



b)

Cluster	Bind. energy [kcal/mol]	Contacting receptor residues	Populated Conformers [%]
A1	3.955	ARG 181, HIS 183, PHE 184, LEU 198, PRO 201, ILE 202, THR 203	70.0
B1	3.5740	PRO 147, PHE 150, ARG 151, LYS 154, LYS 200, PRO 201, ILE 202, THR 203, GLN 204	10.0
C1	3.6320	LYS 165, LYS 166, SER 167, THR 169, LEU 170, PHE 189, GLN 190, PRO 193	15.0
D1	3.5210	GLU 179, ARG 181, THR 203, GLN 204, LEU 205, LEU A 206	5.0