**Supplementary Table 1.** Molecular docking interactions of ligands with binding affinities lower than the benchmark reference inhibitor (ND-2158). For each compound, binding affinity (kcal/mol), hydrogen-bond interactions, and hydrophobic/other contacts are reported.

|  |  |  |  |
| --- | --- | --- | --- |
| Ligand | Binding Affinity (kcal/mol) | Hydrogen Bond interaction | Hydrophobic/Other Interactions |
|  |  | Amino acid | Amino acid |
| 1 | -8.1 | MET30, GLU32 | ALA49, TYR100, VAL38, LEU156 |
| 3 | -8.1 | ASP110, MET103 | MET30, VAL38 |
| 4 | -8 | MET30 | VAL38, ALA49, TYR100, LEU156 |
| 5 | -7.6 | MET103, PRO104 | MET30, ALA49, LEU156, VAL38 |
| 6 | -7.6 | ASN154, ASP110 | MET30, LEU156, VAL38, VAL84, ASP167 |
| 9 | -8.1 | MET103, GLU71, LYS51 | ALA49, VAL38, LEU156, MET30, TYR100 |
| 10 | -7 | ASP110, ALA153, ASN154, SER166, MET103, GLU32 | MET30, VAL38 |
| 11 | -8 | MET30, GLU32 | VAL38, LEU156 |
| 12 | -7.7 | ASN154, MET103, MET30 | LEU156, VAL38, TYR100 |
| 16 | -7.7 | ASP110, TYR100, GLY106 | ALA49, LEU156, MET103, MET30, VAL38 |
| 17 | -8.1 | MET30, MET103, SER166 | LEU156, VAL38, ALA49 |
| 19 | -8 | MET103 | MET30, VAL38, LEU156, TYR100 |
| 20 | -7.8 | ASP110, TYR100 | VAL38, ALA49, LEU156, MET30 |
| 21 | -7.3 |  | VAL38, ALA49, MET30, LEU156, TYR100 |
| 24 | -7.9 | ASN154, ALA153, MET30, MET103 | ALA49, TYR100, VAL38, LEU156 |
| 25 | -7.9 | MET30 | VAL38, ALA49, TYR100, LEU156 |
| 26 | -7.1 | ASN154 | TYR100, VAL38, LEU156 |
| 27 | -7.6 | ASP110, MET30 | TYR102, VAL38, ALA49, LEU156, TYR100 |
| 28 | -8 | ASP116, MET103, MET30 | ALA49, LEU156, VAL38 |
| 29 | -8 | MET103, TYR102 | MET30, ALA49, LEU156, VAL38 |
| 31 | -8.1 | ASP110, TYR100 | VAL38, ALA49, LEU156, MET30, MET103 |
| 32 | -7.7 | MET103, ASN154, SER166 | MET30, LEU156, VAL38, LYS51, ALA49, TYR100 |
| 33 | -7.1 | ASP167, MET30, TYR100 | LEU156, VAL38 |