

US-EPA Chemicals Dashboard – an integrated data hub for environmental science

Antony John Williams

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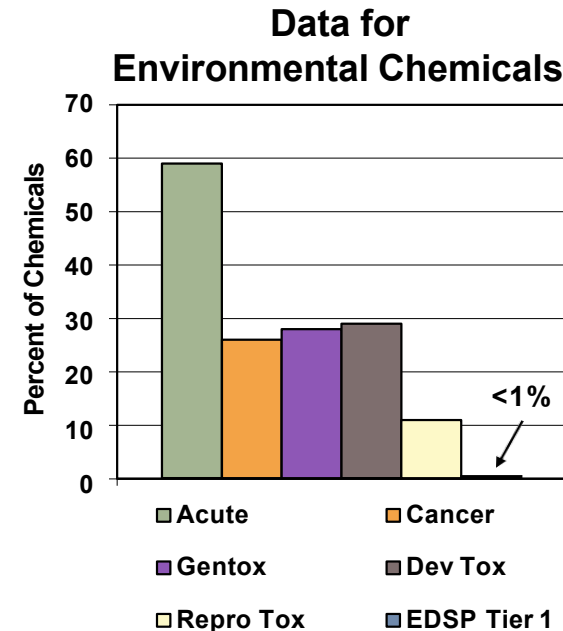
Center for Computational Toxicology and Exposure, US-EPA, RTP, NC

Problem: Too Many Chemicals and Too Few Resources

- Fast characterization of human and ecological risk posed by existing and emerging chemicals is a critical challenge
- Chemistry never stops. But there is sparse and distributed data...



CAS REGISTRY® contains more than **171 million unique organic and inorganic chemical substances**, such as alloys, coordination compounds, minerals, mixtures, polymers and salts, and more than 68 million protein and DNA sequences



Modified from Judson *et al.*, EHP 2010

- 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


If We Database Chemical Structures...

- ...then we can search the dataset by inherent **structural** properties
 - Formula
 - Mass
 - Substructure
 - Structural similarity
- ...we can **integrate** other info into the database for retrieval
- ...available data, both experimental and predicted, is a click away
- ...data can be downloaded, distributed and shared
- ...linking out to other resources enabled by adopting specific standards
- ...structure collections, with associated data, are available for modeling

CompTox Chemicals Dashboard



883k Chemical Substances



United States
Environmental Protection
Agency

HomeAdvanced SearchBatch SearchLists▼PredictionsDownloads

Share▼



Chemicals

Product/Use Categories

Assay/Gene

☐ 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](#).

UNITED STATES


Discover

Connect


Ask

BASIC Search


Chemicals Product/Use Categories Assay/Gene




Benzo(a)pyrene
DTXSID2020139




Benzo(a)pyrene diolepoxide 1
DTXSID9036779




Benzo(a)pyrene- 7,8,9-triol,7,8,9,10-tetrahydro-, (7-alpha,8-beta,9-beta)-
DTXSID00210066




Benzo(a)pyrene-1-methanol
DTXSID40235374




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



Benzo(a)pyrene-11,12-diol
DTXSID70215609



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

- Examples: “perfluoro”

Chemicals

Product/Use Categories

Assay/Gene

perfluoro

☒ Identifier substring search

Search Results

Searched with 'Synonym Substring': Perfluoro

Select all



Download

Send to Batch Search

Substring



DTXSID

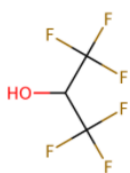
CASRN

TOXCAST

2098 chemicals

Hide chemicals that are:

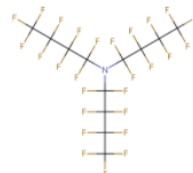
Filter by Name or CASRN



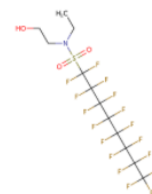
2H-Perfluoro-2-propanol
DTXSID:DTXSID1022134
CASRN:920-66-1
TOXCAST:-



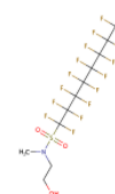
Perfluorooctanesulfonyl fluoride
DTXSID:DTXSID5027140
CASRN:307-35-7
TOXCAST:-



Perfluorotributylamine
DTXSID:DTXSID0027141
CASRN:311-89-7
TOXCAST:-



N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID:DTXSID6027426
CASRN:1691-99-2
TOXCAST:-



N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide
DTXSID:DTXSID7027831
CASRN:24448-09-7
TOXCAST:-

0 related chemical
structures with this
substance

Perfluoro compounds, C5-18
DTXSID:DTXSID5029059
CASRN:86508-42-1
TOXCAST:7/235



Detailed Chemical Pages

One more identifier – the **DTXSID**

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ SAFETY

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS


GENRA (BETA)

RELATED SUBSTANCES

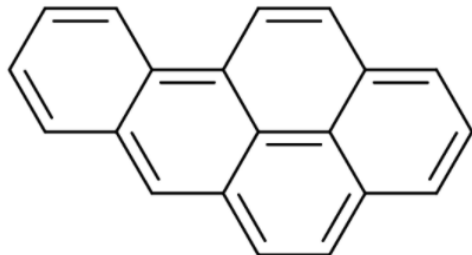
SYNONYMS

▶ LITERATURE

LINKS

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

Searched by DSSTox Substance Id.




Wikipedia


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 (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 C₂₀H₁₂ 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 ...


[Read more](#)


Quality Control Notes


Intrinsic Properties


 **Molecular Formula:** C₂₀H₁₂

 Mol File

 Find All Chemicals

 **Average Mass:** 252.316 g/mol

 Isotope Mass Distribution

 **Monoisotopic Mass:** 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

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

Detailed Chemical Pages

Easy Navigation

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ SAFETY

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS


GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

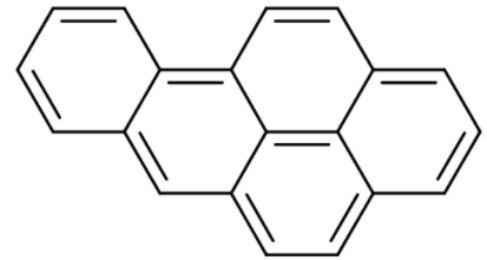
LINKS



Benzo(a)pyrene

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[Read more](#)


Quality Control Notes


Intrinsic Properties


 Molecular Formula: C₂₀H₁₂

 Mol File

 Find All Chemicals

 Average Mass: 252.316 g/mol

 Isotope Mass Distribution

 Monoisotopic Mass: 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

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

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

Intrinsic Properties



Molecular Formula: C₂₀H₁₂




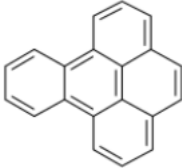
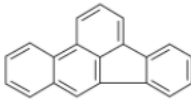
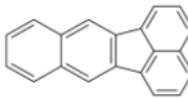
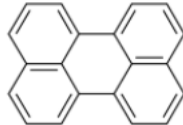
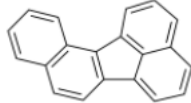
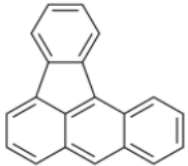
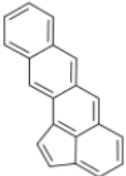
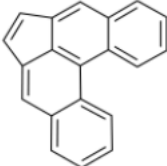
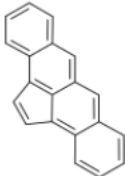
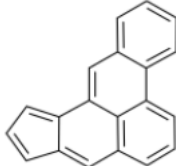
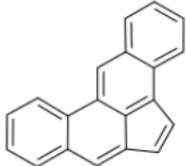
Mol File

Find All Chemicals

Search Results

Searched by Exact Molecular Formula: C₂₀H₁₂.

Download ▾ Send to Batch Search Default ▾ CASRN X DTXSID X ▾ 27 chemicals Hide chemicals that are: ▾ Filter by Name or C

 <p>Benzo(a)pyrene CASRN:50-32-8 DTXSID:DTXSID2020139</p>	 <p>Benzo(e)pyrene CASRN:192-97-2 DTXSID:DTXSID3023764</p>	 <p>Benzo(b)fluoranthene CASRN:205-99-2 DTXSID:DTXSID0023907</p>	 <p>Benzo(k)fluoranthene CASRN:207-08-9 DTXSID:DTXSID0023909</p>	 <p>Perylene CASRN:198-55-0 DTXSID:DTXSID4047753</p>	 <p>Benzo(j)fluoranthene CASRN:205-82-3 DTXSID:DTXSID8052691</p>
 <p>Benzo[a]fluoranthene CASRN:203-33-8 DTXSID:DTXSID4059756</p>	 <p>Cyclopenta(de)naphthalene CASRN:16683-64-0 DTXSID:DTXSID80168197</p>	 <p>Benz(a)acephenanthrylene CASRN:192-28-9 DTXSID:DTXSID70172748</p>	 <p>Cyclopenta(fg)naphthalene CASRN:19770-52-6 DTXSID:DTXSID40173469</p>	 <p>Benzo(de)cyclopent(a)anthracene CASRN:198-46-9 DTXSID:DTXSID60173507</p>	 <p>Benz(e)aceanthrylene CASRN:199-54-2 DTXSID:DTXSID30173675</p>

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

Same Connectivity: [6 records](#) (based on first layer of InChI)

Mixtures, Components and Isotopomers: [DTXCID90112: 25 records;](#)

Similar Compounds: [73 records](#) (based on Tanimoto coefficient >0.8)

Linked Substances

- 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

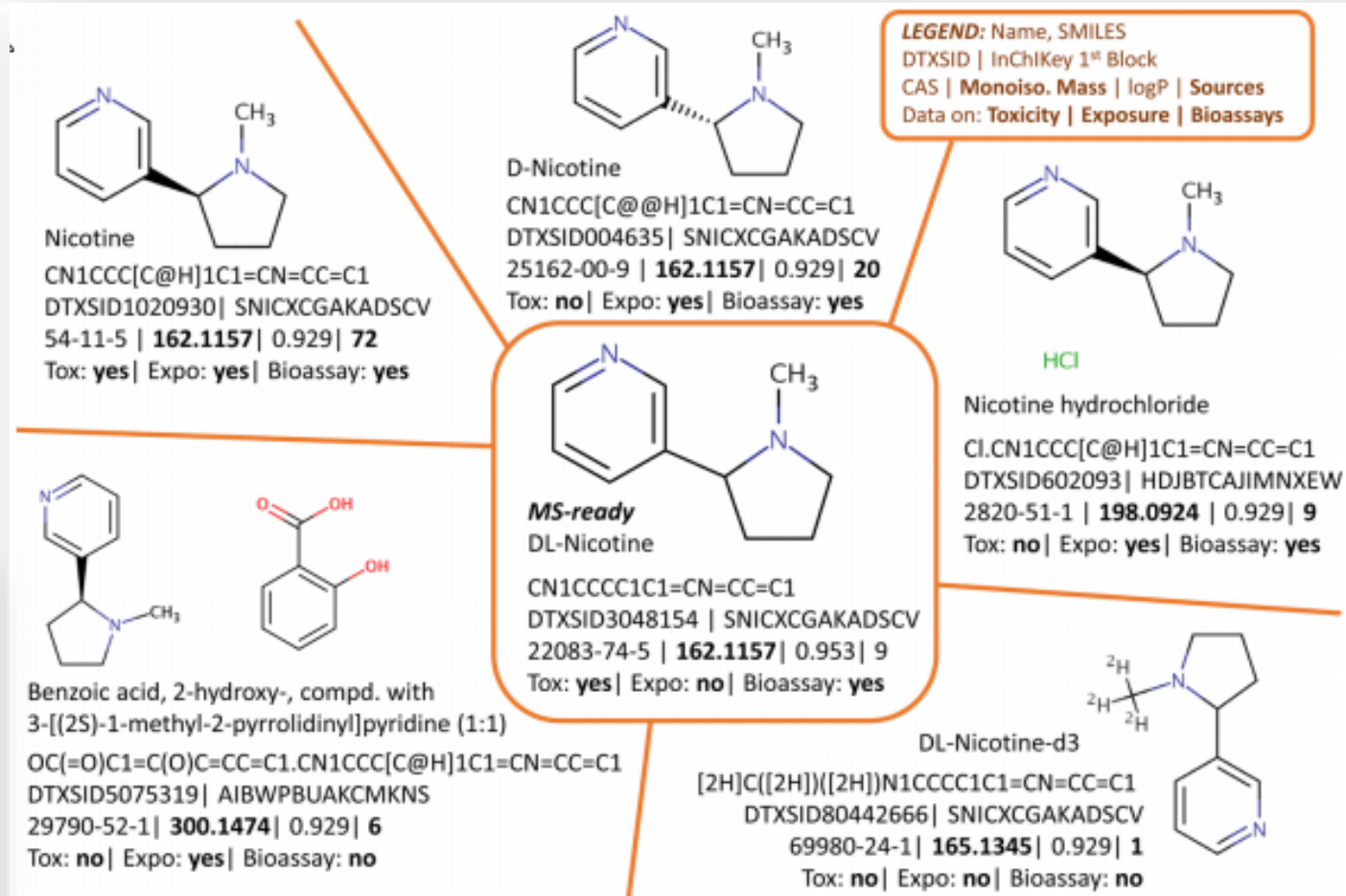
METHODOLOGY

Open Access



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

Andrew D. McEachran^{1,2*}, Kamel Mansouri^{1,2,3}, Chris Grulke², Emma L. Schymanski⁴, Christoph Ruttkies⁵ and Antony J. Williams^{2*}

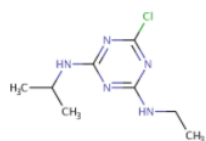


Atrazine Linked Substances

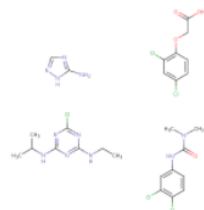
MS-Ready Mappings of Atrazine (Isotopes pre-filtered)

20 of 25 chemicals visible

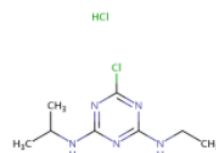
Select all Download Send to Batch Search Default DTXSID CASRN TOXCAST Isotopes Filter by Name or CASRN



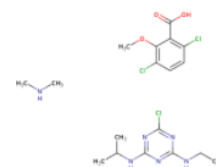
Atrazine
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CASRN:1912-24-9
TOXCAST:62/1024



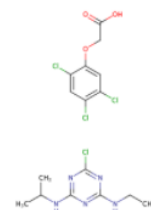
Anox M
DTXSID:DTXSID50156021
CASRN:128996-76-9
TOXCAST:-



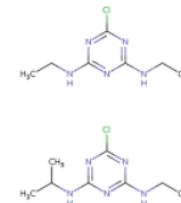
s-Triazine, 2-chloro-4-(ethylamino)-6-(isopropylamino)-
DTXSID:DTXSID30165459
CASRN:15386-47-7
TOXCAST:-



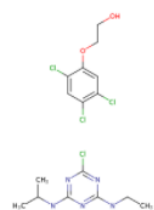
Marksman
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CASRN:160544-50-3
TOXCAST:-



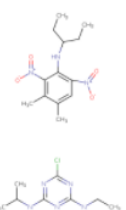
Acetic acid, (2,4,5-trichlorophenoxy)-, methyl ester
DTXSID:DTXSID70192527
CASRN:39283-62-0
TOXCAST:-



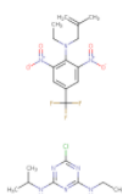
1,3,5-Triazine-2,4-diamine, 6-chloro-N,N-dimethyl-
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TOXCAST:-



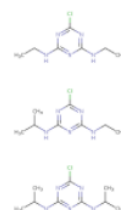
Buvinol
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CASRN:51602-05-2
TOXCAST:-



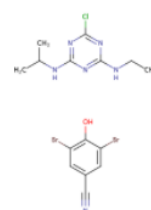
Atrazine mixture with pendimethalin
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CASRN:60704-01-0
TOXCAST:-



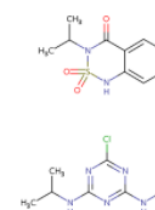
Maizor
DTXSID:DTXSID20215154
CASRN:64867-15-8
TOXCAST:-



Polytriazine
DTXSID:DTXSID00222508
CASRN:72172-70-4
TOXCAST:-




Benzonitrile, 3,5-dibromo-4-hydroxy-, methyl ester
DTXSID:DTXSID20226063
CASRN:75084-56-9
TOXCAST:-



Bentazon / atrazine
DTXSID:DTXSID80226064
CASRN:75084-57-0
TOXCAST:-

Experimental and Predicted Data

Experimental and Predicted Data



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	Predicted average
Water Solubility	8.40e-9 (4)	1.75
LogKow: Octanol-Water	6.13 (2)	6.24
Vapor Pressure	5.49e-9 (1)	3.61e-9
Boiling Point	495 (3)	480
Henry's Law	4.57e-7 (1)	4.59e-7
Melting Point	177 (8)	189
Surface Tension	-	53.9
Flash Point	-	234
Density	-	1.28

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
 - TEST: **T**oxicity **E**stimation **S**oftware **T**ool
 - OPERA: **O**PEn structure–activity/property **R**elationship **A**pp
 - Other commercial algorithms

- What do you trust more? Experimental or predicted data?
- Do you trust individual models or consensus models
- What if there are no experimental data, how good are predictions?

Data Curation Pipelines plus Manual Curation Processes

> SAR QSAR Environ Res. 2016 Nov;27(11):939-965. doi: 10.1080/1062936X.2016.1253611.

An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling

K Mansouri ^{1 2}, C M Grulke ², A M Richard ², R S Judson ², A J Williams ²

Research article | [Open Access](#) | Published: 08 March 2018

OPERA models for predicting physicochemical properties and environmental fate endpoints

[Kamel Mansouri](#) , [Chris M. Grulke](#), [Richard S. Judson](#) & [Antony J. Williams](#)

[Journal of Cheminformatics](#) **10**, Article number: 10 (2018) | [Cite this article](#)

9195 Accesses | **90** Citations | **25** Altmetric | [Metrics](#)

Property and Fate and Transport Data ~25 MILLION pre-predicted values

- We have built QSPR models based on tens of thousands of property data points curated over the past decade
- We push our “QSAR-Ready” chemical structures through predictions to produce property predictions

Methodology | [Open Access](#) | Published: 30 August 2018

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

[Andrew D. McEachran](#) , [Kamel Mansouri](#), [Chris Grulke](#), [Emma L. Schymanski](#), [Christoph Ruttkies](#) & [Antony J. Williams](#) 

[Journal of Cheminformatics](#) **10**, Article number: 45 (2018) | [Cite this article](#)

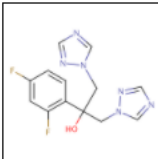
4640 Accesses | **34** Citations | **13** Altmetric | [Metrics](#)

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT



Fluconazole

86386-73-4 | DTXSID3020627

Searched by DSSTox Substance Id.

Property

LogKow: Octanol-Water

Download Summary

Predicted

 Download Predicted Data

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

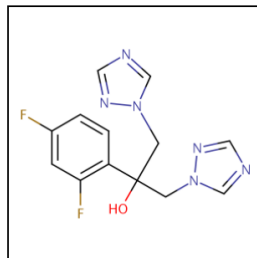
OPERA Reports

OPERA Models: LogKow: Octanol-Water

Fluconazole

86386-73-4 | DTXSID3020627

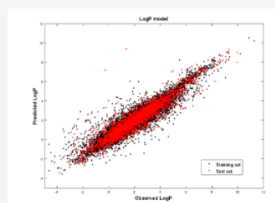
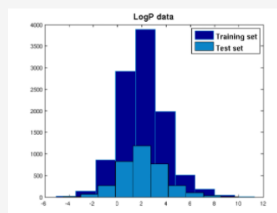
Print PDF



Model Results

Predicted value: 0.501
Global applicability domain: Inside
Local applicability domain index: 0.998
Confidence level: 0.732

Model Performance



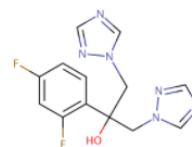
QMRP

Weighted KNN model

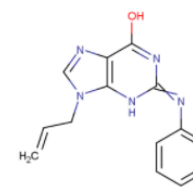
Weighted KNN model

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

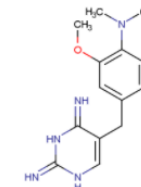
Nearest Neighbors from the Training Set



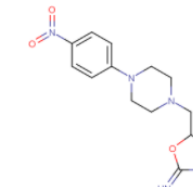
Fluconazole
Measured: 0.5
Predicted: 0.50



GUANINEN2PHENYL9ALLYL
Measured: 1.75
Predicted: 1.75



2,4-PYRIMIDINEDIAMINE, 5-[(4-(DIMETHYLAMINO)-3-M
Measured: 1.87
Predicted: 1.87



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

Similar reports for TEST predictions

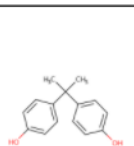
Predicted Normal boiling point for 80-05-7 from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Normal boiling point Å°C	N/A	359.93

Individual Predictions

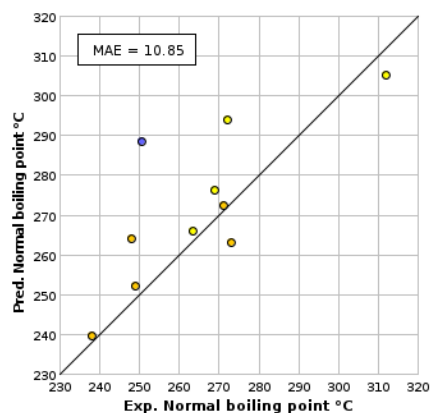
Method	Predicted value Å°C
Hierarchical clustering	372.06
Group contribution	377.41
Nearest neighbor	330.33



Predictions for the test chemical and for the most similar chemicals in the external test set

If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals

Prediction results (colors defined in table below)



Chemicals	MAE*
Entire set	11.46
Similarity coefficient ≥ 0.5	10.85

*Mean absolute error in Å°C

CAS	Structure	Similarity Coefficient	Experimental value Å°C	Predicted value Å°C
80-05-7 (test chemical)			N/A	359.93
14938-35-3		0.81	250.50	288.54
28994-41-4		0.75	312.00	305.28
96-76-4		0.71	263.50	265.93
4130-42-1		0.70	272.00	293.96
616-55-7		0.70	269.00	276.42
2052-14-4		0.69	271.00	272.30

Real-Time Predictions

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CC(C)C1=CC(OC)=C(C2=CC(OC)=C(C)C2)C1

Chiral

Select properties to predict

H **T.E.S.T.**

C

N

O

S

P

F

Cl

Br

I

PT


- ☒ **Toxicological properties**
 - ☒ 96 hour fathead minnow LC50
 - ☒ 48 hour D. magna LC50
 - ☒ 48 hour T. pyriformis IGC50
 - ☒ Oral rat LD50
 - ☒ Bioaccumulation 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

Calculate

- ✓ 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

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<div> Provider: T.E.S.T. <div>Download Summary</div> <div>Calculate</div> </div>						
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/cm ³	0.977 g/cm ³		0.843 g/cm ³	1.057 g/cm ³

Toxicity Data (in vitro *and* in vivo)

ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations

Hazard

DataType
Toxicity Value

Human Eco

Download Columns 10 Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	cancer slope factor	-	chronic	23.5	(mg/kg-day)-1	-	dermal	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.21	(mg/l)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	3.08	(mg/kg-day)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.88	(mg/m3)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	7.3	(mg/kg-day)-1	-	oral	-	Alaska DEC	Alaska DEC
	7	MEG	Short-term Critical Air	short-term	80	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	12	mg/kg	-	Soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, SL/d Negligible Water	chronic	0.0134	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	0.6	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD

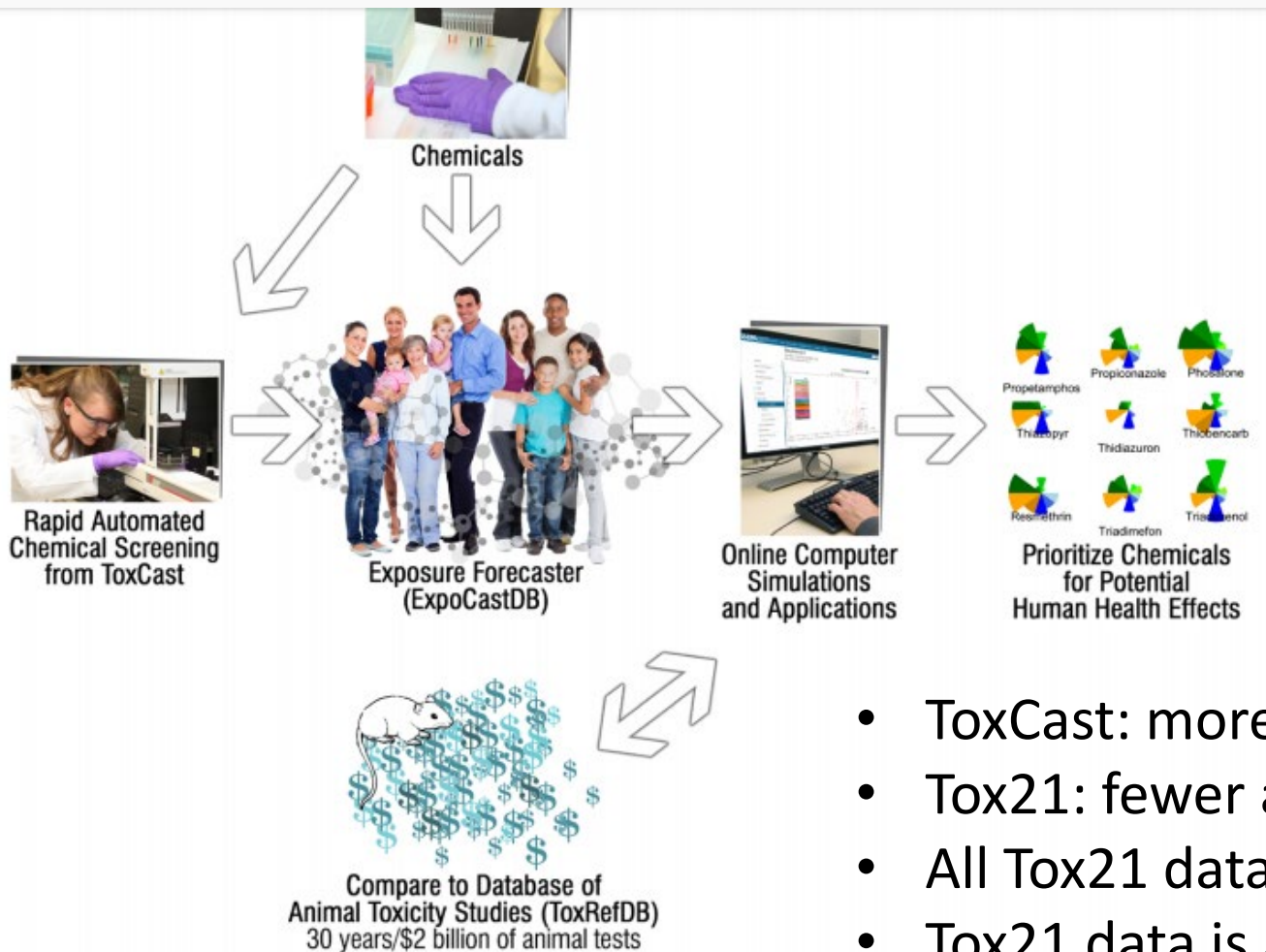
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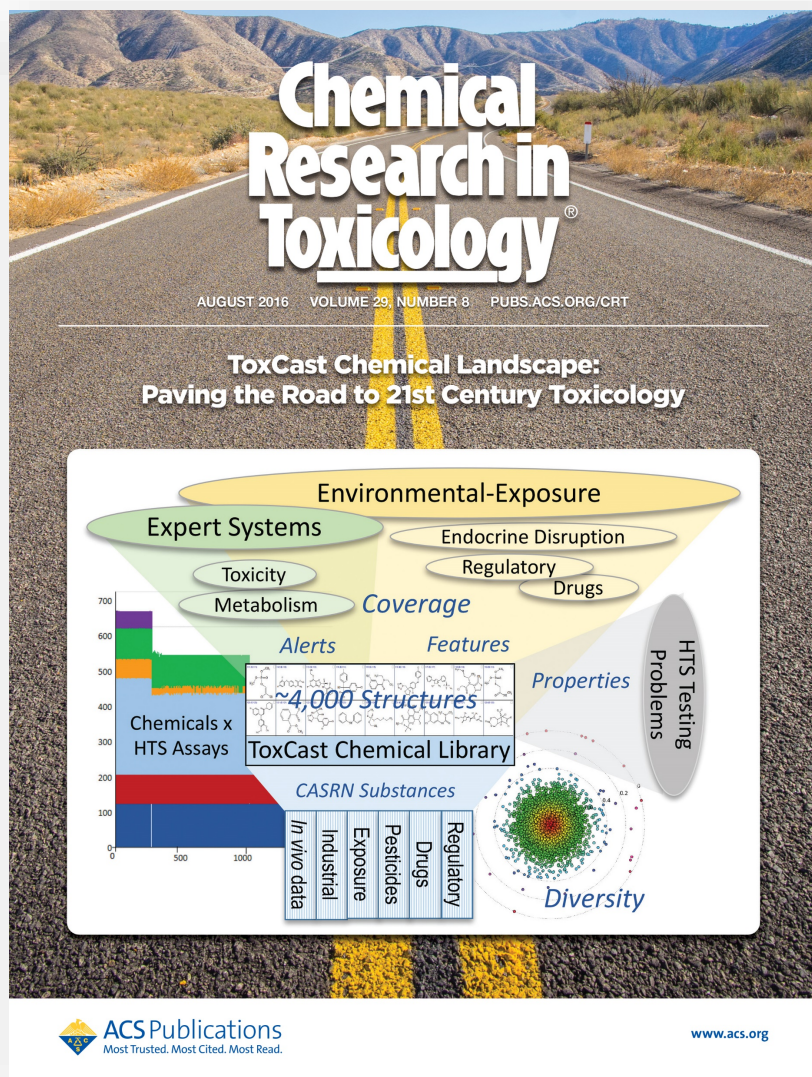
ToxCast and Tox21 bioactivity data for hazard screening and prediction.

EPA's ToxCast program at a glance



Tox21 robot

- ToxCast: more assays, fewer chemicals, EPA-driven
- Tox21: fewer assays, mostly 1536, driven by consortium
- All Tox21 data are analyzed by multiple partners
- Tox21 data is available analyzed in the ToxCast Data Pipeline and other pipelines as well



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

Ann M. Richard^{††}, Richard S. Judson[†], Keith A. Houck[†], Christopher M. Grulke[†], Patra Volarath[†], Inthirany Thillainadarajah[§], Chihae Yang^{||}, James Rathman^{±#}, Matthew T. Martin[†], John F. Wambaugh[†], Thomas B. Knudsen[†], Jayaram Kancherla[▽], Kamel Mansouri[▽], Grace Patlewicz[†], Antony J. Williams[†], Stephen B. Little[†], Kevin M. Crofton[†], and Russell S. Thomas[†]

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Publication Date: July 1, 2016 ▾

<https://doi.org/10.1021/acs.chemrestox.6b00135>

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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 TOXCAST, a reproducible subset of Phase I (ph1v1) chemicals moved into Phase II and later testing phases of the ToxCast program.
TOXCAST_PHASEI	TOXCAST_PhaseI - EPA ToxCast Screening Library (Phase I subset)	2016-01-29	310	TOXCAST_PhaseI corresponds to the ph1v1 subset of TOXCAST (mostly pesticides) screened in Phase I of the ToxCast program.
TOXCAST_PH2	TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset)	2016-01-25	768	TOXCAST_ph2 is the ph2 subset of TOXCAST, added in Phase II of the ToxCast program to increase chemical diversity and coverage of chemicals of concern to EPA programs.
TOXCAST_E1K	TOXCAST_e1k - EPA ToxCast Screening Library (e1k Subset)	2016-01-25	799	TOXCAST_e1k is the e1k subset of TOXCAST, selected for screening in endocrine-related assays.
TOXCAST_PHASEII	TOXCAST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)	2016-01-29	1864	TOXCAST_PhaseII is the full set of chemicals screened in Phase II of the ToxCast program, consisting of TOXCAST_ph1v2, ph2 and e1k sublists.
TOXCAST_PH3	TOXCAST_ph3 - EPA ToxCast Screening Library (ph3 subset)	2018-04-11	2678	TOXCAST_ph3 is the ph3 subset of TOXCAST, added to the most recent Phase III of the ToxCast program to further increase chemical diversity and coverage of chemicals of concern to EPA programs.
TOXCAST_PHASEIII	TOXCAST_PhaseIII - EPA ToxCast Screening Library (Phase III Subset)	2017-04-11	4584	TOXCAST_PhaseIII is the full set of chemicals available for screening in Phase III of the ToxCast program, consisting of the majority of chemicals screened in Phase II and newly added ph3

ToxCast Assays

←

→

↺

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🌐 Apps

📄 Travel Voucher | OR...

📄 ChemReg_v0.9.2a

📄 CCD-INT Dashboard

📄 Jeremy's Admin Pa...


📄 People Plus

📄 Curatr [EMBL - Met...

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Assay Component Endpoint Name ▴▾	Details	Multi Conc. Actives ▴▾	Single Conc. Active	Description	Gene Symbols
ACEA_ER_80hr		456 / 3024	-	Data from the assay component ACEA_ER_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_ER_80hr_Positive, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, measures of the cells for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the subfamily is "steroidal".	ESR1
APR_HepG2_CellCycleArrest_1h_dn		3 / 310	-	Data from the assay component APR_HepG2_CellCycleArrest_1hr was analyzed into 2 assay endpoints. This assay endpoint, APR_HepG2_CellCycleArrest_1h_dn, was analyzed in the negative fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of morphology reporter, measures of all nuclear dna for loss-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene . Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "cell cycle" intended target family, where the subfamily is "proliferation".	
APR_HepG2_CellCycleArrest_1h_up		6 / 310	-	Data from the assay component APR_HepG2_CellCycleArrest_1hr was analyzed into 2 assay endpoints. This assay endpoint, APR_HepG2_CellCycleArrest_1h_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of	

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

Lets look at the data



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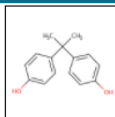
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Bisphenol A

80-05-7 | DTXSID7020182

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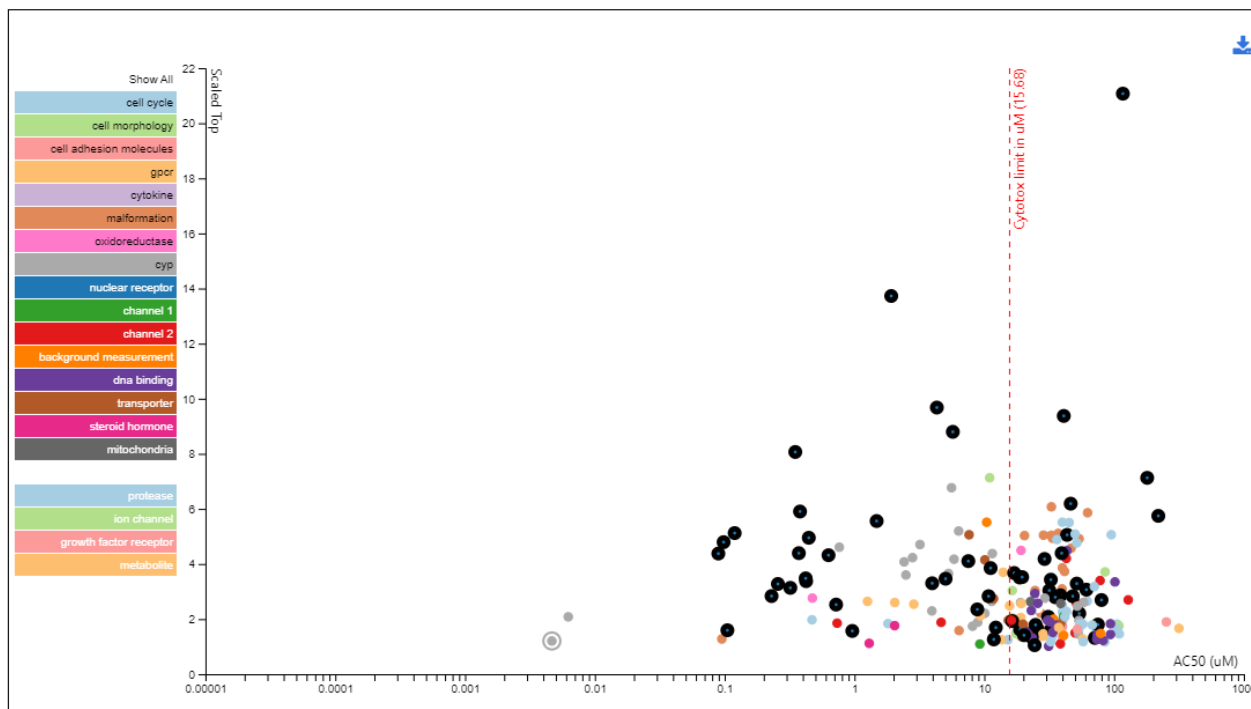
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Chemical Activity Summary i

TOXCAST DATA

ASSAY DETAILS



AC50 (uM): 0.00

Scaled top: 1.21

Assay Endpoint Name: CLD_CYP1A1_6hr

Gene Symbol: CYP1A1

Organism: human

Tissue: liver

Assay Format Type: cell-based

Biological Process Target:

Detection Technology: Quantitative Nuclease Protection Assay (qNPA)

Analysis Direction: positive

Intended Target Family: cyp

Description: inducible reporter assay using Quantitative Nuclease Protection Assay (qNPA) to monitor mRNA in hepatocyte cell line: AED1615 -- CLD_CYP1A1_6hr

Rich data tables – full transparency

217 active of 1152 assays

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







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Name	Modal	SeqAPASS	Gene Symbol	Gene Name	AOP	Event	Hit Call	Top	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
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 	Tspo	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

First

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Bioactivity Data (ToxCast/Tox21)

Data below for Bisphenol A

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Bisphenol A

80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

DC Data ID	Grade	Description
Tox21_2029922	Passe	Purity>90% and MW confirmed
Tox21_450038	Passe	Purity>90% and MW confirmed

Assay Selection 3 Selected

Number of Charts: 18

☒ Active
 ☐ Inactive
 ☐ All

Assay Set: ER (3 of 18 Selected)

- ☒ ACBA 14TU 50hr Positive
- ☒ AIC b1fe CTS up
- ☒ AIC b1fe HKANS up
- ☐ NVS NK BBR
- ☐ NVS NK hBR
- ☐ NVS NK mbR
- ☐ Q1 b1f b1c/b1d 0480
- ☐ Q1 b1f b1c/b1d 1440
- ☐ Q1 b1f b1c/b1d 0480
- ☐ Q1 b1f b1c/b1d 1440
- ☐ Q1 b1f b1c/b1d 0480
- ☐ Q1 b1f b1c/b1d 1440
- ☐ Q1 b1fe b1cGH⁺ 0120
- ☐ Q1 b1fe b1cGH⁺ 0480
- ☐ Tox21 b1fe SLA Agonist ratio
- ☐ Tox21 b1fe SLA Antagonist ratio
- ☐ Tox21 b1fe LUC B21 Agonist
- ☐ Tox21 b1fe LUC B21 Antagonist

Assay Set: AR (0 of 11 Selected)

- ☐ AIC AR HKANS up
- ☐ NVS NK cAR
- ☐ NVS NK hAR
- ☐ NVS NK mAR

A Single Assay Can Have Multiple Charts

#Actives for a chemical

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




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Name	Modal	SeqAPASS	Gene Symbol	Gene Name	AOP	Event	Hit Call	Top	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
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 	Tspo	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

First

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Last

GHS Data

Print Page

[PUBCHEM](#) > [BENZO\[A\]PYRENE](#) > [LABORATORY CHEMICAL SAFETY SUMMARY \(LCSS\)](#) > [GHS CLASSIFICATION](#)




CID 2336

Benzo[a]pyrene

GHS Classification



Showing 6 of 6

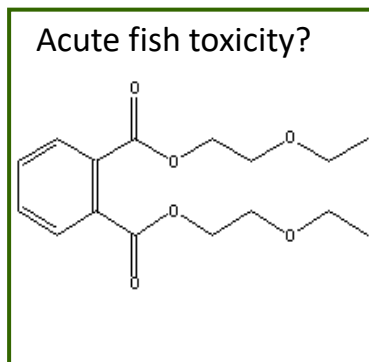
Pictogram(s)	<div></div> <div>Irritant Health Hazard Environmental Hazard</div>
Signal	<u>Danger</u>
GHS Hazard Statements	<div>H317: May cause an allergic skin reaction [<u>Warning</u> Sensitization, Skin]</div> <div>H340: May cause genetic defects [<u>Danger</u> Germ cell mutagenicity]</div> <div>H350: May cause cancer [<u>Danger</u> Carcinogenicity]</div> <div>H360FD: May damage fertility; May damage the unborn child [<u>Danger</u> Reproductive toxicity]</div> <div>H400: Very toxic to aquatic life [<u>Warning</u> Hazardous to the aquatic environment, acute hazard]</div> <div>H410: Very toxic to aquatic life with long lasting effects [<u>Warning</u> Hazardous to the aquatic environment, long-term hazard]</div>
Precautionary Statement Codes	<div>P201, P202, P261, P272, P273, P280, P281, P302+P352, P308+P313, P321, P333+P313, P363, P391, P405, and P501</div> <div>(The corresponding statement to each P-code can be found at the GHS Classification page.)</div>

Generalized Read-Across

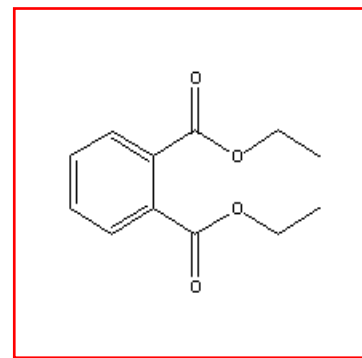
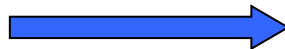
Definitions: Read-Across

- Known information on the property of a substance (source) is used to make a prediction of the same property for another substance (target) that is considered “similar”

	Source chemical	Target chemical	
Property	● → ○		● Reliable data ○ Missing data



Known to be harmful



Predicted to be harmful

GenRA (Generalised Read-Across)

GenRA

Step Two: Data Gap Analysis & Generate Data Matrix

Neighbors by: Chem: Morgan Fgrpts Filter by: invivo data Summary Data Gap Analysis Group: ToxRef By: Tox Fingerprint **Generate Data Matrix**

Select and Review Analogs

Review Available Data

Fingerprint indicating available data

Chemical structures and names: Ethylene glycol, Ethion, Butanal oxime, Myrcene, Ethoprop, Acrolein diethyl..., Chlorothoxyfos, Fosamine amm..., Methyleneugenol, bis(2-Chloro-1-..., 2-Ethoxyethyl a...

		bio h21	bio hct	chm_ct	tox brf
Fluconazole	3	714	15	0	
Hexaconazole	43	819	18	345	
Flusilazole	28	819	9	345	
Cyproconazole	14	819	16	408	
Pyrasulfotole metabolite ...	0	0	18	234	
Myclobutanil	15	818	15	345	
Fenbuconazole	34	819	17	345	
Tetraconazole	35	819	20	345	
Metconazole	35	215	15	82	
Iponazole	46	232	16	180	
Bromuconazole	24	277	13	345	

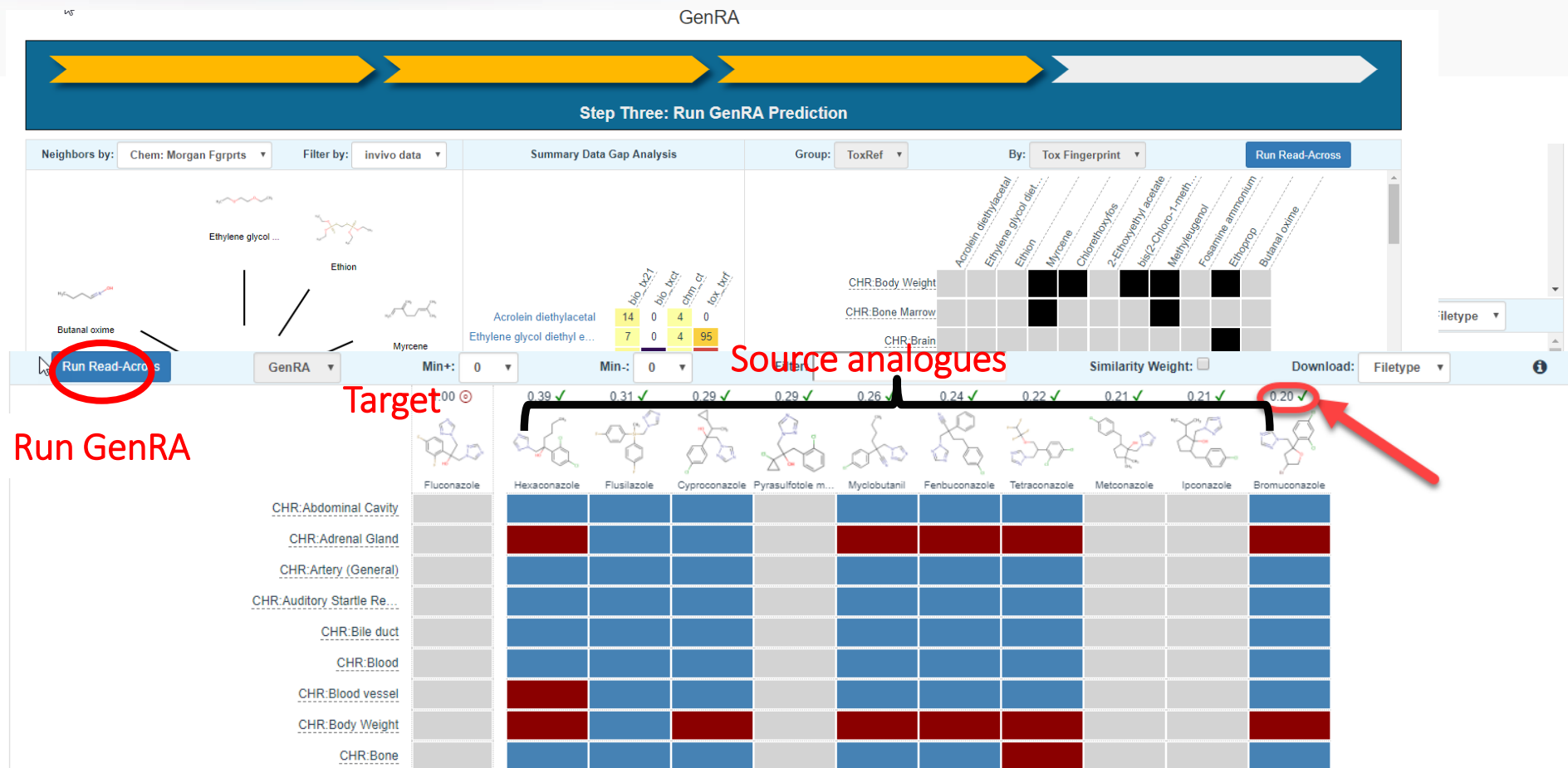
of Analogs: 10

Next

CHR: Abdominal Cavity, CHR: Adrenal Gland, CHR: Artery (General), CHR: Auditory Startle Re..., CHR: Bile duct, CHR: Blood, CHR: Blood vessel, CHR: Body Weight, CHR: Bone, CHR: Bone Marrow, CHR: Brain

Fluconazole, Hexaconazole, Flusilazole, Cyproconazole, Pyrasulfotole metab, Myclobutanil, Fenbuconazole, Tetraconazole, Metconazole, Iponazole, Bromuconazole

GenRA (Generalised Read-Across)

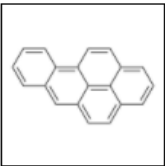


Run GenRA

Red : Toxicity effects.
Blue: No Toxicity effects
Grey : Absence of data

Identifiers and Nomenclature

Identifiers Support Searches in other systems



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Synonyms

Download

25

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

Challenges with Nomenclature

- Be CAREFUL with names! There is a LOT of confusion in the public domain. CHOOSE sources wisely!
- There are MANY public databases but not many are curated
- All public databases have value but not many curate data
- Example: METHANE on PubChem
<https://pubchem.ncbi.nlm.nih.gov/compound/297>

CAS Registry Numbers on PubChem

2.3.1 CAS



74-82-8

- ▶ CAMEO Chemicals; CAS Common Chemistry; ChemIDplus; DrugBank; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECH...

8006-14-2

- ▶ CAMEO Chemicals; EPA Chemicals under the TSCA; EPA DSSTox; European Chemicals Agency (ECHA)

7440-44-0

- ▶ ChemIDplus

7782-40-3

- ▶ ChemIDplus

7782-42-5

- ▶ ChemIDplus

16291-96-6

- ▶ ChemIDplus

64365-11-3

CASRN lookup on the dashboard

Search Results

Searched using Batch Search

8 chemicals

Select all

Download

Send to Batch Search

Default



CASRN

DTXSID

Molecular Formula



Hide chemicals that are:

Filter by Name or CASRN



[Methane](#)

CASRN:74-82-8

DTXSID:DTXSID8025545

Molecular Formula:CH4



[Carbon](#)

CASRN:7440-44-0

DTXSID:DTXSID9027651

Molecular Formula:C

0 related chemical
structures with this
substance

[Natural gas](#)

CASRN:8006-14-2

DTXSID:DTXSID2027676

Molecular Formula:-

2 related chemical
structures with this
substance

[Graphite](#)

CASRN:7782-42-5

DTXSID:DTXSID2049634

Molecular Formula:-

1 related chemical
structure with this
substance

[Charcoal](#)

CASRN:16291-96-6

DTXSID:DTXSID2051217

Molecular Formula:-

1 related chemical
structure with this
substance

[Diamond](#)

CASRN:7782-40-3

DTXSID:DTXSID10905072

Molecular Formula:-

0 related chemical
structures with this
substance

[Activated charcoal](#)

CASRN:64365-11-3

DTXSID:DTXSID801019028

Molecular Formula:-

1 related chemical
structure with this
substance

[Carbon nanotubes](#)

CASRN:308068-56-6

DTXSID:DTXSID301020377

Molecular Formula:-

Methane is Diamond and Nanotubes?

- These are all Depositor Names for Methane ☹️

2.4.2 Depositor-Supplied Synonyms



UN 1971 (Salt/Mix)	Fullerene soot, (as produced)	Carbon Nanotube sponges XFCN01	DTXSID9027651
UN 1972 (Salt/Mix)	MWNTs Butyl acetate suspension	Carbon Nanotube sponges XFCN07	Graphite electrode, rotrode disc
Activated carbon, pellets 3mm	QuadraPure C, 0.3-0.8mm	Carbon Nanotube sponges XFCN08	Carbon conductive cement adhesive
Graphene quantum dots(Powder)	6GRV67N0U2	Carbon, activated, -4+8 mesh	Conductive Flexible TPU Filament
Multiwall Nanotubes 5-15 nm	GO quantum dots yellow(Powder)	Carbon, activated, 2mm & down	GO quantum dots yellow(1mg/ml)
GO quantum dots(C: 1mg/ml)	Graphene electric aqueous slurry	CHEMBL2106049	Graphite powder, -20+84 mesh
;) MWNTs ethyl acetate suspension	Graphene powder Physical methods	Diamond Synthesized, 95% Nano	Carbon black, Super P Conductive
Reduced Graphene Oxide@ SnO2	Reduced Graphene Oxide@ Co3O4	Diethyl Cyanomethyl Phosphonate	DTXSID50179391
Carbon nanotubes aqueous slurry	Carbon Conductive Adhesive Tapes	DTXSID8025545	NanoIntegris metallic SWCNTs70%



A little more about our data quality

- Five full time curators register and curate data to elevate quality

Record Information



Citation: U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. <https://comptox.epa.gov/dashboard/DTXSID0020022> (accessed October 18, 2020), 5-(2-Chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid

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

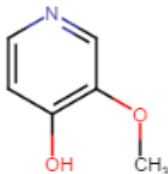
Underneath the Dashboard

View/Edit a Single Record Structure Search Browse/Curate Records Export DSSTox Chemotypes Manage Chemical Lists Manage Property Data Add Deleted Casms

Preferred Name matched null
You are viewing the record associated with
DTXSID80198757
CASRN: 62885-41-0

4-Hydroxy-3-methoxy

Valid license cannot be found



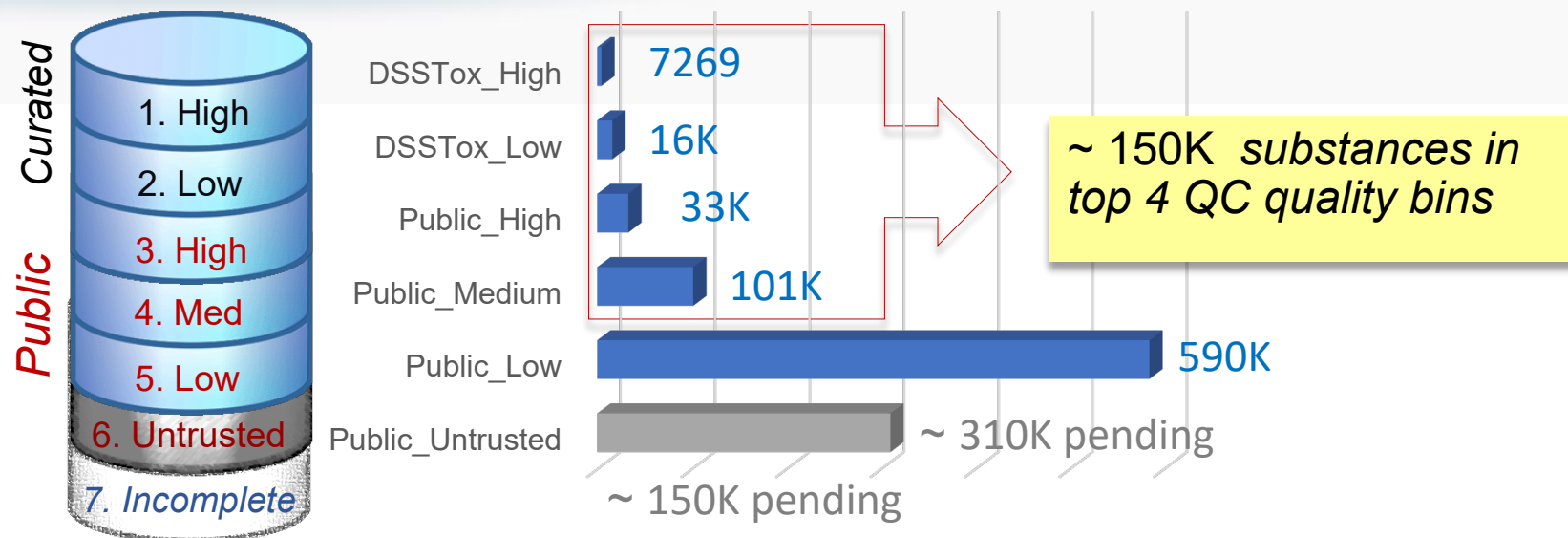
Chemical structure diagram of 4-Hydroxy-3-methoxypyridine, showing a pyridine ring with a hydroxyl group (-OH) at position 4 and a methoxy group (-OCH₃) at position 3.

Calculate from Structure

Substance_ID:	DTXSID80198757	Compound_ID:	DTXCID40121248
CAS:	62885-41-0	Chemical Shown:	Tested Chemical
Name:	4-Hydroxy-3-methoxypyridine	Private Notes:	
Substance Type:	Single Compound	Source of CAS-Compound:	STN(DSSTox)
QC Level:	DSSTox_High	Double Stereo:	None
Data Source:	STN(DSSTox)	Chiral Stereo:	None
QC Notes:	CAS [50700-60-2] assigned by DSSTox to pyridin-one tautomer form, which resolves to hydroxy form thru InChI	Chemical Form:	Organic
		Organic Form:	Parent

Distribution of curated data

Now at >1.2 MILLION substances



QC Levels

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

Computational Toxicology 12 (2019) 100096



ELSEVIER

Contents lists available at ScienceDirect

Computational Toxicology

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

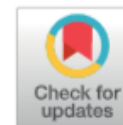


EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke^a, Antony J. Williams^a, Inthirany Thillanadarajah^b, Ann M. Richard^{a,*}

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

^b Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA



What chemicals are in hair care products?

Chemicals

Product/Use Categories

Assay/Gene

Q

hair

CPDat PRODUCT category: hair coloring
general hair coloring products which can not be classified into a more refined category

CPDat PRODUCT category: hair coloring hair bleach
products for lightening or removing color from hair on the head

CPDat PRODUCT category: hair coloring hair color - permanent
hair colors and dyes characterized as permanent

CPDat PRODUCT category: hair coloring hair color - professional
hair colors and dyes characterized as for professional use

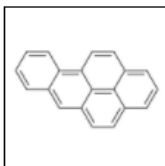
CPDat PRODUCT category: hair coloring hair color activator
chemical activators for hair coloring products

CPDat PRODUCT category: hair coloring hair color developer
chemical developers for hair coloring products

CPDat PRODUCT category: hair styling and care dry shampoo
products for removing oil and dirt from hair

CPDat PRODUCT category: hair styling and care
general hair styling or hair care products which do not fit into a more refined category

Sources of Exposure to Chemicals



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Chemical Weight Fractions

 Download ▾

Columns ▾

10 ▾

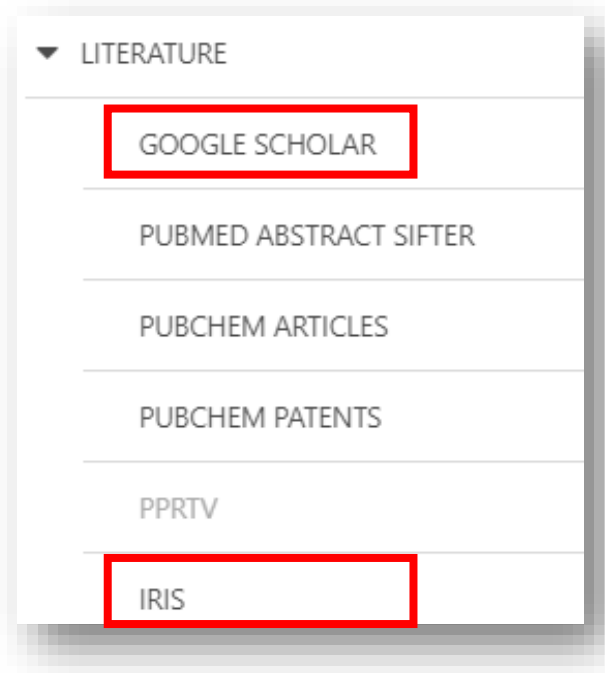
Search query

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
supelprime-hc kit pah mix_48909	Not Yet Categorized:			MSDS	SIRI
supelprime-hc pah mix 1mL_48905	Not Yet Categorized:			MSDS	SIRI

Toxicity Reports and Literature Searching

Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”



EPA United States Environmental Protection Agency

Environmental Topics Laws & Regulations About EPA Search EPA.gov

Contact Us

IRIS

- IRIS Home
- About IRIS
- IRIS Recent Additions
- IRIS Calendar
- IRIS Assessments**
- Advanced Search
- IRIS Program Materials
- Contact Us

Benzo[a]pyrene (BaP)

CASRN 50-32-8 | DTXSID2020139

- [Toxicological Review \(PDF\)](#) (234 pp, 4.67 M)
- [IRIS Executive Summary \(PDF\)](#) (9 pp, 671 K)
- [Supplemental Information on the IRIS Toxicological Review of Benzo\[a\]pyrene](#)

Key IRIS Values Organ/System Specific Values Chemical Documents Other EPA Information

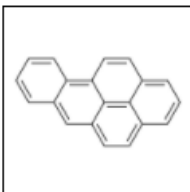
Noncancer Assessment

[Reference Dose for Oral Exposure \(RfD\) \(PDF\)](#) (9 pp, 671 K) Last Updated: 01/19/2017

System	RfD (mg/kg-day)	Basis	PoD

Related Links

- [EPA Chemicals Dashboard - Benzo\[a\]pyrene \(BaP\)](#)




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 

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

Retrieve Articles 


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 find articles quickly, enter terms to sift abstracts. 

dermal cancer pyrene  

<input type="checkbox"/>	dermal	cancer ↓	pyrene	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	0	7	1	8	23922326	2013	Using immunotoxicity information to improve cancer risk a...	Zaccaria, McClure	International journal of toxicology	✓
<input type="checkbox"/>	8	7	2	17	16632147	2006	Development of a dermal cancer slope factor for benzo[a]...	Knafila, Philipps, Brecher, Petrovic, Richardson	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	4	6	2	12	33359623	2020	Testing the validity of a proposed dermal cancer slope fac...	Magee; Forsberg	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	0	5	1	6	28477805	2017	Pollution characteristics, sources and lung cancer risk of ...	Wang; Xia; Wu; Zhang; Sun; Yin; Zhou; Yang	Journal of environmental sciences (China)	
<input type="checkbox"/>	4	4	2	10	20888881	2010	Development and application of a skin cancer slope factor...	Knafila; Petrovic; Richardson; Campbell; Rowat	Regulatory toxicology and pharmacology : RTP	
<input type="checkbox"/>	4	4	1	9	16307791	2005	Health risk assessment on human exposed to environme...	Chen; Liao	The Science of the total environment	
<input type="checkbox"/>	2	4	1	7	11807932	2002	Cancer risk assessment for oral exposure to PAH mixtures.	Schneider; Roller, Kalberlah; Schuhmacher-Wolz	Journal of applied toxicology : JAT	
<input type="checkbox"/>	2	3	1	6	32460055	2020	PAHs in Chinese atmosphere Part II: Health risk assessm...	Ma; Zhu; Liu; Jia; Yang; Li	Ecotoxicology and environmental safety	
<input type="checkbox"/>	0	3	1	4	23379661	2013	Parent and halogenated polycyclic aromatic hydrocarbon...	Ni; Guo	Journal of agricultural and food chemistry	
<input type="checkbox"/>	0	3	1	4	20800879	2010	Health risk assessment on dietary exposure to polycyclic ...	Xia; Duan; Qiu; Liu; Wang; Tao; Jiang; Lu; Song; Hu	The Science of the total environment	
<input type="checkbox"/>	2	3	1	6	16293284	2005	Probabilistic risk assessment for personal exposure to car...	Liao; Chiang	Chemosphere	
<input type="checkbox"/>	0	2	1	3	17544483	2007	Health risk assessment for traffic policemen exposed to p...	Hu; Bai; Zhang; Wang; Zhang; Yu; Zhu	The Science of the total environment	
<input type="checkbox"/>	0	1	1	2	28795279	2017	Human health risk assessment and PAHs in a stretch of ri...	Srivastava; Sreekrishnan; Nema	Environmental monitoring and assessment	
<input type="checkbox"/>	0	1	1	2	12634119	2003	Deviation from additivity in mixture toxicity: relevance of n...	Lutz; Vamvakas; Kopp-Schneider; Schlatter; Stopper	Environmental health perspectives	
<input type="checkbox"/>	0	1	2	3	3709501	1986	The adsorption of polyaromatic hydrocarbons on natural a...	Menard; Noel; Khorami; Jouve; Dunnigan	Environmental research	
<input type="checkbox"/>	0	0	1	1	33136306	2020	Effects on Animal Outcomes of Regulatory Relevance of F...	Crumo; Boulanger; Farhat; Williams; Basu; Hecker	Environmental toxicology and chemistry	

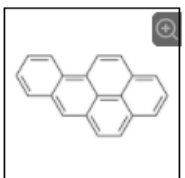
Development of a dermal cancer slope factor for benzo[a]pyrene.
Polycyclic aromatic hydrocarbons (PAHs) are commonly found at environmentally impacted sites in both Canada and the United States, and also occur naturally. Typically, benzo[a]pyrene (B[a]P) is selected as a standard to which the cancer 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 for B[a]P was developed using the benchmark dose approach and the linearized multistage model. The upper 95th CI 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 0.55 (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 which may be used with other carcinogenic PAH in the calculation of total B[a]P equivalent dermal cancer risk estimates. An identified area for further investigation is the consideration of scaling in extrapolating the calculated dermal cancer slope factor from mice to humans.

External Links

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?

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
-  ChempSpider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  ToxPlanet
-  ACS Reagent Chemicals
-  Wolfram Alpha
-  ECHA Infocard
-  ChemAgora
-  Consumer Product Information Database
-  ChEBI
-  NIST Chemistry Webbook
-  WEBWISER
-  PubChem Safety Sheet
-  Consumer Product Information Database
-  PubChem: Chemical Vendors













Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ACToR PDF Report
-  CREST
-  National Air Toxics Assessment
-  ECOTOX
-  ChemView
-  Chemical Checker
-  BindingDB
-  CalEPA OEHHHA
-  NIOSH IDLH Values
-  LactMed
-  ECOTOX






Publications

-  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
-  Google Books (Text Search)
-  Google Patents (Text search)
-  Google Scholar (Text search)
-  Google Patents (Structure search)
-  Google Books (Structure Search)
-  Google Scholar (Structure search)
-  Federal Register

Analytical

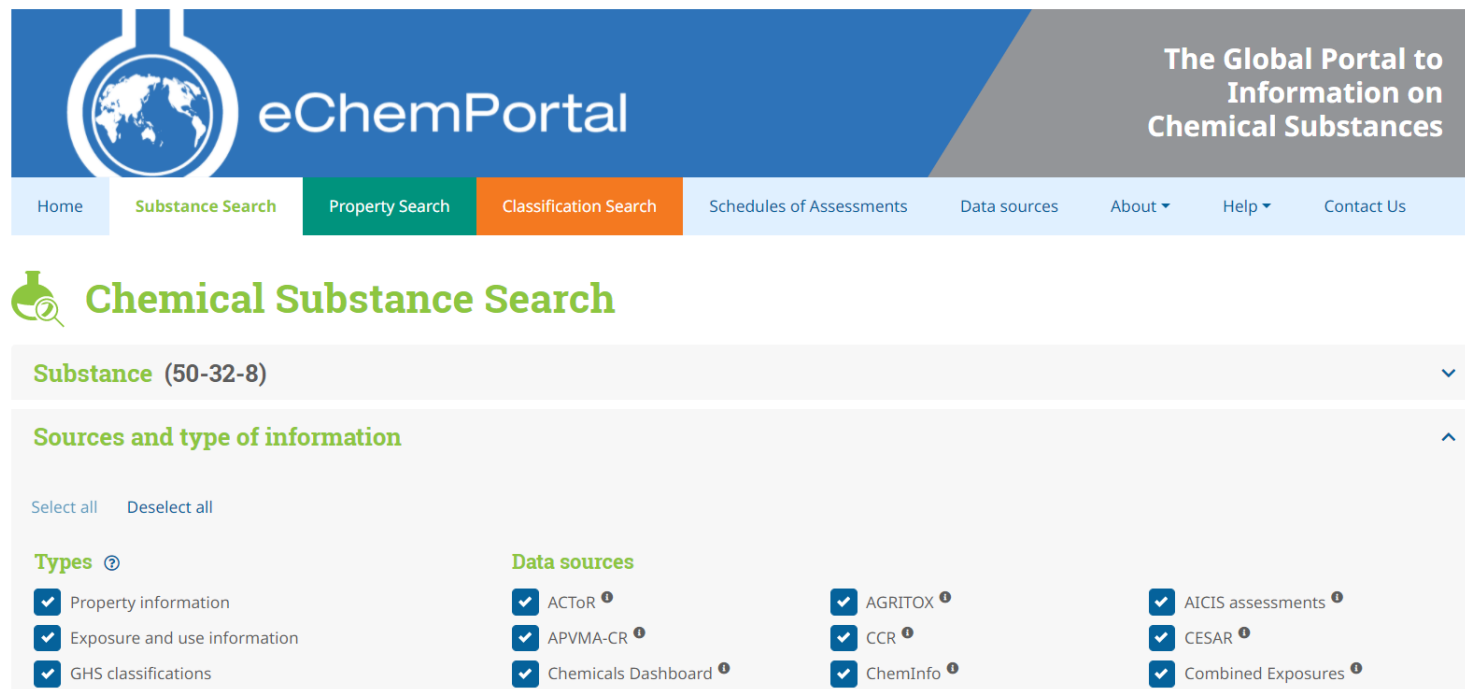
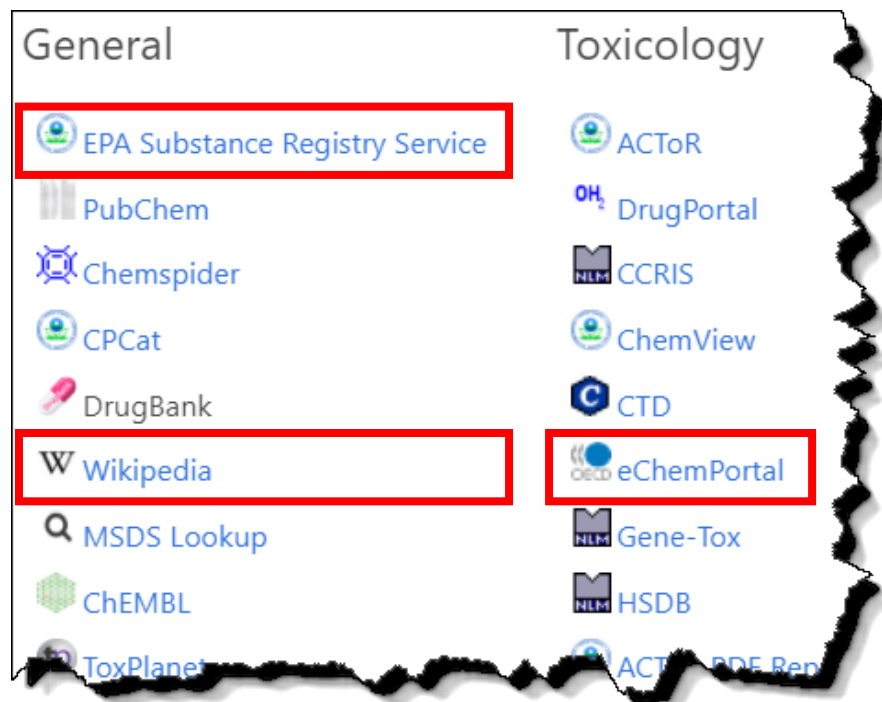
-  RSC Analytical Abstracts
-  Tox21 Analytical Data
-  MONA: MassBank North America
-  mzCloud
-  NIST IR Spectrum
-  NIST MS Spectrum
-  MassBank
-  NIST Antoine Constants
-  IR Spectra on PubChem
-  NIST Kovats Index values
-  Protein DataBank
-  National Environmental Methods Index

Prediction

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

External Links

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



The image is a screenshot of the eChemPortal website. The header features the OECD logo and the text 'The Global Portal to Information on Chemical Substances'. Below the header is a navigation bar with links: Home, Substance Search (highlighted), Property Search, Classification Search, Schedules of Assessments, Data sources, About, Help, and Contact Us. The main content area is titled 'Chemical Substance Search' and shows a search result for 'Substance (50-32-8)'. Under the heading 'Sources and type of information', there are two sections: 'Types' and 'Data sources'. The 'Types' section has checkboxes for 'Property information', 'Exposure and use information', and 'GHS classifications', all of which are checked. The 'Data sources' section has checkboxes for 'ACToR', 'APVMA-CR', 'Chemicals Dashboard', 'AGRITOX', 'CCR', 'ChemInfo', 'AICIS assessments', 'CESAR', and 'Combined Exposures', all of which are checked.



Chemical Lists and Categories

>300 Chemical Lists (and growing)

Home Advanced Search Batch Search Lists ▾ Predictions Downloads

Lists of Chemicals


List of Assays

 Download ▾ Columns ▾  Copy Filtered Lists URL

List Acronym ▾	List Name ▾	Last Updated ▾	Number of Chemicals ▾	List Description ▾
HDXEXCH	MASSPECDB: Hydrogen Deuterium Exchange Standard Set - Under HDX Conditions	2018-11-07	592	Observed species (deuterated and undeuterated) from the HDXNOEX list under hydrogen deuterium exchange conditions (Ruttkies, Schymanski et al. in prep.)
HDXNOEX	MASSPECDB: Hydrogen Deuterium Exchange Standard Set - No Exchange	2018-11-07	765	Environmental standard set used to investigate hydrogen deuterium exchange in small molecule high resolution mass spectrometry (Ruttkies, Schymanski et al. in prep.)
MASSBANKEUSP	MASSPECDB: MassBank.EU Collection: Special Cases	2017-07-16	263	The MassBank.EU list contains curated chemicals (Schymanski/Williams) associated with the literature/tentative/unknown/SI spectra available on MassBank.EU that are not available as part of the full MassBank collection of reference standard spectra.
MASSBANKREF	MASSPECDB: MassBank Reference Spectra Collection	2017-07-13	1267	This MassBank list contains chemicals associated with the full MassBank collection of reference standard spectra available on MassBank.EU, MassBank.JP and MassBank of North America as well as the Open Data collection, curated by Williams/Schymanski.
MYCOTOXINS	MASSPECDB: Mycotoxins from MassBank.EU	2017-08-02	88	This is a set of mycotoxins, initiated by the contribution of spectra of 90 mycotoxins to MassBank.EU by Justin Renaud and colleagues from Agriculture and Agri-Food Canada, Government of Canada

PFAS lists of Chemicals

Select List

 Download ▼

Columns ▼

PFAS

 Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
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 to 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 internal, 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 Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASTRIER	PFAS Community-Compiled List (Trier et al., 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

Curated List of Pesticides

- Find list of interest

- Select list and send to batch

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Select List

PESTICIDES|EPA: Pesticide Chemical Search Database

Search EPAPCS Chemicals

☐ Identifier substring search

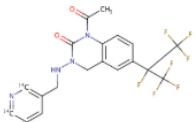
List Details

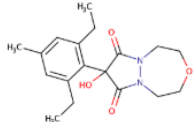
Description: The entries in this list have been classified in the U.S. as pesticidal "active ingredients" (conventional, antimicrobial, or biopesticidal agents), and were sourced from the Pesticide Chemical Search database (<https://iaspub.epa.gov/apex/pesticides/f?p=chemicalsearch:1>) created by EPA's Office of Pesticide Programs. Chemical Search provides a single point of reference for easy access to information previously published in a variety of locations, including various EPA web pages and Regulations.gov. Chemical search contains the following: 1) More than 20,000 regulatory documents; 2) Links to over 800 dockets in Regulations.gov 3) Links to pesticide tolerance (or maximum residue levels) information; 4) A variety of web services providing easy access to other scientific and regulatory information on particular chemicals from other EPA programs and federal government sources.

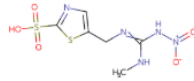
Number of Chemicals: 4012

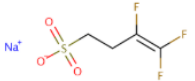
Select all Download **Send to Batch Search** CASRN DTXSID Mono.Mass 3988 chemicals

Hide chemicals that are: Filter by Name or CASRN


1-Acetyl-6-(1,1,1,2,3,3,3-heptafluoro-2-pyridyl)-4-methyl-2-pyridone
CASRN: NOCAS_920532
DTXSID: DTXSID00920532
Mono.Mass: 468.114807


8-(2,6-Diethyl-4-methylphenyl)-8-hydroxy-2,3-dihydro-1,4-benzodioxepine-2-one
CASRN: NOCAS_920508
DTXSID: DTXSID10920508
Mono.Mass: 332.173607


5-(((Methylamino)(nitroamino)methyleneamino)thio)pyridine-2-sulfonate
CASRN: NOCAS_912338
DTXSID: DTXSID20912338
Mono.Mass: 295.004511


Sodium 3,4,4-trifluoro-3-buten-1-sulfonate
CASRN: NOCAS_912336
DTXSID: DTXSID00912336
Mono.Mass: 211.973094

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 CASRN's?
 - 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 in the download file? OPERA?
TEST?
 - Are “these chemicals” screened in Toxcast?
 - I’m a mass spectrometrists and need masses and formulae for a list of chemicals

Batch Search CASRN

Batch Search

Step 1

Step 2

Step 3







Step 4

Step 5






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

Please enter one identifier per line






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 

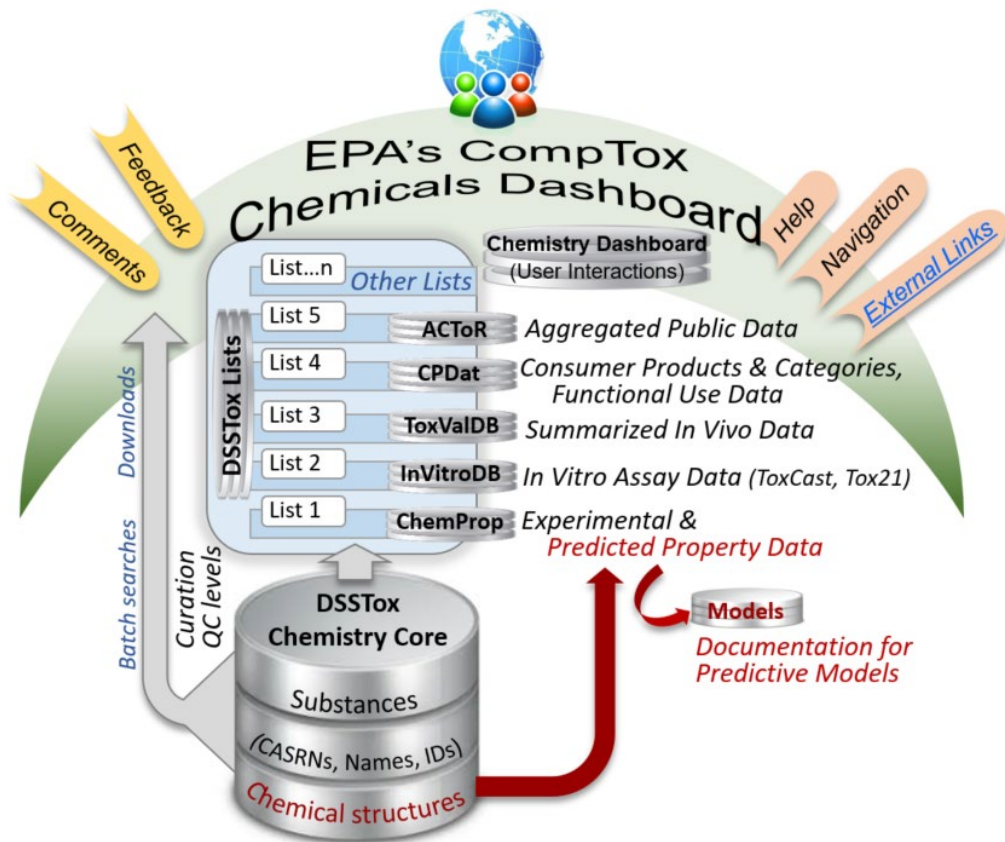
Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☒ Include ToxVal Data Availability 
- ☒ Assay Hit Count 
- ☒ Number of PubMed Articles 

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRED	CASRN	INCHIKEY	IUPAC NAME	MOLECULAR	TOXVAL_D	TOXCAST	TOXCAST	MS_READY	NUMBER_CIRIS	LINK	PPRTV_LIN	ATMOSPHE	BIOCONCE
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,6	534-52-1	ZXVONLUN	2-Methyl-4,6	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	2.88959
3	115-21-9	CAS-RN	DTXSID70	Ethyl silicon	115-21-9	ZOYFEXPF	Trichloro(ethyl)	C2H5Cl3Si	Y	-	-	-	-	-	-	8.289E-12	13.9658
4	111-44-4	CAS-RN	DTXSID90	Bis(2-chloro	111-44-4	ZNSMNVML	1-Chloro-2-(C4H8Cl2O	Y	1.12	10/891	CICCOCCC	12	Y	-	2.647E-12	9.99608
5	2763-96-4	CAS-RN	DTXSID50	Muscimol	2763-96-4	ZJQHPWUV	5-(Aminomethyl)	C4H6N2O2	Y	-	-	NCC1=CC(C	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQ	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-6	ZCJPOPBZ	Ethyl 3-methyl	C13H22NO3	Y	10.8	105/972	CCOP(=O)(C	58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDYQJ	Fluoroacetyl	C2H2ClFO	Y	-	-	FCC(Cl)=O	-	-	-	3.513E-13	4.49379
9	5344-82-1	CAS-RN	DTXSID40	1-(o-Chlorophenyl)	5344-82-1	YZUKKTCD	N-(2-Chlorophenyl)	C7H7ClN2S	Y	-	-	NC(=S)NC1=	-	-	-	2.482E-11	9.95206
10	7446-18-6	CAS-RN	DTXSID10	Thallium (I)	7446-18-6	YTQVHRVI	Dithallium(1-)	O4STI2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluorophenyl)	62207-76-5	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximide	66-81-9	YPHMISFO	4-[(2R)-2-[(2S)-2-oxo-2-phenylpropan-1-ylideneamino]ethyl]piperidine-1-carboxamide	C15H23NO4	Y	32.27	294/911	CC1CC(C)C(C	18709	-	-	1.756E-11	2.81761
13	106-96-7	CAS-RN	DTXSID30	Propargyl bromide	106-96-7	YORCIIVHU	3-Bromoprop-1-ene	C3H3Br	Y	-	-	BrCC#C	-	-	-	1.069E-11	10.4968
14	315-18-4	CAS-RN	DTXSID70	Mexacarbate	315-18-4	YNEVBPNZ	4-(Dimethylamino)	C12H18N2O	Y	5.11	12/235	CNC(=O)OC	27	-	-	1.447E-11	26.2914
15	110-00-9	CAS-RN	DTXSID60	Furan	110-00-9	YLQBMQCI	Furan	C4H4O	Y	0.0	0/235	O1C=CC=C	919	Y	-	4.019E-11	5.01648
16	3037-72-7	CAS-RN	DTXSID20	4-(diethoxyphenyl)	3037-72-7	YHFFINXFN	4-(Diethoxyphenyl)	C9H23NO2	Y	-	-	-	-	-	-	5.95E-12	6.71292
17	75-44-5	CAS-RN	DTXSID00	Phosgene	75-44-5	YGYAWVD	Carbonyl dichloride	CCl2O	Y	-	-	ClC(Cl)=O	489	Y	-	9.994E-16	13.0711
18	2032-65-7	CAS-RN	DTXSID30	Methiocarb	2032-65-7	YFBPRJGD	3,5-Dimethyl-4-isopropylphenyl	C11H15NO2	Y	18.14	88/485	CNC(=O)OC	65	-	-	1.446E-11	34.1692
19	2778-04-3	CAS-RN	DTXSID20	Endothion	2778-04-3	YCAGGFXS	[(5-Methoxy-2-methyl-1,3,4-thioxolan-2-ylideneamino)thio]phosphoric acid	C9H13O6P3	Y	-	-	COC1=COC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyclopentadienyl)tricarbonyliron	12108-13-3	YASXMYPV	Tricarbonyliron(0)	C9H7MnO3	Y	2.56	11/430	-	68	-	-	-	-
21	7803-51-2	CAS-RN	DTXSID20	Phosphine	7803-51-2	XYFCBTPG	Phosphane	H3P	Y	-	-	-	928	Y	-	-	-
22	107-18-6	CAS-RN	DTXSID80	Allyl alcohol	107-18-6	XXROGKLT	Prop-2-en-1-ol	C3H6O	Y	3.99	17/426	OCC=C	627	Y	Y	2.592E-11	4.03901
23	108-05-4	CAS-RN	DTXSID30	Vinyl acetate	108-05-4	XTXRWKR	Ethyl vinyl ether	C4H6O2	Y	1.7	4/235	CC(=O)OC	206	Y	-	2.5E-11	5.52157
24	19624-22-7	CAS-RN	DTXSID10	Pentaborane	19624-22-7	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyllead	75-74-1	XOOGZRUE	Tetramethyllead	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

Worksheet1

Summary and Conclusion



- CompTox Chemicals Dashboard - a central hub for environmental data

- ~900k 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




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



Volume 169, Issue 2

June 2019

The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency FREE

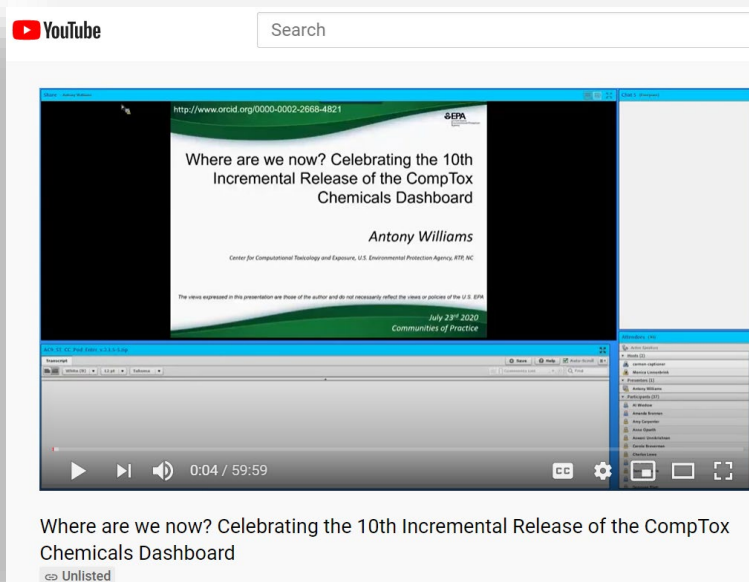
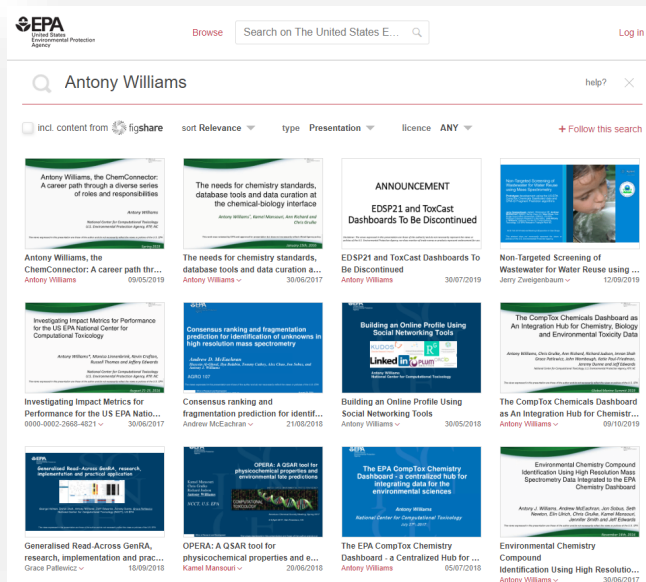
Russell S Thomas ✉, Tina Bahadori, Timothy J Buckley, John Cowden, Chad Deisenroth, Kathie L Dionisio, Jeffrey B Frithsen, Christopher M Grulke, Maureen R Gwinn, Joshua A Harrill ... [Show more](#)

Toxicological Sciences, Volume 169, Issue 2, June 2019, Pages 317–332,
<https://doi.org/10.1093/toxsci/kfz058>

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- Development and Validation of a Computational Model for Androgen Receptor Activity, *Chem. Res. Toxicol.* **30**, 946-964 (2017)
- CERAPP: Collaborative Estrogen Receptor Activity Prediction Project, *Environ. Health Perspect.* **124**, 1023 (2016)
- Abstract Sifter: a comprehensive front-end system to PubMed, *F1000*, **6**, 2164 (2017)

You want to know more...

- Lots of resources available
 - Presentations: <https://tinyurl.com/w5hq55>
 - Communities of Practice Videos: <https://rb.gy/qsbn01>
 - Manual: <https://rb.gy/4fgydc>
 - Latest News: https://comptox.epa.gov/dashboard/news_info

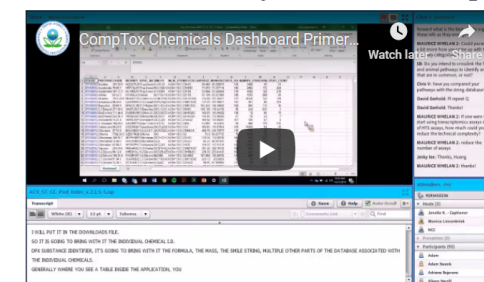


CompTox Chemicals Dashboard primer videos

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 instructional videos narrated by EPA scientists.

General Chemistry and Search Capabilities



Acknowledgments

- Contact: Williams.Antony@epa.gov
- 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