



# MDIPID: Microbiota-drug Interaction and Disease Phenotype Interrelation Databas

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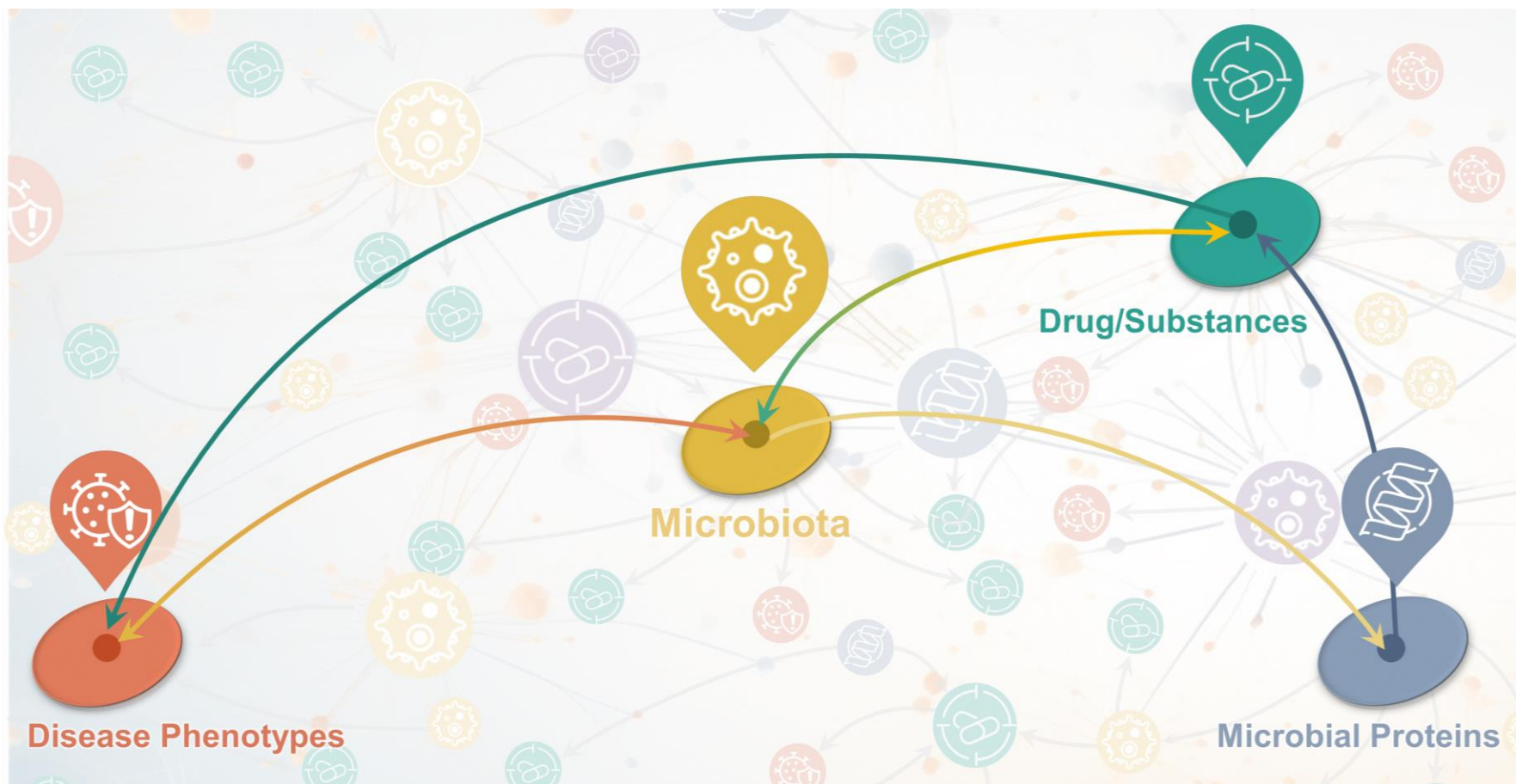


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# Introduction

- Human microbiota plays a vital role in disease development and individualized drug responses
- Existing databases often focus on unidirectional associations, lacking a comprehensive analysis of the complex and bidirectional interactions among microbiota, microbial proteins, drugs, and diseases. This significantly limits in-depth research and the advancement of precision medicine.





# Highlights

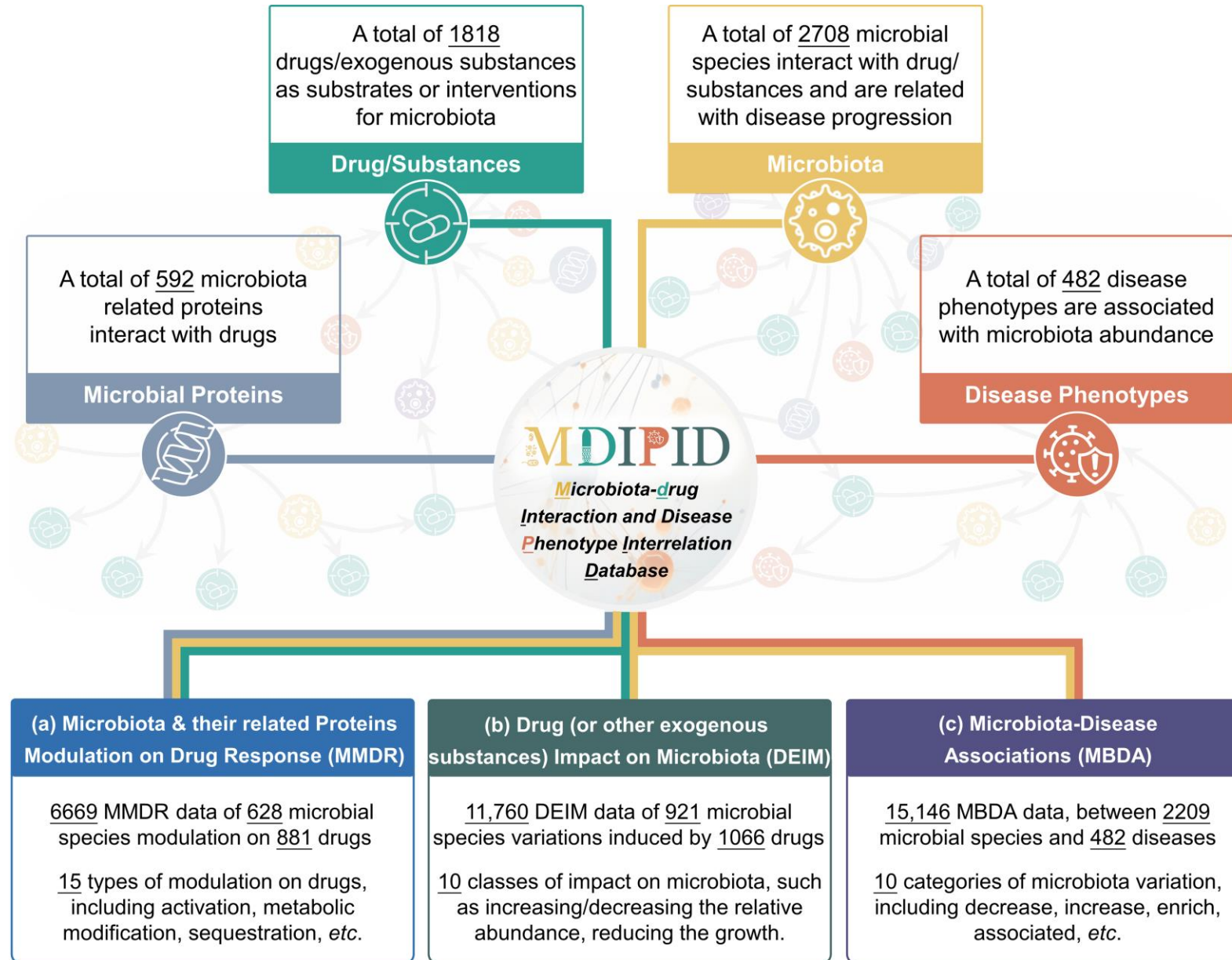


Figure 1. The primary data components of MDIPID and their corresponding statistics.



# Data access and retrieval

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 th...

Keyword search



**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 Info

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

Brief table of specific microbial taxa data

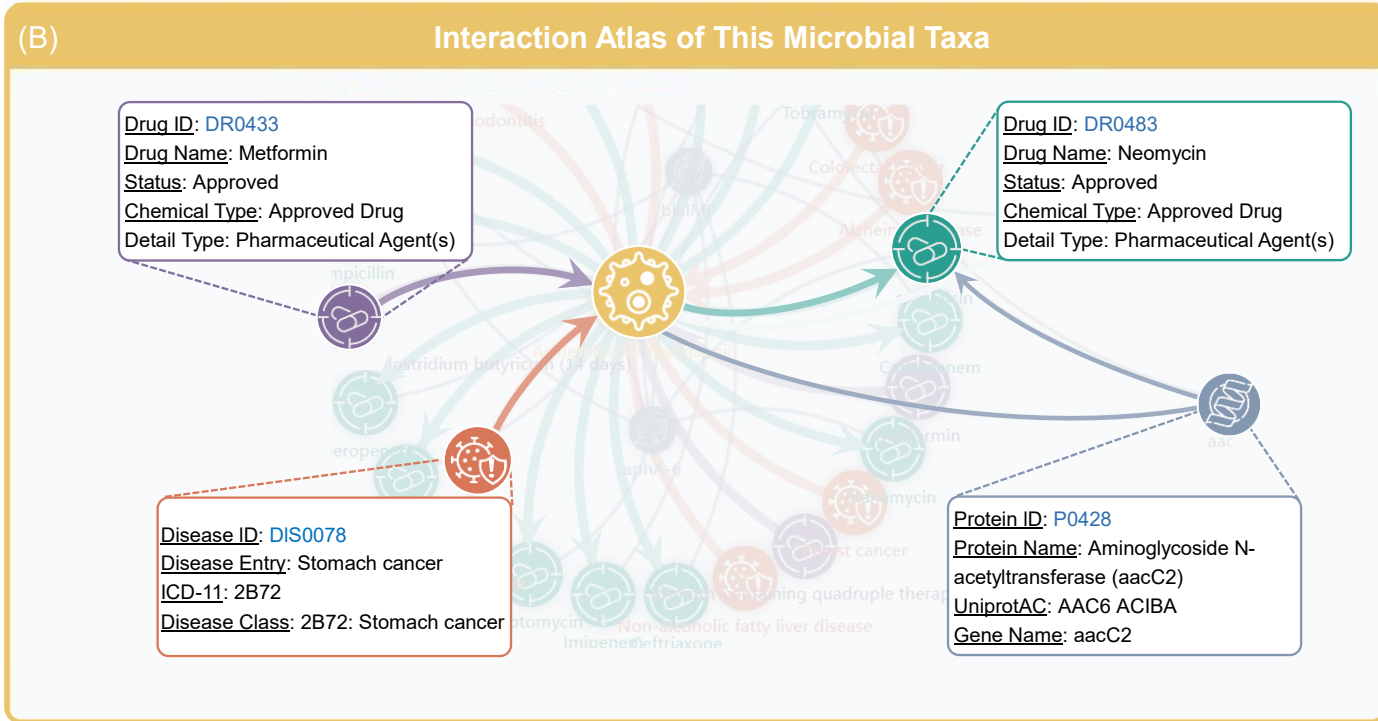
Reset  
Search  
  
Reset  
Search

Drop-down menu search

# Results: for microbiota search and data presentation

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

<b>Species Name</b>	Acinetobacter baumannii	<b>Taxonomy ID</b>	470
<b>Lineage</b>	Kingdom: Bacteria <a href="#">↗</a> ↳ Phylum: Pseudomonadota <a href="#">↗</a> ↳ Class: Gammaproteobacteria <a href="#">↗</a> ↳ Order: Moraxellales <a href="#">↗</a> ↳ Family: Moraxellaceae <a href="#">↗</a> ↳ Genus: Acinetobacter calcoaceticus/baumannii complex <a href="#">↗</a> ↳ Species: Acinetobacter baumannii <a href="#">↗</a>		



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

<b>Approved Drug</b>	Neomycin
<b>Drug Info</b>	DR0483
<b>Related Protein</b>	aacC2 <a href="#">P0428</a>
<b>Mechanism</b>	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**

<b>Approved Drug</b>	Metformin
<b>Drug Info</b>	DR0433
<b>Strain</b>	<i>A. baumannii</i> TCDC-AB0715
<b>Methods</b>	HT incubation assays
<b>Mechanism</b>	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**

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

Figure 2. A typical MDIPID page to provide comprehensive details about a specific microbial taxa.



# Results: for drug search and data presentation



Search for Drug in Whole Database:

### Search for Drug by Keywords:

Please enter your keywords here

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

Search

### 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

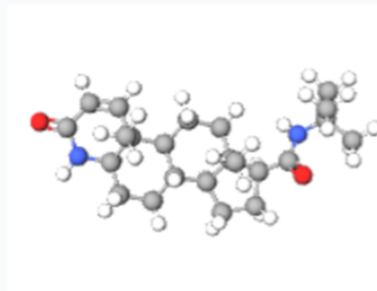
Drug ID	DR0268	Drug Info
Drug Status	Approved	
Drug Class	Pharmaceutical Agent(s)	
Drug Type	Approved Drug	
Representative Indication	Benign prostatic hyperplasia	

(A)

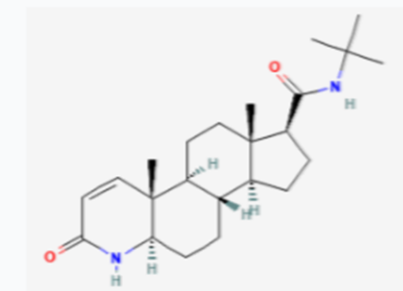
General Information of Drug (ID: DR0268)

Drug Name	Finasteride	Highest Status	Approved
Synonyms	finasteride; 98319-26-7; Proscar; Propecia; Finastid; Prostide; Chibro-Proscar; MK-906; Finasteria; Finasterida; Finasteridum; Finasteridum IINN-I atinI; MK 906; Finasterida IINN-Sp		
Chemical Type	Approved Drug		
Indication	Disease Entry	ICD 11	Status
	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



Figure S1(A). A typical illustrative diagram of the abundant drug information in MDIPID.



# Results: for drug search and data presentation

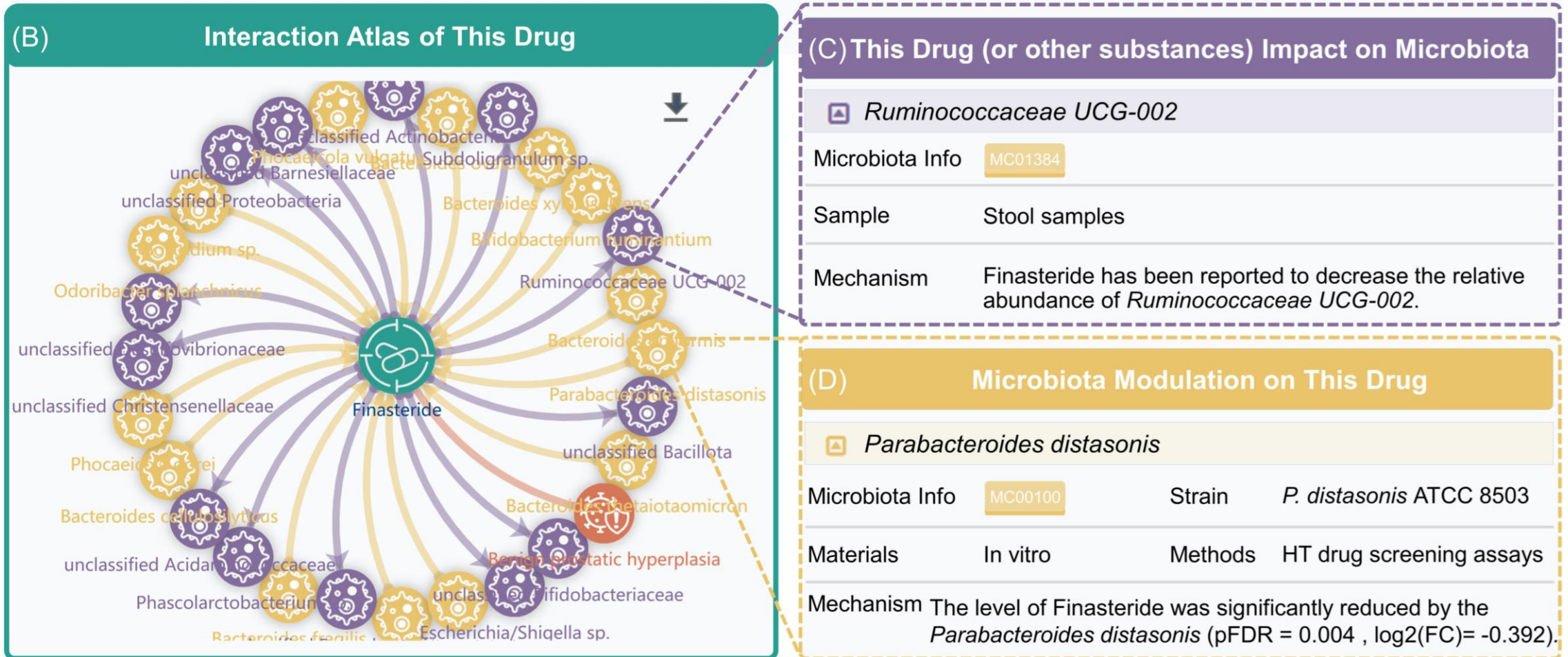


Figure S1(B). The interaction atlas of this drug.

Figure S1(C). This drug impact on microbiota.

Figure S1(D). Microbiota modulation on this drug.



# Results: for disease search and data presentation

- 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

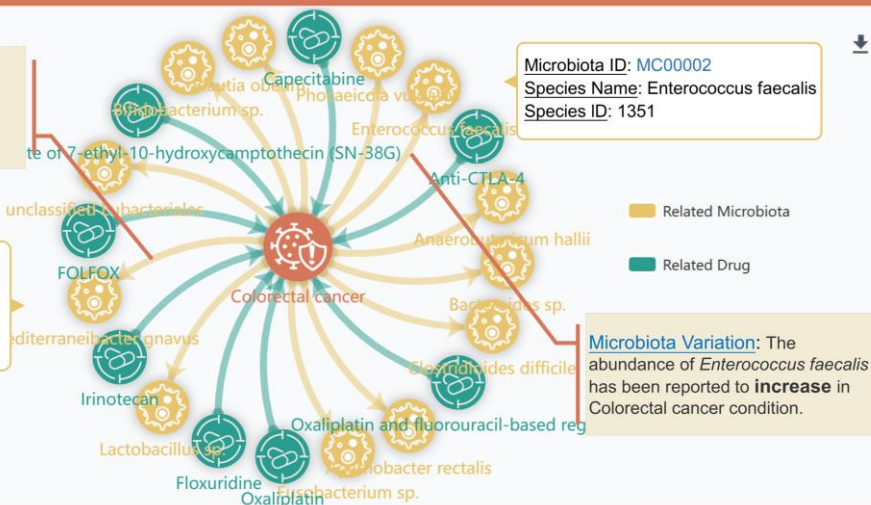
Disease ID	DIS0102	<a href="#">Disease Info</a>
Disease Class	2C60-2C65: Breast cancer	
ICD-11 Code	2C60-2C65	
Representative Drug	<a href="#">Anastrozole</a> ; <a href="#">Doxorubicin</a> ; <a href="#">Gemcitabine</a>	
Related Microbiota	<a href="#">Acholeplasma sp.</a> ; <a href="#">Acidaminococcus sp.</a> ; <a href="#">Acinetobacter baumannii</a>	

## (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:** MC00002  
**Species Name:** *Enterococcus faecalis*  
**Species ID:** 1351

- Related Microbiota
- Related Drug

**Microbiota Variation:** The abundance of *Enterococcus faecalis* has been reported to **increase** in Colorectal cancer condition.

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

<input checked="" type="checkbox"/> Kingdom: Archaea	1 Phylum(s) In Total
<input checked="" type="checkbox"/> Phylum: Euryarchaeota	2 Species(s) In Total
<input checked="" type="checkbox"/> Species: <i>Methanobrevibacter sp.</i>	1 Variation(s) in the Abundance of Microbiota In Total
<input checked="" type="checkbox"/> 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	<a href="#">DR0047</a>	Approved Drug	N.A.	Approved	[78]
Capecitabine	<a href="#">DR0115</a>	Approved Drug	CID: 60953	Approved	[79]
Floxuridine	<a href="#">DR0270</a>	Approved Drug	CID: 5790	Approved	[80]
FOLFOX	<a href="#">DR0277</a>	Approved Drug	CID: 135659064	Approved	[81]

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

Figure S2. A typical page showing the rich disease phenotype information in MDIPID.



# Results: for protein search and data presentation

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

<b>Protein Name</b>	Cytochrome P450 102D1	<b>Gene Name</b>	cyp102A1
<b>Microbial sources</b>	Streptomyces avermitilis <span>MC00128</span>		
<b>Functional Family</b>	EC: 1 <a href="#">Oxidoreductase</a> ↳ EC: 1.14 <a href="#">Oxygen paired donor oxidoreductase</a> ↳ EC: 1.14.14 <a href="#">Flavin/flavoprotein donor oxidoreductase</a> ↳ EC: 1.14.14.1 <a href="#">Flavin/flavoprotein donor oxidoreductase</a>		
<b>EC/TC ID</b>	EC: 1.14.14.1 <a href="#">Oxidoreductase</a>	<b>UniProt AC</b>	CPXB_BACMB <a href="#">Oxidoreductase</a>
<b>Gene ID</b>	Gene ID: 29911283		
<b>PDB ID</b>	1BU7 <a href="#">Oxidoreductase</a> ; 1BVY <a href="#">Oxidoreductase</a> ; 1FAG <a href="#">Oxidoreductase</a> ; 1FAH <a href="#">Oxidoreductase</a> ; 1JME <a href="#">Oxidoreductase</a> ; 1JPZ <a href="#">Oxidoreductase</a> ; 1P0V <a href="#">Oxidoreductase</a> ; 1P0W <a href="#">Oxidoreductase</a> ; 1SMJ <a href="#">Oxidoreductase</a> ; 1YQO <a href="#">Oxidoreductase</a> ; 1YQP <a href="#">Oxidoreductase</a> ; 1ZO4 <a href="#">Oxidoreductase</a> ; 1ZO9 <a href="#">Oxidoreductase</a> ; 1ZOA <a href="#">Oxidoreductase</a> ; 2BMH <a href="#">Oxidoreductase</a> ; <a href="#">Show More</a>		
<b>KEGG Pathway</b>	bmeg00627 (Aminobenzoate degradation) <a href="#">Oxidoreductase</a> <a href="#">Show More</a>		
<b>Tissue Distribution</b>	Primarily distributed in human gut.		
<b>Function</b>	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 <a href="#">Show More</a>		
<b>Sequence</b>	MTIKEMPQPKTFGELKNLPLLNTDKPVQALMKIADELGEIFKFEAPGRVTRYLSSQRLIK EACDESRLFKNLSQALKFVRDFAGDGLFTSWTHEKNWKKAHNILLPSFSQAMKGYHA <a href="#">Show More</a>		

(B) Interaction Atlas of This Microbial Protein

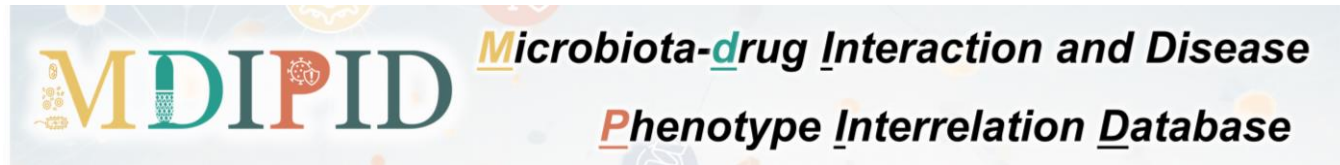
(C) Effect of This Microbial Protein on Drugs

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

Figure S3. A typical page illustrating the microbial protein data in MDIPID.



# Summary






- ❑ In this study, we developed a comprehensive database MDIPID to systematically provide the complex and bidirectional interaction data among microbiota, drugs, diseases, and microbial proteins.
- ❑ Currently, MDIPID includes data on 6,669 MMDR, 11,760 DEIM, and 15,146 MBDA records, collectively forming a comprehensive and interconnected network that encompasses 2,708 microbial species, 1,818 drugs/exogenous substances, 592 microbial proteins, and 482 diseases.
- ❑ MDIPID offers versatile search and data display functions, promising to be a key resource for researchers aiming to identify microbial therapeutic targets, predict drug efficacy, and develop new therapies.
- ❑ Website: <https://idrblab.org/mdipid/>


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