

# US EPA CompTox Chemicals Dashboard Data Integration Hub to Support Environmental Science

*Antony Williams*

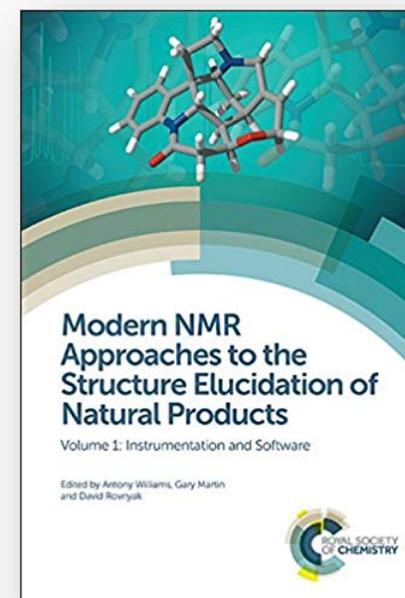
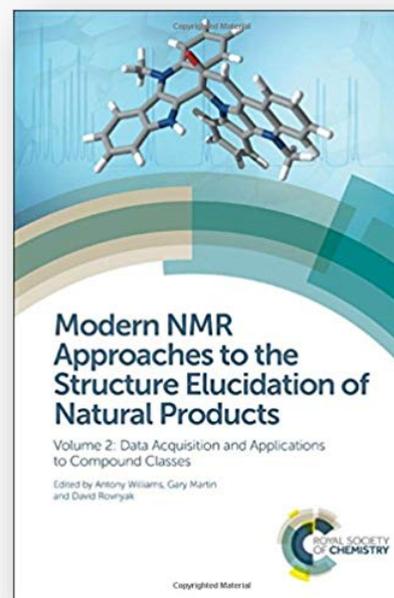
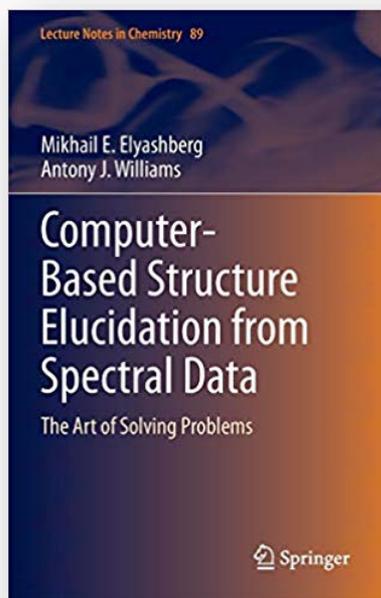
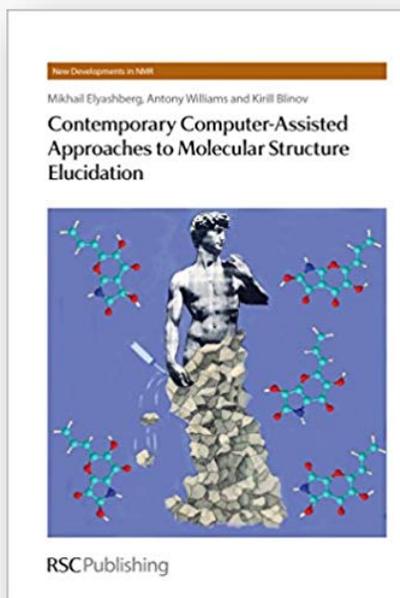
*Center for Computational Toxicology and Exposure, U.S. Environmental Protection Agency, RTP, NC*

*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*

*Global Marine Summit 2019  
UNCW, Wilmington, NC*

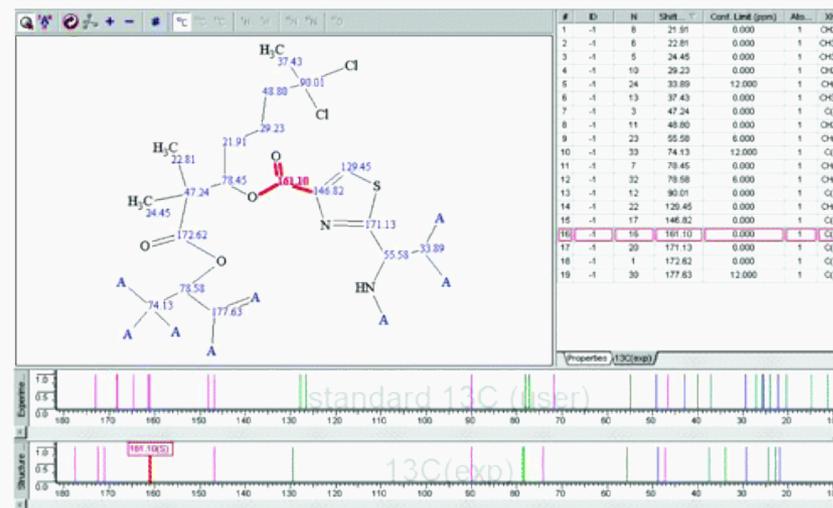
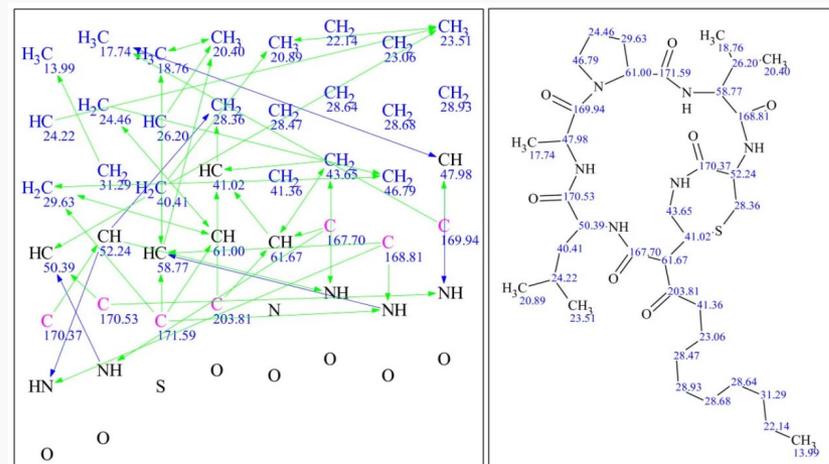
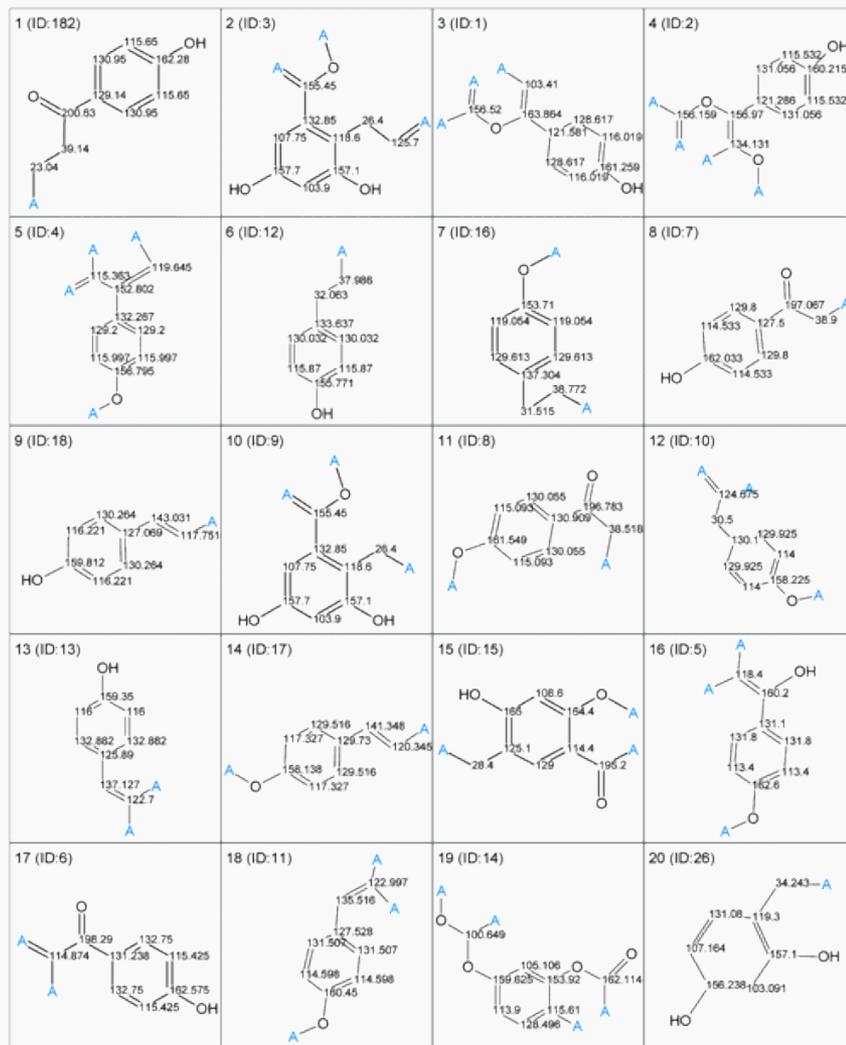
# A little bit about me...

- NMR spectroscopist by training

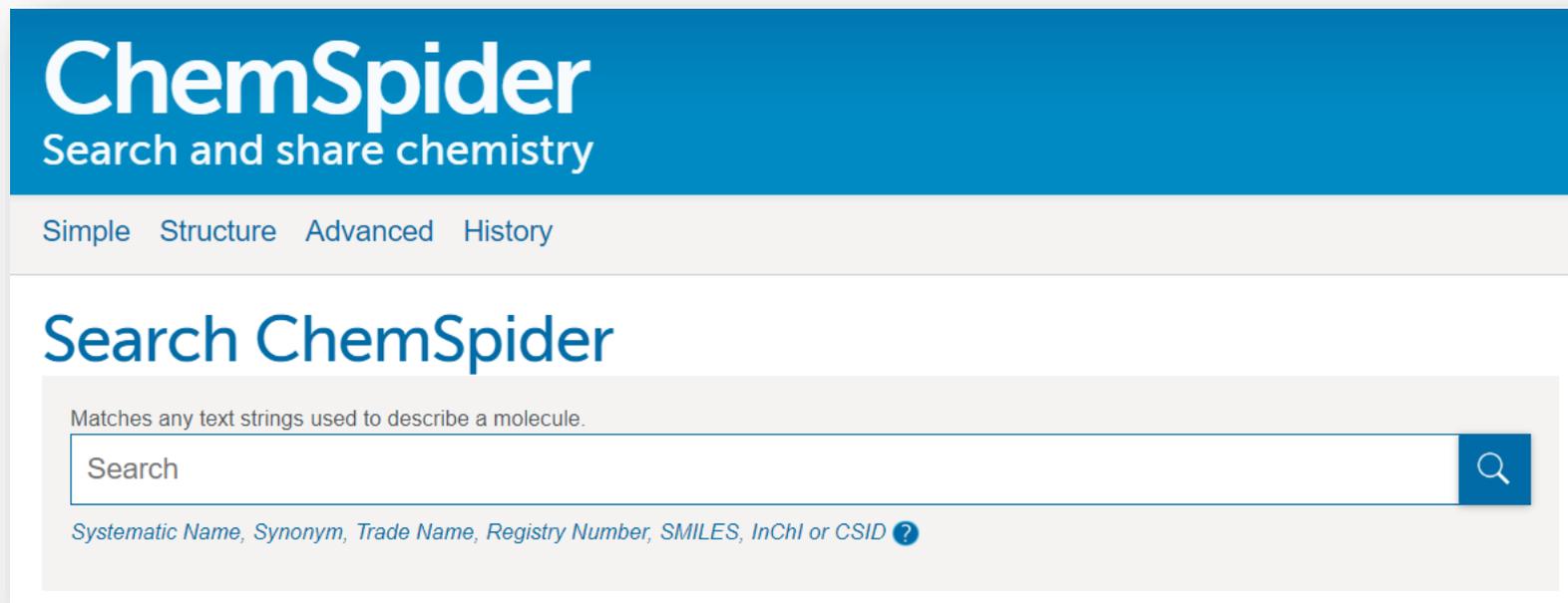


- ...ultimately focused on CASE Analysis  
(Computer-Assisted Structure Elucidation)

# CASE Analysis – Elucidating VERY complex chemical structures



- We built this free website...



- ...that has about 100,000 users a day...

# Bringing large databases and CASE together

## Organic & Biomolecular Chemistry



COMMENT

[View Article Online](#)

[View Journal](#) | [View Issue](#)



click for updates

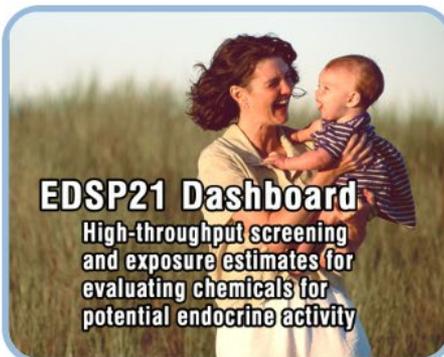
Cite this: *Org. Biomol. Chem.*, 2015, **13**, 9957

### Dereplication of natural products using minimal NMR data inputs†

Russell B. Williams,<sup>a</sup> Mark O'Neil-Johnson,<sup>a</sup> Antony J. Williams,<sup>b</sup> Patrick Wheeler,<sup>c</sup> Rostislav Pol<sup>c</sup> and Arvin Moser<sup>\*c</sup>

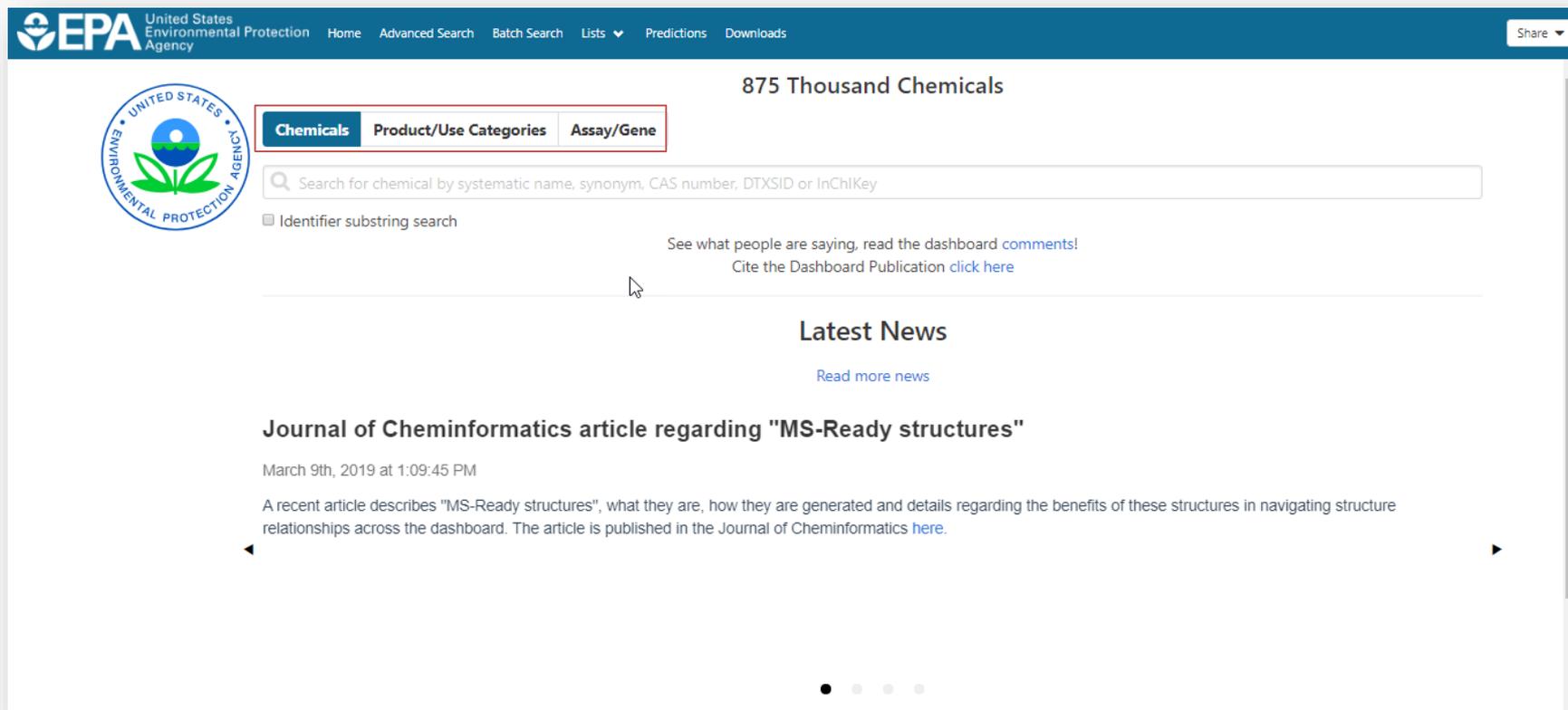
- Application of computer-assisted structure elucidation using ACD/Structure Elucidator and data obtained from the ChemSpider database hosted by the RSC

# Today I represent US EPA...



- 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
  - 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

## 875k Chemical Substances



The screenshot displays the EPA CompTox Chemicals Dashboard. At the top, the EPA logo and navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads) are visible. The main heading is "875 Thousand Chemicals". Below this, there are three tabs: "Chemicals" (selected), "Product/Use Categories", and "Assay/Gene". A search bar is present with the placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey". Below the search bar, there is a checkbox for "Identifier substring search" and a link to "See what people are saying, read the dashboard comments!". A link to "Cite the Dashboard Publication" is also present. The "Latest News" section features an article titled "Journal of Cheminformatics article regarding 'MS-Ready structures'" dated March 9th, 2019. The article text describes "MS-Ready structures" and their benefits in navigating structure relationships. A "Read more news" link is provided. The dashboard includes a "Share" button in the top right corner and a carousel indicator at the bottom.

# Type-ahead Search



Chemicals

Product/Use Categories

Assay/Gene

Q emodin|



Emodin  
*DTXSID5025231*



Emodin anthrone  
*DTXSID80197684*



Emodin-8-o-beta-gentiobioside  
*DTXSID20216681*



Emodin 3-methyl ether  
*DTXSID20200101*



emodin-8-methyl ether  
*DTXSID30191177*



Emodinanthrone  
*DTXSID80197684*



Emodine  
*DTXSID2030695*

# Substring Search: Enniatin (10/29)

Chemicals

Product/Use Categories

Enniatin

Identifier substring search

## Search Results

Searched with 'Synonym Substring': Enniatin

Select all

Download

Send to Batch Search

Substring

↑

DTXSID

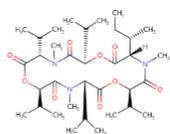
CASRN

TOXCAST

10 chemicals

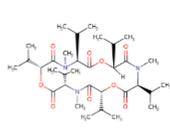
Hide chemicals that are:

Filter by Name or CASRN



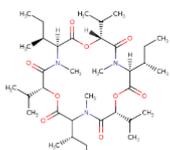
Enniatin B1

DTXSID:DTXSID70891861  
CASRN:19914-20-6  
TOXCAST:-



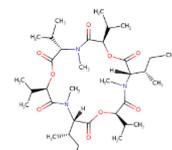
Enniatin B

DTXSID:DTXSID30891862  
CASRN:917-13-5  
TOXCAST:-



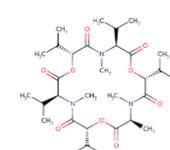
Enniatin A

DTXSID:DTXSID90891863  
CASRN:2503-13-1  
TOXCAST:-



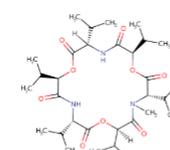
Enniatin A1

DTXSID:DTXSID50891864  
CASRN:4530-21-6  
TOXCAST:-



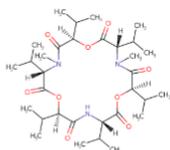
Enniatin J1

DTXSID:DTXSID701017631  
CASRN:19893-15-3  
TOXCAST:-



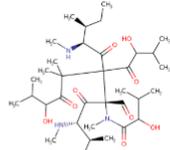
Enniatin B3

DTXSID:DTXSID401017632  
CASRN:864-99-3  
TOXCAST:-



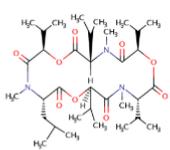
Enniatin B2

DTXSID:DTXSID501017635  
CASRN:632-91-7  
TOXCAST:-



Enniatin F

DTXSID:DTXSID601017690  
CASRN:144446-20-8  
TOXCAST:-



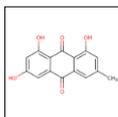
Enniatin B4

DTXSID:DTXSID601017783  
CASRN:19893-21-1  
TOXCAST:-



Enniatin K1

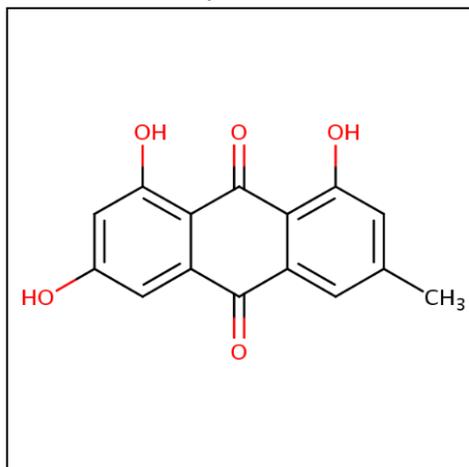
DTXSID:DTXSID801017977  
CASRN:716318-00-2  
TOXCAST:-



## Emodin

518-82-1 | DTXSID5025231

Searched by DSSTox Substance Id.



### Wikipedia

**Emodin (6-methyl-1,3,8-trihydroxyanthraquinone)** is a chemical compound that can be isolated from rhubarb, buckthorn, and Japanese knotweed (*Reynoutria japonica* syn. *Polygonum cuspidatum*). It is also produced by many species of fungi, including members of the genera *Aspergillus*, *Pyrenochaeta*, and *Pestalotiopsis*, inter alia. The common name is derived from *Rheum emodi*, a taxonomic synonym of *Rheum australe*, (Himalayan rhubarb) and synonyms

[Read more](#)

### Quality Control Notes

### Intrinsic Properties

### Structural Identifiers

### Linked Substances

### Presence in Lists

### Record Information

#### DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

# Experimental & Predicted Properties

DETAILS

EXECUTIVE SUMMARY

**PROPERTIES**

ENV. FATE/TRANSPORT

HAZARD

ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

INTERACTIONS

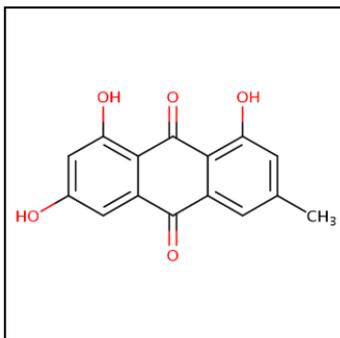
Property

Summary

Download Columns

Property	Experimental average	Predicted average
<a href="#">LogP: Octanol-Water</a>	-	3.59
<a href="#">Melting Point</a>	255 (5)	250
<a href="#">Boiling Point</a>	587 (1)	453
<a href="#">Water Solubility</a>	-	1.13e-4
<a href="#">Vapor Pressure</a>	-	2.28e-10
<a href="#">Flash Point</a>	-	302
<a href="#">Surface Tension</a>	-	85.4
<a href="#">Index of Refraction</a>	-	1.75
<a href="#">Molar Refractivity</a>	-	69.1
<a href="#">Polarizability</a>	-	27.4

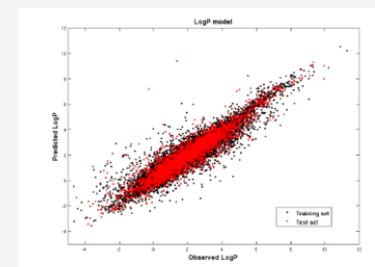
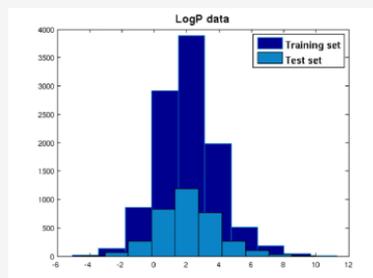
# Open Source Prediction Models



## Model Results

Predicted value: 2.59  
 Global applicability domain: Inside  
 Local applicability domain index: 0.548  
 Confidence level: 0.695

## Model Performance

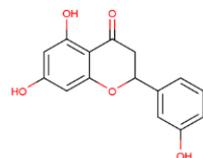


QMRP

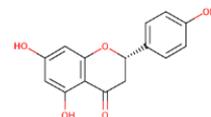
Weighted KNN model

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

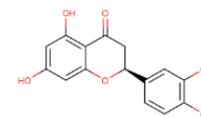
## Nearest Neighbors from the Training Set



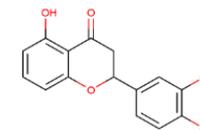
5,7,3'-Trihydroxyflavanone  
 Measured: 2.61  
 Predicted: 2.59



Naringenin  
 Measured: 2.52  
 Predicted: 2.62



ERIODICTYOL  
 Measured: 2.02  
 Predicted: 1.90



5,3',4'-Trihydroxyflavanone  
 Measured: 2.81  
 Predicted: 2.73

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

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams

To cite this article: K. Mansouri et al. *J Cheminform* (2018) 10:10  
An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling  
DOI: [10.1080/1062936X.2018.1461111](https://doi.org/10.1080/1062936X.2018.1461111)

*J Cheminform* (2018) 10:10  
<https://doi.org/10.1186/s13321-018-0263-1>

 Journal of Cheminformatics

To link to this article: <https://doi.org/10.1080/1062936X.2018.1461111>

RESEARCH ARTICLE

Open Access

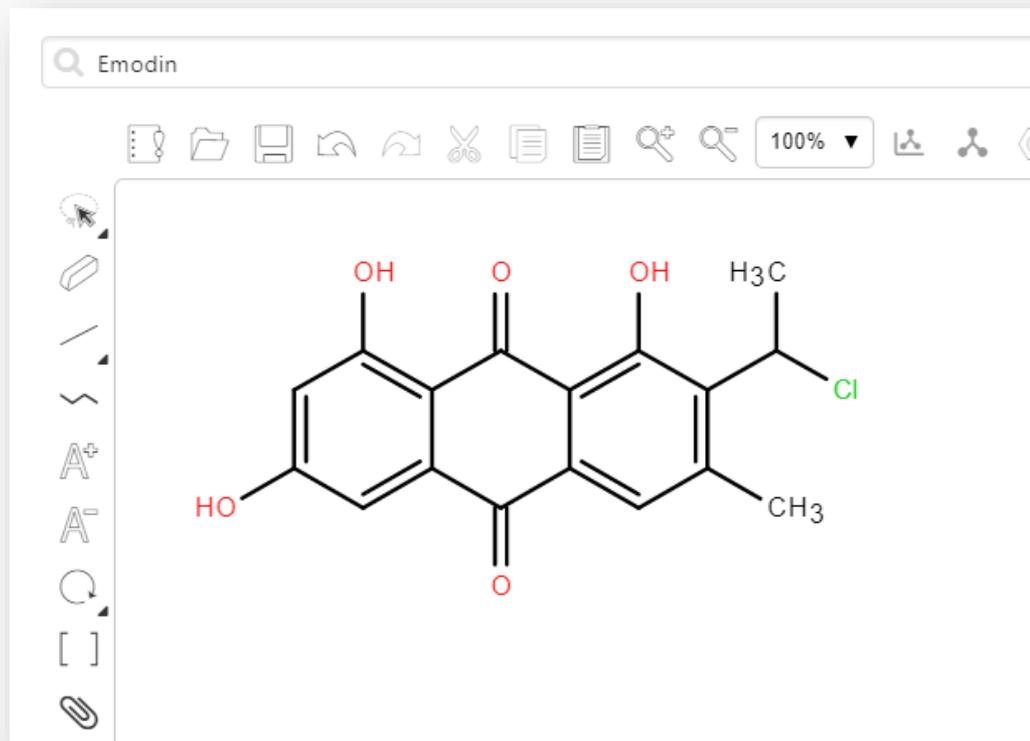
## OPERA models for predicting physicochemical properties and environmental fate endpoints



Kamel Mansouri<sup>1,2,3\*</sup> , Chris M. Grulke<sup>1</sup>, Richard S. Judson<sup>1</sup> and Antony J. Williams<sup>1</sup>

OPERA Models: <https://github.com/kmansouri/OPERA>

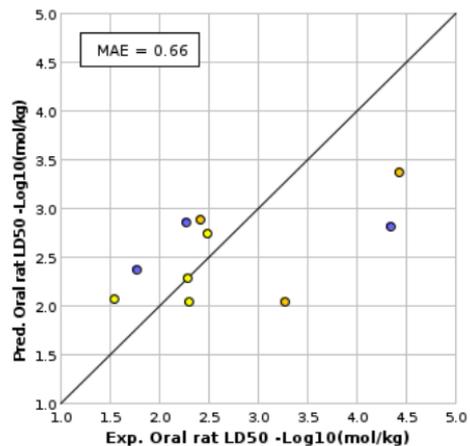
# Plus Real-Time Predictions



- Toxicological properties
  - 96 hour fathead minnow LC50
  - 48 hour *D. magna* LC50
  - 48 hour *T. pyriformis* IGC50
  - Oral rat LD50
  - Bioaccumulation factor
  - Developmental toxicity
  - Ames mutagenicity
  - Estrogen Receptor RBA
  - Estrogen Receptor Binding
  
- Physical properties
  - Normal boiling point
  - Melting point
  - Flash point
  - Vapor pressure
  - Density
  - Surface tension
  - Thermal conductivity
  - Viscosity
  - Water solubility

# Toxicity Estimation Software Tool

Prediction results (colors defined in table below)



Chemicals	MAE*
Entire set	0.43
Similarity coefficient $\geq 0.5$	0.66

\*Mean absolute error in  $-\text{Log}_{10}(\text{mol/kg})$

Structure	Similarity Coefficient	Experimental value $-\text{Log}_{10}(\text{mol/kg})$	Predicted value $-\text{Log}_{10}(\text{mol/kg})$
		N/A	2.96
	0.85	2.27	2.86
	0.83	4.35	2.82
	0.80	1.77	2.37
	0.77	2.48	2.75
	0.74	2.29	2.28

# Access to Chemical Hazard Data

Data Type

Lethality Effect Level ▾

Human Eco

Download ▾ Columns ▾ Search query

More ▾	Priority ▾	Type ▾	Subtype ▾	Risk assessment class ▾	Value ▾	Units ▾	Study type ▾	Exposure route ▾	Species ▾	Subsource ▾	Source ▾
	5	LR50	-	repeat dose	1873	g/ha	chronic	-	predatory mite	EFS OpenFoodTox	<a href="#">EFS</a>
	5	LR50	-	repeat dose	1873	g/ha	acute	-	parasitic wasp	EFS OpenFoodTox	<a href="#">EFS</a>
	5	LD50	-	subacute	100	mg/kg	acute	-	tiger worm	EFS OpenFoodTox	<a href="#">EFS</a>
	5	LD50	-	acute	2000	mg/kg	acute	oral	bobwhite quail	EFS OpenFoodTox	<a href="#">EFS</a>
	5	LD50	-	acute	100	ug/piece	acute	oral	honey bee	EFS OpenFoodTox	<a href="#">EFS</a>
	5	LD50	-	acute	100	ug/piece	acute	oral	honey bee	EFS OpenFoodTox	<a href="#">EFS</a>

LD50: The dose of a toxicant or microbe that will kill 50 percent of the test organisms within a designated period. The lower the LD50, the more toxic the compound.

6 records

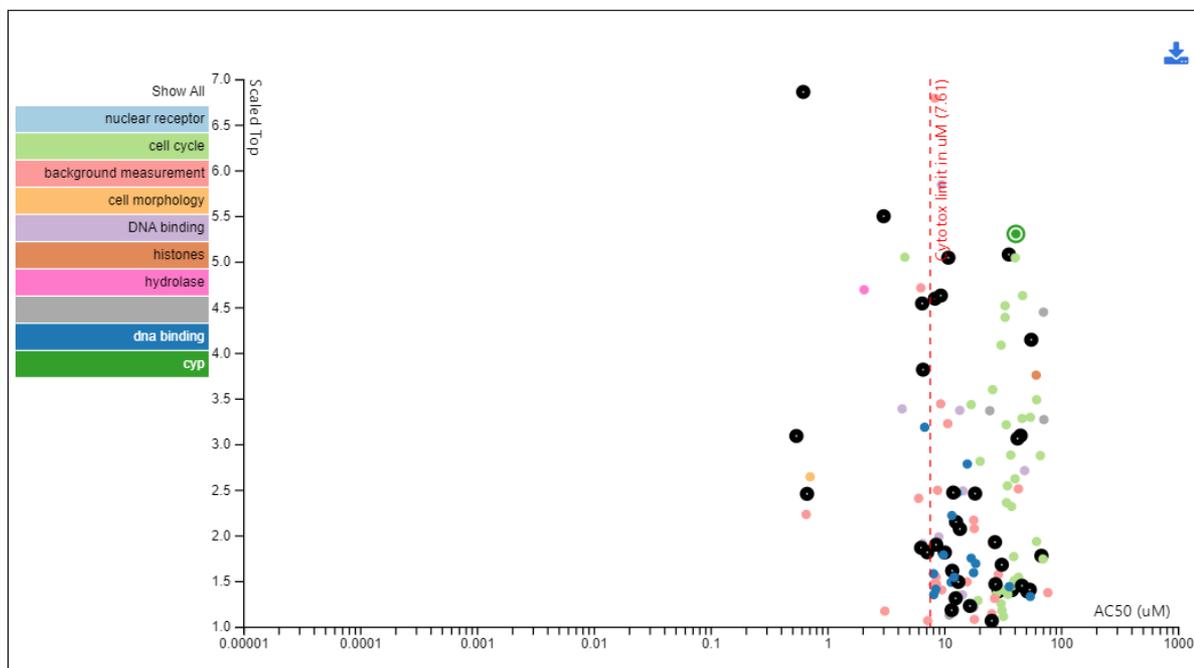
- ToxVal Database contains following data:
  - ~800,000 toxicity values
  - ~30 sources of data
  - ~22,000 sub-sources
  - ~5000 journals cited
  - ~70,000 literature citations

# In Vitro Bioassay Screening

## ToxCast and Tox21

### Chemical Activity Summary

#### TOXCAST DATA



#### ASSAY DETAILS

**AC50 (uM):** 41.17  
**Scaled top:** 5.30 

**Assay Endpoint Name:** TOX21\_Aromatase\_Inhibition  
**Gene Symbol:** CYP19A1  
**Organism:** human  
**Tissue:** breast  
**Assay Format Type:** cell-based  
**Biological Process Target:** regulation of transcription factor activity  
**Detection Technology:** Luciferase-coupled ATP quantitation  
**Analysis Direction:** positive  
**Intended Target Family:** cyp  
**Description:** Data from the assay component TOX21\_Aromatase\_Inhibition was analyzed into 1 assay endpoint. This assay endpoint, TOX21\_Aromatase\_Inhibition, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, loss-of-signal activity can be used to understand changes in the reporter gene as they relate to the gene CYP19A1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the cyp intended target family, where the subfamily is steroidogenesis-related.

# In Vitro Bioassay Screening

## ToxCast and Tox21

123 active of 402 assays

Download ▾

Columns ▾

10 ▾

Search query



Show Inactive



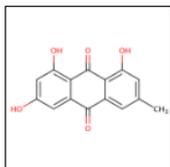
Show Background

Name	Gene Name	Gene Url	Hit Call	AC50	logAC50	Cutoff	ModIAcb	Intended Target Family
ACEA_ER_80hr	estrogen receptor 1	<a href="https://www.ncbi.nlm.nih.gov/gene/2099">https://www.ncbi.nlm.nih.gov/gene/2099</a>	ACTIVE	0.544	-0.265	26.9	-0.387	nuclear receptor
ATG_ERE_CIS_up	estrogen receptor 1	<a href="https://www.ncbi.nlm.nih.gov/gene/2099">https://www.ncbi.nlm.nih.gov/gene/2099</a>	ACTIVE	0.623	-0.206	0.503	-0.570	nuclear receptor
TOX21_MMP_rhodamine		-	ACTIVE	0.659	-0.181	44.6	-0.626	background measurement
ATG_ERa_TRANS_up	estrogen receptor 1	<a href="https://www.ncbi.nlm.nih.gov/gene/2099">https://www.ncbi.nlm.nih.gov/gene/2099</a>	ACTIVE	0.670	-0.174	1.13	-0.235	nuclear receptor
TOX21_MMP_ratio_down		-	ACTIVE	0.713	-0.147	38.7	-0.708	cell morphology
TOX21_HDAC_Inhibition		-	ACTIVE	2.07	0.315	20.0	-0.634	hydrolase
TOX21_ERa_LUC_VM7_Agonist	estrogen receptor 1	<a href="https://www.ncbi.nlm.nih.gov/gene/2099">https://www.ncbi.nlm.nih.gov/gene/2099</a>	ACTIVE	3.04	0.483	20.0	3.00e-2	nuclear receptor

# Identifiers to Support Searches

Synonym	Quality
<b>Emodin</b>	<b>Valid</b>
<b>1,3,8-Trihydroxy-6-methylanthracene-9,10-dione</b>	<b>Valid</b>
<b>9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl-</b>	<b>Valid</b>
<b>518-82-1</b> <span style="background-color: #28a745; color: white; padding: 2px;">Active CAS-RN</span>	<b>Valid</b>
<i>9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl-</i>	<i>Good</i>
<i>1,3,8-trihidroxi-6-metilantraquinona</i>	<i>Good</i>
<i>1,3,8-Trihydroxy-6-methyl-9,10-anthraquinone</i>	<i>Good</i>
<i>1,3,8-Trihydroxy-6-methylanthrachinon</i>	<i>Good</i>
<i>1,3,8-trihydroxy-6-methylanthraquinone</i>	<i>Good</i>
<i>1,6,8-Trihydroxy-3-methylanthraquinone</i>	<i>Good</i>
<i>3-Methyl-1,6,8-trihydroxyanthraquinone</i>	<i>Good</i>
<i>4,5,7-Trihydroxy-2-methylanthraquinone</i>	<i>Good</i>
<i>Anthraquinone, 1,3,8-trihydroxy-6-methyl-</i>	<i>Good</i>
<i>Frangula emodin</i>	<i>Good</i>
<i>Frangulic acid</i>	<i>Good</i>
<i>NSC 408120</i>	<i>Good</i>

***Built in “Modules”***



## Emodin

518-82-1 | DTXSID5025231

Searched by Approved Name.

### Abstract Sifter

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

Select a Query Term

Retrieve Articles 

Select a Query Term

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

Optionally, edit the query before retrieving.

"518-82-1" OR "Emodin"

## Abstract Sifter

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

Cancer  Retrieve Articles 

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

Optionally, edit the query before retrieving.

```
("518-82-1" OR "Emodin") AND (cancer OR neoplasm  
OR carcinogen*)
```

## Abstract Sifter

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

Cancer

Retrieve Articles

568 of 568 articles loaded...

Optionally, edit the query before retrieving.

("518-82-1" OR "Emodin") AND (cancer OR neoplasm OR carcinogen\*)

To find articles quickly, enter terms to sift abstracts.

Download / Send to...

Download Sifter for Excel

<input type="checkbox"/>	PMID	Year	Title	Authors	Journal	Ri	Rev	▲
<input type="checkbox"/>	31572001	2019	Emodin sensitizes human pancreatic cancer cells to EGFR inhibitor through s...	Wang; Chen; Chen; Hong; Liao; Zhang; Tong	Cancer management and research			
<input type="checkbox"/>	31524243	2019	Emodin: Its role in prostate cancer-associated inflammation (Review).	Tu; Wu; Tan; Yang; Fang	Oncology reports			
<input type="checkbox"/>	31462111	2019	Combination of targeted daunorubicin liposomes and targeted emodin liposo...	Fu; Tang; Liu; Gong; Kong; Yao; Jing; Cai; Li; Ju	Journal of drug targeting			
<input type="checkbox"/>	31424332	2019	Components synergy between stilbenes and emodin derivatives contributes to...	Zhang; Liu; Tu; Li; Song; Zhu; Zhou; Wang; Li; Xiao...	Xenobiotica; the fate of foreign compounds in biolo...			
<input type="checkbox"/>	31420258	2019	Anthraquinones and autophagy - Three rings to rule them all?	Deitersen; El-Kashef; Proksch; Stork	Bioorganic & medicinal chemistry		✓	
<input type="checkbox"/>	31349435	2019	Effect of structure in ionised albumin based nanoparticle: Characterisation, E...	Siri; Ruocco; Achilli; Pizzuto; Delgado; Ruyschaert...	Materials science & engineering. C, Materials for bi...			
<input type="checkbox"/>	31325728	2019	Anticancer activity of emodin is associated with downregulation of CD155.	Fang; Zhao; Iwanowycz; Wang; Yin; Wang; Fan	International immunopharmacology			
<input type="checkbox"/>	31308025	2019	β-Dihydroartemisinin-Emodin Promotes Apoptosis by Activating Extrinsic and I...	Li; Gao; Yang; Jin; Sun	Annals of clinical and laboratory science			
<input type="checkbox"/>	31294125	2019	Pharmacological properties of Rheum turkestanicum Janisch.	Ghorbani; Amiri; Hosseini	Heliyon		✓	
<input type="checkbox"/>	31288005	2019	Emodin suppresses growth and invasion of colorectal cancer cells by inhibitin...	Dai; Ding; Cao; Xu; He; Liu; Ju	European journal of pharmacology			
<input type="checkbox"/>	31280208	2019	Peroxiredoxin V Inhibits Emodin-induced Gastric Cancer Cell Apoptosis via th...	Jin; Sun; Liu; Lee; Kim; Kim; Jiao; Han; Jin; Shen; L...	In vivo (Athens, Greece)			
<input type="checkbox"/>	31236404	2019	Anticancer Effects of Emodin on HepG2 Cell: Evidence from Bioinformatic An...	Zhou; Wang; Sun; Ye; Liu; Zhou; Tang	BioMed research international			
<input type="checkbox"/>	31234244	2019	Emodin, as a mitochondrial uncoupler, induces strong decreases in adenosine...	Sugiyama; Shudo; Hosokawa; Watanabe; Nakano; ...	Genes to cells : devoted to molecular & cellular me...			
<input type="checkbox"/>	31190872	2019	Anti-tumor effect of aloe-emodin on cervical cancer cells was associated with ...	Gao; Wu; Huang; Wang; Li; Xu; Ran	OncoTargets and therapy			
<input type="checkbox"/>	31128032	2019	Aloe emodin exerts potent anticancer effects in MIAPaCa-2 and PANC-1 hum...	Du; Zhang; Tao; Wang; Yan; Zhang; Huang	Journal of B.U.ON. : official journal of the Balkan U...			
<input type="checkbox"/>	31114158	2019	Emodin enhances antitumor effect of paclitaxel on human non-small-cell lung ...	Chen; Zhang; Zhang	Drug design, development and therapy			▼

# Sifting retrieved articles

To find articles quickly, enter terms to sift abstracts.




To find articles quickly, enter terms to sift abstracts.








<input type="checkbox"/>	emodin	anti-tumor ↓	gynecol	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	7	4	0	11	22474959	2012	Synthesis and anti-tumor activity evaluation of rhein...	Yuan; Hu; He; Deng	Natural product communications	
<input type="checkbox"/>	0	3	0	3	28922732	2017	Physcion 8-O-β-glucopyranosideregulates cell cycl...	Li; Li; Zhu; Song	Biomedicine & pharmacotherapy = Biomedicine & ...	
<input type="checkbox"/>	0	3	0	3	28570979	2017	Physcion 8-O-β-glucopyranoside suppresses tumor...	Wang; Jiang; Guo; Lv; Liu; Wei; Ming; Tian	Biomedicine & pharmacotherapy = Biomedicine & ...	
<input type="checkbox"/>	0	3	0	3	27694907	2016	Physcion, a naturally occurring anthraquinone deriv...	Dang; Yang; Zhang; Liu; Fan; Zhang	Acta pharmacologica Sinica	
<input type="checkbox"/>	13	3	6	22	26162964	2015	Anti-tumor effect of emodin on gynecological cance...	Wang; Yu; Zhang; Ge; Gao; Zhang; Lou	Cellular oncology (Dordrecht)	
<input type="checkbox"/>	0	2	0	2	29758413	2016	Physcion 8-O-β-glucopyranoside inhibits clear-cell ...	wang; Yan; Zhang; Guo; Xing; wang; Qin; Zeng	Biomedicine & pharmacotherapy = Biomedicine & ...	
<input type="checkbox"/>	3	2	0	5	27062805	2016	[Research progress in anti-tumor effect of emodin].	Lin; Wang; Ling	Zhongguo Zhong yao za zhi = Zhongguo zhongyao...	✓
<input type="checkbox"/>	0	2	0	2	26144377	2015	Physcion induces mitochondria-driven apoptosis in ...	Chen; Gao; Han; Ye; Xie; Wang	European journal of pharmacology	
<input type="checkbox"/>	7	2	0	9	22876305	2012	Antitumor activity of emodin against pancreatic can...	Lin; Wei; Chen; Chen; Tong; Wang; Ni; Liu; Guo; Liu	PloS one	
<input type="checkbox"/>	12	2	0	14	19857484	2009	Anti-tumor activity of emodin against human chroni...	Chun-Guang; Jun-Qing; Bei-Zhong; Dan-Ting; Cho...	European journal of pharmacology	
<input type="checkbox"/>	8	1	0	9	31190872	2019	Anti-tumor effect of aloe-emodin on cervical cancer ...	Gao; Wu; Huang; Wang; Li; Xu; Ran	OncoTargets and therapy	
<input type="checkbox"/>	6	1	0	7	30832378	2019	Design and Synthesis of Novel Anti-Proliferative E...	Yang; Jin; Quan; Piao	Molecules (Basel, Switzerland)	
<input type="checkbox"/>	8	1	0	9	30648710	2019	Magnetic liposomal emodin composite with enhanc...	Song; Sheng; Xu; Dong; Xu; Li; Wang; Wu; Yang; S...	Biomaterials science	
<input type="checkbox"/>	2	1	0	3	30199885	2018	Aloe-Emodin Induces Endoplasmic Reticulum Stres...	Cheng; Dong	Medical science monitor : international medical jour...	
<input type="checkbox"/>	0	1	0	1	28810515	2017	Physcion blocks cell cycle and induces apoptosis in ...	Gao; Liu; Guo; Bai; Yang; Chen	Biomedicine & pharmacotherapy = Biomedicine & ...	
<input type="checkbox"/>	5	1	0	6	28669313	2017	Dose-dependent role of novel agents emodin and B...	Braumann; Koplin; Geier; Höhn; Pohlenz; Dubiel; R...	Acta chirurgica Belgica	

### Anti-tumor effect of emodin on gynecological cancer cells.

**PURPOSE:** Although an anti-tumor effect of emodin has been reported before, its effect on human gynecological cancer cells has so far not been studied. Here, we assessed the effect of emodin on cervical cancer-derived (Hela), choriocarcinoma-derived (JAR) and ovarian cancer-derived (HO-8910) cells, and investigated the possible underlying molecular and cellular mechanisms.

**METHODS AND RESULTS:** The respective cells were treated with 0, 5, 10 or 15 μM emodin for 72 h. Subsequently, MTT and Transwell in vitro migration assays revealed that emodin significantly decreased the viability and invasive capacity of the gynecological cancer-derived cells tested. We found that emodin induced apoptosis and significantly decreased mitochondrial membrane potential and ATP release in these cells. We also found that emodin may exert its apoptotic effects via regulating the activity of caspase-9 and the expression of cleaved-caspase-3. Moreover, we found that emodin induced a cell cycle arrest at the G0/G1 phase, possibly through down-regulating the key cell cycle regulators Cyclin D and Cyclin E. Interestingly, emodin also led to autophagic cell death, as revealed by increased MAP LC3 expression, a marker of the autophagosome, and decreased expression of the autophagy regulators Beclin-1 and Atg12-Atg5. Finally, we found that the protein levels of both VEGF and VEGFR-2 were significantly decreased in emodin-treated cells, suggesting an anti-angiogenic effect of emodin on gynecological cancer-derived cells.



US National Library of Medicine  
National Institutes of Health

PubMed

Advanced

Format: Abstract

Send to

[Cell Oncol \(Dordr\)](#). 2015 Oct;38(5):353-63. doi: 10.1007/s13402-015-0234-8. Epub 2015 Jul 11.

## Anti-tumor effect of emodin on gynecological cancer cells.

Wang Y<sup>1</sup>, Yu H<sup>2</sup>, Zhang J<sup>3</sup>, Ge X<sup>4</sup>, Gao J<sup>1</sup>, Zhang Y<sup>1</sup>, Lou G<sup>5</sup>.

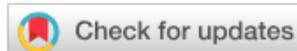
### Author information

- 1 Department of Gynaecology, Harbin Medical University Cancer Hospital, 150 Hapin Road, Harbin, 150081, China.
- 2 Cardiopulmonary Function Room, Harbin Medical University Cancer Hospital, Harbin, China.
- 3 Department of Gynaecology, The Fourth Affiliated Hospital of Harbin Medical University, Harbin, China.
- 4 Department of General Surgery, The Provincial Hospital of Heilongjiang, Harbin, China.
- 5 Department of Gynaecology, Harbin Medical University Cancer Hospital, 150 Hapin Road, Harbin, 150081, China. Gexincom@163.com.

### Abstract

**PURPOSE:** Although an anti-tumor effect of emodin has been reported before, its effect on human gynecological cancer cells has so far not been studied. Here, we assessed the effect of emodin on cervical cancer-derived (Hela), choriocarcinoma-derived (JAR) and ovarian cancer-derived (HO-8910) cells, and investigated the possible underlying molecular and cellular mechanisms.

**METHODS AND RESULTS:** The respective cells were treated with 0, 5, 10 or 15  $\mu$ M emodin for 72 h. Subsequently, MTT and Transwell in vitro migration assays revealed that emodin significantly decreased the viability and invasive capacity of the gynecological cancer-derived cells tested. We found that emodin induced apoptosis and significantly decreased mitochondrial membrane potential and ATP release in



SOFTWARE TOOL ARTICLE

## Abstract Sifter: a comprehensive front-end system to PubMed [version 1; referees: 2 approved]

 [Nancy Baker](#) <sup>1</sup>, [Thomas Knudsen](#)<sup>2</sup>, [Antony Williams](#) <sup>2</sup>

 [Author details](#)



This article is included in the [Chemical Information Science](#) gateway.

### Abstract

The Abstract Sifter is a Microsoft Excel based application that enhances existing search capabilities of PubMed. The Abstract Sifter assists researchers to search effectively, triage results, and keep track of articles of interest. The tool implements an innovative "sifter" functionality for relevance ranking, giving the researcher a way to find articles of interest quickly. The tool also gives



METRICS

629



VIEWS

118



DOWNLOADS



Get PDF



Get XML



Cite



Export



Track

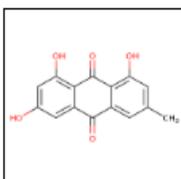


Email

# *Mapped Relationships*

# Relationships in the Data

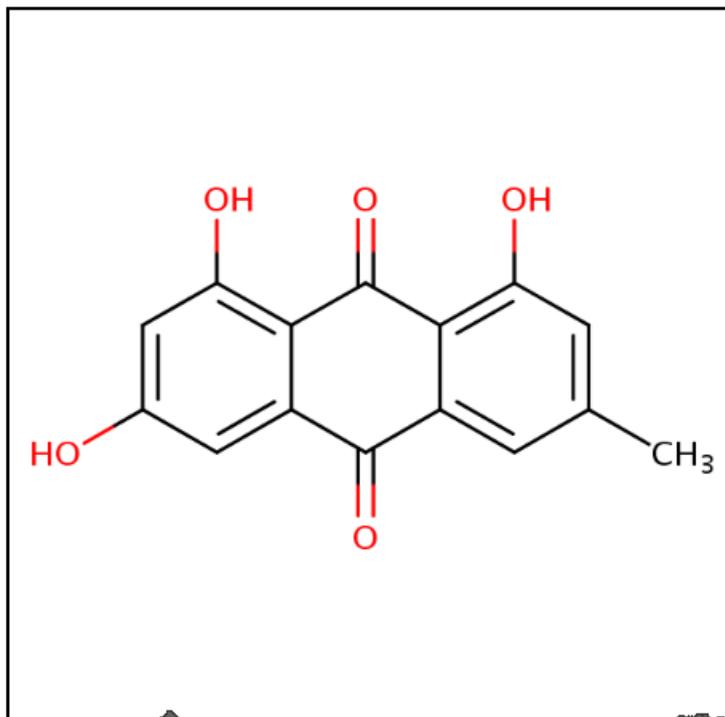
## All chemicals: Same Formula



### Emodin

518-82-1 | DTXSID5025231

Searched by Approved Name.



#### Wikipedia

**Emodin (6-methyl-1,3,8-trihydroxyanthraquinone)** is a chemical compound that can be found in *Rheum japonica* syn. *Polygonum cuspidatum*). It is also produced by many species of fungi, including *Aspergillus nidulans*. The common name is derived from *Rheum emodi*, a taxonomic synonym of *Rheum*

[Read more](#)

#### Quality Control Notes

#### Intrinsic Properties



**Molecular Formula:** C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>



Mol File

[Find All Chemicals](#)



**Average Mass:** 270.24 g/mol



Isotope Mass Distribution



**Monoisotopic Mass:** 270.052823 g/mol

# Relationships in the Data

## All chemicals: Same Formula

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

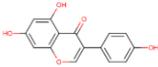
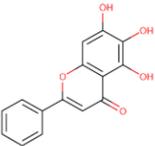
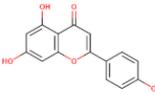
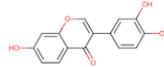
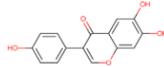
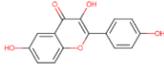
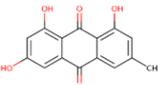
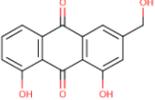
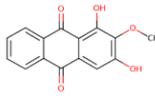
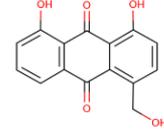
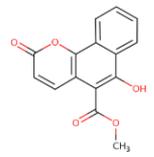
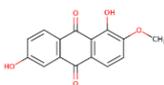
### Search Results

Searched by Exact Molecular Formula: C<sub>15</sub>H<sub>10</sub>O<sub>5</sub>.

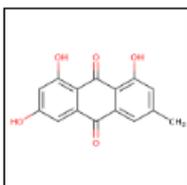
86 chemicals

Select all Download Send to Batch Search Default CASRN DTXSID Mono.Mass

Hide chemicals that are: Filter by Name or CASRN

 <p><b>Genistein</b> CASRN:446-72-0 DTXSID:DTXSID5022308 Mono.Mass:270.052823</p>	 <p><b>Baicalein</b> CASRN:491-67-8 DTXSID:DTXSID2022389 Mono.Mass:270.052823</p>	 <p><b>Apigenin</b> CASRN:520-36-5 DTXSID:DTXSID6022391 Mono.Mass:270.052823</p>	 <p><b>3',4',7-Trihydroxyisoflavone</b> CASRN:485-63-2 DTXSID:DTXSID3022451 Mono.Mass:270.052823</p>	 <p><b>4',6,7-Trihydroxyisoflavone</b> CASRN:17817-31-1 DTXSID:DTXSID8022452 Mono.Mass:270.052823</p>	 <p><b>3,6,4'-Trihydroxyflavone</b> CASRN:NOCAS_22539 DTXSID:DTXSID8022539 Mono.Mass:270.052823</p>
 <p><b>Emodin</b> CASRN:518-82-1 DTXSID:DTXSID5025231 Mono.Mass:270.052823</p>	 <p><b>Aloe-emodin</b> CASRN:481-72-1 DTXSID:DTXSID2030695 Mono.Mass:270.052823</p>	 <p><b>Anthraquinone, 1,3-dihydroxy-2-methoxy-</b> CASRN:10383-63-8 DTXSID:DTXSID70146080 Mono.Mass:270.052823</p>	 <p><b>1,8-Dihydroxy-4-hydroxymethylantraquinone</b> CASRN:128341-04-8 DTXSID:DTXSID70155854 Mono.Mass:270.052823</p>	 <p><b>Rubilactone</b> CASRN:142182-54-5 DTXSID:DTXSID80161966 Mono.Mass:270.052823</p>	 <p><b>1,6-Dihydroxy-2-methoxyanthraquinone</b> CASRN:142878-32-8 DTXSID:DTXSID70162205 Mono.Mass:270.052823</p>

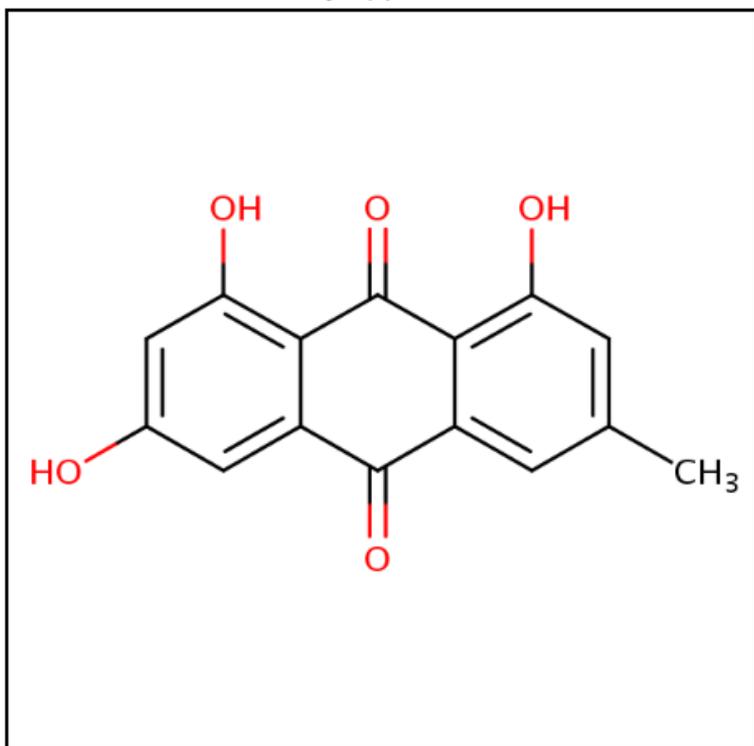
# Relationships in the Data Structure search the web



## Emodin

518-82-1 | DTXSID5025231

Searched by Approved Name.



### Wikipedia

### Quality Control Notes

### Intrinsic Properties

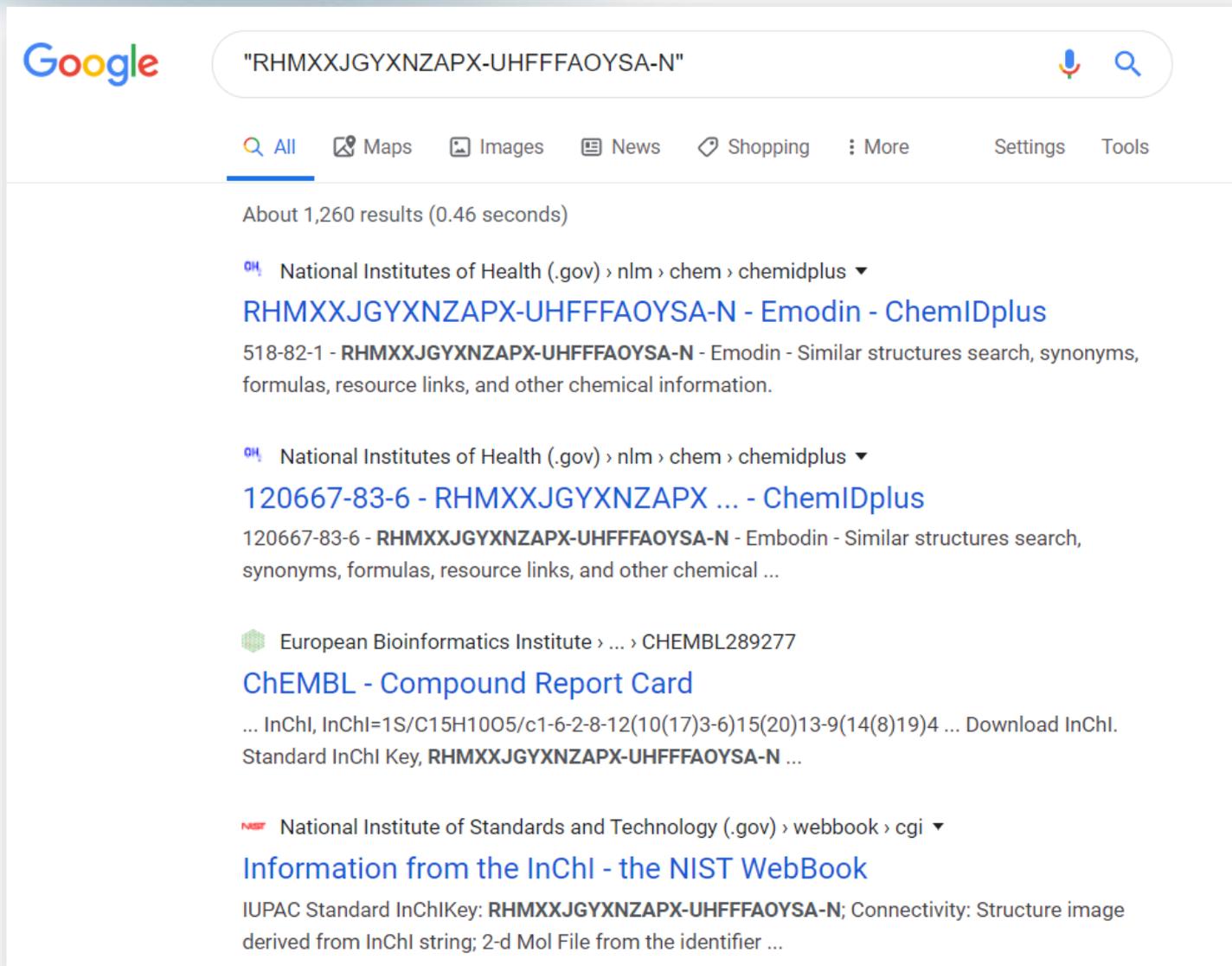
### Structural Identifiers

-  **IUPAC Name:** 1,3,8-Trihydroxy-6-methylantracene-9,10-dione
-  **SMILES:** CC1=CC(O)=C2C(=O)C3=C(O)C=C(O)C=C3C(=O)C2=C1
-  **InChI String:** InChI=1S/C15H10O5/c1-6-2-8-12(10(17)3-6)15(20)13-9(14(8)19)4-7(1)
-  **InChIKey:** RHMXXJGYXNZAPX-UHFFFAOYSA-N

Search Google for:

 Copy All

# Structure search the web



Google

"RHMXXJGYXNZAPX-UHFFFAOYSA-N"

All Maps Images News Shopping More Settings Tools

About 1,260 results (0.46 seconds)

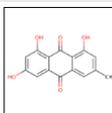
National Institutes of Health (.gov) › nlm › chem › chemidplus ▼  
**RHMXXJGYXNZAPX-UHFFFAOYSA-N - Emodin - ChemIDplus**  
518-82-1 - RHMXXJGYXNZAPX-UHFFFAOYSA-N - Emodin - Similar structures search, synonyms, formulas, resource links, and other chemical information.

National Institutes of Health (.gov) › nlm › chem › chemidplus ▼  
**120667-83-6 - RHMXXJGYXNZAPX ... - ChemIDplus**  
120667-83-6 - RHMXXJGYXNZAPX-UHFFFAOYSA-N - Embodin - Similar structures search, synonyms, formulas, resource links, and other chemical ...

European Bioinformatics Institute › ... › CHEMBL289277  
**ChEMBL - Compound Report Card**  
... InChI, InChI=1S/C15H10O5/c1-6-2-8-12(10(17)3-6)15(20)13-9(14(8)19)4 ... Download InChI. Standard InChI Key, RHMXXJGYXNZAPX-UHFFFAOYSA-N ...

National Institute of Standards and Technology (.gov) › webbook › cgi ▼  
**Information from the InChI - the NIST WebBook**  
IUPAC Standard InChIKey: RHMXXJGYXNZAPX-UHFFFAOYSA-N; Connectivity: Structure image derived from InChI string; 2-d Mol File from the identifier ...

# Similar Compounds



## Emodin

518-82-1 | DTXSID5025231

Searched by Approved Name.

Searched with a similarity threshold of 0.8

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

▶ EXPOSURE

▶ BIOACTIVITY

**SIMILAR COMPOUNDS**

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▼ LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

Pubchem.ncbi.nlm.nih.gov

Select all



Send to Batch Search

Similarity



Similarity



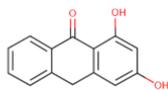
Similarity



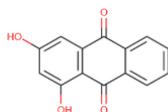
644 chemicals

Hide chemicals that are:

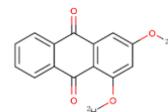
Filter by Name or CASRN



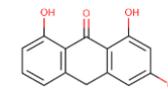
9(10H)-Anthracenone, 1,3-dihydroxy-  
Similarity:1.00  
Similarity:1.00



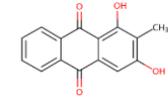
9,10-Anthracenedione, 1,3-dihydroxy-  
Similarity:1.00  
Similarity:1.00



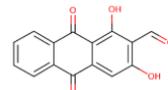
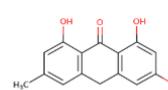
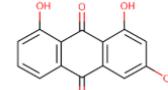
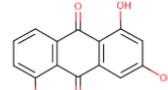
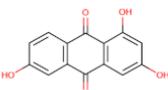
1,3-Bis(2H)hydroxyanthracene-9,10-dio...  
Similarity:1.00  
Similarity:1.00



1,3,8-Trihydroxyanthracen-9(10H)-one  
Similarity:1.00  
Similarity:1.00



Rubiadin  
Similarity:1.00  
Similarity:1.00



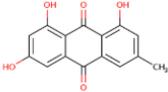
# Related Substances – Metabolites and Transformation Products

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

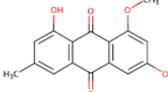
7 chemicals
Select all
Download
Send to Batch Search
Relationship
DTXSID
CASRN
TOXCAST
Hide chemicals that are:
Filter by Name or CASRN

Searched Chemical

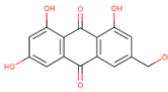
Transformation Product



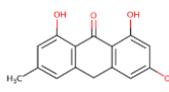
**Emodin**  
DTXSID:DTXSID5025231  
CASRN:518-82-1  
TOXCAST:123/402



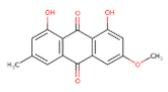
**Questin**  
DTXSID:DTXSID30191177  
CASRN:3774-64-9  
TOXCAST:-



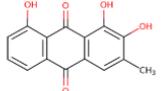
**omega-Hydroxyemodin**  
DTXSID:DTXSID60197420  
CASRN:481-73-2  
TOXCAST:-



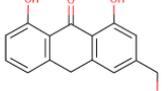
**Emodin anthrone**  
DTXSID:DTXSID80197684  
CASRN:491-60-1  
TOXCAST:-



**Physcione**  
DTXSID:DTXSID20200101  
CASRN:521-61-9  
TOXCAST:-

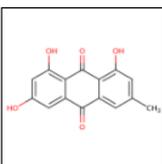


**2-Hydroxychrysophanol**  
DTXSID:DTXSID70207049  
CASRN:58322-78-4  
TOXCAST:-



**Aloe emodin anthrone**  
DTXSID:DTXSID20211510  
CASRN:6247-99-0  
TOXCAST:-

# “External Links” to >70 sites



## Emodin

518-82-1 | DTXSID5025231

Searched by Approved Name.

### General

-  EPA Substance Registry Service
-  Household Products Database
-  PubChem
-  Chemspider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  ToxPlanet
-  ACS Reagent Chemicals
-  ChemHat: Hazards and Alternatives Toolbox
-  Wolfram Alpha
-  ECHA Infocard

### Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ToxCast Dashboard 2
-  LactMed
-  ATSDR Toxic Substances Portal
-  ACToR PDF Report
-  Toxics Release Inventory
-  CREST
-  National Air Toxics Assessment
-  Superfund Chemical Data matrix

### Publications

-  Toxline
-  Google Books
-  Google Scholar
-  Google Patents
-  PPRTVWEB
-  PubMed
-  IRIS Assessments
-  EPA HERO
-  NIOSH Skin Notation Profiles
-  NIOSH Pocket Guide
-  RSC Publications
-  BioCaddie DataMed
-  Springer Materials
-  Federal Register
-  Regulations.gov
-  Bielefeld Academic Search Engine

### Analytical

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

### Prediction

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



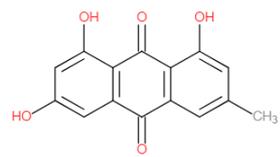
# External Links: MassBank of North America

MoNA - MassBank of North America [Spectra](#) [Downloads](#) [Upload](#) [Help](#) Search... 

    42

10 records/page

Emodin Score: ★★★★★



 collision energy	35.0000
 ionization mode	positive
 ms level	MS2
 instrument type	Linear Ion Trap
 instrument	Thermo Finnigan LTQ
 ms level	MS2
 precursor m/z	288.2516
 precursor type	M-H
 raw filename	NP_C2_12_p1_A09_POS_iTree...
 author	Arpana Vaniya

Originally submitted to the Vaniya/Fiehn Natural Products Library

[VF-NPL](#) [VF-NPL LTQ](#) [LC-MS](#) [Display Full Record](#)

<https://mona.fiehnlab.ucdavis.edu>

# ***Chemical Lists***

# >200 Lists of Chemicals

## Select List

Download Columns 10

Search query Copy page URL

List Acronym	List Name	Number of Chemicals	List Description
WIKICHEMICALS	LIST: Wikipedia Chemicals under constant curation	1926	List of chemicals harvested from Wikipedia and under constant growth and curation
TOXCAST_PHASEII	TOXCAST_PhaseII - EPA ToxCast Screening Library (Phase II Subset)	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.
ERMODEL	EPA ENDOCRINE: Integrated pathway model for the Estrogen Receptor	1812	Dataset associated with 'Integrated Model of Chemical Perturbations of a Biological Pathway Using 18 In Vitro High-Throughput Screening Assays for the Estrogen Receptor' by Judson et al.
UATHTARGETS	NORMAN: University of Athens Target List	1768	A list of target substances measured at the Department of Chemistry, University of Athens. Provided by Nikiforos Alygizakis and Nikos Thomaidis.
EPACONS	EPA: Consumer Products Suspect Screening Result	1705	This is a compiled list of the suspects reported in the supporting information of Phillips et al 2018, DOI: 10.1021/acs.est.7b04781 - Suspect Screening Analysis of Chemicals in Consumer Products with GCxGC-TOF/MS.
EPAHFR	WATER EPA; Chemicals associated with hydraulic fracturing	1640	EPAHFR lists chemicals associated with hydraulic fracturing from 2005-20013, as reported in EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016)
MNDOHTOxFREE	LIST: Minnesota Department of Health Chemicals of High Concern	1620	The Minnesota Department of Health Toxic Free Kids Program Chemicals of High Concern list.

# Filtered Search on Toxins

## Select List

Download ▾

Columns ▾

toxins

Copy Filtered Lists URL

List Acronym	List Name	Number of Chemicals	List Description
ALGALTOX	<a href="#">LIST: Algal Toxins</a>	54	A list of Algal Toxins of potential interest
MYCOTOX2	<a href="#">LIST: Mycotoxins</a>	328	List of mycotoxins collected from public sources
MYCOTOXINS	<a href="#">MASSPECDB: Mycotoxins from MassBank.EU</a>	88	This is a set of mycotoxins, initiated by the contribution of spectra of 90 mycotoxins to MassBank.EU by Justin Renaud and colleagues from Agriculture and Agri-Food Canada, Government of Canada
NEUROTOXINS	<a href="#">NEURO: Neurotoxicants Collection from Public Resources</a>	511	This is a list of chemicals reported as neurotoxins that has been compiled from public resources including Ganfyd, ChEBI, Wikipedia, T3DB and various literature (mining) resources.
PHYTOTOXINS	<a href="#">NORMAN: Toxic Plant Phytotoxin (TPPT) Database</a>	561	A comprehensive toxic plant-phytotoxin (TPPT) database provided by <a href="#">Günthardt et al 2018, DOI: 10.1021/acs.jafc.8b01639</a>

5 records

# Mycotoxins with MS Data

## MASSPECDB: Mycotoxins from MassBank.EU

Search MYCOTOXINS Chemicals

Identifier substring search

### List Details

**Description:** This is a set of mycotoxins, initiated by the contribution of spectra of 90 mycotoxins to [MassBank.EU](#) by Justin Renaud and colleagues from Agriculture and Agri-Food Canada, Government of Canada. This list is also a part of the [MASSBANKREE](#) list and the [NORMAN Suspect Exchange](#) and will be expanded as new contributions arrive.

**Number of Chemicals:** 88

88 chemicals

Select all

Download

Send to Batch Search

Default

↑

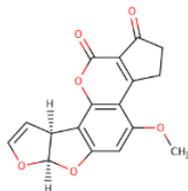
CASRN

DTXSID

Mono.Mass

Hide chemicals that are:

Filter by Name or CASRN

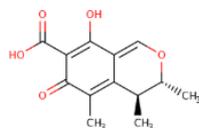


Aflatoxin B1

CASRN:1162-65-8

DTXSID:DTXSID9020035

Mono.Mass:312.063388

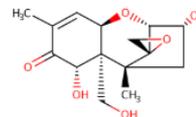


Citrinin

CASRN:518-75-2

DTXSID:DTXSID8020333

Mono.Mass:250.084124

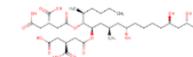


Vomitoxin

CASRN:51481-10-8

DTXSID:DTXSID3020382

Mono.Mass:296.125988



Fumonisin B1

CASRN:116355-83-0

DTXSID:DTXSID6020644

Mono.Mass:721.38847

## Basic Information about

### Monitoring and Analysis



- [Determination of Cyanotoxins in Drinking and Ambient Freshwaters](#)
- [Laboratories that Analyze for Cyanobacteria and Cyanotoxins](#)
- [State HABs Monitoring Programs](#)

## Managing Cyanotoxins in Public Drinking Water

### Research, Collaboration and Other Resources



- [EPA HABs Research](#)
- [EPA Newsletter and Collaboration and Outreach on HABs](#)
- [State HABs Resources](#)
- [Other Federal Agencies and Organizations HABs Resources](#)
- [The Harmful Algal Bloom and Hypoxia Research and Control Amendments Act \(HABHRCA\)](#)
  - [Comment now on EPA's plan to make determinations of HABs or hypoxia an event of national significance in freshwater systems](#)
- [EPA HABs Contacts](#)

## LIST: Algal Toxins

 Identifier substring search

### List Details

**Description:** Algal toxins do not enter the marine environment from an external source but are generated during blooms of particular naturally occurring marine algal species. Such blooms have been referred to as toxic algal blooms, harmful algal blooms (HABs) and red tides. The occurrence of blooms of these and other so-called toxic algae is perfectly natural but there are concerns that increases in the supply of essential nutrients (such as nitrogen, phosphorus) to the marine environment as a result of Man's activities may be contributing to the increased frequency and magnitude of these events.

**Number of Chemicals:** 54

54 chemicals

Select all

Download

Send to Batch Search

Default



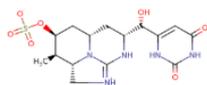
CASRN

DTXSID

Mono.Mass

Hide chemicals that are:

Filter by Name or CASRN

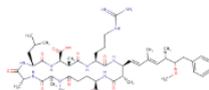


Cylindrospermopsin

CASRN:143545-90-8

DTXSID:DTXSID2031083

Mono.Mass:415.116169

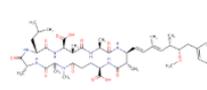


Microcystin LR

CASRN:101043-37-2

DTXSID:DTXSID3031654

Mono.Mass:994.548768

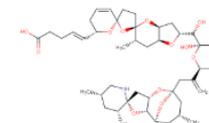


Microcystin LA

CASRN:96180-79-9

DTXSID:DTXSID3031656

Mono.Mass:909.484771



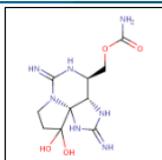
Azaspiracid

CASRN:214899-21-5

DTXSID:DTXSID9040974

Mono.Mass:841.497627

# Hazard Data for 25/54 Algal Toxins



## Saxitoxin

35523-89-8 | DTXSID3074313

Searched by DSSTox Substance Id.

### Hazard

DataType

▾

▾

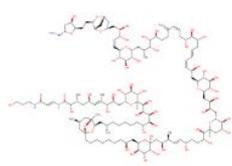
▾

More ▾	Priority ▾	Type ▾	Subtype ▾	Risk assessment class ▾	Value ▾	Units ▾	Study type ▾	Exposure route ▾	Subsource ▾	Source ▾
	7	MEG	Short-term Negligible Air	short-term	0.0001	mg/m3	-	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	0.0006	mg/m3	-	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Critical Air	short-term	0.0035	mg/m3	-	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	5	RfD	-	chronic	0.5	ug/kg-day	-	-	EFSA OpenFoodTox	EFSA

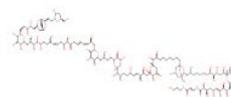
# And who wants to draw these?



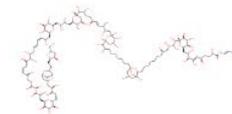
**Maitotoxin**  
CASRN:59392-53-9  
DTXSID:DTXSID10880012  
Mono.Mass:3423.581083



**palytoxin**  
CASRN:77734-91-9  
DTXSID:DTXSID90423027  
Mono.Mass:2678.479594



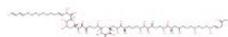
**ovatoxin-a**  
CASRN:1009813-91-5  
DTXSID:DTXSID90880111  
Mono.Mass:2646.489764



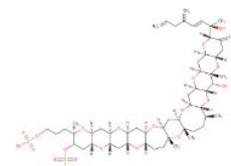
**ostreocin-D**  
CASRN:163648-25-7  
DTXSID:DTXSID50880112  
Mono.Mass:2634.453379



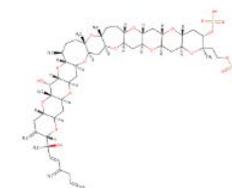
**Prymnesin-2**  
CASRN:168010-52-4  
DTXSID:DTXSID10880113  
Mono.Mass:1967.795848



**Karlotoxin-2**  
CASRN:1138665-35-6  
DTXSID:DTXSID70880114  
Mono.Mass:1344.793633



**Homoyessotoxin**  
CASRN:196309-94-1  
DTXSID:DTXSID20880088  
Mono.Mass:1156.494652



**Yessotoxin**  
CASRN:112514-54-2  
DTXSID:DTXSID20880023  
Mono.Mass:1142.479002

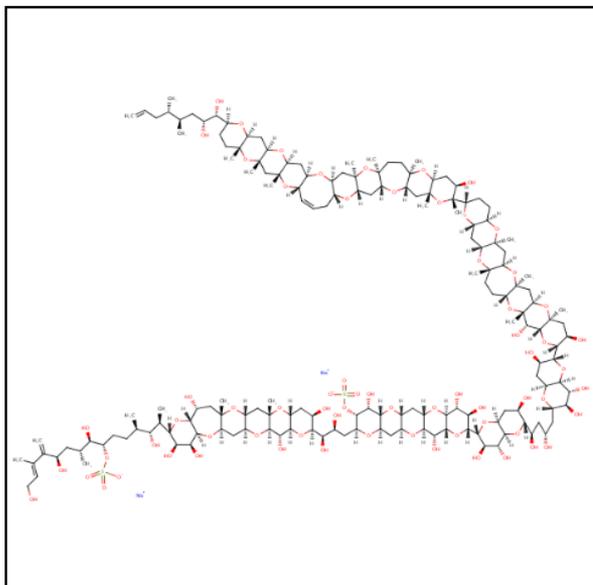
# When you can download them...



## Maitotoxin

59392-53-9 | DTXSID10880012

Searched by DSSTox Substance Id.



### Wikipedia

**Maitotoxin** (or **MTX**) is an extremely potent toxin produced by *Gambierdiscus toxicus*, a dinoflagellate species. Maitotoxin is so potent that it has been demonstrated that an intraperitoneal injection of 130 ng/kg was lethal in mice. Maitotoxin was named from the ciguateric fish *Ctenochaetus striatus*—called "maito" in Tahiti—from which maitotoxin was isolated for the first time. It was later shown that maitotoxin is actually produced by the dinoflagellate *Gambierdiscus*

...  
[Read more](#)

### Quality Control Notes

### Intrinsic Properties



**Molecular Formula:** C<sub>164</sub>H<sub>256</sub>Na<sub>2</sub>O<sub>68</sub>S<sub>2</sub>



**Mol File**

[Find All Chemicals](#)



**Average Mass:** 3425.88 g/mol



**Isotope Mass Distribution**



**Monoisotopic Mass:** 3423.581083 g/mol

# **DO WE REALLY NEED ANOTHER DATABASE?**

# Data Quality is important

- Data quality in free web-based databases!



The screenshot shows two overlapping journal pages from Elsevier's *Drug Discovery Today*. The top page is Volume 17, Issues 13-14, July 2012, Pages 685-701. The bottom page is Volume 16, Issues 17-18, September 2011, Pages 747-750. The bottom page features an editorial by Alex M Clark, Antony J Williams, and Sean Ekins, titled "Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data". The article is published in *Journal of Cheminformatics* 2015, 7:9. The URL <https://doi.org/10.1186/s13321-015-0057-7> is provided. The publication dates are: Received: 24 November 2014, Accepted: 23 February 2015, Published: 22 March 2015.

**Drug Discovery Today**  
Volume 17, Issues 13–14, July 2012, Pages 685-701

**Drug Discovery Today**  
Volume 16, Issues 17–18, September 2011, Pages 747-750

Editorial

**Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data**

Alex M Clark , Antony J Williams and Sean Ekins

*Journal of Cheminformatics* 2015 7:9  
<https://doi.org/10.1186/s13321-015-0057-7> | © Clark et al.; licensee Springer. 2015

Received: 24 November 2014 | Accepted: 23 February 2015 | Published: 22 March 2015

# Will the correct Microcystin LR Stand Up? ChemSpider Skeleton Search

Matches any text strings used to describe a molecule.

ZYZCGGRZINLQBL



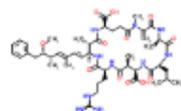
Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

FILTER ▾

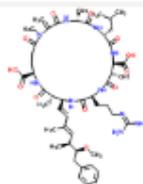
Search Hits Limit: 100 ▾

Found 9 results

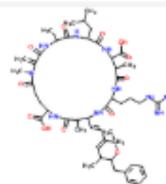
Search term: ZYZCGGRZINLQBL (Found by InChIKey (skeleton match))



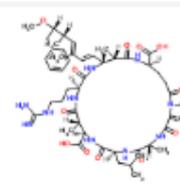
[Cyanoginosin](#)



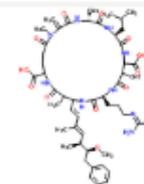
[MCYST-LR](#)



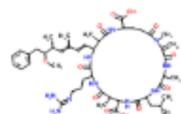
[15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,3E\)-6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-](#)



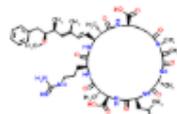
[\(5R,8S,11R,12S,15S,18R,19S,22R\)-15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,3E,5S,6S\)-6-methoxy-3,5-](#)



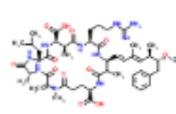
[\(5R,8S,15S\)-15-\(3-\(\(Diaminomethylene\)amino\)propyl\)-8-isobutyl-18-\(\(1E,3E,5S,6S\)-6-methoxy-3,5-](#)



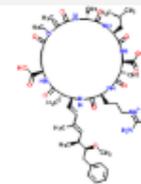
[15-\(3-\(\(Diaminomethylene\)amino\)propyl\)-8-isobutyl-18-\(6-methoxy-3,5-dimethyl-7-](#)



[\(5R,8S,11R,12S,15S,18S,19S,22R\)-15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,5S,6S\)-6-methoxy-3,5-dimethyl-7-](#)

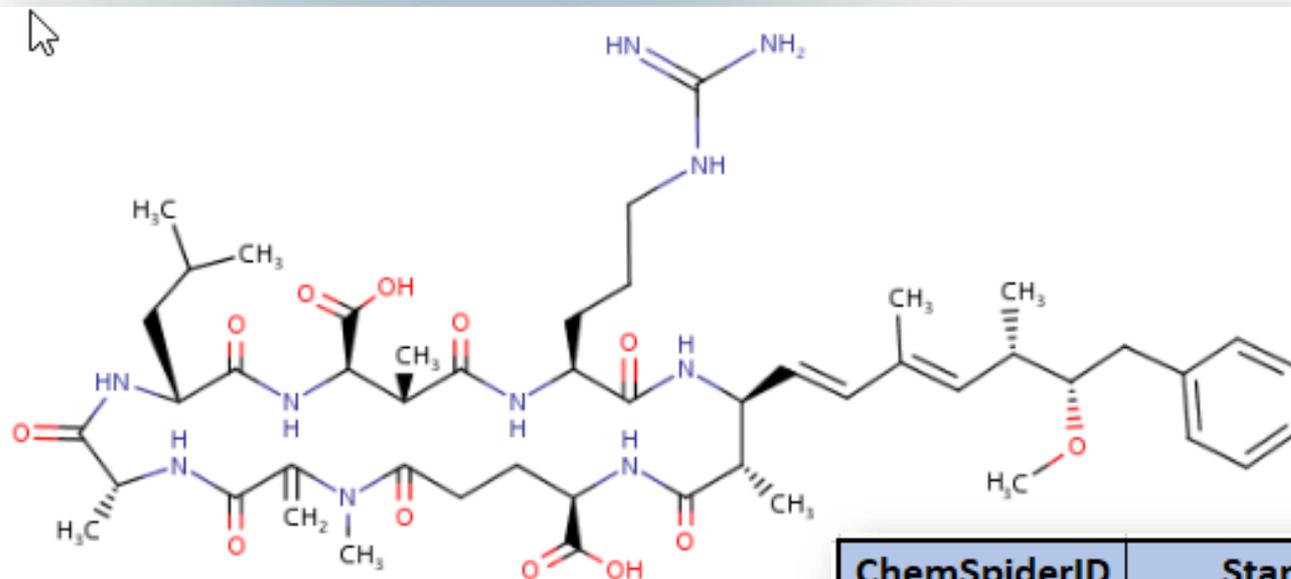


[\(5R,8R,11R,12S,15S,18S,22R\)-15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,3E,5R,6R\)-6-methoxy-3,5-dimethyl-7-](#)



[Diamino-N-\(3-\(\(5R,8S,11R,12S,15S,18S,19S,22R\)-11,2'-dicarboxy-8-isobutyl-18-\(\(1E,3E,5S,6S\)-6-methoxy-3,5-dimethyl-7-](#)

# Comparing ChemSpider Structures



ChemSpiderID	Standard InChIKey Stereolayer
WIKIPEDIA	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
CompTox	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
<a href="#">4941647</a>	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
<a href="#">393078</a>	t28-,29-,30-,31+,34-,35-,36+, <b>37-</b> ,38-,40+
<a href="#">57618348</a>	t28-,29-,30-,31+,34-,35-,36+, <b>37-</b> ,38-,40+
<a href="#">29342071</a>	t28-,29-,30-,31+, <b>34+</b> ,35-,36+, <b>37-</b> ,38-,40+
<a href="#">7987594</a>	t28-, <b>29?</b> , <b>30?</b> ,31+, <b>34?</b> ,35-, <b>36?</b> , <b>37-</b> ,38-, <b>40?</b>
<a href="#">22900854</a>	t28-, <b>29?</b> , <b>30+</b> , <b>31-</b> , <b>34+</b> , <b>35+</b> , <b>36-</b> , <b>37-</b> ,38-, <b>40-</b>
<a href="#">19692240</a>	NONE
<a href="#">2831283</a>	NONE

# Comparing ChemSpider Structures

ChemSpiderID	InChIKey	# Stereocenters	# Different
WIKIPEDIA	ZYZCGGRZINLQBL-JCGNTXOTSA-N	10/10	0
CompTox	ZYZCGGRZINLQBL-JCGNTXOTSA-N	10/10	0
<a href="#">4941647</a>	ZYZCGGRZINLQBL-JCGNTXOTSA-N	10/10	0
<a href="#">393078</a>	ZYZCGGRZINLQBL-GWRQVWKTSA-N	10/10	1
<a href="#">57618348</a>	ZYZCGGRZINLQBL-UPPCHHEJSA-N	10/10	1
<a href="#">29342071</a>	ZYZCGGRZINLQBL-IIJTUTQBSA-N	10/10	2
<a href="#">7987594</a>	ZYZCGGRZINLQBL-BESLYTPASA-N	5/10	6
<a href="#">22900854</a>	ZYZCGGRZINLQBL-QAXSDTKVSA-N	9/10	8
<a href="#">19692240</a>	ZYZCGGRZINLQBL-ORZJCNCZSA-N	0/10	10
<a href="#">2831283</a>	ZYZCGGRZINLQBL-UHFFFAOYSA-N	0/10	10

# Other Searches



**PubChem** About

SEARCH FOR

**ZYZCGGRZINLQBL**

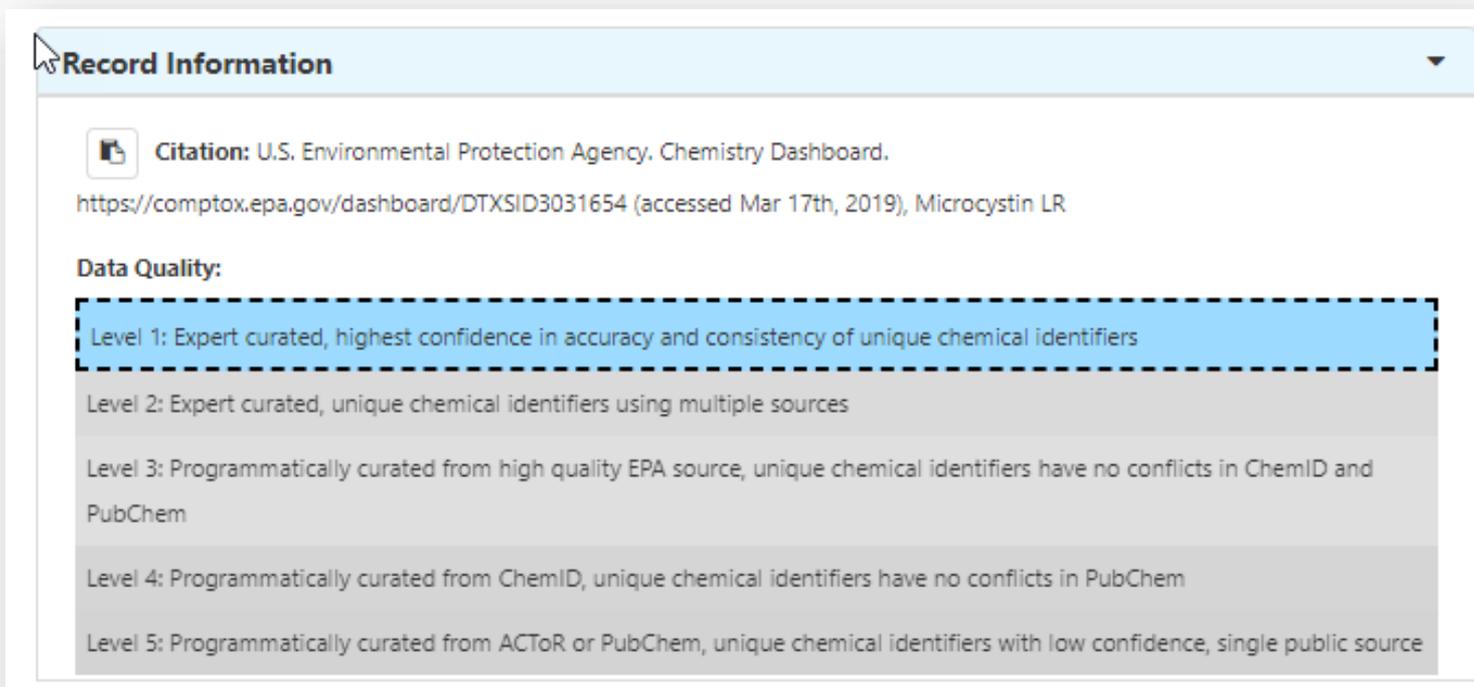
Treating this query as a text search.

**Compounds  
(17)**

Show **All** entries

CMR. Query InChI...	src_id	Source	src_compound_id
...matches...	1	ChEMBL	<a href="#">CHEMBL444092</a>
...matches...	4	Guide to Pharmacology	<a href="#">4735</a>
...matches...	6	KEGG Ligand	<a href="#">C05371</a>
...matches...	7	ChEBI	<a href="#">6925</a>
...matches...	9	ZINC	<a href="#">ZINC000169715525</a>
...matches...	9	ZINC	<a href="#">ZINC000255288110</a>
...matches...	9	ZINC	<a href="#">ZINC000255288111</a>
...matches...	9	ZINC	<a href="#">ZINC000255288112</a>
...matches...	9	ZINC	<a href="#">ZINC000255288113</a>
...matches...	9	ZINC	<a href="#">ZINC000255288114</a>
...matches...	9	ZINC	<a href="#">ZINC000255288115</a>
...matches...	9	ZINC	<a href="#">ZINC000583653042</a>
...matches...	9	ZINC	<a href="#">ZINC000669680403</a>
...matches...	10	eMolecules	<a href="#">26754757</a>
...matches...	10	eMolecules	<a href="#">31239828</a>
...matches...	11	IBM Patent System	<a href="#">DA3C2F25F29692734272194ED0E2C009</a>
...matches...	14	FDA SRS	<a href="#">EQ8332842Y</a>

- An ideal database would provide:
  - Curated CAS Number-Name mappings with “correct” chemical structures
- We have full time curators checking data



**Record Information**

 **Citation:** U.S. Environmental Protection Agency. Chemistry Dashboard.  
<https://comptox.epa.gov/dashboard/DTXSID3031654> (accessed Mar 17th, 2019), Microcystin LR

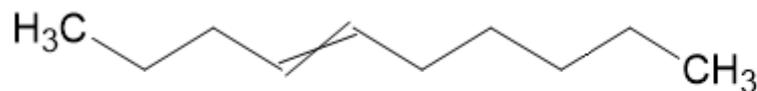
**Data Quality:**

- 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

# Names to CASRN Mappings

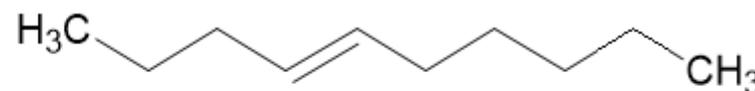
Substance Mapping						
(1 of 66) <span>1</span> <span>2</span> <span>3</span> <span>4</span> <span>5</span> <span>6</span> <span>7</span> <span>8</span> <span>9</span> <span>10</span> <span>25</span>						
	Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
▶	19398-89-1	4-Decene	<u><a href="#">DTXSID50876156</a></u>	19689-18-0	4-Decene	<a href="#">Remove Validation</a>
▶	112926-00-8	silica gel, cryst. - free	<u><a href="#">DTXSID9029851</a></u>	112926-00-8	Hydrated silica	<a href="#">Remove Validation</a>
▶	124-28-7	1-Octadecanamine, N,N-dimethyl-	<u><a href="#">DTXSID4027026</a></u>	124-28-7	N,N-Dimethyl-1-octadecanamine	<a href="#">Remove Validation</a>
▶	1330-43-4	Boron sodium oxide	<u><a href="#">DTXSID2034388</a></u>	1330-43-4	Sodium tetraborate	<a href="#">Remove Validation</a>
▶	13492-26-7	Mono- and di-potassium salts of phosphorous acid	<u><a href="#">DTXSID9035961</a></u>	13492-26-7	Phosphonic acid, potassium salt (1:2)	<a href="#">Remove Validation</a>
▶	135-37-5	Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-, disodium salt	<u><a href="#">DTXSID8042008</a></u>	135-37-5	Ethanoldiglycine disodium salt	<a href="#">Remove Validation</a>

## “4-Decene”



19398-89-1

**E/Z-stereochemistry**



19689-18-0

**E-stereochemistry**

# Crowdsourced Curation

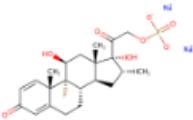
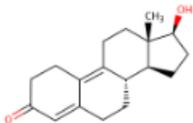
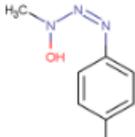
### New Comment

I'm not

## Crowdsourced Comments

Show  entries

Sort Options:

Chemical	Structure	Date	Comment	Status
Dexamethasone sodium phosphate		03-06-2018	This didn't show up when I searched for dexamethasone only when I specifically looked with the CAS number.	★
CHEMBL2311179		03-03-2018	Change preferred name to 9,10-Dehydro-19-nortestosterone (or alternative). See <a href="https://pubchem.ncbi.nlm.nih.gov/compound/11747708">https://pubchem.ncbi.nlm.nih.gov/compound/11747708</a>	★
1-(4-CARBAMOYLPHENYL)-3-METHYL-3-...		03-03-2018	DTXCID601033319 associated with this record has no InChIKey despite SMILES and InChI fields. Change preferred name to "1-(4-Carbamoylphenyl)-3-methyl-3-hydroxytriazene" (remove caps)	★

# ***Batch Searching***

- Singleton searches are useful but people generally want data on LOTS 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?
  - Can I include properties in the download file?

## Emerging Mycotoxins: Beyond Traditionally Determined Food Contaminants

Christiane Gruber-Dorninger,<sup>†</sup> Barbara Novak,<sup>†</sup> Veronika Nagl,<sup>†</sup> and Franz Berthiller<sup>\*,‡</sup>

<sup>†</sup>BIOMIN Research Center, Technopark 1, 3430 Tulln, Austria

<sup>‡</sup>Christian Doppler Laboratory for Mycotoxin Metabolism and Center for Analytical Chemistry, Department of Agrobiotechnology (IFA-Tulln), University of Natural Resources and Life Sciences, Vienna (BOKU), Konrad-Lorenz-Strasse 20, 3430 Tulln, Austria

# Public release had 16/17 mycotoxins. Last one registered

	A	B	C	D
1	<b>INPUT</b>	<b>FOUND_BY</b>	<b>DTXSID</b>	<b>PREFERRED_NAME</b>
2	enniatin A	Approved Name	<a href="#">DTXSID90891863</a>	Enniatin A
3	enniatin B	Approved Name	<a href="#">DTXSID30891862</a>	Enniatin B
4	enniatin A1	Approved Name	<a href="#">DTXSID50891864</a>	Enniatin A1
5	enniatin B1	Approved Name	<a href="#">DTXSID70891861</a>	Enniatin B1
6	beauvericin	Approved Name	<a href="#">DTXSID00891834</a>	Beauvericin
7	moniliformin	Approved Name	<a href="#">DTXSID10185731</a>	Moniliformin
8	<b>fusaproliferin</b>	<b>NO_MATCH</b>	-	-
9	fusaric acid	Approved Name	<a href="#">DTXSID5023085</a>	Fusaric acid
10	culmorin	Approved Name	<a href="#">DTXSID10891805</a>	Culmorin
11	butenolide	Synonym	<a href="#">DTXSID7075422</a>	2(5H)-Furanone
12	sterigmatocystin	Approved Name	<a href="#">DTXSID2021280</a>	Sterigmatocystin
13	emodin	Approved Name	<a href="#">DTXSID5025231</a>	Emodin
14	mycophenolic acid	Approved Name	<a href="#">DTXSID4041070</a>	Mycophenolic acid
15	alternariol	Approved Name	<a href="#">DTXSID80214305</a>	Alternariol
16	alternariol monomethyl ether	Approved Name	<a href="#">DTXSID30178004</a>	Alternariol monomethyl ether
17	tenuazonic acid	Approved Name	<a href="#">DTXSID30893265</a>	Tenuazonic acid

# Add Other Data of Interest

## Intrinsic And Predicted Properties

- Molecular Formula **i**
- Average Mass **i**
- Monoisotopic Mass **i**
- TEST Model Predictions **i**
- OPERA Model Predictions **i**

## Metadata

DTXSID	PREFERRE	MOLECULA	AVERAGE_	TOXVAL_D	TOXCAST_	TOXCAST_	PUBCHEM	WIKIPEDIA	ARTICLE
DTXSID90	Enniatin A	C36H63N3O	681.912	Y	-	-	-	-	
DTXSID30	Enniatin B	C33H57N3O	639.831	Y	-	-	-	-	
DTXSID50	Enniatin A1	C35H61N3O	667.885	Y	-	-	-	-	
DTXSID70	Enniatin B1	C34H59N3O	653.858	Y	-	-	-	-	
DTXSID00	Beauvericin	C45H57N3O	783.963	Y	-	-	-	-	
DTXSID10	Moniliformin	C4H2O3	98.057	Y	-	-	37	Y	
DTXSID00	Terpestacin	C27H40O5	444.612	-	-	-	-	-	
DTXSID50	Fusaric acid	C10H13NO2	179.219	Y	1.27	1/79	115	Y	
DTXSID10	Culmorin	C15H26O2	238.371	-	-	-	-	-	
DTXSID40	Butenolide	C6H7NO3	141.126	-	-	-	-	-	
DTXSID20	Sterigmatoc	C18H12O6	324.288	Y	-	-	23	Y	
DTXSID50	Emodin	C15H10O5	270.24	Y	30.6	123/402	194	Y	
DTXSID40	Mycophenol	C17H20O6	320.341	Y	22.55	53/235	181	Y	
DTXSID80	Alternariol	C14H10O5	258.229	-	-	-	50	Y	
DTXSID30	Alternariol m	C15H12O5	272.256	-	-	-	39	Y	
DTXSID30	Tenuazonic	C10H15NO3	197.234	Y	-	-	-	-	

# Related Substance Relationships

## Enhanced Data Sheets

- MetFrag Input File (Beta) 
- ToxPrint single fingerprints 
- Abstract Sifter Input File (Beta) 
- Synonyms and Identifiers 
- Related Substance relationships 

INPUT	DTXSID	HAS_RELATIONSHIP_WITH	RELATED_DTXSID	RELATED_PREFERRED_NAME	RELATED_CASRN
emodin	<a href="#">DTXSID50</a>	Transformation Product	<a href="#">DTXSID60197420</a>	omega-Hydroxyemodin	481-73-2
emodin	<a href="#">DTXSID50</a>	Transformation Product	<a href="#">DTXSID30191177</a>	Questin	3774-64-9
emodin	<a href="#">DTXSID50</a>	Transformation Product	<a href="#">DTXSID80197684</a>	Emodin anthrone	491-60-1
emodin	<a href="#">DTXSID50</a>	Transformation Product	<a href="#">DTXSID20200101</a>	Physcione	521-61-9
emodin	<a href="#">DTXSID50</a>	Transformation Product	<a href="#">DTXSID70207049</a>	2-Hydroxychrysophanol	58322-78-4
emodin	<a href="#">DTXSID50</a>	Transformation Product	<a href="#">DTXSID20211510</a>	Aloe emodin anthrone	6247-99-0

# MASS AND FORMULA SEARCHING

# Advanced Searches

## Mass and Formula Based Search

### Mass Search

± Min/Max

Adduct

Neutral 

All Adducts



Choose adduct from dropdown

285.1364

Da

±

5

Da

ppm

Search 

### Molecular Formula Search

MS Ready Formula   Exact Formula 

Formula

Please use the format of the following example: C6H8O2 or C6H(8-10)O(0-2)

Search 

# Advanced Searches

## Mass and Formula Based Search

### Search Results

Searched by Mass: 285.1364 +/- 5.0 ppm.

122 of 125 chemicals visible

Select all

Download

Send to Batch Search

Mass Difference

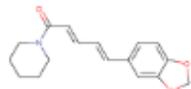
DTXSID

CASRN

TOXCAST

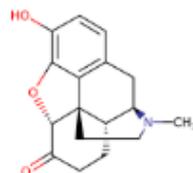
Mass Diff

Multicomponent Chemicals



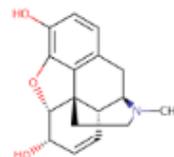
Piperine

DTXSID: DTXSID3021805  
CASRN: 94-62-2  
TOXCAST: 59/374  
Mass Diff: 0.000093



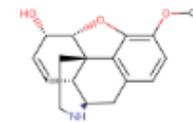
Hydromorphone

DTXSID: DTXSID8023133  
CASRN: 466-99-9  
TOXCAST: -  
Mass Diff: 0.000093



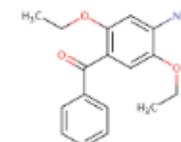
Morphine

DTXSID: DTXSID9023336  
CASRN: 57-27-2  
TOXCAST: -  
Mass Diff: 0.000093



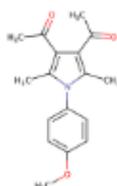
Norcodeine

DTXSID: DTXSID8046327  
CASRN: 467-15-2  
TOXCAST: 0/79  
Mass Diff: 0.000093



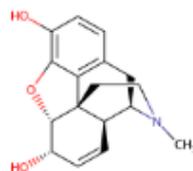
Methanone, (4-amino-2,5-diethoxyphenyl)phenyl

DTXSID: DTXSID3071696  
CASRN: 68568-55-8  
TOXCAST: -  
Mass Diff: 0.000093



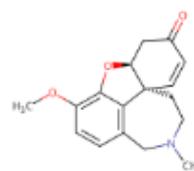
Ethanone, 1-(4-acetyl-1-(4-methoxyphenyl)pyrazol-5-yl)ethane

DTXSID: DTXSID80149860  
CASRN: 112086-82-5  
TOXCAST: -  
Mass Diff: 0.000093



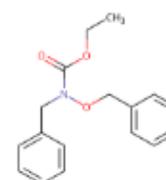
Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-

DTXSID: DTXSID40167308  
CASRN: 16206-77-2  
TOXCAST: -  
Mass Diff: 0.000093



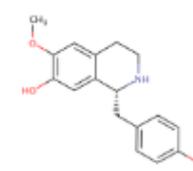
Narwedine, (+/-)-

DTXSID: DTXSID60168190  
CASRN: 1668-86-6  
TOXCAST: -  
Mass Diff: 0.000093



Carbamic acid, (phenylmethoxy)(phenyl)phenyl

DTXSID: DTXSID50171931  
CASRN: 1867-23-8  
TOXCAST: -  
Mass Diff: 0.000093



7-Isoquinolinol, 1,2,3,4-tetrahydro-1-(4-hydroxyphenyl)

DTXSID: DTXSID70176367  
CASRN: 2196-60-3  
TOXCAST: -  
Mass Diff: 0.000093

# Batch Searching Formula/Mass

## Batch Search



### Step Five: Choose Data Fields to Download

Please enter one identifier per line 

+/-  ppm

#### 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 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>.

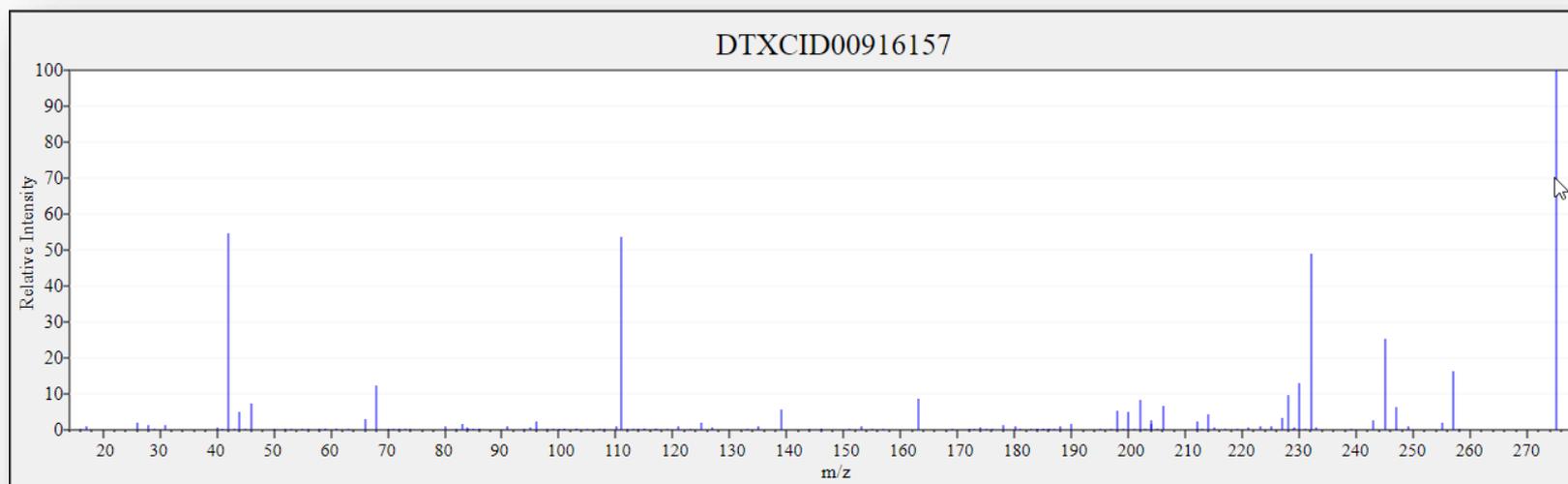
# WORK IN PROGRESS

# Predicted Mass Spectra

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



- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >800,000 structures, to be accessible via Dashboard



# Search Expt. vs. Predicted Spectra

## Non Target Analysis Prototype

### Mass Search

±  Min/Max

Da ±  Da ppm

### Molecular Formula Search

*Mass or Formula must be entered before searching spectrum*

### Ionization Type

ESI+ ▼  
ESI+  
ESI-  
EI

### Spectra Input

Single Energy  Multiple

304.1332052 11.6199475  
198.0913404 7.308439699  
123.0440559 6.538348292  
198.0756904 5.269463115  
216.1019051 4.700461978  
200.1080005 4.800144384

Peak Match Window:  Da ppm

# Search Expt. vs. Predicted Spectra

## Spectra Input

Single Ener

304.1332052 11.61  
198.0913404 7.30  
123.0440559 6.53  
196.0756904 5.28  
216.1019051 4.70  
200.4080005 4.80

## Peak Match

Search

TSV CSV Excel

Chemical Structure ID

DTXCID101048191

DTXCID101181567

DTXCID50879086

DTXCID60686349

DTXCID00830900

DTXCID10971176

DTXCID60301242

DTXCID40703048

DTXCID60349982

DTXCID10316649

Showing 1 to 10 of 38 entries

Chemical Structure ID

Score (10eV)

DTXCID101048191

0.22

DTXCID101181567

0.19

DTXCID50879086

0.17

DTXCID60686349

0.14

DTXCID00830900

0.13

DTXCID10971176

0.12

DTXCID60301242

0.12

DTXCID40703048

0.11

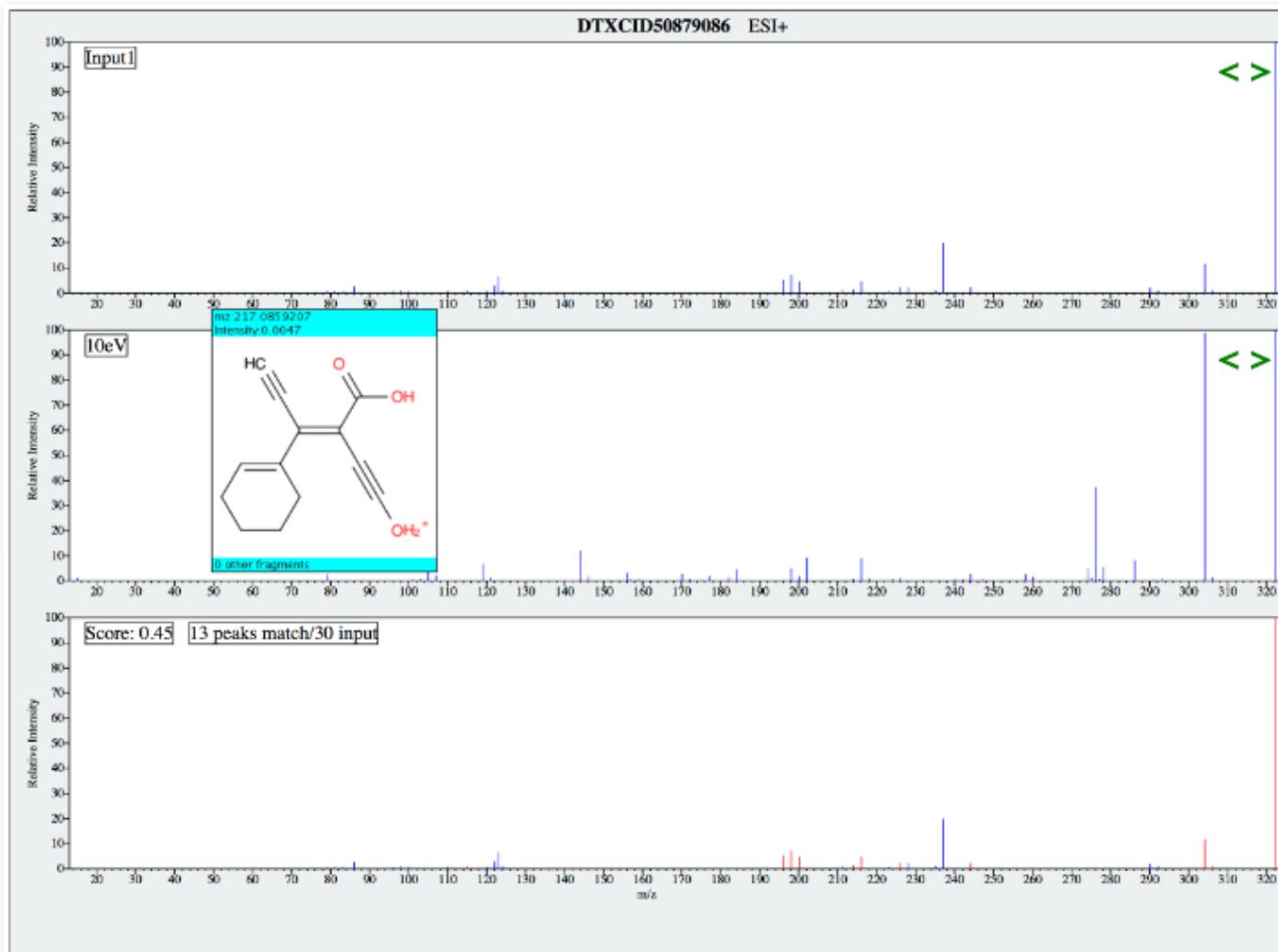
DTXCID60349982

0.11

DTXCID10316649

0.09

# Spectral Viewer Comparison



Peak Window: 2.0 ppm Update Score

Input	10eV	20eV	40eV
1	0.45	0.16	0.029
2	0.45	0.16	0.029
3	0.45	0.16	0.029



# Prototype Development

atrazine Search

Select properties to predict

H T.E.S.T. 18 OPERA Search

C

N

O

S

P

F

Cl

Br

Exact

Substructure

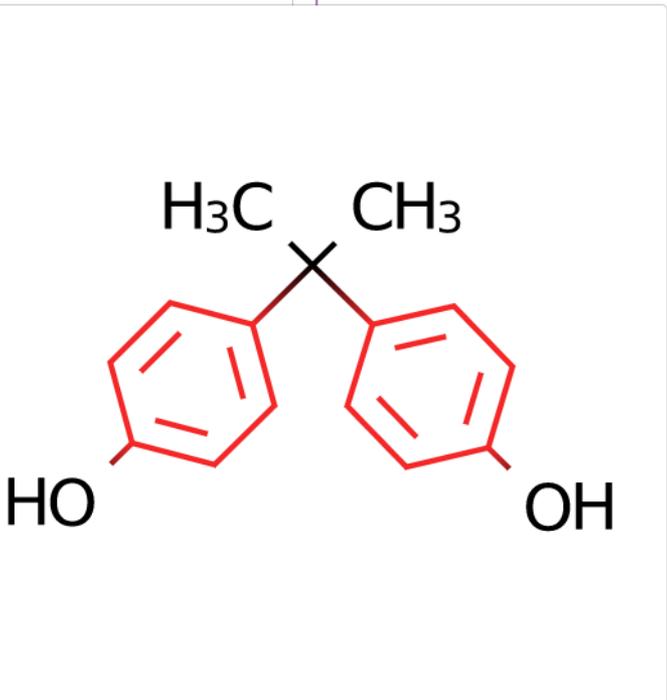
Similarity

Molecular Formula

Molecular Weight

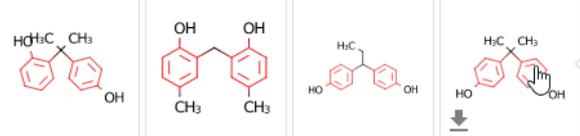
Input formula (e.g. C6 H6):

C15H16O2



Search

Search result 5 Show  Isotopically Labeled  Cl



Elements per page 50

1

- Agilent : “Mycotoxins and Metabolites Personal Compound Database and Library”
- Registered for next release...

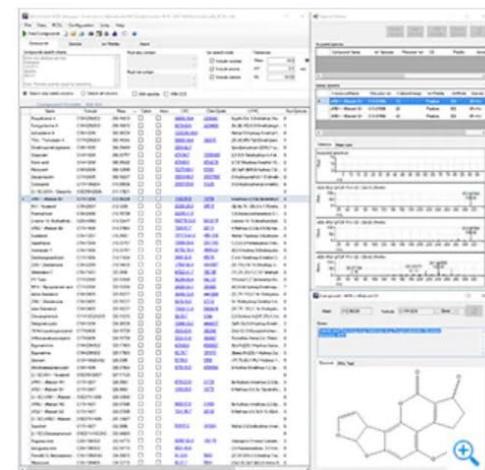
Food

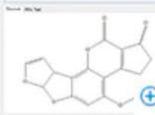
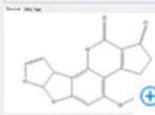
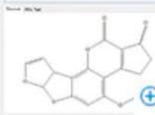
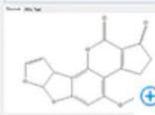
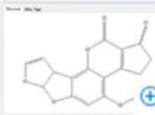
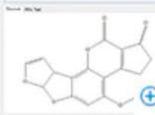
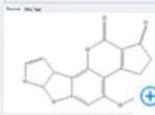
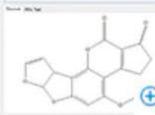
## Mycotoxins PCDL

Perform truly comprehensive mycotoxin screening applications with the Mycotoxins and Related Metabolites Personal Compound Database and Library (PCDL) for TOF and Q-TOF LC/MS systems. Detailed acquisition method setup information allows fast ramp-up to full productivity.

REQUEST QUOTE

RELATED PRODUCTS



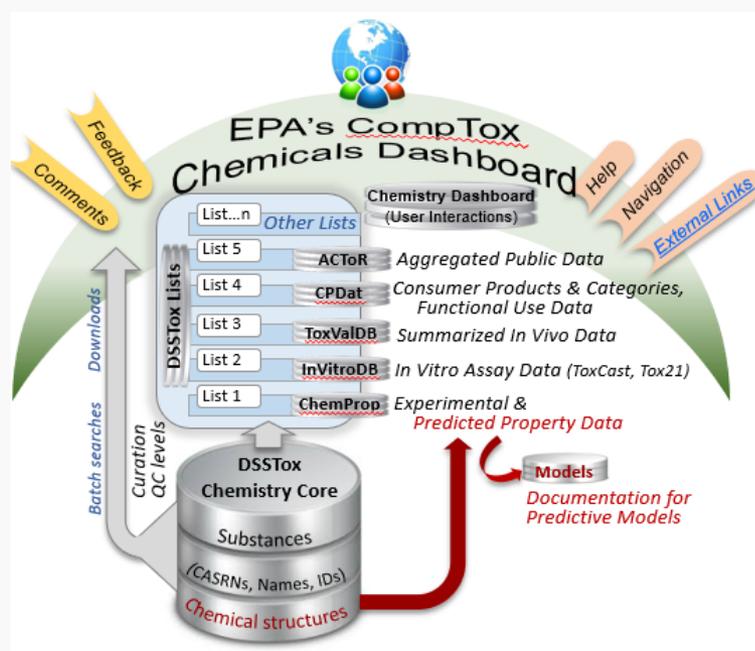
Name	CAS	MW	SMILES	Structure
Aspergillus A	1110000	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus B	1110001	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus C	1110002	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus D	1110003	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus E	1110004	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus F	1110005	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus G	1110006	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus H	1110007	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus I	1110008	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	
Aspergillus J	1110009	384.06	CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4	

MassHunter PCDL Manager Compound view of Mycotoxins PCDL

- Help grow the lists of Mycotoxins and Algal Toxins – please suggest additions
- Next up – structures of microviridins...
- Email me at [williams.antony@epa.gov](mailto:williams.antony@epa.gov)

# Conclusion

- Building an integrated hub for environmental chemistry
- Transparent access to data and models
- Data QUALITY is a key focus - ongoing curation
- Microcystins and algal toxins are two growing “lists”





Credit: the Research Triangle Foundation

## EPA-RTP

- *An enormous team of contributors from NCCT, especially the IT software development team*
- *Our curation team for their care and focus on data quality*
- *Multiple centers and laboratories across the EPA*
- *Many public domain databases and open data contributors*

## Antony Williams

NCCT, US EPA Office of Research and Development,

[Williams.Antony@epa.gov](mailto:Williams.Antony@epa.gov)

**ORCID:** <https://orcid.org/0000-0002-2668-4821>

Williams et al. *J Cheminform* (2017) 9:61  
DOI 10.1186/s13321-017-0247-6

 Journal of Cheminformatics

**DATABASE**

**Open Access**

### The CompTox Chemistry Dashboard: a community data resource for environmental chemistry



Antony J. Williams<sup>1\*</sup>, Christopher M. Grulke<sup>1</sup>, Jeff Edwards<sup>1</sup>, Andrew D. McEachran<sup>2</sup>, Kamel Mansouri<sup>1,2,4</sup>, Nancy C. Baker<sup>3</sup>, Grace Patlewicz<sup>1</sup>, Imran Shah<sup>1</sup>, John F. Wambaugh<sup>1</sup>, Richard S. Judson<sup>1</sup> and Ann M. Richard<sup>1</sup>

<https://doi.org/10.1186/s13321-017-0247-6>