

中药复方乌梅丸网络药理学分析

2024-04-01

LiChuang Huang



@ 立效研究院

Contents

1 摘要	1
1.1 需求	1
1.2 结果	1
2 前言	2
3 材料和方法	2
3.1 材料	2
3.2 方法	2
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	5
6.1.5 富集分析	7
6.1.5.1 与肠道炎症相关的通路和基因	8
6.1.6 与疾病相关的活性成分筛选	9
6.1.6.1 PubMed 文献报道数 (任意领域)	9
6.1.6.2 CTD 数据库记录与肾炎相关的化合物	11
6.2 分子对接	12
6.2.1 Top docking	12
6.2.2 对接可视化	14
6.2.3 局部对接细节	17
6.2.4 Top1 的靶点的富集分析 (参与 hsa05321 靶点)	20
6.2.4.1 TOP1 的结合靶点 (IL1B) 参与的通路	23
Reference	25

List of Figures

1 Intersection of all compounds	3
2 Overall targets number of datasets	4
3 Network pharmacology with disease	6
4 Targets intersect with targets of diseases	6
5 HERBS KEGG enrichment	7

6	HERBS GO enrichment	8
7	HERBS hsa05321 visualization	9
8	Intersection of CTD records with herbs of hsa05321 related	11
9	Overall combining Affinity	13
10	Docking 72326 into 9ilb	15
11	Docking 969516 into 4xfu	16
12	Docking 774 into nod2	17
13	Docking 72326 into 9ilb detail	18
14	Docking 969516 into 4xfu detail	19
15	Docking 774 into nod2 detail	20
16	TOP KEGG enrichment	21
17	TOP GO enrichment	21
18	TOP hsa05321 visualization	22
19	TOP pharmacology visualization	23

List of Tables

1	Herbs information	3
2	Tables of Herbs compounds and targets	4
3	GeneCards used data	5
4	All compounds Literature Count	10
5	Hsa05321 related genes and compounds	10
6	Intersection Herbs compounds and targets	12
7	Combining Affinity	14
8	Metadata of visualized Docking	14
9	IL1B kegg	24
10	IL1B go	24

1 摘要

1.1 需求

中药复方乌梅丸：乌梅，花椒，细辛，黄连，黄柏，干姜，附子，桂枝，人参，当归

疾病：慢性结肠炎，炎性肠病，肠纤维化，可以都包含，也可以单独一种疾病（如果单独疾病可以做出来，优先级按照语序来）

目标：筛选出有效成分 XX，及其作用靶点蛋白 YY，YY 需满足：1、与 XX 能对接 2、富集分析显示 YY 与疾病相关的机制相关（比如炎症，纤维化，再放宽可以免疫细胞调控）

其它：

1、选取中药复方（乌梅丸）中和调控纤维化相关的单体成分，结合 pubchem、chemical book、scifinder 等数据库分析排名靠前的化合物的活性信息，并通过中医网络药理学方法（如 TCMSP 平台和 BATMAN-TCM 数据库），分析有效成分 XXX 的对应靶点 YYY，功能富集分析显示 YYY 调控肠道纤维化。

2.、通过 PubChem 数据库获取中药单体主要活性成分的 2D 化学结构，在 PDB 数据库中查找相关核心靶点蛋白 3D 结构，通过 Autodock 软件进行分子对接，获取结合能最高的位点，最后通过 Pymol 软件进行可视化处理。

交付：

1. 疾病-复方-成分-靶点网络图
2. 成分 XX-靶点网络图
3. XX 与 YY 分子对接 pymol 可视化图，注意细节标注
4. 成分 XX 靶点功能富集分析
5. 总的复方靶点的功能富集分析
6. YY 可能参与的环节需要标注在 4 上或者单独注释分

1.2 结果

1. 利用 BATMAN-TCM 数据库作为成分靶点数据库，并结合 Fig. 2 所示的疾病靶点数据获得的疾病-复方-成分-靶点网络图见 Fig. 3
2. 筛选的成分的靶点关系图见 Fig. 19。这里的成分是后续的分析和分子对接筛选的 TOP 1，其名称等相关信息 (TOP 1-3) 可参考 Tab. 8
3. Pymol 可视化见 Fig. 13 (局部放大加注释), Fig. 10 (全局图)。此外，对接 TOP 2 和 TOP 3 的可视化也附在随后。
4. TOP 1 成分的富集分析见 Fig. 16 和 Fig. 17
5. 总的复方靶点的富集分析见 Fig. 5 和 Fig. 6
6. YY (TOP 1 对应的结合靶点为 IL1B) 参与的环节见 Fig. 18

补充说明：

- TCMSP 网站最近几日都无法打开，所以草药数据来源只选用 BATMAN (这个数据库比 TCMSP 全面)。

- 关于“结合 pubchem、chemical book、scifinder 等数据库分析排名靠前的化合物的活性信息”，chemical book 和 scifinder 为商业工具，预计是无法获取权限的，这里没有使用；而 PubChem，我这里的分析中获取了成分的文献记录，即 LiteratureCount，具体可见 Tab. 4，Tab. 5。此外，还根据 CTD 对疾病相关的成分做了筛选，Fig. 8
- 其它候选成分靶点 Tab. 6
- 分子对接良好的结果汇总表格 Tab. 7

2 前言

3 材料和方法

3.1 材料

3.2 方法

Mainly used method:

- Database BATMAN-TCM was used as source data of TCM ingredients and target proteins¹.
- The Comparative Toxicogenomics Database (CTD) used for finding relationship between chemicals and disease².
- R package `ClusterProfiler` used for gene enrichment analysis³.
- Databases of DisGeNet, GeneCards, PharmGKB used for collating disease related targets⁴⁻⁶.
- The CLI tools of AutoDock vina and ADFR software used for auto molecular docking⁷⁻¹¹.
- R version 4.3.2 (2023-10-31); 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.xlsx)

注：表格共有 10 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‘Pinyin.Name’。

Table 1: Herbs information

Pinyin.Name	Chinese.Name	English.Name	Latin.Name
FU ZI	附子	Prepared common m...	Aconitum carmichaeli
GAN JIANG	干姜	Common ginger dri...	Zingiber officinale
DANG GUI	当归	Chinese angelica ...	Angelica sinensis
REN SHEN	人参	Ginseng	Panax ginseng [s...
XI XIN	细辛	Siebold wildginge...	Asarum sieboldii
GUI ZHI	桂枝	Cassia barktree twig	Cinnamomum cassia...
HUA JIAO	花椒	Bunge pricklyash ...	Zanthoxylum bunge...
WU MEI	乌梅	Japanese apricot	Prunus mume
HUANG LIAN	黄连	Chinese goldthrea...	Coptis chinensis
HUANG BAI	黄柏	Amur corktree equ...	Phellodendron amu...

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](#))

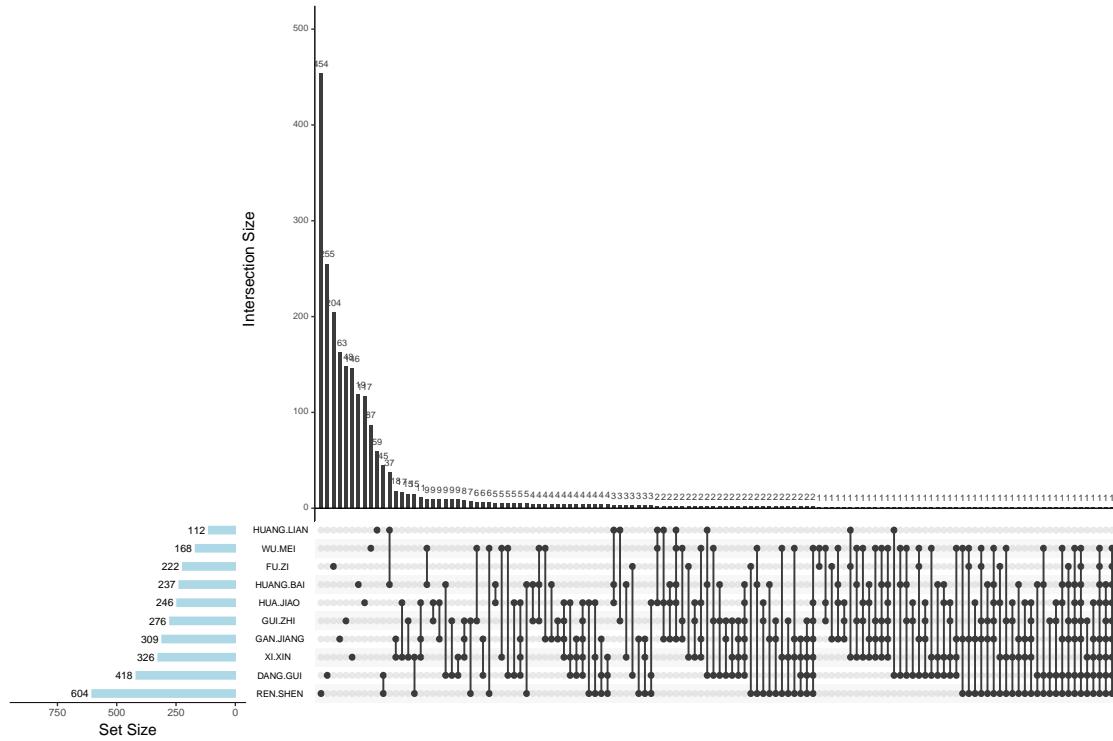


Figure 1: Intersection of all compounds

All_intersection :

(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 2 (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 15264 行 3 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_pinyin_name’。

Table 2: Tables of Herbs compounds and targets

Herb_pinyin_name	Ingredient.name	Target.name
GUI ZHI	3,4-dihydroxybenzoic acid	AKT1
GUI ZHI	3,4-dihydroxybenzoic acid	MGAM
GUI ZHI	[5-(6-aminopurin-9-yl)-4-hy...	NA
GUI ZHI	3-hydroxybenzaldehyde	NA
GUI ZHI	3-phenylpropanoic acid	NA
GUI ZHI	4-hydroxybenzoic acid	HDAC6
GUI ZHI	acetaldehyde	HDAC11
GUI ZHI	acetaldehyde	MMP2
GUI ZHI	acetaldehyde	CDT1
GUI ZHI	acetaldehyde	CAT
GUI ZHI	acetaldehyde	MMP1
GUI ZHI	acetaldehyde	PPARG
GUI ZHI	acetaldehyde	TIMP1
GUI ZHI	acetaldehyde	AGT
GUI ZHI	acetaldehyde	IL1B
...

6.1.3 疾病靶点

Figure 2 (下方图) 为图 Overall targets number of datasets 概览。

(对应文件为 Figure+Table/Overall-targets-number-of-datasets.pdf)

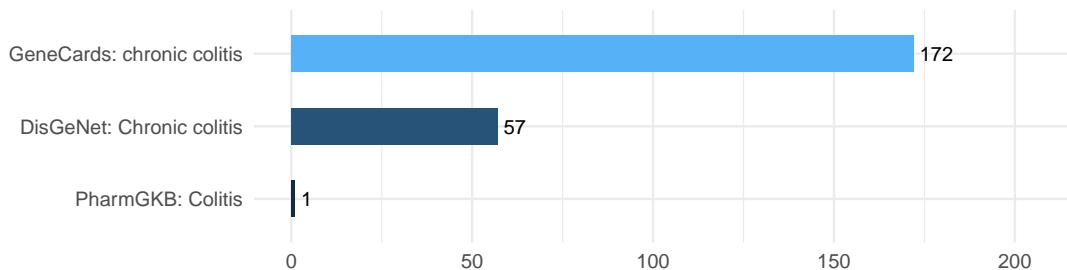


Figure 2: Overall targets number of datasets

The GeneCards data was obtained by querying :

chronic colitis

Restrict (with quotes) :

TRUE

Filtering by Score: :

Score > 0

Table 3 (下方表格) 为表格 GeneCards used data 概览。

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

注：表格共有 172 行 7 列，以下预览的表格可能省略部分数据；表格含有 172 个唯一‘Symbol’。

Table 3: GeneCards used data

Symbol	Description	Category	UniProt_ID	GIFTs	GC_id	Score
CARMIL2	Capping Pr...	Protein Co...	Q6F5E8	43	GC16P067644	3
WAS	WASP Actin...	Protein Co...	P42768	56	GC0XP048676	2.13
IL37	Interleuki...	Protein Co...	Q9NZH6	48	GC02P141239	2.04
LINC02605	Long Inter...	RNA Gene		19	GC08P078838	2.04
TNFSF15	TNF Superf...	Protein Co...	O95150	52	GC09M114784	1.96
LINC01672	Long Inter...	RNA Gene		18	GC01P011469	1.96
STAT3	Signal Tra...	Protein Co...	P40763	62	GC17M042313	1.91
BDNF-AS	BDNF Antis...	RNA Gene		28	GC11P027466	1.91
CERNA3	Competing ...	RNA Gene		19	GC08P056101	1.8
NOS2	Nitric Oxi...	Protein Co...	P35228	58	GC17M027756	1.73
IL17A	Interleuki...	Protein Co...	Q16552	52	GC06P052186	1.69
IFNG	Interferon...	Protein Co...	P01579	59	GC12M068154	1.49
IL23A	Interleuki...	Protein Co...	Q9NP7	48	GC12P059649	1.44
MPO	Myeloperox...	Protein Co...	P05164	61	GC17M058269	1.38
IL7R	Interleuki...	Protein Co...	P16871	55	GC05P035852	1.38
...

6.1.4 疾病-成分-靶点

Figure 3 (下方图) 为图 Network pharmacology with disease 概览。

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

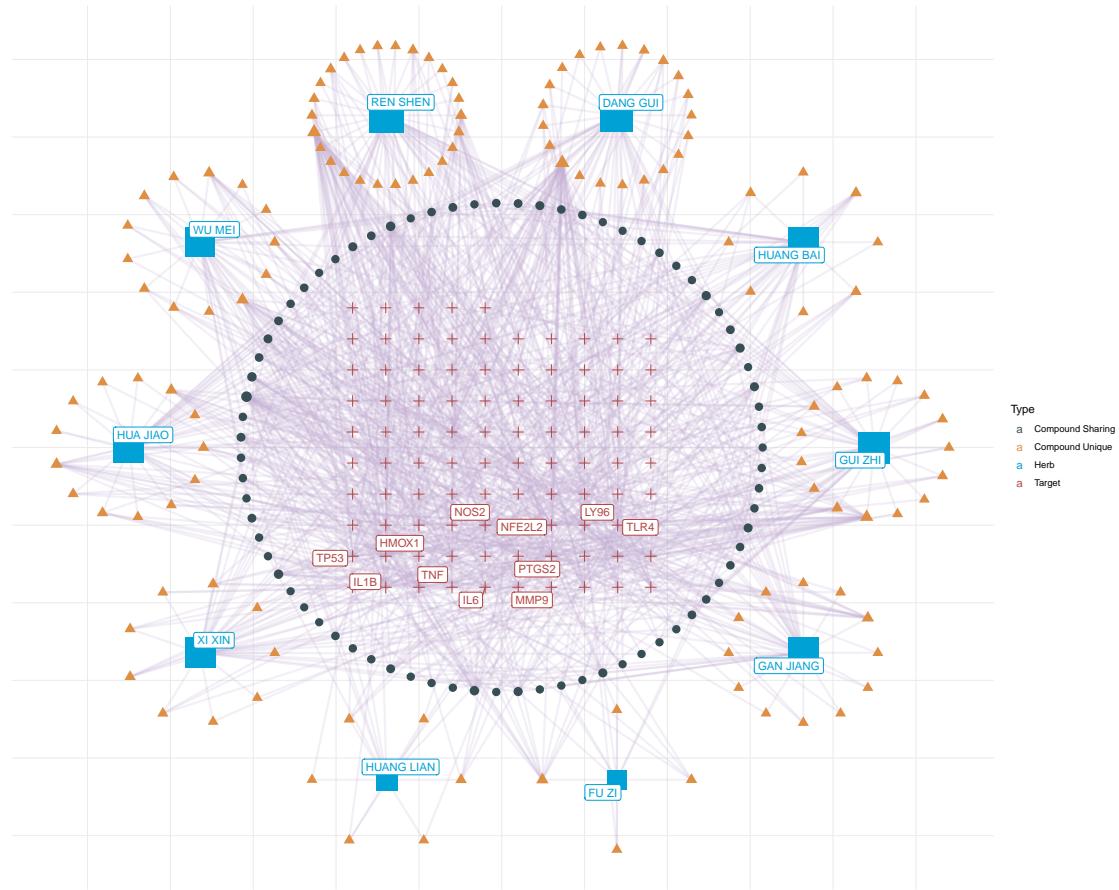


Figure 3: Network pharmacology with disease

Figure 4 (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)

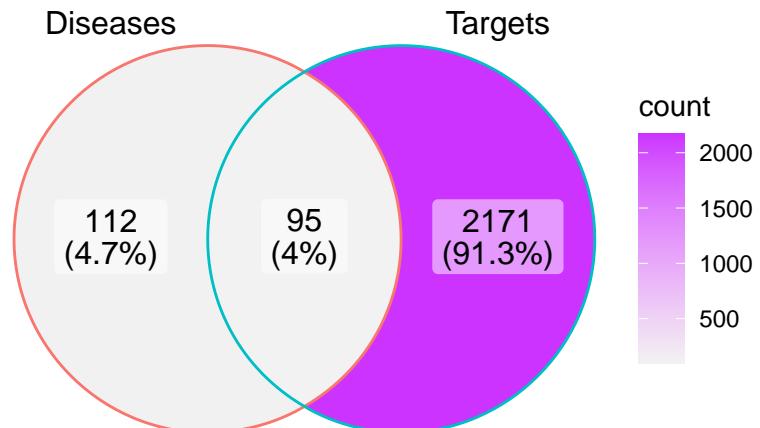


Figure 4: Targets intersect with targets of diseases

Intersection :

IL10, TNF, IL7, ACAD8, IL1B, NLRP3, PRKAB1, PRKAA1, TACR1, SLC7A2, PRKAA2, AKR1B10, NOD2, TLR4, CD44, DCLK1, IL33, TP53, PON1, LY96, SIRT1, ESR2, NR0B1, AGER, CSF3, GABPA, NFE2L2, MUC2, MMP9, MIF, IL17A, CXCL8, PIAS3, STAT3, NOS2, IFNG, MPO, EGF, IL6, VCAM1, MIR18A, TCF4, MST1, MIR155, CA4, EGFR,...

(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 5 (下方图) 为图 HERBS KEGG enrichment 概览。

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

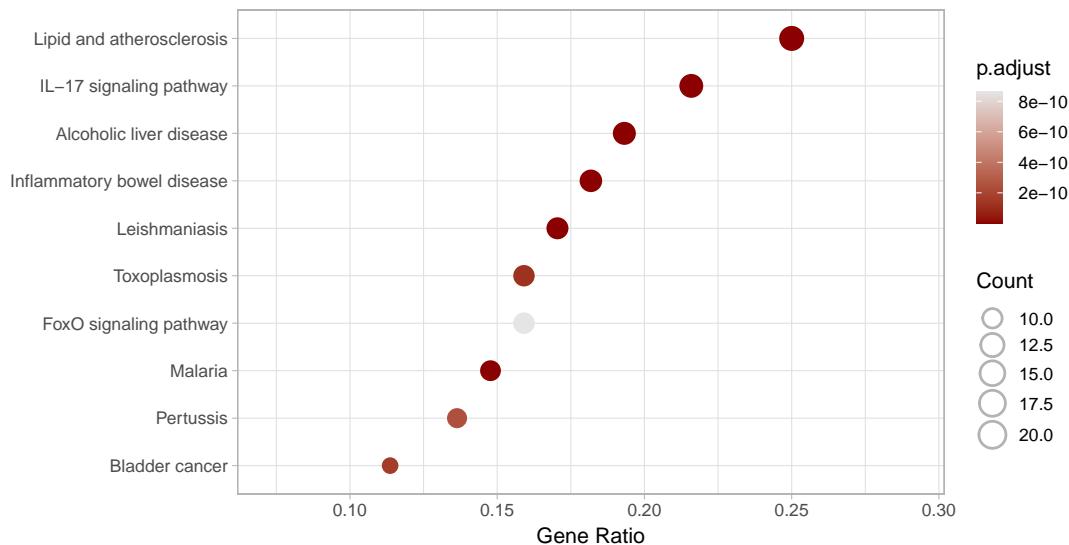


Figure 5: HERBS KEGG enrichment

Figure 6 (下方图) 为图 HERBS GO enrichment 概览。

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

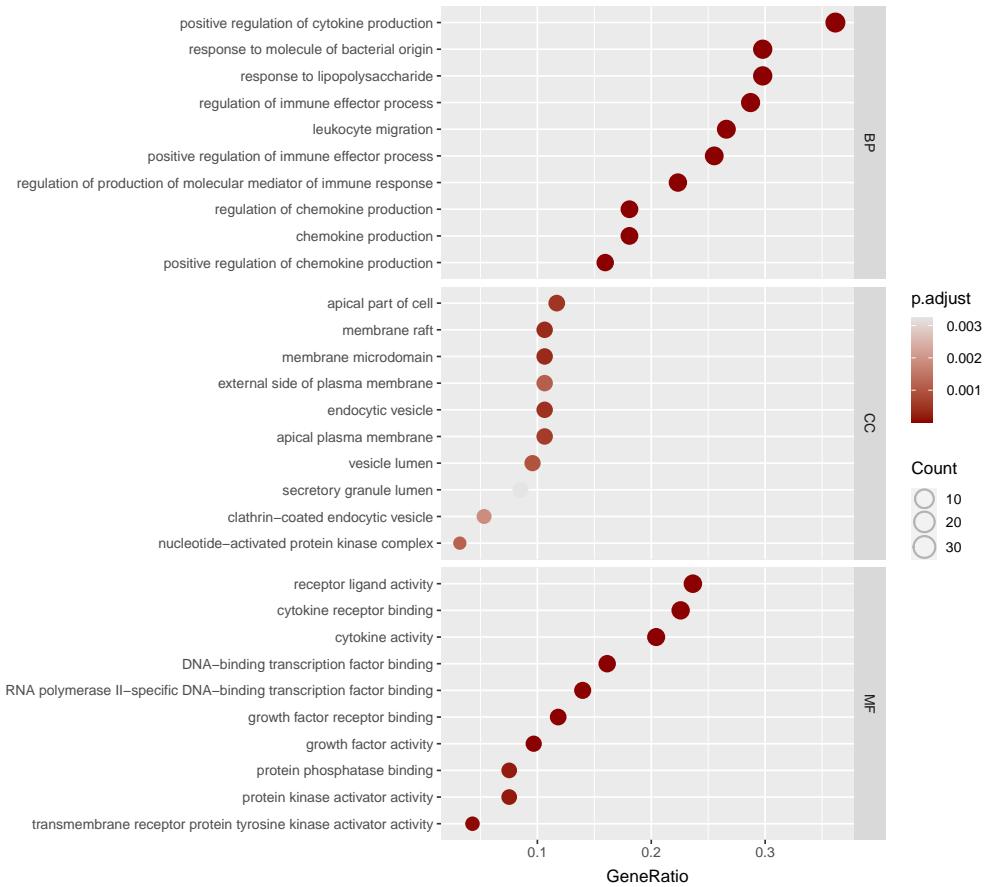


Figure 6: HERBS GO enrichment

6.1.5.1 与肠道炎症相关的通路和基因

Figure 7 (下方图) 为图 HERBS hsa05321 visualization 概览。

(对应文件为 Figure+Table/hsa05321.pathview.png)

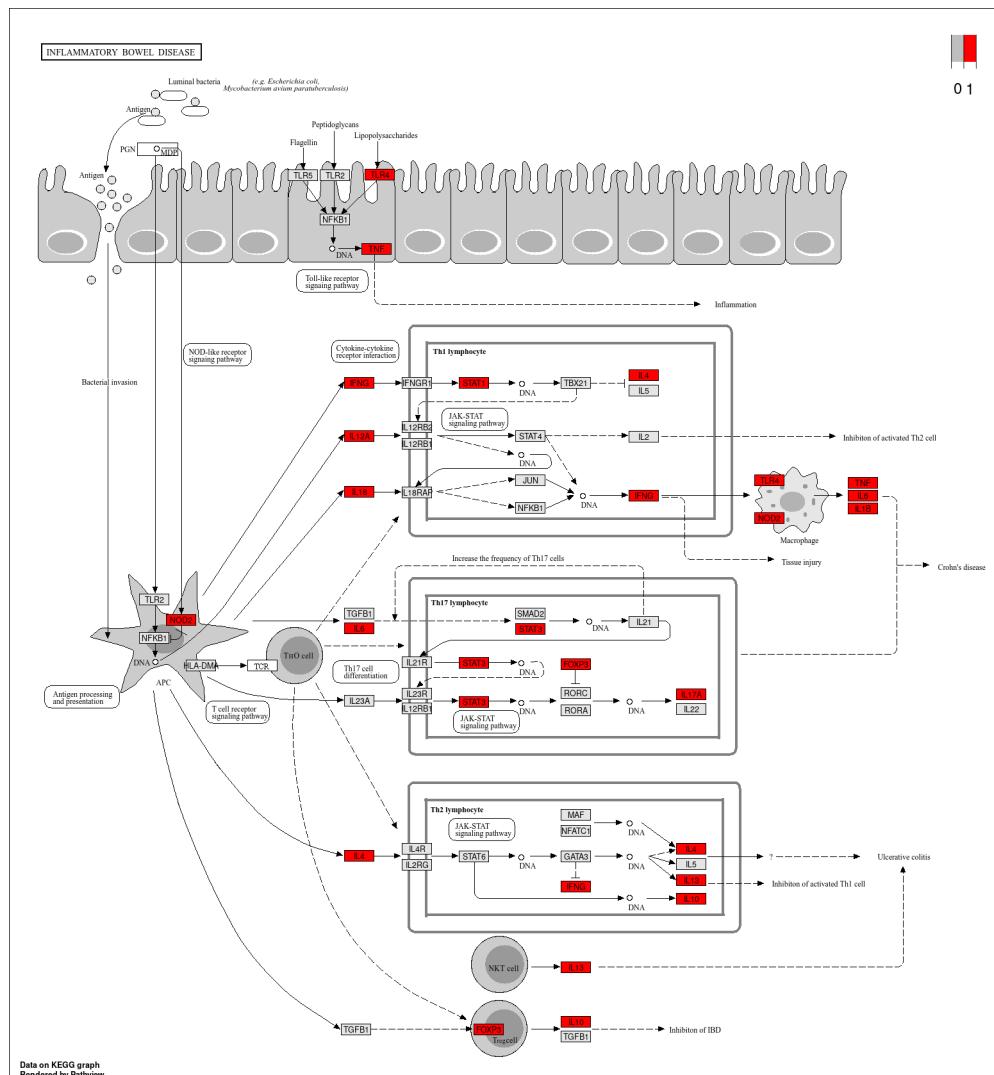


Figure 7: HERBS hsa05321 visualization

Interactive figure :

<https://www.genome.jp/pathway/hsa05321>

6.1.6 与疾病相关的活性成分筛选

6.1.6.1 PubMed 文献报道数 (任意领域)

Table 4 (下方表格) 为表格 All compounds Literature Count 概览。

(对应文件为 Figure+Table/All-compounds-Literature-Count.xlsx)

注：表格共有 2200 行 3 列，以下预览的表格可能省略部分数据；表格含有 2200 个唯一‘cids’。

Table 4: All compounds Literature Count

cids	name	LiteratureCount
702	ethanol	540787
5997	(3S,8S,9S,10R,13R,14S,17R)-...	337620
5988	(2R,3R,4S,5S,6R)-2-[(2S,3S,...	204482
24749	2,3,4,5,6-pentahydroxyhexanal	197377
180	propan-2-one	182194
241	benzene	155727
5957	[(2R,3S,4R,5R)-5-(6-aminop...	151618
5757	(8R,9S,13S,14S,17S)-13-meth...	143457
996	phenol	125953
612	2-hydroxypropanoic acid	115138
8058	hexane	112457
5461108	[(2R,3S,4R,5R)-5-(6-amino...	110671
774	2-(1H-imidazol-5-yl)ethanamine	98412
60961	(2R,3R,4S,5R)-2-(6-aminopur...	90522
311	2-hydroxypropane-1,2,3-tric...	78795
...

Table 5 (下方表格) 为表格 hsa05321 related genes and compounds 概览。

(对应文件为 **Figure+Table/hsa05321-related-genes-and-compounds.xlsx**)

注：表格共有 409 行 5 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_pinyin_name’。

Table 5: Hsa05321 related genes and compounds

Herb_pinyin_name	Ingredient.name	Target.name	LiteratureCount	cids
GUI ZHI	acetaldehyde	IL1B	37277	177
GUI ZHI	acetaldehyde	TNF	37277	177
GUI ZHI	acetaldehyde	IL6	37277	177
HUANG BAI	acetaldehyde	IL1B	37277	177
HUANG BAI	acetaldehyde	TNF	37277	177
HUANG BAI	acetaldehyde	IL6	37277	177
DANG GUI	2-hydroxyethyl(tr...	TNF	24884	305
REN SHEN	2-hydroxyethyl(tr...	TNF	24884	305
GUI ZHI	chromen-2-one	IL6	26252	323
GUI ZHI	chromen-2-one	STAT3	26252	323
REN SHEN	2-hydroxybenzoic ...	IL4	38476	338
GUI ZHI	octanoic acid	TLR4	7352	379

Herb_pinyin_name	Ingredient.name	Target.name	LiteratureCount	cids
HUANG BAI	octanoic acid	TLR4	7352	379
WU MEI	octanoic acid	TLR4	7352	379
XI XIN	octanoic acid	TLR4	7352	379
...

6.1.6.2 CTD 数据库记录与肾炎相关的化合物

Figure 8 (下方图) 为图 Intersection of CTD records with herbs of hsa05321 related 概览。

(对应文件为 [Figure+Table/Intersection-of-CTD-records-with-herbs-of-hsa05321-related.pdf](#))

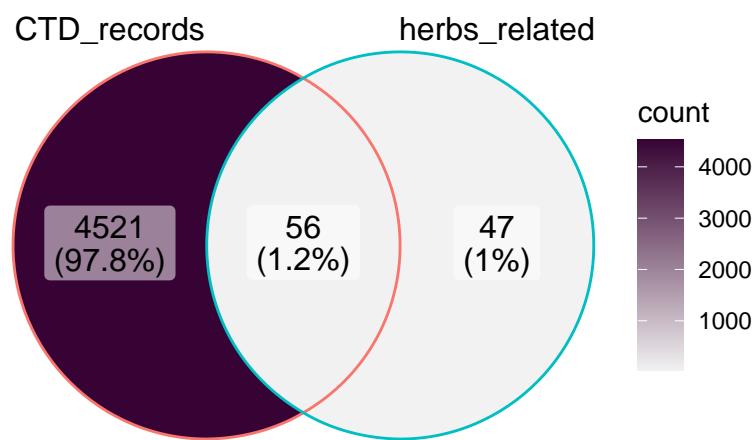


Figure 8: Intersection of CTD records with herbs of hsa05321 related

Intersection :

8530, 54675866, 177, 7847, 119258, 2353, 72326, 64971, 2519, 644019, 2703, 5959, 5280795, 5997, 305, 637511, 638011, 323, 969516, 637568, 5281613, 16078, 5757, 702, 2758, 445070, 5280805, 5280961, 441923, 774, 72303, 5280863, 10255, 3893, 8181, 439246, 6184, 12389, 379, 10228, 11092, 985, 8158, 9...

(上述信息框内容已保存至 [Figure+Table/Intersection-of-CTD-records-with-herbs-of-hsa05321-related-content](#))

Table 6 (下方表格) 为表格 Intersection Herbs compounds and targets 概览。

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

注：表格共有 307 行 5 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_pinyin_name’。

Table 6: Intersection Herbs compounds and targets

Herb_pinyin_name	Ingredient.name	Target.name	LiteratureCount	cids
GUI ZHI	acetaldehyde	IL1B	37277	177
GUI ZHI	acetaldehyde	TNF	37277	177
GUI ZHI	acetaldehyde	IL6	37277	177
HUANG BAI	acetaldehyde	IL1B	37277	177
HUANG BAI	acetaldehyde	TNF	37277	177
HUANG BAI	acetaldehyde	IL6	37277	177
DANG GUI	2-hydroxyethyl(tr...	TNF	24884	305
REN SHEN	2-hydroxyethyl(tr...	TNF	24884	305
GUI ZHI	chromen-2-one	IL6	26252	323
GUI ZHI	chromen-2-one	STAT3	26252	323
REN SHEN	2-hydroxybenzoic ...	IL4	38476	338
GUI ZHI	octanoic acid	TLR4	7352	379
HUANG BAI	octanoic acid	TLR4	7352	379
WU MEI	octanoic acid	TLR4	7352	379
XI XIN	octanoic acid	TLR4	7352	379
...

6.2 分子对接

6.2.1 Top docking

取 Tab. 6 (即, Fig. 8 交集) 成分与靶点, 进行批量分子对接。

以下展示了各个靶点结合度 Top 5 的成分

Figure 9 (下方图) 为图 Overall combining Affinity 概览。

(对应文件为 Figure+Table/Overall-combining-Affinity.pdf)

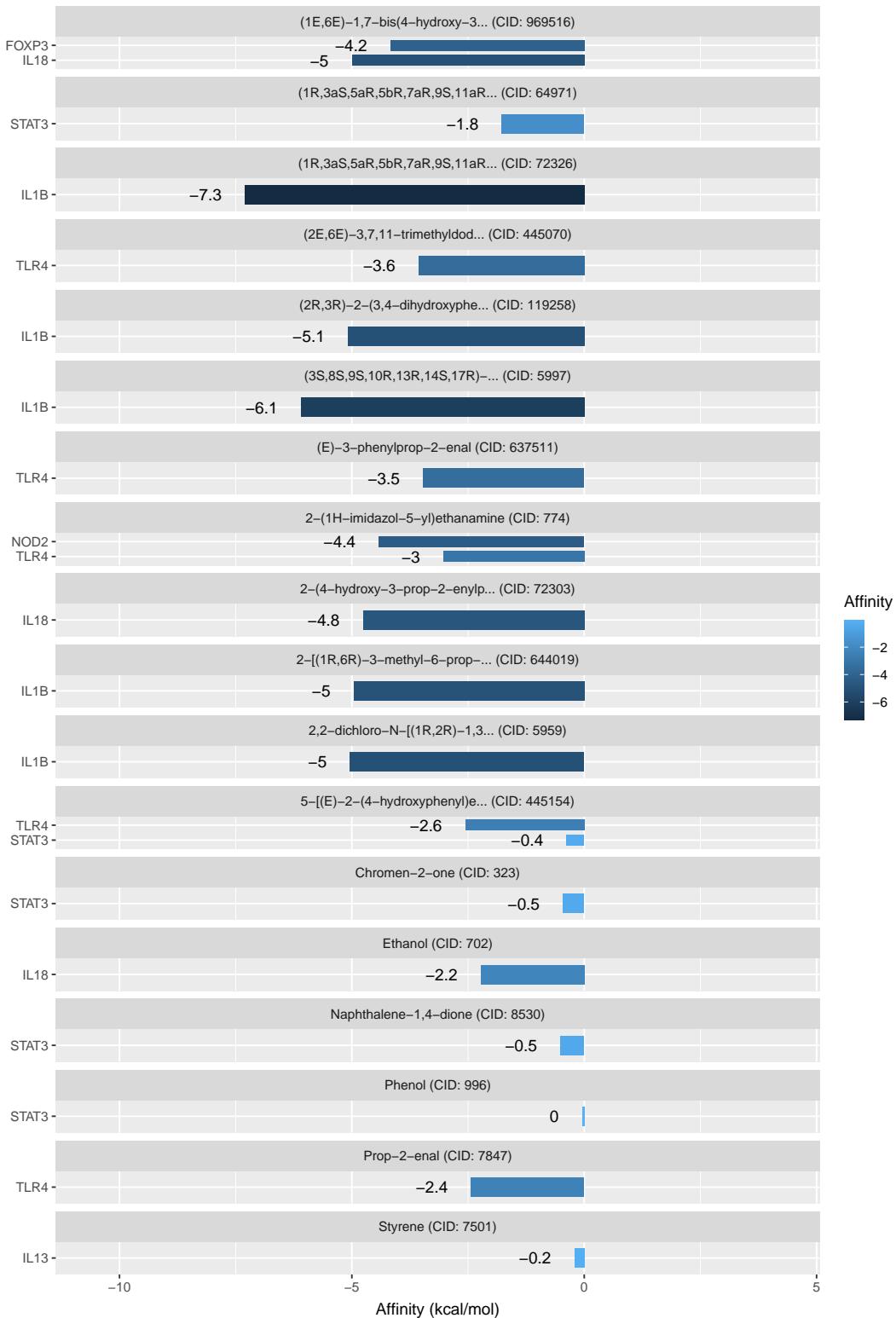


Figure 9: Overall combining Affinity

Table 7 (下方表格) 为表格 Combining Affinity 概览。

(对应文件为 Figure+Table/Combining-Affinity.xlsx)

注：表格共有 35 行 6 列，以下预览的表格可能省略部分数据；表格含有 10 个唯一 ‘hgnc_symbol’。

1. hgnc_symbol: 基因名 (Human)

Table 7: Combining Affinity

hgnc_symbol	Ingredient...	Affinity	PubChem_id	PDB_ID	Combn
IL1B	(1R,3aS,5a...	-7.303	72326	9ilb	72326_into...
IL1B	(3S,8S,9S,...	-6.096	5997	9ilb	5997_into_...
IL1B	(2R,3R)-2...	-5.083	119258	9ilb	119258_int...
IL1B	2,2-dichlo...	-5.038	5959	9ilb	5959_into_...
IL18	(1E,6E)-1,...	-4.999	969516	4xfu	969516_int...
IL1B	2-[(1R,6R)...	-4.959	644019	9ilb	644019_int...
IL18	2-(4-hydro...	-4.76	72303	4xfu	72303_into...
NOD2	2-(1H-imid...	-4.417	774	nod2	774_into_nod2
FOXP3	(1E,6E)-1,...	-4.169	969516	4wk8	969516_int...
TLR4	(2E,6E)-3,...	-3.564	445070	5nao	445070_int...
TLR4	(E)-3-phen...	-3.467	637511	5nao	637511_int...
TLR4	2-(1H-imid...	-3.032	774	5nao	774_into_5nao
TLR4	5-[(E)-2-(...	-2.558	445154	5nao	445154_int...
TLR4	prop-2-enal	-2.434	7847	5nao	7847_into_...
IL18	ethanol	-2.225	702	4xfu	702_into_4xfu
...

6.2.2 对接可视化

Table 8 (下方表格) 为表格 Metadata of visualized Docking 概览。

(对应文件为 **Figure+Table/Metadata-of-visualized-Docking.xlsx**)

注：表格共有 3 行 5 列，以下预览的表格可能省略部分数据；表格含有 3 个唯一 ‘PubChem_id’。

1. hgnc_symbol: 基因名 (Human)

Table 8: Metadata of visualized Docking

PubChem_id	PDB_ID	Affinity	hgnc_symbol	Ingredient_name
72326	9ilb	-7.303	IL1B	(1R,3aS,5aR,5bR,7...
969516	4xfu	-4.999	IL18	(1E,6E)-1,7-bis(4...

PubChem_id	PDB_ID	Affinity	hgnc_symbol	Ingredient_name
774	nod2	-4.417	NOD2	2-(1H-imidazol-5-...

Figure 10 (下方图) 为图 Docking 72326 into 9ilb 概览。

(对应文件为 [Figure+Table/72326_into_9ilb.png](#))



Figure 10: Docking 72326 into 9ilb

Figure 11 (下方图) 为图 Docking 969516 into 4xfu 概览。

(对应文件为 [Figure+Table/969516_into_4xfu.png](#))

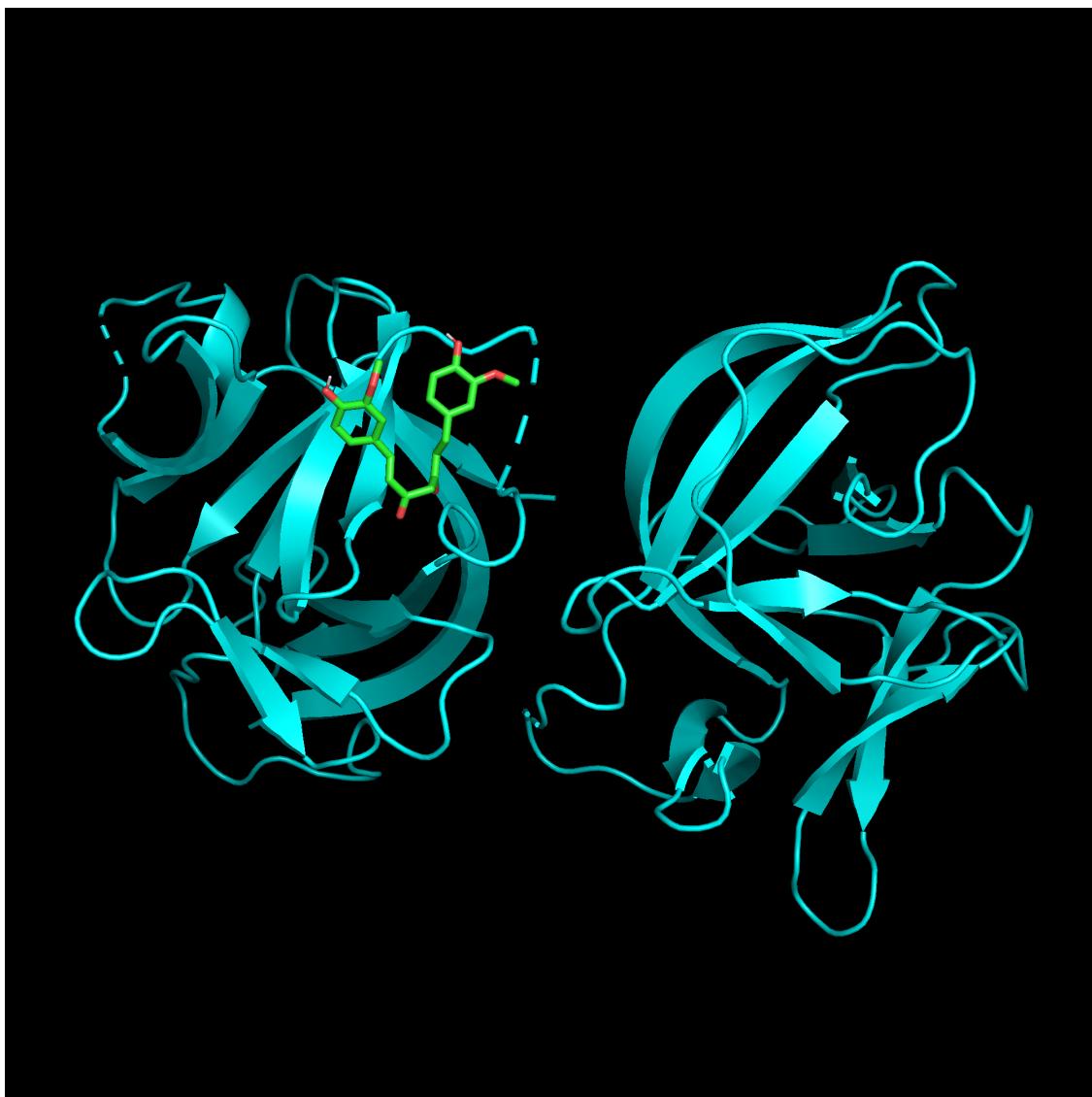


Figure 11: Docking 969516 into 4xfu

Figure 12 (下方图) 为图 Docking 774 into nod2 概览。

(对应文件为 Figure+Table/774_into_nod2.png)

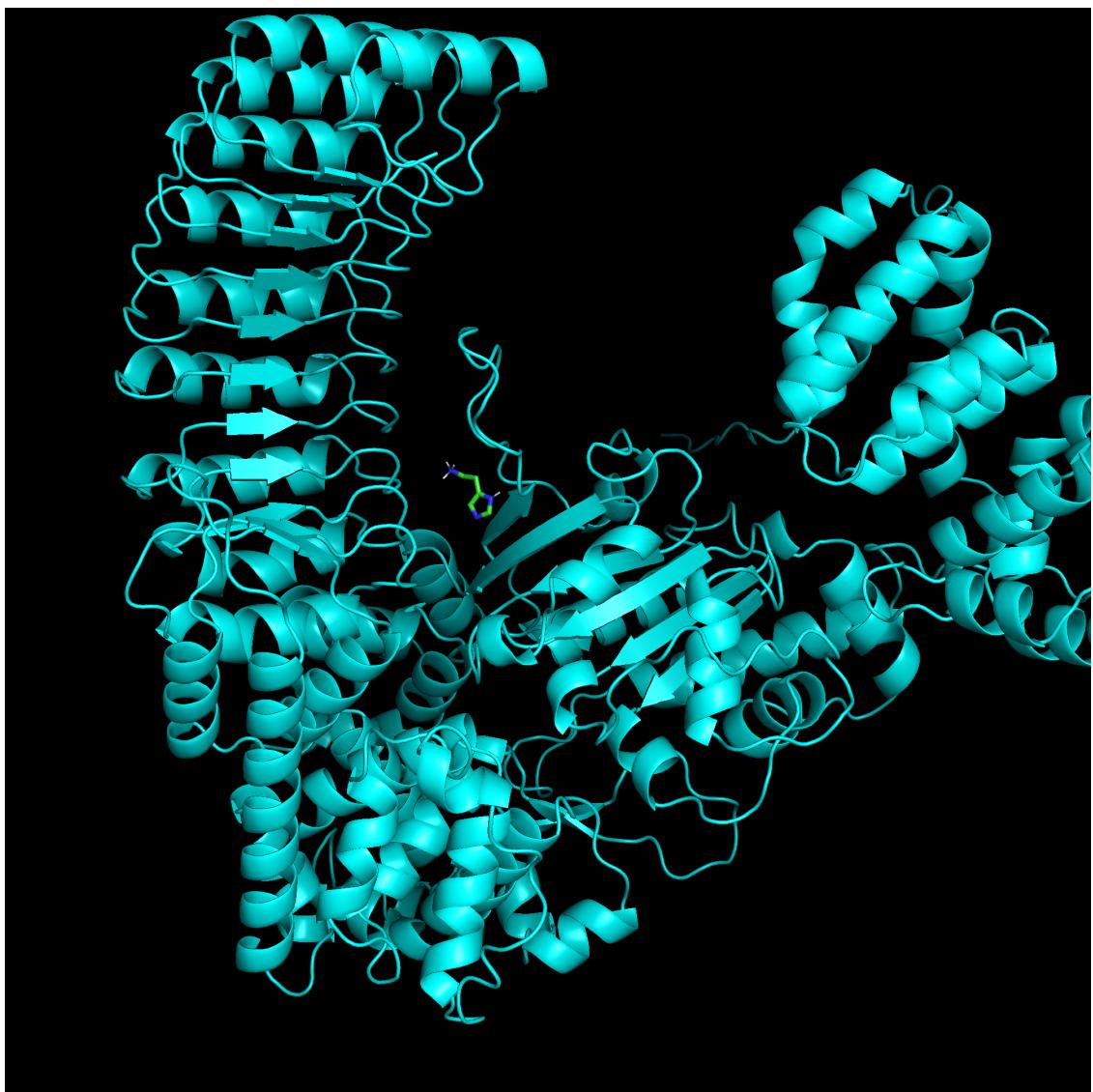


Figure 12: Docking 774 into nod2

6.2.3 局部对接细节

Figure 13 (下方图) 为图 Docking 72326 into 9ilb detail 概览。

(对应文件为 Figure+Table/detail_72326_into_9ilb.png)

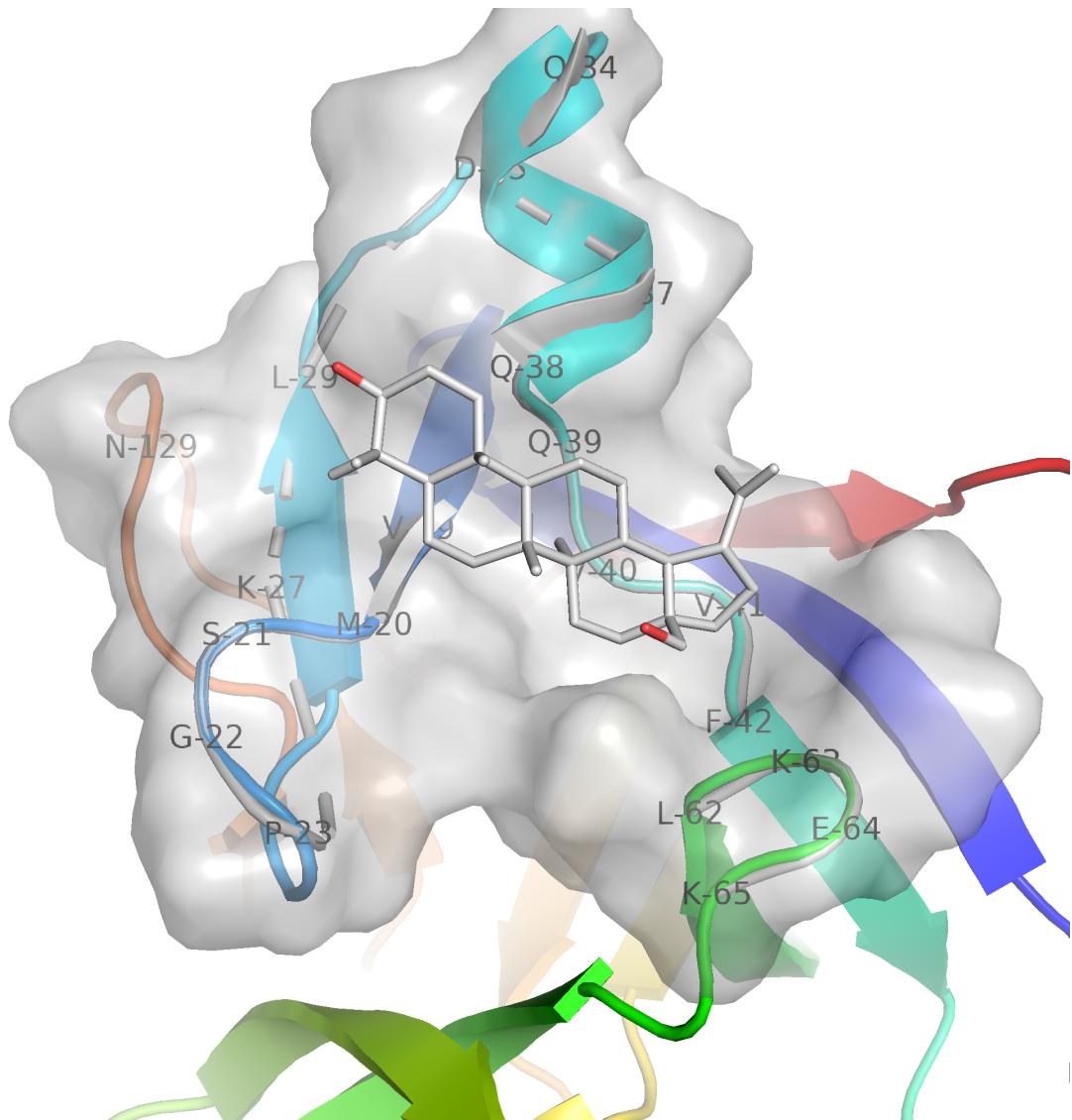


Figure 13: Docking 72326 into 9ilb detail

Figure 14 (下方图) 为图 Docking 969516 into 4xfu detail 概览。

(对应文件为 Figure+Table/detail_969516_into_4xfu.png)

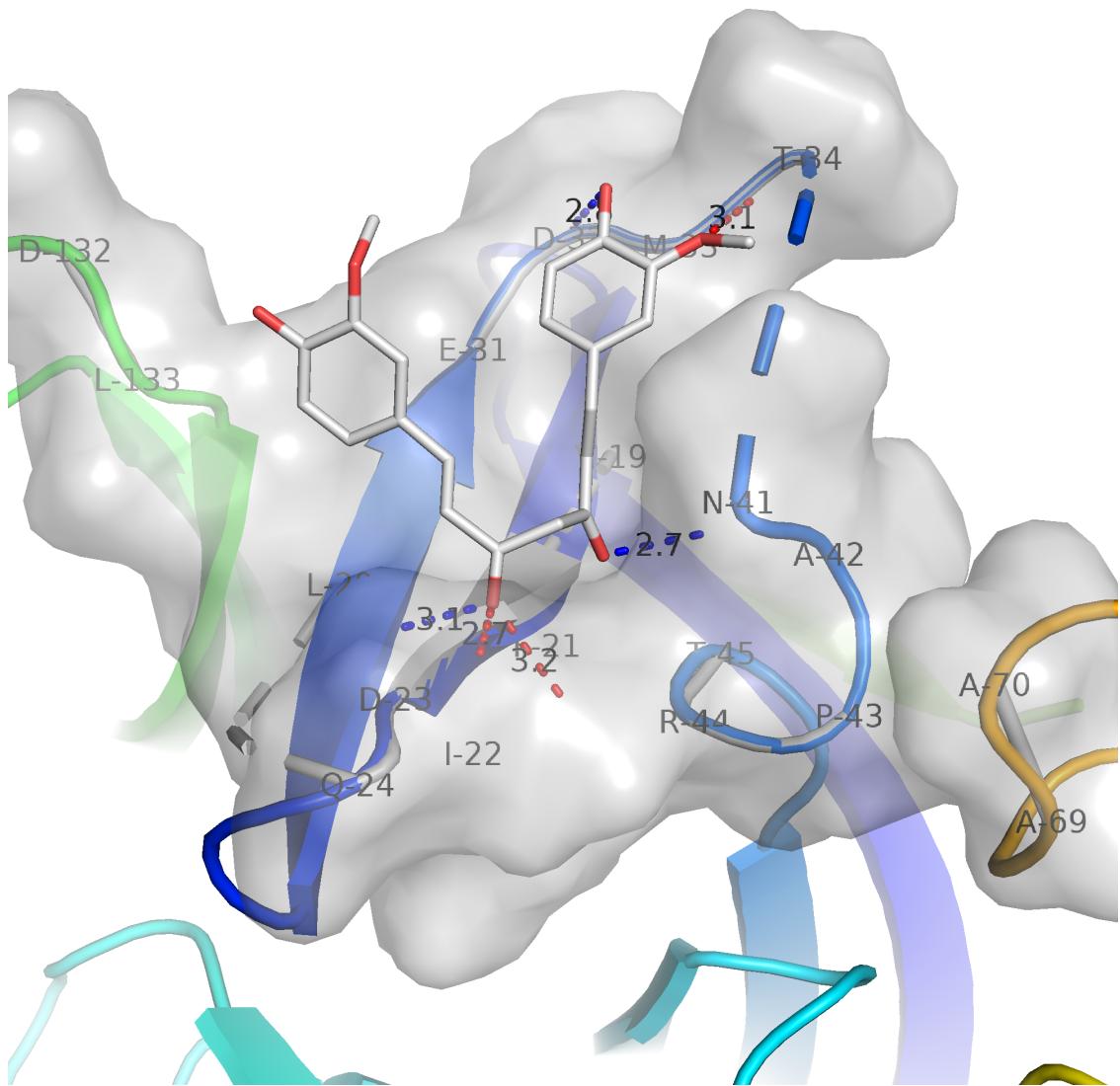


Figure 14: Docking 969516 into 4xfu detail

Figure 15 (下方图) 为图 Docking 774 into nod2 detail 概览。

(对应文件为 [Figure+Table/detail_774_into_nod2.png](#))

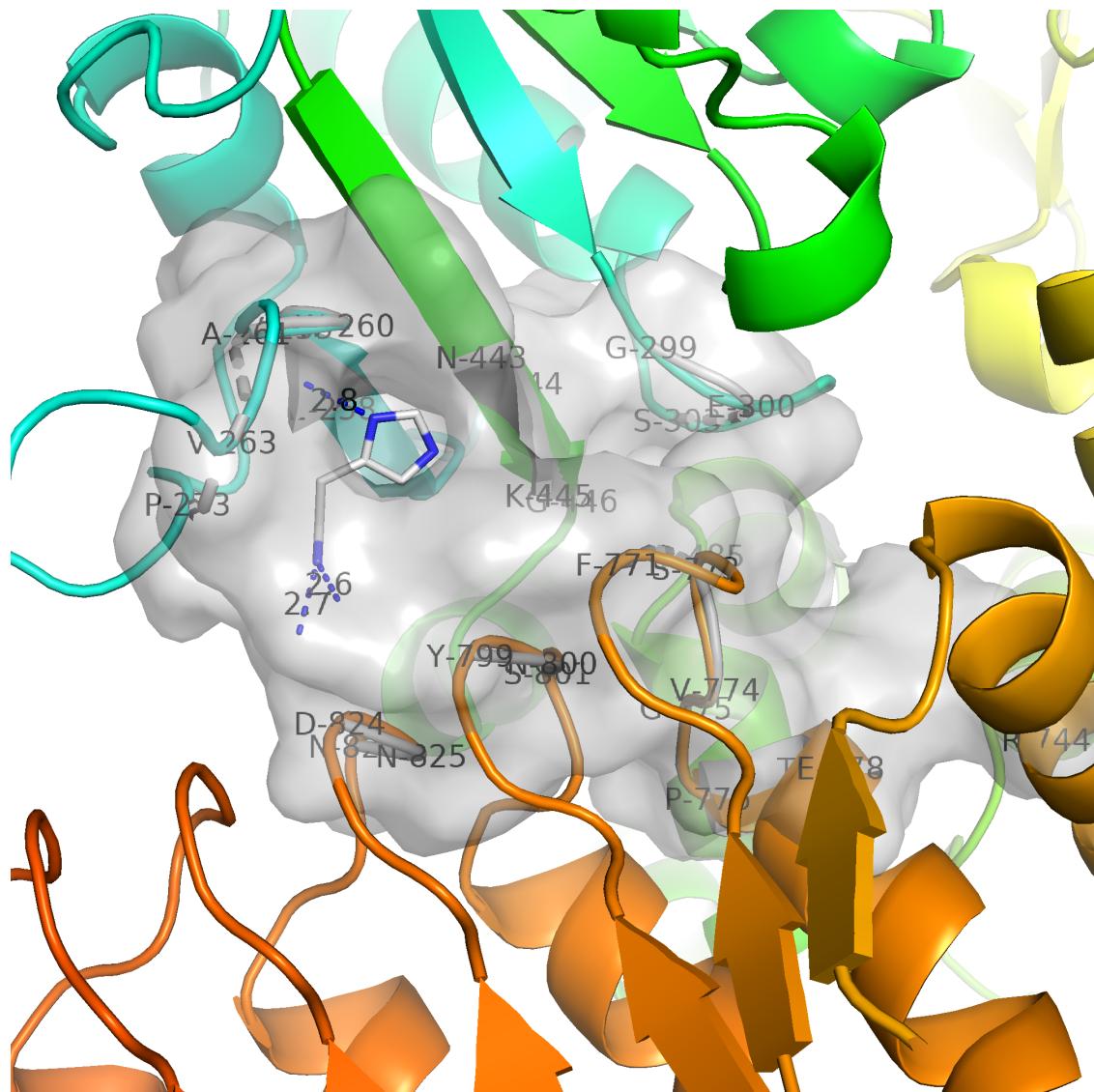


Figure 15: Docking 774 into nod2 detail

6.2.4 Top1 的靶点的富集分析 (参与 hsa05321 靶点)

Figure 16 (下方图) 为图 TOP KEGG enrichment 概览。

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

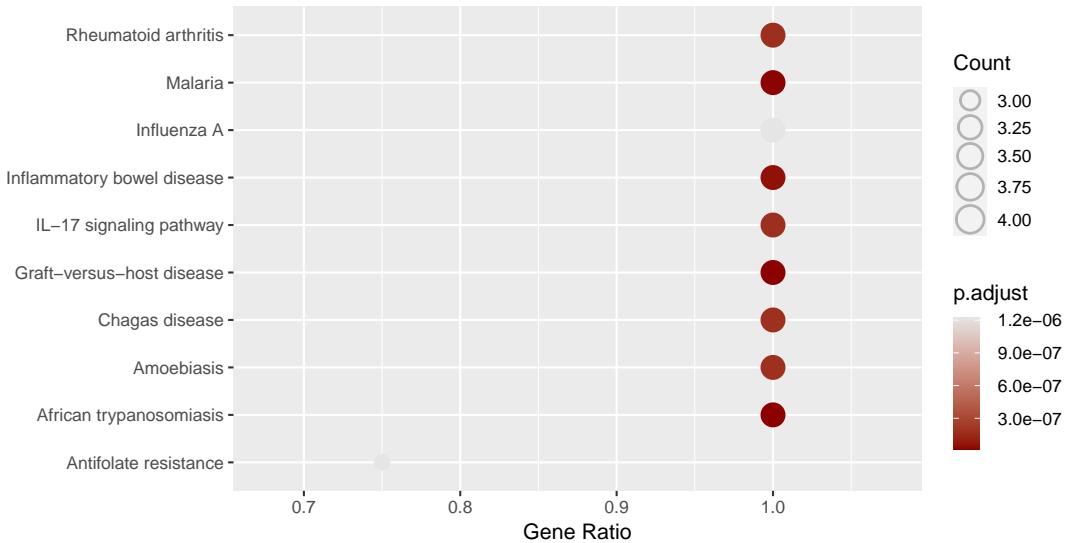


Figure 17 (下方图) 为图 TOP GO enrichment 概览。

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

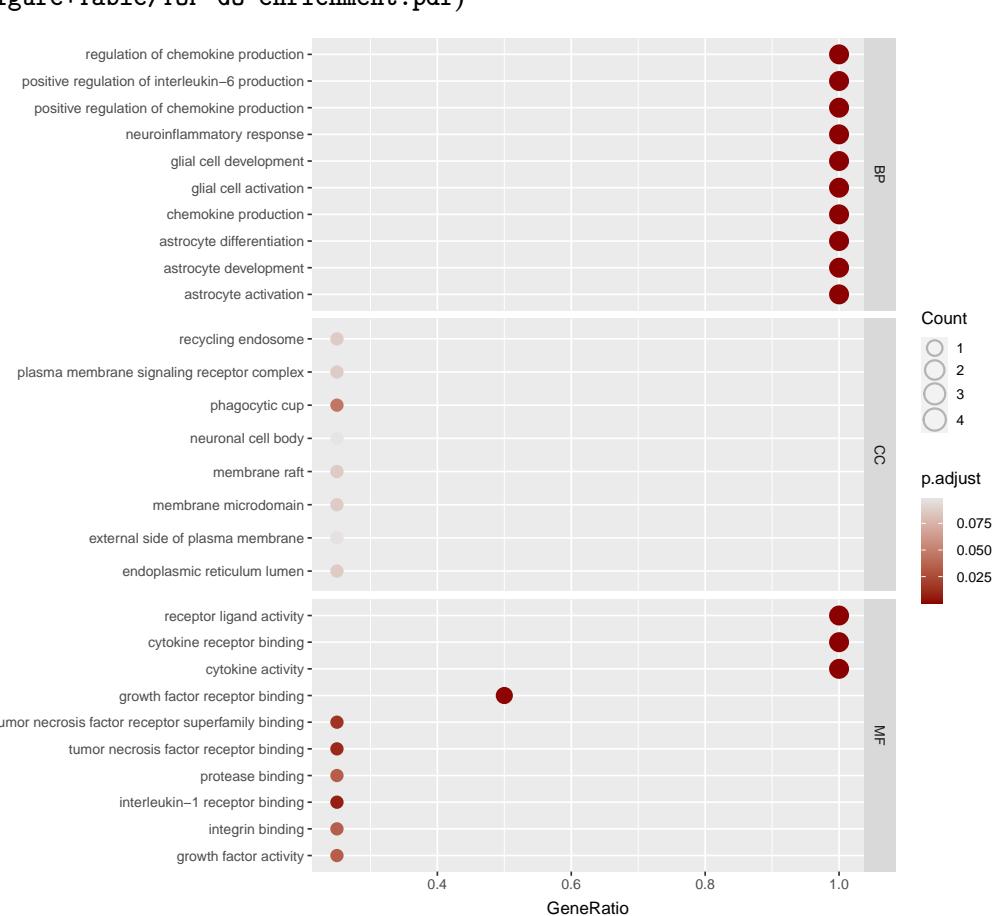


Figure 18 (下方图) 为图 TOP hsa05321 visualization 概览。
 (对应文件为 Figure+Table/hsa05321.pathview.png)

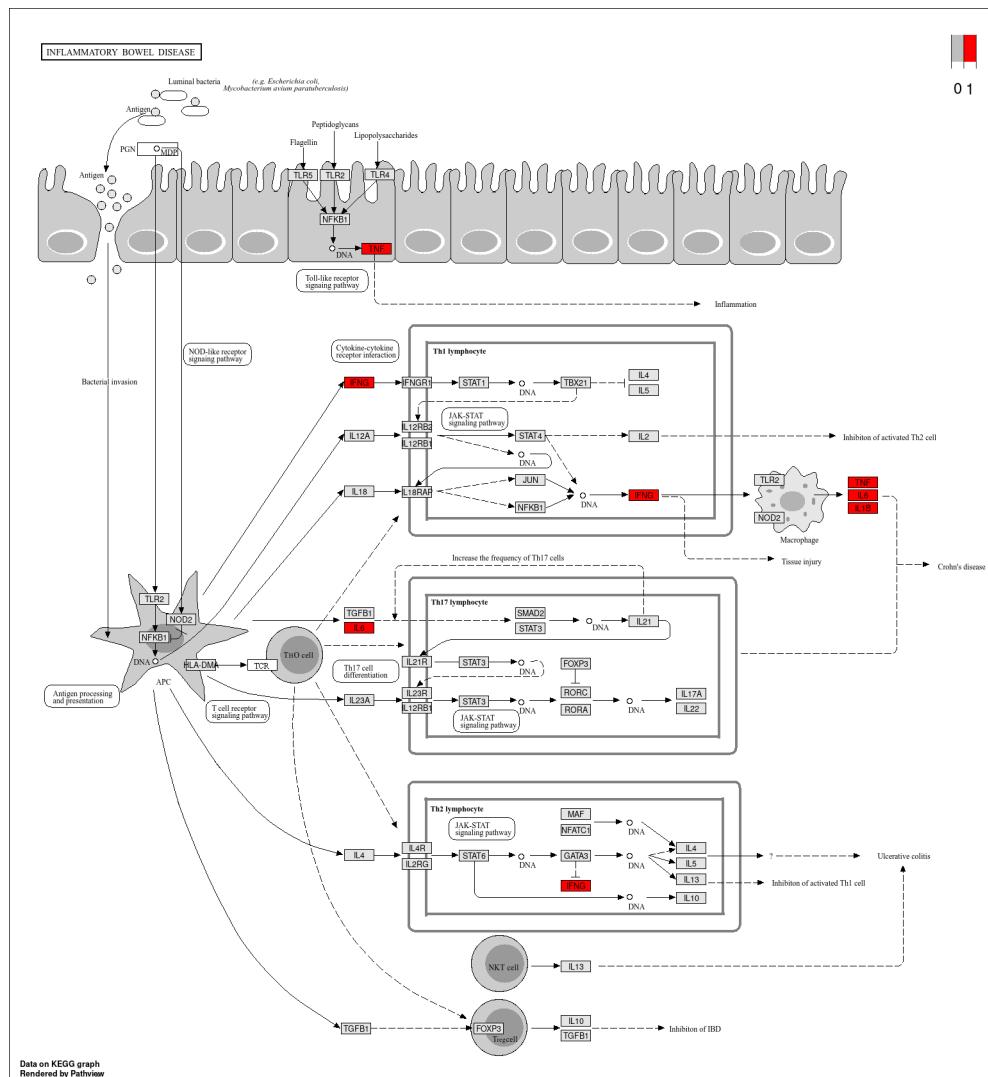


Figure 18: TOP hsa05321 visualization

Interactive figure :

<https://www.genome.jp/pathway/hsa05321>

Figure 19 (下方图) 为图 TOP pharmacology visualization 概览。
 (对应文件为 Figure+Table/TOP-pharmacology-visualization.pdf)

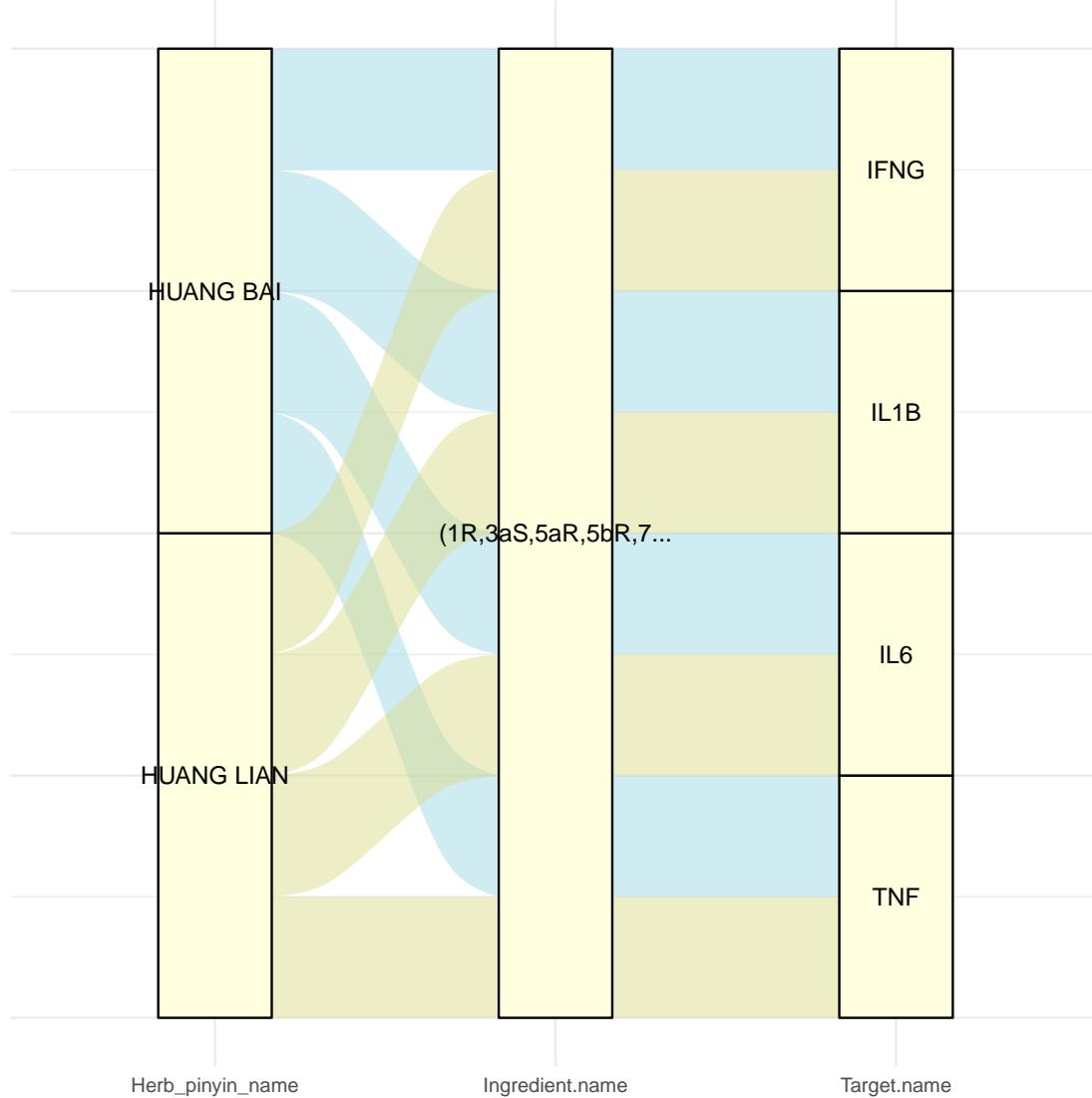


Figure 19: TOP pharmacology visualization

6.2.4.1 TOP1 的结合靶点 (IL1B) 参与的通路

Table 9 (下方表格) 为表格 IL1B kegg 概览。

(对应文件为 Figure+Table/IL1B-kegg.csv)

注：表格共有 43 行 9 列，以下预览的表格可能省略部分数据；表格含有 43 个唯一 ‘ID’。

1. pvalue: 显著性 P。

Table 9: IL1B kegg

ID	Descri...	GeneRatio	BgRatio	pvalue	p.adjust	qvalue	geneID	Count
hsa05143	Africa...	4/4	37/8672	2.8046...	1.9487...	3.0019...	3458/3...	4
hsa05332	Graft...	4/4	42/8672	4.7531...	1.9487...	3.0019...	3458/3...	4
hsa05144	Malaria	4/4	50/8672	9.7797...	2.6731...	4.1177...	3458/3...	4
hsa05321	Inflam...	4/4	65/8672	2.8750...	5.8939...	9.0791...	3458/3...	4
hsa05323	Rheuma...	4/4	93/8672	1.2398...	1.7698...	2.7262...	3458/3...	4
hsa04657	IL-17 ...	4/4	94/8672	1.2949...	1.7698...	2.7262...	3458/3...	4
hsa05142	Chagas...	4/4	102/8672	1.8045...	1.8497...	2.8493...	3458/3...	4
hsa05146	Amoebi...	4/4	102/8672	1.8045...	1.8497...	2.8493...	3458/3...	4
hsa05164	Influe...	4/4	171/8672	1.4603...	1.2227...	1.8835...	3458/3...	4
hsa01523	Antifo...	3/4	30/8672	1.4911...	1.2227...	1.8835...	3553/3...	3
hsa05152	Tuberc...	4/4	180/8672	1.7961...	1.3389...	2.0625...	3458/3...	4
hsa04940	Type I...	3/4	43/8672	4.5273...	3.0937...	4.7656...	3458/3...	3
hsa05134	Legion...	3/4	56/8672	1.0157...	6.4072...	9.8699...	3553/3...	3
hsa04060	Cytoki...	4/4	297/8672	1.3490...	7.9018...	1.2172...	3458/3...	4
hsa05133	Pertussis	3/4	76/8672	2.5716...	1.3712...	2.1123...	3553/3...	3
...

Table 10 (下方表格) 为表格 IL1B go 概览。

(对应文件为 Figure+Table/IL1B-go.xlsx)

注：表格共有 431 行 10 列，以下预览的表格可能省略部分数据；表格含有 2 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 10: IL1B go

ont	ID	Descri...	GeneRatio	BgRatio	pvalue	p.adjust	qvalue	geneID	Count
BP	GO:004...	astroc...	4/4	24/18614	2.1250...	2.5330...	2.0802...	3458/3...	4
BP	GO:001...	astroc...	4/4	43/18614	2.4679...	1.4709...	1.2080...	3458/3...	4
BP	GO:006...	glial ...	4/4	55/18614	6.8205...	2.7100...	2.2256...	3458/3...	4
BP	GO:003...	positi...	4/4	70/18614	1.8336...	5.4642...	4.4875...	3458/3...	4
BP	GO:015...	neuroi...	4/4	76/18614	2.5657...	6.1166...	5.0234...	3458/3...	4
BP	GO:004...	astroc...	4/4	87/18614	4.4514...	8.8434...	7.2628...	3458/3...	4
BP	GO:003...	regula...	4/4	98/18614	7.2239...	1.0385...	8.5296...	3458/3...	4
BP	GO:003...	chemok...	4/4	99/18614	7.5281...	1.0385...	8.5296...	3458/3...	4

ont	ID	Descri...	GeneRatio	BgRatio	pvalue	p.adjust	qvalue	geneID	Count
BP	GO:003...	positi...	4/4	100/18614	7.8417...	1.0385...	8.5296...	3458/3...	4
BP	GO:002...	glial ...	4/4	119/18614	1.5880...	1.8929...	1.5545...	3458/3...	4
BP	GO:005...	positi...	3/4	16/18614	2.0831...	2.2573...	1.8539...	3458/3...	3
BP	GO:015...	positi...	3/4	18/18614	3.0352...	3.0149...	2.4760...	3553/3...	3
BP	GO:005...	positi...	4/4	154/18614	4.5062...	4.1318...	3.3933...	3458/3...	4
BP	GO:006...	positi...	3/4	21/18614	4.9465...	4.2115...	3.4588...	3553/3...	3
BP	GO:005...	regula...	4/4	163/18614	5.6679...	4.5041...	3.6991...	3458/3...	4
...

Reference

- Kong, X. *et al.* BATMAN-tcm 2.0: An enhanced integrative database for known and predicted interactions between traditional chinese medicine ingredients and target proteins. *Nucleic acids research* **52**, D1110–D1120 (2024).
- Davis, A. P. *et al.* Comparative toxicogenomics database (ctd): Update 2023. *Nucleic acids research* **51**, D1257–D1262 (2023).
- Wu, T. *et al.* ClusterProfiler 4.0: A universal enrichment tool for interpreting omics data. *The Innovation* **2**, (2021).
- Piñero, J. *et al.* The disgenet knowledge platform for disease genomics: 2019 update. *Nucleic Acids Research* (2019) doi:10.1093/nar/gkz1021.
- Stelzer, G. *et al.* The genecards suite: From gene data mining to disease genome sequence analyses. *Current protocols in bioinformatics* **54**, 1.30.1–1.30.33 (2016).
- Barbarino, J. M., Whirl-Carrillo, M., Altman, R. B. & Klein, T. E. PharmGKB: A worldwide resource for pharmacogenomic information. *Wiley interdisciplinary reviews. Systems biology and medicine* **10**, (2018).
- Eberhardt, J., Santos-Martins, D., Tillack, A. F. & Forli, S. AutoDock vina 1.2.0: New docking methods, expanded force field, and python bindings. *Journal of Chemical Information and Modeling* **61**, 3891–3898 (2021).
- Zhang, Y., Forli, S., Omelchenko, A. & Sanner, M. F. AutoGridFR: Improvements on autodock affinity maps and associated software tools. *Journal of computational chemistry* **40**, 2882–2886 (2019).
- Zhang, Y. & Sanner, M. F. AutoDock crankpep: Combining folding and docking to predict protein-peptide complexes. *Bioinformatics (Oxford, England)* **35**, 5121–5127 (2019).
- Ravindranath, P. A. & Sanner, M. F. AutoSite: An automated approach for pseudo-ligands prediction-from ligand-binding sites identification to predicting key ligand atoms. *Bioinformatics (Oxford, England)* **32**, 3142–3149 (2016).
- Ravindranath, P. A., Forli, S., Goodsell, D. S., Olson, A. J. & Sanner, M. F. AutoDockFR: Advances

in protein-ligand docking with explicitly specified binding site flexibility. *PLoS computational biology* **11**, (2015).