**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 | ec\_2h2t\_101690\_uff\_E=2034.34 | -6.6 | 0 | 0 |
| 02 | ec\_2h2t\_12302182\_uff\_E=843.90 | -6.3 | 0 | 0 |
| 03 | ec\_2h2t\_11402337\_uff\_E=426.86 | -5.9 | 0 | 0 |
| 04 | ec\_2h2t\_10364\_uff\_E=78.47 | -4.8 | 0 | 0 |
| 05 | ec\_2h2t\_1549778\_uff\_E=108.04 | -4.7 | 0 | 0 |
| 06 | ec\_2h2t\_10231\_uff\_E=304.43 | -4.7 | 0 | 0 |
| 07 | ec\_2h2t\_10607083\_uff\_E=171.94 | -4.6 | 0 | 0 |
| 08 | ec\_2h2t\_10104370\_uff\_E=146.78 | -4.6 | 0 | 0 |
| 09 | ec\_2h2t\_121719\_uff\_E=632.63 | -4.6 | 0 | 0 |
| 10 | ec\_2h2t\_10582\_uff\_E=649.92 | -4.6 | 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 | Num. H-bond acceptors | Num. H-bond donors | Lipophilicity (iLOGP) | Water Solubility (Log S (SILICOS-IT)) | GI absorption | BBB permeant | Lipinski | PAINS |
| **Myristic Acid** | **11005** | **CCCCCCCCCCCCCC(=O)O** | 228.37 g/mol | **2** | **1** | **3.32** | -4.51 | **High** | **yes** | **yes** | **0 aleert** |
| **Myrtenol** | **10582** | **CC1(C2CC=C(C1C2)CO)C** | |  | | --- | | 152.23 g/mol | |  | | **1** | **1** | **2.34** | |  | | --- | | -1.69 | |  | | **High** | **yes** | **yes** | **0 alert** |
| **(3S,4S)-4-ethenyl-4-methyl-3-prop-1-en-2-ylcyclohexene** | **10607083** | **CC(=C)[C@@H]1C=CCC[C@@]1(C)C=C** | |  | | --- | | 162.27 g/mol | |  | | **0** | **0** | **2.84** | |  | | --- | | -2.49 | |  | | **low** | **yes** | **yes** | **O alert** |
| **Beta-Bisabolene** | **10104370** | **CC1=CC[C@H](CC1)C(=C)CCC=C(C)C** | |  | | --- | | **204.35 g/mol** | |  | | **0** | **0** | **3.57** | |  | | --- | | **-3.58** | |  | | **Low** | **no** | **yes** | **0 alert** |
| **o-Cymene** | **10703** | **CC1=CC=CC=C1C(C)C** | |  | | --- | | **134.22 g/mol** | |  | | **0** | **0** | |  | | --- | | **2.43** | |  | | |  | | --- | | **-3.57** | |  | | **Low** | **yes** | **yes** | **0 alert** |
| **m-Cymene** | **10812** | **CC1=CC(=CC=C1)C(C)C** | |  | | --- | | **134.22 g/mol** | |  | | **0** | **0** | |  | | --- | | **2.52** | |  | | |  | | --- | | **-3.57** | |  | | **Low** | **yes** | **yes** | **0 alert** |
| **Dillapiol** | **10231** | **COC1=C(C2=C(C=C1CC=C)OCO2)OC** | |  | | --- | | **222.24 g/mol** | |  | | **4** | **0** | |  | | --- | | **2.82** | |  | | |  | | --- | | **-3.26** | |  | | **High** | **yes** | **yes** | **0 alert** |
| **Thymoquinone** | **10281** | **CC1=CC(=O)C(=CC1=O)C(C)C** | |  | | --- | | **164.20 g/mol** | |  | | **2** | **0** | |  | | --- | | **1.99** | |  | | |  | | --- | | **-2.03** | |  | | **High** | **yes** | **yes** | **1 alert** |
| **Carvacrol** | **10364** | **CC1=C(C=C(C=C1)C(C)C)O** | |  | | --- | | **150.22 g/mol** | |  | | **1** | **1** | **2.24** | |  | | --- | | **-3.01** | |  | | **High** | **yes** | **yes** | **O alert** |
| **Geranylacetone** | **1549778** | **CC(=CCC/C(=C/CCC(=O)C)/C)C** | |  | | --- | | **194.31 g/mol** | |  | | **1** | **0** | **3.09** | **-3.18** | **High** | **yes** | **yes** | **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 |
| **Myristic Acid** | 11005 | CCCCCCCCCCCCCC(=O)O | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| **Myrtenol** | 10582 | CC1(C2CC=C(C1C2)CO)C | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| **(3S,4S)-4-ethenyl-4-methyl-3-prop-1-en-2-ylcyclohexene** | [10607083](https://pubchem.ncbi.nlm.nih.gov/compound/10607083) | CC(=C)[C@@H]1C=CCC[C@@]1(C)C=C | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| **Beta-Bisabolene** | [10104370](https://pubchem.ncbi.nlm.nih.gov/compound/10104370) | CC1=CC[C@H](CC1)C(=C)CCC=C(C)C | **Inactive** | **Inactive** | **Active** | **Inactive** | **Inactive** |
| **o-Cymene** | [10703](https://pubchem.ncbi.nlm.nih.gov/compound/10703) | CC1=CC=CC=C1C(C)C | **Inactive** | **Active** | **Inactive** | **Inactive** | **Inactive** |
| **m-Cymene** | [10812](https://pubchem.ncbi.nlm.nih.gov/compound/10812) | CC1=CC(=CC=C1)C(C)C | **Inactive** | **Active** | **Inactive** | **Inactive** | **Inactive** |
| **Dillapiol** | [10231](https://pubchem.ncbi.nlm.nih.gov/compound/10231) | COC1=C(C2=C(C=C1CC=C)OCO2)OC | **Inactive** | **Active** | **Active** | **Inactive** | **Inactive** |
| **Thymoquinone** | [10281](https://pubchem.ncbi.nlm.nih.gov/compound/10281) | CC1=CC(=O)C(=CC1=O)C(C)C | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| **Carvacrol** | [10364](https://pubchem.ncbi.nlm.nih.gov/compound/10364) | CC1=C(C=C(C=C1)C(C)C)O | **Inactive** | **Inactive** | **Inactive** | **Inactive** | **Inactive** |
| **Geranylacetone** | [1549778](https://pubchem.ncbi.nlm.nih.gov/compound/1549778) | CC(=CCC/C(=C/CCC(=O)C)/C)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 |
| B:GLN171:HE21 - N:UNK1:O | 2.18834 | Hydrogen Bond | Conventional Hydrogen Bond |
| N:UNK1 - B:LEU285 | 5.05526 | Hydrophobic | Alkyl |
| N:UNK1:C - B:LEU285 | 3.83 | Hydrophobic | Alkyl |
| N:UNK1:C - B:LEU285 | 4.45501 | Hydrophobic | Alkyl |