Table S1. Partial atomic charges (in e.u.) for monosaccharides

Atom name	α-D-gal	β-D-gal	α-D-glc	β-D-glc	α-D-man	β-D-man	α-fuc	β-fuc	α-nag	β-nag	α-nga	β-nga	α-L-xyl	β-L-xyl	α-gcu	β-gcu
C1	0.066	0.017	0.083	0.135	-0.036	0.145	0.180	-0.047	0.058	0.129	0.019	-0.050	0.103	0.123	-0.080	-0.128
H1	0.157	0.146	0.157	0.101	0.217	0.073	0.130	0.175	0.184	0.099	0.162	0.162	0.147	0.100	0.173	0.171
C_2	0.115	0.084	0.077	0.055	0.058	0.002	0.144	0.229	-0.057	-0.034	0.003	-0.042	0.064	0.042	0.094	0.079
H_2	0.136	0.165	0.132	0.126	0.098	0.108	0.145	0.125	0.181	0.171	0.185	0.215	0.127	0.126	0.139	0.144
O_2	-0.562	-0.572	-0.563	-0.560	-0.549	-0.519	-0.632	-0.613	-	-	-	-	-0.552	-0.555	-0.575	-0.558
HO2	0.358	0.386	0.369	0.381	0.392	0.386	0.403	0.395	-	-	-	-	0.364	0.381	0.352	0.359
C3	0.102	0.079	0.127	0.100	0.162	0.127	0.090	0.097	0.182	0.125	0.113	0.094	0.107	0.063	0.124	0.036
H3	0.105	0.114	0.108	0.120	0.074	0.088	0.102	0.110	0.117	0.118	0.111	0.121	0.123	0.135	0.118	0.145
O3	-0.567	-0.563	-0.586	-0.560	-0.583	-0.549	-0.594	-0.628	-0.544	-0.551	-0.560	-0.583	-0.558	-0.559	-0.590	-0.562
HO3	0.385	0.386	0.390	0.378	0.378	0.365	0.378	0.404	0.356	0.362	0.366	0.380	0.369	0.376	0.365	0.357
C4	0.017	0.030	0.097	0.101	0.180	0.145	0.078	0.082	-0.002	0.101	0.019	0.058	0.062	0.152	0.052	0.034
H4	0.085	0.118	0.107	0.115	0.111	0.118		0.082	0.148	0.121	0.113	0.109	0.117	0.103	0.103	0.134
O4	-0.530	-0.589	-0.624	-0.632	-0.663	-0.627	-0.661	-0.600	-0.604	-0.627	-0.583	-0.593	-0.579	-0.602	-0.660	-0.606
C5	0.016	0.026	0.089	0.084	0.090	0.021	-0.050	0.150	0.105	0.021	0.037	0.017	0.002	-0.056	0.122	0.055
H5(1)	0.099	0.041	0.137	0.093	0.136	0.120	0.089	0.055	0.131	0.107	0.080	0.069	0.111	0.104	0.070	0.051
H52	-	-	-	-	-	-	-	-	-	-	-	-	0.111	0.104	-	-
C6	0.113	0.099	0.182	0.146	0.094	0.093	0.002	-0.119	0.066	0.053	0.066	0.036	-	-	0.798	0.792
H61	0.065	0.059	0.036	0.043	0.059	0.059	0.035	0.054	0.077	0.081	0.083	0.092	-	-	-	-
H62	0.065	0.059	0.036	0.043	0.059	0.059	0.035	0.054	0.077	0.081	0.083	0.092	-	-	-	-
H63	-	-	-	-	-	-	0.035	0.054	-	-	-	-	-	-	-	-
O6(a)	-0.595	-0.580	-0.626	-0.594	-0.598	-0.598	-	-	-0.587	-0.554	-0.602	-0.579			-0.788	-0.788
O6b	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-0.788	-0.788
HO6	0.395	0.412	0.424	0.415	0.414	0.421	-	-	0.393	0.392	0.391	0.395	-	-	-	-
O5	-0.318	-0.208	-0.441	-0.382	-0.386	-0.330	-0.288	-0.379	-0.410	-0.342	-0.246	-0.203	-0.395	-0.321	-0.336	-0.210
N2	-	-	-	-	-	-	-	-	-0.566	-0.512	-0.562	-0.460	-	-	-	-
HN2	-	-	-	-	-	-	-	-	0.305	0.284	0.316	0.279	-	-	-	-
C7	-	-	-	-	-	-	-	-	0.748	0.691	0.711	0.726	-	-	-	-
O7	-	-	-	-	-	-	-	-	-0.622	-0.575	-0.608	-0.600	-	-	-	-
C8	-	-	-	-	-	-	-	-	-0.296	-0.299	-0.255	-0.321	-	-	-	-
H81	-	-	-	-	-	-	-	-	0.087	0.088	0.077	0.092	-	-	-	-
H82	-	-	-	-	-	-	-	-	0.087	0.088	0.077	0.092	-	-	-	-
H83	-	-	-	-	-	-	-	-	0.087	0.088	0.077	0.092	-	-	-	-

Table S1 (continued).

Atom name	α-sia	β-sia
C2	-0.240	-0.144
C1	0.866	0.875
O1a	-0.759	-0.765
O1b	-0.759	-0.765
C3	-0.068	-0.129
H31	0.092	0.127
H32	0.092	0.127
C4	0.221	0.103
H4	0.110	0.090
O4	-0.634	-0.567
HO4	0.354	0.317
C5	-0.027	0.030
H5	0.146	0.155
N5	-0.502	-0.350
HN5	0.291	0.252
C10	0.669	0.507
O10	-0.622	-0.557
C11	-0.253	-0.128
H111	0.074	0.045
H112	0.074	0.045
H113	0.074	0.045
C_6	0.003	0.017
H_6	0.148	0.080
C_7	0.040	0.039
H7	0.117	0.110
O7	-0.608	-0.541
HO7	0.415	0.353
C8	0.213	0.15
H8	0.089	0.114
O8	-0.734	-0.666
HO8	0.442	0.399
C9	0.148	0.067
H91	0.045	0.069
H92	0.045	0.069
O9	-0.688	-0.661
HO9	0.412	0.410
O5	-0.187	-0.227

Table S2. Relative energies (kcal/mol) for conformations of model molecules used for deriving torsional parameters

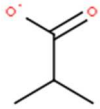
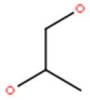
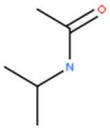
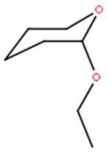
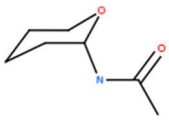
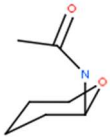
Molecule		dihedral	Conf. (deg.)	MP2/6-31G**	ICMFF
2-methyl-propanoic acid		O-C-C-C	-40	0.00	0.00
			-120	0.37	0.27
2,3-butanediol		C-C-C-C	180	2.75	2.49
			60	0.00	0.00
Propylene glycol		O-C-C-C	60	2.80	2.00
			180	0.00	0.00
N-(1-methylethyl)-ethanamide		C-N-C-C (CCNC trans)	80	0.00	0.00
			-80	0.80	1.66
			180	0.00	0.00
Methoxy-ethane		C-O-C-C	180	0.00	0.00
			75	1.37	1.31
Mol 1		C-O-C1-C2 (CO-CC 180°)	60	0.00	0.00
			150 (saddle point)	4.33	3.46
Mol 2		C-O-C1-C2 (CO-CC 180°)	0	4.53	4.61
			60	0.00	0.00
			180	2.62	2.74
Mol 4		C-N-C1-C2 (C1N-CC trans)	-150	0.29	0.29
			-70	0.00	0.00
Mol 5		C-N-C1-C2 (C1N-CC trans)	-60	2.67	2.90
			80	0.71	0.88

Table S3. Conformational information available for selected di- and tri-saccharides from experimental and theoretical studies

conformation	NMR + MD		This work	
β-D-Glcp-(1→4)-α-D-Glcp-OMe[a)]				
	(ϕ,ψ), deg.	*p*	(ϕ,ψ), deg.	Δ*E,* kcal/mol
Syn	(-60,120)	0.93	(-60,120)	0.0
Anti	(60,0)	0.05	(60,0)	4.5
Anti	(60,120)	0.02	(60,120)	3.0
β-D-Galp-(1→3)-β-D-Glcp-OMe[b)]				
	(ϕ,ψ), deg.	*p*	(ϕ,ψ), deg.	Δ*E,* kcal/mol
Syn	(46,-2)	-	(43,-16)	0.0
Anti	(28,171)	-	(49,173)	3.8
Anti	(178,4)	-	(171,11)	5.0
α-D-Glcp-(1→2)-β-D-Glcp-(1→3)-α-D-Glcp-OMe[c)]				
	(ϕ_2,ψ_2,ϕ_3,ψ_3), deg.	*p*	(ϕ_2,ψ_2,ϕ_3,ψ_3), deg.	Δ*E,* kcal/mol
all-*syn*	(-58,-36,66,17)	-	(-53,-58,53,-3)	0.0
anti-ψ2	(-38,170,90,37)	-	(-21,-151,61,7)	3.4
anti-ψ3	(-48,-18,43,176)	-	(-56,-61,51,179)	5.3
anti-ψ2, ψ3	(-23,-175,73,-158)	-	(-26,-159,61,-158)	7.1
α-D-Glcp-(1→3)-[β-D-Glcp-(1→4)]-α-D-Glcp-OMe[c)]				
	(ϕ_3,ψ_3,ϕ_4,ψ_4), deg.	*p*	(ϕ_3,ψ_3,ϕ_4,ψ_4), deg.	Δ*E,* kcal/mol
all-syn	(-45,-2,63,12)	-	(-42,-12,56,18)	0.0
anti-ψ4	(-45,18,60,-176)	-	(-33,21,49,-162)	6.0
anti-ψ3,ψ4	(-34,-178,72,-166)	-	(-40,137,41,-159)	1.3
β-D-Glcp-(1→2)-β-D-Glcp-(1→3)-α-D-Glcp-OMe[d)]				
	(ϕ_2,ψ_2,ϕ_3,ψ_3), deg.	*p*	(ϕ_2,ψ_2,ϕ_3,ψ_3), deg.	Δ*E,* kcal/mol
all-syn	(~60,~0,~60,~0)	0.91	(49,-4,39,-8)	0.00
anti-ϕ2	(~180,~0,~60,~0)	0.07	(169,4,51,-7)	1.04
anti-ψ2	(~60,~180,~60,~0)	0.02	(43,-153,59,-5)	2.01

a) the NMR+MD values of ϕ/ψ torsional angles and populations (*p*) were taken from: a) Ref.[1]; b) Ref.[2]; c) Ref.[3]; d) Ref. [4]

Table S4. Glycosidic linkage conformers for model oligosaccharides **1-6** (Fig. S1).

torsion	molecule	ϕ,ψ (deg.)*				
		MD(ns)	MD(μs)	NMR	X-ray	This work
α-(1-3)						
Man-Man	5,6	(70,-100)	(70,-100) (160,-80)	(80,-100) (60,180)	(72,-121)	(57,-139)
Fuc-GlcNAc	4	(-70,-100)	(-70,-100) (-150,-145)	(-72,-96)	(-72,-99)	(-66,-97)
Fuc-GlcNAc	1	(-70,-110)	(-75,-105) (-145,-140) (-80,75)	-	-	(-72;-100)
α-(1-4)						
Fuc-GlcNAc	3	(-70,135)	(-70,135)	(-77,142)	-	(-65,150)
α-(1-6)						
Man-Man	5,6	(70,-160)	(70,-160)	(64,180) (64,60)	(67,179) (60,94)	(53,174)
α-(2-3)						
NeuAc-Gal	3,4,2	(60,-120)	(60,-120) (-50,-140)	(60,-120) (-60,-120) (20,170)	(69,-125)	(43,-117) (-22,-143) (25;-164)
β-(1-2)						
GlcNAc-Man$^{(1\rightarrow3)}$	6	(-90,-70)	(-90,-70) (60,-90)	(-92,-83)	(80,-98) (58,-87)	(-85,-90)
GlcNAc-Man$^{(1\rightarrow6)}$	6	(-90,-70)	(-90,-70)	-	-	(-77,-96)
β-(1-3)						
Gal-GlcNAc	3	(-70,-110)	(-70,-110)	(-70,-99)	(-74,-132)	(-68,-102)
β-(1-4)						
Gal-GlcNAc	4	(-70,130)	(-70,130)	(-74,138)	(-71,132)	(-70,137)
Gal-GlcNAc	2	(-70,130)	(-70,130) (-70,-50) (-150,-100)	-	-	

* ϕ and ψ torsions in (1→n) linkages (where n = 2,3,4 or 6) were computed using IUPAC formalism ϕ = O_5-C_1-O-C_n and ψ = C_1-O-C_n-$C_{(n-1)}$. The α(2→3) torsions were defined as ϕ = O_6-C_2-O-C_3 and ψ = C_2-O-C_3-C_2.

Table S5. Probabilities, average positions and sizes of the most populated zones for ϕ/ψ torsional angles in disaccharide "eq-eq" linkages

disaccharide	# of linkages	*p*	ϕ, deg.	Δϕ, deg.	ψ, deg.	Δψ, deg.	zone
β-D-GlcpNAc-(1-4)-β-D-GlcpNAc	3260	0.95	-79.7	16.6	116.6	18.1	I
		0.03	74.9	40.3	122.4	21.9	III
β-D-Manp-(1-4)-β-D-GlcpNAc	1003	0.92	-87.2	19.7	111.4	20.8	I
		0.04	111.0	38.7	105.8	20.2	III
β-D-Glcp-(1-4)-β-D-Glcp	550	0.98	-80.3	19.2	110.5	18.6	I
		0.01	63.2	4.8	124.7	4.7	III
β-D-Galp-(1-4)-β-D-Glcp	264	0.98	-76.7	16.9	117.3	20.7	I
β-D-Xylp-(1-4)-β-D-Xylp	207	0.96	-78.3	21.8	133.2	51.2	I
β-D-Galp-(1-4)-β-D-GlcpNAc	184	0.95	-74.6	13.6	122.4	16.6	I
		0.02	-66.9	11.9	-31.9	9.6	II
a-D-Neup5Ac-(2-3)-β-D-Galp	120	0.65	64.6	15.6	109.7	13.2	III
		0.03	-59.1	12.8	100.8	11.5	I
β-D-GlcpNAc-(1-4)-α-D-GlcpNAc	102	0.71	-86.1	27.2	110.2	19.8	I
		0.23	84.0	28.7	120.0	12.7	III
		0.05	-100.4	18.5	-31.8	16.2	II
β-D-Glcp-(1-3)-β-D-Glcp	76	1.00	-83.0	17.7	120.8	17.1	I
β-D-Manp-(1-4)-β-D-Manp	59	0.76	-77.5	14.9	108.3	22.6	I
β-D-GlcpNAc-(1-3)-β-D-Galp	58	1.00	-83.1	12.1	-140.4	14.3	II
β-D-Galp-(1-4)-α-D-Glcp	56	0.88	-74.0	10.8	120.2	17.3	I
		0.05	49.2	2.1	126.0	1.6	III
β-D-Manp-(1-3)-β-D-Manp	41	0.76	-96.9	41.8	-86.6	43.7	II
β-D-Manp-(1-4)-α-D-Manp	29	0.55	-88.4	34.3	99.1	23.	I
		0.34	-119.9	19.6	-71.1	29.1	II
β-D-Galp-(1-3)-β-D-GalpNAc	46	0.98	-77.4	12.6	-145.4	14.6	II
β-D-Manp-(1-4)-α-D-GlcpNAc	41	0.63	-81.2	16.1	109.9	31.0	I
β-D-Galp-(1-3)-α-D-GalpNAc	42	1.00	-82.7	6.8	-148.8	14.2	II
β-D-Galp-(1-3)-β-D-GlcpNAc	41	1.00	-69.5	14.3	-114.5	19.1	II
β-D-Galp-(1-4)-α-D-GlcpNAc	31	1.00	-72.0	11.1	131.5	11.9	I
β-D-Glcp-(1-4)-α-D-Glcp	28	0.71	-79.1	12.4	119.8	14.5	I
		0.21	-111.5	15.1	-69.7	18.4	II
β-D-Xylp-(1-4)-α-D-Xylp	18	0.94	-69.1	13.4	154.0	9.9	I
β-D-ManpA-(1-4)-β-D-ManpA	19	0.84	-68.1	8.8	116.1	15.5	I
β-D-GlcpA-(1-3)-β-D-GlcpNAc	17	1.00	-76.0	14.1	112.8	10.8	I
β-D-GalpNAc-(1-3)-β-D-Galp	16	1.00	-48.8	24.7	-127.5	8.1	II
β-D-GlcpNAc-(1-4)-β-D-GlcpA	14	1.00	-67.0	9.6	95.9	26.4	I

Table S6. Probabilities, average positions and sizes of the most populated zones for ϕ/ψ torsional angles in disaccharide "ax-eq" linkages.

disaccharide	# of linkages	*p*	ϕ, deg.	Δϕ, deg.	ψ, deg.	Δψ, deg.	zone
α-D-Glcp-(1-4)-α-D-Glcp	789	0.98	96.9	19.	109.1	15.9	I
		0.01	90.2	19.4	-63.4	9.6	II
α-D-Manp-(1-3)-β-D-Manp	542	0.98	79.9	21.6	-115.1	23.7	II
α-D-Glcp-(1-4)-β-D-Glcp	348	0.94	96.4	23.0	110.3	18.5	I
		0.04	105.8	18.5	-58.6	24.8	II
α-D-Manp-(1-3)-α-D-Manp	205	0.97	74.6	14.3	-106.4	18.9	II
α-D-GlcpNAc-(1-4)-β-D-GlcpNAc	165	0.75	48.8	47.7	104.6	32.4	I
		0.23	77.5	13.5	-22.5	17.9	II
α-D-Manp-(1-4)-β-D-GlcpNAc	84	0.79	115.6	44.6	108.2	29.	I
		0.15	97.2	11.9	-14.5	17.7	II
α-D-Galp-(1-3)-β-D-Galp	60	0.95	73.5	24.5	-146.6	27.8	II
α-D-GalpNAc-(1-3)-β-D-Galp	48	1.00	54.2	7.3	-171.9	8.2	II
α-D-Manp-(1-4)-β-D-Manp	31	0.61	84.6	18.1	109.6	20.2	I
α-D-GlcpA-(1-2)-α-D-Manp	18	1.00	73.7	9.11	52.3	17.4	I
α-D-Glcp-(1-3)-α-D-Manp	13	1.00	61.2	22.1	-113.6	29.6	II

Table S7. Probabilities, average positions and sizes of the most populated zones for ϕ/ψ torsional angles in di-saccharide "ax-ax" linkages

disaccharide	# of linkages	*p*	ϕ, deg.	Δϕ, deg.	ψ, deg.	Δψ, deg.
α-D-Manp-(1-2)-α-D-Manp	319	0.92	77.7	19.7	-107.6	32.0
α-D-GalpA-(1-4)-α-D-GalpA	71	1.00	88.0	25.2	-119.1	30.3
α-D-Galp-(1-4)-β-D-Galp	38	0.97	73.2	5.9	-134.0	5.7
α-D-Galp-(1-2)-β-D-Manp	14					

Table S8. Probabilities, average positions and sizes of the most populated zones for ϕ/ψ torsional angles in di-saccharide "eq-ax" linkages

disaccharide	# of linkages	p	ϕ, deg.	Δϕ, deg.	ψ, deg.	Δψ, deg.
β-D-GlcpNAc-(1-2)-α-D-Manp	135	0.93	-79.6	15.4	-93.0	19.1
β-D-Xylp-(1-2)-β-D-Manp	57	0.91	-83.6	10.7	-107.6	7.3
β-D-GalpNAc-(1-4)-β-D-Galp	26	1.00	-85.4	9.6	-111.7	7.7
β-D-Galp-(1-4)-β-D-Galp	21	1.00	-93.9	12.5	-116.5	7.2

Table S9. Probabilities, average positions and sizes of the most populated zones for ϕ/ψ torsional angles in *-6 di-saccharide linkages

	p	ϕ, deg.	Δϕ, deg.	ψ, deg.	Δψ, deg.	ω, deg.	Δω, deg.
α	0.48	65.1	17.9	180.2	18.4	180.3	12.6
(633)	0.31	71.1	17.2	171.8	18.2	60.6	15.1
	0.08	85.1	20.0	88.5	10.8	-167.7	8.9
	0.07	62.7	13.1	89.1	10.6	49.8	21.3
	0.06	-54.5	24.9	185.0	37.2	26.5	75.2
β	0.54	-99.6	41.7	-158.5	41.3	156.7	39.9
(92)	0.46	-92.8	50.1	-170.5	65.3	10.2	48.1

Table S10. Probabilities, average positions and sizes of the most populated zones for ϕ/ψ torsional angles in N- and O- protein-glycan linkages

	# of linkages	p	ϕ, deg.	Δϕ, deg.	ψ, deg.	Δψ, deg.
β-Nag-Asn	1406	0.98	-98.5	20.5	177.7	9.4
		0.02	68.7	12.3	180.1	10.1
α-*-Ser	158	1.00	66.5	17.2	171.9	21.3
α-*-Thr	88	0.91	82.0	17.5	129.7	18.4

Table S11. Parameters of the torsional potential (Eq. 4, kcal/mol) for mono- and di-saccharides.

	angle	k_θ^1	k_θ^2	k_θ^3	phase, deg.
C-O-C linkage					
α-equatorial	ϕ	-3.71	0.15	0.30	-
	ψ	-1.51	1.22	-0.19	-
α-axial	ϕ	-0.65	-1.38	1.24	-
	ψ	-	-	-	-
β-equatorial	ϕ	-1.71	-1.60	0.94	-
	ψ	-	-	-	-
β-axial	ϕ	-1.18	-2.03	0.81	-
	ψ	-	-	-	-
O-linkage					
α	ϕ	-2.13	0.44	0.23	-
β	ϕ	-0.31	0.35	1.85	-
N-linkage					
α	ϕ	-	-	-0.64	160.
β	ϕ	-	-	1.40	-90.
6-linkage	ψ	-0.52	0.70	0.64	-
O5 equatorial	ω	-0.17	1.30	1.50	-
		-1.30	-	-	300.0
O5 axial	ω	-0.59	0.26	1.52	
		1.40	-	-	300.0
α-sia, β-sia	O_9-C_9-C_8-C_7	0.03	0.42	2.18	-
α-sia, β-sia	C_9-C_8-C_7-C_6	-0.44	-0.34	2.29	-
α-gcu, β-gcu, α-sia, β-sia	$O_{1\alpha}$-C_1-C_2-O_5	-	0.89	-	-
α-Nag, β-Nag, α-Nga, β-Nga	C-N-C-C	-1.47	0.64	-0.39	-120.

Table S12. Results of local energy minimizations carried out for crystals of monosaccharides with the ICMFF nonbonded parameters.

Name/ CSD ref. code	Space group	Δa, %[a]	Δb, %[a]	Δc, %[a]	$\Delta\gamma$, %[a]	ΔH_{subl}, kcal/mol	E, kcal/mol
α-D-glucose/ GLUCSA03	$P2_12_12_1$, Z=4	-1.7	-2.3	-0.7	-	33.2±1.9;[5] 46.5±1.2 [6]	-40.0
β-D-glucose /GLUCSE02	$P2_12_12_1$, Z=4	-2.4	4.3	-4.5	-	-	-38.2
α-D-galactose/ ADGALA03	$P2_12_12_1$, Z=4	-0.4	-1.8	-0.4	-	-	-37.5
β-D-galactose/ BDGLOS01	$P2_12_12_1$, Z=4	3.4	-3.8	-2.8	-	-	-44.4
α-D-mannose/ ADMANN	$P2_12_12_1$, Z=8	-2.2	-0.7	-2.9	-	-	-38.3
α-L-fucose/ ALFUCO	$P2_12_12_1$, Z=4	0.9	-2.0	2.9	-	-	-28.8
N-acetyl-α-D-glucosamine/ ACGLUA11	$P2_1$, Z=2	0.2	-2.7	-0.7	1.4	-	-46.7
N-acetyl-α-D-galactosamine/ AGALAM01	$P2_1$, Z=2	-1.1	-3.6	1.3	0.8	-	-46.9

[a] computed as $100\%\cdot(x_{exp}-x)/x_{exp}$, where x is a unit cell parameter a, b, c, or γ.

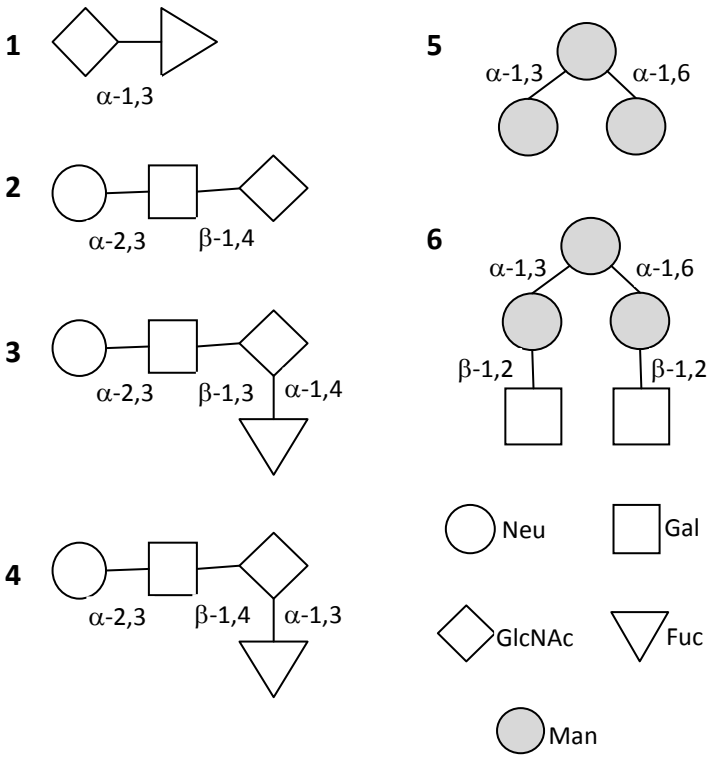


Figure S1. Model oligosaccharides: constituent di and tri-saccharides **1-2**, sialyl Lewis^{a} **3**, sialyl Lewis^{x} **4**, mannotriose **5**, bianntennary N-linked core pentasaccharide **6**. Symbols are N-acetyl-α-D-neuraminic acid (NeuAc), β-D-galactose (Gal), N-acetyl-β-D-glucosamine (GlcNAc), α-L-fucose (Fuc), and α-D-mannose (Man).

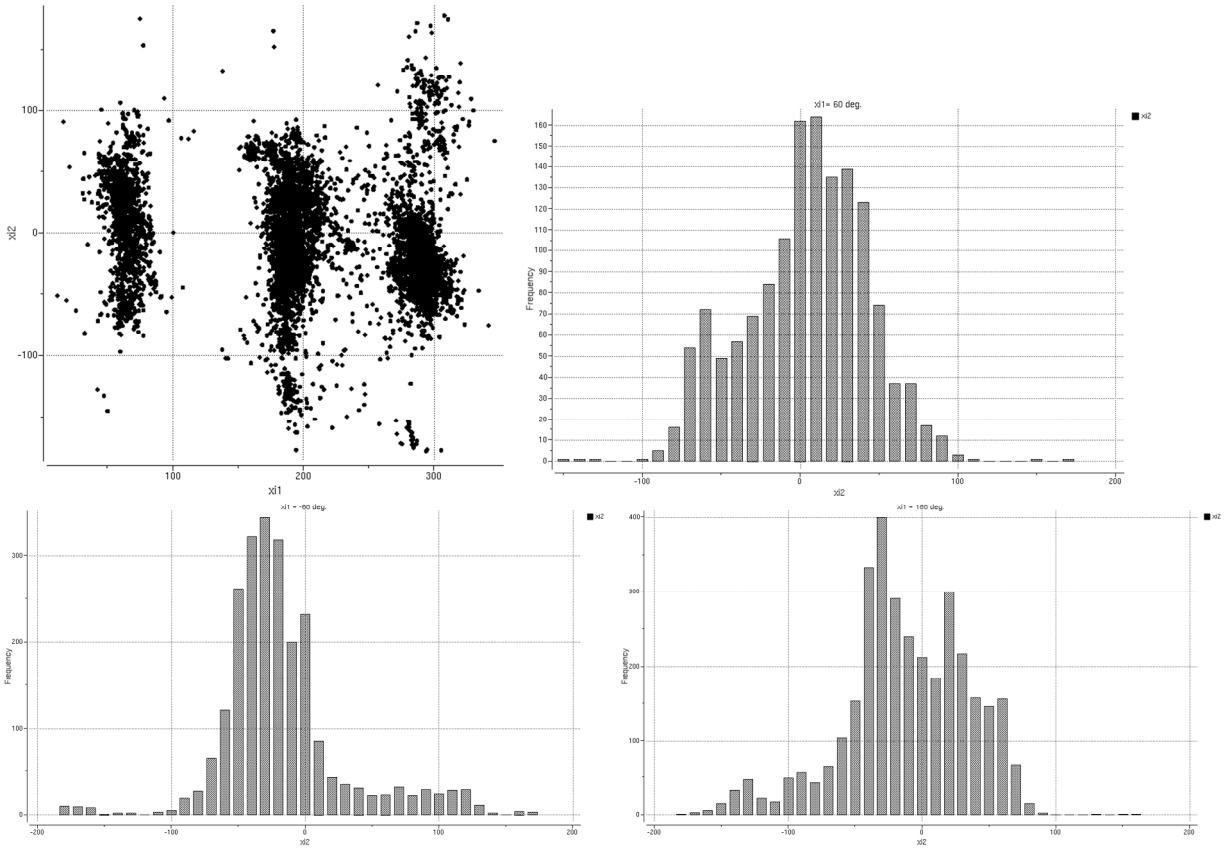


Figure S2. Distribution of χ_1/χ_2 angles in high-resolution PDB structures of glycoproteins with beta*-Asn linkages

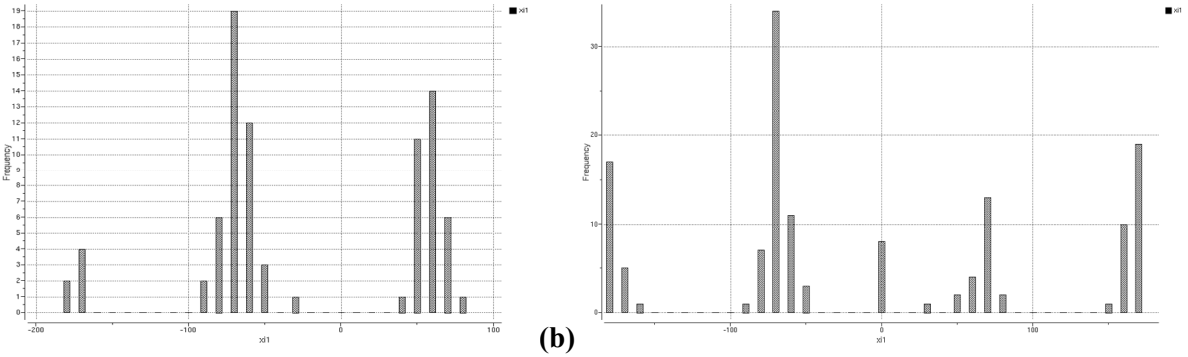


Figure S3. Distribution of χ_1 torsional angles in high-resolution PDB structures of glycoproteins with O-linkages**:** (a) Thr; (b) Ser

(1) Larsson, E. A.; Staaf, M.; Söderman, P.; Höög, C.; Widmalm, G. *J. Phys. Chem. A* **2004**, *108*, 3932.

(2) Dabrowski, J.; Kozar, T.; Grosskurth, H.; Nifant'ev, N. E. *J. Am. Chem. Soc.* **1995**, *117*, 5534.

(3) Dixon, A. M.; Venable, R.; Widmalm, G.; Bull, T. E.; Pastor, R. W. *Biopolymers* **2003**, *69*, 448.

(4) Hoog, C.; Landersjo, C.; Widmalm, G. *Chemistry* **2001**, *7*, 3069.

(5) Kabo, G. J.; Voitkevich, O. V.; Blokhin, A. V.; Kohut, S. V.; Stepurko, E. N.; Paulechka, Y. U. *J. Chem. Thermodynamics.* **2013**, *59*, 87.

(6) Oja, V.; Suuberg, E. M. *J. Chem. Eng. Data* **1999**, *44*, 26.