**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 | E5ce9\_5280343\_uff\_E=380.43 | -6.4 | 0 | 0 |
| 02 | E5ce9\_439246\_uff\_E=195.81 | -6.2 | 0 | 0 |
| 03 | EC2mv9\_101324856\_uff\_E=967.70 | -6.1 | 0 | 0 |
| 04 | EC2mv9\_5280637\_uff\_E=456.82 | -6.1 | 0 | 0 |
| 05 | EC2mv9\_441071\_uff\_E=807.01 | -6.1 | 0 | 0 |
| 06 | E5ce9\_5281643\_uff\_E=608.46 | -6.1 | 0 | 0 |
| 07 | EC2mv9\_12912214\_uff\_E=410.93 | -6 | 0 | 0 |
| 08 | E5ce9\_10742\_uff\_E=181.46 | -6 | 0 | 0 |
| 09 | EC2mv9\_5280445\_uff\_E=242.10 | -5.8 | 0 | 0 |
| 10 | EC2mv9\_5280794\_uff\_E=546.19 | -5.7 | 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 |
| [Anacardic acid](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | [167551](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | Cccccccccccccccc1cccc(c1c(=o)o)o | 348.52 | 3 | 2 | 4.19 | -7.21 | High | No | 1 | 0 |
| [5-pentadecylresorcinol](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | [76617](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | Cccccccccccccccc1cc(o)cc(c1)o | 320.51 | 2 | 2 | 4.53 | -7.28 | High | No | 1 | 0 |
| [Digallic acid](https://pubchem.ncbi.nlm.nih.gov/compound/341) | [341](https://pubchem.ncbi.nlm.nih.gov/compound/341) | O=C(c1cc(O)c(c(c1)O)O)Oc1cc(cc(c1o)O)C(=O)O | 322.22 | 9 | 6 | 0.85 | -1.08 | Low | No | 1 | 1 |
| [Quercetin](https://pubchem.ncbi.nlm.nih.gov/compound/5280343) | [5280343](https://pubchem.ncbi.nlm.nih.gov/compound/5280343) | Oc1cc(o)c2c(c1)oc(c(c2=o)o)c1ccc(c(c1)o)o | 302.24 | 7 | 5 | 1.63 | -3.24 | High | No | 0 | 1 |
| [Ethyl gallate](https://pubchem.ncbi.nlm.nih.gov/compound/13250) | [13250](https://pubchem.ncbi.nlm.nih.gov/compound/13250) | Ccoc(=o)c1cc(o)c(c(c1)o)o | 198.17 | 5 | 3 | 1.21 | -1.16 | High | No | 0 | 1 |
| [Cardanol](https://pubchem.ncbi.nlm.nih.gov/compound/11266523) | [11266523](https://pubchem.ncbi.nlm.nih.gov/compound/11266523) | C=CC/C=C\C/C=C\cccccccc1cccc(c1)O | 298.46 | 1 | 1 | 1.21 | -1.16 | High | No | 0 | 1 |
| [Syringic acid](https://pubchem.ncbi.nlm.nih.gov/compound/10742) | [10742](https://pubchem.ncbi.nlm.nih.gov/compound/10742) | Coc1cc(cc(c1o)oc)c(=o)o | 198.17 | 5 | 2 | 1.54 | -1.46 | High | No | 0 | 0 |
| [Nonanal](https://pubchem.ncbi.nlm.nih.gov/compound/31289) | [31289](https://pubchem.ncbi.nlm.nih.gov/compound/31289) | Ccccccccc=o | 142.24 | 1 | 0 | 2.44 | -3.02 | High | Yes | 0 | 0 |
| [Anacardic acid](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | [167551](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | Cccccccccccccccc1cccc(c1c(=o)o)o | 348.52 | 3 | 2 | 4.19 | -7.21 | High | No | 1 | 0 |
| [5-pentadecylresorcinol](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | [76617](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | Cccccccccccccccc1cc(o)cc(c1)o | 320.51 | 2 | 2 | 4.53 | -7.28 | High | No | 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 |
| [Anacardic acid](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | [167551](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | CCCCCCCCCCCCCCCC1=C(C(=CC=C1)O)C(=O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [5-pentadecylresorcinol](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | [76617](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | CCCCCCCCCCCCCCCC1=CC(=CC(=C1)O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Digallic acid](https://pubchem.ncbi.nlm.nih.gov/compound/341) | [341](https://pubchem.ncbi.nlm.nih.gov/compound/341) | C1=C(C=C(C(=C1O)O)O)C(=O)OC2=CC(=CC(=C2O)O)C(=O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Quercetin](https://pubchem.ncbi.nlm.nih.gov/compound/5280343) | [5280343](https://pubchem.ncbi.nlm.nih.gov/compound/5280343) | C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O | Inactive | Active | Inactive | Active | Inactive |
| [Ethyl gallate](https://pubchem.ncbi.nlm.nih.gov/compound/13250) | [13250](https://pubchem.ncbi.nlm.nih.gov/compound/13250) | CCOC(=O)C1=CC(=C(C(=C1)O)O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Cardanol](https://pubchem.ncbi.nlm.nih.gov/compound/11266523) | [11266523](https://pubchem.ncbi.nlm.nih.gov/compound/11266523) | C=CC/C=C\C/C=C\CCCCCCCC1=CC(=CC=C1)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Syringic acid](https://pubchem.ncbi.nlm.nih.gov/compound/10742) | [10742](https://pubchem.ncbi.nlm.nih.gov/compound/10742) | COC1=CC(=CC(=C1O)OC)C(=O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Nonanal](https://pubchem.ncbi.nlm.nih.gov/compound/31289) | [31289](https://pubchem.ncbi.nlm.nih.gov/compound/31289) | CCCCCCCCC=O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [Anacardic acid](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | [167551](https://pubchem.ncbi.nlm.nih.gov/compound/167551) | CCCCCCCCCCCCCCCC1=C(C(=CC=C1)O)C(=O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| [5-pentadecylresorcinol](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | [76617](https://pubchem.ncbi.nlm.nih.gov/compound/76617) | CCCCCCCCCCCCCCCC1=CC(=CC(=C1)O)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:HIS243:ND1 - N:UNK1:O | 3.28688 | Hydrogen Bond | Conventional Hydrogen Bond |
| A:LEU244:CD1 - N:UNK1 | 3.46991 | Hydrophobic | Pi-Sigma |
| A:LEU244:CD2 - N:UNK1 | 3.69573 | Hydrophobic | Pi-Sigma |
| A:HIS243 - N:UNK1 | 4.23318 | Hydrophobic | Pi-Pi Stacked |
| A:PHE260 - N:UNK1 | 4.34798 | Hydrophobic | Pi-Pi T-shaped |
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