Assignment -02

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	e4u9c_6436348_uff_E=402.80	-6.2	0	0
02	e4u9c_10104370_uff_E=146.78	-5.5	0	0
03	e4u9c_196216_uff_E=215.06	-5.5	0	0
04	e4u9c_14529_uff_E=139.23	-5.5	0	0
05	e4u9c_79035_uff_E=1568.10	-5.4	0	0
06	e4u9c_5315469_uff_E=160.58	-5.3	0	0
07	e4u9c_28930_uff_E=387.47	-5.2	0	0
08	e4u9c_7463_uff_E=91.91	-5	0	0
09	e4u9c_7461_uff_E=63.24	-5	0	0
10	e4u9c_31253_uff_E=90.99	-4.5	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
beta-Bisabolene		CC(=CCCC(=C)[C@H]1CCC(=CC1)C)C	204.35	0	0	3.67	-3.58	Low	No	1	0
2-(4-Methylphenyl)propan-2-ol		Cc1ccc(cc1)C(O)(C)C	150.22	1	1	2.17	-3.01	High	Yes	0	0

Myrcene		C=CC(=C)CCC=C(C)C	136.23	0	0	2.89	-2.42	Low	Yes	0	0
alpha-Fenchene		Cc1ccc(cc1)C(O)(C)C	150.22	1	1	2.17	-3.01	High	Yes	0	0
gamma-Terpinene		CC1=CCC(=CC1)C(C)C	136.23	0	0	2.73	-2.23	Low	Yes	0	0
Bisacumol		CC(=CC(CC(c1ccc(cc1)C)C)O)C	218.33	1	1	2.87	-3.97	High	Yes	0	0
Curlone		CC(C1CCC(=C)C=C1)CC(=O)C=C(C)C	218.33	1	0	3.14	-2.9	High	Yes	0	0
p-Cymene		Cc1ccc(cc1)C(C)C	134.22	0	0	2.51	-3.57	Low	Yes	1	0
Germacrone		C/C/1=CCC(=C(C)C)C(=O)C/C(=C/CC1)/C	218.33	1	0	2.88	-3.64	High	Yes	0	0
Tricyclene		CC12C3C1CC(C2(C)C)C3	136.23	0	0	2.53	-2.23	Low	Yes	1	0

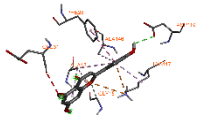
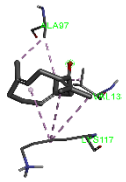
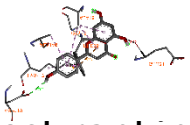
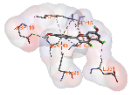
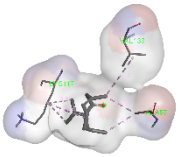
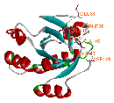
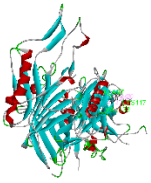
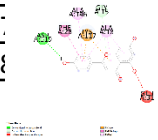
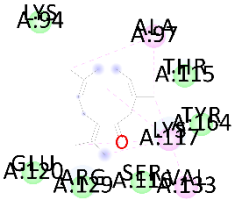
Task 03: Perform Toxicity Prediction on the 10 compounds obtained from the Protein-Ligand Docking and provide the results in the table below.

Toxicity Prediction

Name	CID ID	Canonical SMILES	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
beta-Bisabolene	**10104370**	CC(=CCCC(=C)[C@H]1CCC(=CC1)C)C	**Inactive**	**Active**	**Inactive**	**Inactive**	**Inactive**
2-(4-Methylphenyl)propan-2-ol	**14529**	Cc1ccc(cc1)C(O)(C)C	**Inactive**	**Active**	**Inactive**	**Inactive**	**Inactive**
Myrcene	**31253**	C=CC(=C)CCC=C(C)C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
alpha-Fenchene	**28930**	Cc1ccc(cc1)C(O)(C)C	**Inactive**	**Active**	**Inactive**	**Inactive**	**Inactive**
gamma-Terpinene	**7461**	CC1=CCC(=CC1)C(C)C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
Bisacumol	**5315469**	CC(=CC(CC(c1ccc(cc1)C)C)O)C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
Curlone	**19216**	CC(C1CCC(=C)C=C1)CC(=O)C=C(C)C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
p-Cymene	**7463**	Cc1ccc(cc1)C(C)C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**

Germacrone	**6436348**	C/C/1=CCC(=C(C)C)C(=O)C/C(=C/CC1)/C	**Inactive**	**Inactive**	**Inactive**	**Inactive**	**Inactive**
Tricyclene	**79035**	CC12C3C1CC(C2(C)C)C3	**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		Category	es
N:UNK1:C - A:ALA97		Hydrophobic	
N:UNK1:C - A:ALA97		Hydrophobic	
N:UNK1:C - A:VAL133	5.12826	Hydrophobic	
N:UNK1:C - A:LYS117	4.70026	Hydrophobic	
N:UNK1:C - A:LYS117	4.5107	Hydrophobic	
A:LYS117 - N:UNK1	4.51099	Hydrophobic	Alkyl
N:UNK1:C - A:ALA97		Hydrophobic	Alkyl
N:UNK1:C - A:ALA97		Hydrophobic	Alkyl
N:UNK1:C - A:VAL133		Hydrophobic	Alkyl
N:UNK1:C - A:LYS117	4.70026	Hydrophobic	Alkyl
N:UNK1:C - A:LYS117	4.5107	Hydrophobic	Alkyl
A:LYS117 - N:UNK1	4.51099	Hydrophobic	yl
N:UNK1:C - A:ALA97	3.7	Hydrophobic	yl
N:UNK1:C - A:ALA97	3.68	Hydrophobic	yl