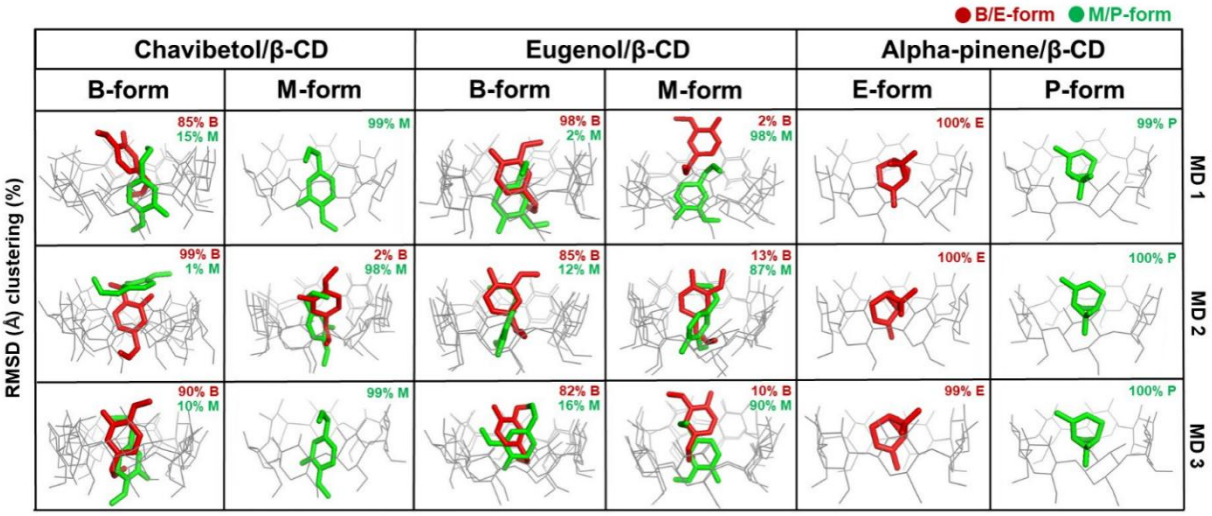

Supplementary Fig. S10. Representative clustered conformations of guest molecules (chavibetol, eugenol, and alpha-pinene) within *β*-cyclodextrin inclusion complexes obtained from RMSD-based clustering analysis over 200 ns molecular dynamics simulations. Each column shows different guest/*β*-CD complexes and their corresponding initial form (B-, M-, E-, or P-form). Each row represents a different independent simulation replica (MD1–MD3). The dominant conformational clusters are illustrated with the guest molecules in red (B/E-form) or green (M/P-form). Percentages indicate the population of each form in the dominant cluster, reflecting the preferred binding orientation and conformational stability throughout the simulations.