**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 | MET192, GLU194 | ALA211, TYR262, VAL200, LEU318 |
| 3 | -8.1 | ASP272, MET265 | MET192, VAL200 |
| 4 | -8 | MET192 | TYR264, VAL200, ALA211, TYR262, LEU318 |
| 5 | -7.6 | ALA315, ASP272 | TYR262, LEU318, VAL200, MET192 |
| 6 | -7.6 | MET192 | VAL200, TYR262, ALA211, LEU318 |
| 9 | -8.1 | SER328, GLU194 MET265 | VAL246, ALA211, VAL200, LEU318, MET192, GLY268, TYR262 |
| 10 | -7 | ASN316, SER328, ALA315, GLU194, ASP272, MET265 | VAL200, MET192 |
| 11 | -8 | GLU194, MET192 | LEU318, VAL200 |
| 12 | -7.7 | ASN316, MET192, MET265 | VAL200, TYR262, LEU318 |
| 16 | -7.7 | TYR262, GLY268, ASP272 | VAL200, ALA211, LEU318, MET265, MET192 |
| 17 | -8.1 | ASP272 | MET192, ALA211, LEU318, VAL246, TYR262, VAL200 |
| 19 | -8 | MET265 | MET192, VAL200, LEU318, TYR262 |
| 20 | -7.8 | MET192 | VAL200, MET265, ALA211, LEU318, VAL246 |
| 21 | -7.3 |  | VAL200, ALA211, MET192, LEU318, TYR262 |
| 24 | -7.9 | MET265, MET192 | VAL200, LEU318, ALA211, VAL246, TYR262, ASP329 |
| 25 | -7.9 | MET192 | VAL200, ALA211, TYR262, LEU318 |
| 26 | -7.1 | ASN316 | ALA211, TYR262, LEU318, VAL200 |
| 27 | -7.6 | ASP272, MET192 | TYR264, VAL200, ALA211, LEU318, TYR262 |
| 28 | -8 | ASP278, MET265, MET192 | LEU318, VAL200, ALA211 |
| 29 | -8 | MET265, VAL263 | MET192, VAL200, LEU318, VAL246, ALA211, TYR262 |
| 31 | -8.1 | TYR262 | ASP272, VAL200, LEU318, ALA211, MET265, MET192 |
| 32 | -7.7 | MET192 | VAL200, LEU318 |
| 33 | -7.1 | MET265, ASP329 | TYR262, VAL246, LEU318, VAL200, MET192 |