

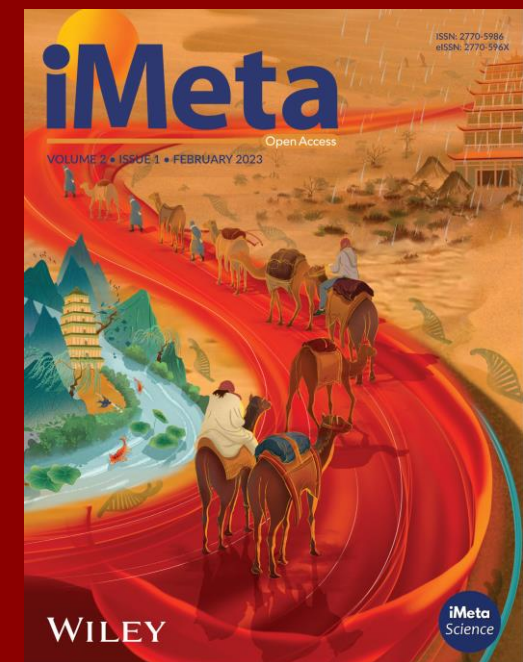


iNAP2.0: 代谢互补在微生物网络分析中的应用

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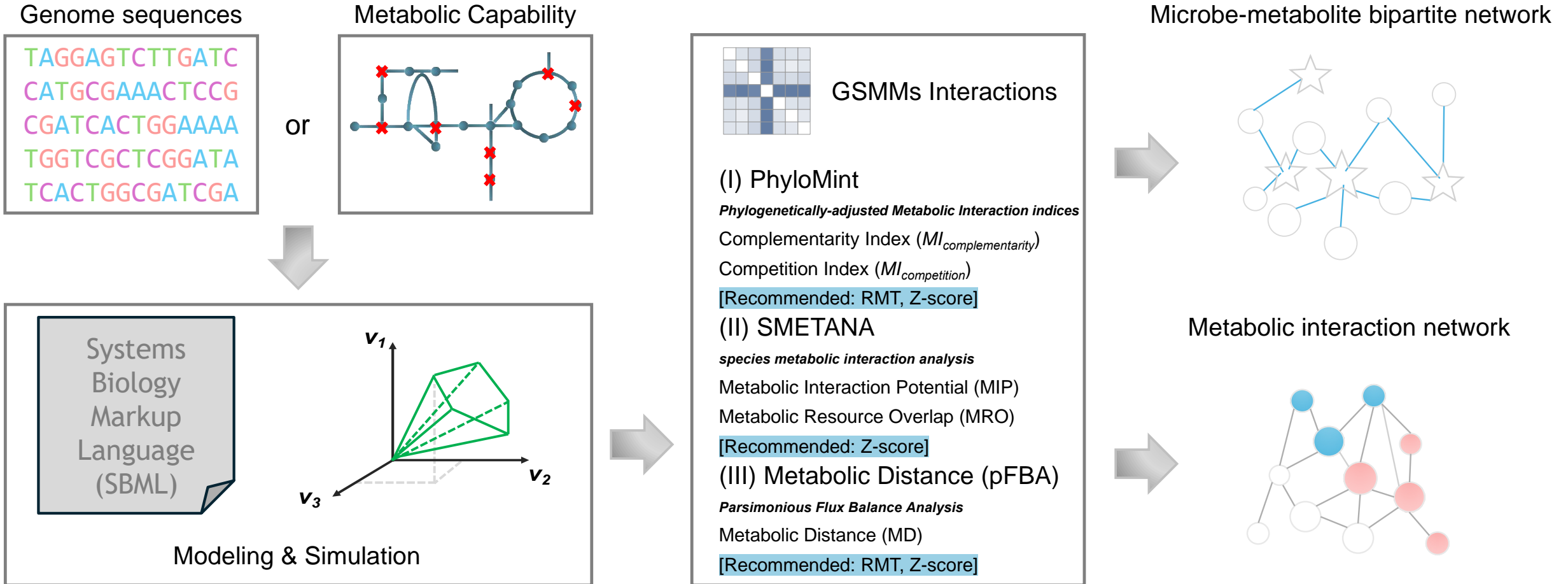
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Peng, Xi, Kai Feng, Xingsheng Yang, Qing He, Bo Zhao, Tong Li, Shang Wang, and Ye Deng. 2024. “iNAP 2.0: Harnessing metabolic complementarity in microbial network analysis.” *iMeta* 3: e235.
<https://doi.org/10.1002/imt2.235>

简介



本研究中提出了更新的iNAP2.0, 其最重要的**进步**是整合了代谢模型的构建与分析模块, 用于根据宏基因组测序数据进行微生物代谢互作的研究。



亮点

METABOLIC MODELINGS (TESTING)

Build metabolic models

Find interactions between models

Construct metabolic network

Analyze metabolic network

- 更新后的iNAP 2.0可以计算各种代谢互补与竞争系数，如PhyloMint指数、SMETANA（物种代谢相互作用分析）分数与基于pFBA的代谢距离，并提供了代谢互作网络的构建与分析模块；
- iNAP 2.0创新性地使用了随机矩阵理论模型（RMT）来选择筛选代谢互作网络的阈值；
- iNAP 2.0中的PhyloMint PTM程序可以显示微生物相互作用间的可能转移的代谢物，并将它们和微生物网络一起构建微生物-代谢物二分网络。

Visualize PTM network Microbe-Metabolite network visualization (Galaxy Version Beta 1.0) ☆ Favorite ▼ Options

PhyloMint PTMs Result (.txt)

📄 📄 📄 96: RMT chi square result of example.txt 📄

✓ Execute

Metabolic Modeling Network function: Get Potentially Transferable Metabolites (PTMs)

[**bigg_models_metabolites.txt**] Download from http://bigg.ucsd.edu/data_access. It provided the namespace of all bigg collected metabolite ids.

[**get_PTM.py**] Modified on the base of <https://github.com/mgtools/PhyloMint/blob/master/lib/BuildGraphNetX.py> because our results are also from this tool.



iNAP2.0主要模块概述（一）：构建基因组规模代谢模型

Build metabolic models

Prokka (Testing) Rapid prokaryotic genome annotation

CarveMe (Testing) Genome-scale metabolic model reconstruction

CarveMe (Gap-filling)(Testing) Genome-scale metabolic model reconstruction (Gap-filling)

第一部分：准备基因组规模代谢模型

步骤1：Prokka蛋白质预测

步骤2：CarveMe构建GSMM

步骤3：Gap filling选项下的CarveMe

CarveMe (Gap-filling)(Testing) Genome-scale metabolic model reconstruction (Gap-filling)
(Galaxy Version CarveMe Release 1.5.2)

☆ Favorite

▼ Options

Prokka Predicted Protein Sequences (Zipped, .zip)

   53: Prokka_faa.zip 

Source of Media Compositions Library

CarveMe's pre-built library of media compositions

Growth Medium for Gap-filling

LB

CarveMe provides with a very small pre-built library of media compositions. You can specify multiple media names by separate them with comma, e.g. LB,M9.

✓ Execute

CarveMe Release 1.5.2

CarveMe is a python-based tool for genome-scale metabolic model reconstruction.

About self-provided media library

CarveMe currently supports 5 pre-built libraries of media compositions:

- **LB** (Lysogeny broth)
- **LB-O2** (Lysogeny broth, anaerobic)
- **M9** (Minimal M9 medium)
- **M9-O2** (Minimal M9 medium, anaerobic)
- **M9-glyc** (Minimal M9 medium, glycerol as carbon source)

PhyloMint 重要步骤：PhyloMint PTM的识别






PhyloMint

重要步骤：PhyloMint PTM的识别






PHYLOMINT
PhyloMint Pathway-based and phylogenetically adjusted quantification of competition and cooperation between microbial species
PhyloMint PTM Find Potentially Transferable Metabolites
Create PhyloMint Matrix (Competition and Complementarity) Create PhyloMint matrix
SMETANA
Create Community List Create input file for SMETANA
SMETANA Global SMETANA (Global Mode)
Iterative SMETANA Global SMETANA (Global Mode, iterative)
SMETANA Detailed SMETANA (Detailed Mode)
Iterative SMETANA Detailed SMETANA (Detailed Mode, iterative)
Create SMETANA Matrix Convert MIP/MRO results to adjacent matrices
METABOLIC DISTANCE
Metabolic Distance Calculates metabolic dissimilarity

PhyloMint PTM Find Potentially Transferable Metabolites (Galaxy Version Beta 1.0) ☆ Favorite ▼ Options


Zipped CarveMe Models (.zip)

   55: CarveMe_models.zip  

PhyloMint Result (txt)

   57: PhyloMint_result.txt  


Genome File Extension

xml (Extensible Markup Language) 

MaxCC

5

Must be equal to the value set in PhyloMint!

 Execute

Metabolic Modeling Network function: Get Potentially Transferable Metabolites (PTMs)

[bigg_models_metabolites.txt] Download from http://bigg.ucsd.edu/data_access. It provided the namespace of all bigg collected metabolite ids.

[get_PTM.py] Modified on the base of <https://github.com/mgtools/PhyloMint/blob/master/lib/BuildGraphNetX.py> because our results are also from this tool.

SMETANA

代谢距离



iNAP2.0主要模块概述 (三) : 构建代谢相互作用网络

Construct metabolic network

Random Matrix Theory (cutoff) To show the cutoff using adjacent matrix

新增方法

Random Matrix Theory (cutoff, Kolmogorov-Smirnov test) RMT cutoff determination using Kolmogorov-Smirnov test

Z-Score Outlier Detection

Standard and modified Z-score for outlier detection

Construct Network Adjacent

Matrix Use RMT cutoff to generate adjacent network

Random Matrix Theory (cutoff, Kolmogorov-Smirnov test) RMT cutoff determination using Kolmogorov-Smirnov test (Galaxy Version 1.1.0)

☆ Favorite

▼ Options

Adjacent Matrix(txt)



96: RMT chi square result of example.txt



✓ Execute

使用Kolmogorov-Smirnov检验的RMT方法

Using Random Matrix Theory (RMT) with Kolmogorov-Smirnov test

Notice your distance matrix must follow the form provided below:

	Species_Apple	Species_Bravo	Species_Candy	Species_Dancing	Species_ET
Species_Apple	1	0.03862660944206009	0.29545454545454547	0.2553191489361702	0.2696629213483146
Species_Bravo	0.03862660944206009	1	0.2839506172839506	0.25	0.25301204819277107
Species_Candy	0.29545454545454547	0.2839506172839506	1	0.05660377358490566	0.04716981132075472
Species_Dancing	0.2553191489361702	0.25	0.05660377358490566	1	0.038834951456310676
Species_ET	0.2696629213483146	0.25301204819277107	0.04716981132075472	0.038834951456310676	1

Z-Score Outlier Detection Standard and modified Z-score for outlier detection (Galaxy Version 1.0.0)

☆ Favorite

▼ Options

基于Z-score检测异常值的网络阈值筛选方法

Adjacent Matrix (tabular file)



96: RMT chi square result of example.txt



Standard or modified Z-score

Modified Z-score





iNAP2.0主要模块概述 (四) : 分析代谢相互作用网络

Analyze metabolic network

Global Network Properties and Individual Nodes' Centrality

Module separation and module hubs Modularization and Z-P result for module hubs

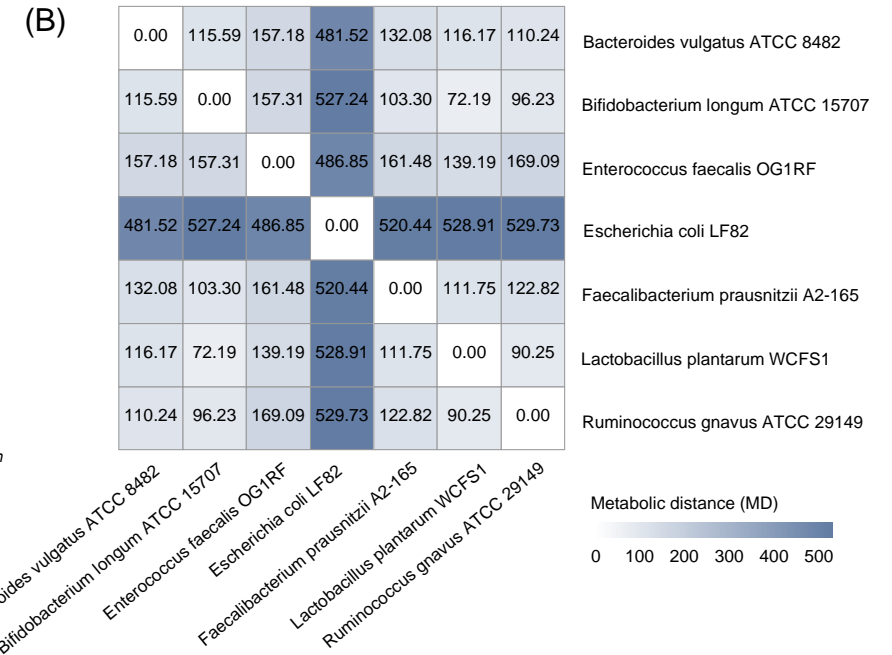
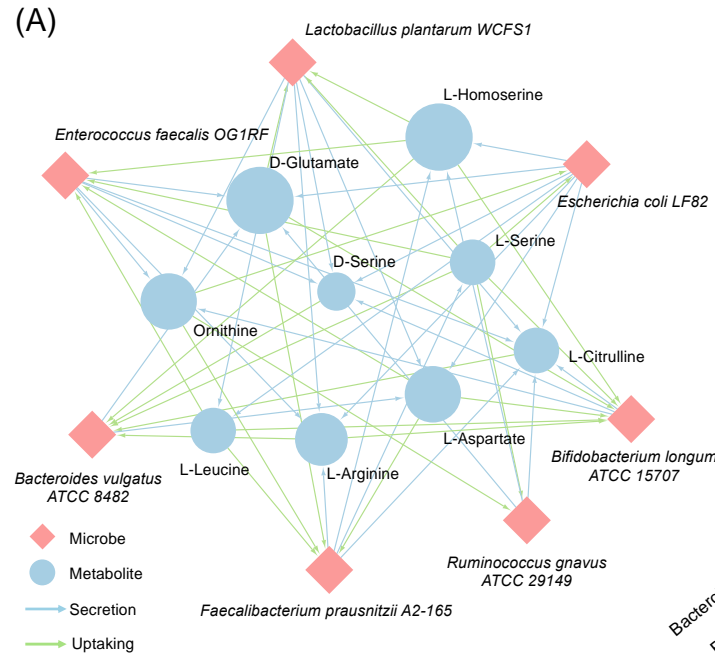
Integrate Node Attribute Put node centrality, modularity and annotation into one table

新增方法

Network Intersection Find shared edges and nodes between two networks

Visualize PTM network Microbe-Metabolite network visualization

Metabolic distance heatmap Visualize metabolic distance



微生物-PTM代谢物二分网络

代谢距离矩阵热图



iNAP2.0的典型应用案例

nature communications



Article

<https://doi.org/10.1038/s41467-024-52532-x>

Metabolic interdependencies in thermophilic communities are revealed using co-occurrence and complementarity networks

Received: 8 March 2024

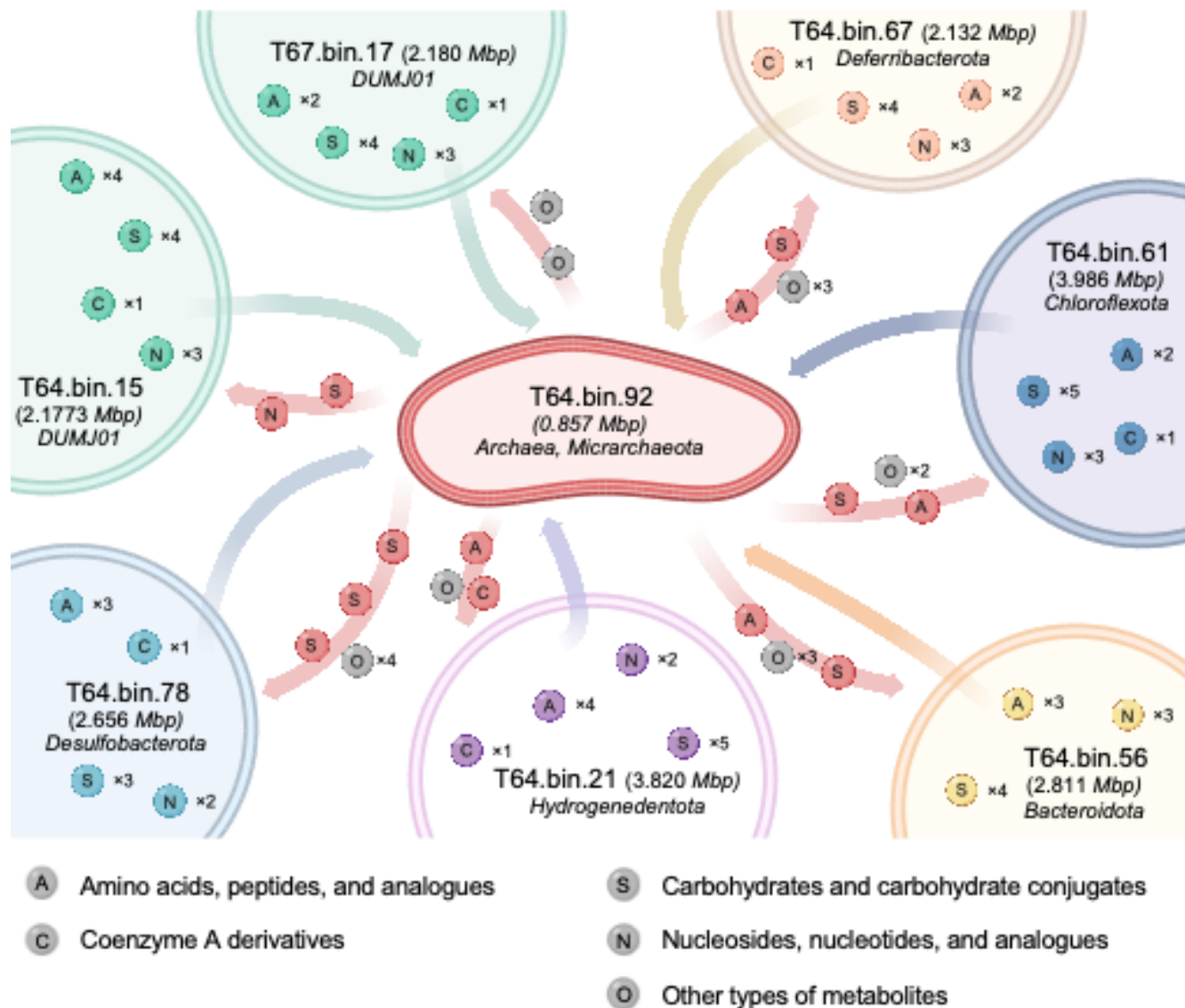
Xi Peng^{1,2}, Shang Wang¹, Miaoxiao Wang^{3,4}, Kai Feng¹, Qing He¹,

Accepted: 9 September 2024

Xingsheng Yang^{1,2}, Weiguo Hou⁵, Fangru Li⁵, Yuxiang Zhao⁶, Baolan Hu^{7,8,9},
Xiao Zou¹⁰ & Ye Deng^{1,2} ✉

利用微生物代谢互补网络与共现网络结合分析的方法解析了热泉环境中嗜热菌群的生存策略以及群落结构变化等特征。

相关成果发表在Nature Communications上。



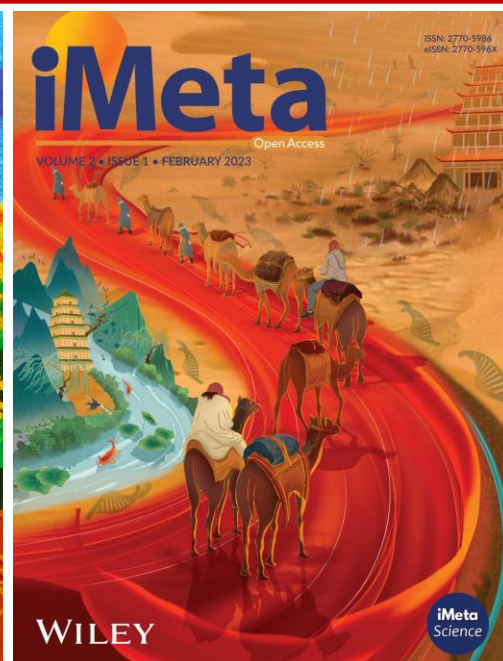
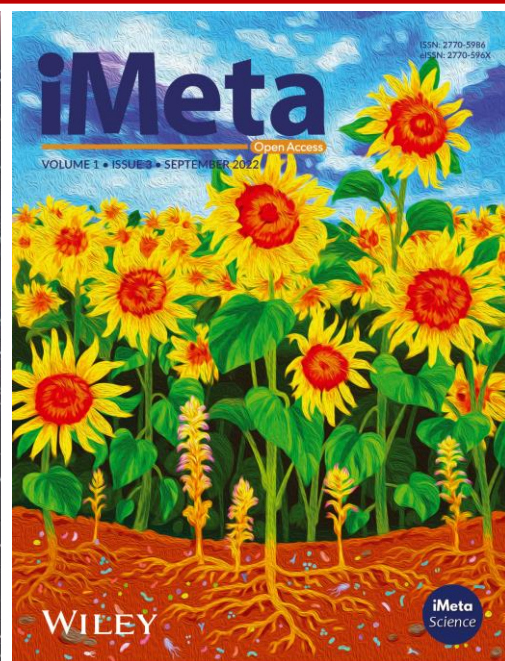
<https://www.nature.com/articles/s41467-024-52532-x>



总结

- ❑ 在这项研究中，我们介绍了更新后的iNAP2.0，其主要功能是将基于宏基因组测序数据的代谢互补分析整合到分子生态网络中；
- ❑ 更新后的iNAP2.0新增了20个工具，使得用户能够完整地**对代谢互补网络进行构建与分析**；
- ❑ 平台开放注册，允许用户上传数据从头分析或使用中间数据开始分析，平台中提供了相应的**测试数据**供研究者学习使用；
- ❑ 平台网址：<https://inap.denglab.org.cn/>

Peng, Xi, Kai Feng, Xingsheng Yang, Qing He, Bo Zhao, Tong Li, Shang Wang, and Ye Deng. 2024. “iNAP 2.0: Harnessing metabolic complementarity in microbial network analysis.” *iMeta* 3: e235.
<https://doi.org/10.1002/imt2.235>



“**iMeta**” (影响因子**23.7**) 由威立、肠菌分会和数千名华人科学家出版的期刊，主编刘双江和傅静远教授。
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影响力：[ESCI/WOS/JCR](#)、[PubMed](#)、[Google](#)、[Scopus](#)收录，**IF 23.7**位列微生物学研究期刊全球第一；
时效性：外审平均21天；投稿至发表中位数57天；
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