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C EURO²

High throughput Virtual Screening with AutoDOCK vina program
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Lesson 1: Preparing protein for docking calculations

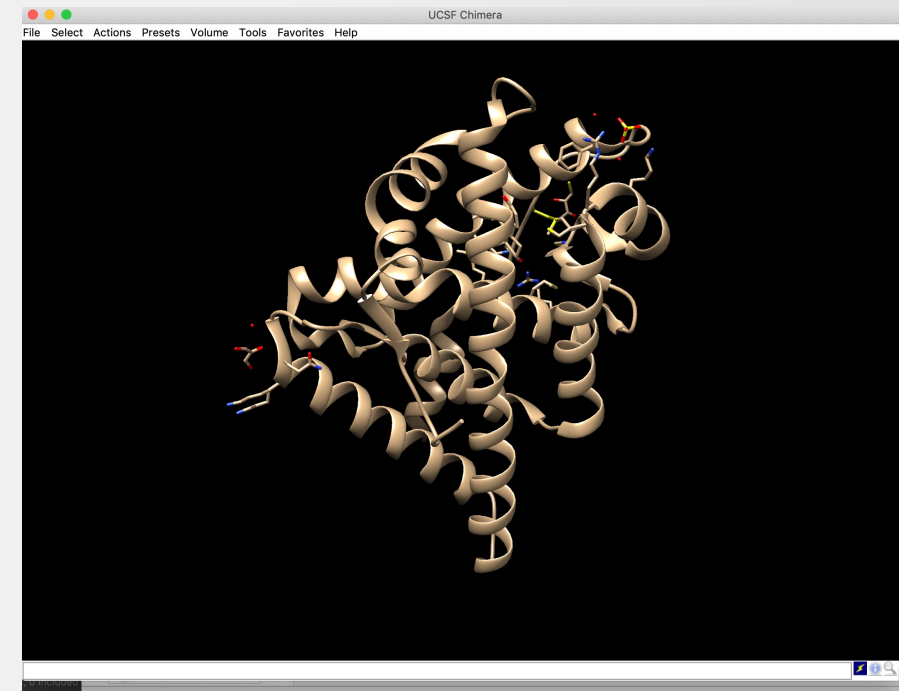
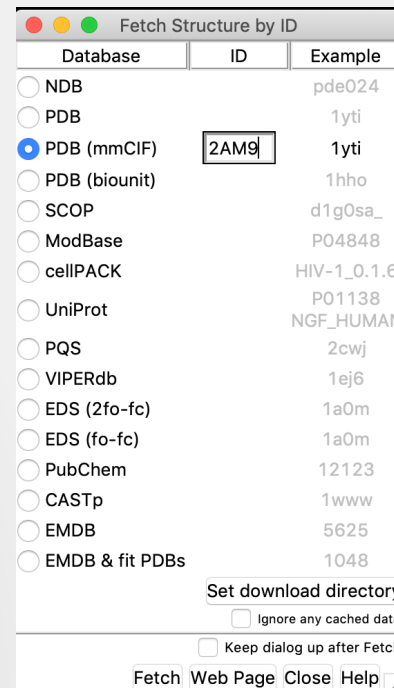
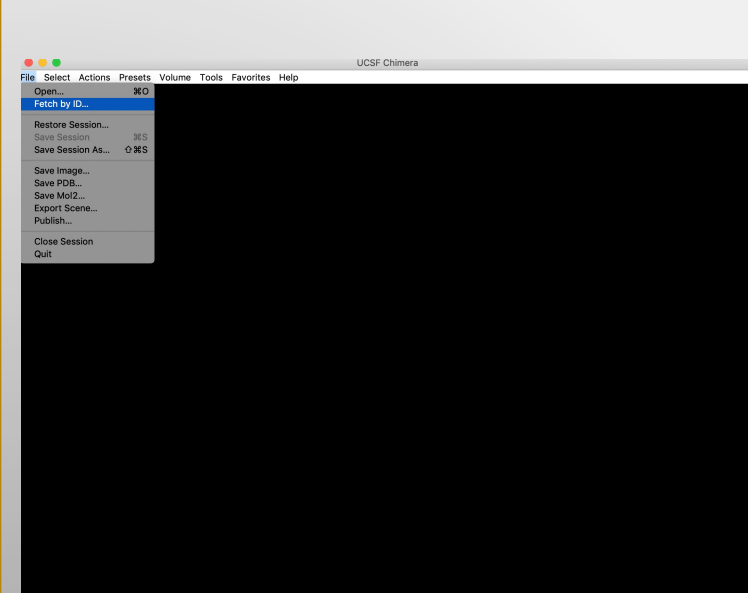


- AutoDock Vina works with a special file format called **pdbqt**.
- We need to create pdbqt file for the protein of interest.
- There are a couple of ways to do this.
- Chimera program, which is a free software, can be used.
- The next slides will guide you how you can create a pdbqt.

Loading the protein pdb file



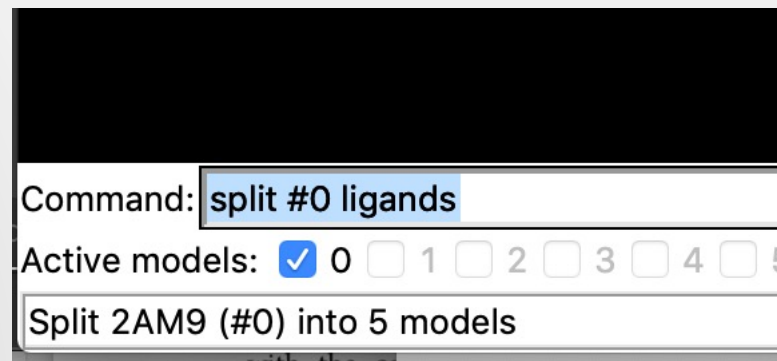
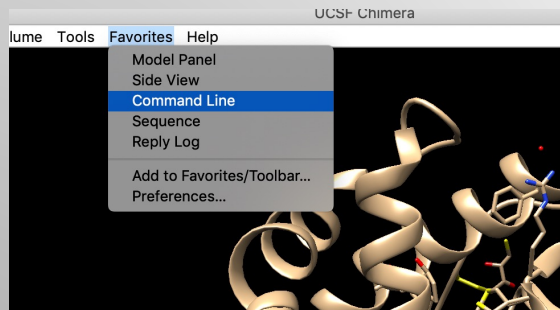
- From File menu select open or Fetch by ID.
- We will download the protein structure from protein data bank (pdb) that is why we selected fetch by ID menu
- Write 2AM9 to the pdb section and click Fetch.
- It will download the pdb file to your local computer



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

The screenshot shows the UCSF Chimera software interface. The main window displays a 3D ribbon model of a protein structure with a ligand. The 'Favorites' menu is open, showing 'Model Panel' as the selected option. To the right, the 'Model Panel' window is open, displaying a table of models and a list of actions.

ID	A	S	Name
0.1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2AM9
0.2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2AM9 TES
0.3	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2AM9 DTT
0.4	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2AM9 GOL
0.5	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	2AM9 SO4

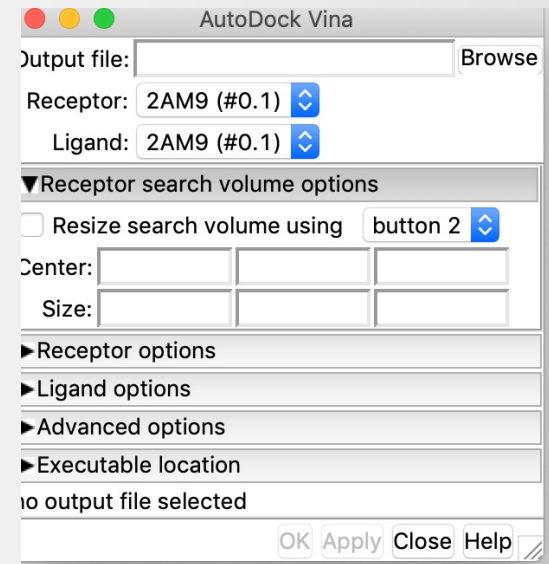
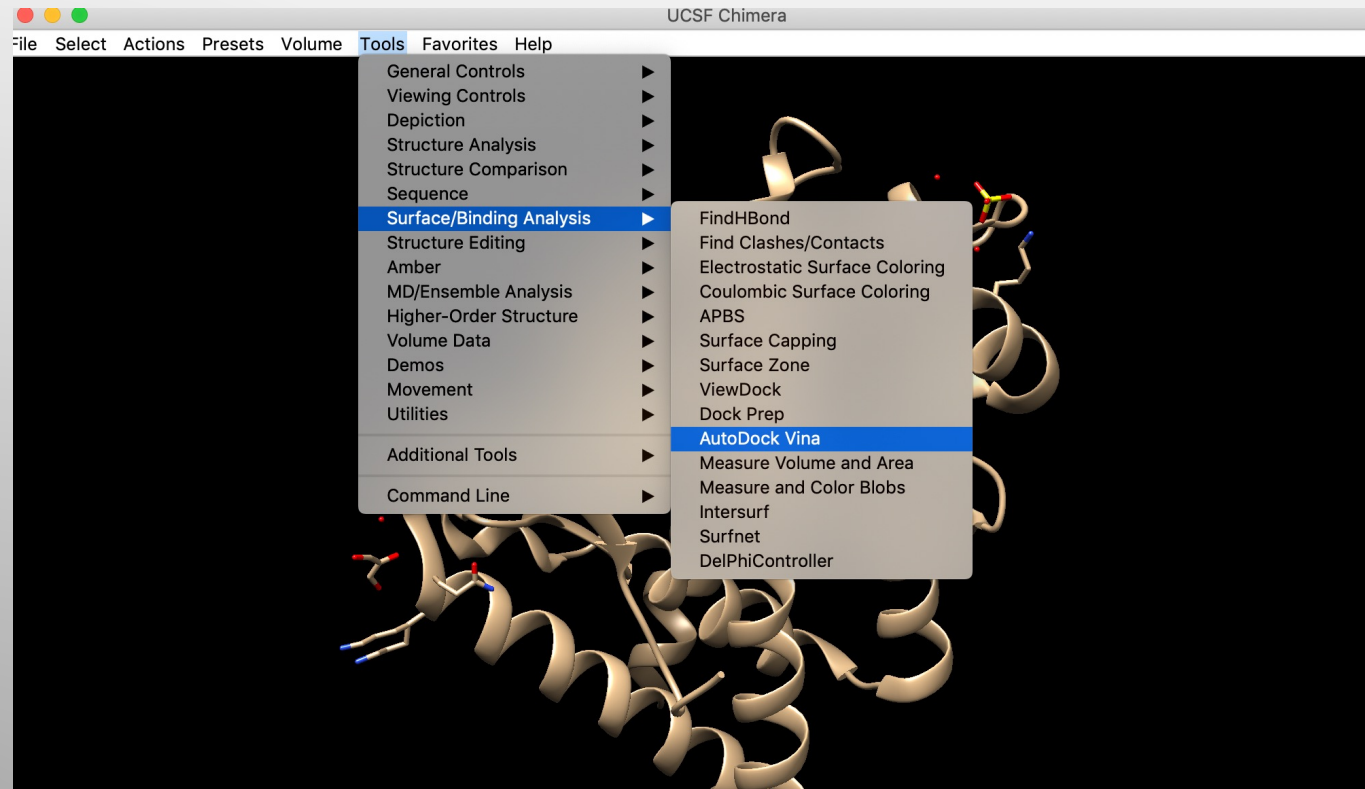
Model Panel actions list:

- activate
- activate all
- activate only
- add/edit note...
- attributes...
- biological unit
- clipping...
- close
- compute SS
- copy/combine...
- deactivate
- group/ungroup
- hide
- match...
- Ramachandran plot...

Creating pdbqt file



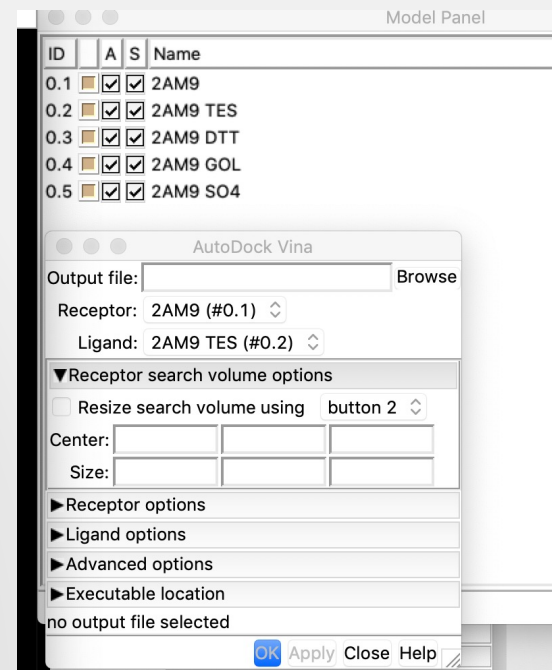
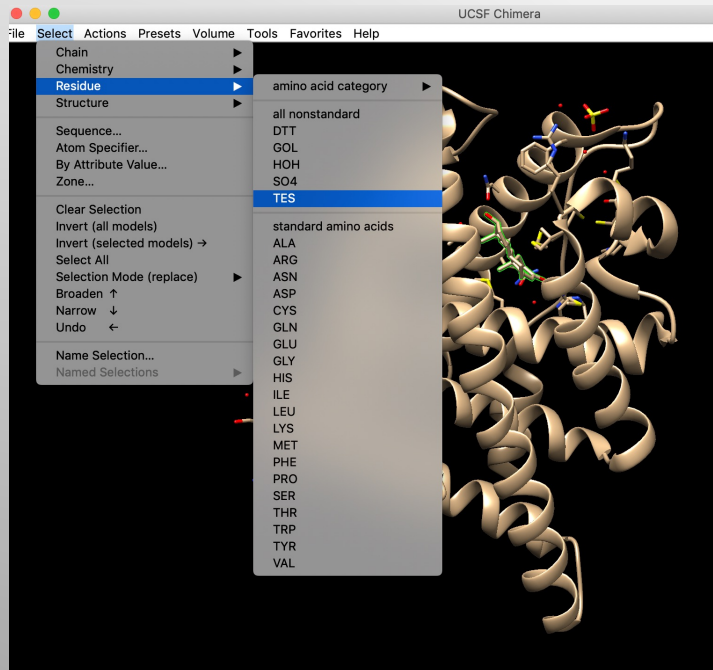
- From **tools** select first **Surface/Binding Analysis** and then **AutoDock Vina**
- Box shown below should appear.



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



Command: `measure center #0.2`

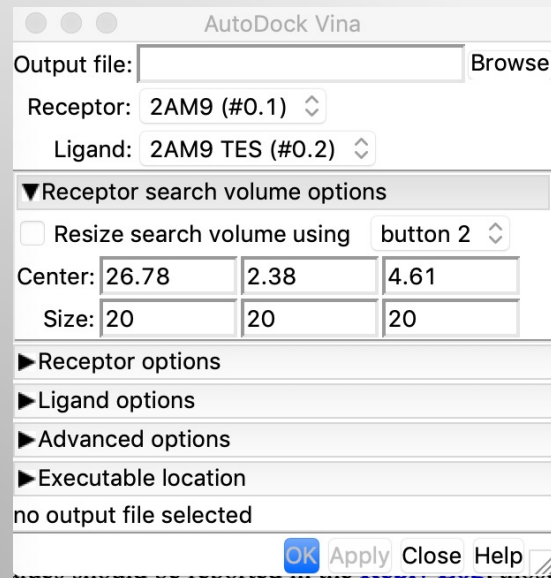
Active models: 0 1 2 3 4 5

Center for 21 atoms = (26.78, 2.36, 4.61)

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

The screenshot shows the AutoDock Vina graphical user interface. The window title is "AutoDock Vina". The "Output file" is set to "fer_imac/Desktop/vina_grid.pdbqt". The "Receptor" is "2AM9 (#0.1)" and the "Ligand" is "2AM9 TES (#0.2)".

Receptor search volume options:

- Resize search volume using: button 2
- Center: 26.78, 2.38, 4.61
- Size: 20, 20, 20

Receptor options:

- Add hydrogens in Chimera: true
- Merge charges and remove non-polar hydrogens: true
- Merge charges and remove lone pairs: true
- Ignore waters: true
- Ignore chains of non-standard residues: true
- Ignore all non-standard residues: true

Ligand options:

- Advanced options

Executable location:

- Opal web service
- Server: <http://nbc-222.ucsd.edu/opal2/service/> [Reset]
- Local
- Path: /Users/sefer_imac/work/programs/autod [Browse...]

Buttons at the bottom: OK, Apply, Close, Help.

References



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

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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