**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 | EC2mv9\_101324856\_uff\_E=967.70 | -6.1 | 0 | 0 |
| 02 | EC2mv9\_5280637\_uff\_E=456.82 | -6.1 | 0 | 0 |
| 03 | EC2mv9\_441071\_uff\_E=807.01 | -6.1 | 0 | 0 |
| 04 | EC2mv9\_12912214\_uff\_E=410.93 | -6 | 0 | 0 |
| 05 | EC2mv9\_5280445\_uff\_E=242.10 | -5.8 | 0 | 0 |
| 06 | EC2mv9\_5280794\_uff\_E=546.19 | -5.7 | 0 | 0 |
| 07 | EC2mv9\_5280443\_uff\_E=233.26 | -5.7 | 0 | 0 |
| 08 | EC2mv9\_15515703\_uff\_E=992.32 | -5.6 | 0 | 0 |
| 09 | EC2mv9\_64971\_uff\_E=793.31 | -5.5 | 0 | 0 |
| 10 | EC2mv9\_222284\_uff\_E=590.88 | -5.4 | 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 |
| Ascorbic acid | 54670067 | OC[C@@H]([C@H]1OC(=O)C(=C1O)O)O | 176.12 | 6 | 4 | -0.31 | 1.49 | High | No | 0 | 0 |
| Nicotinic acid | 938 | OC(=O)c1cccnc1 | 123.11 | 3 | 1 | 0.86 | -1.35 | High | Yes | 0 | 0 |
| Apigenin-7 | 12912214 | OC(=O)[C@H]1O[C@H](Oc2cc(O)c3c(c2)oc(cc3=O)c2ccc(cc2)O)[C@@H]([C@H]([C@@H]1O)O)O | 446.36 | 11 | 6 | 1 | -2.22 | Low | No | 2 | 0 |
| Luteolin | 5280445 | Oc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)O | 286.24 | 6 | 4 | 1.86 | -3.82 | High | No | 0 | 1 |
| Apigenin | 5280443 | Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O | 270.24 | 5 | 3 | 1.89 | -4.40 | High | No | 0 | 0 |
| Nicotine | [89594](https://pubchem.ncbi.nlm.nih.gov/compound/89594) | CN1CCC[C@H]1c1cccnc1 | 162.23 | 2 | 0 | 2.04 | -2.62 | High | Yes | 0 | 0 |
| L-(+)-arabinose | [9847922](https://pubchem.ncbi.nlm.nih.gov/compound/9847922) | OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)O)[C@@H]([C@H]([C@@H]1O)O)OC(=O)/C=C/c1ccc(c(c1)O)O | 478.45 | 11 | 7 | 1.17 | -1.45 | Low | No | 2 | 1 |
| Stigmasterol | [5280794](https://pubchem.ncbi.nlm.nih.gov/compound/5280794) | CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)CC[C@@H](C2)O)C | 412.69 | 1 | 1 | 5.08 | -5.47 | Low | No | 1 | 0 |
| [Stigmastanol](https://pubchem.ncbi.nlm.nih.gov/compound/241572) | [241572](https://pubchem.ncbi.nlm.nih.gov/compound/241572) | CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC[C@@H]2[C@]1(C)CC[C@@H](C2)O)C | 416.72 | 1 | 1 | 5.17 | -6.20 | Low | No | 1 | 0 |
| [Dotriacontane](https://pubchem.ncbi.nlm.nih.gov/compound/11008) | [11008](https://pubchem.ncbi.nlm.nih.gov/compound/11008) | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 450.87 | 0 | 0 | 8.4 | -12.67 | Low | 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 |
| Ascorbic acid | 54670067 | OC[C@@H]([C@H]1OC(=O)C(=C1O)O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Nicotinic acid | 938 | OC(=O)c1cccnc1 | Active | Inactive | Inactive | Inactive | Inactive |
| Apigenin-7 | 12912214 | OC(=O)[C@H]1O[C@H](Oc2cc(O)c3c(c2)oc(cc3=O)c2ccc(cc2)O)[C@@H]([C@H]([C@@H]1O)O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Luteolin | 5280445 | Oc1cc(O)c2c(c1)oc(cc2=O)c1ccc(c(c1)O)O | Inactive | Active | Inactive | Active | Inactive |
| Apigenin | 5280443 | Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O | Inactive | Inactive | Inactive | Inactive | Inactive |
| Nicotine | [89594](https://pubchem.ncbi.nlm.nih.gov/compound/89594) | CN1CCC[C@H]1c1cccnc1 | Inactive | Inactive | Inactive | Inactive | Inactive |
| L-(+)-arabinose | [9847922](https://pubchem.ncbi.nlm.nih.gov/compound/9847922) | OC[C@H]1O[C@@H](OCCc2ccc(c(c2)O)O)[C@@H]([C@H]([C@@H]1O)O)OC(=O)/C=C/c1ccc(c(c1)O)O | Inactive | Inactive | Active | Inactive | Inactive |
| Stigmasterol | [5280794](https://pubchem.ncbi.nlm.nih.gov/compound/5280794) | CC[C@@H](C(C)C)/C=C/[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)CC[C@@H](C2)O)C | Inactive | Inactive | Active | Inactive | Inactive |
| [Stigmastanol](https://pubchem.ncbi.nlm.nih.gov/compound/241572) | [241572](https://pubchem.ncbi.nlm.nih.gov/compound/241572) | CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC[C@@H]2[C@]1(C)CC[C@@H](C2)O)C | Inactive | Inactive | Active | Inactive | Inactive |
| [Dotriacontane](https://pubchem.ncbi.nlm.nih.gov/compound/11008) | [11008](https://pubchem.ncbi.nlm.nih.gov/compound/11008) | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 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:PRO168 - N:UNK1 | 4.69928 | Hydrophobic | Alkyl |
| A:PRO168 - N:UNK1 | 4.3658 | Hydrophobic | Alkyl |
| A:PRO168 - N:UNK1 | 4.08108 | Hydrophobic | Alkyl |
| N:UNK1 - A:MET132 | 5.08623 | Hydrophobic | Alkyl |
| N:UNK1:C - A:ARG231 | 4.24348 | Hydrophobic | Alkyl |
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