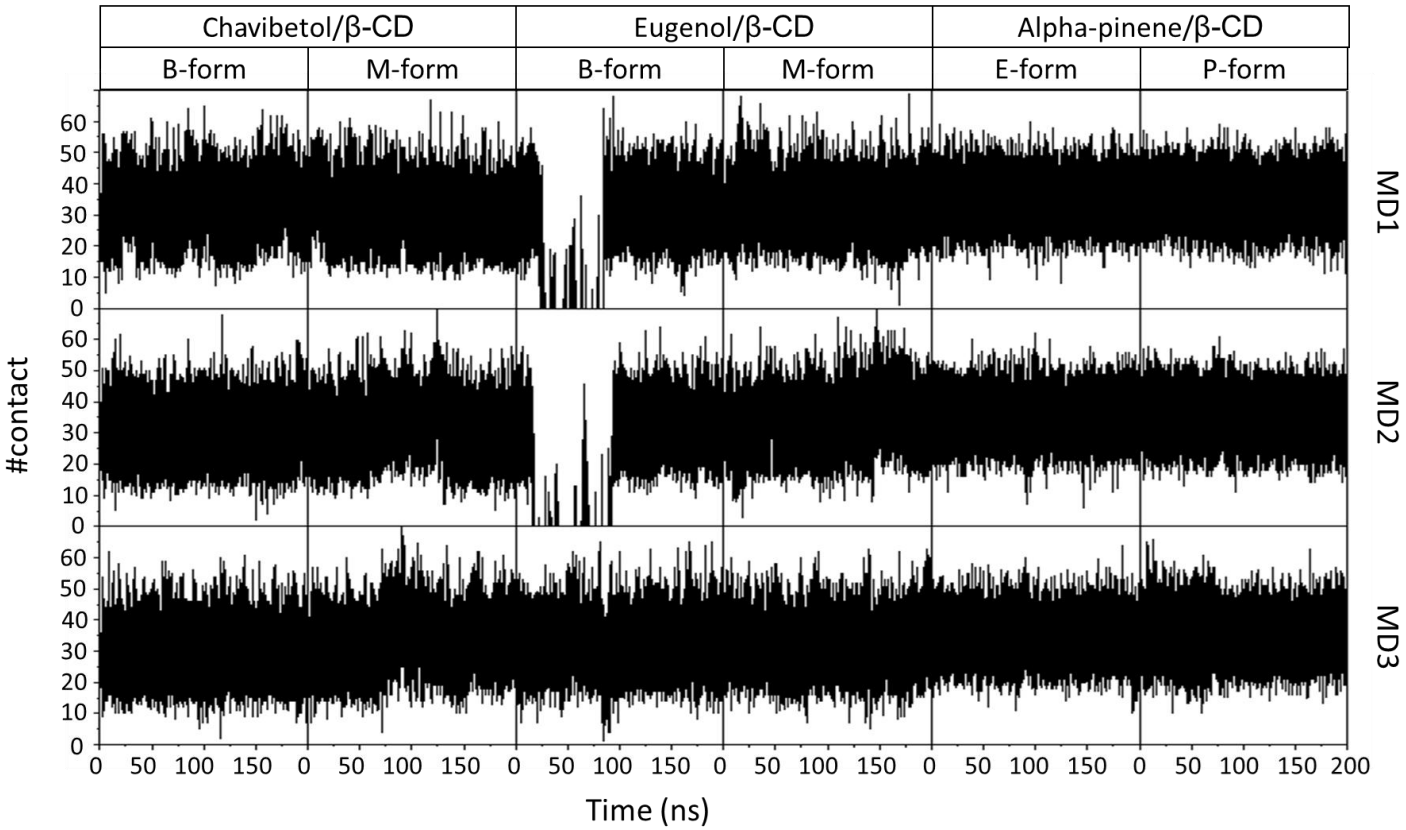

Supplementary Fig. S13. Time evolution of the number of atomic contacts between β-cyclodextrin and guest molecules (chavibetol, eugenol, and alpha-pinene) in various inclusion forms (B-, M-, E-, and P-forms) over 200 ns molecular dynamics simulations. The number of contacts was monitored across three independent replicas (MD1–MD3), indicating the stability and consistency of intermolecular interactions throughout the simulation time. Higher numbers of contacts suggest more extensive host–guest interaction.