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AutoDock Vina tutorial

Method · March 2021

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Docking Vina

Prepare **protein.pdbqt** and **ligand.pdbqt** files from Autodock software.

Create directory folder

The directory folder must contain the followings files:

- 1) Protien.pdbqt
- 2) Ligand.pdbqt
- 3) Conf.txt

➡ Lock at the bellow (Configurations file)

Open **cmd** by:

- 1) Hold **Ctrl+ Shift+ right click** , from pup window select **Open command window here**
OR
- 2) from **RUN** type **cmd**

Then, in the **command window** type following commands: (COPY and PASTE)

Cd space (past the directory folder link)

ENTER

"C:\Program Files (x86)\The Scripps Research Institute\Vina\vina.exe" --config conf.txt --log out.txt

ENTER

Wait to complete 100%

"C:\Program Files (x86)\The Scripps Research Institute\Vina\vina_split.exe" --input result.pdbqt

ENTER

Preparation of the configurations file.

Open the text file (**right click**) and write the followings:

receptor = Protien.pdbqt

ligand = Ligand.pdbqt

out = result.pdbqt

center_x =

center_y =

center_z =

size_x =

size_y =

size_z =

exhaustiveness = 8

Then, save as **conf.txt**

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