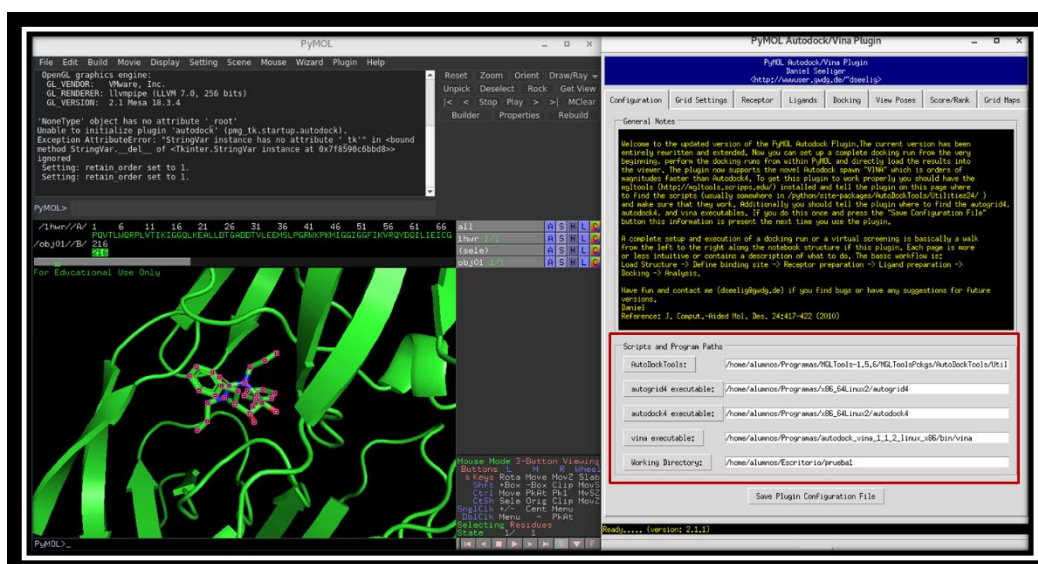
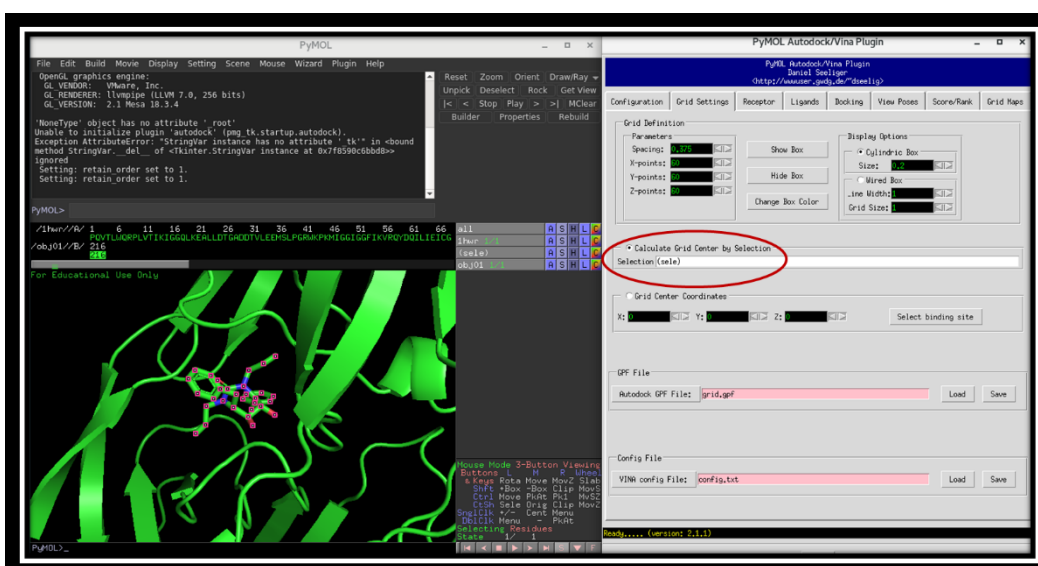


Get your docking done in less than twenty steps!

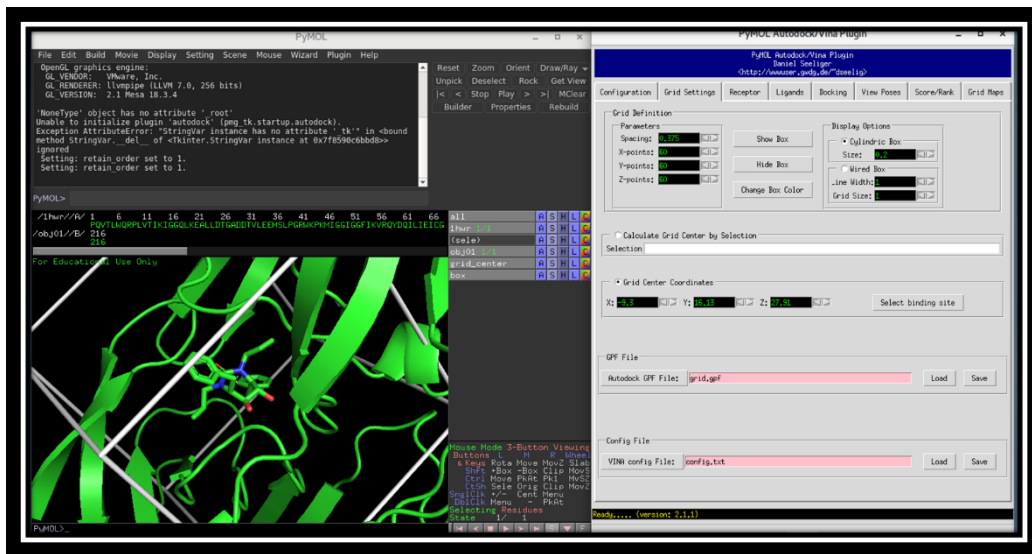
1. Download the desired PDB ID from the RCSB Protein Data Bank.
2. Open the PDB file using PyMOL, extract the ligand and export it in a file with mol2 format; save the receptor in a file with pdb format.
3. **OPTIONAL** Use [H++ server](#) to check the protonation state of ionizable groups in the receptor. Once the calculation is done, download .top and .crd files from the server, and use cpptraj to generate a new pdb file.
4. Using PyMOL, check the structure of the ligand and add hydrogen atoms, if necessary, with PyMOL's Builder module.
5. **OPTIONAL** Use sqm program to optimize the geometry of the ligand and to calculate charges.
6. Open AutoDock Vina plugin using the route Wizard-Plugings-Legacy Plugins-Autodock Vina.
7. Check routes and working directory:



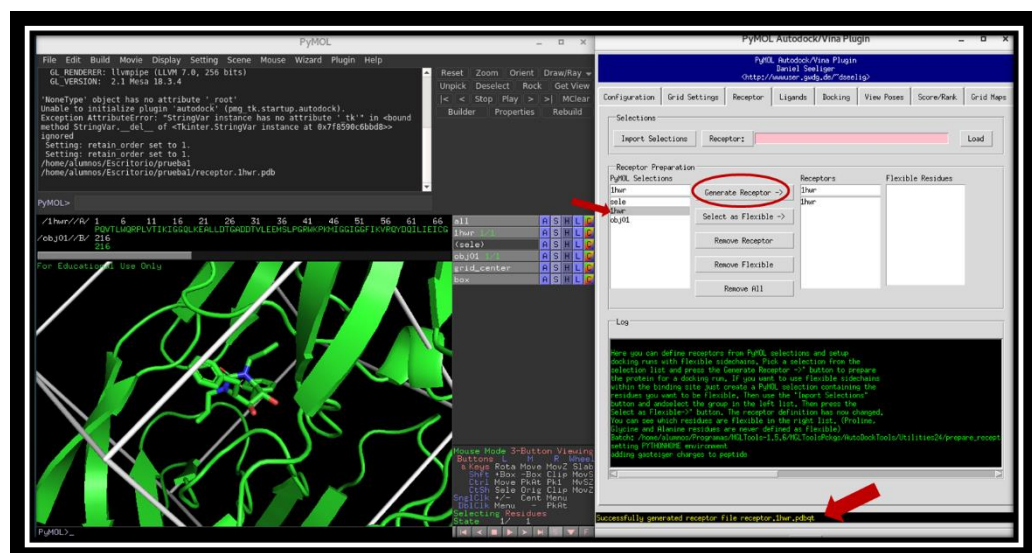
8. Calculate grid center by selection:



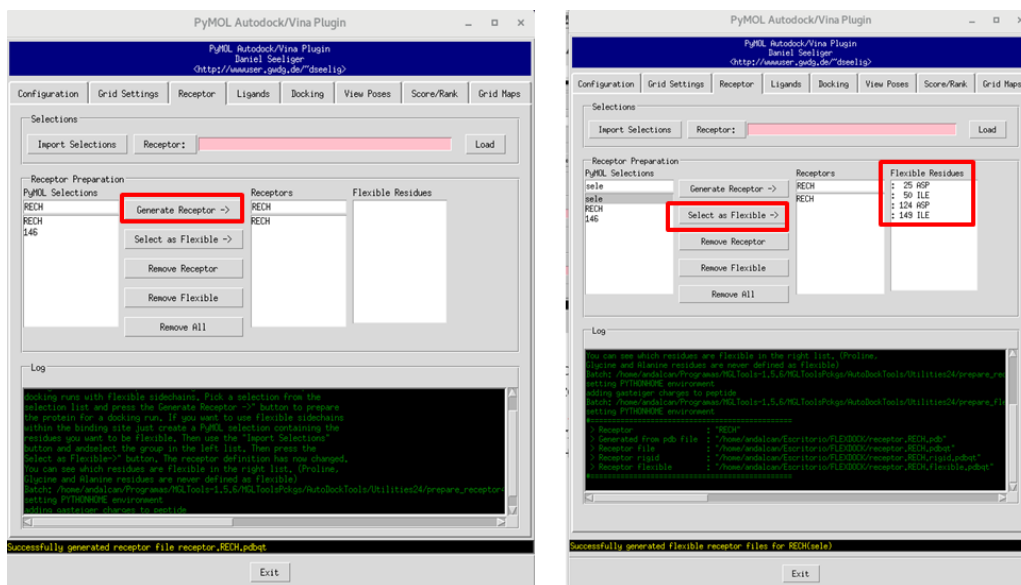
9. Once you enter the selection, do not forget to press the Enter key, and then, the docking box appears:



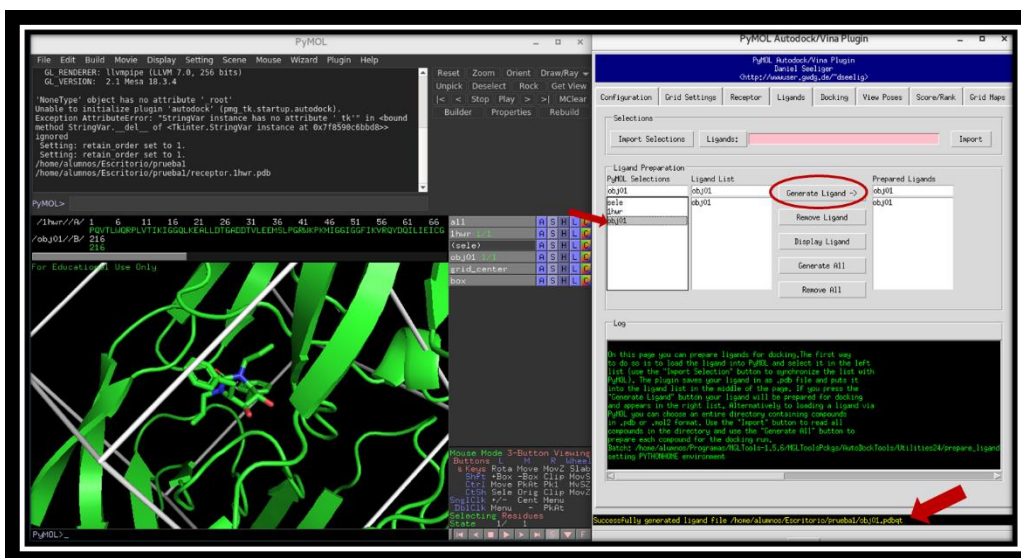
10. Generate receptor:



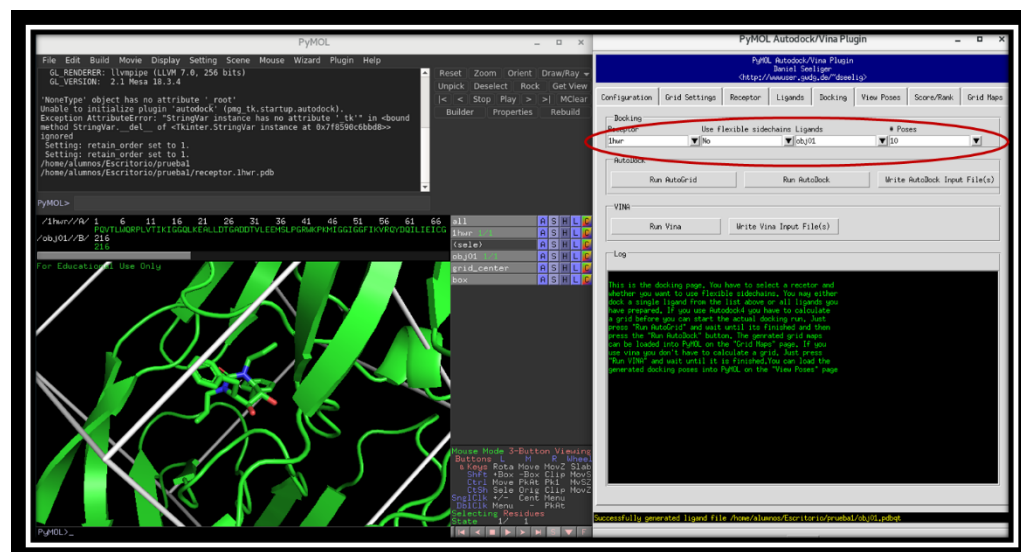
11. OPTIONAL Set up flexible residues. Select residues using PyMOL, generate the receptor and then Select as Flexible. You should see the selected residues on right hand side window:



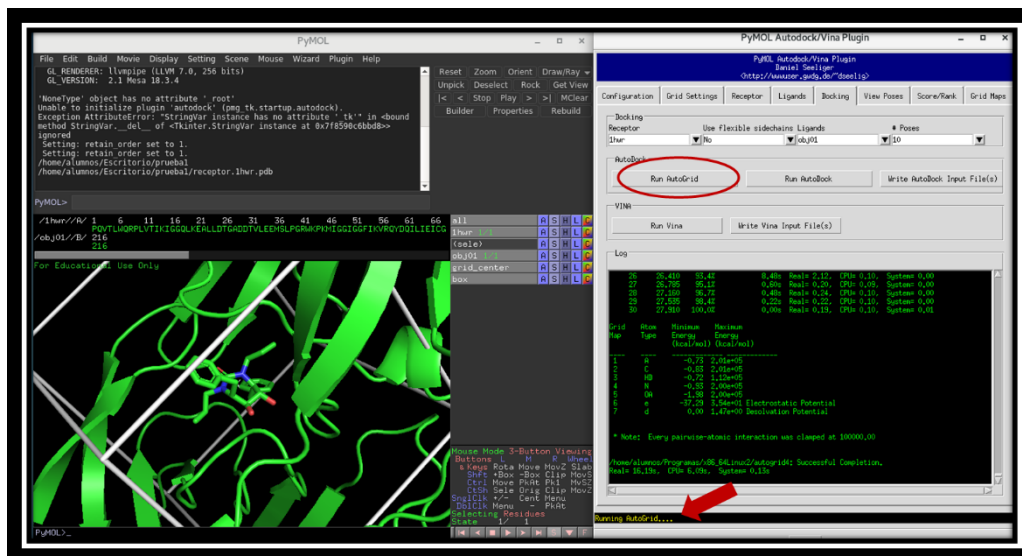
12. Generate ligand:



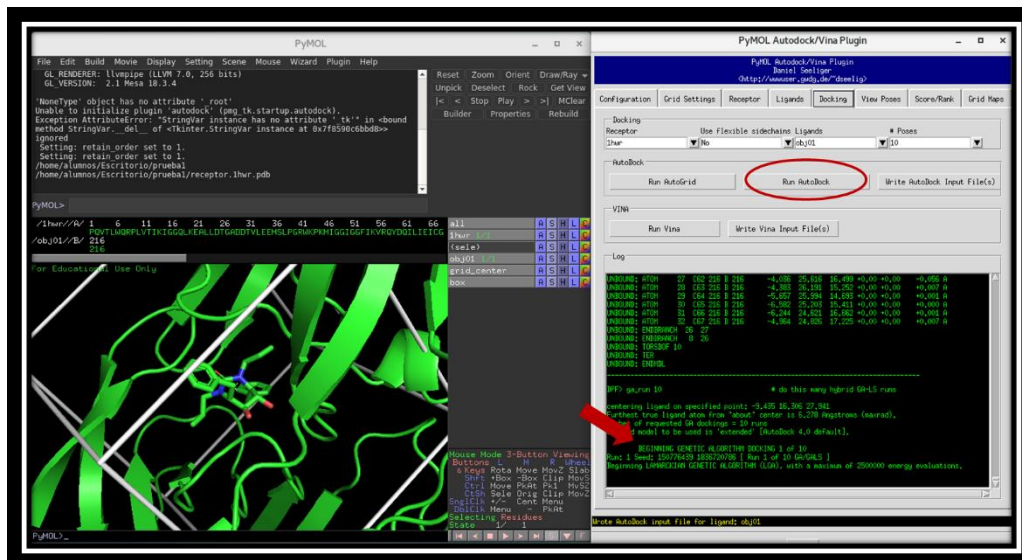
13. Select receptor, ligand and number of poses:



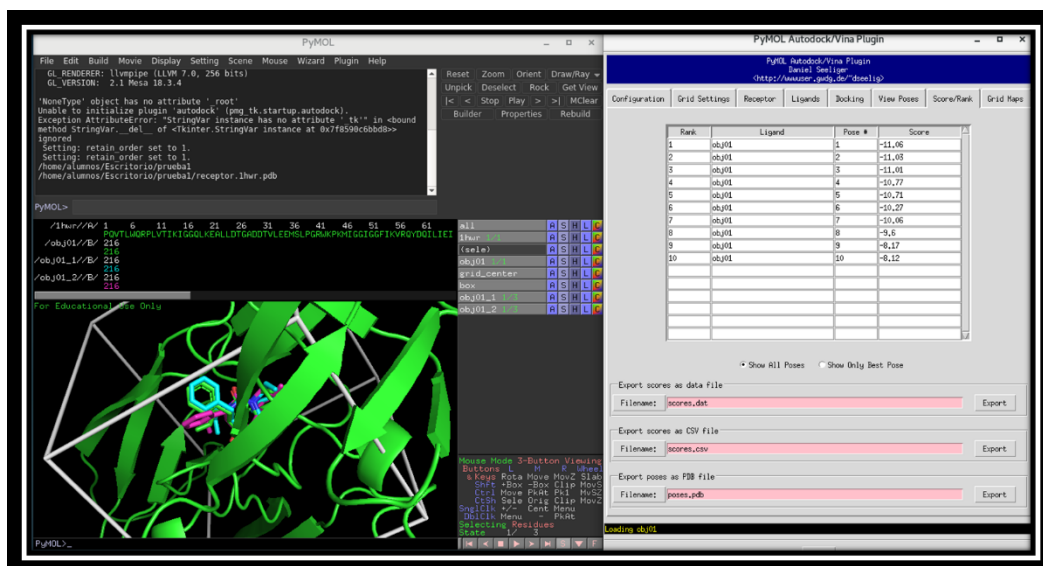
14. Run AutoGrid:



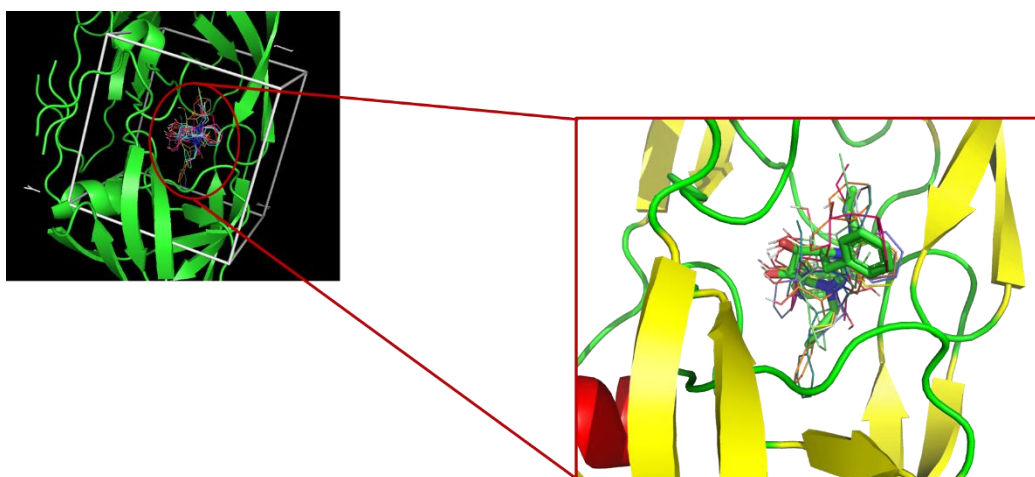
15. Run AutoDock:



16. Or run AutoDock Vina:



19. Visualize results:



20. Write down the center and size of the docking box (will be used later when running Autodock Vina from script):

```

press the "Run AutoDock" button. The generated grid maps
can be loaded into PyMOL on the "Grid Maps" page. If you
use vina you don't have to calculate a grid. Just press
"Run VINA" and wait until it is finished. You can load the
generated docking poses into PyMOL on the "View Poses" page
#-----
# SETTING UP VINA RUN
> RECEPTOR RIGID      : /home/andalcan/Escritorio/FLEXDOCK/receptor.RECH.rigid.pdbqt
> RECEPTOR FLEXIBLE  : /home/andalcan/Escritorio/FLEXDOCK/receptor.RECH.flexible.pdbqt
> CENTER X : -9.06
> CENTER Y : 15.67
> CENTER Z : 27.93
> SIZE X   : 26.25
> SIZE Y   : 22.5
> SIZE Z   : 22.5
> LIGAND(S) : 146
> # POSES    : 10
#####
# If you used AutoDock Vina in your work, please cite:
#
# O. Trott, A. J. Olson,
# AutoDock Vina: improving the speed and accuracy of docking
# with a new scoring function, efficient optimization and
# multithreading, Journal of Computational Chemistry 31 (2010)

```