

BT305 LAB 9

Name: Aditya Jindal

Roll No.: 210106004

1)

A) Binding Energy of most probable conformation: -8.8

B) Residue present in ligand binding sites: Iso-Leucine, Histidine, Alanine



C) Nature of Amino Acids present in ligand binding sites:

Iso-Leucine: Non-polar aromatic amino acids

Histidine: Basic Amino Acid

Alanine: Non-polar amino acid

E)

Target-Based Docking

Binding Energy: 201.2

Number Of Residues: 1
Residues: ASP

Blind Docking

Binding Energy: -8.8
Number Of Residues: 3
Residues: MET, HIS, ILE

Target-Based Docking:

