

**Table S1.** Pyranose ring  $^3J_{\text{HH}}$ -values

Methyl $\alpha$ -(2,8)-disialoside						
	Residue a		Residue b			
	Experiment	Conventional MD	Experiment	Conventional MD	Experiment	Conventional MD
H3ax – H4	12.2 $\pm$ 0.1	11.0 $\pm$ 0.7	12.2 $\pm$ 0.1	11.0 $\pm$ 0.7		
H3eq – H4	4.4 $\pm$ 0.4	4.6 $\pm$ 1.2	4.4 $\pm$ 0.4	4.5 $\pm$ 1.2		
H4 – H5	10.2 $\pm$ 0.1	9.4 $\pm$ 0.8	10.3 $\pm$ 0.1	9.6 $\pm$ 0.7		
H5 – H6	10.2 $\pm$ 0.1	10.4 $\pm$ 0.5	10.3 $\pm$ 0.1	10.4 $\pm$ 0.4		

  

Methyl $\alpha$ -(2,8)-trisialoside						
	Residue a		Residue b		Residue c	
	Experiment	Conventional MD	Experiment	Conventional MD	Experiment	Conventional MD
H3ax – H4	12.3 $\pm$ 0.1	10.8 $\pm$ 1.3	12.3 $\pm$ 0.1	11.0 $\pm$ 0.7	12.3 $\pm$ 0.1	11.0 $\pm$ 0.7
H3eq – H4	4.3 $\pm$ 0.4	4.6 $\pm$ 1.2	4.3 $\pm$ 0.4	4.5 $\pm$ 1.2	4.3 $\pm$ 0.4	4.5 $\pm$ 1.2
H4 – H5	10.3 $\pm$ 0.1	9.4 $\pm$ 0.9	10.3 $\pm$ 0.1	9.5 $\pm$ 0.7	10.3 $\pm$ 0.1	9.6 $\pm$ 0.7
H5 – H6	10.3 $\pm$ 0.1	10.4 $\pm$ 0.4	10.3 $\pm$ 0.1	10.4 $\pm$ 0.4	10.3 $\pm$ 0.1	10.4 $\pm$ 0.4