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

AMOS: the EPA database of analytical methods and open mass spectral database supporting non-targeted analysis

Gregory Janesch[1], Erik Carr[1], Vicente Samano[2], James McCord[3], Jacqueline Bangma[3], Jon Sobus[4] and ***Antony Williams[4]***

1. ORAU Student Services Contractor 2. Senior Environmental Employment Program
3. Center for Environmental Measurement and Modeling and 4. Center for Computational Toxicology & Exposure, ALL at the U.S. Environmental Protection Agency

August 2023: ACS Fall Meeting, San Francisco, CA

Background

- A huge number of openly available sources exist for spectra, documentation of analytical procedures, etc.
- Search engines can easily find high-traffic sources, but maybe not niche-but-high-quality ones. Most are not “structurally-enabled”
- Useful to have complementary types of data alongside each other, **especially** with consistent substance identifiers
- Non-targeted analysis can benefit from a broad, high-quality experimental database as a reference

About AMOS - General

- AMOS is a cheminformatics application integrating spectra and analytical methods
- Developed in ~16 months as a “proof-of-concept” application and **not yet** available publicly
- Provides mappings between substance(s), method documents and experimental spectra

About AMOS - Data

- Three broad categories of records:
  - Spectra (>195,000)
  - Methods (>3500)
  - Fact Sheets (>800)
- Most data are open access, some are just external links
- Data is being continually updated (new datasets & updates)
- Many chemicals of interest to EPA – PFAS, pesticides, etc.

Underpinning Chemistry: DSSTox Database

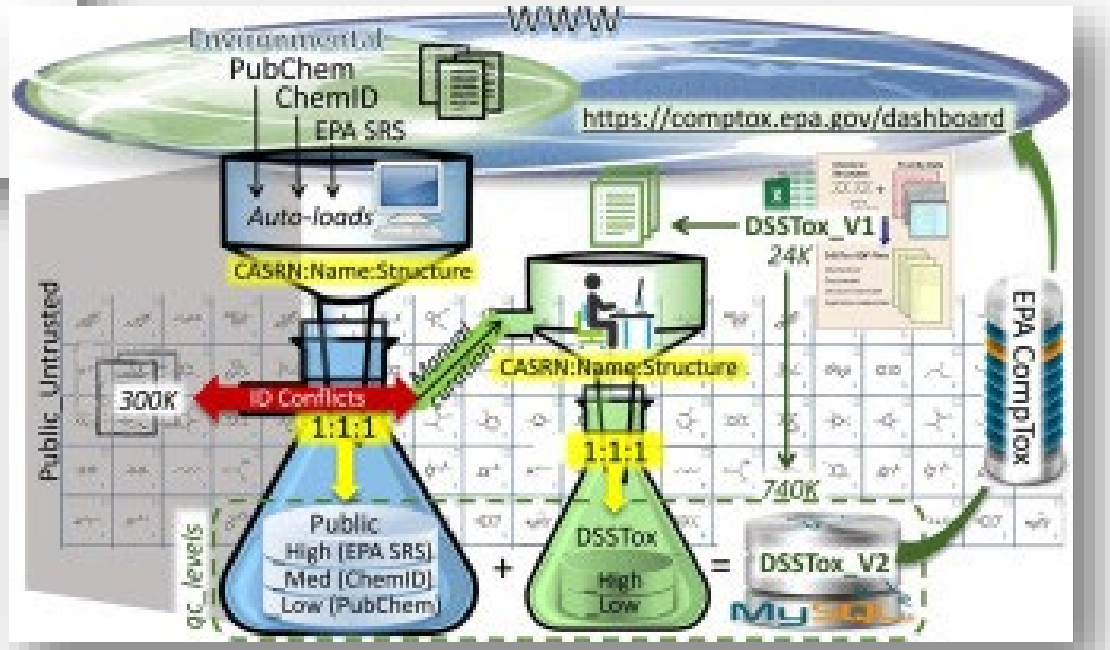
ELSEVIER

Computational Toxicology

Volume 12, November 2019, 100096

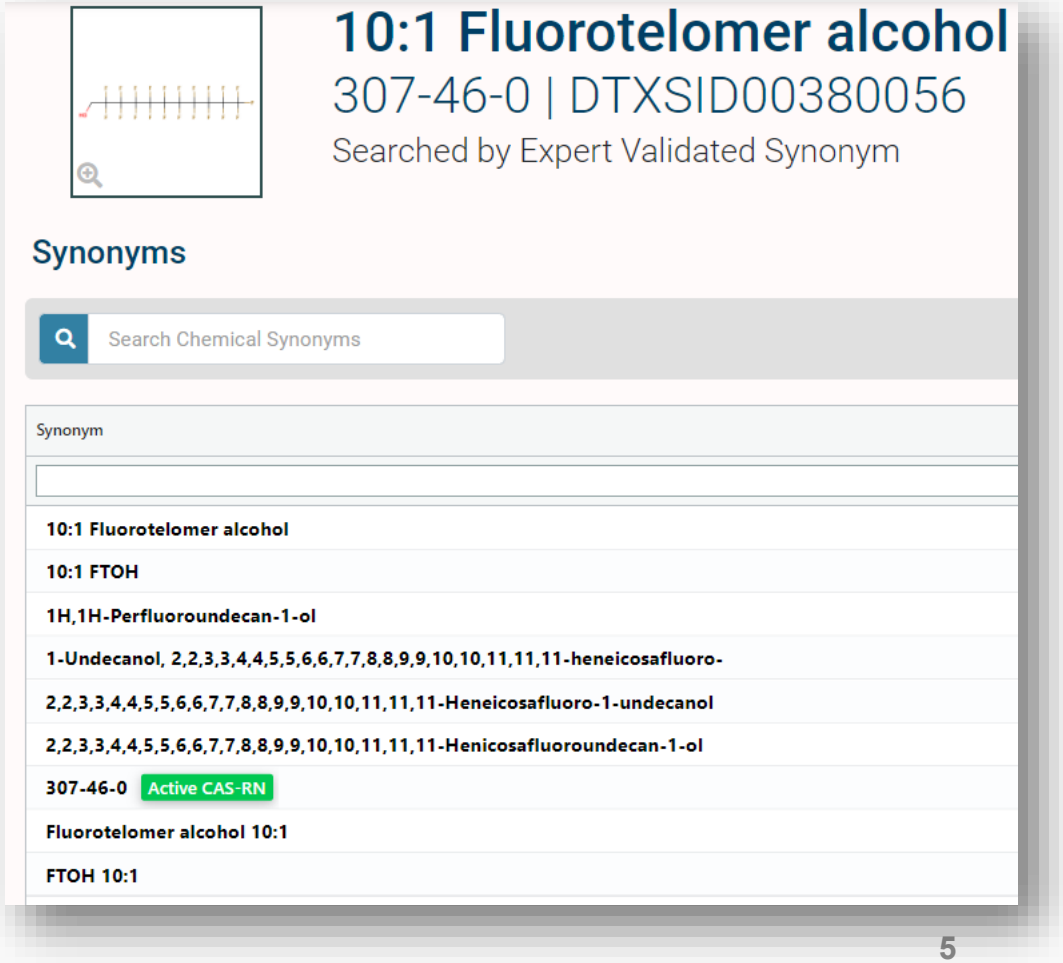
EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke [a], Antony J. Williams [a], Inthirany Thillanadarajah [b], Ann M. Richard [a]



About AMOS - Curation

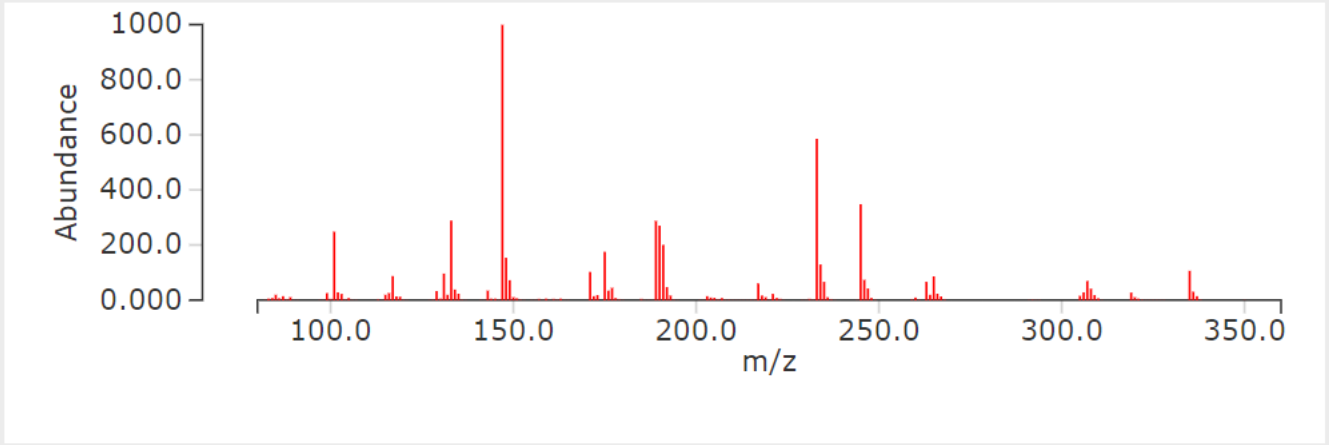
- Identifiers vary between different sources so we must curate
- A single chemical can have dozens of names
  - FTOH 10:1
  - 10:1 FTOH
  - 10:1 Fluorotelomer alcohol
  - 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-Henicosafluoroundecan-1-ol
  - 1-Undecanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heneicosafluoro-
- …and it rarely stops here…



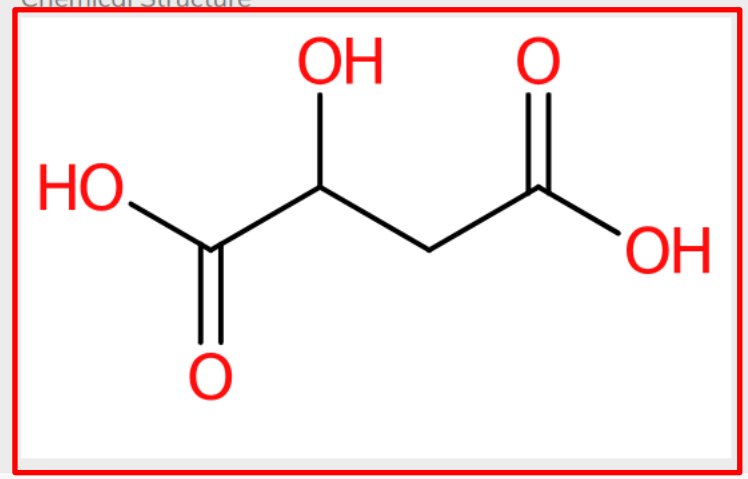
Curation of Structure-Spectra is challenging

L-(-)-Malic acid; GC-EI-TOF; MS; 3 TMS; BP:147

Mass Spectrum

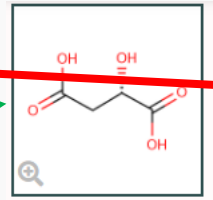


Chemical Structure



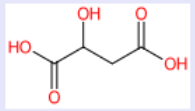
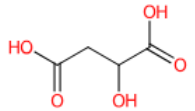
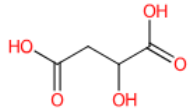
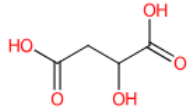
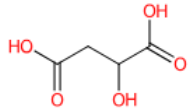
CH$NAME: L-(-)-Malic acid
CH$COMPOUND_CLASS: Natural Product
CH$FORMULA: $C_4H_6O_5$
CH$EXACT_MASS: 134.02152
CH$SMILES: OC(=O)CC(O)C(O)=O
CH$IUPAC: InChI=1S/C4H6O5/c5-2(4(8)9)1-3(6)7/h2,5H,1H2,(H,6,7)(H,8,9)/t2-/m0/s1
CH$LINK: CAS 636-61-3
CH$LINK: KEGG C00497
CH$LINK: INCHIKEY BJEPYKJPYRNKOW-REOHCLBHSA-N
CH$LINK: COMPTOX DTXSID30273987

InChIKey: BJEPYKJPYRNKOW-REOHCLBHSA-N
SMILES: O[C@@H](CC(O)=O)C(O)=O



(2S)-2-Hydroxybutanedioic acid
97-67-6 | DTXSID30273987
Searched by DTXSID30273987.

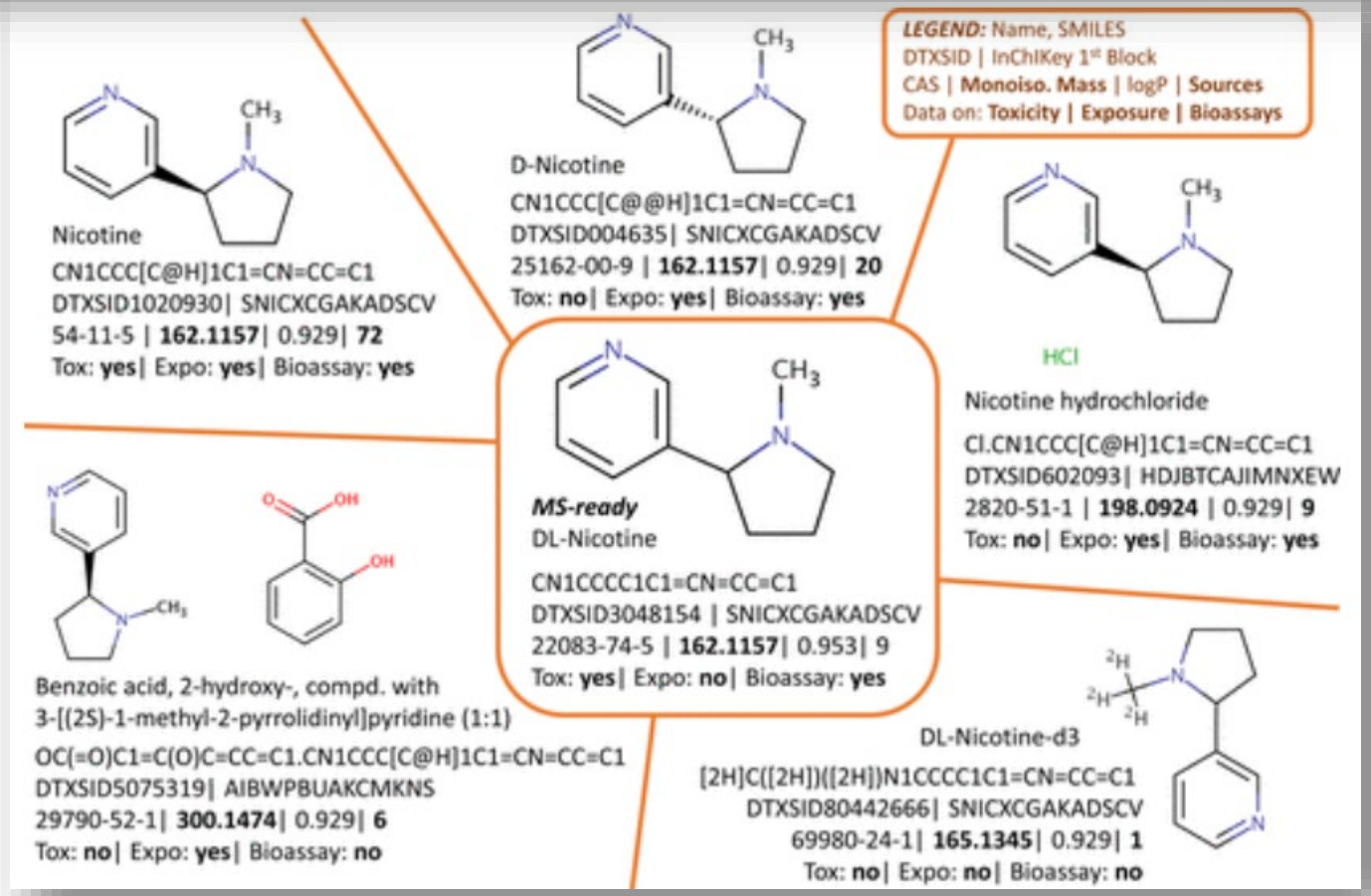
Curation of Structure-Spectra is challenging Multiple Malic Acids

⊞ L-(-)-Malic acid 5 spectra	C4H6O5		134.02151	
⊞ L-Hydroxybutanedioic acid, L-(-)-Malic acid, L-Mal... 2 spectra	C4H6O5		134.08701	
⊞ Malic acid 10 spectra	C4H6O5		134.02153	
⊞ Malic acid-[1,2,3,4-13C4] 6 spectra	C4H6O5		134.02153	
⊞ Malic acid-[1-13C] 6 spectra	C4H6O5		134.02153	

We understand spectra collapse by structure

Open Science for Identifying "Known Unknown" Chemicals

Emma L. Schymanski*† and Antony J. Williams*‡

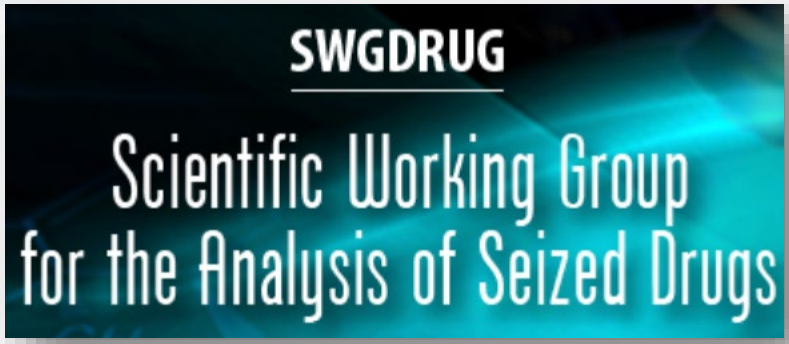


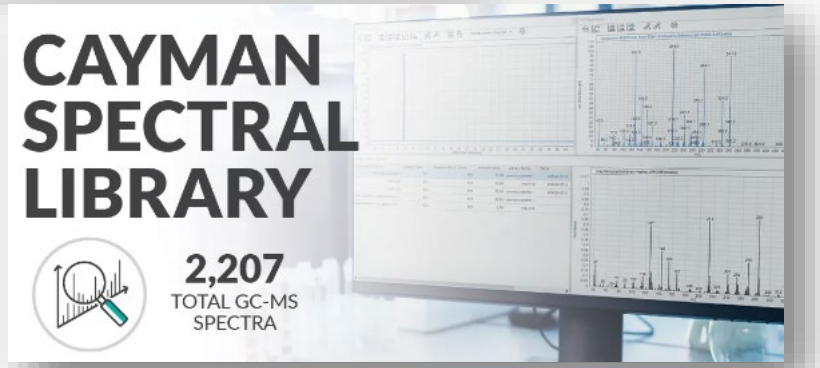
Spectra

- About 195,000 experimental spectra covering almost 25,000 substances (not including externally-linked ones)
- Most are from external, open-access sources
  - About 95% between MassBank EU, MoNA, & HMDB
- EPA labs now providing spectra (especially PFAS)
- Includes metadata like instrument settings (when possible)

Sources of Spectra

- Agency for Toxic Substances and Disease Registry
- Agilent
- Analytical QC
- Cayman Spectral Library
- Center for Forensic Science Research & Education
- Centers for Disease Control and Prevention
- Human Metabolome Database
- Jozef Stefan Institute
- MassBank Europe
- MassBank of North America
- National Environmental Methods Index
- National Institute for Occupational Safety and Health
- National Institute of Standards and Technology
- National Pesticide Information Center
- Scientific Working Group for the Analysis of Seized Drugs
- SCIEX





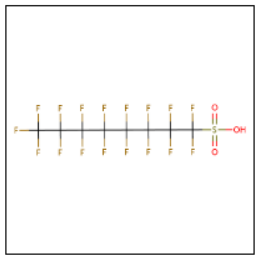
Methods

- Almost 3500 in AMOS so far from an assortment of vendors, publications, and government agencies
  - Agencies include: US-EPA, DEA, CDC, FDA, OSHA, USGS, USDA
  - Vendors include: Agilent, Shimadzu, LECO, Sciex and talking to others
- Methods can be linked to sets of spectra
- Searchable can be filtered by analytes, matrix, analytical methodology, source

General Search

PFOS | Compound Search | Home | Lists | Similar Method Search | Batch Search | Other Pages | About | Related Applications | Toggle Header/Footer

78 Results for "PFOS"



(Preferred) Name: Perfluorooctanesulfonic acid
DTXSID: DTXSID3031864
CASRN: 1763-23-1
InChIKey: YFSUTJLHUFNCNZ-UHFFFAOYSA-N
Molecular Formula: C8HF17O3S
Mass: 499.9375

Download Results

☑ Display Single Point Spectra

All Results (78) | Methods (55) | Spectra (23) | Fact Sheets (0)

Methodology	Source	Record Type	Information
GC/MS	NIST	Method	Determination of fatty acids, electrolytes, vitamins, hormones and amino acic
GC/MS	NIST	Method	Determination of pCB congengers, Chlorinated pesticides and PBDE congene
GC/MS	EPA MS Labs	Method	Determination of pFAS in incinerated soil by GC/MS.
GC/MS, LC/MS, NMR	Analytical QC	Spectrum Link	External link only. Link has 28 file(s).
LC-APCI, LC-ESI	NIST PFAS	Method	Generate PFAS reference spectra using high resolution LC-MS
LC-ESI	NIST PFAS	Spectrum	ESI; MS2; [M-H]-; R=17500; # PEAKS=23
LC-ESI-QFT	MassBank EU	Spectrum	LC-ESI-QFT; MS2; CE:40; R=30000; [M-H]-; # PEAKS=16
LC-ESI-QFT	MassBank EU	Spectrum	LC-ESI-QFT; MS2; CE: 35 NCE; R=35000; [M-H]-; # PEAKS=1
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE10eV; [M-H]-; # PEAKS=13
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE20eV; [M-H]-; # PEAKS=8
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE30eV; [M-H]-; # PEAKS=15
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE40eV; [M-H]-; # PEAKS=14
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE50eV; [M-H]-; # PEAKS=13
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE60eV; [M-H]-; # PEAKS=14
LC-ESI-QTOF	MassBank EU	Spectrum	LC-ESI-QTOF; MS2; CE: 10 eV; R=35000; [M-H]-; # PEAKS=3

Generate PFAS reference spectra using high resolution LC-MS

This method has spectra associated with it. Click here to view.

Author: Benjamin Place
Focus/Analyte: PFAS
Synopsis: Generate PFAS reference spectra using high resolution LC-MS

PDF Viewer | Compounds (141) (grid) | Compounds (141) (table)

1 / 23 | 74%

PFAS150 Data Report

Disclaimer: Certain commercial equipment, instruments, software, or materials are identified in this documentation in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

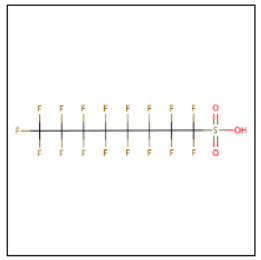
Authors: Benjamin Place
Date: September 19, 2022
Title: Generation of reference data for per- and polyfluoroalkyl substances in the EPA PFAS150 standard set
Methods: liquid chromatography with high resolution tandem mass spectrometry
Constituents: per- and polyfluoroalkyl substances
Date(s) of Analysis: Sample Receipt: November 16, 2021
Sample Preparation: June 6-8, 2022
Instrumental Analysis: June 23-27 and July 6-13, 2022
Data Analysis: July 13 – August 22, 2022

Introduction
The work described in this report was in fulfillment of the material transfer agreement (MTA) with the U.S. Environmental Protection Agency. The set of PFAS solutions will be referred to as

General Search

PFOS | Compound Search | Home | Lists | Similar Method Search | Batch Search | Other Pages | About | Related Applications | Toggle Header/Footer

78 Results for "PFOS"



(Preferred) Name: Perfluorooctanesulfonic acid
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CASRN: 1763-23-1
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☑ Display Single Point Spectra

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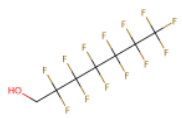
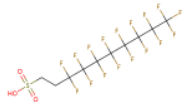
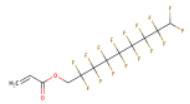
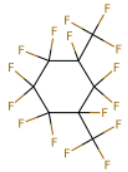
GC/MS, LC/MS, NMR	Analytical QC	Spectrum Link	External link only. Link has 28 file(s).
LC-APCI, LC-ESI	NIST PFAS	Method	Generate PFAS reference spectra using high resolution LC-MS
LC-ESI	NIST PFAS	Spectrum	ESI; MS2; [M-H]-; R=17500; # PEAKS=23
LC-ESI-QFT	MassBank EU	Spectrum	LC-ESI-QFT; MS2; CE:40; R=30000; [M-H]-; # PEAKS=16
LC-ESI-QFT	MassBank EU	Spectrum	LC-ESI-QFT; MS2; CE: 35 NCE; R=35000; [M-H]-; # PEAKS=1
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE10eV; [M-H]-; # PEAKS=13
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE20eV; [M-H]-; # PEAKS=8
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE30eV; [M-H]-; # PEAKS=15
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE40eV; [M-H]-; # PEAKS=14
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE50eV; [M-H]-; # PEAKS=13
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE60eV; [M-H]-; # PEAKS=14
LC-ESI-QTOF	MassBank EU	Spectrum	LC-ESI-QTOF; MS2; CE: 10 eV; R=35000; [M-H]-; # PEAKS=3

Generate PFAS reference spectra using high resolution LC-MS

This method has spectra associated with it. Click here to view.

Author: Benjamin Place
Focus/Analyte: PFAS
Synopsis: Generate PFAS reference spectra using high resolution LC-MS

PDF Viewer | Compounds (141) (grid) | Compounds (141) (table)

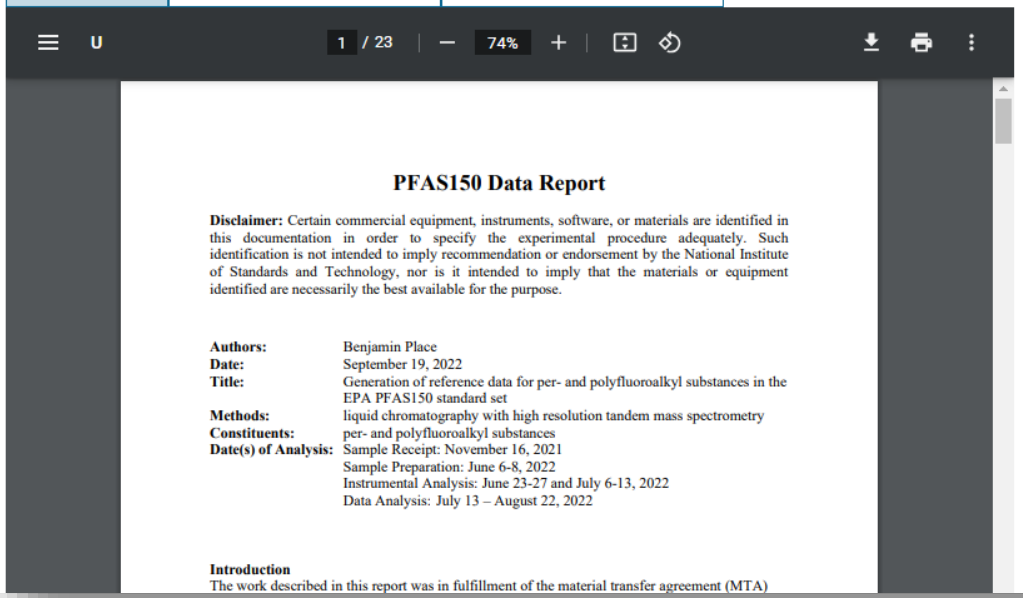
6:1 Fluorotelomer alcohol  DTXSID00190950 ↗	8:2 Fluorotelomer sulfonic ...  DTXSID00192353 ↗	1H,1H,9H-Perfluorononyl ...  DTXSID00194615 ↗
Perfluoro-1,3-dimethylcycl...  DTXSID0036926 ↗	3:3 Fluorotelomer carboxyl...  DTXSID00379268 ↗	10:1 Fluorotelomer alcohol  DTXSID00380056 ↗

Methods can have associated spectra

Generate PFAS reference spectra using high resolution LC-MS

Author: Benjamin Place
Focus/Analyte: PFAS
Synopsis: Generate PFAS reference spectra using high resolution LC-MS

PDF Viewer | Compounds (141) (grid) | Compounds (141) (table)



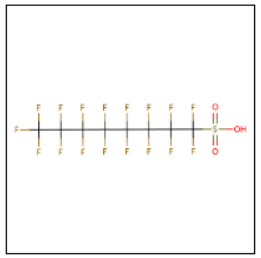
This is a list of the 68 spectra associated with this method, organized by compound identifier. Double-click on a row to show the spectrum in a modal window.

DTXSID	Compound Name
DTXSID00190950	6:1 Fluorotelomer alcohol
DTXSID00194615	1H,1H,9H-Perfluorononyl acrylate
DTXSID0059879	1H,1H,5H-Perfluoropentanol
DTXSID10382147	3-(Perfluoro-2-butyl)propane-1,2-diol
DTXSID20337446	2-(Perfluorooctyl)ethanthiol
DTXSID3066215	(Heptafluorobutanoyl)pivaloylmethane
DTXSID40380797	1H,1H-Perfluoro-3,6,9-trioxadecan-1-ol
DTXSID70381090	1H,1H,8H,8H-Perfluoro-3,6-dioxaoctane-1,8-diol
DTXSID70381151	Perfluorooctanamidine
DTXSID7060332	(Perfluorobutyryl)-2-thenoylmethane
DTXSID80310730	Octafluoroadipamide
DTXSID80375107	11:1 Fluorotelomer alcohol
DTXSID80379721	1H,1H,6H,6H-Perfluorohexane-1,6-diol diacrylate
DTXSID9059832	1H,1H,7H-Dodecafluoro-1-heptanol
DTXSID00192353	8:2 Fluorotelomer sulfonic acid
DTXSID00379268	3:3 Fluorotelomer carboxylic acid
DTXSID1032646	N-Ethylperfluorooctane sulfonamide
DTXSID1037303	Perfluoroheptanoic acid
DTXSID1067629	N-Methylperfluorooctanesulfonamide
DTXSID20179883	2-(Perfluorohexyl)ethylphosphonic acid

General Search finds spectra too

PFOS | Compound Search | Home | Lists | Similar Method Search | Batch Search | Other Pages | About | Related Applications | Toggle Header/Footer

78 Results for "PFOS"



(Preferred) Name: Perfluorooctanesulfonic acid
DTXSID: DTXSID3031864
CASRN: 1763-23-1
InChIKey: YFSUTJLHUFNCNZ-UHFFFAOYSA-N
Molecular Formula: C8HF17O3S
Mass: 499.9375

Download Results

☑ Display Single Point Spectra

All Results (78) | Methods (55) | Spectra (23) | Fact Sheets (0)

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GC/MS, LC/MS, NMR	Analytical QC	Spectrum Link	External link only. Link has 28 file(s).
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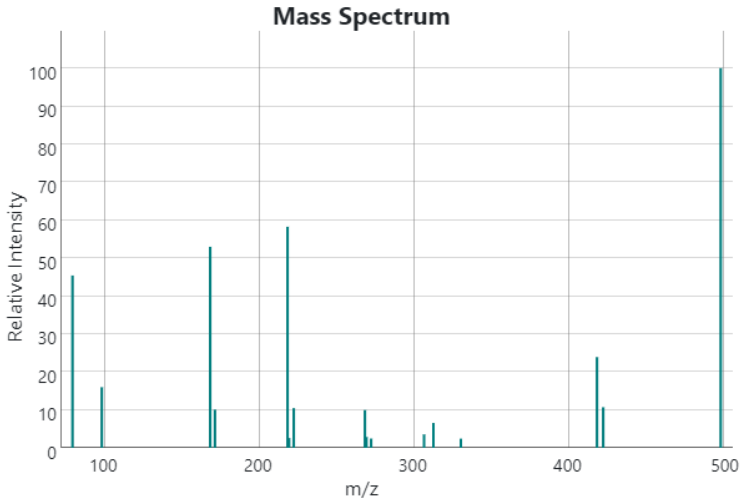
LC-ESI-QFT	MassBank EU	Spectrum	LC-ESI-QFT; MS2; CE:40; R=30000; [M-H]-; # PEAKS=16
LC-ESI-QFT	MassBank EU	Spectrum	LC-ESI-QFT; MS2; CE: 35 NCE; R=35000; [M-H]-; # PEAKS=1
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE10eV; [M-H]-; # PEAKS=13
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE20eV; [M-H]-; # PEAKS=8
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE30eV; [M-H]-; # PEAKS=15
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE40eV; [M-H]-; # PEAKS=14
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE50eV; [M-H]-; # PEAKS=13
LC-ESI-QQ	MassBank EU	Spectrum	LC-ESI-QQ; MS2; CE60eV; [M-H]-; # PEAKS=14
LC-ESI-QTOF	MassBank EU	Spectrum	LC-ESI-QTOF; MS2; CE: 10 eV; R=35000; [M-H]-; # PEAKS=3

Below is a plot of the spectrum as intensities versus mass-to-charge ratios (m/z). Click and drag over a section of the horizontal axis to zoom; double click to zoom back out. Intensities are scaled so that the highest peak has a value of 100.

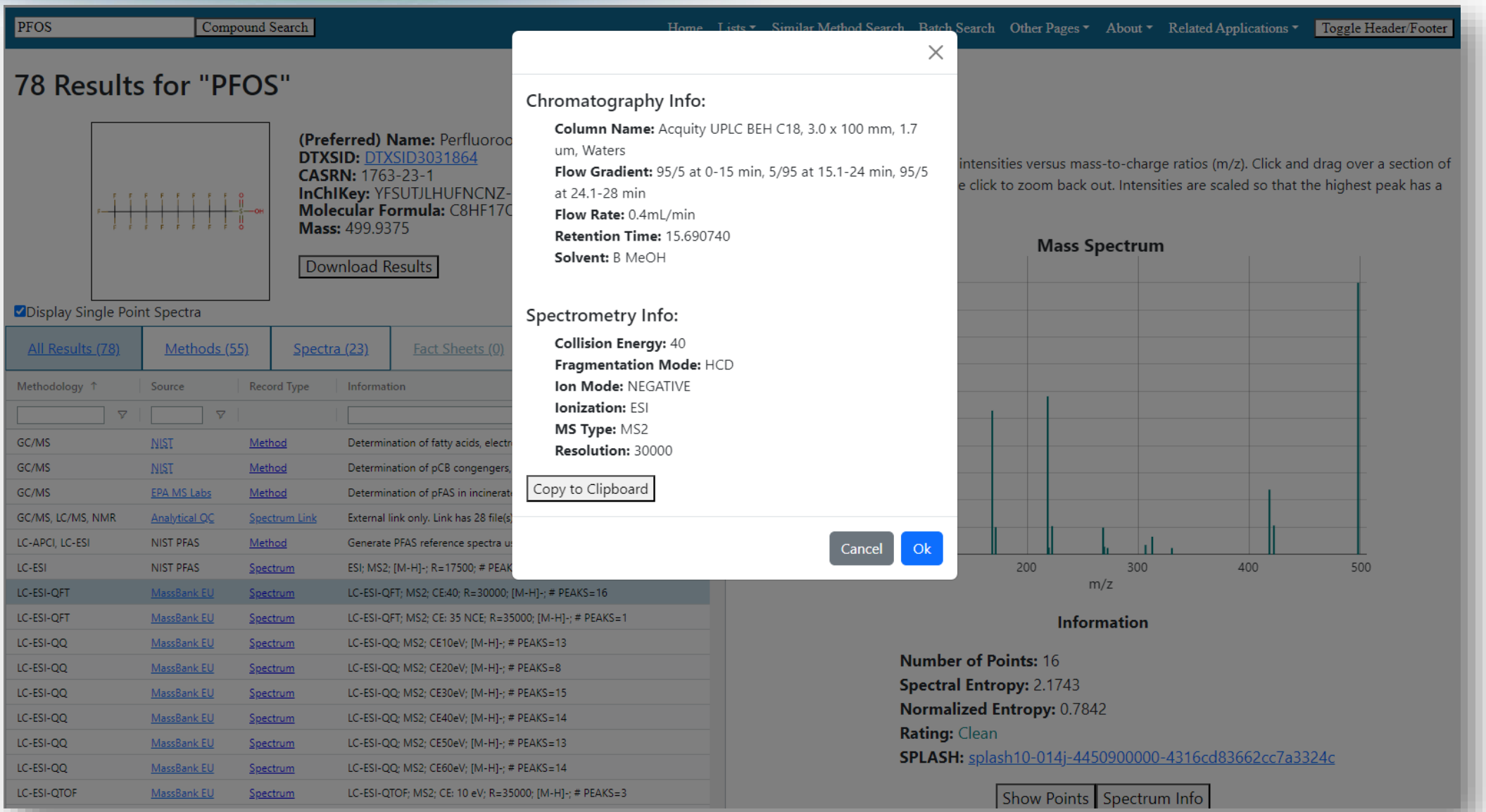


Information

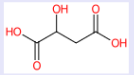
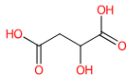
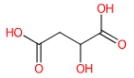
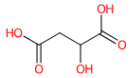
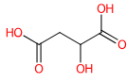
Number of Points: 16
Spectral Entropy: 2.1743
Normalized Entropy: 0.7842
Rating: Clean
SPLASH: splash10-014j-4450900000-4316cd83662cc7a3324c

Show Points | Spectrum Info

Chromatographic and Spectral Parameters



Curation is separating spectra-structures
Spectral Search based on InChI Key

⊞ L-(-)-Malic acid 5 spectra	C4H6O5 	134.02151	
⊞ L-Hydroxybutanedioic acid, L-(-)-Malic acid, L-Mal... 2 spectra	C4H6O5 	134.08701	
⊞ Malic acid 10 spectra	C4H6O5 	134.02153	
⊞ Malic acid-[1,2,3,4-13C4] 6 spectra	C4H6O5 	134.02153	
⊞ Malic acid-[1-13C] 6 spectra	C4H6O5 	134.02153	

Home Page

The search will return records of all three types -- spectra, fact sheets, and methods. The init

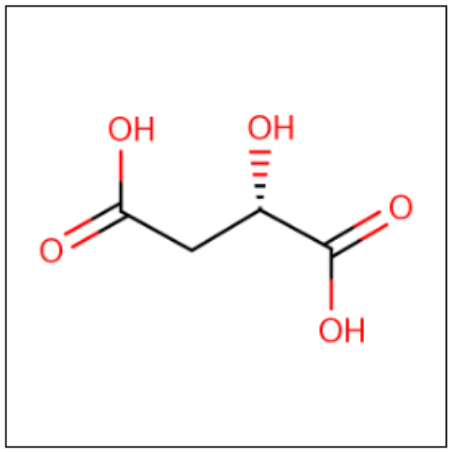
BJEPYKJPYRNKOW-REOHCLBHSA-N | Compound Search

◉All ○Methods ○Fact Sheets ○Spectra

Exact InChIKey Search: 34 spectra/1 method

An exact match for the InChIKey "BJEPYKJPYRNKOW-REOHCLBHSA-N" was found. However, several other InChIKeys with the same first block were discovered, if you were looking for one of those. Click on the InChIKey to be directed to search results for that substance.

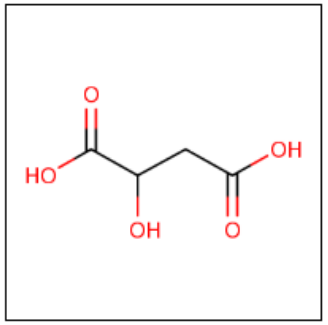
EXACT MATCH:



(Preferred) Name: (2S)-2-Hydroxybutanedioic acid
DTXSID: DTXSID30273987
CASRN: 97-67-6
InChIKey: BJEPYKJPYRNKOW-REOHCLBHSA-N
Molecular Formula: C4H6O5
Mass: 134.02153

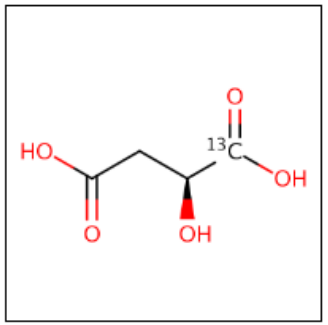
Records available: 34 spectra, 1 methods

Other spectra based on first block InChIKey
We map spectra to specific structures



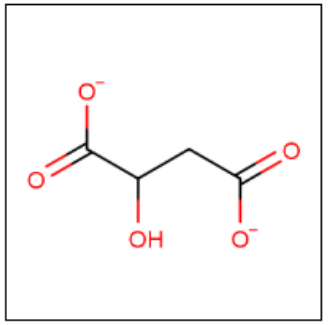
(Preferred) Name: Malic acid
DTXSID: DTXSID0027640
CASRN: 6915-15-7
InChIKey: BJEPYKJPYRNKOW-UHFFFAOYSA-N
Molecular Formula: C4H6O5
Mass: 134.02153

Records available: 66 spectra, 3 methods



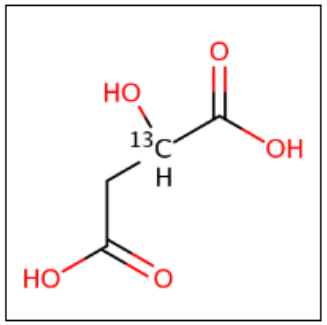
(Preferred) Name: (2S)-2-Hydroxy(1-^{13}C)butanedioic acid
DTXSID: DTXSID60745925
CASRN: 180991-05-3
InChIKey: BJEPYKJPYRNKOW-GZPBOPPUSA-N
Molecular Formula: C3[13C]H6O5
Mass: 135.02487

Records available: 3 spectra



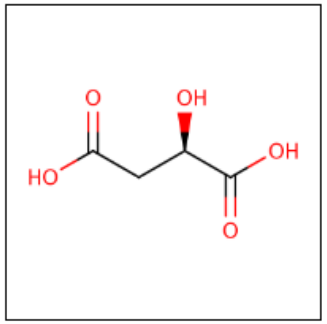
(Preferred) Name: 2-Hydroxybutanedioate
DTXSID: DTXSID00933521
CASRN: 149-61-1
InChIKey: BJEPYKJPYRNKOW-UHFFFAOYSA-L
Molecular Formula: C4H4O5
Mass: 132.00697

Records available: 1 spectra



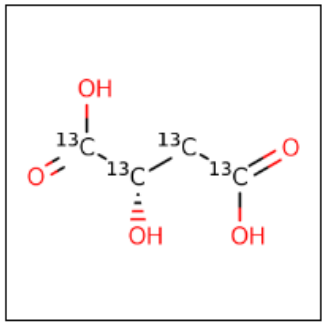
(Preferred) Name: 2-Hydroxy(2-^{13}C)butanedioic acid
DTXSID: DTXSID90745771
CASRN: 143435-96-5
InChIKey: BJEPYKJPYRNKOW-VQEHIDDOSA-N
Molecular Formula: C3[13C]H6O5
Mass: 135.02487

Records available: 5 spectra



(Preferred) Name: (+)-Malic acid
DTXSID: DTXSID90892496
CASRN: 636-61-3
InChIKey: BJEPYKJPYRNKOW-UWTATZPHSA-N
Molecular Formula: C4H6O5
Mass: 134.02153

Records available: 23 spectra



(Preferred) Name: Malic acid-[1,2,3,4-13C4] 2-
DTXSID: DTXSID301353776
CASRN: 1258274-51-9
InChIKey: BJEPYKJPYRNKOW-JCDJMFQYNA-N
Molecular Formula: [13C]4H6O5
Mass: 138.03494

Records available: 6 spectra

Methods List Filtering

Compound Search | Home | Lists | Similar Method Search | Batch Search | Other Pages | About | Related Applications | Toggle Header/Footer

Below is a list of methods currently in the database. Double-click on a row to display the method and its compounds in another tab. Cells in the table with a dashed underline have hovertext, usually for expanding out abbreviations in the cell content (it will take a second or two for the hovertext to appear).

2714 methods in total are present in the database; 2714 are currently displayed.

Full Table Filter

Copy filters to clipboard | Download Compounds | Reset Filters

Method #	Name	Year	Methodology	Source	Analyte	Chemical Class	Matrix	# Compounds
EPA-1656a	Method 1656, Revision A: Organo-Halide I	2020	GC/HSD	USEPA	Organohalide pesticides	Pesticides	Water (waste), soil, sludge, sediment, and fish tissu	31
EPA-1657a	Method 1657, Revision A: Organo-Phosph	2020	GC/FPD	USEPA	Organophosphorus Pesticides	Pesticides	Water (waste), soil, sludge, sediment, and fish tissu	47
EPA-601	Method 601: Purgeable Halocarbons	1994	GC/MS	USEPA	Halocarbons	Halocarbons	Municipal and industrial wastewater	29
CLG-MRM3.03	Screening and Confirmation of Animal Dru	2022	LC/MS	USDA	Drugs	Drugs	Kidney tissue (bovine, avian, porcine, caprine, ovine	108
CLG-PFAS2.03	Screening, Determination and Confirmatic	2021	LC/MS	USDA	PFAS	PFAS	Kidney tissue (bovine, avian, porcine, caprine, ovine	16
CLG-MRM1.08	Screening and Confirmation of Animal Dru	2018	LC/MS	USDA	Drugs	Drugs	Kidney tissue (bovine, avian, porcine, caprine, ovine	97
CLG-AMG2.08	Screening and Confirmation for Aminogly	2021	LC/MS	USDA	Aminoglycosides	Drugs	Kidney tissue (bovine, porcine, avian, ovine, caprine	9
CLG-AMG4.03	Screening for Aminoglycosides by LC-MS-	2020	LC/MS	USDA	Aminoglycosides	Drugs	Kidney tissue (bovine, porcine, avian, ovine, caprine	12
CLG-PST5.09	Screening for Pesticides by LC/MS and GC	2022	GC/MS;LC/MS	USDA	Pesticides	Pesticides	Muscle tissue (bovine, caprine, equine, ovine, porci	117
CLG-AGON1.10	Screening Determination and Confirmatio	2018	LC/MS	USDA	Beta-agonists	Drugs	Liver tissue (bovine, porcine), and muscle tissue (bc	5
CLG-AVR.04	Determination of Ivermectin, Doramectin,	2011	LC/FLD	USDA	Ivermectin, Doramectin and Moxidectin	Drugs	Liver tissue (bovine, ovine, porcine, caprine, equine	7
CLG-AVR1.03	Liquid Chromatography/Atmospheric Pres	2011	LC/MS	USDA	Ivermectin, Doramectin and Moxidectin	Drugs	Liver tissue (bovine, ovine, porcine, caprine, equine	3
CLG-CAM.07	Determination and Confirmation of Chlora	2018	GC/ECD;GC/MS	USDA	Chloramphenicol	Drugs	Muscle tissue (bovine, avian, fish, porcine, equine)	1
CLG-CBX4.02	Screen of Carbadox Metabolite QCA by HI	2016	LC/MS	USDA	Carbadox degradate QCA	Vet drug	Liver tissue (porcine)	2

Methods List: 82 Methods regarding PFAS

3294 methods in total are present in the database; 82 are currently displayed.

Full Table Filter

Copy filters to clipboard | Download Compounds | Reset Filters

Method #	Name	Year	Methodology	Source	Analyte	Chemical Class	Matrix	# Compounds
					PFAS			
CLG-PFAS2.03	Screening, Determinatio	2021	LC/MS	USDA	PFAS	PFAS	Kidney tissue (bovine, avian, p	16
CLG-PFC1.01	Determination and Conf	2009	LC/MS	USDA	PFAS	PFAS	Muscle tissue (bovine), and se	2
EPA-533	Method 533: Determina	2019	LC/MS	USEPA	PFAS	PFAS	Water (drinking)	25
EPA-537.1	Method 537.1 determin	2018	LC/MS	USEPA	PFAS	PFAS	Water (drinking)	18
EPA-1633	2nd Draft Method 1633:	2022	LC/MS	USEPA	PFAS	PFAS	Aqueous, solid (soil, biosolids	40
EPA-8327	Method 8327 – Per- and	2021	LC/MS	USEPA	PFAS	PFAS	Water (waste, surface, ground	41
5994-4926	Analysis of Per- and Poly	2022	LC/MS	Agilent	PFAS	PFAS	Water (waste)	39
5994-4960	Determination of Per an	2022	LC/MS	Agilent	PFAS	PFAS	Water (drinking)	62
5994-4237	Analysis of Perfluoroalky	2022	LC/MS	Agilent	PFAS	PFAS	Hair	21
5994-3920	Simultaneous Quantifica	2021	LC/MS	Agilent	PFAS	PFAS	Biosolids	47
5994-3616	Analysis of Per- and Poly	2021	LC/MS	Agilent	PFAS	PFAS	Water (drinking)	25
5994-3600	Targeted Quantitation o	2021	LC/MS	Agilent	PFAS	PFAS	Water (drinking)	71

Similar Method Search

Compound Identifier: 1-Propionyl-lysergic acid | Method Search

The table below lists methods for compounds that are similar to "1-Propionyl-lysergic acid diethylamide".

Select a row in the table to view the method on the right half of the screen. Bolded rows refer to methods which contain the chemical being searched.

Hover over a method name to see the full text of it. The number in parentheses at the end is the number of similar compounds found in the method (not necessarily the number of compounds present in the method).

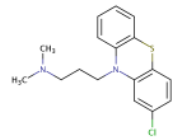
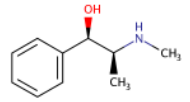
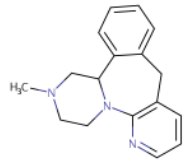
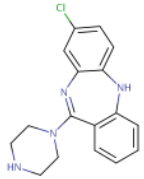
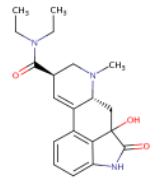
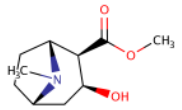
Columns can be hidden by clicking on the menu icon seen when hovering over a column name -- this brings up a menu where column visibility can be toggled.

Method Name (# compounds)	Source	Methodology	Year	Simi... ↓	Similar DTXSID	Compound Na
Highly sensitive determination c	Analytical and	LC/MS	2014	0.88		
	Analytical and	LC/MS	2014	0.88	DTXSID1023231	Lysergide
	Analytical and	LC/MS	2014	0.54	DTXSID00436244	2-Oxo-3-hyc
A fully automated approach for	Journal of Chrc	LC/MS	2018	0.88		
	Journal of Chrc	LC/MS	2018	0.88	DTXSID1023231	Lysergide
Performance Evaluation of LC-M	Journal of AOA	LC/MS	2019	0.84		
Development of a Novel LC-MS/	Molecules	LC/MS	2023	0.84		
Screening and Verifying Mycoto	Agilent	LC/MS	2016	0.64		
Determination of 63 mycotoxins	Food Control	LC/MS	2023	0.64		
Quantitative Screening of Multir	Agilent	LC/MS	2021	0.63		
An End-To-End Workflow for Qu	Agilent	LC/MS	2020	0.63		
Quantitative Screening of Multir	Agilent	LC/MS	2021	0.63		
Fast, rugged and sensitive ultra l	Journal of Chrc	LC/MS	2015	0.59		
Method development and valida	Environmental	LC/MS	2021	0.59		
Quantitation of Microcystins and	SCIEX	LC/MS	2017	0.59		
Identification of Unknown Micrc	Agilent	LC/MS	2014	0.59		
LC-MS/MS Validation and Quant	Toxins	LC/MS	2022	0.59		
On-line solid-phase extraction c	Toxicon	LC/MS	2015	0.59		
Development and Application o	Toxins	LC/MS	2022	0.59		

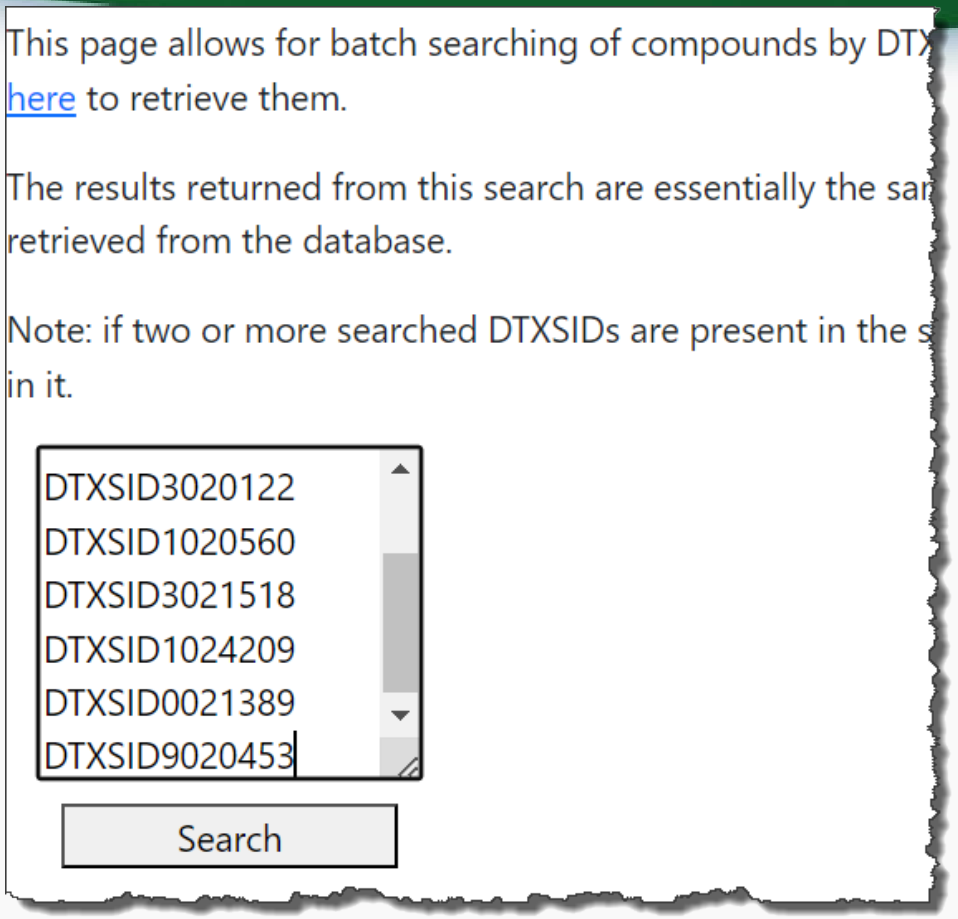
Highly sensitive determination of 68 psychoactive pharmaceuticals, illicit drugs, and related human metabolites in wastewater by liquid chromatography–tandem mass spectrometry

Author: Viola L. Borova, Niki C. Maragou, Pablo Gago-Derrero, Constantinos Pistos, Nikolaos S. Thomaidis
Focus/Analyte: Psychoactive substances
Synopsis: Determination of psychoactive substances in water (waste) by LC/MS.

PDF Viewer | Compounds (68) (grid) | Compounds (68) (table)

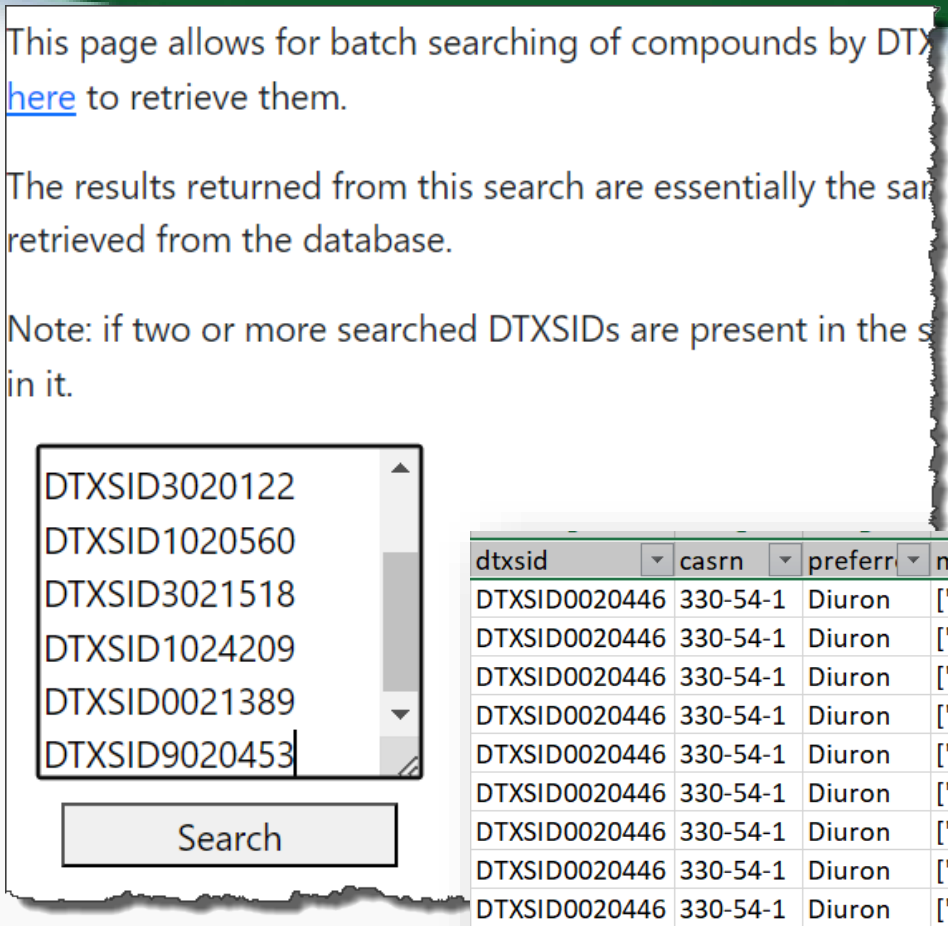
Chlorpromazine  DTXSID0022808 ↗	Ephedrine  DTXSID0022985 ↗	Mirtazapine  DTXSID0023325 ↗
N-Desmethylclozapine  DTXSID0042616 ↗	2-Oxo-3-hydroxy-LSD  DTXSID00436244 ↗	Ecgonine methyl ester  DTXSID00891435 ↗
Oxazepam	Lysergide	Thiopental

Batch Search



- Searching a set of DTXSIDs downloads sets of spectra and methods and links to original data

Batch Search



- Searching a set of DTXSIDs downloads sets of spectra and methods and links to original data

dtxsid	casrn	preferr	methodologies	source	link	record_	description
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DTXSID0020446	330-54-1	Diuron	['LC/MS']	MoNA	https://m	Spectrum	MS2; Positive; # PEAKS=9
DTXSID0020446	330-54-1	Diuron	['LC/MS']	MoNA	https://m	Spectrum	MS2; Negative; # PEAKS=53
DTXSID0020446	330-54-1	Diuron	['LC/MS']	MoNA	https://m	Spectrum	MS2; Positive; # PEAKS=25
DTXSID0020446	330-54-1	Diuron	['LC/MS']	MoNA	https://m	Spectrum	MS2; Positive; # PEAKS=54
DTXSID0020446	330-54-1	Diuron	['GC/MS', 'LC/MS'	USDA	https://w	Method	Determination of pesticides in muscle tissue (bovine, caprine, equine, ovine, p
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	Determination of linuron, diuron and their degradates in water (drinking, grou
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	DER of method for determination of diuron, Linuron, Desmethoxy linuron, Nor
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	Determination of linuron, Diuron and their degradates in soil (loam, silty clay l
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	ILV of method for determination of linuron, Diuron and their degradates in soi
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	DER of method for determination of diuron and its degradates in water (drinki
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	Determination of diuron, Linuron and their degradates in water by LC/MS with
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-EMC	https://w	Method	ILV of method for determination of diuron degradates PDMU and cPMU in wat
DTXSID0020446	330-54-1	Diuron	['LC/MS']	EPA-ECM	https://w	Method	ILV of method for determination of diuron and its degradates DCPMU and mC
DTXSID0020446	330-54-1	Diuron	['LC/MS']	USEPA	https://w	Method	This method covers the use of high-performance liquid chromatography (HPLC

Spectrum Search

This page is intended for searching the database for spectra. Currently, this is just being done by mass (with a margin of error) and the methodology of the spectrum.

Mass Information

194 Da ± 0.1 ◉Da ○ppm

WARNING: Wide mass intervals can severly slow down the app due to retrieving large spectra; there are currently no limits on what mass values can be collected, so be careful.

Methodology

LC/MS

User Spectrum

```
53.84601 0.040218
59.7077 0.039517
69.04531 0.269281
71.112045 0.036707
83.06077 0.233345
110.071434 2.046293
```

Search

Search found 292 spectra covering 27 substances.

DTXSID (Name)	Similarity	Description
DTXSID0020232 (Caffeine) (41)	1.0000	
DTXSID5040673 (Ferulic acid) (34)	0.7781	
DTXSID1049431 (Anthrone) (1)	0.7629	
DTXSID20282301 (5,6-DIMETHOXY-3H-ISOBENZ(	0.7511	
DTXSID601029528 (Quebrachitol) (56)	0.5797	
	0.5797	Orbitrap; MS2; CE=2V; # PEAKS=8
	0.5794	MS2; CE=13V; # PEAKS=8
	0.5498	MS2; CE=13V; # PEAKS=4
	0.4944	Orbitrap; MS2; CE=1V; # PEAKS=5
	0.4799	Orbitrap; MS2; CE=4V; # PEAKS=7
	0.3116	Orbitrap; MS2; CE=2V; # PEAKS=12
	0.3113	Orbitrap; MS2; CE=0V; # PEAKS=2
	0.2911	Orbitrap; MS2; CE=3V; # PEAKS=13

Combined Mass Spectra

Spectrum Search

This page is intended for searching the database for spectra. Currently, this is just being done by mass (with a margin of error) and the methodology of the spectrum.

Mass Information

194 Da ± 0.1 ◉Da ○ppm

WARNING: Wide mass intervals can severly slow down the app due to retrieving large spectra; there are currently no limits on what mass values can be collected, so be careful.

Methodology

LC/MS

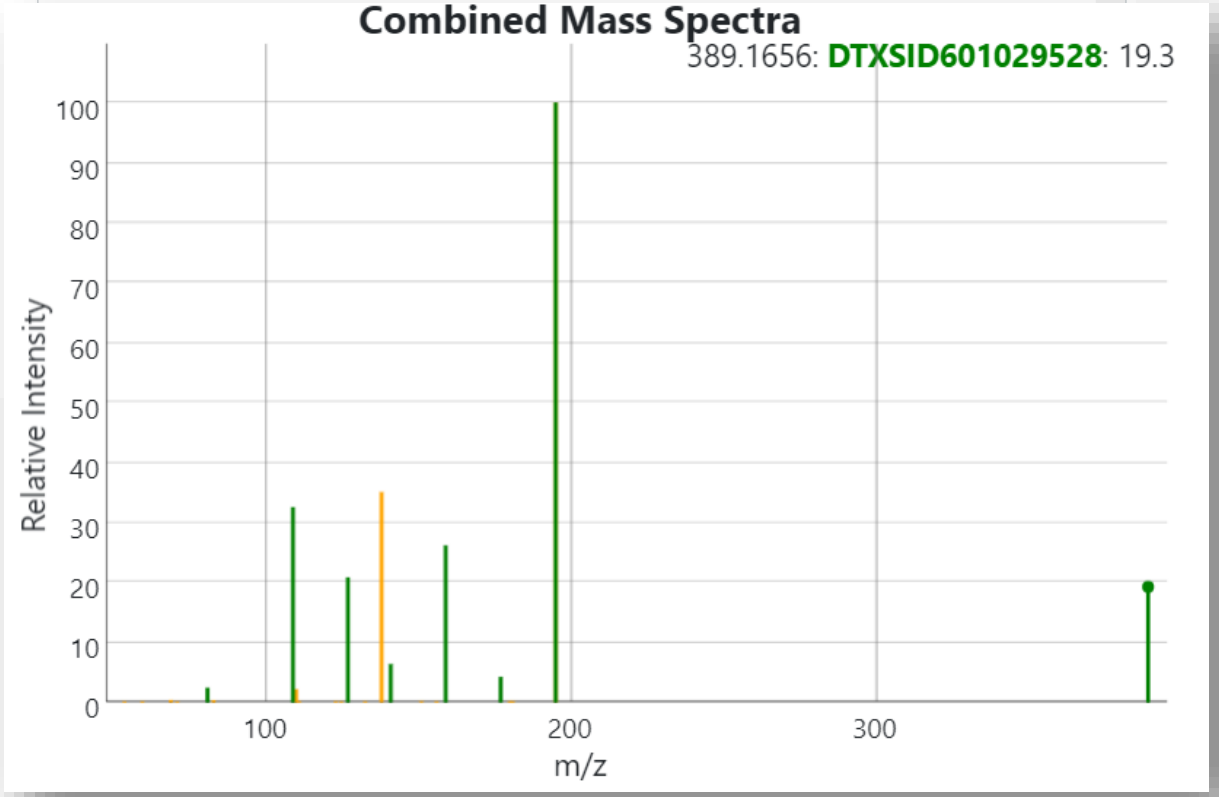
User Spectrum

```
53.84601 0.040218
59.7077 0.039517
69.04531 0.269281
71.112045 0.036707
83.06077 0.233345
110.071434 2.046293
```

Search

Search found 292 spectra covering 27 substances.

DTXSID (Name)	Similarity	Description
DTXSID0020232 (Caffeine) (41)	1.0000	
DTXSID5040673 (Ferulic acid) (34)	0.7781	
DTXSID1049431 (Anthrone) (1)	0.7629	
DTXSID20282301 (5,6-DIMETHOXY-3H-ISOBENZC	0.7511	
DTXSID601029528 (Quebrachitol) (56)	0.5797	
	0.5797	Orbitrap; MS2; CE=2V; # PEAKS=8



How can these data be used?

- Assembling spectral and methods data provides additional data for building training algorithms

Analytical and Bioanalytical Chemistry (2021) 413:7495–7508
https://doi.org/10.1007/s00216-021-03713-w

RESEARCH PAPER

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Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis

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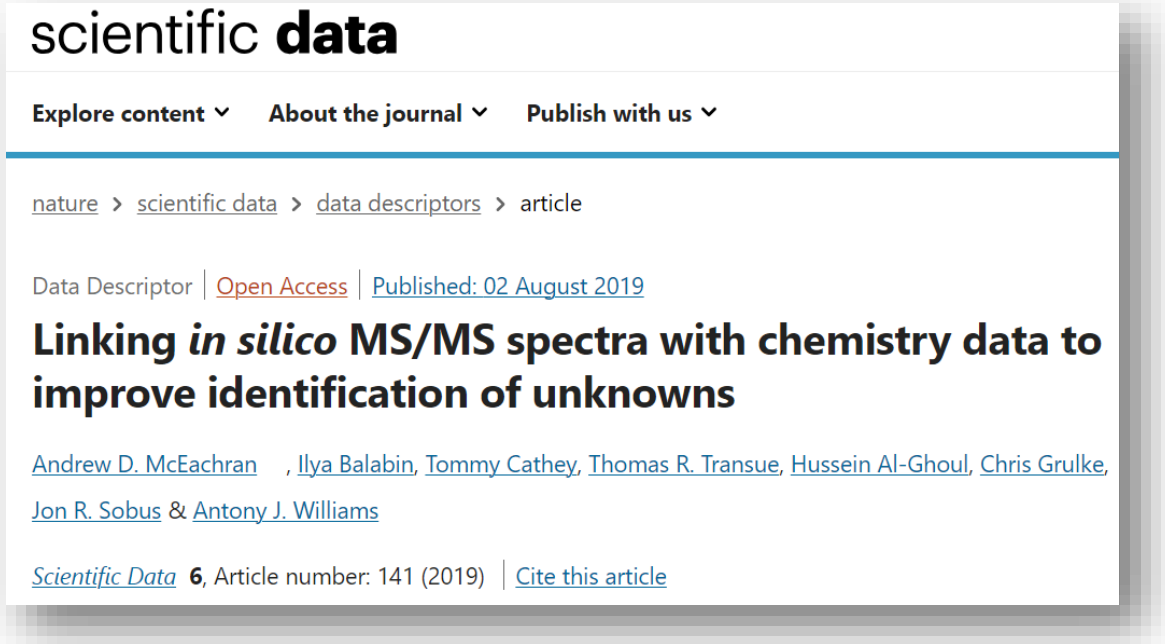
Spectral Searching for the NTA WebApp

- NTA is supported by searching against predicted spectra



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Andrew D. McEachran , Ilya Balabin, Tommy Cathey, Thomas R. Transue, Hussein Al-Ghoul, Chris Grulke, Jon R. Sobus & Antony J. Williams

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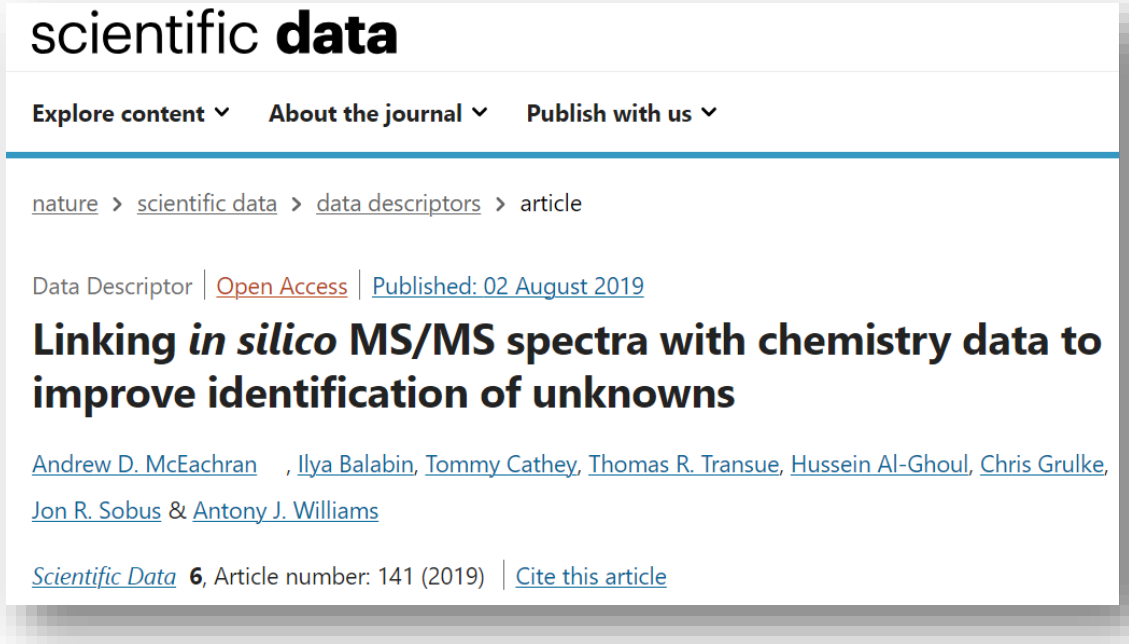
- Now experimental spectral data are being used

Spectral Searching for the NTA WebApp

- NTA is supported by searching against predicted spectra – NTA WebApp



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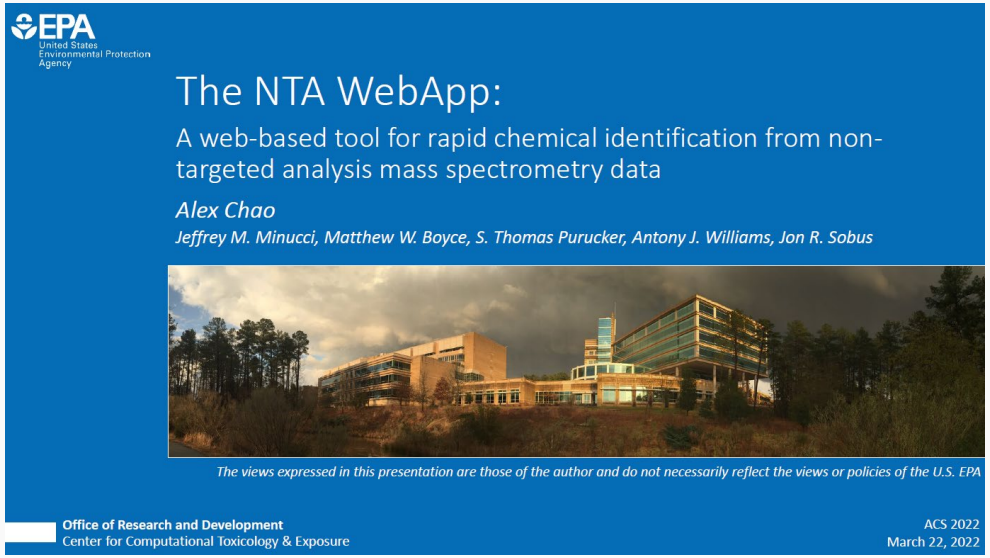


EPA United States Environmental Protection Agency

The NTA WebApp:

A web-based tool for rapid chemical identification from non-targeted analysis mass spectrometry data

Alex Chao

Jeffrey M. Minucci, Matthew W. Boyce, S. Thomas Purucker, Antony J. Williams, Jon R. Sobus

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

Office of Research and Development
Center for Computational Toxicology & Exposure

ACS 2022
March 22, 2022

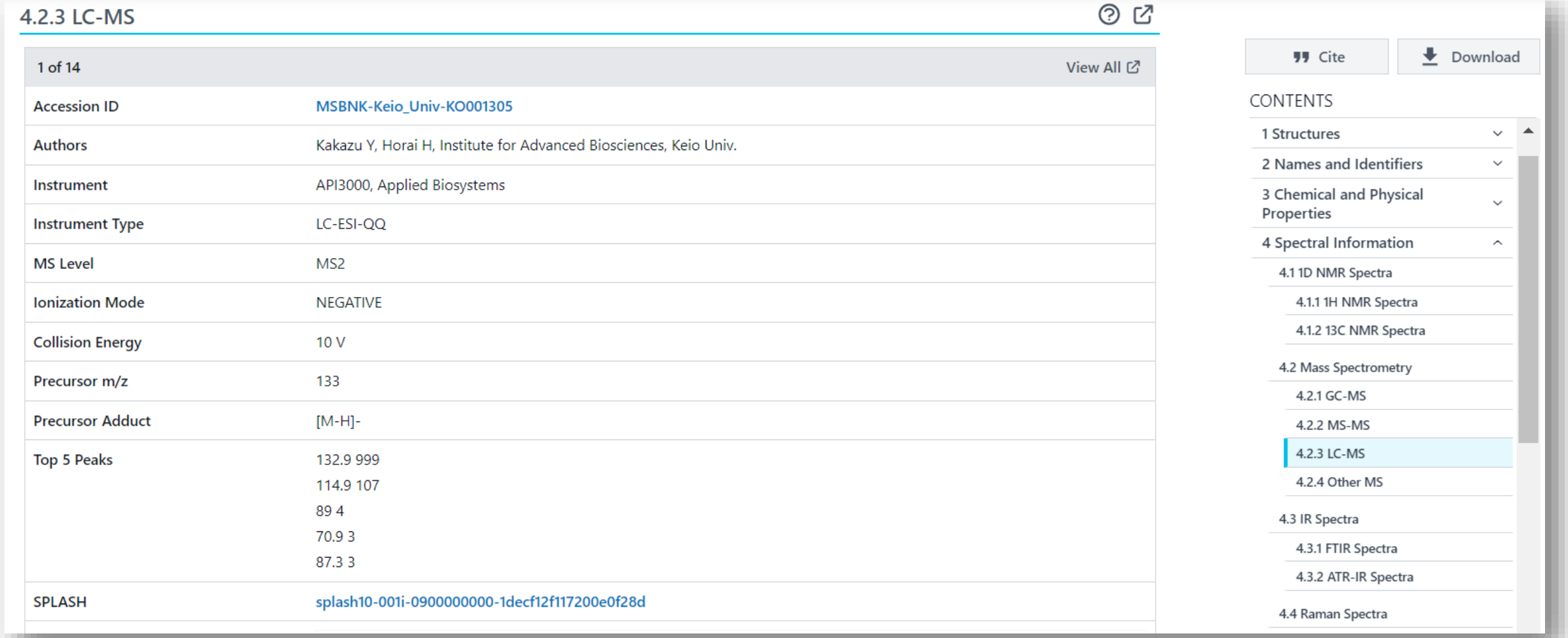
- Now experimental spectral data are being used

Future Work

- Add more data assembled from EPA labs (standards)
- Improvements to spectral searching – in testing
- Expand spectral and chromatographic metadata
- Structure, substructure and similarity searching
- Integration with other EPA applications
  - Chemical transformations database
  - ToxCast/Tox21 Analytical QC dataset for >8,000 chemicals

- ***Hoping to release to the public in 2024***

Other sources of Methods and Spectra PubChem



4.2.3 LC-MS

1 of 14 View All

Accession ID	MSBNK-Keio_Univ-KO001305
Authors	Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio Univ.
Instrument	API3000, Applied Biosystems
Instrument Type	LC-ESI-QQ
MS Level	MS2
Ionization Mode	NEGATIVE
Collision Energy	10 V
Precursor m/z	133
Precursor Adduct	[M-H]-
Top 5 Peaks	132.9 999 114.9 107 89 4 70.9 3 87.3 3
SPLASH	splash10-001i-0900000000-1decf12f117200e0f28d

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CONTENTS

Other sources of Methods and Spectra PubChem

4.2.3 LC-MS

1 of 14	
Accession ID	MSBNK-Keio_Univ-KO001305
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SPLASH	splash10-001i-0900000000-1decf

11 Identification

11.1 Analytic Laboratory Methods

9.123, 22.073. CORDIALS & LIQUEURS /OF/ ... TOTAL MALIC ACID (LEVO & INACTIVE) /DETERMINED/ BY CHROMATOGRAPHIC METHOD. 9.124, 22.081. CORDIALS & LIQUEURS /OF/ LEVO-MALIC ACID /DETERMINED BY/ POLARIZATION. /L-MALIC ACID/

Association of Official Analytical Chemists. Official Methods of Analysis. 10th ed. and supplements. Washington, DC: Association of Official Analytical Chemists, 1965. New editions through 13th ed. plus supplements, 1982., p. 13/160

▸ Hazardous Substances Data Bank (HSDB)

12.020, 22.073. BEVERAGES: NONALCOHOLIC & CONCENTRATES /OF/ TOTAL MALIC ACID /DETERMINED BY/ CHROMATOGRAPHIC METHODS. 12.021, 22.081. BEVERAGES: NONALCOHOLIC & CONCENTRATES /OF/ LEVO MALIC ACID /DETERMINED BY/ POLARIZATION. /L-MALIC ACID/

Association of Official Analytical Chemists. Official Methods of Analysis. 10th ed. and supplements. Washington, DC: Association of Official Analytical Chemists, 1965. New editions through 13th ed. plus supplements, 1982., p. 13/194

▸ Hazardous Substances Data Bank (HSDB)

11.047, 22.088. BEVERAGES: WINES /OF/ ... CITRIC & MALIC ACIDS /DETERMINED BY/ POLARIZATION.

Association of Official Analytical Chemists. Official Methods of Analysis. 10th ed. and supplements. Washington, DC: Association of Official Analytical Chemists, 1965. New editions through 13th ed. plus supplements, 1982., p. 13/160

Conclusions

- The AMOS database combines multiple kinds of data associated with analytical chemistry – primarily MS-related
- DSSTox database provides the underpinning chemistry
- Data can be interrogated via a web-based interface and enabled by cheminformatics
- Methods database is growing by 10-20 methods per day

If you want to help…

- Send information regarding analytical methods and method articles to williams.antony@epa.gov