S1: Rank conformer populations (%) and free energies (G, kcal mol^{-1}) in each 10 μs simulation: TIP3P

α-L-idose			β-L-idose		
Pucker	**%**	***G***	**Pucker**	**%**	***G***
1C4	85.0768	0.10	**1C4**	99.5250	0.00
4C1	5.1057	1.76	**4C1**	0.2935	3.46
B14	3.6629	1.96	**5S1**	0.0951	4.13
5S1	1.8638	2.36	**B14**	0.0216	5.01
3S1	1.6036	2.45	**25B**	0.0136	5.28
2SO	1.0151	2.72	**14B**	0.0116	5.37
1S3	0.5348	3.10	**2SO**	0.0101	5.46
14B	0.4002	3.27	**1S5**	0.0053	5.84
B3O	0.3350	3.38	**3S1**	0.0046	5.92
25B	0.1395	3.90	**1S3**	0.0036	6.07
1S5	0.0992	4.10	**2H1**	0.0036	6.07
E2	0.0276	4.86	**B3O**	0.0024	6.31
1HO	0.0231	4.97	**5HO**	0.0018	6.48
1E	0.0226	4.98	**2E**	0.0013	6.67
3H2	0.0202	5.04	**5E**	0.0009	6.89
1H2	0.0181	5.11	**5H4**	0.0009	6.89
3OB	0.0129	5.31	**3E**	0.0008	6.96
2H1	0.0084	5.57	**1HO**	0.0007	7.04
EO	0.0062	5.75	**3H2**	0.0007	7.04
4H3	0.0044	5.95	**E4**	0.0006	7.13
3E	0.0042	5.98	**3H4**	0.0006	7.13
E1	0.0034	6.10	**EO**	0.0006	7.13
2E	0.0027	6.24	**E1**	0.0003	7.54
OS2	0.0016	6.55	**2H3**	0.0003	7.54
E3	0.0013	6.67	**1H2**	0.0003	7.54
2H3	0.0013	6.67	**1E**	0.0001	8.19
3H4	0.0011	6.77	**E2**	0.0001	8.19
4E	0.0010	6.83	**OS2**	0.0000	-
5HO	0.0007	7.04	**B25**	0.0000	-
OH5	0.0005	7.24	**3OB**	0.0000	-
E5	0.0004	7.37	**OH5**	0.0000	-
OH1	0.0004	7.37	**E5**	0.0000	-
5H4	0.0004	7.37	**4H5**	0.0000	-
E4	0.0004	7.37	**4E**	0.0000	-
4H5	0.0002	7.78	**4H3**	0.0000	-
B25	0.0001	8.19	**OE**	0.0000	-
OE	0.0001	8.19	**E3**	0.0000	-
5E	0.0001	8.19	**OH1**	0.0000	-

S2: Rank conformer populations (%) and free energies (G, kcal mol^{-1}) in each 10 μs simulation: TIP4P

α-L-idose			β-L-idose		
Pucker	**%**	***G***	**Pucker**	**%**	***G***
1C4	83.8761	0.10	**1C4**	99.3885	0.00
4C1	7.4671	1.54	**4C1**	0.4079	3.26
B14	2.7886	2.12	**5S1**	0.0874	4.18
5S1	1.8636	2.36	**25B**	0.0215	5.01
3S1	1.2563	2.60	**B14**	0.0203	5.04
2SO	1.1235	2.66	**2SO**	0.0191	5.08
1S3	0.5407	3.10	**14B**	0.0187	5.09
B3O	0.3525	3.35	**1S3**	0.0085	5.56
14B	0.3413	3.37	**B3O**	0.0057	5.80
25B	0.1729	3.77	**3S1**	0.0048	5.90
1S5	0.0692	4.31	**1S5**	0.0041	5.99
E2	0.0216	5.01	**2H1**	0.0032	6.14
1HO	0.0211	5.02	**3H2**	0.0014	6.63
3H2	0.0193	5.07	**3E**	0.0013	6.67
1E	0.0191	5.08	**5HO**	0.0009	6.89
1H2	0.0136	5.28	**5E**	0.0008	6.96
3OB	0.0115	5.38	**3H4**	0.0008	6.96
2H1	0.0082	5.58	**2E**	0.0007	7.04
EO	0.0051	5.86	**E4**	0.0007	7.04
4H3	0.0044	5.95	**EO**	0.0007	7.04
3E	0.0036	6.07	**1HO**	0.0007	7.04
2H3	0.0034	6.10	**E1**	0.0005	7.24
E1	0.0033	6.12	**5H4**	0.0005	7.24
E3	0.0032	6.14	**E2**	0.0005	7.24
2E	0.0032	6.14	**2H3**	0.0004	7.37
OS2	0.0013	6.67	**E3**	0.0002	7.78
4E	0.0013	6.67	**1H2**	0.0001	8.19
E5	0.0011	6.77	**1E**	0.0001	8.19
5HO	0.0009	6.89	**OS2**	0.0000	-
3H4	0.0006	7.13	**B25**	0.0000	-
4H5	0.0005	7.24	**3OB**	0.0000	-
5H4	0.0005	7.24	**OH5**	0.0000	-
E4	0.0005	7.24	**E5**	0.0000	-
OH5	0.0003	7.54	**4H5**	0.0000	-
OE	0.0002	7.78	**4E**	0.0000	-
OH1	0.0002	7.78	**4H3**	0.0000	-
B25	0.0001	8.19	**OE**	0.0000	-
5E	0.0001	8.19	**OH1**	0.0000	-

S3: Rank conformer populations (%) and free energies (G, kcal mol^{-1}) in each 10 μs simulation: TIP4P-EW

α-L-idose			β-L-idose		
Pucker	**%**	***G***	**Pucker**	**%**	***G***
1C4	83.5423	0.11	**1C4**	99.7812	0.00
4C1	7.7207	1.52	**4C1**	0.1318	3.93
B14	2.9498	2.09	**5S1**	0.0353	4.71
5S1	1.8320	2.37	**25B**	0.0085	5.56
3S1	1.3716	2.54	**2SO**	0.0076	5.62
2SO	1.0413	2.71	**14B**	0.0071	5.66
1S3	0.5036	3.14	**B14**	0.0066	5.71
14B	0.3321	3.38	**1S3**	0.0039	6.02
B3O	0.3209	3.40	**1S5**	0.0029	6.20
25B	0.1578	3.83	**B3O**	0.0027	6.24
1S5	0.0749	4.27	**3S1**	0.0025	6.28
1HO	0.0236	4.95	**5HO**	0.0017	6.51
E2	0.0217	5.00	**2H1**	0.0015	6.59
1E	0.0187	5.09	**3E**	0.0011	6.77
3H2	0.0184	5.10	**5E**	0.0008	6.96
3OB	0.0136	5.28	**5H4**	0.0008	6.96
1H2	0.0127	5.32	**3H2**	0.0007	7.04
2H1	0.0075	5.63	**2E**	0.0006	7.13
EO	0.0052	5.85	**E4**	0.0006	7.13
4H3	0.0047	5.91	**EO**	0.0005	7.24
E1	0.0042	5.98	**E2**	0.0005	7.24
2E	0.0041	5.99	**3H4**	0.0004	7.37
2H3	0.0039	6.02	**3OB**	0.0002	7.78
3E	0.0033	6.12	**1HO**	0.0002	7.78
E3	0.0031	6.16	**E1**	0.0001	8.19
4E	0.0018	6.48	**1H2**	0.0001	8.19
OS2	0.0015	6.59	**1E**	0.0001	8.19
4H5	0.0011	6.77	**OS2**	0.0000	-
E5	0.0006	7.13	**B25**	0.0000	-
OH5	0.0005	7.24	**OH5**	0.0000	-
5HO	0.0005	7.24	**E5**	0.0000	-
E4	0.0005	7.24	**4H5**	0.0000	-
3H4	0.0005	7.24	**4E**	0.0000	-
OE	0.0003	7.54	**4H3**	0.0000	-
OH1	0.0003	7.54	**OE**	0.0000	-
5H4	0.0003	7.54	**E3**	0.0000	-
B25	0.0002	7.78	**OH1**	0.0000	-
5E	0.0002	7.78	**2H3**	0.0000	-

S4: Rank conformer populations (%) and free energies (G, kcal mol^{-1}) in each 10 μs simulation: GAS-PHASE

α-L-idose			β-L-idose		
Pucker	**%**	***G***	**Pucker**	**%**	***G***
1C4	92.3800	0.05	**1C4**	98.6260	0.01
4C1	5.7121	1.70	**4C1**	1.2204	2.61
B3O	0.5734	3.06	**5S1**	0.0406	4.63
1S3	0.3761	3.31	**1S3**	0.0227	4.98
2SO	0.3418	3.37	**5HO**	0.0112	5.39
5S1	0.2542	3.54	**B14**	0.0111	5.40
B14	0.1289	3.95	**B3O**	0.0105	5.43
14B	0.0830	4.21	**14B**	0.0094	5.50
1HO	0.0190	5.08	**EO**	0.0074	5.64
3S1	0.0187	5.09	**2SO**	0.0072	5.66
1S5	0.0179	5.12	**2E**	0.0054	5.83
EO	0.0164	5.17	**5E**	0.0052	5.85
25B	0.0144	5.25	**1S5**	0.0045	5.94
1E	0.0116	5.37	**2H3**	0.0036	6.07
2H3	0.0095	5.49	**25B**	0.0030	6.18
2E	0.0086	5.55	**3S1**	0.0027	6.24
E3	0.0084	5.57	**2H1**	0.0024	6.31
2H1	0.0059	5.77	**E3**	0.0020	6.42
5HO	0.0051	5.86	**5H4**	0.0010	6.83
4H3	0.0048	5.90	**4H3**	0.0009	6.89
3OB	0.0028	6.22	**1HO**	0.0009	6.89
1H2	0.0021	6.39	**3H2**	0.0006	7.13
E2	0.0017	6.51	**3OB**	0.0003	7.54
E1	0.0010	6.83	**1H2**	0.0002	7.78
5E	0.0009	6.89	**OS2**	0.0001	8.19
3H2	0.0004	7.37	**B25**	0.0001	8.19
4E	0.0003	7.54	**4E**	0.0001	8.19
4H5	0.0002	7.78	**1E**	0.0001	8.19
OS2	0.0001	8.19	**E4**	0.0001	8.19
OH1	0.0001	8.19	**3H4**	0.0001	8.19
5H4	0.0001	8.19	**E1**	0.0000	-
3E	0.0001	8.19	**OH5**	0.0000	-
B25	0.0000	-	**E5**	0.0000	-
OH5	0.0000	-	**4H5**	0.0000	-
E5	0.0000	-	**OE**	0.0000	-
OE	0.0000	-	**OH1**	0.0000	-
E4	0.0000	-	**3E**	0.0000	-
3H4	0.0000	-	**E2**	0.0000	-

S5: Averages and standard deviations of computed Cremer-Pople parameters (chair-puckers)

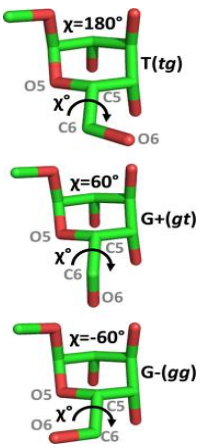
		TIP3P		TIP4P		TIP4P-EW	
		AVE	STDEV	AVE	STDEV	AVE	STDEV
ϑ°	α-$^1C_4$	168.6	5.9	168.8	5.8	168.7	5.8
ϑ°	β-$^1C_4$	170.8	4.9	170.5	4.9	170.5	5.0
ϑ°	α-$^4C_1$	11.4	6.2	11.5	6.3	11.5	6.3
ϑ°	β-$^4C_1$	14.5	7.4	14.2	7.0	14.2	7.4
φ°	α-$^1C_4$	134.4	70.6	137.7	70.2	137.7	70.2
φ°	β-$^1C_4$	195.7	80.1	193.8	76.6	193.9	76.5
φ°	α-$^4C_1$	160.4	103.7	156.8	100.0	156.2	101.1
φ°	β-$^4C_1$	150.5	56.2	151.2	54.4	150.7	56.2
Q	α-$^1C_4$	0.53	0.04	0.53	0.04	0.53	0.04
Q	β-$^1C_4$	0.57	0.04	0.57	0.04	0.57	0.04
Q	α-$^4C_1$	0.54	0.04	0.54	0.05	0.54	0.04
Q	β-$^4C_1$	0.53	0.04	0.53	0.04	0.53	0.04

S6: Hydroxymethyl rotamer state populations (%), calculated and experimental (EXPT)

Isomer	Model	Anomer	T (*tg*)	G+ (*gt*)	G- (*gg*)	
L	TIP3P	α	17	14	69	
L	TIP3P	β	18	8	75	
L	TIP4P	α	16	23	61	
L	TIP4P	β	17	18	65	
L	TIP4P-EW	α	16	23	61	
L	TIP4P-EW	β	17	18	65	
D	EXPT	α	24	76	0	*
D	EXPT	β	29	67	4	*

**gt* and *gg* definitions are reversed in the L-/D-isomers
Estimated experimental error was ±5%
Average populations were calculated from ten 1 μs subsets, standard deviations were all <= 1%

3D-definitions of hydroxymethyl conformations (α-L-idopyranoside):



S7: Expected pyroanse ring vicinal couplings in canonical chair puckers of α- and β-L-idose

α	$^1C_4$	$^4C_1$
$J_{1,2}$	*g*	*t*
$J_{2,3}$	*g*	*t*
$J_{3,4}$	*g*	*t*
$J_{4,5}$	*g*	*g*

β	$^1C_4$	$^4C_1$
$J_{1,2}$	*g*	*g*
$J_{2,3}$	*g*	*t*
$J_{3,4}$	*g*	*t*
$J_{4,5}$	*g*	*g*

g=gauche

t=trans

S8: Two-site models

			α-idose		β-idose	
Model	**Isomer**	**Karplus**	$^4C_1$	$^1C_4$	$^4C_1$	$^1C_4$
Simulation	L	n/a	5	85	0	100
Rigid	L	Ref. 24	61	39	26	74
Flexible	L	Ref. 24	65	35	24	76

Rigid models:
used "ideal" chairs, ring torsions set to ±60°, all other atoms relaxed using MM

Flexible model:
used all $^4C_1$ (θ<30) or $^1C_4$ (θ>150) chairs from the TIP3P simulations

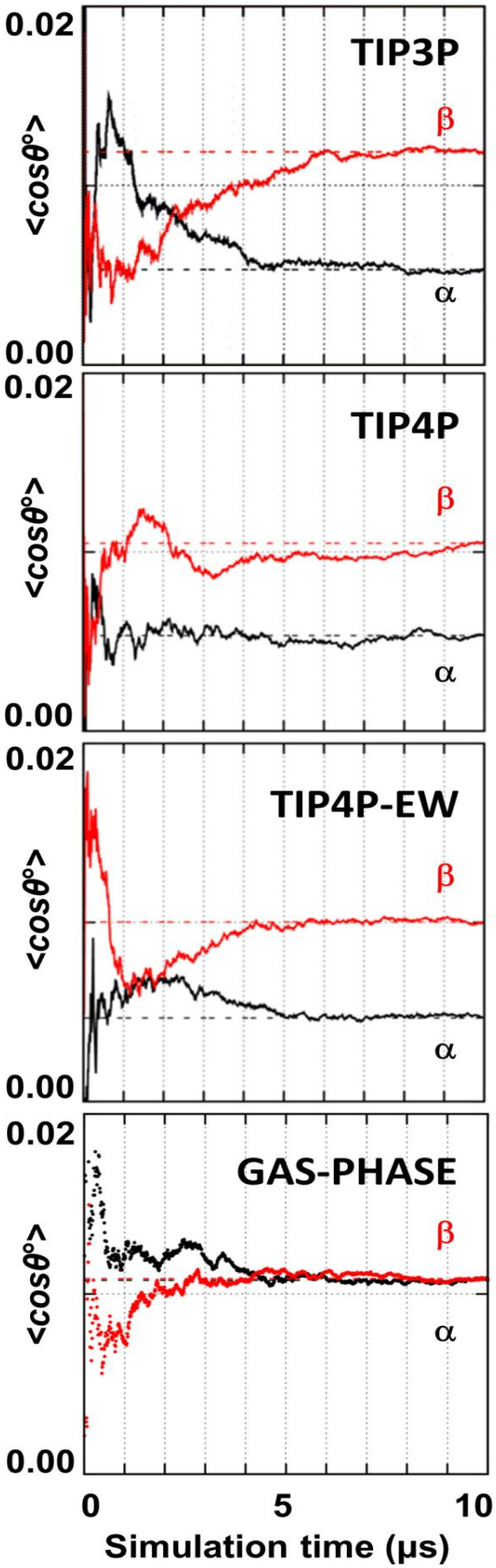
S9: Chemical shifts for synthesized D isomers of compounds 1 and 2

750 MHz	^{1}H chemical shift (ppm)							
Anomer	**H1**	**H2**	**H3**	**H4**	**H5**	**H6**	**H6'**	**OCH_3**
α	4.69	3.53	3.73	3.75	4.09	3.82	3.79	3.45
β	4.74	3.69	3.98	3.66	3.99	3.84	3.79	3.54

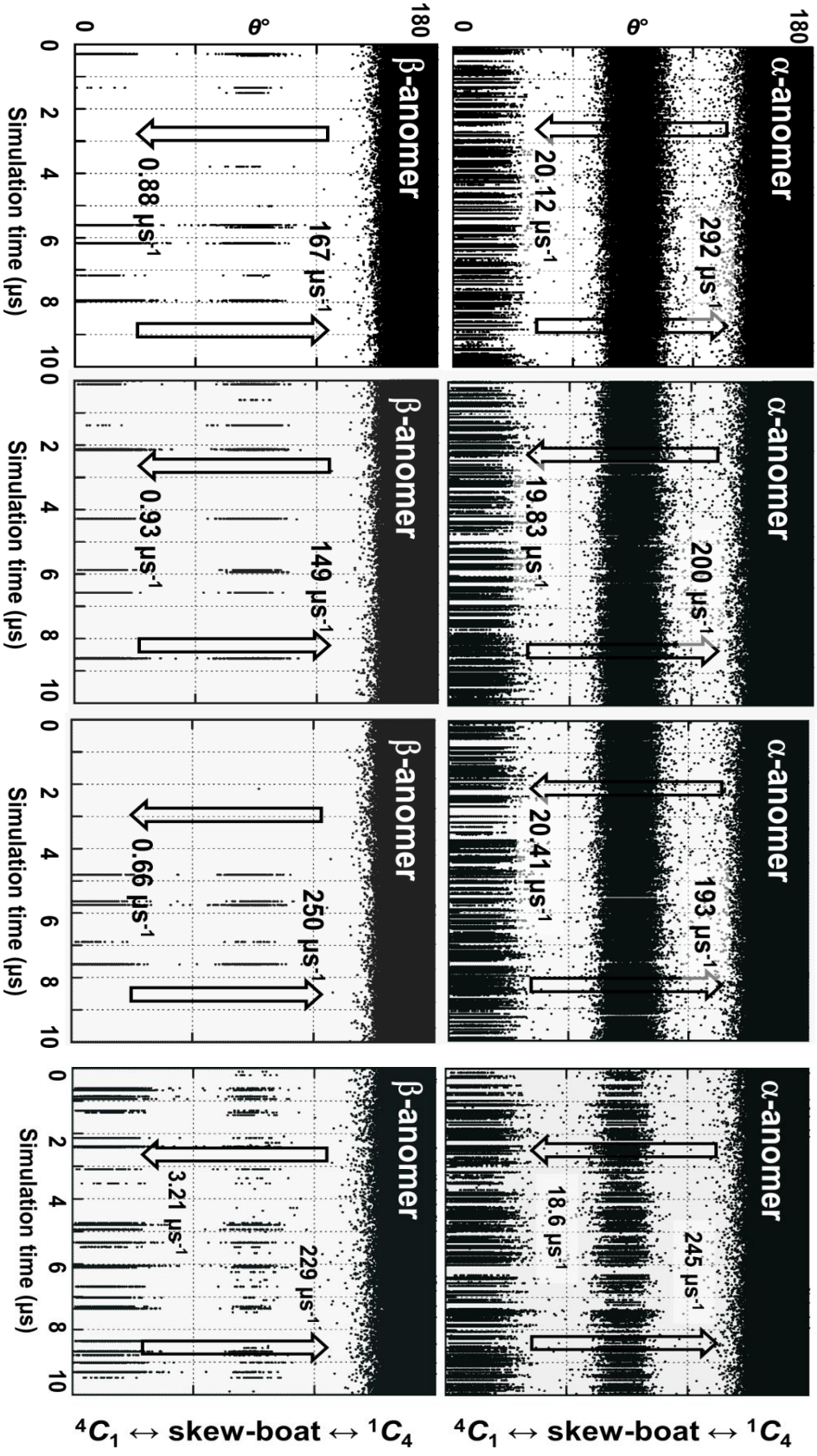
150 MHz	^{13}C chemical shift (ppm)						
Anomer	**C1**	**C2**	**C3**	**C4**	**C5**	**C6**	**OCH_3**
α	102.66	71.96	72.74	71.37	72.37	61.31	57.16
β	101.63	70.88	71.09	69.91	76.72	62.68	58.15

The estimated error in ^{1}H chemical shift values is ± 0.002 ppm

S10: Convergence of pucker in α- and β-L-idose during each 10 μs simulation

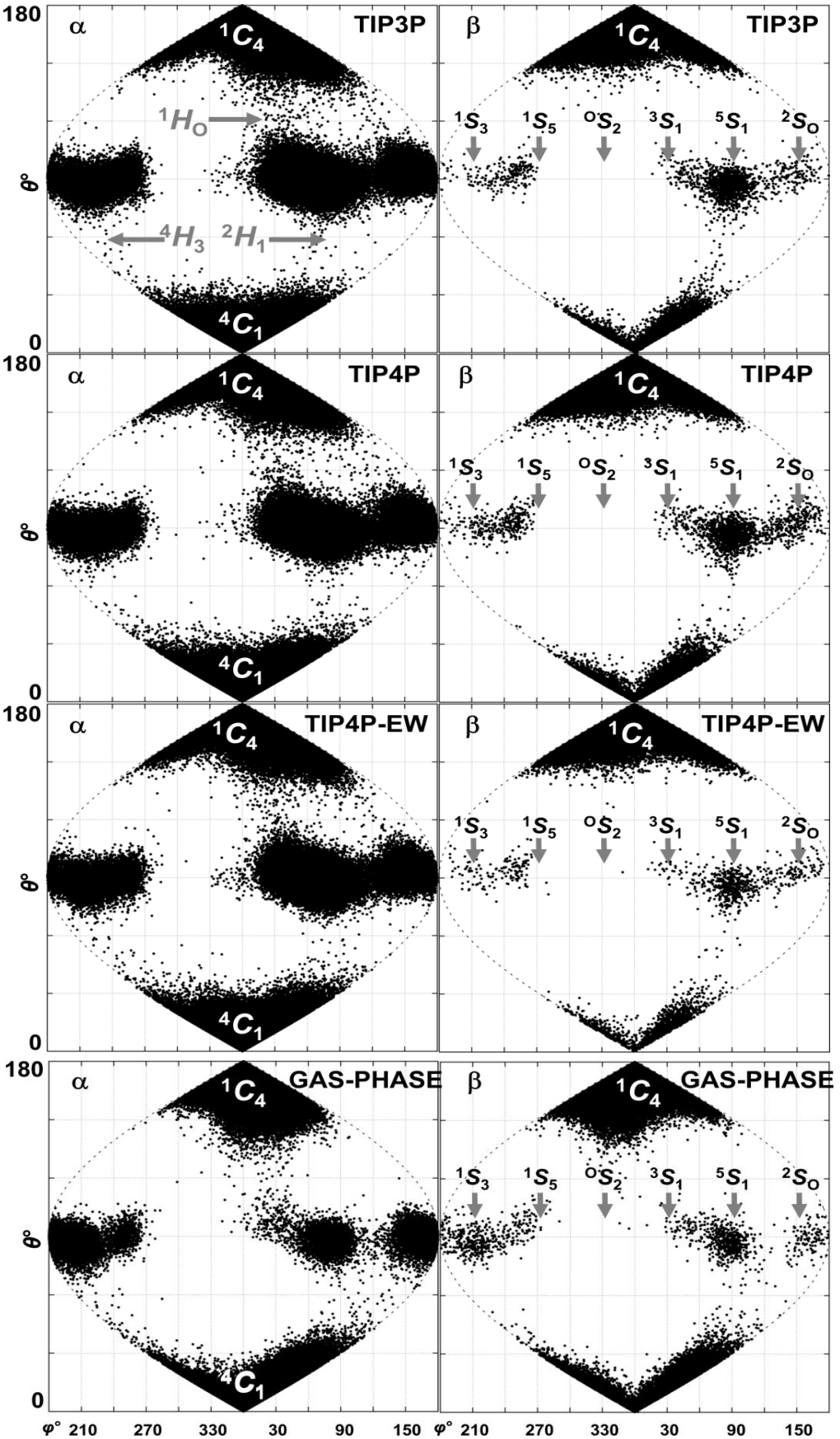


S11: Time series of the Cremer-Pople parameter ϑ in each 10μs simulation

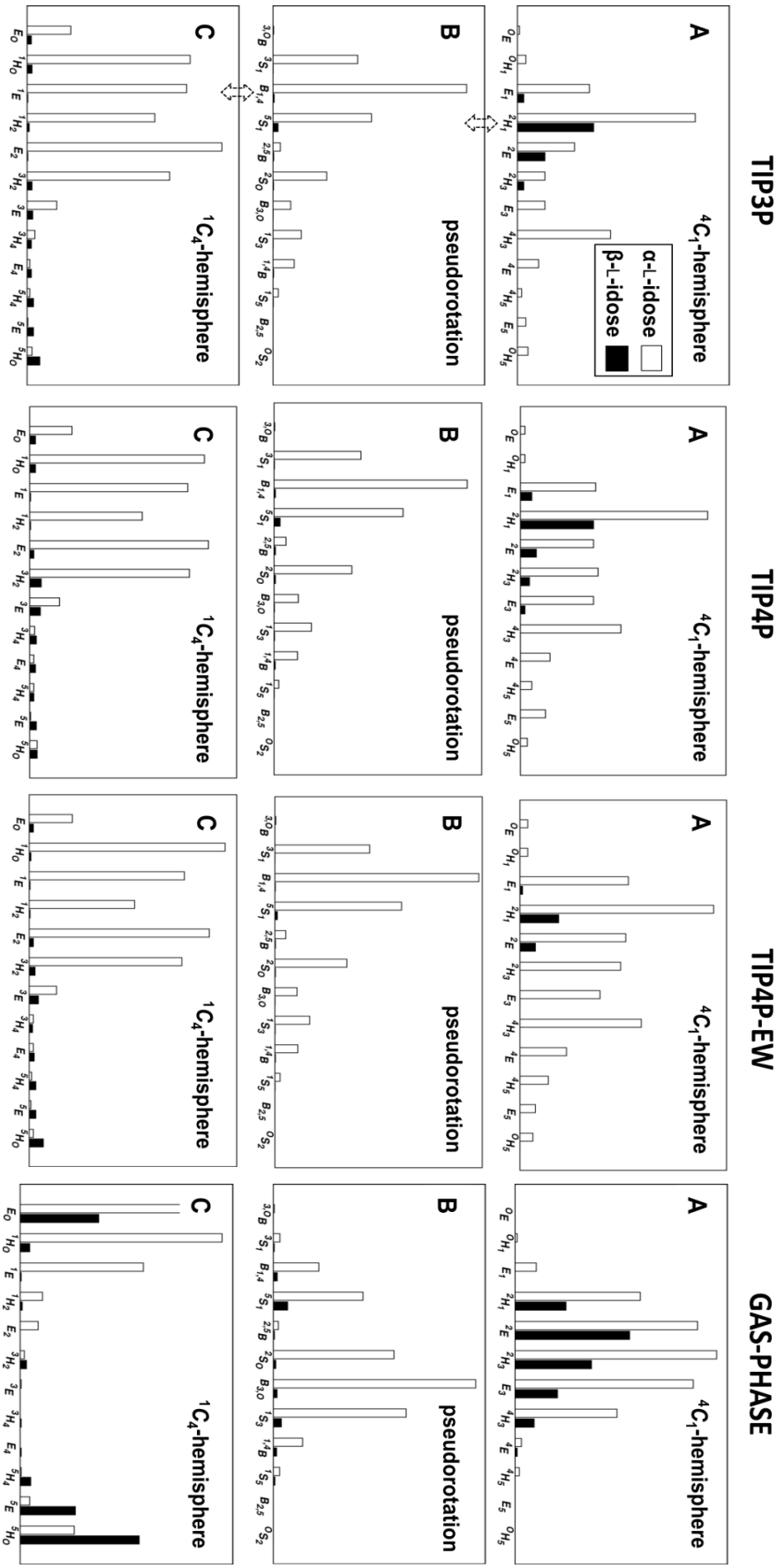


Computed forward ($^1C_4 \rightarrow {}^4C_1$) and backward ($^4C_1 \rightarrow {}^1C_4$) puckering rates are illustrated

S12: Sinusoidal projections of Cremer-Pople spherical phase-space for each 10 μs simulation



S13: Relative occupancy of puckers (arbitrary units) in each 10 μs simulation



S14: Classification of the 36 cannonical non-chair puckers in terms of ϑ and φ angles

4C1	-1	<	ϑ°	<	36	&	-16	<	φ°	<	345
OE	36	<	ϑ°	<	72	&	-16	<	φ°	<	15
OH1	36	<	ϑ°	<	72	&	15	<	φ°	<	45
E1	36	<	ϑ°	<	72	&	45	<	φ°	<	75
2H1	36	<	ϑ°	<	72	&	75	<	φ°	<	105
2E	36	<	ϑ°	<	72	&	105	<	φ°	<	135
2H3	36	<	ϑ°	<	72	&	135	<	φ°	<	165
E3	36	<	ϑ°	<	72	&	165	<	φ°	<	195
4H3	36	<	ϑ°	<	72	&	195	<	φ°	<	225
4E	36	<	ϑ°	<	72	&	225	<	φ°	<	255
4H5	36	<	ϑ°	<	72	&	255	<	φ°	<	285
E5	36	<	ϑ°	<	72	&	285	<	φ°	<	315
OH5	36	<	ϑ°	<	72	&	315	<	φ°	<	345
3OB	72	<	ϑ°	<	108	&	-16	<	φ°	<	15
3S1	72	<	ϑ°	<	108	&	15	<	φ°	<	45
B14	72	<	ϑ°	<	108	&	45	<	φ°	<	75
5S1	72	<	ϑ°	<	108	&	75	<	φ°	<	105
25B	72	<	ϑ°	<	108	&	105	<	φ°	<	135
2SO	72	<	ϑ°	<	108	&	135	<	φ°	<	165
B3O	72	<	ϑ°	<	108	&	165	<	φ°	<	195
1S3	72	<	ϑ°	<	108	&	195	<	φ°	<	225
14B	72	<	ϑ°	<	108	&	225	<	φ°	<	255
1S5	72	<	ϑ°	<	108	&	255	<	φ°	<	285
B25	72	<	ϑ°	<	108	&	285	<	φ°	<	315
OS2	72	<	ϑ°	<	108	&	315	<	φ°	<	345
EO	108	<	ϑ°	<	144	&	-16	<	φ°	<	15
1HO	108	<	ϑ°	<	144	&	15	<	φ°	<	45
1E	108	<	ϑ°	<	144	&	45	<	φ°	<	75
1H2	108	<	ϑ°	<	144	&	75	<	φ°	<	105
E2	108	<	ϑ°	<	144	&	105	<	φ°	<	135
3H2	108	<	ϑ°	<	144	&	135	<	φ°	<	165
3E	108	<	ϑ°	<	144	&	165	<	φ°	<	195
3H4	108	<	ϑ°	<	144	&	195	<	φ°	<	225
E4	108	<	ϑ°	<	144	&	225	<	φ°	<	255
5H4	108	<	ϑ°	<	144	&	255	<	φ°	<	285
5E	108	<	ϑ°	<	144	&	285	<	φ°	<	315
5HO	108	<	ϑ°	<	144	&	315	<	φ°	<	345
1C4	144	<	ϑ°	<	180	&	-16	<	φ°	<	345

S15: Vicinal coupling calculations

Paramaters used (for α- and β-anomers) in the Karplus equation (Ref. 24)

	Δχ1	Δχ2	Δχ3	Δχ4	P1	P2	P3	P4	P5	P6
$^3J_{1-2}$	1.30	1.30	1.30	0.40	13.24	-0.91	0.00	0.53	-2.41	0.27
$^3J_{2-3}$	0.40	1.30	0.40	1.30	13.24	-0.91	0.00	0.53	-2.41	0.27
$^3J_{3-4}$	1.30	0.40	1.30	0.40	13.24	-0.91	0.00	0.53	-2.41	0.27
$^3J_{4-5}$	0.40	1.30	0.40	1.30	13.24	-0.91	0.00	0.53	-2.41	0.27

$^3J_{HH} = P_1 \cos^2\vartheta + P_2 \cos\vartheta + P_3 + \Sigma\Delta\chi_i [P_4 + P_5 \cos^2(\zeta_i \vartheta + P6 |\Delta\chi_i|)]$

ζ_i is +1 or -1 depending on the substituent orientation (see ref. 24 for details)

Pyranose ring vicinal 1H-1H dihedrals

averages (θ°) and standard deviations (±) from the 10 μs simulations

TIP3P

	α		β	
Torsion	**θ°**	**±**	**θ°**	**±**
H1-H2	77	51	-54	11
H2-H3	-80	37	-67	12
H3-H4	73	34	67	11
H4-H5	50	25	54	9

TIP4P

	α		β	
Torsion	**θ°**	**±**	**θ°**	**±**
H1-H2	64	69	-45	34
H2-H3	-68	62	-57	41
H3-H4	63	58	57	41
H4-H5	40	41	46	33

TIP4P-EW

	α		β	
Torsion	**θ°**	**±**	**θ°**	**±**
H1-H2	65	70	-46	33
H2-H3	-68	62	-57	40
H3-H4	64	58	57	40
H4-H5	40	41	46	33

S16: GLYCAM11 paramaters for residue 0iA (α-L-idopyranose)

0iA new atom type OA: endo-anomeric oxygen

1	DUMM	DU	M	0	-1	-2	0	0	0	0
2	DUMM	DU	M	1	0	-1	1.522	0	0	0
3	DUMM	DU	M	2	1	0	1.422	109.5	0	0
4	C1	CG	M	3	2	1	1.4	113.3	-60	0.4405
5	H1	H2	E	4	3	2	1.102	110.7	56.2	0
6	O5	OA	M	4	3	2	1.435	107.9	-66.3	-0.543
7	C5	CG	M	6	4	3	1.434	114.3	-59.5	0.283
8	H5	H1	E	7	6	4	1.105	109.1	60.8	0
9	C6	CG	3	7	6	4	1.517	106.7	177.2	0.264
10	H61	H1	E	9	7	6	1.092	108.3	65.1	0
11	H62	H1	E	9	7	6	1.093	108.8	177.1	0
12	O6	OH	S	9	7	6	1.413	112.7	-56.7	-0.678
13	H6O	HO	E	12	9	7	0.955	108.1	-96	0.4205
14	C4	CG	M	7	6	4	1.519	110.8	-59	0.2625
15	H4	H1	E	14	7	6	1.1	107.7	173.8	0
16	O4	OH	S	14	7	6	1.43	110	-66.6	-0.702
17	H4O	HO	E	16	14	7	0.958	109.2	6.1	0.432
18	C3	CG	M	14	7	6	1.529	110.3	54.4	0.2935
19	H3	H1	E	18	14	7	1.101	109.2	-173.5	0
20	O3	OH	S	18	14	7	1.421	106.9	67.3	-0.733
21	H3O	HO	E	20	18	14	0.976	108.5	-168.6	0.439
22	C2	CG	B	18	14	7	1.524	111.6	-53.4	0.308
23	H2	H1	E	22	18	14	1.105	110.2	172.2	0
24	O2	OH	S	22	18	14	1.415	110.8	-65.2	-0.734
25	H2O	HO	E	24	22	18	0.957	110	-44.9	0.439

S17: GLYCAM11 paramaters for residue 0iB (β-L-idopyranose)

0iB new atom type OA: endo-anomeric oxygen

1	DUMM	DU	M	0	-1	-2	0	0	0	0
2	DUMM	DU	M	1	0	-1	1.522	0	0	0
3	DUMM	DU	M	2	1	0	1.422	109.5	0	0
4	C1	CG	M	3	2	1	1.4	113.3	180	0.469
5	H1	H2	E	4	3	2	1.102	110	-60.7	0
6	C2	CG	M	4	3	2	1.529	109.7	180	0.221
7	H2	H1	E	6	4	3	1.105	108.8	66	0
8	O2	OH	S	6	4	3	1.415	110	-59.2	-0.689
9	H2O	HO	E	8	6	4	0.957	110	-89.3	0.436
10	C3	CG	M	6	4	3	1.519	110.1	-173.1	0.3255
11	H3	H1	E	10	6	4	1.101	109.1	173.3	0
12	O3	OH	S	10	6	4	1.421	109.9	-65.8	-0.737
13	H3O	HO	E	12	10	6	0.976	108.5	-172.4	0.4375
14	C4	CG	M	10	6	4	1.528	110.8	53.3	0.238
15	H4	H1	E	14	10	6	1.1	108.7	-173.1	0
16	O4	OH	S	14	10	6	1.43	110.6	66.4	-0.707
17	H4O	HO	E	16	14	10	0.958	109.2	60	0.432
18	C5	CG	M	14	10	6	1.435	110	-52.7	0.3165
19	H5	H1	E	18	14	10	1.105	109.6	-66.3	0
20	O5	OA	E	18	14	10	1.412	112	54.9	-0.556
21	C6	CG	3	18	14	10	1.517	111.3	174.2	0.262
22	H61	H1	E	21	18	14	1.092	108.9	-63.1	0
23	H62	H1	E	21	18	14	1.093	108.3	55.9	0
24	O6	OH	S	21	18	14	1.413	112.7	172.7	-0.6755
25	H6O	HO	E	24	21	18	0.955	108.1	58.1	0.421

S18: GLYCAM11 torsional paramaters for new atom type OA

Key:

DIV	factor by which torsion is divided
BH/2	barrier height divided by a factor of 2
PH	phase shift angle in the torsional function (°)
PN	torsional barrier periodicity
	if PN is negative (identifies the next term) the absolute vaule is used

Torsion	**DIV**	**BH/2**	**PH**	**PN**
H2-CG-OA-CG	1	-1.20	0	1
	1	0.10	0	2
	1	0.02	0	3
CG-CG-OA-CG	1	-0.70	0	1
	1	-0.30	0	2
	1	-0.33	0	3
OE-CG-OA-CG	1	-0.25	0	1
	1	-0.76	0	2
	1	1.20		3
OA-CG-CG-CG	1	0.19	0	1
	1	-0.11	0	2
	1	0.14	0	3

S19: Reaction scheme for synthesis of (1) and (2)