INSTITUTE OF MOLECULAR AND TRANSLATIONAL MEDICINE

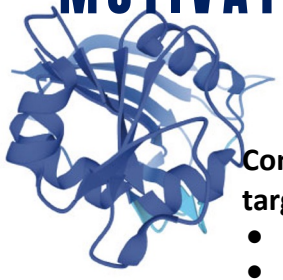
RDKit UGM 2025

EasyDock 1.0: customizable & scalable docking tool

Guzel Minibaeva[1], Vincent Yap [2], Pavel Polishchuk[1]

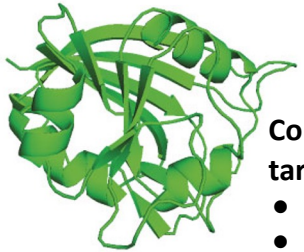
[1]Institute of Molecular and Translational Medicine, Faculty of Medicine and Dentistry, Palacký University, Czech Republic
[2]Nanyang Technological University, Singapore, Singapore

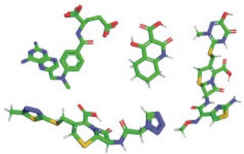
MOTIVATION



Compound and target selection

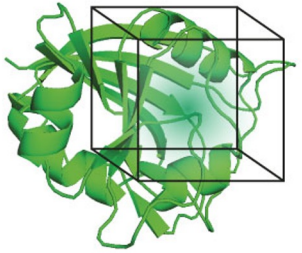
- x-ray protein structure
- SMILES





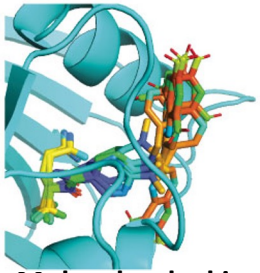
Compound and target preparation

- generate 3D coordinates
- add hydrogens (pH=7.4)



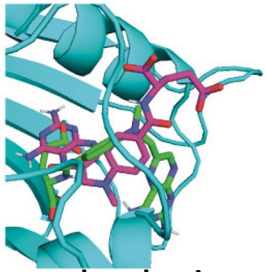
Active site definition

- compute a grid box
- specify the 3D coordinates and box size, based on prospective ligand binding sites



Molecular docking

- explore conformational space
- generate energetically favorable poses



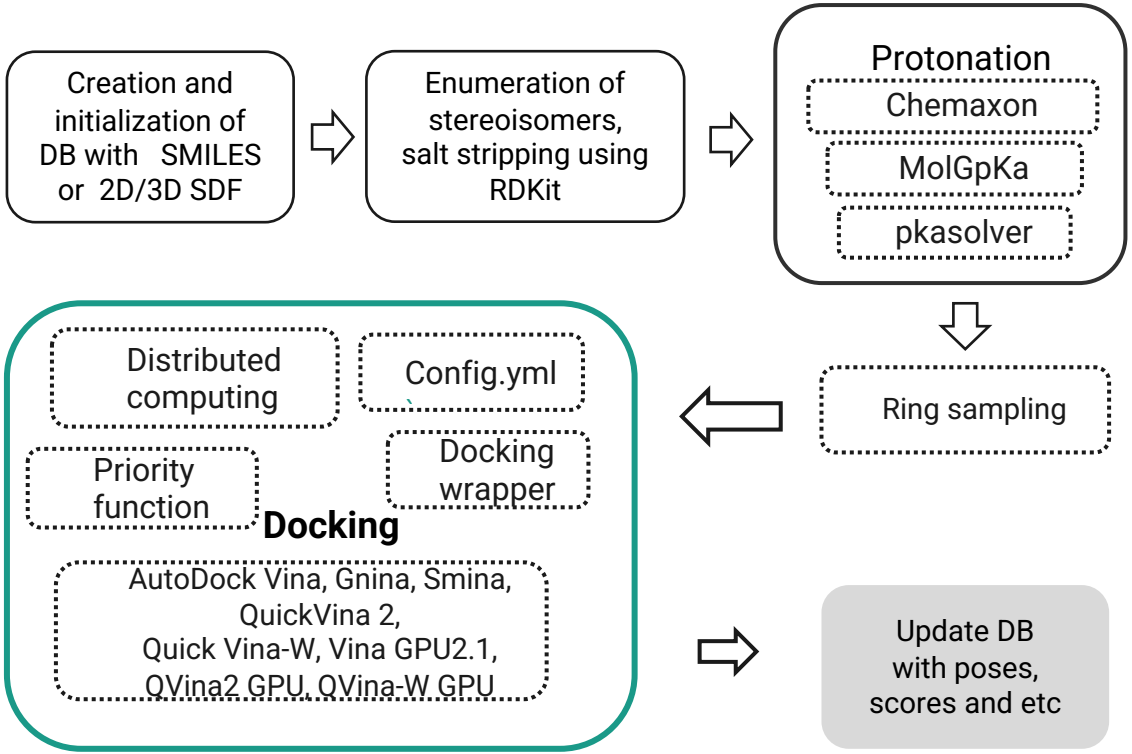
Scoring and evaluation

- rank molecules based on the scoring function

Wong F. et al. Mol Syst Biol. 2022;18(9)

IMTM

EasyDock



- Storage of all input and calculated data in an SQLite DB
- Salt stripping (RDKit)
- Enumeration of stereoisomers (RDKit)
- Optional sampling of saturated rings
- Protonation
- Conversion of conformers into a format for a particular docking program (Meeko)
- Replacement of boron atoms with carbon atoms to enable docking of boron-containing molecule
- Support for interrupted and resumed docking procedures
- Distributed docking with Dask

IMTM

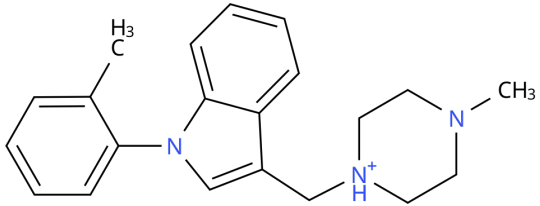
RING SAMPLING

	Program	RMSD ≤ 2	%	Total
The lowest conformer	Vina	644	47.2	1365
The lowest conformer + ring sampling		692	50.9	1360
The lowest conformer	Gnina1.3	907	64.7	1402
The lowest conformer + ring sampling		961	68.5	1402

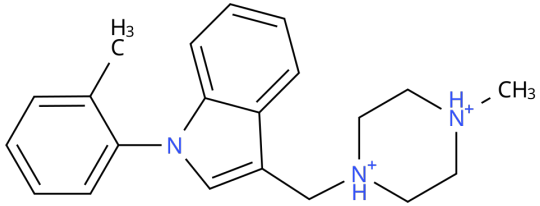
PROTONATION

- Comparison between Chemaxon (commercial license) and MolGpKa (MIT license) at pH 7.4
- Validation on 1,748,091 molecules from ChEMBL33
- 24 hand-crafted rules to fix MolGpKa

Chemaxon

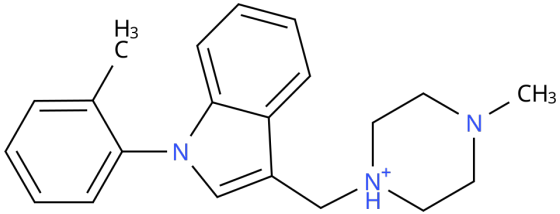


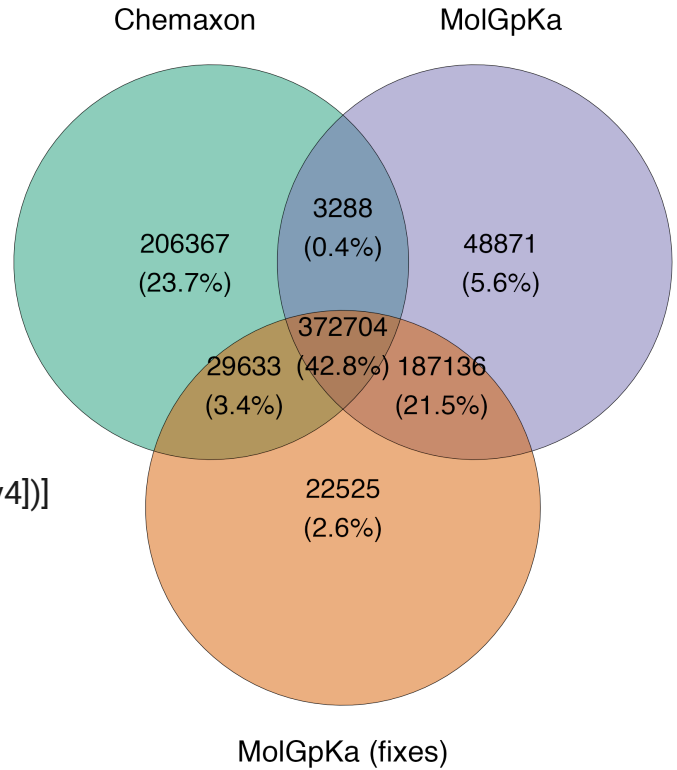
MolGpKa



[#7+;!$([#7+][O-]);!$([#7+H0v4])]**[#7+;!$([#7+][O-]);!$([#7+H0v4])]

MolGpKa (fixes)





https://github.com/ci-lab-cz/easydock

SOFTWARE Open Access

EasyDock: customizable and scalable docking tool

Guzel Minibaeva[1], Aleksandra Ivanova[1] and Pavel Polishchuk[1*]

Operating system(s): Platform independent.
Programming language: Python 3.
Other requirements: RDKit, vina, gnina, dask, meeko, MolGpKa
License: BSD 3-clause.

```
$ pypistats overall easydock
```

category	percent	downloads
with_mirrors	100.00%	4,857
without_mirrors	32.32%	1,570
Total		4,857

```
Date range: 2025-03-12 - 2025-09-08
```

Thank for your attention