Multiple Ligand Docking Procedure

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January 2025

Contents

1 Component

- `vina.exe`
- `vina_split.exe`
- `vina_license.rtf`
- `Vina_windows.pl`
- `conf_vs.txt`
- `Ligand.txt`
- `receptor.pdbqt`
- `ligand *.pdbqt files`

2 Steps

STEP-1 Install mgltools, Autdock vina and perl in the Computer

https://ccsb.scripps.edu/mgltools/downloads/

https://ccsb.scripps.edu/mgltools/1-5-7/

https://www.perl.org/get.html

Step-2 We have to prepare

(1) Ligand files

(2) Receptor file

(3) Vina executables

(4) pearl script for automated docking

Step-3 PBDQT format of Multiple ligand and Receptor* .pdb filem which have to be processed to PBDQT format in Autodock Tools. [Here, One forlder has tobe created only for the docking included receptor file, Ligand file, Perl Script, Vina files]

Step-4 Vina files check, Copy and do paste to the Docking folder with a specific name called vina files.

Step-5 Open perl script, there will be an script don't alter

Step-6 Open the process receptor pdb file into pbdqt format in autodock tools

Step-7 Do prepare the Protein (Receptor) using Autodock tools

Edit ¿ Delete Water

Edit ¿ Charges ¿ Add kollman Charges

Repair missing Atoms

Edit ¿ Hydrogen ¿ Add ¿ Polar Only ¿ Ok

Grid ¿ Macromolecule ¿ Choose ¿ Receptor ¿ Select Molecule

Save as receptor.pbdqt

Step-8 Open the vina files ¿ open conf-vs.txt

We have to set the grid box (define the search space) Grid ¿ Grid Box ¿Do Necessary adjustment

Must carefully record these numbers into conf-vs.txt ¿ do input

After inputing infor save the conf txt and leave the Autodock Tools

Put all ligand.pbdqt, Receptor.pbdtqt, Perl script and vina executants in to the newly prepares file

Step-9 New file that has been created will be containing all the prepared

Now need a list of pbdqt ligand files, in order to use by pearl script during repeated docking process (Loop) — Therefore, new txt file "Ligand.txt" has to be created

Step-10 Open command promt by typing cmd in search but must the path will be the drive within.

Use cd command to navigte to your folder that contains all the files essential for docking

3 times need to use cd till the the path comes fully

$$"i : g : E : \ Dokcing\ New - analysis >"$$

Now have to follow the command

$$dir/B > Ligand.txt$$

it will write the file "Lignad.txt"

Now follow the command :

$$perlVina_{W}indows.pl > enter$$

it will promt you to enter name of the ligand file, just type in ¿

$$> Ligand.txt$$

Step-11 The Docking intiates

At the end will have a series of separate log files that contain binding scores required for your analysis

Step -12 Next have to process and summarize all log files to identify the heighest

3 References:

- Bioforphile, 30 Mar 2023, https://youtu.be/LtULkMiaA68?si=92xcZXkHadNrj2AB