Analysis

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1 摘要

2 研究设计流程图

3 材料和方法

4 分析结果

4.1 网络药理学分析主要活性成分

4.1.1 从 HERB 网站获取中药和成分以及靶点数据

HERB http://herb.ac.cn/

Table 1为表格 TCM information 概览。

(对应文件为 Figure+Table/TCM-information.xlsx)

注: 表格共有 10 行 18 列,以下预览的表格可能省略部分数据;表格含有 10 个唯一'Herb_'。

Table 1: TCM information

Herb_	Herb	Herb	Herb	Herb	Prope	Merid	UsePart	Function	Indic	Toxicity	
HERB0	. CHEN	陈皮	Dried	Peric	Warm;	Lung;	NA	To re	Treat	NA	
	PI										
HERB0	.DA	大黄	root	Radix	Cold;	Splee	root	To	Reple	NA	
	HUANG							ca			
HERB0	.DAN	丹参	root	Radix	Minor	Liver	root	To re	Angin	NA	
	SHEN										
HERB0	.FU	茯苓	India	Poria	$\operatorname{Mild};$	Splee	scler	То	Neura	NA	
	LING							ca			
HERB0	.GAN	甘草	Root	Radix	$\operatorname{Mild}; \dots$	Lung;	root	To re	1. It	NA	
	CAO										
HERB0	.HONG	红花	Saffl	Flos	${\rm Warm;}$	Liver	flower	То	Ameno	NA	
	HUA							ac			
HERB0	.HUANG	黄连	rhizo	Rhizo	$\operatorname{Cold}; \dots$	Large	${\rm rhizome}$	To re	Febri	NA	
HERB0	.NIU	牛膝	root	Radix	$\operatorname{Mild}; \dots$	Liver	root	To re	Achin	NA	
	XI										
HERB0	.TAI	太子	Heter	Radix	$\operatorname{Mild}; \dots$	Lung;	NA	To re	${\bf Treat}$	NA	
	Z	参									
HERB0	.ZHI	制半	Prepa	Rhizo	${\rm Warm;}$	Lung;	Pinel	Treat	Treat	Extre	
	В	夏									

Table 2为表格 TCM compounds 概览。

(对应文件为 Figure+Table/TCM-compounds.xlsx)

注: 表格共有 1761 行 4 列,以下预览的表格可能省略部分数据;表格含有 10 个唯一'herb_id'。

Table 2: TCM compounds

herb_id	Ingre2	Ingre3	Ingre4
HERB0	HBIN0	1-A-t	NA
HERB0	HBIN0	(1S,5	(1S,5
HERB0	HBIN0	1-Und	10268
HERB0	HBIN0	22410	2,6-O
HERB0	HBIN0	2-(2	NA
HERB0	HBIN0	2,5,5	2,5,5
HERB0	HBIN0	2,6,1	2,6,1
HERB0	HBIN0	()-2	Bicyc
HERB0	HBIN0	(2S)	NA
HERB0	HBIN0	(2S)	(2S)
HERB0	HBIN0	3-carene	(1S)
HERB0	HBIN0	3-dec	3-dec
HERB0	HBIN0	[(3R)	butan
HERB0	HBIN0	4-ACE	17745
HERB0	HBIN0	5,7-d	(2R)

Table 3为表格 compounds targets 概览。

(对应文件为 Figure+Table/compounds-targets.csv)

注:表格共有 14888 行 6 列,以下预览的表格可能省略部分数据;表格含有 707 个唯一'Ingredient_id'。

Table 3: Compounds targets

Ingre	Targe2	Targe3	Datab	Paper.id	PubMe
HBIN0	HBTAR	PGR	NA	NA	NA
HBIN0	HBTAR	PTGS2	NA	NA	NA
HBIN0	HBTAR	RXRA	NA	NA	NA
HBIN0	HBTAR	DPP4	NA	NA	NA
HBIN0	HBTAR	AR	NA	NA	NA
HBIN0	HBTAR	NR3C1	NA	NA	NA

Ingre	Targe2	Targe3	Datab	Paper.id	PubMe
HBIN0	HBTAR	PRSS1	NA	NA	NA
HBIN0	HBTAR	CA2	NA	NA	NA
HBIN0	HBTAR	ESR1	NA	NA	NA
HBIN0	HBTAR	GABRA1	NA	NA	NA
HBIN0	HBTAR	NCOA2	NA	NA	NA
HBIN0	HBTAR	ACHE	NA	NA	NA
HBIN0	HBTAR	PRSS1	NA	NA	NA
HBIN0	HBTAR	PRSS1	NA	NA	NA
HBIN0	HBTAR	SLC6A2	NA	NA	NA

将 Tab. 3 的基因信息注释:

Table 4为表格 compounds targets with annotation of biomaRt of ensembl dataset 概览。

(对应文件为 Figure+Table/compounds-targets-with-annotation-of-biomaRt-of-ensembl-dataset.xlsx)

注:表格共有 14888 行 13 列,以下预览的表格可能省略部分数据;表格含有 4230 个唯一'Target.name'。

Table 4: Compounds targets with annotation of biomaRt of ensembl dataset

Targe1	Ingre	Targe3	Datab	Paper.id	PubMe	ensem7	ensem8	entre	
6PGD	HBIN0	HBTAR	NA	HBREF.	. 27270429	NA	NA	NA	
AAMP	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	14	
AANAT	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	15	
AANAT	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	15	
AARS1	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	16	
AARS1	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	16	
AARS1	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	16	
AARS1	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	16	
AARS1	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	16	
AARS2	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	57505	
AASS	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	10157	
AASS	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	10157	
ABAT	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	18	
ABAT	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	18	
ABAT	HBIN0	HBTAR	NA	NA	NA	ENSG0	ENST0	18	

4.1.2 从 Genecards 获取疾病的靶点数据

Genecards https://www.genecards.org/

Table 5为表格 desease targets of diabetic nephropathy 概览。

(对应文件为 Figure+Table/desease-targets-of-diabetic-nephropathy.xlsx)

注: 表格共有 1309 行 7 列,以下预览的表格可能省略部分数据;表格含有 1309 个唯一'Symbol'。

Table 5: Desease targets of diabetic nephropathy

Symbol	Descr	Category	UniPr	GIFtS	GC_id	Score
ACE	Angio	Prote	P12821	55	GC17P	84.68
HNF1B	HNF1	Prote	P35680	47	GC17M	83.38
GCK	Gluco	Prote	P35557	53	GC07M	83.04
KCNJ11	Potas	Prote	Q14654	50	GC11M	80.35
HNF1A	HNF1	Prote	P20823	51	GC12P	78.94
ABCC8	ATP B	Prote	Q09428	50	GC11M	73.88
IL6	Inter	Prote	P05231	55	GC07P	70.31
HNF4A	Hepat	Prote	P41235	53	GC20P	67.73
PPARG	Perox	Prote	P37231	57	GC03P	64.11
PDX1	Pancr	Prote	P52945	50	GC13P	61.95
COL4A5	Colla	Prote	P29400	48	GC0XP	58.60
WFS1	Wolfr	Prote	O76024	50	GC04P	57.65
TCF7L2	Trans	Prote	Q9NQB0	51	GC10P	56.48
VEGFA	Vascu	Prote	P15692	53	GC06P	56.25
COL4A3	Colla	Prote	Q01955	50	GC02P	55.86

Table 6为表格 desease targets with annotation of biomaRt of ensembl dataset 概览。

(对应文件为 Figure+Table/desease-targets-with-annotation-of-biomaRt-of-ensembl-dataset.xlsx)

注:表格共有 674 行 8 列,以下预览的表格可能省略部分数据;表格含有 674 个唯一'hgnc_symbol'。

Table 6: Desease targets with annotation of biomaRt of ensembl dataset

hgnc	ensem2	ensem3	entre	chrom	start	end_p	descr
ABCB1	ENSG0	ENST0	5243	7	87503017	87713323	ATP b
ABCC8	ENSG0	ENST0	6833	11	17392498	17476894	ATP b
ABCG1	ENSG0	ENST0	9619	21	42199689	42297244	ATP b

hgnc	ensem2	ensem3	entre	chrom	start	end_p	descr
ACE	ENSG0	ENST0	1636	17	63477061	63498380	angio
ACHE	ENSG0	ENST0	43	7	10088	10089	acety
ACSL1	ENSG0	ENST0	2180	4	18475	18482	acyl
ACTB	ENSG0	ENST0	60	7	5526409	5563902	actin
ADA	ENSG0	ENST0	100	20	44584896	44652252	adeno
ADA2	ENSG0	ENST0	51816	22	17178790	17258235	adeno
ADAMTS1	3ENSG0	ENST0	11093	HG203	240452	285496	ADAM
ADAR	ENSG0	ENST0	103	1	15458	15462	adeno
ADCY3	ENSG0	ENST0	109	2	24819169	24920237	adeny
ADCY5	ENSG0	ENST0	111	3	12328	12344	adeny
ADD1	ENSG0	ENST0	118	4	2843844	2930076	adduc
ADORA1	ENSG0	ENST0	134	1	20309	20316	adeno

4.1.3 数据透视

以下,以 UpSet 图展示各个数据集之间的交集。

Figure 1为图 intersect of target genes of TCMs 概览。

(对应文件为 Figure+Table/intersect-of-target-genes-of-TCMs.pdf)

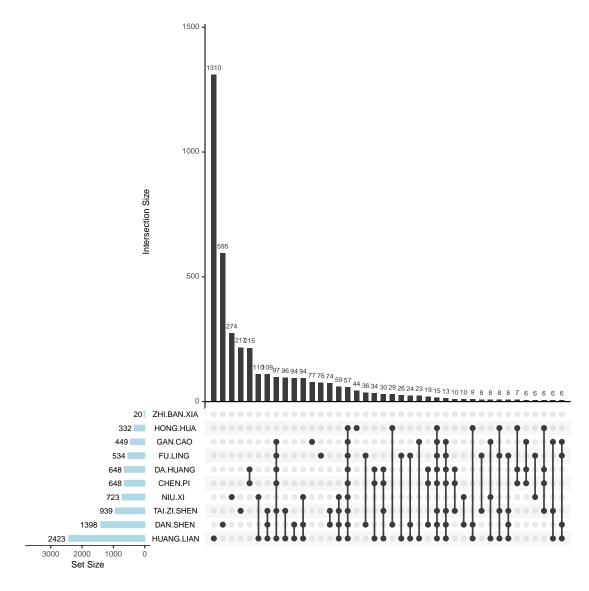


Figure 1: Intersect of target genes of TCMs

Figure 2为图 intersect of compounds of TCMs 概览。

(对应文件为 Figure+Table/intersect-of-compounds-of-TCMs.pdf)

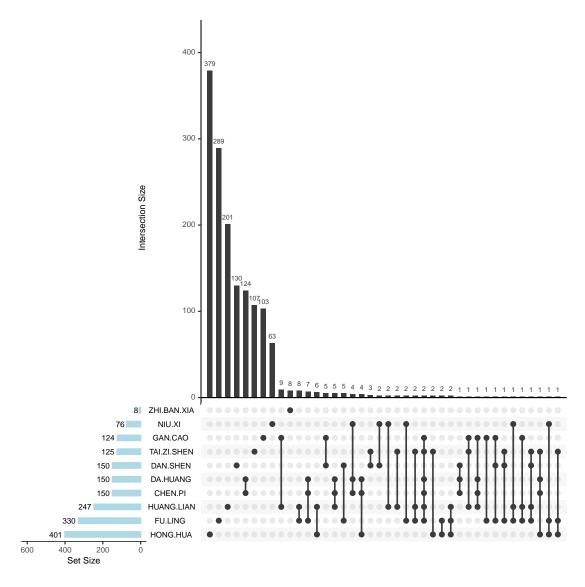


Figure 2: Intersect of compounds of TCMs

Figure 3为图 intersect of targets of compounds and disease targets 概览。

(对应文件为 Figure+Table/intersect-of-targets-of-compounds-and-disease-targets.pdf)

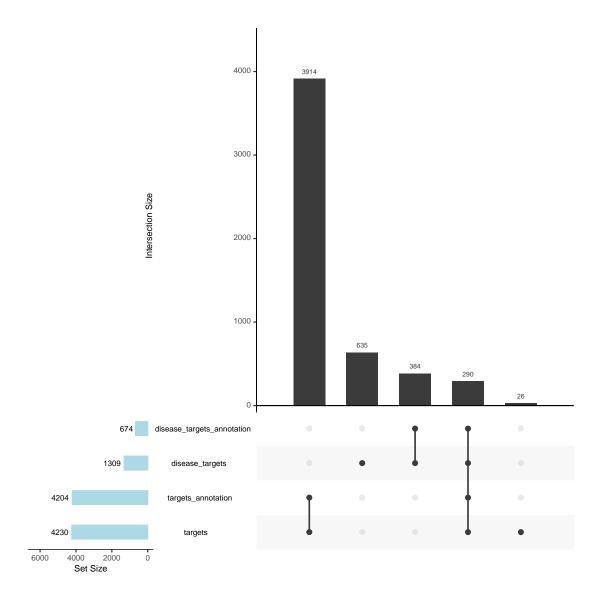


Figure 3: Intersect of targets of compounds and disease targets

4.1.4 以 STRINGdb 构建 PPI 网络

以 Fig. 3 中的四个数据集的交集,以 STRINGdb 创建 PPI 网络。

由于 PPI 网络包含过多节点,这里不展示 PPI 图 (较为混乱)。

Table 7为表格 ID mapped by STRINGdb 概览。

(对应文件为 Figure+Table/ID-mapped-by-STRINGdb.xlsx)

注: 表格共有 292 行 9 列,以下预览的表格可能省略部分数据;表格含有 289 个唯一'hgnc_symbol'。

Table 7: ID mapped by STRINGdb

hgnc	STRIN	ensem3	ensem4	entre	chrom	start	end_p	descr
ABCB1	9606	ENSG0	ENST0	5243	7	87503017	87713323	ATP b
ACE	9606	ENSG0	ENST0	1636	17	63477061	63498380	angio
ACHE	9606	ENSG0	ENST0	43	7	10088	10089	acety
ACSL1	9606	ENSG0	ENST0	2180	4	18475	18482	acyl
ACTB	9606	ENSG0	ENST0	60	7	5526409	5563902	actin
ADA	9606	ENSG0	ENST0	100	20	44584896	44652252	adeno
ADA2	9606	ENSG0	ENST0	51816	22	17178790	17258235	adeno
ADA2	9606	ENSG0	ENST0	51816	22	17178790	17258235	adeno
ADAR	9606	ENSG0	ENST0	103	1	15458	15462	adeno
ADD1	9606	ENSG0	ENST0	118	4	2843844	2930076	adduc
ADORA1	9606	ENSG0	ENST0	134	1	20309	20316	adeno
ADRB1	9606	ENSG0	ENST0	153	10	11404	11404	adren
AGXT	9606	ENSG0	ENST0	189	2	24086	24088	alani
AKR1B10	9606	ENSG0	ENST0	57016	7	13452	13454	aldo
ALAD	9606	ENSG0	ENST0	210	9	11338	11340	amino

4.1.5 筛选 HubGenes

利用 Cytoscape 的插件 CytoHubba¹ 提供的 MCC 算法计算 Hub 基因得分(这里 MCC 算法被集成到 R 中,独立计算)。

Figure 4为图 MCC Top 30 概览。

(对应文件为 Figure+Table/MCC-Top-30.pdf)

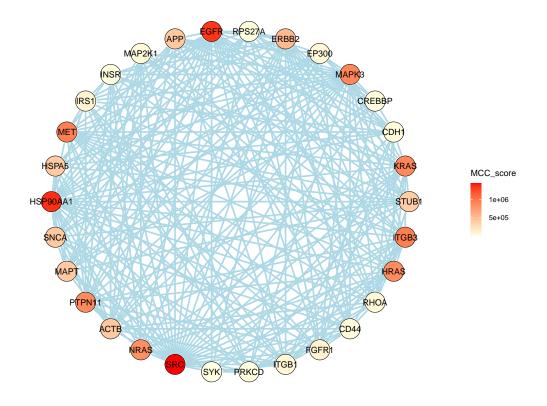


Figure 4: MCC Top 30

Table 8为表格 all MCC scores 概览。

(对应文件为 Figure+Table/all-MCC-scores.xlsx)

注: 表格共有 292 行 10 列,以下预览的表格可能省略部分数据;表格含有 289 个唯一'hgnc_symbol'。

Table 8: All MCC scores

hgnc	MCC_s	.STRIN	ensem4	ensem5	entre	chrom	start	end_p	descr	
SRC	1441311	9606	ENSG0	ENST0	6714	HG410	254187	315552	SRC	
									p	
HSP90A	All353642	9606	ENSG0	ENST0	3320	14	10208	10213	heat	
EGFR	1328596	9606	ENSG0	ENST0	1956	7	55019017	55211628	epide	
ITGB3	941356	9606	ENSG0	ENST0	3690	17	47253827	47313743	integ	
MET	937035	9606	ENSG0	ENST0	4233	7	11667	11679	MET	
									p	
MAPK3	894838	9606	ENSG0	ENST0	5595	16	30114105	30123506	mitog	

hgnc	MCC_s	.STRIN	ensem4	ensem5	entre	chrom	start	end_p	descr	
KRAS	890536	9606	ENSG0	ENST0	3845	12	25205246	25250936	KRAS	
PTPN11	871709	9606	ENSG0	ENST0	5781	12	11241	11250	prote	
HRAS	849299	9606	ENSG0	ENST0	3265	HSCHR	.61883	66928	HRas	
NRAS	828404	9606	${\rm ENSG0}$	ENST0	4893	1	11470	11471	NRAS	
ERBB2	531274	9606	${\rm ENSG0}$	ENST0	2064	17	39687914	39730426	erb-b	
ACTB	420124	9606	ENSG0	ENST0	60	7	5526409	5563902	actin	
APP	417130	9606	${\rm ENSG0}$	ENST0	351	21	25880535	26171128	amylo	
SNCA	416493	9606	ENSG0	ENST0	6622	4	89700345	89838315	synuc	
MAPT	406245	9606	ENSG0	ENST0	4137	HSCHR	.760287	893653	micro	

4.1.6 通路富集分析

使用 clusterProfiler 富集分析 top 30 的基因。

Figure 5为图 GO enrichment of MCC top 30 概览。

(对应文件为 Figure+Table/GO-enrichment-of-MCC-top-30.pdf)

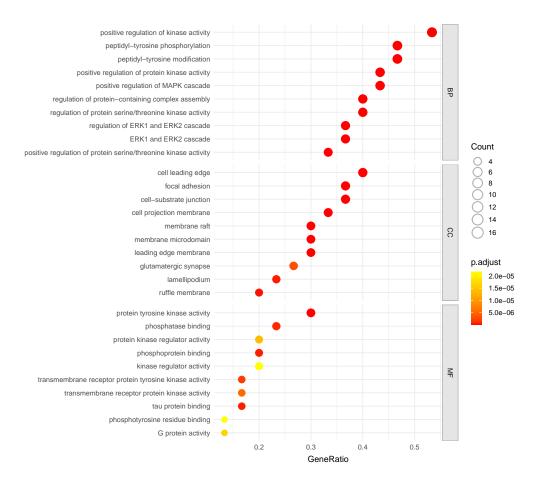


Figure 5: GO enrichment of MCC top $30\,$

Figure 6为图 KEGG enrichment of MCC top 30 概览。

(对应文件为 Figure+Table/KEGG-enrichment-of-MCC-top-30.pdf)

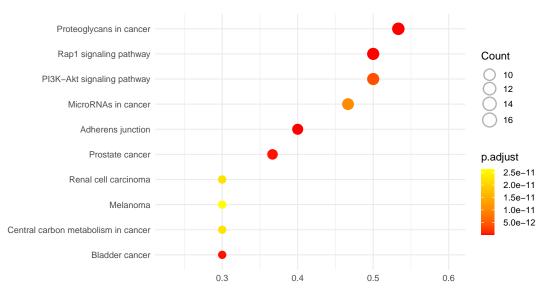


Figure 6: KEGG enrichment of MCC top 30

4.2 分析糖尿病肾病肠道差异菌群

4.2.1 选择公共数据库的 16s rRNA 数据

- 所选数据的文献来源2
 - Title: The Intestinal Microbiota Composition in Early and Late Stages of Diabetic Kidney Disease
 - PMID: 37341590
 - BioProject: PRJNA824185
- 相关信息
 - 引物: 805R (5'-GACTACHVGGGTATCTAATCC-3') and 341F (5'-CCTACGGGNGGCWGCAG-3')

Table 9为表格 metadata of the sra data of PRJNA824185 概览。

(对应文件为 Figure+Table/metadata-of-the-sra-data-of-PRJNA824185.csv)

注: 表格共有 108 行 47 列,以下预览的表格可能省略部分数据;表格含有 108 个唯一'Run'。

Table 9: Metadata of the sra data of PRJNA824185

Run	Relea	LoadDatspo	ots	bases	spots	avgLe	size_	_MBAssem	downl	Exper	Libra12	
SRR18.	2023-	2022- 84	114	4205700	00	500	13	NA	https	SRX14	.C_1	
SRR18.			133	4256650	00	500	13	NA	https	SRX14	.C_10	
SRR18.	2023-	2022- 83	213	4177292	60	502	12	NA	https	SRX14	.C_11	
SRR18.	2023-	2022- 80	525	4042355	00	502	12	NA	https	SRX14	.C_12	
SRR18.	2023-	 2022- 839	961	4198050	00	500	13	NA	https	SRX14	.C_2	
SRR18.	2023-	 2022- 81	782	4089100	00	500	13	NA	https	SRX14	.C_3	
SRR18.	2023-	 2022- 569	959	2847950	00	500	9	NA	https	SRX14	.C_4	
SRR18.	2023-	 2022- 85	406	4270300	00	500	15	NA	https	SRX14	.C_5	
SRR18.	2023-	 2022- 878	838	4391900	00	500	15	NA	https	SRX14	.C_6	
SRR18.	2023-	 2022- 87	784	4389200	00	500	13	NA	https	SRX14	.C_7	
SRR18.	2023-	 2022- 85	552	4277600	00	500	13	NA	https	SRX14	.C_8	

.. ...

Run	Relea	LoadDatepot	s bases	spots	avgLe	size_	_MBAssem	downl	Exper	Libra12	
SRR18.	2023-	2022- 8256	62 412810	0000	500	12	NA	https	SRX14	.C_9	
SRR18.	 2023-	 2022- 8030	09 401545	5000	500	12	NA	https	SRX14	.DM_10	
SRR18.	2023-	2022- 8412	25 420625	6000	500	13	NA	https	SRX14	.DM_11	
SRR18	 2023-	 2022- 8265	32 413160	0000	500	13	NA	https	SRX14	.DM_12	
	•••	•••									

4.2.2 下载和预处理 SRA 数据

使用 sra-toolkit 工具组的 prefetch 下载 SRA 数据,并用 fastq-dump 转化为 fastq 文件。 实际使用的数据为:

- Control 组
- Diabetic Nephropathy 组

Table 10为表格 metadata of used 16s rRNA data 概览。

(对应文件为 Figure+Table/metadata-of-used-16s-rRNA-data.csv)

注:表格共有 78 行 5 列,以下预览的表格可能省略部分数据;表格含有 2 个唯一'group'。

Table 10: Metadata of used 16s rRNA data

sampl	Run	forwa	rever	group
C.1	SRR18	/home	/home	С
C.10	SRR18	/home	/home	\mathbf{C}
C.11	SRR18	/home	/home	\mathbf{C}
C.12	SRR18	/home	/home	\mathbf{C}
C.2	SRR18	/home	/home	\mathbf{C}
C.3	SRR18	/home	/home	\mathbf{C}
C.4	SRR18	/home	/home	\mathbf{C}
C.5	SRR18	/home	/home	\mathbf{C}
C.6	SRR18	/home	/home	\mathbf{C}
C.7	SRR18	/home	/home	\mathbf{C}
C.8	SRR18	/home	/home	\mathbf{C}
C.9	SRR18	/home	/home	\mathbf{C}
DN.16	SRR18	/home	/home	DN
DN.17	SRR18	/home	/home	DN
DN.18	SRR18	/home	/home	DN

sampl	Run	forwa	rever	group
•••		•••		

4.2.3 使用 Qiime2 作为上游分析

以下分析参照³⁻⁷: https://docs.qiime2.org/2023.7/tutorials/moving-pictures-usage/

- importing data
- Demultiplexing sequences
- Sequence quality control and feature table construction
 - DADA2
- FeatureTable and FeatureData summaries
- Generate a tree for phylogenetic diversity analyses
- Alpha and beta diversity analysis
- Alpha rarefaction plotting
- Taxonomic analysis
- Differential abundance testing with ANCOM

4.2.4 使用 MicrobiotaProcess 作为下游分析

关于 LDA8

4.3 分析糖尿病肾病的肠道代谢组学差异

- 4.3.1 数据来源
- 4.3.2 Feature selection
- 4.3.3 富集分析
- 4.4 分析差异菌群与代谢物的相关性
- 4.4.1 使用关联数据

血清代谢物和肠道菌群的关联性9

4.4.2 从差异菌群到差异代谢物

 $Lachnospiraceae^{10}$

Trimethylamine¹¹

4.5 分析糖尿病肾病的转录组学差异

4.5.1 数据来源

• GSE199838

data_processing:

Illumina Bcl2FastQ software used for basecalling.

data_processing.1:

Sequenced reads were trimmed for adaptor sequence, and masked for low-complexity or low-quality sequence. The remaining reads were filtered against the rRNA database to remove possible ribosomal RNA contamination, and then mapped to the hg19 whole genome using Hisat2 v2.1.0 with default parameters.

data_processing.2:

HTSeq v0.11.2 was subsequently employed to convert aligned short reads into read counts for each gene model.

data_processing.3:

Assembly: hg19

data_processing.4:

Supplementary files format and content: tab-delimited text files include RPKM for each Sample

4.5.2 数据标准化

Figure 7为图 RNA filtered genes 概览。

(对应文件为 Figure+Table/RNA-filtered-genes.pdf)

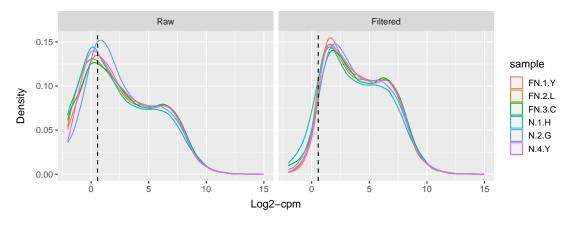


Figure 7: RNA filtered genes

Figure 8为图 RNA nomalization 概览。

(对应文件为 Figure+Table/RNA-nomalization.pdf)

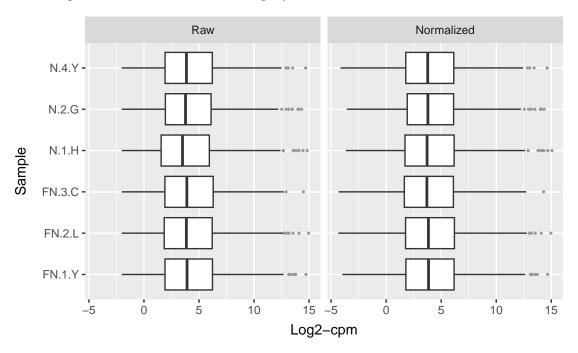


Figure 8: RNA nomalization

4.5.3 差异分析

Figure 9为图 RNA seq DEG 概览。

(对应文件为 Figure+Table/RNA-seq-DEG.pdf)

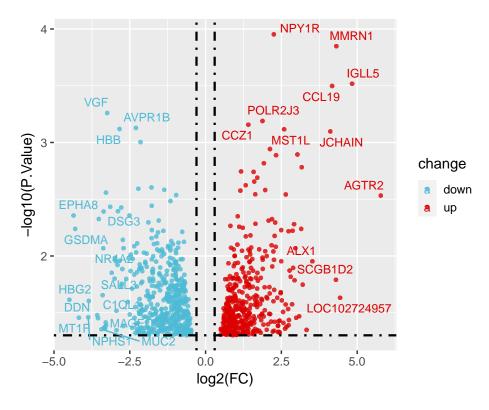


Figure 9: RNA seq DEG

Table 11为表格 RNA DEG top table 概览。

(对应文件为 Figure+Table/RNA-DEG-top-table.csv)

注: 表格共有 865 行 7 列,以下预览的表格可能省略部分数据; 表格含有 865 个唯一'hgnc_symbol'。

Table 11: RNA DEG top table

hgnc	$\log FC$	AveExpr	t	P.Value	adj.P	В
NPY1R	2.251	6.749	7.572	0.000	0.618	-3.90
HBB	-2.83	8.479	-5.57	0.000	0.618	-3.91
COL14A1	2.124	7.990	5.201	0.001	0.618	-3.94
ASAH1	1.170	7.424	4.806	0.001	0.618	-3.97
VARS	-0.96	7.518	-4.40	0.002	0.618	-3.99
RHOB	-1.15	9.861	-4.31	0.003	0.618	-4.01
MT1E	-3.14	8.226	-4.21	0.003	0.618	-4.02
MT2A	-2.89	8.428	-4.14	0.004	0.618	-4.02
FGL2	1.058	8.156	4.069	0.004	0.618	-4.03
C4B	-1.88	7.510	-3.97	0.005	0.618	-4.04
SLC27A4	-0.76	7.183	-3.82	0.006	0.618	-4.06
VASN	-1.13	7.761	-3.68	0.007	0.618	-4.07

hgnc	logFC	AveExpr	t	P.Value	adj.P	В
PABPC1	-0.71	9.322	-3.67	0.007	0.618	-4.08
TTC28	-0.90	8.207	-3.58	0.008	0.618	-4.08
TRABD2B	-1.78	7.019	-3.73	0.006	0.618	-4.08

4.6 转录组学和网络药理学结合

receptors:

DCN IRAK1 CDKN1A FOXO3

4.7 代谢小分子靶点蛋白分析

4.7.1 分子对接数据准备

5 结论

Reference

- 1. Chin, C.-H. *et al.* cytoHubba: Identifying hub objects and sub-networks from complex interactome. *BMC Systems Biology* **8**, S11 (2014).
- 2. Zhang, L. *et al.* The intestinal microbiota composition in early and late stages of diabetic kidney disease. *Microbiology Spectrum* **11**, (2023).
- 3. Bolyen, E. et al. Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2. Nature Biotechnology 37, 852–857 (2019).
- 4. McDonald, D. *et al.* The biological observation matrix (BIOM) format or: How i learned to stop worrying and love the ome-ome. *GigaScience* 1, 7 (2012).
- Callahan, B. J. et al. DADA2: High-resolution sample inference from illumina amplicon data. Nature methods 13, 581 (2016).
- 6. Hamday, M., Walker J., J., Harris, J. K., Gold J., N. & Knight, R. Error-correcting barcoded primers allow hundreds of samples to be pyrosequenced in multiplex. *Nature Methods* 5, 235–237 (2008).
- 7. Hamday, M. & Knight, R. Microbial community profiling for human microbiome projects: Tools, techniques, and challenges. *Genome Research* **19**, 1141–1152 (2009).
- 8. Rai, S. N. et al. Microbiome data analysis with applications to pre-clinical studies using QIIME2: Statistical considerations. Genes \& Diseases 8, (2021).
- 9. Wilmanski, T. et al. Blood metabolome predicts gut microbiome α -diversity in humans. Nature Biotechnology 37, (2019).

- 10. Vacca, M. et al. The controversial role of human gut lachnospiraceae. Microorganisms 8, (2020).
- 11. Praveenraj, S. S. et al. The role of a gut microbial-derived metabolite, trimethylamine n-oxide (TMAO), in neurological disorders. *Molecular neurobiology* **59**, 6684–6700 (2022).