# 中药-有效成分-乳腺癌相关靶点的网药分析

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# ${\bf Contents}$

1	摘要		1
	1.1	需求	1
	1.2	结果	1
	1.3	需求 2	1
	1.4	结果 2	1
2	前言		1
3	材料	和方法	1
	3.1	材料	1
	3.2	方法	1
4	分析	结果	2
5	结论		2
6	附:	分析流程	2
	6.1	网络药理学	2
		6.1.1 成分	2
		6.1.2 成分靶点	4
		6.1.3 疾病靶点	4
		6.1.4 疾病-成分-靶点网络图	5
		6.1.5 富集分析	7
		6.1.6 疾病-成分-靶点-通路网络图	9
	6.2	beta-sitosterol	11
		6.2.1 富集分析	11
		6.2.2 TCGA-BRCA	14
		6.2.3 糖酵解、巨噬细胞极化相关基因	15
		6.2.4 关联分析	17
		6.2.5 韦恩图	17
Re	efere	nce	18
$\mathbf{L}$	ist	of Figures	
	1	Intersection of all compounds	3
	2	Network pharmacology with disease	6
	3	Targets intersect with targets of diseases	6
	4	KEGG enrichment	8
	5	GO enrichment	9
	6	Network pharmacology with disease and pathway	10

7	SITO KEGG enrichment	11
8	SITO GO enrichment	12
9	Correlation heatmap	17
10	Intersection of Baihuasheshecao with Banzhilian with Zhebeimu	18
List	of Tables	
1	Herbs information	
2	Compounds filtered by OB and DL	2
3	Tables of Herbs compounds and targets	4
4	Disease related targets from GeneCards	5
5	Network pharmacology with disease and pathway data	10
6	SITO KEGG enrichment data	12
7	SITO GO enrichment data	13
8	BC metadata	14
9	MP related targets from GeneCards	15
10	GL related targets from GeneCards	16

### 1 摘要

#### 1.1 需求

网络药理学分析

• 药对: 白花蛇舌草, 半枝莲, 浙贝母

• 疾病: 乳腺癌

• 目标: 提供中药-有效成分-乳腺癌相关靶点的网药分析

#### 1.2 结果

- 数据来源于 TCMSP, 以 OB、DL 筛选过化合物 Tab. 2。
- 疾病靶点来源于 GeneCards, Tab. 4
- 疾病成分靶点网络图: Fig. 3
- 包含通路: Fig. 6, Tab. 5

#### 1.3 需求 2

下一步请对 beta-sitosterol 的 60 个靶点做富集分析,并作这些靶点与糖酵解、巨噬细胞极化相关性分析。 意向靶点为 JTK2 (即 FGFR4),请重点关注另外需要提供一个韦恩图表明 beta-sitosterol 就是三种药共有的唯一成分

#### 1.4 结果 2

见 6.2

- 2 前言
- 3 材料和方法
- 3.1 材料
- 3.2 方法

Mainly used method:

- R package ClusterProfiler used for gene enrichment analysis<sup>1</sup>.
- The Human Gene Database GeneCards used for disease related genes prediction<sup>2</sup>.
- R package Limma and edgeR used for differential expression analysis<sup>3,4</sup>.
- Website TCMSP https://tcmsp-e.com/ used for data source<sup>5</sup>.
- The API of UniProtKB (https://www.uniprot.org/help/api\_queries) used for mapping of names or IDs of proteins.
- R version 4.4.0 (2024-04-24); 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 网络药理学

#### 6.1.1 成分

Table 1 (下方表格) 为表格 Herbs information 概览。

#### (对应文件为 Figure+Table/Herbs-information.csv)

注:表格共有3行2列,以下预览的表格可能省略部分数据;含有3个唯一'Herb\_pinyin\_name'。

Table 1: Herbs information

Herb_pinyin_name	Herb_cn_name
Baihuasheshecao	白花蛇舌草
Banzhilian	半枝莲
Zhebeimu	浙贝母

Table 2 (下方表格) 为表格 Compounds filtered by OB and DL 概览。

#### (对应文件为 Figure+Table/Compounds-filtered-by-OB-and-DL.xlsx)

注:表格共有 43 行 15 列,以下预览的表格可能省略部分数据;含有 39 个唯一 'Mol ID;含有 3 个唯一 'Herb\_pinyin\_name'。

#### OB (%) and DL cut-off:

OB >= 30%; DL >= 0.18

Table 2: Compounds filtered by OB and DL

Mol ID	Molecu	MW	AlogP	Hdon	Hacc	OB (%)	Caco-2	BBB	DL
MOL001646	2,3-di	282.310	3.262	0	4	34.858	0.75128	0.17357	0.26255
MOL001659	Porife	412.770	7.640	1	1	43.829	1.43659	1.03472	0.75596
MOL001663	(4aS,6	456.780	6.422	2	3	32.028	0.60932	0.39268	0.75713
MOL001670	2-meth	252.280	3.278	0	3	37.827	0.72896	-0.12795	0.20517

Mol ID	Molecu	MW	AlogP	Hdon	Hacc	OB (%)	Caco-2	BBB	DL
MOL000449	Stigma	412.770	7.640	1	1	43.829	1.44458	1.00045	0.75665
MOL000358	beta-s	414.790	8.084	1	1	36.913	1.32463	0.98588	0.75123
MOL000098	quercetin	302.250	1.504	5	7	46.433	0.04842	-0.76890	0.27525
MOL001040	(2R)-5	272.270	2.298	3	5	42.363	0.37818	-0.47578	0.21141
MOL012245	5,7,4'	302.300	2.281	3	6	36.626	0.43274	-0.31890	0.26833
MOL012246	5,7,4'	302.300	2.281	3	6	74.235	0.37328	-0.43273	0.26479
MOL012248	5-hydr	328.340	2.820	1	6	65.818	0.84750	0.07437	0.32874
MOL012250	7-hydr	298.310	2.836	1	5	43.716	0.95759	0.22129	0.25376
MOL012251	Chrysi	268.280	2.853	1	4	37.268	0.90922	0.15556	0.20317
MOL012252	9,19-c	426.800	7.554	1	1	38.685	1.44891	1.16360	0.78074
MOL002776	Baicalin	446.390	0.639	6	11	40.123	-0.84777	-1.74426	0.75264

Figure 1 (下方图) 为图 intersection of all compounds 概览。

# (对应文件为 Figure+Table/intersection-of-all-compounds.pdf)

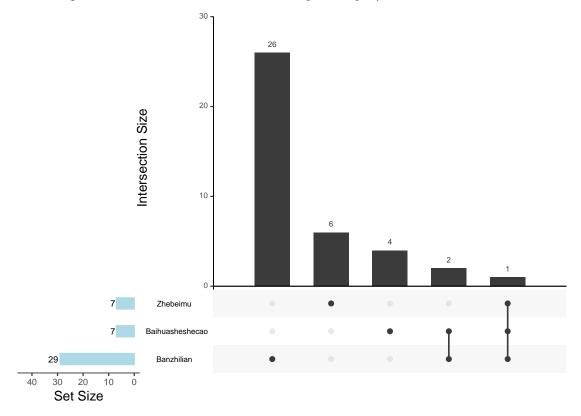


Figure 1: Intersection of all compounds  $\,$ 

All\_intersection:

MOL000358

(上述信息框内容已保存至 Figure+Table/intersection-of-all-compounds-content)

#### 6.1.2 成分靶点

Table 3 (下方表格) 为表格 tables of Herbs compounds and targets 概览。

(对应文件为 Figure+Table/tables-of-Herbs-compounds-and-targets.xlsx)

注:表格共有 1846 行 4 列,以下预览的表格可能省略部分数据;含有 3 个唯一'Herb\_pinyin\_name'。

Table 3: Tables of Herbs compounds and targets

Herb_pinyin_name	Molecule name	symbols	protein.names
Banzhilian	luteolin	NA	NA
Banzhilian	luteolin	MMP2	72 kDa type IV co
Banzhilian	luteolin	CLG4A	72 kDa type IV co
Banzhilian	luteolin	ADCY2	Adenylate cyclase
Banzhilian	luteolin	KIAA1060	Adenylate cyclase
Banzhilian	luteolin	APP	Amyloid-beta prec
Banzhilian	luteolin	A4	Amyloid-beta prec
Banzhilian	luteolin	AD1	Amyloid-beta prec
Banzhilian	luteolin	AR	Androgen receptor
Banzhilian	luteolin	DHTR	Androgen receptor
Banzhilian	luteolin	NR3C4	Androgen receptor
Banzhilian	luteolin	XIAP	E3 ubiquitin-prot
Banzhilian	luteolin	API3	E3 ubiquitin-prot
Banzhilian	luteolin	BIRC4	E3 ubiquitin-prot
Banzhilian	luteolin	IAP3	E3 ubiquitin-prot

#### 6.1.3 疾病靶点

Table 4 (下方表格) 为表格 Disease related targets from GeneCards 概览。

(对应文件为 Figure+Table/Disease-related-targets-from-GeneCards.xlsx)

注: 表格共有 1746 行 7 列, 以下预览的表格可能省略部分数据; 含有 1746 个唯一 'Symbol'。

#### The GeneCards data was obtained by querying:

breast cancer

Restrict (with quotes):

FALSE

Filtering by Score: :

Score > 15

Table 4: Disease related targets from GeneCards

Symbol	Description	Category	UniProt_ID	GIFtS	GC_id	Score
BRCA2	BRCA2 DNA	Protein Co	P51587	56	GC13P032315	584.27
BRCA1	BRCA1 DNA	Protein Co	P38398	59	GC17M043044	565.02
PALB2	Partner An	Protein Co	Q86YC2	53	GC16M023603	366.84
ATM	ATM Serine	Protein Co	Q13315	61	GC11P108223	340.7
CHEK2	Checkpoint	Protein Co	O96017	63	GC22M028687	336.43
BRIP1	BRCA1 Inte	Protein Co	Q9BX63	57	GC17M061679	325.07
CDH1	Cadherin 1	Protein Co	P12830	58	GC16P068737	306.68
BARD1	BRCA1 Asso	Protein Co	Q99728	55	$\mathrm{GC}02\mathrm{M}214725$	291.41
TP53	Tumor Prot	Protein Co	P04637	62	GC17M007661	287.34
MSH6	MutS Homol	Protein Co	P52701	58	GC02P047695	239.29
MSH2	MutS Homol	Protein Co	P43246	57	GC02P047403	231.87
MLH1	MutL Homol	Protein Co	P40692	58	GC03P036993	223.25
C11orf65	Chromosome	Protein Co	Q8NCR3	40	GC11M108308	218.43
LOC126862571	BRD4-Indep	Functional		10	GC17P114574	215.91
APC	APC Regula	Protein Co	P25054	58	GC05P112707	199.23

#### 6.1.4 疾病-成分-靶点网络图

Figure 2 (下方图) 为图 Network pharmacology with disease 概览。

(对应文件为 Figure+Table/Network-pharmacology-with-disease.pdf)

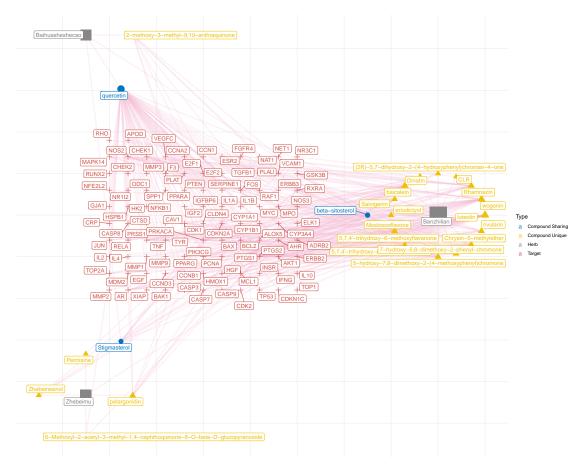


Figure 2: Network pharmacology with disease

Figure 3 (下方图) 为图 Targets intersect with targets of diseases 概览。

#### (对应文件为 Figure+Table/Targets-intersect-with-targets-of-diseases.pdf)

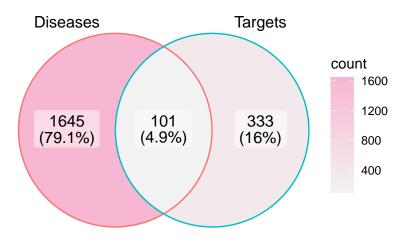


Figure 3: Targets intersect with targets of diseases

#### Intersection:

CHEK2, TP53, PTEN, ERBB2, CDKN2A, AKT1, AR, CASP8, ERBB3, JUN, MYC, IL2, MDM2, CDK2, IL1B, FGFR4, BCL2, BAX, TGFB1, ESR2, IGF2, NFE2L2, PPARG, EGF, PTGS2, TNF, MMP2, MMP9, RAF1, CASP3, CYP1A1, NFKB1, CTSD, PCNA, PLAU, TOP2A, CDK1, MMP1, E2F1, VEGFC, IFNG, CYP1B1, CHEK1, PIK3CG, IL10, CASP9, CAV1,...

(上述信息框内容已保存至 Figure+Table/Targets-intersect-with-targets-of-diseases-content)

#### 6.1.5 富集分析

Figure 4 (下方图) 为图 KEGG enrichment 概览。

(对应文件为 Figure+Table/KEGG-enrichment.pdf)

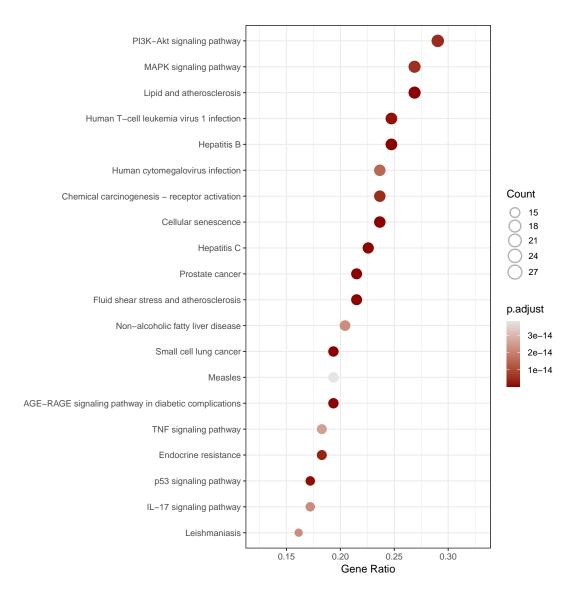


Figure 4: KEGG enrichment

Figure 5 (下方图) 为图 GO enrichment 概览。

(对应文件为 Figure+Table/GO-enrichment.pdf)

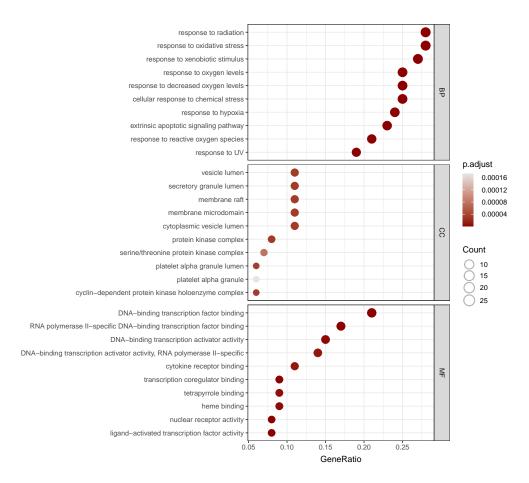


Figure 5: GO enrichment

#### 6.1.6 疾病-成分-靶点-通路网络图

Figure 6 (下方图) 为图 Network pharmacology with disease and pathway 概览。

(对应文件为 Figure+Table/Network-pharmacology-with-disease-and-pathway.pdf)

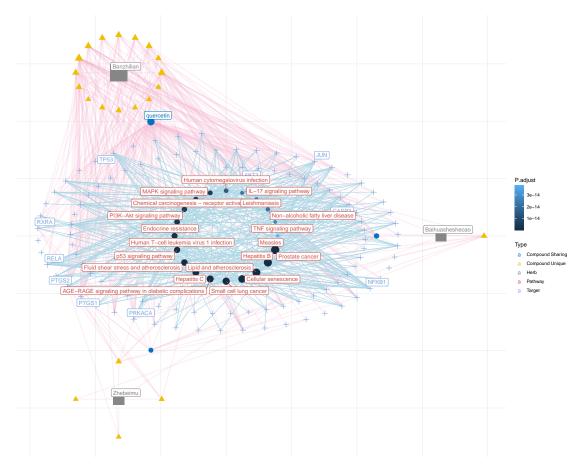


Figure 6: Network pharmacology with disease and pathway

Table 5 (下方表格) 为表格 Network pharmacology with disease and pathway data 概览。

#### (对应文件为 Figure+Table/Network-pharmacology-with-disease-and-pathway-data.xlsx)

注: 表格共有 431 行 5 列,以下预览的表格可能省略部分数据; 含有 3 个唯一'Herb\_pinyin\_name; 含有 24 个唯一'Ingredient.name; 含有 101 个唯一'Target.name'。

Table 5: Network pharmacology with disease and pathway data

Herb_pinyin_name	e Ingredient.name	Target.name	Hit_pathway_number	er Enriched_pathways
Baihuasheshecao	quercetin	NFKB1	18	AGE-RAGE signalin
Baihuasheshecao	quercetin	RELA	18	AGE-RAGE signalin
Banzhilian	baicalein	RELA	18	AGE-RAGE signalin
Banzhilian	luteolin	RELA	18	AGE-RAGE signalin
Banzhilian	quercetin	NFKB1	18	AGE-RAGE signalin
Banzhilian	quercetin	RELA	18	AGE-RAGE signalin
Banzhilian	wogonin	RELA	18	AGE-RAGE signalin
Baihuasheshecao	quercetin	AKT1	17	AGE-RAGE signalin
Banzhilian	baicalein	AKT1	17	AGE-RAGE signalin

Herb_pinyin_name	e Ingredient.name	Target.name	Hit_pathway_numb	er Enriched_pathways
Banzhilian	luteolin	AKT1	17	AGE-RAGE signalin
Banzhilian	quercetin	AKT1	17	AGE-RAGE signalin
Banzhilian	wogonin	AKT1	17	AGE-RAGE signalin
Baihuasheshecao	quercetin	TP53	14	Cellular senescen
Banzhilian	baicalein	TP53	14	Cellular senescen
Banzhilian	luteolin	TP53	14	Cellular senescen

#### 6.2 beta-sitosterol

#### 6.2.1 富集分析

Figure 7 (下方图) 为图 SITO KEGG enrichment 概览。

#### (对应文件为 Figure+Table/SITO-KEGG-enrichment.pdf)

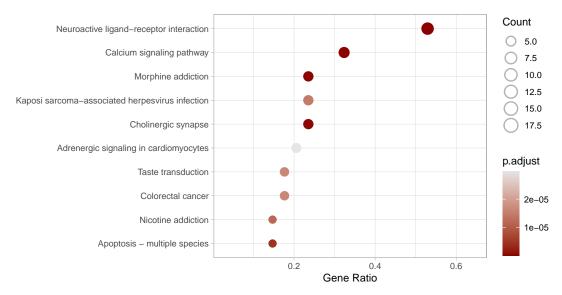


Figure 7: SITO KEGG enrichment

Figure 8 (下方图) 为图 SITO GO enrichment 概览。

#### (对应文件为 Figure+Table/SITO-GO-enrichment.pdf)

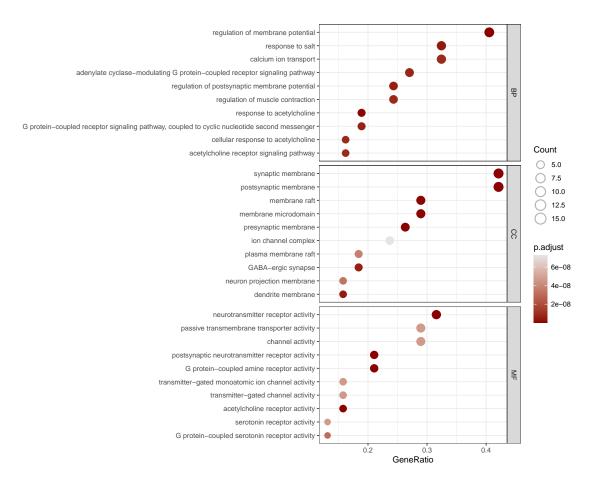


Figure 8: SITO GO enrichment

Table 6 (下方表格) 为表格 SITO KEGG enrichment data 概览。

#### (对应文件为 Figure+Table/SITO-KEGG-enrichment-data.xlsx)

注:表格共有 181 行 9 列,以下预览的表格可能省略部分数据;含有 181 个唯一'ID'。

1. pvalue: 显著性 P。

Table 6: SITO KEGG enrichment data

ID	Descri	GeneRatio	BgRatio	pvalue	p.adjust	qvalue	geneID	Count
hsa04080	Neuroa	18/34	366/8753	1.2099	2.1900	1.1590	148/14	18
$\rm hsa05032$	Morphi	8/34	91/8753	1.4533	9.0812	4.8060	1812/2	8
hsa04020	Calciu	11/34	253/8753	1.5051	9.0812	4.8060	148/14	11
$\rm hsa04725$	Cholin	8/34	113/8753	8.2528	3.7344	1.9763	596/11	8
$\rm hsa04215$	Apopto	5/34	32/8753	1.2159	4.4015	2.3294	581/59	5
$\rm hsa05033$	Nicoti	5/34	40/8753	3.8860	1.1722	6.2040	1139/2	5
$\rm hsa05167$	Kaposi	8/34	194/8753	5.5839	1.4438	7.6411	581/71	8
hsa04742	Taste	6/34	86/8753	8.1367	1.6363	8.6601	1131/2	6

ID	Descri	GeneRatio	BgRatio	pvalue	p.adjust	qvalue	geneID	Count
hsa05210	Colore	6/34	86/8753	8.1367	1.6363	8.6601	581/59	6
hsa04261	Adrene	7/34	154/8753	1.6438	2.9753	1.5746	148/14	7
hsa05161	Hepati	7/34	162/8753	2.3085	3.7986	2.0103	581/59	7
hsa05145	Toxopl	6/34	111/8753	3.6575	5.5167	2.9196	596/83	6
hsa04726	Seroto	6/34	115/8753	4.4952	6.0205	3.1862	836/33	6
$\rm hsa05152$	Tuberc	7/34	180/8753	4.6567	6.0205	3.1862	581/59	7
hsa01524	Platin	5/34	73/8753	8.0960	9.3555	4.9511	581/59	5

Table 7 (下方表格) 为表格 SITO GO enrichment data 概览。

#### (对应文件为 Figure+Table/SITO-GO-enrichment-data.xlsx)

注: 表格共有 2405 行 10 列,以下预览的表格可能省略部分数据;含有 3 个唯一'ont'。

- 1. pvalue: 显著性 P。
- 2. ont: One of "BP", "MF", and "CC" subontologies. The Cellular Component (CC), the Molecular Function (MF) and the Biological Process (BP).

Table 7: SITO GO enrichment data

ont	ID	Descri	GeneRatio	BgRatio	pvalue	p.adjust	qvalue	geneID	Count
BP	GO:004	regula	15/37	433/18614	1.4579	2.9742	1.6528	148/15	15
BP	GO:190	respon	7/37	36/18614	5.3761	5.4836	3.0474	1128/1	7
BP	GO:190	respon	12/37	383/18614	5.6547	3.8452	2.1369	1128/1	12
BP	GO:006	regula	9/37	148/18614	1.0226	5.2155	2.8984	154/11	9
BP	GO:000	G prot	7/37	56/18614	1.4519	5.9240	3.2921	1128/1	7
BP	GO:000	adenyl	10/37	234/18614	2.1044	7.1552	3.9763	148/14	10
BP	GO:009	acetyl	6/37	31/18614	2.8612	8.1337	4.5201	1128/1	6
BP	GO:000	regula	9/37	173/18614	4.1766	8.1337	4.5201	148/14	9
BP	GO:000	calciu	12/37	455/18614	4.1950	8.1337	4.5201	148/58	12
BP	GO:190	cellul	6/37	33/18614	4.2917	8.1337	4.5201	1128/1	6
BP	GO:000	${\it muscle}$	11/37	349/18614	4.7585	8.1337	4.5201	148/14	11
BP	GO:000	phosph	8/37	113/18614	4.7845	8.1337	4.5201	148/14	8
BP	GO:007	calciu	11/37	360/18614	6.6320	1.0407	5.7835	148/58	11
BP	GO:006	excita	8/37	124/18614	1.0137	1.4771	8.2087	154/11	8
BP	GO:009	postsy	6/37	39/18614	1.2534	1.7046	9.4734	1128/1	6

#### 6.2.2 TCGA-BRCA

获取 TCGA-BRCA (RNA-seq) 数据,以备关联分析

Table 8 (下方表格) 为表格 BC metadata 概览。

#### (对应文件为 Figure+Table/BC-metadata.xlsx)

注: 表格共有 1094 行 89 列,以下预览的表格可能省略部分数据;含有 1094 个唯一'sample'。

sample: 样品名称
 group: 分组名称

Table 8: BC metadata

3       3       3       3       3       1	sample	group	lib.size	norm.f	barcode	patient	shortL	defini	sample9	sample10	
TCGA-         Alive         375951791         TCGA-         TCGA-         TP         Primar         TCGA-         01            3         3         3         3         3         3         3         1 </td <td>TCGA-</td> <td>Alive</td> <td>5671450</td> <td>41</td> <td>TCGA-</td> <td>TCGA-</td> <td>TP</td> <td>Primar</td> <td>TCGA-</td> <td>01</td> <td></td>	TCGA-	Alive	5671450	41	TCGA-	TCGA-	TP	Primar	TCGA-	01	
3         3         3         3         3         1 <td< td=""><td>3</td><td></td><td></td><td></td><td>3</td><td>3</td><td></td><td></td><td>3</td><td></td><td></td></td<>	3				3	3			3		
TCGA-         Alive         225981541         TCGA-         TCGA-         TP         Primar         TCGA-         01            3         4         4         4         4         4         4         4         4         4         4         4         4         4         4         4         4         4         4         5         5         5         5         5         5         5         5         5         5         5         5         5         7	TCGA-	Alive	3759517	91	TCGA-	TCGA-	TP	Primar	TCGA-	01	
3       3       3       3       3       1	3				3	3			3		
TCGA-         Alive         527254451         TCGA-         TCGA-         TP         Primar         TCGA-         01            3         4         4         4         4         4         4         4         4         4         4         4         4         4         5	TCGA-	Alive	2259815	41	TCGA-	TCGA-	TP	Primar	TCGA-	01	
3       3       3       3       3       TCGA- TCGA- TP Primar       TCGA- 01          4       4       4       4       4       4       4         TCGA- Alive 342141291       TCGA- TCGA- TCGA- TP Primar       TCGA- 01       5       5       5         TCGA- Alive 242606631       TCGA- TCGA- TCGA- TP Primar       TCGA- 01       5       5       5         TCGA- Alive 335752871       TCGA- TCGA- TCGA- TP Primar       TCGA- 01       5       5       5         TCGA- Alive 475729491       TCGA- TCGA- TCGA- TP Primar       TCGA- 01       6	3				3	3			3		
TCGA-       Alive       474122611       TCGA-       TCGA-       TP       Primar       TCGA-       01          4       5       7       7       7       7       7       7       7       7       7       7       7       7       7       7       7       7       7 </td <td>TCGA-</td> <td>Alive</td> <td>5272544</td> <td>51</td> <td>TCGA-</td> <td>TCGA-</td> <td>TP</td> <td>Primar</td> <td>TCGA-</td> <td>01</td> <td></td>	TCGA-	Alive	5272544	51	TCGA-	TCGA-	TP	Primar	TCGA-	01	
4       4       4       4       4       4       4       4       4       4       4       4       TCGA- TCGA- TP Primar       TCGA- 01       5       7 <td>3</td> <td></td> <td></td> <td></td> <td>3</td> <td>3</td> <td></td> <td></td> <td>3</td> <td></td> <td></td>	3				3	3			3		
TCGA-         Alive         342141291         TCGA-         TCGA-         TP         Primar         TCGA-         01            5         5         5         5         5         5         1         5         5         1	TCGA-	Alive	4741226	11	TCGA-	TCGA-	TP	Primar	TCGA-	01	
5       5       5       5       5       5       1	4				4	4			4		
TCGA-       Alive       242606631       TCGA-       TCGA-       TP       Primar       TCGA-       01          5       5       5       5       5       5       1          TCGA-       Alive       335752871       TCGA-       TCGA-       TP       Primar       TCGA-       01          5       5       5       5       5       5       5       1        A </td <td>TCGA-</td> <td>Alive</td> <td>3421412</td> <td>91</td> <td>TCGA-</td> <td>TCGA-</td> <td>TP</td> <td>Primar</td> <td>TCGA-</td> <td>01</td> <td></td>	TCGA-	Alive	3421412	91	TCGA-	TCGA-	TP	Primar	TCGA-	01	
5       5       5       5       5       5       5       1	5				5	5			5		
TCGA-       Alive       335752871       TCGA-       TCGA-       TP       Primar       TCGA-       01          5       5       5       5       5       5       1          TCGA-       Alive       475729491       TCGA-       TCGA-       TP       Primar       TCGA-       01          A.	TCGA-	Alive	2426066	31	TCGA-	TCGA-	TP	Primar	TCGA-	01	
5       5       5       5       5       7CGA- Alive Af5729491       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- Alive Ar       7CGA- Alive Ar       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- Alive Ar       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- Alive Ar       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- Alive Ar       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- Alive Ar       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- Alive Ar       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- 01       7CGA- TCGA- TCGA- TP Primar       7CGA- 01       7CGA- 01	5				5	5			5		
TCGA-       Alive       475729491       TCGA-       TCGA-       TP       Primar       TCGA-       01          A       A       A       A       A       A       TCGA-       01          TCGA-       Alive       605450031       TCGA-       TCGA-       TP       Primar       TCGA-       01          A       Alive       610323511       TCGA-       TCGA-       TP       Primar       TCGA-       01          TCGA-       Alive       488189181       TCGA-       TCGA-       TP       Primar       TCGA-       01          TCGA-       Alive       564029211       TCGA-       TCGA-       TP       Primar       TCGA-       01	TCGA-	Alive	3357528	71	TCGA-	TCGA-	TP	${\bf Primar}$	TCGA-	01	
A       TCGA-       TP       Primar       TCGA-       01        A       A       TCGA-       TP       Primar       TCGA-       01        A       TCGA-       A       A       TCGA-       TP       Primar       TCGA-       01        A       TCGA-       TCGA-       TP       Primar       TCGA-       01        A       A       TCGA-       TCGA-       TP       Primar       TCGA-       01        A       A       TCGA-       <	5				5	5			5		
TCGA-       Alive       605450031       TCGA-       TCGA-       TP       Primar       TCGA-       01          A       A       A       A       A       A       TCGA-       01          TCGA-       Alive       610323511       TCGA-       TCGA-       TP       Primar       TCGA-       01          TCGA-       Alive       488189181       TCGA-       TCGA-       TP       Primar       TCGA-       01          A       A       A       A       A       A       TCGA-       01	TCGA-	Alive	4757294	91	TCGA-	TCGA-	TP	Primar	TCGA-	01	
A       A       A       A       A       A       TCGA- DTP Primar       TCGA- D1 M       A       A       A       A       A       A       A       TCGA- DTP Primar       TCGA- DTP DTM	A				A	A			A		
TCGA-       Alive       610323511       TCGA-       TCGA-       TP       Primar       TCGA-       01          A       A       A       A       A       A       A       A       A       TCGA-       01          TCGA-       Alive       564029211       TCGA-       TCGA-       TP       Primar       TCGA-       01	TCGA-	Alive	6054500	31	TCGA-	TCGA-	TP	${\bf Primar}$	TCGA-	01	
A A A A A A A A	A				A	A			A		
TCGA-       Alive       488189181       TCGA-       TCGA-       TP       Primar       TCGA-       01          A       A       A       A       A       TCGA-       01          TCGA-       Alive       564029211       TCGA-       TCGA-       TP       Primar       TCGA-       01	TCGA-	Alive	6103235	11	TCGA-	TCGA-	TP	Primar	TCGA-	01	
A A A A A A A TCGA- Alive $564029211$ TCGA- TCGA- TP Primar TCGA- $01$	A				A	A			A		
TCGA- Alive 564029211	TCGA-	Alive	4881891	81	TCGA-	TCGA-	TP	Primar	TCGA-	01	
	A				A	A			A		
A A A	TCGA-	Alive	5640292	11	TCGA-	TCGA-	TP	Primar	TCGA-	01	
	A				A	A			A		

sample	group	lib.size	norm.f	barcode	patient	shortL	defini	sample9	sample10	
TCGA-	Alive	6853493	91	TCGA-	TCGA-	TP	Primar	TCGA-	01	
A				A	A			A		
TCGA-	Alive	7333205	91	TCGA-	TCGA-	TP	Primar	TCGA-	01	
A				A	A			A		
		•••	•••	•••	•••		•••	•••	•••	

#### 6.2.3 糖酵解、巨噬细胞极化相关基因

Table 9 (下方表格) 为表格 MP related targets from GeneCards 概览。

#### (对应文件为 Figure+Table/MP-related-targets-from-GeneCards.xlsx)

注:表格共有 72 行 7 列,以下预览的表格可能省略部分数据;含有 72 个唯一'Symbol'。

#### The GeneCards data was obtained by querying :

Macrophage polarization

#### Restrict (with quotes):

TRUE

#### Filtering by Score: :

Score > 2

Table 9: MP related targets from GeneCards

Symbol	Description	Category	${\bf UniProt\_ID}$	GIFtS	GC_id	Score
MIRLET7C	MicroRNA L	RNA Gene (		29	GC21P018103	6.28
GAS5	Growth Arr	RNA Gene (		31	GC01M173947	4.76
NR4A1AS	NR4A1 Anti	RNA Gene (		13	GC12M052059	4.37
LINC01672	Long Inter	RNA Gene (		19	GC01P020797	4.33
MIR125A	MicroRNA 125a	RNA Gene (		29	GC19P113552	4.23
H19	H19 Imprin	RNA Gene (		34	GC11M001995	3.82
CERNA3	Competing	RNA Gene (		19	GC08P056323	3.76
STAT3	Signal Tra	Protein Co	P40763	62	GC17M042313	3.73
MIR146B	MicroRNA 146b	RNA Gene (		29	GC10P102436	3.7
IL6	Interleukin 6	Protein Co	P05231	60	GC07P022725	3.5
MIR98	MicroRNA 98	RNA Gene (		26	GC0XM053782	3.42
TMX2-CTNND1	TMX2-CTNND	RNA Gene (		23	GC11P057712	3.39

Symbol	Description	Category	UniProt_ID	GIFtS	GC_id	Score
PLA2G5	Phospholip	Protein Co	P39877	46	GC01P020028	3.37
LINC02605	Long Inter	RNA Gene (		18	GC08P078838	3.15
IRF5	Interferon	Protein Co	Q13568	55	GC07P128937	3.14

Table 10 (下方表格) 为表格 GL related targets from GeneCards 概览。

#### (对应文件为 Figure+Table/GL-related-targets-from-GeneCards.xlsx)

注:表格共有 118 行 7 列,以下预览的表格可能省略部分数据;含有 118 个唯一 'Symbol'。

# The GeneCards data was obtained by querying :

glycolysis

Restrict (with quotes):

TRUE

Filtering by Score: :

 $\mathrm{Score} > 3$ 

Table 10: GL related targets from GeneCards

Symbol	Description	Category	$UniProt\_ID$	GIFtS	GC_id	Score
TIGAR	TP53 Induc	Protein Co	Q9NQ88	45	GC12P038924	22.4
PKM	Pyruvate K	Protein Co	P14618	58	GC15M072199	20.77
HK2	Hexokinase 2	Protein Co	P52789	55	GC02P074947	19.42
GAPDH	Glyceralde	Protein Co	P04406	59	GC12P038965	17.14
LDHA	Lactate De	Protein Co	P00338	59	GC11P018394	15.81
HIF1A	Hypoxia In	Protein Co	Q16665	57	GC14P061695	15.1
RRAD	RRAD, Ras	Protein Co	P55042	46	GC16M067483	15.1
HK1	Hexokinase 1	Protein Co	P19367	59	GC10P069269	14.64
PKLR	Pyruvate K	Protein Co	P30613	55	GC01M155289	13.37
ENO1	Enolase 1	Protein Co	P06733	56	GC01M008861	13.36
ENO3	Enolase 3	Protein Co	P13929	54	GC17P004948	13.33
PFKP	Phosphofru	Protein Co	Q01813	53	GC10P003066	13.19
TPI1	Triosephos	Protein Co	P60174	55	GC12P006867	13.18
GLTC1	Glycolysis	RNA Gene (		2	GC11U909607	12.97

Symbol	Description	Category	UniProt_ID	GIFtS	GC_id	Score
PGK1	Phosphogly	Protein Co	P00558	57	GC0XP078166	12.94

#### 6.2.4 关联分析

Figure 9 (下方图) 为图 Correlation heatmap 概览。

#### (对应文件为 Figure+Table/Correlation-heatmap.pdf)

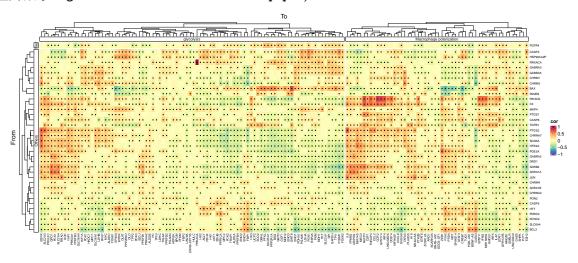


Figure 9: Correlation heatmap

'Linear curve' 数据已全部提供。

#### (对应文件为 Figure+Table/Linear-curve)

注:文件夹 Figure+Table/Linear-curve 共包含 2 个文件。

- 1. 1\_glycolysis.pdf
- 2. 2\_Macrophage polarization.pdf

#### 6.2.5 韦恩图

Figure 10 (下方图) 为图 Intersection of Baihuasheshecao with Banzhilian with Zhebeimu 概览。

(对应文件为 Figure+Table/Intersection-of-Baihuasheshecao-with-Banzhilian-with-Zhebeimu.pdf)

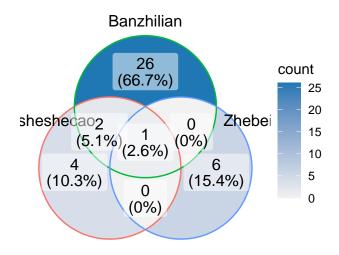


Figure 10: Intersection of Baihuasheshecao with Banzhilian with Zhebeimu

# All\_intersection: beta-sitosterol

(上述信息框内容已保存至 Figure+Table/Intersection-of-Baihuasheshecao-with-Banzhilian-with-Zhebeimu-content

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