

Introduction

Background

- Untargeted metabolomics data generated from LC-HRMS experiments are typically characterized by 1000s of peaks with unknown chemical identities.
- To assist with compound identification, tandem MS (called MS/MS or MS2) spectra are often collected.
- MS2 methods such as DDA and SWATH-DIA are commonly used

Data Formats

Raw spectra files must be saved in common open-source formats and uploaded individually as separate zip files. LC-MS spectra data is mandatory, while MS2 is optional. There are four open-source formats supported:

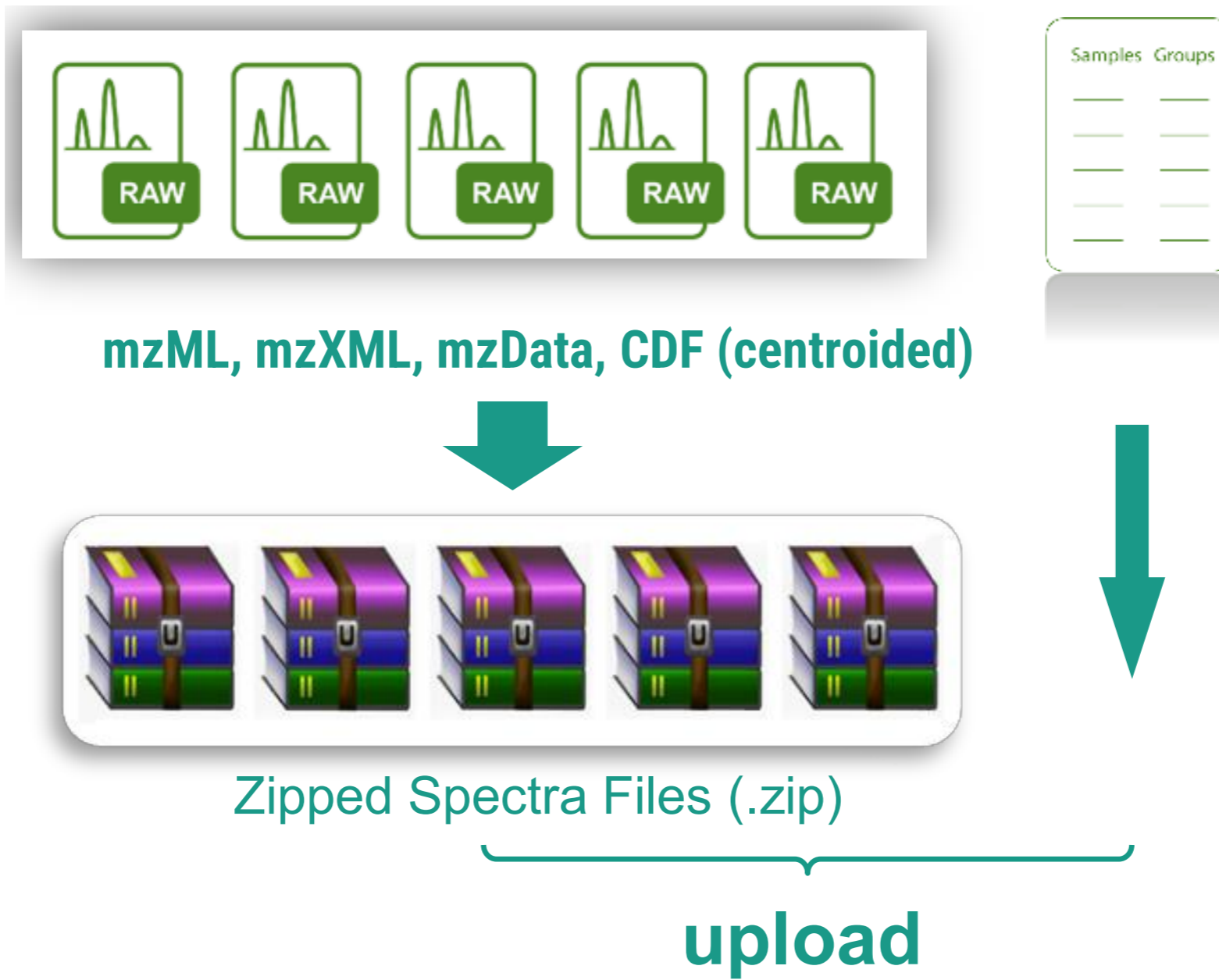
- i. mzML (recommended);
- ii. mzXML;
- iii. cdf/CDF;
- iv. mzData (phasing-out).

Expected Results

LC-MS raw spectra processing module provides user comprehensive results on LC-MS1 features and MS2-based compound identifications:


- i. Compound identification summary table;
- ii. Visualization on MS2 matching pattern and annotation of fragments;

Spectra preparation



Spectra processing and peak calling

Go to MetaboAnalyst (<https://www.metaboanalyst.ca>), and select the module



MetaboAnalyst 6.0 - from raw spectra to biomarkers, patterns, functions and systems biology

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Module Overview

Input Data Type | **Available Modules** (click on a module to proceed, or scroll down to explore a total of 18 modules including **utilities**)

Input Data Type	Available Modules (click on a module to proceed, or scroll down to explore a total of 18 modules including utilities)				
LC-MS Spectra (mzML, mzXML or mzData)			Spectra Processing [LC-MS1 w/wo MS2]		
MS Peaks (peak list or intensity table)		Peak Annotation [MS2-DDA/DIA]	Functional Analysis [LC-MS1]	Functional Meta-analysis [LC-MS1]	
Generic Format (.csv or .txt table files)	Statistical Analysis [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis	Dose Response Analysis
Annotated Features (metabolite list or table)		Enrichment Analysis	Pathway Analysis	Network Analysis	
Link to Genomics & Phenotypes (metabolite list)			Causal Analysis [Mendelian randomization]		

Navigate results

Processing Results:

PCA Scores: Based on all peaks | PCA Loadings: 11433 | Update

View Type: Joint view | Main Background: White | Inset Background: Black | Node Style: Specify | Ticks: Show

Legend: Naive (red), QC (blue), Semi_immune (green)

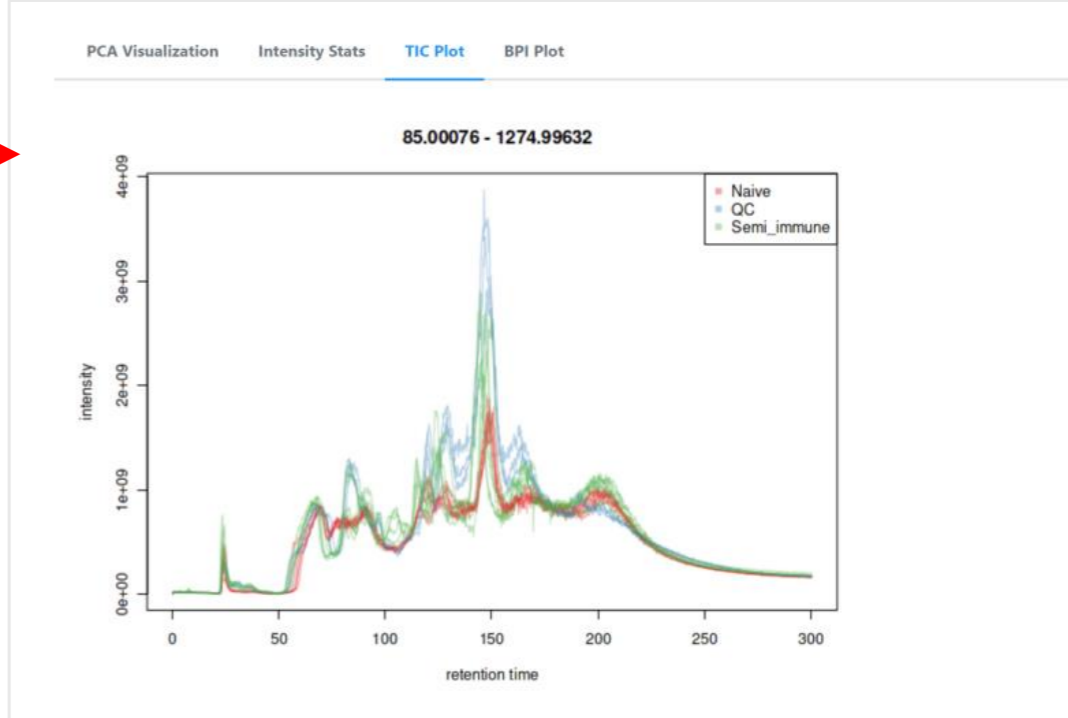
PC2 (26.8%) | PC3 (6.2%)

Result Summary | Spectra / Sample Table | Feature / Peak Table

Raw Spectra Processing Result Summary:
MetaboAnalyst has finished raw spectra processing with OptiLCMS (1.1.0):
There are 15 samples of 3 groups (Naive, QC, Semi-immune) included for processing!
Total of 11433 features have been detected and aligned across the whole sample list.
The mass deviation of this study was estimated/set as 5 ppm.
5228 features (45.72%) have been annotated as isotopes.
5085 features (44.47%) have been annotated as adducts.
346 unique formulas have been matched to HMDB database.

Try to use these functionalities to switch the PCA view, compute ellipse, and download the result figures.

Explore other graphical summaries of the spectral processing results here.

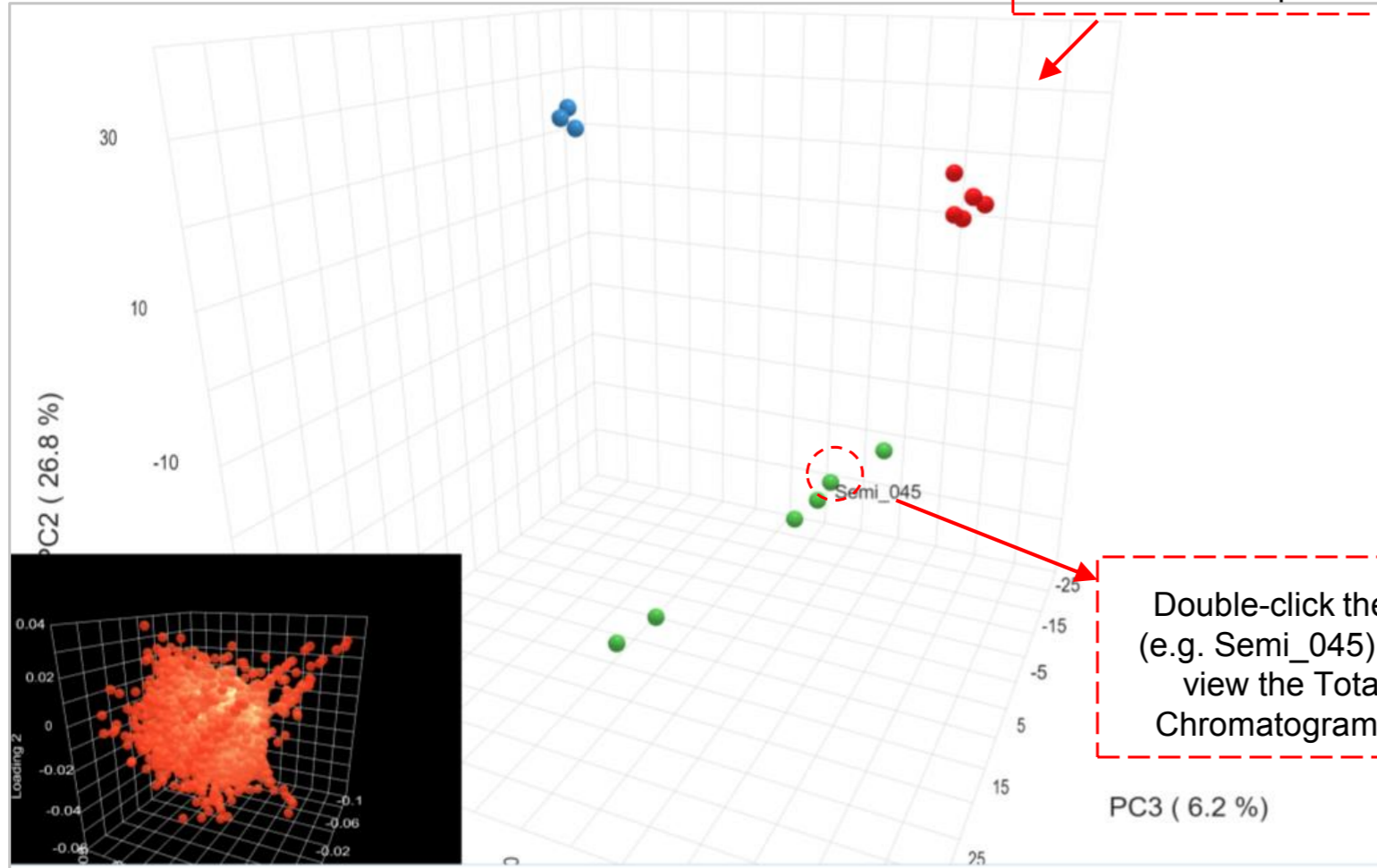


Spectra processing results are visually summarized in 3D PCA view, with all samples displayed in score plot, and all features in loading plot.

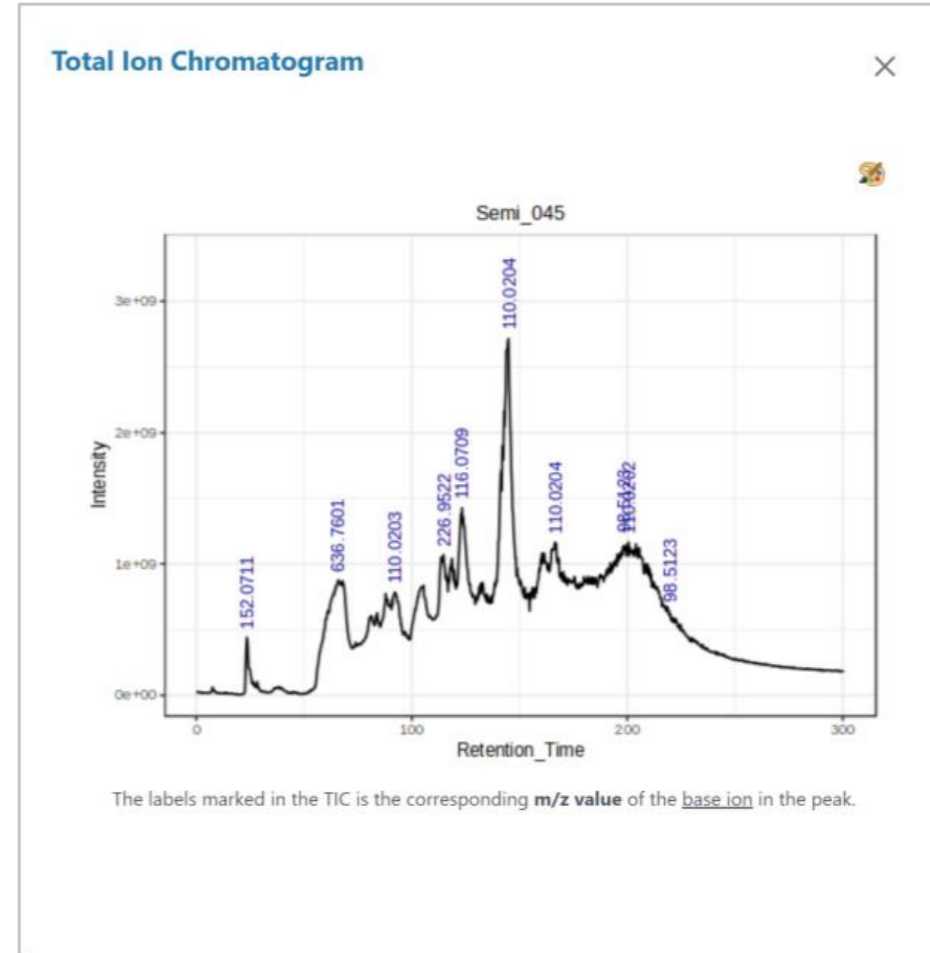
Detailed information including samples and features are summarized at the bottom panel.

Navigate results

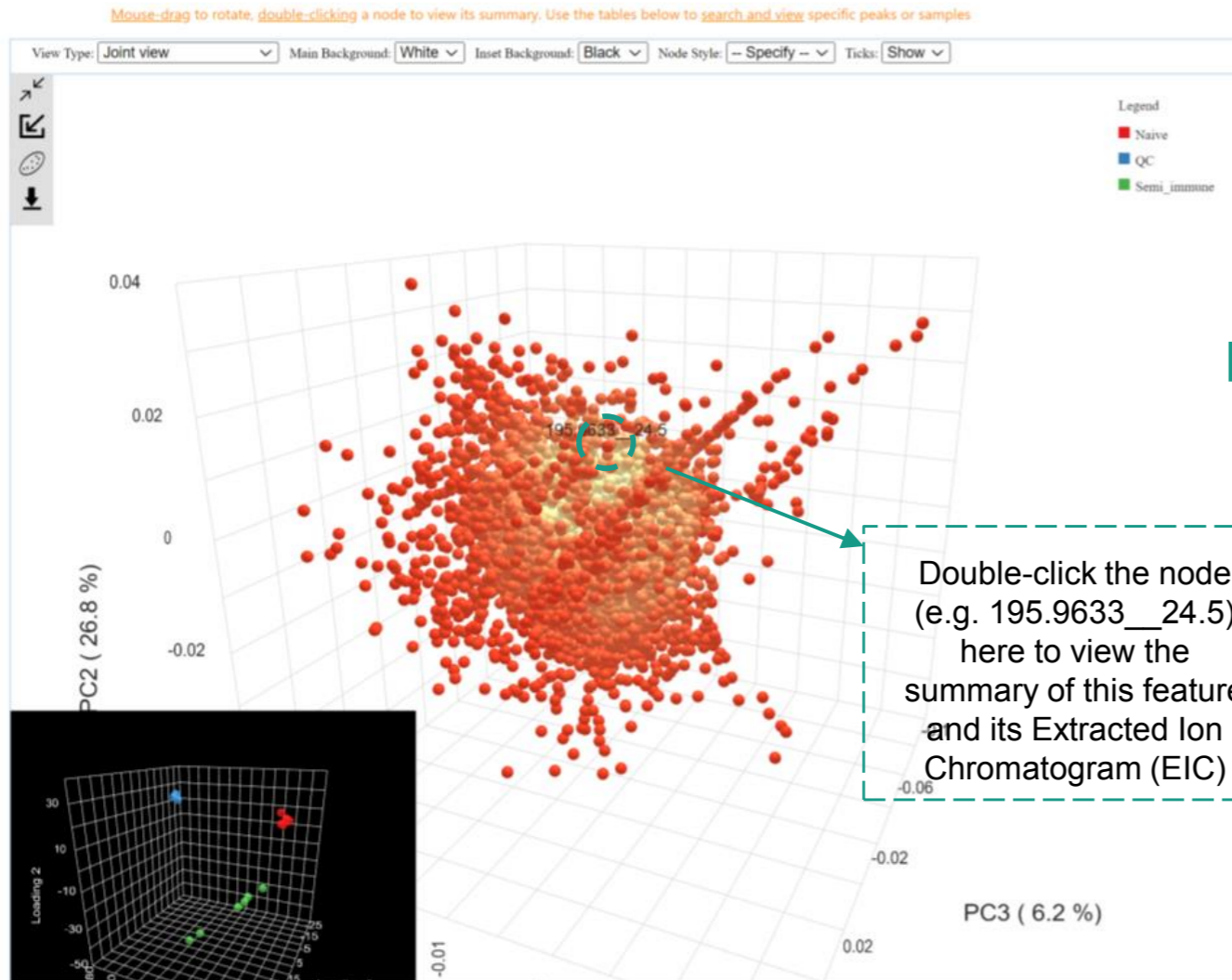
User could use their mouse to scroll and zoom in/out this score plot



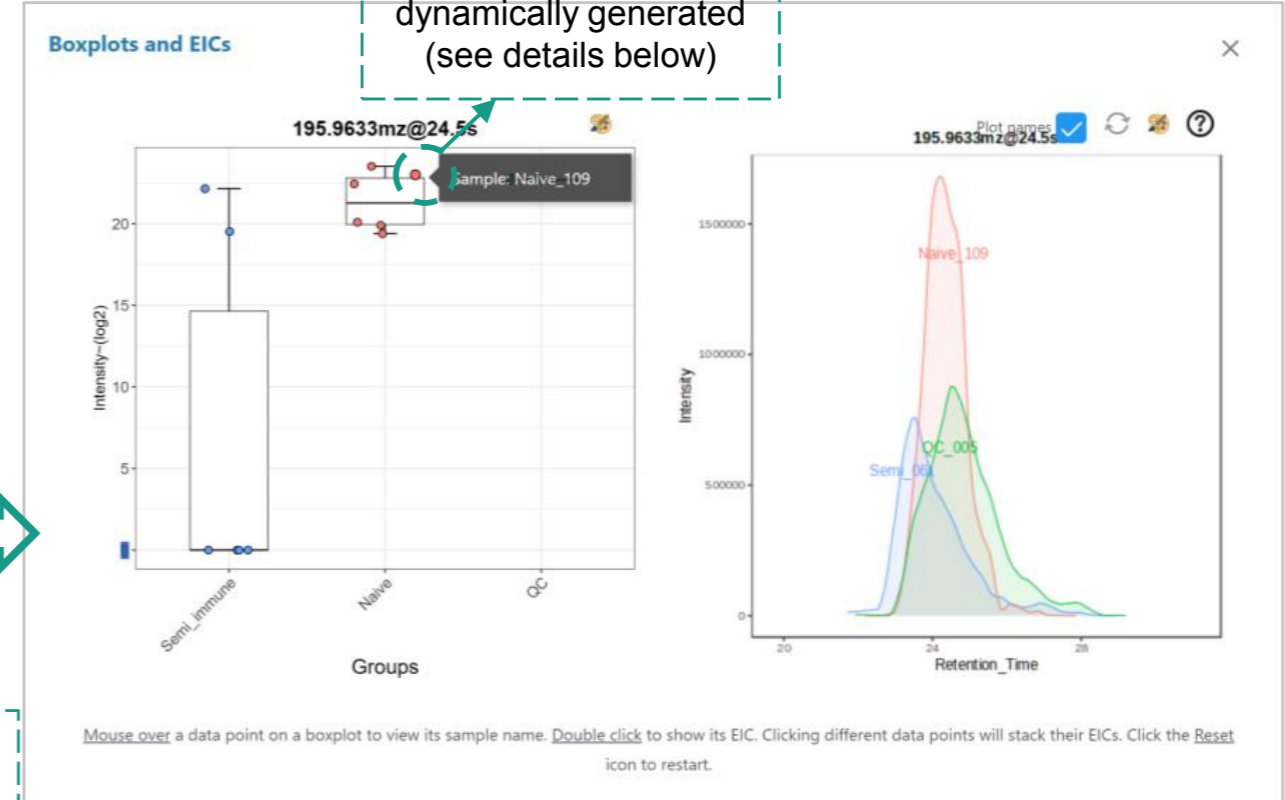
Double-click the node (e.g. Semi_045) here to view the Total Ion Chromatogram (TIC).



Navigate results



Double-click the node (e.g. 195.9633_24.5) here to view the summary of this feature and its Extracted Ion Chromatogram (EIC)



This EIC plot can be dynamically generated (see details below)

How to use the dynamic EIC generation,

1. **Select MS feature.** From the PCA loading plot, double click the node of interest. Then a dialog will be pop-up automatically;
2. **View the boxplot and click the sample node:** The intensity of all samples are statistically summarized as a boxplot. Double any node to add the EIC of the sample to the right panel. By clicking multiple samples, you can dynamically add more layers into the EIC panel.
3. **Reset the EIC:** If you want to reset the EIC plot, click the reset circle to empty the EIC panel.

Navigate results

[Result Summary](#) [Spectra / Sample Table](#) [Feature / Peak Table](#)

Raw Spectra Processing Result Summary:
MetaboAnalyst has finished raw spectra processing with OptiLCMS (1.1.0):
There are 15 samples of 3 groups (Naive, QC, Semi_immune) included for processing!
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The mass deviation of this study was estimated/set as 5 ppm.
5228 features (45.72%) have been annotated as isotopes.
5085 features (44.47%) have been annotated as adducts.
346 unique formulas have been matched to HMDB database.
2813 potential compounds have been matched to HMDB database.



[Result Summary](#) [Spectra / Sample Table](#) [Feature / Peak Table](#)

Click the “**View**” icon to view the corresponding Total Ion Chromatogram of the sample

Spectra ↑↓	Group ↑↓	Peaks No. ↑↓	Missing (%) ↑↓	RT Range	m/z Range	View
Semi_157	Semi_immune	5850	48.83	1.91~296.45	85.048~1264.1306	
Naive_007	Naive	4465	60.95	1.91~297.5	85.0844~1274.5201	
Naive_027	Naive	4497	60.67	1.91~297.5	85.0762~1274.5201	
Naive_071	Naive	4076	64.35	1.91~297.5	85.0844~1270.6334	
Naive_109	Naive	4518	60.48	1.91~297.5	85.0844~1270.6334	
Naive_127	Naive	4500	60.64	1.91~297.5	85.048~1274.5201	
Naive_139	Naive	4364	61.83	1.91~297.5	85.0844~1274.5201	
QC_001	QC	5777	49.47	1.91~296.45	85.048~1264.1306	
QC_003	QC	5836	48.95	19.25~296.45	85.048~1264.1306	
QC_005	QC	5636	50.7	19.25~296.45	85.048~1264.1306	
Semi_025	Semi_immune	5634	50.72	1.91~297.5	85.048~1264.1306	

1. **Result Summary:** This summary box is used to summarize the basic information of this job;
2. **Spectra/Sample Table:** This table offers detailed information on all samples (see the example at the right side).
3. **Feature/Peak Table:** This table provides detailed information on all detected features and its putative annotation (see the example from the next page).

Navigate results

Result Summary Spectra / Sample Table **Feature / Peak Table**

- For isotopes/adducts annotation, the matching is based on the m/z value of its corresponding parent ion. Otherwise, it is considered as in the format of the primary ion.
- All compounds/formulas are matched to [HMDB](#) (v5) based on the mass error (ppm value) for raw spectra processing.
- Intensity is average of all samples. Coefficient of variation (CV) is also the summarized based on all samples.
- When group information is provided, p values will be calculated with t-test/ANOVA based on log transformed data.

m/z ↑↓	RT/s ↑↓	Intensity ↑↓	CV (%) ↑↓	P values ↑↓	FDR	Annotations	Putative IDs	View
544.370236354959	38.6911764	1.1206938E7	45.27	6.2481402E-23	0.0			
684.830841124181	91.503288	4.3811566E7	49.65	1.1195928E-22	0.0			
237.170126537048	28.9694562	8.1026999E7	51.62	8.2754042E-22	0.0	M0 M-H-		
293.196509329594	23.9772402	1.1601194E7	38.33	8.1127794E-21	0.0	13C/12C ACN		
336.945587666283	59.710875	3.4089651E7	48.97	1.199339E-20	0.0	M0 M-H-		
238.173669143381	28.4439942	8563085.0	44.38	1.7304435E-20	0.0	13C/12C M-H-		
830.365552376317	72.322668	4.2872149E7	40.62	1.9462206E-20	0.0			
125.060050295032	275.9517	5525526.0	42.88	2.8978219E-20	0.0			

Putative IDs ×

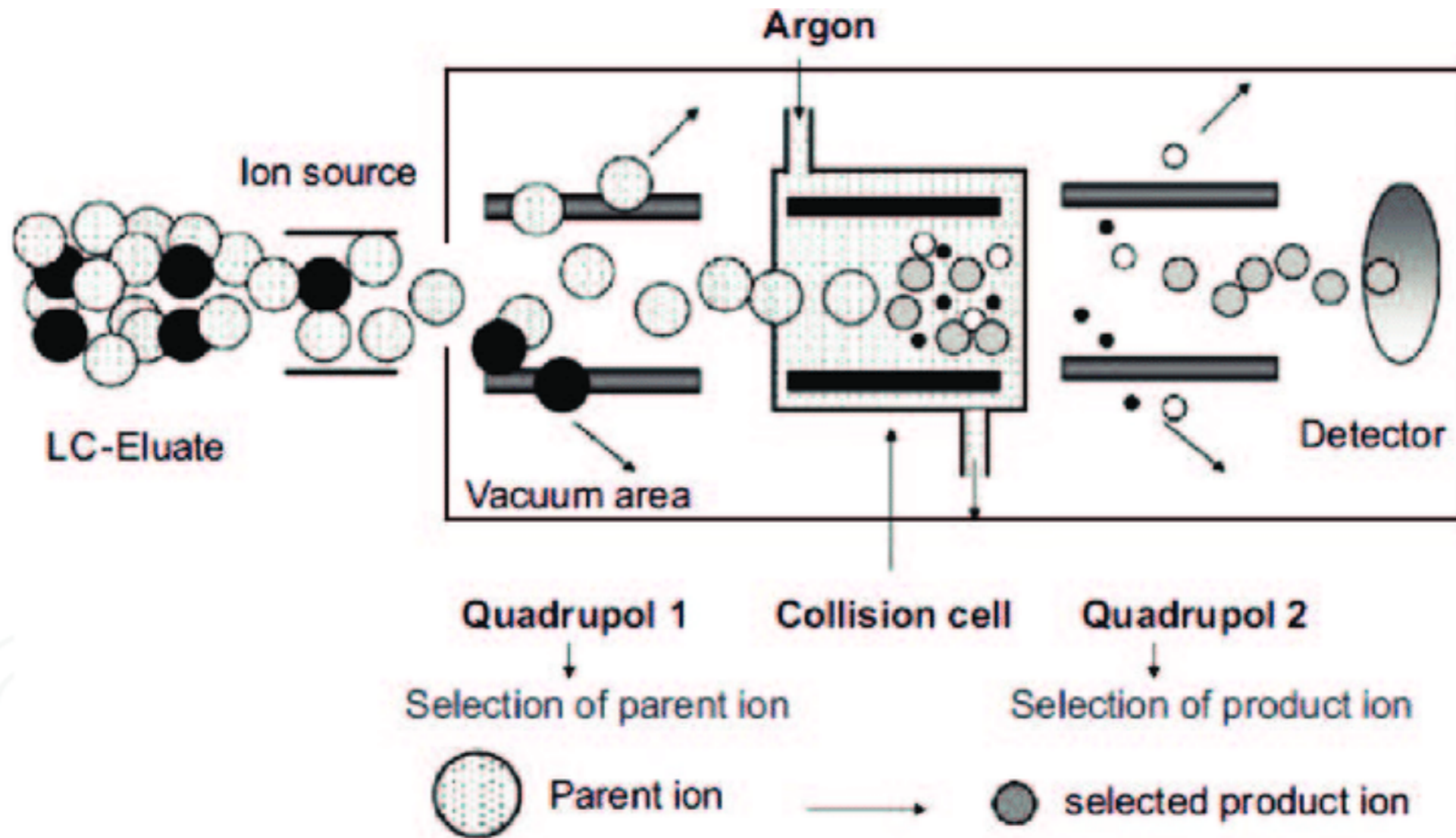
Formulas	Compounds
C15H24O3	1-Hydroxyepiacorone ; Acorusdiol ; 3d->5-Abec-4-11:4-12-diepoxy-3-eudesmanol ; 4R-5S-7R-11R-11,12-Dihydroxy-110-scirovetiven-2-one ; Apotrichodiol ; 6alpha-Carissanol ; alpha-Carissanol ; Epioxyfubimin ; Dihydromyoporone ; Piperolol ; Zedoarondiol ; Hydroxypelenolide ; Toxin FS2 ; Urodienone ; Bisacurone B ; 2,3-Dihydroabscisic alcohol ; 3-Methyl-5-pentyl-2-furanpentanoic acid ; 3-Methyl-5-propyl-2-furanheptanoic acid

Click the **“Putative ID”** icon to view the putative ID results. Please note, this chemical ID is generated based on the MS1 information.

Features without the putative IDs from HMDB database would not show the icon.

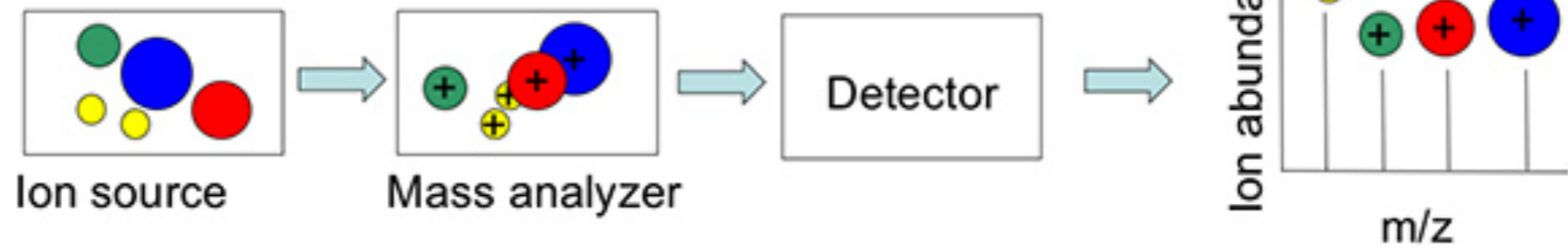
Click the **“View”** icon to start the corresponding dynamic EIC plot panel.

Tandem MS

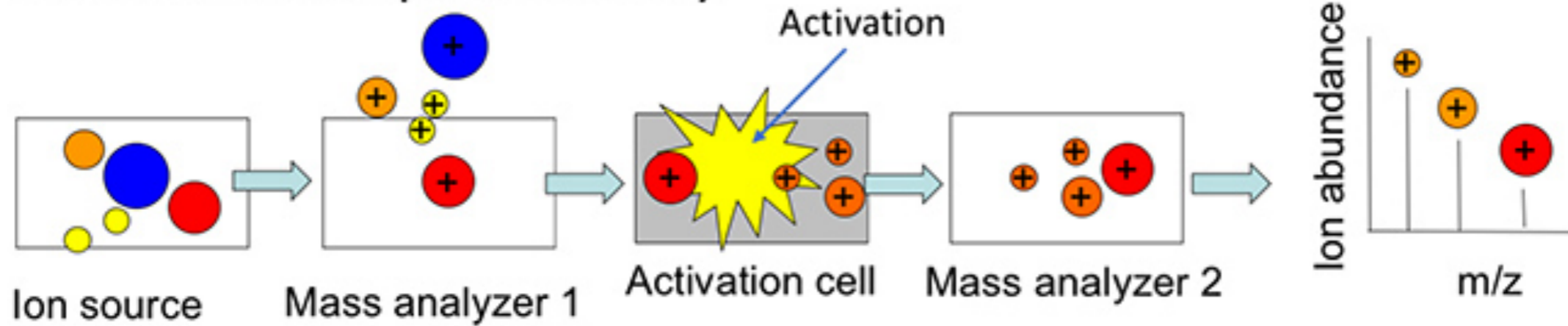


Tandem MS

a) Mass spectrometry




b) Tandem mass spectrometry




Spectra processing and peak calling

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Module Overview

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LC-MS Spectra (mzML, mzXML or mzData)			Spectra Processing [LC-MS1 w/wo MS2]		
MS Peaks (peak list or intensity table)		Peak Annotation [MS2-DDA/DIA]	Functional Analysis [LC-MS1]	Functional Meta-analysis [LC-MS1]	
Generic Format (.csv or .txt table files)	Statistical Analysis [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis	Dose Response Analysis
Annotated Features (metabolite list or table)		Enrichment Analysis	Pathway Analysis	Network Analysis	
Link to Genomics & Phenotypes (metabolite list)			Causal Analysis [Mendelian randomization]		

Spectra processing and peak calling

+ Select

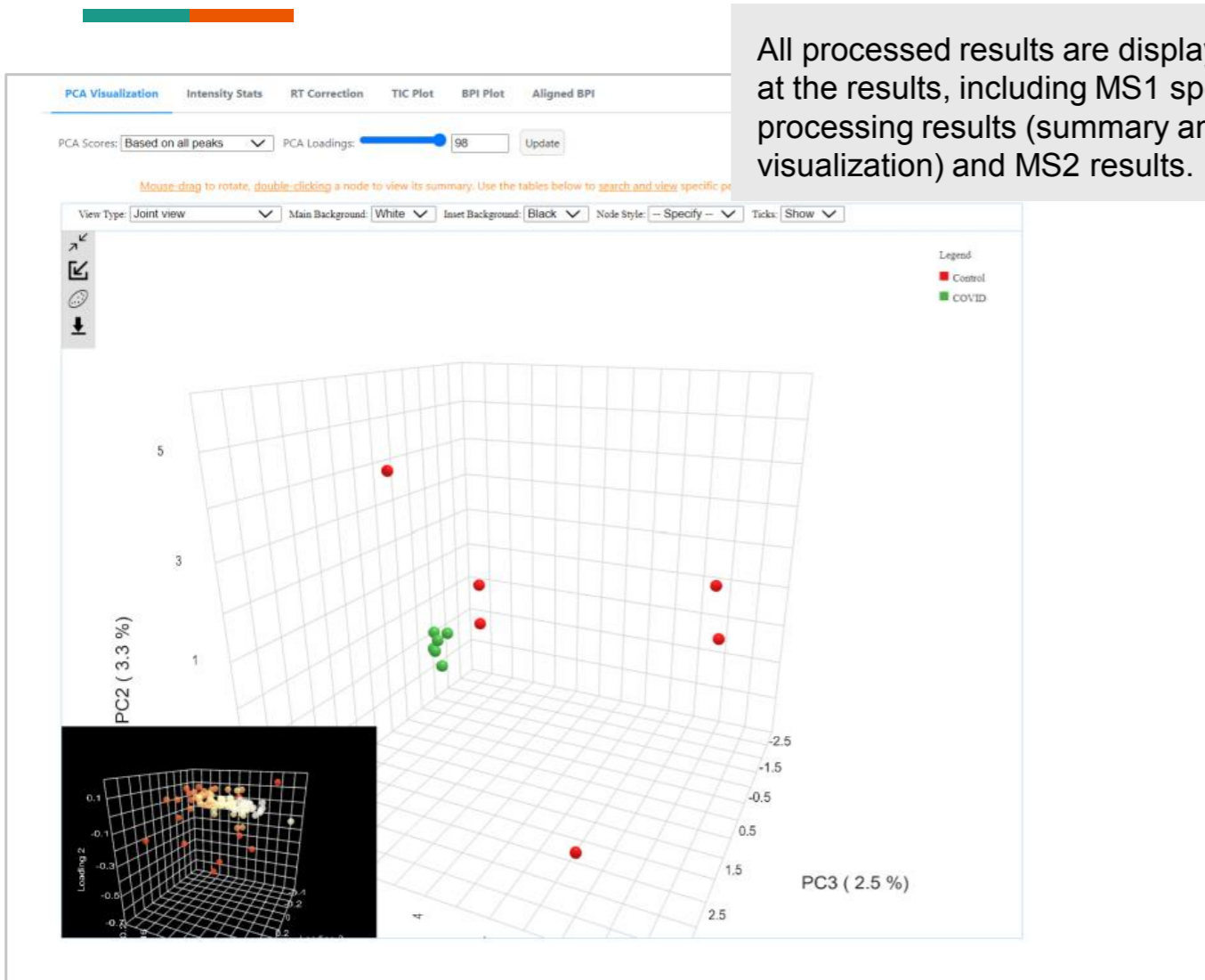
Select Mode: MS1 Only MS1+DDA MS1+SWATH-DIA

For LC-MS1 + SWATH-DIA data processing, you should choose "MS1 + SWATH-DIA"

Reset Proceed

https://new.metaboanalyst.ca/MetaboAnalyst/faces/Share?ID=q2m2bo7wo_12873

Navigate results



All processed results are displayed at the results, including MS1 spectra processing results (summary and visualization) and MS2 results.

Result Summary | Spectra / Sample Table | **Feature / Peak Table** | MS/MS Results

- For isotopes/adducts annotation, the matching is based on the m/z value of its corresponding parent ion. Otherwise, it is considered as in the format of the primary ion.
- All compounds/formulas are matched to HMDB (v5) based on the mass error (ppm value) for raw spectra processing.
- Intensity is average of all samples. Coefficient of variation (CV) is also the summarized based on all samples.
- When group information is provided, p values will be calculated with t-test/ANOVA based on log transformed data.

m/z	RT/s	Intensity	CV (%)	P values	FDR	Annotations	Putative IDs	View
160.8422	79.23	11036.9	46.45	1.5068802E-4	0.01476743			
217.0301	84.55	215276.0	10.02	0.0027741963	0.0659002			
117.0555	138.64	20089.0	25.41	0.0029012625	0.0659002			
96.9598	72.13	38909.9	14.77	0.0036270983	0.0659002			
678.5083	81.66	9218.9	69.89	0.0065294412	0.0659002			
215.0331	84.66	577626.3	8.77	0.0082779721	0.0659002			

MS2 results are summarized in the tab, MS/MS results. (see more details from section 5.4 and 5.5).

Result Summary | Spectra / Sample Table | Feature / Peak Table | **MS/MS Results**

- MS/MS-based compounds identification results are displayed below.
- Similarity of MS/MS are evaluated based on dot-product or spectral entropy methods. Top 5 compounds are listed from high to low (100, perfect match; 0, not matched).
- User could click View button below to view the MS/MS pattern matching results.

Compound	Formula	Matching Score	InchiKey	Database	View
▼ m/z146.0457@74.06sec					
L-Glutamic acid	CSH9NO4	57.16	WHUUTDBJXRKMK-VKHMYHEASA-N	HMDB_experimental	
O-Acetyserine	CSH9NO4	57.16	VZXPDPZARILFQX-BYPYZUCNSA-N	HMDB_experimental	
▶ m/z160.9202@83.59sec					

« 1 » 50

[Download Page](#)

Click "Download Page" to download results

Summary peak calling

- Raw spectra files must be saved in common open-source formats and uploaded individually as separate zip files.
- LC-MS spectra data is mandatory, while MS2 is optional. Upon data uploading, MetaboAnalyst 6.0 automatically validates the status of MS files.
- For SWATH-DIA data, the SWATH window design is automatically extracted from the spectra. If the related information is missing, users will be prompted to enter the window design manually.
- On the parameters setting page, users are given the option to choose the default auto-optimized centWave algorithm or use the *asari* algorithm for LC-MS data processing.
- If MS2 data is included, spectra deconvolution, consensus, and database searching are performed automatically, using the MS features as target list. Once the spectra processing is complete, users can explore both MS and MS2 data processing results.

Functional analysis

Go to MetaboAnalyst (<https://www.metaboanalyst.ca>), and select the module

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Module Overview

Input Data Type	Available Modules (click on a module to proceed, or scroll down to explore a total of 18 modules including utilities)				
LC-MS Spectra (mzML, mzXML or mzData)			Spectra Processing [LC-MS1 w/wo MS2]		
MS Peaks (peak list or intensity table)		Peak Annotation [MS2-DDA/DIA]	Functional Analysis [LC-MS]	Functional Meta-analysis [LC-MS1]	
Generic Format (.csv or .txt table files)	Statistical Analysis [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis	Dose Response Analysis
Annotated Features (metabolite list or table)		Enrichment Analysis	Pathway Analysis	Network Analysis	
Link to Genomics & Phenotypes (metabolite list)			Causal Analysis [Mendelian randomization]		

>> Spectral Processing [LC-MS1 w/wo MS2]

This module allows users to upload raw LC-MS spectra (mzML, mzXML or mzData) to be processed using our optimized workflow based on MetaboAnalystR 4.0 or the

>> Peak Annotation [MS2-DIA/DDA]

This module performs MS2 peak annotation based on a comprehensive list of public databases. Users can either directly enter a two-column peak list containing m/z and

>> Functional Analysis [LC-MS1]

This module accepts high-resolution LC-MS spectral peak data to perform metabolic pathway enrichment analysis and visual exploration based on the [mummichog](#) or [GSEA](#)

Functional analysis

File preparation

Two files need to prepared:

1. **LC-MS1 peak list:** this file should consist of multiple columns containing complete LC-MS1 features. m/z, retention time (rt), and p values are required for accurate functional analysis. Besides, users are recommended to provide t scores column. Please note that this peak list must contain all LC-MS1 features (no matter they are significant or not). Usually, for untargeted metabolomics on a biological sample, the complete features number is over 5,000.
2. **MS2-based compound candidate list:** This file should consist of the MS2-based compound identification results. This table can be in two formats:
 - **Format 1:** A specific column, named as “index” added before the compound candidate columns. The index refers to the corresponding number the LC-MS1 peak list (see example below). Users can provide 3-10 chemical candidate for each MS1 feature;
 - **Format 2:** The number of rows of the two data should be the same and corresponding (see next page).

Functional analysis

File preparation

Header of data is required

	A	B	C	D
1	mz	rt	p.value	
2	139.5311	44.87	5.38E-06	
3	204.056	42.26	2.31E-05	
4	203.1279	784.65	7.5E-05	
5	521.3151	304.9	0.001754	
6	345.1516	577.72	0.002652	
7	250.1777	481.76	0.004474	
8	714.5077	762.3	0.004555	
9	189.0737	53.16	0.004971	
10	307.5487	461.67	0.005336	
11	366.1607	190.66	0.005795	
12	776.3663	782.33	0.005948	
13	486.2957	714.81	0.006051	
14	599.4561	768.32	0.006113	
15	344.2124	512.66	0.006171	
16	492.2939	319.1	0.006195	
17	678.3317	782.33	0.007085	
18	713.422	283.4	0.00759	
19	238.5637	44.38	0.008047	

	A	B	C	D	E	F	G	H
1	Index	InchiKey_1	InchiKey_2	InchiKey_3	InchiKey_4	InchiKey_5		
2	2	MGSKVZVWGBWPBTF	TZJAEGLMLTGRJ-U	OVRNDRQMDRJTHS	NA	NA		
3	8	FWULQXYJOANGSS	JDVGAQPNNXQDW	BJTZATWAPRKXBV-U	LIWMQSWFLXEGMA	VEQOALNAAJBPNY-U	HFFFAOYSA-N	
4	10	LUALTOATIOESLM-U	NA	NA	NA	NA		
5	42	WIYUZYBFCWCCQJ	HGSOUJPIFSDBKJ-O	NA	NA	NA		
6	44	HOVAGTYPDGVJG	RYVLZVUVIJVGH-UI	NA	NA	NA		
7	56	FQZPXSRCOWUEI	YRQOXUDKDCXME	YRQOXUDKDCXME	OTGQIQTPXJQRG	NA		
8	68	RYVLZVUVIJVGH-UI	PXQPEWDEAKTCGB	KSEBMYQBYZTDHS	QURCVMIEKCOAJU	NA		
9	70	HJMQDJPMQIHLPB	AMDPNECWKZZEBQ	IRZVHDLBAYNPCT-U	NA	NA		
10	74	YEJYLHKQOBOSCP	OKJCFMUGMSVJBG	NPJICTMALKLTFW-C	NA	NA		
11	94	XJLSEXAGTJCILF-UH	JWYOAMOZLZXDER	NILQLFBWTXNUOE	PJDFLNIOAUIZSL-UH	DDSLGZOYEPKPSJ-UH	HFFFAOYSA-N	
12	112	DKLKMKYDWHYZTD	SSEBTPPFLCUMN-I	MTFCPNHRBINLRQ	IGLHHSKNBDXCEY	NA		
13	123	IEPGNWMPIFDND	IEPGNWMPIFDND	WECGLUPZRHILCT	NA	NA		
14	129	HXFOXFJUNFFYMO-I	NA	NA	NA	NA		
15	141	OTCCIMWXFLJLIA-B	NXQJDVBMRCQKQ	NRNCYVBFDDJNE	POJWUDADGALRAB	NA		
16	160	IZYCZPAFZQFMCQ-U	NVEPPWDVLBMNME	GHOKWGTUZJEAQD	WTDRDQBEARUVNC	JXXCENBLGFBQJM-UH	HFFFAOYSA-N	
17	161	LUINDDOUWHRIPW	DFQOXFIPAAMFAU-U	NA	NA	NA		
18	186	VLSMHEGGTFMBBZ	NA	NA	NA	NA		
19	198	IRZTUXPRIUZXPMP-UI	RTIXKCRFFJGDFG-U	LCAWNFIKMLXZPQ	NA	NA		
20	205	XUQWWIFROYJHCU	SEKYBDYVXDAPY-A	SEKYBDYVXDAPY-U	IDTCGADOYRIRKB-U	NA		
21	206	CMRNMZJAUFXOQF	FMMOAYVCKXGMF	XSXIVVZCUAHUJO-I	XSXIVVZCUAHUJO-L	XUJWOMMOEHPFP-UT	JQPWESSA-N	

LC-MS1 peak list

LC-MS2-based compound identification results list

Functional analysis

File preparation

The number of rows of the two data should be the same and corresponding to each other;
If there are no MS2-based compound identification results, please fill **NA** in the rows.
You can provide 3-10 chemical candidate for each MS1 feature.

	A	B	C	D	E
1	mz	rt	t.score	p.value	mode
2	52.99813	1202.7	1.4439	0.165	positive
3	53.00038	1295.16	2.474	0.0193	positive
4	53.00228	1291.68	2.7635	0.0094	positive
5	53.00296	1273.08	3.1435	0.0037	positive
6	53.00432	1264.08	2.7164	0.0106	positive
7	59.04659	1076.76	2.1416	0.042	positive
8	59.04682	1106.76	0.9601	0.3477	positive
9	59.04705	992.94	1.3661	0.1827	positive
10	59.04716	871.5	1.6124	0.1168	positive
11	59.04739	1259.94	0.2004	0.8432	positive
12	59.04752	1129.98	0.5856	0.5635	positive
13	59.04757	677.64	0.2032	0.8408	positive
14	59.04778	1002.6	0.1681	0.8682	positive
15	59.048	1302.06	2.0595	0.0483	positive
16	59.04802	968.1	0.2093	0.8358	positive
17	59.04805	1184.76	0.852	0.402	positive
18	59.04829	1122.66	0.2977	0.7684	positive
19	59.04842	865.98	0.387	0.7017	positive
20	59.04854	1069.5	0.8101	0.428	positive
21	59.04856	1033.62	1.0973	0.2836	positive

LC-MS1 peak list

	A	B	C	D	E
1	Inchikey1	Inchikey2	Inchikey3	Inchikey4	Inchikey5
2	NA	NA	NA	NA	NA
3	NA	NA	NA	NA	NA
4	NA	NA	NA	NA	NA
5	NA	NA	NA	NA	NA
6	NA	NA	NA	NA	NA
7	NA	NA	NA	NA	NA
8	XUWHAWMETYGRKENYEZZYQZRQDLEH-I	SECXISVLQFMRJM-U	NA	NA	NA
9	XUWHAWMETYGRKENYEZZYQZRQDLEH-I	SECXISVLQFMRJM-U	NA	NA	NA
10	XUWHAWMETYGRKENYEZZYQZRQDLEH-I	SECXISVLQFMRJM-U	NA	NA	NA
11	PAFZNILMFXTMIY-UI	NA	NA	NA	NA
12	PAFZNILMFXTMIY-UI	NA	NA	NA	NA
13	NA	NA	NA	NA	NA
14	DYDCUQKUCUHJBH	KYCJNUIHWNJNCT-	KHIQJCVGWNEQMI-	DYDCUQKUCUHJBH	NA
15	NA	NA	NA	NA	NA
16	NA	NA	NA	NA	NA
17	NA	NA	NA	NA	NA
18	NA	NA	NA	NA	NA
19	NA	NA	NA	NA	NA
20	NUVWVUPJCXRIIW-I	KFDVPUJYSDEJTH-U	KGIGUEBEKRSTEW-I	YAXKTBLXMTYWDQ-	NA
21	NUVWVUPJCXRIIW-I	KFDVPUJYSDEJTH-U	KGIGUEBEKRSTEW-I	YAXKTBLXMTYWDQ-	NA

LC-MS2-based compound identification results list

Functional analysis

Please upload your data

This module supports functional analysis of untargeted metabolomics data generated from high-resolution mass spectrometry (HRMS). The basic assumption is that putative annotation at individual compound level can collectively predict changes at functional levels as defined by **metabolite sets** or **pathways**. This is because changes at group level rely on "collective behavior" which is more tolerant to random errors in compound annotation as demonstrated by [Li et al.](#) To use this approach,

- The input peak list or peak table must contain the complete data, not just significant data - we need the complete data to estimate the null model (background);
- [Required] Feature or peak names must be their numeric mass (m/z) values for putative annotation;
- [Optional] You can also provide retention time (RT) to further improve peak annotation

A peak list profile A peak intensity table **MS Peak and Annotation lists**

For functional analysis with LC-MS1 + MS2, we should use "MS Peak and Annotation lists"

Upload peak and compound lists

Ion Mode:

Negative Mode

Mass Tolerance (ppm):

5.0

(editable)

Retention Time:

Not present

Annotation ID type:

InchiKeys

Enforce Primary Ions (V2 only):



Peak Data File:

+ Choose

Annotation File:

+ Choose

Parameters on the data and MS instrument need to be specified here. Multiple MS2-based compound ID are supported.

Click "Choose" buttons to upload either peak list or annotation list respectively.

Submit

Click "Submit" to upload your data

Annotation ID type:

InchiKeys

Enforce Primary Ions (V2 only):

Peak Data File:

Annotation File:

Submit

InchiKeys

HMDB ID

PubChem CID

PubChem SID

SMILES

Functional analysis

Data Integrity Check:

- Checking sample names - spaces will be replaced with underscore, and special characters will be removed;
- Checking the class labels - at least three replicates are required in each class.
- The data (except class labels) must not contain non-numeric values.
- If the samples are paired, the pair labels must conform to the specified format.
- The presence of missing values or features with constant values (i.e. all zeros).

Data processing information:

Checking data content ...passed.

A total of 7340 m/z features were found in your uploaded data.

5 compounds found in your uploaded data.

The instrument's mass accuracy is **5** ppm.

The instrument's analytical mode is **positive**.

The uploaded data contains **3** columns.

The column headers of uploaded data are **m.z, p.value, r.t**.

The range of m/z peaks is trimmed to 50-2000. **0** features have been trimmed.

A total of 7340 input m/z features were retained for further analysis.

A total of 1455 InchiKeys Compounds included.

Edit Groups

Missing Values

▶ Proceed

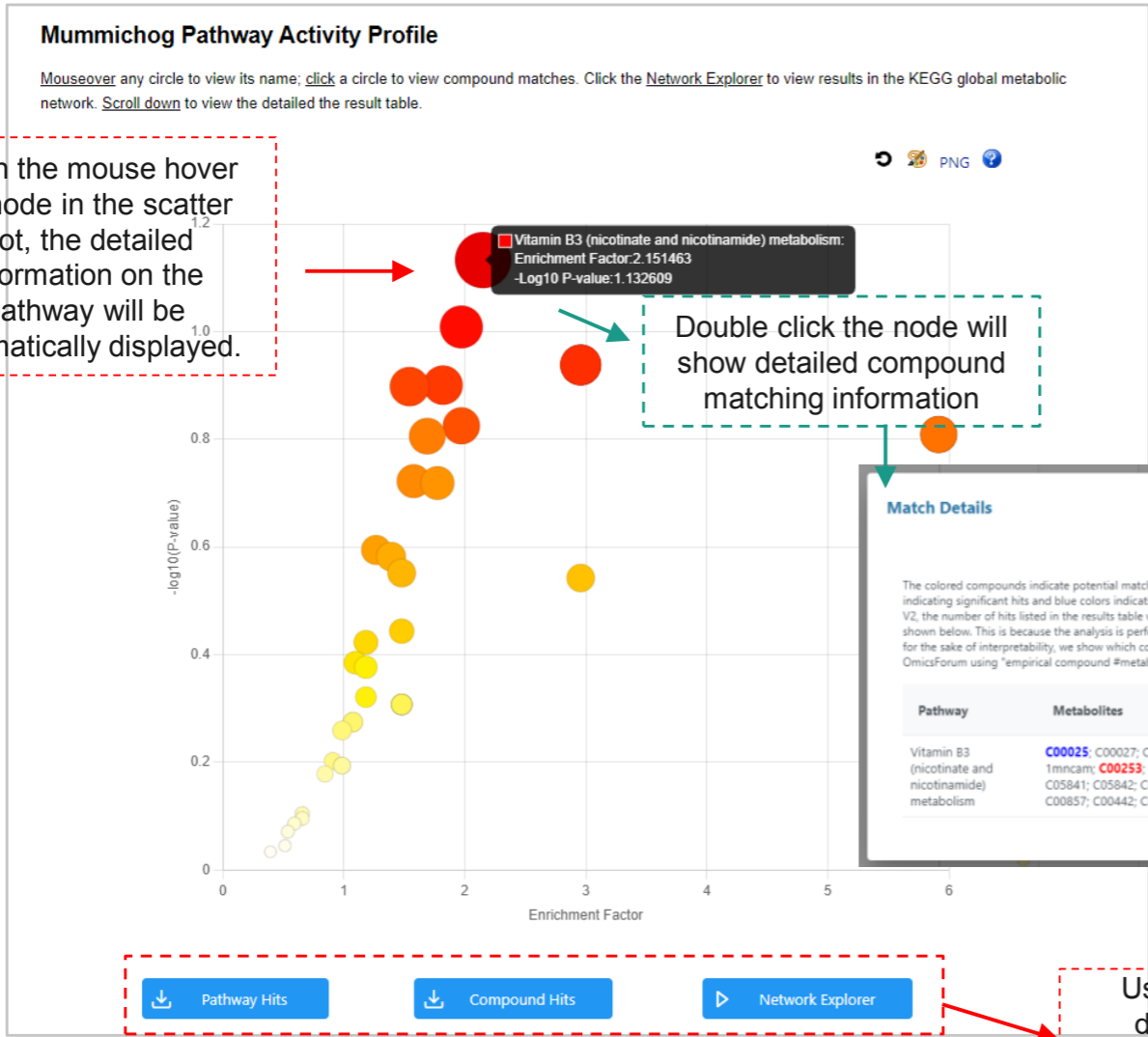
MetaboAnalyst could process your data and do an integrity check at first. The integrity check results are summarized here.

Click "**Proceed**" button to continue.

Navigate results

All pathway enrichment results are summarized in the result table

When the mouse hover the node in the scatter plot, the detailed information on the pathway will be automatically displayed.



Double click the node will show detailed compound matching information

Click the "View" link to see the detailed matching information.

Detailed result table

Mouse over the [Help](#) icon to find more information on each columns

Pathway Name	Total	Hits (all)	Hits (sig.)	Expected	P(Fisher)	P(Gamma)	Details
	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	
Vitamin B3 (nicotinate and nicotinamide) metabolism	28	9	4	1.8592	0.073687	7.9925E-4	View
Histidine metabolism	33	9	4	2.11108	0.1008	8.9292E-4	View
Vitamin B9 (folate) metabolism	33	3	2	0.07606	0.11538	9.6619E-4	View
Fructose and mannose metabolism	33	6	2	0.67606	0.11538	9.6619E-4	View
Ascorbate (Vitamin C) and Aldarate Metabolism	29	3	2	0.67606	0.11538	9.6619E-4	View
Linoleate metabolism	46	13	6	2.1972	0.12579	0.0010133	View
metabolism	114	27	6	3.8873	0.12656	0.0010169	View
	19	7	3	1.5211	0.14969	0.0011306	View
	20	1	1	0.16901	0.15534	0.0011604	View
(min)	9	1	1	0.16901	0.15534	0.0011604	View
ne	4	2	2	0.16901	0.15534	0.0011604	View
metabolism	94	13	4	2.3662	0.15646	0.0011664	View
d threonine	88	14	4	2.5352	0.18967	0.0013597	View
Carnitine shuttle	72	14	3	1.6901	0.19118	0.0013692	View
Tryptophan metabolism	94	25	6	4.7324	0.25451	0.0018401	View
Prostaglandin formation from arachidonate	78	30	4	2.8732	0.26188	0.001905	View

↓ Pathway Hits ↓ Compound Hits ▶ Network Explorer

User could download the results directly here or click "Network Explorer" to explore the results from Global Network view (see next page)