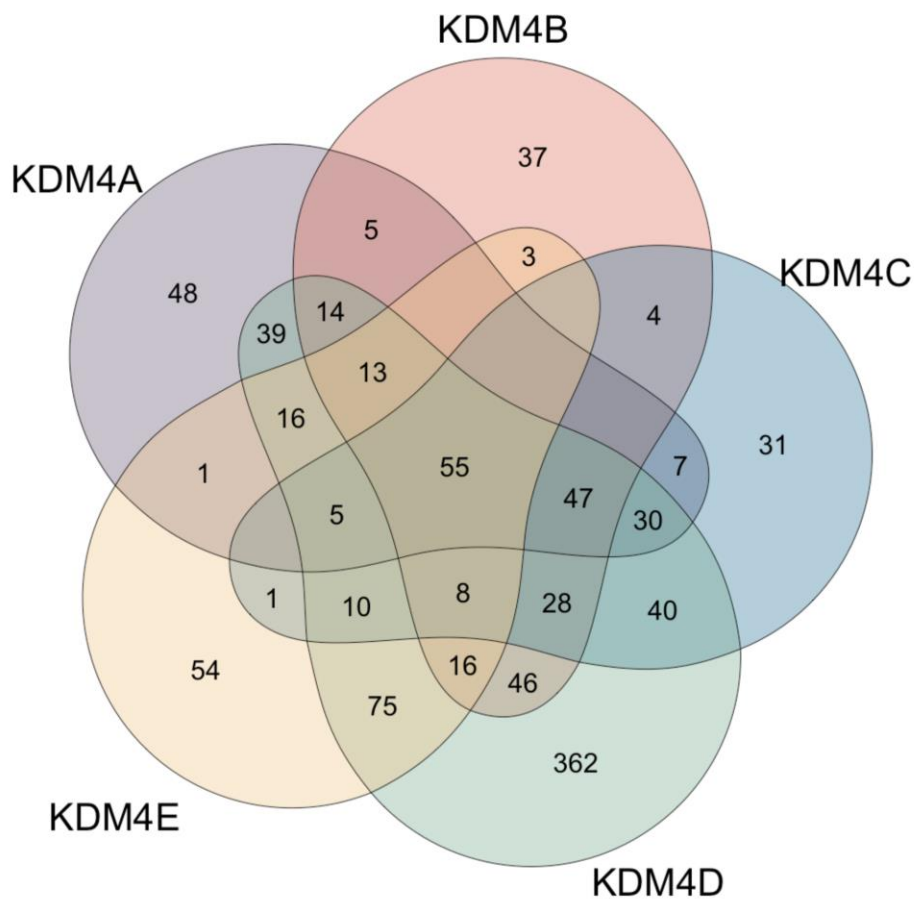
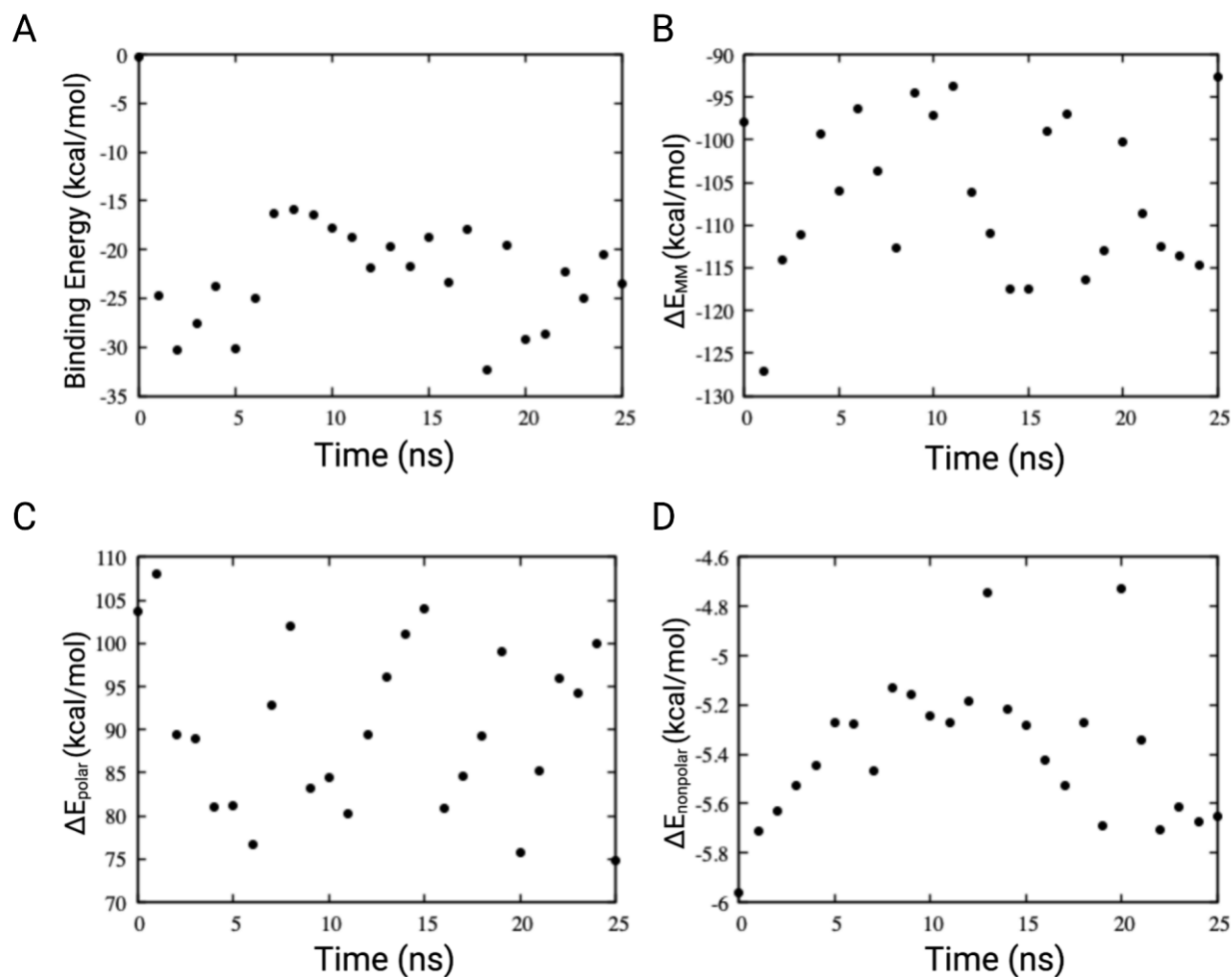


Supplementary Figures



Supplementary Figure 1. Shared ligands between the KDM4 subfamily. The Venn diagram shows the intersections for the top 100 ligands predicted to bind to each KDM4 subfamily member (results are only for the HOLO form). The compounds for each intersection are listed in the Supplementary File 3



Supplementary Figure 2. Binding energies for the KDM4A-CNP0371131 complex through the molecular dynamics simulation. (A) Δ GPBSA binding energy. (B) Molecular Mechanics (MM) energy. (C) polar solvation free energy estimated with the Poisson-Boltzmann (PB) model. (D) Binding nonpolar contribution energy estimated from the solvent accessible surface area.