



MetOrigin 2.0: Advancing the discovery of microbial metabolites and their origins

Gang Yu¹, Cuifang Xu¹, Xiaoyan Wang¹, Feng Ju², Junfen Fu^{1*}, Yan Ni^{1*}

¹Children's Hospital, Zhejiang University School of Medicine,
National Clinical Research Center for Child Health, Hangzhou, China.

²Key Laboratory of Coastal Environment and Resources of Zhejiang Province,
School of Engineering, Westlake University, Hangzhou, China.



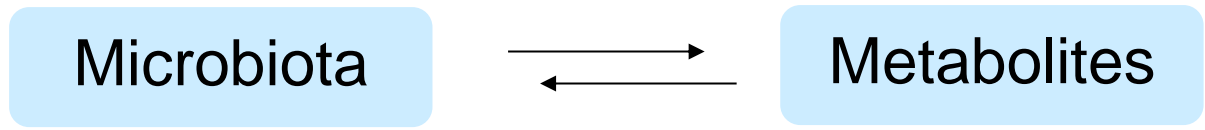
Yu, Gang, Cuifang Xu, Xiaoyan Wang, Feng Ju, Junfen Fu, and Yan Ni. 2024. MetOrigin 2.0: Advancing the Discovery of Microbial Metabolites and their Origins. *iMeta* 3: e246. <https://doi.org/10.1002/imt2.246>



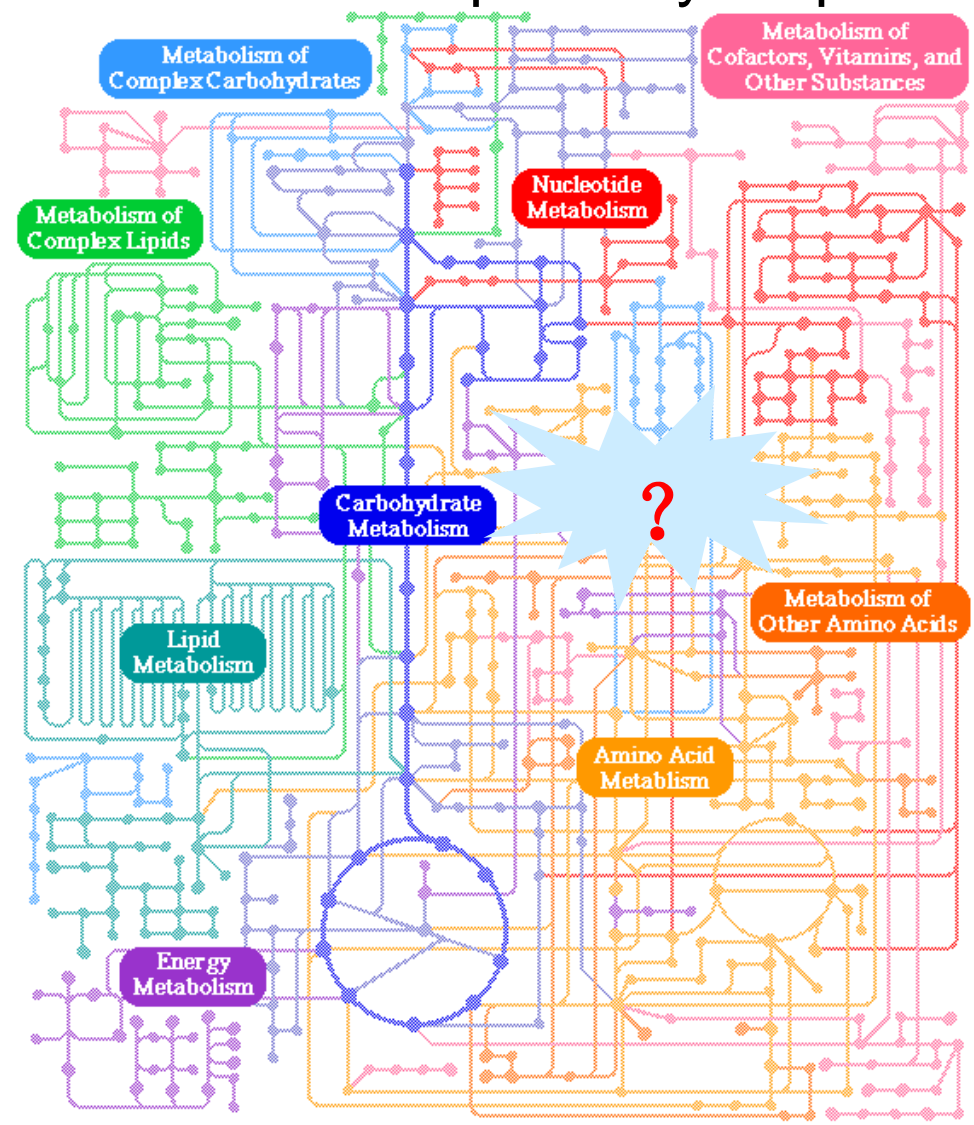
Background

Origins of metabolites:

- Host
- **Microbiota**
- Food
- Drug
- Environment (air, water, living condition)



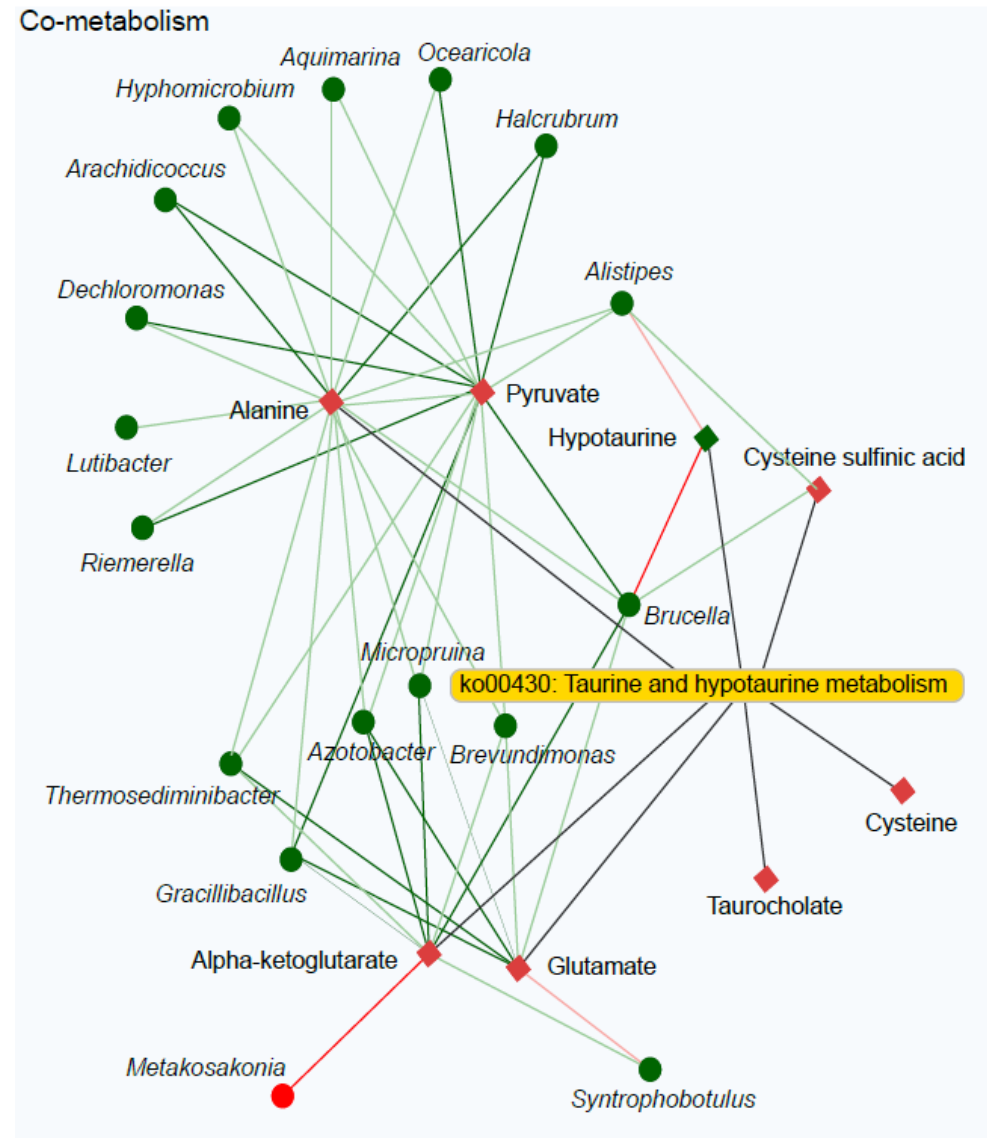
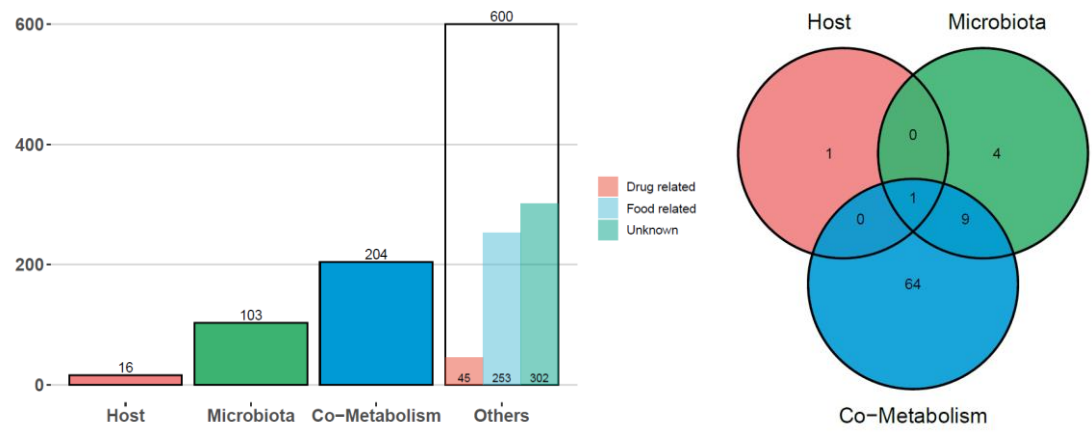
Metabolic pathway map



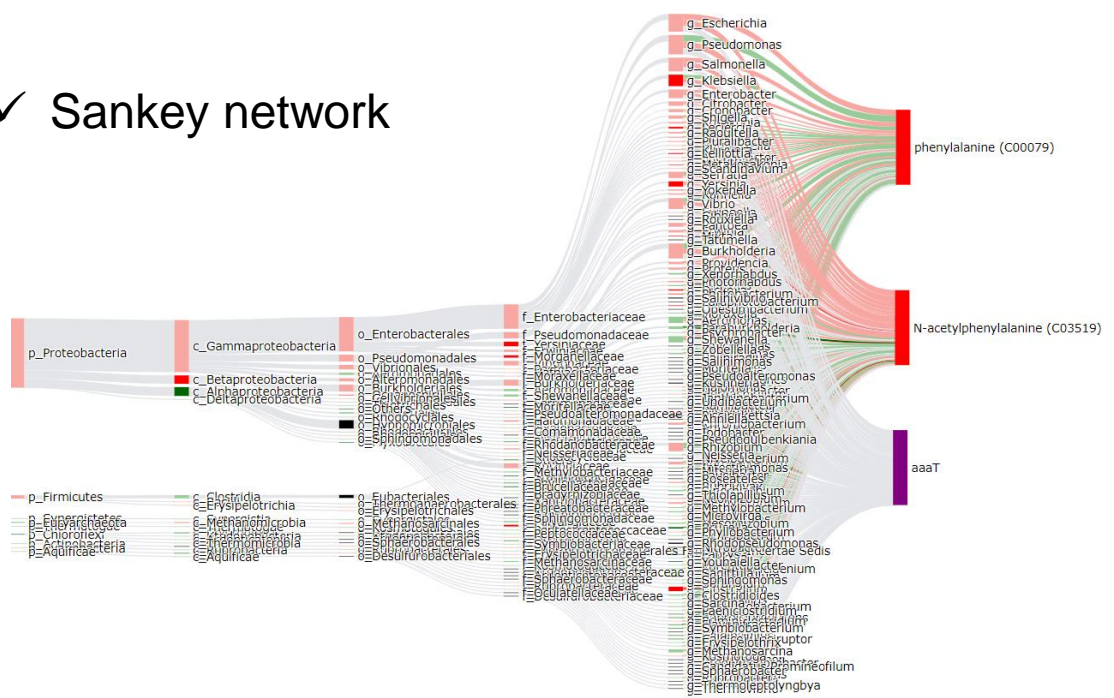


MetOrigin 1.0

- ✓ Origin analysis and metabolic pathway enrichment analysis
- ✓ Microbiome-metabolite co-network visualization



Sankey network





MetOrigin 2.0 Highlights

Mode 1: Quick search

Required datasets: None

Functions:

- Metabolic reactions
- Sankey network

Aims:

- To search and provide metabolic reactions of a metabolite and their related bacteria.

Mode 2: SMOA

Required datasets:

- Differential metabolite table

Functions:

- Origin analysis
- Pathway analysis
- Sankey network

Aims:

- To identify differential metabolic pathways, metabolic reactions, and their related bacteria.

Mode 3: DMOA

Required datasets:

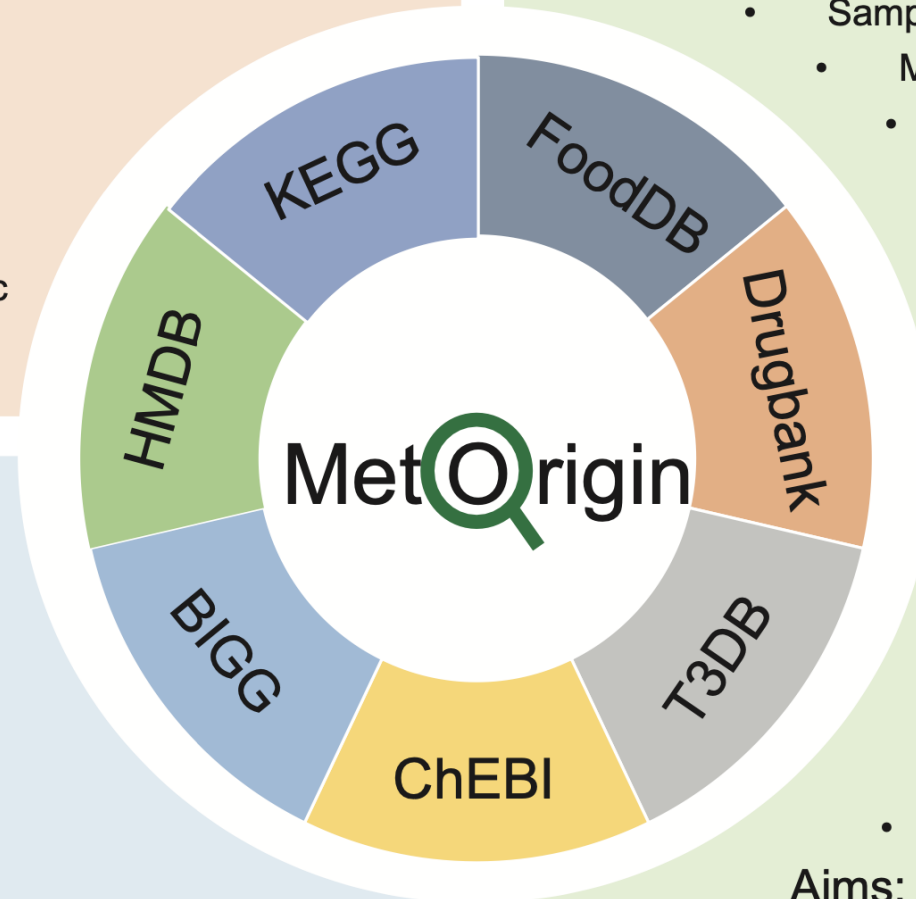
- Sample Information
- Metabolome table
- Microbiome table
- Phenotype table
- KEGG orthology table

Functions:

- Origin analysis
- Pathway analysis
- Correlation analysis
- Sankey network
- Orthology analysis
- Mediation analysis
- Network analysis

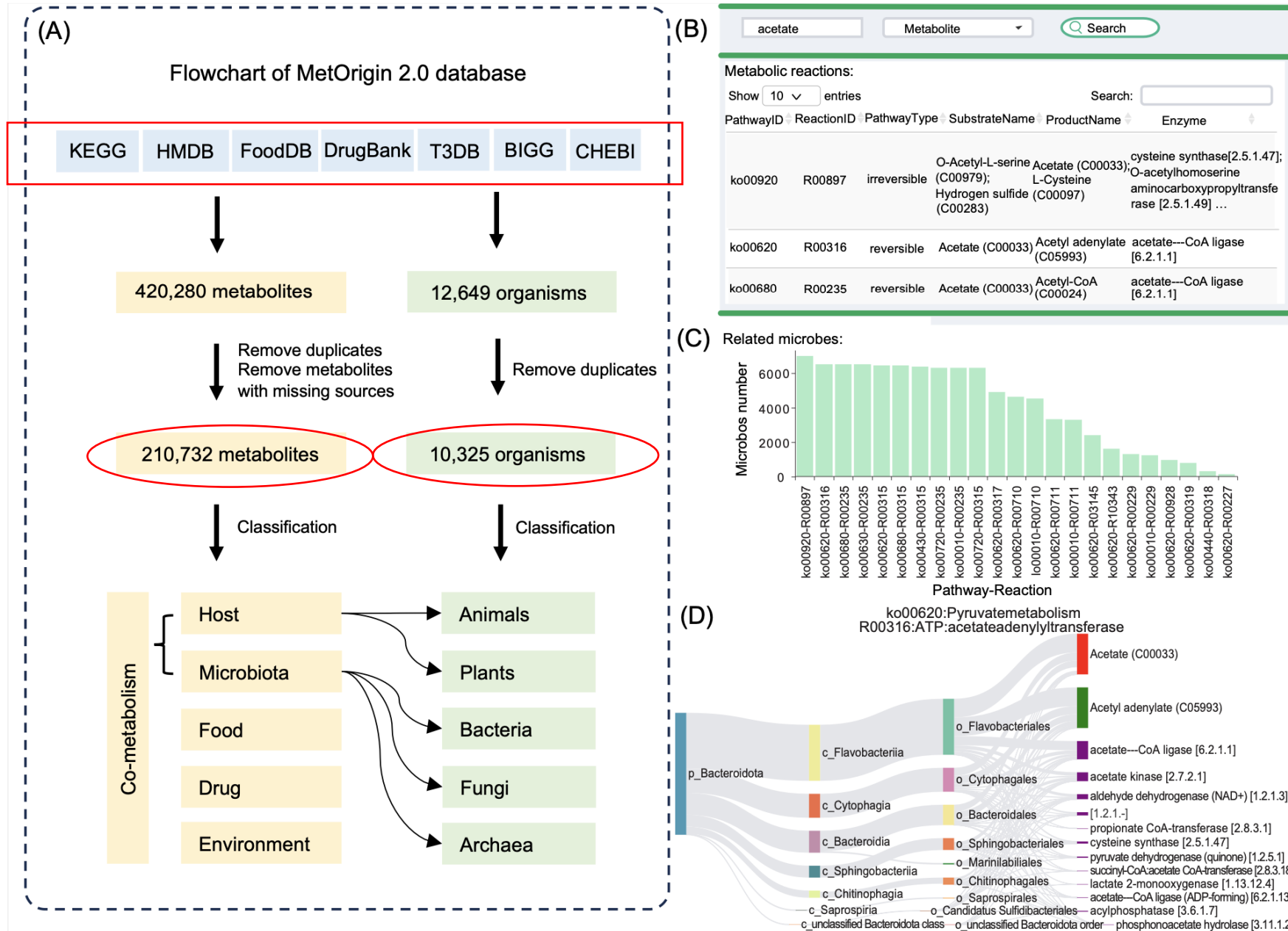
Aims:

- To explore the correlations between microbiome and metabolome step by step, from statistical, biological, to casual relationship.





Database update & Quick search

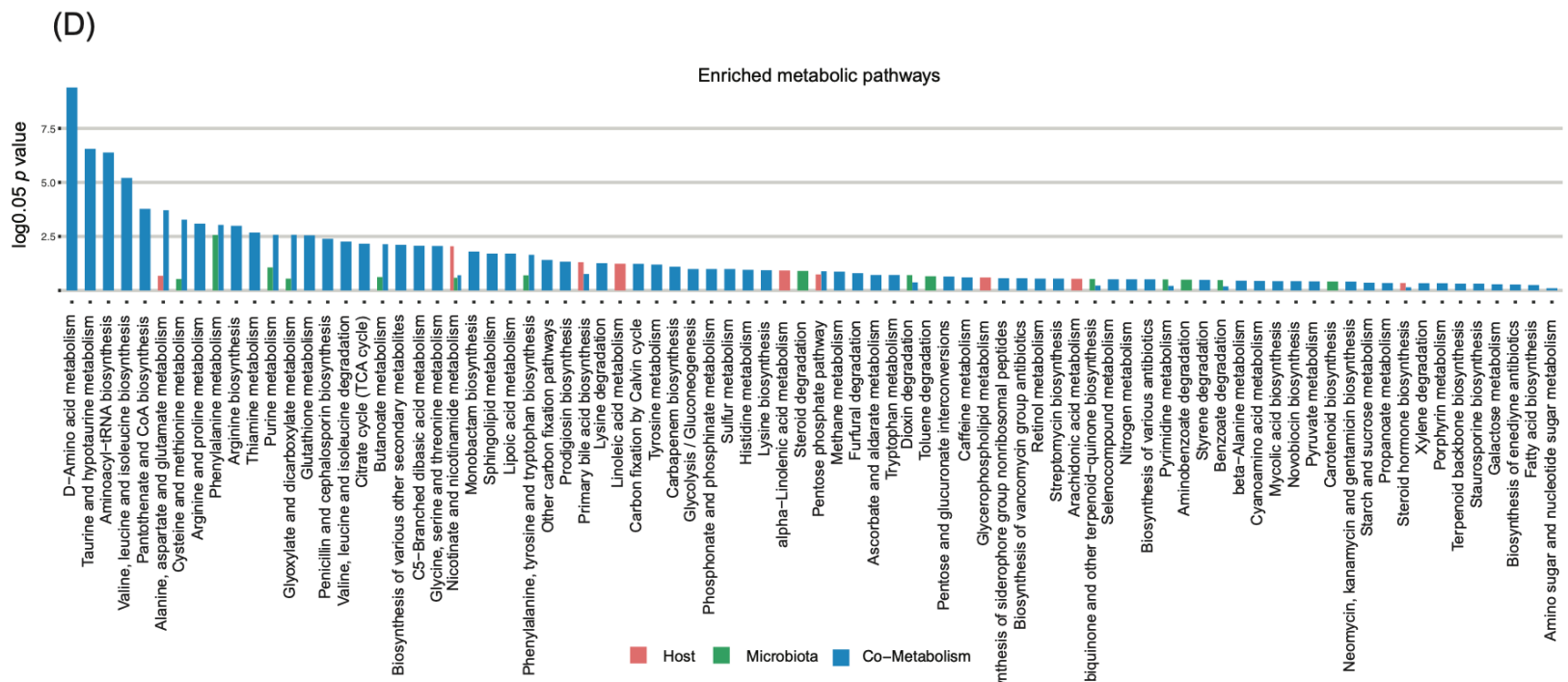
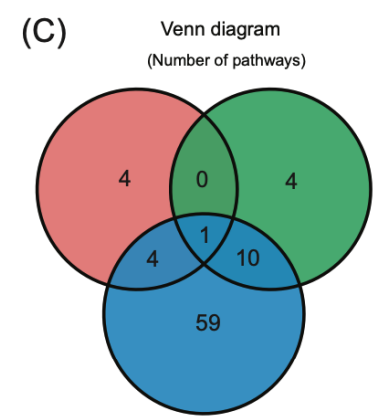
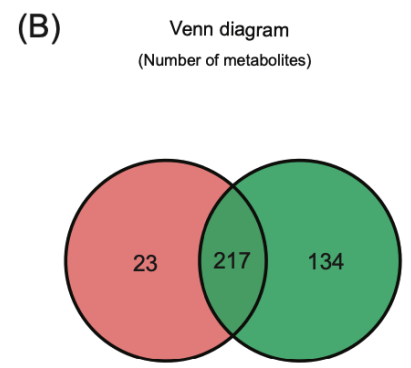
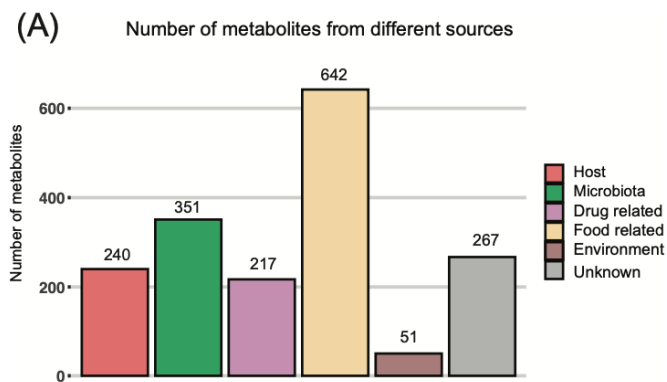


1

2

3

Origin analysis & metabolic pathway enrichment analysis



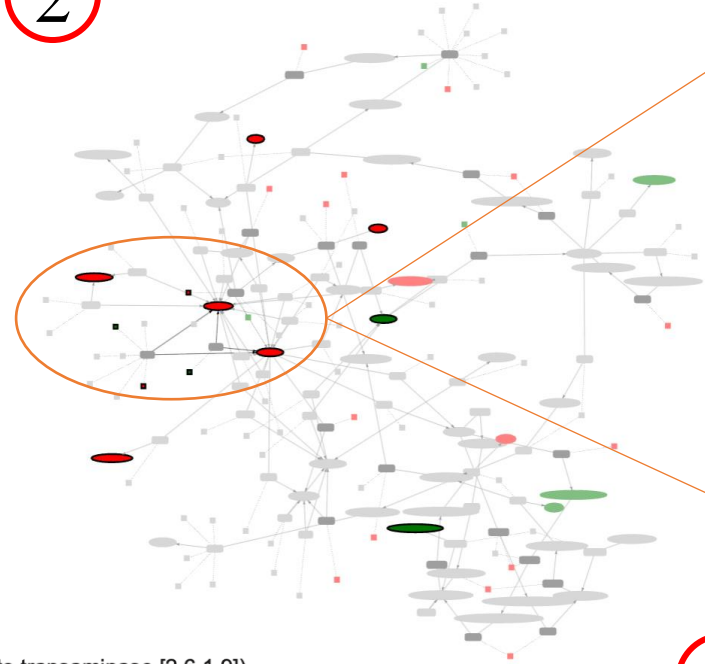


Orthology analysis

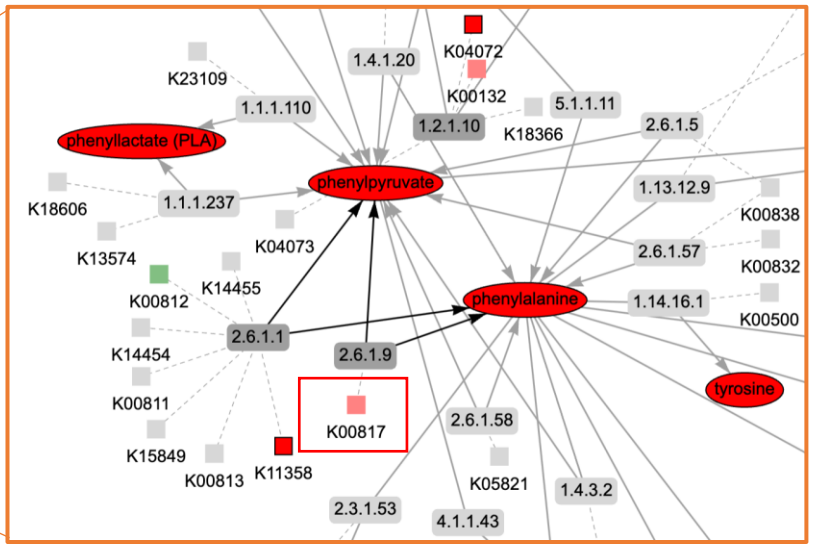
1 Pathway analysis

Microbiota					
Show 10 entries		Search:			
No.	ID	Name	Pvalue	Sig. Metabolite ID	Sig. Metabolites
1	ko00360	Phenylalanine metabolism	5.05e-03	C03519; C05607	N-acetylphenylalanine; phenyllactate (PLA)
2	ko00984	Steroid degradation	0.047	C00599	4-cholesten-3-one
3	ko00621	Dioxin degradation	0.084	C00180	benzoate

2

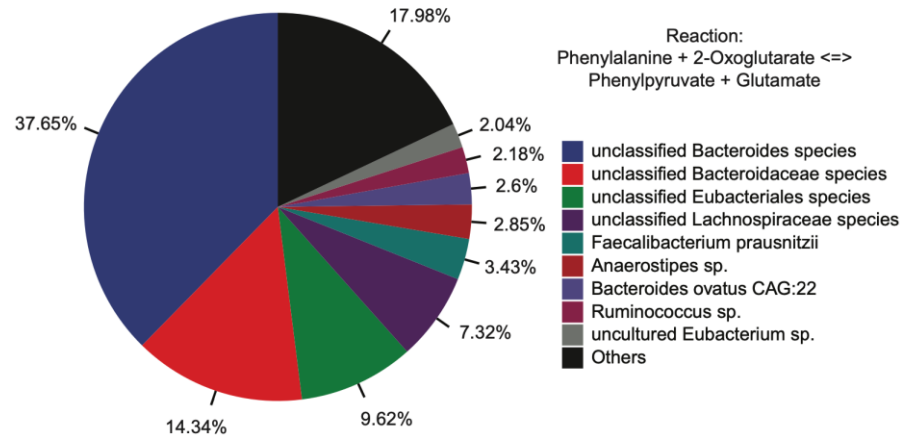


Ko00360 Phenylalanine metabolism

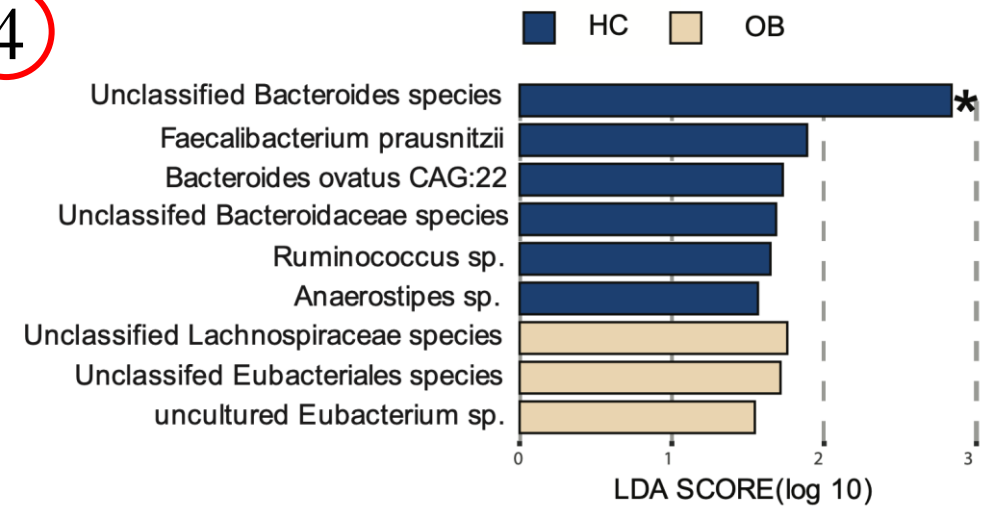


3

K00817 (Enzyme: Histidinol-phosphate transaminase [2.6.1.9])



4



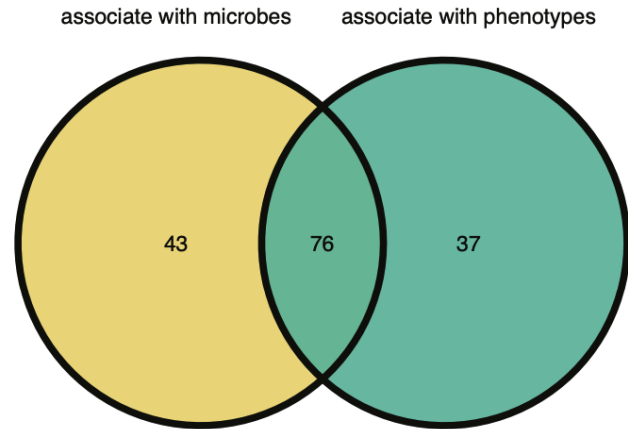


Mediation analysis

1

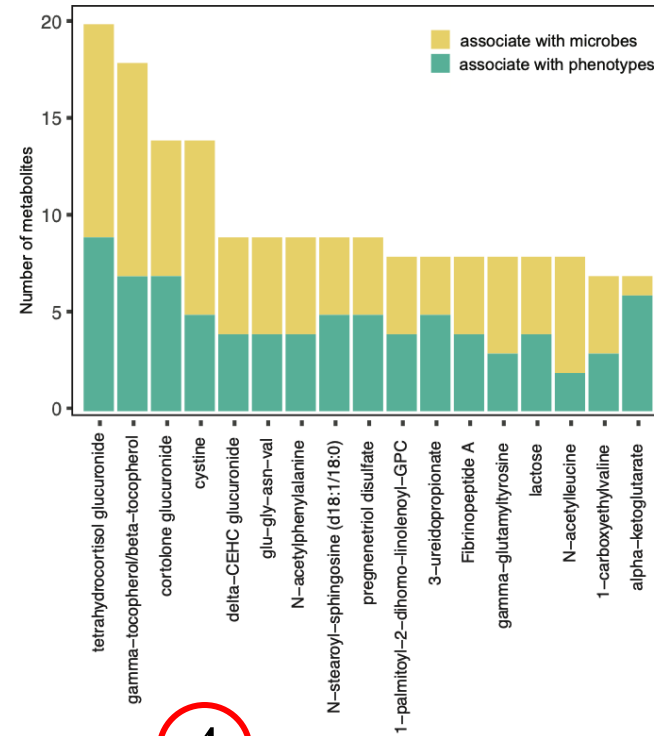
(A)

Venn diagram
(Number of metabolites)



2

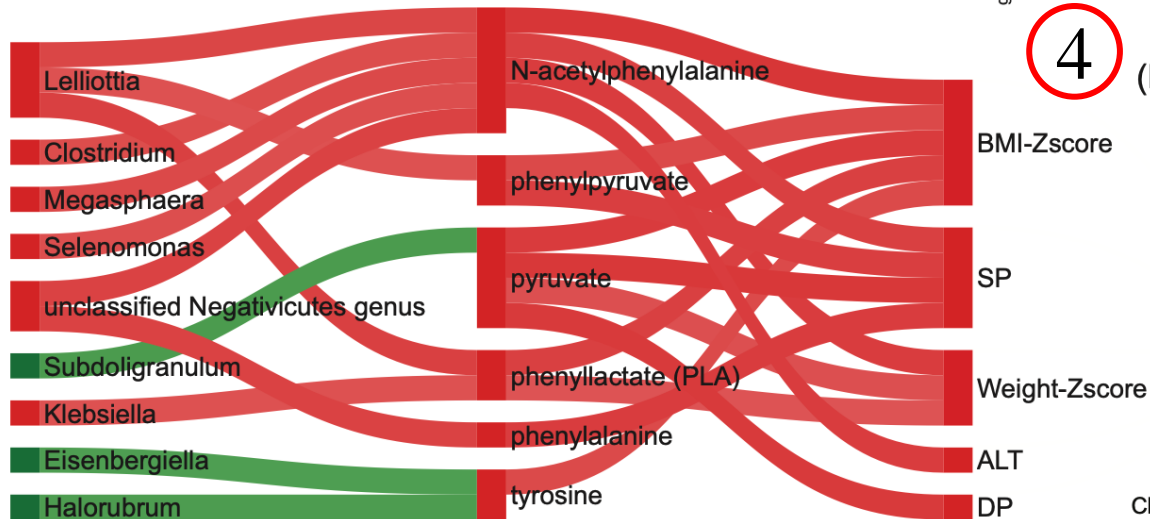
(B)



3

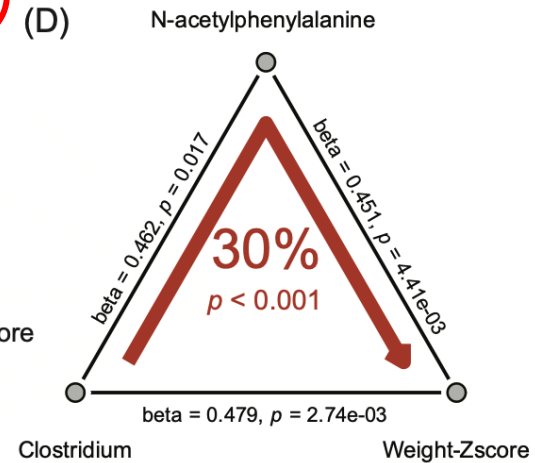
(C)

Correlations between metabolites and microbes/phenotype



4

(D)

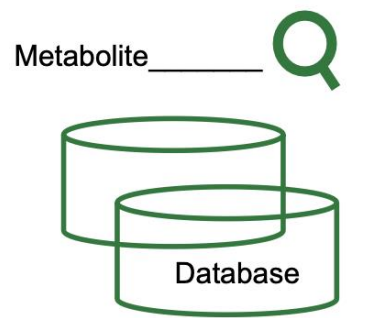




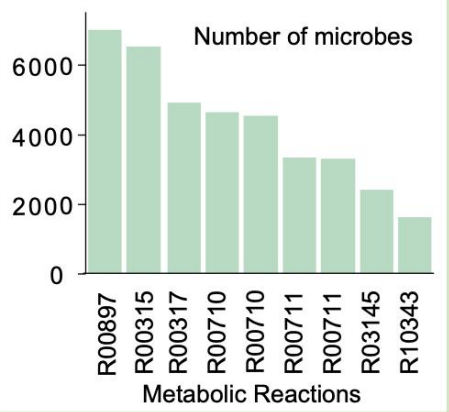
MetOrigin 2.0 : advance the discovery of microbial metabolites and their origins

1. Database search

√ Search a metabolite of interest

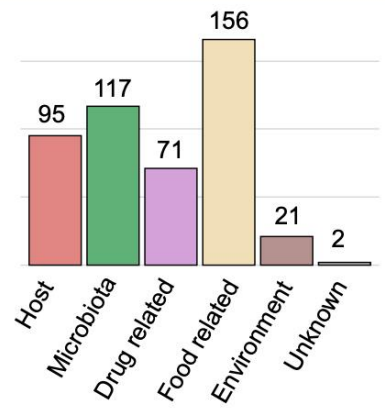


√ A list of metabolic reactions and related bacteria

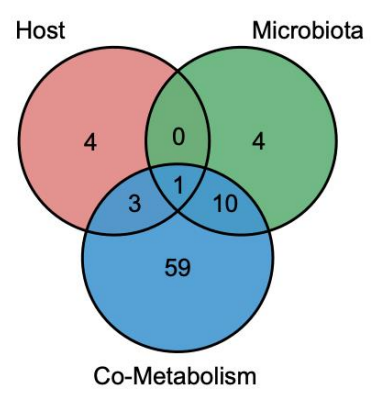


2. Origin classification

√ Classify metabolites into different origins

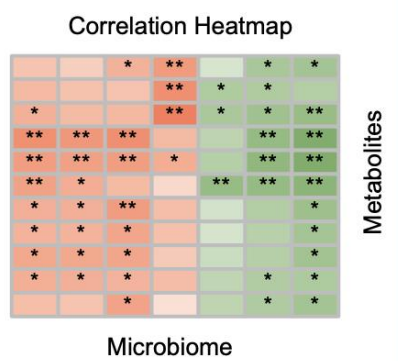


√ Metabolic pathways for microbial metabolites

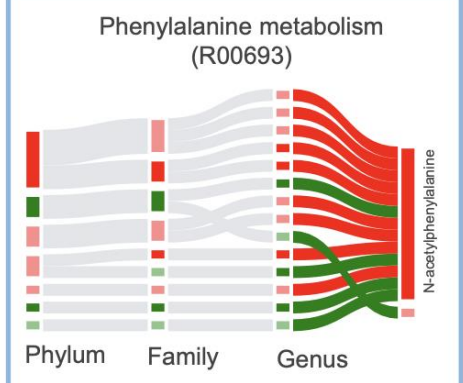


3. Correlation analysis

√ Statistical correlations between microbes & metabolites

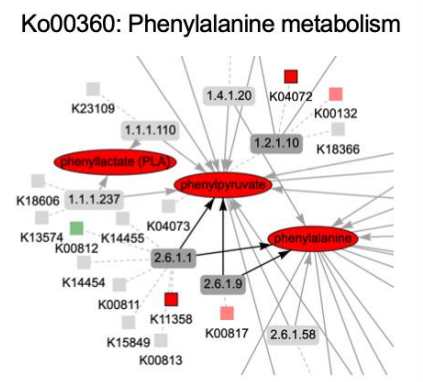


√ Sankey network of biological & statistical correlations

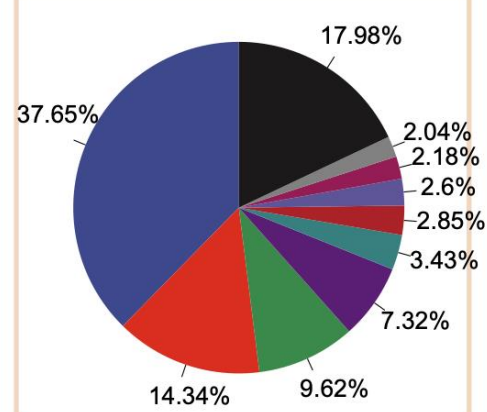


4. Orthology analysis

√ Identify KO genes for a metabolic enzyme

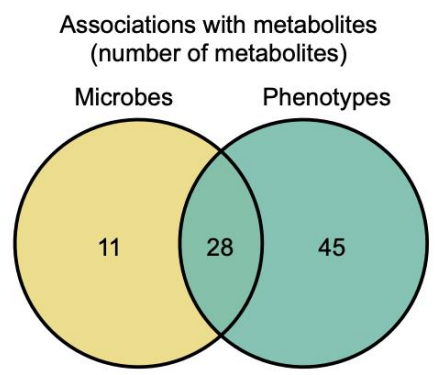


√ Evaluate relative contributions of bacteria

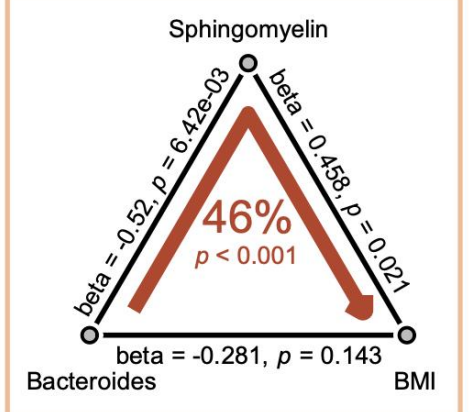


5. Mediation analysis

√ Metabolites to microbes or to phenotype correlations



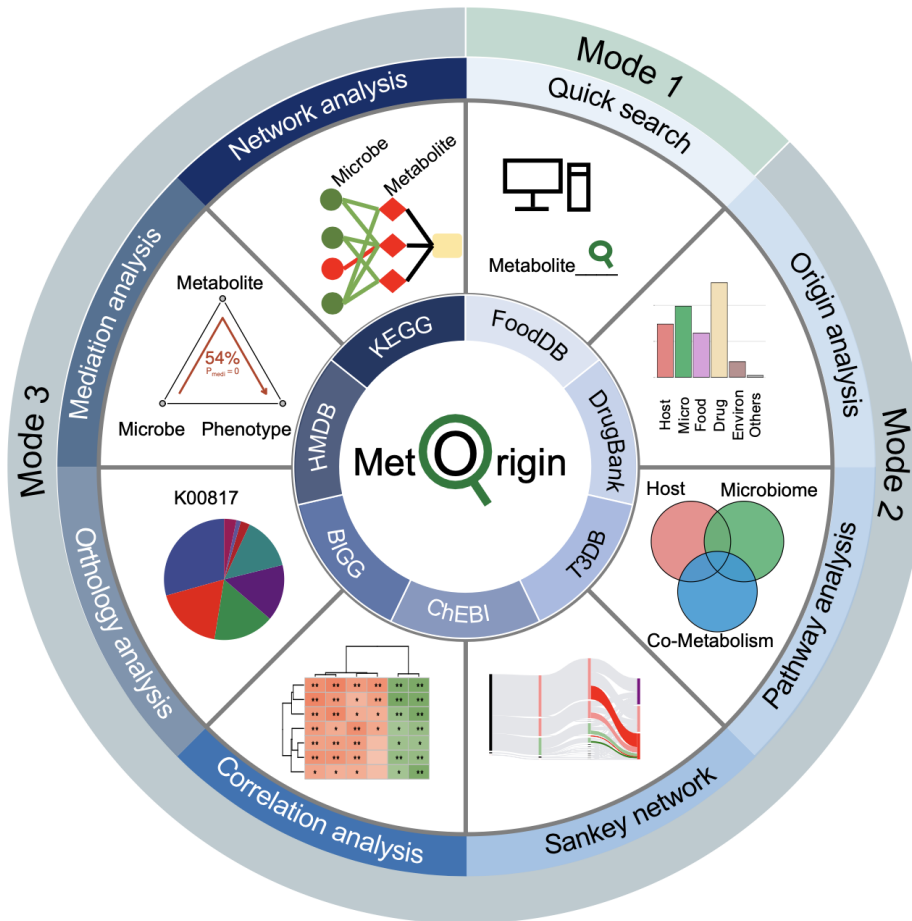
√ Evaluate the mediation effects of metabolites



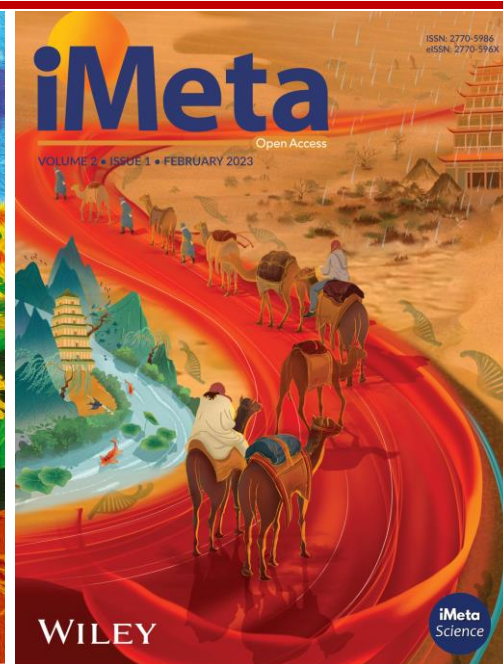


Summary

- MetOrigin 2.0 has integrated three analytical modes and eight distinct modules for advanced microbial metabolite discrimination.
- The updated database and three new features including quick search, orthology analysis, and mediation analysis expand the platform's versatility and functionality.
- MetOrigin 2.0 serves as a comprehensive web server for microbiome-metabolome data integration, streamlining the identification of microbial metabolites and their origins.
- Weblink: <http://metorigin.met-bioinformatics.cn>







Yu, Gang, Cuifang Xu, Xiaoyan Wang, Feng Ju, Junfen Fu, and Yan Ni. 2024. MetOrigin 2.0: Advancing the Discovery of Microbial Metabolites and their Origins. *iMeta* 3: e246. <https://doi.org/10.1002/imt2.246>



“***iMeta***” is a Wiley partner journal launched by iMeta Science Society in 2022, first **impact factor (IF) 23.8** in 2024, ranking 2/165 in the **microbiology field**. It aims to publish innovative and high-quality papers with broad and diverse audiences. **Its scope is similar to *Nature Biotechnology, Nature Methods, Nature Microbiology, Nature Food, etc.*** Its unique features include video abstract, bilingual publication, and social media dissemination, with more than 600,000 followers. It has published 220+ papers and been cited for 5000+ times, and has been indexed by **ESCI/WOS, PubMed, Google Scholar, and Scopus**.

“***iMetaOmics***” is a sister journal of “***iMeta***” launched in 2024, with a **target IF>10**, and its **scope is similar to *Nature Communications, Microbiome, ISME J, Nucleic Acids Research, Briefings in Bioinformatics, etc.*** All contributes are welcome!

 Society: <http://www.imeta.science>
 Publisher: <https://wileyonlinelibrary.com/journal/imeta>
 Submission: <https://wiley.atyponrex.com/journal/IMT2>
<https://wiley.atyponrex.com/journal/IMO2>

 office@imeta.science
imetaomics@imeta.science

 [Promotion Video](#)

 [iMetaScience](#)

 [iMetaScience](#)