|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Pdb id of protein** | **Lead structure of compound** | **Binding affinity**  **(kCal/mol)** | **Interaction of amino acid** | |
| **Hydrogen bond** | **Hydrophobic bond** |
| **4af3** | **CID:**16274282 | -10.6 | TYR A:141, LEU A:210, ARG A:139, | TYR A:141, LEU A:210, PRO A:158, TYR D:859, LEU D:865 |
| **4af3** | CID: 16273736 | -10.5 | ARG A:139, TYR A:141, GLN D:858, LYS A:215, SER A:338 | GLU A:155, LEU D:865, ILE D:855, PRO A:158, GLU A:213 |
| **4af3** | CID: 16345668 | -9.4 | LYS A:215, ARG A: 139, GLN D:858 | GLU A:155, LEU D:865, PRO D:862, LEU A: 210, PRO A:158, TYR D:859 |
| **4af3** | CID: 8895340 | -9.9 | GLN D:858, ARG A:139, HIS A:134, LYS A:215 | LEU D:865, GLU A:155, TYR D:859, PRO A:158, |
| **4af3** | CID: 16272857 | -9.9 | ARG A:139, GLU A:155, PRO D:862, PRO D863, | TYR D:859, PRO A:158 |
| **4af3** | CID: 16273739 | -9.8 | HIS A:134, LYS A:215, ARG:139 | LEU D:865, SER A:338, GLU A:155, GLU A:213 |