|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ZINC ID | Protein | Replicate | Binding free energy as predicted during | |
| AMBER simulation (kJ/mol) | CHARMM simulation(kJ/mol) |
| ZINC94258558 | N | 1 | - | -114+/-10 |
| 2 | - | -86+/-4 |
| 3 | - | - |
| ZINC73641145 | N | 1 | - | - |
| 2 | - | - |
| 3 | - | - |
| ZINC12362922 | N | 1 | -96+/-8 |  |
| 2 | -100+/-10 |  |
| 3 | -69+/-6 |  |
| ZINC04829362 | N | 1 | -37+/-7 |  |
| 2 | 86+/-7 |  |
| 3 | -101+/-8 |  |
| ZINC72462705 | P | 1 | - | 106+/-4 |
| 2 | - | 86+/-4 |
| 3 | - | 98+/-5 |
| ZINC86098248 | P | 1 | 39+/-5 |  |
| 2 | -65+/-7 |  |
| 3 | 37+/-3 |  |
| ZINC77285117 | P | 1 | - | - |
| 2 | - | - |
| 3 | - | - |
| ZINC86095599 | P | 1 | -196+/-7 |  |
| 2 | -149+/-10 |  |
| 3 | -153+/-14 |  |
| ZINC35605802 | P | 1 | -14+/-0.5 |  |
| 2 | 1+/-1 |  |
| 3 | -98+/-8 |  |
| ZINC01725633 | M | 1 | - | - |
| 2 | - | - |
| 3 | - | - |