

Dissolution of cellulose in ionic liquids: an *ab-initio* molecular dynamics simulation study

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Supporting Information

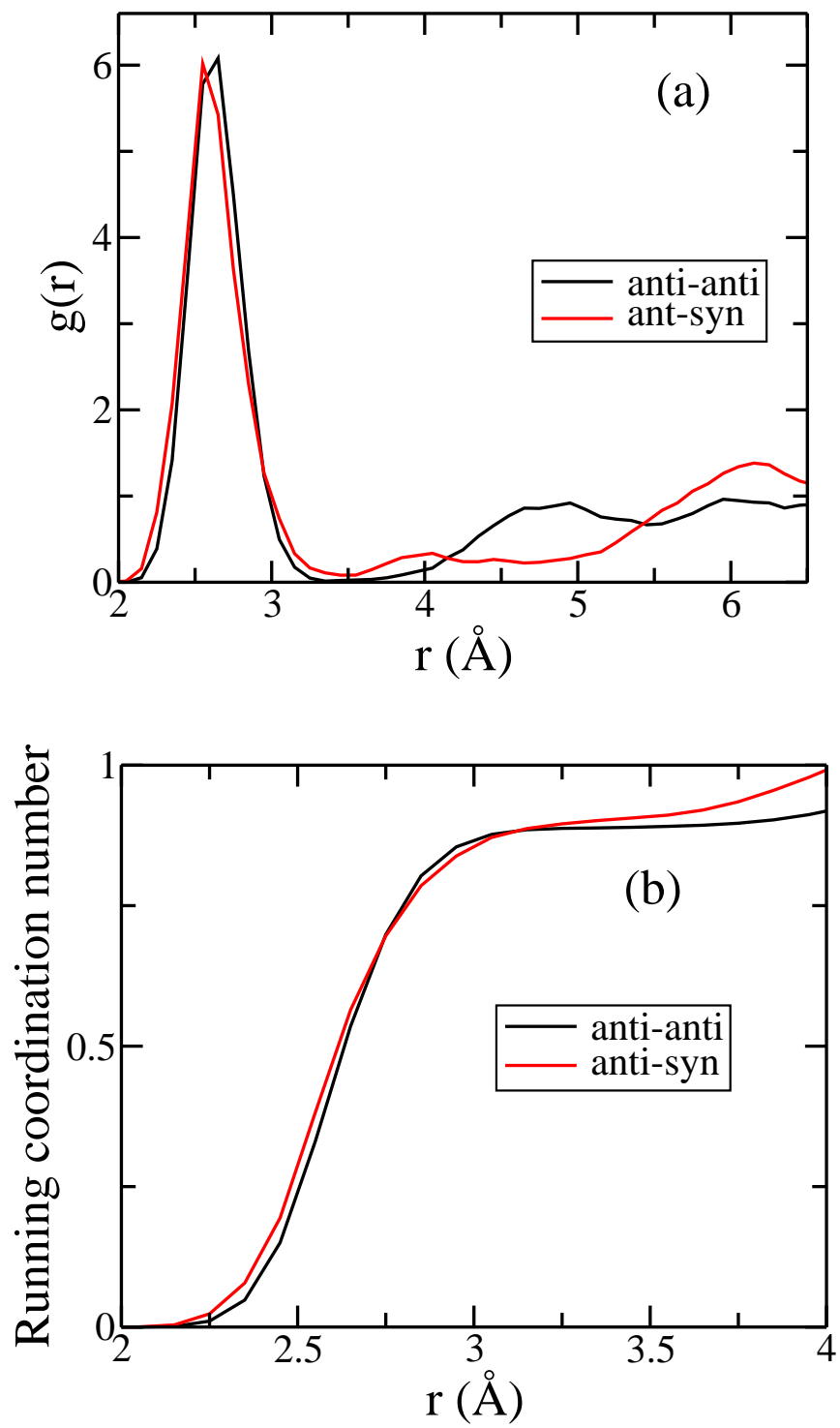


Figure S1: (a) Radial distribution function and (b) running coordination number between HC of cellobiose and carboxylate carbon of anion.

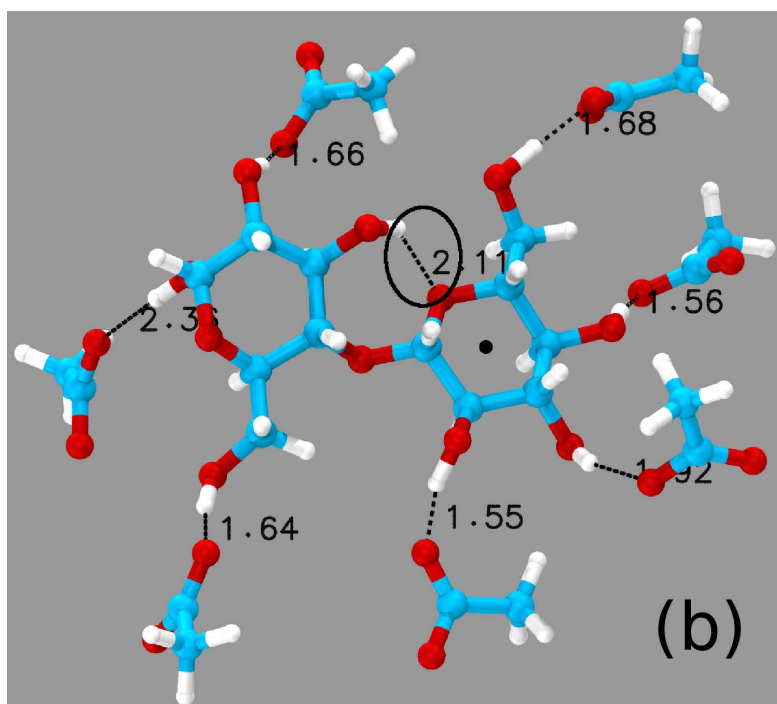
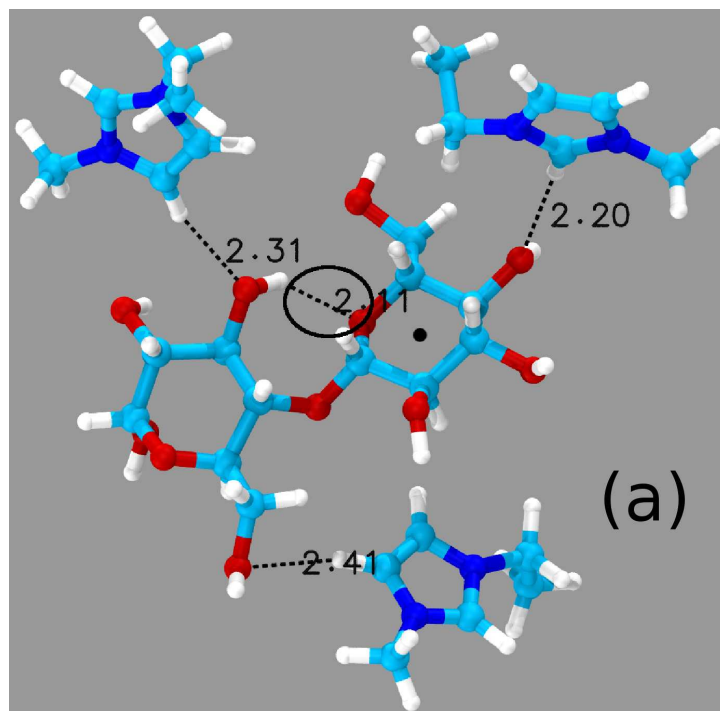


Figure S2: Snapshot of environment around anti-anti conformer of cellobise showing the formation of hydrogen bonds with (a) cation and (b) anion. Intramolecular hydrogen bond of the cellobiose unit is also shown. Colour scheme Nitrogen : Blue, Carbon : Cyan, Oxygen : Red and Hydrogen : White. Black dot can be used to identify the specific pentose ring of the cellobiose across the two panels.

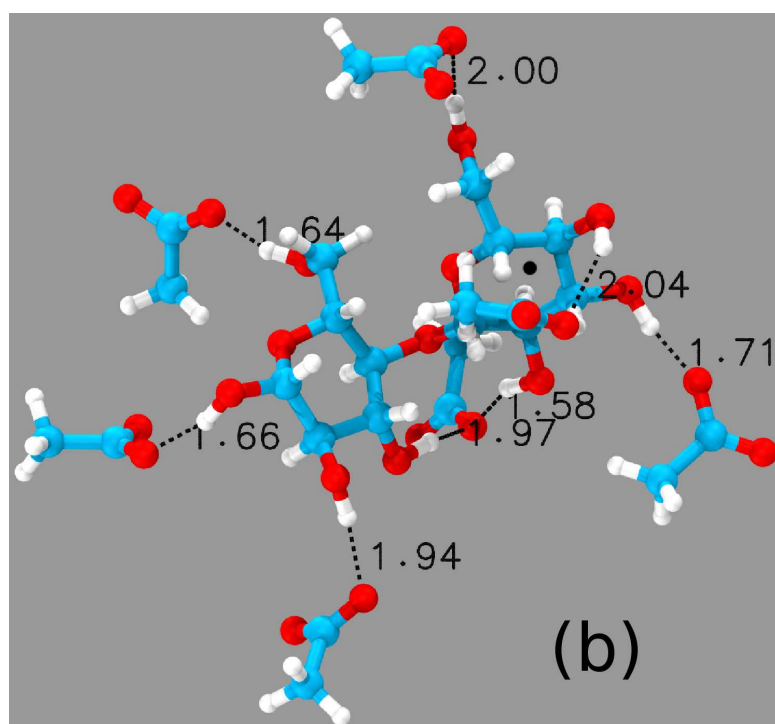
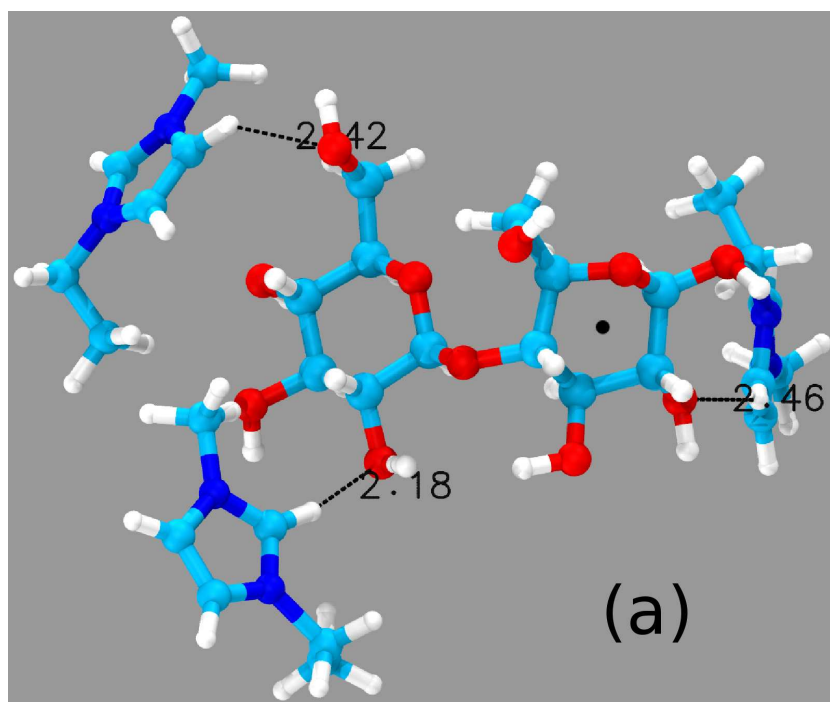


Figure S3: Snapshot of environment around anti-syn conformer of cellobise showing the formation of hydrogen bonds with (a) cation and (b) anion. Colour scheme is the same as in earlier figures. Black dot can be used to identify the specific pentos ring of the cellobiose across the two panels.

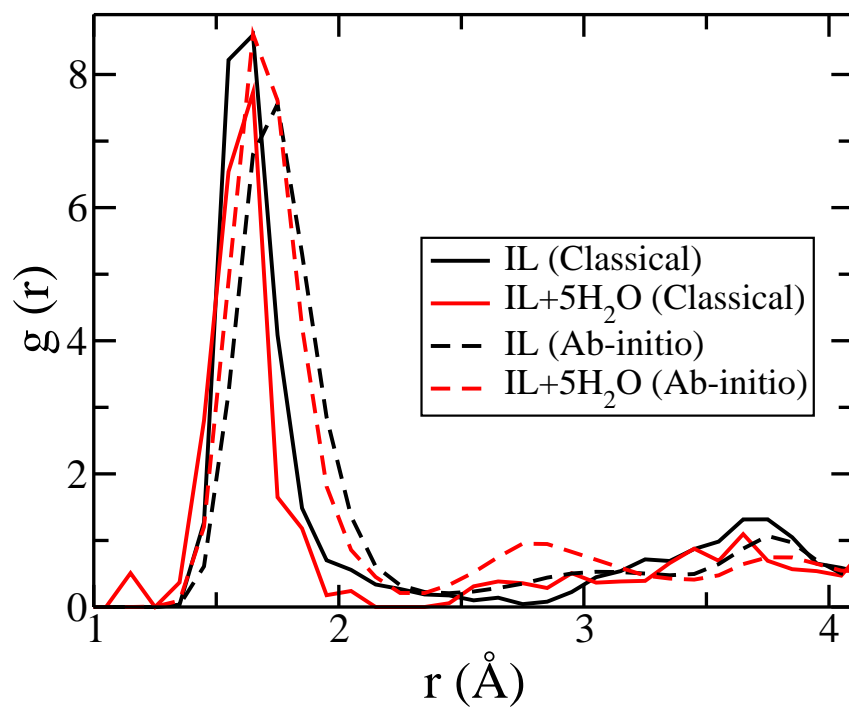


Figure S4: Comparison of OA-HC RDFs obtained from classical and ab-initio MD simulations for the anti - syn conformer of cellobiose.

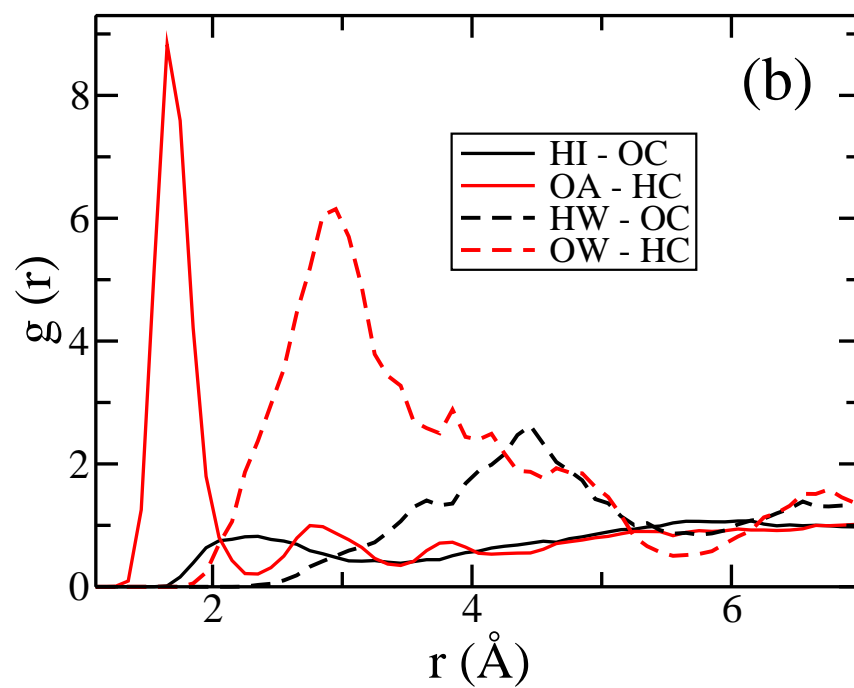
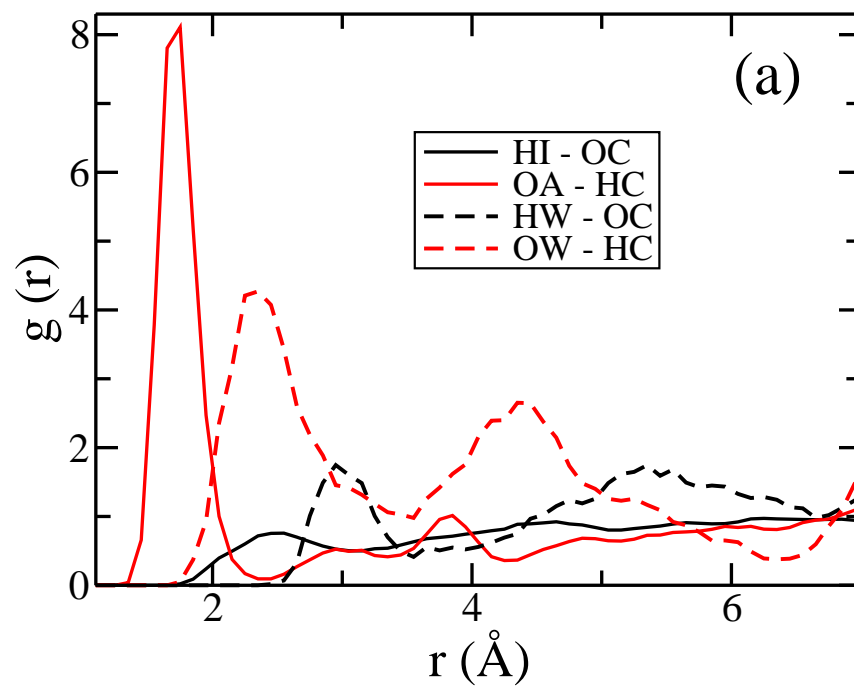


Figure S5: Radial distribution functions for (a) anti - anti and (b) anti -syn conformer of cellobiose solvated in IL+H₂O.

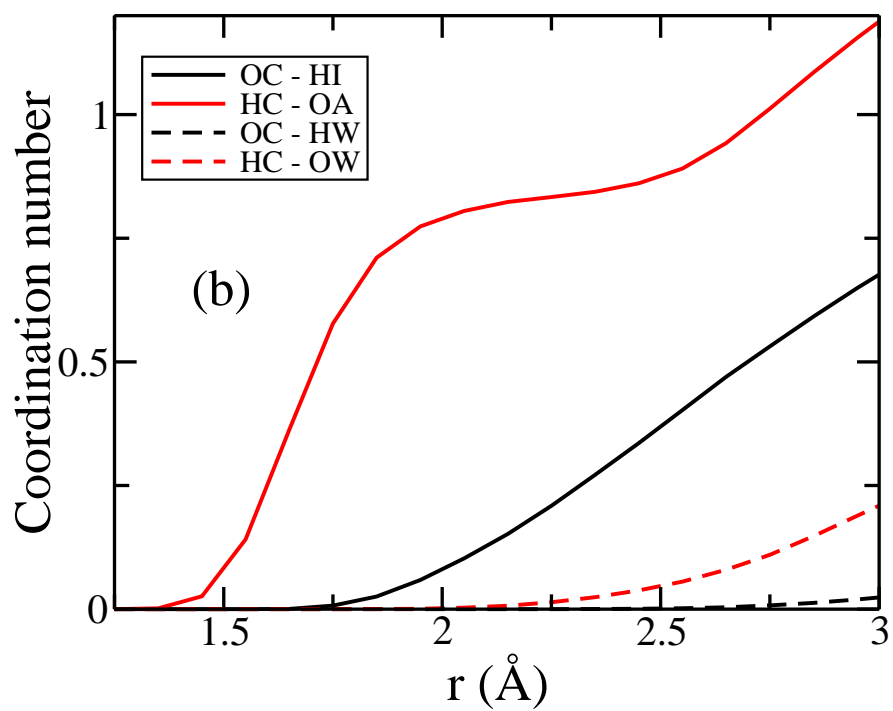
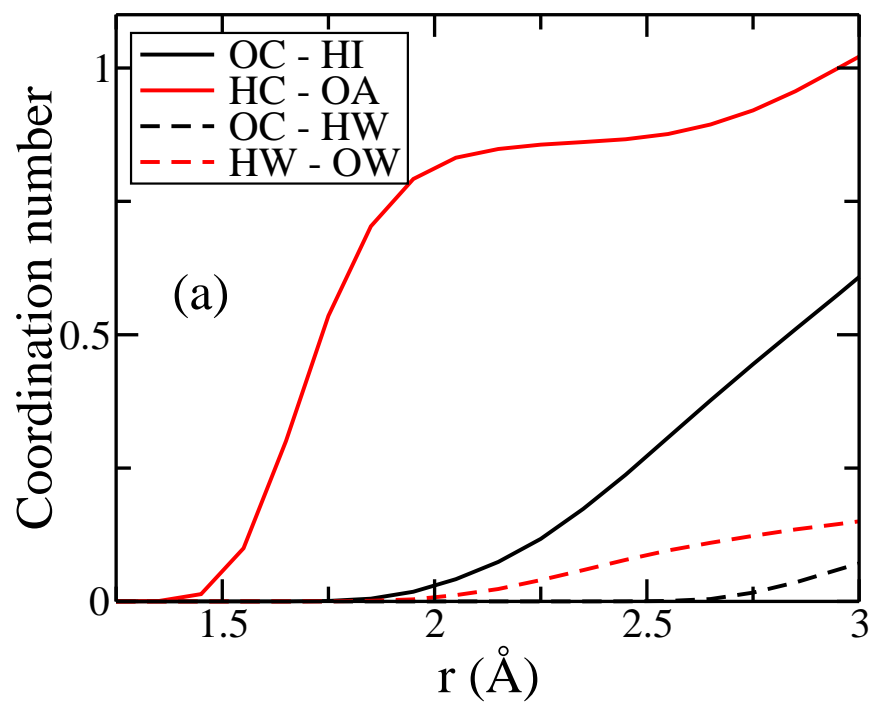


Figure S6: Running coordination number for (a) anti - anti and (b) anti - syn conformers of cellobiose solvated in IL+5H₂O.

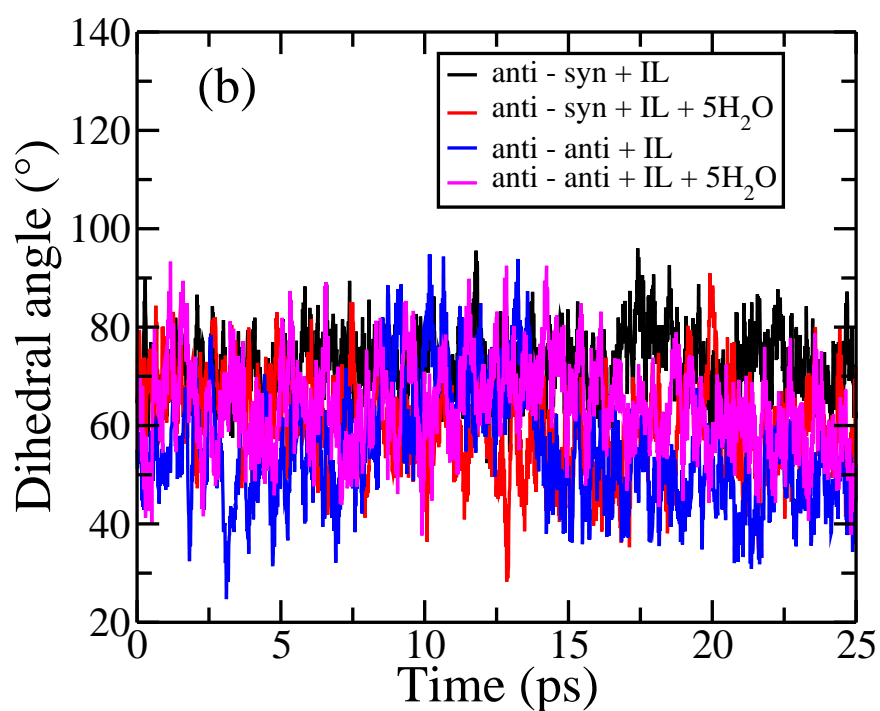
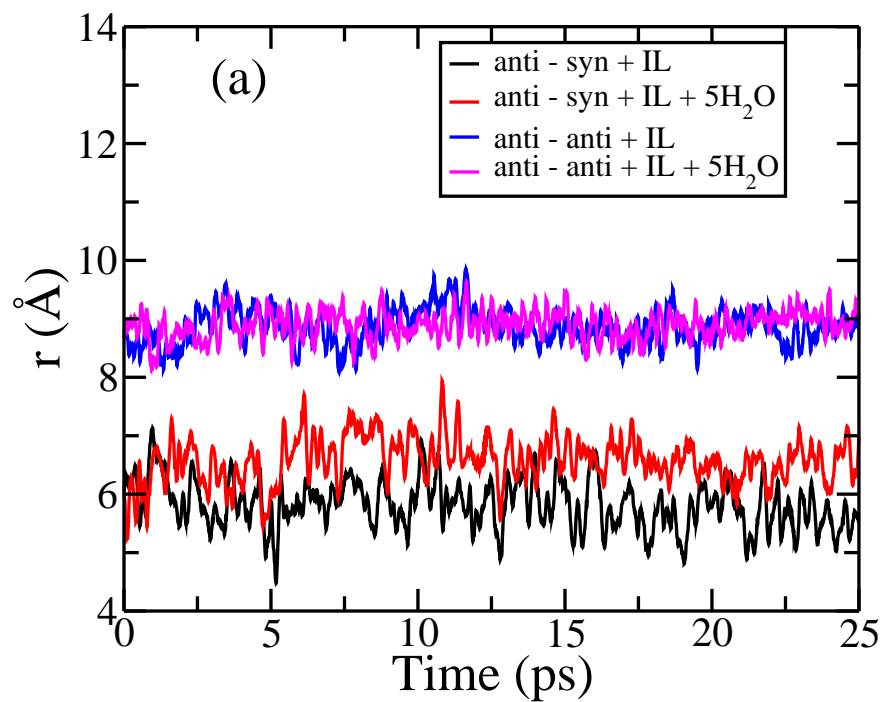


Figure S7: Distribution of (a) distance between oxygen atoms of two CH₂OH in cellobiose conformers (b) dihedral angle between two pentos rings of cellobiose conformers as function of time.