Steps for Docking

Packages Required:-

Install Anaconda , Jupyter Notebook , Open Babel . MGL Tools 1.5.7 , Vina.exe

Step 1 :-

* Open Anaconda Prompt
* Type Jupyter Notebook

Step 2 :- Inside Jupyter Notebook

* Create a new Notebook
* Inside that new Notebook , create a new environment

Step 3 :-

* Install Open Babel from its official website or from Github repository.
  + Website :- <https://sourceforge.net/projects/openbabel/>
  + Github Repo:- <https://github.com/openbabel/openbabel>
* Install MGL Tools from Its official website.
  + Website:- <https://ccsb.scripps.edu/mgltools/downloads/>
* Install Vina.exe from its official website or from its official Github repository.
  + Website :- <https://vina.scripps.edu/downloads/>
  + Github:- <https://github.com/ccsb-scripps/AutoDock-Vina/releases>

Step 4 :-

* Download Ligand and Receptor in .pdb form

Step 5 :-

* Put that Ligand and Receptor file in the Jupyter Notebook home page .

Step 6 :-

* Inside the new Notebook , in a new shell , remove the impurities of the ligand and convert the ligand and receptor in .pdbqt format through Open babel.

Step 7 :-

* In a new shell , add hydrogen and hydrogen and gastienger charge in the ligand.pdbqt and receptor.pdbqt through MGL Tools.
* For using MGL Tools you have to install Python 2.7 version.

Step 8 :-

* Now Dock using Vina.