

Glycosidic α -linked mannopyranose disaccharides: An NMR spectroscopy and molecular dynamics simulation study employing additive and Drude polarizable force fields

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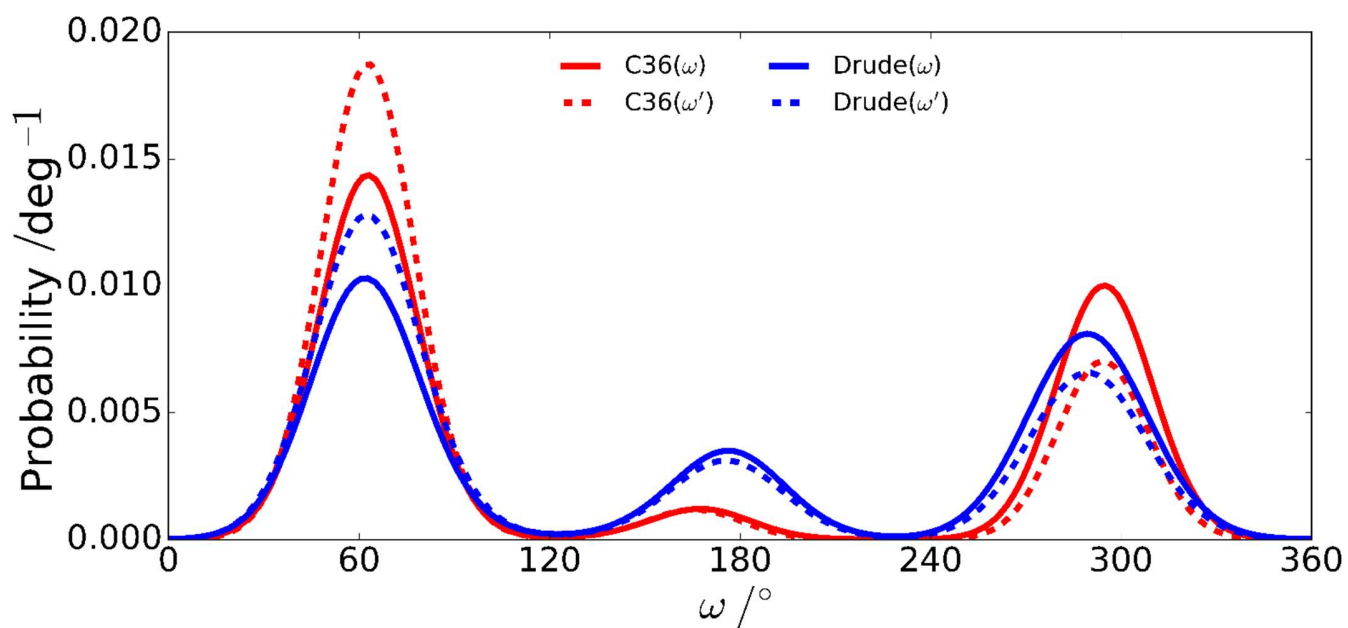


Figure S1. Rotameric distributions of the ω torsion angles in **M2M** for the additive C36 and the polarizable Drude force fields.

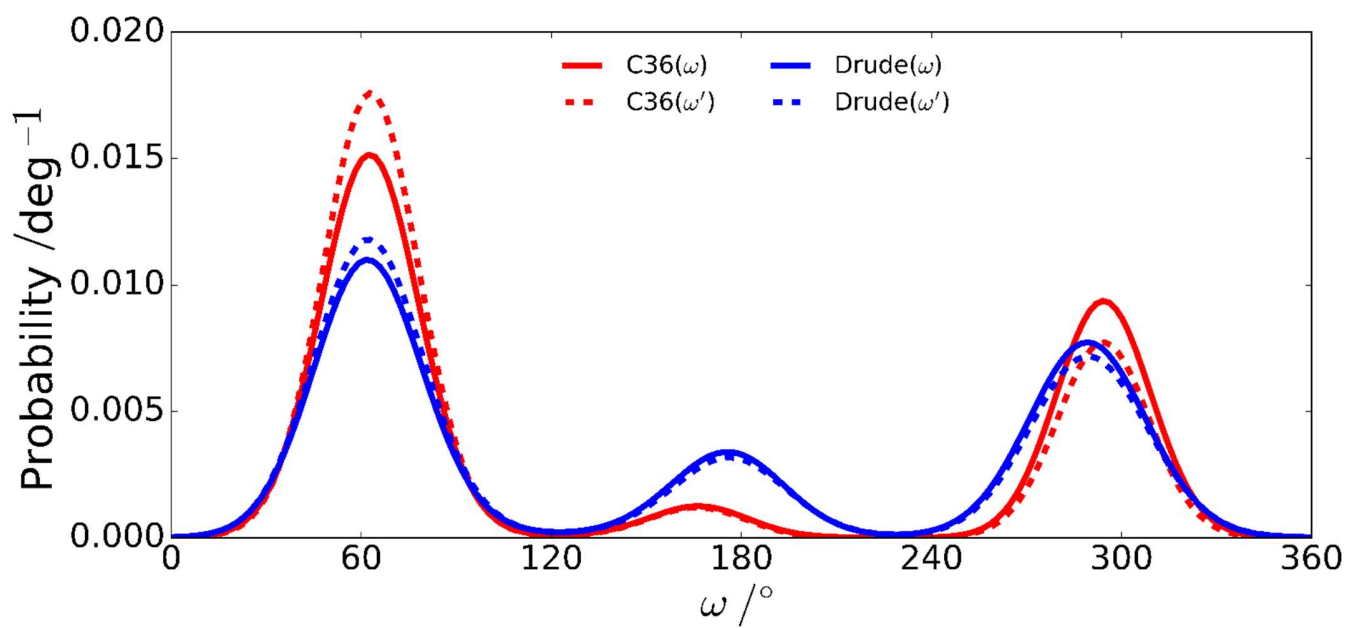


Figure S2. Rotameric distributions of the ω torsion angles in **M3M** for the additive C36 and the polarizable Drude force fields.

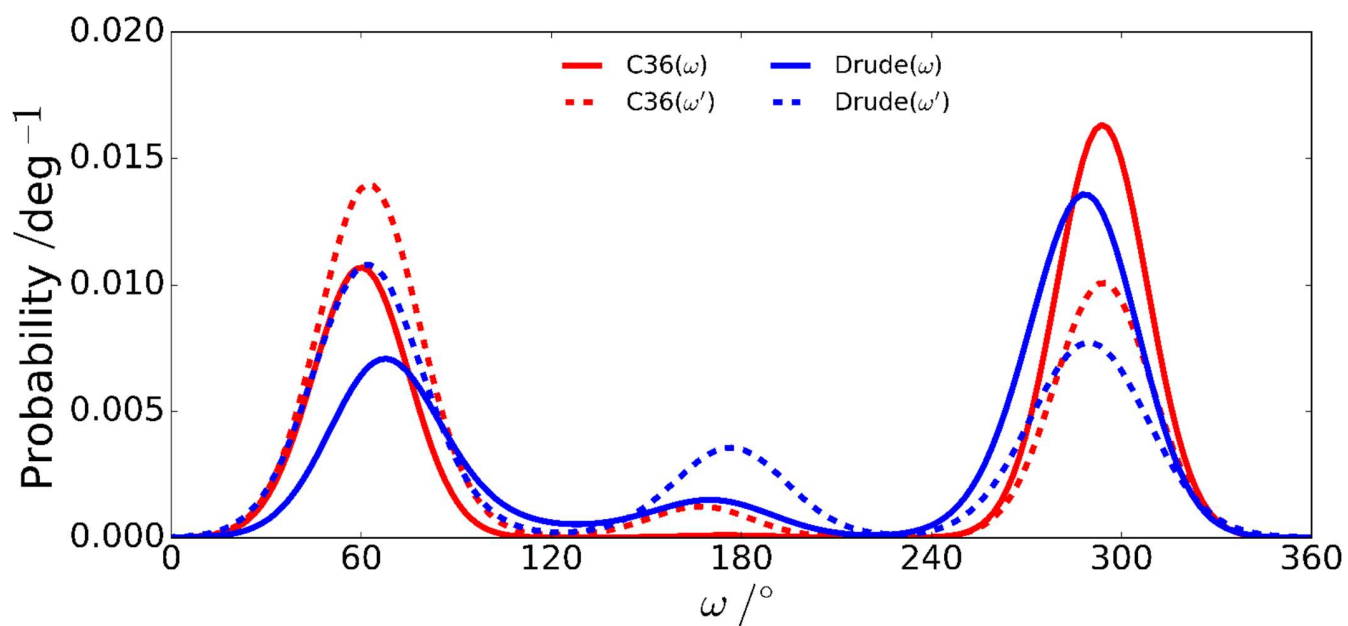


Figure S3. Rotameric distributions of the ω torsion angles in **M6M** for the additive C36 and the polarizable Drude force fields.

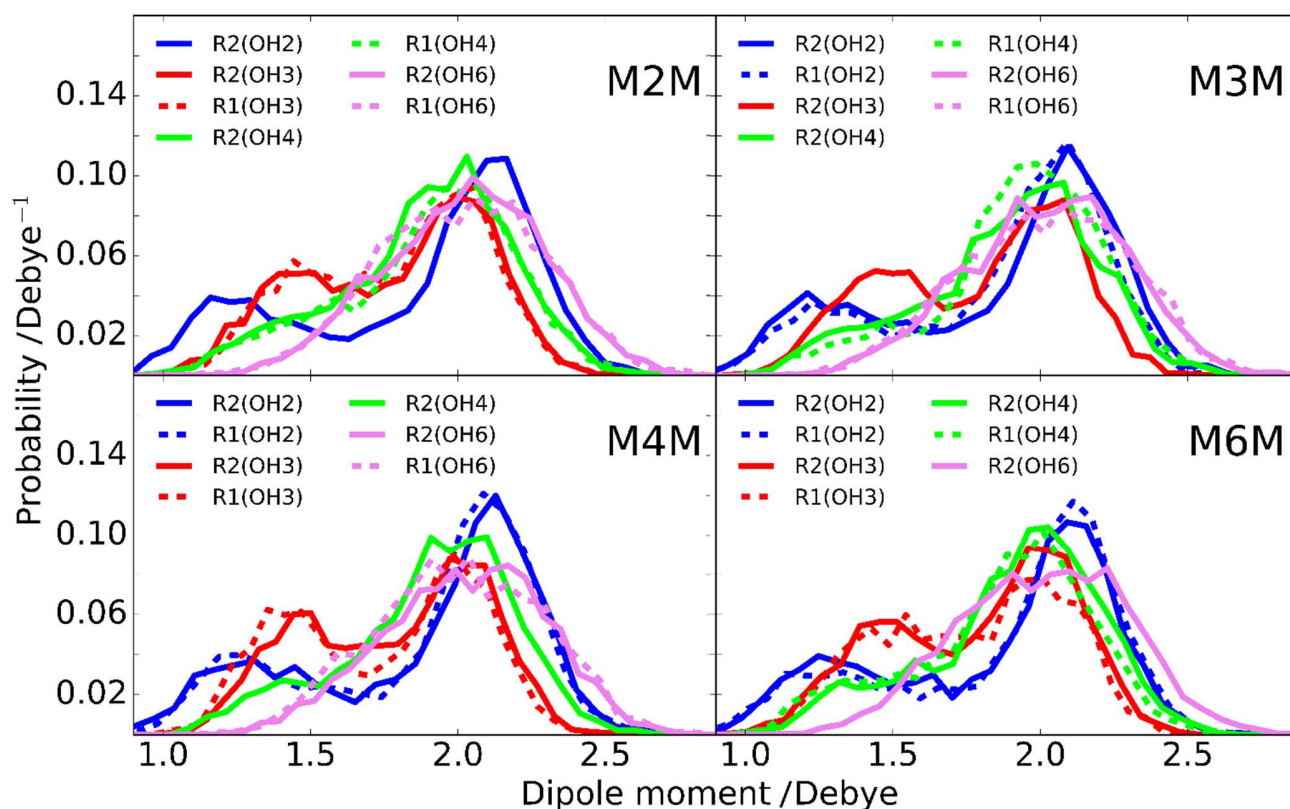


Figure S4. Individual dipole moment distributions of the hydroxyl groups of the α -linked mannopyranose disaccharides from the Drude simulations for the for the reducing end residue (R1, solid line) and the terminal residue (R2, dashed line). Results are shown for hydroxyl groups at positions 2 (blue), 3 (red), 4 (green) and 6 (purple). Hydroxyl dipole moments include contributions from the OH group, covalently linked CH_n atoms, and lone pairs as their charges sum to zero. Note that each panel is devoid of a dashed line, since the oxygen atom of the missing hydroxyl group is part of the pertinent glycosidic linkage.

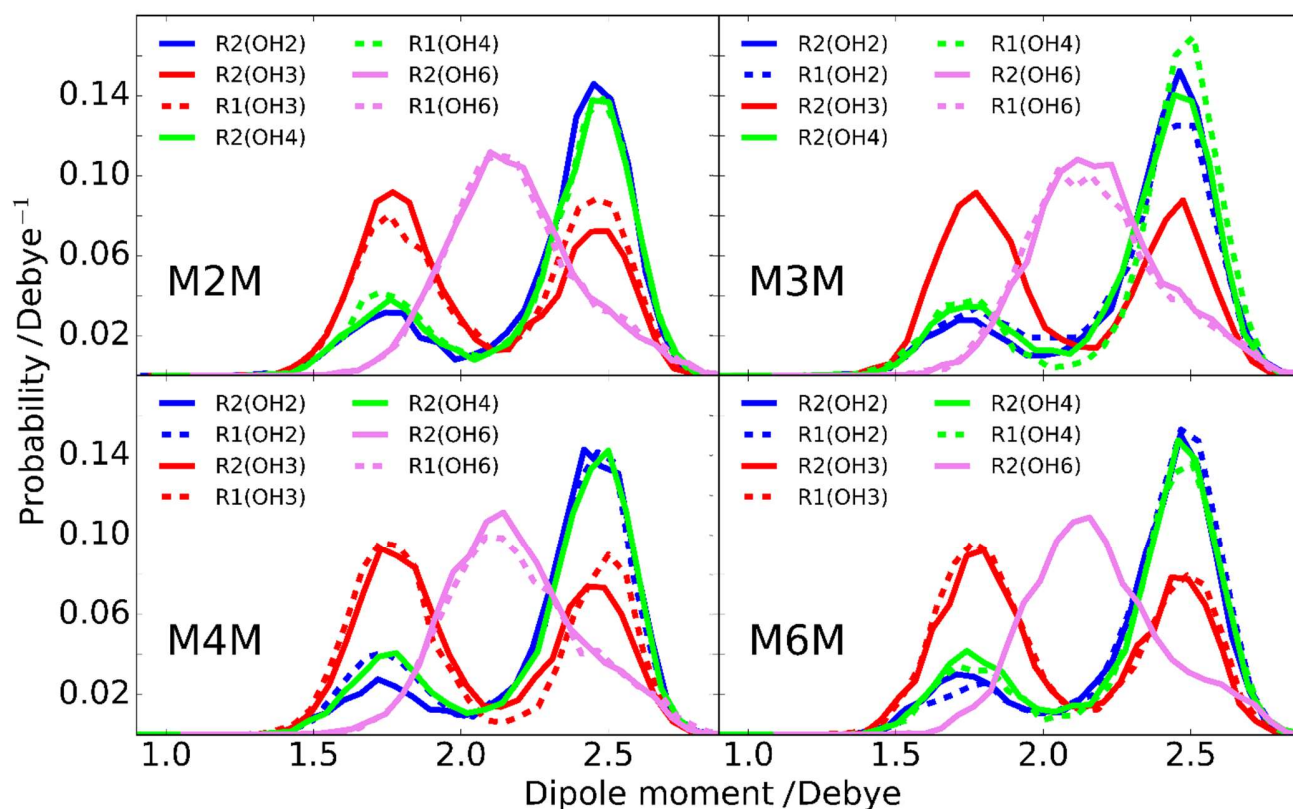
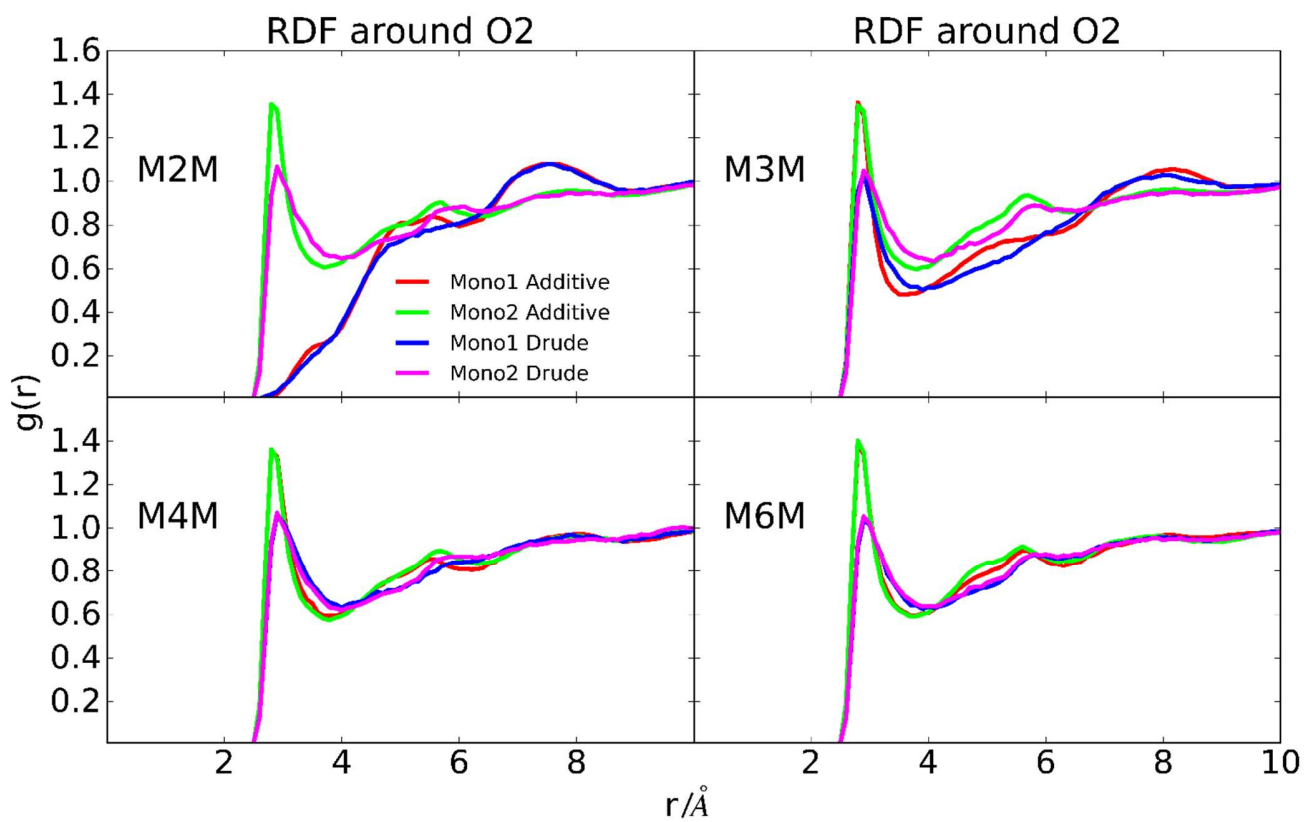
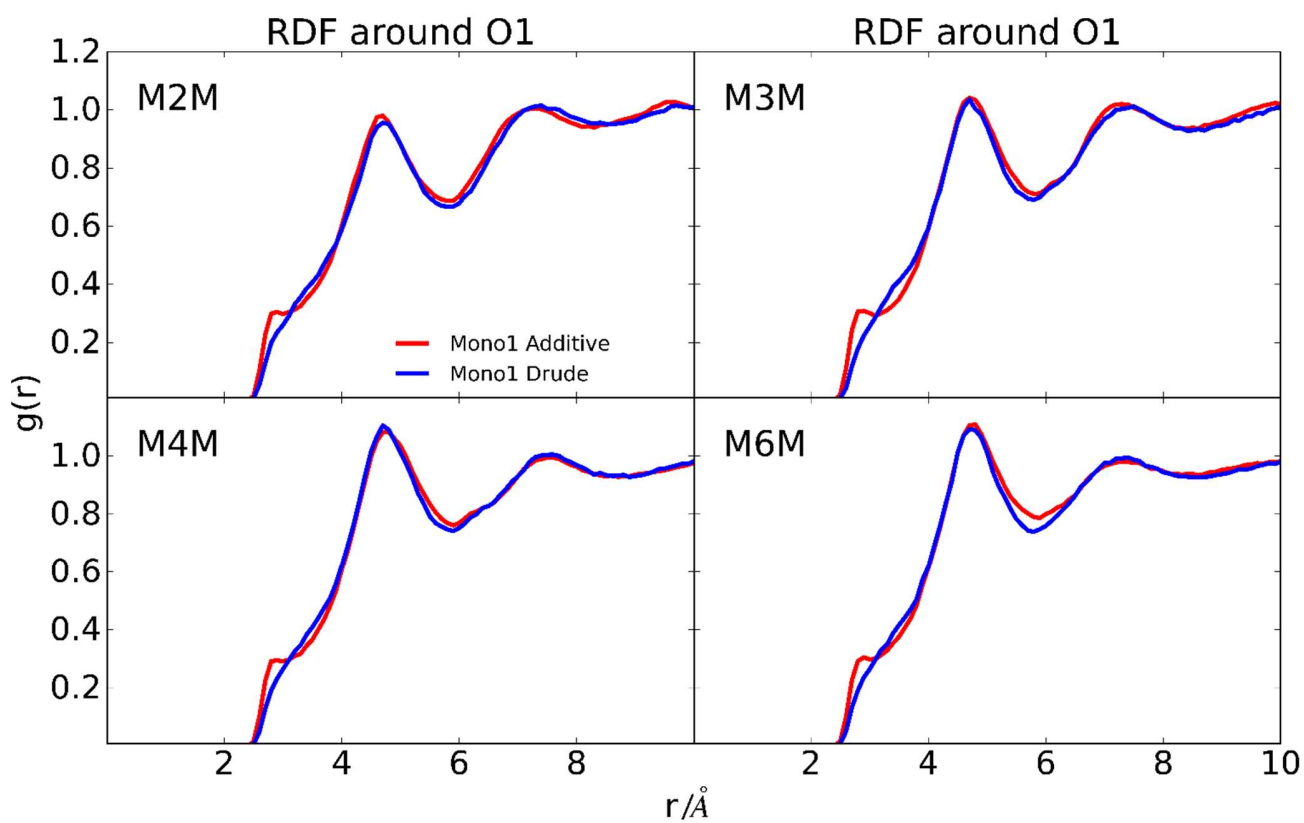
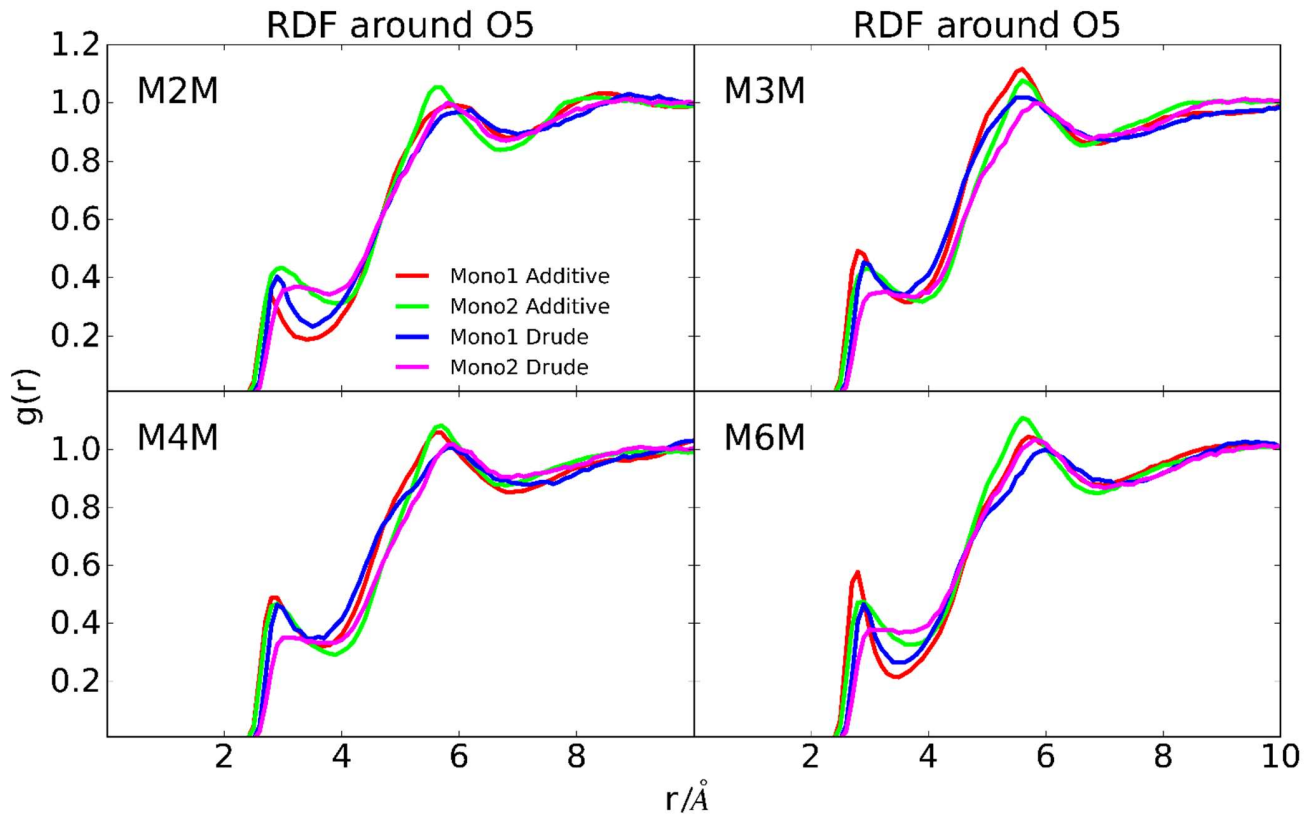
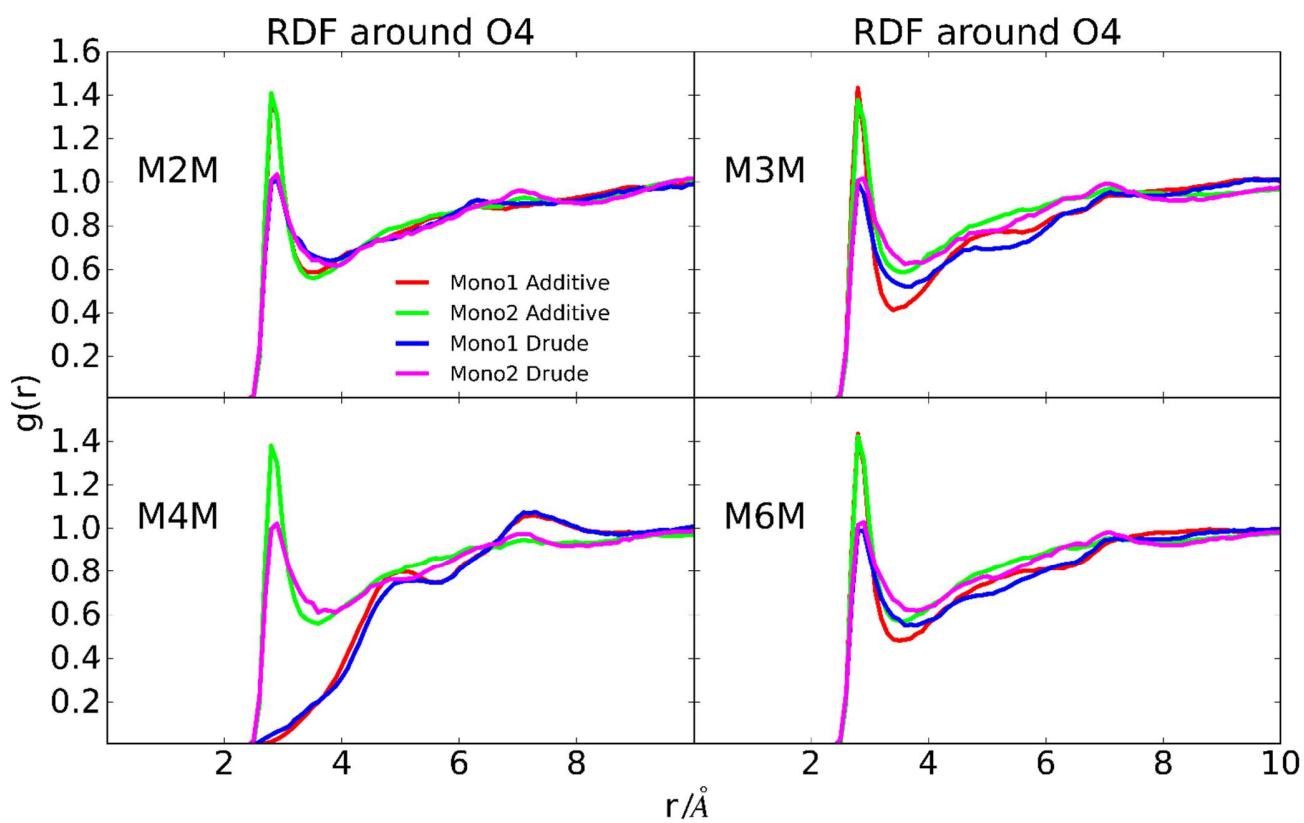


Figure S5. Individual dipole moment distributions of the hydroxyl groups of the α -linked mannopyranose disaccharides from the Additive C36 simulations for the reducing end residue (R1, solid line) and the terminal residue (R2, dashed line). Results are shown for hydroxyl groups at positions 2 (blue), 3 (red), 4 (green) and 6 (purple). Hydroxyl dipole moments include contributions from the OH group and covalently linked CH_n atoms as their charges sum to zero. Note that each panel is devoid of a dashed line, since the oxygen atom of the missing hydroxyl group is part of the pertinent glycosidic linkage.





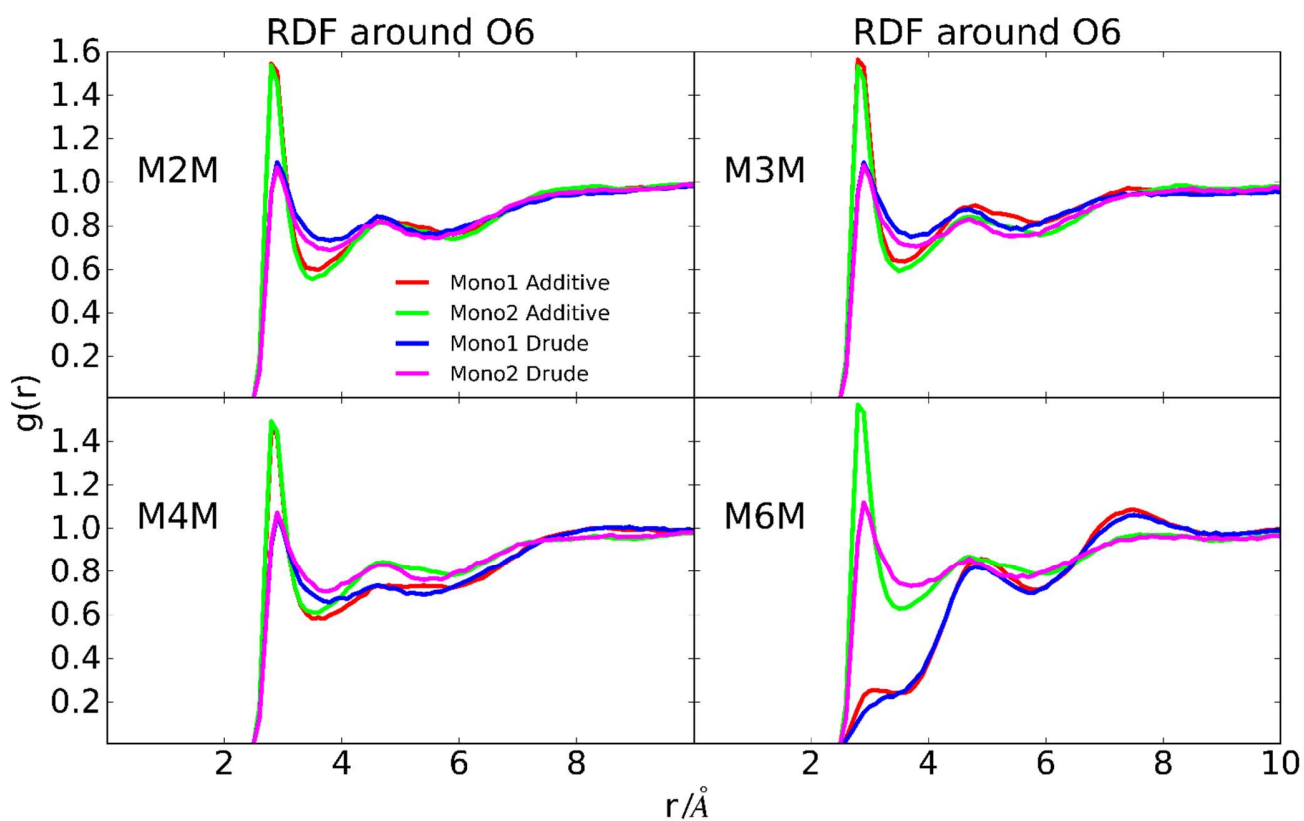


Figure S6. Radial distribution functions of water oxygen around the sugar oxygen atoms of the four disaccharides. Top to bottom panels depict RDFs for O1, O2, O4, O5 and O6. Monosaccharide 1 and 2 correspond to the reducing and terminal end residues of the disaccharides, respectively, for the additive C36 and Drude force fields as indicated by the labels the figure.