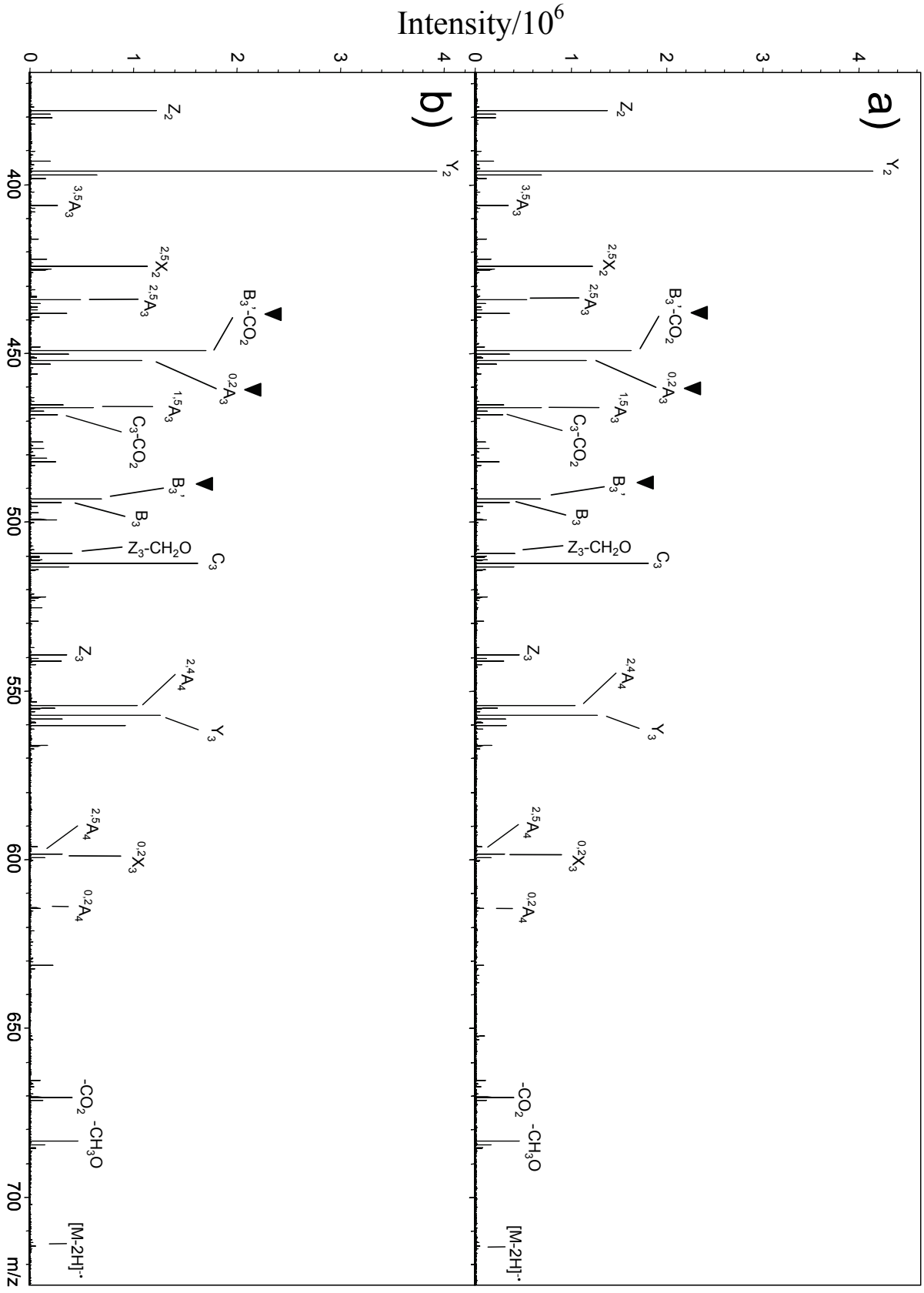
Supplemental Data for IdoA/GlcA Paper

Figure. EDD mass spectra of the $[M-2H]^{2-}$ precursor ion of tetrasaccharide ***3*** acquired 4 months apart, which demonstrate the excellent reproducibility of EDD fragmentation. (a) EDD of tetrasaccharide ***3*** on 3/20/06. (b) EDD of tetrasaccharide ***3*** on 8/1/06. Fragmentation is identical and all diagnostic product ions are observed at similar intensities. The ▼above the peak labels indicates product ions unique the GlcA containing HS tetrasaccharide, ***3***.

Figure 4


Intensity/10^6
a)
b)
Z2
Y2
3,5A3
2,5X2
2,5A3
B3'-CO2
0,2A3
1,5A3
C3-CO2
B3'
B3
Z3-CH2O
C3
Z3
2,4A4
Y3
2,5A4
0,2X3
0,2A4
-CO2
-CH3O
[M-2H]-·
400
450
500
550
600
650
700
m/z

Mass-to-charge/intensity table for the spectra in Figure 1

Tetrasaccharide 1		Tetrasaccharide 2		
m/z	RI	m/z	RI	ID
157.0142	0.112716	157.0143	0.067786	B_1
173.009	0.097941	173.0091	0.035066	
175.0248	0.322369	175.0248	0.19351	C_1
202.0722	0.021727	202.072	0.011405	Z_1
202.9892	0.036285	202.9893	0.036676	
210.9916	0.020361	210.9917	0.016768	
211.9867	0.047084	211.9995	0.016947	
220.0825	0.042944	220.0825	0.02381	Y_1
222.0076	0.165805	222.0076	0.065311	
240.0181	0.064112	240.0183	0.049768	
258.0287	0.08546	258.0289	0.087397	
259.046	0.083033	259.0458	0.016507	$^{2,5}A_2$
272.0533	0.017359	272.0536	0.016875	
273.0616	0.049677	273.0614	0.038031	
277.0563	0.020017	277.0563	0.029097	$^{0,2}A_2$
286.0282	0.12203	286.0236	0.035332	
286.0362	0.114487	286.0362	0.087895	
286.5324	0.1132	286.5321	0.019578	B_3^{2-}
294.5297	0.021432	294.5298	0.06232	$C_3\text{-}2H^{2-}$
295.5375	1.682314	295.5375	0.489193	C_3^{2-}
296.5343	0.108313	296.5345	0.037169	
316.5428	0.052768	316.5427	0.069672	$^{2,4}A_4^{2-}$
332.0618	0.04182	332.0623	0.04146	
333.0697	0.466127	333.0699	0.415616	
333.1062	0.110742	333.1062	0.146384	
337.548	0.571004	337.548	0.284969	$^{2,5}A_4^{2-}$
346.5535	0.473739	346.5536	0.400564	$^{0,2}A_4^{2-}$
369.037	0.03023	369.037	0.023211	
370.0454	0.218213	370.0455	0.108467	
372.0605	0.115679	372.0605	0.133251	
376.0882	0.347461	376.0884	0.042075	
377.0959	0.859294	377.0969	0.128271	$Z_2\text{-}H$
378.0994	0.132182	378.1044	0.046084	Z_2
382.5763	0.116335	382.5756	0.015266	
383.0789	0.074438	383.0795	0.027275	
388.0718	0.124535	388.0711	0.076885	
388.5768	0.259511	388.5771	0.078436	
389.0714	0.193642	389.0753	0.119948	$[M\text{-}2H\text{-}H_2O]^{2-}$
397.076	119.0124	397.0761	49.67004	precursor ion^{2-}
413.0265	0.035083	413.0267	0.035649	
414.0346	0.319661	414.0347	0.25647	
415.0423	0.866599	415.0424	1.10527	$C_2\text{-}H$
415.0785	0.671537	415.0788	0.857938	

416.0508	1	416.0507	1	C_2
440.0508	0.213258	440.0509	0.017395	
442.0659	0.168046	442.0662	0.027032	$^{3,5}A_3$-CO_2
459.0684	1.474862	459.0687	0.426186	$^{2,4}A_3$
470.0609	0.034169	470.0612	0.022625	
486.0558	0.605093	486.0562	0.089661	$^{3,5}A_3$
496.0403	0.065192			
504.0661	0.044209	504.0663	0.008438	
505.0737	0.105901	505.0744	0.195637	
506.0798	0.111196			
510.1097	0.022053	510.1089	0.036161	
512.1265	0.019443	512.1265	0.012311	
514.0505	0.212771	514.0494	0.011424	$^{2,4}A_3$
527.0596	0.01794			
528.0665	0.034526	528.0677	0.015911	
529.0743	0.099136			B_3'-CO_2
532.0609	0.051666			$^{0,2}A_3$
		544.0631	0.026706	
546.0775	0.140355	546.0767	0.224703	$^{1,5}A_3$
548.0926	0.0189	548.0958	0.014196	C_3-CO_2
		554.1358	0.01818	
555.0542	0.022023			
571.1051	0.004772	571.1086	0.011917	
572.0561	0.027979	572.057	0.013618	
573.065	0.1553	573.0643	0.011704	B_3'
574.0712	0.116286	574.0721	0.088508	B_3
589.1184	0.084124	589.1198	0.045367	Z_3-CH_2O
590.0673	0.118777	590.0671	0.357035	C_3"
592.0827	0.176393	592.0828	0.119569	C_3
600.1117	0.040436	600.1117	0.077216	
619.1298	0.298629	619.1297	0.191542	Z_3
634.0936	0.026323	634.0928	0.044409	$^{2,4}A_4$
637.1413	0.035836	637.1397	0.061999	Y_3
646.0941	0.017687	646.0941	0.057862	$^{3,5}A_4$
		668.1925	0.047264	
678.1436	0.032454	678.1446	0.02704	$^{0,2}X_3$
694.1144	0.063871	694.1135	0.040289	$^{0,2}A_4$
749.1584	0.020902	749.1572	0.038651	$[M-2H-CHO_2]^{-\bullet}$
750.1646	0.084904	750.1627	0.033485	$[M-2H-CO_2]^{-\bullet}$
794.153	0.01702	794.1541	0.015973	$[M-2H]^{-\bullet}$

Mass-to-charge/intensity table for the spectra in Figure 2

Tetrasaccharide 3		Tetrasaccharide 4		
m/z	I	m/z	I	ID
157.0129	0.186454	157.013	0.196726	B_1
175.0233	1.530121	175.0233	1.084135	C_1
202.0703	0.016441	202.0704	0.030469	Z_1
220.0804	0.045258	220.0804	0.043652	Y_1
255.5566	0.741483	255.5565	0.192901	C_3^{2-}
259.0432	0.091871	259.043	0.13015	$^{2,5}A_2$
276.5615	0.05698	276.5614	0.271499	$^{2,4}A_4^{2-}$
277.0536	0.26103	277.0531	0.325279	$^{0,2}A_2$
297.5666	0.293569	297.5663	0.435	$^{2,4}A_4^{2-}$
306.5717	0.263051	306.5715	0.616931	$^{0,2}A_4^{2-}$
		307.5172	0.572409	
318.0803	0.037498	318.0785	0.032269	B_2
		327.576	0.108505	
		328.0296	0.166245	
333.1026	0.165318	333.1022	0.144204	
334.0748	0.050872			
334.1104	0.282425	334.11	0.259808	
336.0898	0.519693	336.0891	0.371991	C_2
342.5938	0.104351			
348.0897	4.206264			$[M-2H-H_2O]^{2-}$
		349.0348	0.891572	
357.0944	56.56165	357.0937	61.28651	precursor ion^{2-}
378.0996	0.339766	378.0988	0.777172	Z_2
380.1158	0.053156	380.1145	0.052732	
396.1097	1	396.1088	1	Y_2
406.0942	0.082536	406.0933	0.074242	$^{3,5}A_3$
		416.0441	0.228481	
422.125	0.038511			
424.1044	0.292544	424.1033	0.112623	$^{1,5}X_2$
434.0883	0.128579	434.0563	0.038016	$^{2,5}A_3$
434.1481	0.08973	434.147	0.064724	
438.12	0.084592			
449.1113	0.39374			B_3'-CO_2
452.0985	0.277125			$^{0,2}A_3$
		458.0527	0.34884	
465.1056	0.074956			
466.1142	0.164485	466.1123	0.152779	$^{1,5}A_3$
468.1296	0.072664	468.1284	0.036573	C_3-CO_2
476.1587	0.028059	476.0629	0.133457	
478.174	0.035609			
482.1448	0.059947			
493.1016	0.176727			B_3'
494.1078	0.087772	494.1068	0.217245	B_3
499.1225	0.028704			
509.155	0.098856	509.153	0.089634	Z_3-CH_2O
510.1028	0.027485	510.1003	0.103916	C_3"
512.1185	0.433624	512.1162	0.403658	C_3

522.1621	0.031508			
		536.0802	0.065892	
539.165	0.114891	539.1649	0.044245	Z_3
541.1807	0.075062	541.1777	0.089119	
554.1283	0.248965	554.1251	0.212519	$^{2,4}A_4$
557.1755	0.306407	557.1725	0.142909	Y3
560.1751	0.078029			
566.1294	0.042324			
596.137	0.019679	596.1358	0.051822	$^{2,5}A_4$
598.1778	0.078654	598.1743	0.314978	$^{0,2}X_3$
614.15	0.021088	614.1444	0.123784	$^{0,2}A_4$
652.1886	0.023747			
665.1599	0.025538			
670.1965	0.095483	670.1927	0.078937	$[M-2H-CO_2]^{-\bullet}$
683.1676	0.111147	683.1668	0.082506	$[M-2H-CH_3O]^{-\bullet}$
714.1835	0.014958	714.179	0.034296	$[M-2H]^{-\bullet}$