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Where are we now? Celebrating the 10th Incremental Release of the CompTox Chemicals Dashboard

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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

July 23rd 2020
Communities of Practice

Outline

- A Short History of the Dashboard
- What is the dashboard used for?
- New capabilities, data and lists
- Linkages – outbound and inbound
- Contributing to Data Quality
- Prototypes in progress
- What's the Next Big Change?

But first

EPA United States Environmental Protection Agency

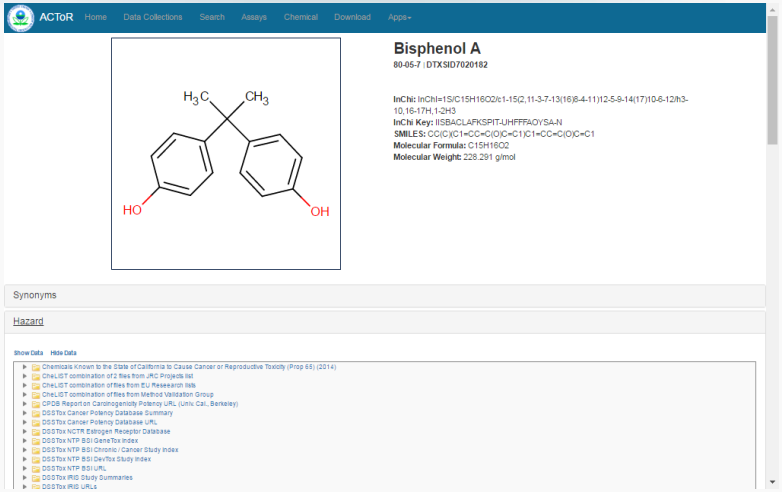
THANK YOU TO ALL CONTRIBUTORS

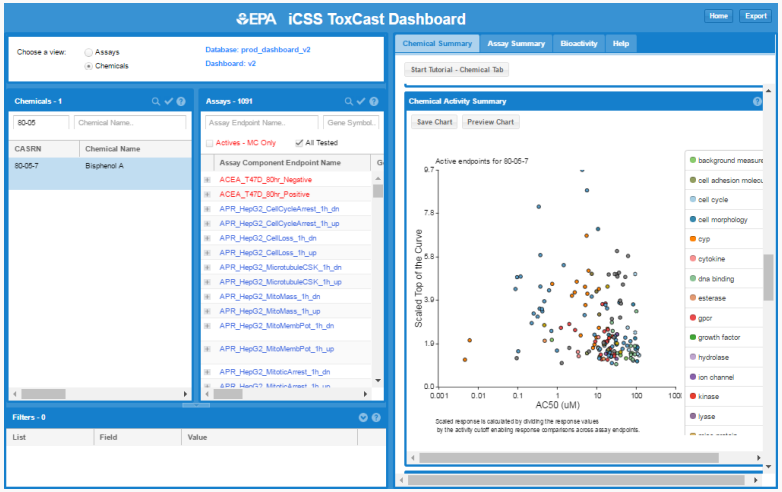
Acknowledgments upfront…

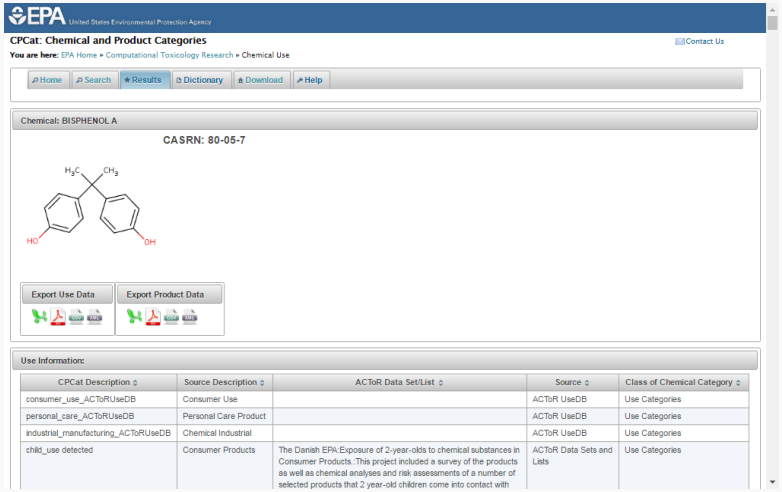
- CCTE Members
  - CompTox Chemicals Dashboard Development Team
  - Principal Investigators and postdocs
  - Curation Team
- Collaborators across the agency for data sets, testing and cross-linking
- Contributors of datasets for registration
- And you, the users for support and feedback

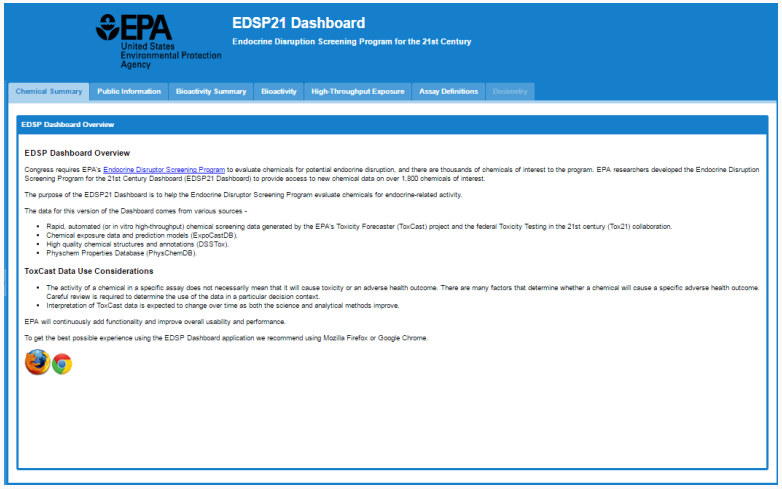
A SHORT HISTORY of the DASHBOARD

Earlier Dashboard Applications

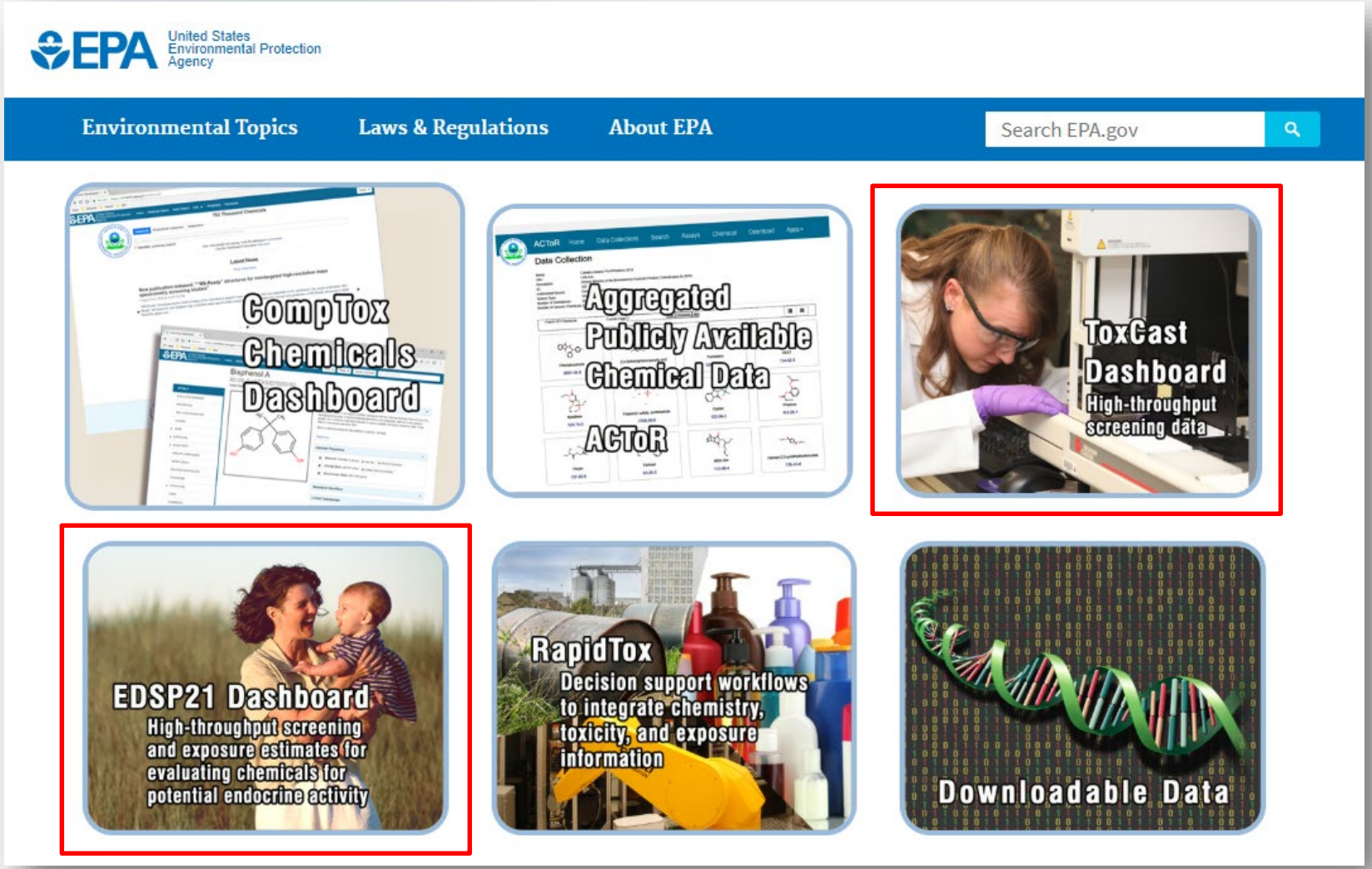






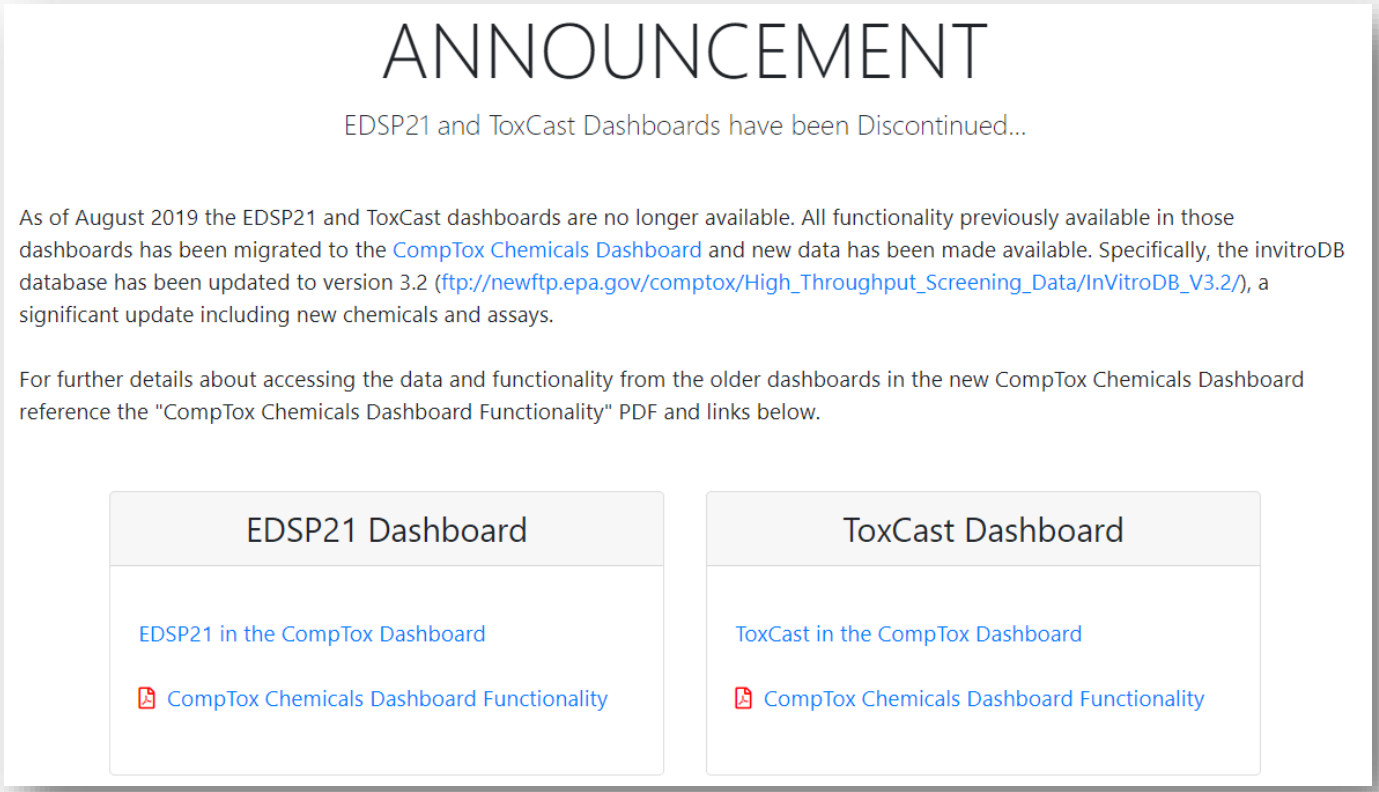


Retired Dashboards – Two Gone



ToxCast and EDSP21 Dashboards

- Both dashboards served valuable purposes for a number of years but blended in now



ANNOUNCEMENT

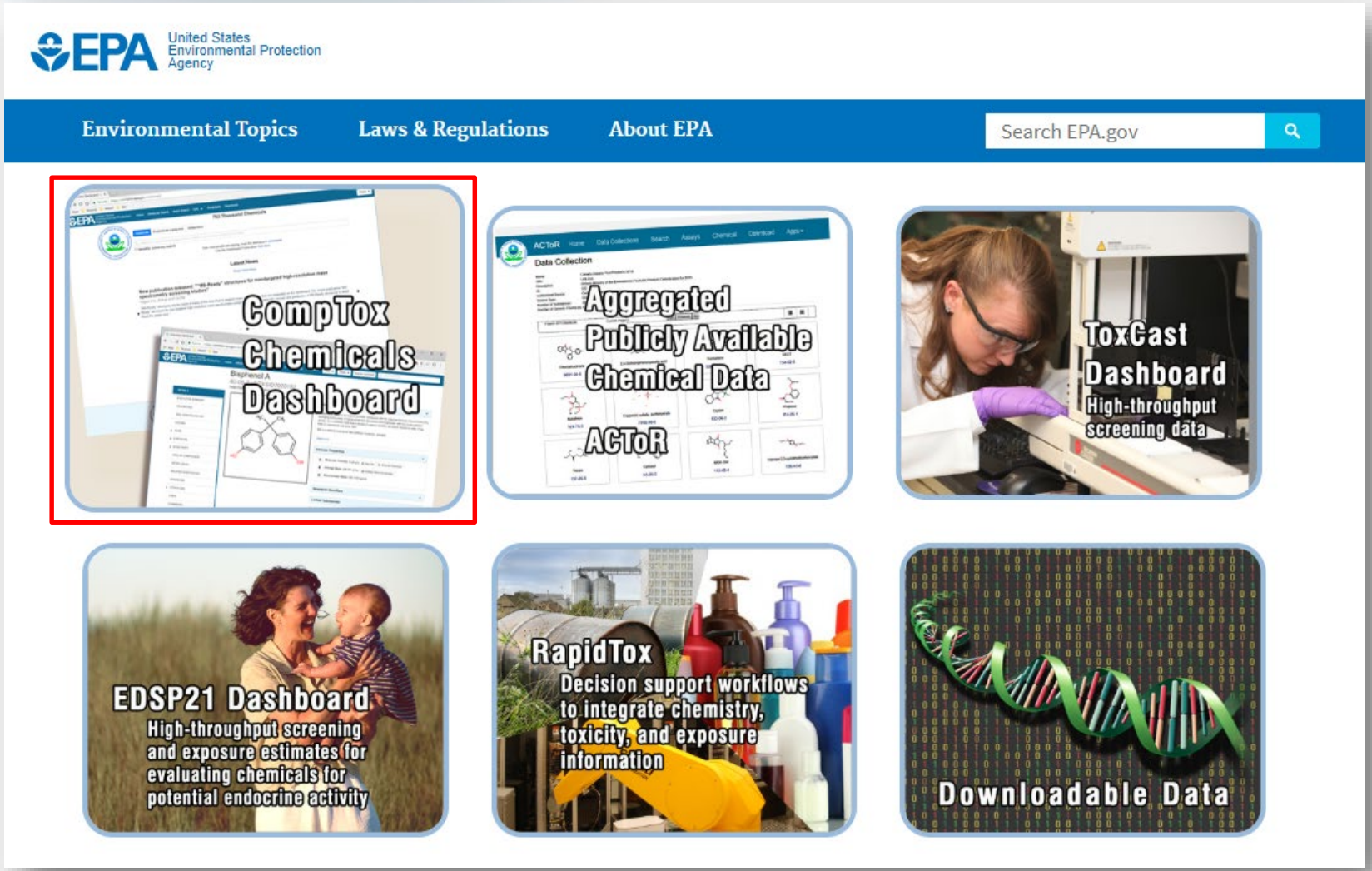
EDSP21 and ToxCast Dashboards have been Discontinued...

As of August 2019 the EDSP21 and ToxCast dashboards are no longer available. All functionality previously available in those dashboards has been migrated to the CompTox Chemicals Dashboard and new data has been made available. Specifically, the invitroDB database has been updated to version 3.2 (ftp://newftp.epa.gov/comptox/High_Throughput_Screening_Data/InVitroDB_V3.2/), a significant update including new chemicals and assays.

For further details about accessing the data and functionality from the older dashboards in the new CompTox Chemicals Dashboard reference the "CompTox Chemicals Dashboard Functionality" PDF and links below.

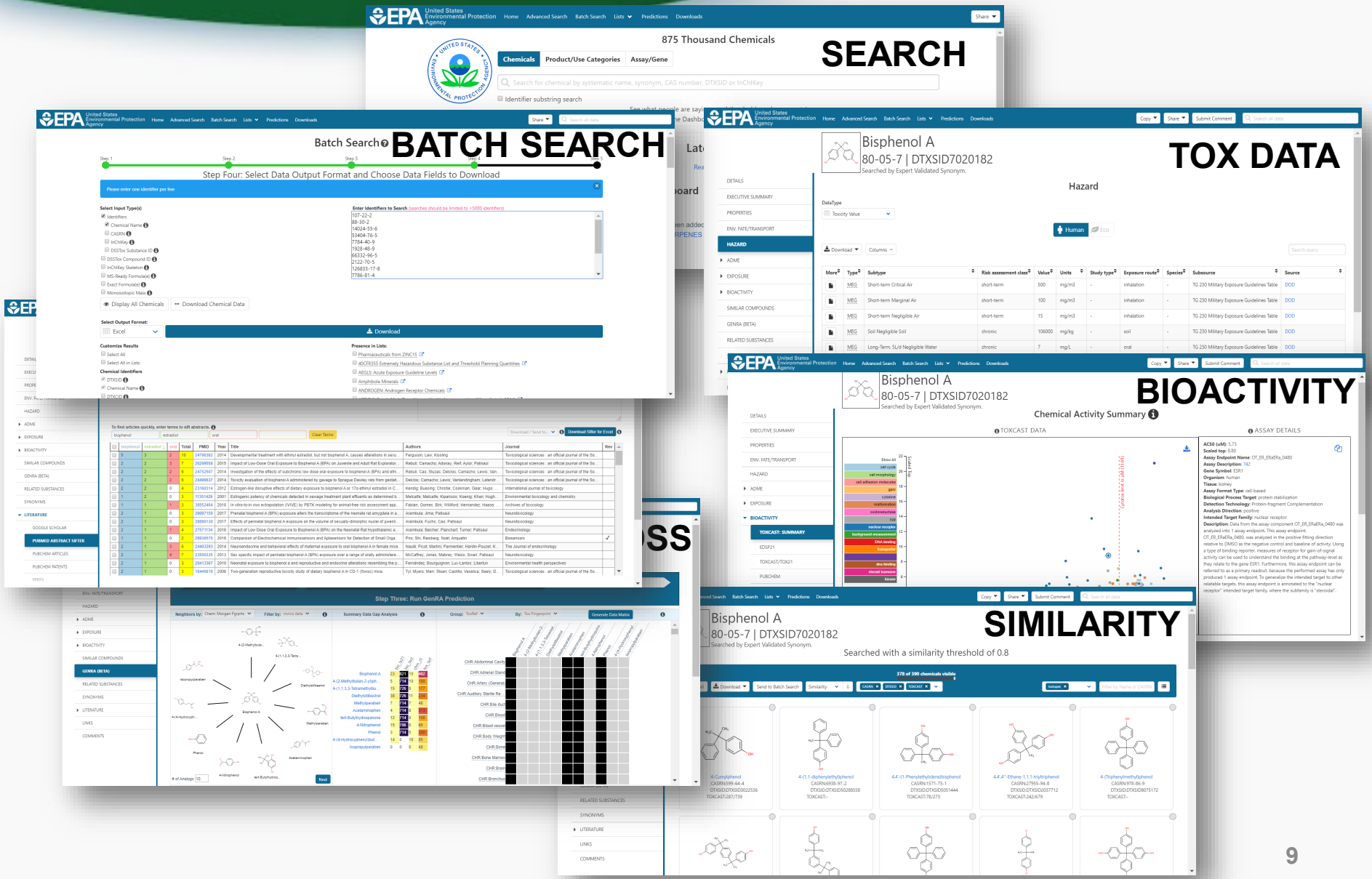
EDSP21 Dashboard	ToxCast Dashboard
EDSP21 in the CompTox Dashboard	ToxCast in the CompTox Dashboard
CompTox Chemicals Dashboard Functionality	CompTox Chemicals Dashboard Functionality

The CompTox Portal – get it here https://comptox.epa.gov/



CompTox Chemicals Dashboard

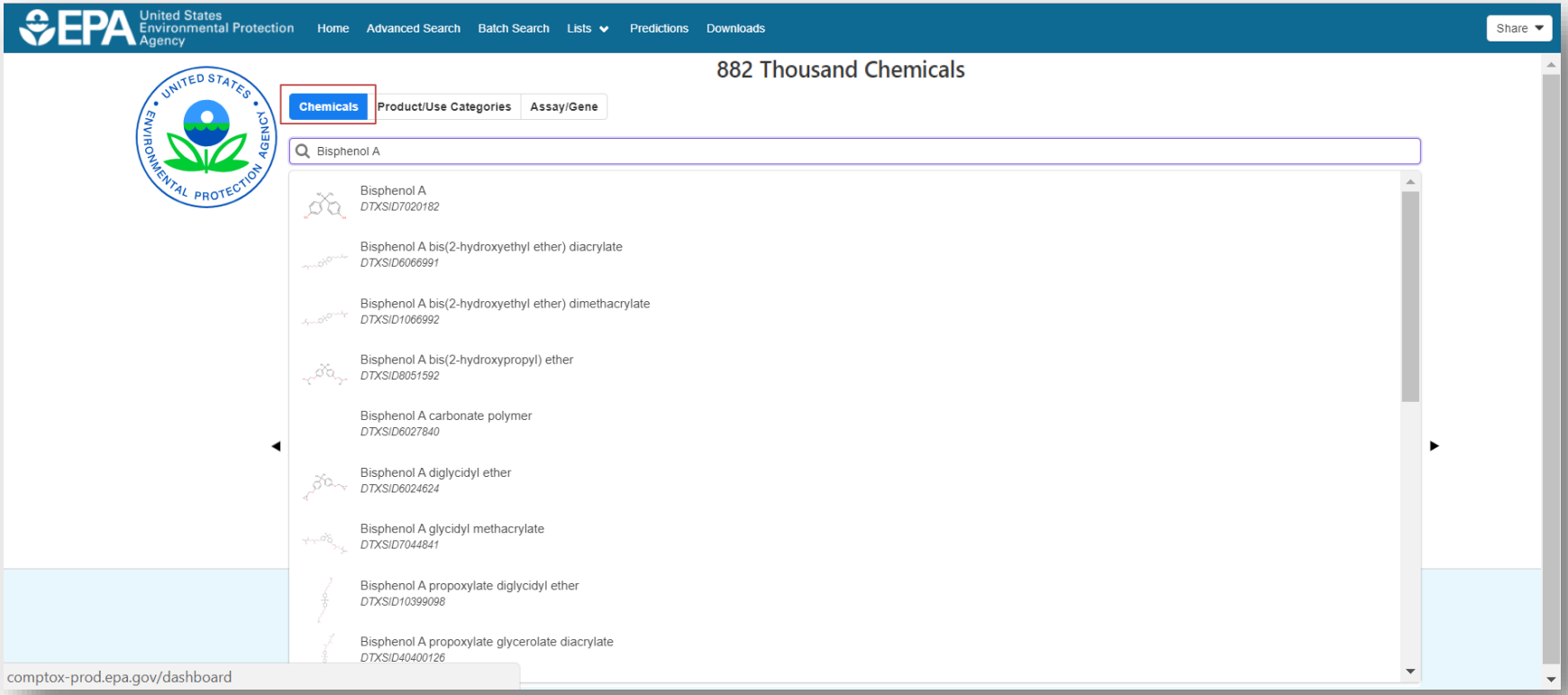
https://comptox.epa.gov/dashboard



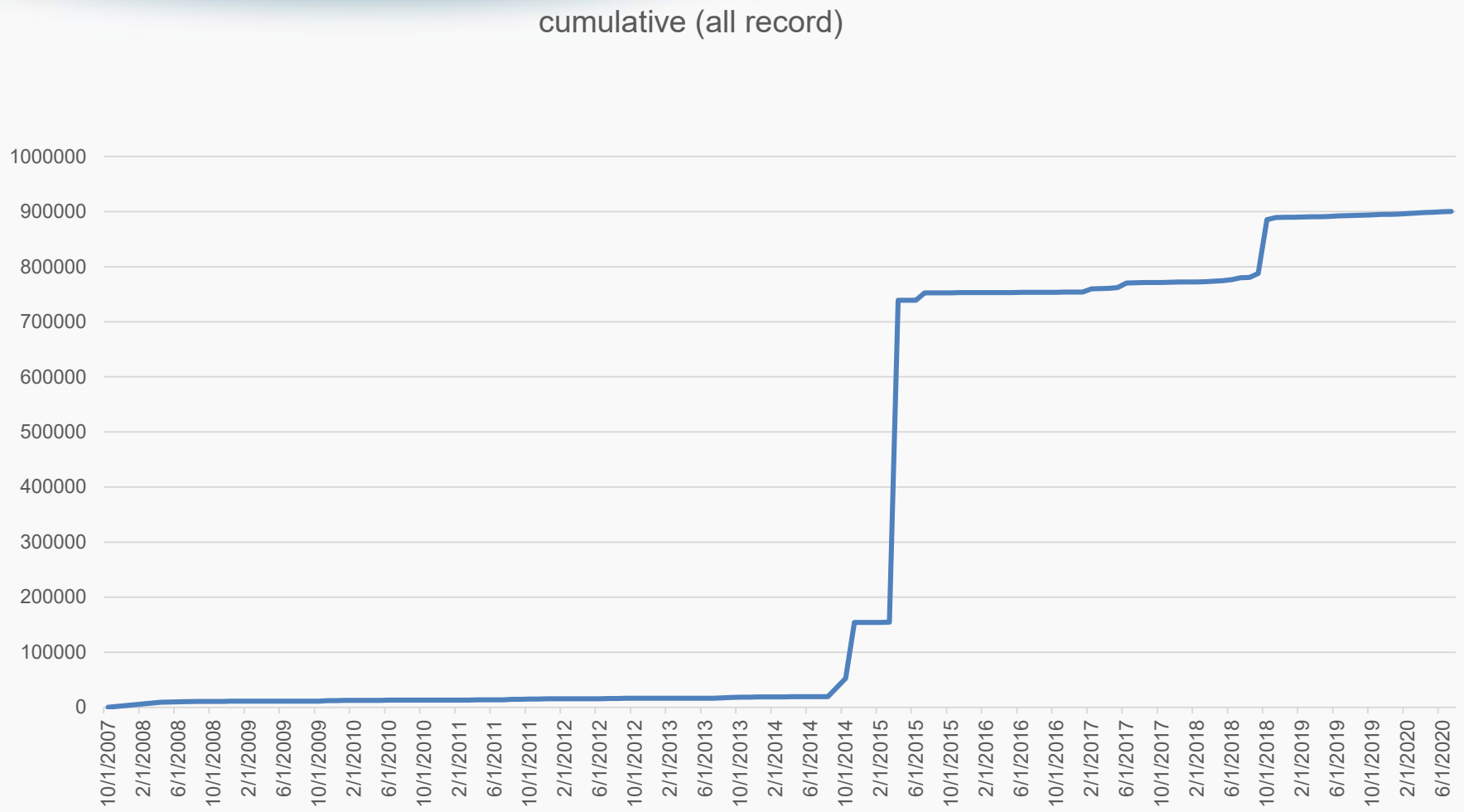
WHAT IS THE DASHBOARD USED FOR?

(and some what's new)

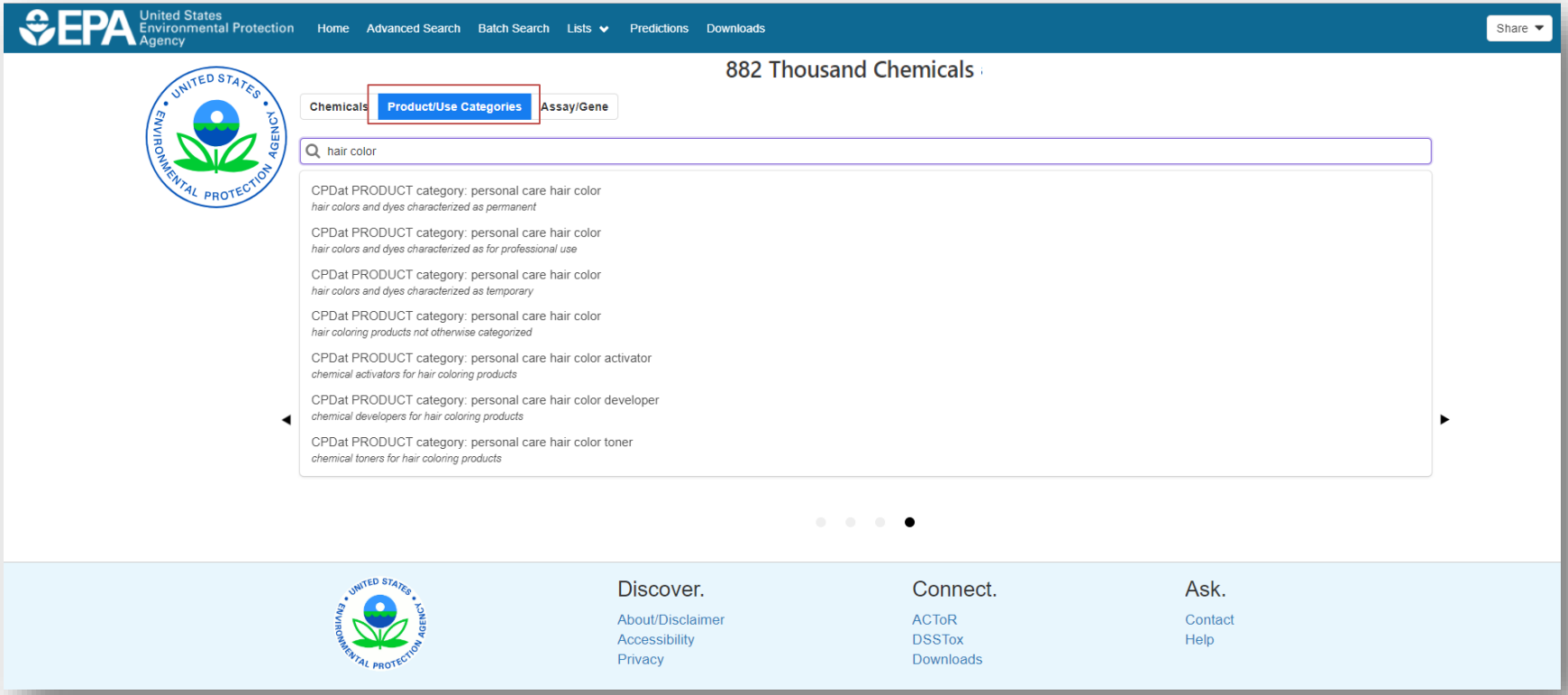
CompTox Dashboard Chemicals



DSSTox growth – 2007 to 2020
>7000 new chemicals added

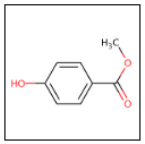


CompTox Dashboard
Products and Use Categories



Additional Exposure Data

588k consumer products now in the database.
Under constant curation and expansion…



Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

Chemical Weight Fractions

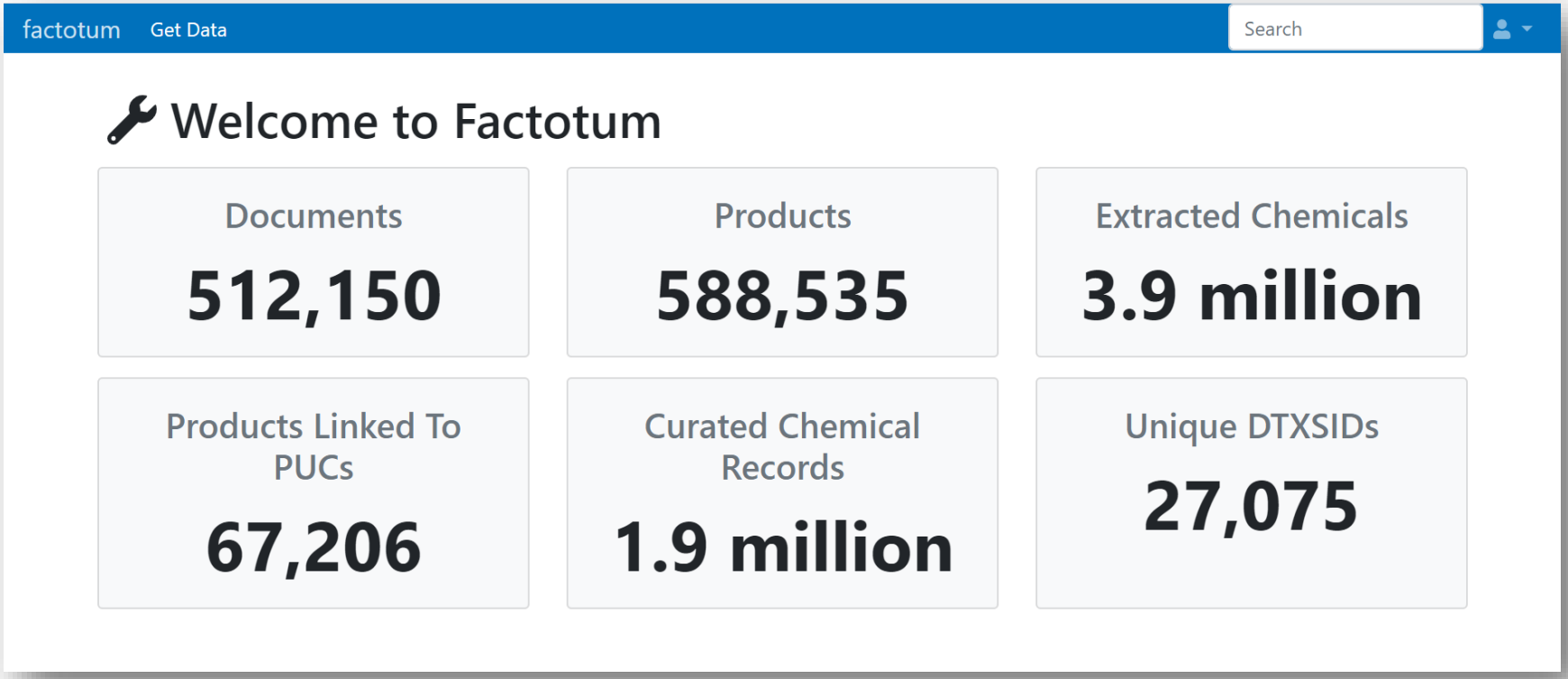
Download | Columns | 10 | Search query

Product Name	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
114 9764 kodak ektachem calibrator kit 5-calibrator 1	0.00	1.00e-2	MSDS	SIRI
114 9764 kodak ektachem calibrator kit 5-calibrator 2	0.00	1.00e-2	MSDS	SIRI
173 6594 ektachem liquid calibrator 16	0.00	1.00e-2	MSDS	SIRI
2540 gabe's grit	0.00	5.00e-3	MSDS	SIRI
276300_ solution_ a e r pads	0.00	1.00e-3	MSDS	SIRI
420 rp super filter coat_ ready-to-use	0.00	1.00e-2	MSDS	SIRI
421 rp super filter coat_ ready-to-use	0.00	1.00e-2	MSDS	SIRI
422 rp super filter coat_ bulk ready-to-use	0.00	1.00e-2	MSDS	SIRI
846 6492 ektachem liquid performance verifier i	0.00	1.00e-2	MSDS	SIRI
846 6492 kodak ektachem liquid performance verifier	0.00	1.00e-2	MSDS	SIRI

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 21 to 30 of 462 records

The Factotum Database



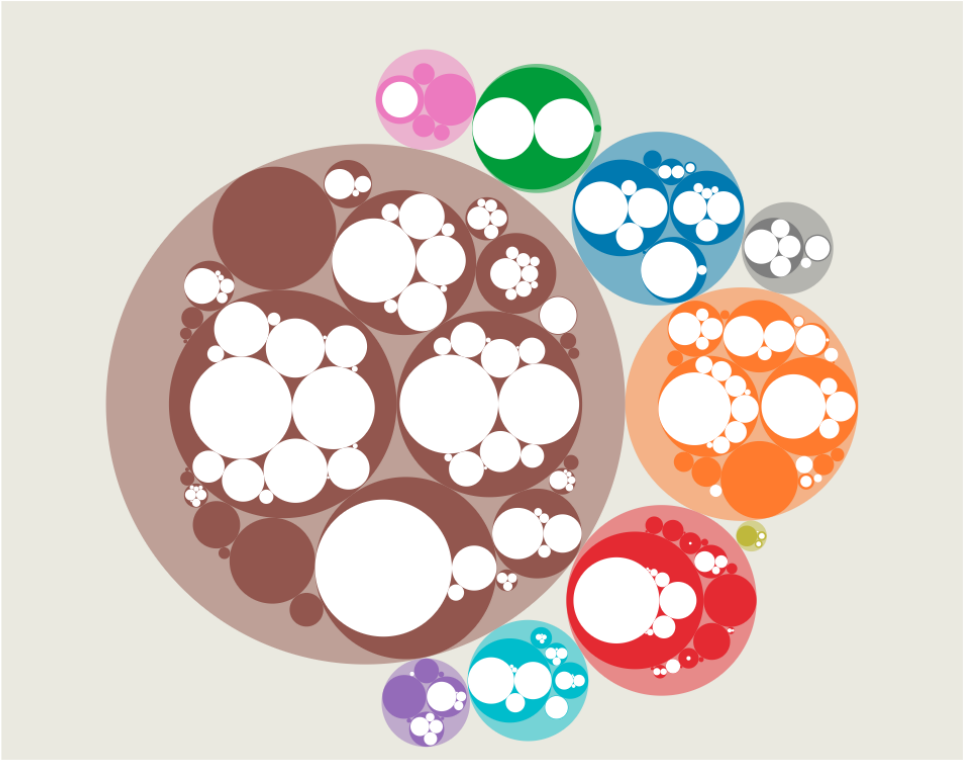
The Factotum Database

EPA United States Environmental Protection Agency

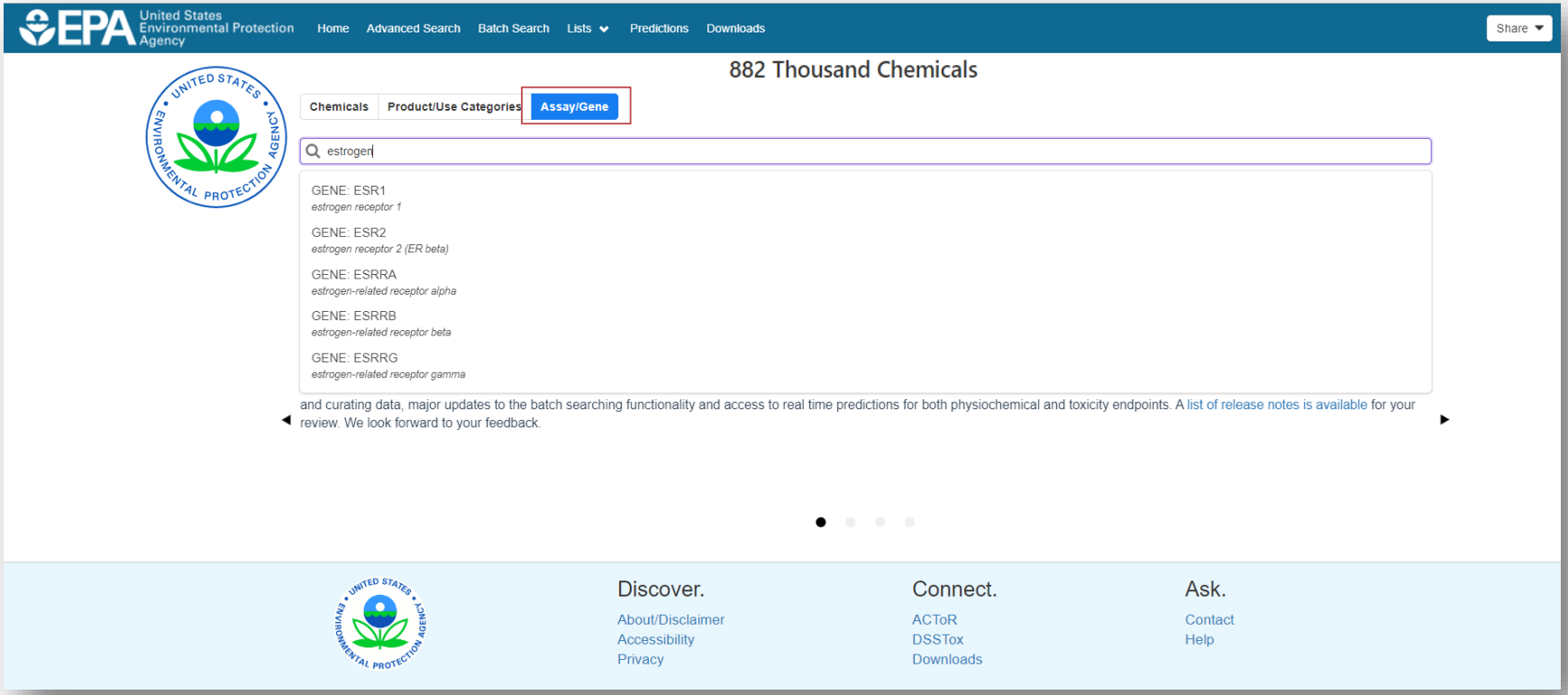
Formulation PUCs

General Category - Product Family - Product Type

Arts and crafts/Office supplies	3962
Cleaning products and household care	7917
Electronics/small appliances	2184
Home maintenance	5089
Landscape/Yard	1113
Personal care	38626
Pesticides	1472
Pet care	1076
Sports equipment	139
Vehicle	1743



CompTox Dashboard
Assays and Genes



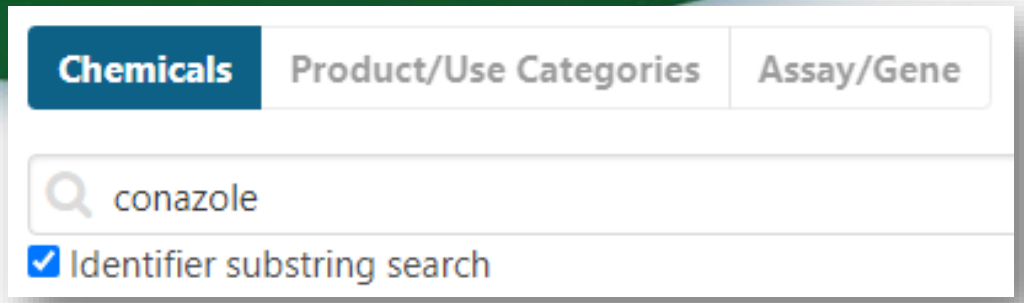
Growth in *invitrodb* data 2015:2020
~150 new assay endpoints

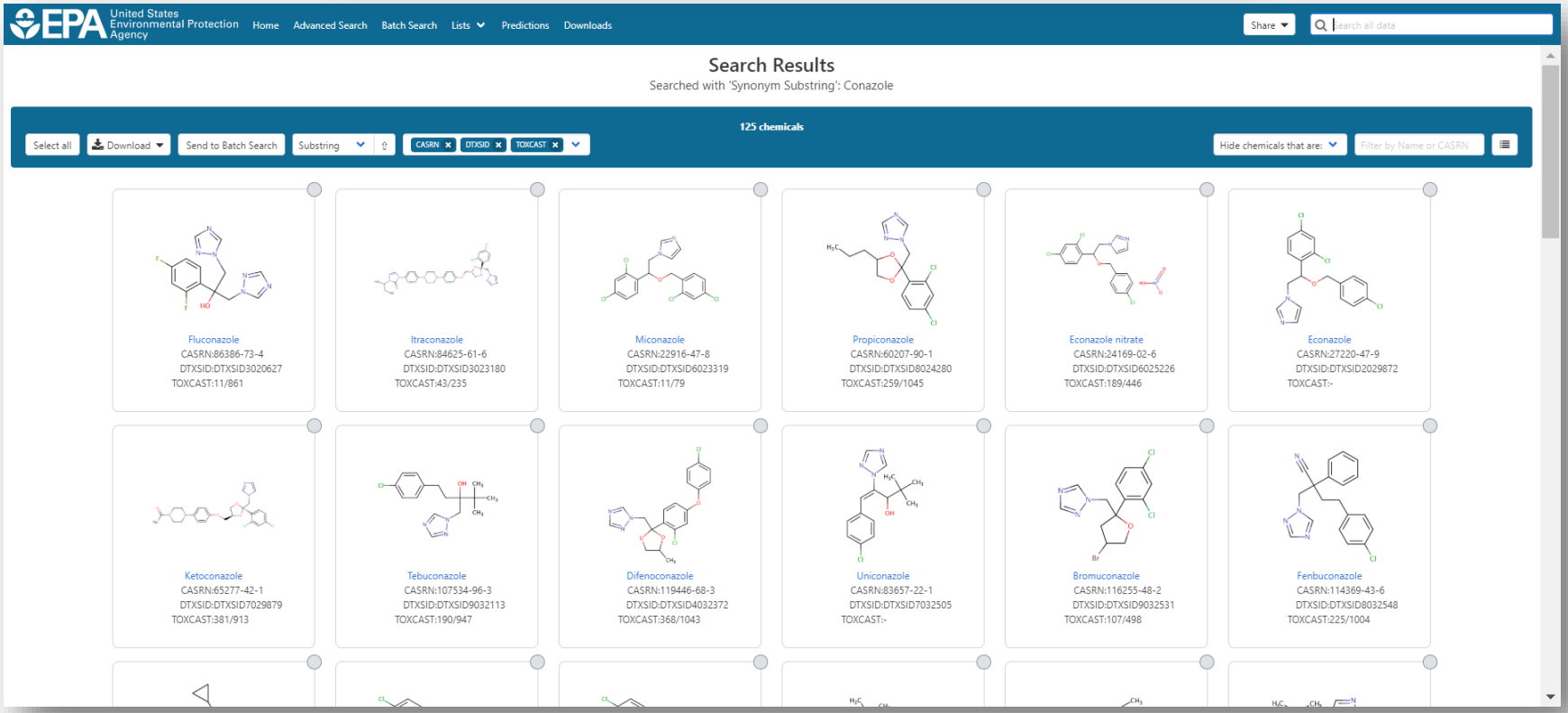
- >140 assay endpoints and >700 chemicals added
- Data re-pipelined with new fitting procedures and ~200k new curve fits released with this version
- >140 endpoints annotated to genes

Approx Year	Invitrodb Version (Public)	# assay endpoints	#chemicals (total)	#curve fits (chemical-aeid pairs)	#assay endpoints annotated to gene	#unique target genes annotated
2015	2.0	1192	9076	2,244,647	737	377
2018	3.1	1399	9214	3,281,340	1215	442
2019	3.2	1473	9224	3,525,844	1255	443
2020	3.3	1614	9949	3,720,594	1398	492

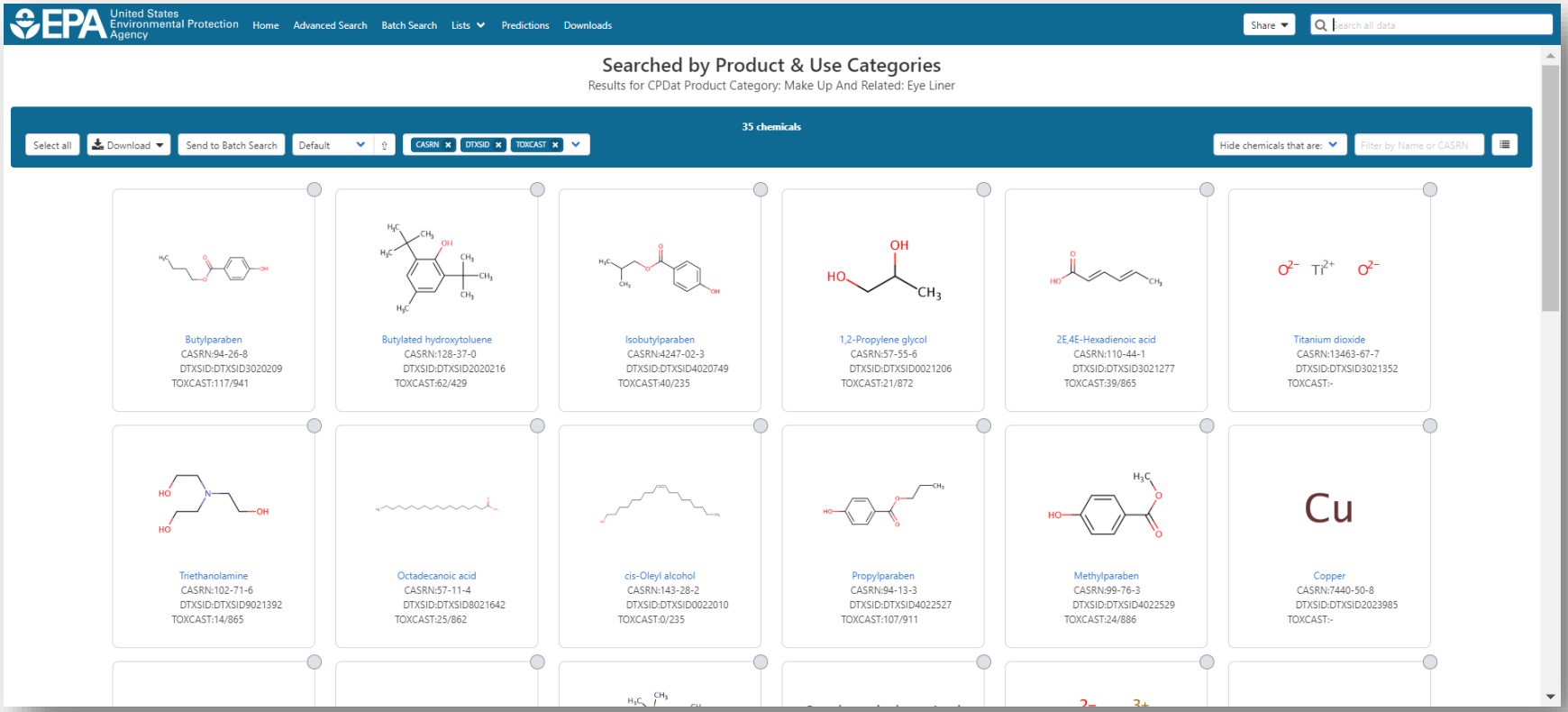
SOME EXAMPLES OF USAGE

Find me all “conazoles”



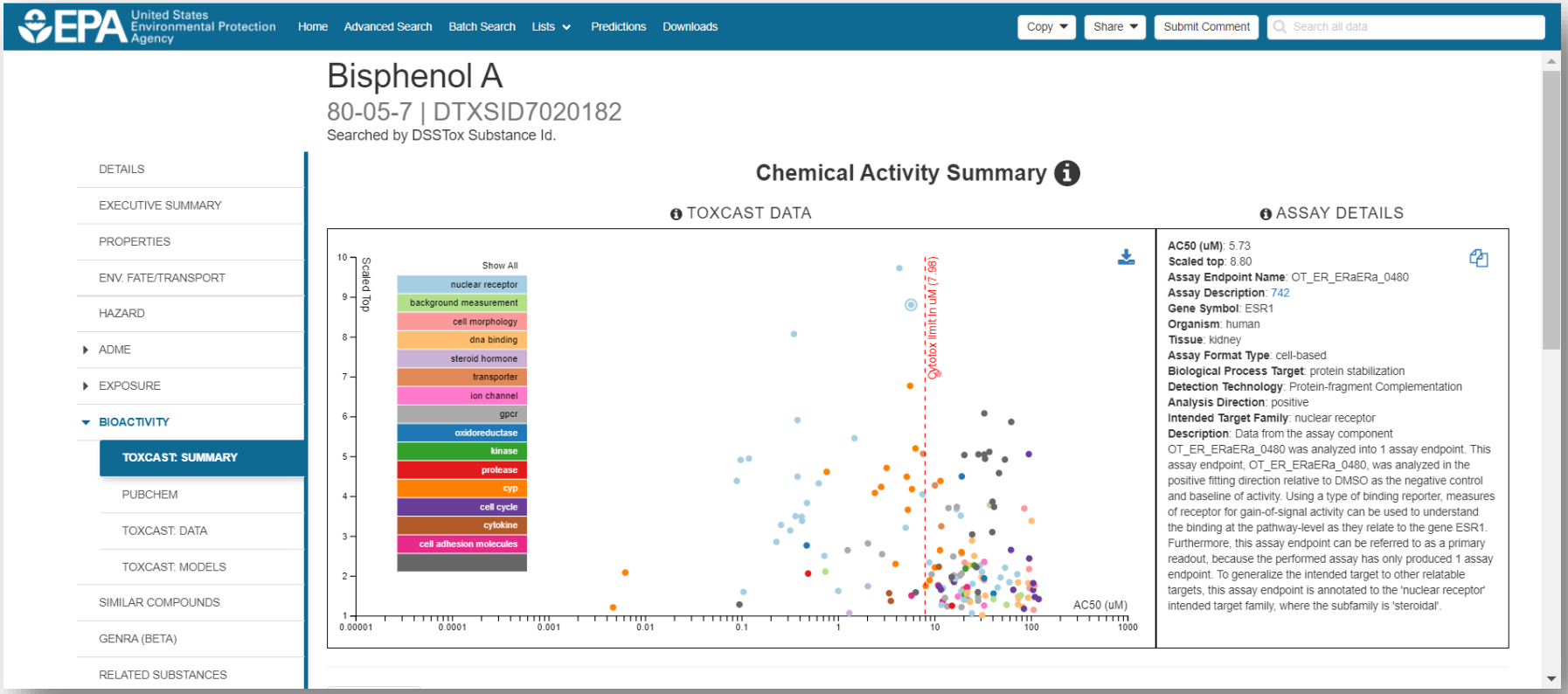


What chemicals in what use category?
"What's in eye liner?"



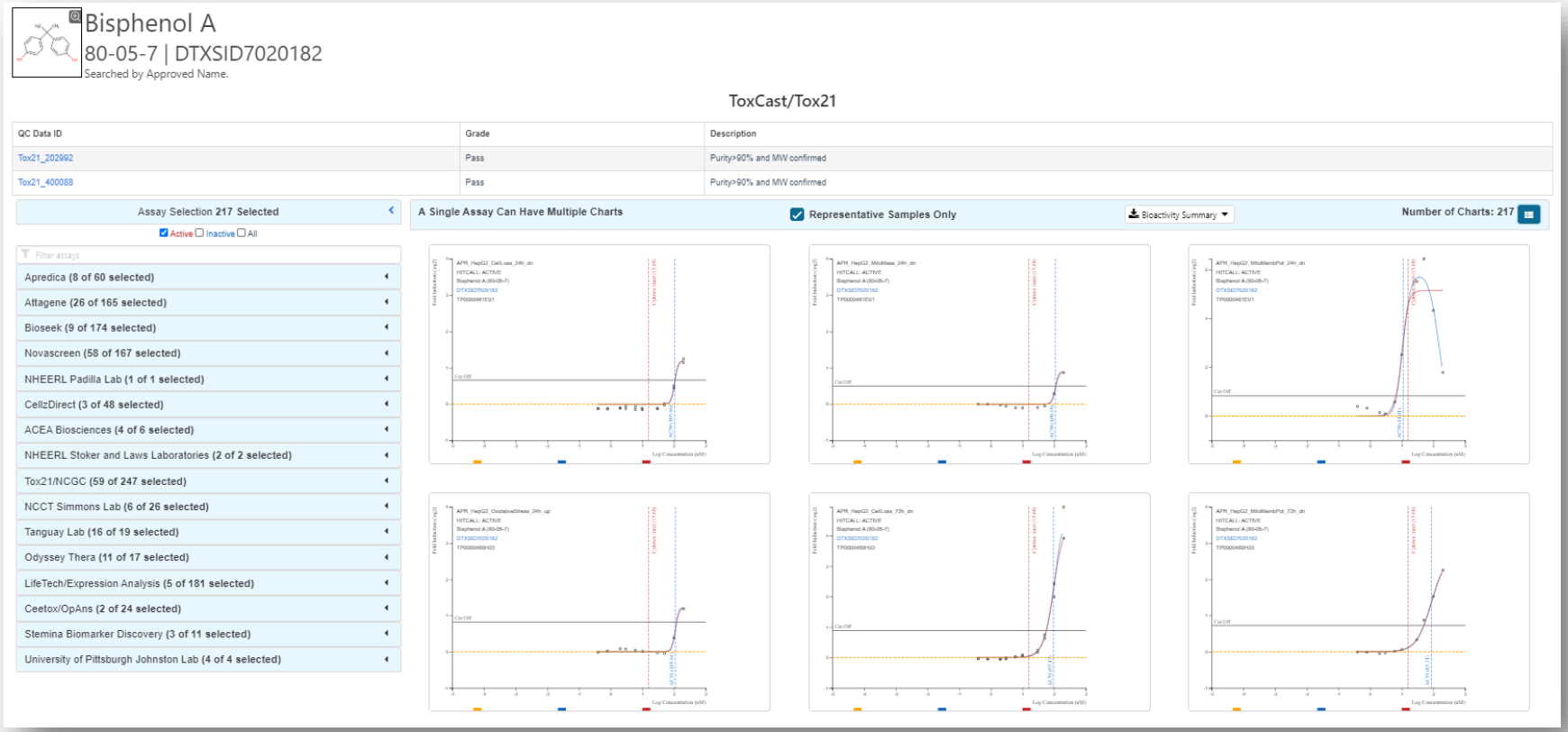
Access *In Vitro* Bioactivity Data

ToxCast and Tox21

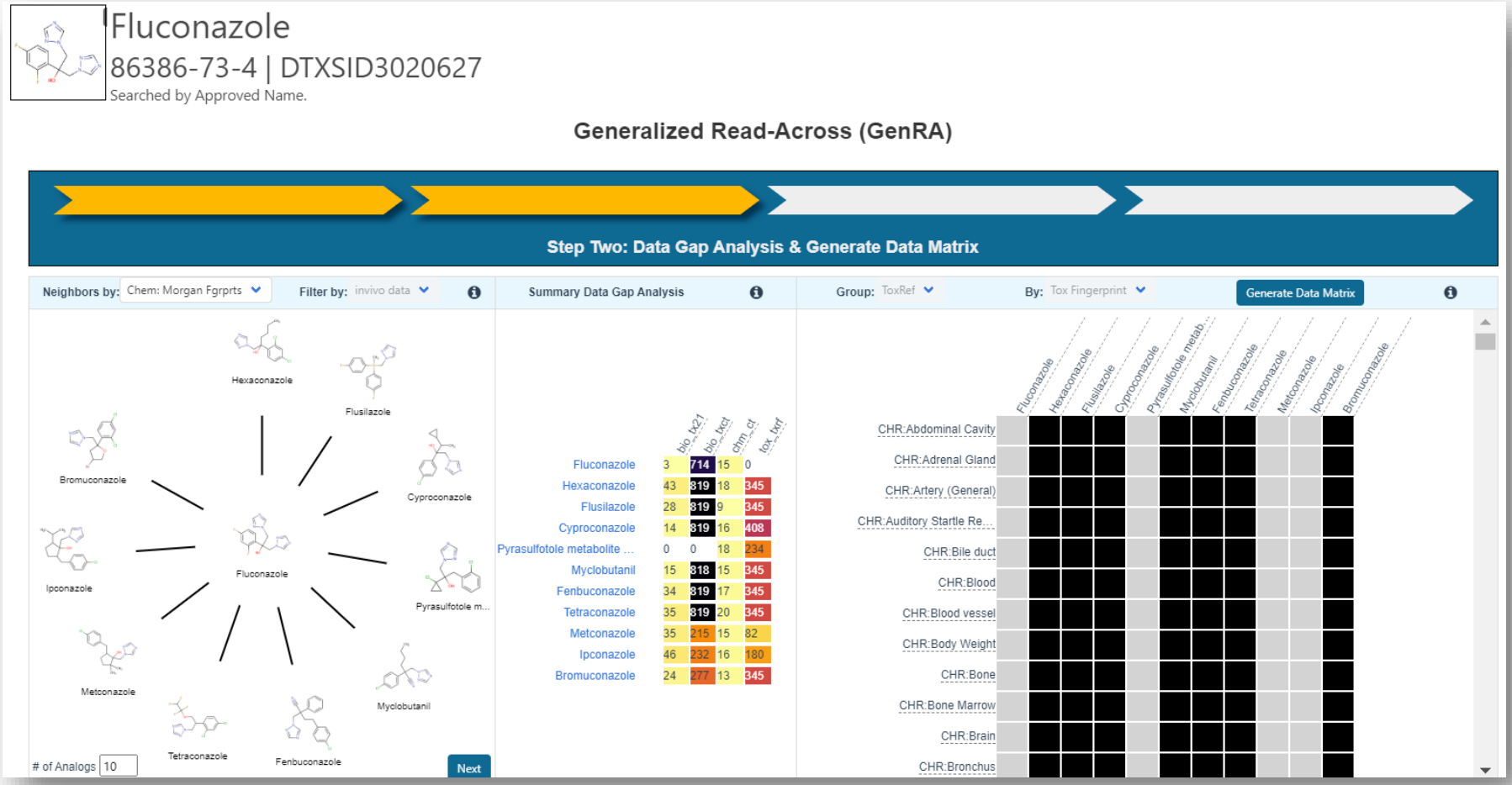


Access *In Vitro* Bioactivity Data

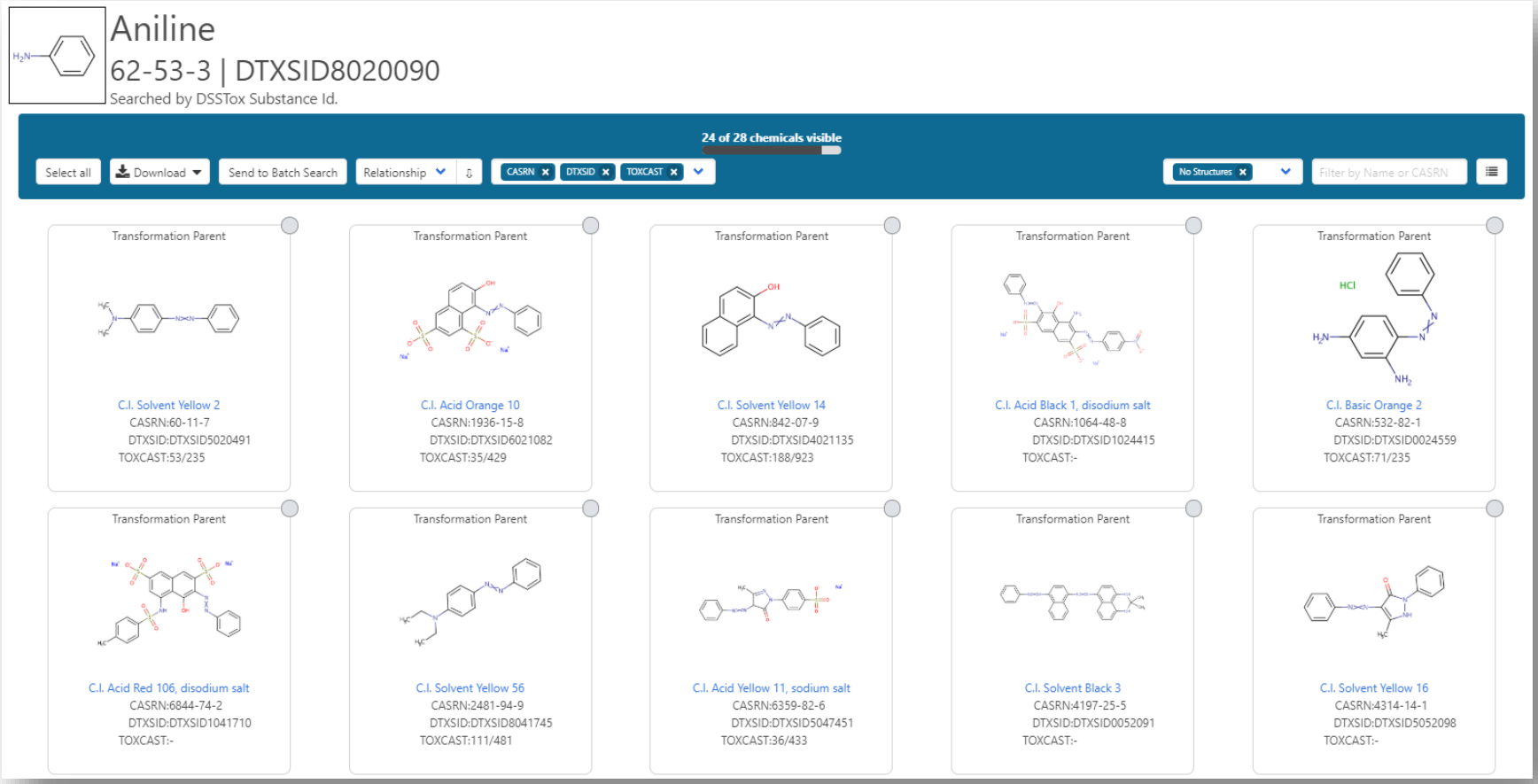
ToxCast and Tox21



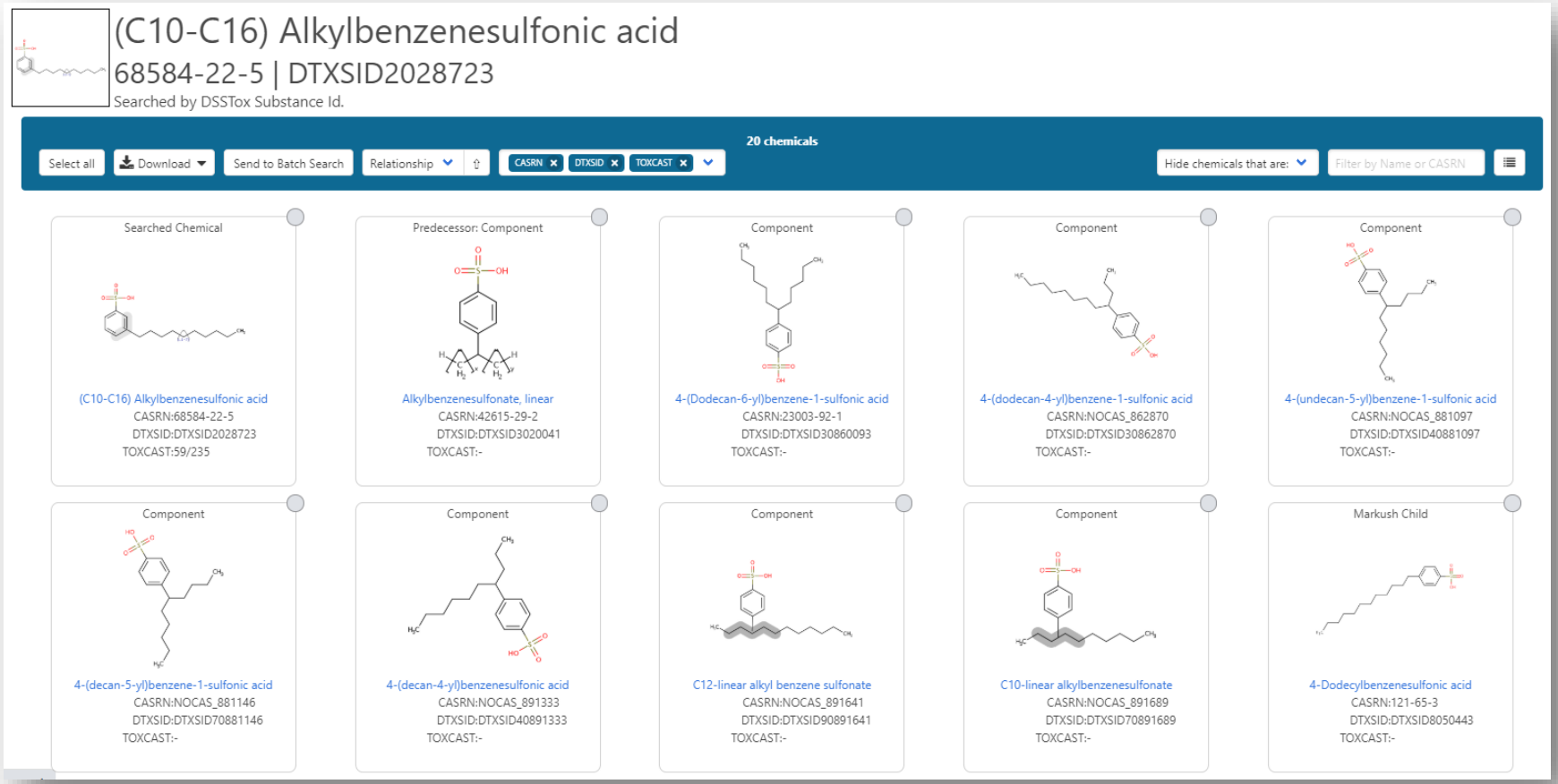
GenRA (Generalised Read-Across)



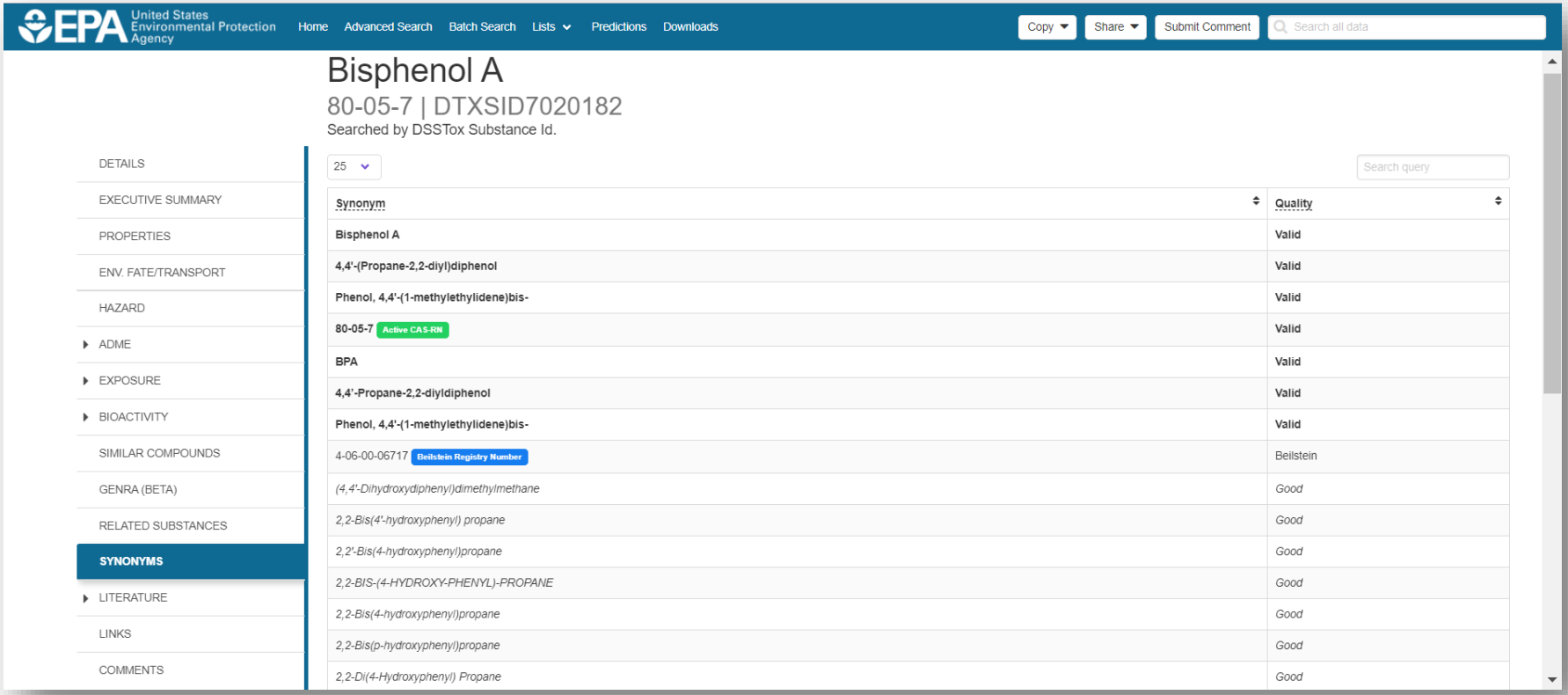
Related Substances
e.g. Transformation Products



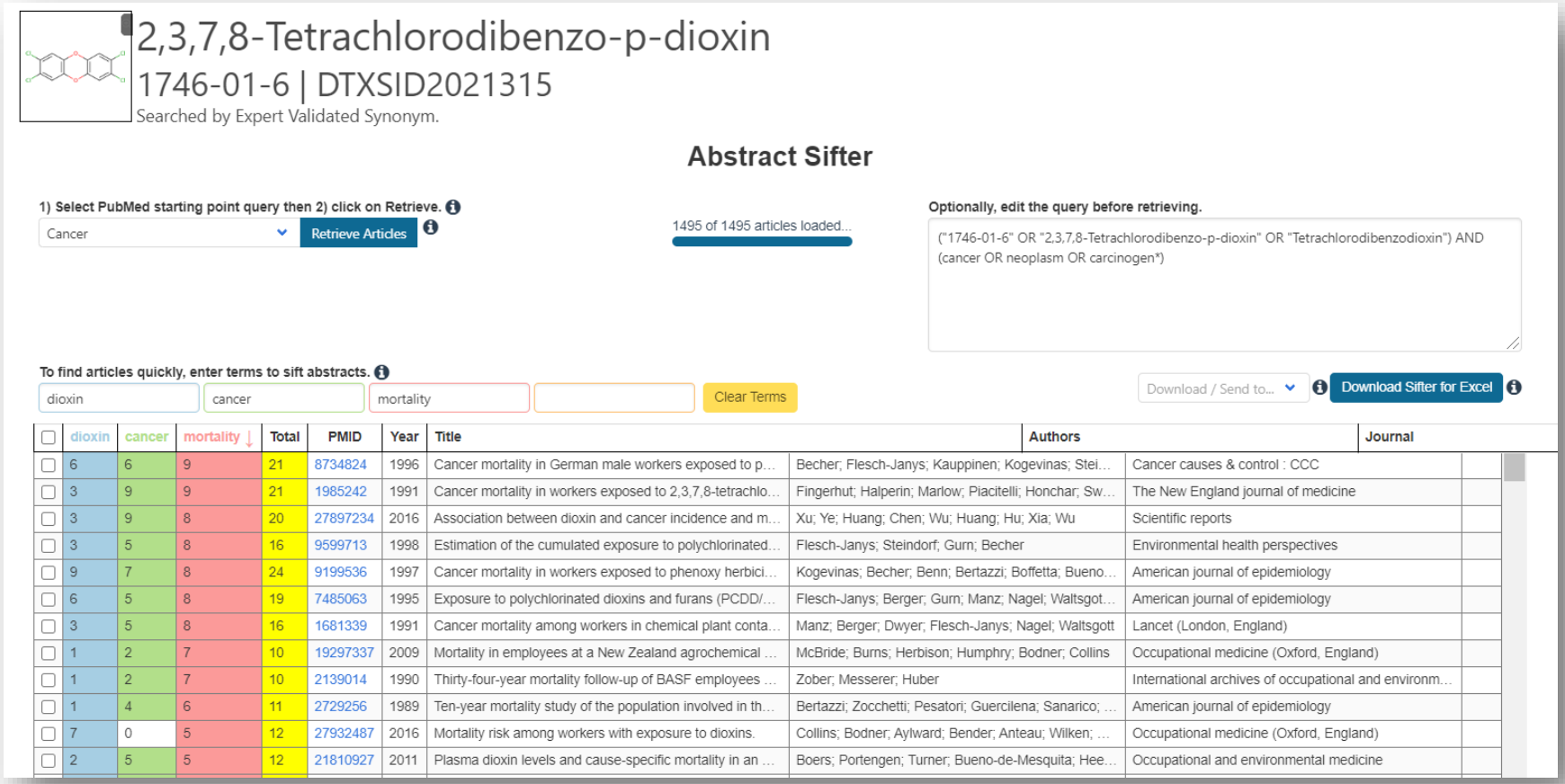
Related Substances for Markush



Identifiers to Support Searches

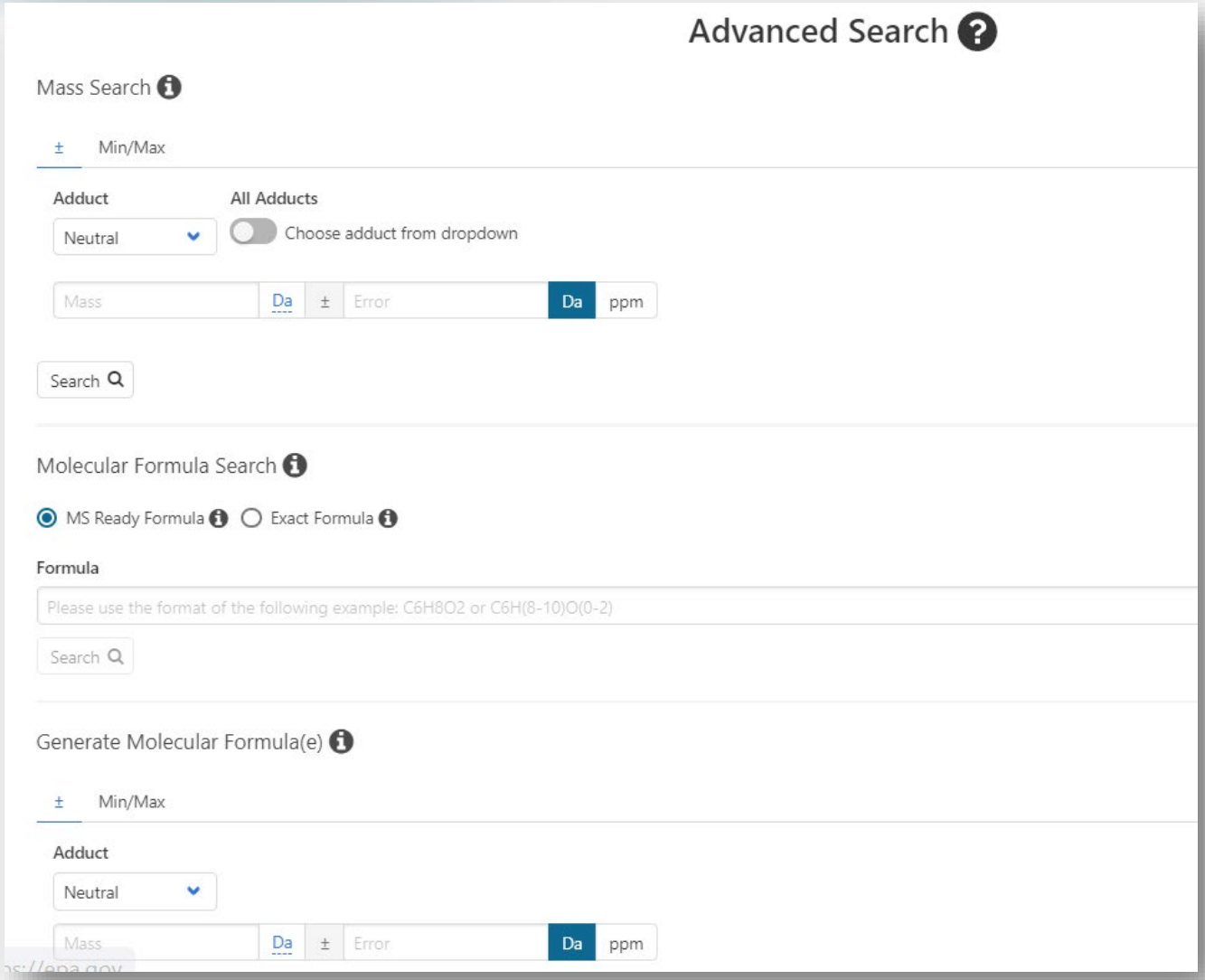


Abstract Sifter – PubMed Integration searching >30 million abstracts

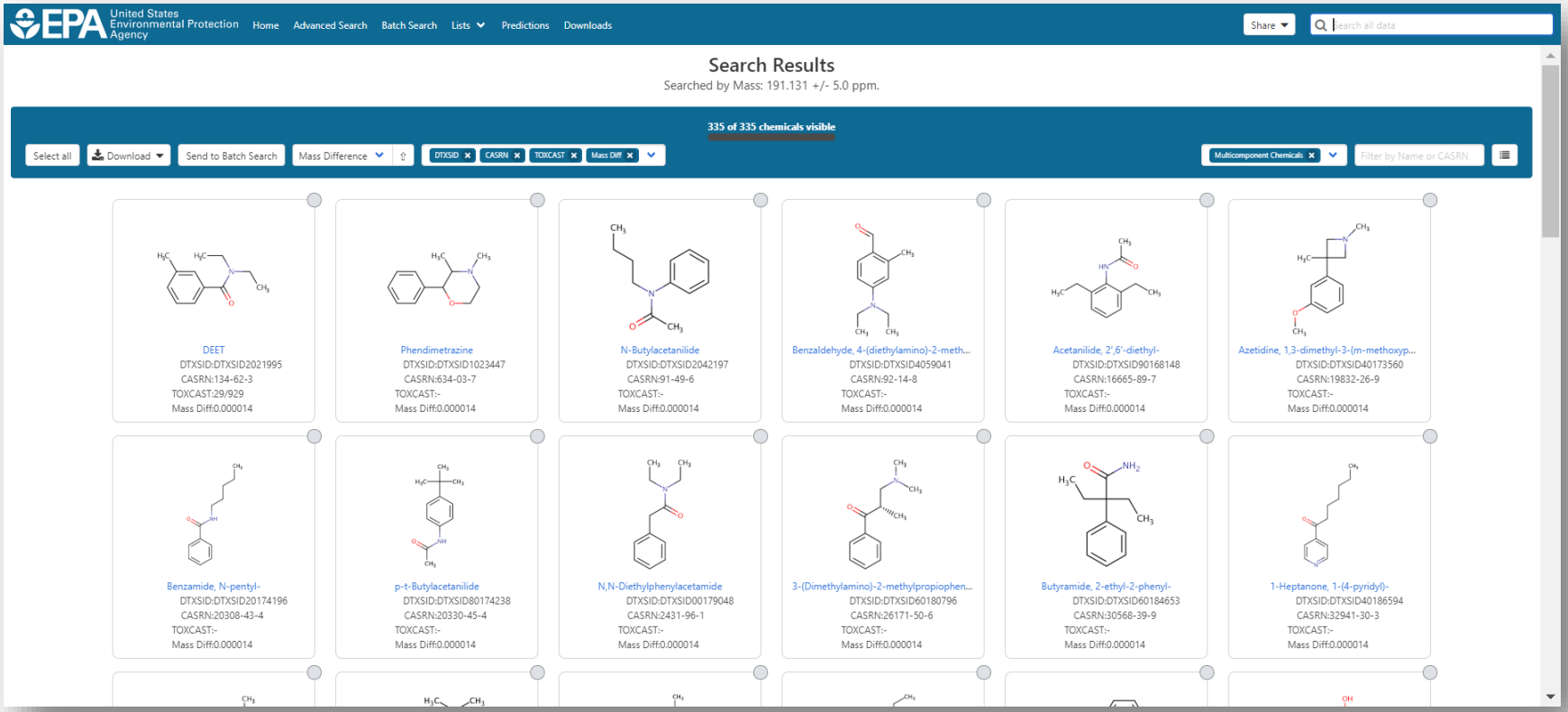


dioxin	cancer	mortality	Total	PMID	Year	Title	Authors	Journal
6	6	9	21	8734824	1996	Cancer mortality in German male workers exposed to p…	Becher; Flesch-Janys; Kauppinen; Kogevinas; Stei…	Cancer causes & control : CCC
3	9	9	21	1985242	1991	Cancer mortality in workers exposed to 2,3,7,8-tetrachlo…	Fingerhut; Halperin; Marlow; Piacitelli; Honchar; Sw…	The New England journal of medicine
3	9	8	20	27897234	2016	Association between dioxin and cancer incidence and m…	Xu; Ye; Huang; Chen; Wu; Huang; Hu; Xia; Wu	Scientific reports
3	5	8	16	9599713	1998	Estimation of the cumulated exposure to polychlorinated…	Flesch-Janys; Steindorf; Gurn; Becher	Environmental health perspectives
9	7	8	24	9199536	1997	Cancer mortality in workers exposed to phenoxy herbici…	Kogevinas; Becher; Benn; Bertazzi; Boffetta; Bueno…	American journal of epidemiology
6	5	8	19	7485063	1995	Exposure to polychlorinated dioxins and furans (PCDD/…	Flesch-Janys; Berger; Gurn; Manz; Nagel; Waltsgot…	American journal of epidemiology
3	5	8	16	1681339	1991	Cancer mortality among workers in chemical plant conta…	Manz; Berger; Dwyer; Flesch-Janys; Nagel; Waltsgott	Lancet (London, England)
1	2	7	10	19297337	2009	Mortality in employees at a New Zealand agrochemical …	McBride; Burns; Herbison; Humphry; Bodner; Collins	Occupational medicine (Oxford, England)
1	2	7	10	2139014	1990	Thirty-four-year mortality follow-up of BASF employees …	Zober; Messerer; Huber	International archives of occupational and environm…
1	4	6	11	2729256	1989	Ten-year mortality study of the population involved in th…	Bertazzi; Zocchetti; Pesatori; Guercilena; Sanarico; …	American journal of epidemiology
7	0	5	12	27932487	2016	Mortality risk among workers with exposure to dioxins.	Collins; Bodner; Aylward; Bender; Anteau; Wilken; …	Occupational medicine (Oxford, England)
2	5	5	12	21810927	2011	Plasma dioxin levels and cause-specific mortality in an …	Boers; Portengen; Turner; Bueno-de-Mesquita; Hee…	Occupational and environmental medicine

Mass and Formula Searches Supporting Mass Spectrometry

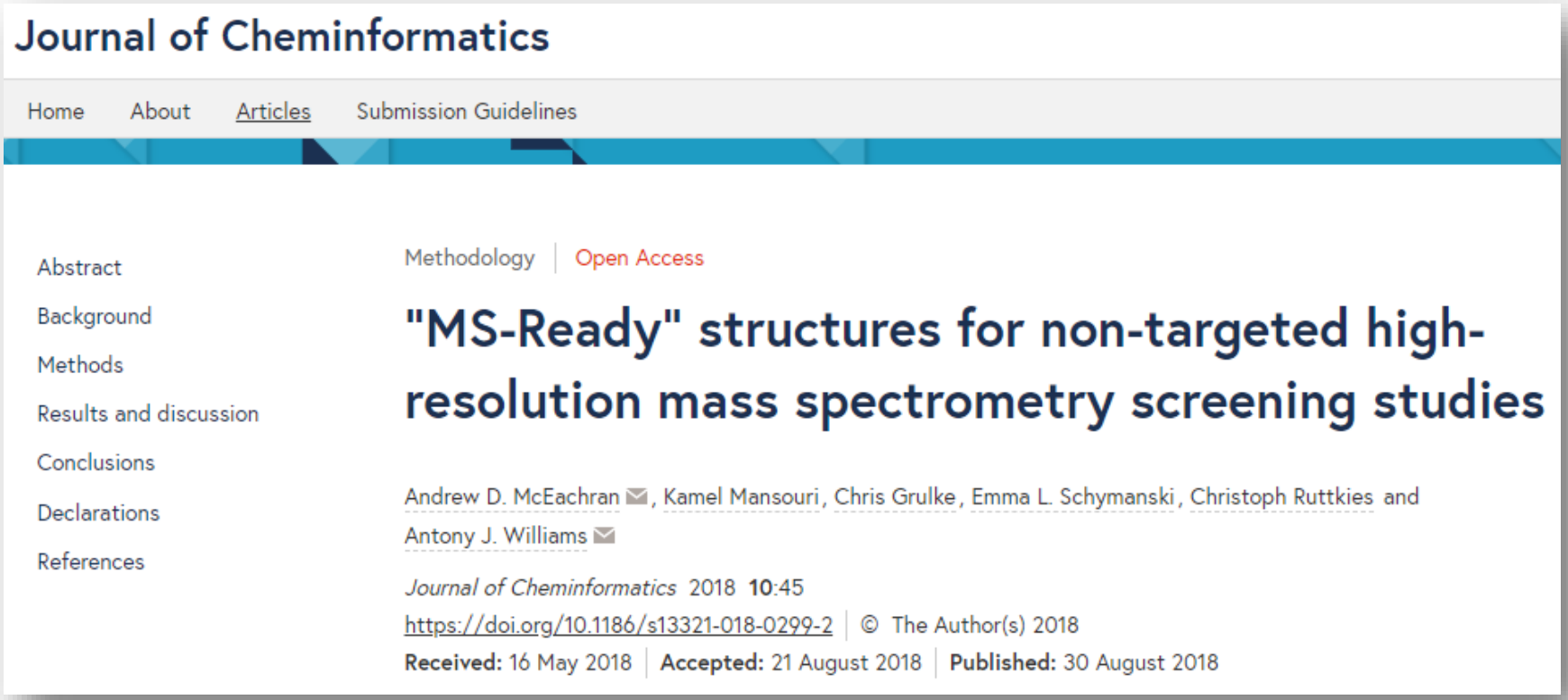


Advanced Searches
Mass Based Search



MS-Ready Structures

https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0299-2



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"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran, Kamel Mansouri, Chris Grulke, Emma L. Schymanski, Christoph Ruttkies and Antony J. Williams

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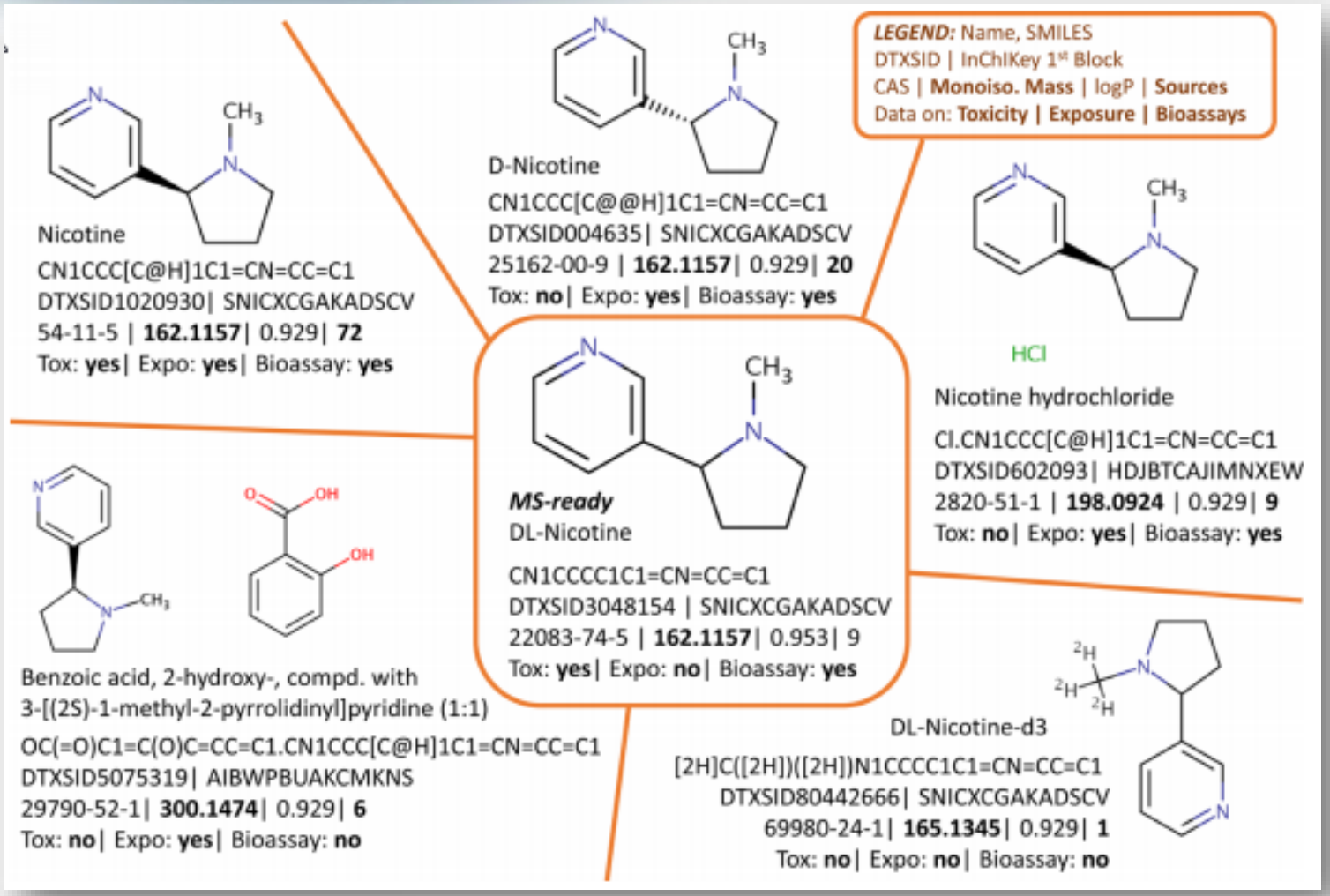
MS-Ready Structures

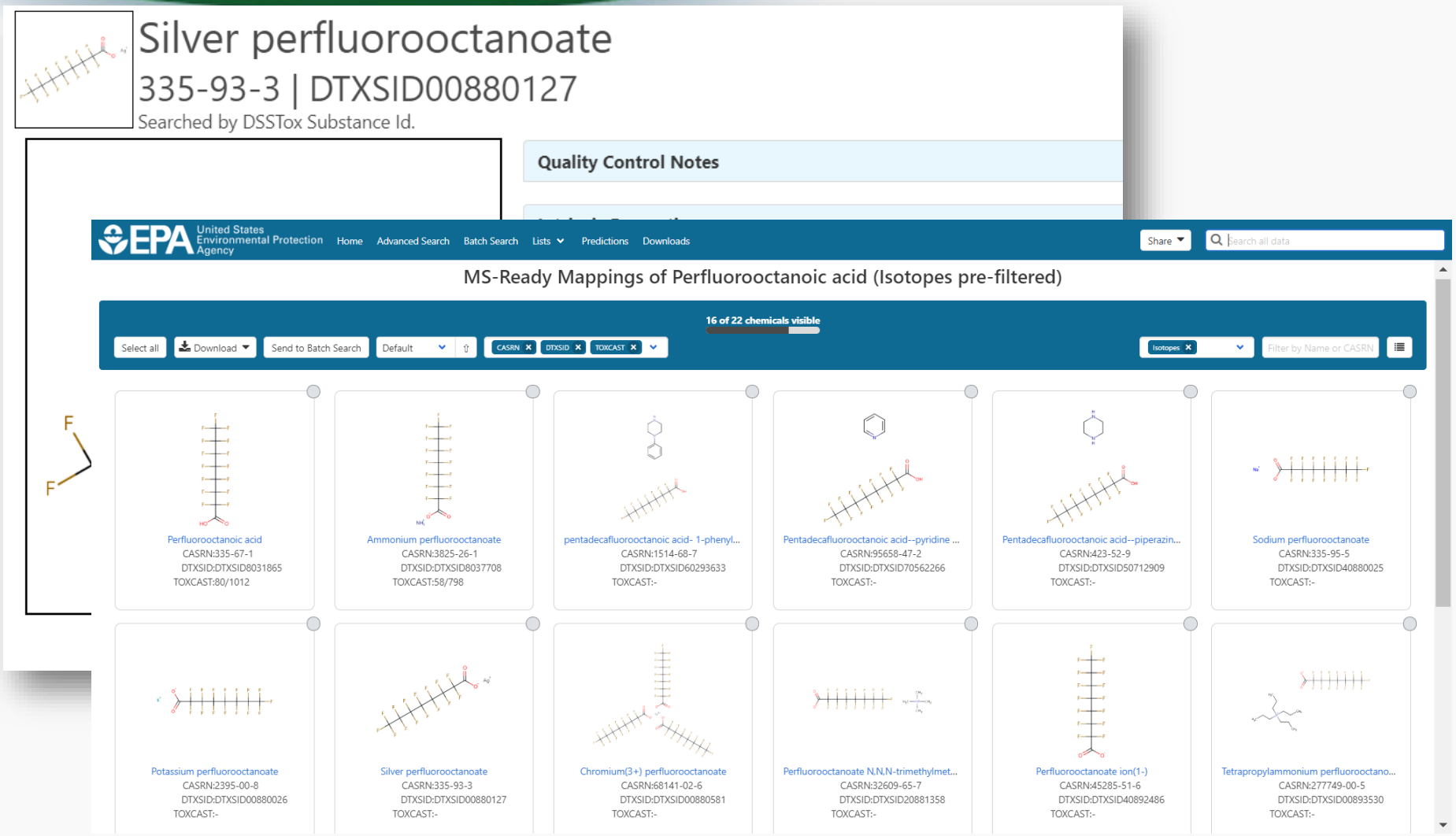


Environmental Science & Technology
Viewpoint
pubs.acs.org/est

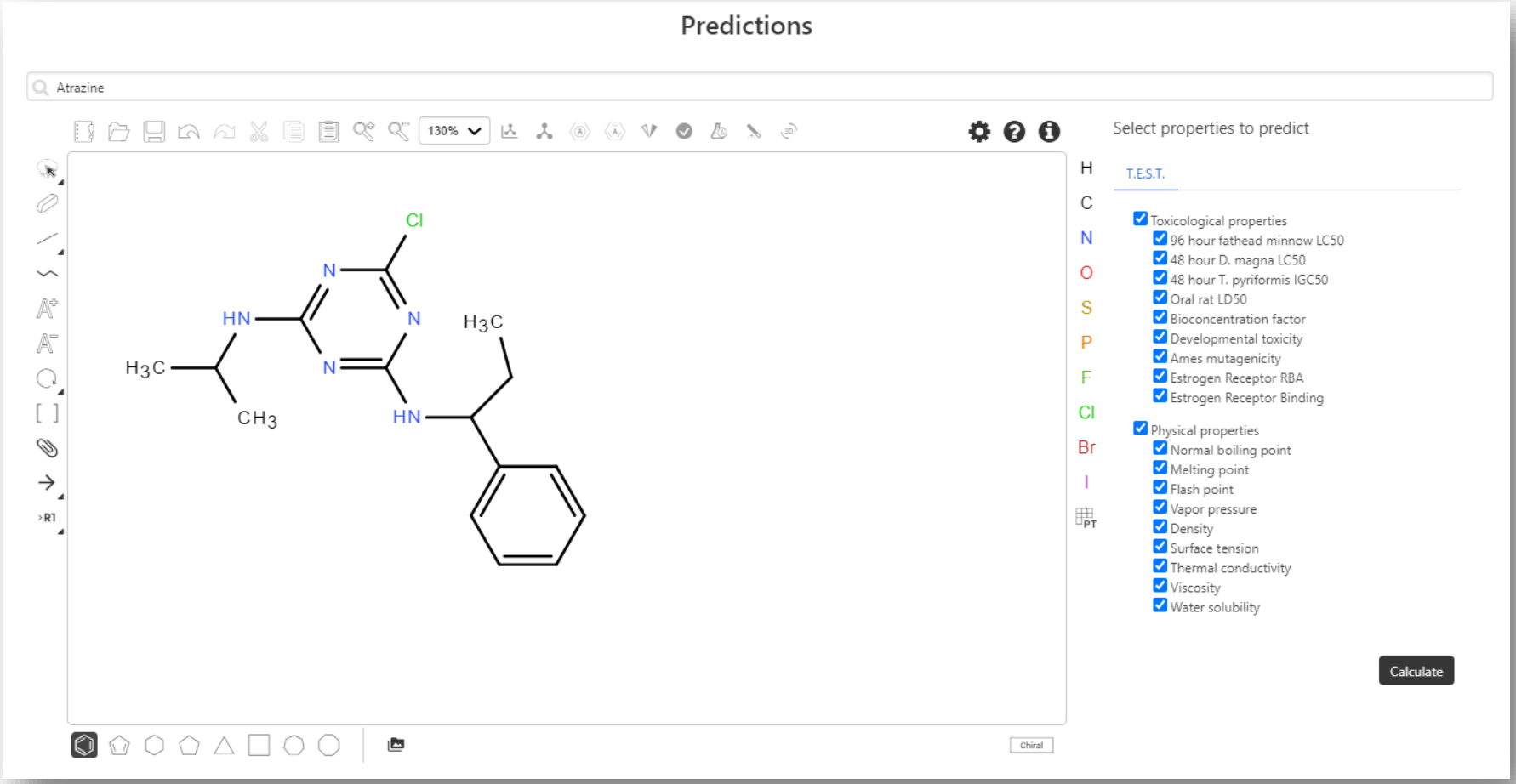
Open Science for Identifying "Known Unknown" Chemicals

Emma L. Schymanski*,† and Antony J. Williams*,‡

Find me all salts of…



Real-Time Predictions



Real-Time Predictions

Provider: T.E.S.T.

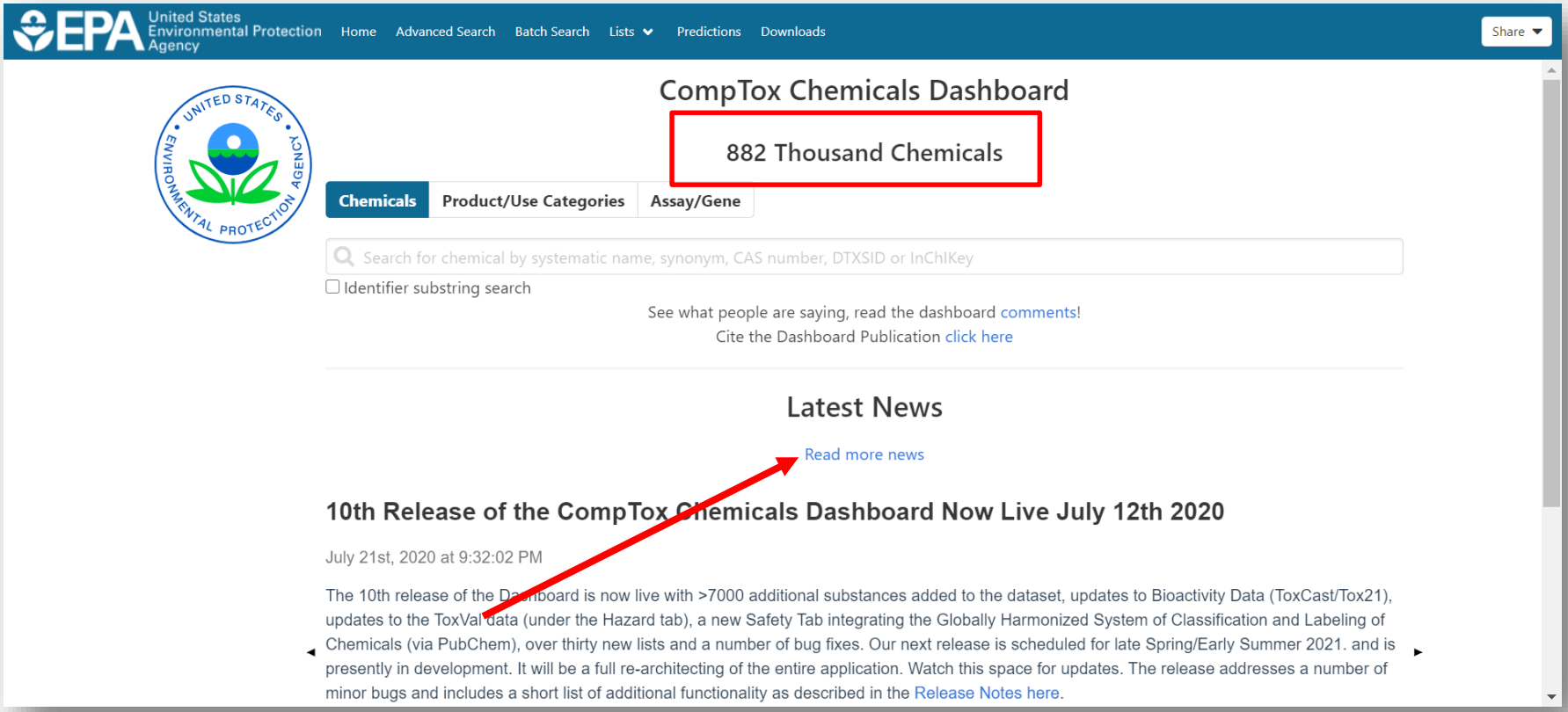
Download Summary

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		5.000 -Log10(mol/L) 3.057 mg/L	5.194 -Log10(mol/L) 1.958 mg/L	5.592 -Log10(mol/L) 0.783 mg/L	5.151 -Log10(mol/L) 2.158 mg/L	4.064 -Log10(mol/L) 26.414 mg/L
48 hour D. magna LC50		4.827 -Log10(mol/L) 4.553 mg/L	4.920 -Log10(mol/L) 3.679 mg/L	5.266 -Log10(mol/L) 1.657 mg/L	5.317 -Log10(mol/L) 1.473 mg/L	3.806 -Log10(mol/L) 47.846 mg/L
48 hour T. pyriformis IGC50		5.209 -Log10(mol/L) 1.892 mg/L	5.074 -Log10(mol/L) 2.581 mg/L			5.343 -Log10(mol/L) 1.387 mg/L
Oral rat LD50		2.059 -Log10(mol/kg) 2669.702 mg/kg	2.028 -Log10(mol/kg) 2869.132 mg/kg			2.090 -Log10(mol/kg) 2484.135 mg/kg
Bioconcentration factor		1.285 Log10 19.279	1.328 Log10 21.270	1.592 Log10 39.048	1.716 Log10 51.953	0.505 Log10 3.201
Developmental toxicity		true	true	true		
Ames mutagenicity		false	false			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		372.1 °C	331.0 °C		479.8 °C	305.5 °C
Melting point		133.9 °C	126.4 °C		138.6 °C	136.7 °C
Flash point		232.7 °C	282.4 °C		240.2 °C	175.7 °C

NEW CAPABILITIES, DATA AND LISTS

Watch for our news

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



Release Notes

https://comptox.epa.gov/dashboard/resources/cdn/release_notes_march2020.pdf

- A detailed list of new functionality and fixes

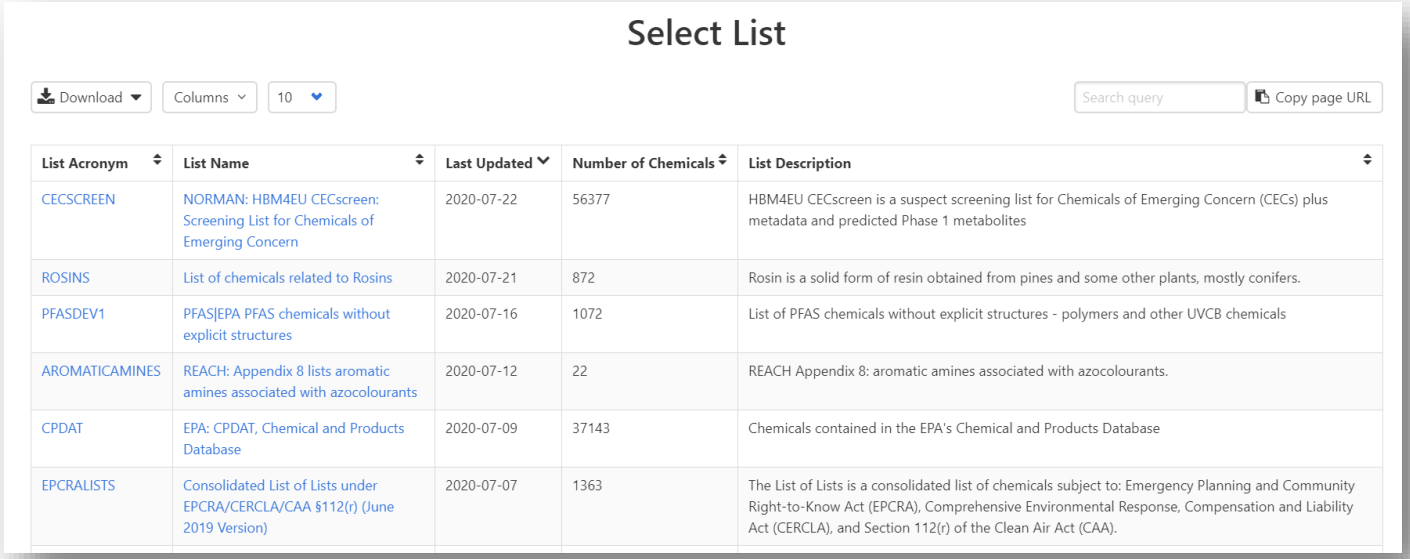
NEW FUNCTIONALITY

ICD-4105	Add new Safety Tab and load data from PubChem mapped GHS data
ICD-4294	Insert Safety tab and GHS data subtab into dev database
ICD-4147	CompTox Dashboard - Null Search string should Return Message "Please input search string""
ICD-4248	Close QC Notes by Default when there are no notes: Open Intrinsic properties by default
ICD-4233	Collapse MS-Ready and Mixtures, Components and Neutralized Forms under Linked Substances
ICD-4103	Make Genra Front End handle lack of data
ICD-4140	assays on EDSP21 tab would be easier to use if alpha-sorted
ICD-4153	Create Redirect page for legacy Toxcast and EDSP Dashboards
ICD-4255	Edit text in batch to insist on "one per row"
ICD-4159	Use PIPE instead of comma to separate names in name export in Batch Search
ICD-4222	Integrate Toxval_v8 into dashboard for next release
ICD-4234	Switch off ToxCast and EDSP21 dashboards
ICD-4241	Add Date filter to Chemical List Ag-Grid
ICD-4235	Remove Google Plus from share dropdown on home page
ICD-4242	Add toolbar to chemical-lists page
ICD-4238	update AG-GRID to version 21.2.0
ICD-4216	Update nuxtjs version
ICD-4201	Modify navigation bar
ICD-4017	Change hitcall=-1 to NO CALL instead of ACTIVE or INACTIVE
ICD-4285	Add "CompTox Chemicals Dashboard" to home page

New Safety Tab
Integrating PubChem GHS Data

Over 260 Lists Now Available

- Lists ranging from 3 to >62,200 chemicals
- 27 different PFAS lists – structures and non-structure lists
- Lists added to support specific programs

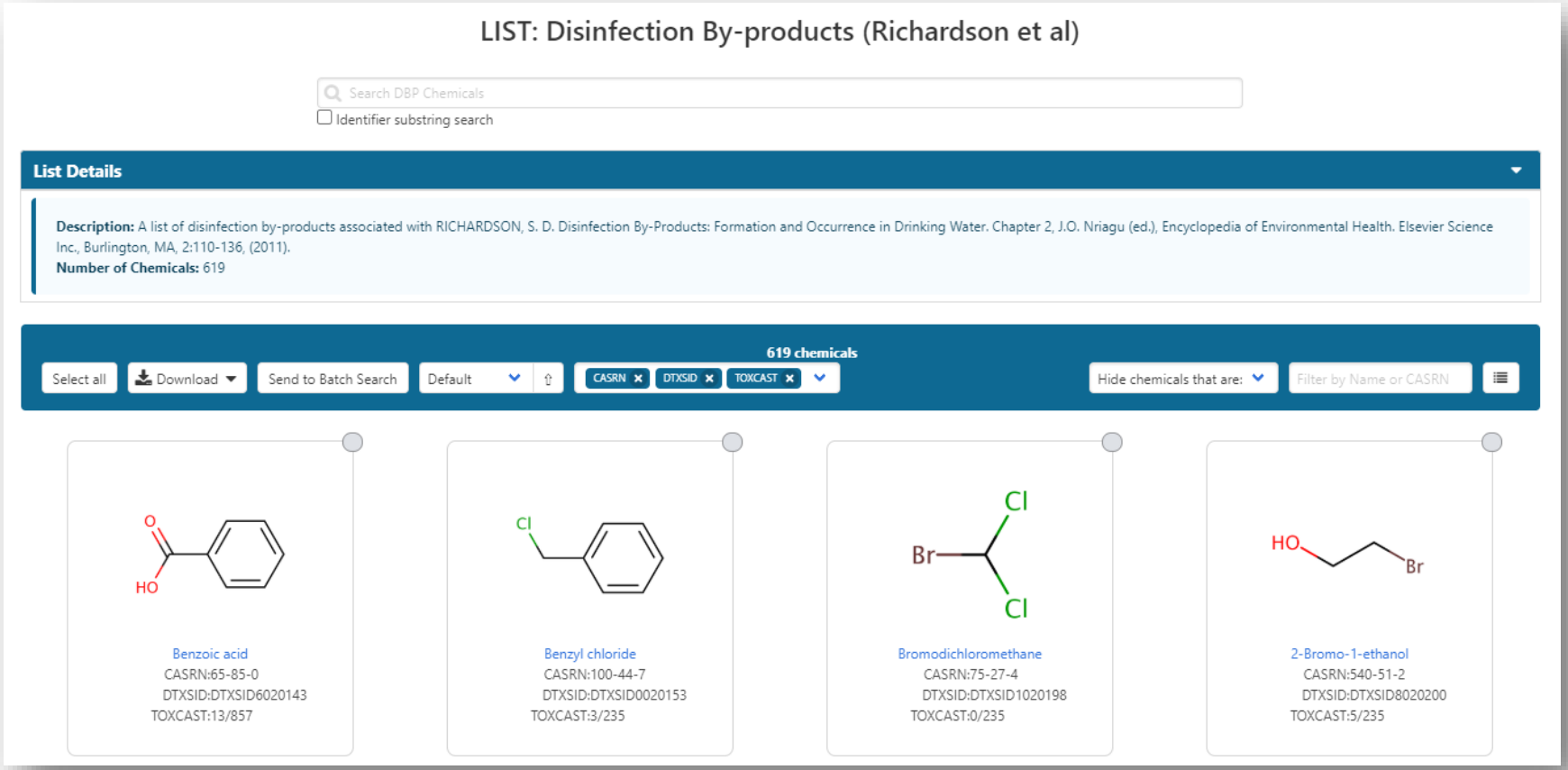


Select List

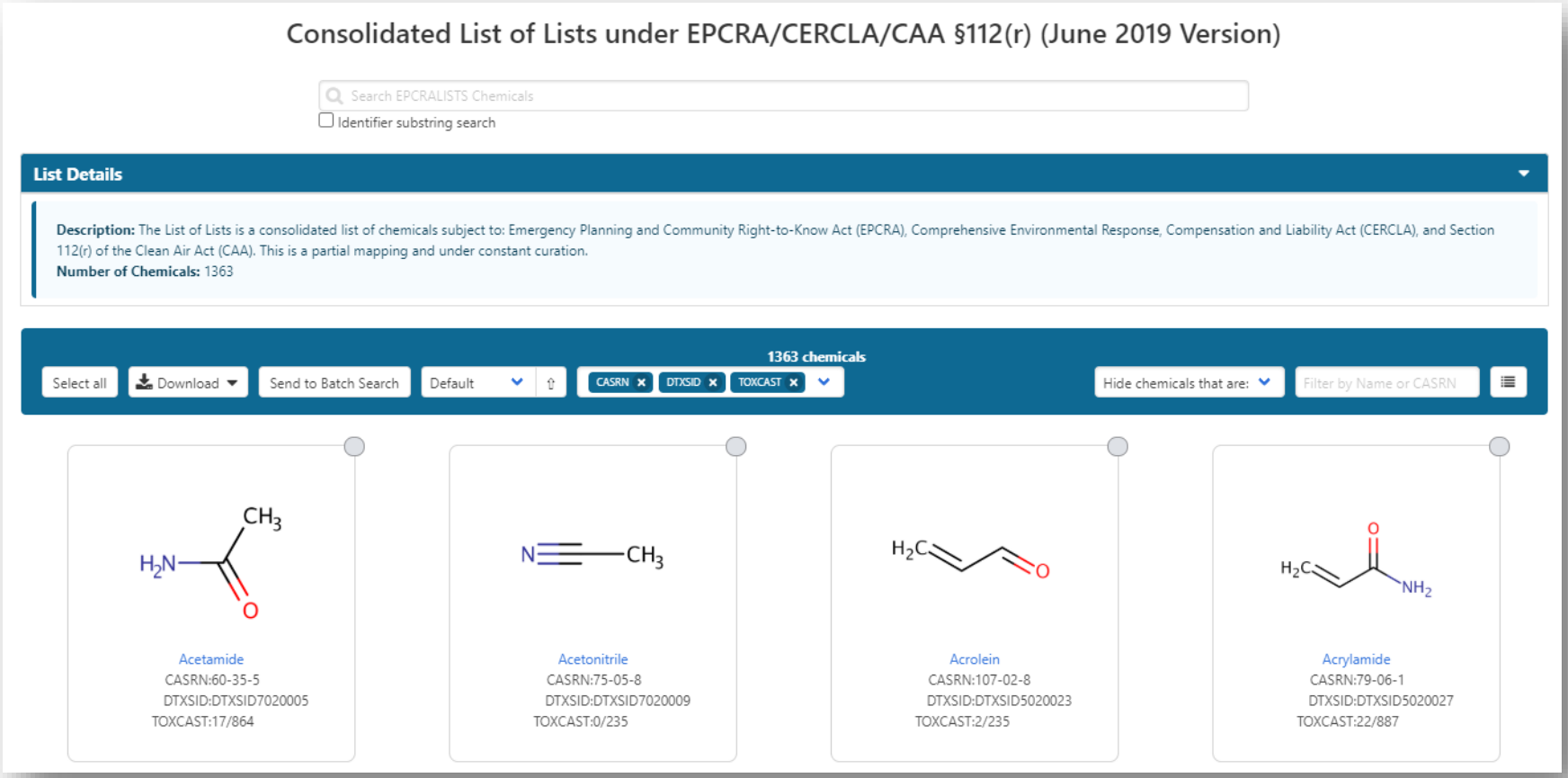
Download | Columns | 10 | Search query | Copy page URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
CECSCREEN	NORMAN: HBM4EU CECscreen: Screening List for Chemicals of Emerging Concern	2020-07-22	56377	HBM4EU CECscreen is a suspect screening list for Chemicals of Emerging Concern (CECs) plus metadata and predicted Phase 1 metabolites
ROSINS	List of chemicals related to Rosins	2020-07-21	872	Rosin is a solid form of resin obtained from pines and some other plants, mostly conifers.
PFASDEV1	PFAS|EPA PFAS chemicals without explicit structures	2020-07-16	1072	List of PFAS chemicals without explicit structures - polymers and other UVCB chemicals
AROMATICAMINES	REACH: Appendix 8 lists aromatic amines associated with azocolourants	2020-07-12	22	REACH Appendix 8: aromatic amines associated with azocolourants.
CPDAT	EPA: CPDAT, Chemical and Products Database	2020-07-09	37143	Chemicals contained in the EPA's Chemical and Products Database
EPCRALISTS	Consolidated List of Lists under EPCRA/CERCLA/CAA §112(r) (June 2019 Version)	2020-07-07	1363	The List of Lists is a consolidated list of chemicals subject to: Emergency Planning and Community Right-to-Know Act (EPCRA), Comprehensive Environmental Response, Compensation and Liability Act (CERCLA), and Section 112(r) of the Clean Air Act (CAA).

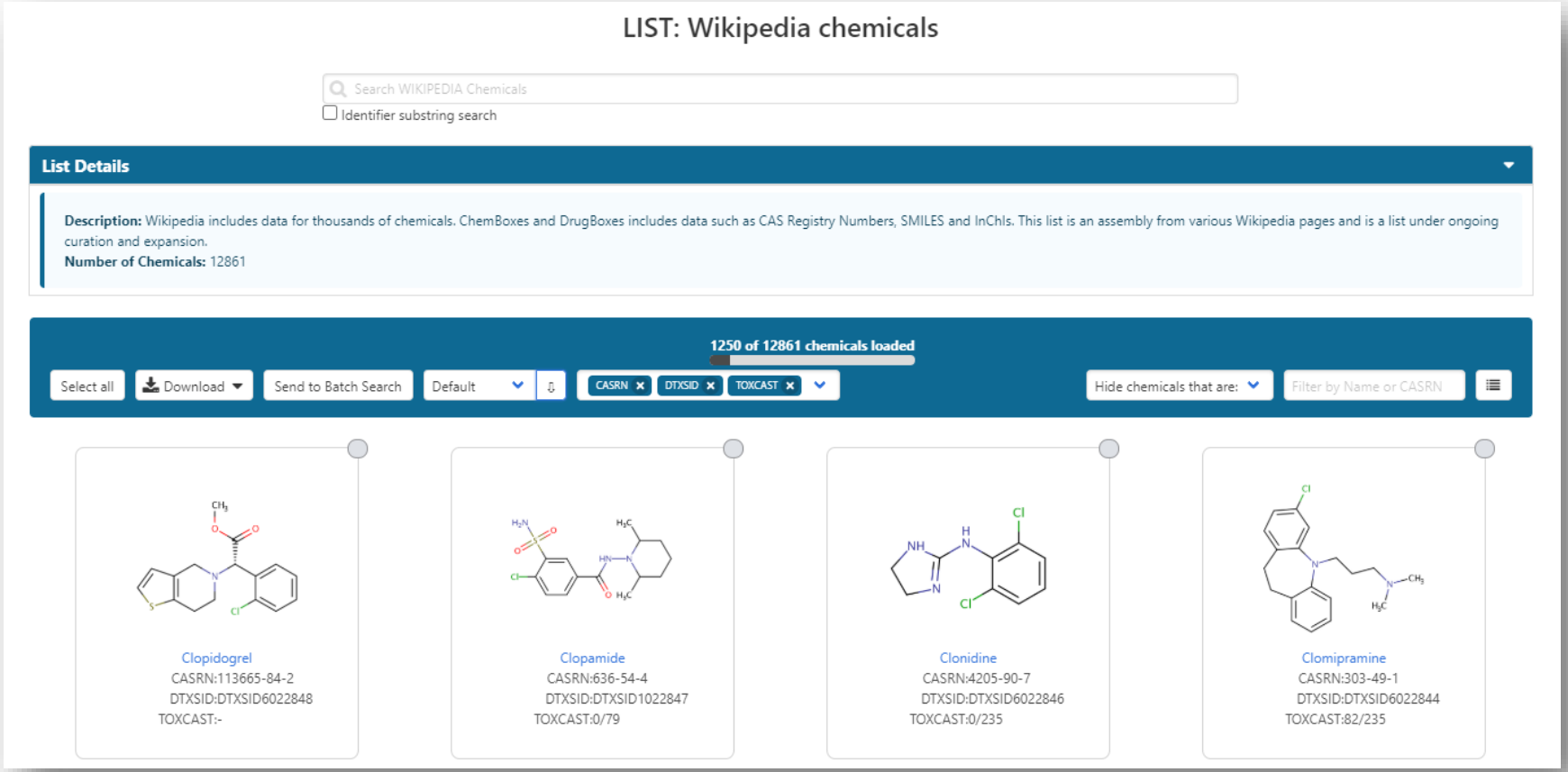
Disinfectant By-Products
82 to 619 chemicals



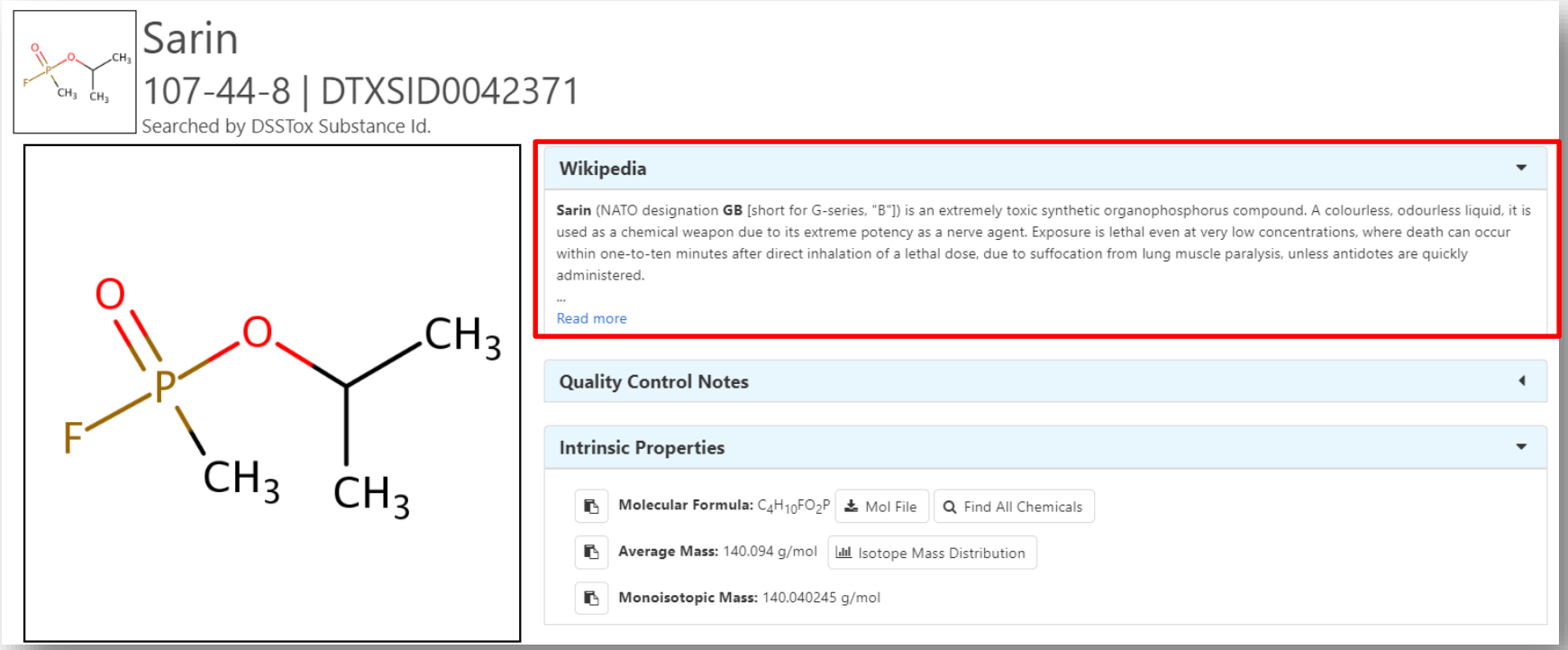
EPCRA/CERCLA/CAA Lists



Curated Wikipedia
>12,000 chemicals



Wikipedia serves the “snippet”



Other Lists of Interest

- Storage Tanks – Above Ground/Underground
- IRIS Chemicals refreshed to >600 chemicals
- Azo dyes (decompose to aromatic amines)
- Curated CASMI (Critical Assessment of Small Molecule Identification) datasets

Metabolites. 2020 Jun; 10(6): 260.
Published online 2020 Jun 23. doi: 10.3390/metabo10060260
PMCID: PMC7345619
PMID: 32585902

Revisiting Five Years of CASMI Contests with EPA Identification Tools

Andrew D. McEachran,[1,*] Alex Chao,[1] Hussein Al-Ghoul,[1] Charles Lowe,[2] Christopher Grulke,[2] Jon R. Sobus,[2] and Antony J. Williams[2,*]

Lists provide a landscape overview

EPA United States Environmental Protection Agency

Presence in Lists

Federal

TOXCASST_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)
CHEMINV: EPA Chemical Inventory for ToxCast
TOXCAST: EPA ToxCast Screening Library
ENDOCRINE: EDSP Universe of Chemicals
ECOTOX; Ecotoxicology knowledgebase
WATER|EPA; Chemicals in hydraulic fracturing fluids Table H-2
WATER|EPA; Chemicals associated with hydraulic fracturing
EPA: Consumer Products Suspect Screening Result
TOXCAST: EPA ToxCast Screening Assay In Vitro DB Version 3
EPA: High Production Volume List
CHEMINV; ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
TOX21SL: Tox21 Screening Library
LIST: Substances Added to Food (formerly EAFUS)
TSCA Active Inventory non-confidential portion (updated March 20th 2020).

US State

None.

International

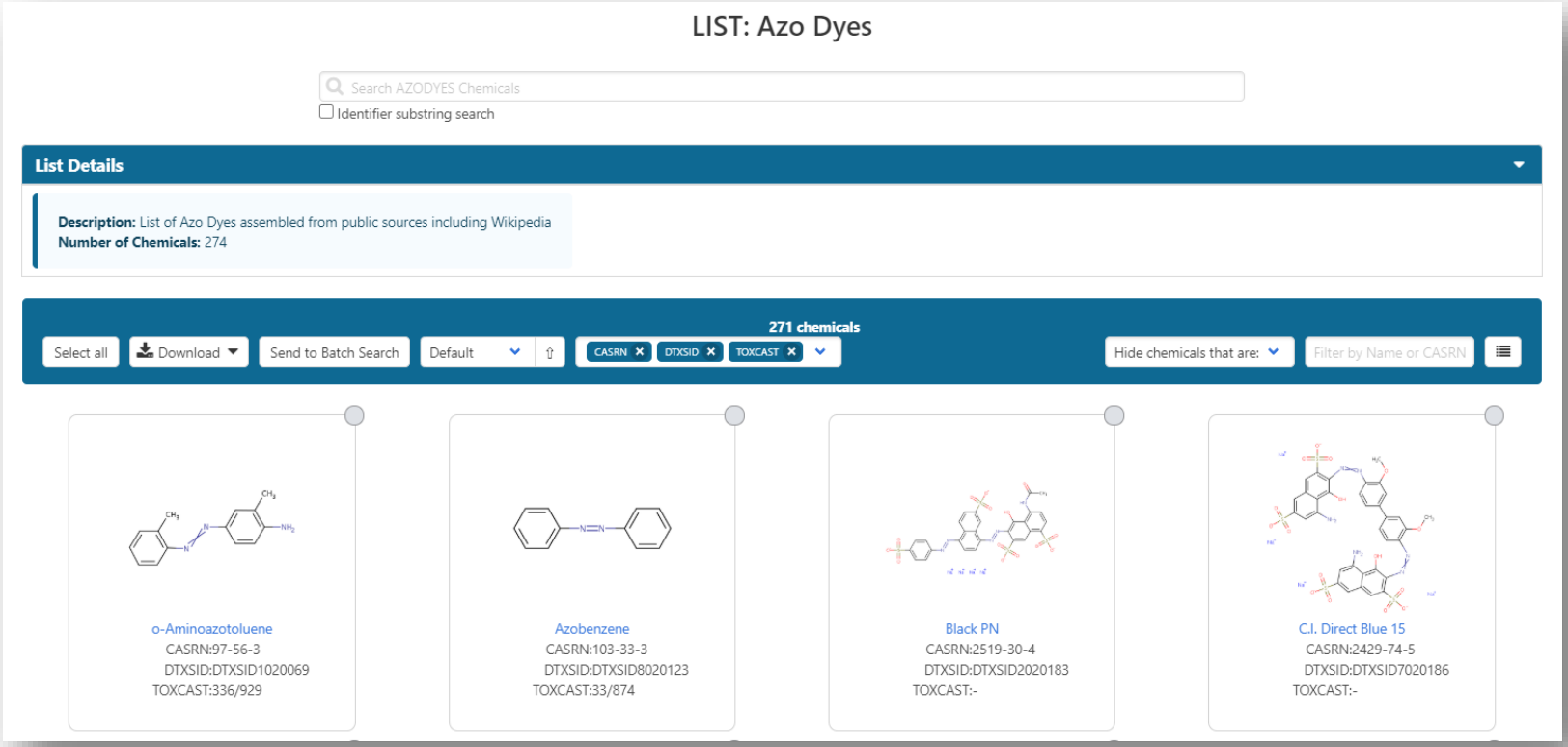
Canadian Domestic Substances List 2019
FOOD: EFSA OpenFoodTox
NORMAN: KEMI List of Substances on the Market

Other

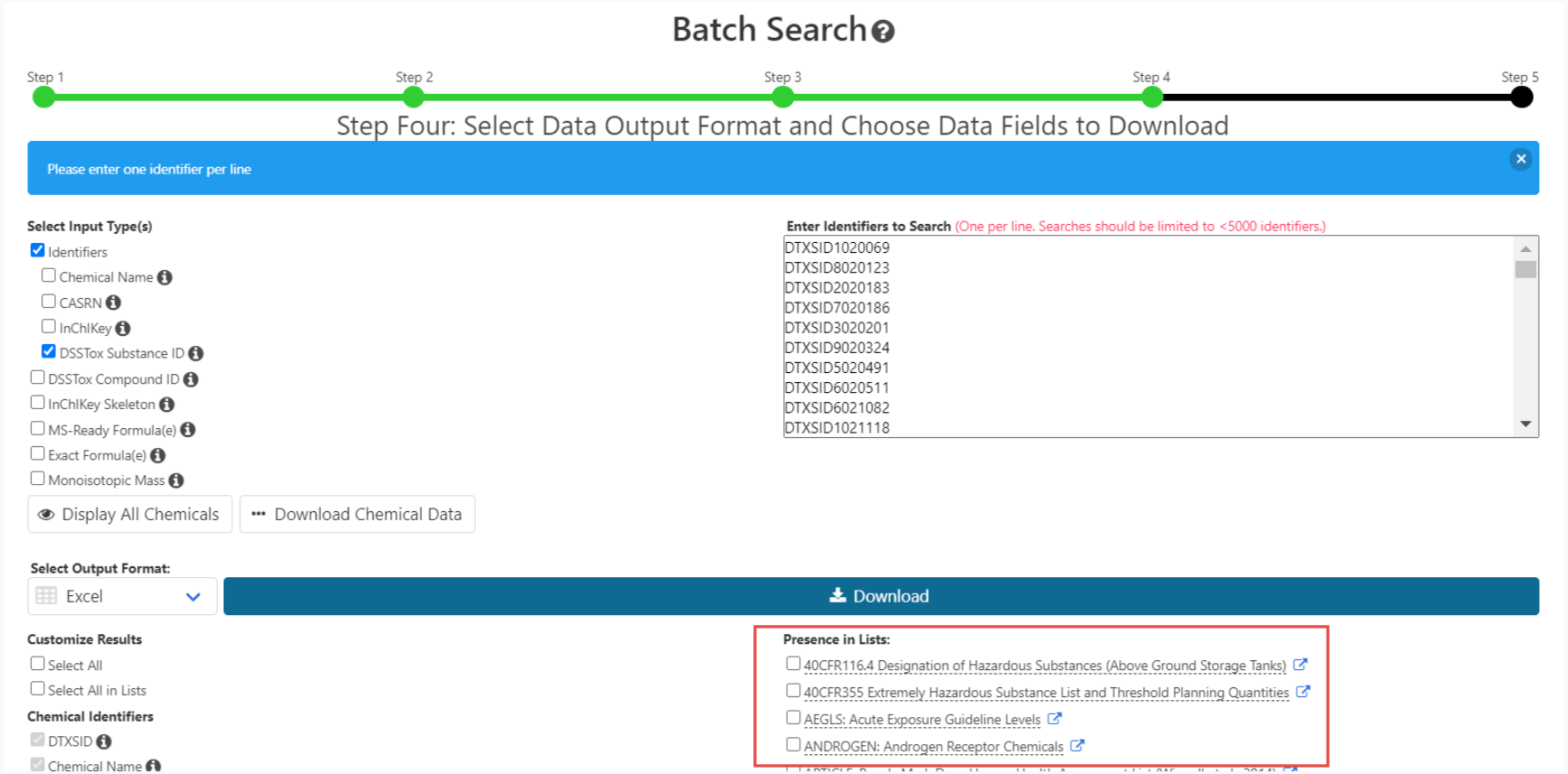
COSMOS DB cosmetics database
EPA|LIST: Article "Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays"
NORMAN: REACH Chemicals List Provided to NORMAN Network
NORMAN: Norman Network Suspect Screening List (SUSDAT)
EPA: CPDAT, Chemical and Products Database
Global harmonization system aggregated chemical data list (skin and eyes)
MASSPECDB: Thermo's mzCloud Database
NORMAN: Combined 2000/2006 EU Cosmetic Ingredients Inventory
WATER: STOFF-IDENT Database of Water-Relevant Substances
ESTROGEN: Integrated pathway model for the Estrogen Receptor
NEURO: DNT Screening Library
PESTICIDES|EPA: Pesticide Chemical Search Database
ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
EPA: Toxicity Values Version 5 (Aug 2018)
LIST: Wikipedia chemicals
LIST:Hazardous Substances Data Bank
PESTICIDES|EPA: List of Inert Ingredients Food and Nonfood Use UPDATED 10/25/2019

Potential Use Cases

- Batch search a list of chemicals to identify presence in >280 lists



Select lists of Interest & Export File



Cross-walking lists of interest

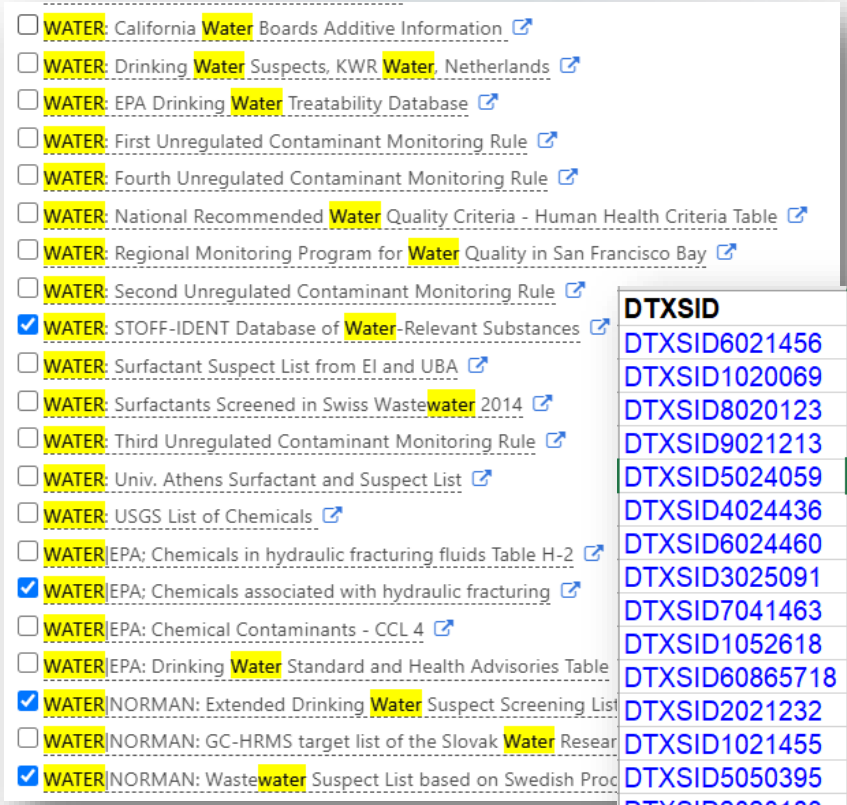
	A	B	C	D	E	F	G	H	I
1	DTXSID	PREFERRED_NAME	CANADADSL	OEHHA	EPCRALISTS	ECOTOX_V2	EDSPUOC	CPDAT	TRIRELEASE
2	DTXSID1020069	o-Aminoazotoluene	Y	Y	Y	Y	Y	Y	Y
3	DTXSID8020123	Azobenzene	Y	Y	-	Y	Y	Y	-
4	DTXSID2020183	Black PN	-	-	-	-	-	Y	-
5	DTXSID7020186	C.I. Direct Blue 15	Y	Y	-	-	Y	Y	-
6	DTXSID3020201	C.I. Direct Brown 95	Y	Y	Y	Y	Y	Y	Y
7	DTXSID9020324	Chocolate Brown HT	-	-	-	-	-	Y	-
8	DTXSID5020491	4-(Dimethylamino)azober	Y	Y	Y	Y	Y	Y	Y
9	DTXSID6020511	3,3'-Dimethylbenzidine di	Y	Y	Y	Y	Y	Y	Y
10	DTXSID6021082	C.I. Acid Orange 10	Y	-	-	-	Y	Y	-
11	DTXSID1021118	Phenazopyridine hydroch	Y	Y	-	Y	Y	Y	-
12	DTXSID4021135	C.I. Solvent Yellow 14	Y	Y	Y	-	Y	Y	Y
13	DTXSID9021213	SX purple	Y	-	-	Y	Y	Y	-
14	DTXSID8021224	C.I. Acid Red 114	Y	Y	Y	Y	Y	Y	Y
15	DTXSID8021228	Ponceau MX	Y	Y	Y	Y	Y	Y	Y
16	DTXSID7021231	Ponceau 3R	-	Y	-	Y	Y	Y	-
17	DTXSID2021232	Amaranth	Y	-	-	Y	Y	Y	-
18	DTXSID6021450	C.I. Disperse Yellow 3	Y	Y	Y	Y	Y	Y	Y
19	DTXSID1021455	FD&C Yellow 5	Y	-	-	Y	Y	Y	-
20	DTXSID6021456	FD&C Yellow 6	Y	-	-	Y	Y	Y	-
21	DTXSID9022815	Evans blue	Y	-	-	Y	-	Y	-
22	DTXSID4022816	C.I. Direct Red 28	Y	-	-	Y	-	Y	-
23	DTXSID5024059	3,3'-Dimethylbenzidine	Y	Y	Y	Y	Y	Y	Y
24	DTXSID1024415	C.I. Acid Black 1, disodiu	Y	-	-	Y	Y	Y	-

Are there azo dye mass spectra?

- MASSPECDB: MassBank Reference Spectra Collection
- MASSPECDB: MassBank.EU Collection: Special Cases
- MASSPECDB: Mycotoxins from MassBank.EU
- MASSPECDB: National Environmental Methods Index
- MASSPECDB: SWGDRUG Mass Spectral Library Chemical Collection
- MASSPECDB: Thermo's n
- MASSPECDB: Wiley Regi
- MASSPECDB|NORMAN:I

DTXSID	PREFERRED_NAME	MASSBANK	NEMILIST	MZCLOUD	WRTMSD	INDOORCT16
DTXSID1020069	o-Aminoazotoluene	-	-	Y	-	-
DTXSID8020123	Azobenzene	-	Y	Y	-	Y
DTXSID5020491	4-(Dimethylamino)azobe	-	Y	Y	-	-
DTXSID4021135	C.I. Solvent Yellow 14	-	-	Y	-	-
DTXSID6021450	C.I. Disperse Yellow 3	-	-	Y	-	-
DTXSID1021455	FD&C Yellow 5	-	-	Y	-	-
DTXSID5024059	3,3'-Dimethylbenzidine	Y	Y	Y	-	-
DTXSID6024460	4-Aminoazobenzene	Y	Y	Y	-	-
DTXSID3025091	3,3'-Dimethoxybenzidine	Y	Y	Y	Y	-
DTXSID5040706	C.I. Solvent Orange 7	-	-	Y	-	-
DTXSID3041742	C.I. Solvent Red 23	Y	-	Y	-	-
DTXSID8041743	Scarlet red	Y	-	Y	-	-
DTXSID1042154	Methyl red	-	-	Y	-	-
DTXSID1059238	N-Phenyl-4-(phenylazo)a	-	-	Y	-	-
DTXSID7062536	Benzenamine, 4-[(4-nitrc	-	-	Y	-	-
DTXSID9066883	C.I. Disperse Brown 1	-	-	Y	-	-
DTXSID2020183	Black PN	-	-	-	-	-
DTXSID7020186	C.I. Direct Blue 15	-	-	-	-	-
DTXSID3020201	C.I. Direct Brown 95	-	-	-	-	-

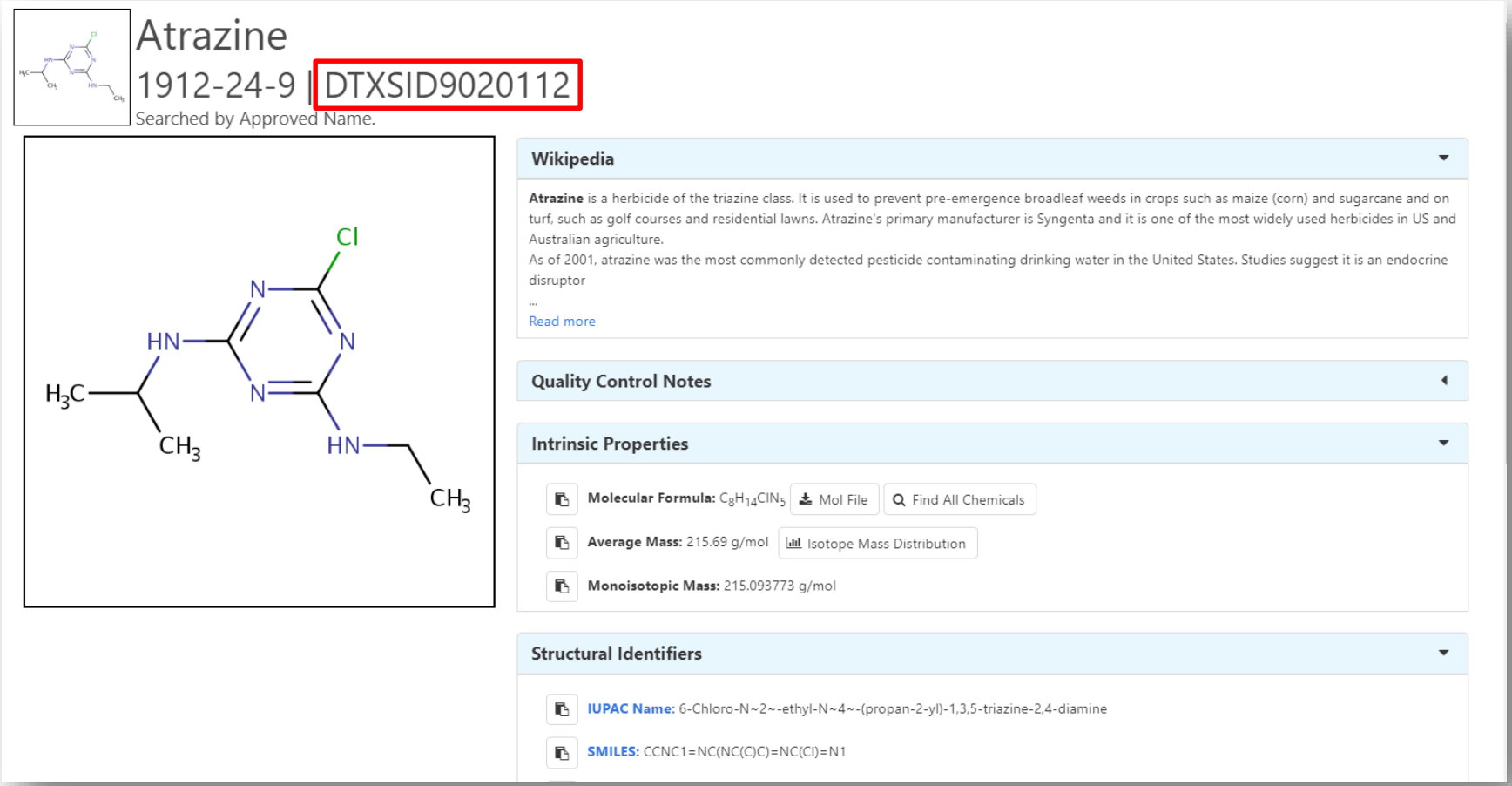
Azo dyes listed in “water” lists



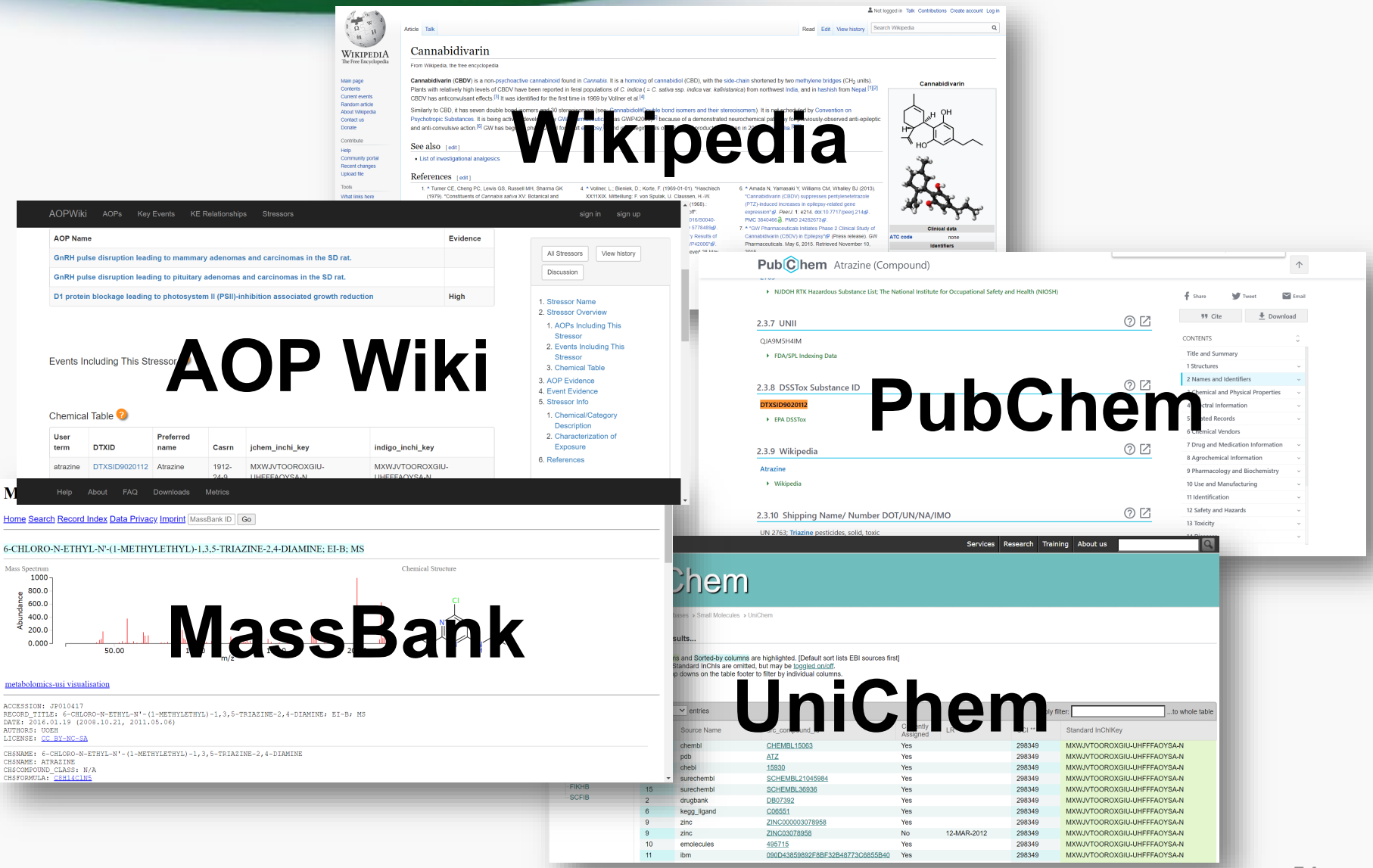
DTXSID	PREFERRED_NAMI	STOFFIDENT	EPAHFR	KWRSJERPS2	KEMIWWSUS
DTXSID6021456	FD&C Yellow 6	-	Y	Y	Y
DTXSID1020069	o-Aminoazotoluene	-	-	Y	-
DTXSID8020123	Azobenzene	Y	-	Y	-
DTXSID9021213	SX purple	-	-	Y	-
DTXSID5024059	3,3'-Dimethylbenzidir	-	-	Y	-
DTXSID4024436	Allura Red C.I.16035	-	-	Y	-
DTXSID6024460	4-Aminoazobenzene	Y	-	Y	-
DTXSID3025091	3,3'-Dimethoxybenzic	Y	-	Y	-
DTXSID7041463	3,3'-Dimethyl-4,4'-dip	Y	-	Y	-
DTXSID1052618	3-Hydroxy-2-naphtha	Y	-	Y	-
DTXSID60865718	N-Ethyl-N-(2-(1-(2-m	Y	-	Y	-
DTXSID2021232	Amaranth	-	Y	-	-
DTXSID1021455	FD&C Yellow 5	-	Y	-	Y
DTXSID5050395	C.I. Solvent Red 26	-	Y	-	-
DTXSID2020183	Black PN	-	-	-	-
DTXSID7020186	C.I. Direct Blue 15	-	-	-	-
DTXSID3020201	C.I. Direct Brown 95	-	-	-	-
DTXSID9020324	Chocolate Brown HT	-	-	-	-
DTXSID5020491	4-(Dimethylamino)az	Y	-	-	-
DTXSID6020511	3,3'-Dimethylbenzidir	-	-	-	-
DTXSID6021082	C.I. Acid Orange 10				

LINKAGES OUTBOUND and INBOUND

Increasingly important identifier
The **DTXSID**



In-links from various sources



The DTXSID Identifier

English Not logged in Talk Contributions Create account Log in

WIKIDATA

Project page Discussion Read Edit View history Search Wikidata

Wikidata:Property proposal/DTXSID

< Wikidata:Property proposal

Main page
Community portal
Project chat
Create a new Item
Create a new Lexeme
Recent changes
Random Item
Query Service
Nearby
Help
Donate

Tools

What links here
Related changes
Special pages
Permanent link
Page information

In Wikipedia

Add links

DSSTOX substance identifier [edit]

Originally proposed at Wikidata:Property proposal/Natural science

Done: DSSTox substance ID (P3117) (Talk and documentation)

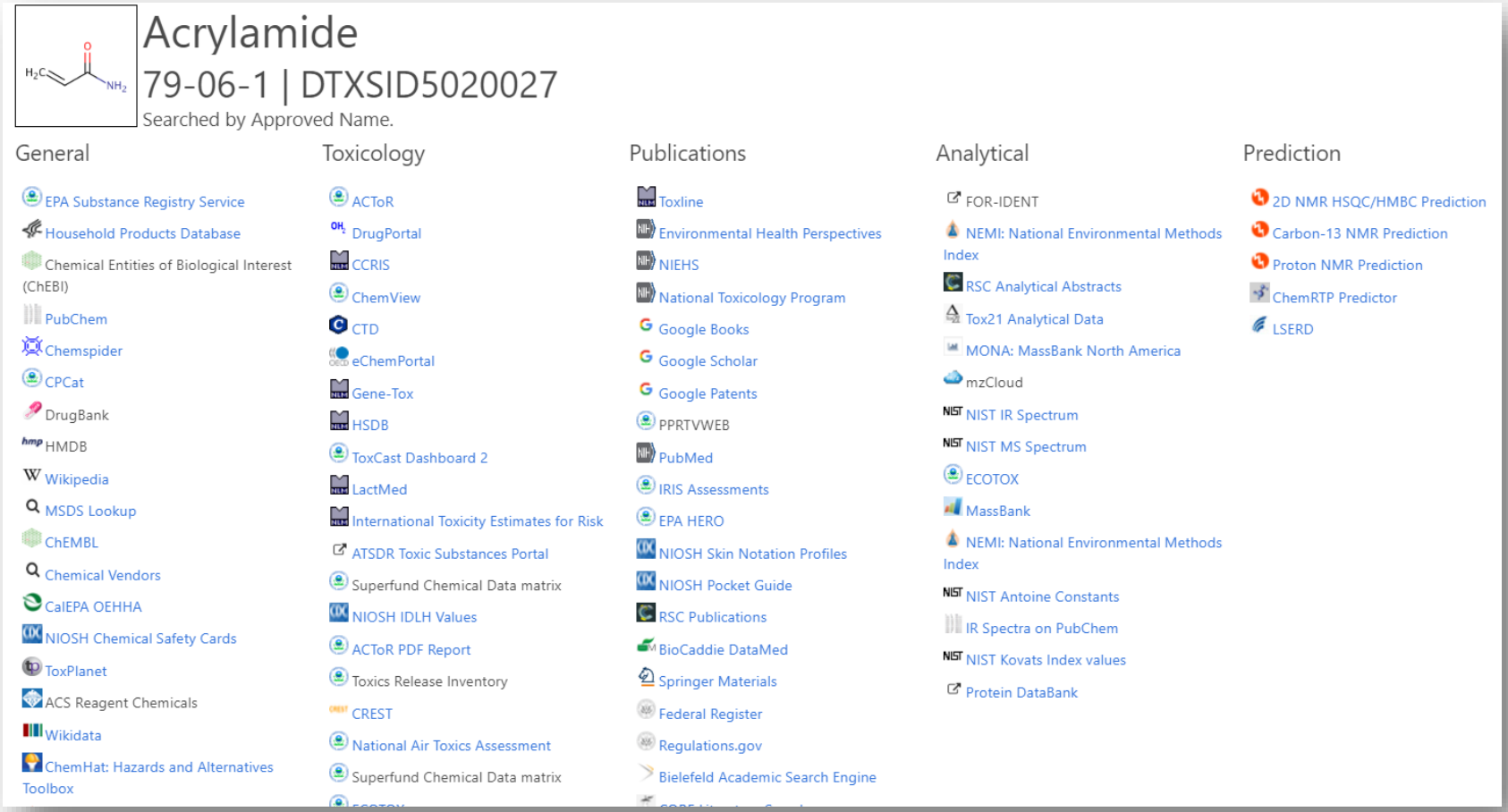
Description	Ths DTXSID is the DSSTox substance identifier used in the Environmental Protection Agency CompTox Dashboard.
Data type	External identifier
Domain	chemical substance (Q79529)
Example	benzene (Q2270) → DTXSID3039242
Planned use	Adding DTXSIDs to @wikidata using a bot or possible Mix&Match, based on InChIKey matches and this CCZero data on Figshare: https://figshare.com/articles/Mapping_file_of_InChIStrings_InChIKeys_and_DTXSIDs_for_the_EPA_CompTox_Dashboard/3578313/1 .
Formatter URL	https://comptox.epa.gov/dashboard/**$1**

Motivation

The Environmental Protection Agency (Q16919823)'s CompTox Dashboard is a fairly new website, but the DSSTox project exists for much longer (Distributed structure-searchable toxicity (DSSTox) public database network: a proposal (Q26701395)). The Dashboard aggregates over 720 thousand chemical substances and is open data. The CompTox dashboard also provides access to synonyms, experimental and predicted property data, product and functional use details and EPA's Toxcast Bioassay data. The DTXSIDs are unique substance identifiers, already been included into PubChem and the EBI Unichem InChIKey mapping files. The DTXSIDs will also be included into the BridgeDb metabolite mapping databases on short notice. Egon Willighagen (talk) 17:48, 24 August 2016 (UTC)

Increasing number of outlinks

- External Links reduce time to discovery



New Outlinks of Interest
State-Specific Water Quality Standards

EPA United States Environmental Protection Agency

State-Specific Water Quality Standards Effective under the Clean Water Act (CWA)

EPA has compiled state, territorial, and authorized tribal water quality standards that EPA has approved or are otherwise in effect for Clean Water Act purposes. This compilation is continuously updated as EPA approves new or revised WQS.

In instances when state-specific water quality standards have not been developed or approved by EPA, the Agency will propose and/or promulgate standards for a state until such time as the state submits and EPA approves their own standards. Any federally-proposed or promulgated replacement water quality standards are also identified.

Please note the water quality standards may contain additional provisions outside the scope of the Clean Water Act, its implementing federal regulations, or EPA's authority. In some cases, these additional provisions have been included as supplementary information.

EPA is posting the water quality standards as a convenience to users and has made a reasonable effort to assure their accuracy. Additionally, EPA has made a reasonable effort to identify parts of the standards that are approved, disapproved, or are otherwise not in effect for Clean Water Act purposes.

- See EPA's CompTox Chemical Dashboard for more information on this chemical.

Modernizing Public Hearings for WQS Reviews

The document below suggests how states and authorized tribes can conduct online public hearings in lieu of in-person public hearings, consistent with federal public hearing requirements.

- Modernizing Public Hearings for Water Quality Standard Decisions Consistent with 40 CFR 25.5 (PDF) (31 pp, 686 K)

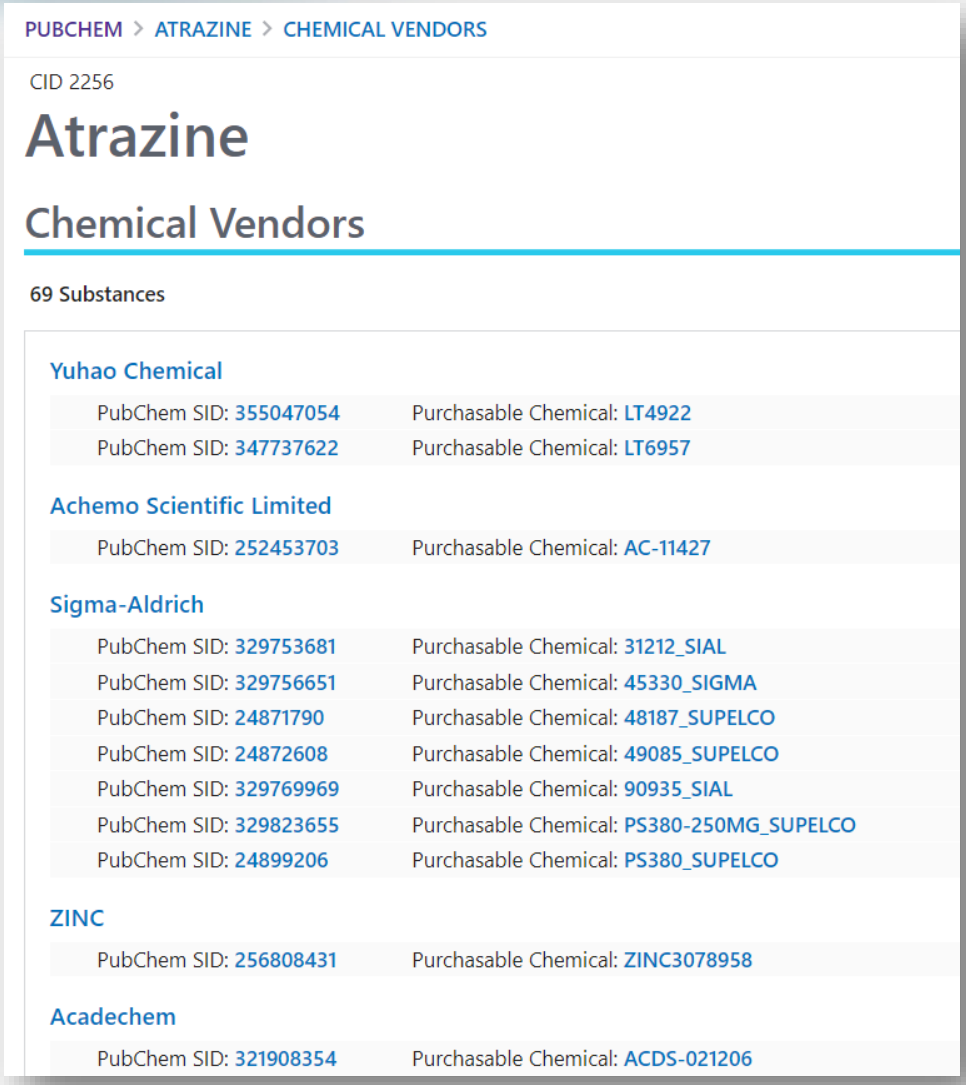
Show 10 entries — Search this table.

State (Search this column.)	Parameter (the name used by the state) (Search this column.)	Application (Search this column.)	Criteria Magnitude (Search this column.)
Alaska	atrazine Source Page 5	drinking water MCL {water supply (drinking, culinary and food processing); contact recreation} *(Human Health)*	0.0030 mg/l
Arizona	atrazine Source Page 20	Domestic Water Source (DWS) *(Human Health)*	3 µg/l
Arizona	atrazine Source Page 20	Full-Body Contact (FBC) *(Human Health)*	32667 µg/l
Arizona	atrazine Source Page 20	Partial-Body Contact (PBC) *(Human Health)*	32667 µg/l
California Region 1 - North Coast	atrazine Source Page 47	municipal or domestic supply *(Human Health)*	0.0030 mg/l
California Region 2 - San Francisco Bay	atrazine Source Page 54	municipal supply	0.0030 mg/l
California Region 3 - Central Coast	atrazine Source Page 48	domestic or municipal supply	0.0030 mg/l
California Region 4 - Los Angeles	atrazine Source Page 135	municipal and domestic water supply *(Human Health)*	0.001 mg/l
California Region 9 - San Diego	atrazine Source Page 162	municipal or domestic supply *(Human Health)*	0.0030 mg/l
Colorado	atrazine Source Page 31	drinking water supply *(Human Health)*	3 µg/l

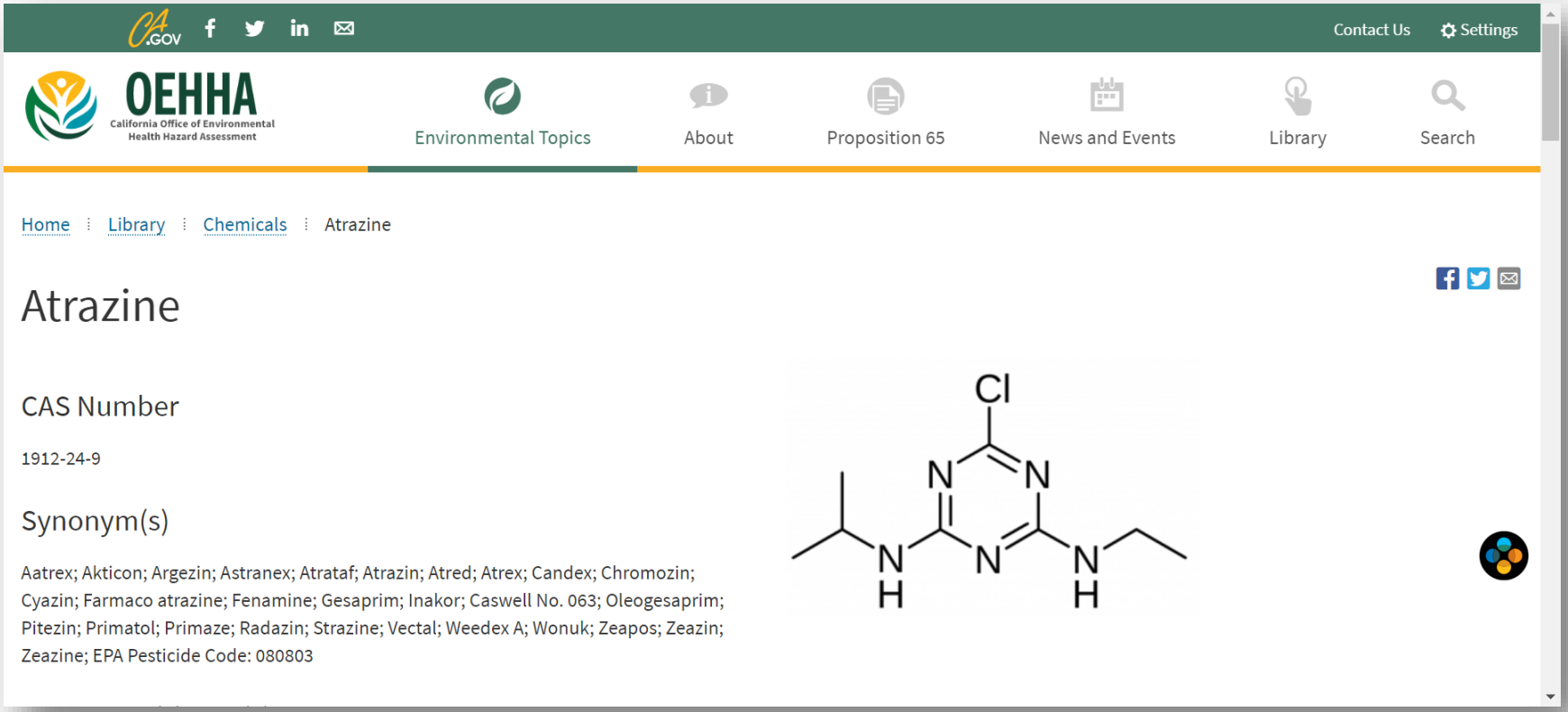
Showing 1 to 10 of 41 entries — Previous 1 2 3 4 5 Next

Top of Page

New Outlinks of Interest
PubChem Chemical Vendors



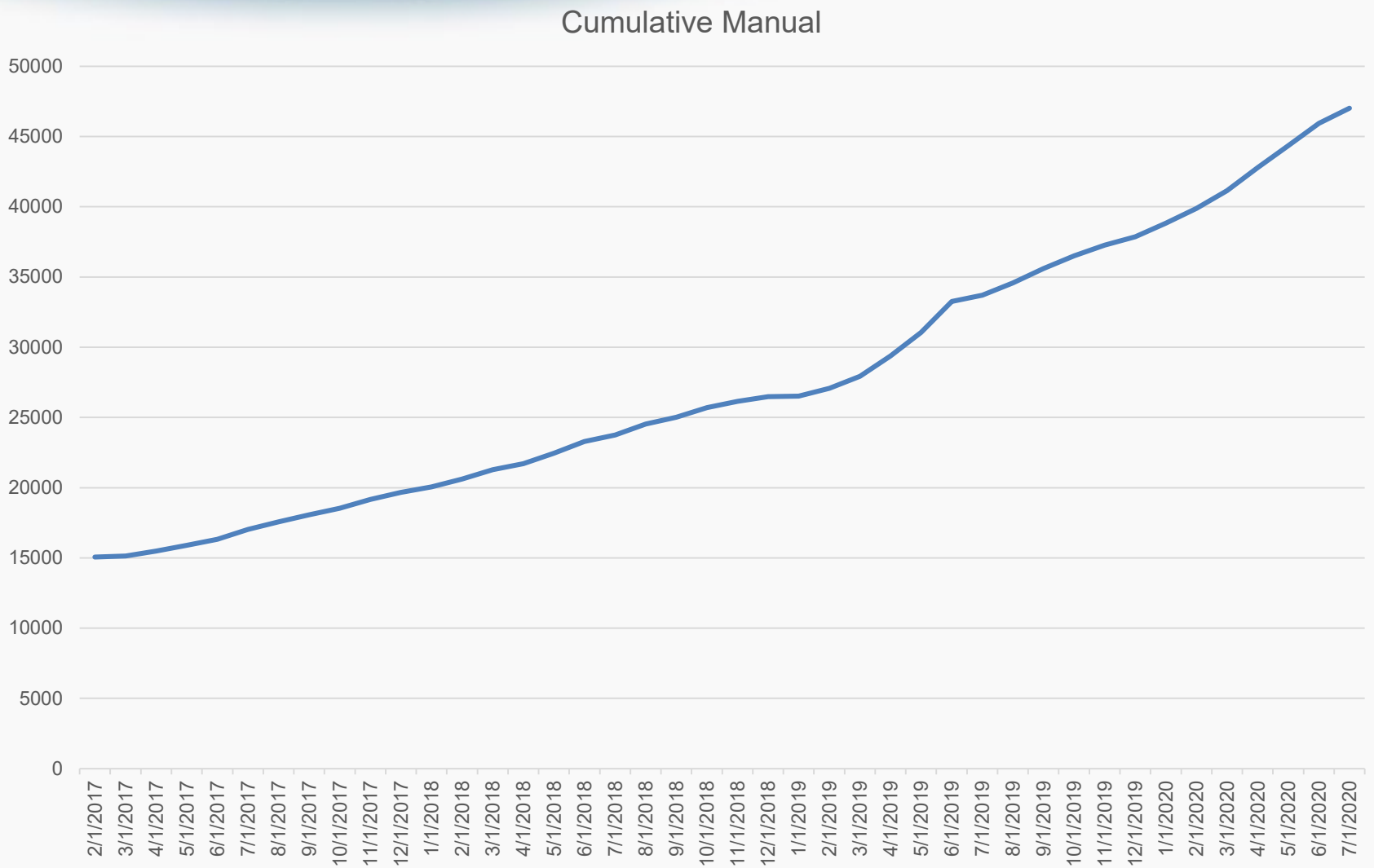
New Outlinks of Interest
California EPA OEHHA



EPA United States Environmental Protection Agency

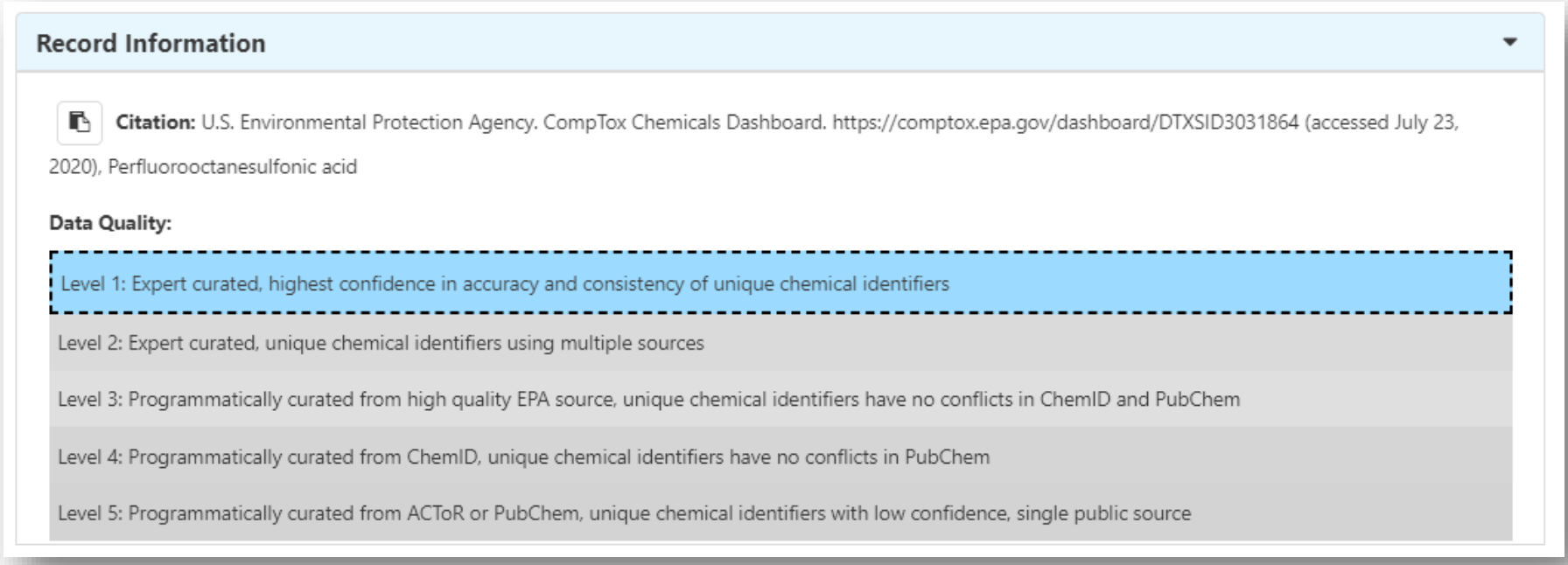
CONTRIBUTING to DATA QUALITY

Ongoing Data Review
Thanks to our curators!



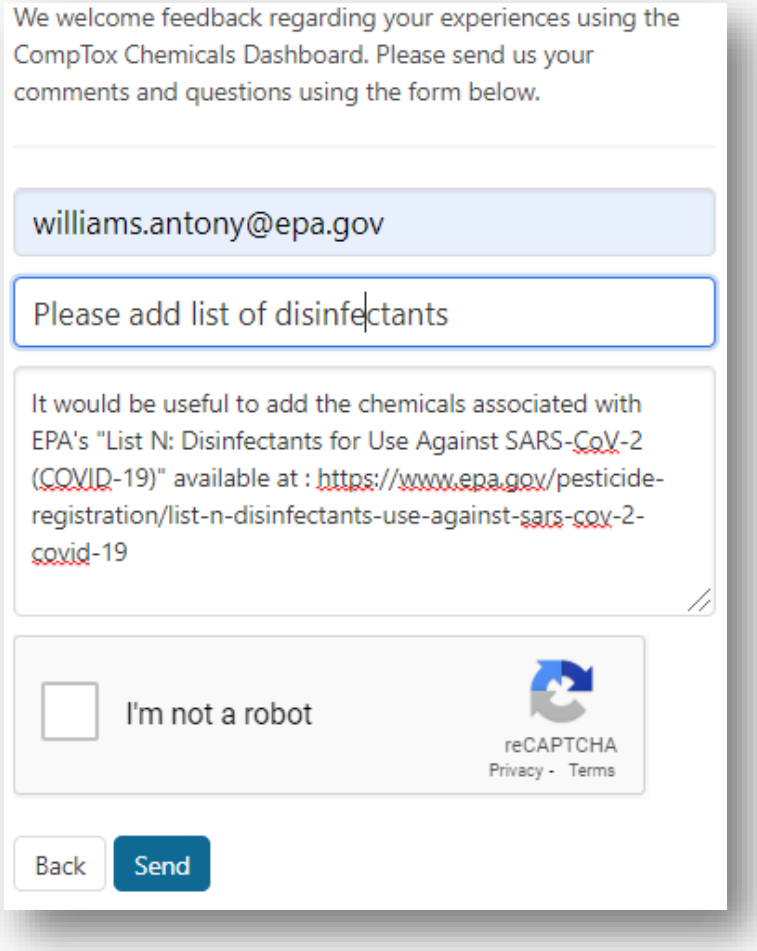
Data Curation Level

- View the level of curation for any chemical
- If you see any issues let us know



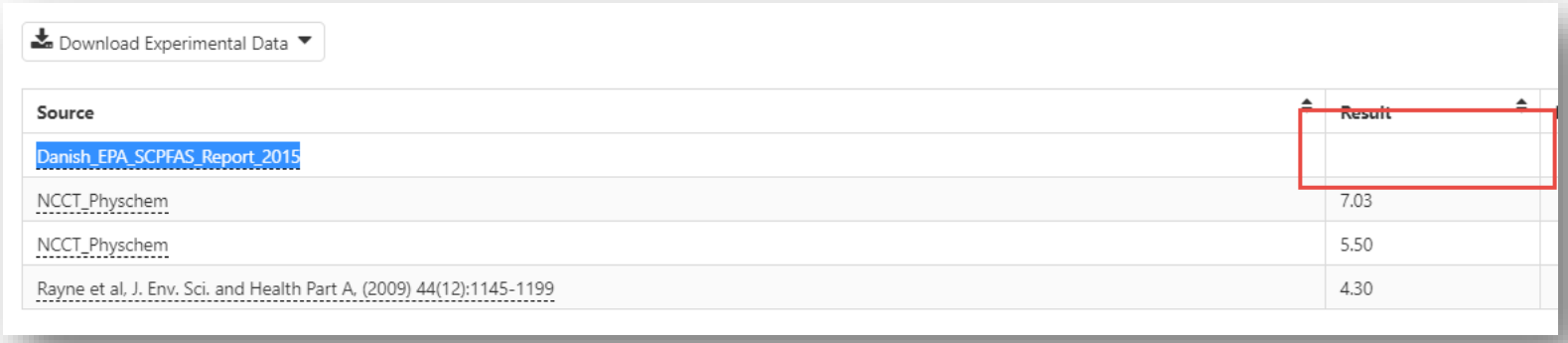
As users, please **contribute**

- We welcome your comments: https://comptox.epa.gov/dashboard/contact_us

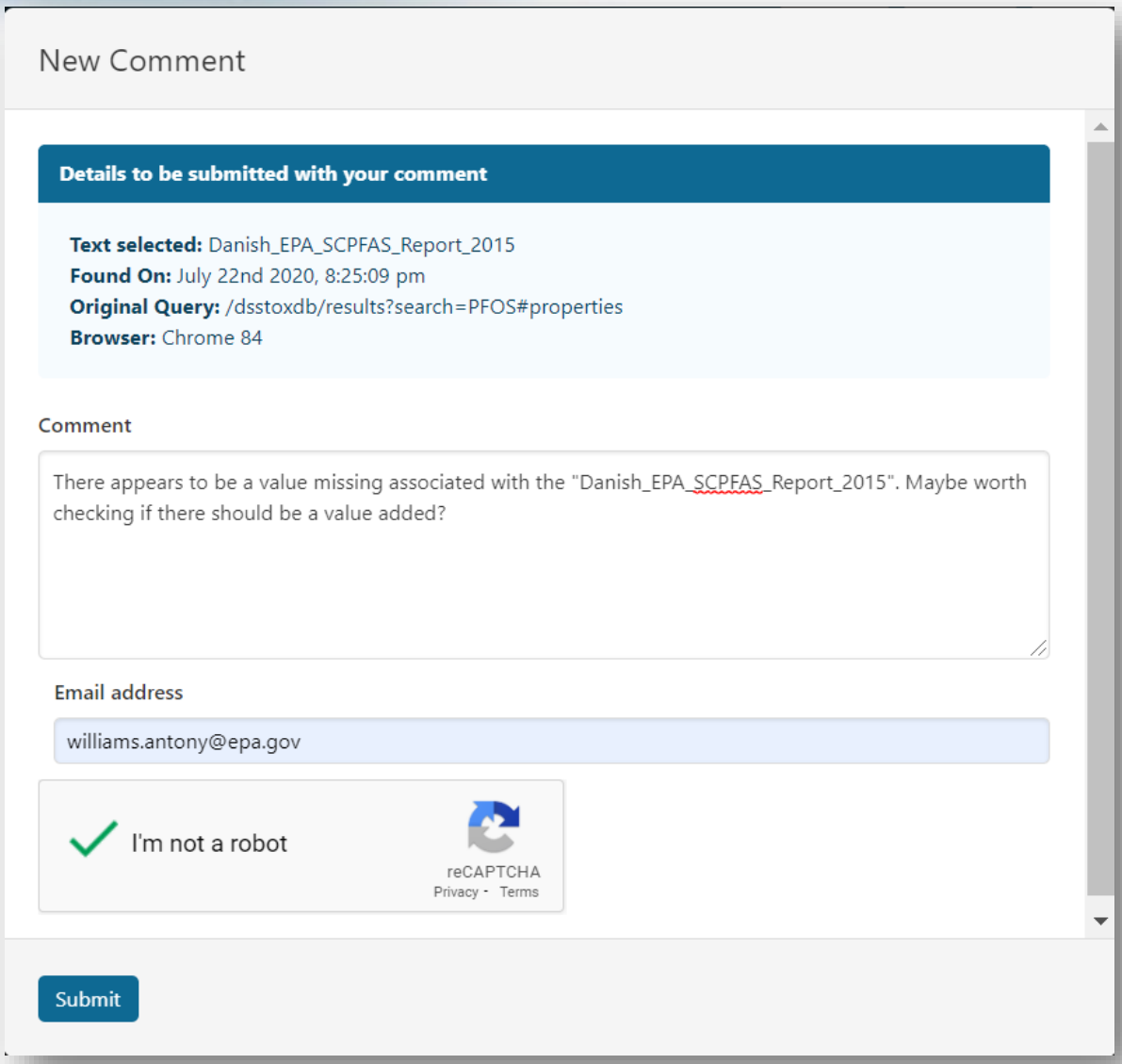


Please help curate the data…

- Users can identify issues with all of our data
  - Suggest chemicals to add to lists
  - Suggest related substances – e.g. metabolites, degradants
  - Flag errors in the data – e.g. properties
- We are now receiving daily feedback – "Submit Comment"



Submit Comments
We will provide feedback…



>400 Comments to Date
Cleaning chemistry one at a time

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Crowdsourced Comments

25

Search query

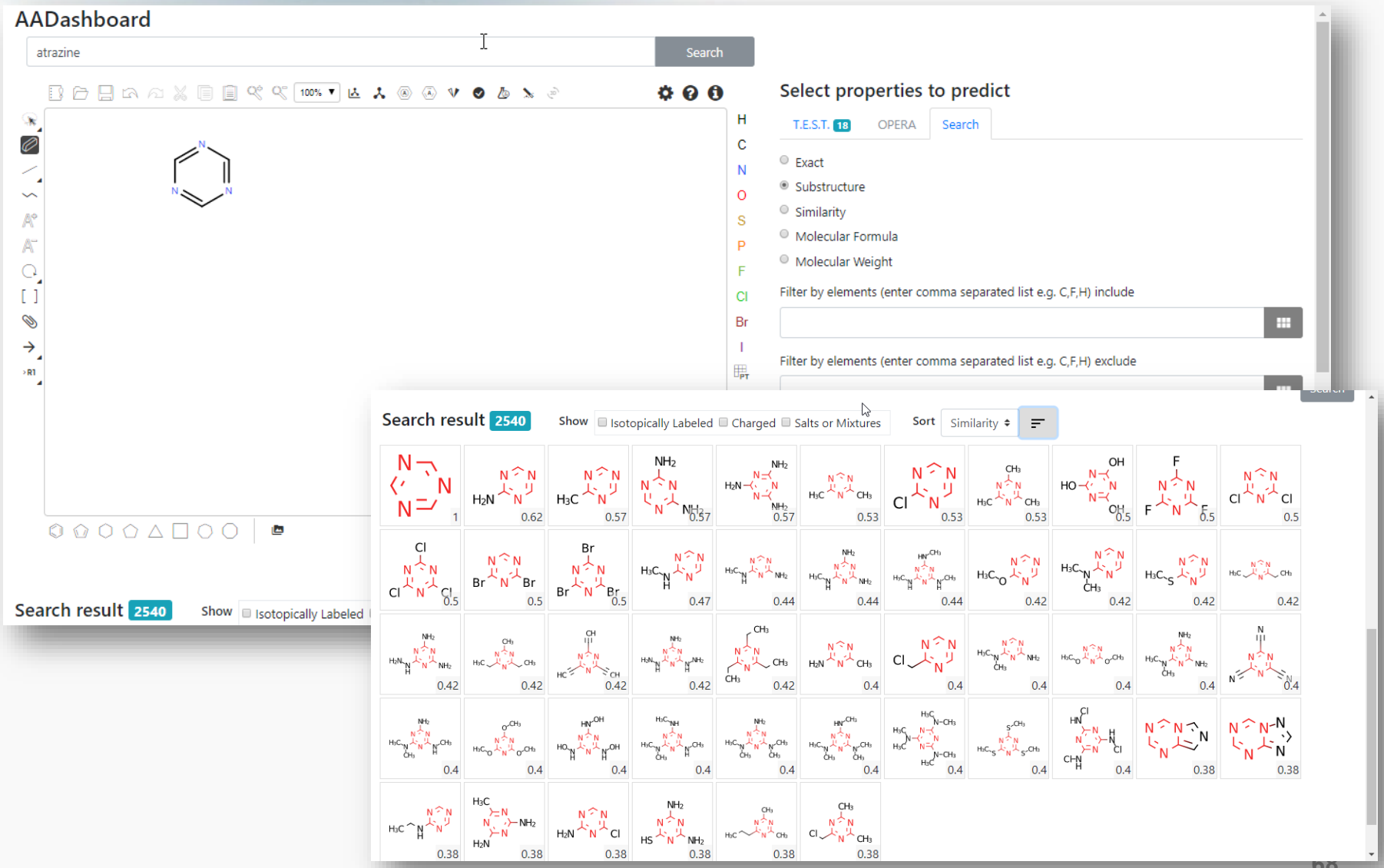
Chemical	Structure	Date	Comment	Resolution
Oxazole, 2-ethyl-4,5-dimethyl-		2020-07-22	4,5-Dimethyl-2-ethyloxazole is just a BAD name - remove ? Add 2-Ethyl-4,5-dimethyloxazole WLN is T5N COJ B2 D1 E1 REAXYS/BRN is 507360 FEMA 3672 MFCD00036664 Barrie	Resolved
4-Decenoic acid, ethyl ester, (4E)-		2020-07-22	Add names Ethyl (4E)-4-decenoate (uninverted CAS name) Ethyl (E)-dec-4-enoate (IUPAC) FEMA 3642 REAXYS/BRN 1770966 WLN 6U3VO2 &&E or trans Form REACH 278-509-4 (ex EINECS) PubChem CID 5362583 MFCD00015574 UNII-3I89X5937N Barrie	Resolved
Hexanedioic acid, diisononyl ester	No Chemical Structure Associated with this Substance	2020-07-21	the tox cast curves for some chemicals will not display, specifically the toxcast/tox21 tab is missing from the left side menu on the dashboard. You can only display the toxcast summary (that shows that there are results from toxcast/tox21) or the toxcast models. Examples are 33703-08-1 and 27178-16-1 .	Resolved
2-Pentenal, 5-(methylthio)-2-[(methylthio)methyl...		2020-07-20	2,8-Dithianon-4-en-4-carboxaldhyde should be..aldehyde 2-Methylthiomethyl-5-methylthiopent-2-enal BAD name - remove, on corrected as below 5-(Methylthio)-2-(methylthio)methylpent-2-en-1-al 5-(Methylthio)-2-(methylthio)methylpent-2-enal known trivially as Methialdol REAXYS/BRN is 2241044 WLN is 1S3UYVH1S1 Barrie	Resolved
Dipentyl 2-hydroxybutanedioate		2020-07-20	well known as Dipentyl malate WLN 5OVYQ1VO5 Barrie	Resolved
Tricyclo[1.1.0.0~2,4~]tetraphosphane		2020-07-20	This comment or question is asked of me somewhat frequently, is DTXSID1024382 white phosphorus as it is listed as a synonym, or is it more appropriate to say DTXSID90923991 is white phosphorus? Any clarification that could be provided on DTXSID90923991's entry on the Dashboard would be appreciated.	Resolved

EPA United States Environmental Protection Agency

PROTOTYPES in PROGRESS

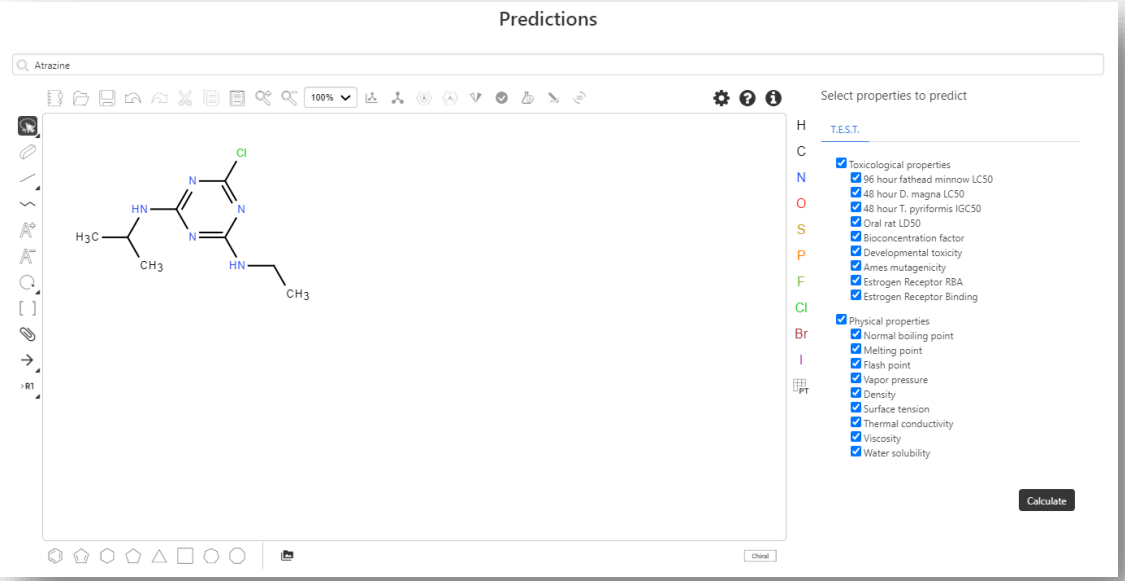
Proof-of-Concept: Structure/ Substructure/Similarity Searches

EPA United States Environmental Protection Agency

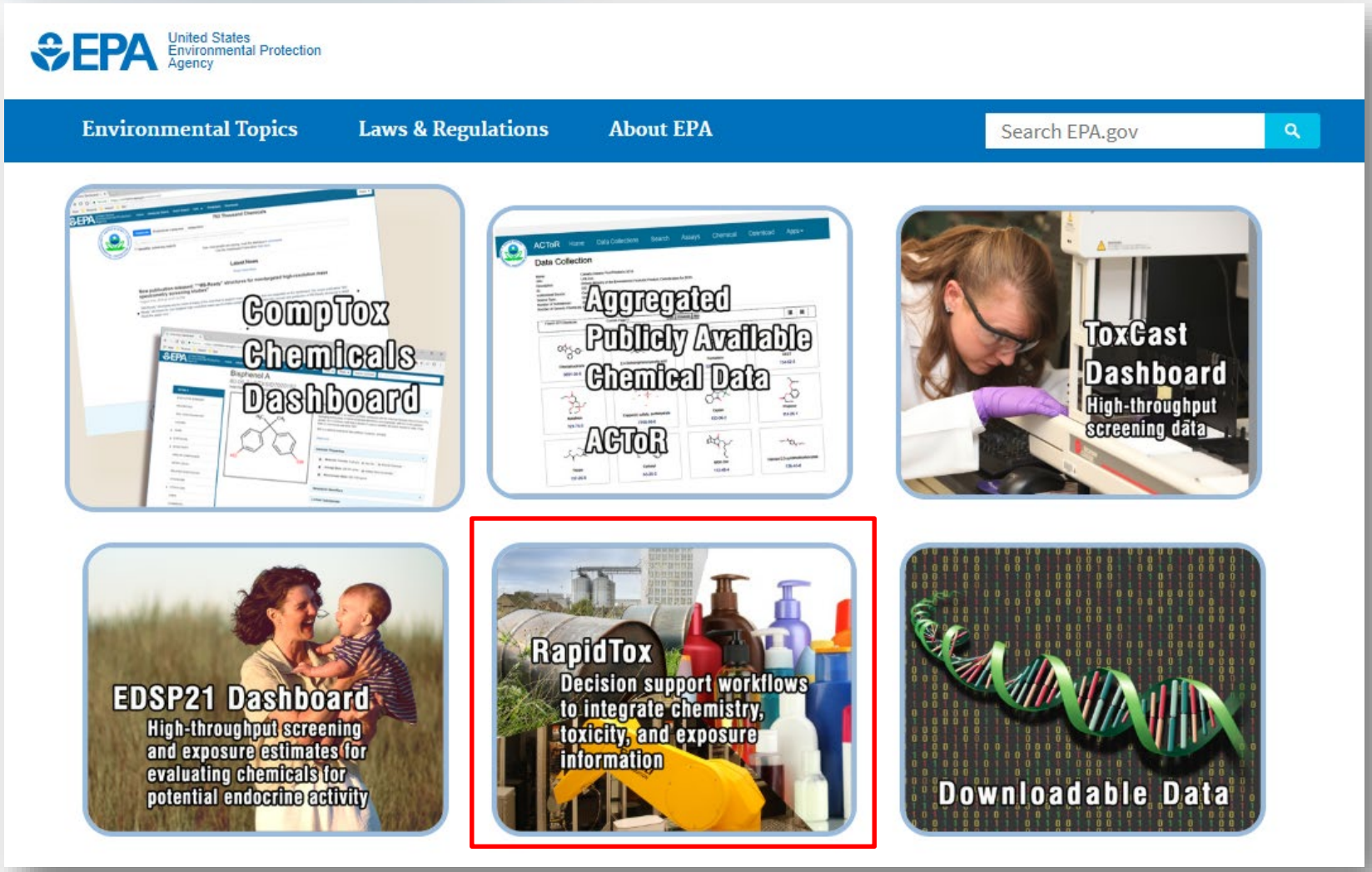


Other Prototypes in Progress

- “Structure Standardization” services to produce MS-Ready and QSAR-ready data
- Single predictions already available. Batch predictions in development.



"RapidTox" *Proof-of-Concept*



RapidTox Dashboard

RapidTox Dashboard

Decision-support tool to integrate chemistry, toxicity and exposure information

Under different federal statutes, EPA makes a broad range of decisions to protect public health and the environment from unintended consequences of using chemicals. Decisions about chemicals are also made by other Federal Agencies, State Environmental and Health Agencies, International Governmental Agencies and Industry. As examples, there are specific federal laws for pesticides, drinking water contaminants, commercial and industrial chemicals, chemicals found on contaminated sites and endocrine disrupting chemicals.

These laws give EPA the authority to gather health, safety and exposure data on chemicals, require necessary testing, and control human and environmental exposures. EPA's computational toxicology researchers are integrating available chemical information including chemistry, toxicity and exposure information into an online tool called RapidTox to help decision-makers quickly and efficiently evaluate chemicals. To help decision-makers leverage this information effectively, researchers are now customizing this tool to help EPA and states meet the requirements under various federal statutes as well as state and local laws.

Alternatives Assessment Dashboard - a foundation technology

Clean Technologies and Environmental Policy (2020) 22:441–458
https://doi.org/10.1007/s10098-019-01795-w

ORIGINAL PAPER

An automated framework for compiling and integrating chemical hazard data

Leora Vegosen[1,2] · Todd M. Martin[2]

Received: 3 October 2019 / Accepted: 13 December 2019 / Published online: 21 January 2020

Now: “Hazard Comparison Dashboard”

- Watch this space….

WHAT'S THE NEXT BIG CHANGE?

First - An Announcement

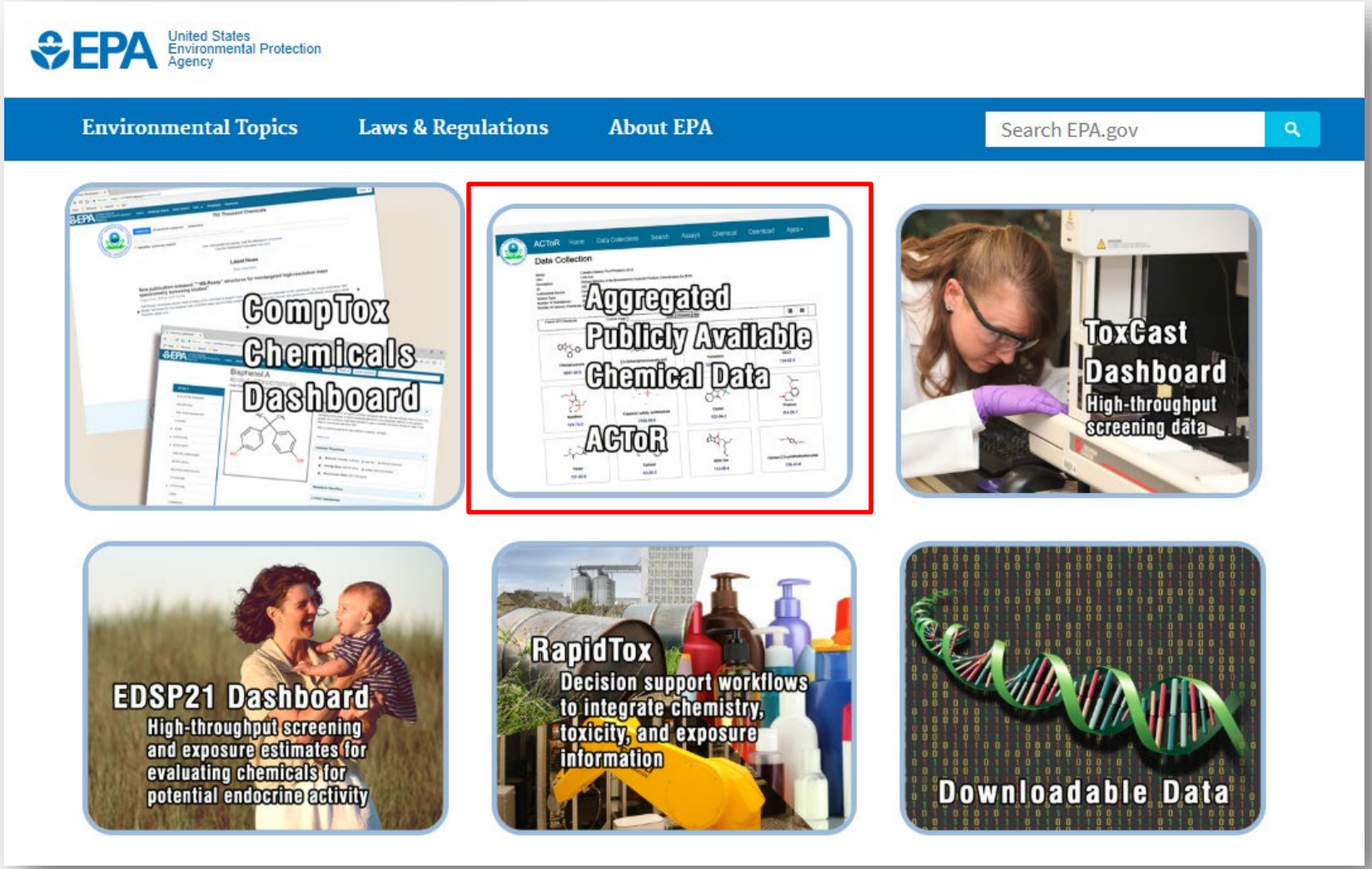
- After 5 years & 10 releases, we have reached the end of *this* technology architecture
- The dashboard: a prototype that kept growing
- We are starting ***afresh*** with a new architecture based on a datahub and new user experience
- First release scheduled for March 2021
  - migration of existing capabilities
  - supporting increased frequency of data releases
  - existing dashboard will remain online for smooth transition

Short Term Goals for Release

EPA United States Environmental Protection Agency

- Using new table widgets to unify tabulated data handling across the application
- Rebuilding visualization widgets to support multiple applications
- Service-based architecture will ultimately provide **public API** to access datahub
- Faster, more flexible searching

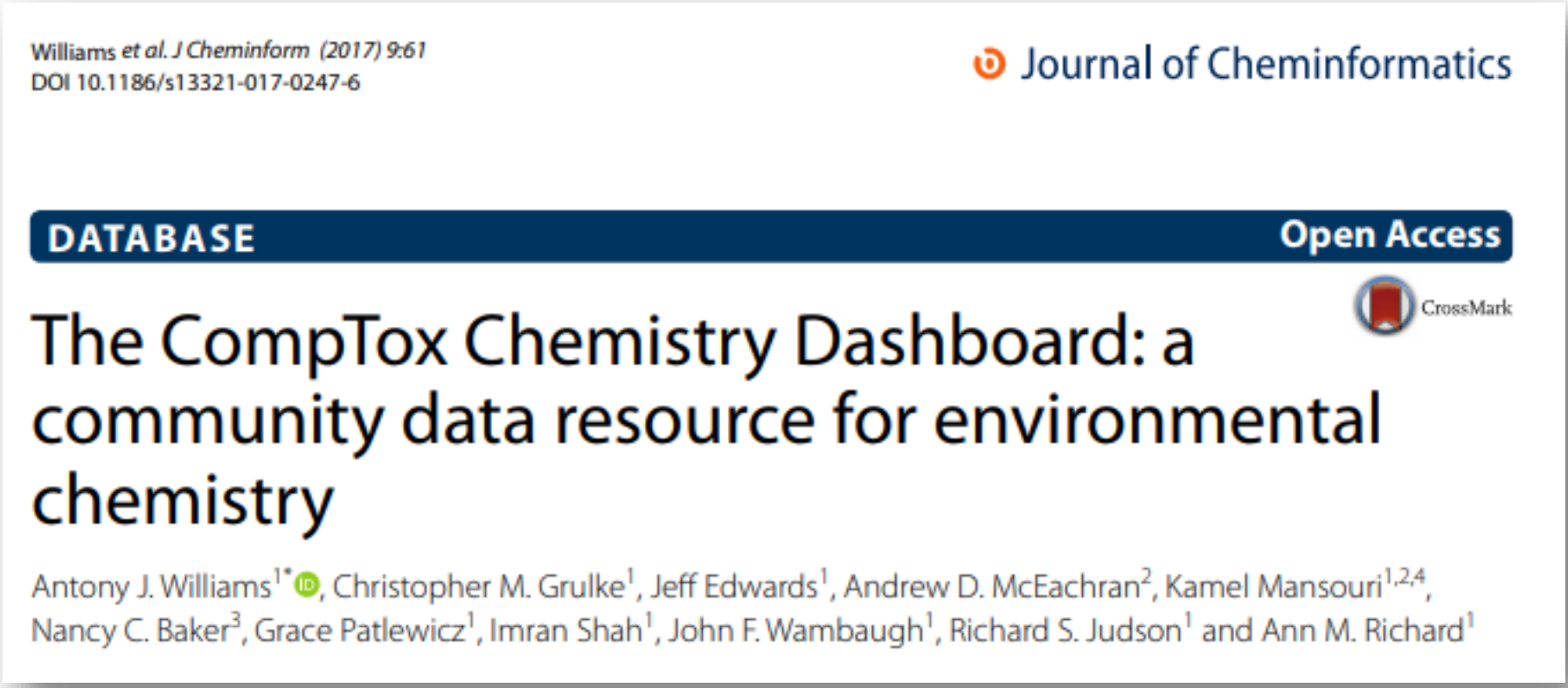
Future Integration Planned…
The ACToR Database



The early days of the dashboard

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

CrossMark

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]

The many years of data curation…

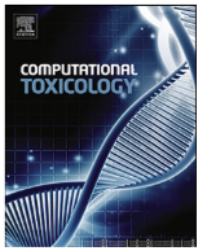
https://www.sciencedirect.com/science/article/pii/S2468111319300234

Computational Toxicology 12 (2019) 100096

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox

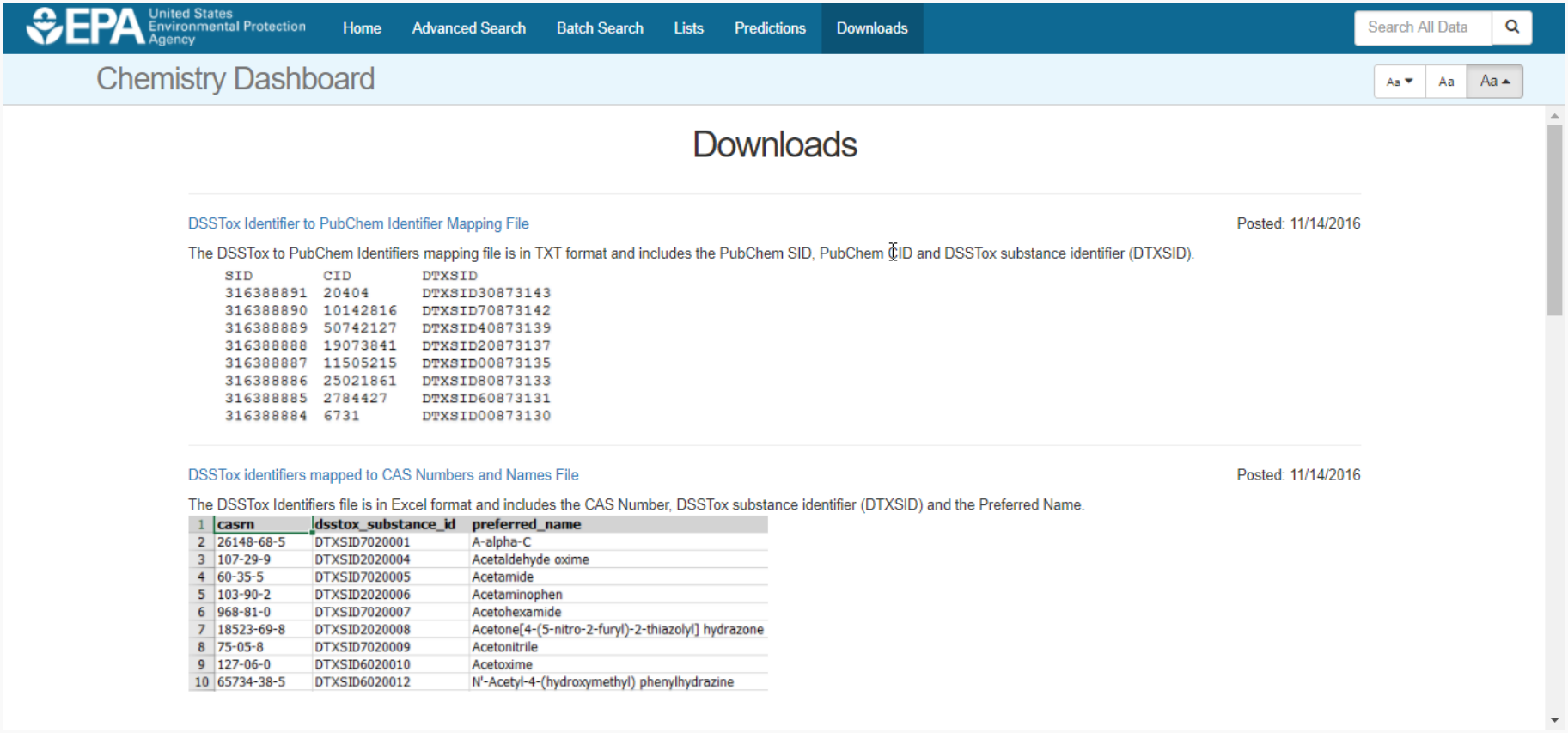


EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke[a], Antony J. Williams[a], Inthirany Thillanadarajah[b], Ann M. Richard[a,*]

- We owe a great debt to the curators who have invested efforts over ~20 years

Downloadable Data Will Be Updated



Conclusion

- The Dashboard is our primary web-based tool for delivering data to the community
- Data growth continues unabated – new chemicals, toxicity data, products, predictions, *in vitro* data…
- Data curation is a **critical** aspect of the project
- Proof-of-concept applications in development
  - Structure standardization (MS-Ready/QSAR-Ready)
  - Structure-substructure-similarity searching
  - Hazard Comparison Dashboard and RapidTox workflows
- Next release (March 2021) will be a full **rebuild** of the architecture. Public API in development

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(Please note I am one *small* cog in the engine that makes the dashboard happen…)