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 | -10.38 | -11.63 | -10.92 | -14.1 | -14.14 | -11.48 | -14.31 | -10.07 | -10.54 | -10.21 |
| Ligand efficiency | -0.32 | -0.36 | -0.34 | -0.44 | -0.44 | -0.36 | -0.45 | -0.31 | -0.33 | -0.32 |
| Ihib constant, Ki (uM) | 24.57 | 2.99 | 9.95 | 46.51 | 43.25 | 3.87 | 32.48 | 41.67 | 18.81 | 32.84 |
| Intermol energy | -13.66 | -14.91 | -14.2 | -17.38 | -17.42 | -14.76 | -17.59 | -13.35 | -13.82 | -13.49 |
| Vdw-hb-desolv energy | -13.66 | -14.91 | -14.2 | -17.38 | -17.42 | -14.76 | -17.59 | -13.35 | -13.82 | -13.49 |
| Electrostatic energy | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Total internal energy | -5.21 | -4.98 | -5.07 | -3.73 | -4.69 | -4.77 | -4.73 | -4.84 | -4.92 | -5.2 |
| 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 | -4.28 | -5.63 | -5.34 | -6.42 | -4.72 | -5.98 | -5.61 | -6.09 | -4.89 | -3.95 |
| Ligand efficiency | -0.14 | -0.19 | -0.18 | -0.21 | -0.16 | -0.2 | -0.19 | -0.2 | -0.16 | -0.13 |
| Ihib constant, Ki (uM) | 727.87 | 74.75 | 121.21 | 19.65 | 347.25 | 41.59 | 77.23 | 34.25 | 261.11 | 1.27 |
| Intermol energy | -8.16 | -9.51 | -9.22 | -10.3 | -8.6 | -9.85 | -9.49 | -9.97 | -8.77 | -7.83 |
| Vdw-hb-desolv energy | -7.62 | -8.5 | -8.48 | -9.64 | -8.39 | -9.12 | -8.63 | -9.37 | -8.16 | -7.57 |
| Electrostatic energy | -0.54 | -1.01 | -0.74 | -0.65 | -0.2 | -0.73 | -0.86 | -0.6 | -0.6 | -0.26 |
| Total internal energy | -5.16 | -4.38 | -5.69 | -4.48 | -5.03 | -4.7 | -5.24 | -4.75 | -5.23 | -4.85 |
| Torional energy | 3.88 | | | | | | | | | |