Assignment -02

Task 01: Conduct multiple Protein-Ligand Docking and provide the top 10 results in the following table.

	Ligands	Binding Affinity	Rmsd/ub	Rmsd/ib
01	7di7minimizedenergy_101281364_uff_E=2207.71	-8.3	0	0
02	7di7minimizedenergy_25090669_uff_E=2156.77	-8.3	0	0
03	7di7minimizedenergy_21679023_uff_E=771.19	-8.2	0	0
04	7di7minimizedenergy_265237_uff_E=2170.87	-8.1	0	0
05	7di7minimizedenergy_101281365_uff_E=770.69	-7.8	0	0
06	7di7minimizedenergy_23266146_uff_E=724.36	-7.8	0	0
07	7di7minimizedenergy_44567123_uff_E=836.12	-7.6	0	0
08	7di7minimizedenergy_108065_uff_E=551.24	-7.5	0	0
09	7di7minimizedenergy_9823926_uff_E=599.99	-7.5	0	0
10	7di7minimizedenergy_101289844_uff_E=1112.05	-7.4	0	0

Task 02: **ADME analysis on the 10 compounds obtained from the Protein-Ligand Docking and provide the results in the table below.**

ADME Analysis								Pharmacokinetics		Drug likeness	Medicinal Chemistry
Name	CID ID	Canonical SMILES	Molecular weight (g/mol)	Num. H-bond acceptors	Num. H-bond donors	Lipophilicity (iLOGP)	Water Solubility (Log S (SILICOS-IT))	GI absorption	BBB permeant	Lipinski	PAINS
Withanolide R	101281364	O=C1O[C@H]([C@H](C(=C1C)C)O)[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2[C@@H]2O[C@@H]2[C@@]2([C@]1(C)C(=O)C=CC2)O)C	470.60	6	2	3.69	-3.55	High	No	Yes; 0 violation	0 alert
Withanolide M	25090669	CC1=C(C)C(=O)O[C@H](C1)[C@@]([C@@]1(O)C[C@H]2[C@@]3([C@]1(C)CC[C@H]1[C@H]3CC=C3[C@]1(C)C(=O)C=CC3)O2)(O)C	468.58	6	2	3.72	-4.21	High	No	Yes; 0 violation	0 alert
Withanolide G	21679023	CC1=C(C)C(=O)O[C@H](C1)[C@@]([C@H]1CC[C@@]2([C@]1(C)CC[C	454.60	5	2	3.74	-4.50	High	No	Yes; 0 violation	0 alert

		@H]1[C@H]2CC=C2[C@]1(C)C(=O)C=CC2)O)(O)C									
Withaferin A	265237	OCC1=C(C)C[C@@H](OC1=O)[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]2[C@]3([C@]1(C)C(=O)C=C[C@@H]3O)O2)C	470.60	6	2	3.24	-3.79	High	No	Yes; 0 violation	0 alert
Withanolide Q	101281365	OCC1=C(C)[C@@H]([C@@H](OC1=O)[C@H]([C@@]1(O)CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)C(=O)C=CC2)C)O	470.60	6	3	3.36	-3.70	High	No	Yes; 0 violation	0 alert
Kulactone	101289844	CC(=CCC[C@H]1C(=O)O[C@@H]2[C@@H]1[C@]1(C)CC[C@H]3C(=CC[C@@H]4[C@]3(C)CCC(=O)C4(C)C)[C@]1(C2)C)C	452.67	3	0	4.47	-6.70	Low	No	Yes; 1 violation: MLOGP >4.15	0 alert
Withanolide O	23266146	OCC1=C(C)C[C@@H](OC1=O)[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]2[C@]3([C@]1(C)C(	470.60	6	2	3.24	-3.79	High	No	Yes; 0 violation	0 alert

		=O)C=C[C@@H]3O)O2)C									
Methyl kulonate	44567123	COC(=O)[C@@H]([C@@H]1[C@@H](O)C[C@]2([C@@]1(C)CC[C@H]1C2=CC[C@@H]2[C@]1(C)CCC(=O)C2(C)C)C)CCC=C(C)C	484.71	4	1	4.58	-6.27	High	No	Yes; 1 violation: MLOGP>4.15	0 alert
Proanthocyanidin	108065	COc1c(O)cc(cc1O)C1Oc2c(C[C@H]1O)c(O)cc(c2[C@@H]1[C@@H](O)[C@H](Oc2c1c(O)cc(c2)O)c1ccc(cc1)O)O	592.55	12	9	2.17	-4.60	Low	No	No; 3 violations: MW>500, NorO>10, NHorOH>5	0 alert
6beta-Hydroxystigmast-4-en-3-one	9823926	CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@H](C2=CC(=O)CC[C@]12C)O)C	428.69	2	1	4.68	-6.06	Low	No	Yes; 1 violation: MLOGP>4.15	0 alert

Task 03: Performing Toxicity Prediction on the 10 compounds obtained from the Protein-Ligand Docking and provide the results in the table below.

Toxicity Prediction

Name	CID ID	Canonical SMILES	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
Withanolide R	101281364	O=C1O[C@H]([C@H](C(=C1C)C)O)[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2[C@@H]2O[C@@H]2[C@@]2([C@]1(C)C(=O)C=CC2)O)C	0.85	0.54	0.99	0.75	0.94
Withanolide M	25090669	CC1=C(C)C(=O)O[C@H](C1)[C@@]([C@@]1(O)C[C@H]2[C@@]3([C@]1(C)CC[C@H]1[C@H]3CC=C3[C@]1(C)C(=O)C=CC3)O2)(O)C	0.85	0.53	0.85	0.74	0.59
Withanolide G	21679023	CC1=C(C)C(=O)O[C@H](C1)[C@@]([C@H]1CC[C@@]2([C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)C(=O)C=CC2)O)(O)C	0.83	0.52	0.82	0.90	0.80
Withaferin A	265237	OCC1=C(C)C[C@@H](OC1=O)[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]2[C@]3([C@]1(C)C(=O)C=C[C@@H]3O)O2)C	0.93	0.55	0.99	0.79	0.87
Withanolide Q	101281365	OCC1=C(C)[C@@H]([C@@H](OC1=O)[C@H]([C@@]1(O)CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)C(=O)C=CC2)C)O	0.96	0.66	0.98	0.84	0.67
Kulactone	101289844	CC(=CCC[C@H]1C(=O)O[C@@H]2[C@@H]1[C@]1(C)CC[C@H]3C(=CC[C@@H]4[C@]3(C)CCC(=O)C4(C)C)[C@]1(C2)C)C	0.83	0.59	0.91	0.95	0.82
Withanolide O	23266146	OCC1=C(C)C[C@@H](OC1=O)[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@@H]2[C@]3([C@]1(C)C(=O)C=C[C@@H]3O)O2)C	0.93	0.55	0.99	0.79	0.87
Methyl kulonate	44567123	COC(=O)[C@@H]([C@@H]1[C@@H](O)C[C@]2([C@@]1(C)CC[C@H]1C2=CC[C@	0.83	0.50	0.92	0.93	0.72

		@H]2[C@]1(C)CCC(=O)C2(C)C)C)CCC=C(C)C					
Proanthocyanidin	108065	COc1c(O)cc(cc1O)C1Oc2c(C[C@H]1O)c(O)cc(c2[C@@H]1[C@@H](O)[C@H](Oc2c1c(O)cc(c2)O)c1ccc(cc1)O)O	0.73	0.70	0.98	0.73	0.81
6beta-Hydroxystigmast-4-en-3-one	9823926	CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C[C@H](C2=CC(=O)CC[C@]12C)O)C	0.79	0.53	0.99	0.91	0.88

Task 04: Identifying the highest-ranking Protein – ligand complex and input the corresponding figures into the table below.

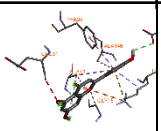
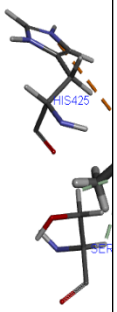
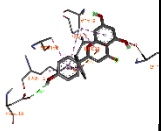
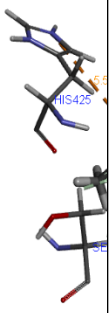
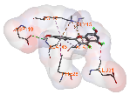
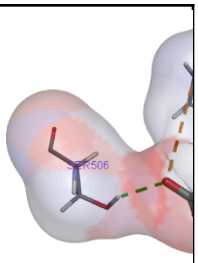
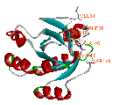
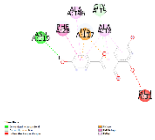
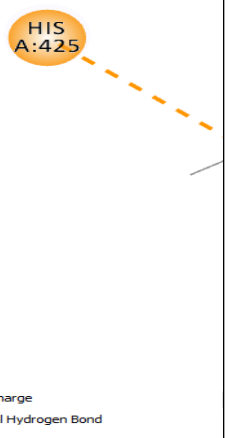
Figure Name	Sample Figure	Input your Docking Figure
Figure 01		
Figure 02		

Figure 03		
Figure 04		
Figure 05		

Task 05: Identify the highest-ranking Protein – ligand complex and input the Interaction details into the table below.

Name	Distance	Category	Types
A: HIS425:NE2 - A: ACT1201: OXT	5.59194	Electrostatic	Attractive Charge
A: SER506: HG - A: ACT1201: OXT	2.55319	Hydrogen Bond	Conventional Hydrogen Bond
A: SER429: HA - A: ACT1201:O	3.05025	Hydrogen Bond	Carbon Hydrogen Bond
A: SER429:HB2 - A: ACT1201:O	2.94711	Hydrogen Bond	Carbon Hydrogen Bond

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