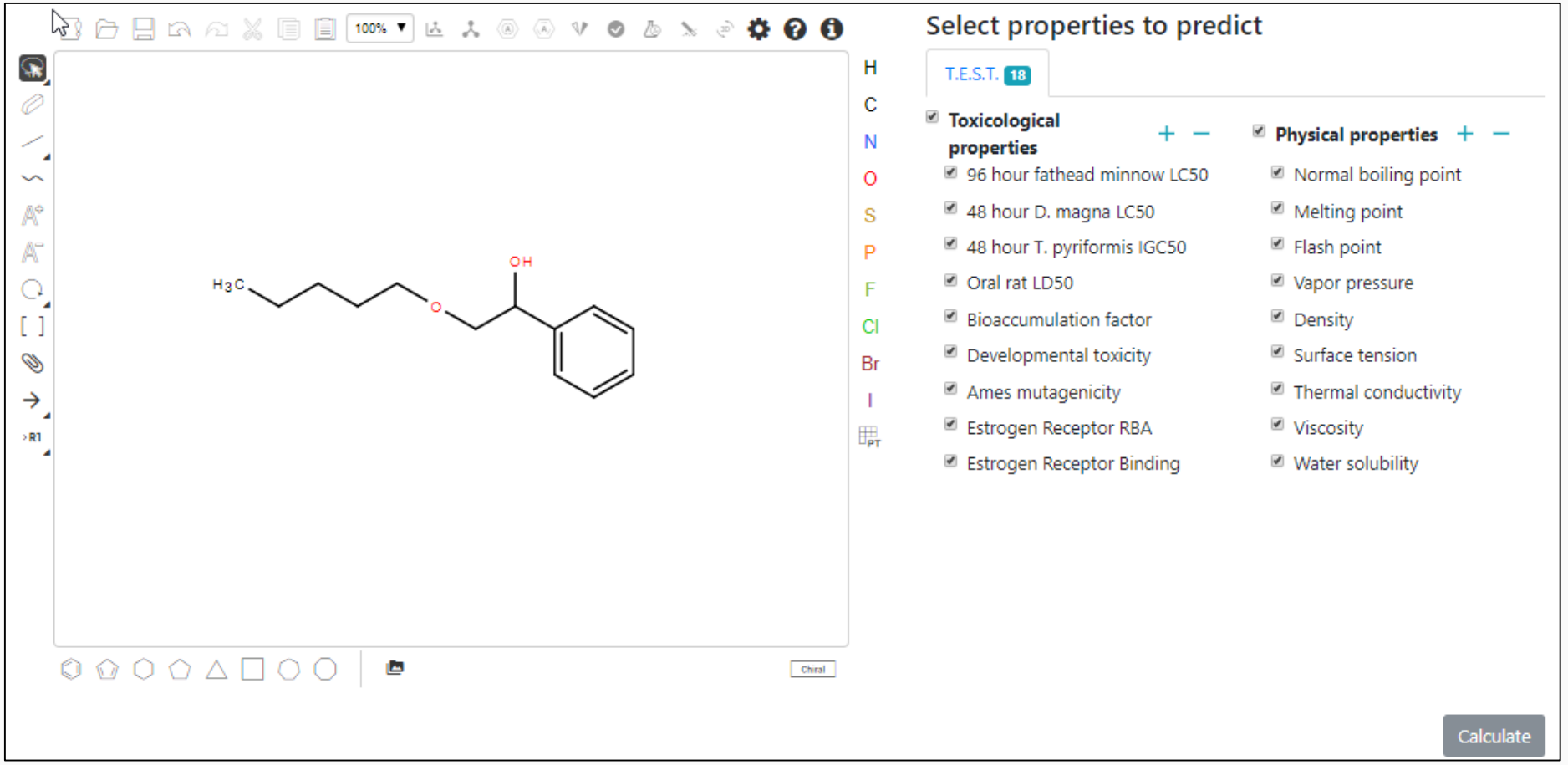
Diisononyl phthalate
28553-12-0

Enumeration of Markush

- Markush structures can be enumerated into chemical families



Real-Time Predictions



Real-Time Predictions

Property	Experimental Value	Prediction				
		Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.477 -Log10(mol/L) 6.954 mg/L	4.195 -Log10(mol/L) 13.288 mg/L	3.994 -Log10(mol/L) 21.110 mg/L	3.478 -Log10(mol/L) 69.224 mg/L	6.238 -Log10(mol/L) 0.120 mg/L
48 hour D. magna LC50		4.398 -Log10(mol/L) 8.328 mg/L	3.877 -Log10(mol/L) 27.677 mg/L	4.039 -Log10(mol/L) 19.026 mg/L	4.084 -Log10(mol/L) 17.173 mg/L	5.593 -Log10(mol/L) 0.532 mg/L
48 hour T. pyriformis IGC50		4.063 -Log10(mol/L) 18.039 mg/L	3.731 -Log10(mol/L) 38.668 mg/L		3.386 -Log10(mol/L) 85.610 mg/L	5.070 -Log10(mol/L) 1.773 mg/L
Oral rat LD50		1.758 -Log10(mol/kg) 3640.950 mg/kg	1.982 -Log10(mol/kg) 2172.756 mg/kg			1.533 -Log10(mol/kg) 6101.245 mg/kg
Bioaccumulation factor		1.797 Log10 62.700	2.202 Log10 159.310	1.287 Log10 19.346	1.181 Log10 15.157	2.520 Log10 330.834
Developmental toxicity		false	false	false		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-3.075 Log10 $8.418*10^{-4}$	-3.078 Log10 $8.356*10^{-4}$	-3.720 Log10 $1.907*10^{-4}$		-2.427 Log10 0.004
Estrogen Receptor Binding		true	true	true	false	true

Real-Time Predictions

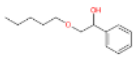
Predicted Water solubility at 25°C for OC(C=1C=CC=CC1)COCCCCC from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Water solubility at 25°C -Log10(mol/L)	N/A	2.46
Water solubility at 25°C mg/L	N/A	723.26

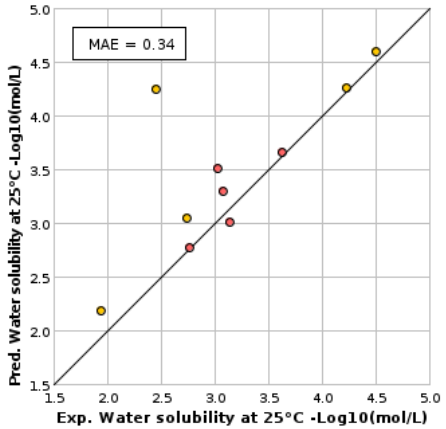
Individual Predictions

Method	Predicted value -Log10(mol/L)
Hierarchical clustering	2.42
Group contribution	2.32
Nearest neighbor	2.64



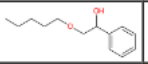
Predictions for the test chemical and for the most similar chemicals

Prediction results (colors defined in table below)

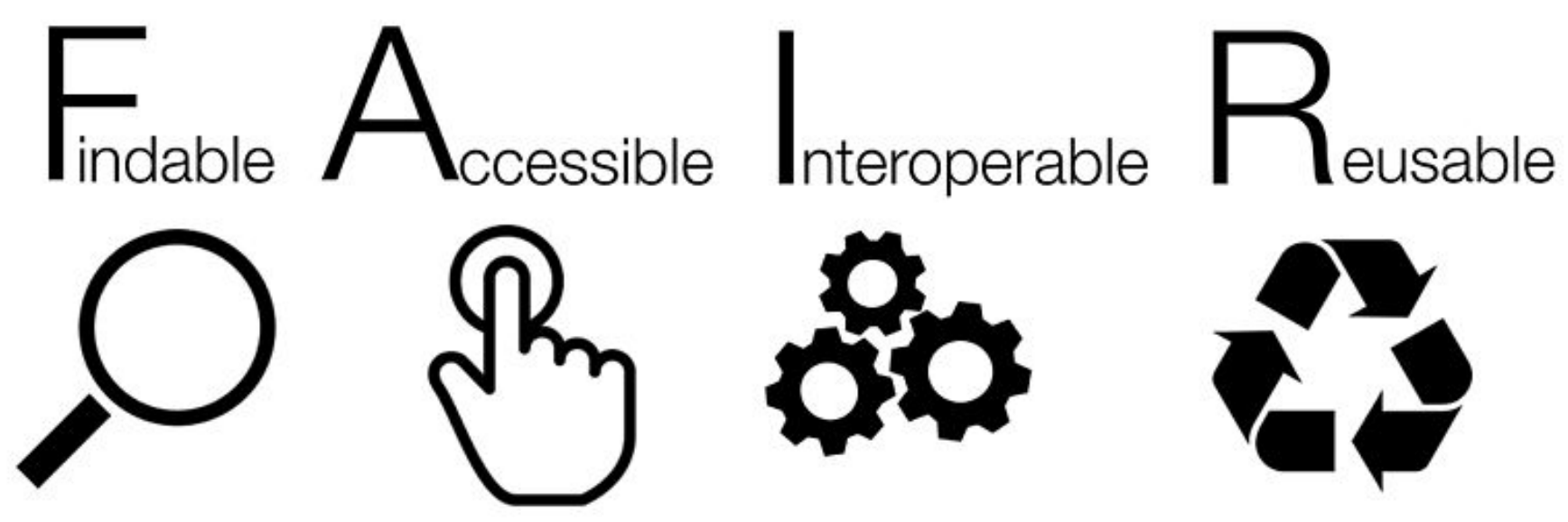


Chemicals	MAE*
Entire set	0.58
Similarity coefficient ≥ 0.5	0.34

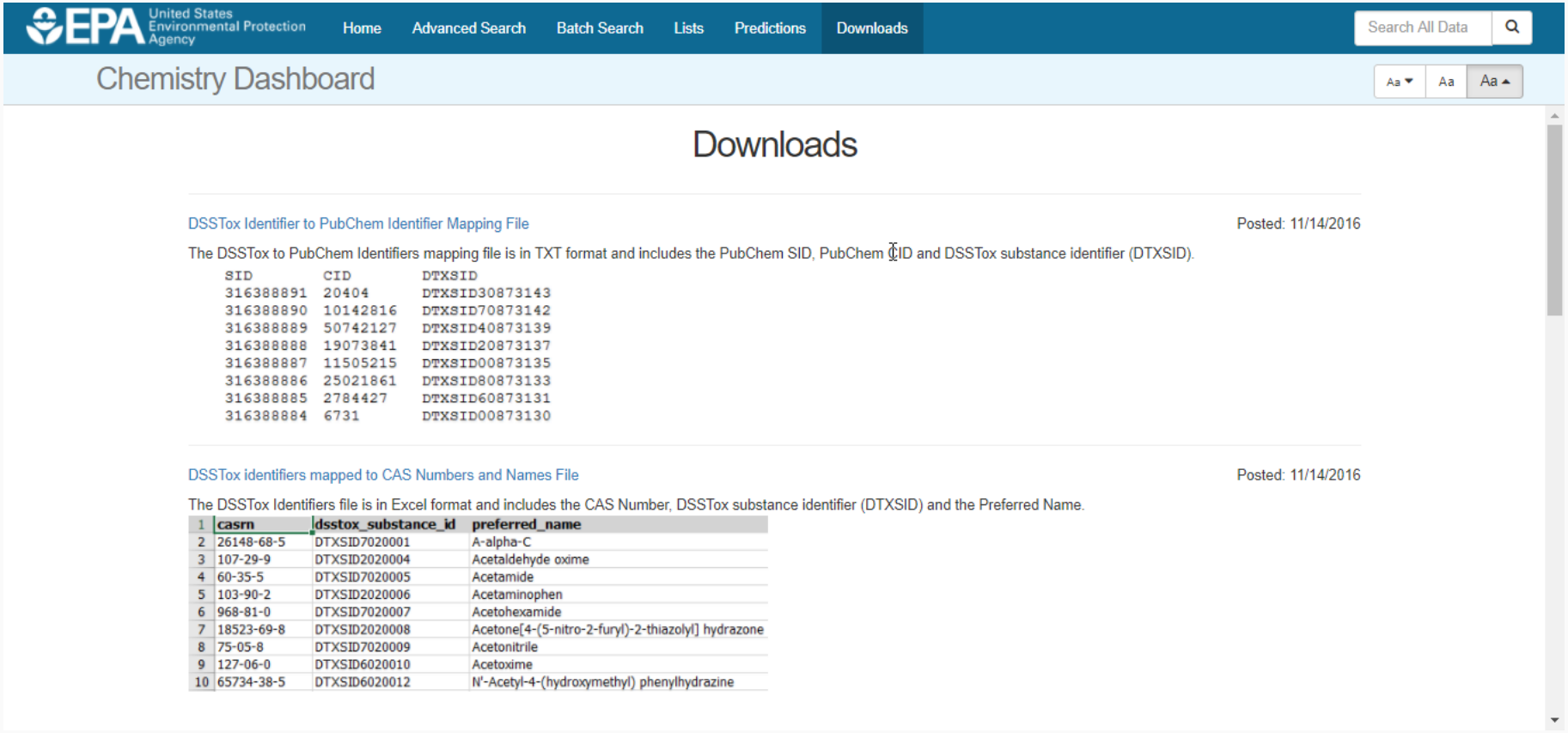
*Mean absolute error in -Log10(mol/L)

CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
OC(C=1C=CC=CC1)COCCCCC (test chemical)			N/A	2.46
104-40-5		0.68	4.50	4.60
1219-38-1		0.67	4.22	4.26

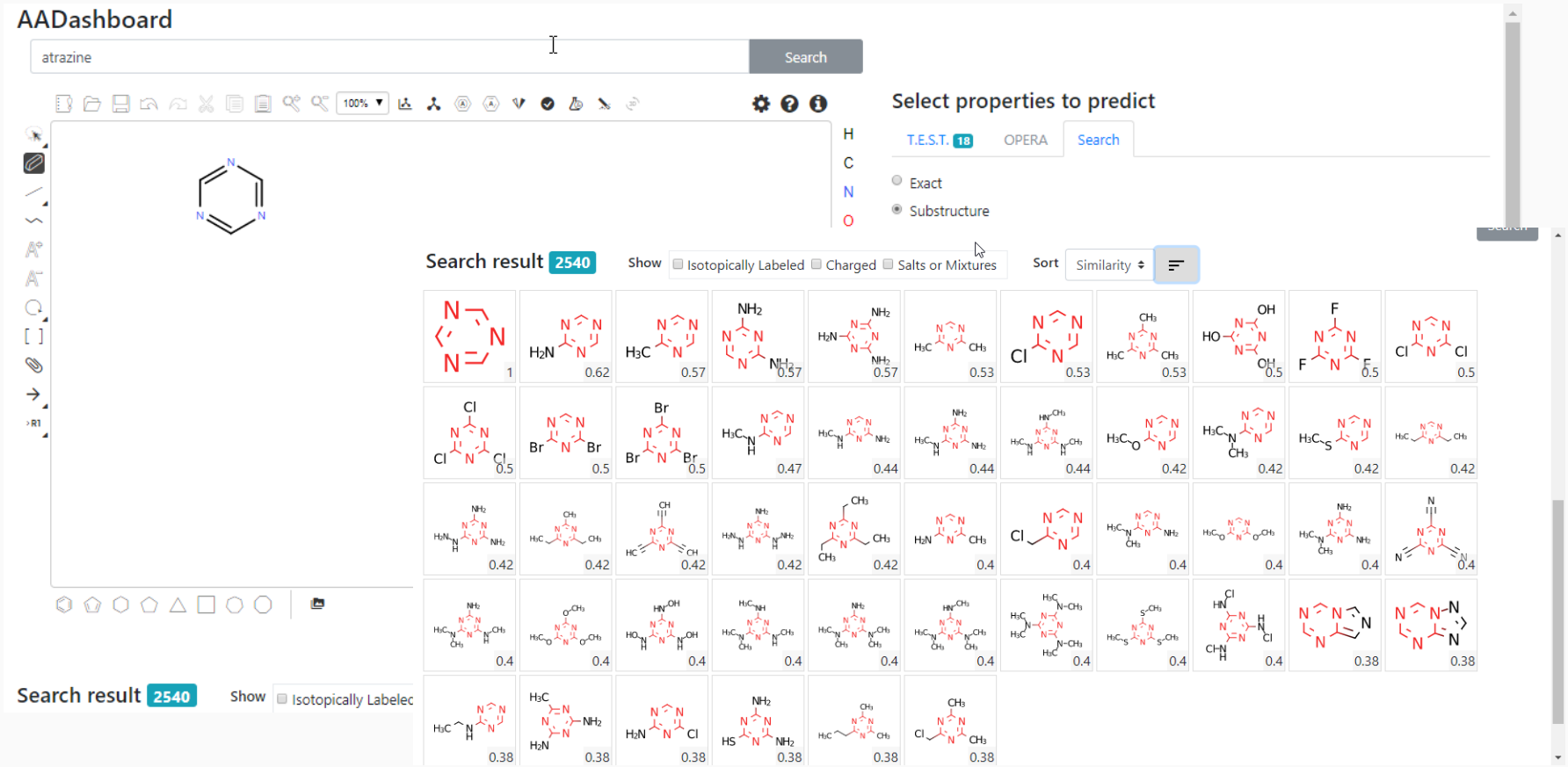
Our support for FAIR Data



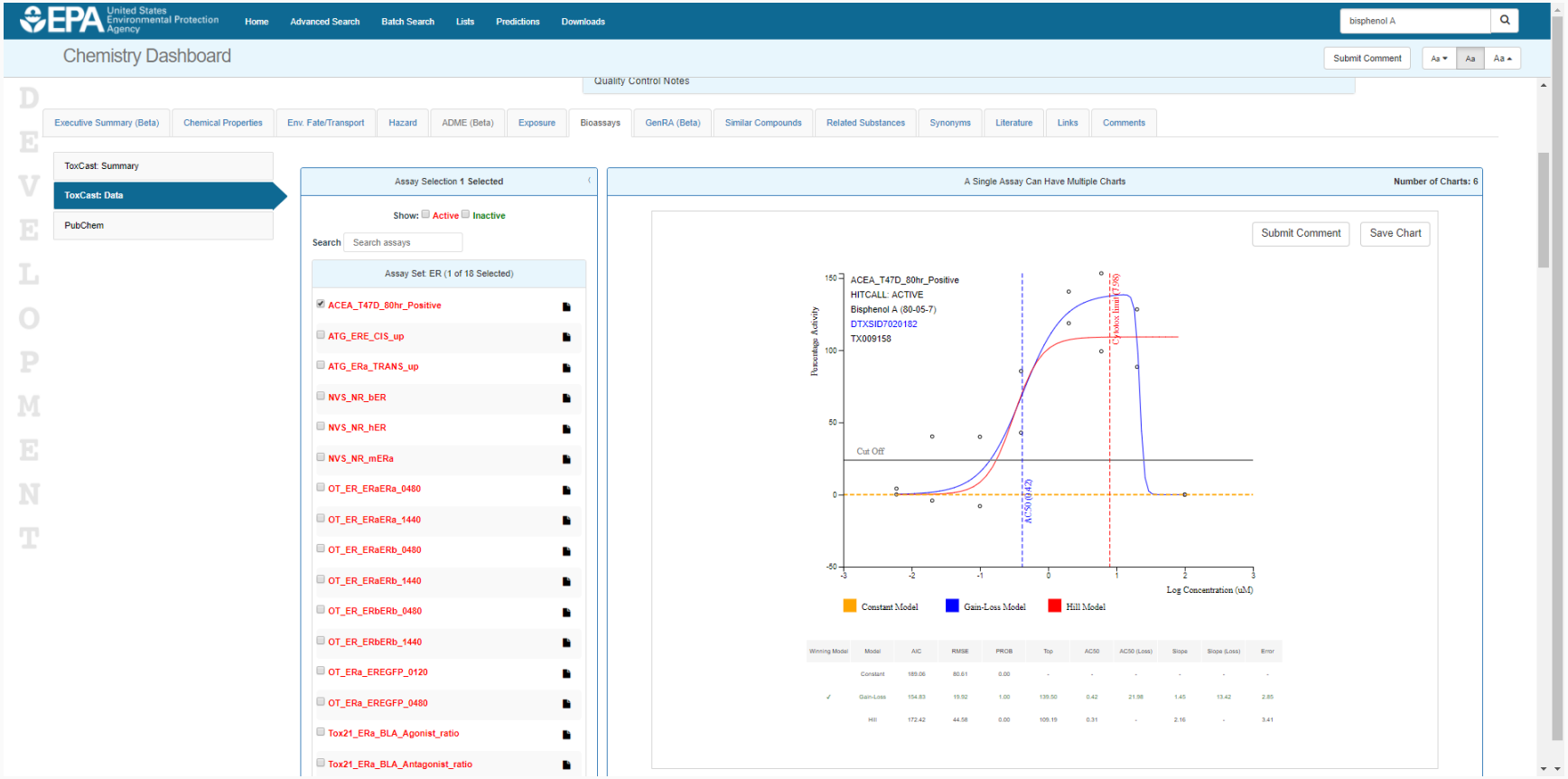
Downloadable Data



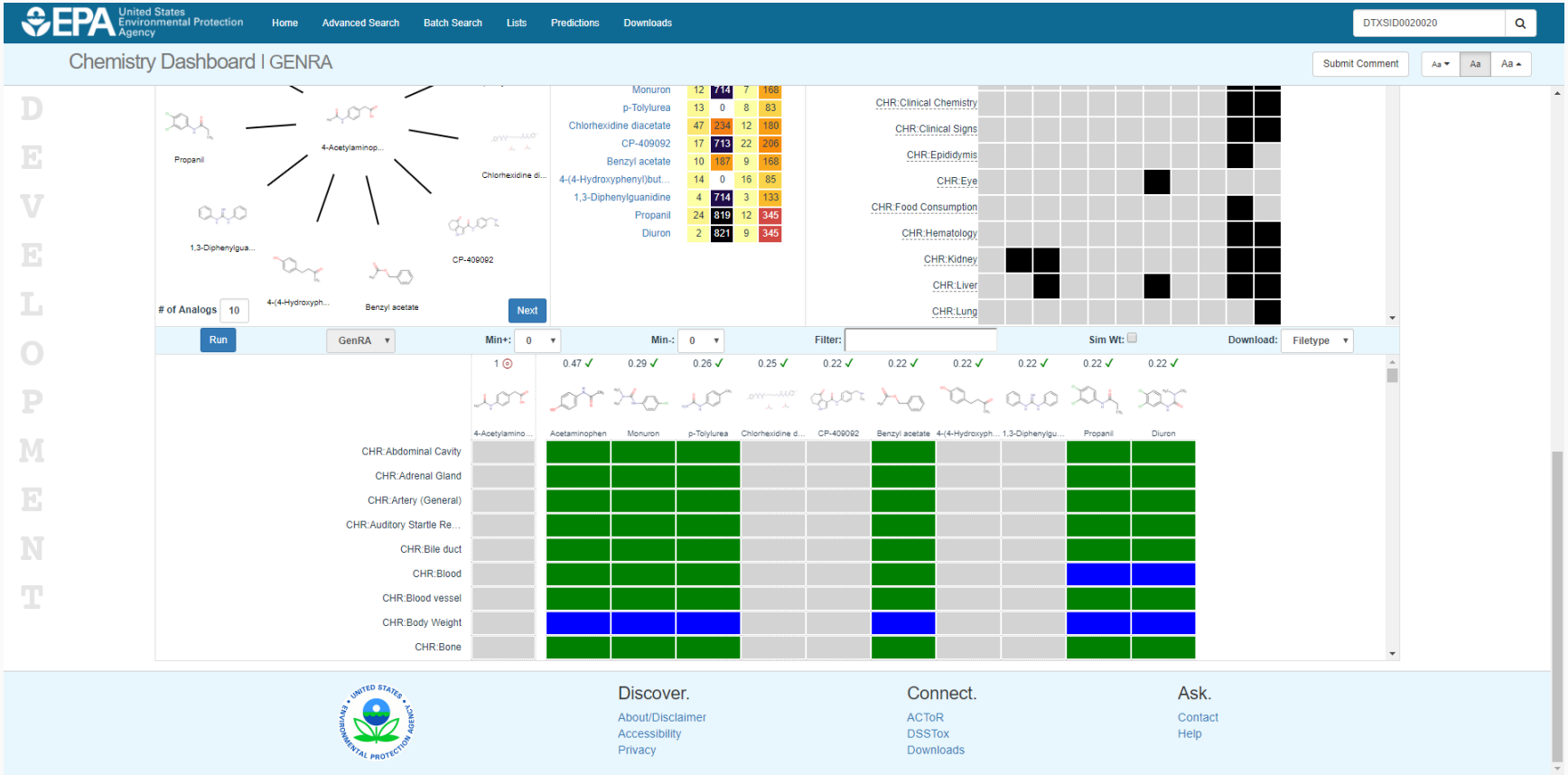
Prototype Development



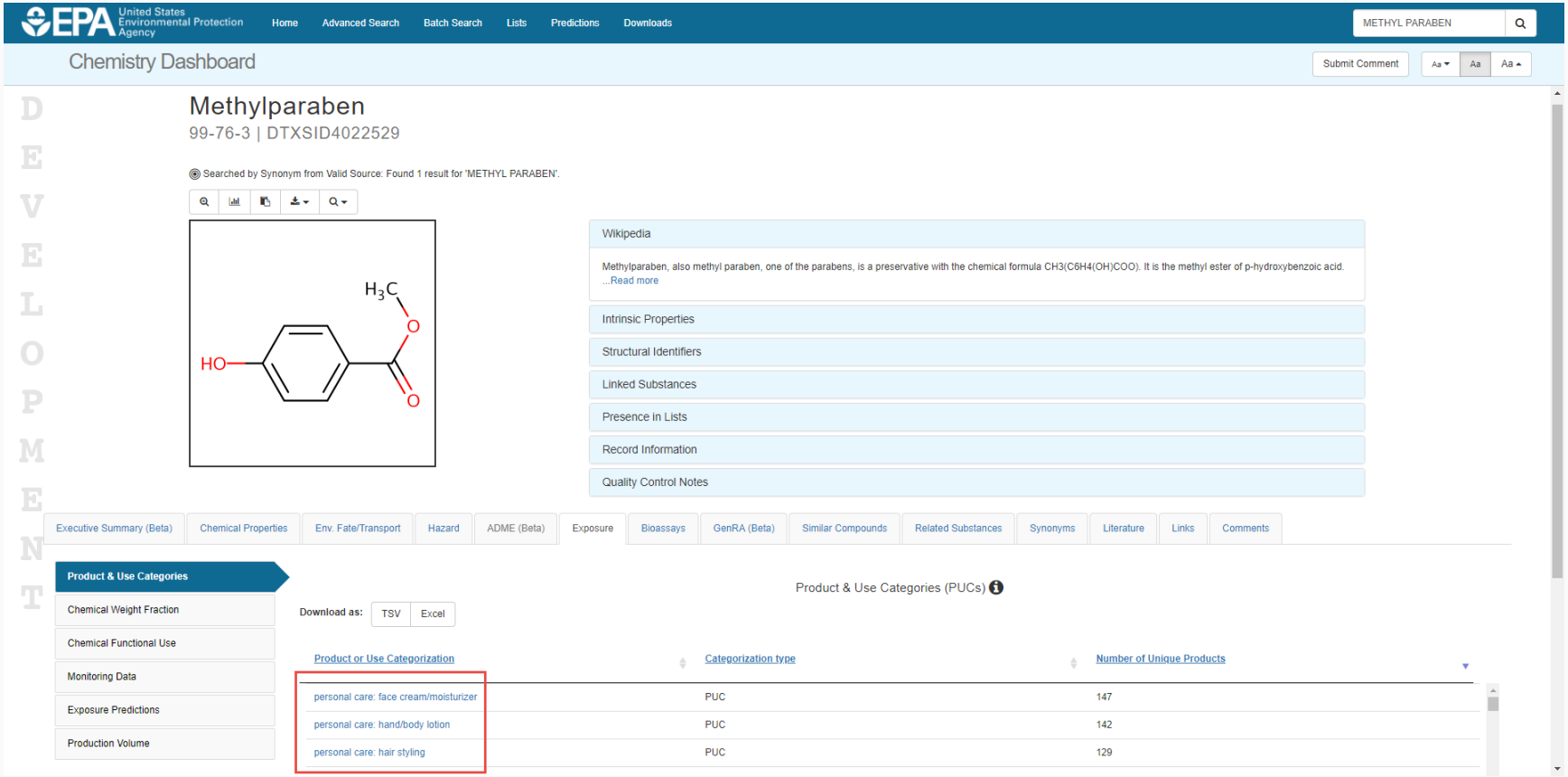
Work in Progress – ToxCast Data
Early start transferring EDSP



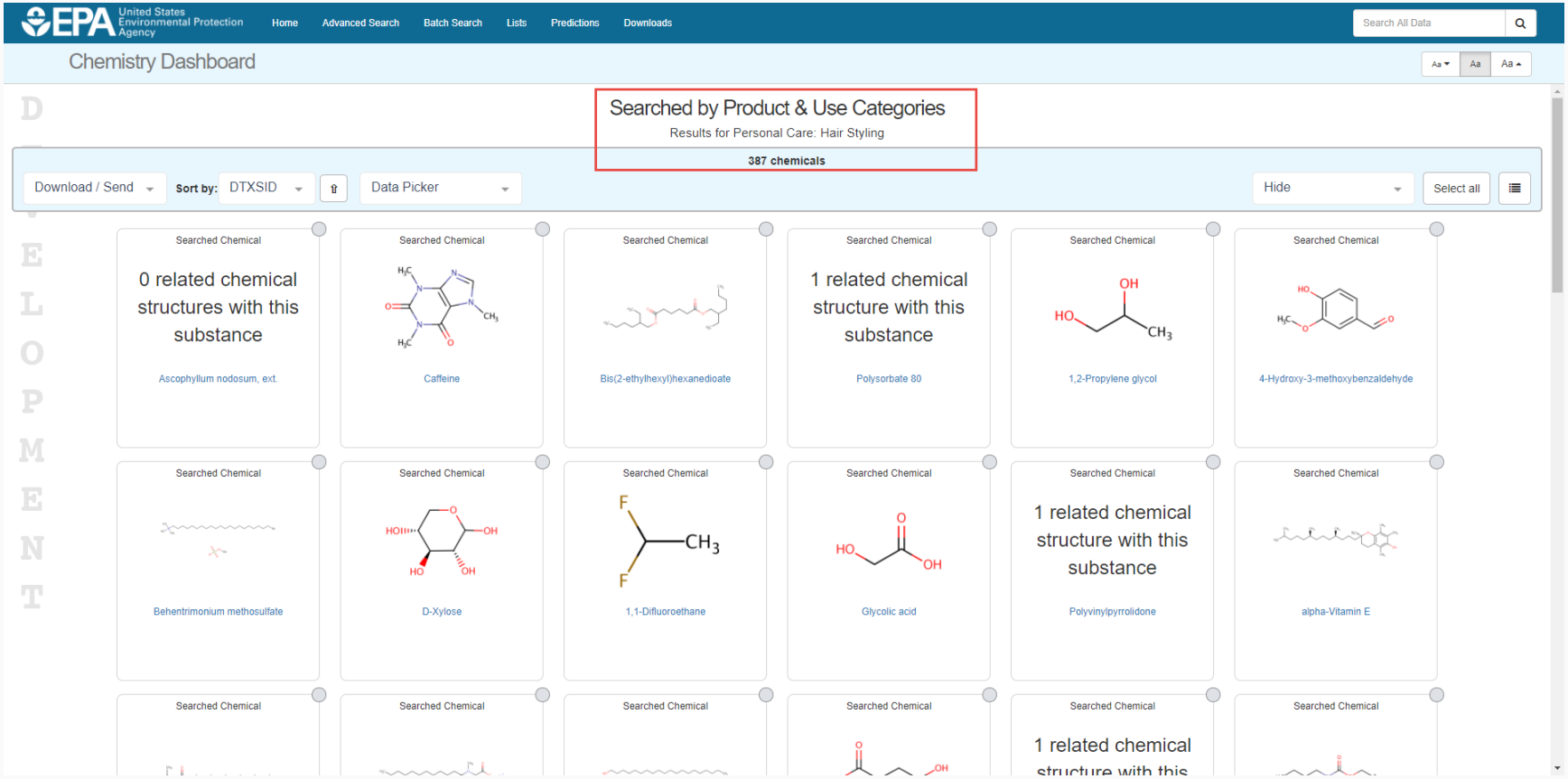
Work in Progress – GenRA



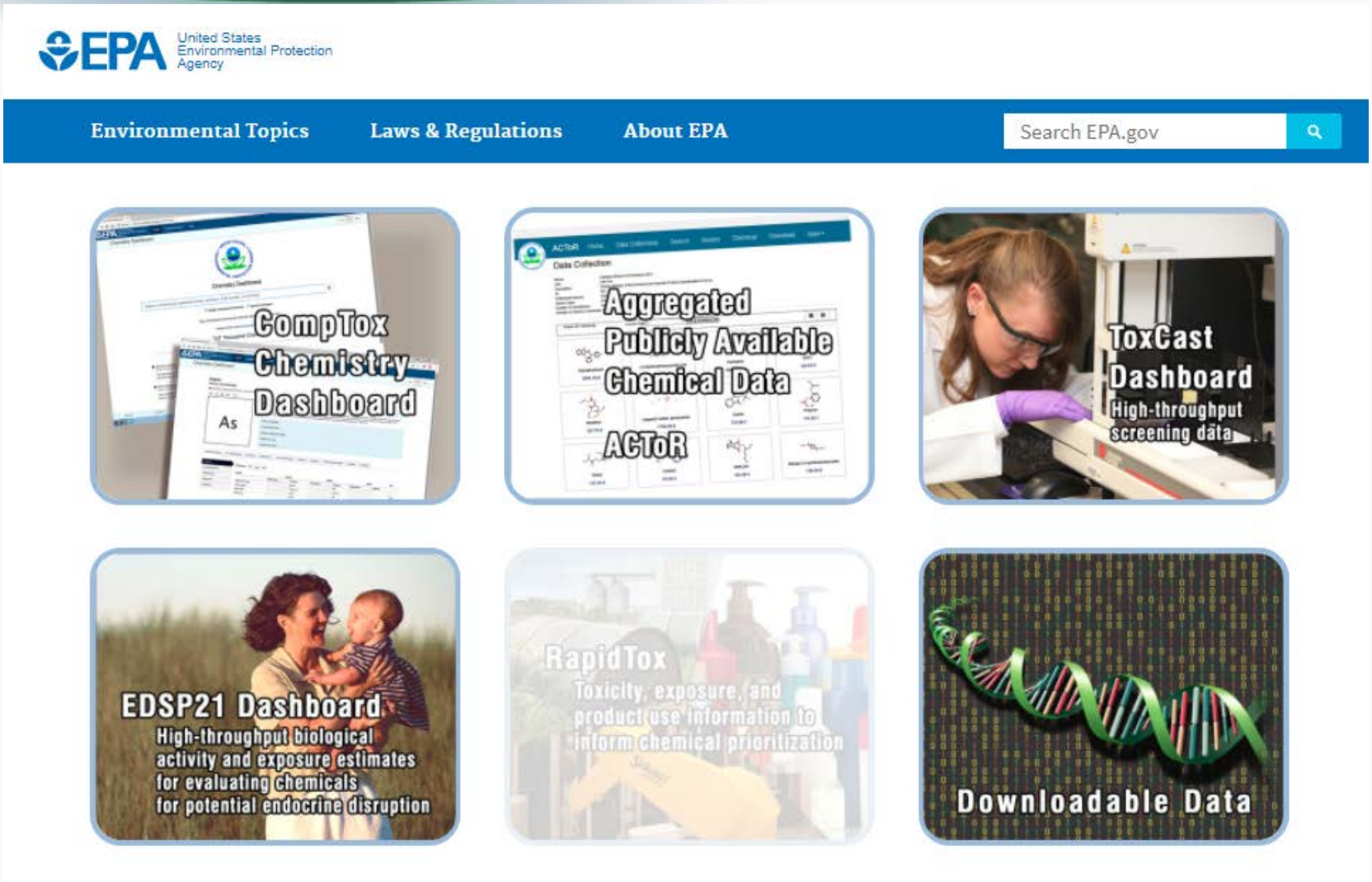
What chemicals in What Products?



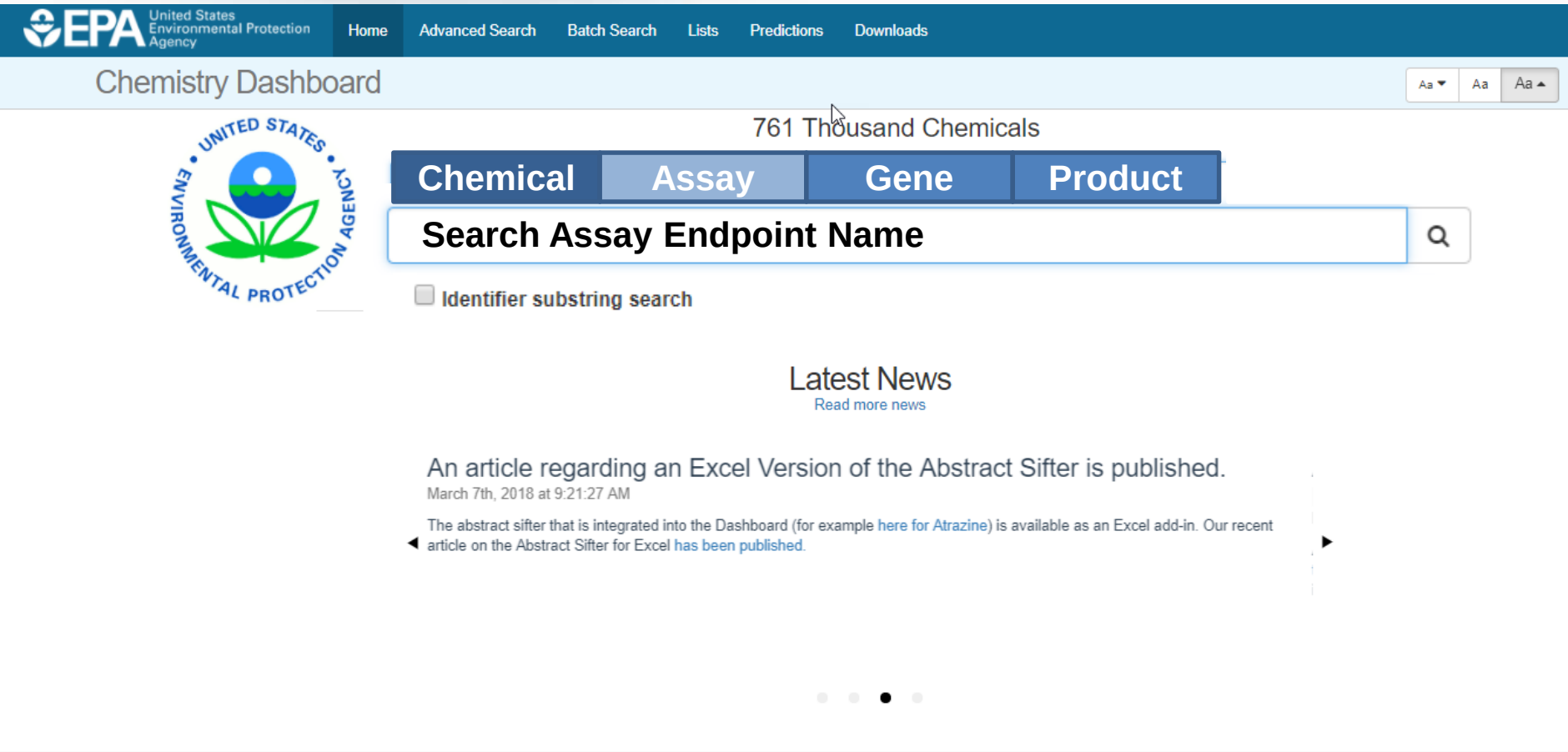
What chemicals in What Products?



Coming Soon


United States Environmental Protection Agency
Environmental Topics
Laws & Regulations
About EPA
Search EPA.gov
CompTox Chemistry Dashboard
Aggregated Publicly Available Chemical Data
ACToR
ToxCast Dashboard
High-throughput screening data
EDSP21 Dashboard
High-throughput biological activity and exposure estimates for evaluating chemicals for potential endocrine disruption
RapidTox
Toxicity, exposure, and product use information to inform chemical prioritization
Downloadable Data

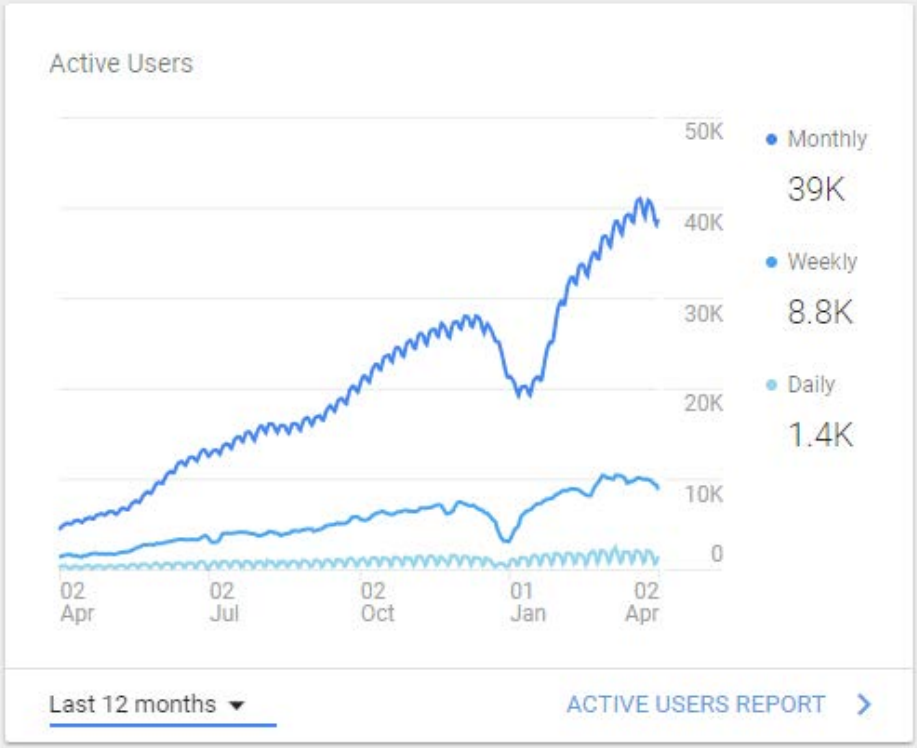
Future Search Possibilities



April 1st was the 2nd birthday

Take up

How are your active users trending over time?



Country	Acquisition	
	Users ↓	New Users
	8,766 % of Total: 100.00% (8,766)	7,268 % of Total: 100.06% (7,264)
1. United States	**3,153** (35.97%)	2,611 (35.92%)
2. India	**910** (10.38%)	741 (10.20%)
3. South Korea	**450** (5.13%)	370 (5.09%)
4. Canada	**334** (3.81%)	267 (3.67%)
5. United Kingdom	**287** (3.27%)	241 (3.32%)
6. Japan	**285** (3.25%)	221 (3.04%)
7. Germany	**239** (2.73%)	188 (2.59%)
8. France	**227** (2.59%)	183 (2.52%)
9. China	**177** (2.02%)	136 (1.87%)
10. Brazil	**140** (1.60%)	117 (1.61%)

Conclusion

- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules”
  - Experimental and predicted properties
  - Human and Ecological Hazard data
  - Exposure data – products, data in the environment
  - *In vitro* bioassay data – ToxCast/Tox21
  - Literature searching – Google Scholar and PubMed
  - Specialized searches – mass/formula for analytical support
  - Batch searching and Real Time Predictions
- The primary architecture for NCCT data

Acknowledgments

- The NCCT CompTox Chemistry Dashboard Development Team
- The NCCT Team
- NERL scientists – MS, Exposure, CPDat
- Kamel Mansouri – OPERA models
- Todd Martin – TEST predictions

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