

Applications of the US EPA's CompTox Chemicals Dashboard to support structure identification and chemical forensics using mass spectrometry

Antony Williams¹ and Andrew D. McEachran^{2,3}

1) *National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC*

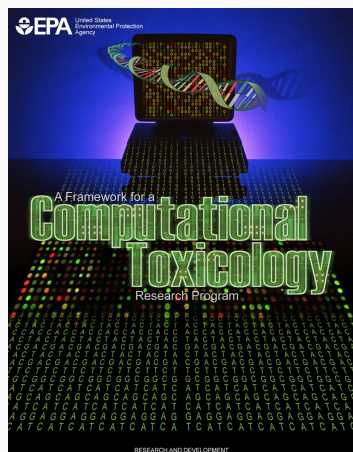
2) *Oak Ridge Institute of Science and Education (ORISE) Research Participant, RTP, NC*

3) *Present Address: Agilent Inc., Santa Clara, CA*

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

*March 2019
Pittcon, Philadelphia*

National Center for Computational Toxicology




- National Center for Computational Toxicology established in 2005 to integrate:
 - High-throughput and high-content technologies
 - Modern molecular biology
 - Data mining and statistical modeling
 - Computational biology and chemistry
- Researching computational approaches to quickly evaluate the safety of chemicals for potential risk.
- Outputs: a lot of data, models, algorithms and software applications

- A publicly accessible website delivering access:
 - ~**875,000** chemicals with related property data
 - Searchable by chemical, product use, gene and assay (ToxCast)
 - Experimental and predicted physicochemical property data
 - “Bioactivity data” for the ToxCast/Tox21 project
 - Generalized Read-Across (GenRA) module
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals
 - **DOWNLOADABLE** Open Data for reuse and repurposing


CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>

 EPA
United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists ▼ Predictions Downloads

Share ▼



875 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](#)

Journal of Cheminformatics article regarding "MS-Ready structures"


March 9th, 2019 at 1:09:45 PM

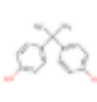
A recent article describes "MS-Ready structures", what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#).




Search Chemicals


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

 Bisphenol




Bisphenol A
DTXSID7020182






Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991




Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992




Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592

Bisphenol A carbonate polymer
DTXSID6027840



Bisphenol A diglycidyl ether
DTXSID6024624



Bisphenol A glycidyl methacrylate
DTXSID7044841

Detailed Chemical Pages

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

► ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

► LITERATURE

LINKS

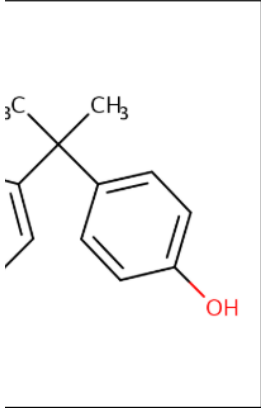
COMMENTS

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

Bisphenol A

05-7 | DTXSID7020182

Identified by DSSTox Substance Id.








Wikipedia


Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(\text{CH}_3)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water (0.344 wt % at 83 °C). BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates

[Read more](#)

Intrinsic Properties

 **Molecular Formula:** $\text{C}_{15}\text{H}_{16}\text{O}_2$  **Mol File**  **Find All Chemicals**

 **Average Mass:** 228.291 g/mol  **Isotope Mass Distribution**

 **Monoisotopic Mass:** 228.11503 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Access to Chemical Hazard Data

DETAILS

EXECUTIVE SUMMARY

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GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

Hazard

DataType

Toxicity Value

Human

Eco

Download

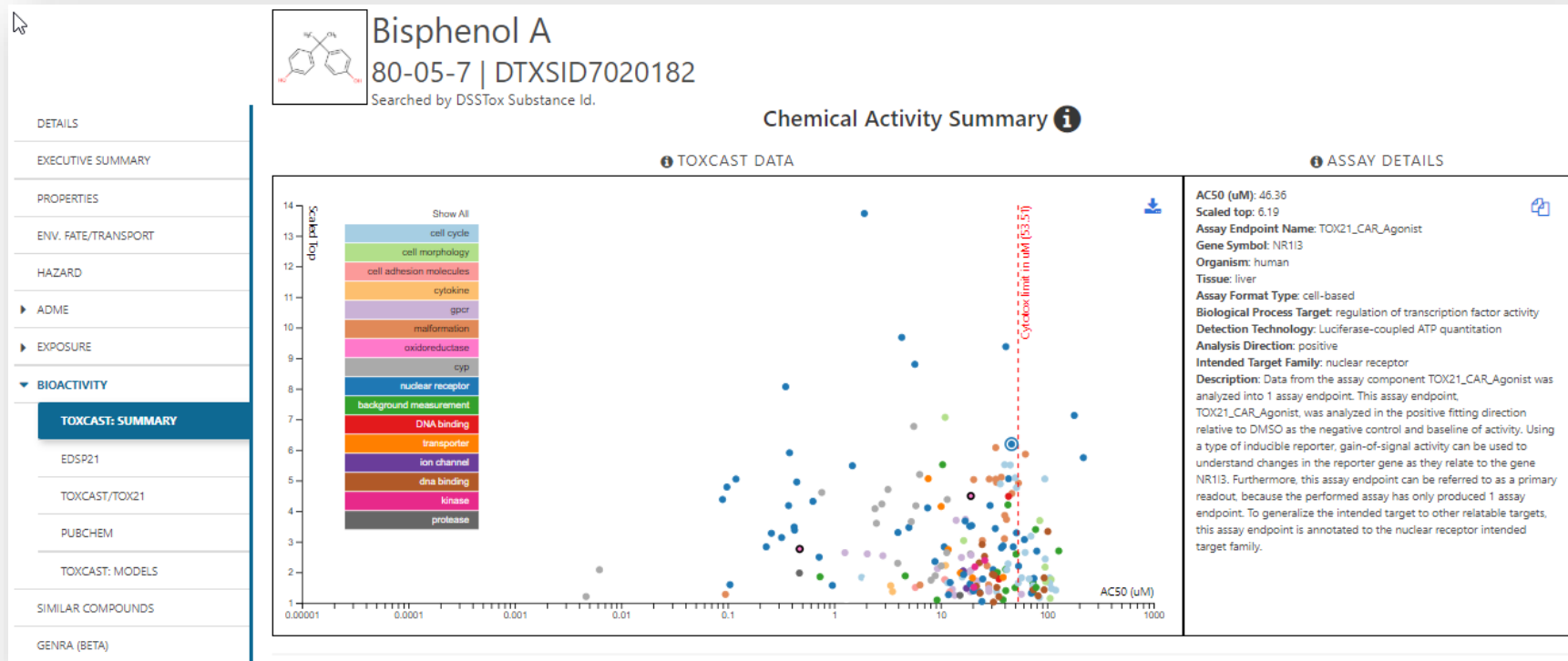
Columns

Search query


More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	106000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, SL/d Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	6	RfD	-	chronic	0.05	mg/kg-day	-	oral	rat	Wignall	Wignall
	5	RfD	-	chronic	0.05	mg/kg-day	-	-	-	MSC Table 5	Pennsylvania DEP ToxValues
	4	RfD	-	chronic	0.05	mg/kg-day	chronic	oral	rat	IRIS	Chiu
	3	RfD	-	chronic	0.6	mg/kg-day	-	oral	rat	EPA/ORNL/OLEM	HEAST
	1	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

In Vitro Bioassay Screening

ToxCast and Tox21



Sources of Exposure to Chemicals

 United States
Environmental Protection
Agency

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Search all data

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

Download ▼

Columns ▼10 ▼

Search query

Product and Use Categories (PUCs)

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
	CPCat Cassette	16
	CPCat Cassette	12
	CPCat Cassette	11
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	7
	CPCat Cassette	6

First<<<12345678910>>>Last

EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE


TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

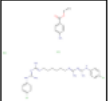
PRODUCTION VOLUME

MS-Ready Mappings

 **EPA** United States
Environmental Protection
Agency

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Progaron

108532-15-6 | DTXSID20148579

Searched by DSSTox Substance Id.

DETAILS

[EXECUTIVE SUMMARY](#)

[PROPERTIES](#)

[ENV. FATE/TRANSPORT](#)

[HAZARD](#)

[ADME](#)

[EXPOSURE](#)

[BIOACTIVITY](#)

[SIMILAR COMPOUNDS](#)

[GENRA \(BETA\)](#)

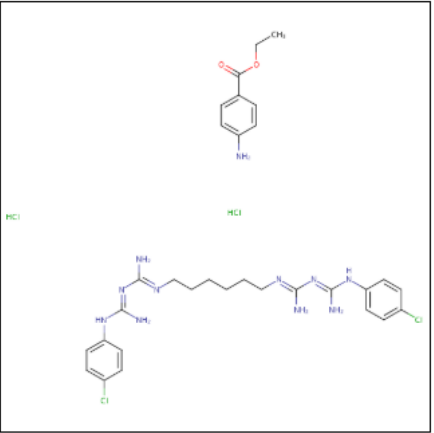
[RELATED SUBSTANCES](#)

[SYNONYMS](#)

[LITERATURE](#)




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[COMMENTS](#)



Chemical structure of Progaron (108532-15-6) is displayed, showing the molecule and its hydrochloride salt (HCl).

Intrinsic Properties

 **Molecular Formula:** C₃₁H₄₃Cl₄N₁₁O₂  Mol File  Find All Chemicals

 **Average Mass:** 743.56 g/mol  Isotope Mass Distribution

Structural Identification

Linked Substances

Same Connectivity: 1 record (nChl)

Mixtures, Component records

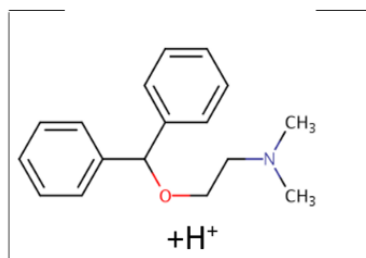
MS-Ready Mappings: DTXCID301804: 12 records; DTXCID0013314: 11 records;

Similar Compounds: 0 records

Quality Control Notes

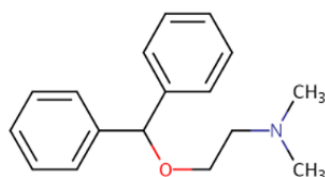
Specific Data-Mappings “MS-Ready Structures”

A) Molecular Ion



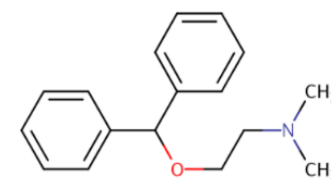
m/z ≈ 256.1702

B) MS-Ready Form

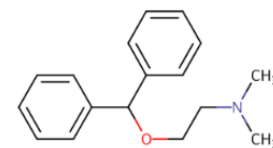


monoisotopic mass= 255.1623
C₁₇H₂₁NO
DTXCID802949

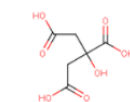
C) Mappings from MS-Ready



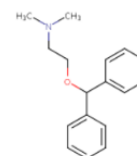
Diphenhydramine
C₁₇H₂₁NO | 255.1623
DTXCID4022949



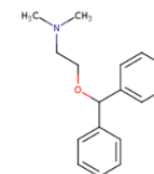
Diphenhydramine
hydrochloride
C₁₇H₂₂ClNO | 291.1390
DTXCID4020537



Diphenhydramine citrate
C₂₃H₂₉NO₈ | 447.1893
DTXCID80237211



Diphenhydramine salicylate
C₂₄H₂₇NO₄ | 393.1940
DTXCID10225883



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

Journal of Cheminformatics

METHODOLOGY

Open Access



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

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

MS-Ready Mappings Set

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

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

10 of 12 chemicals visible

Select all Download Send to Batch Search Default DTXSID PubChem CPDAT

Isotopes Filter by Name or CASRN

Benzocaine
DTXSID: DTXSID8021804
PubChem: 184
CPDAT: 42

Anesthesine succinate
DTXSID: DTXSID60148336
PubChem: 10
CPDAT: 0

Anesthesine oxalate
DTXSID: DTXSID20148337
PubChem: 6
CPDAT: 0

Progaron
DTXSID: DTXSID20148579
PubChem: 5
CPDAT: 0

Benzocaine hydrochloride
DTXSID: DTXSID50177812
PubChem: 33
CPDAT: 0

Antipyrine mixture with benzocaine
DTXSID: DTXSID80212886
PubChem: 9
CPDAT: 0

Almagel A-neo
DTXSID: DTXSID60227559
PubChem: 9
CPDAT: 0

Almagel
DTXSID: DTXSID70227560
PubChem: 9
CPDAT: 0

Ethyl 4-aminobenzoate--2,4,6-trinitroph...
DTXSID: DTXSID70787033
PubChem: 5
CPDAT: 0

1-Hexadecylpyridin-1-ium 2-butoxy-N-[-...
DTXSID: DTXSID50997335
PubChem: 0
CPDAT: 0

Mass and Formula Searches

Supporting Mass Spectrometry

Advanced Search?

Mass Search?

Select Adduct: ▼

Da \pm

Molecular Formula Search?

☒ MS Ready Formula? ☐ Exact Formula?

Generate Molecular Formula(e)?

Da \pm

Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]

Include Halogens: ☐ F[0-20] ☐ Cl[0-20] ☐ Br[0-20] ☐ I[0-20]

Advanced Searches

Mass Based Search

Mass Search

± Min/Max

Adduct

Neutral



All Adducts



Choose adduct from dropdown

191.131

Da

±

5

Da

ppm

Search 

Advanced Searches

Mass Based Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

Select all

Download

Send to Batch Search

Mass Difference

DTXSID

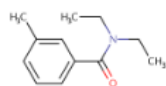
CASRN

TOXCAST

Mass Diff

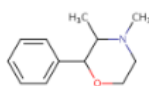
Multicomponent Chemicals

Filter by Name or CASRN



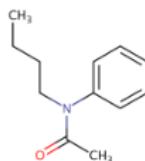
DEET

DTXSID: DTXSID2021995
CASRN: 134-62-3
TOXCAST: 12/768
Mass Diff: 0.000014



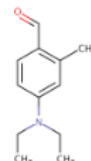
Phendimetrazine

DTXSID: DTXSID1023447
CASRN: 634-03-7
TOXCAST: -
Mass Diff: 0.000014



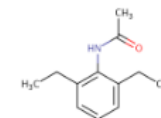
N-Butylacetanilide

DTXSID: DTXSID2042197
CASRN: 91-49-6
TOXCAST: -
Mass Diff: 0.000014



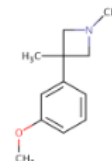
Benzaldehyde, 4-(diethylamino)-2-meth...

DTXSID: DTXSID4059041
CASRN: 92-14-8
TOXCAST: -
Mass Diff: 0.000014



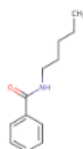
Acetanilide, 2',6'-diethyl-

DTXSID: DTXSID90168148
CASRN: 16665-89-7
TOXCAST: -
Mass Diff: 0.000014



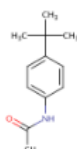
Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)-

DTXSID: DTXSID40173560
CASRN: 19832-26-9
TOXCAST: -
Mass Diff: 0.000014



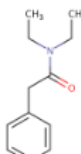
Benzamide, N-pentyl-

DTXSID: DTXSID20174196
CASRN: 20308-43-4
TOXCAST: -
Mass Diff: 0.000014



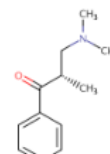
p-t-Butylacetanilide

DTXSID: DTXSID80174238
CASRN: 20330-45-4
TOXCAST: -
Mass Diff: 0.000014



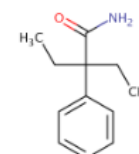
N,N-Diethylphenylacetamide

DTXSID: DTXSID00179048
CASRN: 2431-96-1
TOXCAST: -
Mass Diff: 0.000014



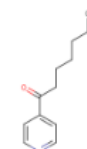
3-(Dimethylamino)-2-methylpropionophenone

DTXSID: DTXSID60180796
CASRN: 26171-50-6
TOXCAST: -
Mass Diff: 0.000014



Butyramide, 2-ethyl-2-phenyl-

DTXSID: DTXSID60184653
CASRN: 30568-39-9
TOXCAST: -
Mass Diff: 0.000014



1-Heptanone, 1-(4-pyridyl)-

DTXSID: DTXSID40186594
CASRN: 32941-30-3
TOXCAST: -
Mass Diff: 0.000014

Advanced Searches

Mass Based Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

Select all

Download

Send to Batch Search

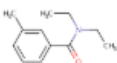
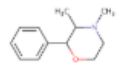
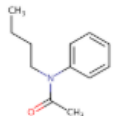
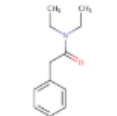
Sources



Multicomponent Chemicals


Filter by Name or CASRN



Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass	Mass Difference
	DTXSID2021995 ToxCast™	DEET	134-62-3	Level 1	111	135	155	753	191.131014	0.000014
	DTXSID1023447	Phendimetrazine	634-03-7	Level 2	12	34	35	50	191.131014	0.000014
	DTXSID2042197	N-Butylacetanilide	91-49-6	Level 2	1	32	50	1	191.131014	0.000014
	DTXSID00179048	N,N-Diethylphenylacetamide	2431-96-1	Level 4	0	21	52	34	191.131014	0.000014

- Singleton searches are useful but we work with thousands of chemicals!
- Typical questions
 - What is the list of chemicals for the formula $C_xH_yO_z$
 - What is the list of chemicals for a mass +/- error
 - Can I get chemical lists in Excel files? In SDF files?

Batch Searches

 United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Batch Search?

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6

Step Six: Click "Download"

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

Display All Chemicals Download Chemical Data

Select Output Format:

Excel

Download

Customize Results

- ☐ Select All
- ☐ Select All in Lists


Enter Identifiers to Search (searches should be limited to <5000 identifiers)

107-02-8
79-06-1
107-13-1
309-00-2
107-18-6
62-53-3
7631-89-2
1327-53-3
7784-46-5
26628-22-8

Presence in Lists:

- ☐ 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
- ☐ AEGLs: Acute Exposure Guideline Levels

Batch Searches

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6

Step Six: Click "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

Presence in Lists:

- ☐ 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)
- ☐ ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances
- ☐ ATSDR: Toxic Substances Portal Chemical List
- ☐ California Office of Environmental Health Hazard Assessment
- ☐ CERAPP: Collaborative Estrogen Receptor Activity Prediction Project
- ☐ CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
- ☐ CHEMINV: EPA Chemical Inventory for ToxCast
- ☐ CHEMINV: EPA ToxCast CHEMINV list of volatiles
- ☐ CHEMINV: EPA ToxCast Cheminventory chemicals with stability problems
- ☐ CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
- ☐ CHEMINV: EPA ToxCast Cheminventory List of Reactives
- ☐ DRUGS: DrugBank database from the University of Alberta
- ☐ DRUGS: ITNANTIBIOTIC list of antibiotics
- ☐ DRUGS: Pharmaceutical List with EU, Swiss, US Consumption Data
- ☐ DRUGS: Statin drugs
- ☐ ECOTOX: Ecotoxicology knowledgebase
- ☐ Endocrine Disruptor Screening Program (EDSP) Universe of Chemicals
- ☐ ENDOCRINE: EDSR21 Tier 1 Screening Chemicals List 1

Batch Searching Formula/Mass

Batch Search ?












Step Five: Choose Data Fields to Download

Please enter one identifier per line

Select Input Type(s)

+/- 5 ppm

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

 Display All Chem

Enter Identifiers to Search (searches should be limited to <5000 identifiers)

41.0265
56.02621
53.0265
58.0418|
93.0578
113.9639
151.8754
69.9377
77.9872

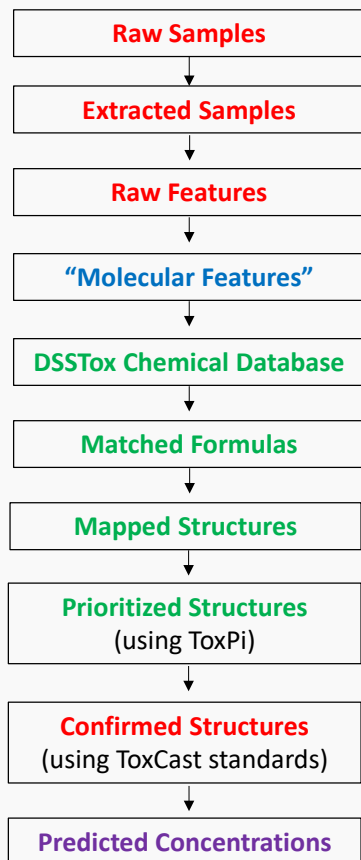
This search is based on what we refer to as "Mass Spec (MS) Ready" structures. All chemicals within the database are treated in a manner such that all are desalted, mixtures are separated, and stereochemistry is removed as Mass Spectrometry detects the major components of a salt or mixture and is insensitive to stereochemistry. As an example, a search for the monoisotopic mass of phenol will return phenol, sodium phenolate and calcium phenoxide. See the publication for more details: <https://doi.org/10.1186/s13321-018-0299-2>.

Excel Output

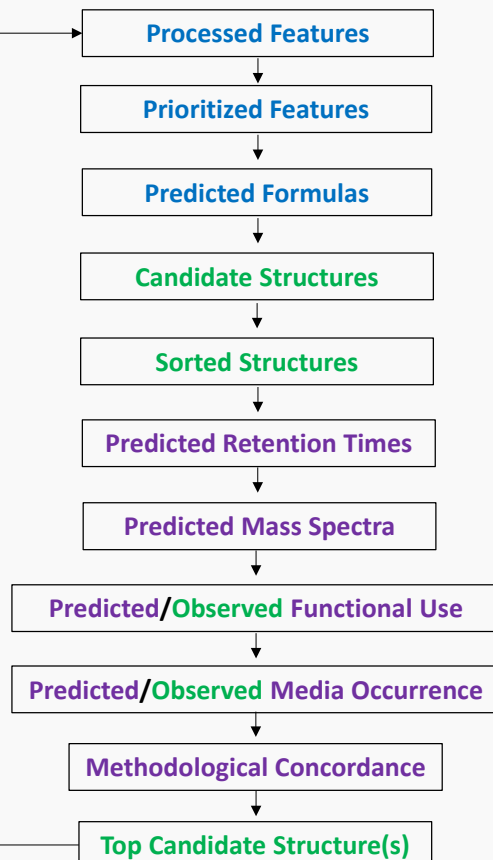
PREFERRED	CASRN	DATA_SOURCE	TOXVAL_D	TOXCAST	TOXCAST	NUMBER_OF_PUBMED	PUBCHEM_DATA_S	CPDAT_COUNT
Aniline	62-53-3	148	Y	0.47	1/211	1932	284	80
3-Methylpyr	108-99-6	93	Y	2.8	16/571	16	120	16
2-Methylpyr	109-06-8	88	Y	0.0	0/211	1395	112	12
4-Methylpyr	108-89-4	82	Y	0.52	2/381	1	118	4
Aniline hydr	142-04-1	54	Y	2.23	9/404	1932	66	5
Anilinium ni	542-15-4	13	-	2.37	5/211	1932	4	-
Benzenami	542-16-5	13	-	-	-	-	-	5
1,3,5-Trinitr	3101-79-9	10	-	-	-	-	10	1
Di-2-propyn	6921-28-4	10	-	-	-	-	43	-
Benzenami	542-14-3	8	-	-	-	-	15	-
Butanal--an	68411-20-1	8	-	-	-	-	-	6
Benzenami	37832-42-1	7	-	-	-	1932	27	-
2,4-Hexadie	1516-01-4	6	-	-	-	-	25	-
Cyclobutan	15760-35-7	6	-	-	-	-	79	2
Aniline hydr	542-13-2	6	-	-	-	1932	6	-
Benzenami	542-11-0	6	-	-	-	-	-	-
Tris(4-amin	68389-46-8	6	-	-	-	-	-	3
4-[(2-Chloro	71566-74-0	6	-	-	-	-	-	4
Heptanal--a	9003-50-3	6	-	-	-	-	-	1

Suspect Screening and Non-Targeted Analysis Workflow

Suspect Screening



Non-Targeted Analysis



Color Key

Red = Analytical Chemistry

Blue = Data Processing & Analysis

Purple = Mathematical & QSPR Modeling

Green = Informatics & Web Services



MS-Ready Structures Underpin Analysis

Mass

Search 

Molecular Formula Search

☒ MS Ready Formula 

Formula

Please use the format of C1=CC=C(C=C1)O

Search 

Generate Molecular Formula










This search is based on what we refer to as "Mass Spec (MS) Ready" structures. All chemicals within the database are treated in a manner such that all are desalted, mixtures are separated, and stereochemistry is removed as Mass Spectrometry detects the major components of a salt or mixture and is insensitive to stereochemistry. As an example, a search for the formula of phenol will return phenol, sodium phenolate and calcium phenoxide. See the publication for more details:

<https://doi.org/10.1186/s13321-018-0299-2>

C1=CC=C(C=C1)O

MS-Ready Structures Underpin Analysis

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 

 Display All Chemicals

+/- 5 ppm

Enter Identifiers to Search [\(search\)](#)

41.0265
56.02621
53.0265
58.0418|
93.0578
113.9639
151.8754
69.9377
77.9872

This search is based on what we refer to as "Mass Spec (MS) Ready" structures. All chemicals within the database are treated in a manner such that all are desalted, mixtures are separated, and stereochemistry is removed as Mass Spectrometry detects the major components of a salt or mixture and is insensitive to stereochemistry. As an example, a search for the monoisotopic mass of phenol will return phenol, sodium phenolate and calcium phenoxide. See the publication for more details: <https://doi.org/10.1186/s13321-018-0299-2>.

The Dashboard to Support MS-Analysis

MS-Ready Structures Underpin Analysis

Mass Search

±

Min/Max

M

Mass

Da

±


Error

Da

ppm

Molecular Formula Search

Molecular Formula

☒ MS Ready Formula 

☐ Exact Formula 

Generate Molecular Formula(e)

±

Min/Max

Mass

Da

Step One

Step Two

Step Three

Step Four

Step Five


Step Six


Step Five: Choose Data Fields to Download

Please enter one identifier per line


×

Select Input Type(s)

☐ Chemical Name 

☐ CASRN 

☐ InChIKey  ☐ Skeleton 

☐ DSSTox Substance ID 

☒ MS-Ready Formula(e) 

☐ Exact Formula(e) 

☐ Monoisotopic Mass

Enter Identifiers to Search (searches should be limited to <1000 identifiers)



C14H22N2O3
C10H12N2O
C14H18N4O3
C12H11N7
C8H9NO2

Display All Chemicals

Download Chemical Data


MS-Ready Mappings

- Input Formula: C₁₀H₁₆N₂O₈: 3 Hits


☐ MS Ready Formula 
☒ Exact Formula 


Formula

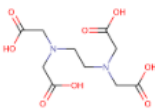
C₁₀H₁₆N₂O₈

Search 

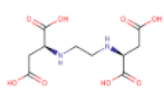
3 of 3 chemicals visible

Select all Download Send to Batch Search Default 
 DTXSID PubChem CPDAT

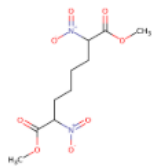
Multicomponent Chemicals Filter by Name or CASR 



Ethylenediaminetetraacetic acid
DTXSID: DTXSID6022977
PubChem: 158
CPDAT: 387



N,N'-Ethylenedi-L-aspartic acid
DTXSID: DTXSID1051852
PubChem: 25
CPDAT: 8



Dimethyl 2,7-dinitrooctanedioate
DTXSID: DTXSID20498864
PubChem: 5
CPDAT: 0

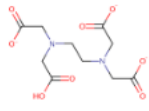
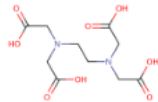
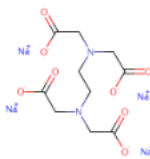
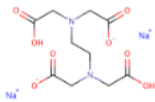
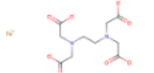
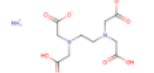
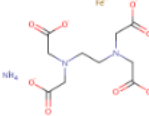
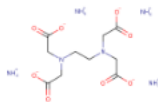
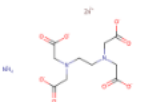
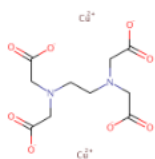
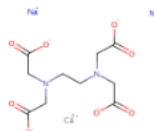
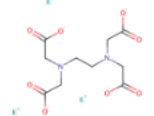
MS-Ready Mappings

- **Same Input Formula: C₁₀H₁₆N₂O₈**
- **MS Ready Formula Search: 125 Chemicals**

125 chemicals

Select all Download Send to Batch Search Default DTXSID PubChem CPDAT

Hide chemicals that are: Filter by Name or CASR

 <p>Trisodium ethylenediaminetetraacetate DTXSID: DTXSID7020556 PubChem: 33 CPDAT: 82</p>	 <p>Ethylenediaminetetraacetic acid DTXSID: DTXSID6022977 PubChem: 158 CPDAT: 387</p>	 <p>Ethylenediaminetetraacetic acid tetrasod... DTXSID: DTXSID3026350 PubChem: 57 CPDAT: 1227</p>	 <p>Ethylenediaminetetraacetic acid, disodiu... DTXSID: DTXSID9027073 PubChem: 56 CPDAT: 1359</p>	 <p>Ethylenediaminetetraacetic acid ferric so... DTXSID: DTXSID5027774 PubChem: 53 CPDAT: 62</p>	 <p>Diammonium dihydrogen ethylenediami... DTXSID: DTXSID9027813 PubChem: 12 CPDAT: 17</p>
 <p>Ferrate(1-), [[N,N'-1,2-ethanediy]bis[N-]]... DTXSID: DTXSID9027815 PubChem: 24 CPDAT: 20</p>	 <p>Tetraammonium ethylenediaminetetraac... DTXSID: DTXSID8027820 PubChem: 11 CPDAT: 12</p>	 <p>Zincate(2-), [[N,N'-1,2-ethanediy]bis[N-]]... DTXSID: DTXSID8028343 PubChem: 5 CPDAT: 10</p>	 <p>EDTA, copper salt DTXSID: DTXSID0034564 PubChem: 8 CPDAT: 10</p>	 <p>Calcium disodium ethylenediaminetetra... DTXSID: DTXSID2036409 PubChem: 42 CPDAT: 29</p>	 <p>Tetrapotassium ethylenediaminetetraac... DTXSID: DTXSID3036442 PubChem: 25 CPDAT: 36</p>

- 125 chemicals returned in total
 - 8 of the 125 are single component chemicals
 - 3 of the 8 are isotope-labeled
 - 3 are neutral compounds and 2 are charged

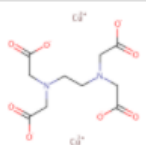

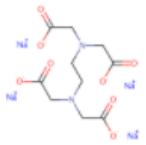

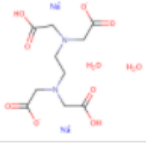

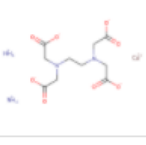

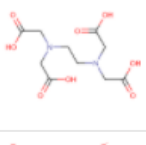

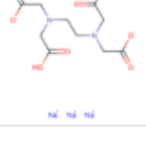

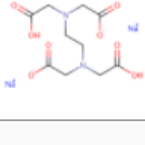

Complexity to Simplicity

93 Chemicals – 7 in EPAHFR

1	INPUT	DTXCID_INDIVID	FORMULA	SMILES	DTXSID	CASRN	EXPOCAST	MEXPOCAST	DATA_SOURCE	TOXVAL	DTXCAST	TOXCAST	# OF PUBMED	PUBCHEM	EPAHFR
2	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID6022977	60-00-4	7.96e-05	Y		71	Y	2.65	3/113	25251	158	Y
3	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID9027073	139-33-3	-	-		41	Y	-	-	25251	56	Y
4	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID3026350	64-02-8	-	-		37	Y	-	-	-	57	Y
5	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID7020556	150-38-9	-	-		30	Y	-	-	-	33	Y
6	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID5049609	67989-88-2	-	-		20	Y	-	-	-	8	Y
7	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID5049576	6381-92-6	-	-		19	Y	-	-	25251	31	Y
8	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID0034564	12276-01-6	-	-		11	-	-	-	-	8	Y
9	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID5027774	15708-41-5	-	-		48	Y	1.98	6/303	241	53	-
10	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID2036409	62-33-9	4.64e-06	Y		37	Y	0.0	0/64	25251	42	-
11	C10H16N2O8	DTXCID00197424	C10H16N2(OC(=O)Cl	DTXSID1051852	20846-91-7	-	-		36	Y	-	-	89	25	-
12	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID6042107	15375-84-5	-	-		25	Y	-	-	97	25	-
13	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID3036442	5964-35-2	-	-		23	Y	-	-	25251	25	-
14	C10H16N2O8	DTXCID00197424	C10H16N2(OC(=O)Cl	DTXSID1051806	178949-82-1	-	-		22	Y	-	-	-	5	-
15	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID0065696	14025-21-9	-	-		22	Y	-	-	-	43	-
16	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID9027813	20824-56-0	-	-		21	Y	-	-	-	12	-
17	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID9027815	21265-50-9	-	-		20	Y	-	-	241	24	-
18	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID5058272	17421-79-3	-	-		19	Y	-	-	25251	25	-
19	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID3058612	2001-94-7	-	-		18	Y	-	-	25251	19	-
20	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID8027820	22473-78-5	-	-		16	Y	-	-	-	11	-
21	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID8058324	17572-97-3	-	-		15	-	-	-	-	36	-
22	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID8028343	67859-51-2	-	-		14	Y	-	-	-	5	-
23	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID4051328	13235-36-4	-	-		14	-	-	-	-	18	-
24	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID6070980	68015-77-0	-	-		14	Y	-	-	-	13	-
25	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID9058317	15934-01-7	-	-		11	-	-	-	-	5	-
26	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID0066163	17099-81-9	-	-		11	-	-	-	241	14	-
27	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID1068988	54959-35-2	-	-		11	-	-	-	241	14	-
28	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID5074266	60816-63-9	-	-		11	-	-	-	1	10	-
29	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID4048197	39208-15-6	-	-		10	-	-	-	-	28	-
30	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID2065830	14931-83-0	-	-		10	-	-	-	47	9	-
31	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID70189997	36499-65-7	-	-		10	-	-	-	25298	26	-
32	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID7051420	61916-40-3	-	-		9	-	-	-	-	4	-
33	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID2051425	73513-47-0	-	-		8	Y	-	-	-	3	-
34	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID7051426	73637-19-1	-	-		8	Y	-	-	-	5	-
35	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID2051427	73637-20-4	-	-		8	Y	-	-	-	-	-
36	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID3058741	10378-23-1	-	-		8	Y	-	-	-	31	-
37	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID6065925	15708-48-2	-	-		8	-	-	-	-	19	-
38	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID20217976	6766-87-6	-	-		8	-	-	-	-	13	-
39	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID5065807	14689-29-3	-	-		7	-	-	-	-	12	-
40	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID6069408	60544-70-9	-	-		7	-	-	-	-	12	-
41	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID00153984	123354-94-9	-	-		7	-	-	-	2	6	-
42	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID70190705	37209-61-3	-	-		7	-	-	-	6	9	-
43	C10H16N2O8	DTXCID902977	C10H16N2(OC(=O)Cl	DTXSID7051424	67401-50-7	-	-		6	-	-	-	-	4	-

Complexity to Simplicity

93 Chemicals – 7 in the list

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Source	PubMed Data Source	Monoisotopic Mass
	DTXSID0034564	EDTA, copper salt	12276-01-6	Level 1	10	11	8	0	413.918561 
	DTXSID3026350	Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	Level 1	1227	37	57	0	380.018442 
	DTXSID5049576	Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	Level 1	93	19	31	25251	372.075683 
	DTXSID5049609	Ethylenediaminetetraacetic acid, diammonium copper salt	67989-88-2	Level 2	9	20	8	0	387.057712 
	DTXSID6022977	Ethylenediaminetetraacetic acid	60-00-4	Level 1	346	71	158	25251	292.090665 
	DTXSID7020556	Trisodium ethylenediaminetetraacetate	150-38-9	Level 1	85	30	33	0	358.036498 
	DTXSID9027073	Ethylenediaminetetraacetic acid, disodium salt	139-33-3	Level 1	1358	41	56	25251	336.054554 

Searching batches

Formula (or mass) searching

	A	B	C	D	E	F	G
1	INPUT	DTXSID	CASRN	PREFERRED NAME	MOL FORMULA	MONOISOTOPIC MASS	DATA SOURCES
2	C14H22N2O3	DTXSID2022628	29122-68-7	Atenolol	C14H22N2O3	266.163042576	46
3	C14H22N2O3	DTXSID0021179	6673-35-4	Practolol	C14H22N2O3	266.163042576	32
4	C14H22N2O3	DTXSID4048854	841-73-6	Bucolome	C14H22N2O3	266.163042576	20
5	C14H22N2O3	DTXSID1045407	13171-25-0	Trimetazidine dihydrochloride	C14H24Cl2N2O3	338.116398	19
6	C14H22N2O3	DTXSID0045753	56715-13-0	R-(+)-Atenolol	C14H22N2O3	266.163042576	19
7	C14H22N2O3	DTXSID2048531	5011-34-7	Trimetazidine	C14H22N2O3	266.163042576	14
8	C14H22N2O3	DTXSID10239405	93379-54-5	Esatenolol	C14H22N2O3	266.163042576	12
9	C14H22N2O3	DTXSID50200634	52662-27-8	N-(2-Diethylaminoethyl)-2-(4-hydroxyphenoxy)acetamide	C14H22N2O3	266.163042576	7
10	C14H22N2O3	DTXSID4020111	51706-40-2	dl-Atenolol hydrochloride	C14H23ClN2O3	302.1397203	6
11	C14H22N2O3	DTXSID1068693	51963-82-7	Benzenamine, 2,5-diethoxy-4-(4-morpholinyl)-	C14H22N2O3	266.163042576	5
12	C18H34N2O6S	DTXSID3023215	154-21-2	Lincomycin	C18H34N2O6S	406.213757997	35
13	C18H34N2O6S	DTXSID7047803	859-18-7	Lincomycin hydrochloride	C18H35ClN2O6S	442.1904357	22
14	C18H34N2O6S	DTXSID20849438	1398534-62-7	PUBCHEM_71432748	C18H35ClN2O6S	442.1904357	1
15	C10H12N2O	DTXSID1047576	486-56-6	Cotinine	C10H12N2O	176.094963014	40
16	C10H12N2O	DTXSID8075330	50-67-9	Serotonin	C10H12N2O	176.094963014	22
17	C10H12N2O	DTXSID8044412	2654-57-1	4-Methyl-1-phenylpyrazolidin-3-one	C10H12N2O	176.094963014	18
18	C10H12N2O	DTXSID80165186	153-98-0	Serotonin hydrochloride	C10H13ClN2O	212.0716407	11
19	C10H12N2O	DTXSID2048870	29493-77-4	(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-amine	C10H12N2O	176.094963014	10
20	C10H12N2O	DTXSID10196105	443-31-2	6-Hydroxytryptamine	C10H12N2O	176.094963014	9
21	C10H12N2O	DTXSID90185693	31822-84-1	1,4,5,6-Tetrahydro-5-phenoxypyrimidine	C10H12N2O	176.094963014	7
22	C10H12N2O	DTXSID40178777	2403-66-9	2-Benzimidazolepropanol	C10H12N2O	176.094963014	7
23	C10H12N2O	DTXSID80157026	13140-86-8	N-Cyclopropyl-N'-phenylurea	C10H12N2O	176.094963014	6
24	C10H12N2O	DTXSID30205607	570-14-9	4-Hydroxytryptamine	C10H12N2O	176.094963014	6
25	C14H18N4O3	DTXSID5023900	17804-35-2	Benomyl	C14H18N4O3	290.137890456	68
26	C14H18N4O3	DTXSID3023712	738-70-5	Trimethoprim	C14H18N4O3	290.137890456	51
27	C14H18N4O3	DTXSID40209671	60834-30-2	Trimethoprim hydrochloride	C14H19ClN4O3	326.1145682	8
28	C14H18N4O3	DTXSID70204210	55687-49-5	Benzenemethanol, 4-((2,4-diamino-5-pyrimidinyl)methyl)-2-	C14H18N4O3	290.137890456	5
29	C14H18N4O3	DTXSID20152671	120075-57-2	6-Methoxy-4-(3-(N,N-dimethylamino)propylamino)-5,8-quinaz	C14H18N4O3	290.137890456	4
30	C14H18N4O3	DTXSID30213742	63931-79-3	1H-1,2,4-Benzotriazepine-3-carboxylic acid, 4,5-dihydro-4-	C14H18N4O3	290.137890456	3
31	C14H18N4O3	DTXSID30219608	69449-07-6	2,4-Pyrimidinediamine, 5-((3,4,5-trimethoxyphenyl)methyl)-	C14H20N4O4	308.14845514	3
32	C14H18N4O3	DTXSID20241155	94232-27-6	L-Aspartic acid, compound with 5-((3,4,5-trimethoxyphenyl	C18H25N5O7	423.175398165	3
33	C14H18N4O3	DTXSID80241156	94232-28-7	L-Glutamic acid, compound with 5-((3,4,5-trimethoxyphenyl	C19H27N5O7	437.191048229	3
34	C14H18N4O3	DTXSID20143781	101204-93-7	1H-Pyrido(2,3-e)-1,4-diazepine-2,3,5-trione, 4-(2-(diethylam	C14H18N4O3	290.137890456	3
35	C12H11N7	DTXSID6021373	396-01-0	Triamterene	C12H11N7	253.107593382	52
36	C12H11N7	DTXSID00204465	5587-93-9	Ampyrimine	C12H11N7	253.107593382	7
37	C12H11N7	DTXSID5064621	7300-26-7	Benzenamine, 4-azido-N-(4-azidophenyl)-	C12H9N7	251.091943318	4
38	C12H11N7	DTXSID00848025	90293-82-6	Sulfuric acid-6-phenylpteridine-2,4,7-triamine (1/1)	C12H13N7O4S	351.074973101	1
39	C12H11N7	DTXSID50575293	92310-83-3	(1E)-N-Phenyl-1,2-bis(1H-1,2,4-triazol-1-yl)ethan-1-imine	C12H11N7	253.107593382	1
40	C8H9NO2	DTXSID2020006	103-90-2	Acetaminophen	C8H9NO2	151.063328534	75
41	C8H9NO2	DTXSID6025567	134-20-3	Methyl 2-aminobenzoate	C8H9NO2	151.063328534	50

Downloadable Data



[DSSTox identifiers mapped to CAS Numbers and Names File](#)

Posted: 11/14/2016

The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] hydrazone
8	75-05-8	DTXSID7020009	Acetonitrile
9	127-06-0	DTXSID6020010	Acetoxime
10	65734-38-5	DTXSID6020012	N'-Acetyl-4-(hydroxymethyl) phenylhydrazine

[DSSTox MS Ready Mapping File](#)

Posted: 11/14/2016

The CompTox Chemistry Dashboard can be used by mass spectrometrists for the purpose of structure identification. A normal formula search would search the exact formula associated with any chemical, whether it include solvents of hydration, salts or multiple components. However, mass spectrometry detects ionized chemical structures and molecular formulae searches should be based on desalted, and desolvated structures with stereochemistry removed. We refer to these as "MS ready structures" and the MS-ready mappings are delivered as Excel Spreadsheets containing the Preferred Name, CAS-RN, DTXSID, Formula, Formula of the MS-ready structure and associated masses, SMILES and InChI Strings/Keys.

[DSSTox SDF File](#)

Posted: 12/14/2016

This zip file contains the entire chemical structure collection of over 700,000 chemicals from the DSSTox database contained in one large SDF file. The file contains the structure, The DSSTox Structure Identifier (DTXCID), The DSSTOX Substance Identifier (DTXSID listed as PubChem External Data Source), the associated Dashboard URL, associated synonyms and Quality Control Level details. In order to view an SDF file you will need to have access to the appropriate piece of software to open an SDF file. Examples include ChemDraw, IChem

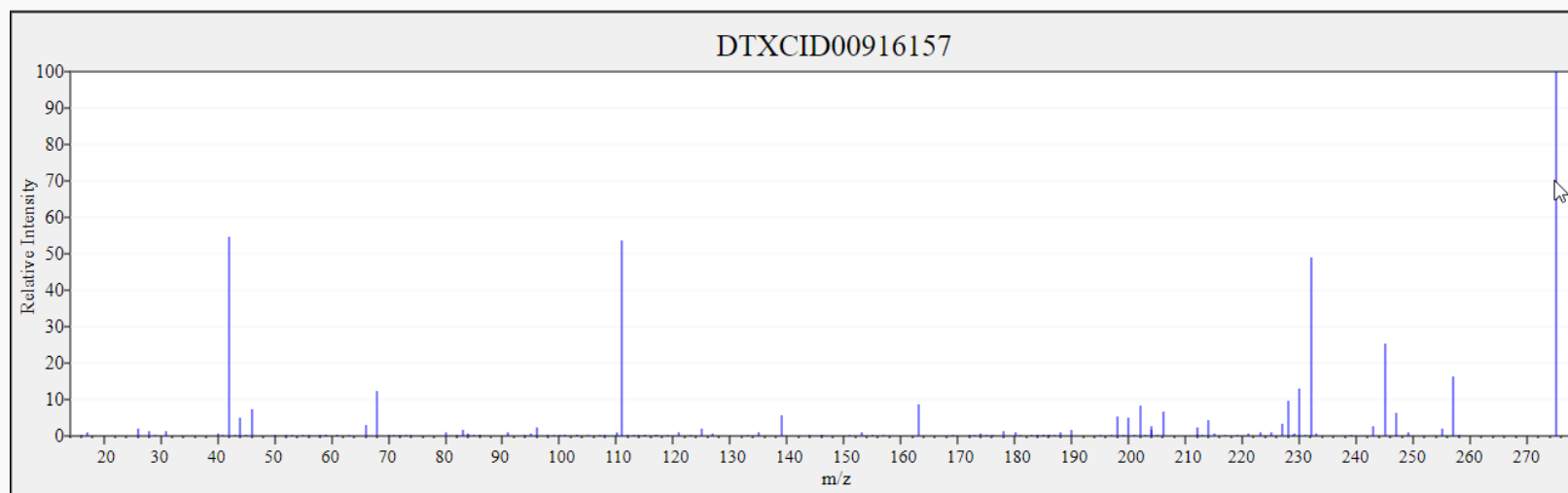
- CFM-ID
 - Viewing and Downloading pre-predicted spectra
 - Search spectra against the database
- Retention Time Index Prediction
- Structure/substructure/similarity search
- Generation of MS-ready structures:
 - Upload file, download results
 - Service based generation

Predicted Mass Spectra

<http://cfmid.wishartlab.com/>

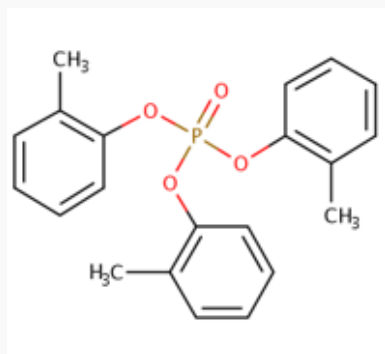


- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >700,000 structures, to be accessible via Dashboard

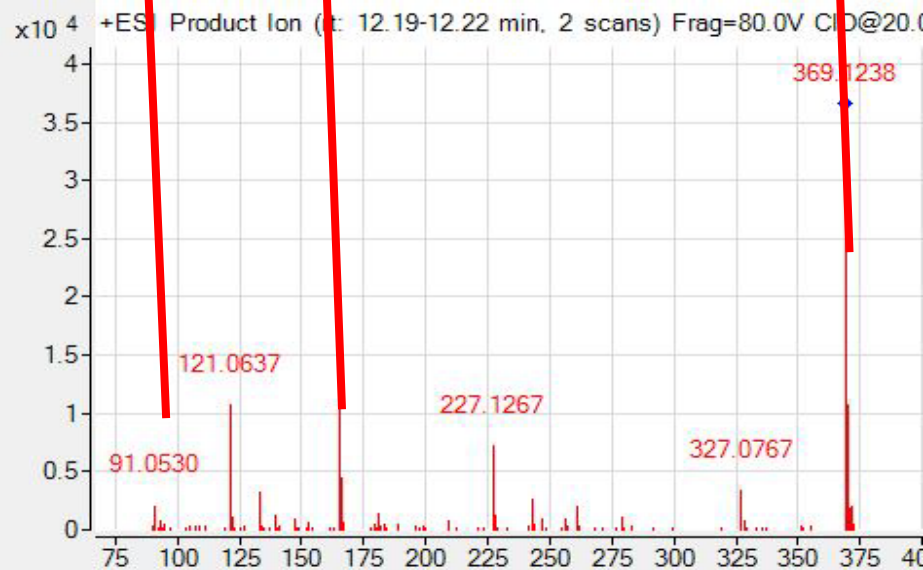
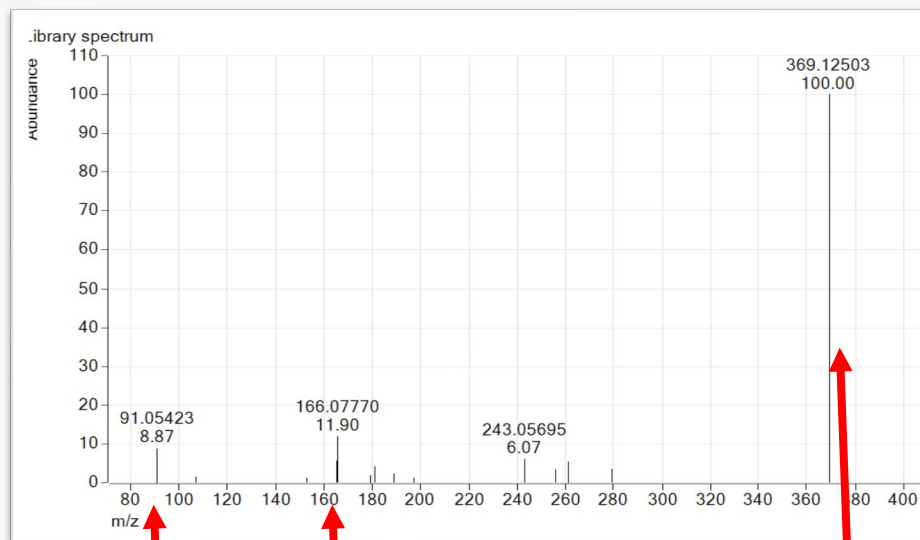


Predicted Mass Spectra

Library Fragmentation
Spectra (20eV)



Observed Fragmentation
Spectra (20eV)



**Match
Score**

Search Expt. vs. Predicted Spectra

Mass Search

±

Min/Max

Mass

Da

±

Error

Da

ppm

Molecular Formula Search

Molecular Formula

Mass or Formula must be entered before searching spectrum

Ionization Type

ESI+ ▼

Spectra Input

Single Energy

Multiple

Peak Match Window:

0.02

Da

ppm

Search

Prototype Development

AADashboard

atrazine Search

100%

Select properties to predict
H T.E.S.T. 18 OPERA Search
C
N ☐ Exact
O ☒ Substructure

Search result 2540 Show ☐ Isotopically Labeled ☐ Charged ☐ Salts or Mixtures Sort Similarity

 1	 0.62	 0.57	 0.57	 0.57	 0.53	 0.53	 0.53	 0.5	 0.5	 0.5
 0.5	 0.5	 0.5	 0.47	 0.44	 0.44	 0.44	 0.42	 0.42	 0.42	 0.42
 0.42	 0.42	 0.42	 0.42	 0.42	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4
 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.38	 0.38
 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38

Search result 2540 Show ☐ Isotopically Labeled

Prototype Development

atrazine Search

100%

Select properties to predict

T.E.S.T. 18 OPERA Search

- ☐ Exact
- ☐ Substructure
- ☐ Similarity
- ☒ Molecular Formula
- ☐ Molecular Weight

Input formula (e.g. C6 H6):

Search

Search result **5** Show ☐ Isotopically Labeled ☐ Chiral

Elements per page 50

1

<https://comptox.epa.gov/dashboard/DTXSID7020182>

- The CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals
- Multiple prediction models available for data gap filling
 - OPERA models and TEST models – PhysChem and Tox endpoints
 - Models based on *in vitro* data – classification models
 - Generalized Read-Across development in progress
- 2 years development as a CompTox Integration Hub

- IT Development team – especially Jeff Edwards and Jeremy Dunne
- Chris Grulke for the ChemReg system
- NERL colleagues – Jon Sobus, Elin Ulrich, Mark Strynar, Seth Newton

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