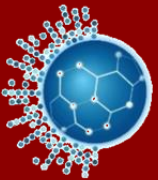


iMetaLab Suite: A One-stop Toolset for Metaproteomics

Leyuan Li¹, Zhibin Ning¹, Kai Cheng, Xu Zhang,
Caitlin M.A. Simopoulos, Daniel Figeys*



uOttawa

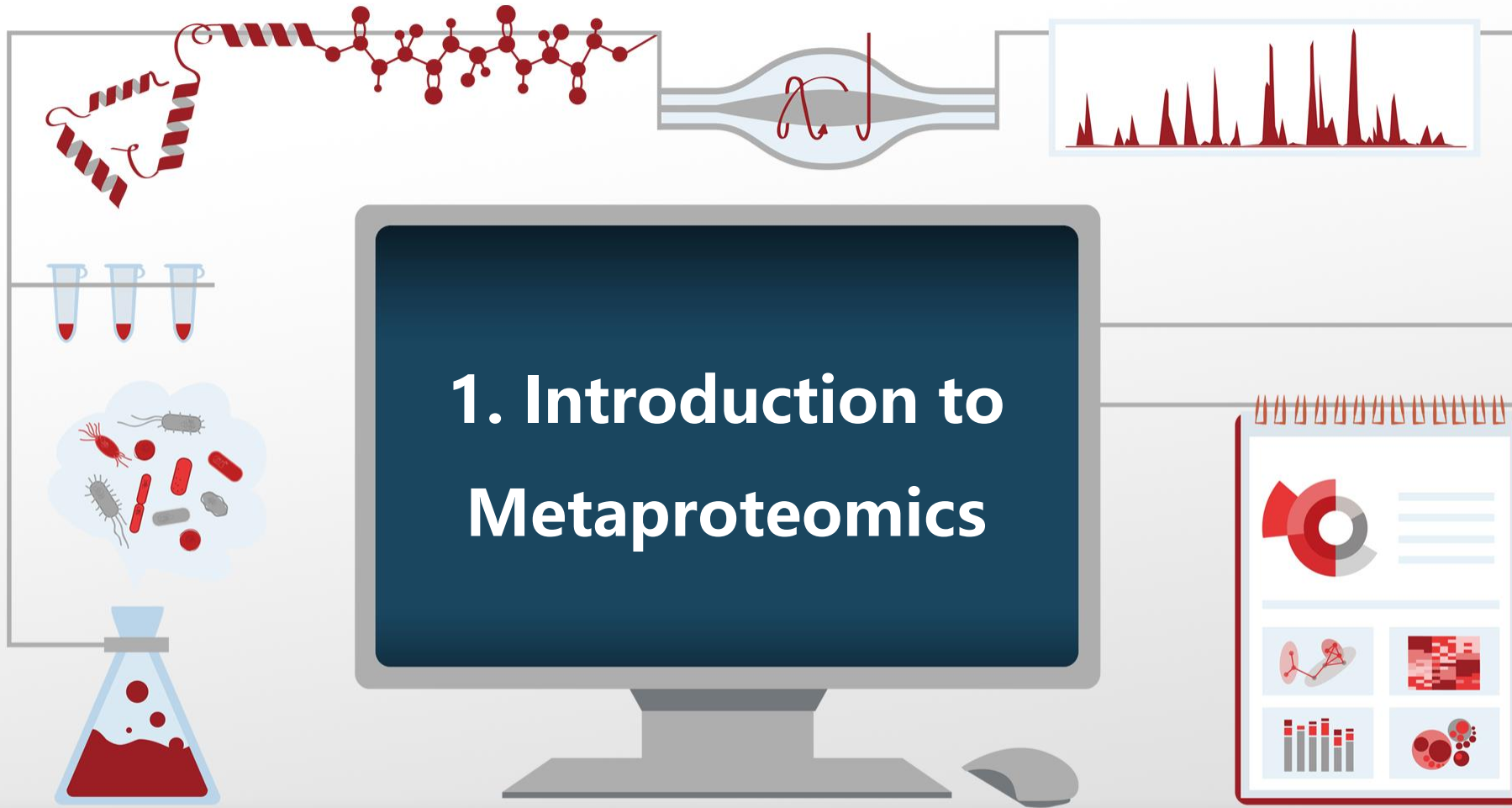


School of Pharmaceutical Sciences, Faculty of Medicine, University of Ottawa,
Ottawa, ON, Canada

Ottawa Institute of Systems Biology, University of Ottawa, Ottawa, ON, Canada

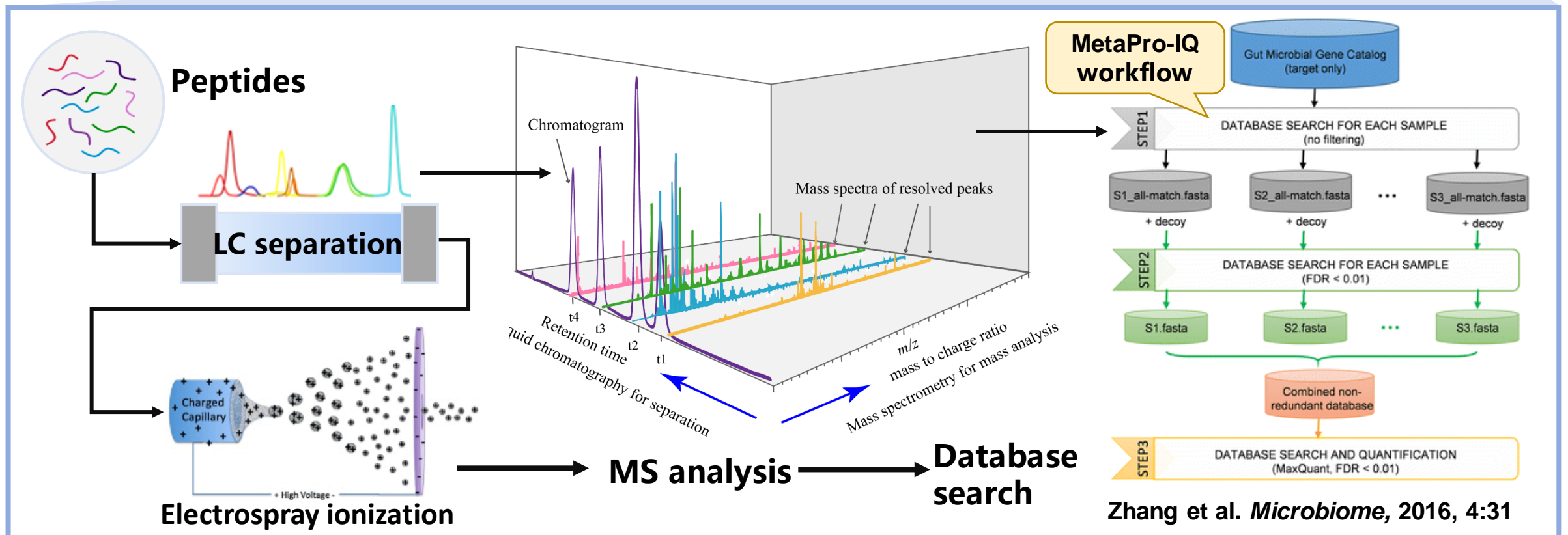
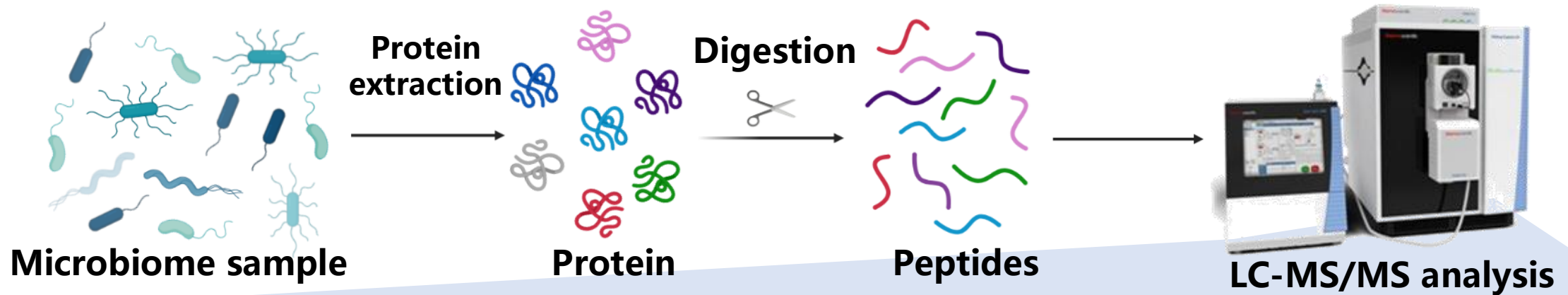


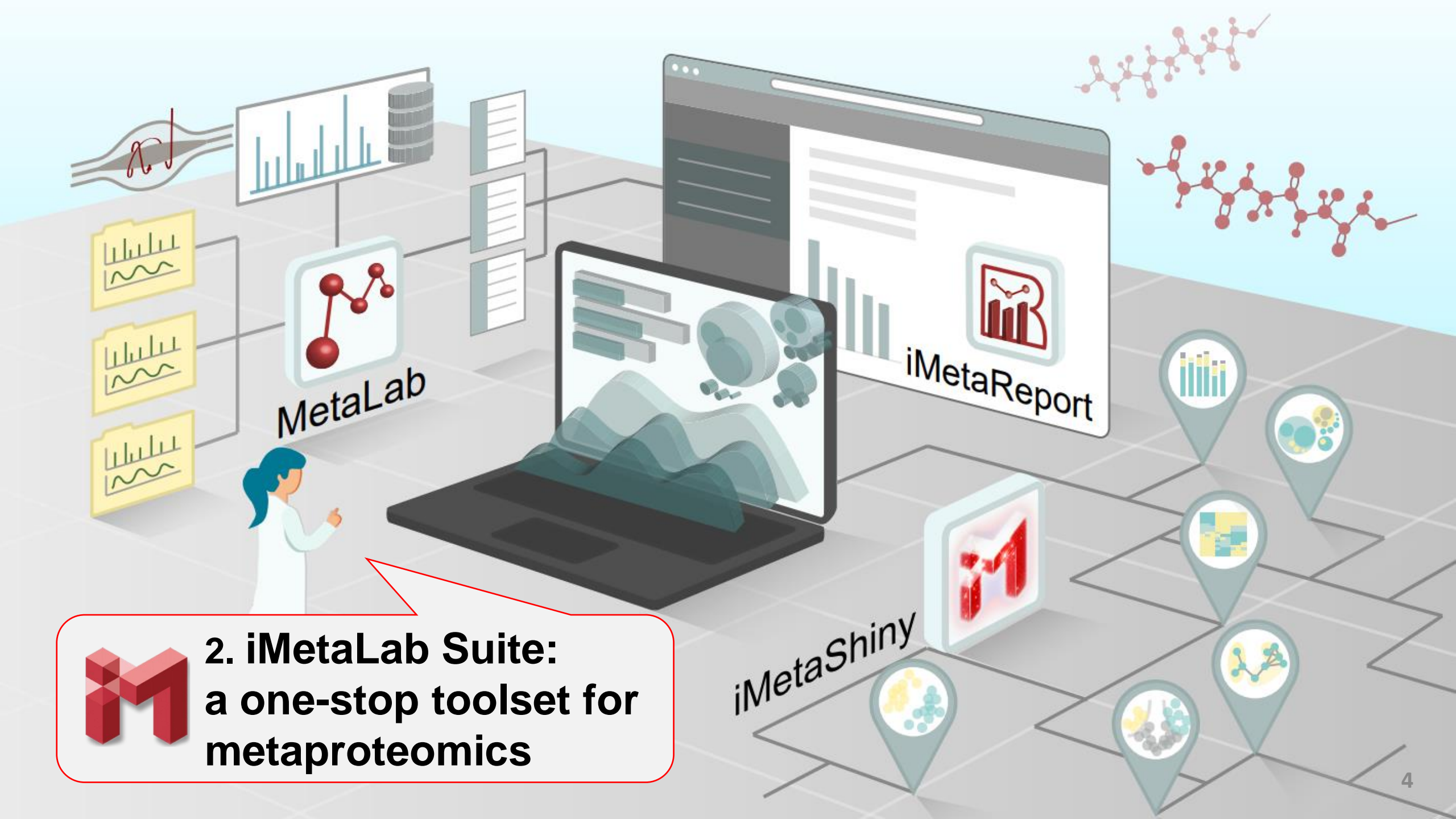
Li, Leyuan, Zhibin Ning, Kai Cheng, Xu Zhang, Caitlin M. A. Simopoulos, and Daniel Figeys. 2022.
iMetaLab Suite: A one-stop toolset for metaproteomics. iMeta e25. <https://doi.org/10.1002/imt2.25>



1. Introduction to Metaproteomics

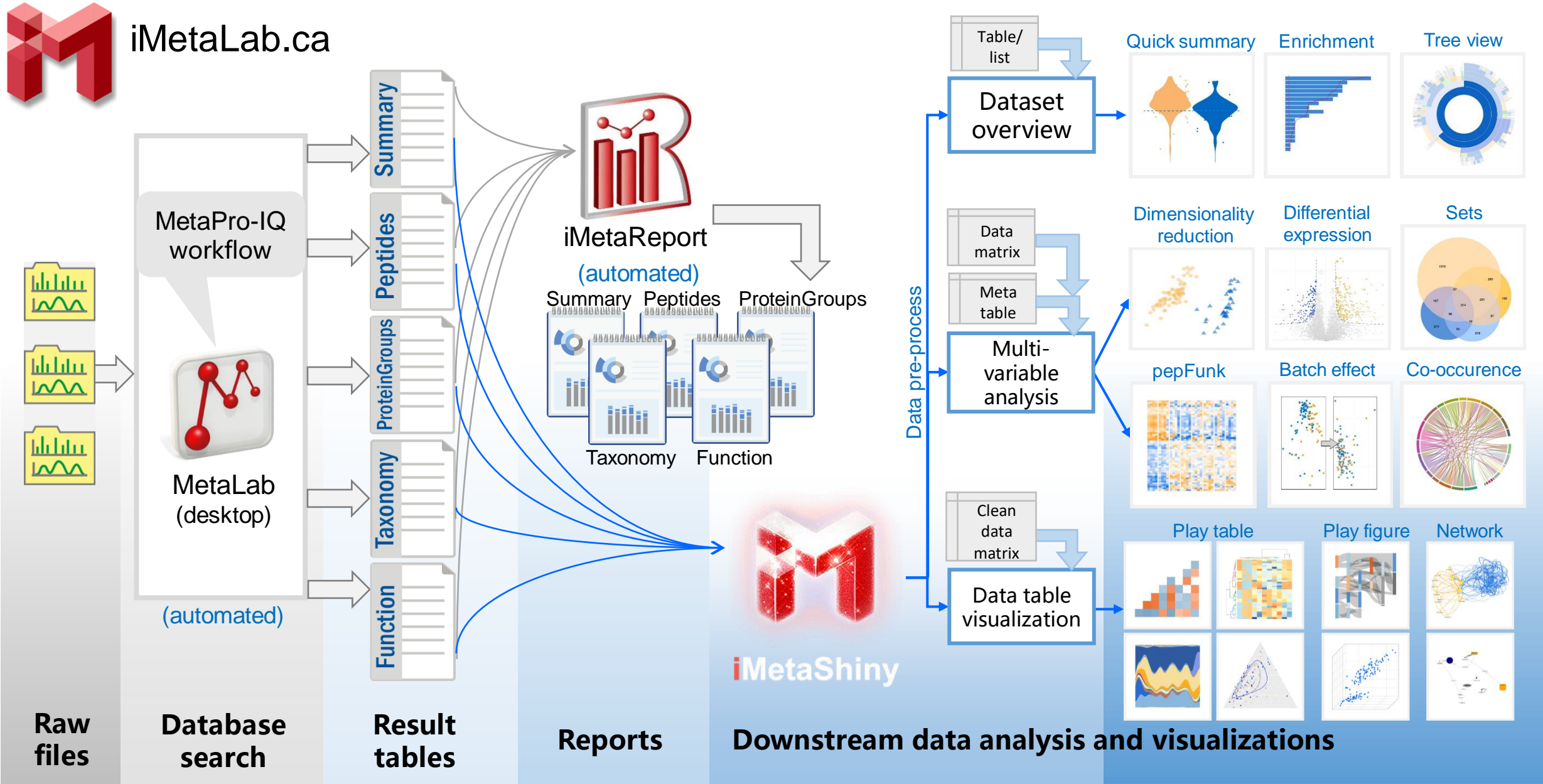
A typical workflow of metaproteomic analysis

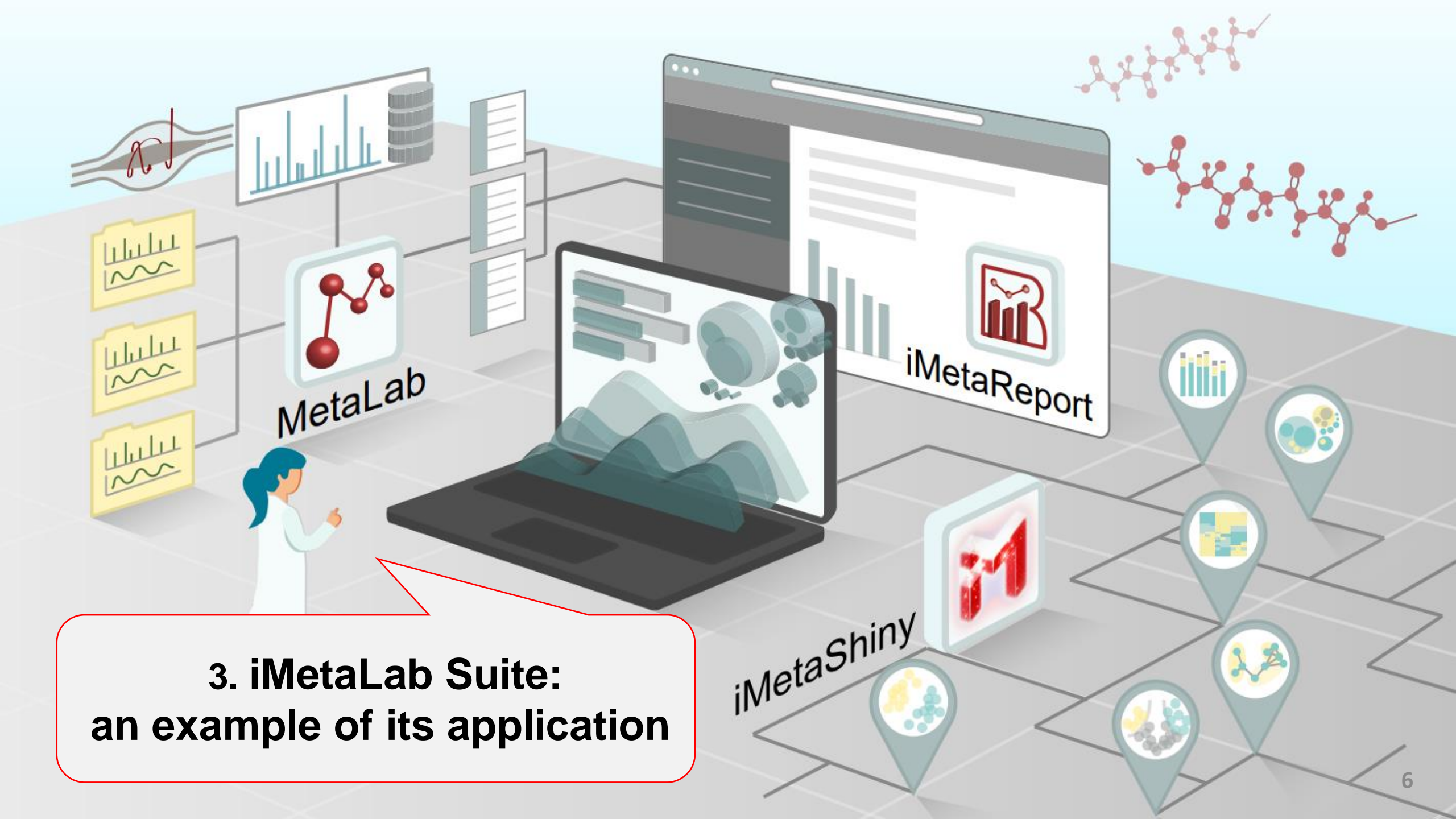




**2. iMetaLab Suite:
a one-stop toolset for
metaproteomics**

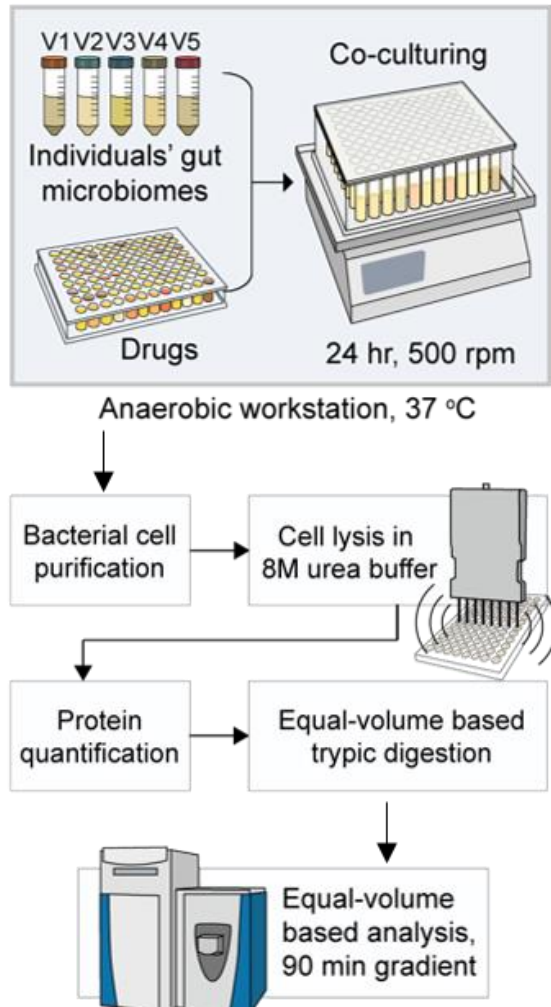
MetaLab software, iMetaReport and iMetaShiny apps





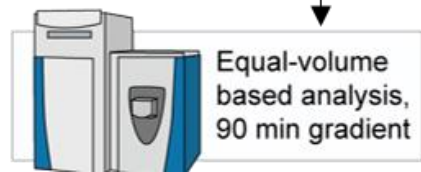
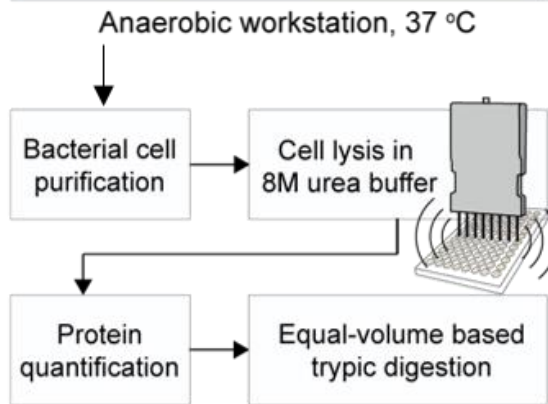
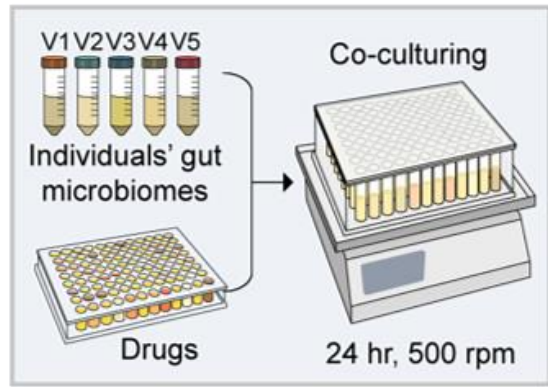
**3. iMetaLab Suite:
an example of its application**

iMetaLab Suite: an example of its application



Diclofenac vs DMSO

iMetaLab Suite: an example of its application



Diclofenac vs DMSO

MetaLab 2.2.1
File Tools Setting Help

MaxQuant workflow
MSFragger workflow
pFind workflow
Taxonomy analysis
Functional annotation

Input data Parameters Setting Run

| Exist | Index | File | Experiment | Fraction |
|-------|-------|------|------------|----------|
|-------|-------|------|------------|----------|

Experiment name editing
Split symbol
Keep in experiment name Content
Reset

Add Remove Clear Edit exp in xlsx Edit exp in tsv Load exp info

Result
Output Z:\Leyuan\3-paper\20220223_iMetaLabSuite\data\MetaLab

Database
Microbiome database C:\database\human_IGC.pep.fasta.pep.fasta
 Append host database to the generated sample-specific database
Host database

Running time: CPU state: Memory (used/max):

iMetaReport automated report

The screenshot displays the iMetaLab 2.2 Result Summary interface. The top header shows the iMetaLab logo and the text "MetaLab 2.2 Result Summary". A sidebar on the left contains a "Reports" section with the following items: ID Summary, Peptides Summary, ProteinGroups Summary, Taxon Summary, Function Summary, and MetaMep for Taxon Vis. Below this are "ShinyApps" and "iMetaLab" sections. The main content area features a network visualization background with blue nodes and lines. In the center, the text "MetaLab Reports Portal" is displayed, followed by the instruction "Click the left panel menu to check the MetaLab analysis reports".

MetaLab 2.2 Result Summary

Reports

- ID Summary
- Peptides Summary
- ProteinGroups Summary
- Taxon Summary
- Function Summary
- MetaMep for Taxon Vis

ShinyApps

iMetaLab

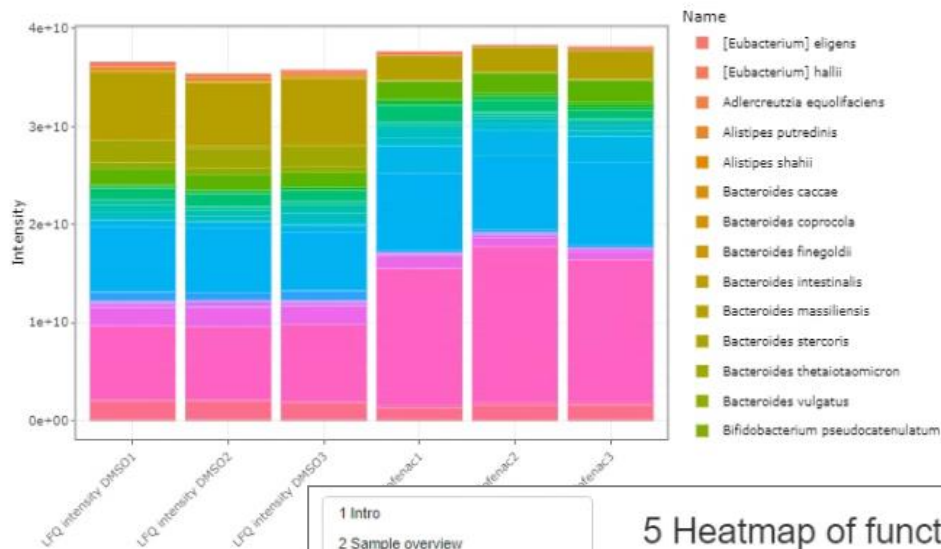
MetaLab Reports Portal

Click the left panel menu to check the MetaLab analysis reports

iMetaReport automated report

- 1 Intro
- 2 Sample overview
- 3 Identification per sample
- 4 Alpha diversity
- 5 Beta diversity
- 6 Sample Clustering
- 7 Taxonomic composition bar plots
- 7.1 Composition bar plot, species-level:
- 7.2 Composition bar plot, genus-level:
- 7.3 Composition bar plot, family-level:
- 7.4 Composition bar plot, order-level:
- 7.5 Composition bar plot, class-level:
- 7.6 Composition bar plot, phylum-level:

7.1 Composition bar plot, species-level:

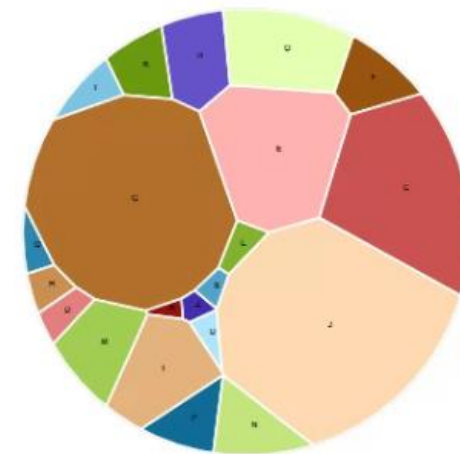


- 1 Intro
- 2 Sample overview
- 3 Overview with voronoi plots
- 3.1 Overview of COG categories
- 3.2 Overview of NOG categories
- 4 Overview with composition bar plots
- 5 Heatmap of functional composition
- 6 PCA plots

3.1 Overview of COG categories

The figure below displays the composition of COG categories in your dataset. Areas in the voronoi plot are based on summed proteinGroup intensities across all samples.

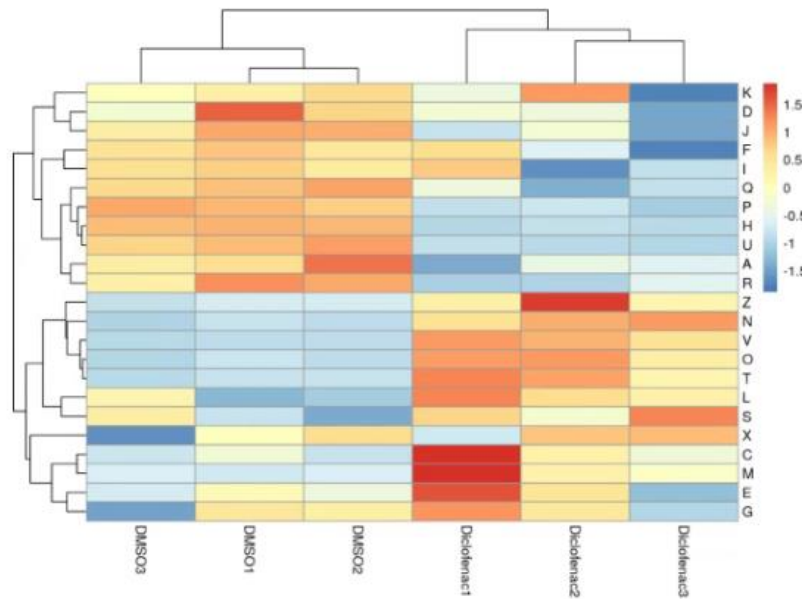
- COG categories**
- A
 - C
 - D
 - E
 - F
 - G
 - H
 - I
 - J
 - K
 - L
 - M
 - N
 - O
 - P
 - Q
 - R



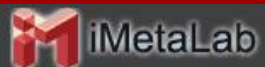
- 1 Intro
- 2 Sample overview
- 3 Overview with voronoi plots
- 4 Overview with composition bar plots
- 5 Heatmap of functional composition
- 5.1 Heatmap of COG composition
- 5.2 Heatmap of NOG composition
- 6 PCA plots

5 Heatmap of functional composition

5.1 Heatmap of COG composition



.....



iMetaShiny Apps

Analyze your metaproteomic data and generate publishable scientific figures

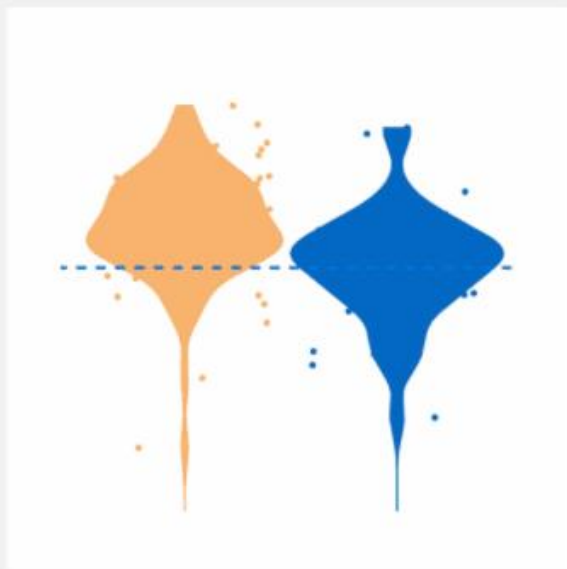
All

Metaproteomics

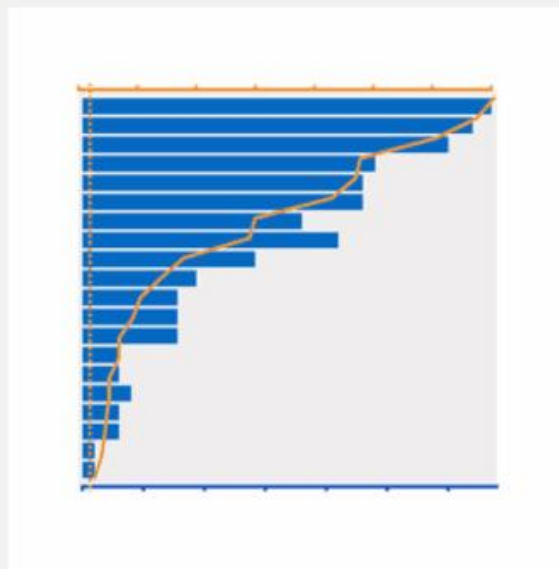
Statistics

Simply plotting

Special analysis



Quick MQ summary



Enrichment analysis



Phylo explorer

iMetaShiny for data analysis and visualization: pepFunk as an example

- Upload Data
- Analysis
- Gallery
- About
- iMetaLab
- pepFunk on GitHub

1. Data input

A. Import peptide file:

Input data type:

- Upload your own data
- Use our sample data

Choose the peptide intensity file to be analyzed

Browse... No file selected

File format:

- peptide.txt
- CSV with peptide sequences and intensities

File format: The peptide.txt output file from MaxQuant or MetaLab.

B. Add treatment information

Manual or auto condition formatting?

- Manual
- Auto

Auto condition formatting will try and match your treatment conditions with your samples. If your sample names contain your treatment, this is a great option. Try typing your control and treatment names in the boxes above. If you have more than one treatment, please push the button to add another treatment option.

Input control condition

Enter control/reference condition name

Input condition 1

Enter test condition name

Add additional condition Remove added condition

2. Check sample names and sample conditions

Please upload a file of peptide intensity values.

Note: you can update your sample names here. Condition names are either auto filled or can be typed in. Please use the drop down options for conditions.

3. Analysis options

A. Data Normalization

Would you like pepFunk to normalize your data by depth?

- Yes
- No

Note: If you opt for no normalization, we highly recommend you normalize your data using your own methods before uploading to pepFunk. If you'd like to know more about our normalization technique, please see our manuscript (<https://doi.org/10.1093/bioinformatics/btaa289>).

B. Choose log transformation

Transform intensity values using:

- Log10
- Log2
- No transformation

C. Choose peptide-to-KEGG database

Peptide-to-KEGG database:

- Curated human microbiome
- Upload your own database

Please upload a file of peptide intensity values.

Welcome to iMetaWiki



- [Metalab HGM 1.0](#) version released, [Quick Setup Manual](#)
- MetaLab: 2.2.1, [Quick setup for 2.2.1 Desktop](#)
- [Release Notes](#), [Register to download](#), [Which version to choose?](#)
- [TERMS](#) for usage.
- [Reference](#) for details about how Metalab works.
- [FAQs](#), [Frequent errors to avoid](#)
- Result/Outputs files for(2.x, HGM)

Tutorials and FAQ:

wiki.imetalab.ca

Tech support team:

techteam.metalab@gmail.com

Your feedbacks and suggestions are welcome!

iMeta: Integrated meta-omics to change the understanding of the biology and environment



“iMeta” is an open-access Wiley partner journal and launched by scientists of the Chinese Academy of Sciences. iMeta aims to promote metagenomics, microbiome and bioinformatics development by publishing original researches, methods or protocols, and reviews. The goal is to publish highly quality papers (Top 10%, IF > 15) targeting broad audience. Unique features including video submission, reproducible analysis, figure polishing, APC waiver, and promotion by social media with 500,000 followers. The first issue will be released in March 2022.

 Society: <http://www.imeta.science>
Publisher: <https://onlinelibrary.wiley.com/journal/2770596x>

 Submission: <https://mc.manuscriptcentral.com/imeta>

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