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The CompTox Chemistry Dashboard v2.6 – Delivering Improved Access to Data and Real Time Predictions

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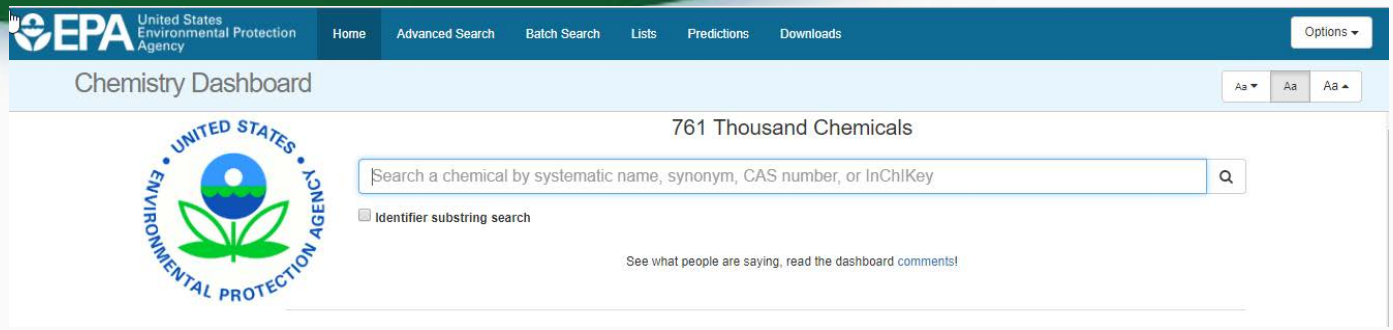
The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

March 29th 2018
Communities of Practice

Outline

- A *very* basic intro to the dashboard
- Our latest release – Getting to What's New?
- New data and functionality
- From data to real data predictions
- Work in progress

The CompTox Chemistry Dashboard



- A **publicly accessible website** delivering access:
  - ~**760,000 chemicals** with related property data
  - Experimental and predicted physicochemical property data
  - Experimental Human and Ecological hazard 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
  - Real time prediction of physchem and toxicity endpoints

How is it built?

https://jcheminf.springeropen.com/articles/10.1186/s13321-017-0247-6

EPA United States Environmental Protection Agency

Williams et al. J Cheminform (2017) 9:61
DOI 10.1186/s13321-017-0247-6

Journal of Cheminformatics

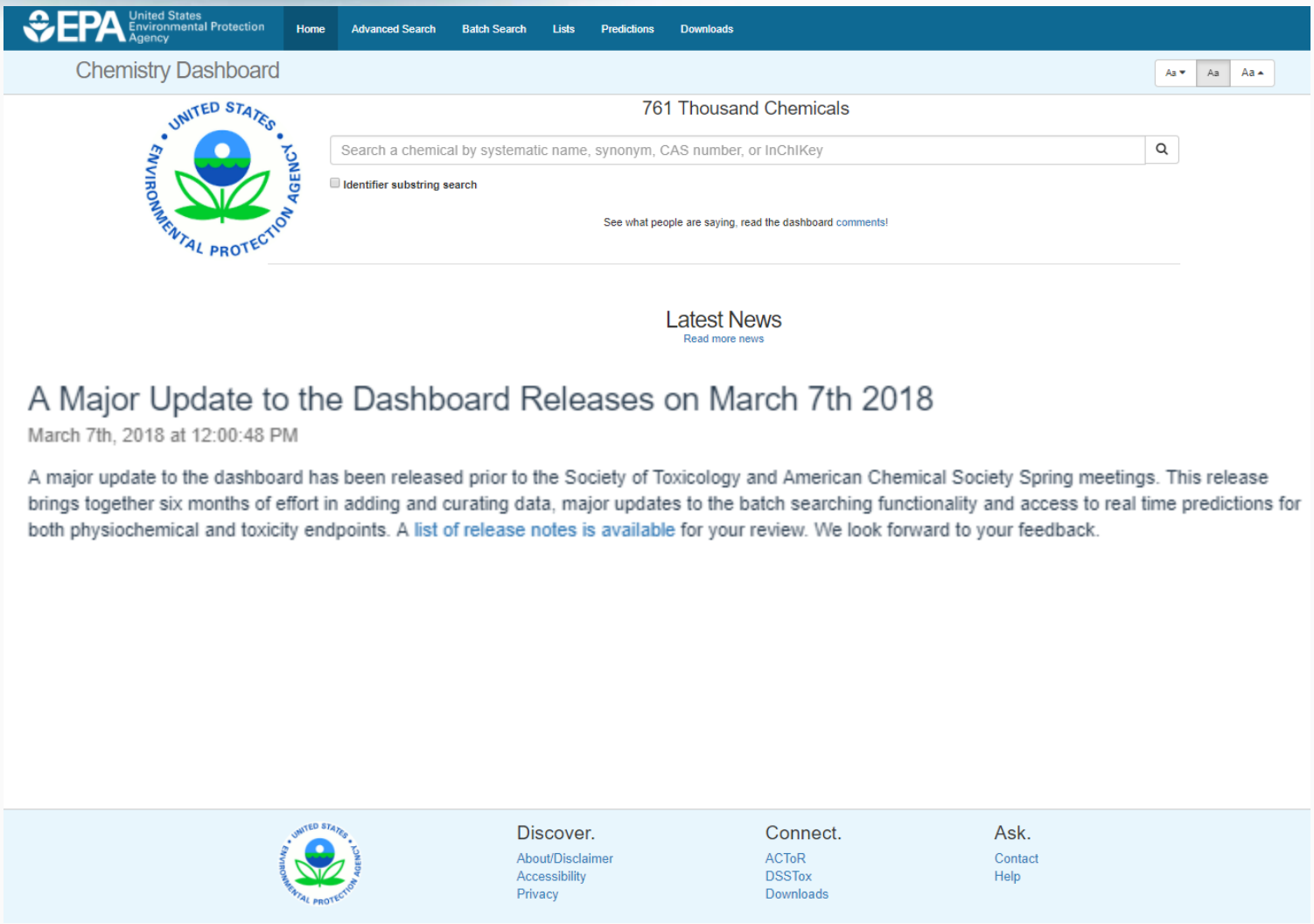
DATABASE Open Access

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

Antony J. Williams[1*], Christopher M. Grulke[1], Jeff Edwards[1], Andrew D. McEachran[2], Kamel Mansouri[1,2,4], Nancy C. Baker[3], Grace Patlewicz[1], Imran Shah[1], John F. Wambaugh[1], Richard S. Judson[1] and Ann M. Richard[1]

Release Notes

https://comptox.epa.gov/dashboard/resources/comptox_release_notes.pdf



Release Notes

https://comptox.epa.gov/dashboard/resources/comptox_release_notes.pdf

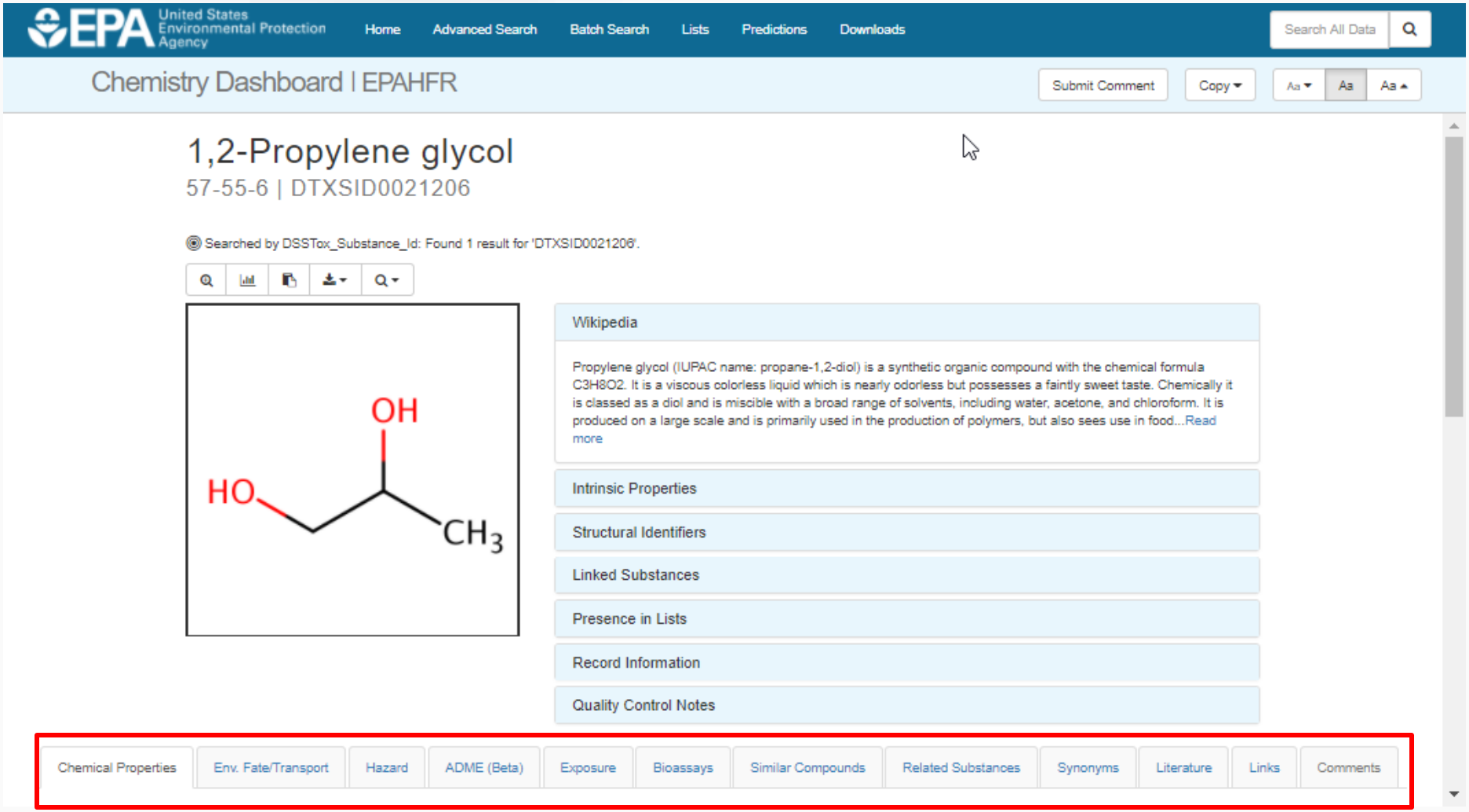
- A detailed list of new functionality and fixes

** New Functionality
* [ICD-756] - Produce link from ToxCast In Vitro Data Assay into AOP
* [ICD-851] - Improve generation of molecular formulae
* [ICD-929] - Include Monoisotopic Mass as Input for Batch Searching
* [ICD-975] - Batch Search export for Batch Mass searching of MS Ready Structures
* [ICD-977] - Add ability to download "QSAR-Ready SMILES" presently used by OPERA in the batch search
* [ICD-1011] - Provide Download of PubMed ID and Article Title from Abstract Sifter Page
* [ICD-1070] - Provide ability to perform batch search based on First Layer of InChIKey Only
* [ICD-1106] - Add option to search MS-Ready Formulae or Exact Formulae
* [ICD-1136] - Add Bioassay data plot display for selected assays
* [ICD-1192] - Add Ranking Based on number of articles found in PubMed

New Data

- ~3000 chemicals added since last release
- Additional experimental physchem data from literature added
- T.E.S.T predictions made across all data – physicochemical predictions
- Human and Ecological hazard data added and curated (always ongoing)
- Production volume data added

Detailed Chemical Pages



Presence in Lists

EPA United States Environmental Protection Agency

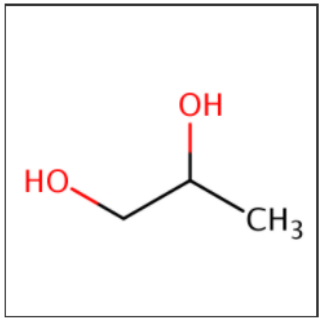
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Search All Data

Chemistry Dashboard | Submit Comment | Share | Copy | Aa

1,2-Propylene glycol

57-55-6 | DTXSID0021206

Searched by Approved Name: Found 1 result for '1,2-propylene glycol'.



- Wikipedia
- Intrinsic Properties
- Structural Identifiers
- Linked Substances
- Presence in Lists

Federal: TOX21SL: Tox21 Screening Library; ATSDR Toxic Substances Portal Chemical List; NIOSH International Chemical Safety Cards; HERO: Health and Environmental Research Online; EPA Integrated Risk Information System (IRIS); Provisional Peer Reviewed Toxicity Values; EPAHFR - EPA Chemicals associated with hydraulic fracturing; TOXCAST - EPA ToxCast Screening Library; TOXCAST_PhaseII - EPA ToxCast Screening Library (Phase II Subset); TOXCAST_PhaseIII - EPA ToxCast Screening Library (Phase II Subset); TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset)

US State

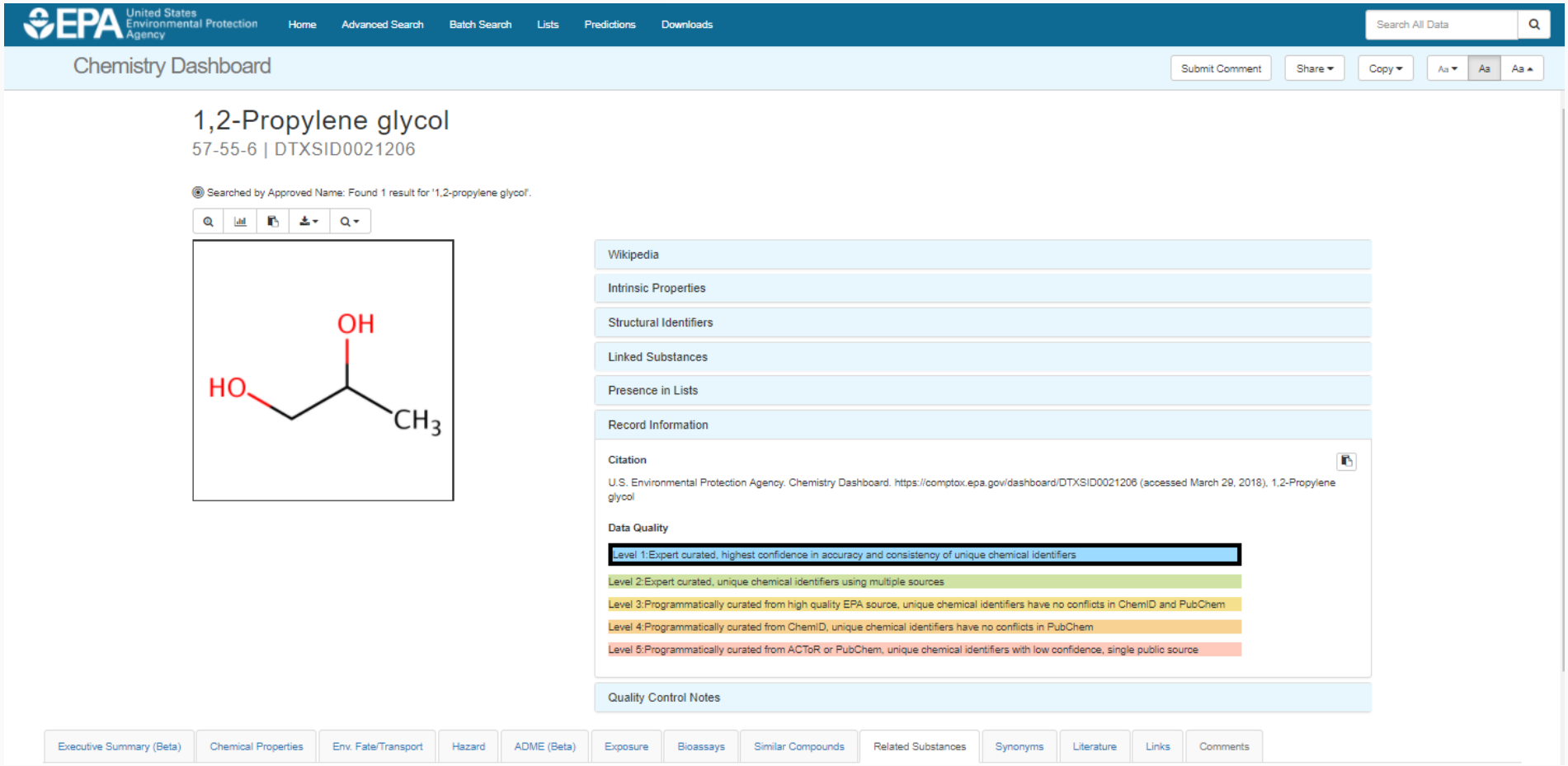
International: EU Cosmetic Ingredients Inventory (Combined 2000/2006); KEMI List of Substances on the Market; Pharmaceutical List with EU, Swiss and US Consumption Data

Other: EPA Consumer Products Suspect Screening Results; STOFF-IDENT Database of Water-Relevant Substances

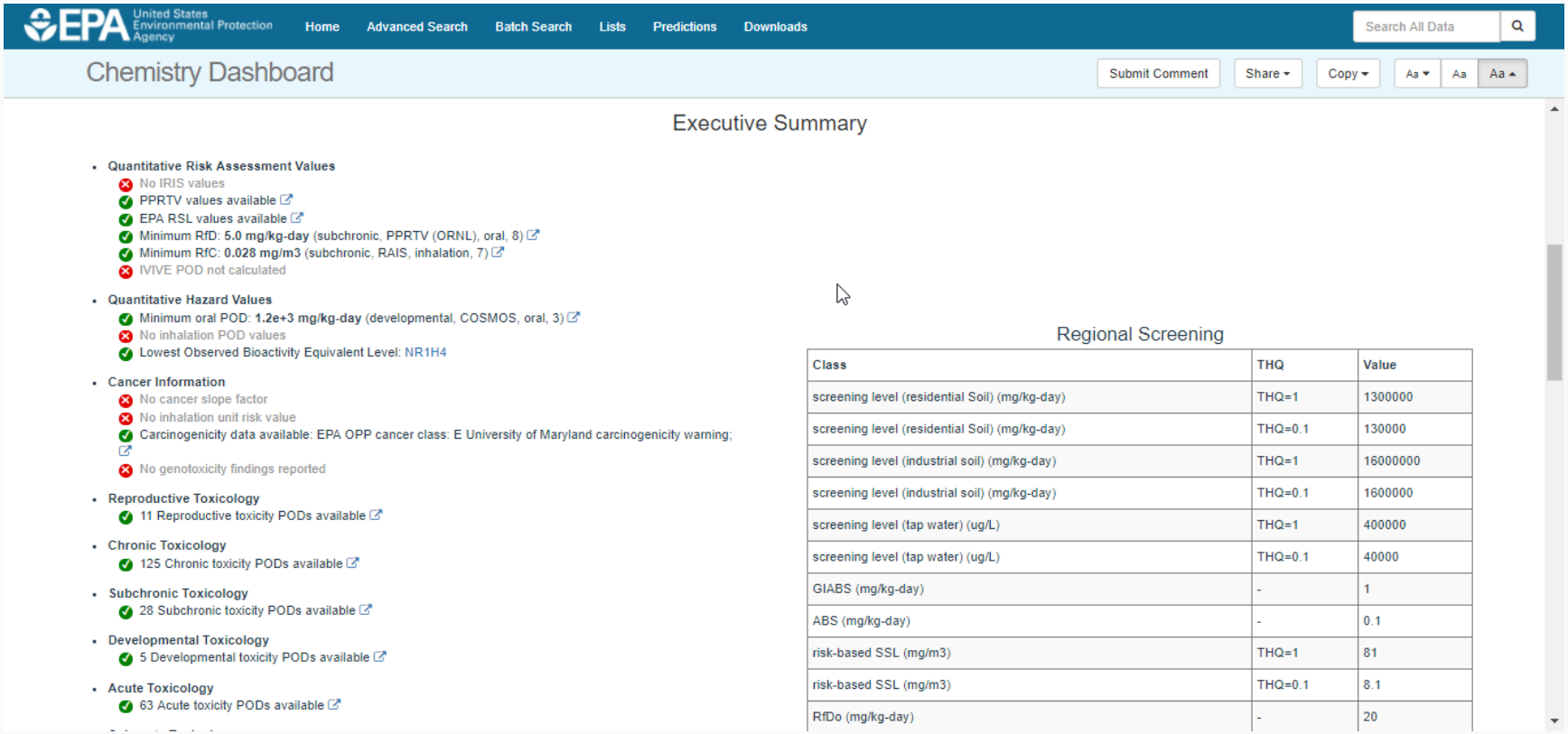
- Record Information
- Quality Control Notes

Executive Summary (Beta) | Chemical Properties | Env. Fate/Transport | Hazard | ADME (Beta) | Exposure | Bioassays | Similar Compounds | Related Substances | Synonyms | Literature | Links | Comments

Data Quality

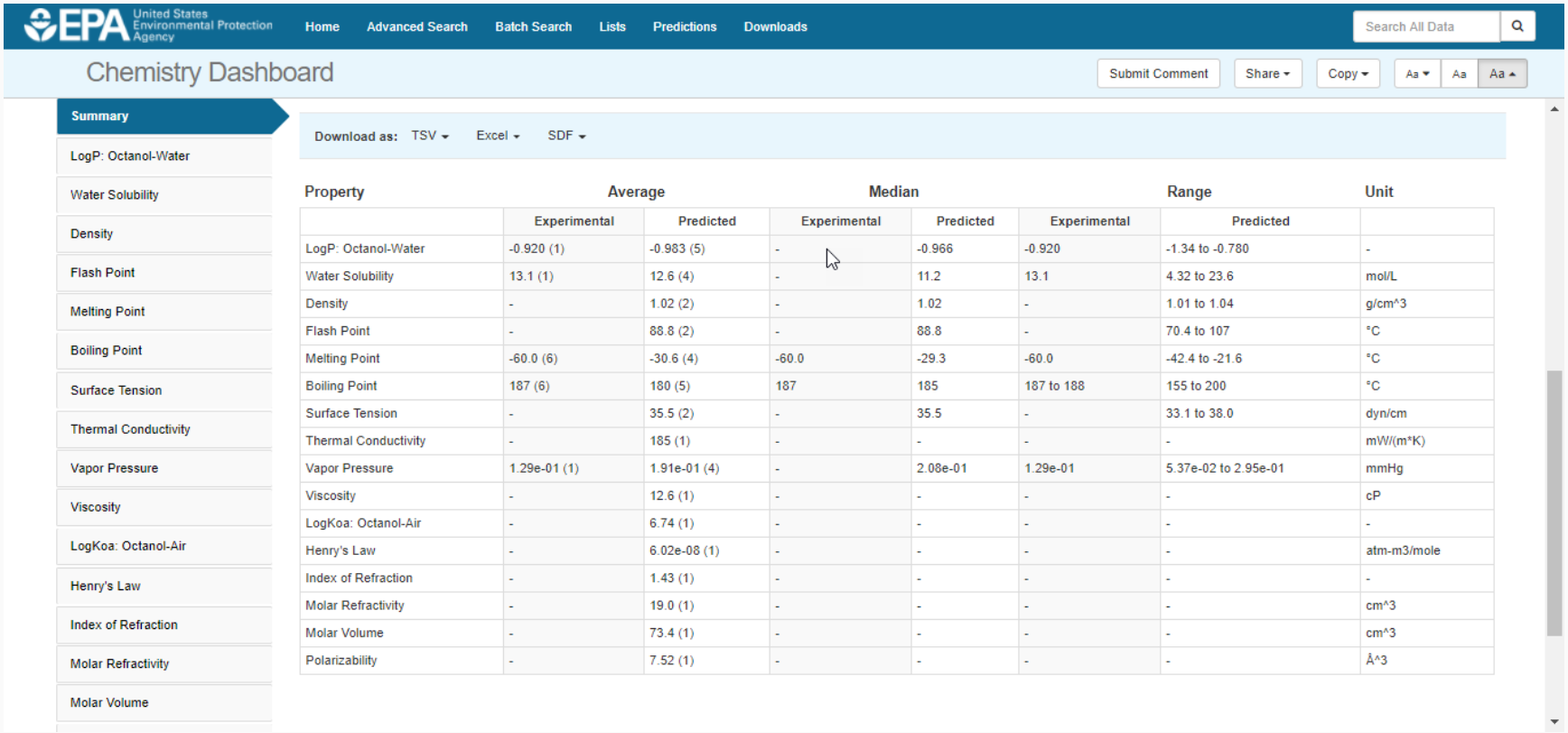


The Executive Summary (NEW)



The Executive Summary (NEW)

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

Properties, Fate and Transport

- When we don't have experimental data we predict it…

Property	Average	
	Experimental	Predicted
Soil Adsorp. Coeff.	2.29 (1)	1.94 (2)
Atmos. Hydroxylation Rate	1.20e-11 (1)	1.30e-11 (1)
Biodeg. Half-Life	-	4.28 (1)
Fish Biotrans. Half-Life (Km)	-	8.30e-02 (1)
Bioaccumulation Factor	-	8.96e-01 (1)
Bioconcentration Factor	-	2.13 (5)

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]

Model Performance Details
(Redesigned display)

EPA United States Environmental Protection Agency

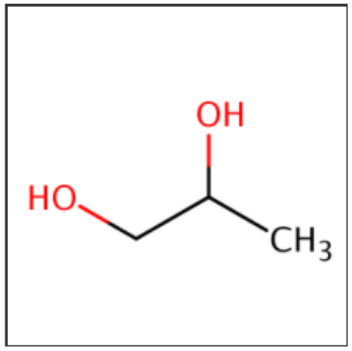
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | 21206

Chemistry Dashboard

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

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

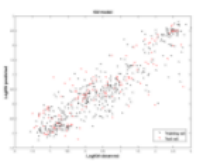
Save PDF

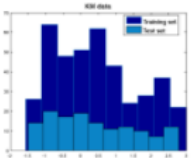


Model Results

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

Model Performance



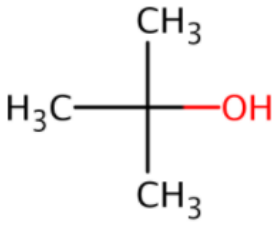


Weighted KNN model

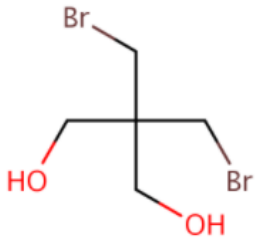
QMRF

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

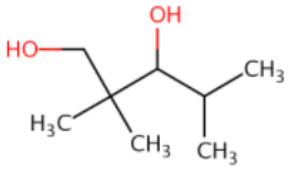
Nearest Neighbors from the Training Set



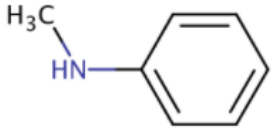
tert-Butyl alcohol
Measured: 7.41e-02
Predicted: 7.66e-02



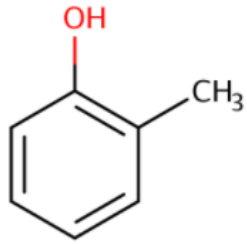
Pentaerythritol dibromide
Measured: 3.98e-02
Predicted: 5.44e-02



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

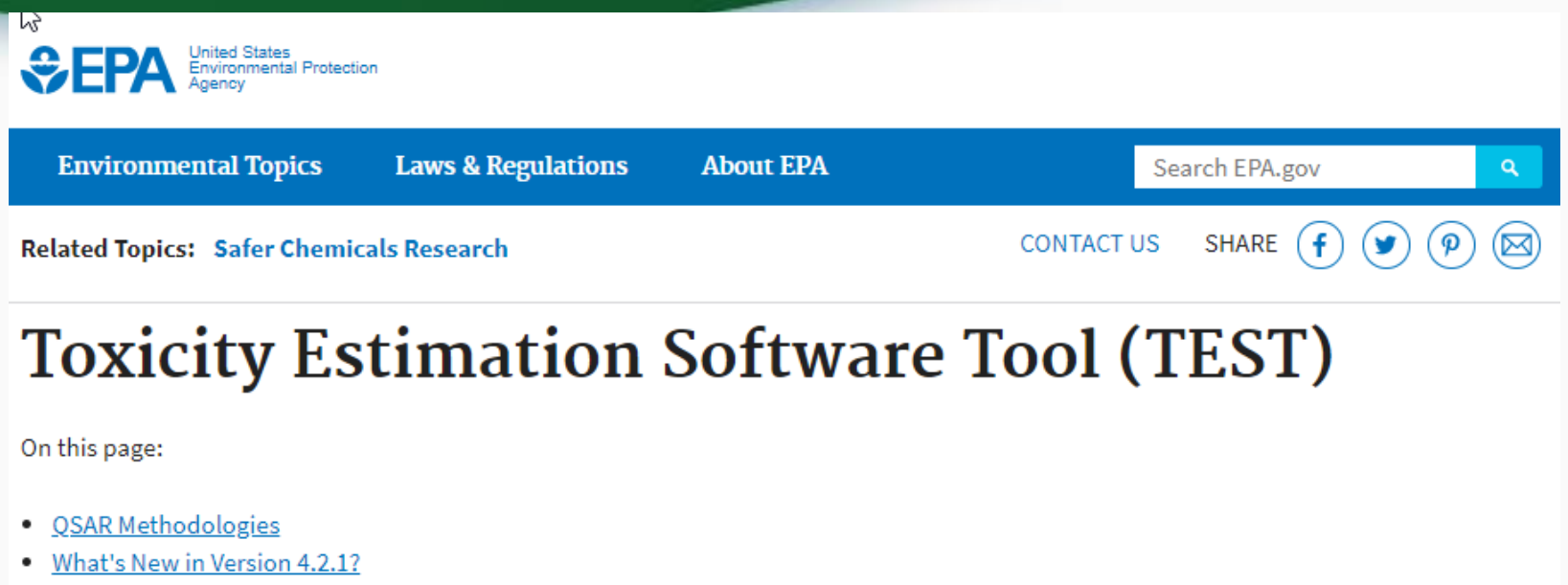


N-Methylaniline
Measured: 1.32e-01
Predicted: 1.50e-01



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

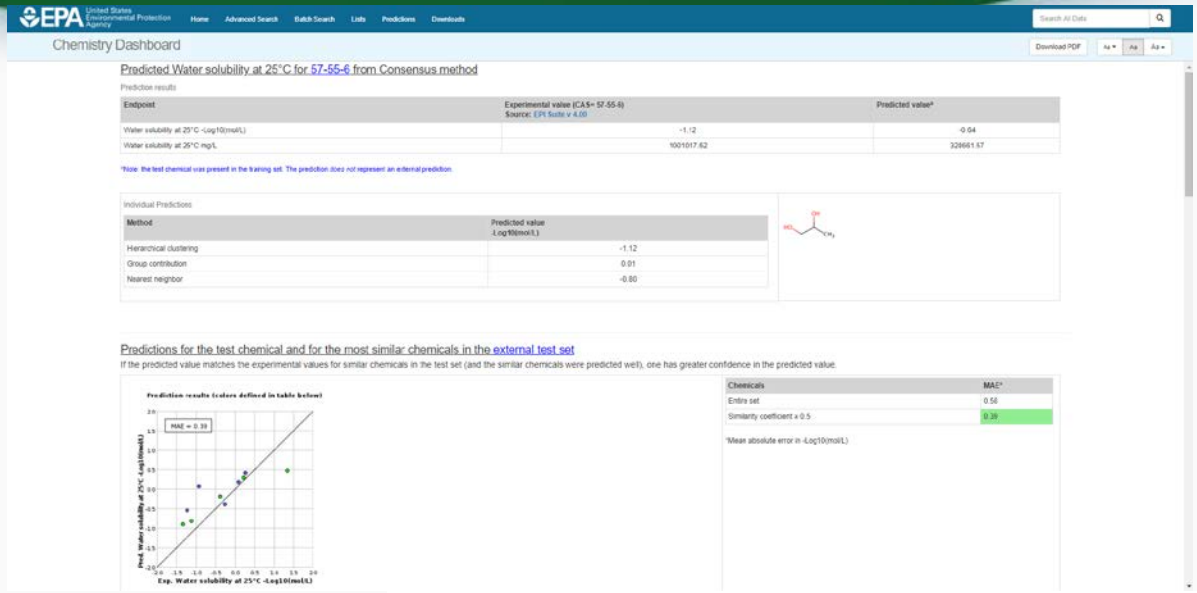
T.E.S.T Models



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

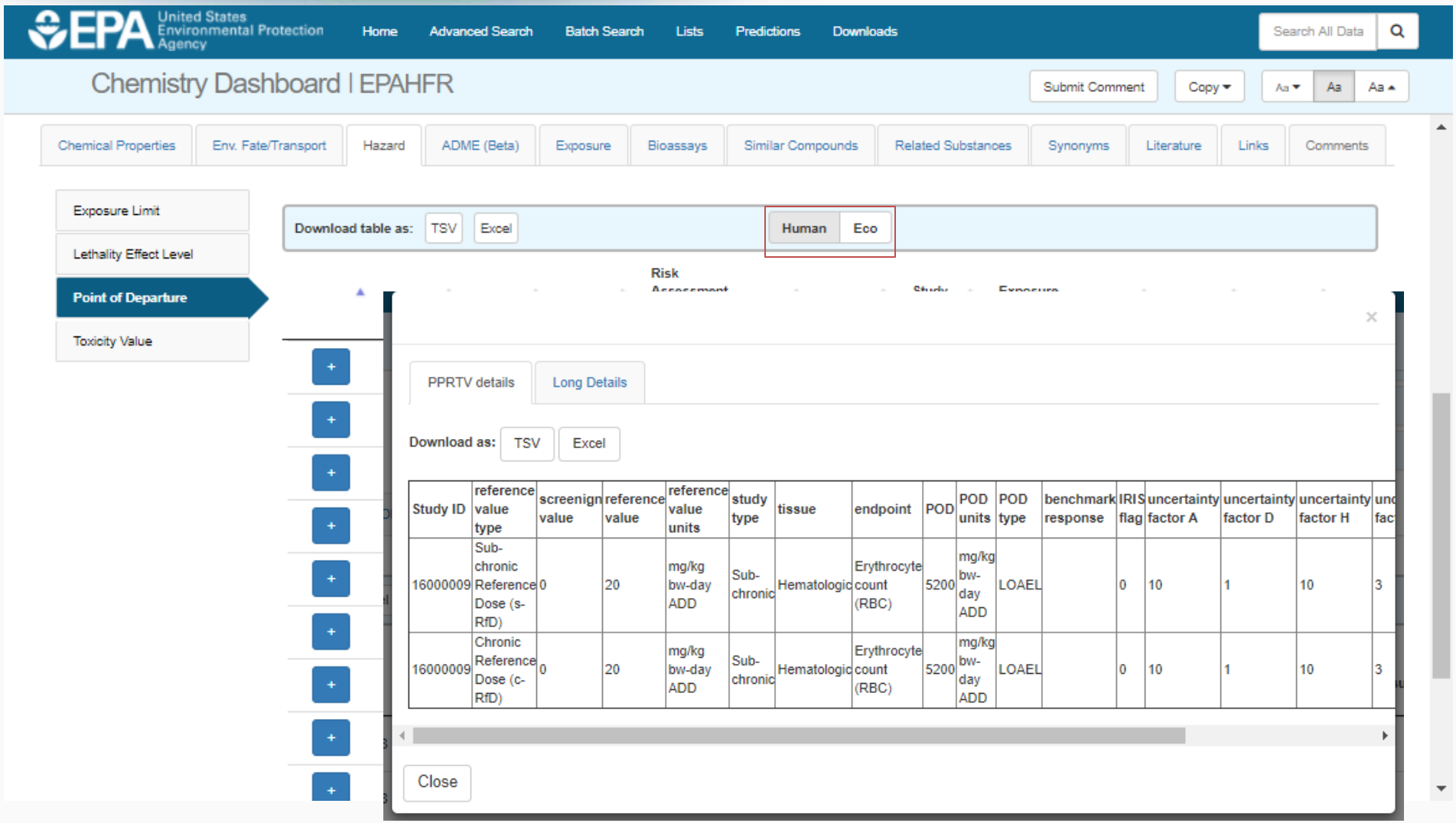
T.E.S.T Calculation Reports

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

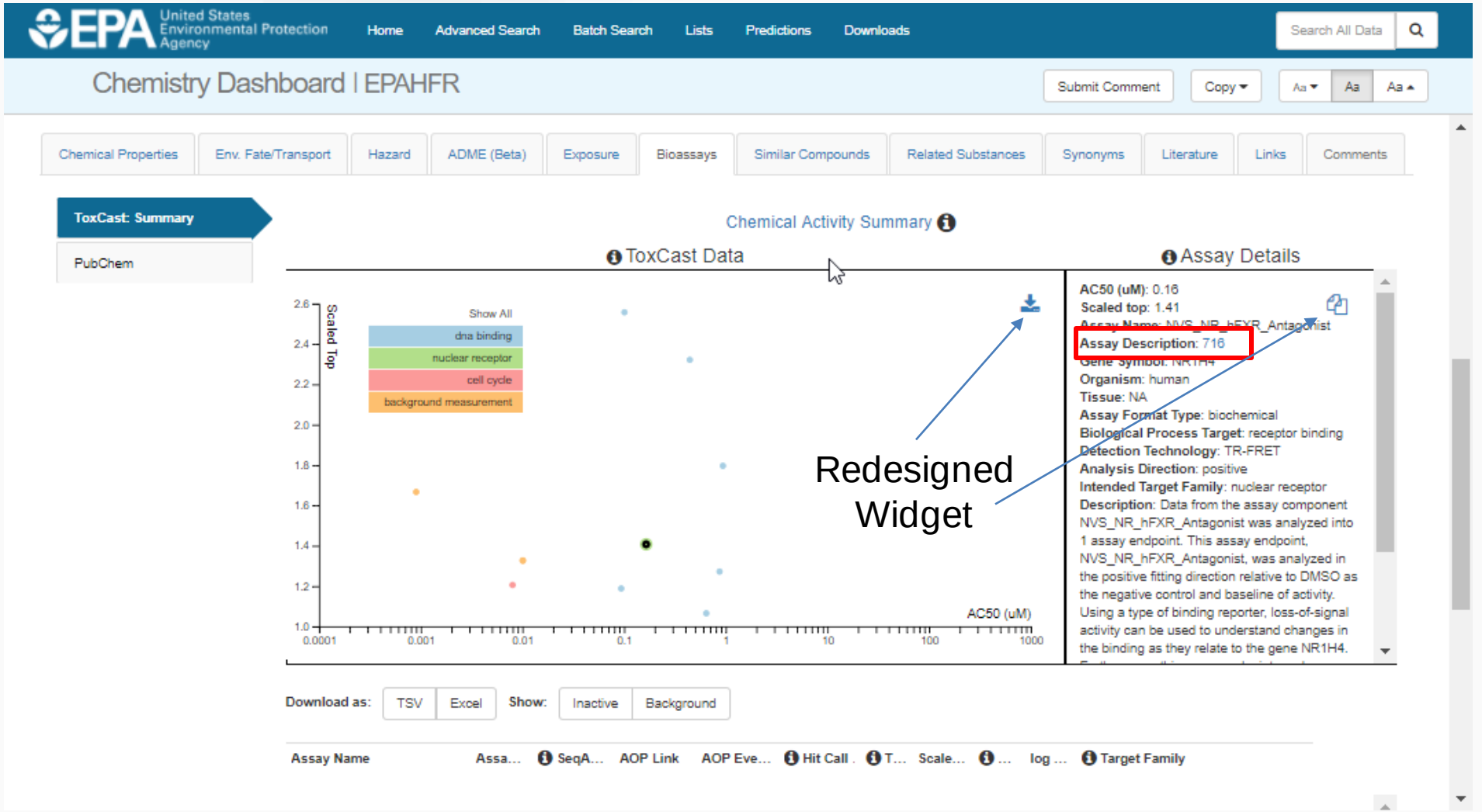
Access to Chemical Hazard Data



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:

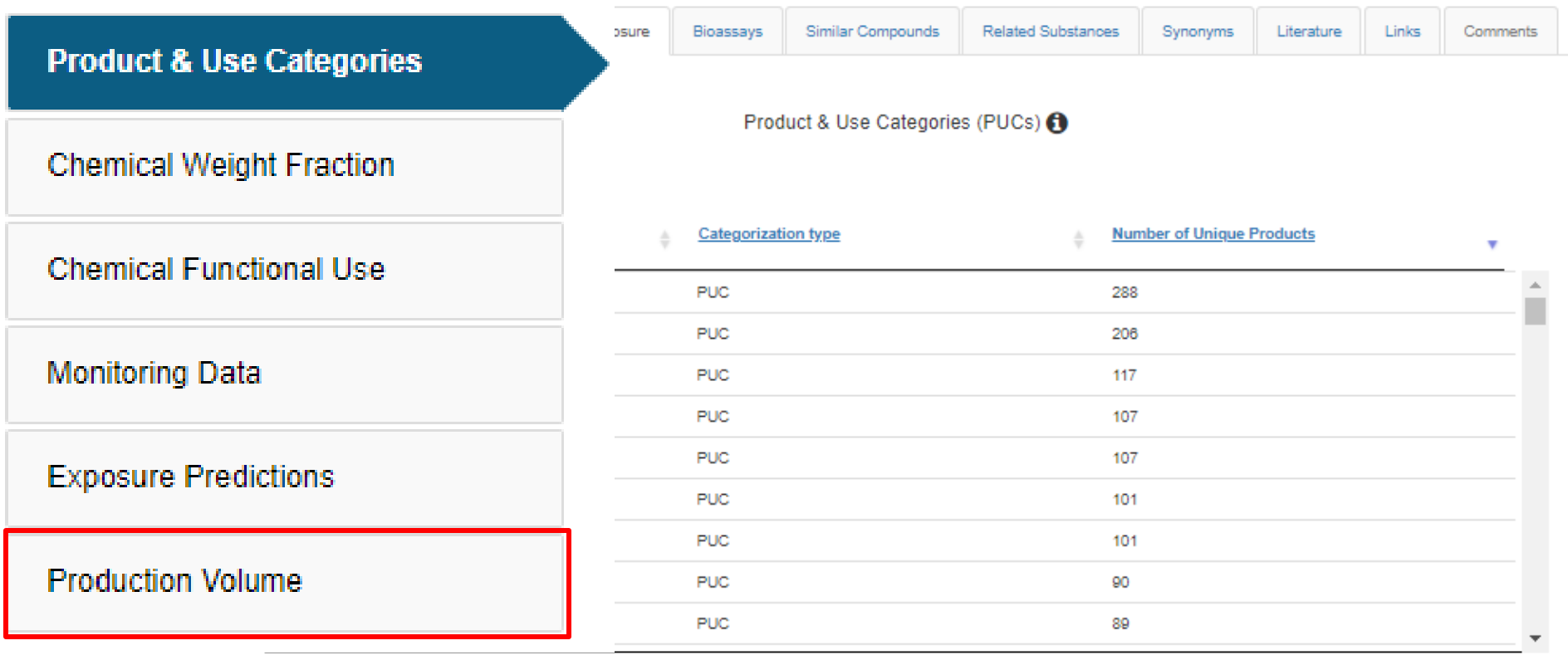
High-throughput screening of in vitro chemical-target interactions across a wide variety of compounds through a broad range of biochemical interactions will help describe the chemical-assay bioactivity space for chemicals with limited available information. There exists a large number of environmental 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

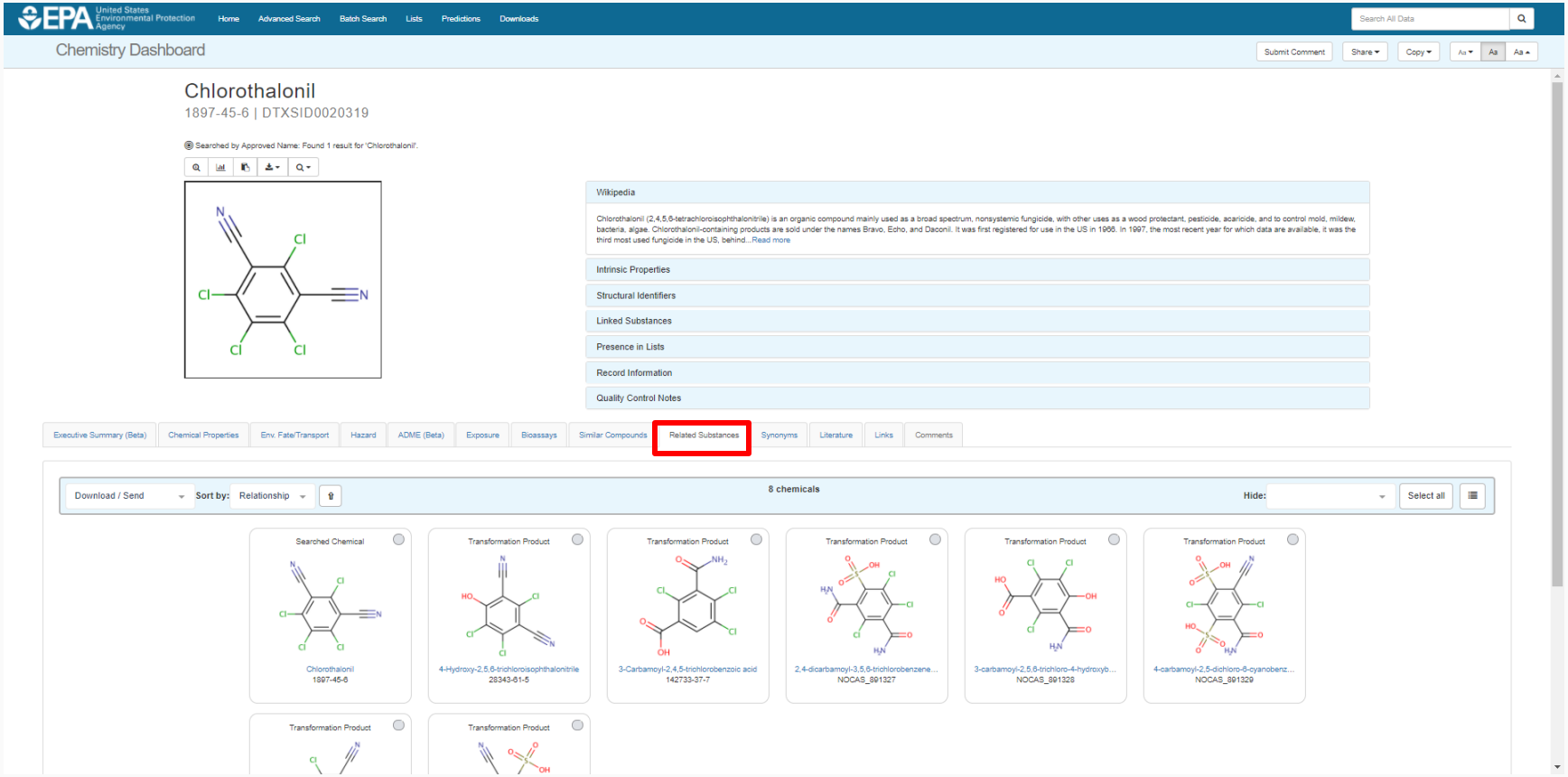
Assay Throughput:

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.

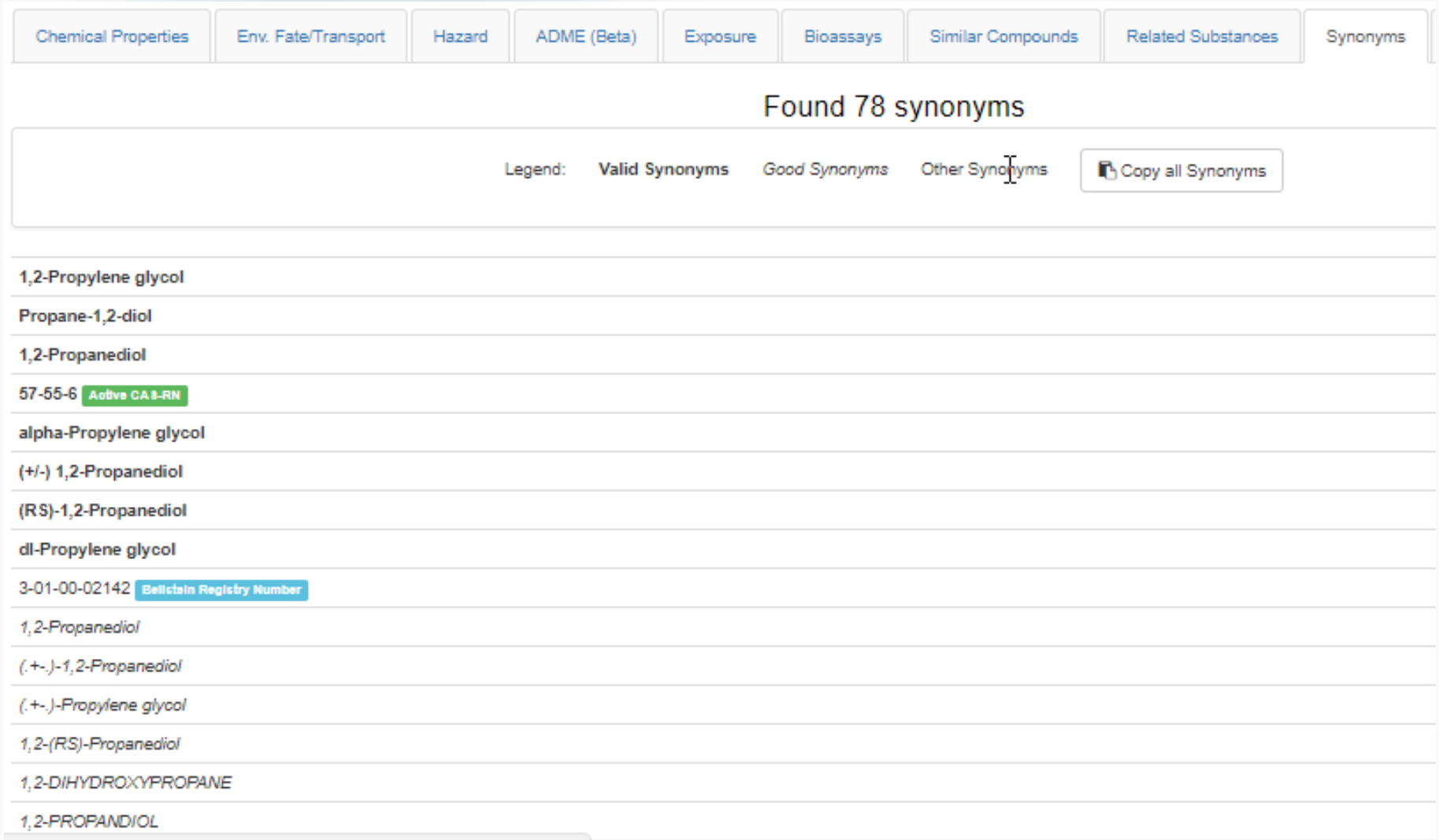
Sources of Exposure to Chemicals



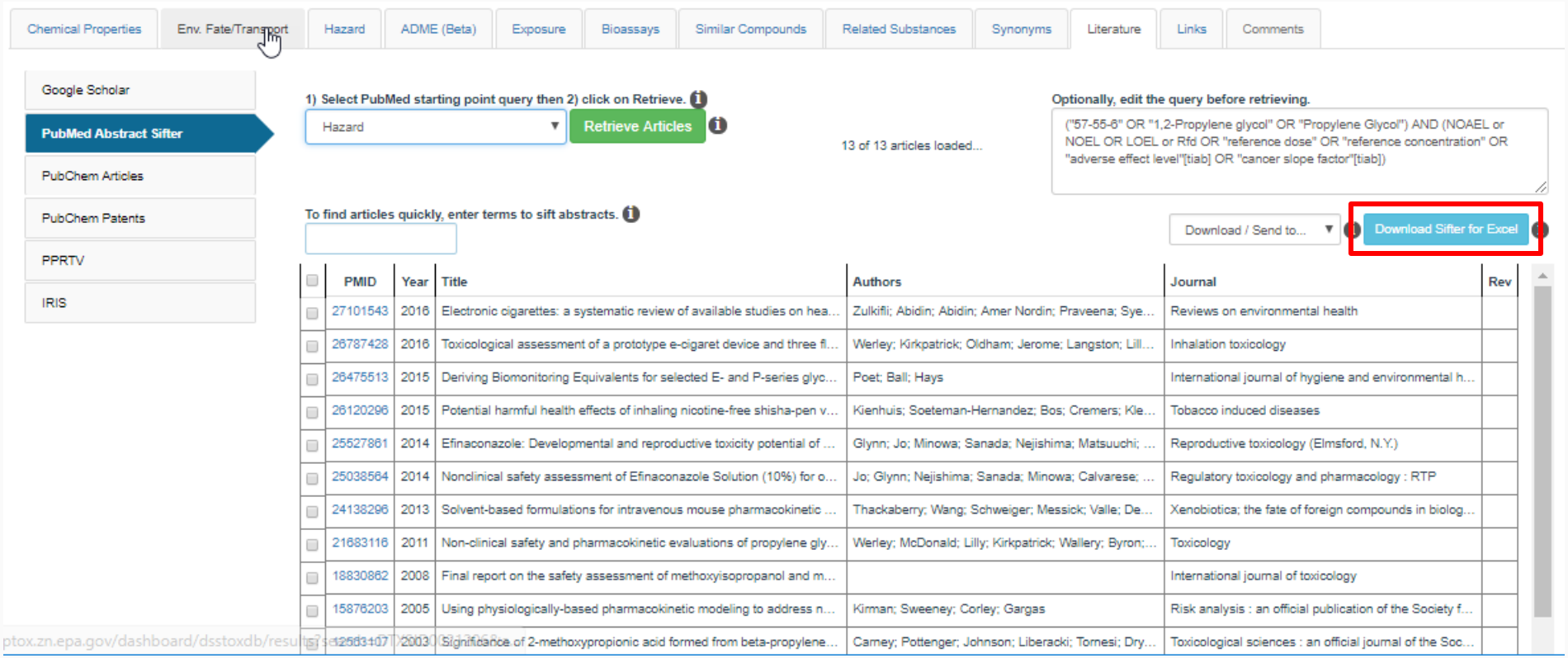
Related Substances
Mappings to Transformation Products



Identifiers to Support Searches



Literature Searches and Links



Abstract Sifter for Excel

https://f1000research.com/articles/6-2164/v1

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

Check for updates

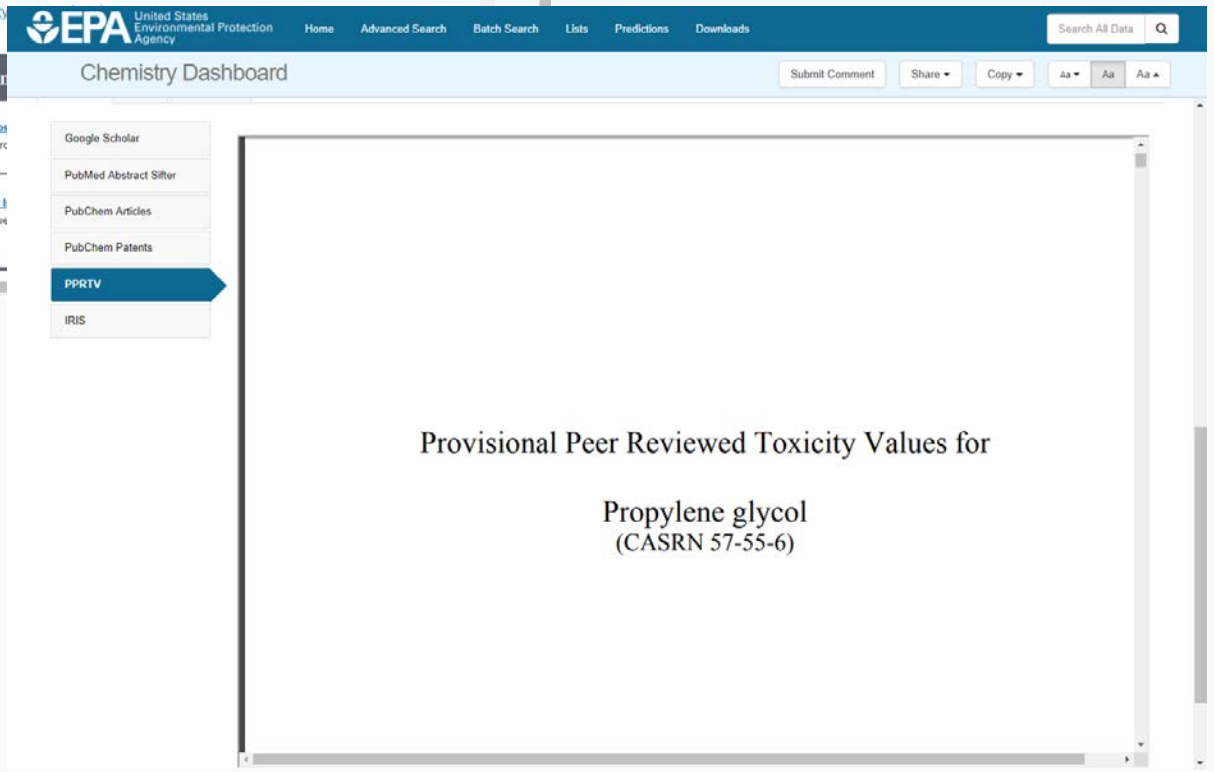
SOFTWARE TOOL ARTICLE

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

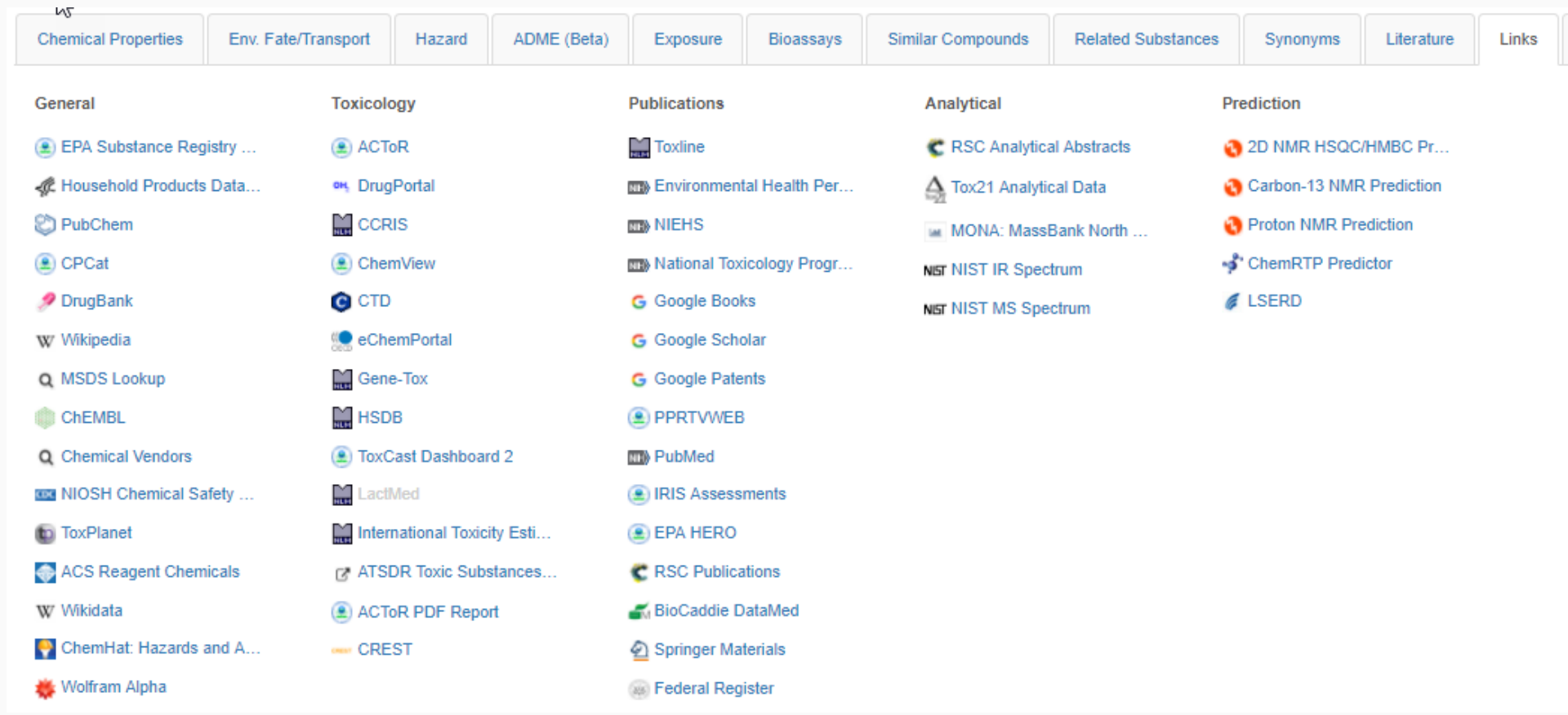
Nancy Baker [1], Thomas Knudsen[2], Antony Williams [2]

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

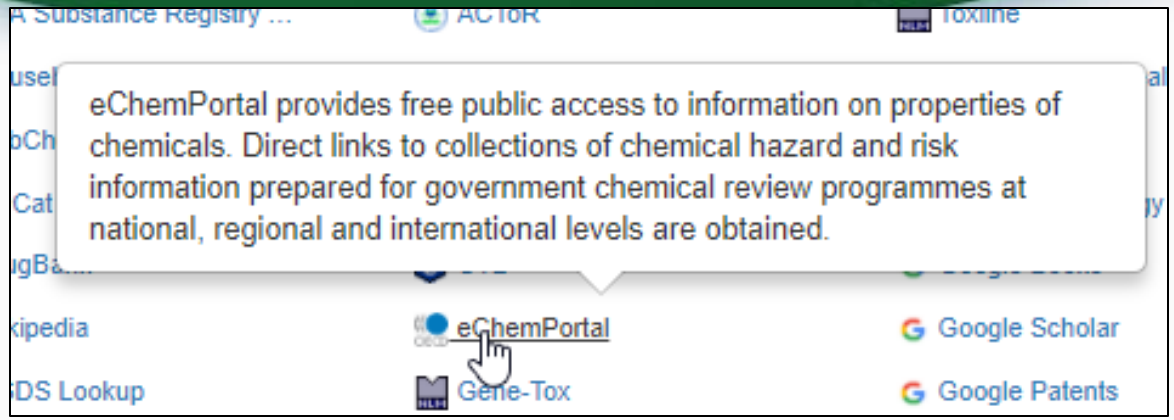
Links to PPRTV and IRIS

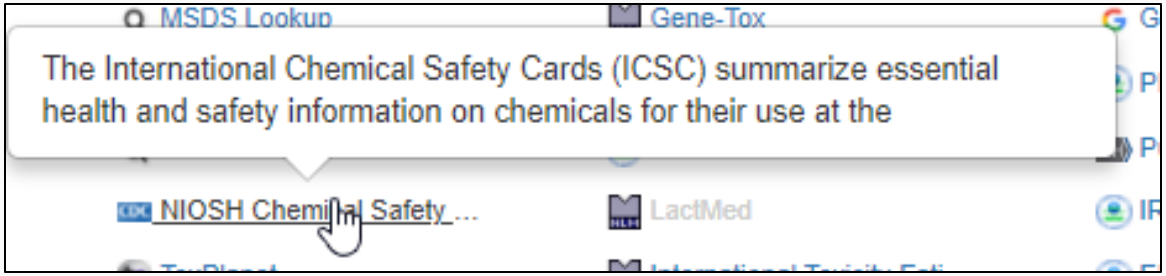


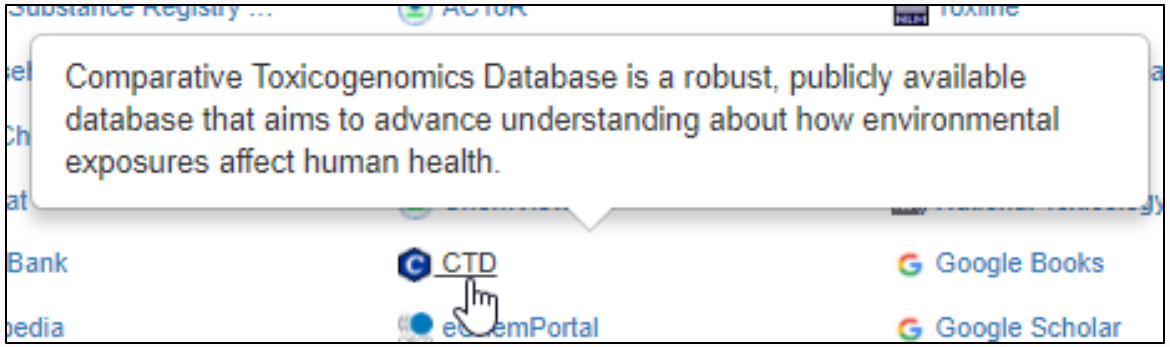
External Links to Data and Services



Integrated Linkouts



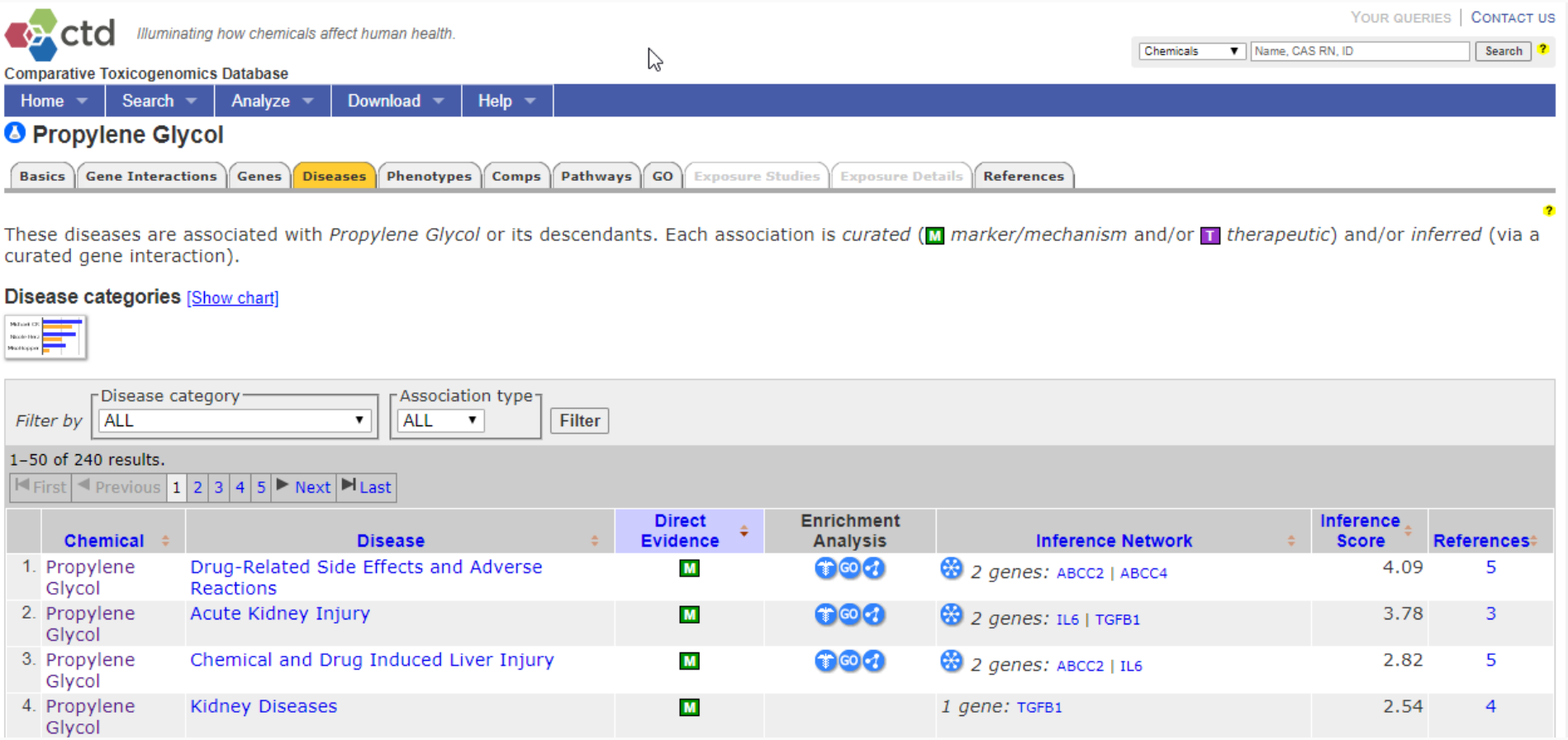




Integrated Linkouts

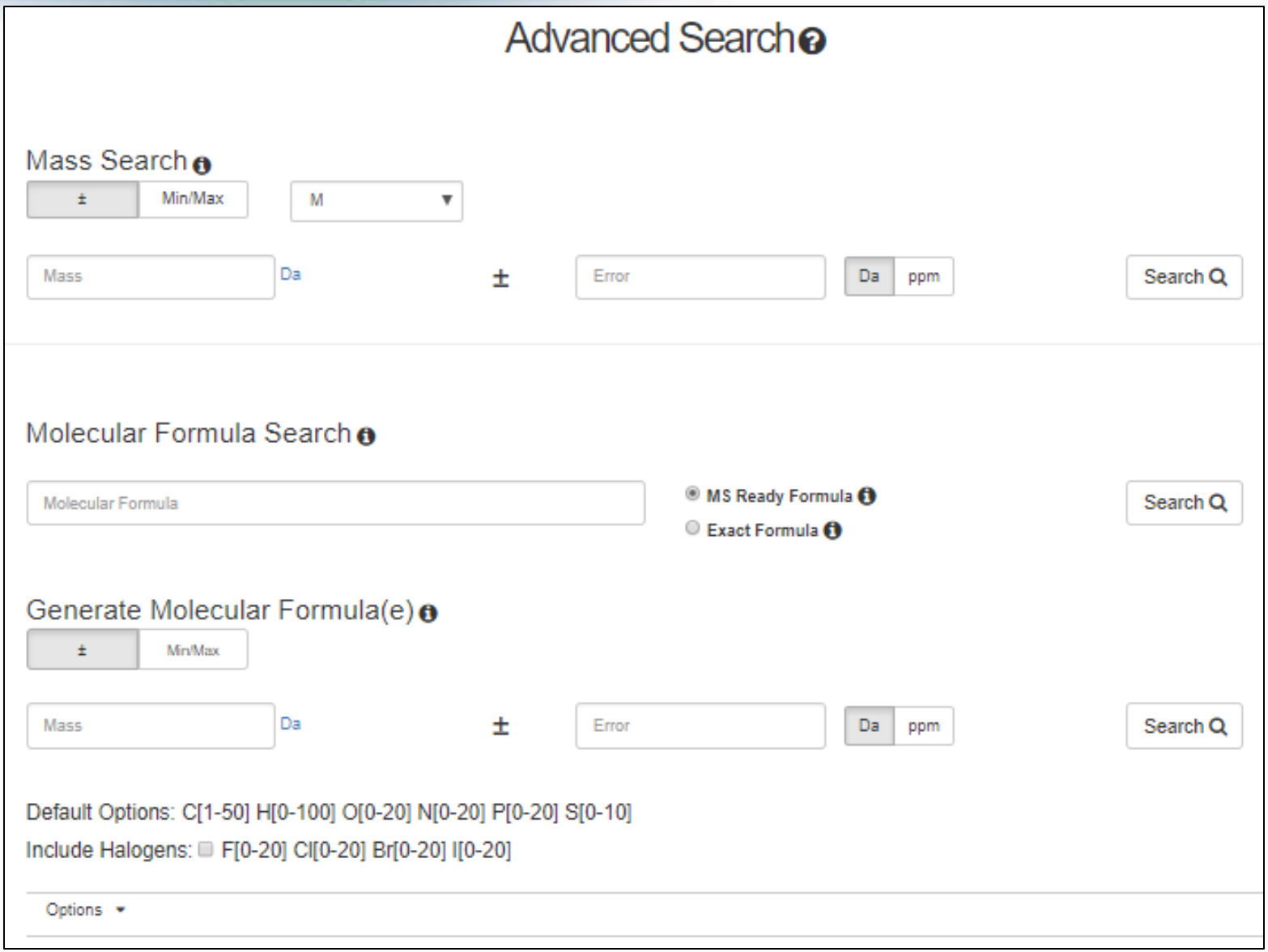
Comparative Toxicogenomics DB

EPA United States Environmental Protection Agency



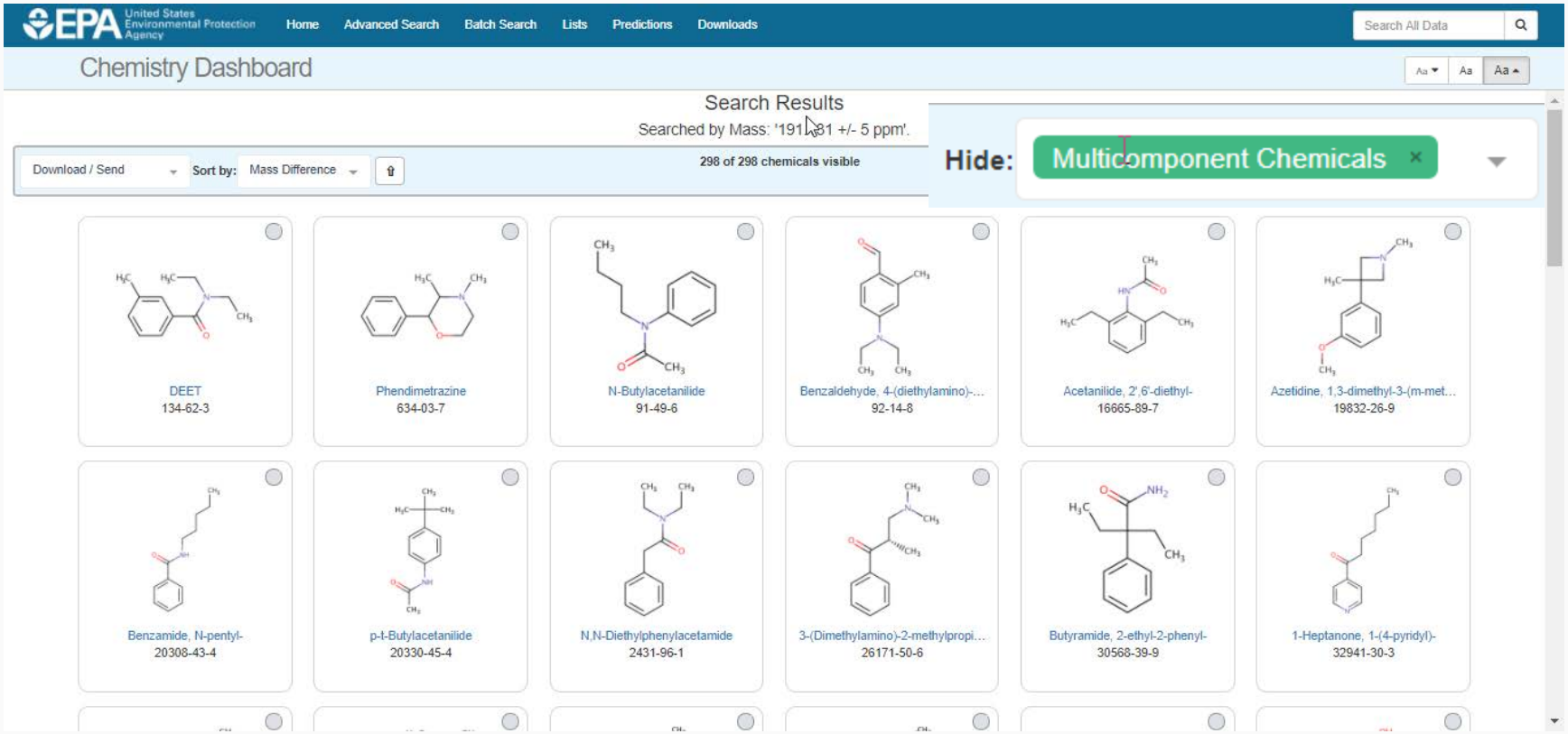
	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M		2 genes: ABCC2 | ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M		2 genes: IL6 | TGFB1	3.78	3
3.	Propylene Glycol	Chemical and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

Advanced Searches

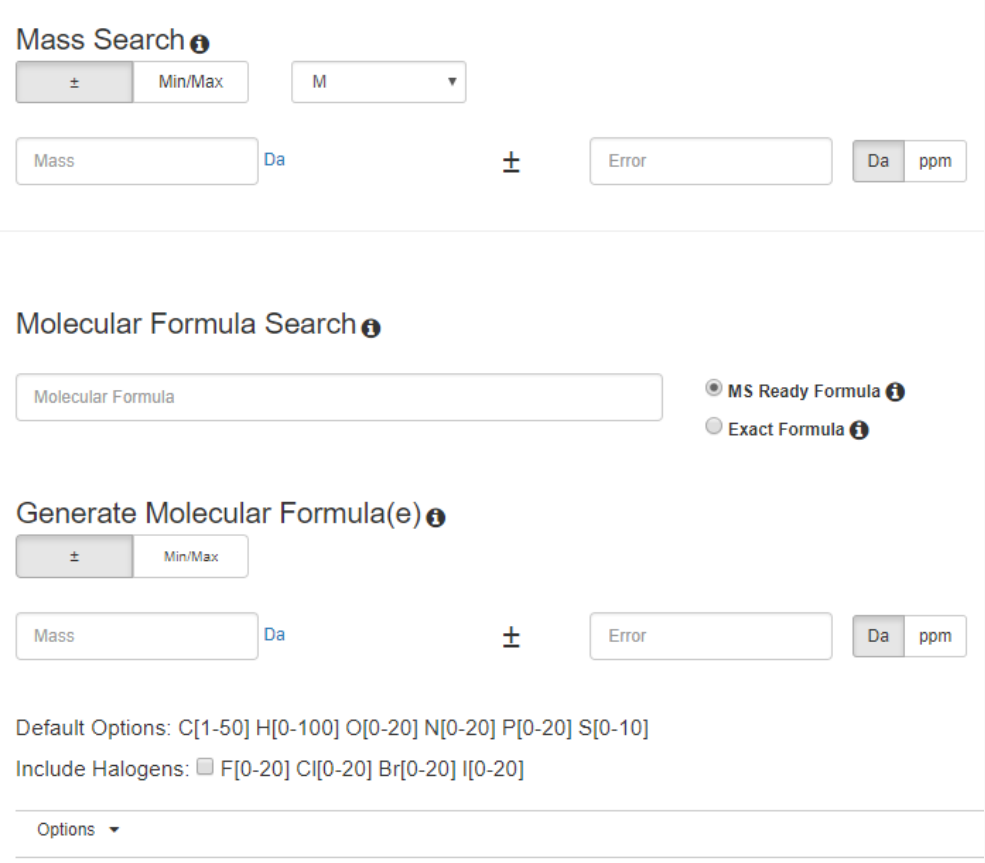


Advanced Searches
Mass Based Search

Advanced Searches

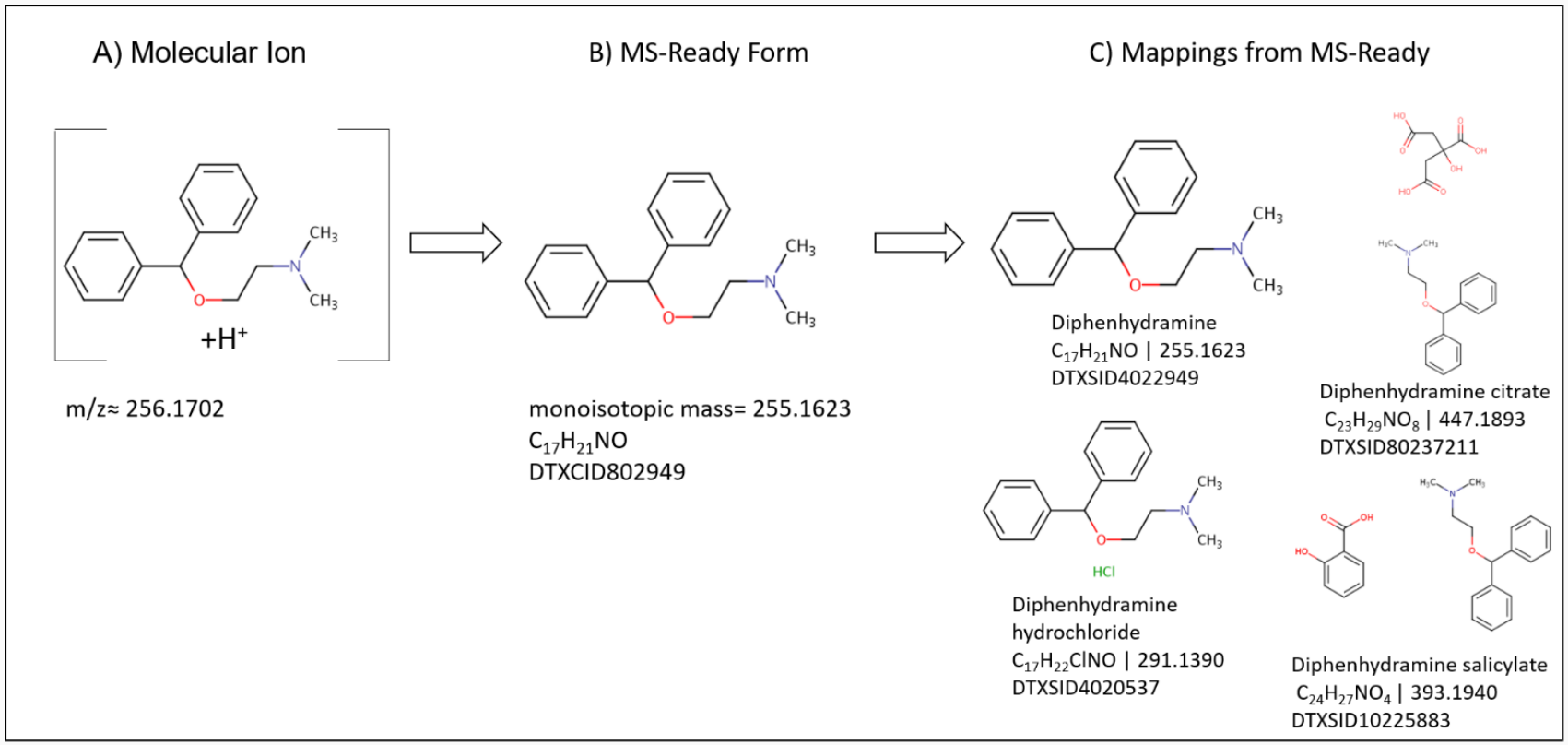


The Dashboard to Support MS-Analysis



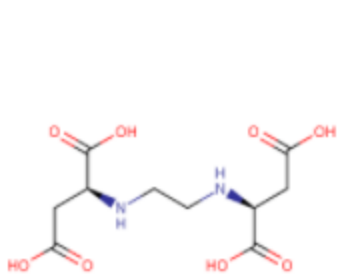
MS-Ready Structures Underpin Analysis

Specific Data-Mappings "MS-Ready Structures"

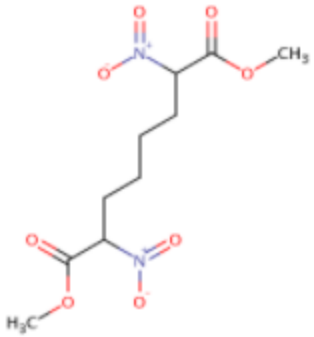


MS-Ready Mappings

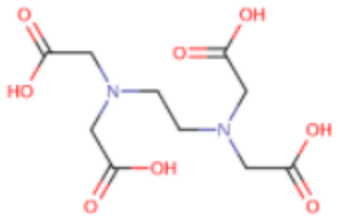
- Input Formula: C10H16N2O8
- EXACT Formula Search: 3 Chemicals



N,N'-Ethylenedi-L-aspartic acid
20846-91-7



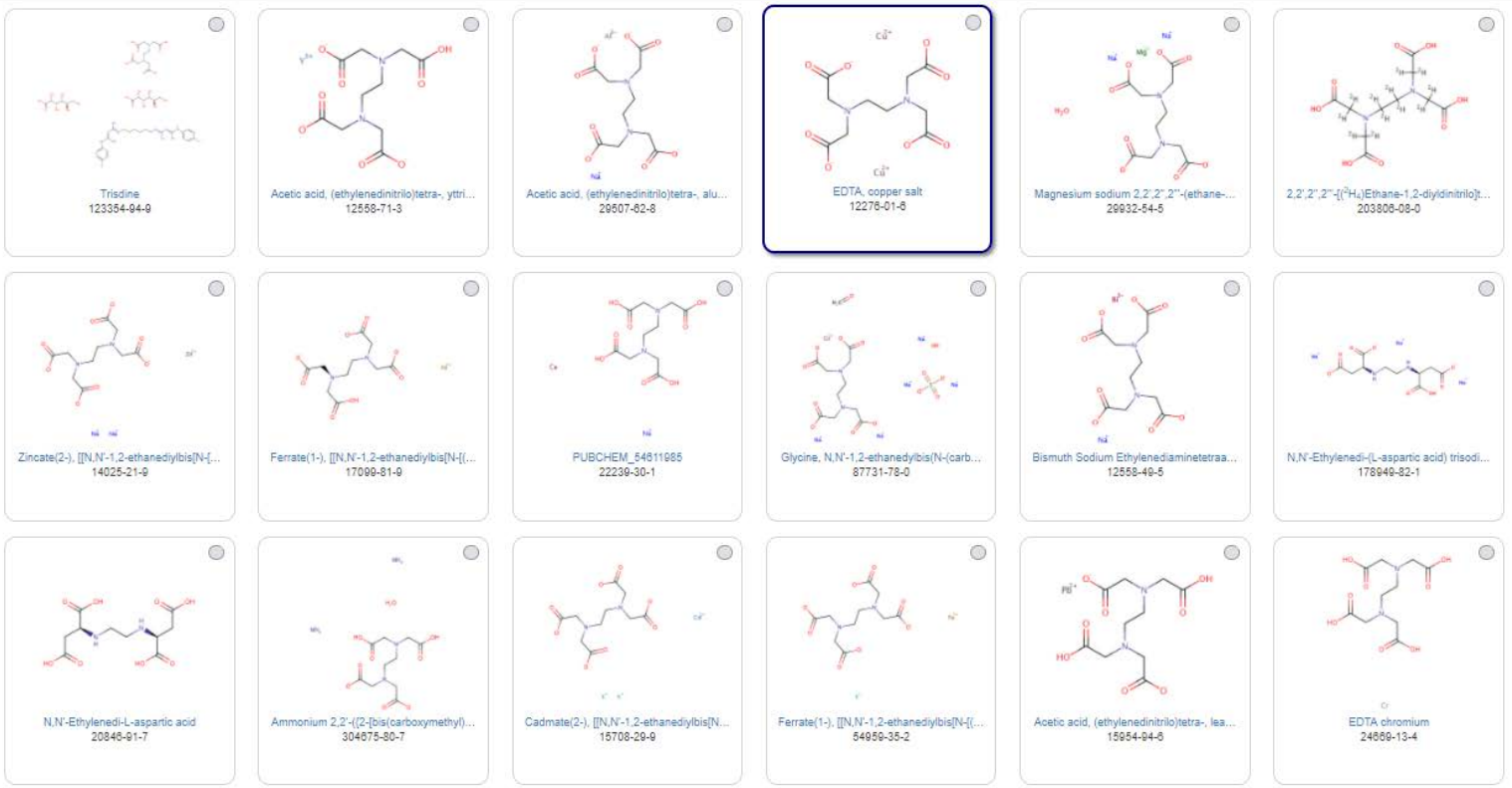
Dimethyl 2,7-dinitrooctanedioate
67404-09-5



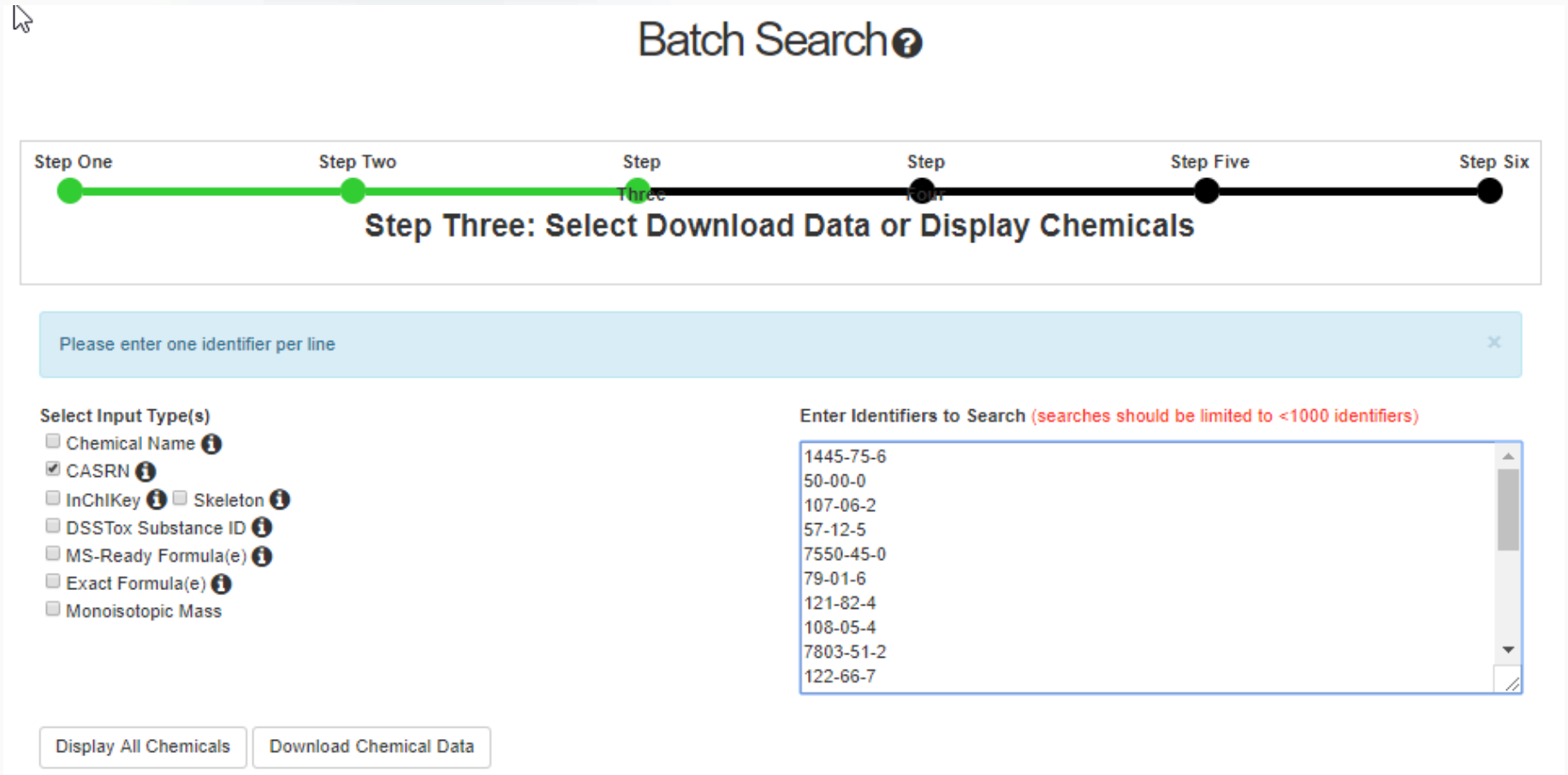
Ethylenediaminetetraacetic acid
60-00-4

MS-Ready Mappings

- **Same** Input Formula: C10H16N2O8
- MS Ready Formula Search: 88 Chemicals



Batch Searches



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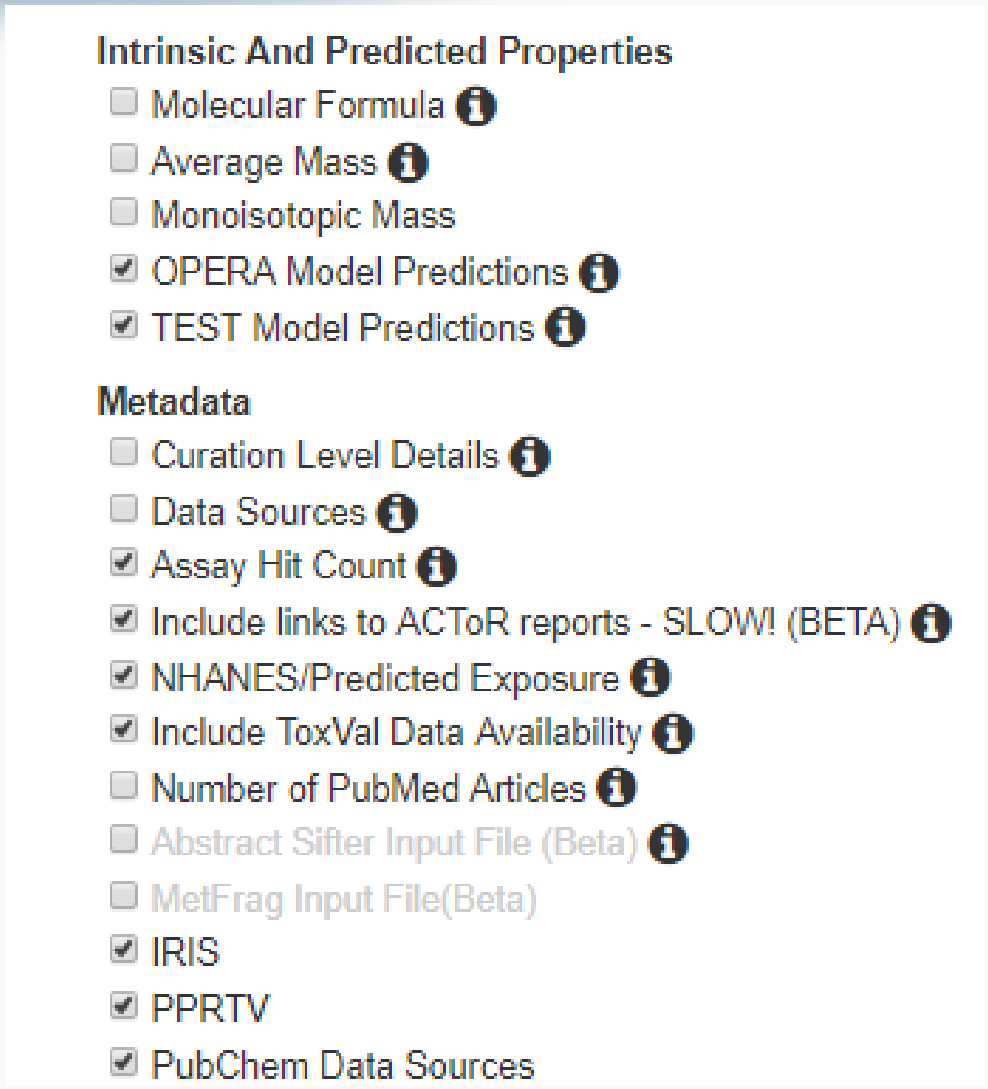
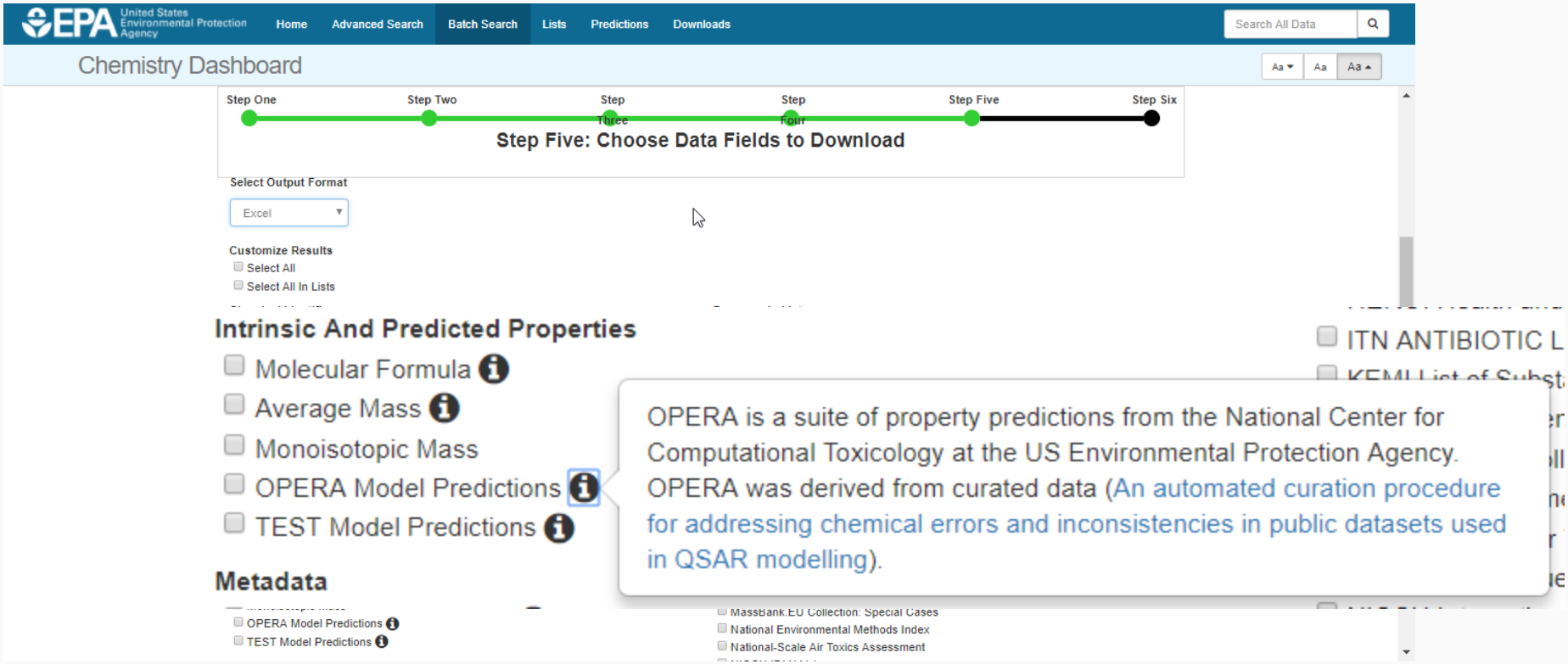
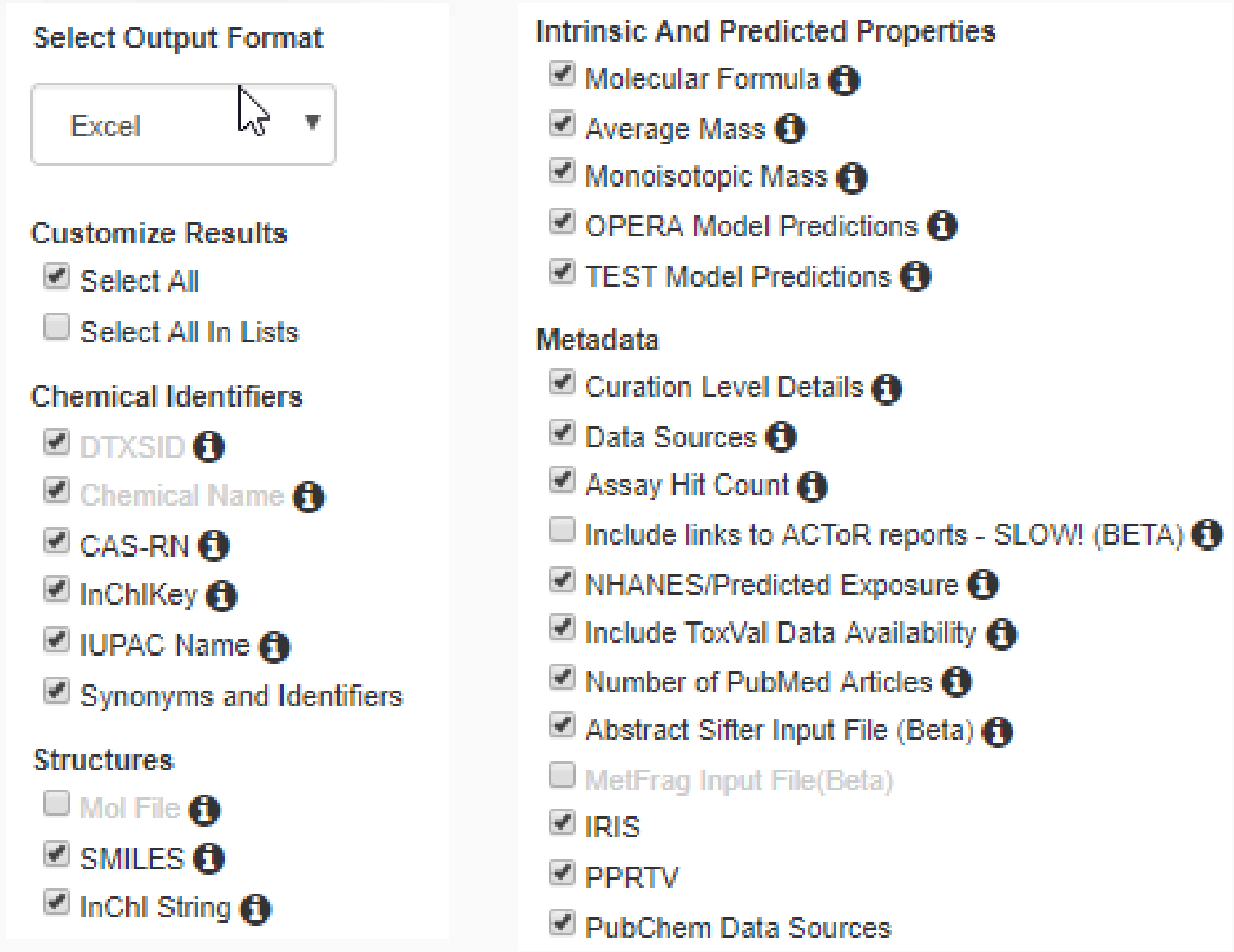


OPERA and TEST in Batch



Batch Search



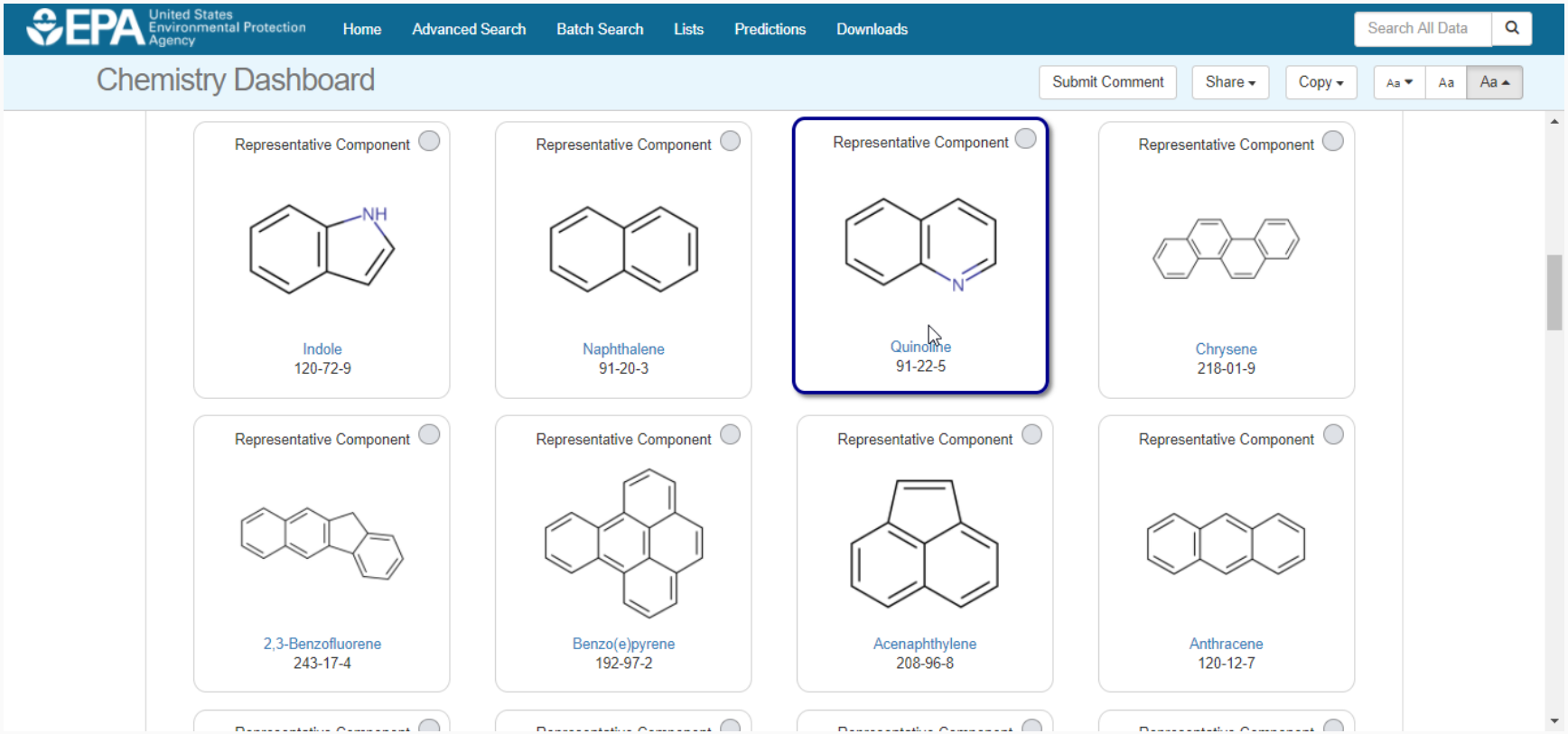
Excel Output

	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

Searching Families of chemicals

- Families of chemicals of interest
  - Polychlorinated biphenyls (PCBs)
  - Polybrominated diphenyl ethers (PBDEs)
  - Polyaromatic hydrocarbons (PAHs)

Searching Families of chemicals Polyaromatic Hydrocarbons



Surfacing Lists of Chemicals

- Specific subsets of chemicals, “lists”, can be displayed on the dashboard
- If there are chemicals that map together then these link to existing:
  - Property data
  - Hazard data
  - Exposure data
  - *In vitro* bioassay data
  - Documents and Literature

A List of Lists of Chemicals

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

EPA United States Environmental Protection Agency

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

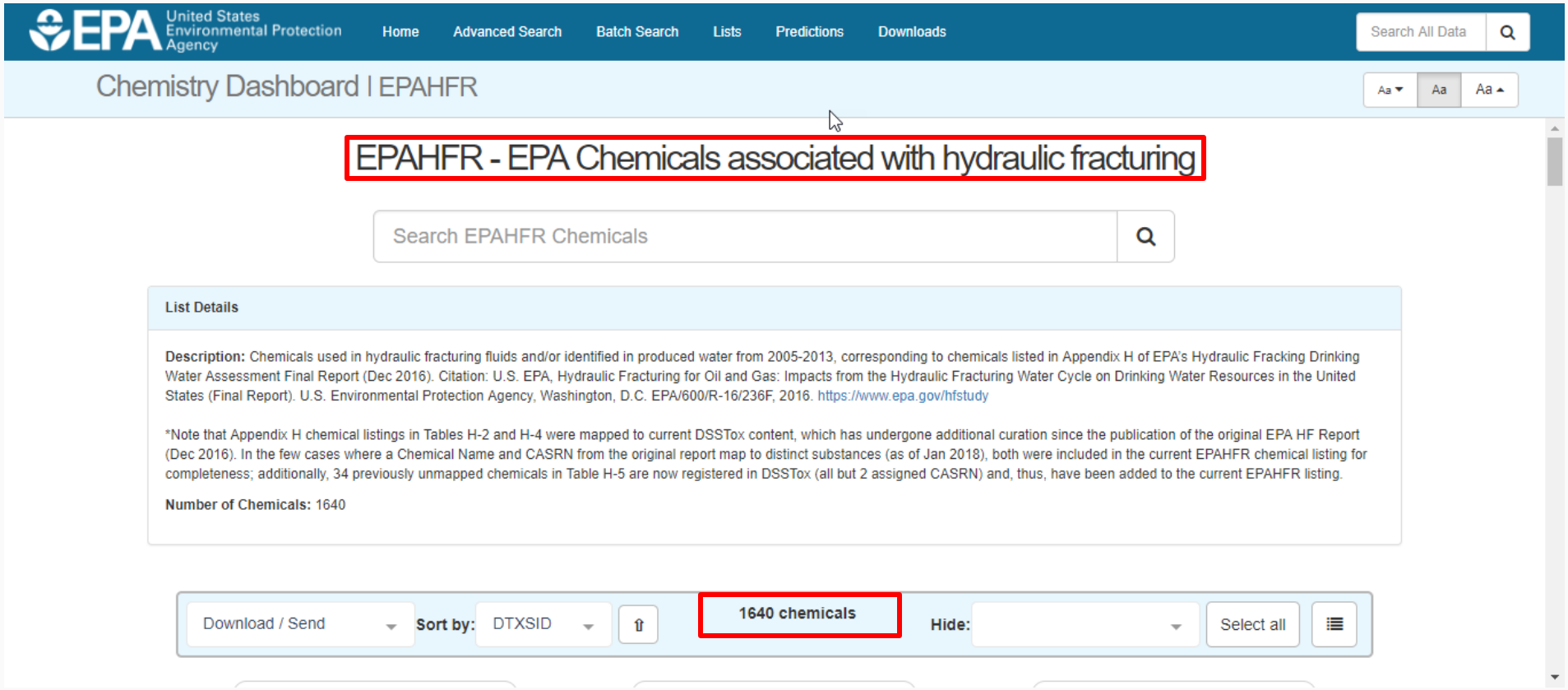
Chemistry Dashboard

Aa | Aa | Aa

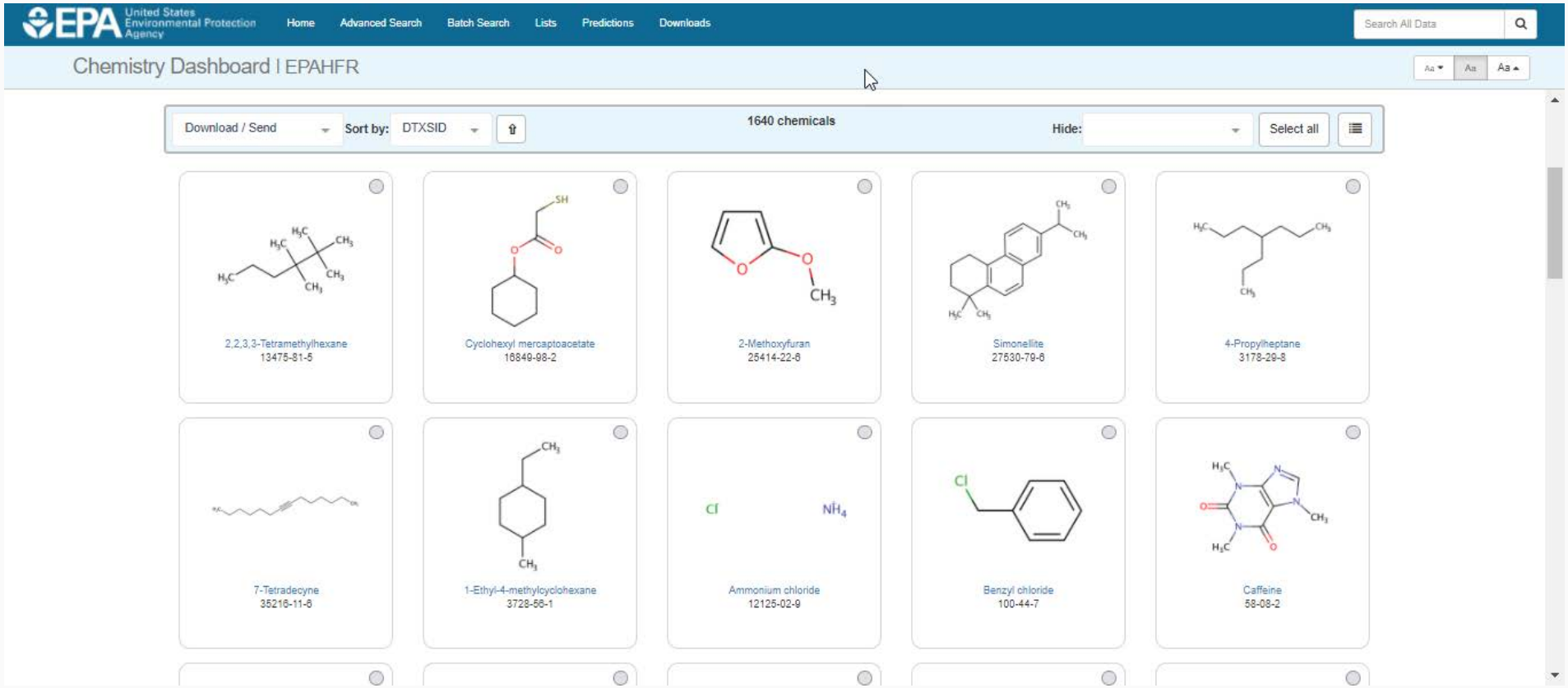
Select List

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

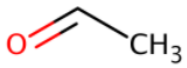
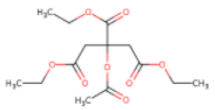
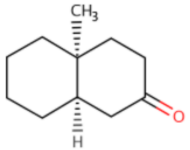
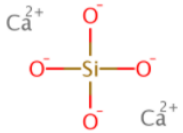
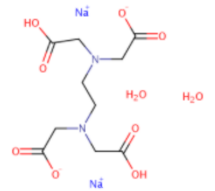


The List as “Structures”



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

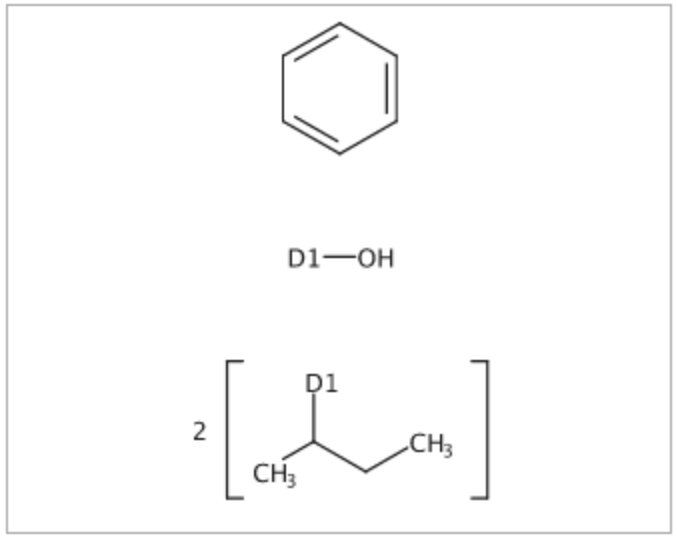
Not all chemicals are “structures”

- UVCBs are chemical substances of unknown or variable composition, complex reaction products and biological materials
  - Surfactants (C11-14 linear alkyl sulfonates)
  - Reaction mass of p-t-butylphenyldiphenyl phosphate and bis(p-t-butylphenyl)phenyl phosphate and triphenyl phosphate
  - Almond Oil

Di-sec-butylphenol

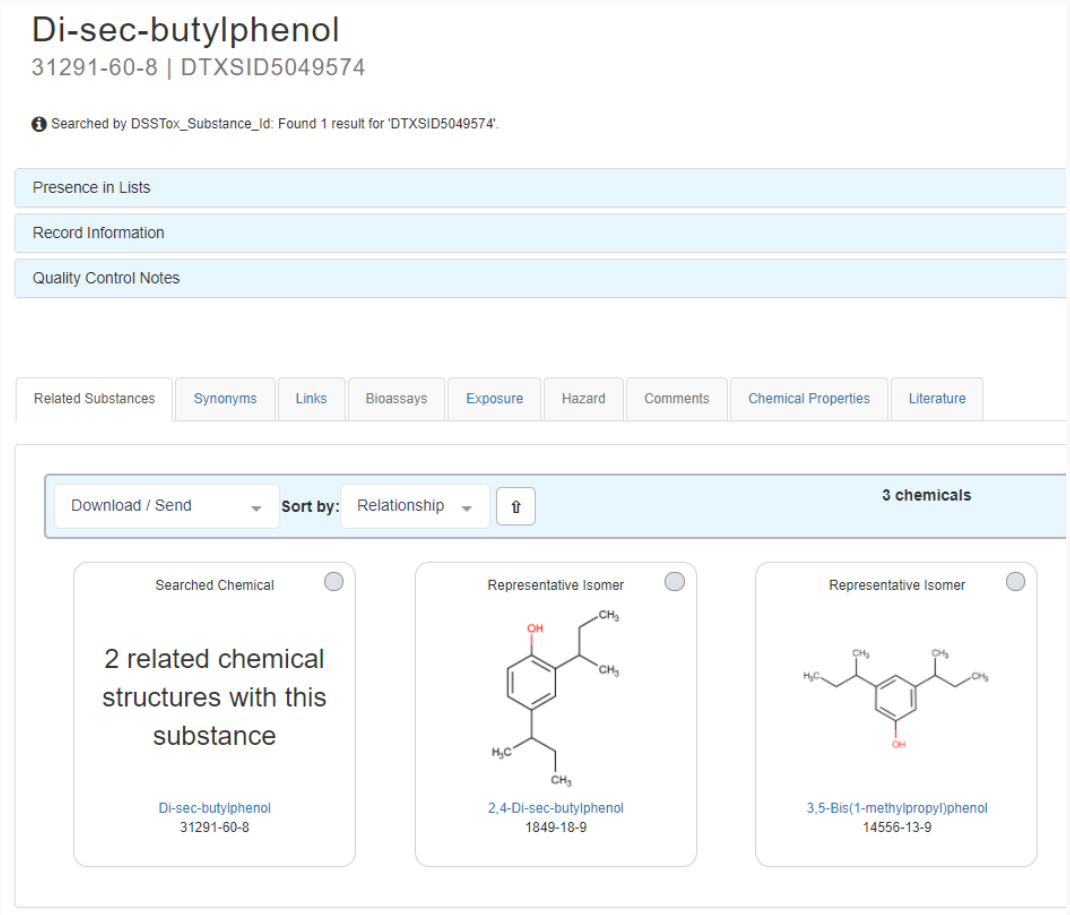
CAS Representation

1. 31291-60-8



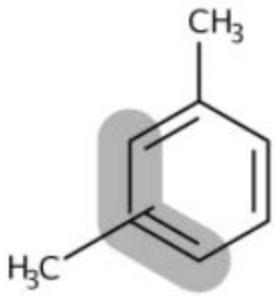
$C_{14}H_{22}O$
Phenol, bis(1-methylpropyl)-

Dashboard Representation

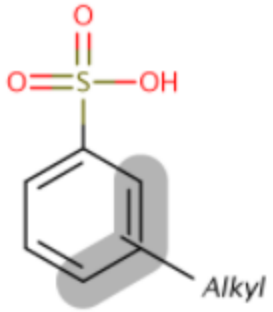


“Markush Structures”

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

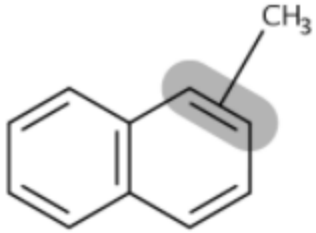


Xylenes
1330-20-7

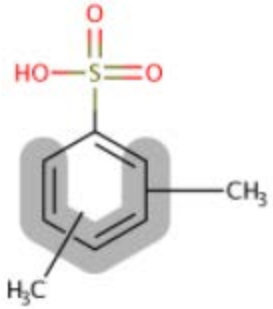


(C10-C16) Alkylbenzenesulfonic acid
68584-22-5

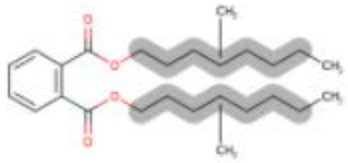
n-Nonylphenol
25154-52-3



Methylnaphthalene
1321-94-4



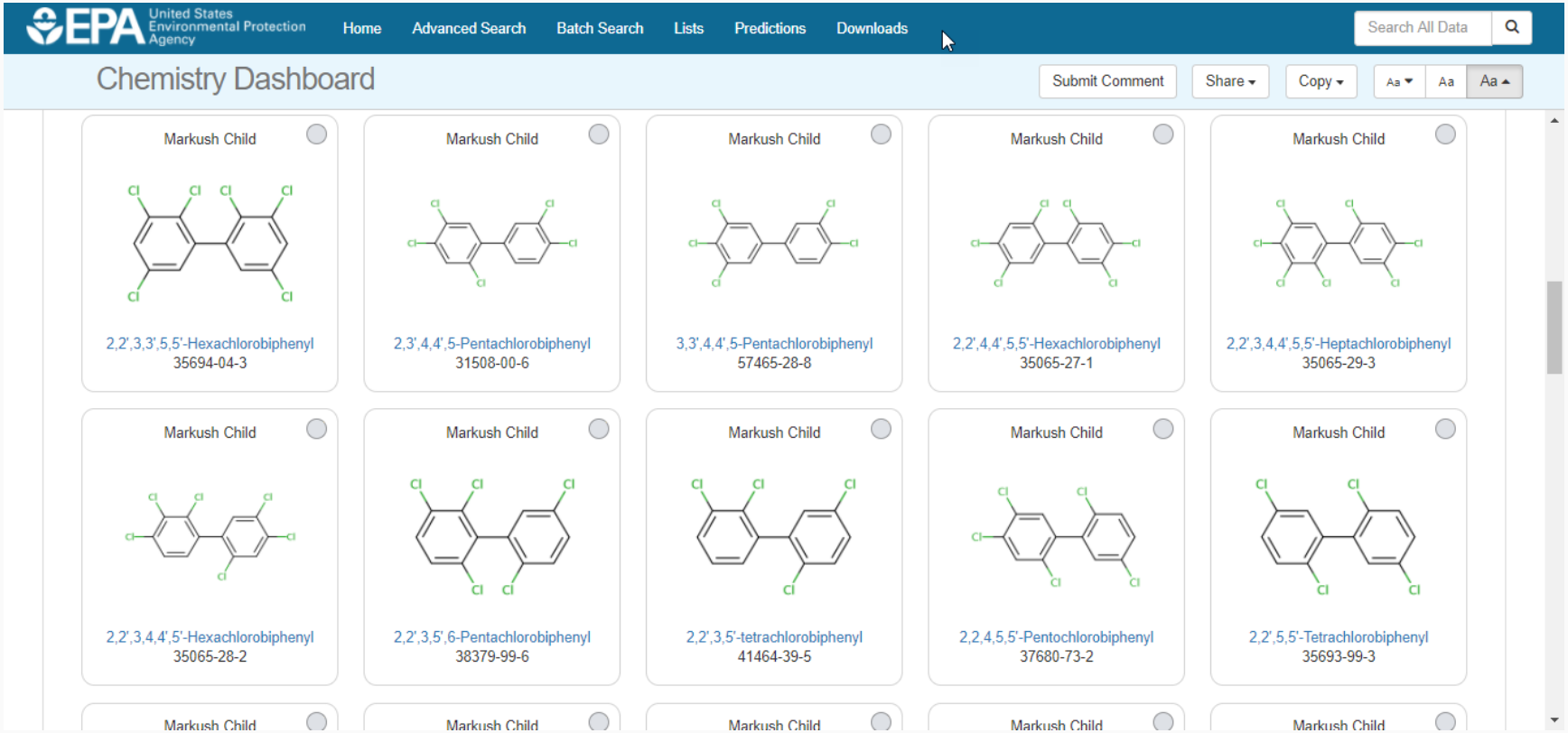
Sodium xylenesulfonate
1300-72-7



Diisononyl phthalate
28553-12-0

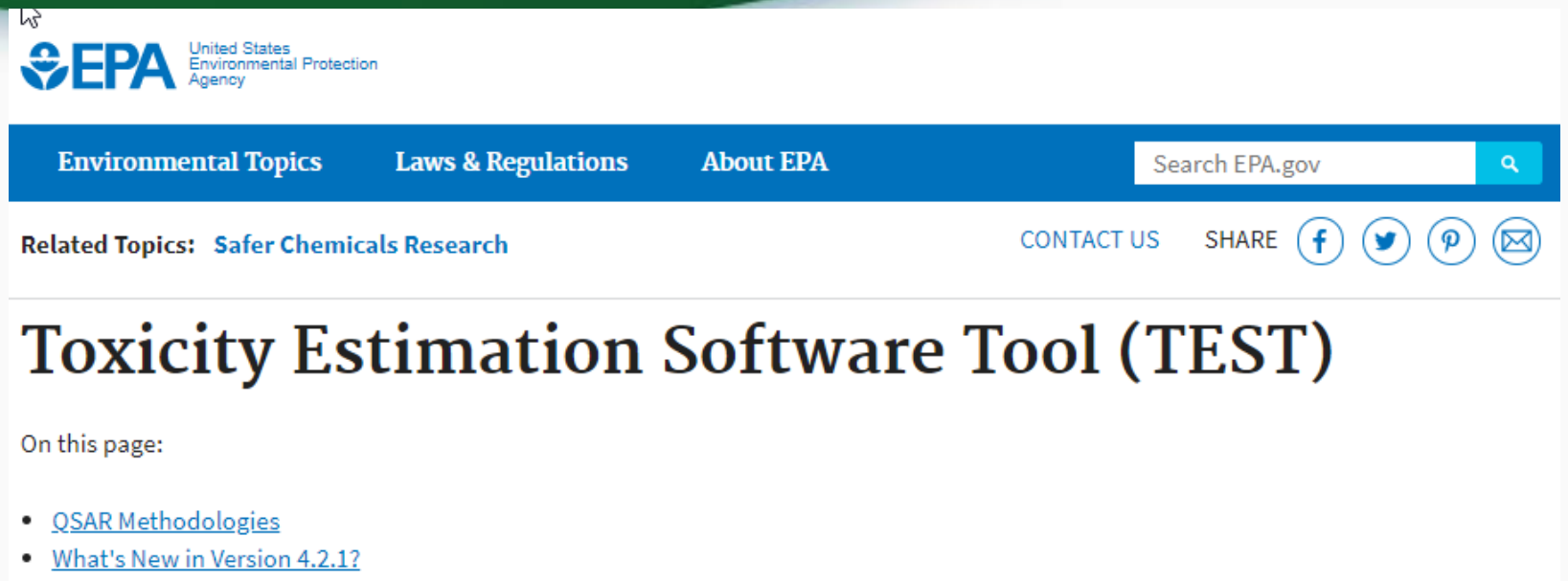
Enumeration of Markush

- Markush structures can be enumerated into chemical families



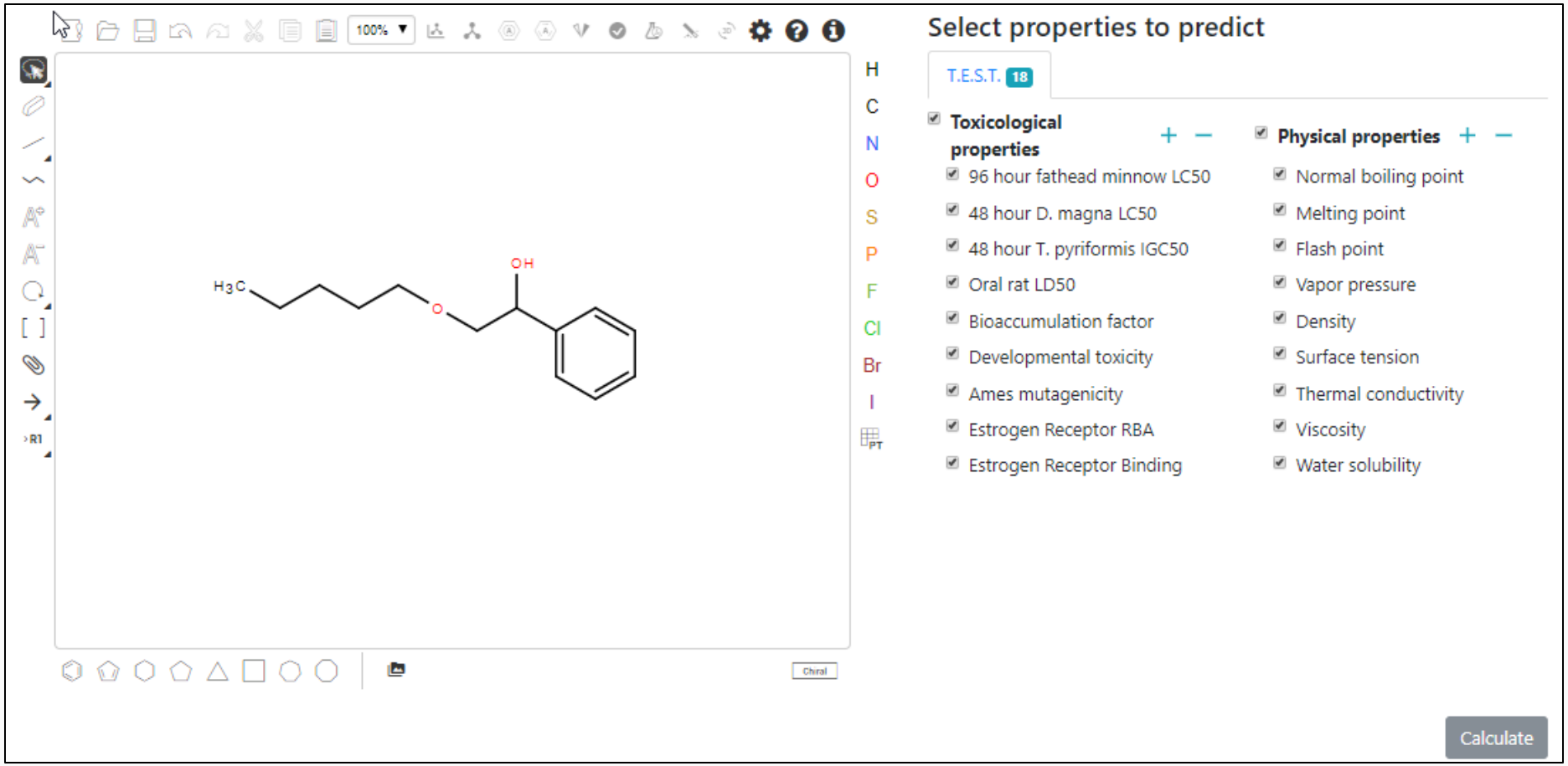
Real Time Predictions

10 Years of EPA T.E.S.T Models



- Over 10 years of QSAR modeling at the desktop – installable Java module (from National Risk Management Research Laboratory)
- Now 750,000 chemicals predicted and real time predictions are available

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

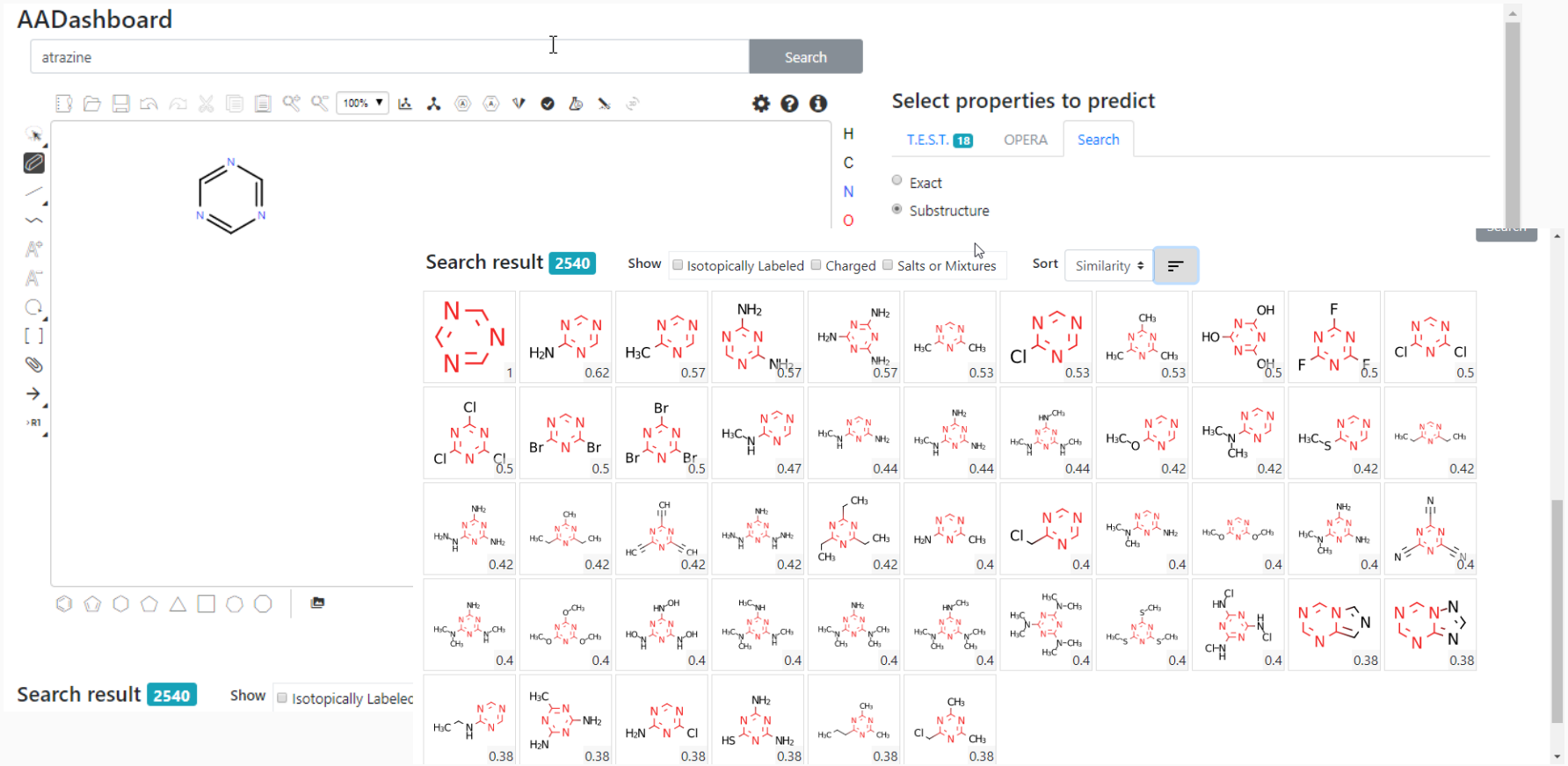
Work in Progress

- Present work in development
  - Real time OPERA predictions – TEST predictions done

Work in Progress

- Present work in development
  - Real time OPERA prediction
  - Structure/substructure/similarity search

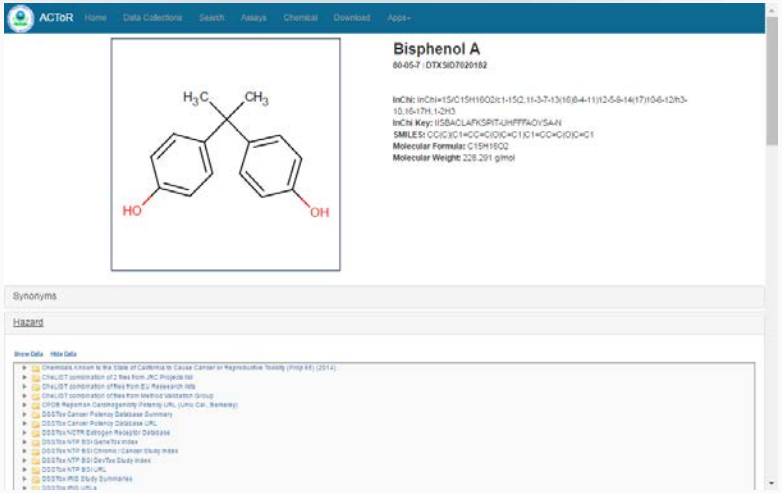
Prototype Development

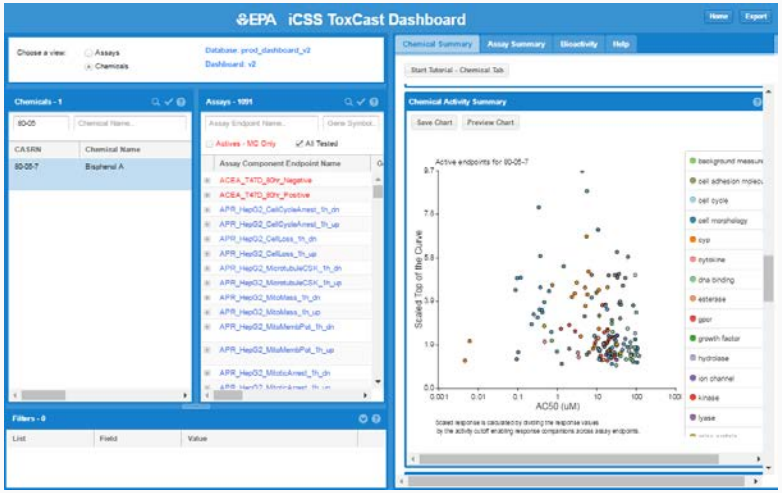


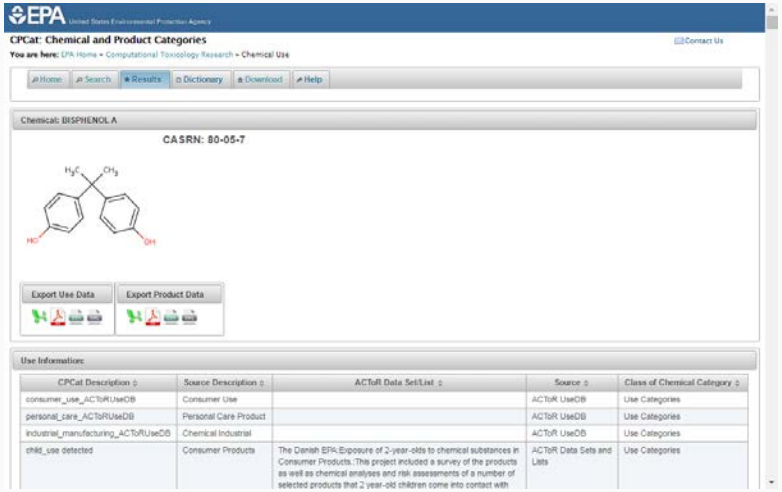
Work in Progress

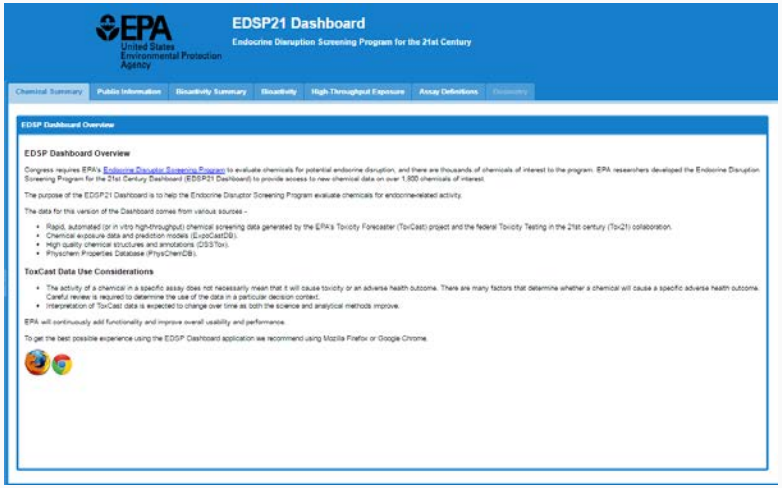
- Present work in development
  - Real time OPERA prediction
  - Structure/substructure/similarity search
  - Merging in other NCCT dashboard capabilities

Earlier Dashboard Applications

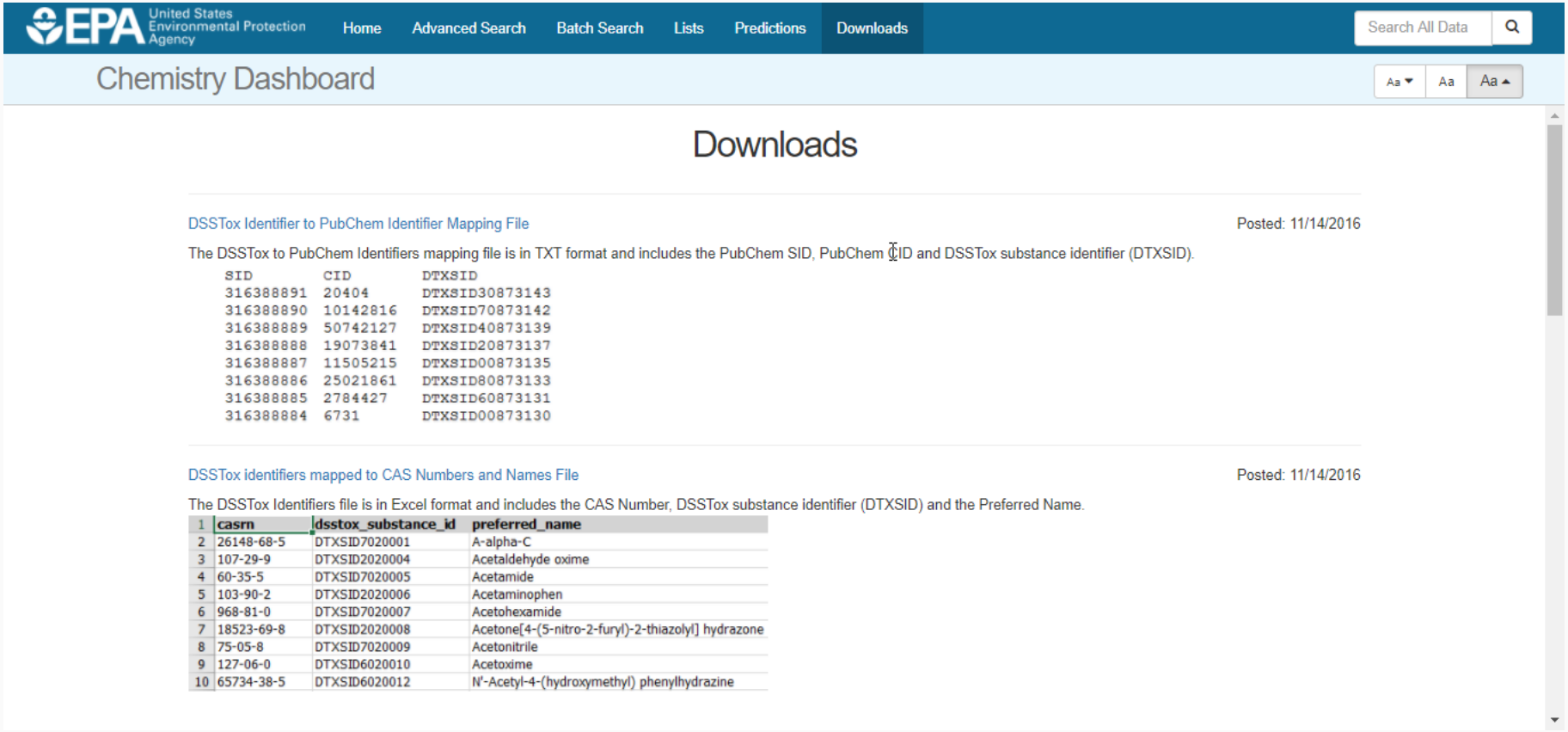








Downloadable Data



Conclusion

- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- An expanding list of data types and sources has been integrated
- The chemical lists of interest grows with each release
- Real time prediction models rollout has started

- Exciting array of additional searches in development

April 1st is the 2nd birthday

Acknowledgments

- The NCCT CompTox Chemistry Dashboard Development Team
- The NCCT Team of Scientists
- NERL scientists - Mass Spectrometry
- Kamel Mansouri – OPERA models
- Todd Martin – TEST predictions

Contact

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ORCID: https://orcid.org/0000-0002-2668-4821