

Supporting Information

Fast and Comprehensive N- and O-glycoproteomics analysis with MSFragger-Glyco

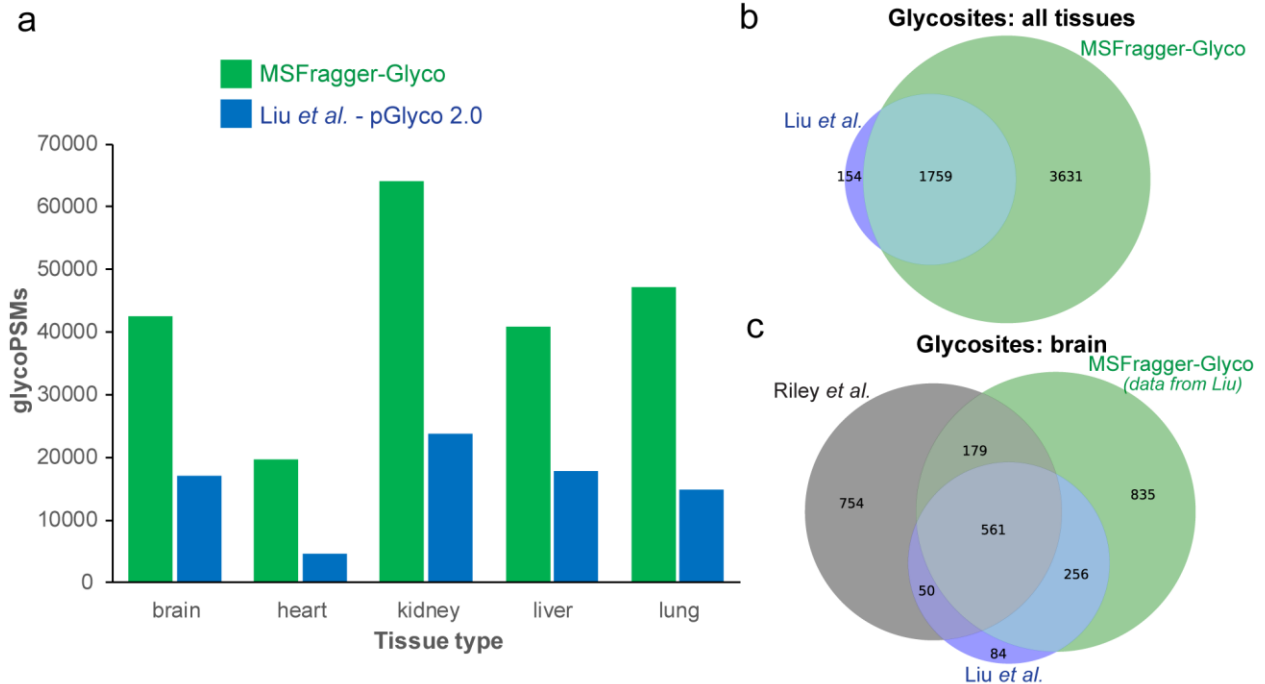
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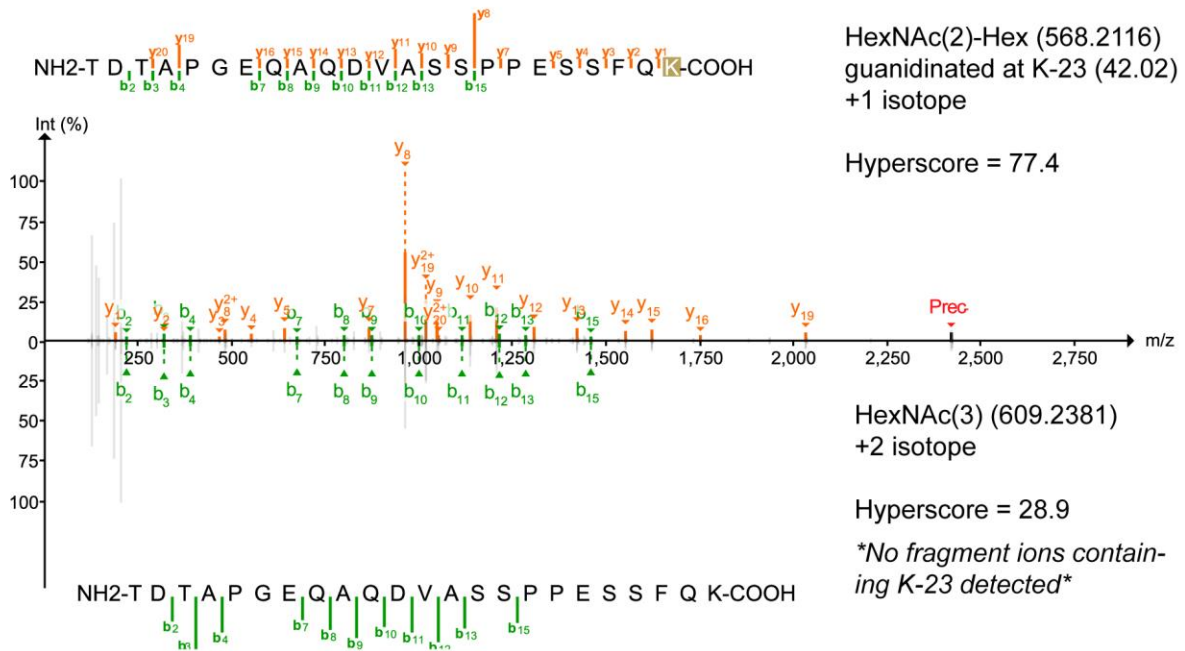
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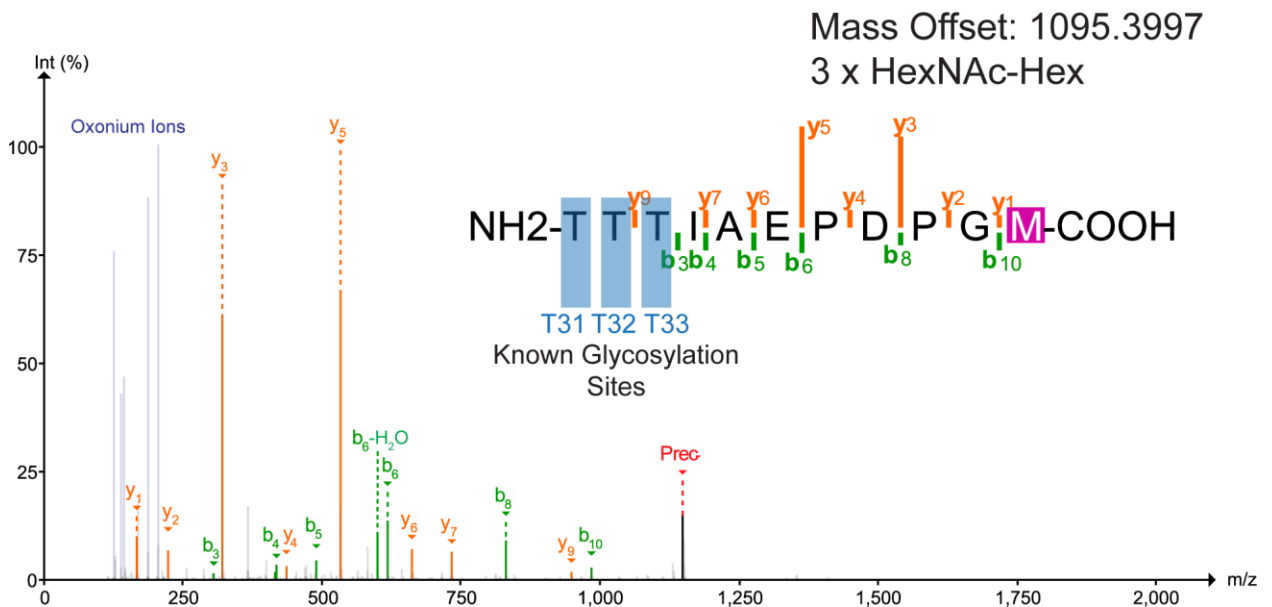
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Supplementary Figure 1. Comparison with Liu *et al.* mouse N-glycoproteomics data processed with pGlyco 2.0. Raw data from Liu *et al.* was searched using the same glycan database (8,093 entries corresponding to 1,670 unique masses) as a mass offset glyco search in MSFragger-Glyco. a) MSFragger-Glyco annotated 2.3 to 4.2 times as many glyco PSMs as pGlyco 2.0 in the various tissue types, generating in total approx. 214,000 glycoPSMs to the 78,000 reported in Liu *et al.* b) MSFragger-Glyco identified more than twice as many glycosites (summed across all 5 tissue types) while showing excellent agreement with sites annotated in the original analysis. c) Comparison of glycosites annotated in mouse brain tissue with data of Riley *et al.*, Liu *et al.*, and MSFragger-Glyco reanalysis of Liu *et al.* data. Many of the additional sites annotated by MSFragger-Glyco appear in the Riley *et al.* data.



Supplementary Figure 2. Comparison of guanidinated peptide (Hex + guanidinyll group) vs HexNAc. The mass of HexNAc + 1 isotope is nearly identical to that of Hex + guanidinyllation of Lys. Guanidinyllation is not labile whereas O-glycosyllation is highly labile, allowing us to clearly distinguish between them based on whether fragment ions retain the guanidinyllation mass shift or not. Example peptide with guanidinyllation (top) shows clear series of y-ions resulting in a hyperscore of 77.4. Considering the same peptide with HexNAc instead of Hex+guanidinyll group matches only b-ions with a much lower score of 28.9 (bottom), indicating that all y-ions are shifted by the guanidinyll group mass and that the top spectrum contains the correct ID.



Supplementary Figure 3. Example spectrum of a peptide containing multiple known sites of O-glycosylation. No fragment ions bearing partial or intact glycan can be observed in the spectrum. All ions observed correspond to the fragmentation of the peptide sequence with no modifications aside from oxidation of Met-11. The mass offset of 1095.3997 corresponds to 3 copies of the common glycan HexNAcHex, which are likely present at the 3 Thr residues at the peptide N-terminus. All 3 Thr residues are known glycosylation sites of the protein (glycophorin-C).

			Time/File (min)	
Activation Type	Shifted Ions?	MS2 Scans/File	Average	St. Dev.
HCD	no	10,000 - 15,000	0.14	0.001
AI-ETD	yes	4,000 - 5,000	1.40	0.004
Total			1.54	

Supplementary Table 1. Time for MSFragger-Glyco searches of Riley *et al.* data. Raw files were split into HCD and AI-ETD scans and analyzed separately. Testing was performed in triplicate on a Windows 10 desktop computer with an Intel Core i7-8700 CPU (3.2 GHz, 6 cores) and 32 GB RAM. HCD scans averaged 0.14 min per raw file and AI-ETD scans averaged 1.4 min per raw file. The much larger time for AI-ETD files is a result of the shifted ion search (used for c/z-type ions with glycan intact).

Supplementary Table 2. Y ions used in MSFragger searches

Mass	Composition
203.07937	HexNAc(1)
406.15874	HexNAc(2)
568.21156	HexNAc(2)Hex(1)
730.26438	HexNAc(2)Hex(2)
892.3172	HexNAc(2)Hex(3)
1095.39657	HexNAc(3)Hex(3)
1257.44939	HexNAc(3)Hex(4)
349.137279	HexNAc(1)Fuc(1)
552.216649	HexNAc(2)Fuc(1)

Supplementary Table 3. Oxonium ions used in MSFragger searches

Composition	Mass (MH+)
HexNAc(1)	204.0866
HexNAc(1) - H ₂ O	186.0761
HexNAc(1)Hex(1)	366.1395
C ₆ H ₁₀ NO ₃	144.0656
C ₇ H ₈ NO ₂	138.0550
C ₆ H ₈ NO ₂	126.0550
HexNAc(1) - H ₂ O(2)	168.0655
Hex(1)	163.0601
NeuAc(1)	292.1027
NeuAc(1) - H ₂ O	274.0921
HexNAc(1)Hex(1)NeuAc(1)	657.2349
Phospho(1)Hex(1)	243.0264
Phospho(2)Hex(1)	405.0792
Phospho(2)Hex(2)	485.0456
HexNAc(1)Sulfo(1)	284.0435
HexNAc(1)Hex(1)Sulfo(1)	446.0963
HexNAc(2)Hex(2)Sulfo(1)	811.2285
NeuGc(1)	308.0976

Supplementary Table 4. Results of decoy offset search for N-glycan data. The 10 most abundant mass offsets were searched along with 10 decoy offsets generated by adding 20 Da to each target mass offset. 0.6% of PSMs corresponded to decoy offsets, within the expected PSM FDR of 1%.

Mass	Composition	PSMs	Decoy Mass	Decoy PSMs	FDR%
892.3172	HexNAc-2_Hex-3	926	912.3172	20	2.2%
1038.3751	HexNAc-2_Hex-3_Fuc-1	1417	1058.3751	21	1.5%
1054.37	HexNAc-2_Hex-4	2277	1074.37	11	0.5%
1216.4228	HexNAc-2_Hex-5	13485	1236.4228	45	0.3%
1378.4757	HexNAc-2_Hex-6	5999	1398.4757	19	0.3%
1540.5285	HexNAc-2_Hex-7	3846	1560.5285	8	0.2%
1565.5601	HexNAc-3_Hex-5_Fuc-1	392	1585.5601	9	2.3%
1702.5813	HexNAc-2_Hex-8	4140	1722.5813	50	1.2%
1768.6395	HexNAc-4_Hex-5_Fuc-1	602	1788.6395	17	2.8%
1864.6341	HexNAc-2_Hex-9	2048	1884.6341	14	0.7%
	Target Total:	35132	Decoy Total:	214	0.6%

Supplementary Table 5. Results of decoy offset search for O-glycan kidney data. The 10 most abundant mass offsets were searched along with 10 decoy offsets generated by adding 10 Da to each target mass offset. 10 Da was chosen to avoid conflicts with other known glycan composition masses and isotope distributions. In total, 1.3% of PSMs corresponded to decoy offsets, close to the expected PSM FDR of 1%. High FDRs for decoy masses 781 and 943 result from overlap with common glycans and amino acid substitutions, illustrating the challenge of choosing appropriate decoys. Despite this, the overall FDR remains close to 1% as expected.

Mass	Composition	PSMs	Decoy Mass	Decoy PSMs	FDR%
203.0794	HexNAc-1	5425	213.0794	62	1.1%
365.1322	HexNAc-1_Hex-1	45900	375.1322	201	0.4%
568.2116	HexNAc-2_Hex-1	2783	578.2116	65	2.3%
730.2644	HexNAc-2_Hex-2	12322	740.2644	113	0.9%
771.2909	HexNAc-3_Hex-1	1172	781.2909	160	13.7%
933.3438	HexNAc-3_Hex-2	964	943.3438	163	16.9%
1095.3966	HexNAc-3_Hex-3	6379	1105.3966	113	1.8%
1298.4759	HexNAc-4_Hex-3	441	1308.4759	23	5.2%
1460.5288	HexNAc-4_Hex-4	1702	1470.5288	100	5.9%
1825.6609	HexNAc-5_Hex-5	885	1835.6609	17	1.9%
	Target Total:	77973	Decoy Total:	1017	1.3%

Supplementary Table 6. 182 N-glycan compositions searched in Riley *et al.* data.

Mass	Composition	Mass	Composition
203.07937	HexNAc(1)	2715.962512	HexNAc(5)Hex(6)Fuc(1)NeuAc(2)
349.137279	HexNAc(1)Fuc(1)	3007.057929	HexNAc(5)Hex(6)Fuc(1)NeuAc(3)
406.15874	HexNAc(2)	2279.829588	HexNAc(5)Hex(6)Fuc(2)
552.216649	HexNAc(2)Fuc(1)	2570.925005	HexNAc(5)Hex(6)Fuc(2)NeuAc(1)
568.21156	HexNAc(2)Hex(1)	2425.887497	HexNAc(5)Hex(6)Fuc(3)
714.269469	HexNAc(2)Hex(1)Fuc(1)	2716.982914	HexNAc(5)Hex(6)Fuc(3)NeuAc(1)
2026.68694	HexNAc(2)Hex(10)	3008.07833	HexNAc(5)Hex(6)Fuc(3)NeuAc(2)
2188.73976	HexNAc(2)Hex(11)	3299.173747	HexNAc(5)Hex(6)Fuc(3)NeuAc(3)
2350.79258	HexNAc(2)Hex(12)	2571.945406	HexNAc(5)Hex(6)Fuc(4)
730.26438	HexNAc(2)Hex(2)	2863.040823	HexNAc(5)Hex(6)Fuc(4)NeuAc(1)
876.322289	HexNAc(2)Hex(2)Fuc(1)	2278.809187	HexNAc(5)Hex(6)NeuAc(1)
892.3172	HexNAc(2)Hex(3)	2569.904603	HexNAc(5)Hex(6)NeuAc(2)
1038.375109	HexNAc(2)Hex(3)Fuc(1)	2861.00002	HexNAc(5)Hex(6)NeuAc(3)
1054.37002	HexNAc(2)Hex(4)	2586.919916	HexNAc(5)Hex(7)Fuc(1)NeuAc(1)
1200.427929	HexNAc(2)Hex(4)Fuc(1)	2878.015332	HexNAc(5)Hex(7)Fuc(1)NeuAc(2)
1216.42284	HexNAc(2)Hex(5)	2311.81941	HexNAc(5)Hex(8)
1362.480749	HexNAc(2)Hex(5)Fuc(1)	2457.877319	HexNAc(5)Hex(8)Fuc(1)
1378.47566	HexNAc(2)Hex(6)	2619.930139	HexNAc(5)Hex(9)Fuc(1)
1524.533569	HexNAc(2)Hex(6)Fuc(1)	1704.63468	HexNAc(6)Hex(3)
1458.44199	HexNAc(2)Hex(6)Phospho(1)	1850.692589	HexNAc(6)Hex(3)Fuc(1)
1540.52848	HexNAc(2)Hex(7)	2141.788006	HexNAc(6)Hex(3)Fuc(1)NeuAc(1)
1686.586389	HexNAc(2)Hex(7)Fuc(1)	2432.883422	HexNAc(6)Hex(3)Fuc(1)NeuAc(2)
1702.5813	HexNAc(2)Hex(8)	1996.750498	HexNAc(6)Hex(3)Fuc(2)
1864.63412	HexNAc(2)Hex(9)	1866.6875	HexNAc(6)Hex(4)
1095.39657	HexNAc(3)Hex(3)	2012.745409	HexNAc(6)Hex(4)Fuc(1)
1241.454479	HexNAc(3)Hex(3)Fuc(1)	2158.803318	HexNAc(6)Hex(4)Fuc(2)
1257.44939	HexNAc(3)Hex(4)	2157.782917	HexNAc(6)Hex(4)NeuAc(1)
1403.507299	HexNAc(3)Hex(4)Fuc(1)	2028.74032	HexNAc(6)Hex(5)
1694.602716	HexNAc(3)Hex(4)Fuc(1)NeuAc(1)	2174.798229	HexNAc(6)Hex(5)Fuc(1)
1549.565208	HexNAc(3)Hex(4)Fuc(2)	2465.893646	HexNAc(6)Hex(5)Fuc(1)NeuAc(1)
1840.660625	HexNAc(3)Hex(4)Fuc(2)NeuAc(1)	2756.989062	HexNAc(6)Hex(5)Fuc(1)NeuAc(2)
1548.544807	HexNAc(3)Hex(4)NeuAc(1)	3048.084479	HexNAc(6)Hex(5)Fuc(1)NeuAc(3)
1419.50221	HexNAc(3)Hex(5)	2320.856138	HexNAc(6)Hex(5)Fuc(2)
1565.560119	HexNAc(3)Hex(5)Fuc(1)	2611.951555	HexNAc(6)Hex(5)Fuc(2)NeuAc(1)
1856.655536	HexNAc(3)Hex(5)Fuc(1)NeuAc(1)	2466.914047	HexNAc(6)Hex(5)Fuc(3)
2147.750952	HexNAc(3)Hex(5)Fuc(1)NeuAc(2)	2190.79314	HexNAc(6)Hex(6)
1710.597627	HexNAc(3)Hex(5)NeuAc(1)	2336.851049	HexNAc(6)Hex(6)Fuc(1)
1581.55503	HexNAc(3)Hex(6)	2627.946466	HexNAc(6)Hex(6)Fuc(1)NeuAc(1)
1727.612939	HexNAc(3)Hex(6)Fuc(1)	2482.908958	HexNAc(6)Hex(6)Fuc(2)
2018.708356	HexNAc(3)Hex(6)Fuc(1)NeuAc(1)	2774.004375	HexNAc(6)Hex(6)Fuc(2)NeuAc(1)
1872.650447	HexNAc(3)Hex(6)NeuAc(1)	3065.099791	HexNAc(6)Hex(6)Fuc(2)NeuAc(2)
1298.47594	HexNAc(4)Hex(3)	2481.888557	HexNAc(6)Hex(6)NeuAc(1)
1444.533849	HexNAc(4)Hex(3)Fuc(1)	2772.983973	HexNAc(6)Hex(6)NeuAc(2)
1589.571357	HexNAc(4)Hex(3)NeuAc(1)	3064.07939	HexNAc(6)Hex(6)NeuAc(3)

1460.52876	HexNAc(4)Hex(4)	2352.84596	HexNAc(6)Hex(7)
1606.586669	HexNAc(4)Hex(4)Fuc(1)	2789.999286	HexNAc(6)Hex(7)Fuc(1)NeuAc(1)
1897.682086	HexNAc(4)Hex(4)Fuc(1)NeuAc(1)	3081.094702	HexNAc(6)Hex(7)Fuc(1)NeuAc(2)
1752.644578	HexNAc(4)Hex(4)Fuc(2)	2644.961778	HexNAc(6)Hex(7)Fuc(2)
1751.624177	HexNAc(4)Hex(4)NeuAc(1)	2936.057195	HexNAc(6)Hex(7)Fuc(2)NeuAc(1)
1622.58158	HexNAc(4)Hex(5)	2791.019687	HexNAc(6)Hex(7)Fuc(3)
1768.639489	HexNAc(4)Hex(5)Fuc(1)	3082.115104	HexNAc(6)Hex(7)Fuc(3)NeuAc(1)
2059.734906	HexNAc(4)Hex(5)Fuc(1)NeuAc(1)	2643.941377	HexNAc(6)Hex(7)NeuAc(1)
2350.830322	HexNAc(4)Hex(5)Fuc(1)NeuAc(2)	2935.036793	HexNAc(6)Hex(7)NeuAc(2)
1914.697398	HexNAc(4)Hex(5)Fuc(2)	3226.13221	HexNAc(6)Hex(7)NeuAc(3)
2205.792815	HexNAc(4)Hex(5)Fuc(2)NeuAc(1)	3517.227626	HexNAc(6)Hex(7)NeuAc(4)
2496.888231	HexNAc(4)Hex(5)Fuc(2)NeuAc(2)	2952.052106	HexNAc(6)Hex(8)Fuc(1)NeuAc(1)
2351.850724	HexNAc(4)Hex(5)Fuc(3)NeuAc(1)	2805.994197	HexNAc(6)Hex(8)NeuAc(1)
2642.94614	HexNAc(4)Hex(5)Fuc(3)NeuAc(2)	2676.9516	HexNAc(6)Hex(9)
1913.676997	HexNAc(4)Hex(5)NeuAc(1)	3114.104926	HexNAc(6)Hex(9)Fuc(1)NeuAc(1)
2204.772413	HexNAc(4)Hex(5)NeuAc(2)	3405.200342	HexNAc(6)Hex(9)Fuc(1)NeuAc(2)
1784.6344	HexNAc(4)Hex(6)	1907.71405	HexNAc(7)Hex(3)
1930.692309	HexNAc(4)Hex(6)Fuc(1)	2053.771959	HexNAc(7)Hex(3)Fuc(1)
2221.787726	HexNAc(4)Hex(6)Fuc(1)NeuAc(1)	2069.76687	HexNAc(7)Hex(4)
2076.750218	HexNAc(4)Hex(6)Fuc(2)	2215.824779	HexNAc(7)Hex(4)Fuc(1)
2075.729817	HexNAc(4)Hex(6)NeuAc(1)	2393.87251	HexNAc(7)Hex(6)
1946.68722	HexNAc(4)Hex(7)	2539.930419	HexNAc(7)Hex(6)Fuc(1)
2092.745129	HexNAc(4)Hex(7)Fuc(1)	2555.92533	HexNAc(7)Hex(7)
2237.782637	HexNAc(4)Hex(7)NeuAc(1)	2701.983239	HexNAc(7)Hex(7)Fuc(1)
1501.55531	HexNAc(5)Hex(3)	3575.269489	HexNAc(7)Hex(7)Fuc(1)NeuAc(3)
1647.613219	HexNAc(5)Hex(3)Fuc(1)	2717.97815	HexNAc(7)Hex(8)
1938.708636	HexNAc(5)Hex(3)Fuc(1)NeuAc(1)	2864.036059	HexNAc(7)Hex(8)Fuc(1)
1793.671128	HexNAc(5)Hex(3)Fuc(2)	3155.131476	HexNAc(7)Hex(8)Fuc(1)NeuAc(1)
1663.60813	HexNAc(5)Hex(4)	4028.417725	HexNAc(7)Hex(8)Fuc(1)NeuAc(4)
1809.666039	HexNAc(5)Hex(4)Fuc(1)	3009.073567	HexNAc(7)Hex(8)NeuAc(1)
2100.761456	HexNAc(5)Hex(4)Fuc(1)NeuAc(1)	2110.79342	HexNAc(8)Hex(3)
2391.856872	HexNAc(5)Hex(4)Fuc(1)NeuAc(2)	2256.851329	HexNAc(8)Hex(3)Fuc(1)
1955.723948	HexNAc(5)Hex(4)Fuc(2)	2272.84624	HexNAc(8)Hex(4)
1954.703547	HexNAc(5)Hex(4)NeuAc(1)	2434.89906	HexNAc(8)Hex(5)
2245.798963	HexNAc(5)Hex(4)NeuAc(2)	2580.956969	HexNAc(8)Hex(5)Fuc(1)
1825.66095	HexNAc(5)Hex(5)	2759.0047	HexNAc(8)Hex(7)
1971.718859	HexNAc(5)Hex(5)Fuc(1)	2921.05752	HexNAc(8)Hex(8)
2262.814276	HexNAc(5)Hex(5)Fuc(1)NeuAc(1)	3083.11034	HexNAc(8)Hex(9)
2553.909692	HexNAc(5)Hex(5)Fuc(1)NeuAc(2)	3229.168249	HexNAc(8)Hex(9)Fuc(1)
2117.776768	HexNAc(5)Hex(5)Fuc(2)	3448.24253	HexNAc(9)Hex(10)
2408.872185	HexNAc(5)Hex(5)Fuc(2)NeuAc(1)	2313.87279	HexNAc(9)Hex(3)
2263.834677	HexNAc(5)Hex(5)Fuc(3)	2459.930699	HexNAc(9)Hex(3)Fuc(1)
2116.756367	HexNAc(5)Hex(5)NeuAc(1)	2475.92561	HexNAc(9)Hex(4)
2407.851783	HexNAc(5)Hex(5)NeuAc(2)	2621.983519	HexNAc(9)Hex(4)Fuc(1)
1987.71377	HexNAc(5)Hex(6)	2800.03125	HexNAc(9)Hex(6)
2133.771679	HexNAc(5)Hex(6)Fuc(1)	2946.089159	HexNAc(9)Hex(6)Fuc(1)
2424.867096	HexNAc(5)Hex(6)Fuc(1)NeuAc(1)	3432.247619	HexNAc(9)Hex(9)Fuc(1)

Supplementary Table 7. 300 O-glycan compositions searched in Yang *et al.* data.

Mass	Composition	Mass	Composition
146.0579	Fuc(1)	1387.4695	HexNAc(5)Fuc(2)Sulf(1)
203.0794	HexNAc(1)	1387.5124	HexNAc(3)Hex(3)Fuc(2)
226.0147	Fuc(1)Sulf(1)	1392.4120	HexNAc(2)Hex(2)NeuAc(2)Sulf(1)
283.0362	HexNAc(1)Sulf(1)	1393.4324	HexNAc(2)Hex(2)Fuc(2)NeuAc(1)Sulf(1)
308.1107	Hex(1)Fuc(1)	1395.5287	HexNAc(4)Fuc(2)NeuAc(1)
349.1373	HexNAc(1)Fuc(1)	1401.4110	HexNAc(1)Hex(6)Fuc(1)Sulf(1)
365.1322	HexNAc(1)Hex(1)	1403.5073	HexNAc(3)Hex(4)Fuc(1)
388.0675	Hex(1)Fuc(1)Sulf(1)	1419.4593	HexNAc(5)Hex(2)Sulf(1)
406.1587	HexNAc(2)	1427.5185	HexNAc(4)Hex(2)NeuAc(1)
429.0941	HexNAc(1)Fuc(1)Sulf(1)	1428.5389	HexNAc(4)Hex(2)Fuc(2)
445.0890	HexNAc(1)Hex(1)Sulf(1)	1433.4386	HexNAc(3)Hex(1)NeuAc(2)Sulf(1)
486.1155	HexNAc(2)Sulf(1)	1434.4589	HexNAc(3)Hex(1)Fuc(2)NeuAc(1)Sulf(1)
494.1748	HexNAc(1)NeuAc(1)	1442.4375	HexNAc(2)Hex(5)Fuc(1)Sulf(1)
511.1901	HexNAc(1)Hex(1)Fuc(1)	1444.5338	HexNAc(4)Hex(3)Fuc(1)
527.1850	HexNAc(1)Hex(2)	1450.4539	HexNAc(3)Hex(2)Fuc(1)NeuAc(1)Sulf(1)
568.2116	HexNAc(2)Hex(1)	1451.4743	HexNAc(3)Hex(2)Fuc(3)Sulf(1)
574.1316	HexNAc(1)NeuAc(1)Sulf(1)	1458.4325	HexNAc(2)Hex(6)Sulf(1)
591.1469	HexNAc(1)Hex(1)Fuc(1)Sulf(1)	1458.5131	HexNAc(2)Hex(2)Fuc(1)NeuAc(2)
607.1418	HexNAc(1)Hex(2)Sulf(1)	1460.5288	HexNAc(4)Hex(4)
609.2381	HexNAc(3)	1466.4488	HexNAc(3)Hex(3)NeuAc(1)Sulf(1)
640.2327	HexNAc(1)Fuc(1)NeuAc(1)	1467.4692	HexNAc(3)Hex(3)Fuc(2)Sulf(1)
648.1684	HexNAc(2)Hex(1)Sulf(1)	1474.5080	HexNAc(2)Hex(3)NeuAc(2)
656.2276	HexNAc(1)Hex(1)NeuAc(1)	1475.4855	HexNAc(4)Fuc(2)NeuAc(1)Sulf(1)
673.2429	HexNAc(1)Hex(2)Fuc(1)	1483.4641	HexNAc(3)Hex(4)Fuc(1)Sulf(1)
689.1949	HexNAc(3)Sulf(1)	1501.5553	HexNAc(5)Hex(3)
689.2378	HexNAc(1)Hex(3)	1507.4754	HexNAc(4)Hex(2)NeuAc(1)Sulf(1)
697.2541	HexNAc(2)NeuAc(1)	1508.4958	HexNAc(4)Hex(2)Fuc(2)Sulf(1)
698.2746	HexNAc(2)Fuc(2)	1515.5346	HexNAc(3)Hex(2)NeuAc(2)
714.2695	HexNAc(2)Hex(1)Fuc(1)	1517.5754	HexNAc(3)Hex(2)Fuc(4)
720.1895	HexNAc(1)Fuc(1)NeuAc(1)Sulf(1)	1524.4906	HexNAc(4)Hex(3)Fuc(1)Sulf(1)
730.2644	HexNAc(2)Hex(2)	1524.5336	HexNAc(2)Hex(6)Fuc(1)
736.1844	HexNAc(1)Hex(1)NeuAc(1)Sulf(1)	1532.5499	HexNAc(3)Hex(3)Fuc(1)NeuAc(1)
753.1997	HexNAc(1)Hex(2)Fuc(1)Sulf(1)	1533.5703	HexNAc(3)Hex(3)Fuc(3)
755.2960	HexNAc(3)Fuc(1)	1538.4699	HexNAc(2)Hex(2)Fuc(1)NeuAc(2)Sulf(1)
769.1946	HexNAc(1)Hex(3)Sulf(1)	1540.4856	HexNAc(4)Hex(4)Sulf(1)
771.2909	HexNAc(3)Hex(1)	1540.5285	HexNAc(2)Hex(7)
777.2109	HexNAc(2)NeuAc(1)Sulf(1)	1548.5448	HexNAc(3)Hex(4)NeuAc(1)
778.2314	HexNAc(2)Fuc(2)Sulf(1)	1554.4648	HexNAc(2)Hex(3)NeuAc(2)Sulf(1)
786.2906	HexNAc(1)Fuc(2)NeuAc(1)	1557.5815	HexNAc(4)Hex(1)Fuc(2)NeuAc(1)
794.2263	HexNAc(2)Hex(1)Fuc(1)Sulf(1)	1565.5601	HexNAc(3)Hex(5)Fuc(1)
802.2855	HexNAc(1)Hex(1)Fuc(1)NeuAc(1)	1573.5764	HexNAc(4)Hex(2)Fuc(1)NeuAc(1)

810.2212	HexNAc(2)Hex(2)Sulf(1)	1574.5968	HexNAc(4)Hex(2)Fuc(3)
812.3175	HexNAc(4)	1581.5121	HexNAc(5)Hex(3)Sulf(1)
818.2804	HexNAc(1)Hex(2)NeuAc(1)	1589.5713	HexNAc(4)Hex(3)NeuAc(1)
835.2528	HexNAc(3)Fuc(1)Sulf(1)	1590.5918	HexNAc(4)Hex(3)Fuc(2)
835.2957	HexNAc(1)Hex(3)Fuc(1)	1595.4914	HexNAc(3)Hex(2)NeuAc(2)Sulf(1)
843.3120	HexNAc(2)Fuc(1)NeuAc(1)	1597.5322	HexNAc(3)Hex(2)Fuc(4)Sulf(1)
851.2477	HexNAc(3)Hex(1)Sulf(1)	1604.4904	HexNAc(2)Hex(6)Fuc(1)Sulf(1)
851.2907	HexNAc(1)Hex(4)	1606.5867	HexNAc(4)Hex(4)Fuc(1)
859.3070	HexNAc(2)Hex(1)NeuAc(1)	1612.5067	HexNAc(3)Hex(3)Fuc(1)NeuAc(1)Sulf(1)
860.3274	HexNAc(2)Hex(1)Fuc(2)	1613.5271	HexNAc(3)Hex(3)Fuc(3)Sulf(1)
866.2474	HexNAc(1)Fuc(2)NeuAc(1)Sulf(1)	1620.4853	HexNAc(2)Hex(7)Sulf(1)
876.3223	HexNAc(2)Hex(2)Fuc(1)	1622.5816	HexNAc(4)Hex(5)
882.2423	HexNAc(1)Hex(1)Fuc(1)NeuAc(1)Sulf(1)	1628.5016	HexNAc(3)Hex(4)NeuAc(1)Sulf(1)
892.2743	HexNAc(4)Sulf(1)	1637.5383	HexNAc(4)Hex(1)Fuc(2)NeuAc(1)Sulf(1)
892.3172	HexNAc(2)Hex(3)	1645.5169	HexNAc(3)Hex(5)Fuc(1)Sulf(1)
898.2372	HexNAc(1)Hex(2)NeuAc(1)Sulf(1)	1647.6132	HexNAc(5)Hex(3)Fuc(1)
915.2525	HexNAc(1)Hex(3)Fuc(1)Sulf(1)	1653.5332	HexNAc(4)Hex(2)Fuc(1)NeuAc(1)Sulf(1)
917.3488	HexNAc(3)Hex(1)Fuc(1)	1654.5536	HexNAc(4)Hex(2)Fuc(3)Sulf(1)
923.2688	HexNAc(2)Fuc(1)NeuAc(1)Sulf(1)	1663.6081	HexNAc(5)Hex(4)
931.2475	HexNAc(1)Hex(4)Sulf(1)	1669.5281	HexNAc(4)Hex(3)NeuAc(1)Sulf(1)
933.3438	HexNAc(3)Hex(2)	1670.5486	HexNAc(4)Hex(3)Fuc(2)Sulf(1)
939.2638	HexNAc(2)Hex(1)NeuAc(1)Sulf(1)	1677.5874	HexNAc(3)Hex(3)NeuAc(2)
940.2842	HexNAc(2)Hex(1)Fuc(2)Sulf(1)	1686.5435	HexNAc(4)Hex(4)Fuc(1)Sulf(1)
956.2791	HexNAc(2)Hex(2)Fuc(1)Sulf(1)	1686.5864	HexNAc(2)Hex(7)Fuc(1)
972.2740	HexNAc(2)Hex(3)Sulf(1)	1702.5384	HexNAc(4)Hex(5)Sulf(1)
974.3703	HexNAc(4)Hex(1)	1704.6347	HexNAc(6)Hex(3)
989.3700	HexNAc(2)Fuc(2)NeuAc(1)	1727.5700	HexNAc(5)Hex(3)Fuc(1)Sulf(1)
997.3056	HexNAc(3)Hex(1)Fuc(1)Sulf(1)	1727.6129	HexNAc(3)Hex(6)Fuc(1)
997.3486	HexNAc(1)Hex(4)Fuc(1)	1743.5649	HexNAc(5)Hex(4)Sulf(1)
1005.3649	HexNAc(2)Hex(1)Fuc(1)NeuAc(1)	1751.6242	HexNAc(4)Hex(4)NeuAc(1)
1006.3853	HexNAc(2)Hex(1)Fuc(3)	1752.6446	HexNAc(4)Hex(4)Fuc(2)
1013.3006	HexNAc(3)Hex(2)Sulf(1)	1757.5442	HexNAc(3)Hex(3)NeuAc(2)Sulf(1)
1013.3435	HexNAc(1)Hex(5)	1766.5432	HexNAc(2)Hex(7)Fuc(1)Sulf(1)
1015.3969	HexNAc(5)	1768.6395	HexNAc(4)Hex(5)Fuc(1)
1021.3598	HexNAc(2)Hex(2)NeuAc(1)	1784.5915	HexNAc(6)Hex(3)Sulf(1)
1022.3802	HexNAc(2)Hex(2)Fuc(2)	1806.6300	HexNAc(3)Hex(2)NeuAc(3)
1038.3751	HexNAc(2)Hex(3)Fuc(1)	1807.5697	HexNAc(3)Hex(6)Fuc(1)Sulf(1)
1046.3914	HexNAc(3)Fuc(1)NeuAc(1)	1823.6453	HexNAc(3)Hex(3)Fuc(1)NeuAc(2)
1054.3271	HexNAc(4)Hex(1)Sulf(1)	1825.6609	HexNAc(5)Hex(5)
1054.3700	HexNAc(2)Hex(4)	1831.5810	HexNAc(4)Hex(4)NeuAc(1)Sulf(1)
1062.3863	HexNAc(3)Hex(1)NeuAc(1)	1831.6239	HexNAc(2)Hex(7)NeuAc(1)
1063.4067	HexNAc(3)Hex(1)Fuc(2)	1832.6014	HexNAc(4)Hex(4)Fuc(2)Sulf(1)
1069.3268	HexNAc(2)Fuc(2)NeuAc(1)Sulf(1)	1848.5963	HexNAc(4)Hex(5)Fuc(1)Sulf(1)

1077.3054	HexNAc(1)Hex(4)Fuc(1)Sulf(1)	1850.6926	HexNAc(6)Hex(3)Fuc(1)
1079.4017	HexNAc(3)Hex(2)Fuc(1)	1864.6719	HexNAc(4)Hex(2)Fuc(1)NeuAc(2)
1085.3217	HexNAc(2)Hex(1)Fuc(1)NeuAc(1)Sulf(1)	1866.6875	HexNAc(6)Hex(4)
1086.3421	HexNAc(2)Hex(1)Fuc(3)Sulf(1)	1886.5868	HexNAc(3)Hex(2)NeuAc(3)Sulf(1)
1093.3003	HexNAc(1)Hex(5)Sulf(1)	1903.6021	HexNAc(3)Hex(3)Fuc(1)NeuAc(2)Sulf(1)
1095.3537	HexNAc(5)Sulf(1)	1905.6177	HexNAc(5)Hex(5)Sulf(1)
1095.3966	HexNAc(3)Hex(3)	1905.6607	HexNAc(3)Hex(8)
1101.3166	HexNAc(2)Hex(2)NeuAc(1)Sulf(1)	1911.5807	HexNAc(2)Hex(7)NeuAc(1)Sulf(1)
1102.3370	HexNAc(2)Hex(2)Fuc(2)Sulf(1)	1913.6770	HexNAc(4)Hex(5)NeuAc(1)
1118.3319	HexNAc(2)Hex(3)Fuc(1)Sulf(1)	1914.6974	HexNAc(4)Hex(5)Fuc(2)
1126.3482	HexNAc(3)Fuc(1)NeuAc(1)Sulf(1)	1930.6494	HexNAc(6)Hex(3)Fuc(1)Sulf(1)
1134.3268	HexNAc(2)Hex(4)Sulf(1)	1930.6923	HexNAc(4)Hex(6)Fuc(1)
1136.4231	HexNAc(4)Hex(2)	1938.7086	HexNAc(5)Hex(3)Fuc(1)NeuAc(1)
1142.3432	HexNAc(3)Hex(1)NeuAc(1)Sulf(1)	1944.6287	HexNAc(4)Hex(2)Fuc(1)NeuAc(2)Sulf(1)
1143.3636	HexNAc(3)Hex(1)Fuc(2)Sulf(1)	1946.6443	HexNAc(6)Hex(4)Sulf(1)
1150.4024	HexNAc(2)Hex(1)NeuAc(2)	1969.7032	HexNAc(3)Hex(3)Fuc(2)NeuAc(2)
1151.4228	HexNAc(2)Hex(1)Fuc(2)NeuAc(1)	1971.7189	HexNAc(5)Hex(5)Fuc(1)
1159.3585	HexNAc(3)Hex(2)Fuc(1)Sulf(1)	1985.6175	HexNAc(3)Hex(8)Sulf(1)
1159.4014	HexNAc(1)Hex(5)Fuc(1)	1987.7138	HexNAc(5)Hex(6)
1167.4177	HexNAc(2)Hex(2)Fuc(1)NeuAc(1)	1993.6338	HexNAc(4)Hex(5)NeuAc(1)Sulf(1)
1168.4381	HexNAc(2)Hex(2)Fuc(3)	1994.6542	HexNAc(4)Hex(5)Fuc(2)Sulf(1)
1175.3534	HexNAc(3)Hex(3)Sulf(1)	2010.6491	HexNAc(4)Hex(6)Fuc(1)Sulf(1)
1183.4126	HexNAc(2)Hex(3)NeuAc(1)	2018.6655	HexNAc(5)Hex(3)Fuc(1)NeuAc(1)Sulf(1)
1192.4493	HexNAc(3)Fuc(2)NeuAc(1)	2018.7083	HexNAc(3)Hex(6)Fuc(1)NeuAc(1)
1200.4279	HexNAc(2)Hex(4)Fuc(1)	2028.7403	HexNAc(6)Hex(5)
1208.4443	HexNAc(3)Hex(1)Fuc(1)NeuAc(1)	2042.7196	HexNAc(4)Hex(4)NeuAc(2)
1216.3799	HexNAc(4)Hex(2)Sulf(1)	2043.7400	HexNAc(4)Hex(4)Fuc(2)NeuAc(1)
1216.4228	HexNAc(2)Hex(5)	2049.6600	HexNAc(3)Hex(3)Fuc(2)NeuAc(2)Sulf(1)
1218.4762	HexNAc(6)	2051.6757	HexNAc(5)Hex(5)Fuc(1)Sulf(1)
1224.4391	HexNAc(3)Hex(2)NeuAc(1)	2060.7553	HexNAc(4)Hex(5)Fuc(3)
1225.4596	HexNAc(3)Hex(2)Fuc(2)	2067.6706	HexNAc(5)Hex(6)Sulf(1)
1230.3592	HexNAc(2)Hex(1)NeuAc(2)Sulf(1)	2083.7461	HexNAc(5)Hex(3)NeuAc(2)
1231.3796	HexNAc(2)Hex(1)Fuc(2)NeuAc(1)Sulf(1)	2092.7451	HexNAc(4)Hex(7)Fuc(1)
1239.3582	HexNAc(1)Hex(5)Fuc(1)Sulf(1)	2098.6651	HexNAc(3)Hex(6)Fuc(1)NeuAc(1)Sulf(1)
1241.4545	HexNAc(3)Hex(3)Fuc(1)	2108.6971	HexNAc(6)Hex(5)Sulf(1)
1247.3745	HexNAc(2)Hex(2)Fuc(1)NeuAc(1)Sulf(1)	2117.7768	HexNAc(5)Hex(5)Fuc(2)
1248.3949	HexNAc(2)Hex(2)Fuc(3)Sulf(1)	2122.6764	HexNAc(4)Hex(4)NeuAc(2)Sulf(1)
1257.4494	HexNAc(3)Hex(4)	2123.6968	HexNAc(4)Hex(4)Fuc(2)NeuAc(1)Sulf(1)
1263.3694	HexNAc(2)Hex(3)NeuAc(1)Sulf(1)	2133.7717	HexNAc(5)Hex(6)Fuc(1)
1272.4061	HexNAc(3)Fuc(2)NeuAc(1)Sulf(1)	2140.7121	HexNAc(4)Hex(5)Fuc(3)Sulf(1)
1280.3847	HexNAc(2)Hex(4)Fuc(1)Sulf(1)	2163.7030	HexNAc(5)Hex(3)NeuAc(2)Sulf(1)
1282.4810	HexNAc(4)Hex(2)Fuc(1)	2171.7622	HexNAc(4)Hex(3)NeuAc(3)
1288.4011	HexNAc(3)Hex(1)Fuc(1)NeuAc(1)Sulf(1)	2172.7019	HexNAc(4)Hex(7)Fuc(1)Sulf(1)

1296.3796	HexNAc(2)Hex(5)Sulf(1)	2174.7982	HexNAc(6)Hex(5)Fuc(1)
1296.4603	HexNAc(2)Hex(1)Fuc(1)NeuAc(2)	2189.7979	HexNAc(4)Hex(4)Fuc(3)NeuAc(1)
1298.4330	HexNAc(6)Sulf(1)	2190.7931	HexNAc(6)Hex(6)
1298.4759	HexNAc(4)Hex(3)	2197.7336	HexNAc(5)Hex(5)Fuc(2)Sulf(1)
1304.3959	HexNAc(3)Hex(2)NeuAc(1)Sulf(1)	2213.7285	HexNAc(5)Hex(6)Fuc(1)Sulf(1)
1305.4164	HexNAc(3)Hex(2)Fuc(2)Sulf(1)	2213.7714	HexNAc(3)Hex(9)Fuc(1)
1307.5127	HexNAc(5)Fuc(2)	2251.7190	HexNAc(4)Hex(3)NeuAc(3)Sulf(1)
1312.4552	HexNAc(2)Hex(2)NeuAc(2)	2254.7550	HexNAc(6)Hex(5)Fuc(1)Sulf(1)
1313.4756	HexNAc(2)Hex(2)Fuc(2)NeuAc(1)	2269.7547	HexNAc(4)Hex(4)Fuc(3)NeuAc(1)Sulf(1)
1321.4113	HexNAc(3)Hex(3)Fuc(1)Sulf(1)	2270.7499	HexNAc(6)Hex(6)Sulf(1)
1321.4542	HexNAc(1)Hex(6)Fuc(1)	2293.7282	HexNAc(3)Hex(9)Fuc(1)Sulf(1)
1337.4062	HexNAc(3)Hex(4)Sulf(1)	2352.8460	HexNAc(6)Hex(7)
1339.5025	HexNAc(5)Hex(2)	2393.8725	HexNAc(7)Hex(6)
1353.4818	HexNAc(3)Hex(1)NeuAc(2)	2432.8028	HexNAc(6)Hex(7)Sulf(1)
1354.5021	HexNAc(3)Hex(1)Fuc(2)NeuAc(1)	2432.8834	HexNAc(6)Hex(3)Fuc(1)NeuAc(2)
1362.4378	HexNAc(4)Hex(2)Fuc(1)Sulf(1)	2473.8293	HexNAc(7)Hex(6)Sulf(1)
1362.4807	HexNAc(2)Hex(5)Fuc(1)	2498.9039	HexNAc(6)Hex(7)Fuc(1)
1370.4971	HexNAc(3)Hex(2)Fuc(1)NeuAc(1)	2512.8402	HexNAc(6)Hex(3)Fuc(1)NeuAc(2)Sulf(1)
1371.5175	HexNAc(3)Hex(2)Fuc(3)	2555.9253	HexNAc(7)Hex(7)
1376.4171	HexNAc(2)Hex(1)Fuc(1)NeuAc(2)Sulf(1)	2578.8607	HexNAc(6)Hex(7)Fuc(1)Sulf(1)
1378.4327	HexNAc(4)Hex(3)Sulf(1)	2635.8821	HexNAc(7)Hex(7)Sulf(1)
1378.4757	HexNAc(2)Hex(6)	2701.9832	HexNAc(7)Hex(7)Fuc(1)
1386.4920	HexNAc(3)Hex(3)NeuAc(1)	2781.9400	HexNAc(7)Hex(7)Fuc(1)Sulf(1)

Supplementary Table 8. FDR for each mass offset for N-glycan data from Riley *et al.*

Modification Mass	Target PSMs	Decoy PSMs	FDR %	Modification Mass	Target PSMs	Decoy PSMs	FDR %
0	54599	11	0	2864	5	0	0
16	42657	11	0	2466.9	5	0	0
1216.4	9516	17	0.2	1851.7	5	0	0
1378.5	4297	13	0.3	1987.8	5	0	0
1217.4	3312	7	0.2	2223.8	5	1	20
1702.6	2773	3	0.1	2217.9	5	0	0
1540.5	2627	0	0	2459.9	5	0	0
1054.4	1810	9	0.5	2947.1	5	0	0
1379.5	1466	2	0.1	3067.1	5	0	0
1864.6	1310	0	0	2013.7	5	0	0
1703.6	1215	1	0.1	2679	4	0	0
1038.4	1144	0	0	3576.3	4	0	0
1541.5	1081	2	0.2	2936	4	0	0
1218.4	929	4	0.4	1526.5	4	0	0
892.3	807	5	0.6	2436.9	4	0	0
1865.7	720	1	0.1	1696.6	4	0	0
1704.6	440	0	0	2569.9	4	0	0
1380.5	432	1	0.2	3085.1	4	0	0
1055.4	420	0	0	2281.9	4	0	0
42	420	0	0	1608.6	4	0	0
1768.7	403	0	0	2191.9	4	0	0
1241.5	389	1	0.3	2407.8	4	0	0
-17	350	2	0.6	3432.2	4	0	0
1458.5	339	1	0.3	1665.6	4	0	0
1542.6	336	0	0	2581.9	4	0	0
1565.6	276	2	0.7	570.2	4	0	0
1362.5	249	2	0.8	2257.8	4	0	0
1419.5	243	0	0	2238.8	4	0	0
1622.6	241	0	0	1794.7	4	0	0
1727.6	240	1	0.4	2110.7	4	0	0
1039.4	228	0	0	3227.1	4	0	0
730.3	226	0	0	1916.7	3	0	0
1873.7	212	0	0	1591.5	3	0	0
1866.6	207	0	0	2030.8	3	0	0
1930.7	192	1	0.5	2118.8	3	0	0
2018.7	170	0	0	2257	3	0	0
1459.5	162	0	0	2427.9	3	0	0
203.1	153	0	0	2761	3	0	0
893.3	149	0	0	1825.7	3	0	0
2433.9	138	0	0	2012.7	3	0	0

1769.7	136	0	0	2541	3	0	0
1444.5	126	0	0	3517.3	3	0	0
2076.8	117	1	0.9	2192.7	3	0	0
1874.7	115	0	0	2149.7	3	0	0
1566.6	114	0	0	2612	3	0	0
1897.7	113	0	0	2644	3	0	0
1420.5	109	0	0	2141.7	3	0	0
1872.7	105	0	0	2094.8	3	0	0
2432.9	104	0	0	3229.2	3	0	0
1623.6	103	0	0	2613.9	3	0	0
1931.7	101	0	0	2410.8	3	0	0
2019.7	97	0	0	1811.6	3	0	0
568.2	97	0	0	3066	3	0	0
1056.4	88	0	0	1957.7	3	0	0
2077.8	84	0	0	1947.7	3	0	0
1728.6	81	0	0	715.3	3	0	0
1752.7	81	0	0	1097.5	3	0	0
1242.5	80	0	0	2245.8	3	0	0
1705.6	77	0	0	2800	3	0	0
1040.4	76	0	0	2029.7	3	0	0
1363.5	76	0	0	3010.1	3	0	0
1200.4	75	0	0	2935	3	0	0
1581.6	74	0	0	2190.9	3	0	0
2434.9	68	0	0	2807.9	3	0	0
1095.4	66	0	0	3300.3	3	0	0
1257.5	61	0	0	2111.8	2	0	0
1784.7	55	0	0	1988.7	2	0	0
1445.5	53	0	0	2553.9	2	0	0
1460.5	52	0	0	2147.7	2	0	0
406.2	52	0	0	1711.6	2	0	0
2758	52	0	0	2716	2	0	0
2027.7	51	0	0	2677	2	0	0
1403.5	50	0	0	1590.6	2	0	0
1898.7	48	0	0	1842.7	2	0	0
1867.7	47	0	0	2720	2	0	0
1770.7	45	0	0	2938	2	0	0
2026.7	44	0	0	2702	2	0	0
1606.6	42	0	0	1827.7	2	0	0
1932.7	41	0	0	2542	2	0	0
731.3	40	0	0	2258.8	2	0	0
2757	38	0	0	1686.6	2	0	0
876.3	38	0	0	3228.1	2	0	0
1729.6	37	0	0	349.1	2	0	0

2020.7	36	0	0	2160.8	2	0	0
1582.6	35	0	0	2143.8	2	0	0
1201.4	35	0	0	1857.7	2	0	0
1421.5	33	0	0	2392.9	2	0	0
1753.7	33	0	0	3231.1	2	0	0
1624.6	33	0	0	2206.7	2	0	0
1785.7	33	0	0	2321.8	2	0	0
894.3	32	0	0	2496.9	2	0	0
2078.8	32	0	0	878.3	2	0	0
1243.5	31	0	0	3155.1	2	0	0
1647.6	30	0	0	552.2	2	0	0
1567.6	29	0	0	2354.9	2	0	0
204.1	29	0	0	2623.9	2	0	0
2435.9	29	0	0	2117.7	2	0	0
3082.1	28	0	0	2952	2	0	0
569.2	28	0	0	2801	2	0	0
2865.1	27	0	0	2425.9	2	0	0
1786.6	26	0	0	2189.7	2	0	0
2221.8	25	0	0	3115.1	2	0	0
732.3	25	0	0	2588.9	2	0	0
2921	24	0	0	1664.6	2	0	0
1549.6	22	0	0	3226.1	2	0	0
2759	22	0	0	2937	2	0	0
3083.1	22	0	0	1971.8	2	0	0
1364.5	21	0	0	2205.8	2	0	0
1648.6	21	0	0	1996.8	2	0	0
1259.4	20	0	0	3434.2	2	0	0
1298.5	20	0	0	2719	2	0	0
2866.1	20	0	0	1300.5	2	0	0
1649.6	19	0	0	2014.8	2	0	0
1938.7	18	0	0	1989.7	2	0	0
2222.8	18	0	0	2158.8	2	0	0
2946.1	18	0	0	2133.7	2	0	0
1913.7	18	0	0	2481.9	2	0	0
1460.4	17	0	0	1850.6	2	0	0
1751.6	17	0	0	2395	2	0	0
2351.8	17	1	5.9	2772.9	2	0	0
205.1	16	0	0	3114.2	1	0	0
1607.5	15	0	0	3065	1	0	0
2100.8	15	0	0	1840.6	1	0	0
1706.6	15	0	0	2054.7	1	0	0
1694.6	15	0	0	2279.8	1	0	0
1258.5	15	0	0	3448.3	1	0	0

1899.7	14	0	0	2313.8	1	0	0
2060.8	14	0	0	2393.8	1	0	0
2580.9	14	0	0	2702.9	1	0	0
1525.5	14	0	0	2135.8	1	0	0
1583.5	13	0	0	2776	1	0	0
1589.5	13	0	0	2337.9	1	0	0
2352.9	13	0	0	2477	1	0	0
1461.5	12	0	0	1972.8	1	0	0
2759.9	12	0	0	2467.9	1	0	0
2237.8	12	0	0	2424.9	1	0	0
2059.7	12	0	0	2247.7	1	0	0
1868.7	12	0	0	1300.6	1	0	0
1502.6	12	0	0	2571	1	0	0
1501.6	11	0	0	2678	1	0	0
1550.6	11	0	0	1548.6	1	0	0
1754.7	11	0	0	2426.9	1	0	0
1695.6	11	0	0	2791.9	1	0	0
3407.2	11	0	0	2557.9	1	0	0
1939.7	11	0	0	1998.8	1	0	0
1914.7	11	0	0	3156.2	1	0	0
1404.5	11	0	0	2555.8	1	0	0
1096.4	11	0	0	2322.8	1	0	0
2075.7	11	0	0	2336.8	1	0	0
1858.7	10	0	0	1694.5	1	0	0
1446.6	10	0	0	1826.7	1	0	0
2028.7	10	0	0	2704.1	1	0	0
2311.9	10	0	0	1462.5	1	0	0
2350.8	10	0	0	1909.7	1	0	0
1202.4	10	0	0	2642.9	1	0	0
1405.5	9	0	0	2070.7	1	0	0
1956.7	9	0	0	3433.2	1	0	0
1915.7	9	0	0	2408.9	1	0	0
2621.9	9	0	0	3519.2	1	0	0
1524.5	9	0	0	1809.7	1	0	0
877.3	9	0	0	1940.7	1	0	0
3084.1	9	0	0	4028.5	1	0	0
1503.6	9	0	0	2717.9	1	0	0
2093.7	8	0	0	2469	1	0	0
2922	8	0	0	2802	1	0	0
2239.8	8	0	0	2461.9	1	0	0
2612.9	8	0	0	3301.1	1	0	0
2620.9	8	0	0	2582.9	1	0	0
1551.6	7	0	0	2948.1	1	0	0

2879	7	0	0	1856.6	1	0	0
3406.2	7	0	0	3011.1	1	0	0
408.2	7	0	0	3008	1	0	0
1299.5	7	0	0	2774	1	0	0
2272.8	7	0	0	3299.3	1	0	0
1710.6	7	0	0	553.2	1	0	0
1793.7	7	0	0	2112.8	1	0	0
2273.8	7	0	0	2263.8	1	0	0
2458.8	6	0	0	1954.7	1	0	0
2457.8	6	0	0	2053.7	1	0	0
3081.1	6	0	0	2877.9	1	0	0
1097.4	6	0	0	2793	1	0	0
2775	6	0	0	2646	1	0	0
1810.7	6	0	0	3048.2	1	0	0
407.2	6	0	0	2587	1	0	0
2216.9	6	0	0	3116.1	1	0	0
2622.9	6	0	0	3009	1	0	0
1955.7	6	0	0	2483.9	1	0	0
714.3	6	0	0	2497.9	1	0	0
1852.6	6	0	0	2571.8	1	0	0
2207.7	6	0	0	716.3	1	0	0
2092.7	6	0	0	2274.9	1	0	0
1907.7	6	0	0	2880.1	1	0	0
2159.9	6	0	0	2314.9	1	0	0
1687.6	5	0	0	2574	1	0	0
1946.7	5	0	0	4029.5	1	0	0
2069.9	5	0	0	2278.7	1	0	0
2353.8	5	0	0	3230.2	1	0	0
2482.9	5	0	0	2175.8	1	0	0
2061.7	5	0	0	3050.1	1	0	0
2312.8	5	0	0	2391.9	1	0	0
1712.6	5	0	0	3405.2	1	0	0
2465.9	5	0	0	554.2	1	0	0
2619.9	5	0	0	2116.8	1	0	0
1663.6	5	0	0				

Supplementary Table 9: FDR for each mass offset for O-glycan main search (300 glycans) from Yang *et al.*

Modification Mass	Target PSMs	Decoy PSMs	FDR %	Modification Mass	Target PSMs	Decoy PSMs	FDR %
365.1	45598	57	0.1	844.3	29	0	0
42	30878	24	0.1	1232.4	29	0	0
1	22065	369	1.7	1629.5	29	0	0
16	16131	209	1.3	2637.9	29	0	0
730.3	13015	2	0	940.3	28	0	0
57	12664	24	0.2	1258.5	28	0	0
366.1	8949	12	0.1	488.2	28	0	0
0	5808	0	0	1216.4	28	0	0
203.1	5517	2	0	227	28	0	0
1095.4	5224	7	0.1	836.3	27	11	40.7
367.1	4536	3	0.1	1192.5	27	0	0
731.3	3254	0	0	1554.5	27	0	0
1096.4	2670	0	0	794.2	27	0	0
568.2	2508	8	0.3	1392.3	27	2	7.4
933.3	1431	1	0.1	1656.6	27	0	0
1461.5	1410	24	1.7	2053.6	27	0	0
445.1	1169	0	0	1120.4	27	0	0
732.3	1043	0	0	1048.4	26	0	0
1460.5	1013	39	3.8	737.1	26	0	0
771.3	854	3	0.4	1217.4	26	0	0
810.2	847	2	0.2	1274.4	26	0	0
1097.4	807	0	0	753.2	26	1	3.8
569.2	765	0	0	2018.8	26	0	0
2135.8	738	0	0	852.3	25	0	0
1462.5	732	4	0.5	722.2	25	0	0
1826.7	723	15	2.1	721.2	25	0	0
1136.4	700	7	1	972.3	25	0	0
1827.7	677	2	0.3	1322.5	25	1	4
204.1	642	0	0	866.2	25	0	0
934.3	637	0	0	1645.5	25	0	0
406.2	570	0	0	1289.5	25	0	0
1298.4	557	24	4.3	228	25	0	0
2500.9	539	0	0	1823.6	25	0	0
1299.5	524	9	1.7	1323.5	25	0	0
1175.4	499	0	0	2556	25	0	0
2134.8	469	0	0	1628.5	25	0	0
408.1	449	0	0	1574.6	24	0	0
570.2	433	0	0	1080.4	24	0	0
1137.4	432	1	0.2	1459.5	24	0	0

690.2	373	0	0	1085.3	24	0	0
446.1	351	0	0	1160.4	24	0	0
1176.4	351	0	0	1444.5	24	0	0
859.3	330	0	0	1850.6	24	0	0
772.3	325	1	0.3	1308.5	23	0	0
308.1	320	0	0	1831.7	23	0	0
2192.8	318	0	0	1848.5	23	0	0
811.2	305	0	0	1354.5	23	0	0
1502.6	305	4	1.3	1297.5	23	0	0
689.2	292	0	0	1248.4	23	0	0
1989.7	286	0	0	2395.9	23	0	0
205.1	285	0	0	2092.7	23	0	0
1300.5	281	2	0.7	2393.9	23	0	0
494.2	280	0	0	1757.5	23	0	0
511.2	276	1	0.4	700.3	23	0	0
2558	276	0	0	1524.5	23	0	0
1664.6	274	11	4	1948.7	22	0	0
1241.5	273	2	0.7	1851.7	22	0	0
1501.6	270	7	2.6	1183.4	22	0	0
812.2	245	0	0	1209.4	22	0	0
1825.7	239	2	0.8	1364.5	22	0	0
935.4	235	0	0	973.3	22	0	0
876.3	230	0	0	1559.6	22	0	0
2215.8	229	0	0	1419.5	21	0	0
1988.7	222	0	0	1679.6	21	0	0
1242.5	221	0	0	1401.4	21	1	4.8
1138.5	216	0	0	1312.4	21	0	0
974.4	216	0	0	2294.7	21	0	0
1606.6	206	0	0	1646.6	21	1	4.8
2354.9	201	0	0	1686.6	21	0	0
2499.9	199	0	0	1807.6	21	0	0
1224.4	196	0	0	2172.7	21	0	0
2191.8	193	0	0	591.2	21	0	0
1607.6	189	0	0	1903.6	21	0	0
860.3	187	0	0	1687.5	21	0	0
349.1	187	0	0	2702	21	0	0
1663.6	185	3	1.6	1087.4	20	1	5
1665.6	180	2	1.1	574.1	20	0	0
1541.5	177	0	0	608.2	20	0	0
1340.5	172	0	0	1007.4	20	0	0
1503.5	171	1	0.6	1008.4	20	0	0
1339.5	171	0	0	1655.6	20	0	0
2704	170	0	0	1930.7	19	1	5.3

656.2	163	0	0	1313.5	19	0	0
773.3	160	0	0	1575.6	19	0	0
609.3	158	0	0	1428.5	19	0	0
1079.3	153	0	0	916.3	19	0	0
755.3	153	0	0	1102.3	19	0	0
769.2	153	0	0	1373.5	19	0	0
2133.8	149	0	0	1395.5	19	0	0
611.3	148	0	0	720.2	19	0	0
407.2	147	0	0	1688.5	19	0	0
714.3	145	0	0	915.3	19	0	0
429.1	144	0	0	1994.6	19	0	0
1177.4	139	0	0	1538.4	19	0	0
803.3	135	0	0	1483.4	19	0	0
447.1	134	0	0	1887.6	19	0	0
512.2	133	0	0	1421.5	19	0	0
716.3	131	0	0	1443.5	18	0	0
2353.9	130	0	0	837.3	18	0	0
845.3	130	0	0	2256.8	18	0	0
877.4	130	0	0	2085.8	18	0	0
1623.6	129	0	0	1377.4	18	1	5.6
691.3	127	0	0	819.3	18	0	0
1540.5	126	0	0	1231.4	18	1	5.6
495.1	123	0	0	1280.4	18	0	0
642.2	122	0	0	2578.9	18	0	0
527.2	118	3	2.5	1508.5	18	0	0
1973.7	118	0	0	1702.5	18	0	0
1134.3	118	0	0	1403.4	18	2	11.1
2176.8	117	0	0	957.2	18	0	0
513.2	115	1	0.9	1389.5	18	0	0
786.3	115	0	0	1088.3	18	0	0
1907.6	114	0	0	2171.7	18	0	0
1055.4	114	0	0	736.1	17	0	0
975.4	113	0	0	1047.4	17	0	0
389.1	113	0	0	1556.5	17	0	0
715.2	112	0	0	1220.5	17	0	0
1152.4	111	1	0.9	1219.5	17	0	0
2580.9	111	0	0	2174.7	17	0	0
648.2	110	4	3.6	1233.4	17	0	0
147.1	110	0	0	1996.6	17	0	0
1153.4	110	0	0	1094.3	17	0	0
1769.6	109	0	0	1806.6	17	0	0
1542.5	109	0	0	1307.3	17	0	0
2214.8	108	0	0	1284.5	17	0	0

351.1	108	0	0	1888.6	16	0	0
1315.5	107	0	0	1932.7	16	0	0
1972.7	106	0	0	1259.5	16	0	0
788.3	106	0	0	1227.5	16	1	6.2
1341.5	106	0	0	1606.5	16	0	0
1021.4	105	0	0	1630.5	16	0	0
1592.6	104	0	0	2253.7	16	0	0
1430.6	104	0	0	1766.5	16	0	0
802.3	103	0	0	1754.6	15	0	0
787.3	101	0	0	1402.5	15	1	6.7
390.1	100	0	0	2295.7	15	0	0
1225.4	98	0	0	1396.5	15	0	0
310.1	98	0	0	1833.6	15	0	0
640.2	93	0	0	1239.4	15	0	0
757.3	92	0	0	575.2	15	0	0
997.4	92	1	1.1	1809.6	15	0	0
1912.6	92	0	0	1101.3	15	0	0
1868.7	91	0	0	2067.6	15	0	0
1751.6	90	0	0	1397.5	15	0	0
892.2	90	0	0	2272.8	15	0	0
1770.7	89	1	1.1	1638.5	14	0	0
1150.4	88	0	0	1567.6	14	0	0
649.2	88	2	2.3	1677.6	14	0	0
496.2	88	0	0	2093.7	14	0	0
1077.3	87	0	0	1548.6	14	0	0
673.2	87	0	0	1786.6	14	0	0
939.3	87	0	0	1849.6	14	0	0
1128.4	84	0	0	1429.5	14	0	0
779.2	84	2	2.4	1273.4	14	0	0
350.1	84	0	0	1745.5	14	0	0
1314.5	83	0	0	1703.6	14	0	0
1608.6	81	0	0	2094.7	14	1	7.1
1906.6	81	0	0	2271.8	14	0	0
1078.3	80	0	0	1103.3	14	0	0
1054.4	80	0	0	2122.6	14	0	0
283.1	79	0	0	2252.7	14	0	0
1243.5	79	0	0	1532.5	14	0	0
1065.4	78	0	0	2784	14	0	0
1987.7	78	0	0	1566.6	13	0	0
893.3	77	0	0	1516.6	13	0	0
1624.6	76	0	0	2255.7	13	0	0
813.4	75	0	0	1475.5	13	0	0
2213.7	75	0	0	1784.6	13	0	0

1867.7	73	0	0	1548.5	13	0	0
641.3	72	0	0	820.3	13	0	0
1304.4	72	0	0	2514.9	13	0	0
1017.4	71	0	0	2394.9	13	0	0
610.3	70	0	0	2045.7	13	0	0
1768.6	69	1	1.4	2068.7	13	0	0
1288.4	69	0	0	1886.5	13	0	0
1752.7	68	0	0	1852.7	12	0	0
1622.6	68	0	0	1210.5	12	0	0
528.2	66	0	0	958.3	12	0	0
1039.4	66	5	7.6	1785.6	12	0	0
1706.6	66	0	0	1405.5	12	0	0
657.2	66	0	0	1515.6	12	0	0
1911.6	65	0	0	1393.4	12	0	0
2498.9	64	0	0	1526.6	12	0	0
1038.4	64	0	0	1678.6	12	0	0
1305.4	64	0	0	1450.5	12	0	0
650.2	63	0	0	2164.8	12	0	0
917.4	63	0	0	1944.7	12	0	0
1169.5	62	0	0	1886.6	12	0	0
576.1	62	0	0	1931.7	12	0	0
2556.9	62	0	0	1573.6	12	0	0
835.3	61	0	0	1834.6	12	0	0
878.3	61	0	0	941.3	12	0	0
804.3	61	0	0	1435.4	12	0	0
894.3	61	0	0	2044.7	12	0	0
2190.8	61	0	0	1230.3	12	0	0
1151.4	60	0	0	1832.5	12	0	0
309.1	60	0	0	2043.7	12	0	0
1167.4	60	1	1.7	900.3	11	0	0
998.3	59	5	8.5	1458.4	11	0	0
1905.6	59	0	0	1729.6	11	0	0
884.2	59	0	0	1069.3	11	0	0
1362.5	58	3	5.2	2293.8	11	0	0
989.4	58	0	0	486.1	11	0	0
976.3	58	0	0	1864.6	11	0	0
430.1	58	0	0	1758.5	11	0	0
1022.3	58	0	0	2141.7	11	0	0
1015.4	57	0	0	1071.3	11	0	0
1704.7	55	0	0	1599.5	11	0	0
2030.8	55	0	0	1433.4	11	0	0
738.1	54	0	0	1272.4	11	0	0
1705.6	54	0	0	1947.7	11	0	0

919.3	53	0	0	1126.3	11	0	0
898.2	53	0	0	1184.5	11	0	0
1534.5	53	0	0	2432.8	11	0	0
861.3	53	0	0	2189.8	11	0	0
2703	53	0	0	2473.8	11	0	0
1477.5	53	0	0	942.4	10	0	0
1380.5	52	0	0	1532.6	10	0	0
1046.4	52	0	0	1613.5	10	0	0
388.1	52	0	0	2010.6	10	0	0
1168.4	52	0	0	2012.6	10	0	0
658.3	52	0	0	1549.5	10	0	0
1403.5	52	0	0	1865.6	10	0	0
1363.5	51	0	0	2173.7	10	0	0
1518.6	50	0	0	1484.4	10	0	0
756.3	50	0	0	1265.4	10	0	0
956.2	50	0	0	1290.4	10	0	0
778.3	50	0	0	1458.5	10	0	0
1590.6	49	0	0	1118.3	10	0	0
1006.4	49	0	0	2028.7	10	0	0
226	49	0	0	1533.6	10	0	0
1145.4	48	1	2.1	2269.8	10	0	0
1218.5	47	0	0	2251.7	10	0	0
1282.5	47	0	0	1565.6	10	0	0
1201.4	47	2	4.3	1621.5	10	0	0
795.2	47	0	0	1247.4	10	0	0
1517.5	46	0	0	1159.4	9	0	0
1969.7	46	0	0	2069.7	9	0	0
754.2	46	1	2.2	2052.6	9	0	0
1445.6	46	0	0	2140.7	9	0	0
818.2	45	0	0	1986.7	9	0	0
2117.8	45	0	0	1185.4	9	0	0
1356.5	45	0	0	1597.5	9	0	0
1355.5	45	0	0	487.1	9	0	0
699.3	45	0	0	1539.4	9	0	0
999.3	45	0	0	2142.7	9	0	0
1013.4	45	0	0	1250.4	9	0	0
990.4	45	0	0	1582.5	9	0	0
1647.6	45	0	0	1916.7	9	0	0
1202.4	45	0	0	2434.8	9	0	0
1056.3	44	0	0	1583.6	9	0	0
1024.4	44	0	0	1612.5	9	0	0
1226.4	44	0	0	1938.7	9	0	0
1649.6	44	0	0	1469.5	9	0	0

284.1	43	0	0	2165.7	8	0	0
1727.6	43	1	2.3	2084.8	8	0	0
1376.5	43	0	0	2100.7	8	0	0
285	43	0	0	1824.7	8	0	0
2029.7	42	0	0	2019.7	8	0	0
796.3	42	0	0	1337.4	8	0	0
1442.5	42	0	0	1614.6	8	0	0
1866.7	42	0	0	1766.6	8	0	0
1387.5	41	0	0	2042.7	8	0	0
851.3	41	0	0	1081.4	8	0	0
1372.5	41	0	0	2636.9	8	0	0
882.3	41	0	0	1743.5	8	0	0
674.2	41	2	4.9	1557.6	7	0	0
1144.4	40	0	0	1281.4	7	1	14.3
1576.6	40	0	0	2110.7	7	0	0
148.1	40	0	0	899.2	7	0	0
1379.5	40	1	2.5	923.3	7	0	0
1555.5	40	0	0	1525.5	7	0	0
675.3	39	0	0	1353.5	7	0	0
1193.5	39	0	0	1589.5	7	0	0
1589.6	39	0	0	1672.6	7	0	0
431.1	39	0	0	2020.7	7	0	0
593.2	39	0	0	1604.5	7	0	0
1476.5	39	0	0	1671.6	7	0	0
1127.4	39	1	2.6	931.3	7	0	0
814.4	39	0	0	1452.4	7	0	0
883.2	39	0	0	867.2	7	0	0
1249.4	39	1	2.6	2050.6	7	0	0
2118.8	38	0	0	1143.4	7	0	0
1086.3	38	0	0	1453.5	7	0	0
853.3	38	0	0	2049.6	6	0	0
770.2	38	0	0	1468.5	6	0	0
1595.4	38	1	2.6	1394.4	6	0	0
1971.7	37	0	0	2125.7	6	0	0
1519.6	37	0	0	2011.6	6	0	0
2119.8	37	0	0	1421.4	6	0	0
843.3	37	0	0	1142.4	6	0	0
1062.4	37	0	0	1743.6	6	0	0
592.2	37	0	0	1993.6	6	0	0
1507.5	37	0	0	1550.6	6	0	0
1386.5	36	0	0	1485.4	6	0	0
1309.5	36	0	0	1940.7	6	0	0
1194.5	36	0	0	2163.7	6	0	0

1753.7	36	0	0	2062.8	6	0	0
1913.6	36	0	0	1946.6	6	0	0
1014.3	36	0	0	2254.8	5	0	0
1296.4	35	0	0	1525.6	5	0	0
1767.5	35	0	0	1558.6	5	0	0
991.4	35	0	0	2051.6	5	0	0
1434.4	35	0	0	1620.5	5	0	0
146.1	35	0	0	1669.5	5	0	0
1005.3	34	0	0	1639.6	5	0	0
1283.5	34	0	0	1615.5	5	0	0
529.2	34	0	0	1995.6	5	0	0
607.2	34	0	0	932.2	5	1	20
2352.9	34	0	0	2198.8	5	0	0
777.2	34	0	0	2199.8	5	0	0
1596.5	34	0	0	1070.4	5	0	0
780.2	34	0	0	1985.6	5	0	0
925.3	34	0	0	1904.6	5	0	0
1321.5	34	0	0	2197.8	5	0	0
1451.5	33	0	0	1240.3	5	0	0
1370.5	33	0	0	1686.5	5	0	0
1064.5	33	0	0	2635.9	5	0	0
698.3	33	0	0	1581.5	5	0	0
2175.8	33	0	0	2083.7	4	0	0
1444.4	33	0	0	1509.5	4	0	0
1170.5	32	0	0	1338.4	4	0	0
1637.6	32	0	0	1744.6	4	0	0
2579.9	32	0	0	1466.4	4	0	0
1161.4	32	0	0	2109.7	4	0	0
1016.4	32	0	0	2475.8	4	0	0
1378.5	32	0	0	2124.7	4	0	0
1040.4	31	0	0	2270.7	4	0	0
1970.7	31	0	0	2513.8	3	0	0
697.3	31	0	0	2061.8	3	0	0
1135.3	31	0	0	2099.7	3	0	0
1535.6	31	0	0	1474.6	3	0	0
918.4	31	0	0	2060.8	3	0	0
924.3	31	0	0	1542.6	3	0	0
1023.4	31	0	0	1467.5	3	0	0
1104.3	31	2	6.5	1654.6	3	0	0
1446.6	31	0	0	1605.4	3	0	0
1427.5	30	0	0	1093.3	3	0	0
1622.4	30	0	0	2123.7	3	0	0
868.3	30	0	0	1670.6	3	0	0

862.3	30	0	0	1436.5	3	0	0
1257.5	30	0	0	1263.4	3	0	0
1420.5	30	0	0	2512.8	3	0	0
1591.6	30	0	0	2783	3	0	0
1728.6	30	0	0	1264.4	3	0	0
1598.6	30	0	0	1759.6	2	0	0
1808.7	30	0	0	1939.7	2	0	0
1648.6	30	0	0	1395.4	2	0	0
1914.7	30	0	0	1653.5	2	0	0
1119.3	30	0	0	1583.5	2	0	0
1388.5	30	0	0	2474.8	2	0	0
1063.4	29	0	0	2433.8	2	0	0
1915.8	29	0	0	1453.4	1	0	0
1200.4	29	0	0	2098.7	1	0	0
1306.4	29	0	0	2108.6	1	0	0
1208.5	29	0	0	1945.6	1	0	0
				2781.9	1	0	0