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BioInformatics Practical - 4

1. Ligand Selection – Aspirin

Docking with Attracting Cavities | Docking with AutoDock Vina

Don't know where to start? Try with an example: binding of **SNJ-1715 (PDB ID 0m6) to calpain-1 catalytic subunit (PDB ID 2g8e)**, of **WRR-99 (r99) to cruzipain (1ewl)**, or of **dabrafenib (p06) to B-Raf (5hie)**.

1 - Submit a ligand

Provide a SMILES `C(CC/C=C\C[C@@H]([C@@H](/C=C/C=C/C=C\C=C\[C@@H](C/C=C\CC)O)O)O)(`

. . . or upload a Mol2 file or a PDBQT file [Choose File]

. . . or input, or modify, or check the molecule **using the sketcher**

. . . or use the **advanced search**

✓ [Prepare ligand] **Reset ligand**

2. Target Protein Search – 1MH1

2 - Submit a target

Provide a PDB id *(e.g. 5hie)* `1MH1`

Choose chain(s) to keep*: Select all, A

Choose heteroatom(s) to keep*: MG A 201, GNP A 200

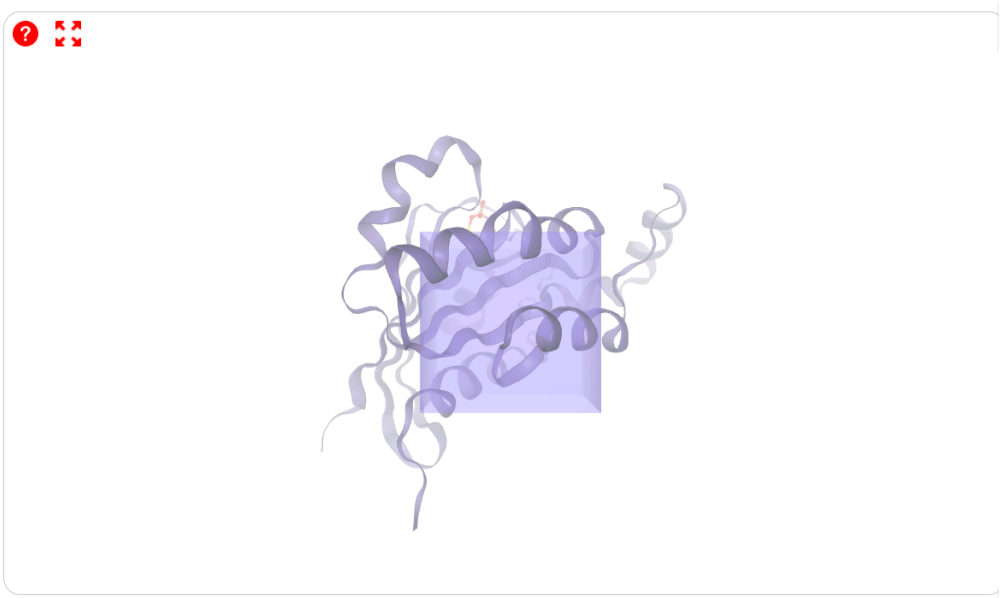
. . . or upload a PDB file or a PDBQT file [Choose File]

. . . or use the **advanced search**

✓ [Prepare target] **Reset target**

3 - Define search space

Search box center	2	32	7	Å
Search box size	20	20	20	Å



Hydrogen bonds | Ionic interactions | Cation-π interactions | Hydrophobic contacts | π-stacking interactions | Show protein surface | Reset

3. Docking Parameters Setup

4 - Select parameters

Sampling exhaustivity 4

Check parameters

This job is estimated to take 0:02:25 (h:mm:ss).

5 - Start docking

Enter an email (optional) gaurangvaghela674@gmail.com

Enter a docking name (optional) Practical 4

START DOCKING **Reset form**

4. Docking Results Summary

Query

Ligand	C(CC/C=C\C[C@@H]([C@@H](/C=C/C=C/C=C\C=C\[C@@H](C/C=C\CC)O)O)O)(O...
Target	1mh1_modified.pdb
Method	AutoDock Vina
Date	October 12, 2025, 7:13 am UTC

Parameters:

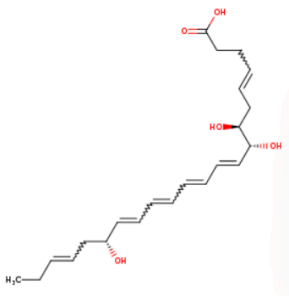
Box center:	2 - 32 - 10	Sampling exhaustivity:	4
Box size:	20 - 20 - 20		

If you publish these results, please, cite the following papers:

Bugnon M, Röhrig UF, Goullieux M, Perez MAS, Daina A, Michielin O, Zoete V. SwissDock 2024: major enhancements for small-molecule docking with Attracting Cavities and AutoDock Vina. *Nucleic Acids Res.* **2024**

Eberhardt J, Santos-Martins D, Tillack AF, Forli S.. AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. *J. Chem. Inf. Model.*, **2021**

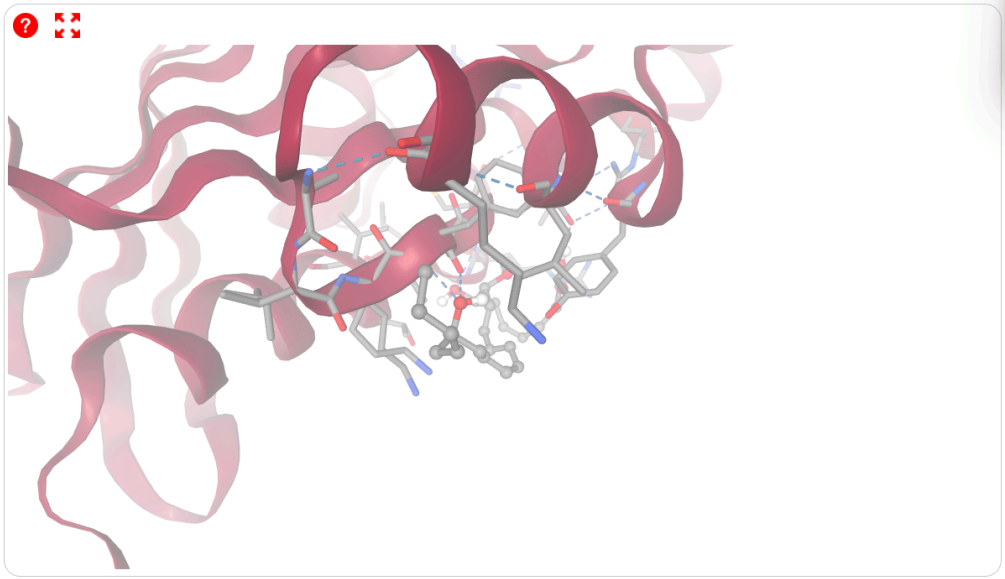
Ligand



5. Best Docking Pose Visualization

Results

Export your results:



Hydrogen bonds | Ionic interactions | Cation-π interactions | Hydrophobic contacts | π-stacking interactions | Show protein surface | Reset

Model	Calculated affinity (kcal/mol)
1	-4.832
2	-4.390
3	-4.380
4	-4.226
5	-4.094
6	-4.032
7	-3.137
8	-2.375