Polarizable AMOEBA force field predicts thin and dense hydration layer around monosaccharides.

Luke A. Newman, Mackenzie Patton, Breyanna Rodriguez, Ethan Sumner, and Valerie Vaissier Welborn*

E-mail: vwelborn@vt.edu

MD input file availability

Poltype 2 and Tinker 9 input with parameters files are available at https://github.com/WelbornGroup/.

Average bond, angle and dihedrals for monosaccharides in water

Table 1: Bond lengths reported in Å as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	β-Glc		β-GlcN		β-GlcNAc		Exp
Bond	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2	1.54 ± 0.04	1.53 ± 0.03	1.53 ± 0.04	1.53 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.52
C2-C3	1.55 ± 0.04	1.54 ± 0.03	1.56 ± 0.04	1.56 ± 0.04	1.53 ± 0.04	1.53 ± 0.04	1.53
C3-C4	1.55 ± 0.04	1.55 ± 0.03	1.53 ± 0.04	1.53 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.52
C4-C5	1.57 ± 0.04	1.57 ± 0.03	1.56 ± 0.04	1.57 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.53
C5-C6	1.54 ± 0.04	1.53 ± 0.04	1.54 ± 0.04	1.55 ± 0.04	1.54 ± 0.04	1.55 ± 0.04	1.51
C1-O1	1.41 ± 0.03	1.41 ± 0.03	1.42 ± 0.03	1.42 ± 0.03	1.40 ± 0.03	1.40 ± 0.03	1.40
C2-O2	1.45 ± 0.04	1.44 ± 0.03	1.48 ± 0.03	1.49 ± 0.03	1.47 ± 0.03	1.47 ± 0.03	1.43
C3-O3	1.45 ± 0.04	1.43 ± 0.03	1.47 ± 0.04	1.46 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43

C4-O4	1.45 ± 0.04	1.44 ± 0.03	1.45 ± 0.04	1.45 ± 0.04	1.46 ± 0.04	1.46 ± 0.04	1.43
C5-O5	1.44 ± 0.04	1.46 ± 0.05	1.44 ± 0.04	1.44 ± 0.04	1.46 ± 0.04	1.46 ± 0.04	1.45
C6-O6	1.45 ± 0.04	1.43 ± 0.03	1.45 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.42
O5-C1	1.45 ± 0.04	1.43 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.46 ± 0.04	1.46 ± 0.04	1.43

Table 2: Bond lengths reported in Å as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	β-Gal		β-GalN		β-GalNAc		Exp
Bond	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2	1.54 ± 0.04	1.55 ± 0.04	1.53 ± 0.04	1.55 ± 0.04	1.56 ± 0.04	1.57 ± 0.04	1.52
C2-C3	1.55 ± 0.04	1.55 ± 0.04	1.56 ± 0.04	1.54 ± 0.04	1.54 ± 0.04	1.54 ± 0.04	1.53
C3-C4	1.56 ± 0.04	1.57 ± 0.04	1.53 ± 0.04	1.57 ± 0.04	1.56 ± 0.04	1.57 ± 0.04	1.52
C4-C5	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.53 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.53
C5-C6	1.54 ± 0.04	1.55 ± 0.04	1.54 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.51
C1-O1	1.41 ± 0.03	1.41 ± 0.03	1.42 ± 0.03	1.41 ± 0.03	1.40 ± 0.03	1.41 ± 0.03	1.40
C2-O2	1.45 ± 0.04	1.45 ± 0.04	1.48 ± 0.03	1.48 ± 0.03	1.47 ± 0.04	1.47 ± 0.03	1.43
C3-O3	1.45 ± 0.04	1.44 ± 0.04	1.47 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43
C4-O4	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43
C5-O5	1.44 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.43 ± 0.04	1.43 ± 0.04	1.43 ± 0.04	1.45
C6-O6	1.45 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.44 ± 0.04	1.42
O5-C1	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43

Table 3: Bond lengths reported in Å as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	α-Glc		α-GlcN		α-GlcNAc		Exp
Bond	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2	1.56 ± 0.04	1.57 ± 0.04	1.53 ± 0.04	1.53 ± 0.04	1.55 ± 0.04	1.56 ± 0.04	1.52

C2-C3	1.52 ± 0.04	1.53 ± 0.04	1.54 ± 0.04	1.54 ± 0.04	1.54 ± 0.04	1.54 ± 0.04	1.53
C3-C4	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.52
C4-C5	1.58 ± 0.04	1.58 ± 0.04	1.58 ± 0.04	1.58 ± 0.04	1.57 ± 0.04	1.57 ± 0.04	1.53
C5-C6	1.54 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.51
C1-O1	1.41 ± 0.03	1.41 ± 0.03	1.41 ± 0.03	1.41 ± 0.03	1.43 ± 0.03	1.43 ± 0.03	1.40
C2-O2	1.44 ± 0.04	1.45 ± 0.04	1.49 ± 0.03	1.49 ± 0.03	1.48 ± 0.03	1.48 ± 0.03	1.43
C3-O3	1.45 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43
C4-O4	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.46 ± 0.04	1.45 ± 0.04	1.43
C5-O5	1.48 ± 0.04	1.48 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.44 ± 0.04	1.45
C6-O6	1.44 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.44 ± 0.04	1.42
O5-C1	1.45 ± 0.04	1.45 ± 0.04	1.46 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43

Table 4: Bond lengths reported in Å as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	α-Gal		α-GalN		α-GalNAc		Exp
Bond	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.56 ± 0.04	1.57 ± 0.04	1.52
C2-C3	1.55 ± 0.04	1.55 ± 0.04	1.54 ± 0.04	1.54 ± 0.04	1.53 ± 0.04	1.54 ± 0.04	1.53
C3-C4	1.56 ± 0.04	1.56 ± 0.04	1.52 ± 0.04	1.53 ± 0.04	1.56 ± 0.04	1.57 ± 0.04	1.52
C4-C5	1.55 ± 0.04	1.55 ± 0.04	1.57 ± 0.04	1.58 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.53
C5-C6	1.54 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.55 ± 0.04	1.51
C1-O1	1.43 ± 0.03	1.43 ± 0.03	1.41 ± 0.03	1.41 ± 0.03	1.43 ± 0.03	1.43 ± 0.03	1.40
C2-O2	1.45 ± 0.04	1.45 ± 0.04	1.49 ± 0.04	1.49 ± 0.04	1.47 ± 0.04	1.48 ± 0.03	1.43
C3-O3	1.46 ± 0.04	1.45 ± 0.04	1.46 ± 0.04	1.46 ± 0.04	1.46 ± 0.04	1.46 ± 0.04	1.43
C4-O4	1.46 ± 0.04	1.45 ± 0.04	1.47 ± 0.04	1.46 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.43
C5-O5	1.44 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.48 ± 0.04	1.48 ± 0.04	1.45
C6-O6	1.45 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.45 ± 0.04	1.44 ± 0.04	1.42

O5-C1	1.46 ± 0.04	1.45 ± 0.04	1.48 ± 0.04	1.48 ± 0.04	1.44 ± 0.04	1.45 ± 0.04	1.43

Table 5: Angle values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	β-Glc		β-GlcN		β-GlcNAc		Exp
Angle	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3	109 ± 3	109 ± 3	108 ± 2	109± 3	109 ± 3	110 ± 3	110
C2-C3-C4	110 ± 3	112 ± 3	111 ± 3	112 ± 3	111 ± 3	111 ± 3	110
C3-C4-C5	110 ± 3	109 ± 3	109 ± 3	109 ± 3	110 ± 3	110 ± 3	110
C4-C5-C6	114 ± 3	115 ± 3	114 ± 3	114 ± 3	114 ± 3	114 ± 3	113
C4-C5-O5	109 ± 3	103 ± 3	109 ± 3	109 ± 3	109 ± 3	108 ± 3	109
C5-O5-C1	113 ± 3	109 ± 3	113 ± 3	113 ± 3	113 ± 3	114 ± 3	113
C5-C6-O6	108 ± 3	110 ± 3	109 ± 3	109 ± 3	114 ± 3	114 ± 3	111
O5-C1-C2	109 ± 3	104 ± 3	109 ± 3	110 ± 3	110 ± 3	110 ± 3	110
O5-C5-C6	107 ± 3	104 ± 3	107 ± 3	107 ± 3	107 ± 3	107 ± 3	107
O5-C1-O1	107 ± 3	108 ± 3	105 ± 3	106 ± 3	105 ± 3	105 ± 3	109
C2-C1-O1	108 ± 3	108± 3	109± 3	109± 3	109 ± 3	110 ± 3	110
C1-C2-O2	112 ± 3	112 ± 3	110 ± 2	110 ± 3	112 ± 3	112 ± 3	109
C3-C2-O2	107 ± 3	108 ± 3	110 ± 2	110 ± 3	111 ± 3	111 ± 3	111
C2-C3-O3	110 ± 3	112 ± 3	112 ± 3	112 ± 3	109 ± 3	109 ± 3	108
C4-C3-O3	107 ± 3	107 ± 3	107 ± 3	107 ± 3	111 ± 3	111 ± 3	111
C3-C4-O4	110 ± 3	109 ± 3	110 ± 3	110 ± 3	105 ± 3	105 ± 3	110
C5-C4-O4	110 ± 3	111 ± 3	110 ± 3	109 ± 3	113 ± 3	113 ± 3	110

Table 6: Angle values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	β-Gal	β-GalN	β-GalNAc	Exp

Angle	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3	110 ± 3	110 ± 3	109 ± 2	109± 2	109 ± 3	110 ± 3	110
C2-C3-C4	109 ± 3	110 ± 3	110 ± 2	111 ± 3	110 ± 3	110 ± 3	110
C3-C4-C5	109 ± 3	109 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110
C4-C5-C6	113 ± 3	113 ± 3	114 ± 3	114 ± 3	115 ± 3	115 ± 3	113
C4-C5-O5	110 ± 3	110 ± 3	110 ± 3	110 ± 3	109 ± 3	109 ± 3	109
C5-O5-C1	112 ± 3	113 ± 3	113 ± 3	113 ± 3	114 ± 3	114 ± 3	113
C5-C6-O6	108 ± 3	109 ± 3	109 ± 3	109 ± 3	111 ± 3	112 ± 3	111
O5-C1-C2	109 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110
O5-C5-C6	108 ± 3	108 ± 3	108 ± 3	108 ± 3	106 ± 3	107 ± 3	107
O5-C1-O1	107 ± 3	107 ± 3	106 ± 3	106 ± 3	105 ± 3	105 ± 3	109
C2-C1-O1	108 ± 3	108± 3	109± 3	109± 3	109 ± 3	109 ± 3	110
C1-C2-O2	112 ± 3	112 ± 3	116 ± 3	116 ± 3	111 ± 3	112 ± 3	109
C3-C2-O2	107 ± 3	107 ± 3	109 ± 2	109 ± 2	112 ± 3	113 ± 3	111
C2-C3-O3	112 ± 3	112 ± 3	112 ± 3	112 ± 3	109 ± 3	109 ± 3	108
C4-C3-O3	108 ± 3	108 ± 3	108 ± 3	108 ± 3	110 ± 3	110 ± 3	111
C3-C4-O4	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110
C5-C4-O4	109 ± 3	109 ± 3	108 ± 3	108 ± 3	109 ± 3	109 ± 3	110

Table 7: Angle values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	α-Glc		α-GlcN		α-GlcNAc		Exp
Angle	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3	111 ± 3	111 ± 3	110 ± 2	110 ± 2	110 ± 3	111 ± 3	110
C2-C3-C4	110 ± 3	110 ± 3	111 ± 3	112 ± 2	111 ± 2	111 ± 3	110
C3-C4-C5	109 ± 3	109 ± 3	109 ± 3	110 ± 3	112 ± 2	110 ± 3	110

C4-C5-C6	112 ± 3	112 ± 3	113 ± 3	114 ± 3	113 ± 3	112 ± 3	113
C4-C5-O5	113 ± 3	113 ± 3	112 ± 3	112 ± 3	112 ± 3	110 ± 3	109
C5-O5-C1	115 ± 3	115 ± 3	114 ± 3	114 ± 3	117 ± 3	115 ± 3	113
C5-C6-O6	109 ± 3	109 ± 3	108 ± 3	108 ± 3	108 ± 3	108 ± 3	111
O5-C1-C2	112 ± 3	112 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110
O5-C5-C6	111 ± 3	111 ± 3	113 ± 3	114 ± 3	110 ± 3	107 ± 3	107
O5-C1-O1	110 ± 3	109 ± 3	107 ± 4	107 ± 3	110 ± 3	113 ± 3	109
C2-C1-O1	109 ± 3	109 ± 3	110 ± 3	110 ± 3	107 ± 3	108 ± 3	110
C1-C2-O2	111 ± 3	111 ± 3	116 ± 3	116 ± 2	114 ± 3	113 ± 3	109
C3-C2-O2	108 ± 3	108 ± 3	108 ± 2	108 ± 2	110 ± 3	110 ± 3	111
C2-C3-O3	112 ± 3	112 ± 3	111 ± 3	111 ± 3	111 ± 3	111 ± 3	108
C4-C3-O3	109 ± 3	109 ± 3	111 ± 3	111 ± 3	110 ± 3	109 ± 3	111
C3-C4-O4	114 ± 3	114 ± 3	114 ± 3	114 ± 3	112 ± 3	111 ± 3	110
C5-C4-O4	111 ± 3	111 ± 3	110 ± 3	110 ± 3	110 ± 3	112 ± 3	110

Table 8: Angle values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	α-Gal		α-GalN		α-GalNAc		Exp
Angle	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3	110 ± 3	110 ± 3	111 ± 2	111 ± 2	110 ± 3	111 ± 3	110
C2-C3-C4	109 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110 ± 3	110
C3-C4-C5	109 ± 3	109 ± 3	110 ± 3	109 ± 3	110 ± 3	110 ± 3	110
C4-C5-C6	113 ± 3	113 ± 3	112 ± 3	112 ± 3	115 ± 3	115 ± 3	113
C4-C5-O5	111 ± 3	111 ± 3	112 ± 3	111 ± 3	110 ± 3	110 ± 3	109
C5-O5-C1	114 ± 3	114 ± 3	113 ± 3	113 ± 3	115 ± 3	115 ± 3	113
C5-C6-O6	108 ± 3	109 ± 3	107 ± 3	108 ± 3	111 ± 3	111 ± 3	111
O5-C1-C2	110 ± 3	110 ± 3	112 ± 3	112 ± 3	111 ± 3	111 ± 3	110

O5-C5-C6	108 ± 3	108 ± 3	110 ± 3	110 ± 3	105 ± 3	106 ± 3	107
O5-C1-O1	113 ± 3	113 ± 3	109 ± 3	108 ± 3	112 ± 3	112 ± 3	109
C2-C1-O1	109 ± 3	109 ± 3	112 ± 3	112 ± 3	109 ± 3	109 ± 3	110
C1-C2-O2	114 ± 3	114 ± 3	111 ± 2	111 ± 2	113 ± 3	113 ± 3	109
C3-C2-O2	107 ± 3	107 ± 3	109 ± 2	109 ± 2	110 ± 3	110 ± 3	111
C2-C3-O3	111 ± 3	111 ± 3	111 ± 3	112 ± 3	110 ± 3	110 ± 3	108
C4-C3-O3	107 ± 3	107 ± 3	110 ± 3	107 ± 3	108 ± 3	108 ± 3	111
C3-C4-O4	109 ± 3	110 ± 3	107 ± 3	111 ± 3	110 ± 3	110 ± 3	110
C5-C4-O4	109 ± 3	109 ± 3	114 ± 3	114 ± 3	110 ± 3	109 ± 3	110

Table 9: Torsion values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	β-Glc		β-GlcN		β-GlcNAc		Exp
Torsion	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3-C4	-55± 6	-50± 6	-55 ± 5	-55± 6	-54± 6	-52± 6	-54
C2-C3-C4-C5	53 ± 6	50 ± 6	54 ± 5	53 ± 6	54 ± 6	53 ± 6	55
C3-C4-C5-O5	-55 ± 6	-58± 6	-55± 4	-55± 6	-55± 6	-56± 6	-57
C4-C5-O5-C1	62 ± 5	75 ± 6	62 ± 5	62 ± 6	61 ± 6	62 ± 6	62
C5-O5-C1-C2	-65 ± 6	-77± 6	-65 ± 5	-64± 6	-63± 5	-62± 6	-62
O5-C1-C2-C3	59 ± 6	61 ± 6	58 ± 5	57 ± 6	57 ± 6	55 ± 6	57
O1-C1-O5-C5	178± 6	168± 6	178± 6	178± 7	180± 7	180± 7	N/A
O2-C2-C1-O5	178± 6	180± 6	179± 5	178± 7	180± 7	180± 7	N/A
O3-C3-C2-C1	-174± 6	-170± 6	-175± 6	-174± 6	-177± 6	-175± 6	N/A
O4-C4-C3-C2	174± 6	170± 6	174± 6	174± 6	176± 6	176± 6	N/A

Table 10: Torsion values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	β-Gal		β-GalN		β-GalNAc		Exp
Torsion	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3-C4	-55 ± 5	-54 ± 5	-53 ± 5	-52± 5	-53± 5	-52± 6	-54
C2-C3-C4-C5	53 ± 5	53 ± 5	54 ± 5	53 ± 5	54 ± 5	54± 5	55
C3-C4-C5-O5	-57 ± 5	-57± 5	-57± 5	-57± 5	-57 ± 5	-57± 5	-57
C4-C5-O5-C1	63 ± 6	63 ± 6	63 ± 6	63± 6	62± 6	62± 5	62
C5-O5-C1-C2	-64 ± 6	-63 ± 6	-62 ± 6	-61 ± 6	-62 ± 5	-61± 6	-62
O5-C1-C2-C3	59 ± 6	57 ± 6	56 ± 6	55 ± 6	56 ± 6	54± 6	57
O1-C1-O5-C5	179 ± 6	180 ± 6	180 ± 6	-179 ± 6	-179 ± 6	-179± 6	N/A
O2-C2-C1-O5	178 ± 6	176 ± 6	180 ± 6	178 ± 6	180 ± 6	-179± 6	N/A
O3-C3-C2-C1	-175 ± 6	-174 ± 6	-173 ± 6	-172 ± 6	-174 ± 6	-173± 6	N/A
O4-C4-C3-C2	-66 ± 6	-66 ± 6	-66 ± 6	-66 ± 6	-66 ± 6	-66± 6	N/A

Table 11: Torsion values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	α-Glc		α-GlcN		α-GlcNAc		Exp
Torsion	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3-C4	-57 ± 9	-52 ±13	13 ± 52	52 ± 13	55 ± 5	-52± 6	-54
C2-C3-C4-C5	56 ± 8	57 ± 7	-8 ± 52	-46 ± 17	-49 ± 5	52± 6	55
C3-C4-C5-O5	-49 ±15	-48 ±14	11 ± 48	47 ± 13	45 ± 6	-54± 6	-57
C4-C5-O5-C1	43 ±29	35 ±36	-21 ± 51	-57 ± 7	-51 ± 6	59± 7	62
C5-O5-C1-C2	-42 ±33	-28 ±47	27 ± 54	61 ± 6	58 ± 6	-59± 6	-62
O5-C1-C2-C3	49 ±22	37 ±34	-22 ± 51	-58 ± 7	-58 ± 5	54± 6	57
O1-C1-O5-C5	80 ±33	94 ±46	147 ± 51	-179 ± 6	176 ± 6	62± 7	N/A
O2-C2-C1-O5	170±22	158 ±35	102 ± 51	66 ± 7	66 ± 6	178± 6	N/A
O3-C3-C2-C1	-178±9	-173 ±13	-111 ± 51	-73 ± 13	-68 ± 6	-174± 6	N/A

O4-C4-C3-C2	-179± 8	-179 ± 7	116 ± 53	77 ± 17	75 ± 6	176± 7	N/A

Table 12: Torsion values reported in ° as averages over 145 ns of MD in the NPT ensemble (after 5 ns equilibration). The error is the standard deviation.

	α-Gal		α-GalN		α-GalNAc		Exp
Torsion	mutual pol.	no pol.	mutual pol.	no pol.	mutual pol.	no pol	
C1-C2-C3-C4	-55 ± 5	-54 ± 5	-52 ±10	-54 ± 5	-55 ± 5	-54± 5	-54
C2-C3-C4-C5	55 ± 5	54 ± 5	55 ± 6	55 ± 5	55 ± 5	55± 5	55
C3-C4-C5-O5	-56 ± 6	-56 ± 5	-56 ± 8	-57 ± 6	-55 ± 6	-56± 5	-57
C4-C5-O5-C1	59 ± 6	60 ± 6	54 ±15	57 ± 6	57 ± 6	58± 6	62
C5-O5-C1-C2	-57 ± 7	-58 ± 6	-50 ±20	-55 ± 6	-56 ± 6	-57± 6	-62
O5-C1-C2-C3	55 ± 6	54 ± 6	49 ±18	53 ± 6	55 ± 6	54± 6	57
O1-C1-O5-C5	65 ± 8	64 ± 7	71 ± 9	68 ± 7	65 ± 7	65± 7	N/A
O2-C2-C1-O5	175± 7	175 ± 6	172 ± 6	174 ± 6	178 ± 6	177± 6	N/A
O3-C3-C2-C1	-173± 6	-172 ± 6	-173 ± 6	-177 ± 6	-174 ± 6	-173± 6	N/A
O4-C4-C3-C2	-65± 6	-65 ± 6	-66 ± 6	-69 ± 6	-65 ± 6	-65± 6	N/A

Radial distribution function for α anomers

Table 13: First peak position (r_0), first minimum position ($r_{\min}$) and coordination number (CN) for hydroxyl-water radial distribution function of $\alpha-$Glc with and without mutual polarization.

	Mutual pol.			No pol.		
Oxygen	r_0 (Å)	$r_{\min}$ (Å)	CN	r_0 (Å)	$r_{\min}$ (Å)	CN
O_1	2.85	3.65	4.07	3.05	3.95	4.41
O_2	2.85	3.35	3.33	3.05	4.05	4.84
O_3	2.85	3.65	4.42	3.05	3.95	4.63
O_4	2.85	3.45	3.39	3.05	3.85	3.93
Average	2.85	3.45	3.51	3.05	4.05	4.82
O_6	2.85	3.35	3.33	3.05	3.95	4.73

Mean square displacement of $\beta-$Glc center-of-mass as a function of concentration

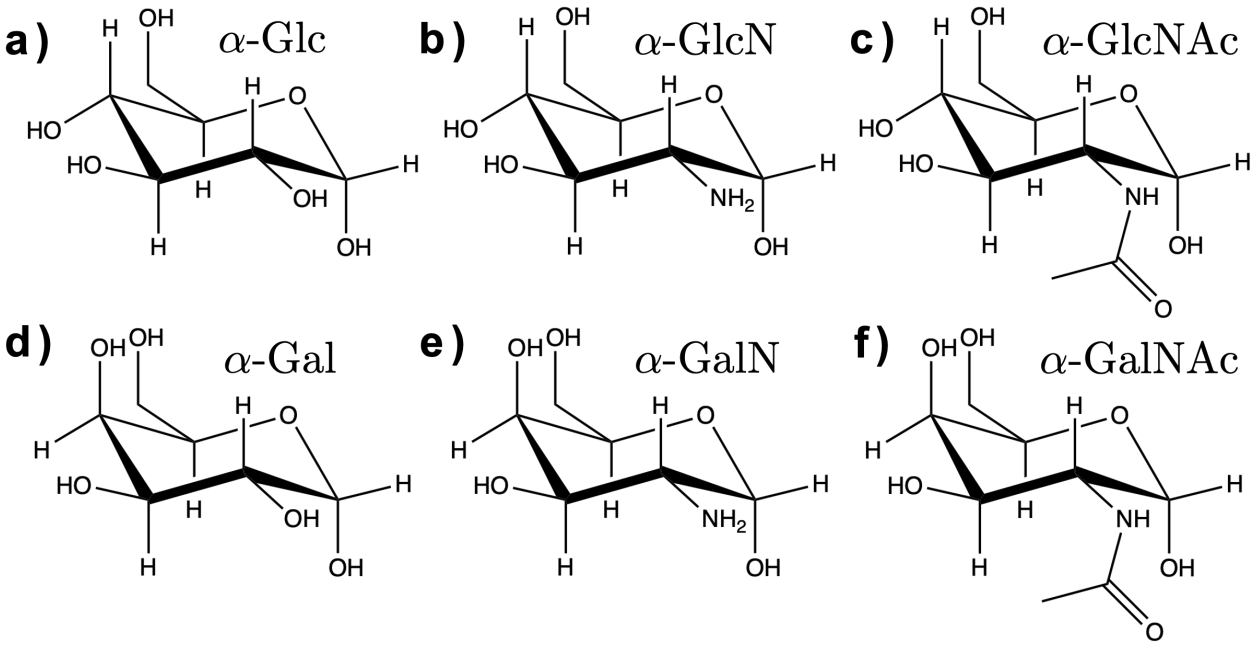

Figure S1: Chemical structure of the α anomers of the six monosaccharides studied here. a) Glc, b) GlcN, c) GlcNAc, d) Gal, e) GalN, f) GalNAc.

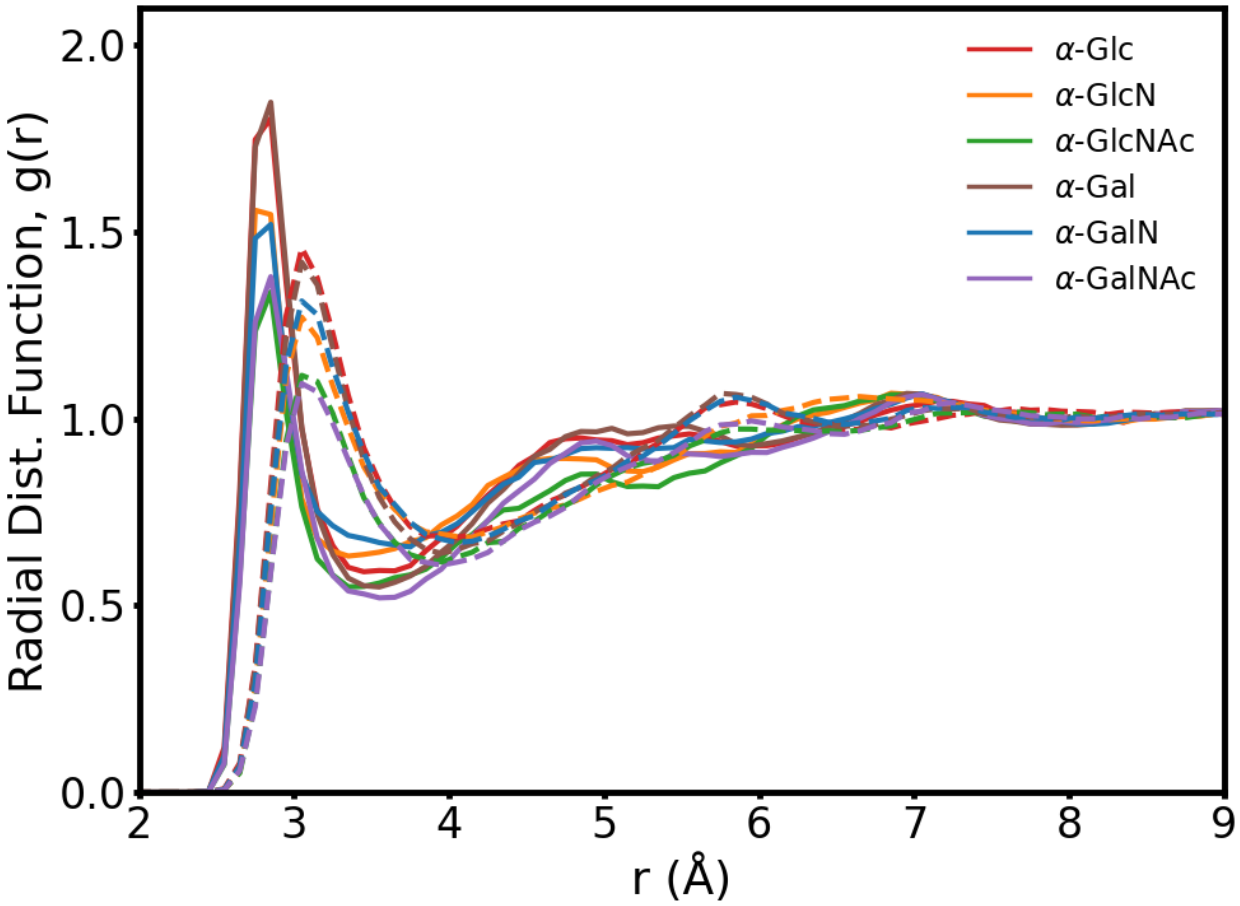

Figure S2: Carbohydrate-water radial distribution function for the six α anomers, with (solid lines) and without (dotted lines) mutual polarization. Each curve is an average of the $O_1 - O_w$, $O_2/N_2 - O_w$, $O_3 - O_w$ and $O_4 - O_w$ distribution functions, where O_w is the water oxygen.

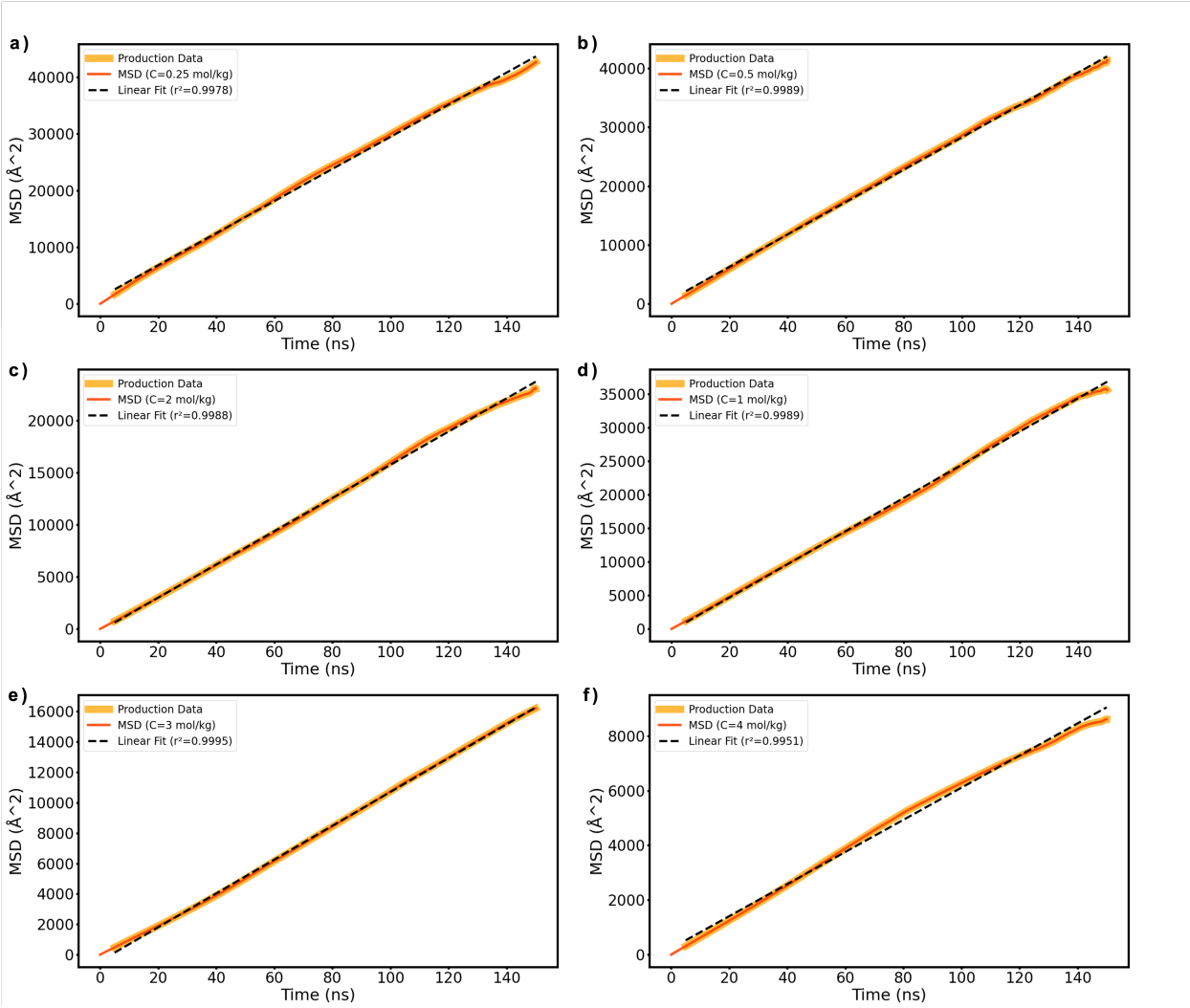

Figure S3: Mean square displacement of $\beta-$Glc center-of-mass as a function of MD time and linear fit a) c=0.25 mol/kg (29 $\beta-$Glc molecules), b) c=0.5 mol/kg (56 $\beta-$Glc molecules), c) c=1 mol/kg (105 $\beta-$Glc molecules), d) c=2 mol/kg (188 $\beta-$Glc molecules), e) c=3 mol/kg (255 $\beta-$Glc molecules), f) c=4 mol/kg (305 $\beta-$Glc molecules).

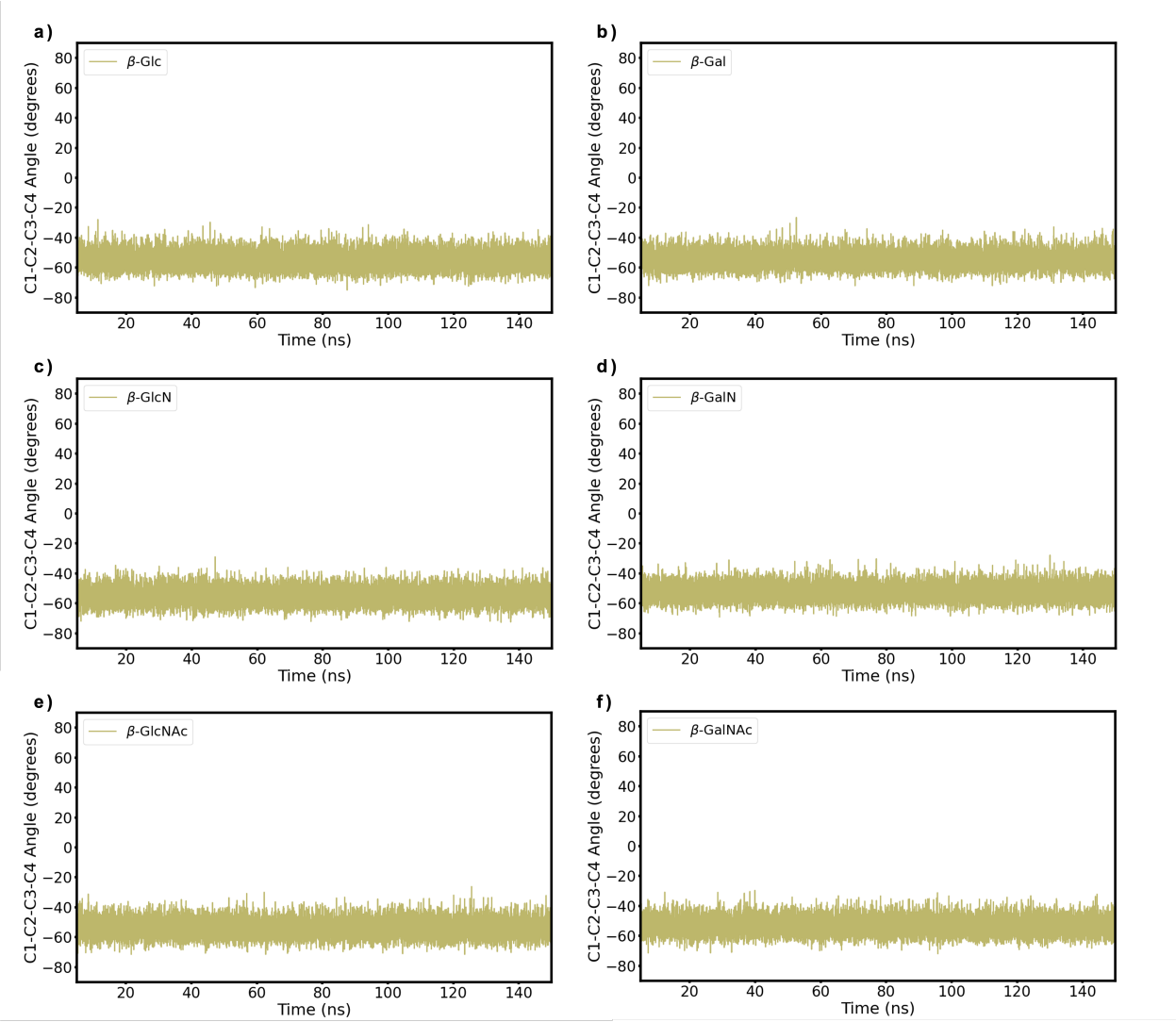

Figure S4: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\beta-$ anomers during 145 ns production MD with AMOEBA (mutual polarization, β parameters). $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) β-Glc, b) β-GlcN, c) β-GlcNAc, d) β-Gal, e) β-GalN, f) β-GalNAc.

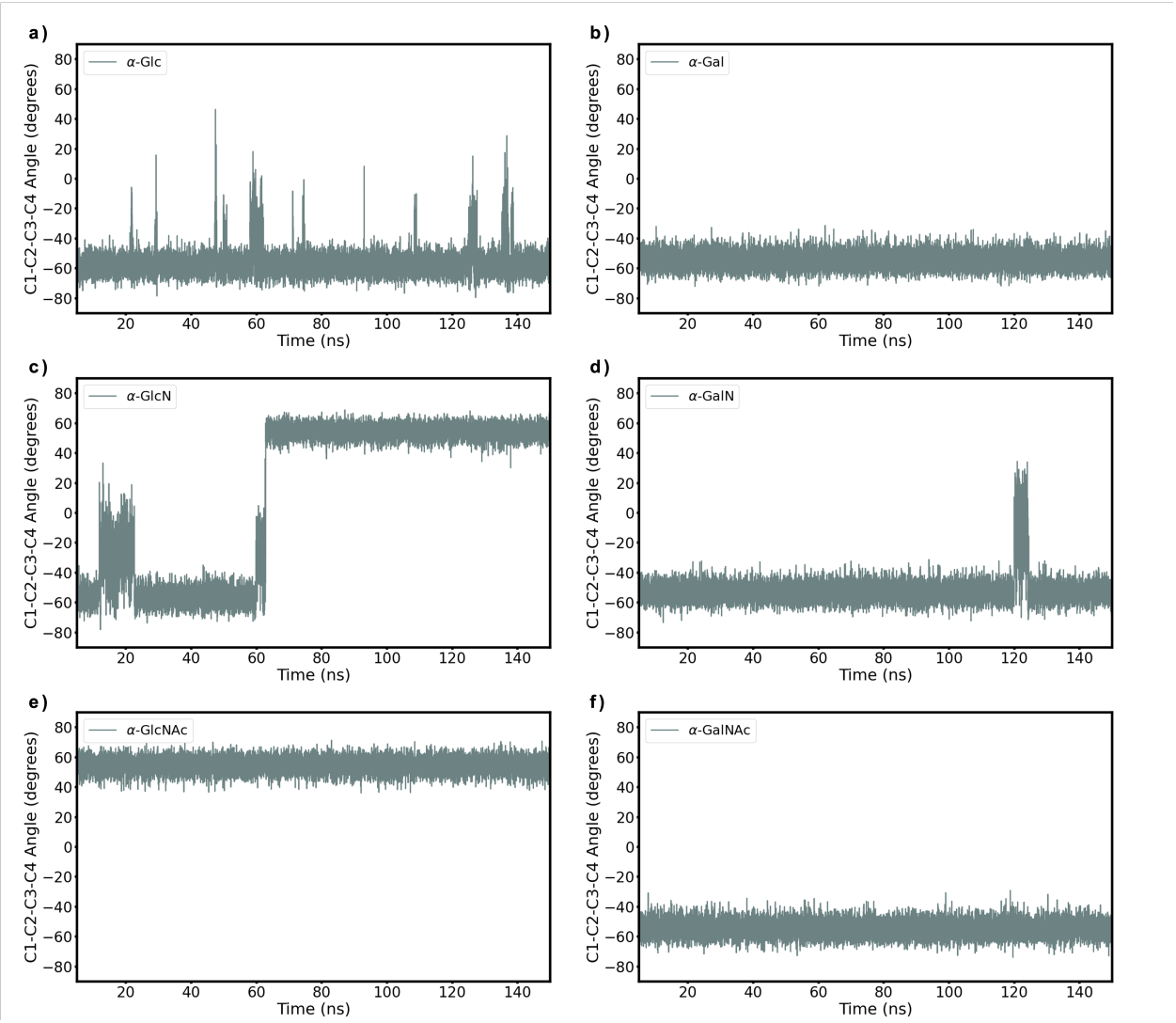

Figure S5: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\alpha-$ anomers during 145 ns production MD with AMOEBA (mutual polarization, α parameters). $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) α-Glc, b) α-GlcN, c) α-GlcNAc, d) α-Gal, e) α-GalN, f) α-GalNAc. Overall, α-Glc, α-GlcN, α-GlcNAc, α-Gal, α-GalN and α-GalNAc spends 2.9, 7.4, 0.09, 0.07, 2.6 and 0.05% of the time, respectively, in a conformation other than chair.

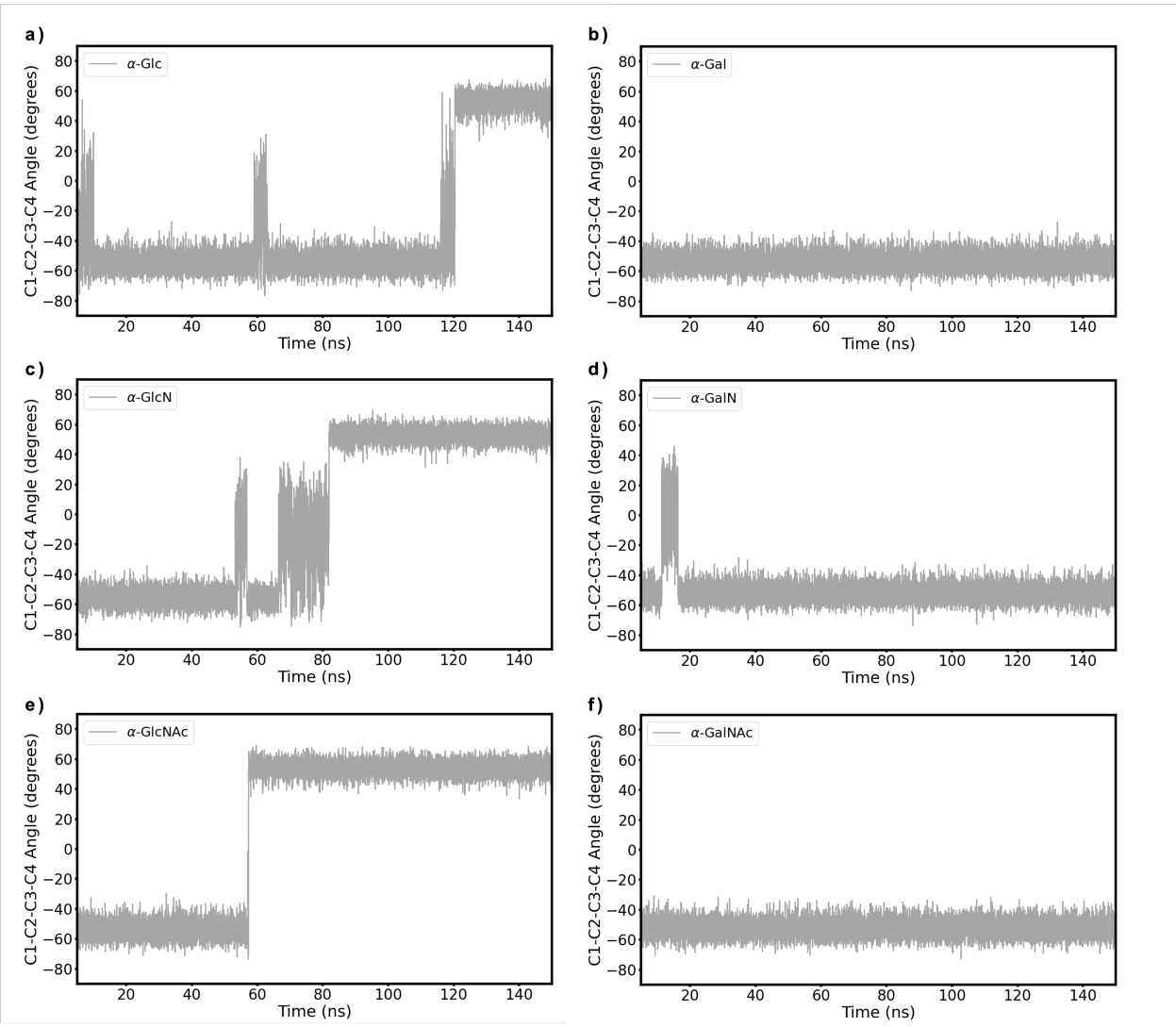

Figure S6: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\alpha-$ anomers during 145 ns production MD with AMOEBA (mutual polarization, β parameters). $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) α-Glc, b) α-GlcN, c) α-GlcNAc, d) α-Gal, e) α-GalN, f) α-GalNAc. Overall, α-Glc, α-GlcN, α-GlcNAc, α-Gal, α-GalN and α-GalNAc spends 7.6, 10.9, 0.1, 0.1, 4.1 and 0.2% of the time, respectively, in a conformation other than chair.

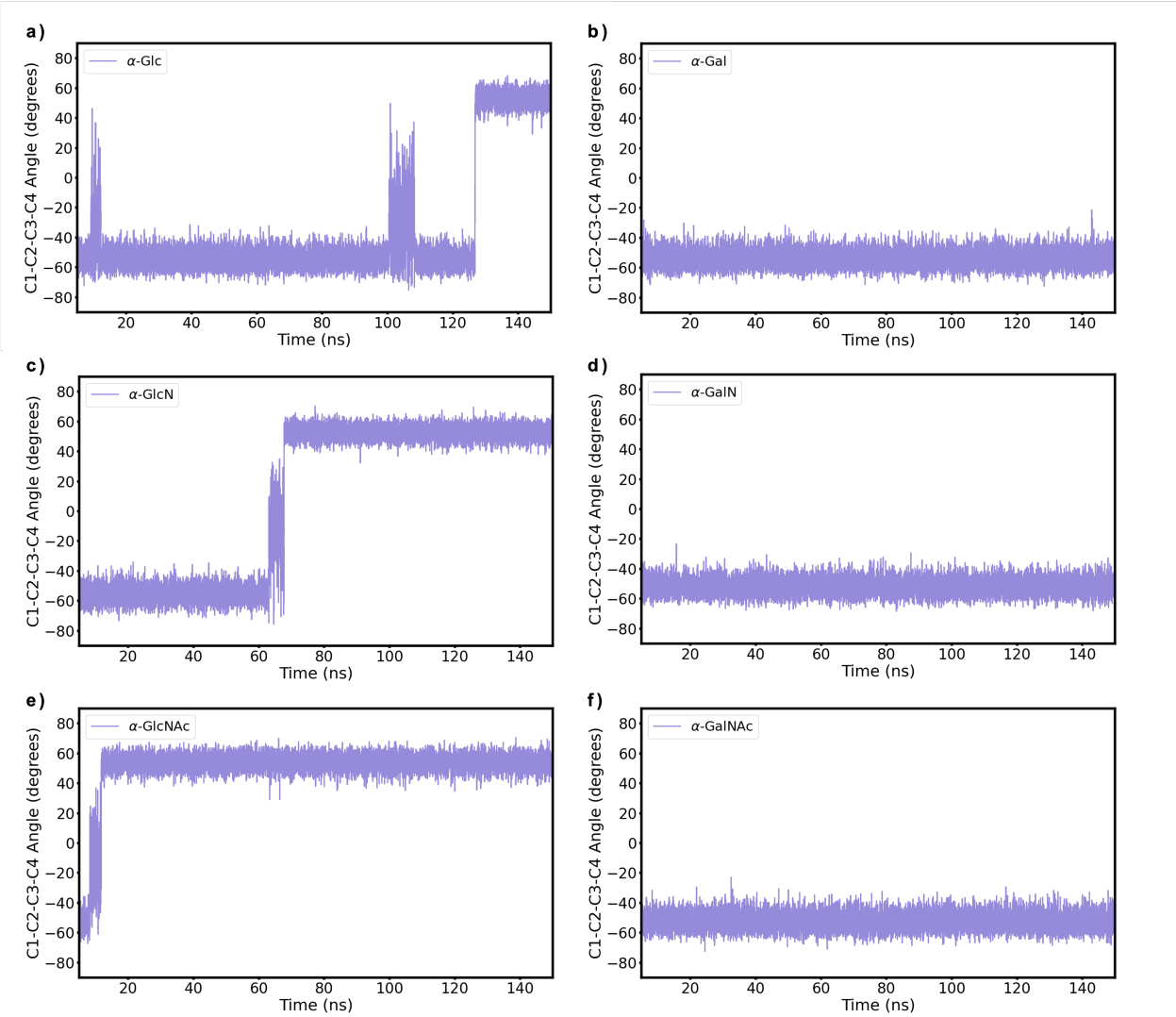

Figure S7: Time evolution of the torsion angle $C_1-C_2-C_3-C_4$ in $\alpha-$ anomers during 145 ns production MD with AMOEBA (mutual polarization, α parameters, no energy minimization prior to MD). $C_1-C_2-C_3-C_4$ is -55° when in chair conformation. a) α-Glc, b) α-GlcN, c) α-GlcNAc, d) α-Gal, e) α-GalN, f) α-GalNAc. Overall, α-Glc, α-GlcN, α-GlcNAc, α-Gal, α-GalN and α-GalNAc spends 4.9, 2.7, 2.4, 0.1, 0.2 and 0.2% of the time, respectively, in a conformation other than chair.

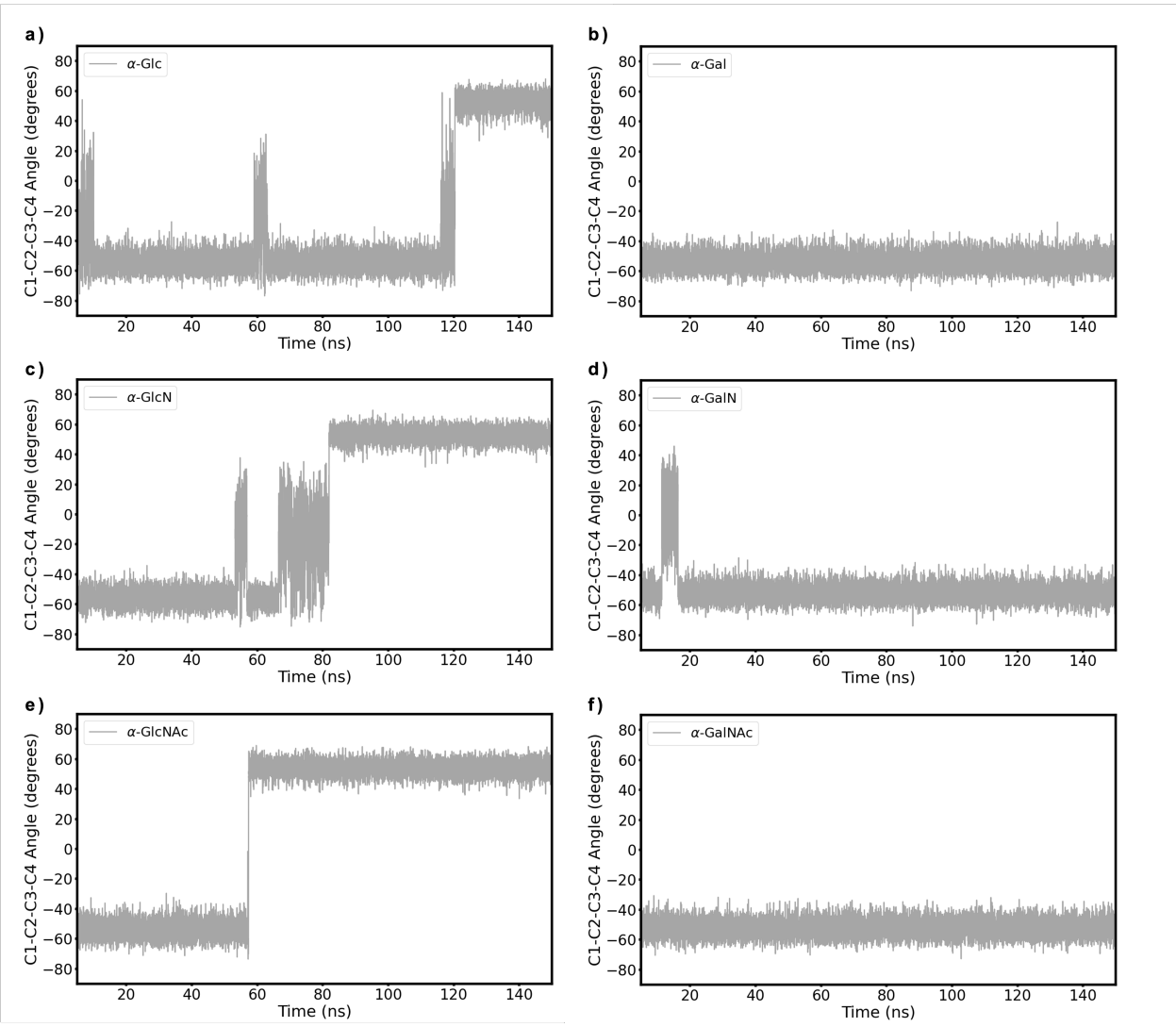

Figure S8: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\alpha-$ anomers during 145 ns production MD with AMOEBA (mutual polarization, β parameters). $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) α-Glc, b) α-GlcN, c) α-GlcNAc, d) α-Gal, e) α-GalN, f) α-GalNAc. Overall, α-Glc, α-GlcN, α-GlcNAc, α-Gal, α-GalN and α-GalNAc spends 7.6, 10.9, 0.1, 0.1, 4.1 and 0.2% of the time, respectively, in a conformation other than chair.

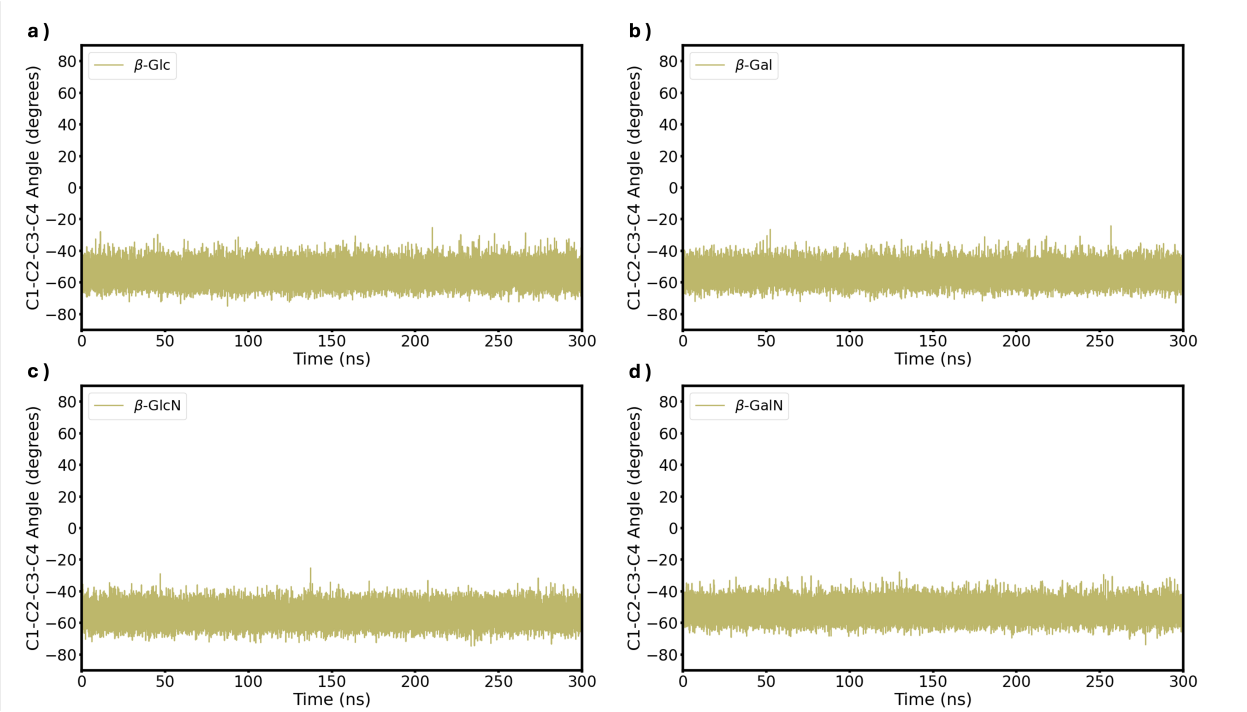

Figure S9: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\beta-$Glc, GlcN, Gal, and GalN during 300 ns (extension of the previous 145 ns presented in Figure S4), first replicate. $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) β-Glc, b) β-GlcN, c) β-GlcNAc, d) β-Gal.

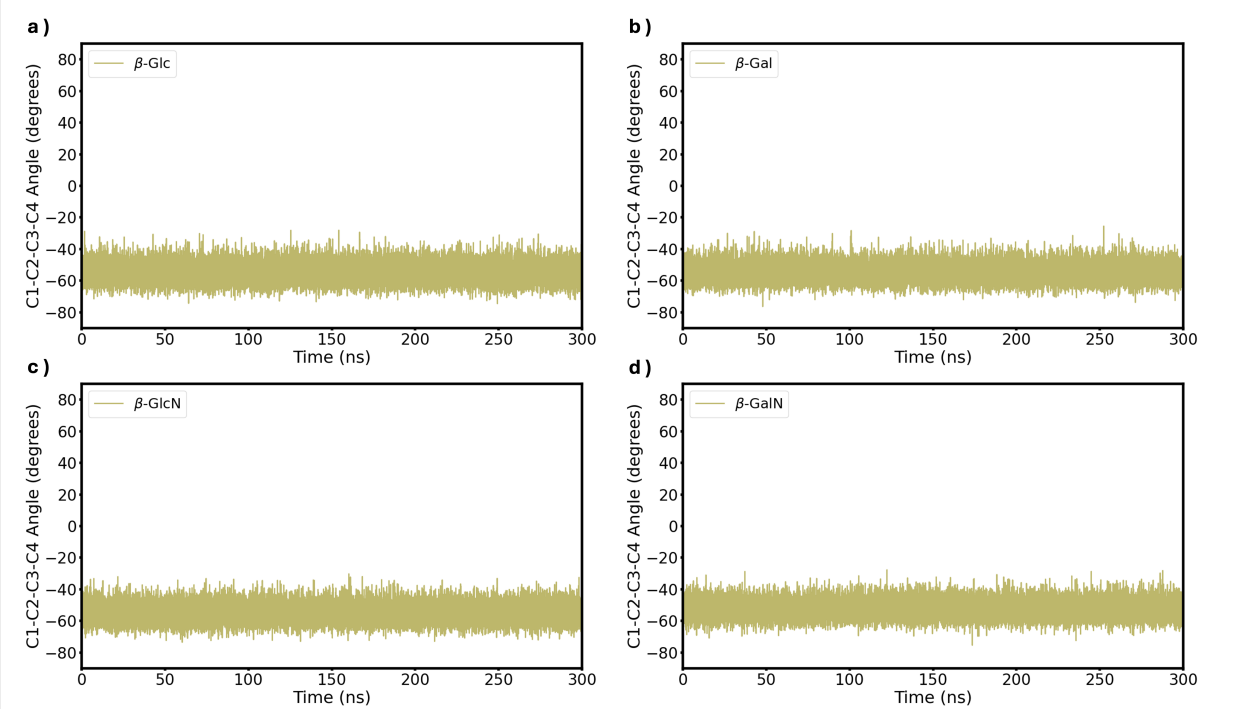

Figure S10: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\beta-$Glc, GlcN, Gal, and GalN during 300 ns, second replicate. $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) β-Glc, b) β-GlcN, c) β-GlcNAc, d) β-Gal.

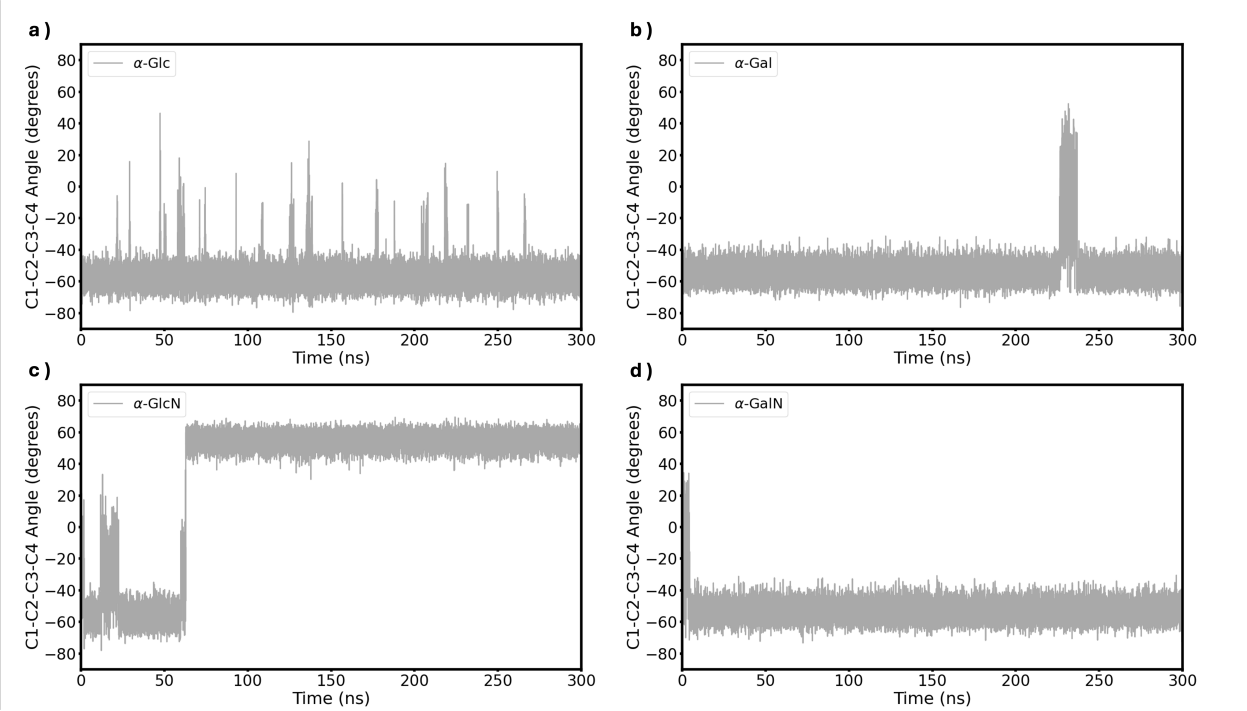

Figure S11: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\alpha-$Glc, GlcN, Gal, and GalN during 300 ns (extension of the previous 145 ns presented in Figure S5), first replicate. $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) α-Glc, b) α-GlcN, c) α-GlcNAc, d) α-Gal. Overall, α-Glc, α-GlcN, α-Gal, and α-GalN spends 2.3, 3.7, 3.1, 1.3% of the time, respectively, in a conformation other than chair.

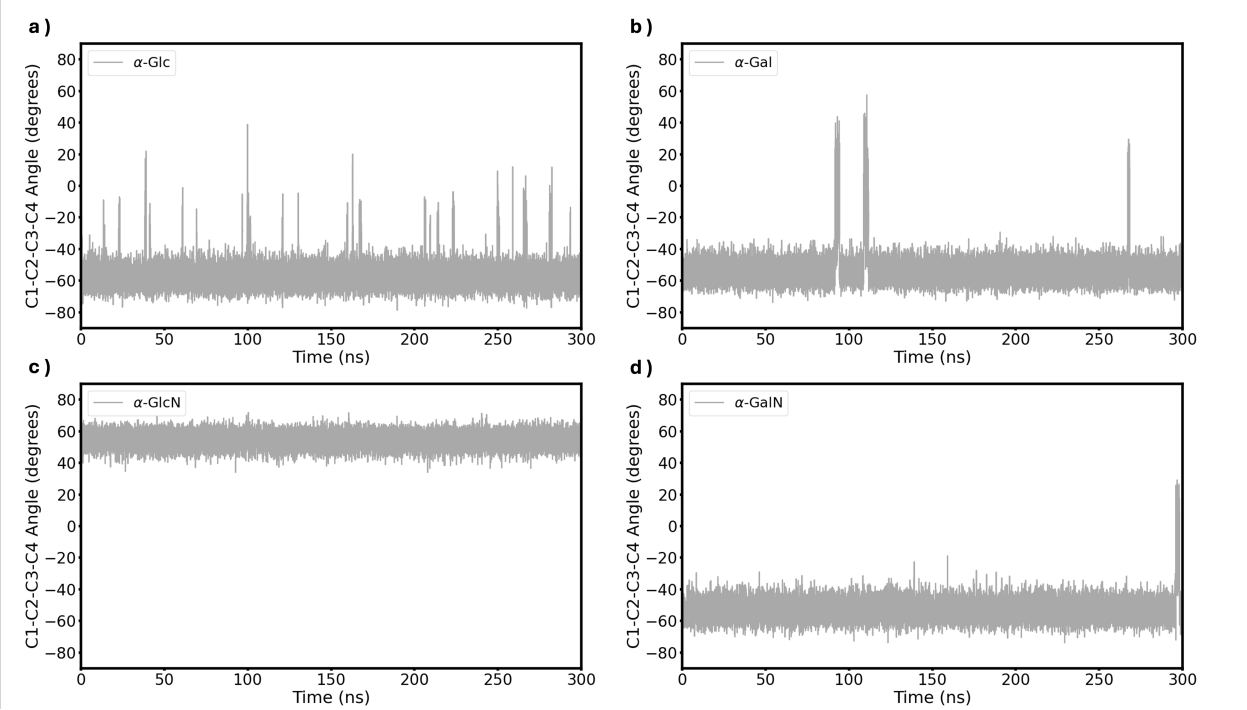

Figure S12: Time evolution of the torsion angle $C_1 - C_2 - C_3 - C_4$ in $\alpha-$Glc, GlcN, Gal, and GalN during 300 ns, second replicate. $C_1 - C_2 - C_3 - C_4$ is -55° when in chair conformation. a) α-Glc, b) α-GlcN, c) α-GlcNAc, d) α-Gal. Overall, α-Glc, α-GlcN, α-Gal, and α-GalN spends 1.7, 0.01, 2.0, 0.8% of the time, respectively, in a conformation other than chair.