**Assignment -02**

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| **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 | E\_C\_4nfn\_440933\_uff\_E=244.68 | -4.3 | 0 | 0 |
| 02 | E\_C\_4nfn\_92987\_uff\_E=68.07 | -4.6 | 0 | 0 |
| 03 | E\_C\_4nfn\_1201543\_uff\_E=486.38 | -4.8 | 0 | 0 |
| 04 | E\_C\_4nfn\_5793\_uff\_E=184.96 | -4.9 | 0 | 0 |
| 05 | E\_C\_4nfn\_442877\_uff\_E=539.07 | -6 | 0 | 0 |
| 06 | E\_C\_4nfn\_21679027\_uff\_E=2243.34 | -7.8 | 0 | 0 |
| 07 | E\_C\_4nfn\_44562999\_uff\_E=940.38 | -8.1 | 0 | 0 |
| 08 | E\_C\_4nfn\_23266146\_uff\_E=724.36 | -8.2 | 0 | 0 |
| 09 | E\_C\_4nfn\_11049407\_uff\_E=945.72 | -8.2 | 0 | 0 |
| 10 | E\_C\_4nfn\_301751\_uff\_E=2375.14 | -8.2 | 0 | 0 |

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| **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 |
| Hygrine | CID\_440933 | CC(=O)C[C@H]1CCCN1C | **141.21 g/mol** | **2** | **0** | **2.11** | **-1.20** | **High** | **No** | **Yes; 0 violation** | **0 alert** |
| Pelletierine | CID\_92987 | CC(=O)CC1CCCCN1 | **141.21 g/mol** | **2** | **1** | **1.90** | **-1.80** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |
| Cuscohygrine | CID\_1201543 | O=C(C[C@@H]1CCCN1C)C[C@H]1CCCN1C | **224.34 g/mol** | **3** | **0** | **2.90** | **-1.85** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |
| D-Glucose | CID\_5793 | OC[C@H]1OC(O)[C@@H]([C@H]([C@@H]1O)O)O | **180.16 g/mol** | **6** | **5** | **0.35** | **2.62** | **Low** | **No** | **Yes; 0 violation** | **0 alert** |
| Withasomnine | CID\_442877 | c1ccc(cc1)c1cnn2c1CCC2 | **184.24 g/mol** | **1** | **0** | **2.10** | **-3.76** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |
| Withanone | CID\_21679027 | CC1=C(C)C(=O)O[C@H](C1)[C@H] | **138.16 g/mol** | **2** | **0** | **0.00** | **-1.77** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |
| (2R)-2-[(1R)-1-[(4S,9S,10R,13S,17S)-4,17-dihydroxy-10,13-dimethyl-1-oxo-7,9,11,12,15,16-hexahydro-4H-cyclopenta[a]phenanthren-17-yl]ethyl]-4,5-dimethyl-2,3-dihydropyran-6-one | CID\_44562999 | CC1=C(C(=O)O[C@H](C1)[C@@H](C)[C@]2(CCC3=C4CC=C5[C@H](C=CC(=O)[C@@]5([C@H]4CC[C@@]32C)C)O)O)C | **452.58 g/mol** | **5** | **2** | **3.34** | **-4.71** | **High** | **No** | **Yes; 0 violation** | **0 alert** |
| 2R)-2-[(1S)-1-[(8R,9S,10R,13S,14R,17S)-14,17-dihydroxy-10,13-dimethyl-1-oxo-4,7,8,9,11,12,15,16-octahydrocyclopenta[a]phenanthren-17-yl]-1-hydroxyethyl]-4,5-dimethyl-2,3-dihydropyran-6-one | CID\_23266146 | CC1=C(C)C(=O)O[C@H](C1)[C@@] | **137.16 g/mol** | **2** | **0** | **0.00** | **-1.77** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |
| Withanolide S | CID\_11049407 | CC1=C(C)C(=O)O[C@H](C1)[C@@]([C@]1(O)CC[C@@]2([C@]1(C)CC[C@H]1[C@H]2C[C@H] | **138.16 g/mol** | **2** | **0** | **0.00** | **-1.57** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |
| Withanolide E | CID\_301751 | CC1=C(C)C(=O)O[C@H](C1)[C@@] | **137.16 g/mol** | **2** | **0** | **0.00** | **-1.77** | **High** | **Yes** | **Yes; 0 violation** | **0 alert** |

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| **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 |
| Hygrine | CID\_440933 | CC(=O)C[C@H]1CCCN1C | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| Pelletierine | CID\_92987 | CC(=O)CC1CCCCN1 | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| Cuscohygrine | CID\_1201543 | O=C(C[C@@H]1CCCN1C)C[C@H]1CCCN1C | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| D-Glucose | CID\_5793 | OC[C@H]1OC(O)[C@@H]([C@H]([C@@H]1O)O)O | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| Withasomnine | CID\_442877 | c1ccc(cc1)c1cnn2c1CCC2 | **Inactive** | **Active** | **Inactive** | **Inactive** | **Inactive** |
| Withanone | CID\_21679027 | CC1=C(C)C(=O)O[C@H](C1)[C@H] | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| (2R)-2-[(1R)-1-[(4S,9S,10R,13S,17S)-4,17-dihydroxy-10,13-dimethyl-1-oxo-7,9,11,12,15,16-hexahydro-4H-cyclopenta[a]phenanthren-17-yl]ethyl]-4,5-dimethyl-2,3-dihydropyran-6-one | CID\_44562999 | CC1=C(C(=O)O[C@H](C1)[C@@H](C)[C@]2(CCC3=C4CC=C5[C@H](C=CC(=O)[C@@]5([C@H]4CC[C@@]32C)C)O)O)C | **Inactive** | **Active** | **Active** | **Inactive** | **Inactive** |
| 2R)-2-[(1S)-1-[(8R,9S,10R,13S,14R,17S)-14,17-dihydroxy-10,13-dimethyl-1-oxo-4,7,8,9,11,12,15,16-octahydrocyclopenta[a]phenanthren-17-yl]-1-hydroxyethyl]-4,5-dimethyl-2,3-dihydropyran-6-one | CID\_23266146 | CC1=C(C)C(=O)O[C@H](C1)[C@@] | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| Withanolide S | CID\_11049407 | CC1=C(C)C(=O)O[C@H](C1)[C@@]([C@]1(O)CC[C@@]2([C@]1(C)CC[C@H]1[C@H]2C[C@H] | **Active** | **Inactive** | **Active** | **Inactive** | **Inactive** |
| Withanolide E | CID\_301751 | CC1=C(C)C(=O)O[C@H](C1)[C@@] | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |

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| **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** | A picture containing sketch, drawing, clipart, cartoon  Description automatically generated |  |
| **Figure 03** | A picture containing cartoon, art  Description automatically generated |  |
| **Figure 04** | A picture containing clipart, illustration, design  Description automatically generated |  |
| **Figure 05** | A picture containing text, diagram, font, screenshot  Description automatically generated |  |

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| **Task 05:** Identify the highest-ranking Protein – ligand complex and input the Interaction details into the table below. | | | |
| Name | Distance | Category | Types |
| A:GLU215:HN - N:UNK1:O | 2.02599 | Hydrogen Bond | Conventional Hydrogen Bond |
| A:ARG214 - N:UNK1 | 4.81092 | Hydrophobic | Alkyl |
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