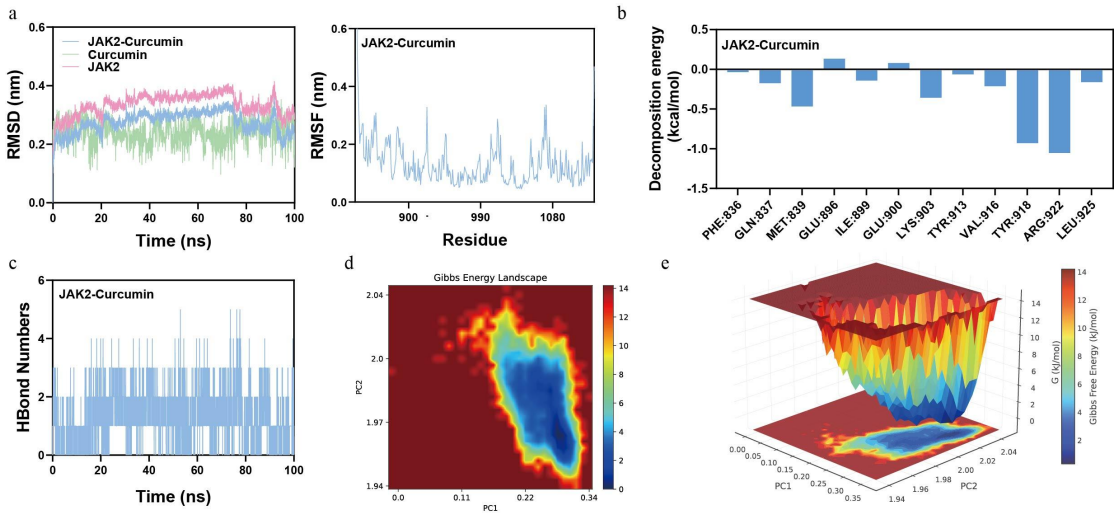


Supplementary Figure S6. Molecular dynamics simulation of the JAK2-curcumin complex over 100 ns.

(a) RMSD time series. (b) Per-residue binding free energy decomposition showing Leu892 and Glu896 as key binding residues. (c) Intermolecular hydrogen bond count over time. (d) Two-dimensional free energy landscape along PC1/PC2. (e) Three-dimensional FEL