Developing a Predictive Mass Spectra Database for Structural Elucidation and Identification of Novel Arsenolipids in Seafood

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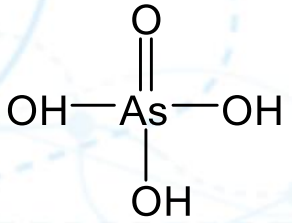
All Things Lab and Testing (ATLT) Insight Series | 4th September 2025.

What is Arsenic?

14 4A	15 5A	16 6A
6 **C** Carbon 12.011	7 **N** Nitrogen 14.007	8 **O** Oxygen 15.999
14 **Si** Silicon 28.086	15 **P** Phosphorus 30.974	16 **S** Sulfur 32.06
32 **Ge** Germanium 72.61	33 **As** Arsenic 74.922	34 **Se** Selenium 78.96
50 **Sn** Tin 118.710	51 **Sb** Antimony 121.757	52 **Te** Tellurium 127.60

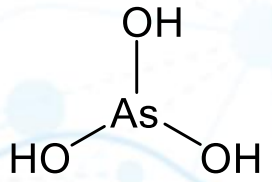
Ubiquitous, toxic, naturally occurring element

Exists in 4 oxidation states:



Arsenic acid

$H_3AsO_4 = (As^{V})$

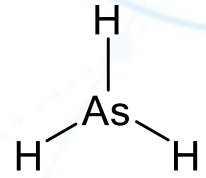


Arsenous acid

$H_3AsO_3 = (As^{III})$

As

Arsenic = (As^{0})



Arsane

$H_3As = (As^{-III})$

Not all Arsenic is Toxic

LD_{50} of Arsenicals in mice or rats (mg/kg)

Species	AsIII	AsV	MMA	DMA	AC	AsSugar	AB
LD_{50}	4.5	14 – 18	1,800	1,200	6000	*	10,000

Toxic → Moderately toxic → Nontoxic

*Kaise, T, et al., J. Food Hyg. Soc. Jpn. 1996, 37, 135-141.

Kenya Bureau of Standards
Standards for Quality life

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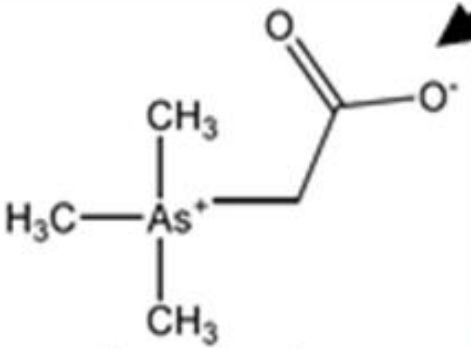
Toxicological Profile of Arsenicals

Seafood

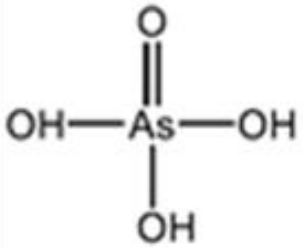


Arsenobetaine
(AsB)

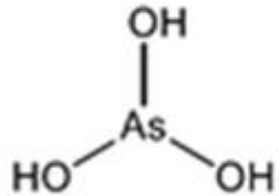
Non-toxic

Organoarsenicals

Unknown toxicity



Arsenic acid
(As^{V})



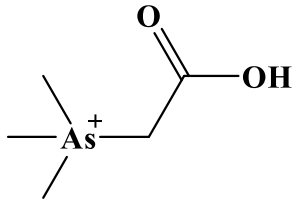
Arsenous acid
(As^{III})

Toxic

Luvonga, C., Rimmer C. A., Yu, L. L., Lee S. B., J. Agric. Food Chem. **2020**, 68, 943−960

Arsenobetaine

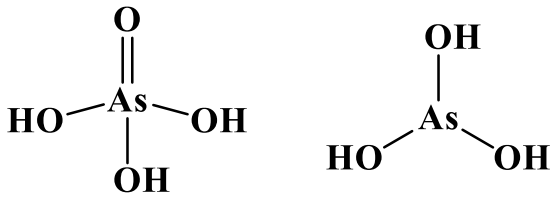
Most abundant Arsenic species in shellfish and finfish, non-toxic



Inorganic arsenic (iAs)

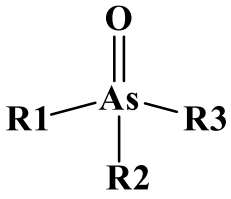
Minor component in most seafood, known carcinogen

Arsenate (As^{V}) **Arsenite (As^{III})**



Methylated Arsenicals

Minor constituents of seafood, metabolites of iAs, AsSugars & AsLipids



Examples:

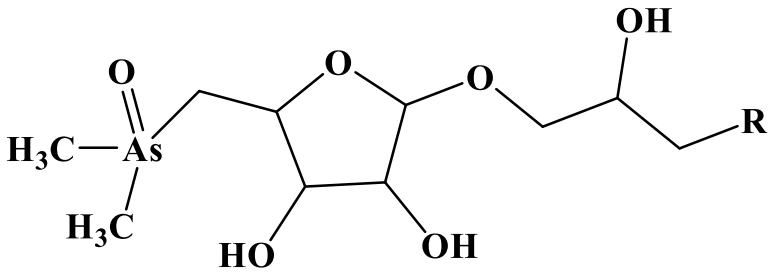
MMA: R_1=CH_3, R_{2-3}=OH

DMA: R_{1-2}=CH_3, R_3=OH

TMAO: R_{1-3}=CH_3

Arsenosugars (AsSugars)

Major arsenic compound in seaweed; metabolized by humans



Examples:

AsSugar 328: R=OH

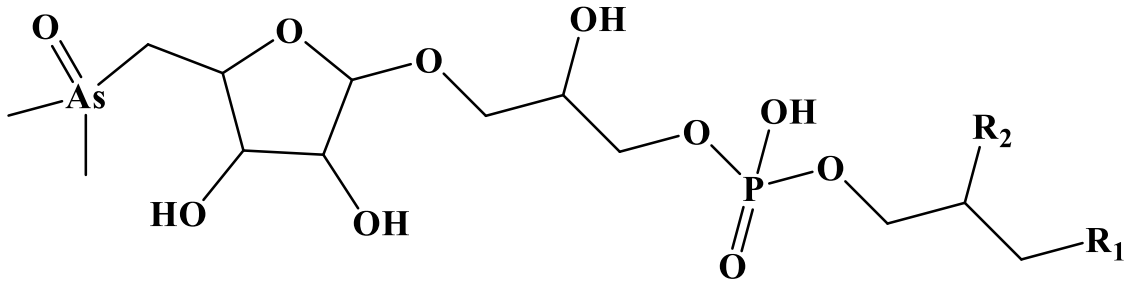
AsSugar 392: R=SO_3

AsSugar 408: R=SO_4

AsSugar 482: R=$OPO_3CH_2CHOHCH_2OH$

Arsenic-containing Phospholipids (AsPLs)

Identified in seaweed

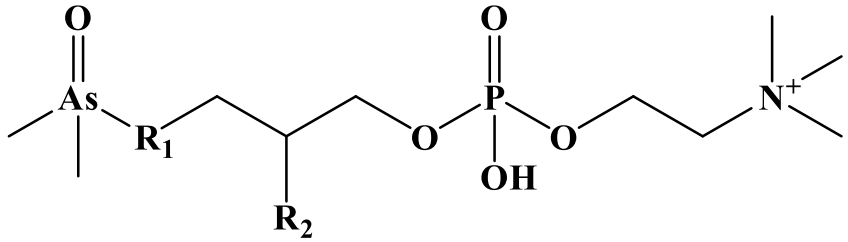


R_1 = Fatty Acid

R_2 = Fatty Acid

Arsenic-containing Phosphatidylcholines (AsPCs)

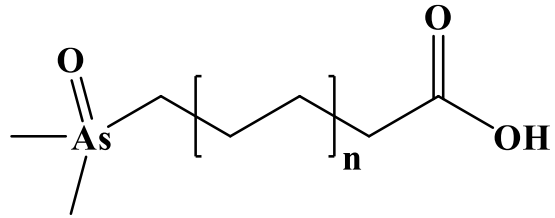
Identified in Roe



R_1 = Fatty Acid; **R_2** = Fatty Acid

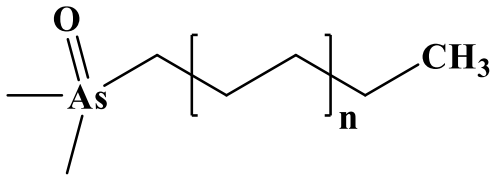
Arsenic-containing Fatty Acids (AsFAs)

Identified in fish oils; metabolized by humans



Arsenic-containing hydrocarbons (AsHCs)

Identified in fish oils; metabolized by humans



Toxicity Studies of Organoarsenicals

Metallomics

COMMUNICATION

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Arsenic-containing hydrocarbons are toxic in the *in vivo* model *Drosophila melanogaster*†

S. Meyer,[ab] J. Schulz,[c] A. Jeibmann,[c] M. S. Taleshi,[de] F. Ebert,[b] K. A. Francesconi[d] and T. Schwerdtle*[b]

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www.rsc.org/metallomics

Arsenic-containing hydrocarbons (AsHC) constitute one group of arsenolipids that have been identified in seafood. In this first *in vivo* toxicity study for AsHCs, we show that AsHCs exert toxic effects in *Drosophila melanogaster* in a concentration range similar to that of arsenite. In contrast to arsenite, however, AsHCs cause developmental toxicity in the late developmental stages of *Drosophila melanogaster*. This work illustrates the need for a full characterisation of the toxicity of AsHCs in experimental animals to finally assess the risk to human health related to the presence of arsenolipids in seafood.

fatty alcohols (TMAsFOH)[7] and the arsenic-containing hydrocarbons (AsHC).[8]

AsHCs consist of a polar dimethylarsinoyl group and a long hydrocarbon chain, which is important for the lipophilic character of these compounds. AsHCs have been identified in edible fish oils,[7–9] several fish meat samples, including herring,[10] tuna[11] and cod[12,13] and also in some edible brown algae.[5]

Recently, three AsHCs (Fig. 1) have been shown to exert toxic effects in cultured human urothelial and liver cells with IC_{50} values similar to that of arsenite (iAs^{III}). However, the toxic

Toxicology Research

PAPER

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In vitro toxicological characterisation of arsenic-containing fatty acids and three of their metabolites†

S. Meyer,[a,b] G. Raber,[c] F. Ebert,[b] L. Leffers,[a] S. M. Müller,[b,d] M. S. Taleshi,[e] K. A. Francesconi[c] and T. Schwerdtle*[a,b]

Cite this: *Toxicol. Res.*, 2015, **4**, 1289

Arsenic-containing fatty acids are a group of fat-soluble arsenic species (arsenolipids) which are present in marine fish and other seafood. Recently, it has been shown that arsenic-containing hydrocarbons, another group of arsenolipids, exert toxicity in similar concentrations comparable to arsenite although the toxic modes of action differ. Hence, a risk assessment of arsenolipids is urgently needed. In this study the cellular toxicity of a saturated (AsFA 362) and an unsaturated (AsFA 388) arsenic-containing fatty acid and three of their proposed metabolites (DMA^V, DMAPr and thio-DMAPr) were investigated in human liver cells (HepG2). Even though both arsenic-containing fatty acids were less toxic as compared to arsenic-containing hydrocarbons and arsenite, significant effects were observable at μM concentrations. DMA^V causes effects in a similar concentration range and it could be seen that it is metabolised to its highly toxic thio analogue thio-DMA^V in HepG2 cells. Nevertheless, DMAPr and thio-DMAPr did not exert any cytotoxicity. In summary, our data indicate that risks to human health related to the presence of arsenic-

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Arch Toxicol
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ORGAN TOXICITY AND MECHANISMS

Toxicity of two classes of arsenolipids and their water-soluble metabolites in human differentiated neurons

Barbara Witt[1] · Sören Meyer[1] · Franziska Ebert[1] · Kevin A. Francesconi[2] · Tanja Schwerdtle[1]

Received: 26 September 2016 / Accepted: 12 January 2017

Abstract Arsenolipids are lipid-soluble organoarsenic compounds, mainly occurring in marine organisms, with arsenic-containing hydrocarbons (AsHCs) and arsenic-containing fatty acids (AsFAs) representing two major subgroups. Recently, toxicity studies of several arsenolipids showed a high cytotoxic potential of those arsenolipids into account the substantial in vitro neurotoxic potential of the AsHCs and the fact that they could transfer across the physiological barriers of the brain, a neurotoxic potential in vivo for the AsHCs cannot be excluded and needs to be urgently characterized.

Metallomics

PAPER

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In vitro toxicological characterisation of three arsenic-containing hydrocarbons

S. Meyer,[ab] M. Matissek,[c] S. M. Müller,[c] M. S. Taleshi,[d] F. Ebert,[b] K. A. Francesconi[d] and T. Schwerdtle*[b]

Cite this: *Metallomics*, 2014, 6, 1023

Arsenic-containing hydrocarbons are one group of fat-soluble organic arsenic compounds (arsenolipids) found in marine fish and other seafood. A risk assessment of arsenolipids is urgently needed, but has not been possible because of the total lack of toxicological data. In this study the cellular toxicity of three arsenic-containing hydrocarbons was investigated in cultured human bladder (UROtsa) and liver (HepG2) cells. Cytotoxicity of the arsenic-containing hydrocarbons was comparable to that of arsenite, which was applied as the toxic reference arsenical. A large cellular accumulation of arsenic, as measured by ICP-MS/MS, was observed after incubation of both cell lines with the arsenolipids. Moreover, the toxic mode of action shown by the three arsenic-containing hydrocarbons seemed to differ from that observed for arsenite. Evidence suggests that the high cytotoxic potential of the lipophilic arsenicals results from a decrease in the cellular energy level. This first *in vitro* based risk assessment cannot exclude a risk to human health related to the presence of arsenolipids in seafood, and indicates the urgent need for further toxicity studies in experimental animals to fully assess this possible risk.

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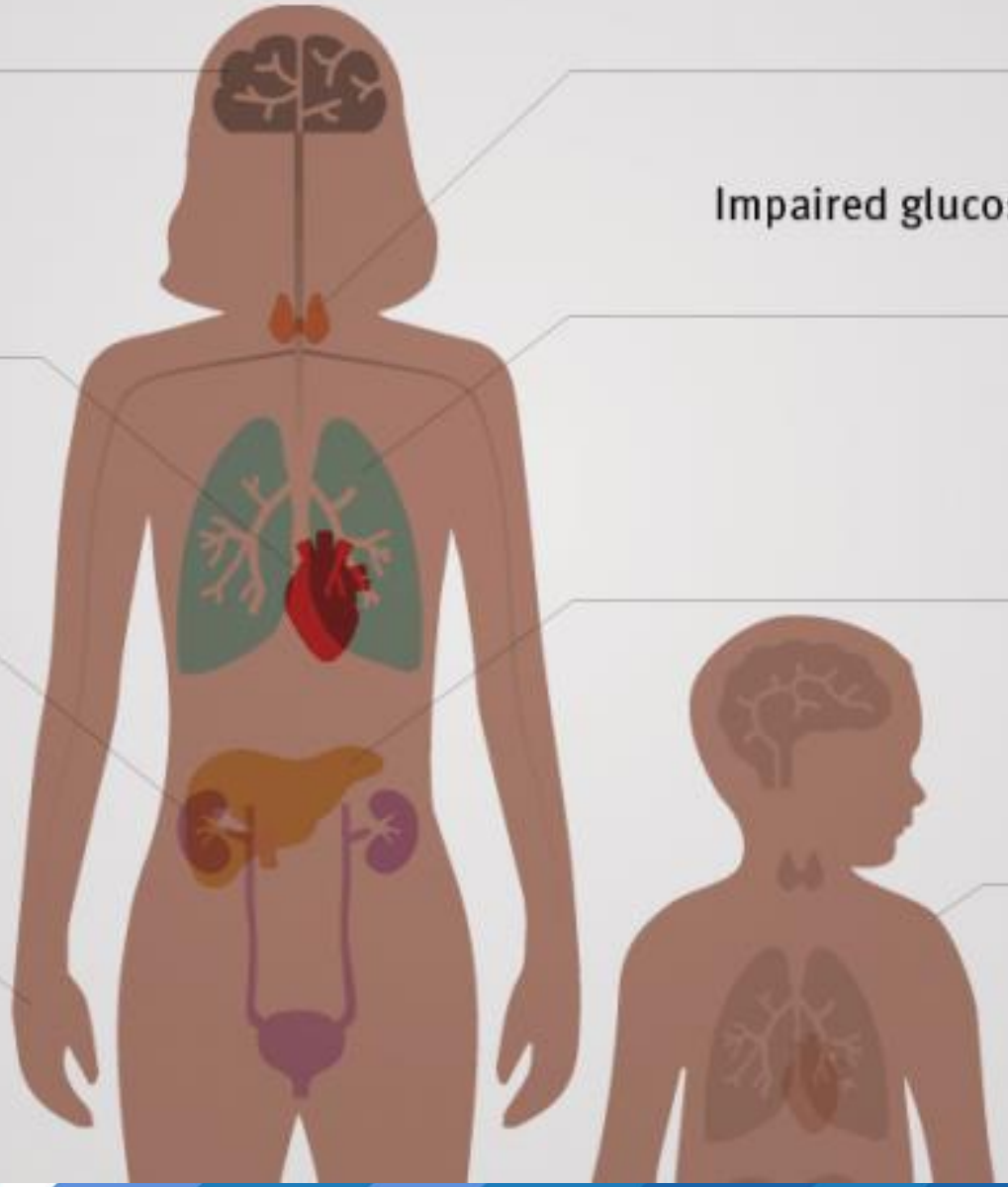
Health Effects of Arsenic Exposure



Nervous System

Impaired intellectual function
Impaired motor function
Neuropathy

Cardiovascular System

Coronary heart disease
Hypertension
Heart attack

Renal System

Kidney cancer
Bladder cancer

Skin

Skin lesions
Skin cancer

Endocrine System

Diabetes
Impaired glucose tolerance in pregnant women

Respiratory System

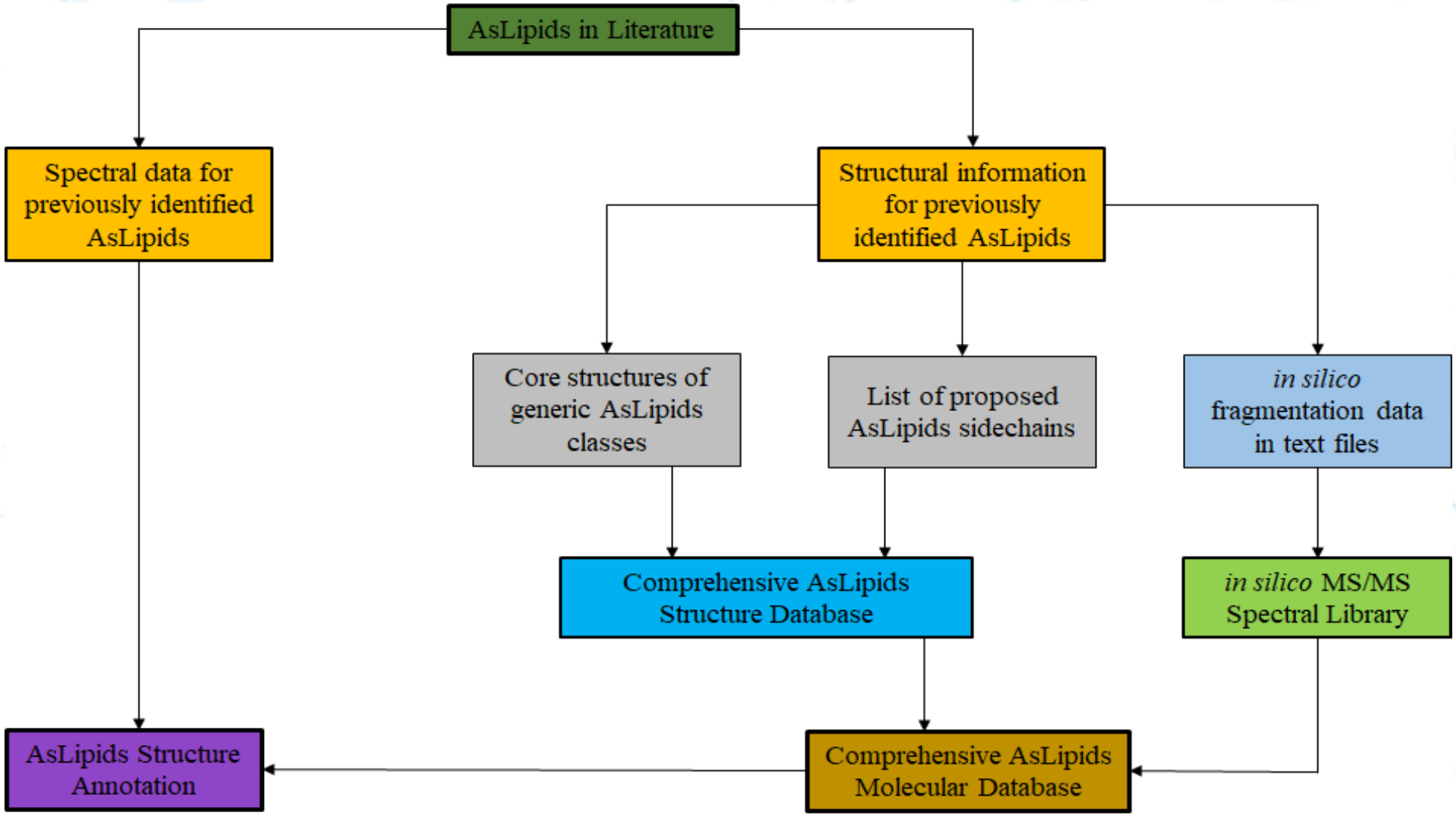
Pulmonary tuberculosis
Bronchiectasis
Lung cancer

Liver cancer

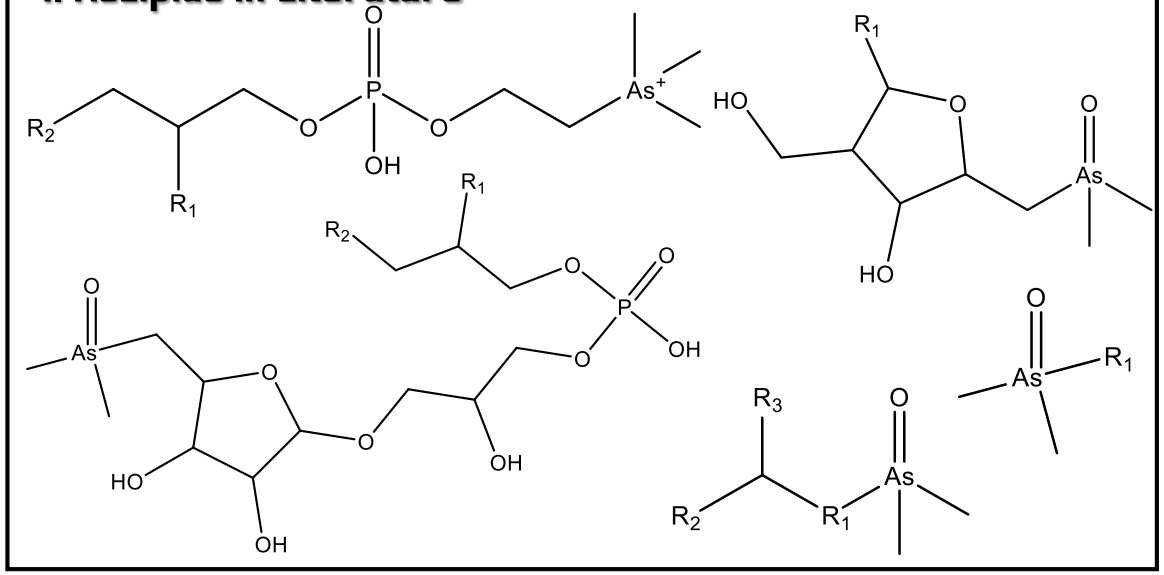
Developmental Process

Increased cancer risk as adults
Increased infant mortality
Neurological impairment
Reduced birth weight

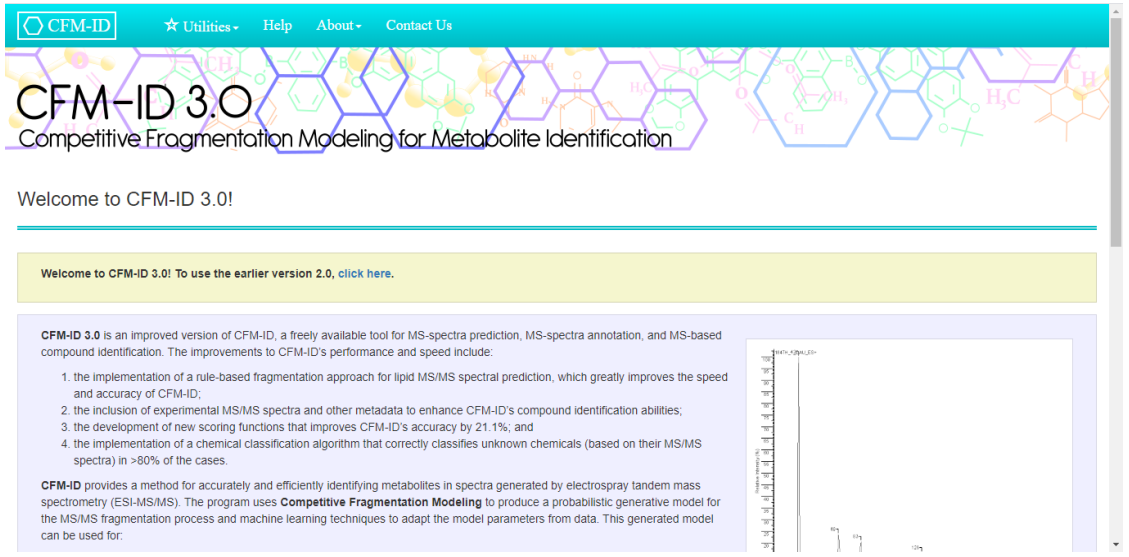
Development of AsLipids *in silico* Library



1. AsLipids in Literature

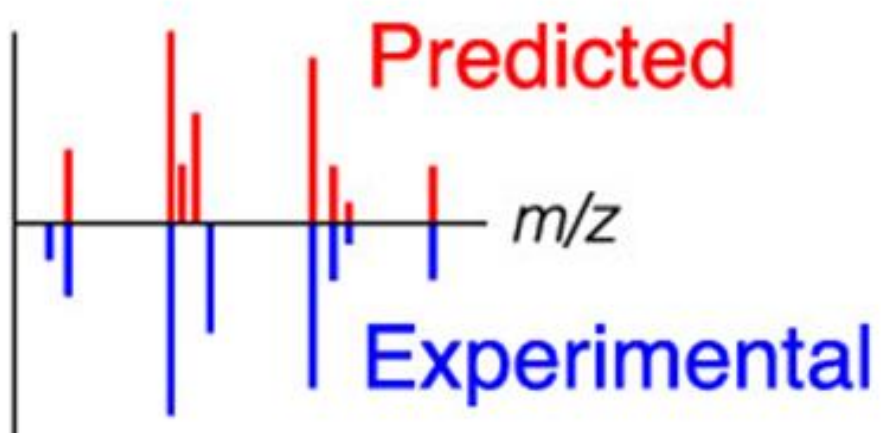


2. Prediction



3. *in silico* MS/MS Library

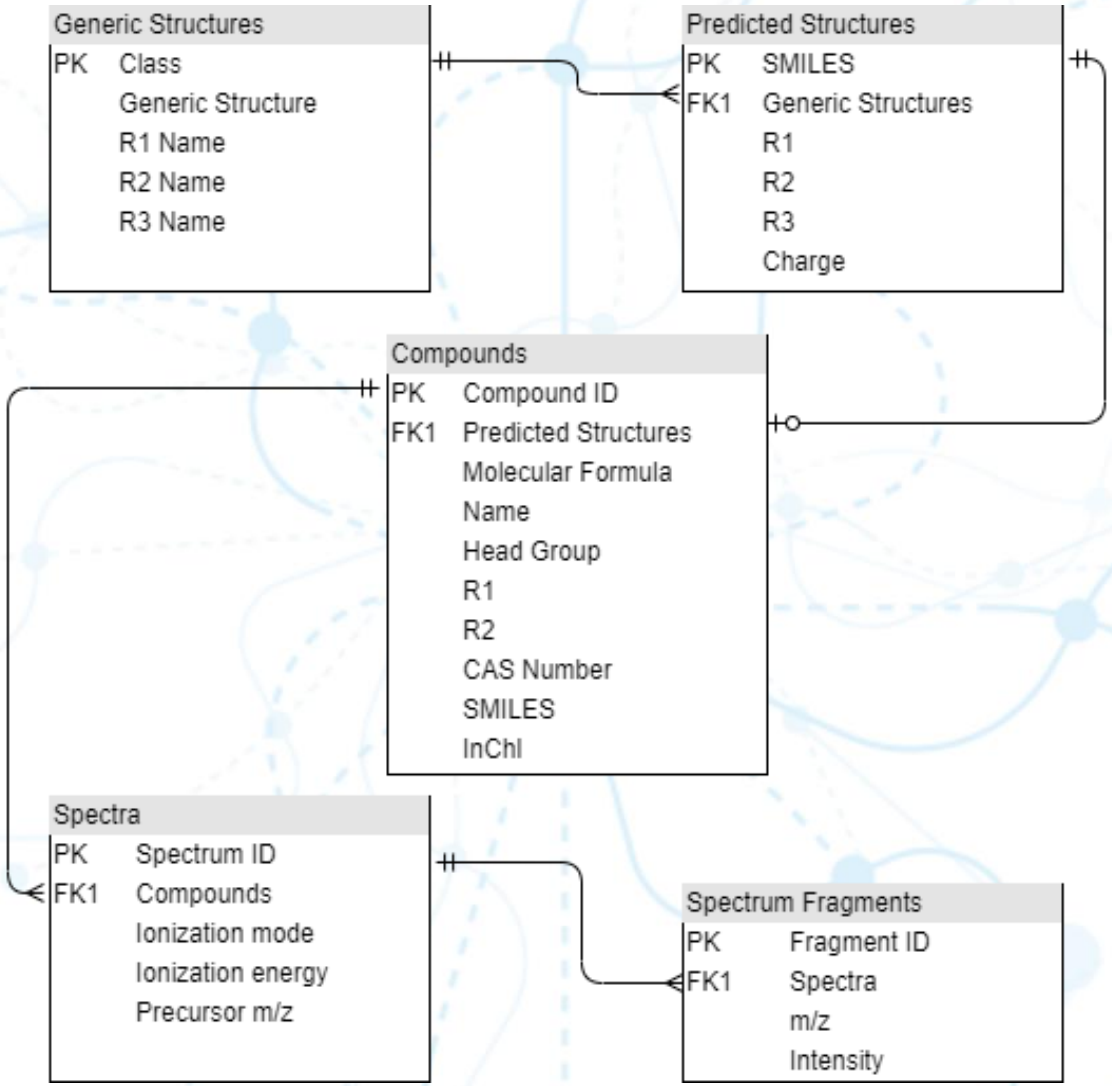
4. Assessing utility of spectral library for structure annotation



Core Structures of Generic AsLipids Classes

SNo.	Class	SMILES	R Type		
			R1	R2	R3
1	AsHCs	C[As](C)([R1])=O	Hydrocarbon		
2	AsFAs	C[As](C)([R1])=O	Reverse Fatty Acid		
3	TMAsFOHs	C[As+](C)(C)[R1]	Fatty Alcohol		
4	DMAsFOHs	C[As](C)([R1])=O	Fatty Alcohol		
5	AsPCs	O=P(OCC[As+](C)(C)C)(OCC([R1])C[R2])O	Fatty Acid	Fatty Acid/ OH	
6	AsPEs	O=P(OCC[N+]([H])([H])[H])(OCC([R2])C[R1][As](C)(C)=O)O	Fatty Acid	Fatty Acid/ OH	
7	AsSugar-PL	O=P(OCC(COC1OC(C(C1O)O)C[As](C)(C)=O)O)(OCC([R2])C[R1])O	Fatty Acid	Fatty Acid/ OH	
8	AsSugar-Phytol	OC(C(OC1[R2])C[As](C)(C)=O)C1[R1]	CH3O / OH	Terpene	
9	AsTAG	[R3]C([R2])[R1][As](C)(C)=O	Fatty Acid	Fatty Acid	Fatty Acid
10	AsDAG	[R3]C([R2])[R1][As](C)(C)=O	Fatty Acid	Fatty Acid	OH

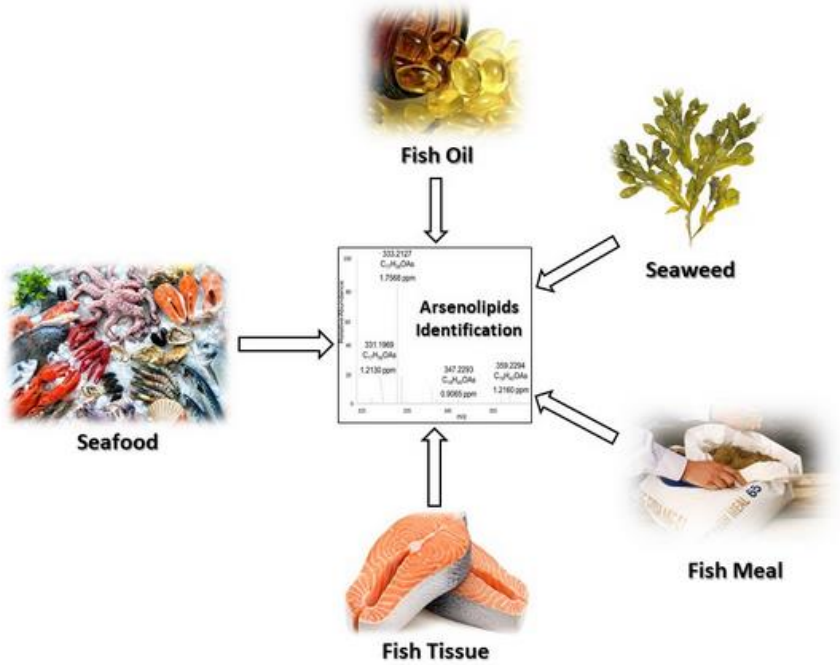
Schema of the Relational Database



AsLipids in silico Web-based Library

Home Search By Compound Search By Spectrum

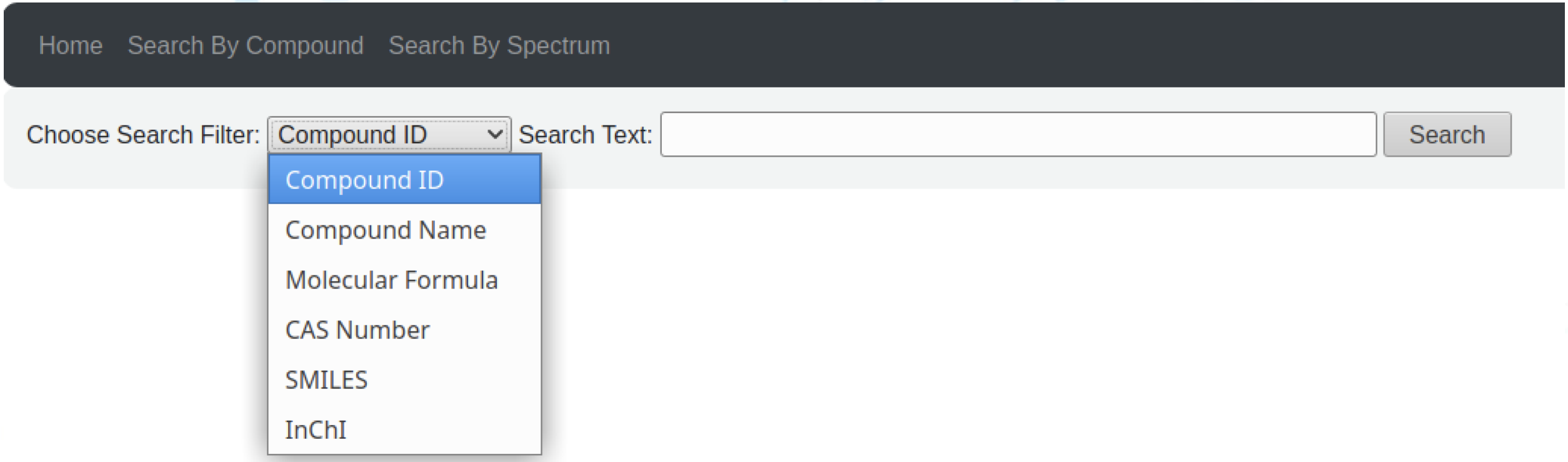
Arsenolipids in silico tandem mass spectral library



Lipophilic organic arsenic compounds, generally known as arsenolipids (AsLipids) elicit research interest due to their novel structures, likely role in membrane biochemistry, and since they exist in common seafood with potential health concerns based on arsenic toxicity. Characterization of AsLipids has been hampered by the lack of experimentally collected reference spectra from tandem mass spectrometry (MS/MS) due to lack of authentic standards, certified reference materials (CRMs), and spectral libraries.

AsLipID is a computationally derived mass spectral library for identification of AsLipids. It is developed from extant compound structures, previously identified, and reported in literature, and ESI-MS/MS spectra generated in silico using competitive fragmentation modeling for metabolite identification (CFM-ID) online software version 3.0. The in silico spectral data is generated at low (10V), medium (20V), and high (40V) collision energies, in both positive and negative ionization modes. The library is searchable based on the compound information like the compound name, molecular formular, AsLipids class, CAS Number, SMILES or InChI notations. The database can also be searched based on spectral data. This is not a comprehensive list of all known AsLipids, the library will be updated as new information becomes available.

Search by Compound Identification



Search by Compound ID Output

Home Search By Compound Search By Spectrum

Choose Search Filter: Compound ID Search Text: AsHC Search

Compound ID	Compound Name	Class	Molecular Formula	SMILES	CAS Number	InChI
AsHC 332	dimethyl(pentadecyl)arsine oxide	Arsenic-containing hydrocarbon	C17H37AsO	C[As](C)(CCCCCCCCCCCCCCC)=O	1083077-42-2	1S/C17H37AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(2,3)19/h4-17H2,1-3H3
AsHC 360	heptadecyldimethylarsine oxide	Arsenic-containing hydrocarbon	C19H41AsO	C[As](C)(CCCCCCCCCCCCCCCCC)=O	1083077-43-3	1S/C19H41AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)21/h4-19H2,1-3H3
AsHC 404	((2Z,5Z,8Z,11Z,14Z,17Z)-henicosa-2,5,8,11,14,17-hexaen-1-yl)dimethylarsine oxide	Arsenic-containing hydrocarbon	C23H37AsO	C[As](C)(C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCC)=O	1083077-44-4	1S/C23H37AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24(2,3)25/h6-7,9-10,12-13,15-16,18-19,21-22H,4-5,8,11,14,17,20,23H2,1-3H3/b7-6-,10-9-,13-12-,16-15-,19-18-,22-21-
AsHC 358	(Z)-heptadec-10-en-1-yldimethylarsine oxide	Arsenic-containing hydrocarbon	C19H39AsO	C[As](C)(CCCCCCCCC/C=C\CCCCCC)=O	1456610-45-9	1S/C19H39AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)21/h9-10H,4-8,11-19H2,1-3H3/b10-9-
AsHC 346	hexadecyldimethylarsine oxide	Arsenic-containing hydrocarbon	C18H39AsO	C[As](C)(CCCCCCCCCCCCCCCC)=O	1423745-41-8	1S/C18H39AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2,3)20/h4-18H2,1-3H3
AsHC 304	dimethyl(tridecyl)arsine oxide	Arsenic-containing hydrocarbon	C15H33AsO	C[As](C)(CCCCCCCCCCCCC)=O	1456610-35-7	1S/C15H33AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16(2,3)17/h4-15H2,1-3H3

Search by Compound – Compound Name

Home Search By Compound Search By Spectrum

Choose Search Filter: Compound Name Search Text: dimethyl(pentadecyl)arsine oxide Search

Compound ID	Compound Name	Class	Molecular Formula	SMILES	CAS Number	InChI
AsHC 332	dimethyl(pentadecyl)arsine oxide	Arsenic-containing hydrocarbon	C17H37AsO	C[As](C)(CCCCCCCCCCCCCCC)=O	1083077-42-2	1S/C17H37AsO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(2,3)19/h4-17H2,1-3H3

Partial Search Text Matching

Home Search By Compound Search By Spectrum

Choose Search Filter: Compound Name Search Text: dimethylarsoryl Search

Compound ID	Compound Name	Class	Molecular Formula	SMILES	CAS Number
AsFA 362	15-(dimethylarsoryl)pentadecanoic acid	Arsenic-containing fatty acids	C17H35AsO3	C[As](C)(CCCCCCCCCCCCCCC(=O)O)=O	1032052-02-0
AsFA 334	13-(dimethylarsoryl)tridecanoic acid	Arsenic-containing fatty acids	C15H31AsO3	C[As](C)(CCCCCCCCCCCCC(=O)O)=O	1032052-00-8
AsFA 390	17-(dimethylarsoryl)heptadecanoic acid	Arsenic-containing fatty acids	C19H39AsO3	C[As](C)(CCCCCCCCCCCCCCCCC(=O)O)=O	1032052-04-2
AsFA 418	19-(dimethylarsoryl)nonadecanoic acid	Arsenic-containing fatty acids	C21H43AsO3	C[As](C)(CCCCCCCCCCCCCCCCCCC(=O)O)=O	1032052-06-4
AsFA 388	(Z)-17-(dimethylarsoryl)heptadec-9-enoic acid	Arsenic-containing fatty acids	C19H37AsO3	C[As](C)(CCCCCCC/C=C\CCCCCCCC(=O)O)=O	1032052-08-6

Search by Compound - SMILES

Home Search By Compound Search By Spectrum

Choose Search Filter: SMILES Search Text: C[As](C)(CCCCCCCCCCCCCCC(=O)O)=O Search

- Compound ID
- Compound Name
- Molecular Formula
- CAS Number
- SMILES
- InChI

Compound ID	Com	Class	Molecular Formula	SMILES	CAS Number	InChI
AsFA 362	15-(di	Arsenic-containing fatty acids	C17H35AsO3	C[As](C)(CCCCCCCCCCCCCCC(=O)O)=O	1032052-02-0	1S/C17H35AsO3/c1-18(2,21)16-14-12-10-8-6-4-3-5-7-9-11-13-15-17(19)20/h3-16H2,1-2H3,(H,19,20)

Search by Compound – CAS Number

Home Search By Compound Search By Spectrum

Choose Search Filter: CAS Number Search Text: 1032052-02-0 Search

- Compound ID
- Compound Name
- Molecular Formula
- CAS Number
- SMILES
- InChI

Compound ID	Com	Class	Molecular Formula	SMILES	CAS Number	InChI
AsFA 362	15-(di	Arsenic-containing fatty acids	C17H35AsO3	C[As](C)(CCCCCCCCCCCCCCC(=O)O)=O	1032052-02-0	1S/C17H35AsO3/c1-18(2,21)16-14-12-10-8-6-4-3-5-7-9-11-13-15-17(19)20/h3-16H2,1-2H3,(H,19,20)

Search by Compound – Molecular Formula

Home Search By Compound Search By Spectrum

Choose Search Filter: Molecular Formula Search Text: C45H88AsPO14 Search

Compound ID	Compound Name	Class	Molecular Formula	SMILES	CAS Number	InChI
AsSugar-PL 958	3-(((3-((5-((dimethylarsoryl)methyl)-3,4-dihydroxytetrahydrofuran-2-yl)oxy)-2-hydroxypropoxy)(hydroxy)phosphoryl)oxy)propane-1,2-diyl dipalmitate	AsSugar-Phospholipids	C45H88AsPO14	O=P(OCC(COC1OC(C(C1O)O)C[As](C)(C)=O)O)(OCC(OC(=O)CCCCCCCCCCCCCCC)COC(=O)CCCCCCCCCCCCCCC)O	115921-38-5	1S/C45H88AsO14P/c1-5-7-9-11-13-15-17-19-21-23-25-27-29-31-41(48)55-36-39(59-42(49)32-30-28-26-24-22-20-18-16-14-12-10-8-6-2)37-58-61(53,54)57-35-38(/h38-40,43-45,47,50-51H,5-37H2,1-4H3,(H,53,54)

Search by Compound – InChI

Home Search By Compound Search By Spectrum

Choose Search Filter: InChI Search Text: 1S/C24H40AsO/c1-25(2,3)23-21-19-17-15-13-11-9-7-5-4-6-8-10-: Search

Compound ID	Compound Name	Class	Molecular Formula	SMILES	CAS Number	InChI
TMAsFOH 419	((2Z,5Z,8Z,11Z,14Z,17Z)-21-hydroxyhenicosa-2,5,8,11,14,17-hexaen-1-yl)trimethylarsonium	Arsenic-containing fatty alcohols	C24H40As+O	C[As+](C)(C)C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCO	1456610-52-8	1S/C24H40AsO/c1-25(2,3)23-21-19-17-15-13-11-9-7-5-4-6-8-10-12-14-16-18-20-22-24-26/h4,6-7,9-10,12-13,15-16,18-19,21,26H,5,8,11,14,17,20,22-24H2,1-3H3/q+1/b6-4-,9-7-,12-10-,15-13-,18-16-,21-19-

Search by Spectral Data

Home Search By Compound Search By Spectrum

Unknown Spectrum:

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15.02402368 0.9801898837 21 (0.98019)
17.00328823 1.934348764 22 (1.9343)
99.11792406 0.5820599405 138 (0.58206)
100.9377951 1.700319708 38 (1.7003)
102.9170597 1.105802015 37 (1.1058)
102.9534452 0.8171927206 36 (0.81719)
104.9327098 27.26990034 35 (27.27)
104.9690953 0.7647204459 34 (0.76472)
106.9483598 1.139179209 33 (1.1392)
111.1179241 1.197748749 143 (1.1977)
118.9483598 10.11267348 12 (10.113)
```

Ionization Mode: Negative

Molecular Ion Resolution:

Precursor Ion: 547.2985345

Precursor Ion Resolution:

Submit

Compound ID	Compound Name	Class	Precursor Ion	Match	Ionization Mode	Ionization Energy	Molecular Formula	SMILES	CAS Number	InChI
AsSugar-Phytol 548_3-4	((5-((8-(3-(heptan-2-yl)oxiran-2-yl)-3,7-dimethyloctyl)oxy)-3-hydroxy-4-methoxytetrahydrofuran-2-yl)methyl)dimethylarsine oxide	AsSugar-Phytols	547.2985345	100 %	Negative	10V	C27H53AsO6	OC(C1OC)C(C[As](C)(C)=O)OC1[O]CCC(CCCC(C)CC1C(C(CCCCC)C)O1)C	None	1S/C27H53AsO6/c1-8-9-10-14-21(4)25-22(33-25)17-20(3)13-11-12-19(2)15-16-32-27-26(31-7)24(29)23(34-27)18-28(5,6)30/h19-27,29H,8-18H2,1-7H3
AsSugar-Phytol 548_3-3	16-((5-((dimethylarsoryl)methyl)-4-hydroxy-3-methoxytetrahydrofuran-2-yl)oxy)-6,10,14-trimethylhexadecan-7-one	AsSugar-Phytols	547.2985345	74 %	Negative	10V	C27H53AsO6	OC(C1OC)C(C[As](C)(C)=O)OC1[O]CCC(CCCC(C)CCC(C(CCCCC)C)=O)C	None	1S/C27H53AsO6/c1-8-9-10-14-22(4)23(29)16-15-20(2)12-11-13-21(3)17-18-33-27-26(32-7)25(30)24(34-27)19-28(5,6)31/h20-22,24-27,30H,8-19H2,1-7H3

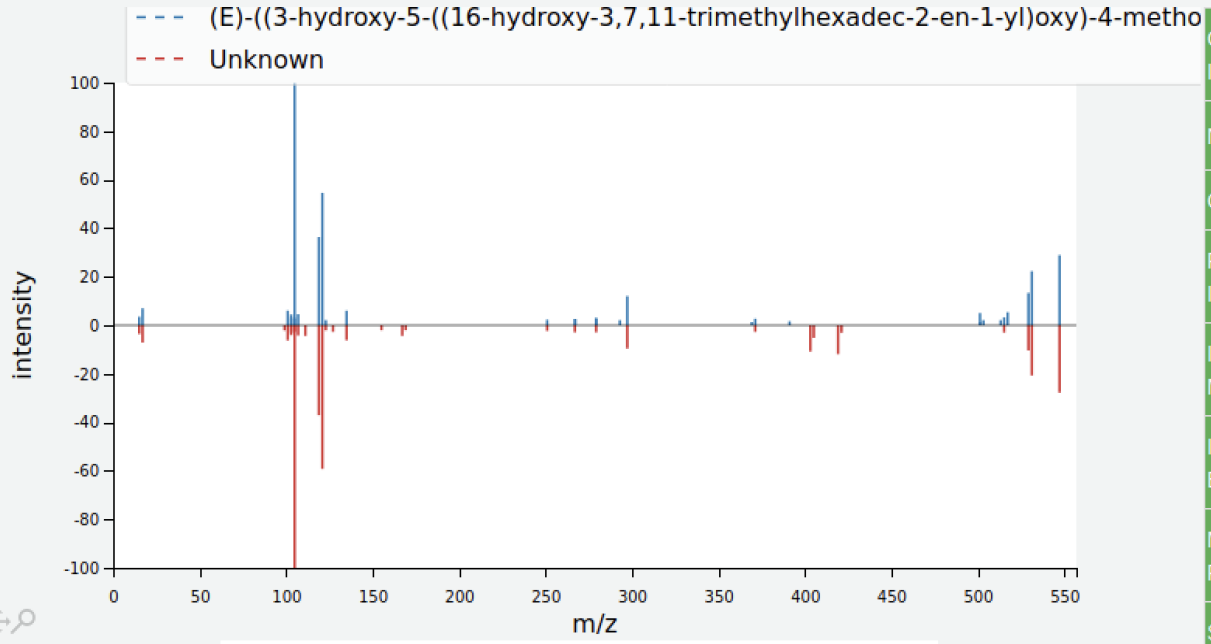
Search by Spectral Data

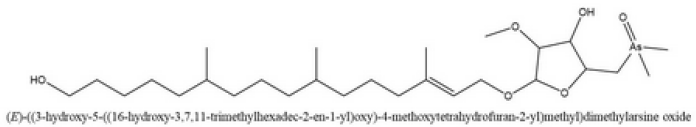
Home Search By Compound Search By Spectrum

Compound ID	Compound Name	Class	Precursor Ion	Match	Ionization Mode	Ionization Energy	Molecular Formula	SMILES	CAS Number
AsFA 306	11-(dimethylarsoryl)undecanoic acid	Arsenic-containing fatty acids	305.1103398	100 %	Negative	10V	C13H27AsO3	C[As](C)(CCCCCCCCCCC(=O)O)=O	1971874-33-5
AsFA 264	8-(dimethylarsoryl)octanoic acid	Arsenic-containing fatty acids	263.0633896	65 %	Negative	10V	C10H21AsO3	C[As](C)(CCCCCCCC(=O)O)=O	1431731-55-3
AsFA 278	9-(dimethylarsoryl)nonanoic acid	Arsenic-containing fatty acids	277.0790396	65 %	Negative	10V	C11H23AsO3	C[As](C)(CCCCCCCCC(=O)O)=O	1448014-29-6

Search by Spectrum - Visual Output 1

Home Search By Compound Search By Spectrum

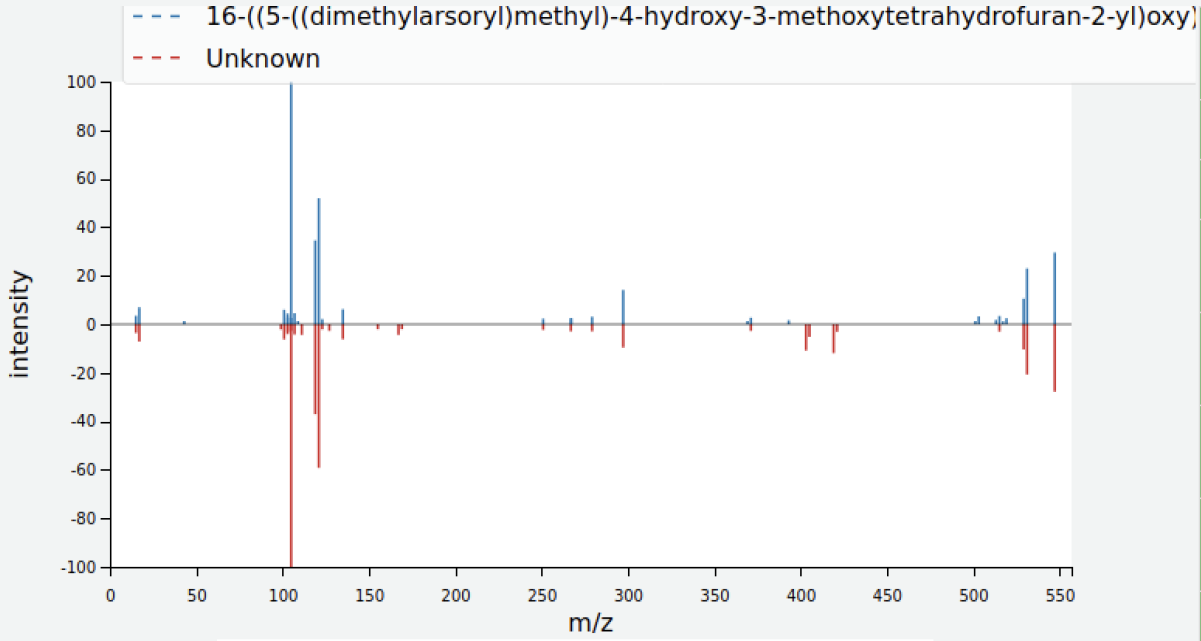


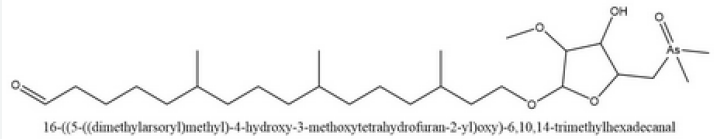


Compound ID	AsSugar-Phytol 548_3-1
Name	(E)-((3-hydroxy-5-((16-hydroxy-3,7,11-trimethylhexadec-2-en-1-yl)oxy)-4-methoxytetrahydrofuran-2-yl)methyl)dimethylarsine oxide
Class	AsSugar-Phytols
Precursor Ion	547.2985345
Ionization Mode	Negative
Ionization Energy	10V
Molecular Formula	C27H53AsO6
SMILES	OC(C1OC)C(C[As](C)(C)=O)OC1[O]C/C=C(CCCC(C)CCCC(CCCCCO)C)\C
CAS Number	None
InChI	1S/C27H53AsO6 /c1-21(12-8-7-9-18-29)13-10-14-22(2)15-11-16-23(3)17-19-33-27-26(32-6)25(30)24(34-27)20-28(4,5)31 /h17,21-22,24-27,29-30H,7-16,18-20H2,1-6H3/b23-17+

Search by Spectrum – Visual Output 2

Home Search By Compound Search By Spectrum

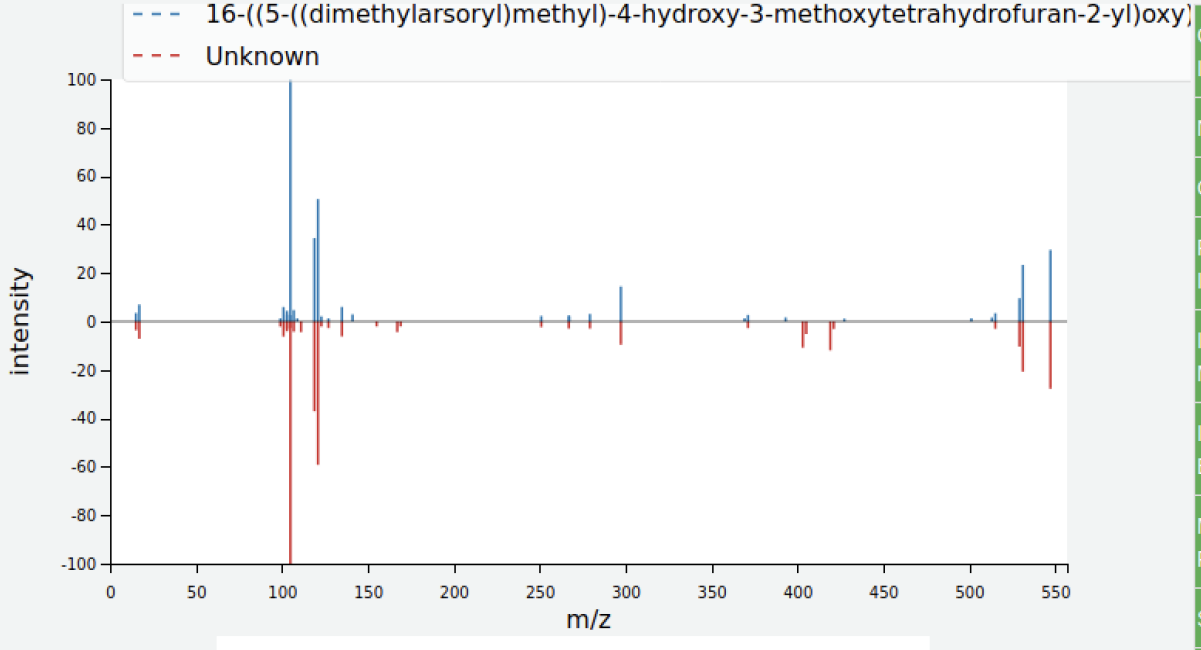


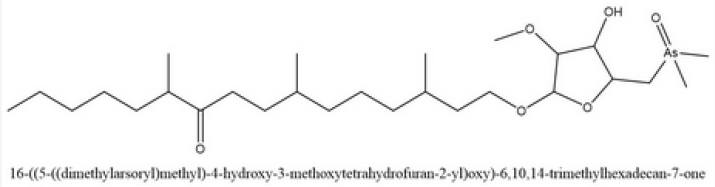


Compound ID	AsSugar-Phytol 548_3-2
Name	16-((5-((dimethylarsoryl)methyl)-4-hydroxy-3-methoxytetrahydrofuran-2-yl)oxy)-6,10,14-trimethylhexadecanal
Class	AsSugar-Phytols
Precursor Ion	547.2985345
Ionization Mode	Negative
Ionization Energy	10V
Molecular Formula	C27H53AsO6
SMILES	OC(C1OC)C(C[As](C)(C)=O)OC1[O]CCC(CCCC(C)CCCC(CCCCC=O)C)C
CAS Number	None
InChI	1S/C27H53AsO6 /c1-21(12-8-7-9-18-29)13-10-14-22(2)15-11-16-23(3)17-19-33-27-26(32-6)25(30)24(34-27)20-28(4,5)31 /h18,21-27,30H,7-17,19-20H2,1-6H3

Search by Spectrum - Visual Output 3

Home Search By Compound Search By Spectrum

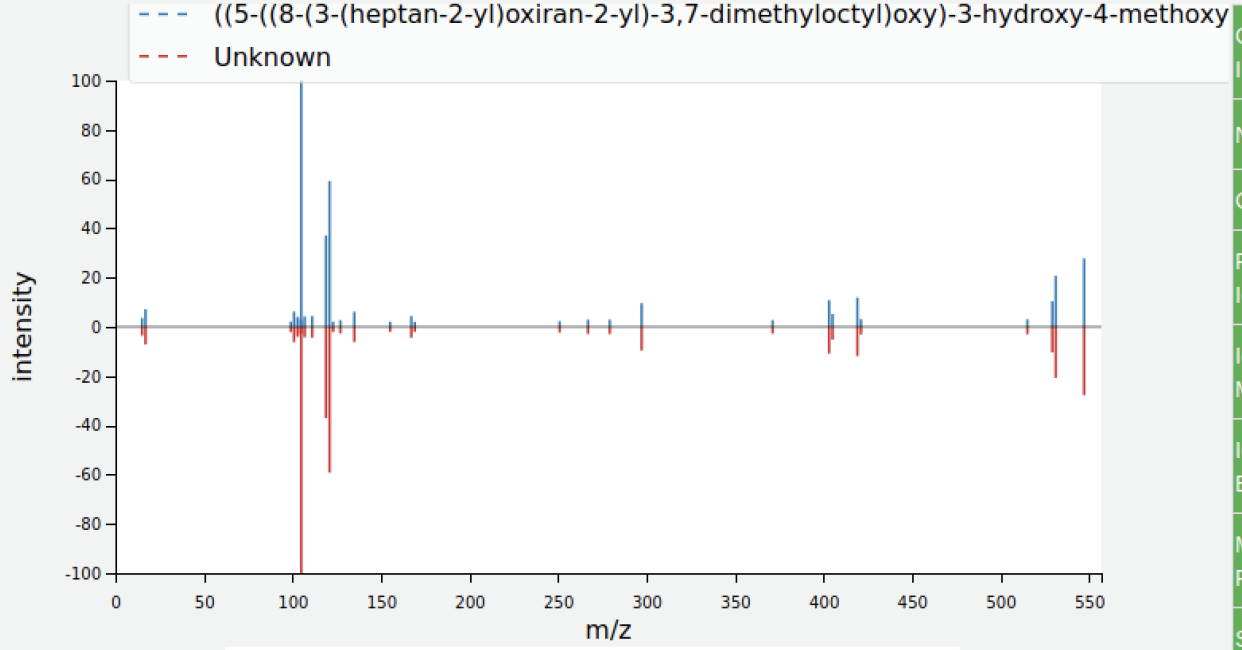


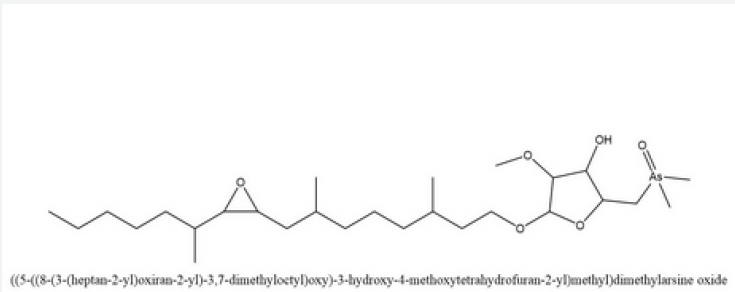


Compound ID	AsSugar-Phytol 548_3-3
Name	16-((5-((dimethylarsoryl)methyl)-4-hydroxy-3-methoxytetrahydrofuran-2-yl)oxy)-6,10,14-trimethylhexadecan-7-one
Class	AsSugar-Phytols
Precursor Ion	547.2985345
Ionization Mode	Negative
Ionization Energy	10V
Molecular Formula	C27H53AsO6
SMILES	OC(C1OC)C(C[As](C)(C)=O)OC1[O]CCC(CCCC(C)CCC(C(CCCCC)C)=O)C
CAS Number	None
InChI	1S/C27H53AsO6 /c1-8-9-10-14-22(4)23(29)16-15-20(2)12-11-13-21(3)17-18-33-27-26(32-7)25(30)24(34-27)19-28(5,6)31 /h20-22,24-27,30H,8-19H2,1-7H3

Search by Spectrum - Visual Output 4

Home Search By Compound Search By Spectrum





Compound ID	AsSugar-Phytol 548_3-4
Name	((5-((8-(3-(heptan-2-yl)oxiran-2-yl)-3,7-dimethyloctyl)oxy)-3-hydroxy-4-methoxytetrahydrofuran-2-yl)methyl)dimethylarsine oxide
Class	AsSugar-Phytols
Precursor Ion	547.2985345
Ionization Mode	Negative
Ionization Energy	10V
Molecular Formula	C27H53AsO6
SMILES	OC(C1OC)C(C[As](C)(C)=O)OC1[O]CCC(CCCC(C)CC1C(C(CCCCC)C)O1)C
CAS Number	None
InChI	1S/C27H53AsO6 /c1-8-9-10-14-21(4)25-22(33-25)17-20(3)13-11-12-19(2)15-16-32-27-26(31-7)24(29)23(34-27)18-28(5,6)30 /h19-27,29H,8-18H2,1-7H3

Error Message

Home Search By Compound Search By Spectrum

Choose Search Filter: Compound ID Search Text: dimethyl(pentadecyl)arsine oxide Search

Alert! No results found in the database for your query.

Click on the "x" symbol to close the alert message.

Conclusions and Future Perspectives

- More than 270,000 AsLipids structures were predicted and were used to generate an *in silico* spectral search engine, which is in good agreement with the experimental data that is reported in literature.
- Work presented here serves as proof of concept of the operation and functionality of the AsLipids search engine.
- The tool is deployed on a web-based platform, which enhances the usability and accessibility of the system on online.
- Provides a cheaper means of identification of arsenic-containing compounds using their tandem mass spectral data.
- The technique for development of the tool is simple, transferable and applicable to other analytical fields.

Thank You

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