|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Binding enery**  **(kcal/mol)** | **Ligand efficiency** | **Ihib constant, Ki (uM)** | **Intermol energy**  **(kcal/mol)** | **Vdw-hb-desolv energy**  **(kcal/mol)** | **Electrostatic energy**  **(kcal/mol)** | **Total internal energy**  **(kcal/mol)** | **Torional energy**  **(kcal/mol)** |
| Acarbose (3) | -3.27 | -0.11 | 4.02 | -7.15 | -6.88 | -0.26 | -5.84 | 3.88 |
| Cynaroside (8) | -11.27 | -0.35 | 5.45 | -14.55 | -14.55 | 0 | -4.53 | 3.28 |
| Rutin (1) | -4.38 | -0.1 | 619.4 | -9.15 | -8.58 | -0.57 | -6.92 | 4.77 |
| Rosavin (6) | -5.45 | -0.18 | 100.42 | -9.33 | -8.63 | -0.71 | -5.6 | 3.88 |
| Salidrodside (10) | -4.39 | -0.16 | 245.4 | -8.8 | -7.93 | -0.88 | -5.36 | 3.88 |