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

	Ligands	Binding Affinity	Rmsd/ub	Rmsd/ib
01	Petunidin	-9.1	0	0
02	Epigallocatechin	-8.5	0	0
03	(-)-Epicatechin	-8.3	0	0
04	Retinol	-8.2	0	0
05	Riboflavin	-8.1	0	0
06	Resveratrol	-7.9	0	0
07	Thiamine	-6.4	0	0
08	beta-Bisabolene	-6.2	0	0
09	1-Hexanol	-4.3	0	0
10	1,3-Propanediol	-3.7	0	0

Task 02: Please perform 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	Num. H-bond acceptors	Num. H-bond donors	Lipophilicity (iLOGP)	Water Solubility (Log S (SILICOS-IT))	GI absorption	BBB permeant	Lipinski	PAINS
Petunidin	4417774	COc1cc(cc(c1O)O)c1[o+]c2cc(O)cc(c2cc1O)O	317.27	7	5	-2.01	-2.77	High	No	0	1
Epigallocatechin	7227277	Oc1cc2O[C@H](c3cc(O)c(c(c3)O)O)[C@@H](Cc2c(c1)O)O	306.27	7	6	0.98	-1.56	High	No	1	1
(-)-Epicate	7227276	Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@@H](Cc2c(c1)O)O	290.27	6	5	1.47	-2.14	High	No	0	1

chin											
Retinol	445354	OC/C=C(/C=C/C=C(/C=C/C1=C(C)CCCC1(C)C)\C)\C	286.45	1	1	1.47	-2.14	High	No	0	1
Riboflavin	493570	OC[C@H]([C@H]([C@H](Cn1c2cc(C)c(cc2nc2c1nc(=O)[nH]c2=O)C)O)O)O	376.36	8	5	1.63	-2.62	Low	No	0	0
Resveratrol	445154	Oc1ccc(cc1)/C=C/c1cc(O)cc(c1)O	228.24	3	3	1.71	-3.29	High	Yes	0	0
Thiamine	1010437 0	CC(=CCCC(=C)[C@H]1CCC(=CC1)C)C	204.35	0	0	3.67	-3.58	Low	No	1	0
beta-Bisabolene	1130	OCCc1sc[n+](c1C)Cc1cnc(nc1N)C	265.35	3	2	-1.6	-3.3	High	No	0	0
1-Hexanol	8103	CCCCCCO	102.17	1	1	2.03	-1.64	High	Yes	0	0
1,3-Propanediol	10442	OCCCO	76.09	2	2	1.02	0.18	High	No	0	0

Task 03: Perform 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
Petunidin	441774	COc1cc(cc(c1O)O)c1[o+]c2cc(O)cc(c2cc1O)O	**Inactive**	**Active**	**Active**	**Inactive**	**Inactive**
Epigallocatechin	72277	Oc1cc2O[C@H](c3cc(O)c(c(c3)O)O)[C@@H](Cc2c(c1)O)O	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**

(-)-Epicatechin	72276	Oc1cc2O[C@H](c3ccc(c(c3)O)O)[C@@H](Cc2c(c1)O)O	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
Retinol	445354	OC/C=C(/C=C/C=C(/C=C/C1=C(C)CCCC1(C)C)\C)\C	**Inactive**	**Inactive**	**Inactive**	**Active**	**Inactive**
Riboflavin	493570	OC[C@H]([C@H]([C@H](Cn1c2cc(C)c(cc2nc2c1nc(=O)[nH]c2=O)C)O)O)O	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
Resveratrol	445154	Oc1ccc(cc1)/C=C/c1cc(O)cc(c1)O	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
Thiamine	10104370	CC(=CCCC(=C)[C@H]1CCC(=CC1)C)C	**Inactive**	**Inactive**	**Active**	**Inactive**	**Inactive**
beta-Bisabolene	1130	OCCc1sc[n+](c1C)Cc1cnc(nc1N)C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
1-Hexanol	8103	CCCCCCO	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
1,3-Propanediol	10442	OCCCO	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**

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

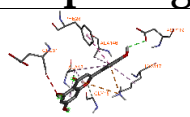
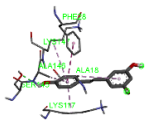
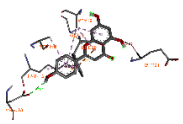
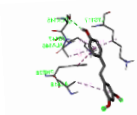
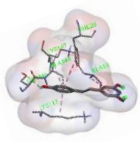
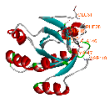
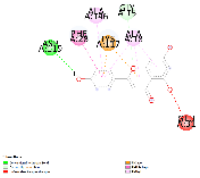
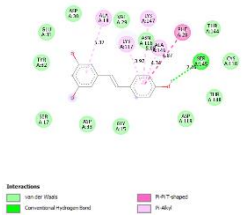
Figure Name	Sample Figure	Input your Docking Figure
Figure 01		
Figure 02		
Figure 03		

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
N:UNK1:H - A:SER145:OG	2.45525	Hydrogen Bond	Conventional Hydrogen Bond
N:UNK1 - A:PHE28	4.86738	Hydrophobic	Pi-Pi T-shaped
N:UNK1 - A:ALA18	5.36973	Hydrophobic	Pi-Alkyl
N:UNK1 - A:LYS117	3.96965	Hydrophobic	Pi-Alkyl
N:UNK1 - A:ALA146	4.34331	Hydrophobic	Pi-Alkyl
N:UNK1 - A:LYS147	5.08459	Hydrophobic	Pi-Alkyl