

# An Introduction (and Demo) of the CompTox Chemicals Dashboard

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**A4 Short Course – Tour de Force of Tools from the US Environmental Protection Agency to Support Assessments of Alternatives**



Environment International

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Review article

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

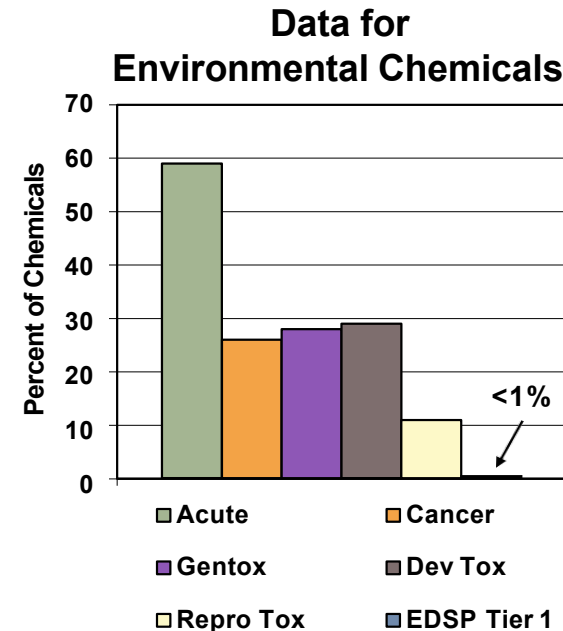
Antony J. Williams <sup>a</sup>  , Jason C. Lambert <sup>a</sup>, Kris Thayer <sup>b</sup>, Jean-Lou C.M. Dorne <sup>c</sup>

# 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

# The Charge for the Dashboard



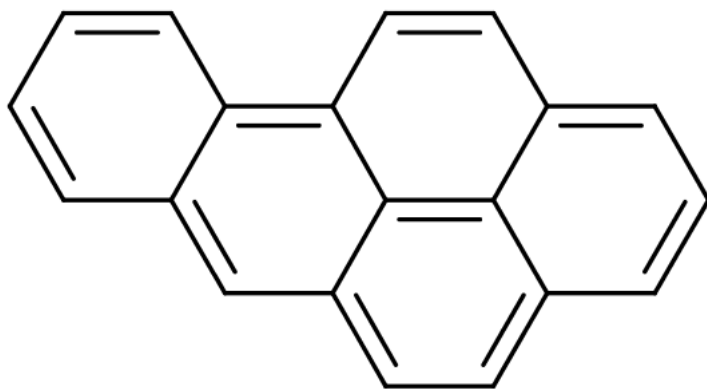
- Develop a “first-stop-shop” for environmental chemical data to support EPA and partner decision making:
  - **Centralized location** for relevant chemical data
  - Chemistry, exposure, hazard and dosimetry
  - Combination of existing data and predictive models
  - Publicly accessible, periodically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



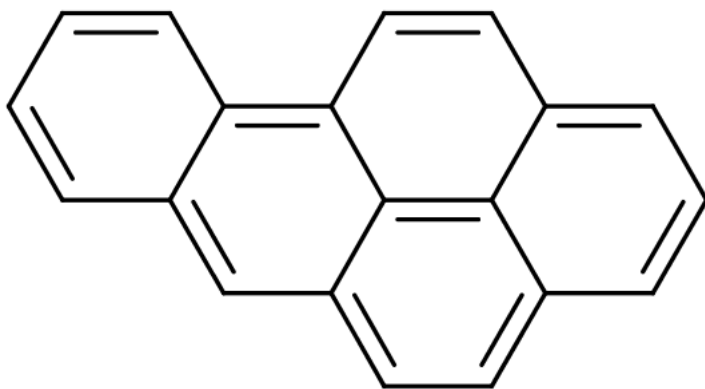
# Cheminformatics and the Dashboard

- Cheminformatics is the application of computer science and informatics-based approaches to:
  - Represent chemical structures, substances and reactions
  - Store chemistry-related data
  - Search for chemistry related data
  - Model data sets to provide predictive capabilities
  - Visualize and analyse chemistry related data
- The US-EPA uses cheminformatics (and bioinformatics) to manipulate, integrate, store, model and deliver access to our data. The CompTox Chemicals Dashboard is built on a solid cheminformatics foundation

# Types of Chemical Identifiers



- Structural Identifiers
- The visual depiction
- Multiple electronic formats
- InChI (Key): FMMWHPNWAFFZXNH-UHFFFAOYSA-N
- Common Name: Benzo(a)pyrene
- Systematic Name: Benzo[*pqr*]tetraphene
- CAS Registry Number(s) : 50-32-8
- Lots of other “common names and trade names”



## INTRINSIC PROPERTIES

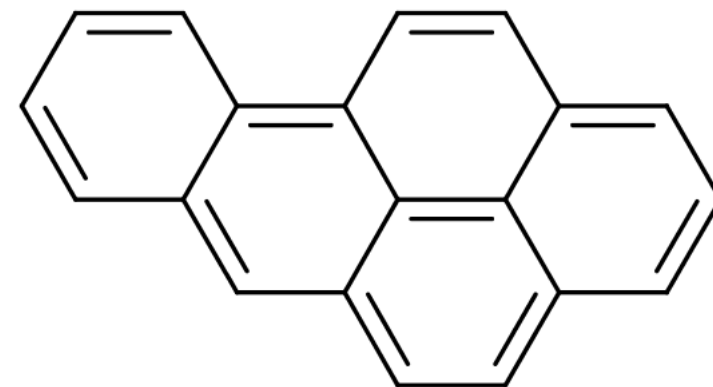
- Formula :  $C_{20}H_{12}$
- Molecular weight: 252.316 g/mol
- Monoisotopic Mass: 252.093900 g/mol

## MEASURED PROPERTIES

- LogKow 6.13
- Melting Pt 177°C
- Boiling Pt 485°C
- ....and many more

# How to Store a Chemical Structure

- Multiple approaches:
  - Names and identifiers
  - 2D or 3D structure “molfile”



```
Mrv1533009301517202D
  0  0  0      0  0      999 V3000
M  V30 BEGIN CTAB
M  V30 COUNTS 20 24 0 0 0
M  V30 BEGIN ATOM
M  V30 1 C 5.3801 0 0 0
M  V30 2 C 6.9201 0 0 0
M  V30 3 C 7.6901 -1.33 0 0
M  V30 4 C 9.2302 -1.33 0 0
M  V30 5 C 10.0003 -2.67 0 0
M  V30 6 C 9.2302 -4.0001 0 0
M  V30 7 C 7.6901 -4.0001 0 0
M  V30 8 C 6.9201 -5.3301 0 0
M  V30 9 C 5.3801 -5.3301 0 0
M  V30 10 C 4.6201 -4.0001 0 0
M  V30 11 C 5.3801 -2.67 0 0
M  V30 12 C 6.9201 -2.67 0 0
M  V30 13 C 4.6201 -1.33 0 0
M  V30 14 C 3.0801 -1.33 0 0
M  V30 15 C 2.31 -2.67 0 0
M  V30 16 C 3.0801 -4.0001 0 0
M  V30 17 C 0.77 -2.67 0 0
M  V30 18 C 0 -1.33 0 0
M  V30 19 C 0.77 0 0 0
M  V30 20 C 2.31 0 0 0
M  V30 END ATOM
M  V30 BEGIN BOND
M  V30 1 2 1 2
M  V30 2 1 1 13
M  V30 3 1 2 3
M  V30 4 2 3 4
M  V30 5 1 3 12
M  V30 6 1 4 11
```

- SMILES:
  - c1cc2c3ccc4cccc5ccc(cc2cc1)c3c45
  - C1=CC2=CC3=CC=C4C=CC=C5C=CC(=C2C=C1)C3=C45
  - and many other variants....
- InChI=1S/C20H12/c1-2-7-17-15(4-1)12-16-9-8-13-5-3-6-14-10-11-18(17)20(16)19(13)14/h1-12H
- InChIKey: FMMWHPNWAFFZXNH-UHFFFAOYSA-N


# 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▼



### CompTox Chemicals Dashboard

883 Thousand Chemicals

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

**Chemicals** Product/Use Categories Assay/Gene


Q Benzo(a)pyrene




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

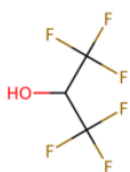
CASRN

TOXCAST

2098 chemicals

Hide chemicals that are:

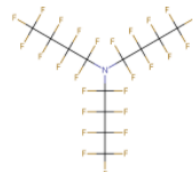
Filter by Name or CASRN



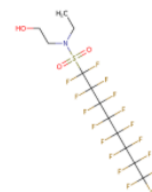
2H-Perfluoro-2-propanol  
DTXSID:DTXSID1022134  
CASRN:920-66-1  
TOXCAST:-



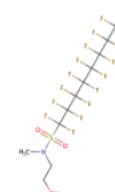
Perfluorooctanesulfonyl fluoride  
DTXSID:DTXSID5027140  
CASRN:307-35-7  
TOXCAST:-



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



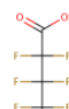
N-Ethyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide  
DTXSID:DTXSID6027426  
CASRN:1691-99-2  
TOXCAST:-



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

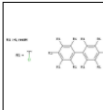




# Search for classes of chemicals

Examples:

- PCBs (or polychlorinated biphenyls)



### Polychlorinated biphenyls

1336-36-3 | DTXSID5024267

Searched by DSSTox Substance Id.

**Quality Control Notes**

biphenyl with multiple (unknown number) chlorines attached at unknown locations

**Intrinsic Properties**

**Presence in Lists**

Federal





- National Recommended Water Quality Criteria Aquatic Life chemical list
- EPA Region 10
- EPA: Toxics Release Inventory
- EPA: Underground Storage Tanks (USTs)
- EPA: IRIS
- State-Specific Water Quality Standards Effective under the Clean Water Act (CWA)
- ENDOCRINE: EDSP21 Tier 1 Screening Chemicals: List 2
- ENDOCRINE: EDSP Universal Screening Chemicals: List 1



- Polycyclic aromatic hydrocarbons

### Polycyclic aromatic hydrocarbons

130498-29-2 | DTXSID3044043

Searched by Expert Validated Synonym.

Select all Download Send to Batch Search Relationship     73 chemicals

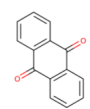
Hide chemicals that are:  Filter by Name or CASRN 

Searched Chemical


73 related chemical structures with this substance

Polycyclic aromatic hydrocarbons  
DTXSID:DTXSID3044043  
CASRN:130498-29-2  
TOXCAST:-

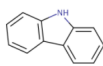
Component

  
Anthraquinone  
DTXSID:DTXSID020095  
CASRN:84-65-1  
TOXCAST:235

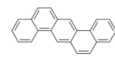
Component

  
Benzofluorene  
DTXSID:DTXSID020139  
CASRN:86-32-8  
TOXCAST:72/235

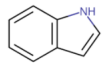
Component

  
Carbazole  
DTXSID:DTXSID4020248  
CASRN:86-74-8  
TOXCAST:39/598

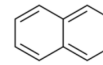
Component

  
Dibenz(a,h)anthracene  
DTXSID:DTXSID9020409  
CASRN:53-70-3  
TOXCAST:61/621

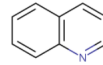
Component

  
Indole  
DTXSID:DTXSID002737


Component

  
Naphthalene  
DTXSID:DTXSID002813

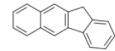
Component

  
Quinoline  
DTXSID:DTXSID002138

Component

  
Chrysene  
DTXSID:DTXSID002437

Component

  
2,3-Benzofluorene  
DTXSID:DTXSID002477

# Detailed Chemical Pages

## One more identifier – the **DTXSID**

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

SAFETY

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS


GENRA (BETA)

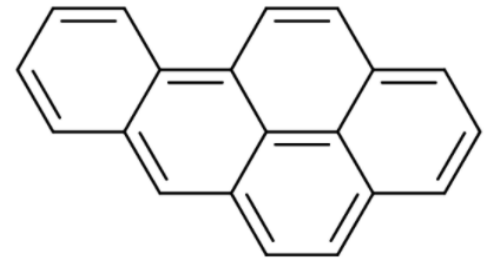
RELATED SUBSTANCES

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 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 ...  
[Read more](#)

Quality Control Notes

Intrinsic Properties

Molecular Formula: C<sub>20</sub>H<sub>12</sub> [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

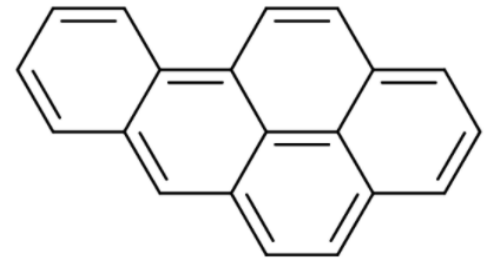
- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

# Detailed Chemical Pages

## Easy Navigation



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



**DETAILS**




- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ▶ SAFETY
- ▶ ADME
- ▶ EXPOSURE
- ▶ BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- ▶ LITERATURE
- LINKS



**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 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 ...  
[Read more](#)

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 **Molecular Formula:** C<sub>20</sub>H<sub>12</sub>  **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:  $C_{20}H_{12}$




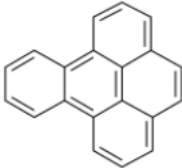
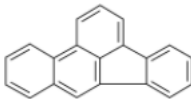
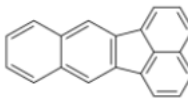

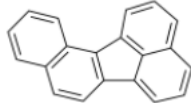
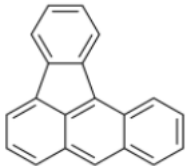
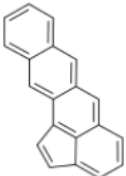
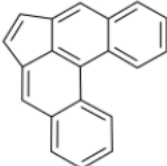
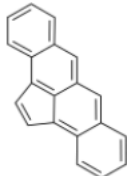
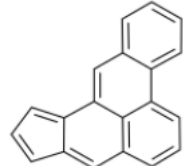
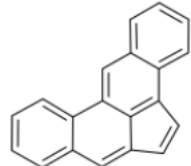
Mol File

 Find All Chemicals

## Search Results

Searched by Exact Molecular Formula:  $C_{20}H_{12}$ .

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 – 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

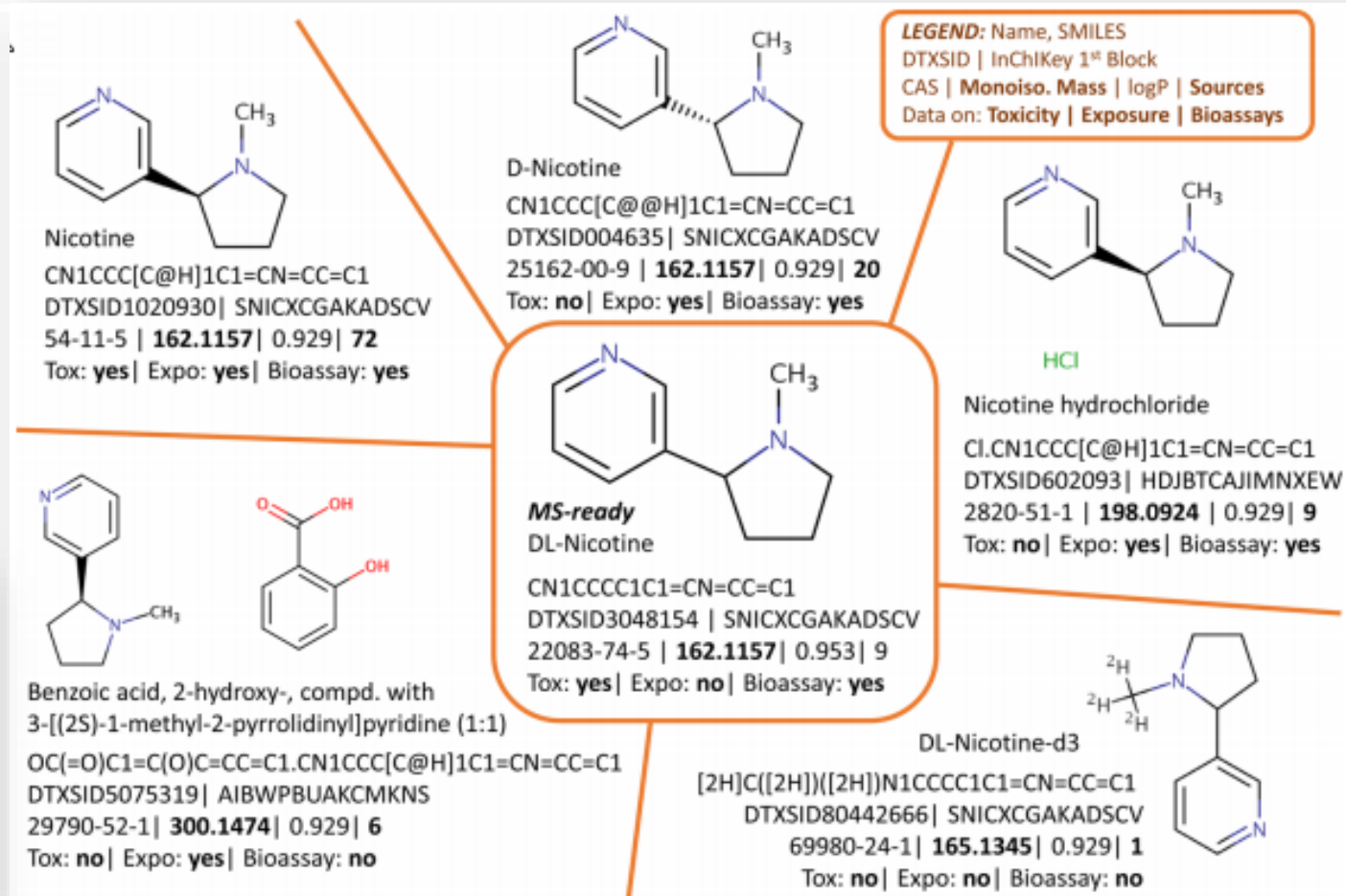
## METHODOLOGY

Open Access



### “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>

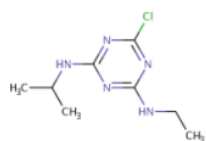


# Atrazine Linked Substances

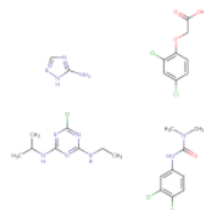
## MS-Ready Mappings of Atrazine (Isotopes pre-filtered)

20 of 25 chemicals visible

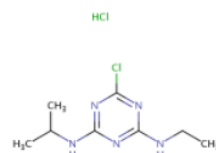
Select all Download Send to Batch Search Default DTXSID CASRN TOXCAST Isotopes Filter by Name or CASRN



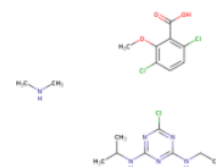
**Atrazine**  
DTXSID:DTXSID9020112  
CASRN:1912-24-9  
TOXCAST:62/1024



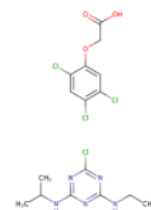
**Anox M**  
DTXSID:DTXSID50156021  
CASRN:128996-76-9  
TOXCAST:-



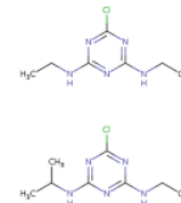
**s-Triazine, 2-chloro-4-(ethylamino)-6-(isopropylamino)-**  
DTXSID:DTXSID30165459  
CASRN:15386-47-7  
TOXCAST:-



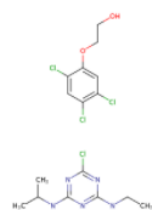
**Marksman**  
DTXSID:DTXSID80166936  
CASRN:160544-50-3  
TOXCAST:-



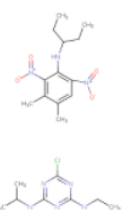
**Acetic acid, (2,4,5-trichlorophenoxy)-, methyl ester**  
DTXSID:DTXSID70192527  
CASRN:39283-62-0  
TOXCAST:-



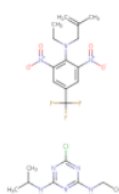
**1,3,5-Triazine-2,4-diamine, 6-chloro-N,N-dimethyl-**  
DTXSID:DTXSID60192556  
CASRN:39331-45-8  
TOXCAST:-



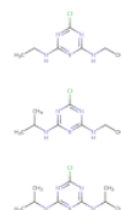
**Buvinol**  
DTXSID:DTXSID10199555  
CASRN:51602-05-2  
TOXCAST:-



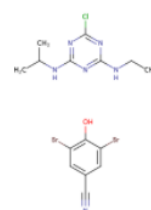
**Atrazine mixture with pendimethalin**  
DTXSID:DTXSID10209527  
CASRN:60704-01-0  
TOXCAST:-



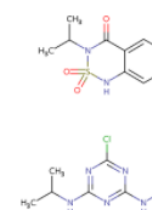
**Maizor**  
DTXSID:DTXSID20215154  
CASRN:64867-15-8  
TOXCAST:-



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



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



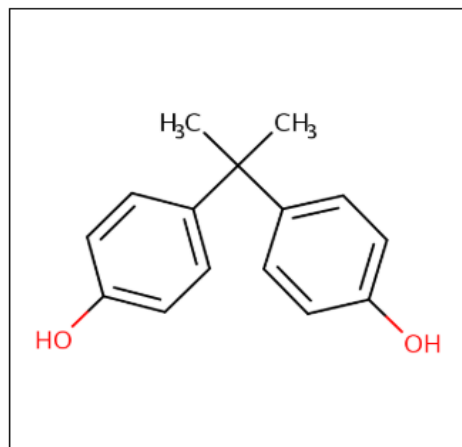
**Bentazon / atrazine**  
DTXSID:DTXSID80226064  
CASRN:75084-57-0  
TOXCAST:-

# Record Information Quality Flags

## Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.



Wikipedia


Intrinsic Properties

Structural Identifiers

Linked Substances

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

## Record Information

 **Citation:** U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID7020182> (accessed Aug 20th, 2018), Bisphenol A

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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



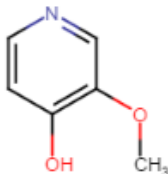
# Underneath the Dashboard

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

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

4-Hydroxy-3-methoxy

Valid license cannot be found



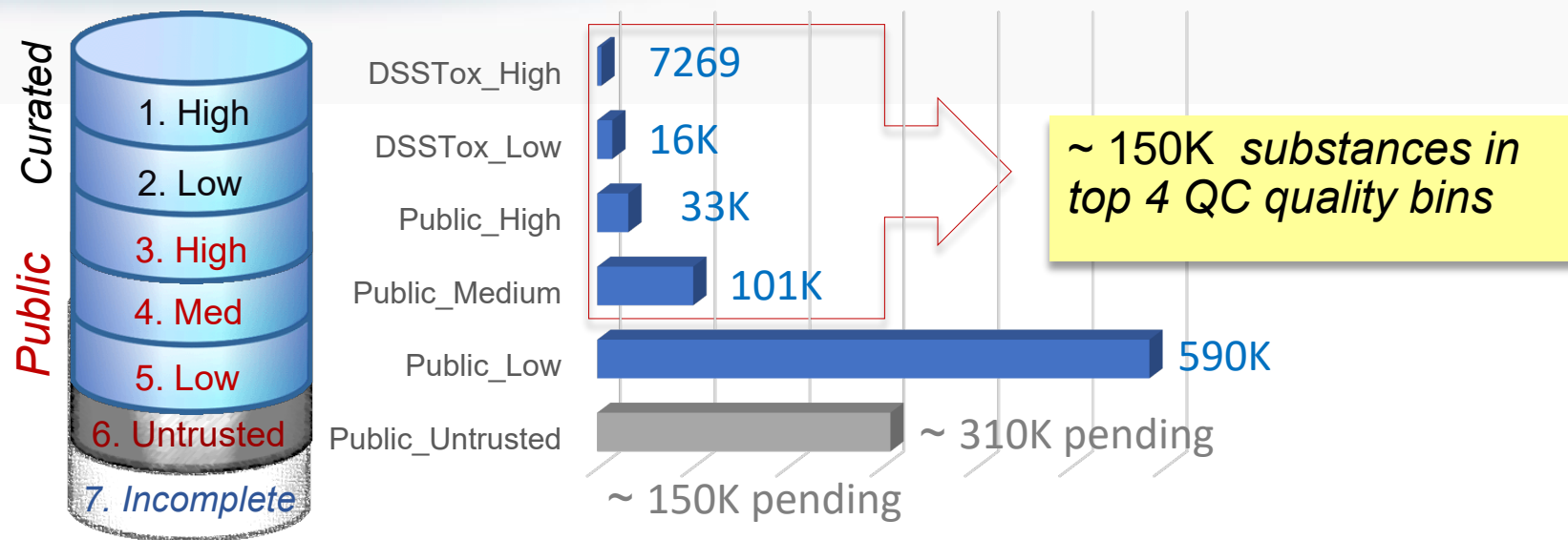
Chemical structure of 4-Hydroxy-3-methoxypyridine is displayed. The structure shows a pyridine ring with a hydroxyl group (-OH) at the 4-position and a methoxy group (-OCH<sub>3</sub>) at the 3-position.

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 >910k 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](http://www.elsevier.com/locate/comtox)



### 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

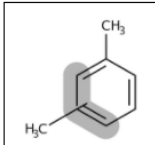
<sup>b</sup> Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA



# If you find an error, or want to comment...

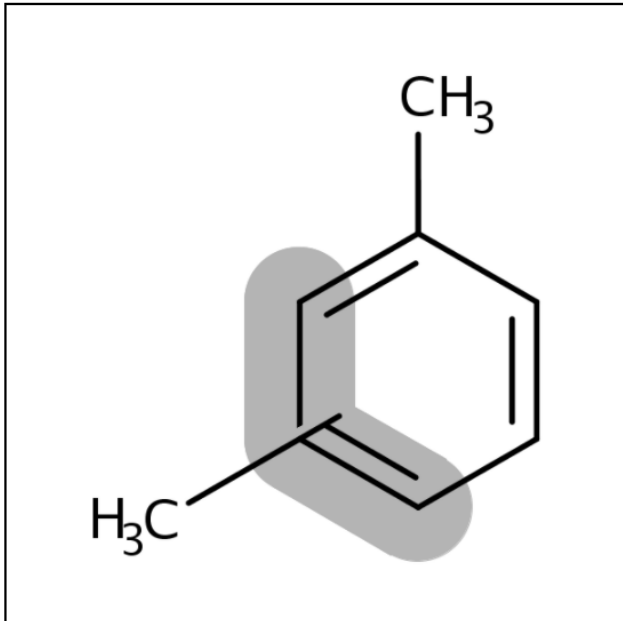
## Select text and "Submit Comment"

[Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#) [Copy](#) [Share](#) [Submit Comment](#)



## Xylenes

**1330-20-7** | DTXSID2021446  
Searched by DSSTox Substance Id.



### Wikipedia




**Xylene** (from Greek ξύλον *xylon*, "wood"), **xylol** or **dimethylbenzene** is any one of the three isomers of dimethylbenzene, or a combination thereof. With the formula  $(\text{CH}_3)_2\text{C}_6\text{H}_4$ , each of the three isomers consists of a central benzene ring with two methyl groups attached at substituents. They are all of which are of great industrial value



...  
[Read more](#)


### Quality Control Notes

Ill-defined substance;

### Intrinsic Properties

 **Molecular Formula:** Not Found  Mol File  Find All Chemicals

 **Average Mass:** 0 g/mol  Isotope Mass Distribution

 **Monoisotopic 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?

Email address

williams.antony@epa.gov

 I'm not a robot



[Submit](#)

comptox.epa.gov says

Your comment has been submitted and will be reviewed.

[OK](#)

# “Executive Summary”

## Executive Summary

### Quantitative Risk Assessment Values

- ✓ IRIS values available
- ✗ No PPRTV values
- ✓ EPA RSL values available
- ✓ Minimum RfD: **0.00030 mg/kg-day** (chronic, IRIS, oral, 8)
- ✓ Minimum RfC: **0.0000020 mg/m3** (chronic, IRIS, inhalation, 8)
- ✗ IVIVE POD not calculated

### 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**

### Cancer Information

- ✓ Cancer slope factor: **23.5 (mg/kg-day)<sup>-1</sup>** (ACToR, dermal, 4)
- ✓ Inhalation unit risk: **2.4 (mg/m3)<sup>-1</sup>** (IRIS, inhalation, 8)
- ✓ Carcinogenicity data available: IARC: undefinedEPA OPP cancer class: undefinedNTP Report on Carcinogens (ROC 12): undefinedNLM ToxNet HSDB carcinogenicity warningUniversity of Maryland carcinogenicity warning
- ✗ No genotoxicity findings reported

### Reproductive Toxicology

- ✓ Reproductive toxicity PODs available

### Chronic Toxicology

- ✓ Chronic toxicity PODs available

### Subchronic Toxicology

- ✓ Subchronic toxicity PODs available

### Developmental Toxicology

- ✗ No developmental toxicity data available.

### Acute Toxicology

- ✓ Acute toxicity PODs available

### Subacute Toxicology

- ✗ No subacute toxicity data available.

### Neurotoxicology

- ✗ No neurotoxicology data available.

### Endocrine System

- ✓ 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).

### ADME

- ✗ No HTTK data

### Fate and Transport

- ✗ No bioaccumulation concern.
- ✗ No volatility concern
- ✓ Biodegradation predictions are available
- ✓ BCF predictions are available
- ✓ Vapor Pressure predictions are available

### Exposure

- ✓ Exposure Estimates have been predicted using the SEEM modeling methodology

### AOP Information

- ✓ AOP Links: 36, 61, 66, 107, 150, 163, 187, 200

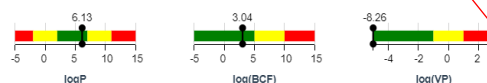
### Other Notes

- ✗ No water quality values available.
- ✓ 18 Air quality values available
- ✓ Occupational exposure values available

### REGIONAL SCREENING

Class	THQ	Value
GIABS (-)	THQ = 0.1	1
ABS (-)	THQ = 0.1	0.13
MCL (ug/L)	THQ = 0.1	0.2
MCLbased SSL (mg/kg)	THQ = 0.1	0.24
cancer slope factor ((mg/kg-day) <sup>-1</sup> )	THQ = 0.1	1
cancer unit risk ((ug/m3) <sup>-1</sup> )	THQ = 0.1	0.0006
RfDo (mg/kg-day)	THQ = 0.1	0.0003
RfCi (mg/m3)	THQ = 0.1	0.000002
Resident soil (mg/kg)	THQ = 0.1	0.11
Industrial soil (mg/kg)	THQ = 0.1	2.1
Resident air (ug/m3)	THQ = 0.1	0.00021
Industrial air (ug/m3)	THQ = 0.1	0.00088
Tapwater (ug/L)	THQ = 0.1	0.025
Riskbased SSL (mg/kg)	THQ = 0.1	0.029
GIABS (-)	THQ = 1	1
ABS (-)	THQ = 1	0.13
MCL (ug/L)	THQ = 1	0.2
MCLbased SSL (mg/kg)	THQ = 1	0.24
cancer slope factor ((mg/kg-day) <sup>-1</sup> )	THQ = 1	1
cancer unit risk ((ug/m3) <sup>-1</sup> )	THQ = 1	0.0006
RfDo (mg/kg-day)	THQ = 1	0.0003
RfCi (mg/m3)	THQ = 1	0.000002
Resident soil (mg/kg)	THQ = 1	0.11
Industrial soil (mg/kg)	THQ = 1	2.1
Resident air (ug/m3)	THQ = 1	0.0017
Industrial air (ug/m3)	THQ = 1	0.0088
Tapwater (ug/L)	THQ = 1	0.025
Riskbased SSL (mg/kg)	THQ = 1	0.029

### PHYSICHEM PARAMETERS



- Overview of toxicity-related info
  - Quantitative values
  - Info re. toxicology subsets
  - Physchem. and Fate & Transport
  - Adverse Outcome Pathway links
  - *In vitro* bioactivity summary plot


### Quantitative Risk Assessment Values

- ✓ IRIS values available
- ✗ No PPRTV values
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- ✓ Lowest Observed Bioactivity Equivalent Level: **AR**

# 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
<a href="#">Water Solubility</a>	8.40e-9 (4)	1.75
<a href="#">LogKow: Octanol-Water</a>	6.13 (2)	6.24
<a href="#">Vapor Pressure</a>	5.49e-9 (1)	3.61e-9
<a href="#">Boiling Point</a>	495 (3)	480
<a href="#">Henry's Law</a>	4.57e-7 (1)	4.59e-7
<a href="#">Melting Point</a>	177 (8)	189
<a href="#">Surface Tension</a>	-	53.9
<a href="#">Flash Point</a>	-	234
<a href="#">Density</a>	-	1.28

- 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: **O**PEn 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
- ***TODD MARTIN will cover this later***



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



## 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	<a href="#">Alaska DEC</a>
	7	cancer unit risk	-	chronic	0.21	(mg/l)-1	-	inhalation	-	Alaska DEC	<a href="#">Alaska DEC</a>
	7	cancer slope factor	-	chronic	3.08	(mg/kg-day)-1	-	inhalation	-	Alaska DEC	<a href="#">Alaska DEC</a>
	7	cancer unit risk	-	chronic	0.88	(mg/m3)-1	-	inhalation	-	Alaska DEC	<a href="#">Alaska DEC</a>
	7	cancer slope factor	-	chronic	7.3	(mg/kg-day)-1	-	oral	-	Alaska DEC	<a href="#">Alaska DEC</a>
	7	MEG	Short-term Critical Air	short-term	80	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	7	MEG	Short-term Marginal Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	7	MEG	Soil Negligible Soil	chronic	12	mg/kg	-	Soil	-	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	7	MEG	Long-Term, SL/d Negligible Water	chronic	0.0134	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>
	7	MEG	Short-term Negligible Air	short-term	0.6	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	<a href="#">DOD</a>

<< < 1 2 3 4 > >>

Showing 1 to 10 of 32 records

[advanced search/index](#)

# Let's talk about Export Formats

- 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”

- ***Katherine Phillips will cover this later***

## ▼ EXPOSURE

### PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

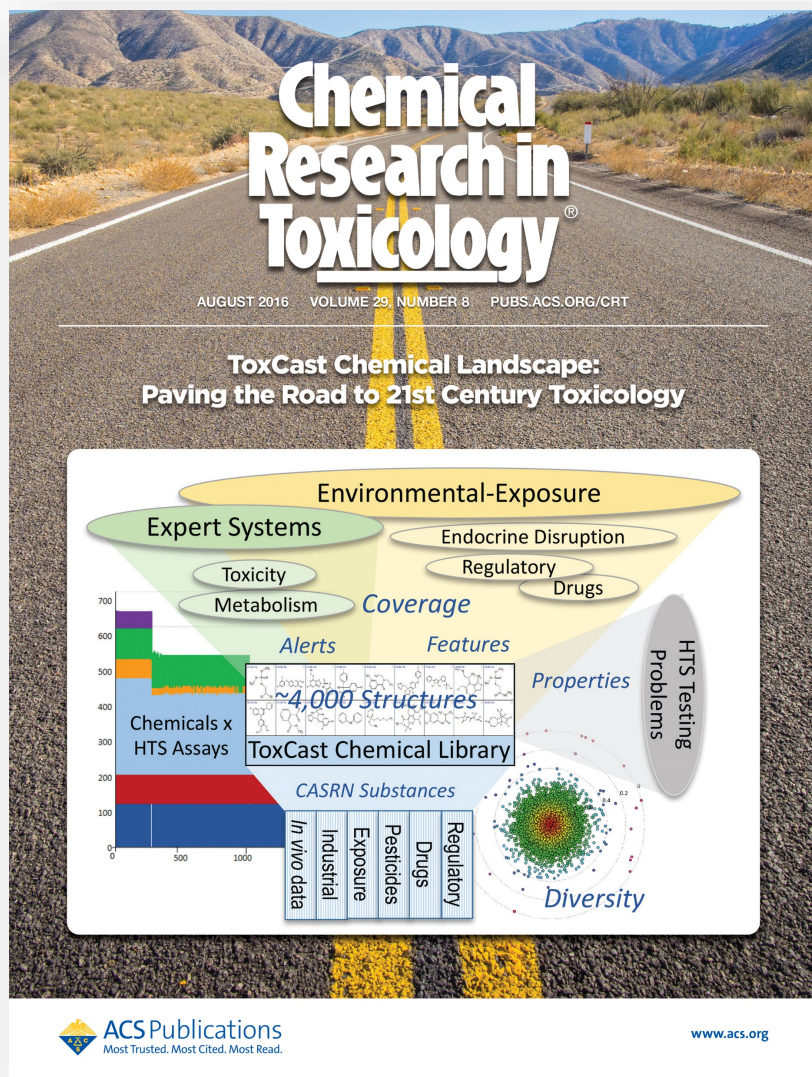
CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME



## 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>

**View Author Information** ▾

✓ **Cite this:** *Chem. Res. Toxicol.* 2016, 29, 8, 1225–1251

Publication Date: July 1, 2016 ▾

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

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Citations

244

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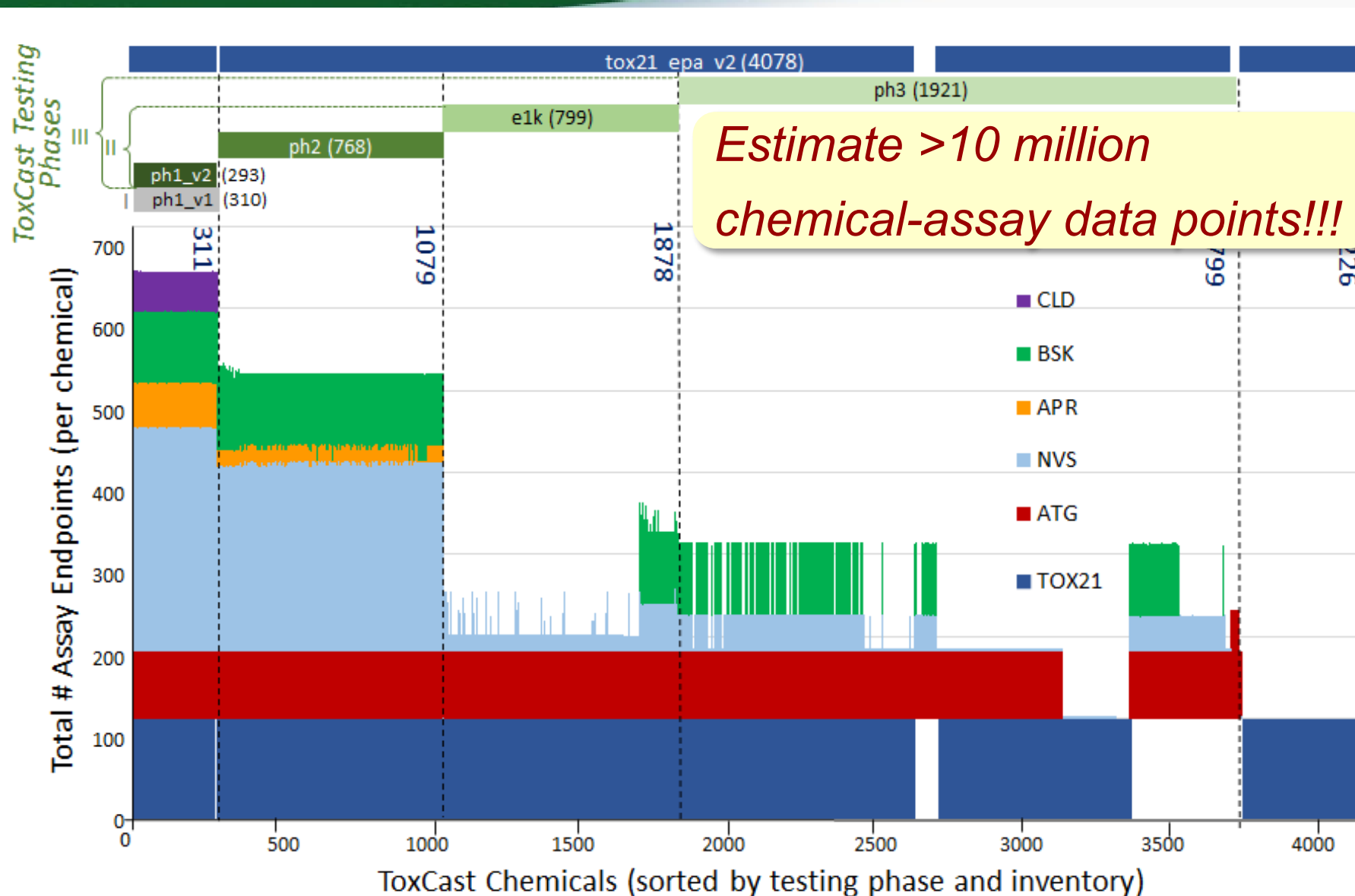
Add to



Export



# ToxCast/To21 HTS data



# ToxCast Chemicals and Assays

## Select List

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 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 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
OT	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	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	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 identify potential environmental toxicants.	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.	Endocrine (AR related)


# The Tox21 Screening Library

## Select List

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tox21

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List Acronym ⬆	List Name ⬆	Last Updated ⬆	Number of Chemicals ⬆	List Description ⬆
<a href="#">EPACHEMINV_AVAIL</a>	<a href="#">CHEMINV; ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)</a>	2018-11-21	6408	EPACHEMINV_AVAIL is list of unique DSSTox substances available as DMSO solutions for ToxCast and Tox21 partner projects, managed by EPA Chemical Contract Services.
<a href="#">TOX21SL</a>	<a href="#">TOX21SL: Tox21 Screening Library</a>	2017-02-23	8947	TOX21SL is list of unique substances comprising the screening library for the Tox21 program, a multi-federal agency collaborative among the US EPA, NIH/NTP, NIH/NCATS, and the US FDA.

2 records



# Let's look at the data



United States  
Environmental Protection  
Agency

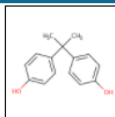
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## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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**TOXCAST: SUMMARY**

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[TOXCAST/TOX21](#)

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[GENRA \(BETA\)](#)

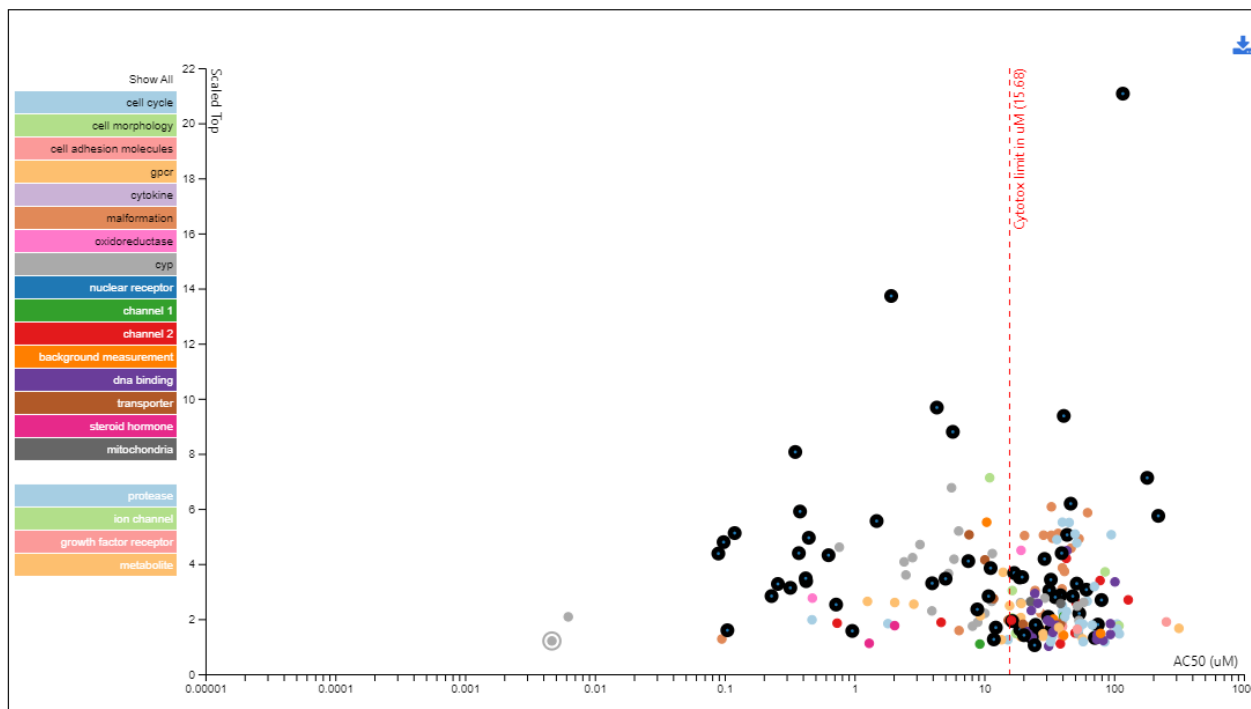
[RELATED SUBSTANCES](#)

[SYNONYMS](#)

## 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

 Download

Columns

10





















Search query



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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		<a href="#">NP_005071.2</a> 	<a href="#">XBP1</a>	X-box binding protein 1	-	-	ACTIVE	1.08	1.83	93.8	1.97	0.118	0.590	dna binding
ATG_VDRE_CIS_up		<a href="#">NP_000367.1</a> 	<a href="#">VDR</a>	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		<a href="#">NP_001069.1</a> 	<a href="#">VCAM1</a>	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		<a href="#">NP_001069.1</a> 	<a href="#">VCAM1</a>	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		<a href="#">NP_000537.3</a> 	<a href="#">TP53</a>	tumor protein p53	-	-	ACTIVE	35.5	1.78	73.7	1.87	0.959	20.0	dna binding
TOX21_p53_BLA_p4_ratio		<a href="#">NP_000537.3</a> 	<a href="#">TP53</a>	tumor protein p53	-	-	ACTIVE	28.6	1.43	73.8	1.87	1.02	20.0	dna binding
ATG_p53_CIS_dn		<a href="#">NP_000537.3</a> 	<a href="#">TP53</a>	tumor protein p53	-	-	ACTIVE	0.789	1.23	82.4	1.92	0.129	0.643	dna binding
NVS_MP_rPBR		<a href="#">NP_036647.1</a> 	<a href="#">Tspo</a>	translocator protein	-	-	ACTIVE	61.5	1.96	15.3	1.19	5.24	31.4	transporter
ATG_AP_2_CIS_dn		<a href="#">NP_003211.1</a> 	<a href="#">TFAP2A</a>	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		<a href="#">NP_003193.2</a> 	<a href="#">TCF7</a>	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*

**Bisphenol A**

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

QC Data ID	Grade	Description
Tox21_2029922	Pure	Purity>90% and MW confirmed
Tox21_450038	Pure	Purity>90% and MW confirmed

Assay Selection 3 Selected
A Single Assay Can Have Multiple Charts
Number of Charts: 18

☒ Active ☐ Inactive ☐ All

Filter

Assay Set: ER (3 of 18 Selected)

- ☒ ACBA 14TU 50hr Positive
- ☒ AIG b1fe C1S up
- ☒ AIG b1fe HANS up
- ☐ NVS NK BBR
- ☐ NVS NK hBR
- ☐ NVS NK mbR
- ☐ Q1 b1f b1e/b1o 0480
- ☐ Q1 b1f b1e/b1o 1440
- ☐ Q1 b1f b1e/b1o 0480
- ☐ Q1 b1f b1e/b1o 1440
- ☐ Q1 b1f b1e/b1o 0480
- ☐ Q1 b1f b1e/b1o 1440
- ☐ Q1 b1fe b1eGHP 0120
- ☐ Q1 b1fe b1eGHP 0480
- ☐ Tox21 b1fe SLA Agonist ratio
- ☐ Tox21 b1fe SLA Antagonist ratio
- ☐ Tox21 b1fe LUC B1C1 Agonist
- ☐ Tox21 b1fe LUC B1C1 Antagonist

Assay Set: AR (0 of 11 Selected)

- ☐ AIG AR HANS up
- ☐ NVS NK cAR
- ☐ NVS NK hAR
- ☐ NVS NK mbR

# #Actives for a chemical

217 active of 1152 assays

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




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# Cytotoxicity Threshold



United States  
Environmental Protection  
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Volume 152, Issue 2

August 2016

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▼ BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

PUBCHEM

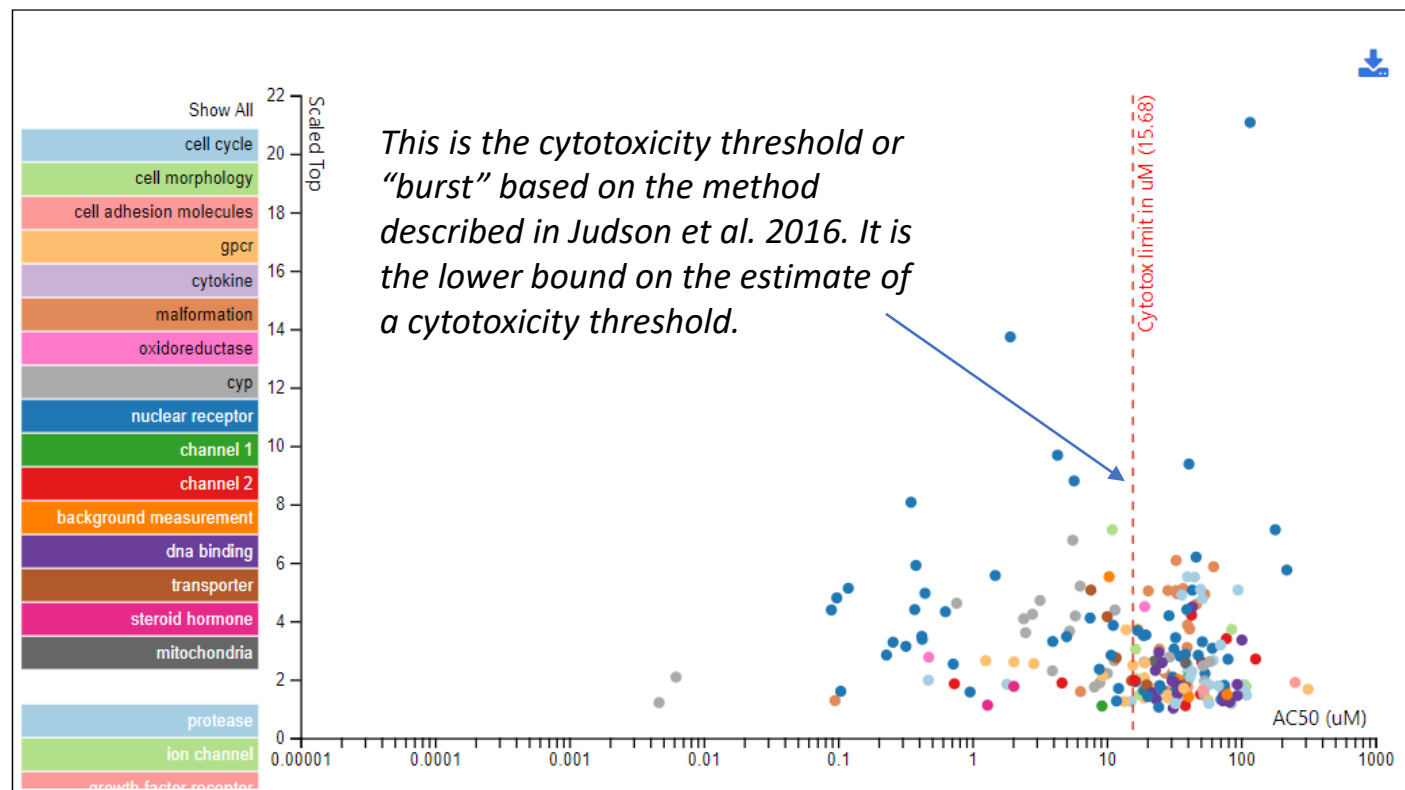
TOXCAST: MODELS



## Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity on *In Vitro* Assay Activity Across a Diverse Chemical and Assay Space <sup>FREE</sup>

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](#)

TOXCAST DATA



- 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\_80hr

### Assay Details

Assay Endpoint Name: ACEA\_ER\_80hr



Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell growth assay system called xCELLigence based on a microelectronic impedance readout.

### Histograms

175 of 3031 chemicals visible

Select all



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DTXSID

CASRN

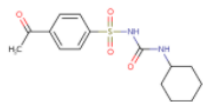
TOXCAST



Inactive



Filter by Name or CASRN

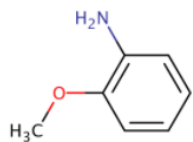


Acetohexamide

DTXSID:DTXSID7020007

CASRN:968-81-0

TOXCAST:7/403



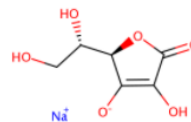
HCl

2-Methoxyaniline hydrochloride

DTXSID:DTXSID8020092

CASRN:134-29-2

TOXCAST:17/412



Sodium L-ascorbate

DTXSID:DTXSID0020105

CASRN:134-03-2

TOXCAST:22/890

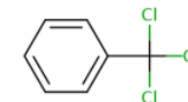


Sodium azide

DTXSID:DTXSID8020121

CASRN:26628-22-8

TOXCAST:84/864



Benzotrichloride

DTXSID:DTXSID1020148

CASRN:98-07-7

TOXCAST:10/866

# High-Level Visualizations of Data

## Assay Endpoint Name: ACEA\_ER\_80hr

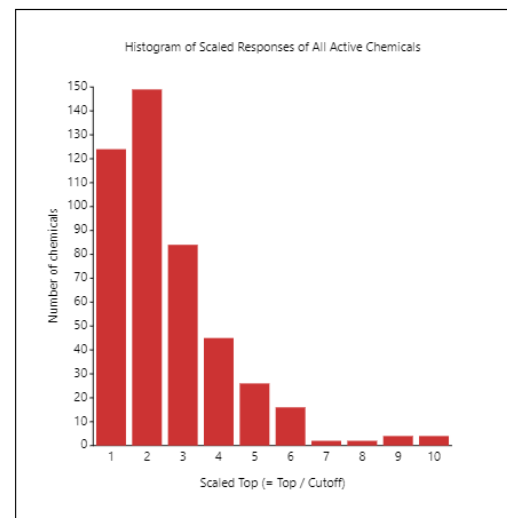
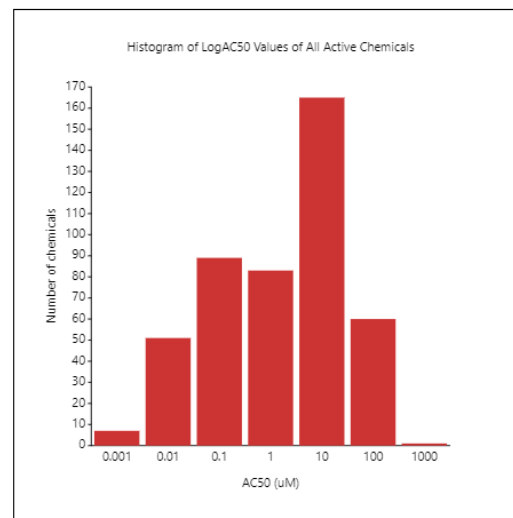
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Assay Endpoint Name: ACEA\_ER\_80hr



**Assay Source Description:** ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell growth assay system called xCELLigence based on a microelectronic impedance readout .

### Histograms





# Filtering by vendor....or Gene Symbol




## Assay List

Download ▾

ACEA ✕ ▾

Search query

Copy filtered page URL

Assay Component Endpoint Name ▴ ▾	Details	Multi Conc. Actives ▴ ▾	Single Conc. Active	Description	Gene Symbols
<a href="#">ACEA_ER_80hr</a>		456 / 3024	-	Data from the assay component ACEA endpoint, ACEA_ER_80hr_Positive, was negative control and baseline of activity of-signal activity can be used to understand ESR1. Furthermore, this assay endpoint produced multiple assay endpoints with intended target to other relatable target intended target family, where the subfamily is	<a href="#">ESR1</a>
<a href="#">ACEA_AR_agonist_AUC_viability</a>		609 / 1830	-	Data from the assay component ACEA relative to DMSO as the negative control of-signal activity can be used to understand where this one serves a viability function this assay endpoint is annotated to the "cytotoxicity".	
<a href="#">ACEA_ER_AUC_viability</a>		1051 / 3025	-	Data from the assay component ACEA relative to DMSO as the negative control of-signal activity can be used to understand where this one serves a viability 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	

# 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>||</sup>, and Russell S. Thomas<sup>‡</sup>

[View Author Information](#) ▾

✓ **Cite this:** *Environ. Sci. Technol.* 2015, 49, 14, 8804–8814

Publication Date: June 12, 2015 ▾

<https://doi.org/10.1021/acs.est.5b02641>

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## 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 Wedeby, Francesca Grisoni, Giuseppe F. Mangiatordi, ... [See all authors](#) ▾

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>||</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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✓ **Cite this:** *Chem. Res. Toxicol.* 2017, 30, 4, 946–964

Publication Date: November 18, 2016 ▾

<https://doi.org/10.1021/acs.chemrestox.6b00347>

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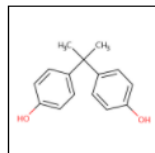
[Vol. 128, No. 2](#) | Research

## 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 Bhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, ... [See all authors](#)

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



Bisphenol A

80-05-7 | DTXSID7020182





Searched by DSSTox Substance Id.

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

ToxCast: Models

ToxCast Model Predictions

 Download ToxCast Model Predictions ▾

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)

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► SAFETY

► ADME

► EXPOSURE

▼ BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

TOXCAST/TOX21

PUBCHEM

TOXCAST: MODELS

# Where do we look for assay details?

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

Chemicals	Product/Use Categories	Assay/Gene
-----------	------------------------	------------

GENE: NR3C1  
*nuclear receptor subfamily 3, group C, member 1 (glucocorticoid receptor)*

GENE: SGK1  
*serum/glucocorticoid regulated kinase 1*

# Generalized Read-Across

# GenRA (Generalised Read-Across)

DETAILS

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▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

**GENRA (BETA)**

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

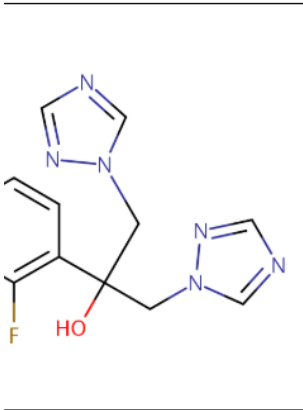
LINKS

COMMENTS

Batch Search Lists Predictions Downloads Copy Share Submit Comment Search all data

## azole

-4 | DTXSID3020627  
STox Substance Id.



Wikipedia

Fluconazole is an antifungal medication used for a number of fungal infections. This includes candidiasis, blastomycosis, coccidioidomycosis, cryptococcosis, histoplasmosis, dermatophytosis, and pityriasis versicolor. It is also used to prevent candidiasis in those who are at high risk such as following organ transplantation, low birth weight babies, and those with low blood neutrophil counts. It is given either by mouth or by injection into a vein. Common side effects include vomiting

...  
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Intrinsic Properties

Molecular Formula:  $C_{12}H_{12}F_2N_6O$  Mol File Find All Chemicals

Average Mass: 306.277 g/mol [Isotope Mass Distribution](#)

Monoisotopic Mass: 306.104065 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

50

# GenRA (Generalised Read-Across)

**Fluconazole**  
86386-73-4 | DTXSID3020627  
Searched by DSSTox Substance Id.

DETAILS  
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**GENRA**  
RELATED SUBSTANCES  
SYNONYMS  
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COMMENTS

**Step One: Analog Identification and Evaluation**

Neighbors by: Chem: Morgan Fgrprts Filter by: invivo data

Structure Similarity

Fluconazole

Bromuconazole  
Flusilazole  
Cyproconazole  
Pyrasulfotole m...  
Myclobutanil  
Fenbuconazole  
Tetraconazole  
Metonazole  
Ipconazole

# of Analogs 10

Next

Select and Review Analogs

# 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	
Ipconazole	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, Ipconazole, Bromuconazole



# GenRA (Generalised Read-Across)



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

## Chemical Research in Toxicology

Cite This: Chem. Res. Toxicol. 2017, 30, 2046-2059

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



## 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>



## Regulatory Toxicology and Pharmacology

Volume 79, August 2016, Pages 12-24



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

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



Contents lists available at ScienceDirect

## Computational Toxicology

journal homepage: [www.elsevier.com](http://www.elsevier.com)

Journal  
Cover  
Image

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

Grace Patlewicz<sup>a, \*</sup>, Mark T.D. Cronin<sup>b</sup>, George Helman<sup>a, c</sup>, Jason C. Lambert<sup>d</sup>, Lucina E. Lizarraga<sup>d</sup>, Imran Shah<sup>a</sup>

<sup>a</sup> National Center for Computational Toxicology (NCCT), Office of Research and Development, US Environmental Protection Agency (US EPA), 109 TW Alexander Dr, Research Triangle Park (RTP), NC 27711, USA

<sup>b</sup> School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK

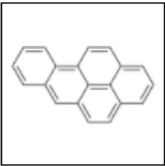
<sup>c</sup> Oak Ridge Institute for Science and Education (ORISE), 1299 Bethel Valley Road, Oak Ridge, TN 37830, USA

<sup>d</sup> National Center for Evaluation Assessment (NCEA), US Environmental Protection Agency (US EPA), 26 West Martin Luther King Dr, Cincinnati, OH 45268, USA

# 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.

## Synonyms

Download

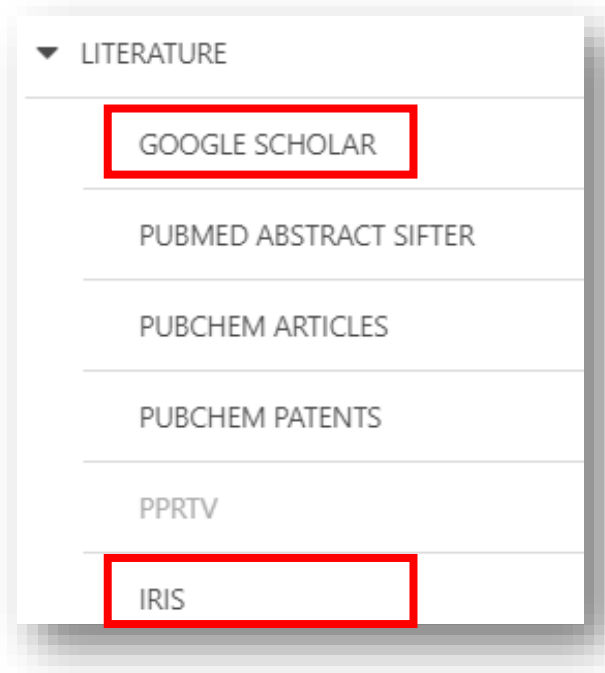
25

Search query

Synonym	Quality
Benzo(a)pyrene	Valid
Benzo[pqr]tetraphene	Valid
Benzo[a]pyrene	Valid
50-32-8 <span>Active CAS-RN</span>	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”



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

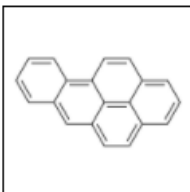
#### Noncancer Assessment

[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)<sup>-1</sup> was calculated for mice, which was converted to a dose-equivalent slope factor of 25 (mg/kg day)<sup>-1</sup>. 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 – 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

### General

-  EPA Substance Registry Service
-  PubChem
-  Chempider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  ToxPlanet

### Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ACToR



## eChemPortal

The Global Portal to  
Information on  
Chemical Substances

[Home](#) [Substance Search](#) [Property Search](#) [Classification Search](#) [Schedules of Assessments](#) [Data sources](#) [About](#) [Help](#) [Contact Us](#)

### Chemical Substance Search

**Substance** (50-32-8) ▼

**Sources and type of information** ▲

Select all Deselect all

**Types** ⓘ

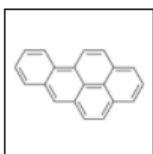
- ☒ Property information
- ☒ Exposure and use information
- ☒ GHS classifications

**Data sources**

<input checked="" type="checkbox"/> ACToR ⓘ	<input checked="" type="checkbox"/> AGRITOX ⓘ	<input checked="" type="checkbox"/> AICIS assessments ⓘ
<input checked="" type="checkbox"/> APVMA-CR ⓘ	<input checked="" type="checkbox"/> CCR ⓘ	<input checked="" type="checkbox"/> CESAR ⓘ
<input checked="" type="checkbox"/> Chemicals Dashboard ⓘ	<input checked="" type="checkbox"/> ChemInfo ⓘ	<input checked="" type="checkbox"/> Combined Exposures ⓘ



# Similarity Searching



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Searched with a similarity threshold of 0.8

237 of 276 chemicals visible

Select all

Download

Send to Batch Search

Similarity



DTXSID

CASRN

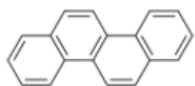
Similarity



Isotopes

Multicomponent Chemicals

Filter by Name or CASRN

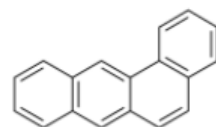


Chrysene

DTXSID:DTXSID0022432

CASRN:218-01-9

Similarity:1.00

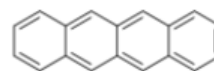


Benz(a)anthracene

DTXSID:DTXSID5023902

CASRN:56-55-3

Similarity:1.00

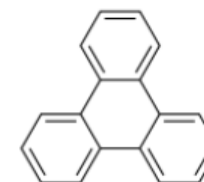


Naphthalene

DTXSID:DTXSID4059045

CASRN:92-24-0

Similarity:1.00

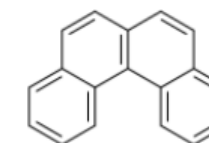


Triphenylene

DTXSID:DTXSID9059757

CASRN:217-59-4

Similarity:1.00



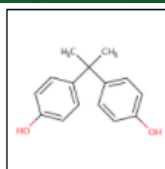
Benzo[c]phenanthrene

DTXSID:DTXSID4075459

CASRN:195-19-7

Similarity:1.00

# Related Substances



## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

9 chemicals

Select all

Download

Send to Batch Search

Relationship



DTXSID

CASRN

TOXCAST

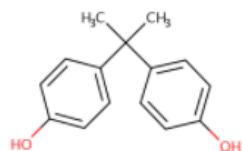


Hide chemicals that are:

Filter by Name or CASRN



Searched Chemical



Bisphenol A

DTXSID:DTXSID7020182

CASRN:80-05-7

TOXCAST:217/1152

Polymer

2 related chemical  
structures with this  
substance

Formaldehyde, polymer with bisphenol A

DTXSID:DTXSID3049627

CASRN:25085-75-0

TOXCAST:-

Polymer

2 related chemical  
structures with this  
substance

Bisphenol A/ Epichlorohydrin resin

DTXSID:DTXSID0050479

CASRN:25068-38-6

TOXCAST:-

Polymer

3 related chemical  
structures with this  
substance

Bisphenol A-epichlorohydrin-polyformal...

DTXSID:DTXSID9050480

CASRN:28906-96-9

TOXCAST:-

Predecessor: Component

4 related chemical  
structures with this  
substance

Fatty acids, C18-unsatd., dimers, polyme...

DTXSID:DTXSID40105886

CASRN:106906-26-7

TOXCAST:-

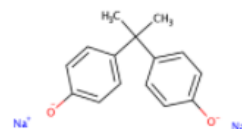
Predecessor: Component

3 related chemical  
structures with this  
substance

Predecessor: Component

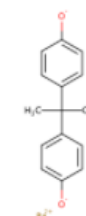
2 related chemical  
structures with this  
substance

Salt Form



Disodium 4,4'-isopropylidenediphenolate

Salt Form



Barium(2+) 4,4'-isopropylidenebispheno...

# Chemical Lists and Categories

# Example: AEGLs list

Home Advanced Search Batch Search Lists ▾ Predictions Downloads

Lists of Chemicals  
List of Assays

## AEGLs: Acute Exposure Guideline Levels

Search AEGLVALUES Chemicals

☐ Identifier substring search

### List Details

**Description:** Acute Exposure Guideline Level (AEGLs) values are intended to protect most individuals in the general population, including those that might be particularly susceptible to the harmful effects of the chemicals. Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals. Used by emergency responders when dealing with chemical spills or other catastrophic exposures, AEGLs are set through a collaborative effort of the public and private sectors worldwide.

**Number of Chemicals:** 174

174 chemicals

Select all

Download ▾

Send to Batch Search

Name ▾

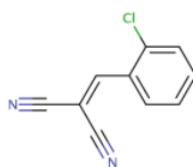


CASRN ✕

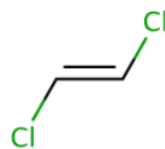
DTXSID ✕ ▾

Hide chemicals that are: ▾

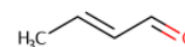
Filter by Name or CASRN



(2-Chlorobenzylidene)propanedinitrile  
CASRN:2698-41-1  
DTXSID:DTXSID9020297



(E)-1,2-Dichloroethylene  
CASRN:156-60-5  
DTXSID:DTXSID7024031




(E)-Crotonaldehyde  
CASRN:123-73-9  
DTXSID:DTXSID6020351



(Z)-1,2-Dichloroethylene  
CASRN:156-59-2  
DTXSID:DTXSID2024030

# 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

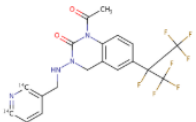
**List Details**

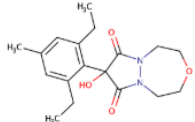
**Description:** The entries in this list have been classified in the U.S. as pesticidal "active ingredients" (conventional, antimicrobial, or biopesticidal agents), and were sourced from the Pesticide Chemical Search database (<https://iaspub.epa.gov/apex/pesticides/f?p=chemicalsearch:1>) created by 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.

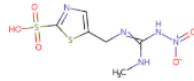
**Number of Chemicals:** 4012

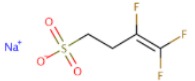
Select all Download **Send to Batch Search** CASRN DTXSID Mono.Mass 3988 chemicals

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-benzodioxepin-2-one  
CASRN: NOCAS\_920508  
DTXSID: DTXSID10920508  
Mono.Mass: 332.173607

  
5-(((Methylamino)(nitroamino)methylene)amino)-2-methylthiophene-3-sulfonic acid  
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 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....

## Batch Search ?



### Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

#### Select Input Type(s)

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

#### Enter Identifiers to Search (One per line. Searches should be limited to <5000 identifiers.)

Sodium azide  
O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate  
(Trichloromethyl)benzene  
100-44-7  
(Chloromethyl)benzene  
98-07-7  
111-44-4  
1-Chloro-2-(2-chloroethoxy)ethane  
Chloro(chloromethoxy)methane  
2-(Butan-2-yl)-4,6-dinitrophenol

Display All Chemicals

Download Chemical Data

# Select Output Format and Content

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

### Select Output Format:







 Excel 

 Download






### Customize Results

- ☐ Select All
- ☐ Select All in Lists






### 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 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS 
- ☐ PPRTV 
- ☐ Wikipedia Article
- ☐ QC Notes 
- ☐ Include links to ACToR reports - SLOW! (BETA) 

### Presence in Lists:

- ☐ 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks) 
- ☐ 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities 
- ☐ AEGLs: Acute Exposure Guideline Levels 
- ☐ ANDROGEN: Androgen Receptor Chemicals 
- ☐ ARTICLE: Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014) 
- ☐ ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP) 
- ☐ ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA) 
- ☐ ATSDR Toxicological Profiles 
- ☐ ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances 
- ☐ ATSDR: Toxic Substances Portal Chemical List 
- ☐ California Office of Environmental Health Hazard Assessment 
- ☐ Canadian Domestic Substances List 2019 
- ☐ CATEGORY: Amino acids 
- ☐ CATEGORY: Color Index dyes 
- ☐ CATEGORY: Flame Retardants 

# 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 WEIGHT	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)	C12H18N2C	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]	C9H23NO2S	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-Methoxyphenyl)thio]methyl	C9H13O6P	Y	-	-	COC1=COCC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyclopentadienyl)tricarbonyliron	12108-13-3	YASXMYPV	Tricarbonyliron	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 acetate	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

# Send to batch and select....

## 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 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ 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	B	C	D	E	F	G	H	I	J	K	L	M
DTXSID	PREFERRED_NAME	EXPOCAST_ME	EXPOCAST_NH	ANES	TOXVAL_DATA	TOXCAST_%_ACT	TOXCAST_	#PUBMED	PUBCHEM_	CPDAT_COU	IRIS_LINK	PPRTV_LINK
DTXSID2021105	Pentachloronitrobenzene	1.14e-07	Y	Y	Y	11.8	99/839	69	96	164	Y	-
DTXSID4022527	Propylparaben	1.4e-05	Y	Y	Y	13.77	99/719	201	121	1476	-	-
DTXSID4024064	Dinex	8.29e-08	Y	-	Y	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	-	Y	14.02	98/699	284	16	98	Y	Y
DTXSID6025355	Glutaraldehyde	2.03e-05	Y	-	Y	14.35	98/683	6515	139	1144	-	-
DTXSID8032417	Isofenphos	1.87e-08	Y	-	Y	16.28	98/602	30	42	60	-	-
DTXSID6032352	Chlorpyrifos-methyl	1.07e-07	Y	Y	Y	11.27	97/861	72	50	116	-	-
DTXSID8020620	Fenthion	8.99e-08	Y	Y	Y	11.56	97/839	354	100	99	-	-
DTXSID2020189	FD&C Blue No. 1	0.000178	Y	-	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	-	Y	11.23	96/855	476	91	105	Y	-
DTXSID9020247	Carbaryl	5.61e-08	Y	Y	Y	11.51	96/834	1135	117	245	Y	-
DTXSID8024109	Flutolanil	1.63e-08	Y	-	Y	11.4	95/833	6	59	80	-	-
DTXSID1023998	Cypermethrin	1.62e-06	Y	Y	Y	10.78	94/872	1148	148	246	-	-
DTXSID2024242	Paclobutrazol	9.19e-08	Y	-	Y	11.11	94/846	139	-	40	Y	-
DTXSID1020807	2-Mercaptobenzothiazole	4.7e-05	Y	-	Y	12.82	94/733	111	181	86	-	Y