Supporting information

CHARMM Additive All-Atom Force Field for Aldopentofuranoses, Methyl-Aldopentofuranosides and Fructofuranose

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Table S1. Errors in calculated average bond lengths and angles from simulations of infinite crystals of aldopentofuranoses relative the experimental crystal values. Here α-arabinofuranose is denoted α-Ara, α-xylofuranose is denoted α-Xyl, α-lyxofuranose is denoted α-Lyx, β-arabinofuranose is denoted β-Ara and β-ribofuranose is β-Rib.

	α-Ara	α-Xyl	α-Lyx	β-Ara	β-Rib	avg
bonds						
c1c2	0.002	0.005	0.007	-0.002	0.013	0.005
c1o1	0.005	0.002	0.007	-0.002	0.001	0.003
c2c3	0.014	0.008	0.010	-0.001	0.021	0.010
c2o2	-0.012	-0.002	-0.007	0.010	0.006	-0.001
c3c4	-0.006	0.004	0.009	-0.004	0.007	0.002
c3o3	-0.012	-0.014	-0.011	-0.008	0.001	-0.009
c4c5	-0.003	-0.005	0.007	-0.002	0.013	0.002
c4o4	0.004	-0.010	-0.010	-0.016	-0.001	-0.007
c5o5	0.001	0.005	-0.006	0.011	0.008	0.004
o1cm	0.001	0.004	-0.019	0.011	0.006	0.000
o4c1	-0.014	-0.002	0.003	0.003	0.003	-0.001
angles						
c1c2c3	-0.49	-0.46	-1.25	1.67	-1.43	-0.39
c2c1o1	1.28	1.86	-0.95	2.61	-1.38	0.68
c2c3c4	0.72	-0.62	1.10	0.97	0.21	0.48
c3c2o2	-1.58	-0.98	0.34	-0.74	5.44	0.50
c3c4o4	-0.60	1.39	0.07	0.23	0.29	0.28
c4c3o3	-0.16	1.66	2.77	1.97	0.06	1.26
c4c5o5	0.49	0.09	0.10	-1.20	1.18	0.13
c4o4c1	-0.19	-1.37	-0.76	-0.72	-1.23	-0.85

o4c1c2	-0.52	0.50	1.72	-0.63	0.50	0.31
o4c4c5	2.79	0.81	2.09	-2.00	-1.18	0.50
o4c1o1	0.30	-1.54	0.83	-0.69	0.54	-0.11
c1o1cm	-0.47	0.01	-0.71	0.05	-0.88	-0.40
dihedrals						
c1c2c3c4	-3.3	0.6	-3.3	-9.5	-3.5	-3.8
c1o4c4c5	2.7	4.5	2.8	-9.7	-5.3	-1.0
c2c1o1cm	1.2	1.5	16.9	0.9	6.2	5.3
c2c3c4o4	1.2	-0.8	0.5	10.4	5.6	3.4
c3c2o2ho2	-1.5	-2.7	0.7	-6.7	2.1	-1.6
c3c4o4c1	2.0	1.0	1.5	-10.3	-6.4	-2.5
c4c3o3ho3	-2.5	8.3	7.0	19.7	-0.48	6.4
c4c5o5ho5	-19.6	-8.5	13.0	7.1	-2.3	-2.1
o4c1c2c3	4.7	0.5	4.1	4.2	-0.8	2.5
o4c4c5o5	6.3	1.2	-3.4	-7.0	1.9	-0.2

Table S2. Vibrational analysis of α-arabinofuranose. QM frequencies were calculated the MP2/6-31G(d) level. A scaling factor of 0.9434 was applied to the QM frequencies to account for the limitations in the level of theory.[2] The internal coordinate system in the Pulay methodology was used for the vibrational modes.[3]

QM			MM		
frequency	vibrational mode[a]	contribution	frequency	vibrational mode[a]	contribution
88.4	tC5OH	30	70.3	tRing	78
	tC4C5	27		tC4C5	18
	tRing	21	121.9	tCOH	84
	tRing'	16	129.9	tRing'	35
121.9	tRing	43		tCOH	32
	tC5OH	36	145.9	tC4C5	67
	tRing'	18		tRing	16
140	tC4C5	54	193.5	tCOH	48
	tC5OH	26		tRing'	19
	tRing	16	222.9	rC4	22
184.1	tRing'	50		tRing'	16
	tRing	30	278.3	scCCO	22
229.1	rC4	36	285.6	rRing	38
	scCCO	22	339.4		
249.5	rRing	45	364.3	twRing	27
269.4	twRing	18		tC5OH	27
	twC4	17		wRing	19
	wC4	17	388.3	twRing	28
302	twRing	34		wRing	22
	rRing	22	426.8	rRing	30
	wRing	19		tC5OH	15
357.7	twRing	35	479.6	twRing	41
	wRing	17		wRing	30
367.6	tCOH	75	504.1	rRing	37
406.2	twRing	22		sC-Oh	24
	tCOH	22	579.6	dRing'	25
	wRing	20		scCCO	21
466.6	twRing	25		rRing	15
	scCCO	17	604.1	tCOH	43
532.7	tCOH	96		dRing'	24
562.5	sC-Oh	25	619.7	tCOH	39
	rRing	24	661.9	dRing	42
592.9	tCOH	84		rRing	22
635.8	scCCO	15	860.8	rCH2	54
694.7	dRing'	42	873.6	rCH2	22
796.6	dRing	40		sC4-O4	16
	rRing	17	950.8	sC4-C5	18
849	sC4-O4	35	1017.9	sO4-C1	26
	sO4-C1	20		sC2-C3	17
	rCH2	17	1035	sC2-C3	17
873.8	sC3-C4	18	1072.4	sC5-O5	29
	sC5-O5	16	1083.3	sC-Oh	39
913.4	sC1-C2	28		dCOHr	20
965.3	sO4-C1	20	1109.4	sC-Oh	23
	sC2-C3	19		dCOHr	17
	sC-Oh	15	1138	sC-Oh	25

981.6	sC5-O5	24	1161.3	scRing	35
	sC3-C4	18		sC-Oh	29
1021.8	sC-Oh	37	1168.1	sC4-O4	23
	twRing	20		dCOHr	15
1042.9	sC-Oh	21	1235.8	dC5OH	31
	rCH2	15		twCH2	22
1058.8	sC-Oh	26		dCOHr	16
	sC4-O4	16	1237.5	wRing	35
1064.9	sC-Oh	62		dCOHr	21
1081	sC-Oh	30		twRing	17
	sC5-O5	17	1267.9	dCOHr	29
1094.2	sC-Oh	30		twCH2	17
1153.8	dCOHr	24	1272.6	twCH2	36
	dC5OH	23		dC5OH	25
1182.7	wRing	22	1290	dCOHr	43
	dC5OH	18	1317.5	dCOHr	33
1212.7	dCOHr	34		wRing	26
1232.3	twCH2	23	1348.9	wRing	24
	scRing	16		dCOHr	23
1238.3	twCH2	37	1370.4	scC4	28
	wRing	23	1393.8	scRing	31
1255.7	scRing	47		wRing	24
	wRing	21	1413	scCH2	73
1278.2	wC4	25		wCH2	18
	scRing	19	1469.9	scRing	35
1316.6	rRing	21		sC-Oh	23
	dCOHr	21	1519	wC4	33
	scRing	19		twC4	16
1322.9	wRing	22	1563.7	sC-Oh	21
	scC4	21		scRing	20
	dCOHr	16	1566.8	wCH2	40
1337.6	wRing	20		sC5-O5	27
	wC4	16		scCH2	25
	scC4	16	1613.9	scRing	27
1385	scRing	23		sC-Oh	24
	dCOHr	15		rRing	21
	scC4	15	2855.1	sCH2	99
1396.5	wCH2	68	2865.5	sCH	99
	dC5OH	15	2889.2	sCH2a	99
1409.6	dCOHr	57	2907.1	sCH	100
	scRing	35	2913.5	sCH	99
1429	dCOHr	62	2919.1	sCH	100
	scRing	28	3661.3	sOHring	86
1476.7	scCH2	100	3683.7	sOHring	99
2906.6	sCH2	63	3688.7	sOHring	100
	sCH	33	3690.2	sO5-H	85
2918	sCH	67			
	sCH2	32			
2951.5	sCH	99			
2969.7	sCH	96			
2971.9	sCH2a	91			
3020.9	sCH	100			
3429.2	sOHring	100			

3466.4	sOHring	100			
3530.7	sOHring	100			
3579.5	sO5-H	100			

[a] where t=torsion, tw=twisting, r=rocking, w=wagging, sc=scissoring, s=stretching and d=deformation

Table S3. Table of all of the aldopentofuranose parametrized torsion. “F” represents the fit dihedrals, “V” represents the dihedrals used to validate the dihedral parameters. “T” represents the dihedrals transferred. “X” represents a non-existent dihedral

	α-Ara	β-Ara	α-Rib	β-Rib	α-Lyx	β-Lyx	α-Xyl	β-Xyl	α-Deo	β-Deo
c1c2c3c4	F	F	F	F	T	T	T	T	F	F
c1c2c3o3	F	F	F	F	T,V	T	T	T	F	F
c1c2o2ho2	F	F	F	F	T	T	T	T	X	X
c1o4c4c3	F	F	F	F	T	T	T	T	T	T
c1o4c4c5	F	F	F	F	T	T	T	T	T	T
c2o1o1ho1	F	F	F	F	T	T	T	T,V	F	F
c2c3c4o4	F	F	F	F	T	T	T	T	F	F
c2c3o3ho3	F	F	F	F	T	T	T	T	F	F
c3c2c1o1	F	F	F	F	T	T	T	T	F	F
c3c2c1o4	F	F	F	F	T	T	T	T	F	F
c3c2o2ho2	F	F	F	F	T,V	T	T	T	X	X
c3c4c5o5	F	F	F	F	T	T	T	T	T	T
c4c3c2o2	F	F	F	F	T	T	T	T	X	X
c4c3o3ho3	F	F	F	F	T	T	T,V	T	T	T
c4c5o5ho5	F	F	F	F	T,V	T	T	T,V	T	T
c4o4c1c2	F	F	F	F	T	T	T	T	F	F
c4o4c1o1	F	F	F	F	T	T	T,V	T	T	T
c5c4c3o3	F	F	F	F	T	T	T	T	T	T
o1c1c2o2	F	F	F	F	T	T	T	T	X	X
o2c2c3o3	F	F	F	F	T	T	T	T	X	X
o2c2c1o4	F	F	F	F	T	T	T	T,V	X	X
o3c3c4o4	F	F	F	F	T	T	T,V	T	T	T
o4c1o1ho1	F	F	F	F	T	T	T	T	T	T
o4c4c5o5	F	F	F	F	T	T	T	T	T	T

Table S4. ϕ/ψ values of the two lowest energy North and South conformations and QM (MP2/cc-pVTZ//MP2/6-31G(d)) and MM energies from the 2D ring pucker surfaces. Both QM and MM energies have been zeroed for comparison purposes. Energies are in kcal/mol

	QM North ϕ/ψ	MM North ϕ/ψ	E_{QM}	E_{MM}	E_{MM}-E_{QM}	QM South ϕ/ψ	MM South ϕ/ψ	E_{QM}	E_{MM}	E_{MM}-E_{QM}
α-Ara	-30/40	-30/40	0.38	0.65	0.27	40/-30	40/-30	0.00	0.00	0.00
β-Ara	-40/40	-40/40	0.00	0.00	0.00	20/-40	40/-40	0.44	0.20	-0.24
α-Rib	-30/40	-30/40	0.31	0.00	-0.31	40/-40	40/-40	0.00	0.65	0.65
β-Rib	-40/30	-40/30	0.00	0.00	0.00	0/-20	0/-20	1.65	1.28	-0.37
α-Deo	-10/30	-20/40	2.46	0.70	-1.76	40/-40	40/-30	0.00	0.01	0.01
β-Deo	-40/30	-40/30	0.00	0.16	0.16	-10/-10	-10/-10	0.04	0.00	-0.04

Table S5. Comparison of water interaction energies and O…H distance by HF/6-31G(d) QM calculations and CHARMM force field for the pair conformations shown in Figure S1.

		E_{QM} (kcal/mol)	E_{MM} (kcal/mol)	$E_{MM} - E_{QM}$ (kcal/mol)	R_{QM} (Å)[a]	R_{MM} (Å)	$R_{MM} - R_{QM}$ (Å)
O-methyl-THF	Pair 1	-7.44	-7.14	0.30	1.80	1.75	-0.05
	Pair 2	-5.70	-5.46	0.24	1.84	1.77	-0.07
	Pair 3	-5.92	-5.79	0.13	1.85	1.78	-0.07
	Pair 4	-5.83	-6.58	-0.76	1.86	1.74	-0.11
	Pair 5	-4.88	-4.63	0.25	1.95	1.84	-0.11
	Pair 6	-5.55	-5.75	-0.20	1.92	1.80	-0.12
	Pair 7	-4.50	-4.03	0.47	1.95	1.85	-0.10
	Pair 8	-7.30	-7.40	-0.10	1.85	1.76	-0.09
Average				0.07			-0.06
RMSE				0.37			0.26

[a] E_{QM} values are scaled by 1.16, and 0.2 is subtracted from the R_{QM} values

Table S6. Average pseudorotation angles and amplitudes from the crystal simulations compared to the experimental crystal structure results.

Pseudorotation angle and amplitude	Expt P	Calc P	Diff	Expt Φ_m	Calc Φ_m	Diff
Me-α-arabinofuranoside	61	65	4	41	42	1
Me-β-arabinofuranoside	322	305	-18	40	39	-1
Me-β-ribofuranoside	350	339	-11	38	39	1
Me-α-lyxofuranoside	28	34	6	44	43	-1
Me-α-xylofuranoside	156	154	-2	40	41	1

Tables S7 and S8 (topology and parameter files) are appended after the references

Figure S1. Water-*O*-methyl-THF interaction pairs. For simplicity the water molecules are shown simultaneously, but during the calculations the individual monohydrate pairs were analyzed. Molecular graphics prepared with VMD.[1]

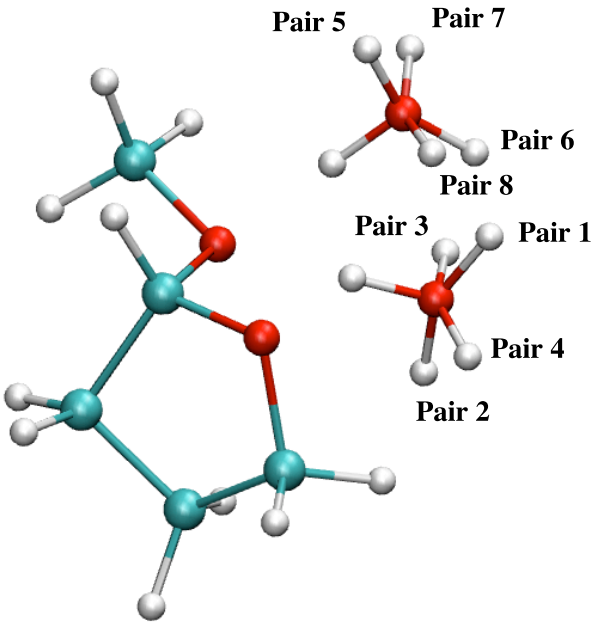


Figure S2. Potential energy scans of 146 conformations of α-lyxofuranose, α-xylofuranose, β-xylofuranose. QM results given with an energy cutoff at 12 kcal/mol. QM is black, MM using transferred arabinofuranose and ribofuranose parameters is red.

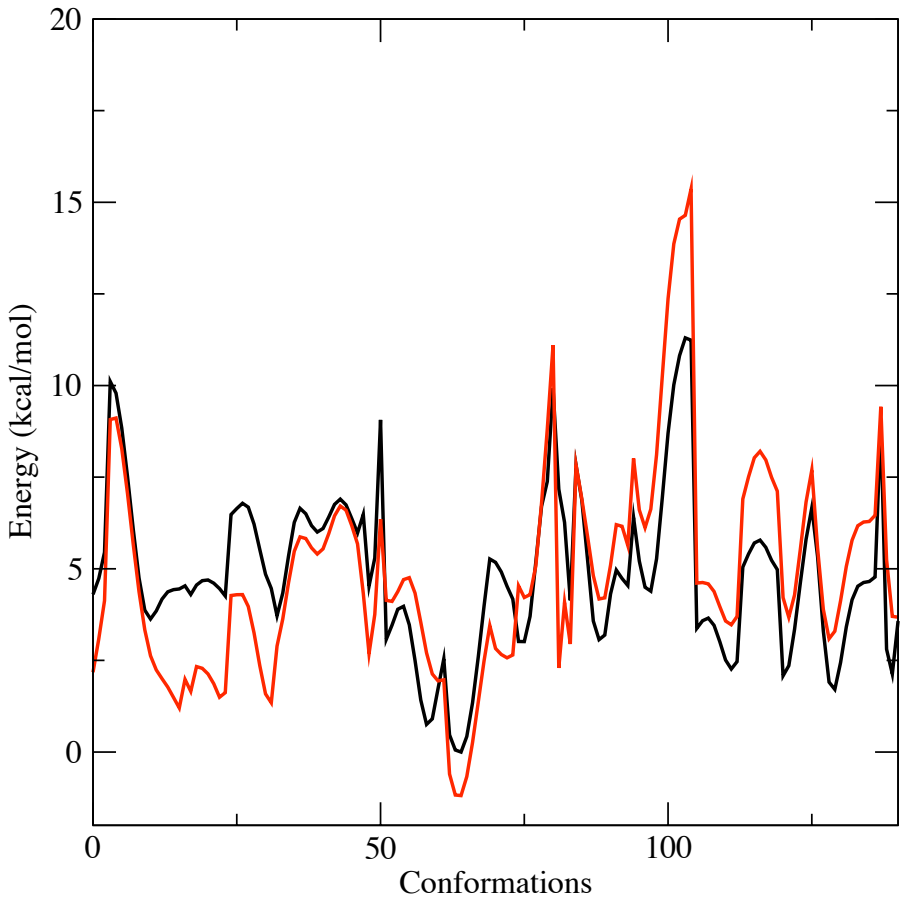


Figure S3. Potential energy scan *O*-methyl-THF. QM results are in black and MM results are in red.

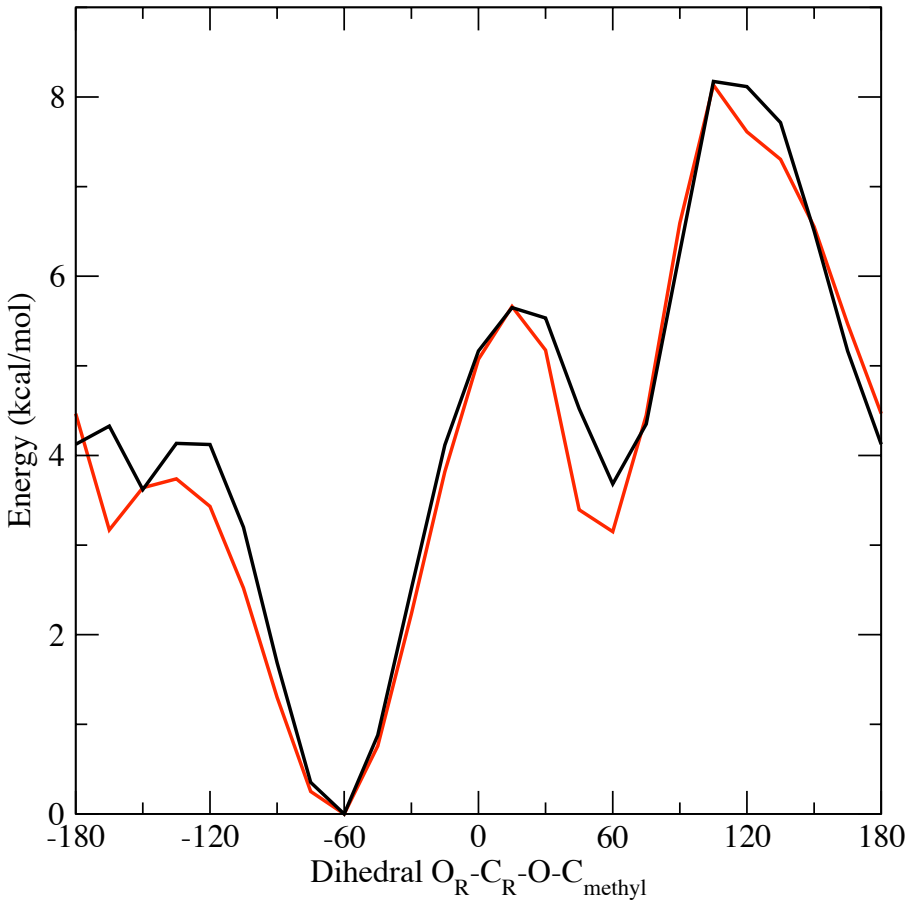


Figure S4. Time series of the pseudorotation rotation of 1 molecule of α-arabinofuranose from solution simulations.

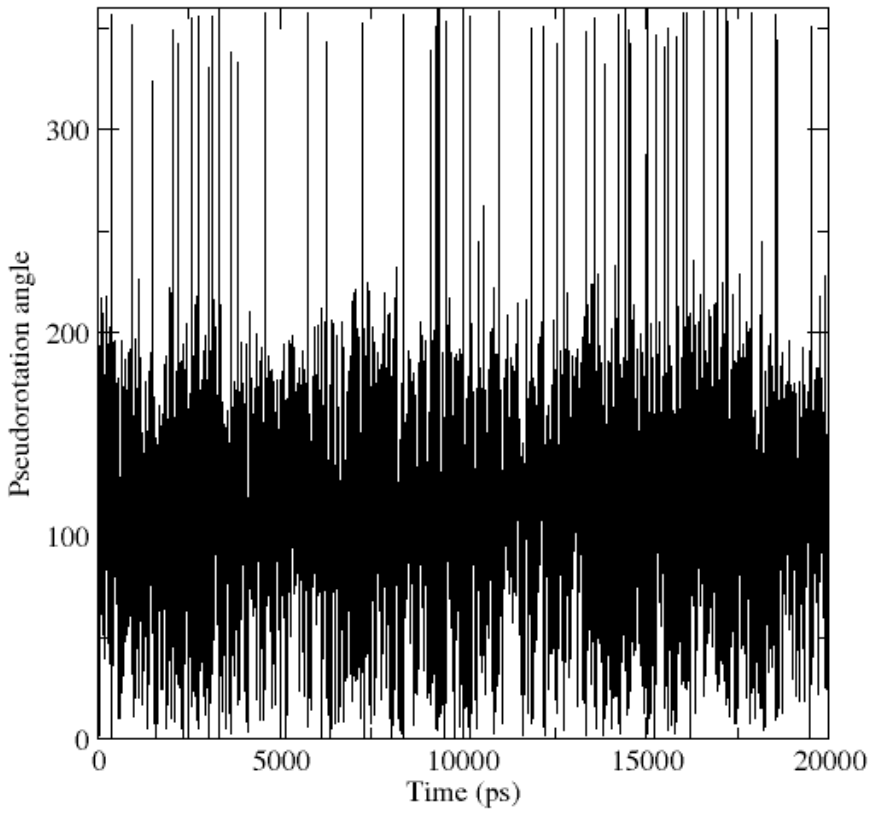
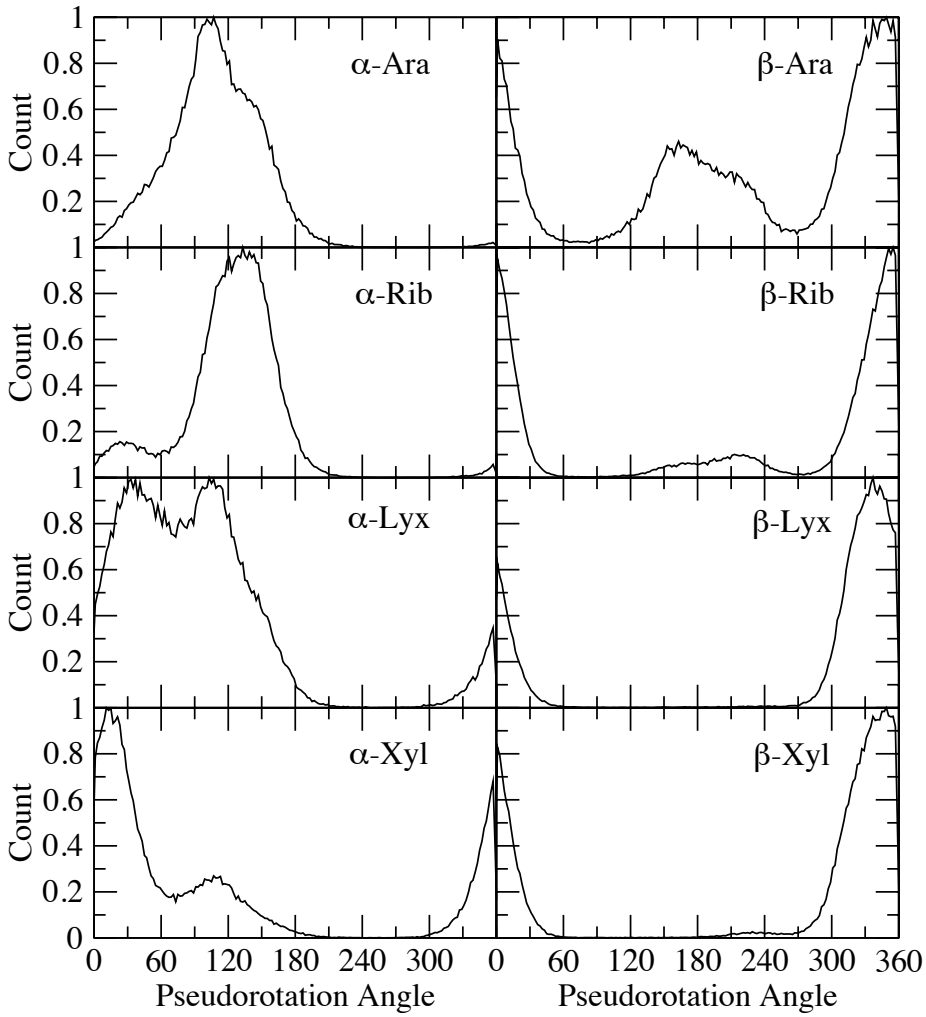


Figure S5. Histogram of the pseudorotation angle of the aldopentofuranoses from solution simulations. The distributions are normalized to one.



References:

(1) Humphrey, W.; Dalke, A.; Schulten, K. *J. Mol. Graph.* **1996**, *14*, 33.
(2) Scott, A. P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502.
(3) Pulay, P.; Fogarasi, G.; Pang, F.; Boggs, 16. E. *J. Am. Chem. Soc.* **1979**, *101*, 2550.

Table S7. Topology file for furanose compounds

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* $Id: top_allxx_sugar.inp,v 1.79 2009-05-07 01:31:31 oguvench Exp $
* Topology file for carbohydrates
* IC coordinates are for thermalized structures
* Guvench, Hatcher, Greene, and MacKerell
*
32 1

MASS    18 CC331   12.01100  C ! generic acyclic CH3 carbon
MASS    25 HCA3     1.00800  H ! aliphatic proton, CH3
MASS    33 OC301   15.99940  O ! generic linear ether
MASS    91 OC3C51  15.99940  O ! furan ring oxygen
MASS    92 CC3152  12.01100  C ! furan ring carbon
MASS    93 CC3153  12.01100  C ! furan ring carbon
MASS    94 CC3251  12.01100  C ! furan ring carbon; C2 deoxy
MASS    95 CC3151  12.01100  C ! furan ring carbon
MASS    96 CC3051  12.01100  C ! furan ring carbon; C2 fructose
AUTOGENERATE angles dihedrals
! DEFAults for patching FIRSt and LAST residues
DEFA FIRS NONE LAST NONE
RESI ADEO        0.0  !  alpha-Deoxy-Ribose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !
ATOM O1   OC311  -0.65  !
ATOM HO1  HCP1    0.42  !
ATOM C4   CC3153  0.11  !
ATOM H4   HCA1    0.09  !
GROUP                   !
ATOM C5   CC321   0.05  !
ATOM H51  HCA2    0.09  !
ATOM H52  HCA2    0.09  !
ATOM O5   OC311  -0.65  !
ATOM HO5  HCP1    0.42  !
GROUP                   !
ATOM C2   CC3251 -0.18  !
ATOM H21  HCA2    0.09  !
ATOM H22  HCA2    0.09  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
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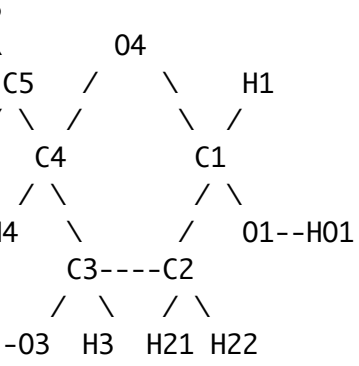

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BOND C1 C2  C2 H21  C2 H22  C2 C3
BOND C3 H3  C3 O3   O3 HO3  C3 C4
BOND C4 H4  C4 O4   C4 C5   C5 H51
BOND C5 H52  C5 O5  O5 HO5
IC C4   O4   C1   C2   1.4309  108.67  -19.01  106.25   1.5278
IC O4   C1   C2   C3   1.4258  106.25   -8.82  103.23   1.5178
IC C1   C2   C3   C4   1.5278  103.23   31.05  101.83   1.5232
IC C3   O4  *C4   C5   1.5232  101.44  124.05  113.01   1.5448
IC C3   O4  *C4   H4   1.5232  101.44 -115.42  106.74   1.1134
IC O4   C4   C5   O5   1.4309  113.01 -178.27  111.12   1.4304
IC C4   C5   O5   HO5  1.5448  111.12  -87.73  110.40   0.9643
IC O4   C4  *C5   H51  2.4824   32.04   59.71  109.84   1.1020
IC O4   C4  *C5   H52  2.4824   32.04  -58.37  108.86   1.1027
IC C2   O4  *C1   O1   1.5278  106.25  119.87  110.66   1.3905
IC O4   C1   O1   HO1  1.4258  110.66   60.11  106.63   0.9584
IC C2   O4  *C1   H1   1.5278  106.25 -119.86  107.45   1.1137
IC C3   C1  *C2   H21  1.5178  103.23  118.42  111.24   1.1030
IC C3   C1  *C2   H22  1.5178  103.23 -122.05  112.95   1.0962
IC C2   C4  *C3   O3   1.5178  101.83 -120.07  112.49   1.4116
IC C4   C3   O3   HO3  1.5232  112.49  -53.93  107.21   0.9673
IC C2   C4  *C3   H3   1.5178  101.83  117.41  109.93   1.1144
RESI BDEO         0.0  !  beta-Deoxy-Ribose
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    O1--HO1
ATOM C4   CC3153  0.11  !                / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                   / \        / \
ATOM C5   CC321   0.05  !                 H4   \      /   H1
ATOM H51  HCA2    0.09  !                      C3----C2
ATOM H52  HCA2    0.09  !                     /  \   / \
ATOM O5   OC311  -0.65  !              HO3--O3  H3  H21 H22
ATOM HO5  HCP1    0.42  !
GROUP                   !
ATOM C2   CC3251 -0.18  !
ATOM H21  HCA2    0.09  !
ATOM H22  HCA2    0.09  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H21  C2 H22  C2 C3
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BOND C3 H3  C3 O3   O3 HO3  C3 C4
BOND C4 H4  C4 O4   C4 C5   C5 H51
BOND C5 H52  C5 O5  O5 HO5
IC C4   O4   C1   C2   1.4309  108.67  -19.01  106.25   1.5278
IC O4   C1   C2   C3   1.4258  106.25   -8.82  103.23   1.5178
IC C1   C2   C3   C4   1.5278  103.23   31.05  101.83   1.5232
IC C3   O4  *C4   C5   1.5232  101.44  124.05  113.01   1.5448
IC C3   O4  *C4   H4   1.5232  101.44 -115.42  106.74   1.1134
IC O4   C4   C5   O5   1.4309  113.01 -178.27  111.12   1.4304
IC C4   C5   O5   HO5  1.5448  111.12  -87.73  110.40   0.9643
IC O4   C4  *C5   H51  2.4824   32.04   59.71  109.84   1.1020
IC O4   C4  *C5   H52  2.4824   32.04  -58.37  108.86   1.1027
IC C2   O4  *C1   O1   1.5278  106.25 -119.87  110.66   1.3905
IC O4   C1   O1   HO1  1.4258  110.66   60.11  106.63   0.9584
IC C2   O4  *C1   H1   1.5278  106.25  119.86  107.45   1.1137
IC C3   C1  *C2   H21  1.5178  103.23  118.42  111.24   1.1030
IC C3   C1  *C2   H22  1.5178  103.23 -122.05  112.95   1.0962
IC C2   C4  *C3   O3   1.5178  101.83 -120.07  112.49   1.4116
IC C4   C3   O3   HO3  1.5232  112.49  -53.93  107.21   0.9673
IC C2   C4  *C3   H3   1.5178  101.83  117.41  109.93   1.1144
RESI ARIB          0.0  !  alpha-Ribose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                   / \        / \
ATOM C5   CC321   0.05  !                 H4   \      /   O1--HO1
ATOM H51  HCA2    0.09  !                      C3----C2
ATOM H52  HCA2    0.09  !                     /  \   / \
ATOM O5   OC311  -0.65  !              HO3--O3  H3  O2 H2
ATOM HO5  HCP1    0.42  !                           |
GROUP                   !                          HO2
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
```

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BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4343  107.06  -43.51  102.91   1.5564
IC O4   C1   C2   C3   1.4227  102.91   29.68  103.27   1.5615
IC C1   C2   C3   C4   1.5564  103.27   -6.90  103.97   1.5386
IC C3   O4  *C4   C5   1.5386  104.85  125.17  112.30   1.5446
IC C3   O4  *C4   H4   1.5386  104.85 -116.42  106.12   1.1143
IC O4   C4   C5   O5   1.4343  112.30 -178.59  110.88   1.4293
IC C4   C5   O5   HO5  1.5446  110.88  -86.85  110.49   0.9639
IC O5   C4  *C5   H51  1.4293  110.88  119.78  108.95   1.1027
IC O5   C4  *C5   H52  1.4293  110.88 -122.02  109.96   1.1020
IC C2   O4  *C1   O1   1.5564  102.91  122.54  109.76   1.4025
IC O4   C1   O1   HO1  1.4227  109.76   66.79  107.33   0.9584
IC C2   O4  *C1   H1   1.5564  102.91 -117.68  108.69   1.1117
IC C3   C1  *C2   H2   1.5615  103.27 -113.35  106.87   1.1124
IC C3   C1  *C2   O2   1.5615  103.27  127.46  116.16   1.4278
IC C1   C2   O2   HO2  1.5564  116.16  -81.77  106.00   0.9665
IC C2   C4  *C3   O3   1.5615  103.97 -125.04  111.07   1.4263
IC C2   C4  *C3   H3   1.5615  103.97  115.28  109.94   1.1126
IC C4   C3   O3   HO3  1.5386  111.07  -77.15  108.40   0.9644
IC C2   C4  *C3   H4   1.5615  103.97  -95.69   28.61   2.1867
RESI BRIB          0.0  !  beta-Ribose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !
ATOM O1   OC311  -0.65  !
ATOM HO1  HCP1    0.42  !
ATOM C4   CC3153  0.11  !
ATOM H4   HCA1    0.09  !
GROUP                   !
ATOM C5   CC321   0.05  !
ATOM H51  HCA2    0.09  !
ATOM H52  HCA2    0.09  !
ATOM O5   OC311  -0.65  !
ATOM HO5  HCP1    0.42  !
GROUP                   !
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
```

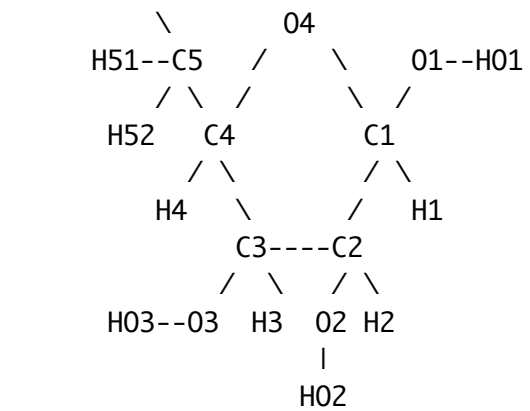

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ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4440  110.08   18.97  105.48   1.5227
IC O4   C1   C2   C3   1.4297  105.48  -35.29  101.04   1.5223
IC C1   C2   C3   C4   1.5227  101.04   37.68  102.70   1.5258
IC C3   O4  *C4   C5   1.5258  105.50  121.77  111.20   1.4950
IC C3   O4  *C4   H4   1.5258  105.50 -118.83  108.63   0.9263
IC O4   C4   C5   O5   1.4440  111.20   64.86  111.55   1.4236
IC C4   C5   O5   HO5  1.4950  111.55 -127.57  107.69   0.8505
IC O5   C4  *C5   H51  1.4236  111.55 -124.94  108.14   0.9881
IC O5   C4  *C5   H52  1.4236  111.55  119.60  108.76   0.9311
IC C2   O4  *C1   O1   1.5227  105.48 -116.55  111.30   1.3905
IC O4   C1   O1   HO1  1.4227  109.76   66.79  107.33   0.9584
IC C2   O4  *C1   H1   1.5227  105.48  122.60  106.81   0.9349
IC C3   C1  *C2   H2   1.5223  101.04 -123.72  113.32   0.9736
IC C3   C1  *C2   O2   1.5223  101.04  114.67  111.40   1.4145
IC C1   C2   O2   HO2  1.5227  111.40   80.30  105.08   0.8475
IC C2   C4  *C3   O3   1.5223  102.70 -122.33  110.28   1.4117
IC C2   C4  *C3   H3   1.5223  102.70  114.19  111.24   0.9813
IC C4   C3   O3   HO3  1.5258  110.28 -141.24  107.85   0.8418
IC C2   C4  *C3   H4   1.5223  102.70  -89.81   25.03   2.0467
RESI AARB          0.0  !  alpha-Arabinose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                 / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                   / \       / \
ATOM C5   CC321   0.05  !                 H4   \      /   O1--HO1
ATOM H51  HCA2    0.09  !                      C3----C2
ATOM H52  HCA2    0.09  !                     /  \   / \
ATOM O5   OC311  -0.65  !              HO3--O3  H3  H2 O2
ATOM HO5  HCP1    0.42  !                              |
GROUP                   !                             HO2
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
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GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4306  107.10  -26.49  106.34   1.5438
IC O4   C1   C2   C3   1.4340  106.34    1.12  104.02   1.5260
IC C1   C2   C3   C4   1.5438  104.02   22.34  102.46   1.5303
IC C3   O4  *C4   C5   1.5303  103.09  123.36  110.44   1.5159
IC C3   O4  *C4   H4   1.5303  103.09 -115.64  113.85   1.0086
IC O4   C4   C5   O5   1.4306  110.44  -56.37  112.04   1.4264
IC C4   C5   O5   HO5  1.5159  112.04  102.19  102.06   0.9067
IC O5   C4  *C5   H51  1.4264  112.04  127.49  104.59   0.9921
IC O5   C4  *C5   H52  1.4264  112.04 -122.48  106.02   1.0363
IC C2   O4  *C1   O1   1.5438  106.34  115.42  111.62   1.4003
IC O4   C1   O1   HO1  1.4302  110.02   65.19  106.88   0.9590
IC C2   O4  *C1   H1   1.5438  106.34 -122.53  103.21   0.8654
IC C3   C1  *C2   H2   1.5260  104.02  116.77  107.88   0.9738
IC C3   C1  *C2   O2   1.5260  104.02 -125.34  114.46   1.4292
IC C1   C2   O2   HO2  1.5438  114.46   76.69  114.36   0.8703
IC C2   C4  *C3   O3   1.5260  102.46 -119.30  112.98   1.4288
IC C2   C4  *C3   H3   1.5260  102.46  117.20  112.99   1.0436
IC C4   C3   O3   HO3  1.5303  112.98  -92.09  109.45   0.8415
IC C2   C4  *C3   H4   1.5260  102.46  -81.75   27.82   2.0656
RESI BARB          0.0  !  beta-Arabinose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                  / \        / \
ATOM C5   CC321   0.05  !                 H4   \      /   O1--HO1
ATOM H51  HCA2    0.09  !                      C3----C2
ATOM H52  HCA2    0.09  !                     /  \   / \
ATOM O5   OC311  -0.65  !              HO3--O3  H3  H2 O2
ATOM HO5  HCP1    0.42  !                              |
GROUP                   !                             HO2
ATOM C2   CC3151  0.14  !
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```
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4548  108.97   34.73  103.97   1.5359
IC O4   C1   C2   C3   1.4109  103.97  -41.14  100.87   1.5393
IC C1   C2   C3   C4   1.5359  100.87   31.90  103.23   1.5403
IC C3   O4  *C4   C5   1.5403  106.18  122.06  111.54   1.5130
IC C3   O4  *C4   H4   1.5403  106.18 -117.66  107.50   1.1035
IC O4   C4   C5   O5   1.4548  111.54   73.00  112.71   1.4167
IC C4   C5   O5   HO5  1.5130  112.71  -63.34  111.90   0.9759
IC O5   C4  *C5   H51  1.4167  112.71  118.93  109.63   1.0973
IC O5   C4  *C5   H52  1.4167  112.71 -123.60  108.79   1.1016
IC C2   O4  *C1   O1   1.5359  103.97 -116.48  112.55   1.4080
IC O4   C1   O1   HO1  1.4302  110.02   65.19  106.88   0.9590
IC C2   O4  *C1   H1   1.5359  103.97  122.08  107.20   1.1084
IC C3   C1  *C2   H2   1.5393  100.87  114.97  107.92   1.0994
IC C3   C1  *C2   O2   1.5393  100.87 -123.41  116.28   1.4042
IC C1   C2   O2   HO2  1.5359  116.28   69.52  111.91   0.9792
IC C2   C4  *C3   O3   1.5393  103.23 -122.92  110.55   1.4162
IC C2   C4  *C3   H3   1.5393  103.23  114.63  110.37   1.0999
IC C4   C3   O3   HO3  1.5403  110.55 -146.15  107.12   0.9899
IC C2   C4  *C3   H4   1.5393  103.23 -103.11   28.42   2.1796
RESI ALYF          0.0  !  alpha-Lyxofuranose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                 / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                   / \       / \
ATOM C5   CC321   0.05  !                  H4   \      /   O1--HO1
ATOM H51  HCA2    0.09  !                       C3----C2
ATOM H52  HCA2    0.09  !                      /  \   / \
ATOM O5   OC311  -0.65  !                    H3  O3  H2 O2
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```
ATOM HO5  HCP1    0.42  !                          |       |
GROUP                   !                        HO3     HO2
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4508  108.66   -7.71  105.45   1.5350
IC O4   C1   C2   C3   1.4423  105.45  -20.33  103.34   1.5260
IC C1   C2   C3   C4   1.5350  103.34   38.67   99.49   1.5213
IC C3   O4  *C4   C5   1.5213  103.18  123.49  110.50   1.5094
IC C3   O4  *C4   H4   1.5213  103.18 -116.37  110.06   0.9177
IC O4   C4   C5   O5   1.4508  110.50   64.45  111.91   1.4362
IC C4   C5   O5   HO5  1.5094  111.91 -100.83  106.52   0.8229
IC O5   C4  *C5   H51  1.4362  111.91 -122.96  111.22   0.9610
IC O5   C4  *C5   H52  1.4362  111.91  118.00  105.92   0.9981
IC C2   O4  *C1   O1   1.5350  105.45  117.18  111.33   1.3990
IC O4   C1   O1   HO1  1.4298  109.95   66.51  107.28   0.9594
IC C2   O4  *C1   H1   1.5350  105.45 -122.79  104.35   0.9461
IC C3   C1  *C2   H2   1.5260  103.34  114.87  109.77   0.9507
IC C3   C1  *C2   O2   1.5260  103.34 -124.11  111.80   1.4233
IC C1   C2   O2   HO2  1.5350  111.80 -137.09  106.49   0.8342
IC C2   C4  *C3   O3   1.5260   99.49  115.69  108.16   1.4208
IC C2   C4  *C3   H3   1.5260   99.49 -120.13  112.07   0.9599
IC C4   C3   O3   HO3  1.5213  108.16  166.83  108.82   0.7802
IC C2   C4  *C3   H4   1.5260   99.49  -73.23   25.44   2.0181
RESI BLYF          0.0  !  beta-Lyxofuranose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                 / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                   / \       / \
ATOM C5   CC321   0.05  !                  H4   \     /   O1--HO1
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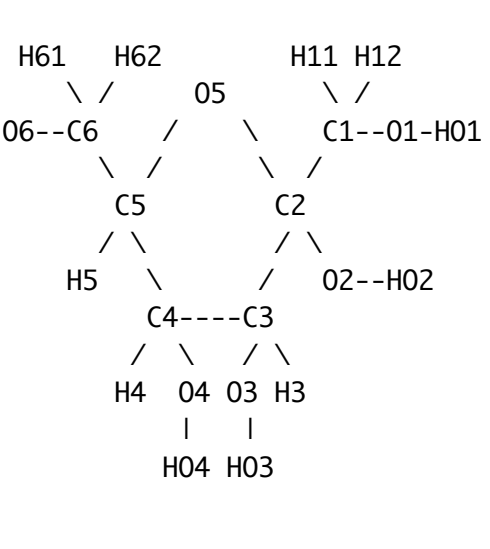
```
ATOM H51  HCA2    0.09  !                      C3----C2
ATOM H52  HCA2    0.09  !                     /  \   / \
ATOM O5   OC311  -0.65  !                   H3  O3  H2 O2
ATOM HO5  HCP1    0.42  !                       |      |
GROUP                   !                      HO3    HO2
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4315  107.76  -22.45  106.42   1.5606
IC O4   C1   C2   C3   1.4298  106.42   -6.06  102.41   1.5494
IC C1   C2   C3   C4   1.5606  102.41   29.67  101.01   1.5315
IC C3   O4  *C4   C5   1.5315  102.23  127.07  113.37   1.5469
IC C3   O4  *C4   H4   1.5315  102.23 -114.55  106.16   1.1145
IC O4   C4   C5   O5   1.4315  113.37  172.78  110.88   1.4279
IC C4   C5   O5   HO5  1.5469  110.88  -89.23  111.11   0.9627
IC O5   C4  *C5   H51  1.4279  110.88  120.67  109.96   1.1012
IC O5   C4  *C5   H52  1.4279  110.88 -120.92  109.55   1.1021
IC C2   O4  *C1   O1   1.5606  106.42 -121.62  109.95   1.3992
IC O4   C1   O1   HO1  1.4298  109.95   66.51  107.28   0.9594
IC C2   O4  *C1   H1   1.5606  106.42  119.08  107.39   1.1123
IC C3   C1  *C2   H2   1.5494  102.41  115.35  109.45   1.1122
IC C3   C1  *C2   O2   1.5494  102.41 -123.37  114.05   1.4282
IC C1   C2   O2   HO2  1.5606  114.05  104.03  106.69   0.9675
IC C2   C4  *C3   O3   1.5494  101.01  118.58  111.21   1.4279
IC C2   C4  *C3   H3   1.5494  101.01 -119.18  112.30   1.1095
IC C4   C3   O3   HO3  1.5315  111.21  -32.26  108.53   0.9635
IC C2   C4  *C3   H4   1.5494  101.01  -68.34   28.96   2.1721
RESI AXYF          0.0  !  alpha-Xylofuranose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
ATOM O1   OC311  -0.65  !                 \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                 / \  /      \  /
```

```
ATOM H4   HCA1    0.09  !               H52   C4        C1
GROUP                   !                    / \        / \
ATOM C5   CC321   0.05  !                  H4   \      /   O1--HO1
ATOM H51  HCA2    0.09  !                       C3----C2
ATOM H52  HCA2    0.09  !                      /  \   / \
ATOM O5   OC311  -0.65  !                     H3  O3 O2 H2
ATOM HO5  HCP1    0.42  !                         |   |
GROUP                   !                        HO3 HO2
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4499  110.14  -28.22  104.00   1.5265
IC O4   C1   C2   C3   1.4186  104.00   40.39  101.04   1.5264
IC C1   C2   C3   C4   1.5265  101.04  -36.87  102.46   1.5422
IC C3   O4  *C4   C5   1.5422  105.44  125.67  107.30   1.5196
IC C3   O4  *C4   H4   1.5422  105.44 -122.50  107.03   0.9837
IC O4   C4   C5   O5   1.4499  107.30  -67.21  114.12   1.4235
IC C4   C5   O5   HO5  1.5196  114.12   69.48  106.22   0.7593
IC O5   C4  *C5   H51  1.4235  114.12 -117.13  109.10   0.9433
IC O5   C4  *C5   H52  1.4235  114.12  125.77  106.78   0.9482
IC C2   O4  *C1   O1   1.5265  104.00  116.88  112.60   1.4045
IC O4   C1   O1   HO1  1.4288  110.19   60.16  106.38   0.9603
IC C2   O4  *C1   H1   1.5265  104.00 -124.86  106.28   0.9211
IC C3   C1  *C2   H2   1.5264  101.04 -115.23  105.83   0.9677
IC C3   C1  *C2   O2   1.5264  101.04  124.69  114.86   1.4186
IC C1   C2   O2   HO2  1.5265  114.86  -77.13  109.68   0.7338
IC C2   C4  *C3   O3   1.5264  102.46  123.87  113.27   1.4234
IC C2   C4  *C3   H3   1.5264  102.46 -112.51  113.63   0.9361
IC C4   C3   O3   HO3  1.5422  113.27  154.10  106.17   0.8221
IC C2   C4  *C3   H4   1.5264  102.46 -138.78   24.60   2.1476
RESI BXYF          0.0  !  beta-Xylofuranose
GROUP
ATOM O4   OC3C51 -0.40  !
ATOM C1   CC3152  0.34  !
ATOM H1   HCA1    0.09  !           HO5--O5
```

```
ATOM O1   OC311  -0.65  !                \       O4
ATOM HO1  HCP1    0.42  !             H51--C5   /    \    H1
ATOM C4   CC3153  0.11  !                / \  /      \  /
ATOM H4   HCA1    0.09  !              H52   C4        C1
GROUP                   !                   / \        / \
ATOM C5   CC321   0.05  !                 H4   \      /   O1--HO1
ATOM H51  HCA2    0.09  !                      C3----C2
ATOM H52  HCA2    0.09  !                     /  \   / \
ATOM O5   OC311  -0.65  !                   H3  O3 O2 H2
ATOM HO5  HCP1    0.42  !                       |   |
GROUP                   !                     HO3 HO2
ATOM C2   CC3151  0.14  !
ATOM H2   HCA1    0.09  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
BOND O4 C1  C1 H1   C1 O1   O1 HO1
BOND C1 C2  C2 H2   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 C5   C4 O4
BOND C5 H51 C5 H52  C5 O5   O5 HO5
IC C4   O4   C1   C2   1.4368  109.21    7.17  106.92   1.5609
IC O4   C1   C2   C3   1.4288  106.92  -29.31  100.61   1.5256
IC C1   C2   C3   C4   1.5609  100.61   38.33  101.22   1.5366
IC C3   O4  *C4   C5   1.5366  105.95  126.07  111.10   1.5466
IC C3   O4  *C4   H4   1.5366  105.95 -115.62  106.41   1.1129
IC O4   C4   C5   O5   1.4368  111.10 -170.12  111.17   1.4292
IC C4   C5   O5   HO5  1.5466  111.17  -86.81  110.69   0.9637
IC O5   C4  *C5   H51  1.4292  111.17  119.44  108.73   1.1031
IC O5   C4  *C5   H52  1.4292  111.17 -122.76  110.12   1.1017
IC C2   O4  *C1   O1   1.5609  106.92 -123.12  110.19   1.4024
IC O4   C1   O1   HO1  1.4288  110.19   60.16  106.38   0.9603
IC C2   O4  *C1   H1   1.5609  106.92  117.24  106.84   1.1130
IC C3   C1  *C2   H2   1.5256  100.61 -119.80  111.22   1.1086
IC C3   C1  *C2   O2   1.5256  100.61  116.99  113.84   1.4299
IC C1   C2   O2   HO2  1.5609  113.84   25.15  106.11   0.9678
IC C2   C4  *C3   O3   1.5256  101.22  116.82  111.32   1.4223
IC C2   C4  *C3   H3   1.5256  101.22 -120.45  112.39   1.1104
IC C4   C3   O3   HO3  1.5366  111.32   68.17  107.50   0.9664
IC C2   C4  *C3   H4   1.5256  101.22  -77.82   29.09   2.1676
RESI AFRU          0.0  !  alpha-Fructofuranose
GROUP
```

```
ATOM O5   OC3C51 -0.40  !
ATOM C2   CC3051  0.43  !
ATOM O2   OC311  -0.65  !
ATOM HO2  HCP1    0.42  !
ATOM C5   CC3153  0.11  !
ATOM H5   HCA1    0.09  !
GROUP                   !
ATOM C6   CC321   0.05  !
ATOM H61  HCA2    0.09  !
ATOM H62  HCA2    0.09  !
ATOM O6   OC311  -0.65  !
ATOM HO6  HCP1    0.42  !
GROUP                   !
ATOM C1   CC321   0.05  !
ATOM H11  HCA2    0.09  !
ATOM H12  HCA2    0.09  !
ATOM O1   OC311  -0.65  !
ATOM HO1  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
GROUP                   !
ATOM C4   CC3151  0.14  !
ATOM H4   HCA1    0.09  !
ATOM O4   OC311  -0.65  !
ATOM HO4  HCP1    0.42  !
BOND O5 C2  C2 C1   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 O4   O4 HO4
BOND C4 C5  C5 H5   C5 C6   C5 O5
BOND C6 H61 C6 H62  C6 O6   O6 HO6
BOND C1 H11 C1 H12  C1 O1   O1 HO1
IC C5   O5   C2   C3   1.4395  110.18   -3.87  105.48    1.5648
IC O5   C2   C3   C4   1.4336  105.48  -22.42  101.84    1.5306
IC C2   C3   C4   C5   1.5648  101.84   38.32  100.70    1.5279
IC C4   O5  *C5   C6   1.5279  103.59  125.05  112.69    1.5464
IC C4   O5  *C5   H5   1.5279  103.59 -115.88  106.71    1.1148
IC O5   C5   C6   O6   1.4395  112.69   61.06  111.04    1.4266
IC C5   C6   O6   HO6  1.5464  111.04  -54.34  109.23    0.9640
IC O6   C5  *C6   H61  1.4266  111.04  120.13  109.35    1.1026
IC O6   C5  *C6   H62  1.4266  111.04 -121.07  109.82    1.1014
IC C3   O5  *C2   O2   1.5648  105.48  118.28  109.92    1.4008
IC O5   C2   O2   HO2  1.4336  109.92   74.40  106.34    0.9587
IC C4   C2  *C3   H3   1.5306  101.84  113.46  108.58    1.1157
```



```
IC C4   C2  *C3   O3   1.5306  101.84 -124.07  116.26    1.4342
IC C2   C3   O3   HO3  1.5648  116.26 -110.77  108.92    0.9651
IC C3   C5  *C4   O4   1.5306  100.70 -121.44  112.56    1.4204
IC C3   C5  *C4   H4   1.5306  100.70  116.39  109.75    1.1135
IC C5   C4   O4   HO4  1.5279  112.56 -173.27  109.31    0.9636
IC C3   C5  *C4   H5   1.5306  100.70  -71.96   28.83    2.1752
IC C5   O5   C2   C1   1.4395  110.18 -125.10  106.36    1.5716
IC O5   C2   C1   H11  1.4336  106.36   64.27  108.72    1.1000
IC O5   C2   C1   H12  1.4336  106.36  -52.00  108.02    1.1012
IC O5   C2   C1   O1   1.4336  106.36 -172.81  115.31    1.4354
IC C2   C1   O1   HO1  1.5716  115.31  -62.37  108.51    0.9672
IC O1   C2  *C1   H11  1.4354  115.31 -122.91  108.72    1.1000
IC O1   C2  *C1   H12  1.4354  115.31  120.81  108.02    1.1012
RESI BFRU          0.0  !  beta-Fructofuranose
GROUP
ATOM O5   OC3C51 -0.40  !
ATOM C2   CC3051  0.43  !              H61   H62        H11 H12
ATOM O2   OC311  -0.65  !                 \ /     O5      \ /
ATOM HO2  HCP1    0.42  !           HO6-O6--C6   /    \    C1--O1-HO1
ATOM C5   CC3153  0.11  !                     \  /      \  /
ATOM H5   HCA1    0.09  !                      C5        C2
GROUP                   !                     / \        / \
ATOM C6   CC321   0.05  !                   H5   \      /   O2--HO2
ATOM H61  HCA2    0.09  !                        C4----C3
ATOM H62  HCA2    0.09  !                       /  \   / \
ATOM O6   OC311  -0.65  !                      H4  O4 O3 H3
ATOM HO6  HCP1    0.42  !                          |   |
GROUP                   !                         HO4 HO3
ATOM C1   CC321   0.05  !
ATOM H11  HCA2    0.09  !
ATOM H12  HCA2    0.09  !
ATOM O1   OC311  -0.65  !
ATOM HO1  HCP1    0.42  !
GROUP                   !
ATOM C3   CC3151  0.14  !
ATOM H3   HCA1    0.09  !
ATOM O3   OC311  -0.65  !
ATOM HO3  HCP1    0.42  !
GROUP                   !
ATOM C4   CC3151  0.14  !
ATOM H4   HCA1    0.09  !
ATOM O4   OC311  -0.65  !
ATOM HO4  HCP1    0.42  !
BOND O5 C2  C2 C1   C2 O2   O2 HO2
BOND C2 C3  C3 H3   C3 O3   O3 HO3
BOND C3 C4  C4 H4   C4 O4   O4 HO4
```

```
BOND C4 C5  C5 H5   C5 C6   C5 O5
BOND C6 H61 C6 H62  C6 O6   O6 HO6
BOND C1 H11 C1 H12  C1 O1   O1 HO1
IC C5   O5   C2   C3   1.4445  110.17   24.54  103.90    1.5535
IC O5   C2   C3   C4   1.4287  103.90  -39.46  100.37    1.5308
IC C2   C3   C4   C5   1.5535  100.37   38.82  101.99    1.5367
IC C4   O5  *C5   C6   1.5367  106.18  125.52  112.09    1.5470
IC C4   O5  *C5   H5   1.5367  106.18 -116.60  106.00    1.1142
IC O5   C5   C6   O6   1.4445  112.09   59.25  111.08    1.4266
IC C5   C6   O6   HO6  1.5470  111.08  -58.47  108.57    0.9643
IC O6   C5  *C6   H61  1.4266  111.08  120.33  109.39    1.1023
IC O6   C5  *C6   H62  1.4266  111.08 -120.82  109.55    1.1021
IC C3   O5  *C2   O2   1.5535  103.90 -118.22  109.18    1.4035
IC O5   C2   O2   HO2  1.4287  109.18  159.12  104.91    0.9617
IC C4   C2  *C3   H3   1.5308  100.37  114.40  108.58    1.1131
IC C4   C2  *C3   O3   1.5308  100.37 -122.50  115.94    1.4351
IC C2   C3   O3   HO3  1.5535  115.94  -76.65  108.79    0.9673
IC C3   C5  *C4   O4   1.5308  101.99 -122.06  112.87    1.4204
IC C3   C5  *C4   H4   1.5308  101.99  116.11  109.34    1.1142
IC C5   C4   O4   HO4  1.5367  112.87 -177.81  108.59    0.9641
IC C3   C5  *C4   H5   1.5308  101.99  -88.31   28.76    2.1807
IC C5   O5   C2   C1   1.4445  110.17  145.62  109.90    1.5622
IC O5   C2   C1   H11  1.4287  109.90   62.33  108.75    1.1018
IC O5   C2   C1   H12  1.4287  109.90  -54.09  107.90    1.1015
IC O5   C2   C1   O1   1.4287  109.90 -174.69  113.93    1.4392
IC C2   C1   O1   HO1  1.5622  113.93  -99.33  109.99    0.9653
IC O1   C2  *C1   H11  1.4392  113.93 -122.98  108.75    1.1018
IC O1   C2  *C1   H12  1.4392  113.93  120.60  107.90    1.1015
PRES FOMEA          0.11 ! alpha O-methyl to C1 on aldopentose
dele atom HO1
ATOM C1   CC3152    0.29 !
ATOM O1   OC301    -0.36 !
ATOM CM   CC331    -0.09 !
ATOM HM1  HCA3      0.09 !
ATOM HM2  HCA3      0.09 !
ATOM HM3  HCA3      0.09 !
BOND O1 CM
BOND CM HM1  CM HM2  CM HM3
IC O4   C1   O1   CM   1.4477  109.89   66.08  108.74   1.4244
IC C1   O1   CM   HM1  1.4355  108.74   59.11  111.44   1.0883
IC HM1  O1  *CM   HM2  1.0883  111.44  119.69  113.64   1.0586
IC HM3  O1  *CM   HM2  1.1131  110.64 -122.99  113.64   1.0586
PRES FOMEB          0.11 ! beta O-methyl to C1 on aldopentose
dele atom HO1
ATOM C1   CC3152    0.29 !
ATOM O1   OC301    -0.36 !
```

```
ATOM CM   CC331    -0.09 !
ATOM HM1  HCA3      0.09 !
ATOM HM2  HCA3      0.09 !
ATOM HM3  HCA3      0.09 !
BOND O1 CM
BOND CM HM1  CM HM2  CM HM3
IC O4   C1   O1   CM   1.4138  114.30  -66.36  108.55   1.4077
IC C1   O1   CM   HM1  1.4353  108.55   41.11  109.39   1.0734
IC HM1  O1  *CM   HM2  1.0734  109.39  129.90  119.45   1.0441
IC HM3  O1  *CM   HM2  1.1148  107.24 -121.74  119.45   1.0441
END
```

Table S8.Parameter file for furanose compounds

```
* $Id: par_allxx_sugar.inp,v 1.106 2009-03-16 16:03:28 ehatcher Exp $
* Parameter file for furanose carbohydrates
* Hatcher, Guvench, and MacKerell
*
BONDS
OC3C51  CC3152   350.00  1.425
OC3C51  CC3051   350.00  1.425
OC3C51  CC3153   350.00  1.425
OC311   CC3152   428.00  1.395
OC311   CC3051   428.00  1.395
OC311   CC3151   410.00  1.395
CC3152  HCA1     309.00  1.111
CC3251  HCA2     307.00  1.100
CC3151  HCA1     309.00  1.111
CC3153  HCA1     309.00  1.111
CC3152  CC3251   195.00  1.508
CC3051  CC3251   195.00  1.508
CC3251  CC3151   195.00  1.508
CC3151  CC3153   195.00  1.508
CC3151  CC3152   195.00  1.508
CC3151  CC3051   195.00  1.508
CC3151  CC3151   195.00  1.508
CC3153  CC321    222.50  1.490
CC3051  CC321    222.50  1.490
CC3152  OC301    360.00  1.395
CC331   OC301    360.00  1.415
CC331   HCA3     322.00  1.111
ANGLES
OC3C51 CC3152 CC3251     45.00   111.10
OC3C51 CC3051 CC3251     45.00   111.10
OC3C51 CC3152 CC3151     45.00   111.10
OC3C51 CC3051 CC3151     45.00   111.10
OC3C51 CC3153 CC3151     45.00   111.10
OC3C51 CC3153 CC321      45.000  108.00
OC3C51 CC3051 CC321      45.000  108.00
OC311  CC3151 CC3251     75.700  110.10
OC311  CC3151 CC3153     75.700  110.10
OC311  CC3151 CC3152     75.700  110.10
OC311  CC3151 CC3051     75.700  110.10
OC311  CC3151 CC3151     75.700  110.10
OC311  CC321  CC3153     75.700  110.10
OC311  CC321  CC3152     75.700  110.10
OC311  CC321  CC3051     75.700  110.10
OC311  CC3152 CC3251     75.700  110.10
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OC311  CC3051 CC3251     75.700  110.10
OC311  CC3152 CC321      75.700  110.10
OC311  CC3051 CC321      75.700  110.10
OC311  CC3152 CC3151     75.700  110.10
OC311  CC3051 CC3151     75.700  110.10
OC3C51 CC3152 OC311      45.000  116.50
OC3C51 CC3051 OC311      45.000  116.50
OC3C51 CC3152 HCA1       70.00   107.30
OC3C51 CC3153 HCA1       70.00   107.30
OC311  CC3152 HCA1       55.000  108.89
OC311  CC3151 HCA1       55.000  108.89
CC3152 OC311  HCP1       50.000  109.00
CC3051 OC311  HCP1       50.000  109.00
CC3151 OC311  HCP1       50.000  109.00
CC3153 OC3C51 CC3152     95.00   111.00
CC3153 OC3C51 CC3051     95.00   111.00
CC3152 CC3251 CC3151     58.00   109.50   11.16   2.561
CC3051 CC3251 CC3151     58.00   109.50   11.16   2.561
CC3152 CC3151 CC3151     58.00   109.50   11.16   2.561
CC3051 CC3151 CC3151     58.00   109.50   11.16   2.561
CC3251 CC3151 CC3153     58.00   109.50   11.16   2.561
CC3151 CC3151 CC3153     58.00   109.50   11.16   2.561
CC3151 CC3153 CC321      58.35   113.50   11.16   2.561
CC3151 CC3051 CC321      58.35   113.50   11.16   2.561
CC3152 CC3251 HCA2       35.00   111.40   22.53   2.179
CC3051 CC3251 HCA2       35.00   111.40   22.53   2.179
CC3251 CC3152 HCA1       35.00   111.40   22.53   2.179
CC3251 CC3151 HCA1       35.00   111.40   22.53   2.179
CC3151 CC3251 HCA2       35.00   111.40   22.53   2.179
CC3153 CC3151 HCA1       35.00   111.40   22.53   2.179
CC3152 CC3151 HCA1       35.00   111.40   22.53   2.179
CC3051 CC3151 HCA1       35.00   111.40   22.53   2.179
CC3151 CC3151 HCA1       35.00   111.40   22.53   2.179
CC3151 CC3152 HCA1       35.00   111.40   22.53   2.179
CC3151 CC3153 HCA1       35.00   111.40   22.53   2.179
CC3153 CC321  HCA2       33.43   110.10   22.53   2.179
CC3152 CC321  HCA2       33.43   110.10   22.53   2.179
CC3051 CC321  HCA2       33.43   110.10   22.53   2.179
CC321  CC3153 HCA1       34.50   110.10   22.53   2.179
HCA2   CC3251 HCA2       38.50   106.80    5.40   1.802
HCA1   CC3152 OC301      60.00   109.50
OC301  CC3152 CC3151     45.00   105.00
CC3152 OC301  CC331      95.00   111.00
OC301  CC3152 OC3C51     90.00   112.00
OC301  CC331  HCA3       60.00   109.50
DIHEDRALS
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```
OC3C51 CC3152 OC311  HCP1      1.17  1    0.0
OC3C51 CC3152 OC311  HCP1      0.85  2    0.0
OC3C51 CC3152 OC311  HCP1      0.37  3    0.0
OC3C51 CC3051 OC311  HCP1      0.90  1    0.0
OC3C51 CC3051 OC311  HCP1      1.14  2    0.0
OC3C51 CC3051 OC311  HCP1      0.11  3  180.0
OC3C51 CC3152 CC3251 HCA2      0.20  3    0.0
OC3C51 CC3051 CC3251 HCA2      0.20  3    0.0
OC3C51 CC3152 CC3151 HCA1      0.20  3    0.0
OC3C51 CC3051 CC3151 HCA1      0.20  3    0.0
OC3C51 CC3153 CC3151 HCA1      0.20  3    0.0
OC3C51 CC3153 CC321  HCA2      0.20  3    0.0
OC3C51 CC3152 CC321  HCA2      0.20  3    0.0
OC3C51 CC3051 CC321  HCA2      0.20  3    0.0
OC311  CC3152 CC3251 HCA2      0.14  3    0.0
OC311  CC3051 CC3251 HCA2      0.14  3    0.0
OC311  CC3051 CC321  HCA2      0.14  3    0.0
OC311  CC3151 CC3251 HCA2      0.14  3    0.0
OC311  CC3151 CC3153 HCA1      0.14  3    0.0
OC311  CC3151 CC3152 HCA1      0.14  3    0.0
OC311  CC3151 CC3151 HCA1      0.14  3    0.0
OC311  CC3152 CC3151 HCA1      0.14  3    0.0
OC311  CC3051 CC3151 HCA1      0.14  3    0.0
OC311  CC321  CC3153 HCA1      0.14  3    0.0
OC3C51 CC3153 CC3151 OC311     0.14  1    0.0
OC3C51 CC3153 CC3151 OC311     0.70  2    0.0
OC3C51 CC3153 CC3151 OC311     0.18  3    0.0
OC3C51 CC3152 CC3151 OC311     1.26  1  180.0
OC3C51 CC3152 CC3151 OC311     1.27  2    0.0
OC3C51 CC3152 CC3151 OC311     0.53  3    0.0
OC3C51 CC3051 CC3151 OC311     0.32  1  180.0
OC3C51 CC3051 CC3151 OC311     0.65  2  180.0
OC3C51 CC3051 CC3151 OC311     2.62  3    0.0
OC3C51 CC3153 CC321  OC311     1.50  1  180.0
OC3C51 CC3153 CC321  OC311     0.58  2    0.0
OC3C51 CC3153 CC321  OC311     0.54  3    0.0
OC3C51 CC3051 CC321  OC311     0.52  1    0.0
OC3C51 CC3051 CC321  OC311     1.16  2  180.0
OC3C51 CC3051 CC321  OC311     0.33  3  180.0
OC311  CC3152 CC3151 OC311     2.87  1  180.0
OC311  CC3152 CC3151 OC311     0.03  2    0.0
OC311  CC3152 CC3151 OC311     0.23  3    0.0
OC311  CC3051 CC3151 OC311     0.12  1  180.0
OC311  CC3051 CC3151 OC311     1.87  2  180.0
OC311  CC3051 CC3151 OC311     1.64  3  180.0
OC311  CC3151 CC3151 OC311     2.87  1  180.0
```

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OC311  CC3151 CC3151 OC311     0.03  2    0.0
OC311  CC3151 CC3151 OC311     0.23  3    0.0
OC311  CC3051 CC321  OC311     0.07  1    0.0
OC311  CC3051 CC321  OC311     1.99  2  180.0
OC311  CC3051 CC321  OC311     1.72  3  180.0
OC311  CC3152 OC3C51 CC3153    0.76  1  180.0
OC311  CC3152 OC3C51 CC3153    1.25  2    0.0
OC311  CC3152 OC3C51 CC3153    0.48  3  180.0
OC311  CC3051 OC3C51 CC3153    0.19  1  180.0
OC311  CC3051 OC3C51 CC3153    2.85  2  180.0
OC311  CC3051 OC3C51 CC3153    0.86  3    0.0
CC3152 CC3251 CC3151 CC3153    1.83  3    0.0
CC3051 CC3251 CC3151 CC3153    1.83  3    0.0
CC3152 CC3151 CC3151 CC3153    0.64  3  180.0
CC3051 CC3151 CC3151 CC3153    2.37  3    0.0
CC3251 CC3151 CC3153 CC321     0.20  3    0.0
CC3151 CC3151 CC3153 CC321     0.20  3    0.0
CC3151 CC3151 CC3051 CC321     0.20  3    0.0
CC3152 CC3251 CC3151 OC311     0.39  1    0.0
CC3152 CC3251 CC3151 OC311     1.20  2    0.0
CC3152 CC3251 CC3151 OC311     1.42  3  180.0
CC3051 CC3251 CC3151 OC311     0.39  1    0.0
CC3051 CC3251 CC3151 OC311     1.20  2    0.0
CC3051 CC3251 CC3151 OC311     1.42  3  180.0
CC3153 CC3151 CC3151 OC311     0.01  1  180.0
CC3153 CC3151 CC3151 OC311     0.72  2    0.0
CC3153 CC3151 CC3151 OC311     0.73  3    0.0
CC3152 CC3151 CC3151 OC311     0.81  1  180.0
CC3152 CC3151 CC3151 OC311     1.07  2    0.0
CC3152 CC3151 CC3151 OC311     0.11  3    0.0
CC3051 CC3151 CC3151 OC311     2.07  1    0.0
CC3051 CC3151 CC3151 OC311     2.13  2    0.0
CC3051 CC3151 CC3151 OC311     2.71  3  180.0
CC3151 CC3251 CC3152 OC311     0.56  1  180.0
CC3151 CC3251 CC3152 OC311     0.30  2  180.0
CC3151 CC3251 CC3152 OC311     0.35  3  180.0
CC3151 CC3251 CC3051 OC311     0.56  1  180.0
CC3151 CC3251 CC3051 OC311     0.30  2  180.0
CC3151 CC3251 CC3051 OC311     0.35  3  180.0
CC3151 CC3151 CC3152 OC311     0.11  1  180.0
CC3151 CC3151 CC3152 OC311     0.66  2    0.0
CC3151 CC3151 CC3152 OC311     0.02  3  180.0
CC3151 CC3151 CC3051 OC311     2.23  1    0.0
CC3151 CC3151 CC3051 OC311     3.00  2    0.0
CC3151 CC3151 CC3051 OC311     0.88  3  180.0
CC3151 CC3153 CC321  OC311     0.01  1    0.0
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CC3151 CC3153 CC321  OC311     0.14  2    0.0
CC3151 CC3153 CC321  OC311     0.70  3  180.0
CC3151 CC3051 CC321  OC311     1.59  1    0.0
CC3151 CC3051 CC321  OC311     0.95  2  180.0
CC3151 CC3051 CC321  OC311     1.95  3    0.0
CC321  CC3153 CC3151 OC311     0.76  1  180.0
CC321  CC3153 CC3151 OC311     0.40  2  180.0
CC321  CC3153 CC3151 OC311     0.40  3  180.0
CC321  CC3051 CC3151 OC311     0.94  1    0.0
CC321  CC3051 CC3151 OC311     1.59  2  180.0
CC321  CC3051 CC3151 OC311     0.84  3    0.0
CC3151 CC3151 CC3153 OC3C51    1.24  3    0.0
CC3151 CC3151 CC3152 OC3C51    1.24  3    0.0
CC3251 CC3151 CC3153 OC3C51    0.94  3    0.0
CC3151 CC3251 CC3152 OC3C51    0.94  3    0.0
CC3151 CC3251 CC3051 OC3C51    0.94  3    0.0
CC3151 CC3151 CC3051 OC3C51    0.62  3    0.0
CC3251 CC3152 OC311  HCP1      0.59  1    0.0
CC3251 CC3152 OC311  HCP1      0.38  2    0.0
CC3251 CC3152 OC311  HCP1      0.13  3    0.0
CC3251 CC3051 OC311  HCP1      0.59  1    0.0
CC3251 CC3051 OC311  HCP1      0.38  2    0.0
CC3251 CC3051 OC311  HCP1      0.13  3    0.0
CC321  CC3051 OC311  HCP1      0.40  1  180.0
CC321  CC3051 OC311  HCP1      0.48  2    0.0
CC321  CC3051 OC311  HCP1      0.19  3    0.0
CC3151 CC3152 OC311  HCP1      0.29  1    0.0
CC3151 CC3152 OC311  HCP1      0.55  2    0.0
CC3151 CC3152 OC311  HCP1      0.08  3    0.0
CC3151 CC3051 OC311  HCP1      0.40  1  180.0
CC3151 CC3051 OC311  HCP1      0.48  2    0.0
CC3151 CC3051 OC311  HCP1      0.19  3    0.0
CC3151 CC3151 OC311  HCP1      0.29  1    0.0
CC3151 CC3151 OC311  HCP1      0.55  2    0.0
CC3151 CC3151 OC311  HCP1      0.08  3    0.0
CC3152 CC3151 OC311  HCP1      0.29  1    0.0
CC3152 CC3151 OC311  HCP1      0.55  2    0.0
CC3152 CC3151 OC311  HCP1      0.08  3    0.0
CC3051 CC3151 OC311  HCP1      0.40  1  180.0
CC3051 CC3151 OC311  HCP1      0.48  2    0.0
CC3051 CC3151 OC311  HCP1      0.19  3    0.0
CC3251 CC3151 OC311  HCP1      0.59  1    0.0
CC3251 CC3151 OC311  HCP1      0.38  2    0.0
CC3251 CC3151 OC311  HCP1      0.13  3    0.0
CC3153 CC3151 OC311  HCP1      0.29  1    0.0
CC3153 CC3151 OC311  HCP1      0.55  2    0.0
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CC3153 CC3151 OC311  HCP1      0.08  3    0.0
CC3153 CC321  OC311  HCP1      0.12  1    0.0
CC3153 CC321  OC311  HCP1      0.42  2    0.0
CC3153 CC321  OC311  HCP1      0.29  3    0.0
CC3051 CC321  OC311  HCP1      0.40  1  180.0
CC3051 CC321  OC311  HCP1      0.48  2    0.0
CC3051 CC321  OC311  HCP1      0.19  3    0.0
CC3152 CC3251 CC3151 HCA1      0.20  3    0.0
CC3051 CC3251 CC3151 HCA1      0.20  3    0.0
CC3151 CC3251 CC3152 HCA1      0.20  3    0.0
CC3151 CC3151 CC3152 HCA1      0.20  3    0.0
CC3151 CC3151 CC3153 HCA1      0.20  3    0.0
CC3151 CC3153 CC321  HCA2      0.20  3    0.0
CC3151 CC3152 CC321  HCA2      0.20  3    0.0
CC3151 CC3051 CC321  HCA2      0.20  3    0.0
CC3153 CC3151 CC3251 HCA2      0.20  3    0.0
CC3153 CC3151 CC3151 HCA1      0.20  3    0.0
CC3152 CC3151 CC3151 HCA1      0.20  3    0.0
CC3051 CC3151 CC3151 HCA1      0.20  3    0.0
CC321  CC3153 CC3151 HCA1      0.20  3    0.0
CC321  CC3152 CC3151 HCA1      0.20  3    0.0
CC321  CC3051 CC3151 HCA1      0.20  3    0.0
CC3251 CC3151 CC3153 HCA1      0.20  3    0.0
CC3152 OC3C51 CC3153 CC3151    1.00  3    0.0
CC3153 OC3C51 CC3152 CC3151    1.00  3    0.0
CC3153 OC3C51 CC3152 CC3251    0.45  3    0.0
CC3153 OC3C51 CC3051 CC3151    0.61  3    0.0
CC3153 OC3C51 CC3051 CC3251    0.61  3    0.0
CC3051 OC3C51 CC3153 CC3151    0.43  3    0.0
CC3152 OC3C51 CC3153 CC321     0.30  3    0.0
CC3051 OC3C51 CC3153 CC321     2.58  1    0.0
CC3051 OC3C51 CC3153 CC321     0.24  2  180.0
CC3051 OC3C51 CC3153 CC321     0.36  3  180.0
CC3153 OC3C51 CC3051 CC321     0.24  1    0.0
CC3153 OC3C51 CC3051 CC321     3.00  2  180.0
CC3153 OC3C51 CC3051 CC321     1.38  3  180.0
CC3152 OC3C51 CC3153 HCA1      0.30  3    0.0
CC3051 OC3C51 CC3153 HCA1      0.30  3    0.0
CC3153 OC3C51 CC3152 HCA1      0.30  3    0.0
HCA1   CC3152 CC3251 HCA2      0.20  3    0.0
HCA2   CC3251 CC3151 HCA1      0.20  3    0.0
HCA1   CC3151 CC3153 HCA1      0.20  3    0.0
HCA1   CC3151 CC3152 HCA1      0.20  3    0.0
HCA1   CC3151 CC3151 HCA1      0.20  3    0.0
HCA1   CC3153 CC321  HCA2      0.20  3    0.0
HCP1   OC311  CC3152 HCA1      0.18  3    0.0
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HCP1   OC311  CC3151 HCA1      0.18  3    0.0
OC301  CC3152 CC3151 OC311     2.87  1  180.0
OC301  CC3152 CC3151 OC311     0.03  2    0.0
OC301  CC3152 CC3151 OC311     0.23  3    0.0
CC3152 OC301  CC331  HCA3      0.284 3    0.0
HCA1   CC3152 OC301  CC331     0.284 3    0.0
OC301  CC3152 CC3151 HCA1      0.20  3    0.0
CC3151 CC3151 CC3152 OC301     0.11  1  180.0
CC3151 CC3151 CC3152 OC301     0.66  2    0.0
CC3151 CC3151 CC3152 OC301     0.02  3  180.0
CC3151 CC3151 CC3051 OC301     2.23  1    0.0
CC3151 CC3151 CC3051 OC301     3.00  2    0.0
CC3151 CC3151 CC3051 OC301     0.88  3  180.0
OC301  CC3152 OC3C51 CC3153    0.76  1  180.0
OC301  CC3152 OC3C51 CC3153    1.25  2    0.0
OC301  CC3152 OC3C51 CC3153    0.48  3  180.0
CC3153 OC3C51 CC3051 OC301     0.19  1  180.0
CC3153 OC3C51 CC3051 OC301     2.85  2  180.0
CC3153 OC3C51 CC3051 OC301     0.86  3    0.0
CC3151 CC3152 OC301  CC331     0.21  1  180.0
CC3151 CC3152 OC301  CC331     0.34  2  180.0
CC3151 CC3152 OC301  CC331     0.74  3  180.0
CC331  OC301  CC3152 OC3C51    0.08  1    0.0
CC331  OC301  CC3152 OC3C51    0.76  2    0.0
CC331  OC301  CC3152 OC3C51    1.18  3    0.0
NONBONDED  NBXMOD 5  ATOM CDIEL FSHIFT VATOM VDISTANCE VFSWITCH -
     CUTNB 14.0  CTOFNB 12.0  CTONNB 10.0  EPS 1.0  E14FAC 1.0  WMIN 1.5
CC331     0.0  -0.0780   2.040 0.0 -0.01 1.9
HCA3      0.0  -0.0240   1.340
OC301     0.0  -0.1000   1.650
OC3C51    0.0  -0.1000   1.650
CC3152    0.0  -0.0320   2.000 0.0 -0.01 1.9
CC3051    0.0  -0.0320   2.000 0.0 -0.01 1.9
CC3251    0.0  -0.0600   2.020 0.0 -0.01 1.9
CC3151    0.0  -0.0320   2.000 0.0 -0.01 1.9
CC3153    0.0  -0.0320   2.000 0.0 -0.01 1.9
END
```