

Integrating Mass Spectrometry Non-Targeted Analysis and Computational Toxicology to Characterize Chemicals

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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

June 2022

Medical Device and Combination Product Specialty Section webinar

CompTox Chemicals Dashboard

>906k chemicals

CompTox Chemicals Dashboard Home Search ▾ Lists ▾ About ▾ Tools ▾ Submit Comments

Welcome to the new EPA CompTox Chemicals Dashboard

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2020. ⓘ

CompTox Chemicals Dashboard

Search 906,511 Chemicals

Chemicals

Products/Use Categories

Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey 

Start typing to search.

☐ Identifier substring search

Latest News
[Read More News](#)

The Charge for the Dashboard

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

United States
Environmental Protection
Agency



BPDA



4-Cumylphenol
CASRN:599-64-4
DTXSID:DTXSID0018242
TOXCAST-287/739

Detailed Chemical Pages

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

Similar Compounds

GenRA

Related Substances

Synonyms

Literature

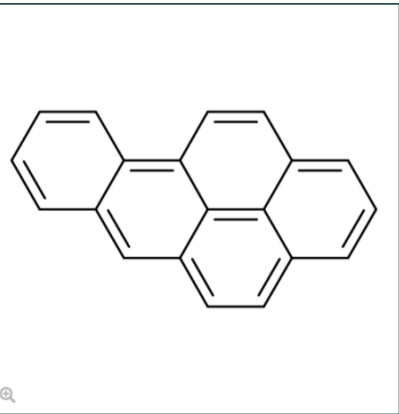
Links

Comments



Benzo(a)pyrene
50-32-8 | DTXSID2020139
Searched by Approved Name.

Chemical Details



Wikipedia

Benzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C (1,112 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula C₂₀H₁₂ is one of the benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to

[Read more](#)

Quality Control Notes

Intrinsic Properties

Molecular Formula: C₂₀H₁₂

MOL FILE

FIND ALL CHEMICALS

Average Mass: 252.316 g/mol

ISOTOPE MASS DISTRIBUTION

Monoisotopic Mass: 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

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

“Executive Summary”

Executive Summary

Quantitative Risk Assessment Values

✓ IRIS values available [↗](#)

✗ No PPRTV values

✓ EPA RSL values available [↗](#)

✓ Minimum RfD: 0.0003 mg/kg-day (chronic,) [↗](#)

✓ Minimum RfC: 2e-06 mg/m³ (chronic,) [↗](#)

Chronic Toxicology

✓ Chronic toxicity PODs available [↗](#)

Subchronic Toxicology

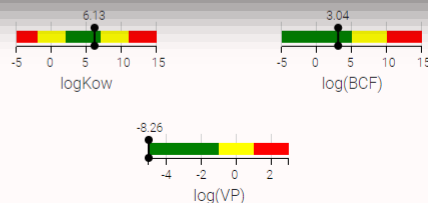
✗ No subchronic toxicity data available

Developmental Toxicology

✗ No developmental toxicity data available

Acute Toxicology

✗ No acute toxicity data available



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

Experimental and Predicted Data

Summary ▾

Search Chemical P

EXPORT ▾

Property	Experimental average	Predicted average
Polarizability	-	35.8 (1)
Henry's Law	4.57e-7 (1)	4.59e-7 (1)
Boiling Point	495 (3)	480 (4)
Flash Point	-	234 (2)
Melting Point	177 (8)	189 (3)
Molar Refractivity	-	90.3 (1)
Molar Volume	-	196 (1)
Surface Tension	-	53.9 (2)
Density	-	1.28 (2)
Vapor Pressure	5.49e-9 (1)	3.61e-9 (3)

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files

Chemical Hazard Data

ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations

Point of Departure

Search Hazard

☒ human
 ☐ eco

EXPORT

More	Priority	Source	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Critical effect	Species	Year
	1	IRIS	LOAEL	-	chronic	=	9.10e-3	mg/m3	-	inhalation	reduced ovulation rate and ovary weight	-	-
	1	IRIS	LOAEL	-	chronic	=	4.60e-3	mg/m3	-	inhalation	reduced embryo/fetal survival	-	-
	3	ECOTOX	NOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical, ...	Weight	house ...	1990
	3	ECOTOX	NOEL	-	chronic growth	-	50.0	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical, ...	Weight	house ...	1990
	3	ECOTOX	NOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	50.0	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	LOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	LOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical, ...	Weight	house ...	1990

Rows: 58
 Total Rows: 58

GHS Data

Print Page

[PUBCHEM](#) > [BENZO\[A\]PYRENE](#) > [LABORATORY CHEMICAL SAFETY SUMMARY \(LCSS\)](#) > [GHS CLASSIFICATION](#)

CID 2336

Benzo[a]pyrene

GHS Classification



Showing 6 of 6

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

United States
Environmental Protection
Agency

Search Chemical Weight Fractions											
Product Name	Product Use Category	Categorization Subtype	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source	Product Count				
48743 pah mixture	Not yet Categorized	-	-	reported	SIRI	1					
asphalt cement penetration 60-70	Not yet Categorized	-	-	reported	SIRI	1					
base-neutral 4 1ml methylene chl...	Not yet Categorized	-	-	reported	SIRI	1					
base neutral calibration checkco...	Not yet Categorized	-	-	reported	SIRI	1					
benzo (a) pyrene_ 98%_ b1008-0	Not yet Categorized	-	-	reported	SIRI	1					
benzo (a) pyrene_md-1956	Not yet Categorized	0.990	1.00	reported	SIRI	1					
blasocut 2000 cf art no 875	Not yet Categorized	0.00	1.00e-3	reported	SIRI	1					
blasocut 2000 universal_ 870	Not yet Categorized	-	-	reported	SIRI	1					
blasocut 2000 universal art_ 870	Not yet Categorized	0.00	1.00e-3	reported	SIRI	1					
blasocut 4000 strong_ 872	Not yet Categorized	-	-	reported	SIRI	1					
blasocut 4000 universal art_ 872	Not yet Categorized	0.00	1.00e-3	reported	SIRI	1					
clp-011a clp base/neutrals check ...	Not yet Categorized	-	-	reported	SIRI	1					

Searching Literature and the Internet

Literature Searching

Literature - PubMed Abstract Sifter

Abstract Sifter Instructions

1 Select PubMed starting point query

Hazard

Choose 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

2 Optionally, enter any PubMed query or edit the query from step 1

("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL
OR Rfd OR "reference dose" OR "reference concentration" OR
"adverse effect level"[tiab] OR "cancer slope factor"[tiab])

3 Click Retrieve Articles to begin download.

RETRIEVE ARTICLES

4 Optionally, export articles

SEND TO

- Real-time retrieval of data from PubMed ~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Markup of abstracts

To find articles quickly, enter terms to sift abstracts. 

Atrazine metabol

Download / Send to...  

☐	Atrazine	metabol	Total ↓	PMID	Year	Title	Authors	Journal	Rev	Rev
☐	19	10	29	16527233	2006	Determination of atrazine and its metabolites in mouse urine and...	Ross, Filipov	Analytical biochemistry		
☐	13	10	23	16656648	1967	Atrazine metabolism and herbicidal selectivity.	Shimabukuro	Plant physiology		
☐	13	10	23	8481106	1993	In vitro percutaneous absorption and metabolism in man of 2-chl...	Ademola; Sedik; Wester; Maibach	Archives of toxicology		
☐	19	3	22	33421427	2021	Transcriptomic profiling of atrazine phytotoxicity and comparativ...	Qu; Mei; Liu; Zhao; Liu; Li; Huang; Zhu	Environmental research		
☐	19	3	22	23102724	2012	Fate of atrazine in switchgrass-soil column system.	Albright; Murphy; Anderson; Coats	Chemosphere		
☐	15	7	22	11476505	2001	Anaerobic degradation of atrazine and metolachlor and metaboli...	Seybold; Mersie; McNamee	Journal of environmental quality		
☐	16	5	21	20830925	2010	Enhanced degradation and soil depth effects on the fate of atrazi...	Krutz; Shaner; Zablutowicz	Journal of environmental quality		
☐	16	5	21	14674556	2003	Infiltration and adsorption of dissolved atrazine and atrazine met...	Krutz; Senseman; Dozier; Hoffman; Tierney	Journal of environmental quality		
☐	19	2	21	2761262	1989	Testosterone metabolism in neuroendocrine organs in male rats ...	Babić-Gojmerac; Kniewald; Kniewald	Journal of steroid biochemistry		
☐	20	0	20	33254405	2020	Removal of atrazine in catalytic degradation solutions by microal...	Hu; Xu; Sun; Zhu; Sun; Zhao; Hu	Ecotoxicology and environmental safety		
☐	17	3	20	24062064	2013	Biodegradation of atrazine by Rhodococcus sp. BCH2 to N-isopr...	Kolekar; Phugare; Jadhav	Environmental science and pollution research intern...		
☐	18	2	20	21121649	2010	Metabolism and persistence of atrazine in several field soils with...	Jablonowski; Hamacher; Martinazzo; Langen; Köpp...	Journal of agricultural and food chemistry		
☐	20	0	20	18848368	2008	Nitrogen limited biobarriers remove atrazine from contaminated ...	Hunter; Shaner	Journal of contaminant hydrology		
☐	20	0	20	16595379	2006	Mixed-effect models for evaluating multiple measures of atrazine...	Hines; Deddens; Lu; Fenske; Striley	Journal of occupational and environmental hygiene		
☐	12	8	20	16349478	2005	Molecular basis of a bacterial consortium: interspecies catabolis...	de Souza; Newcombe; Alvey; Crowley; Hay; Sadow...	Applied and environmental microbiology		
☐	11	8	19	16656991	1968	Atrazine metabolism in resistant corn and sorghum	Shimabukuro	Plant physiology		

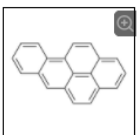
Determination of atrazine and its metabolites in mouse urine and plasma by LC-MS analysis.

Atrazine is a herbicide widely used on agricultural commodities. Existing analytical methods to analyze atrazine and its metabolites in biological matrices have various drawbacks. Thus, further development of such methods will be needed to correlate the growing number of toxicological effects associated with atrazine exposure with the concentrations of this compound and its metabolites in plasma, urine, and tissues. The purpose of this study was to develop a broad and sensitive LC-MS method for the analysis of atrazine and its metabolites in mouse urine and plasma. We were able to simultaneously measure atrazine and its major mammalian metabolites, which include didealkyl atrazine, desisopropyl atrazine, desethyl atrazine, atrazine-glutathione conjugate, and atrazine-mercaptopurine, using preparation procedures that used small sample volumes of plasma and urine (0.25 and 0.5 ml, respectively). Furthermore, derivatization of analytes prior to analysis was unnecessary. This method was used to analyze plasma and urine samples following single in vivo oral exposures of a limited number of mice to atrazine (doses, 5-250 mg/kg body weight) to demonstrate the utility of this LC-MS method. The data obtained from this study suggest that atrazine is rapidly metabolized in mice. Didealkyl atrazine was the most abundant metabolite detected in the urine and plasma samples (approximately 1000 microM in 24-h urine and approximately 100 microM in plasma following the highest dose of atrazine), with lesser quantities of mono N-dealkylated metabolites and thio conjugates of atrazine observed. We also used this methodology in a preliminary study of cytochrome P450-catalyzed metabolism of atrazine in vitro. The results obtained in this study suggest that this method will be a useful tool for the determination of atrazine and its metabolites in future pharmacokinetic studies and for the subsequent development and refinement of biologically based models of atrazine disposition.

What's the best way to search the internet for chemical data?

- We know how complex identifiers are...
 - CASRN(s)
 - Hundreds of names (maybe)
 - SMILES
 - InChIs
 - EINECS, EC numbers
- What can WE do to help navigate the internet?

External Links – Also use Identifiers Names, CASRN, PubChem IDs, InChIs...



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

 EPA Substance Registry Service
 PubChem
 Chemspider
 CPat
 DrugBank
 Wikipedia
 MSDS Lookup
 ChEMBL
 ToxPlanet
 ACS Reagent Chemicals
 Wolfram Alpha
 ECHA Infocard
 ChemAgora
 Consumer Product Information Database
 ChEBI
 NIST Chemistry Webbook
 WEBWISER
 PubChem Safety Sheet
 Consumer Product Information Database
 PubChem: Chemical Vendors

Toxicology

 ACToR
 DrugPortal
 CCRIS
 ChemView
 CTD
 eChemPortal
 Gene-Tox
 HSDB
 ACToR PDF Report
 CREST
 National Air Toxics Assessment
 ECOTOX
 ChemView
 Chemical Checker
 BindingDB
 CalEPA OEHA
 NIOSH IDLH Values
 LactMed
 ECOTOX

Publications

 Toxline
 PPRTVWEB
 PubMed
 IRIS Assessments
 EPA HERO
 NIOSH Skin Notation Profiles
 NIOSH Pocket Guide
 RSC Publications
 BioCaddie DataMed
 Springer Materials
 Bielefeld Academic Search Engine
 CORE Literature Search
 Google Books (Text Search)
 Google Patents (Text search)
 Google Scholar (Text search)
 Google Patents (Structure search)
 Google Books (Structure Search)
 Google Scholar (Structure search)
 Federal Register

Analytical

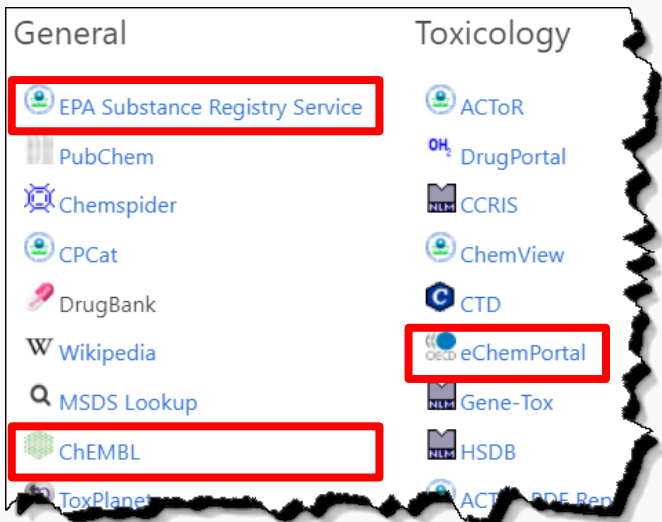
 RSC Analytical Abstracts
 Tox21 Analytical Data
 MONA: MassBank North America
 mzCloud
 NIST NIST IR Spectrum
 NIST NIST MS Spectrum
 MassBank
 NIST NIST Antoine Constants
 IR Spectra on PubChem
 NIST NIST Kovats Index values
 Protein DataBank
 National Environmental Methods Index

Prediction

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

External Links

- Links to ~90 websites providing access to additional data on the chemical of interest



 **OECD**
BETTER POLICIES FOR BETTER LIVES

Print  English 

 **eChemPortal**

The Global Portal to Information on Chemical Substances

Home **Substance Search** Property Search Classification Search Schedules of Assessments Data sources About  Help  Contact Us

 **Chemical Substance Search**

Substance (50-32-8) 

Sources and type of information 

Select all  Deselect all 

Types 

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

Data sources

☒ ACToR 	☒ AGRITOX 	☒ AICIS assessments 
☒ APVMA-CR 	☒ CCR 	☒ CESAR 
☒ Chemicals Dashboard 	☒ ChemInfo 	☒ Combined Exposures 



Analytical

 FOR-IDENT

 NEMI: National Environmental
Methods Index

 RSC Analytical Abstracts

 Tox21 Analytical Data

 MONA: MassBank North
America

 mzCloud

 NIST IR Spectrum

 NIST MS Spectrum

Mass spectrum (electron ionization)

[Go To: Top, References, Notes](#)

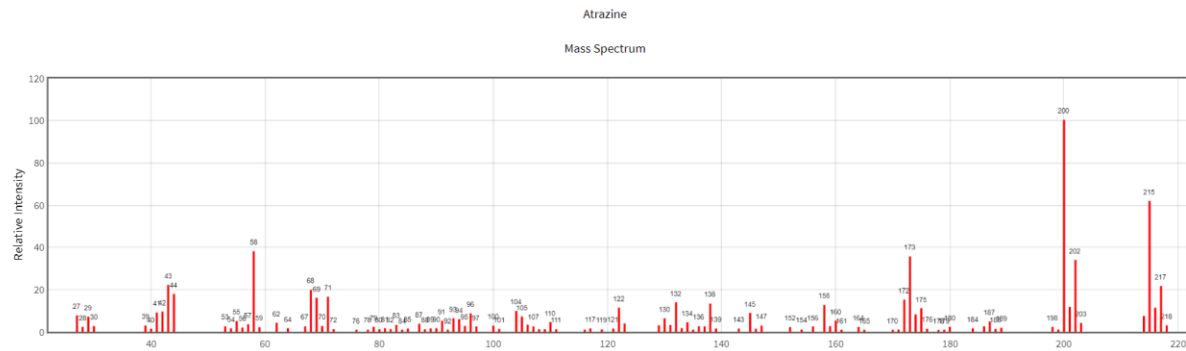
Data compilation [copyright](#) by the U.S. Secretary of Commerce on behalf of the U.S.A. All rights reserved.

Data compiled by: NIST Mass Spectrometry Data Center, William E. Wallace, director

Spectrum

[Plot](#)

[Help / Software credits](#)



MassBank of North America

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

Analytical

- FOR-IDENT
- NEMI: National Environmental Methods Index
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America**
- mzCloud
- NIST NIST IR Spectrum
- NIST NIST MS Spectrum

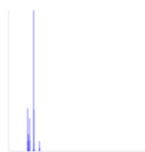
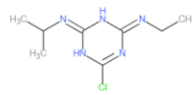
MoNA - MassBank of North America

Search...

51

Atrazine

Score: ★★★★★

Originally submitted to the MassBank High Quality Mass Spectral Database

MassBank LC-MS

Display Full Record

instrument	Bruker maXis Impact
instrument type	LC-ESI-QTOF
ms level	MS2
ionization	ESI
collision energy	30 eV
retention time	8.0 min
ionization mode	positive
precursor m/z	216.1010
precursor type	[M+H] ⁺
accession	AU310903

Chemical Lists of Interest...

Lists of Extractables and Leachables

<https://comptox.epa.gov/dashboard/chemical-lists?filtered=&search=extractables>

- Chemical lists with extractables & leachables
- Expands with literature extraction

Chemical Lists

 extractables

 EXPORT

 COPY URL

Showing 3 of 323 Records

List Acronym	List Name	# Chemicals	Updated	List Description
ELSIE	EXTRACTABLES: Extractables & Leachables ...	457	2019-11-16	The Extractables and Leachables Safety Information Exchange (ELSIE: https://www.elsiedata.org/) was established by scientists in pharmaceuticals companies to advance the concept of sharing pre-competitive safety information on extractables and leachables, among industry. The vision was that such a collaborative effort would reduce duplicative safety studies across companies, streamline development projects, and allow industry and other stakeholders to share experiences and information to help advance the practice and science of extractables, leachables and materials evaluation.
EXTRACTPIPES	EXTRACTABLES: Leachable Chemical Substa...	151	2019-11-16	List of chemicals from the article "Characterization of Leachable Chemical Substances from Common Drinking Water Piping Materials" by Pizzurro et al [https://esemag.com/wp-content/uploads/2018/06/Pizzurro-et-al_2018_Piping-Review-White-Paper.pdf]
FOODPLASTICS	EXTRACTABLES: Chemical migrants in plasti...	81	2019-11-16	List of chemical migrants in plastic food contact products listed in the article "Detection and quantification analysis of chemical migrants in plastic food contact products" by Qian et al (https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0208467)

The ELSIE Database

<https://comptox.epa.gov/dashboard/chemical-lists/ELSIE>



EXTRACTABLES: Extractables & Leachables Safety Information Exchange (ELSIE)

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Start typing to search.

☐ Identifier substring search

List Details

Description: The Extractables and Leachables Safety Information Exchange (ELSIE: <https://www.elsiedata.org/>) was established by scientists in pharmaceuticals companies to advance the concept of sharing pre-competitive safety information on extractables and leachables, among industry. The vision was that such a collaborative effort would reduce duplicative safety studies across companies, streamline development projects, and allow industry and other stakeholders to share experiences and information to help advance the practice and science of extractables, leachables and materials evaluation.

Number of Chemicals: 457

EXTRACTABLES: Leachable Chemical Substances from Common Drinking Water Piping Materials

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey



Start typing to search.

☐ Identifier substring search

List Details



Description: List of chemicals from the article "Characterization of Leachable Chemical Substances from Common Drinking Water Piping Materials" by Pizzurro et al [https://esemag.com/wp-content/uploads/2018/06/Pizzurro-et-al_2018_Piping-Review-White-Paper.pdf]

Number of Chemicals: 151

EXTRACTABLES: Chemical migrants in plastic food contact products

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey



Start typing to search.

☐ Identifier substring search

List Details

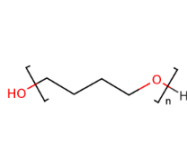
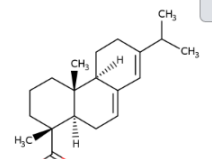
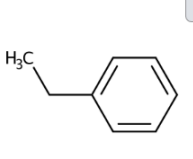
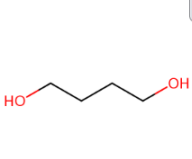
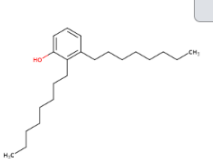
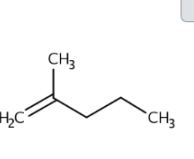
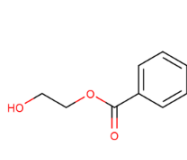
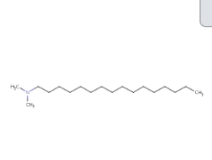
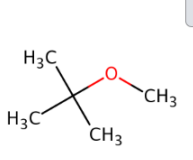
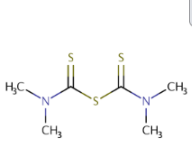
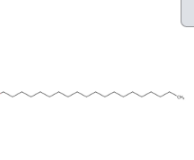


Description: List of chemical migrants in plastic food contact products listed in the article "Detection and quantification analysis of chemical migrants in plastic food contact products" by Qian et al (<https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0208467>)

Number of Chemicals: 81

Download data, send to batch search for data harvesting

Showing 457 of 457 chemicals

 Polytetramethylene glycol DTXSID : DTXSID2042307 CASRN : 25190-06-1 TOXCAST :	 Abietic acid DTXSID : DTXSID7022047 CASRN : 514-10-3 TOXCAST :	 Ethylbenzene DTXSID : DTXSID3020596 CASRN : 100-41-4 TOXCAST : 1/235	 1,4-Butanediol DTXSID : DTXSID2024666 CASRN : 110-63-4 TOXCAST : 7/430	 Phenol, dioctyl- DTXSID : DTXSID7067534 CASRN : 29988-16-7 TOXCAST :	 2-Methyl-1-pentene DTXSID : DTXSID901017356 CASRN : 763-29-1 TOXCAST :
 1,2-ETHANEDIOL, MONOBENZOATE DTXSID : DTXSID20879477 CASRN : 94-33-7 TOXCAST :	 N,N-Dimethyl-1-hexadecylamine DTXSID : DTXSID9026924 CASRN : 112-69-6 TOXCAST : 2/235	 Methyl tert-butyl ether DTXSID : DTXSID3020833 CASRN : 1634-04-4 TOXCAST : 5/235	 Tetramethylthiuram monosulfide DTXSID : DTXSID0021333 CASRN : 97-74-5 TOXCAST : 173/628	0 related chemical structures with this substance Soybean oil, epoxidized DTXSID : DTXSID1027687 CASRN : 8013-07-8 TOXCAST :	 1-Eicosanol DTXSID : DTXSID0027272 CASRN : 629-96-9 TOXCAST :



“MS-ready” structures

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

Journal of Cheminformatics

METHODOLOGY

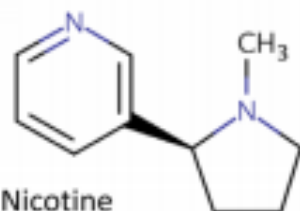
Open Access

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



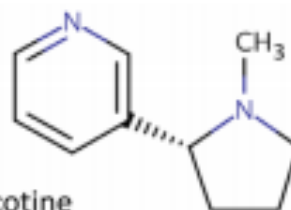
Andrew D. McEachran^{1,2*}, Kamel Mansouri^{1,2,3}, Chris Grulke², Emma L. Schymanski⁴, Christoph Ruttkies⁵
and Antony J. Williams^{2*}

- All structure-based chemical substances are algorithmically processed to
 - Split multicomponent chemicals into individual structures
 - Desalt and neutralize individual structures
 - Remove stereochemical bonds from all chemicals
- MS-Ready structures are then mapped to original substances to provide a path between chemicals detected by mass spectrometry to original substances



Nicotine

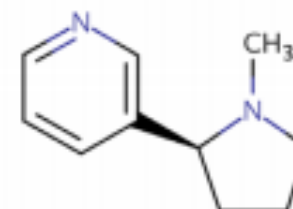
CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID1020930 | SNICXCGAKADSCV
 54-11-5 | **162.1157** | 0.929 | **72**
 Tox: **yes** | Expo: **yes** | Bioassay: **yes**



D-Nicotine

CN1CCC[C@@H]1C1=CN=CC=C1
 DTXSID004635 | SNICXCGAKADSCV
 25162-00-9 | **162.1157** | 0.929 | **20**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**

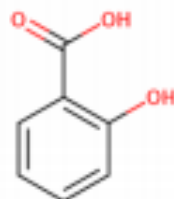
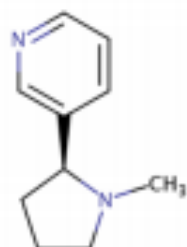
LEGEND: Name, SMILES
 DTXSID | InChIKey 1st Block
 CAS | **Monoiso.** Mass | logP | **Sources**
 Data on: **Toxicity** | **Exposure** | **Bioassays**



HCl

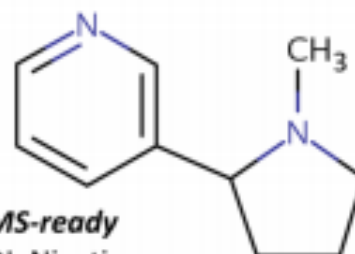
Nicotine hydrochloride

Cl.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID602093 | HDJBTCAJIMNXEW
 2820-51-1 | **198.0924** | 0.929 | **9**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**



Benzoic acid, 2-hydroxy-, compd. with
3-[(2S)-1-methyl-2-pyrrolidiny]pyridine (1:1)

OC(=O)C1=CC=C(C=C1)C(=O)C1=CC=C(C=C1)C1=CN=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID5075319 | AIBWPBUAKCMKNS
 29790-52-1 | **300.1474** | 0.929 | **6**
 Tox: **no** | Expo: **yes** | Bioassay: **no**

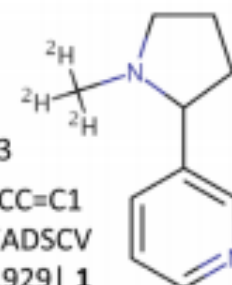


MS-ready
DL-Nicotine

CN1CCCC1C1=CN=CC=C1
 DTXSID3048154 | SNICXCGAKADSCV
 22083-74-5 | **162.1157** | 0.953 | **9**
 Tox: **yes** | Expo: **no** | Bioassay: **yes**

DL-Nicotine-d3

[2H]C([2H])([2H])N1CCCC1C1=CN=CC=C1
 DTXSID80442666 | SNICXCGAKADSCV
 69980-24-1 | **165.1345** | 0.929 | **1**
 Tox: **no** | Expo: **no** | Bioassay: **no**



Mass and Formula Searching

Advanced Searches: Mass Search

Mass Search

± Min/Max

Adduct

Neutral



All Adducts



Choose adduct from dropdown

215.093

Da

±

5

Da

ppm

Search 

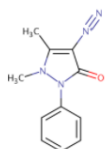
Advanced Searches: Mass Search

Search Results

Searched by Mass: 215.093 +/- 5.0 ppm.

27 of 30 chemicals visible

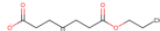
Select all Download Send to Batch Search Mass Difference DTXSID CASRN TOXCAST Mass Diff Multicomponent Chemicals Filter by Name or CASRN



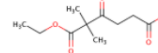
1H-Pyrazole-4-diazonium, 2,3-dihydro-1-phenyl-
DTXSID:DTXSID20480103
CASRN:14051-47-9
TOXCAST:-
Mass Diff:0.000263



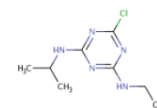
4-[(2-Hydroxyhexyl)oxy]-4-oxobut-2-enal
DTXSID:DTXSID90751433
CASRN:89036-55-5
TOXCAST:-
Mass Diff:0.000503



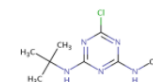
4,7-Dioxo-7-propoxyheptanoate
DTXSID:DTXSID50763416
CASRN:111044-04-3
TOXCAST:-
Mass Diff:0.000503



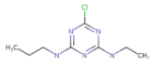
6-Ethoxy-5,5-dimethyl-4,6-dioxohexanoic acid
DTXSID:DTXSID50790348
CASRN:69527-64-6
TOXCAST:-
Mass Diff:0.000503



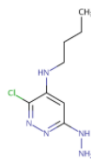
Atrazine
DTXSID:DTXSID9020112
CASRN:1912-24-9
TOXCAST:62/1024
Mass Diff:0.000773



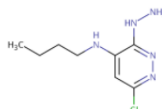
GS 18183
DTXSID:DTXSID00187906
CASRN:34333-27-2
TOXCAST:-
Mass Diff:0.000773



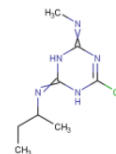
6-Chloro-N²-ethyl-N⁴-propyl-1,3,5-triazine
DTXSID:DTXSID60536638
CASRN:90952-64-0



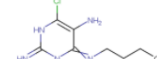
N-Butyl-3-chloro-6-hydrazinylpyridazin-4-amine
DTXSID:DTXSID90615440
CASRN:61261-46-9



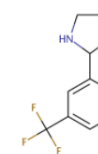
N-Butyl-6-chloro-3-hydrazinylpyridazin-4-amine
DTXSID:DTXSID70615443
CASRN:61261-44-7



N²-(Butan-2-yl)-6-chloro-N⁴-methyl-1,3,5-triazine
DTXSID:DTXSID60955305
CASRN:33692-99-8



4-(Butylimino)-6-chloro-2-imino-1,2,3,4-tetrahydropyrimidin-5(1H)-one
DTXSID:DTXSID90978320
CASRN:6270-25-3



2-[3-(Trifluoromethyl)phenyl]pyrrolidine
DTXSID:DTXSID20392717
CASRN:109086-17-1

Advanced Searches: Formula Search

Search Results

Searched by Exact Molecular Formula: C₈H₁₄ClN₅.

7 chemicals

Select all

Download

Send to Batch Search

Default

⬇

DTXSID ✕

CASRN ✕

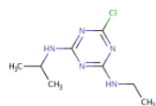
TOXCAST ✕

⬇

Hide chemicals that are: ⬇

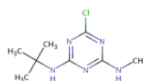
Filter by Name or CASRN

☰



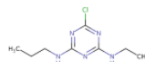
Atrazine

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



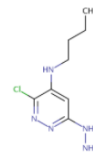
GS 18183

DTXSID:DTXSID00187906
CASRN:34333-27-2
TOXCAST:-



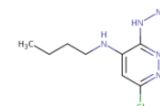
6-Chloro-N²-ethyl-N⁴-propyl-1,3,5-triazi...

DTXSID:DTXSID60536638
CASRN:90952-64-0
TOXCAST:-



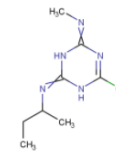
N-Butyl-3-chloro-6-hydrazinylpyridazin-...

DTXSID:DTXSID90615440
CASRN:61261-46-9
TOXCAST:-



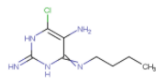
N-Butyl-6-chloro-3-hydrazinylpyridazin-...

DTXSID:DTXSID70615443
CASRN:61261-44-7
TOXCAST:-



N²-(Butan-2-yl)-6-chloro-N⁴-methyl-1,3,...

DTXSID:DTXSID60955305
CASRN:33692-99-8
TOXCAST:-



4-(Butylimino)-6-chloro-2-imino-1,2,3,4-...

DTXSID:DTXSID90978320
CASRN:6270-25-3
TOXCAST:-

Batch Searching

- Singleton searches are useful but we work with **thousands** of masses and formulae!
- 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 Search

Batch Search

1 Select Input Type(s)

☒ Substance Identifiers

☒ Chemical Name

☒ CASRN

☒ InChIKey

☒ DSSTox Substance ID

☐ DSSTox Compound ID

☐ InChIKey Skeleton

☐ MS-Ready Formula(e)

☐ Exact Formula(e)

☐ Monoisotopic Mass

2 Enter Identifiers to Search

(Please enter one identifier per line. Processing time increases with number of inputs.)

DTXSID9020374
DTXSID9020827
DTXSID2022678
DTXSID4023381
DTXSID9044164
DTXSID7032004
DTXSID4022361
DTXSID8021771

3

 DISPLAY ALL CHEMICALS

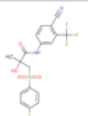
or

 CHOOSE EXPORT OPTIONS

45% loaded

45 Chemicals Found from 110 Input(s)

REPLACE IDENTIFIERS WITH SELECTED CHEMICALS

☐ Structure	DTXSID	Preferred Name	CASRN	Mono. Mass	Mol. Formula
☐		DTXSID2022678  Bicalutamide	90357-06-5	430.061041	C ₁₈ H ₁₄ F ₄ N ₂ O ₄ S
☐		DTXSID3020621  (R,R)-Fenvalerate	67614-33-9	419.128821	C ₂₅ H ₂₂ ClNO ₃

Batch Search – Excel, CSV, SDF file

Customize Export Results

4

CHOOSE EXPORT FORMAT

Your file will be exported in Microsoft Excel Format (.xlsx)

☐ Select All columns available

Chemical Identifiers

☒ DTXSID

☒ Chemical Name

☐ DTXCID

☒ CAS-RN

☒ InChIKey

☐ IUPAC Name

Structures

☐ Mol File

☒ SMILES

☐ InChI String

☐ MS-Ready SMILES

☐ QSAR-Ready SMILES

Intrinsic and Predicted Properties

☒ Molecular Formula

☒ Average Mass

☒ Monoisotopic Mass

☐ TEST Model Predictions

☒ OPERA Model Predictions

Metadata

☐ Curation Level Details

☒ Safety Data

☐ NHANES/Predicted Exposure

☒ Data Sources

☐ Include ToxVal Data Availability

☒ Assay Hit Count

☒ Number of PubMed Articles

☐ PubChem Data Sources

☐ OPDat Product Occurrence Count

☒ IRIS

☒ PPRTV

☐ Wikipedia Article

☒ QC Notes

☐ Include links to ACToR reports

Enhanced Data Sheets

☐ MetFrag Input File (Beta)

☐ ToxPrint single fingerprints

☐ Abstract Sifter Input File

☐ Synonyms and Identifiers

☐ Related Substance relationships

☐ ToxPrint fingerprints (ChemoTyper)

☐ Associated ToxCast Assays

Presence in Lists

☐	Title	Description
☐	40CFR116.4	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
☐	40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
☐	ACSREAG	LIST: ACS Reagent Chemicals
☐	AEGVALUES	AEGLS: Acute Exposure Guideline Levels
☐	ALGALTOX	LIST: Algal Toxins
☐	ALLSURFACTANTS	CATEGORY: Surfactants
☐	AMINOACIDS	CATEGORY: Amino acids
☐	AMPHIBOLES	Amphibole minerals
☐	ANTIBIOTICS	CATEGORY(PHARMACEUTICALS): Antibiotics
☐	ANTIMICROBIALS	CATEGORY(WIKILIST)ANTIMICROBIALS: Antimicrobials from Wikipedia
☐	AOPSTRESSORS	List of Adverse Outcome Pathway Stressors
☐	APCRARETRO	LIST: APCRA Chemicals for Retrospective Analysis
☐	APCRARETRO	APCRARETRO Adverse Outcome Chemicals

Rows: 319

Download Export file for the chemicals selected

5

DOWNLOAD EXPORT FILE

Batch Search

AutoSave Off CCD-Batch-Search_2022-03-27_05_36_52.xlsx Williams, Antony WA

File Home Insert Draw Page Layout Formulas Data Review View Developer Help

Paste Font Alignment Number Styles Cells Editing Sensitivity

Clipboard Font Alignment Number Styles Cells Editing Sensitivity

A2 DTXSID9020299

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
	DTXSID	PREFERRED_NAME	INCHIKEY	CASRN	SMILES	MOLECULAR_FORMULA	AVERAGE	MONOISOTOPE	SAFETY_D	DATA_SOURCE	NUMBER	IRIS_LINK	ATMOSPHERIC	BIOCONCENTRATION	BIODEGRADABILITY	BOILING
1	DTXSID9020299	Chlorobenzilate	RAPBNVD	510-15-6	CCOC(=O)C16H14Cl2O3		325.19	324.032	Y		154	16 Y	1.37E-11	477.542	4.6243	349.9
2	DTXSID6034712	Mesosulfuron-methyl	NIFKBBMC	208465-21	COC(=O)C C17H21N5O9S2		503.5	503.0781	Y		95	10	1.79E-11	3.2453	4.26547	254.0
3	DTXSID7034753	Foramsulfuron	PXDNXJSD	173159-57	COC1=CC(C17H20N6O7S		452.44	452.1114	Y		95		2.35E-11	3.84639	5.67465	265.1
4	DTXSID1033664	17-Methyltestosterone	GCKMFJBC	58-18-4	C[C@]1(O C20H30O2		302.458	302.2246	Y		145	1377	3.99E-11	62.2298	97.9166	294.8
5	DTXSID8034401	Buprofezin	PRLVTUNV	69327-76-	CC(C)N1C(C16H23N3OS		305.44	305.1562	Y		134	42	1.38E-11	52.49	6.89035	353.7
6	DTXSID0020529	2,4-Dinitrotoluene	RMBFBMJ	121-14-2	CC1=C(C=C(C7H6N2O4		182.135	182.0328	Y		198	379 Y	1.63E-12	9.12436	3.5609	299.8
7	DTXSID2034673	Iodosulfuron methyl ester	JUJFQMPK	144550-36	[Na+].COC C14H13IN5NaO6S		529.24	528.9529	Y		88		1.77E-11	3.51252	4.73647	265.0
8	DTXSID7024247	Pentachlorobenzene	CEOCDNV	608-93-5	C1C1=CC(C C6HCl5		250.32	247.8521	Y		170	84 Y	2.25E-13	5620.75	6.16855	277.0
9	DTXSID0034227	Icaridin	QLHULAH	119515-38	CCC(C)OC(C12H23NO3		229.32	229.1678	Y		111	67	1.82E-11	3.81105	5.17405	251.8
10	DTXSID0020440	Dichlorprop	MZHCENG	120-36-5	CC(OC1=C C9H8Cl2O3		235.06	233.985	Y		164	89	1.16E-11	3.54397	3.53597	298.4
11	DTXSID9034816	Monocrotophos	KRTSDMXI	6923-22-4	CNC(=O)\(C7H14NO5P		223.165	223.061	Y		152	274	2.77E-11	0.922318	4.13837	301.7
12	DTXSID8021301	Tamoxifen citrate	FQZTYWI	54965-24-	OC(=O)CC C32H37NO8		563.647	563.2519	Y		90	17257	2.9E-11	1209.93	3.36316	419.3
13	DTXSID7032553	Flumetralin	PWNAWO	62924-70-	CCN(CC1=C C16H12ClF4N3O4		421.73	421.0452	Y		117		1.38E-11	35265.1	3.54617	347.7
14	DTXSID6024048	Difenzoquat metilsulfate	XQEMNBN	43222-48-	COS([O-])(C18H20N2O4S		360.43	360.1144	Y		79	20 Y	1.93E-11	565.107	13.7793	335.0
15	DTXSID3024104	Fluoranthene	GVEPBHJC	206-44-0	C1=CC2=C C16H10		202.256	202.0783	Y		211	398 Y	4.98E-11	3528.4	147.199	393.9
16	DTXSID8023890	Asulam	VGPYEHKC	3337-71-1	COC(=O)N C8H10N2O4S		230.24	230.0361	Y		133	19 Y	1.21E-11	2.50573	4.63676	254.8
17	DTXSID4032532	Carfentrazone-ethyl	MLKCGVH	128639-02	CCOC(=O)C15H14Cl2F3N3O3		412.19	411.0364	Y		133	9	2.16E-11	192.141	4.88739	352.4
18	DTXSID5032498	Triclosan	XEFQLINVI	3380-34-5	OC1=C(OC C12H7Cl3O2		289.54	287.9512	Y		246	2221	1.74E-11	52.8927	4.50619	342.3
19	DTXSID1021160	Picloram	NQQVFXU	1918-02-1	NC1=C(Cl) C6H3Cl3N2O2		241.45	239.926	Y		186	133 Y	8.15E-12	2.72427	4.09513	296.1
20	DTXSID9020160	Bifenthrin	OMFRMAI	82657-04-	CC1=C(C=C(C23H22ClF3O2		422.87	422.126	Y		172	246 Y	3.32E-11	4990.65	3.54377	370.9

Cover Sheet Main Data

Ready 100%

Work in Progress

New lists added regularly

In progress

- New chemicals registered daily and released with each new version of the Dashboard



The screenshot shows the ACS Publications website interface. At the top is the ACS Publications logo with the tagline "Most Trusted. Most Cited. Most Read." and a search bar. Below the header, navigation links include "RETURN TO ARTICLES ASAP", "< PREV", "CONTAMINANTS IN AQUA...", and "NEXT >". The main title of the article is "Prediction of Collision Cross-Section Values for Extractables and Leachables from Plastic Products". The authors listed are "Xue-Chao Song, Nicola Dreolin, Elena Canellas, Jeff Goshawk, and Cristina Nerin*". On the left, there is a "Cite this:" section with the citation "Environ. Sci. Technol. 2022, XXXX, XXX, XXX-XXX", the publication date "June 22, 2022", the DOI "https://doi.org/10.1021/acs.est.2c02853", and the copyright notice "© 2022 The Authors. Published by American Chemical Society". In the center, a table displays article metrics: "Article Views" (342), "Altmetric" (2), and "Citations" (-). Below the metrics is a link "LEARN ABOUT THESE METRICS". On the right, there are "Share" and "Add" buttons with corresponding icons. At the bottom left, there is a "RIGHTS & PERMISSIONS" link and icons for ACS, CC, and a person.

ACS Publications
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Prediction of Collision Cross-Section Values for Extractables and Leachables from Plastic Products

Xue-Chao Song, Nicola Dreolin, Elena Canellas, Jeff Goshawk, and Cristina Nerin*

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<https://doi.org/10.1021/acs.est.2c02853>
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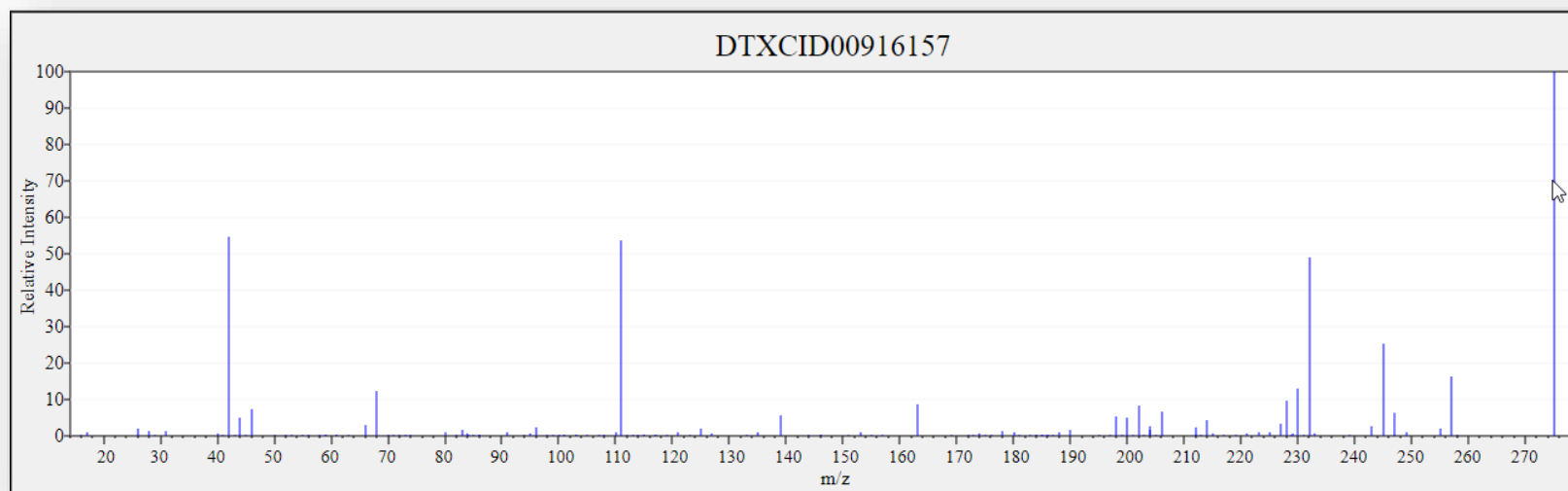
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Predicted Mass Spectra

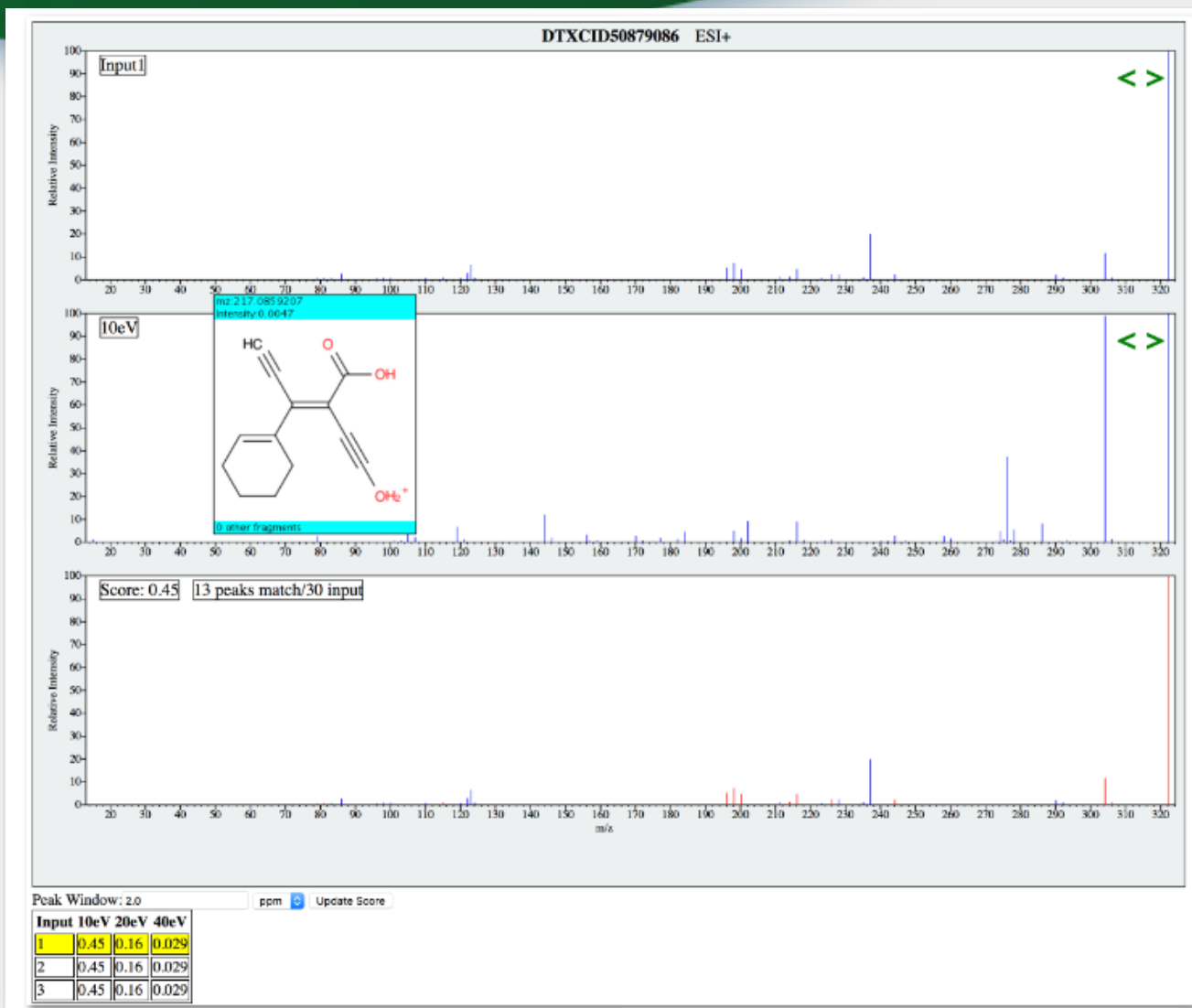
<http://cfmid.wishartlab.com/>



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



Spectral Viewer Comparison



Analytical and Bioanalytical Chemistry

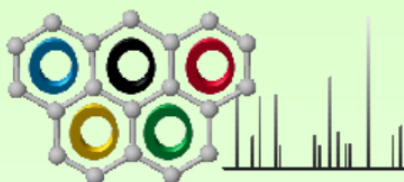
<https://doi.org/10.1007/s00216-019-02351-7>

In silico MS/MS spectra for identifying unknowns: a critical examination using CFM-ID algorithms and ENTACT mixture samples

Alex Chao^{1,2} • Hussein Al-Ghoul^{1,2} • Andrew D. McEachran^{1,3} • Ilya Balabin⁴ • Tom Transue⁴ • Tommy Cathey⁴ • Jarod N. Grossman^{2,3} • Randolph Singh^{1,5} • Elin M. Ulrich² • Antony J. Williams⁶ • Jon R. Sobus²

Received: 4 October 2019 / Revised: 27 November 2019 / Accepted: 11 December 2019

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CASMI 2017

CASMI 2017

Important Dates
Contest Rules
Challenge Data
Solutions
Preliminary results
Results
About the Team

CASMI 2016

CASMI 2014

CASMI 2013

CASMI 2012

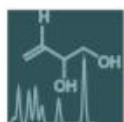
Critical Assessment of Small Molecule Identification

The experimental and computational mass spectrometry communities are invited to participate in the fifth round of an open contest on the identification of small molecules from mass spectrometry data.

This year the contest will test the applicability of MS and MS/MS on natural products chemistry identifications. With 45 (Category 1) and up to 243 (Categories 2&3) natural products challenges - including a few tricky ones - there's something for everyone!

CASMI 2017 is organised by Dr. Dejan Nikolic (University of Illinois at Chicago, USA), Dr. Nir Shahaf (Weizmann Institute of Science, Israel), Dr. Emma Schymanski (Eawag, Switzerland) and Dr. Steffen Neumann (IPB Halle, Germany).

Mailing lists



metabolites



Article

Revisiting Five Years of CASMI Contests with EPA Identification Tools

Table 2. Percentage of the total number of compounds from each CASMI contest year that were ranked in the top 5 by Competitive Fragmentation Modeling for Metabolite Identification (CFM-ID) only and by the summation of CFM-ID and DSSTox Data Source Counts (DS), alongside the percentage in the top 5 reported by the contest years' winning entry. Complete ranking results are provided in Supplemental File S1.

CASMI Year	CFM-ID Only	CFM-ID + DS	Winners' Results ¹	Total in DB/Total in Dataset ²
2012	36%	64%	36%	14/14
2013	81%	88%	88%	16/16
2014	57%	76%	71%	42/42
2016-training	63%	96%		312/312
2016-challenge	66%	94%	81%	208/208
2017	59%	53%	74% ³	227/243

Hazard Module

HAZARD																			
PREDICT																			
SEARCH																			
STANDARD																			
Hazard assessment profile																			
Full																			
Full																			
Custom																			
Emergency Response																			
Site-Specific Screening																			
Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable Authority: Authorita																			
CAS Name	Human Health Effects																		
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure							
60-35-5 Acetamide	L	I	I	VH	VH	L	M	M	I	I	L	I	I	I	I	L	L	L	L
107-13-1 Acrylonitrile	H	H	H	VH	VH	L	H	H	H	H	H	M	H	H	VH	H	H	H	L
1912-24-9 Atrazine	M	H	L	VH	L	H	H	H	H	M	M		H	L	M	VH	VH	H	L

United States
Environmental Protection
Agency

Chiral

- Metadata ranking of candidates based on mass/formula searching was a starting point
- Searching experimental spectra against *in silico* predictions was next.
- Searching experimental spectra against experimental spectra is the next phase.
- Assembling experimental mass spec data from the internet, homogenize formats and database – includes curation

- There are hundreds of methods distributed across the EPA website – that can be enabled by cheminformatics
 - Focus: Aggregate MS method documents and extract chemicals to make methods structure searchable
 - Vision: Search by structure/substructure/similarity to find existing method(s) as a starting point

- Presently working with scientists from NIST

Unified mass spectrometry approach for identifying plastics-related contaminant: Chemical coverage, applications and web resources

Mar 23, 2022 7:00pm - Mar 23, 2022 9:00pm

Overview

Comments

Description

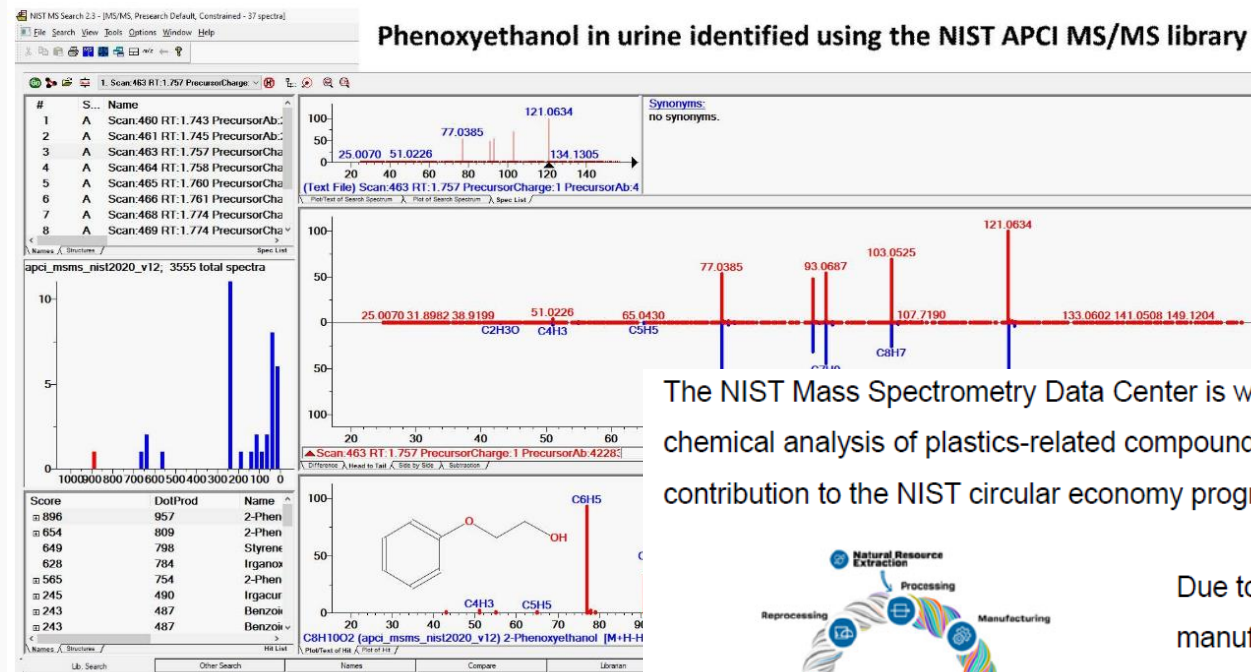
A comprehensive list of plastic monomers, additives, and processing aids containing more than 10,000 compounds has been published recently (Environ. Sci. Technol. 2021, 55, 9339-9351). According to ISO standards, USP compliant testing, and FDA/EPA

- Dataset to be released as a list
- Spectra will be added to our experimental spectral database for searching

Collaboration with NIST

>10,000 plastic related chemicals

We have identified phenoxyethanol, several phthalates and phthalate metabolites, and bisphenol A in pooled human urine samples (NIST/SRMs), together with other contaminants in need of further analysis. A similar study was conducted for extracts from orthopedic casts using 16 polymer extracts.



The NIST Mass Spectrometry Data Center is working on a comprehensive approach to the chemical analysis of plastics-related compounds (PRC) using mass spectrometry as a contribution to the NIST circular economy program (<https://www.nist.gov/circular-economy>).



Due to the versatility of plastics, many manufactured products and environmental pollutants are associated with PRC. 10,547 compounds including monomers, additives, and processing aids of the plastics industry (Environ. Sci. Technol. 2021, 55,9339-9351) and three types of ionizations has been used in this work to obtain mass spectra and build standard libraries of PRC.

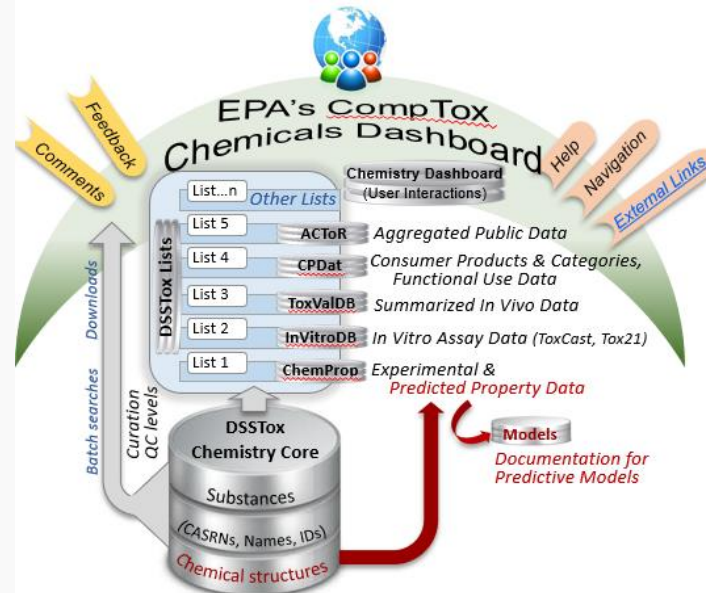
Request for participation

- Please point us to relevant datasets and articles
- Nothing is perfect – so please flag issues

The screenshot displays the EPA Dashboard interface. The top navigation bar includes links for Dashboard, Home, Search, Lists, About, and Tools. A 'Submit Comments' button is visible in the top right. The main content area features a chemical details page for Azithromycin, identified by the number 83905-01-5 and searched by DTXSID8. The chemical structure is shown with stereochemistry. A 'New Comment' modal is open, displaying details to be submitted with the comment: 'Text selected: Azithromycin', 'Found On: February 23 2022, 10:01:19 AM', 'Original Query: /dashboard/chemical/details/DTXSID8030760', and 'Browser: Mozilla on Win32'. The user's email, williams.antony@epa.gov, is shown. The comment text reads: 'It would be ideal to map other Azithromycin isomers as related substances for this chemical'. A 'SEND' button is at the bottom of the modal. The background page also shows sections for 'Quality Control Notes', 'Intrinsic Properties', and 'Molecular Formula: C₃₈H₇₂N₂O₁₂'.

Conclusion

- Dashboard access to data for ~900,000 chemicals, next release will update to **1.2 million** substances
- Extractable and leachables lists continue to expand
- “MS-Ready data” facilitates structure identification
- Data continues to grow with ongoing curation activities
- Proof-of-concept developments will release in future versions
- ***Do you want to learn more?***

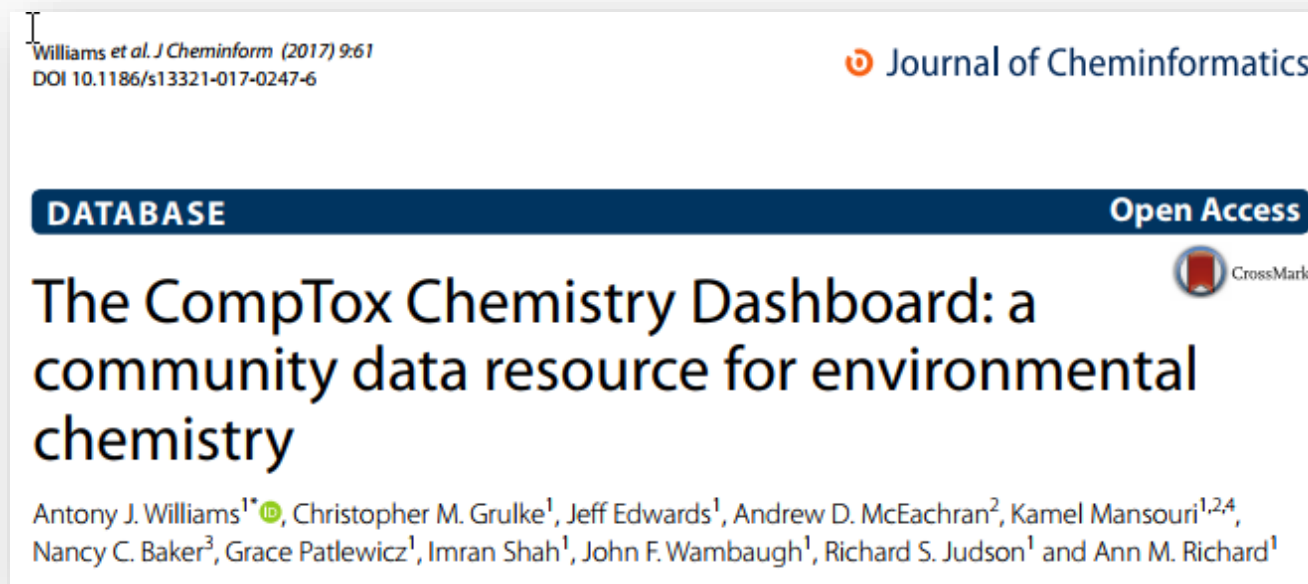


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<https://doi.org/10.1186/s13321-017-0247-6>