MetaboAnalyst 5.0

A Web-based Tool for Sreamlined Metabolomics Data Analysis

2022.07.12

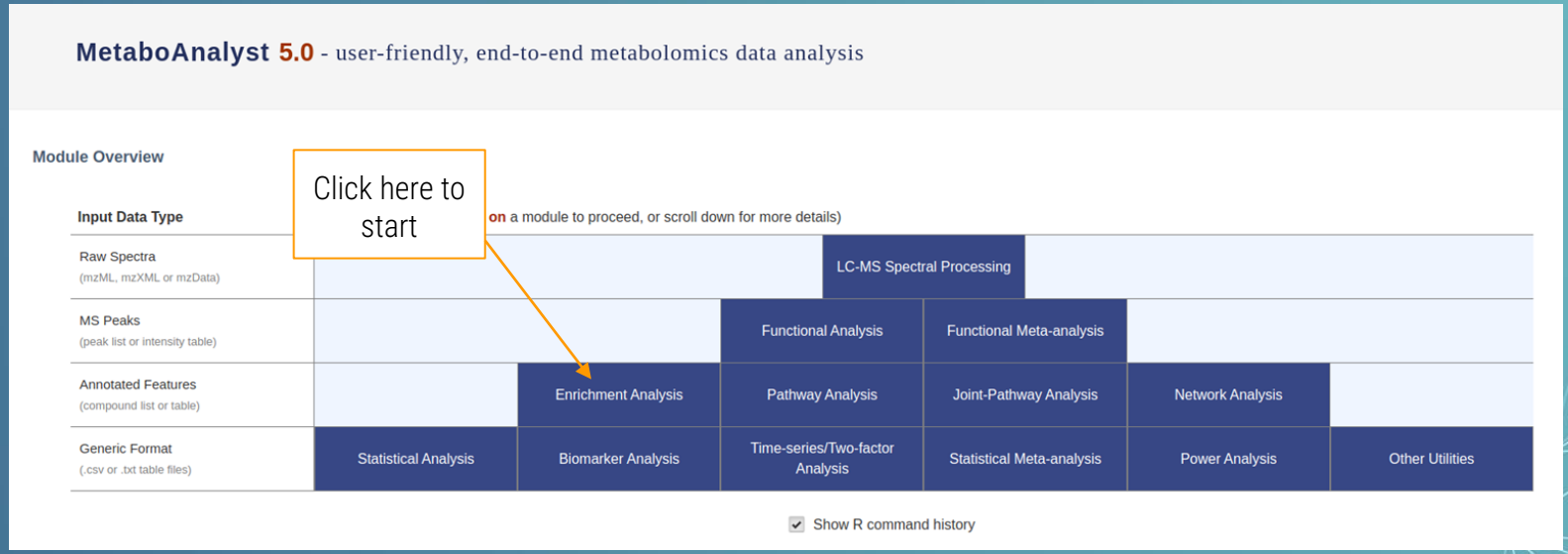
5. Enrichment Analysis

Metabolite Enrichment Analysis is used to directly investigates if a group of functionally related metabolites are significantly enriched, eliminating the need to preselect compounds based on some arbitrary cut-off threshold. The Enrichment Analysis module of MetaboAnalyst has added multiple enhancements for Version 5.

Highlights:

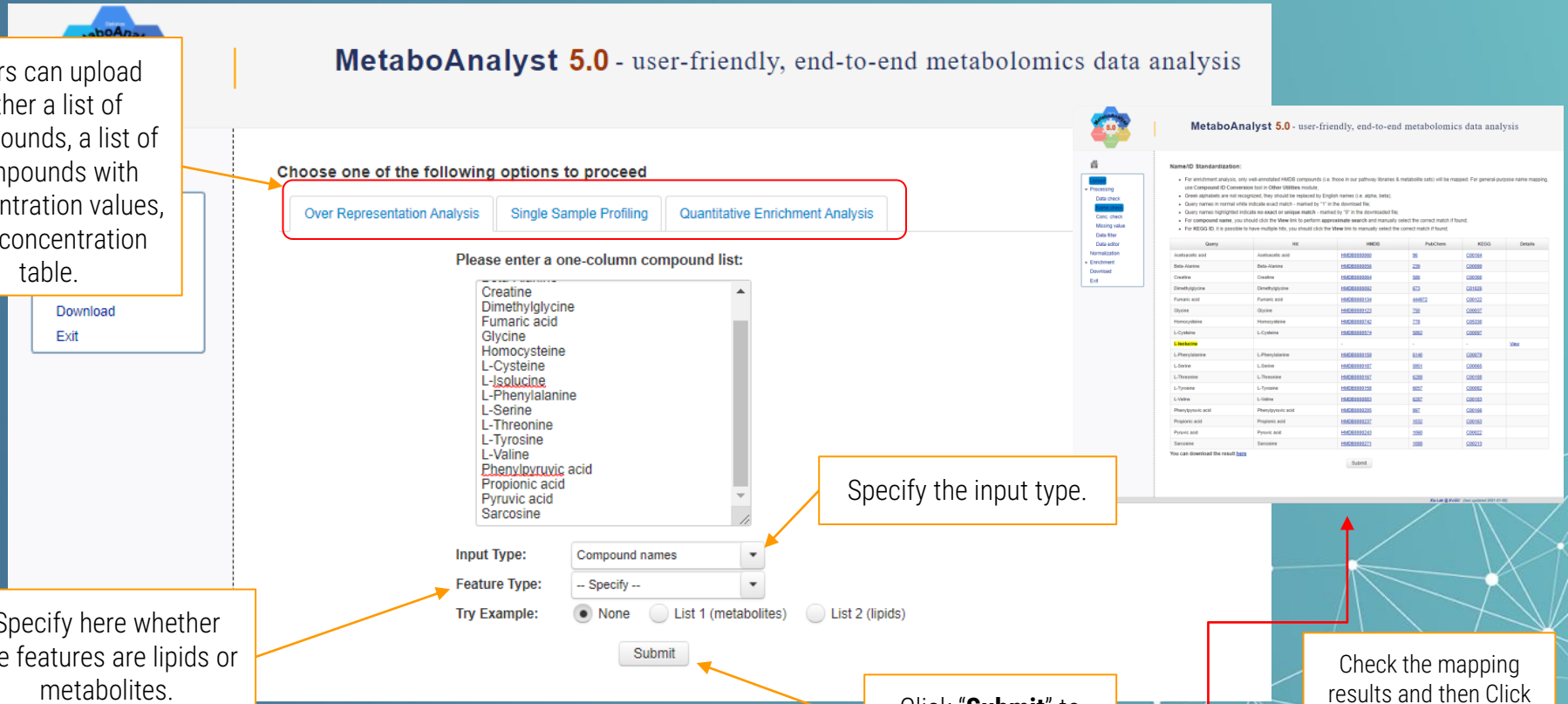
- Added 1615 new chemical class metabolite sets
- Enhanced enrichment analysis visualizations ~ interactive bar-chart, bubble plot, and interactive pie-chart
- Enhanced support for lipidomics data
    - Expanded our underlying database to cover 197 854 lipids
    - Implemented a smart-matching algorithm to enhance the matching of user-uploaded lipids to our internal compound database.

5.1 Start Enrichment Analysis



5.2.1 Enrichment Analysis (Upload one column compound list)

Users can upload either a list of compounds, a list of compounds with concentration values, or a concentration table.



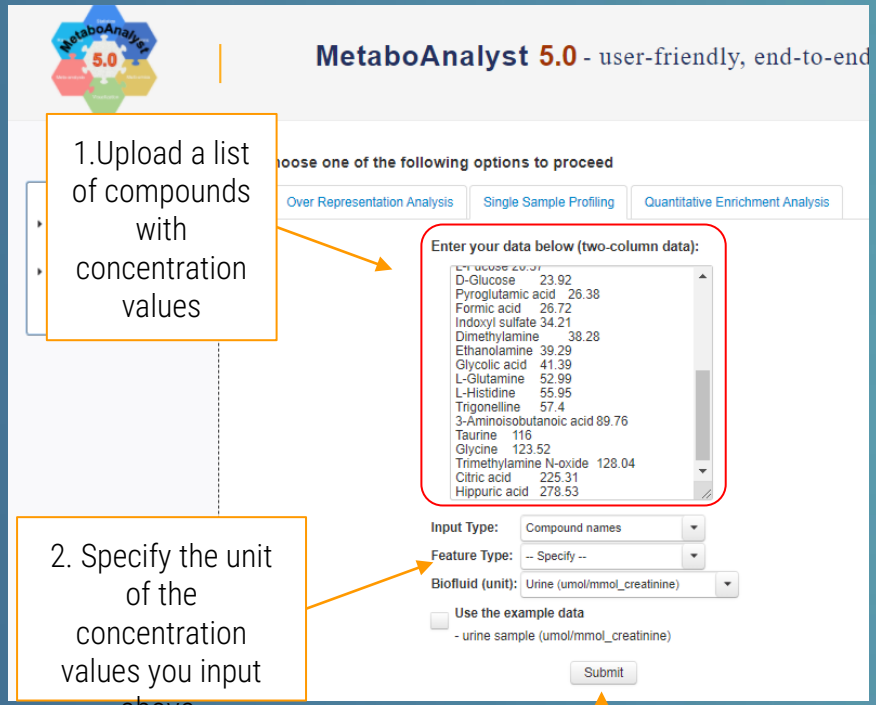
Specify the input type.

Specify here whether the features are lipids or metabolites.

Click "**Submit**" to upload your data.

Check the mapping results and then Click "**Submit**" to process your data.

5.2.2 Enrichment Analysis (Upload two column compound list)

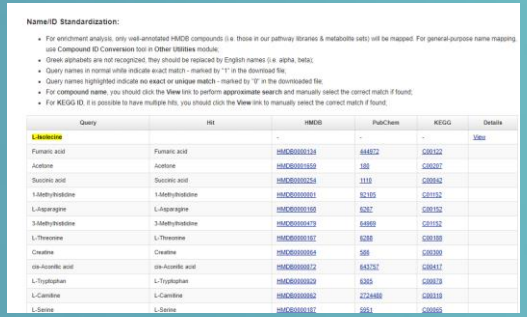


1.Upload a list of compounds with concentration values

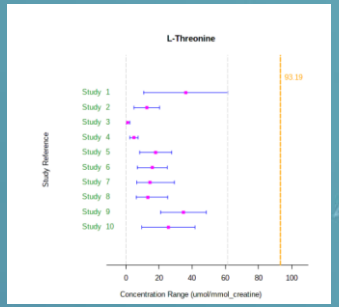
2. Specify the unit of the concentration values you input above.

3. Click "**Submit**" to upload your data.

4. Check the compound mapping results.



5. Check the concentration comparison results.

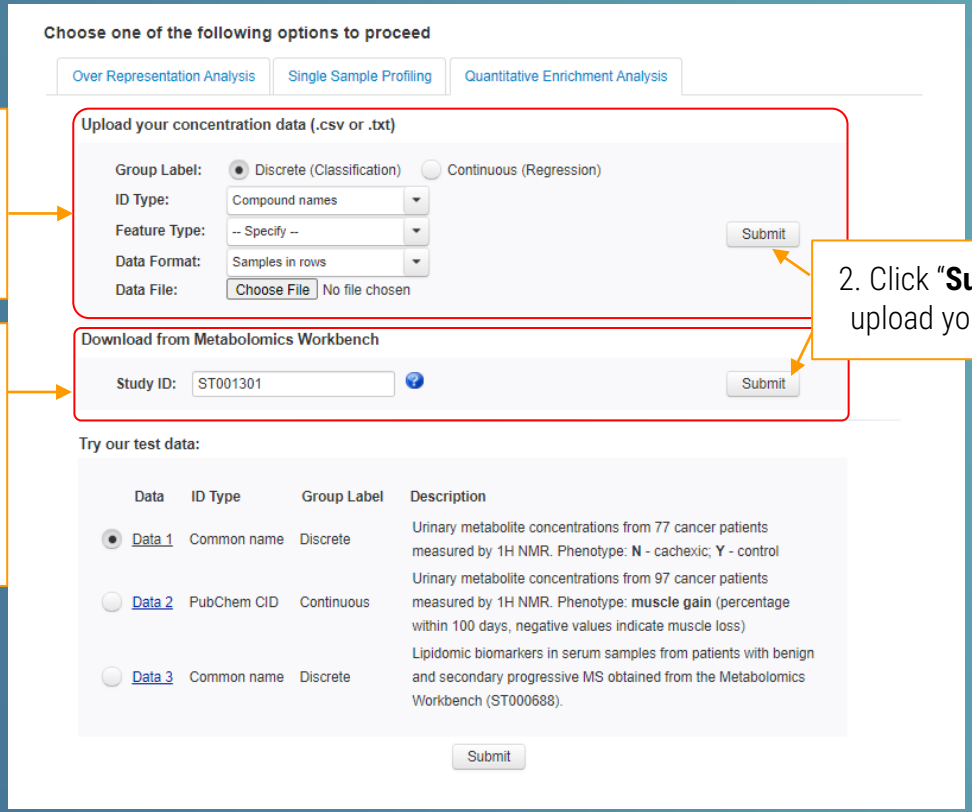


6. Click view to inspect the compound comparison.

5.2.3 Enrichment Analysis (Upload concentration table)

1.Upload your data table and specify the format etc.

1.Input the Metabolomic Workbench Study ID to import the data.

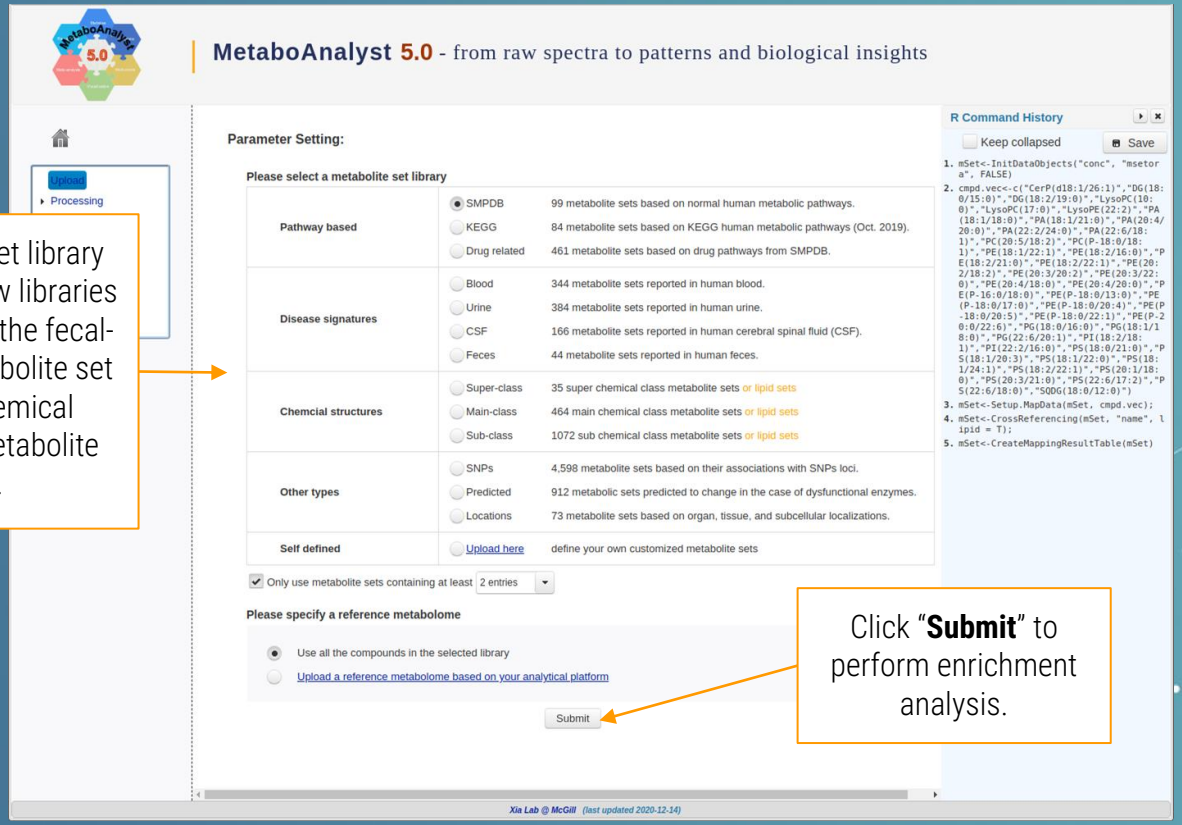


2. Click "**Submit**" to upload your data.

TIP1: MetaAnalyst now allows users to use the study results from Metabolomics Workbench directly by simply providing the STUDY ID.

TIP2: The data pre-processing steps, including data integrity check, ID standardization, and normalization need to be performed step by step.

5.3 Parameter Selection



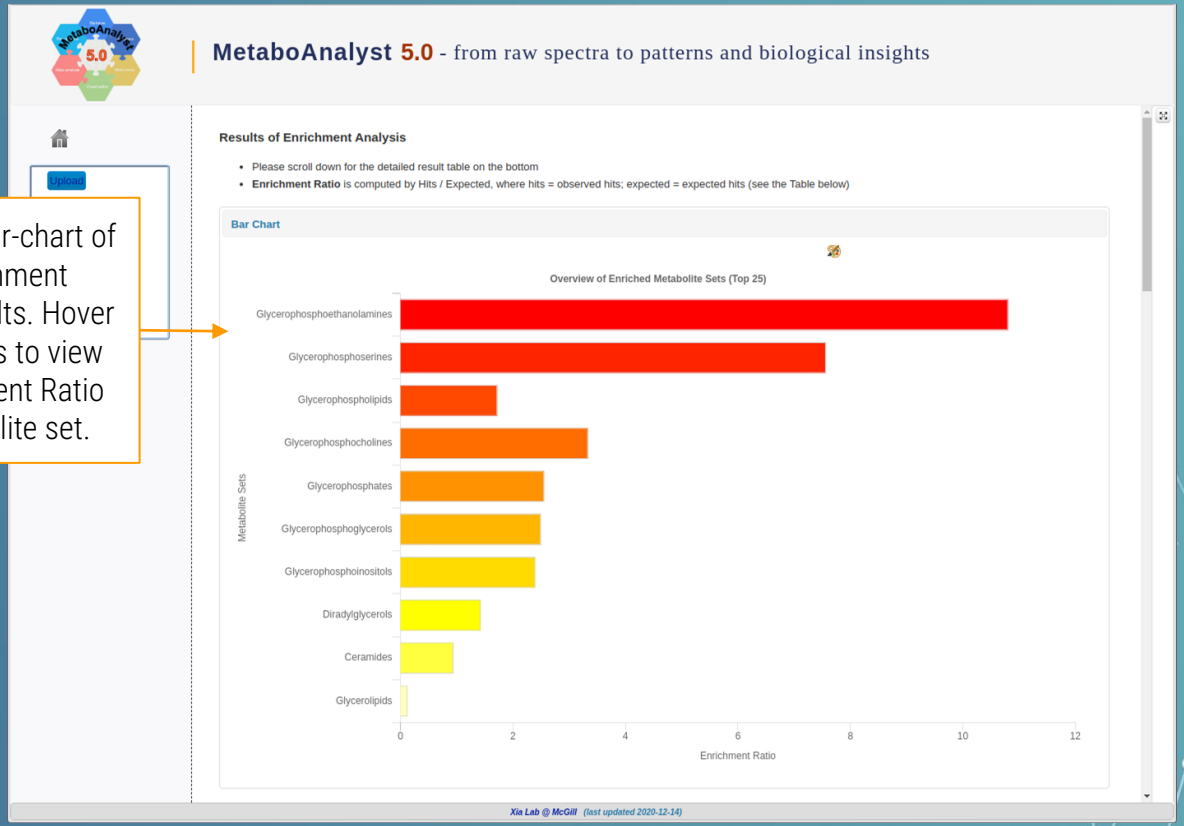
Metabolite set library selection. New libraries in V5 include the fecal-disease metabolite set and all chemical structure metabolite sets.

Click "**Submit**" to perform enrichment analysis.

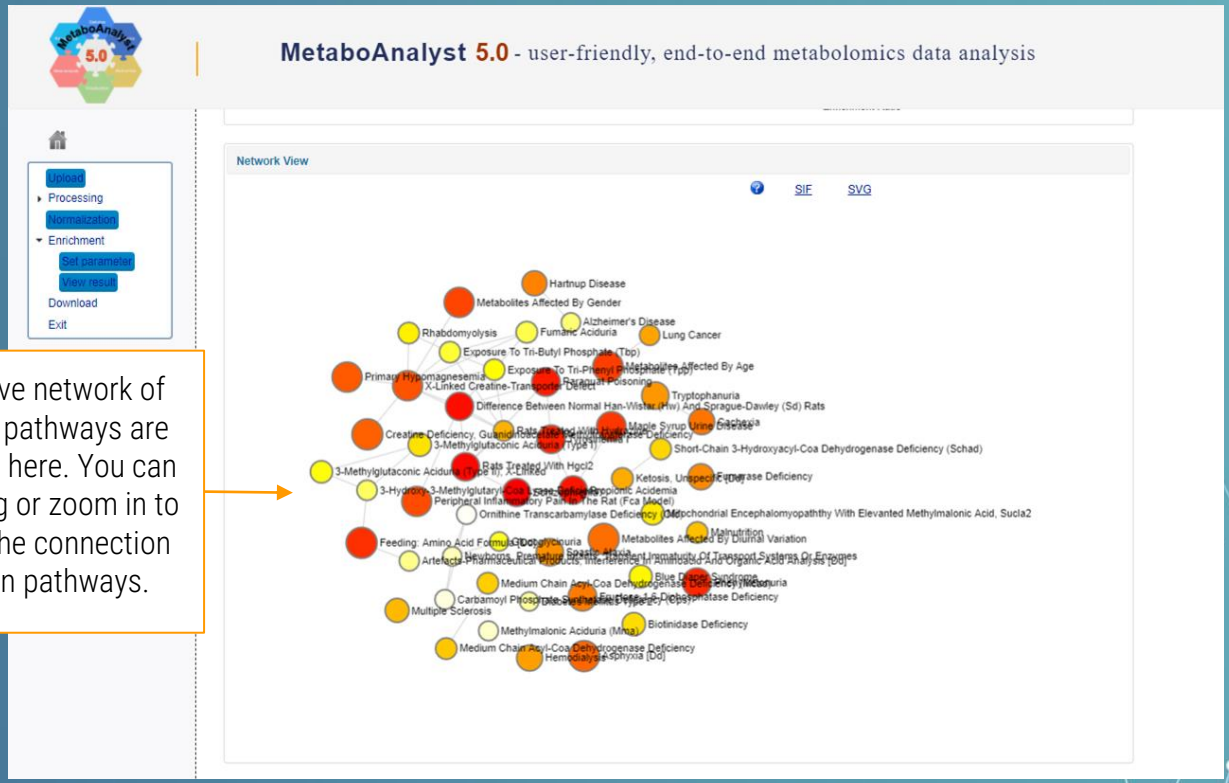
TIP1: Select the metabolites sets you are going to explore or upload a self-defined sets.

5.4.1 Enrichment Analysis Results – Bar Chart

Interactive bar-chart of the enrichment analysis results. Hover over the bars to view the Enrichment Ratio per metabolite set.



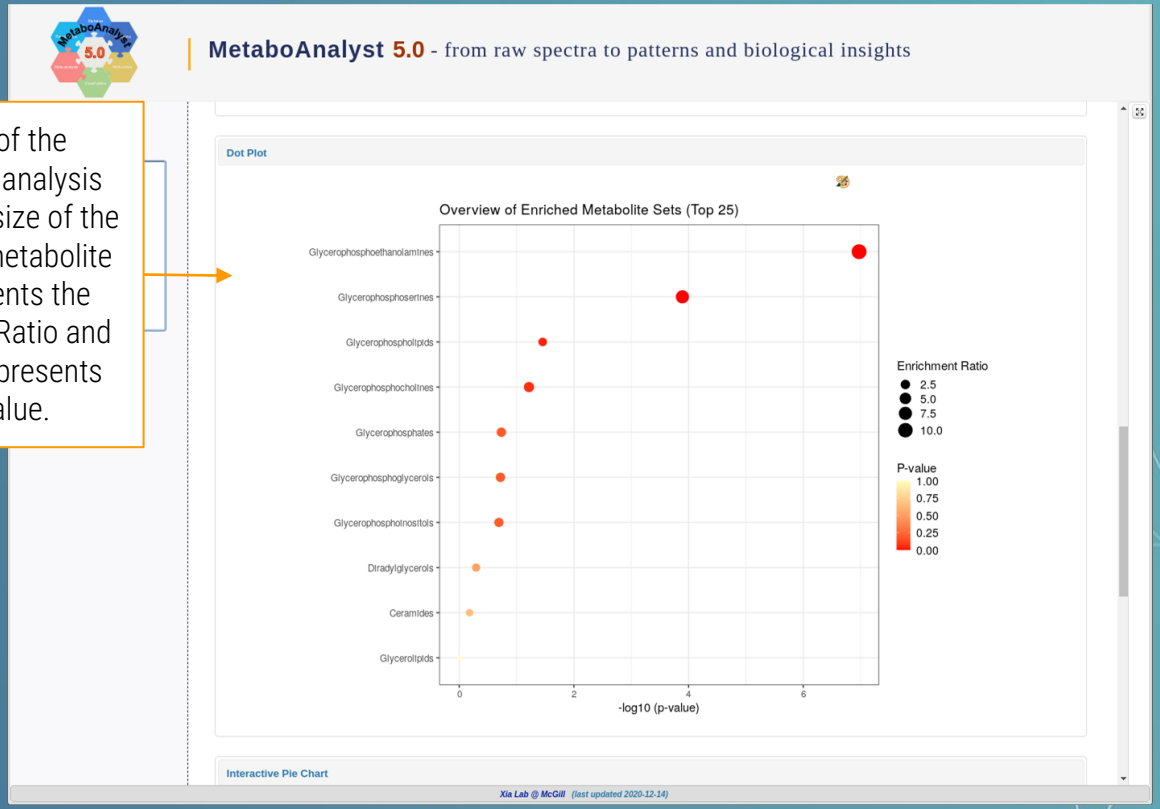
5.4.2 Enrichment Analysis Results – Network View



Interactive network of different pathways are displayed here. You can try to drag or zoom in to explore the connection between pathways.

5.4.3 Enrichment Analysis Results – Dot Plot

Dot plot of the enrichment analysis results. The size of the circles per metabolite set represents the Enrichment Ratio and the color represents the p-value.



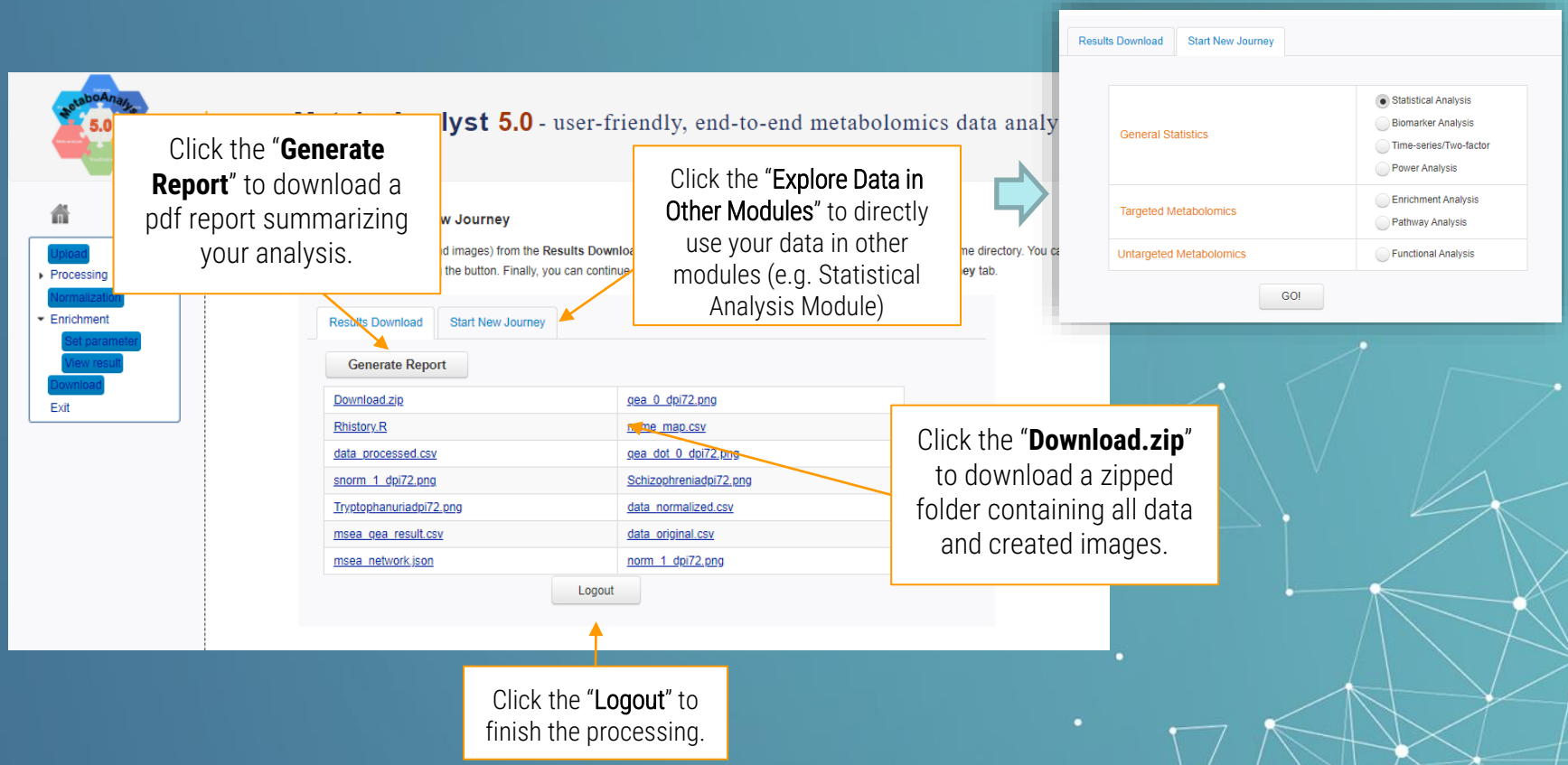
5.4.4 Enrichment Analysis Results – Summary table

Metabolite Set	Total	Hits	Statistic	Expected	P value	Holm P	FDR	Details
Schizophrenia	32	17	12.55	1.3158	3.5583E-4	0.039141	0.003311	View
Rats Treated With Hgcl2	13	13	12.814	1.3158	3.6236E-4	0.039497	0.003311	View
Difference Between Normal Han-Wistar (Hw) And Sprague-Dawley (Sd) Rats	10	10	12.763	1.3158	3.633E-4	0.039497	0.003311	View
Propionic Acidemia	20	11	12.843	1.3158	3.8979E-4	0.041708	0.003311	View
Paraquat Poisoning	7	7	13.083	1.3158	3.9458E-4	0.041825	0.003311	View
Tyrosinemia I	8	6	12.992	1.3158	3.9493E-4	0.041825	0.003311	View
Phenylketonuria	12	4	13.466	1.3158	4.0033E-4	0.041825	0.003311	View
Feeding: Amino Acid Formula [Dd]	5	2	14.973	1.3158	4.695E-4	0.048358	0.003311	View
Maple Syrup Urine Disease	9	7	13.855	1.3158	4.9515E-4	0.050506	0.003311	View
Metabolites Affected By Age	12	12	14.547	1.3158	4.9763E-4	0.050506	0.003311	View
Metabolites Affected By Gender	8	5	14.234	1.3158	5.0144E-4	0.050506	0.003311	View
Peripheral Inflammatory Pain In The Rat (Fca Model)	10	7	14.169	1.3158	5.0252E-4	0.050506	0.003311	View
X-Linked Creatine-Transporter Defect	4	4	14.205	1.3158	5.027E-4	0.050506	0.003311	View
Primary Hypomagnesemia	4	2	14.251	1.3158	5.0295E-4	0.050506	0.003311	View
Creatine Deficiency, Guanidinoacetate Methyltransferase Deficiency	4	3	14.933	1.3158	5.115E-4	0.050506	0.003311	View
Asphyxia [Dd]	12	4	14.902	1.3158	5.115E-4	0.050506	0.003311	View
Metabolites Affected By Diurnal Variation	6	5	14.928	1.3158	5.117E-4	0.050506	0.003311	View
Cachexia	3	3	11.205	1.3158	7.428E-4	0.06908	0.0045393	View
Fructose-1,6-Diphosphatase Deficiency	3	1	13.16	1.3158	0.0011854	0.10905	0.0068627	View
Hartnup Disease	12	10	10.35	1.3158	0.001424	0.12958	0.007832	View
Fumarase Deficiency	5	2	11.176	1.3158	0.0018152	0.16337	0.0090793	View
Spastic Ataxia	5	1	12.143	1.3158	0.0018984	0.16896	0.0090793	View
Tryptophanuria	2	1	12.143	1.3158	0.0018984	0.16896	0.0090793	View
Hemodialysis	12	1	11.154	1.3158	0.002993	0.26039	0.01359	View
Lung Cancer	32	27	6.9615	1.3158	0.0030887	0.26563	0.01359	View
Ketosis, Unspecific [Dd]	8	3	7.9804	1.3158	0.0042017	0.35715	0.017776	View
Rats Treated With Hydrazine	9	7	7.0029	1.3158	0.0047579	0.39966	0.019384	View
Multiple Sclerosis	21	1	9.6108	1.3158	0.0060732	0.50408	0.023859	View
Malnutrition	10	2	7.7399	1.3158	0.0066558	0.54577	0.024601	View
Medium Chain Acyl Coa Dehydrogenase Deficiency	15	2	7.7731	1.3158	0.0075441	0.61107	0.024601	View

Tabular summary of the enrichment analysis results. Click "**Details**" to view which features were hits in the metabolite set.

You can click the 'submit' button at the bottom of this page to finish the analysis this time.

5.5 Result Downloading & New Journey



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