Supporting Information

Table 1
Calculated $^{2}J_{C1,O1,C4'}$ Values[a] in Geometrically-Optimized **1-4**

Disaccharide	$^{2}J_{C1,O1,C4'}$	ϕ[b]	ψ[c]	$\angle_{C1\text{-}O1\text{-}C4'}$	Energy[d]
1 60R	- 1.9	43.4	21.7	115.4°	0.1
1 60S	- 2.0	47.5	-17.1	116.3°	0.0
1 AP	- 2.4	31.9	170.7	118.9°	2.6
2 60S	- 2.1	31.7	-25.5	118.3°	0.0
2 AP	- 2.1	17.6	179.6	119.4°	2.4
3 60S	- 2.1	43.8	-19.4	116.9°	0.0
3 AP	- 2.8	51.9	-159.6	120.1°	3.2
4 60S	- 2.3	32.0	-22.1	118.7°	0.0
4 AP	- 2.1	16.5	-178.9	119.9°	2.8

[a]In Hz; *uncorrected* computed values. [b]Defined as H1-C1-O1-C4'. [c]Defined as C1-O1-C4'-H4'. [d]Relative energy within each group (in kcal/mol).

Supporting Information

Table 2

Calculated $^2J_{C1,O1,C4'}$ Values[a] in ψ-Constrained **1**

Disaccharide	$^2J_{C1,O1,C4'}$	φ[b]	ψ[c]	$\angle_{C1\text{-}O1\text{-}C4'}$	Energy[d]
1 60	-2.4	54.9°	60°	117.3°	1.5
1 80	-2.5	58.1°	80°	118.2°	2.4
1 110	-2.8	47.6°	110°	120.6°	4.4
1 130	-2.9	43.8°	130°	121.0°	4.6
1 150	-2.7	38.1°	150°	119.5°	3.4

[a]In Hz; *uncorrected* computed values. [b]Defined as H1-C1-O1-C4'. [c]Defined as C1-O1-C4'-H4'; held constant in the calculation (all other structural parameters were optimized). [d]Relative to the (most stable) 60S geometry of **1** (see Table 1).