Lab Session 9: Docking

Date: April 2024

1. Download structures of Dihydrofolate Reductase (PDB ID: 4DFR) from Protein Data Bank and Folic acid from PubChem. Perform molecular docking (blind and target-based) using Autodock.
   A. Find the binding energy of the most probable docked conformation.
   B. Find the residues present in this ligand binding site.
   C. What is the nature of amino acids present in the ligand binding site? Represent the docked structure in your lab report.
   D. If 50% of the residues that are acidic in nature are replaced with the basic ones. What will be the change in docking result? Explain and demonstrate with an example.
   E. Compare the results of Target-based docking and Blind docking.

Please find the links of the tools that are needed for docking demonstration.

1. Autodock Vina

   https://vina.scripps.edu/downloads/

2. Chimera

   https://www.cgl.ucsf.edu/chimera/download.html

3. LIgplot (academic license needed, which will be mailed after registration.)

   https://www.ebi.ac.uk/thornton-srv/software/LigPlus/download2.html