| #Ligand | TotalEnergy | VDW | AverConPair |
|---|---|---|---|
| 6xs6-Roccustyrna_gs1-0.pdb | -926.867 | -926.867 | 171.667 |
| 6xs6-Roccustyrna_gs4-0.pdb | -103.451 | -826.471 | 136.735 |
| 6xs6-Roccustyrna_gs5-0.pdb | -873.398 | -873.398 | 15.275 |
| 6xs6-Roccustyrna_gs6-0.pdb | -785.159 | -785.159 | 130.732 |
| 6xs6-Acalabrutinib_CID_71226662 (1)-0.pdb | -867.968 | -867.968 | 160.857 |
| 6xs6-Ursolic acid-0.pdb | -722.477 | -722.477 | 145.758 |
| 6xs6-Valsartan-0.pdb | -795.093 | -795.093 | 165.625 |