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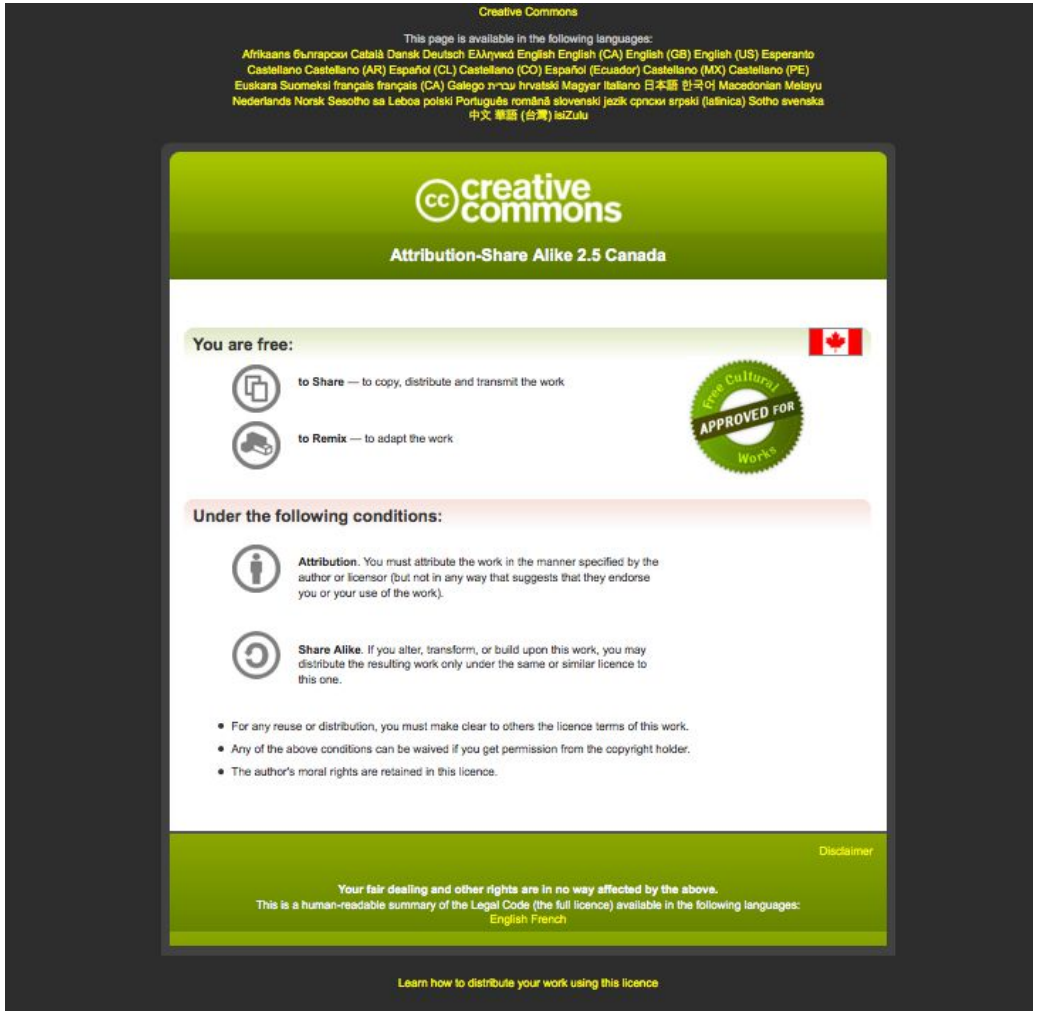
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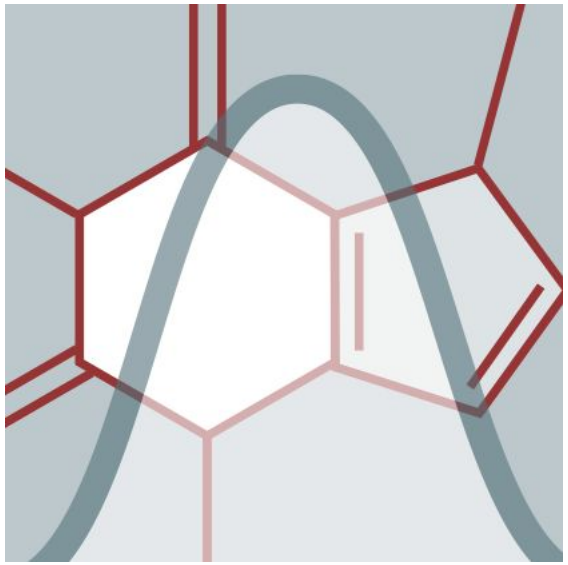
Data analytics for untargeted metabolomics

Jianguo (Jeff) Xia
Metabolomics Analysis
July 6-7, 2023

bioinformatics.ca



McGill

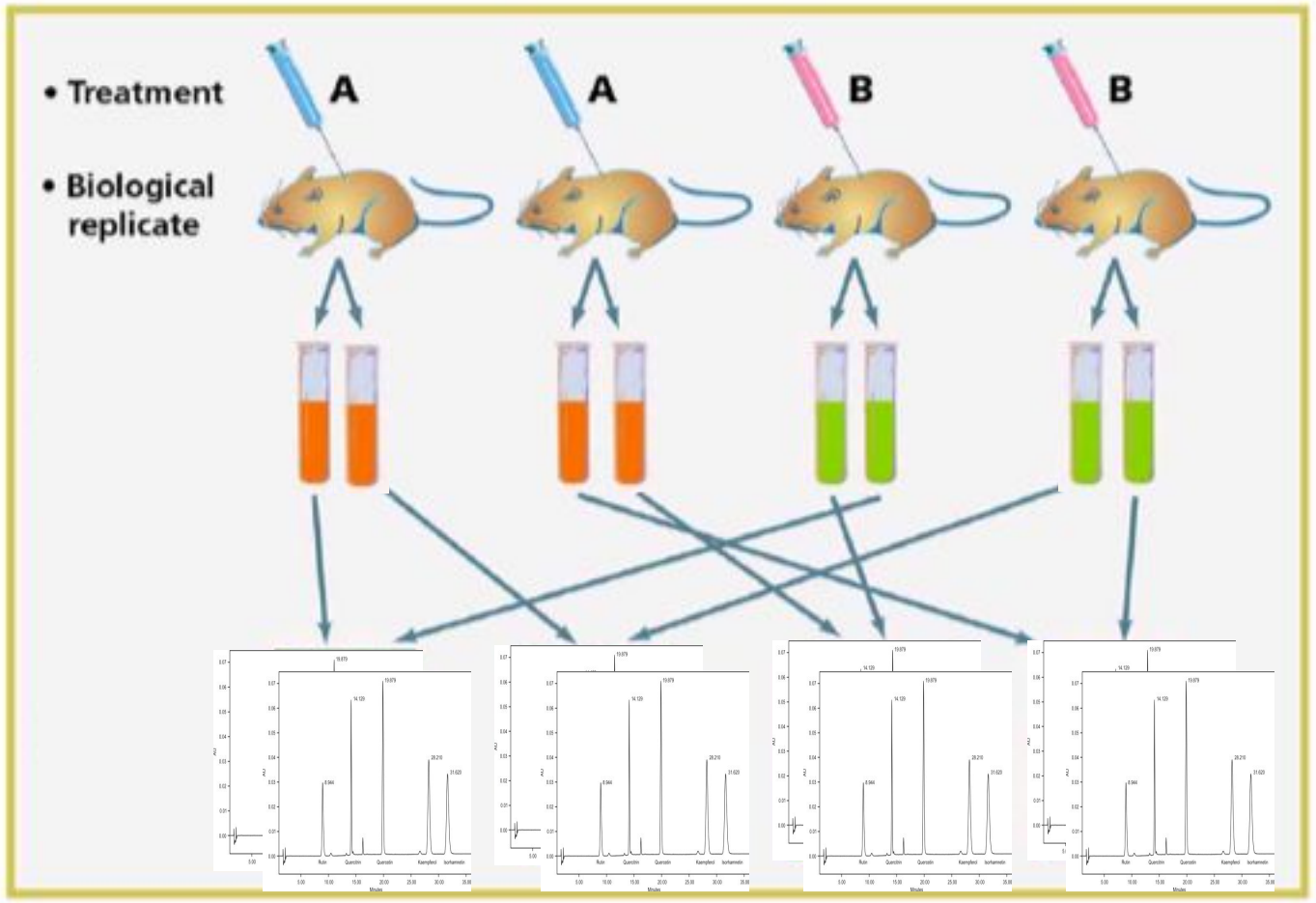
Learning Objectives

1. Become familiar with basic steps in LC-MS spectral processing
2. Become familiar with enrichment analysis for quantitative metabolomics data
3. Become familiar with enrichment analysis from LC-MS untargeted data

A Typical Metabolomics Experiment

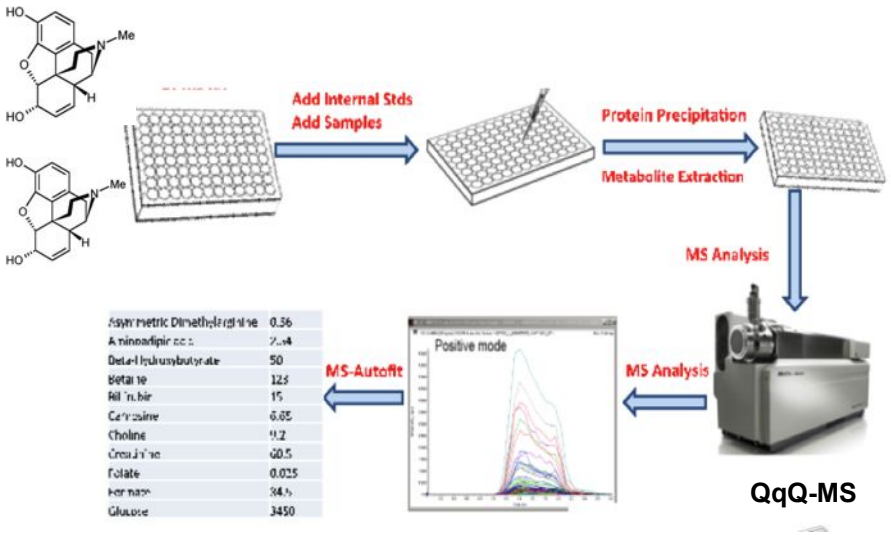
Biological replicates

Technical replicates

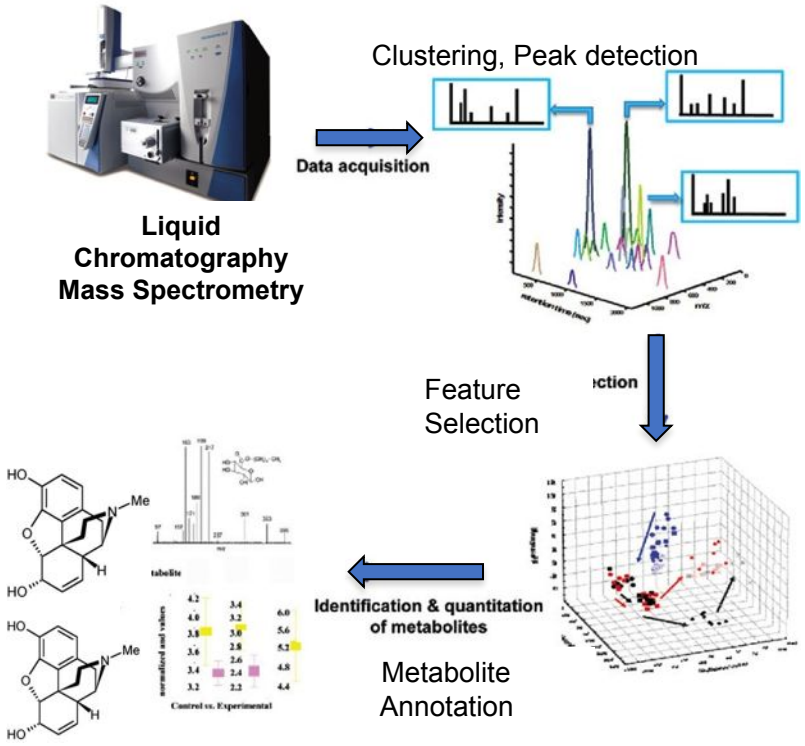


Data generation: two routes to metabolomics

Targeted / Quantitative



Untargeted / Global

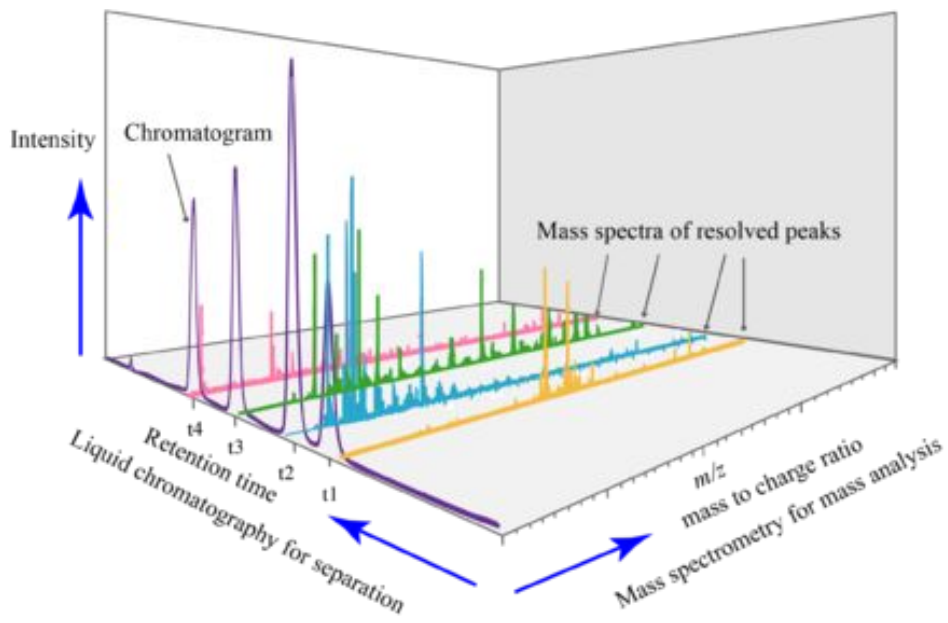


Common Tasks

- Purpose: to convert various raw data forms into data matrices suitable for statistical / functional analysis
- Supported data formats
  - Concentration tables (Targeted Analysis)
  - Spectral bins (Untargeted)
  - Peak lists (Untargeted)
  - Raw spectra (Untargeted, in mzML/mzXML/mzData/CDF)

LC-MS Raw Spectral Data Processing

MS Features



Raw spectral data is large and noisy

Features: LC-MS signals (m/z, RT, intensity) produced by the same molecular ion

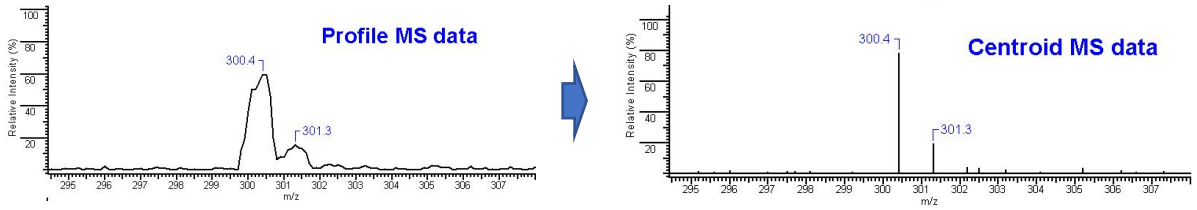
Single compound can give rise to multiple of mass signals (adducts, fragments, isotopes)

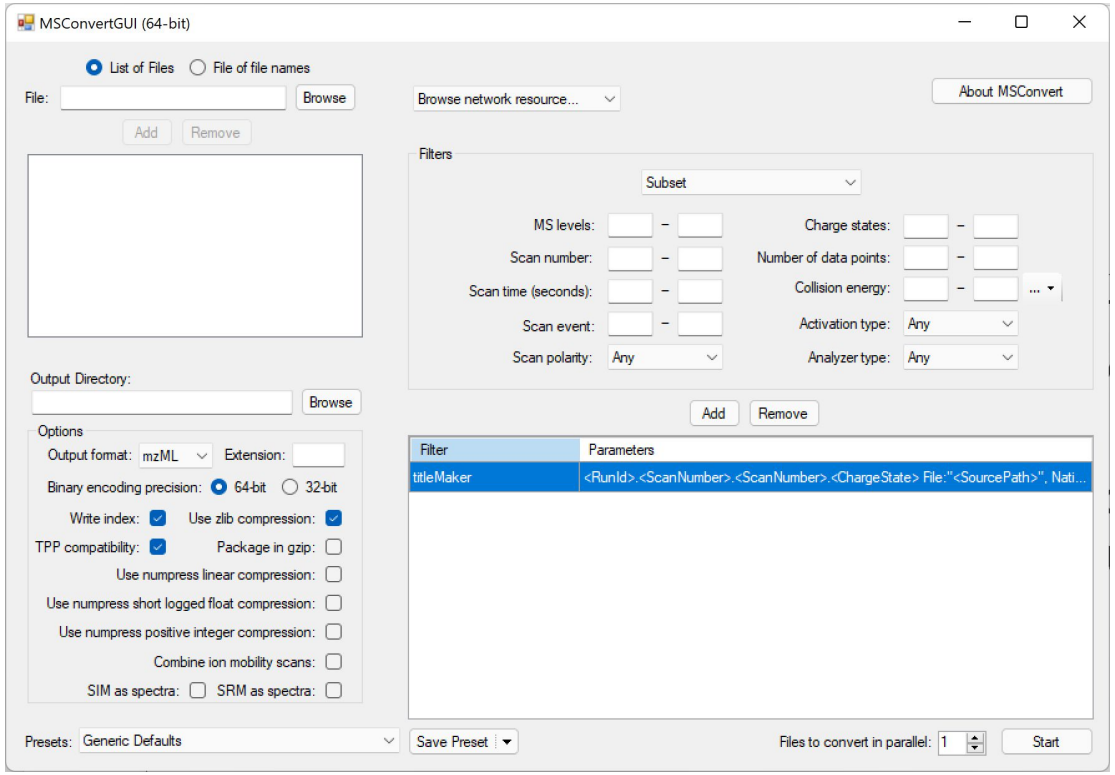
Processing MS data

- Identify, quantify, and align all possible features (peaks) across samples
- Output: a table of features (RT, m/z) with their quantitative information for subsequent statistical analysis

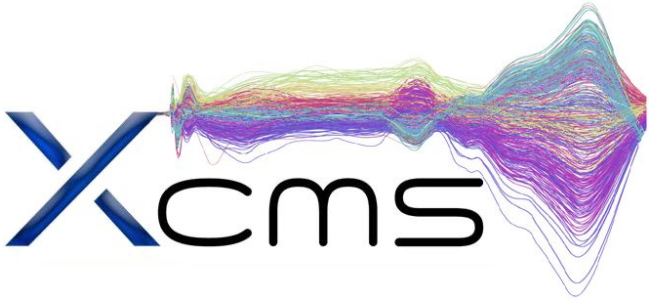
Profile or Centroid?

- The vendor raw spectra data is usually in profile format, which is redundant for regular LC-MS based metabolomics analysis;
- We need to convert the MS data into centroid mode to condense the Gaussian Profile peaks into centroids.
- Open-source formats (.mzML/ etc.)..

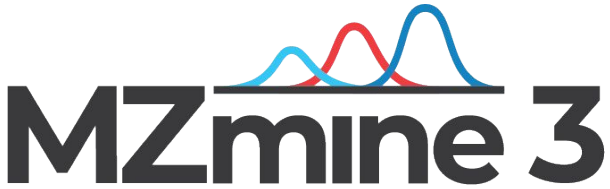


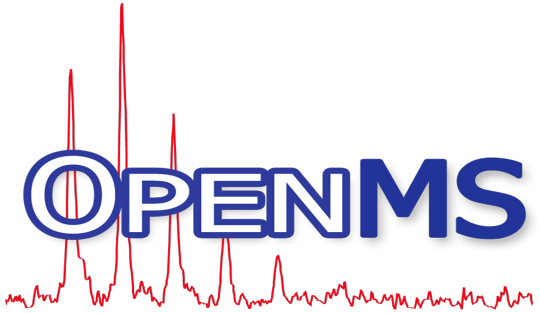


Open-source software for spectra processing..



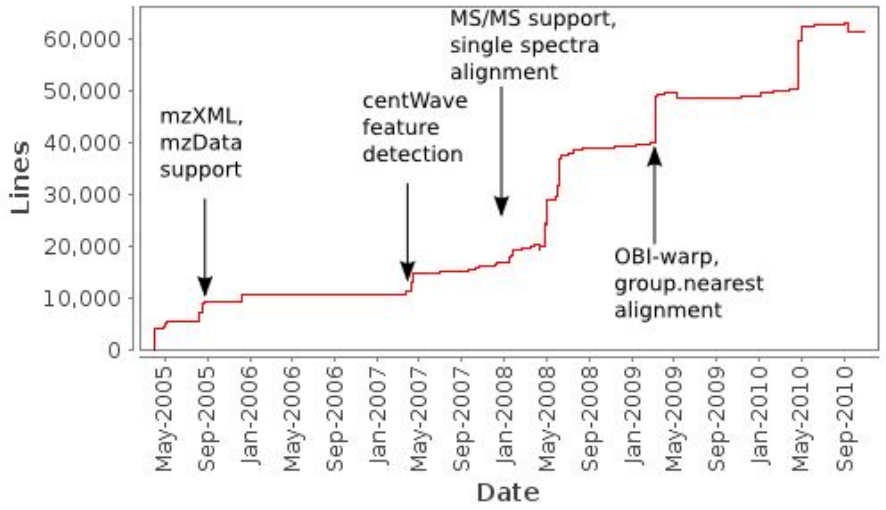
MS-DIAL





Why XCMS?

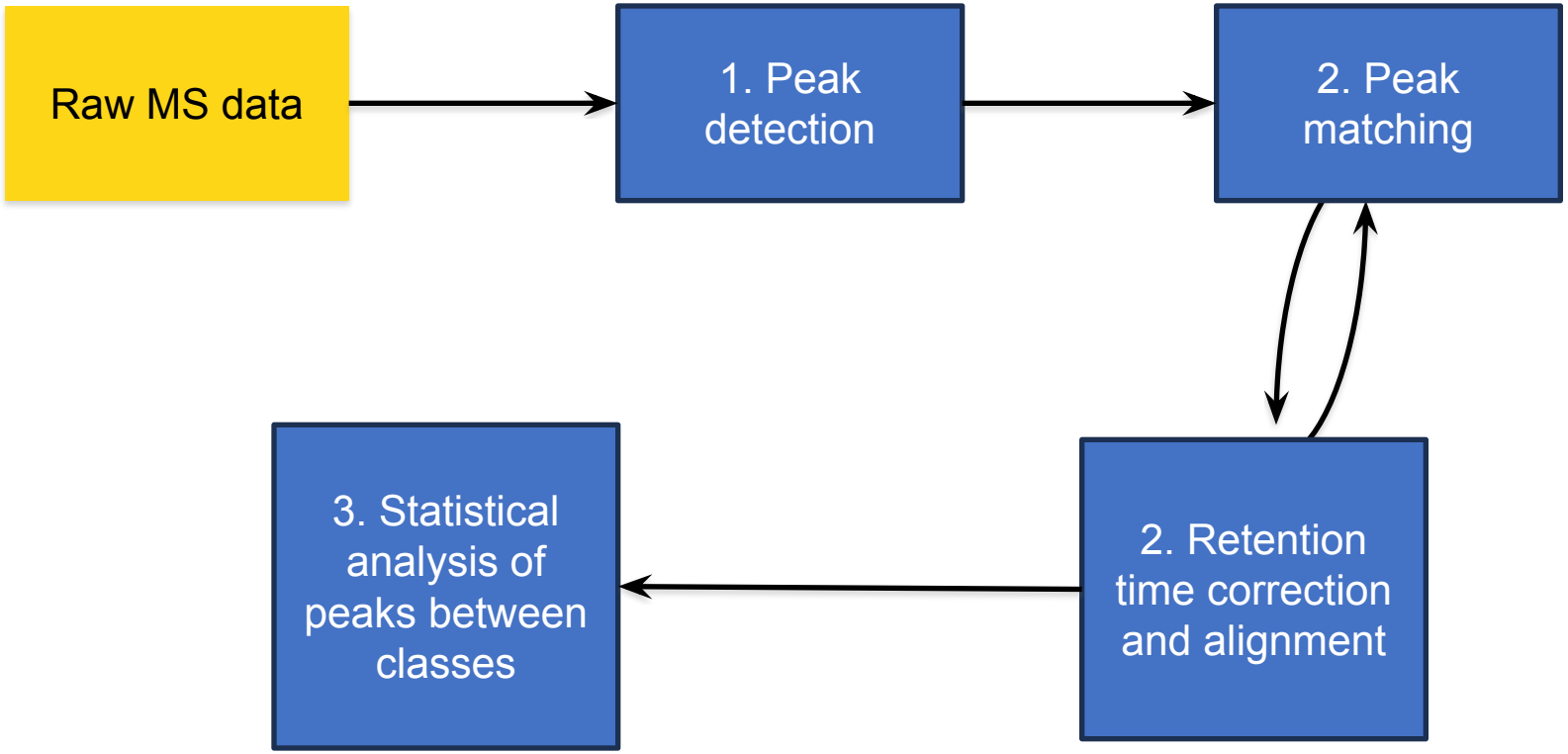
- First open-source software (R package) developed in 2006 by Siuzdak lab to process LC/GC-MS spectra
- Permits batch processing
- Widely used by metabolomics community for untargeted LC-MS based metabolomics



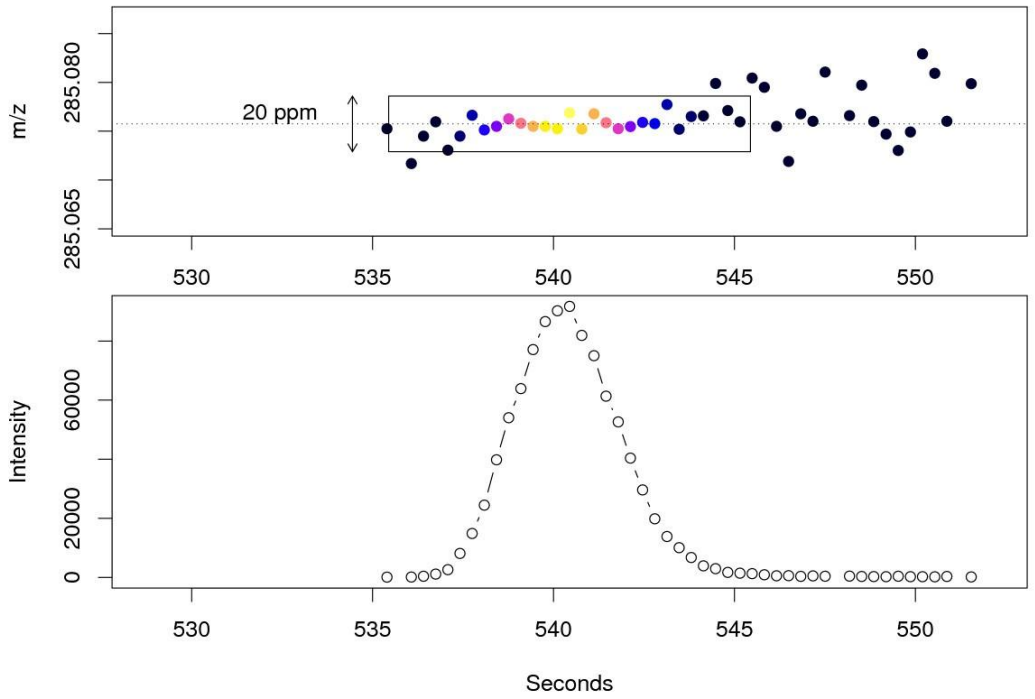
- LC-MS, MS/MS, MRM

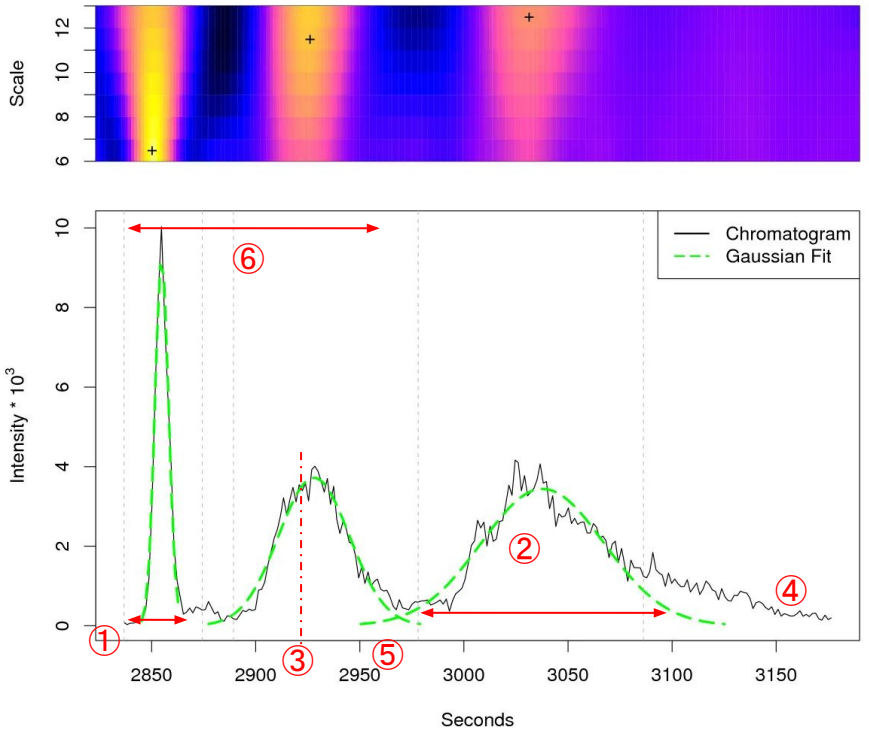
http://metablogomics.blogspot.com/2010/11/short-history-of-xcms.html

XCMS Flowchart



The centWave algorithm



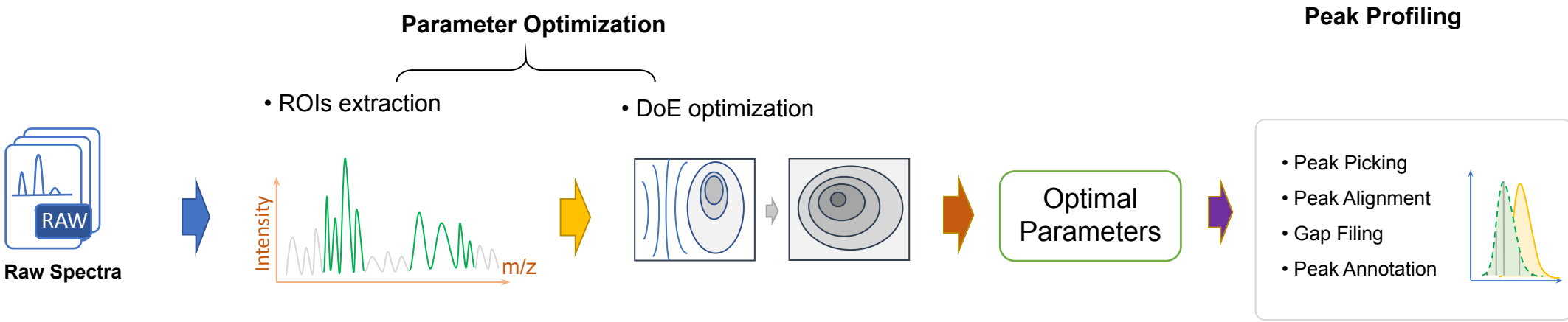


Many parameters need to be manually tuned to work well for your data
Need to be familiar with with instrument and analytics

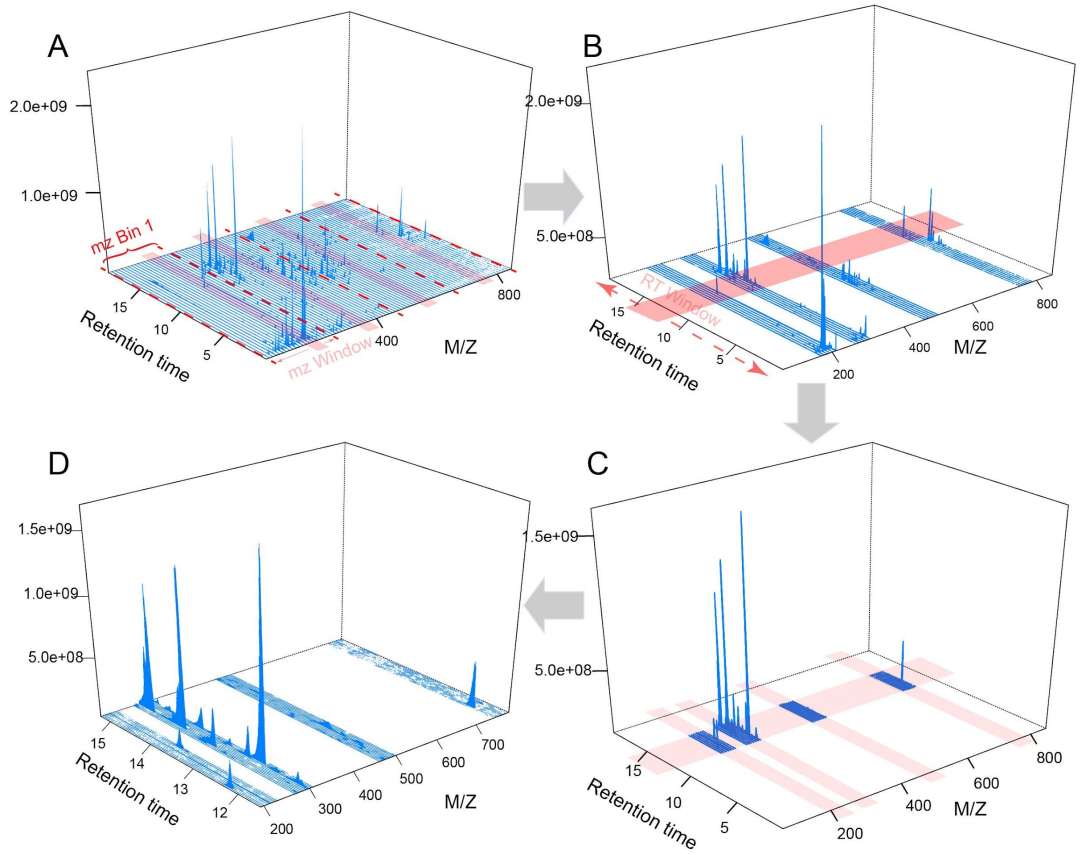
- Can we make this automatic?

Auto-optimization workflow

Our optimization approach is designed to extract a region abundant with MS signals for a design of experiment (DoE)-based optimization.



ROI Extraction



- Data-driven ROI extraction;
- Regions with high abundance of MS signals;
- Both low intensity peaks as well as high intensity peaks will be retained;

DoE-based Parameter Optimization

DoE -- central composite design

44 runs

Order	Peakwith_min	Peakwith_max	mzdiff	snthresh	bw
1	-1	-1	-1	-1	-1
2	1	-1	-1	-1	-1
3	-1	1	-1	-1	-1
...	...	...	...	...	...
43	0	0	0	0	1
44	0	0	0	0	0

3 level for every parameters (-1, 0, 1)

Relative reliable peaks ratio (identified by their isotopes)

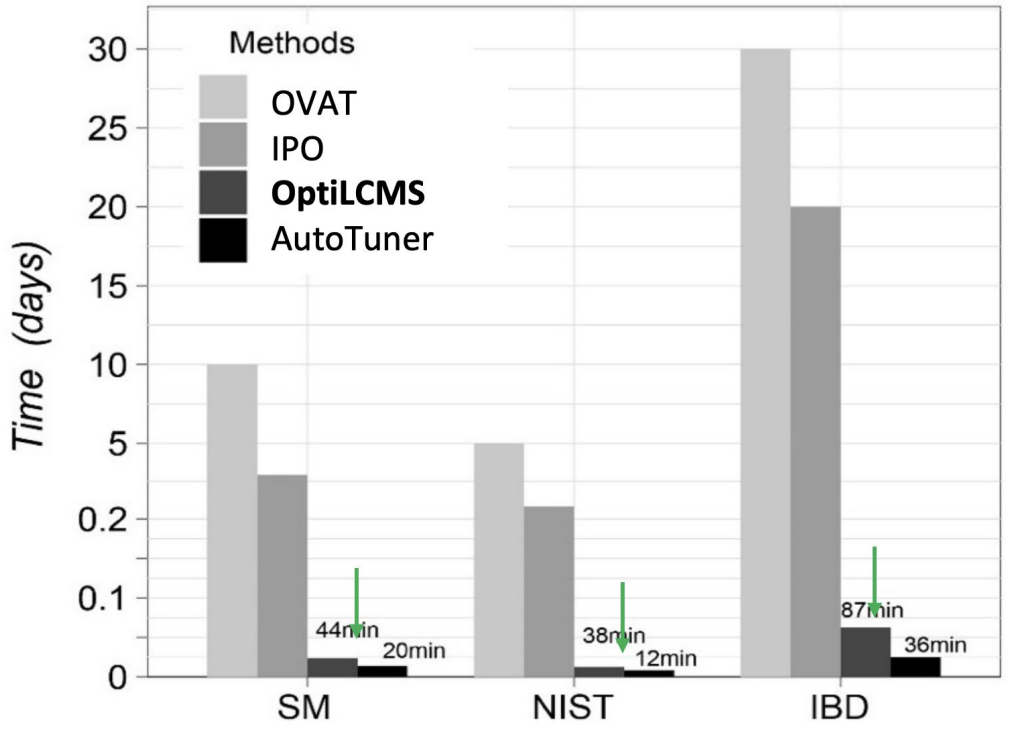
A co-efficient describing the stability of a grouped feature

$$QS = \frac{RP^{3/2}}{'all\ peaks' - LIP} * GR^2 * QcoE$$

Gaussian peaks ratio

- The most important parameters are evaluated with 44 DoE runs
- Instead of $3^8 = 6561$ one-variable-at-a-time runs.

Performance Evaluation – fast & better results

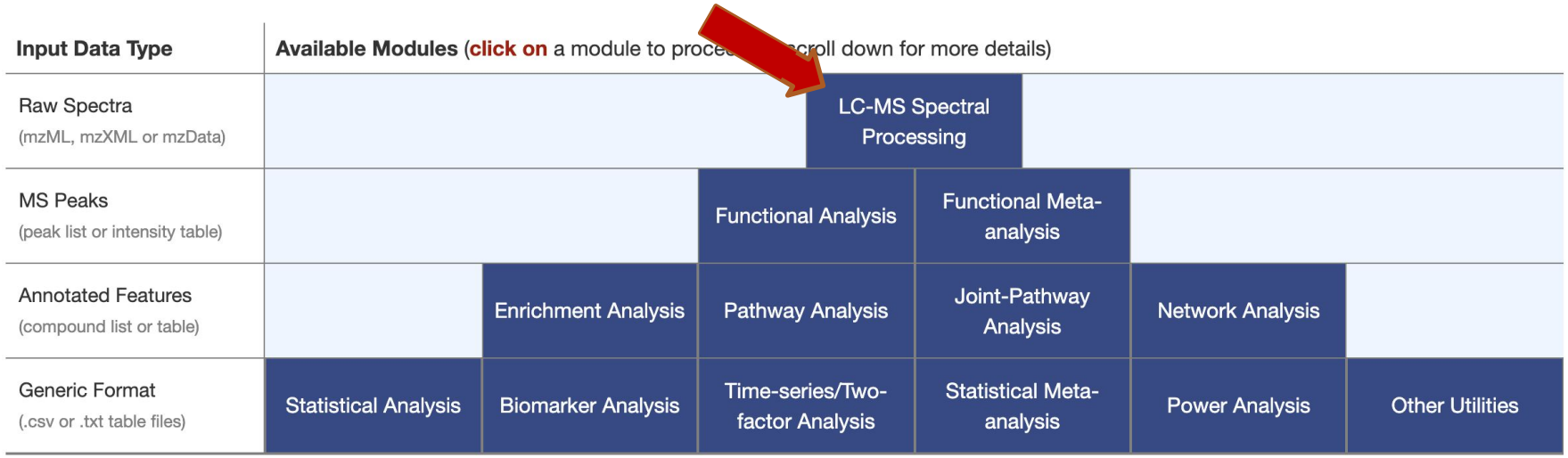


	Default	Optimized
Total peaks	4,344	5,113 (+18%)
Isotopes	760	1,274 (+68%)
Adducts	927	1,132 (+22%)
Formulas assigned	632	687 (+8.7%)
Potential matches	1,587	1,803 (+14%)
Variance explained	76.5%	81.3% (+5%)

Three datasets: Standard Mixture (SM), NIST-SRM 1950 and IBD data from iHMP2.

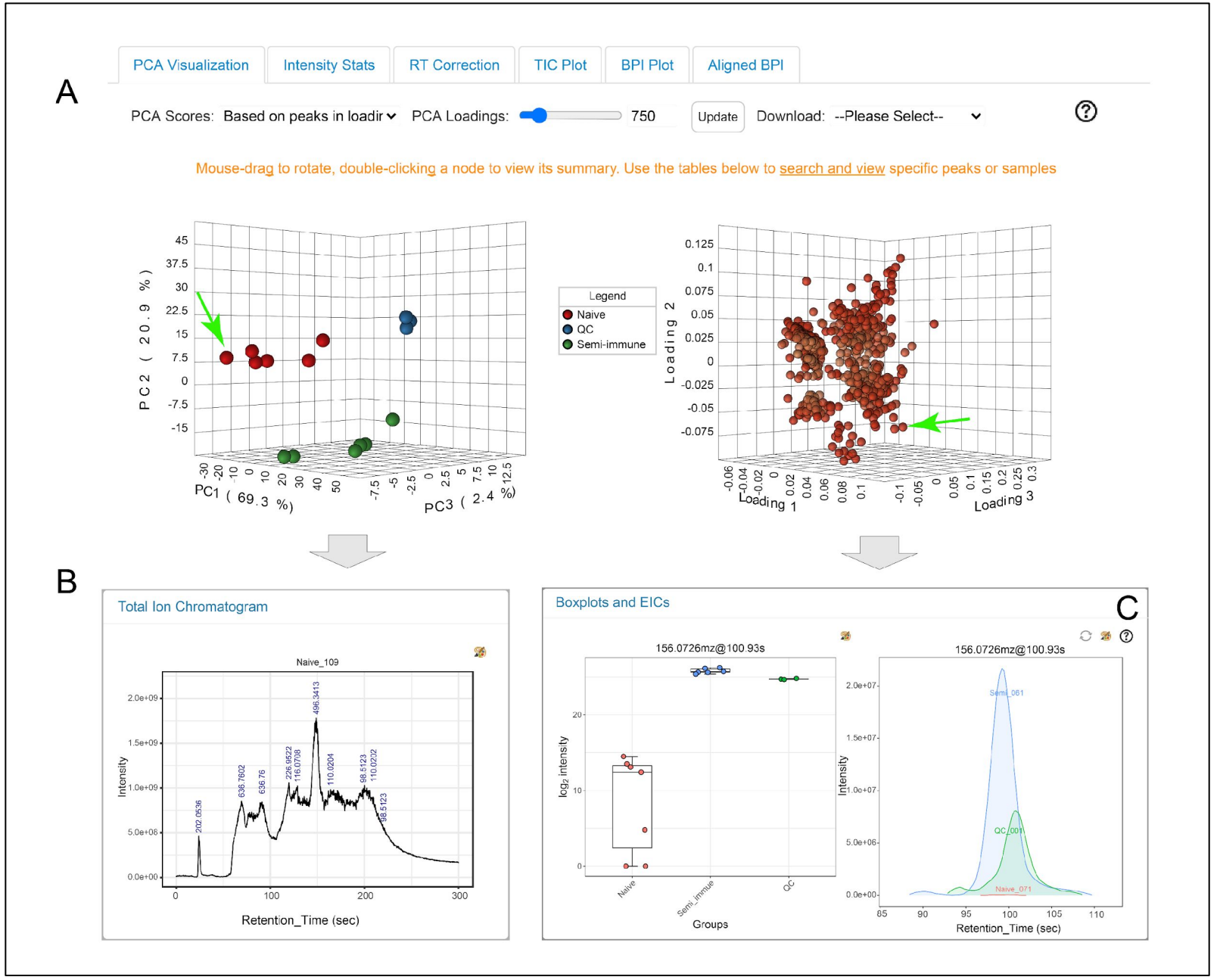
Pang, Z.; Chong, J.; Li, S.; Xia, J. MetaboAnalystR 3.0: Toward an Optimized Workflow for Global Metabolomics. *Metabolites* **2020**, *10*, 186

Raw LC-MS spectra processing



- From raw LC-MS spectra to peak abundance table
- Accept mzML, mzXML, CDF or mzData formats

Results

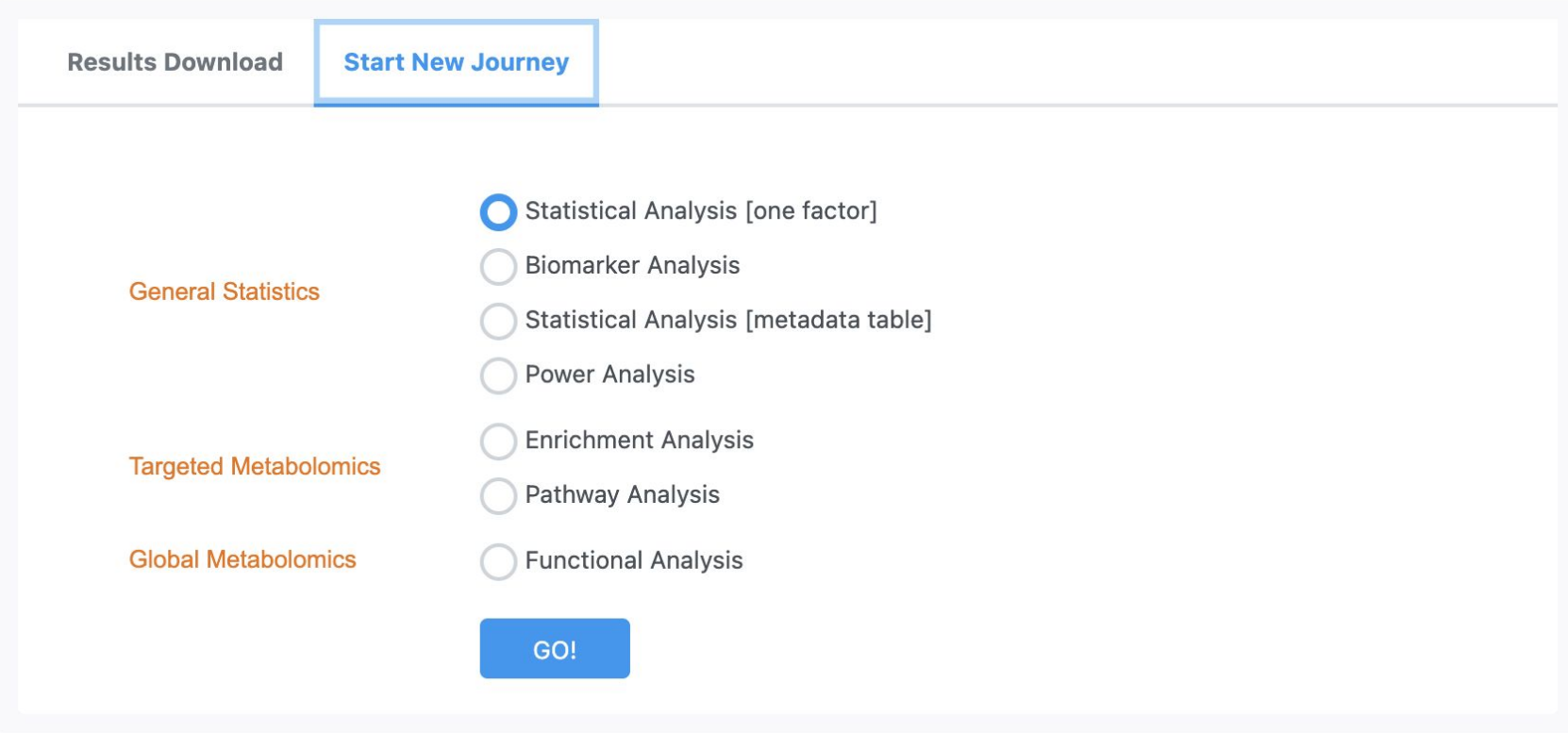


TIC: Total Ion Chromatography; EIC, Extracted Ion Chromatography.

After spectral processing, you can now ...

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.



New-generation spectra processing: **asari**

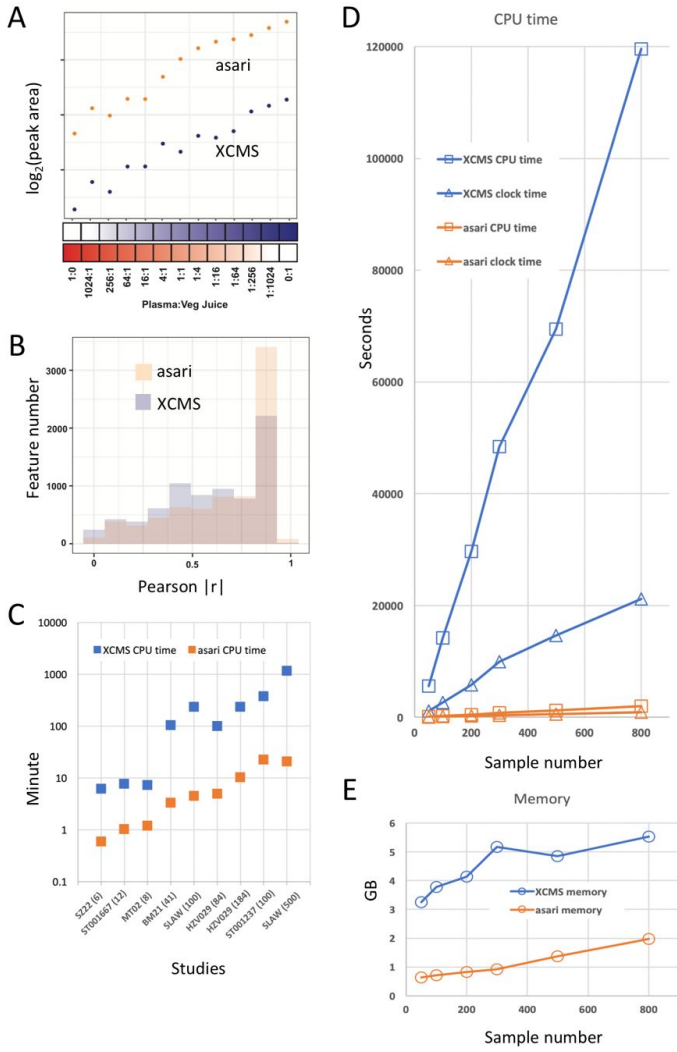
Trackable and scalable LC-MS metabolomics data processing using asari

Shuzhao Li*, Amnah Siddiqa, Maheshwor Thapa, Shujian Zheng
Jackson Laboratory for Genomic Medicine, Farmington, CT 06032, USA

*Corresponding author, E-mail: shuzhao.li@jax.org

Metabolomics holds the pr
comprehensively in biolog
mass spectrometry) has b
challenges still exist in the
experiments into metaboli
current software tools. We
MS metabolomics data processing. Asari is designed with a set of new algorithmic framework and data structures, and all steps are explicitly trackable. It offers substantial improvement of computational performance over current tools, and is highly scalable.

asari vs. XCMS
=
kallisto vs. HISAT



BioRxiv https://doi.org/10.1101/2022.06.10.495665

From compounds / peaks to functions

Compound	Retention Time (min)	Conc. in Urine (µM)
Dns-o-phospho -L-serine	0.92	<D.L.*
Dns-o-phospho -L-tyrosine	0.95	<D.L.
Dns-adnosine monophosphate	0.99	<D.L.
Dns-o-phosphoethanolamine	1.06	16
Dns-glucosamine	1.06	22
Dns-o-phospho -L-threonine	1.09	<D.L.
Dns-6-dimet hylamine purine	1.20	<D.L.
Dns-3-methyl -histidine	1.22	80
Dns-taurine	1.25	834
Dns-carnosine	1.34	28
Dns-Arg	1.53	36
Dns-Asn	1.55	133
Dns-hypotaurine	1.58	10
Dns-homocarnosine	1.61	3.9
Dns-guanidine	1.62	<D.L.
Dns-Gln	1.72	633
Dns-allantoin	1.83	3.8
Dns-L-citrulline	1.87	2.9

m.z	p.value	t.score
304.2979	1.02E-10	14.7179316
177.1024	1.62E-10	14.2666
345.0277	1.72E-10	-14.209195
491.0325	1.83E-10	-14.146348
258.0048	2.17E-10	-13.987636
483.1205	2.22E-10	-13.967634
694.9937	2.81E-10	-13.745172
270.9767	3.27E-10	13.6060705
371.604	3.53E-10	-13.534483
316.5773	3.71E-10	13.4893333
451.0505	4.04E-10	-13.412347
257.0543	4.09E-10	-13.401887
762.9787	4.71E-10	-13.274141
231.0422	5.14E-10	-13.195677
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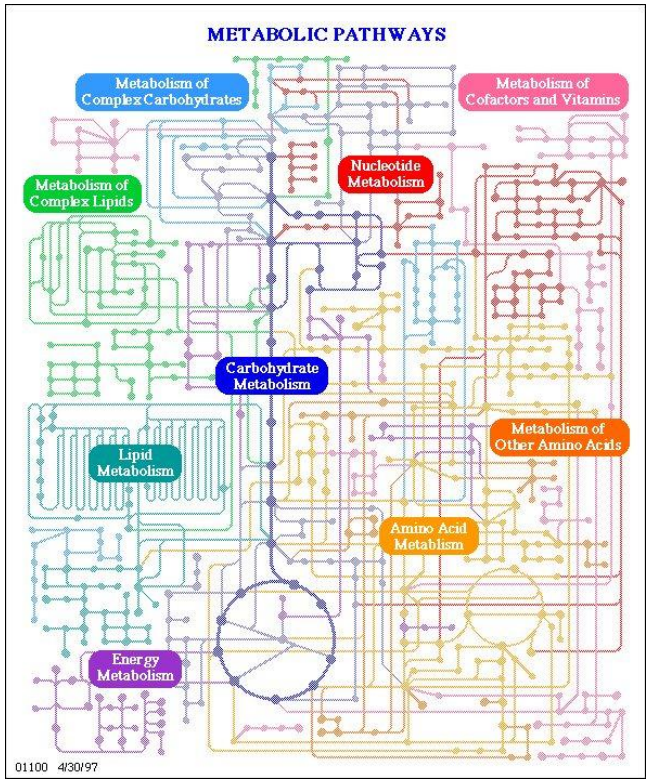
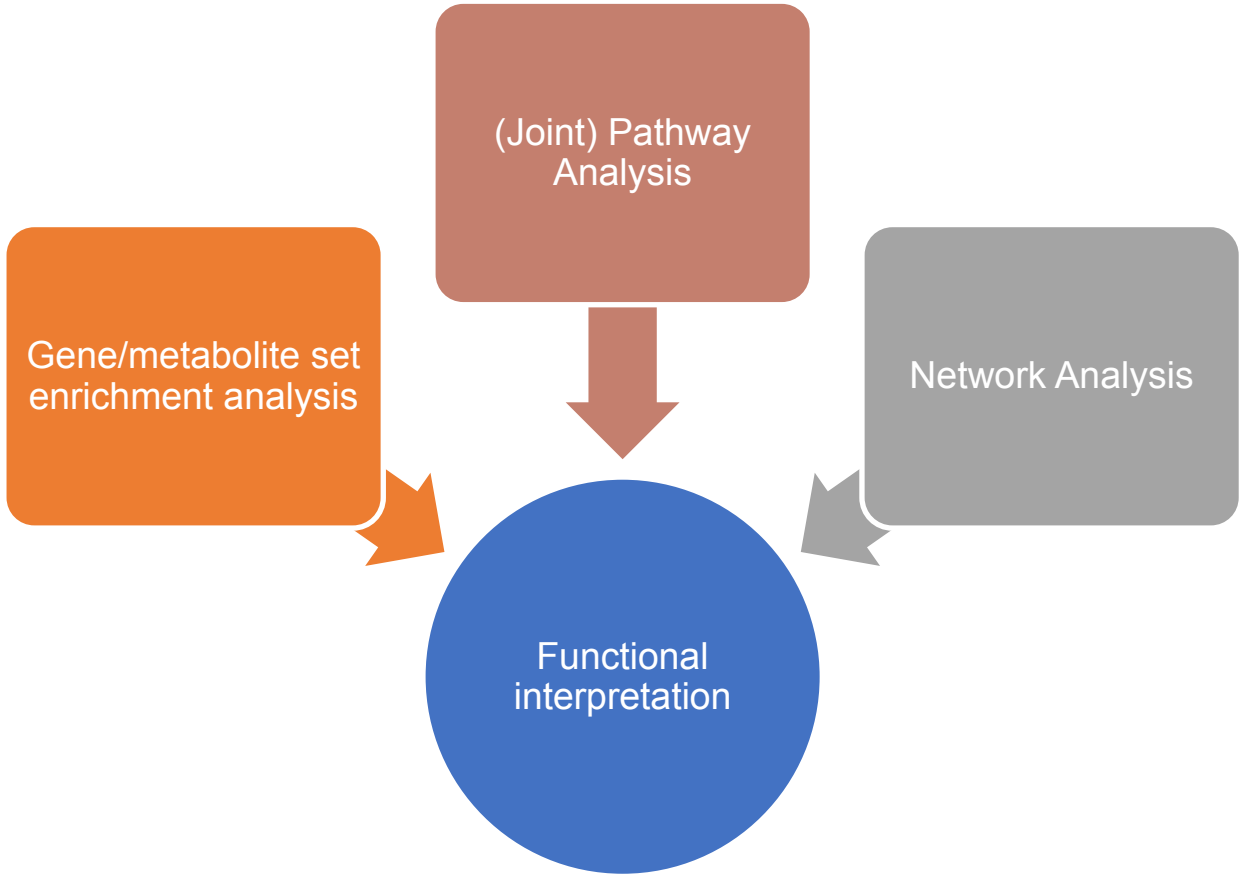
213.0066	6.79E-10	12.9471714
416.2122	7.92E-10	12.8119438



Strategies for omics data interpretation



Enrichment Analysis

- Purpose: To test if there are biologically meaningful groups of metabolites that are significantly enriched in your data
- Biological meaningful in terms of:
  - Pathways
  - Disease associated metabolite signatures
  - Localization
  - SNP associated metabolites
  - …..

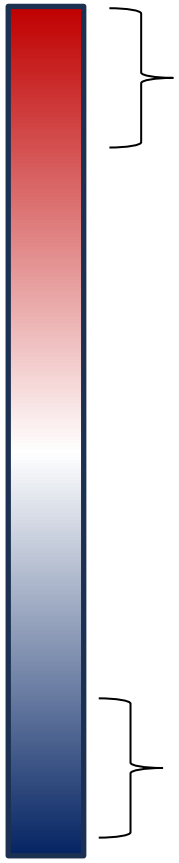
We need to define functions first

Please select a metabolite set library

Pathway based	◉ SMPDB	99 metabolite sets based on normal human metabolic pathways.
	○ KEGG	84 metabolite sets based on KEGG human metabolic pathways (Oct. 2019).
	○ Drug related	461 metabolite sets based on drug pathways from SMPDB.
Disease signatures	○ Blood	344 metabolite sets reported in human blood.
	○ Urine	384 metabolite sets reported in human urine.
	○ CSF	166 metabolite sets reported in human cerebral spinal fluid (CSF).
	○ Feces	44 metabolite sets reported in human feces.
Chemcial structures	○ Super-class	35 super chemical class metabolite sets or lipid sets
	○ Main-class	464 main chemical class metabolite sets or lipid sets
	○ Sub-class	1072 sub chemical class metabolite sets or lipid sets
Other types	○ SNPs	4,598 metabolite sets based on their associations with SNPs loci.
	○ Predicted	912 metabolic sets predicted to change in the case of dysfunctional enzymes.
	○ Locations	73 metabolite sets based on organ, tissue, and subcellular localizations.
Self defined	○ Upload here	define your own customized metabolite sets

☑ Only use metabolite sets containing at least 2 entries

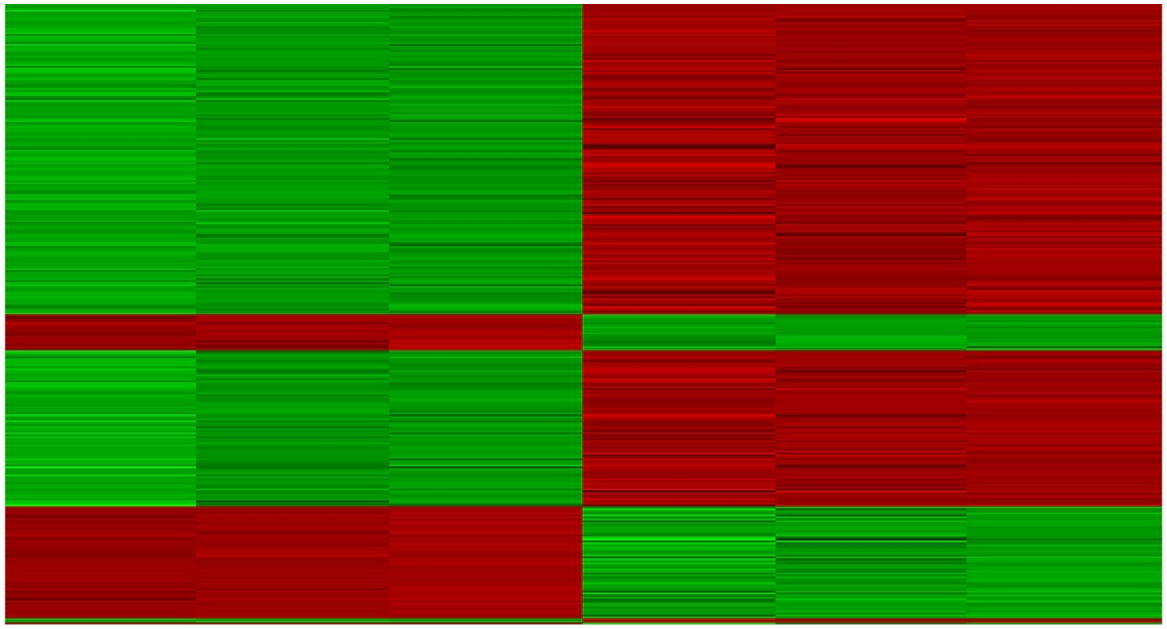
Functions are coordinated changes



Upregulated

Downregulated

- Multiple molecules work together to finish a task



Clustered (co-regulated) compounds

Detecting functional changes

- To test whether members involved in a function have more consistent changes (i.e. most move in one direction) compared to random changes
- Enrichment analysis
  - Over representation analysis (ORA)
    - Starting from significant compounds
    - Different cutoff could get different results
  - Gene Set Enrichment Analysis (GSEA)
    - A complete ranked compound list
    - Cutoff-free

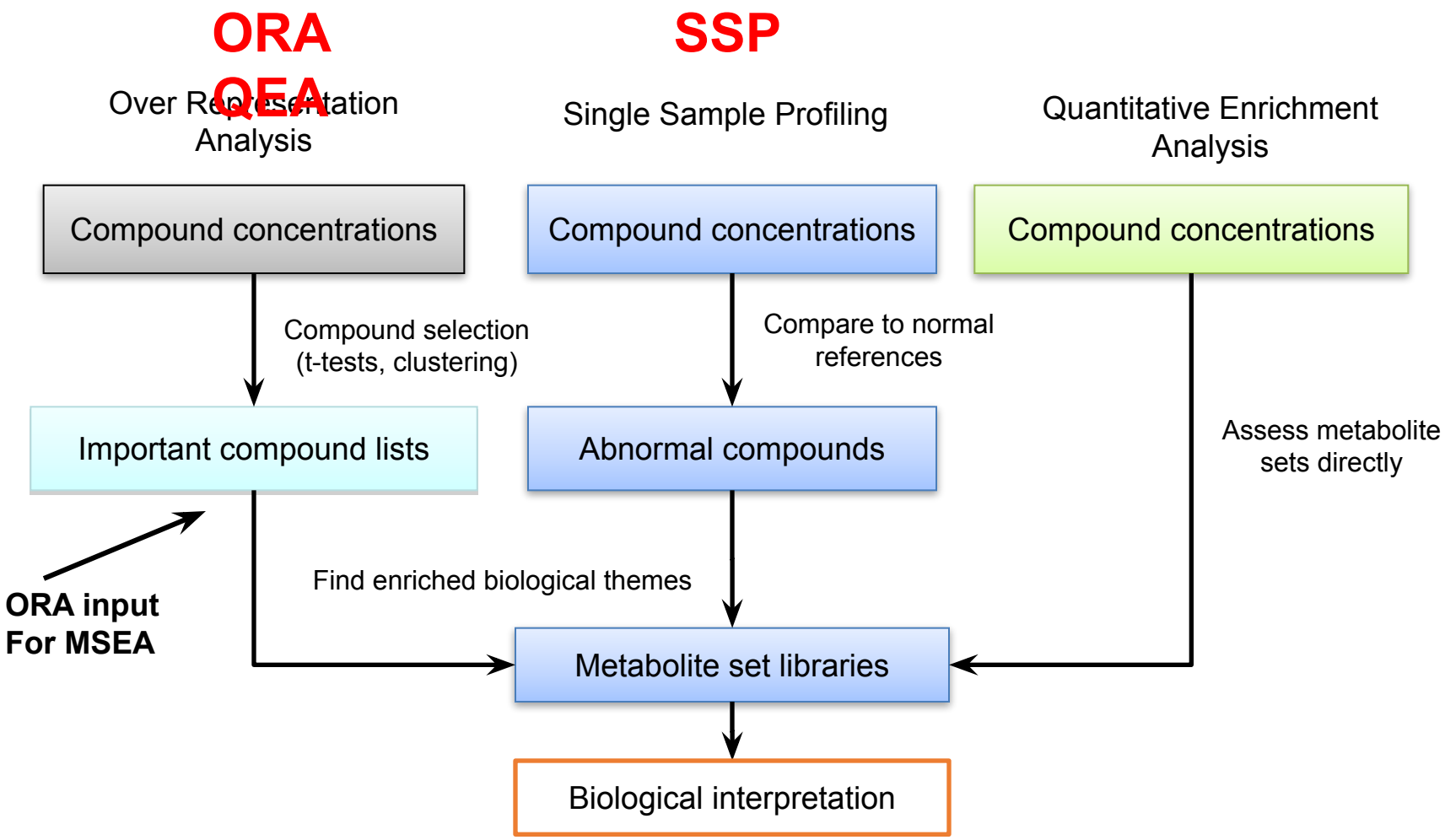
Functional analysis in metabolomics

- Targeted metabolomics is similar to gene expression profiling.
  - The compound concentration table can be used for enrichment analysis against pathways to identify which pathways or biological processes are changed significantly under the conditions.
- It is more challenging to perform functional analysis for untargeted metabolomics, as peaks cannot be directly mapped to pathways
  - Can we predict functions from peaks in a similar manner?

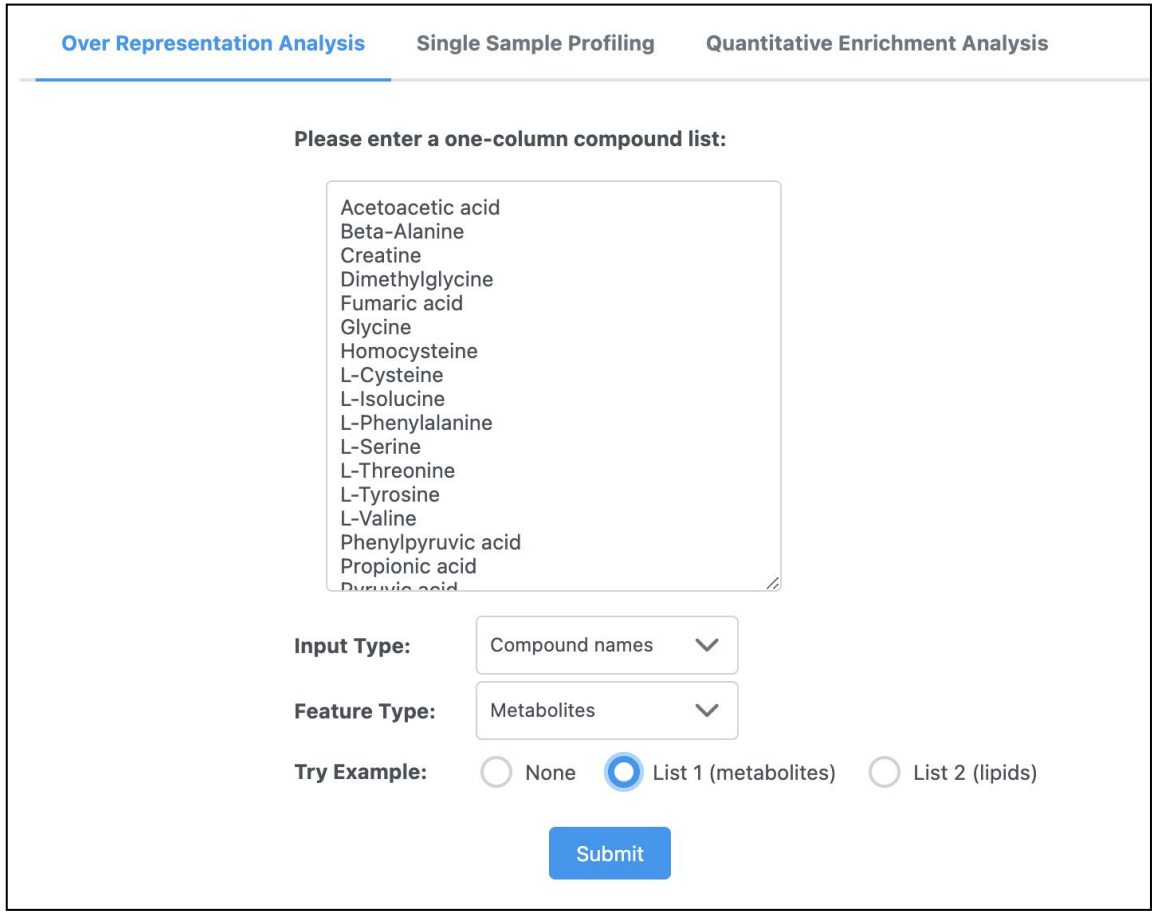
Metabolite Set Enrichment Analysis

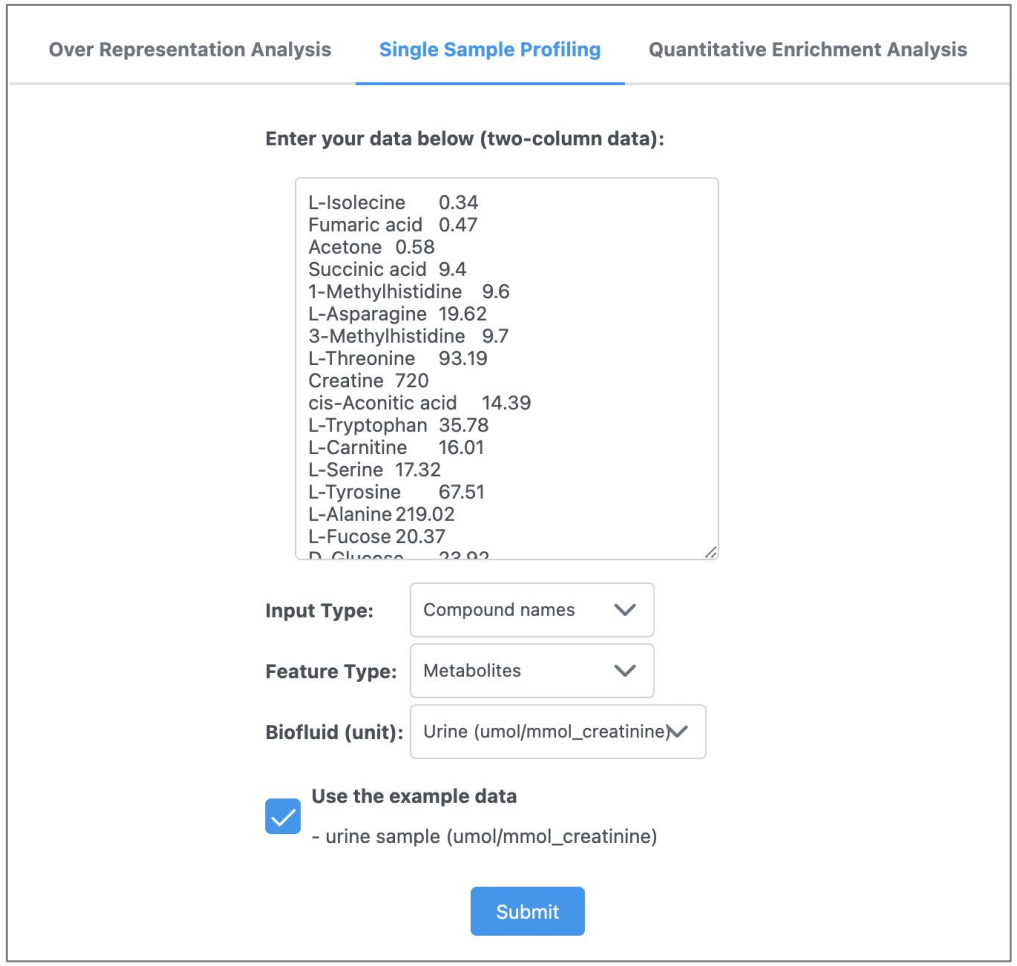
- **Similar to Gene Set Enrichment Analysis (GSEA)**
- **Accepts 3 kinds of input files**
  - list of metabolite names only (ORA – over representation analysis)
  - list of metabolite names + concentration data from a single sample (SSP – single sample profiling)
  - a concentration table with a list of metabolite names + concentrations for multiple samples/patients (QEA – quantitative enrichment analysis)

The MSEA Approach



Upload a compound list, or sample concentration





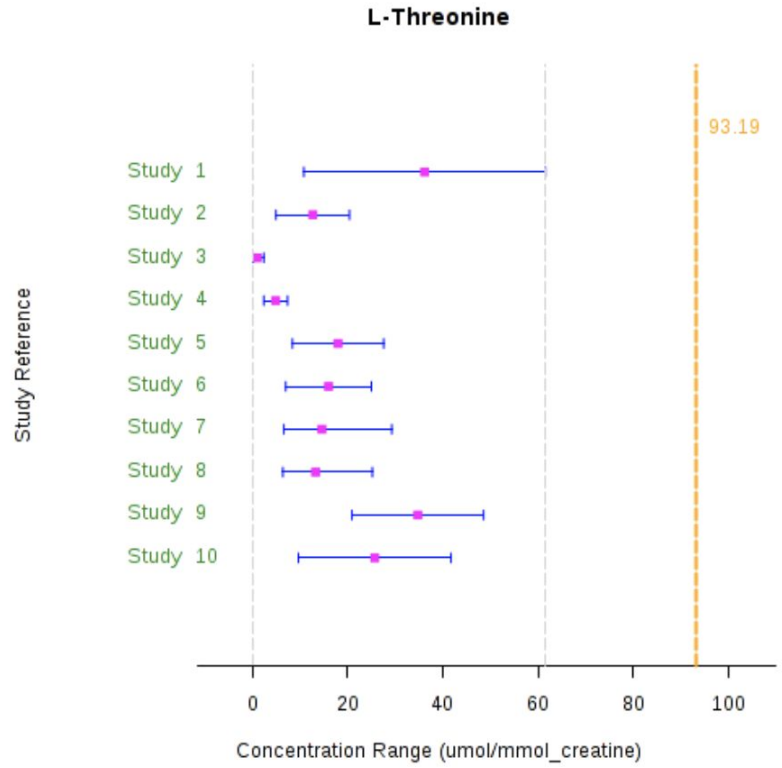
Concentration Comparison (Single Sample Profiling)

Comparison with Reference Concentration

Note: *reference concentrations* are in the form of **mean(min - max)** format. In cases where the ranges were not reported in the original literature, the min and max were calculated using the 95% confidence intervals. In the *Comparison* column, **H, M, L** means **higher, medium (within range), lower** compared to the reference concentrations. Click the **Image Icon** link to see a graphical summary for the comparisons.

Compound	Concentration	Reference concentrations	Comparison	Detail	Include
Fumaric acid	0.47	0.95 (0.02 - 1.88); 10.4 (2.8 - 53.7); 0.5 (0.1 - 1.7); 10.7 (0.1 - 28.2); 0.4 (0.2 - 0.8); 0.7 (0.2 - 1.7); 1.342 (0.025 - 2.659)	M	View	☐
Acetone	0.58	4.2 (0.98 - 15.3); 0.92 (0.2 - 2.8); 3.9 (0.8 - 17.6); 2.24 (0 - 6.37); 3.914 (0 - 7.843)	M	View	☐
Succinic acid	9.4	7.7 (1.9 - 20); 197.2 (29.4 - 486.2); 185.4 (6 - 342.6); 11.6 (4 - 27.3); 8.25 (0.5 - 16); 9.9 (4.9 - 14.9); 14.4 (9.5 - 19.3); 12.6 (0.47 - 24.73); 3.8 (1.25 - 6.7); 14.48 (11.28 - 17.68); 7.5 (0.5 - 16); 5.6 (1.8 - 9.4); 6.2 (2.5 - 13.5); 4.7 (1.1 - 14.5); 6 (0.3 - 33.3); 14.581 (4.918 - 24.244); 163.491 (0 - 355.25)	M	View	☐
1-Methylhistidine	9.6	4.6 (1.9 - 7.3); 2.3 (0 - 7.4); 46.1 (0 - 99.6); 15.9 (0 - 35.4); 28.1 (0 - 59.9); 1.3 (0 - 4.06); 45.5 (3.9 - 87.1); 33.6 (0 - 70); 30 (0 - 73); 8.3 (2.4 - 28.4); 15.9 (0 - 35.4); 21.329 (8.358 - 34.3); 46.0833 (0 - 99.5153); 45.473 (3.856 - 87.09); 15.919 (0 - 35.422); 33.624 (0 - 69.984); 28.0954 (0 - 59.9214); 2.34 (0 - 7.4164); 1.334 (0 - 4.093)	M	View	☐
L-Asparagine	19.62	0.96 (0.31 - 1.61); 9.211 (3.289 - 15.1); 10 (4.6 - 16.32); 10.52 (6.67 - 14.37); 8.8 (4.6 - 17.7); 9.5 (3 - 26); 10.1 (4.6 - 17.8); 35.7098 (23.0844 - 48.3352); 25.158 (1.696 - 48.62)	M	View	☐
3-Methylhistidine	9.7	12.5 (8.3 - 16.7); 42.76 (19.92 - 65.6); 16.5 (2.8 - 59.8); 44.944 (3.626 - 86.262); 17.977 (12.075 - 23.879); 18.191 (11.1587 - 25.2233); 15.806 (10.402 - 21.21); 13.556 (11.069 - 16.043); 18.203 (11.691 - 24.715); 17.705 (11.70151 - 23.70849); 16.0206 (11.1256 - 20.9156); 17.0268 (15.4548 - 18.5988)	M	View	☐
L-Threonine	93.19	36.2 (10.82 - 61.58); 12.7 (4.934 - 20.4); 1 (0.16 - 2.4); 4.9 (2.4 - 7.4); 18 (8.4 - 27.6); 16 (7 - 25); 14.6 (6.6 - 29.3); 13.3 (6.4 - 25.2); 34.7611 (20.9314 - 48.5908); 25.712 (9.672 - 41.752)	H	View	☑

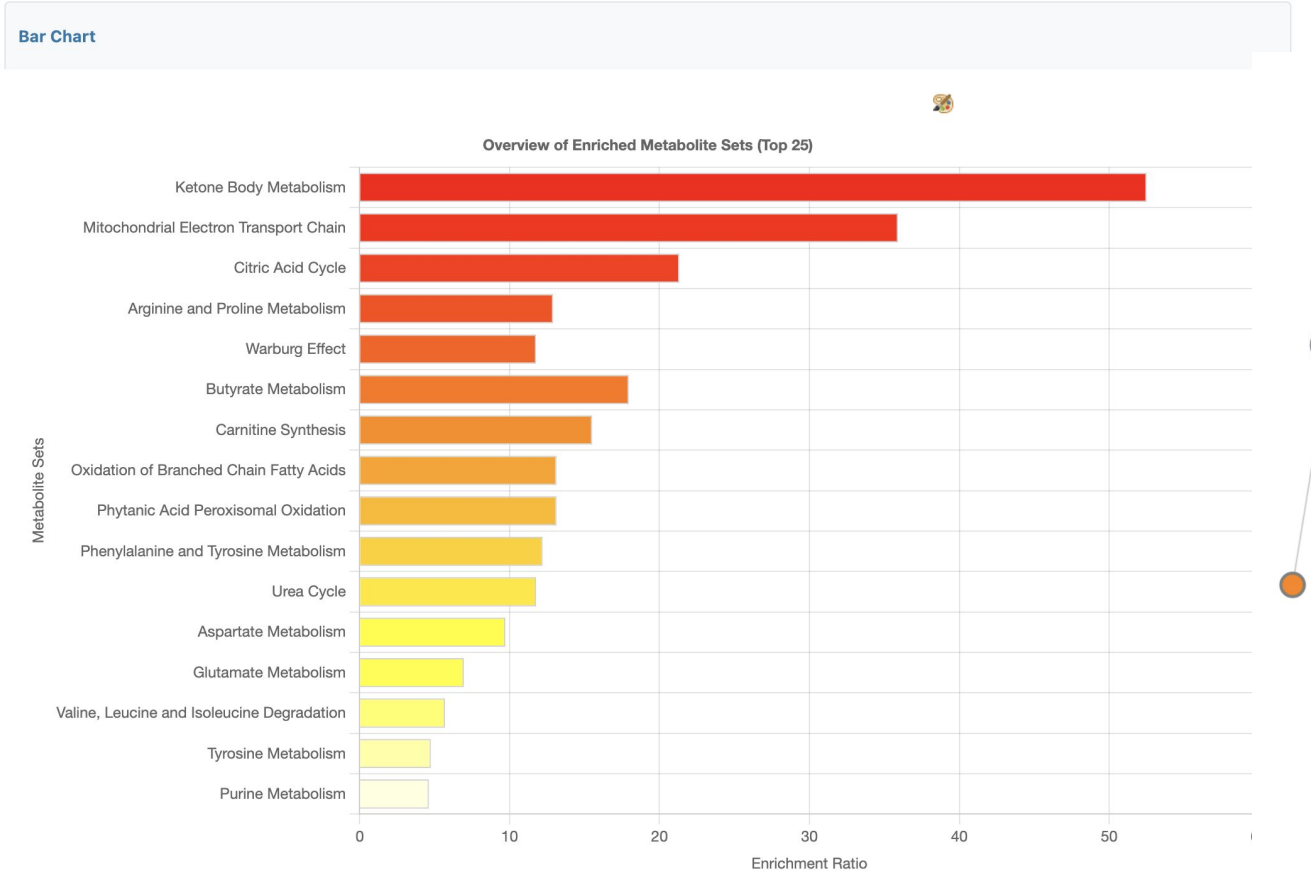
Concentration comparison (cont.)

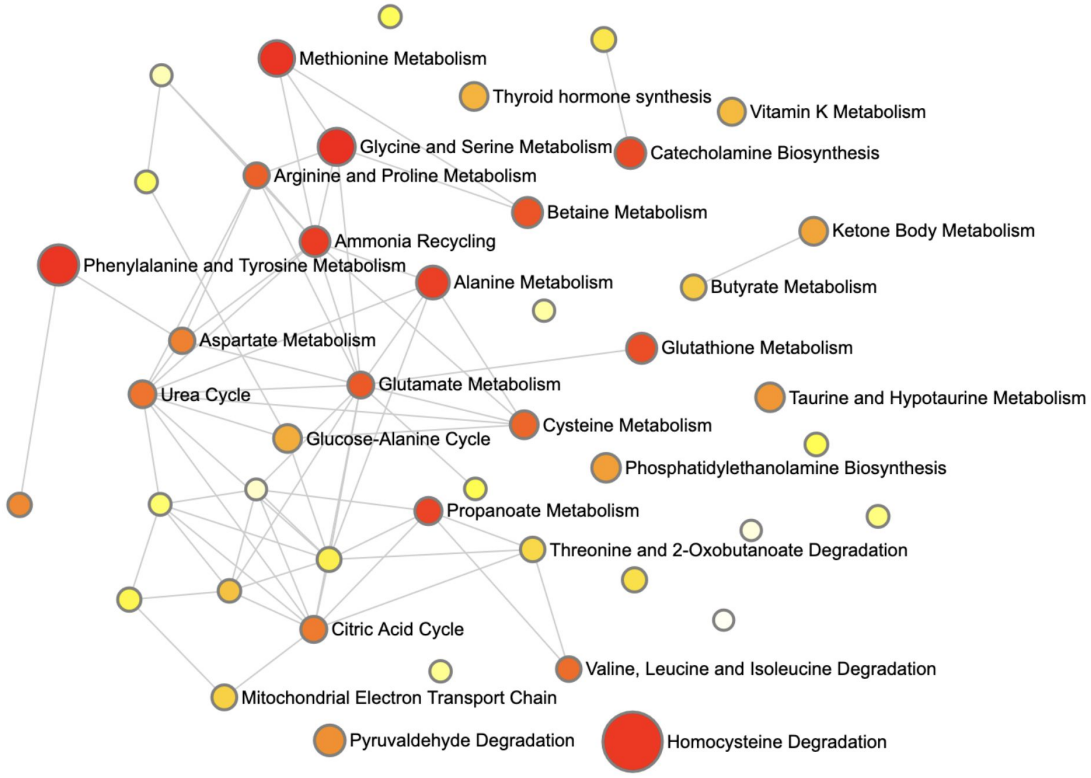


Study	Concentration	Reference	Note
Study 1	36.2 (10.82 - 61.58)	(Pubmed)	Both
Study 2	12.7 (4.934 - 20.4)	(Pubmed)	Both
Study 3	1 (0.16 - 2.4)	Geigy Scientific Tables, 8th Rev edition, pp. 165-177. Edited by Cornelius Lentner.; West Cadwell, N.J. : Medical education Div., Ciba-Geigy Corp.; Basel, Switzerland c1981-1992. (Pubmed)	Both
Study 4	4.9 (2.4 - 7.4)	Geigy Scientific Tables, 8th Rev edition, pp. 165-177. Edited by Cornelius Lentner.; West Cadwell, N.J. : Medical education Div., Ciba-Geigy Corp.; Basel	Female

Normal ranges based on reports from literature from HMDB

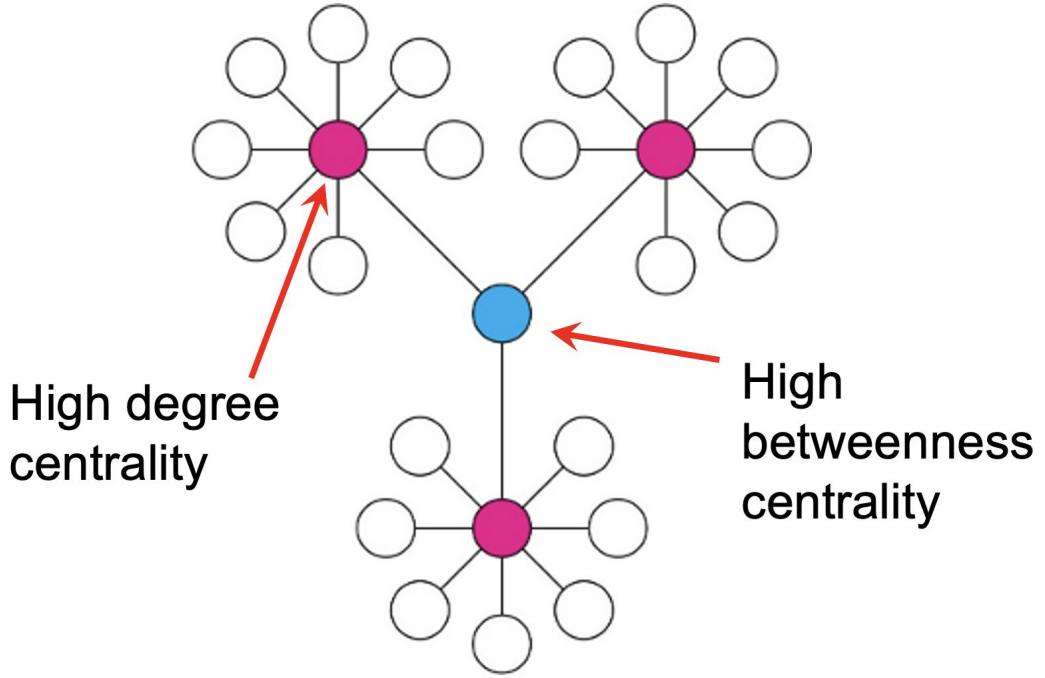
Results from Enrichment Analysis (targeted)





Pathway analysis – consider structures

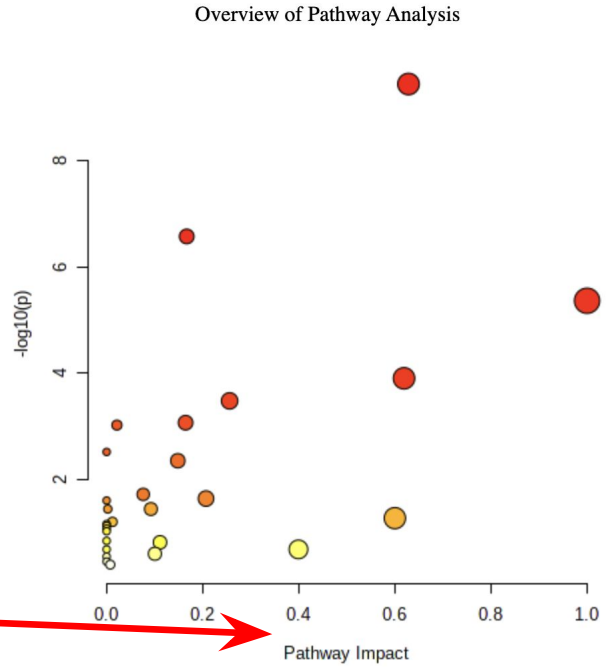
- Which positions are important?
  - Hubs
    - Nodes that are highly connected (red ones)
  - Bottlenecks
    - Nodes on many shortest paths between other nodes (blue ones)
- Graph theory
  - Degree centrality
  - Betweenness centrality

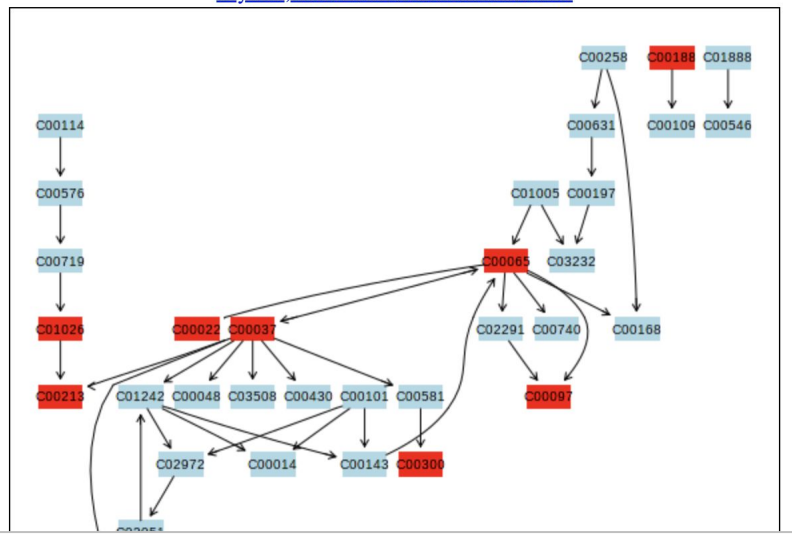


Junker *et al. BMC Bioinformatics* 2006

Pathway Results

Pathway Impact: normalized sum of degree / betweenness values of matched nodes within each pathway





Click the corresponding **Pathway Name** to view its graphical presentation:

Pathway Name	Match
Glycine, serine and threonine metabolism	8/33
Aminoacyl-tRNA biosynthesis	7/48
Phenylalanine, tyrosine and tryptophan biosynthesis	3/4

Matched metabolites:

Pathway	Metabolites
Glycine, serine and threonine metabolism	**L-Serine**; Choline; Betaine aldehyde; Betaine; Guanidinoacetate; 3-Phospho-D-glycerate; **N,N-Dimethylglycine**; L-Cystathionine; **Glycine**; O-Phospho-L-serine; **Sarcosine**; 5,10-Methylenetetrahydrofolate; **L-Threonine**; Lipoylprotein; Aminoacetone; D-Glycerate; [Protein]-S8-aminomethyldihydrolipoyllysine; Tetrahydrofolate; Dihydrolipoylprotein; 2-Phospho-D-glycerate; D-Serine; Hydroxypyruvate; **Creatine**; 3-Phosphonooxypyruvate; **L-Cysteine**; 2-Oxobutanoate; Glyoxylate; L-2-Amino-3-oxobutanoic acid; **Pyruvate**; CO2; 5-Aminolevulinate; Methylglyoxal; Ammonia

OK

Generate report & download results

Metabolomic Data Analysis with MetaboAnalyst 4.0

Name: guest7188993447605746741

June 11, 2020

1 Background

The Pathway Analysis module combines results from powerful pathway enrichment analysis with pathway topology analysis to help researchers identify the most relevant pathways involved in the conditions under study.

There are many commercial pathway analysis software tools such as Pathway Studio, MetaCore, or Ingenuity Pathway Analysis (IPA), etc. Compared to these commercial tools, the pathway analysis module was specifically developed for metabolomics studies. It uses high-quality KEGG metabolic pathways as the backend knowledgebase. This module integrates many well-established (i.e. univariate analysis, over-representation analysis) methods, as well as novel algorithms and concepts (i.e. Global Test, GlobalAncova, network topology analysis) into pathway analysis. Another feature is a Google-Map style interactive visualization system to deliver the analysis results in an intuitive manner.

2 Data Input

The Pathway Analysis module accepts either a list of compound labels (common names, HMDB IDs or KEGG IDs) with one compound per row, or a compound concentration table with samples in rows and compounds in columns. The second column must be phenotype labels (binary, multi-group, or continuous). The table is uploaded as comma separated values (.csv).

3 Compound Name Matching

The first step is to standardize the compound labels used in user uploaded data. This is a necessary step since these compounds will be subsequently compared with compounds contained in the pathway library. There are three outcomes from the step - exact match, approximate match (for common names only), and no match. Users should click the textbfView button from the approximate matched results to manually select the correct one. Compounds without match will be excluded from the subsequently pathway analysis.

Table 1 shows the conversion results. Note: *1* indicates exact match, *2* indicates approximate match, and *0* indicates no match. A text file contain the result can be found the downloaded file *name_map.csv*

Table 1: Result from Compound Name Mapping

	Query	Match	HMDB	PubChem	KEGG	SMILES
1	1,6-Anhydro-beta-D-glucose	Levoglucosan	HMDB0000640	2724705		C1[C@@H]2[C@H]([C@@H][C@
2	1-Methylnicotinamide	1-Methylnicotinamide	HMDB0000699	457	C02918	C[N+]1=CC=CC(=C1)C(=O)N
3	2-Aminobutyrate	L-Alpha-aminobutyric acid	HMDB0000452	80283	C02356	CC[C@@H](C(=O)O)N
4	2-Hydroxyisobutyrate	Alpha-Hydroxyisobutyric acid	HMDB0000729	11671		CC(C)(C(=O)O)O
5	2-Oxoglutarate	Oxoglutaric acid	HMDB0000208	51	C00026	C(CC(=O)O)C(=O)C(=O)O

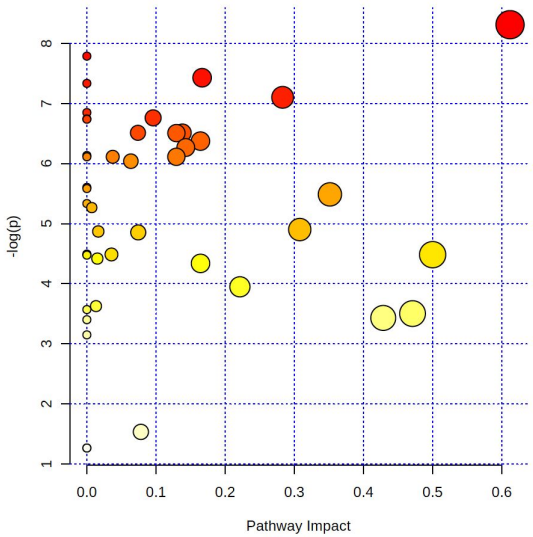
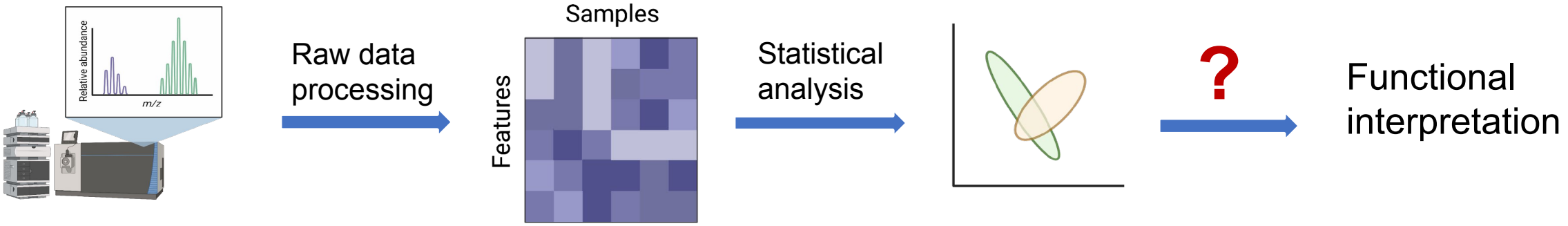
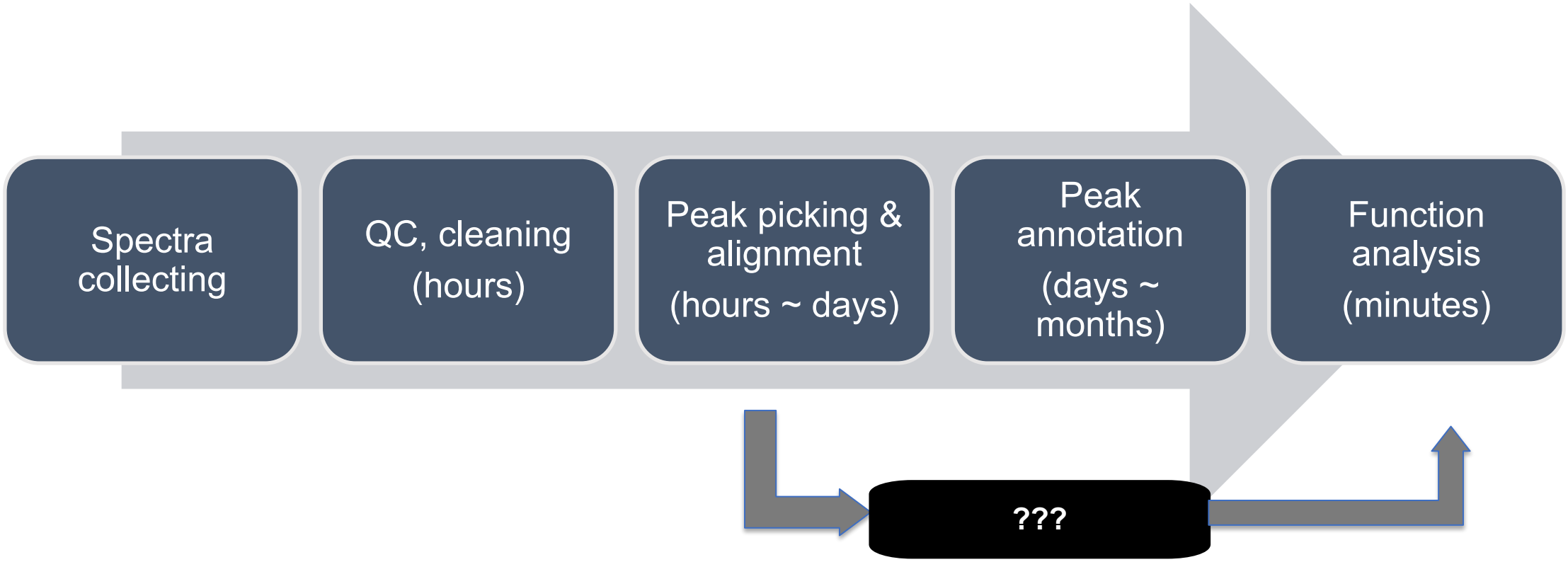


Figure 1: Summary of Pathway Analysis

Can we do the same to untargeted metabolomics?

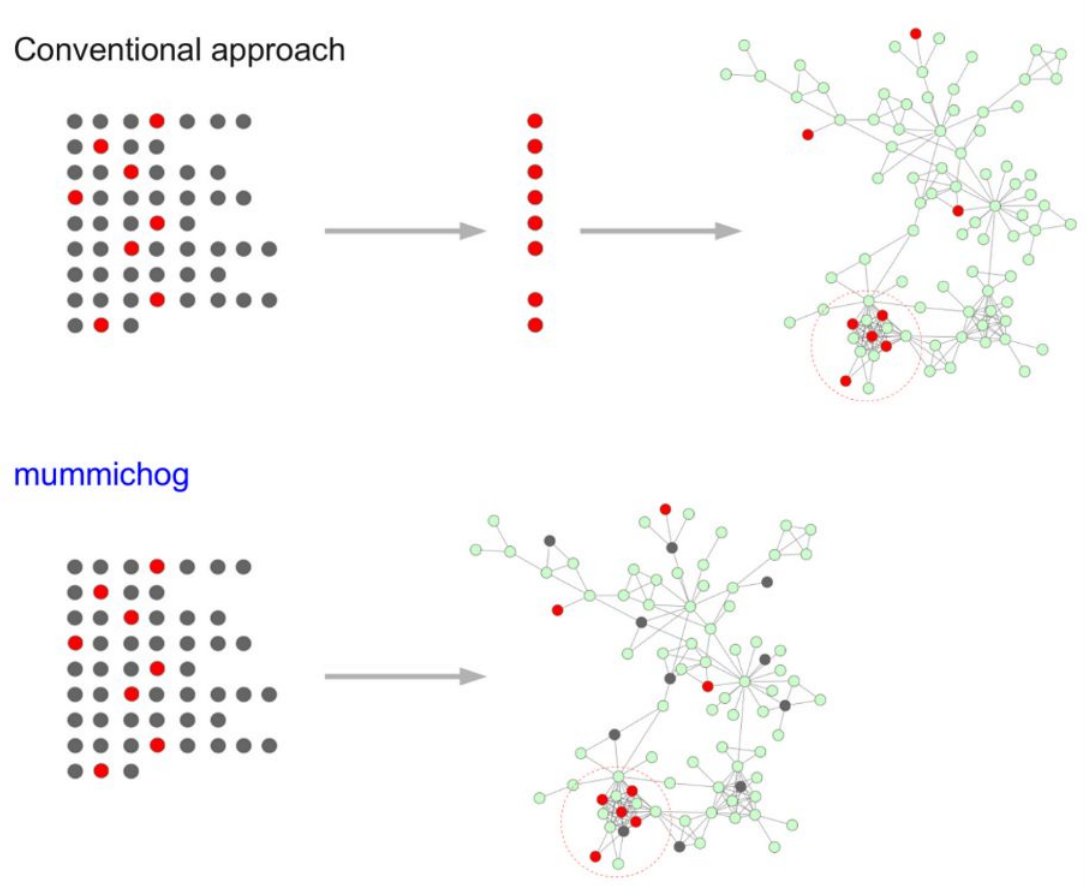


Conventional approaches requires compound ID known



Can we perform enrichment analysis direct from peaks?

Mummichog



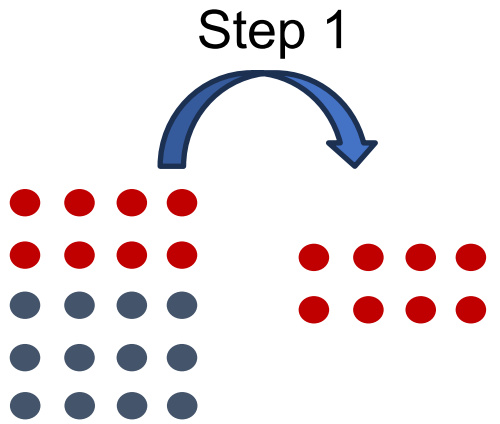
- We have a general idea what each peak is
- We have an idea of how each compound in a pathway could look like as peaks
- Mummichog: map many possible matches to a background pathway and look for consistent functional patterns
- Pathway-level results will be robust

S. Li *et al.*, *Plos Computational Biology* (2013).

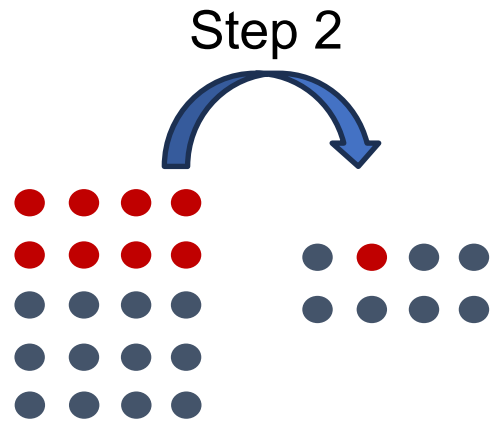
How does mummichog work?

Input requirement:

- Significant list: selected by t-test or fold change
- Reference list: all features detected



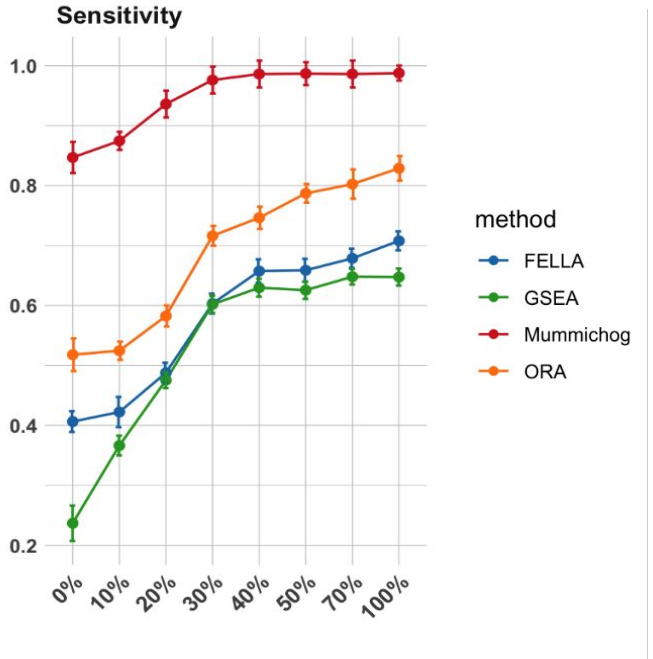
Step 1: Match the peaks to tentative metabolites. Looked up all the significant metabolites in each pathway and calculate the p-value using Fisher's exact test



Step 2: Randomly pull features with the same length as the significant ones, and repeat Step 1 for 100 ~ 1000 times

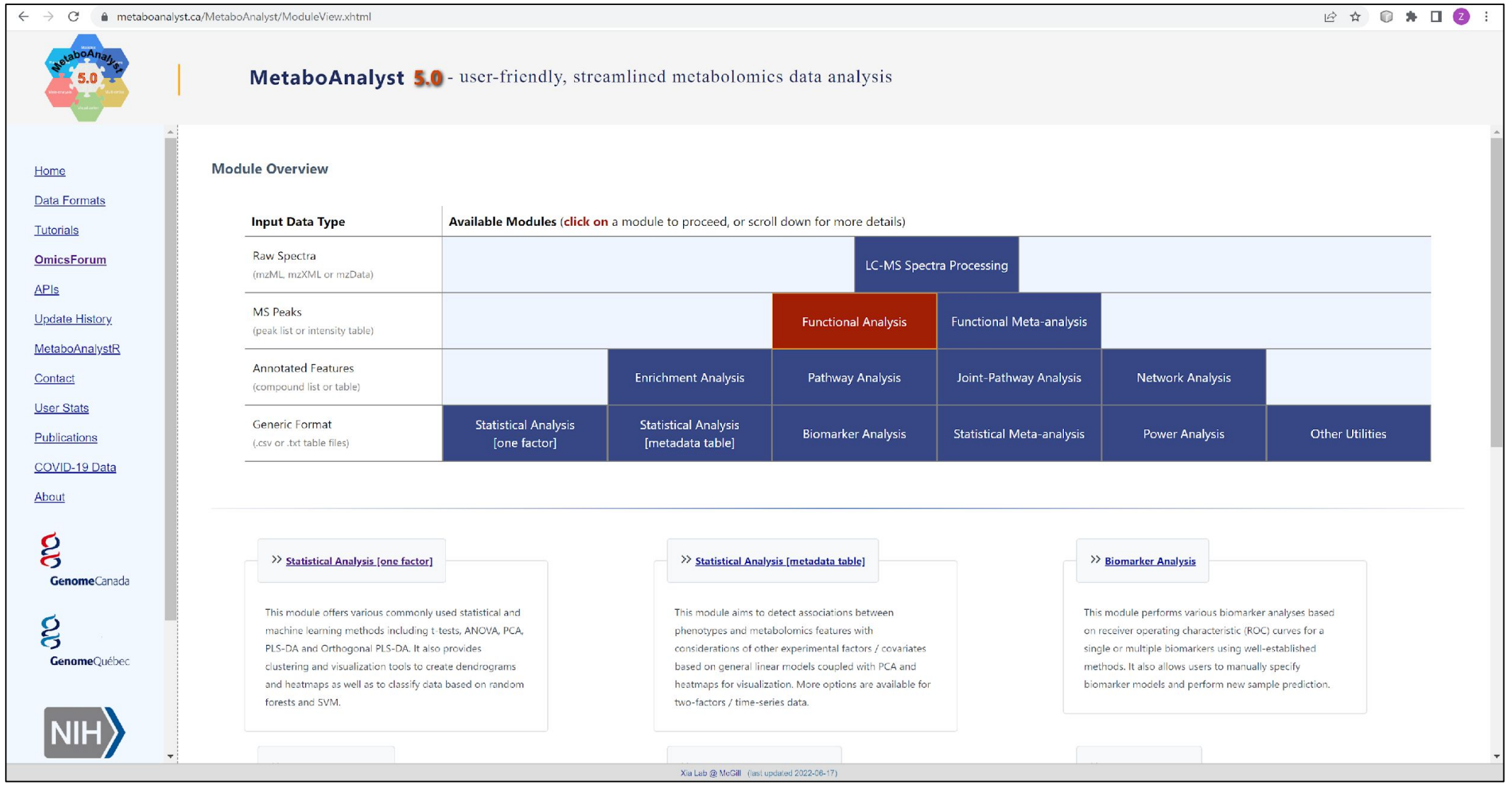
Step3: Test if certain pathways are enriched in the significant peaks as compared to null models (Gamma distribution)

Mummichog – sensitive, robust enrichment analysis for untargeted metabolomics



Y. Lu *et al.*, *Briefings in Bioinformatics* (2023).

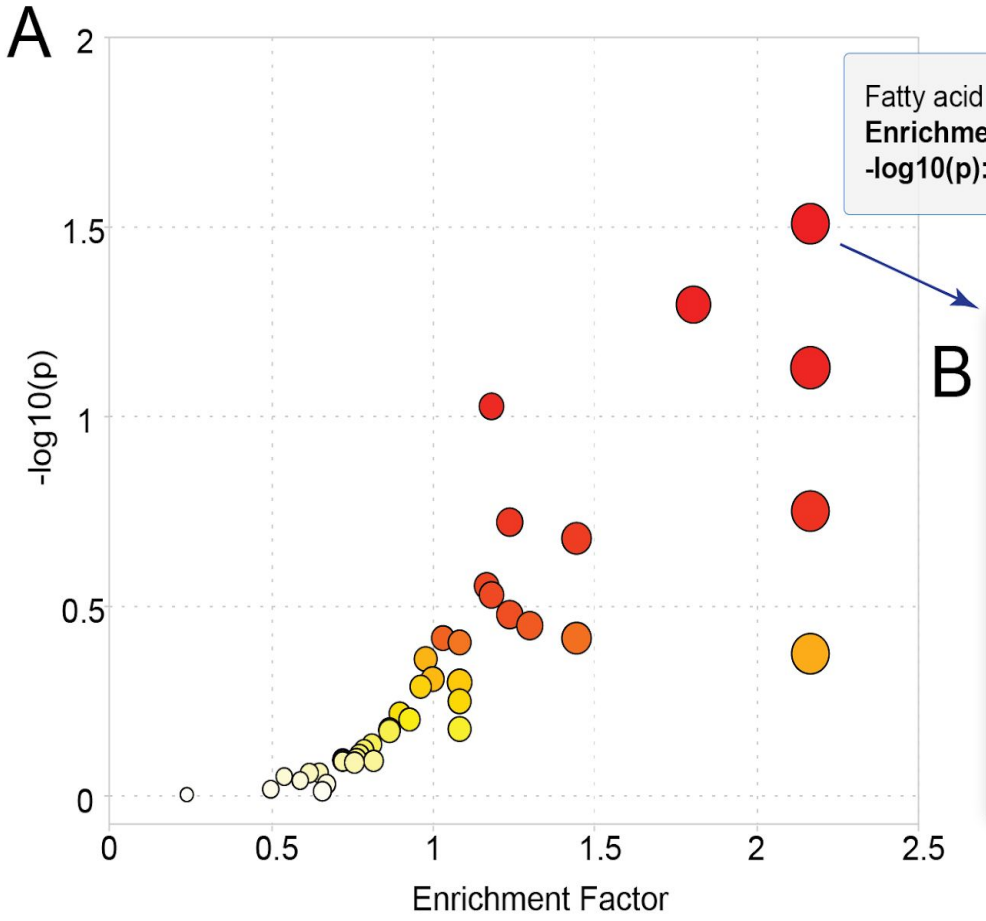
Implementation in MetaboAnalyst



Critical: input preparation

- LC - **high-resolution** MS (HR-MS)
  - Orbitrap, Q-TOF
  - Reason: putative annotation needs to be approximately correct (better guess leads to more accurate functional analysis)
- Needs to be **complete** peak list or peak intensity table
  - Not just significant peaks
  - Reason: mummichog using permutation to estimate the null/background distribution
- In general, the algorithm works well for **> 3000** peaks (assuming human plasma samples).

From ranked peak lists to functions



Fatty acid oxidation
Enrichment Factor: 2.168962
-log10(p): 1.506919

B

Functional Analysis

Match Details

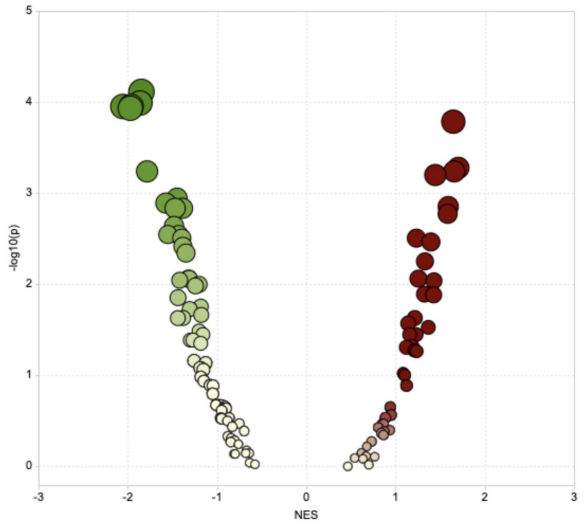
Pathway	Metabolites
Fatty acid oxidation	C00024; C00027; strdnccoa; C00100; C01944; q10h2; dmhptcoa; etfrd; C03035; etfox; dmnoncoa; arachdcoa; dcsptn1coa; ptdcacoa; C00412; od2coa; hdcoa; C02593 ; dlnlcgcoa; vacccoa; C00010; C00016; adrncoa; C00154; lneldccoa; lnlccoa; c226coa; lnlncacoa ; C00399; odecoa; hpdcacoa; C01352; eicostetcoa; tmndnccoa; arachcoa;

How to interpret result table (key parameters)

Pathway Name	Total	Hits (all)	Hits (sig.)	Expected	P(Fisher)	P(Gamma)	Details
Vitamin E metabolism	54	38	15	5.0563	0.030024	0.025523	View
Carnitine shuttle	72	25	10	6.7418	0.06554	0.028334	View

- **Total**: the total number of the given pathway
- **Hits (all)**: all the peaks mapped to the pathway
- **Hits (sig)**: all the significant peaks mapped to the pathway
- **Expected:** The expected number of metabolite hits in the pathway.
- **P(Fischer)**: The Fisher's exact p-value for the pathway
- **P(Gamma)**: P-values derived from Gamma distribution based on permutation tests for the pathway.

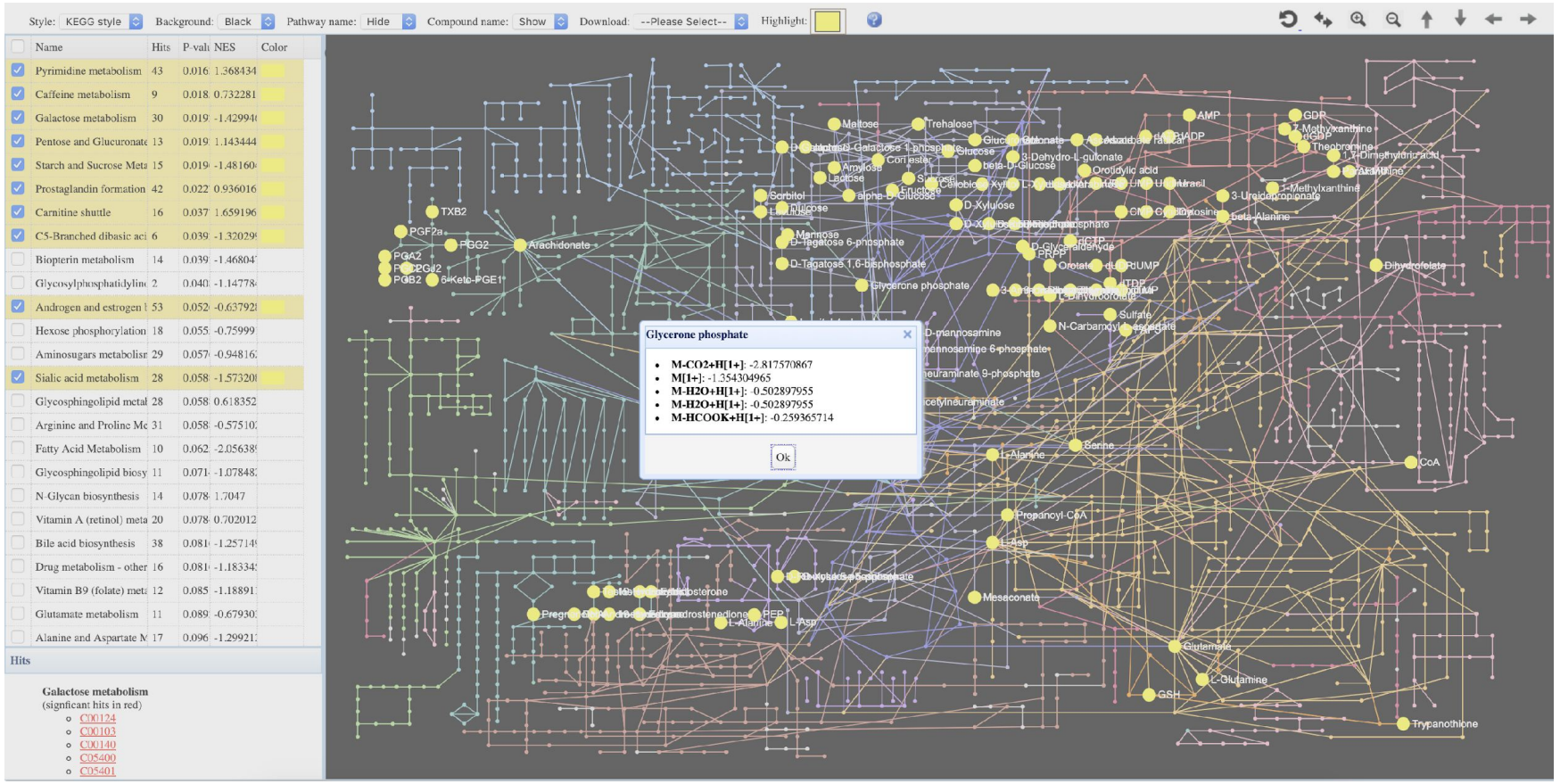
From pathways to “candidate” compounds



The red compounds indicate all potential matches from the user's input to the selected pathway.

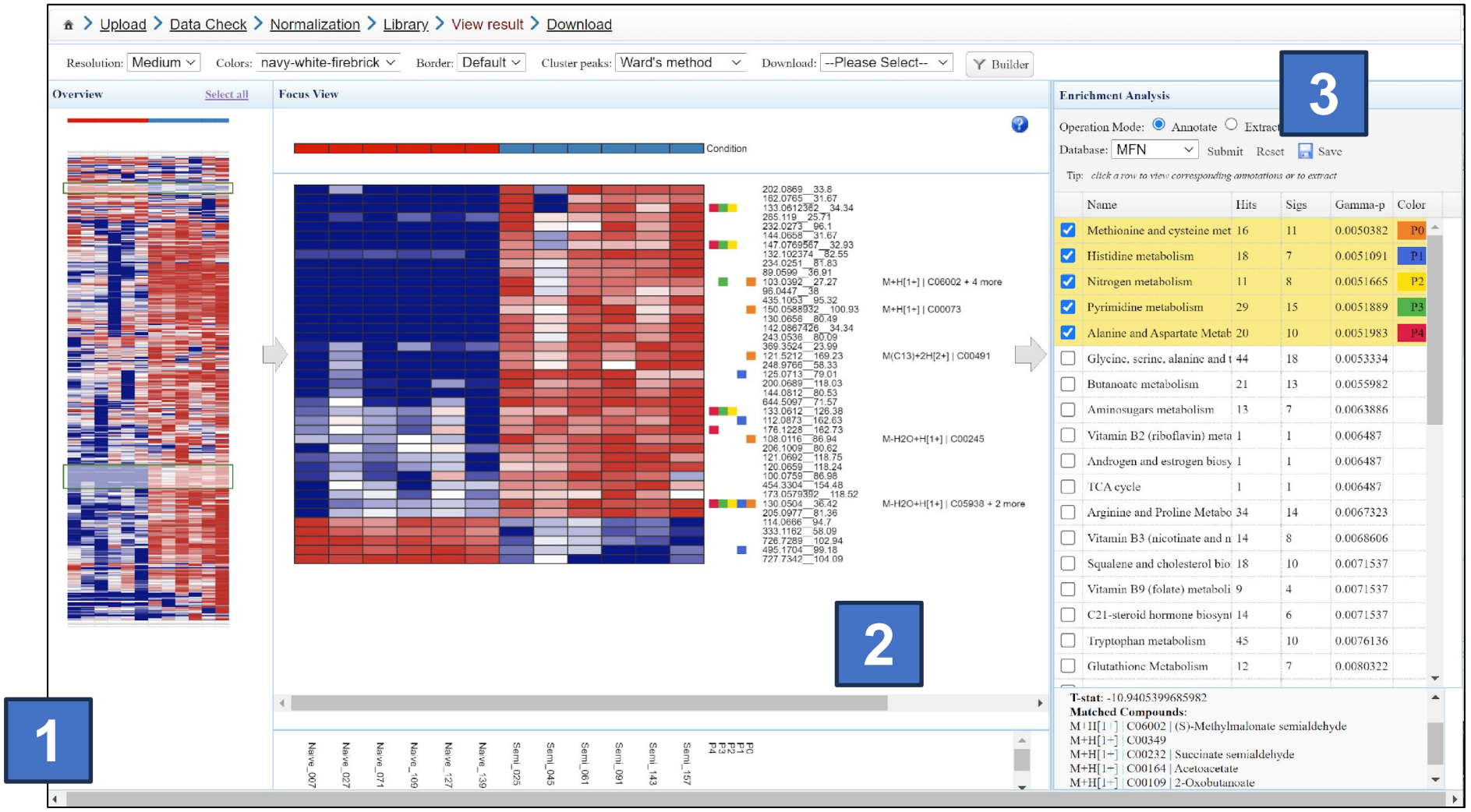
Pathway	Metabolites
Prostaglandin formation from arachidonate	**CE5703**; CE5700; CE6238; **C00425**; CE5707; **CE5704**; **CE5705**; CE5724; CE5708; CE1243; CE6236; C00584; **CE5535**; **C00959**; **CE5537**; **CE5925**; **CE5533**; C13856; **CE0955**; **CE4980**; C01312; CE5304; **C04686**; CE4938; **C05963**; **C04741**; **CE5931**; **CE0737**; **C01041**; CE4878; **CE5926**; **C00051**; **CE5924**; **C00219**; C00704; **CE5928**; **CE5929**; **C00020**; CE4876; **C00010**; **C05954**; C00024; **C05962**; C00030; **C00072**; CE7107; CE7105; C00028; C00696; **CE1447**; **C04685**; **C11695**; CE6244; CE6245; CE6242; CE6243; **CE6240**; CE6241; **C05953**; C00027; **C05956**; **C05957**; C00427; **C05955**; CE4877; CE6235; **C05959**; **C00639**; CE5730; **CE5534**; **CE5930**; C00282; **CE3481**; C00189; CE7054; C11304; C02198; **CE5828**

OK

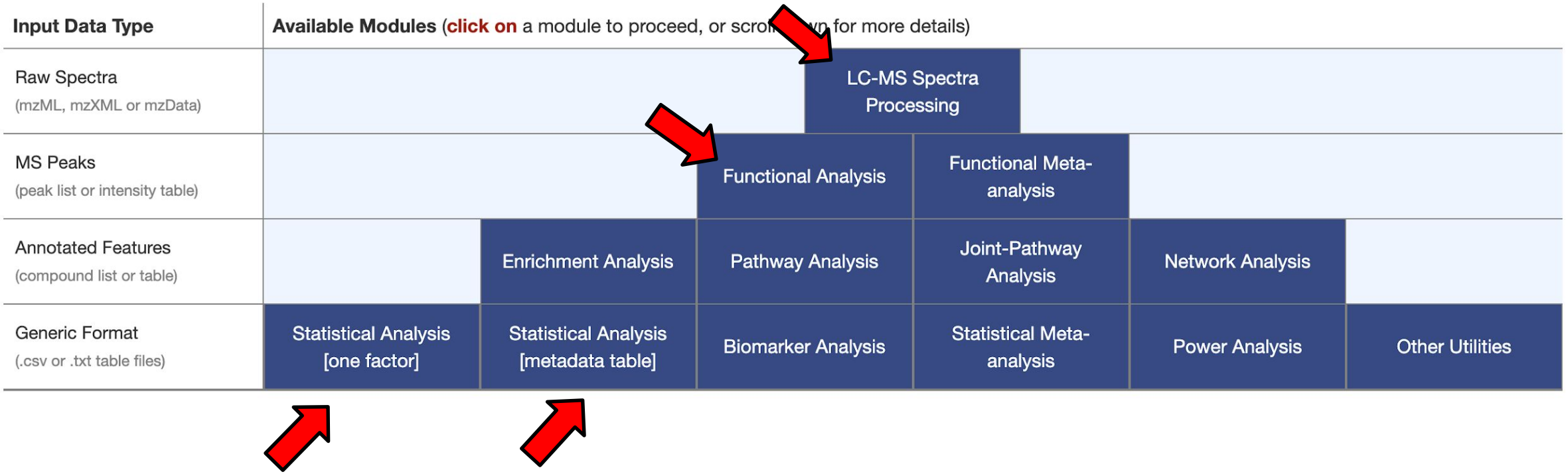


Both mummichog and GSEA are available in MetaboAnalyst 5.0

From patterns to functions



MetaboAnalyst 5.0 Lab



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