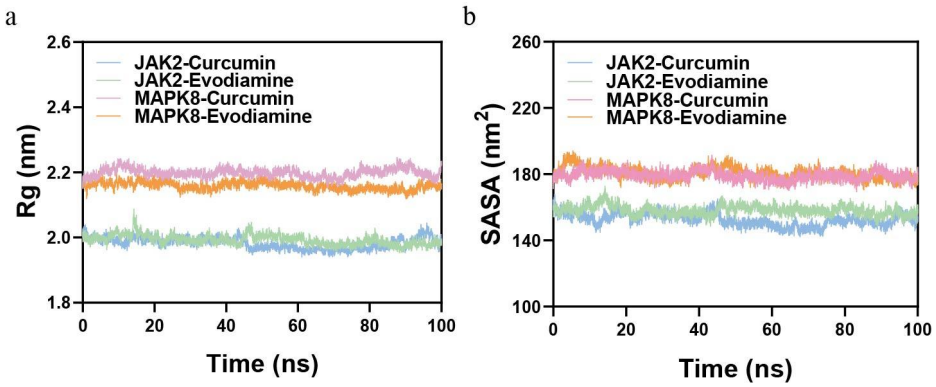


Supplementary Figure S7. Structural compactness of the four protein-ligand complexes over 100 ns molecular dynamics simulations.

(a) Radius of gyration (Rg) trajectories for each complex; (b) solvent-accessible surface area (SASA) profiles indicating stable global structure with no substantial expansion or unfolding.