1. **Acarbose Vina results**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| **Affinity (kcal/mol)** | -7.6 | -7.6 | -7.5 | -7.4 | -7.4 | -7.4 | -7.3 | -7.2 | -7 |
| **Rmsd l.b.** | 0 | 2.2 | 1.727 | 2.025 | 2.075 | 2.457 | 1.984 | 2.396 | 1.937 |
| **Rmsd u.b.** | 0 | 2.858 | 2.794 | 3.562 | 8.667 | 4.176 | 3.105 | 3.508 | 2.596 |
| **Amino acid residue (Conf. 1)** | **TRP59, TYR62, LEU162, LYS200, HIS201, ILE235** | | | | | | | | |

**Acarbose Autodock results**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| **Binding enery** | -5.18 | -4.33 | -3.27 | -3.9 | -4.5 | -5.29 | -4.32 | -3.81 | -4.18 | -4.78 |
| **Ligand efficiency** | -0.17 | -0.14 | -0.11 | -0.13 | -0.15 | -0.18 | -0.14 | -0.13 | -0.14 | -0.16 |
| **Ihib constant, Ki (uM)** | 158.33 | 674.62 | 4.02 | 1.38 | 502.33 | 133.3 | 679.21 | 1.6 | 869.37 | 312.81 |
| **Intermol energy** | -9.06 | -8.2 | -7.15 | -7.78 | -8.38 | -9.16 | -8.2 | -7.69 | -8.05 | -8.66 |
| **Vdw-hb-desolv energy** | -8.62 | -7.49 | -6.88 | -7.19 | -7.69 | -8.51 | -7.77 | -6.95 | -7.89 | -8.19 |
| **Electrostatic energy** | -0.45 | -0.71 | -0.26 | -0.59 | -0.69 | -0.66 | -0.43 | -0.74 | -0.16 | -0.47 |
| **Total internal energy** | -4.49 | -4.56 | -5.84 | -5.63 | -5.74 | -4.06 | -4.45 | -5.09 | -4.84 | -4.41 |
| **Torional energy** | 3.88 | | | | | | | | | |

1. **Cynaroside Vina results**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| **Affinity (kcal/mol)** | -9.1 | -9 | -8.8 | -8.7 | -8.7 | -8.3 | 8.1 | -7.9 | -7.8 |
| **Rmsd l.b.** | 0 | 1.951 | 2.626 | 2.063 | 3.582 | 3.118 | 3.661 | 3.78 | 3.853 |
| **Rmsd u.b.** | 0 | 8.294 | 5.237 | 3.014 | 9.564 | 6.47 | 10.106 | 9.135 | 9.115 |
| **Amino acid residue (Conf. 1)** | **TRP59, TYR62, GLN63, LEU165, ASP197, ALA198, GLU233, ASP300, HIS305, ASP356** | | | | | | | | |

**Cynaroside Autodock results**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| **Binding enery** | -11.06 | | -14.35 | -10.48 | -10.24 | -10.28 | -9.87 | -11.59 | -11.27 | -9.65 | -11.27 |
| **Ligand efficiency** | -0.35 | | -0.45 | -0.33 | -0.32 | -0.32 | -0.31 | -0.36 | -0.35 | -0.3 | -0.35 |
| **Ihib constant, Ki (uM)** | 7.87 | | 30.23 | 20.7 | 31.2 | 28.97 | 58.5 | 3.2 | 5.45 | 84.26 | 5.46 |
| **Intermol energy** | -14.34 | | -17.63 | -13.76 | -13.52 | -13.57 | -13.15 | -14.87 | -14.55 | -12.93 | -14.55 |
| **Vdw-hb-desolv energy** | -14.34 | | -17.63 | -13.76 | -13.52 | -13.57 | -13.15 | -14.87 | -14.55 | -12.93 | -14.55 |
| **Electrostatic energy** | 0 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Total internal energy** | -5.09 | | -4.71 | -4.79 | -5.21 | -4.94 | -5.01 | -4.69 | -4.53 | -5.17 | -4.39 |
| **Torional energy** | 3.28 | | | | | | | | | | |

1. **Rutin Vina results**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| **Affinity (kcal/mol)** | -8.5 | -8.3 | -8 | -8 | -7.9 | -7.8 | -7.6 | -7.5 | -7.4 |
| **Rmsd l.b.** | 0 | 2.035 | 2.783 | 4.414 | 4.94 | 1.761 | 2.037 | 4.991 | 7.302 |
| **Rmsd u.b.** | 0 | 2.876 | 6.312 | 8.303 | 10.295 | 6.859 | 7.697 | 8.173 | 11.928 |
| **Amino acid residue (Conf. 1)** | **TRP59, GLN63, LEU162, LEU165, ASP197, HIS305, ASP356** | | | | | | | | |

**Rutin Autodock results**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| **Binding enery** | -4.38 | | -2.44 | -2.12 | -1.76 | -2.92 | -2.89 | -2.24 | -4.99 | -4.17 | -3.95 |
| **Ligand efficiency** | -0.1 | | -0.06 | -0.05 | -0.04 | -0.07 | -0.07 | -0.05 | -0.12 | -0.1 | -0.09 |
| **Ihib constant, Ki (uM)** | 619.4 | | 16.21 | 27.84 | 51.32 | 7.26 | 7.58 | 22.92 | 221.45 | 879.25 | 1.27 |
| **Intermol energy** | -9.15 | | -7.22 | -6.89 | -6.53 | -7.69 | -7.67 | -7.01 | -9.76 | -8.94 | -8.72 |
| **Vdw-hb-desolv energy** | -8.58 | | -6.57 | -6.38 | -6.53 | -7.32 | -7.44 | -6.41 | -9.34 | -8.08 | -8.09 |
| **Electrostatic energy** | -0.57 | | -0.64 | -6.38 | 0.02 | -0.37 | -0.23 | -0.6 | -0.42 | -0.86 | -0.63 |
| **Total internal energy** | -6.92 | | -6.81 | -8.44 | -9.08 | -8.45 | -7.14 | -8.53 | -7.98 | -7.61 | -6.86 |
| **Torional energy** | 4.77 | | | | | | | | | | |

1. **Rosavin Vina results**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| **Affinity (kcal/mol)** | -7.7 | -7.7 | -7.7 | -7.6 | -7.5 | -7.4 | -7.4 | -7.3 | -7.3 |
| **Rmsd l.b.** | 0 | 2.336 | 2.069 | 2.089 | 1.919 | 1.597 | 2.69 | 2.498 | 2.429 |
| **Rmsd u.b.** | 0 | 3.162 | 8.571 | 3.169 | 2.816 | 2.302 | 5.141 | 4.311 | 8.891 |
| **Amino acid residue (Conf. 1)** | **TRP59,TYR151, LEU162, ARG195, LYS200, HIS201, ILE235, ASP300** | | | | | | | | |

**Rosavin Autodock results**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| **Binding enery** | -4.96 | -5.53 | -4.91 | -3.28 | -5.22 | -5.45 | -6.54 | -4.61 | -4.69 | -4.21 |
| **Ligand efficiency** | -0.17 | -0.18 | -0.16 | -0.11 | -0.17 | -0.18 | -0.22 | -0.15 | -0.16 | -0.14 |
| **Ihib constant, Ki (uM)** | 233 | 88.96 | 250.27 | 3.96 | 149.81 | 100.42 | 16.05 | 417.23 | 364.84 | 820.37 |
| **Intermol energy** | -8.83 | -9.4 | -8.79 | -7.16 | -9.1 | -9.33 | -10.42 | -8.49 | -8.57 | -8.09 |
| **Vdw-hb-desolv energy** | -8.67 | -8.84 | -8.41 | -6.95 | -8.71 | -8.63 | -9.57 | -7.77 | -8.2 | -7.52 |
| **Electrostatic energy** | -0.17 | -0.56 | -0.38 | -0.21 | -0.39 | -0.71 | -0.85 | -0.72 | -0.36 | -0.57 |
| **Total internal energy** | -6.58 | -4.54 | -5.17 | -6.06 | -5.06 | -5.6 | -4.99 | -5.6 | -5.21 | -5.19 |
| **Torional energy** | 3.88 | | | | | | | | | |

1. **Salidrodside Vina results**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| **Affinity (kcal/mol)** | -7.6 | -7.5 | -7.5 | -7.5 | -7.5 | -7.4 | -7.3 | -7.2 | -7.1 |
| **Rmsd l.b.** | 0 | 1.435 | 1.326 | 2.336 | 1.733 | 1.764 | 2.01 | 2.628 | 1.778 |
| **Rmsd u.b.** | 0 | 2.32 | 1.925 | 3.054 | 2.487 | 3.052 | 3.17 | 4.522 | 3.036 |
| **Amino acid residue (Conf. 1)** | **TRP59, TYR62, LEU165, ASP197, GLU233, HIS305, GLY306, ALA307** | | | | | | | | |

**Salidrodside Autodock results**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| **Binding enery** | -5.9 | -4.23 | -4.19 | -5.62 | -6.54 | -4.44 | -5.62 | -5.31 | -7.39 | -4.39 |
| **Ligand efficiency** | -0.2 | -0.14 | -0.14 | -0.19 | -0.22 | -0.15 | -0.19 | -0.18 | -0.25 | -0.16 |
| **Ihib constant, Ki (uM)** | 47.62 | 788.59 | 848.16 | 75.61 | 16.18 | 552.31 | 75.68 | 128.4 | 3.83 | 245.4 |
| **Intermol energy** | -9.77 | -8.11 | -8.07 | -9.5 | -10.41 | -8.32 | -9.5 | -9.19 | -11.27 | -8.8 |
| **Vdw-hb-desolv energy** | -9.08 | -7.88 | -7.83 | -8.65 | -9.72 | -7.91 | -8.65 | -8.55 | -10.51 | -7.93 |
| **Electrostatic energy** | -0.69 | -0.23 | -0.24 | -0.85 | -0.69 | -0.41 | -0.85 | -0.63 | -0.76 | -0.88 |
| **Total internal energy** | -3.83 | -6.37 | -5.61 | -5.23 | -4.37 | -4.22 | -4.55 | -4.35 | -3.33 | -5.36 |
| **Torional energy** | 3.88 | | | | | | | | | |

**Table 1: Binding energies of the compounds based on their rank**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **Binding energies of the compounds based on their rank (kcal/mol)** | | | | | | | | | |
| **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| Cynaroside | -10.38 | -11.63 | -10.92 | -14.1 | -14.14 | -11.48 | -14.31 | -10.07 | -10.54 | -10.21 |
| Salidrodside | -4.28 | -5.63 | -5.34 | -6.42 | -4.72 | -5.98 | -5.61 | -6.09 | -4.89 | -3.95 |
| Rosavin | -4.96 | -5.53 | -4.91 | -3.28 | -5.22 | -5.45 | -6.54 | -4.61 | -4.69 | -4.21 |
| Acarbose | -5.18 | -4.33 | -3.27 | -3.9 | -4.5 | -5.29 | -4.32 | -3.81 | -4.18 | -4.78 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **Binding energies of the compounds based on their rank (kcal/mol)** | | | | | | | | |
| **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| Cynaroside | -9.1 | -9 | -8.8 | -8.7 | -8.7 | -8.3 | 8.1 | -7.9 | -7.8 |
| Salidrodside | -7.6 | -7.5 | -7.5 | -7.5 | -7.5 | -7.4 | -7.3 | -7.2 | -7.1 |
| Rosavin | -7.7 | -7.7 | -7.7 | -7.6 | -7.5 | -7.4 | -7.4 | -7.3 | -7.3 |
| Acarbose | -7.6 | -7.6 | -7.5 | -7.4 | -7.4 | -7.4 | -7.3 | -7.2 | -7 |

**Table 2: Inhibition Constant of the compounds based on their rank**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **Inhibition Constant of the compounds based on their rank (µM, mM\*** | | | | | | | | | |
| **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** |
| Cynaroside | 24.57 | 2.99 | 9.95 | 46.51 | 43.25 | 3.87 | 32.48 | 41.67 | 18.81 | 32.84 |
| Salidrodside | 727.87 | 74.75 | 121.21 | 19.65 | 347.25 | 41.59 | 77.23 | 34.25 | 261.11 | 1.27 |
| Rosavin | 233 | 88.96 | 250.27 | 3.96 | 149.81 | 100.42 | 16.05 | 417.23 | 364.84 | 820.37 |
| Acarbose | 158.33 | 674.62 | 4.02 | 1.38 | 502.33 | 133.3 | 679.21 | 1.6 | 869.37 | 312.81 |

1. Sinoroside &salidrodside
2. A-amilase activator
3. Ligand+membrane kanal – actin, miosine, kalmadulin (oqsil)