**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 | 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 |

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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 |
| 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 |

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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 |
| 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** |

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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 |
| N:UNK1:C - A:ALA97 | 3.77101 | Hydrophobic | Alkyl |
| N:UNK1:C - A:ALA97 | 3.68404 | Hydrophobic | Alkyl |
| N:UNK1:C - A:VAL133 | 5.12826 | 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 | Alkyl |
| N:UNK1:C - A:ALA97 | 3.77101 | Hydrophobic | Alkyl |
| N:UNK1:C - A:ALA97 | 3.68404 | Hydrophobic | Alkyl |
| N:UNK1:C - A:VAL133 | 5.12826 | 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 | Alkyl |
| N:UNK1:C - A:ALA97 | 3.77101 | Hydrophobic | Alkyl |
| N:UNK1:C - A:ALA97 | 3.68404 | Hydrophobic | Alkyl |