

MassBank User's Manual

Version 2.4, 7 February 2012

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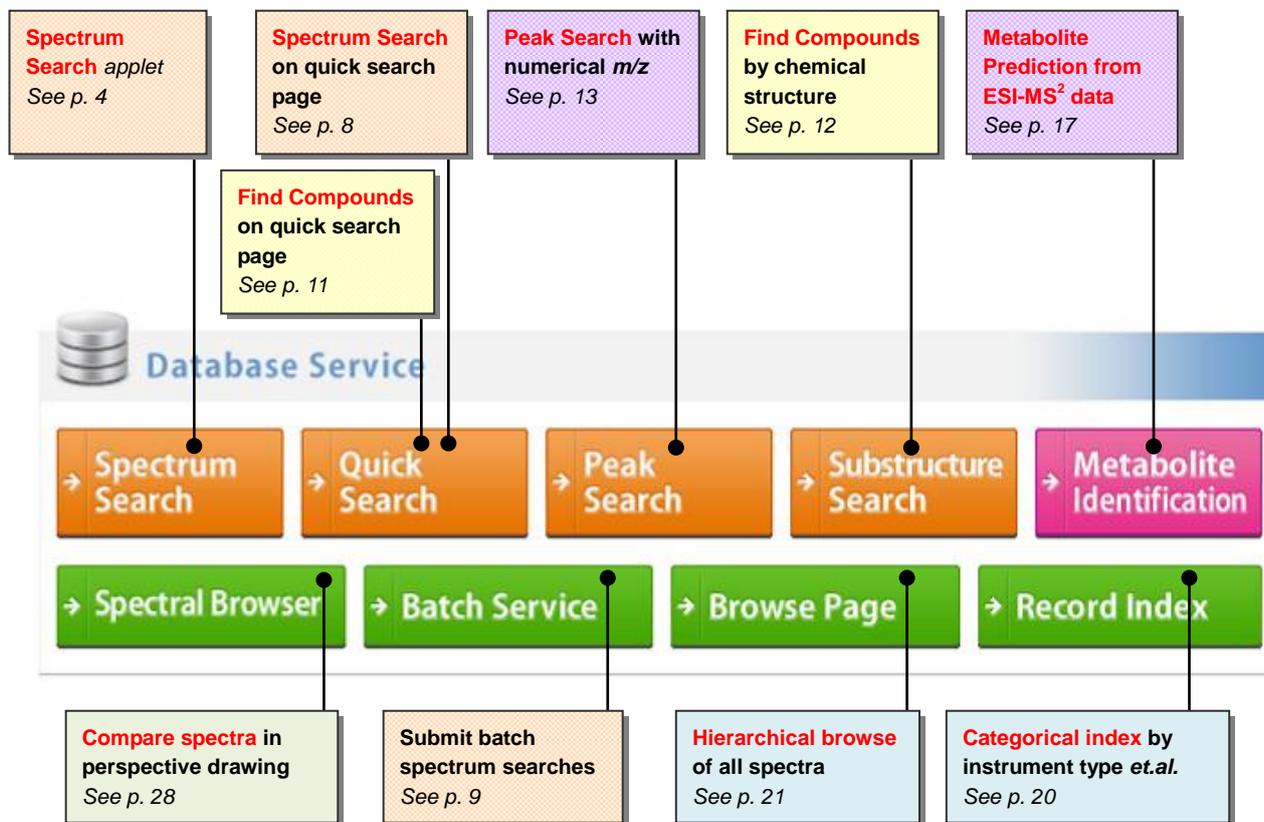
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1. Introduction

This manual mainly describes the operation of the MassBank database services.

1.1 Overview of the Database Services

MassBank provides the following database services.



1.2 System Requirements

Below are the system requirements for using the MassBank database services.

(1) Web Browser

We recommend using Internet Explorer 6 or higher, or Firefox 2 or higher as your browser.

(2) Web Browser Settings

Make sure that your Web browser is configured as follows.

[1] JavaScript execution enabled

[2] Popups enabled

- See the page below for instructions on how to check this (URL to allow: <http://www.massbank.jp>)
http://www.microsoft.com/japan/windowsxp/using/web/sp2_popupblocker.msp

(3) Install Java runtime environment

The Java Runtime Environment (JRE) Version 5 or higher must be installed.

- You can use the page below to check your installation status and download Java.

<http://www.java.com/en/download/>

2. Searching for Similar Spectra

2.1 Spectrum Search Applet

Spectrum Search enables you to perform GUI-based spectrum searches in a Web browser. Spectra in the MassBank similar to one provided by the user as a query are retrieved and displayed in a list. It is also possible to graphically compare the query spectrum with the retrieved spectrum.

(1) Prepare the query file

When performing a spectrum search with the applet, you must prepare a query file in one of the following formats. A sample can be downloaded from <http://www.massbank.jp/sample/sample.zip>

Name
Write an arbitrary name, such as the name of the compound. (Optional)

Peak information
Write the *m/z* and intensity, separated by spaces. You can write all the peak information on a multiple lines, writing one peak per line.

Empty line
If you include peak information for more than one spectrum, put a blank line between each one.

[Query File Contents]

```

Name: Sample Compound 1
70 24
71 10
72 68
73 999
74 107

Name: Sample_Compound 2
73.1 15008
78.54 4456
79.45 2158311
85.3 964800
86.11 150
90.0 804911

Name: Sample Compound 3
178.876379147 15
186.884786287 8
229.504276894 9
                    
```

Single space

Name : Δ Sample...

Arbitrary name

When entering a name, always begin the line with "Name:"

Single space

78.54 Δ 4456

m/z Intensity
(Absolute or relative value can be used)

(2) Load the query and configure the search parameters

After selecting your query file, click **File Read**.

Click **Search Parameter Setting**

Search Parameter Setting Window

[1] Load the query file

Click **Browse**, and select the query file you have prepared. Click **File Read** to load the file. After the file finishes loading, a list of queries appears.

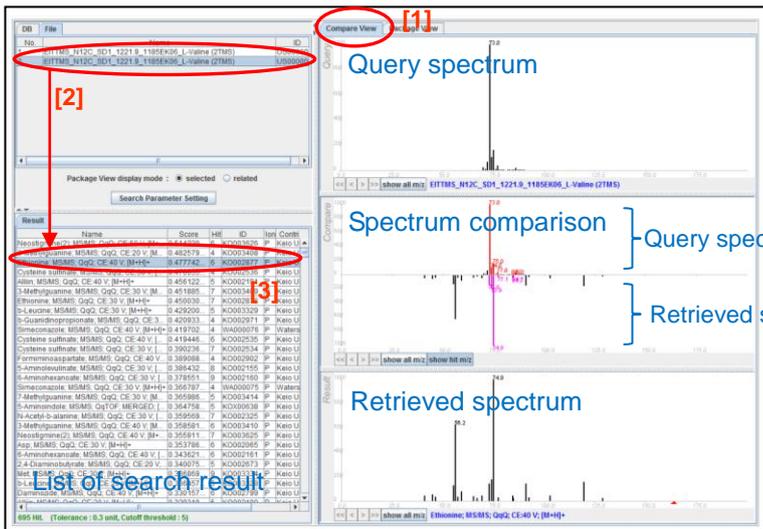
[2] Set the search parameters

Click **Search Parameter Setting**. The Setting window opens.

- Settings**
- **Precursor *m/z* :**
Precursor ion specified by *m/z*
 - **Tolerance:**
m/z error range
 - **Cutoff Threshold:**
Relative intensity threshold
 - **Instrument Type:**
Type of instrument
 - **Ionization Mode:**
Mode of ionization

(3) Perform the search

Compare View: Compare query and retrieved spectrums one to one.



[1] Select "Compare View"

Click to select.
It is selected by default.

[2] Select the query spectrum

Click to select the spectrum to use in the query. As soon as it is selected, similar spectrums are retrieved.

[3] Select a retrieved spectrum

Click to select any spectrum in the list of search result.

Package View: Compare query and retrieved spectrums one to many.



[1] Select "Package View"

Click to select.

[2] Select package view display mode

Click "selected" or "related".

[3] Select the query spectrum

Click to select the spectrum to use in the query. As soon as it is selected, similar spectrums are retrieved.

[4] Select a retrieved spectrum

Click to select any spectrum in the list of search result. If you chose "selected" in step 2, then you can hold down Ctrl + Shift to select multiple rows. If you chose "related" in step 2, then only one row can be selected.

Different Display Modes in Package View

There are two display modes in Package View.

selected

Multiple spectrums can be selected from the list of search results. The selected spectrums and the query spectrum are shown in a tiled view.

related

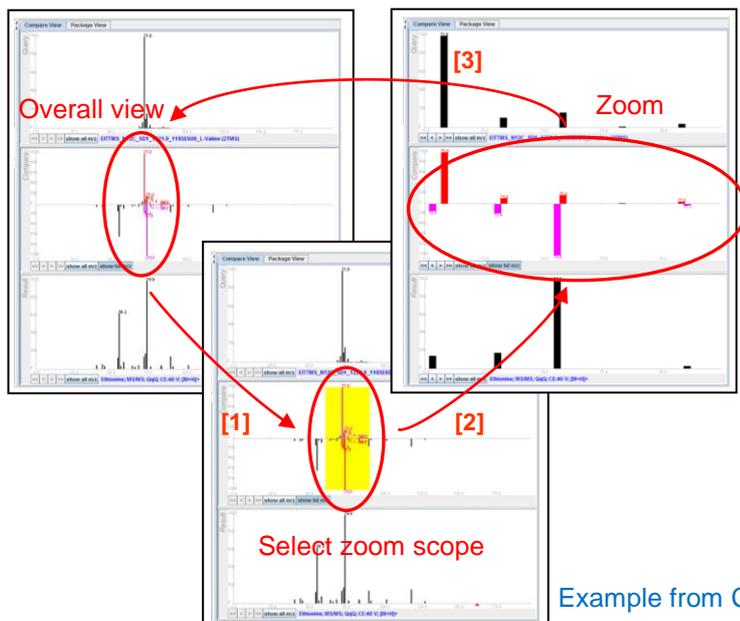
Only one spectrum can be selected from the list of search results. The selected spectrum, a spectrum with different collision energy than the selected spectrum (detected automatically), and the query spectrum are displayed in tiled view.

Peak Color in Spectrum Comparison Window

In the spectrum comparison windows in Compare View and Package View, matching peaks can be distinguished by color.

| | Matching m/z on query peak | Perfect Match | Match within Error Margin |
|--------------------|----------------------------|---------------|---------------------------|
| Peak | | | |
| Query Spectrum | | Red | Red |
| Retrieved Spectrum | | Red | Pink |

<<Handy Feature 1: Spectrum Zoom>>



- [1] Select location to zoom**
Drag from the location of the start of the zoom.
- [2] Set zoom position**
Drop to set the location on the spectrum to zoom.
- [3] End zoom**
Double click on the spectrum.

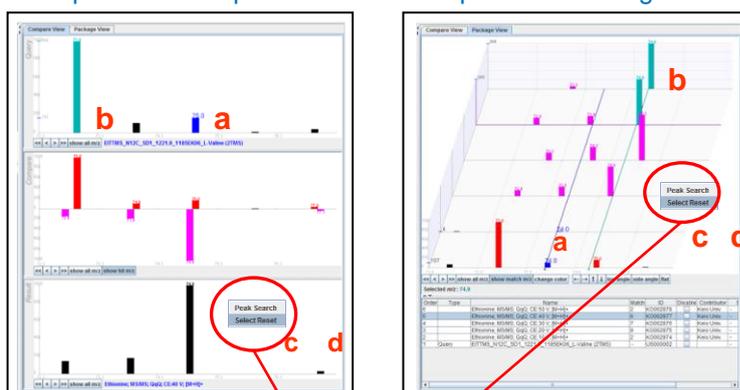
Note: You can also zoom on spectrums from the Package View.

Example from Compare View

<<Handy Feature 2: Peak Manipulation>>

Example from Compare View

Example from Package View



- a. Highlight peak**
Place the cursor over a peak. It is highlighted in blue, and the *m/z* and intensity values appear.
- b. Select peak**
Click on a peak. It is rendered in blue to indicate that it is selected. Up to 6 peaks can be selected.
- c. Search for peaks**
If you right click while one or more peaks are selected, a menu appears, and "Peak Search" can be selected. The peak search begins immediately after selection.
- d. Cancel peak selection**
When you right click on the spectrum, a menu appears. Chose "Select Reset".

Peak Search Results

Search Parameters:
m/z: 73.0 RelInt: 5 Tol(amt): 0
 Instrument Type: All
 Ionization Mode: Both

Results: 140 Hit (1 - 36 Displayed)

| First | Prev | 1 | 2 | 3 | 4 | Next | Last | (Total 4 Page) | Results End |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| <input type="checkbox"/> |
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| <input type="checkbox"/> |
| 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| <input type="checkbox"/> |
| 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |
| <input type="checkbox"/> |
| 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 |
| <input type="checkbox"/> |
| 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 |
| <input type="checkbox"/> |
| 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 |
| <input type="checkbox"/> |
| 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 |
| <input type="checkbox"/> |
| 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 |
| <input type="checkbox"/> |
| 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 |
| <input type="checkbox"/> |
| 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 |
| <input type="checkbox"/> |
| 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 |
| <input type="checkbox"/> |
| 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 |
| <input type="checkbox"/> |
| 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 |
| <input type="checkbox"/> |
| 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 |
| <input type="checkbox"/> |

Peak Search Results Window

Peak Rendering Color
 Highlighted: Blue
 Selected: Light blue

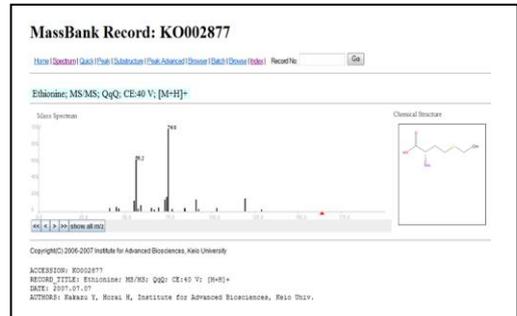
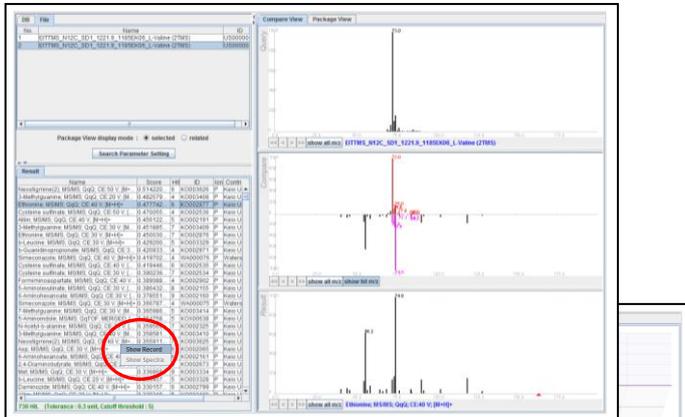
Highlighting and Selecting Peaks in Package View
 When multiple spectrums are displayed in Package View, you can highlight or select the peaks in any spectrum. When you do so, if there is a peak in another spectrum with a perfectly matching *m/z*, then that peak is also highlighted or selected.

<<Handy Feature 3: Show Record>>

a. Show record

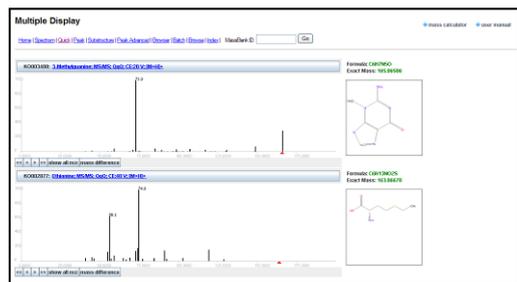
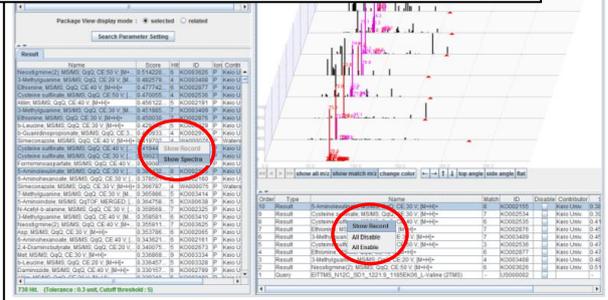
When you right click with one spectrum selected, the **"Show Record"** command appears on the menu. Select this to view details about the spectrum.

Example from Compare View



b. Show multiple spectra

When you right click with two or more spectra selected, the **"Show Spectra"** command appears on the menu. Select this to display multiple spectra in tiled view.



Example from Package View

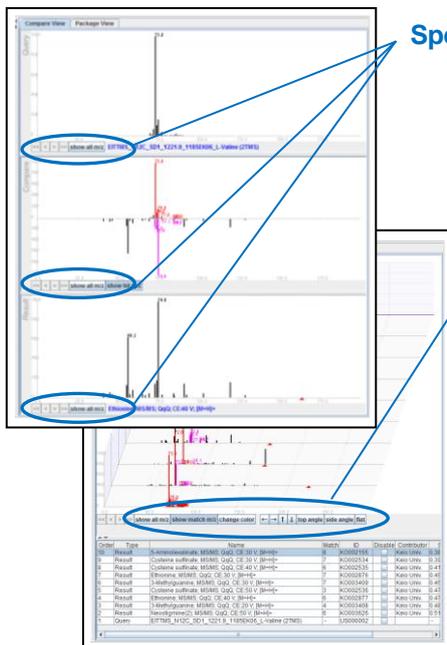
<<Handy Feature 4: Spectrum Manipulation>>

Spectrum Manipulation Buttons in Compare View

- <<, <, >, >> Move display location (only when zoomed on spectrum)
- show all m/z Display m/z values of all peaks
- show hit m/z Display m/z values of matching peaks

Spectrum Manipulation Buttons in Package View

- <<, <, >, >> Move display location (only when zoomed on spectrum)
- show all m/z Display m/z values of all peaks
- show match m/z Display m/z values of matching peaks
- change color Change color of entire spectrum
- ←, →, ↑, ↓ Change angle (manual manipulation)
- top angle Change angle (top perspective)
- side angle Change angle (side perspective)
- flat Change angle (all spectrums in flat view)



2.2 Spectrum Search on Quick Search Page

The Quick Search feature allows you to search for similar spectrums just using simple input.

>> Enter Search Parameters

Quick Search

[manual \(in Japanese\)](#)

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | Record No:

Search by Keyword
 Search by Peak
 Select this

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 |

Enter peak data

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

Example1 Example2

Instrument Type

- EI EI-MS
- GC-EI-TOF-MS
- ESI CE-ESI-TOF-MS
- ESI-IT-(MS)n
- ESI-IT-MS/MS
- ESI-QqIT-MS/MS
- ESI-QqQ-MS/MS
- ESI-QqTOF-MS/MS
- LC-ESI-IT-TOF-MS
- LC-ESI-Q-MS
- LC-ESI-TOF-MS/MS

Ionization Mode

Positive Negative Both

[1] Cutoff threshold of relative intensities

[2] Number of Results

Single space

273.096 22

m/z
Intensity
(Absolute or relative value can be used)

[1] Cutoff threshold of relative intensities
Relative intensity threshold
Ignore peaks with intensity lower than specified value.

[2] Number of Results
Number of retrieved spectrums to be displayed

You can narrow your results by selecting the Instrument type or Ionization Mode.

>> Display Search Results

Quick Search Results

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | Record No:

Query :

Display query spectrum

[Previous Query](#)

Results : 20 Hit.

Up to top 20 scores displayed

| | Name | Formula / Structure | Hit | Score |
|--------------------------|---|---------------------|-----|--------|
| <input type="checkbox"/> | (+)-3'3'4'5'7-Pentahydroxyflavan; LC-TOF/MS | C15H14O6 | 8 | 1.0000 |
| <input type="checkbox"/> | (-)-3'3'4'5'7-Pentahydroxyflavan; LC-TOF/MS | C15H14O6 | 8 | 0.9054 |
| <input type="checkbox"/> | Desalkylfurazepam; LC-Q/MS; POS: 15 V, 45 V | C15H10ClFN2O | 4 | 0.6845 |

Hit: Number of peaks in the retrieved spectrums matched to those in a query data

Score: Similarity score of retrieved spectrum to a query data

2.3 Conduct Batch Spectrum Searches

Batch Service conducts a batch spectrum search, and emails you the results.

Use this in such cases as when you would like to search for a large number of spectra.

Batch Service

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

This service will appear as a part of Quick Search Page.

[1] Query File: C:\Users% Desktop%\Neg 参照... sample file

[2] Mail Address: yttck.keio.ac.jp

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[1] Load the query file

Prepare a query file with the same format as the one described in "2.1 (1) Spectrum Search Applet". Click **Browse**, and select the query file you have prepared.

[2] Enter email address

Enter the email address to which you would like the search results sent.



Click **Submit** to perform the batch query. A message appears indicating that the query has been accepted.

Batch Service

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#)

[2009/09/25 18:41:51]
Your batch search is accepted.
The results will be sent to ynihei@ttck.keio.ac.jp later.



Search results are sent to the specified address by e-mail. The following files are attached to the e-mail: (1) Search Results; and (2) Summary of Results.

(1) Search Results (Text Format)

```

***** MassBank Batch Service Results *****

Request Date: 2010/10/15 14:07:51 JST
# Instrument Type:
CE-ESI-TOF-MS,ESI-IT-(MS)n,ESI-IT-MS/MS,ESI-QTOF-MS/MS,ESI-QqIT-MS/MS,ESI-QqQ-MS/MS,ESI-QqTOF-MS/MS,LC-ESI-FT-MS,LC-ESI-IT-MS/M
S,LC-ESI-IT-TOF-MS,LC-ESI-Q-MS,LC-ESI-QTOF-MS/MS,LC-ESI-QqQ-MS/MS,LC-ESI-TOF-MS
# Ion Mode: Negative

### Query 1 ###
# Name: Scan530
# Hit: 37
    
```

List of search results (at most 20 high-scored spectra)

| Top 20 List Accession | Title | Formula | Mass | Score | Hit |
|--------------------------|--|---------|-----------|-----------|----------|
| KNA00756 | L-Aspartate; LC-ESI-FT-MS; NEG | | C4H7NO4 | 133.03751 | 0.3545 2 |
| KNA00487 | L-Aspartate; LC-ESI-FT-MS; NEG | | C4H7NO4 | 133.03751 | 0.3104 2 |
| KNA00752 | L-Serine; LC-ESI-FT-MS; NEG | | C3H7NO3 | 105.04259 | 0.3041 2 |
| KNA00542 | cis-Aconitate; LC-ESI-FT-MS; NEG | | C6H6O6 | 174.01644 | 0.2955 2 |
| KNA00475 | L-Serine; LC-ESI-FT-MS; NEG | | C3H7NO3 | 105.04259 | 0.2942 2 |
| KNA00628 | L-Glutamine; LC-ESI-FT-MS; NEG | | C5H10N2O3 | 146.06914 | 0.2911 2 |
| KNA00728 | L-Homoserine; LC-ESI-FT-MS; NEG | | C4H9NO3 | 119.05824 | 0.2904 2 |
| KNA00812 | Citrate; LC-ESI-FT-MS; NEG | | C6H8O7 | 192.027 | 0.2885 2 |
| KNA00820 | 3-Phospho-D-glycerate; LC-ESI-FT-MS; NEG | | C3H7O7P | 185.99294 | 0.2844 2 |
| KNA00554 | L-Homoserine; LC-ESI-FT-MS; NEG | | C4H9NO3 | 119.05824 | 0.2823 2 |
| KNA00538 | sn-Glycerol 3-phosphate; LC-ESI-FT-MS; NEG | | C3H9O6P | 172.01367 | 0.2756 2 |
| KNA00527 | (S)-Malate; LC-ESI-FT-MS; NEG | | C4H6O5 | 134.02152 | 0.2746 2 |
| KNA00648 | L-Threonine; LC-ESI-FT-MS; NEG | | C4H9NO3 | 119.05824 | 0.2716 2 |
| KNA00736 | L-Asparagine; LC-ESI-FT-MS; NEG | | C4H8N2O3 | 132.05349 | 0.2713 2 |
| KNA00808 | cis-Aconitate; LC-ESI-FT-MS; NEG | | C6H6O6 | 174.01644 | 0.2673 2 |
| KNA00491 | L-Glutamine; LC-ESI-FT-MS; NEG | | C5H10N2O3 | 146.06914 | 0.2663 2 |
| KNA00483 | L-Asparagine; LC-ESI-FT-MS; NEG | | C4H8N2O3 | 132.05349 | 0.2650 2 |
| KNA00696 | 4-Hydroxy-L-proline; LC-ESI-FT-MS; NEG | | C5H9NO3 | 131.05824 | 0.2646 2 |
| KNA00546 | D-Gluconic acid; LC-ESI-FT-MS; NEG | | C6H12O7 | 196.0583 | 0.2616 2 |
| KNA00530 | 2-Oxoglutarate; LC-ESI-FT-MS; NEG | | C5H6O5 | 146.02152 | 0.2587 2 |

3. Compound Search

3.1 Find Compounds on Quick Search Page

The Quick Search feature allows you to search for compounds by compound name, molecular formula, etc.

>> Enter Search Parameters

Quick Search

[manual \(in Japanese\)](#)

Select this : [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | Record No:

Search by Keyword Search by Peak

[1] Compound Name

AND **[2] Exact Mass** **Tolerance**

AND **[3] Formula**
(e.g. C6H7N5, C5H*N5, C5*)

Instrument Type

EI EI-MS
 GC-EI-TOF-MS

ESI CE-ESI-TOF-MS
 ESI-IT-(MS)n
 ESI-IT-MS/MS
 ESI-QqIT-MS/MS
 ESI-QqQ-MS/MS
 ESI-QqTOF-MS/MS
 LC-ESI-IT-TOF-MS
 LC-ESI-Q-MS
 LC-ESI-TOF-MS/MS

Ionization Mode

Positive Negative Both

You can narrow your results by selecting the Instrument type and Ionization Mode.

[1] Compound Name

Enter the compound name. Names with substring matches on the string you entered are retrieved.

[2] Exact Mass/Tolerance

Enter the exact mass and error tolerance.

[3] Formula

Enter the molecular formula of the compound. Enter the formula starting with "C", followed by "H", and then the other letters in alphabetical order. Add wildcards ("*") to find partial matches.

Example: C5H*N5



>> Display Search Results

Quick Search Results

[mass calculator](#) [user manual](#)

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

Search Parameters :
Compound Name: **acetate**
Instrument Type: **GC-EI-TOF-MS**
Ionization Mode: **Positive**

[Edit / Resubmit Query](#)

Results : 4 Hit. (1 - 4 Displayed)

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

| Name | Formula / Structure | ExactMass | ID |
|---|--|-----------|----|
| <input type="checkbox"/> 3,4-dihydroxyphenylacetic acid <small>1 spectrum</small> | C8H8O4  | 168.04226 | |
| <input type="checkbox"/> 4-Hydroxyphenylacetic acid <small>1 spectrum</small> | C8H8O3  | 152.04734 | |
| <input type="checkbox"/> Indole-3-acetic acid <small>2 spectra</small> | C10H9NO2  | 175.06333 | |

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

Matching items (including synonyms) are displayed

3.2 Find Compounds by Chemical Structure

The Substructure Search enables you to find compounds including the specified chemical structure.

>> Enter Search Parameters

(1) Number of π electrons
 Comparison of pi-electron for each atom. **number in query = number in target**
 * Double and triple bound is translated to pi-electrons of the bonded atoms.

Peak Search (Option)
 m/z: , ,
 Tolerance of m/z: 0.3
 Search

(2) Peak Search option

(1) Number of π electrons

- Query structure = target structure (default)
- Query structure \leq target structure
- No comparison

(2) Peak Search option

Specify *m/z* values to perform peak search at same time.

You can also narrow your results by selecting the Instrument type or Ionization Mode.

>> Display Search Results

[Edit / Resubmit Query](#)

Results: 48 Hit. (1 - 42 Displayed)

[Open All Tree](#) [Multiple Display](#) [Spectrum Search](#)

First Prev 1 2 Next Last (Total 2 Page)

Results End

| <input type="checkbox"/> | Name | Formula / Structure | ExactMass | ID |
|-------------------------------------|-------------------------------------|--|-----------|----|
| <input checked="" type="checkbox"/> | (R)-(-)-Phenylephrine 1 spectrum | C ₉ H ₁₃ NO ₂ | 167.09463 | |
| <input type="checkbox"/> | 1,10-Phenanthroline 2 spectra | C ₁₂ H ₈ N ₂ | 180.06875 | |

Enter query structure

[1] Write in editor

Or:
 [2] Load Molfile

Read Molfile

(1) Click Browse

(2) Select a file

The loaded structure formula can be modified in the editor as well.

4. Peak Search

4.1 Peak Search by *m/z* values

Peak Search enables you to find peaks by specifying the *m/z* or *m/z* difference as numerical values.

>> Enter Search Parameters

- [1] Search of Peaks Peak Differences
- [2] Search by *m/z*-Value Molecular Formula

[1] Search of "Peaks" or "Peak Differences"

- "Peaks": search of the *m/z* value.
- "Peak Differences": search of the *m/z* differences.

[2] Search by "*m/z*-Value" or "Molecular Formula"

Select "*m/z*-Value" for Peak Search by *m/z* values.

[3] *m/z*

Specify the peak *m/z* value. You can specify up to 6, and connect them via AND or OR conditions.

[4] Rel. Intensity

Ignore peaks with intensity lower than specified value. Specify a relative intensity from 1 to 999.

[5] Tolerance

Specify the *m/z* error range.

Converting from molecular formula to *m/z*

Enter a molecular formula the exact calculated mass in the *m/z* text box. The exact calculated mass is truncated to 5 decimal place.

You can also narrow your results by selecting the Instrument type or Ionization Mode.

>> Display Search Results

Results : 313 Hit. (1 - 46 Displayed)

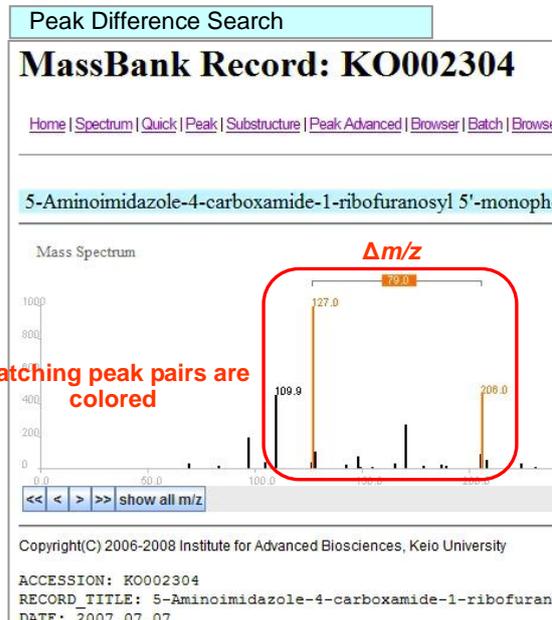
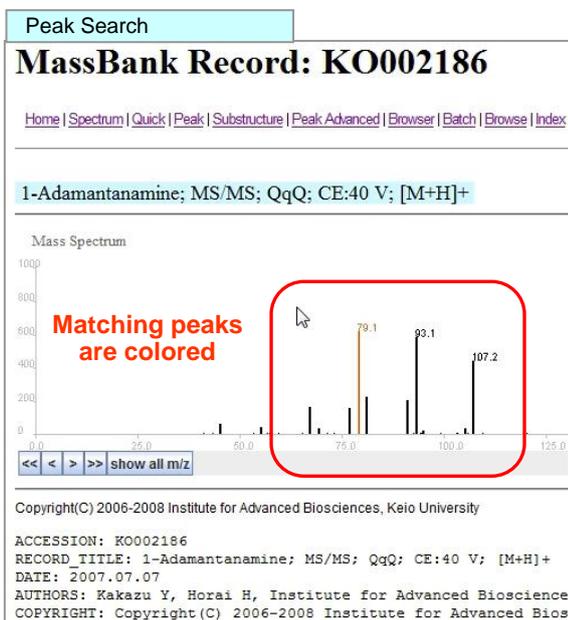
Close All Tree Show Spectra

First Prev 1 2 3 4 5 6 7 8 9 Next Last (Total 9 Page)

| Name | Formula / Structure | ExactMass |
|--|---------------------|-----------|
| 1-Adamantanamine | C10H17N | 151.13610 |
| MS/MS: QqQ: CE:40 V: [M+H] ⁺ | C10H17N | 151.13610 |
| MS/MS: QqQ: CE:50 V: [M+H] ⁺ | C10H17N | 151.13610 |
| MS/MS: QqTOF: MERGED: [M+H] ⁺ | C10H17N | 151.13610 |
| 1-Methyladenine | C6H7N5 | 149.07015 |
| MS/MS: QqQ: CE:40 V: [M+H] ⁺ | C6H7N5 | 149.07015 |
| MS/MS: QqQ: CE:50 V: [M+H] ⁺ | C6H7N5 | 149.07015 |

Click link.

>> Spectrum View



4.2 Peak Search with Molecular Formulas

Peak Search Advanced enables you to find peaks by specifying an ion or neutral loss by molecular formulas instead of a numerical *m/z* values.

>> Enter Search Parameters

Searching via ion

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

Ion 1 Formula: C5H6N5 AND Ion 2 Formula: C3H6N AND Ion 3 Formula: AND Ion 4 Formula: AND

AND OR

Enter molecular formula

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

Search

If CH3COOH is entered, it is converted internally to C2H4O2 for the search.

Searching via neutral loss

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

Neutral Loss 1 Formula: C4H7NO2 → Neutral Loss 2 Formula: CH4S → Neutral Loss 3 Formula: → Neutral Loss 4 Formula: →

AND SEQUENCE

Enter molecular formula

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

Search

If "SEQUENCE" is selected, peak pairs, whose *m/z* difference is matched to the molecular formula, are retrieved in the order of Neutral Loss 1, 2, and 3. (In the example above, order of CH4H7NO2, then CH4S)

>> Display Search Results

Query :

Ion 1 Formula: C5H6N5 AND Ion 2 Formula: C3H6N

[Edit / Resubmit Query](#)

Results : 1 Hit. (1 - 1 Displayed)

First Prev 1 Next Last (Total 1 Page)

| Name | 1 spectrum | C15H2 |
|---|------------|-------|
| S-Adenosylmethionine | | |
| MS/MS: QqTOF: MERGED: [M+H]⁺ | | |

Click link

Query :

Neutral Loss 1 Formula: C4H7NO2 → Neutral Loss 2 Formula: CH4S

[Edit / Resubmit Query](#)

Results : 1 Hit. (1 - 1 Displayed)

First Prev 1 Next Last (Total 1 Page)

| Name | 1 spectrum | C15H2 |
|---|------------|-------|
| S-Adenosylmethionine | | |
| MS/MS: QqTOF: MERGED: [M+H]⁺ | | |

Click link

>> Spectrum View

Searching by Ion

MassBank Record: KOX00710 **MERGED SPECTRUM**

Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | Record No: _____

Dihydrospingosine; MS/MS; QqTOF; MERGED; [M+H]⁺

Mass Spectrum

Molecular formulas with matching peaks appear

C18H40NO2

C17H38N

Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University
 ACCESSION: KOX00710
 RECORD TITLE: Dihydrospingosine; MS/MS; QqTOF; MERGED; [M+H]⁺

Searching by Neutral Loss

MassBank Record: KOX00636 **MERGED SPECTRUM**

Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | Record No: _____

S-Adenosylmethionine; MS/MS; QqTOF; MERGED; [M+H]⁺

Mass Spec:

CH4S CH4S C4H7NO2

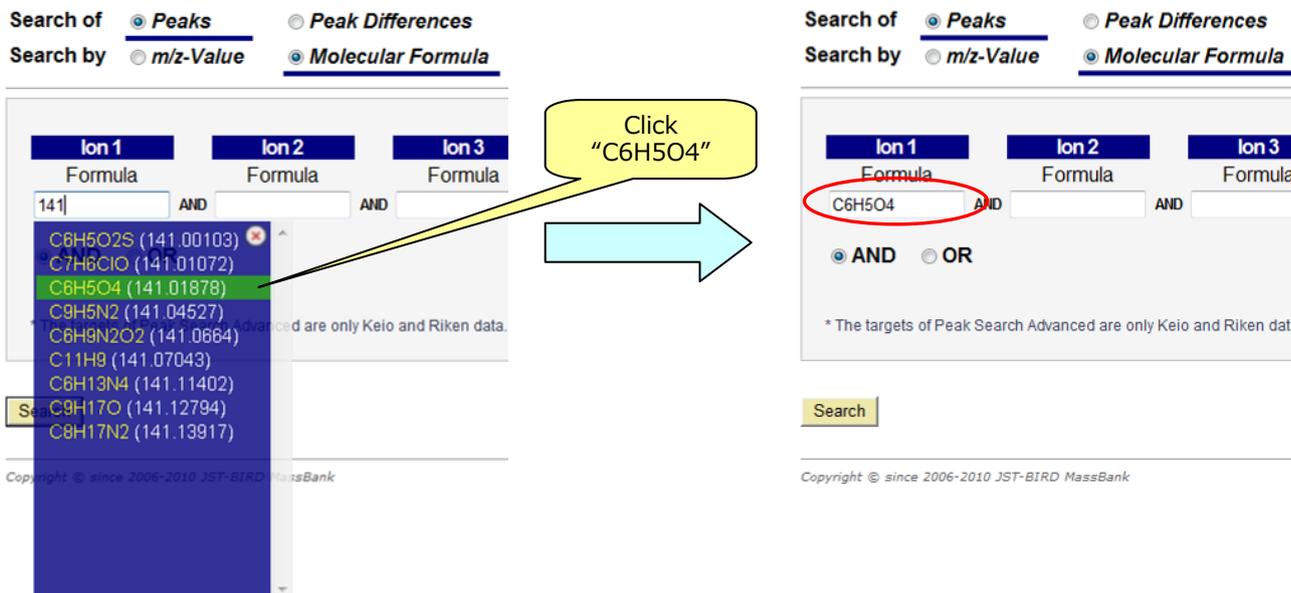
Molecular formulas with matching peak pairs

Copyright(C) 2006-2008
 ACCESSION: KOX006
 RECORD TITLE: S-Adenosylmethionine; MS/MS; QqTOF; MERGED; [M+H]⁺

* Assist in the Input of Molecular Formulas

When m/z values instead of molecular formulas are entered in the "Formula" boxes, a list of candidate molecular formulas, whose exact masses are close to the entered m/z values, is shown in the pull-down menu.

Following example shows a case when a value, 141, was entered in a Formula box on the "Search of Peaks" and "Search by Molecular Formula" mode.



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

lon 1 lon 2 lon 3
Formula Formula Formula

141 AND AND

C6H5O2S (141.00103)
C7H6ClO (141.01072)
C6H5O4 (141.01878)
C9H5N2 (141.04527)
C6H9N2O2 (141.0664)
C11H8 (141.07043)
C6H13N4 (141.11402)
C9H17O (141.12794)
C8H17N2 (141.13917)

Click "C6H5O4"

Search

lon 1 lon 2 lon 3
Formula Formula Formula

C6H5O4 AND AND

AND OR

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

Search

Copyright © since 2006-2010 JST-BIRD MassBank

Pull-down menu shows a list of the molecular formulas, whose exact masses is starting from the value 141. No molecular formula such as 140.9 are listed because prefix string match algorithm is applied.

5. Prediction of Metabolites from ESI-MS² Data

5.1 Metabolite prediction by using peak-chemical substructure relationships

Currently this tool is adapted to predict primary metabolites and their derivatives from the query ESI-MS² data. MassBank has analyzed and accumulated the relationships between peaks (product ions) and chemical substructures by chemically annotating ESI-MS² data of primary metabolites.

The present tool elucidates possible chemical substructures of the unknown metabolite from the query ESI-MS² data by using the relationships that linked the observed product ions to chemical substructures. Additionally possible molecular formulae of the unknown metabolite are predicted from the precursor ion. KNApSack database < http://kanaya.naist.jp/knapsack_jsp/top.html > provides a list of metabolites that satisfy the predicted molecular formula with the possible chemical substructures. Finally the prediction tool outputs the list as the candidates of the unknown metabolite.

A reliable prediction is expected when (1) the query ESI-MS² data should be analyzed on high resolution mass analyzers, (2) the precursor ion observed is a type of "M ± H", (3) more than ten product ions with the relative intensity higher than 5 % are observed, (4) a query data that was prepared by merging two or more ESI-MS² data analyzed on the same unknown metabolite at different CID conditions gives a good result. The present tool automatically merges them into a single query data.

>> Input the query data and set the parameters

The following procedure shows a case when three ESI-MS² data analyzed on the same unknown metabolite at different CID conditions are uploaded, merged into a single query data, and predicted.

Metabolite Identification

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

[1]

by Peak-Substructure Relationships

by Annotated Neutral Losses

[2]

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



A list of the ESI-MS² data uploaded is shown.

[1] Select "by Peak-Substructure Relationships"

[2] Load the query file*

- Select the query file.
- Click "File Read".

*To prepare the query ESI-MS² file, see "2.1 (1) Prepare the query file".

| Query List | | | |
|-------------------------------------|------------------|------|--|
| No | Name | Peak | |
| <input checked="" type="checkbox"/> | 1 sample1_CE10eV | 4 | |
| <input checked="" type="checkbox"/> | 2 sample1_CE20eV | 4 | |
| <input checked="" type="checkbox"/> | 3 sample1_CE30eV | 5 | |
| <input checked="" type="checkbox"/> | 4 sample2_CE10eV | 4 | |
| <input checked="" type="checkbox"/> | 5 sample2_CE20eV | 5 | |

5 spectra

[3']



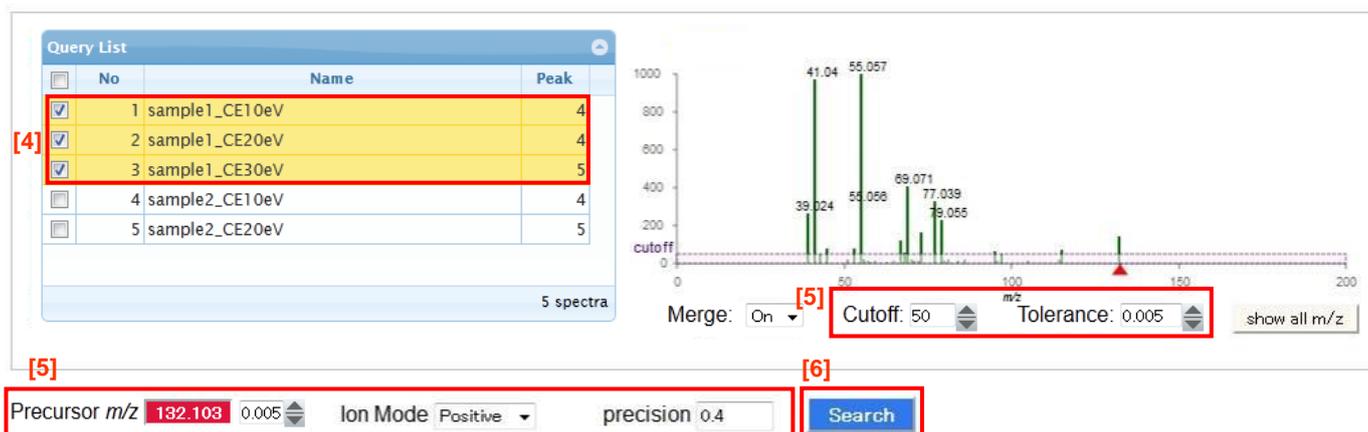
[3] Merge: Cutoff: 50 Tolerance: 0.005

Precursor m/z Ion Mode
precision



[3] Set "Merge On"

- A check box [3'] is appeared at each data.



The screenshot displays the MassBank software interface. On the left, a 'Query List' table contains five entries. The first three entries are selected with checkboxes. On the right, a mass spectrum plot shows relative intensity versus m/z, with several peaks labeled. Below the plot, there are controls for 'Merge', 'Cutoff', and 'Tolerance'. At the bottom, there is a search bar with a 'Precursor m/z' field containing '132.103', an 'Ion Mode' dropdown set to 'Positive', a 'precision' field set to '0.4', and a 'Search' button.

| No | Name | Peak |
|-------------------------------------|------------------|------|
| <input checked="" type="checkbox"/> | 1 sample1_CE10eV | 4 |
| <input checked="" type="checkbox"/> | 2 sample1_CE20eV | 4 |
| <input checked="" type="checkbox"/> | 3 sample1_CE30eV | 5 |
| <input type="checkbox"/> | 4 sample2_CE10eV | 4 |
| <input type="checkbox"/> | 5 sample2_CE20eV | 5 |

Mass Spectrum Plot Parameters:

- Merge: On
- Cutoff: 50
- Tolerance: 0.005

Search Parameters:

- Precursor m/z: 132.103
- Ion Mode: Positive
- precision: 0.4

[4] By checking the box, select the data files of the metabolite to be identified.

- As one data is selected by checking the box, it is added and merged into the query.
- With each selection, the merged ESI-MS² data generated is shown in the right window

[5] Set parameters (see the table below)

- All the parameters should be set correctly.
- Input "Precursor m/z".

[6] Click "Search" button to start.

– Parameters settings–

• **Merge:**

Select "ON" when two or more ESI-MS² data are merged into the query. Check box is appeared at each data. Select the data by checking their boxes.
Leave "OFF" (default) to predict the metabolite from a single data.

• **Cutoff:**

This selects the product ions for the prediction.
Only the peaks larger than the cutoff value are considered in the prediction.
Cutoff value is indicated by the red dotted line on the merged spectra in the write window.
Precursor ion is always included in the prediction independent of the cutoff value.

• **Tolerance:**

This defines the mass accuracy of the product ions in the query data. Within the tolerance, substructure-peak relationships give possible substructures to each product ion.

• **Precursor m/z in the red box:**

Check whether the precursor m/z is correct.
When the m/z value is not correct, correct it manually.

• **Precursor m/z in the white box:**

This defines the mass accuracy of the precursor m/z.

• **Ion Mode:**

Select either "Positive" or "Negative".

• **Precision:**

This is the precision of an empirical relationship between a peak and a chemical substructure that is used for prediction. False positive decreases with the precision. See the next page for details.

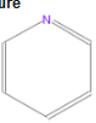
>> Search Results

Matched Formulae : 4

| m/z | 78.0355 | 80.0508 | 96.0458 | 123.0560 |
|---------|--------------|--------------|------------------------------|--------------|
| Formula | C5H4N | C5H6N | C5H6NO | C6H7N2O |
| No. | ion-pos-0013 | ion-pos-0013 | ion-pos-0013 ion-pos-0028 | ion-pos-0013 |

Hit Relationships : 2

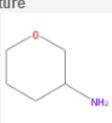
ion-pos-0013
Substructure



Formula, Precision & Recall, TP

| | | | | |
|---------|-------|------|------|----|
| C5H4N | 0.66 | 0.68 | 27 | |
| C6H7N2O | 0.67 | 0.1 | 4 | |
| C5H6N | C5H4N | 0.71 | 0.38 | 15 |

ion-pos-0028
Substructure



Formula, Precision & Recall, TP

| | | | |
|--------|------|------|----|
| C5H6NO | 0.55 | 0.55 | 11 |
|--------|------|------|----|

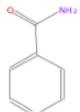
A

- **m/z**: Product ions used for prediction
- **Formula**: Possible molecular formulae assigned to the ions
- **No.**: ID numbers of the substructures predicted by the relationships between peaks and chemical substructures

* By placing the cursor on an ID number, the corresponding substructure is shown as "A".

Results : 3 Hit.

Isonicotineamide

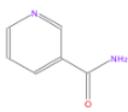


Formula : C6H6N2O
Exact Mass : 122.048

DB Links
KEGG : [C02421](#)

Hit Relationship-No.
ion-pos-0013

Nicotinamide

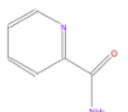


Formula : C6H6N2O
Exact Mass : 122.04801

DB Links
KNApSack : [C00000209](#)
KEGG : [C00153](#)

Hit Relationship-No.
ion-pos-0013

Picolinamide



Formula : C6H6N2O
Exact Mass : 122.048

DB Links
KEGG : [C01950](#)

Hit Relationship-No.
ion-pos-0013

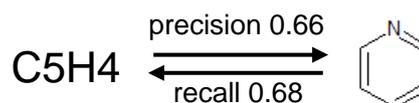
B

A: Possible substructures that are embedded in the structure of the unknown metabolite are predicted by using the relationships between peaks and chemical substructures.

B: Candidates of the unknown metabolite are shown. The KNApSack database outputs the candidates that satisfy the following conditions; they have one or more of the substructures shown in **A** and the molecular formula is the same to that predicted from the mass of the precursor ion. A substructure in the gray box in **A** is not applicable in the candidates in **B**.

Formula, Precision & Recall, TP

| | | | |
|-------|------|------|----|
| C5H4N | 0.66 | 0.68 | 27 |
|-------|------|------|----|



Formula, Precision & Recall, TP: ("C5H4N", "0.66", "0.68", "27" in the above example)

Formula: Chemical formula of a peak

Precision: Ratio of the number of ESI-MS² data (pyrimidine substructure & C5H4N) to that of ESI-MS² data (C5H4N), where among the ESI-MS² data (C5H4N), in which the peak C5H4N was observed, ESI-MS² data (pyrimidine substructure & C5H4N) are those analyzed on chemical compounds with the pyrimidine substructure.

In the above example, the ratio is 0.66.

Recall: Ratio of the number of ESI-MS² data (pyrimidine substructure & C5H4N) to that of ESI-MS² data (pyrimidine substructure), where the ESI-MS² data (pyrimidine substructure) were analyzed on chemical compounds with the pyrimidine substructure. In the above example, the ratio is 0.68.

TP: Total number of the ESI-MS² data (pyrimidine substructure & C5H4N). In the above example, it is 27.

5.2 Metabolite prediction by spectrum search in terms of neutral loss

Chemical compounds are often synthesized from a common chemical compound by slight chemical modifications. Such derivatives share the chemical structure of the common chemical compound. Their mass spectra are also similar, although their similarity cannot be detected by conventional spectral similarity search. Peaks observed in the mass spectrum of one derivative are shifted by Δu from the corresponding peaks of the other one where Δ is the mass difference between their chemical structures. Such a similarity is searchable by comparing not the m/z of the corresponding peaks but the mass difference between the corresponding peak pairs because Δ is unknown. Thus this tool searches the ESI-MS² data in MassBank that are similar to the query one by comparing the m/z difference between the corresponding peak pairs. Here “**neutral loss**” is defined as the m/z difference between peak pairs. Search results suggest the users the common chemical compound among the target and query chemical compounds. However, this comparison has such a general difficulty that many possible peak pairs should be compared within the mass accuracy of m/z . To escape the difficulty, the targets in the present method are limited to the high resolution MassBank ESI-MS2 data with chemical annotation on peaks. All possible peak differences in each target data have been calculated not by m/z but by the assigned molecular formulae. MassBank recommends the query data that is enough high in the resolution to assign the molecular formula to peaks. All possible peak differences in the target are also calculated by the molecular formulae. Peak differences between the target and the query are compared by the molecular formulae. Additionally the present tool evaluates the matching peaks observed in the range of m/z 50-99.

>> Input the query data and set the parameters

Metabolite Identification

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

by Peak-Substructure Relationships

[1] *by Annotated Neutral Losses*

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

Search similar spectra on a neutral loss-to-neutral loss basis
Retrieves spectra similar to user's spectrum in terms of molecular formulae.
This search is helpful to predict the chemical structure of unknown metabolites.

[1] Select “by Annotated Neutral Losses”.

[2] - [6] the same in the Section 5.1 “Metabolite prediction based on peak-chemical substructure relationships”.

>> Search Results

Matched neutral losses : 6
 H3N(17.027), CH2N2(42.022), C4H6(54.047), CH5N3(59.048), C3H7O(59.05), C4H9N(71.074)

A list of the peak differences that were annotated with the molecular formula in the query data.

Results : In descending order of rank of matched neutral loss.

hide (4)

| | | |
|---|--|--|
| <p>No. 1 PR100307 Agmatine, LC-ESI-QTOF-MS/MS, CE, Ramp, 5-6 ...</p> <p>Neutral Loss Hits : 5 H3N(17.027) CH2N2(42.022) C4H6(54.047) CH5N3(59.048) C4H9N(71.074)</p> <p>Ion :CH6N3(60.05617) :C4H10N(72.08132)</p> <p>Formula : C5H14N4 Exact Mass : 130.12185</p> | <p>No. 2 KOX00653 Agmatine, MS/MS, QqTOF, MERGED, [M+H]⁺</p> <p>Neutral Loss Hits : 5 H3N(17.027) CH2N2(42.022) C4H6(54.047) CH5N3(59.048) C4H9N(71.074)</p> <p>Ion :CH6N3(60.05617) :C4H10N(72.08132)</p> <p>Formula : C5H14N4 Exact Mass : 130.12185</p> | <p>No. 3 KOX00672 Bufornin, MS/MS, QqTOF, MERGED, [M+H]⁺</p> <p>Neutral Loss Hits : 4 H3N(17.027) CH2N2(42.022) CH5N3(59.048) C4H9N(71.074)</p> <p>Ion :CH6N3(60.05617) :C4H10N(72.08132)</p> <p>Formula : C6H15N5 Exact Mass : 157.13275</p> |
| <p>No. 4 KOX00641 N-Acetylputrescine, MS/MS, QqTOF, MERGED, [M+H]⁺</p> <p>Neutral Loss Hits : 3 H3N(17.027) C4H6(54.047) C4H9N(71.074)</p> <p>Ion C4H10N(72.08132)</p> <p>Formula : C6H14N2O Exact Mass : 130.11061</p> | <p>No. 5 KOX00781 Metformin, MS/MS, QqTOF, MERGED, [M+H]⁺</p> <p>Neutral Loss Hits : 3 H3N(17.027) CH2N2(42.022) CH5N3(59.048)</p> <p>Ion CH6N3(60.05617)</p> <p>Formula : C4H11N5 Exact Mass : 129.10145</p> | <p>No. 6 KOX00737 b-Guanidinopropionate, MS/MS, QqTOF, MERGED, [M+H]⁺</p> <p>Neutral Loss Hits : 3 H3N(17.027) CH2N2(42.022) CH5N3(59.048)</p> <p>Ion :CH6N3(60.05617) :C4H10N(72.08132)</p> <p>Formula : C4H9N3O2 Exact Mass : 131.06948</p> |

* MassBank data similar to the query one are shown (max. 30 data).

- (1) **Neutral Loss:** Here "Neutral Loss" is defined as the difference of the corresponding peak pairs in terms of molecular formulae. The target data are listed by a total number (Hits) of the molecular formulae that were matched between the query and target ESI-MS² data.
- (2) **Ion:** The matching peaks ($50 < m/z < 99$) are listed by molecular formulae.
 - A. They are shown in a dotted red box when the target data have the maximum number of matching peaks.
 - B. The target data that have no matching peak are shown in a grey box. They are not shown when the "hide" button was clicked.
 - C. "Results: **NO peaks within m/z 50-99 in query.**" is shown when no peak ($50 < m/z < 99$) was observed in the query data.
 - D. "Results: **NO matched ions to peaks within m/z 50-99 in query.**" is shown when no peak ($50 < m/z < 99$) has no annotated molecular formulae.
- (3) **Exact Mass:** Molecular mass of the target data is shown in white characters in the red box or in the grey box when it is equal to "Precursor $m/z + 1$ " or "Precursor $m/z - 1$ " in the positive or negative mode, respectively.
- (4) **Rank:** The target data are listed by the rank which is scored by a total number of matching peak pairs with matching peaks.

Minimum requirements that target data are matched or similar to the query are as follows.

- Target data are ranked at high.
- They have one or more matching peaks ($50 < m/z < 99$).
- Their molecular mass is equal to that of the query.

6. Browsing All Data

6.1 Categorical Index

In Record Index, all data is categorized into contributor, instrument type, MS type, merged type, ion mode and compound name categories. Click a link in this page, then the whole data in the category is displayed in the same format as other search results.

Record Index

[mass calculator](#) [user manual](#)

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

| | | |
|------------------------|---|------------|
| Contributor | Chubu Univ. (2,628) Fac. Eng. Univ. Tokyo (12,379) Fukuyama Univ. (340) IMM, CAMS & PUMC, China (67) Kazusa (273) Keio Univ. (5,629) Kyoto Univ. (185) Leibniz IPB (528) Metabolon (149) NAIST (817) Nihon Univ. (75) Osaka MCHRI (20) Osaka Univ. (502) PFOS research group (277) RIKEN (1,722) Tottori Univ. (16) UOEH (35) Univ. Connecticut (510) Univ. Toyama (253) Waters (2,994) | [1] |
| Instrument Type | CE-ESI-TOF (20) CL-B (796) EL-B (11,636) EL-EBEB (12) ESI-IT-MS/MS (149) ESI-QqIT-MS/MS (15) ESI-QqQ-MS/MS (52) ESI-QqTOF-MS/MS (510) FAB-B (26) FAB-EB (5) FAB-EBEB (173) FD-B (41) FL-B (1) GC-EL-TOF (1,016) LC-APPI-QQ (277) LC-ESI-IT (515) LC-ESI-ITFT (3,006) LC-ESI-ITTOF (253) LC-ESI-Q (2,721) LC-ESI-QIT (378) LC-ESI-QQ (5,038) LC-ESI-QTOF (2,742) MALDI-TOF (17) | [2] |
| MS Type | MS (16,898) MS2 (11,505) MS3 (926) MS4 (70) | [3] |
| Merged Type | Normal (28,560) Merged (839) | [4] |
| Ion Mode | Positive (22,721) Negative (6,678) | [5] |
| Compound Name | A (1,273) B (1,117) C (1,478) D (1,887) E (760) F (395) G (747) H (565) I (777) J (3) K (216) L (1,371) M (1,552) N (1,389) O (471) P (3,762) Q (140) R (262) S (948) T (1,491) U (118) V (137) W (3) X (50) Y (8) Z (75) 1-9 (7,781) Others (623) | [6] |

[1] Contributor

Number of data listed by contributors.

Each link is followed by the parenthesized number of spectra in the category.

[2] Instrument Type

Number of data listed by the types of chromatography and mass spectrometer.

[3] MS Type

Number of data listed by the types of mass spectrometry.

[4] Merged Type

Number of merged ESI-MS2 data and that of the other data.

[5] Ionization Mode

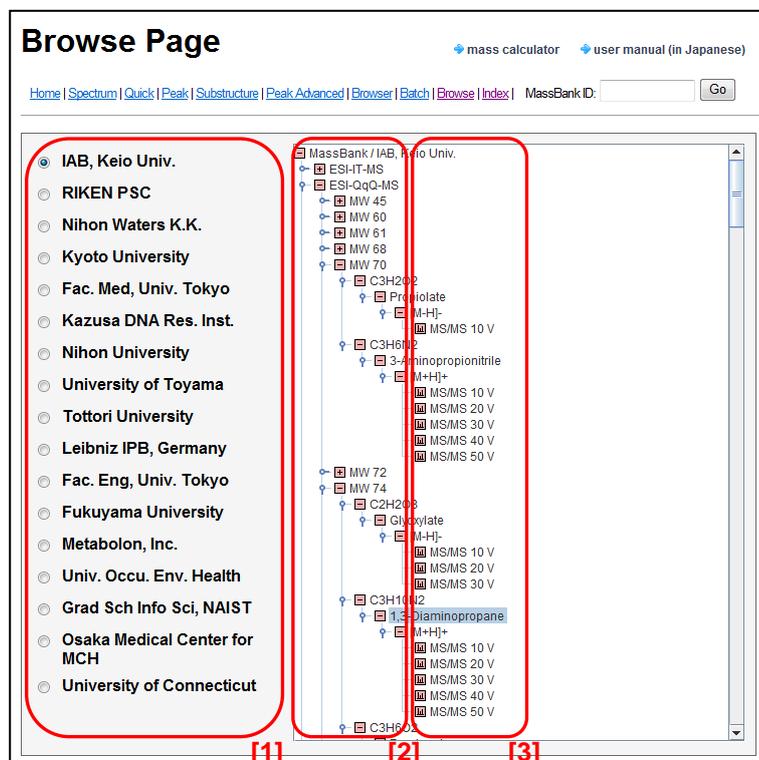
Number of data analyzed by positive and negative modes.

[6] Compound Name

Number of data listed by the first letters of compound names.

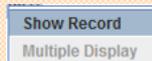
6.2 Hierarchical Browse

In Browse Page, all data are hierarchically displayed for each data provider. You can go up and down the hierarchy (tree) and find a specific data you want.



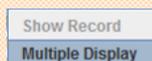
After selecting a spectrum by clicking , you can select multiple spectra by clicking  with Ctrl key or Shift key. After that, a right button click shows the following popup menu.

[case of single selection]



Click "Show Record", then the details of the MassBank Record are displayed.

[case of multiple selection]



Click "Multiple Display", then multiple spectra are displayed in tiled view.

[1] Select Provider

Click a radio button, then display the hierarchy of the selected provider is displayed in right hand side.

[2] Browse Tree

-  : open the lower layer.
-  : close the lower layer.

[3] Display Spectrum

View detailed MassBank Record: Double click of ; or "Show Record" in popup menu by right button click when a spectrum is selected.

Display multiple spectra in a tiled view: "Multiple Display" in popup menu by right button click when multiple spectra are selected.

7. Others

7.1 Search Results

When you conduct a search via "Quick Search", "Substructure Search", "Peak Search", "Peak Search Advanced", or "Record Index", the search results are displayed in a common format.

<<Operation 1>>

List of Search Results

Compound list

Results : 25 Hit. (1 - 25 Displayed)

First Prev 1 Next Last (Total 1 Page)

| Name | Formula / Structure | ExactMass | ID |
|---|---------------------|-----------|----|
| <input checked="" type="checkbox"/> 2,4-Dimethylaniline | C8H11N | 121.08915 | |
| <input type="checkbox"/> 2,6-Dimethylaniline | C10H15N | | |
| <input type="checkbox"/> 2,6-Diethylaniline | C8H11N | 121.08915 | |

Buttons: Open All Tree, Multiple Display, Spectrum Search

Callouts: "Expand all trees" points to "Open All Tree"; "Click the '+' icon to expand an individual tree." points to the checked box; "Click on a column heading to sort (by name, molecular formula, or exact mass)." points to the "ExactMass" header.

Spectrum list

Results : 25 Hit. (1 - 25 Displayed)

Close All Tree Multiple Display Spectrum Search

First Prev 1 Next Last (Total 1 Page)

| Name | Formula / Structure | ExactMass | ID |
|---|---------------------|-----------|----------|
| <input checked="" type="checkbox"/> 2,4-Dimethylaniline | C8H11N | 121.08915 | |
| <input type="checkbox"/> - MS/MS: QqQ, CE:10 V, [M+H] ⁺ | | | KO002806 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:20 V, [M+H] ⁺ | | | KO002807 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:30 V, [M+H] ⁺ | | | KO002808 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:40 V, [M+H] ⁺ | | | KO002809 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:50 V, [M+H] ⁺ | | | KO002810 |
| <input type="checkbox"/> 2,6-Diethylaniline | C10H15N | 149.12045 | |
| <input type="checkbox"/> - MS/MS: QqQ, CE:10 V, [M+H] ⁺ | | | KO002677 |
| <input checked="" type="checkbox"/> - MS/MS: QqQ, CE:20 V, [M+H] ⁺ | | | KO002678 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:30 V, [M+H] ⁺ | | | KO002679 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:40 V, [M+H] ⁺ | | | KO002680 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:50 V, [M+H] ⁺ | | | KO002681 |
| <input type="checkbox"/> 2,6-Dimethylaniline | C8H11N | 121.08915 | |
| <input type="checkbox"/> - MS/MS: QqQ, CE:10 V, [M+H] ⁺ | | | KO002801 |
| <input checked="" type="checkbox"/> - MS/MS: QqQ, CE:20 V, [M+H] ⁺ | | | KO002802 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:30 V, [M+H] ⁺ | | | KO002803 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:40 V, [M+H] ⁺ | | | KO002804 |
| <input type="checkbox"/> - MS/MS: QqQ, CE:50 V, [M+H] ⁺ | | | KO002805 |

Callouts: "Click link" points to the selected spectrum link.

MassBank Record: KO002806

Home | Spectrum | Quick | Peak | Substructure | Peak-Advanced | Browse | Batch | Browse | Index | Record No: Go

2,4-Dimethylaniline; MS/MS: QqQ, CE:10 V, [M+H]⁺

Mass Spectrum

Chemical Structure

Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University

ACCESSION: KO002806
 RECORD TITLE: 2,4-Dimethylaniline; MS/MS: QqQ, CE:10 V, [M+H]⁺
 DATE: 2007.07.07
 AUTHORS: Rikazu Y, Hozai H, Institute for Advanced Biosciences, Keio Univ.
 COPYRIGHT: Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University

MassBank record of an individual spectral data is displayed.

<<Operation 3>>

Brief display of chemical structure

Results : 5,704 Hit. (1 - 182 Displayed)

Open All Tree Multiple Display Spectrum Search

First Prev 1 2 3 4 5 6 7 8 9 10 Next Last (Total 28 Page) Results End

| Name | Formula / Structure | ExactMass | ID |
|---|---------------------|-----------|----|
| (9Z, 12Z)-Octadecadienoate 6 spectra | C18H32O2 | 280.24023 | |
| (Aminomethyl)phosphonate 12 spectra | CH6NO3P | | |
| (Methylthio)acetate | | | |
| (R)-Mandelate | | 152.04734 | |
| (S)-2-Aminobutyrate | | 103.06333 | |

1) Move mouse pointer onto a thumbnail of chemical structure

2) The structure is enlarged. If mouse pointer leaves from the thumb nail, then it disappears

Results : 5,704 Hit. (1 - 182 Displayed)

Open All Tree Multiple Display Spectrum Search

Total 28 Page) Results End

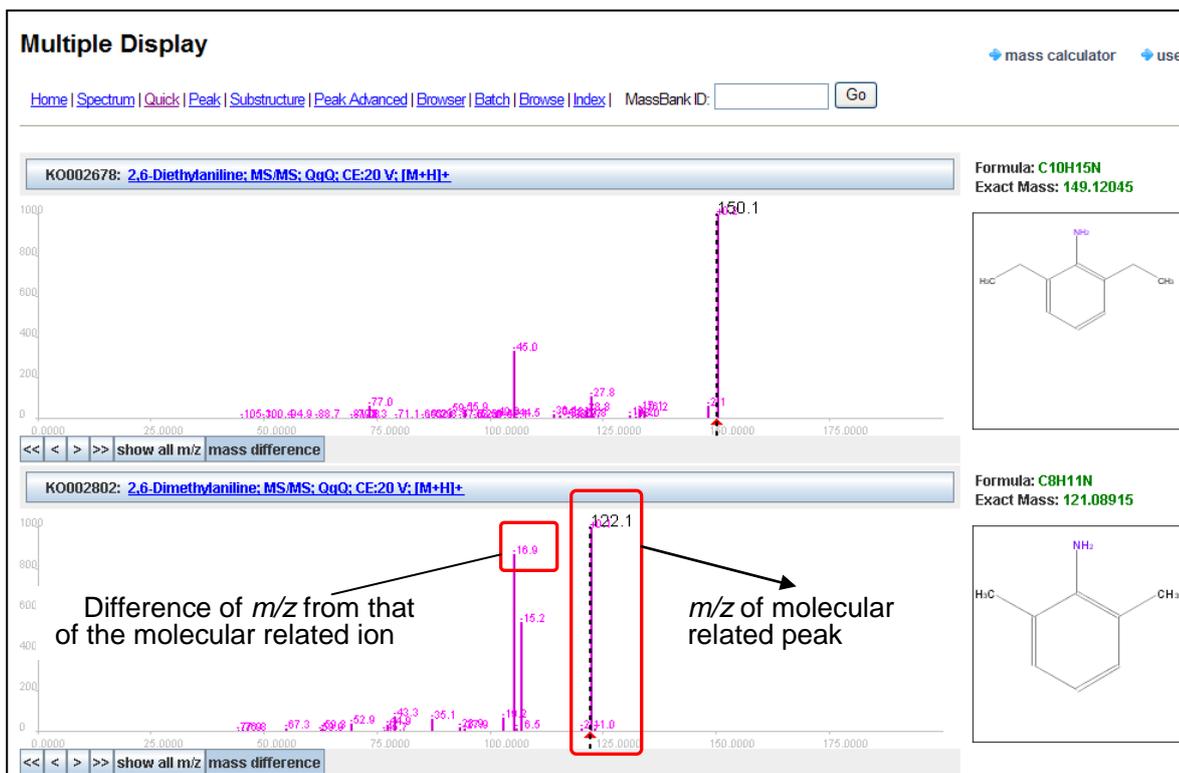
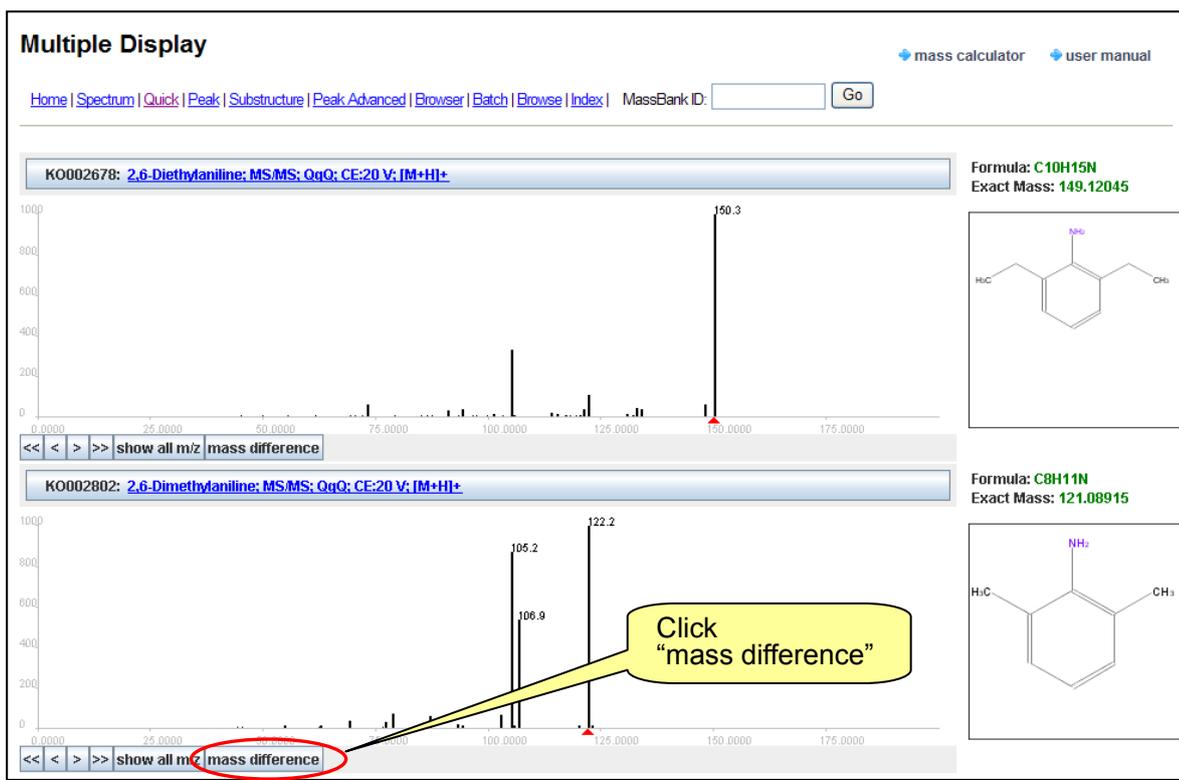
| Name | Formula / Structure | ExactMass | ID |
|---|---------------------|-----------|----|
| (9Z, 12Z)-Octadecadienoate 6 spectra | C18H32O2 | 280.24023 | |
| (Aminomethyl)phosphonate 12 spectra | CH6NO3P | | |
| (Methylthio)acetate 6 spectra | C3H6O2S | | |
| (R)-Mandelate 5 spectra | C8H8O3 | 152.04734 | |
| (S)-2-Aminobutyrate 11 spectra | | 103.06333 | |

1) Click a thumbnail of chemical structure.

2) Large structure is shown in another window. If another thumbnail is clicked, then a new window does not appear and the new structure is shown in the window. It does not disappear automatically, then you must close the window by yourself

>> mass difference

When click the “mass difference” button on the “Multiple Display” panel of “Compound and Peak Search Results”, spectra display the peaks with the value of m/z difference from that of the molecular related ion.



7.2 MassBank Record Detailed Display

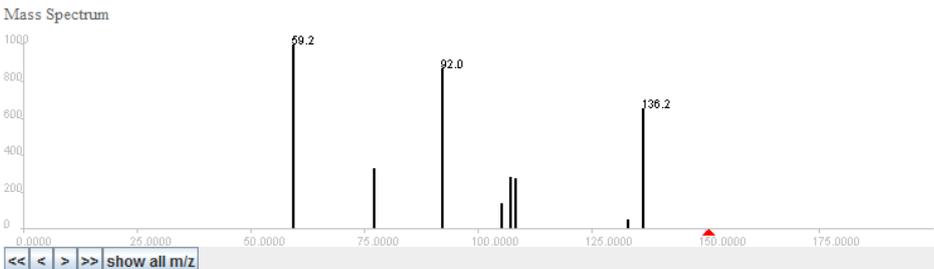
The MassBank record is the fundamental unit of data in the MassBank database. Each mass spectrum has one MassBank record. In addition to peak data, each record includes the compound information (CH\$), test conditions (AC\$), etc. (To see "Record Editor Manual" for more details)

MassBank Record: KO001419

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

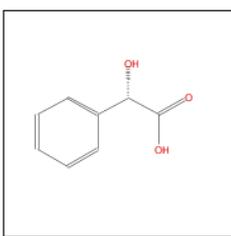
(S)-Mandelic acid; LC-ESI-QQ; MS2; CE:30 V; [M-H]-

Mass Spectrum



show all m/z

Chemical Structure

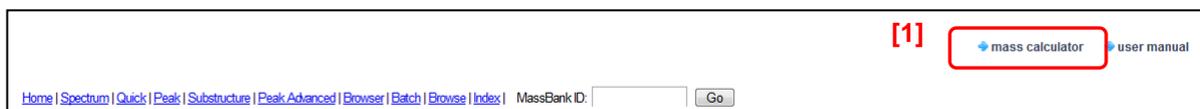


| | | | |
|---|---|-----------------------|---|
| <pre> ACCESSION: KO001419 RECORD_TITLE: (S)-Mandelic acid; LC-ESI-QQ; MS2; CE:30 V; [M-H]- DATE: 2011.05.10 (Created 2007.07.07) AUTHORS: Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio LICENSE: CC BY-NC-SA COMMENT: KEIO_ID M057 </pre> | } | Base Info | <p>ACCESSION: "record ID" RECORD_TITLE: "title (compound name, method, etc.)" DATE: "Date last updated (Create date)" AUTHORS: "Record creators" LICENSE: "Creative Commons or Copyright"</p> |
| <pre> CH\$NAME: (S)-Mandelate CH\$NAME: (S)-Mandelic acid CH\$NAME: (S)-2-Hydroxy-2-phenylacetic acid CH\$NAME: (S)-2-Hydroxy-2-phenylacetate CH\$COMPOUND_CLASS: Non-Natural Product CH\$FORMULA: C8H8O3 CH\$EXACT_MASS: 152.04734 CH\$SMILES: OC(=O)[C@H](O)c1ccccc1 CH\$IUPAC: InChI=1S/C8H8O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7,9H,(H,10) CH\$LINK: CAS 90-64-2 611-72-3 CH\$LINK: CHEBI 32800 CH\$LINK: ChEMBL SMN CH\$LINK: KEGG C01984 CH\$LINK: PUBCHEM SID:5081 </pre> | } | Compound Info | <p>CH\$NAME: "name (can include multiple names, including variants)" CH\$FORMULA: "Molecular formula" CH\$EXACT_MASS: "Exact mass (to five decimal places)" CH\$SMILES: "SMILES code" CH\$IUPAC: "InChI code"</p> |
| <pre> AC\$INSTRUMENT: API3000, Applied Biosystems AC\$INSTRUMENT_TYPE: LC-ESI-QQ AC\$MASS_SPECTROMETRY: MS_TYPE MS2 AC\$MASS_SPECTROMETRY: ION_MODE NEGATIVE AC\$MASS_SPECTROMETRY: COLLISION_ENERGY 30 V </pre> | } | Analytical Conditions | <p>AC\$INSTRUMENT: "instrument name" AC\$INSTRUMENT_TYPE: "instrument type" AC\$MASS_SPECTROMETRY: MS_TYPE "ms type" AC\$MASS_SPECTROMETRY: ION_MODE "ion mode"</p> |
| <pre> MS\$FOCUSED_ION: PRECURSOR_M/Z 151 MS\$FOCUSED_ION: PRECURSOR_TYPE [M-H]- </pre> | } | Peak Data | <p>PK\$NUM_PEAK: number of peaks PK\$PEAK: array of m/z, measured intensity, and relative intensity for each peak</p> |
| <pre> PK\$NUM_PEAK: 8 PK\$PEAK: m/z int. rel.int. 59.200 707921.5 999 77.200 232673.5 328 92.000 613862.0 866 105.100 99010.0 140 107.200 198020.0 279 108.300 193069.5 272 133.000 34653.5 49 136.200 460396.5 650 // </pre> | } | Peak Data | <p>PK\$NUM_PEAK: number of peaks PK\$PEAK: array of m/z, measured intensity, and relative intensity for each peak</p> |

* For details of MassBank Record, see "Record Editor Manual".

7.3 Basic Mass Calculation Tool

Mass Calculator on the upper right corner is a basic mass calculation tool that you can use everywhere in MassBank. It calculates m/z (i.e. exact mass) of the input formula or displays a list of chemical formulae corresponding to m/z .

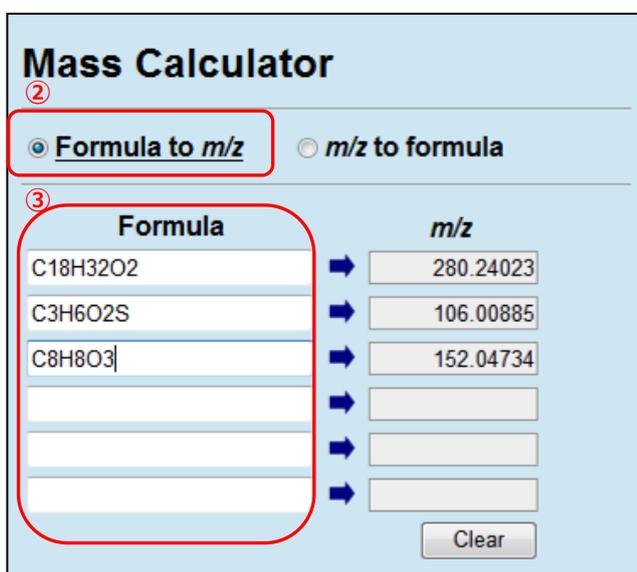


[1] Click "mass calculator"

MassCalculator appears in a separate window.



Calculation of m/z from chemical formula.



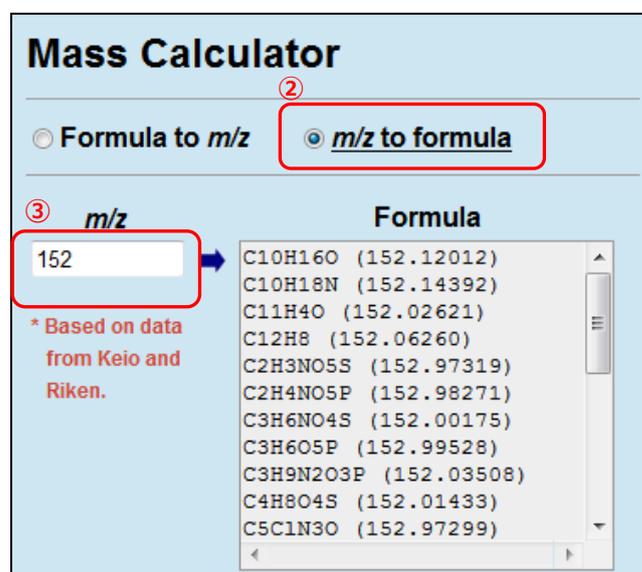
| Formula | m/z |
|----------|-----------|
| C18H32O2 | 280.24023 |
| C3H6O2S | 106.00885 |
| C8H8O3 | 152.04734 |
| | |
| | |
| | |

[1] Select "Formula to m/z "

[3] Input Formula

When a formula is entered, m/z is calculated and displayed.

Listing of chemical formulae corresponding to m/z .



| m/z | Formula |
|-------|-----------------------|
| 152 | C10H16O (152.12012) |
| | C10H18N (152.14392) |
| | C11H4O (152.02621) |
| | C12H8 (152.06260) |
| | C2H3NO5S (152.97319) |
| | C2H4NO5P (152.98271) |
| | C3H6NO4S (152.00175) |
| | C3H6O5P (152.99528) |
| | C3H9N2O3P (152.03508) |
| | C4H8O4S (152.01433) |
| | C5C1N3O (152.97299) |

* Based on data from Keio and Riken.

[2] Select " m/z to formula"

[3] Input m/z

When a m/z value is entered, the chemical formulae that were observed in the MassBank annotated ESI-QTOF-MS² data are shown.

Chemical formulae listed are those that were actually observed in Keio and RIKEN ESI-QTOF-MS² data, but not possible chemical formulae.

Mass Calculator window can be closed by ESC key.

7.4 Comparison Tool of User Spectra

Spectral Browser is a comparison tool of spectra which reads a file which consists of a set of user spectra and displays them in perspective drawing. The upper limit of user spectra is 20. It also compare input spectra each other.

(1) Prepare the spectral file

The format of an input of Spectral Browser, so-called a spectral file, is as follows. You can download a sample from <http://www.massbank.jp/sample/sample.zip>. The format of this spectral file is same as the format of a query file of Spectrum Search, then a spectral file is commonly used in Spectrum Search、Spectral Browser.

Name
Write an arbitrary name, such as the name of the compound. (Optional)

Peak Information
Write the *m/z* and intensity, separated by spaces. You can write all the peak information on a multiple lines, writing one peak per line.

Empty line
If you include peak information for more than one spectrum, put a blank line between each one.

[Spectral File]

```
Name: Sample Compound 1
70 24
71 10
72 68
73 999
74 107

Name: Sample_Compound 2
73.1 15008
78.54 4456
79.45 2158311
85.3 964800
86.11 150
90.0 804911

Name: Sample Compound 3
178.876379147 15
186.884786287 8
229.504276894 9
```

Single space

Name : Δ Sample...

Arbitrary name

When entering a name, always begin the line with "Name:"

Single space

78.54 Δ 4456

m/z Intensity
(Absolute or relative value can be used)

(2) Load spectral file and set the compare parameters

After selecting your spectral file, click **File Read**.

Click **Compare Parameter**.

| Order | Query | Name | Hit | Match | Disable | Peak | Precursor | ID |
|-------|-------------|------|-----|-------|---------|------|-----------|----------|
| 9 | Compound_09 | | - | 0 | | 57 | | US000009 |
| 8 | Compound_08 | | - | 0 | | 12 | | US000008 |
| 7 | Compound_07 | | - | 0 | | 108 | | US000007 |
| 6 | Compound_06 | | - | 0 | | 31 | | US000006 |
| 5 | Compound_05 | | - | 0 | | | | |
| 4 | Compound_04 | | - | 0 | | | | |
| 3 | Compound_03 | | - | 0 | | | | |
| 2 | Compound_02 | | - | 0 | | | | |
| 1 | Compound_01 | | - | 0 | | | | |

Compare Parameter

Tolerance: unit ppm Help

Cutoff threshold: Help

OK Cancel

[1] Load the spectral file

Click "**Browse**", and select a spectral file. Afterwards, click "**File Read**", then Spectral Browser reads the spectral file and display the spectra in it

[2] Set the compare parameters

Click **Compare Parameter**. The Setting window opens.

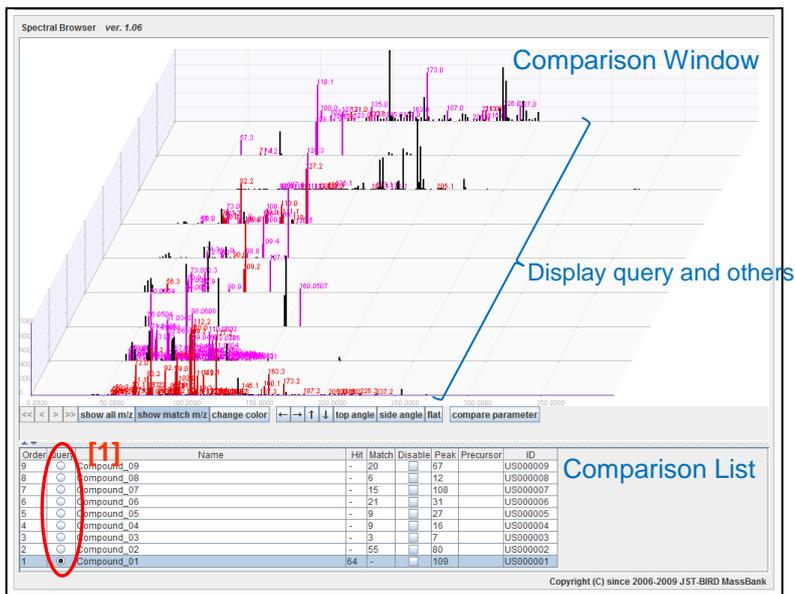
Settings

- **Tolerance:**
m/z error range
- **Cutoff Threshold:**
Relative intensity threshold

Compare Parameter Setting Window

(3) Perform the compare

When you specify an arbitrary spectrum as a query, then you can compare input spectra in one-to-many manner.



[1] Select query spectrum

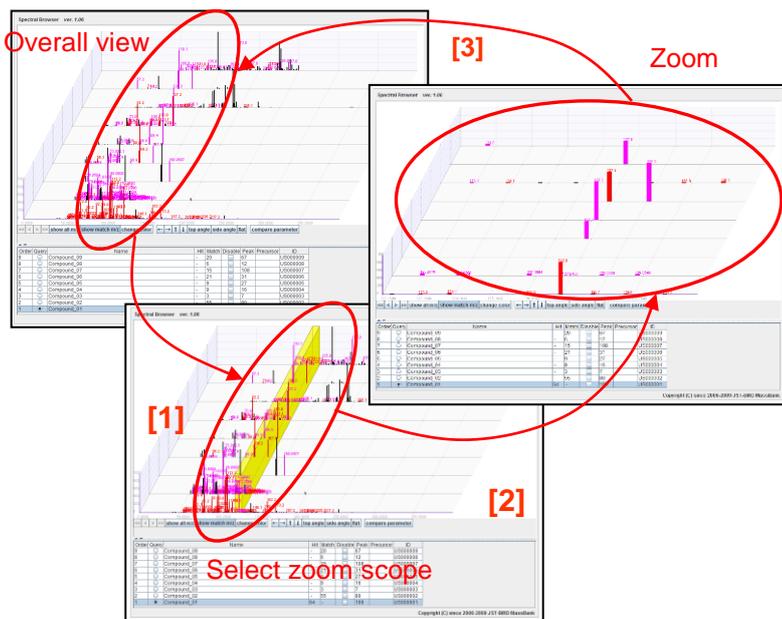
Click a radio button for selecting a query. The one-to-many comparison is suddenly executed and its results are reflected automatically.

Peak Color in Spectrum Comparison Window

In the spectrum comparison windows in Compare View and Package View, matching peaks can be distinguished by color.

| Peak | Matching m/z on query peak | |
|--------------------|----------------------------|---------------------------|
| | Perfect Match | Match within Error Margin |
| Query Spectrum | Red | Red |
| Retrieved Spectrum | Red | Pink |

<<Handy Feature 1: Spectrum Zoom>>



[1] Select location to zoom

Drag from the location of the start of the zoom.

[2] Set zoom position

Drop to set the location on the spectrum to zoom.

[3] End zoom

Double click in comparison window, then return to the initial size without zooming

<< Handy Feature 2: Peak Manipulation >>



a Highlight peak

Place the cursor over a peak. It is highlighted in blue, and the m/z and intensity values appear.

b Select peak

Click on a desired peak. It is rendered in blue to indicate that it is selected. Up to 6 peaks can be selected.

Peak Rendering Color

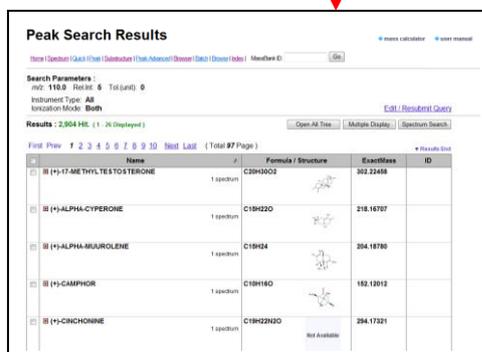
Highlighted: Blue
Selected: Light blue

c Search for peaks

If you right click while one or more peaks are selected, a menu appears, and "Peak Search" can be selected. The peak search begins immediately after selection.

d Cancel peak selection

Select "Select Reset" from a menu popped up by a right button click in graphic area.

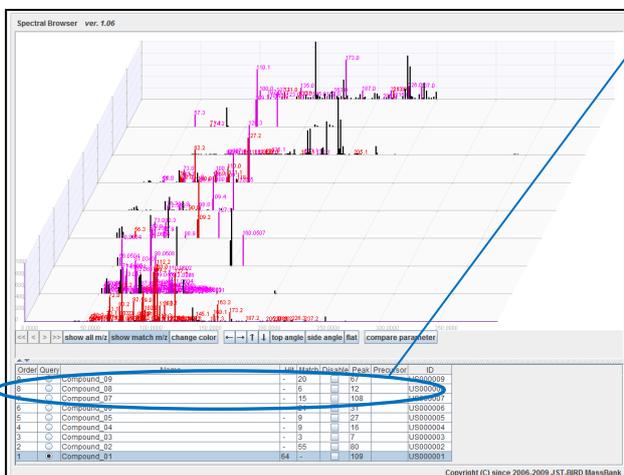


Peak Search Results Window

- Highlight & select peak in Spectral Browser -

In Spectral Browser, when you highlight or select a peak in a spectrum, peaks in other spectra are also highlighted or selected if whose m/z are completely equal to the m/z of the highlighted/selected peak.

<< Handy Feature 3: Spectrum Manipulation >>



Spectrum Manipulation Buttons

<< < > >>

... Move display location (only when zoomed on spectrum)

show all m/z

... Display m/z values of all peaks

show match m/z

... Display m/z values of matching peaks

change color

... Change color of entire spectrum

↖ ↗ ↕ ↘

... Change angle (manual manipulation)

top angle

... Change angle (top perspective)

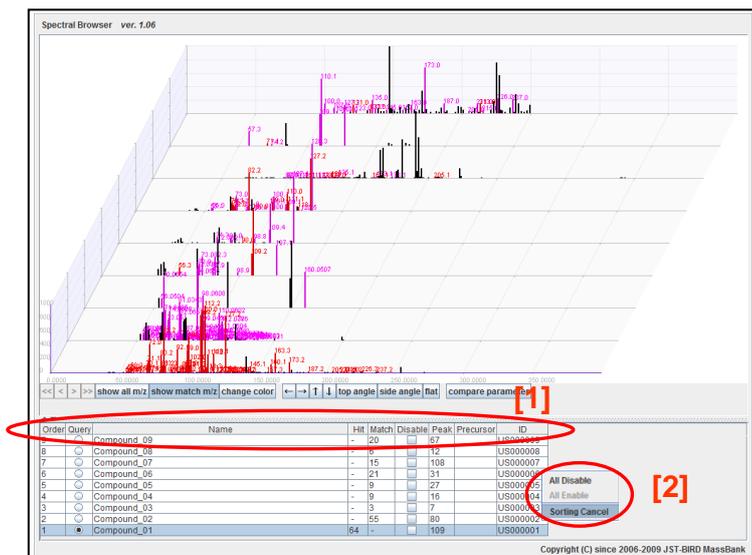
side angle

... Change angle (side perspective)

flat

... Change angle (all spectrums in flat view)

<< Handy Feature 4: Sort Spectra >>



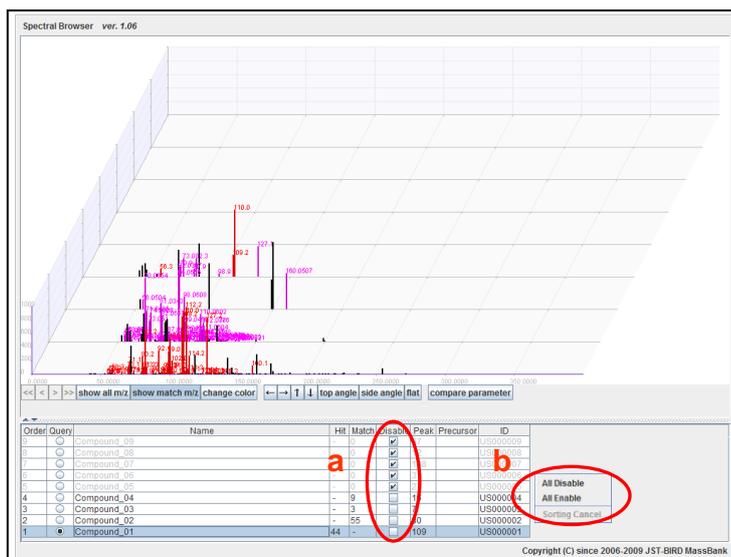
[1] Sort Spectra

Click one of header items in comparison list (i.e. "Order", "Query", "Name", "Hit", "Match", "Disable", "Peak", "Precursor", and "ID"), then the list is sorted by the item. Consecutive clicks of an item change the order of sorting cyclically in ascending, descending and without sorting

[2] Cancel sorting

Select "Sorting Cancel" in a menu popped up by right button click on comparison list.

<< Handy Feature 5: Spectrum Hiding >>



a Hide/show spectrum

For each item in comparison list, tick its checkbox "Disable", then the corresponding spectrum is hidden. Untick the checkbox, then it appears again

b Hide/show all spectra

Select "All Disable" in a menu popped up by right button click on comparison list, then all spectra are hidden. Select "All Enable" in the same menu, then all spectra appear again.

- Comparison window and comparison list -
 Comparison window and Comparison list are operated simultaneously. For example, spectra are sorted in comparison list, the results is suddenly reflected to comparison window and spectra in comparison window are also sorted in same order.

Contact

Please contact the MassBank Group if you have any problems or questions.

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