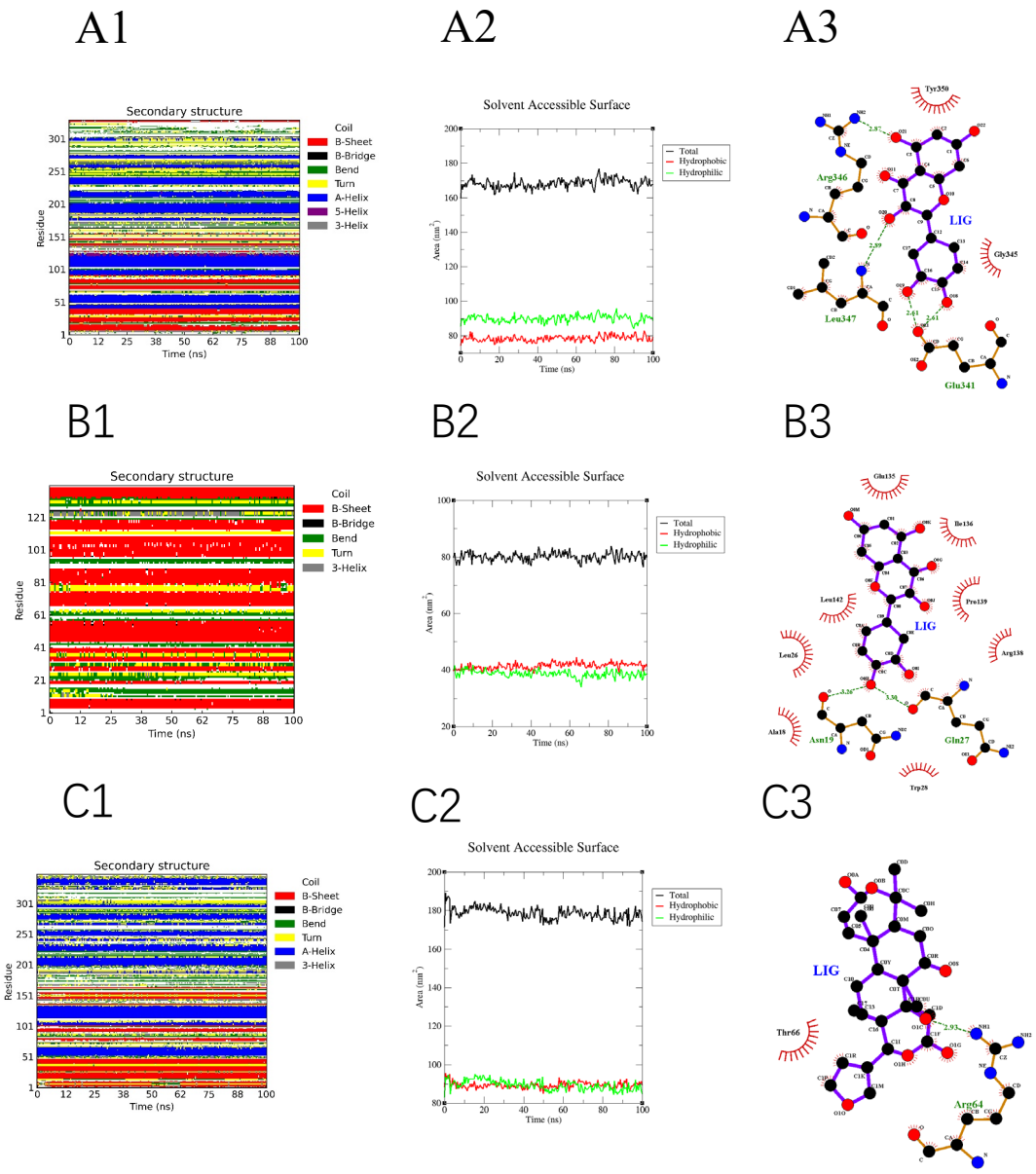
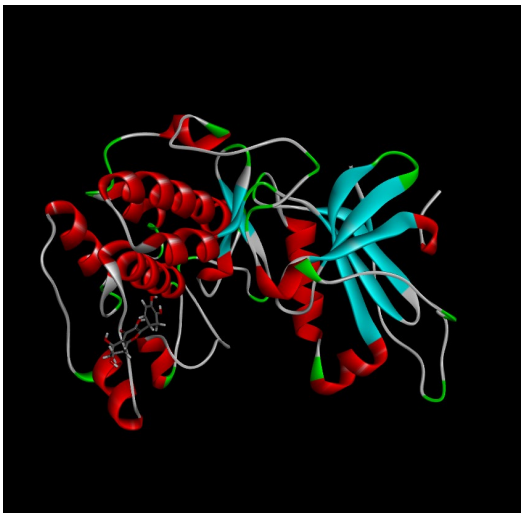
Supplementary Figure 1



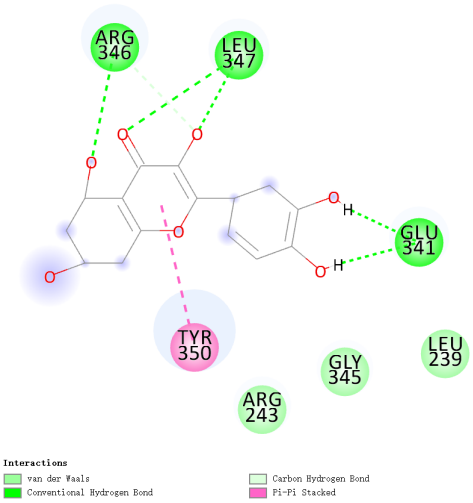
Supplementary Figure 1 Molecular dynamics(MD) simulations of HL10(Obacunone)-MAPK3, HQ10(Quercetin)-AKT1, and HQ10(Quercetin)-TNF. A1,A2: The secondary structure and solvent accessible surface area of HQ10(Quercetin)-AKT1 after 100ns molecular dynamics simulation; B1,B2: Secondary structure and solvent accessible surface area of HQ10(Quercetin)-TNF after 100ns molecular dynamics simulation; C1,C2 : Secondary structure and solvent accessible surface area of 100ns molecular dynamics simulation of HL10(Obacunone)-MAPK3; A3, B3, and C3 are two-dimensional bond pattern diagrams respectively.

Supplementary Figure 2

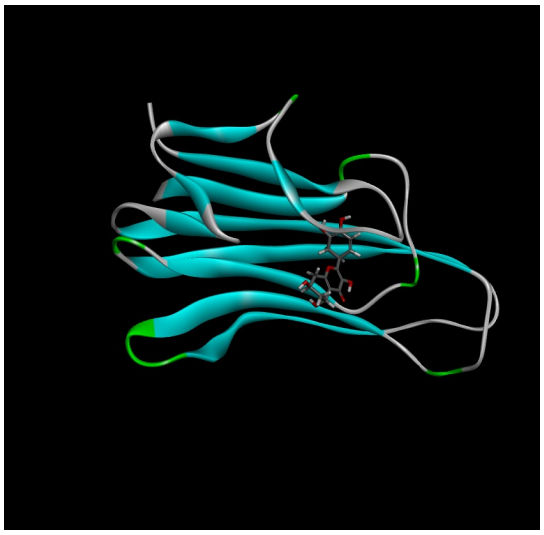
A



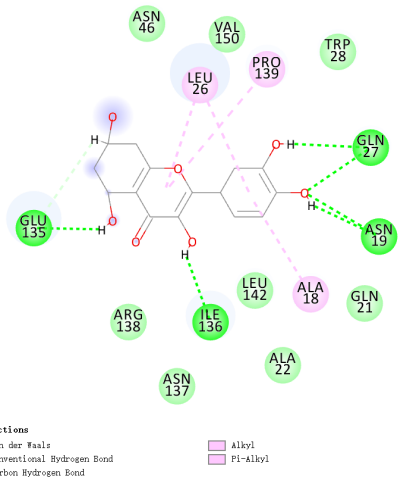
B

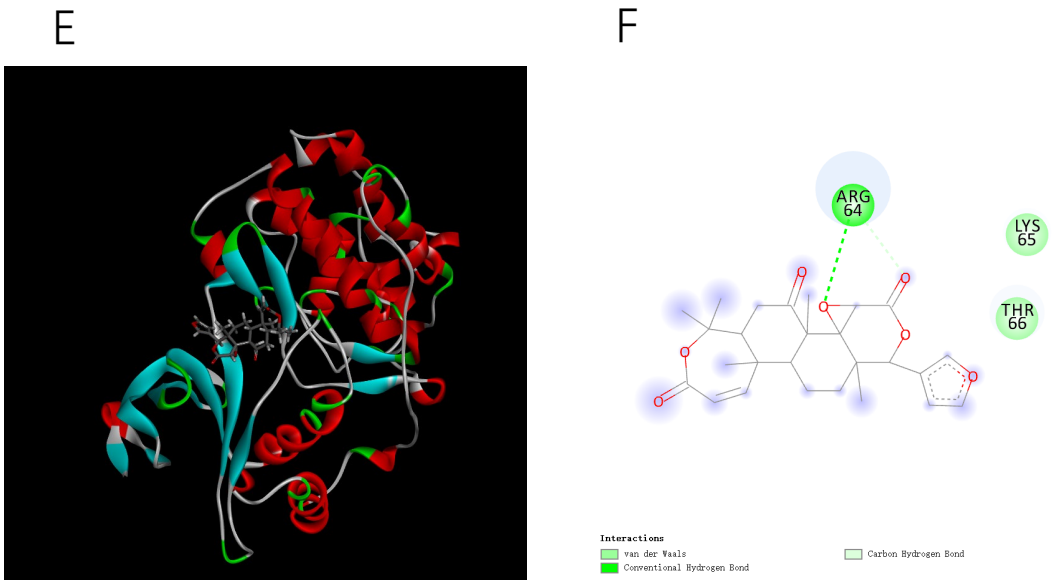


C



D





Supplementary Figure 2 100ns stable binding diagrams of HL10(obacunone)-MAPK3, HQ10(quercetin)-AKT1, and HQ10(quercetin)-TNF. A, C, and E are 100ns combined three-dimensional model diagrams of HQ10-AKT1, HQ10-TNF, and HL10-MAPK3, respectively. The colors red and cyan both represent receptors, with A, B, and C representing AKT1, TNF, and MAPK3, respectively. The gray color represents the ligands, where A, B, and C correspond to quercetin, quercetin, and obacunone, respectively. B, D, and F are 100ns combined two-dimensional bond pattern diagrams of HQ10-AKT1, HQ10-TNF, and HL10-MAPK3, respectively.