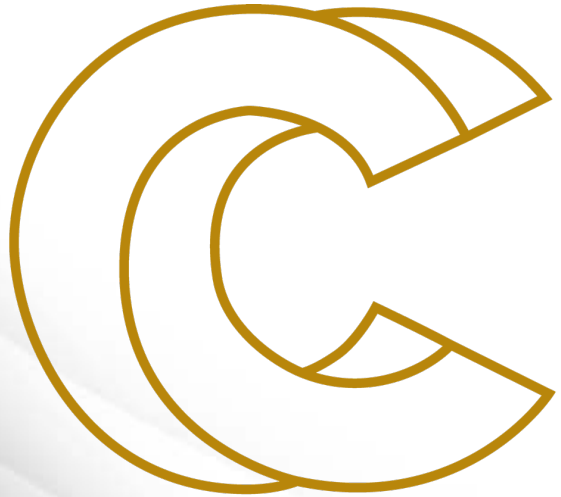

EURO^2

High throughput Virtual Screening with AutoDOCK vina program

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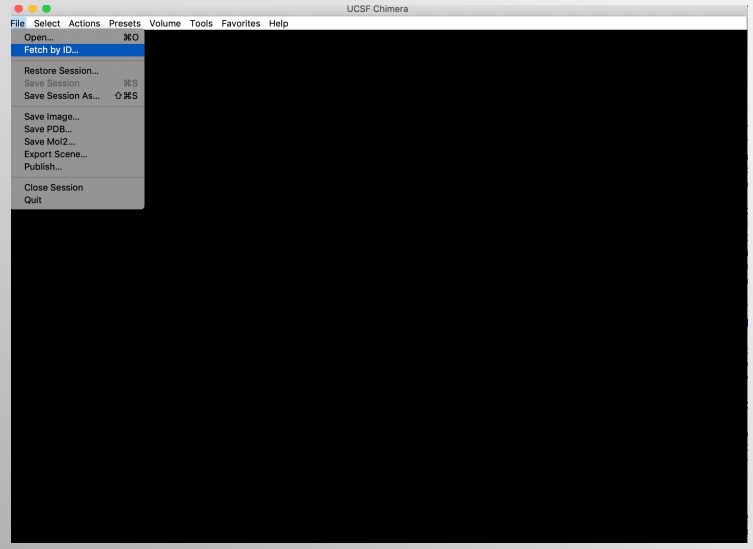
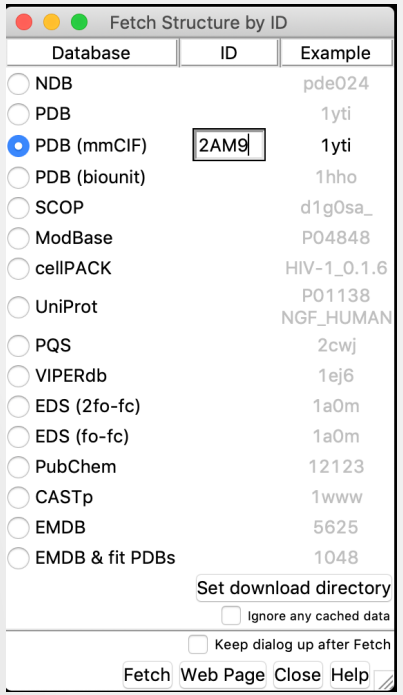
Lesson 1: Preparing protein for docking calculations

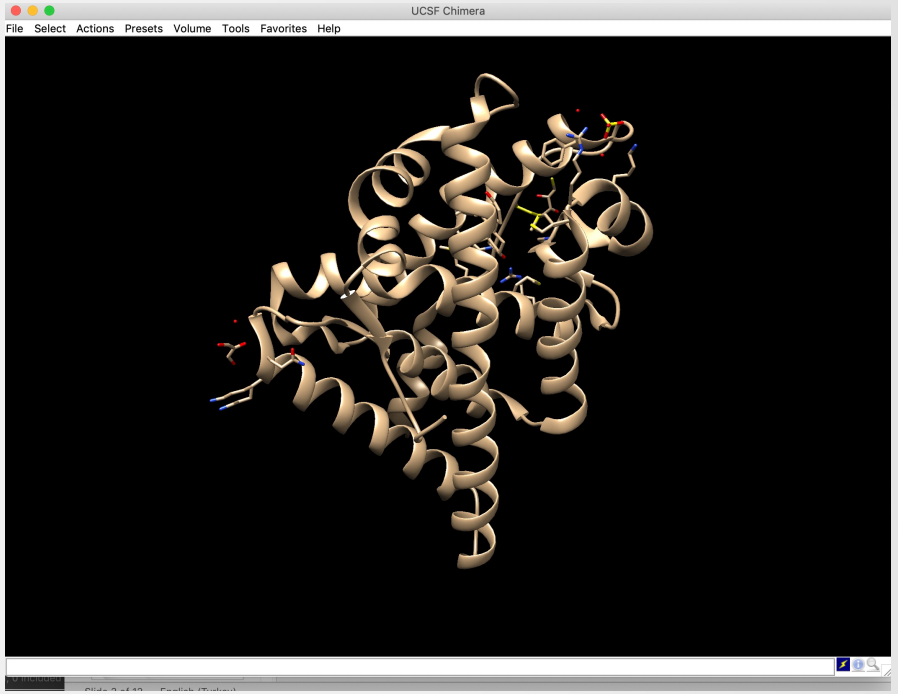
- AutoDock Vina works with a special file format called **pdbqt**.
- We need to create pdbqt file for the protein of interest.
- There are a couple of ways to do this.
- Chimera program, which is a free software, can be used.
- The next slides will guide you how you can create a pdbqt.

Loading the protein pdb file

- From File menu select open or Fetch by ID.
- We will download the protein structure from protein data bank (pdb) that is why we selected fetch by ID menu
- Write 2AM9 to the pdb section and click Fetch.
- It will download the pdb file to your local computer

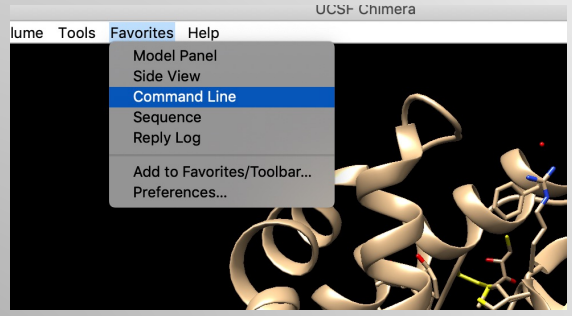


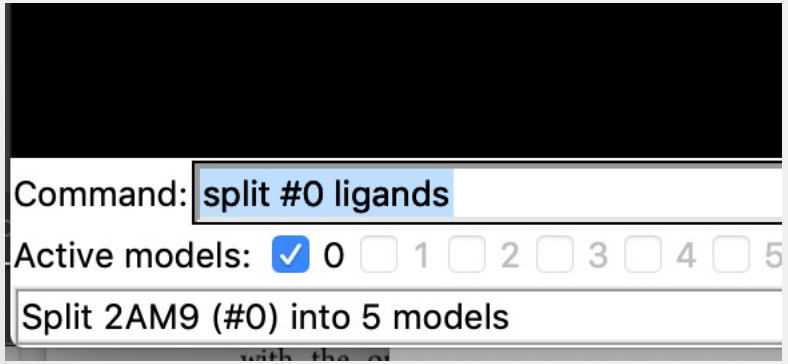




Splitting ligand in the pdb file

- In this pdb file there is ligand in the binding site.
- We will split the pdb file into protein and ligands, this will be useful later when we want to create grid box
- If there is no ligand in the pdb file you work with you can skip this stage
- From Favorites select Command Line
- Type split #0 ligands and press enter
- This will create a separate models for protein and other ligands



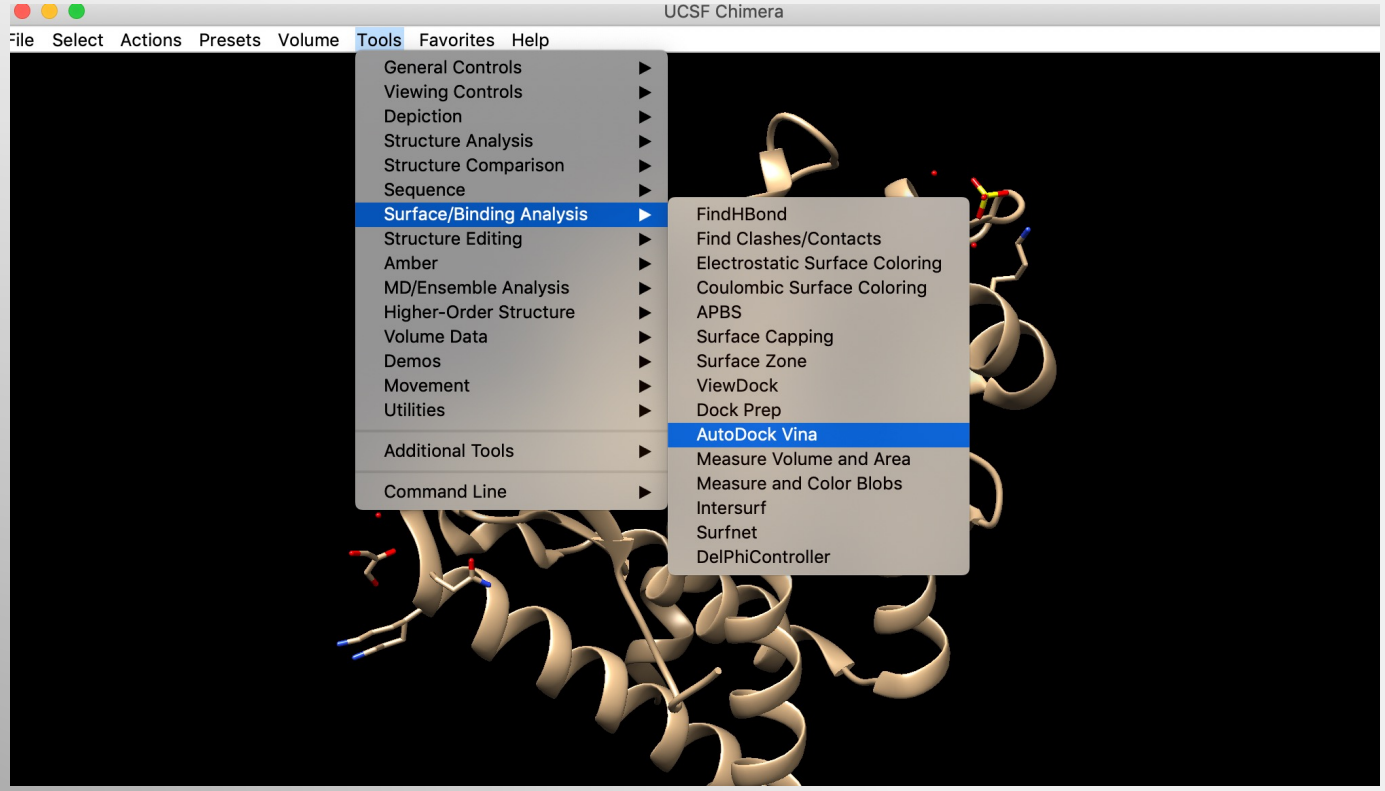


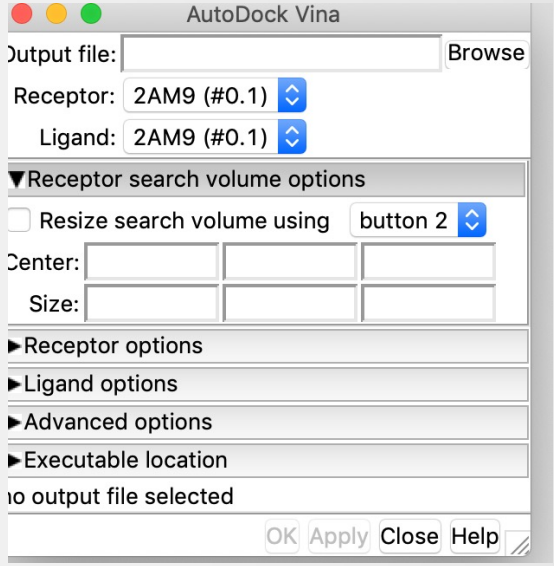
Splitting ligand in the pdb file

- If you click Model Panel under Favorites menu you can see separate models for protein and ligands

Creating pdbqt file

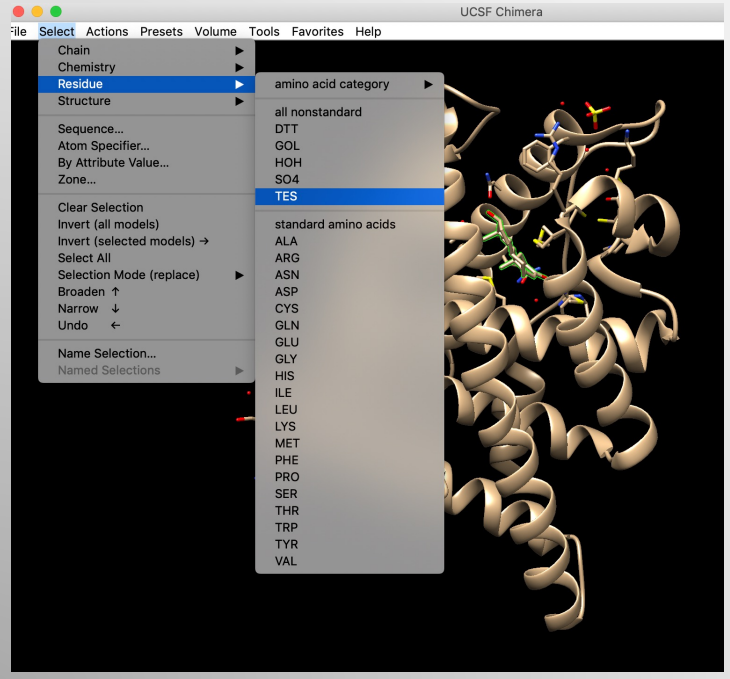
- From tools select first Surface/Binding Analysis and then AutoDock Vina
- Box shown below should appear.

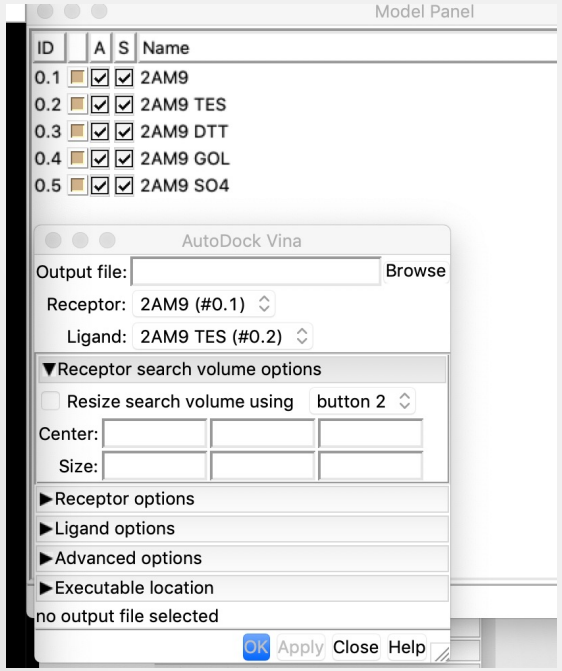


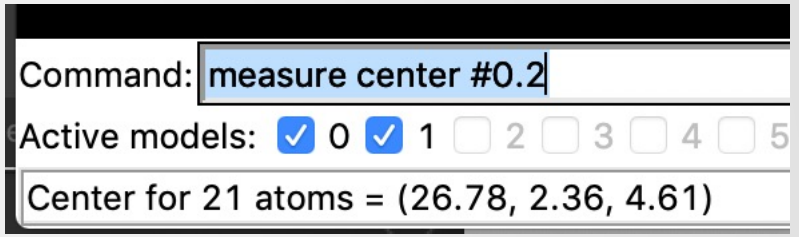


Calculate the center of grid box

- In this protein we will use the center of the ligand as the center of grid box.
- To calculate the center of the grid box in the command line you can type:
- Measure center #0.2
- #0.2 We got this from ID on the Model Panel
- Also you can select the ligand from Select,Residue,TES options

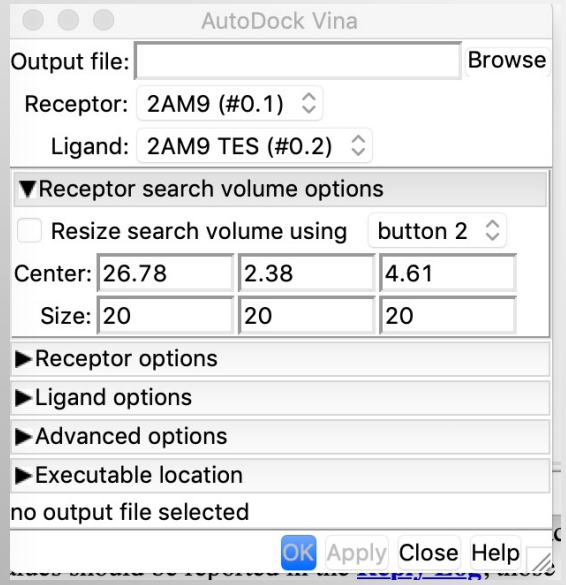


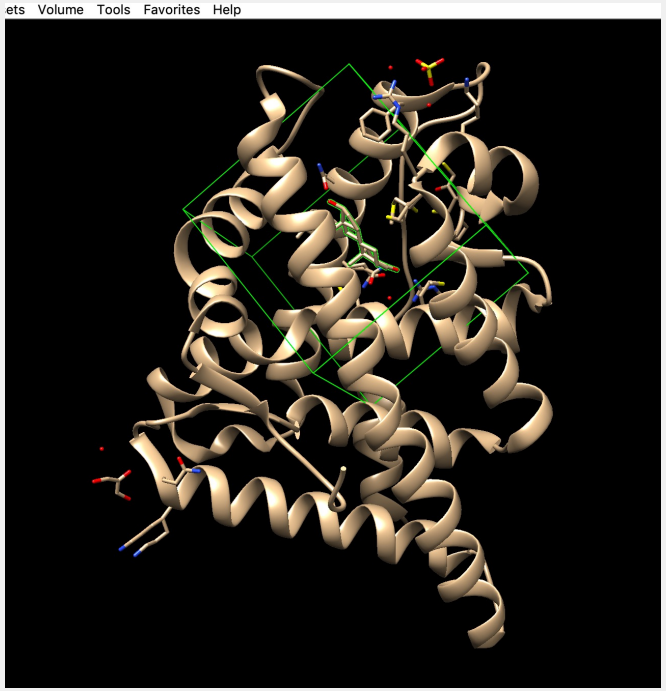




Calculate the center of grid box

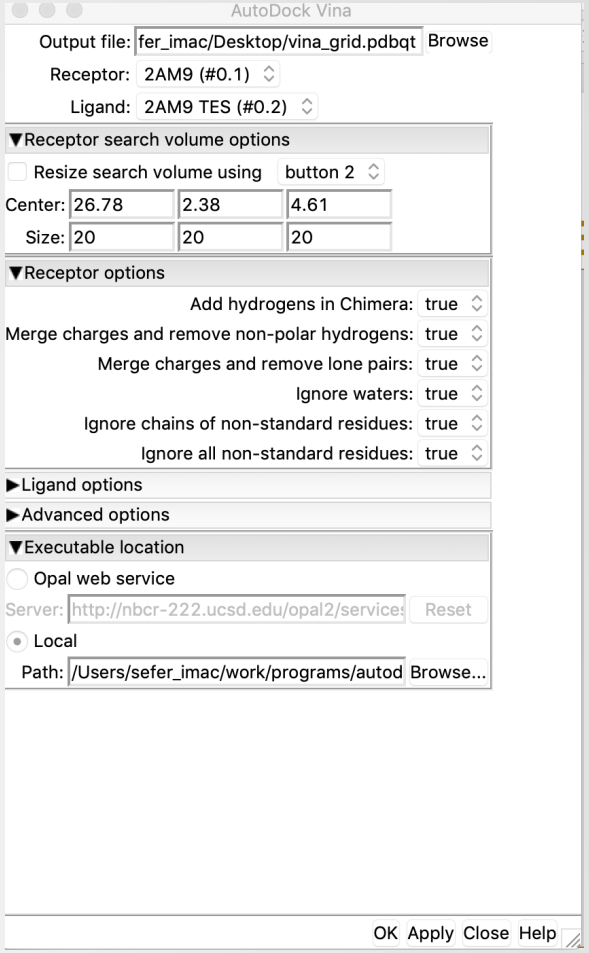
- We write the coordinates of the center we got in the previous slide here Receptor Search Volume options center section.
- For size we can write 20 for each dimension
- Chimera displays the grid box as in green
- You can increase the size depends on the protein you are working.





Calculate the center of grid box

- From the Outputfile menu select the folder you want to write the files
- You can check Receptor and Ligand options menu
- Depend on your protein/ligand you may want to change some parameters.
- Here we continued with default options.
- Last executable location you should put the path for the vina executable file.
- You can get the link in the references to download vina executable.
- Basically, this will dock the ligand to the protein, while docking it will also create receptor pdbqt file



References

- Vina executable file link:
- https://vina.scripps.edu/downloads/
- Chimera program download link
- https://www.cgl.ucsf.edu/chimera/download.html

Copyright

None

Thanks.

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101101903. The JU receives support from the Digital Europe Programme and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia