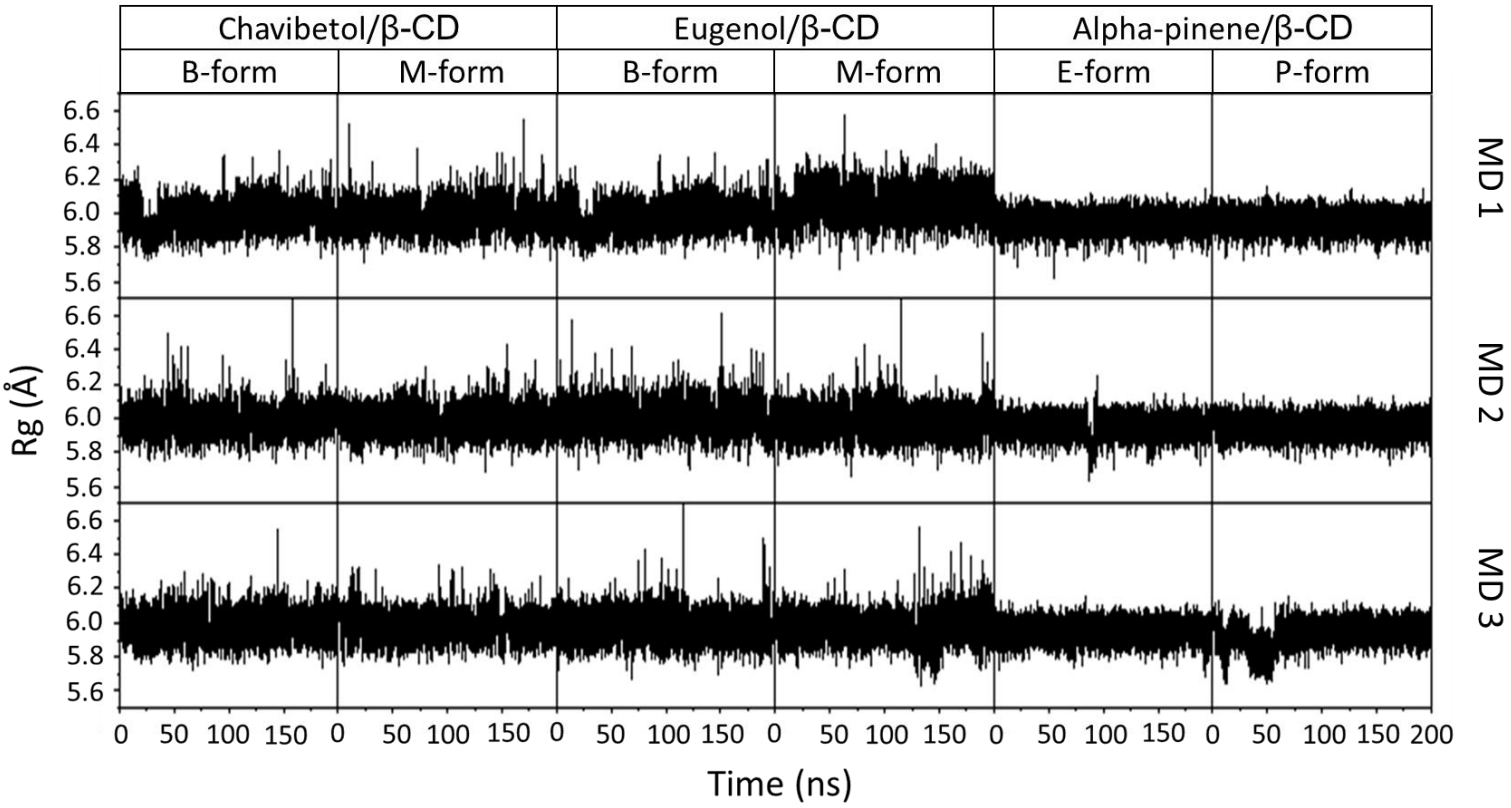

Supplementary Fig. S11. Time evolution of the radius of gyration (Rg) of β-cyclodextrin in complex with chavibetol, eugenol, and alpha-pinene in different conformational forms (B-, M-, E-, and P-forms) over 200 ns molecular dynamics simulations. The plots are shown for three independent simulation replicas (MD1, MD2, and MD3). Fluctuations in Rg values reflect the conformational stability and compactness of each inclusion complex during the simulation.