Supporting Information for:

Evidence for two populated conformations for the dimeric Le^X and Le^ALe^X tumour associated carbohydrate antigens.

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Table 1. Proton chemical shifts (ppm) for compounds **2**, **4** and **5** in D_2O at 300 K.

	2	**4**	**5**
H-1*A*	4.62	4.62	4.46
H-2*A*	3.94	3.93	3.88
H-3*A*	3.87	3.87	3.84
H-4*A*	3.94	3.94	3.90
H-5*A*	3.61	3.60	3.58
H-6a*A*	4.01	4.01	4.00
H-6b*A*	3.86	3.85	3.83
H-1*B*	5.11	5.11	5.08
H-2*B*	3.70	3.69	3.67
H-3*B*	3.90	3.89	3.88
H-4*B*	3.79	3.79	3.77
H-5*B*	4.82	4.82	4.80
H-6*B*	1.16	1.16	1.14
H-1*C*	4.45	4.45	4.42
H-2*C*	3.52	3.52	3.50
H-3*C*	3.72	3.72	3.70
H-4*C*	4.06	4.07	4.09
H-5*C*	3.60	3.59	3.58
H-6a*C*	3.72–3.75	3.72–3.75	3.70
H-6b*C*	3.72–3.75	3.72–3.75	3.70
H-1*A'*	4.72	4.71	4.68
H-2*A'*	3.97	3.96	3.74
H-3*A'*	3.89	4.08	3.54
H-4*A'*	3.98	3.76	3.46
H-5*A'*	3.59	3.54	3.43
H-6a*A'*	3.99	3.96	3.88
H-6b*A'*	3.88	3.87	3.75
H-1*B'*	5.15	5.04	–[a]
H-2*B'*	3.71	3.81	–[a]
H-3*B'*	3.92	3.89	–[a]
H-4*B'*	3.80	3.80	–[a]
H-5*B'*	4.84	4.88	–[a]
H-6*B'*	1.19	1.19	–[a]
H-1*C'*	4.47	4.52	–[a]
H-2*C'*	3.51	3.49	–[a]
H-3*C'*	3.66	3.62	–[a]
H-4*C'*	3.91	3.89	–[a]
H-5*C'*	3.61	3.57	–[a]
H-6a*C'*	3.72–3.75	3.72–3.75	–[a]
H-6b*C'*	3.72–3.75	3.72–3.75	–[a]

[a] Not applicable

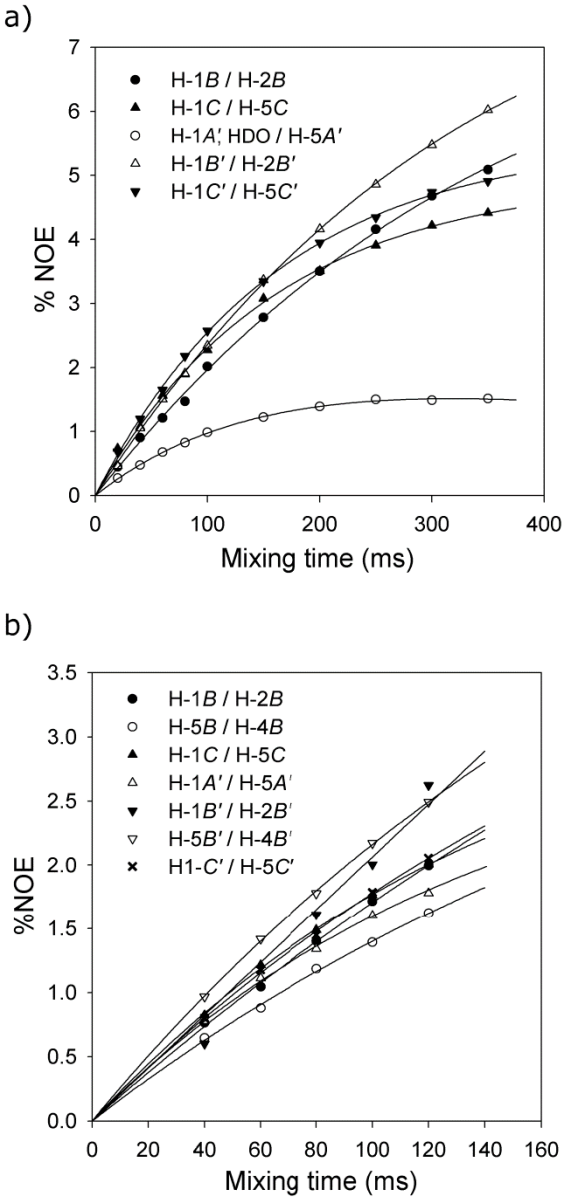

Figure 1. Normalized cross-relaxation buildup curves for signals used as references in distance calculation: a) hexasaccharide dimLe^x (**2**) at 800 MHz, b) hexasaccharide Le^aLe^x (**4**) at 600 MHz (cryoprobe).

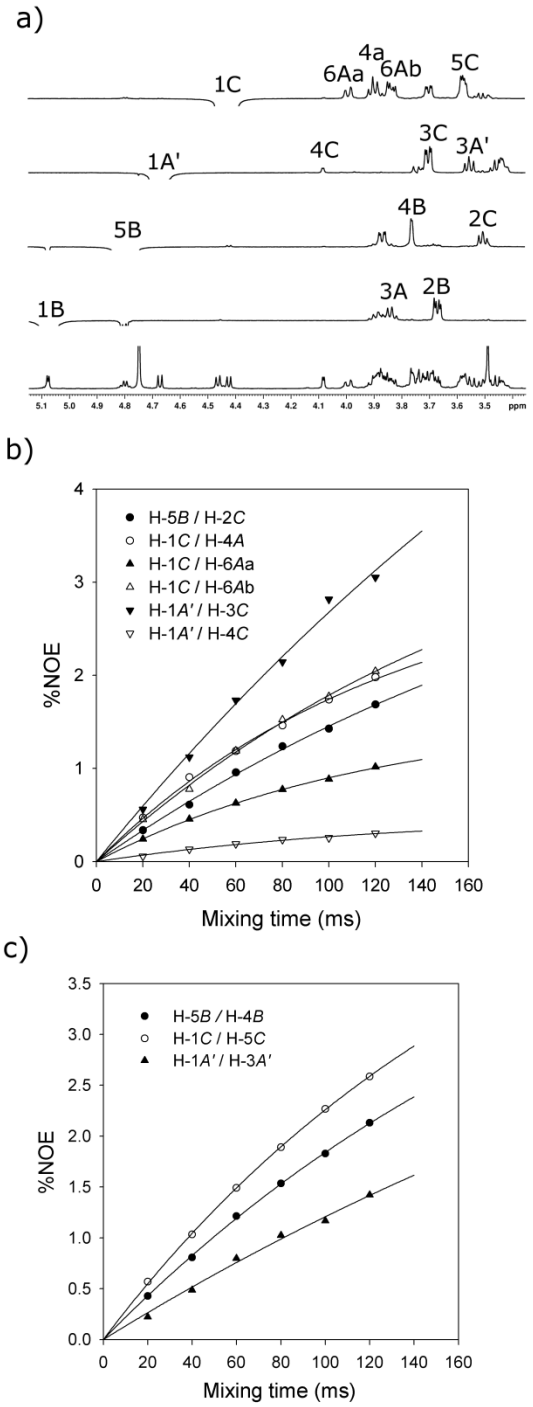

Figure 2. NMR data for tetrasaccharide **5** at 600 MHz (cryoprobe) and 300 K: a) ^{1}H NMR spectrum and ^{1}H, ^{1}H ROESY spectra upon selective excitation of protons H-1*B*, H-5*B*, H-1*C*, H-1*A'* (mixing time 120 ms), b) normalized cross-relaxation buildup curves used for distance calcultation, c) normalized cross-relaxation buildup curves for signals used as references in distance calculation.

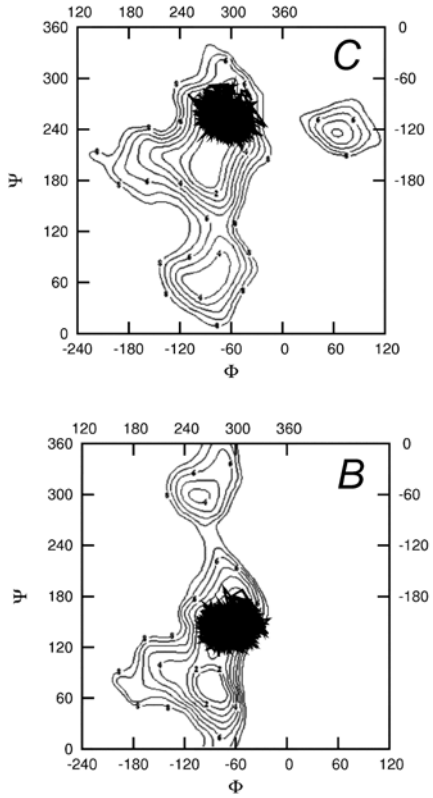

Figure 3. Trajectories (20 ns dynamics simulations, 300 K) of the fucosidic (Φ_B/Ψ_B) and galactosidic (Φ_C/Ψ_C) linkages in the Le^x trisaccharides portions of tetrasaccharide **5** superimposed on the MM3 grid search energy maps obtained for the disaccharide linkages (contours, text ref. 11a).