

iMetaLab Suite宏蛋白质组学一站式工具集

iMetaLab Suite: A One-stop Toolset for Metaproteomics

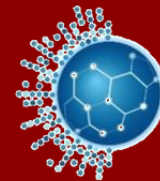
李乐园¹, 宁志斌¹, 程凯, 张旭,
Caitlin M.A. Simopoulos, Daniel Figeys*



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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>



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Leyuan Li, Zhibin Ning, Kai Cheng, Xu Zhang, Caitlin M. A. Simopoulos, Daniel Figeys

First published: 21 May 2022 | <https://doi.org/10.1002/imt2.25>

Leyuan Li and Zhibin Ning contributed equally to the manuscript.

SECTIONS

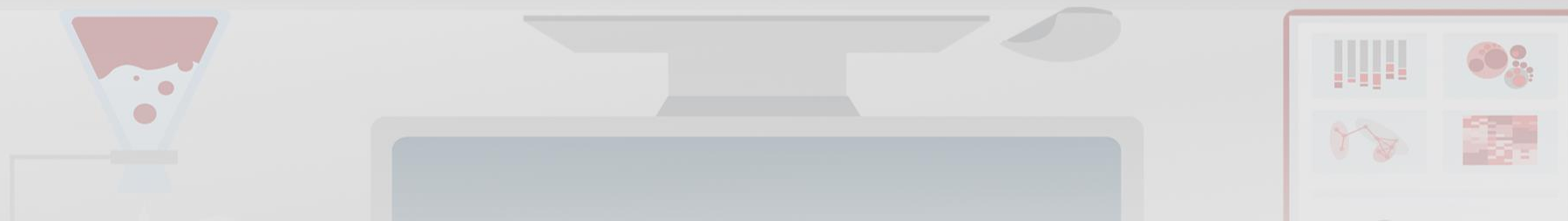
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Abstract

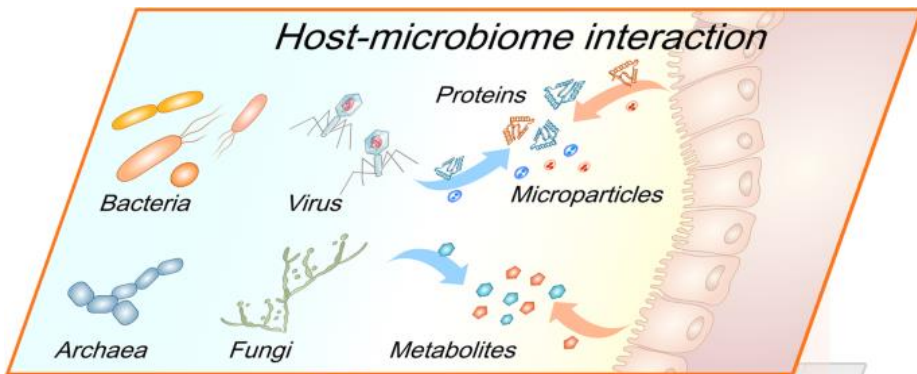
Metaproteomics is a recently thriving technique that studies the collection of proteins in complex microbiomes of the human, animal, plant, and environment. The bioinformatics workflow required for metaproteomics research, from the database search and protein quantification to downstream functional and taxonomic analysis has been challenging and thus limiting the accessibility of metaproteomics to microbiome researchers. To overcome these challenges, we have developed a set of tools named iMetaLab Suite. iMetaLab Suite includes the following components: (1) MetaLab Desktop, an automated database search software that facilitates proteins identification and quantitation from microbiomes; (2) the automated iMetaReport that allows users to quickly access database search results and data set profiles; and (3) an interactive online toolset, iMetaShiny, covering most frequently used functional, taxonomic, and statistical analysis in metaproteomics. iMetaLab Suite is a free, easily accessible, and actively updated toolset available to assist researchers to explore metaproteomic data.

Highlights

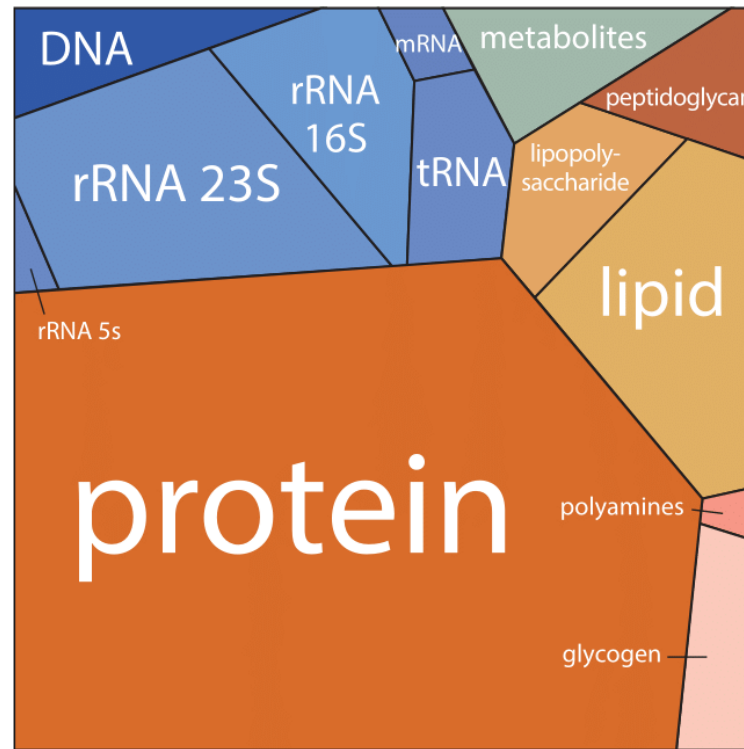
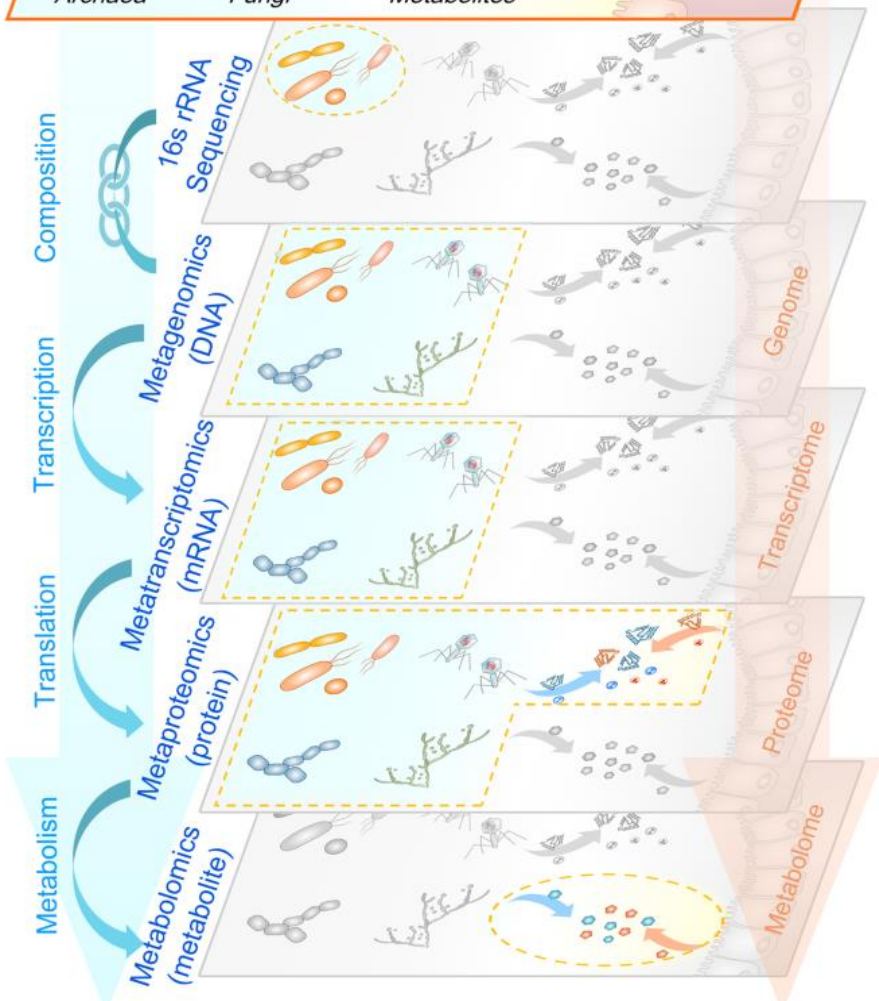
- A one-stop solution for metaproteomics data analysis for nonexpert.
- Database search and result reports that include taxonomy and function.
- Interactive tools for frequently used metaproteomics data analysis tools.



宏蛋白质组学：宏多组学中经常缺席的成员



- 微生物组学研究中，不同宏组学技术提供不同层面的解析

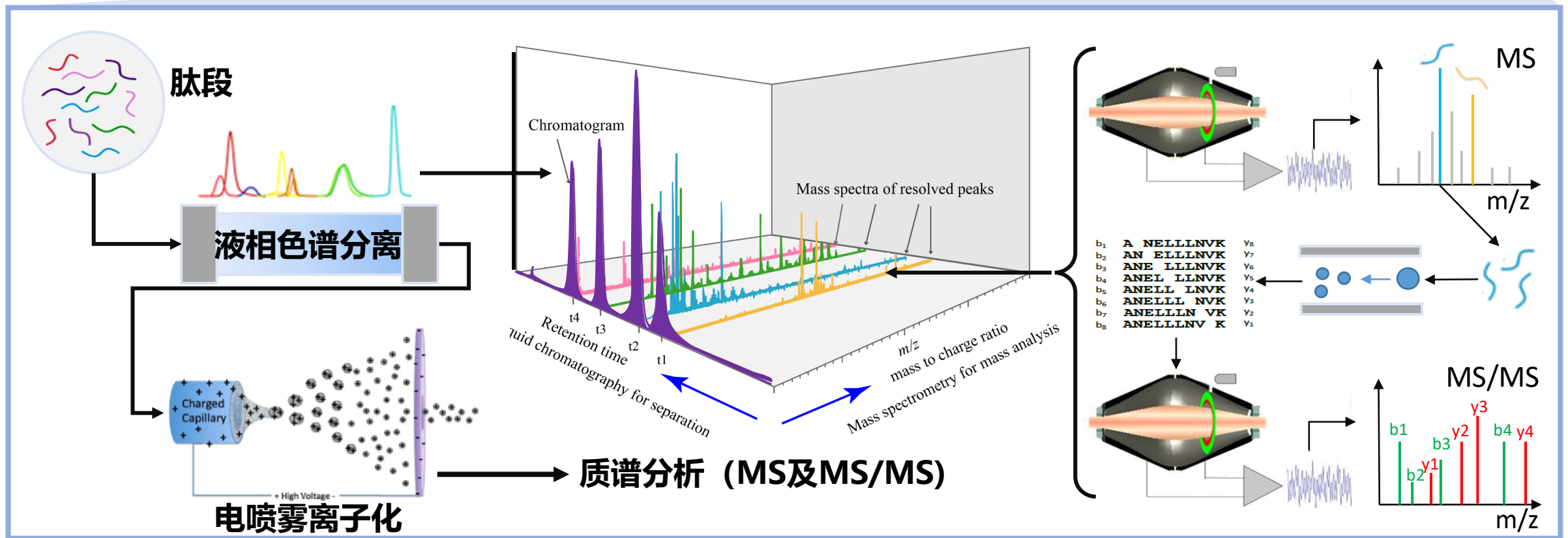
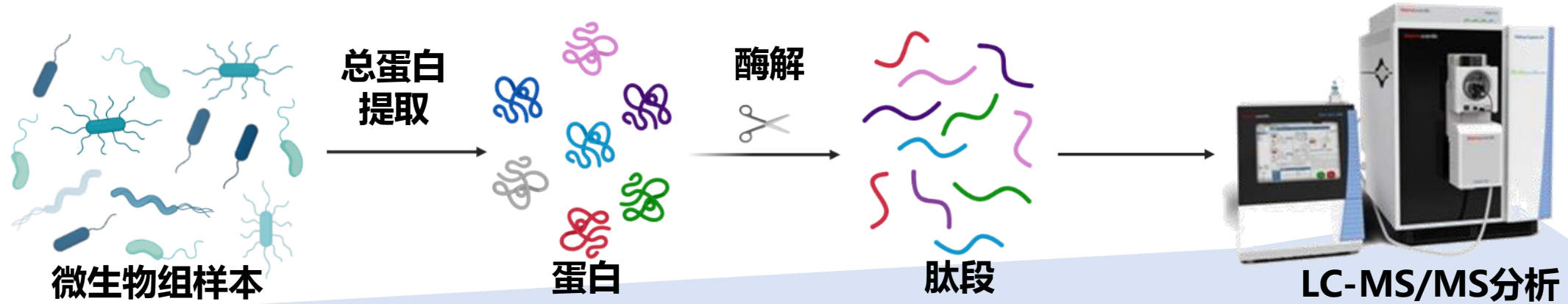


图片来源<https://bionumbers.hms.harvard.edu>

- 宏蛋白质组学：
 - 在微生物细胞中，蛋白质大约占细胞干重的50%。这些蛋白质是细胞生物过程的基本功能单元
 - 宏蛋白质组学分析复杂微生物组的蛋白质组成，对理解其功能非常重要

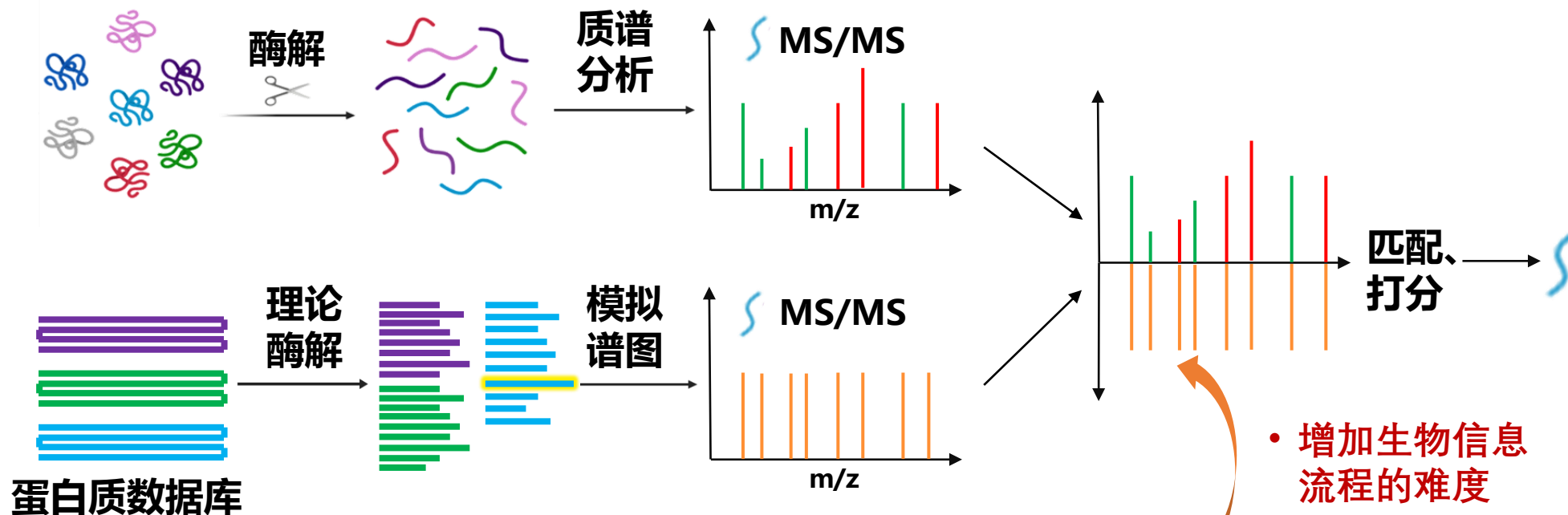
- 然而在目前的宏多组学研究中，宏蛋白质组学普遍缺席

宏蛋白质组学：基于液相色谱-串联质谱的测序技术



宏蛋白质组学生物信息流程比传统蛋白质组学更具挑战

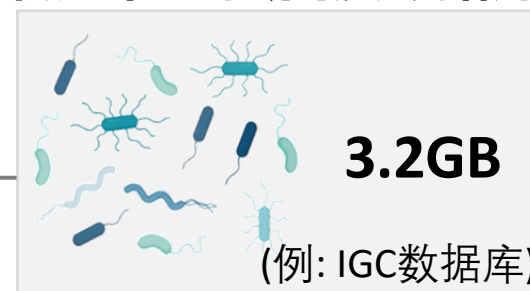
传统蛋白质组学生物信息流程：



单个微生物物种蛋白质数据库



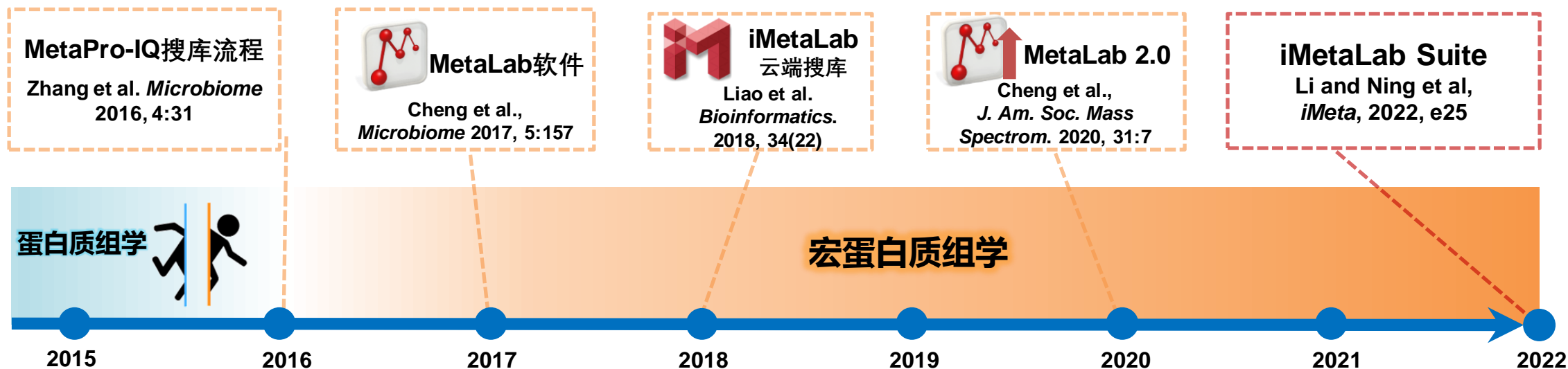
微生物组蛋白质数据库



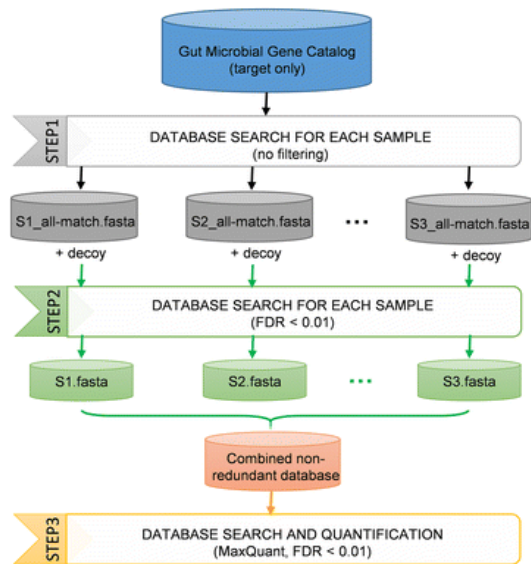
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宏蛋白质组学
搜库面临挑战：

本团队的宏蛋白质组学技术发展



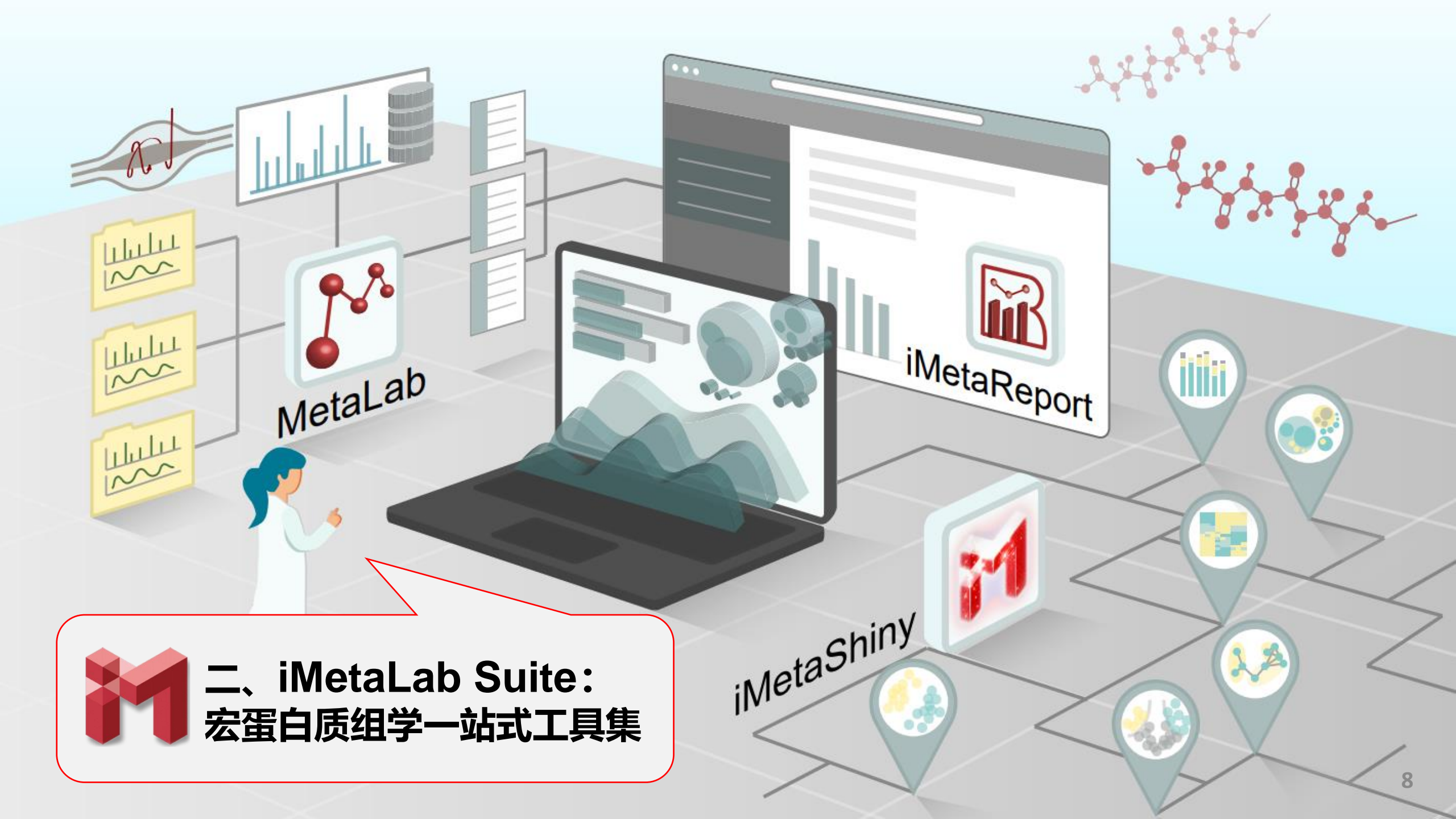
渥太华大学
Daniel Figeys教授团队



MetaPro-IQ搜库流程

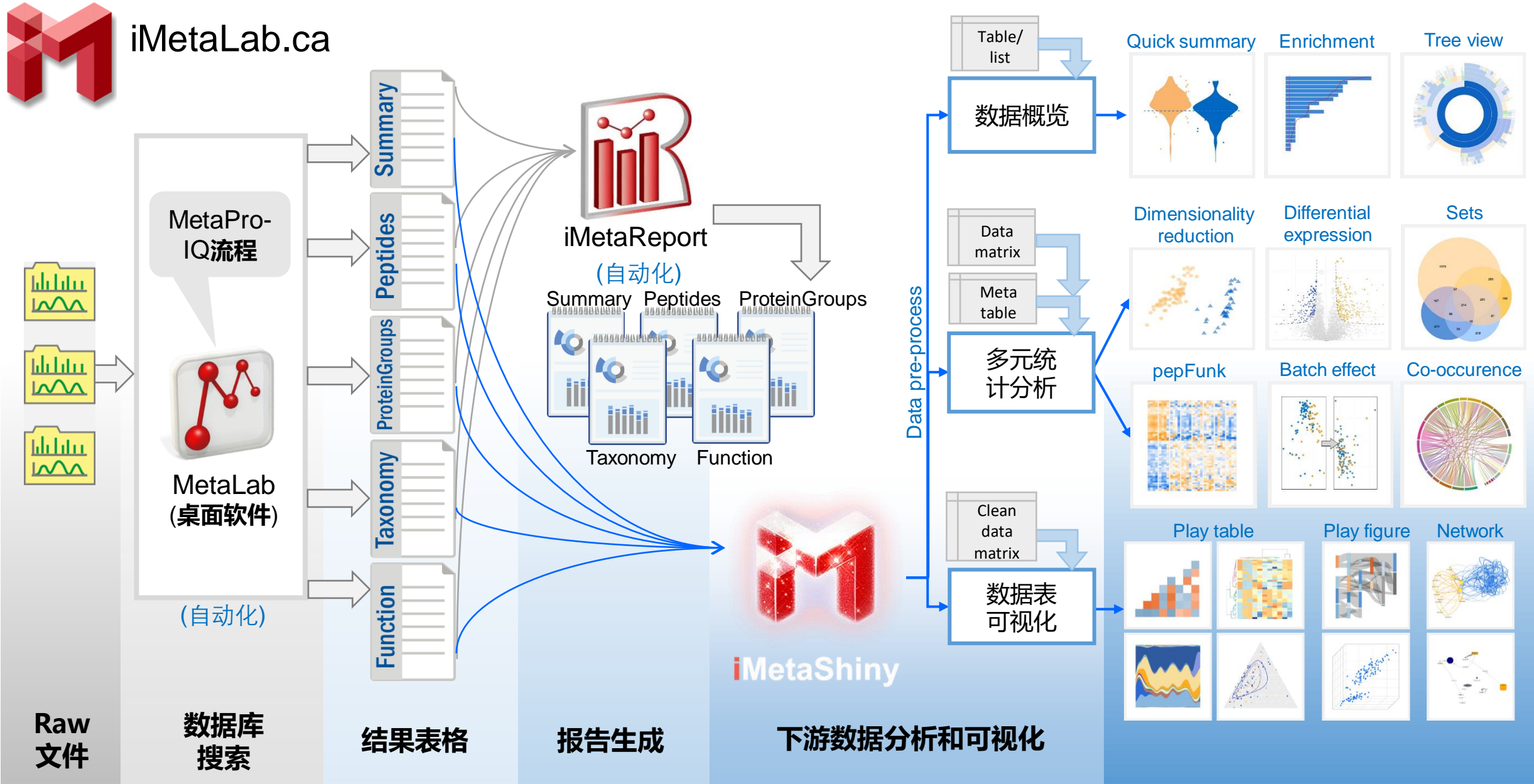


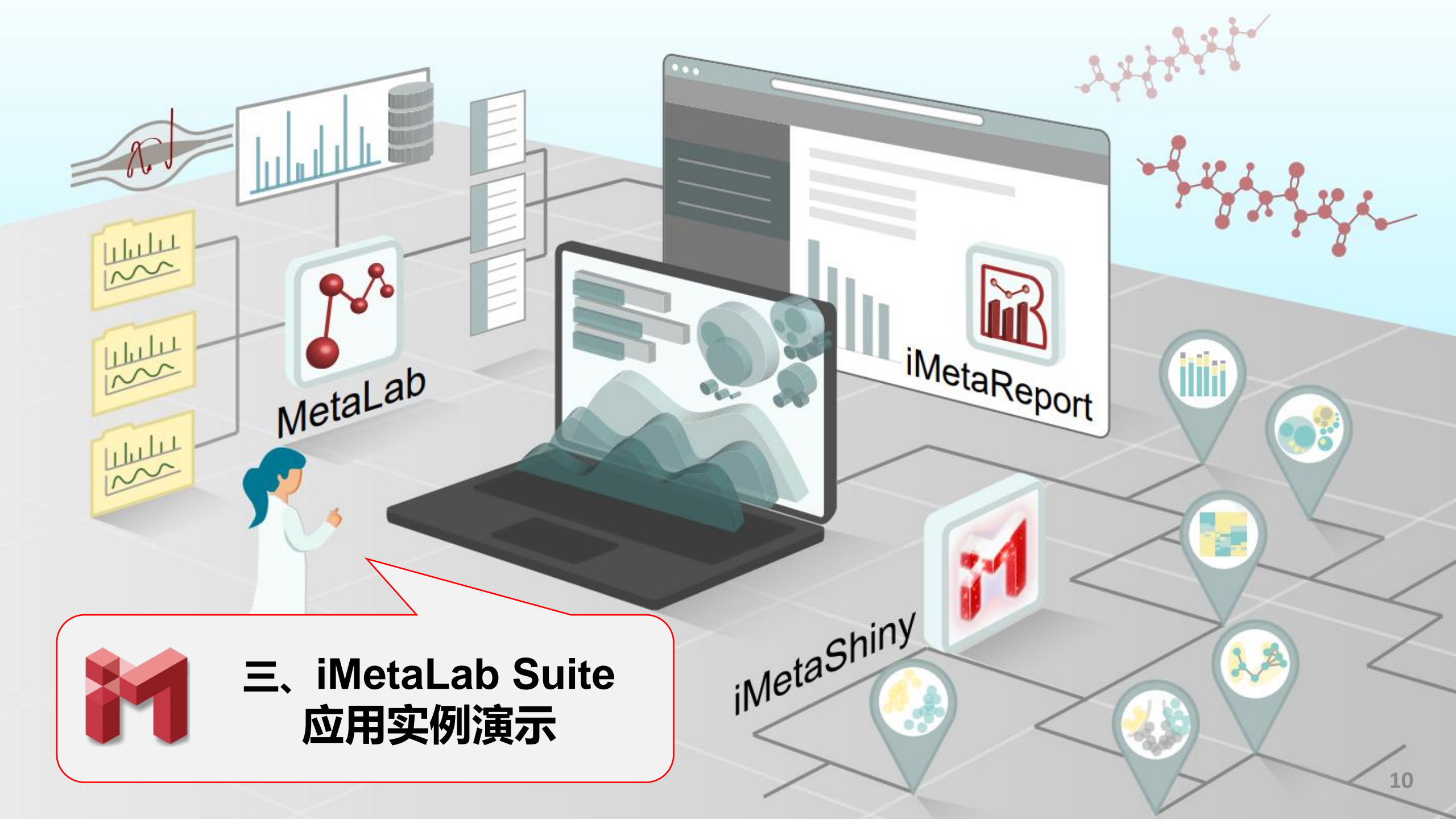
iMetaLab Suite



二、iMetaLab Suite： 宏蛋白质组学一站式工具集

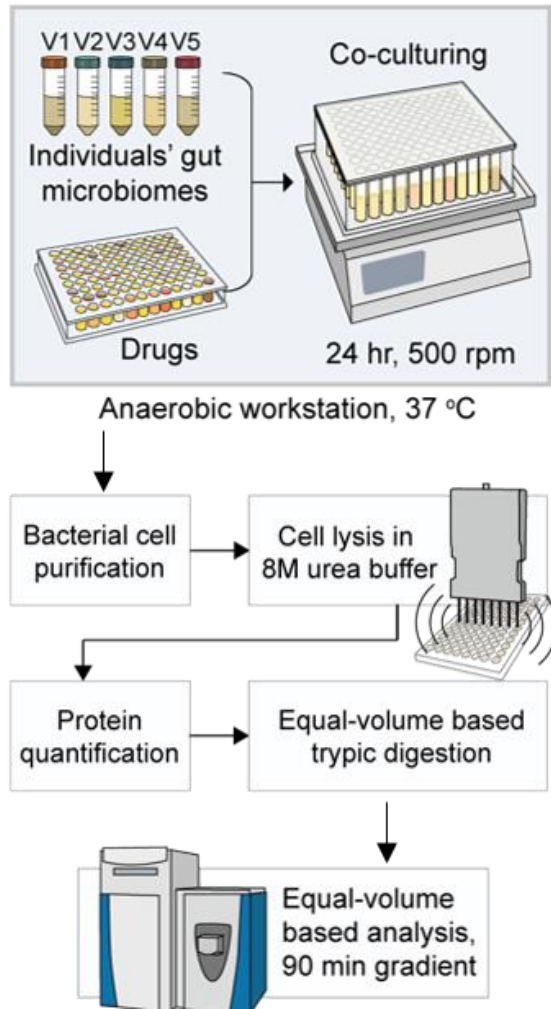
MetaLab自动化搜库、iMetaReport自动报告、iMetaShiny交互式数据分析应用





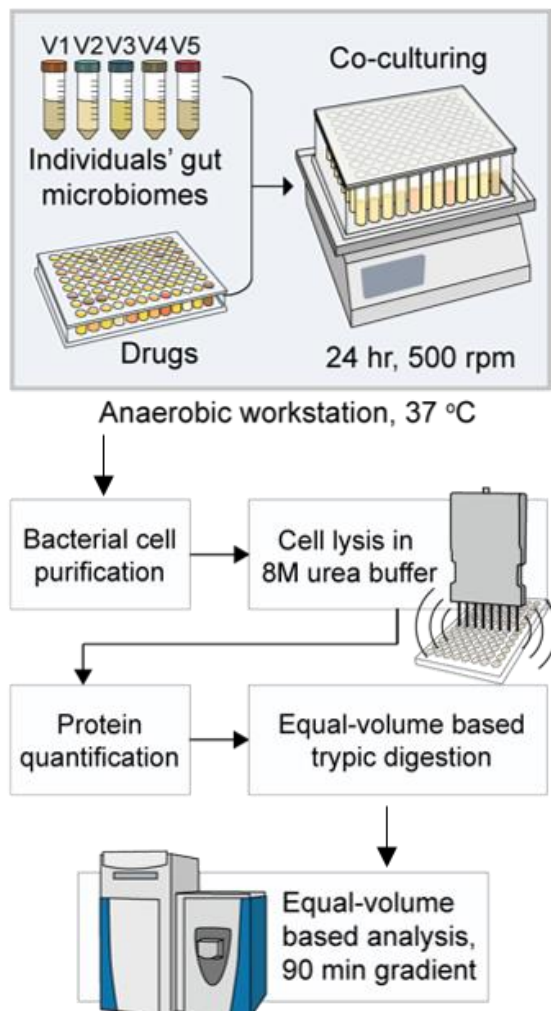
三、iMetaLab Suite 应用实例演示

iMetaLab Suite应用实例



以双氯芬酸vs对照为例
(Diclofenac vs DMSO)

iMetaLab Suite应用实例



以双氯芬酸vs对照为例
(Diclofenac vs DMSO)

Li et al., *Microbiome* 8:33, 2020

The screenshot shows the iMetaLab Suite 2.2.1 interface with the following components:

- Workflow Selection:** MaxQuant workflow, MSFragger workflow, pFind workflow, Taxonomy analysis, Functional annotation.
- Raw files Table:**

Exist	Index	File	Experiment	Fraction
-------	-------	------	------------	----------
- Buttons:** Add, Remove, Clear, Edit exp in xlsx, Edit exp in tsv, Load exp info.
- Result Section:** Output path: Z:\Leyuan\3-paper\20220223_iMetaLabSuite\data\MetaLab
- Database Section:** Microbiome database: C:\database\human_IGC.pep.fasta.pep.fasta. Includes a checkbox for "Append host database to the generated sample-specific database".
- System Status:** Running time, CPU state, Memory (used/max).

iMetaReport自动报告

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

iMetaShiny Apps

Analyze your metaproteomic data and generate publishable scientific figures

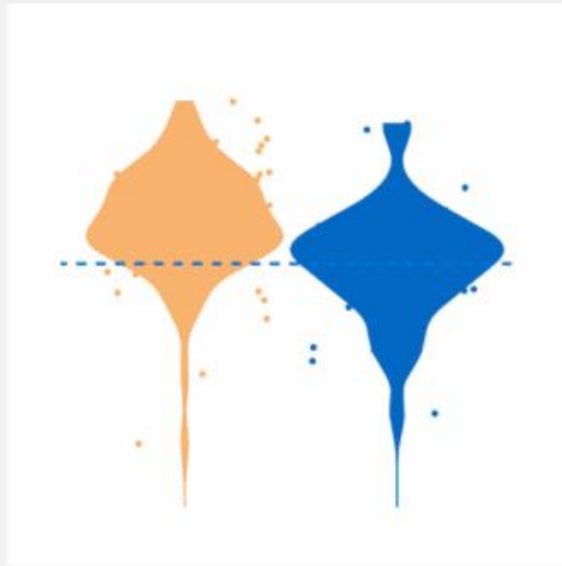
All

Metaproteomics

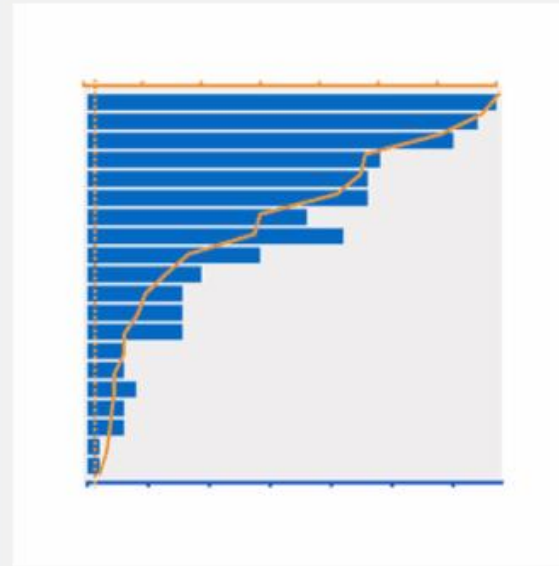
Statistics

Simply plotting

Special analysis



Quick MQ summary



Enrichment analysis



Phylo explorer

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



使用教程网站:

wiki.imetalab.ca

技术支持团队:

techteam.metalab@gmail.com

- [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)

欢迎您的宝贵反馈和建议!



“iMeta”是由威立、肠菌分会和本领域数百位华人科学家合作出版的开放获取期刊，主编由中科院微生物所刘双江研究员和荷兰格罗宁根大学傅静远教授担任。目的是发表原创研究、方法和综述以促进宏基因组学、微生物组和生物信息学发展。目标是发表前10%(IF > 15)的高影响力论文。期刊特色包括视频投稿、可重复分析、图片打磨、青年编委、前3年免出版费、50万用户的社交媒体宣传等。2022年2月正式创刊发行!



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