

Primer on New Version of CompTox Chemicals Dashboard

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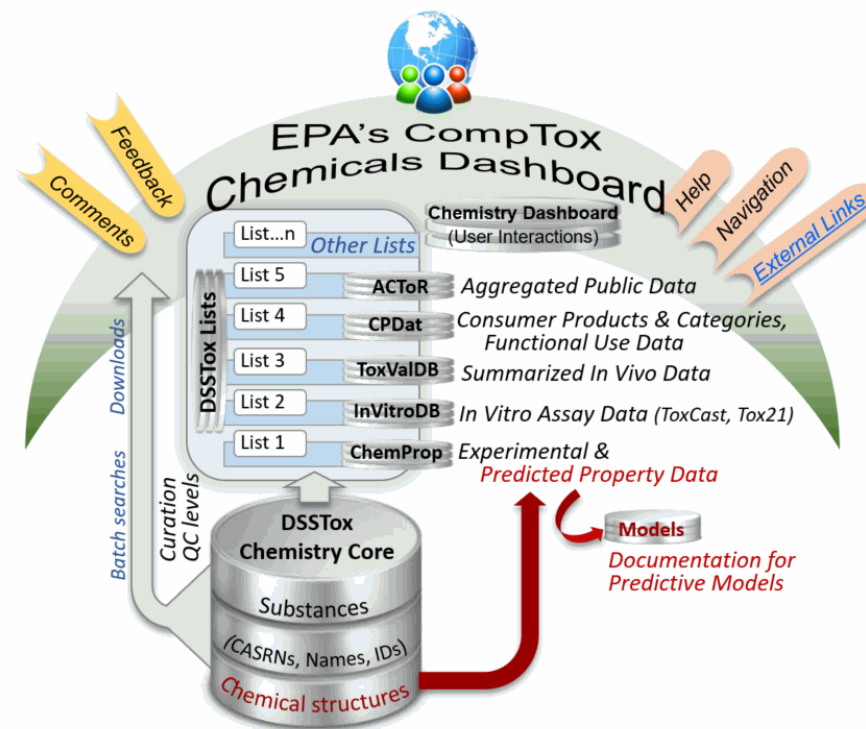
Center for Computational Toxicology and Exposure, US-EPA, RTP, NC

Communities of Practice, February 23rd 2022

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

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



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 ✉

Show more ▾

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

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Search text, DOI, authors, etc.



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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>

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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](#)



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

- 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



- VISION: Rearchitected 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

CompTox Chemicals Dashboard

HomeSearch ▾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

Important Dashboard Information

Check out the new CCD Dashboard [About Page](#) for details about the CCD Dashboard. [The CCD Users Manual](#) can help get you started.

Please log issues or questions using the Submit Comments function/button in the Menu bar.

Known Issues

1. Browser Cache: In order to properly load the new Comptox Chemical Dashboard and data, please clear the browser cache. We are observing issues caused by browser cache. Refer to the specific instructions on how to clear the cache for the various browsers.
2. Chemical Lists:
 1. Issue: Some hyperlinks for the list acronyms (e.g. toxcast_phasel, etc.) in the chemical list description are not functional i.e. all chemicals in the list are not displayed.
 2. Workaround: To select a particular list in the chemical list, perform the following steps:
 - Select Chemical Lists from the Comptox Dashboard home page
 - Enter the list acronym in the filter box below the "List Acronym" header
 - Select the list to see all of the chemicals in that list
3. Chemical Result Sets:
 1. Issue: Anywhere within the Comptox Chemicals Dashboard that displays a list of chemicals, either from a user entered search or preconfigured lists linked from a searched chemical details. The sort function on the upper toolbar does not always work.
 2. Workaround: The initial view of all these result sets is the Ag-grid view. Use the column header sort function to get your desired sort:
 - Click on the header of the column you desire to sort on.
 - Once you click on the header it will show an arrow icon pointing up for an ascending order sort or down for descending order sort.
 - Clicking on the column header multiple times will cycle through ascending, descending, and then removing the sort order.

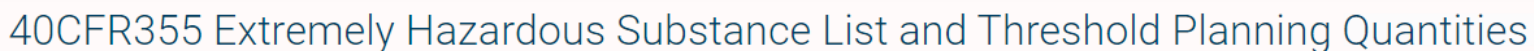
- On-click informational icon gives latest important information

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, HHTK)	Factotum 9/11/202 SEEM3 HHTK	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/hhtk/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

<http://ccte-cdd.epa.gov/dashboard/chemical-lists/40CFR355>



Start typing to search.

☐ Identifier substring search

List Details

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

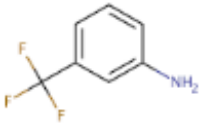
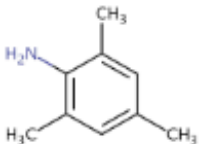
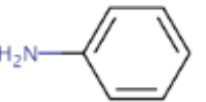
Find all chemicals with N2 in formula

Showing 47 of 353 chemicals

CASRN	QC Level	#ToxCast Active	%ToxCast Active	#CPDat	#Sources	#PubChem	#PubMed	Mono. Mass	Mol. Formula
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text" value="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...

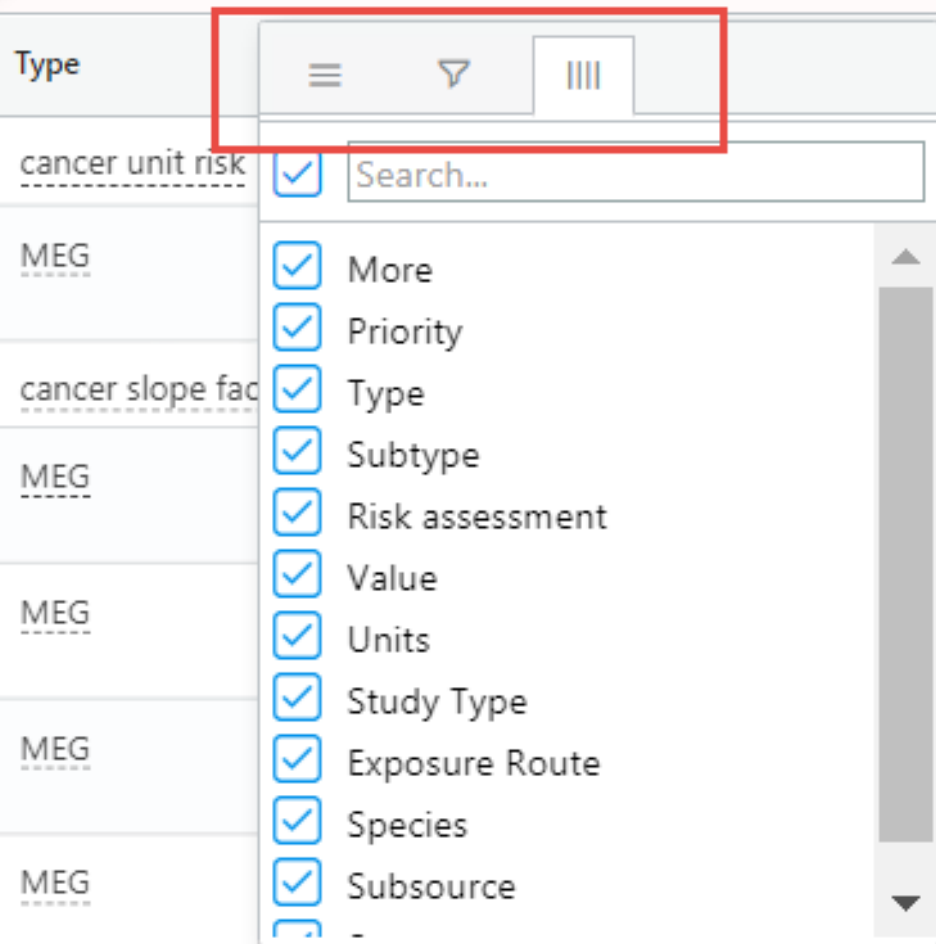
Find “aniline” in the names

Substructure searching is better

<input type="checkbox"/> Structure	DTXSID	Preferred Name ▼
	<input type="text"/>	<input type="text" value="aniline"/>
<input type="checkbox"/> 	DTXSID9024512	<u>3-(Trifluoromethyl)aniline</u>
<input type="checkbox"/> 	DTXSID5043847	<u>2,4,6-Trimethylaniline</u>
<input type="checkbox"/> 	DTXSID8020090	<u>Aniline</u>

Capabilities to switch columns on/off

- Table functionality for selecting columns for view is built in



Type		Value
cancer unit risk	<input checked="" type="checkbox"/>	0.0097
MEG	<input checked="" type="checkbox"/>	0.007
cancer slope fac	<input checked="" type="checkbox"/>	0.34
MEG	<input checked="" type="checkbox"/>	0.245
MEG	<input checked="" type="checkbox"/>	0.0494
MEG	<input checked="" type="checkbox"/>	2
MEG	<input checked="" type="checkbox"/>	0.00233
cancer slope factor	-	0.34

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

EXPORT

More	Priority	Type		
	7	LOAEL		
	7	LOEL		
	7	LOAEL		
	7	LOAEL		
	7	LOEL		repeat dose
	7	LOEL	BPA	short-term
	7	LOAEL	-	repeat dose
	7	LOAEL	Repeated dose toxicity: oral	repeat dose
	7	LOEC	-	chronic
	7	LOAEL	-	repeat dose
	6	LOAEL	-	chronic
	4	LOAEL	-	developmental neurotoxicity
	4	LOAEL	-	subchronic
	4	LOAEL	-	reproductive
			-	developmental

Not contains

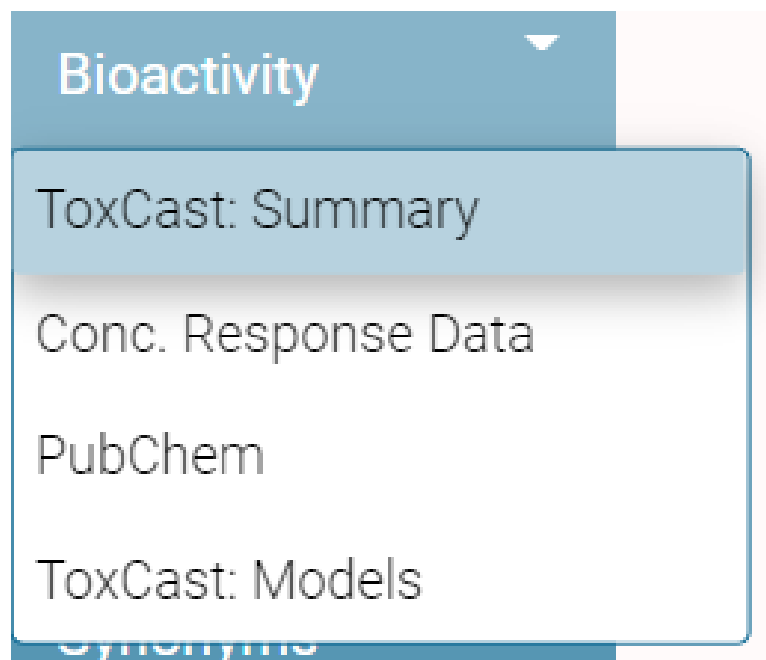
EC50

AND OR

Contains

LO

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





United States
Environmental Protection
Agency

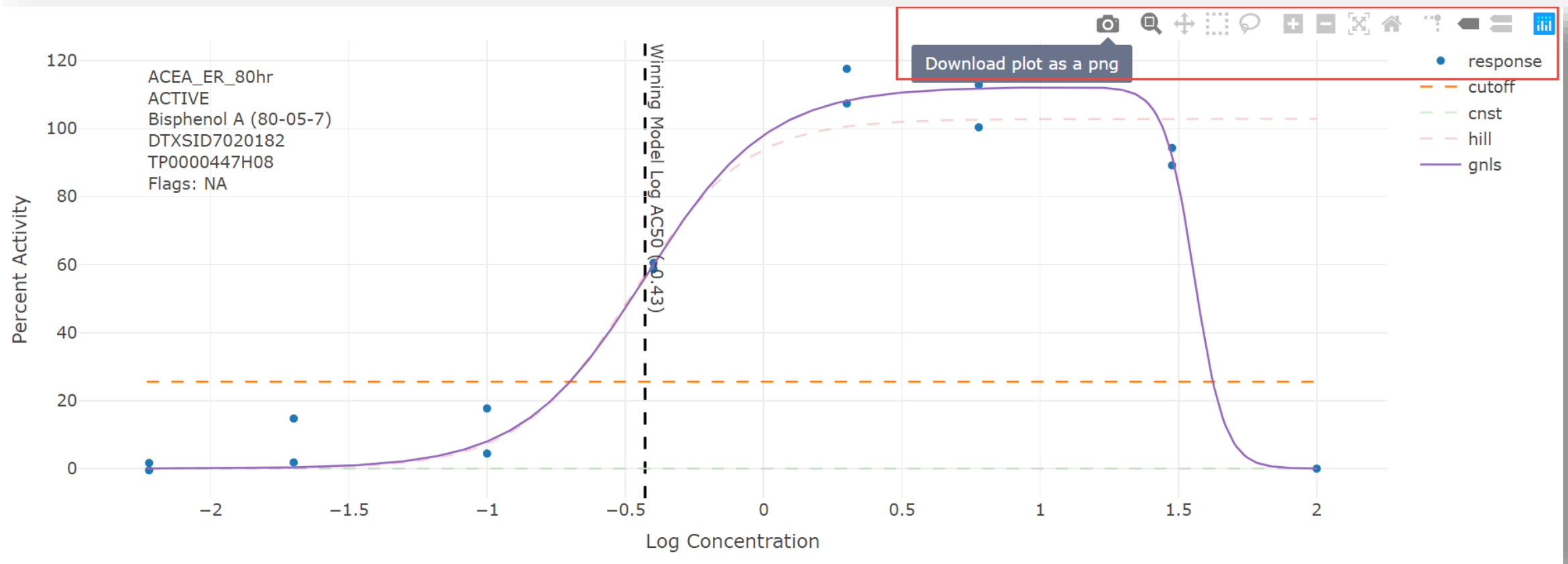
- ## Concentration Response Data

EXPORT ▾

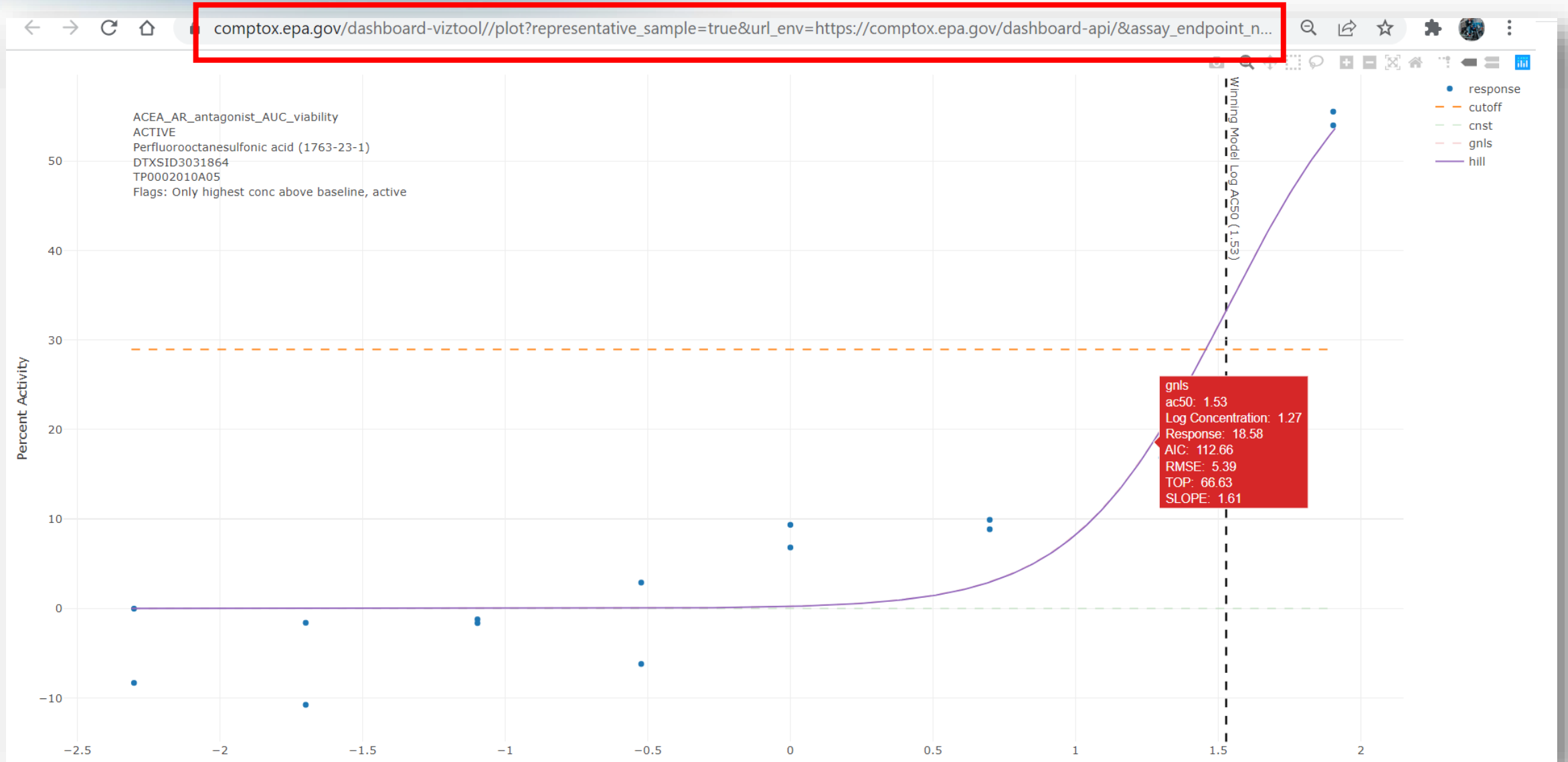
<input type="checkbox"/>	Name ↑	Description	Endpoint Name	Active	Det...	Rep...	All P...	Gene	Intended Target	Cell Line	Cell For...
<input type="checkbox"/>											
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive				AR	steroidal	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active				null	cytotoxicity	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active				AR	steroidal	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active				null	cytotoxicity	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_80hr	Active				ESR1	steroidal	breast	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_AUC_viability	Inactive				null	cytotoxicity	breast	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_dn	Inactive				null	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_up	Inactive				null	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_dn	Inactive				null	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_up	Inactive				null	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_dn	Inactive				null	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_up	Inactive				null	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_dn	Inactive				null	cytotoxicity	liver	cell line
<input type="checkbox"/>	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

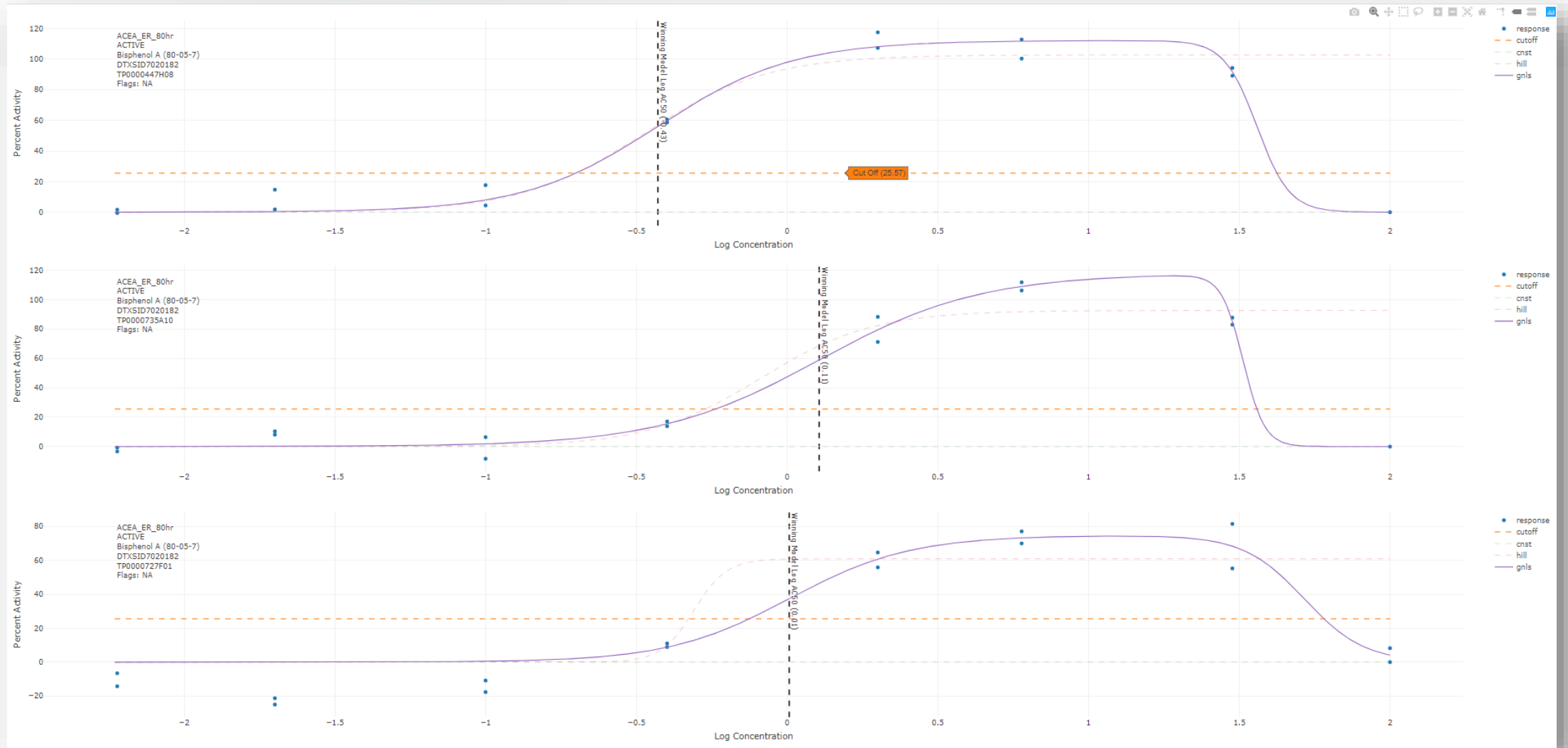


Direct URL access – useful for referencing in publications



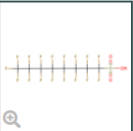
Multiple plots available via URL

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

 **Perfluorooctanesulfonic acid**
1763-23-1 | DTXSID3031864
Searched by DTXSID3031864.

Concentration Response Data ⓘ


Analytical Data on Tox21 Browser  



<input type="checkbox"/>	Name ↑	Description	Endpoint Name	Active	Details
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive	
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active	
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active	
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active	

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

tripod.nih.gov/tox21/search?q=DTXSID3031864



Home / Tox21 Samples

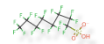
QC Grade T0

☐ **U** 1

QC Grade T4

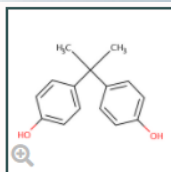
☐ **U** 1

Query: DTXSID3031864

Structure	Tox21 ID	Name	QC Grade T0	QC Grade T4
	Tox21_400083	PFOS	U Unknown/Inconclusive	U Unknown/Inconclusive

Molecular Weight

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
- NIH 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 OEHHHA
- 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 NIST Antoine Constants
- NIST NIST IR Spectrum
- NIST NIST Kovats Index values
- NIST 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... ↓↑	<input type="checkbox"/>	PubMe...	Y... ↓↑	Title ↓↑	≡	Authors ↓↑	≡	Journal ↓↑	≡	Rev ↓↑	DOI ↓↑
							▽		▽		▽		
2	4	6	<input type="checkbox"/>	34147626	2021	Modulation of Folliculogenesis in Adult Laying ...		Eldefrawy; Xu; Pusch; Karkoura; Alsafy; Elgendy; ...		Reproductive toxicology (Elmsford, N.Y.)			10.1016/j.repr...
0	9	9	<input type="checkbox"/>	34146661	2021	Effects of bisphenols on Blood-Testis Barrier pro...		Peña-Corona; Vásquez Aguirre; Vargas; Juárez; ...		Reproductive toxicology (Elmsford, N.Y.)		✓	10.1016/j.repr...
3	2	5	<input type="checkbox"/>	33802611	2021	Characterization of Estrogenic Activity and Site-...		Chioccarelli; Migliaccio; Suglia; Manfredola; Porr...		International journal of molecular sciences			10.3390/ijms2
0	2	2	<input type="checkbox"/>	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	<input type="checkbox"/>	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	<input type="checkbox"/>	33516155	2021	Update on the Health Effects of Bisphenol A: O...		Vom Saal; Vandenberg		Endocrinology			10.1210/endoc
0	2	2	<input type="checkbox"/>	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	<input type="checkbox"/>	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	<input type="checkbox"/>	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	<input type="checkbox"/>	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	<input type="checkbox"/>	31952086	2020	Bisphenol A exposure is involved in the develop...		Murachio; Araújo; Bortolotto; de Freitas Couto;		Food and chemical toxicology : an international			10.1016/j.fct.20

Abstract Sifter as a TOOL

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... ↓↑	<input type="checkbox"/> PubM...	Y... ↓↑	Title ↓↑	Authors ↓↑	Journal ↓↑	Rev ↓↑	DOI ↓↑
			<input type="checkbox"/>						
0	0	3223	<input type="checkbox"/>	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	<input type="checkbox"/>	34124416	2021	Using Chemical Structure Information to De...	Pradeep; Patlewicz; Pearce; Wambaugh; We...	Computational toxicology (Amsterdam, Net...	10.1016/j.com
0	0	147	<input type="checkbox"/>	34101097	2021	Correction to: Notch regulates vascular coll...	Gross; Webb; Peterlin; Durrant; Judson; Raz...	Angiogenesis	10.1007/s104
0	0	2115	<input type="checkbox"/>	34017928	2021	Structure-based QSAR Models to Predict R...	Pradeep; Friedman; Judson	Computational toxicology (Amsterdam, Net...	10.1016/j.com
0	0	1736	<input type="checkbox"/>	33855360	2021	Machine Learning Models for Predicting the	Gao; Wu; Bai; Fan; Ding; Li; Zhang; Zhang...	Angiogenesis	10.1007/s104

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

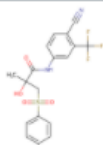
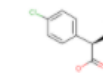
or

 CHOOSE EXPORT OPTIONS

45% loaded

45 Chemicals Found from 110 Input(s)

REPLACE IDENTIFIERS WITH SELECTED CHEMICALS

<input type="checkbox"/>	Structure	DTXSID	Preferred Name	CASRN	Mono. Mass	Mol. Formula
<input type="checkbox"/>		DTXSID2022678	Bicalutamide	90357-06-5	430.061041	C ₁₈ H ₁₄ F ₄ N ₂ O ₄ S
<input type="checkbox"/>		DTXSID3020621	(R,R)-Fenvalerate	67614-33-9	419.128821	C ₂₅ H ₂₂ ClNO ₃

Batch Search – *List Filtering*

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

<input type="checkbox"/> Title	Description
<input type="checkbox"/> 40CFR116.4	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
<input type="checkbox"/> 40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
<input type="checkbox"/> ACSREAG	LIST: ACS Reagent Chemicals
<input type="checkbox"/> AEGLVALUES	AEGLS: Acute Exposure Guideline Levels
<input type="checkbox"/> ALGALTOX	LIST: Algal Toxins
<input type="checkbox"/> ALLSURFACTANTS	CATEGORY: Surfactants
<input type="checkbox"/> AMINOACIDS	CATEGORY: Amino acids
<input type="checkbox"/> AMPHIBOLES	Amphibole minerals
<input type="checkbox"/> ANTIBIOTICS	CATEGORY(PHARMACEUTICALS): Antibiotics
<input type="checkbox"/> ANTIMICROBIALS	CATEGORY(WIKILIST)ANTIMICROBIALS: Antimicrobials from Wikipedia
<input type="checkbox"/> AOPSTRESSORS	List of Adverse Outcome Pathway Stressors
<input type="checkbox"/> APCRARETRO	LIST: APCRA Chemicals for Retrospective Analysis
<input type="checkbox"/> 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		
<input type="checkbox"/> Title ▾		Description ▾
<input type="text" value="PFAS"/>	▾	<input type="text" value="Water"/>
<input type="checkbox"/> EPAPFASDW ↗		PFAS EPA: New EPA Method Drinking Water
<input type="checkbox"/> EPAPFASDW537 ↗		PFAS EPA WATER: Existing EPA DW Method 537.1
<input type="checkbox"/> EPAPFASDWTREAT ↗		PFAS EPA WATER: Drinking Water Treatment Technology
<input type="checkbox"/> EPAPFASNONDW ↗		PFAS EPA: New EPA Method Non-Drinking Water
<input type="checkbox"/> EPAPFASVALDW ↗		PFAS EPA WATER: PFAS with Validated EPA Drinking Water Methods
<input type="checkbox"/> 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	EPAPFASNNDW	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-dioxahexanoic 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

- 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

Chemical Identifiers

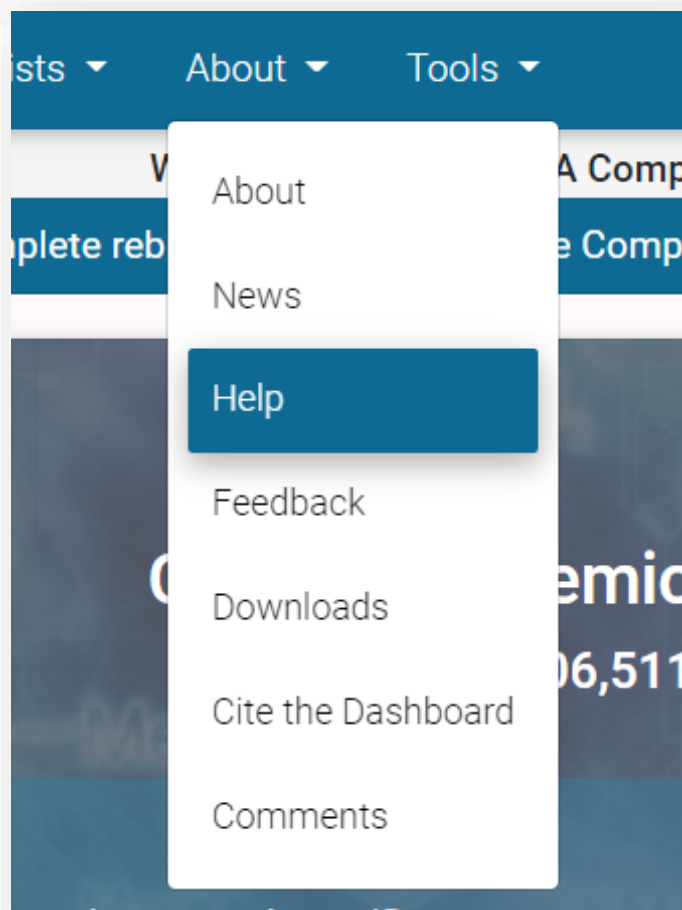
- ☒ DTXSID
- ☒ Chemical Name
- ☒ DTXCID
- ☒ CAS-RN
- ☒ InChIKey
- ☒ IUPAC Name

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



CCD Help Pages Searching CCD

Introduction

Common Navigational
Tips

Searching CCD

Simple search

Advanced Search

Advanced: Mass
Search

Advanced:
Molecular Formula
Search

Advanced:
Generate
Molecular
Formula(e)

Batch Search

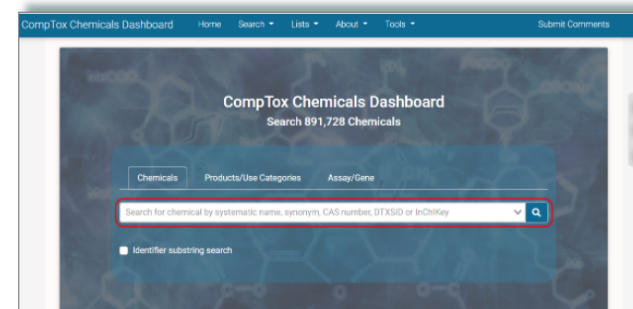
Details

Executive Summary

For information about the CCD Batch Search tool, see [Batch Search](#).

Simple search

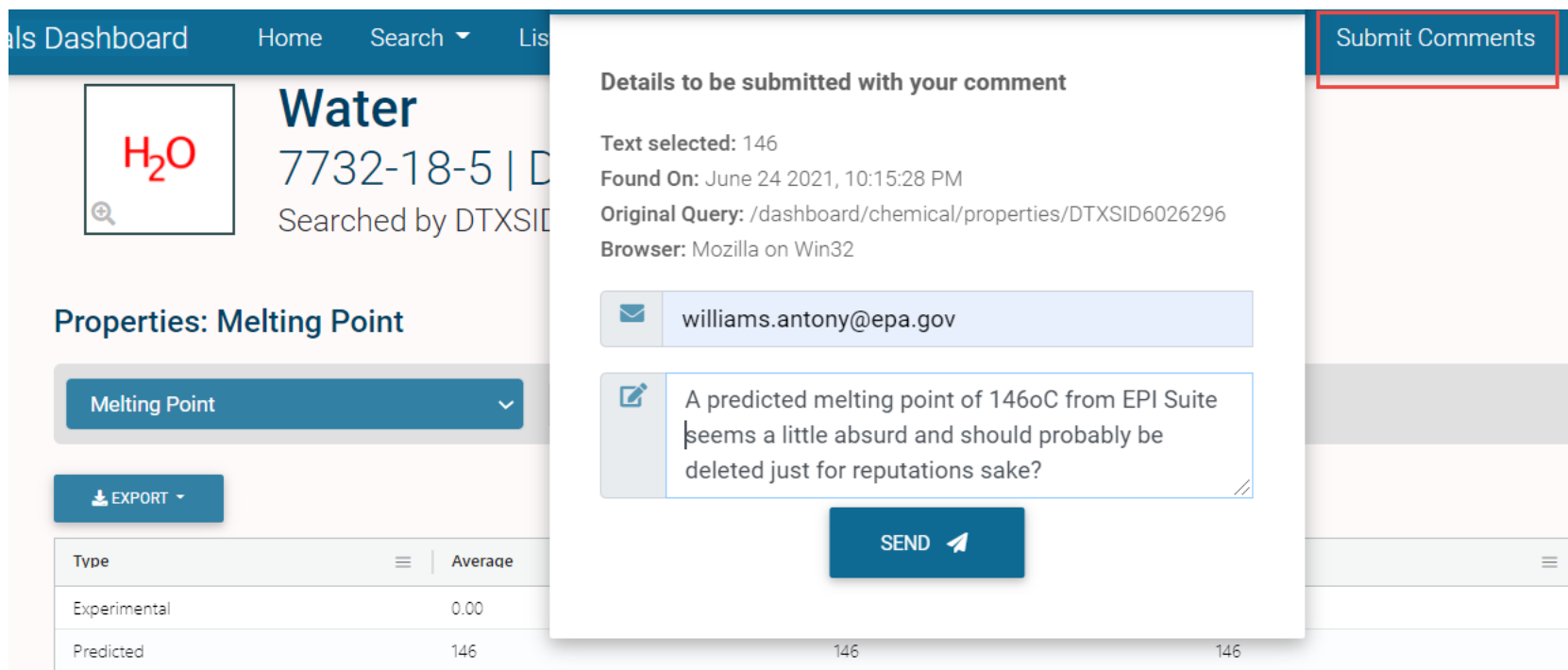
Simple (single chemical) searches can be done from either the [Dashboard homepage](#), or from the search box present at the top right of most Dashboard pages. For chemicals, simple searches are based on preferred name, synonym, CASRN, DSSTOX substance identifier (DTXSID), InChIKey, or IUPAC name. From 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



The screenshot shows the EPA Chemical Dashboard interface. A modal window is open for submitting a comment on the 'Water' chemical page. The modal displays details about the selected text and the user's email address. The comment text is: 'A predicted melting point of 146oC from EPI Suite seems a little absurd and should probably be deleted just for reputations sake?'. The 'Submit Comments' button is highlighted with a red box in the top right corner of the dashboard.

Details to be submitted with your comment

Text selected: 146
Found On: June 24 2021, 10:15:28 PM
Original Query: /dashboard/chemical/properties/DTXSID6026296
Browser: Mozilla on Win32

williams.antony@epa.gov

A predicted melting point of 146oC from EPI Suite seems a little absurd and should probably be deleted just for reputations sake?

SEND

Submit Comments

Water
7732-18-5 | D
Searched by DTXSID

Properties: Melting Point

Melting Point

EXPORT

Type	Average
Experimental	0.00
Predicted	146

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...	-
-	chronic			-

Search ▾ Lists ▾ About ▾ Tools ▾ Submit Comment

New Comment

Details to be submitted with your comment

Text selected: 106000
Found On: January 21 2021, 7:15:53 AM
Original Query: /dashboard/chemical/hazard/DTXSID7020182
Browser: Mozilla on Win32

williams.antony@epa.gov

This value should be 106 mg/kg based on Global Assessment of Bisphenol A in the Environment Review and Analysis of Its Occurrence and Bioaccumulation:
<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4674187/>

SEND ↗

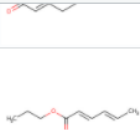
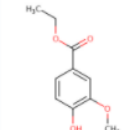
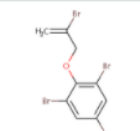
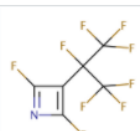
Comments are all viewable

<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 ether		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

- 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.

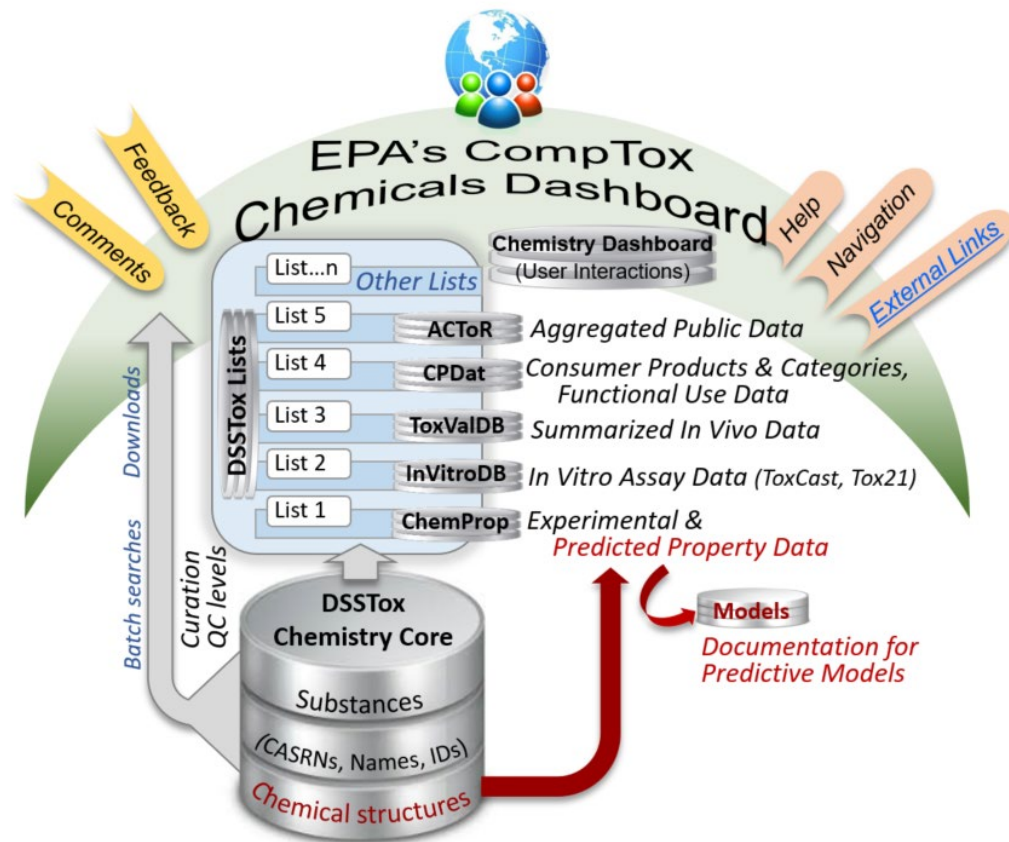
- Incorporation of *some* of the Common Chemistry™ data, specifically without structures
- Addition of structures is ongoing methodical curation
- Increased efforts mapping parents to metabolites and degradants and polymers to monomers
- 10s of new lists added and existing lists updated where possible

- Structure/substructure/similarity search module in development

The screenshot displays a web-based chemical structure search interface. At the top, a search bar allows queries by Name, CAS, SMILES, DTXSID, DTXCID, InChI, or InChIKey. Below the search bar is a toolbar with icons for file operations (open, save, copy, paste, delete), zooming (100%), and other functions. The main workspace shows a chemical structure of 1-(4-chlorophenyl)-2-methyl-5-methylamino-1H-imidazole. The structure is rendered with atoms color-coded: Carbon (grey), Hydrogen (white), Nitrogen (blue), Oxygen (red), Sulfur (yellow), Phosphorus (orange), Fluorine (green), Chlorine (dark green), Bromine (brown), and Iodine (purple). To the right of the workspace is a sidebar with a vertical list of elements (H, C, N, O, S, P, F, Cl, Br, I) and a 'PT' (Point) button. Below the workspace is a row of geometric shapes (hexagon, pentagon, square, triangle, circle, etc.). On the right side of the interface, there is a 'Search' panel. It includes tabs for 'Substructure', 'Similarity' (selected), 'Molecular Formula', and 'Molecular Weight'. The 'Similarity' section has a 'Min similarity' slider set to 0.85 and a 'Similarity-type' dropdown menu set to 'Tanimoto'. Below these are two input fields for 'Elements must be included' and 'Elements must be excluded', both containing the example 'e.g. C,F,H'. A 'Search' button is located at the bottom of this panel.

- 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 screenshot shows the EPA Comptox Dashboard homepage. At the top is the EPA logo and a search bar. Below the navigation bar are nine tool tiles arranged in a 3x3 grid:

- Computational Toxicology Chemicals Dashboard (CompTox Dashboard)**: Shows a screenshot of the dashboard interface with 'As' (Arsenic) selected.
- Ecological Toxicity Tool (EcoTox)**: Features a logo with a bird, a fish, and a plant, with the text 'ECOTOX KNOWLEDGEBASE'.
- Rapid Exposure and Dose Tools (ExpoCast)**: Shows a baby playing with colorful blocks.
- Rapid Toxicity Tool (RapidTox)**: Shows a collection of household cleaning products.
- Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)**: Shows a 3D protein structure.
- Toxicity Estimation Software Tool (TEST)**: Shows the word 'TEST' in large red letters with a magnifying glass over it.
- Literature Mining Tool (Abstract Sifter)**: Shows a stack of papers with colorful tabs.
- Downloadable Data**: Shows a DNA double helix structure.
- GenRA**: Shows a 3D molecular model of a chemical structure.

- 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...

