

Supplementary Information:

Enforced conformational changes in the structural units of glycosaminoglycan (non-sulfated heparin-based oligosaccharides)

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Tab. 1S Results for IdoA^c

Stretched structure			Relaxed structure					conformer
f	E	L	E[L	tau1	tau2	tau3	
[au]	[au]	[Å]	[au]	[Å]		[°]		
0.0000	-761.2197815	4.589	-761.2197815	4.589	51.58	-58.84	54.47	1C4
0.0150	-761.2155966	4.878	-761.2197819	4.589	51.81	-52.87	54.51	1C4
0.0200	-761.2122035	4.906	-761.2197820	4.589	51.82	-52.87	54.51	1C4
0.0250	-761.2076174	5.088	-761.2197821	4.589	51.82	-52.87	54.51	1C4
0.0285	-761.2031995	5.175	-761.2197813	4.589	51.81	-52.82	54.45	1C4
0.0300	-761.1959319	5.626	-761.2158000	5.011	66.01	-44.52	-7.19	0S2
0.0350	-761.1917532	5.636	-761.2157988	5.012	66.01	-44.48	-7.26	0S2
0.0400	-761.1875858	5.753	-761.2157974	5.011	66.01	-44.52	-7.29	0S2
0.0450	-761.1829080	5.811	-761.2157983	5.011	66.01	-44.51	-7.20	0S2
0.0475	-761.1773748	5.836	-761.2157931	5.011	66.01	-44.52	-7.20	0S2
0.0500	-761.1744160	5.868	-761.2157929	5.011	66.01	-44.52	-7.20	0S2
0.0550	-761.1679212	5.934	-761.2157917	5.011	66.04	-44.55	-7.19	0S2
0.0600	-761.1605011	6.020	-761.2157910	5.011	66.03	-44.51	-7.14	0S2
0.0615	-761.1576998	6.026	-761.2157922	5.495	66.02	-44.52	-7.22	4C1
0.0650	-761.1719270	6.082	-761.2105139	5.495	-53.18	54.70	-57.66	4C1
0.0700	-761.1637925	6.146	-761.2105139	5.495	-53.18	54.70	-57.66	4C1
0.0750	-761.1538774	6.218	-761.2105139	5.494	-53.18	54.72	-57.65	4C1

Tab. 2S Results for IdoA^s

Stretched structure			Relaxed structure					conformer
f	E	L	E[L	tau1	tau2	tau3	
[au]	[au]	[Å]	[au]	[Å]		[°]		
0.0000	-761.210445	5.101	-761.210445	5.101	-61.49	34.32	28.53	2SO
0.0200	-761.204007	5.486	-761.210464	5.110	-62.02	35.54	27.17	2SO
0.0250	-761.200829	5.543	-761.210465	5.110	-62.04	35.48	27.24	2SO
0.0300	-761.197085	5.615	-761.210465	5.110	-62.05	35.47	27.24	2SO
0.0350	-761.192763	5.685	-761.210466	5.110	-62.03	35.46	27.29	2SO
0.0375	-761.190355	5.720	-761.210466	5.110	-62.02	35.47	27.26	2SO
0.0400	-761.210139	5.808	-761.222963	5.482	-55.34	56.10	-57.57	4C1
0.0450	-761.206281	5.856	-761.222964	5.482	-55.34	56.11	-57.38	4C1
0.0500	-761.201727	5.907	-761.222963	5.482	-55.34	56.11	-57.59	4C1
0.0550	-761.196365	5.961	-761.222961	5.482	-55.33	56.13	-57.64	4C1
0.0600	-761.190041	6.019	-761.222961	5.482	-55.34	56.14	-57.64	4C1
0.0650	-761.182486	6.083	-761.222964	5.482	-55.33	56.09	-57.55	4C1
0.0700	-761.173274	6.155	-761.222963	5.483	-55.34	56.08	-57.53	4C1
0.0750	-761.161414	6.241	-761.222963	5.482	-55.34	56.14	57.64	4C1

Tab. 3S Results for GlcN

Stretched structure			Relaxed structure					conformer
f	E	L	E[L	tau1	tau2	tau3	
[au]	[au]	[Å]	[au]	[Å]		[°]		
0.0000	-667.321493	4.565	-667.321493	4.565	-53.08	56.37	-57.56	4C1
0.0050	-667.320417	4.800	-667.321492	4.565	-52.34	59.38	-61.02	4C1
0.0100	-667.317414	5.013	-667.321493	4.565	-53.07	56.36	-57.55	4C1
0.0150	-667.312961	5.202	-667.321493	4.565	-53.07	56.37	-57.55	4C1
0.0200	-667.307523	5.367	-667.321493	4.565	-53.07	56.36	-57.55	4C1
0.0250	-667.301479	5.510	-667.321493	4.564	-53.08	56.36	-57.53	4C1
0.0275	-667.301496	5.660	-667.307180	5.477	-37.39	64.68	-26.11	1S3
0.0300	-667.300330	5.681	-667.307179	5.447	-37.41	64.69	-26.10	1S3
0.0350	-667.297590	5.726	-667.307179	5.447	-37.35	64.69	-26.15	1S3
0.0400	-667.294273	5.773	-667.307179	5.447	-37.35	64.68	-26.14	1S3
0.0450	-667.290307	5.822	-667.307179	5.447	-37.36	64.48	-26.14	1S3
0.0500	-667.285602	5.874	-667.307179	5.447	-37.34	64.48	-26.15	1S3
0.0550	-667.280044	5.930	-667.307178	5.447	-37.35	64.48	-26.14	1S3
0.0600	-667.273468	5.991	-667.307178	5.447	-37.36	64.49	-26.15	1S3
0.0650	-667.265636	6.057	-667.307177	5.447	-37.41	64.70	-26.13	1S3
0.0700	-667.254437	6.151	-667.307177	5.447	-32.14	63.89	-30.29	1S3
0.0750	-667.304638	6.234	-667.307177	5.471	-32.17	63.88	-30.27	1S3

Tab. 4S Results for GluA

Stretched structure				Relaxed structure				conformer
f	E	L	E[L	tau1	tau2	tau3	
[au]	[au]	[Å]	[au]	[Å]		[°]		
0.0000	-761.215755	5.462	-761.215755	5.462	-52.85	47.07	-50.17	4C1
0.0200	-761.212663	5.624	-761.215755	5.462	-52.85	47.08	-50.19	4C1
0.0300	-761.208674	5.709	-761.215755	5.462	-52.64	47.07	-50.18	4C1
0.0400	-761.202734	5.798	-761.215755	5.462	-52.85	47.06	-50.16	4C1
0.0500	-761.194415	5.896	-761.215755	5.462	-52.85	47.07	-50.18	4C1
0.0600	-761.182997	6.006	-761.215755	5.462	-52.85	47.08	-50.19	4C1
0.0700	-761.167069	6.135	-761.215755	5.462	-52.85	47.08	-50.20	4C1
0.0750	-761.156433	6.213	-761.215755	5.462	-52.84	47.08	-50.21	4C1

Tab 5S. Results for IdoA^c-GlcN

Stretched structure					Relaxed structure											
f	E	IdoAc	GlcN	Total	E[[au]	IdoAc				conformer	GlcN				L(tot) [Å]	
[au]	[au]	L [Å]	L [Å]	L [Å]		L [Å]	tau1 [°]	tau2 [°]	tau3 [°]		L [Å]	tau1 [°]	tau2 [°]	tau3 [°]		conformer
0.0000	-1352.116617	4.656	4.559	8.956	-1352.116617	4.656	51.04	-53.60	54.08	1C4	4.559	-53.86	57.11	-58.27	4C1	8.956
0.0200	-1352.094513	4.932	5.279	10.159	-1352.116622	4.656	51.04	-53.60	54.09	1C4	4.559	-53.85	57.09	-58.23	4C1	8.956
0.0250	-1352.083519	5.029	5.421	10.418	-1352.116624	4.656	51.04	-53.63	54.08	1C4	4.558	-53.85	57.07	-58.22	4C1	8.956
0.0300	-1352.070958	5.139	5.543	10.661	-1352.116625	4.656	51.03	-53.66	54.12	1C4	4.558	-53.83	57.06	-58.22	4C1	8.956
0.0315	-1352.063769	5.595	5.530	11.091	-1352.112366	5.054	65.14	-45.28	-7.35	0S2	4.513	-52.13	54.67	-56.92	4C1	9.317
0.0325	-1352.061693	5.607	5.555	11.125	-1352.112366	5.054	65.12	-45.48	-7.34	0S2	4.513	-52.14	54.68	-56.92	4C1	9.317
0.0350	-1352.060196	5.636	5.691	11.290	-1352.097949	5.047	65.20	-45.20	-7.22	0S2	5.445	-38.04	64.14	-25.10	1S3	9.974
0.0400	-1352.052809	5.697	5.733	11.395	-1352.097948	5.047	65.28	-45.20	-7.22	0S2	5.445	-37.98	64.14	-25.14	1S3	9.973
0.0425	-1352.048631	5.723	5.754	11.445	-1352.097947	5.047	65.28	-45.20	-7.29	0S2	5.450	37.95	64.14	-25.16	1S3	9.974
0.0450	-1352.062079	5.824	5.771	11.559	-1352.095424	5.528	-57.28	53.81	-54.21	4C1	5.444	-41.02	61.30	-19.46	1S3	10.715
0.0500	-1352.053916	5.866	5.818	11.650	-1352.095423	5.528	-57.24	53.78	-54.19	4C1	5.444	-40.97	61.31	-19.51	1S3	10.714
0.0550	-1352.044460	5.911	5.867	11.745	-1352.095422	5.528	-57.21	53.72	-54.13	4C1	5.444	-40.73	61.35	-19.71	1S3	10.712
0.0600	-1352.033488	5.958	5.919	11.846	-1352.095424	5.528	-57.23	53.69	-54.10	4C1	5.444	-40.69	61.33	-19.75	1S3	10.711
0.0650	-1352.020706	6.007	5.976	11.954	-1352.095425	5.528	-57.23	53.70	-54.11	4C1	5.444	-40.69	61.36	-19.76	1S3	10.712
0.0700	-1352.003993	6.061	6.0585	12.092	-1352.095425	5.527	-57.02	53.89	-54.35	4C1	5.444	-32.91	60.067	-25.39	1S3	10.713

Tab. 6S. Results for IdoA^s-GlcN

Stretched structure					Relaxed structure											
f	E	IdoA ^s	GlcN	L(tot)	E[IdoA ^s				GlcN					L(tot)	
[au]	[au]	L	L	[au]	L	tau1	tau2	tau3	conformer	L	tau1	tau2	tau3	conformer	[Å]	
		[Å]	[Å]		[Å]		[°]			[Å]		[°]				
0.0000	-1352.106222	5.105	4.592	9.321	-1352.106222	5.105	-62.02	44.14	16.03	2S0	4.592	-55.14	58.06	-59.03	4C1	9.321
0.0200	-1352.083828	5.464	5.273	10.688	-1352.106251	5.112	-62.04	44.31	17.10	2S0	4.602	-55.16	58.34	-59.28	4C1	9.314
0.0250	-1352.075099	5.527	5.414	10.893	-1352.106251	5.112	-62.03	43.29	17.13	2S0	4.603	-55.16	58.36	-59.29	4C1	9.313
0.0275	-1352.070153	5.556	5.483	10.993	-1352.106250	5.112	-62.03	43.31	17.10	2S0	4.603	-55.14	58.35	-59.29	4C1	9.314
0.0300	-1352.066997	5.587	5.662	11.209	-1352.104656	5.084	-60.72	41.95	19.32	2S0	5.021	-66.04	50.15	3.76	2S0	9.656
0.0325	-1352.063739	5.621	5.682	11.264	-1352.104657	5.084	-60.69	41.97	19.28	2S0	5.022	-66.03	50.16	3.72	2S0	9.657
0.0350	-1352.081331	5.721	5.687	11.352	-1352.113107	5.482	-55.85	55.38	-56.29	4C1	5.467	-41.70	63.58	-21.35	1S3	10.302
0.0400	-1352.074910	5.763	5.730	11.443	-1352.113111	5.482	-55.83	55.38	-56.28	4C1	5.465	-42.69	63.30	-20.61	1S3	10.314
0.0450	-1352.067402	5.763	5.730	11.537	-1352.113110	5.482	-57.04	55.03	-57.68	4C1	5.465	-42.62	63.50	-20.61	1S3	10.314
0.0500	-1352.058665	5.823	5.852	11.632	-1352.113109	5.482	-55.59	55.40	-56.28	4C1	5.465	-42.74	63.50	-20.57	1S3	10.315
0.0550	-1352.048499	5.873	5.901	11.736	-1352.113109	5.482	-55.83	55.39	-56.29	4C1	5.466	-42.29	63.53	-20.90	1S3	10.310
0.0600	-1352.036648	5.927	5.954	11.845	-1352.113109	5.482	-55.83	55.40	-56.30	4C1	5.466	-42.42	63.52	-20.79	1S3	10.311
0.0650	-1352.022672	6.012	5.985	11.964	-1352.113108	5.483	-55.85	55.42	-56.35	4C1	5.467	-42.00	63.55	-21.15	1S3	10.308
0.0700	-1352.003861	6.077	6.062	12.107	-1352.113110	5.482	-55.82	55.38	-56.29	4C1	5.465	-42.51	63.55	-20.83	1S3	10.312

Tab. 7S. Results for GlcN-GluA

Stretched structure					Relaxed structure											
f	E	IdoAc	GlcN	L(tot)	E[GlcN			GluA						L(tot)	
						L	tau1	tau2	tau3	conformer	L	tau1	tau3	tau3		conformer
[au]	[au]		[Å]		[au]	[Å]	[°]	[°]		[Å]	[°]	[°]	[°]		[Å]	
0.0000	-1352.115789	4.487	5.464	9.891	-1352.115789	4.485	-51.90	52.00	-54.43	4C1	5.464	-54.32	52.33	-54.7	4C1	9.891
0.0200	-1352.100091	5.223	5.604	10.761	-1352.115789	4.485	-51.89	51.92	-54.33	4C1	5.464	-54.31	52.34	-54.71	4C1	9.891
0.0250	-1352.092321	5.366	5.640	10.944	-1352.115789	4.485	-51.89	51.92	-54.33	4C1	5.464	-54.31	52.34	-54.71	4C1	9.890
0.0300	-1352.083218	5.499	5.678	11.119	-1352.115789	4.485	-51.91	51.90	-54.29	4C1	5.464	-54.33	52.38	-54.75	4C1	9.891
0.0325	-1352.080399	5.670	5.692	11.305	-1352.099978	5.469	-33.39	63.62	-30.15	1S3	5.467	-54.11	52.61	-55.07	4C1	10.356
0.0350	-1352.077648	5.711	5.690	11.348	-1352.099978	5.469	-33.41	63.67	-30.20	1S3	5.467	-54.09	52.58	-55.04	4C1	10.354
0.0400	-1352.071422	5.732	5.751	11.436	-1352.099978	5.469	-33.38	63.66	-30.22	1S3	5.467	-54.09	52.59	-55.05	4C1	10.353
0.0450	-1352.064143	5.777	5.793	11.527	-1352.099978	5.469	-33.43	63.65	-30.17	1S3	5.467	-54.10	52.57	-55.02	4C1	10.355
0.0500	-1352.055663	5.823	5.837	11.612	-1352.099978	5.469	-33.44	63.64	-30.15	1S3	5.467	-54.10	52.58	-55.03	4C1	10.356
0.0550	-1352.045804	5.873	5.884	11.720	-1352.099979	5.469	-33.35	63.64	-30.21	1S3	5.467	-54.12	52.60	-13.75	4C1	10.353
0.0600	-1352.034353	5.926	5.934	11.826	-1352.099979	5.469	-33.40	63.63	-30.16	1S3	5.467	-54.11	52.58	-55.02	4C1	10.354
0.0650	-1352.020961	5.983	5.988	11.939	-1352.099979	5.469	-33.41	63.62	-30.13	1S3	5.467	-54.11	52.58	-55.03	4C1	10.355
0.0700	-1352.005153	6.046	6.047	12.063	-1352.099980	5.469	-33.39	63.61	-30.12	1S3	5.667	-54.12	52.59	-55.02	4C1	10.355
0.0750	-1351.986057	6.118	6.112	12.202	-1352.099980	5.469	-33.41	63.64	-30.17	1S3	5.667	-54.10	52.57	-55.01	4C1	10.354

Tab. 8S(a). Results for GlcN-IdoA^c-GlcN-GluA-GlcN

f	Stretched structure							Relaxed structure						
	E	GlcN	IdoA ^c	GlcN	GluA	GlcN	Total	E	GlcN	IdoA ^c	GlcN	GluA	GlcN	Total
	[au]	L					[au]	L						
	[au]	[Å]						[au]	[Å]					
0.0000	-3218.723162	4.556	4.598	4.413	5.477	4.536	20.207	-3218.723162	4.564	4.554	4.436	5.481	4.628	20.701
0.0200	-3218.669227	5.272	4.867	5.205	5.582	5.526	25.941	-3218.723162	4.564	4.554	4.436	5.481	4.628	22.204
0.0250	-3218.636262	5.418	4.974	5.318	5.618	5.438	26.577	-3218.723146	4.564	4.554	4.434	5.481	4.628	22.198
0.0275	-3218.624146	5.482	5.037	5.366	5.632	5.476	26.820	-3218.723164	4.564	4.554	4.436	5.481	4.628	22.201
0.0300	-3218.599553	5.507	5.406	5.376	5.646	5.675	27.434	-3218.675041	4.522	5.080	4.472	5.468	5.467	23.126
0.0325	-3218.589393	5.561	5.439	5.414	5.663	5.694	27.606	-3218.675046	4.521	5.080	4.473	5.467	5.467	23.134
0.0340	-3218.579527	5.617	5.468	5.449	5.677	5.710	27.762	-3218.675034	4.522	5.080	4.469	5.467	5.469	23.130
0.0350	-3218.582201	5.698	5.469	5.458	5.681	5.714	27.862	-3218.660787	5.450	5.074	4.490	5.467	5.467	24.047
0.0365	-3218.578412	5.709	5.471	5.478	5.691	5.726	27.914	-3218.655775	5.454	5.043	4.475	5.468	5.470	22.542
0.0375	-3218.572397	5.719	5.503	5.501	5.698	5.735	28.006	-3218.677342	5.450	5.073	4.452	5.475	5.452	23.751
0.0400	-3218.580629	5.729	5.736	5.549	5.721	5.752	28.312	-3218.680154	5.449	5.485	4.298	5.474	5.451	20.838
0.0425	-3218.571584	5.750	5.754	5.581	5.739	5.774	28.428	-3218.662906	5.449	5.485	4.351	5.470	5.462	21.827
0.0450	-3218.561982	5.772	5.772	5.612	5.757	5.796	28.544	-3218.662914	5.448	5.485	4.351	5.470	5.463	21.843
0.0475	-3218.551705	5.795	5.791	5.643	5.775	5.819	28.661	-3218.662920	5.448	5.484	4.356	5.470	5.463	21.871
0.0500	-3218.540787	5.819	5.809	5.673	5.794	5.843	28.780	-3218.662920	5.448	5.485	4.353	5.470	5.464	21.846
0.0525	-3218.529120	5.843	5.829	5.702	5.813	5.868	28.900	-3218.662907	5.448	5.485	4.350	5.470	5.462	21.830
0.0550	-3218.516638	5.867	5.848	5.732	5.832	5.893	29.023	-3218.662902	5.449	5.485	4.347	5.470	5.462	21.801
0.0600	-3218.488915	5.920	5.889	5.792	5.874	5.948	29.278	-3218.662972	5.448	5.485	4.347	5.471	5.469	21.815
0.0625	-3218.477360	5.948	5.904	5.831	5.892	5.977	29.401	-3218.680197	5.448	5.485	4.311	5.476	5.451	21.059
0.0650	-3218.461115	5.977	5.927	5.857	5.914	6.008	29.535	-3218.680198	5.448	5.485	4.313	5.476	5.451	21.062
0.0675	-3218.437184	6.028	5.954	5.884	5.941	6.042	29.713	-3218.660277	5.478	5.486	4.341	5.470	5.464	21.739
0.0700	-3218.422857	6.059	5.973	5.910	5.962	6.077	29.842	-3218.660224	5.479	5.486	4.383	5.470	5.468	22.265
0.0730	-3218.397421	6.099	6.044	5.945	5.993	6.125	30.030	-3218.660236	5.479	5.486	4.388	5.470	5.469	22.312
0.0745	-3218.383061	6.121	6.019	5.965	6.010	6.151	30.134	-3218.660214	5.479	5.486	4.377	5.470	5.467	22.193

Tab. 8S (b). Results for GlcN-IdoA^c-GlcN-GluA-GlcN

Relaxed structure																				
f	GlcN				IdoA ^c				GlcN				GluA				GlcN			
	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer
[au]	[°]				[°]				[°]				[°]				[°]			
0.0000	-53.95	57.08	-58.02	4C1	46.49	-52.08	54.45	1C4	-52.06	49.90	-51.77	4C1	-54.79	52.45	-57.0	4C1	-50.57	54.53	-55.52	4C1
0.0200	-52.93	55.63	-58.21	4C1	53.07	-52.15	52.10	1C4	-51.90	49.84	-51.76	4C1	-53.42	50.94	-55.0	4C1	-48.67	55.28	-59.88	4C1
0.0250	-52.92	55.61	-58.21	4C1	53.06	-52.17	52.12	1C4	-51.85	49.73	-51.64	4C1	-53.44	50.95	-55.0	4C1	-48.71	55.27	-59.74	4C1
0.0275	-52.97	55.66	-58.21	4C1	53.06	-52.16	52.11	1C4	-51.91	49.85	-51.75	4C1	-53.39	50.99	-55.1	4C1	-48.69	55.25	-59.85	4C1
0.0300	-52.18	55.01	-57.22	4C1	61.32	-42.86	-10.52	0S2	-53.14	51.36	-52.95	4C1	-53.84	50.87	-54.4	4C1	14.97	41.52	-62.60	1S5
0.0325	-52.21	55.02	-57.19	4C1	61.32	-42.88	-10.51	0S2	-53.16	51.42	-53.00	4C1	-53.83	50.86	-54.4	4C1	15.05	41.46	-62.63	1S5
0.0340	-52.17	55.02	-57.23	4C1	61.30	-42.90	-10.48	0S2	-53.23	51.33	-52.81	4C1	-53.81	50.77	-54.3	4C1	16.21	40.67	-63.40	1S5
0.0350	-37.58	64.34	-25.71	4C1	61.53	-42.65	-10.49	0S2	-53.18	51.84	-53.52	4C1	-53.79	50.77	-54.3	4C1	15.28	41.31	-62.82	1S5
0.0365	-39.44	63.89	-24.13	1S3	63.02	-39.57	-12.32	0S2	-53.02	51.31	-52.96	4C1	-53.88	50.75	-54.2	4C1	16.13	40.65	-63.48	1S5
0.0375	-37.73	64.36	-25.64	1S3	61.56	-42.59	-10.43	0S2	-52.47	49.92	-51.56	4C1	-53.23	48.23	-51.3	4C1	-12.13	55.54	-40.03	1S3
0.0400	-39.02	61.57	-21.68	1S3	-52.48	50.94	-52.07	4C1	-53.57	47.45	-44.75	4C1	-54.05	49.16	-51.9	4C1	-11.85	55.53	-40.34	1S3
0.0425	-38.76	61.47	-21.74	1S3	-52.33	51.29	-52.53	4C1	-53.20	48.40	-46.31	4C1	-55.10	51.26	-54.2	4C1	11.41	43.89	-60.04	1S3
0.0450	-39.05	61.54	-21.64	1S3	-52.36	51.33	-52.54	4C1	-53.20	48.41	-46.33	4C1	-55.12	51.27	-54.2	4C1	12.21	43.39	-69.70	1S3
0.0475	-38.84	61.52	-21.76	1S3	-52.35	51.32	-52.54	4C1	-53.18	48.57	-46.60	4C1	-55.14	51.28	-54.2	4C1	12.49	43.22	-69.90	1S3
0.0500	-39.11	61.55	-21.61	1S3	-52.38	51.33	-52.51	4C1	-53.24	48.51	-46.46	4C1	-55.14	51.30	-54.2	4C1	12.69	43.07	-61.04	1S3
0.0525	-39.06	61.55	-21.64	1S3	-52.34	51.31	-52.52	4C1	-53.21	48.39	-46.29	4C1	-55.11	51.27	-54.2	4C1	11.79	43.66	-60.35	1S3
0.0550	-38.81	61.49	-21.74	1S3	-52.37	51.31	-52.51	4C1	-53.22	48.35	-46.24	4C1	-55.11	51.29	-54.2	4C1	11.77	43.64	-60.28	1S3
0.0600	-39.22	61.56	-21.55	1S3	-52.45	51.31	-52.47	4C1	-53.20	48.34	-46.28	4C1	-55.08	51.34	-54.4	4C1	15.90	40.83	-63.56	1S3
0.0625	-39.04	61.50	-21.56	1S3	-52.46	51.18	-52.30	4C1	-53.44	47.65	-45.16	4C1	-53.87	49.18	-52.2	4C1	-11.53	55.37	-40.44	1S3
0.0650	-39.10	61.50	-21.53	1S3	-52.49	51.18	-52.28	4C1	-53.44	47.68	-45.20	4C1	-53.86	49.19	-52.2	4C1	-11.54	55.36	-40.40	1S3
0.0675	-31.26	60.24	-26.61	1S3	-52.43	51.25	-52.37	4C1	-53.26	48.20	-45.96	4C1	-55.13	51.31	-54.2	4C1	12.94	42.88	-61.28	1S5
0.0700	-31.36	60.24	-26.54	1S3	-52.22	51.37	-52.71	4C1	-53.08	49.16	-47.51	4C1	-54.96	50.91	-54.0	4C1	15.50	41.15	-63.25	1S5
0.0730	-31.34	60.22	-26.52	1S3	-52.23	51.38	-52.72	4C1	-52.06	49.28	-47.70	4C1	-54.96	50.84	-53.9	4C1	16.03	40.75	-63.62	1S5
0.0745	-31.54	60.29	-26.46	1S3	-52.29	51.41	-52.68	4C1	-53.14	49.03	-47.29	4C1	-54.96	50.99	-54.1	4C1	14.84	41.61	-62.73	1S5

Tab 9s (a) Results for GlcN-IdoA^s-GlcN-GluA-GlcN

f	Stretched structure							Relaxed structure						
	E	GlcN	IdoA ^s	GlcN	GluA	GlcN	Total	E	GlcN	IdoA ^s	GlcN	GluA	GlcN	Total
[au]	[au]	[Å]				[au]	[Å]							
0.0000	-3218.700529	4.555	5.172	4.459	5.475	4.532	22.809	-3218.700529	4.555	5.172	4.459	5.475	4.532	22.809
0.0100	-3218.684507	4.921	5.281	4.642	5.529	5.066	24.931	-3218.700529	4.558	5.173	4.478	5.477	4.626	22.745
0.0150	-3218.669762	5.098	5.351	4.767	5.553	5.181	25.562	-3218.700529	4.557	5.172	4.479	5.477	4.625	22.736
0.0200	-3218.648729	5.263	5.438	4.933	5.580	5.280	26.201	-3218.700535	4.557	5.172	4.480	5.478	4.625	22.730
0.0225	-3218.629983	5.344	5.505	5.310	5.602	5.397	26.963	-3218.702302	4.579	5.131	4.627	5.480	4.626	22.392
0.0230	-3218.628209	5.358	5.510	5.319	5.605	5.406	27.005	-3218.702299	4.579	5.131	4.626	5.480	4.625	22.390
0.0250	-3218.620919	5.413	5.531	5.354	5.616	5.439	27.165	-3218.702298	4.579	5.131	4.627	5.480	4.625	22.391
0.0275	-3218.611407	5.484	5.556	5.395	5.631	5.477	27.357	-3218.702297	4.579	5.131	4.631	5.480	4.625	22.394
0.0285	-3218.607252	5.515	5.565	5.411	5.637	5.492	27.436	-3218.702294	4.579	5.131	4.632	5.480	4.624	22.391
0.0300	-3218.595222	5.663	5.579	5.439	5.645	6.170	27.810	-3218.676584	4.946	5.111	4.637	5.471	5.451	23.490
0.0325	-3218.587248	5.682	5.598	5.496	5.662	5.995	27.947	-3218.693200	5.423	5.138	4.593	5.472	5.451	23.629
0.0350	-3218.579402	5.703	5.621	5.533	5.679	5.715	28.070	-3218.693222	5.421	5.140	4.592	5.472	5.451	23.613
0.0400	-3218.582495	5.733	5.741	5.628	5.716	5.754	28.364	-3218.668861	5.469	5.473	3.924	5.463	5.470	18.685
0.0425	-3218.574003	5.755	5.759	5.650	5.734	5.776	28.473	-3218.668868	5.469	5.473	3.916	5.463	5.470	18.682
0.0450	-3218.564855	5.778	5.778	5.672	5.752	5.798	28.584	-3218.668916	5.469	5.473	3.908	5.463	5.468	18.706
0.0460	-3218.561014	5.787	5.785	5.681	5.759	5.807	28.629	-3218.660871	5.472	5.484	5.463	5.464	5.469	24.000
0.0485	-3218.550872	5.811	5.804	5.704	5.778	5.831	28.743	-3218.660872	5.472	5.485	5.463	5.464	5.469	23.972
0.0500	-3218.544398	5.825	5.816	5.718	5.789	5.845	28.813	-3218.660856	5.472	5.485	5.462	5.463	5.470	23.923
0.0525	-3218.532997	5.850	5.836	5.741	5.808	5.870	28.931	-3218.660885	5.472	5.485	5.463	5.464	5.470	23.959
0.0600	-3218.493109	5.929	5.899	5.817	5.870	5.951	29.306	-3218.660895	5.472	5.485	5.463	5.463	5.470	23.968
0.0625	-3218.477559	5.957	5.922	5.845	5.892	5.981	29.441	-3218.660943	5.472	5.484	5.463	5.464	5.471	24.033
0.0635	-3218.470992	5.969	5.931	5.856	5.900	5.993	29.496	-3218.660957	5.472	5.484	5.463	5.464	5.470	24.055
0.0650	-3218.460737	5.987	5.945	5.873	5.914	6.012	29.580	-3218.660953	5.472	5.484	5.463	5.464	5.470	24.055

Tab 9S (b) Results for GlcN-IdoA^s-GlcN-GluA-GlcN

<i>f</i>	Relaxed structure																			
	GlcN				IdoA ^s				GlcN				GluA				GlcN			
	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer	tau1	tau2	tau3	conformer
[au]	[°]				[°]				[°]				[°]				[°]			
0.0000	-54.33	56.36	-57.57	4C1	-62.81	36.36	26.38	2S0	-51.62	51.97	-55.43	4C1	-54.83	51.10	-55.64	4C1	-50.65	54.51	-55.50	4C1
0.0100	-54.36	56.41	-57.60	4C1	-62.85	36.22	26.63	2S0	-51.68	52.45	-55.99	4C1	-53.79	50.27	-54.39	4C1	-48.59	55.26	-60.05	4C1
0.0150	-54.42	56.45	-57.60	4C1	-62.81	36.16	26.71	2S0	-51.68	52.49	-56.05	4C1	-53.80	50.30	-54.42	4C1	-48.63	55.27	-60.02	4C1
0.0200	-54.41	56.43	-57.59	4C1	-62.81	36.14	26.74	2S0	-51.65	52.51	-56.10	4C1	-53.79	50.31	-54.45	4C1	-48.62	55.26	-60.02	4C1
0.0225	-54.53	57.28	-58.46	4C1	-62.07	37.09	24.77	2S0	-52.77	54.92	-55.81	4C1	-53.46	50.49	-54.82	4C1	-48.57	55.17	-59.96	4C1
0.0230	-54.52	57.28	-58.47	4C1	-62.06	37.07	24.78	2S0	-52.77	54.90	-55.79	4C1	-53.46	50.49	-54.83	4C1	-48.57	55.17	-59.95	4C1
0.0250	-54.52	57.28	-58.47	4C1	-62.08	37.03	24.84	2S0	-52.79	54.95	-55.84	4C1	-53.47	50.49	-54.82	4C1	-48.60	55.18	-59.93	4C1
0.0275	-54.51	57.28	-58.49	4C1	-62.10	37.07	24.80	2S0	-52.77	55.02	-55.93	4C1	-53.48	50.47	-54.79	4C1	-48.65	55.20	-59.91	4C1
0.0285	-54.49	57.27	-58.49	4C1	-62.10	37.06	24.81	2S0	-52.75	55.02	-55.94	4C1	-53.48	50.50	-54.83	4C1	-48.68	55.20	-59.88	4C1
0.0300	-66.71	49.70	4.54	2S0	-61.13	36.63	25.62	2S0	-52.98	55.15	-55.68	4C1	-53.40	47.95	-51.12	4C1	-12.66	55.86	-39.88	1S3
0.0325	-49.67	63.82	-17.66	1S3	-61.25	15.24	43.54	2,5B	-52.40	53.81	-54.05	4C1	-53.26	48.11	-51.22	4C1	-12.14	55.56	-40.00	1S3
0.0350	-49.97	63.80	-17.49	1S3	-61.38	15.40	43.33	2,5B	-52.44	53.75	-54.05	4C1	-53.32	48.12	-51.27	4C1	-11.86	55.43	-40.18	1S3
0.0400	-41.47	63.81	-22.08	1S3	-55.83	50.29	-49.56	4C1	-55.33	15.11	33.62	2,5B	-53.00	51.11	-54.28	4C1	16.66	40.24	-64.00	1S5
0.0425	-41.41	63.88	-22.23	1S3	-55.79	50.23	-49.50	4C1	-55.20	14.87	33.75	2,5B	-52.98	51.10	-54.30	4C1	16.92	40.05	-64.10	1S5
0.0450	-41.27	63.94	-22.43	1S3	-55.80	50.27	-49.52	4C1	-55.21	14.75	33.82	2,5B	-53.04	51.28	-54.43	4C1	15.77	40.92	-63.35	1S5
0.0460	-40.23	64.16	-23.43	1S3	-56.39	51.01	-49.89	4C1	-37.57	67.49	-33.55	1S3	-53.81	49.89	-53.07	4C1	15.25	41.23	-63.01	1S5
0.0485	-40.26	64.17	-23.44	1S3	-56.38	51.03	-49.92	4C1	-37.41	67.50	-33.68	1S3	-53.80	49.80	-52.97	4C1	15.94	40.75	-63.52	1S5
0.0500	-40.25	64.17	-23.45	1S3	-56.39	51.25	-50.22	4C1	-37.41	67.53	-33.75	1S3	-53.79	49.72	-52.88	4C1	16.57	40.28	-64.01	1S5
0.0525	-40.19	64.16	-23.48	1S3	-56.39	51.09	-50.00	4C1	-37.44	67.51	-33.67	1S3	-53.80	49.80	-52.97	4C1	16.22	40.54	-63.73	1S5
0.0600	-40.14	64.15	-23.50	1S3	-56.39	51.02	-49.92	4C1	-37.37	67.47	-33.65	1S3	-53.82	49.80	-52.91	4C1	16.35	40.43	-63.82	1S5
0.0625	-40.34	64.14	-23.35	1S3	-56.37	50.80	-49.63	4C1	-37.73	67.42	-33.28	1S3	-53.83	49.85	-53.02	4C1	16.48	40.33	-63.90	1S5
0.0635	-40.35	64.14	-23.34	1S3	-56.38	50.76	-49.57	4C1	-37.85	67.40	-33.17	1S3	-53.84	49.91	-53.08	4C1	16.26	40.50	-63.72	1S5
0.0650	-40.34	64.14	-23.34	1S3	-56.36	50.80	-49.65	4C1	-38.00	67.39	-33.08	1S3	-52.83	49.90	-53.09	4C1	16.29	40.47	-63.70	1S5