**Supplementary Table 6.** **Key interacting residues of oleacein mimetics to the catalytic site of mTOR.** Interactions other than electrostatic are highlighted in yellow (possible) or green (reliable).

|  |  |  |
| --- | --- | --- |
| Oleacein mimetic | Main catalytic residues | Other relevant residues |
| CHEMBL2172394 | Leu2185Lys2187Ile2356Ser2342Trp2239 (π-π stacking) | Pro2169Asp2244Thr2245Asn2343Asp2357Met2345Gln2167 |
| CHEMBL1085246 | Trp2239 (π-πstacking/cation-π stacking)Ser2342 | Ile2163Pro2169Leu2185Thr2245Met2345Ile2356 |
| CHEMBL357073 | Pro2169Leu2185Lys2187Thr2245 | Ile2163Leu2192Ile2337Trp2239 Ile2356Asp2357 |
| CHEMBL1632504 | Leu2185Trp2239 (cation-π stacking)Val2240Met2345Ile2356 | Leu2187Ile2237Gly2238Thr2245 |
| CHEMBL126593 | Trp2239 (π-π stacking)Val2240Met2345Ile2356 | Ile2163Leu2169Tyr2225Leu2354 |
| CHEMBL1950046 | Leu2187Leu2192Trp2239 (π-π stacking)Ile2356Asp2357 | Leu2195Tyr2225Ile2237Val2240 |
| CHEMBL1440472 | Lys2187Asn2343Asp2357 | Pro2169Leu2185Leu2192Tyr2225 (halogen bonding)Ile2337Ile2356 |
| CHEMBL1300434 | Lys2187Leu2192Asp2195Ile2356Asp2357Phe2358 | Leu2185Asp2191Gln2194Tyr2225Ile2237Gly2359 |
| CHEMBL1890048 | Trp2239(π-π stacking)Val2240Met2345 | Leu2185Tyr2225 (cation-π stacking) |
| CHEMBL1180264 | Leu2185Lys2187Ile2237Ile2356Asp2357 | Ile2167Pro2169Glu2190Leu2192 |
| CHEMBL165714 | Leu2185Ile2237Trp2239Val2240Ile2356 | Lys2187Tyr2225Cys2243Met2345 |
| CHEMBL1621113 | Asp2195Tyr2225 (cation-π stacking)Ile2237Asp2357 | Gln2167Pro2169Leu2185Lys2187Ile2356Phe2358 |
| CHEMBL1079062 | Leu2185Trp2239 (π-π stacking/cation-π stacking)Val2240 | Met2345Ile2356 |
| CHEMBL267516 | Leu218Gln2194Asp2195Trp2239 (cation-π stacking)Ile2356 | Leu2192Ile2237Met2345Asp2357 |
| CHEMBL1545778 | Lys2187Asp2195Ile2237Tyr2225 (π-πstacking)Val2240Ile2356Asp2357 | Glu2190Leu2192Met2345 |
| CHEMBL1366164 | Leu2185Trp2239 (cation-π stacking)Val2240Met2345Ile2356 | Ile2163Pro2169Lys2185Cys2243 |
| CHEMBL1642794 | Ile2163Leu2185Tyr2225 (cation-π stacking)Ile2237Trp2239 (π-π stacking)Val2240Thr2245Ile2356 | Pro2169Met2345Ser2342 |
| CHEMBL2165395 | Tyr2225 (cation-π stacking)Trp2239 (cation-π/π-π stacking)Val2240Met2345 | Ile2163Leu2185Gly2238 |
| CHEMBL45196 | Lys2187Glu2190Leu2192Asp2195Asp2357Phe2358 (π-π stacking) | Gln2194Ile2237Gly2359 |
| CHEMBL2143987 | Trp2239 (π-πstacking/cation-π stacking)Ser2342 | Ile2163Pro2169Leu2185Thr2245Met2345 |