Setup and run automated docking docking

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

Install (on own laptops/computers)

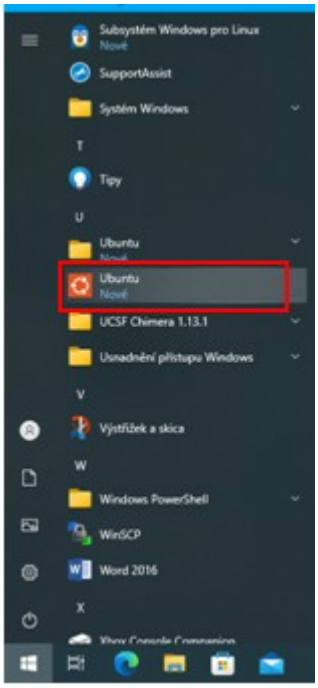
```
conda create -n vina-c conda-forge python=3.9 numpy=1.20 rdkit scipy dask distributed vina
```

```
conda activate vina
```

```
pip install meeko moldock
```

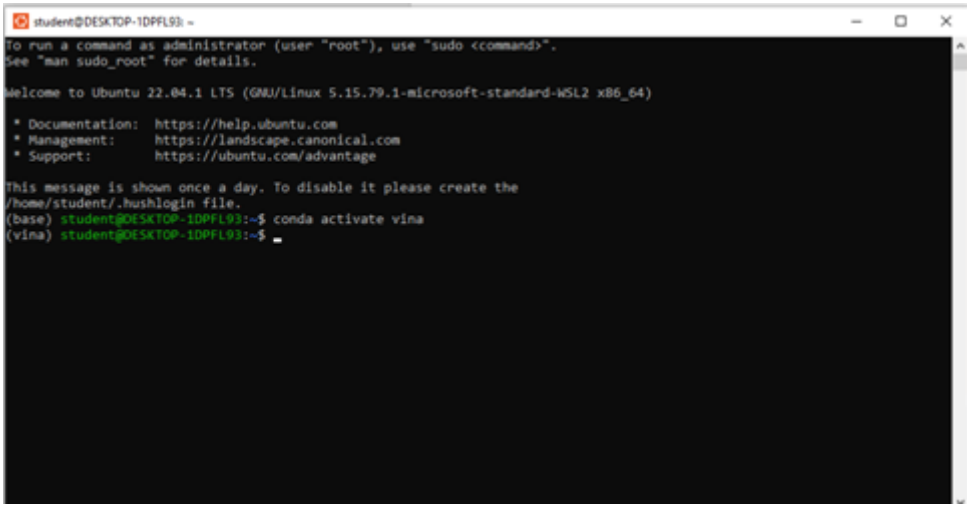
Run on computers:

Run Ubuntu on Windows machines



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

```
conda activate vina
```

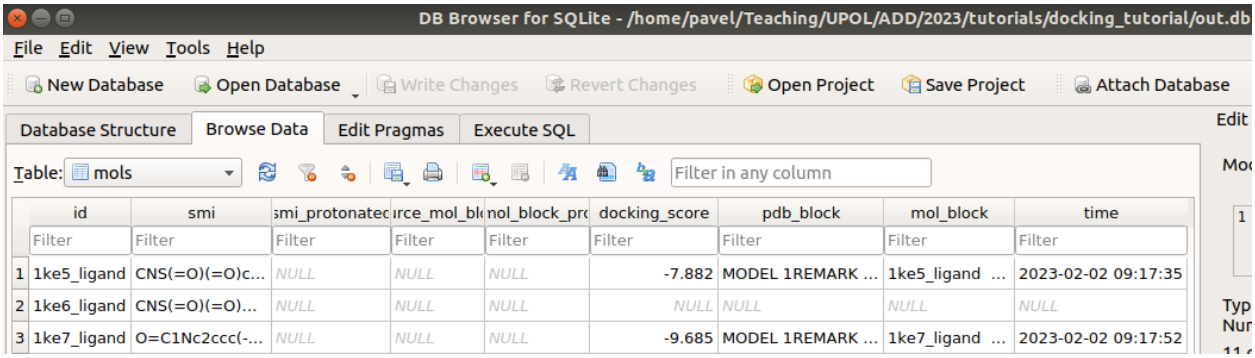


To run docking on a local machine:

```
vina_dock -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:



- 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
```