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** | | | | | | | | |

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** | | | | | | | | |

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** | | | | | | | | |

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** | | | | | | | | |

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** | | | | | | | | |