

白茅根-IgA 网络药理学分析

2023-12-08

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1 摘要

- 白茅根绘制活性成分-靶点图。
 - 结果见 Fig. 1
- 靶点与 IgA 肾病差异基因 Venn 图。
 - 结果见 Fig. 2

2 材料和方法

2.1 方法

Mainly used method:

- GEO <https://www.ncbi.nlm.nih.gov/geo/> used for expression dataset acquisition .
- Website HERB <http://herb.ac.cn/> used for data source.¹
- Limma and edgeR used for differential expression analysis.^{2,3}
- Other R packages (eg., dplyr and ggplot2) used for statistic analysis or data visualization.

3 分析结果

4 结论

5 附：分析流程

5.1 白茅根网络药理学分析

5.1.1 成分

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

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

注：表格共有 1 行 18 列，以下预览的表格可能省略部分数据；表格含有 1 个唯一 ‘Herb_’。

Table 1: Herbs information

Herb_	Herb_...	Herb_...	Herb_...	Herb_...	Prope...	Merid...	UsePart	Function	Indic...
HERB0...	BAI M...	白茅根	Lalan...	Rhizo...	Sweet...	Lung;...	NA	To ar...	1. It...

Table 2 (下方表格) 为表格 Components of Herbs 概览。

(对应文件为 `Figure+Table/Components-of-Herbs.xlsx`)

注：表格共有 89 行 4 列，以下预览的表格可能省略部分数据；表格含有 89 个唯一‘Ingredient.name’。

Table 2: Components of Herbs

herb_id	Ingre.....2	Ingre.....3	Ingre.....4
HERB0...	HBIN0...	1-mon...	Glyce...
HERB0...	HBIN0...	20,23...	NA
HERB0...	HBIN0...	2,3-b...	(2R,3...
HERB0...	HBIN0...	23-hy...	NA
HERB0...	HBIN0...	23-hy...	NA
HERB0...	HBIN0...	3beta...	3beta...
HERB0...	HBIN0...	3 ,23...	NA
HERB0...	HBIN0...	3 ,23...	NA
HERB0...	HBIN0...	3 -ac...	3 -ac...
HERB0...	HBIN0...	3-O-a...	3-o-a...
HERB0...	HBIN0...	3-o- ...	3-o- ...
HERB0...	HBIN0...	3-oxo...	NA
HERB0...	HBIN0...	4,5-D...	AIDS0...
HERB0...	HBIN0...	4-Met...	AI3-2...
HERB0...	HBIN0...	5alph...	5 ,9 ...
...

5.1.2 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 1593 行 9 列，以下预览的表格可能省略部分数据；表格含有 89 个唯一‘Ingredient.id’。

Table 3: Tables of Herbs compounds and targets

Ingre.....1	Herb_...	Ingre.....3	Ingre.....4	Targe.....5	Targe.....6	Datab...	Paper.id	...
HBIN0...	BAI M...	1-mon...	Glyce...	HBTAR...	PTGS1	NA	NA	...
HBIN0...	BAI M...	1-mon...	Glyce...	HBTAR...	PPARG	NA	NA	...
HBIN0...	BAI M...	1-mon...	Glyce...	HBTAR...	PTGS1	NA	NA	...
HBIN0...	BAI M...	1-mon...	Glyce...	HBTAR...	PPARG	NA	NA	...
HBIN0...	BAI M...	1-mon...	Glyce...	HBTAR...	PTGS1	NA	NA	...
HBIN0...	BAI M...	1-mon...	Glyce...	HBTAR...	PPARG	NA	NA	...
HBIN0...	BAI M...	20,23...	NA	NA	NA	NA	NA	...

Ingre.....1	Herb_...	Ingre.....3	Ingre.....4	Targe.....5	Targe.....6	Datab...	Paper.id	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	ANPEP	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	CDC34	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	COMT	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	ENPEP	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	GRK6	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	UBE2K	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	LNPEP	NA	NA	...
HBIN0...	BAI M...	2,3-b...	(2R,3...	HBTAR...	LTA4H	NA	NA	...
...

Figure 1 (下方图) 为图 BaiMaoGen network pharmacology visualization 概览。

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

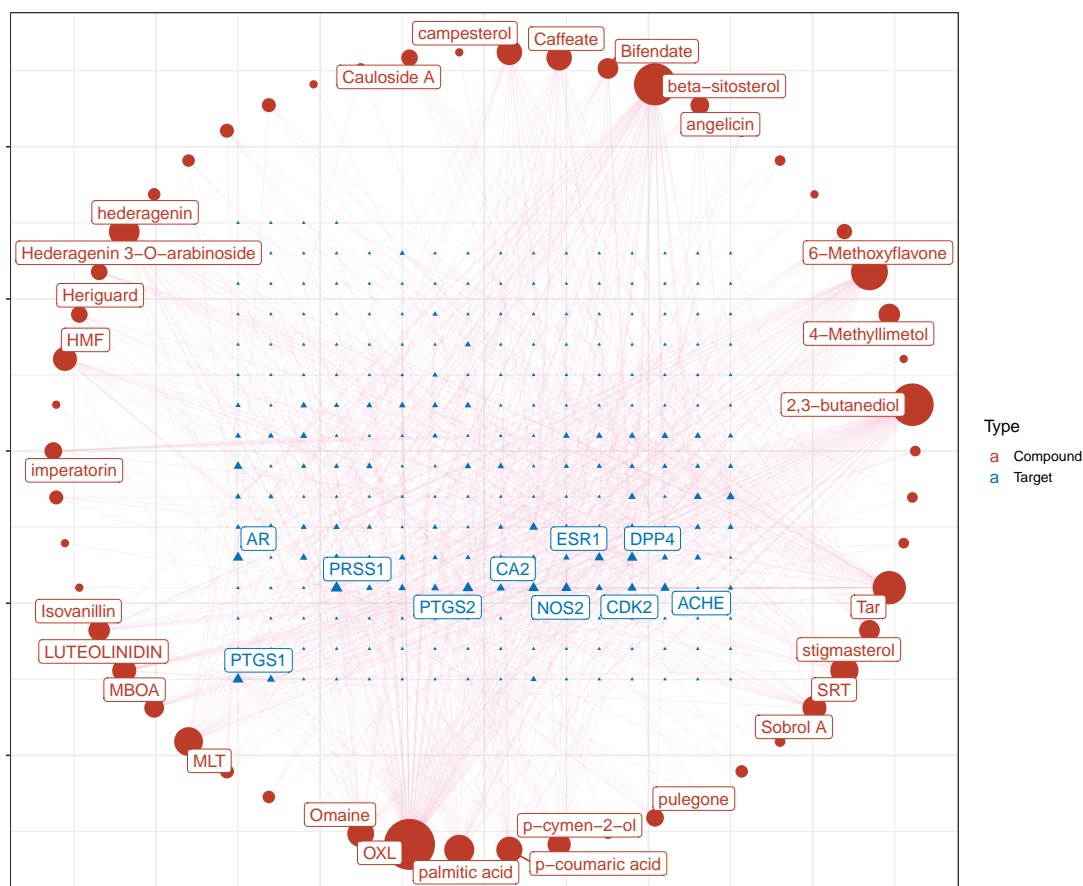


Figure 1: BaiMaoGen network pharmacology visualization

5.2 IgA 肾炎 (IgA Nephropathy) 差异基因

Table 4 (下方表格) 为表格 metadata of used samples 概览。

(对应文件为 Figure+Table/metadata-of-used-samples.csv)

注：表格共有 65 行 9 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 4: Metadata of used samples

rownames	group	lib.size	norm....	sample	title	estim...	techn...	tissu...
GSM53...	IgAN	40893...	1.057...	GSM53...	IgAN_...	76.6	No	Kidne...
GSM53...	IgAN	49316...	1.331...	GSM53...	IgAN_...	68.8	No	Kidne...
GSM53...	IgAN	35208...	1.009...	GSM53...	IgAN_...	70.5	No	Kidne...
GSM53...	IgAN	41500...	1.271...	GSM53...	IgAN_...	46.8	No	Kidne...
GSM53...	IgAN	50748...	1.286...	GSM53...	IgAN_...	63.0	No	Kidne...
GSM53...	IgAN	43491...	1.145...	GSM53...	IgAN_...	114.8	No	Kidne...
GSM53...	IgAN	31920...	0.885...	GSM53...	IgAN_...	77.0	No	Kidne...
GSM53...	IgAN	29243...	0.877...	GSM53...	IgAN_...	81.1	No	Kidne...
GSM53...	IgAN	33622...	0.941...	GSM53...	IgAN_...	70.5	No	Kidne...
GSM53...	IgAN	33555...	0.986...	GSM53...	IgAN_...	67.1	No	Kidne...
GSM53...	IgAN	33784...	1.044...	GSM53...	IgAN_...	77.7	No	Kidne...
GSM53...	IgAN	40344...	1.195...	GSM53...	IgAN_...	64.6	No	Kidne...
GSM53...	IgAN	59431...	1.175...	GSM53...	IgAN_...	74.8	No	Kidne...
GSM53...	IgAN	41323...	1.121...	GSM53...	IgAN_...	68.3	No	Kidne...
GSM53...	IgAN	35019...	0.890...	GSM53...	IgAN_...	104.5	No	Kidne...
...

Table 5 (下方表格) 为表格 tables of DEGs 概览。

(对应文件为 Figure+Table/tables-of-DEGs.xlsx)

注：表格共有 4526 行 15 列，以下预览的表格可能省略部分数据；表格含有 4526 个唯一 ‘rownames’。

Table 5: Tables of DEGs

rownames	ensem...	hgnc_...	entre...	refse...	chrom...	start...	end_p...	descr...	logFC
5045	ENSG0...	DUSP1	1843	NM_00...	5	17276...	17277...	dual ...	-3.87...
12927	ENSG0...	FOS	2353	NM_00...	14	75278826	75282230	Fos p...	-5.85...
8356	ENSG0...	CCN1	3491	NM_00...	1	85580761	85584589	cellu...	-2.40...
5412	ENSG0...	NR4A1	3164		12	52022832	52059507	nucle...	-4.27...
5129	ENSG0...	EGR1	1958	NM_00...	5	13846...	13846...	early...	-4.07...
6021	ENSG0...	ZFP36	7538	NM_00...	19	39406847	39409412	ZFP36...	-2.51...
4348	ENSG0...	CISH	1154		3	50606489	50611774	cytok...	-1.71...
14506	ENSG0...	JUN	3725		1	58776845	58784048	Jun p...	-2.19...

rownames	ensem...	hgnc_...	entre...	refse...	chrom...	start...	end_p...	descr...	logFC
8271	ENSG0...	SIK1	150094	NM_17...	21	43414483	43427131	salt ...	-2.04...
3578	ENSG0...	RASD1	51655	NM_01...	17	17494437	17496395	ras r...	-2.89...
10442	ENSG0...	BTG2	7832		1	20330...	20330...	BTG a...	-1.99...
7869	ENSG0...	DUSP6	1848	NM_00...	12	89347235	89352501	dual ...	-1.24...
20500	ENSG0...	PPP1R10	5514	NM_00...	6	30600413	30618612	prote...	-0.64...
9152	ENSG0...	SLC25A25	114789	NM_00...	9	12806...	12810...	solut...	-1.13...
10648	ENSG0...	IER2	9592	NM_00...	19	13150411	13154911	immed...	-1.63...
...

5.3 白茅根靶点和 IgA 肾病差异基因的交集

去除缺失数据后，交集为：

Figure 2 (下方图) 为图 intersection venn plot 概览。

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

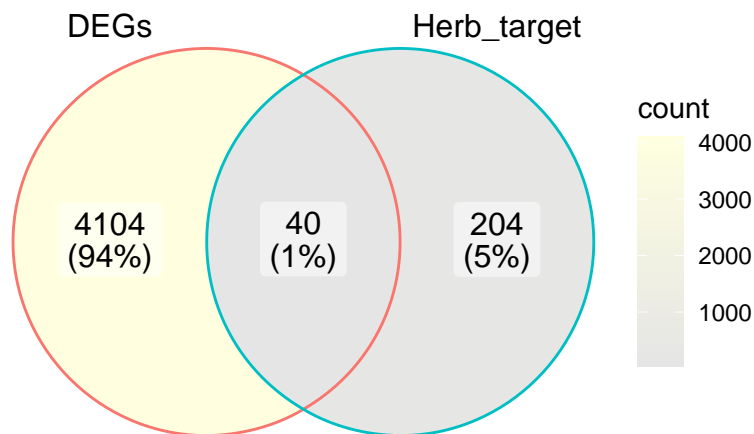


Figure 2: Intersection venn plot

intersection :

JUN, ADRA2A, ESR2, TNF, NFKB1, GOT2, PRKCB, CHRM1, CCNA2, PTGS2, AR, CA2, IGHG1, TLR8, CASP9, TOP3B, COL1A1, TOP2A, TPI1, LYZ, PGR, CTSD, LTF, ADRB1, NR3C1, ALOX5, COMTD1, NOS2, ADRA1B, PDE3A, SLC6A4, TRPV3, ALDH4A1, PYGL, PYGM, TRPM2, UBE2S, ADRB2, TLR4, CDC34

Reference

1. Fang, S. *et al.* HERB: A high-throughput experiment- and reference-guided database of traditional chinese medicine. *Nucleic Acids Research* **49**, D1197–D1206 (2021).
2. Ritchie, M. E. *et al.* Limma powers differential expression analyses for rna-sequencing and microarray studies. *Nucleic Acids Research* **43**, e47 (2015).
3. Chen, Y., McCarthy, D., Ritchie, M., Robinson, M. & Smyth, G. EdgeR: Differential analysis of sequence read count data user’s guide. 119.