

The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data

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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

*August 21-25, 2016
ACS Fall Meeting, Philadelphia, PA*

Who is NCCT?

- National Center for Computational Toxicology – part of EPA’s Office of Research and Development
- Research driven by EPA’s *Chemical Safety for Sustainability Research Program*
 - Develop new approaches to **evaluate the safety of chemicals**
 - Integrate advances in biology, biotechnology, chemistry, exposure science and computer science
- Goal - To identify **chemical exposures** that may disrupt biological processes and cause adverse outcomes.

Introducing Our Latest Dashboard

<https://comptox.epa.gov>

- >720,000 chemicals
- >10 years assembling data



CompTox Dashboard

- Bisphenol
- Bisphenol A
- Bisphenol A (BPA)
- BISPHENOL A ANHYDRIDE
- Bisphenol A bis(2-hydroxyethyl)ether
- Bisphenol A bis(2-hydroxyethyl ether) diacrylate
- Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
- Bisphenol A bis(2-hydroxy-3-methacryloxypropyl) ether
- Bisphenol A bis(2-hydroxy-3-methacryloyloxypropyl ether)

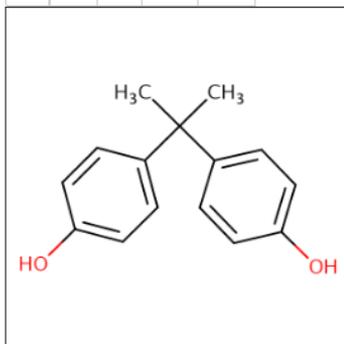
Help

Bisphenol A

Bisphenol A

80-05-7 | DTXSID7020182

i Searched by Approved Name: Found 1 result for 'bisphenol A'.



Intrinsic Properties

Molecular Formula: C₁₅H₁₆O₂

Q Find All Chemicals 

Average Mass: 228.291 g/mol



Monoisotopic Mass: 228.115030 g/mol



Structural Identifiers

Record Information

Chemical Properties

External Links

Synonyms

Product Composition

ToxCast in Vitro Data

Exposure

Analytical

PubChem

Comments

Physicochemical Properties

Summary

Download as:

CSV

Excel

SDF

Octanol-Water
Partition Coefficient
(LogP)

Water Solubility

Melting Point

Boiling Point

Vapor Pressure

Soil Adsorption
Coefficient

Octanol-Air Partition
Coefficient

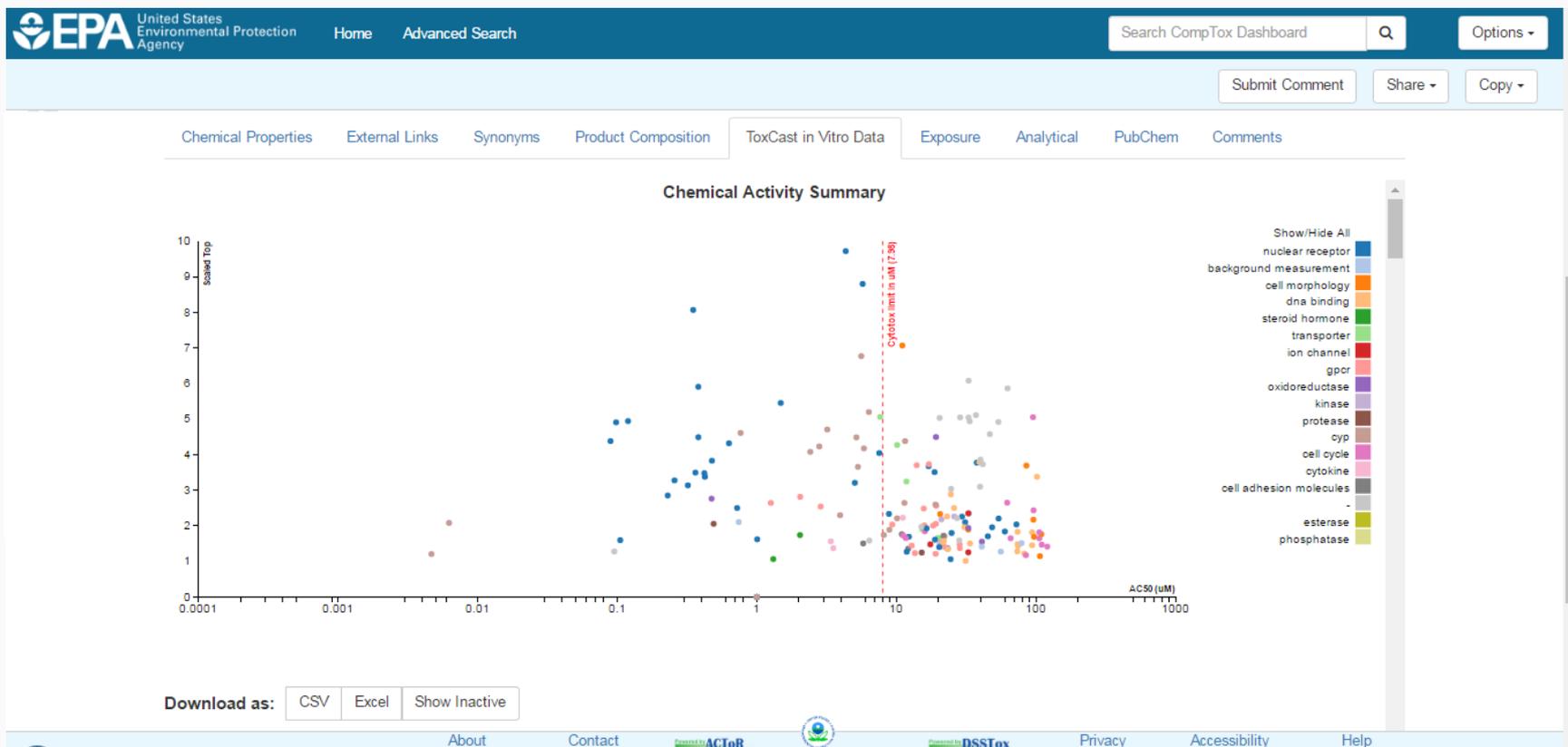
Atmospheric
Hydroxylation Rate

Biodegradation Half
Life

Bioaccumulation

Property	Average (Exp.)	Median (Exp.)	Range (Exp.)	Average (Pred.)	Median (Pred.)	Range (Pred.)	Result Unit
Octanol-Water Partition Coefficient (LogP)	3.38 (2)	3.43	3.43	3.42 (2)	3.42	3.20 to 3.64	-
Water Solubility	5.26e-04 (1)	5.26e-04	5.26e-04	2.22e-03 (2)	2.22e-03	7.56e-04 to 3.68e-03	mol/L
Melting Point	155 (7)	156	153 to 158	138 (2)	138	132 to 144	°C
Boiling Point	200 (1)	200	200	349 (2)	349	334 to 364	°C
Vapor Pressure	-	-	-	7.06e-08 (1)	7.06e-08	-	mmHg
Soil Adsorption Coefficient	-	-	-	2.92 (2)	2.92	2.74 to 3.10	-
Octanol-Air Partition Coefficient	-	-	-	8.39 (1)	8.39	-	-
Atmospheric Hydroxylation Rate	-	-	-	-10.4 (1)	-10.4	-	-
Biodegradation Half Life	-	-	-	15.1 (1)	15.1	-	days
Bioaccumulation Factor	-	-	-	173 (1)	173	-	-
Bioconcentration Factor	1.64 (1)	1.64	1.64	82.0 (3)	82.0	1.38 to 173	-

Bioassay Screening Data



Functional Use and Composition

EPA United States Environmental Protection Agency Home Advanced Search Search CompTox Dashboard Q Options

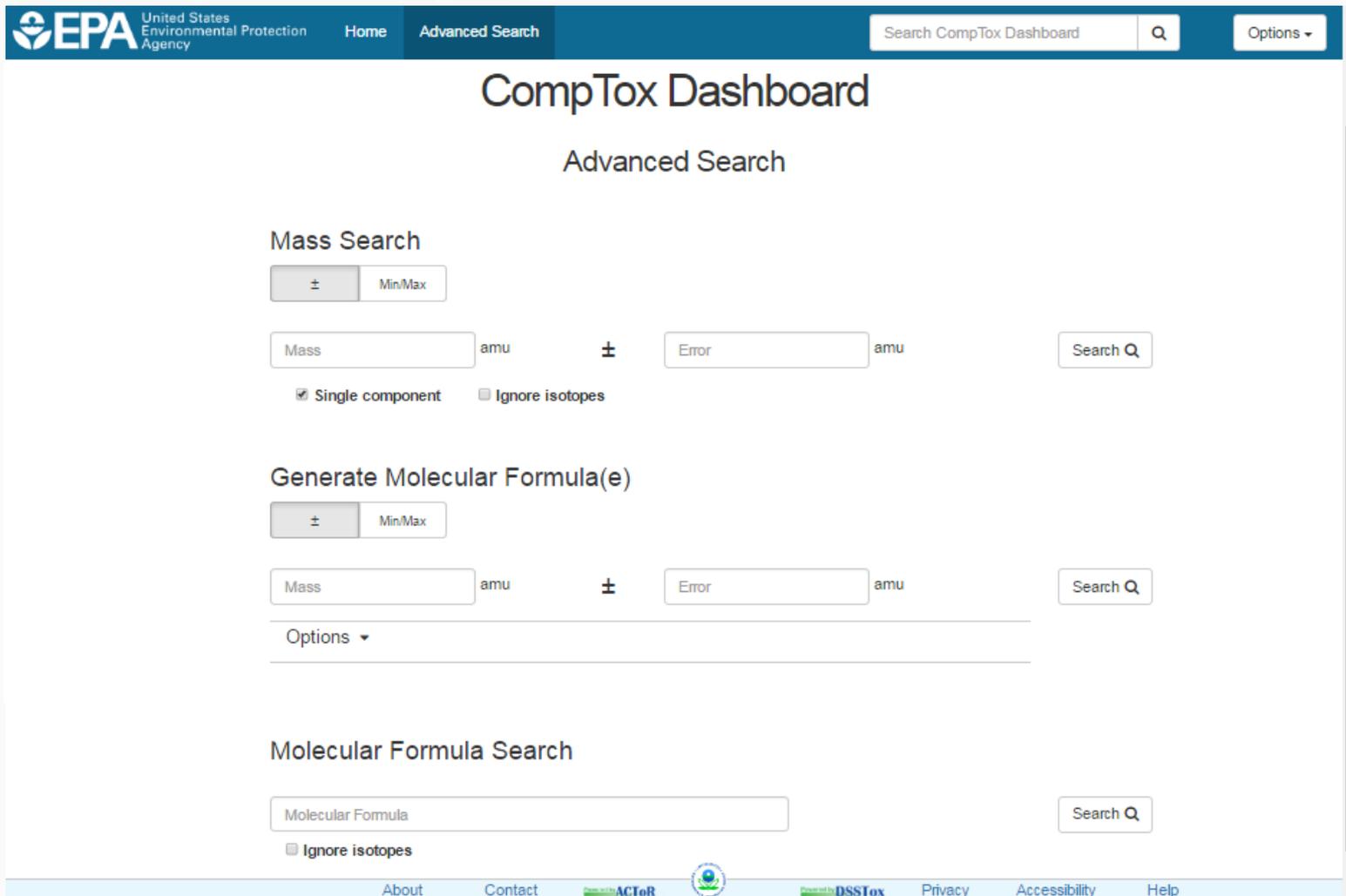
Submit Comment Share Copy

Chemical Properties External Links Synonyms **Product Composition** ToxCast in Vitro Data Exposure Analytical PubChem Comments

Product Composition

Product	Percent Composition ↓	Manufacturer
BISPHENOL-A (BPA)	100%	GENERAL ELECTRIC COMPANY
EPOXY PASTE PIGMENTS, 3402-3408	<100%PPM	SYSTEM THREE RESINS
ISOPROPYLIDENEDIPHENOL, 99+%, 23965-8	99%+	ALDRICH CHEMICAL CO
BISPHENOL A (RESIN GRADE) (43106)	97.8%	SHELL OIL COMPANY
4,4-ISOPROPYLIDENEDIPHENOL, 97%, 13302-7	97%	ALDRICH CHEMICAL CO
ICO-PATCH EPOXY RESIN HARDENER, PART B	80%	INTERNATIONAL COATINGS CO
ADHESIVE-SCOTCH-WELD (R) 2216 B GRAY	72%	3M COMPANY
EPOCAST HARDENER 946, FPC 5000	45%	CIBA-GEIGY CORP
EPOLITE 1350 HANDENER	35-50	HEXCEL CORP, RESINS GROUP
EL-CHEM NO 200 PRIMER PART.B	32.5%	ELECTRO CHEMICAL ENGINEERING &

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The screenshot shows the EPA CompTox Dashboard's Advanced Search page. At the top, there is a navigation bar with the EPA logo, 'Home', 'Advanced Search', a search box for 'Search CompTox Dashboard', and an 'Options' dropdown. The main heading is 'CompTox Dashboard' followed by 'Advanced Search'. There are three main search sections: 'Mass Search', 'Generate Molecular Formula(e)', and 'Molecular Formula Search'. Each section has a '±' button and a 'Min/Max' button. The 'Mass Search' and 'Generate Molecular Formula(e)' sections have input fields for 'Mass' and 'Error' in 'amu', a 'Search Q' button, and checkboxes for 'Single component' and 'Ignore isotopes'. The 'Molecular Formula Search' section has a 'Molecular Formula' input field, a 'Search Q' button, and an 'Ignore isotopes' checkbox. The footer contains links for 'About', 'Contact', 'ACToR', 'DSSTox', 'Privacy', 'Accessibility', and 'Help'.

Mass Search

± Min/Max

Mass amu ± Error amu Search Q

Single component Ignore isotopes

Generate Molecular Formula(e)

± Min/Max

Mass amu ± Error amu Search Q

Options ▾

Molecular Formula Search

Molecular Formula Search Q

Ignore isotopes

About Contact   Privacy Accessibility Help

Monoisotopic Mass Search

Mass Search

± Min/Max

amu

±

amu

Single component

Ignore isotopes

Monoisotopic Mass Search

Mass Search

± Min/Max

Found 344 results for '215.096 ± 0.005 amu'

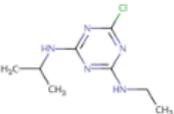
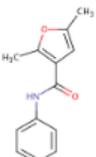
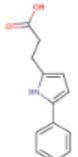
amu ± amu

Single component Ignore isotopes

Number of
Sources ↑↓

 Searched by Mass and single component chemicals: Found 344 res

Download as:

Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	Number of Sources	Monoisotopic Mass ↑↓	Mass Difference ↑↓	
	Atrazine	1912-24-9	DSSTox Low	59	5.093773	-0.0022	<input type="checkbox"/>
	Furcarbanil [ISO]	28562-70-1	Public Medium		5.094629	-0.0014	<input type="checkbox"/>
	5-Phenylpyrrole-2-propionic acid	79720-70-0	Public Medium	5	5.094629	-0.0014	<input type="checkbox"/>

0

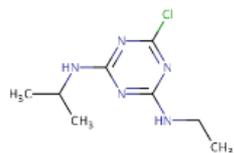
Formula Search

Molecular Formula Search

Molecular Formula Search

Found 8 results for 'C8H14ClN5'

Number of
Sources ↑↓



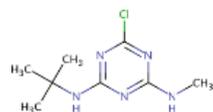
Atrazine

1912-24-9

DSSTox Low

59

215.093773



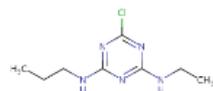
GS 18183

34333-27-2

Public Medium

3

215.093773



6-Chloro-N²-ethyl-N⁴-pr...

90952-64-0

Public Low

1

215.093773



Formula Searching

Formulae matching Bisphenol A

Intrinsic Properties

Molecular Formula: C₁₅H₁₆O₂

Average Mass: 228.291 g/mol

Monoisotopic Mass: 228.115030 g/mol

Q Find All Chemicals

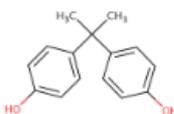
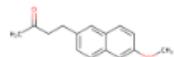
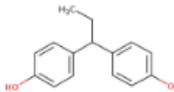
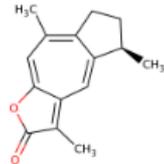
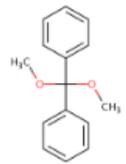
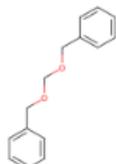
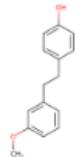
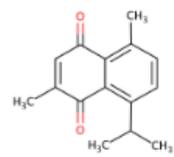
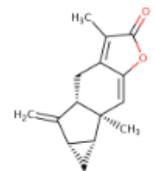
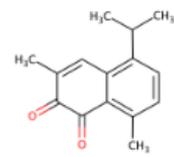
Search
across all
content
contained
within the
iCSS
CompTox
Dashboard

Formula Search Results

Search Results

Searched by Molecular Formula Found 215 results for 'C15H16O2'.

Download as: CSV Excel SDF

Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	Number of Sources ↑↓	Monoisotopic Mass ↑↓
 <p>Bisphenol A 80-05-7</p>	 <p>Nabumetone 42924-53-8</p>	 <p>4,4'-Propane-1,1-diylidiphenol 1576-13-2</p>	 <p>Gweicurculactone 123914-43-2</p>	 <p>1,1'-(Dimethoxymethylene)bisbe... 2235-01-0</p>
 <p>Preventol D2 2749-70-4</p>	 <p>4-Hydroxy-3'-methoxybibenzyl 59586-27-5</p>	 <p>Stahlianthusone 87018-26-6</p>	 <p>CHLORANTHALACTONE A 66395-02-6</p>	 <p>1,2-Naphthalenedione, 3,8-dime... 5574-34-5</p>

Download to Excel

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CompToxAdvancedSearch_2016-08-14_23-46-20.xls - Excel Williams, Antony

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW ESRI MAPS ACROBAT

Clipboard Font Alignment Number Styles Cells Editing

	A	B	C	D	E	F	G	H	I
1	DTXSID	CAS RN	PREFERRED NAME	IUPAC NAME	FORMULA	MONOISOTOPIC	AVERAGE MASS	SMILES	INCHI KEY
2	DTXSID7020182	80-05-7	Bisphenol A	4,4'-(Propane-2,2-diyl)diphenol	C15H16O2	228.1150298	228.2910004	CC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	IISBACLAFKSPIT-UHFFFAOYSA-N
3	DTXSID7042275	837-08-1	Phenol, 2-[1-(4-hydroxyphenyl)-1-	Hydroxyphenyl)propan-2-	C15H16O2	228.1150298	228.2910004	CC(C)(C1=CC=C(O)C=C1)C1=C(O)C=CC=C1	MLCQXUZAXKTSG-UHFFFAOYSA-N
4	DTXSID3044594	1576-13-2	4,4'-Propane-1,1-	4,4'-(Propane-1,1-(6-Methoxynaphthalen-2-yl)butan-2-one	C15H16O2	228.1150298	228.2910004	CCC(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1	YKPAABNCNAGAAJ-UHFFFAOYSA-N
5	DTXSID4045472	42924-53-8	Nabumetone	2,2'-Methylenebis(4-methylphenol)	C15H16O2	228.1150298	228.2910004	COC1=CC2=CC=C(CCC(C)=O)C=C2C=C1	BLXJMDCKKMKV-UHFFFAOYSA-N
6	DTXSID0062923	3236-63-3	methylenebis[4-methyl-	(5R)-3,5,8-Trimethyl-6,7-dihydroazuleno[6,5-	C15H16O2	228.1150298	228.2910004	CC1=CC(CC2=C(O)C=CC(C)=C2)=C(O)C=C1	XZXYQEHISUMZAT-UHFFFAOYSA-N
7	DTXSID50154143	123914-43-2	Gweicurculactone	3-Methoxy-5-(2-methylphenol)	C15H16O2	228.1150298	228.2910004	3C=C12	OGJFTQVVQMGJG-MRVPVSSYSA-N
8	DTXSID80170114	17635-59-5	Phenol, 3-methoxy-5-(2-1,1'-	3-Methoxy-5-(2-1,1'-(Dimethoxymethylene)bis[4-methylphenol]	C15H16O2	228.1150298	228.2910004	COC1=CC(CCC2=CC=CC=C2)=C(O)C=C1	HPEFWCAKFRCLBD-UHFFFAOYSA-N
9	DTXSID90176884	2235-01-0	(Dimethoxymethylene)bis[4-methylphenol]	(Dimethoxymethylene)bis[4-methylphenol]	C15H16O2	228.1150298	228.2910004	COC(OC)(C1=CC=CC=C1)C1=CC=CC=C1	NYRVXYOKUZSUDA-UHFFFAOYSA-N
10	DTXSID60181905	2749-70-4	Preventol D2	1-Methoxy-2-((4-methoxyphenyl)methyl)-1,2-Naphthalenedione,	C15H16O2	228.1150298	228.2910004	C(OCC1=CC=CC=C1)OCC1=CC=CC=C1	JCTHGPXQLMSDK-UHFFFAOYSA-N
11	DTXSID00184652	30567-87-4	methoxyphenyl)methyl)	3,8-Dimethyl-5-(propan-2-yl)naphthalene-1,2-dione	C15H16O2	228.1150298	228.2910004	COC1=CC=C(CC2=CC=CC=C2OC)C=C1	KVCVHSGCINIKCE-UHFFFAOYSA-N
12	DTXSID80204286	5574-34-5	3,8-dimethyl-5-(1-methoxyphenyl)methyl)	1,1'-Methylenebis(2-hydroxy-3-	C15H16O2	228.1150298	228.2910004	C1	GREWJSSEUGRGIT-UHFFFAOYSA-N
13	DTXSID10206935	5819-93-2	Methane, bis-(o-	4-[2-(3-	C15H16O2	228.1150298	228.2910004	COC1=CC=CC=C1CC1=CC=CC=C1OC	DPRFNHUMLZXNR-UHFFFAOYSA-N
14	DTXSID40208245	59586-27-5	4-Hydroxy-3'		C15H16O2	228.1150298	228.2910004	COC1=CC=CC(CCC2=CC=C(O)C=C2)=C1	QHWSNPUNTSCHIE-UHFFFAOYSA-N

Download as SDF file

Download as:

CSV ▾

Excel ▾

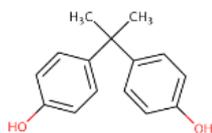
SDF ▾

All Results

Selected Chemicals

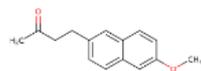
View Selected

Hide Multicomponent Chemicals



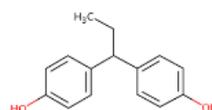
Bisphenol A

80-05-7



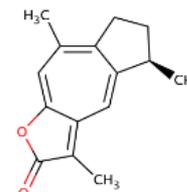
Nabumetone

42924-53-8



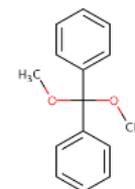
4,4'-Propane-1,1'-diylidenebis(4-hydroxyphenyl)

1576-13-2



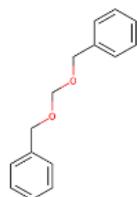
Gweicurculactone

123914-43-2



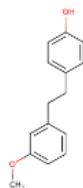
1,1'-(Dimethoxymethyl)bis(4-phenyleneoxy)

2235-01-0



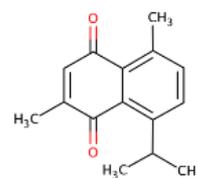
Preventol D2

2749-70-4



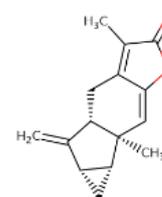
4-Hydroxy-3'-methoxybenzyl 4-methoxybenzoate

59586-27-5



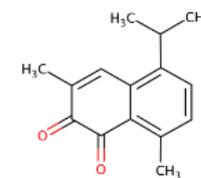
Stahlianthusone

87018-26-6



CHLORANTHALACTONE

66395-02-6



1,2-Naphthalenedione, 1,4-dimethyl-3-isopropyl-

5574-34-5

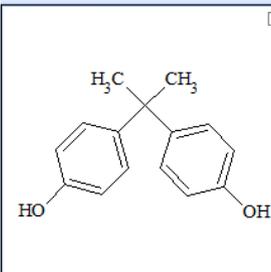
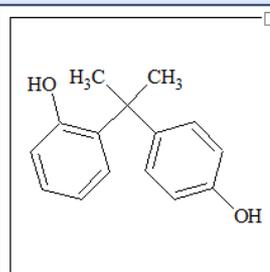
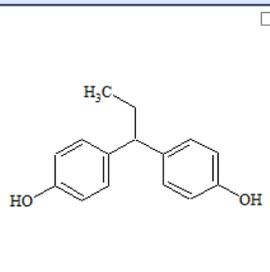
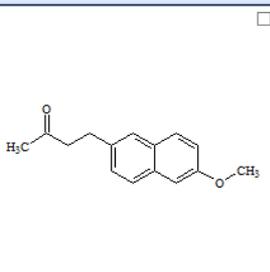
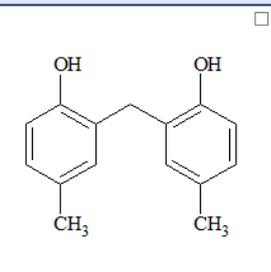
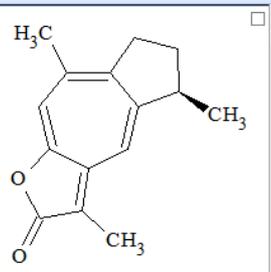
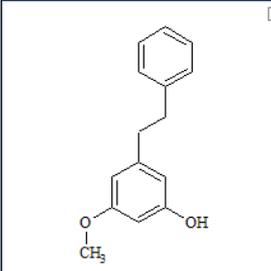
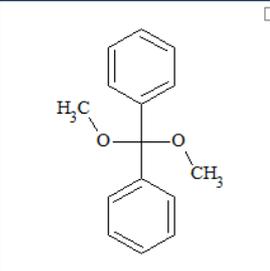
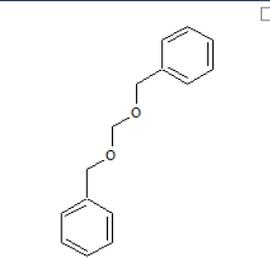
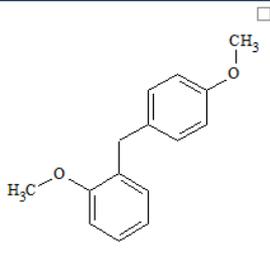
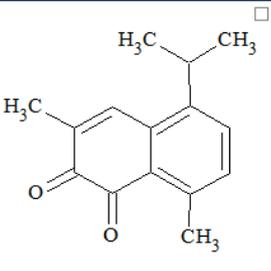
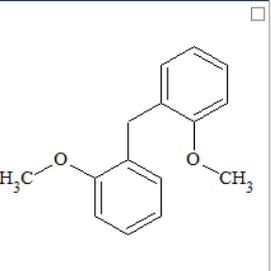


SDF file downloaded to desktop

ACD/ChemFolder: Database Window - [C:\USERS\AWILLID\DOWNLOADS\COMPTOXADVANCEDSEARCH_2016-08-20_17-49-02.SDF]

Database View Record Search Lists Plates Options ACD/Labs Help

Tile Table Default with User Data Screen Form 1

					
DTXSID: DTXSID7020182 CAS.RN: 80-05-7 PREFERRED.NAME: Bisphenol A IUPAC.NAME: 4,4'-(Propane-2,2-diy)ldiphenol MOLECULAR.FORMULA: C15H16O2 MONOISOTOPIC.MASS: 228.115029755	DTXSID: DTXSID7042275 CAS.RN: 837-08-1 PREFERRED.NAME: Phenol, 2-[1-(4-hydroxyphenyl)propan IUPAC.NAME: 2-[2-(4-Hydroxyphenyl)propan MOLECULAR.FORMULA: C15H16O2 MONOISOTOPIC.MASS: 228.115029755	DTXSID: DTXSID3044594 CAS.RN: 1576-13-2 PREFERRED.NAME: 4,4'-(Propane-1,1-diyl)diph IUPAC.NAME: 4,4'-(Propane-1,1-diyl)diphenol MOLECULAR.FORMULA: C15H16O2 MONOISOTOPIC.MASS: 228.115029755	DTXSID: DTXSID4045472 CAS.RN: 42924-53-8 PREFERRED.NAME: Nabumetone IUPAC.NAME: 4-(6-Methoxynaphthalen-2-yl) MOLECULAR.FORMULA: C15H16O2 MONOISOTOPIC.MASS: 228.115029755	DTXSID: DTXSID0062923 CAS.RN: 3236-63-3 PREFERRED.NAME: Phenol, 2,2'-methylenebi IUPAC.NAME: 2,2'-Methylenebis(4-methylphe MOLECULAR.FORMULA: C15H16O2 MONOISOTOPIC.MASS: 228.115029755	DTXSID: DTXSID50154143 CAS.RN: 123914-43-2 PREFERRED.NAME: Gweicurcylactone IUPAC.NAME: (5R)-3,5,8-Trimethyl-6,7-dihydr MOLECULAR.FORMULA: C15H16O2 MONOISOTOPIC.MASS: 228.115029755
					
DTXSID: DTXSID80170114	DTXSID: DTXSID90176884	DTXSID: DTXSID60181905	DTXSID: DTXSID00184652	DTXSID: DTXSID80204286	DTXSID: DTXSID10206935

ID: 2 A: 2/214 B: 214 Last Updated: 20/08/2016 17:49 Single DB

1-ChemSketch 2-Database

Rank-Ordering of “Known-Unknowns” using ChemSpider

RESEARCH ARTICLE

Identification of “Known Unknowns” Utilizing Accurate Mass Data and ChemSpider

Table 1. Searching ChemSpider by Elemental Composition then Sorting by Number of Associated References

Class of compounds	Number compounds in class	Position of compound sorted in de		
		#1	#2	#3
Drugs	45	43	1	1
Pesticides	8	7	1	
Toxins	2	2		
Polymer antioxidants	15	15		
Polymer UV stabilizers	10	8	1	1
Polymer clarifying agent (Irgaclear DM)	1			
Polyurethane additives	4	2	1	
Natural products	3	2		1
Herbicide (clofibric acid)	1	1		
Artificial sweetener (sucralose)	1	1		
Total compounds ChemSpider	90	81	4	3
Total compounds CAS Registry [1]	90	84	4	1

Comparing Performance



57 Million
chemical structures



CompTox Dashboard **721k structures**

- Remember:
 - Focus on high quality data and curation
 - Data sources include EPA data sources and a focus on environmental chemistry
- No “dilution” by chemical vendors

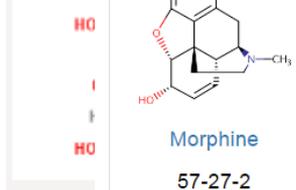
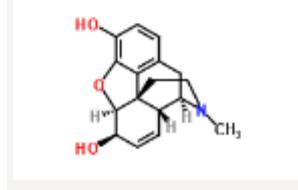
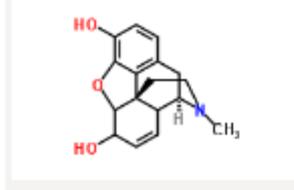
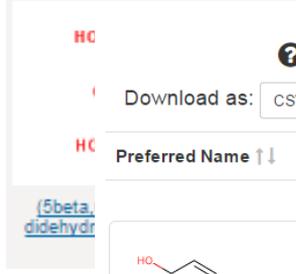
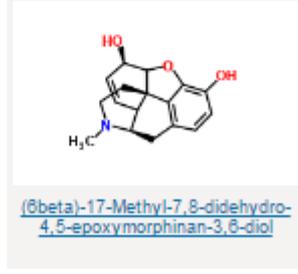
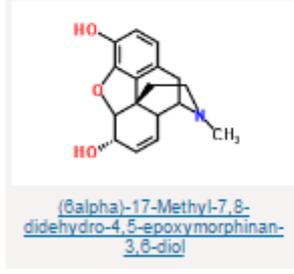
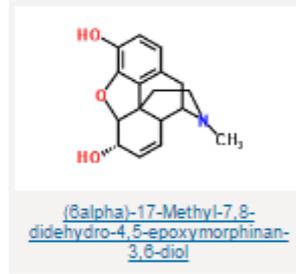
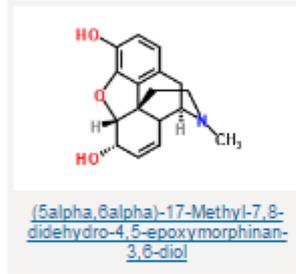
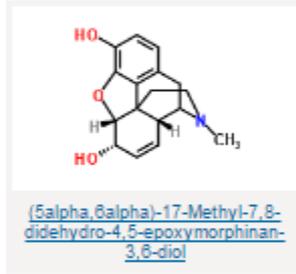
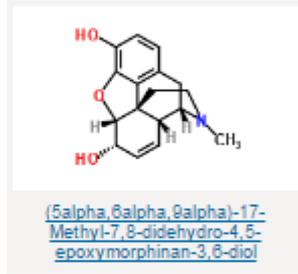
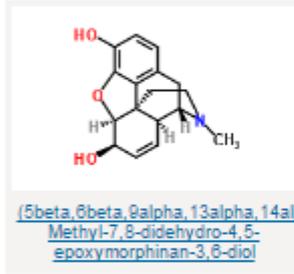
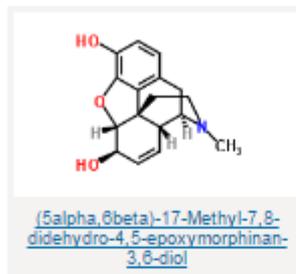
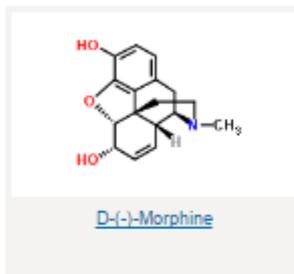
< Data Sources

<u>Data Source</u>	<u>Count</u>	<u>Date Created</u>	<u>Last Updated</u>
Aurora Feinchemie	25288289	13/04/2009	12/06/2016
PubChem	10881750	15/04/2008	25/06/2015
AKos	8226932	15/04/2008	15/06/2016
Mcule	5649548	21/01/2014	30/10/2015
Molport	5292029	09/02/2010	02/09/2014

Dilution Example... Morphine Skeleton

Found 32 results

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



HC Searched by InchiKey Skeleton: Found 3 results for 'BQJCRHHNABKAKU'.

Download as:

HC	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	Number of Sources ↑↓	Monoisotopic Mass ↑↓
HC	Morphine	57-27-2			
	Morphinan-3,6-d...	16206-77-2			
	Morphinan-3,6-a...	67293-88-3			

Bisphenol A as an example

ChemSpider: 1564 Structures

FILTER ▾

Search Hits Limit: 100 ▾

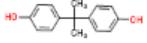
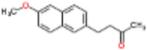
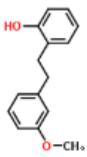
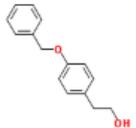
CLEAR FORM

SEARCH

Found 1564 results

Search term: MF = 'C_{15}H_{16}O_{2}'

1 2 3 4 5

ID	Structure	Molecular Formula	Molecular Weight	# of Data Sources ▾	# of References	# of PubMed	# of RSC
6371 		C ₁₅ H ₁₆ O ₂	228.2863	117	1631	3029	423
4256 		C ₁₅ H ₁₆ O ₂	228.2863	110	420	368	23
8760824		C ₁₅ H ₁₆ O ₂	228.2863	58	67	0	1
2285031		C ₁₅ H ₁₆ O ₂	228.28634	48	57	0	0

Bisphenol A as an example Dashboard: 215 Structures

 United States Environmental Protection Agency

Home Advanced Search

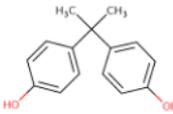
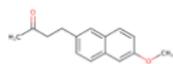
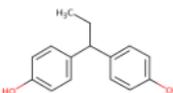
Search CompTox Dashboard

Options ▾

Search Results

 Searched by Molecular Formula, ignoring isotopes. Found 215 results for 'C15H16O2'.

Download as:

Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	Number of Sources ↑↓	Monoisotopic Mass ↑↓	
	Bisphenol A	80-05-7	DSSTox High	60	228.115030	<input type="checkbox"/>
	Nabumetone	42924-53-8	DSSTox Low	16	228.115030	<input type="checkbox"/>
	4,4'-Propane-1,1-di...	1576-13-2	DSSTox Low	5	228.115030	<input type="checkbox"/>

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Chemical Identification Dashboard vs ChemSpider

Monoisotopic Mass (± 0.005 amu) Search

Sorted by number of references (ChemSpider) or data sources (Dashboard)

Source of List	# of Compounds	Search Tool	Mean Position	Median Position	Position of compound sorted				
					#1	#2	#3	#4	#5+
McEachran et al Wastewater	34	ChemSpider	1.8	1	28	5	0	0	1
		Dashboard	1.3	1	31	2	0	0	1
Misc. NTA Compounds	13	ChemSpider	2	1	7	5	0	0	1
		Dashboard	1.7	1	10	2	0	0	1
Bade et al (2016)	19	ChemSpider	2.1	1	11	2	5	0	1
		Dashboard	1.6	1	12	3	3	1	0
Rager et al (2016)	24	ChemSpider	2.25	1	15	2	1	2	4
		Dashboard	1.08	1	22	2	0	0	0

Dashboard vs ChemSpider Ranking Summary

- Selected peer-reviewed publications
- 162 total individual chemicals in search

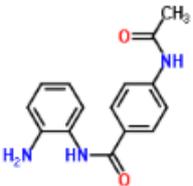
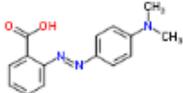
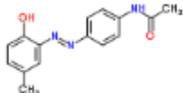
	Mass-based Searching		Formula Based Searching	
	<i>Dashboard</i>	<i>ChemSpider</i>	<i>Dashboard</i>	<i>ChemSpider</i>
Cumulative Average Position	1.3	2.2	1.2	1.4
% in #1 Position	85%	70%	88%	80%

ChemSpider 6926 Results!!

Found 6926 results

Search term: MF = 'C_{15}H_{15}N_{3}O_{2}'

1 2 3 4 5

ID	Structure	Molecular Formula	Molecular Weight	# of Data Sources	
<input type="checkbox"/> 2644		C ₁₅ H ₁₅ N ₃ O ₂	269.2985	86	Tacedinaline
<input type="checkbox"/> 9881 		C ₁₅ H ₁₅ N ₃ O ₂	269.2985	85	Methyl Red
<input type="checkbox"/> 10468668 		C ₁₅ H ₁₅ N ₃ O ₂	269.2985	33	C.I. Disperse Yellow 3

Using Functional Use to Sort Candidates

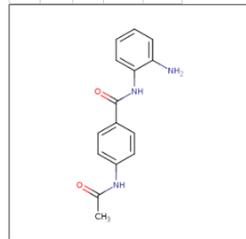
Tacedinaline

112522-64-2 | DTXSID60150095

Anti-cancer Drug

Searched by Approved Name: Found 1 result for 'tacedinaline'.

Q [] [] [] [] [] []



Intrinsic Properties

Molecular Formula: C₁₅H₁₅N₃O₂

Q Find All Chemicals

Average Mass: 269.304 g/mol

[]

Monoisotopic Mass: 269.116427 g/mol

[]

Structural Identifiers

Record Information

Chemical Properties External Links Synonyms Product Composition ToxCast in Vitro Data Exposure Analytical PubChem Comments

Frequent Uses and Functions



No product composition data found.

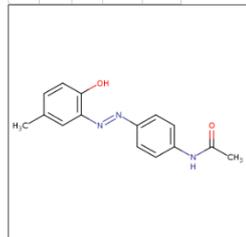
C.I. Disperse Yellow 3

2832-40-8 | DTXSID6021450

Textile/Product Dye

Searched by Approved Name: Found 1 result for 'C.I. Disperse Yellow 3'.

Q [] [] [] [] [] []



Intrinsic Properties

Molecular Formula: C₁₅H₁₅N₃O₂

Q Find All Chemicals

Average Mass: 269.304 g/mol

[]

Monoisotopic Mass: 269.116427 g/mol

[]

Structural Identifiers

Record Information

Chemical Properties External Links Synonyms Product Composition ToxCast in Vitro Data Exposure Analytical PubChem Comments

Frequent Uses and Functions



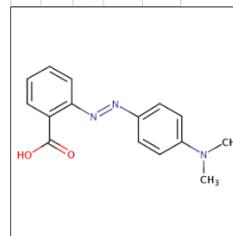
Methyl red

493-52-7 | DTXSID1042154

Microbiological Indicator Dye

Searched by Approved Name: Found 1 result for 'Methyl red'.

Q [] [] [] [] [] []



Intrinsic Properties

Molecular Formula: C₁₅H₁₅N₃O₂

Q Find All Chemicals

Average Mass: 269.304 g/mol

[]

Monoisotopic Mass: 269.116427 g/mol

[]

Structural Identifiers

Record Information

Chemical Properties External Links Synonyms Product Composition ToxCast in Vitro Data Exposure Analytical PubChem Comments

Frequent Uses and Functions



UNIVERSAL INDICATOR SOLUTION	0.05%	CENTRAL SCIENTIFIC CO
UNIVERSAL INDICATOR SOLUTION	0.05 %	SCIENCE KIT
UNIVERSAL INDICATOR SOLUTION,38826-16	0.05%	CENTRAL SCIENTIFIC CO
0098 TOTAL ALKALINITY TABLETS	0.04%	INDUSTRIAL MUNICIPAL EQUIP INC
84-8265 BOGEN UNIVERSAL INDICATOR SOLUTION	0.0185%	CAROLINA BIOGOLICAL SUPPLY CO
HTH 5-Way Test Kit - Hardness Indicator		
HTH 5-Way Test Kit - Cyanuric Acid Reagent		Arch Chemicals, Inc.
HTH 5-Way Test Kit - Cyanuric Acid Reagent		Arch Chemicals, Inc.

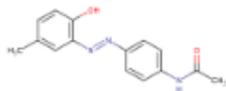
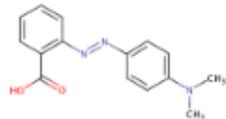
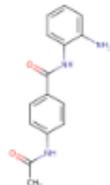
Same top hits – different ranking

90 hits only versus 6926 hits

Search Results

🔍 Searched by Molecular Formula, ignoring isotopes: Found 90 results for 'C15H15N3O2'.

Download as:

Structure	Preferred Name ↑↓	CAS-RN ↑↓	QC Level ↑↓	Number of Sources ↑↓	Monoisotopic Mass ↑↓
	C.I. Disperse Yellow 3	2832-40-8	DSSTox Low	18	269.116427
	Methyl Red	493-52-7	DSSTox Low	17	269.116427
	Tacedinaline	112522-64-2	Public Medium	4	269.116427

Dashboard: External Links to Analytical Methods

Chemical Properties External Links Synonyms Produ

General

-  EPA Substance Registry...
-  NIST Chemistry Webbook
-  Household Products Dat...
-  PubChem
-  Chemspider
-  CPCat
-  DrugBank
-  HMDB
-  Wikipedia
-
-  ToxPlanet
-  ChemHat: Hazards and ...

Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  EDSP Dashboard
-  Gene-Tox
-  HSDB
-  ToxCast Dashboard 2
-  LactMed
-  International Toxicity Esti

Publications

-  Toxline
-  Environmental Health P...
-  NIEHS
-  National Toxicology Prog...
-  Google Books
-  Google Scholar
-  Google Patents
-  PubMed

Analytical

-  National Environmental ...
-  RSC Analytical Abstracts

National Environmental Methods Index



NEMI National Environmental Methods Index

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Modify your search:

Search

RESULTS: Your search for "80-05-7" returned: 3 results.

Back to search

Page 1 of 1

Method ID	Method Source	Descriptive Method Name	Get Method	Search Ranking
O-1433-01	USGS-NWQL	Wastewater compounds in water by SPE and GC/MS	Download full method now (PDF file)	11
O-4434-12	USGS-NWQL	Steroid Hormones in Unfiltered Water by GC-MS/MS	Download full method now (PDF file)	11
O-4433-06	USGS-NWQL	Wastewater Compounds in Water by CLLE and GC-MS	Download full method now (PDF file)	11

RESULTS: Your search for "80-05-7" returned: 3 results.

Back to search

Page 1 of 1

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Search

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ACWI

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Accessibility

FOIA

Privacy

Google Analytics

Publishing

Journals, books and databases

Network access to this resource provided by

US Environmental Protection Agency



Journals ▾ Books ▾ Databases ▾ Alerts ▾ Other ▾ Help ▾ Feedback

Log in Register

Full Text ▾ 80-05-7

Advanced Search

Home > Search results

For Authors & Referees | For Librarians | For Members

Search results

You searched for : Keywords: 80-05-7

Modify Search | Search History

All (894) Journal Articles (17) Book Chapters (4) More abstracts (873)

Sort By: Relevance ▾ Results Per Page: 25 ▾

Save This Search ▾

Page 1 of 36 Go »

Select All Download Citation: RIS ▾ Go ? Check Access Expand All

Extractive - spectrophotometric determination of phenol in dian [4,4'-isopropylidenediphenol; bisphenol A].
Analytical Abstracts Abstract

Quantitative analysis of industrial products by capillary gas chromatography with on-column sample introduction.
Analytical Abstracts Abstract

Filters Applied

Content Type- all

Author

A. M. Calafat (23)
K. Sissell (17)
H. Nakazawa (15)
K. Hosoya (11)
X. Wang (11)

More

Integrated Google Chemical Searches

Web Images More...

Google

"80-05-7" OR "Bisphenol A"

Scholar About 17,100 results (0.09 sec)

Articles

Case law

My library

Any time

Since 2016

Since 2015

Since 2012

Custom range...

Sort by relevance

Sort by date

include patents

include citations

A review of the environmental fate, effects, and exposures of bisphenol A
CA Staples, PB Dome, GM Klecka, ST Oblock... - Chemosphere, 1998 - Elsevier
Bisphenol A (CAS 85-05-7) may be released into the environment through its use and handling, and permitted discharges. BPA is moderately soluble (120 to 300 mg/L at pH 7), may adsorb to sediment (Koc 314 to 1524), has low volatility, and is not persistent based ...
Cited by 1315 Related articles All 10 versions Web of Science: 821 Cite Save More

Environmental toxins: exposure to bisphenol A advances puberty
KL Howdeshell, AK Hotchkiss, KA Thayer... - Nature, 1999 - nature.com
Abstract Plastics and pesticides are examples of products that contain oestrogenic endocrine-disrupting chemicals, or EEDCs, which can interfere with mammalian development by mimicking the action of the sex hormone oestradiol 1. For instance, the ...
Cited by 739 Related articles All 10 versions Web of Science: 482 Cite Save More

Bisphenol-A: an estrogenic substance is released from polycarbonate flasks during autoclaving.
AV Krishnan, P Stathis, SF Permuth, L Tokes... - ..., 1993 - press.endocrine.org
In studies to determine whether Saccharomyces cerevisiae produced estrogens, the organism was grown in culture media prepared using distilled water autoclaved in polycarbonate flasks. The yeast-conditioned media showed the presence of a substance ...
Cited by 1504 Related articles All 10 versions Web of Science: 1069 Cite Save More

Google Chemical Searches Enhanced with Query Terms

"Mass Spectrometry" AND "80-05-7" OR "Bisphenol A"



... of estrogens, pesticides and **bisphenol A** in natural waters and drinking water treatment plants by solid-phase extraction–liquid chromatography–**mass spectrometry**

[S Rodriguez-Mozaz](#), [MJL de Alda](#), [D Barceló](#) - *Journal of Chromatography ...*, 2004 - Elsevier

A multi-residue analytical method has been developed for the determination of various classes of selected endocrine disruptors. This method allows the simultaneous extraction and quantification of different estrogens (estradiol, estrone, estriol, estradiol-17- ...

Cited by 344 [Related articles](#) [All 8 versions](#) [Web of Science: 228](#) [Cite](#) [Save](#) [More](#)

... compounds nonylphenol, nonylphenol ethoxylates, triclosan and **bisphenol A** in wastewater and sewage sludge by gas chromatography–**mass spectrometry**

[G Gatidou](#), [NS Thomaidis](#), [AS Stasinakis](#)... - ... of *Chromatography A*, 2007 - Elsevier

An integrated analytical method for the simultaneous determination of 4-n-nonylphenol (4-n-NP), nonylphenol monoethoxylate (NP1EO), nonylphenol diethoxylate (NP2EO), **bisphenol A** (BPA) and triclosan (TCS) in wastewater (dissolved and particulate phase) and sewage ...

Cited by 266 [Related articles](#) [All 11 versions](#) [Web of Science: 177](#) [Cite](#) [Save](#) [More](#)

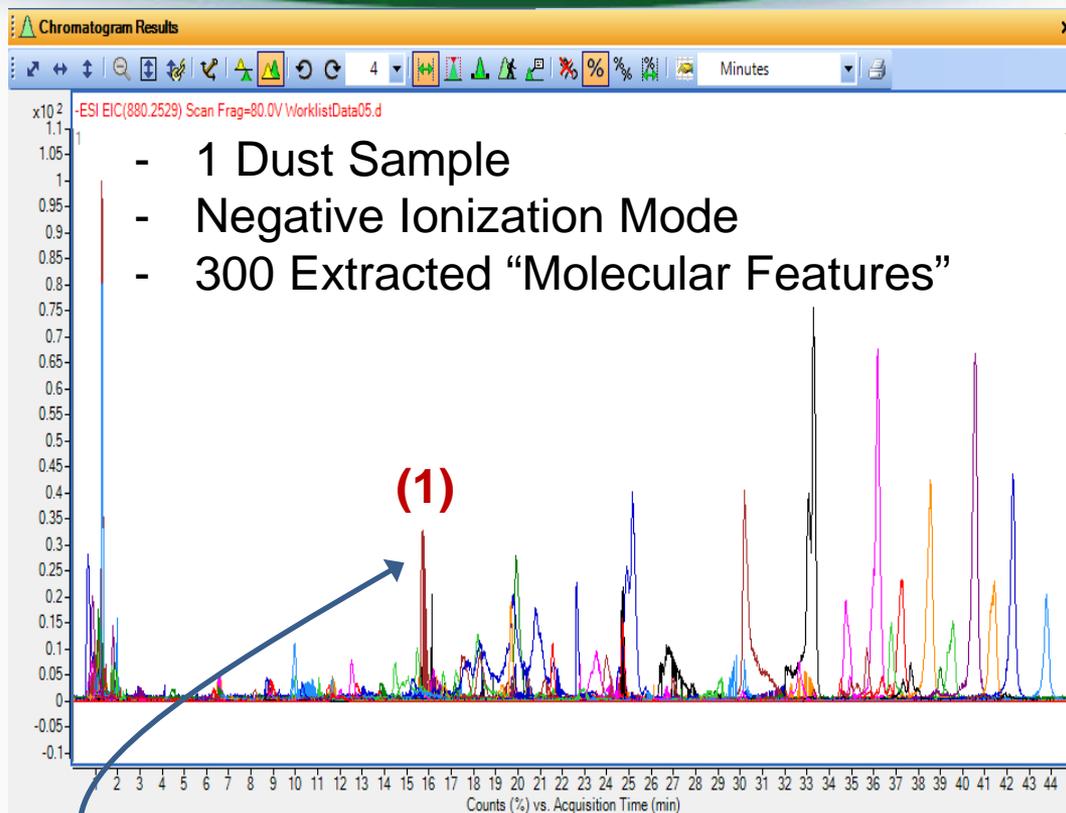
Quantitation of **bisphenol A** and **bisphenol A** glucuronide in biological samples by high performance liquid chromatography-tandem **mass spectrometry**

[W Völkel](#), [N Bittner](#), [W Dekant](#) - *Drug Metabolism and Disposition*, 2005 - ASPET

Abstract **Bisphenol A** (BPA) is a weak estrogen. Pharmacokinetic studies of BPA have demonstrated a rapid and extensive metabolism of BPA to the nonestrogenic BPA-monoglucuronide (BPA-gluc). Some investigators have reported that BPA was found at ...

Cited by 183 [Related articles](#) [All 5 versions](#) [Web of Science: 122](#) [Cite](#) [Save](#) [More](#)

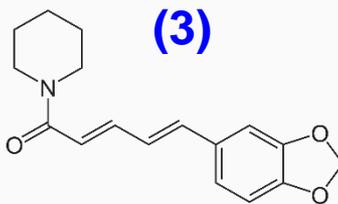
Non-Targeted Analysis Research



What is contained in house dust, waste streams etc???

- 1) Prioritize “Molecular Features”
- 2) Correctly assign formulas
- 3) Correctly assign structures
- 4) Determine chemical sources
- 5) Predict chemical concentrations

(2)
C₁₇H₁₉NO₃



(5)
12 µg/g

Previous Work with Suspect-Screening

Environment International 88 (2016) 269–280



Contents lists available at ScienceDirect

Environment International

journal homepage: www.elsevier.com/locate/envint



Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring



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The dashboard is being enhanced to support Non-targeted Analysis

- Presently researching rank-ordering based on other criteria – Pubmed
- Additional links to methods – CDC NIOSH
- Links to Mass Spec databases – Thermo’s mzCloud, Massbank. Metlin etc.
- Consider predicting metabolites and degradants
- Searching based on “MS-ready” structures

- Many compounds are salts – searches should be on the “neutral form”
- Need to search for adducts (+Na, +K, +NH₄), decarboxylation, loss of water etc.

- Dashboard support for MS is focused on NTA research – related to chemical exposure
- Dashboard outperforms ChemSpider for ranking chemicals of environmental concern
- New searches developed with Non-targeted Analysis in mind - new rank-ordering approaches in development

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