|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ZINC ID | Protein | Replicate | Binding free energy as predicted from (kJ/mol) | |
| DOCK pose (kJ/mol) | Autodock pose (kJ/mol) |
| ZINC00814199 | M | 1 | -153+/-6 | -119+/-8 |
| 2 | - | -184+/-3 |
| 3 | -203+/-6 | - |
| ZINC63411510 | G | 1 | - | -44+/-4 |
| 2 | - | -79+/-4 |
| 3 | - | -59+/-4 |
| ZINC91252717 | P | 1 | -158+/-9 | -187+/-8 |
| 2 | -256+/-10 | -196+/-8 |
| 3 | -251+/-7 | - |