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ENVIRONMENTAL
RESEARCH - UFZ



Interactive Demonstration

NORMAN-MassBank



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Contents of Demonstration

- NORMAN MassBank
 - Record Structure and the Record Index
 - Quick Search
 - Peak Search
 - Spectrum Search
 - Substructure Search
 - Administration of NORMAN MassBank
- MassBank in NIST

Mass Spectral Database Searching

Some Definitions

- Compound Database (e.g. ChemSpider, PubChem):
 - A collection of structures, basic properties and associated information¹
 - Generally, no spectral data – but >32,000,000 structures

- Mass Spectral Databases (or Libraries)
 - A collection of structures, their mass spectra and associated information
 - NIST and Wiley Mass Spectral Libraries for GC-EI-MS
 - NIST14: 276,259 spectra; Wiley 10th: >719,000 spectra²
 - MS/MS databases are growing; none are yet “established”
 - MassBank: 40,899 spectra (mixed origin);
 - METLIN: 61,872 HR-ESI-MS/MS, Agilent TOF-MS of 12,057 cmpds
 - NIST MS/MS: 193,164 MS/MS spectra of ~8,000 compounds
 - mzCloud.org: 134,029 HR-MS/MS spectra of 1,840 compounds

¹<http://www.chemspider.com/About.aspx>.

²<http://www.sisweb.com/software/ms/wiley.htm>

Using NORMAN MassBank

What do you really want to achieve?









- Flexible exchange of data within NORMAN
 - Upload of data from different instruments, different resolutions, ...
 - Reduce standard purchase via sharing of data
 - Extension to tentative / unknown spectra

- Purpose of a Mass Spectral Search
 - I have a compound of interest
 - Are there any spectra? What do they look like?
 - I want to identify an unknown
 - Features of MassBank that may be useful
 - Using MetFusion for identification
 - I want to perform routine confirmation and quantification of targets
 - MassBank is not the best stand-alone solution for you (yet?!)
 - *Talk to vendors to value-add instrument software with MassBank*

MassBank: www.massbank.jp

Horai et al. 2010: DOI 10.1002/jms.1777



-  Database Service
-  Statistics
-  Documents
-  Download
-  Manuals
-  About MassBank
-  Contact
-  Consortium Members

-  Site Map
-  Use Restrictions

News

- Sep 25, 2012 [Record Editor 2.1](#) was updated. new
- Sep 21, 2012 [Document](#) page was updated. new
- Sep 20, 2012 MassBank service will stop on Sep 27 for the server maintenance. new
- Sep 03, 2012 [Manuals](#) page was updated. new
- Aug 24, 2012 [Record Editor 2.1](#) was updated. new

[→ All news](#)



Database Service

→ Spectrum Search	→ Quick Search	→ Peak Search	→ Substructure Search	→ Metabolite Identification
→ Spectral Browser	→ Batch Service	→ Browse Page	→ Record Index	

MassBank is financially supported from [National Bioscience Database Center, Japan Science and Technology Agency](#) (2011-2013).

[The Mass Spectrometry Society of Japan](#) officially supports MassBank.

Please cite the article ([DOI](#)) when using MassBank.

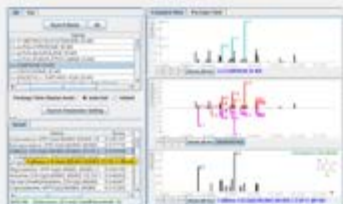
NORMAN MassBank

<http://massbank.normandata.eu/MassBank/>



NORMAN MassBank

Spectrum Search



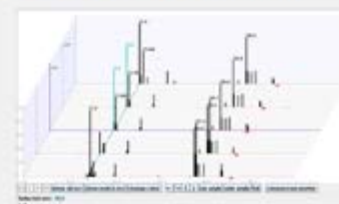
Quick Search

Substructure Search

Browse Page

Peak Search

Spectral Browser



Record Index

NORMAN MassBank

<http://massbank.normandata.eu/MassBank/>



NORMAN MassBank

[Spectrum Search](#)

[Quick Search](#)

[Substructure Search](#)

[Browse Page](#)

[Peak Search](#)

[Spectral Browser](#)

Search your spectrum through here

Search many other options here

[Record Index](#)

Browse through the records here

Searching MassBank

What do you want to achieve?

- MassBank is a mixed database
 - Be careful to pick and mix your settings
 - Adjust the thresholds to the data you have
 - ...but also to the data in MassBank
 - Tolerance is in Da (i.e. one mass unit)
- Quality of spectra is quite mixed
 - ...as is the information provided in them

Instrument Type

<input type="checkbox"/> EI	<input type="checkbox"/> EI-B <input type="checkbox"/> EI-EBEB <input type="checkbox"/> GC-EI-MS <input type="checkbox"/> GC-EI-TOF
<input checked="" type="checkbox"/> ESI	<input checked="" type="checkbox"/> CE-ESI-TOF <input checked="" type="checkbox"/> ESI-IT-MS/MS <input checked="" type="checkbox"/> ESI-ITFT <input checked="" type="checkbox"/> ESI-QQ <input checked="" type="checkbox"/> ESI-QqIT-MS/MS <input checked="" type="checkbox"/> ESI-QqQ-MS/MS <input checked="" type="checkbox"/> ESI-QqTOF-MS/MS

Ionization Mode

Positive
 Negative
 Both

More details in the next slides!

MassBank Record Format

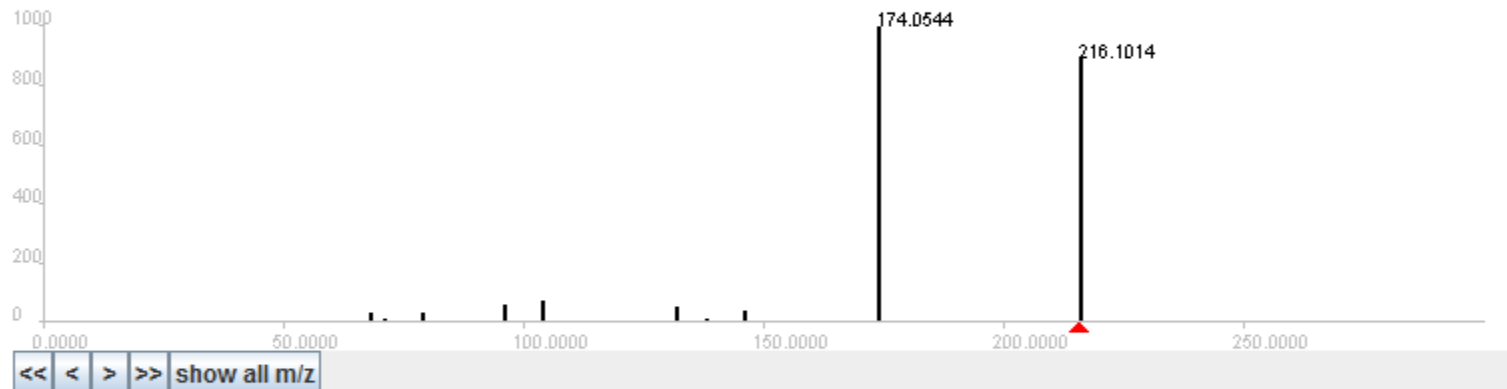
MassBank Record: EA028804

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#)

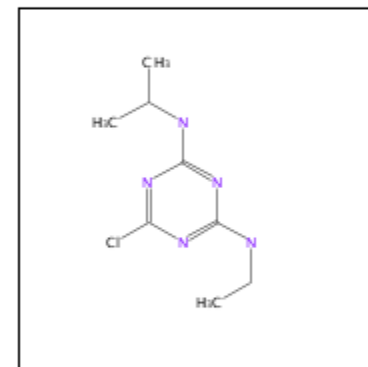
MassBank ID:

Atrazine; LC-ESI-ITFT; MS2; 45%; R=7500; [M+H]⁺

Mass Spectrum



Chemical Structure



ACCESSION: EA028804

RECORD_TITLE: Atrazine; LC-ESI-ITFT; MS2; 45%; R=7500; [M+H]⁺

DATE: 2012.08.02

AUTHORS: Stravs M, Schymanski E, Singer H, Department of Environmental Chemistry, Eawag

LICENSE: <http://massbank.ufz.de/MassBank/files/1.0/>

COPYRIGHT: Copyright (C) 2011 Eawag, Duebendorf, Switzerland

COMMENT: CONFIDENCE standard compound

COMMENT: EAWAG_UCHEM_ID 288

Authors, licence, copyright, etc

CH\$NAME: Atrazine

MassBank Record Format

Compound Information

CH\$NAME: Atrazine

CH\$NAME: 6-chloro-N-ethyl-N'-isopropyl-1,3,5-triazine-2,4-diamine

CH\$NAME: 6-chloranyl-N4-ethyl-N2-propan-2-yl-1,3,5-triazine-2,4-diamine

CH\$COMPOUND_CLASS: N/A; Environmental Standard

CH\$FORMULA: C8H14ClN5

CH\$EXACT_MASS: 215.0932

CH\$SMILES: c1(nc(nc(n1)Cl)NCC)NC(C)C

CH\$IUPAC: InChI=1S/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,

CH\$LINK: CAS [1912-24-9](#)

CH\$LINK: CHEBI [15930](#)

CH\$LINK: KEGG [C06551](#)

CH\$LINK: PUBCHEM CID:[2256](#)

CH\$LINK: INCHIKEY MXWJVTOOROXGIU-UHFFFAOYSA-N

CH\$LINK: CHEMSPIDER [10774593](#)

MassBank Record Format

Instrument and Measurement Information

```

AC$INSTRUMENT: LTQ Orbitrap XL Thermo Scientific
AC$INSTRUMENT_TYPE: LC-ESI-ITFT
AC$MASS_SPECTROMETRY: MS_TYPE MS2
AC$MASS_SPECTROMETRY: IONIZATION ESI
AC$MASS_SPECTROMETRY: ION_MODE POSITIVE
AC$MASS_SPECTROMETRY: FRAGMENTATION_MODE HCD
AC$MASS_SPECTROMETRY: COLLISION_ENERGY 45 % (nominal)
AC$MASS_SPECTROMETRY: RESOLUTION 7500
AC$CHROMATOGRAPHY: COLUMN_NAME XBridge C18 3.5um, 2.1x50mm, Waters
AC$CHROMATOGRAPHY: FLOW_GRADIENT 90/10 at 0 min, 50/50 at 4 min, 5/95 at
AC$CHROMATOGRAPHY: FLOW_RATE 200 ul/min
AC$CHROMATOGRAPHY: RETENTION_TIME 8.3 min
AC$CHROMATOGRAPHY: SOLVENT A water with 0.1% formic acid
AC$CHROMATOGRAPHY: SOLVENT B methanol with 0.1% formic acid

```

```

MS$FOCUSED_ION: BASE_PEAK 216.1012
MS$FOCUSED_ION: PRECURSOR_M/Z 216.101
MS$FOCUSED_ION: PRECURSOR_TYPE [M+H]+
MS$DATA_PROCESSING: DEPROFILE Spline
MS$DATA_PROCESSING: RECALIBRATE loess on assigned fragments and MS1
MS$DATA_PROCESSING: WHOLE RMassBank

```

MassBank Record Format - Peaks

PK\$ANNOTATION: m/z num {formula mass error(ppm) }

```
68.0243 1 C2H2N3+ 68.0243 0.24
71.0603 1 C3H7N2+ 71.0604 -0.35
79.0058 1 CH4C1N2+ 79.0058 0.35
96.0557 1 C4H6N3+ 96.0556 0.48
104.001 1 C2H3C1N3+ 104.001 0.28
132.0324 1 C4H7C1N3+ 132.0323 0.37
138.0779 1 C5H8N5+ 138.0774 3.1
138.1029 1 C7H12N3+ 138.1026 2.36
146.0228 1 C3H5C1N5+ 146.0228 0.01
146.0481 1 C5H9C1N3+ 146.048 0.95
174.0544 1 C5H9C1N5+ 174.0541 1.9
216.1014 1 C8H15C1N5+ 216.101 1.81
```

PK\$NUM_PEAK: 12

PK\$PEAK: m/z int. rel.int.

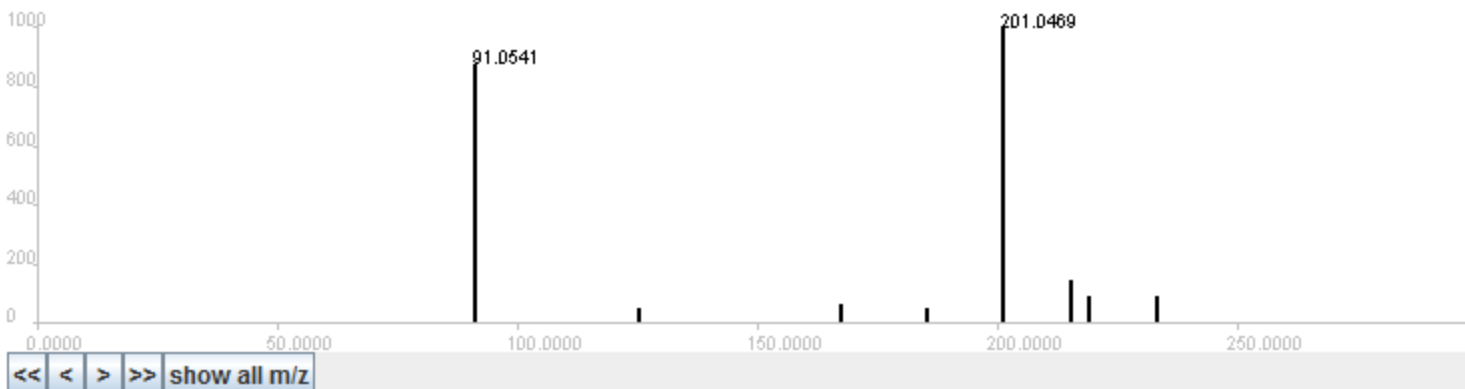
```
68.0243 949141.4 28
71.0603 167093.1 5
79.0058 1014555.8 30
96.0557 1956578 59
104.001 2256202.5 68
132.0324 1805661.3 54
138.0779 349329.9 10
138.1029 280901.6 8
146.0228 1313633.2 39
146.0481 263134.4 7
174.0544 32958196.3 999
216.1014 29362258.7 890
```

//

MassBank Record – Example Unknown (so far)

CASMI2012 LC Challenge 13; APCI-ITFT; MS2; CE:45 CID;

Mass Spectrum



Chemical Structure

Not Available

ACCESSION: SMI00131

RECORD_TITLE: CASMI2012 LC Challenge 13; APCI-ITFT; MS2; CE:45 CID;

DATE: 2012.08.31 (Created 2012.08.31)

AUTHORS: S. Neumann: IPB-Halle, Germany & E. Schymanski: Eawag, Switzerland

COPYRIGHT: CASMI2012

COMMENT: Unknown

COMMENT: <http://casmi-contest.org/challenges-cat1-2.shtml>

MS\$FOCUSED_ION: PRECURSOR_M/Z N/A

MS\$FOCUSED_ION: PRECURSOR_TYPE N/A

CH\$NAME: CASMI2012 LC Challenge 13

CH\$COMPOUND_CLASS: N/A; Unknown for CASMI

CH\$FORMULA: N/A

CH\$EXACT_MASS: N/A

CH\$SMILES: N/A

CH\$IUPAC: N/A

PK\$NUM_PEAK: 8

PK\$PEAK: m/z int. rel.int.

91.0541 2211410.3 873

125.0152 130666.3 52

167.0859 161086.1 64

185.0519 125915.7 50

201.0469 2531123 999

215.0626 371698.1 147

219.0576 223408.9 88

233.0733 226928.3 90

//

AC\$INSTRUMENT: LTQ-Orbitrap

AC\$INSTRUMENT_TYPE: APCI-ITFT

AC\$ANALYTICAL_CONDITION: MODE POSITIVE

AC\$MASS_SPECTROMETRY: MS_TYPE MS2

AC\$MASS_SPECTROMETRY: ION_MODE POSITIVE

MassBank Record Index

Have a look at what is in MassBank:

Contributor

: NORMAN EMPOMASS (2,081)	: CASMI (42)	: Eawag (944)
: UFZ (2,509)	: Keio Univ. (5,629)	: RIKEN (1,721)
: Waters (2,993)	: Kyoto Univ. (185)	: Chubu Univ. (2,628)
: Kazusa (273)	: Nihon Univ. (75)	: Univ. Toyama (253)
: Tottori Univ. (16)	: IPB Halle (528)	: Fukuyama Univ. (340)
: Metabolon (149)	: UOEH (35)	: NAIST (680)
: Osaka MCHRI (20)	: Univ. Connecticut (510)	: Osaka Univ. (502)
: IMM, CAMS & PUMC, China (192)	: PFOS research group (365)	: MPI for Chemical Ecology (691)

Contributor:

Instrument Type:
(Orbitrap = ITFT)

Instrument Type

: GC-EI-MS (2,097)	: LC-ESI-QTOF (2,750)	: LC-APCI-ITFT (10)
: APCI-ITFT (1,206)	: LC-ESI-ITFT (4,504)	: ESI-ITFT (1,310)
: LC-ESI-IT (515)	: LC-ESI-QQ (5,038)	: CE-ESI-TOF (20)
: GC-EI-TOF (1,016)	: LC-ESI-Q (2,720)	: EI-EBEB (12)
: FAB-EBEB (173)	: LC-ESI-QIT (378)	: EI-B (91)
: LC-ESHTTOF (253)	: FAB-EB (5)	: ESI-MS/MS (149)
: CI-B (1)	: FAB-B (26)	: FD-B (3)
: MALDI-TOF (17)	: ESI-QqTOF-MS/MS (510)	: ESI-QqIT-MS/MS (140)
: ESI-Qq-MS/MS (52)	: APPI-Qq-MS (2)	: APPI-Qq-MS/MS (27)
: ESI-QQ (78)	: LC-APPI-QQ (258)	

Compound Name: watch out for numbers...

Ionization Mode

: Positive (16,197)	: Negative (7,164)
-------------------------------------	------------------------------------

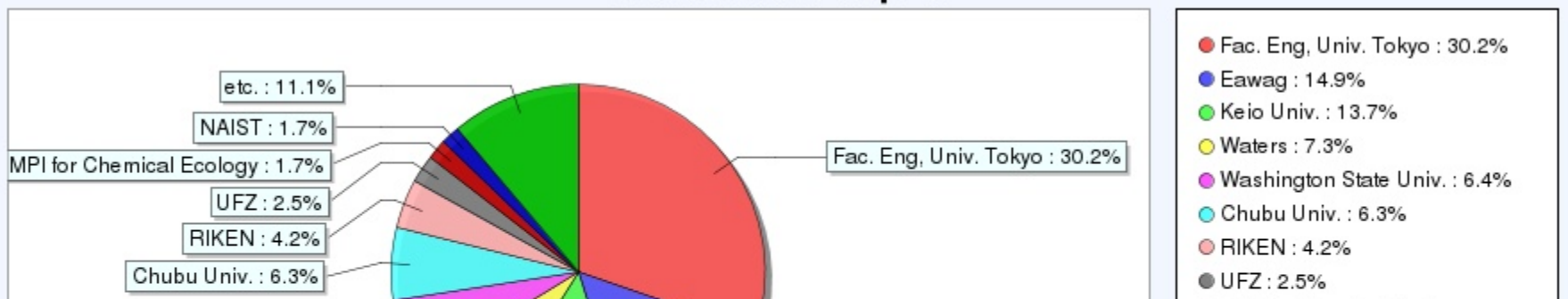
Compound Name

: A (1,185)	: B (1,122)	: C (1,372)	: D (1,559)	: E (426)	: F (421)
: G (793)	: H (429)	: I (657)	: J (2)	: K (223)	: L (1,254)
: M (996)	: N (1,005)	: O (388)	: P (3,687)	: Q (184)	: R (287)
: S (941)	: T (1,249)	: U (887)	: V (128)	: W (3)	: X (51)
: Y (5)	: Z (72)	: 1-9 (3,844)	: Others (191)		

MassBank Record Index

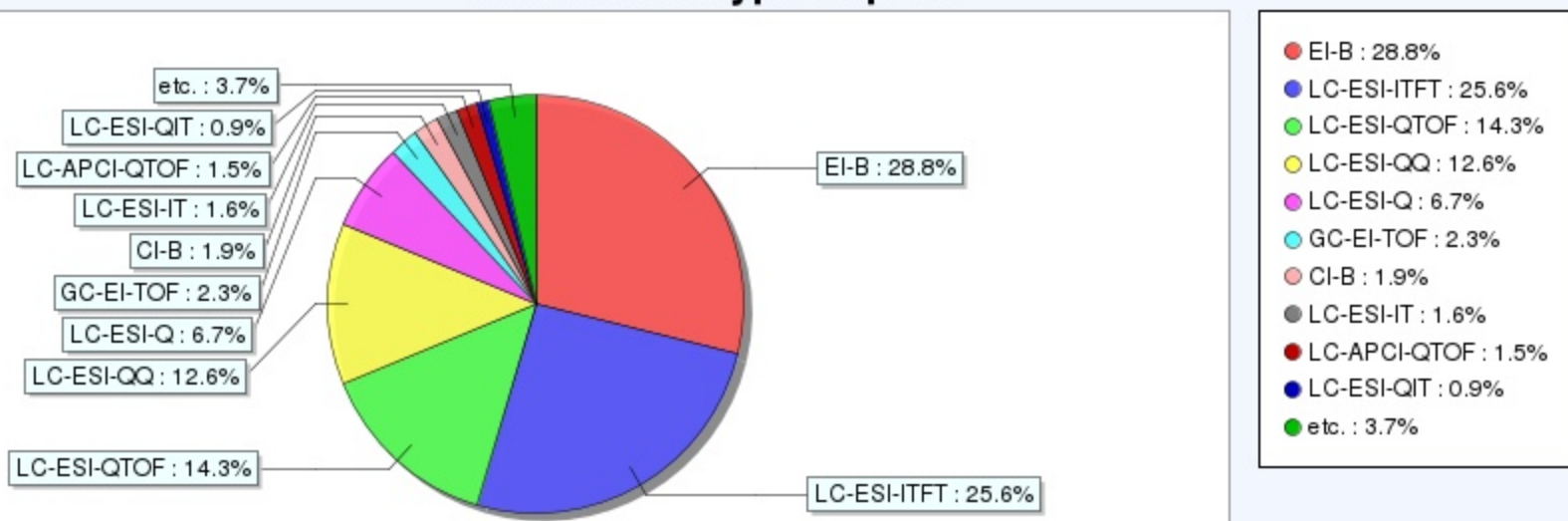
Scroll to see the contents (and see if your institute is in the top 10!)

Contributor top 10



Wast

Instrument Type top 10



MassBank Quick Search

Search compounds or peaks

Quick Search

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) |
 MassBank ID:

Search by Keyword

Search by Peak

Compound Name

Exact Mass **Tolerance**

Formula

(e.g. C₆H₇N₅, C₅H*N₅, C₅*)

REMEMBER:

Tolerance is in Da (one mass unit)

Instrument Type

<input checked="" type="checkbox"/> EI	<input checked="" type="checkbox"/> EI-B
	<input checked="" type="checkbox"/> EI-EBEB
	<input checked="" type="checkbox"/> GC-EI-TOF
<hr/>	
<input checked="" type="checkbox"/> ESI	<input checked="" type="checkbox"/> CE-ESI-TOF
	<input checked="" type="checkbox"/> ESI-QqIT-MS/MS
	<input checked="" type="checkbox"/> ESI-QqQ-MS/MS
	<input checked="" type="checkbox"/> LC-ESI-IT
	<input checked="" type="checkbox"/> LC-ESI-ITFT

MS Type

All
 MS
 MS2
 MS3
 MS4

Ion Mode

Positive
 Negative
 Both

Quick Search Results

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID:

Search Parameters :

Compound Name: **carbazole**

Instrument Type:

EI-B ,	EI-EBEB ,	GC-EI-TOF
CE-ESI-TOF ,	ESI-QqIT-MS/MS ,	ESI-QqQ-MS/MS
LC-ESI-IT ,	LC-ESI-ITFT ,	LC-ESI-ITTOF
LC-ESI-Q ,	LC-ESI-QIT ,	LC-ESI-QQ
LC-ESI-QTOF ,	CI-B ,	FAB-B
FAB-EB ,	FAB-EBEB ,	FD-B
FI-B ,	LC-APPI-QQ ,	MALDI-TOF
MALDI-TOFTOF		

MS Type: **All**



Ion Mode: **Both**

[Edit / Resubmit Query](#)

Results : **34 Hit.** (1 - 34 Displayed)

First [Prev](#) **1** [Next](#) [Last](#) (Total **1** Page)

▼ Results End

<input type="checkbox"/>	Name		Formula / Structure	ExactMass	ID
<input type="checkbox"/>	1,6-DINITROCARBAZOLE	1 spectrum	C12H7N3O4 	257.04366	
<input type="checkbox"/>	1-METHYLCARBAZOLE	1 spectrum	C13H11N 	181.08915	
<input type="checkbox"/>	2-METHYLCARBAZOLE		C13H11N	181.08915	

MassBank Quick Search

Search compounds or peaks

Quick Search

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Browser](#) | [Browse](#) | [Index](#) | MassBank ID:

Search by Keyword

Search by Peak

Peak Data

```
273.096 22
289.086 107
290.118 14
291.096 999
292.113 162
293.054 34
579.169 37
580.179 15
```

m/z and relative intensities(0-999), delimited by a space.

Cutoff threshold of relative intensities

Number of Results

Instrument Type

- | | |
|-----------------------------------------|-----------------------------------------------------|
| <input type="checkbox"/> EI | <input type="checkbox"/> EI-B |
| | <input type="checkbox"/> EI-EBEB |
| | <input type="checkbox"/> GC-EI-MS |
| | <input type="checkbox"/> GC-EI-TOF |
| <hr/> | |
| <input checked="" type="checkbox"/> ESI | <input checked="" type="checkbox"/> CE-ESI-TOF |
| | <input checked="" type="checkbox"/> ESI-IT-MS/MS |
| | <input checked="" type="checkbox"/> ESI-ITFT |
| | <input checked="" type="checkbox"/> ESI-QQ |
| | <input checked="" type="checkbox"/> ESI-QqIT-MS/MS |
| | <input checked="" type="checkbox"/> ESI-QqQ-MS/MS |
| | <input checked="" type="checkbox"/> ESI-QqTOF-MS/MS |

Ionization Mode

- Positive Negative Both

MassBank Peak Search

Different to Quick Search → Search by Peak!

Peak Search

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) |
 MassBank ID:

Search of **Peaks** *Peak Differences*
 Search by **m/z-Value** *Molecular Formula*

	<i>m/z</i>	←	Formula
AND ▾	<input type="text" value="105.04527"/>	←	<input type="text" value="C6H5N2"/>
AND	<input type="text" value="77.03912"/>	←	<input type="text" value="C6H5"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>

Rel.Intensity Tolerance

Instrument Type

- EI
 - EI-B
 - EI-EBEB
 - GC-EI-TOF
- ESI
 - CE-ESI-TOF
 - ESI-QqIT-MS/MS
 - ESI-QqQ-MS/MS
 - LC-ESI-IT
 - LC-ESI-ITFT

MS Type

- All
- MS
- MS2
- MS3
- MS4

Ion Mode

- Positive
- Negative
- Both

Peak Search Results (Peaks by m/z value)

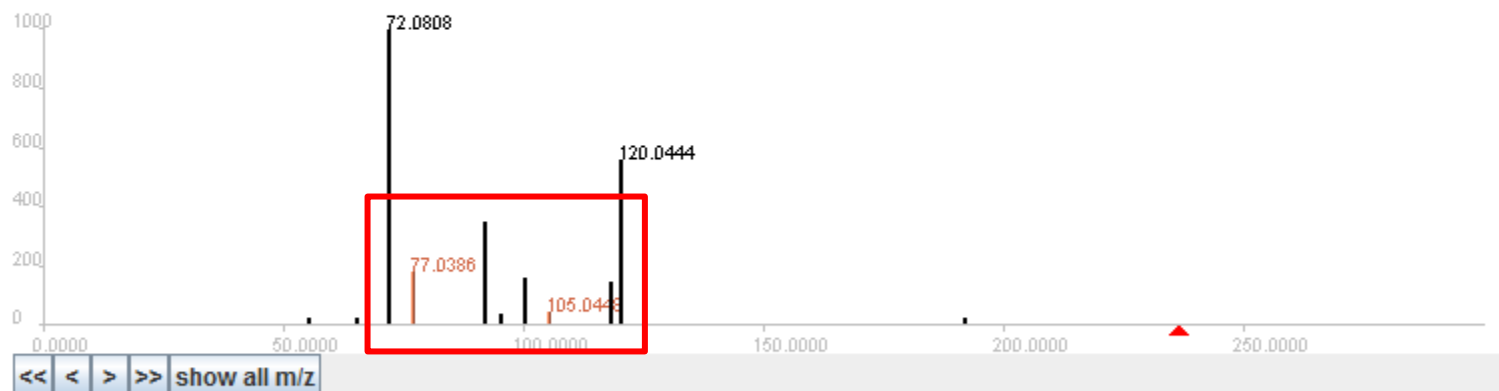
[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID:

MassBank Record: EA013612

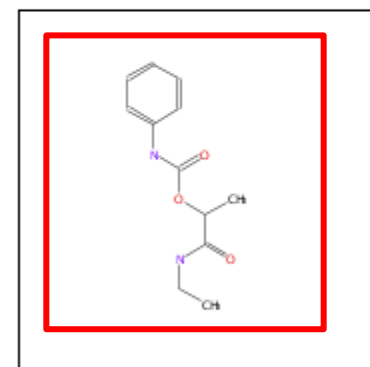
[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID:

Carbetamide; LC-ESI-ITFT; MS2; 75%; R=15000; [M+H]⁺

Mass Spectrum



Chemical Structure



ACCESSION: EA013612

RECORD_TITLE: Carbetamide; LC-ESI-ITFT; MS2; 75%; R=15000; [M+H]⁺

DATE: 2012.08.02

AUTHORS: Stravs M, Schymanski E, Singer H, Department of Environmental Chemistry, Eawag

<input type="checkbox"/>	<input checked="" type="checkbox"/> Aminocaproic acid	1 spectrum	<chem>C6H13NO2</chem>		131.09463
--------------------------	-------------------------------------------------------	------------	-----------------------	--	-----------

MassBank Peak Search

By Peak Differences and m/z value

Peak Search

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) |
 MassBank ID:

Search of Peaks Peak Differences
 Search by m/z-Value Molecular Formula

	m/z Diff.	←	Formula
AND ▾	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>
AND	<input type="text"/>	←	<input type="text"/>

Rel.Intensity Tolerance

Instrument Type

EI
 EI-B
 EI-EBEB
 GC-EI-TOF

ESI
 CE-ESI-TOF
 ESI-QqIT-MS/MS
 ESI-QqQ-MS/MS
 LC-ESI-IT
 LC-ESI-ITFT

MS Type

All MS MS2 MS3 MS4

Ion Mode

Positive Negative Both

MassBank Peak Search

By Peak Differences and Molecular Formula

Peak Search

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Prediction](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID:

Search of Peaks Peak Differences
 Search by *m/z-Value* Molecular Formula

Neutral Loss 1

Formula

AND

Neutral Loss 2

Formula

AND

Neutral Loss 3

Formula

AND

Neutral Loss 4

Formula

AND

Neutral Loss 5

Formula

AND SEQUENCE

* The targets of Peak Search Advanced are only Keio and Riken data.

Instrument Type

ESI

LC-ESI-QTOF

MS Type

All

MS2

Ion Mode

Positive

Negative

B

MassBank Spectrum Search

<http://www.massbank.jp/sample/sample.txt>

```
// Specification of file format
// - A line started by '//' is a comment line.
// - A peak is denoted by its m/z and intensity
  separated by one or more spaces.
// - Delimiter of spectra: one or more empty lines is
  needed between spectra.
If you saved the data before the workshop, you can try
this example with “SpectrumSearch_EnvEgs.txt”
// - A line started by 'ID:' specifies the value of the
  ID column in the spectrum table for each spectrum.
// - A line started by 'Name:' specifies the value of the
  name column in the spectrum table for each spectrum.
// - A "Nist Format" file can be used without any
  modification.
```

MassBank Spectrum Search Results

Spectrum Search

Home | Spectrum | Quick | Peak | Substructure | Prediction | Browser | Batch | Browse | Index | MassBank ID:

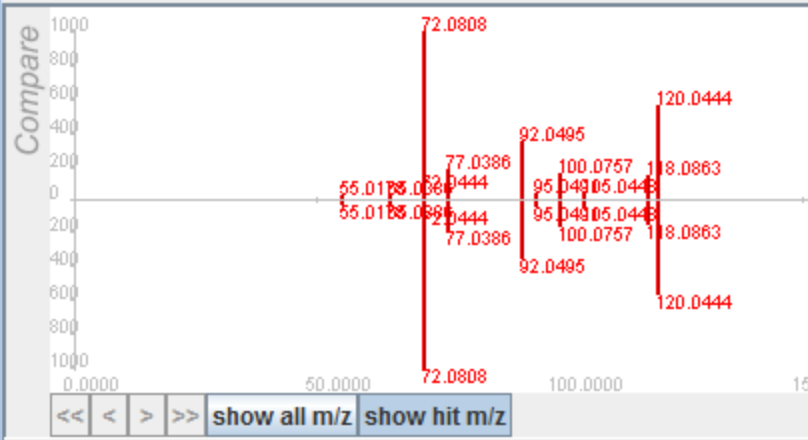
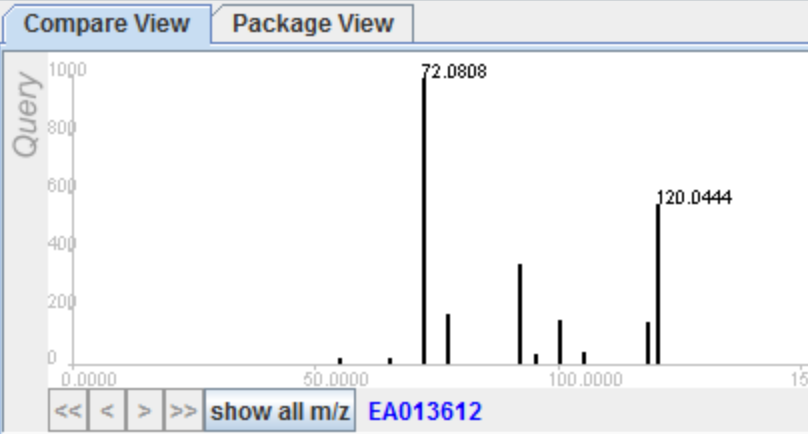
[sample file](#) [sample archive](#)

No.	Name	ID
1	EA013612	US000001
2	EA008812	US000002

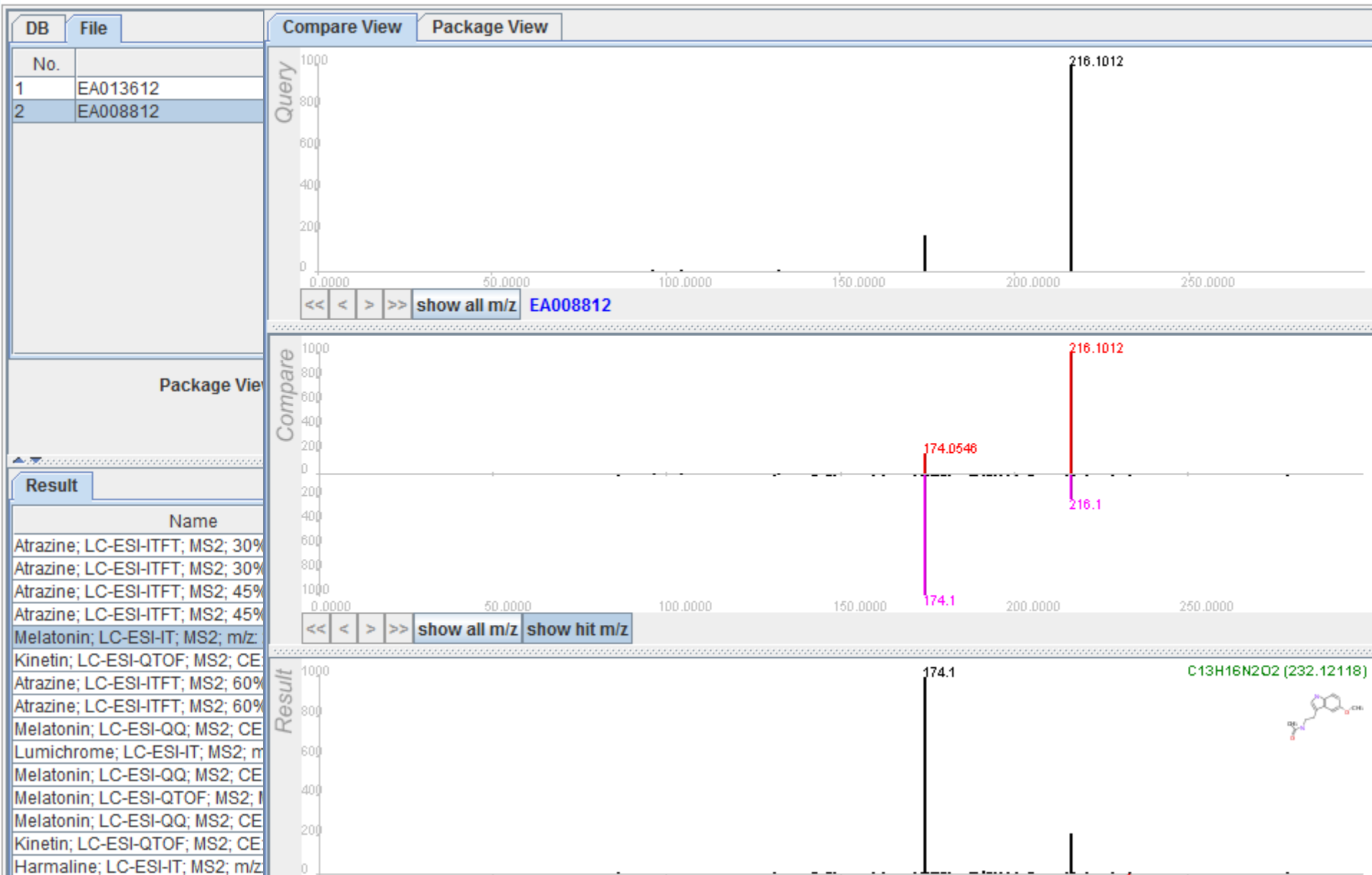
Click on file name to search

Package View display mode : selected related

Name	Score	Hit	ID	Ion	Contributor
Carbetamide; LC-ESI-ITFT; MS2; 75%; R=1...	0.941860...	12	EA013612	P	Eawag
Carbetamide; LC-ESI-ITFT; MS2; 75%; R=7...	0.937374...	12	EA013606	P	Eawag
Carbetamide; LC-ESI-ITFT; MS2; 60%; R=7...	0.908825...	11	EA013605	P	Eawag
Carbetamide; LC-ESI-ITFT; MS2; 60%; R=1...	0.903718...	10	EA013611	P	Eawag
Carbetamide; LC-ESI-ITFT; MS2; 90%; R=3...	0.893760...	12	EA013613	P	Eawag



MassBank Spectrum Search Results



MassBank Spectrum Search with NIST Format

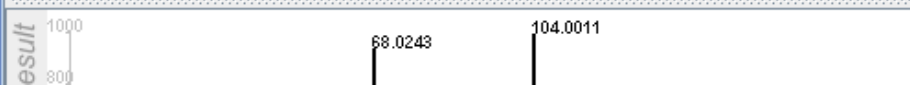
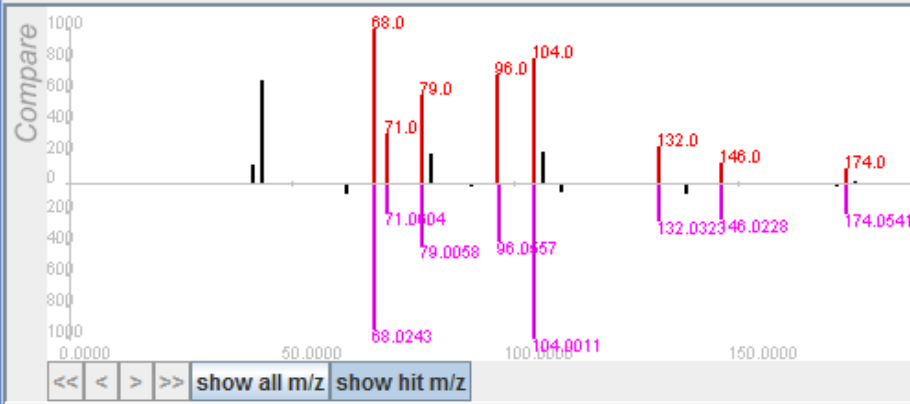
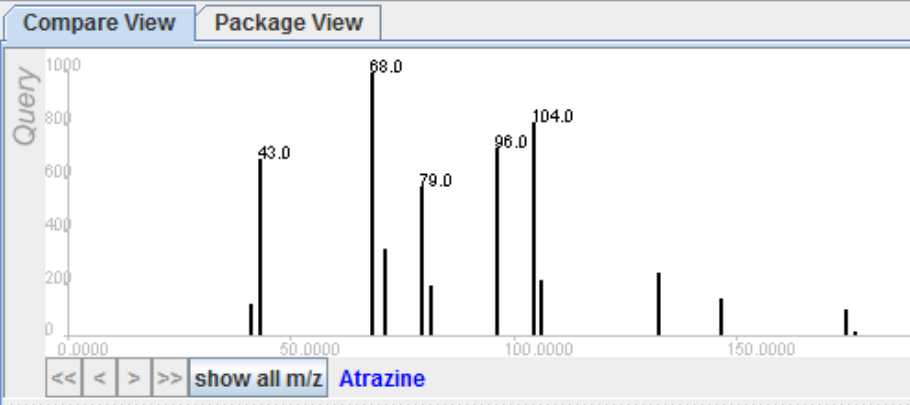
Example Spectrum "atrazine_msms_1563.msp"

sample file
 sample archive

No.	Name	ID
1	Atrazine	US000001

Package View display mode : selected related

Name	Score	Hit	ID	Ion	Contributor
Atrazine; LC-ESI-ITFT; MS2; 90%; R=30000; [...]	0.877605...	8	EA028813	P	Eawag
Terbutylazine; LC-ESI-ITFT; MS2; 90%; R=3...	0.876831...	8	EA028413	P	Eawag
Terbutylazine; LC-ESI-ITFT; MS2; 90%; R=7...	0.869507...	8	EA028407	P	Eawag
Deisopropylatrazine; LC-ESI-QQ; MS2; CE:...	0.846463...	11	KO002380	P	Keio Univ.
Atrazine; LC-ESI-ITFT; MS2; 90%; R=7500; [...]	0.841599...	7	EA028807	P	Eawag
Simazine; LC-ESI-ITFT; MS2; 90%; R=7500; [...]	0.830011...	8	EA026207	P	Eawag
Simazine; LC-ESI-ITFT; MS2; 90%; R=3000...	0.824303...	8	EA026213	P	Eawag
Atrazine; LC-ESI-ITFT; MS2; 75%; R=7500; [...]	0.820171...	8	EA028806	P	Eawag



MassBank Substructure Search

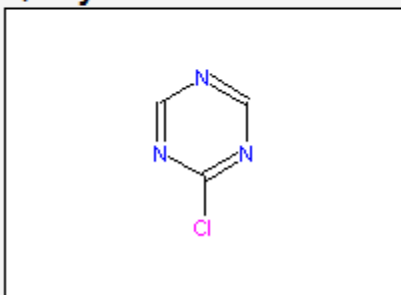
How many spectra in MassBank have the atrazine backbone?

Search MassBank

Search KNApSack

Substructure

Query1



Edit

Molfile

Clear

Query2

Empty search box for Query2.

Edit

Molfile

Clear

AND

Comparison of pi-electron for each atom

number in query = number in target

* Double and triple bond is translated to pi-electrons of the bonded atoms.

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Instrument Type

- EI
 - EI-B
 - EI-EBEB
 - GC-EI-TOF

- ESI
 - CE-ESI-TOF
 - ESI-QqIT-MS/MS
 - ESI-QqQ-MS/MS
 - LC-ESI-IT
 - LC-ESI-ITFT

MS Type

- All
- MS
- MS2
- MS3
- MS4

Ion Mode

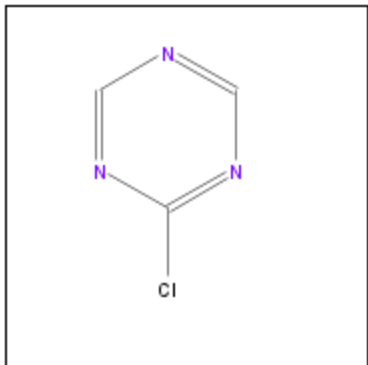
- Positive
- Negative
- Both

Peak Search (Option)

m/z , ,

Tolerance of m/z

Search



MassBank Substructure Search Results

[Edit / Resubmit Query](#)

Results : **59 Hit.** (1 - 59 Displayed)

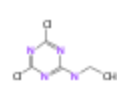
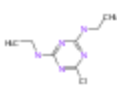
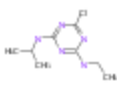
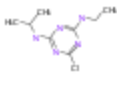
[Open All Tree](#)

[Multiple Display](#)

[Spectrum Search](#)

First Prev **1** Next Last (Total 1 Page)

▼ Results End

<input type="checkbox"/>	Name ▲	Formula / Structure	ExactMass	ID
<input type="checkbox"/>	+ 2,6-DICHLORO-4-(N-ETHYL)AMINO-1,3,5-TRIAZINE 1 spectrum	C5H6Cl2N4 	191.99695	
<input type="checkbox"/>	+ 2-CHLORO-4,6-BIS(ETHYLAMINO)-1,3,5-TRIAZINE 1 spectrum	C7H12ClN5 	201.07812	
<input type="checkbox"/>	+ 6-CHLORO-N-ETHYL-N'-(1-METHYLETHYL)-1,3,5-TRIAZINE... 1 spectrum	C8H14ClN5 	215.09377	
<input type="checkbox"/>	+ Atrazine 15 spectra	C8H14ClN5 	215.09320	
<input type="checkbox"/>	+ Deisopropylatrazine	C5H8ClN5	173.04682	

Internal MassBank Administration

Eawag Uchem-MassBank

• [MassBank Administration Tool](#)

→ **User and Password...**

• [WEB-API WSDL](#)

Internal MassBank Administration

MassBank Administration Tool

Main Menu

Record Validator

Validator

ADMIN MENU	Record Validator	Record Registration	Structure Registration	File Upload	Sql File Generator	Version Information	HOME
	Instrument Editor	Record List	Structure List	Validator	Record List Generator	Dababase Manager	

Record Validator

Database : ▼

Record Version : 2 1 (old record version)

Record Archive :

Browse_

Validation

** please specify your [recdata.zip] or [*.msbk].*

Internal MassBank Administration

Database Manager

No.	DB Name	Short Label	Long Label
2 ▾	UchemA	Eawag Uchem Adducts	Uchem EZ records of adduct spectra
	URL Type	URL	
	<input checked="" type="radio"/> internal <input type="radio"/> external	http://uchem-massbank/MassBank/	
		Add	Edit
		Delete	

26 database (20 external database)

No.	DB Name	URL	Short Label	Long Label	Status	Details
0	MassBank	http://uchem-massbank/MassBank/	EQ Uchem Q Ex	Eawag Uchem-MassBank	ok	
1	UchemEZ	http://uchem-massbank/MassBank/	EA Uchem Orbi Test	Annotated Uchem Standard Spectra for Approval	ok	
2	UchemA	http://uchem-massbank/MassBank/	Eawag Uchem Adducts	Uchem EZ records of adduct spectra	ok	
3	EA	http://uchem-massbank/MassBank/	EA Uchem Orbi	Annotated Uchem Standard Spectra	ok	
4	Waters	http://www.massbank.jp/	Waters	Nihon Waters K.K.	ok	external database.
5	Kyoto	http://www.massbank.jp/	Kyoto Univ.	Kyoto University	ok	external database.
6	MassBank	http://157.110.6.77/MassBank/	Chubu Univ.	College. Life and Health Sci, Chubu U	ok	external database.

MassBank in NIST

The beginning of a collaboration...

NIST MS Search 2.2 - [Name search]

File Search View Tools Options Window Help

ATRAZINE Clear a-z massbank_eawag

Atraton [M+H] ⁺ 90% P=212.2
Atrazine [M+H] ⁺ 15% P=216.1
Atrazine [M+H] ⁺ 15% P=216.1
Atrazine [M+H] ⁺ 30% P=216.1
Atrazine [M+H] ⁺ 30% P=216.1
Atrazine [M+H] ⁺ 35% P=216.1
Atrazine [M+H] ⁺ 35% P=216.1
Atrazine [M+H] ⁺ 45% P=216.1
Atrazine [M+H] ⁺ 45% P=216.1
Atrazine [M+H] ⁺ 60% P=216.1
Atrazine [M+H] ⁺ 60% P=216.1
Atrazine [M+H] ⁺ 75% P=216.1
Atrazine [M+H] ⁺ 90% P=216.1
Atrazine [M+H] ⁺ 90% P=216.1
Atrazine-2-hydroxy [M+H] ⁺ 15% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 15% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 30% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 30% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 35% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 35% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 45% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 45% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 60% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 60% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 75% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 75% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 90% P=198.1
Atrazine-2-hydroxy [M+H] ⁺ 90% P=198.1
Atrazine-2-hydroxy [M-H] ⁻ 15% P=196.1
Atrazine-2-hydroxy [M-H] ⁻ 15% P=196.1
Atrazine-2-hydroxy [M-H] ⁻ 30% P=196.1
Atrazine-2-hydroxy [M-H] ⁻ 30% P=196.1
Atrazine-2-hydroxy [M-H] ⁻ 35% P=196.1
Atrazine-2-hydroxy [M-H] ⁻ 45% P=196.1

(massbank_eawag) Atrazine [M+H]⁺ 75% P=216.1

Name: Atrazine
Formula: C₈H₁₄ClN₅
MW: 215 Exact Mass: 215.0932 CAS#: 1912-24-9 ID#: 2283 DB: massbank_eawag
Other DBs: None
Contributor: Stravs M, Schymanski E, Singer H, Department of Environmental Chemistry, Eawag
Comment: ID=EA028812 License="CC BY-SA" Record_title="Atrazine; LC-ESI-ITFT; MS2; CE: 75%; R=15000; [M+H]⁺ RT="8.3 min" Derivative_formula=C8H14
Notes: c1(nc(nc(n1)Cl)NCC)NC(C)C
Collision energy: 75%
Instrument: LTQ Orbitrap XL Thermo Scientific
Instrument type: LC-ESI-ITFT
Precursor m/z: 216.101
Precursor type: [M+H]⁺
Ion mode: P
Spectrum type: ms2
10 largest peaks:
174.054 999 | 104.001 962 | 68.0243 791 | 96.0557 570 | 132.032 485 |

Names Structures PlotText Plot

Lib. Search Other Search Names Compare Librarian MSMS

MassBank in NIST

The beginning of a collaboration...

NIST MS Search 2.2 - [Ident, Presearch Default - InLib = 1030, 85 spectra]

File Search View Tools Options Window Help

MS m/z

1. Atrazine

1 (ma) Atrazine 2 (ni) Atrazine

Names Structures Spec List

mainlib; replib; massbank_eawag; massbank_msms; nist_msms;
nist_msms2: 528385 total spectra

#	Lib.	Match	R.Match	Prob. (%)	RI	Name
1	ma	999	999	65.2	-	Atrazine [M
2	ma	977	980	23.8	-	Sebutylazi
3	ma	954	955	8.69	-	Terbutylazir
4	ma	949	959	23.8	-	Sebutylazi
5	ma	942	942	8.69	-	Terbutylazir
6	ma	941	943	65.2	-	Atrazine [M
7	ma	921	923	2.27	-	Atrazine-de
8	ma	918	920	2.27	-	Atrazine-de
9	ni	915	917	65.2	-	Atrazine [M
10	ma	907	909	8.69	-	Terbutylazir
11	ma	901	902	8.69	-	Terbutylazir

Names Structures InLib = 1030, Hit List

(massbank_eawag) Atrazine [M+H]⁺ 75% P=216.1

Plot/Text of Search Spectrum Plot of Search Spectrum Spec List

Name: Atrazine
Formula: C₈H₁₄ClN₅
MW: 215 Exact Mass: 215.0932 CAS#: 1912-24-9 ID#: 2283 DB: ma
Other DBs: None
Contributor: Stravs M, Schymanski E, Singer H, Department of Environm
Comment: ID=EA028812 License="CC BY-SA" Record_title="Atrazin
Notes: c1(nc(nc(n1)Cl)NCC)NC(C)C
Collision energy: 75%
Instrument: LTQ Orbitrap XL Thermo Scientific

Atrazine Head to Tail MF=999 RMF=999 Atrazine

Difference Head to Tail Side by Side Subtraction 999 999R 65.2

(massbank_eawag) Atrazine [M+H]⁺ 75% P=216.1

Plot/Text of Hit Plot of Hit

Name: Atrazine
Formula: C₈H₁₄ClN₅
MW: 215 Exact Mass: 215.0932 CAS#: 1912-24-9 ID#: 2283 DB: ma
Other DBs: None
Contributor: Stravs M, Schymanski E, Singer H, Department of Environm
Comment: ID=EA028812 License="CC BY-SA" Record_title="Atrazin
Notes: c1(nc(nc(n1)Cl)NCC)NC(C)C
Collision energy: 75%
Instrument: LTQ Orbitrap XL Thermo Scientific

Lib. Search Other Search Names Compare Librarian MSMS

MassBank in NIST

The beginning of a collaboration

- Currently a few sub-sets of MassBank available
 - massbank_ei – all EI spectra up to July 2012
 - massbank_msms – all MS/MS spectra up to July 2012
 - massbank_eawag – all Eawag MS/MS spectra

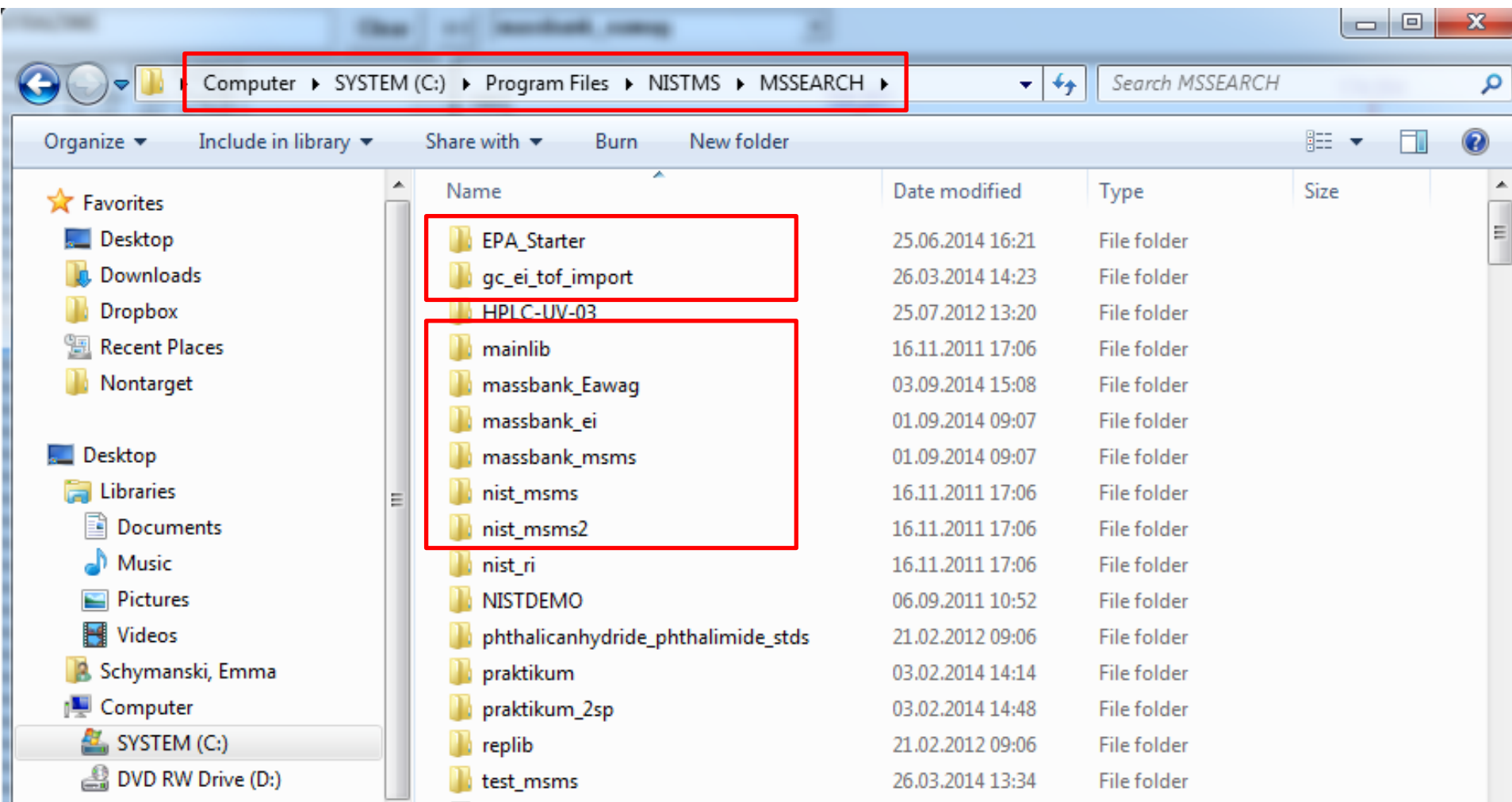
- NIST do not want to add our spectra into NIST distribution
 - “Standard spectral library” – reference laboratory
 - License is creative commons, but NIST is commercial => incompatible
 - BUT, NIST want to improve access to alternative databases within NIST
 - Several other libraries also available to download

- Very easy install for NIST users
 - Download zip file, unzip, copy to NIST folder and it's there!
 - Can browse straight away
 - Need to add to search path manually

MassBank in NIST

“Installing” MassBank

Simply copy unzipped folder into NISTMS/MSSEARCH path



MassBank in NIST

Adding MassBank to the search path

The screenshot shows the NIST software interface with the 'Library Search Options' dialog box open. The 'Options' menu in the top bar is highlighted. The dialog box has tabs for 'Search', 'MS/MS', 'Libraries', 'Automation', 'Limits', 'Constraints', and 'RI (GC)'. The 'Libraries' tab is active, showing two lists: 'Available Libs' and 'Included Libs'. An arrow points from 'massbank_eawag' in the 'Available Libs' list to the 'Included Libs' list. The 'Included Libs' list contains 'mainlib', 'replib', 'massbank_eawag', 'massbank_msms', 'nist_msms', and 'nist_msms2'. Below the lists, it shows '640110 Spectra in 15 Libraries' and '528385 Spectra in 6 Libraries'. A 'Spectrum search' dropdown is also visible. In the background, a mass spectrum plot shows peaks at 174.054 and 180.124, and a chemical structure of Atrazine is displayed.

Library Search Options

Search | MS/MS | Libraries | Automation | Limits | Constraints | RI (GC)

Available Libs:

- mainlib
- replib
- epa_starter
- gc_ei_tof_import
- hplc-uv-03
- massbank_eawag
- massbank_ei
- massbank_msms
- nist_msms
- nist_msms2

>> Add >>

Included Libs:

- mainlib
- replib
- massbank_eawag
- massbank_msms
- nist_msms
- nist_msms2

640110 Spectra in 15 Libraries 528385 Spectra in 6 Libraries

Spectrum search

OK Cancel Help

ATRAZINE

Atrazine [M+H]⁺ 90% P=212.2

Atrazine [M+H]⁺ 15% P=216.1

Atrazine [M+H]⁺ 15% P=216.1

Atrazine [M+H]⁺ 30% P=216.1

Atrazine [M+H]⁺ 30% P=216.1

Atrazine [M+H]⁺ 35% P=216.1

Atrazine [M+H]⁺ 35% P=216.1

Atrazine [M+H]⁺ 45% P=216.1

Atrazine [M+H]⁺ 45% P=216.1

Atrazine [M+H]⁺ 60% P=216.1

Atrazine [M+H]⁺ 60% P=216.1

Atrazine [M+H]⁺ 75% P=216.1

Atrazine [M+H]⁺ 75% P=216.1

Atrazine [M+H]⁺ 90% P=216.1

Atrazine [M+H]⁺ 90% P=216.1

Atrazine-2-hydroxy [M+H]⁺ 15% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 15% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 30% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 30% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 35% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 35% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 45% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 45% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 60% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 60% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 75% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 75% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 90% P=198.1

Atrazine-2-hydroxy [M+H]⁺ 90% P=198.1

Atrazine-2-hydroxy [M-H]⁻ 15% P=196.1

Atrazine-2-hydroxy [M-H]⁻ 15% P=196.1

Atrazine-2-hydroxy [M-H]⁻ 30% P=196.1

Atrazine-2-hydroxy [M-H]⁻ 30% P=196.1

Atrazine-2-hydroxy [M-H]⁻ 35% P=196.1

Atrazine-2-hydroxy [M-H]⁻ 45% P=196.1

174.054

180.124

R=15000; [M+H]⁺ RT="8.3 min" Derivative_formu

Chemical Structure: CC1=NC(=C(N1)N)N

MassBank in NIST

The beginning of a collaboration

- Details under discussion
 - Easy install for NIST users => hard for “MassBank” to generate files
 - NIST will provide this service for the moment
 - Available to download via MassBank website
 - How to (best) split up the databases
 - Information in MassBank records not available in NIST 1:1
 - Current files are “work in progress”
 - Conversion will need to be optimized in the coming months before “going public”
 - Increasing the accessibility will improve usability
 - Web interface of MassBank complementary to offline MSSearch
 - Future developments to MassBank to improve functionality



Thank you for listening

Any Questions?



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