Inclusion Complexes of Norepenephrine with $\beta$-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) βCD (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.
Figure S6a Hydrogen bonding interaction obtained from MD trajectories for binary complexes.
(b) NP-βCD-18C6

Figure S6b Hydrogen bonding interaction obtained from MD trajectories for NP-βCD-18C6 complex.
Figure S6c Hydrogen bonding interaction obtained from MD trajectories for NP-βCD-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-βCD complex.

**Figure S8** The RDF of center of mass of βCD and NP plotted as a function of separation distance $r$ (Å) in NP-βCD-18C6 complex.
Figure S9 Snapshots of NP-βCD-18C6 complex taken from the simulation at (a) 5 ns (b) 10 ns (c) 13 ns.