Supplement to
"Cysteine S-linked N-acetylglucosamine (S-GlcNAcylation), a new post-translational modification in mammals."
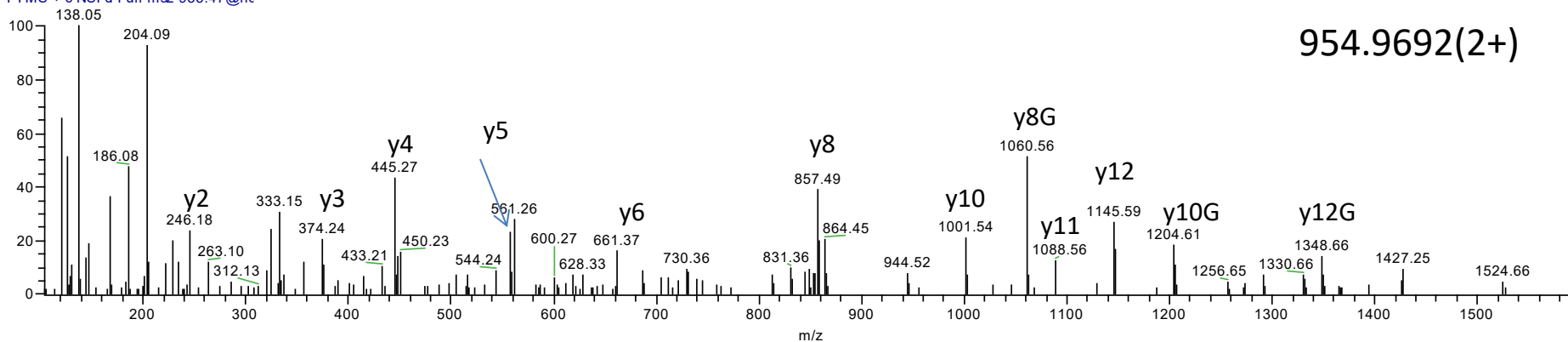
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Department of Pharmaceutical Chemistry, School of Pharmacy, University of California San Francisco, 600 16th Street Genentech Hall, N474A, Box 2240, San Francisco, California 94158-2517, United States
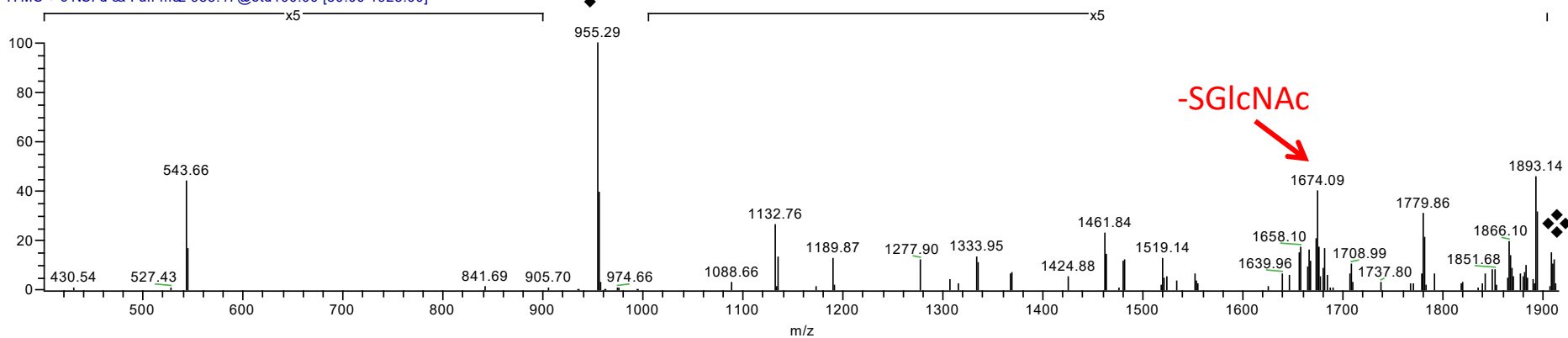
Legend

- We listed the UniProt accession number of the S-GlcNAcylated proteins, their name, the species they were isolated from, the glycopeptide sequence and the sequence position of the modified Cys-residue

- Both the beam-type CID spectrum (HCD) (upper panel) and the ETD data (lower panel) are presented for each S-GlcNAcylated peptide

- In most database searches an unspecified 203-203.1Da modification was permitted on Cys residues – thus, the exact mass of the modification was reported by Protein Prospector and this information is listed in S Table 1. Here the modification is shown according to the final assignment, i.e. GlcNAc. However, in some later searches a user-specified exactly defined modification was introduced: Cgly that stands for a HexNAc on Cys.

- For the O-GlcNAcylated peptides the Prospector output was copied, where "HexNAc' was assigned as the modification. Since isomeric GalNAc and GlcNAc both may derivatize peptides this generic assignment is used in database searches.

- The measured precursor ion masses were included.

- In the HCD spectra we assigned just enough fragment ions to indicate that the sequence identification is reliable.

- In the ETD spectra we labeled the precursor ion and its charge-reduced forms (❖), it was also indicated (*) if the charge reduced form of a coeluting ion of different charge in the precursor selection window was detected. The characteristic side-chain loss from the charge-reduced form(s) of the precursor ion is pointed out.

- Protein Prospector output, i.e. the masses used in the database search and their assignments, including the mass measurement error, is presented in the Tables. These assignments were manually implemented to indicate the w ion formation from the Cys-residues.

S Figure 1A

Bassoon   O88737

LDFGQGSGSPVC(GlcNAc)LAQVK

Cys-1775   *Mouse*

V20141119-37 #7387 RT: 71.74 AV:
T: FTMS + c NSI d Full ms2 955.47@hc

954.9692(2+)

138.05
204.09
186.08
y2 246.18
333.15
y3 374.24
263.10
312.13
y4 445.27
433.21
450.23
y5 561.26
544.24
600.27
y6 661.37
628.33
730.36
y8 857.49
864.45
831.36
944.52
y10 1001.54
y8G 1060.56
y11 1088.56
y12 1145.59
y10G 1204.61
1256.65
y12G 1348.66
1330.66
1427.25
1524.66

m/z

V20141119-37 #7388 RT: 71.76 AV: 1 NL: 1.29E3
T: ITMS + c NSI d sa Full ms2 955.47@etd100.00 [50.00-1925.00]

x5   x5

955.29

-SGlcNAc

430.54
527.43
543.66
841.69
905.70
974.66
1088.66
1132.76
1189.87
1277.90
1333.95
1424.88
1461.84
1519.14
1639.96
1658.10
1674.09
1708.99
1737.80
1779.86
1851.68
1866.10
1893.14

m/z

[−] Peak Matches

335.3340	430.6260	543.5050	849.8690	948.6410	956.9750	1132.2410	1132.9600	1275.7680	1276.8060
	$z+1_4(0.36)$	$z+1_5(0.15)$	$z+1_6(0.44)$ $b_9(0.50)$	$z+1_7(0.14)$		$z+1_9(-0.34)$ $z_9(0.66)$	$z+1_9(0.37)$	$z_{11}(0.14)$	$z+1_{11}(0.17)$

1461.8090	1480.6320	1519.0390	1532.7390	1552.7280	1656.9390	1664.9660	1673.0230	1680.7850	1688.3240
$z+1_{13}(0.090)$	$c-1_{13}(-0.048)$	$z+1_{14}(0.30)$		$c_{14}(0.0029)$		$z_{15}(0.16)$		$c_{15}(0.0013)$ $y_{15}(-0.035)$	

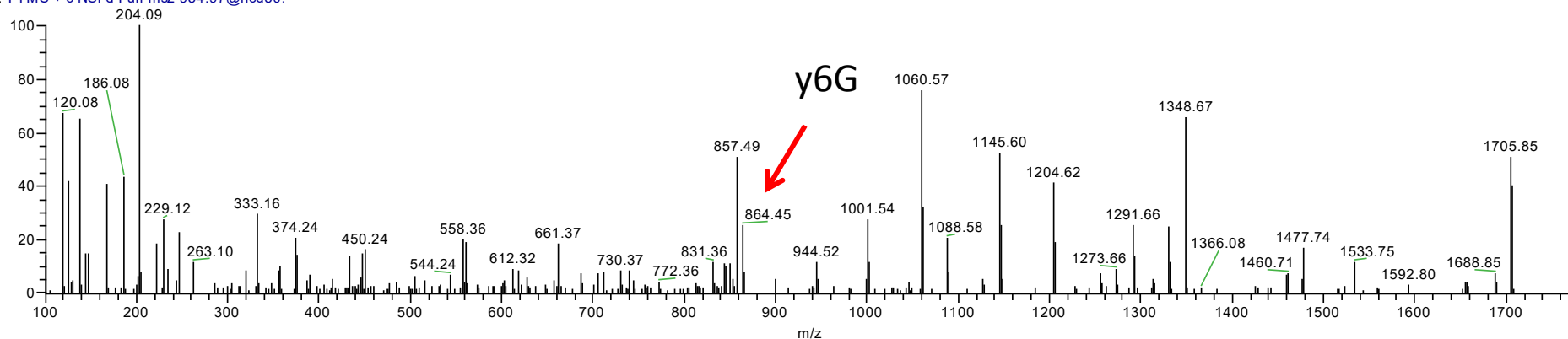| 1690.9060	1707.9940	1780.9910
		$z+1_{16}(0.15)$

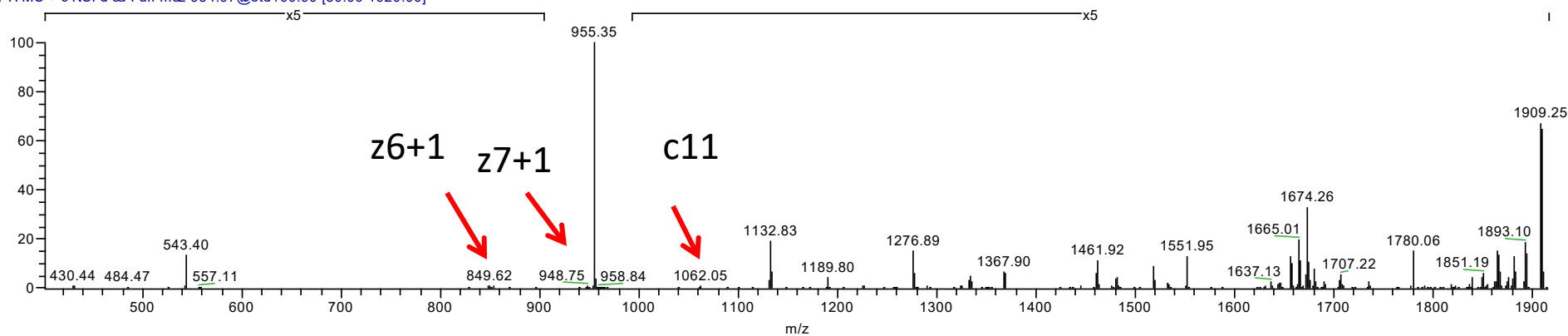## S Figure 1B

In vitro GlcNAcylated
LDFGQGSGSPVC(GlcNAc)LAQVK

The modified peptide eluted slightly earlier than the unmodified sequence; fragment ions making the site-assignment unambiguous are labeled
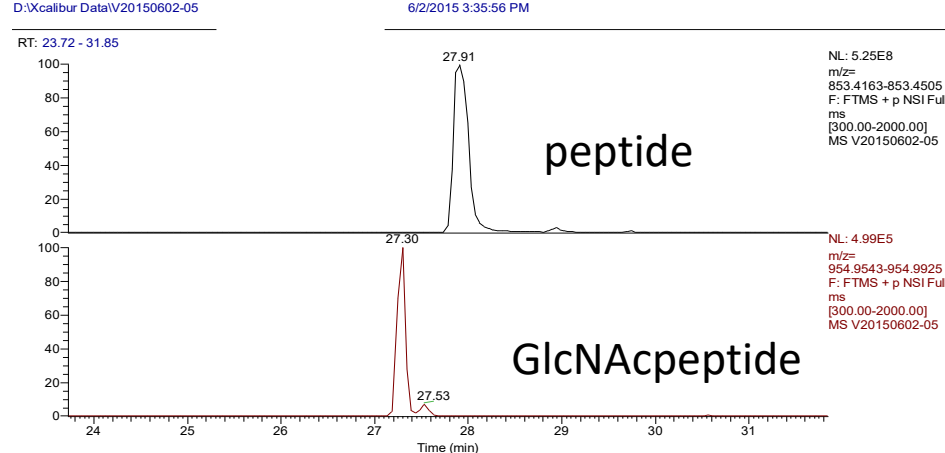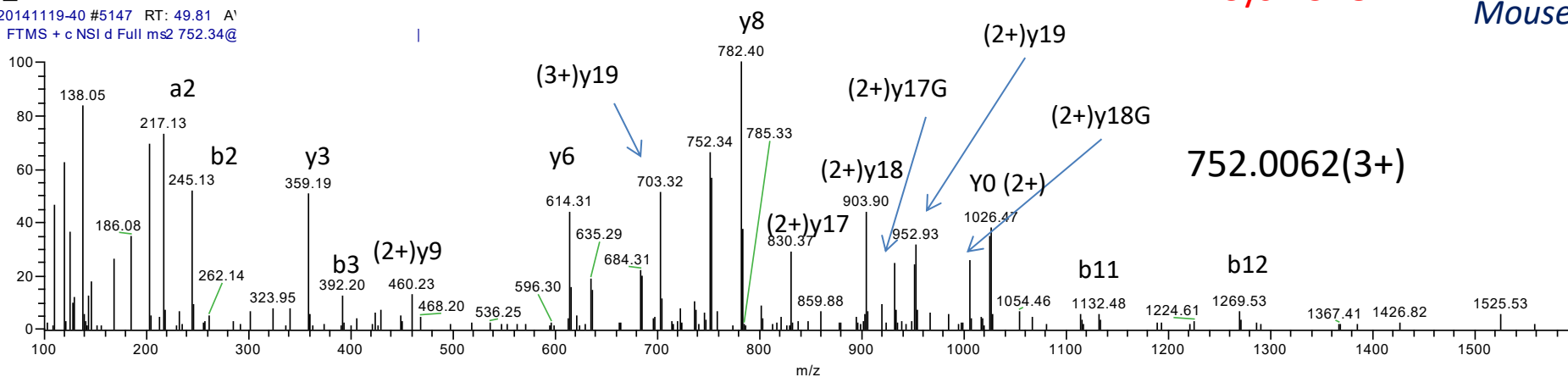
S Figure 2

FPFGSSC(GlcNAc)TGTFHPAPSAPDK

Bassoon   O88737

Cys-1918   *Mouse*

752.0062(3+)
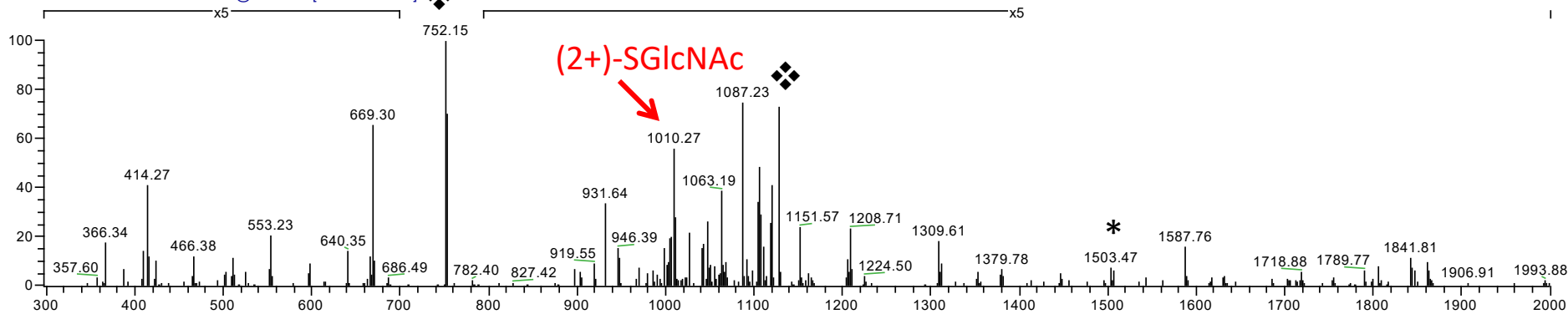
Peak Matches

366.3370	387.4930	409.3060	414.2670	423.2910	465.1910	466.3790	501.2540	509.0700	510.3430
	$c_3(0.083)$	$z_4(0.056)$			$c\text{-}1_4(-0.046)$	$c_4(0.13)$	$z_5(0.011)$		
525.3170	**552.3750**	**553.2300**	**596.3030**	**597.3930**	**640.3470**	**666.6050**	**669.3020**	**761.4710**	**782.4050**
$z_{10}^{+2}(-0.44)$	$c\text{-}1_5(0.11)$	$c_5(-0.047)$			$c_6(0.038)$		$z_7(-0.031)$		$y_8(7.1e\text{-}4)$
931.6430	**946.3880**	**997.8630**	**1005.3880**	**1010.2670**	**1026.5580**	**1041.2670**	**1047.5250**	**1063.1870**	**1087.2280**
$y_{17}^{+2}(-0.27)$	$c_7(-0.0014)$	$z+1_{18}^{+2}(-0.077)$ $z_{18}^{+2}(0.43)$	$y_{18}^{+2}(-0.057)$ $c_{18}^{+2}(-0.065)$ $c\text{-}1_{18}^{+2}(0.44)$				$c_8(0.088)$	$c_{19}^{+2}(0.22)$ $c\text{-}1_{19}^{+2}(0.72)$	$b_9(-0.20)$
1104.4660	**1107.5970**	**1111.2260**	**1120.9960**	**1151.5700**	**1205.6510**	**1208.7050**	**1309.6100**	**1586.7850**	**1841.8050**
$c_9(0.0074)$				$z_{11}(0.0094)$	$c_{10}(0.14)$	$z_{12}(0.12)$	$z_{13}(-0.020)$	$c_{13}(0.099)$	$c_{16}(-0.0032)$

S Figure 3

Bassoon   O88737

MC(GlcNAc)AALNSMDQYGGR

Cys-2107   *Mouse*

860.3623(2+)

Peak Matches

359.5970	437.6530	485.5280	515.4290	564.6510	565.5830	628.7120	680.5750	810.6460	811.6490
	$z+1_4(0.44)$ $b_2(-0.49)$			$z_5(0.39)$ $z+1_5(-0.62)$	$z+1_5(0.31)$		$z+1_6(0.28)$	$z_7(0.31)$ $z+1_7(-0.69)$	$z+1_7(0.31)$
897.6540	898.6620	1011.7150	1012.6370	1124.7610	1196.8130	1266.8350	1267.8420	1281.9080	1289.2640
$z_8(0.29)$ $z+1_8(-0.72)$	$z+1_8(0.29)$	$z_9(0.31)$ $z+1_9(-0.70)$	$z+1_9(0.22)$	$z_{10}(0.27)$ $z+1_{10}(-0.74)$	$z+1_{11}(0.28)$	$z_{12}(0.27)$ $z+1_{12}(-0.74)$	$z+1_{12}(0.27)$ $b_{10}(-0.66)$	$y_{12}(-0.68)$	
1336.7800	1467.8330	1484.0020	1484.8760	1518.7920	1561.8880	1646.8150			
w13				$c-1_{13}(0.26)$ $c_{13}(-0.74)$					

S Figure 4A

Bassoon   O88737

Cys-2489   Mouse

QKAPFPAT(GlcNAc)C(GlcNAc)EAPSR

S Figure 4B
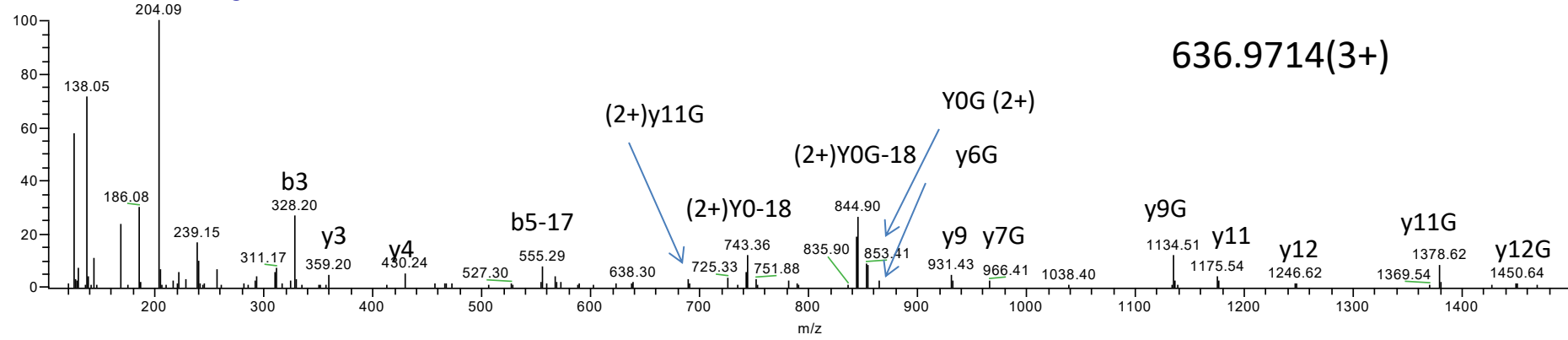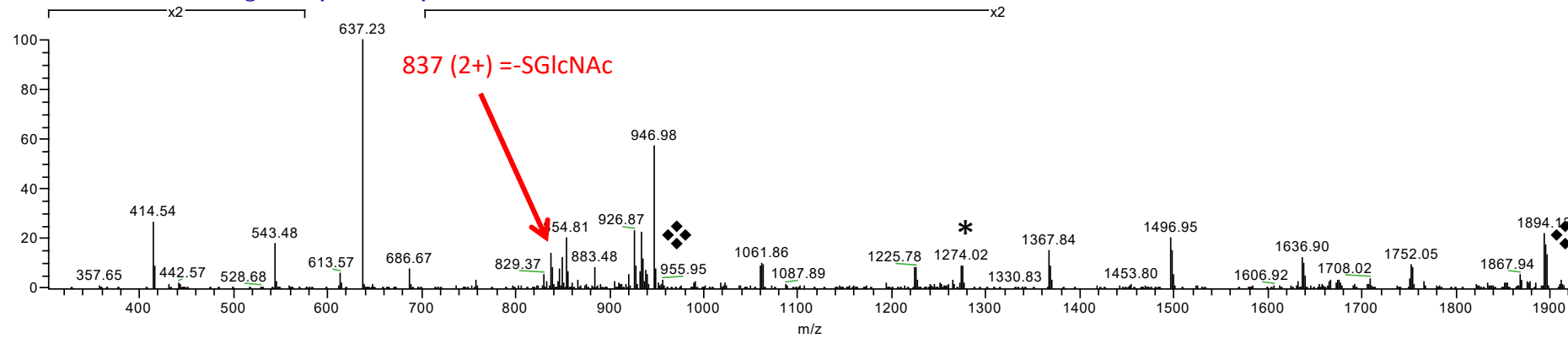
QKAPFPAT(GlcNAc)C(GlcNAc)EAPSR

Peak Matches

414.5430	430.6040	442.5660	543.4830	559.6430	579.5750	612.5930	613.5750	639.1620	647.6000
$z_4(0.32)$ $z+1_4(-0.69)$	$y_4(0.36)$	$c_4(0.29)$	$z_5(0.22)$ $z+1_5(-0.79)$	$y_5(0.36)$			w6		
658.6090	**686.6670**	**736.1520**	**757.7700**	**802.5220**	**822.7940**	**828.4890**	**829.3730**	**832.9140**	**837.0300**
	$c_6(0.27)$		$c_7(0.33)$					$c_{12}^{+2}(0.019)$ $c-1_{12}^{+2}(0.52)$	
837.9480	**846.3930**	**849.2250**	**854.0380**	**883.4770**	**920.2940**	**927.7070**	**935.3730**	**938.5850**	**948.7850**
		$z_6(-0.13)$		$z+1_{13}^{+2}(0.058)$ $z_{13}^{+2}(0.56)$					
1060.7300	**1224.7560**	**1274.0190**	**1367.8360**	**1496.9520**	**1636.8970**	**1674.0060**	**1708.0170**	**1751.2130**	**1752.0460**
$c-1_8(0.18)$	$z_8(0.24)$ $z+1_8(-0.77)$		$c_9(0.19)$	$c_{10}(0.26)$	$z_{12}(0.17)$			$c-1_{13}(0.41)$ $c_{13}(-0.60)$	$c_{13}(0.23)$

S Figure 5

QKAPFPATC(GlcNAc)EAPSR

Bassoon   O88737

Cys-2489   *Mouse*

V20141119-08 #2451 RT: 25.79 AV
T: FTMS + c NSI d Full ms2 569.28@l

569.2800(3+)

138.06, 144.07, 204.09, 186.08, 239.15, 257.16, 311.17, 328.20, 359.20, 408.22, 430.24, 466.22, 527.30, 555.29, 559.29, 662.29, 734.36, 743.37, 763.34, 834.38, 913.42, 931.43, 966.42, 1037.47, 1078.50, 1127.52, 1175.55, 1246.59, 1367.63

y3, y4, y5, y6, y6G, y7, y7G, y8, y8G, y9, y10, y11, y12
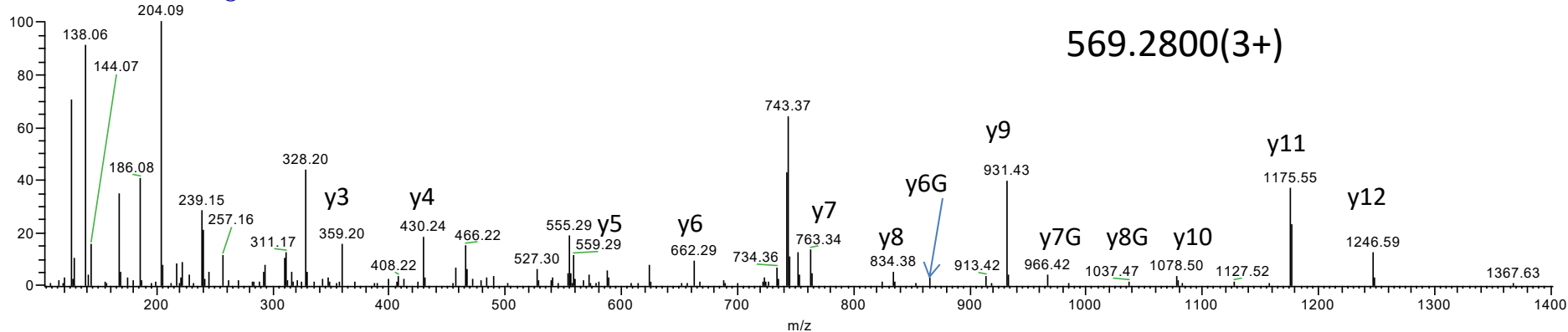
V20141119-08 #2452 RT: 25.80 AV: 1 NL: 1.51E5
T: ITMS + c NSI d sa Full ms2 569.28@etd66.67 [50.00-1720.00]

(2+)-SGlcNAc

160.53, 274.79, 359.55, 414.65, 442.78, 527.72, 543.61, 569.85, 613.73, 652.77, 686.82, 736.45, 781.99, 825.68, 845.86, 858.89, 951.77, 1021.69, 1146.65, 1164.86, 1265.85, 1294.00, 1321.93, 1434.84, 1505.07, 1549.99, 1665.11, 1691.12
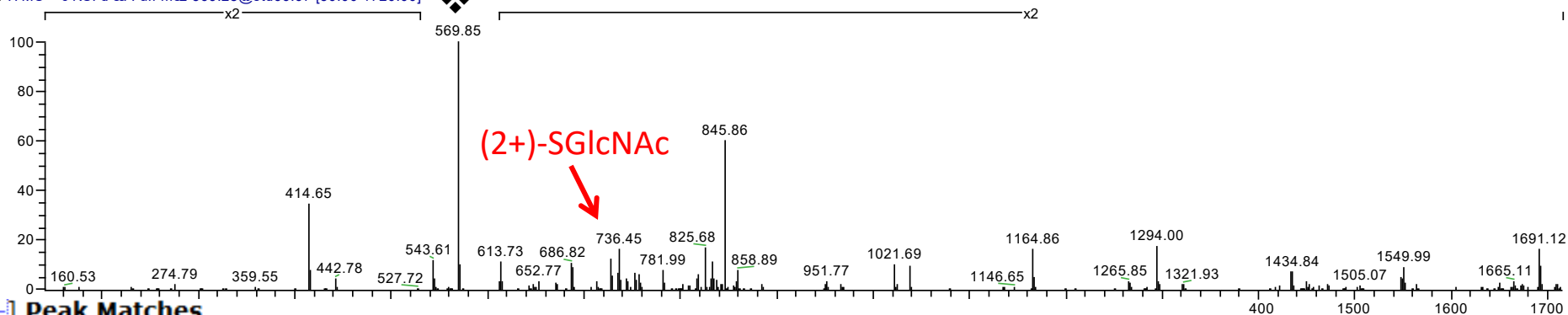
Peak Matches

160.5280	230.5830	274.7860	414.6510	442.7810	543.6080	547.7330	559.6500	570.6450	612.7170
$z+1_1(0.42)$		$c_2(0.60)$	$z_4(0.43)$ $z+1_4(-0.58)$	$c_4(0.50)$	$z_5(0.34)$ $z+1_5(-0.66)$		$y_5(0.37)$		
613.7340	**642.8470**	**647.6690**	**652.7690**	**670.7010**	**686.8250**	**713.8050**	**728.1750**	**735.5960**	**736.4540**
w6		$c_{10}^{+2}(0.36)$			$c_6(0.43)$				
744.3780	**752.5620**	**757.8470**	**781.9940**	**817.4440**	**826.3750**	**833.9940**	**836.9880**	**846.8170**	**858.1290**
		$c_7(0.41)$	$z+1_{13}^{+2}(0.11)$ $z_{13}^{+2}(0.62)$						$c_8(-0.35)$ $c-1_8(0.65)$
858.8910	**1021.6870**	**1037.8730**	**1164.8590**	**1265.8490**	**1294.0020**	**1433.8440**	**1450.0330**	**1548.2830**	**1549.9860**
$c_8(0.41)$	$z_8(0.24)$ $z+1_8(-0.76)$	$y_8(0.41)$	$c_9(0.28)$	$z_{10}(0.29)$ $z+1_{10}(-0.72)$	$c_{10}(0.38)$	$z_{12}(0.19)$	$y_{12}(0.36)$	$c_{13}(-0.46)$ $c-1_{13}(0.55)$	

S Figure 6   Piccolo   Q9QYX7
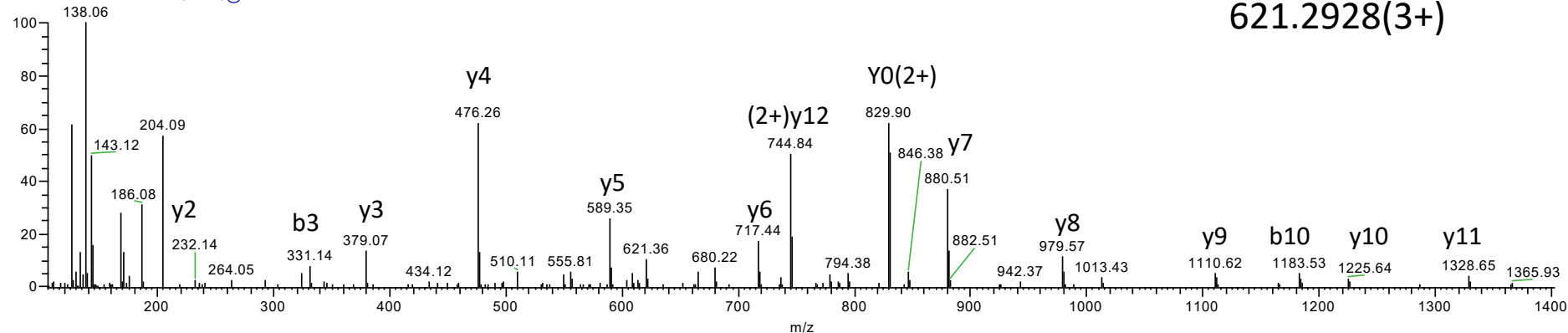
AVC(Carbamidomethyl)C(GlcNAc)DMVYKLPFGR   Cys-2870   Mouse

621.2928(3+)

V20141119-53 #5810 RT: 58.03 AV: 1
T: FTMS + c NSI d Full ms2 621.29@hc...

138.06
143.12
204.09
186.08
y2 232.14
264.05
b3 331.14
y3 379.07
434.12
y4 476.26
510.11
555.81
y5 589.35
621.36
y6 717.44
680.22
(2+)y12 744.84
794.38
Y0(2+) 829.90
846.38
y7 880.51
882.51
942.37
y8 979.57
1013.43
y9 1110.62
b10 1183.53
y10 1225.64
y11 1328.65
1365.93

m/z

V20141119-53 #5811 RT: 58.04 AV: 1 NL: 1.39E4
T: ITMS + c NSI d sa Full ms2 621.29@etd66.67 [50.00-1875.00]

x5
621.61
923.67
931.66
(2+)-SGlcNAc
813.77
902.72
363.37
160.19 232.43 348.42 379.46 476.47
573.47
654.35
702.51
769.35 793.67 878.58
999.43
1056.47
1095.60
1243.65
1290.52
1304.63
1456.83
1500.64
1587.81 1648.84
1704.71
1777.86
1846.85
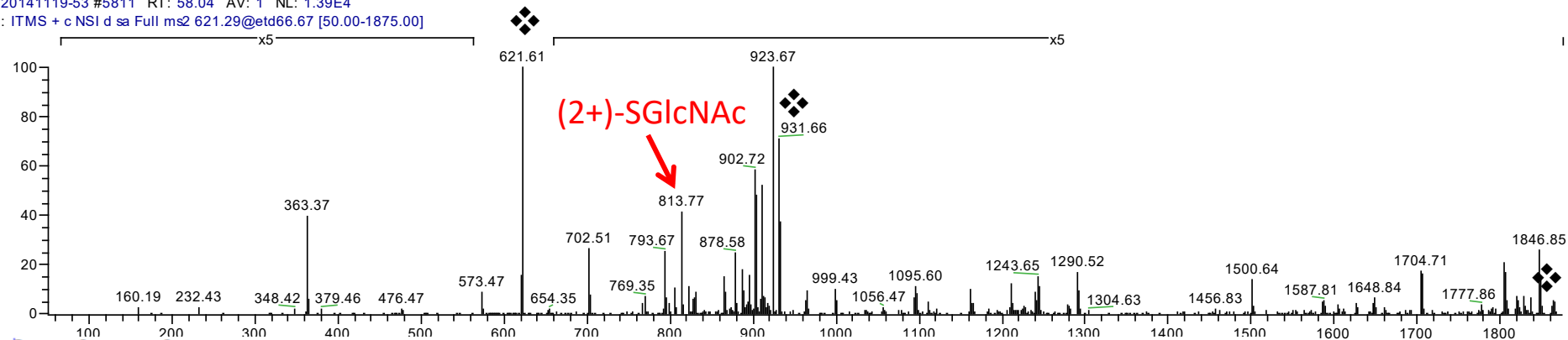
⊟ **Peak Matches**

160.1910	232.4270	348.4180	363.3730	379.4640	476.4730	573.4660	622.4480	638.9160	653.2450
$z+1_1(0.083)$	$y_2(0.29)$	$c_3(0.25)$	$z_3(0.18)$	$y_3(0.26)$	$y_4(0.21)$	$z_5(0.14)$			$c-1_4(-0.0051)$
701.5450	702.5130	766.2110	767.0860	769.3510	792.0770	793.6700	799.4460	806.1740	813.7730
$z_6(0.12)$	$z+1_6(0.083)$	$y_{11}^{+2}(-0.16)$	$y_{11}^{+2}(0.72)$	$c_5(0.066)$		w12(2+)			
822.2850	864.6450	865.5570	878.5770	887.1440	895.3800	904.7110	912.0240	914.7920	964.6050
	$z_7(0.16)$	$z+1_7(0.064)$		$z_{13}^{+2}(-0.76)$	$y_{13}^{+2}(-0.54)$				$z+1_8(0.044)$
999.4270	1094.6590	1095.5980	1162.5580	1210.7750	1240.2630	1243.6510	1290.5200	1500.6420	1704.7100
$c_7(0.033)$	$z_9(0.065)$	$z+1_9(-0.0039)$	$c_8(0.10)$	$z+1_{10}(0.15)$			$c_9(-0.032)$	$c_{11}(-0.047)$	$c_{13}(-0.069)$

Cys-2906   *Mouse*

IQTDTC(GlcNAc)HSTVVHSPEVYSVIIR

S Figure 7B
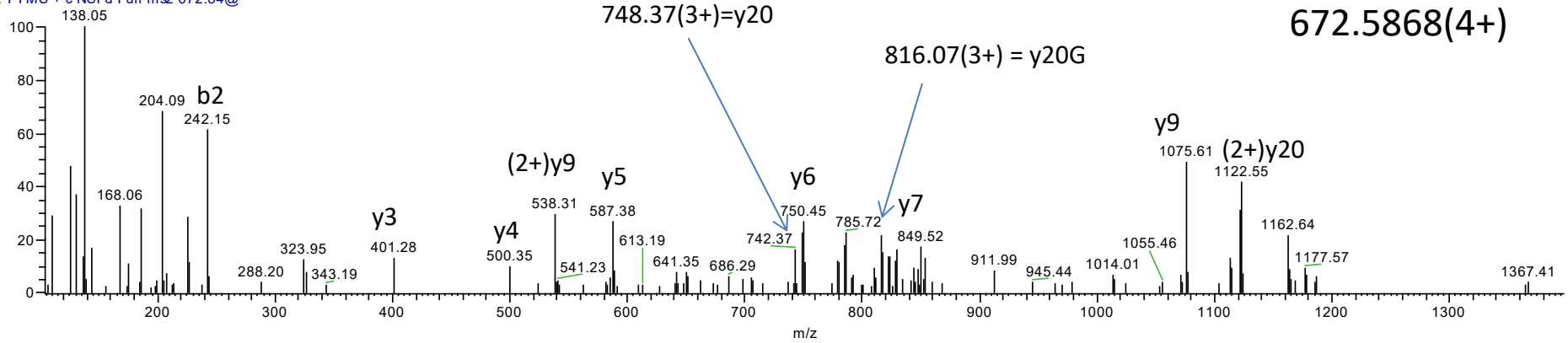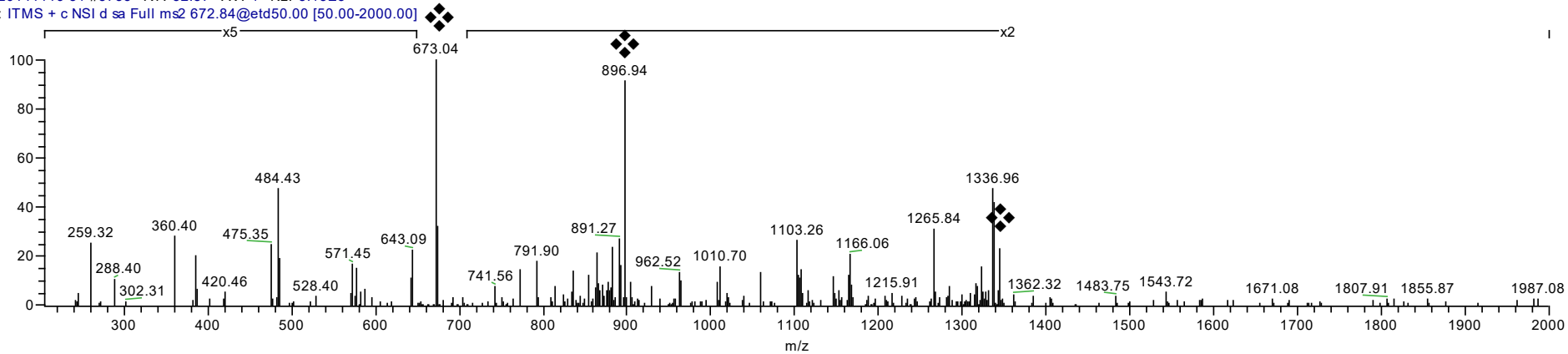
IQTDTC(GlcNAc)HSTVVHSPEVYSVIIR

Peak Matches

259.3170	360.4030	385.4340	475.3530	484.4330	571.4500	576.3280	643.0950	673.9720	703.5850
$c_2(0.14)$	$c_3(0.18)$	$z_3(0.17)$	$c_4(0.10)$	$z_4(0.096)$	$z_5(0.081)$	$c_5(0.029)$ $c_{14}^{+3}(0.057)$ $c\text{-}1_{14}^{+3}(0.39)$	$z+1_{11}^{+2}(0.24)$ $z_{11}^{+2}(0.75)$		$c_{11}^{+2}(0.25)$ $c\text{-}1_{11}^{+2}(0.76)$

741.5560	772.1180	791.8960	813.5690	835.7440	853.8260	861.8640	864.2790	867.9370	870.1260
$z_{13}^{+2}(0.14)$ $z+1_{13}^{+2}(-0.36)$	$c_{12}^{+2}(0.26)$ $c\text{-}1_{12}^{+2}(0.76)$	$z_{14}^{+2}(-0.043)$ $z+1_{14}^{+2}(-0.55)$		$z+1_{15}^{+2}(-0.22)$ $z_{15}^{+2}(0.29)$	$z+1_{21}^{+3}(0.078)$ $z_{21}^{+3}(0.41)$		$c_{14}^{+2}(0.38)$		

875.3980	883.3300	904.4260	928.9490	962.5170	1007.3400	1010.6990	1059.3710	1059.9840	1103.2620
		$z+1_{16}^{+2}(-0.063)$ $z_{16}^{+2}(0.44)$	$c_{15}^{+2}(0.53)$	$z_8(-0.026)$			$c_{17}^{+2}(-0.12)$ $c\text{-}1_{17}^{+2}(0.39)$	$c_{17}^{+2}(0.49)$	$c_{18}^{+2}(0.26)$ $c\text{-}1_{18}^{+2}(0.76)$

1106.5210	1116.6750	1146.3870	1153.7160	1165.0410	1166.0590	1265.8390	1284.6590	1317.7700	1338.5170
$c_8(0.052)$		$z_{10}(-0.24)$		$z_{19}^{+2}(-0.021)$ $z+1_{19}^{+2}(-0.52)$	$z+1_{19}^{+2}(0.49)$	$c_{21}^{+2}(0.22)$ $c\text{-}1_{21}^{+2}(0.72)$	$z+1_{11}(-0.036)$		

S Figure 8

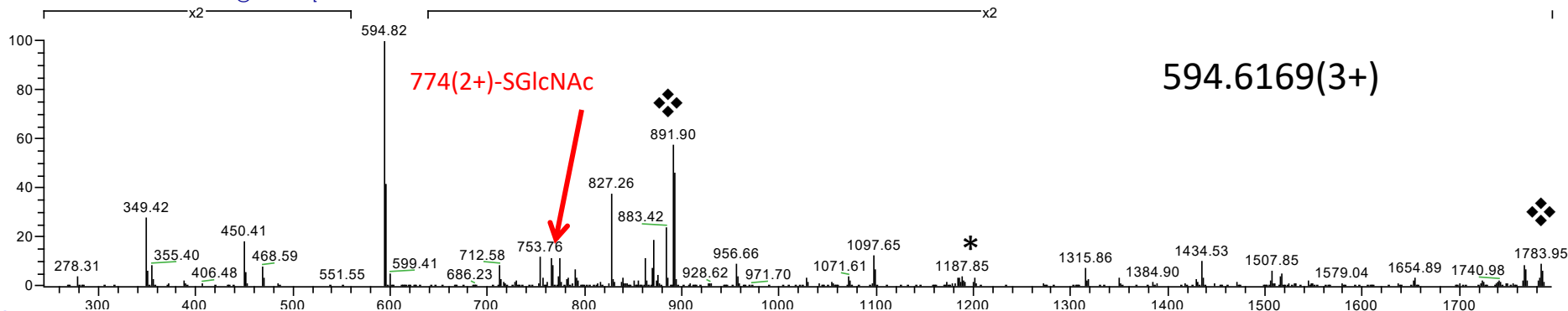YPATC(GlcNAc)VTDIMLSHK

Serine/threonine-protein kinase SIK3   Q6P4S6

Cys-1289   *Mouse*

Peak Matches

269.5640	278.3140	306.4360	349.4190	355.3960	371.4170	387.8580	388.5280	406.4800	449.3990
$z+1_2(0.40)$	$c_2(0.16)$		$c_3(0.23)$	$z_3(0.21)$ $z+1_3(-0.80)$	$y_3(0.21)$				$c-1_4(0.17)$
450.4060	468.5870	484.5590	596.2800	599.4150	686.2270	711.4680	712.5770	717.3170	728.7080
$c_4(0.17)$	$z_4(0.32)$ $z+1_4(-0.69)$	$y_4(0.27)$		$z_5(0.11)$			$z_6(0.18)$	$z_{11}^{+2}(-0.52)$	$y_6(0.30)$
753.7570	765.9480	773.4090	774.2720	790.2110	827.2610	871.7530	875.2170	885.1120	956.6600
$z+1_{12}^{+2}(-0.10)$ $z_{12}^{+2}(0.40)$					$z_7(-0.16)$ $c_{13}^{+2}(0.38)$				$c_7(0.23)$
1027.7150	1071.6120	1097.6510	1184.6650	1187.8480	1200.8160	1315.8580	1434.5270	1506.8330	1515.8800
$z_9(0.18)$	$c_8(0.15)$	w10	$c_9(0.12)$		$c_{10}(0.28)$	$z_{11}(-0.14)$	$z+1_{12}(0.12)$	$c_{12}(0.18)$	

S Figure 9

Trafficking kinesin-binding protein 1   Q6PD31

VTPSLNSAPAPAC(GlcNAc)SSTSHLK   Cys-695   *Mouse*

V20141119-21 #3454 RT: 34.05 A
T: FTMS + c NSI d Full ms2 724.70@

204.09
138.06
186.08
201.1=b2
228.13 280.17 273.12
PSLN
412.22 420.22 499.25
(2+)y10 515.75
PSLNSA
570.29 590.29
(2+)y10G 617.29 657.65
(2+)y12G
PSLNSAPA 701.34 738.38
y7 770.41
811.38
875.93 894.43 934.96
(2+)y18 884.44
(2+)y18G 985.98
y10 1030.50 1065.49 1101.51
y12 1198.59
y10G 1233.58
1180.58 1269.62
323.95 384.22

m/z

V20141119-21 #3455 RT: 34.06 AV: 1 NL: 9.53E3
T: ITMS + c NSI d sa Full ms2 724.70@etd66.67 [50.00-2000.00]
x5   x5

724.74
(2+)-SGlcNAc
1086.29
968.58 1029.20
724.3612(3+)
245.30 315.34 381.36 437.28 469.28 514.43 570.30 657.34 744.43 809.41 884.43 929.86 1121.55 1228.70 1289.70 1407.51 1429.68 1544.76 1658.64 1705.71 1858.91 1929.80

Peak Matches

202.1490	245.2990	315.3430	381.3560	468.3720	469.2780	514.4250	568.3470	570.3030	628.4820
	$z+1_2(0.11)$	$c_3(0.14)$	$z_3(0.12)$	$z_4(0.10)$	$z+1_4(0.0011)$	$c-1_5(0.11)$	$y_9^{+2}(-0.42)$	$z+1_5(-0.022)$	$c-1_6(0.13)$
629.3780	**656.4650**	**657.3350**	**716.4700**	**725.8880**	**743.4990**	**744.4290**	**770.5110**	**809.4090**	**884.4300**
$c_6(0.016)$	$z_6(0.12)$	$z+1_6(-0.022)$	$c_7(0.076)$		$z_7(0.12)$	$z+1_7(0.040)$	$b_8(0.11)$		$c_9(-0.054)$
929.8600	**941.8340**	**960.7070**	**964.8200**	**968.5840**	**982.9330**	**985.3320**	**1021.6740**	**1028.2050**	**1029.2020**
$z+1_{17}^{+2}(-0.088)$ $z_{17}^{+2}(0.42)$			$c_{18}^{+2}(-0.14)$ $c-1_{18}^{+2}(0.37)$			$y_{18}^{+2}(-0.65)$	$c_{19}^{+2}(0.18)$ $c-1_{19}^{+2}(0.68)$	$z_{19}^{+2}(-0.29)$ $z+1_{19}^{+2}(-0.79)$	$z+1_{19}^{+2}(0.20)$ $z_{19}^{+2}(0.71)$
1037.8650	**1052.1530**	**1058.8110**	**1066.1390**	**1079.4190**	**1288.6590**	**1428.5890**	**1456.6470**	**1544.7640**	**1658.6420**
	$c_{11}(-0.42)$ $c-1_{11}(0.59)$		$y_8(0.65)$		$z_{11}(0.059)$	$c-1_{13}(-0.11)$	$z_{13}(-0.043)$	$z+1_{14}(0.034)$	$z+1_{15}(-0.13)$

S Figure 10A

MLX-interacting protein Q2VPU4

NAC(GlcNAc)IAPAAFSGQPQK

Cys-579

Mouse

S Figure 10B

NAC(GlcNAc)IAPAAFSGQPQK

[−] Peak Matches

322.6670	326.0350	372.6160	373.5250	391.2560	485.6090	507.5850	509.6740	526.7310	542.7060
		$y_3(0.39)$			$z+1_4(0.34)$	$c-1_3(-0.62)$	$c_3(0.46)$		$z+1_5(0.41)$
559.8100	**595.8510**	**612.8390**	**626.7150**	**628.6710**	**629.7490**	**776.7390**	**847.8870**	**854.8150**	**917.8200**
				$z_6(0.35)$ $z+1_6(-0.65)$	$z+1_6(0.42)$	$z+1_7(0.35)$	$z+1_8(0.46)$		$z_9(0.36)$ $z+1_9(-0.65)$
1085.9550	**1198.9600**	**1250.3300**	**1269.0430**	**1279.0000**	**1448.0080**	**1454.0630**	**1469.9520**	**1470.9810**	**1488.4730**
$z_{11}(0.40)$ $z+1_{11}(-0.60)$	$z_{12}(0.33)$ $z+1_{12}(-0.68)$		w13		$c-1_{13}(0.32)$ $c_{13}(-0.68)$				
1502.9210	**1522.2060**	**1533.8910**	**1576.0370**	**1577.0140**	**1641.9130**				
			$z_{14}(0.27)$ $c-1_{14}(0.30)$ $c_{14}(-0.71)$ $z+1_{14}(-0.74)$	$z+1_{14}(0.24)$ $c_{14}(0.26)$					

Dihydropyrimidinase-related protein 2   P47942

GLYDGPVC(GlcNAc)EVSVTPK   Cys-504   *Rat*

V20150211-10 #3444   RT: 35.79   AV: 1
T: FTMS + c NSI d Full ms2 884.43@hcd

883.9311(2+)
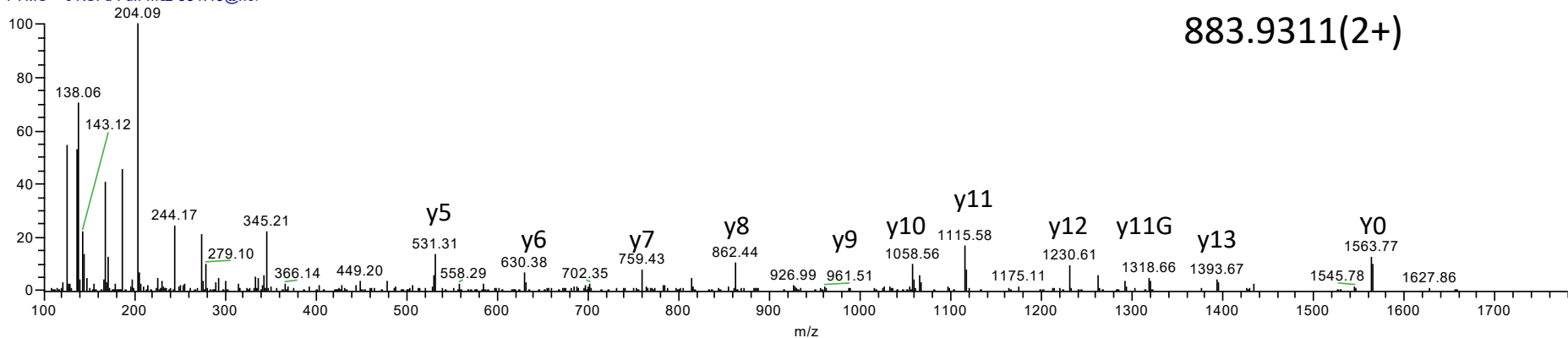
V20150211-10 #3445   RT: 35.80   AV: 1   NL: 3.83E1
T: ITMS + c NSI d sa Full ms2 884.43@etd100.00 [50.00-1780.00]

-SGlcNAc
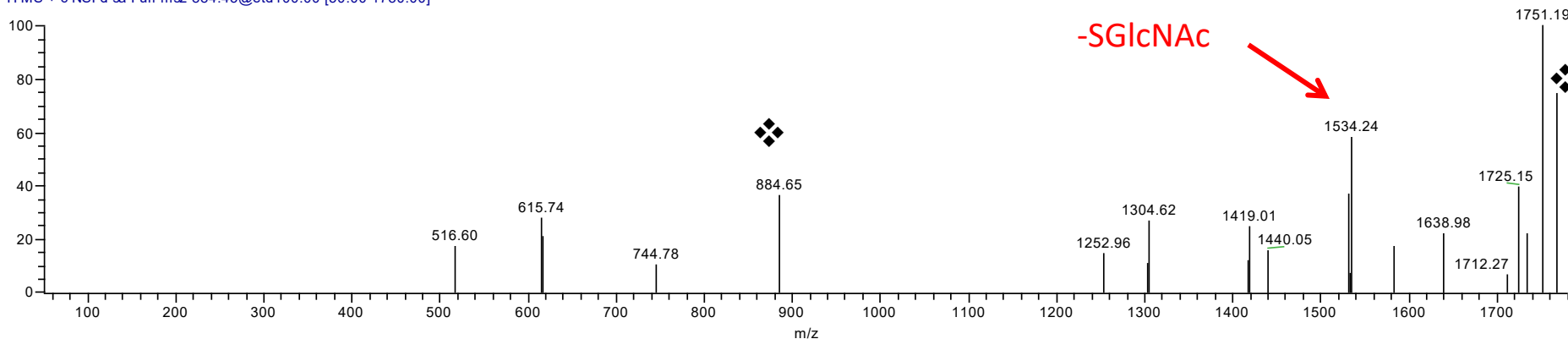
[−] **Peak Matches**

516.5990	615.7390	744.7780	1252.9620	1302.9580	1304.6230	1417.8910	1419.0100	1440.0460	1531.2700
$z+1_5(0.30)$	$z+1_6(0.37)$	$z+1_7(0.36)$	$c-1_{10}(0.39)$ $c_{10}(-0.61)$	$z_{11}(0.32)$ $z+1_{11}(-0.69)$		$z_{12}(0.22)$ $z+1_{12}(-0.78)$	$z+1_{12}(0.33)$	$c_{12}(0.37)$	

1534.2380	1582.2560	1638.9790
	$z+1_{13}(0.52)$	
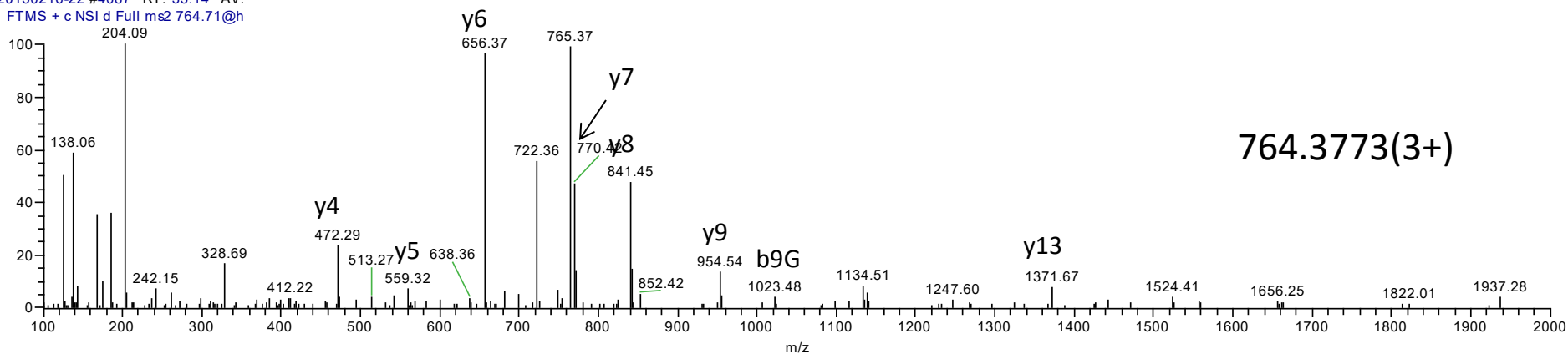
S Figure 12

AGISTTSVC(GlcNAc)EGQIANPSPISR

Protein Fam222b — D3ZPE2

Cys-288 — *Rat*

764.3773(3+)

(2+)-SGlcNAc
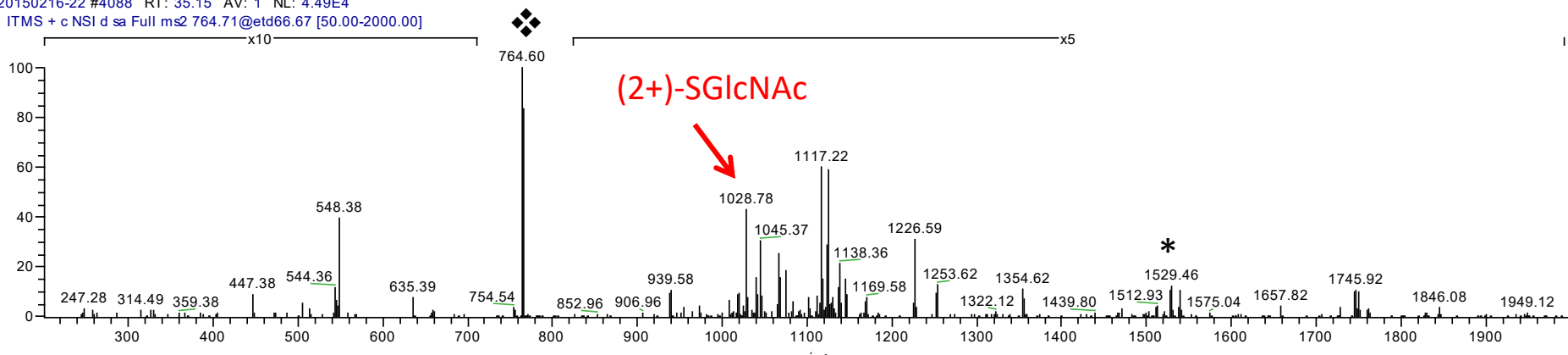
Peak Matches

247.2830	258.3390	314.4940	327.2890	330.3090	447.3790	505.3890	513.3300	543.4690	547.4420
$z+1_2(0.14)$	$c-1_3(0.17)$				$c_5(0.12)$			$z_5(0.17)$	$c-1_6(0.15)$
548.3840	635.3950	659.7130	734.4570	754.5380	766.0160	770.5030	783.0920	802.7370	852.9600
$c_6(0.080)$	$c_7(0.059)$		$c_8(0.053)$	$z_7(0.14)$		$y_7(0.087)$			
938.5690	1008.6550	1017.8850	1020.3330	1027.8080	1028.7820	1040.5460	1044.3980	1066.7000	1074.5690
$z_9(0.051)$						$c_9(0.054)$		$z_{10}(0.12)$	
1102.4340	1111.2470	1125.8730	1226.5870	1252.7170	1354.6170	1528.2240	1538.7710	1744.9750	1749.9660
			$c_{11}(0.031)$	$z_{12}(0.076)$	$c_{12}(0.0025)$		$c_{14}(0.035)$	$z_{15}(0.15)$	$c_{16}(0.13)$

Glucocorticoid receptor   P06536

LGPVYC(GlcNAc)QASFSGTNIIGNK

Cys-322

Rat

V20150213-12 #4145 RT: 41.19 AV
T: FTMS + c NSI d Full ms2 725.03@l

724.6932(3+)

204.09

y3 318.18
y4 431.26
b5 530.30
y6 658.39
y7 759.44
y8 816.46
y9 903.49
y10 1050.56
y11 1137.59
y12 1208.62
y14 1439.70
y15 1602.75

207.11 283.14 339.24 367.23 485.28 591.26 832.40 919.43 985.49 1119.58 1319.67 1525.14 1662.90

m/z
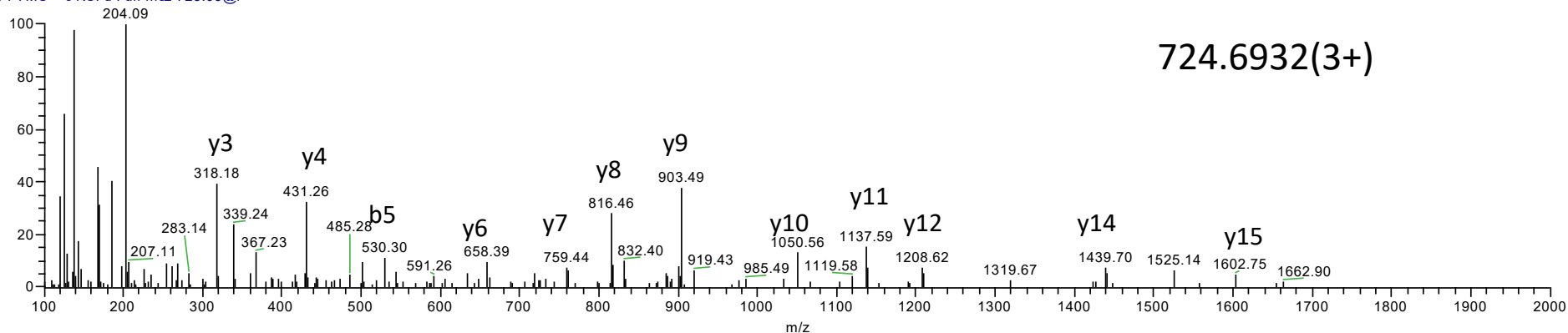
V20150213-12 #4146 RT: 41.20 AV: 1 NL: 2.58E4
T: ITMS + c NSI d sa Full ms2 725.03@etd66.67 [50.00-2000.00]

x10   x5

724.92

(2+)-SGlcNAc

1064.76

1022.01

1086.78

-SGlcNAc

1937.69

246.17 285.30 384.39 504.30 528.31 547.40 642.40 658.57 800.45 853.49 937.45 960.75 968.79 1139.63 1192.63 1208.96 1286.75 1320.77 1449.74 1489.70 1531.69 1645.88 1790.82 1890.04 1970.02

*
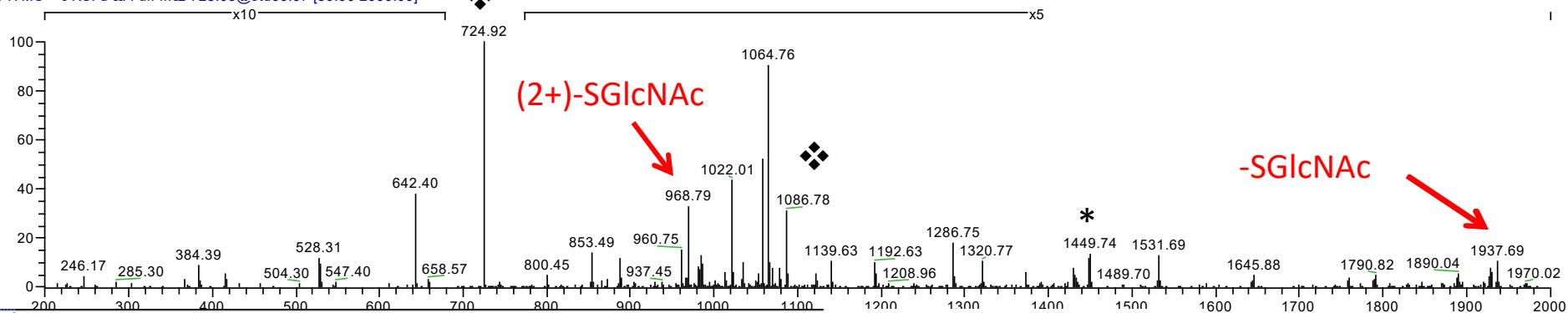
Peak Matches

246.1680	285.2950	367.3390	384.3930	415.4020	528.3110	547.4010	642.4010	658.5650	718.9750
$z+1_2(0.023)$	$c_3(0.10)$	$b_4(0.11)$	$c_4(0.13)$	$z_4(0.16)$	$z_5(-0.016)$	$c_5(0.077)$	$z_6(0.031)$	$y_6(0.18)$	
725.8380	730.0400	742.6010	743.5360	800.4470	852.5430	853.4900	866.3440	872.3020	887.5470
			$z_7(0.12)$	$z_8(0.0083)$	$c\text{-}1_6(0.14)$	$c_6(0.077)$			$z_9(0.076)$
960.7500	968.7880	981.4990	985.2580	1012.8490	1022.0130	1034.6060	1069.8090	1121.6730	1139.6340
	$c_7(0.027)$					$z_{10}(0.067)$		$z_{11}(0.10)$	$c_9(0.093)$
1192.6300	1286.7490	1320.7740	1373.7140	1430.6770	1448.0430	1448.9160	1531.6900	1929.0300	1937.6850
$z_{12}(0.022)$	$c_{10}(0.14)$	$z_{13}(0.11)$	$c_{11}(0.072)$	$c_{12}(0.014)$			$c_{13}(-0.021)$	$c_{17}(0.087)$	

S Figure 14

SAC(GlcNAc)IAPAAFTGQPQK

Cys-579   *Rat*

846.9171(2+)
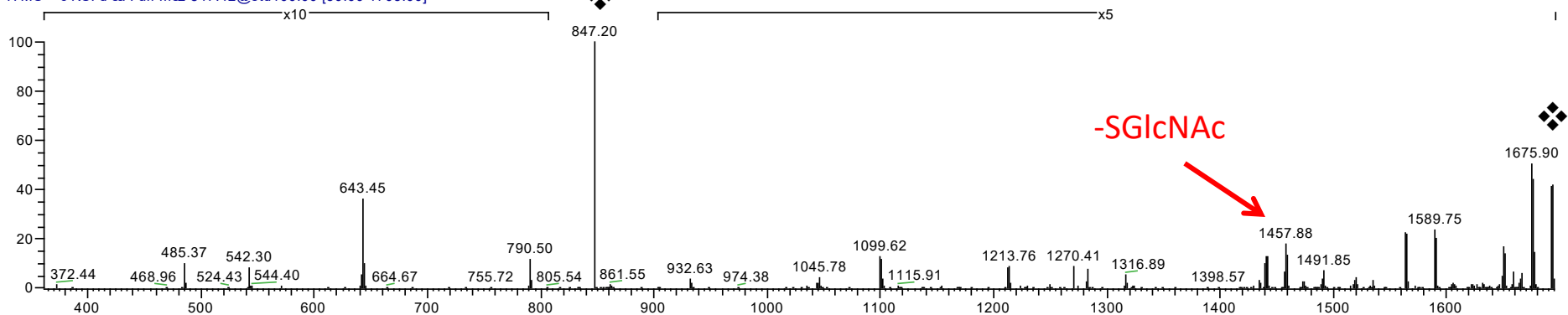
[−] Peak Matches

337.3100	372.4450	386.2340	468.9610	483.5210	485.3670	524.4270	541.3470	542.2970	571.2910
	$y_3(0.22)$			$z_4(-0.74)$	$z+1_4(0.095)$		$z_5(0.062)$		$z+1_5(0.0037)$
611.3440	**626.3580**	**640.8660**	**642.0770**	**643.4500**	**790.4950**	**861.5480**	**932.6250**	**1045.7770**	**1099.6240**
			$z_6(-0.26)$	$z+1_6(0.11)$	$z+1_7(0.086)$	$z+1_8(0.10)$	$z+1_9(0.14)$		$z_{11}(0.058)$
1212.8690	**1270.4060**	**1281.8010**	**1282.7700**	**1316.8890**	**1434.9590**	**1439.9030**	**1456.7820**	**1457.8790**	**1490.8820**
$z_{12}(0.22)$ $z+1_{12}(-0.79)$			w13		$c-1_{13}(0.28)$ $c_{13}(-0.73)$				
1491.8500	**1518.5750**	**1535.3330**	**1563.7370**	**1589.7490**					
$z_{13}(-0.16)$	$y_{13}(0.58)$	$c_{14}(-0.011)$	$z_{14}(-0.027)$						

S Figure 15

YEATS domain-containing protein 2   Q3TUF7

TPGQPQVC(GlcNAc)VSQATMATC(Cm)K

Cys-980   *Mouse*

703.9929(3+)

V20150116-16 #2304 RT: 30.46 AV:
T: FTMS + c NSI d Full ms2 704.33@hc

204.09

138.05

226.12

b4
384.19

273.16   408.19
356.19

y4
479.23

y5
610.26   527.26

690.36

y6
711.32

y7
782.35   811.38

Y0
953.94 y9
997.44

y8
910.43

y10
1096.51

y11
1199.52

y12
1298.59   1372.80

y14
1523.69

1659.36   1928.75

m/z
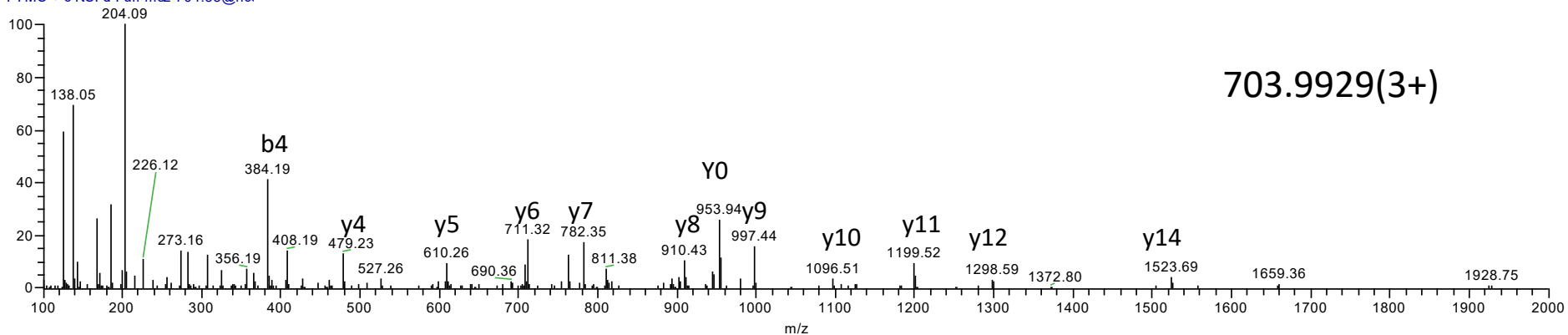
V20150116-16 #2305 RT: 30.46 AV: 1 NL: 3.20E4
T: ITMS + c NSI d sa Full ms2 704.33@etd66.67 [50.00-2000.00]

❖   *

x5   594.26   704.26   x5   1517.71

(2+)-S-HexNAc

❖
1027.09
1055.64

930.55

463.26   766.42
504.27
184.12   273.28   357.42   581.53   626.32   808.31   894.25   1150.67   1345.51 1416.75   1585.84   1648.80   1839.94   1981.94
695.28   1217.56   1719.76   1965.97
1778.82
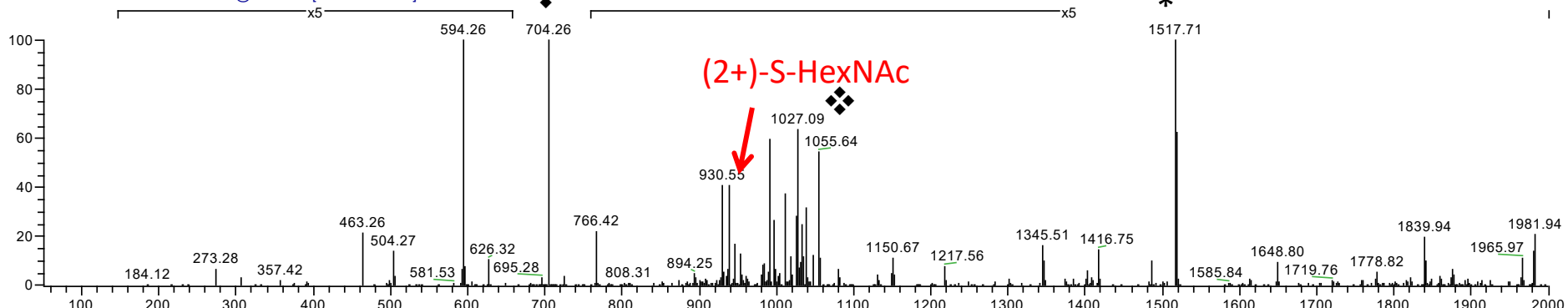
[−] Peak Matches

273.2800	307.1550	357.4210	463.2620	498.3460	504.2660	593.3880	594.2570	626.3240	681.5120
$c_3(0.12)$	$y_2(0.012)$		$z_4(0.052)$	$c_5(0.079)$			$z_5(0.0070)$	$c_6(-0.0017)$	
694.3440	695.2850	705.2080	711.3900	724.5390	725.4460	766.4150	874.0200	894.2540	901.3130
	$z_6(-0.013)$		$y_6(0.074)$	$c{-1}_7(0.15)$	$c_7(0.052)$	$z_7(0.080)$		$z_8(-0.14)$	
930.5490	938.2180	946.0280	954.2940	982.4700	990.6710	997.1600	1010.8230	1019.1080	1025.1600
				$z+1_9(0.037)$		$y_9(-0.28)$			
1038.7150	1150.6670	1345.5140	1416.7520	1485.6030	1517.7070	1648.8020	1839.1630	1965.9730	1980.9040
		$c_{11}(-0.13)$	$c_{12}(0.070)$	$z_{12}(-0.051)$	$c_{13}(-0.022)$	$c_{14}(0.032)$	$z_{15}(0.34)$ $z+1_{15}(-0.67)$		$c_{17}(0.019)$

S Figure 16A

MLX-interacting protein   Q2VPU4

NAC(GlcNAc)IAPAAFSGQPQK

Cys-579

Mouse
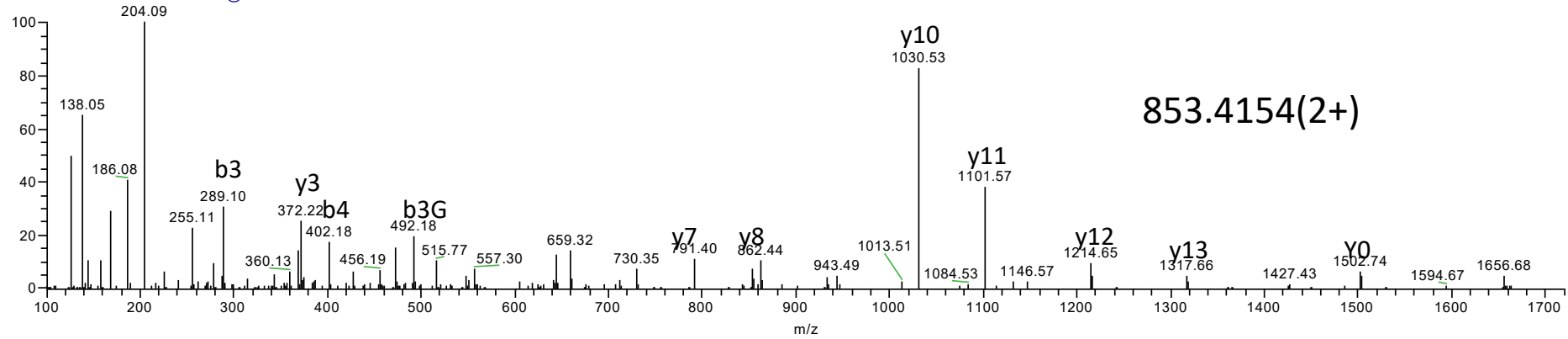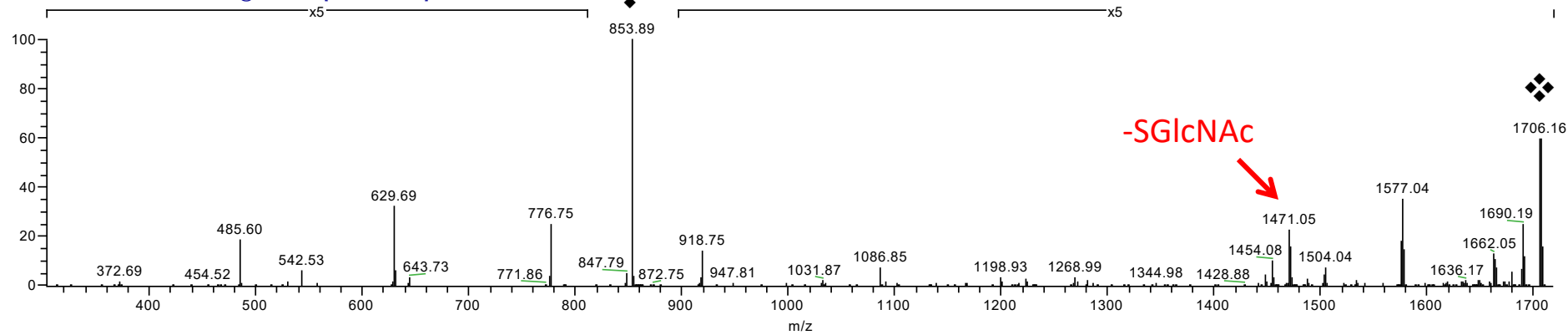
NAC(GlcNAc)IAPAAFSGQPQK

[−] Peak Matches

312.5530	325.7990	366.5980	370.7740	372.6940	421.4680	454.5180	466.6710	483.6150	485.6000
				$y_3(0.47)$				$z_4(-0.65)$	$z+1_4(0.33)$
499.6160	**514.7640**	**524.8190**	**529.7200**	**542.5330**	**557.6130**	**628.7810**	**629.6940**	**642.8330**	**643.7290**
$y_4(-0.67)$				$z+1_5(0.24)$	$y_5(0.31)$	$z_6(0.46)$ $z+1_6(-0.54)$	$z+1_6(0.37)$		$y_6(-0.61)$
775.7820	**776.7470**	**846.7940**	**847.7910**	**854.8630**	**917.7180**	**918.7540**	**1085.8200**	**1198.9340**	**1222.9480**
$z_7(0.40)$ $z+1_7(-0.61)$	$z+1_7(0.35)$	$z_8(0.37)$ $z+1_8(-0.64)$	$z+1_8(0.36)$		$z_9(0.26)$ $z+1_9(-0.75)$	$z+1_9(0.29)$	$z_{11}(0.27)$ $z+1_{11}(-0.74)$	$z_{12}(0.30)$ $z+1_{12}(-0.71)$	$c-1_{11}(0.38)$ $c_{11}(-0.63)$
1268.9910	**1448.0450**	**1454.0830**	**1469.9460**	**1471.0500**	**1488.0740**	**1503.1710**	**1504.0430**	**1576.0690**	**1577.0370**
w13	$c-1_{13}(0.37)$ $c_{13}(-0.64)$						$z_{13}(-0.68)$	$z_{14}(0.31)$ $c-1_{14}(0.33)$ $c_{14}(-0.68)$ $z+1_{14}(-0.70)$	$z+1_{14}(0.27)$ $c_{14}(0.29)$

S Figure 16B

AGISTTSVC(GlcNAc)EGQIANPSPISR

Protein Fam222b   Q6P539

Cys-288   *Mouse*

V20150116-16 #2794 RT: 35.09 AV
T: FTMS + c NSI d Full ms2 764.71@

764.3790(3+)

100 —
80 —
60 — 204.09
138.06
656.37
770.42 841.45
472.29
328.69
600.30
433.17 559.32 765.37 852.42 954.54
262.15 385.71 681.36 1023.48 1134.51 1371.68 1524.96 1659.74 1936.17
1191.51 1268.66

m/z
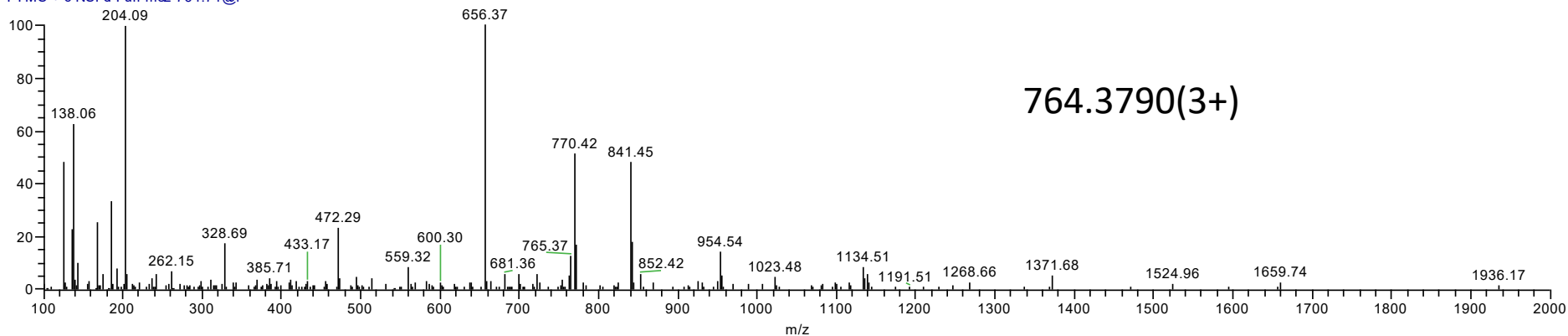
V20150116-16 #2795 RT: 35.11 AV: 1 NL: 1.66E4
T: ITMS + c NSI d sa Full ms2 764.71@etd66.67 [50.00-2000.00]

x10   ❖❖   x5

764.54

(2+)-SGlcNAc

1124.72

*

1028.26   1226.58   1528.71

548.32   938.51   1252.55   1354.70   1538.86

447.31 544.32   635.32   754.38   872.36   1169.54   1470.56   1744.82

299.35 375.48   617.53   825.53   1455.64   1574.96 1657.35   1846.96 1947.92
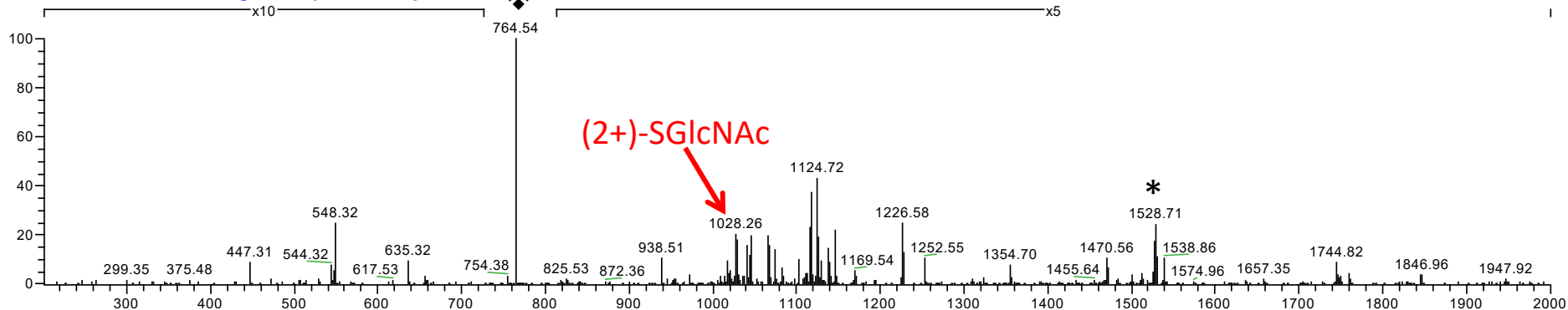
[−] Peak Matches

247.2160	299.3520	446.3520	447.3080	472.3580	529.3720	543.3710	544.3220	547.2850	548.3230
$z+1_2$(0.076)		$c-1_5$(0.10)	c_5(0.052)	y_4(0.070)		z_5(0.070)	$z+1_5$(0.013)	$c-1_6$(−0.011)	c_6(0.019)
635.3180	656.3720	734.4910	754.3750	766.4370	770.5660	802.5610	818.7000	825.5260	872.3620
c_7(−0.018)	y_6(−6.0e-4)	c_8(0.087)	z_7(−0.022)		y_7(0.15)			z_8(0.092)	
938.5140	1017.5970	1028.2590	1040.4610	1044.2860	1045.1530	1066.5490	1074.3270	1082.1060	1102.3540
z_9(−0.0040)			c_9(−0.036)			z_{10}(−0.028)		y_{10}(−0.49)	
1129.6820	1169.5440	1226.5770	1252.5500	1354.6980	1470.5570	1526.6390	1527.5600	1538.8570	1744.8190
	c_{10}(0.0044)	c_{11}(0.016)	z_{12}(−0.091)	c_{12}(0.078)				c_{14}(0.12)	z_{15}(−0.015)

LDFGQGSGSPVC(Cgly)LAQVK^{+3}
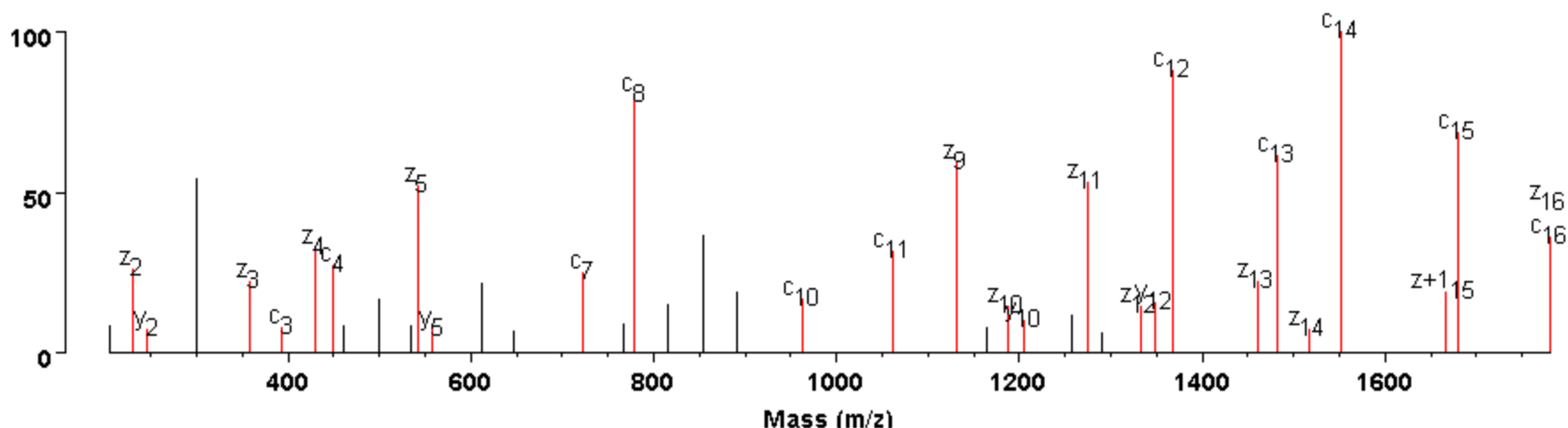
MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)	MH^{+3}(av)	MH^{+3}(mono)
1910.1664	1908.9372	955.5869	954.9722	637.3938	636.9839

[−] Peak Matches

204.0854	230.1621	246.1809	300.1911	358.2204	393.2123	429.2573	450.2340	461.2473	499.2864
204.0854	230.1621	246.1809	300.1911	358.2204	393.2123	429.2573	450.2340	461.2473	499.2864
	z_2(-1.7)	y_2(-1.2)		z_3(-2.0)	c_3(-2.3)	z_4(-2.1)	c_4(-1.6)		
534.2790	542.3415	558.3599	612.3708	646.3556	722.3460	779.3673	963.4535	1062.5193	1131.5818
534.2790	542.3415	558.3599	612.3708	646.3556	722.3460	779.3673	963.4535	1062.5193	1131.5818
	z_5(-1.4)	y_5(-2.0)	w6		c_7(-1.1)	c_8(-1.3)	c_{10}(0.47)	c_{11}(-2.0)	z_9(-2.0)
1163.5720	1188.6041	1204.6219	1257.6377	1275.6346	1290.6464	1332.6576	1348.6752	1368.6078	1460.7142
1163.5720	1188.6041	1204.6219	1257.6377	1275.6346	1290.6464	1332.6576	1348.6752	1368.6078	1460.7142
	z_{10}(-1.1)	y_{10}(-1.9)		z_{11}(-2.2)		z_{12}(-1.0)	y_{12}(-1.9)	c_{12}(-1.6)	z_{13}(-2.3)
1481.6910	1517.7363	767.3810^{+2}	1552.7289	814.9349^{+2}	1665.8119	1680.7867	853.4307^{+2}	890.4230^{+2}	1779.8525
1481.6910	1517.7363	1533.7547	1552.7289	1628.8625	1665.8119	1680.7867	1705.8540	1779.8388	1779.8525
c_{13}(-2.0)	z_{14}(-1.8)		c_{14}(-1.5)		$z+1_{15}$(-2.0)	c_{15}(-1.8)			c_{16}(-3.2) z_{16}(10)

FPFGSSC(Cgly)TGTFHPAPSAPDK^{+3}
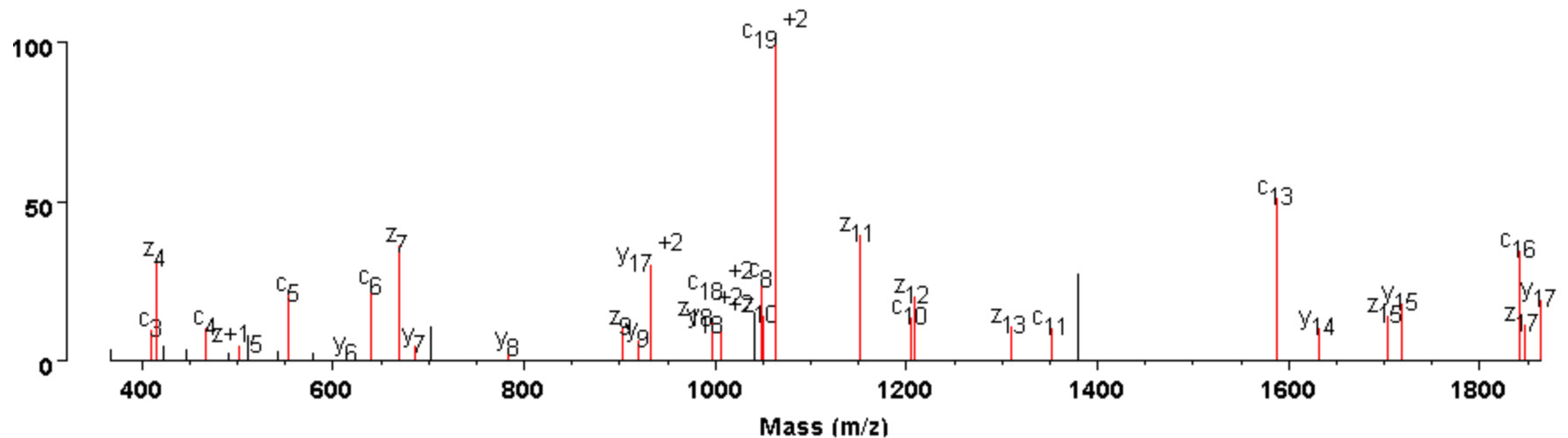
MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)	MH^{+3}(av)	MH^{+3}(mono)
2255.4828	2254.0121	1128.2451	1127.5097	752.4992	752.0089

[−] Peak Matches

366.2163	409.2221	414.2099	423.2375	446.1989	466.2436	491.2521	502.2491	510.2699	541.2519
366.2163	409.2221	414.2099	423.2375	446.1989	466.2436	491.2521	502.2491	510.2699	541.2519
	c_3(-3.3)	z_4(-2.3)			c_4(-2.7)		$z+1_5$(-3.3)		

553.2757	578.2842	614.3126	640.3077	669.3314	685.3494	701.3209	782.4053	903.4428	919.4624
553.2757	578.2842	614.3126	640.3077	669.3314	685.3494	701.3209	782.4053	903.4428	919.4624
c_5(-2.2)		y_6(-3.0)	c_6(-2.0)	z_7(-2.2)	y_7(-3.2)		y_8(1.3)	z_9(-1.9)	y_9(-0.88)

1047.4430	1050.5118	1151.5575	1205.5111	1208.5778	1309.6335	1352.5765	1379.6552	1586.6908	1631.7328
1047.4430	1050.5118	1151.5575	1205.5111	1208.5778	1309.6335	1352.5765	1379.6552	1586.6908	1631.7328
c_8(-2.1)	z_{10}(-1.0)	z_{11}(-2.7)	c_{10}(-2.7)	z_{12}(-3.5)	z_{13}(2.9)	c_{11}(-4.6)	w14	c_{13}(-2.3)	y_{14}(-2.6)

1702.7417	1718.7629	1841.8104	1846.8008	1862.8112	931.9115^{+2}	997.4388^{+2}	1005.4485^{+2}	1040.9637^{+2}	1062.9673^{+2}
1702.7417	1718.7629	1841.8104	1846.8008	1862.8112	1862.8157	1993.8703	2009.8898	2080.9202	2124.9273
z_{15}(-5.1)	y_{15}(-3.5)	c_{16}(-3.2)	z_{17}(-1.6)	y_{17}(-6.1)	y_{17}^{+2}(-3.6)	z_{18}^{+2}(-0.96)	y_{18}^{+2}(-0.55) c_{18}^{+2}(-8.1)		c_{19}^{+2}(-2.7)

QKAPFPATC(Cgly)EAPSR^{+3}
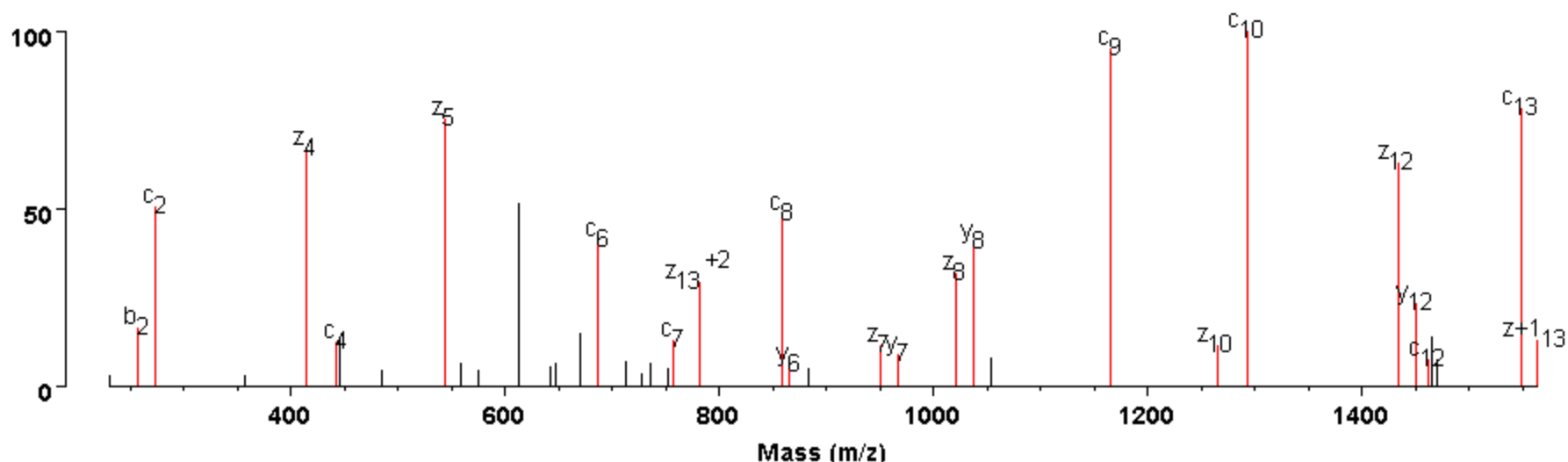
MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)	MH^{+3}(av)	MH^{+3}(mono)
1706.9266	1705.8214	853.9670	853.4143	569.6472	569.2786

[−] Peak Matches

230.1730	257.1602	274.1867	357.1863	414.2212	442.2765	446.2110	484.2502	543.2637	575.2530
230.1730	257.1602	274.1867	357.1863	414.2212	442.2765	446.2110	484.2502	543.2637	575.2530
	b_2(-2.4)	c_2(-2.4)		z_4(-2.3)	c_4(-1.7)			z_5(-1.9)	
613.2925	642.3842	647.2810	670.3787	686.3970	713.4205	757.4342	858.4800	865.3687	883.4885
613.2925	642.3842	647.2810	670.3787	686.3970	713.4205	757.4342	858.4800	865.3687	883.4885
w6				c_6(-2.0)		c_7(-1.8)	c_8(-3.7)	y_6(-3.9)	
950.3987	966.4172	1021.4356	1037.4546	1053.4243	559.2821^{+2}	1164.5691	1265.5574	1293.6112	1433.6451
950.3987	966.4172	1021.4356	1037.4546	1053.4243	1117.5569	1164.5691	1265.5574	1293.6112	1433.6451
z_7(-2.3)	y_7(-2.5)	z_8(-2.5)	y_8(-2.1)			c_9(-2.3)	z_{10}(-1.5)	c_{10}(-2.4)	z_{12}(-2.8)
1449.6639	727.3712^{+2}	1461.6992	1465.6362	1470.7635	735.8876^{+2}	751.8695^{+2}	1548.7319	781.3744^{+2}	1562.7479
1449.6639	1453.7352	1461.6992	1465.6362	1470.7635	1470.7680	1502.7316	1548.7319	1561.7415	1562.7479
y_{12}(-2.7)		c_{12}(-3.4)					c_{13}(-2.8)	z_{13}^{+2}(-1.7)	$z+1_{13}$(-2.6)

LDFGQGS(HexNAc)GSPVC(Carbamidomethyl)LAQVK^{+2}
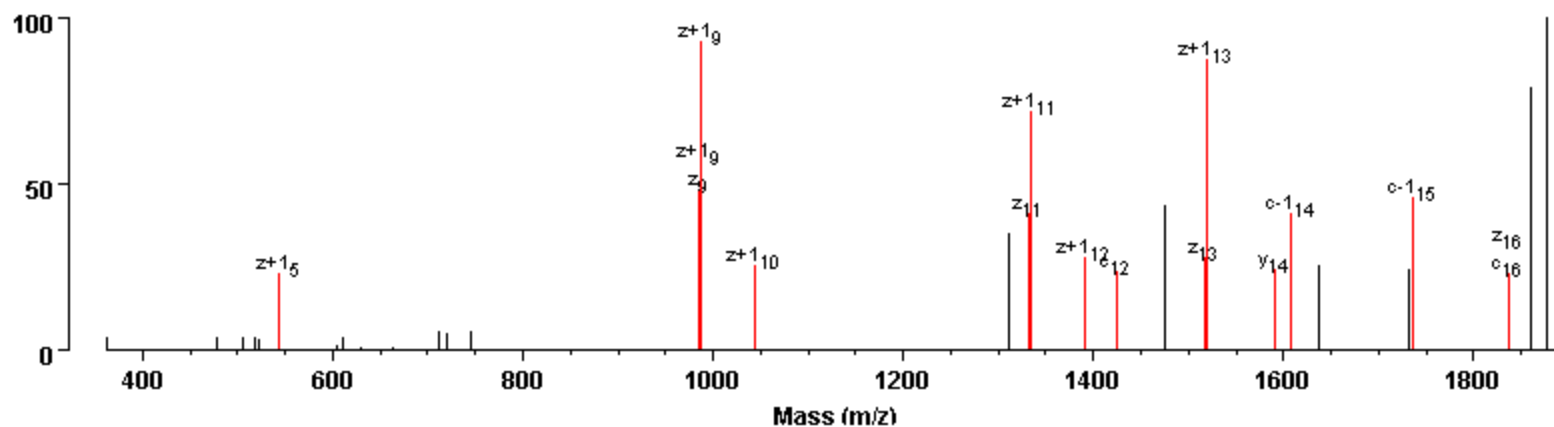
MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)
1967.2186	1965.9586	984.1130	983.4829

[−] **Peak Matches**

361.3270	478.4100	505.2610	517.7150	521.3960	543.3550	603.3420	610.3990	629.3110	663.4130
					z+1$_5$(0.0049)				
711.6010	720.4410	744.3460	985.8490	986.5520	1043.6110	1310.5170	1332.6080	1333.6380	1390.5070
			z$_9$(0.32) z+1$_9$(-0.68)	z+1$_9$(0.018)	z+1$_{10}$(0.056)		z$_{11}$(-0.051)	z+1$_{11}$(-0.029)	z+1$_{12}$(-0.18)
1425.7370	1474.4510	1517.7350	1518.7530	1590.8830	1608.7190	1638.1760	1730.9030	1736.7500	1837.0530
c$_{12}$(0.11)		z$_{13}$(-0.0040)	z+1$_{13}$(0.0062)	y$_{14}$(0.10)	c-1$_{14}$(-0.026)			c-1$_{15}$(-0.053)	c$_{16}$(0.17) z$_{16}$(0.20)
1859.8980	1876.9580	1897.0270							

FPFGS(HexNAc)SC(Carbamidomethyl)TGTFHPAPSAPDK^{+3}

MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)	MH^{+3}(av)	MH^{+3}(mono)
2312.5351	2311.0336	1156.7713	1156.0204	771.5166	771.0160

[−] Peak Matches

366.3130	409.3820	414.3060	465.5430	466.3360	502.3570	552.4280	614.3650	642.5390	669.4480
	c_3(0.16)	z_4(0.095)	$c\text{-}1_4$(0.31) c_4(-0.70)	c_4(0.091)	$z+1_5$(0.11)		y_6(0.051)		z_7(0.12)
685.5650	**756.3360**	**758.5800**	**773.0420**	**786.0310**	**800.4170**	**811.5690**	**816.6280**	**843.3780**	**845.2560**
y_7(0.21)	c_5(-0.020)							c_6(-0.010)	
903.4820	**1003.3980**	**1026.2660**	**1033.6010**	**1047.6730**	**1050.4970**	**1069.5130**	**1070.4660**	**1091.6400**	**1103.2840**
z_9(0.038)	c_7(-0.021)	$z+1_{18}^{+2}$(-0.19) z_{18}^{+2}(0.32)	$c\text{-}1_{18}^{+2}$(0.14) y_{18}^{+2}(-0.36) c_{18}^{+2}(-0.37)		z_{10}(-0.016)			c_{19}^{+2}(0.16) $c\text{-}1_{19}^{+2}$(0.66)	$c\text{-}1_8$(-0.17)
1104.3660	**1110.8630**	**1111.7760**	**1115.7130**	**1128.5670**	**1149.7890**	**1161.4690**	**1262.4980**	**1379.8270**	**1643.6400**
c_8(-0.10)						c_9(-0.019)	c_{10}(-0.038)	w14	c_{13}(-0.076)

FPFGSS(HexNAc)C(Carbamidomethyl)TGTFHPAPSAPDK^{+3}
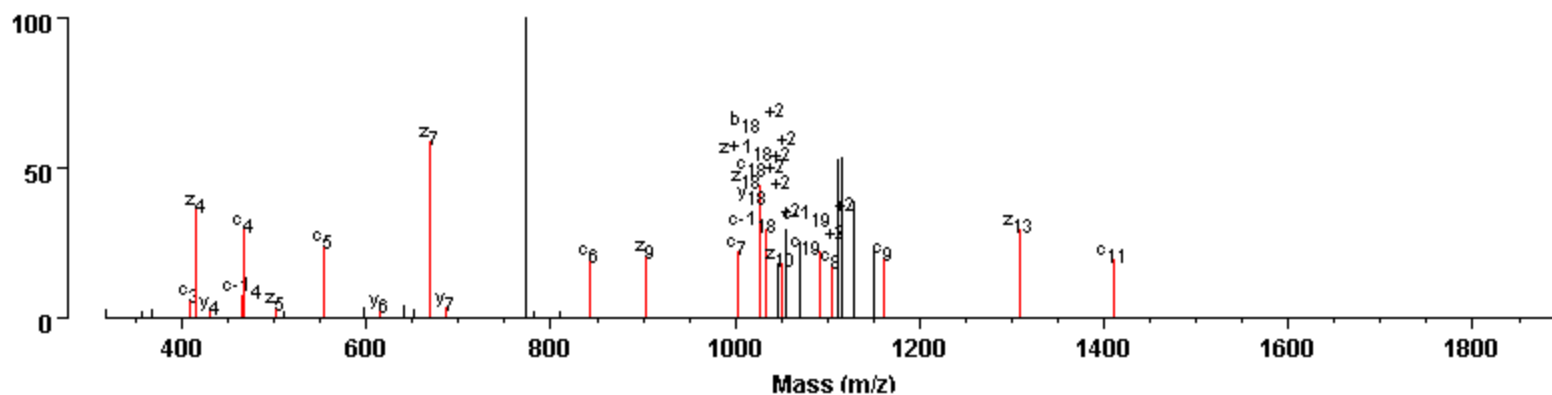
MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)	MH^{+3}(av)	MH^{+3}(mono)
2312.5351	2311.0336	1156.7713	1156.0204	771.5166	771.0160

[−] Peak Matches

316.2680	357.3900	366.3410	409.3500	414.3240	430.3440	465.2000	466.3310	501.4210	510.3470
			c_3(0.13)	z_4(0.11)	y_4(0.11)	$c\text{-}1_4$(-0.037)	c_4(0.086)	z_5(0.18)	
553.3380	**597.2920**	**614.3770**	**640.4390**	**652.3400**	**669.3240**	**685.4680**	**772.2940**	**781.6040**	**809.5640**
c_5(0.061)		y_6(0.063)			z_7(-0.0088)	y_7(0.12)			
843.4030	**903.4860**	**1003.3770**	**1026.1930**	**1033.6970**	**1046.6600**	**1050.5060**	**1055.8500**	**1069.6780**	**1091.4120**
c_6(0.015)	z_9(0.042)	c_7(-0.042)	z_{18}^{+2}(0.24) $z\text{+}1_{18}^{+2}$(-0.26) b_{18}^{+2}(0.74)	$c\text{-}1_{18}^{+2}$(0.23) y_{18}^{+2}(-0.26) c_{18}^{+2}(-0.27)		z_{10}(-0.0069)			c_{19}^{+2}(-0.069) $c\text{-}1_{19}^{+2}$(0.43)
1104.7640	**1111.4910**	**1112.1080**	**1115.7350**	**1128.4580**	**1149.5050**	**1161.5660**	**1309.6950**	**1409.6790**	**1899.8690**
c_8(0.30)						c_9(0.078)	z_{13}(0.065)	c_{11}(0.075)	

MC(Carbamidomethyl)AALNS(HexNAc)MDQYGGR^{+2}
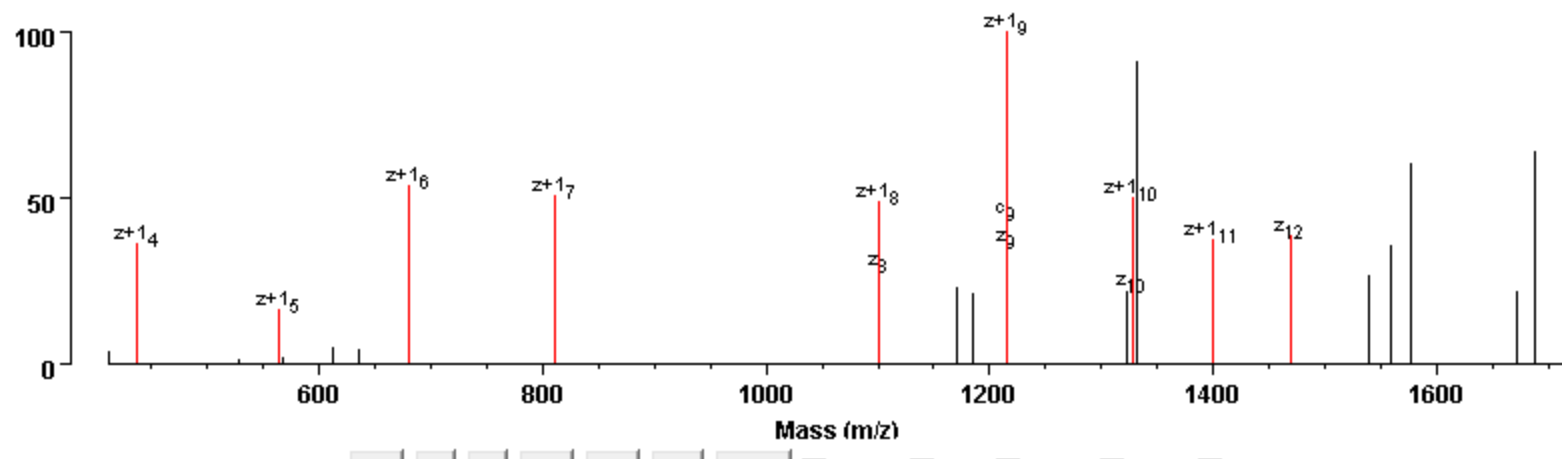
Elemental Composition: C70 H114 N21 O27 S3

MH^{+1}(av)	MH^{+1}(mono)	MH^{+2}(av)	MH^{+2}(mono)
1778.0036	1776.7350	889.5055	888.8711

[−] Peak Matches

411.6260	437.3740	529.5180	565.3280	567.3720	612.5470	636.5120	680.4120	811.4750	1100.5150
	z+1$_4$(0.16)		z+1$_5$(0.055)				z+1$_6$(0.11)	z+1$_7$(0.13)	z$_8$(0.071)
1101.5260	1170.9160	1184.8830	1214.5880	1215.4930	1323.4250	1327.6050	1328.5370	1331.6040	1399.6640
z+1$_8$(0.074)			z$_9$(0.10) c$_9$(0.10)	z+1$_9$(-0.0016)		z$_{10}$(0.034)	z+1$_{10}$(-0.042)		z+1$_{11}$(0.048)
1469.6840	1539.6730	1558.7920	1575.6380	1670.5870	1687.8580	1716.7740			
z$_{12}$(0.039)	w13								

S Figure 25

Estimating the relative amount of (**1**)FPFGSSC(Carbamidomethyl)T(GlcNAc)GTFHPAPSAPDK and (**2**)FPFGSSC(GlcNAc)TGTFHPAPSAPDK from the LC/MS data of a WGA-enriched but further not fractionated mouse synaptosome glycopeptide mixture

Host cell factor 1   P51610
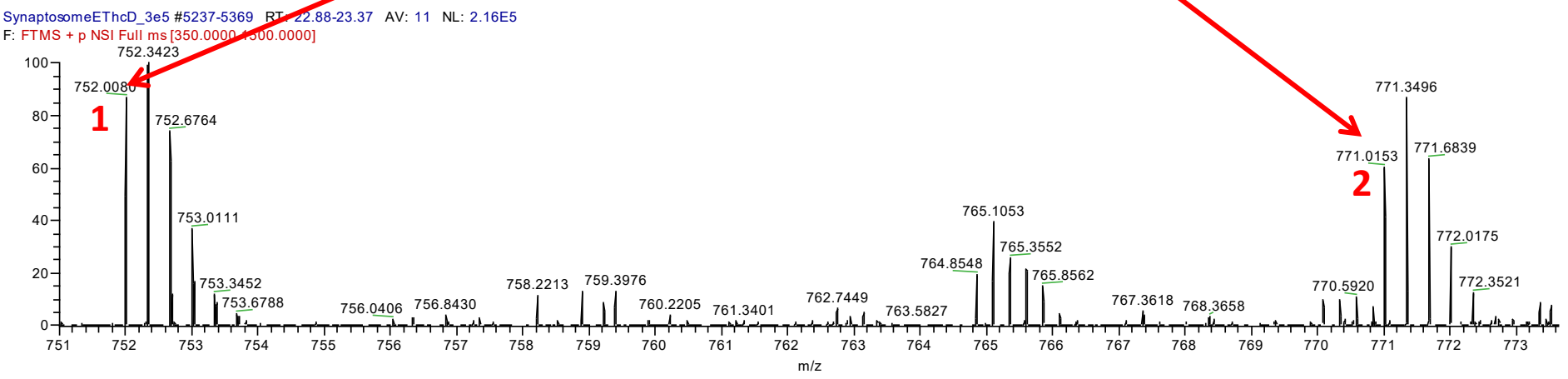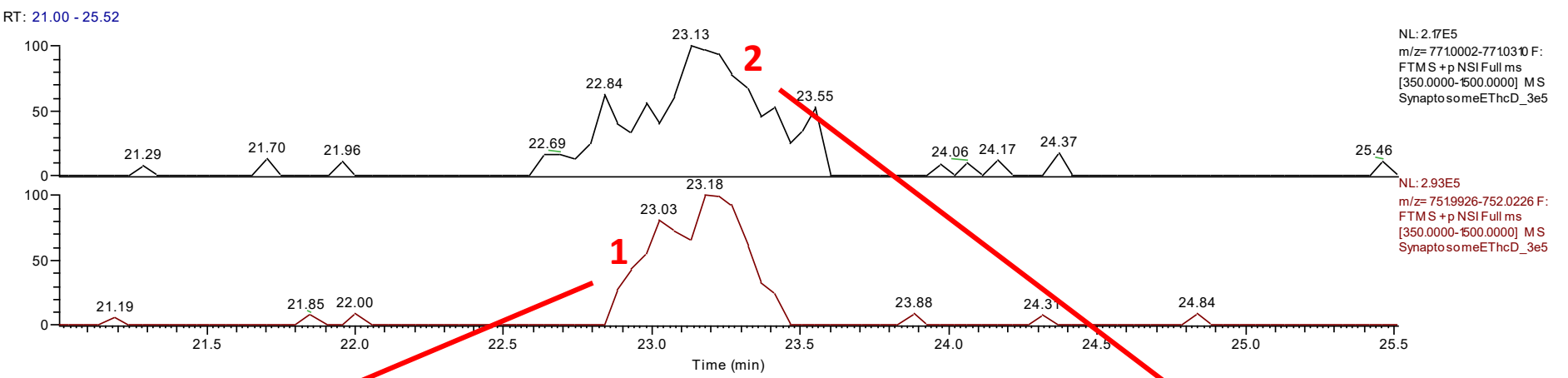
RAC(GlcNAc)AAGTPAVIR

Cys-1139   *Human*
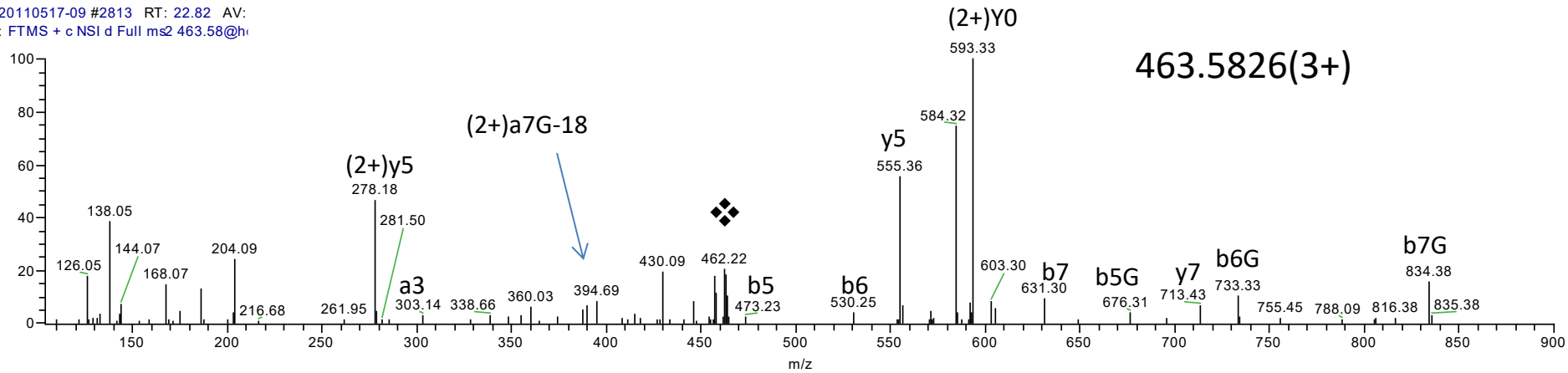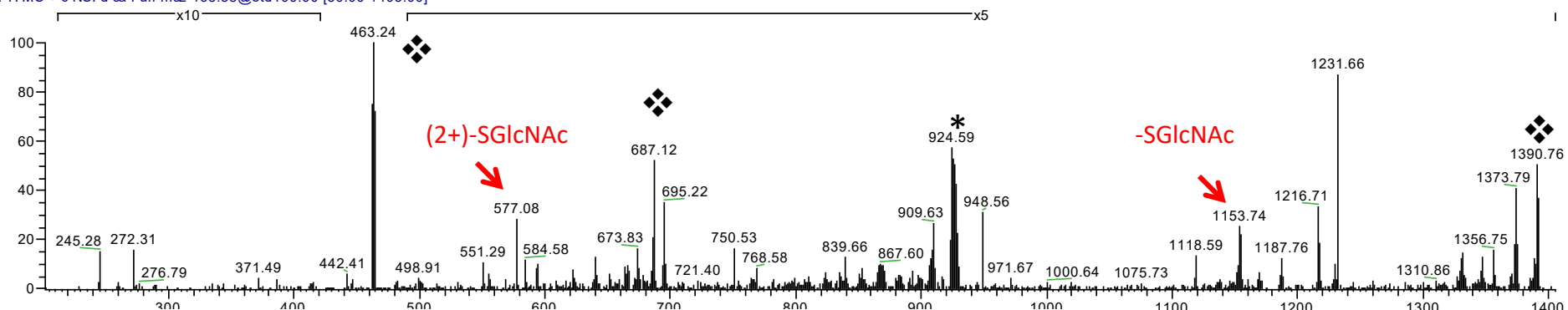
Peak Matches

245.2810	260.2860	272.3070	276.7880	371.4900	386.4300	415.3410	429.3400	442.4120	446.2080
$c_2(0.11)$		$z_2(0.12)$		$z_3(0.24)$				$z_4(0.12)$	

453.2990	472.9240	475.4640	481.9580	488.3840	498.9110	514.0640	530.3490	551.2880	555.3700
								$b_{10}^{+2}(0.016)$ $c_3(0.026)$	$y_5(0.0087)$

577.0810	584.5790	594.1340	622.4320	640.4630	664.1320	750.5270	768.5790	839.6640	852.6380
			$c_4(0.13)$	$z_6(0.073)$		$c_6(0.17)$	$z_8(0.13)$	$z_9(0.18)$	

867.6030	892.6370	909.6330	924.5920	948.5600	1118.5940	1153.7350	1187.7620	1216.7080	1231.6650
	w10			$c_8(0.10)$	$c_{10}(0.030)$			$z_{11}(0.095)$	$c_{11}(0.017)$
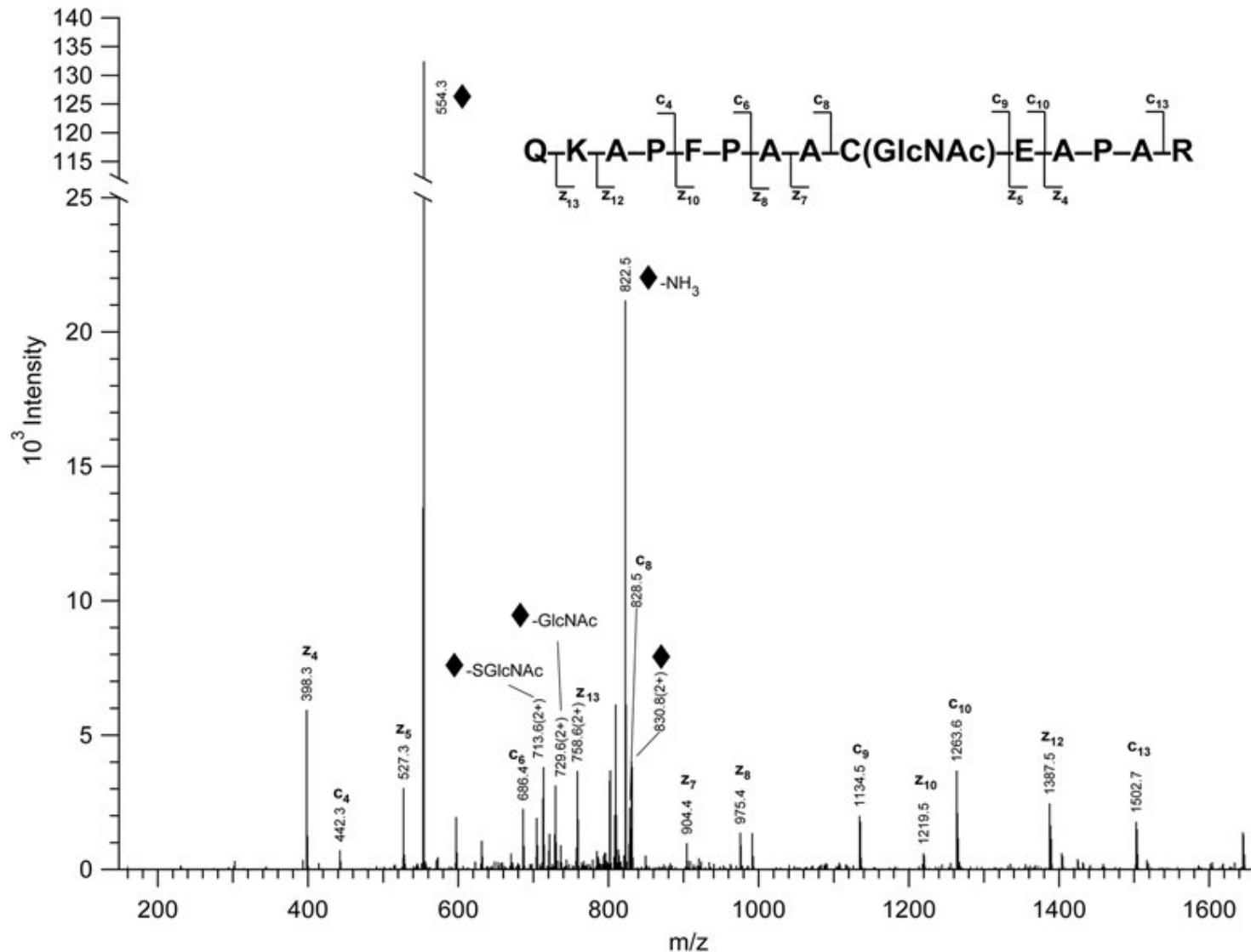
A) ETD spectrum of synthetic peptide QKAPFPAACEAPAR. '◆' labels the precursor ion and its charge-reduced form. The insert shows the bond cleavages detected.

S Figure 27B
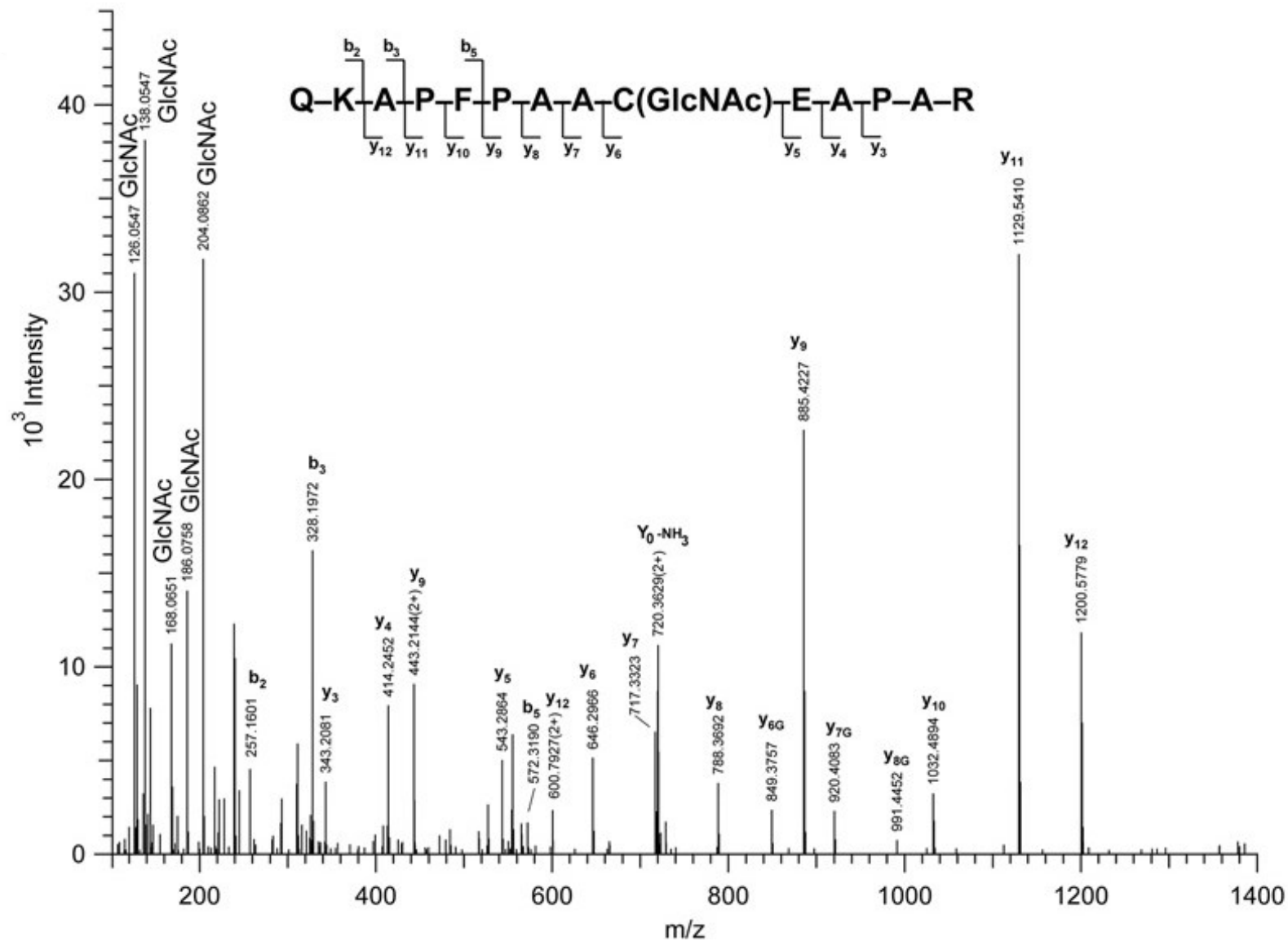
B) HCD spectrum of synthetic peptide QKAPFPAACEAPAR. The insert shows the bond cleavages detected. y ions containing GlcNAc are labeled with a G.

S Figure 28A
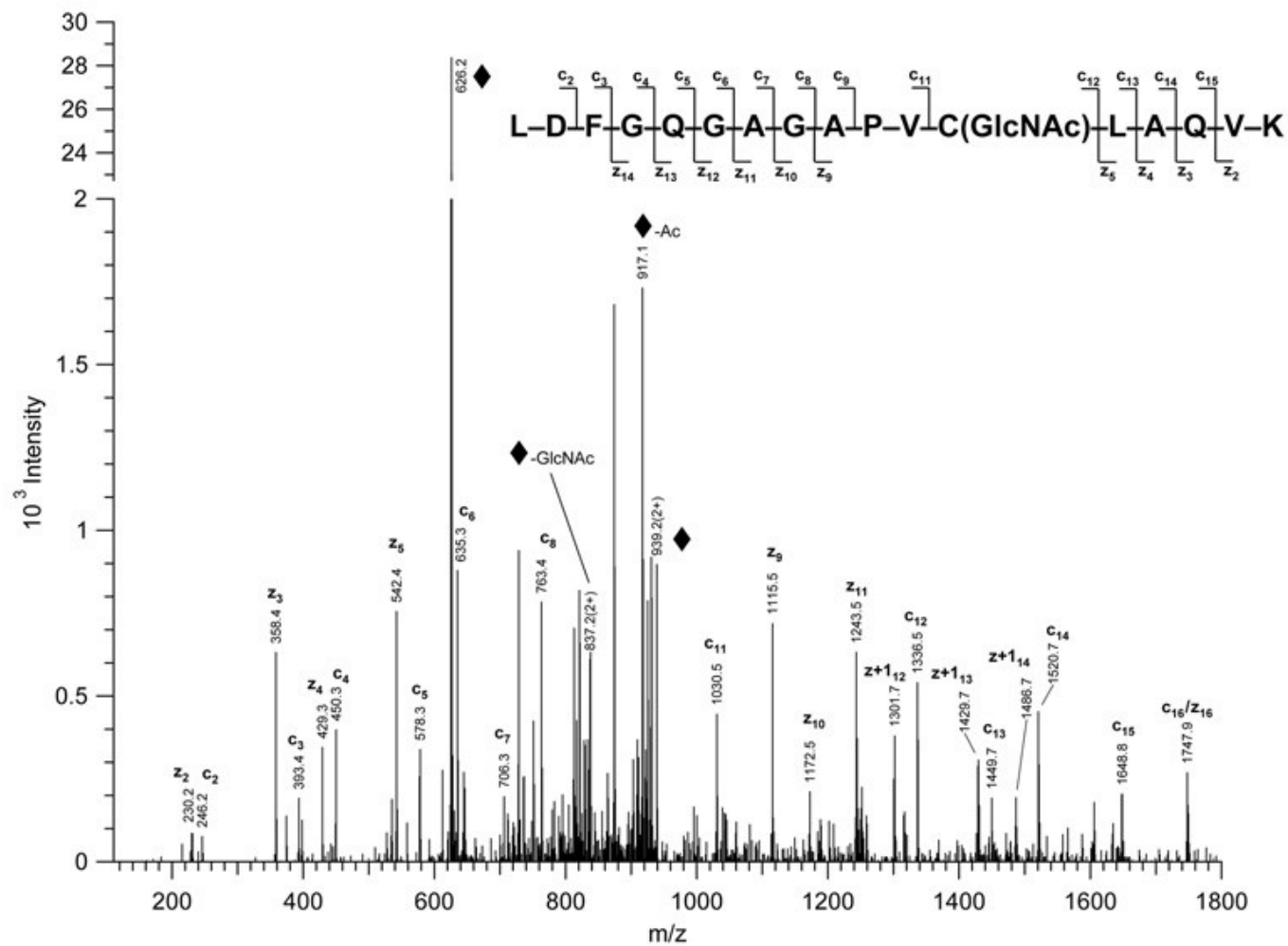
A) ETD spectrum of synthetic peptide LDFGQGAGAPVCLAQVK. '♦' labels the precursor ion and its charge-reduced form. The insert shows the bond cleavages detected.

S Figure 28B

B) HCD spectrum of synthetic peptide QKAPFPAACEAPAR. The insert shows the bond cleavages detected. y ions containing GlcNAc are labeled with a G.

S Figure 29A
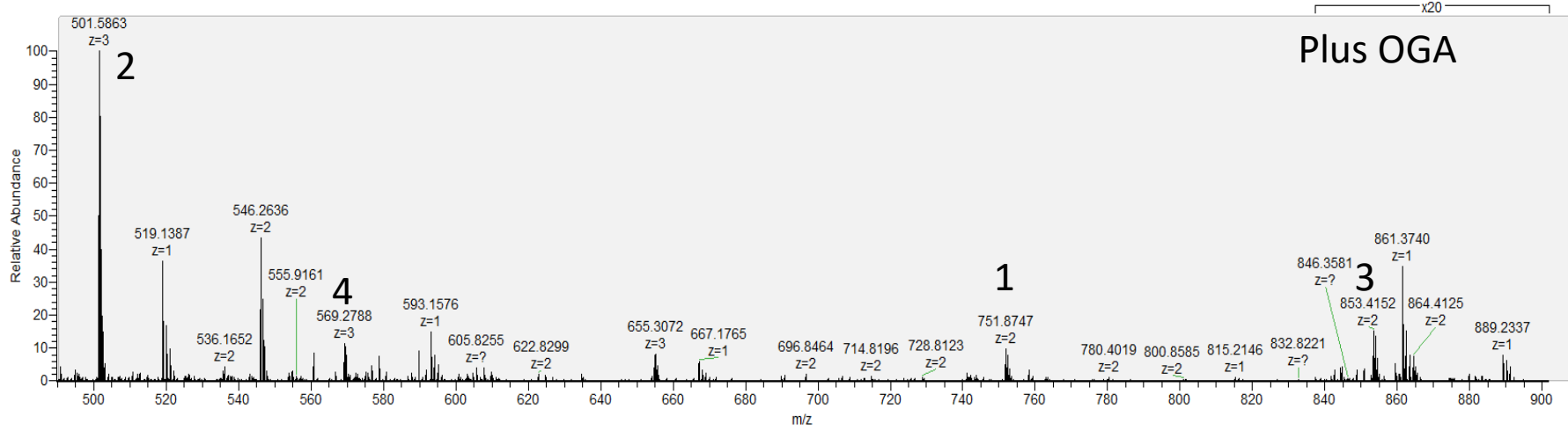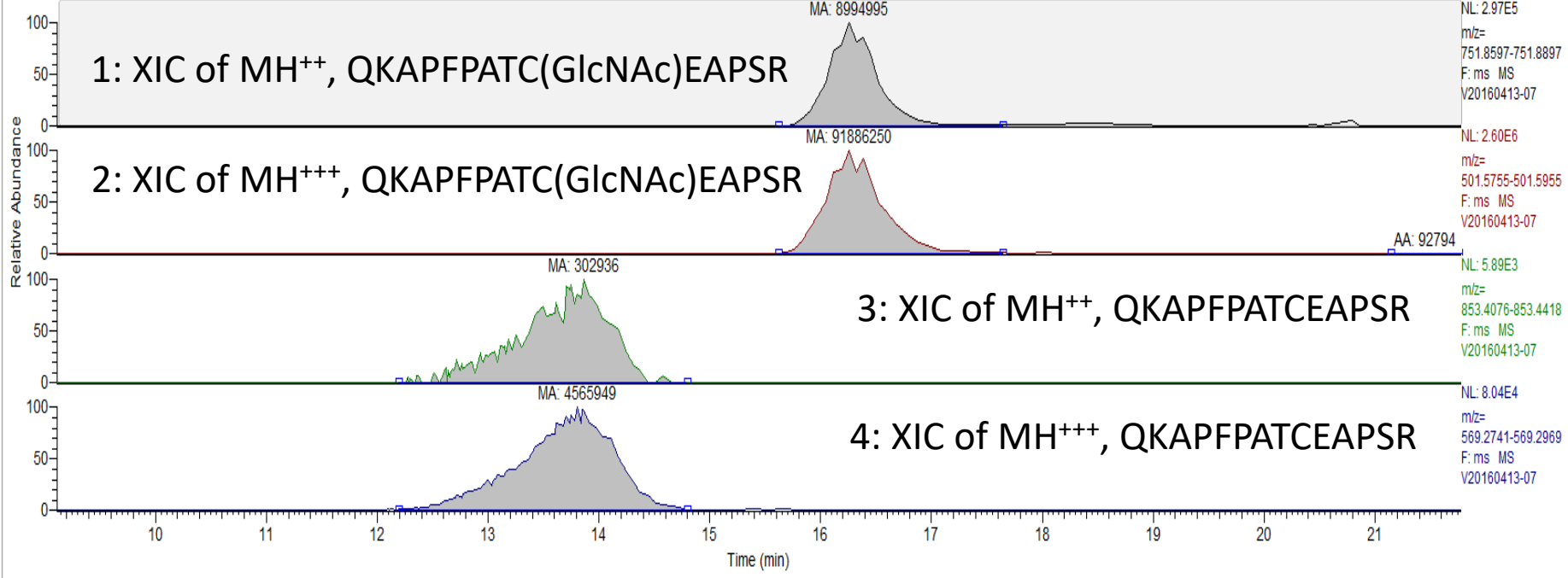

A) Mass spectrum across XIC peaks and extracted ion chromatograms of control peptide TAPTS(GlcNAc)TIAPG (modified and unmodified) after incubation with no OGA. Spectrum peaks are labeled to match XIC peaks. Peak areas are labeled above XIC peaks.

S Figure 29B

B) Mass spectrum across XIC peaks and extracted ion chromatograms of control peptide TAPTS(GlcNAc)TIAPG (modified and unmodified) after incubation with OGA. Spectrum peaks are labeled to match XIC peaks. Peak areas are labeled above XIC peaks.
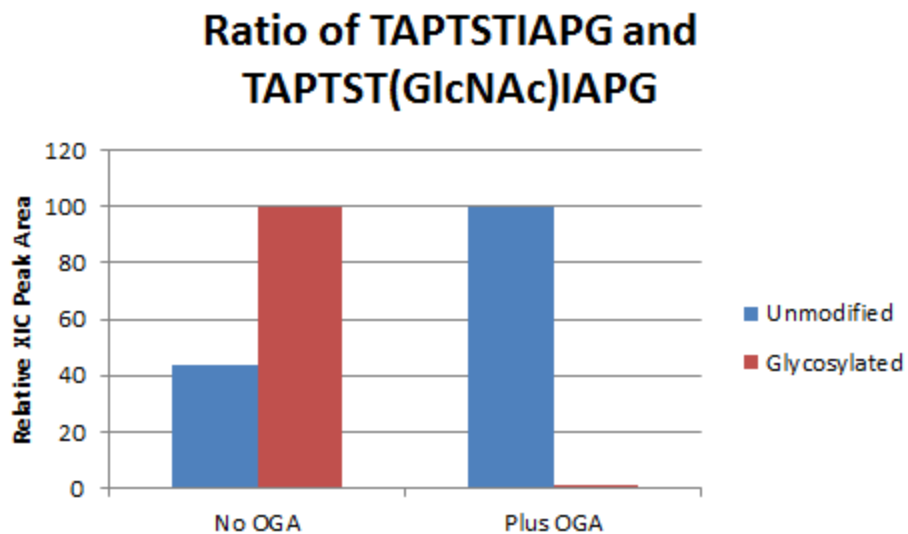
S Figure 29C

C) Mass spectrum across XIC peaks and extracted ion chromatograms of control peptide QKAPFPATC(GlcNAc)EAPSR (modified and unmodified) after incubation with no OGA. Spectrum peaks are labeled to match XIC peaks. Peak areas are labeled above XIC peaks.
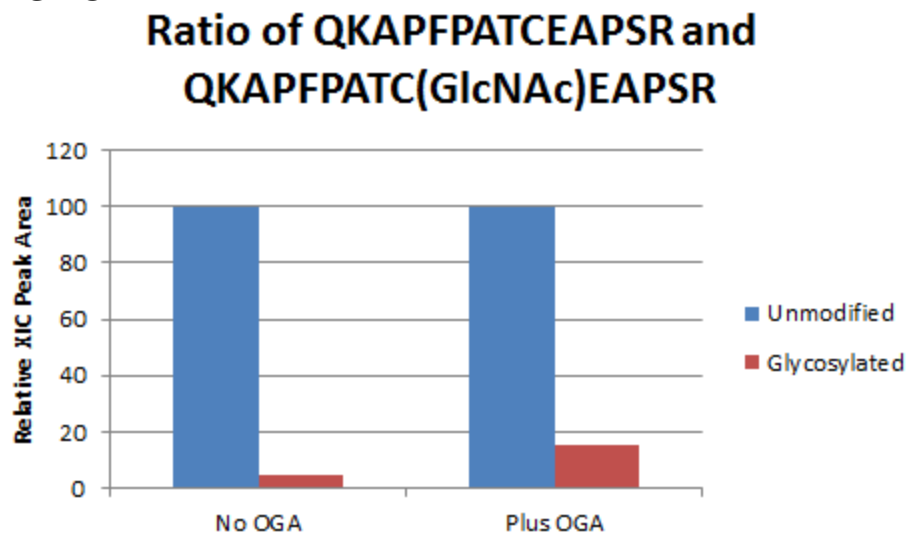
D) Mass spectrum across XIC peaks and extracted ion chromatograms of control peptide QKAPFPATC(GlcNAc)EAPSR (modified and unmodified) after incubation with OGA. Spectrum peaks are labeled to match XIC peaks. Peak areas are labeled above XIC peaks.

S Figure 29E

Ratio of TAPTSTIAPG and TAPTST(GlcNAc)IAPG

S Figure 29F

Ratio of QKAPFPATCEAPSR and QKAPFPATC(GlcNAc)EAPSR

E and F) Relative XIC peak areas of modified and unmodified GlcNAc standard peptide (TAPTSTIAPG) and synthetic peptide (QKAPFPATCEAPSR) with and without incubation with OGA.