**Supplementary Table 7.** **Key interacting residues of oleacein mimetics to the catalytic site of DNMT.** Interactions other than electrostatic are highlighted in yellow (possible) or green (reliable).

|  |  |  |
| --- | --- | --- |
| Oleacein mimetic | Main catalytic residues | Other relevant residues |
| CHEMBL2172394 | Asn1578Pro1225Asn1267 | Gly1223Ala1579Ser1146Glu1266Val1268Arg1310Phe1145 (π-π stacking) |
| CHEMBL1085246 | Asn1578Ala1579Val1580Phe1145Ser1146Gly1147Gly1223Pro1224Pro1225Asn1267 | Cys1148Glu1266 |
| CHEMBL357073 | Val1580Phe1145 (π-π stacking)Ser1146 | Asn1578Ala1579Leu1151Pro1225 |
| CHEMBL1632504 | Ala1579Val1580Phe1145Ser1146Gly1147Leu1151Glu1168 | Asn1578Trp1170Gly1223Met1169Pro1225 Glu1266 |
| CHEMBL126593 | Ala1579Val1580Phe114Ser1146Gly1150Pro1225 | Asn1578Gly1147Cys1148Leu1151Glu1168Gly1219Pro1224Leu1247 |
| CHEMBL1950046 | Ala1579Val1580Asp1143Ser1146Gly1150Leu1151 | Asn1578Gly1147Glu1266Ser1152 |
| CHEMBL1440472 | Asn1578Ala1579Gly1147Glu1168Gly1223Pro1225Trp1170 (halogen bond) | Phe1145Ser1146Gln1575Val1580Cys1148Gly1150Leu1151Pro1224 |
| CHEMBL1300434 | Val1580Phe1145Ser1146Glu1168Trp1170Pro1225  | Asn1578Met1169Gly1226Glu1266Ala1579Gly1147Asn1267 |
| CHEMBL1890048 | Phe1145Gly1147Glu1168Trp1170 (π-π stacking) | Gln1575Arg1574Ala1579Ser1146Met1169Pro1225Leu1247 |
| CHEMBL1180264 | Asn1578Phe1145Glu1266Ala1579Ser1146Gly1147 | Met1169Arg1574Val1580Leu1151Ser1146Trp1170Gly1173 |
| CHEMBL165714 | Val1580 | Ala1579Pro1225Asn1267Asn1578Arg1147Ser1146Gly1150Trp1170Gly1223Pro1224Glu1266 |
| CHEMBL1621113 | Asn1578Gly1223Asn1267Pro1225 (π-π stacking)Pro1224 (halogen bond) | Glu1266Arg1310Arg1312Ala1579Val1580Phe1145Ser1146Gln1227Val1268 |
| CHEMBL1079062 | Asn1578Ala1579Val1580Gly1150Leu1151Gly1223Glu1266Asn1267 | Ser1146Gly1146Pro1225Arg1310 |
| CHEMBL267516 | Ala1579Met1169Gly1223Pro1225Trp1170 (π-π stacking) | Glu1168Asn1578Phe1145Ser1146Gly1147Pro1224Leu1247Glu1266Asn1267 |
| CHEMBL1545778 | Asn1578Phe1145 (π-π stacking)Ser1146Gly1222Gly1223Pro1225 | Val1580Pro1224Ala1579Val1144Leu1151Met1169Leu1247 |
| CHEMBL1366164 | Asn1578Ser1146Gly1223Pro1225Glu1266Phe1145Pro1224 (π-π stacking) | Val1580Asn1267Ala1579Leu1151 |
| CHEMBL1642794 | Asn1578Phe1145Pro1225 | Ser1146Ala1579Val1153Gly1223 |
| CHEMBL2165395 | Ala1579Val1580Phe1145Ser1146Gly1147Leu1151Glu1168Met1169Trp1170 (halogen bond) | Gly1150Gly1223Pro1225Arg1147Asn1578Leu1247 |
| CHEMBL45196 | Gln1575Asn1578Gly1147Glu1168Trp1170 | Arg1574Ala1579Met1169Phe1148Ser1149Cys1148Gly1150Ala1173Gly1223Pro1225Leu1247 |
| CHEMBL2143987 | Asn1578Ala1579Val1580Gly1150Gly1223Pro1225Asn1267 | Ser1146Phe1145Gly1147Cys1148Leu1151Pro1224Glu1266Val1268 |