菌群 + 对应代谢产物介导 + 机制研究

2024-02-23

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Contents

1	摘安	•			1
	1.1	需求概			
	1.2	分析结	5果		1
2	前言	Í			2
3	材料	l和方法			2
	3.1	材料			2
	3.2	方法			2
4	分析	结果			2
5	结论	÷			2
			f ii		2
6	ры: 6.1	分析流 Microl		RNA	_
	0.1	6.1.1		OC	
		6.1.2			
		6.1.3		分析	
		6.1.4	-	otaProcess 分析	
		0.1.1	6.1.4.1	样本聚类	
			6.1.4.2	Alpha 多样性	
			6.1.4.3	Alpha 稀疏曲线	
			6.1.4.4	Beta 多样性	
			6.1.4.5		
		6.1.5	差异菌	- 	
			6.1.5.1	从 gutMDisorder 数据库检索关联代谢物	11
			6.1.5.2	尝试从已发表研究 (孟德尔随机化相关) 中寻找关联代谢物	
		6.1.6	代谢物的	的富集分析	12
		6.1.7	从结肠组	炎或结肠癌已发表的代谢物研究中验证	15
			6.1.7.1	DepressionAndYuan2021 结肠炎 (肠道菌)	15
			6.1.7.2	AlterationsInScovil2018 结肠炎 (代谢物)	16
			6.1.7.3	LossOfSymbiotSadegh2024 结肠癌 (肠道菌)	16
			6.1.7.4	IntegratedAnalChen2022 结肠癌 (肠道菌和代谢物)	17
R	efere	ence			19
${f L}$	\mathbf{ist}	of Fi	${ m gures}$		
					,
	1 2				
	_	- I PII a			-

3	Alpha rarefaction	5
4	Beta diversity group test	6
5	Ancom test group level 2 volcano	7
6	Ancom test group level 2 Percentile abundance	8
7	Ancom test group level 6 volcano	9
8	Ancom test group level 6 Percentile abundance	10
9	MetaboAnalyst kegg enrichment	13
10	Enrichment with algorithm PageRank	14
List	of Tables	
1	Microbiota metadata	3
2	GutMDisorder database	11
3	MendelianRandoLiuX2022 matched data	12
4		
	Compounds ID	13
5		
5 6	Data of enrichment with algorithm PageRank	13
-	Data of enrichment with algorithm PageRank	13 14
6	Data of enrichment with algorithm PageRank	13 14 15 16
6 7	Data of enrichment with algorithm PageRank	13 14 15 16 17
6 7 8	Data of enrichment with algorithm PageRank	13 14 15 16 17

1 摘要

1.1 需求概要

数据分组:

- con: Control
- A: colitis
- B: colon precancerous lesions

肠道菌群测序结果 + 生信分析,得出:菌群 + 对应代谢产物介导 + 机制研究 + 再闭环回到临床。

具体:

溃疡性结肠炎和结肠癌的肠道菌群之间的区别和关联,进而研究其对应的机制,研究结肠炎向结肠癌发展的 关键机制,为临床早期筛查提供理论支持

1.2 分析结果

- 基本分析:
 - alpha、beta 多样性, A、B、C 组均无显著性差异 (6.1.4.2, 6.1.4.4)。
 - 差异菌筛选 (level 6, Species),筛得差异菌 (Fig. 7):d___Bacteria;p___Proteobacteria;c___Alphaproteobacteria;o_
 Methylorubrum 该差异菌主要存在于 A、B 组,不存在 (或少量于) 于 C (对照) 组。含量见 Fig.
 8
 - **...**
 - 差异菌 (level 2, Phylum) (Fig. 5), 同样的有: d___Bacteria;p___Proteobacteria 该差异菌主要存在于 A、B 组,不存在 (或少量于) 于 C (对照) 组。含量见 Fig. 6
- 从肠道菌到相关代谢物:
 - 使用 gutMDisorder 未发现相关代谢物。
 - 从一孟德尔随机化相关研究中¹,发现了与差异菌相关的代谢物,见 Tab. 3。这些代谢物为 (详细信息见 Tab. 4): 5-methyltetrahydrofolic acid, selenium, L-cystine, Glutamic acid
 - 用 MetaboAnalystR 对相关代谢物进行富集分析, 富集到两条通路 (见 Fig. 9)
 - 用 FELLA 对相关代谢物富集分析, 可以发现相关联的更多通路或反应模块 (结果见 Fig. 10, Tab. 5)
- 尝试从已有的关于结肠炎或结肠癌的研究中验证上述发现:
 - 从结肠癌相关研究中匹配到² (Tab. 9): d___Bacteria;p___Proteobacteria (注: 在 Phylum 水平 上得到验证)
 - 未从其它文献中匹配到代谢物或差异肠道菌 (见 6.1.7。
- 结肠炎向结肠癌之间的转化:
 - A 为结肠炎,B 为结肠癌前病变;A 与 B 组间无显著差异菌,因此无法从这一批数据探究可能的 发展机制 (A -> B)。

2 前言

3 材料和方法

3.1 材料

Other data obtained from published article (e.g., supplementary tables):

• Supplementary file from article refer to¹.

3.2 方法

Mainly used method:

- R package FELLA used for metabolite enrichment analysis³.
- Fastp used for Fastq data preprocessing⁴.
- Database gutMDisorder used for finding associations between gut microbiota and metabolites⁵.
- R package MicrobiotaProcess used for microbiome data visualization⁶.
- MetaboAnalyst used for metabolomic data analysis⁷.
- Qiime2 used for gut microbiome 16s rRNA analysis⁸⁻¹².
- Other R packages (eg., dplyr and ggplot2) used for statistic analysis or data visualization.

4 分析结果

- 5 结论
- 6 附:分析流程
- 6.1 Microbiota 16s RNA

6.1.1 Fastp QC

原始数据质控:

'Fastp QC'数据已全部提供。

(对应文件为 ./fastp_report/)

注:文件夹./fastp_report/共包含 23 个文件。

- 1. A1.338F_806R..html
- $2. \ A2.338F_806R..html$
- 3. A3.338F_806R..html
- 4. A4.338F_806R..html
- 5. A5.338F 806R..html
- 6. ...

6.1.2 元数据

Table 1 (下方表格) 为表格 microbiota metadata 概览。

(对应文件为 Figure+Table/microbiota-metadata.csv)

注: 表格共有 22 行 7 列,以下预览的表格可能省略部分数据;表格含有 22 个唯一'SampleName'。

1. group: 分组名称

Table 1: Microbiota metadata

SampleName	group	dirs	reports	Run	forward-ab	reverse-ab
A1	A	./material	./material	rawData	/home/echo	/home/echo
A2	A	./material	./material	rawData	/home/echo	/home/echo
A3	A	./material	./material	rawData	/home/echo	/home/echo
A4	A	./material	./material	rawData	/home/echo	/home/echo
A5	A	./material	./material	rawData	/home/echo	/home/echo
A6	A	$./ {\rm material}$	$./{\rm material}$	rawData	/home/echo	/home/echo
A7	A	$./ {\rm material}$	$./{\rm material}$	rawData	/home/echo	/home/echo
A8	A	$./ {\rm material}$	$./ {\rm material}$	rawData	/home/echo	/home/echo
B1	В	$./ {\rm material}$	$./{\rm material}$	rawData	/home/echo	/home/echo
B2	В	$./ {\rm material}$	$./{\rm material}$	rawData	/home/echo	/home/echo
В3	В	./material	./material	rawData	/home/echo	/home/echo
B4	В	./material	./material	rawData	/home/echo	/home/echo
B5	В	./material	./material	rawData	/home/echo	/home/echo
B6	В	./material	./material	rawData	/home/echo	/home/echo
B7	В	$./ {\rm material}$	$./ {\rm material}$	rawData	/home/echo	/home/echo

6.1.3 Qiime2 分析

Microbiota 数据经 Qiime2 分析后,由 MicrobiotaProcess 下游分析和可视化。

6.1.4 MicrobiotaProcess 分析

6.1.4.1 样本聚类

Figure 1 (下方图) 为图 PCoA 概览。

(对应文件为 Figure+Table/PCoA.pdf)

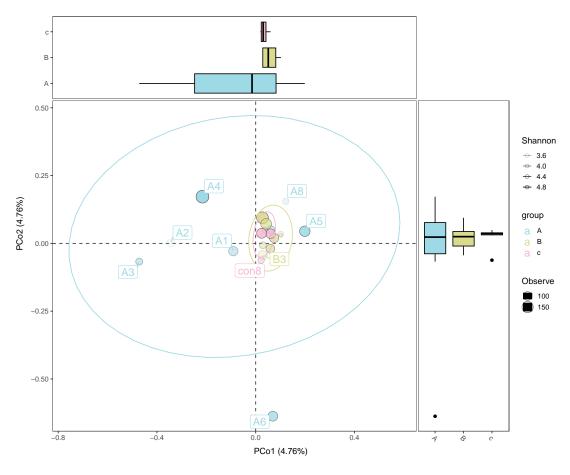


Figure 1: PCoA

6.1.4.2 Alpha 多样性

三组 alpha 多样性没有显著差异。

Figure 2 (下方图) 为图 Alpha diversity 概览。

(对应文件为 Figure+Table/Alpha-diversity.pdf)

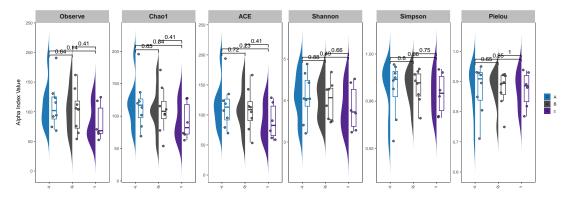


Figure 2: Alpha diversity

^{&#}x27;Taxonomy abundance' 数据已全部提供。

(对应文件为 Figure+Table/Taxonomy-abundance)

注:文件夹 Figure+Table/Taxonomy-abundance 共包含 6 个文件。

- $1.\ 1_Phylum.pdf$
- 2. 2_Class.pdf
- $3. 3_{Order.pdf}$
- $4.\ 4_Family.pdf$
- $5.\ 5_Genus.pdf$
- 6. ...

6.1.4.3 Alpha 稀疏曲线

Figure 3 (下方图) 为图 Alpha rarefaction 概览。

(对应文件为 Figure+Table/Alpha-rarefaction.pdf)

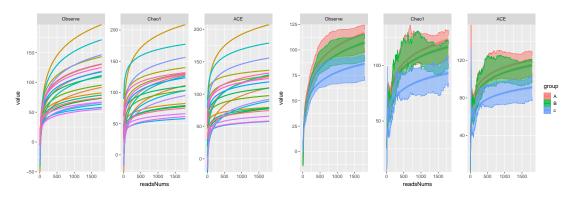


Figure 3: Alpha rarefaction

6.1.4.4 Beta 多样性

Beta 多样性无显著差异。

Figure 4 (下方图) 为图 Beta diversity group test 概览。

(对应文件为 Figure+Table/Beta-diversity-group-test.pdf)

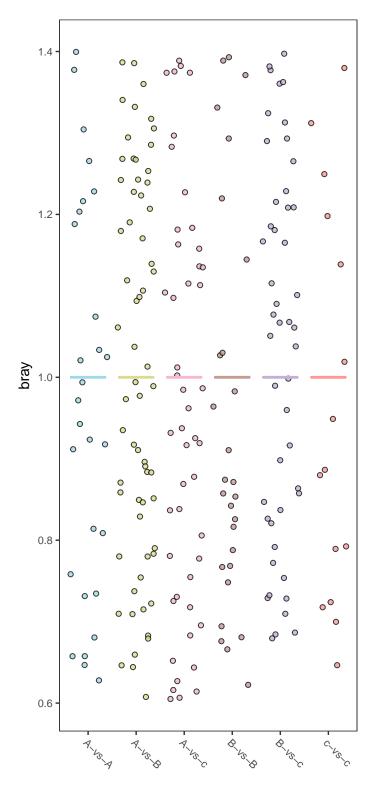


Figure 4: Beta diversity group test

'Taxonomy hierarchy' 数据已全部提供。

(对应文件为 Figure+Table/Taxonomy-hierarchy)

注:文件夹 Figure+Table/Taxonomy-hierarchy 共包含 6 个文件。

- $1.\ 1_Phylum.pdf$
- 2. 2_Class.pdf
- $3. 3_{Order.pdf}$
- 4. 4_Family.pdf
- 5. 5_Genus.pdf
- 6. ...

6.1.4.5 差异分析

MicrobiotaProcess 的差异分析 (MicrobiotaProcess::mp_diff_analysis) 未发现差异菌,因此这里主要用的 Qiime2 的差异分析结果 (accom test)。

注: 关于 ancom test 的结果的解释, 可以参考:

- 1. https://forum.qiime2.org/t/how-to-interpret-ancom-results/1958
- 2. https://forum.qiime2.org/t/specify-w-cutoff-for-anacom/1844

Figure 5 (下方图) 为图 Ancom test group level 2 volcano 概览。

(对应文件为 Figure+Table/Ancom-test-group-level-2-volcano.pdf)

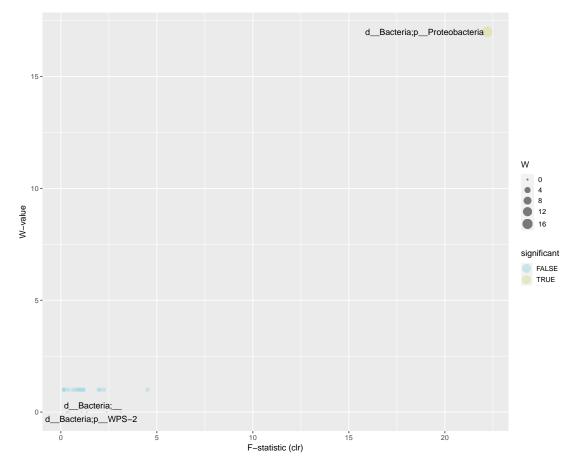


Figure 5: Ancom test group level 2 volcano

Figure 6 (下方图) 为图 Ancom test group level 2 Percentile abundance 概览。

(对应文件为 Figure+Table/Ancom-test-group-level-2-Percentile-abundance.pdf)

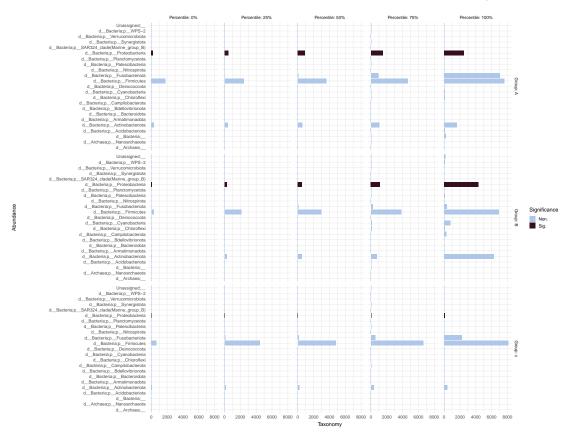


Figure 6: Ancom test group level 2 Percentile abundance

Figure 7 (下方图) 为图 Ancom test group level 6 volcano 概览。

(对应文件为 Figure+Table/Ancom-test-group-level-6-volcano.pdf)

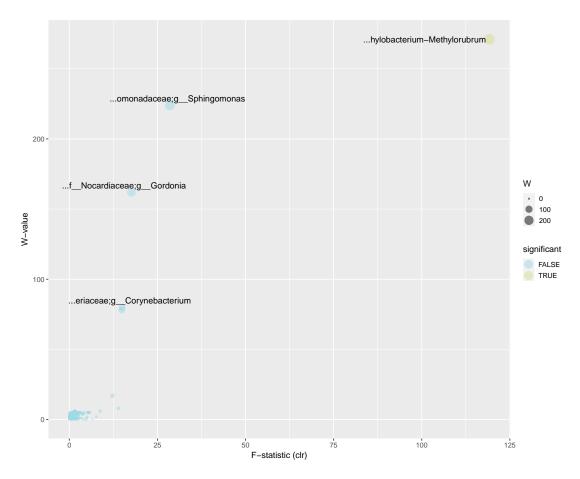


Figure 7: Ancom test group level 6 volcano

Figure 8 (下方图) 为图 Ancom test group level 6 Percentile abundance 概览。

(对应文件为 Figure+Table/Ancom-test-group-level-6-Percentile-abundance.pdf)

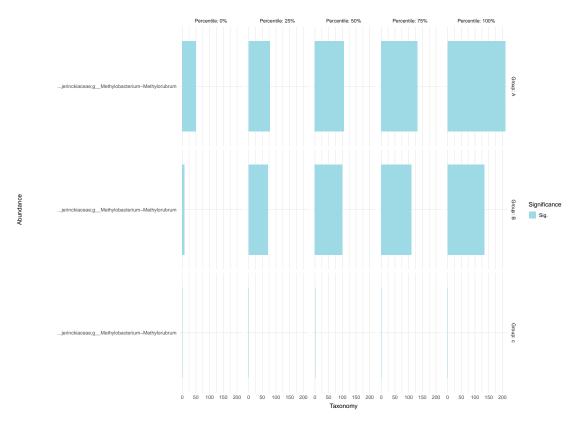


Figure 8: Ancom test group level 6 Percentile abundance

'level 2' 对应 Ontology 中的 Phylum。'level 6' 对应 Ontology 中的 Species。

其余结果的可视化见:

'Ancom test visualization' 数据已全部提供。

(对应文件为 Figure+Table/Ancom-test-visualization)

注:文件夹 Figure+Table/Ancom-test-visualization 共包含 3 个文件。

- 1. 1_ancom_test_group_level_4.pdf
- 2. 2 ancom test group level 5.pdf
- 3. 3_ancom_test_group_level_6.pdf

'Ancom test Percentile abundance' 数据已全部提供。

(对应文件为 Figure+Table/Ancom-test-Percentile-abundance)

注:文件夹 Figure+Table/Ancom-test-Percentile-abundance 共包含 5 个文件。

- 1. 1_ancom_test_group_level_2.pdf
- 2. 2 ancom test group level 3.pdf
- 3. 3 ancom test group level 4.pdf
- 4. 4_ancom_test_group_level_5.pdf
- $5.\ 5_ancom_test_group_level_6.pdf$

'Ancom test results' 数据已全部提供。

(对应文件为 Figure+Table/Ancom-test-results)

注:文件夹 Figure+Table/Ancom-test-results 共包含 3 个文件。

- 1. 1_ancom_test_group_level_4.csv
- $2.\ 2_ancom_test_group_level_5.csv$
- 3. 3_ancom_test_group_level_6.csv

6.1.5 差异菌关联到代谢物

6.1.5.1 从 gutMDisorder 数据库检索关联代谢物

使用的数据库如下:

Table 2 (下方表格) 为表格 GutMDisorder database 概览。

(对应文件为 Figure+Table/GutMDisorder-database.xlsx)

注: 表格共有 724 行 12 列,以下预览的表格可能省略部分数据;表格含有 289 个唯一'Gut.Microbiota'。

Table 2: GutMDisorder database

Gut.Mi1	Gut.Mi2	Gut.Mi3	Classi	Substrate	Substr6	Substr7	
Christ	NA	gm0883	strain	D-Glucose	5793	HMDB00	
Christ	NA	gm0883	strain	Salicin	439503	HMDB00	
Christ	NA	gm0883	strain	D-Xylose	135191	HMDB00	
Christ	NA	gm0883	strain	L-Arab	439195	HMDB00	
Christ	NA	gm0883	strain	L-Rham	25310	HMDB00	
Christ	NA	gm0883	strain	D-Mannose	18950	HMDB00	
Christ	NA	gm0883	strain	D-Glucose	5793	HMDB00	
Christ	NA	gm0883	strain	Salicin	439503	HMDB00	
Christ	NA	gm0883	strain	D-Xylose	135191	HMDB00	
Christ	NA	gm0883	strain	L-Arab	439195	HMDB00	
Christ	NA	gm0883	strain	L-Rham	25310	HMDB00	
Christ	NA	gm0883	strain	D-Mannose	18950	HMDB00	
Entero	1343173	gm0884	species	Orientin	5281675	HMDB00	
Clostr	29347	gm0885	strain	Bile acid	439520		
Clostr	29347	gm0885	strain	Cholic	221493	HMDB00	

使用差异肠道菌匹配:

Content:

Proteobacteria, Alphaproteobacteria, Rhizobiales, Beijerinckiaceae, Methylo
bacterium Methylorubrum

未找到相关代谢物。

6.1.5.2 尝试从已发表研究 (孟德尔随机化相关) 中寻找关联代谢物

请参考1

匹配到 Phylum 水平的菌群关联的代谢物:

Content:

5-methyltetrahydrofolic acid, selenium, Cystine, Glutamic acid

Table 3 (下方表格) 为表格 MendelianRandoLiuX2022 matched data 概览。

(对应文件为 Figure+Table/MendelianRandoLiuX2022-matched-data.csv)

注:表格共有 4 行 25 列,以下预览的表格可能省略部分数据;表格含有 1 个唯一'X1'。

Table 3: MendelianRandoLiuX2022 matched data

X1	X2	beta	se	p	beta.1	se.1	p.1	p_MRPI	Rbeta.2
p_Prot	5-	-	0.0313679	0 1.0532	-0.097	0.0417018	3 0.0188806	0.1756	-0.166
	meth	0.15312							
p_Prot	selenium	-	0.0289698	3 2.3772	-0.032	0.0412256	0.431953	0.189	-0.192
		0.122431							
p_Prot	Cystine	-0.097	0.0221977	71.0141	-0.045	0.0323047	0.16131	0.4752	-0.101
p_Prot	Glutam	0.175275	0.0392992	2 8.1952	0.0363522	0.0368746	0.324216	0.0082	0.1929

6.1.6 代谢物的富集分析

将匹配到的代谢物 (6.1.5.2) 进行代谢物富集分析。

以下是代谢物的数据库匹配:

Table 4 (下方表格) 为表格 compounds ID 概览。

(对应文件为 Figure+Table/compounds-ID.csv)

注:表格共有 4 行 7 列,以下预览的表格可能省略部分数据;表格含有 4 个唯一'Query'。

Table 4: Compounds ID

Query	Match	HMDB	PubChem	KEGG	SMILES	Comment
5-methylte	5-Methylte	HMDB0001396	439234	C00440	CN1C(CNC2=	1
selenium	Selenium	HMDB0001349	NA	C01529	[Se++]	1
L-cystine	L-Cystine	HMDB0000192	67678	C00491	N[C@@H](CS	1
Glutamic acid	Glutamic acid	HMDB0000148	33032	C00302	N[C@@H](CC	1

Figure 9 (下方图) 为图 MetaboAnalyst kegg enrichment 概览。

(对应文件为 Figure+Table/metabolites_ORA_dot_kegg_pathway_dpi72.pdf)

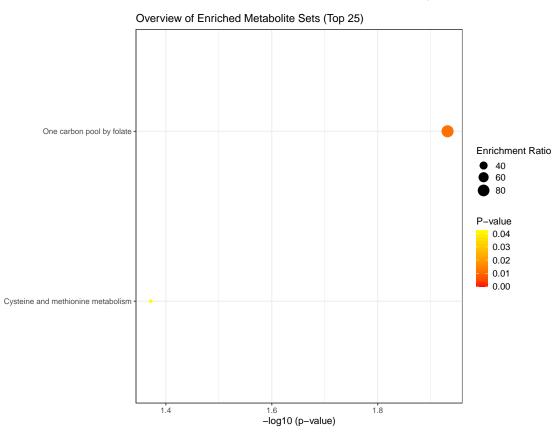


Figure 9: Metabo Analyst kegg enrichment

Figure 10 (下方图) 为图 Enrichment with algorithm PageRank 概览。

(对应文件为 Figure+Table/Enrichment-with-algorithm-PageRank.pdf)

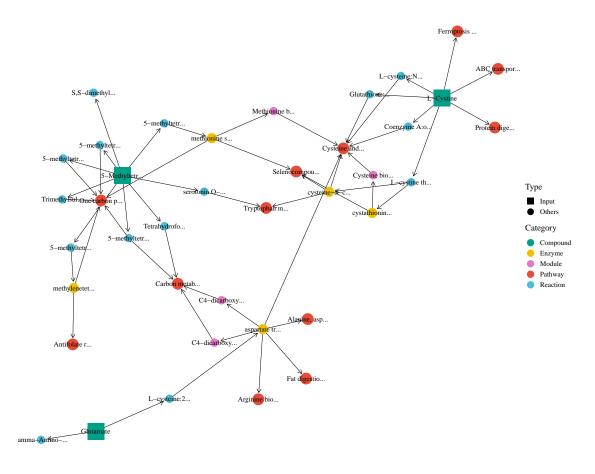


Figure 10: Enrichment with algorithm PageRank

Table 5 (下方表格) 为表格 Data of enrichment with algorithm PageRank 概览。

(对应文件为 Figure+Table/Data-of-enrichment-with-algorithm-PageRank.xlsx)

注:表格共有 39 行 7 列,以下预览的表格可能省略部分数据;表格含有 39 个唯一'name'。

Table 5: Data of enrichment with algorithm PageRank

name	com	NAME	label	input	abbrev.name	type
hsa00220	1	Arginine b	Arginine b	Others	Arginine b	Pathway
hsa00250	1	Alanine, a	Alanine, a	Others	Alanine, a	Pathway
hsa00270	1	Cysteine a	Cysteine a	Others	Cysteine a	Pathway
hsa00380	1	Tryptophan	Tryptophan	Others	Tryptophan	Pathway
hsa00450	1	Selenocomp	Selenocomp	Others	Selenocomp	Pathway
hsa00670	1	One carbon	One carbon	Others	One carbon	Pathway
hsa01200	1	Carbon met	Carbon met	Others	Carbon met	Pathway
hsa01523	1	Antifolate	Antifolate	Others	Antifolate	Pathway
hsa02010	1	ABC transp	ABC transp	Others	ABC transp	Pathway
hsa04216	1	Ferroptosi	Ferroptosi	Others	Ferroptosi	Pathway

name	com	NAME	label	input	abbrev.name	type
hsa04974	1	Protein di	Protein di	Others	Protein di	Pathway
hsa04975	1	Fat digest	Fat digest	Others	Fat digest	Pathway
M00017	2	Methionine	Methionine	Others	Methionine	Module
M00170	2	C4-dicarbo	C4-dicarbo	Others	C4-dicarbo	Module
M00171	2	C4-dicarbo	C4-dicarbo	Others	C4-dicarbo	Module

6.1.7 从结肠炎或结肠癌已发表的代谢物研究中验证

6.1.7.1 DepressionAndYuan2021 结肠炎 (肠道菌)

Depression and anxiety in patients with active ulcerative colitis: crosstalk of gut microbiota, metabolomics and proteomics 13

以下是整理自该文献的差异肠道菌汇总:

Table 6 (下方表格) 为表格 DepressionAndYuan2021 published data significant microbiota 概览。

(对应文件为 Figure+Table/DepressionAndYuan2021-published-data-significant-microbiota.xlsx)

注: 表格共有 91 行 4 列,以下预览的表格可能省略部分数据;表格含有 91 个唯一'Taxonomy'。

Table 6: DepressionAndYuan2021 published data significant microbiota

Taxonomy	p.value	MRA.in.UC	MRA.in.HC
pGemmatimonadetes	0.00049553252446827	0.00171119907683608	0.000160190585722501
pActinobacteria	0.00834784591709094	0.0617033057472256	0.0389112516772091
pFirmicutes	0.00478686441960355	0.589610871565727	0.499806265231797
pBacteroidetes	$9.60337999115942 \mathrm{e}\text{-}05$	0.250752809840626	0.403687121772228
punidentified	$1.40986578996555\mathrm{e}\text{-}07$	0.000640301130981834	$2.05372545798078 \mathrm{e}\text{-}06$
cActinobacteria	0.00353055167754535	0.046725454341533	0.0237116295626934
cLongimicrobia	7.16632518063251e-07	0.00145496100157866	0
cBacteroidia	$6.38198131772293 \mathrm{e}\text{-}05$	0.24518920382048	0.403287329883075
cDeinococci	$3.17450175630301\mathrm{e}\text{-}06$	0.00131123215732429	0
cBacilli	0.00330587139663399	0.0649165901033199	0.0154563377967633
cCytophagia	$2.10636789003367\mathrm{e}\text{-}05$	0.0016664310495747	4.24436594649361e-05
cunidentified	$2.64154914758447\mathrm{e}\text{-}08$	0.0016652538833675	$8.83101946931736\mathrm{e}\text{-}05$
cFlavobacteriia	$5.26714172360768\mathrm{e}\text{-}05$	0.00167703418517471	$5.95580382814426\mathrm{e}\text{-}05$
oOceanospirillales	0.00495867783478051	0.000461817587592187	$2.05372545798077 \mathrm{e}\text{-}06$
oBifidobacteriales	0.00354779153342515	0.0443044462799416	0.0224465346805772

未从 Fig. 6 中匹配到客户数据筛选出的肠道菌。

6.1.7.2 AlterationsInScovil2018 结肠炎 (代谢物)

Alterations in Lipid, Amino Acid, and Energy Metabolism Distinguish Crohn's Disease from Ulcerative Colitis and Control Subjects by Serum Metabolomic Profiling.¹⁴

以下是整理自该文献的代谢物汇总:

Table 7 (下方表格) 为表格 AlterationsInScovil2018 published data metabolites 概览。

(对应文件为 Figure+Table/AlterationsInScovil2018-published-data-metabolites.xlsx)

注: 表格共有 565 行 22 列,以下预览的表格可能省略部分数据;表格含有 565 个唯一'Metabolite'。

Table 7: AlterationsInScovil2018 published data metabolites

Metabo	Pathway	Sub-Pa	Platform	RI	Mass	MSI Id	PUBCHEM	KEGG	HMDB
alanine	Amino	Alanin	LC/MS	2780.3	88.0404	1	5950	C00041	HMDB00161
aspara	Amino	Alanin	$LC/MS \dots$	2951.1	131.0462	1	6267	C00152	HMDB00168
aspartate	Amino	Alanin	LC/MS Neg	640	132.0302	1	5960	C00049	HMDB00191
N-acet	Amino	Alanin	$LC/MS \dots$	1564.8	130.051	1	88064	C02847	HMDB00766
N-acet	Amino	Alanin	$LC/MS \dots$	785	175.0713	1	99715	NA	${\rm HMDB06028}$
N-acet	Amino	Alanin	$LC/MS \dots$	3143	174.0408	1	65065	C01042	${\rm HMDB00812}$
creatine	Amino	Creati	$LC/MS \dots$	2920	130.0622	1	586	C00300	${\rm HMDB00064}$
creati	Amino	Creati	$LC/MS \dots$	2055	114.0662	1	588	C00791	${\rm HMDB00562}$
guanid	Amino	Creati	$LC/MS \dots$	2884	116.0466	1	763	C00581	${\rm HMDB00128}$
glutamate	Amino	Glutam	$LC/MS \dots$	1500	148.0604	1	611	C00025	HMDB00148
glutamine	Amino	Glutam	$LC/MS \dots$	1291	147.0764	1	5961	C00064	${\rm HMDB00641}$
N-acet	Amino	Glutam	$LC/MS \dots$	1035	305.098	1	5255	C12270	${\rm HMDB01067}$
N-acet	Amino	Glutam	$LC/MS \dots$	3106	188.0564	1	70914	C00624	HMDB01138
N-acet	Amino	Glutam	LC/MS Neg	771	187.0724	1	182230	C02716	${\rm HMDB06029}$
pyrogl	Amino	Glutam	$LC/MS \dots$	1900	129.0659	2	134508	NA	NA

未从 Tab. 7 中匹配到 6.1.5.2 中的关联代谢物。

6.1.7.3 LossOfSymbiotSadegh2024 结肠癌 (肠道菌)

Loss of symbiotic and increase of virulent bacteria through microbial networks in Lynch syndrome colon $carcinogenesis^2$

以下是整理自该文献的关联肠道菌汇总:

Table 8 (下方表格) 为表格 LossOfSymbiotSadegh2024 published data microbiota 概览。

(对应文件为 Figure+Table/LossOfSymbiotSadegh2024-published-data-microbiota.csv)

注: 表格共有 34 行 6 列, 以下预览的表格可能省略部分数据; 表格含有 34 个唯一 'taxon'。

Table 8: LossOfSymbiotSadegh2024 published data microbiota

taxon	proportion	position.i	mean.auc	sd.auctest.	Value.with
k_Bacteria	0.992	numerator	1	0	stool
k_Bacteria	0.998	numerator	1	0	stool
$k_Bacteria$	0.956	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool
$k_Bacteria$	0.982	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool
${\bf k_Bacteria}$	1	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool
${\bf k_Bacteria}$	1	numerator	1	0	stool
${\bf k_Bacteria}$	1	numerator	1	0	stool
$k_Bacteria$	0.996	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool
$k_Bacteria$	1	numerator	1	0	stool

匹配到的肠道菌 (Phylum 水平):

Table 9 (下方表格) 为表格 LossOfSymbiotSadegh2024 matched Phylum microbiota 概览。

(对应文件为 Figure+Table/LossOfSymbiotSadegh2024-matched-Phylum-microbiota.csv)

注: 表格共有 3 行 6 列,以下预览的表格可能省略部分数据;表格含有 3 个唯一'taxon'。

Table 9: LossOfSymbiotSadegh2024 matched Phylum microbiota

taxon	proportion	position.i	mean.auc	sd.auctest.	Value.with
k_Bacteria	1	denominator	1	0	stool
$k_Bacteria$	1	denominator	1	0	stool
k_Bacteria	1	denominator	1	0	stool

6.1.7.4 IntegratedAnalChen2022 结肠癌 (肠道菌和代谢物)

Integrated analysis of the faecal metagenome and serum metabolome reveals the role of gut microbiome-associated metabolites in the detection of colorectal cancer and adenoma 15

以下是整理自该文献的肠道菌和代谢物数据 (PDF 识别结果):

Table 10 (下方表格) 为表格 IntegratedAnalChen2022 published data microbiota 概览。

(对应文件为 Figure+Table/IntegratedAnalChen2022-published-data-microbiota.csv)

注:表格共有 782 行 4 列,以下预览的表格可能省略部分数据;表格含有 3 个唯一'Type'。

1. pvalue: 显著性 P。

Table 10: Integrated Anal
Chen2022 published data microbiota

Туре	Species	Metabolites	pvalue	
Tumor_promoting_b	Alistipes_finegoldii	X23.4_476.011mz_pos	3.87e-07	
$Tumor_promoting_b$	Alistipes_finegoldii	$X21.4_494.68mz_pos$	0.000232816	
Tumor_promoting_b	Alistipes_finegoldii	$X24.5_504.692mz_pos$	0.000162744	
$Tumor_promoting_b$	Alistipes_finegoldii	$X26.1_509.03 mz_pos$	0.000793675	
Tumor_promoting_b	Alistipes_finegoldii	$X26.3_514.705mz_pos$	0.000881926	
$Tumor_promoting_b$	$Bilophila_wadswor$	$X23.4_476.011 mz_pos$	4.45 e - 05	
$Tumor_promoting_b$	$Fusobacterium_nuc$	$X21.2_512.336mz_neg$	0.000581862	
$Tumor_promoting_b$	$Fusobacterium_nuc$	$X19.2_536.299 mz_neg$	0.000431165	
$Tumor_promoting_b$	$Fusobacterium_sp$	$X21.2_512.336mz_neg$	0.000850936	
$Tumor_promoting_b$	$Fusobacterium_sp$	$X19.2_536.299 mz_neg$	9.61 e-05	
$Tumor_promoting_b$	$Odoribacter_splan$	$X23.4_476.011 mz_pos$	1.93 e-06	
$Tumor_promoting_b$	$Odoribacter_splan$	$X21.4_494.68mz_pos$	3.38e-05	
$Tumor_promoting_b$	$Odoribacter_splan$	$X24.8_495.024 mz_pos$	0.000618015	
Tumor_promoting_b	$Odoribacter_splan$	$X22.9_499.686 mz_pos$	0.000395014	
Tumor_promoting_b	$Odoribacter_splan$	$X24.5_504.692mz_pos$	0.000898428	

Table 11 (下方表格) 为表格 IntegratedAnalChen2022 published data metabolites 概览。

(对应文件为 Figure+Table/IntegratedAnalChen2022-published-data-metabolites.xlsx)

注: 表格共有 969 行 19 列,以下预览的表格可能省略部分数据;表格含有 905 个唯一'V1'。

Table 11: IntegratedAnalChen2022 published data metabolites

V1	V2	V3	V4	V5	V6	V7	V8	V9	V10
Supple	material	placed	on	this	supple	material	which	has	been
Table	S2.	List	of	colore	abnormal	associ	metabo		
Metabo	feature	Metabo	annota	approach	F meanN	F meanC	F meanA	anova	anova

V1	V2	V3	V4	V5	V6	V7	V8	V9	V10
X10.3	(-)-Fo	exact	mass	match	7748.8	5053.5	5527.3	0.0000	7.36E-08
X12.4	(-)-Or	exact	mass	match	45226	31316	27721	0.0000	0.0000327
X10.9	(-)-tr	glucos	mass	match	364.39	8542.0151	9965.7	0.0026	0.0009
X15_26	(+)-2,	Goniot	mass	match	32595	22986	25975	0.0012	0.0013
X20.8	(+/-)	mass	match	6812.3	10133	3573.2	0.0042	0.0002535	0.1164
X12.5	$(\pm)15$	exact	mass	match	11931	8063.3	8309.9	3.99E-10	3.99E-10
X14.9	(±)-Go	exact	mass	match	24851	16540	15696	0.0022	0.0001
X15.1	(±)-Pa	exact	mass	match	78154	37693	61456	0.0000	0.0004
X24_35	(1S)-1	mass	match	2067.0	6783.2	10613	0.0000	0.0001	0.5843
X20.7	(20R)	Rh2	exact	mass	match	19519	12756	12327	4.39E-10
X11_42	(22E)								
exact	mass	match	97120						

未从上述数据中匹配到客户数据的差异肠道菌或其关联的代谢物。

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