

X 药方-草药-单体-靶点

2023-12-25

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1 摘要

- 做药方-草药-单体-靶点图，着重显示单体-木兰花碱（magnoflorine）和靶点 OPRM1。
- 木兰花碱与 OPRM1 的分子对接。

药理学结果见 Fig. 2、

分子对接见（亲和度为正值，对接不成功）Fig. 4

2 材料和方法

2.1 方法

Mainly used method:

- Website HERB <http://herb.ac.cn/> used for data source.¹
- AutoDock vina used for molecular docking.²
- 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 药方-草药-单体-靶点

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 14 行 18 列，以下预览的表格可能省略部分数据；表格含有 14 个唯一‘Herb_’。

Table 1: Herbs information

Herb_	Herb_p...	Herb_c...	Herb_e...	Herb_l...	Proper...	Meridians	UsePart	Function	Indica...
HERB00...	BAI SHAO	白芍	White ...	Radix ...	Minor ...	Spleen...	root	1. To ...	Headac...
HERB00...	BAI ZHU	白术	rhizom...	Rhizom...	Warm; ...	Spleen...	root	To inv...	Spleen...
HERB00...	BO HE	薄荷	Mentha...	herba ...	Cool; ...	Lung; ...	dried ...	To dis...	Chroni...
HERB00...	CHAI HU	柴胡	root o...	Radix ...	Minor ...	Liver;...	root	To rel...	Common...
HERB00...	DANG GUI	当归	root o...	Radix ...	Warm; ...	Spleen...	root	To enr...	Women'...
HERB00...	FU LING	茯苓	Indian...	Poria	Mild; ...	Spleen...	sclero...	To cau...	Neuras...

Herb_	Herb_p...	Herb_c...	Herb_e...	Herb_l...	Proper...	Meridians	UsePart	Function	Indica...
HERB00...	GAN CAO	甘草	Root o...	Radix ...	Mild; ...	Lung; ...	root a...	To rei...	1. Its...
HERB00...	HUANG BO	黃柏	Phello...	Cortex...	Cold; ...	Bladde...	bark	1. To ...	NA
HERB00...	MU DAN PI	牡丹皮	Tree P...	Cortex...	Minor ...	Liver;...	root c...	To rem...	Append...
HERB00...	SHAN YAO	山药	Common...	Rhizom...	Mild; ...	Lung; ...	rhizome	To rep...	Reduce...
HERB00...	SHAN Z...	山茱萸	Asiati...	Fructu...	Warm; ...	Liver;...	fruit	To rep...	Dizzin...
HERB00...	SHU DI...	熟地黃	Prepar...	Radix ...	Minor ...	Liver;...	steame...	To nou...	Blood ...
HERB00...	ZE XIE	泽泻	rhizom...	Rhizom...	Cold; ...	Bladde...	tuber	To cau...	Hyperl...
HERB00...	ZHI MU	知母	rhizom...	Rhizom...	Cold; ...	Lung; ...	rhizome	To rem...	Diabet...

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 2620 行 4 列，以下预览的表格可能省略部分数据；表格含有 2203 个唯一‘Ingredient.name’。

Table 2: Components of Herbs

herb_id	Ingredient.id	Ingredient.name	Ingredient.alias
HERB000309	HBIN000715	12-(-methyl buty...	12-(-methyl buty...
HERB000309	HBIN000716	12-(-methyl buty...	[(4E,6Z,12E)-1-ac...
HERB000309	HBIN000959	12-Oxoarundoin	(5aR,9S,11aS,13bR...
HERB000309	HBIN000978	12-senecioyl-2E,8...	NA
HERB000309	HBIN001001	13,15-Dideoxyacon...	13,15-dideoxyacon...
HERB000309	HBIN001355	14-acetyl-12-sene...	NA
HERB000309	HBIN001356	14-acetyl-12-sene...	NA
HERB000309	HBIN001365	14(-methyl butyr...	14(-methyl butyr...
HERB000309	HBIN001366	14(-methyl butyr...	14(-methyl butyr...
HERB000309	HBIN003030	(1R)-2-methyl-1-p...	ZINC02508056; (1R...
HERB000309	HBIN003207	(1S,2R,4R)-Neoiso...	(1R,2S,5R)-2-meth...
HERB000309	HBIN003599	2-[(1R,3S,4S)-3-i...	EINECS 211-360-5;...
HERB000309	HBIN003763	2-[(2R,5S,6S)-6,1...	2-[(2R,5S,6S)-6,1...
HERB000309	HBIN005273	2alpha-(alpha-met...	NA
HERB000309	HBIN008151	3 -acetoxyatracty...	NA
...

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**)

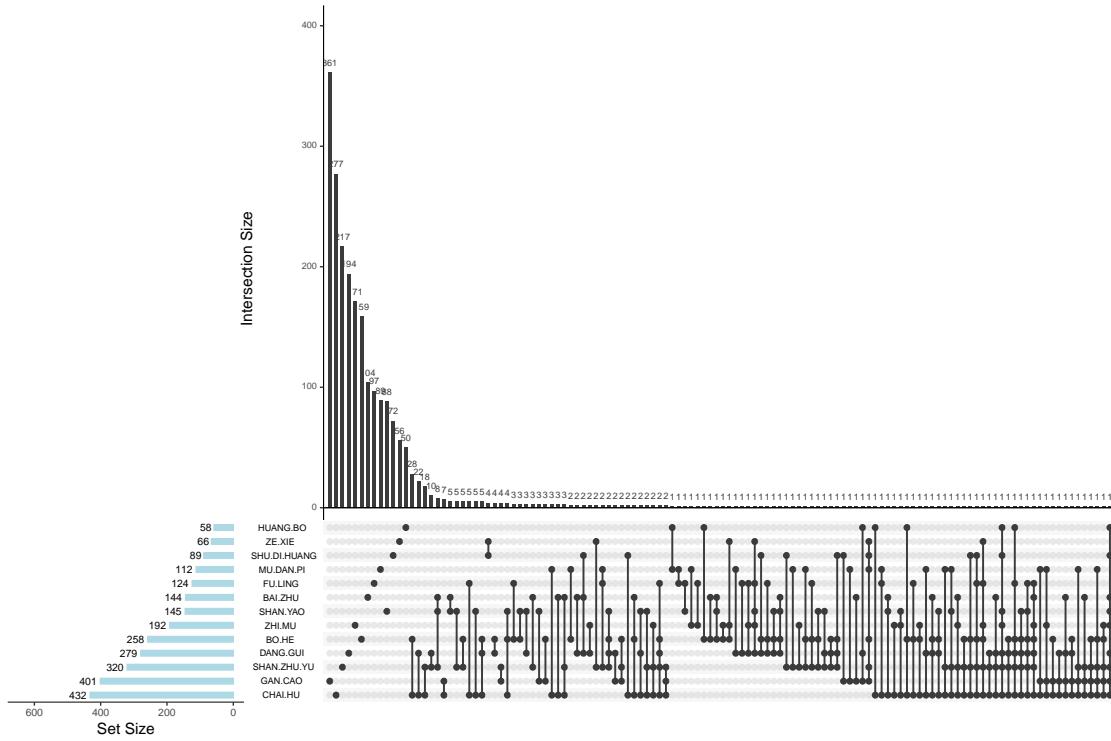


Figure 1: Intersection of all compounds

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.tsv](#))

注：表格共有 57402 行 9 列，以下预览的表格可能省略部分数据；表格含有 2203 个唯一‘Ingredient.id’。

Table 3: Tables of Herbs compounds and targets

Ingred.....1	Herb_p...	Ingred.....3	Ingred.....4	Target.id	Target...	Databa...	Paper.id	...
HBIN00...	FU LING	10-hyd...	NA	NA	NA	NA	NA	...
HBIN00...	SHAN Z...	11,14-...	(11E,1...	HBTAR0...	NCOA2	NA	NA	...
HBIN00...	SHAN Z...	11,14-...	(11E,1...	HBTAR0...	ACHE	NA	NA	...
HBIN00...	SHAN Z...	11,14-...	(11E,1...	HBTAR0...	PPARG	NA	NA	...
HBIN00...	SHAN Z...	11,14-...	(11E,1...	HBTAR0...	CA2	NA	NA	...
HBIN00...	DANG GUI	1,1,5-...	1,1,5-...	HBTAR0...	PRSS1	NA	NA	...
HBIN00...	CHAI HU	11alph...	11 -me...	NA	NA	NA	NA	...
HBIN00...	CHAI HU	11 -me...	11alph...	NA	NA	NA	NA	...
HBIN00...	SHAN Z...	11-Cyc...	Heneic...	NA	NA	NA	NA	...
HBIN00...	ZE XIE	11-deo...	NA	NA	NA	NA	NA	...
HBIN00...	GAN CAO	11-deo...	11-Deo...	HBTAR0...	NR3C1	NA	NA	...

Ingred.....1	Herb_p...	Ingred.....3	Ingred.....4	Target.id	Target...	Databa...	Paper.id	...
HBIN00...	GAN CAO	11-deo...	11-Deo...	HBTAR0...	AR	NA	NA	...
HBIN00...	GAN CAO	11-deo...	11-Deo...	HBTAR0...	NR3C1	NA	NA	...
HBIN00...	GAN CAO	11-deo...	11-Deo...	HBTAR0...	AR	NA	NA	...
HBIN00...	GAN CAO	11-deo...	11-Deo...	HBTAR0...	NR3C1	NA	NA	...
...

Figure 2 (下方图) 为图 Herbs compounds and targets Network 概览。

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

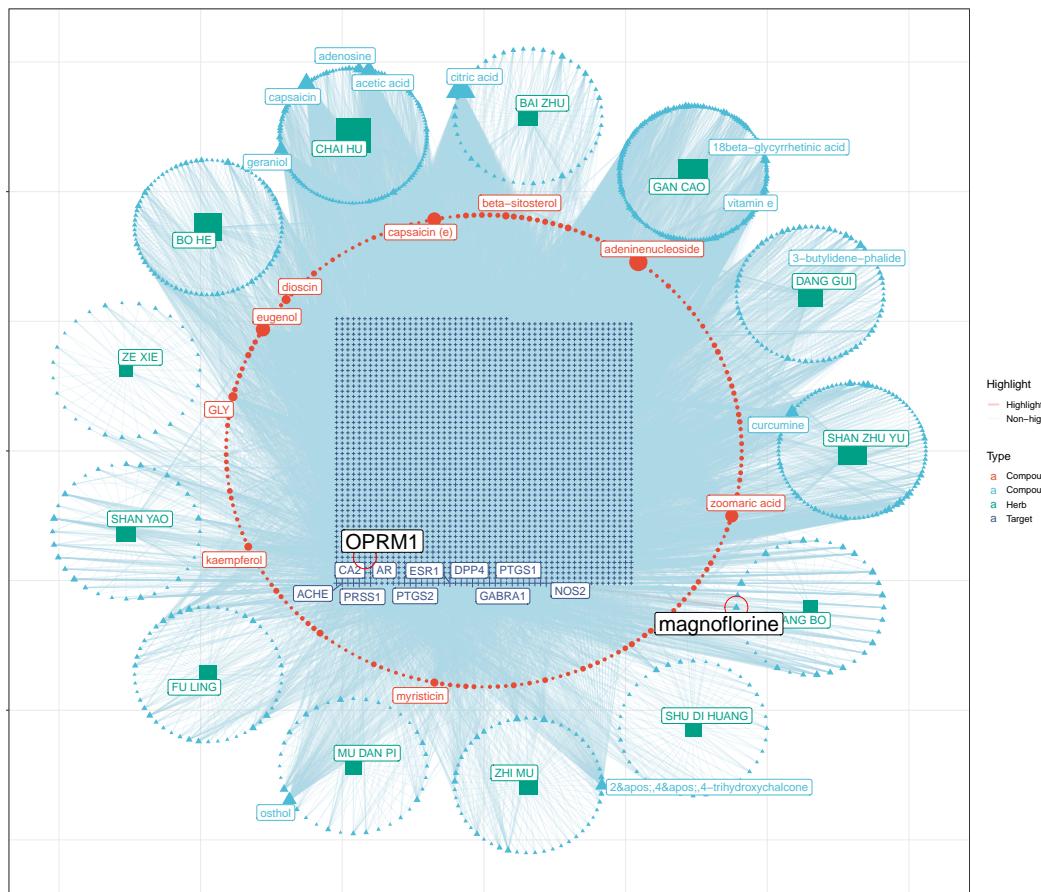


Figure 2: Herbs compounds and targets Network

5.2 分子对接

结合效果不佳 (Affinity 应为负值为佳)

Figure 3 (下方图) 为图 Overall combining Affinity 概览。

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

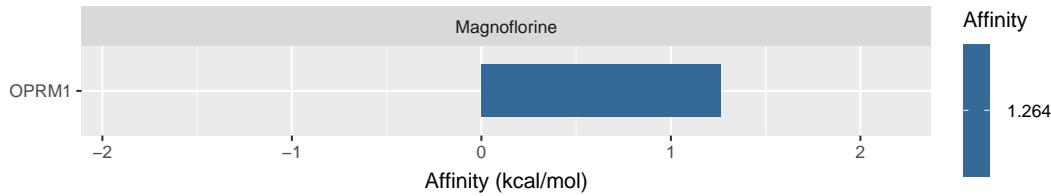


Figure 3: Overall combining Affinity

以下为对接结果示意图 (没有成功，因此没有显示化合物 magnoflorine)

Figure 4 (下方图) 为图 magnoflorine combining with OPRM1 概览。

(对应文件为 ./figs/73337_into_6dde.png)

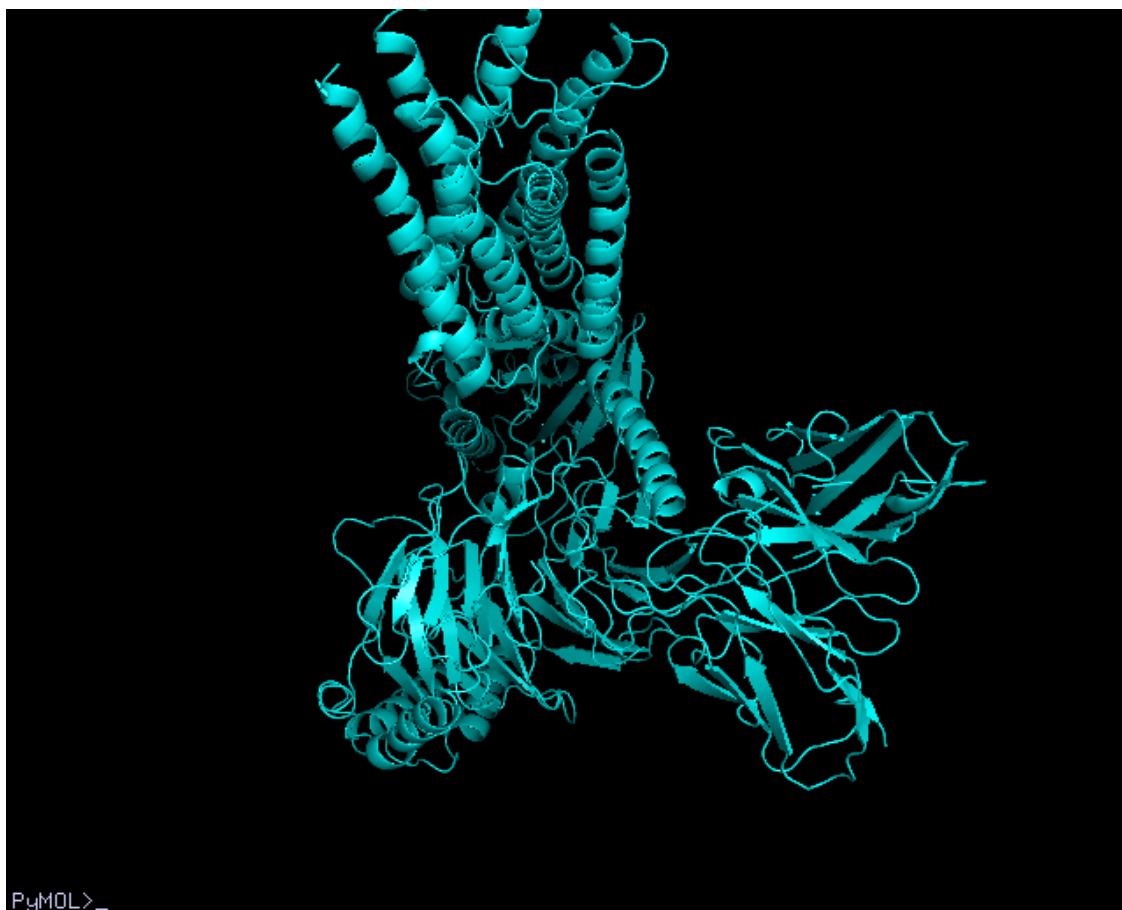


Figure 4: Magnoflorine combining with OPRM1

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. 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).