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Primer on New Version of CompTox Chemicals Dashboard

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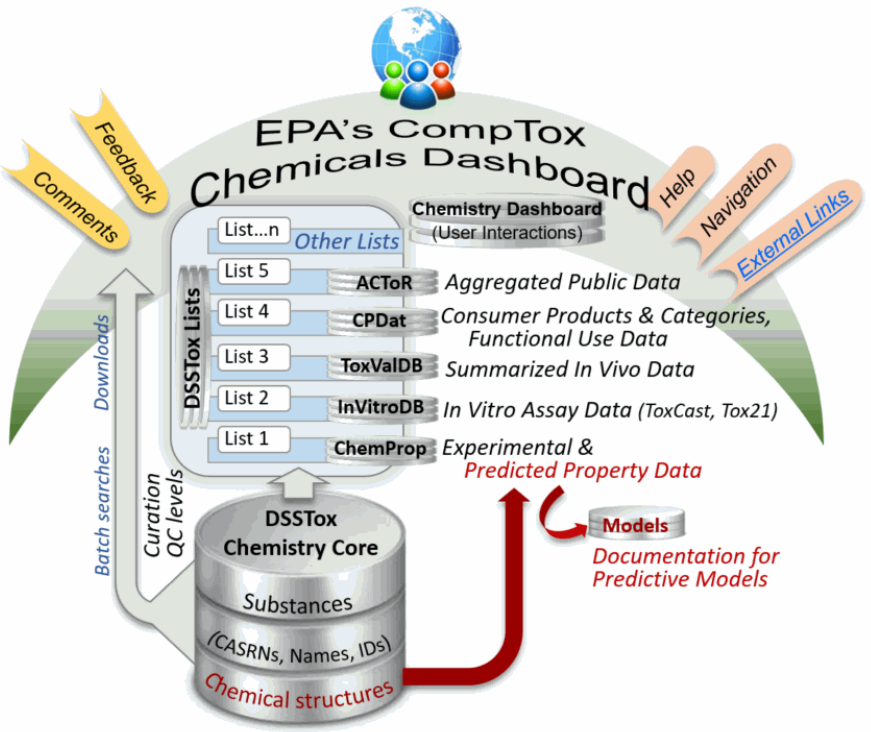
Communities of Practice, February 23rd 2022

The CompTox Chemicals Dashboard

- Our primary tool for integrating and delivering our data to the community *plus* connect across agency resources
- Online since April 2016 with new releases – Spring and Fall every year (to coincide with conference seasons)
- Number of chemical substances has grown from 560k to 906k since first release and from ~40 to ~320 chemical lists
- Replaced multiple other Dashboards unifying data and making support easier



Some Related Publications of Interest

EPA United States Environmental Protection Agency

ELSEVIER

Computational Toxicology
Volume 12, November 2019, 100096

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]

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https://doi.org/10.1016/j.comtox.2019.100096

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Journal of Cheminformatics

Home About Articles Submission Guidelines About The Editors Calls For Papers

Database | Open Access | Published: 28 November 2017

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

Antony J. Williams, Christopher M. Grulke, Jeff Edwards, Andrew D. McEachran, Kamel Mansouri, Nancy C. Baker, Grace Patlewicz, Imran Shah, John F. Wambaugh, Richard S. Judson & Ann M. Richard

Journal of Cheminformatics **9**, Article number: 61 (2017) | Cite this article

ACS Publications
Most Trusted. Most Cited. Most Read.

Search text, DOI, authors, etc. My Activi

RETURN TO ISSUE < PREV **APPLICATION NOTE** NEXT >

Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard

Charles N. Lowe* and Antony J. Williams*

Cite this: *J. Chem. Inf. Model.* 2021, 61, 2, 565–570
Publication Date: January 22, 2021
https://doi.org/10.1021/acs.jcim.0c01273

Article Views	Altmetric	Citations
802	2	7

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ELSEVIER

Environment International
Volume 154, September 2021, 106566

Review article

Sourcing data on chemical properties and hazard data from the US-EPA CompTox Chemicals Dashboard: A practical guide for human risk assessment

Antony J. Williams [a], Jason C. Lambert [a], Kris Thayer [b], Jean-Lou C.M. Dorne [c]

Rearchitecting the Dashboard

- After 5 years and 10 releases of expanding data and functionality performance was degrading
- User experience and feedback encouraged redesign
- Multiple applications requiring underlying data needed unifying approach to facilitate development of other tools: e.g., GenRA, RapidTox

- The Dashboard was a successful "*proof-of-concept*" tool that required rearchitecting for ongoing support and performance

The Vision for the Rebuild

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- VISION: Rearchitect the entire application using a data hub/data mart foundation, API to access and serve the data to the user interface

- GUIDANCE: “1-to-1 mapping of new dashboard to old dashboard”

- EXPECTATIONS:
  - Improved search performance
  - Improved documentation and help manual
  - Unify navigation *especially* in regards to tabular data handling
  - Make *future* development easier with a new foundation

New Design - >906,000 chemicals

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments

Welcome to the new EPA CompTox Chemicals Dashboard

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2020.

CompTox Chemicals Dashboard

Search 906,511 Chemicals

Chemicals | Products/Use Categories | Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

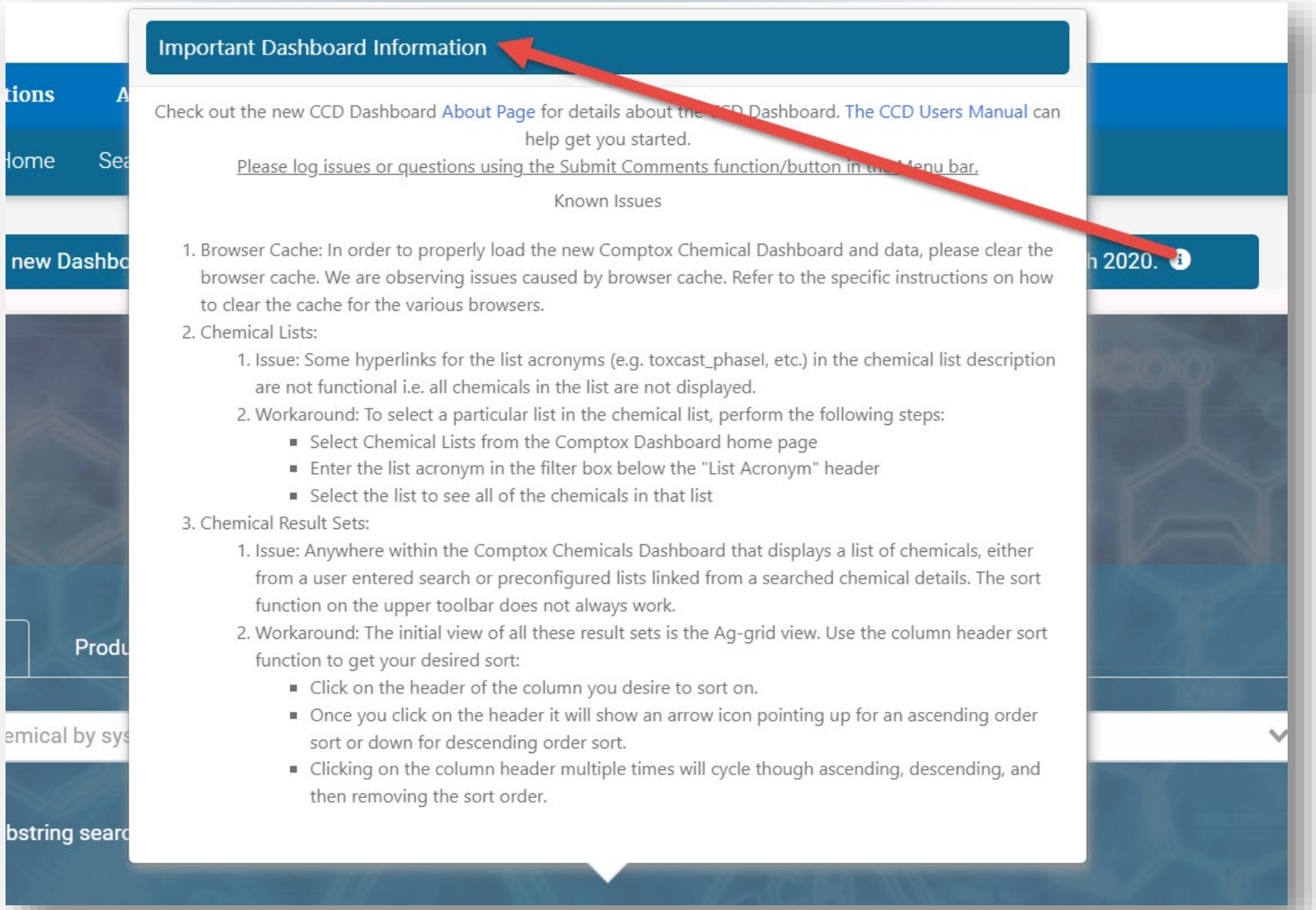
Start typing to search.

Identifier substring search

Latest News

Read More News

Updated information available



- On-click informational icon gives latest important information

Data updates across the board

- Data have been updated across the application
  - Chemistry data and lists
  - ToxVal
  - Exposure
  - Bioactivity
- Data versioning is under: https://comptox.epa.gov/dashboard/about

Data Sources

Source Name	Version	Description	URL
ChemReg/ DSSTox	20210426_DSSTOX	Cheminformatics backbone of the CCTE's ToxCast and the multi-agency Tox21 HTS screening programs	https://www.epa.gov/chemical-research/distributed-structure-searchable-toxicity-dsstox-database https://doi.org/10.23645/epacomptox.5491516.v5
Invitro	V.3.4	Data generated by the ToxCast and Tox21 in vitro high-throughput screening (HTS) programs	https://www.epa.gov/chemical-research/toxicity-forecasting https://doi.org/10.23645/epacomptox.6062623.v5
ToxVal	V.9.1.1	Collection of animal (in vivo) toxicity study data,	https://gaftp.epa.gov/Comptox/Staff/rjudson/datasets/ToxValDB/
Rapid, Exposure and Dose Data (Factotum, SHEDS-HT, SEEM, HTTK)	Factotum 9/11/202 SEEM3 HTTK	Provides data for exposure estimates for thousands of chemicals.	https://www.epa.gov/chemical-research/rapid-chemical-exposure-and-dose-research#10 https://cran.r-project.org/web/packages/httk/index.html https://github.com/HumanExposure/SEEM3RPackage
ChemProp/ QSAR	20191118_ChemPROP	Capture measured or predicted property data associated with a particular source substance or list of chemicals	https://www.epa.gov/chemical-research/chemical-safety-analytics

New Table Capabilities

http://ccte-ccd.epa.gov/dashboard/chemical-lists/40CFR355

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40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Start typing to search.

Identifier substring search

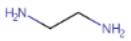
List Details

Description: Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378) This FR notice contains the EHS list of chemicals as published in 1987. This list has been revised over time and should not be used for current compliance purposes. The current EHS list can be found at 40 CFR 355.

Number of Chemicals: 354

Search Results | Default | SEND 353 TO BATCH SEARCH | FILTER | EXPORT

Showing 353 of 353 chemicals

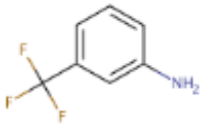
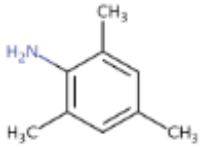
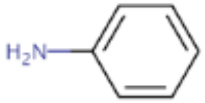
Structure	DTXSID	Preferred Name	CASRN	QC Level	#ToxCast Active	%ToxCast Active	#CPDat	#Sources	#PubChem	#PubMed	Mono. Mass	Mol. Formula
	DTXSID5021881	Ethylenediamine	107-15-3	2	9/398	2%	218	170	272	745	60.068748	C2H8N2
												

Find all chemicals with N2 in formula

Showing 47 of 353 chemicals

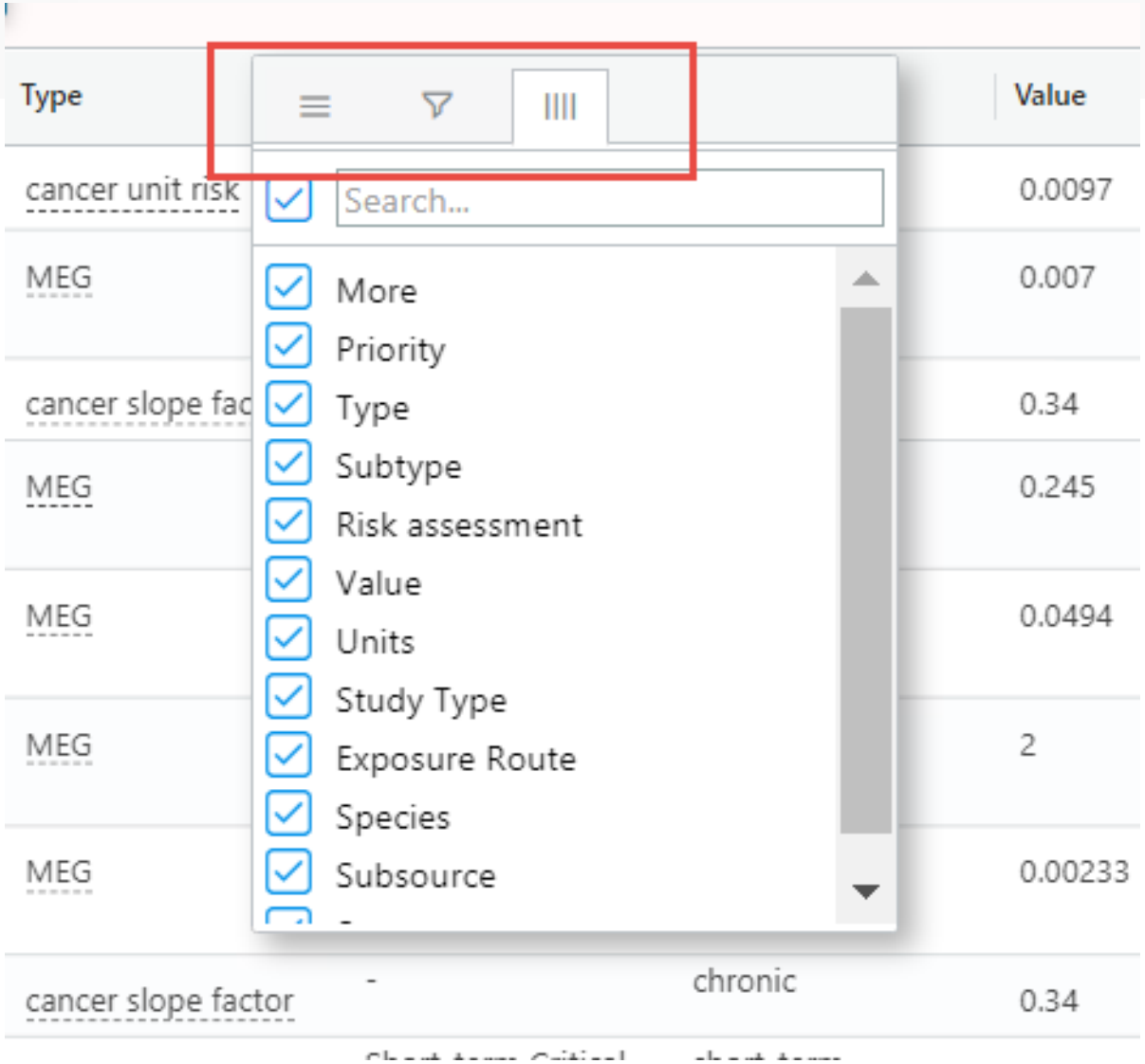
CASRN	QC Level	#ToxCast Active	%ToxCast Active	#CPDat	#Sources	#PubChem	#PubMed	Mono. Mass	Mol. Formula
									N2
107-15-3	2	9/398	2%	218	170	272	745	60.068748	C2H8N2
77-81-6	2	-	-	-	54	36	271	162.055815	C5H11N2O2P
26419-73-8	2	-	-	-	38	15	-	234.049670	C8H14N2O2...

Find “aniline” in the names
Substructure searching is better

Structure	DTXSID	Preferred Name
		aniline
	DTXSID9024512	3-(Trifluoromethyl)aniline
	DTXSID5043847	2,4,6-Trimethylaniline
	DTXSID8020090	Aniline

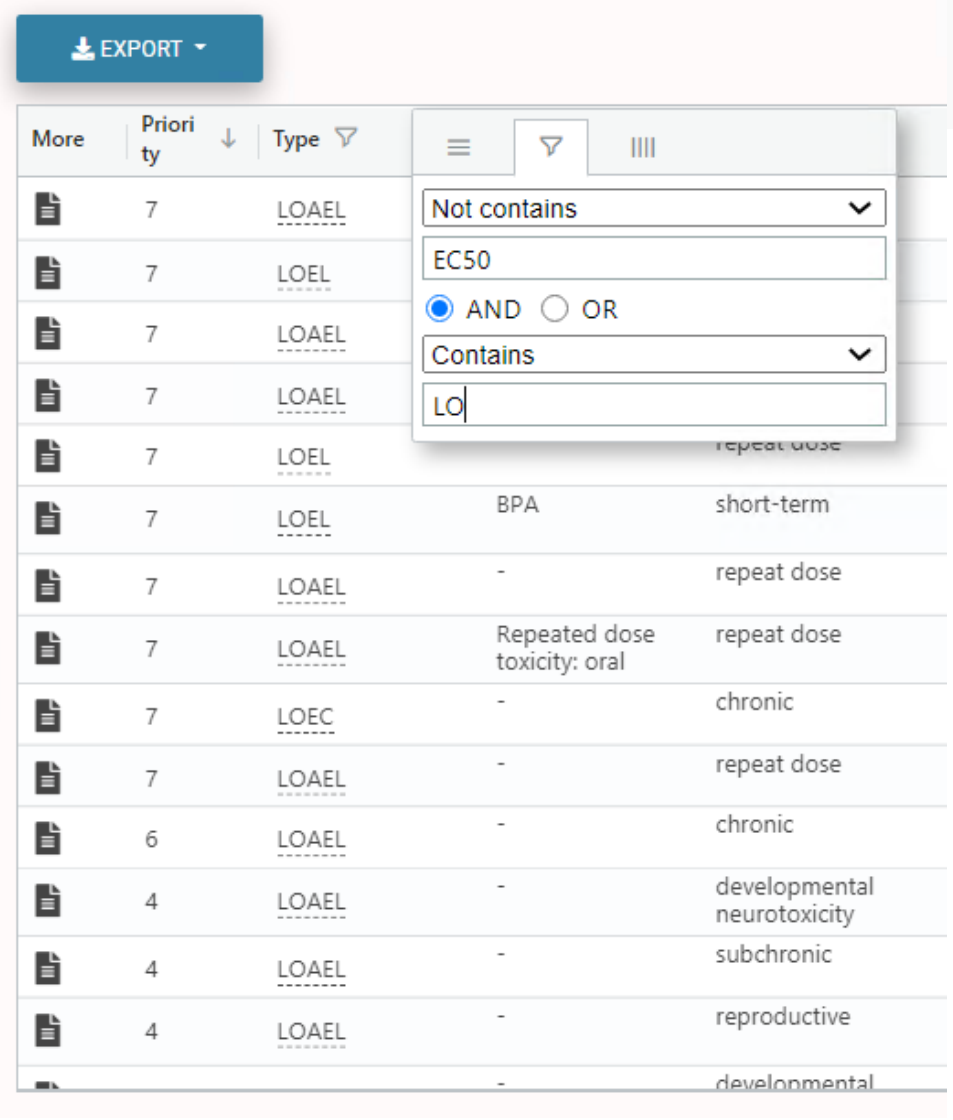
Capabilities to switch columns on/off

- Table functionality for selecting columns for view is built in



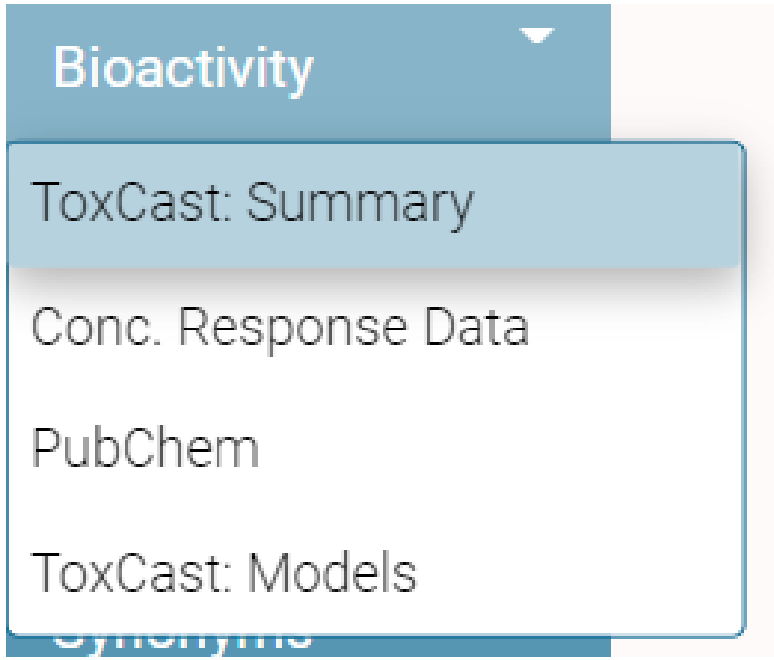
Capabilities to Filter the Table

- Filtering on the tables is possible
- It is not available on every column on every table and in many cases probably doesn't make sense
- While using please highlight where it might be of value



Bioactivity Refresh

- We have collapsed EDSP21 and ToxCast/Tox21
- Concentration Response Data views have been rebuilt
- New display of ToxCast Summary view and Conc. Response curves



Bioactivity Refresh

- Concentration Response fully reworked

Concentration Response Data

Analytical Data on Tox21 Browser

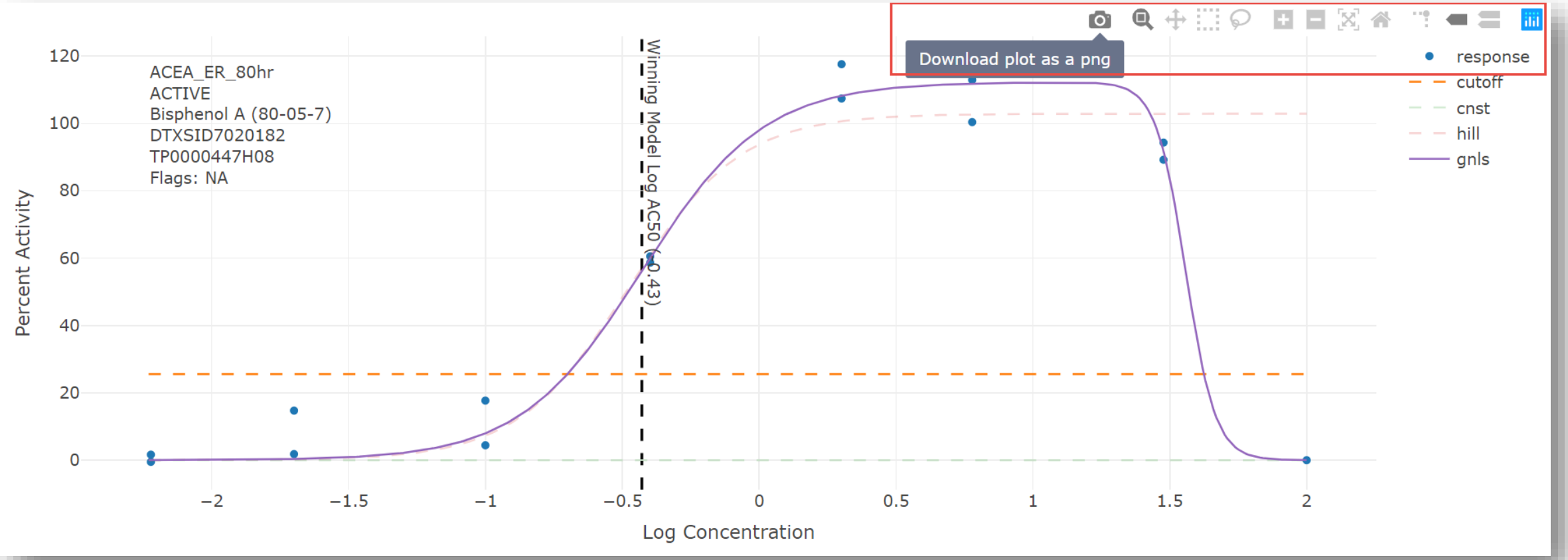
EXPORT

Name	Description	Endpoint Name	Active	Deta...	Rep....	All P...	Gene	Intended Target	Cell Line	Cell For...
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active				null	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active				null	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_80hr	Active				ESR1	steroidal	breast	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_AUC_viability	Inactive				null	cytotoxicity	breast	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_dn	Inactive				null	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_up	Inactive				null	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_dn	Inactive				null	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_up	Inactive				null	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_dn	Inactive				null	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_up	Inactive				null	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_dn	Inactive				null	cytotoxicity	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_up	Inactive				null	proliferation	liver	cell line

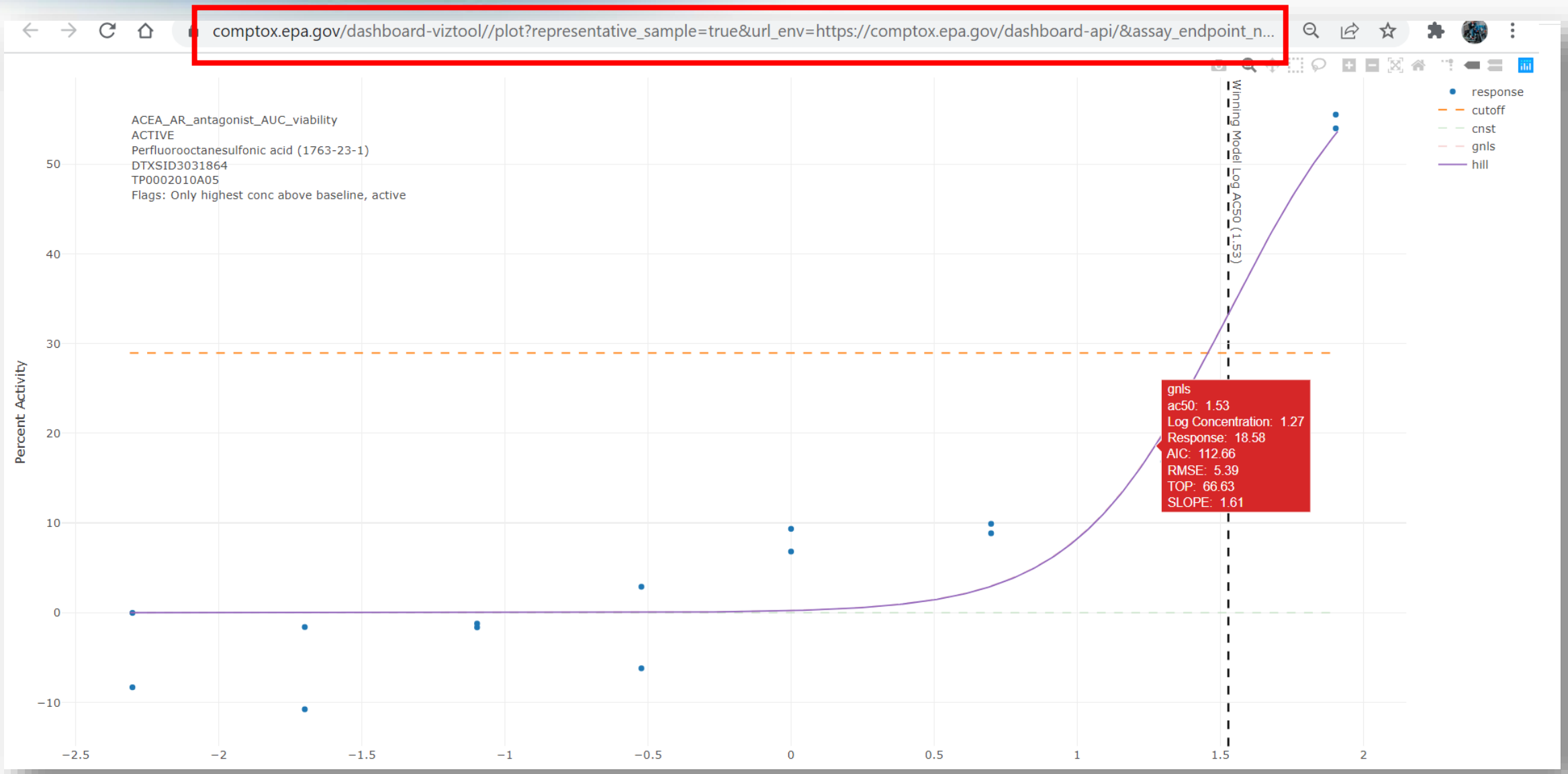
Rows: 1,398 Total Rows: 1,398

More flexible interface for data viewing
Based on Plotly

- All the advantages of Plotly visualization now built into bioactivity

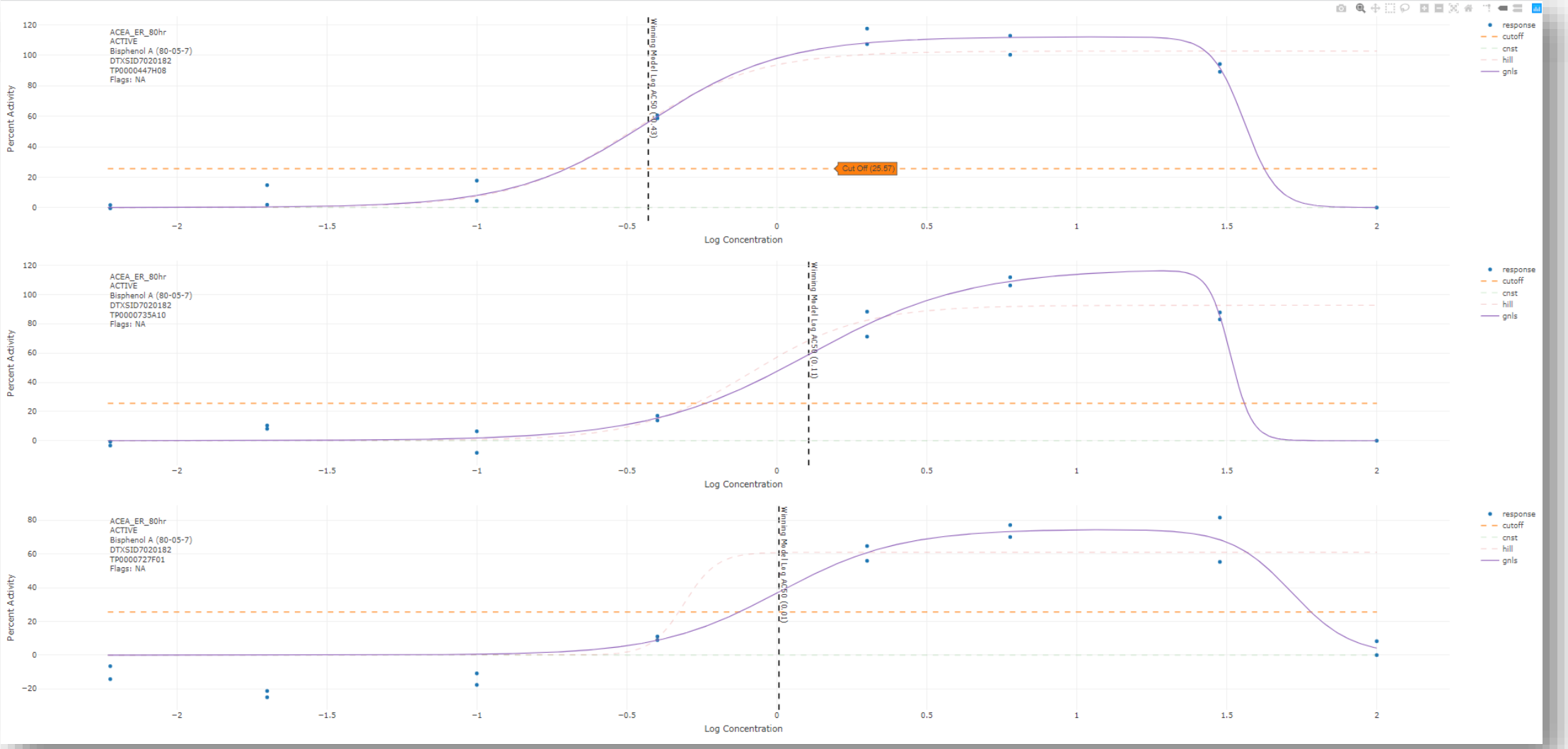


Direct URL access – useful for referencing in publications



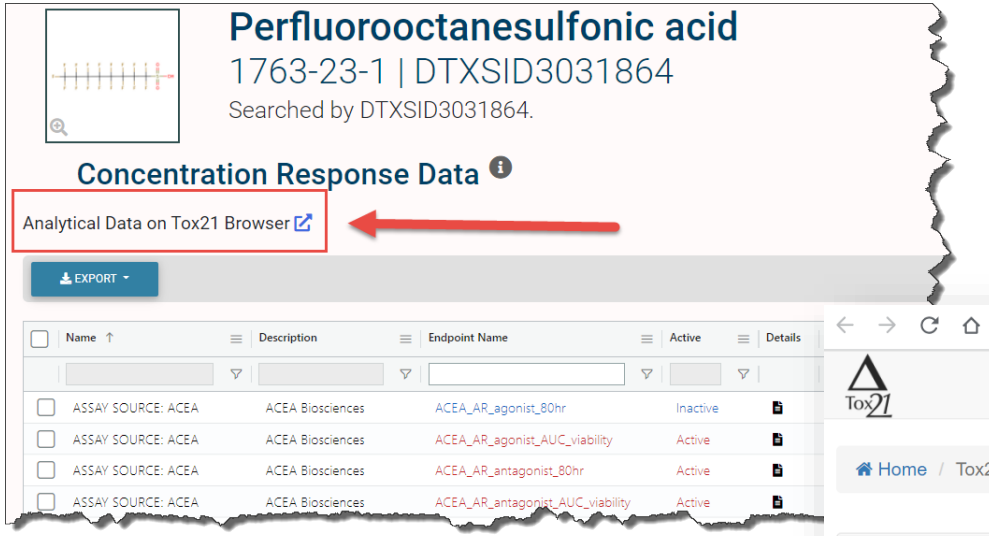
Multiple plots available via URL

https://comptox.epa.gov/dashboard-viztool//plot?representative_sample=false&url_env=https://comptox.epa.gov/dashboard-api/&assay_endpoint_nm=ACEA_ER_80hr&dsstox_id=DTXSID7020182

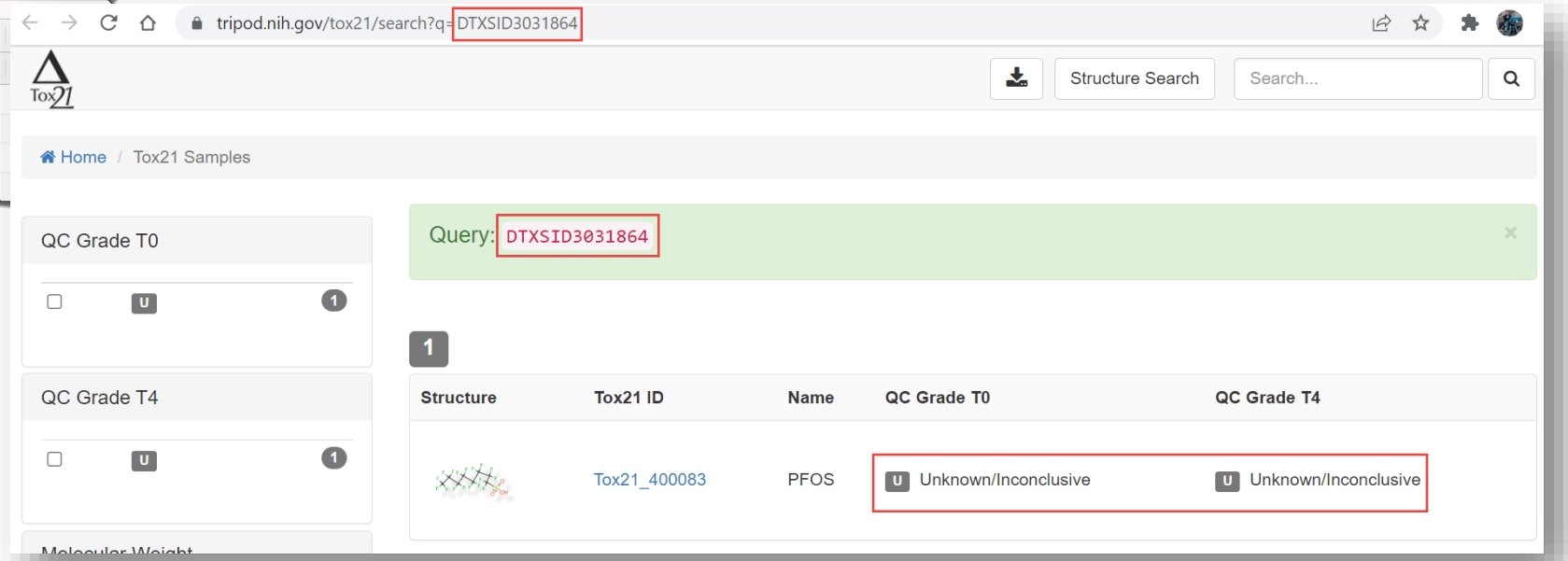


Analytical QC Data updated

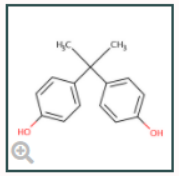
- Previous Analytical QC data was out of date so now linked to the latest data update on the Tox21 browser



- Tox21 browser data now searchable based on DTXSID
- New grade added “Unknown/Inconclusive”



External Links Updated and Expanded



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DTXSID7020182.

General

- ACS Reagent Chemicals
- CAMEO Chemicals
- ChEBI
- ChemAgora
- ChEMBL
- Chemspider
- Consumer Product Information Database
- CPCat
- DrugBank
- ECHA Brief Profile
- ECHA Infocard
- EPA Substance Registry Service
- MSDS Lookup
- NIOSH Chemical Safety Cards
- NIST Chemistry Webbook
- PubChem
- PubChem 3D conformer download
- PubChem 3D Structure Display
- PubChem: Chemical Vendors
- PubChem Safety Sheet
- State-Specific Water Quality Standards
- ToxPlanet
- WEBWISER
- Wikidata
- Wikipedia
- Wolfram Alpha

Toxicology

- ACToR
- ACToR PDF Report
- BindingDB
- CalEPA OEHHA
- Chemical Checker
- ChemView
- CTD
- DrugPortal
- eChemPortal
- ECOTOX
- National Air Toxics Assessment
- NIOSH IDLH Values

Publications

- Bielefeld Academic Search Engine
- BioCaddie DataMed
- CORE Literature Search
- Federal Register
- Google Books (Structure Search)
- Google Books (Text Search)
- Google Patents (Structure search)
- Google Patents (Text search)
- Google Scholar (Structure search)
- Google Scholar (Text search)
- IRIS Assessments
- NIOSH Pocket Guide
- NIOSH Skin Notation Profiles
- PPRTVWEB
- PubMed
- Regulations.gov
- RSC Publications
- Springer Materials

Analytical

- IR Spectra on PubChem
- MassBank
- MONA: MassBank North America
- mzCloud
- National Environmental Methods Index
- NIST Antoine Constants
- NIST IR Spectrum
- NIST Kovats Index values
- NIST MS Spectrum
- Protein DataBank
- RSC Analytical Abstracts
- Tox21 Analytical Data

Prediction

- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- ChemRTP Predictor
- LSERD
- Proton NMR Prediction

- Link decay is an ongoing issue and URLs need updating
- New resources added by request

Abstract Sifter Refresh

Literature - PubMed Abstract Sifter

Abstract Sifter Instructions

1. Select PubMed starting point query

Hazard

2. Optionally, edit the query before retrieving.

("80-05-7" OR "Bisphenol A") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level" [tiab] OR "cancer slope factor"[tiab])

3. Click Retrieve Articles to begin download.

RETRIEVE ARTICLES

143 of 143 articles loaded

4. Optionally, export articles

SEND TO

To find articles quickly, enter terms to sift abstracts.

estrogen | Bisphenol | CLEAR TERMS

estrogen	Bisphenol	T...	PubMe...	Y...	Title	Authors	Journal	Rev	DOI
2	4	6	34147626	2021	Modulation of Folliculogenesis in Adult Laying ...	Eldefrawy; Xu; Pusch; Karkoura; Alsafy; Elgendy; ...	Reproductive toxicology (Elmsford, N.Y.)		10.1016/j.repro
0	9	9	34146661	2021	Effects of bisphenols on Blood-Testis Barrier pro...	Peña-Corona; Vásquez Aguire; Vargas; Juárez; ...	Reproductive toxicology (Elmsford, N.Y.)	✓	10.1016/j.repro
3	2	5	33802611	2021	Characterization of Estrogenic Activity and Site-...	Chioccarelli; Migliaccio; Suglia; Manfrevola; Porr...	International journal of molecular sciences		10.3390/ijms2
0	2	2	33666848	2021	A comprehensive review on the carcinogenic p...	Khan; Correia; Adiga; Rai; Dsouza; Chakrabarty; ...	Environmental science and pollution research in...	✓	10.1007/s1135
0	2	2	33640550	2021	A reconnaissance study of pharmaceuticals, pes...	Picó; Campo; Alfarhan; El-Sheikh; Barceló	The Science of the total environment		10.1016/j.scito
0	2	2	33516155	2021	Update on the Health Effects of Bisphenol A: O...	Vom Saal; Vandenberg	Endocrinology		10.1210/endo
0	2	2	33212759	2020	Gestational Exposure to Bisphenol A Affects Test...	Karmakar; Ahn; Kim; Jung; Kim; Lee; Ryu	International journal of molecular sciences		10.3390/ijms2
2	2	4	33010594	2020	Effects of bisphenol A at the safe reference dos...	Li; Gao; Tan; Miao; Fan; Gao; Liu; Ding; Shi; Song	Ecotoxicology and environmental safety		10.1016/j.ecoe
2	9	11	33010167	2020	Bisphenol AF and Bisphenol F Induce Similar Fe...	Mentor; Wänn; Brunström; Jönsson; Mattsson	Toxicological sciences : an official journal of the ...		10.1093/toxsci
0	2	2	32751382	2020	Paternal Exposure to Bisphenol-A Transgenerati...	Karmakar; Ahn; Kim; Jung; Kim; Lee; Kim; Rahm...	International journal of molecular sciences		10.3390/ijms2
0	2	2	31952986	2020	Bisphenol A exposure is involved in the develop...	Musachio; Araujo; Bortolotto; de Freitas Couto;	Food and chemical toxicology : an international		10.1016/j.fct.2

Abstract Sifter as a TOOL

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Literature - PubMed Abstract Sifter

Abstract Sifter Instructions

1 Select PubMed starting point query

Choose Query Term

2 Optionally, edit the query before retrieving.

Some examples are: Fauci AS[au]
covid-19 spike protein OECD AND qsar
migraine AND 2020[dp]
fipronil or 120068-37-3

3 Click Retrieve Articles to begin download.

RETRIEVE ARTICLES

4 Optionally, export articles

SEND TO

1 Select PubMed starting point query

Choose Query Term

2 Optionally, edit the query before retrieving.

Judson R[AU]

3 Click Retrieve Articles to begin download.

RETRIEVE ARTICLES

246 of 246 articles loaded

4 Optionally, export articles

SEND TO

To find articles quickly, enter terms to sift abstracts.

Judson | Estrogen | CLEAR TERMS

Juds...	Estrogen	T...	PubM...	Y...	Title	Authors	Journal	Rev	DOI
0	0	3223	34140756	2021	Exposure and Toxicity Characterization of C...	Fantke; Chiu; Aylward; Judson; Huang; Jang;...	The international journal of life cycle assess...		10.1007/s1136
0	0	2042	34124416	2021	Using Chemical Structure Information to De...	Pradeep; Patlewicz; Pearce; Wambaugh; We...	Computational toxicology (Amsterdam, Net...		10.1016/j.com
0	0	147	34101097	2021	Correction to: Notch regulates vascular coll...	Gross; Webb; Peterlin; Durrant; Judson; Raz...	Angiogenesis		10.1007/s104
0	0	2115	34017928	2021	Structure-based QSAR Models to Predict R...	Pradeep; Friedman; Judson	Computational toxicology (Amsterdam, Net...		10.1016/j.com

Batch Search Refresh

Batch Search

1 Select Input Type(s)

- Substance Identifiers
  - Chemical Name
  - CASRN
  - InChIKey
  - DSSTox Substance ID
- DSSTox Compound ID
- InChIKey Skeleton
- MS-Ready Formula(e)
- Exact Formula(e)
- Monoisotopic Mass

2 Enter Identifiers to Search

(Please enter one identifier per line. Processing time increases with number of inputs.)

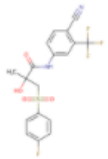
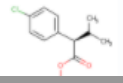
DTXSID9020374
DTXSID9020827
DTXSID2022678
DTXSID4023381
DTXSID9044164
DTXSID7032004
DTXSID4022361
DTXSID8021771

3 DISPLAY ALL CHEMICALS or CHOOSE EXPORT OPTIONS

45% loaded

45 Chemicals Found from 110 Input(s)

REPLACE IDENTIFIERS WITH SELECTED CHEMICALS

Structure	DTXSID	Preferred Name	CASRN	Mono. Mass	Mol. Formula
	DTXSID2022678	Bicalutamide	90357-06-5	430.061041	C18H14F4N2O4S
	DTXSID3020621	(R,R)-Fenvalerate	67614-33-9	419.128821	C25H22ClNO3

Batch Search – *List Filtering*

EPA United States Environmental Protection Agency

Customize Export Results

4 CHOOSE EXPORT FORMAT

Your file will be exported in Microsoft Excel Format (.xlsx)

Select All columns available

Chemical Identifiers

- DTXSID
- Chemical Name
- DTXCID
- CAS-RN
- InChIKey
- IUPAC Name

Structures

- Mol File
- SMILES
- InChI String
- MS-Ready SMILES
- QSAR-Ready SMILES

Intrinsic and Predicted Properties

- Molecular Formula
- Average Mass
- Monoisotopic Mass
- TEST Model Predictions
- OPERA Model Predictions

Metadata

- Curation Level Details
- Safety Data
- NHANES/Predicted Exposure
- Data Sources
- Include ToxVal Data Availability
- Assay Hit Count
- Number of PubMed Articles
- PubChem Data Sources
- CPDat Product Occurrence Count
- IRIS
- PPRTV
- Wikipedia Article
- QC Notes
- Include links to ACToR reports

Enhanced Data Sheets

- MetFrag Input File (Beta)
- ToxPrint single fingerprints
- Abstract Sifter Input File
- Synonyms and Identifiers
- Related Substance relationships
- ToxPrint fingerprints (ChemoTyper)
- Associated ToxCast Assays

Presence in Lists

Title	Description
[illegible]	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
ACSREAG	LIST: ACS Reagent Chemicals
AEGLVALUES	AEGLS: Acute Exposure Guideline Levels
ALGALTOX	LIST: Algal Toxins
ALLSURFACTANTS	CATEGORY: Surfactants
AMINOACIDS	CATEGORY: Amino acids
AMPHIBOLES	Amphibole minerals
ANTIBIOTICS	CATEGORY|PHARMACEUTICALS: Antibiotics
ANTIMICROBIALS	CATEGORY|WIKILIST|ANTIMICROBIALS: Antimicrobials from Wikipedia
AOPSTRESSORS	List of Adverse Outcome Pathway Stressors
APCRARETRO	LIST: APCRA Chemicals for Retrospective Analysis
ARCHEMICALS	ANDROGEN: Androgen Receptor Chemicals

Rows: 319

Download Export file for the chemicals selected

List Filtering

- List filtering is *very* beneficial
- Now ~320 lists so new functionality quickly filters
- Select the lists to push flags into the export file

Presence in Lists

Title	Description
PFAS	Water
EPAPFASDW	PFAS|EPA: New EPA Method Drinking Water
EPAPFASDW537	PFAS|EPA|WATER: Existing EPA DW Method 537.1
EPAPFASDWTREAT	PFAS|EPA|WATER: Drinking Water Treatment Technology
EPAPFASNONDW	PFAS|EPA: New EPA Method Non-Drinking Water
EPAPFASVALDW	PFAS|EPA|WATER: PFAS with Validated EPA Drinking Water Methods
PFASTDB	WATER|PFAS: PFAS Chemicals contained in the EPA Drinking Water Treatability Database

Batch Search Output File… includes new "Cover Sheet"

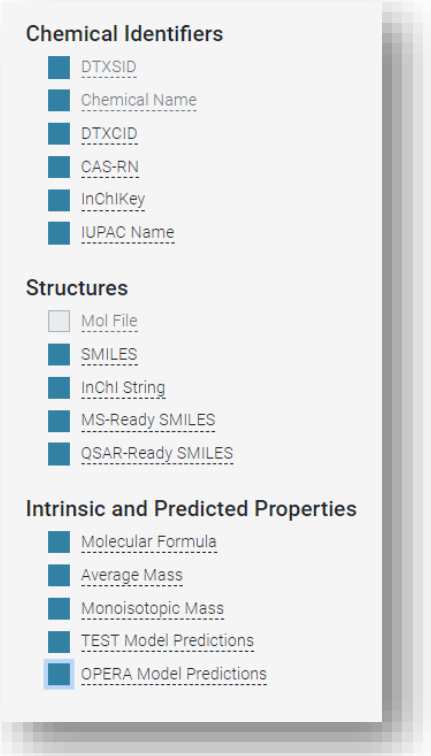
2	WARNING	DO NOT COPY / PASTE THIS DATA Some search terms returned multiple values, copy/paste will result in misaligned data
3	Search datestamp	2022-02-23 12:18:17
4	Search term count	21
5	Found count	15
6	Not found count	6
7	Duplicate count	0
8		

DTXSID	PREFERRED_NAME	EPAPFASDW	EPAPFASDW537	EPAPFASDWTREAT	EPAPFASNONDW	EPAPFASVALDW	PFASTDB
DTXSID4059916	Perfluorobutanoic acid	Y	-	Y	Y	Y	Y
DTXSID70191136	Perfluoro-3-methoxypropanoic acid	Y	-	-	-	Y	Y
DTXSID6067331	6:2 Fluorotelomer sulfonic acid	Y	-	-	Y	Y	Y
DTXSID6062599	Perfluoropentanoic acid	Y	-	-	Y	Y	Y
DTXSID3031862	Perfluorohexanoic acid	Y	Y	Y	Y	Y	Y
DTXSID1037303	Perfluoroheptanoic acid	Y	Y	-	Y	Y	Y
DTXSID00192353	8:2 Fluorotelomer sulfonic acid	Y	-	-	Y	Y	Y
DTXSID60500450	Perfluoro(4-methoxybutanoic acid)	Y	-	-	-	Y	Y
DTXSID8031865	Perfluorooctanoic acid	Y	Y	Y	Y	Y	-
DTXSID30382063	Perfluoro-3,6-dioxaheptanoic acid	Y	-	-	-	Y	-
DTXSID8031863	Perfluorononanoic acid	Y	Y	Y	Y	Y	Y
DTXSID8062600	Perfluoropentanesulfonic acid	Y	-	-	Y	Y	-
DTXSID5030030	Perfluorobutanesulfonic acid	Y	Y	Y	Y	Y	Y
DTXSID5062760	2-(N-Ethylperfluorooctanesulfonamido)acetic acid	-	Y	-	Y	Y	Y
DTXSID3031860	Perfluorodecanoic acid	Y	Y	Y	Y	Y	Y

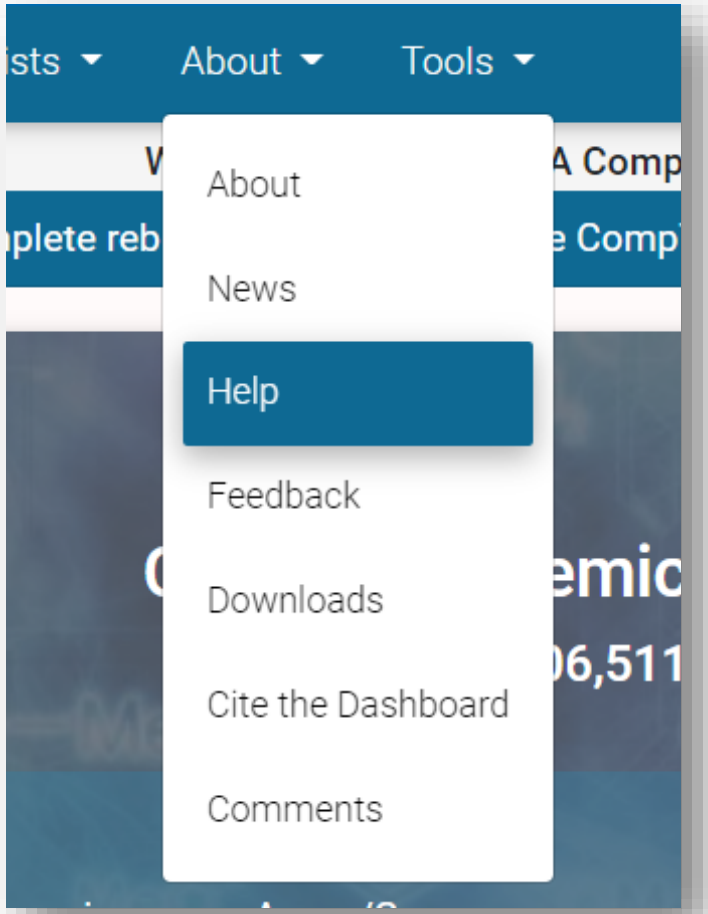
Performance Improvement

- The new architecture brings significant performance enhancements *especially* for list loading and batch searching
- List Loading: 5000 chemicals: 7secs vs 21secs

- Batch Search: 5000 chemicals: 2.5 secs vs 81 secs!
- Search limitation lifted from 5000 to 10,000 inputs



New Online Help



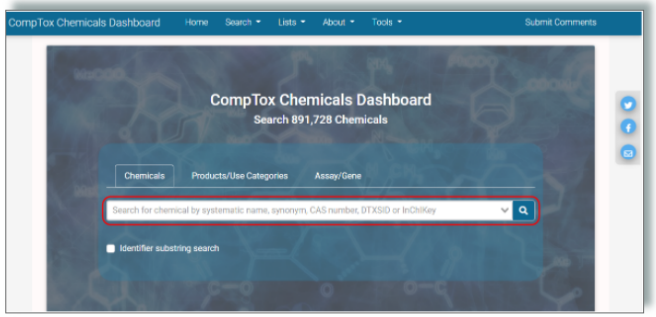
CCD Help Pages

Searching CCD

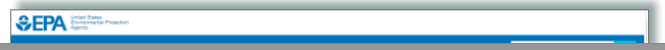
For information about the CCD Batch Search tool, see Batch Search.

Simple search

Simple (single chemical) searches can be done from either the Dashboard homepage, or from the search box present at the top right of most Dashboard pages. For chemicals, simple searches are based on preferred name, synonym, CASRN, DSSTOX substance identifier (DTXSID), InChIKey, or IUPAC name. From the homepage, there are also tabs above the search box to search by product use category or assay / gene. Product use and assay / gene can only be searched from the homepage.

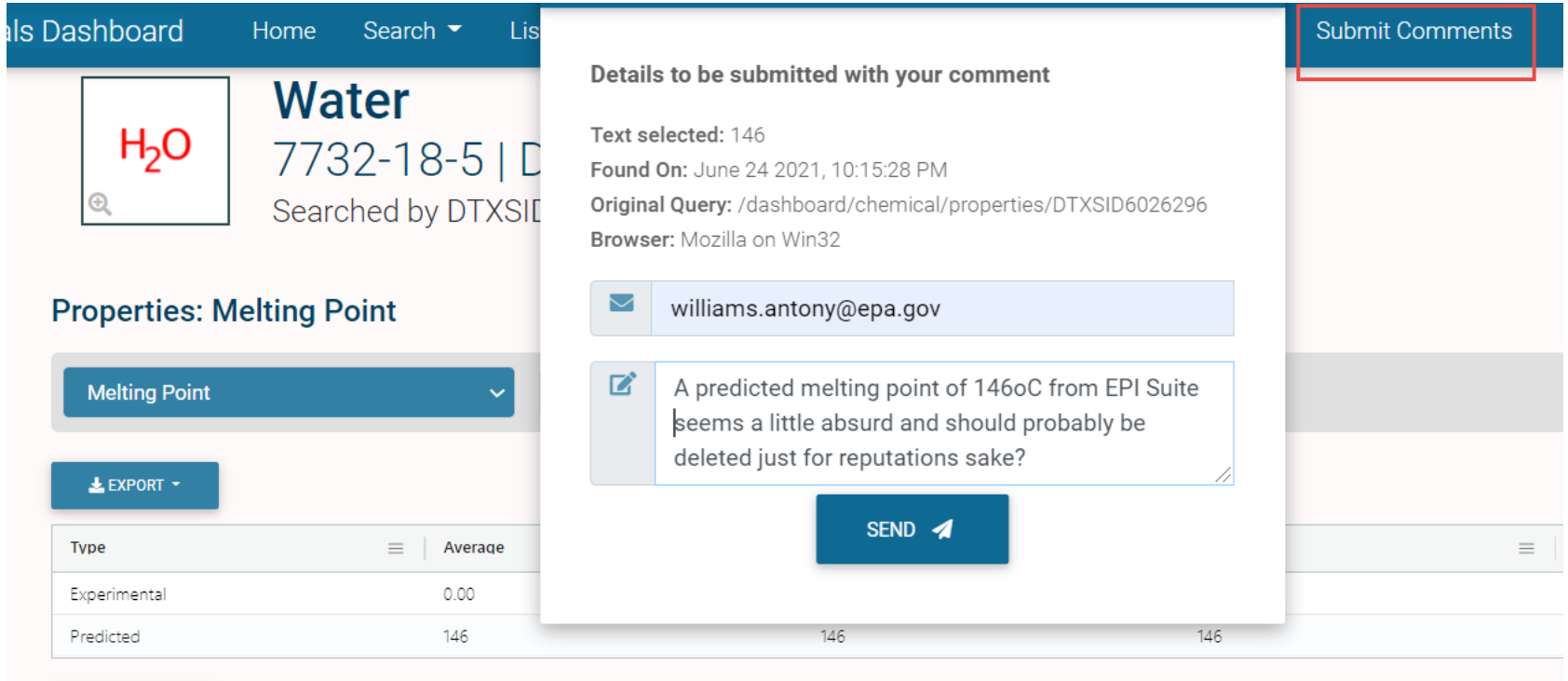


CompTox Chemicals Dashboard home page, https://ccte-ccd.epa.gov, with search box marked in red. Note tabs for product use category and assay / gene above the search box.



How to report comments and bugs

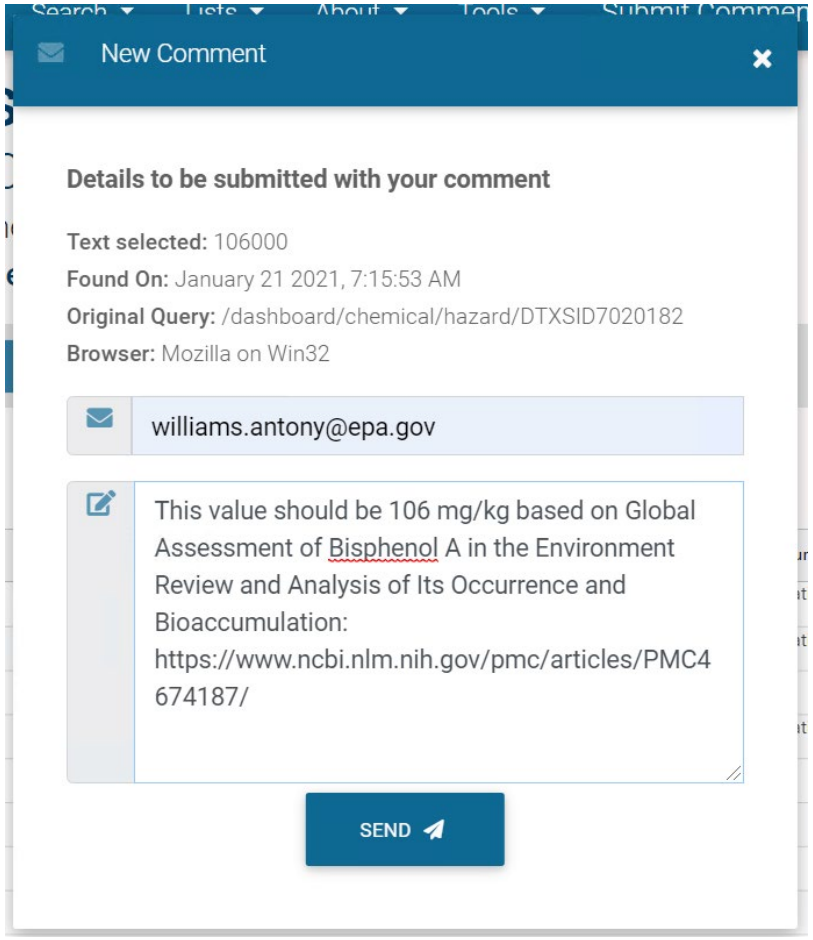
- Please note that Submit Comments is how we want feedback for CHEMICAL LEVEL detail. *Select* relevant text and submit.
- All comments will go directly into Jira for tracking and metrics



Highlight text and describe issue

- Highlight any part of the screen and submit comments will capture the context, URL, date and time etc.

Subtype	Risk assessment	Value	Units	Study Type
Short-term Criti...	short-term	500	mg/m3	-
Short-term Negl...	short-term	15	mg/m3	-
Long-Term, 5L/...	chronic	7	mg/L	-
Short-term Mar...	short-term	100	mg/m3	-
Soil Negligible S...	chronic	106000	mg/kg	-
-	chronic	0.05	mg/k...	-



Comments are all viewable

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

Comments

EXPORT

Chemical Comments

Chemical Name	Structure	DTXSID	Date Submitted	Comment	Status
(E,E)-Propyl 2,4-hexadienoate		DTXSID80883111	January 21, 2022	You seem to have the name 2,4-Hexadienoic acid, propyl ester, (2E,4E)- 2,4-Hexadienoic acid, propyl ester, (2E,4E)- on file twice as a synonym !! The name (E,E)-Propyl 2,4-hexadienoate is a bad one, stereo belongs with the acid end, not the ester/alcohol end ?? I would remove it ! You could add FEMA-4614 UNII-1579567HXI PubChem CID 5368950 MFCD00457385 Barrie	Resolved
Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester		DTXSID2060670	January 21, 2022	Consider adding Ethyl vanillate as a common synonym. See for example: https://www.sigmaaldrich.com/US/en/product/aldrich/s459267	Resolved
2-bromoallyl 2,4,6-tribromophenyl ethe		DTXSID00904130	January 21, 2022	Should be "ether", not "ethe"	Resolved
2,4-Difluoro-3-(1,1,1,2,3,3,3-heptafluoropropan-2-yl)azete		DTXSID90804377	January 20, 2022	https://comptox.epa.gov/dashboard/calculation-details?model_id=22&search=804377 This link is not loading the page	

Rows: 885

Work in Progress

- Data updates in preparation – >1.2M chemicals release next

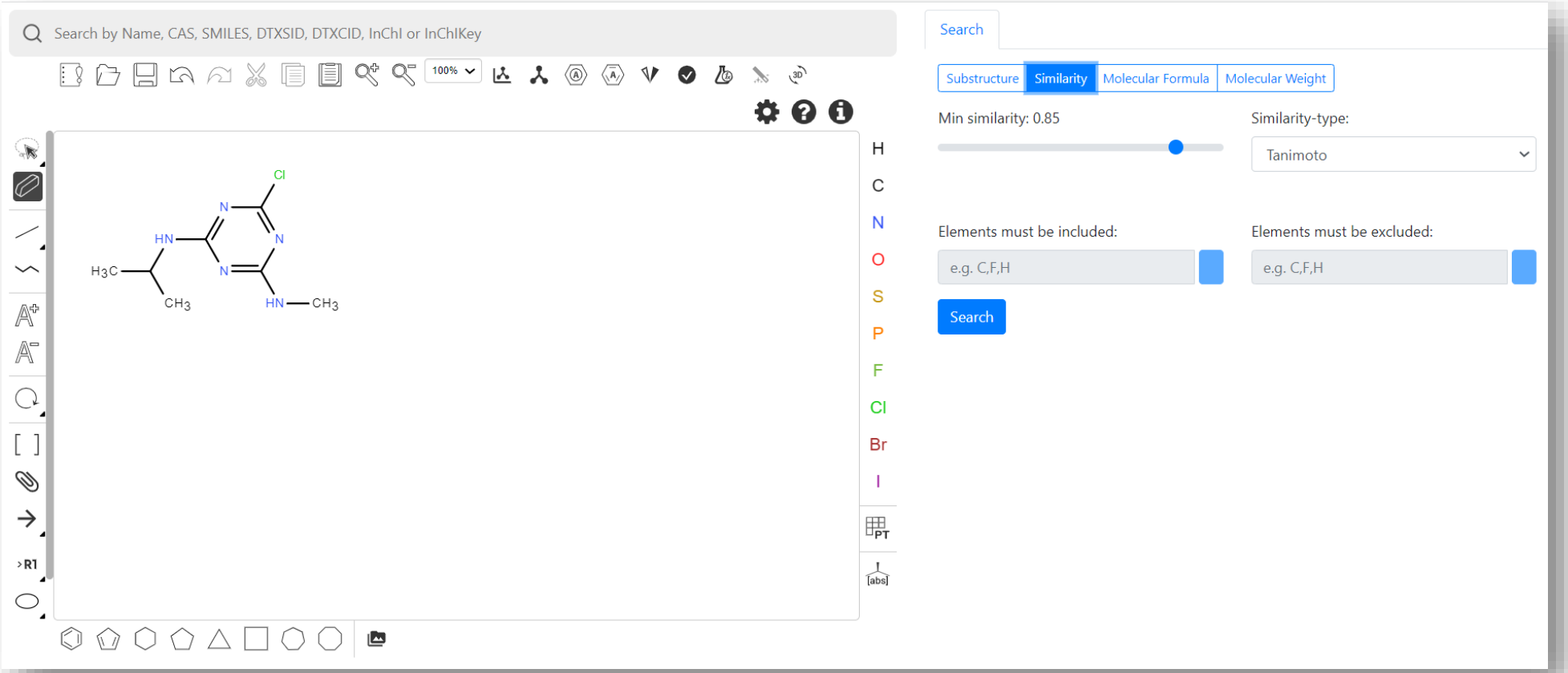
CAS Common Chemistry™ expands collection of publicly available chemical information

COLUMBUS, Ohio, March 17, 2021 — CAS, a division of the American Chemical Society (ACS) that specializes in scientific information solutions, has expanded the CAS Common Chemistry resource. To strengthen the accuracy of publicly available scientific information, CAS Common Chemistry now provides authoritative information on nearly 500,000 substances from CAS REGISTRY®. The collection represents substances commonly found in consumer products, on regulatory lists and as part of introductory chemistry curricula.

- Incorporation of *some* of the Common Chemistry™ data, specifically without structures
- Addition of structures is ongoing methodical curation
- Increased efforts mapping parents to metabolites and degradants and polymers to monomers
- 10s of new lists added and existing lists updated where possible

Work in Progress

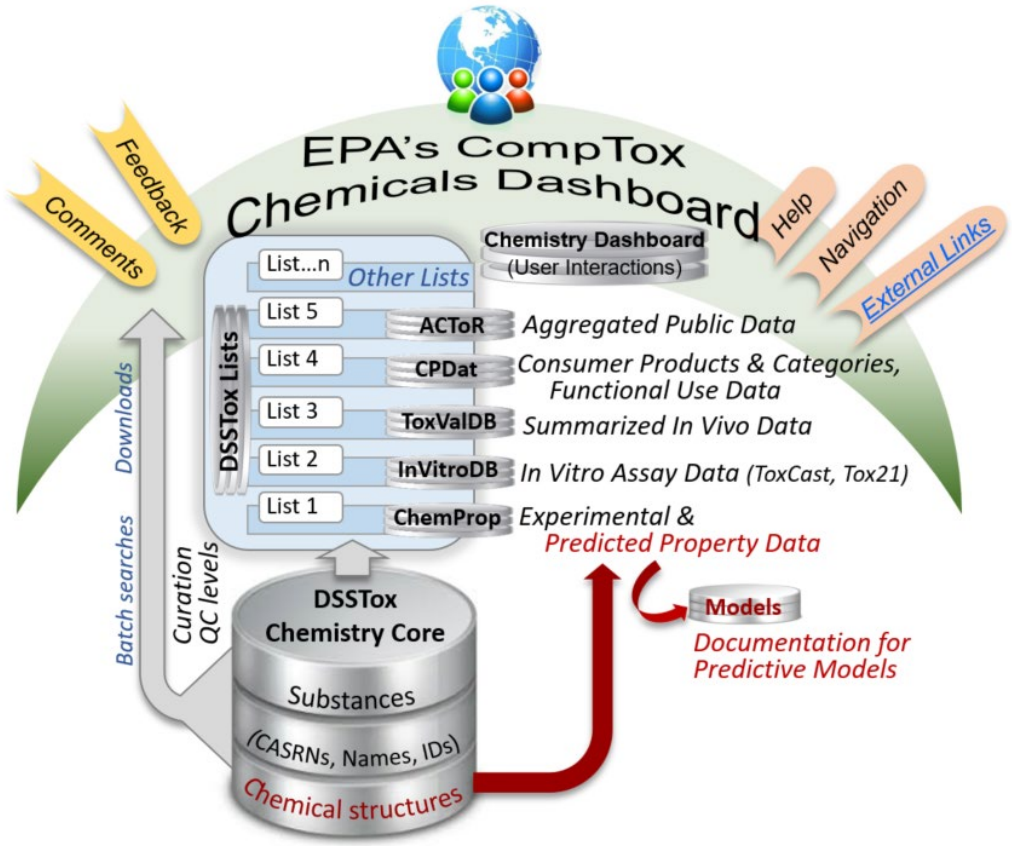
- Structure/substructure/similarity search module in development



Access the CCD-API

- We WANT you to use the underlying data
- API (application programming interface) servicing the Dashboard will go public this year
- Previous users of ACToR web services are encouraged to use the CompTox Chemicals Dashboard API (CCD-API) when available

Summary and Conclusion



- A much-needed rearchitecture has been successfully delivered
- This sets us up for more frequent data releases and is a foundation for new functionality
- Thank you for all of your feedback and support to this point

Acknowledgments

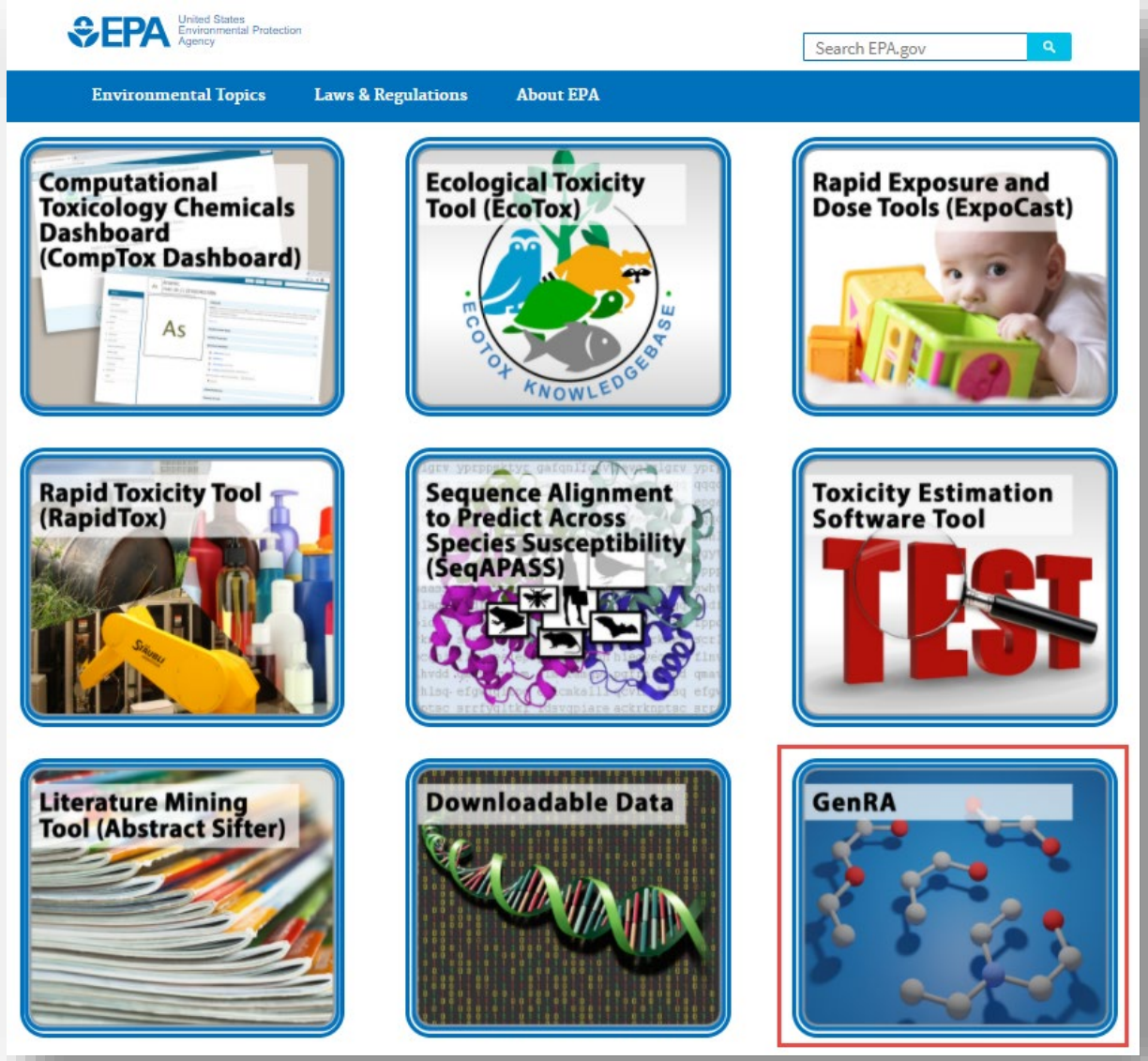
- Feedback and follow-up is welcomed! Your questions help
- Use the comments system to provide feedback
- The dashboard is based on the efforts of so many, those still here and those that have gone
- Thanks to all data providers, developers infrastructure staff, management staff for support and guidance

Transition of Product Owners

- AJW has been Dashboard product owner for 6 years & 11 releases
- A whiteboard idea went proof-of-concept to production application

- The NEW product owner is Dr Nisha Sipes. Assistant Center Director for Research Translations & Program/Regulatory Support for the US EPA Center for Computational Toxicology and Exposure (CCTE)
- Sipes.Nisha@epa.gov

New Tools in Development



- The center continues to work on new tools available via the portal https://comptox.epa.gov/
- The latest tool added is the new GenRA release…