

Supplementary

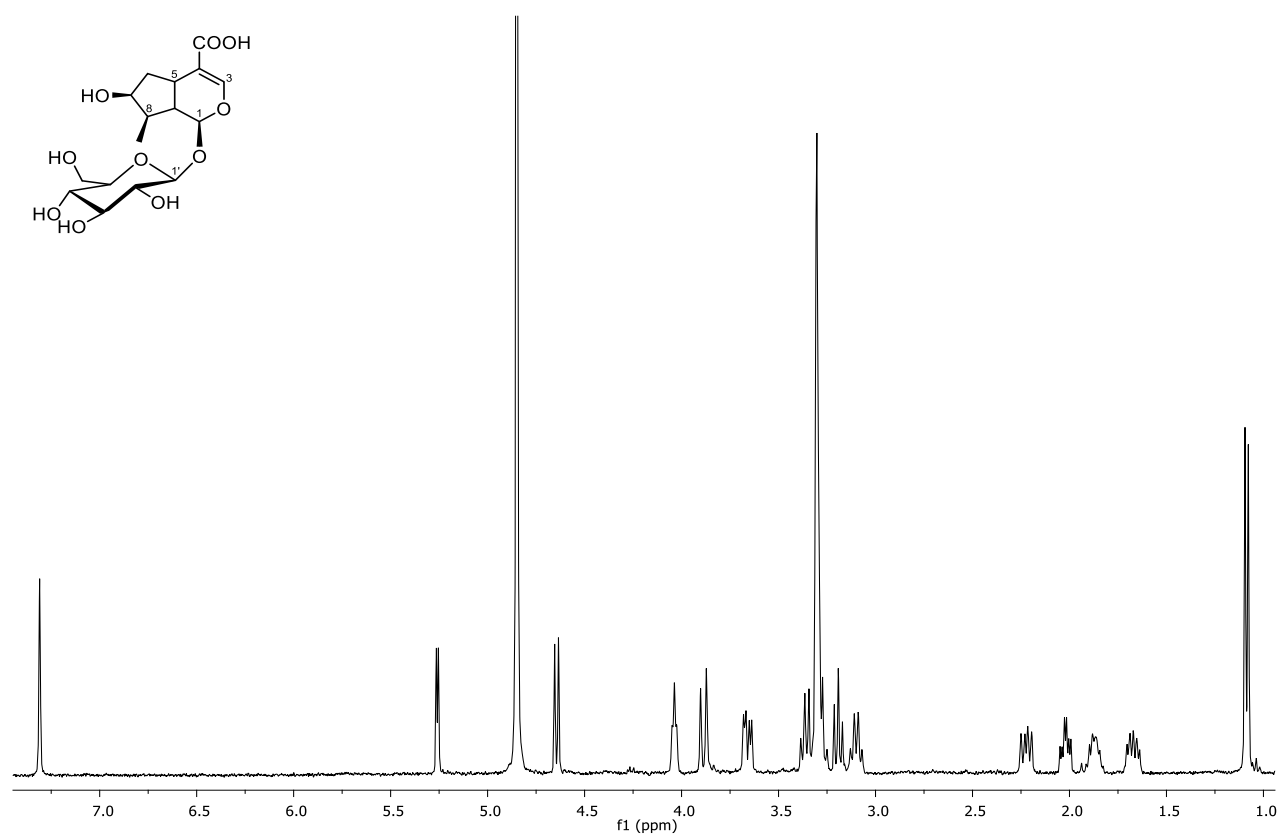


Figure S1. ^1H NMR spectra of loganic acid (**1**) (400 MHz, CD_3OD).

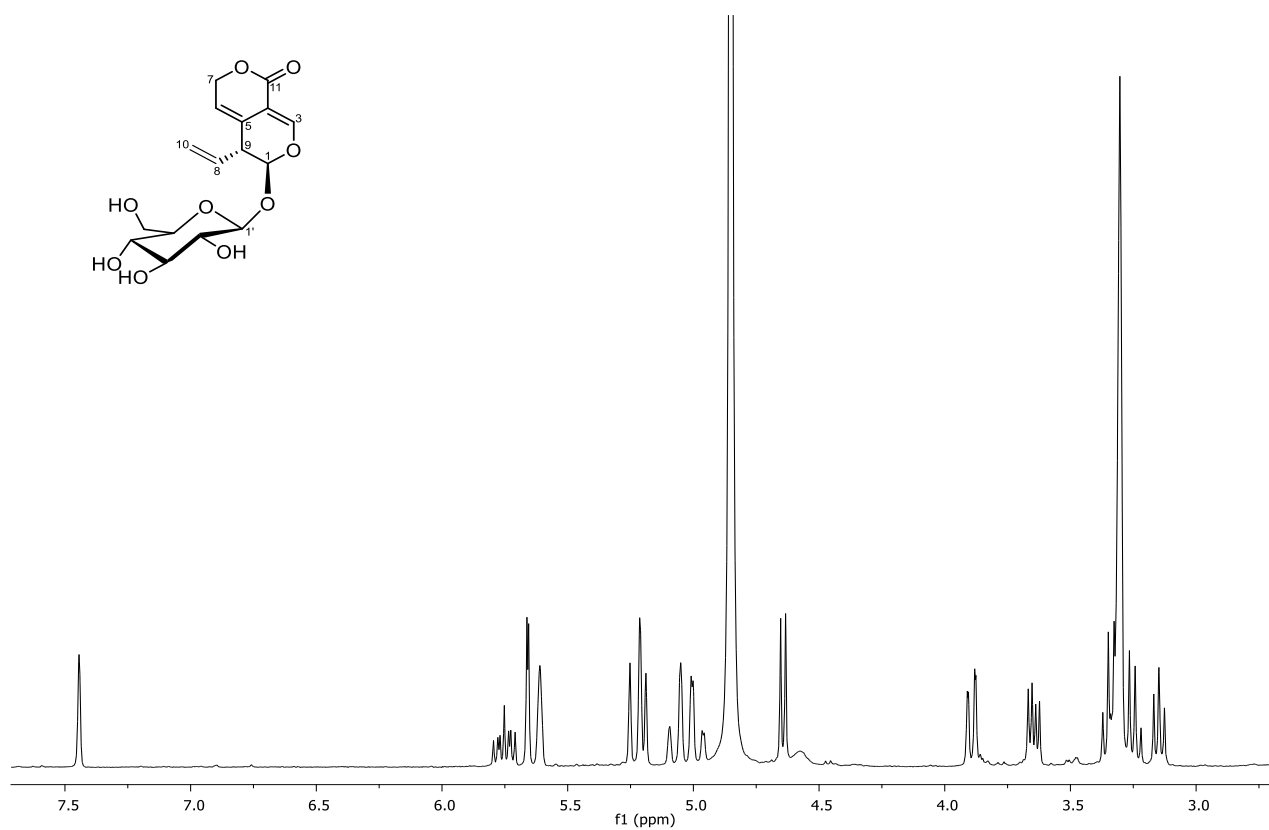


Figure S2. ^1H NMR of gentiopicroside (**2**) (400 MHz, CD_3OD).

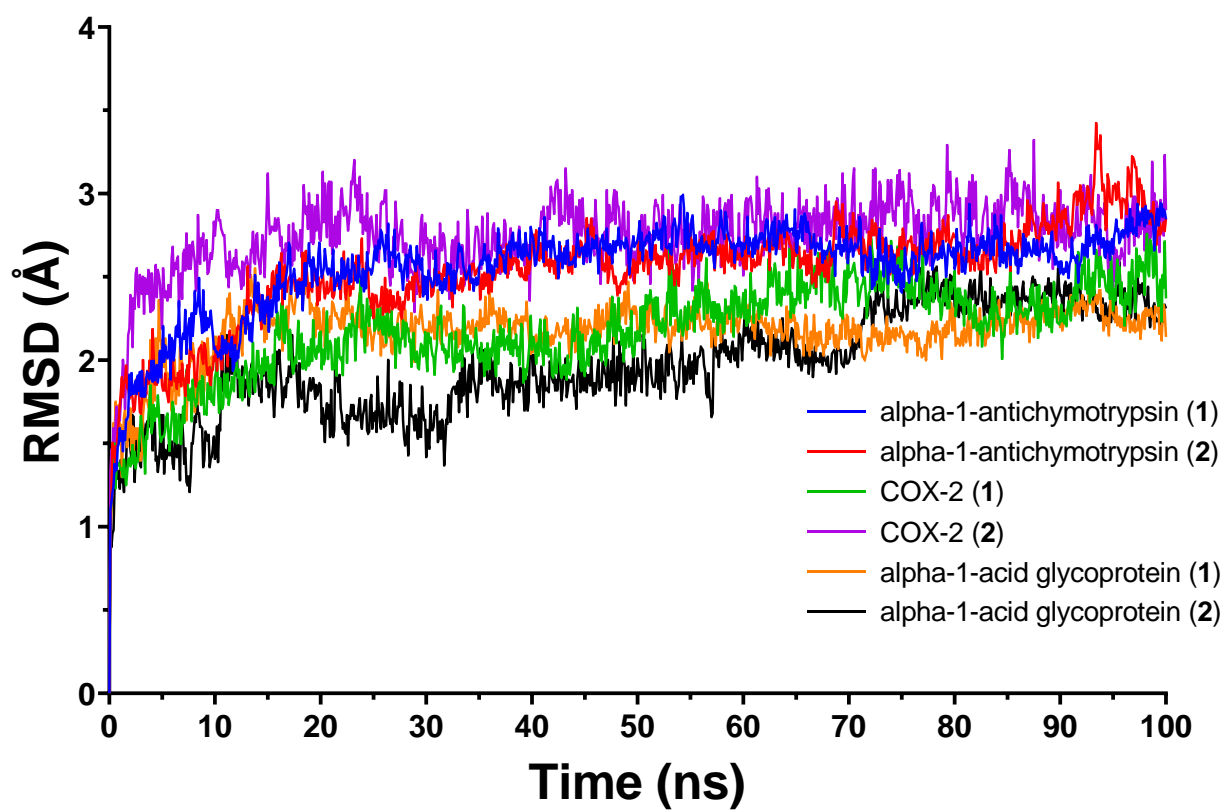


Figure S3. RMSD trend for the six complexes during the 100 ns MD simulation.