Assignment -02

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| **Task 01: Please conduct multiple Protein-Ligand Docking and provide the top 10 results in the following table.** | | | | |
|  | Ligand | Binding Affinity | rmsd/ub | rmsd/lb |
| 01 | EC5e1s\_5281855\_uff\_E=227.58 | -8.6 | 0 | 0 |
| 02 | EC5e1s\_453214\_uff\_E=631.82 | -7 | 0 | 0 |
| 03 | EC5e1s\_445858\_uff\_E=177.42 | -5.8 | 0 | 0 |
| 04 | EC5e1s\_637542\_uff\_E=90.83 | -5.7 | 0 | 0 |
| 05 | EC5e1s\_338\_uff\_E=73.50 | -5.1 | 0 | 0 |
| 06 | EC5e1s\_72\_uff\_E=70.72 | -5.1 | 0 | 0 |
| 07 | EC5e1s\_7478\_uff\_E=80.31 | -5.1 | 0 | 0 |
| 08 | EC5e1s\_8655\_uff\_E=168.50 | -5.1 | 0 | 0 |
| 09 | EC5e1s\_11635\_uff\_E=56.94 | -4.5 | 0 | 0 |
| 10 | EC5e1s\_72\_uff\_E=70.72 | -5.1 | 2.26 | 1.034 |

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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** | | | | | | | | Pharmacok inetics |  | Drug likene ss | Medic inal Chemi stry |
| Na me | CID ID | Canonical SMILES | Molec ular weight | Nu m.  H-  bo nd acc ept ors | Nu m.  H-  bon d don ors | Lipophi licity (iLOGP  ) | Water Solubi lity (Log S (SILI COS- IT)) | GI  absorption | BBB  perme ant | Lipin ski | PAIN S |
| 01 | 453 | COC(=O)C1= |  | 12 | 5 | 2.14 | 1.77 | low | no | Yes; 1 |  |
|  | 214 | CO[C@H]([C | 456.40 |  |  |  |  |  |  | violat | 0 alert |
|  |  | @H]2[C@@ | g/mol |  |  |  |  |  |  | ion: |  |
|  |  | H]1C=C[C@ |  |  |  |  |  |  |  | NorO |  |
|  |  | @]23C=C(C( |  |  |  |  |  |  |  | >10 |  |
|  |  | =O)O3)CO)O |  |  |  |  |  |  |  |  |  |
|  |  | [C@H]4[C@ |  |  |  |  |  |  |  |  |  |
|  |  | @H]([C@H]( |  |  |  |  |  |  |  |  |  |
|  |  | [C@@H]([C |  |  |  |  |  |  |  |  |  |
|  |  | @H](O4)CO) |  |  |  |  |  |  |  |  |  |
|  |  | O)O)O |  |  |  |  |  |  |  |  |  |

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| 02 | 528  185  5 | C1=C2C3=C( C(=C1O)O)O C(=O)C4=CC (=C(C(=C43) OC2=O)O)O | 302.19  g/mol | 8 | 4 | 0.79 | -3.35 | high | no | Yes; 0 violat ion | 1  alert: catech ol\_A |
| 03 | 865  5 | COC1=CC(= CC(=C1O)OC  )C=O | 182.17  g/mol | 4 | 1 | 1.66 | -2.03 | high | yes | Yes; 0 violat ion | 0 alert |
| 04 | 135 | C1=CC(=CC  =C1C(=O)O) O | 138.12  g/mol | 3 | 2 | 0.85 | -1.17 | high | yes | Yes; 0 violat ion | 0 alert |
| 05 | 747  8 | COC1=CC=C (C=C1)C(=O) O | 152.15  g/mol | 3 | 1 | 1.56 | -1.88 | high | yes | Yes; 0 violat ion | 0 alert |
| 06 | 338 | C1=CC=C(C(  =C1)C(=O)O) O | 138.12  g/mol | 3 | 2 | 1.13 | -1.17 | high | yes | Yes; 0 violat ion | 0 alert |
| 07 | 445  858 | COC1=C(C= CC(=C1)/C= C/C(=O)O)O | 194.18  g/mol | 4 | 2 | 1.62 | -1.42 | high | yes | Yes; 0 violat ion | 0 alert |
| 08 | 72 | C1=CC(=C(C  =C1C(=O)O) O)O | 154.12  g/mol | 4 | 3 | 0.66 | -0.60 | high | no | Yes; 0 violat ion | 1  alert: catech ol\_A |
| 09 | 637  542 | C1=CC(=CC  =C1/C=C/C(= O)O)O | 164.16  g/mol | 3 | 2 | 0.95 | -1.28 | high | yes | Yes; 0 violat ion | 0 alert |
| 10 | 445  858 | COC1=C(C= CC(=C1)/C= C/C(=O)O)O | 194.18  g/mol | 4 | 2 | 1.62 | -1.42 | high | yes | Yes; 0 violat ion | 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 | Carcin ogenic ity | Immunotoxic ity | Mutagenici ty | | | Cytotoxic ity | | |
| 01 | 4532  14 | COC(=O)C1=CO[C@H  ]([C@H]2[C@@H]1C= C[C@@]23C=C(C(=O) O3)CO)O[C@H]4[C@  @H]([C@H]([C@@H]  ([C@H](O4)CO)O)O)O | Inactive | Inactiv e | Active | Inactive | | | nactive | | |
| 02 | 5281  855 | C1=C2C3=C(C(=C1O)  O)OC(=O)C4=CC(=C( C(=C43)OC2=O)O)O | Inactive | Active | Inactive |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 03 | 8655 | COC1=CC(=CC(=C1O) OC)C=O | Inactive | Inactiv e | Inactive |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 04 | 135 | C1=CC(=CC=C1C(=O) O)O | Inactive | Inactiv e | Inactive |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 05 | 7478 | COC1=CC=C(C=C1)C(  =O)O | Active | Inactiv e | Inactive |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 06 | 338 | C1=CC=C(C(=C1)C(= O)O)O | Active | Inactiv e | Inactive |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 07 | 4458  58 | COC1=C(C=CC(=C1)/ C=C/C(=O)O)O | Inactive | Inactiv e | Active |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 08 | 72 | C1=CC(=C(C=C1C(=O  )O)O)O | Inactive | Active | Inactive |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 09 | 6375  42 | C1=CC(=CC=C1/C=C/ C(=O)O)O | Active | Inactiv e | Active |  | Inactive |  |  | Inactive |  |
|  | | |  | | |
| 10 | 4458  58 | COC1=C(C=CC(=C1)/ C=C/C(=O)O)O | Inactive | Inactiv e | Active |  | 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** |  |  |

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| **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 |
| N:UNK1:H - A:GLY1003:O | 2.86292 | Hydrogen Bond | Conventional Hydrogen Bond |
| N:UNK1:H - A:GLN1004:O | 2.34832 | Hydrogen Bond | Conventional Hydrogen Bond |
| A:LEU1002:CD1 - N:UNK1 | 3.46423 | Hydrophobic | Pi-Alkyl |
| A:VAL1010:CG1 - N:UNK1 | 3.73158 | Hydrophobic | Pi-Alkyl |
| A:VAL1010:CG2 - N:UNK1 | 3.87256 | Hydrophobic | Pi-Alkyl |
| A:MET1139:CE - N:UNK1 | 3.52589 | Hydrophobic | Pi-Alkyl |
| A:MET1139:CE - N:UNK1 | 3.82239 | Hydrophobic | Pi-Alkyl |
| N:UNK1 - A:LEU1002 | 4.59424 | Hydrophobic | Pi-Alkyl |
| N:UNK1 - A:LEU1002 | 5.21322 | Hydrophobic | Pi-Sigma |
| N:UNK1 - A:VAL1010 | 4.73698 | Hydrophobic | Pi-Sigma |
| N:UNK1 - A:VAL1010 | 4.72553 | Hydrophobic | Pi-Sigma |
| N:UNK1 - A:ALA1028 | 5.29282 | Hydrophobic | Pi-Sigma |
| N:UNK1 - A:ALA1028 | 4.37613 | Hydrophobic | Pi-Sigma |