

Inclusion Complexes of Norepenephrine with β -Cyclodextrin, 18-Crown-6 and Cucurbit[7]uril: Experimental and Molecular Dynamic Study

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Supplementary information

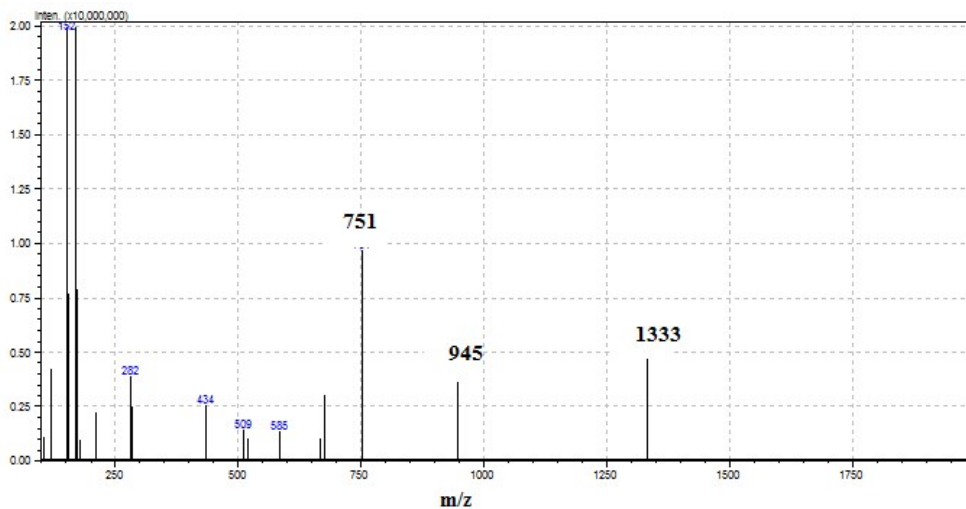


Figure S1 ESI-MS Spectra of NP-CB7.

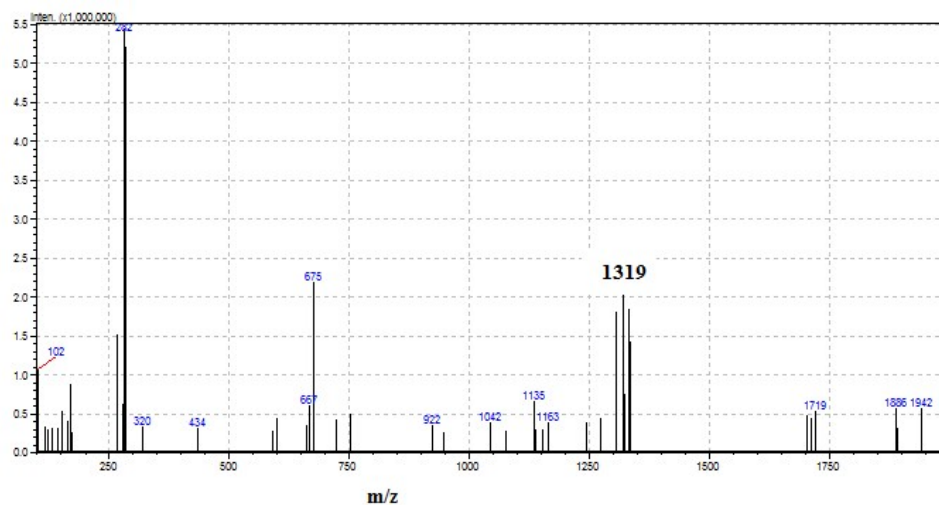


Figure S2 ESI-MS Spectra of NP-CB7-βCD.

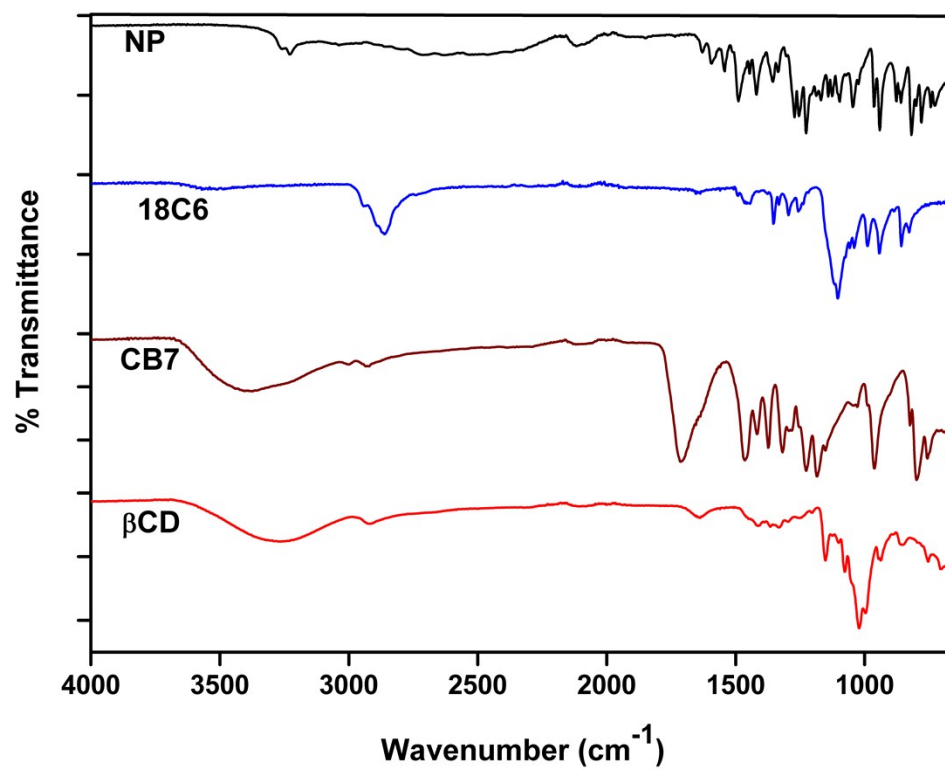


Figure S3 FT-IR spectra of pure substances.

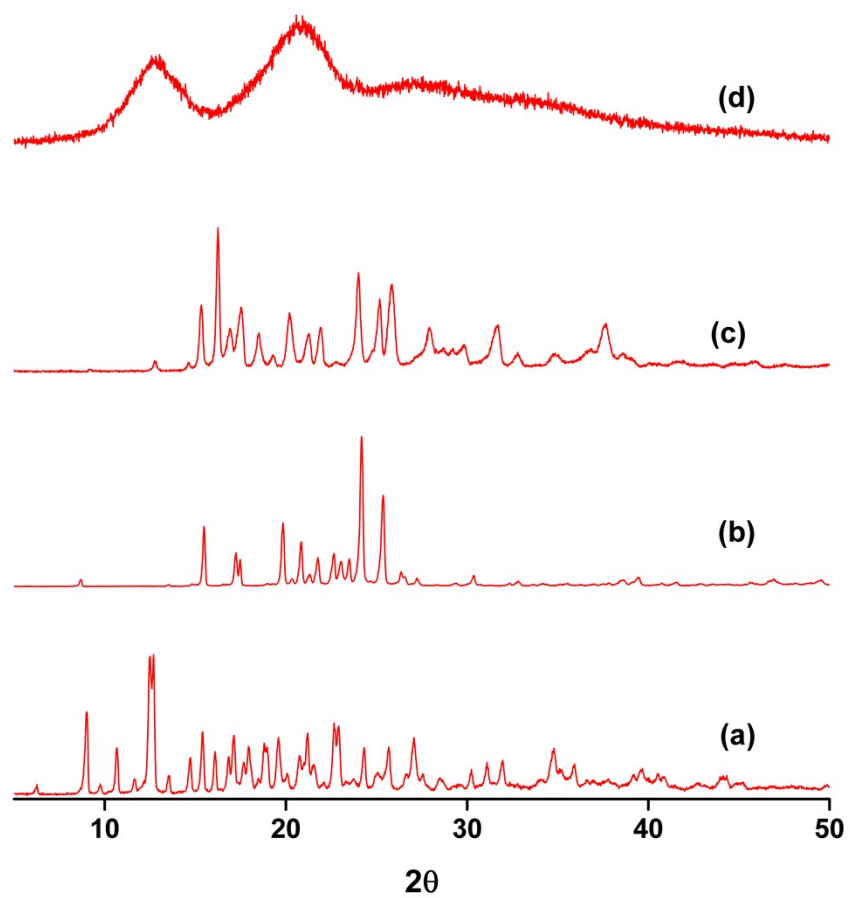


Figure S4 PXRD patterns of (a) β CD (b) 18C6 (c) NP (d) CB7

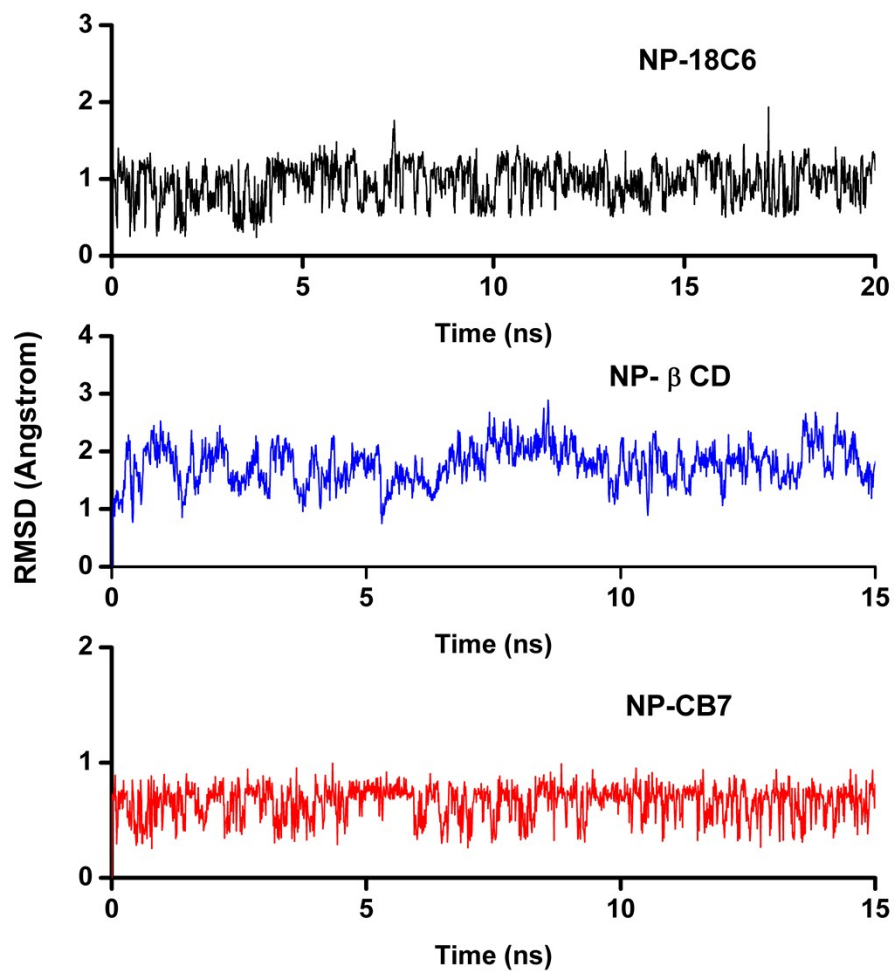


Figure S5a The time dependence of the root-mean-square deviations (RMSD) of atomic positions in the MD simulated binary complexes from those in the corresponding energy minimized structures.

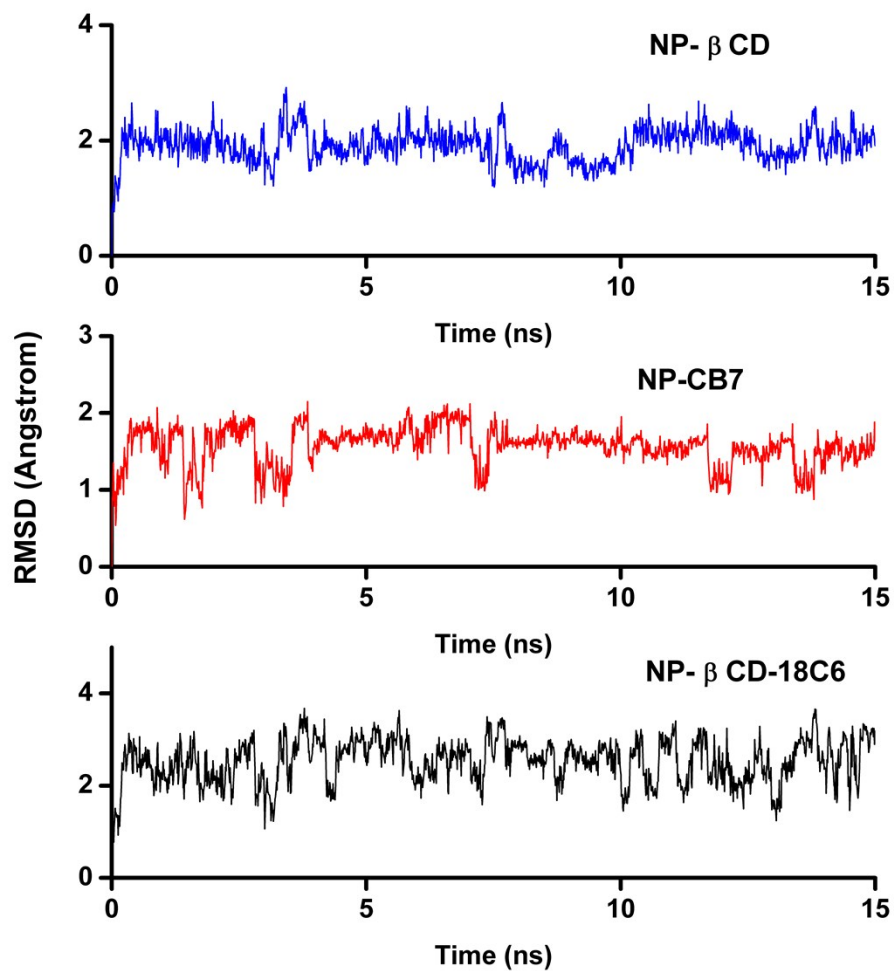


Figure S5b The time dependence of the root-mean-square deviations (RMSD) of atomic positions in the MD simulated ternary NP-βCD-18C6 complex from those in the corresponding energy minimized structure.

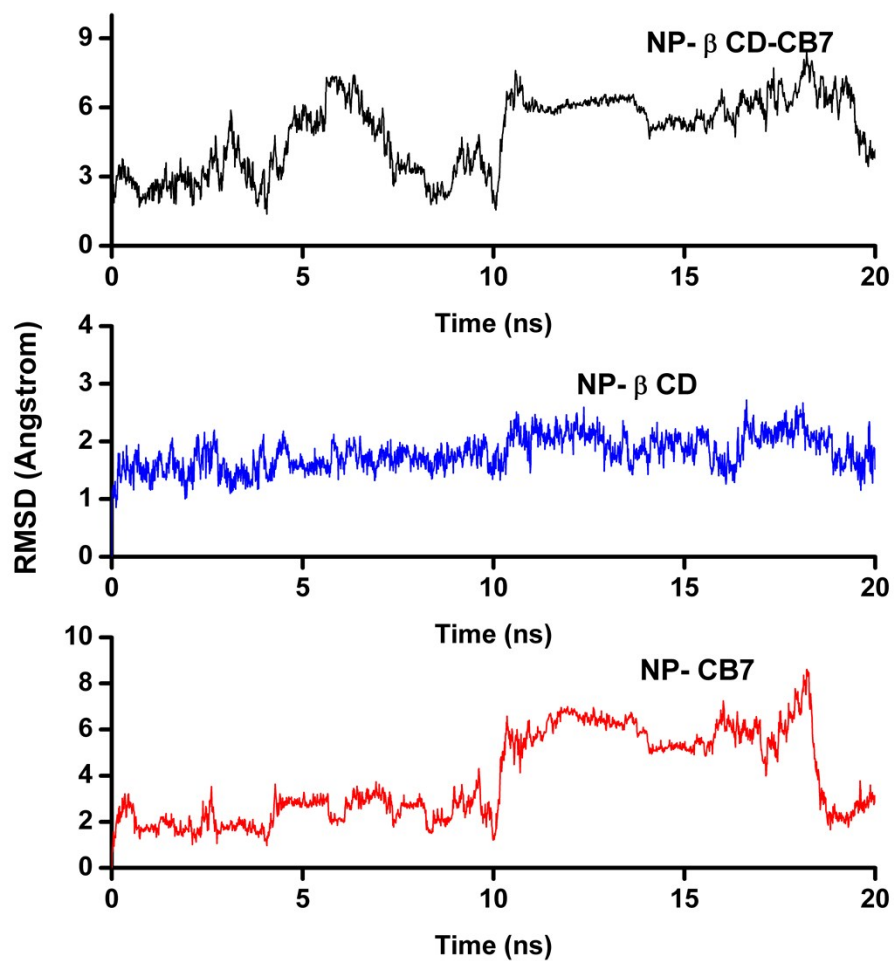


Figure S5c The time dependence of the root-mean-square deviations (RMSD) of atomic positions in the MD simulated ternary NP-βCD-CB7 complex from those in the corresponding energy minimized structure.

Hydrogen Bonding Analysis

(a) Binary complexes

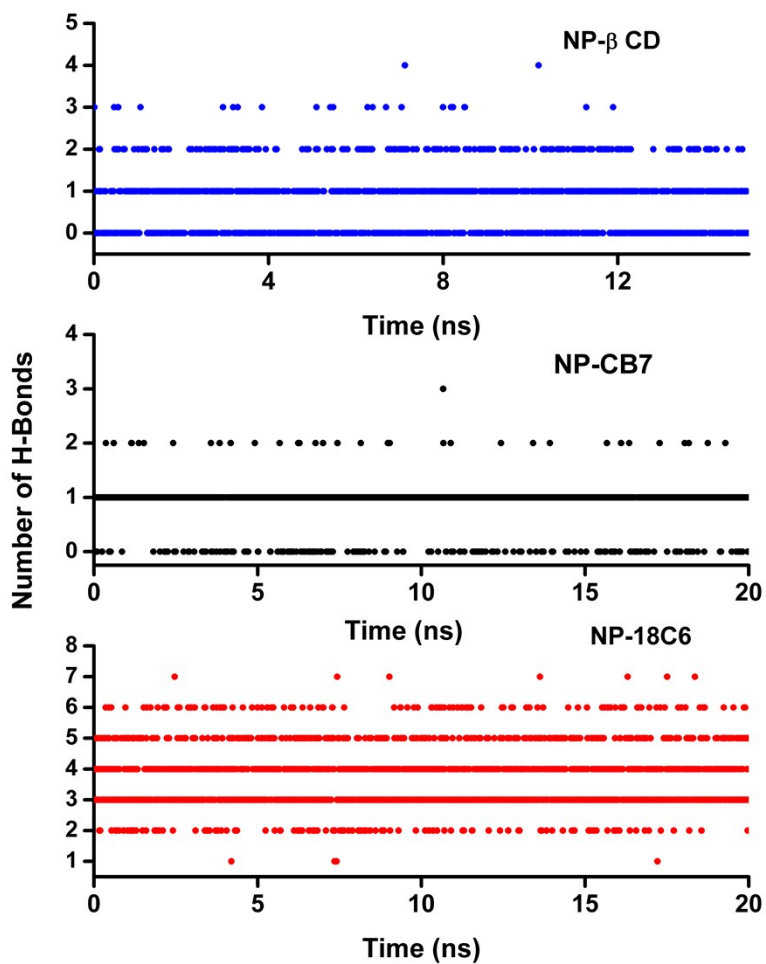


Figure S6a Hydrogen bonding interaction obtained from MD trajectories for binary complexes.

(b) NP- β CD-18C6

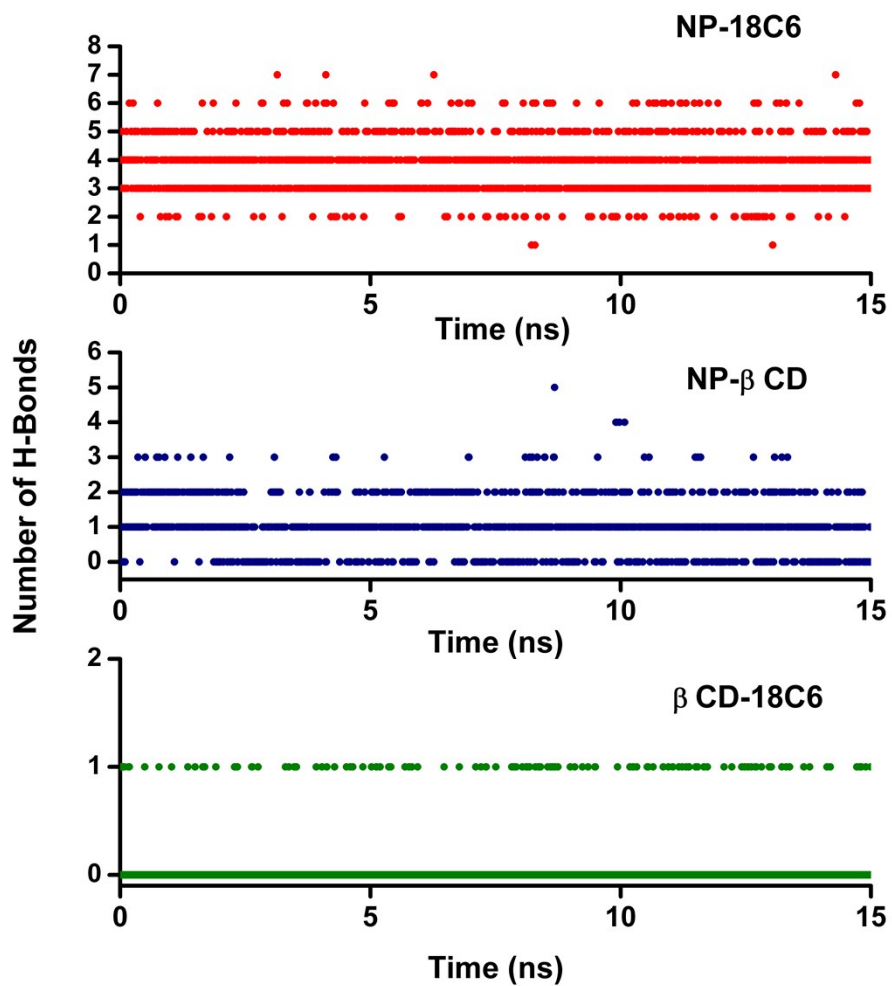


Figure S6b Hydrogen bonding interaction obtained from MD trajectories for NP- β CD-18C6 complex.

(c) NP- β CD-CB7 (NP-Face β CD)

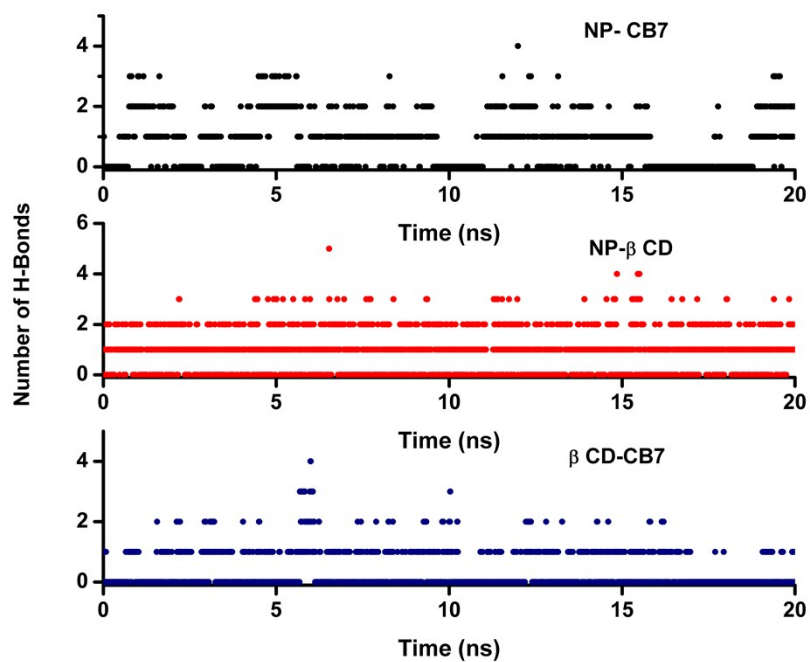


Figure S6c Hydrogen bonding interaction obtained from MD trajectories for NP- β CD-CB7 complex.

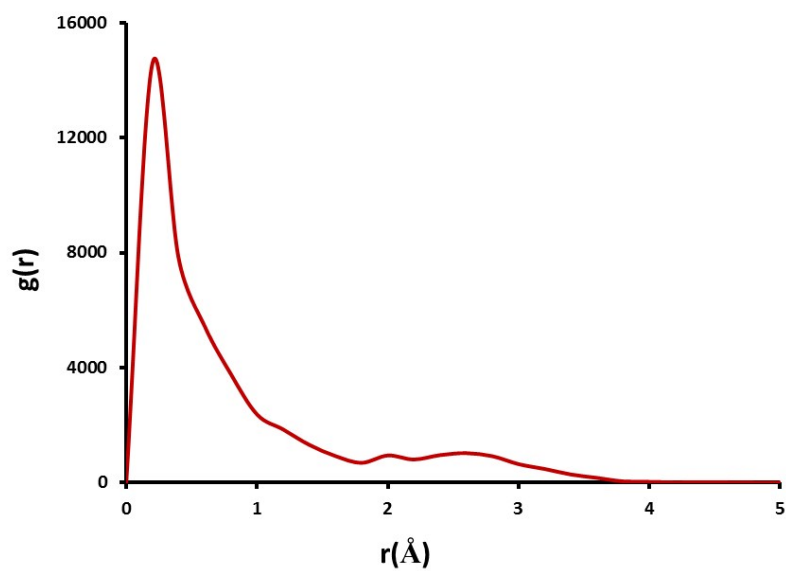


Figure S7 The RDF of center of mass of host and guest plotted as a function of separation distance r (Å) in NP- β CD complex.

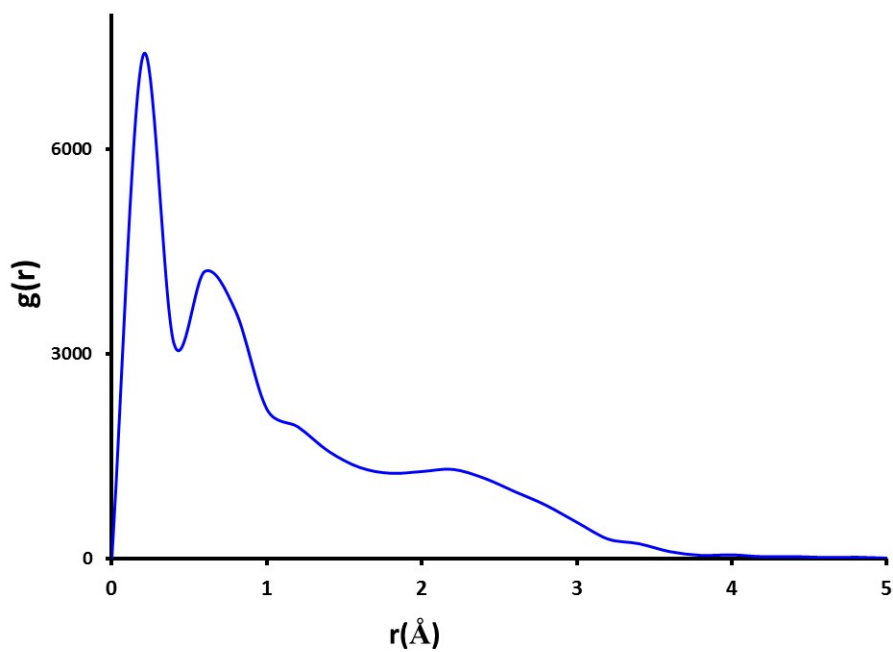
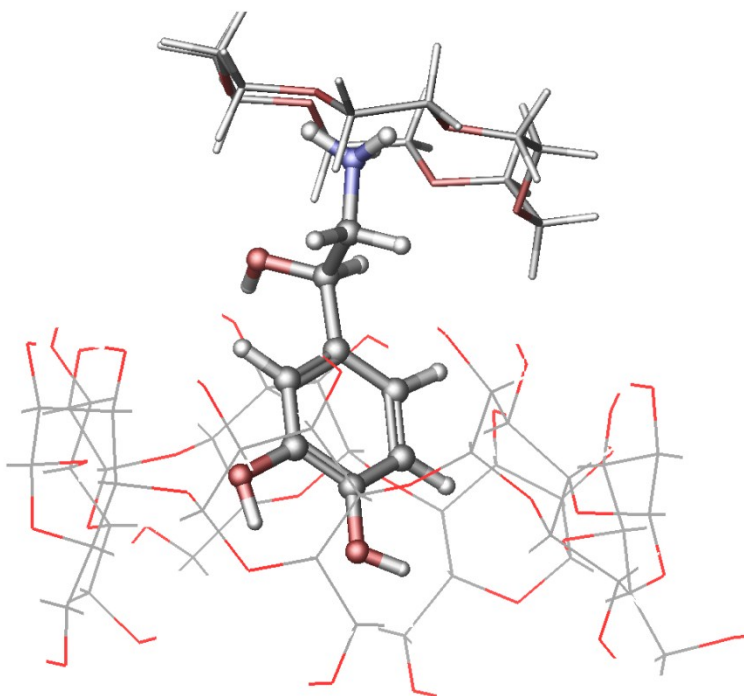
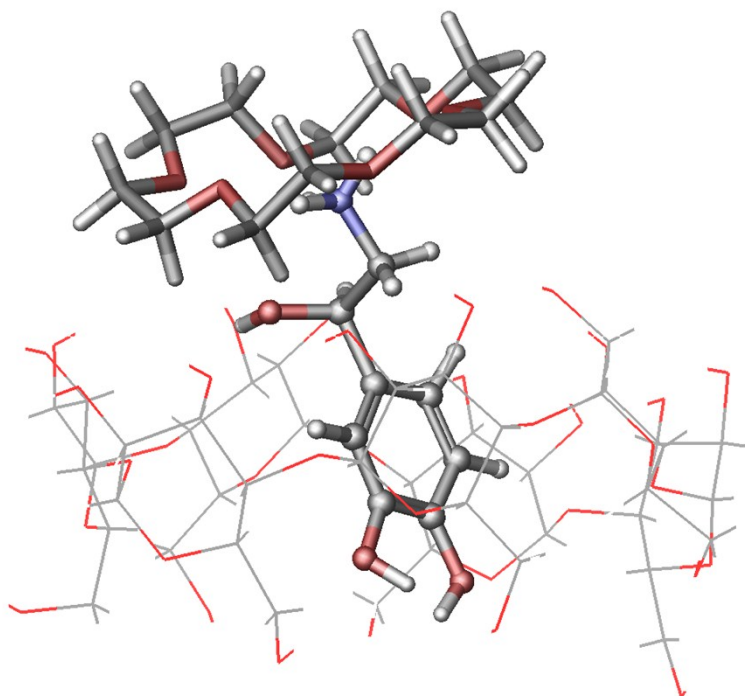


Figure S8 The RDF of center of mass of β CD and NP plotted as a function of separation distance r (Å) in NP- β CD-18C6 complex.

(a)



(b)



(c)

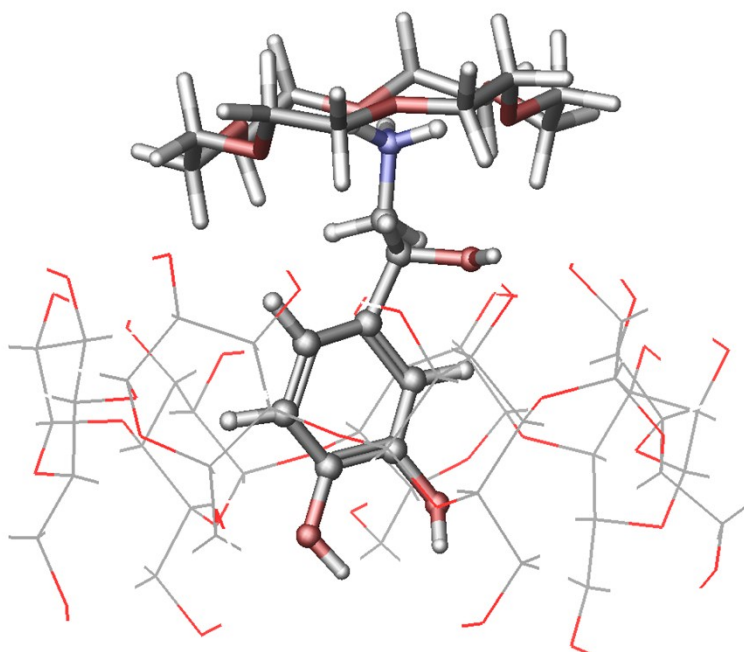


Figure S9 Snapshots of NP-βCD-18C6 complex taken from the simulation at (a) 5 ns (b) 10 ns (c) 13 ns.