

## Supplemental Figure Legends

**Supplemental Figure 1.** Manatee graphical user interface showing (1) Main program hub, able to invoke separate instances of each analysis, or view the About/Help, (2) A preview of the raw data files (mzXML) ; includes file names, paths, and extensions, (3) the chosen targets file (with path and extension), (4) analysis parameter settings options, and (5) the command toolbar.

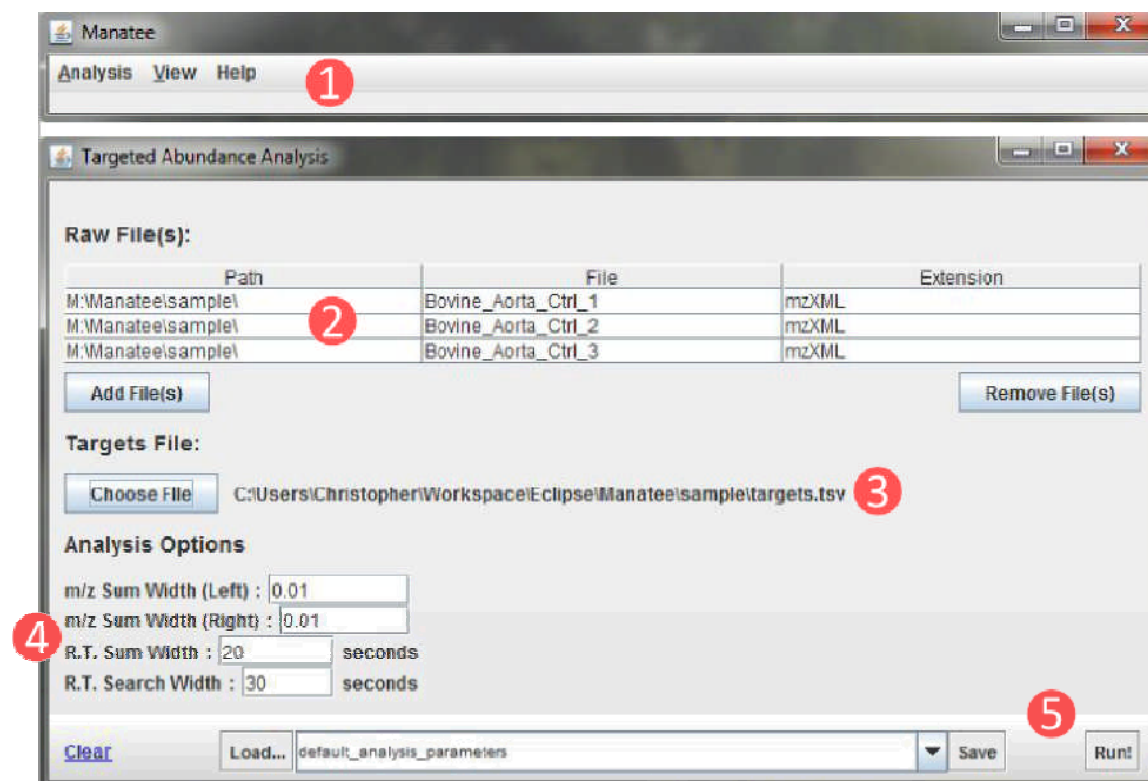
**Supplemental Figure 2.** List of HS compositions defining the chemical space for dp6-dp12 used for targeted analysis of LC/MS data generated on HS samples following exhaustive digestion using heparin lyase III. HS compositions are give as [ $\Delta$ HexA, HexA, acetate,  $\text{SO}_3$ ].

**Supplemental Figure 3.** Compositions of aorta HS oligosaccharides generated by Manatee, (A) saturated dp 11, (B) saturated dp12 and (C)  $\Delta$ -unsaturated dp12. HS co2mpositions are give as [ $\Delta$ HexA, HexA, acetate,  $\text{SO}_3$ ].

**Supplemental Figure 4.** Percent abundances of  $\Delta$ -unsaturated NS domains as a function of dp and organ. The data reconstructed using Manatee show the same trend as that obtained by manual interpretation [4].

## Supplemental Figures

### Supplemental Figure 1



**Supplemental Figure 2.** List of targeted NS domain compositions for HS chains.

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
<b><math>\Delta</math>-unsat dp4</b>										
674.2018	1	1	2	0	0	24	38	2	20	0
754.1586	1	1	2	1	0	24	38	2	23	1
834.1154	1	1	2	2	0	24	38	2	26	2
914.0722	1	1	2	3	0	24	38	2	29	3
994.0291	1	1	2	4	0	24	38	2	32	4
1073.9859	1	1	2	5	0	24	38	2	35	5
1153.9427	1	1	2	6	0	24	38	2	38	6
1233.8995	1	1	2	7	0	24	38	2	41	7
1313.8563	1	1	2	8	0	24	38	2	44	8
716.2124	1	1	2	0	1	26	40	2	21	0
796.1692	1	1	2	1	1	26	40	2	24	1
876.1260	1	1	2	2	1	26	40	2	27	2
956.0828	1	1	2	3	1	26	40	2	30	3
1036.0396	1	1	2	4	1	26	40	2	33	4
1115.9964	1	1	2	5	1	26	40	2	36	5
1195.9532	1	1	2	6	1	26	40	2	39	6
1275.9101	1	1	2	7	1	26	40	2	42	7
758.2229	1	1	2	0	2	28	42	2	22	0
838.1797	1	1	2	1	2	28	42	2	25	1
918.1366	1	1	2	2	2	28	42	2	28	2
998.0934	1	1	2	3	2	28	42	2	31	3
1078.0502	1	1	2	4	2	28	42	2	34	4
1158.0070	1	1	2	5	2	28	42	2	37	5
1237.9638	1	1	2	6	2	28	42	2	40	6
<b><math>\Delta</math>-unsat dp6</b>										
1011.3027	1	2	3			36	57	3	30	0
1091.2595	1	2	3	1		36	57	3	33	1
1171.2163	1	2	3	2		36	57	3	36	2
1251.1731	1	2	3	3		36	57	3	39	3
1331.1299	1	2	3	4		36	57	3	42	4
1411.0868	1	2	3	5		36	57	3	45	5
1491.0436	1	2	3	6		36	57	3	48	6
1571.0004	1	2	3	7		36	57	3	51	7
1650.9572	1	2	3	8		36	57	3	54	8
1730.9140	1	2	3	9		36	57	3	57	9
1053.3133	1	2	3		1	38	59	3	31	0
1133.2701	1	2	3	1	1	38	59	3	34	1
1213.2269	1	2	3	2	1	38	59	3	37	2
1293.1837	1	2	3	3	1	38	59	3	40	3
1373.1405	1	2	3	4	1	38	59	3	43	4
1453.0973	1	2	3	5	1	38	59	3	46	5
1533.0541	1	2	3	6	1	38	59	3	49	6
1613.0110	1	2	3	7	1	38	59	3	52	7
1692.9678	1	2	3	8	1	38	59	3	55	8
1772.9246	1	2	3	9	1	38	59	3	58	9
1095.3238	1	2	3		2	40	61	3	32	0
1175.2806	1	2	3	1	2	40	61	3	35	1
1255.2374	1	2	3	2	2	40	61	3	38	2
1335.1943	1	2	3	3	2	40	61	3	41	3
1415.1511	1	2	3	4	2	40	61	3	44	4
1495.1079	1	2	3	5	2	40	61	3	47	5
1575.0647	1	2	3	6	2	40	61	3	50	6
1655.0215	1	2	3	7	2	40	61	3	53	7
1734.9783	1	2	3	8	2	40	61	3	56	8
1814.9351	1	2	3	9	2	40	61	3	59	9
<b><math>\Delta</math>-unsat dp8</b>										
1348.4036	1	3	4			48	76	4	40	0
1428.3604	1	3	4	1		48	76	4	43	1
1508.3172	1	3	4	2		48	76	4	46	2
1588.2740	1	3	4	3		48	76	4	49	3
1668.2308	1	3	4	4		48	76	4	52	4
1748.1877	1	3	4	5		48	76	4	55	5
1828.1445	1	3	4	6		48	76	4	58	6
1908.1013	1	3	4	7		48	76	4	61	7
1988.0581	1	3	4	8		48	76	4	64	8
2068.0149	1	3	4	9		48	76	4	67	9
2147.9717	1	3	4	10		48	76	4	70	10
2227.9285	1	3	4	11		48	76	4	73	11
2307.8854	1	3	4	12		48	76	4	76	12
1390.4141	1	3	4		1	50	78	4	41	0
1470.3710	1	3	4	1	1	50	78	4	44	1
1550.3278	1	3	4	2	1	50	78	4	47	2



## Supplemental Figure 2, continued

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
2022.6054	1	5	6			72	114	6	60	0
2102.5622	1	5	6	1		72	114	6	63	1
2182.5190	1	5	6	2		72	114	6	66	2
2262.4758	1	5	6	3		72	114	6	69	3
2342.4326	1	5	6	4		72	114	6	72	4
2422.3894	1	5	6	5		72	114	6	75	5
2502.3463	1	5	6	6		72	114	6	78	6
2582.3031	1	5	6	7		72	114	6	81	7
2662.2599	1	5	6	8		72	114	6	84	8
2742.2167	1	5	6	9		72	114	6	87	9
2822.1735	1	5	6	10		72	114	6	90	10
2902.1303	1	5	6	11		72	114	6	93	11
2982.0872	1	5	6	12		72	114	6	96	12
3062.0440	1	5	6	13		72	114	6	99	13
3142.0008	1	5	6	14		72	114	6	102	14
3221.9576	1	5	6	15		72	114	6	105	15
3301.9144	1	5	6	16		72	114	6	108	16
3381.8712	1	5	6	17		72	114	6	111	17
3461.8280	1	5	6	18		72	114	6	114	18
2064.6159	1	5	6		1	74	116	6	61	0
2144.5728	1	5	6	1	1	74	116	6	64	1
2224.5296	1	5	6	2	1	74	116	6	67	2
2304.4864	1	5	6	3	1	74	116	6	70	3
2384.4432	1	5	6	4	1	74	116	6	73	4
2464.4000	1	5	6	5	1	74	116	6	76	5
2544.3568	1	5	6	6	1	74	116	6	79	6
2624.3136	1	5	6	7	1	74	116	6	82	7
2704.2705	1	5	6	8	1	74	116	6	85	8
2784.2273	1	5	6	9	1	74	116	6	88	9
2864.1841	1	5	6	10	1	74	116	6	91	10
2944.1409	1	5	6	11	1	74	116	6	94	11
3024.0977	1	5	6	12	1	74	116	6	97	12
3104.0545	1	5	6	13	1	74	116	6	100	13
3184.0113	1	5	6	14	1	74	116	6	103	14
3263.9682	1	5	6	15	1	74	116	6	106	15
3343.9250	1	5	6	16	1	74	116	6	109	16
3423.8818	1	5	6	17	1	74	116	6	112	17
2106.6265	1	5	6		2	76	118	6	62	0
2186.5833	1	5	6	1	2	76	118	6	65	1
2266.5401	1	5	6	2	2	76	118	6	68	2
2346.4969	1	5	6	3	2	76	118	6	71	3
2426.4538	1	5	6	4	2	76	118	6	74	4
2506.4106	1	5	6	5	2	76	118	6	77	5
2586.3674	1	5	6	6	2	76	118	6	80	6
2666.3242	1	5	6	7	2	76	118	6	83	7
2746.2810	1	5	6	8	2	76	118	6	86	8
2826.2378	1	5	6	9	2	76	118	6	89	9
2906.1947	1	5	6	10	2	76	118	6	92	10
2986.1515	1	5	6	11	2	76	118	6	95	11
3066.1083	1	5	6	12	2	76	118	6	98	12
3146.0651	1	5	6	13	2	76	118	6	101	13
3226.0219	1	5	6	14	2	76	118	6	104	14
3305.9787	1	5	6	15	2	76	118	6	107	15
3385.9355	1	5	6	16	2	76	118	6	110	16
<b>sat dp4</b>										
692.2124	0	2	2	0	0	24	40	2	21	0
772.1692	0	2	2	1	0	24	40	2	24	1
852.1260	0	2	2	2	0	24	40	2	27	2
932.0828	0	2	2	3	0	24	40	2	30	3
1012.0396	0	2	2	4	0	24	40	2	33	4
1091.9964	0	2	2	5	0	24	40	2	36	5
1171.9532	0	2	2	6	0	24	40	2	39	6
1251.9101	0	2	2	7	0	24	40	2	42	7
1331.8669	0	2	2	8	0	24	40	2	45	8
734.2229	0	2	2	0	1	26	42	2	22	0
814.1797	0	2	2	1	1	26	42	2	25	1
894.1366	0	2	2	2	1	26	42	2	28	2
974.0934	0	2	2	3	1	26	42	2	31	3
1054.0502	0	2	2	4	1	26	42	2	34	4
1134.0070	0	2	2	5	1	26	42	2	37	5
1213.9638	0	2	2	6	1	26	42	2	40	6
1293.9206	0	2	2	7	1	26	42	2	43	7
776.2335	0	2	2	0	2	28	44	2	23	0

## Supplemental Figure 2, continued

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
856.1903	0	2	2	1	2	28	44	2	26	1
936.1471	0	2	2	2	2	28	44	2	29	2
1016.1039	0	2	2	3	2	28	44	2	32	3
1096.0607	0	2	2	4	2	28	44	2	35	4
1176.0176	0	2	2	5	2	28	44	2	38	5
1255.9744	0	2	2	6	2	28	44	2	41	6
sat dp6										
1029.3133		3	3			36	59	3	31	0
1109.2701		3	3	1		36	59	3	34	1
1189.2269		3	3	2		36	59	3	37	2
1269.1837		3	3	3		36	59	3	40	3
1349.1405		3	3	4		36	59	3	43	4
1429.0973		3	3	5		36	59	3	46	5
1509.0541		3	3	6		36	59	3	49	6
1589.0110		3	3	7		36	59	3	52	7
1668.9678		3	3	8		36	59	3	55	8
1748.9246		3	3	9		36	59	3	58	9
1071.3238		3	3		1	38	61	3	32	0
1151.2806		3	3	1	1	38	61	3	35	1
1231.2374		3	3	2	1	38	61	3	38	2
1311.1943		3	3	3	1	38	61	3	41	3
1391.1511		3	3	4	1	38	61	3	44	4
1471.1079		3	3	5	1	38	61	3	47	5
1551.0647		3	3	6	1	38	61	3	50	6
1631.0215		3	3	7	1	38	61	3	53	7
1710.9783		3	3	8	1	38	61	3	56	8
1790.9351		3	3	9	1	38	61	3	59	9
1113.3344		3	3		2	40	63	3	33	0
1193.2912		3	3	1	2	40	63	3	36	1
1273.2480		3	3	2	2	40	63	3	39	2
1353.2048		3	3	3	2	40	63	3	42	3
1433.1616		3	3	4	2	40	63	3	45	4
1513.1185		3	3	5	2	40	63	3	48	5
1593.0753		3	3	6	2	40	63	3	51	6
1673.0321		3	3	7	2	40	63	3	54	7
1752.9889		3	3	8	2	40	63	3	57	8
1832.9457		3	3	9	2	40	63	3	60	9
sat dp8										
1366.4141		4	4			48	78	4	41	0
1446.3710		4	4	1		48	78	4	44	1
1526.3278		4	4	2		48	78	4	47	2
1606.2846		4	4	3		48	78	4	50	3
1686.2414		4	4	4		48	78	4	53	4
1766.1982		4	4	5		48	78	4	56	5
1846.1550		4	4	6		48	78	4	59	6
1926.1119		4	4	7		48	78	4	62	7
2006.0687		4	4	8		48	78	4	65	8
2086.0255		4	4	9		48	78	4	68	9
2165.9823		4	4	10		48	78	4	71	10
2245.9391		4	4	11		48	78	4	74	11
2325.8959		4	4	12		48	78	4	77	12
1408.4247		4	4		1	50	80	4	42	0
1488.3815		4	4	1	1	50	80	4	45	1
1568.3383		4	4	2	1	50	80	4	48	2
1648.2952		4	4	3	1	50	80	4	51	3
1728.2520		4	4	4	1	50	80	4	54	4
1808.2088		4	4	5	1	50	80	4	57	5
1888.1656		4	4	6	1	50	80	4	60	6
1968.1224		4	4	7	1	50	80	4	63	7
2048.0792		4	4	8	1	50	80	4	66	8
2128.0360		4	4	9	1	50	80	4	69	9
2207.9929		4	4	10	1	50	80	4	72	10
2287.9497		4	4	11	1	50	80	4	75	11
2367.9065		4	4	12	1	50	80	4	78	12
1450.4353		4	4		2	52	82	4	43	0
1530.3921		4	4	1	2	52	82	4	46	1
1610.3489		4	4	2	2	52	82	4	49	2
1690.3057		4	4	3	2	52	82	4	52	3
1770.2625		4	4	4	2	52	82	4	55	4
1850.2194		4	4	5	2	52	82	4	58	5
1930.1762		4	4	6	2	52	82	4	61	6
2010.1330		4	4	7	2	52	82	4	64	7
2090.0898		4	4	8	2	52	82	4	67	8

## Supplemental Figure 2, continued

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
2170.0466		4	4	9	2	52	82	4	70	9
2250.0034		4	4	10	2	52	82	4	73	10
2329.9602		4	4	11	2	52	82	4	76	11
2409.9171		4	4	12	2	52	82	4	79	12
<b>sat dp10</b>										
1703.5150		5	5			60	97	5	51	0
1783.4719		5	5	1		60	97	5	54	1
1863.4287		5	5	2		60	97	5	57	2
1943.3855		5	5	3		60	97	5	60	3
2023.3423		5	5	4		60	97	5	63	4
2103.2991		5	5	5		60	97	5	66	5
2183.2559		5	5	6		60	97	5	69	6
2263.2127		5	5	7		60	97	5	72	7
2343.1696		5	5	8		60	97	5	75	8
2423.1264		5	5	9		60	97	5	78	9
2503.0832		5	5	10		60	97	5	81	10
2583.0400		5	5	11		60	97	5	84	11
2662.9968		5	5	12		60	97	5	87	12
2742.9536		5	5	13		60	97	5	90	13
2822.9104		5	5	14		60	97	5	93	14
2902.8673		5	5	15		60	97	5	96	15
1745.5256		5	5		1	62	99	5	52	0
1825.4824		5	5	1	1	62	99	5	55	1
1905.4392		5	5	2	1	62	99	5	58	2
1985.3961		5	5	3	1	62	99	5	61	3
2065.3529		5	5	4	1	62	99	5	64	4
2145.3097		5	5	5	1	62	99	5	67	5
2225.2665		5	5	6	1	62	99	5	70	6
2305.2233		5	5	7	1	62	99	5	73	7
2385.1801		5	5	8	1	62	99	5	76	8
2465.1369		5	5	9	1	62	99	5	79	9
2545.0938		5	5	10	1	62	99	5	82	10
2625.0506		5	5	11	1	62	99	5	85	11
2705.0074		5	5	12	1	62	99	5	88	12
2784.9642		5	5	13	1	62	99	5	91	13
2864.9210		5	5	14	1	62	99	5	94	14
2944.8778		5	5	15	1	62	99	5	97	15
1787.5362		5	5		2	64	101	5	53	0
1867.4930		5	5	1	2	64	101	5	56	1
1947.4498		5	5	2	2	64	101	5	59	2
2027.4066		5	5	3	2	64	101	5	62	3
2107.3634		5	5	4	2	64	101	5	65	4
2187.3202		5	5	5	2	64	101	5	68	5
2267.2771		5	5	6	2	64	101	5	71	6
2347.2339		5	5	7	2	64	101	5	74	7
2427.1907		5	5	8	2	64	101	5	77	8
2507.1475		5	5	9	2	64	101	5	80	9
2587.1043		5	5	10	2	64	101	5	83	10
2667.0611		5	5	11	2	64	101	5	86	11
2747.0179		5	5	12	2	64	101	5	89	12
2826.9748		5	5	13	2	64	101	5	92	13
2906.9316		5	5	14	2	64	101	5	95	14
2986.8884		5	5	15	2	64	101	5	98	15
<b>sat dp12</b>										
2040.6159		6	6			72	116	6	61	0
2120.5728		6	6	1		72	116	6	64	1
2200.5296		6	6	2		72	116	6	67	2
2280.4864		6	6	3		72	116	6	70	3
2360.4432		6	6	4		72	116	6	73	4
2440.4000		6	6	5		72	116	6	76	5
2520.3568		6	6	6		72	116	6	79	6
2600.3136		6	6	7		72	116	6	82	7
2680.2705		6	6	8		72	116	6	85	8
2760.2273		6	6	9		72	116	6	88	9
2840.1841		6	6	10		72	116	6	91	10
2920.1409		6	6	11		72	116	6	94	11
3000.0977		6	6	12		72	116	6	97	12
3080.0545		6	6	13		72	116	6	100	13
3160.0113		6	6	14		72	116	6	103	14
3239.9682		6	6	15		72	116	6	106	15
3319.9250		6	6	16		72	116	6	109	16
3399.8818		6	6	17		72	116	6	112	17
3479.8386		6	6	18		72	116	6	115	18

## Supplemental Figure 2, continued

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
2082.6265		6	6		1	74	118	6	62	0
2162.5833		6	6	1	1	74	118	6	65	1
2242.5401		6	6	2	1	74	118	6	68	2
2322.4969		6	6	3	1	74	118	6	71	3
2402.4538		6	6	4	1	74	118	6	74	4
2482.4106		6	6	5	1	74	118	6	77	5
2562.3674		6	6	6	1	74	118	6	80	6
2642.3242		6	6	7	1	74	118	6	83	7
2722.2810		6	6	8	1	74	118	6	86	8
2802.2378		6	6	9	1	74	118	6	89	9
2882.1947		6	6	10	1	74	118	6	92	10
2962.1515		6	6	11	1	74	118	6	95	11
3042.1083		6	6	12	1	74	118	6	98	12
3122.0651		6	6	13	1	74	118	6	101	13
3202.0219		6	6	14	1	74	118	6	104	14
3281.9787		6	6	15	1	74	118	6	107	15
3361.9355		6	6	16	1	74	118	6	110	16
3441.8924		6	6	17	1	74	118	6	113	17
2124.6371		6	6		2	76	120	6	63	0
2204.5939		6	6	1	2	76	120	6	66	1
2284.5507		6	6	2	2	76	120	6	69	2
2364.5075		6	6	3	2	76	120	6	72	3
2444.4643		6	6	4	2	76	120	6	75	4
2524.4211		6	6	5	2	76	120	6	78	5
2604.3780		6	6	6	2	76	120	6	81	6
2684.3348		6	6	7	2	76	120	6	84	7
2764.2916		6	6	8	2	76	120	6	87	8
2844.2484		6	6	9	2	76	120	6	90	9
2924.2052		6	6	10	2	76	120	6	93	10
3004.1620		6	6	11	2	76	120	6	96	11
3084.1188		6	6	12	2	76	120	6	99	12
3164.0757		6	6	13	2	76	120	6	102	13
3244.0325		6	6	14	2	76	120	6	105	14
3323.9893		6	6	15	2	76	120	6	108	15
3403.9461		6	6	16	2	76	120	6	111	16
3323.9893		6	6	15	2	76	120	6	108	15
3403.9461		6	6	16	2	76	120	6	111	16
<b>sat dp5</b>										
853.2812		2	3			30	51	3	25	0
933.2380		2	3	1		30	51	3	28	1
1013.1948		2	3	2		30	51	3	31	2
1093.1516		2	3	3		30	51	3	34	3
1173.1084		2	3	4		30	51	3	37	4
1253.0652		2	3	5		30	51	3	40	5
1333.0221		2	3	6		30	51	3	43	6
1412.9789		2	3	7		30	51	3	46	7
1492.9357		2	3	8		30	51	3	49	8
1572.8925		2	3	9		30	51	3	52	9
895.2917		2	3		1	32	53	3	26	0
975.2485		2	3	1	1	32	53	3	29	1
1055.2054		2	3	2	1	32	53	3	32	2
1135.1622		2	3	3	1	32	53	3	35	3
1215.1190		2	3	4	1	32	53	3	38	4
1295.0758		2	3	5	1	32	53	3	41	5
1375.0326		2	3	6	1	32	53	3	44	6
1454.9894		2	3	7	1	32	53	3	47	7
1534.9462		2	3	8	1	32	53	3	50	8
1614.9031		2	3	9	1	32	53	3	53	9
937.3023		2	3		2	34	55	3	27	0
1017.2591		2	3	1	2	34	55	3	30	1
1097.2159		2	3	2	2	34	55	3	33	2
1177.1727		2	3	3	2	34	55	3	36	3
1257.1296		2	3	4	2	34	55	3	39	4
1337.0864		2	3	5	2	34	55	3	42	5
1417.0432		2	3	6	2	34	55	3	45	6
1497.0000		2	3	7	2	34	55	3	48	7
1576.9568		2	3	8	2	34	55	3	51	8
1656.9136		2	3	9	2	34	55	3	54	9
<b>sat dp7</b>										
1190.3821		3	4			42	70	4	35	0
1270.3389		3	4	1		42	70	4	38	1
1350.2957		3	4	2		42	70	4	41	2
1430.2525		3	4	3		42	70	4	44	3



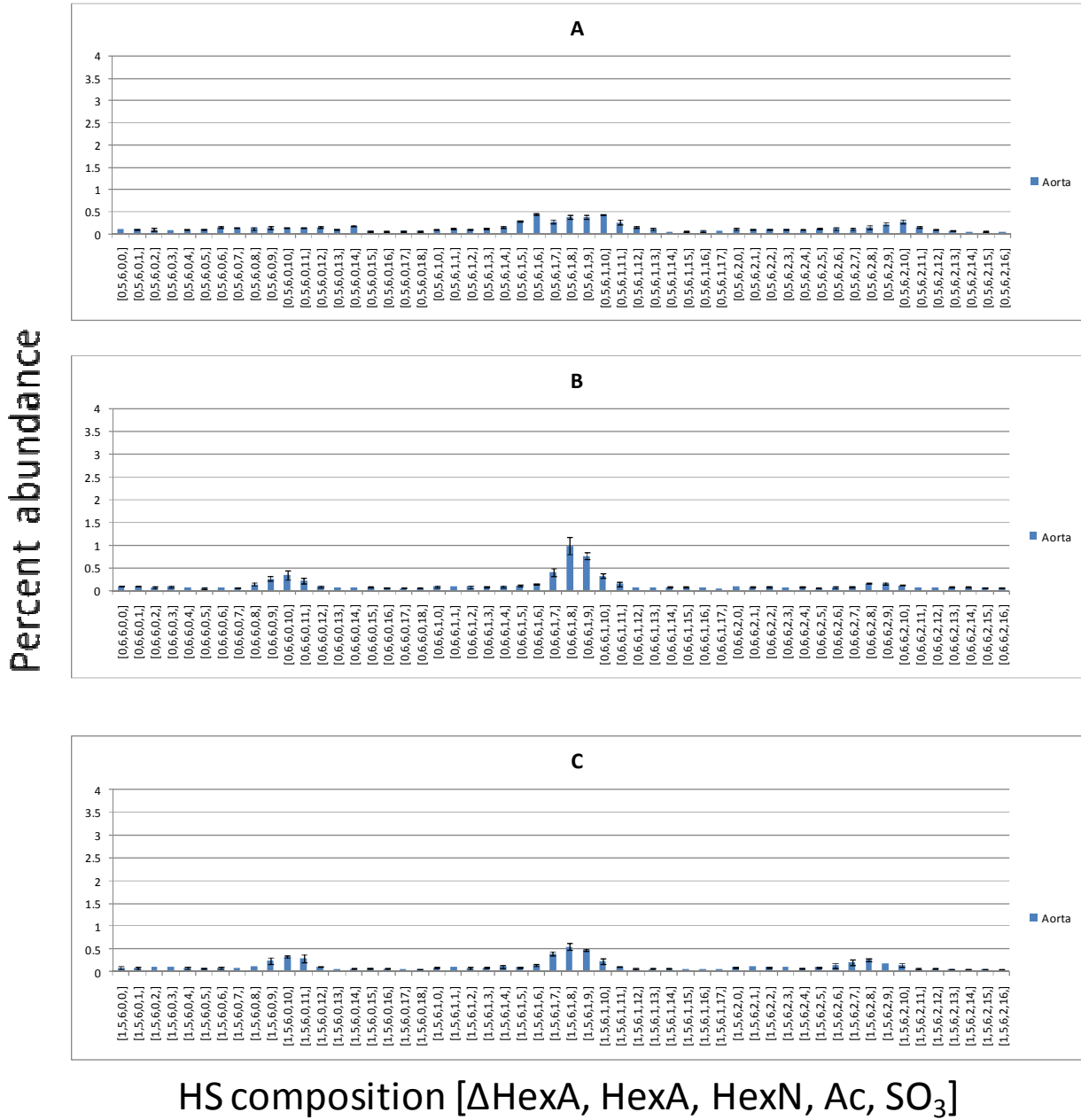
## Supplemental Figure 2, continued

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
1510.2093		3	4	4		42	70	4	47	4
1590.1661		3	4	5		42	70	4	50	5
1670.1229		3	4	6		42	70	4	53	6
1750.0798		3	4	7		42	70	4	56	7
1830.0366		3	4	8		42	70	4	59	8
1909.9934		3	4	9		42	70	4	62	9
1989.9502		3	4	10		42	70	4	65	10
2069.9070		3	4	11		42	70	4	68	11
2149.8638		3	4	12		42	70	4	71	12
1232.3926		3	4		1	44	72	4	36	0
1312.3494		3	4	1	1	44	72	4	39	1
1392.3063		3	4	2	1	44	72	4	42	2
1472.2631		3	4	3	1	44	72	4	45	3
1552.2199		3	4	4	1	44	72	4	48	4
1632.1767		3	4	5	1	44	72	4	51	5
1712.1335		3	4	6	1	44	72	4	54	6
1792.0903		3	4	7	1	44	72	4	57	7
1872.0471		3	4	8	1	44	72	4	60	8
1952.0040		3	4	9	1	44	72	4	63	9
2031.9608		3	4	10	1	44	72	4	66	10
2111.9176		3	4	11	1	44	72	4	69	11
2191.8744		3	4	12	1	44	72	4	72	12
1274.4032		3	4		2	46	74	4	37	0
1354.3600		3	4	1	2	46	74	4	40	1
1434.3168		3	4	2	2	46	74	4	43	2
1514.2736		3	4	3	2	46	74	4	46	3
1594.2304		3	4	4	2	46	74	4	49	4
1674.1873		3	4	5	2	46	74	4	52	5
1754.1441		3	4	6	2	46	74	4	55	6
1834.1009		3	4	7	2	46	74	4	58	7
1914.0577		3	4	8	2	46	74	4	61	8
1994.0145		3	4	9	2	46	74	4	64	9
2073.9713		3	4	10	2	46	74	4	67	10
2153.9282		3	4	11	2	46	74	4	70	11
2233.8850		3	4	12	2	46	74	4	73	12
sat dp9										
1527.4830		4	5			54	89	5	45	0
1607.4398		4	5	1		54	89	5	48	1
1687.3966		4	5	2		54	89	5	51	2
1767.3534		4	5	3		54	89	5	54	3
1847.3102		4	5	4		54	89	5	57	4
1927.2670		4	5	5		54	89	5	60	5
2007.2238		4	5	6		54	89	5	63	6
2087.1807		4	5	7		54	89	5	66	7
2167.1375		4	5	8		54	89	5	69	8
2247.0943		4	5	9		54	89	5	72	9
2327.0511		4	5	10		54	89	5	75	10
2407.0079		4	5	11		54	89	5	78	11
2486.9647		4	5	12		54	89	5	81	12
2566.9215		4	5	13		54	89	5	84	13
2646.8784		4	5	14		54	89	5	87	14
2726.8352		4	5	15		54	89	5	90	15
1569.4935		4	5			56	91	5	46	0
1649.4503		4	5	1	1	56	91	5	49	1
1729.4072		4	5	2	1	56	91	5	52	2
1809.3640		4	5	3	1	56	91	5	55	3
1889.3208		4	5	4	1	56	91	5	58	4
1969.2776		4	5	5	1	56	91	5	61	5
2049.2344		4	5	6	1	56	91	5	64	6
2129.1912		4	5	7	1	56	91	5	67	7
2209.1480		4	5	8	1	56	91	5	70	8
2289.1049		4	5	9	1	56	91	5	73	9
2369.0617		4	5	10	1	56	91	5	76	10
2449.0185		4	5	11	1	56	91	5	79	11
2528.9753		4	5	12	1	56	91	5	82	12
2608.9321		4	5	13	1	56	91	5	85	13
2688.8889		4	5	14	1	56	91	5	88	14
2768.8457		4	5	15	1	56	91	5	91	15
1611.5041		4	5		2	58	93	5	47	0
1691.4609		4	5	1	2	58	93	5	50	1
1771.4177		4	5	2	2	58	93	5	53	2
1851.3745		4	5	3	2	58	93	5	56	3
1931.3313		4	5	4	2	58	93	5	59	4

## Supplemental Figure 2, continued

Mass	Monosaccharide Composition					Elemental Composition				
	$\Delta$ HexA	HexA	HexN	SO <sub>3</sub>	Ac	C	H	N	O	S
2011.2882		4	5	5	2	58	93	5	62	5
2091.2450		4	5	6	2	58	93	5	65	6
2171.2018		4	5	7	2	58	93	5	68	7
2251.1586		4	5	8	2	58	93	5	71	8
2331.1154		4	5	9	2	58	93	5	74	9
2411.0722		4	5	10	2	58	93	5	77	10
2491.0290		4	5	11	2	58	93	5	80	11
2570.9859		4	5	12	2	58	93	5	83	12
2650.9427		4	5	13	2	58	93	5	86	13
2730.8995		4	5	14	2	58	93	5	89	14
2810.8563		4	5	15	2	58	93	5	92	15
sat dp11										
1864.5839		5	6			66	108	6	55	0
1944.5407		5	6	1		66	108	6	58	1
2024.4975		5	6	2		66	108	6	61	2
2104.4543		5	6	3		66	108	6	64	3
2184.4111		5	6	4		66	108	6	67	4
2264.3679		5	6	5		66	108	6	70	5
2344.3247		5	6	6		66	108	6	73	6
2424.2816		5	6	7		66	108	6	76	7
2504.2384		5	6	8		66	108	6	79	8
2584.1952		5	6	9		66	108	6	82	9
2664.1520		5	6	10		66	108	6	85	10
2744.1088		5	6	11		66	108	6	88	11
2824.0656		5	6	12		66	108	6	91	12
2904.0224		5	6	13		66	108	6	94	13
2983.9793		5	6	14		66	108	6	97	14
3063.9361		5	6	15		66	108	6	100	15
3143.8929		5	6	16		66	108	6	103	16
3223.8497		5	6	17		66	108	6	106	17
3303.8065		5	6	18		66	108	6	109	18
1906.5944		5	6		1	68	110	6	56	0
1986.5512		5	6	1	1	68	110	6	59	1
2066.5080		5	6	2	1	68	110	6	62	2
2146.4649		5	6	3	1	68	110	6	65	3
2226.4217		5	6	4	1	68	110	6	68	4
2306.3785		5	6	5	1	68	110	6	71	5
2386.3353		5	6	6	1	68	110	6	74	6
2466.2921		5	6	7	1	68	110	6	77	7
2546.2489		5	6	8	1	68	110	6	80	8
2626.2057		5	6	9	1	68	110	6	83	9
2706.1626		5	6	10	1	68	110	6	86	10
2786.1194		5	6	11	1	68	110	6	89	11
2866.0762		5	6	12	1	68	110	6	92	12
2946.0330		5	6	13	1	68	110	6	95	13
3025.9898		5	6	14	1	68	110	6	98	14
3105.9466		5	6	15	1	68	110	6	101	15
3185.9035		5	6	16	1	68	110	6	104	16
3265.8603		5	6	17	1	68	110	6	107	17
1948.6050		5	6		2	70	112	6	57	0
2028.5618		5	6	1	2	70	112	6	60	1
2108.5186		5	6	2	2	70	112	6	63	2
2188.4754		5	6	3	2	70	112	6	66	3
2268.4322		5	6	4	2	70	112	6	69	4
2348.3891		5	6	5	2	70	112	6	72	5
2428.3459		5	6	6	2	70	112	6	75	6
2508.3027		5	6	7	2	70	112	6	78	7
2588.2595		5	6	8	2	70	112	6	81	8
2668.2163		5	6	9	2	70	112	6	84	9
2748.1731		5	6	10	2	70	112	6	87	10
2828.1299		5	6	11	2	70	112	6	90	11
2908.0868		5	6	12	2	70	112	6	93	12
2988.0436		5	6	13	2	70	112	6	96	13
3068.0004		5	6	14	2	70	112	6	99	14
3147.9572		5	6	15	2	70	112	6	102	15
3227.9140		5	6	16	2	70	112	6	105	16

Supplemental Figure 3.



**Supplemental Figure 4.**