

## An Introduction and Demo of the CompTox Chemicals Dashboard

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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

### **Recommended Reading**





#### **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 <sup>a</sup> A 🖾, Jason C. Lambert <sup>a</sup>, Kris Thayer <sup>b</sup>, Jean-Lou C.M. Dorne <sup>c</sup>



- Develop a "first-stop-shop" for environmental chemical data to support EPA and partner decision making:
  - Centralized location for relevant chemical data
  - Chemistry, exposure, hazard and dosimetry
  - Combination of existing data and predictive models
  - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

#### CompTox Chemicals Dashboard



#### 883k Chemical Substances

Separation United States Environmental Protection Ho Agency	ome Advanced Search Batch Search Lists 🛩 Predictions Downloads	Share 🔻
UNITED STATED	CompTox Chemicals Dashboard	Í
AGENCY AGENCY	Chemicals     Product/Use Categories     Assay/Gene	
	Q Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey	
	Identifier substring search See what people are saying, read the dashboard comments! Cite the Dashboard Publication click here	
	Latest News	
	Read more news	
	10th Release of the CompTox Chemicals Dashboard Now Live July 12th 2020	
	July 21st, 2020 at 9:32:02 PM	
	The 10th release of the Dashboard is now live with >7000 additional substances added to the dataset, updates to Bioactivity Data (ToxCast/Tox21), updates to the ToxVal data (under the Hazard tab), a new Safety Tab integrating the Globally Harmonized System of Classification and Labeling of Chemicals (via PubChem), over thirty new lists and a number of bug fixes. Our next release is scheduled for late Spring/Early Summer 2021. and is presently in development. It will be a full re-architecting of the entire application. Watch this space for updates. The release addresses a number of minor bugs and includes a short list of additional functionality as described in the Release Notes here.	
	M <sup>ED STA</sup>	

#### **BASIC Search**



Chemic	als Product/Use Categories Assay/Gene
Q Benz	o(a)pyrene
<b>8</b> 80	Benzo(a)pyrene DTXSID2020139
-8-A-	Benzo(a)pyrene diolepoxide 1 DTXSID9036779
ý.	Benzo(a)pyrene- 7,8,9-triol,7,8,9,10-tetrahydro-, (7-alpha,8-beta,9-beta)- DTXSID00210066
3	Benzo(a)pyrene-1-methanol DTXSID40235374
ŝ	Benzo(a)pyrene-1,6-dione, 7-methyl- DTXSID70229645
~£	Benzo(a)pyrene-10-methanol DTXSID20235817
×¥	Benzo(a)pyrene-10-sulfonic acid, 7,8,9,10-tetrahydro-7,8,9-trihydroxy-, (7alpha,8beta,9beta DTXSID80154378
<del>}</del>	Benzo(a)pyrene-11,12-diol DTXSID70215609
춿	Benzo(a)pyrene-11,12-diol, 11,12-dihydro-, cis- DTXSID20214501

- Type ahead search using Names, synonyms and CASRNs
- Millions of identifiers
- Substring search

#### Search Results

Searched with 'Synonym Substring': Benzo(A)Pyrene

**183 chemicals** 

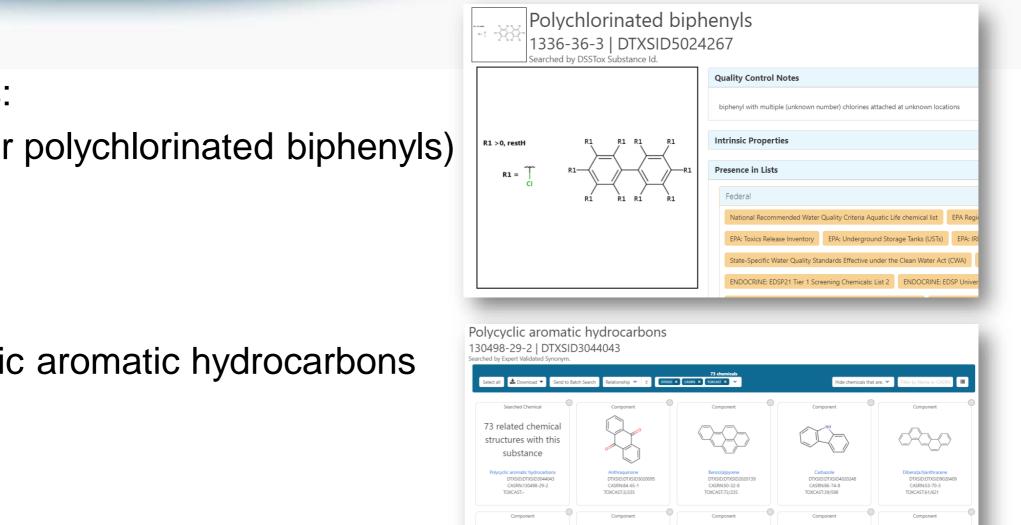
#### Search for classes of chemicals



Chemicals Product/Use Categories Assay/Gene Examples: "perfluoro" **Q** perfluoro Identifier substring search Search Results Searched with 'Synonym Substring': Perfluoro 2098 chemicals 📩 Download 🔻 DTXSID X CASRN X TOXCAST X ≣ Hide chemicals that are: 💙 Select all Send to Batch Search Substring ~ 0 related chemical structures with this substance N-Ethyl-N-(2-hydroxyethyl)perfluorooct... Perfluoro compounds, C5-18 2H-Perfluoro-2-propanol Perfluorooctanesulfonyl fluoride Perfluorotributylamine N-Methyl-N-(2-hydroxyethyl)perfluoroo... DTXSID:DTXSID1022134 DTXSID:DTXSID5027140 DTXSID:DTXSID0027141 DTXSID:DTXSID6027426 DTXSID:DTXSID7027831 DTXSID:DTXSID5029059 CASRN:920-66-1 CASRN:307-35-7 CASRN:311-89-7 CASRN:1691-99-2 CASRN:24448-09-7 CASRN:86508-42-1 TOXCAST:-TOXCAST:-TOXCAST:-TOXCAST:-TOXCAST:-TOXCAST:7/235 11111114 o=<u>s</u>-<u>-</u> 

### Search for classes of chemicals





- Examples:
- PCBs (or polychlorinated biphenyls)

Polycyclic aromatic hydrocarbons

#### Detailed Chemical Pages One more identifier – the DTXSID



	Benzo(a)pyrene	
	50-32-8   DTXSID2020139	
DETAILS	· · · · · · · · · · · · · · · · · · ·	ikipedia 👻
EXECUTIVE SUMMARY	Be	nzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C
PROPERTIES		12 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula C <sub>20</sub> H <sub>12</sub> is one of benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to
ENV. FATE/TRANSPORT		ad more
HAZARD		uality Control Notes
► SAFETY		
► ADME		trinsic Properties 👻
► EXPOSURE		Molecular Formula: C <sub>20</sub> H <sub>12</sub> Anol File Q Find All Chemicals
► BIOACTIVITY		Average Mass: 252.316 g/mol Idd Isotope Mass Distribution
SIMILAR COMPOUNDS		Monoisotopic Mass: 252.0939 g/mol
GENRA (BETA)	st	ructural Identifiers
RELATED SUBSTANCES		
SYNONYMS	Li	nked Substances
▶ LITERATURE	Pi	resence in Lists
LINKS		

 Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

#### Detailed Chemical Pages Easy Navigation

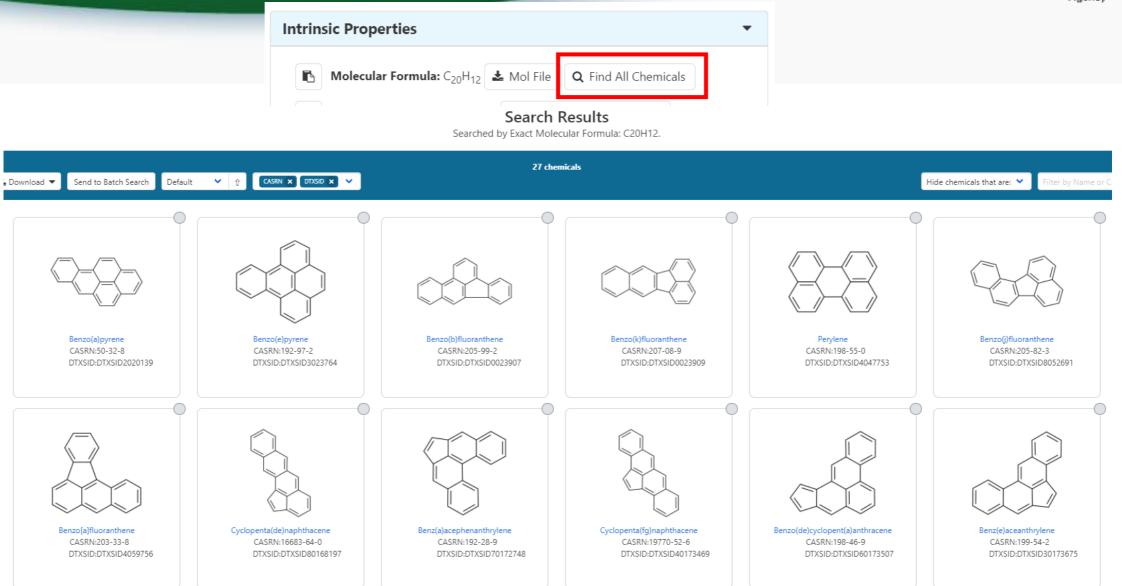


	Benzo(a)pyrene 50-32-8   DTXSID20201 Searched by DSSTox Substance Id.	39
DETAILS		Wikipedia
EXECUTIVE SUMMARY		Benzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C
PROPERTIES		(1,112 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula C <sub>20</sub> H <sub>12</sub> is one of the benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to
ENV. FATE/TRANSPORT		 Read more
HAZARD		Quality Control Notes
► SAFETY		
▶ ADME		Intrinsic Properties
► EXPOSURE		Molecular Formula: C <sub>20</sub> H <sub>12</sub> Mol File Q. Find All Chemicals
BIOACTIVITY		Average Mass: 252.316 g/mol Lul Isotope Mass Distribution
SIMILAR COMPOUNDS		Monoisotopic Mass: 252.0939 g/mol
GENRA (BETA)		Structural Identifiers
RELATED SUBSTANCES		
SYNONYMS		Linked Substances
► LITERATURE		Presence in Lists
LINKS		

 Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

### From the Chemical Details Page... all chemicals with same FORMULA





# How many chemicals are associated through LINKED SUBSTANCES?



- Atrazine, is a herbicide in MANY commercial products
- The dashboard has salt forms, isotopically labelled forms, multicomponent forms
- How do we identify what they are???



### Linked Substances – more interesting



- We map chemicals together
   using cheminformatics
   approaches
- Use desalting, destereo, split multicomponents etc to map chemicals together

McEachran et al. J Cheminform (2018) 10:45 https://doi.org/10.1186/s13321-018-0299-2

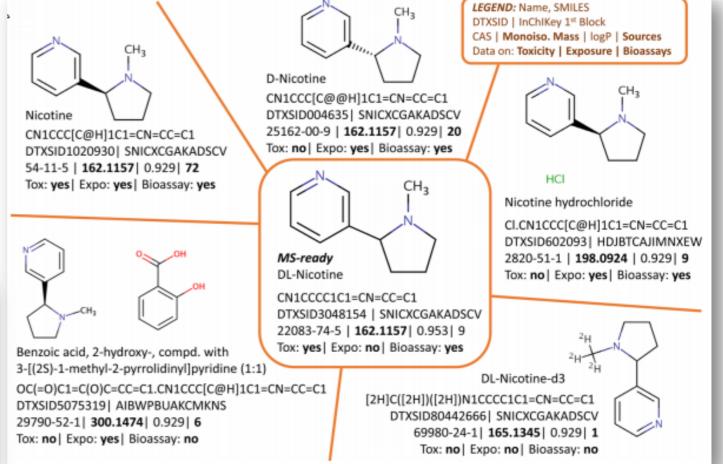
Journal of Cheminformatics

**Open Access** 

#### METHODOLOGY

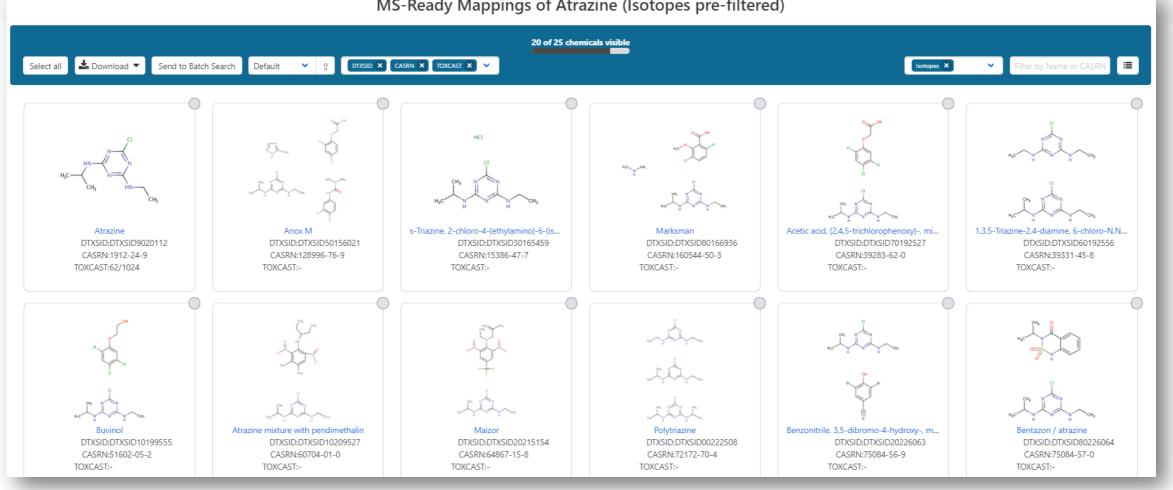
## "MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran<sup>1,2\*</sup>, Kamel Mansouri<sup>1,2,3</sup>, Chris Grulke<sup>2</sup>, Emma L. Schymanski<sup>4</sup>, Christoph Ruttkies<sup>5</sup> and Antony J. Williams<sup>2\*</sup>



#### **Atrazine Linked Substances**





MS-Ready Mappings of Atrazine (Isotopes pre-filtered)

#### **Record Information Quality Flags**



#### Record Information Citation: U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID7020182 (accessed Aug 20th, R 2018), Bisphenol A Bisphenol A Da Quality: 80-05-7 | DTXSID7020182 Searched by Approved Name. Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers Wikipedia Level 2: Expert curated, unique chemical identifiers using multiple sources Intrinsic Properties H<sub>3</sub>C Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem Structural Identifiers Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem Linked Substances Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source Presence in Lists Record Information Citation: U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID7020182 (accessed Aug 20th, 2018), Bisphenol A Data Quality: Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers Level 2: Expert curated, unique chemical identifiers using multiple sources Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem

Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem

Level 5: Programmatically curated from ACTOR or PubChem, unique chemical identifiers with low confidence, single public source

14

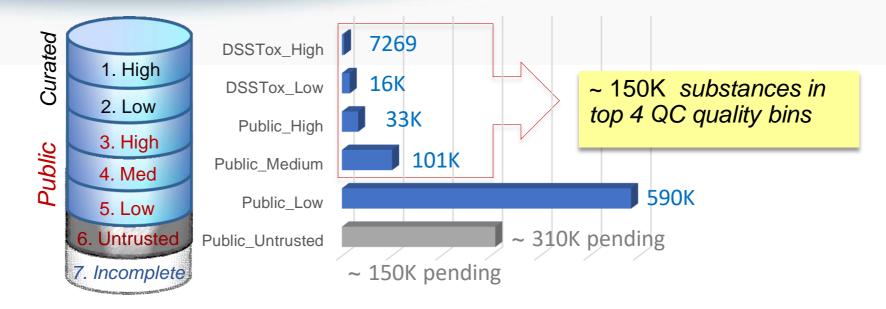
#### Underneath the Dashboard



View/Edit a Structure Se Single Record	arch Browse/Curate Export DSSTox Chemotypes Manage Records Chemical Lists	Manage Property Add Deleted Data Casrns
Preferred Name matched <b>null</b>	<u>□ ◁ ⊟ &gt; ⊂ × ロ ů € € € &lt; </u> # # @ @	
You are viewing the record associated with	Valid license cannot be found	it.pl
DTXSID80198757 CASRN: 62885-41-0		с
Q 4-Hydroxy-3-methox	2 L	N
C Hydroxy 5 metrics	[]	o
	+	s
	-	F
	П СН <sub>3</sub>	P
	→ OH CH <sub>3</sub>	CI Br
		1
		A
		$O_{\pm}$
	Calculate from Structure         Substance_ID:       DTXSID80198757         CAS:       62885-41-0         Name:       4-Hydroxy-3-methoxypyridine	Compound_ID: DTXCID40121248 Chemical Shown: Tested Chemical
	Substance Type: Single Compound ▼ QC Level: DSSTox_High ▼	Private Notes:
	Data Source: STN(DSSTox) ▼ CAS [50700-60-2] assigned by DSSTox to pyridin-one tautomer	Source of CAS-Compound: STN(DSSTox) Double Stereo: None Chiral Stereo: None
	QC Notes: form, which resolves to hydroxy form thru InChI	Chemical Form: Organic   Organic Form: Parent

### Distribution of curated data Now at >910k substances





OC I	Leve	s

DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem
Public_Untrusted	: Postulated, but found to have conflicts in public sources

### A little more about our data quality



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

Christopher M. Grulke<sup>a</sup>, Antony J. Williams<sup>a</sup>, Inthirany Thillanadarajah<sup>b</sup>, Ann M. Richard<sup>a,\*</sup>

<sup>a</sup> National Center for Computational Toxicology, Office of Research & Development, US Environmental Protection Agency, Mail Drop D143-02, Research Triangle Park, NC 27711, USA

<sup>b</sup> Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA





#### "Executive Summary"



**Executive Summarv** Quantitative Risk Assessment Values IRIS values available No PPRTV values REGIONAL SCREENING EPA RSL values available Class THQ Minimum RfD: 0.00030 mg/kg-day (chronic, IRIS, oral, 8) Minimum RfC: 0.0000020 mg/m3 (chronic, IRIS, inhalation, 8) GIABS (-IVIVE POD not calculated ABS (-) Quantitative Hazard Values MCL (ug/L) Minimum oral POD: 0.070 mg/kg-day (chronic, EFSA, oral, 5) Minimum inhalation POD: 0.0046 mg/m3 (chronic, IRIS, inhalation, 8) MCLbased.SSL (mg/kg) Lowest Observed Bioactivity Equivalent Level: AR cancer slope factor ((mg/kg-day)-1 Cancer Information cancer unit risk ((ug/m3)-1) Cancer slope factor: 23.5 (mg/kg-day)-1 (ACToR, dermal, 4) 2 Inhalation unit risk: 2.4 (mg/m3)-1 (IRIS, inhalation, 8) RFDo (mg/kg-day) Carcinogenicity data available: IARC: undefinedEPA OPP cancer class: undefinedNTP Report on Carcinogen RFCi (mg/m3) (ROC 12): undefinedNLM ToxNet HSDB carcinognicity warningUniversity of Maryland carcinogenicity warning; 😣 No aenotoxicity findinas reported Resident.soil (ma/ka) Reproductive Toxicology Industrial.soil (mg/kg) Reproductive toxicity PODs available Resident air (ug/m3) Chronic Toxicology Industrial.air ug/m3 Chronic toxicity PODs available Tapwater (ug/L) Subchronic Toxicology Riskbased.SSL (mg/k Subchronic toxicity PODs available GIABS (-) Developmental Toxicology ABS (-) 😣 No developmental toxicity data available. MCL (ua/L) Acute Toxicology Acute toxicity PODs available MCLbased.SSL (mg/kg cancer slope factor ((mg/kg-day)-1 Subacute Toxicology 😣 No subacute toxicity data available cancer unit risk ((ug/m3)-1) Neurotoxicology RFDo (mg/kg-day) 😣 No neurotoxicology data available RFCi (mg/m3) Endocrine System Resident soil (ma/ka C Endocrine Disruption Potential. Significant Estrogen Receptor activity seen. Chemical was positive in 7 ER assays (out of 12) and was positive in 3 AR assays (tested in 6). Industrial.soil (mg/kg ADME Resident.air (ug/m3) 😣 No HTTK data Industrial.air (ug/m3 THQ = Fate and Transport Tapwater (ug/L) No bioaccumulation concern Riskbased.SSL (mg/kg 😣 No volatility concern. Biodegradation predictions are available BCF predictions are available Vapor Pressure predictions are available **O**PHYSCHEM PARAMETERS Exposure Sexposure Estimates have been predicted using the SEEM modeling methodology AOP Information AOP Links: 36, 61, 66, 107, 150, 163, 187, 200 5 0 5 10 10 Other Notes log(BCF) 😵 No water quality values available I8 Air quality values available.

Occupational exposure values available.

#### Value THQ = 0.1 1 THQ = 0.1 0.13 THQ = 0.1 0.2 THQ = 0.1 0.24 THQ = 0.1 1 THQ = 0.1 0.0006 THO = 0.10.0003 THQ = 0.1 0.000002 THQ = 0.1 0.11 THQ = 0.1 21 THQ = 0.1 0.00021 THO = 0.10.00088 THQ = 0.1 0.025 THQ = 0.1 0.029 THQ = 1 1 THQ = 1 0.13 THQ = 1 0.2 THQ = 1 0.24 THQ = 11 THQ = 10.0006 Quantitative Risk Assessment Values THQ = 10.0003 THQ = 1 0.000002 🕜 IRIS values available 🗹 THQ = 10.11 THQ = 1 21 No PPRTV values THQ = 10.0017 EPA RSL values available 0.0088 THQ = 1 0.025 Minimum RfD: 0.00030 mg/kg-day (chronic, IRIS, oral, 8) THQ = 1 0.029 Minimum RfC: 0.0000020 mg/m3 (chronic, IRIS, inhalation, 8) IVIVE POD not calculated

2 0 2

log(VP

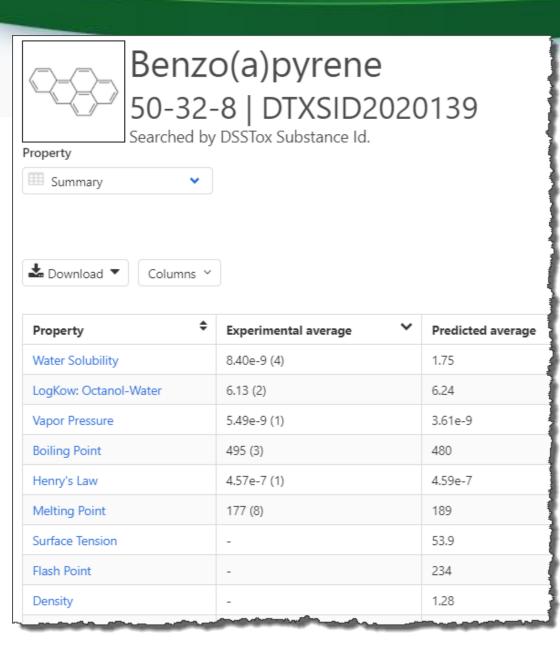
#### Quantitative Hazard Values

- 🕑 Minimum oral POD: 0.070 mg/kg-day (chronic, EFSA, oral, 5) 🗹
- Minimum inhalation POD: 0.0046 mg/m3 (chronic, IRIS, inhalation, 8)
- Lowest Observed Bioactivity Equivalent Level: AR

### **Overview of toxicity-related info**

- Quantitative values
- Info re. toxicology subsets
- Physchem. and Fate & Transport
- Adverse Outcome Pathway links
- In vitro bioactivity summary plot

#### **Experimental and Predicted Data**



- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
  - EPI Suite: Estimation Program Interface
  - ACD/Labs (commercial)
  - TEST: Toxicity Estimation Software Tool
  - OPERA: **OPE**n structure—activity/ property **R**elationship **A**pp

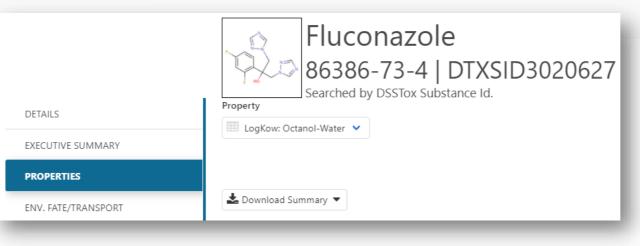




- There are many different "QSAR-related" predictions available
  - QSPR: quantitative structure-**property** relationships
  - QSAR: quantitative structure-activity relationships
  - QSUR: quantitative structure-**use** relationships

#### Access to Predictions





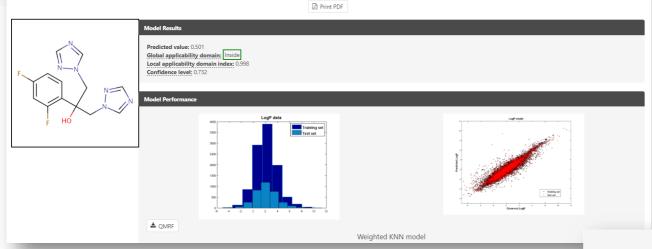
➡ Download Predicted Data ▼		Predicted	
Source \$	Result \$	Calculation Details \$	QMRF
EPISUITE	0.250	Not Available	Not Available
ACD/Labs Consensus	0.698	Not Available	Not Available
ACD/Labs	0.500	Not Available	Not Available
OPERA	0.501	OPERA Model Report [Inside AD]	Available

### **OPERA** Reports



OPERA Models: LogKow: Octanol-Water

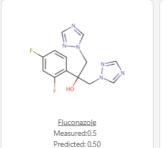
#### Fluconazole 86386-73-4 | DTXSID3020627

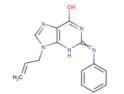


Weighted	KNN	model

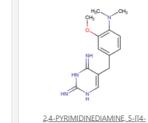
5-fold CV (75%)		Trainir	ng (75%)	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670	0.860	0.780

#### Nearest Neighbors from the Training Set





GUANINEN2PHENYL9ALLYL Measured:1.75 Predicted: 1.75



(DIMETHYLAMINO)-3-M

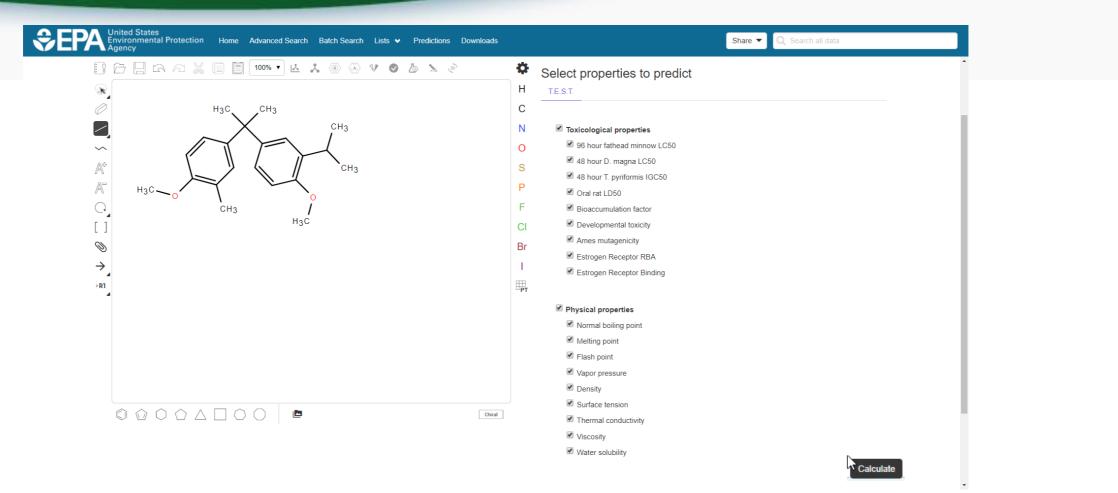
Measured:1.87

Predicted: 1.87

5-(1-P-NITROPHENYL-4-PIPERAZINYL)METHYL-2-AMINO-Measured:1.23 Predicted: 1.23

#### **Real-Time Predictions**





### **Toxicity and Properties**



Toxicological properties ✓ 96 hour fathead minnow LC50 48 hour D. magna LC50 ✓ 48 hour T. pyriformis IGC50 ✓ Oral rat LD50 Bioconcentration factor Developmental toxicity Ames mutagenicity Estrogen Receptor RBA Estrogen Receptor Binding

Physical properties
Normal boiling point
🗹 Melting point
🗹 Flash point
🗹 Vapor pressure
🗹 Density
🗹 Surface tension
🗹 Thermal conductivity
Viscosity
🗹 Water solubility

#### **Real-Time Predictions**



SEPA United States Environmental Protection Home Advanced Search Batch Search Lists - Predictions Downloads

Share 🔻 🔍 Search all data

valculate

Provider: T.E.S.T.

📩 Download Summary 🔻						
Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		6.051 -Log10(mol/L) 0.278 mg/L	5.678 -Log10(mol/L) 0.656 mg/L	5.572 -Log10(mol/L) 0.836 mg/L	5.908 -Log10(mol/L) 0.386 mg/L	7.047 -Log10(mol/L) 0.028 mg/L
48 hour D. magna LC50		5.591 -Log10(mol/L) 0.802 mg/L	5.548 -Log10(mol/L) 0.884 mg/L	6.169 -Log10(mol/L) 0.212 mg/L	5.518 -Log10(mol/L) 0.948 mg/L	5.128 -Log10(mol/L) 2.329 mg/L
48 hour T. pyriformis IGC50		5.590 -Log10(mol/L) 0.804 mg/L	6.390 -Log10(mol/L) 0.127 mg/L		5.588 -Log10(mol/L) 0.806 mg/L	4.790 -Log10(mol/L) 5.068 mg/L
Oral rat LD50		2.400 -Log10(mol/kg) 1243.951 mg/kg	2.232 -Log10(mol/kg) 1829.942 mg/kg			2.568 -Log10(mol/kg) 845.609 mg/kg
Bioaccumulation factor		3.066 Log10 1164.438	3.090 Log10 1230.849	2.717 Log10 521.420	3.257 Log10 1806.262	3.200 Log10 1585.959
Developmental toxicity		true	true	true		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-0.710 Log10 0.195	-1.692 Log10 0.020	-1.515 Log10 0.031		1.077 Log10 11.931
Estrogen Receptor Binding		false	false	false		true
Normal boiling point		345.2 °C	306.6 °C		408.2 °C	320.7 °C
Melting point		74.3 °C	63.8 °C		41.0 °C	118.2 °C
Flash point		161.7 °C	143.5 °C		152.7 °C	188.9 °C
Vapor pressure		-5.955 Log10(mmHg) 1.109*10^-6 mmHg	-5.534 Log10(mmHg) 2.925*10^-6 mmHg		-5.903 Log10(mmHg) 1.249*10^-6 mmHg	-6.428 Log10(mmHg) 3.735*10^-7 mmHg
Density		0.959 g/cm³	0.977 g/cm³		0.843 g/cm <sup>3</sup>	1.057 g/cm <sup>3</sup>



- We are continuously gathering data...where from?
  - How do we validate?
  - What can we check?
- Projects underway at present that may be of interest
  - Water Solubility dataset
  - Mass Spec Amenability
  - Eye and Skin Sensitization and Irritation
  - PFAS chemicals



- Property predictions can be used for
  - Experimental design what chemicals are too volatile to perform bioactivity screens on?
  - As inputs to other models for example toxicokinetic models, exposure models (we cannot measure all the properties we need to build models)
  - To use as flags related to persistence and bioaccumulation

### Safety Data



,	GHS Data	
int Page		
PUBCHEM > BENZO[A]PYREN	E > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION	
CID 2336		
Benzo[a]py	vrene	
GHS Classificati	on	?
howing 6 of 6		
Pictogram(s)	Irritant Health Hazard Hazard	
Signal	Danger	
	H317: May cause an allergic skin reaction [Warning Sensitization, Skin]	
	H340: May cause genetic defects [ <b>Danger</b> Germ cell mutagenicity]	
GHS Hazard Statements	H350: May cause cancer [ <b>Danger</b> Carcinogenicity]	
	H360FD: May damage fertility; May damage the unborn child [Danger Reproductive toxicity]	
	H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]	
	H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]	
Precautionary Statement	P201, P202, P261, P272, P273, P280, P281, P302+P352, P308+P313, P321, P333+P313, P363, P391, P405, and P501	
Codes	(The corresponding statement to each P-code can be found at the GHS Classification page.)	

### **Chemical Hazard Data**



#### **ToxVal Database** Hazard DataType Toxicity Value $\sim$ 🛉 Human 💋 Eco 📥 Download 🔻 Columns 🗸 10 💙 >50k chemicals ♦ Source ♥ More Priority Subtype Risk assessment class Value Study type Exposure route 🗘 Type Units Species 🗘 Subsource 23.5 Alaska DEC Alaska DEC cancer slope factor chronic (mg/kg-day)-1 dermal Ľ >770k tox. values 7 chronic 0.21 (mg/l)-1 Alaska DEC Alaska DEC Ŀ cancer unit risk inhalation 7 3.08 Alaska DEC Alaska DEC Ľ cancer slope factor chronic (mg/kg-day)-1 inhalation Ľ 7 0.88 (mg/m3)-1 inhalation Alaska DEC Alaska DEC cancer unit risk chronic >30 sources of data 7 cancer slope factor chronic 7.3 (mg/kg-day)-1 Alaska DEC Alaska DEC oral 7 MEG Short-term Critical Air short-term 80 inhalation TG 230 Military Exposure Guidelines Table DOD Ŀ mg/m3 ~5k journals cited Ŀ 7 MEG Short-term Marginal Air short-term 15 mg/m3 inhalation TG 230 Military Exposure Guidelines Table DOD Ľ 7 MEG Soil Negligible Soil chronic 12 mg/kg -Soil -TG 230 Military Exposure Guidelines Table DOD Ľ MEG Long-Term, 5L/d Negligible Water chronic 0.0134 mg/L oral TG 230 Military Exposure Guidelines Table DOD ~70k citations MEG Short-term Negligible Air short-term 0.6 mg/m3 inhalation TG 230 Military Exposure Guidelines Table DOD Ŀ 2 3 4 > >> <<

Showing 1 to 10 of 32 records



- Anywhere you see a table you can export
  - CSV is great for integration with other applications (plus read into Excel)
  - Excel file is generally the best for "viewing" as it can have multiple worksheets, color flagging of cells and offers all
- If you have cheminformatics tools SDF files are the best view structures directly as concatenated "molfiles"

### Let's Talk Exposure



- Types of Exposure Data on the Dashboard
  - Consumer product categories and uses
  - Products containing the chemical
  - Predicted exposure levels from modeling

#### Sources of Exposure to Chemicals





#### Benzo(a)pyrene 50-32-8 | DTXSID2020139 Searched by DSSTox Substance Id.

#### Chemical Weight Fractions 🚺

📥 Download 🔻

Columns 🐃 10 💙

Search query

Product Name \$	Product Use Category \$	Minimum Weight Fraction	Maximum Weight Fraction	Data Type 🗘	Source \$
m-525-1-5x pah mixtures 0.5 mg/ml for method 525	Not Yet Categorized:			MSDS	SIRI
mm6125 surface conditioner	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
monolithic membrane 6125 (mm6125) / monolithic membrane	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
organic potablewatr pw 32_component h:reg semi-volatile 690	Not Yet Categorized:	0.00	1.00e-3	MSDS	SIRI
polynuclear aromatic hydrocarbon mixture_ep84627	Not Yet Categorized:			MSDS	SIRI
prestone(r) power steering fluid	engine maintenance: auto fluids and additives			MSDS	CPCPdb
r-12 shield tite wet surface coating	Not Yet Categorized:	0.00	0.500	MSDS	SIRI
sea tar 1010_ 0028	Not Yet Categorized:			MSDS	SIRI
supelpreme-hc kit pah mix_ 48909	Not Yet Categorized:			MSDS	SIRI
supelpreme-hc pah mix 1ml_ 48905	Not Yet Categorized:			MSDS	SIRI

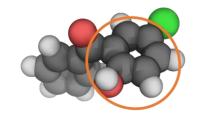


Showing 11 to 20 of 21 records

### Machine Learning NAMS



Chemical Structure and Property Descriptors



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Rectoreverselle van bieter andere		File Cherobase In II. 199 K (Incheror	1/28 5 5 10 10	

						•		Agency
Positive Examples Vegative Examples								
0.6	additive	additive_for_liquid_system	additive_for_rubber	adhesion_promoter	antimicrobial	antioxidant	antistatic_agent	
0.4	additive	additive for liquid system	additive for rubber	adhesion promoter	anti- microbial	anti- oxidant	antistatic agent	Successful
0.6	buffer	catalyst	chelator	colorant	crosslinker	emollient	emulsifier	Madal
0.4	buffer	catalyst	chelator	colorant	crosslinker	emollient	emulsifier	Model
	emulsion_stabilizer	film_forming_agent	flame_retardant	flavorant	foam_boosting_agent	foamer	fragrance	Failed
0.6 0.4 0.2 0.0	emulsion stabilizer	film forming a <mark>gent</mark>	flame retardant	flavorant	foam boosting agent	foamer	fragrance	Model
	hair_conditioner	hair_dye	heat_stabilizer	humectant	lubricating_agent	masking_agent	monomer	
0.6 0.4 0.2	hair condi- tioner	hair dye	heat stabilizer	humectant	lubricating agent	masking agent	monomer	Probabilistic Predictions of
0.0	oral_care	organic_pigment	oxidizer	perfumer	ph_stabilizer	photoinitiator	plastic	Potential Chemical
0.6	oral care	organic pigment	oxidizer	perfumer	pH stabilizer	photo- initiator	plasticizer	Uses
0.0	preservative	reducer	rheology_modifer	skin_conditioner	skin_protectant	soluble_dye	solvent	
0.6 0.4 0.2 0.0	pre- servative	reducer	rheology modifier	skin condi- tioner	skin protectant	soluble dye	solvent	
0.6	surfactant	ubiquitous	uv_absorber	vinyl	viscosity_controlling_agent	wetting_agent	whitener	
0.4	surfactant	ubiquitous	UV absorber	vinyl	viscosity controlling agent	wetting agent	whitener	Phillips <i>et al.</i> (2017)

**Chemical Functional Use Database (FUSE)** 

### QSUR modeling



High-throughput screening of chemicals as functional substitutes using structure-based classification models<sup>†</sup>



Katherine A. Phillips, (b \* ac John F. Wambaugh, b Christopher M. Grulke, b Kathie L. Dionisio<sup>c</sup> and

Kristin K. Isaacs<sup>c</sup>

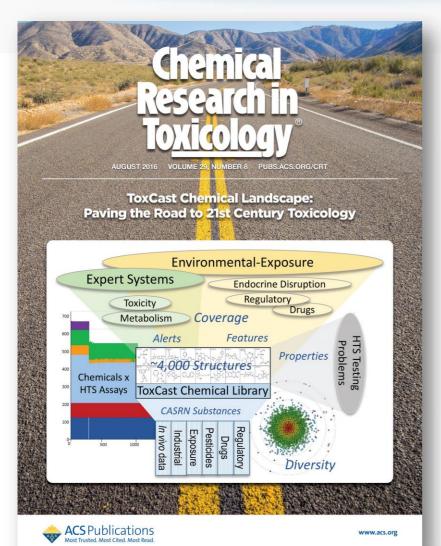
Predicted Probability of Associated Functional Use QSAR Version/Date: 2015-11-06

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Harmonized functional use	Probability
preservative	0.988
UV absorber	0.885
fragrance	0.653
antioxidant	0.608
skin conditioner	0.475
skin protectant	0.411
chelator	0.364
colorant	0.285
antimicrobial	0.279
crosslinker	0.187







#### ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

Ann M. Richard<sup>\*†</sup>, Richard S. Judson<sup>†</sup>, Keith A. Houck<sup>†</sup>, Christopher M. Grulke<sup>†</sup>, Patra Volarath<sup>‡</sup>, Inthirany Thillainadarajah<sup>§</sup>, Chihae Yang<sup>∥⊥</sup>, James Rathman<sup>⊥#</sup>, Matthew T. Martin<sup>†</sup>, John F. Wambaugh<sup>†</sup>, Thomas B. Knudsen<sup>†</sup>, Jayaram Kancherla<sup>⊽</sup>, Kamel Mansouri<sup>⊽</sup>, Grace Patlewicz<sup>†</sup>, Antony J. Williams<sup>†</sup>, Stephen B. Little<sup>†</sup>, Kevin M. Crofton<sup>†</sup>, and Russell S. Thomas<sup>†</sup>

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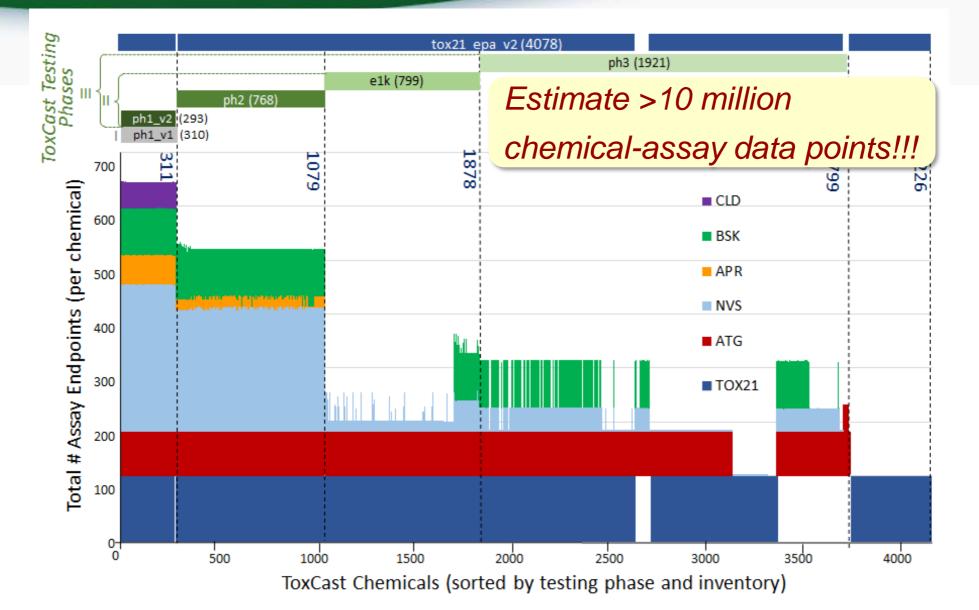
Cite this: Chem. Res. Toxicol. 2016, 29, 8, 1225-	Article Views
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Publication Date: July 1, 2016 🗸	0007
https://doi.org/10.1021/acs.chemrestox.6b00135	LEARN A

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### ToxCast/To21 HTS data





### ToxCast Chemicals and Assays



Ł Download ▼	Columns ~				toxcast_	Copy Filtered Lists URL
List Acronym 🗘	List Name 🗘	Last Updated 🗘	Number of Chemicals	List Description		÷
TOXCAST_PH1V2	TOXCAST_ph1v2 - EPA ToxCast Screening Library (ph1v2 Subset)	2016-01-25	293	TOXCAST_ph1v2 is the ph1v2 subset of TO chemicals moved into Phase II and later te	1	., .
TOXCAST_PHASEI	TOXCAST_Phasei - EPA ToxCast Screening Library (Phase I subset)	2016-01-29	310	TOXCAST_Phasel corresponds to the ph1v1 Phase I of the ToxCast program.	subset of TOXCAST (m	ostly pesticides) screened in
TOXCAST_PH2	TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset)	2016-01-25	768	TOXCAST_ph2 is the ph2 subset of TOXCAS chemical diversity and coverage of chemica		1 5
TOXCAST_E1K	TOXCAST_e1k - EPA ToxCast Screening Library (e1k Subset)	2016-01-25	799	TOXCAST_e1k is the e1k subset of TOXCAS	T, selected for screening	g in endocrine-related assays.
TOXCAST_PHASEII	TOXCASST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)	2016-01-29	1864	TOXCAST_PhaseII is the full set of chemical consisting of TOXCAST_ph1v2, ph2 and e11		f the ToxCast program,
TOXCAST_PH3	TOXCAST_ph3 - EPA ToxCast Screening Library (ph3 subset)	2018-04-11	2678	TOXCAST_ph3 is the ph3 subset of TOXCAS program to further increase chemical diver programs.		
TOXCAST_PHASEIII	TOXCAST_PhaseIII - EPA ToxCast Screening Library (Phase II Subset)	2017-04-11	4584	TOXCAST_PhaseIII is the full set of chemica program, consisting of the majority of cher		5

## ToxCast covers a lot of biology but not all ToxCast is growing over time.



### Invitrodb version 3.3 (released August 2020) contained **17 different assay sources**, covering (at least) **491 unique gene-related** targets with **1600 unique** assay endpoints.

Assay source	Long name	Truncated assay source description	Some rough notes on the biology covered
ACEA	ACEA Biosciences	real-time, label-free, cell growth assay system based on a microelectronic impedance readout	Endocrine (ER-induced proliferation)
APR	Apredica	CellCiphr High Content Imaging system	Hepatic cells (HepG2)
ATG	Attagene	multiplexed pathway profiling platform	Nuclear receptor and stress response profile
BSK	Bioseek	BioMAP system providing uniquely informative biological activity profiles in complex human primary co-culture systems	Immune/inflammation responses
NVS	Novascreen	large diverse suite of cell-free binding and biochemical assays.	Receptor binding; transporter protein binding; ion channels; enzyme inhibition; many targets
ОТ	Odyssey Thera	novel protein:protein interaction assays using protein-fragment complementation technology	Endocrine (ER and AR)
TOX21	Tox21/NCGC	Tox21 is an interagency agreement between the NIH, NTP, FDA and EPA. NIH Chemical Genomics Center (NCGC) is the primary screening facility running ultra high-throughput screening assays across a large interagency-developed chemical library	<sup>/</sup> Many – with many nuclear receptors
CEETOX	Ceetox/OpAns	HT-H295R assay	Endocrine (steroidogenesis)
CLD	CellzDirect	Formerly CellzDirect, this Contract Research Organization (CRO) is now part of the Invitrogen brand of Thermo Fisher providing cell-based in vitro assay screening services using primary hepatocytes.	Liver (Phase I/Phase II/ Phase III expression)
NHEERL_PADILLA	A NHEERL Padilla Lab	The Padilla laboratory at the EPA National Health and Environmental Effects Research Laboratory focuses on the development and screening of zebrafish assays.	Zebrafish terata
NCCT	NCCT Simmons Lab	The Simmons Lab at the EPA National Center for Computational Toxicology focuses on developing and implementing in vitro methods to identif potential environmental toxicants.	y Endocrine (thyroid - thyroperoxidase inhibition)
TANGUAY	Tanguay Lab	The Tanguay Lab, based at the Oregon State University Sinnhuber Aquatic Research Laboratory, uses zebrafish as a systems toxicology model.	Zebrafish terata/phenotypes
NHEERL_NIS	NHEERL Stoker & Laws	The Stoker and Laws laboratories at the EPA National Health and Environmental Effects Research Laboratory work on the development and implementation of high-throughput assays, particularly related to the sodium-iodide cotransporter (NIS).	Endocrine (thyroid - NIS inhibition)
UPITT	University of Pittsburgh	The Johnston Lab at the University of Pittsburgh ran androgen receptor nuclear translocation assays under a Material Transfer Agreement (MTA for the ToxCast Phase 1, Phase 2, and E1K chemicals.	<sup>N)</sup> Endocrine (AR related)

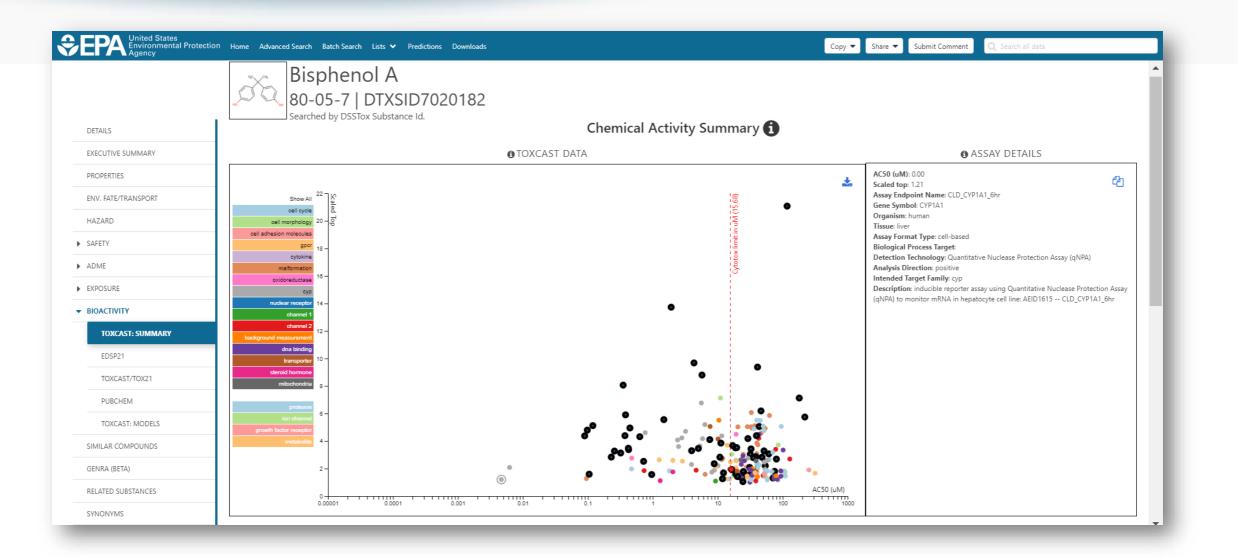
### The Tox21 Screening Library



•					
📩 Download 🔻	Columns 🗸			tox21	Copy Filtered Lists URL
List Acronym 🗘	List Name 🗘	Last Updated 🗘	Number of Chemicals 🕈	List Description	\$
EPACHEMINV_AVAIL	CHEMINV; ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)	2018-11-21	6408	EPACHEMINV_AVAIL is list of unique DSSTox substances availated ToxCast and Tox21 partner projects, managed by EPA Chemic	
TOX21SL	TOX21SL: Tox21 Screening Library	2017-02-23	8947	TOX21SL is list of unique substances comprising the screening a multi-federal agency collaborative among the US EPA, NIH/	

### Let's look at the data





### Rich data tables – full transparency

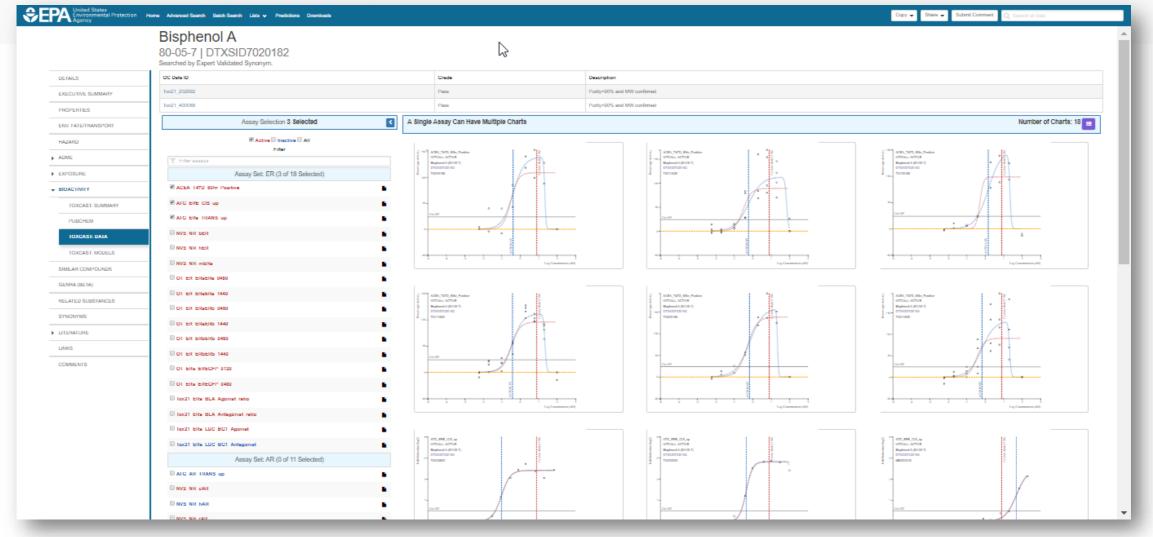


Name 🗘	Modal	SeqAPASS 🗘	Gene Symbol 🗘	Gene Name 🗸	AOP \$	Event \$	Hit Call ₽	Тор≑	Scaled Top 🗘	AC50	logAC50 \$	Bmad ¢	Cutoff ‡	Intended Target Family
ATG_Xbp1_CIS_up		NP_005071.2	XBP1	X-box binding protein 1	-	-	ACTIVE	1.08	1.83	93.8	1.97	0.118	0.590	dna binding
ATG_VDRE_CIS_up		NP_000367.1	VDR	vitamin D (1,25- dihydroxyvitamin D3) receptor	-	-	ACTIVE	1.71	2.35	8.84	0.946	0.146	0.728	nuclear receptor
BSK_hDFCGF_VCAM1_down		NP_001069.1	VCAM1	vascular cell adhesion molecule 1	-	-	ACTIVE	0.248	1.72	40.0	1.60	4.81e- 2	0.144	cell adhesion molecules
BSK_LPS_VCAM1_down		NP_001069.1	VCAM1	vascular cell adhesion molecule 1	-	-	ACTIVE	0.107	1.35	40.0	1.60	2.31e- 2	7.92e-2	cell adhesion molecules
TOX21_p53_BLA_p2_ratio		NP_000537.3	TP53	tumor protein p53	-	-	ACTIVE	35.5	1.78	73.7	1.87	0.959	20.0	dna binding
TOX21_p53_BLA_p4_ratio		NP_000537.3	TP53	tumor protein p53	-	-	ACTIVE	28.6	1.43	73.8	1.87	1.02	20.0	dna binding
O ATG_p53_CIS_dn		NP_000537.3	TP53	tumor protein p53	-	-	ACTIVE	0.789	1.23	82.4	1.92	0.129	0.643	dna binding
• NVS_MP_rPBR		NP_036647.1	Тѕро	translocator protein	-	-	ACTIVE	61.5	1.96	15.3	1.19	5.24	31.4	transporter
ATG_AP_2_CIS_dn		NP_003211.1	TFAP2A	transcription factor AP-2 alpha (activating enhancer binding protein 2 alpha)	-	-	ACTIVE	0.458	1.44	93.8	1.97	6.35e- 2	0.317	dna binding
ATG_TCF_b_cat_CIS_dn		NP_003193.2	TCF7	transcription factor 7 (T-cell specific, HMG-box)	-	-	ACTIVE	1.34	1.96	30.7	1.49	0.137	0.687	dna binding

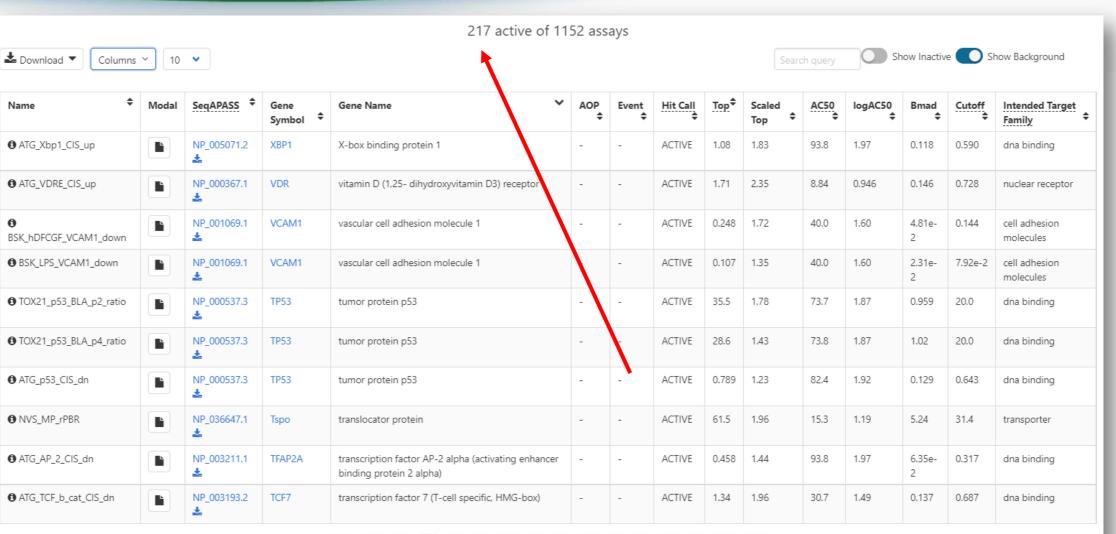
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### Bioactivity Data (ToxCast/Tox21) Data below for Bisphenol A





### #Actives for a chemical



Environmental Protection

Agency

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### Cytotoxicity Threshold

**Jnited States** 

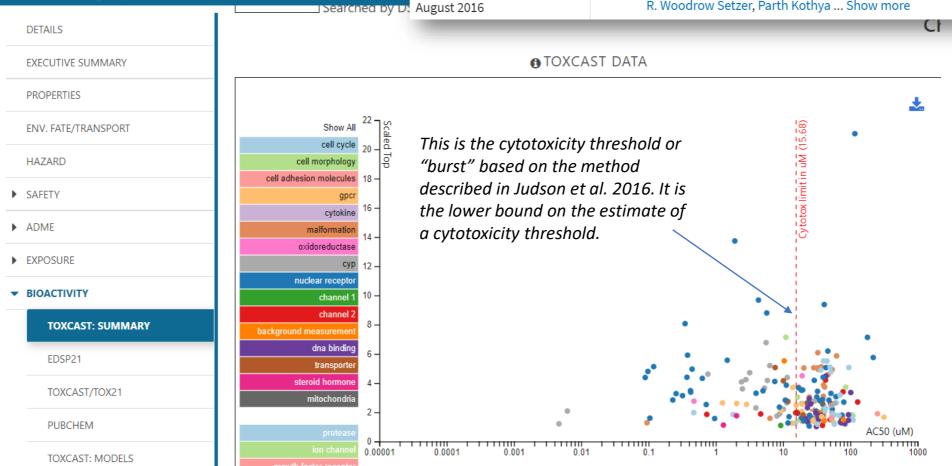
ental Protection Home



Advanced Search Batch Se Volume 152, Issue 2

Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity on *In Vitro* Assay Activity Across a Diverse Chemical and Assay tion Space 🕮

Richard Judson ∞, Keith Houck, Matt Martin, Ann M. Richard, Thomas B. Knudsen, Imran Shah, Stephen Little, John Wambaugh, R. Woodrow Setzer, Parth Kothya ... Show more





- Bisphenol A clearly has some *in vitro* nuclear receptor activity at concentrations that may be below or near cytotoxicity.
  - It has moderate ToxCast ER agonist and AR antagonist scores.
  - The cytotoxicity threshold or "burst" seems to support selectivity of some nuclear receptor responses.
  - Diving a little deeper into the intended target family supports this analysis.

## Let's look at the assay table ACEA\_ER



	Assay	Endpoint Name: ACEA_ER_8	80hr	
ay Details				•
Assay Endpoint Name: ACEA_ER_80hr	(ACEA) is a privately owned biotechnology company that	developed a real-time, label-free, cell growth assay system	n called xCELLigence based on a microelectronic impedance	readout .
stograms				4
elect all 📩 Download 🔻 Send to Batch Searci	ch Default 💙 û DTXSID 🗙 CASRN 🗙 T	175 of 3031 chemicals visible	Inactive X	✓ Filter by Name or CASRN III
elect all Cownload Send to Batch Search	ch Default V û DTXSID X CASRN X			
	H <sub>2</sub> N H <sub>3</sub> C HCI		Nī—N <sup>⊾</sup> —N na <sup>+</sup>	
Acetohexamide DTXSID:DTXSID7020007 CASRN:968-81-0 TOXCAST:7/403	2-Methoxyaniline hydrochloride DTXSID:DTXSID8020092 CASRN:134-29-2 TOXCAST:17/412	Sodium L-ascorbate DTXSID:DTXSID0020105 CASRN:134-03-2 TOXCAST:22/890	Sodium azide DTXSID:DTXSID8020121 CASRN:26628-22-8 TOXCAST:84/864	Benzotrichloride DTXSID:DTXSID1020148 CASRN:98-07-7 TOXCAST:10/866

### High-Level Visualizations of Data



Details			
	Inc. (ACEA) is a privately owned biotechnology company that developed a real-time	e, label-free, cell growth assay system called xCELLigence based on a microelectronic im	pedance readout .
ograms	Histogram of LogAC50 Values of All Active Chemicals	Histogram of Scaled Responses of All Active Chemicals	

### Filtering by vendor....or Gene Symbol



La Download ▼					ACEA X Y Search o	query	Copy filtered page URL
					ACEA Biosciences		
Assay Component Endpoint Name 🗘	Details	Multi Conc. Actives	Single Conc. Active	Description	Apredica		Gene Symbols
ACEA_ER_80hr		456 / 3024	-	Data from the assay component ACE/ endpoint, ACEA_ER_80hr_Positive, wa negative control and baseline of activ of-signal activity can be used to unde ESR1. Furthermore, this assay endpoint produced multiple assay endpoints w intended target to other relatable tark intended target family, where the sub	Bioseek Novascreen Odyssey Thera Tox21/NCGC Centox/OnApr	points. This assay n relative to DMSO as the asures of the cells for gain- el as they relate to the gene ut, because this assay has n. To generalize the the "nuclear receptor"	
ACEA_AR_agonist_AUC_viability		609 / 1830	-	Data from the assay component ACE/ relative to DMSO as the negative con of-signal activity can be used to unde can be referred to as a secondary rea where this one serves a viability funct this assay endpoint is annotated to th "cytotoxicity".	CellzDirect NHEERL Padilla Lab NCCT Simmons Lab	negative fitting direction e of growth reporter, loss- nore, this assay endpoint nultiple assay endpoints o other relatable targets, ere the subfamily is	
ACEA_ER_AUC_viability		1051 / 3025	-	Data from the assay component ACE/ relative to DMSO as the negative con of-signal activity can be used to unde can be referred to as a secondary real where this one serves a viability functi this assay endpoint is annotated to th "cytotoxicity".	NHEERL Mid-Continent Ecology Division University of Pittsburgh Johnston Lab ion. To generalize the intended target	2	

### Use Models Derived from the Data



#### Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model

Patience Browne<sup>\*†</sup>, Richard S. Judson<sup>‡</sup>, Warren M. Casey<sup>§</sup>, Nicole C. Kleinstreuer<sup>II</sup>, and Russell S. Thomas<sup>‡</sup>

#### View Author Information $^{\sim}$

 Cite this: Environ. Sci. Technol. 2015, 49, 14, 8804– 8814
 Publication Date: June 12, 2015 ~ https://doi.org/10.1021/acs.est.5b02641 Article Views Altmetric Citations 3796 27 157



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#### Vol. 124, No. 7 | Research

#### CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

Kamel Mansouri, Ahmed Abdelaziz, Aleksandra Rybacka, Alessandra Roncaglioni, Alexander Tropsha, Alexandre Varnek, Alexey Zakharov, Andrew Worth, Ann M. Richard, Christopher M. Grulke, Daniela Trisciuzzi, Denis Fourches, Dragos Horvath, Emilio Benfenati, Eugene Muratov, Eva Bay Wedebye, Francesca Grisoni, Giuseppe F. Mangiatordi, <u>... See all authors</u> V

Published: 1 July 2016 | https://doi.org/10.1289/ehp.1510267 | Cited by: 76

#### Development and Validation of a Computational Model for Androgen Receptor Activity

Nicole C. Kleinstreuer<sup>\*†</sup>, Patricia Ceger<sup>‡</sup>, Eric D. Watt<sup>§</sup>, Matthew Martin<sup>§</sup>, Keith Houck<sup>§</sup>, Patience Browne<sup>II</sup>, Russell S. Thomas<sup>§</sup>, Warren M. Casey<sup>†</sup>, David J. Dix<sup>⊥</sup>, David Allen<sup>‡</sup>, Srilatha Sakamuru<sup>#</sup>, Menghang Xia<sup>#</sup>, Ruili Huang<sup>#</sup>, and Richard Judson<sup>§</sup>

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#### Vol. 128, No. 2 | Research

#### CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

Kamel Mansouri 🔄, Nicole Kleinstreuer, Ahmed M. Abdelaziz, Domenico Alberga, Vinicius M. Alves, Patrik L. Andersson, Carolina H. Andrade, Fang Bai, Ilya Balabin, Davide Ballabio, Emilio Benfenati, Barun Bhhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, ... <u>See all authors</u>

Published: 7 February 2020 | CID: 027002 | https://doi.org/10.1289/EHP5580 | Cited by: 2

### For Endocrine (AR and ER) better to use summary models

Download ToxCast Model Predictions



H,C CH3	Bispher	nol A
	80-05-7	DTXSID7020182
	Searched by DSS	Tox Substance Id.

### *Positive ToxCast ER pathway agonist* and ToxCast AR antagonist scores.

ToxCast: Models ToxCast Model Predictions

ENV. FATE/TRANSPORT

EXECUTIVE SUMMARY

HAZARD

DETAILS

PROPERTIES

SAFETY

ADMF

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

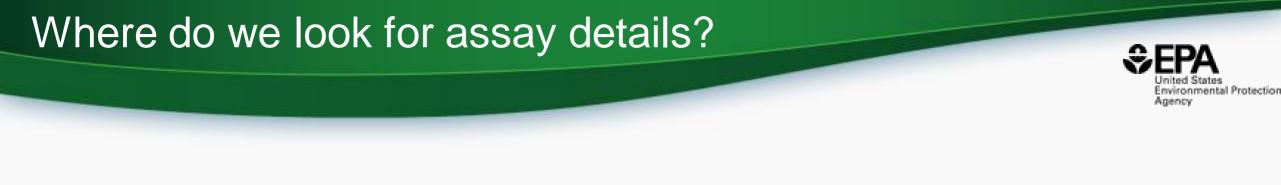
PUBCHEM

TOXCAST: MODELS

Model	Receptor	Agonist	Antagonist	Binding
ToxCast Pathway Model (AUC)	Androgen	0.00	0.345	-
ToxCast Pathway Model (AUC)	Estrogen	0.450	0.00	-
COMPARA (Consensus)	Androgen	Inactive	Active	Active
CERAPP Potency Level (From Literature)	Estrogen	Active (Weak)	-	Active (Weak)
CERAPP Potency Level (Consensus)	Estrogen	Active (Weak)	Active (Strong)	Active (Weak)

CERAPP = consensus ER QSAR (from 17 groups) COMPARA = consensus AR QSAR

ToxCast Pathway Model AUC ER = full ER model (18 assays) ToxCast Pathway Model AUC AR = full AR model (11 assays)



- How do we search the 100s of genes mapped against assays
- Home page: Assay/Gene Search

Chemicals	Product/Use Categories Assay/Gene	
<b>Q</b> gluco		
GENE: SGK1	subfamily 3, group C, member 1 (glucocorticoid receptor) coid regulated kinase 1	



# Generalized Read-Across



#### DETAILS

PROPERTIES

HAZARD

EXPOSURE

BIOACTIVITY

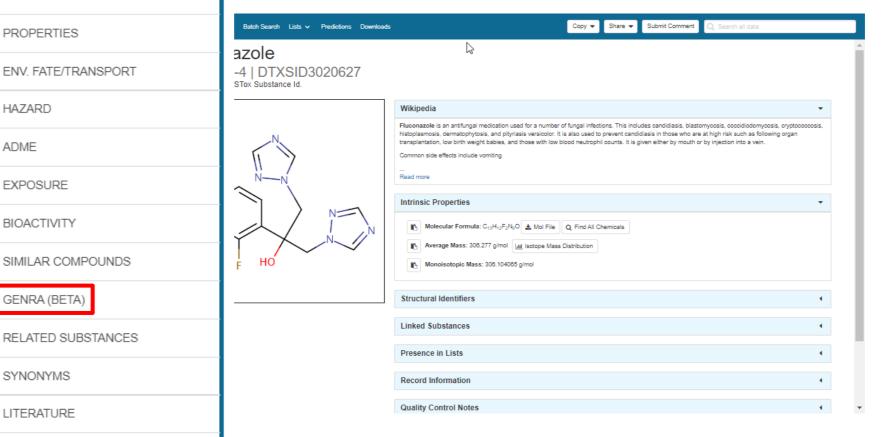
GENRA (BETA)

SYNONYMS

LITERATURE

ADME

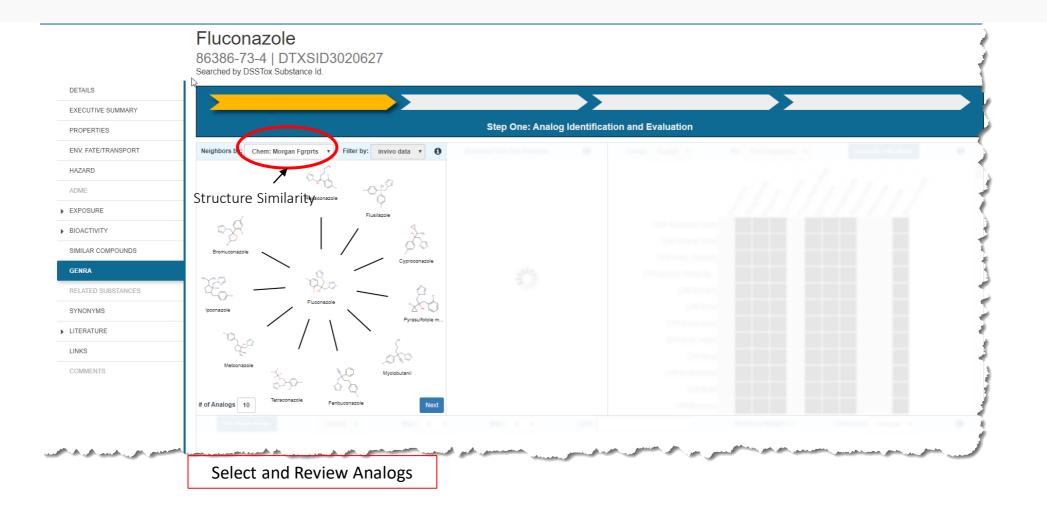
EXECUTIVE SUMMARY



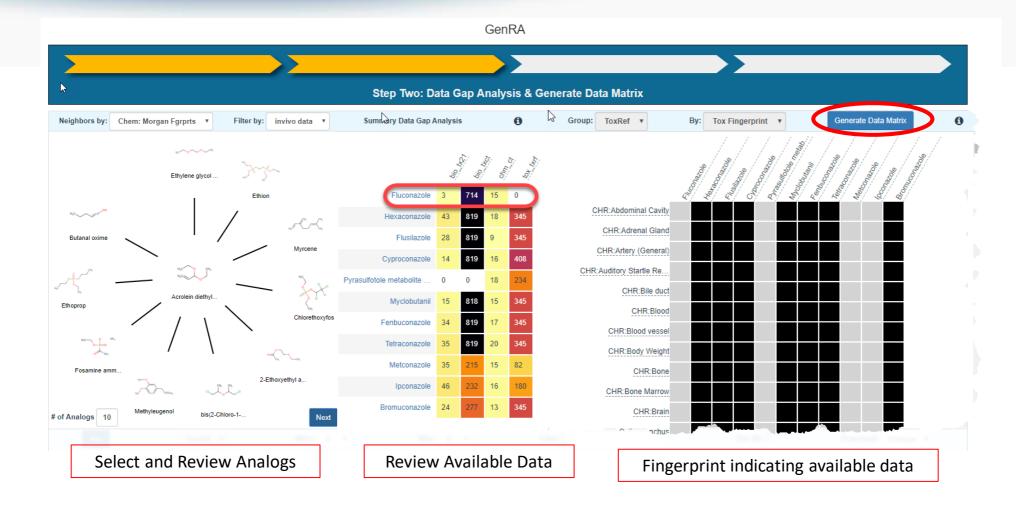
LINKS

COMMENTS

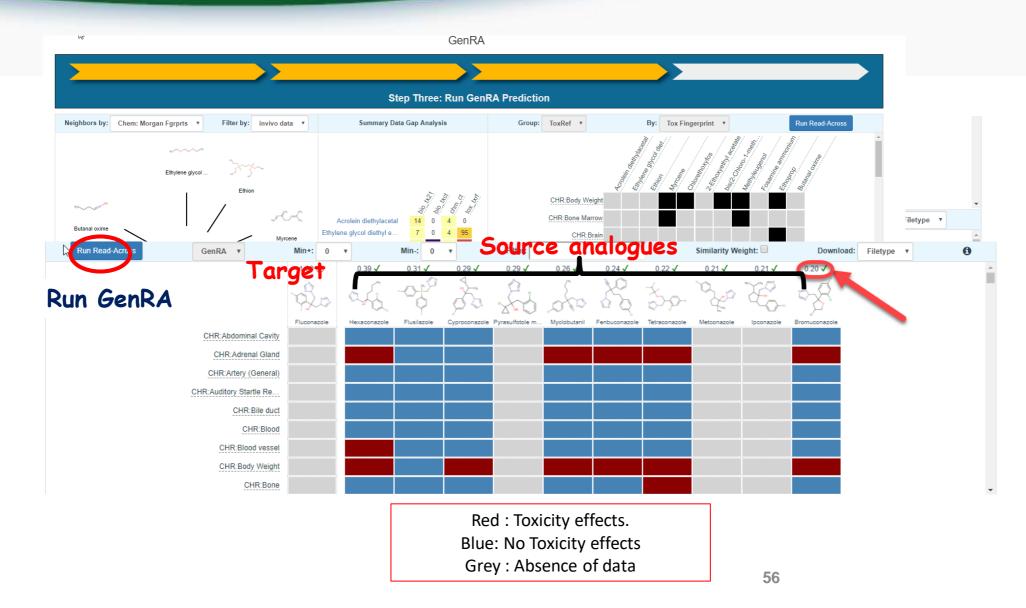












### **Related Publications**



#### Chemical Research in Toxicology

Cite This: Chem. Res. Toxicol. 2017, 30, 2046-205

pubs.acs.org/crt

### Predicting Organ Toxicity Using *in Vitro* Bioactivity Data and Chemical Structure

Jie Liu,<sup>‡,§</sup> Grace Patlewicz,<sup>†</sup> Antony J. Williams,<sup>†</sup> Russell S. Thomas,<sup>†</sup> and Imran Shah\*<sup>†</sup>

<sup>†</sup>National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States

<sup>‡</sup>Department of Information Science, University of Arkansas at Little Rock, Arkansas 72204, United States

<sup>§</sup>Oak Ridge Institute for Science Education, National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States



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Journal

Cover

Image

Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information

Imran Shah <sup>a</sup> A 🖾, Jie Liu <sup>b, c</sup>, Richard S. Judson <sup>a</sup>, Russell S. Thomas <sup>a</sup>, Grace Patlewicz <sup>a</sup>



Computational Toxicology Available online 23 July 2018 In Press, Corrected Proof (?)



Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance

George Helman <sup>a, b</sup>, Imran Shah <sup>b</sup>, Grace Patlewicz <sup>b</sup> <sup>A</sup> ⊠



Computational Toxicology

journal homepage: www.elsevier.com

Contents lists available at ScienceDirect

Navigating through the minefield of read-across frameworks: A commentary perspective

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## What's the best way to search the internet for chemical data?



- We know how complex chemicals identifiers are...
  - CASRN(s)
  - Hundreds of names (maybe)
  - SMILES
  - InChIs
  - EINECS, EC numbers
- What can WE do to help you navigate the internet?

## Identifiers Support Searches in other systems



Benzo(a)pyrene 50-32-8   DTXSID2020139 Searched by DSSTox Substance Id.		
Syn	onyms	
La Download ▼ 25 V	Search query	
Synonym	Quality	\$
Benzo(a)pyrene	Valid	
Benzo[pqr]tetraphene	Valid	
Benzo[a]pyrene	Valid	
50-32-8 Active CAS-RN	Valid	
BaP	Valid	
Benzo[a]pyrene	Good	
3,4-Benz[a]pyrene	Good	
3,4-Benzopyrene	Good	
3,4-Benzpyrene	Good	
6,7-Benzopyrene	Good	
BENZ(A)PYREN	Good	
Benz(a)pyrene	Good	
Benz[a]pyrene	Good	

### Identifiers are used in the app



### • Identifiers are used to feed and link into "Literature"

	Environmental Topics Laws & Regulations About EPA Sea	rch EPA.gov
GOOGLE SCHOLAR	IRIS	<u>Contact Us</u>
PUBMED ABSTRACT SIFTER	IRIS Home Bonzo[] DIVITORO (B-D)	
	IRIS Home     Benzo[a]pyrene (BaP)       About IRIS     Benzo[a]pyrene (BaP)	
PUBCHEM ARTICLES	IRIS Recent Additions CASRN 50-32-8   DTXSID202013	9
	IRIS Calendar • <u>Toxicological Review (PDF)</u> (234 pp, 4.67 M)	
PUBCHEM PATENTS	IRIS Assessments         IRIS Executive Summary (PDF). (9 pp, 671 K)           Supplemental Information on the IRIS Toxicological Review of Benzieway	<u>zo[a]pyrene</u>
	Advanced Search	
PPRTV	IRIS Program Materials Values Specific Values Documents Information	Related Links
	Contact Us	
IRIS	Noncancer Assessment	EPA Chemicals     Dashboard -
	Reference Dose for Oral Exposure (RfD) (PDF) (9 pp, 671 K) Last Updated: 01/19/20	<u>Benzo[a]pyren</u> <u>e (BaP)</u> 17

### Literature Searching





#### Benzo(a)pyrene 50-32-8 | DTXSID2020139 Searched by DSSTox Substance Id.

#### Abstract Sifter

#### 1) Select PubMed starting point query then 2) click on Retrieve.

Hazard 🗸	Retrieve Articles
Select a Query Term	
Hazard	
Fate and Transport	
Metabolism/PK/PD	
Chemical Properties	
Exposure	
Mixtures	
Male Reproduction	
Androgen Disruption	
Female Reproduction	
GeneTox	
Cancer	
Clinical Trials	
Embryo and embryonic development	
Child (infant through adolescent)	
Dust and Exposure	
Food and Exposure	
Water and Exposure	
Algae	
Disaster / Emergency	

#### Optionally, edit the query before retrieving.

("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

- Real-time retrieval of data from PubMed ~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

### Literature Searching



- "Sifting" of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID

To f	ind articl	es quickly,	enter tern	ns to sif	t abstracts.	0					-	
de	rmal		cancer			pyrene	2	Clear 1	Download / Send to V Download S	THE TOP EXC	iel	0
	dermal	cancer ↓	pyrene	Total	PMID	Year	Title		uthors Journal	Re	ev	
	0	7	1	8	23922326	2013	Using immunotoxi	city information to improve cancer risk	Zaccaria; McClure International journal of toxicology	1	7	
	8	7	2	17	16632147	2006	Development of a	dermal cancer slope factor for benzo[	Knafla; Phillipps; Brecher; Petrovic; Richardson Regulatory toxicology and pharmacology : RTP	1		
	4	6	2	12	33359623	2020	Testing the validity	/ of a proposed dermal cancer slope fa	Magee; Forsberg Regulatory toxicology and pharmacology : RTP	1	r	
	0	5	1	6	28477805	2017	Pollution characte	ristics, sources and lung cancer risk o	. Wang; Xia; Wu; Zhang; Sun; Yin; Zhou; Yang Journal of environmental sciences (China)			
	4	4	2	10	20888881	2010	Development and	application of a skin cancer slope fact	Knafla; Petrovic; Richardson; Campbell; Rowat Regulatory toxicology and pharmacology : RTP			
	4	4	1	9	16307791	2005	Health risk assess	ment on human exposed to environm	. Chen; Liao The Science of the total environment			
	2	4	1	7	11807932	2002	Cancer risk asses	sment for oral exposure to PAH mixtu	Schneider; Roller; Kalberlah; Schuhmacher-Wolz Journal of applied toxicology : JAT			
	2	3	1	6	32460055	2020	PAHs in Chinese a	atmosphere Part II: Health risk assess	Ma; Zhu; Liu; Jia; Yang; Li Ecotoxicology and environmental safety			
	0	3	1	4	23379661	2013	Parent and haloge	enated polycyclic aromatic hydrocarbo	. Ni; Guo Journal of agricultural and food chemistry			
	0	3	1	4	20800879	2010	Health risk assess	ment on dietary exposure to polycycli	Xia; Duan; Qiu; Liu; Wang; Tao; Jiang; Lu; Song; Hu The Science of the total environment			
	2	3	1	6	16293284	2005	Probabilistic risk a	essessment for personal exposure to c	Liao; Chiang Chemosphere			
	0	2	1	3	17544483	2007	Health risk assess	ment for traffic policemen exposed to	Hu; Bai; Zhang; Wang; Zhang; Yu; Zhu The Science of the total environment			
	0	1	1	2	28795279	2017	Human health risk	assessment and PAHs in a stretch of	Srivastava; Sreekrishnan; Nema Environmental monitoring and assessment			
	0	1	1	2	12634119	2003	Deviation from ad	ditivity in mixture toxicity: relevance of	Lutz; Vamvakas; Kopp-Schneider, Schlatter; Stopper Environmental health perspectives			
	0	1	2	3	3709501	1986	The adsorption of	polyaromatic hydrocarbons on natura	Menard; Noel; Khorami; Jouve; Dunnigan Environmental research			
$\square$	0	0	1	1	33136306	2020	Effects on Anical (	Outcomes of Regulatory Relevance of	Crumo: Boulander: Farhat: Williams: Basu: Hecker: Environmental toxicology and chemistry			•

#### Development of a dermal cancer slope factor for benzo[a] pyrene.

Polycyclic aromatic hydrocarbons (PAHs) are commonly found at environmentally impacted sites in both Canada and the United States, and also occur naturally. Typically, benzo[a] pyrene (B[a]P) is selected as a standard to which the cancer potencies of other carcinogenic PAHs are compared. Cancer potency estimates for B[a]P have been published for the oral and inhalation routes of exposure, however, no such estimate has been established by a regulatory agency for dermal exposure. The main objectives of the current investigation were to: evaluate approaches used to examine the relative carcinogenicity of PAHs; to conduct a review of mammalian dermal carcinogenicity studies for B[a]P, and derive a cancer slope factor for dermal exposure to PAHs using B[a]P as a surrogate for other PAHs. The toxicological database of dermal B[a]P studies was examined for relevant animal bioassays. Seven relevant studies were identified. A cancer slope factor of D[a]P was developed using the benchmark dose approach and the linearized multistage model. The upper 95th C1 at the 5% effect level above background incidence was used as the point of departure for low-dose linear extrapolation. An average slope factor of 0.5 (microg/animal day)(-1) was calculated for mice, which was converted to a dose-equivalent slope factor of 25 (mg/kg day)(-1). This latter slope factor is proposed for application to human health risk assessment with no scaling adjustment. Dermal potency equivalency factor values were identified area for further investigation is the consideration of scaling in extrapolating the calculated dermal cancer slope factor from mice to humans.

### External Links – Also use Identifiers Names, CASRN, PubChem IDs, InChIs



Benzo(a)pyrene 50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

EPA Substance Registry Service

PubChem

Chemspider

CPCat

🥖 DrugBank

W Wikipedia

Q MSDS Lookup

ChEMBL

😨 ToxPlanet

ACS Reagent Chemicals

🜞 Wolfram Alpha

🔀 ECHA Infocard

🖳 ChemAgora

Consumer Product Information Database

ChEBI

NIST Chemistry Webbook

WEBWISER

PubChem Safety Sheet

PubChem: Chemical Vendors

Consumer Product Information Database

Toxicology

ACToR

on DrugPortal

CCRIS

ChemView

CTD

Gene-Tox

HSDB

ACToR PDF Report

CREST
 National Air Toxics Assessment

ECOTOX

ChemView

BindinaDB

Chemical Checker

MIOSH IDLH Values

actMed

ECOTOX

Publications

and Toxline

PPRTVWEB

🕪 PubMed

IRIS Assessments

🖲 EPA HERO

NIOSH Skin Notation Profiles

🗰 NIOSH Pocket Guide

RSC Publications

🕌 BioCaddie DataMed

 Springer Materials

Bielefeld Academic Search Engine

CORE Literature Search

G Google Books (Text Search)

Google Patents (Text search)

Google Scholar (Text search)

G Google Patents (Structure search)

G Google Books (Structure Search)

Google Scholar (Structure search)

Federal Register

#### Analytical

RSC Analytical Abstracts

🗟 Tox21 Analytical Data

MONA: MassBank North America

imzCloud 🌰

NIST IR Spectrum

NIST MS Spectrum

🛋 MassBank

NIST Antoine Constants

IR Spectra on PubChem

NIST Kovats Index values

Protein DataBank

🍐 National Environmental Methods Index

#### Prediction

2D NMR HSQC/HMBC Prediction

Carbon-13 NMR Prediction

Proton NMR Prediction

\* ChemRTP Predictor

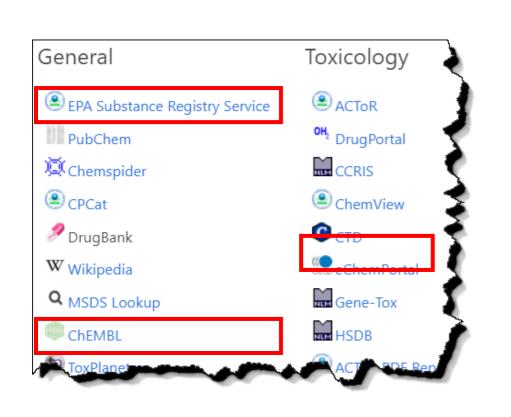
LSERD

SEPA United States Environmental Protection

### External Links



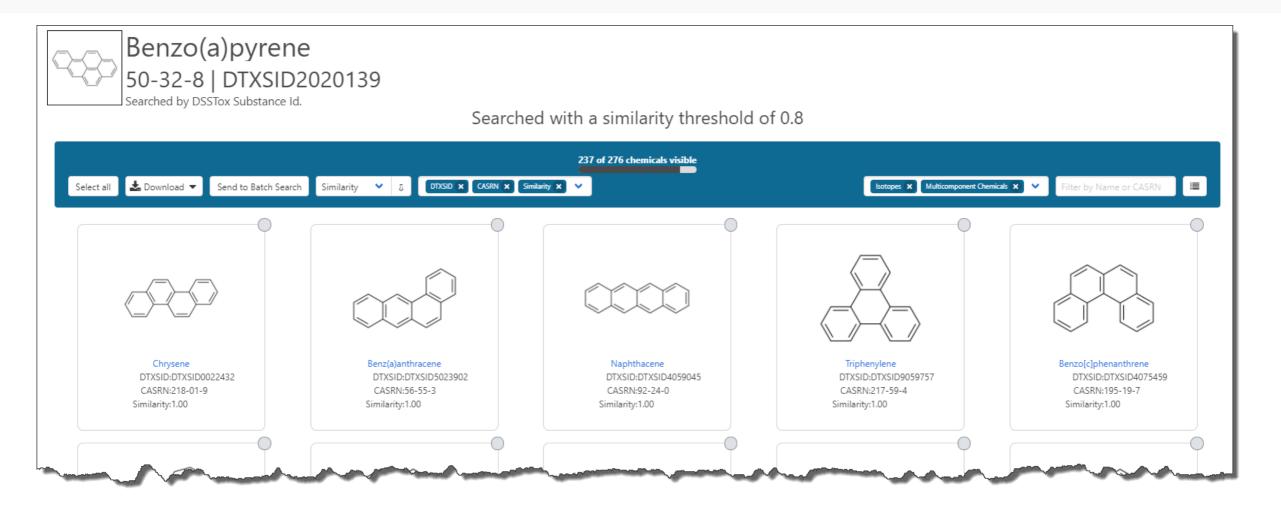
### Links to ~90 websites providing access to additional data on the chemical of interest



Schedules of Assessments	s Data sources At	bout ▼ Help ▼	Contact Us
h			
Irces			
R 🔮 💽 AGRI	ITOX <sup>1</sup>	<ul> <li>AICIS assessm</li> </ul>	ents <sup>1</sup>
1A-CR • CCR	0	CESAR <sup>0</sup>	
F	AGR	A GRITOX •	AGRITOX AGRITOX AICIS assessm

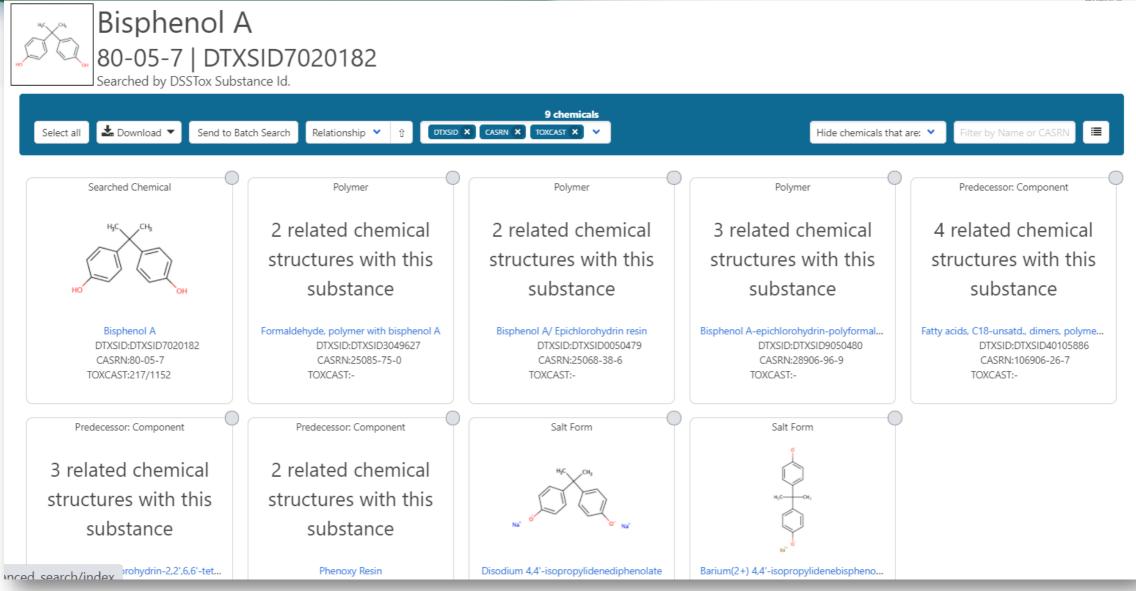
### Similarity Searching





### **Related Substances**







# Chemical Lists and Categories

### Example: AEGLs list



				Lists of Che	micals from			
				List of Assay	/5			
		AEG	LS: Acute Expos	ure Guidelin	e Levels			
		GLVALUES Chemicals						
<b>.</b> .	Identifier sub	usung search						
Details								
Description: Acute Exposure Guideline								
	man health effects	from once-in-a-lifetime, or ra						
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu	man health effects	from once-in-a-lifetime, or ra						
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu	man health effects	from once-in-a-lifetime, or ra						
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic				other catastrophic expos	
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic	cals. Used by emergency		g with chemical spills or c	other catastrophic expos	ures, AEGLs are set
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic	cals. Used by emergency		g with chemical spills or c	other catastrophic expos	ures, AEGLs are set
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic	cals. Used by emergency		g with chemical spills or c	other catastrophic expos	ures, AEGLs are set
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic	cals. Used by emergency		g with chemical spills or c	other catastrophic expos	ures, AEGLs are set
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic	cals. Used by emergency		g with chemical spills or c	other catastrophic expos	ures, AEGLs are set
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or ra tors worldwide.	are, exposure to airborne chemic	cals. Used by emergency		g with chemical spills or c	other catastrophic expos	ures, AEGLs are set
Description: Acute Exposure Guideline uideline levels (AEGLs) describe the hu hrough a collaborative effort of the pu lumber of Chemicals: 174	man health effects blic and private sec	from once-in-a-lifetime, or rators worldwide.	are, exposure to airborne chemic	74 chemicals		g with chemical spills or c	other catastrophic expos	lame or CASRN

### PFAS lists of Chemicals



Copy Filtered Lists URL

#### Select List

PFAS

Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS

PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

📥 Download 🔻 🛛 Columns 🗸

Global Database PFAS Community-

2015)

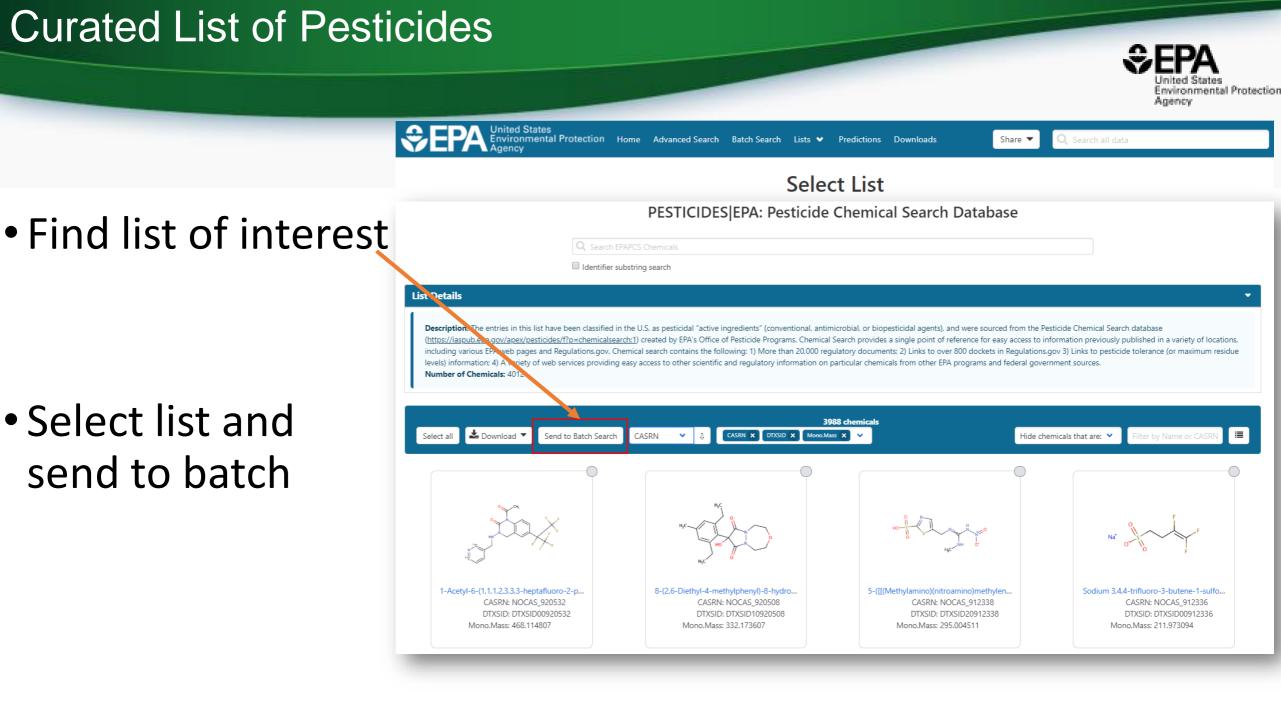
Compiled List (Trier et al.,

2017-07-16

597

PFASTRIER

List Acronym \$	List Name 🗘	Last Updated 🗢	Number of Chemicals 🕈	List Description $\diamond$			
EPAPFAS75S1	PFAS EPA: List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.			
EPAPFAS75S2	PFAS EPA: List of 75 Test Samples (Set 2)	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.			
EPAPFASCAT	PFAS EPA Structure- based Categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.			
EPAPFASINSOL	PFAS[EPA: Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found be insoluble in DMSO above 5mM.			
EPAPFASINV	PFAS EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.			
EPAPFASRL	PFAS EPA: Cross-Agency Research List	2017-11-16	199	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various interna literature and public sources by EPA researchers and program office representatives.			
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.			
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.			
PFASOECD	PFAS: Listed in OECD	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and			





# **Batch Searching**

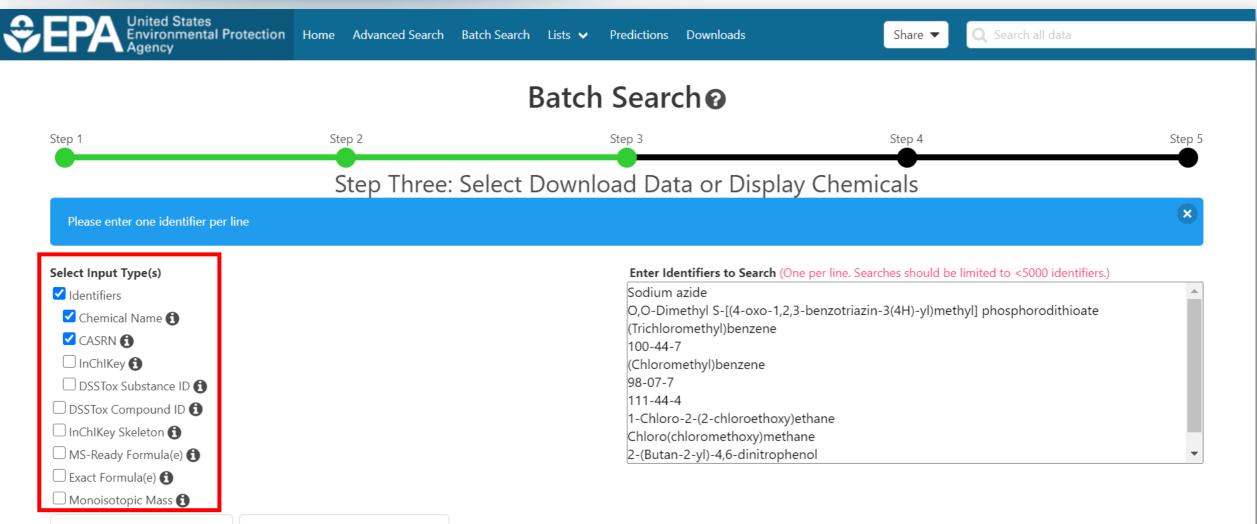
### **Batch Searching**



- Singleton searches are great but...
- ...we generally want data on LOTS of chemicals!
- Typical questions
  - What are the structures for a set of chemical names? Set of CASRNs?
  - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
  - Can I include predicted properties? OPERA? TEST?
  - Are "these chemicals" screened in Toxcast?
  - I need masses and formulae for a list of chemicals

### Access data en masse for thousands of chemicals.





### Select Output Format and Content



#### Step Four: Select Data Output Format and Choose Data Fields to Download

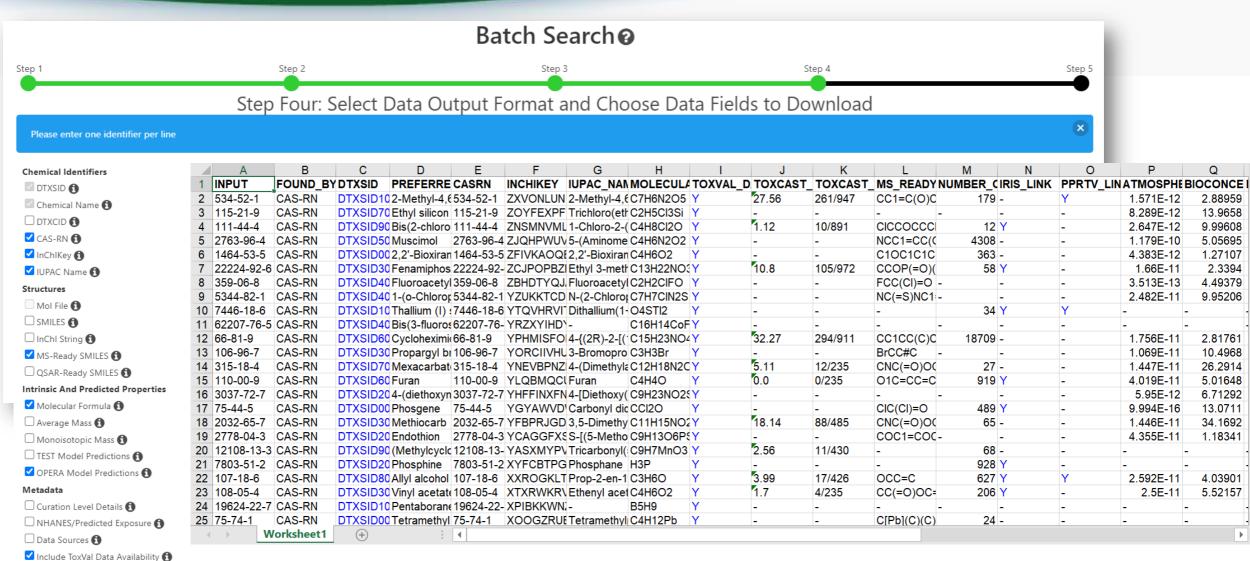
#### Select Output Format:

📰 Excel 🗸 🗸		📩 Download
Customize Results	Intrinsic And Predicted Properties	Presence in Lists:
Select All	🗌 Molecular Formula 🕄	🗌 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks) 🖸
Select All in Lists	Average Mass 🚯	□ 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities 🗹
Chemical Identifiers	🗌 Monoisotopic Mass 🚯	AEGLS: Acute Exposure Guideline Levels 🗹
DTXSID 🚯	TEST Model Predictions ①	ANDROGEN: Androgen Receptor Chemicals 🗹
Chemical Name 🚯	OPERA Model Predictions 🚯	ARTICLE; Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014) 🖸
	Metadata	ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)
CAS-RN (	Curation Level Details 🚯	ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
InChlKey	□ NHANES/Predicted Exposure <b>(</b> )	$\square$ ATSDR Toxicological Profiles $\square$
UPAC Name	Data Sources 🕄	□ ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances ☑
Structures	Include ToxVal Data Availability 🕄	$\square$ ATSDR: Toxic Substances Portal Chemical List $\square$
Mol File	Assay Hit Count 🕄	California Office of Environmental Health Hazard Assessment
	Number of PubMed Articles 🕄	
InChl String	PubChem Data Sources	Canadian Domestic Substances List 2019
	CPDat Product Occurrence Count 🕄	CATEGORY: Amino acids
MS-Ready SMILES		CATEGORY: Color Index dyes
QSAR-Ready SMILES 🚺	PPRTV	CATEGORY: Flame Retardants 🗹
	🗌 Wikipedia Article	

QC Notes
CONTENDED
CONTENDE
CONTENTE
C

### **Batch Search CASRNs**





Assay Hit Count 🚯

✓ Number of PubMed Articles 🚯

### Send to batch and select....



#### Intrinsic And Predicted Properties

- 🔲 Molecular Formula 🚯
- 🔲 Average Mass 🚯
- 🔲 Monoisotopic Mass 🚯
- TEST Model Predictions (1)
- OPERA Model Predictions

#### Metadata

- Curation Level Details (1)
- NHANES/Predicted Exposure 3
- 🔲 Data Sources 🚯
- 🔲 Include ToxVal Data Availability 🚯
- 🗏 Assay Hit Count 🚯
- Number of PubMed Articles 1
- PubChem Data Sources (1)
- CPDat Product Occurrence Count (1)
- 🗆 iris 🕄
- 🗆 PPRTV 🕄

- A few seconds to assemble
  - ToxCast data #actives/#assays and % active
  - # articles in PubMed
  - Links to IRIS or PPRTV reports
  - TEST or OPERA predictions
  - Exposure data: predictions and CPDat

A	В	С	D	E	F	G	н			K L	М
DTXSID		-	MEL EXPOCAST					#PUBMED	PUBCHEM	CPDAT COUNIRIS LIN	
DTXSID2021105	Pentachloronitrobenzene		Y	Y		11.8	99/839	69	96	164 Y	-
DTXSID4022527	Propylparaben	1.4e-05	Y	Y	Υ	13.77	99/719	201	121	1476 -	-
DTXSID4024064	Dinex	8.29e-08	Y	-	Υ	42.13	99/235	-	35	5 Y	-
DTXSID0032493	Triadimenol	1.73e-08	Y	-	Y	10.54	98/930	163	74	83 -	-
DTXSID4032667	Esfenvalerate	1.7e-06	Y	-	Y	11.45	98/856	483	45	198 -	-
DTXSID6020561	Endrin	1.29e-07	Y	-	Υ	14.02	98/699	284	16	98 <mark>Y</mark>	Υ
DTXSID6025355	Glutaraldehyde	2.03e-05	Y	-	Υ	14.35	98/683	6515	139	1144 -	-
DTXSID8032417	Isofenphos	1.87e-08	Y	-	Υ	16.28	98/602	30	42	60 -	-
DTXSID6032352	Chlorpyrifos-methyl	1.07e-07	Y	Y		11.27	97/861	72	50	116 -	-
DTXSID8020620	Fenthion	8.99e-08	Y	Y	Υ	11.56	97/839	354	100	99 -	-
DTXSID2020189	FD&C Blue No. 1	0.000178	Y	-		13.72	97/707	174	49	672 -	-
DTXSID7044843	Erythrosin B	6.3e-07	Y	-	-	24.25	97/400	14843	51	7 -	-
DTXSID5041778	Chloropropylate	1.05e-07	Y	-	Y	40.93	97/237	-	36	12 -	-
DTXSID5023900	Benomyl	1.11e-07	Y	-		11.23	96/855	476	91	105 <mark>Y</mark>	-
DTXSID9020247	Carbaryl	5.61e-08	Y	Υ	Υ	11.51	96/834	1135	117	245 <mark>Y</mark>	-
DTXSID8024109	Flutolanil	1.63e-08	Y	-		11.4	95/833	6	59	80 -	-
DTXSID1023998	Cypermethrin	1.62e-06	Y	Y		10.78	94/872	1148	148	246 -	-
DTXSID2024242	Paclobutrazol	9.19e-08	Y	-		11.11	94/846	139	-	40 Y	-
DTXSID1020807	2-Mercaptobenzothiazole	4.7e-05	Υ	-	Υ	12.82	94/733	111	181	86 -	Υ

### Coming Soon....NEW DASHBOARD https://ccte-ccd.epa.gov/dashboard/



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. This documentation can help get you started.	
CompTox Chemicals Dashboard Search Chemicals	•
Chemicals Products/Use Categories Assay/Gene	
Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey	
Identifier substring search	
Latest News Read More News	
Dashboard update release 3.0.5 - March 2019 Updated at October 14, 2021 An update to the dashboard has been released in March 2019 to coincide with the Society of Toxicology and American Chemical Society Spring meetings. Six months of effort has resulted in the addition of 110,000 new chemical substances being added, improved support for Toxcast bioassay data (integrating data from the invitroDB_v3 release), the addition of multiple chemical lists and new user interface	

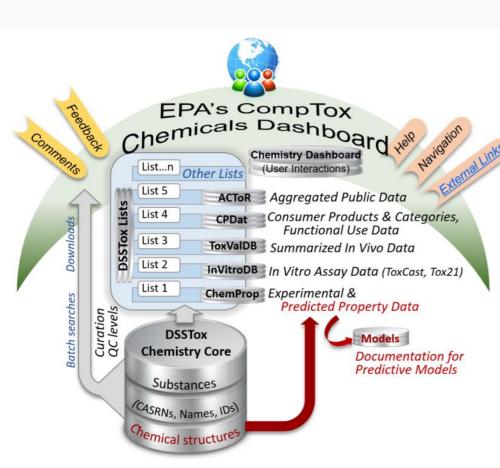
### Proof-of-Concept Apps



- Structure-substructure-similarity searching of Dashboard
- Batch prediction of physicochemical properties and toxicity
- "Hazard Comparison Dashboard" for comparing hazard profiles for chemicals Hazard Comparison Dashboard

zard Comparison Dashb ion: DEV, build: 2021-10-14 13:20:4											*	HAZARD	P	REDICT	5	SEARC	нĘ	🖗 STAI	NDARD	IZE (	🖗 тох	PRINT	og
<b>↑</b>																Full			¢	V	ŀ	X	Ĩ
					Toxici	ity: VH -		_		Nedium L Effects	- Low I	- Inconclusi	ive N/A -N	lot Applic	able Au	thority: Au		<b>ive</b> (i) Sci oxicity	reening (	D <i>QSAR</i> Fate	Model 🛈		
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107-02-8 Acrolein	AHIGB	VH	VH	н	н	VH	L	L	L		н	н	н	I	VH	VH	VH	VH	L	м	_		
107-13-1 Acrylonitri		н	н	н	VH	VH	L	н	н	н	н	н	м	н	н	VH	н	н	н	L			
309-00-2 Aldrin	IGBTP	н	VH	н	VH	н	Н	М	М	Н	н	н			М	М	VH	VH		VH			
107-18-6 Allyl alcoh	ol	н	н	н	н	VH	Н	н	н		н	L	М	T	н	н	VH	VH	L	L			
12125-02- Ammonium ch		М	I	L	I	VH	н	L	I		М	н		L	М	н	VH	νн	н	L			
3012-65-5 Diammonium						VH											L		L	L			

### Summary and Conclusion





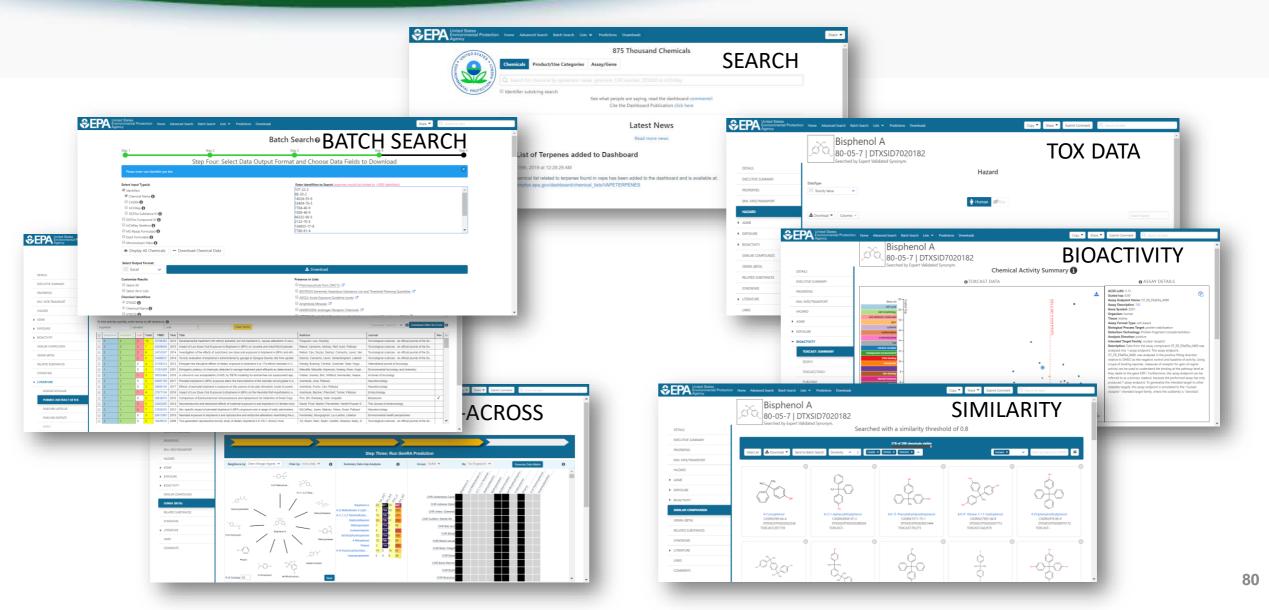
- CompTox Chemicals Dashboard a central hub for environmental data
  - ~875k chemical substances
  - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
  - Interrogation of bioactivity data -
  - Multiple types of searches



- Batch search for thousands of chemicals
- Real-time property and toxicity predictions
- Downloadable files CSV, TSV and Excel

### CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard





### If you find an error, or want to comment... Select text and "Submit Comment"



Home Advanced Search Batch Search Lists 🛩 Predictions Down	loads	Сору 🔻	Share 🔻	Submit Comment	<b>Q</b> Search a
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	Wikipedia				
CH <sub>3</sub>	dimethylbenzene	, or a combin ing with two	ation thereof methyl group	<b>cylol</b> or <b>dimethylbenze</b> . With the formula (CH <sub>3</sub> os attached at substitue	) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> , each of t
	Quality Cont	rol Notes			
	III-defined subs	tance;			
	Intrinsic Prop	perties			
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	Monois	otopic Mass	:0 g/mol		

#### New Comment

#### Details to be submitted with your comment

#### Text selected: 1330-20-7

Found On: July 14th 2021, 7:08:59 am Original Query: /dsstoxdb/results?search=DTXSID2021446 Browser: Chrome 91

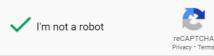
#### Comment

This does not match the CASRN I have for Xylene. I have 95-47-6. Are you sure your CASRN is correct?

6

#### Email address

williams.antony@epa.gov



#### Submit

#### comptox.epa.gov says

Your comment has been submitted and will be reviewed.

### You want to know more...

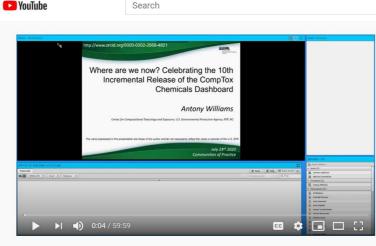


- Lots of resources available
  - Presentations: https://tinyurl.com/w5hqs55
  - Communities of Practice Videos: <a href="https://rb.gy/qsbno1">https://rb.gy/qsbno1</a>

Search

- Manual: https://rb.gy/4fgydc
- Latest News: https://comptox.epa.gov/dashboard/news\_info

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

#### **CompTox Chemicals Dashboard primer videos**

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for over 875,000 chemicals. Data and models within the Dashboard also help with efforts to identify chemicals of most need of further testing and reducing the use of animals in chemical testing.

Explore the wealth of data and features available in the CompTox Chemicals Dashboard with these insructional videos narrated by EPA scientists

#### **General Chemistry and Search Capabilities**



### Acknowledgments



### Contact: <u>Williams.Antony@epa.gov</u>

- Feedback and follow-up is welcomed! Your questions help
- The dashboard is based on the efforts of many more team members than us. Many collaborators provide data also.



EPA's Center for Computational Toxicology and Exposure