



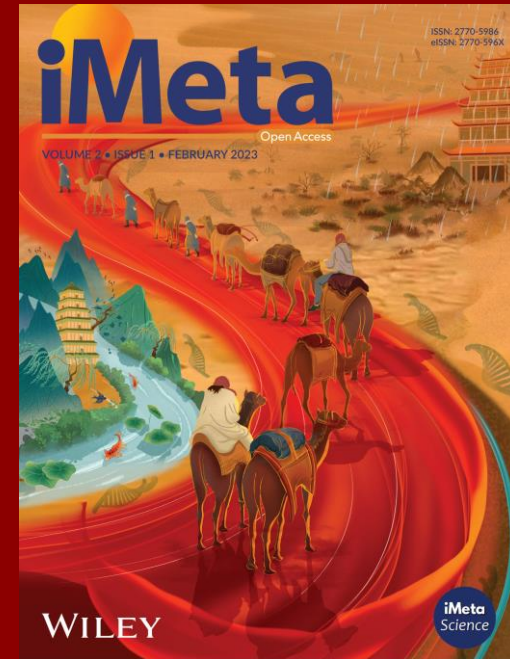
MDIPID: 微生物-药物相互作用及其与疾病表型关联数据库

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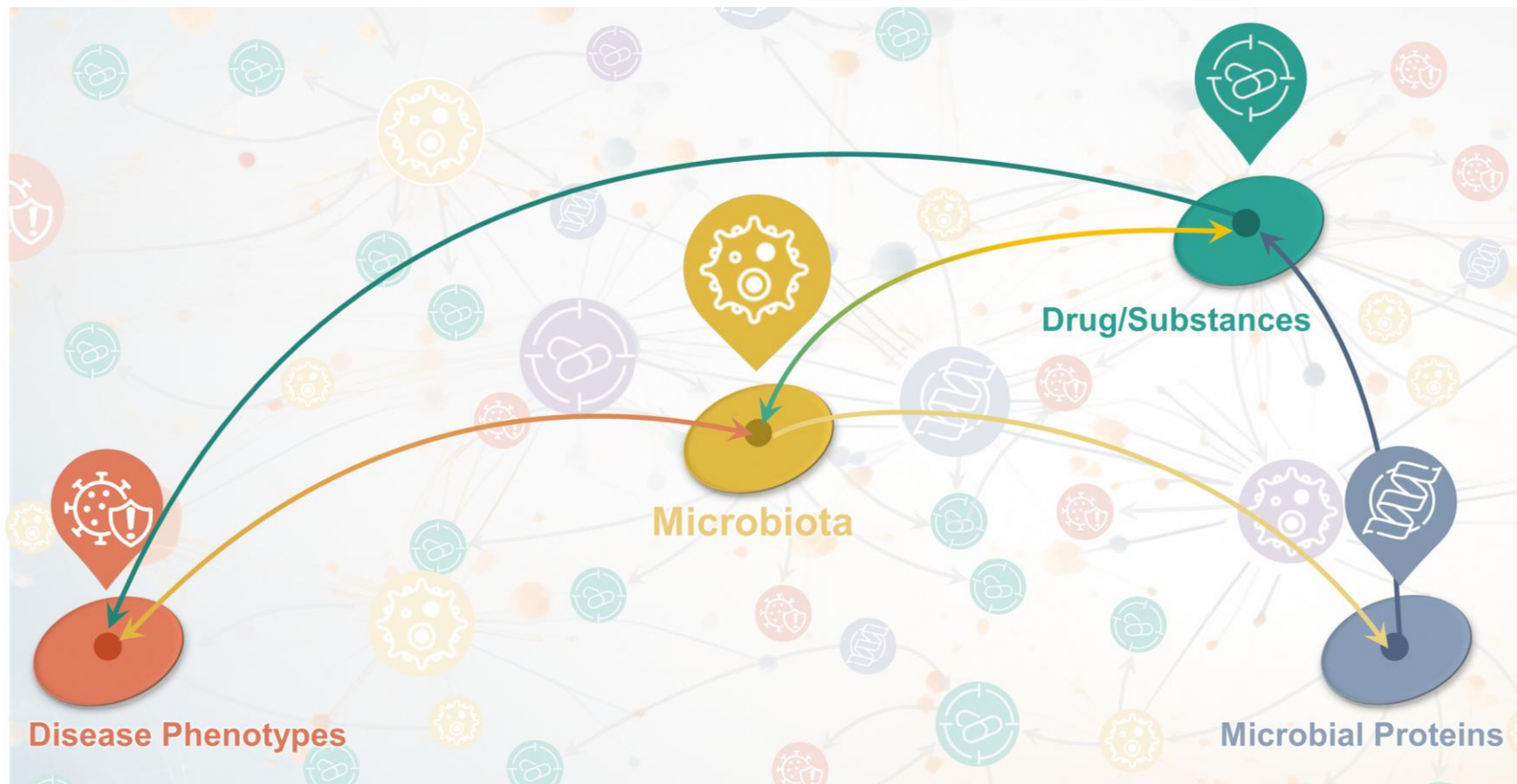


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引言

- 微生物组在疾病发生发展以及个体化药物反应中扮演着极为重要的角色
- 现有数据库多聚焦单一方向，缺乏对微生物、药物与疾病之间复杂双向互作关系的全面解析，极大地限制了相关研究的深入和精准医学的发展





亮点

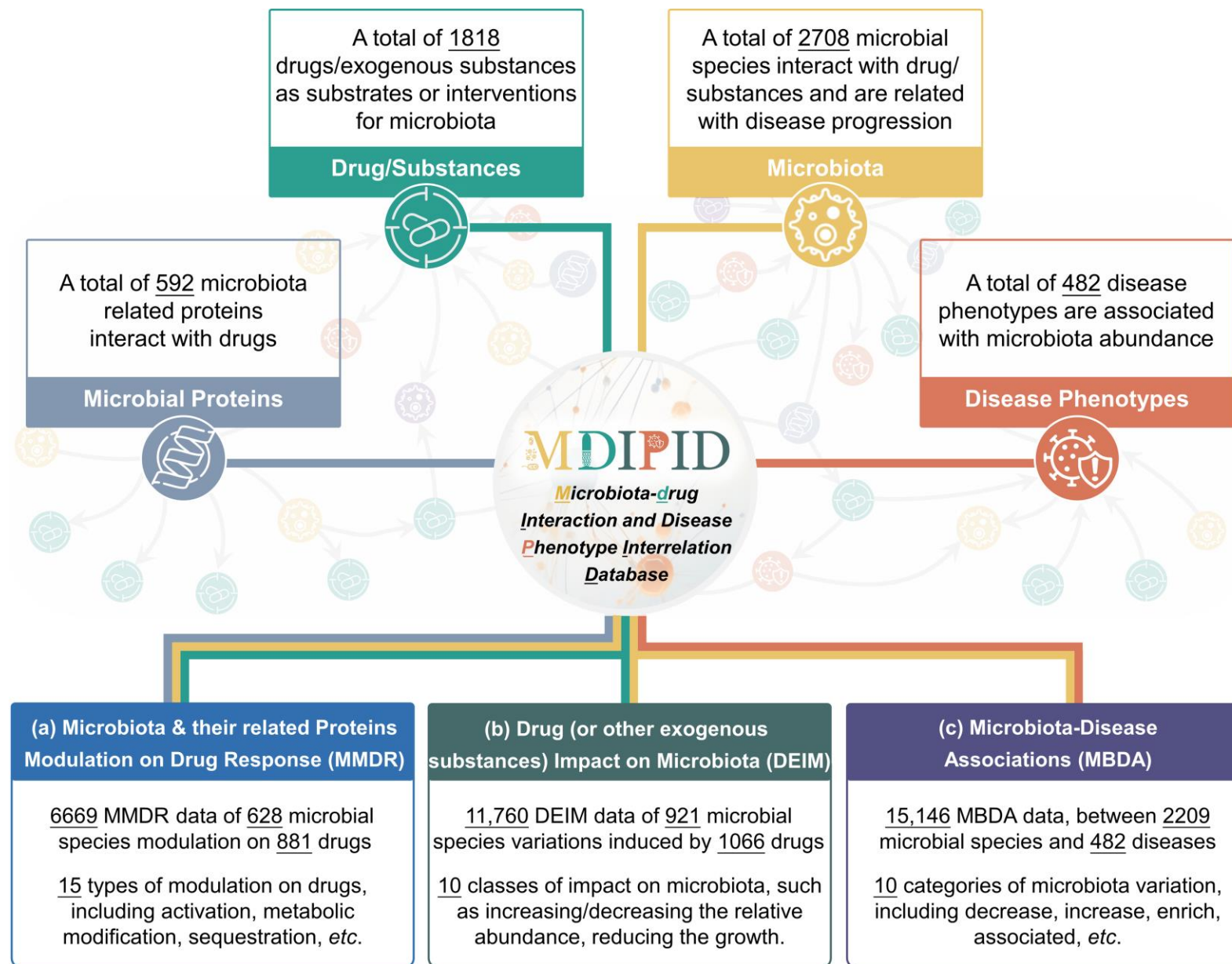


图1. MDIPID的核心数据结构及其统计数据



多种检索方式



Microbiota



Drug



Disease



Protein

About Microbiota

Microbiota, a diverse community of microorganisms, plays a crucial role in health and disease development, significantly impacting individualized drug responses. Understanding the intricate relationships between microbiota, drugs, and diseases, especially the

关键词检索



Search for Microbiota in Whole Database:

Search for Microbiota by Keywords:

Please enter your keywords here

Try example: *Acinetobacter baumannii*; Anti-CTLA-4; Colorectal cancer ...

Search for Microbiota Entries by Microbiota Genus & Species Name:

> Tip: Please select the microbiota genus first, then a list of microbiota with selected genus will be available for selection.

1: Please select a microbiota genus name

2: Please select a microbiota species name

Search for Microbiota Entries by Drug Status & Name:

> Tip: Please select the clinical status first, then a list of drugs under the selected status will be available for selection.

1: Please select a drug status

2: Please select a drug name

Search for Microbiota Entries by Disease Class & Name:

> Tip: Please select the Disease Class first, then a list of disease entries will be available for selection.

1: Please select a disease class

2: Please select a disease entry



Acinetobacter baumannii

| | | |
|------------------------|---|---------------------------------|
| Microbiota ID | MC00073 | Microbiota Info |
| Microbiota Type | Bacteria (Pseudomonadota) | |
| Microbiota Genus | <i>Acinetobacter calcoaceticus/baumannii</i> complex | |
| Species ID | 470 | |
| Representative Protein | Aminoglycoside N-acetyltransferase (aacC2) ; Aminoglycoside O-phosphotransferase (aphA-6) ; Beta-lactamase (blaIMP) | |

具体的微生物信息简表

Reset

Search

Reset

Search

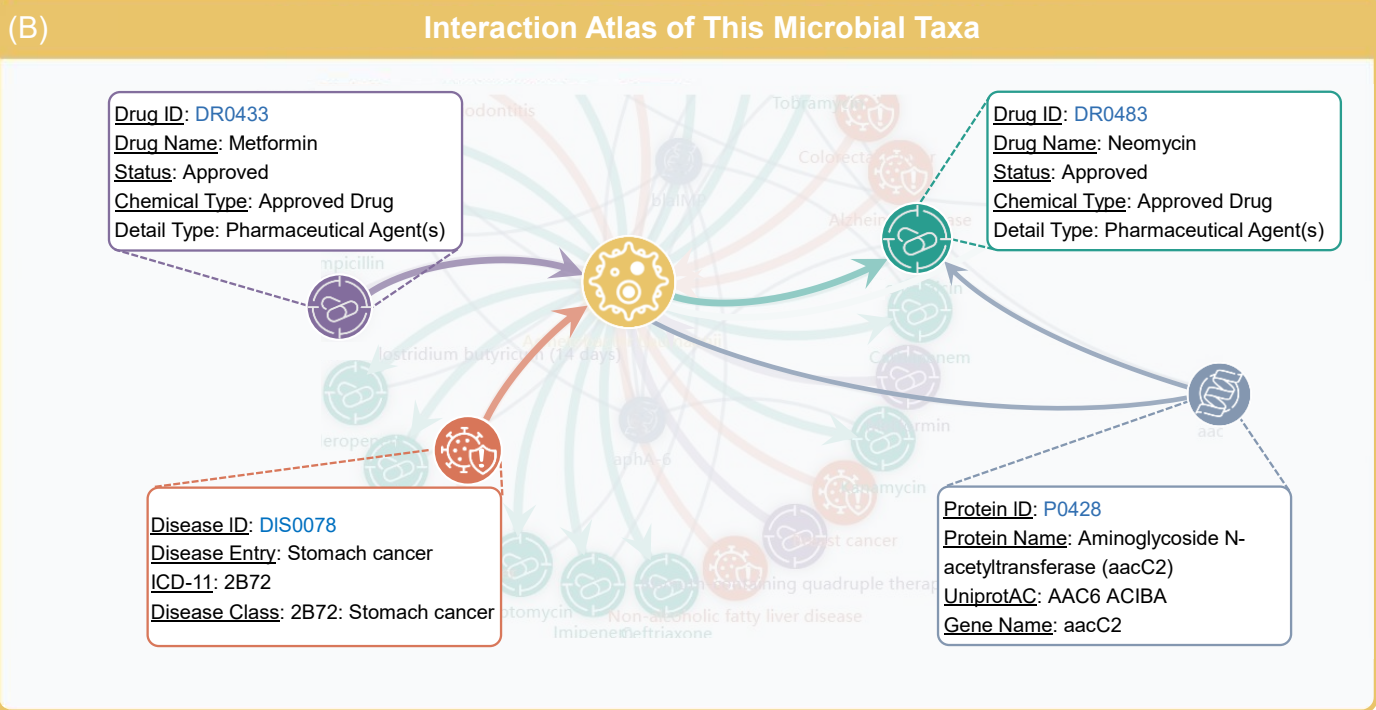
下拉菜单检索



结果：微生物信息

(A) General Information of Microbial Taxa (ID: MC00073)

| | | | |
|--------------|---|-------------|-----|
| Species Name | Acinetobacter baumannii | Taxonomy ID | 470 |
| Lineage | Kingdom: Bacteria ↗ ↳ Phylum: Pseudomonadota ↗ ↳ Class: Gammaproteobacteria ↗ ↳ Order: Moraxellales ↗ ↳ Family: Moraxellaceae ↗ ↳ Genus: Acinetobacter calcoaceticus/baumannii complex ↗ ↳ Species: Acinetobacter baumannii ↗ | | |



(a) Microbiota Taxa & its related Proteins Modulation on Drug Response

| | |
|-----------------|---|
| Approved Drug | Neomycin |
| Drug Info | DR0483 |
| Related Protein | aacC2 P0428 |
| Mechanism | The protein aacC2 of <i>Acinetobacter baumannii</i> has been reported to metabolic modification of Neomycin, thereby affecting drug activity. |

(b) Drug (or other substances) Impact on This Microbial Taxa

| | |
|---------------|---|
| Approved Drug | Metformin |
| Drug Info | DR0433 |
| Strain | <i>A. baumannii</i> TCDC-AB0715 |
| Methods | HT incubation assays |
| Mechanism | Metformin has been reported to increase the relative abundance of <i>Acinetobacter baumannii</i> TCDC-AB0715. |

(c) Variation in the Abundance of This Microbial Taxa Across Phenotypes

| | |
|----------------------|--|
| 2B72: Stomach cancer | Stomach cancer |
| Phenotype Info | DIS0078 |
| Studied Sample | Stomach mucosa tissue |
| Compared Sample | Superficial gastritis |
| Variation | The abundance of <i>Acinetobacter baumannii</i> has been reported to increase in Stomach cancer condition. |

图2. MDIPID中特定微生物的详细信息展示界面



结果：药物信息



Search for Drug in Whole Database:

Search for Drug by Keywords:

Please enter your keywords here

Search

Try example: Finasteride; Akkermansia muciniphila; Triclosan ...

Search for Drug Entries by Drug Indication & Name:

> Tip: Please select the indication first, then a list of drugs with selected indication will be available for selection.

1: Please select a drug indication

Reset

2: Please select a drug name

Search

Search for Substrate Drug Entries by Microbiota Genus & Species Name:

> Tip: Please select the microbiota genus first, then a list of microbiota with selected genus will be available for selection.

1: Please select a microbiota genus name

Reset

2: Please select a microbiota species name

Search

Search for Intervention Drug Entries by Microbiota Genus & Species Name:

> Tip: Please select the microbiota genus first, then a list of microbiota with selected genus will be available for selection.

1: Please select a microbiota genus name

Reset

2: Please select a microbiota species name

Search

Finasteride

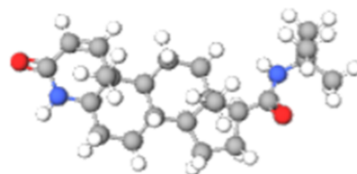
| | | |
|----------------------------------|------------------------------|---------------------------|
| Drug ID | DR0268 | Drug Info |
| Drug Status | Approved | |
| Drug Class | Pharmaceutical Agent(s) | |
| Drug Type | Approved Drug | |
| Representative Indication | Benign prostatic hyperplasia | |

(A)

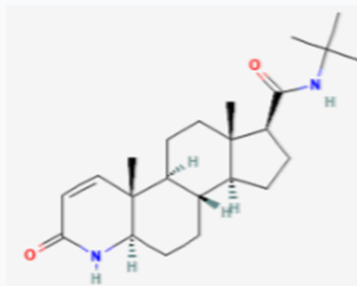
General Information of Drug (ID: DR0268)

| | | | |
|----------------------|--|--------------------------|--------------------------|
| Drug Name | Finasteride | Highest Status | Approved |
| Synonyms | finasteride; 98319-26-7; Proscar; Propecia; Finastid; Prostide; Chibro-Proscar; MK-906; Finneria; Finasterida; Finasteridum; Finasteridum [INN-Latin]; MK 906; Finasterida [INN-Spanish] Show More | | |
| Chemical Type | Approved Drug | | |
| Indication | Disease Entry | ICD 11 | Status REF |
| | Benign prostatic hyperplasia | GA90 | Approved [3] |
| Drug Type | Small molecular drug | Therapeutic Class | Antihyperplasia Agents |

Structure



3D MOL [↓](#)



2D MOL [↓](#)

#Ro5 Violations (Lipinski): 0

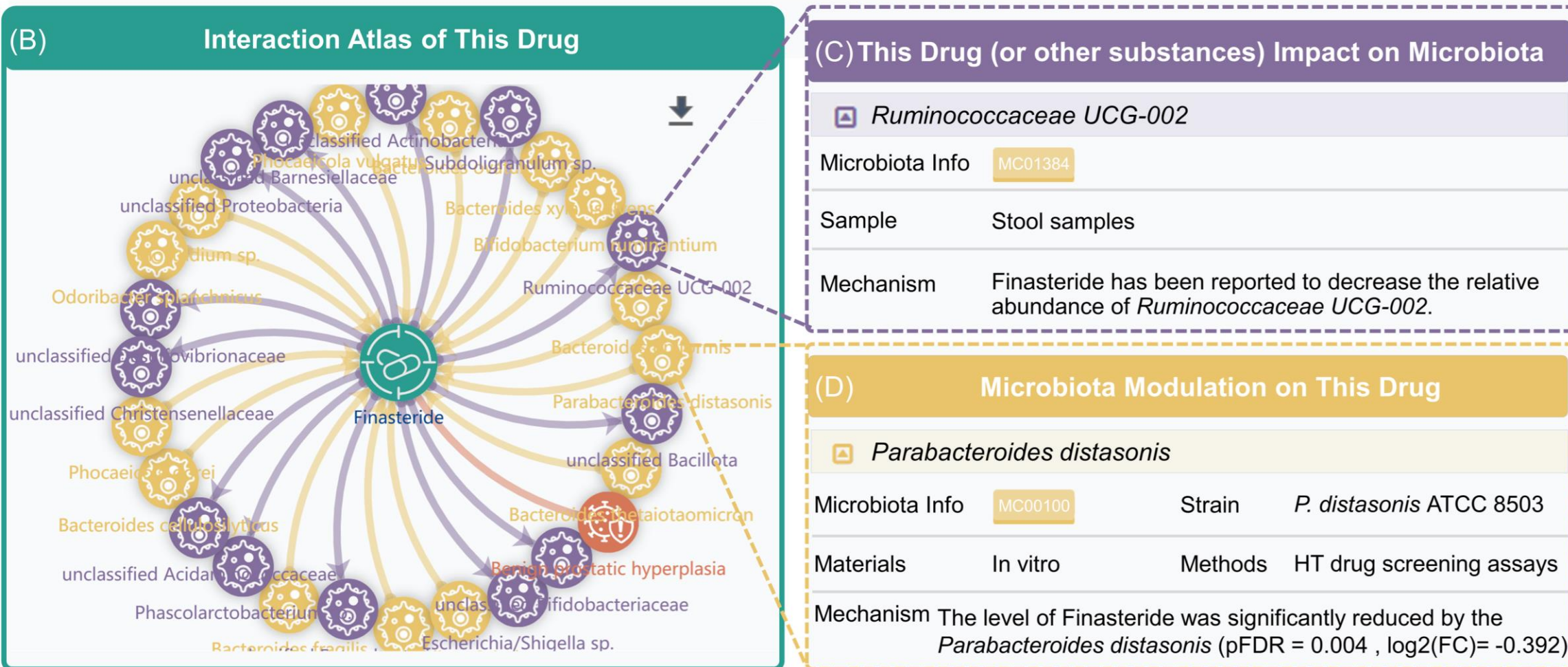
| | |
|--|-------|
| Molecular Weight (mw) | 372.5 |
| Logarithm of the Partition Coefficient (xlogp) | 3 |
| Rotatable Bond Count (rotbonds) | 2 |
| Hydrogen Bond Donor Count (hbonddonor) | 2 |
| Hydrogen Bond Acceptor Count (hbondacc) | 2 |



图S1(A). MDIPID中药物信息页面的示意图



结果：药物信息



图S1(B). 药物的相互作用图谱

图S1(C). 该药物影响微生物的详细信息

图S1(D). 微生物调节该药物的详细数据



结果：疾病表型信息

- Microbiota
- Drug
- Disease
- Protein

About Disease Phenotype

Disease, a complex phenomenon influenced by multiple factors including the microbiota, is key for identifying biomarkers and personalizing treatment. Understanding microbiota's role in disease can lead to new therapeutic targets and effective treatments, emphasizing the need for a holistic approach.

Breast cancer

| | | |
|---------------------|--|------------------------------|
| Disease ID | DIS0102 | Disease Info |
| Disease Class | 2C60-2C65: Breast cancer | |
| ICD-11 Code | 2C60-2C65 | |
| Representative Drug | Anastrozole ; Doxorubicin ; Gemcitabine | |
| Related Microbiota | Acholeplasma sp. ; Acidaminococcus sp. ; Acinetobacter baumannii | |

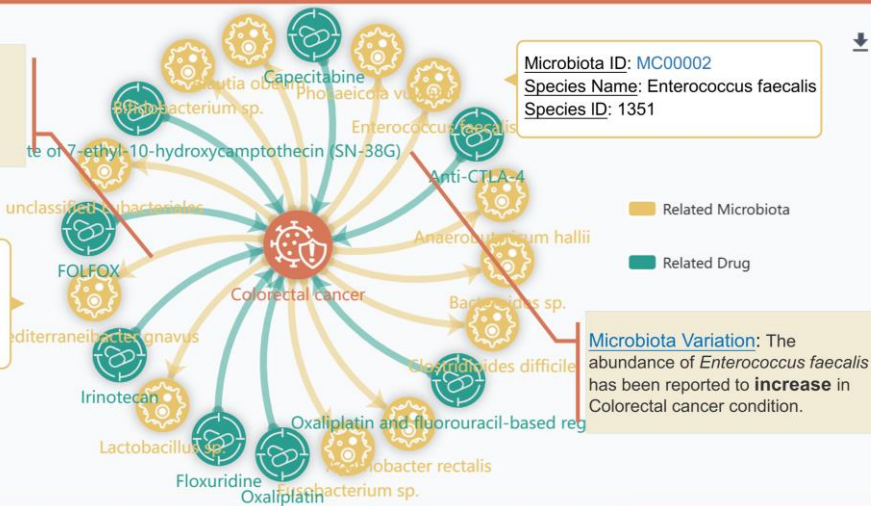
(A) General Information of Disease Phenotype (ID: DIS0082)

| | | | |
|---------------|-------------------------|-------------|------|
| Disease Name | Colorectal cancer | ICD-11 Code | 2B91 |
| Disease Class | 2B91: Colorectal cancer | | |

(B) Interaction Atlas of This Disease Phenotype

Microbiota Variation: The abundance of *Mediterraneibacter gnavus* has been reported to **decrease** in Colorectal cancer condition.

Microbiota ID: MC00011
Species Name: *Mediterraneibacter gnavus*
Species ID: 33038



(C) Variation in the Abundance of Microbiota Across This Disease Phenotype

| | |
|--|--|
| Kingdom: Archaea | 1 Phylum(s) In Total |
| Phylum: Euryarchaeota | 2 Species(s) In Total |
| Species: <i>Methanobrevibacter sp.</i> | 1 Variation(s) in the Abundance of Microbiota In Total |
| Species: unclassified Methanobacteriales | 1 Variation(s) in the Abundance of Microbiota In Total |

[Show the Full List of 654 Microbial Species](#)

(D) List of Drug(s) That Treat This Disease As An Indication

8 Pharmaceutical Agent(s) Treating This Disease As An Indication

| Drug Name | Drug ID | Chemical Type | PubChem CID | Highest Status | REF |
|--------------|------------------------|---------------|----------------|----------------|------|
| Anti-CTLA-4 | DR0047 | Approved Drug | N.A. | Approved | [78] |
| Capecitabine | DR0115 | Approved Drug | CID: 60953 | Approved | [79] |
| Floxuridine | DR0270 | Approved Drug | CID: 5790 | Approved | [80] |
| FOLFOX | DR0277 | Approved Drug | CID: 135659064 | Approved | [81] |

[Show the Full List of 8 Pharmaceutical Agent\(s\)](#)

图S2. MDIPID 中疾病表型信息页面的示例图

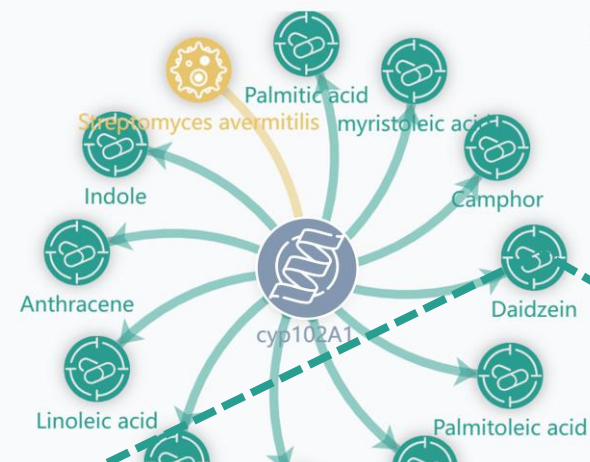


结果：相关蛋白信息

(A) General Information of Microbial Protein (ID: P0024)

| | | | |
|----------------------------|---|-------------------|---|
| Protein Name | Cytochrome P450 102D1 | Gene Name | cyp102A1 |
| Microbial sources | Streptomyces avermitilis MC00128 | | |
| Functional Family | EC: 1 Oxidoreductase ↳ EC: 1.14 Oxygen paired donor oxidoreductase ↳ EC: 1.14.14 Flavin/flavoprotein donor oxidoreductase ↳ EC: 1.14.14.1 Flavin/flavoprotein donor oxidoreductase | | |
| EC/TC ID | EC: 1.14.14.1 Oxidoreductase | UniProt AC | CPXB_BACMB Oxidoreductase |
| Gene ID | Gene ID: 29911283 | | |
| PDB ID | 1BU7 Oxidoreductase ; 1BVY Oxidoreductase ; 1FAG Oxidoreductase ; 1FAH Oxidoreductase ; 1JME Oxidoreductase ; 1JPZ Oxidoreductase ; 1P0V Oxidoreductase ; 1P0W Oxidoreductase ; 1SMJ Oxidoreductase ; 1YQO Oxidoreductase ; 1YQP Oxidoreductase ; 1ZO4 Oxidoreductase ; 1ZO9 Oxidoreductase ; 1ZOA Oxidoreductase ; 2BMH Oxidoreductase ; Show More | | |
| KEGG Pathway | bmeg00627 (Aminobenzoate degradation) Oxidoreductase Show More | | |
| Tissue Distribution | Primarily distributed in human gut. | | |
| Function | This enzyme is P-450 heme-thiolate protein, acting on a wide range of substrates including many xenobiotics, steroids, fatty acids, vitamins and prostaglandins; reactions Show More | | |
| Sequence | MTIKEMPQPKTFGELKLNPLLLNTDKPVQALMKIADELGEIFKFEAPGRVTRYLSSQRLIK EACDESFRFDKNSQALKFVRDFAGDGLFTSWTHEKNWKKAHNILLPSFSQAMKGYHAI Show More | | |

(B) Interaction Atlas of This Microbial Protein



(C) Effect of This Microbial Protein on Drugs

| | |
|--|---|
| <input checked="" type="checkbox"/> Drug in Clinical Trial | |
| <input checked="" type="checkbox"/> Daidzein | |
| Protein Influence | Metabolic modification of Daidzein |
| Drug Info | DR0186 |
| Microbiota Info | MC00128 |
| Metabolic Reaction | Hydroxylation |
| Affinity Data | Kcat/KM values of Daidzein was $6.8 \pm 2.44 \mu\text{M}^{-1}\cdot\text{min}^{-1}$ |
| Mechanism | The protein cyp102A1 of <i>Streptomyces avermitilis</i> has been reported to metabolic modification of Daidzein, thereby affecting drug activity. |

图S3. MDIPID中微生物蛋白信息页面的示意图

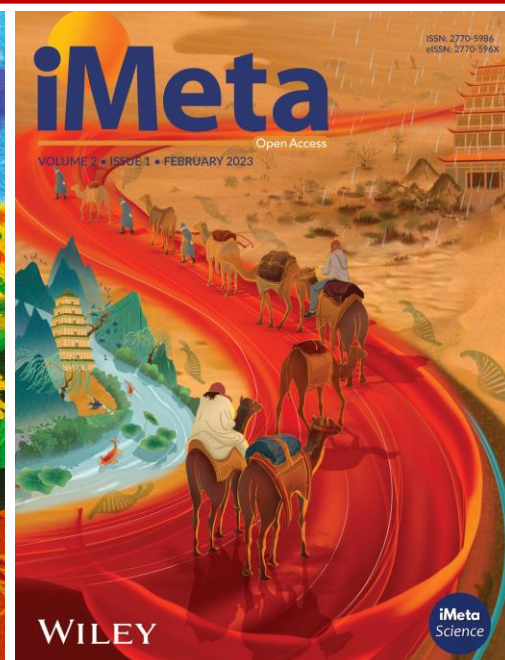
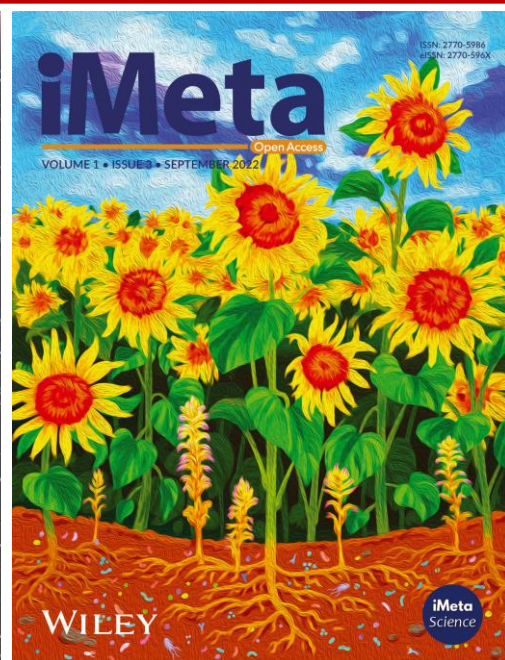


总结



- ❑ 本研究系统性整合了微生物、药物、疾病及微生物蛋白间复杂的双向互作数据，构建了全面的微生物-药物-疾病相互作用图谱MDIPID。
- ❑ MDIPID详细描述了微生物对药物作用、药物对微生物影响及微生物与疾病关联的各种数据及其相关机制，这些数据共同组成了一个包括 1818 种药物/外源性物质、2708 种微生物物种、482 种疾病和 592 种微生物蛋白的综合网络。
- ❑ MDIPID提供多种搜索和数据展示功能，有望成为研究药物、微生物与人类疾病关系的重要资源，促进精准医学发展和新型治疗策略的探索。
- ❑ 数据库网址：<https://idrblab.org/mdipid/>

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