**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 | EC4tzk\_160799\_uff\_E=213.66 | -4.3 | 0 | 0 |
| 02 | EC4tzk\_6436348\_uff\_E=402.80 | -4.2 | 0 | 0 |
| 03 | EC4tzk\_969516\_uff\_E=272.07 | -4.2 | 0 | 0 |
| 04 | EC4tzk\_5281520\_uff\_E=195.77 | -4 | 0 | 0 |
| 05 | EC4tzk\_10364\_uff\_E=78.47 | -3.9 | 0 | 0 |
| 06 | EC4tzk\_20055538\_uff\_E=115.03 | -3.9 | 0 | 0 |
| 07 | EC4tzk\_442343\_uff\_E=218.81 | -3.8 | 0 | 0 |
| 08 | EC4tzk\_10104370\_uff\_E=146.78 | -3.7 | 0 | 0 |
| 09 | EC4tzk\_3314\_uff\_E=169.59 | -3.6 | 0 | 0 |
| 10 | EC4tzk\_5315469\_uff\_E=160.58 | -3.6 | 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  (g/mol) | Num. H-bond acceptors | Num. H-bond donors | Lipophilicity (iLOGP) | Water Solubility (Log S (SILICOS-IT)) | GI absorption | BBB permeant | Lipinski | PAINS |
| Cedrelanol | 160799 | CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C | 222.37 | 1 | 1 | 3.21 | -2.73, Soluble | High | Yes | Yes; 0 violation | 0 alert |
| Germacrone | 6436348 | C/C/1=C\CC(=C(C)C)C(=O)C/C(=C/CC1)/C | 218.33 | 1 | 0 | 2.88 | -3.64, Soluble | High | Yes | Yes; 0 violation | 0 alert |
| Curcumin | 969516 | COC1=C(C=CC(=C1)/C=C/C(=O)CC(=O)/C=C/C2=CC(=C(C=C2)O)OC)O | 368.38 | 6 | 2 | 3.27 | -4.45, Moderately soluble | High | No | Yes; 0 violation | 0 alert |
| Humulene | 5281520 | C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C | 204.35 | 0 | 0 | 3.29 | -3.52, Soluble | Low | No | Yes; 1 violation: MLOGP>4.15 | 0 alert |
| Carvacrol | 10364 | CC1=C(C=C(C=C1)C(C)C)O | 150.22 | 1 | 1 | 2.24 | -3.01, Soluble | High | Yes | Yes; 0 violation | 0 alert |
| Turmerol | 20055538 | CC1=CCC(=CC1)C(C)CC(C=C(C)C)O | 220.35 | 1 | 1 | 3.29 | -2.62, Soluble | High | Yes | Yes; 0 violation | 0 alert |
| Levomenol | 442343 | CC1=CC[C@H](CC1)[C@](C)(CCC=C(C)C)O | 222.37 | 1 | 1 | 3.61 | -3.00, Soluble | High | Yes | Yes; 0 violation | 0 alert |
| Beta-Bisabolene | 10104370 | CC1=CC[C@H](CC1)C(=C)CCC=C(C)C | 204.35 | 0 | 0 | 3.67 | -3.58, Soluble | Low | No | Yes; 1 violation: MLOGP>4.15 | 0 alert |
| Eugenol | 3314 | COC1=C(C=CC(=C1)CC=C)O | 164.20 | 2 | 1 | 2.37 | -2.79, Soluble | High | Yes | Yes; 0 violation | 0 alert |
| Bisacumol | 5315469 | CC1=CC=C(C=C1)C(C)CC(C=C(C)C)O | 218.33 | 1 | 1 | 2.87 | -3.97, Soluble | 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 |
| Cedrelanol | 160799 | CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C | Inactive | Inactive | Active | Inactive | Inactive |
| Germacrone | 6436348 | C/C/1=C\CC(=C(C)C)C(=O)C/C(=C/CC1)/C | Inactive | Inactive | Inactive | Inactive | Inactive |
| Curcumin | 969516 | COC1=C(C=CC(=C1)/C=C/C(=O)CC(=O)/C=C/C2=CC(=C(C=C2)O)OC)O | Inactive | Inactive | Active | Inactive | Inactive |
| Humulene | 5281520 | C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C | Inactive | Inactive | Inactive | Inactive | Inactive |
| Carvacrol | 10364 | CC1=C(C=C(C=C1)C(C)C)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Turmerol | 20055538 | CC1=CCC(=CC1)C(C)CC(C=C(C)C)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Levomenol | 442343 | CC1=CC[C@H](CC1)[C@](C)(CCC=C(C)C)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Beta-Bisabolene | 10104370 | CC1=CC[C@H](CC1)C(=C)CCC=C(C)C | Inactive | Inactive | Active | Inactive | Inactive |
| Eugenol | 3314 | COC1=C(C=CC(=C1)CC=C)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Bisacumol | 5315469 | CC1=CC=C(C=C1)C(C)CC(C=C(C)C)O | 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:THR101:HN - N:UNK1:O | 2.17176 | Hydrogen Bond | Conventional Hydrogen Bond |
| N:UNK1:C - A:PRO99 | 4.54195 | Hydrophobic | Alkyl |
| N:UNK1:C - A:PRO99 | 4.74639 | Hydrophobic | Alkyl |
| A:PHE97 - N:UNK1:C | 5.29759 | Hydrophobic | Pi-Alkyl |
| A:PHE97 - N:UNK1:C | 5.18936 | Hydrophobic | Pi-Alkyl |