http://www.orcid.org/0000-0002-2668-4821

The CompTox Chemicals Dashboard as An Integration Hub for Chemistry, Biology and Environmental Toxicity Data

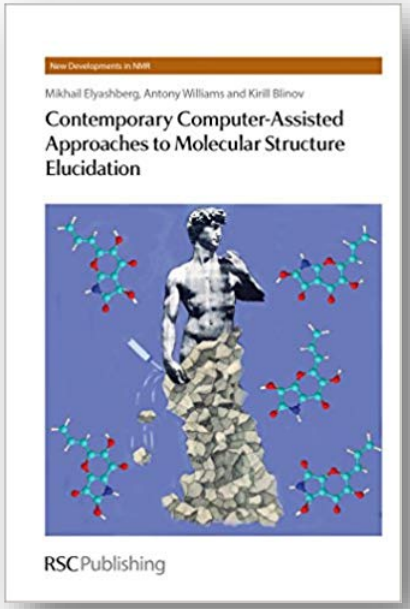
Antony Williams, Chris Grulke, Ann Richard, Richard Judson, Imran Shah
Grace Patlewicz, John Wambaugh, Katie Paul-Friedman,
Jeremy Dunne and Jeff Edwards
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

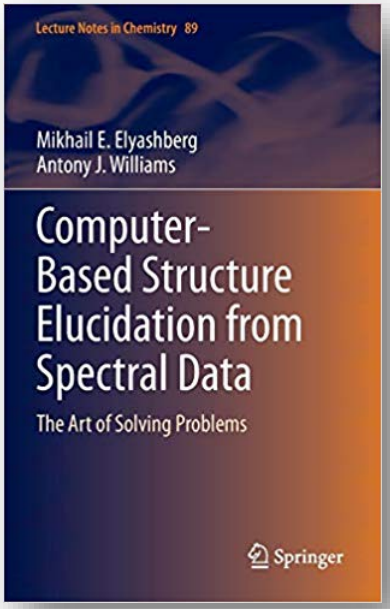
Global Marine Summit 2019
UNCW, Wilmington, NC

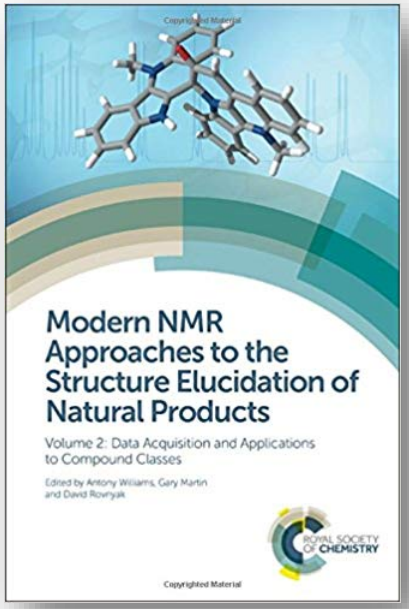
A little bit about me…

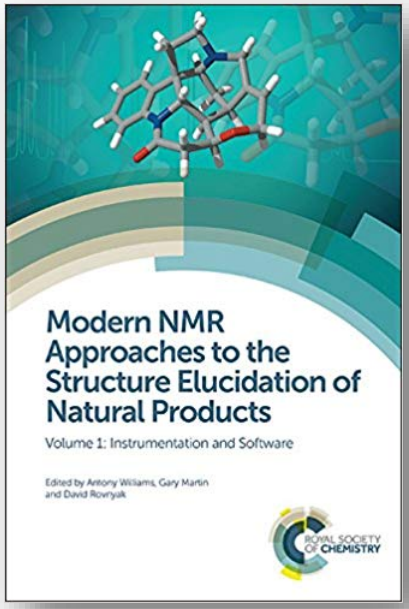
EPA United States Environmental Protection Agency

- NMR spectroscopist by training





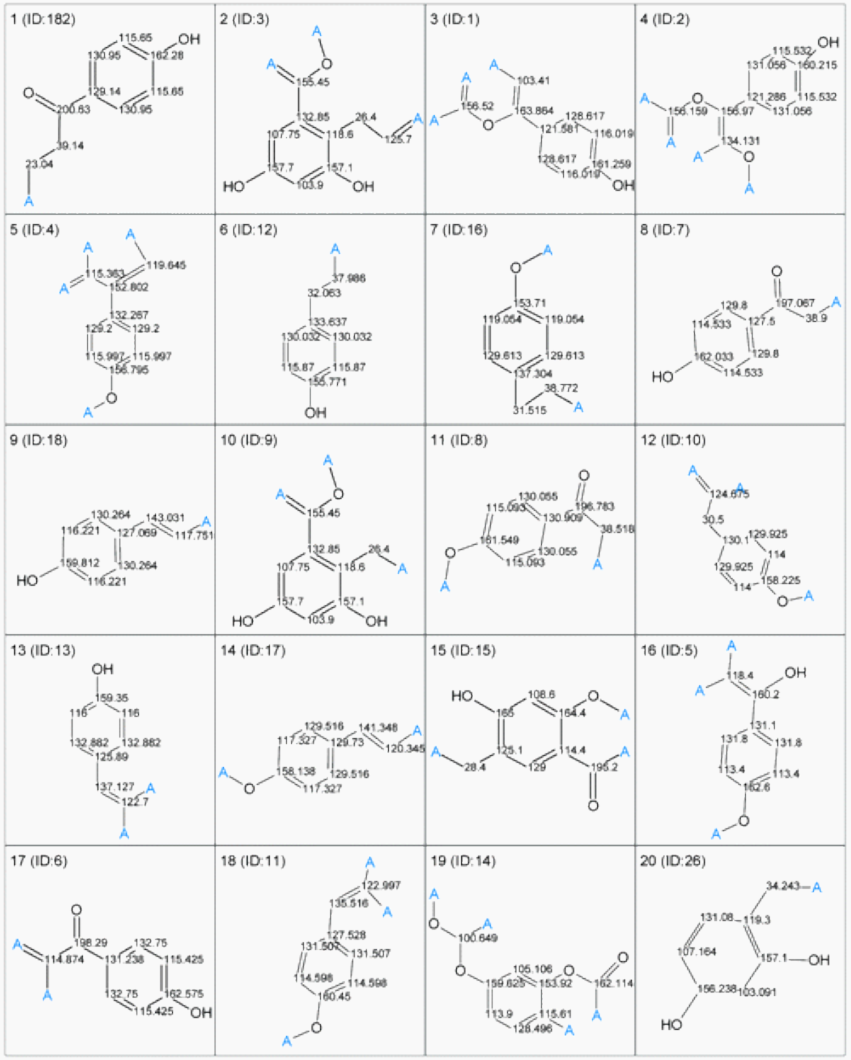


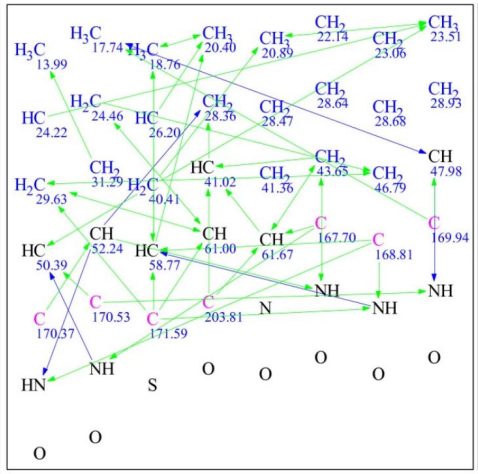


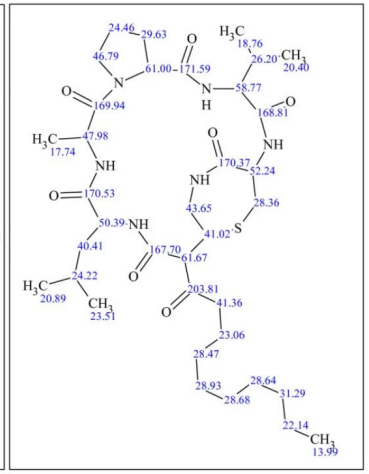
- …ultimately focused on CASE Analysis (Computer-Assisted Structure Elucidation)

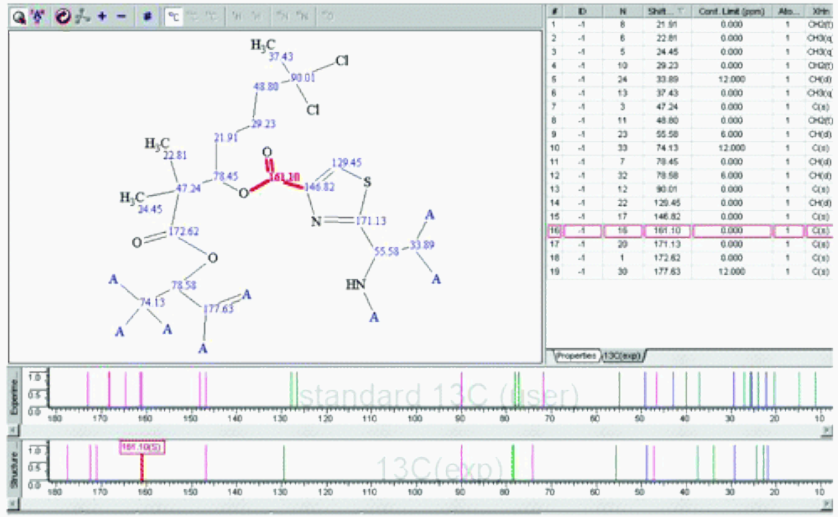
CASE Analysis – Elucidating VERY complex chemical structures

EPA United States Environmental Protection Agency



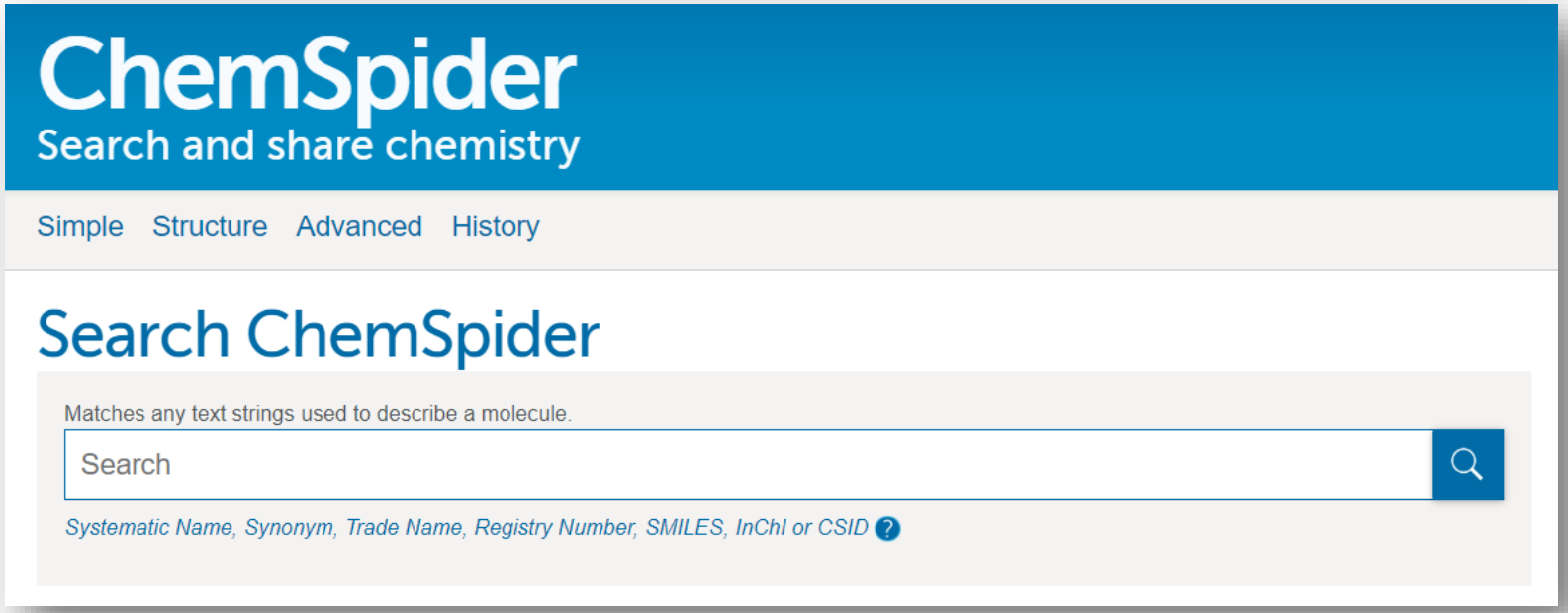






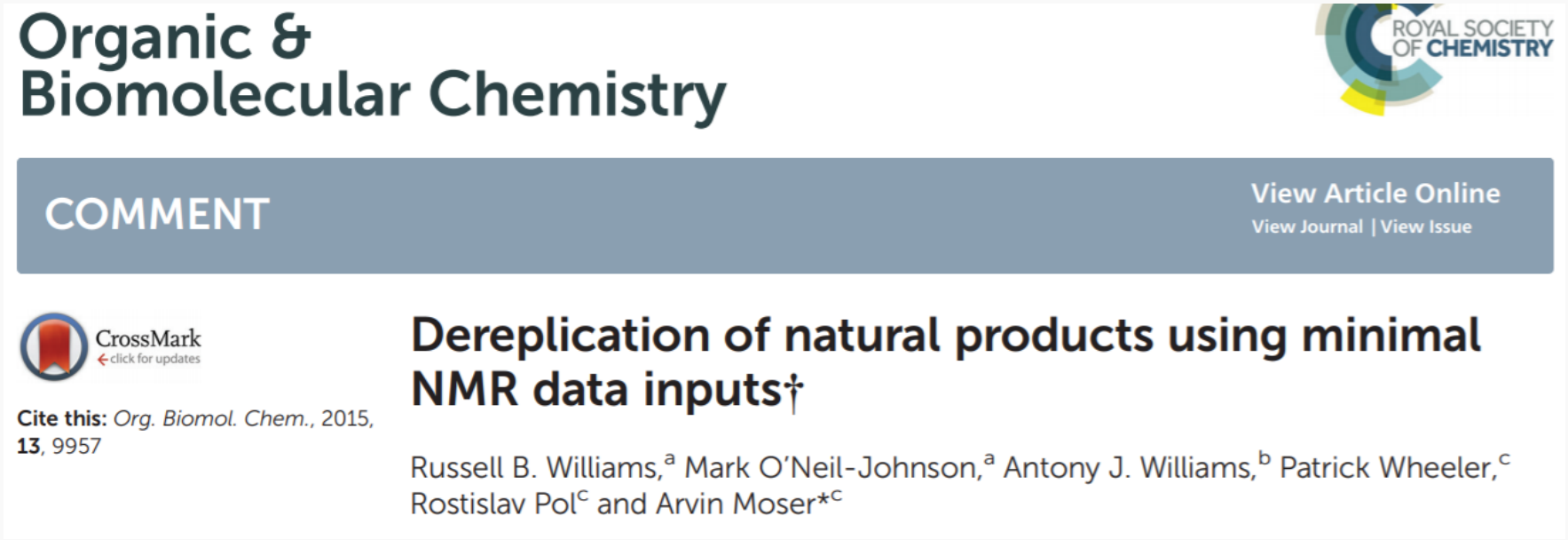
A little bit about me…

- We built this free website…



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

Bringing large databases and CASE together



Organic & Biomolecular Chemistry

ROYAL SOCIETY OF CHEMISTRY

COMMENT

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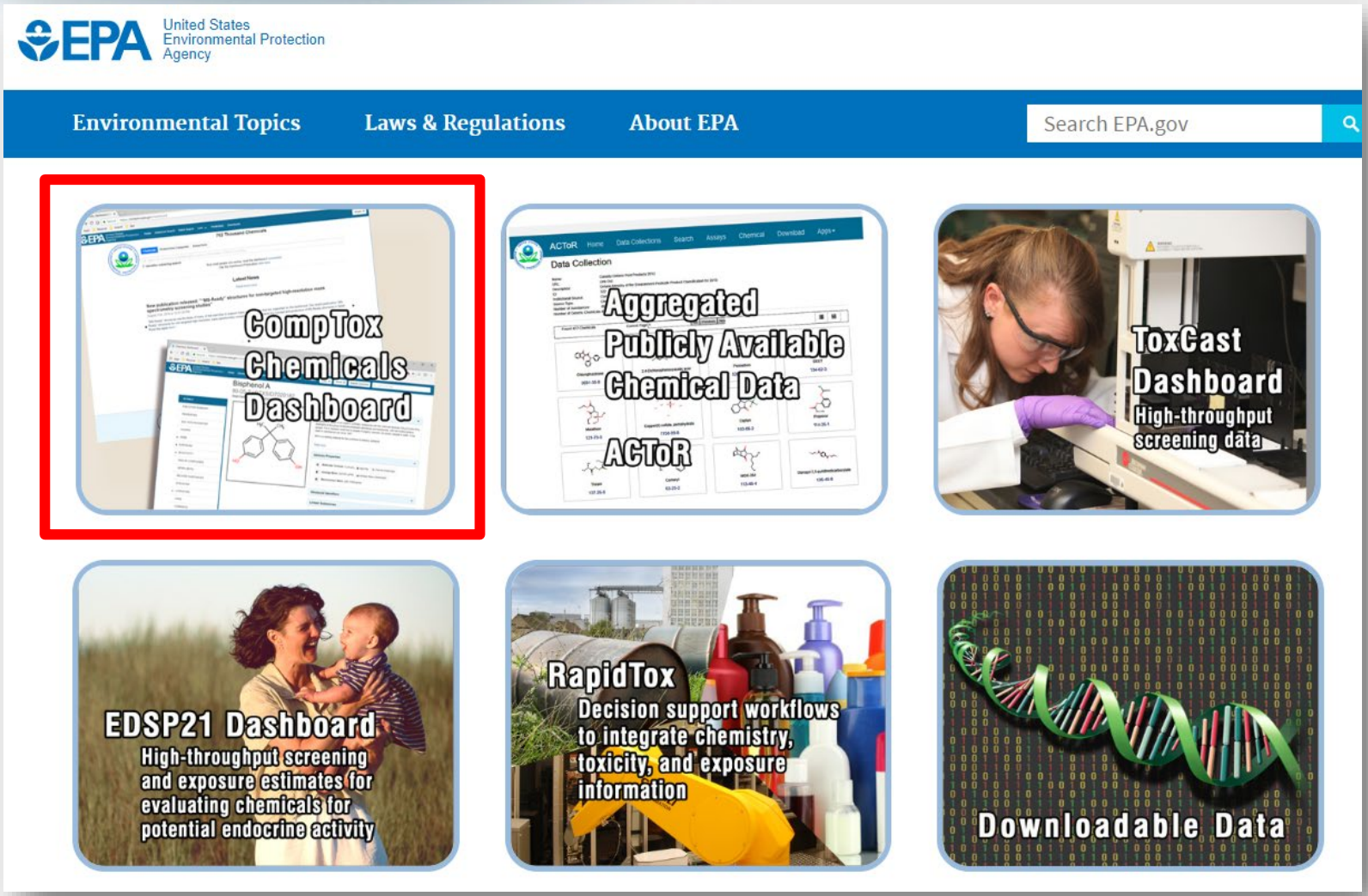
Cite this: *Org. Biomol. Chem.*, 2015, **13**, 9957

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…



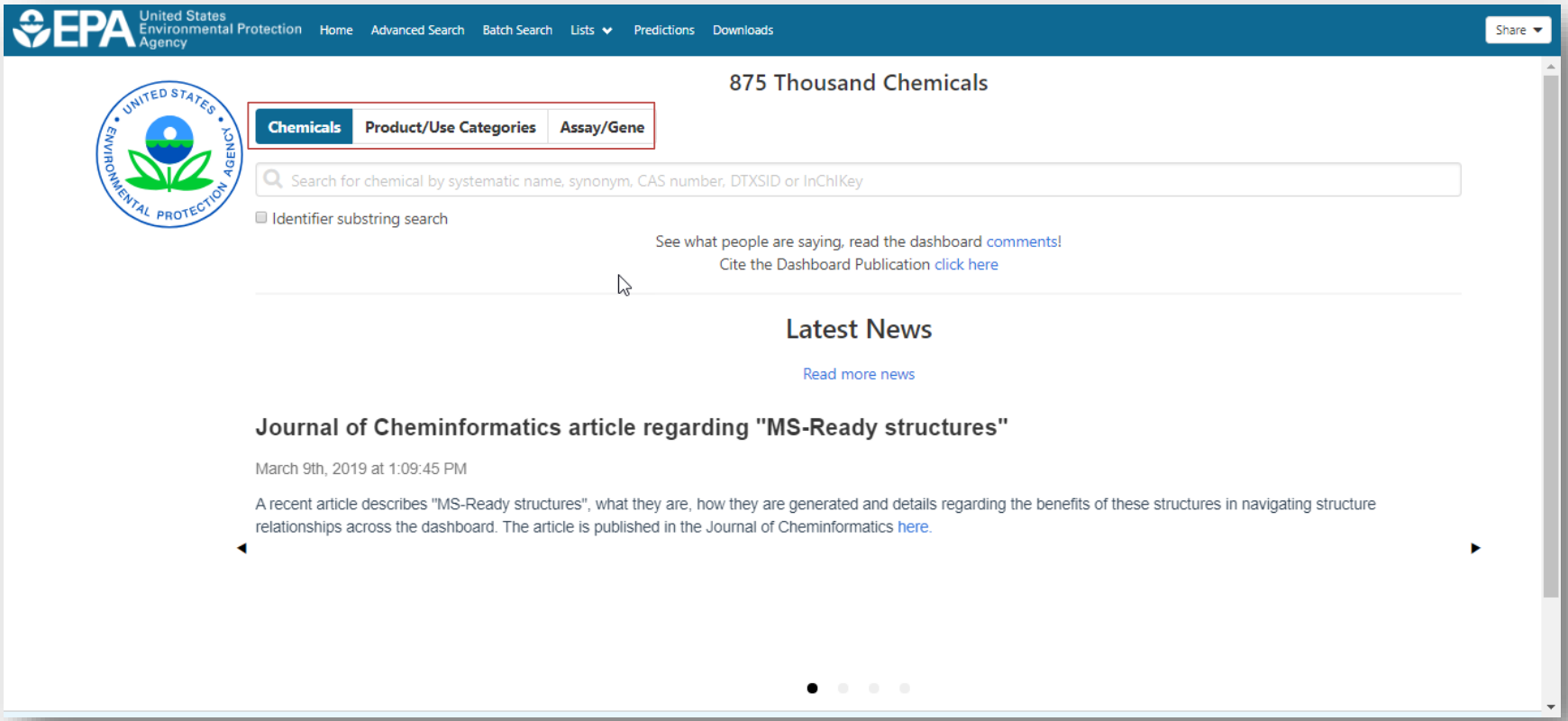
CompTox Chemicals Dashboard

- 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

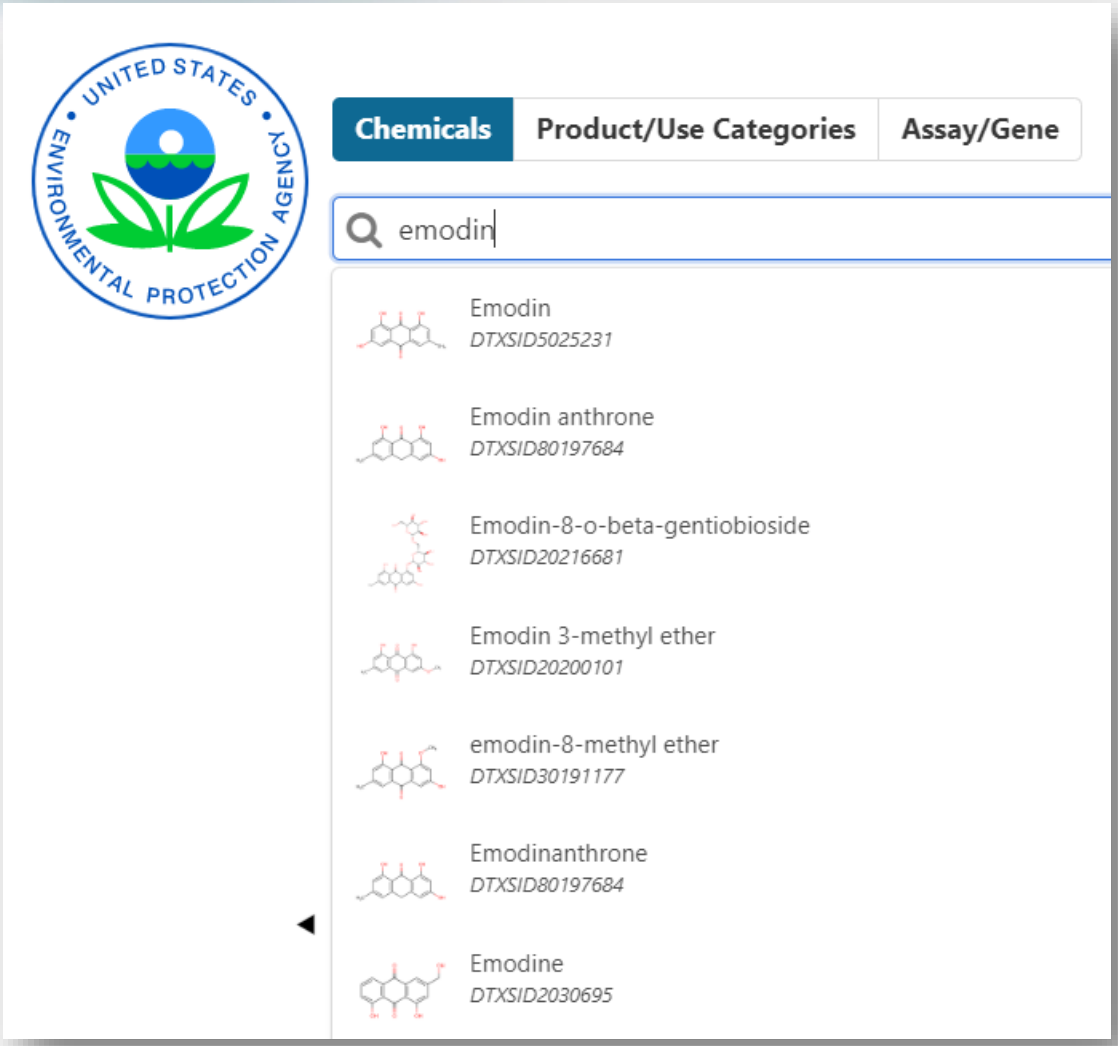
CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard

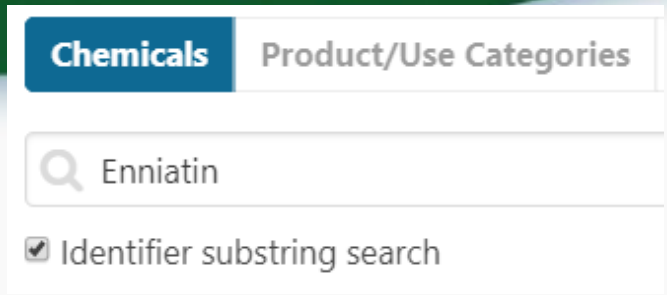
875k Chemical Substances



Type-ahead Search



Substring Search: Enniatin (10/29)

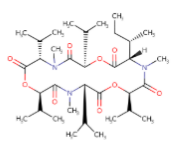


Search Results

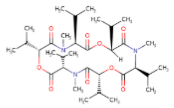
Searched with 'Synonym Substring': Enniatin

10 chemicals

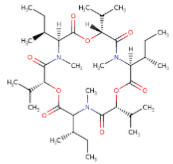
Select all | Download | Send to Batch Search | Substring | DTXSID | CASRN | TOXCAST | Hide chemicals that are: | Filter by Name or CASRN



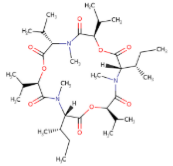
Enniatin B1
DTXSID:DTXSID70891861
CASRN:19914-20-6
TOXCAST:-



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



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



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CASRN:4530-21-6
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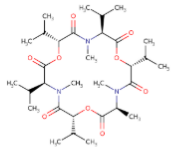
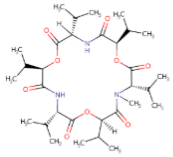
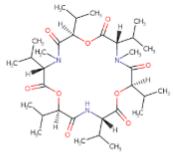


Enniatin J1
DTXSID:DTXSID701017631
CASRN:19893-15-3
TOXCAST:-



Enniatin B3
DTXSID:DTXSID401017632
CASRN:864-99-3
TOXCAST:-



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CASRN:632-91-7
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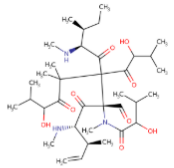

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CASRN:144446-20-8
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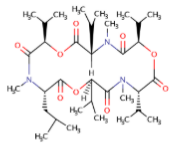

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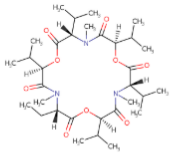
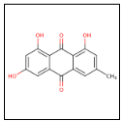


Enniatin K1
DTXSID:DTXSID801017977
CASRN:716318-00-2
TOXCAST:-

Chemical Details Page

EPA United States Environmental Protection Agency

Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data

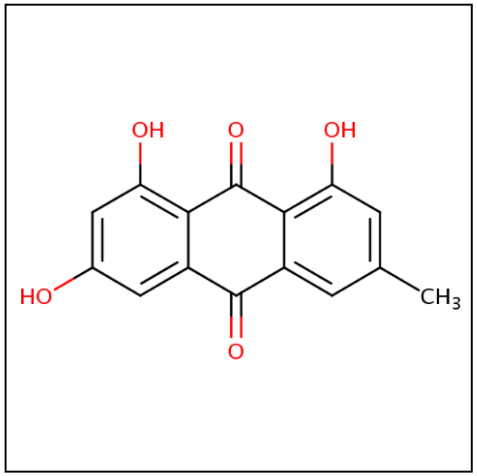


Emodin

518-82-1 | DTXSID5025231

Searched by DSSTox Substance Id.

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



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

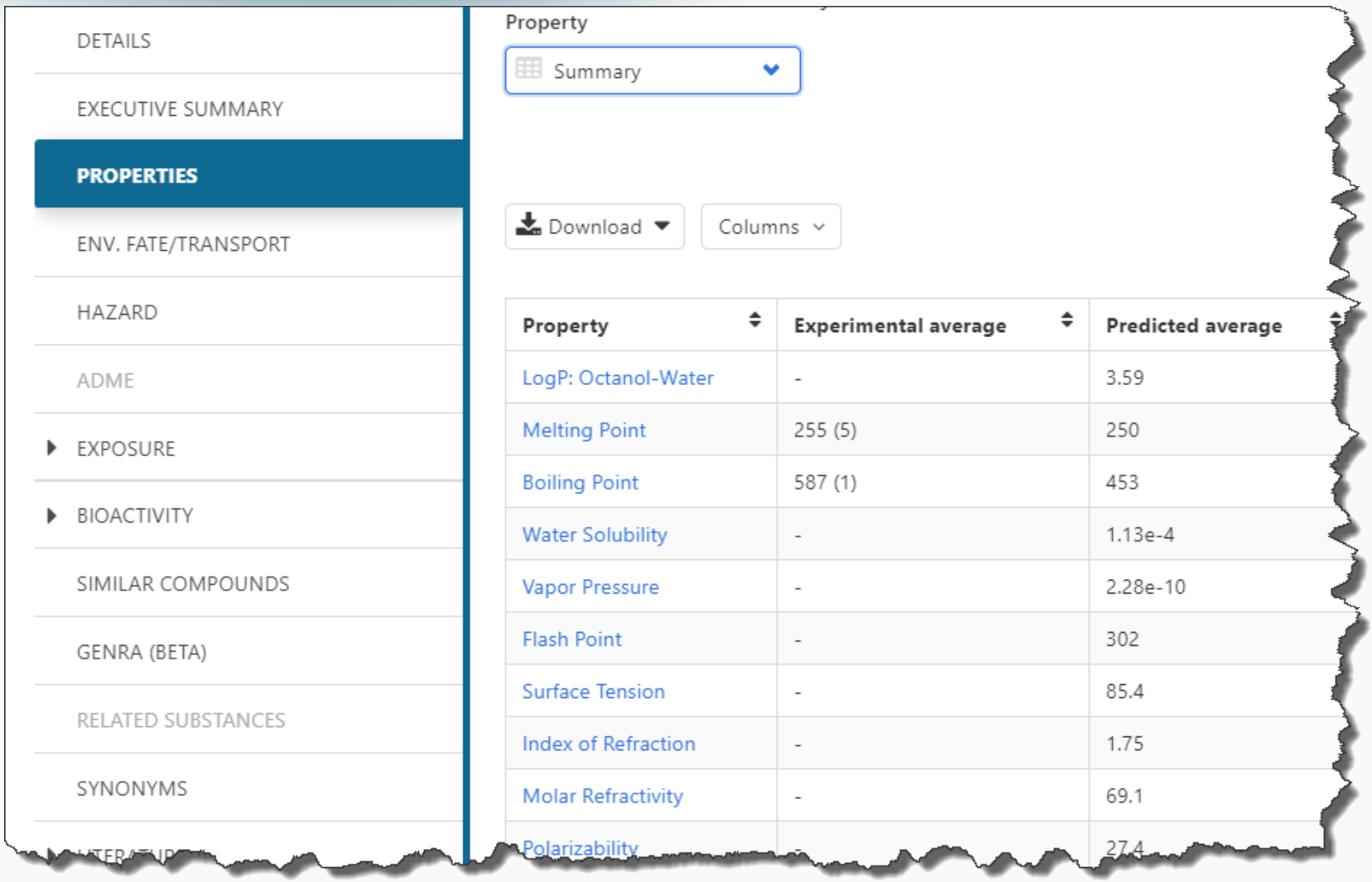
Structural Identifiers

Linked Substances

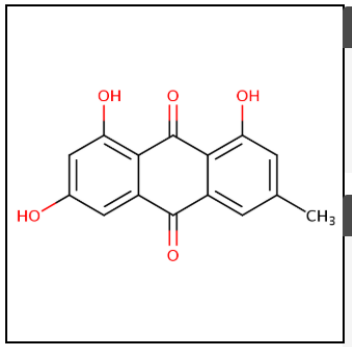
Presence in Lists

Record Information

Experimental & Predicted Properties



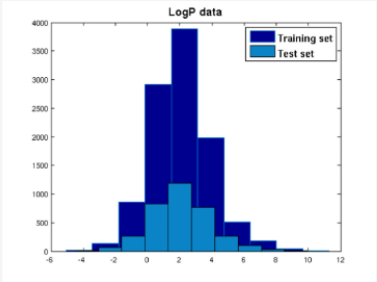
Open Source Prediction Models

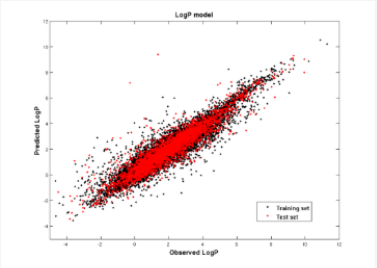


Model Results

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

Model Performance



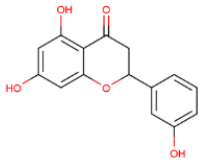


QMRF

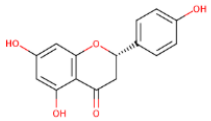
Weighted KNN model

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

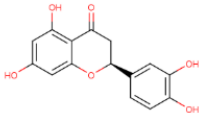
Nearest Neighbors from the Training Set



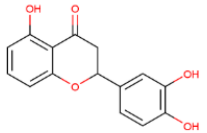
5,7-3'-Trihydroxyflavanone
Measured:2.61
Predicted: 2.59



Naringenin
Measured:2.52
Predicted: 2.62



ERIODICTYOL
Measured:2.02
Predicted: 1.90



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

OPERA Predicted Properties

EPA United States Environmental Protection Agency

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 m
DOI: 10.1080/1062936X.

To link to this article: h

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

Journal of Cheminformatics

RESEARCH ARTICLE Open Access

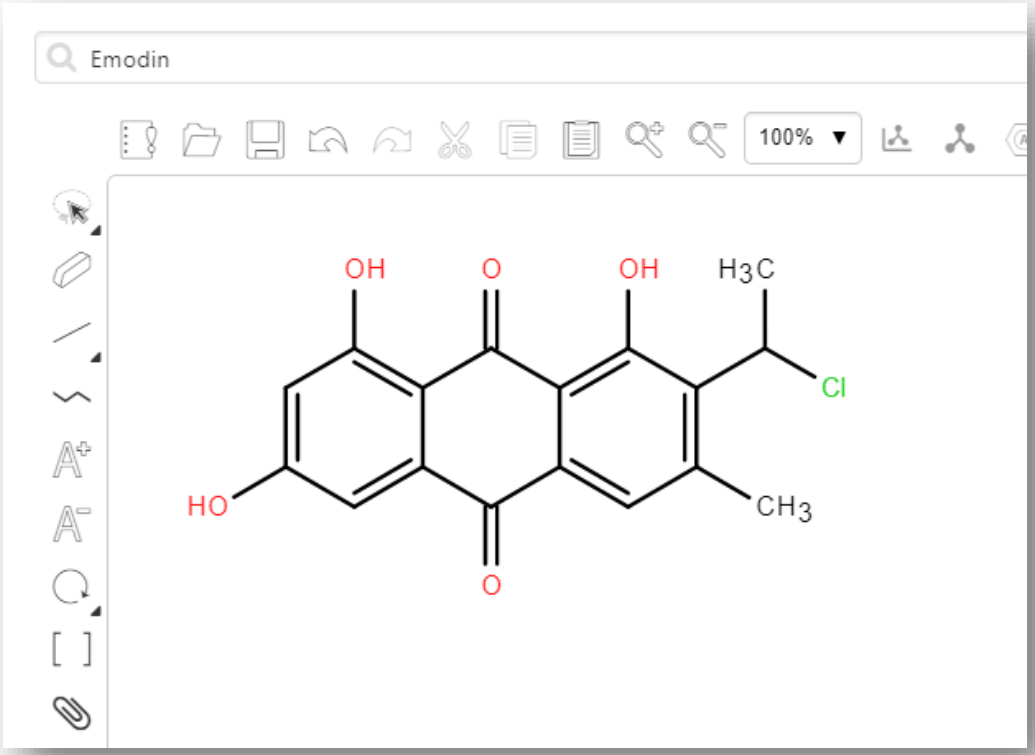
CrossMark

OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri[1,2,3*], Chris M. Grulke[1], Richard S. Judson[1] and Antony J. Williams[1]

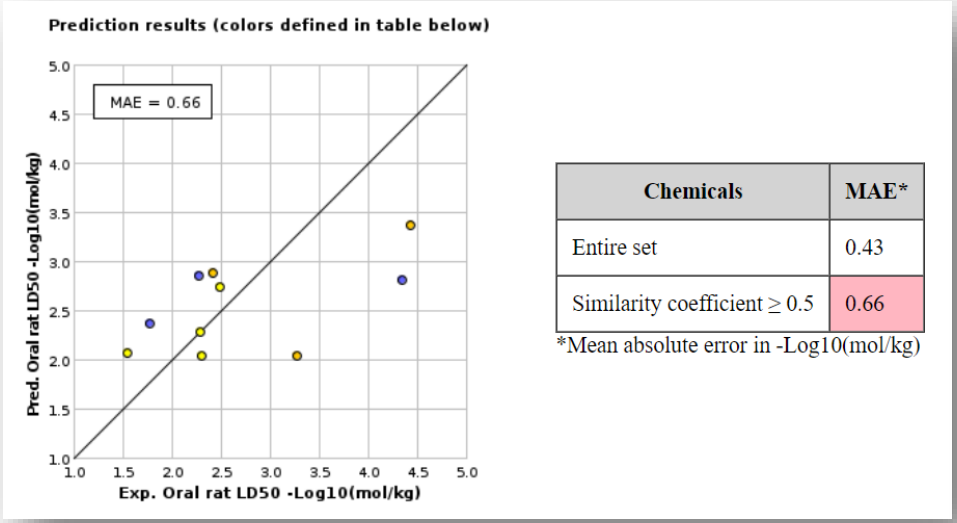
OPERA Models: https://github.com/kmansouri/OPERA

Plus Real-Time Predictions



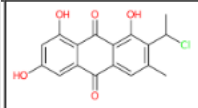
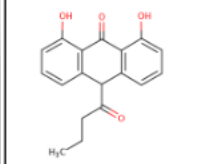
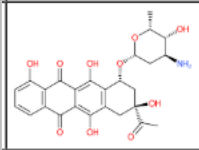
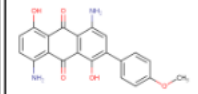
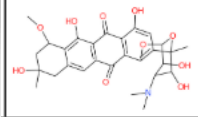
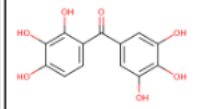
- [x] Toxicological properties
  - [x] 96 hour fathead minnow LC50
  - [x] 48 hour D. magna LC50
  - [x] 48 hour T. pyriformis IGC50
  - [x] Oral rat LD50
  - [x] Bioaccumulation factor
  - [x] Developmental toxicity
  - [x] Ames mutagenicity
  - [x] Estrogen Receptor RBA
  - [x] Estrogen Receptor Binding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

Toxicity Estimation Software Tool

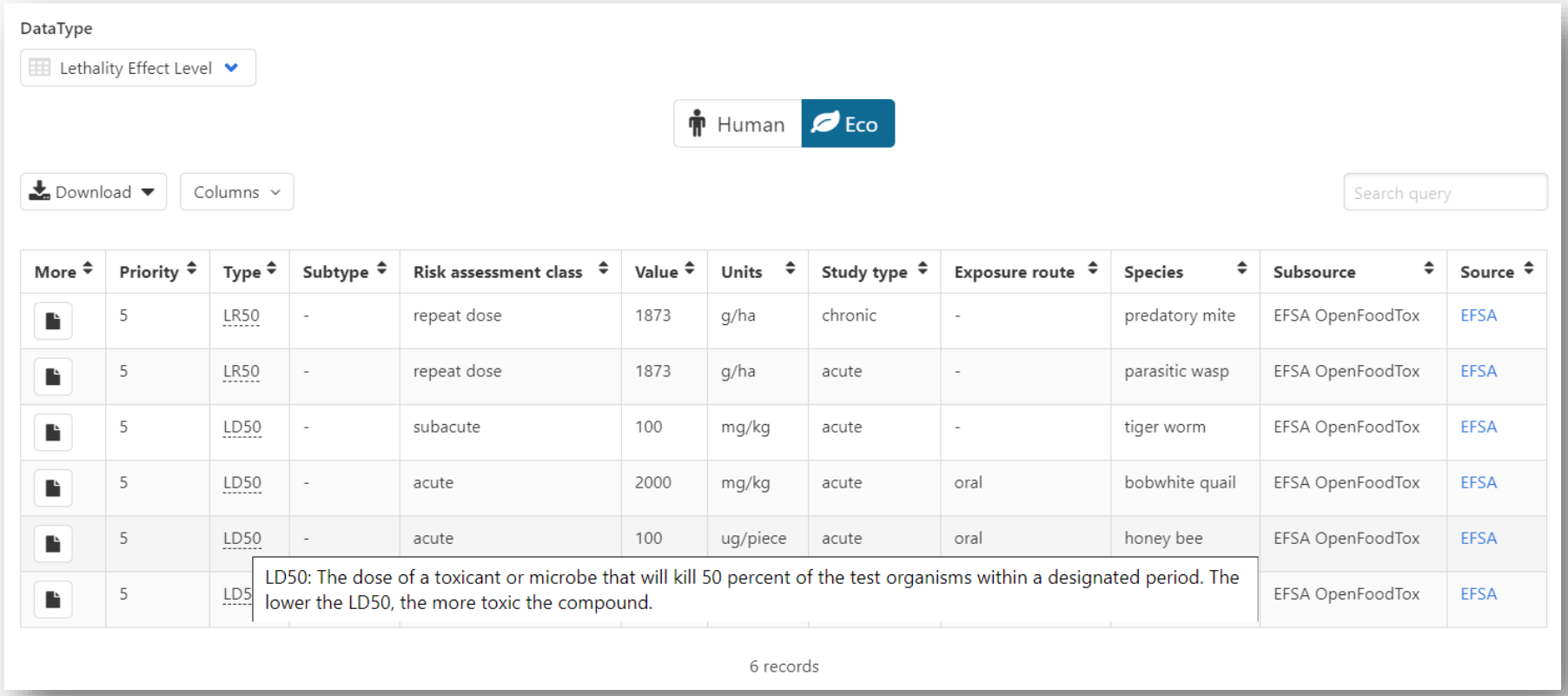


Chemicals	MAE*
Entire set	0.43
Similarity coefficient ≥ 0.5	0.66

*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



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	LD5								EFSA OpenFoodTox	EFSA

Hazard Data from “ToxVal_DB”

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

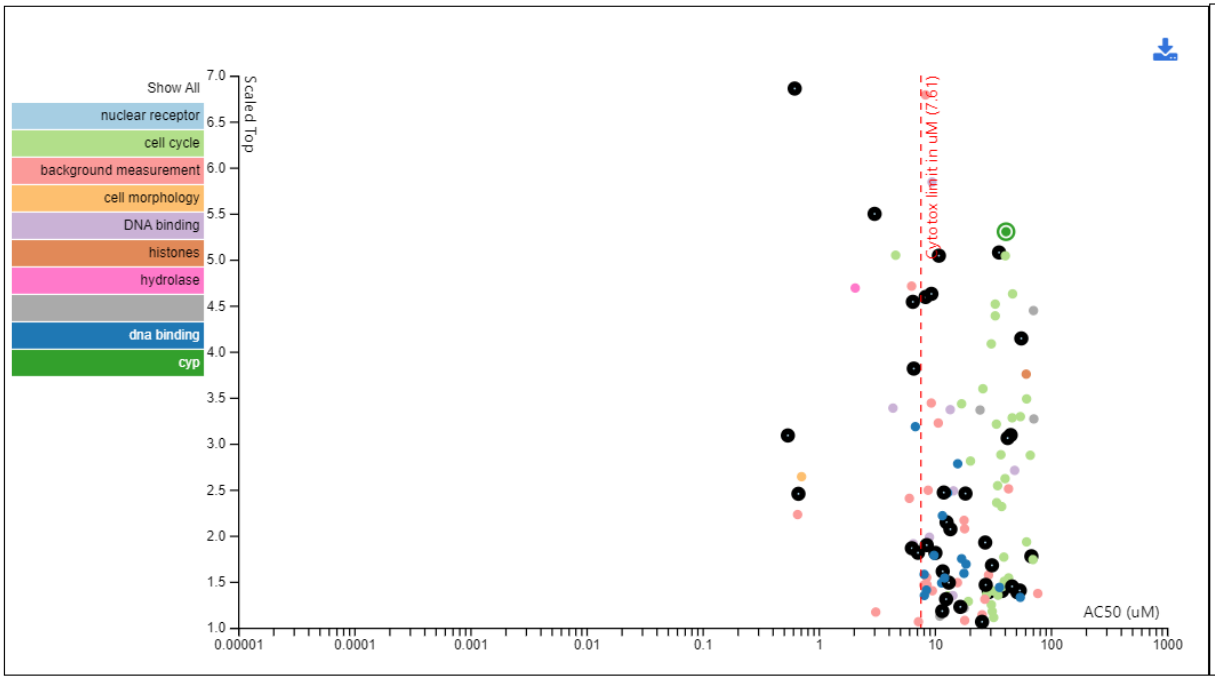
In Vitro Bioassay Screening

ToxCast and Tox21

EPA United States Environmental Protection Agency

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

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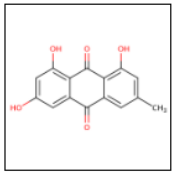
Name	Gene Name	Gene Url	Hit Call	AC50	logAC50	Cutoff	ModlAcb	Intended Target Family
ACEA_ER_80hr	estrogen receptor 1	https://www.ncbi.nlm.nih.gov/gene/2099	ACTIVE	0.544	-0.265	26.9	-0.387	nuclear receptor
ATG_ERE_CIS_up	estrogen receptor 1	https://www.ncbi.nlm.nih.gov/gene/2099	ACTIVE	0.623	-0.206	0.503	-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**
9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl-	*Good*
1,3,8-trihidroxi-6-metilantraquinona	*Good*
1,3,8-Trihydroxy-6-methyl-9,10-anthraquinone	*Good*
1,3,8-Trihydroxy-6-methylanthrachinon	*Good*
1,3,8-trihydroxy-6-methylanthraquinone	*Good*
1,6,8-Trihydroxy-3-methylanthraquinone	*Good*
3-Methyl-1,6,8-trihydroxyanthraquinone	*Good*
4,5,7-Trihydroxy-2-methylanthraquinone	*Good*
Anthraquinone, 1,3,8-trihydroxy-6-methyl-	*Good*
Frangula emodin	*Good*
Frangulic acid	*Good*
NSC 408120	*Good*

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

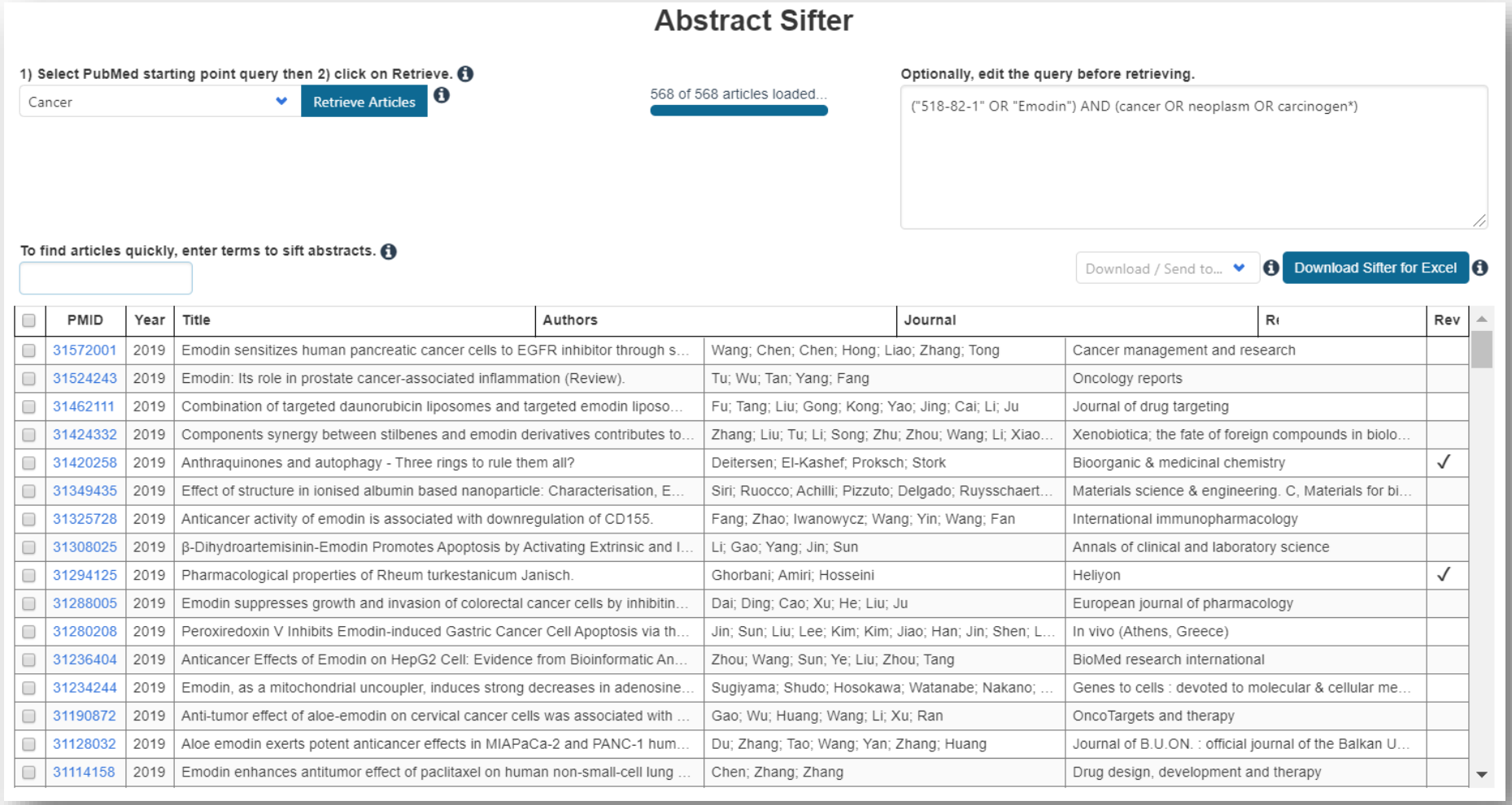
- Select a Query Term
- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Cancer
- Clinical Trials
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure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

Optionally, edit the query before retrieving.

"518-82-1" OR "Emodin"

Literature Searching

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*)

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PMID	Year	Title	Authors	Journal	Rev
31572001	2019	Emodin sensitizes human pancreatic cancer cells to EGFR inhibitor through s...	Wang; Chen; Chen; Hong; Liao; Zhang; Tong	Cancer management and research	
31524243	2019	Emodin: Its role in prostate cancer-associated inflammation (Review).	Tu; Wu; Tan; Yang; Fang	Oncology reports	
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	
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...	
31420258	2019	Anthraquinones and autophagy - Three rings to rule them all?	Deitersen; El-Kashef; Proksch; Stork	Bioorganic & medicinal chemistry	✓
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...	
31325728	2019	Anticancer activity of emodin is associated with downregulation of CD155.	Fang; Zhao; Iwanowycz; Wang; Yin; Wang; Fan	International immunopharmacology	
31308025	2019	β-Dihydroartemisinin-Emodin Promotes Apoptosis by Activating Extrinsic and I...	Li; Gao; Yang; Jin; Sun	Annals of clinical and laboratory science	
31294125	2019	Pharmacological properties of Rheum turkestanicum Janisch.	Ghorbani; Amiri; Hosseini	Heliyon	✓
31288005	2019	Emodin suppresses growth and invasion of colorectal cancer cells by inhibitin...	Dai; Ding; Cao; Xu; He; Liu; Ju	European journal of pharmacology	
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)	
31236404	2019	Anticancer Effects of Emodin on HepG2 Cell: Evidence from Bioinformatic An...	Zhou; Wang; Sun; Ye; Liu; Zhou; Tang	BioMed research international	
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...	
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	
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...	
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

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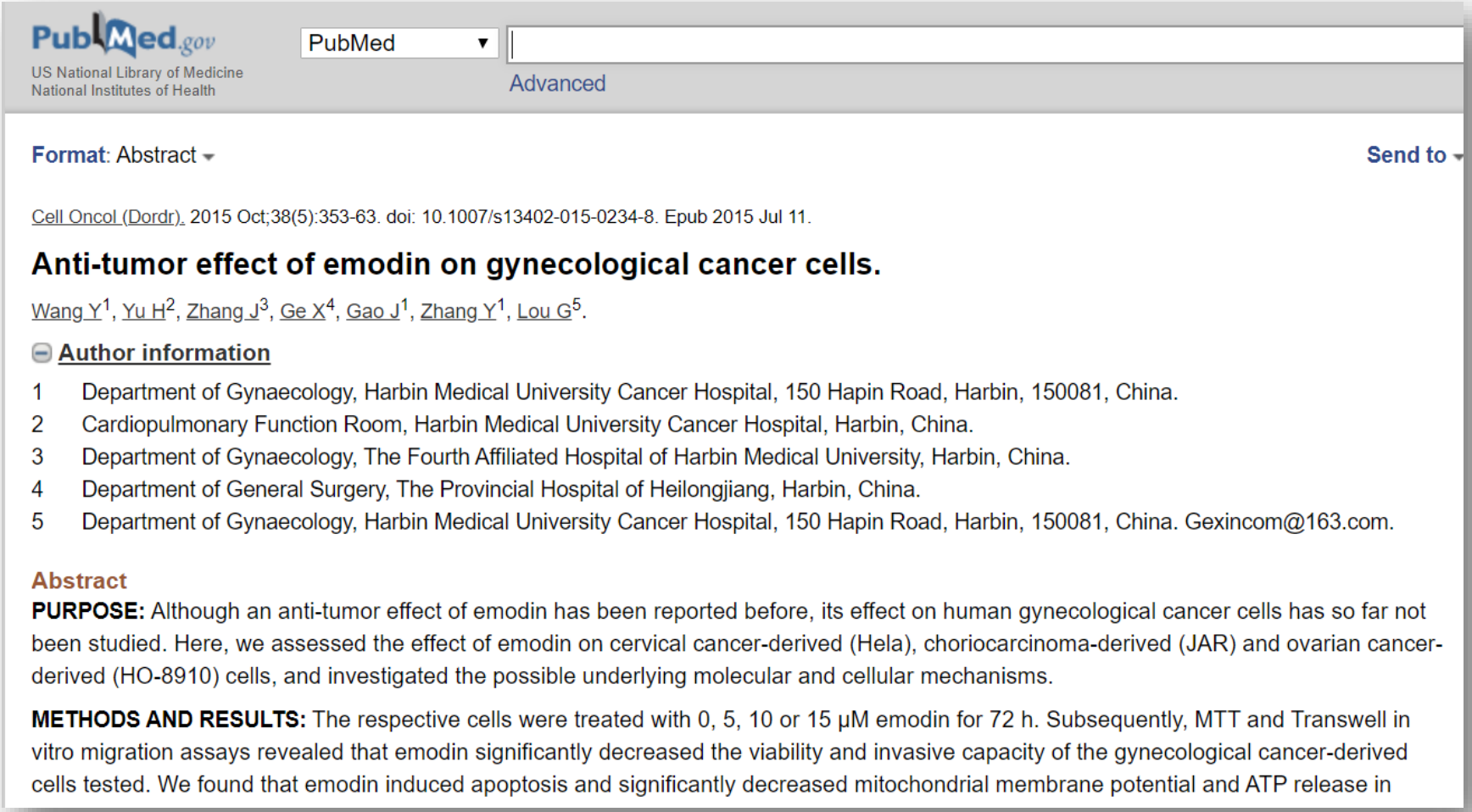
	emodin	anti-tumor	gynecol	Total	PMID	Year	Title	Authors	Journal	Rev
	7	4	0	11	22474959	2012	Synthesis and anti-tumor activity evaluation of rhein...	Yuan; Hu; He; Deng	Natural product communications	
	0	3	0	3	28922732	2017	Physcion 8-O-β-glucopyranosideregulates cell cycl...	Li; Li; Zhu; Song	Biomedicine & pharmacotherapy = Biomedecine & ...	
	0	3	0	3	28570979	2017	Physcion 8-O-β-glucopyranoside suppresses tumor...	Wang; Jiang; Guo; Lv; Liu; Wei; Ming; Tian	Biomedicine & pharmacotherapy = Biomedecine & ...	
	0	3	0	3	27694997	2016	Physcion, a naturally occurring anthraquinone deriv...	Pang; Yang; Zhang; Liu; Fan; Zhang	Acta pharmacologica Sinica	
	13	3	6	22	26162964	2015	Anti-tumor effect of emodin on gynecological cance...	Wang; Yu; Zhang; Ge; Gao; Zhang; Lou	Cellular oncology (Dordrecht)	
	0	2	0	2	29758413	2018	Physcion 8-O-β-glucopyranoside inhibits clear-cell f...	Wang; Yan; Zhang; Guo; Xing; Wang; Qin; Zeng	Biomedicine & pharmacotherapy = Biomedecine & ...	
	3	2	0	5	27062805	2016	[Research progress in anti-tumor effect of emodin].	Lin; Wang; Ling	Zhongguo Zhong yao za zhi = Zhongguo zhongyao...	✓
	0	2	0	2	26144377	2015	Physcion induces mitochondria-driven apoptosis in ...	Chen; Gao; Han; Ye; Xie; Wang	European journal of pharmacology	
	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	
	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	
	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	
	6	1	0	7	30832378	2019	Design and Synthesis of Novel Anti-Proliferative E...	Yang; Jin; Quan; Piao	Molecules (Basel, Switzerland)	
	8	1	0	9	30648710	2019	Magnetic liposomal emodin composite with enhanc...	Song; Sheng; Xu; Dong; Xu; Li; Wang; Wu; Yang; S...	Biomaterials science	
	2	1	0	3	30199885	2018	Aloe-Emodin Induces Endoplasmic Reticulum Stres...	Cheng; Dong	Medical science monitor : international medical jour...	
	0	1	0	1	28810515	2017	Physcion blocks cell cycle and induces apoptosis in...	Gao; Liu; Guo; Bai; Yang; Chen	Biomedicine & pharmacotherapy = Biomedecine & ...	
	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.

Direct Link to PubMed



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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[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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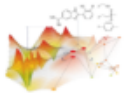
Nancy Baker [1], Thomas Knudsen[2], Antony Williams [2]

Author details



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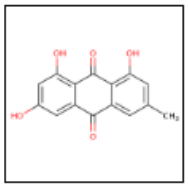
Mapped Relationships

Relationships in the Data
All chemicals: Same Formula



Emodin

518-82-1 | DTXSID5025231

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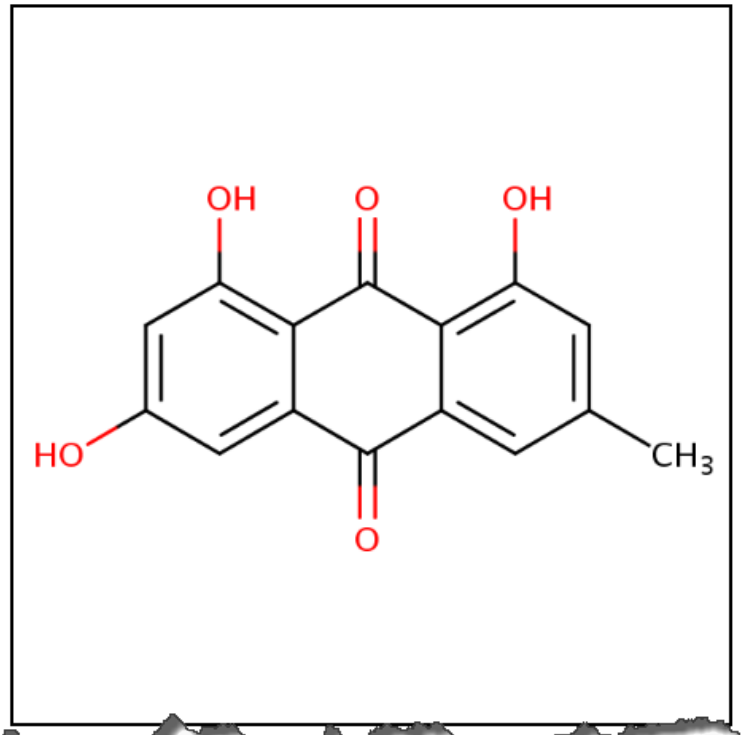


Wikipedia

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

Read more

Quality Control Notes

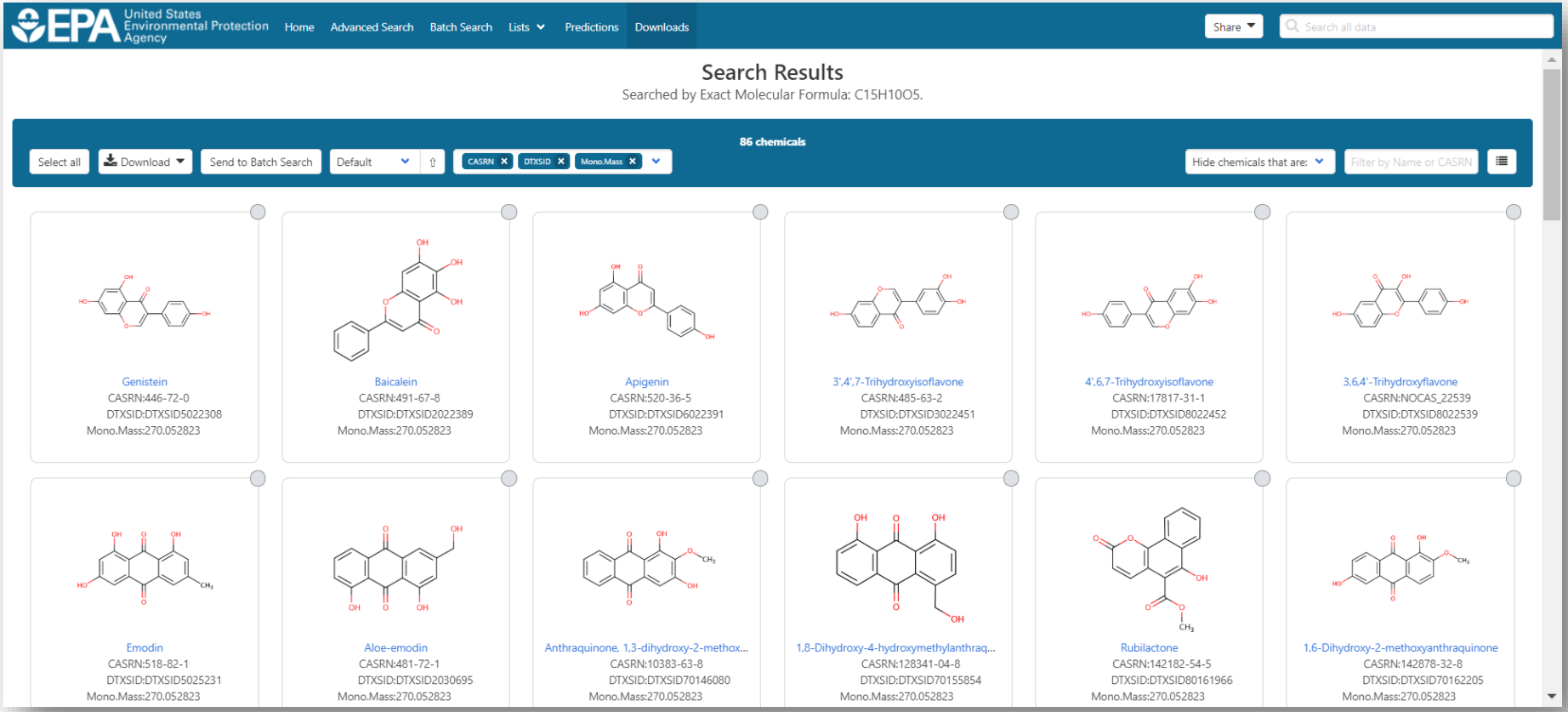
Intrinsic Properties

Molecular Formula: $C_{15}H_{10}O_5$ | 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



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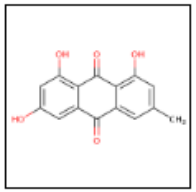

Emodin

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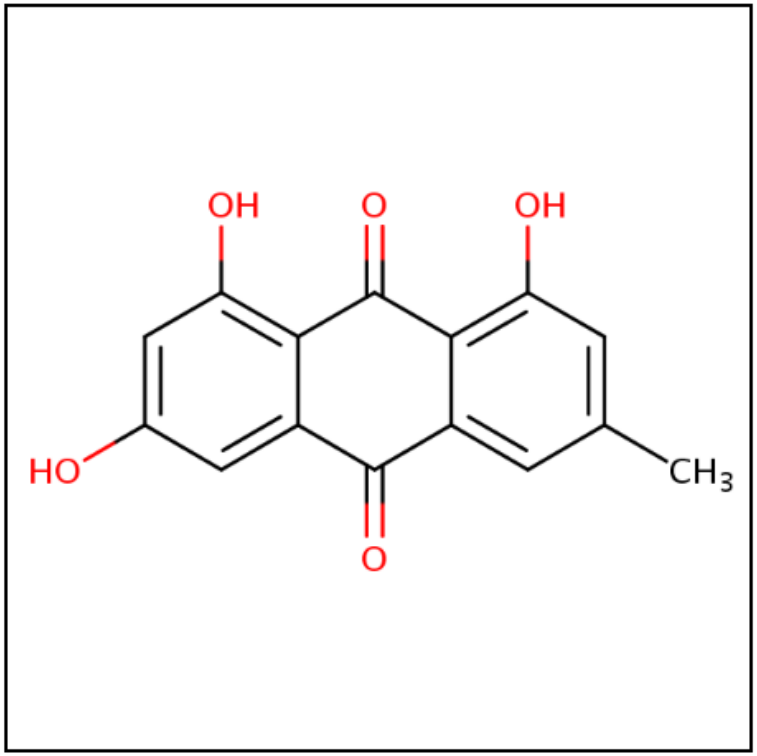

Wikipedia

Quality Control Notes

Intrinsic Properties

Structural Identifiers

IUPAC Name: 1,3,8-Trihydroxy-6-methylanthracene-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

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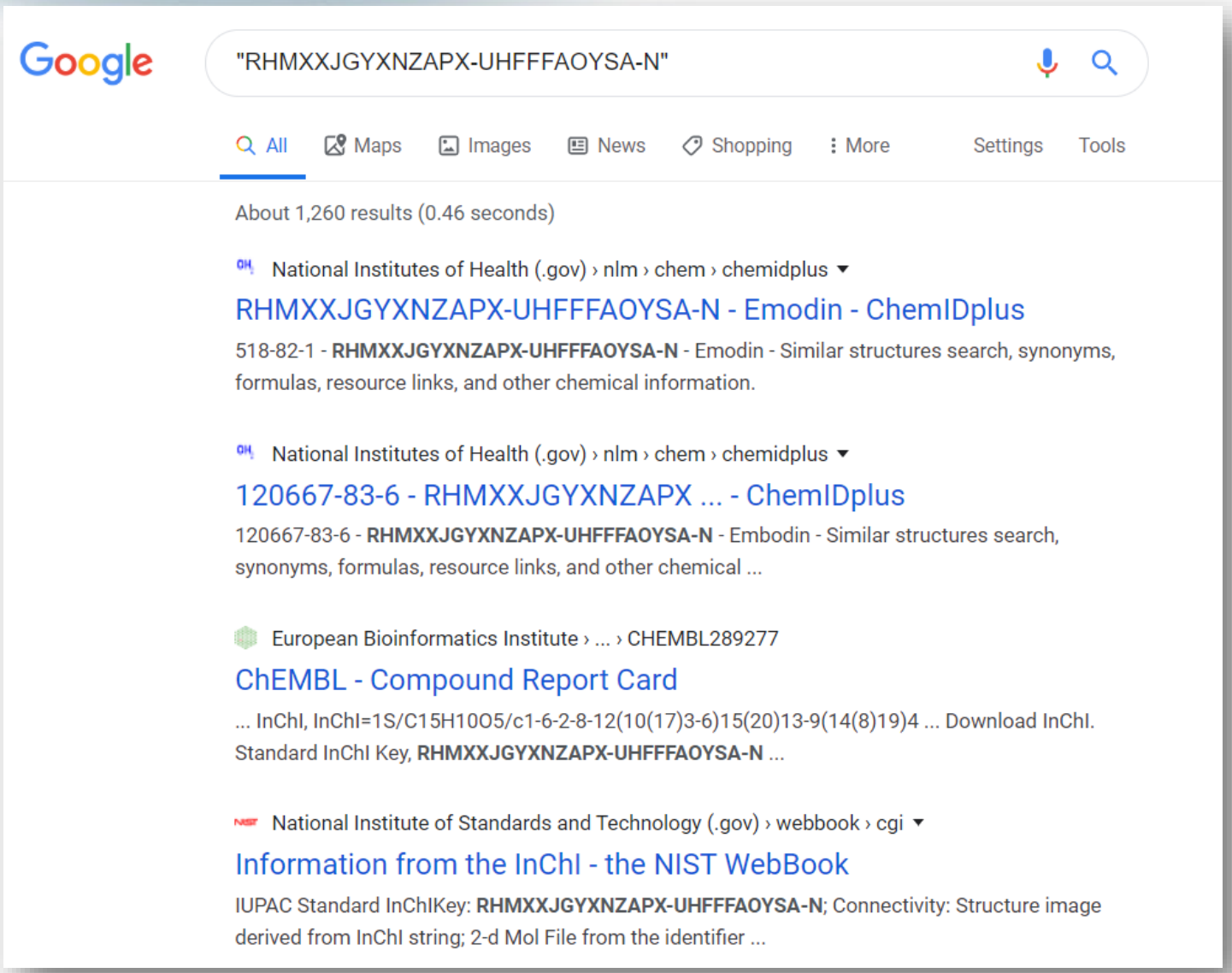
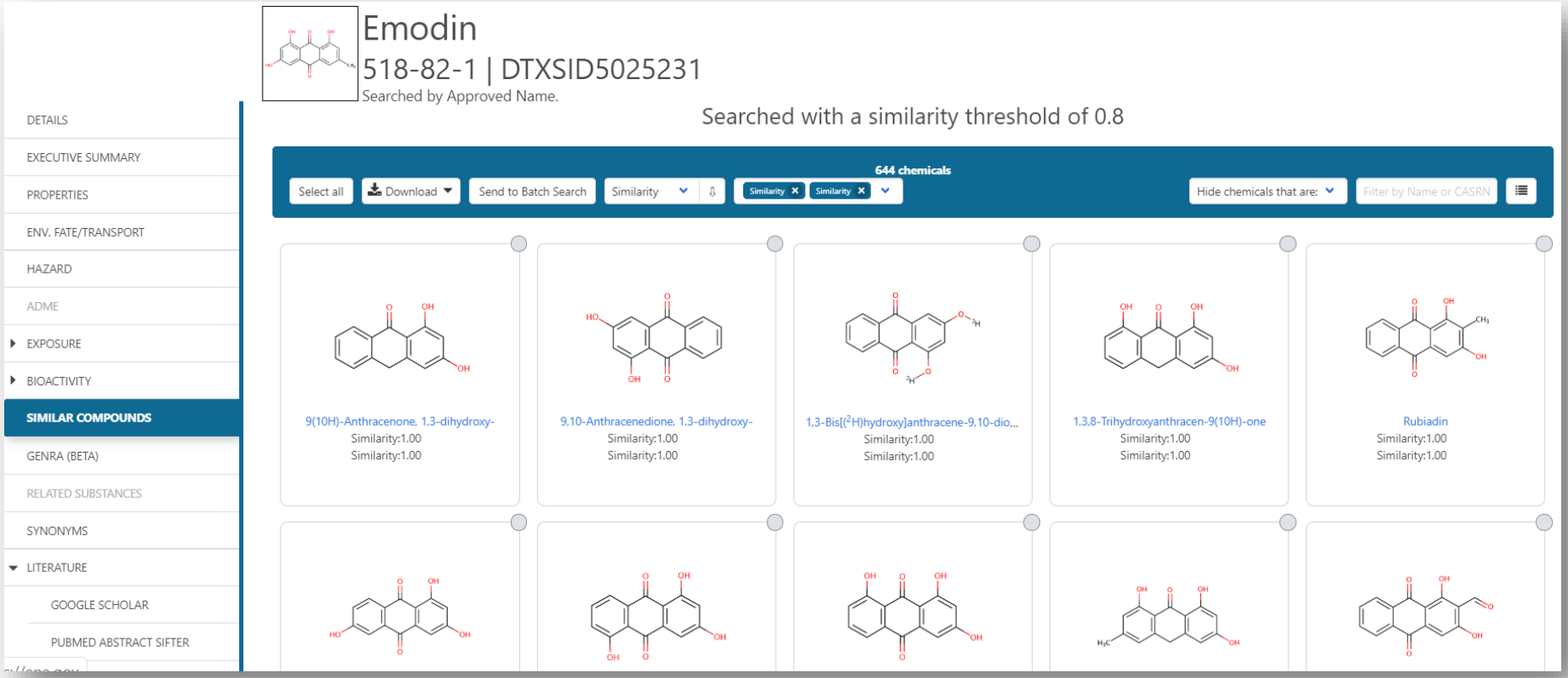
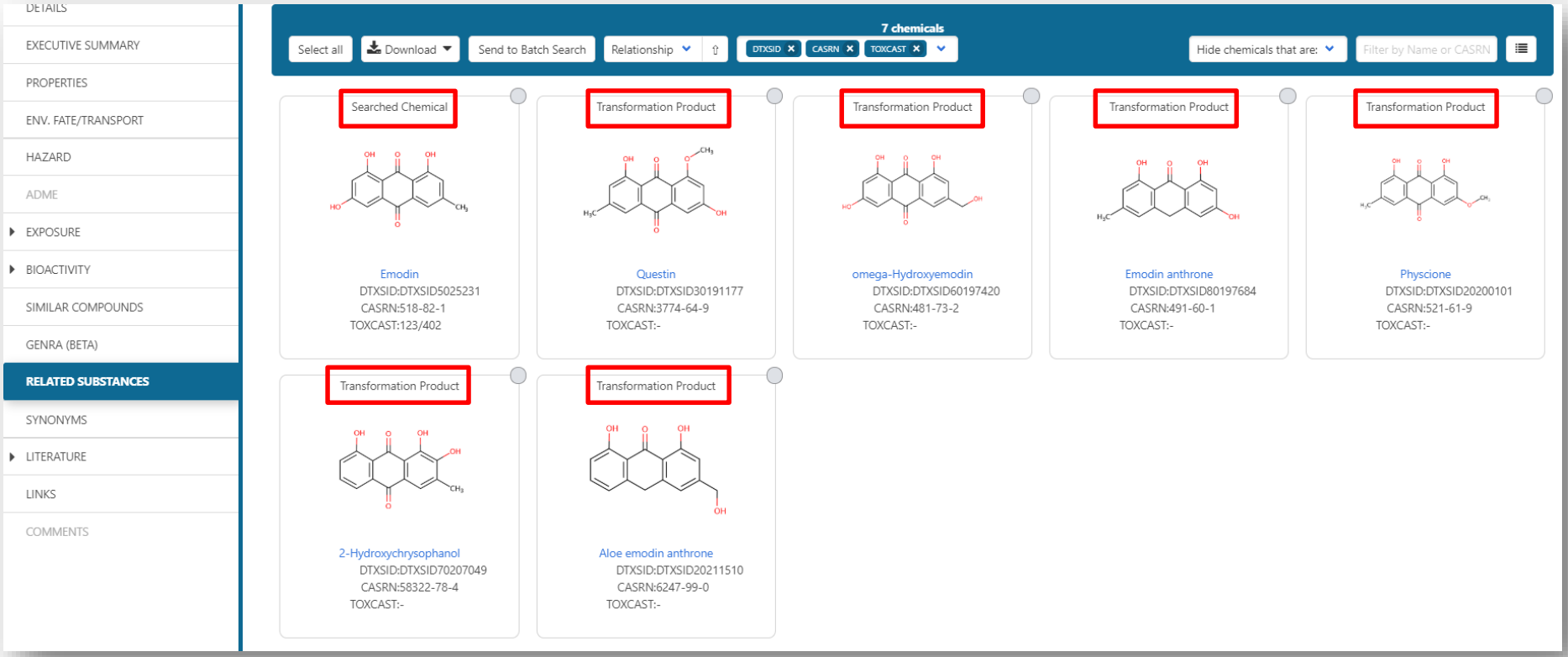
Structure search the web



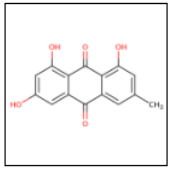
Similar Compounds



Related Substances – Metabolites and Transformation Products



“External Links” to >70 sites



Emodin

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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 IR Spectrum
- NIST MS Spectrum
- MassBank
- NEMI: National Environmental Methods Index
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values

Prediction

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

External Links: CTD

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Comparative Toxicogenomics Database

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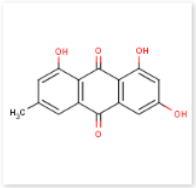
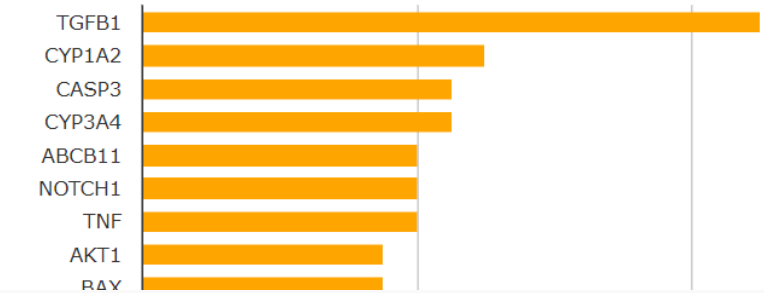
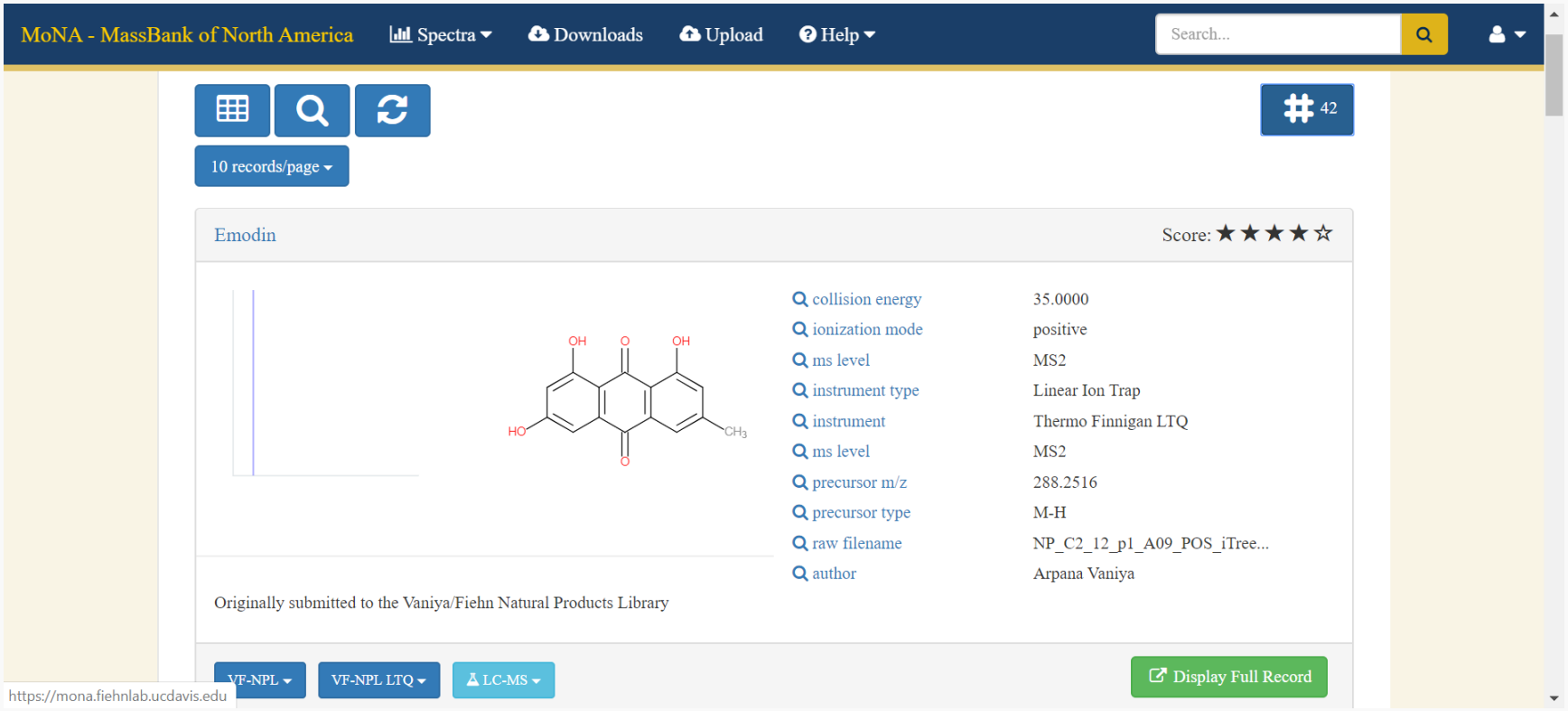
Emodin

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 Emodir
CAS Registry Number	518-82-1
CTD-Curated Synonym	Aloe-emodin
Definition	Purgative anthraquinone found in several plants, especially Rhamnus frangula. It was formerly u in toxicity studies.
Structure	
Top Interacting Genes	

External Links: MassBank of North America



EPA United States Environmental Protection Agency

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>200 Lists of Chemicals

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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

EPA United States Environmental Protection Agency

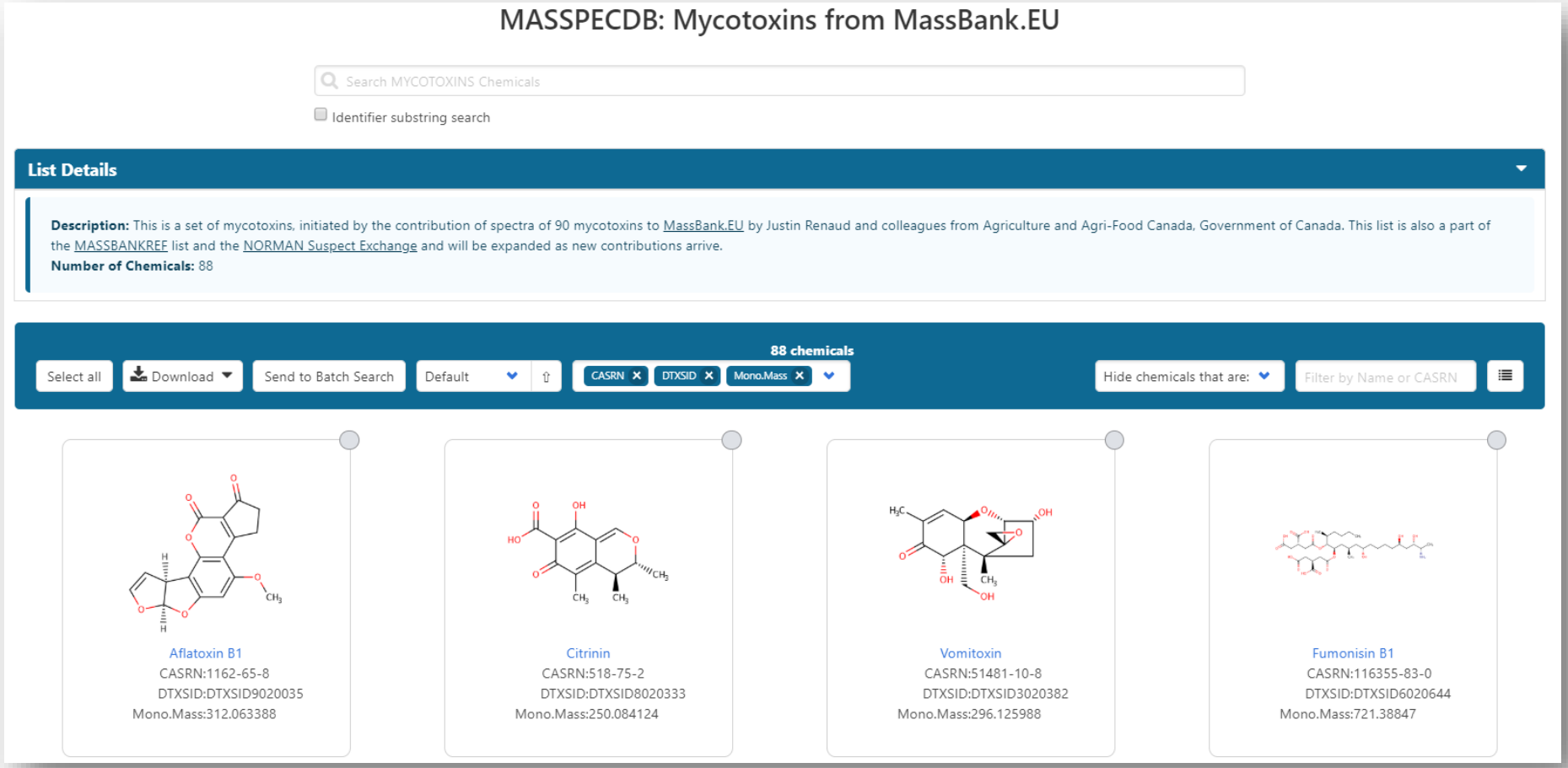
Select List

Download | Columns | toxins | Copy Filtered Lists URL

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



EPA Algal Toxins

https://www.epa.gov/cyanohabs

EPA United States Environmental Protection Agency

Environmental Topics | Laws & Regulations | About EPA | Search EPA.gov

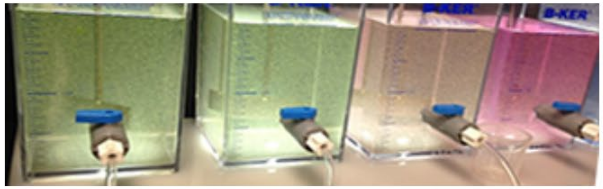
Basic Information about

Managing Cyanotoxins in Public Drinking Water

Monitoring and Analysis

- Determination of Cyanotoxins in Drinking and Ambient Freshwaters
- Laboratories that Analyze for Cyanobacteria and Cyanotoxins
- State HABs Monitoring Programs

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

Algal Toxins

EPA United States Environmental Protection Agency

LIST: Algal Toxins

Search ALGALTOX Chemicals

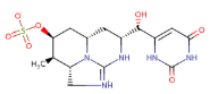
Identifier substring search

List Details

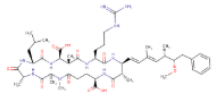
Description: Algal toxins do not enter the marine environment from an external source but are generated during blooms of particular naturally occurring marine algal species. Such blooms have been referred to as toxic algal blooms, harmful algal blooms (HABs) and red tides. The occurrence of blooms of 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

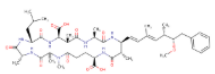
Select all | Download | Send to Batch Search | Default | CASRN | DTXSID | Mono.Mass | Hide chemicals that are: | Filter by Name or CASRN



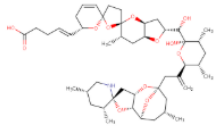
Cylindrospermopsin
CASRN:143545-90-8
DTXSID:DTXSID2031083
Mono.Mass:415.116169



Microcystin LR
CASRN:101043-37-2
DTXSID:DTXSID3031654
Mono.Mass:994.548768

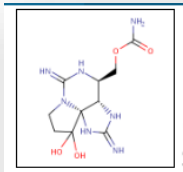


Microcystin LA
CASRN:96180-79-9
DTXSID:DTXSID3031656
Mono.Mass:909.484771



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

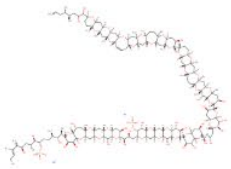
Toxicity Value

Human | Eco

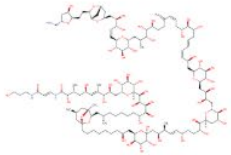
Download | Columns | Search query

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

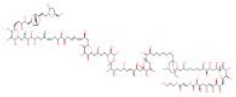
And who wants to draw these?



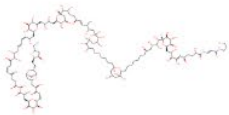
Maitotoxin
CASRN:59392-53-9
DTXSID:DTXSID10880012
Mono.Mass:3423.581083



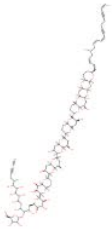
palytoxin
CASRN:77734-91-9
DTXSID:DTXSID90423027
Mono.Mass:2678.479594



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

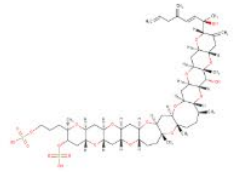


ostreocin-D
CASRN:163648-25-7
DTXSID:DTXSID50880112
Mono.Mass:2634.453379

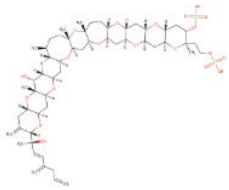


Prymnesin-2
CASRN:168010-52-4
DTXSID:DTXSID10880113
Mono.Mass:1967.795848

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…

DO WE REALLY NEED ANOTHER DATABASE?

Data Quality is important

- Data quality in free web-based databases!

Will the correct Microcystin LR Stand Up? ChemSpider Skeleton Search

EPA United States Environmental Protection Agency

Matches any text strings used to describe a molecule.

ZYZCGGRZINLQBL

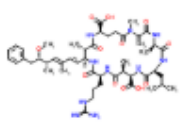
Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID

FILTER

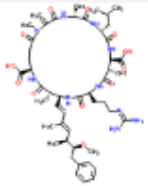
Search Hits Limit: 100

Found 9 results

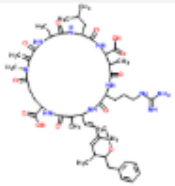
Search term: **ZYZCGGRZINLQBL** (Found by InChIKey (skeleton match))



Cyanoginosin

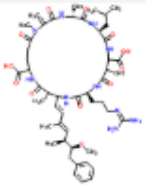


MCYST-LR

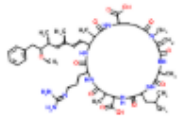


15-(3-Carbamimidamidopropyl)-8-isobutyl-18-[(1E,3E)-6-methoxy-3,5-dimethyl-7-phenyl-1,3-heptadien-1-

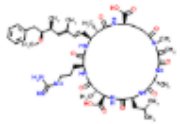
(5R,8S,11R,12S,15S,18R,19S,22R)-15-(3-Carbamimidamidopropyl)-8-isobutyl-18-[(1E,3E,5S,6S)-6-methoxy-3,5-



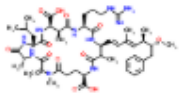
(5R,8S,15S)-15-{3-[(Diaminomethylene)amino]propyl}-8-isobutyl-18-[(1E,3E,5S,6S)-6-methoxy-



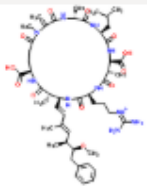
15-{3-[(Diaminomethylene)amino]propyl}-8-isobutyl-18-(6-methoxy-3,5-dimethyl-7-



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

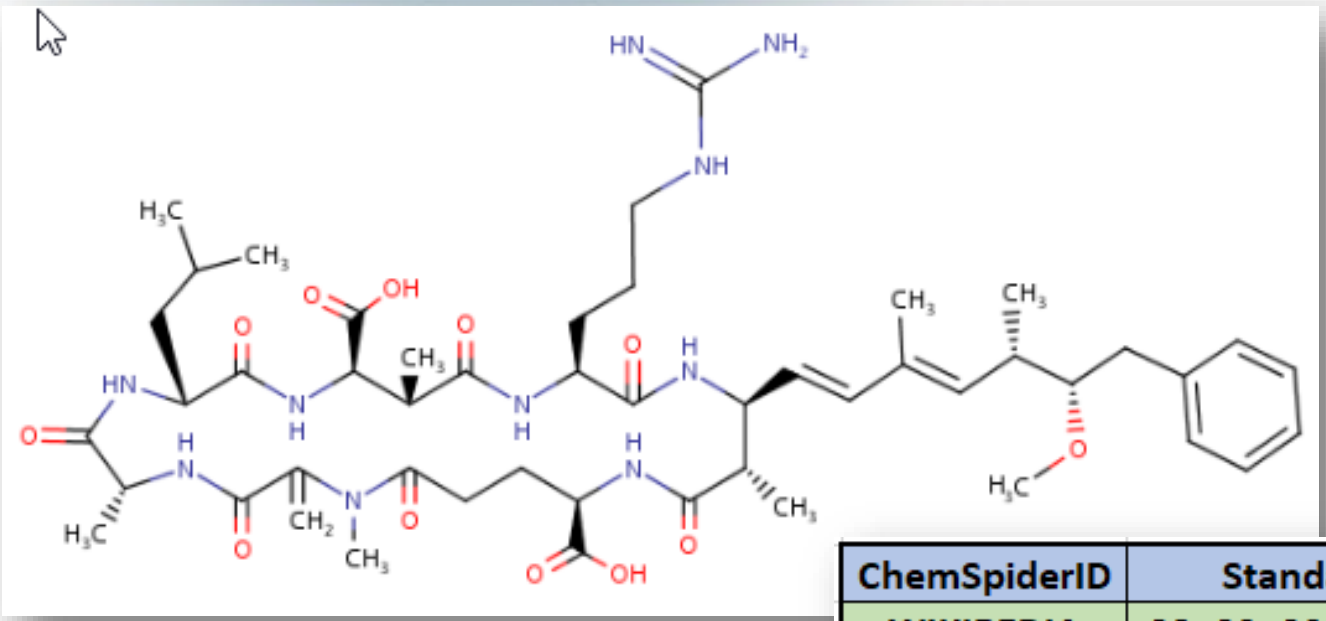


(5R,8R,11R,12S,15S,18S,22R)-15-(3-Carbamimidamidopropyl)-8-isobutyl-18-[(1E,3E,5R,6R)-6-methoxy-3,5-dimethyl-



Diamino-N-(3-{(5R,8S,11R,12S,15S,18S,19S,22R)-11,22-dicarboxy-8-isobutyl-18-

Comparing ChemSpider Structures

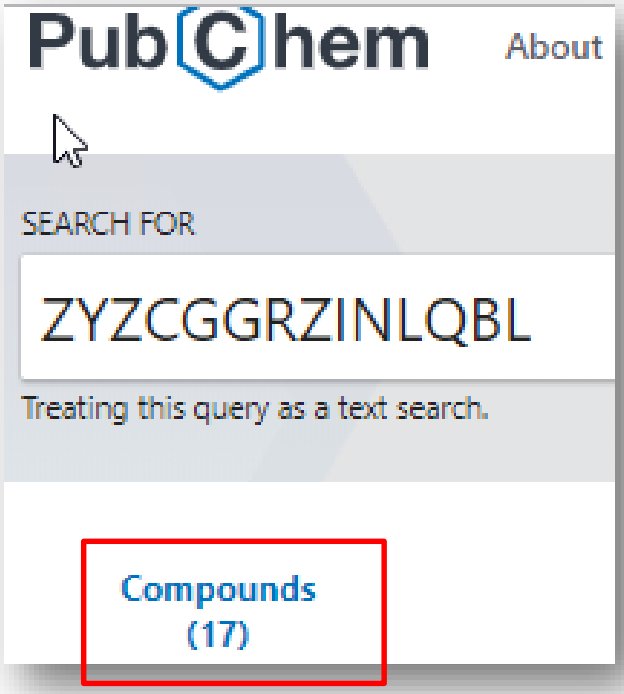


ChemSpiderID	Standard InChIKey Stereolayer
WIKIPEDIA	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
CompTox	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
4941647	t28-,29-,30-,31+,34-,35-,36+,37+,38-,40+
393078	t28-,29-,30-,31+,34-,35-,36+,**37-**,38-,40+
57618348	t28-,29-,30-,31+,34-,35-,36+,**37-**,38-,40+
29342071	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



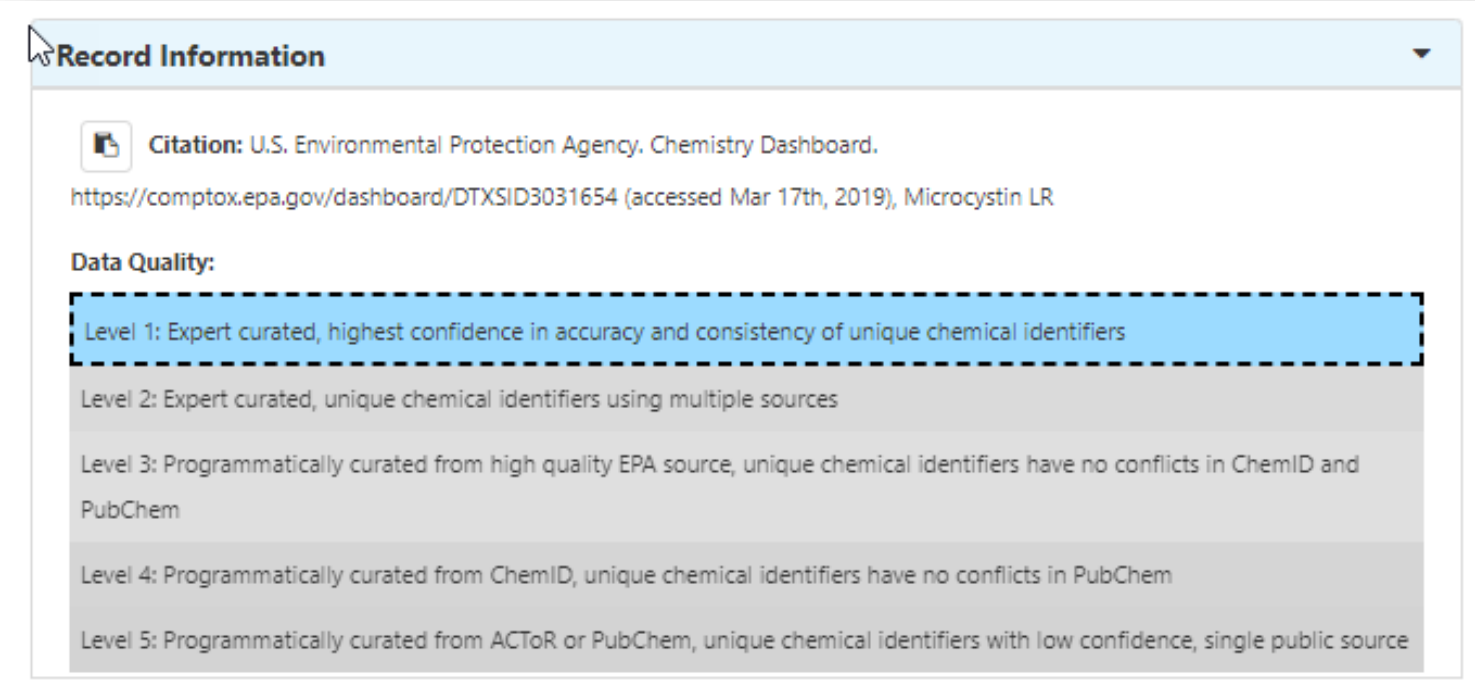
UniChem

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

Delivering a Better Database

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



Names to CASRN Mappings

EPA United States Environmental Protection Agency

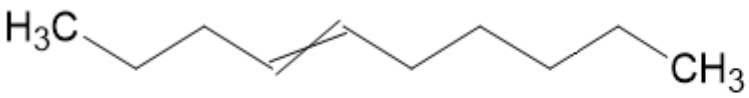
Substance Mapping

(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

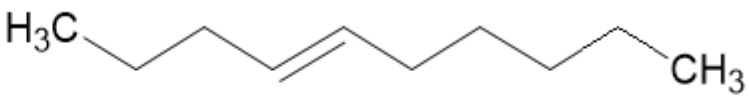
Subtleties

“4-Decene”



19398-89-1

E/Z-stereochemistry



19689-18-0

E-stereochemistry

Crowdsourced Curation

EPA United States Environmental Protection Agency

Submit Comment

New Comment

Comment

Describe the issue you're seeing here...

Email address

Enter email addr

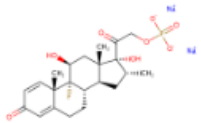
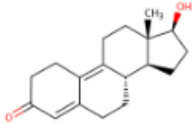
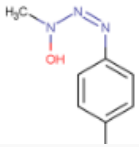
I'm not

Submit

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-Dehydro-19-nortestosterone (or alternative). See https://pubchem.ncbi.nlm.nih.gov/compound/11747706	★
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)	★

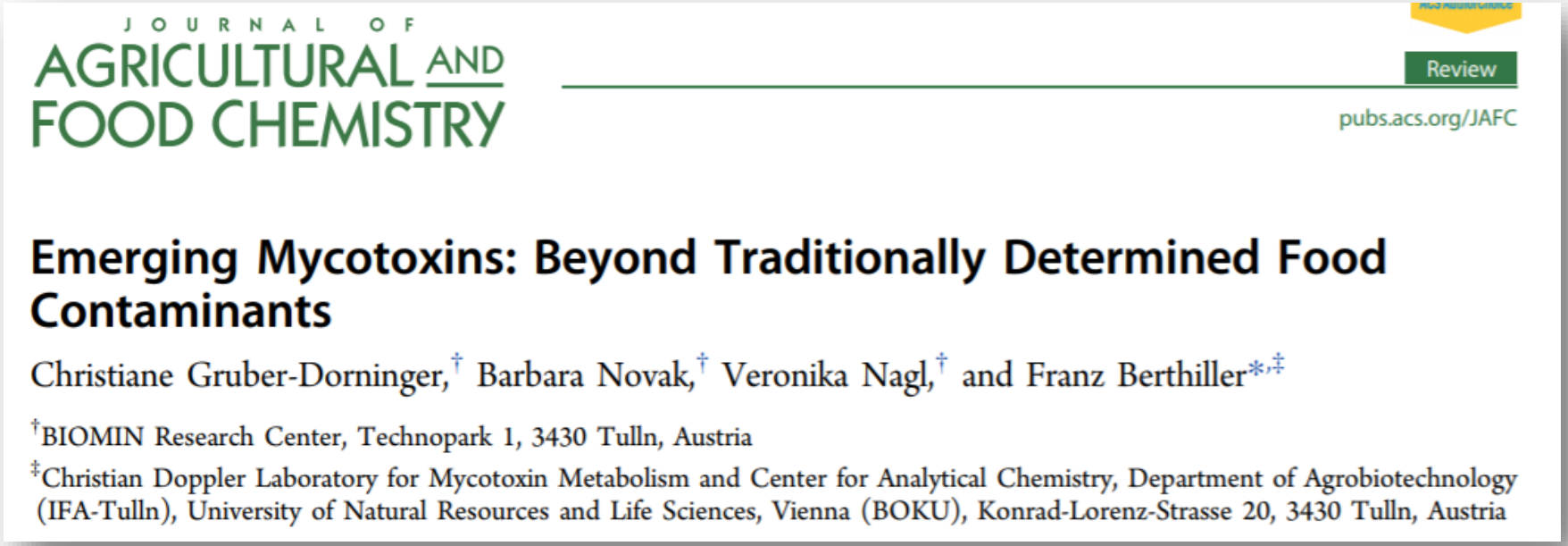
Batch Searching

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?

Batch searching



JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

Review

pubs.acs.org/JAFC

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

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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

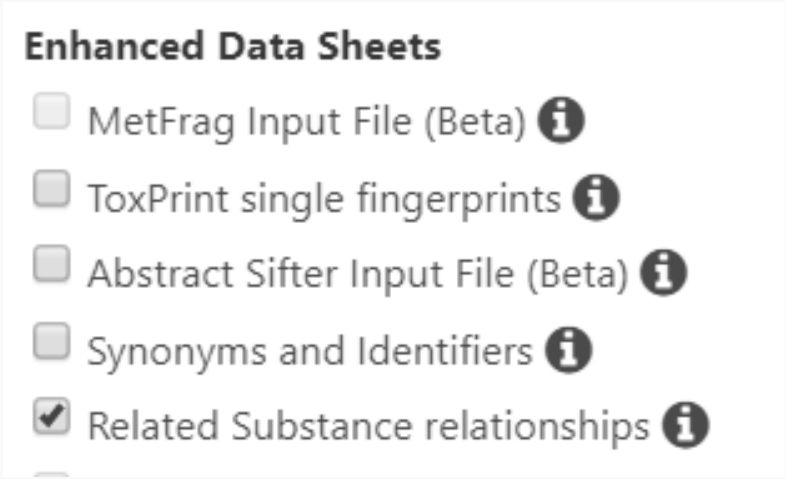
Intrinsic And Predicted Properties

- [x] Molecular Formula
- [x] 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	C36H63N3C	681.912	Y	-	-	-	-	
DTXSID30	Enniatin B	C33H57N3C	639.831	Y	-	-	-	-	
DTXSID50	Enniatin A1	C35H61N3C	667.885	Y	-	-	-	-	
DTXSID70	Enniatin B1	C34H59N3C	653.858	Y	-	-	-	-	
DTXSID00	Beauvericin	C45H57N3C	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	-	-	-	-	

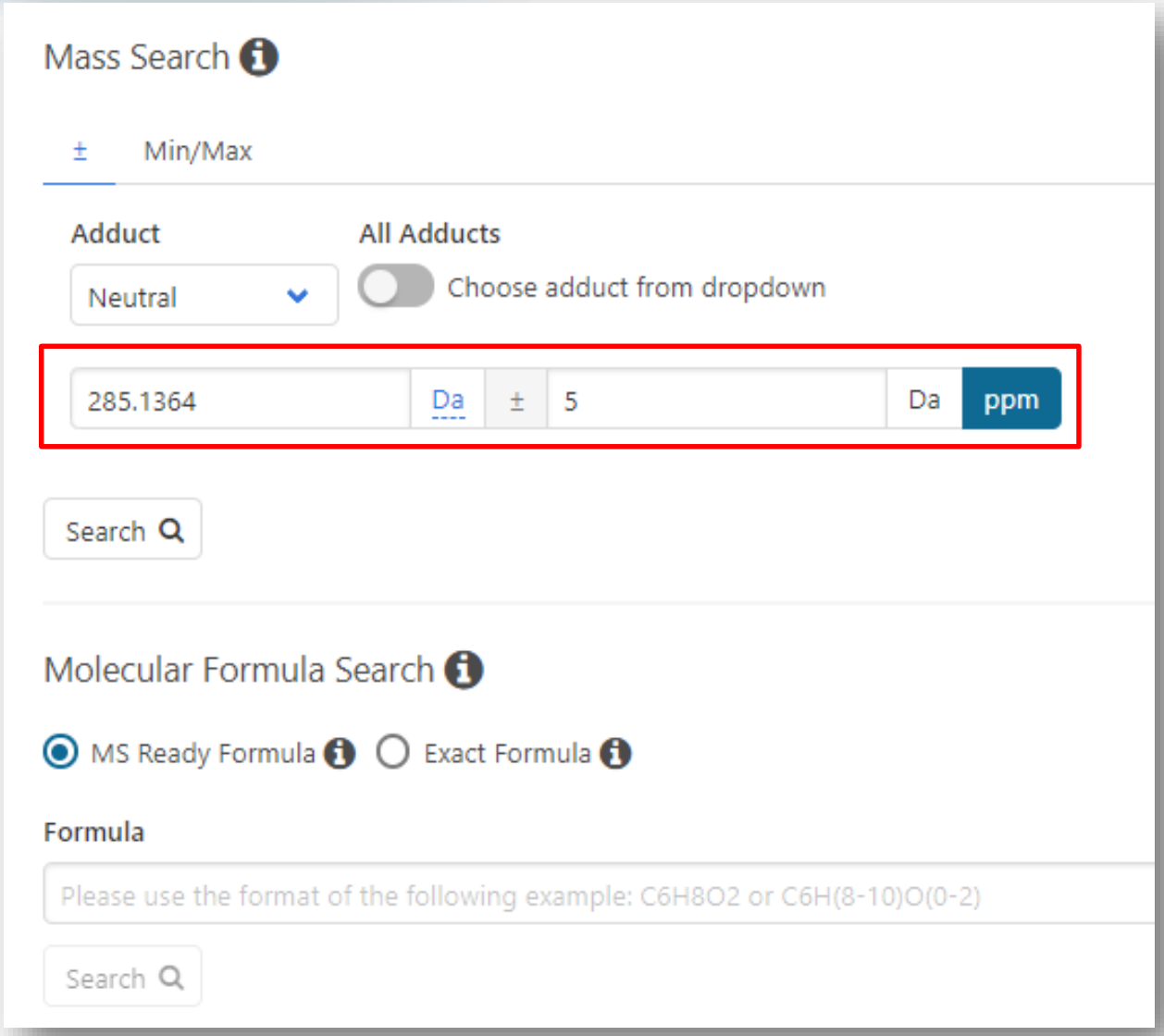
Related Substance Relationships



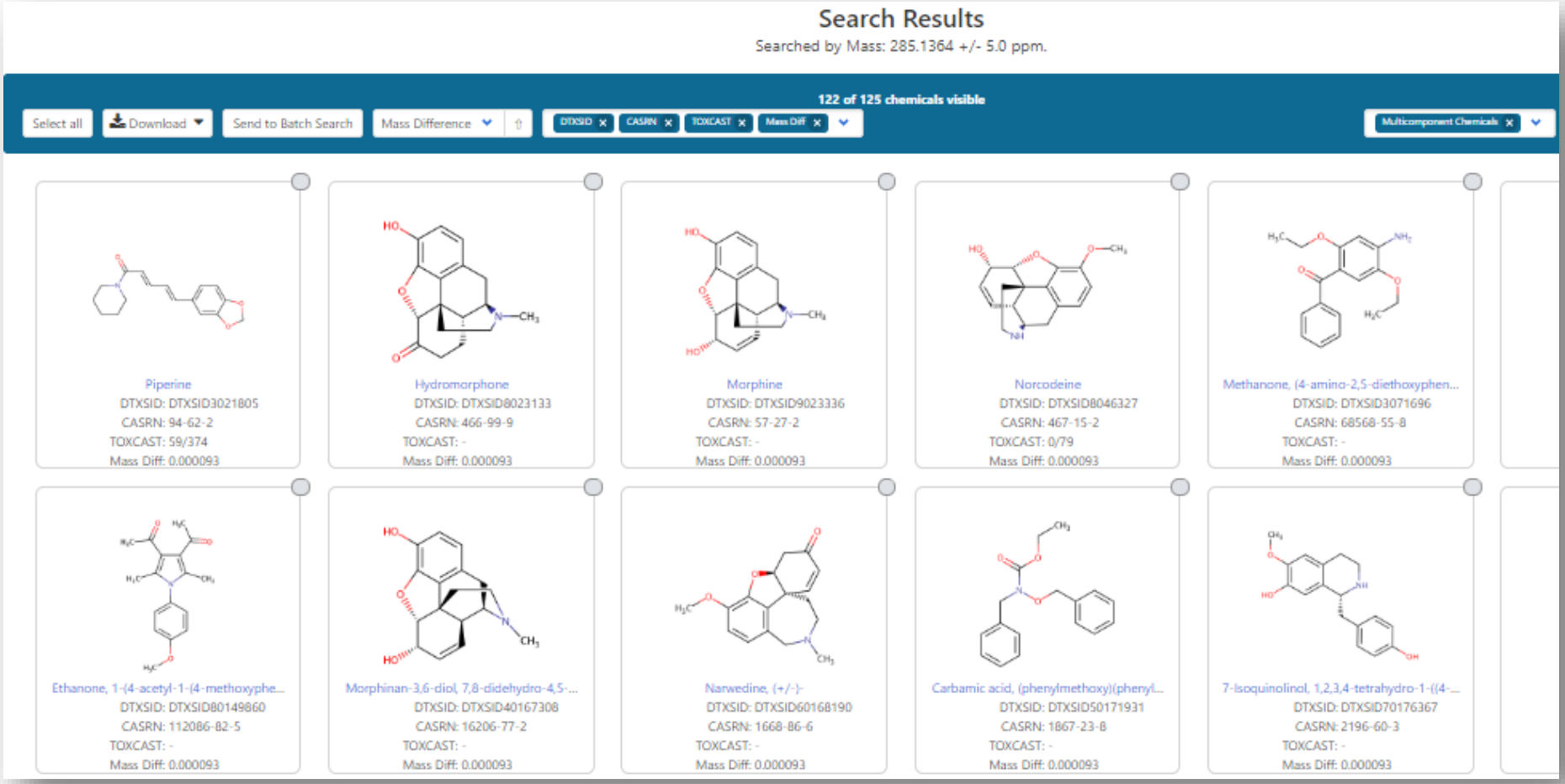
INPUT	DTXSID	HAS_RELATIONSHIP_WITH	RELATED_DTXSID	RELATED_PREFERRED_NAME	RELATED_CASRN
emodin	DTXSID50	Transformation Product	DTXSID60197420	omega-Hydroxyemodin	481-73-2
emodin	DTXSID50	Transformation Product	DTXSID30191177	Questin	3774-64-9
emodin	DTXSID50	Transformation Product	DTXSID80197684	Emodin 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

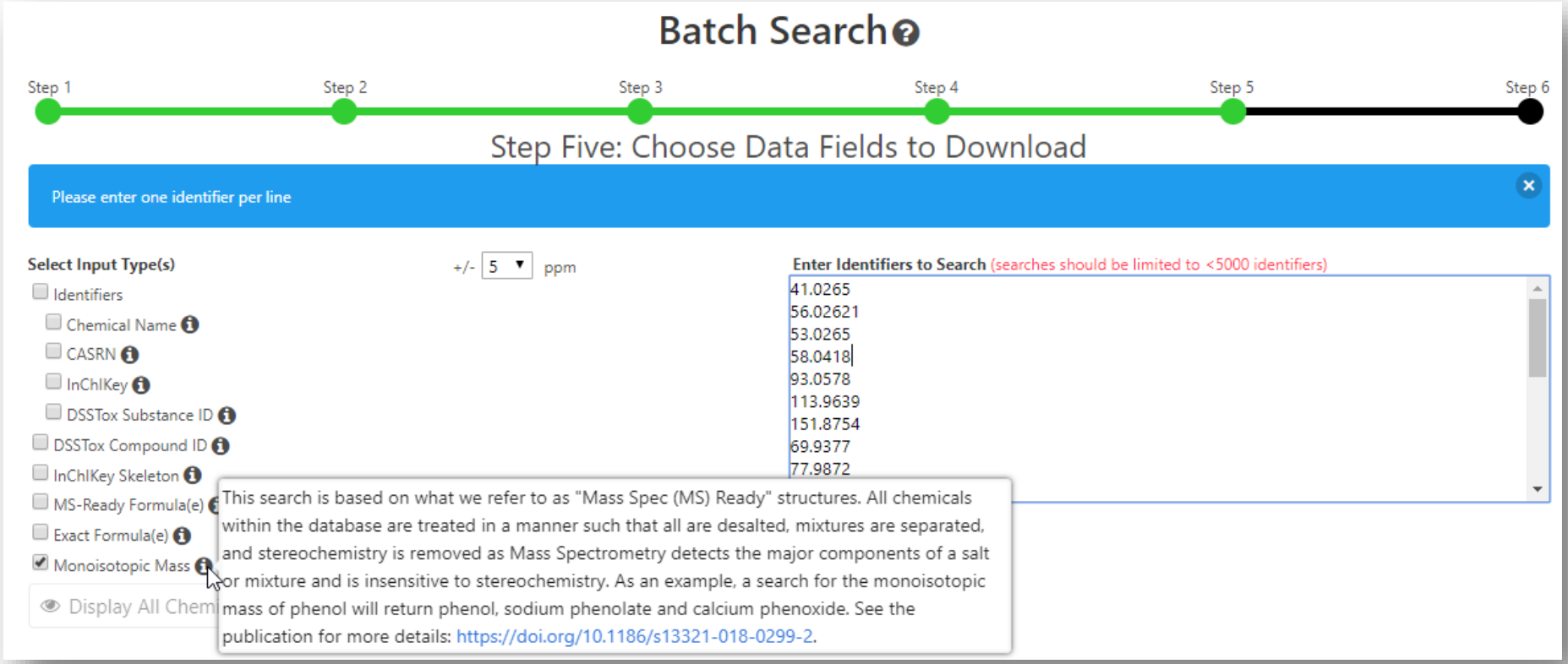
Advanced Searches
Mass and Formula Based Search



Advanced Searches
Mass and Formula Based Search



Batch Searching Formula/Mass



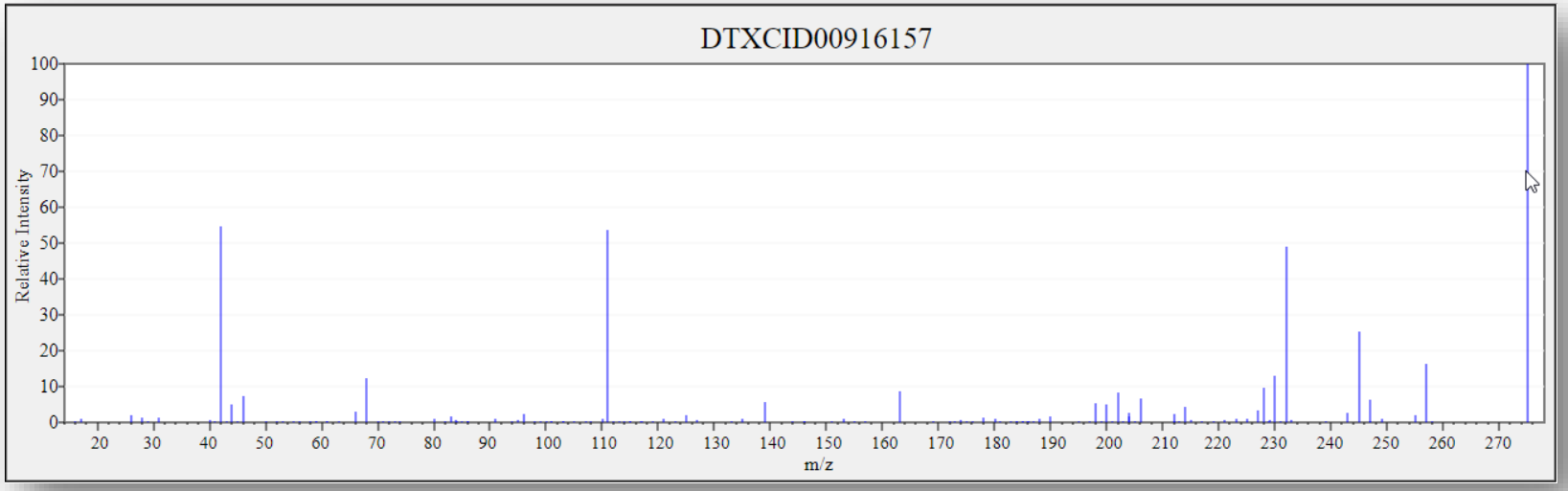
EPA United States Environmental Protection Agency

WORK IN PROGRESS

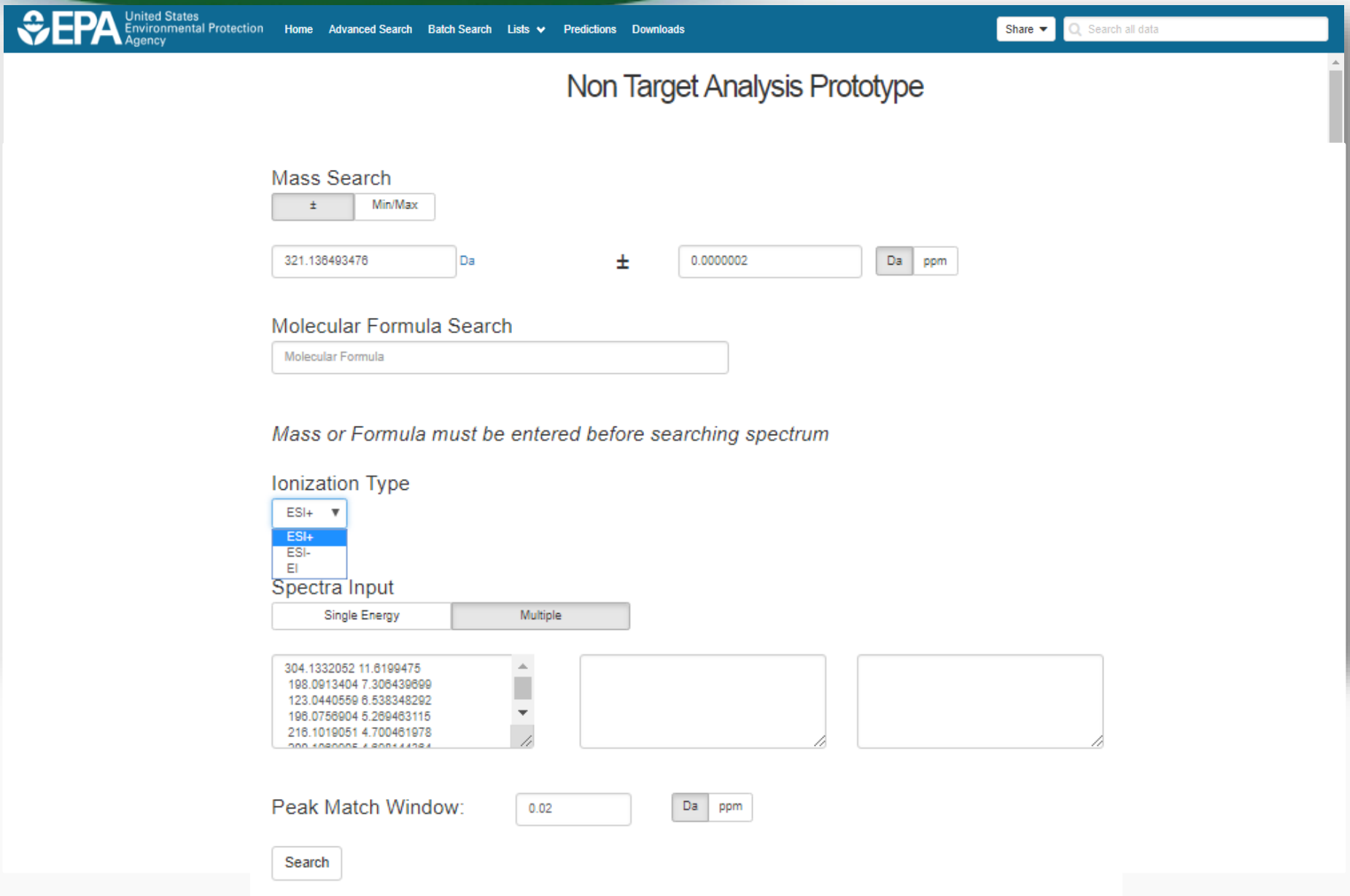
Predicted Mass Spectra

http://cfmid.wishartlab.com/

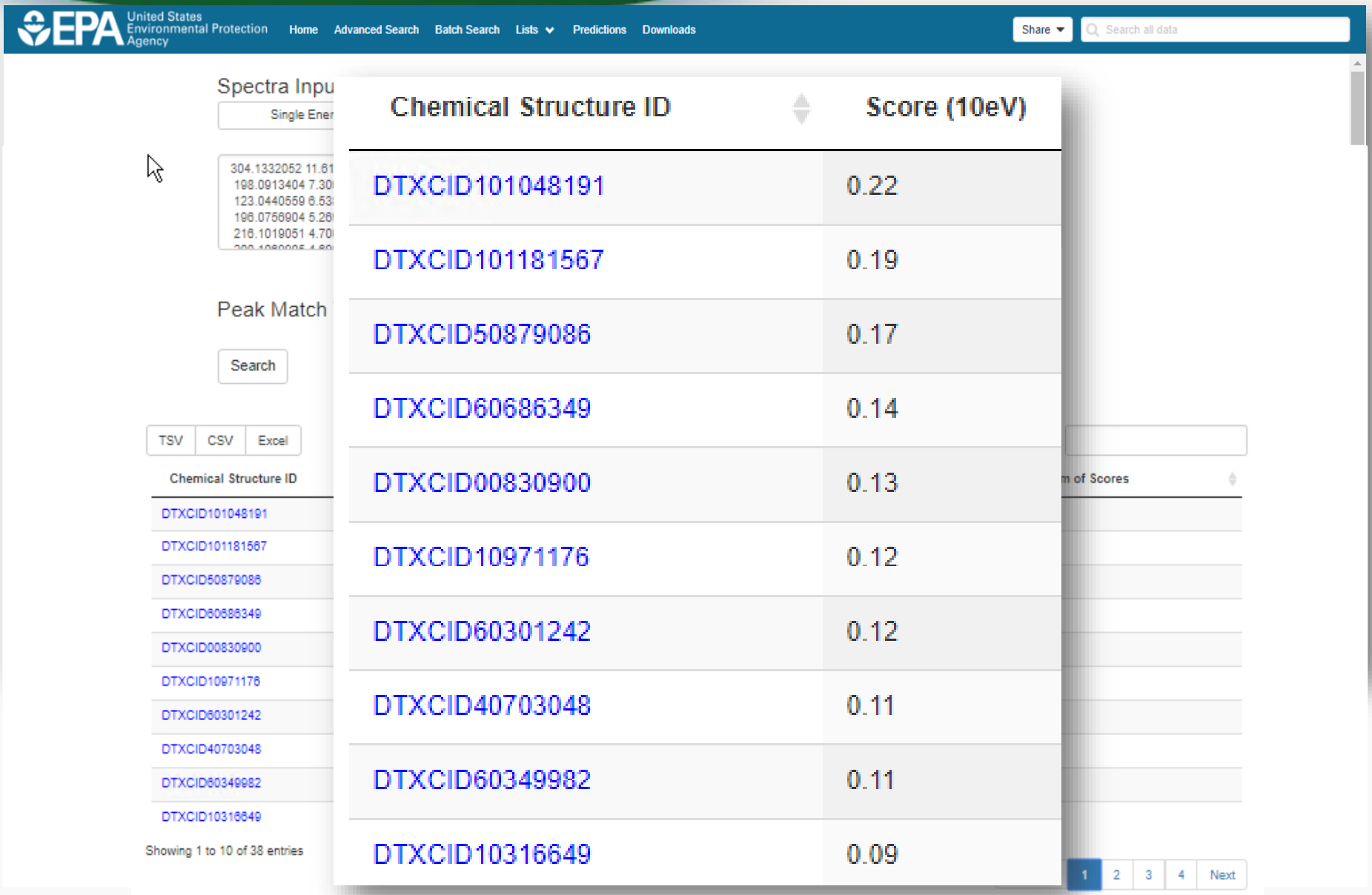
- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >800,000 structures, to be accessible via Dashboard



Search Expt. vs. Predicted Spectra

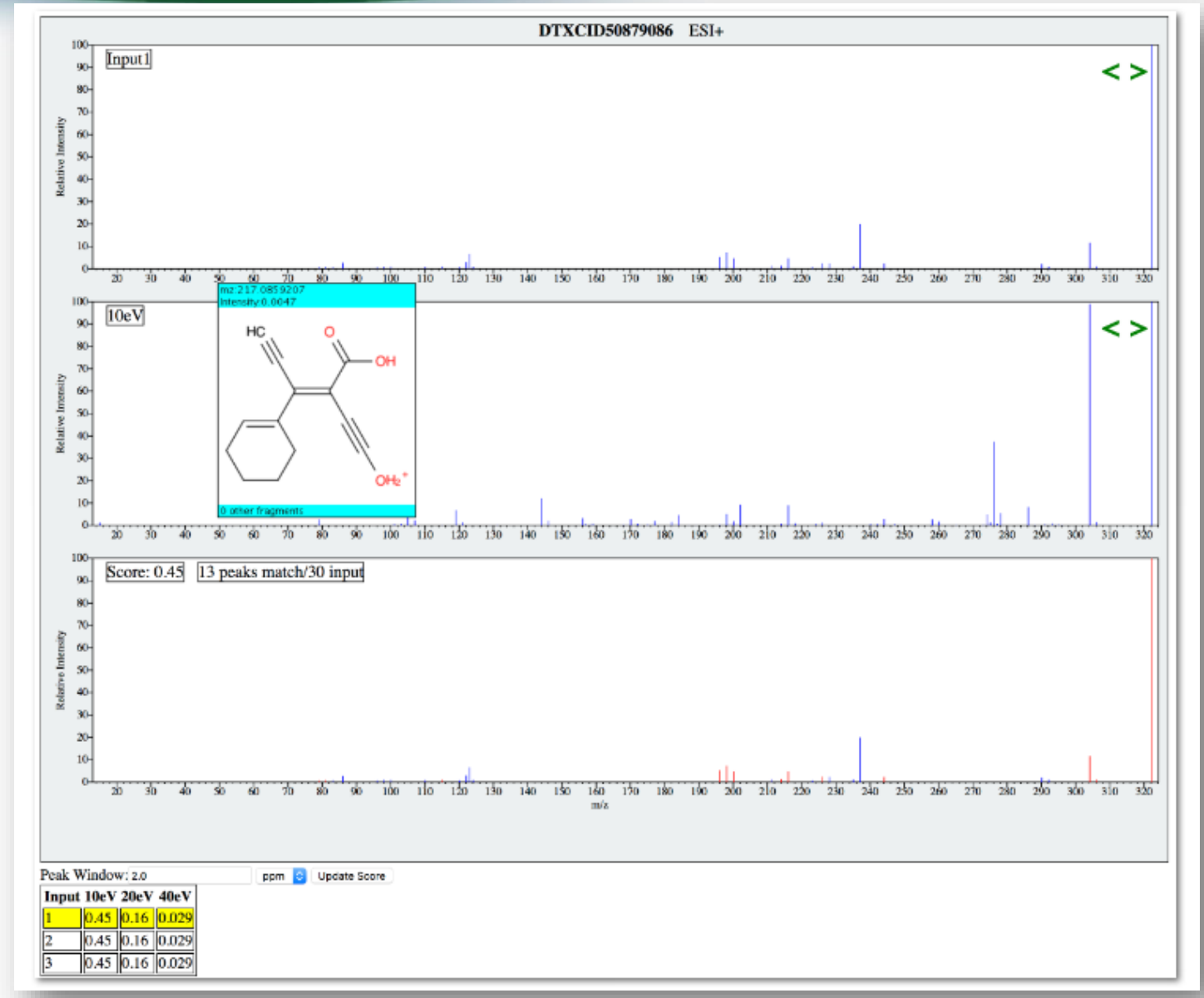


Search Expt. vs. Predicted Spectra

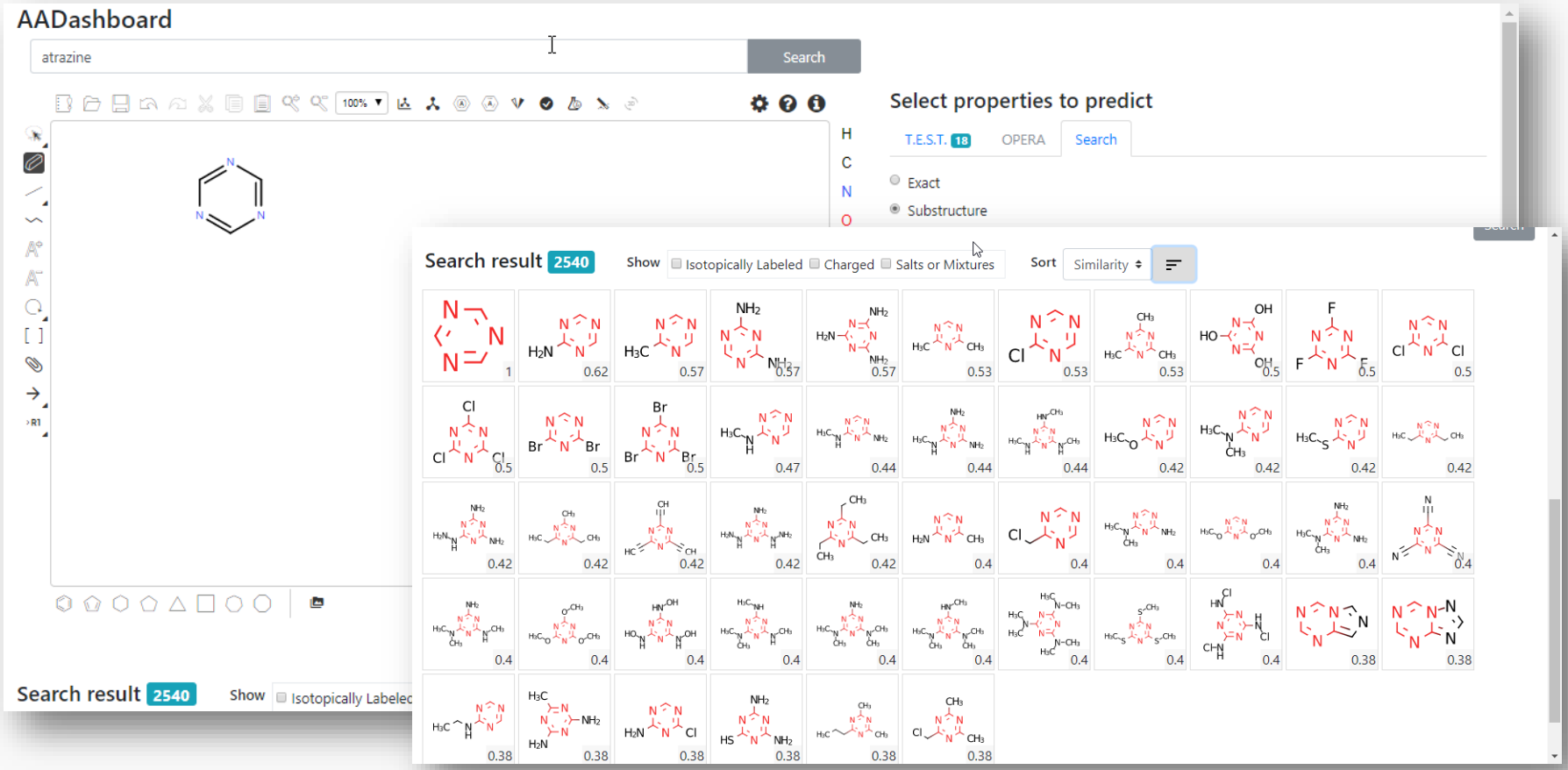


Chemical Structure ID	Score (10eV)
DTXCID101048191	0.22
DTXCID101181567	0.19
DTXCID50879086	0.17
DTXCID60686349	0.14
DTXCID00830900	0.13
DTXCID10971176	0.12
DTXCID60301242	0.12
DTXCID40703048	0.11
DTXCID60349982	0.11
DTXCID10316649	0.09

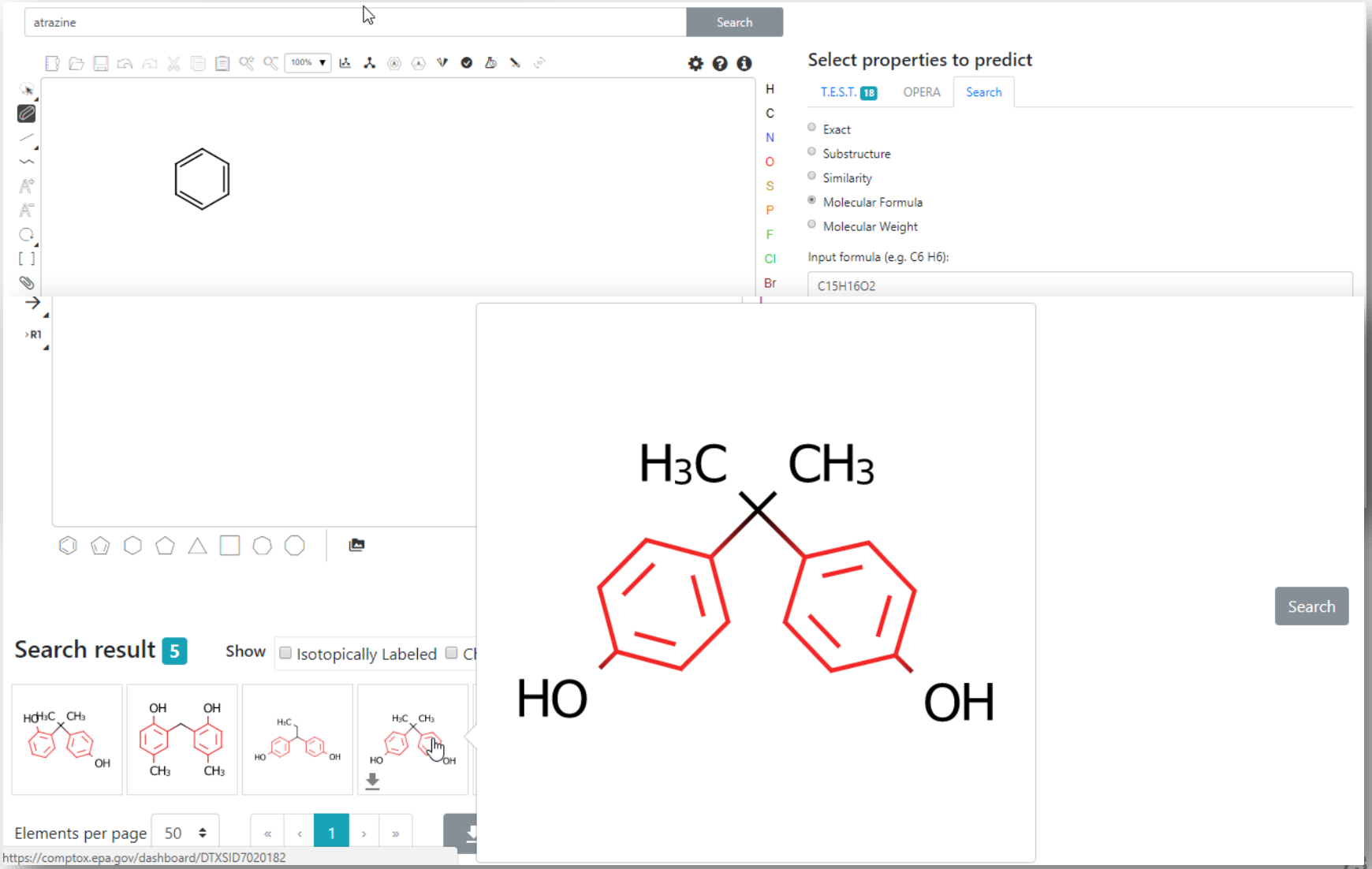
Spectral Viewer Comparison



Prototype Development



Prototype Development



Agilent Dataset

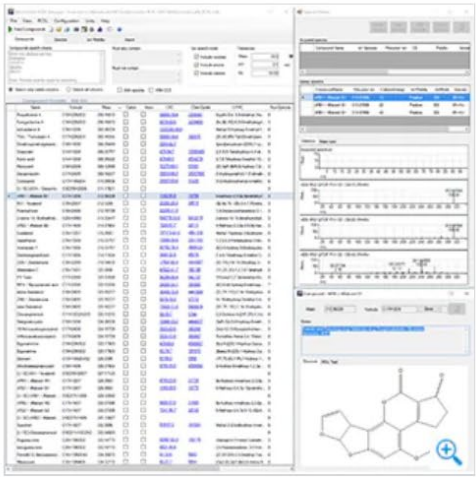
- Agilent : “Mycotoxins and Metabolites Personal Compound Database and Library”
- Registered for next release…

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



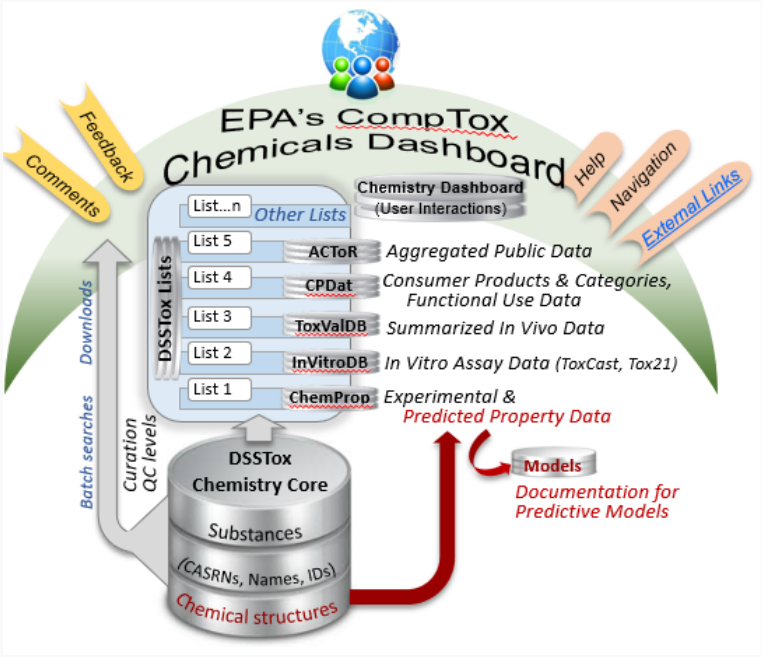
MassHunter PCDL Manager Compound view of Mycotoxins PCDL

Please help

- 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”



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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*

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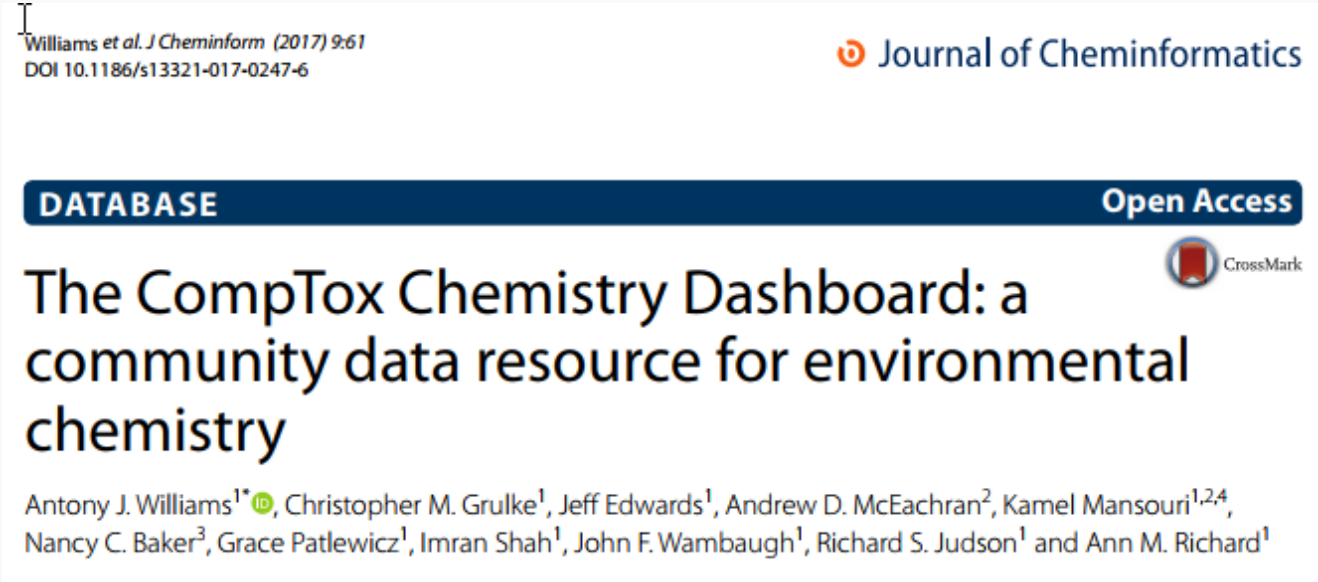

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DOI 10.1186/s13321-017-0247-6

Journal of Cheminformatics

DATABASE Open Access

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

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

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