

红豆杉和养阴解毒汤的共同活性成分和作用靶点 (m6A、铁死亡相关)

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1 摘要

注：关于南方红豆杉的成分数据，使用的是 *Taxus mairei* (<https://plantaedb.com/taxa/phylum/gymnosperms/order/cupressales/family/taxaceae/genus/taxus/species/taxus-mairei>) 记录。更多关于红豆杉的记录可见 <https://plantaedb.com/search?src=Taxus>。

1.1 需求

co-targets > ATF3 > pathway (m6A) > ferroptosis 根据研究基础，养阴解毒汤能够促进 IGFIBP2 表达，抑制 METTL3 表达，如果红豆杉和养阴解毒汤都靶向 m6A 甲基化修饰相关的作用靶点 XXX。推测：红豆杉和养阴解毒汤通过 XXX/YYY 途径调控基因 m6A 甲基化修饰，促进肺癌细胞铁死亡，从而抑制肺癌的发展。(机制尽可能的结合 ATF3)

1.2 结果

注：红豆杉的靶点未发现 ATF3，因此红豆杉和养阴解毒的共同靶点未包括 ATF3。

- 分别分析了养阴解毒汤 (YYJD) 和红豆杉 (HDS) 的成分和靶点。
 - YYDS：由于 YYDS 的南方红豆杉成分，多数中药数据库 (HERB、TCMSP 等) 没有该条目，这里使用了 PlantaeDb 中的成分记录 (Tab. 1)。
 - YYDS：由于 PlantaeDb 中的成分没有靶点信息，因此这里用 Super-Pred 预测了这些化合物的靶点 (先以 HOB 预测 20% 口服利药度，过滤了一部分成分) (Tab. 2)。
 - YYDS：最终的成分靶点数据整合了来自于 HERB 的其它中药的成分靶点数据 (这里，也用 Super-Pred 补充了它们的靶点)，和来自于 PlantaeDb 的南方红豆杉的成分靶点。最终图和表见 Fig. 5, Tab. 5
 - HDS：分析思路同 YYDS，结合了 HERB 数据库的记录和 Super-Pred 的预测。Fig. 7, Tab. 8
- YYDS 和 HDS 的共同靶点见 Fig. 8
- 铁死亡相关的基因集来自于 FerrDb v2。Tab. ??
- 肺癌和 m6A 相关的基因集都来自于 GeneCards (Tab. 9, Tab. 10)。
- 最终结果采取交集方式：共同靶点 + 驱动铁死亡的调控基因 + 肺癌靶点 + m6A 相关，见 Fig. 11 和 Fig. 12。筛选出的基因为：PRKAA1

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 analysis¹.
- Website HERB <http://herb.ac.cn/> used for data source².

- Python tool of **HOB** was used for prediction of human oral bioavailability³.
- The API of **m6A-Atlas** used for obtaining m6A related data from the website⁴.
- The Database **PlantaeDB** <https://plantaedb.com/> used for collating data of herbal ingredients.
- Web tool of **Super-PRED** used for drug-targets prediction⁵.
- R package **STEINGdb** used for PPI network construction^{6,7}.
- The Human Gene Database **GeneCards** used for disease related genes prediction⁸.
- R package **UniProt.ws** used for querying Gene or Protein information.
- Database of **FerrDb V2** used for obtaining ferroptosis regulators⁹.
- Database of **MSigDB** (c2, curated gene sets) was used for signature screening.
- 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

<https://plantaedb.com/> <https://bidd.group/NPASS/index.php> <https://plantaedb.com/>

6.1 网络药理学分析

6.1.1 养阴解毒汤

6.1.1.1 南方红豆杉 *Taxus-mairei*

Table 1 (下方表格) 为表格 *Taxus mairei* compounds from plantaeDb 概览。

(对应文件为 **Figure+Table/Taxus-mairei-compounds-from-plantaedb.xlsx**)

注：表格共有 302 行 8 列，以下预览的表格可能省略部分数据；表格含有 1 个唯一 ‘id’。

Table 1: *Taxus mairei* compounds from plantaeDb

.id	classes	Name	PubChe...	Canoni...	MW	Found in	Proof
Taxus ...	> Alka...	CID 30956	30956	CC1CC=...	507.60	unknown	https:...
Taxus ...	> Alka...	cytoch...	5458428	CC1CC=...	507.60	unknown	https:...
Taxus ...	> Benz...	3,4-Di...	72	C1=CC(...	154.12	unknown	https:...
Taxus ...	> Benz...	(3S)-8...	486250	CC1CC2...	222.19	unknown	https:...
Taxus ...	> Benz...	8-Hydr...	5242129	CC1CC2...	222.19	unknown	https:...
Taxus ...	> Benz...	Methyl...	7456	COC(=O...	152.15	unknown	https:...
Taxus ...	> Benz...	Honokiol	72303	C=CCC1...	266.30	unknown	https:...
Taxus ...	> Benz...	3-(4-H...	82452	C1=CC(...	152.19	unknown	https:...
Taxus ...	> Benz...	2-Prop...	9984	COCl=C...	178.18	unknown	https:...

.id	classes	Name	PubChe...	Canoni...	MW	Found in	Proof
Taxus ...	> Benz...	4-[(5...	163079914	CC1(OC...	402.50	unknown	https:...
Taxus ...	> Benz...	4-[(6-...	141864758	CC1(OC...	402.50	unknown	https:...
Taxus ...	> Benz...	4-Hydr...	5280536	COCl=C...	178.18	unknown	https:...
Taxus ...	> Benz...	Dihydr...	16822	COCl=C...	182.22	unknown	https:...
Taxus ...	> Benz...	Isovan...	12127	COCl=C...	152.15	unknown	https:...
Taxus ...	> Lign...	4-[(5a...	137796452	CC1(OC...	386.40	unknown	https:...
...

Figure 1 (下方图) 为图 Taxus mairei compounds HOB 20 prediction 概览。

(对应文件为 [Figure+Table/Taxus-mairei-compounds-HOB-20-prediction.pdf](#))

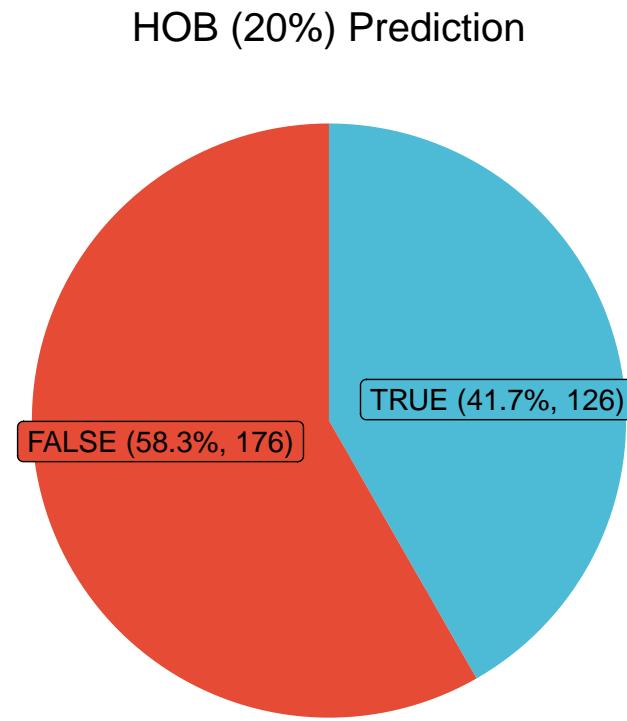


Figure 1: Taxus mairei compounds HOB 20 prediction

Table 2 (下方表格) 为表格 Taxus mairei compounds targets predicted by Super Pred 概览。

(对应文件为 [Figure+Table/Taxus-mairei-compounds-targets-predicted-by-Super-Pred.xlsx](#))

注：表格共有 13879 行 9 列，以下预览的表格可能省略部分数据；表格含有 126 个唯一 ‘.id’。

Table 2: Taxus mairei compounds targets predicted by Super Pred

.id	Target...	ChEMBL-ID	UniPro...	PDB Vi...	TTD ID	Probab...	Model ...	symbols
CC[C@H...]	Nuclea...	CHEMBL...	P19838	1SVC	Not Av...	97.23%	96.09%	NFKB1
CC[C@H...]	Cathep...	CHEMBL...	P07339	4OD9	T67102	96.37%	98.95%	CTSD
CC[C@H...]	Adenos...	CHEMBL226	P30542	5N2S	T92072	94.33%	95.93%	ADORA1
CC[C@H...]	Cannab...	CHEMBL253	P34972	6KPF	Not Av...	93.89%	97.25%	CNR2
CC[C@H...]	Dual s...	CHEMBL...	Q9HAZ1	6FYV	Not Av...	92.7%	94.45%	CLK4
CC[C@H...]	Cycloo...	CHEMBL221	P23219	6Y3C	Not Av...	91.59%	90.17%	PTGS1
CC[C@H...]	Minera...	CHEMBL...	P08235	4PF3	Not Av...	90.65%	100%	NR3C2
CC[C@H...]	Glutam...	CHEMBL...	Q05586	5EWM	Not Av...	90.47%	95.89%	GRIN1
CC[C@H...]	G-prot...	CHEMBL...	Q9Y2T6	Not Av...	T87670	90.05%	78.15%	GPR55
CC[C@H...]	Formyl...	CHEMBL...	P21462	Not Av...	T87831	89.44%	93.56%	FPR1
CC[C@H...]	Glycin...	CHEMBL...	P23415	4X5T	T50269	89.42%	90.71%	GLRA1
CC[C@H...]	LSD1/C...	CHEMBL...	O60341	5L3D	Not Av...	88.56%	97.09%	KDM1A
CC[C@H...]	DNA-(a...	CHEMBL...	P27695	6BOW	T13348	87.72%	91.11%	APEX1
CC[C@H...]	NT-3 g...	CHEMBL...	Q16288	6KZD	Not Av...	83.36%	95.89%	NTRK3
CC[C@H...]	Androg...	CHEMBL...	P10275	3V49	T11211	83.21%	96.43%	AR
...

6.1.1.2 其它中药 MIX

以下靶点数据来源于 HERB 数据库：

Table 3 (下方表格) 为表格 MIX Herbs compounds and targets from HERB 概览。

(对应文件为 Figure+Table/MIX-Herbs-compounds-and-targets-from-HERB.xlsx)

注：表格共有 20801 行 9 列，以下预览的表格可能省略部分数据；表格含有 835 个唯一‘Ingredient.id’。

Table 3: MIX Herbs compounds and targets from HERB

Ingred.....1	Herb_p...	Ingred.....3	Ingred.....4	Target.id	Target...	Databa...	Paper.id	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	ATIC	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	FPGS	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	GART	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	MTHFD1	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	MTHFD2	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	ALDH1L1	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	MTHFD1L	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	MTFMT	NA	NA	...
HBIN00...	SHI HU	10,12-...	NA	HBTAR0...	ALDH1L2	NA	NA	...

Ingred.....1	Herb_p...	Ingred.....3	Ingred.....4	Target.id	Target...	Databa...	Paper.id	...
HBIN00...	SHI HU	10,12...	NA	HBTAR0...	MTHFD2L	NA	NA	...
HBIN00...	SHI HU	10 ,13...	NA	NA	NA	NA	NA	...
HBIN00...	BEI SH...	10-epi...	NA	NA	NA	NA	NA	...
HBIN00...	DANG SHEN	11alph...	11 -me...	NA	NA	NA	NA	...
HBIN00...	DANG SHEN	11-Hyd...	Spiro(...	HBTAR0...	CDK2	NA	NA	...
HBIN00...	DANG SHEN	11-Hyd...	Spiro(...	HBTAR0...	ESR1	NA	NA	...
...

Figure 2 (下方图) 为图 MIX HOB 20 prediction 概览。

(对应文件为 [Figure+Table/MIX-HOB-20-prediction.pdf](#))

HOB (20%) Prediction

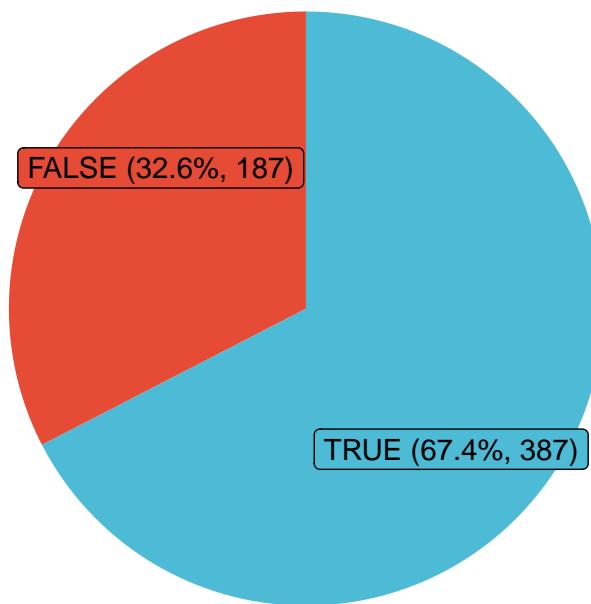


Figure 2: MIX HOB 20 prediction

补充了预测的靶点数据：

Table 4 (下方表格) 为表格 MIX compounds targets predicted by Super Pred 概览。

(对应文件为 [Figure+Table/MIX-compounds-targets-predicted-by-Super-Pred.xlsx](#))

注：表格共有 42305 行 9 列，以下预览的表格可能省略部分数据；表格含有 387 个唯一 ‘id’。

Table 4: MIX compounds targets predicted by Super Pred

.id	Target...	ChEMBL-ID	UniPro...	PDB Vi...	TTD ID	Probab...	Model ...	symbols
C1=CC(...	Transc...	CHEMBL...	O15164	4YBM	Not Av...	94.7%	95.56%	TRIM24
C1=CC(...	Endopl...	CHEMBL...	Q99714	2O23	Not Av...	93.9%	70.16%	HSD17B10
C1=CC(...	Monoam...	CHEMBL...	P21397	2Z5Y	Not Av...	90.07%	91.49%	MAOA
C1=CC(...	Transt...	CHEMBL...	P02766	6SUG	T86462	88.39%	90.71%	TTR
C1=CC(...	DNA-(a...	CHEMBL...	P27695	6BOW	T13348	87.23%	91.11%	APEX1
C1=CC(...	Serine...	CHEMBL...	O75460	6W39	Not Av...	81.09%	98.11%	ERN1
C1=CC(...	Dual s...	CHEMBL...	Q9HAZ1	6FYV	Not Av...	80.64%	94.45%	CLK4
C1=CC(...	Pregna...	CHEMBL...	O75469	6TFI	T82702	79.78%	94.73%	NR1I2
C1=CC(...	Estrog...	CHEMBL242	Q92731	1QKM	T80896	79.45%	98.35%	ESR2
C1=CC(...	Kruppe...	CHEMBL...	Q13887	Not Av...	Not Av...	79.32%	86.33%	KLF5
C1=CC(...	Protea...	CHEMBL...	P20618	6KWW	Not Av...	77.67%	90%	PSMB1
C1=CC(...	Cytoch...	CHEMBL...	P11509	2FDV	T06455	76.23%	71.78%	CYP2A6
C1=CC(...	C-X-C ...	CHEMBL...	P61073	3ODU	T96079	76.12%	93.1%	CXCR4
C1=CC(...	Tyrosy...	CHEMBL...	Q9NUW8	6N0D	Not Av...	75.1%	71.22%	TDP1
C1=CC(...	Cathep...	CHEMBL...	P07339	4OD9	T67102	75.01%	98.95%	CTSD
...

6.1.1.3 合并 MERGE

Figure 3 (下方图) 为图 MERGE Intersection of herbs all targets 概览。

(对应文件为 Figure+Table/MERGE-Intersection-of-herbs-all-targets.pdf)

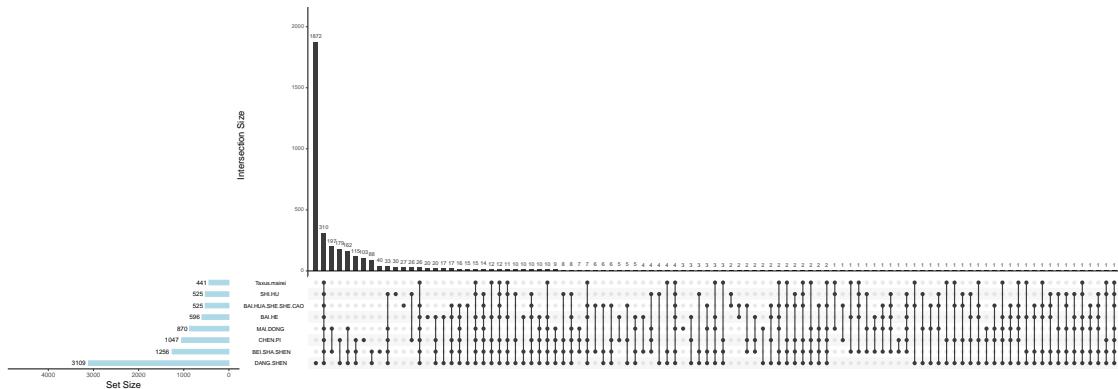


Figure 3: MERGE Intersection of herbs all targets

All_intersection :

ACHE, GRIA2, PRSS1, PTGS2, NOS2, DPP4, GABRA1, CHRM2, CNR2, CTSD, NFKB1, APEX1, TDP1, TRIM24, FPR1, BLM, GRIN1, KDM1A, NR3C2, NR1I2, ADAM10, DPP8, NTRK3, FCGRT, KLF5, TOP2A, S1PR5, CYP3A4, PIK3R1, DRD1, SLC6A5, CSNK2B, CDK5, FPR2, CACNA1B, HSD17B10, GPR55, PLA2G2A, GPBAR1, DPP9, TLR4, ACACA, CHRM...

(上述信息框内容已保存至 Figure+Table/MERGE-Intersection-of-herbs-all-targets-content)

Figure 4 (下方图) 为图 MERGE Intersection of herbs compounds 概览。

(对应文件为 Figure+Table/MERGE-Intersection-of-herbs-compounds.pdf)

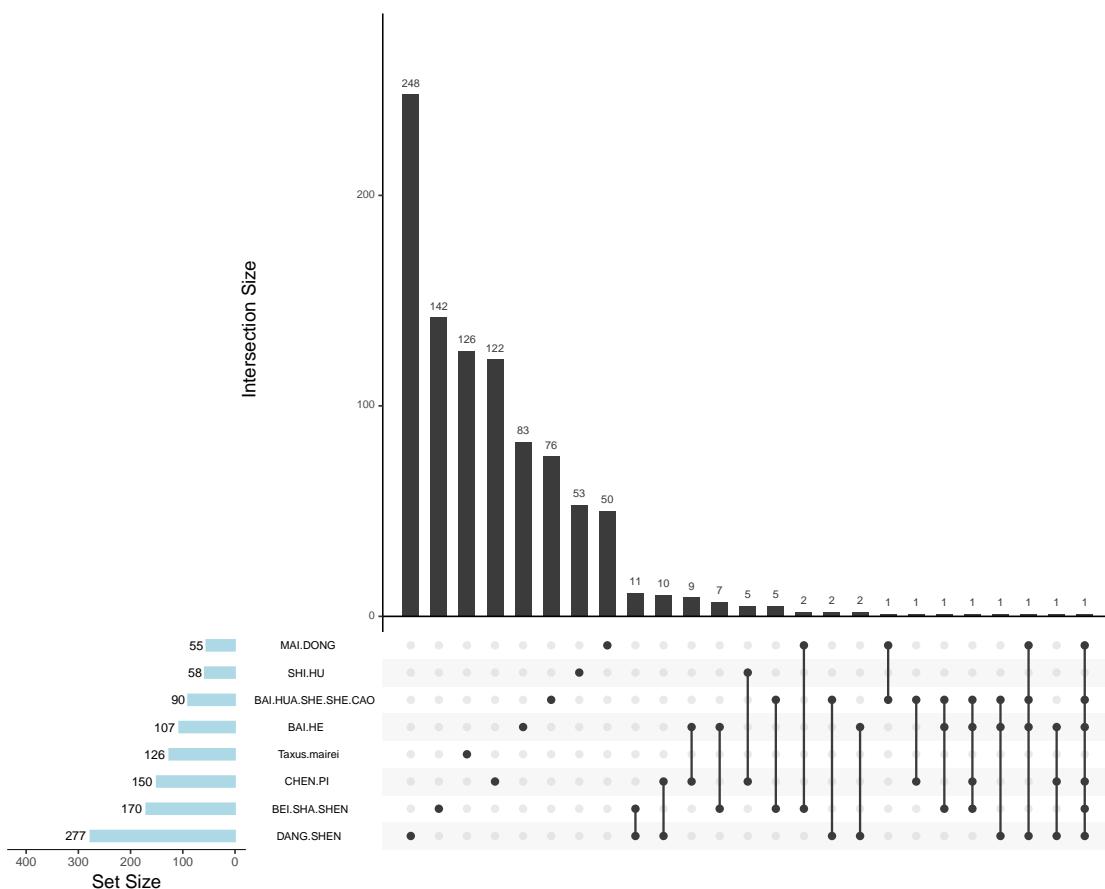


Figure 4: MERGE Intersection of herbs compounds

All_intersection :

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

Figure 5 (下方图) 为图 MERGE network pharmacology visualization 概览。

(对应文件为 Figure+Table/MERGE-network-pharmacology-visualization.pdf)

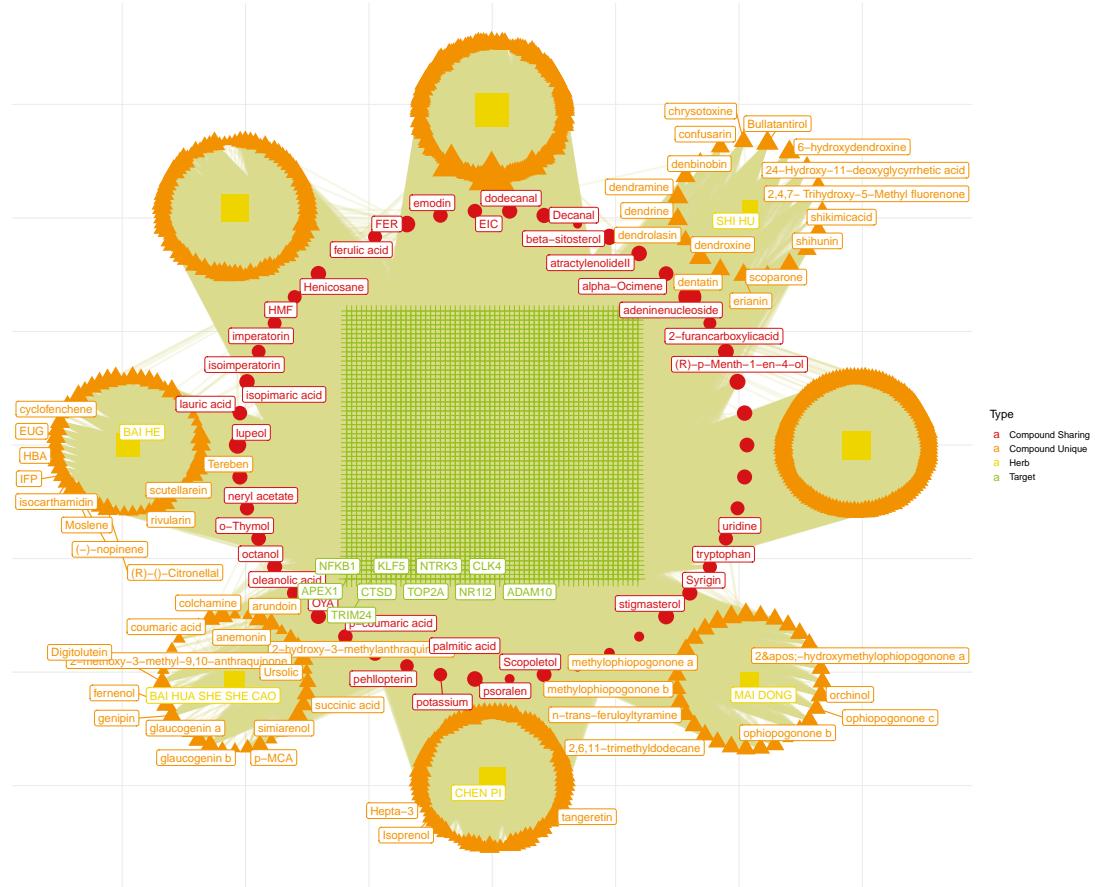


Figure 5: MERGE network pharmacology visualization

药方所有的成分、靶点数据:

Table 5 (下方表格) 为表格 MERGE Herbs compounds and targets 概览。

(对应文件为 Figure+Table/MERGE-Herbs-compounds-and-targets.tsv)

注: 表格共有 70759 行 10 列, 以下预览的表格可能省略部分数据; 表格含有 961 个唯一 'Ingredient.id'。

Table 5: MERGE Herbs compounds and targets

Ingred.....1	Herb_p...	Ingred.....3	Ingred.....4	Target.id	Target.....6	Databa...	Paper.id	...
10022393	Taxus ...	(7R)-7...	NA	NA	APEX1	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	NFKB1	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	KDM1A	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	HTR2C	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	HIF1A	NA	NA	...

Ingred.....1	Herb_p... ...	Ingred.....3	Ingred.....4	Target.id	Target.....6	Databa... ...	Paper.id
10022393	Taxus ...	(7R)-7...	NA	NA	TRIM24	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	BLM	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	SLC6A5	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	GPR55	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	CTSD	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	KLF5	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	PRCP	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	C5AR1	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	THRA	NA	NA	...
10022393	Taxus ...	(7R)-7...	NA	NA	PSMB1	NA	NA	...
...

6.1.2 红豆杉

以下是收集自 HERB 数据库的成分、靶点数据：

Table 6 (下方表格) 为表格 HDS Herbs compounds and targets from HERB 概览。

(对应文件为 [Figure+Table/HDS-Herbs-compounds-and-targets-from-HERB.xlsx](#))

注：表格共有 128 行 7 列，以下预览的表格可能省略部分数据；表格含有 105 个唯一‘Ingredient.id’。

Table 6: HDS Herbs compounds and targets from HERB

Ingredient.id	Herb_pinyi... ...	Ingredient.....3	Ingredient.....4	Target.id	Target.nameDatabase.s...
HBIN000081	HONG DOU SHAN	10-deacety...	NA	NA	NA	NA
HBIN000084	HONG DOU SHAN	10-deacety...	NA	NA	NA	...
HBIN001104	HONG DOU SHAN	1,3,7,8-te...	1,3,7,8-te...	NA	NA	NA
HBIN001125	HONG DOU SHAN	13-acetyl...	NA	NA	NA	...
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	NA	...

Ingredient.id	Herb_pinyi...	Ingredient.....3	Ingredient.....4	Target.id	Target.nameDatabase.s...	...
HBIN001379	HONG DOU SHAN	14 -benzoy...	NA	NA	NA	NA
HBIN001380	HONG DOU SHAN	14 -benzoy...	NA	NA	NA	NA
HBIN001381	HONG DOU SHAN	14 -benzoy...	NA	NA	NA	NA
HBIN001385	HONG DOU SHAN	14 -hydrox...	NA	NA	NA	NA
HBIN002352	HONG DOU SHAN	1 ,2 ,9 -t...	1beta,2bet...	NA	NA	NA
HBIN002387	HONG DOU SHAN	1beta-dehy...	1 -dehydro...	NA	NA	NA
HBIN002399	HONG DOU SHAN	1 -hydroxy...	NA	NA	NA	NA
HBIN002663	HONG DOU SHAN	1-hydroxyt...	NA	NA	NA	NA
HBIN005241	HONG DOU SHAN	2alpha,5al...	NA	NA	NA	NA
HBIN005242	HONG DOU SHAN	2 ,5 ,10 -...	2alpha,5al...	NA	NA	NA
...

Figure 6 (下方图) 为图 HDS HOB 20 prediction 概览。

(对应文件为 Figure+Table/HDS-HOB-20-prediction.pdf)

HOB (20%) Prediction

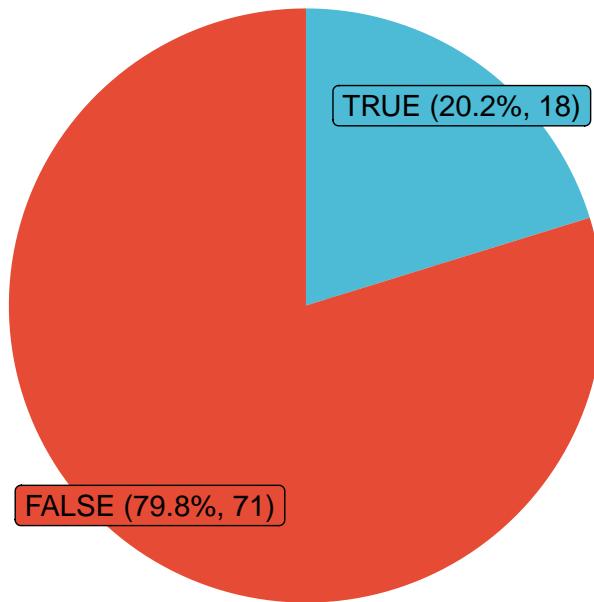


Figure 6: HDS HOB 20 prediction

以 Super-Pred 预测更多的靶点：

Table 7 (下方表格) 为表格 HDS compounds targets predicted by Super Pred 概览。

(对应文件为 [Figure+Table/HDS-compounds-targets-predicted-by-Super-Pred.xlsx](#))

注：表格共有 2050 行 9 列，以下预览的表格可能省略部分数据；表格含有 18 个唯一 ‘id’。

Table 7: HDS compounds targets predicted by Super Pred

.id	Target...	ChEMBL-ID	UniPro...	PDB Vi...	TTD ID	Probab...	Model ...	symbols
CC1=CC...	Bloom ...	CHEMBL...	P54132	4O3M	Not Av...	98.7%	70.06%	BLM
CC1=CC...	Tyrosy...	CHEMBL...	Q9NUW8	6N0D	Not Av...	97.89%	71.22%	TDP1
CC1=CC...	Nuclea...	CHEMBL...	P19838	1SVC	Not Av...	97.37%	96.09%	NFKB1
CC1=CC...	DNA-(a...	CHEMBL...	P27695	6BOW	T13348	93.58%	91.11%	APEX1
CC1=CC...	Cannab...	CHEMBL253	P34972	6KPF	Not Av...	91.48%	97.25%	CNR2
CC1=CC...	Cathep...	CHEMBL...	P07339	4OD9	T67102	91.07%	98.95%	CTSD
CC1=CC...	Protei...	CHEMBL...	Q05655	1YRK	T44861	88.96%	97.79%	PRKCD
CC1=CC...	Dual s...	CHEMBL...	Q9HAZ1	6FYV	Not Av...	88.61%	94.45%	CLK4
CC1=CC...	Kruppe...	CHEMBL...	Q13887	Not Av...	Not Av...	85.83%	86.33%	KLF5
CC1=CC...	Glutam...	CHEMBL...	P42262	2WJW	T42392	82.94%	86.92%	GRIA2
CC1=CC...	Transc...	CHEMBL...	O15164	4YBM	Not Av...	82.59%	95.56%	TRIM24
CC1=CC...	DNA to...	CHEMBL...	P11388	6ZY5	T17048	82.58%	89%	TOP2A

.id	Target...	ChEMBL-ID	UniPro...	PDB Vi...	TTD ID	Probab...	Model ...	symbols
CC1=CC...	Cytoch...	CHEMBL340	P08684	5VCC	T37848	82.47%	91.19%	CYP3A4
CC1=CC...	Minera...	CHEMBL...	P08235	4PF3	Not Av...	82.02%	100%	NR3C2
CC1=CC...	Muscar...	CHEMBL...	P08912	6OL9	T79961	81.06%	94.62%	CHRM5
...

合并了预测的靶点后的数据：

Figure 7 (下方图) 为图 HDS network pharmacology visualization 概览。

(对应文件为 Figure+Table/HDS-network-pharmacology-visualization.pdf)

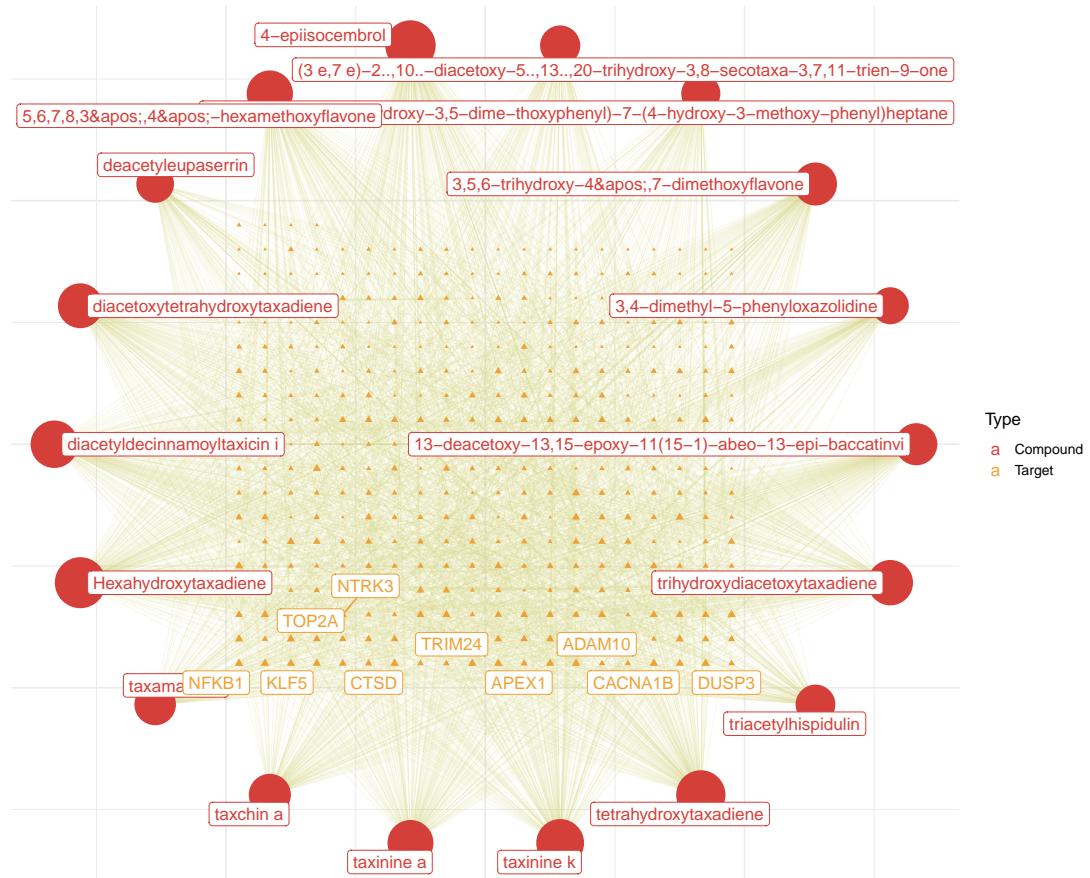


Figure 7: HDS network pharmacology visualization

Table 8 (下方表格) 为表格 HDS Herbs compounds and targets 概览。

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

注：表格共有 2139 行 7 列，以下预览的表格可能省略部分数据；表格含有 105 个唯一‘Ingredient.id’。

Table 8: HDS Herbs compounds and targets

Ingredient.id	Herb_pinyi...	Ingredient.....3	Ingredient.....4	Target.id	Target.nameDatabase.s...	...
HBIN000081	HONG DOU SHAN	10-deacety...	NA	NA	NA	NA
HBIN000084	HONG DOU SHAN	10-deacety...	NA	NA	NA	NA
HBIN001104	HONG DOU SHAN	1,3,7,8-te...	1,3,7,8-te...	NA	NA	NA
HBIN001125	HONG DOU SHAN	13-acetyl...	NA	NA	NA	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	NFKB1	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	KLF5	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	TDP1	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	RORB	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	PTGS1	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	NPC1	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	CTSD	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	CHRM5	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	MAOA	NA

Ingredient.id	Herb_pinyi...	Ingredient.....3	Ingredient.....4	Target.id	Target.nameDatabase.s...	...
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	TRIM24	NA
HBIN001159	HONG DOU SHAN	13-deaceto...	NA	NA	APEX1	NA
...

6.1.3 养阴解毒汤和红豆杉共同靶点 coSig

Figure 8 (下方图) 为图 Intersected targets of YYJD and HDS 概览。

(对应文件为 Figure+Table/Intersected-targets-of-YYJD-and-HDS.pdf)

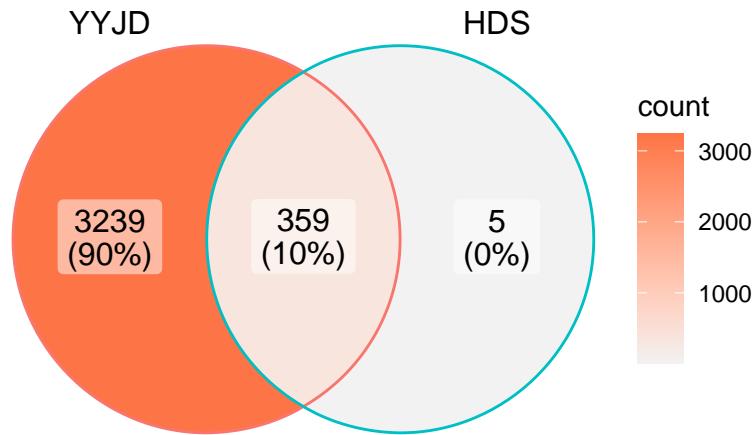


Figure 8: Intersected targets of YYJD and HDS

Intersection :

APEX1, NFKB1, KDM1A, HTR2C, HIF1A, TRIM24, BLM, SLC6A5, GPR55, CTSD, KLF5, PRCP, C5AR1, THRA, PSMB1, HSD17B10, TOP2A, GUSB, NTRK3, NFE2L2, GRIA2, HDAC8, SLC2A1, NR1I2, CACNA1B, ALOX12, PRKCZ, CYP3A4, DUSP3, KIF11, CLK4, GRIN1, KCNA5, ADAM10, SCD, PDE3A, CCR1, HDAC9, DPP8, TTR, SLC9A1, GLS, S1PR5,...

(上述信息框内容已保存至 Figure+Table/Intersected-targets-of-YYJD-and-HDS-content)

6.2 铁死亡

6.2.1 FerrDb V2 基因集

‘Ferroptosis regulators’ 数据已全部提供。

(对应文件为 Figure+Table/Ferroptosis-regulators)

注：文件夹 Figure+Table/Ferroptosis-regulators 共包含 4 个文件。

1. 1_marker.csv
2. 2_driver.csv
3. 3_suppressor.csv
4. 4_uncharger.csv

6.2.2 Ferroptosis Driver 与 coSig 交集

Figure 9 (下方图) 为图 The common Targets related to ferroptosis driver 概览。

(对应文件为 Figure+Table/The-common-Targets-related-to-ferroptosis-driver.pdf)

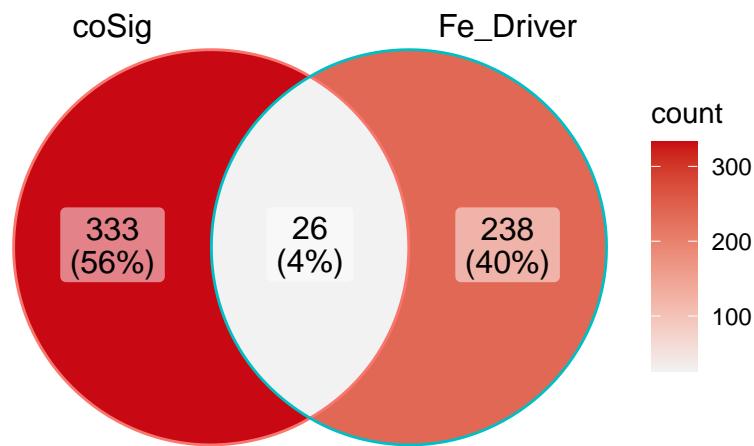


Figure 9: The common Targets related to ferroptosis driver

Intersection :

HIF1A, ALOX12, NOX1, MDM4, TLR4, KEAP1, ABCC1, IDO1, PRKAA1, MAP3K11, KDM5C, KDM5A, MAPK1, PIK3CA, STING1, MAP3K14, TBK1, ALOX5, PPARG, PRKCA, CTSB, DPP4, GSK3B, MAPK14, SIRT1, FLT3

(上述信息框内容已保存至 Figure+Table/The-common-Targets-related-to-ferroptosis-driver-content)

6.3 肺癌

6.3.1 肺癌相关基因集

GeneCards Score > 3

Table 9 (下方表格) 为表格 Lung cancer GeneCards used data 概览。

(对应文件为 Figure+Table/Lung-cancer-GeneCards-used-data.xlsx)

注：表格共有 945 行 7 列，以下预览的表格可能省略部分数据；表格含有 945 个唯一‘Symbol’。

Table 9: Lung cancer GeneCards used data

Symbol	Description	Category	UniProt_ID	GIFtS	GC_id	Score
KRAS	KRAS Proto...	Protein Co...	P01116	61	GC12M028437	74.63
BRAF	B-Raf Prot...	Protein Co...	P15056	62	GC07M140762	73.07
EGFR-AS1	EGFR Antis...	RNA Gene		23	GC07M055179	64.72
PIK3CA	Phosphatid...	Protein Co...	P42336	61	GC03P179148	63.70
ALK	ALK Recept...	Protein Co...	Q9UM73	59	GC02M029190	61.05
ERBB2	Erb-B2 Rec...	Protein Co...	P04626	63	GC17P039687	61.00
CDKN2A	Cyclin Dep...	Protein Co...	Q8N726	60	GC09M021967	58.81
CTNNB1	Catenin Be...	Protein Co...	P35222	62	GC03P041194	58.62
MYC	MYC Proto...	Protein Co...	P01106	61	GC08P127735	52.43
LUCAT1	Lung Cance...	RNA Gene		23	GC05M091054	52.39
AKT1	AKT Serine...	Protein Co...	P31749	62	GC14M104769	52.22
HRAS	HRas Proto...	Protein Co...	P01112	61	GC11M010201	51.36
PTEN	Phosphatas...	Protein Co...	P60484	60	GC10P106636	50.58
ERCC6	ERCC Excis...	Protein Co...	Q03468	55	GC10M049454	50.54
STK11	Serine/Thr...	Protein Co...	Q15831	59	GC19P001177	50.19
...

6.3.2 coSig-ferroptosis 与肺癌交集

Figure 10 (下方图) 为图 Intersection of coSigFe genes with Lung cancer signatures 概览。

(对应文件为 Figure+Table/Intersection-of-coSigFe-genes-with-Lung-cancer-signatures.pdf)

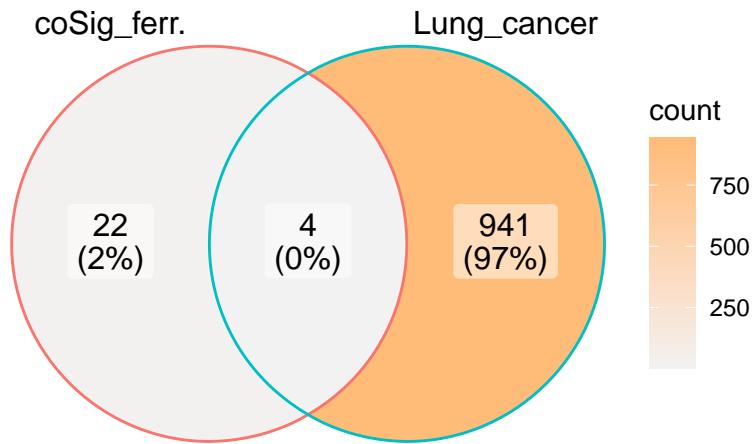


Figure 10: Intersection of coSigFe genes with Lung cancer signatures

Intersection :

IDO1, PRKAA1, PIK3CA, ALOX5

(上述信息框内容已保存至 [Figure+Table/Intersection-of-coSigFe-genes-with-Lung-cancer-signatures-content](#))

6.4 m6A 相关

6.4.1 N6-Methyladenosine 基因集

GeneCards Score > 1

Table 10 (下方表格) 为表格 M6A GeneCards used data 概览。

(对应文件为 [Figure+Table/M6A-GeneCards-used-data.xlsx](#))

注：表格共有 1460 行 7 列，以下预览的表格可能省略部分数据；表格含有 1460 个唯一‘Symbol’。

Table 10: M6A GeneCards used data

Symbol	Description	Category	UniProt_ID	GIFtS	GC_id	Score
YTHDF2	YTH N6-Met...	Protein Co...	Q9Y5A9	45	GC01P034802	46.37
YTHDF1	YTH N6-Met...	Protein Co...	Q9BYJ9	44	GC20M063195	41.09
YTHDF3	YTH N6-Met...	Protein Co...	Q7Z739	43	GC08P063168	40.02
YTHDC1	YTH N6-Met...	Protein Co...	Q96MU7	46	GC04M068310	37.59
YTHDC2	YTH N6-Met...	Protein Co...	Q9H6S0	44	GC05P113513	37.19
METTL3	Methyltran...	Protein Co...	Q86U44	50	GC14M021498	22.54
METTL14	Methyltran...	Protein Co...	Q9HCE5	46	GC04P118685	13.41
VIRMA	Vir Like M...	Protein Co...	Q69YN4	41	GC08M094496	11.79

Symbol	Description	Category	UniProt_ID	GIFtS	GC_id	Score
XIST	X Inactive...	RNA Gene		30	GC0XM073820	11.78
METTL16	Methyltran...	Protein Co...	Q86W50	41	GC17M002405	10.84
ZC3H13	Zinc Finge...	Protein Co...	Q5T200	39	GC13M045954	10.16
ALKBH5	AlkB Homol...	Protein Co...	Q6P6C2	43	GC17P018183	9.99
FTO	FTO Alpha-...	Protein Co...	Q9C0B1	55	GC16P067676	9.67
IGF2BP2	Insulin Li...	Protein Co...	Q9Y6M1	53	GC03M185643	9.60
WTAP	WT1 Associ...	Protein Co...	Q15007	45	GC06P159725	9.31
...

6.4.2 coSig-ferroptosis-cancer 与 m6A 相关

Figure 11 (下方图) 为图 m6A related of alls 概览。

(对应文件为 Figure+Table/m6A-related-of-all.pdf)

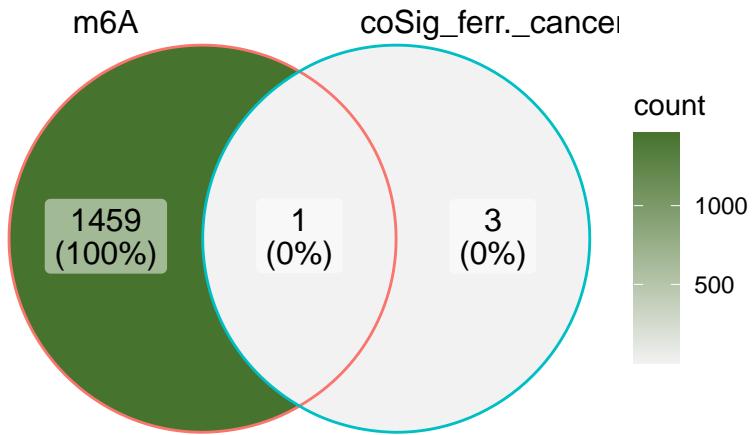


Figure 11: M6A related of alls

Intersection :

PRKAA1

(上述信息框内容已保存至 Figure+Table/m6A-related-of-all-content)

6.5 汇总

Figure 12 (下方图) 为图 All intersection 概览。

(对应文件为 Figure+Table/All-intersection.pdf)

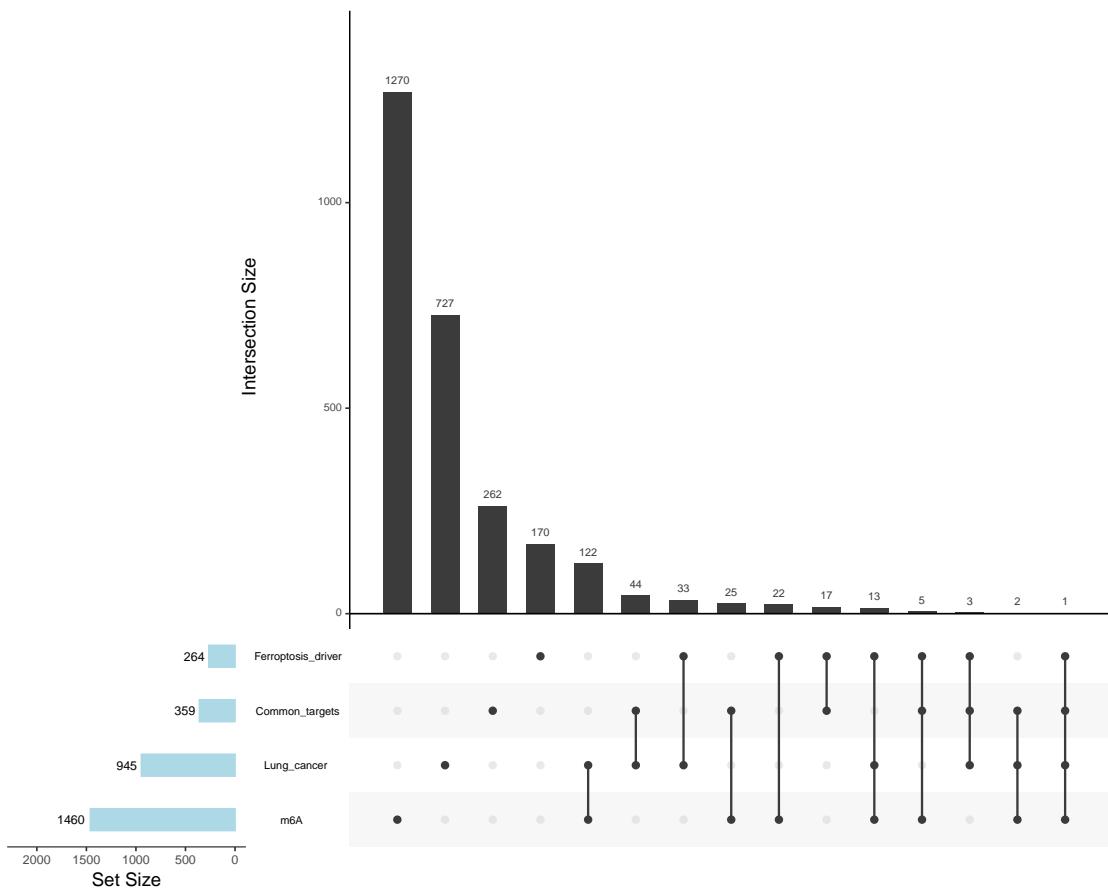


Figure 12: All intersection

All_intersection :

PRKAA1

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

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