Hydroxysafflor Yellow A 与 Piezo1 对接

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1 摘要

需求：

Hydroxysafflor Yellow A（InChIKey：IAVUBSCVWHLRGE-UXEKTNMQSA-N）与 Piezo1 对接

结果：

见 Fig. 1

2 前言

3 材料和方法

3.1 材料

3.2 方法

Mainly used method:

- The CLI tools of `AutoDock vina` and `ADFR` software used for auto molecular docking[1–5].
- 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 分子对接

Figure 1 (下方图) 为图 Overall combining Affinity 概览。

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

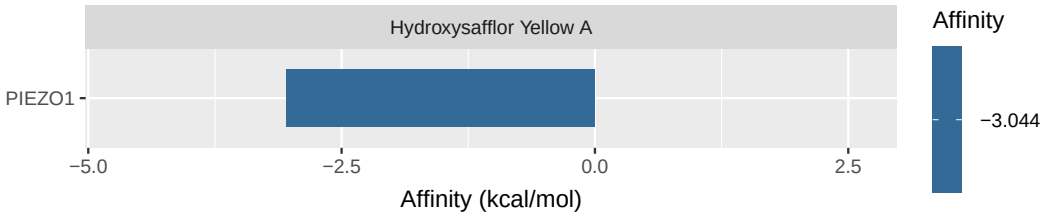

Figure 1: Overall combining Affinity

Figure 2 (下方图) 为图 HYA binding PIEZO1 概览。

(对应文件为 `Figure+Table/6443665_into_piezo1.png`)

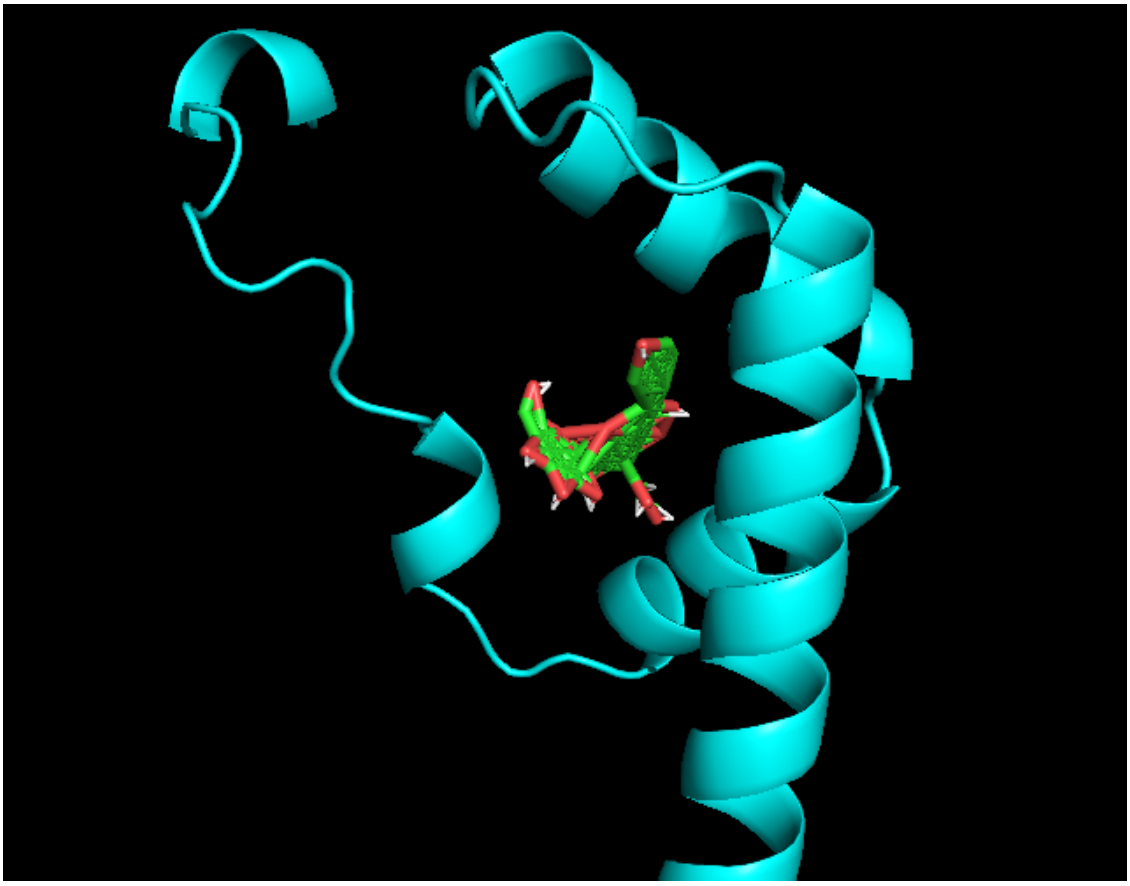

Figure 2: HYA binding PIEZO1

Reference

1. 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).

2. 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).

3. Zhang, Y. & Sanner, M. F. AutoDock crankpep: Combining folding and docking to predict protein-peptide complexes. *Bioinformatics (Oxford, England)* **35**, 5121–5127 (2019).

4. 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).

5. 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).