

Setup and run automated docking

<https://github.com/ci-lab-cz/docking-scripts>

Install (on own laptops/computers)

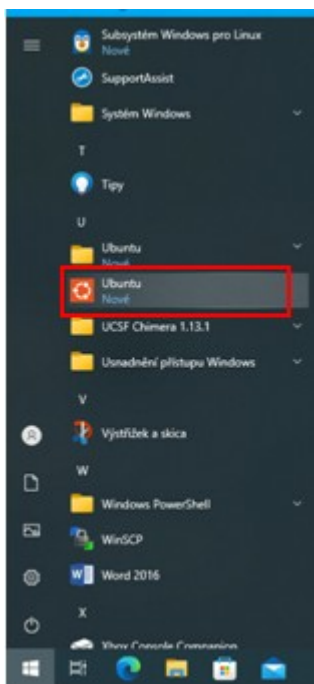
```
conda create -n vina-c conda-forge python=3.9 numpy=1.20 rdkit scipy  
dask distributed vina
```

```
conda activate vina
```

```
pip install meeko moldock
```

Run on computers:

Run Ubuntu on Windows machines



The Ubuntu console will be opened and you have to activate the environment by

```
conda activate vina
```

```

student@DESKTOP-1DPFL93: ~
To run a command as administrator (user "root"), use "sudo <command>".
See "man sudo_root" for details.

Welcome to Ubuntu 22.04.1 LTS (GNU/Linux 5.15.79.1-microsoft-standard-WSL2 x86_64)

 * Documentation:  https://help.ubuntu.com
 * Management:    https://landscape.canonical.com
 * Support:       https://ubuntu.com/advantage

This message is shown once a day. To disable it please create the
/home/student/.hushlogin file.
(base) student@DESKTOP-1DPFL93:~$ conda activate vina
(vina) student@DESKTOP-1DPFL93:~$

```

To run docking on a local machine:

```
vinaDock -i ligands.smi -o out.db -p protein_prepared.pdbqt -s
config.txt --sdf -c 3 -v --no_protonation
```

Top 1 docked poses will be stored in out.sdf file at the same directory as out.db when the docking will finish

To retrieve some other data from db one may use SQLiteBrowser (free cross-platform tool) or by a script:

id	smi	smi_protonated	rce_mol_block	mol_block	docking_score	pdb_block	mol_block	time
1	1ke5_ligand	CNS(=O)(=O)c...	NULL	NULL	-7.882	MODEL 1REMARK ...	1ke5_ligand ...	2023-02-02 09:17:35
2	1ke6_ligand	CNS(=O)(=O)c...	NULL	NULL	NULL	NULL	NULL	NULL
3	1ke7_ligand	O=C1Nc2ccc(-...	NULL	NULL	-9.685	MODEL 1REMARK ...	1ke7_ligand ...	2023-02-02 09:17:52

- get top 2 poses for every ligand

```
get_sdf_from_dock_db -i out.db -o 2.sdf --poses 1 2
```

- apply some additional conditions when retrieving of sdf – retrieve top poses of molecules having docking score below -8:

```
get_sdf_from_dock_db -i out.db -o 3.sdf --add_sql 'docking_score < -8'
--fields docking_score
```