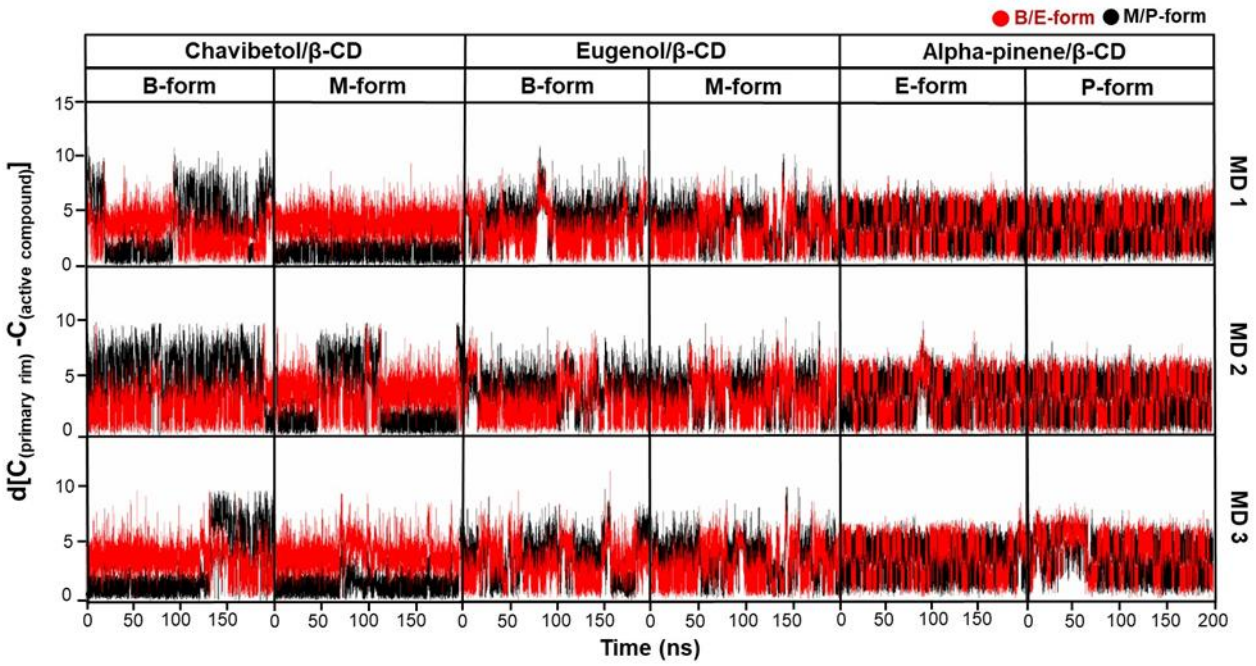

Supplementary Fig. S9. Time evolution of the center-of-mass distance between the active compound and the primary rim of *β*-cyclodextrin ($d[C_{m(\text{primary rim})} - C_{m(\text{active compound})}]$) during 200 ns molecular dynamics simulations for each guest/*β*-CD complex (chavibetol, eugenol, and alpha-pinene) in different conformational forms. Each panel displays results from one of three independent replicas (MD1–MD3). Distances are plotted separately for B/E-forms (red) and M/P-forms (black). The metric reflects the depth and orientation of guest insertion within the *β*-CD cavity, with smaller distances indicating deeper penetration toward the primary rim.