Supporting Information

for

"A hydration study of (1→4) and (1→6) linked α-glucans by comparative 10 ns molecular dynamics simulations and 500 MHz NMR"

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Table S1. Van der Waals radii in Ångstrøm of the different atoms for the non-bonding interaction

	Glycam2000a[a]	HGFB	CSFF
C	1.908	1.800	2.275
O	1.831	1.600	1.770
H	1.387 (H1)[b] 1.287 (H2)	1.468	1.320
O (hydroxyl)	1.961	1.600	1.770
H (hydroxyl)	0.000	0.800	0.2245

[a] Distances are given in Å.
[b] H2= anomeric hydrogen, H1= sugar aliphatic hydrogen

Table S2. Partial charges of the methanol atoms used in this work in the three force fields (Gycam_2000a, HGFB and CSFF)

	Partial Charges[a]
C	0.272
O	-0.699
HO	0.409
H	0.006

[a] Calculated using HF/6-31g* Resp0.000