MetaboAnalyst 5.0

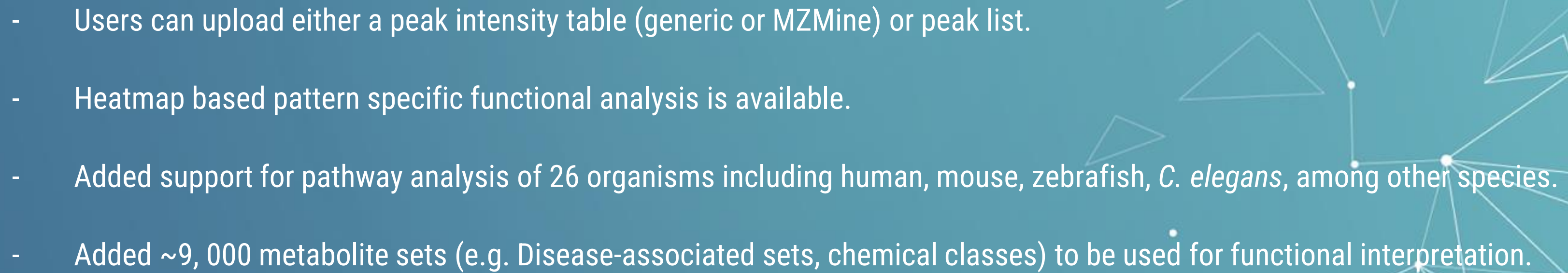
A Web-based Tool for streamlined metabolomics data analysis

2022.07.12

2. Functional Analysis

The **Functional Analysis** module of MetaboAnalyst has undergone several major updates since it's introduction in Version 4. First, it includes a modified Gene Set Enrichment Analysis method, which considers the overall ranks of uploaded peaks and is capable of detecting more subtle and consistent changes than the original mummichog algorithm (Li et al. 2013). Second, it supports the inclusion of retention time when performing functional analysis to increase the confidence and robustness of putative compound annotation. Finally, MetaboAnalyst 5.0 has included an interactive heatmap visualization of a user's peak intensity table to help users perform functional interpretation of manually identified patterns of interest.

Other Highlights:



- Users can upload either a peak intensity table (generic or MZMine) or peak list.
- Heatmap based pattern specific functional analysis is available.
- Added support for pathway analysis of 26 organisms including human, mouse, zebrafish, *C. elegans*, among other species.
- Added ~9, 000 metabolite sets (e.g. Disease-associated sets, chemical classes) to be used for functional interpretation.

2.0 Knowledge & Background

- Mass spectrometry based untargeted metabolomics traditionally require metabolites to be identified before any biological meaning can be drawn from the data. Metabolite identification is a challenging and low throughput process, therefore becomes the bottleneck of the filed. Li et al. report here a novel approach to predict biological activity directly from mass spectrometry data without a priori identification of metabolites by unifying network analysis and metabolite prediction under the same computational framework. (version 1)

- The algorithm has been further enhanced to version 2 by considering the retention time information for more accuracy by introducing empirical compounds. Empirical Compounds are intermediaries between m/z features and compounds. The steps for how they are formed are as follows:

First, all m/z features are matched to potential compounds considering different adducts. Then, per compound, all matching m/z features are split into Empirical Compounds based on whether they match within an expected retention time window. The retention time window (in seconds) is calculated as the maximum retention time * 0.02. This results in the initial Empirical Compounds list.

Next, Empirical Compounds are merged if they have the same m/z, matched form/ion, and retention time. This results in the merged Empirical Compounds list.

Then, if primary ions are enforced, only Empirical Compounds containing at least 1 primary ion are kept. Primary ions considered are 'M+H[1+]', 'M+Na[1+]', 'M-H2O+H[1+]', 'M-H[-]', 'M-2H[2-]', 'M-H2O-H[-]', 'M+H [1+]', 'M+Na [1+]', 'M-H2O+H [1+]', 'M-H [1-]', 'M-2H [2-]', and 'M-H2O-H [1-]'. This results in the final Empirical Compounds list.

Finally, pathway libraries are converted from "Compound" space to "Empirical Compound" space. This is done by converting all compounds in each pathway to all Empirical Compound matches. Then the mummichog/GSEA algorithms work as before to calculate pathway enrichment.

2.1 Start Functional Analysis

MetaboAnalyst 5.0 - user-friendly, streamlined metabolomics data analysis

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Module Overview

Click here to start

Input Data Type	Available Modules (click on a roll down for more details)					
Raw Spectra (mzML, mzXML or mzData)			LC-MS Spectra Processing			
MS Peaks (peak list or intensity table)			Functional Analysis	Functional Meta-analysis		
Annotated Features (compound list or table)		Enrichment Analysis	Pathway Analysis	Joint-Pathway Analysis	Network Analysis	
Generic Format (.csv or .txt table files)	Statistical Analysis [one factor]	Statistical Analysis [metadata table]	Biomarker Analysis	Statistical Meta-analysis	Power Analysis	Other Utilities

2.2 Starting from a list

From peak list to pathways

2.2.1 Peak Uploading – peak list

TIP1 : Multiple examples are provided here. Please try to download one and follow the style of the example rigorously. Please make sure that the list header is consistently same as the example.

Upload
Processing
Set parameter
View result
Download
Exit

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**

1. Switch the different uploading data type from here (peak list or table)

Upload a peak list file

Ion Mode: Negative Mode

Mass Tolerance (ppm): 5.0 (editable)

Retention Time: Not present

Ranked by (1 column only): P values / T scores

Enforce Primary Ions (V2 only):

Data File: Choose

2. Set parameters (mass error and ion mode) based your instrument

Submit

3. Click submit to continue

Try our example datasets

	Data	Format	
◉	IBD	Three columns (m.z, p.value, t.score)	…trols) obtained using a Q-Exactive Plus Orbitrap (negative ion mode) from the Integrative Human Microbiome Project (iHMP).
○	IBD 2	Four columns (m.z, p.value, t.score, rt)	Same as above

2.2.2 Data Integrity Check

Upload
Processing
Data check
Set parameter
View result
Download
Exit

Data Integrity Check:

1. Checking the class labels - at least three replicates are required in each class.
2. If the samples are paired, the pair labels must conform to the specified format.
3. The data (except class labels) must not contain non-numeric values.
4. The presence of missing values or features with constant values (i.e. all zeros).

Data processing information:

Checking data content ...passed.

A total of 4187 m/z features were found in your uploaded data.

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

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

The uploaded data contains **3** columns.

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

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

A total of 4187 input mz features were retained for further analysis.

Edit Groups | Missing Values | Proceed

1. Check **Data Integrity Result** to make sure correct

2. Click **Proceed** to continue

2.2.3 Set Parameters

Upload

Processing

Data check

Exit

Set corresponding parameters/Library

Specify analysis parameters:

Algorithms	☑ Mummichog P-value cutoff: 0.2 (default top 10% peaks) ☐ GSEA (using the overall rank based on t.score)
Visual analytics:	◉ Scatter plot - test significant peaks ○ Heatmaps - test peaks in a visual pattern (good for multiple groups)
Advanced options	Edit Currency Metabolites Edit Adducts

Select a pathway library: *(KEGG pathway info were obtained in Oct. 2019)*

Mammals	◉ Homo sapiens (human) [MFN] ○ Homo sapiens (human) [BioCyc] ○ Homo sapiens (human) [KEGG] ○ Mus musculus (mouse) [BioCyc] ○ Mus musculus (mouse) [KEGG] ○ Rattus norvegicus (rat) [KEGG]

Customize the Metabolites

Customize the Adducts

Currency Metabolite Customization

Use the panels below to select metabolites to include as currency:

Available	Include
Acetoacetyl CoA (C00332)	Water (C00001)
Acetyl coenzyme A (C00024)	Proton (C00080)
Adenosine diphosphate (C00008)	Oxygen (C00007)
Adenosine monophosphate (C00020)	NADPH (C00005)
Carbon monoxide (C00237)	NADP (C00006)
Coenzyme A (C00010)	NADH (C00004)
Flavin adenine dinucleotide (C00016)	NAD (C00003)
FADH2 (C00016)	Adenosine triphosphate (C00002)
Guanosine triphosphate (C00044)	Pyrophosphate (C00013)
Guanosine diphosphate (C00035)	Phosphate (C00009)
Guanosine monophosphate (C00144)	Carbon dioxide (C00011)
Hydrogen (C00282)	
Hydrogen peroxide (C00027)	
Carbonic acid (C01353)	

Submit

Adduct Customization

Use the panels below to select adducts to consider:

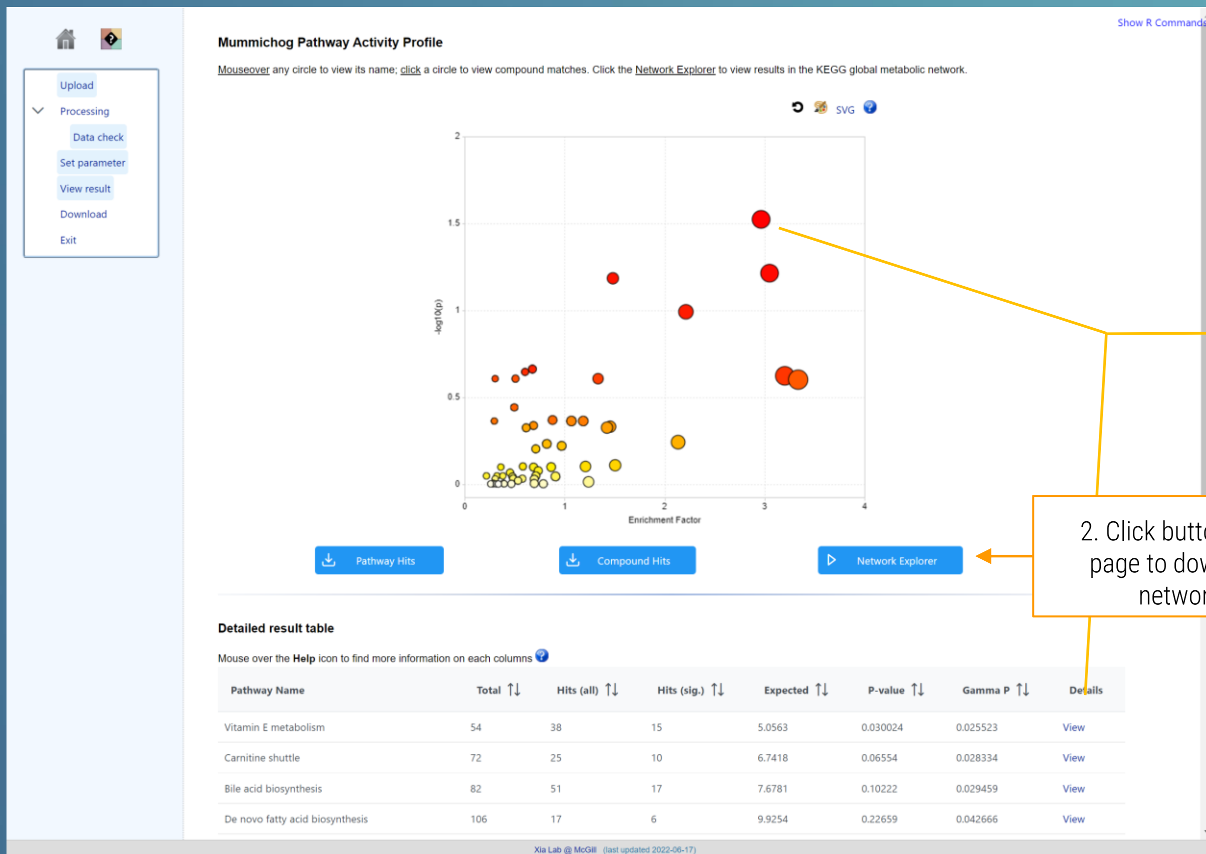
Available	Include
M-3H [3-]	M-H [1-]
M+FA-H [1-]	M-2H [2-]
M+Hac-H [1-]	M-H2O-H [1-]
M+TFA-H [1-]	M-H+O [1-]
2M-H [1-]	M+K-2H [1-]
2M+FA-H [1-]	M+Na-2H [1-]
2M+Hac-H [1-]	M+Cl [1-]
3M-H [1-]	M+Cl37 [1-]
	M+Br [1-]
	M+Br81 [1-]
	M+ACN-H [1-]
	M+HCOO [1-]
	M+CH3COO [1-]
	M(C13)-H [1-]

Submit

TIP1 : You can manually customize the abundant substances as 'Currency Metabolites' and adducts for not considering at the pathway analysis.

TIP2 : Heatmap analysis only works if users upload a peak table If you want to do the heatmap based analysis, please see 6.3.

2.2.4 Pathway analysis results



1. The compounds/empirical compounds hits in this pathway

The colored compounds/empirical compounds indicate potential matches from the user's input, with red colors indicating significant hits and blue colors indicating non-significant hits.

Pathway	Metabolites
Vitamin E metabolism	CE5849; C00024; C00027; CE0812; CE5643; C00020; C00100; CE5848; CE5841; CE5840; CE5843; CE5842; CE5845; CE5721; CE5847; CE5723; CE6000; CE6219; CE5022; C11378; CE5021; CE5844; C02477; CE5838; CE7144; CE7145; C00601; C14153; CE7047; C00010; CE5986; CE5835; CE5837; CE5719; CE5718; CE5850; CE5851; CE5856; CE5855; CE1926; CE5899; CE1924; CE1925; CE5017; CE5846; CE4898; CE1928; CE7101; CE5655; C00088; CE7072; CE7073; CE7074; CE5839

2. Click buttons at the bottom of this page to download results or go the network exploration page

2.3 Starting from a table

2.3.1 Peak uploading – peak table

Upload
Processing
Set parameter
View result
Download
Exit

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 complate 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

Upload a peak intensity table

Ion Mode: Negative Mode
Mass Tolerance (ppm): 5.0 (editable)
Retention Time: Not present
Data Source: Generic
Data Format: Samples in columns
Data File: Choose File No file chosen

Submit

Try our example datasets

Data	Format	
Immune Cell	Generic peak intensity table (… retention time)	…elial cells treated in DSS.
Covid-19	Peak intensity table with retention time	Peak intensity table of COVID-19 global metabolomics study with over 9,000 peaks.

1. Switch to uploading peak intensity table tab

2. Set parameters (mass error and ion mode) based your instrument

3. Click submit to continue

TIP1 : Currently, 2 types of peaks are supported (MetaboAnalyst generic and MZmine style). Users could coerce you table manually to make it applicable here.

2.3.2 Peak uploading – Preprocessing

Data Integrity Check:

1. Checking the class labels - at least three replicates are required in each class.
2. If the samples are paired, the pair labels must conform to the specified format.
3. The data (except class labels) must not contain non-numeric values.
4. The presence of missing values or features with constant values (i.e. all zeros).

Data processing information:

Checking data content ...passed.
Samples are in columns and features in rows.
The uploaded file is in comma separated values (.csv) format.
The uploaded data file contains 12 (samples) by 4353 (peaks(mz/rt)) data matrix.
Samples are not paired.
4 groups were detected in samples.
Only English letters, numbers, underscore, hyphen and forward slash (/) are allowed.
Other special characters or punctuations (if any) will be stripped off.
All data values are numeric.
404 features with a constant or single value across samples were found and deleted.
A total of 1869 (3.9%) missing values were detected.
By default, missing values will be replaced by 1/5 of min positive values of their corresponding variables
Click the **Skip** button if you accept the default practice;
Or click the **Missing value imputation** to use other methods.

Edit Groups | Missing Values | Proceed

Data Filtering:

The purpose of the data filtering is to identify and remove variables that are unlikely to be of use when modeling the data. No phenotype information are used in the filtering process, so the result can be used with any downstream analysis. This step is strongly recommended for untargeted metabolomics datasets (i.e. spectral binning data, peak lists) with large number of variables, many of them are from baseline noises. Filtering can usually improve the results. For details, please refer to the paper by Hackstadt, et al.

Non-informative variables can be characterized in three groups: 1) variables of **very small values** (close to baseline or detection limit) - these variables can be detected using mean or median; 2) variables that are **near-constant values** throughout the experiment conditions (housekeeping or homeostasis) - these variables can be detected using standard deviation (SD); or the robust estimate such as interquantile range (IQR); and 3) variables that show **low repeatability** - this can be measured using QC samples using the relative standard deviation(RSD = SD/mean). Features with high percent RSD should be removed from the subsequent analysis (the suggested threshold is 20% for LC-MS and 30% for GC-MS). For data filtering based on the first two categories, the following empirical rules are applied during data filtering:

- **Less than 250 variables**: 5% will be filtered;
- **Between 250 - 500 variables**: 10% will be filtered;
- **Between 500 - 1000 variables**: 25% will be filtered;
- **Over 1000 variables**: 40% will be filtered;

Please note, in order to reduce the computational burden to the server, the **None** option is only for less than 5000 features. The maximum allowed number of variables is 5000. For power analysis, the max number is 2500 to improve power and to control computing time. Over that, the IQR filter will still be applied to keep only top maximum features, even if you choose None option.

Filtering features if their RSDs are > 25 % in QC samples

None (less than 5000 features)
Interquantile range (IQR)
Standard deviation (SD)
Median absolute deviation (MAD)
Relative standard deviation (RSD = SD/mean)
Non-parametric relative standard deviation (MAD/median)
Mean intensity value
Median intensity value

Submit | Proceed

Normalization overview:

The normalization procedures are grouped into three categories. The sample normalization allows general-purpose adjustment for differences among your sample; data transformation and scaling are two different approaches to make individual features more comparable. You can use one or combine them to achieve better results.

Sample Normalization

None
Sample-specific normalization (i.e. weight, volume) Specify
Normalization by sum
Normalization by median
Normalization by reference sample (PQN) Specify
Normalization by a pooled sample from group Specify
Normalization by reference feature Specify
Quantile normalization

Data transformation

None
Log transformation (generalized logarithm transformation or glog)
Cube root transformation (takes the cube root of data values)

Data scaling

None
Mean centering (mean-centered only)
Auto scaling (mean-centered and divided by the standard deviation of each variable)
Pareto scaling (mean-centered and divided by the square root of the standard deviation of each variable)
Range scaling (mean-centered and divided by the range of each variable)

1. Perform Data Integrity Check

2. Perform Data Filtering

3. Perform Data Normalization

2.3.3 Set parameters

MetaboAnalyst 5.0 - user-friendly, end-to-end metabolomics data analysis

- Upload
- Processing
  - Data check
  - Missing value
  - Data filter
  - Data editor
- Normalization
- Set parameter
- View result
- Metabolic network
- Heatmap viewer
- Download
- Exit

Specify analysis parameters:

Algorithms	☑ Mummichog P-value cutoff: 1.0E-5 (default top 10% peaks) ☐ GSEA (using the overall rank based on t.score)
View options:	◉ Scatter plot (Test significant features) ○ Heatmaps (Test manually selected patterns)
Advanced options	Edit Currency Metabolites Edit Adducts

Select a pathway library: *(KEGG pathway info were obtained in Oct. 2019)*

Mammals	◉ Homo sapiens (human) [MFN] ○ Homo sapiens (human) [BioCyc] ○ Homo sapiens (human) [KEGG] ○ Mus musculus (mouse) [BioCyc] ○ Mus musculus (mouse) [KEGG] ○ Rattus norvegicus (rat) [KEGG] ○ Bos taurus (cow) [KEGG]
Birds	○ Gallus gallus (chicken) [KEGG]
Fish	○ Danio rerio (zebrafish) [KEGG] ○ Danio rerio (zebrafish) [MTF]
Insects	○ Drosophila melanogaster (fruit fly) [KEGG] ○ Drosophila melanogaster (fruit fly) [BioCyc]
Nematodes	○ Caenorhabditis elegans (nematode) [KEGG]
Fungi	○ Saccharomyces cerevisiae (yeast) [KEGG] ○ Saccharomyces cerevisiae (yeast) [BioCyc]

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Set corresponding parameters/Library

TIPs : Most parameters are same as the ones used for processing the peak list, as described in 6.2.3. The only difference is that peak table allow the heatmap based pattern specific functional analysis.

2.3.4 Heatmap based pattern specific analysis

TIPs : The scatter plot and its corresponding functions for peak table uploading is totally same the one of peak list uploading. Please refer to 6.2.4.

MetaboAnalyst 5.0 - user-friendly, end-to-end metabolomics data analysis

- Upload
- Processing
  - Data check
  - Missing value
  - Data filter
  - Data editor
- Normalization
- Set parameter
- View result
- Metabolic network
- Heatmap viewer
- Download
- Exit

Specify analysis parameters:

Algorithms	☑ Mummichog P-value cutoff: 5.0E-5 (default top 10% peaks) ☐ GSEA (using the overall rank based on t.score)
View options:	○ Scatter plot (Test significant features) ● Heatmaps (Test manually selected patterns)
Advanced options	Edit Currency Metabolites Edit Adducts

1. Select **Heatmaps** radio to start !

Select a pathway library: *(KEGG pathway info were obtained in Oct. 2019)*

Mammals	● Homo sapiens (human) [MFN] ○ Homo sapiens (human) [BioCyc] ○ Homo sapiens (human) [KEGG] ○ Mus musculus (mouse) [BioCyc] ○ Mus musculus (mouse) [KEGG] ○ Rattus norvegicus (rat) [KEGG] ○ Bos taurus (cow) [KEGG]
Birds	○ Gallus gallus (chicken) [KEGG]
Fish	○ Danio rerio (zebrafish) [KEGG] ○ Danio rerio (zebrafish) [MTF]
Insects	○ Drosophila melanogaster (fruit fly) [KEGG] ○ Drosophila melanogaster (fruit fly) [BioCyc]
Nematodes	○ Caenorhabditis elegans (nematode) [KEGG]
	○ Saccharomyces cerevisiae (yeast) [KEGG]

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2.3.5 Heatmap based pattern specific analysis - result

This section maybe too complicated to easily understand/follow for beginners, why not watch a **video** first?

Upload ▸ Data Check ▸ Normalization ▸ Library ▸ Heatmap Viewer ▸ Download

Resolution: Medium Colors: navy-white-firebrick Border: Default Cluster peaks: P value Download: --Please Select-- Builder

Overview Select all

Focus View

Enrichment Analysis

Operation Mode: Annotate Extract

Database: KEGG Submit Reset Save

Tip: click a row to view corresponding annotations or to extract

Name	Hits	Sigs	Gamma-p	Color

Tip

By default, peaks are ordered by p-value (t-tests or ANOVA). To perform functional analysis on a peak cluster:

1. From the top menu bar, select a method under **Cluster peaks**;
2. From the left panel, **drag-and-select** a region of interest;
3. From the right panel, set a database and click the Submit button;
4. From the result table, **click a row** to show pathway annotations (color squares);
5. From the heatmap, **click a color square** to show matching details (bottom right)

Ok

Click a row (an enriched pathway) from the result table above to show peak annotations (indicated by color squares next to the heatmap), then click a colored square to show that feature's **annotation details** here.

Read these tips and click **Ok** to start

2.3.6 Heatmap interface introduction

Controller panel to adjust parameters for clustering.

Overview of the peak across the spectrum. Default is clustered based on p value.

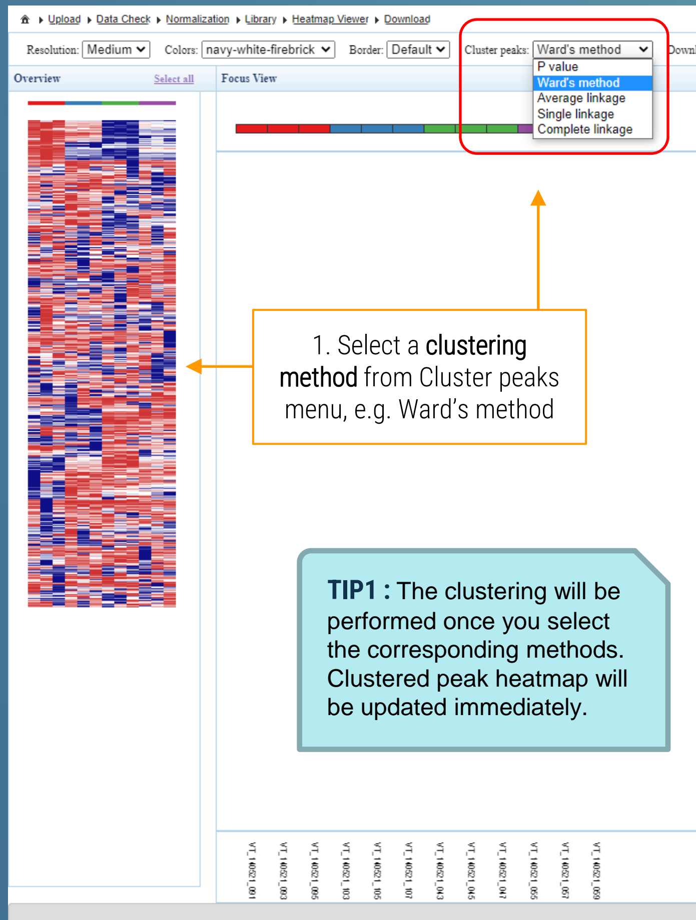
Pattern based **Enrichment analysis** panel.

Focus view of the specific peak pattern from the whole spectrum. Default is the top 50 peaks.

Sample Names View panel.

Dynamic Display panel, used to show the peak/sample information dynamically.

2.3.7 Heatmap peak clustering



Upload Data Check Normalization Library Heatmap Viewer Download

Resolution: Medium Colors: navy-white-firebrick Border: Default Cluster peaks: Ward's method Download: --Please Sele

Overview Select all Focus View

Condition

2. Left click your mouse, don't release and **move your cursor over** a certain area across the spectrum until finish. Then release the left click.

3. The selected specific spectral peaks' **pattern** appears in the focus view panel.

TIP2 : In present example, we selected a consistently down-regulated pattern in 'green' group, and consistently upregulated in 'red' group.

2.3.7 Peak patterns' stitch -1

1. If you want to stitch the different peak patterns. Click the **Builder Button** and the stitch tools appears.

2. Hold the left click of your mouse and move over the whole area as the selected part. The selected part will appear at the bottom panel.

Continue at the next page

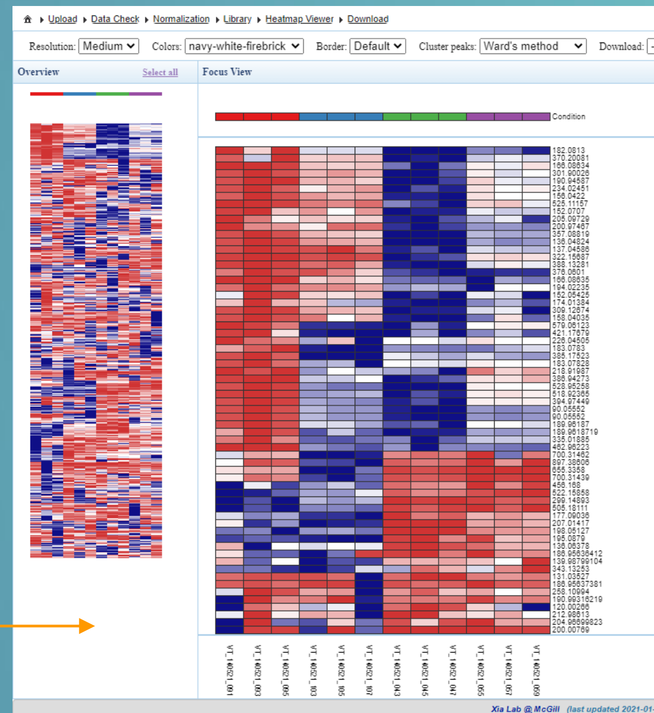
2.3.7 Peak patterns' stitch -2

3. Left click and move your mouse over a new pattern from the overview panel.

4. New pattern appears immediately at the top focus view panel. Hold your left click mouse and move over from this focus view to confirm the area.

5. Newly selected area will be stitched with the previously selected pattern at the bottom focus view.

6. Click To Focus view.



7. The stitched peaks' pattern will be presented at the Focus view.

2.3.8 Enrichment Analysis -1

Upload ▸ Data Check ▸ Normalization ▸ Library ▸ Heatmap Viewer ▸ Download

Resolution: Medium | Colors: navy-white-firebrick | Border: Default | Cluster peaks: Ward's method | Download: --Please Select-- | Builder

Overview | Select all

Focus View

Condition

Enrichment Analysis

Operation Mode: Annotate / Extract

Database: KEGG | Submit | Reset

Tip: *click a row to view corresponding annotation*

Name	Hits	Sigs	
Nicotinate and nicotinamide	4	4	
Phenylalanine metabolism	6	4	
Tyrosine metabolism	4	3	
Aminoacyl-tRNA biosynthes	4	3	
Glycolysis / Gluconeogenesi	5	4	0.041719
Arginine and proline metabo	5	3	0.041719
Glyoxylate and dicarboxylate	5	5	0.041719
Pantothenate and CoA biosyn	5	4	0.041719
Glycerolipid metabolism	2	2	0.042528
Pentose phosphate pathway	6	3	0.052185
beta-Alanine metabolism	3	2	0.058117
Fatty acid biosynthesis	4	2	0.074959
Steroid hormone biosynthesi	9	4	0.09083
Fructose and mannose metab	5	2	0.092589
Pyrimidine metabolism	5	2	0.092589
Drug metabolism - cytochror	5	2	0.092589
Glycine, serine and threonine	7	4	0.12894
Inositol phosphate metabolis	7	2	0.12894
Purine metabolism	12	4	0.13585
Cysteine and methionine met	8	3	0.14725
Biosynthesis of unsaturated f	9	2	0.16548

ID: 388.13281
P-val: 2.4438289969452853e-7
T-stat: 147.2839

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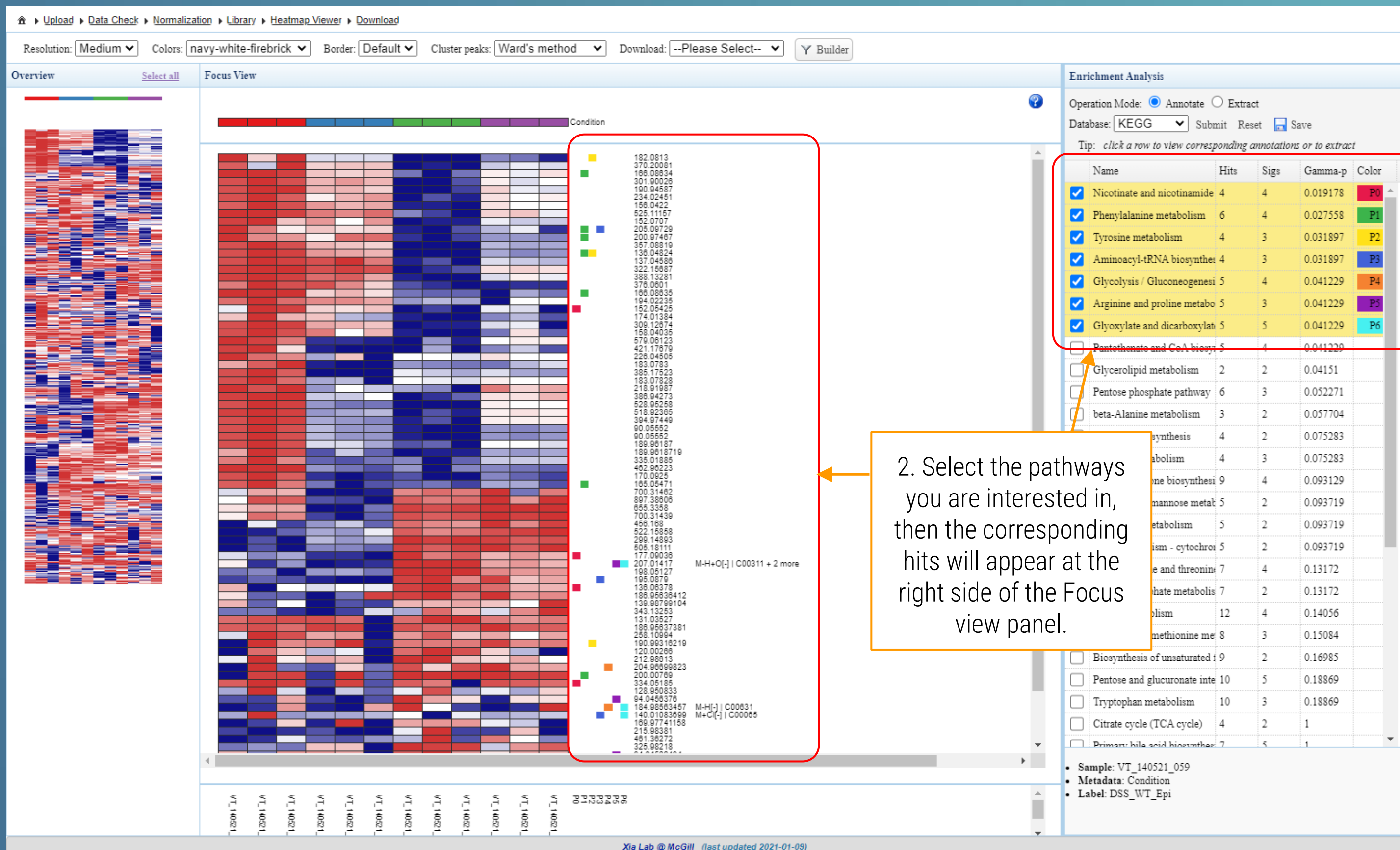
1. Select database and submit to do the enrichment analysis

TIP1 : Operation Mode could show the hits in different way. Annotate will annotate directly on the heatmap, while the 'Extract' will extract the ions hits and hide other non-hits.

Continue at the next page

2.3.8 Enrichment Analysis -2



2.3.9 Result Download

Upload ▸ Data Check ▸ Normalization ▸ Library ▸ Heatmap Viewer ▸ Download

Resolution: Medium (Low / Medium / High) Colors: navy-white-firebrick Border: Default Cluster peaks: Ward's method Download: --Please Select-- (--Please Select-- / Focusview PNG / Overview PNG / Customview PNG / Result table) Builder

Overview Select all | Focus View | Enrichment Analysis

Condition

M-H+O[-] | C00311 + 2 more

M-H[-] | C00631

M+Cl^{-} | C00065

1. Set the resolution of the image in Focus view

2. Download the images from Download menu and click to download it!

Operation Mode: Annotate Extract

Database: KEGG Submit Reset Save

Tip: *click a row to view corresponding annotations or to extract*

	Name	Hits	Sigs	Gamma-p	Color
☑	Nicotinate and nicotinamide	4	4	0.019178	P0
☑	Phenylalanine metabolism	6	4	0.027558	P1
☑	Tyrosine metabolism	4	3	0.031897	P2
☑	Aminoacyl-tRNA biosynthes	4	3	0.031897	P3
☑	Glycolysis / Gluconeogenesi	5	4	0.041229	P4
☑	Arginine and proline metabo	5	3	0.041229	P5
☑	Glyoxylate and dicarboxylat	5	5	0.041229	P6
☐	Pantothenate and CoA biosy	5	4	0.041229	
☐	Glycerolipid metabolism	2	2	0.04151	
☐	Pentose phosphate pathway	6	3	0.052271	
☐	beta-Alanine metabolism	3	2	0.057704	
☐	Fatty acid biosynthesis	4	2	0.075283	
☐	Histidine metabolism	4	3	0.075283	
☐	Steroid hormone biosynthesi	9	4	0.093129	
☐	Fructose and mannose metab	5	2	0.093719	
☐	Pyrimidine metabolism	5	2	0.093719	
☐	Drug metabolism - cytochroi	5	2	0.093719	
☐	Glycine, serine and threonin	7	4	0.13172	
☐	Inositol phosphate metabolis	7	2	0.13172	
☐	Purine metabolism	12	4	0.14056	
☐	Cysteine and methionine me	8	3	0.15084	
☐	Biosynthesis of unsaturated	9	2	0.16985	
☐	Pentose and glucuronate inte	10	5	0.18869	

- **Sample**: VT_140521_057
- **Metadata**: Condition
- **Label**: DSS_WT_Epi

Xia Lab @ McGill (last updated 2021-01-09)

2.3.9 Result Download

MetaboAnalyst 5.0 - user-friendly, end-to-end metabolomics data analysis

- Upload
- Processing
  - Data check
  - Missing value
  - Data filter
  - Data editor
- Normalization
- Set parameter

Download Results & Start New Journey

Please download the results (tables and images) from the **Results Download** tab below. The **Download.zip** contains all the files in your home directory. You can also generate a PDF **analysis report** using the button. Finally, you can continue to explore other compatible modules using the **Start New Journey** tab.

Results Download | Start New Journey

Generate Report

Download.zip	data_original.csv
Rhistory.R	mummichog_enrichment_3.csv
data_processed.csv	mummichog_matched_compound_all.csv
snorm_1_dpi72.png	norm_1_dpi72.png
mummichog_enrichment_3.json	metaboanalyst_heatmap_2.json

Logout

Click the "**Generate Report**" to download a pdf report summarizing your analysis.

Thanks

If you have any questions please read through the FAQs or contact us at Zhiqiang.pang[at]xialab.ca or Jeff.xia[at]xialab.ca