Supporting Information

"Structure and stability of (α-CD)$_3$ agregate and OEG@(α-CD)$_3$ pseudo-rotaxane in aqueous solution: A molecular dynamics study"

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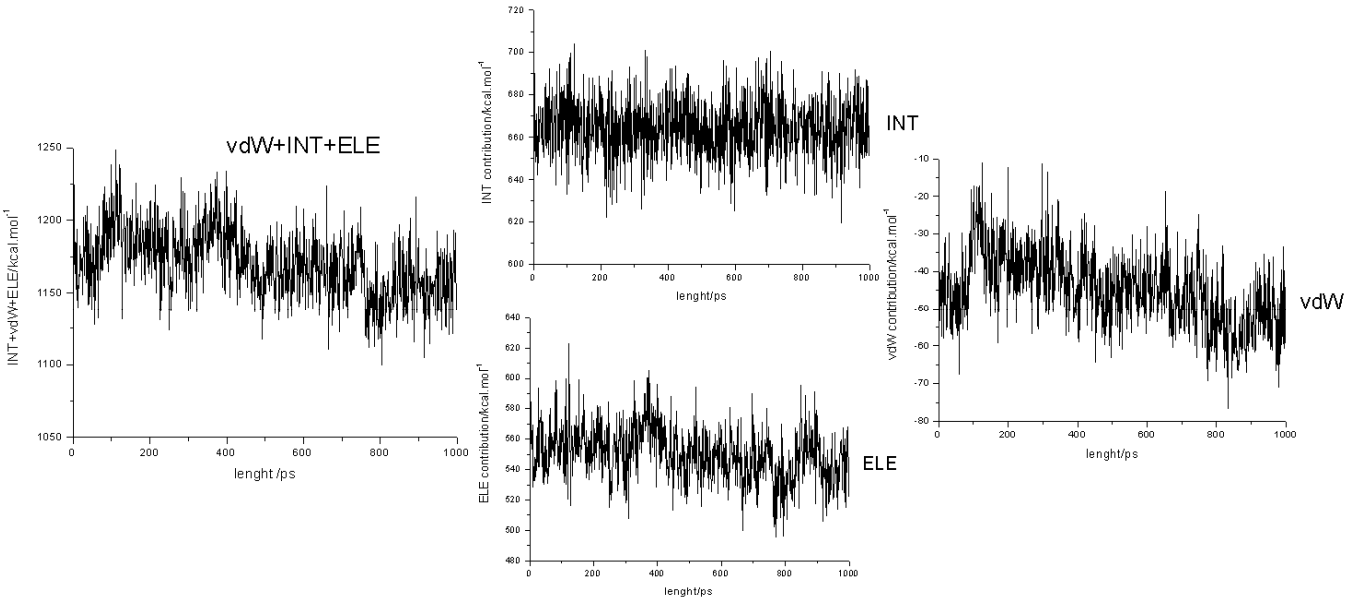
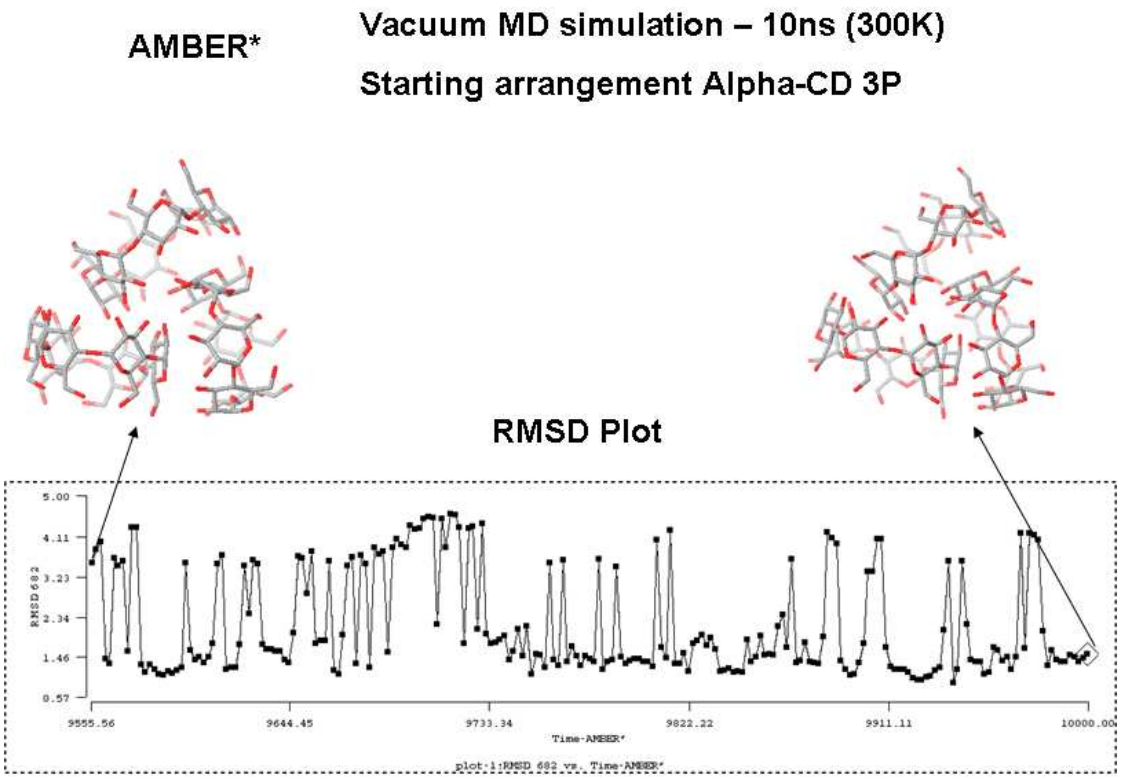
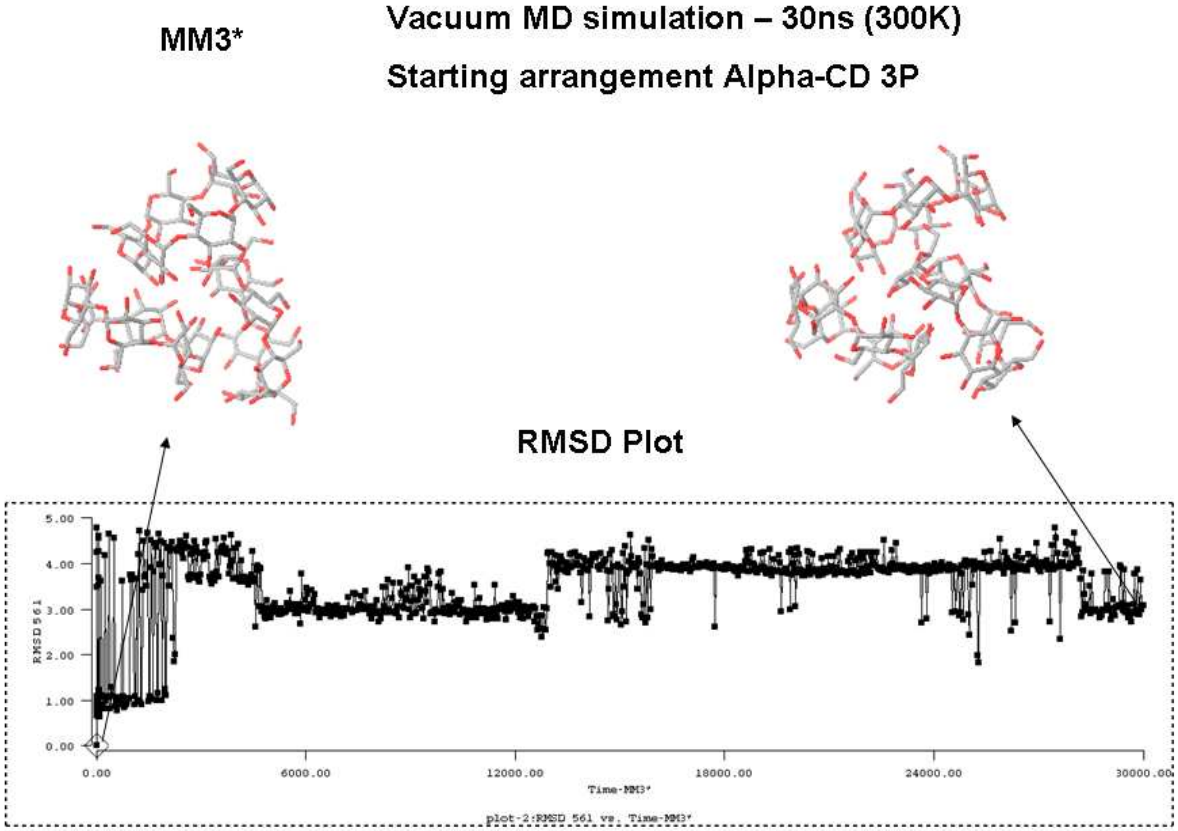
Contents:

S1. Gas phase total energy and their contributions evaluated for the C empty sequence snapshots collected along MD simulations. The plots show that vdW and ELE terms are more sensitive to the formation of a 3P based arrangement that take place at approximately 4ns of simulation.



S2. Root mean square deviation (RMSD) plots for vacuum simulations performed with AMBER*, MM3*, GAFF, GLYCAM_06 and parm99 force fields, for the 3P starting association at 300K.

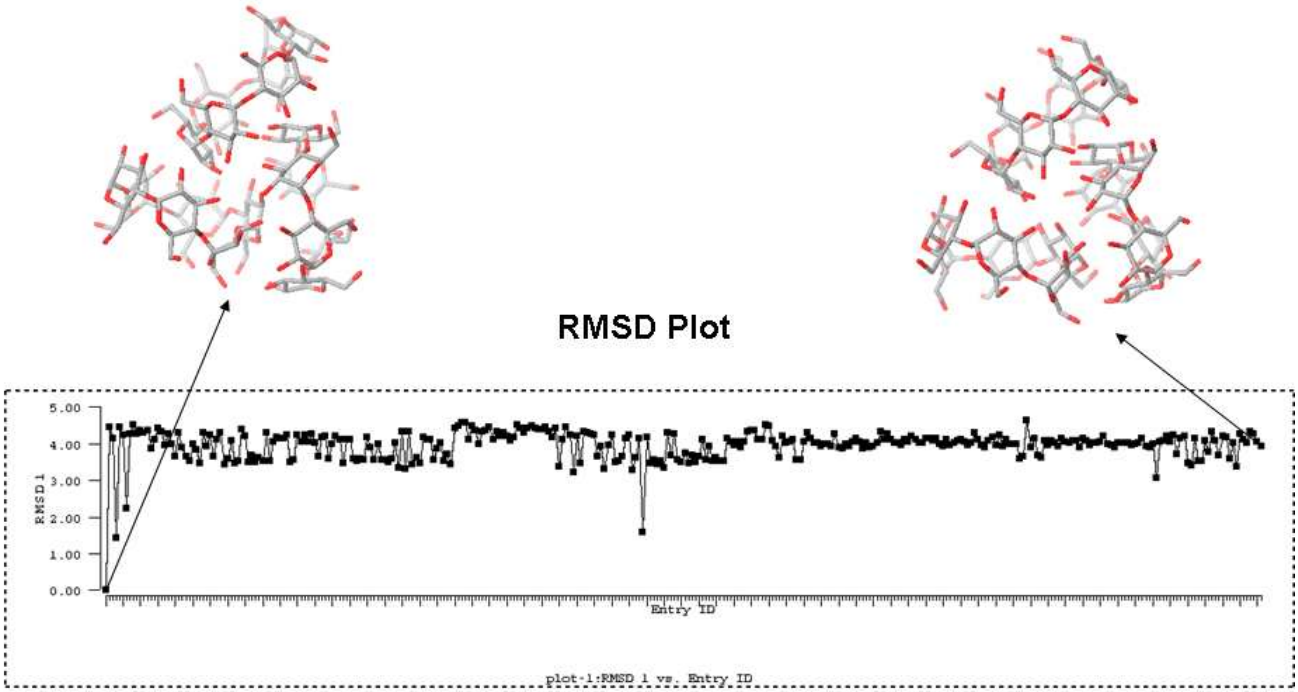




GAFF

Vacuum MD simulation – 10ns (300K)

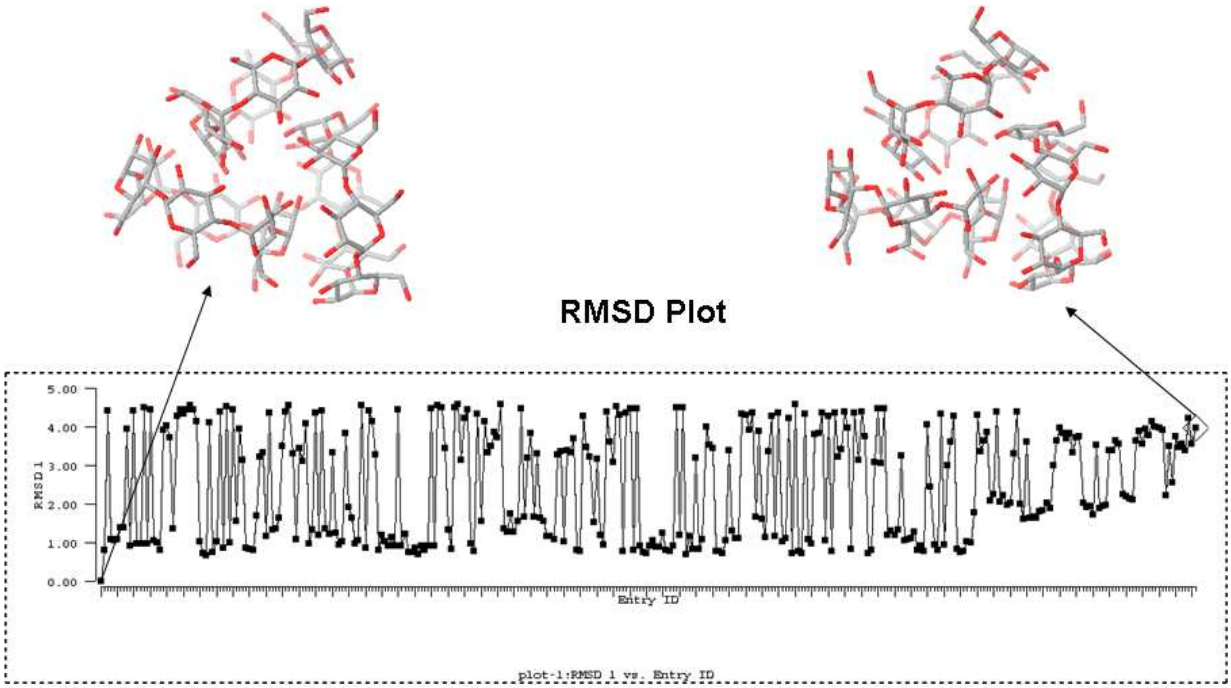
Starting arrangement Alpha-CD 3P



GLYCAM_06

Vacuum MD simulation – 10ns (300K)

Starting arrangement Alpha-CD 3P



parm99

Vacuum MD simulation – 10ns (300K)

Starting arrangement Alpha-CD 3P