Electronic Supporting Information

Molecular Dynamics Study of Conformations of Beta-Cyclodextrin and its Eight Derivatives in Four Different Solvents

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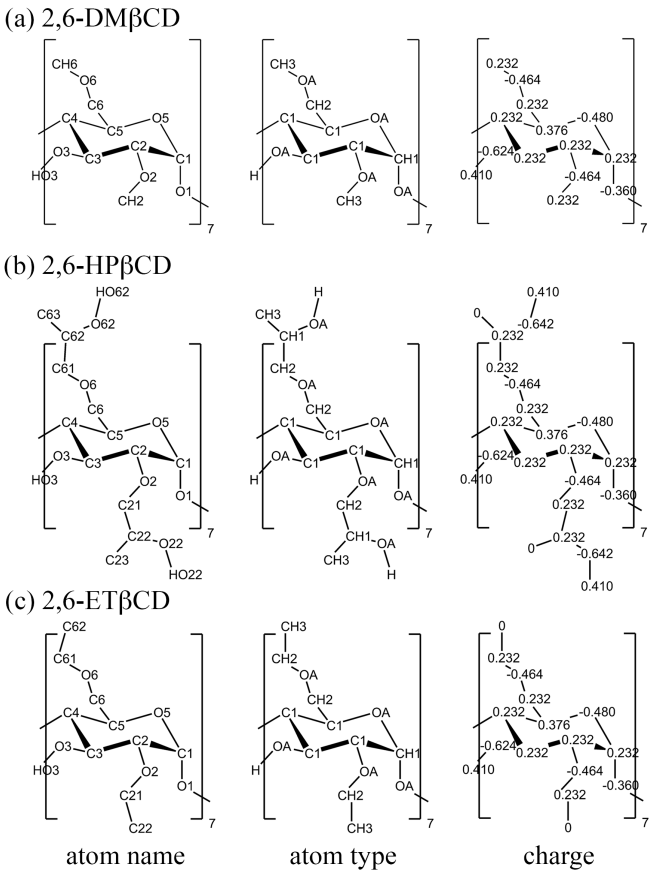


Figure S1: Charge modifications of methyl and 2-hydroxypropyl groups in glucose subunits in (a) 2,6-DMβCD, (b) 2,6-HPβCD and (c) 2,6-ETβCD

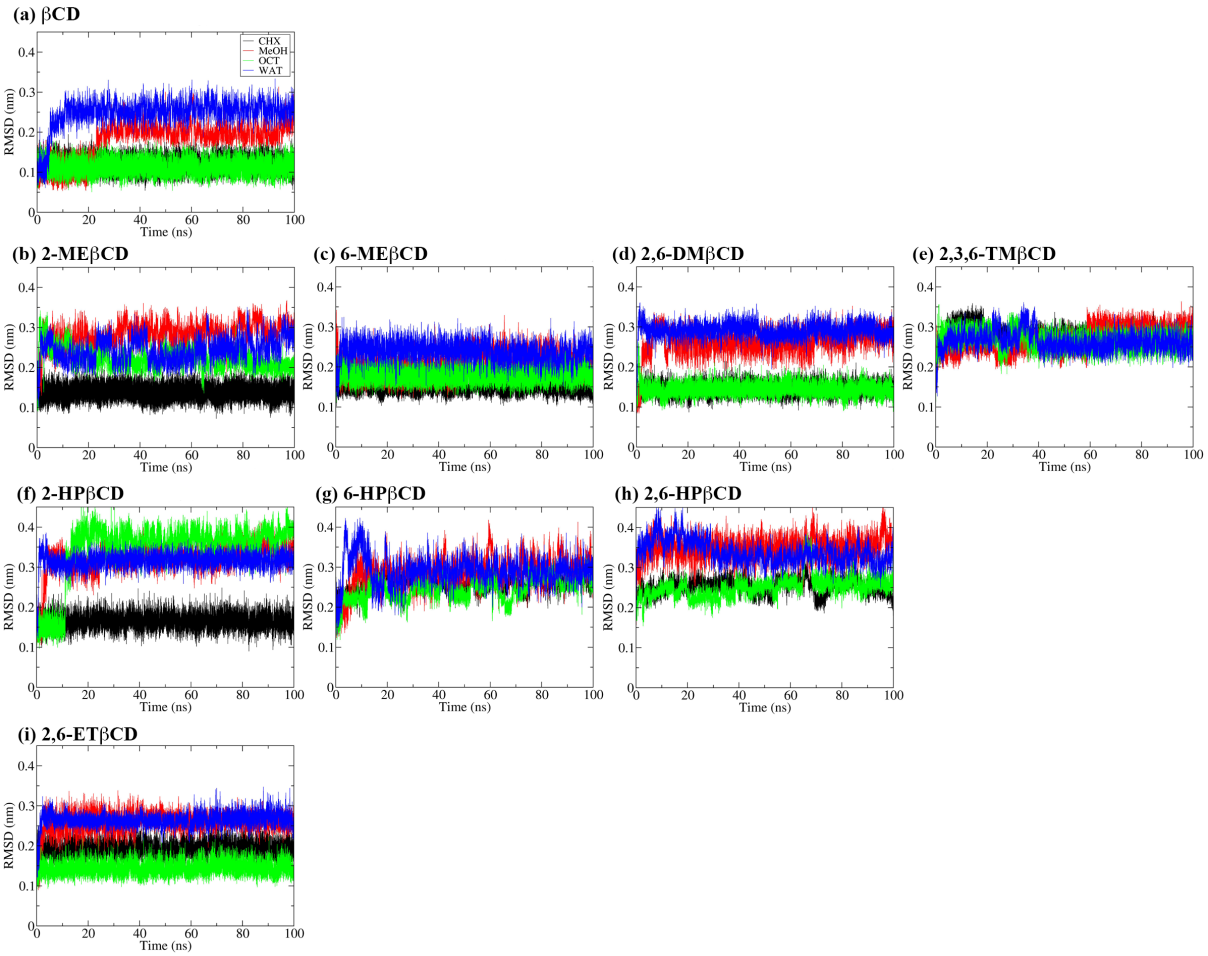


Figure S2: (a)-(i) Time evolution of the root mean square displacement (rmsd) of the atoms in the different βCD derivatives.

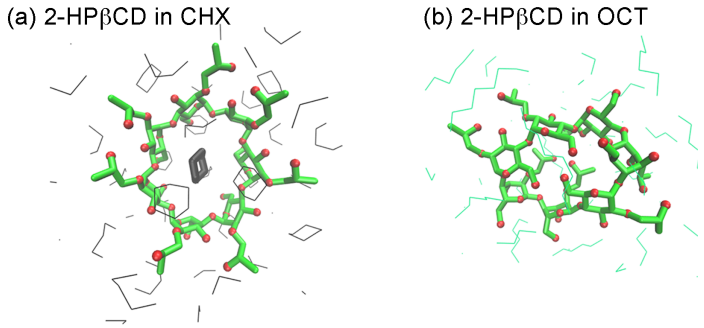
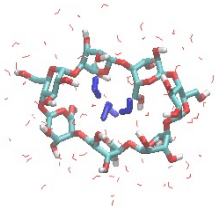
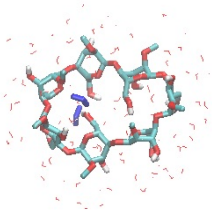


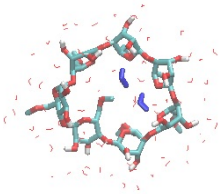
Figure S3: Snapshots of 2-HPβCD in non-polar solvents, CHX and OCT. The inclusion of a CHX in 2-HPβCD' s cavity and the deformation of the 2-HPβCD in OCT are observed.



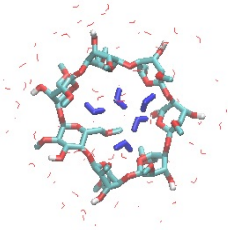
βCD



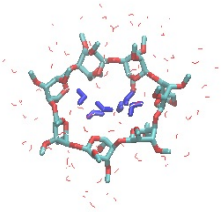
2-MEβCD



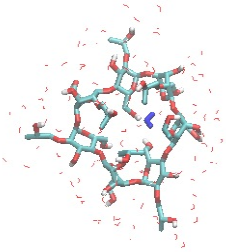
6-MEβCD



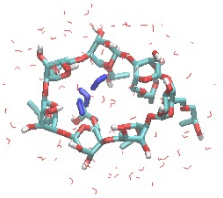
2,6-DMβCD



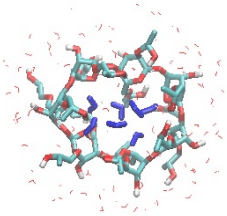
2,3,6-TMβCD



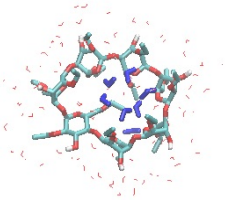
2-HPβCD



6-HPβCD

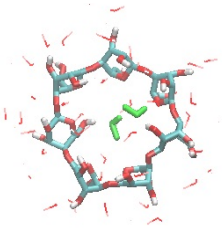


2,6-HPβCD

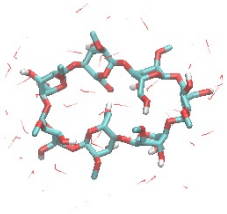


2,6-ETβCD

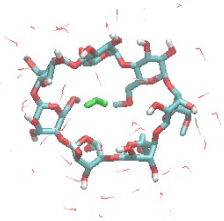
Figure S4: Snapshot of the βCD derivatives solvated in water. Water molecules when present inside the cavity are shown in blue.



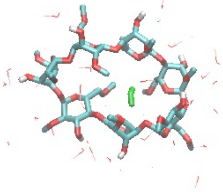
βCD



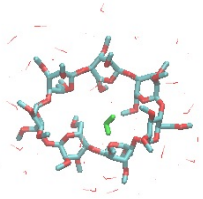
2-MEβCD



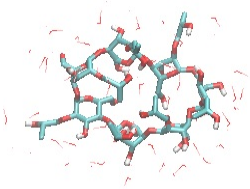
6-MEβCD



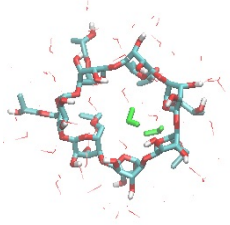
2,6-DMβCD



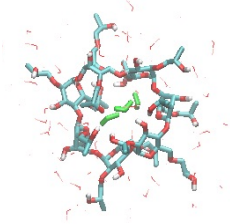
2,3,6-TMβCD



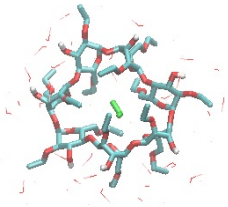
2-HPβCD



6-HPβCD



2,6-HPβCD



2,6-ETβCD

Figure S5: Snapshots of the βCD derivatives in MeOH. The MeOH molecules inside the cavity, when present, are highlighted in green.

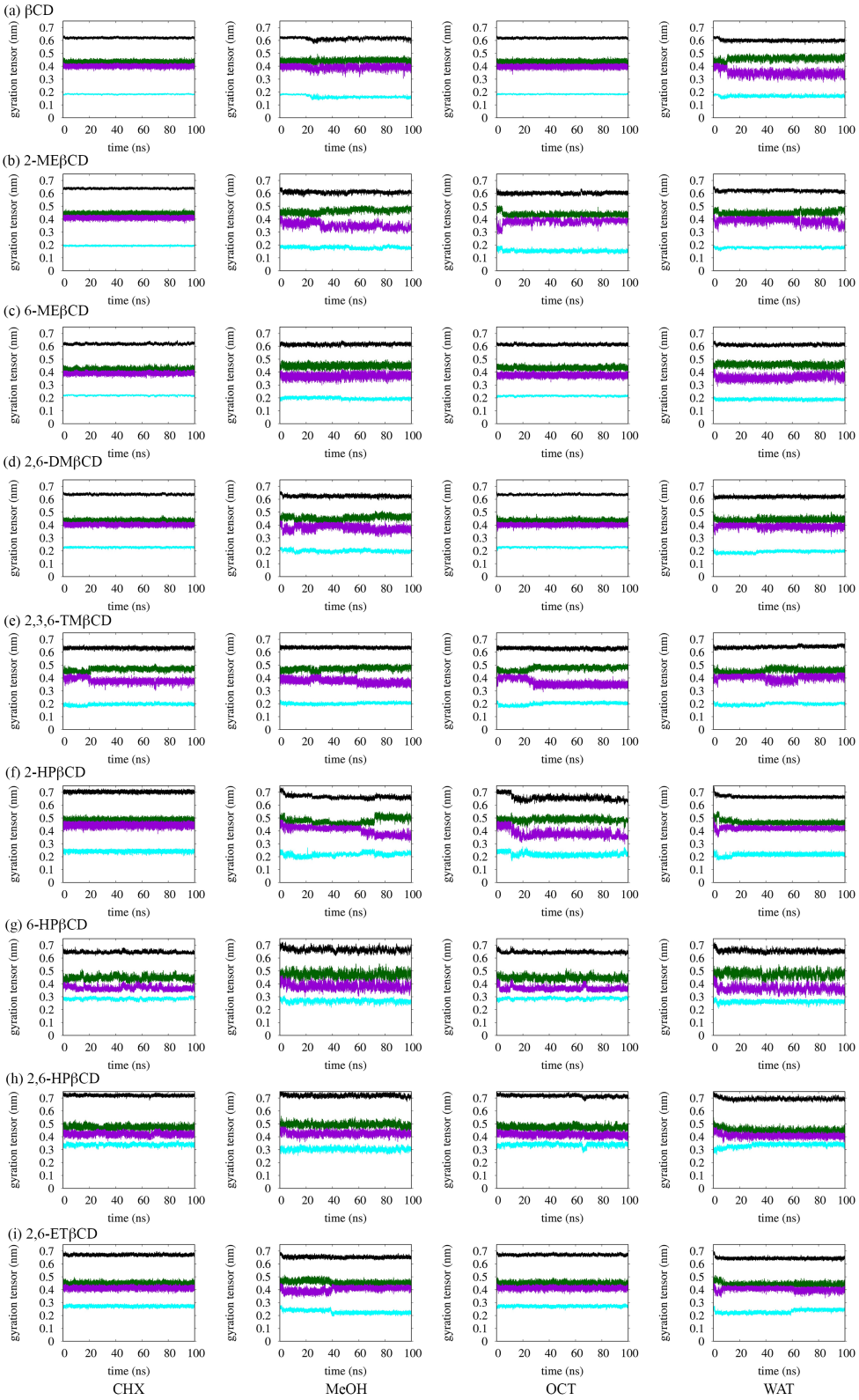


Figure S6: (a)-(i) The time evolutions of R_g (black) and the three principal components, λ_1 (green), λ_2 (violet) and λ_3 (cyan), of each βCD type in different solvents.

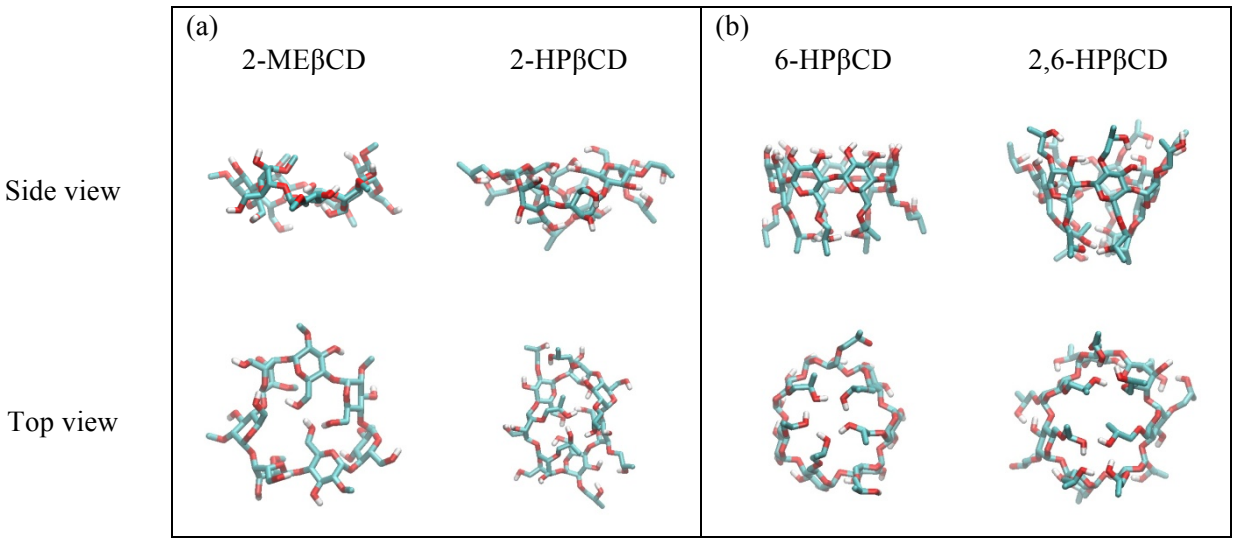


Figure S7: Snapshots at the end of the simulation: (a) 2-MEβCD and 2-HPβCD in OCT. Their structures were deformed. (b) 6-HPβCD and 2,6-HPBCD in OCT.

Table S1: The number of solvent molecules (cyclohexane; CHX; methanol; MeOH; octane; OCT and water; WAT) and the simulation box sizes

Solvents	Number of solvent molecules	Box size (nm^3)
CHX	2000	7.1×7.9×7.7
MeOH	1728	4.8×4.8×4.8
OCT	1000	7.1×7.9×7.7
WAT	7000 (single point charge; SPC)	6.0×6.0×6.0

Table S2: The average peak rmsd position for each βCD type in different solvents. Error is given as standard deviation.

System	Average rmsd (nm)			
	CHX	MeOH	OCT	WAT
βCD	0.12±0.02	0.20±0.02	0.11±0.02	0.26±0.02
2-MEβCD	0.14±0.02	0.29±0.03	0.21±0.02	0.26±0.03
6-MEβCD	0.15±0.01	0.22±0.02	0.18±0.02	0.23±0.02
2,6-DMβCD	0.14±0.01	0.28±0.02	0.14±0.01	0.29±0.02
2,3,6-TMβCD	0.28±0.01	0.30±0.01	0.26±0.02	0.26±0.02
2-HPβCD	0.16±0.02	0.35±0.02	0.37±0.02	0.32±0.01
6-HPβCD	0.26±0.02	0.30±0.03	0.27±0.02	0.29±0.02
2,6-HPβCD	0.25±0.02	0.36±0.03	0.26±0.02	0.32±0.02
2,6-ETβCD	0.19±0.02	0.26±0.01	0.15±0.02	0.27±0.02

Table S3: The full width at half maximum (FWHM) of the RMSD distributions

System	FWHM			
	CHX	MeOH	OCT	WAT
βCD	0.039	0.052	0.043	0.050
2MEβCD	0.040	0.057	0.029	0.064
6MEβCD	0.028	0.051	0.040	0.051
2,6DMβCD	0.029	0.044	0.030	0.042
2,3,6-TMβCD	0.026	0.034	0.054	0.043
2-HPβCD	0.042	0.042	0.056	0.034
6-HPβCD	0.027	0.078	0.060	0.051
2,6-HPβCD	0.044	0.056	0.047	0.052
2,6-ETβCD	0.044	0.030	0.036	0.035