For building carbohydrate molecules

GLYCAM-Web | Utilities for molecular modeling of carbohydrates

For building chitin oligomer (tetramer) with Beta1-4 linkage

Click GlcNAc → configuration beta → linkage 1-4 → Click GlcNAc → configuration beta → linkage 1-4 → Click GlcNAc → configuration beta → linkage 1-4 → Click GlcNAc → configuration beta → linkage 1-4 → Aglycon -- OH

Convert chitin to chitosan (by deleting acetyl group) using Pymol or Avogadro program → Avogadro - Free cross-platform molecular editor - Avogadro

Docking

Download MGLtool Autodock Downloads – mgltools (scripps.edu)

Create a folder on your desktop (name it - mgl), install the program in it

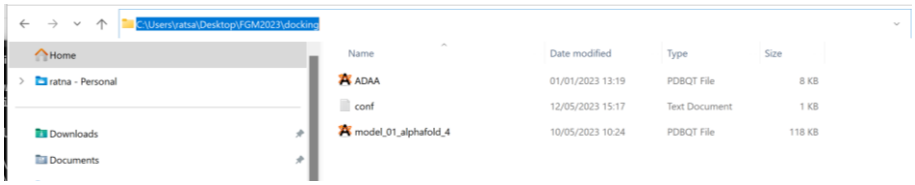
Download autodock vina Downloads – AutoDock Vina (scripps.edu)

Install vina in the mgl folder

i) Open powershell cmd

ii) copy the path of your **docking** folder , as shown below

iii)



In your powershell cmd enter the path like this

cd C:\Users\ratsa\Desktop\FGM2023\docking

(note: cd – change directory)

From mgl folder drag the adt (window batch file) in the powershell window

(note: this step will open the GUI version of mgltool)

1) Preparing protein pdb file for docking in mgltool

In folder docking, move your protein and ligand

Follow the below steps

File --> read molecule -->load protein structure

i) adding hydrogen

edit ---> hydrogens --> add --> polar ----> no bond order

when its required use option edit ---> hydrogens ----> histidine hydrogens

ii) adding charges

edit ----> charges --> kollman charges (for protein)

save the pdb file --> file --> save ---> write pdb

2) Ligand preparation

file ---> open ---> ligand file --> edit add hydrogens all--> atom assign AD4 atomtype ---> add charges (gastegier) --> save ligand

Ligand ----> input --->open (in the right corner from dropdown select pdb or mol2 (depending on your ligand extension) ---> select ligand ----> click ok

ligand ---> torsion tree ---> detect root

ligand --> torsion tree ----> choose torsion ---> green.rotatable --> red.unrotatable--> purple.nonrotatable (purple can be changed to rotable) ---> done

ligand ---> output ----> save as pdbqt

ligand and protein both are prepared for the docking

(ATOM types ---> all hydrogen are assumed able to form a single hydrogen bond so are assigned type ‘HD’ and all oxygens are assumed able to accept hydrogen bonds so are assigned type ‘OA’. Sulphur atoms which can hydrogen-bond are assigned type ‘SA’ while those that cannot are assigned type ‘S’. Nitrogens that can accept hydrogen bonds are assigned type ‘NA’ while those that cannot are assigned ‘N’)

3) Defining docking site

GRId ---> Macromolecule-> open --> (your prepared pdb file)

Grid --> set map---> choose ligand ---> (ligand pdbqt file)

Grid ----> Grid Box--> spacing angstrom 1.000 and then adjust grid box and x,y,z center (adjust grid size)

(hint : usually mgl tool automatically identify the AD4.1_bound.dat but some time not than go to grid --> other options --->parameter file --> D:\mgl\Lib\site-packages\AutoDocktools choose AD4_parameters.dat)

output ---> save gpf (e.g. grid.gpf)

run ----> autogrid ---> choose the saved grid file (grid.gpf) ---> click launch

this take a minute to run and will generate new (grid) files in your folder

(Command line autogrid4 -p grid.gpf -l grid.glg &)

Docking preparation

Docking---->macromolecule ---> set rigid filename

Ligand ----> choose --> open ligand.pdbqt

Docking ---> search parameters ---> choose Genetic Algorithms (leave default settings) click accept

save dock.dpf file

Run- run autodock -- open dock.dfg file and click on launch

this step generate a dock.dfg file in your folder containing all of your docking results

(Command line autodock4 -p dock.dpf -l dock.dlg)

Analysis

Analyze -----> docking ----->open ----> dock.dlg

Analyze --> conformations ---> play and ranked by energy

Docking with autodock VINA

(Note: VINA is better for carbohydrate molecules than Autodock, and it is also easy to handle).

For running VINA, you need a protein and ligand file in pdbqt format generated with MGLtools, and a config file in the following format

conf. txt sample file content

receptor = 2iw0.pdbqt
ligand = A4.pdbqt
center_x =
center_y =
center_z =

size_x =
size_y =
size_z =
#(note: get the above parameters from MGLtool by following the steps **Defining docking site)**

num_modes = 5
out = A4_result1.pdbqt
log = A4_com1.txt
seed = 10
exhaustiveness = 20

To start AutoDock Vina from the command line:

1) Start Vina using a configuration file
2) Open powershell , give the path of vina.exe, e.g.

D:\mgl\vina.exe --config conf.txt

./vina --config conf.txt (on linux or ubuntu)

conf. txt sample file content

receptor = 2iw0.pdbqt
ligand = A4.pdbqt
center_x =
center_y =
center_z =

size_x =
size_y =
size_z =

num_modes = 5
out = A4_result1.pdbqt
log = A4_com1.txt
seed = 10
exhaustiveness = 20

2). Start Vina by explicitly specifying all input parameters:

./vina --receptor protein.pdbqt --ligand ligand.pdbqt \ --center_x 2.5 --center_y 6.5 --center_z -7.5 \ --size_x 22.5 --size_y 22.5 --size_z 22.5 \ --out ind_vina.pdbqt

Jupyter hub muenster

Running the vina on University server → WWU jupyter notebook

https://jupyterhub.wwu.de

1) login with your id

2) create a folder docking and upload the protein, ligand and config file in docking folder
3) upload the vina installation file

enter chmod 777 vina

4) File → new -→ terminal

cd docking

5) run vina by issuing command
   ./vina –config conf.txt

Automatic docking

For automatic docking of several ligand use the script the VS02_f.sh
Put this script in the same folder where you have the docking file
And issue the command

chmod 777 VS02_f.sh

./VS02_f.sh

For opening docking results (On Chimera)

For receptor -→ File → open → receptor file (select pdb from options)

Tools → Binding analysis → View dock -→ *.pdbqt.pdbdt

Open complex.pdb → -→ File → open → complex.pdb

Tools → structure → comparison → match maker -→ receptor protein superimposed on complex.pdb