

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

Antony Williams

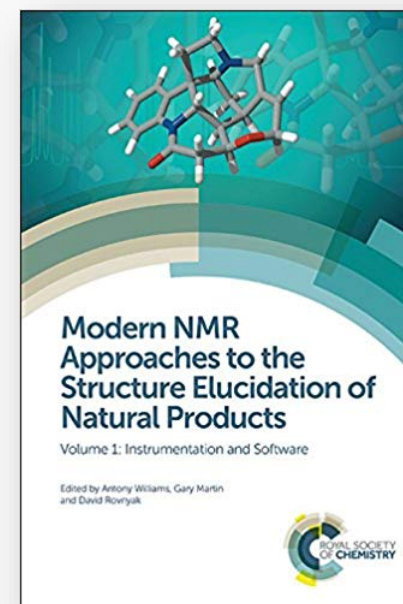
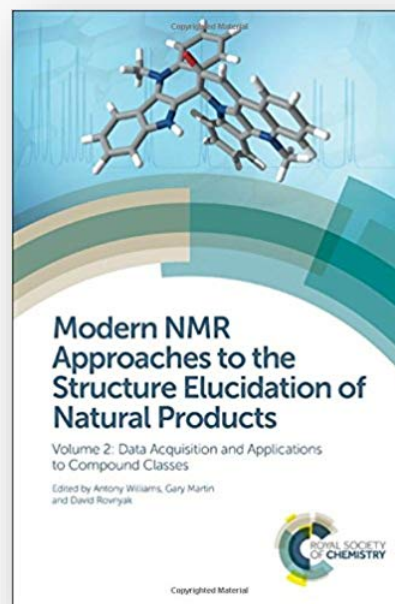
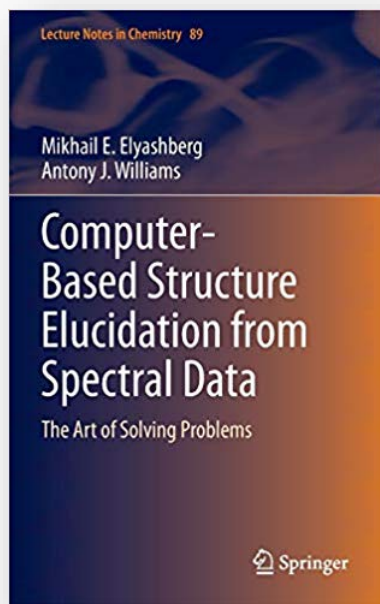
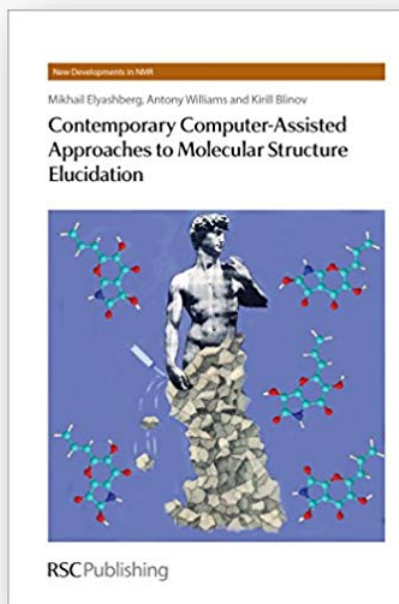
Center for Computational Toxicology and Exposure, U.S. Environmental Protection Agency, RTP, NC

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*

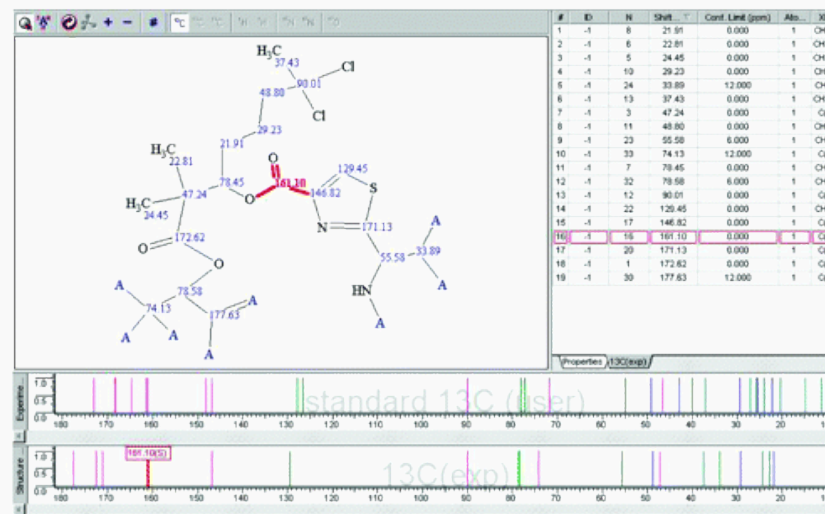
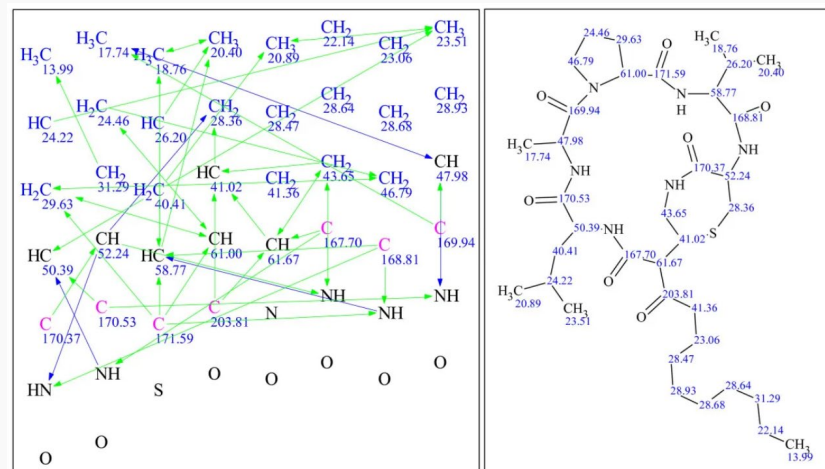
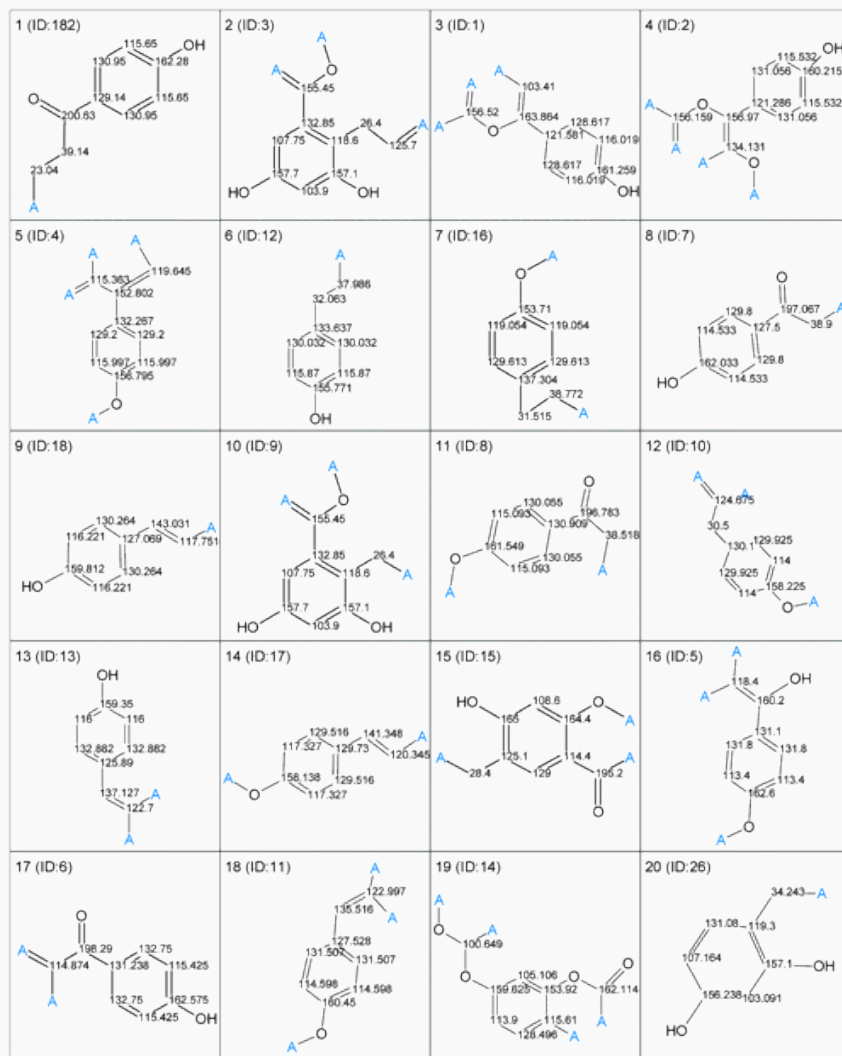
A little bit about me...

- NMR spectroscopist by training



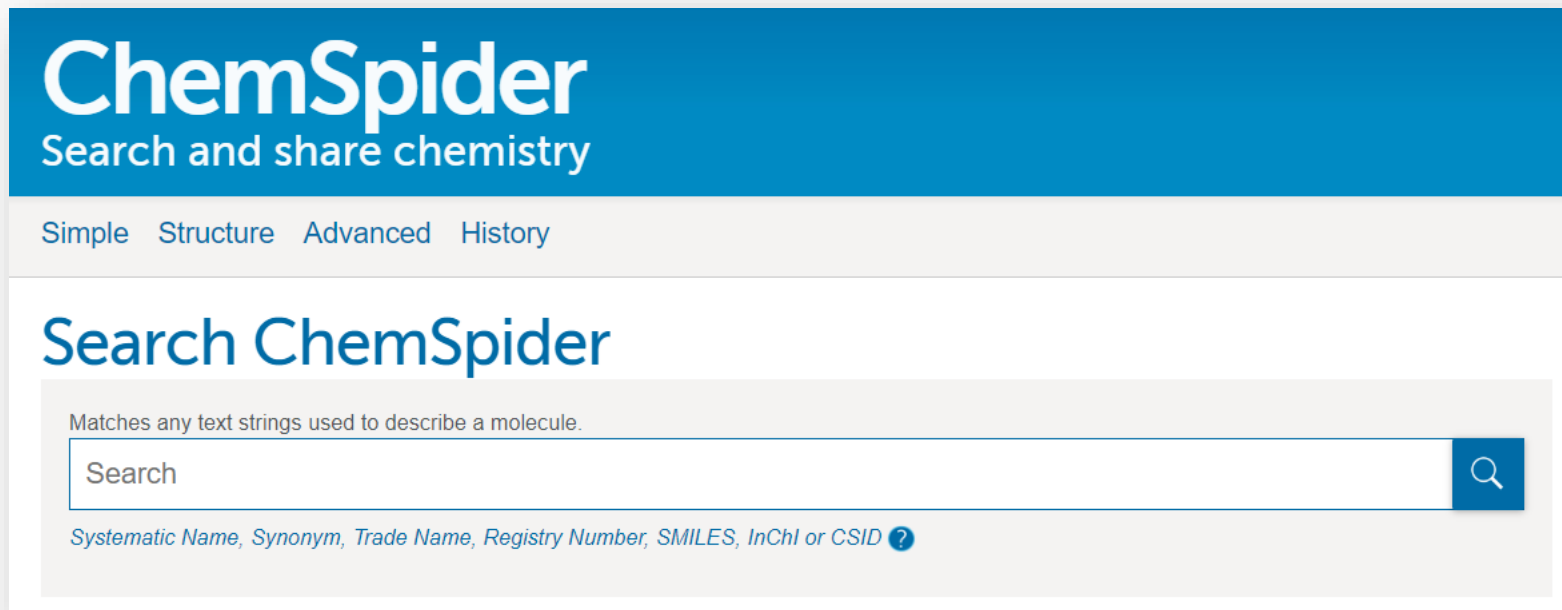
- ...ultimately focused on CASE Analysis
(Computer-Assisted Structure Elucidation)

CASE Analysis – Elucidating VERY complex chemical structures



A little bit about me...

- We built this free website...



The screenshot shows the ChemSpider website. At the top is a blue header with the text "ChemSpider" in large white font and "Search and share chemistry" in smaller white font below it. Below the header is a navigation bar with links: "Simple", "Structure", "Advanced", and "History". The main content area has the heading "Search ChemSpider" in blue. Below this is a search box with the placeholder text "Search". Above the search box, it says "Matches any text strings used to describe a molecule." To the right of the search box is a blue button with a white magnifying glass icon. Below the search box, there is a line of text: "Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID" followed by a question mark icon.

- ...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](#)



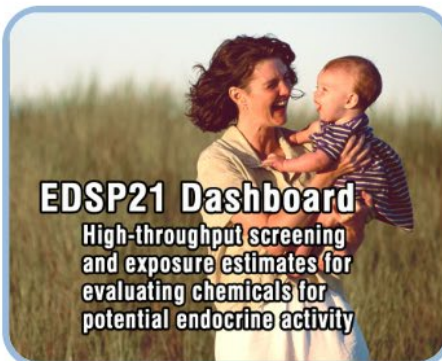
Cite this: *Org. Biomol. Chem.*, 2015, **13**, 9957

Dereplication of natural products using minimal NMR data inputs†

Russell B. Williams,^a Mark O'Neil-Johnson,^a Antony J. Williams,^b Patrick Wheeler,^c Rostislav Pol^c and Arvin Moser^{*c}

- 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...

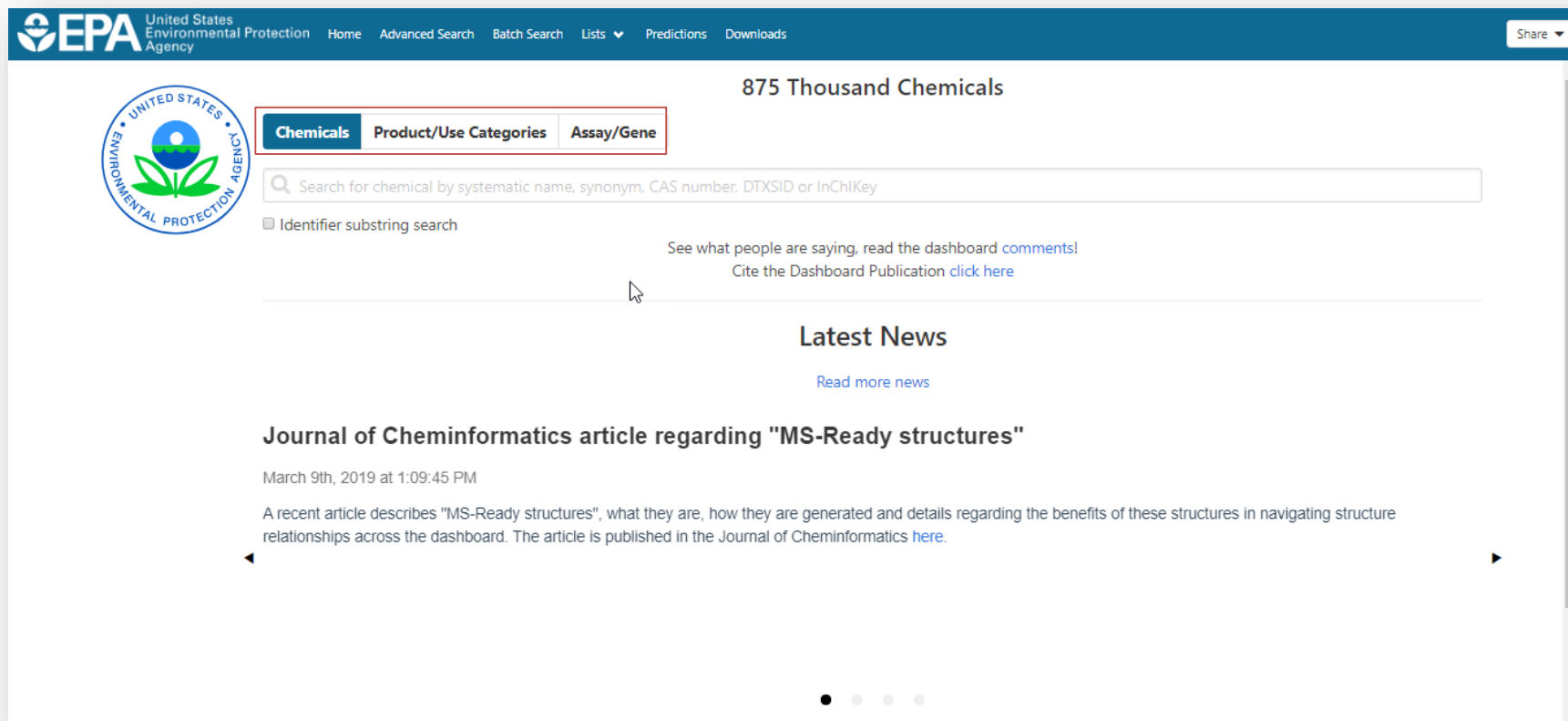


- A publicly accessible website delivering access:
 - ~**875,000** chemicals with related property data
 - Searchable by chemical, product use, gene and assay (ToxCast)
 - Experimental and predicted physicochemical property data
 - “Bioactivity data” for the ToxCast/Tox21 project
 - Links to other agency 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

CompTox Chemicals Dashboard

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

875k Chemical Substances



The screenshot shows the CompTox Chemicals Dashboard interface. At the top is a blue navigation bar with the EPA logo, the text "United States Environmental Protection Agency", and links for Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A "Share" button is on the right. Below the navigation bar is a white header area with the EPA seal on the left and the text "875 Thousand Chemicals" on the right. Under the seal are three tabs: "Chemicals" (selected), "Product/Use Categories", and "Assay/Gene". Below the tabs is a search bar with the placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey". To the left of the search bar is a checkbox for "Identifier substring search". To the right of the search bar are two links: "See what people are saying, read the dashboard [comments!](#)" and "Cite the Dashboard Publication [click here](#)". Below this is a section titled "Latest News" with a link "Read more news". The first news item is titled "Journal of Cheminformatics article regarding 'MS-Ready structures'" and is dated "March 9th, 2019 at 1:09:45 PM". The text of the article states: "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](#)." At the bottom of the news section are four small circular icons.

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

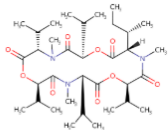
CASRN

TOXCAST

10 chemicals

Hide chemicals that are:

Filter by Name or CASRN

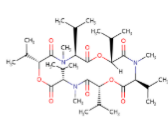


Enniatin B1

DTXSID:DTXSID70891861

CASRN:19914-20-6

TOXCAST:-

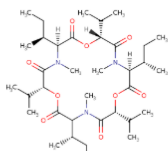


Enniatin B

DTXSID:DTXSID30891862

CASRN:917-13-5

TOXCAST:-

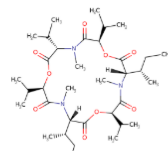


Enniatin A

DTXSID:DTXSID90891863

CASRN:2503-13-1

TOXCAST:-

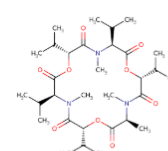


Enniatin A1

DTXSID:DTXSID50891864

CASRN:4530-21-6

TOXCAST:-

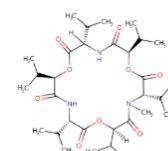


Enniatin J1

DTXSID:DTXSID701017631

CASRN:19893-15-3

TOXCAST:-

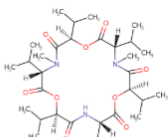


Enniatin B3

DTXSID:DTXSID401017632

CASRN:864-99-3

TOXCAST:-

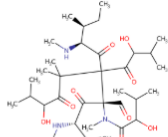


Enniatin B2

DTXSID:DTXSID501017635

CASRN:632-91-7

TOXCAST:-

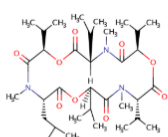


Enniatin F

DTXSID:DTXSID601017690

CASRN:144446-20-8

TOXCAST:-

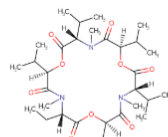


Enniatin B4

DTXSID:DTXSID601017783

CASRN:19893-21-1

TOXCAST:-

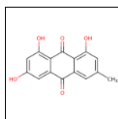


Enniatin K1

DTXSID:DTXSID801017977

CASRN:716318-00-2

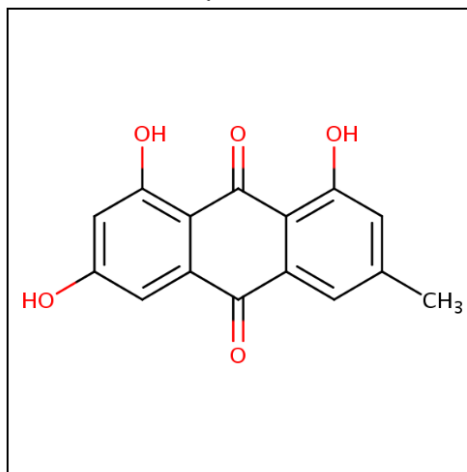
TOXCAST:-



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

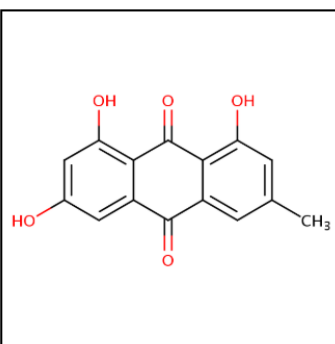
Property

Summary

Download Columns

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

Open Source Prediction Models



Model Results

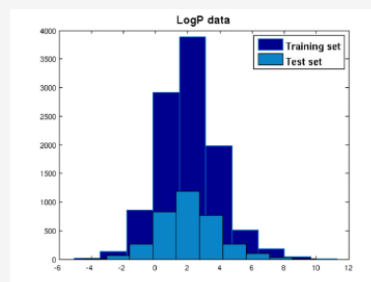
Predicted value: 2.59

Global applicability domain: Inside

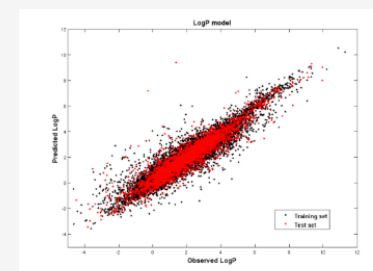
Local applicability domain index: 0.548

Confidence level: 0.695

Model Performance



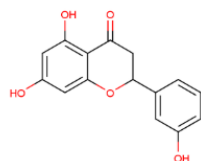
QMRP



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

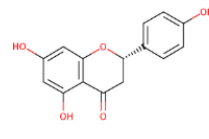
Nearest Neighbors from the Training Set



5,7,3'-Trihydroxyflavanone

Measured: 2.61

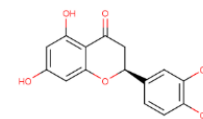
Predicted: 2.59



Naringenin

Measured: 2.52

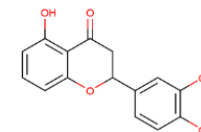
Predicted: 2.62



FRIODICTYOL

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. M.
An automated curation pr
datasets used in QSAR n
DOI: [10.1080/1062936X.](https://doi.org/10.1080/1062936X.)

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

 Journal of Cheminformatics

To link to this article: [h](#)

RESEARCH ARTICLE

Open Access

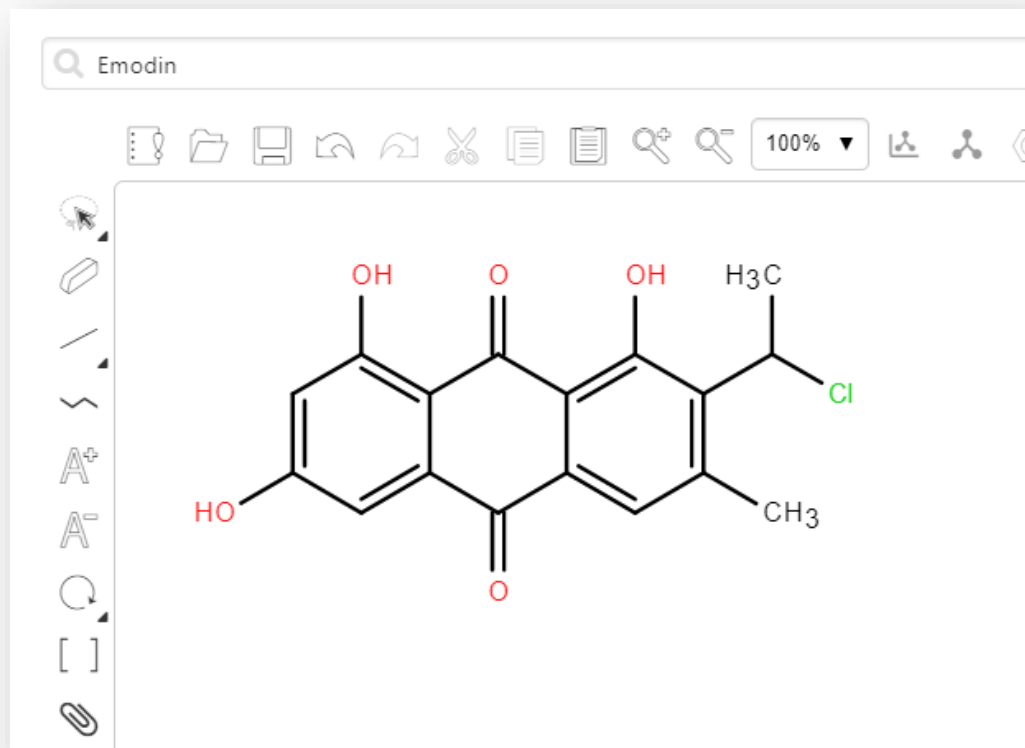


OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri^{1,2,3*} , Chris M. Grulke¹, Richard S. Judson¹ and Antony J. Williams¹

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

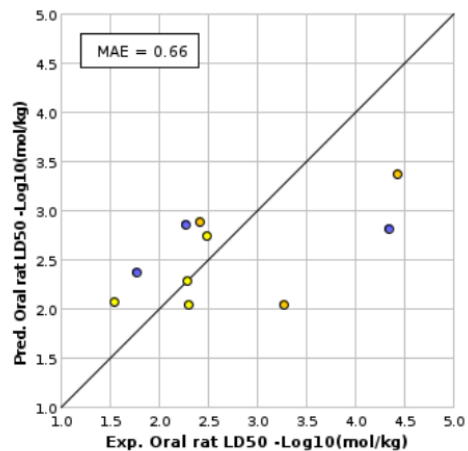
Plus Real-Time Predictions



- ☒ 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 ≥ 0.5	0.66

*Mean absolute error in -Log10(mol/kg)

Structure	Similarity Coefficient	Experimental value -Log10(mol/kg)	Predicted value -Log10(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

DataType

 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	EFSA OpenFoodTox	EFSA
	5	LR50	-	repeat dose	1873	g/ha	acute	-	parasitic wasp	EFSA OpenFoodTox	EFSA
	5	LD50	-	subacute	100	mg/kg	acute	-	tiger worm	EFSA OpenFoodTox	EFSA
	5	LD50	-	acute	2000	mg/kg	acute	oral	bobwhite quail	EFSA OpenFoodTox	EFSA
	5	LD50	-	acute	100	ug/piece	acute	oral	honey bee	EFSA OpenFoodTox	EFSA
	5	LD50	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.							EFSA OpenFoodTox	EFSA

6 records

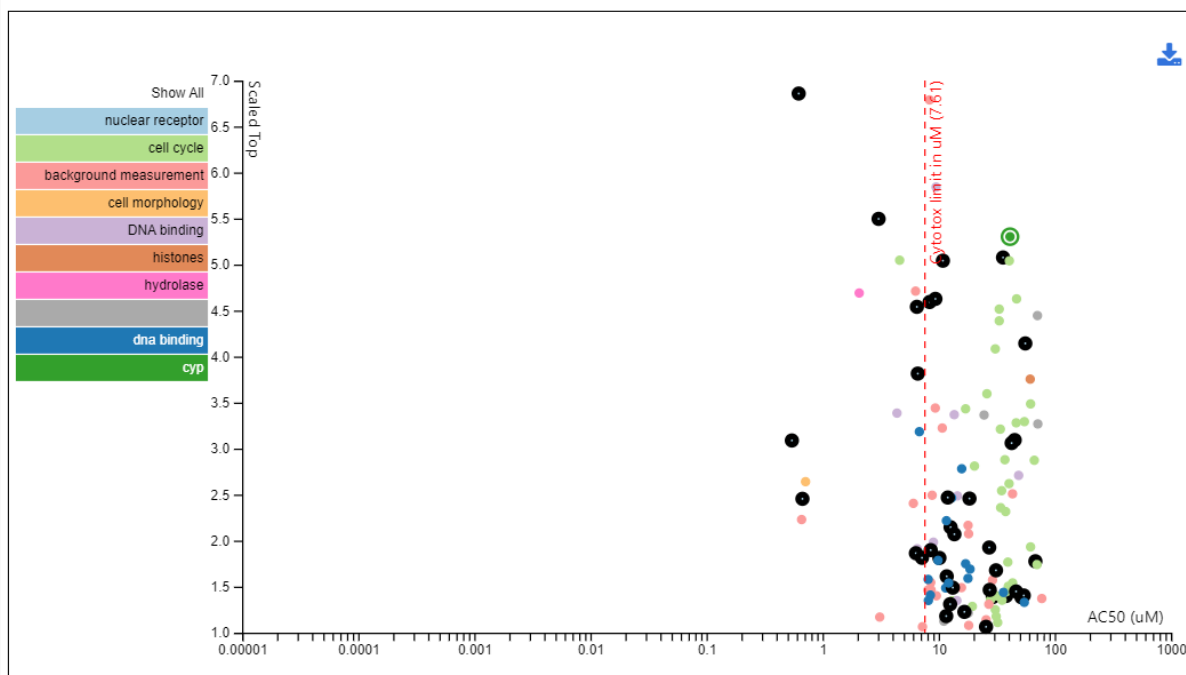
- ToxVal Database contains following data:
 - ~800,000 toxicity values
 - ~30 sources of data
 - ~22,000 sub-sources
 - ~5000 journals cited
 - ~70,000 literature citations

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

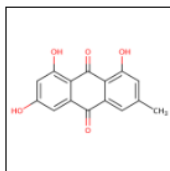
Name	Gene Name	Gene Url	Hit Call	AC50	logAC50	Cutoff	ModlAcb	Intended Target Family
ACEA_ER_80hr	estrogen receptor 1	https://www.ncbi.nlm.nih.gov/gene/2099	ACTIVE	0.544	-0.265	26.9	-0.387	nuclear receptor
ATG_ERE_CIS_up	estrogen receptor 1	https://www.ncbi.nlm.nih.gov/gene/2099	ACTIVE	0.623	-0.206	0.503	-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	https://www.ncbi.nlm.nih.gov/gene/2099	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	https://www.ncbi.nlm.nih.gov/gene/2099	ACTIVE	3.04	0.483	20.0	3.00e-2	nuclear receptor

Identifiers to Support Searches

Synonym	Quality
Emodin	Valid
1,3,8-Trihydroxy-6-methylanthracene-9,10-dione	Valid
9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl-	Valid
518-82-1 Active CAS-RN	Valid
<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”

Literature Searching




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*)

Literature Searching

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; Ruysschaert...	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		

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<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-glucopyranoside regulates cell cycl...	Li; Li; Zhu; Song	Biomedicine & pharmacotherapy = Biomedecine & ...	
<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 = Biomedecine & ...	
<input type="checkbox"/>	0	3	0	3	27604007	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	2018	Physcion 8-O-β-glucopyranoside inhibits clear-cell l...	Wang; Yan; Zhang; Guo; Xing; Wang; Qin; Zeng	Biomedicine & pharmacotherapy = Biomedecine & ...	
<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...	✓
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<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	
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<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.



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Anti-tumor effect of emodin on gynecological cancer cells.

[Wang Y](#)¹, [Yu H](#)², [Zhang J](#)³, [Ge X](#)⁴, [Gao J](#)¹, [Zhang Y](#)¹, [Lou G](#)⁵.


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- 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.

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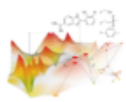
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 Nancy Baker ¹, Thomas Knudsen², Antony Williams ²

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
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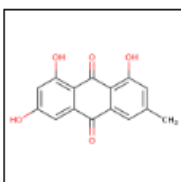
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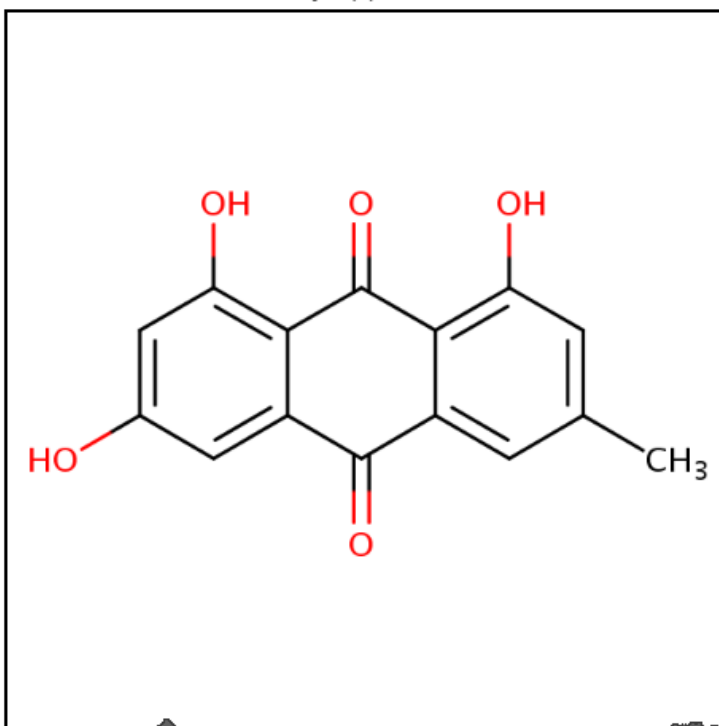
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Emodin

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 *Polygonum japonicum* syn. *Polygonum cuspidatum*). It is also produced by many species of fungi, including *Aspergillus* and *Penicillium*. The common name is derived from *Rheum emodi*, a taxonomic synonym of *Rheum*...

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Intrinsic Properties



Molecular Formula: C₁₅H₁₀O₅



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Average Mass: 270.24 g/mol



Isotope Mass Distribution



Monoisotopic Mass: 270.052823 g/mol

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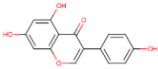
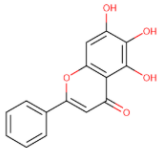
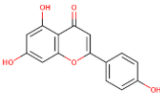
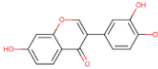
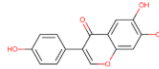
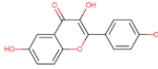
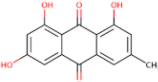
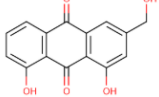
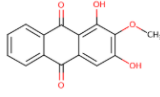
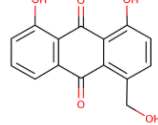
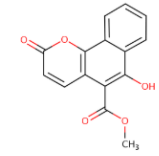
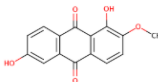
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86 chemicals

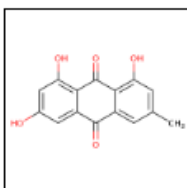
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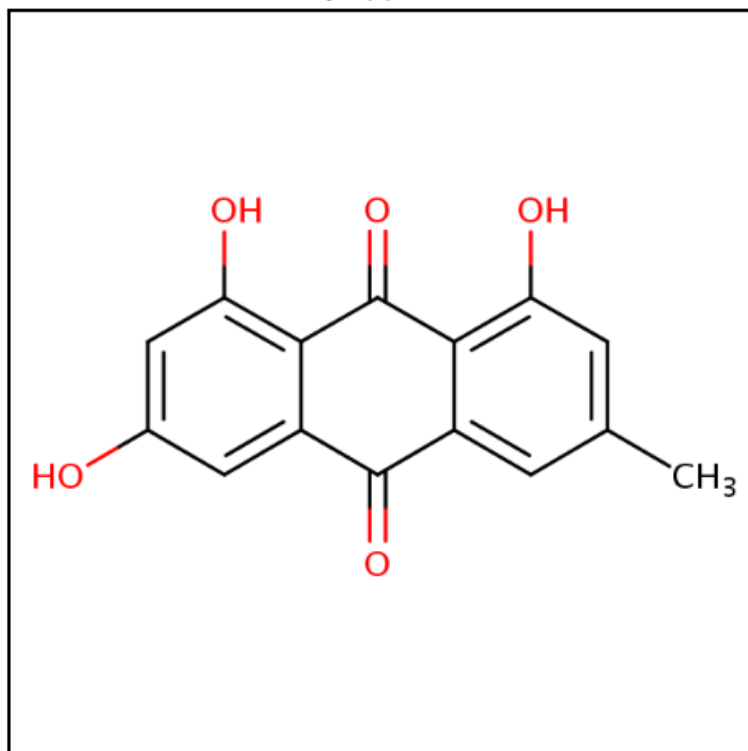
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Wikipedia

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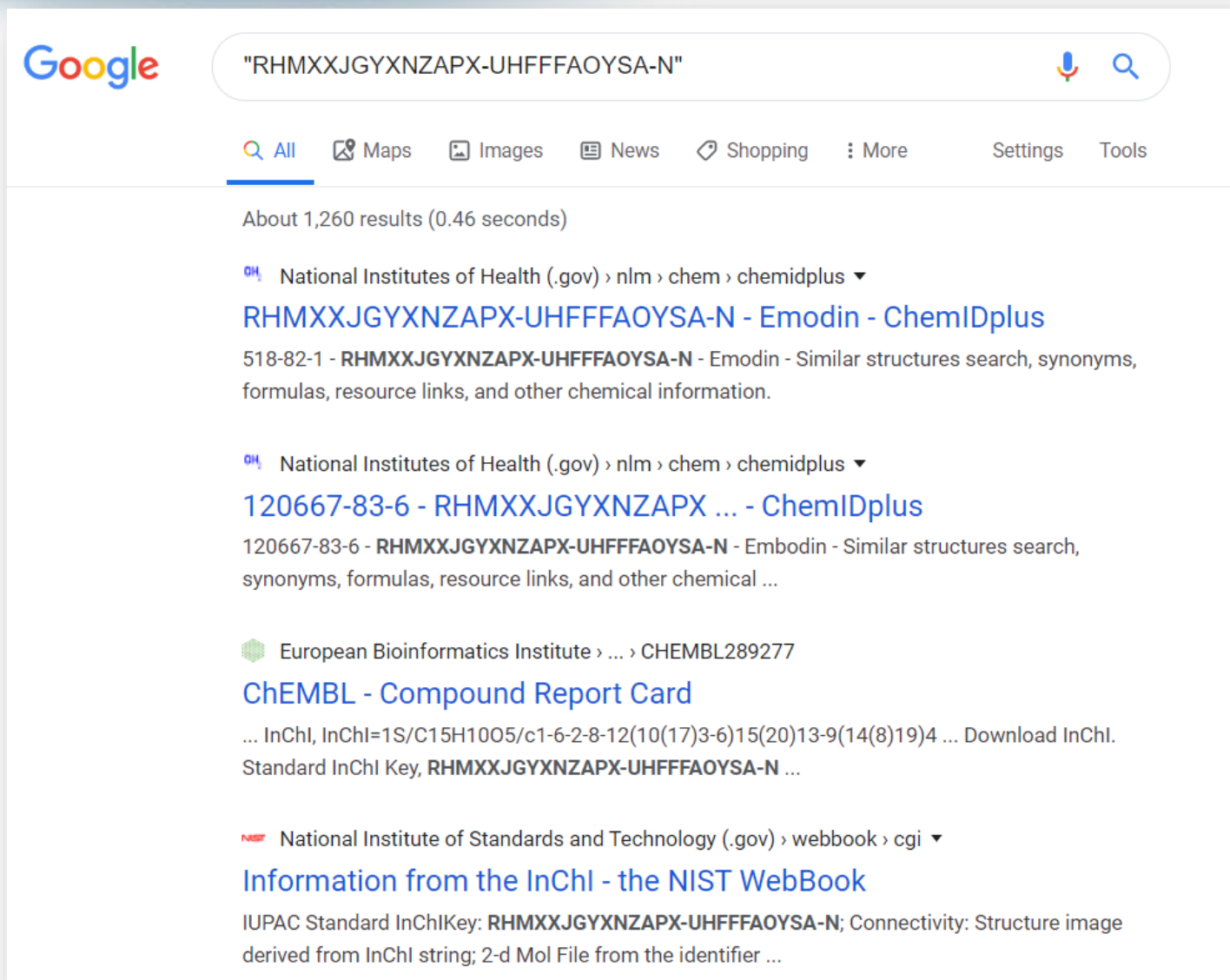
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-  **InChI String:** InChI=1S/C15H10O5/c1-6-2-8-12(10(17)3-6)15(20)13-9(14(8)19)4-7(1
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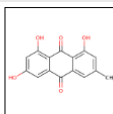
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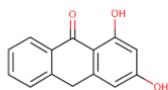
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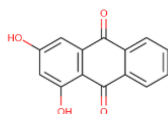
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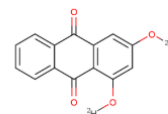
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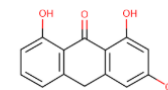
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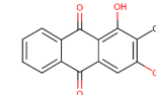
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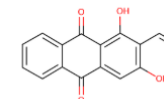
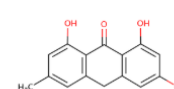
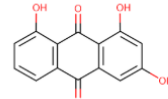
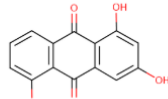
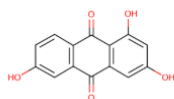
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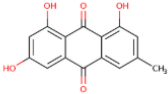
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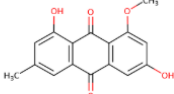
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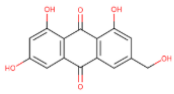
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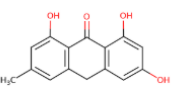
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Transformation Product



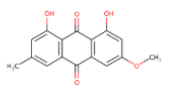
omega-Hydroxyemodin
DTXSID:DTXSID60197420
CASRN:481-73-2
TOXCAST:-

Transformation Product



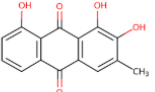
Emodin anthrone
DTXSID:DTXSID80197684
CASRN:491-60-1
TOXCAST:-

Transformation Product



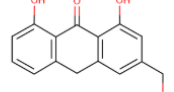
Physcione
DTXSID:DTXSID20200101
CASRN:521-61-9
TOXCAST:-

Transformation Product



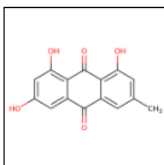
2-Hydroxychrysophanol
DTXSID:DTXSID70207049
CASRN:58322-78-4
TOXCAST:-

Transformation Product



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: CTD



Illuminating how chemicals affect human health.

Comparative Toxicogenomics Database

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Emodin

Basics

Gene Interactions

Genes

Diseases

Phenotypes

Comps

Pathways

GO

Exposure Studies

Exposure Details

References

Name ? Emodin

CAS Type 1 Name ? 9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl-

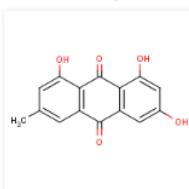
Equivalent Terms ? Archin | Emodin, Frangula | Emodin, Rheum | Frangula Emodin | Frangulic Acid | Rheum Emodin

CAS Registry Number ? 518-82-1

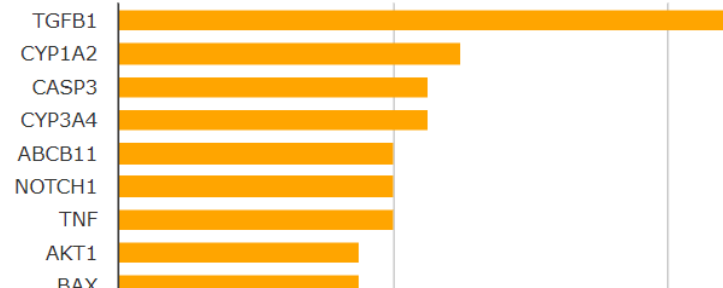
CTD-Curated Synonym ? Aloe-emodin

Definition ? Purgative anthraquinone found in several plants, especially Rhamnus frangula. It was formerly used in toxicity studies.





Structure ?








Top Interacting Genes ?



External Links: MassBank of North America


MoNA - MassBank of North America  Spectra  Downloads  Upload  Help

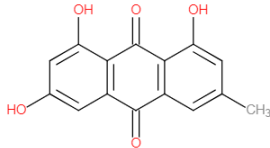
Search...  











   # 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

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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

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Columns ▼

toxins

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List Acronym	List Name	Number of Chemicals	List Description
ALGALTOX	LIST: Algal Toxins	54	A list of Algal Toxins of potential interest
MYCOTOX2	LIST: Mycotoxins	328	List of mycotoxins collected from public sources
MYCOTOXINS	MASSPECDB: Mycotoxins from MassBank.EU	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	NEURO: Neurotoxicants Collection from Public Resources	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	NORMAN: Toxic Plant Phytotoxin (TPPT) Database	561	A comprehensive toxic plant-phytotoxin (TPPT) database provided by Günthardt et al 2018, DOI: 10.1021/acs.jafc.8b01639

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](https://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

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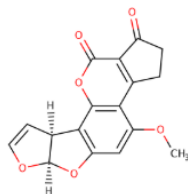
CASRN 

DTXSID 

Mono.Mass 

Hide chemicals that are: 

Filter by Name or CASRN

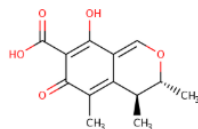


Aflatoxin B1

CASRN:1162-65-8

DTXSID:DTXSID9020035

Mono.Mass:312.063388

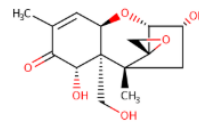


Citrinin

CASRN:518-75-2

DTXSID:DTXSID8020333

Mono.Mass:250.084124

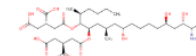


Vomitoxin

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

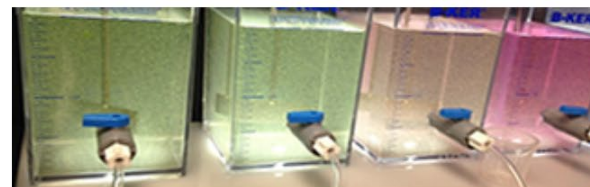
Monitoring and Analysis



- [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

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Default



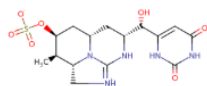
CASRN

DTXSID

Mono.Mass

Hide chemicals that are:

Filter by Name or CASRN

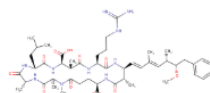


Cylindrospermopsin

CASRN:143545-90-8

DTXSID:DTXSID2031083

Mono.Mass:415.116169

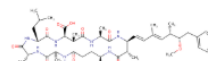


Microcystin LR

CASRN:101043-37-2

DTXSID:DTXSID3031654

Mono.Mass:994.548768

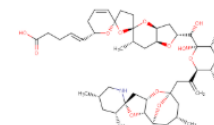


Microcystin LA

CASRN:96180-79-9

DTXSID:DTXSID3031656

Mono.Mass:909.484771



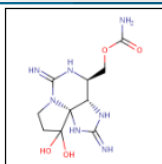
Azaspiracid

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



 Toxicity Value

 Human  Eco

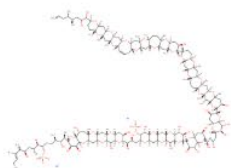
 Download

Columns

Search query

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?

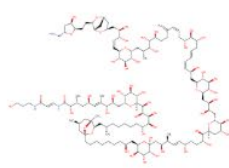


Maitotoxin

CASRN:59392-53-9

DTXSID:DTXSID10880012

Mono.Mass:3423.581083

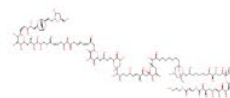


palytoxin

CASRN:77734-91-9

DTXSID:DTXSID90423027

Mono.Mass:2678.479594

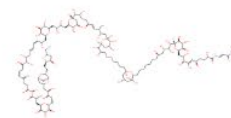


ovatoxin-a

CASRN:1009813-91-5

DTXSID:DTXSID90880111

Mono.Mass:2646.489764

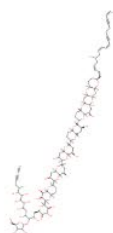


ostreocin-D

CASRN:163648-25-7

DTXSID:DTXSID50880112

Mono.Mass:2634.453379

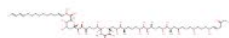


Prymnesin-2

CASRN:168010-52-4

DTXSID:DTXSID10880113

Mono.Mass:1967.795848

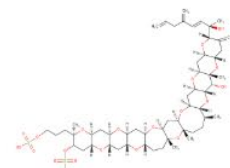


Karlotoxin-2

CASRN:1138665-35-6

DTXSID:DTXSID70880114

Mono.Mass:1344.793633

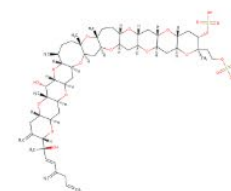


Homoyessotoxin

CASRN:196309-94-1

DTXSID:DTXSID20880088

Mono.Mass:1156.494652



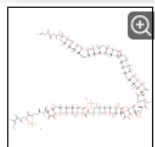
Yessotoxin

CASRN:112514-54-2

DTXSID:DTXSID20880023

Mono.Mass:1142.479002

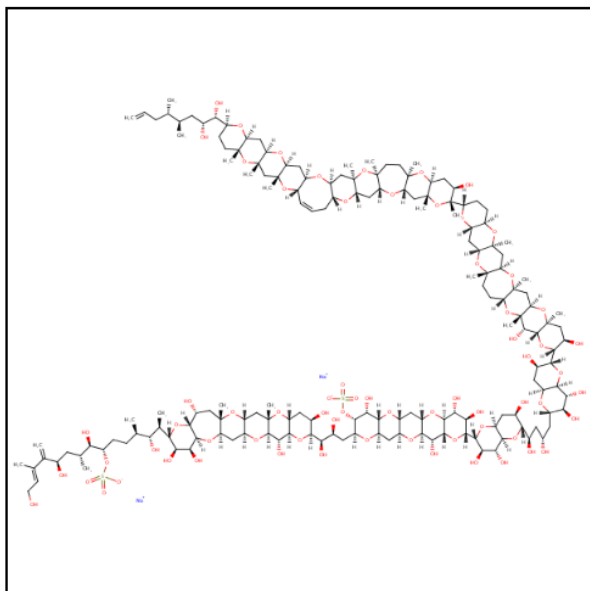
When you can download them...



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: C₁₆₄H₂₅₆Na₂O₆₈S₂



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!



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


Review
Keynote

Towards a gold standard:
quality in public domain
databases and approaches
the

Antony J. Williams
Show
<https://doi.org/10.1186/s13321-015-0057-7>

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

and content

Will the correct Microcystin LR Stand Up? ChemSpider Skeleton Search

Matches any text strings used to describe a molecule.

ZYZCGGRZINLQBL



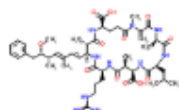
Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

FILTER ▾

Search Hits Limit: 100 ▾

Found 9 results

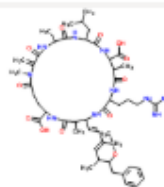
Search term: ZYZCGGRZINLQBL (Found by InChIKey (skeleton match))



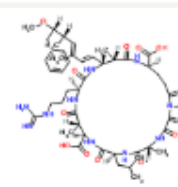
[Cyanoginosin](#)



[MCYST-LR](#)



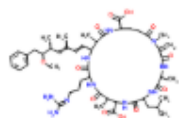
[15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,3E\)-6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-yl\)](#)



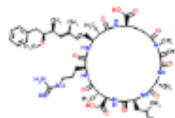
[\(5R,8S,11R,12S,15S,18R,19S,22R\)-15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,3E,5S,6S\)-6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-yl\)](#)



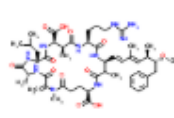
[\(5R,8S,15S\)-15-\(3-\(\(Diaminomethylene\)amino\)propyl\)-8-isobutyl-18-\(\(1E,3E,5S,6S\)-6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-yl\)](#)



[15-\(3-\(\(Diaminomethylene\)amino\)propyl\)-8-isobutyl-18-\(6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-yl\)](#)



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

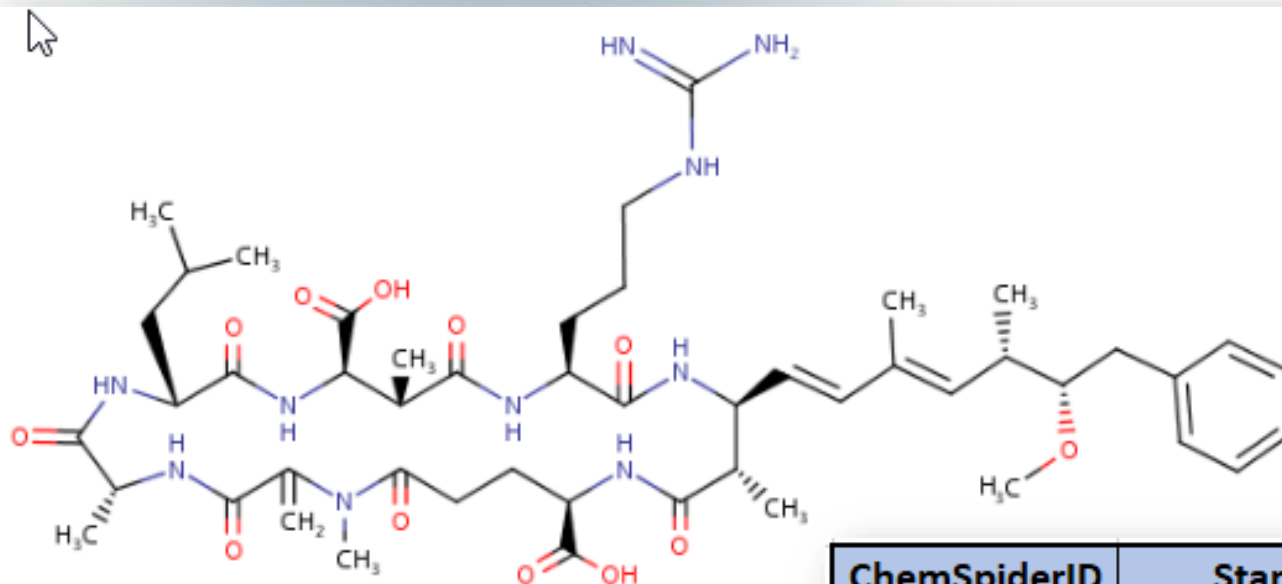


[\(5R,8R,11R,12S,15S,18S,22R\)-15-\(3-Carbamimidamidopropyl\)-8-isobutyl-18-\(\(1E,3E,5R,6R\)-6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-yl\)](#)



[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-phenyl-1,3-heptadien-1-yl\)](#)

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+
4941647	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
393078	t28-,29-,30-,31+,34-,35-,36+, 37- ,38-,40+
57618348	t28-,29-,30-,31+,34-,35-,36+, 37- ,38-,40+
29342071	t28-,29-,30-,31+, 34+ ,35-,36+, 37- ,38-,40+
7987594	t28-, 29? , 30? ,31+, 34? ,35-, 36? , 37- ,38-, 40?
22900854	t28-, 29? , 30+ , 31- , 34+ , 35+ , 36- , 37- ,38-, 40-
19692240	NONE
2831283	NONE

Comparing ChemSpider Structures

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

Other Searches



PubChem [About](#)

SEARCH FOR

ZYZCGGRZINLQBL

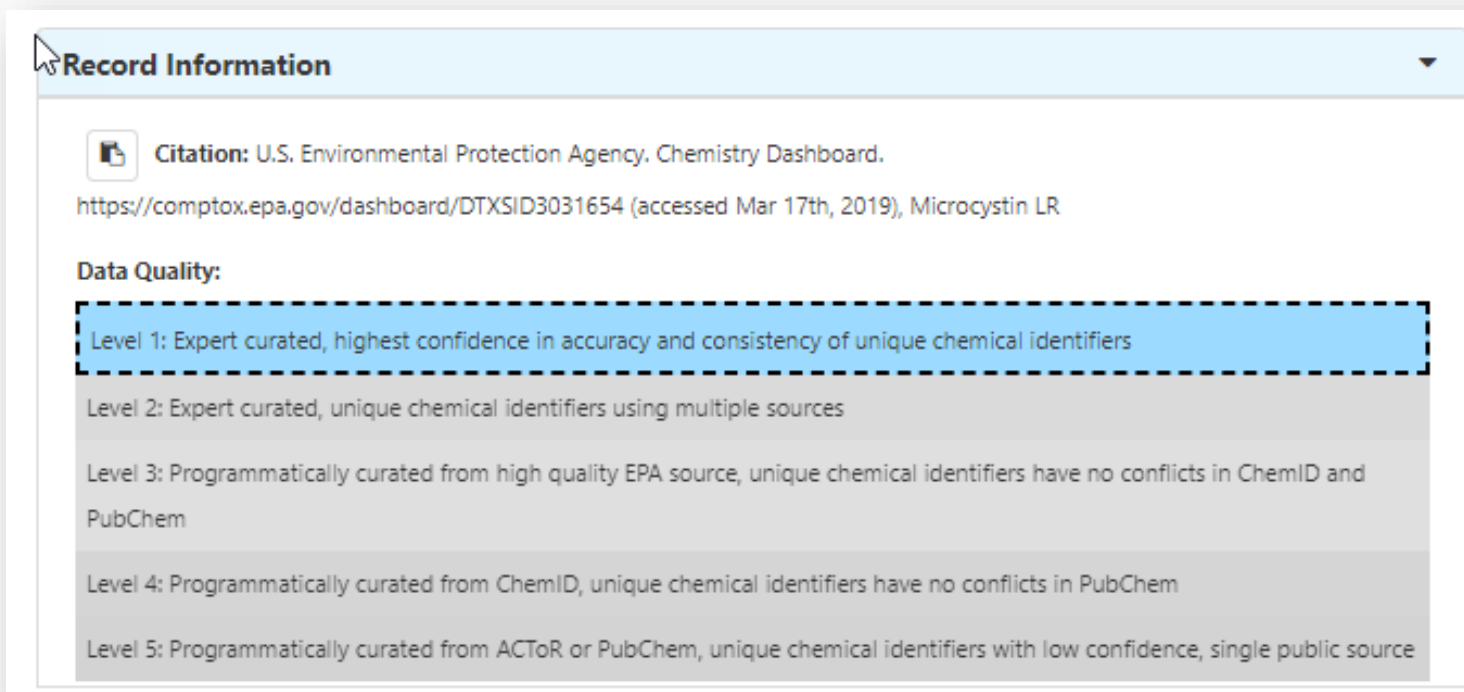
Treating this query as a text search.

Compounds
(17)


Show **All** entries

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

- 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

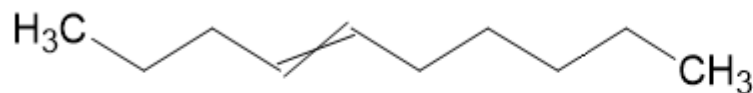
Data Quality:

- 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

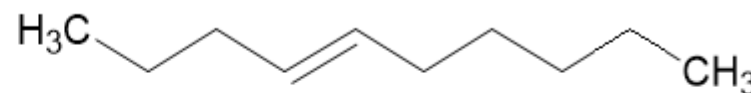
Substance Mapping						
(1 of 66) 1 2 3 4 5 6 7 8 9 10 25						
	Source Casrn	Source Name	Hit Substance_ID	Hit Casrn	Hit Name	
▶	19398-89-1	4-Decene	DTXSID50876156	19689-18-0	4-Decene	Remove Validation
▶	112926-00-8	silica gel, cryst. - free	DTXSID9029851	112926-00-8	Hydrated silica	Remove Validation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

“4-Decene”



19398-89-1

E/Z-stereochemistry



19689-18-0

E-stereochemistry

Crowdsourced Curation

New Comment

Comment

Describe the issue you're seeing here...

Email address

Enter email address

☐ I'm not

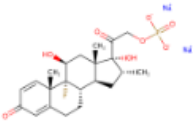
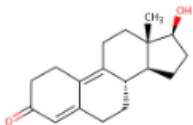
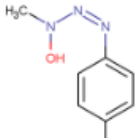
Submit

Submit Comment

Crowdsourced Comments

Show 25 entries

Sort Options: original order ↑ date chemical status

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-Dihydro-19-nortestosterone (or alternative). See https://pubchem.ncbi.nlm.nih.gov/compound/11747708	★
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-hydroxy-1,2,4-triazene" (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,[†] Barbara Novak,[†] Veronika Nagl,[†] and Franz Berthiller^{*,‡}

[†]BIOMIN Research Center, Technopark 1, 3430 Tulln, Austria






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

Add Other Data of Interest

Intrinsic And Predicted Properties






- ☒ Molecular Formula 
- ☒ Average Mass 
- ☐ Monoisotopic Mass 
- ☐ TEST Model Predictions 
- ☐ OPERA Model Predictions 

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	DTXSID50	Transformation Product	DTXSID60197420	omega-Hydroxyemodin	481-73-2
emodin	DTXSID50	Transformation Product	DTXSID30191177	Questin	3774-64-9
emodin	DTXSID50	Transformation Product	DTXSID80197684	Emodin anthrone	491-60-1
emodin	DTXSID50	Transformation Product	DTXSID20200101	Physcione	521-61-9
emodin	DTXSID50	Transformation Product	DTXSID70207049	2-Hydroxychrysophanol	58322-78-4
emodin	DTXSID50	Transformation Product	DTXSID20211510	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

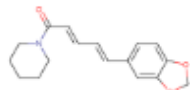
DTXSID

CASRN

TOXCAST

Mass Diff

Multicomponent Chemicals



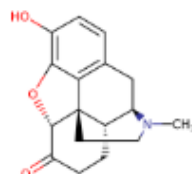
Piperine

DTXSID: DTXSID3021805

CASRN: 94-62-2

TOXCAST: 59/374

Mass Diff: 0.000093



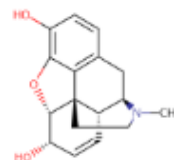
Hydromorphone

DTXSID: DTXSID8023133

CASRN: 466-99-9

TOXCAST: -

Mass Diff: 0.000093



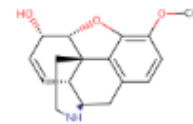
Morphine

DTXSID: DTXSID9023336

CASRN: 57-27-2

TOXCAST: -

Mass Diff: 0.000093



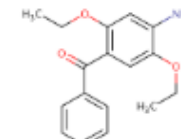
Norcodeine

DTXSID: DTXSID8046327

CASRN: 467-15-2

TOXCAST: 0/79

Mass Diff: 0.000093



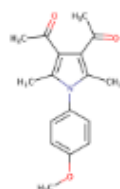
Methanone, (4-amino-2,5-diethoxyphenyl)-

DTXSID: DTXSID3071696

CASRN: 68568-55-8

TOXCAST: -

Mass Diff: 0.000093



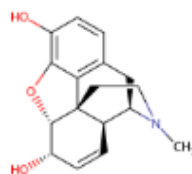
Ethanone, 1-(4-acetyl-1-(4-methoxyphenyl)-1H-pyrazol-5-yl)-

DTXSID: DTXSID80149860

CASRN: 112086-82-5

TOXCAST: -

Mass Diff: 0.000093



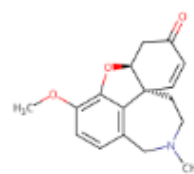
Morphinan-3,6-diol, 7,8-didehydro-4,5-dihydro-

DTXSID: DTXSID40167308

CASRN: 16206-77-2

TOXCAST: -

Mass Diff: 0.000093



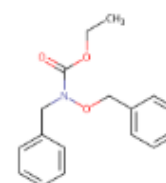
Narwedine, (+/-)-

DTXSID: DTXSID60168190

CASRN: 1668-86-6

TOXCAST: -

Mass Diff: 0.000093



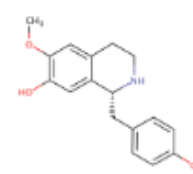
Carbamic acid, (phenylmethoxy)(phenyl)-

DTXSID: DTXSID50171931

CASRN: 1867-23-8

TOXCAST: -

Mass Diff: 0.000093



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

DTXSID: DTXSID70176367

CASRN: 2196-60-3

TOXCAST: -


Mass Diff: 0.000093

Batch Searching Formula/Mass










Batch Search


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

Step Five: Choose Data Fields to 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

+/- ppm

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>.

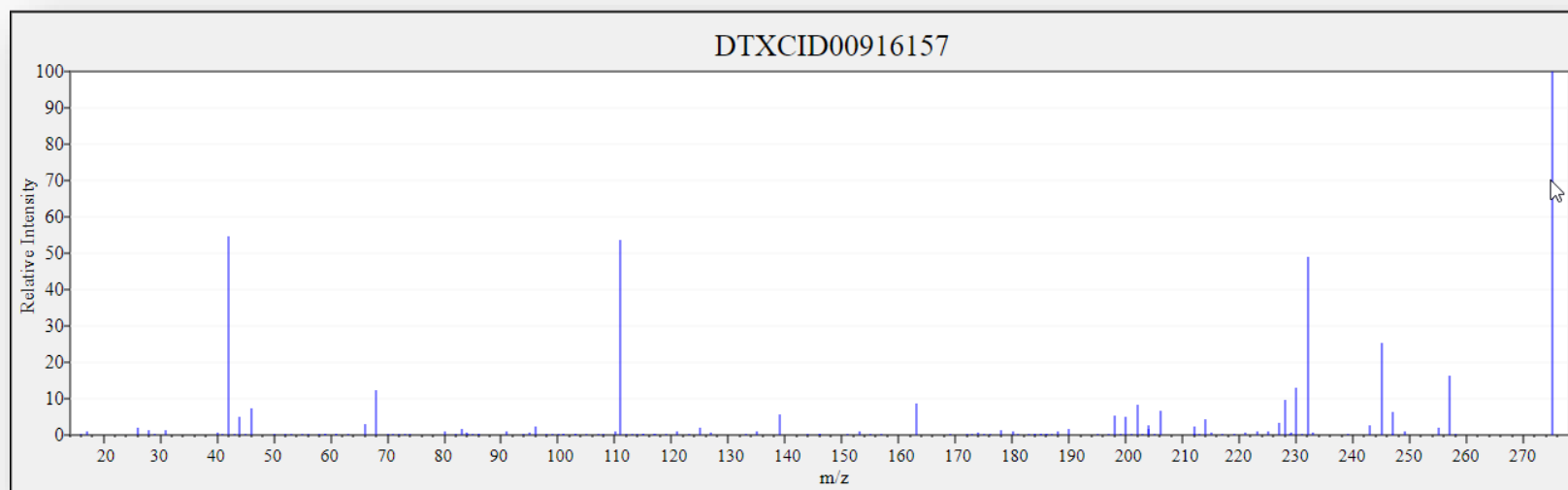
WORK IN PROGRESS

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

321.136493476

Da

±

0.0000002

Da

ppm

Molecular Formula Search

Molecular Formula

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
196.0756904 5.269463115
216.1019051 4.700461978
200.1080005 4.800144384

Peak Match Window:

0.02

Da

ppm

Search

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
200.1080005 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

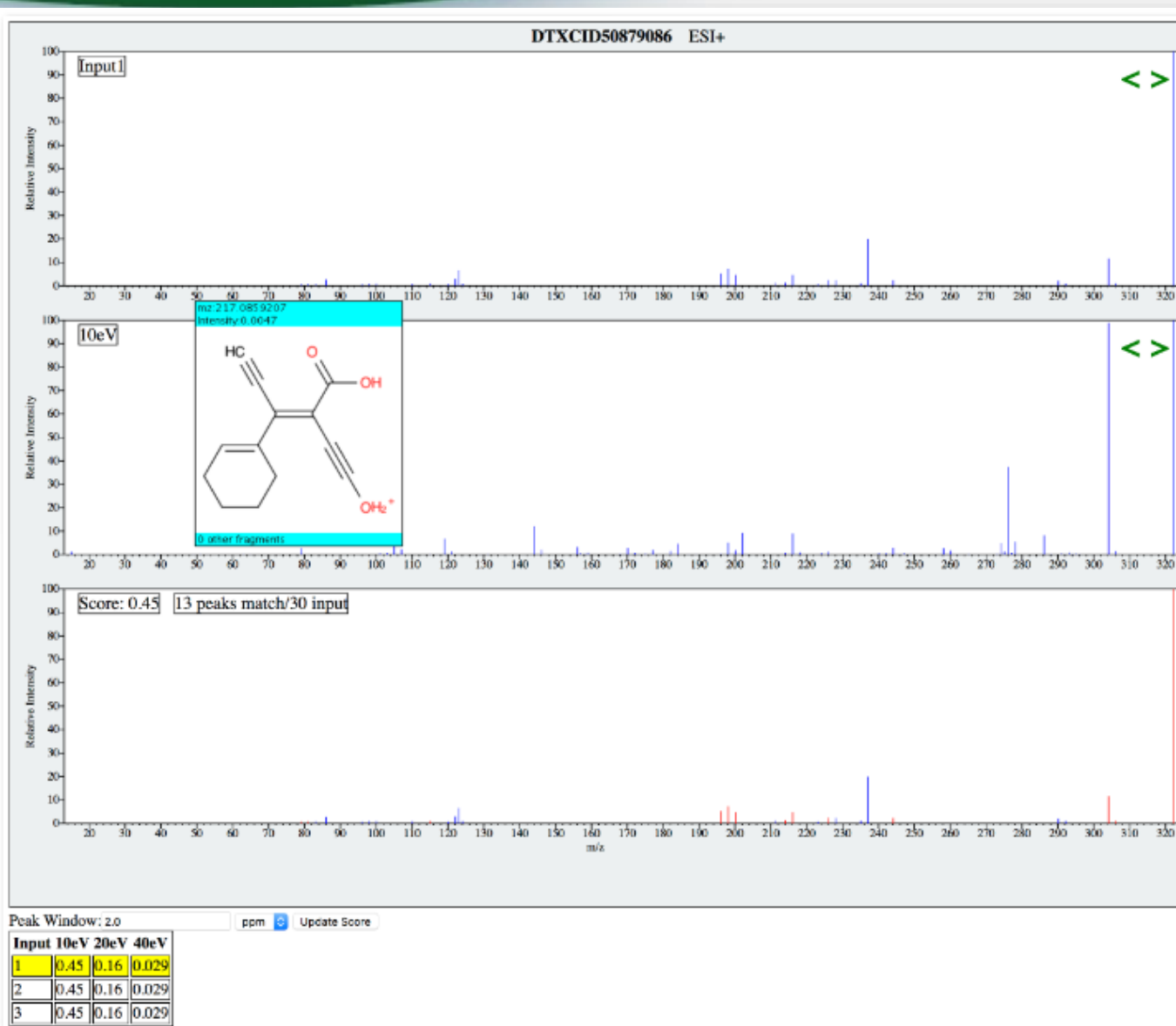
[DTXCID60349982](#)

0.11

[DTXCID10316649](#)

0.09

Spectral Viewer Comparison



Prototype Development

AADashboard

atrazine

Search



Select properties to predict

H

T.E.S.T. 18

OPERA

Search

C

Exact

N

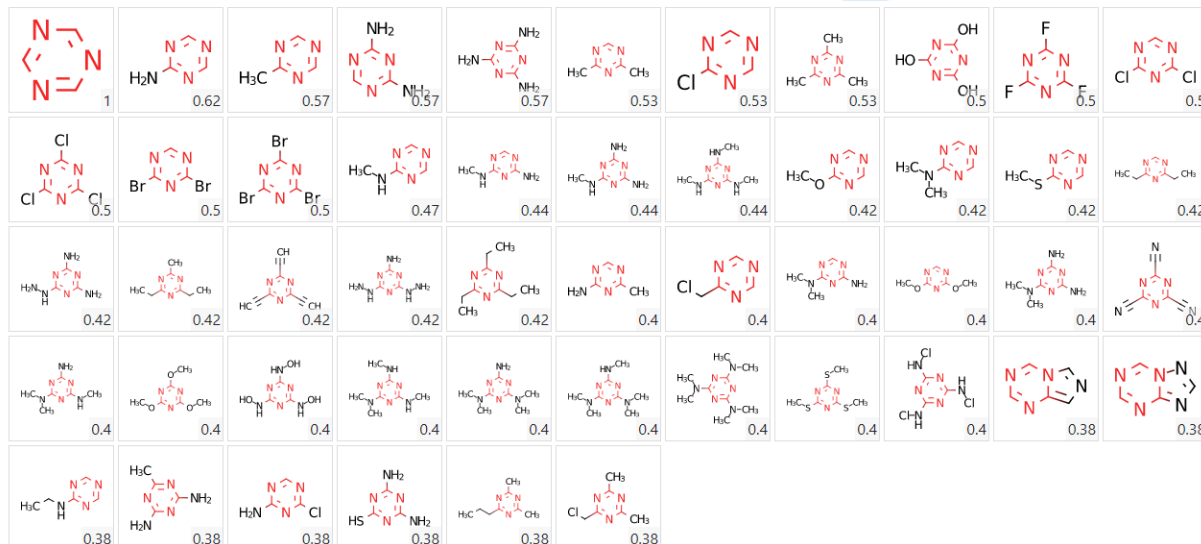
Substructure

O

Search result 2540

Show ☐ Isotopically Labeled ☐ Charged ☐ Salts or Mixtures

Sort Similarity



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):
C₁₅H₁₆O₂

Search result 5 Show ☐ Isotopically Labeled ☐ Chiral

Elements per page 50 << < 1 > >>

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

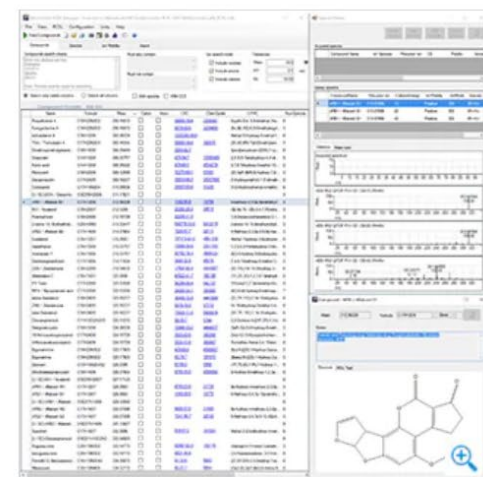
Chemical Structure: A large chemical structure is displayed in the center, showing two phenol rings connected by a central carbon atom bonded to two methyl groups (H₃C and CH₃). The phenol rings are highlighted in red, and the hydroxyl groups (HO) are labeled.

Search: A "Search" button is located in the bottom right corner of the interface.

- Food
Mycotoxins PCDL

REQUEST QUOTE

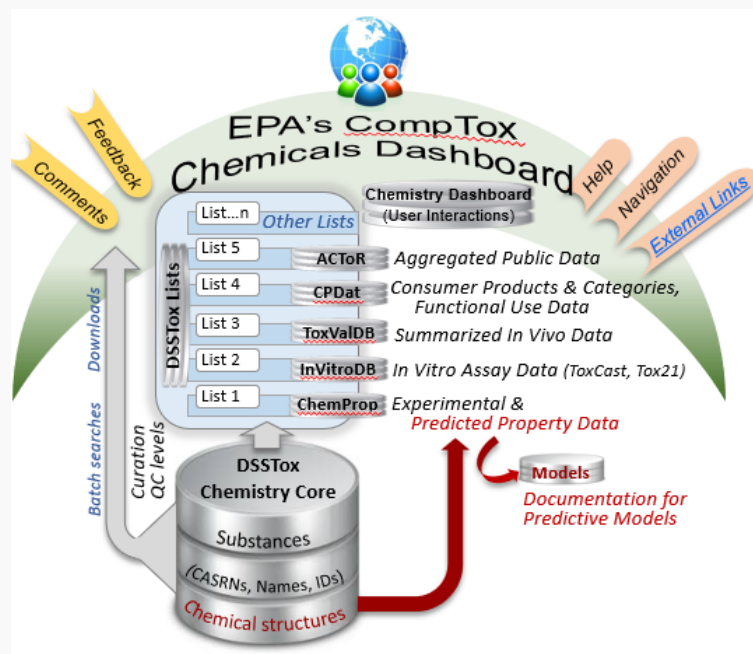
RELATED PRODUCTS

O=C1C(=O)C2=C(C(=O)C3=C2C(=O)C=C3)C(=O)C1

- Help grow the lists of Mycotoxins and Algal Toxins – please suggest additions
- Next up – structures of microviridins...
- Email me at 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”



Acknowledgements



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

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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^{1*} , Christopher M. Grulke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri^{1,2,4}, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹

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