| #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 |
| 6xs6-Betrixaban-0.pdb | -832.592 | -832.592 | 165.313 |
| 6xs6-Gemigliptin-0.pdb | 411.916 | 411.916 | 132.424 |
| 6xs6-Raltegravir-0.pdb | -897.648 | -897.648 | 199.375 |
| 6xs6-Ribavirin-0.pdb | -826.374 | -826.374 | 299.412 |
| 6xs6-Doxycycline-0.pdb | -163.781 | -163.781 | 10.25 |
| 6xs6-Histrelin-0.pdb | 667.201 | 667.201 | 134.896 |
| 6xs6-Eflornithine-0.pdb | -51.409 | -51.409 | 250.833 |
| 6xs6-Cycloserine-0.pdb | -501.861 | -501.861 | 482.857 |
| 6xs6-Colchicine-0.pdb | 326.766 | 326.766 | 26.069 |
| 6xs6-Bleomycin-0.pdb | 275.752 | 275.752 | 623.958 |
| 6xs6-Azathioprine-0.pdb | -790.178 | -790.178 | 331.579 |
| 6xs6-Ritonavir-0.pdb | 404.602 | 404.602 | 20.38 |
| 6xs6-Umifenovir-0.pdb | -760.054 | -760.054 | 180.345 |