We, research group at Andhra University humbly present here AUDocker, a self executable software tool to aid virtual screening using AUTODOCK Vina, one of the most useful Docking software available online.

Problems with Vina:

1. Usage is not flexible for virtual screening of larger libraries
2. No continuity in case of power failure or accidental shutdown – very common in common computer labs
3. Alignment of docking results, especially for larger libraries.

Although some tools are available like VcPPT are available to answer this problem, continuity of work remained a problem, which is very common in degree colleges. You cannot expect a continuous power supply in most of the desktops running with UPS (home versions can hold upto 1hour).

THIS PROGRAM IS DESIGNED TO ENCOURAGE STUDENTS AND RESEARCHERS TO EVEN WORK AT HOME AND DOCK USING ORDINERY DESKTOPS

Things to remember:

1. Keep all files (protein rigid file, protein flexible file, ligand files) in the same folder
2. Always name flexible file as protein nameflex.pdbqt. **example-** proteaseflex.pdbqt, for the protein protease.
3. Install Python 2.5, PyMol, ADT, Vina and .net framework in your system by following their respective installation instructions.
4. Vina installation in systems running on Windows 7 is not successful, so you may copy the installation folder given in the software and copy it into C:\ folder.

This manual is prepared presuming that the user is familiar with AUTODOCK environment and steps.

How to use this software?

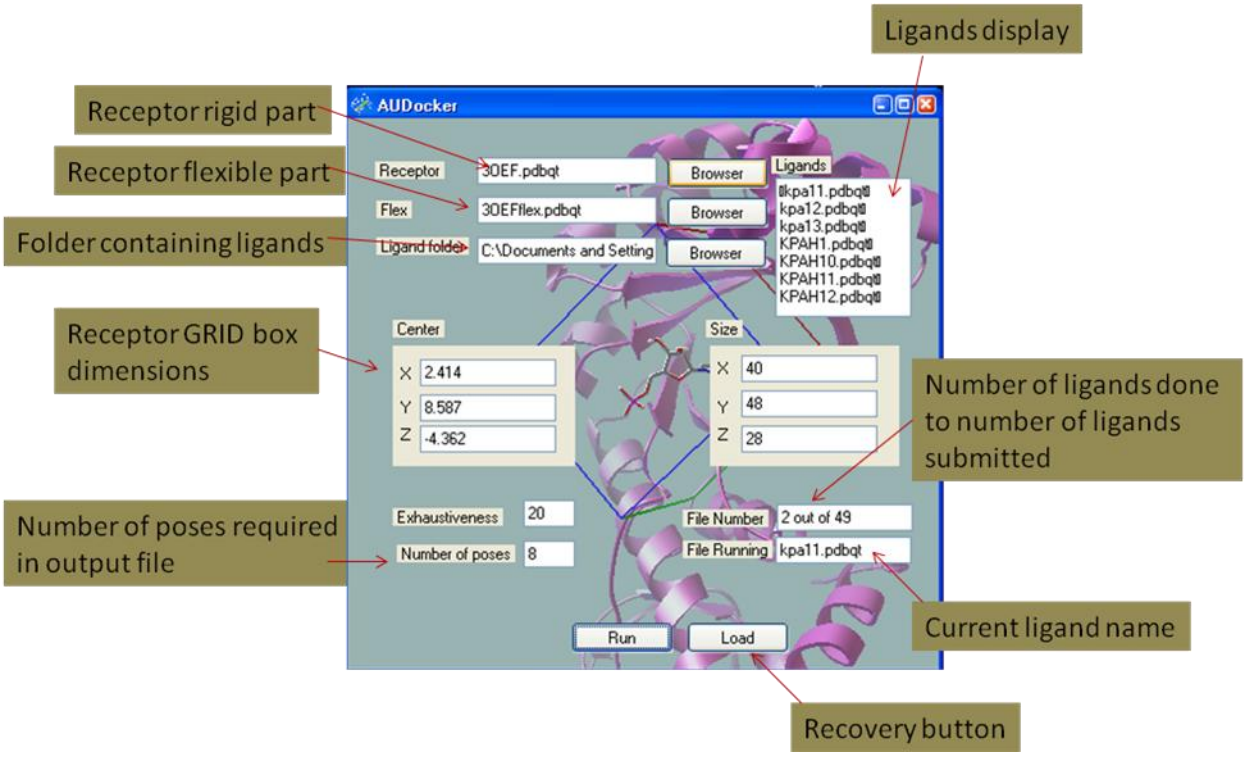
Download the software tool AUDocker.rar and double click on the file to see the GUI of AUDocker

The Standard Steps using AUTODOCK Vina, which are to be performed prior to usage – (Please consult AUTODOCK user manual for detailed information)

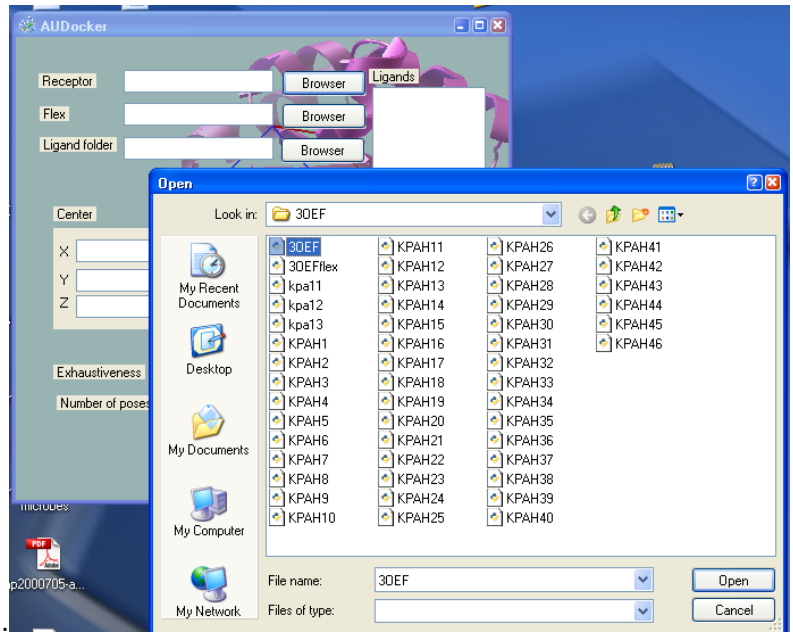
1. protein.pdbqt (rigid file)
2. prepare flexible part of protein and save it as flex.pdbqt file (you may give any name but ***don't forget*** to use flex in the file name)
3. Prepare library of compounds to be docked in .pdbqt.

#keep all these files in the same folder and give it the name of your protein (CONSIDER THIS AS WORKING DIRECTORY).

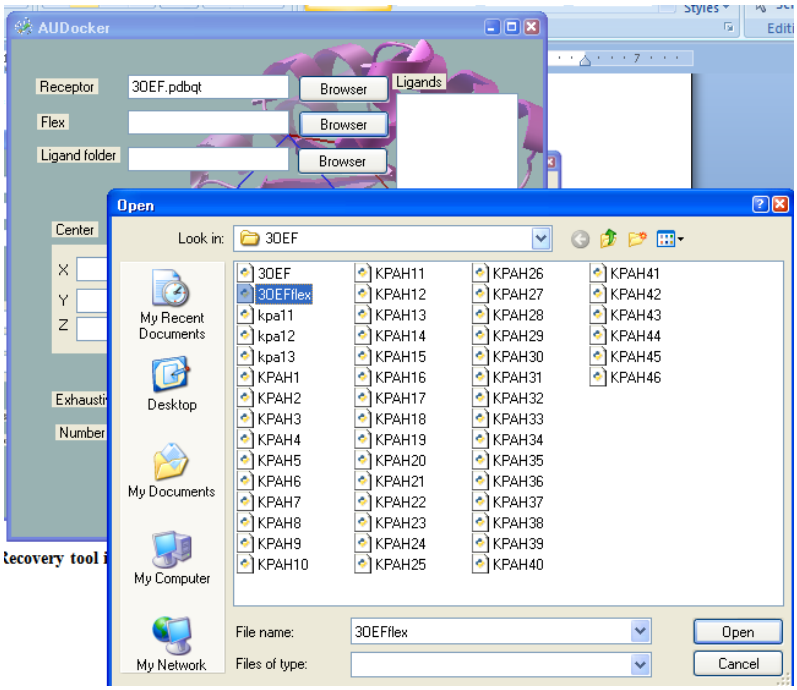
4. Optimize the GRID parameters for the receptor pocket and note down the center_x, center_y, center_z and size_x, size_y, size_z values.
5. Select exhaustiveness value depending on the computational power of your system and requirement (1 to 100)
6. Select the number of poses depending on your requirement (1 to 20)



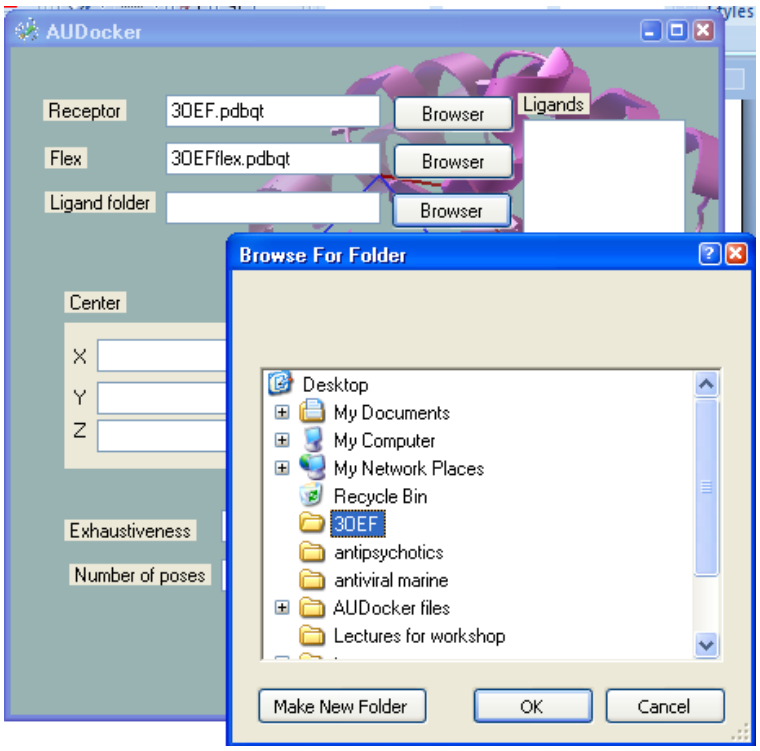
1. Selection of protein – Click on the ‘browse’ button for receptor and open the folder in which you have saved your protein rigid file and select the file.



2. Flex file- Select the flex.pdbqt file in the same manner. This entry is required only for flexible docking.

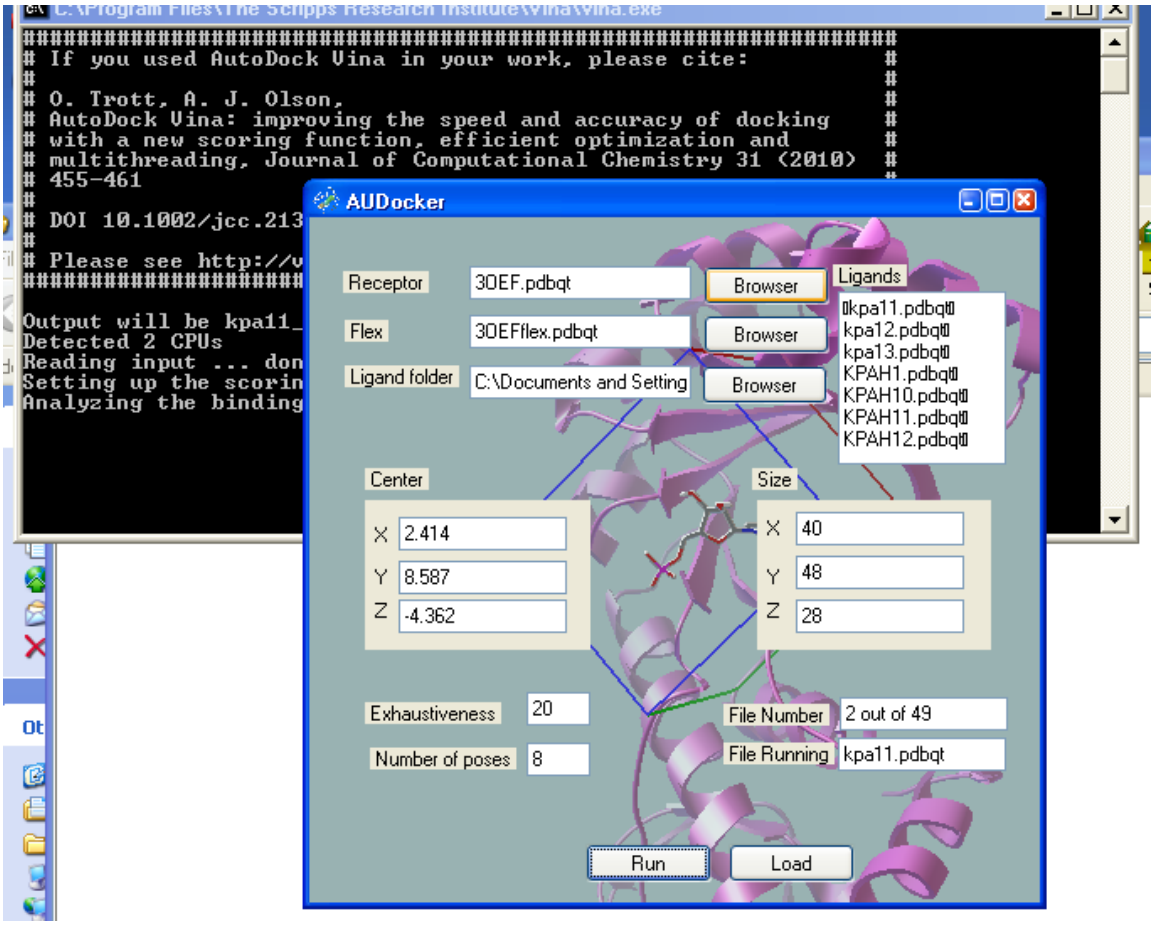


3. Ligand input – Click on the browse button for ligands and select the folder in which ligandfiles were kept. (You need not select each ligand. This program automatically recognizes the ligand files and dock them)

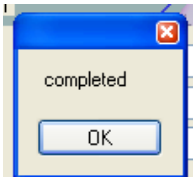


4. Enter the optimized GRID parameters into the respective boxes. Enter the exhaustive ness and number poses required also into their respective boxes. If you donot enter any number here the default values will be taken. Exhaustiveness = 8 and poses = 9

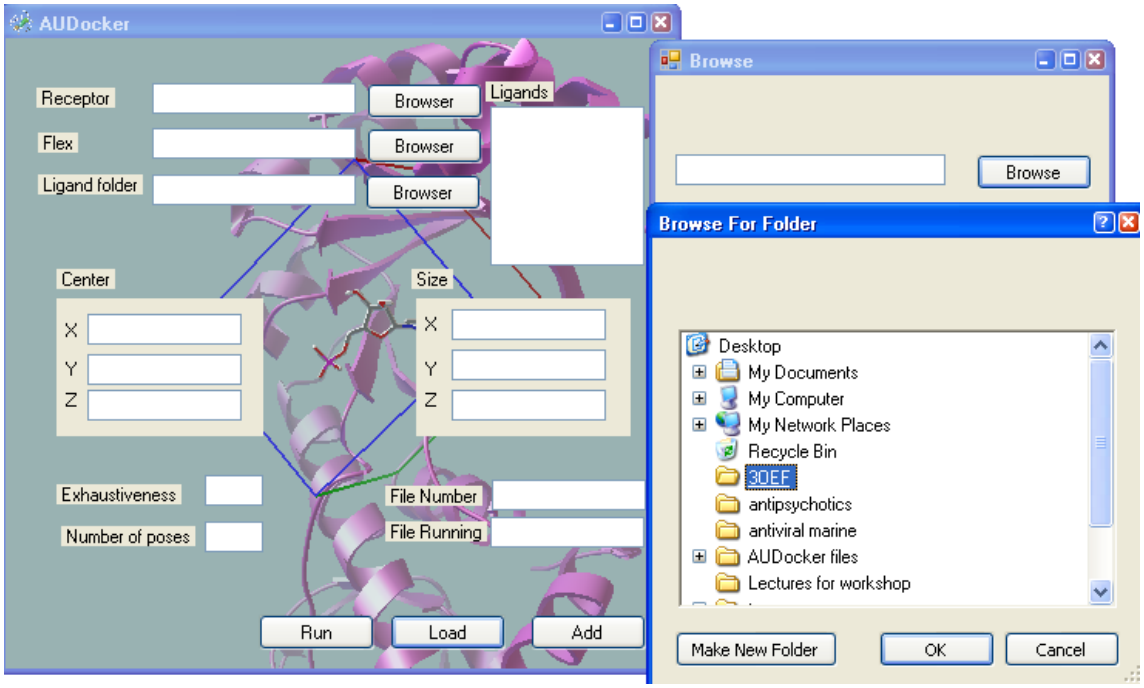
5. Then click run



6. You will see a pop-up window showing complete at the end of the virtual screening of the entire ligand library.

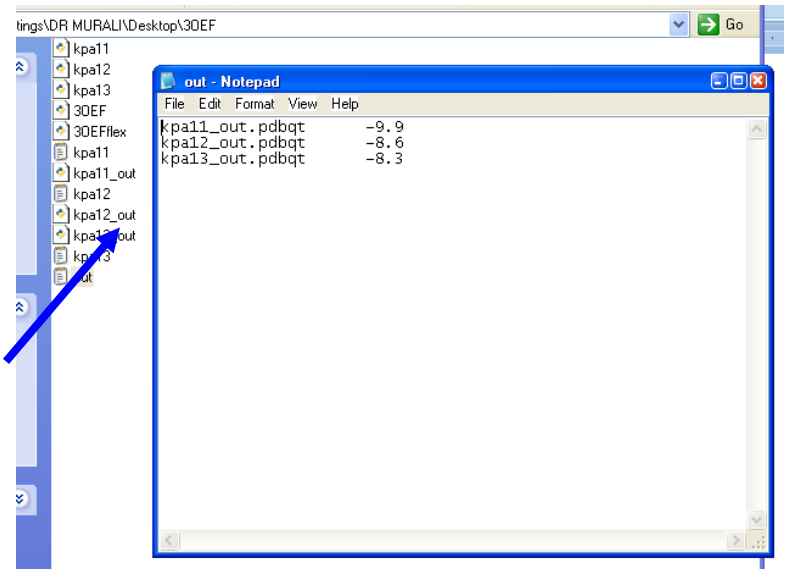


7. If it is shutdown in the middle then click load button to see another window with ‘browse’ button.



Select the original folder in which you will have all required files for backup. Then click 'Add' on the main console and close the browse window. All parameters will be loaded, then click 'Run' the screening will start from the point where it stopped.

8. At the end of the successful Virtual screening run, open your folder and find the file 'out.txt' and open it. You will find the docking scores aligned in the ascending order. The top one is obviously your best ligand. Eg: *picture below shows the result obtained for three ligands*



HAPPY DOCKING