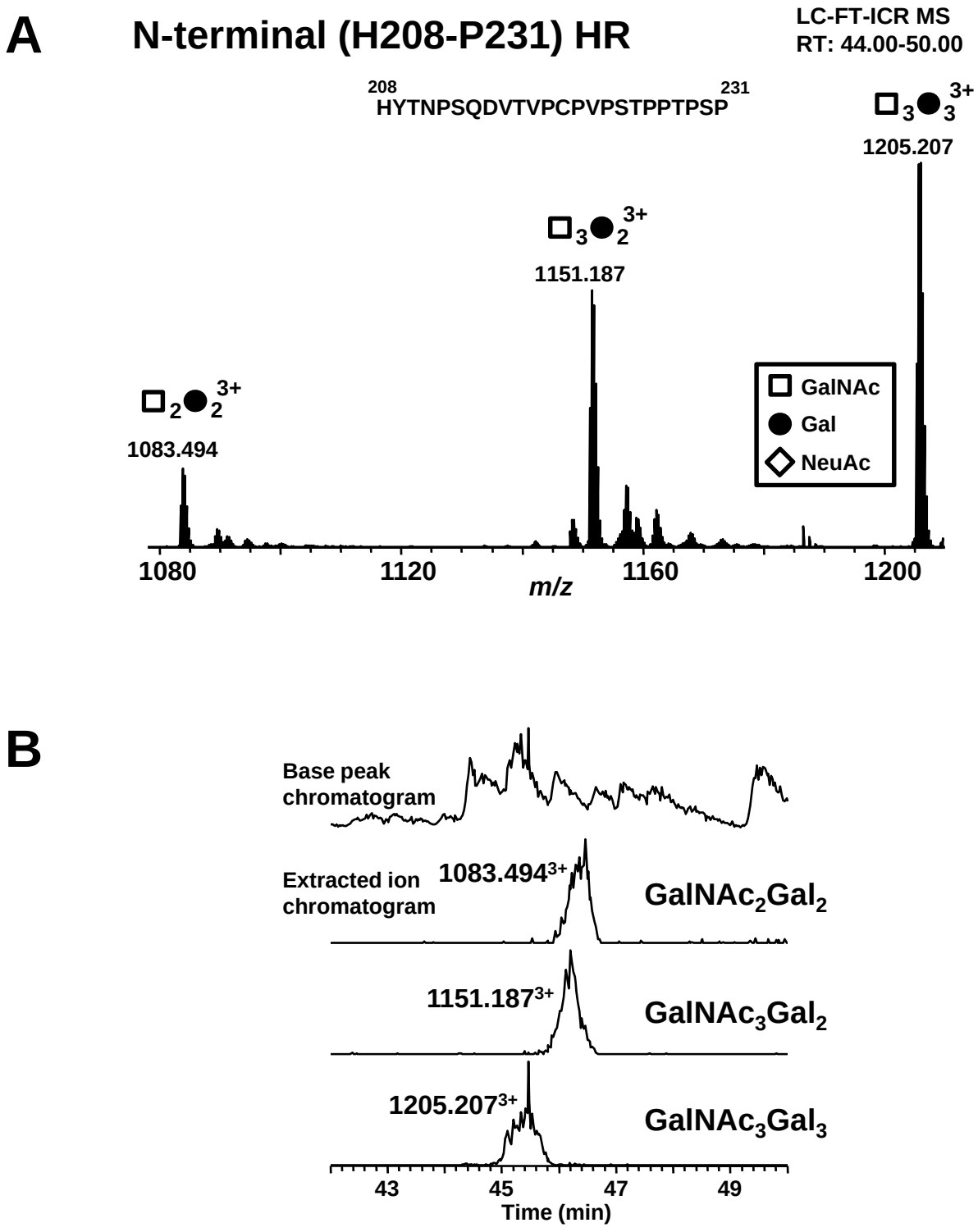
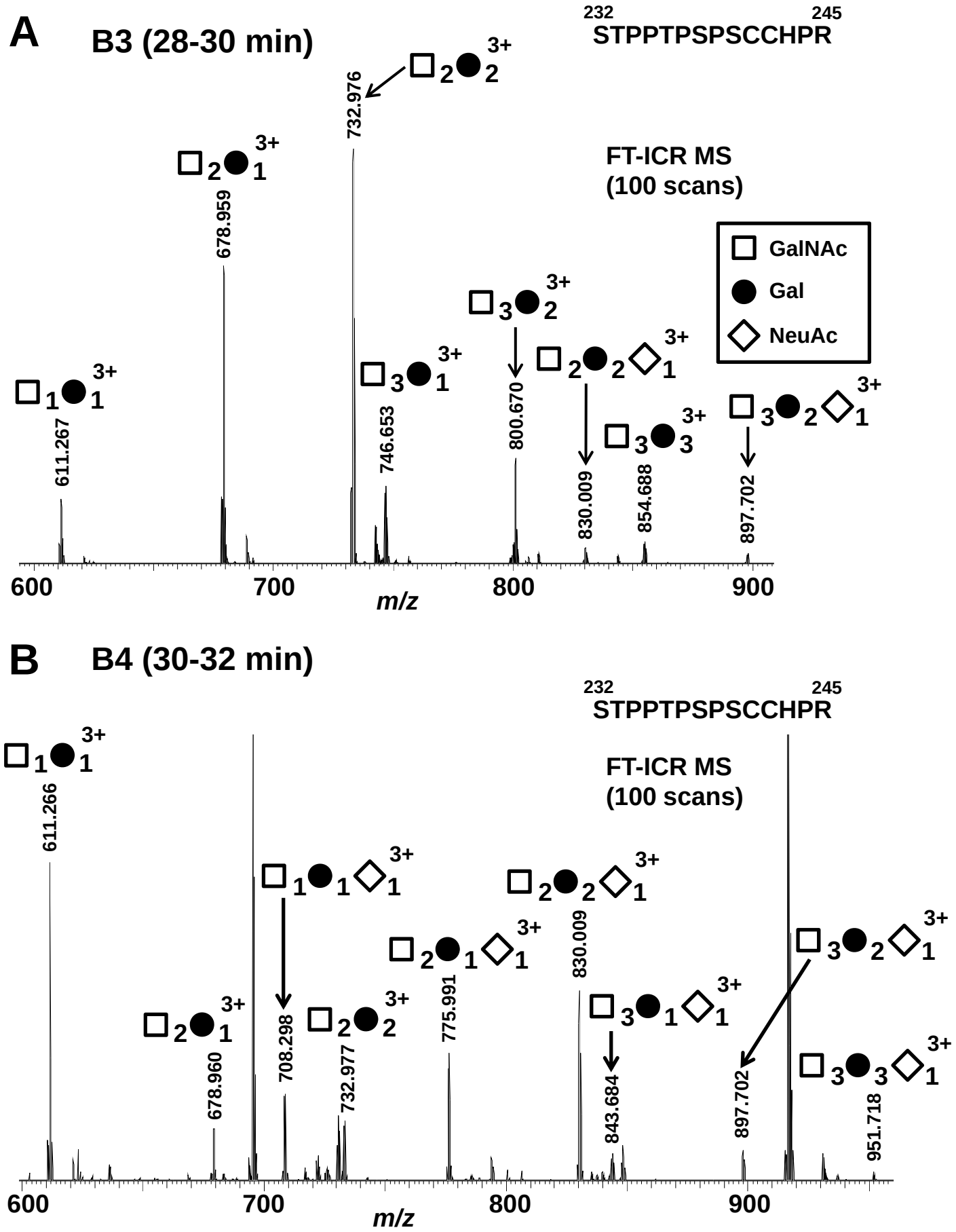
Supplemental Fig. 1



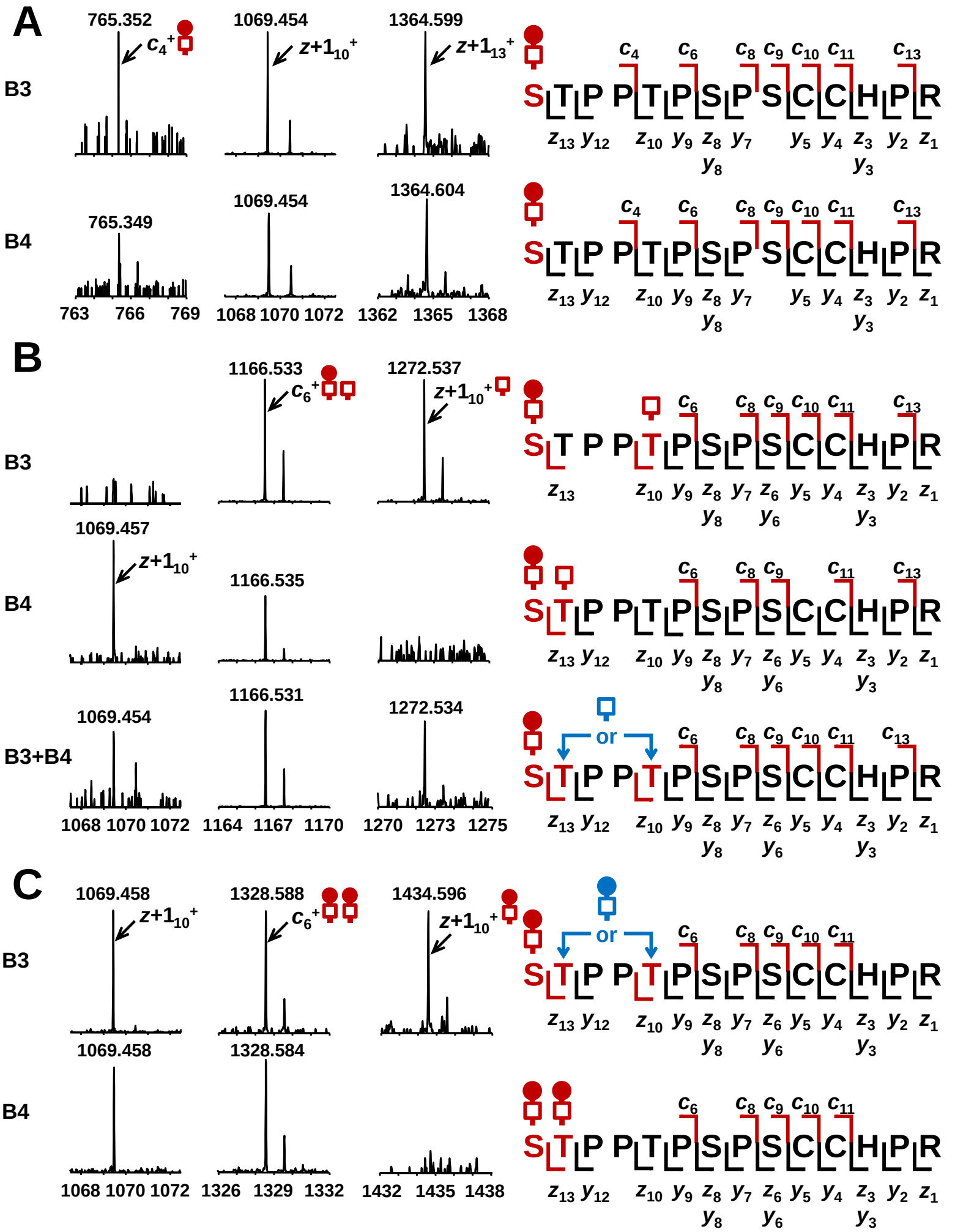
Supplemental Fig. 1. Online LC FT-ICR MS analysis of His^{208}-Pro^{231} (*A*) HR glycopeptides of IgA1 (Mce1) myeloma protein. All glycopeptides were detected as triply charged ions. The number of *O*-glycan chains was assigned based on the masses of the amino-acid sequence, GalNAc (open squares), and Gal (full circles). The *m/z* values for the observed glycopeptides, retention time, relative abundance, mass error, and site-specific *O*-glycosylation are summarized in Supplemental Table 1. XIC of three dominant glycopeptides in N-terminal (*B*) HR fragments were individually extracted for the specific *m/z* of glycopeptides. Single peak was observed for the each of the His^{208}-Pro^{231} glycoforms.

Supplemental Fig. 2



Supplemental Fig. 2. The NanoMate^{TM} ESI FT-ICR mass spectrum of IgA1 (Mce1) myeloma protein HR Ser^{232}-Arg^{245} glycopeptides, fractionated into the wells B3 (28-30 min) (*A*) and B4 (30-32 min) (*B*) by offline LC revealed the same series of HR *O*-glycopeptides seen for the *O*-glycopeptides in Fig. 1B. Monosialylated glycopeptides were detected in spite of neuraminidase treatment. All glycopeptides were detected as triply charged ions. Each spectrum represents the sum of 100 individual FT-ICR MS scans.

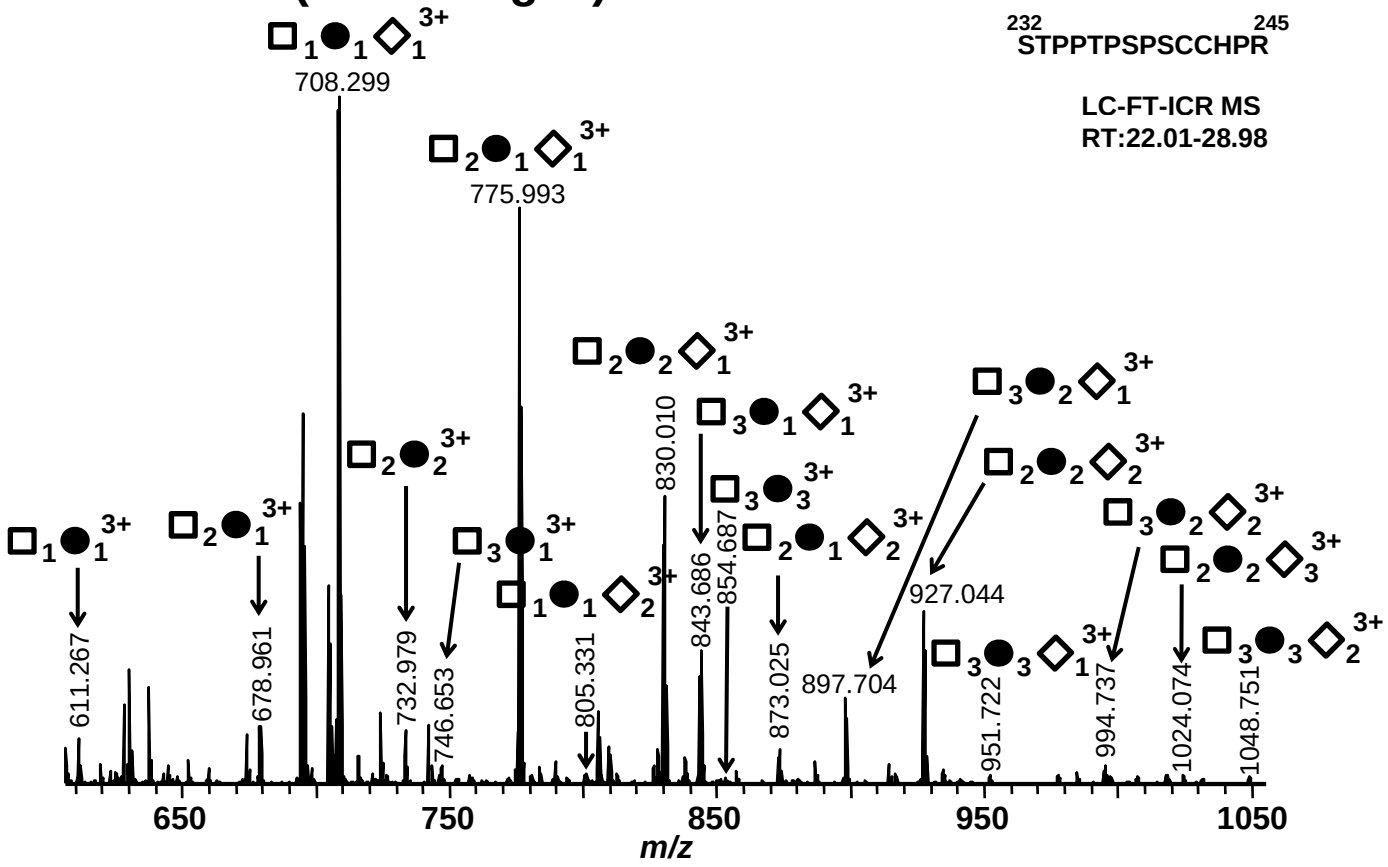
Supplemental Fig. 3



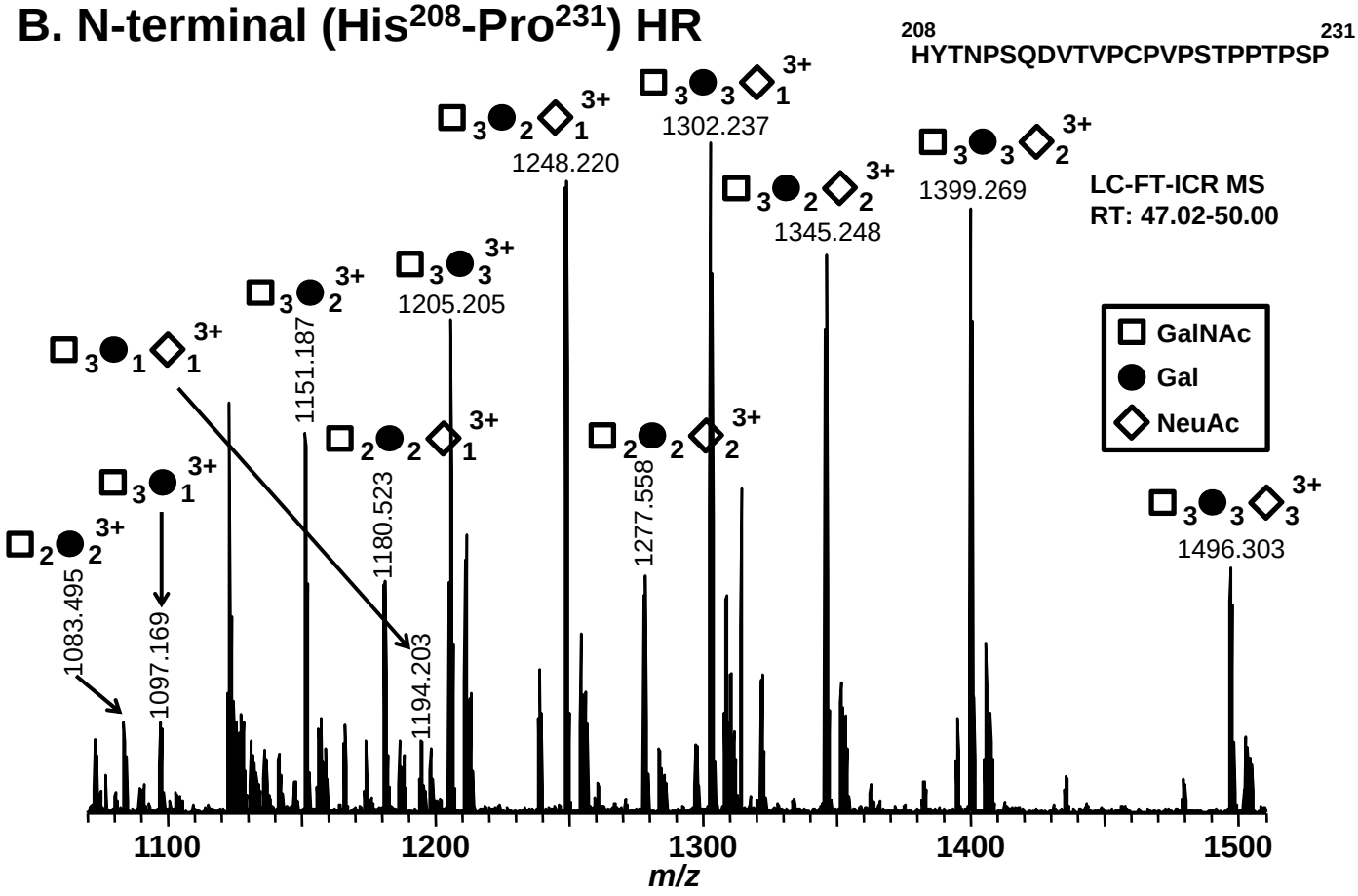
Supplemental Fig. 3. AI-ECD FT-ICR tandem MS of the IgA1 HR Ser^{232}-Arg^{245} with $GalNAc_1Gal_1$ (*A*), $GalNAc_2Gal_1$ (*B*), and $GalNAc_2Gal_2$ (*C*). Each AI-ECD fragmentation was performed using a triply charged precursor ion and 100 individual FT-ICR tandem MS scans were collected for each spectrum. Arrows in the spectra denote the key fragments that allowed assignment of glycan attachment sites and identification of amio acid positional isomers. The observed *c*, *z*, and *y* fragments for each *O*-glycopeptide are indicated above and below the sequences. Arrows in the amino-acid sequence point the alternative attachment sites in the isomeric structural variants of glycopeptides (panels *B*, *C*).

Supplemental Fig. 4

A. C-terminal (Ser^{232}-Arg^{245}) HR

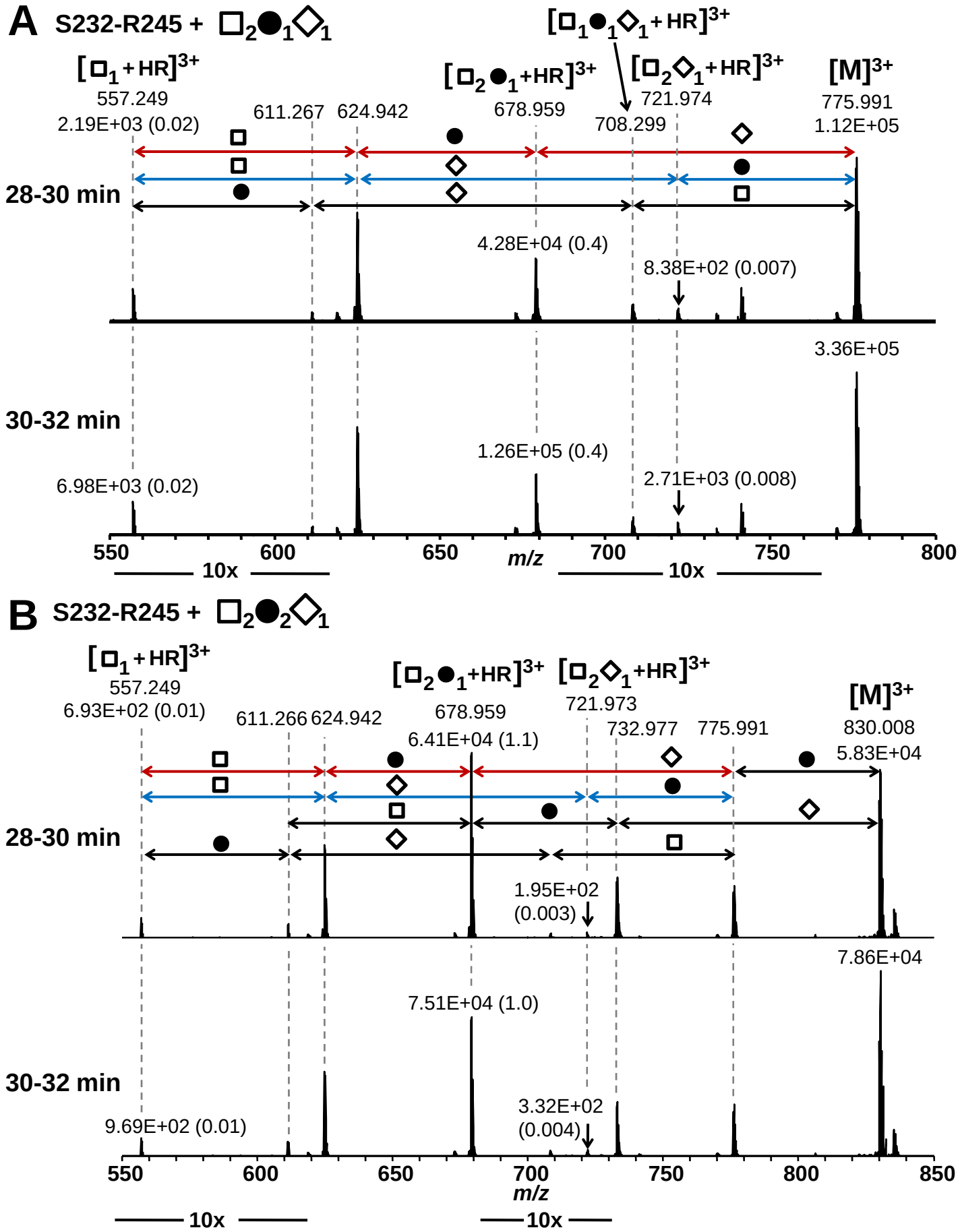


B. N-terminal (His^{208}-Pro^{231}) HR



Supplemental Fig. 4. Online LC FT-ICR MS analysis of Ser^{232}-Arg^{245} (*A*) and His^{208}-Pro^{231} (*B*) HR glycopeptides of normal human IgA1. All glycopeptides were detected as triply charged ions. The number of *O*-glycan chains was assigned based on the masses of the amino-acid sequence, GalNAc (open squares), Gal (full circles), and NeuAc (open diamonds). The *m/z* values for the observed glycopeptides, their respective retention times, relative abundance, and mass error are summarized in Table 2 and Supplemental Table 4.

Supplemental Fig. 5

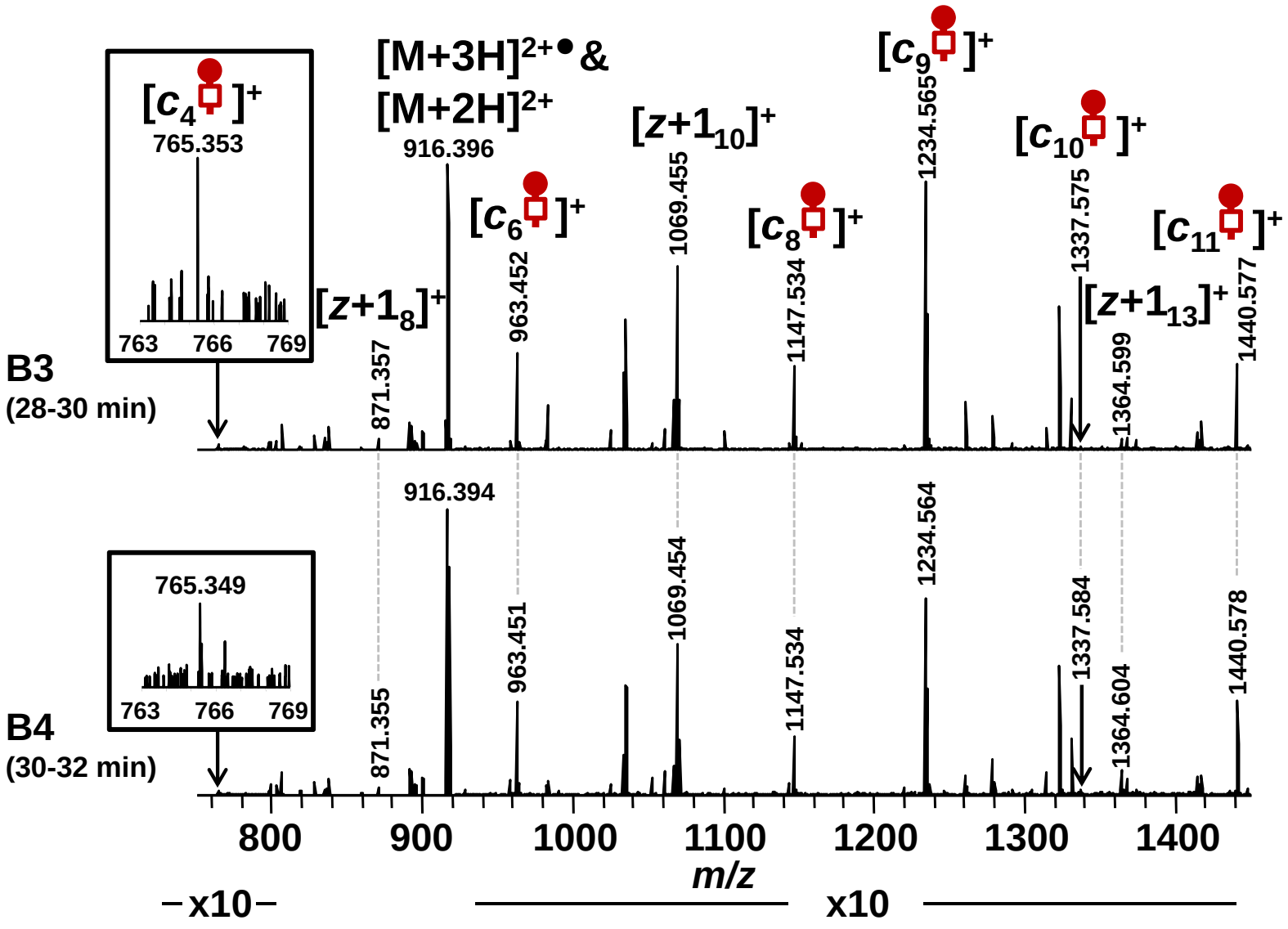


Supplemental Fig. 5. IRMPD FT-ICR tandem MS of the normal human serum IgA1 HR Ser^{232}-Arg^{245} with $GalNAc_2Gal_1NeuAc_1$ (A) and $GalNAc_2Gal_2NeuAc_1$ (B) fractionated into 28-30 min and 30-32 min fractions by off-line RP LC. Red fragmentation pathway indicates NeuAc (open diamond) attachment to Gal (filled circle), whereas blue fragmentation pathway shows GalNAc (open rectangle) with NeuAc.

Supplemental MS spectra

IgA1 (Mce1) myeloma protein

Ser^{232}-Arg^{245} + $GalNAc_1Gal_1$



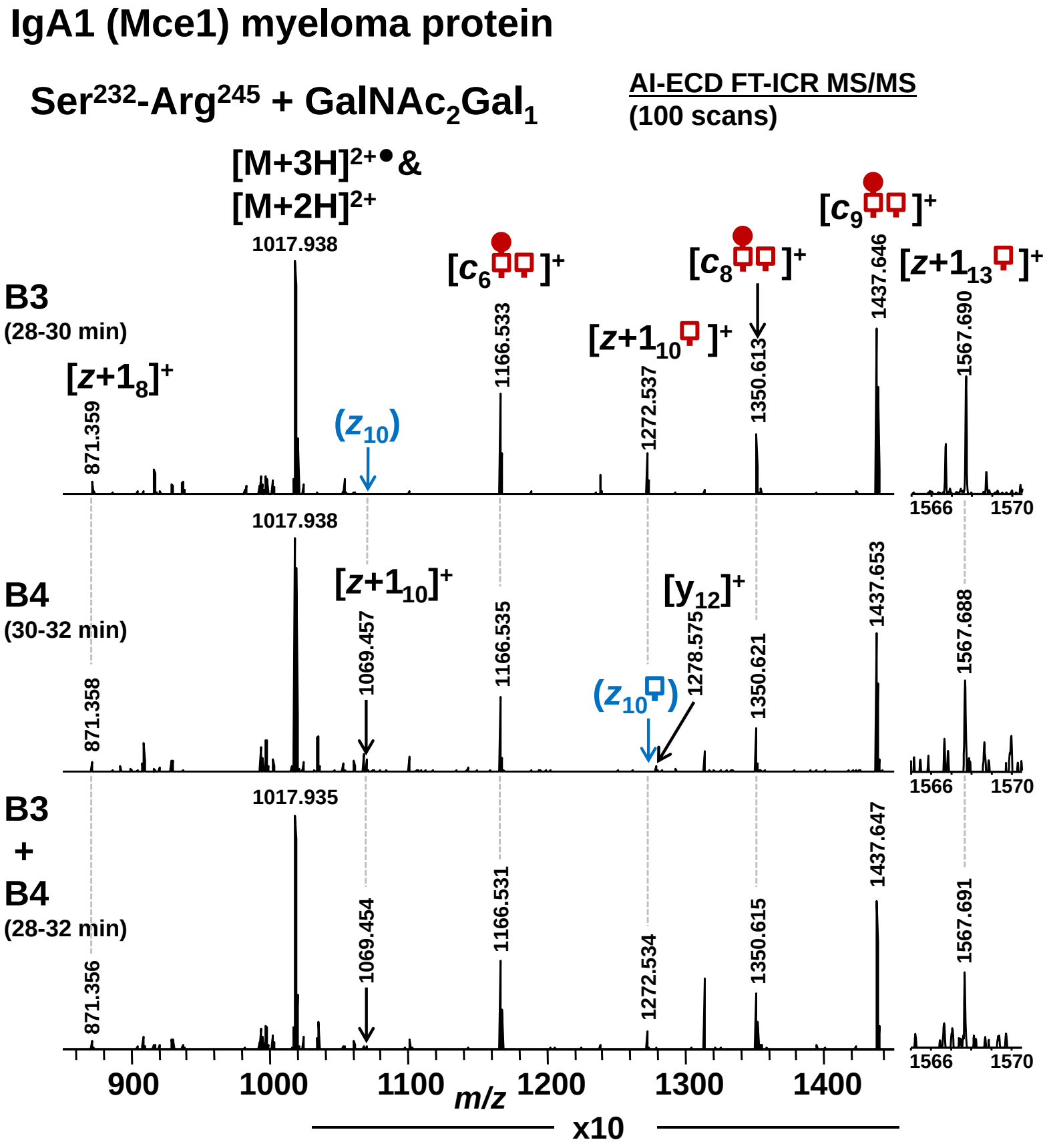
Ser^{232}-Arg^{245} + $GalNAc_1Gal_1$

B3 (28-30 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
765.353	1	765.351	c_4 + □ 1 ● 1	2.22
871.357	1	871.354	$z+1_8$	3.01
916.396	2	1831.784	M	0.56
963.452	1	963.452	c_6 + □ 1 ● 1	0.31
1069.455	1	1069.455	$z+1_{10}$	0.21
1147.534	1	1147.537	c_8 + □ 1 ● 1	-2.18
1234.565	1	1234.569	c_9 + □ 1 ● 1	-2.83
1337.575	1	1337.578	c_{10} + □ 1 ● 1	-2.02
1364.599	1	1364.608	$z+1_{13}$	-6.58
1440.577	1	1440.587	c_{11} + □ 1 ● 1	-6.59

B4 (30-32 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
765.349	1	765.351	c_4 + □ 1 ● 1	-2.48
871.355	1	871.354	$z+1_8$	0.71
916.394	2	1831.784	M	-1.63
963.451	1	963.452	c_6 + □ 1 ● 1	-0.73
1069.454	1	1069.455	$z+1_{10}$	-0.73
1147.534	1	1147.537	c_8 + □ 1 ● 1	-2.18
1234.564	1	1234.569	c_9 + □ 1 ● 1	-3.64
1337.584	1	1337.578	c_{10} + □ 1 ● 1	4.71
1364.604	1	1364.608	$z+1_{13}$	-2.92
1440.578	1	1440.587	c_{11} + □ 1 ● 1	-5.90


IgA1 (Mce1) myeloma protein
Ser232-Arg245 + GalNAc2Gal1
AI-ECD FT-ICR MS/MS
(100 scans)
[M+3H]2+• &
[M+2H]2+
1017.938
[c6]+
[c8]+
[c9]+
[z+113]+
1437.646
1567.690
[z+110]+
1166.533
1272.537
1350.613
[z+18]+
871.359
(z10)
B3
(28-30 min)
1566
1570
1017.938
[z+110]+
[y12]+
1437.653
1567.688
1069.457
1166.535
1278.575
1350.621
871.358
(z10)
B4
(30-32 min)
1566
1570
1017.935
1437.647
1567.691
1069.454
1166.531
1272.534
1350.615
871.356
B3
+
B4
(28-32 min)
1566
1570
900
1000
1100
m/z
1200
1300
1400
x10

Ser^{232}-Arg^{245} + $GalNAc_2Gal_1$

B3 (28-30 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
871.359	1	871.354	$z+1_8$	5.30
1017.938	2	2034.863	M	2.76
1166.533	1	1166.531	c_6 + □ 2 ● 1	1.63
1272.537	1	1272.534	$z+1_{10}$ + □ 1	2.22
1350.613	1	1350.616	c_8 + □ 2 ● 1	-2.15
1437.646	1	1437.648	c_9 + □ 2 ● 1	-1.32
1567.69	1	1567.687	$z+1_{13}$ + □ 1	1.67

B4 (30-32 min)

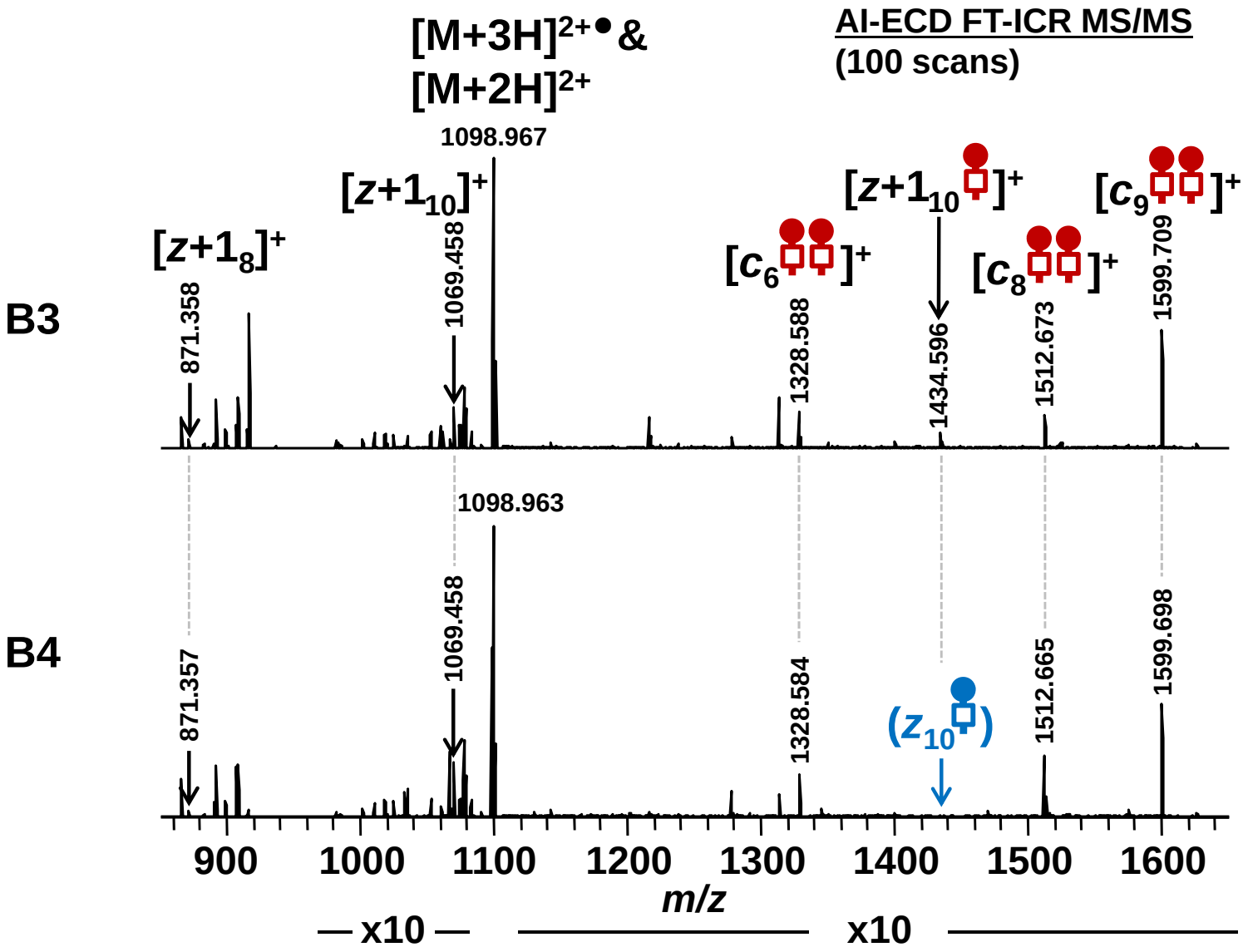
m/z	Charge	Theoretical MW	Assignment	Mass error
871.358	1	871.354	$z+1_8$	4.15
1017.938	2	2034.863	M	2.76
1069.457	1	1069.455	$z+1_{10}$	2.08
1166.535	1	1166.531	c_6 + □ 2 ● 1	3.34
1278.575	1	1278.572	y_{12}	2.50
1350.621	1	1350.616	c_8 + □ 2 ● 1	3.78
1437.653	1	1437.648	c_9 + □ 2 ● 1	3.55
1567.688	1	1567.687	$z+1_{13}$ + □ 1	0.40

B3 + B4 (28-32 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
871.356	1	871.354	$z+1_8$	1.86
1017.935	2	2034.863	M	-0.19
1069.454	1	1069.455	$z+1_{10}$	-0.73
1166.531	1	1166.531	c_6 + □ 2 ● 1	-0.09
1272.534	1	1272.534	$z+1_{10}$ + □ 1	-0.14
1350.615	1	1350.616	c_8 + □ 2 ● 1	-0.67
1437.647	1	1437.648	c_9 + □ 2 ● 1	-0.63
1567.691	1	1567.687	$z+1_{13}$ + □ 1	2.31

IgA1 (Mce1) myeloma protein

Ser^{232}-Arg^{245} + $GalNAc_2Gal_2$



Ser^{232}-Arg^{245} + $GalNAc_2Gal_2$

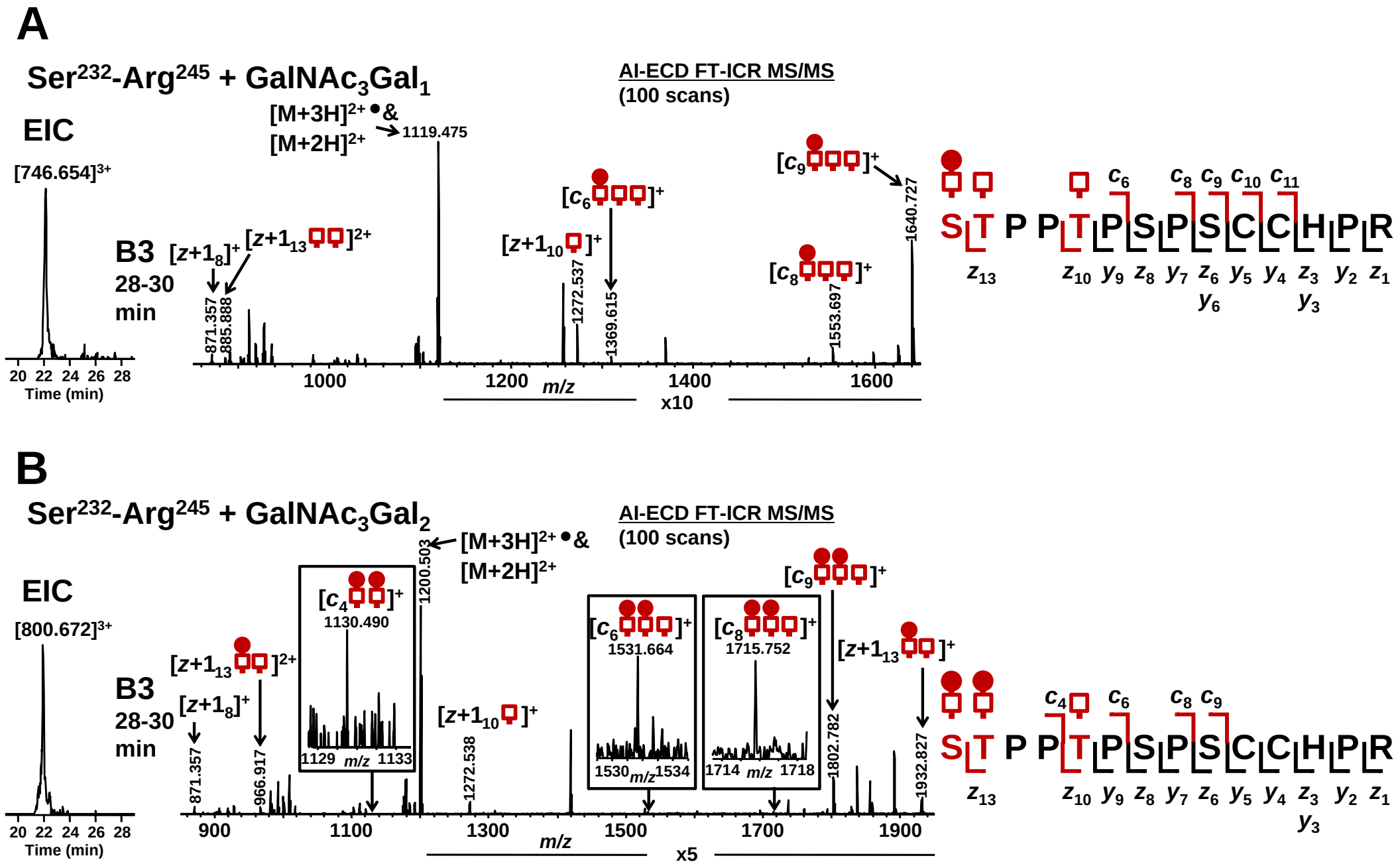
B3 (28-30 min)

m/z	Charge	Theoretical MW	Assignment			Mass error
871.358	1	871.354	$z+1_8$			4.15
1069.458	1	1069.455	$z+1_{10}$			3.01
1098.967	2	2196.916	M			4.93
1328.588	1	1328.584	c_6	+	□ 2 ● 2	3.09
1434.596	1	1434.587	$z+1_{10}$	+	□ 1 ● 1	5.94
1512.673	1	1512.669	c_8	+	□ 2 ● 2	2.84
1599.709	1	1599.701	c_9	+	□ 2 ● 2	5.19

B4 (30-32 min)

m/z	Charge	Theoretical MW	Assignment			Mass error
871.357	1	871.354	$z+1_8$			3.01
1069.458	1	1069.455	$z+1_{10}$			3.01
1098.963	2	2196.916	M			1.28
1328.584	1	1328.584	c_6	+	□ 2 ● 2	0.08
1512.665	1	1512.669	c_8	+	□ 2 ● 2	-2.45
1599.698	1	1599.701	c_9	+	□ 2 ● 2	-1.69

IgA1 (Mce1) myeloma protein



A

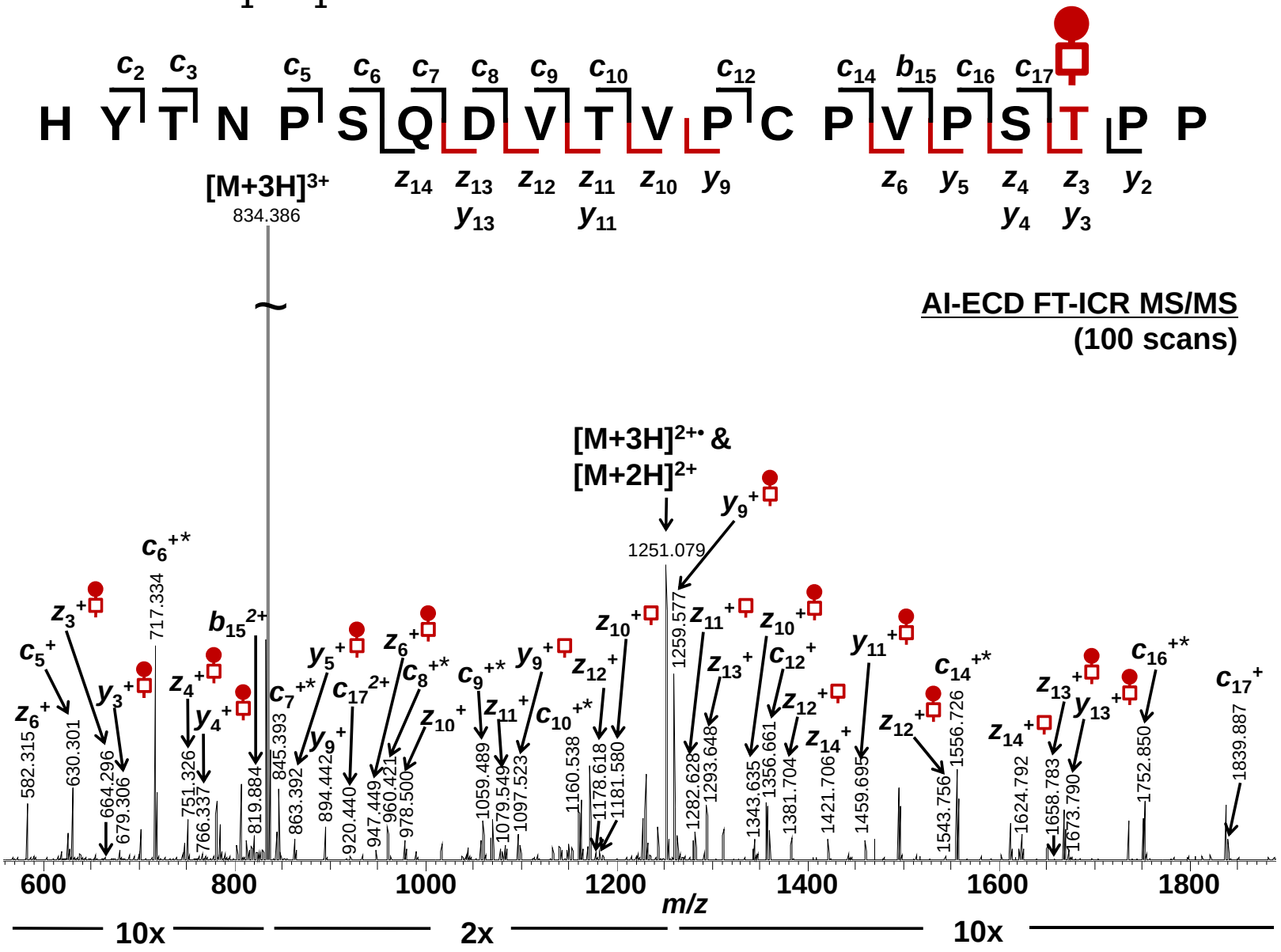
m/z	Charge	Theoretical MW	Assignment	Mass error
871.357	1	871.354	$z+1_8$	3.01
885.888	2	1770.767	$z+1_{13}$ + ☐ 2	1.10
1119.475	2	2237.943	M	0.10
1272.537	1	1272.534	$z+1_{10}$ + ☐ 1	2.22
1369.615	1	1369.611	c_6 + ☐ 3 ● 1	3.29
1553.697	1	1553.695	c_8 + ☐ 3 ● 1	1.09
1640.727	1	1640.727	c_9 + ☐ 3 ● 1	-0.18

B

m/z	Charge	Theoretical MW	Assignment	Mass error
871.357	1	871.354	$z+1_8$	3.01
966.917	2	1932.820	$z+1_{13}$ + ☐ 2 ● 1	3.69
1130.490	1	1130.484	c_4 + ☐ 2 ● 2	5.31
1200.503	2	2399.995	M	1.43
1272.538	1	1272.534	$z+1_{10}$ + ☐ 1	3.00
1531.664	1	1531.663	c_6 + ☐ 3 ● 2	0.46
1715.752	1	1715.748	c_8 + ☐ 3 ● 2	2.27
1802.782	1	1802.780	c_9 + ☐ 3 ● 2	1.05
1932.827	1	1932.820	$z+1_{13}$ + ☐ 2 ● 1	3.68

IgA1 (Mce1) myeloma protein

His^{208}-Pro^{227} + $GalNAc_1Gal_1$

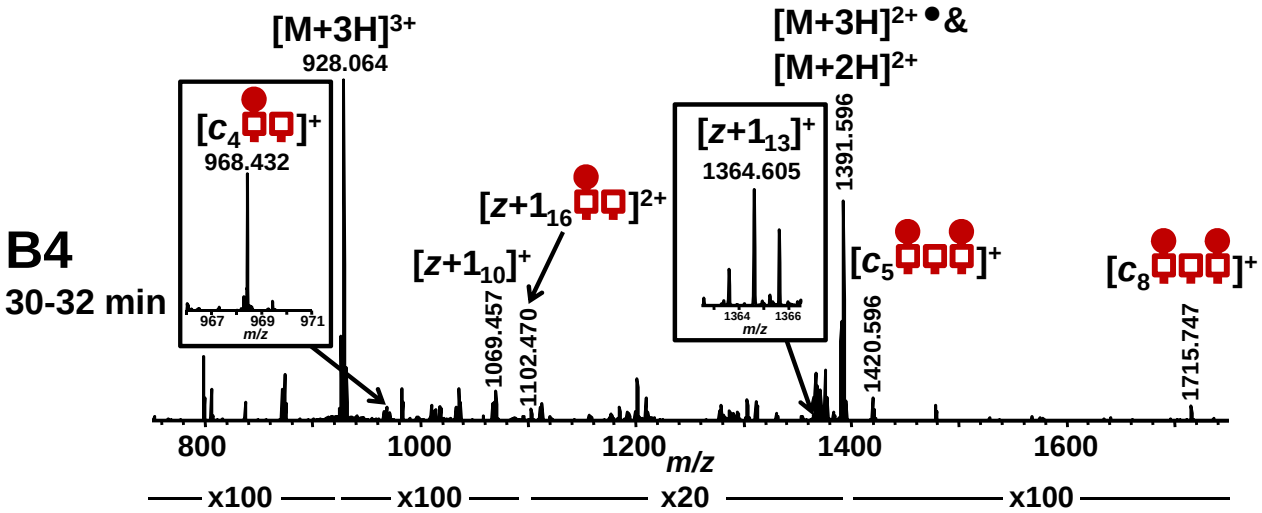


*Mixture of *c* and *c*-1 fragments were observed.

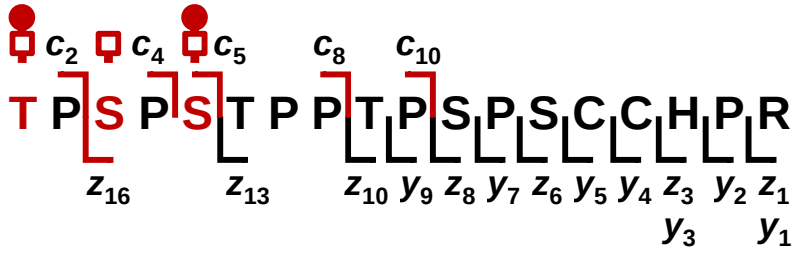
IgA1 (Mce1) myeloma protein

Thr^{228}-Arg^{245} + GalNAc$_3$Gal$_2$

AI-ECD FT-ICR MS/MS
(100 scans)



B4
30-32 min



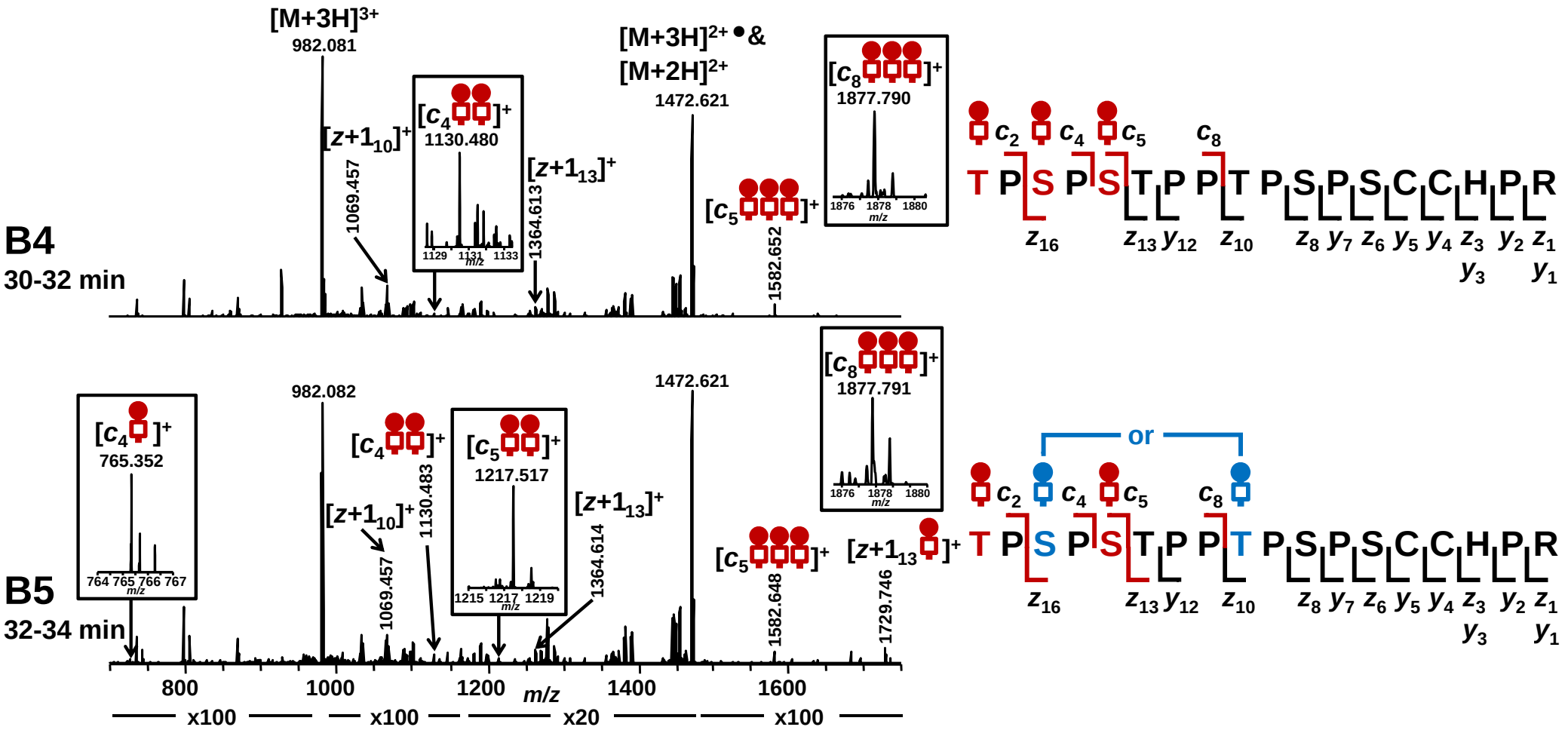
Thr^{228}-Arg^{245} + $GalNAc_3Gal_2$

B4 (30-32 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
968.432	1	968.431	c_4 + □ 2 ● 1	1.34
928.064	3	2782.181	M	-1.10
1069.457	1	1069.455	$z+1_{10}$	2.08
1102.470	2	2203.936	$z+1_{16}$ + □ 2 ● 1	-1.71
1364.605	1	1364.608	$z+1_{13}$	-2.18
1391.596	2	2782.181	M	1.52
1420.596	1	1420.595	c_5 + □ 3 ● 2	0.77
1715.747	1	1715.748	c_8 + □ 3 ● 2	-0.64

IgA1 (Mce1) myeloma protein

Thr^{228}-Arg^{245} + $GalNAc_3Gal_3$



Thr^{228}-Arg^{245} + $GalNAc_3Gal_3$

B4 (30-32 min)

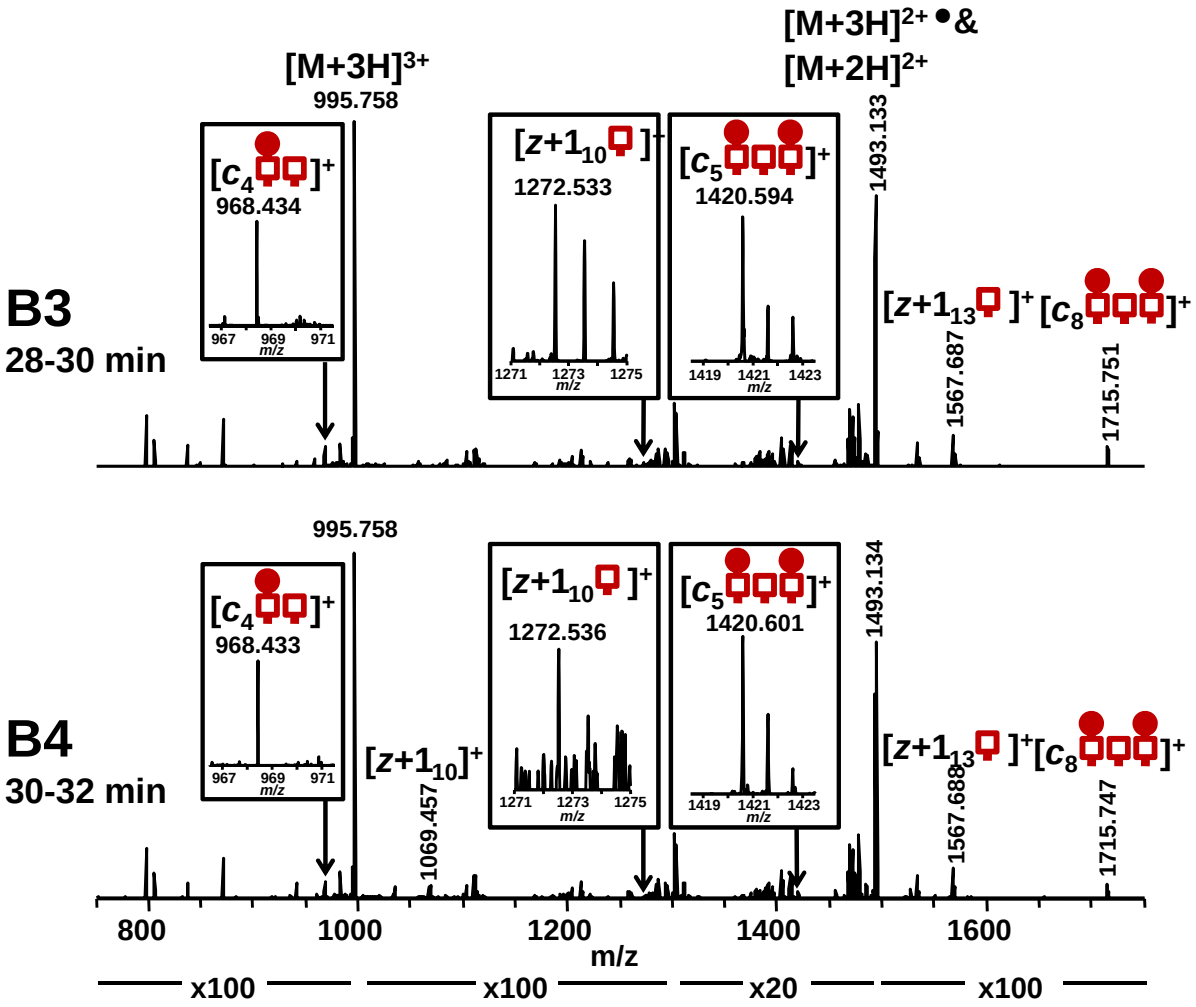
m/z	Charge	Theoretical MW	Assignment	Mass error
982.081	3	2944.233	M	-1.65
1069.457	1	1069.455	$z+1_{10}$	2.08
1130.480	1	1130.484	c_4 + □ 2 ● 2	-3.10
1364.613	1	1364.608	$z+1_{13}$	3.68
1472.621	2	2944.233	M	0.48
1582.652	1	1582.648	c_5 + □ 3 ● 3	2.72
1877.790	1	1877.801	c_8 + □ 3 ● 3	-5.80

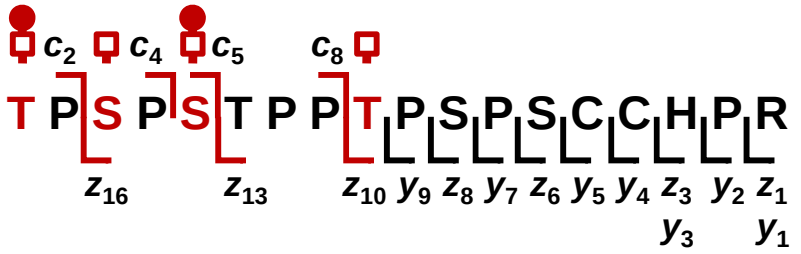
B5 (32-34 min)

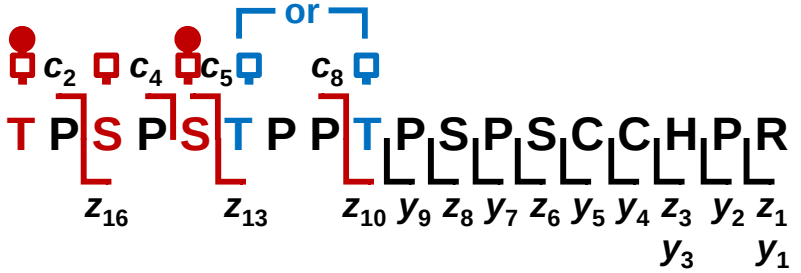
m/z	Charge	Theoretical MW	Assignment	Mass error
765.352	1	765.351	*c*4 + □ 1 ● 1	0.91
982.082	3	2944.233	M	-0.63
1069.457	1	1069.455	$z+1_{10}$	2.08
1130.483	1	1130.484	c_4 + □ 2 ● 2	-0.44
1217.517	1	1217.516	c_5 + □ 2 ● 2	1.23
1364.614	1	1364.608	$z+1_{13}$	4.41
1472.621	2	2944.233	M	0.48
1582.648	1	1582.648	c_5 + □ 3 ● 3	0.13
1729.746	1	1729.740	$z+1_{13}$ + □ 1 ● 1	3.36
1877.791	1	1877.801	c_8 + □ 3 ● 3	-5.27

IgA1 (Mce1) myeloma protein

Thr^{228}-Arg^{245} + $GalNAc_4Gal_2$







Thr^{228}-Arg^{245} + $GalNAc_4Gal_2$

B3 (28-30 min)

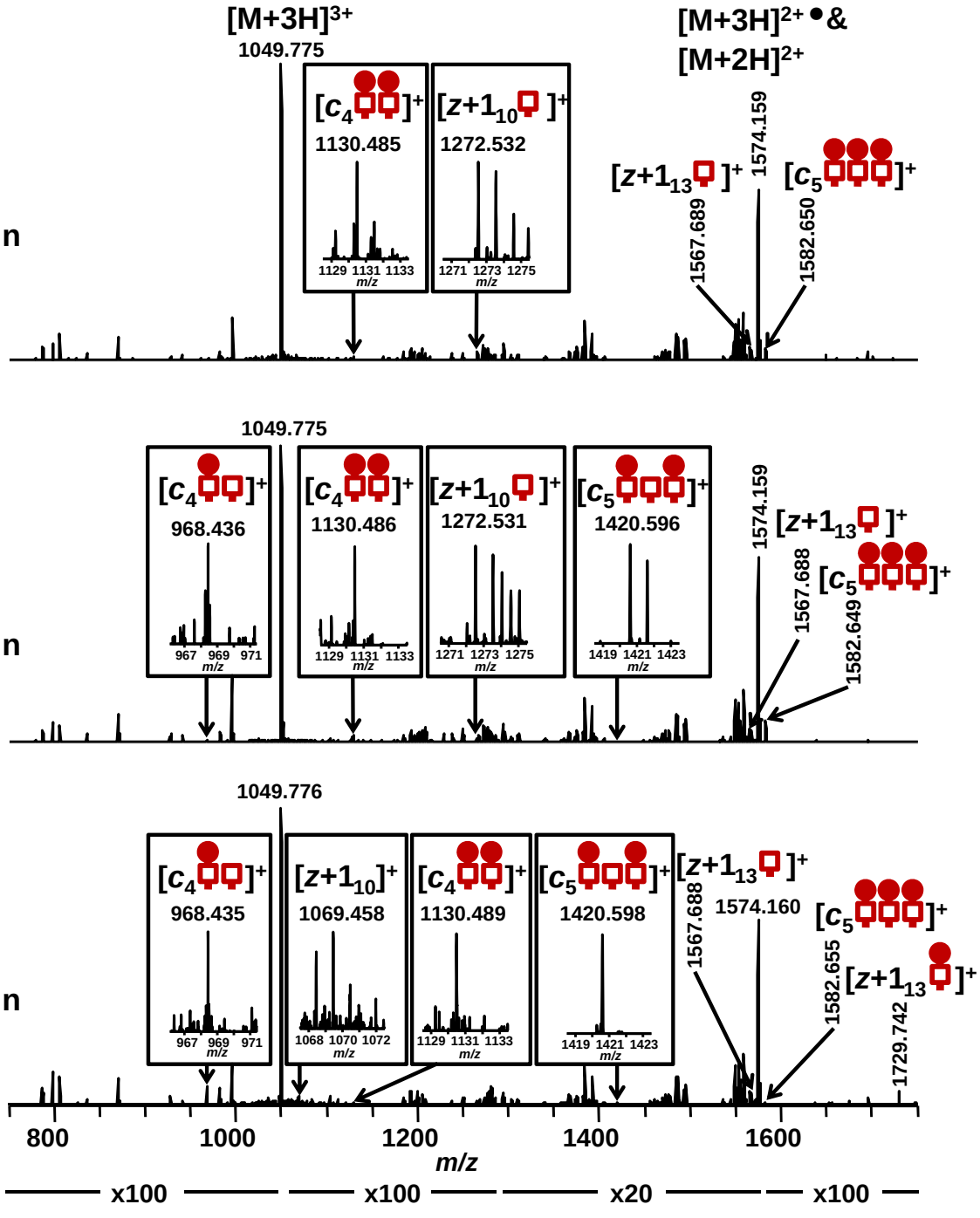
m/z	Charge	Theoretical MW	Assignment	Mass error
968.434	1	968.431	c_4 + ☐ 2 ● 1	3.41
995.759	3	2985.260	M	0.85
1272.533	1	1272.534	$z+1_{10}$ + ☐ 1	-0.93
1420.594	1	1420.595	c_5 + ☐ 3 ● 2	-0.63
1493.133	2	2985.260	M	-0.40
1567.687	1	1567.687	$z+1_{13}$ + ☐ 1	-0.24
1715.751	1	1715.748	c_8 + ☐ 3 ● 2	1.69

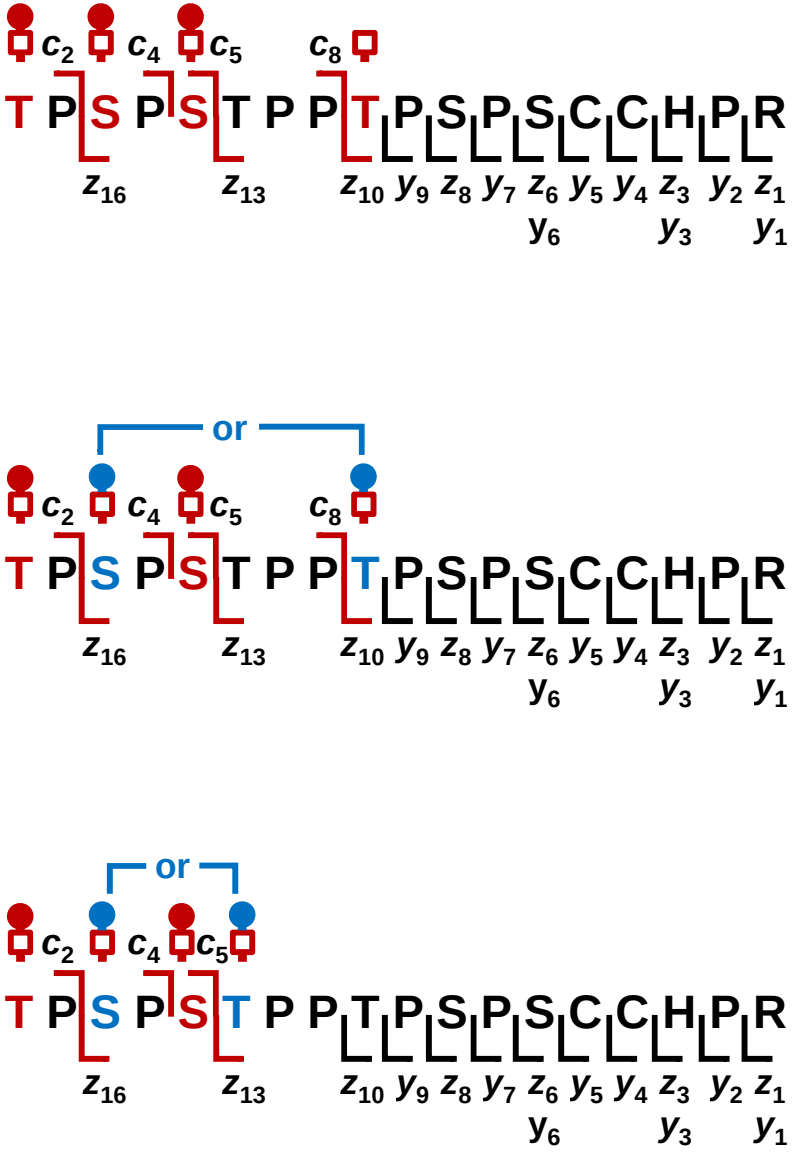
B4 (30-32 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
968.433	1	968.431	c_4 + ☐ 2 ● 1	2.37
995.758	3	2985.260	M	-0.15
1069.457	1	1069.455	$z+1_{10}$	2.08
1272.536	1	1272.534	$z+1_{10}$ + ☐ 1	1.43
1420.601	1	1420.595	c_5 + ☐ 3 ● 2	4.29
1493.134	2	2985.260	M	0.27
1567.688	1	1567.687	$z+1_{13}$ + ☐ 1	0.40
1715.747	1	1715.748	c_8 + ☐ 3 ● 2	-0.64

IgA1 (Mce1) myeloma protein

Thr^{228}-Arg^{245} + $GalNAc_4Gal_3$





Thr^{228}-Arg^{245} + $GalNAc_4Gal_3$

B2 (26-28 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
1049.775	3	3147.313	M	-0.72
1130.485	1	1130.484	c_4 + □ 2 ● 2	1.33
1272.532	1	1272.534	$z+1_{10}$ + □ 1	-1.71
1567.689	1	1567.687	$z+1_{13}$ + □ 1	1.03
1574.159	2	3147.313	M	-0.63
1582.650	1	1582.648	c_5 + □ 3 ● 3	1.45

B3 (28-30 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
968.436	1	968.431	c_4 + □ 2 ● 1	5.47
1049.775	3	3147.313	M	-0.72
1130.486	1	1130.484	c_4 + □ 2 ● 2	2.21
1272.531	1	1272.534	$z+1_{10}$ + □ 1	-2.50
1420.596	1	1420.595	c_5 + □ 3 ● 2	0.77
1567.688	1	1567.687	$z+1_{13}$ + □ 1	0.40
1574.159	2	3147.313	M	-0.63
1582.649	1	1582.648	c_5 + □ 3 ● 3	0.82

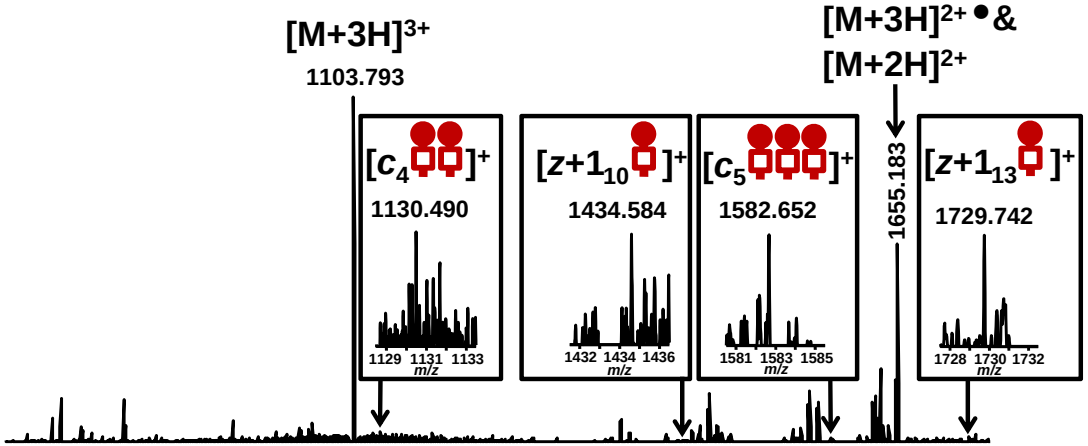
B4 (30-32 min)

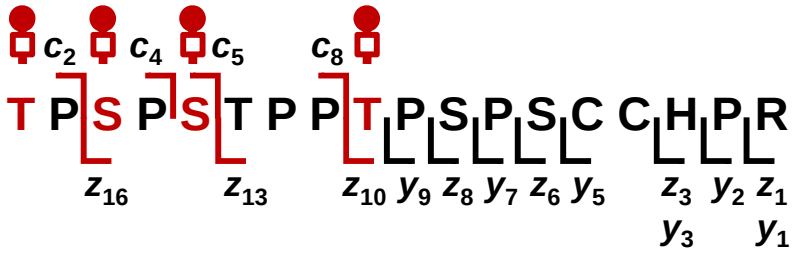
m/z	Charge	Theoretical MW	Assignment	Mass error
968.435	1	968.431	c_4 + □ 2 ● 1	4.44
1049.776	3	3147.313	M	0.24
1069.458	1	1069.455	$z+1_{10}$	3.01
1130.489	1	1130.484	c_4 + □ 2 ● 2	4.87
1420.598	1	1420.595	c_5 + □ 3 ● 2	2.18
1567.688	1	1567.687	$z+1_{13}$ + □ 1	0.40
1574.160	2	3147.313	M	0.01
1582.655	1	1582.648	c_5 + □ 3 ● 3	4.61
1729.742	1	1729.740	$z+1_{13}$ + □ 1 ● 1	1.05

IgA1 (Mce1) myeloma protein

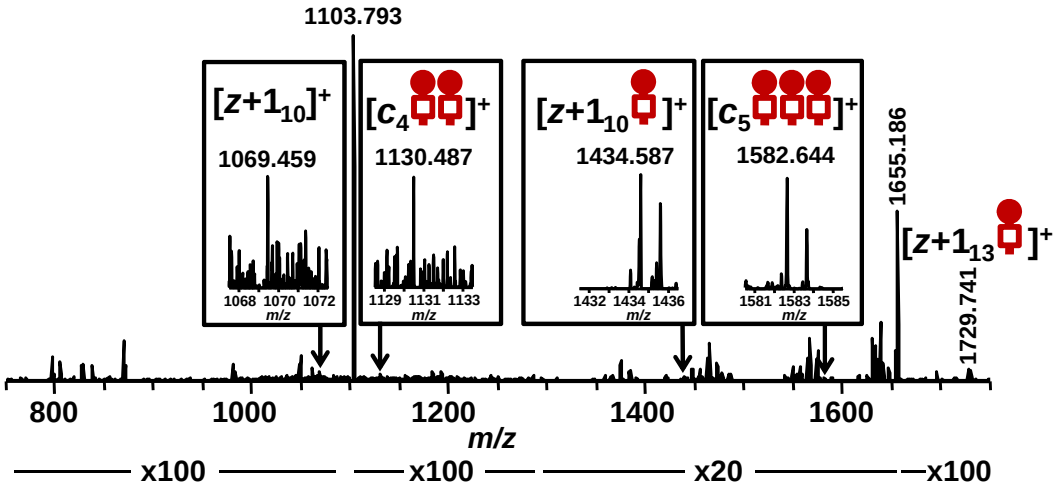
Thr^{228}-Arg^{245} + $GalNAc_4Gal_4$

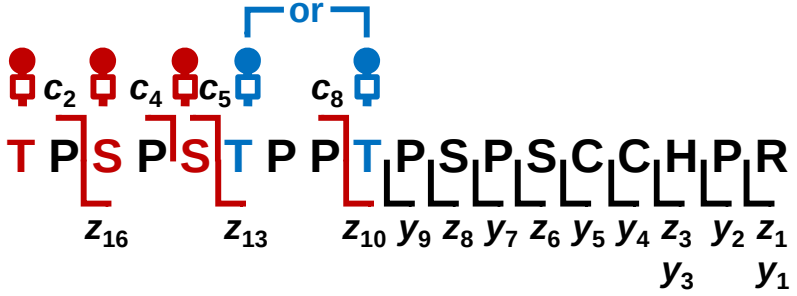
B2
26-28 min





B3
28-30 min





Thr^{228}-Arg^{245} + $GalNAc_4Gal_4$

B2 (26-28 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
1103.793	3	3309.366	M	-0.32
1130.490	1	1130.484	c_4 + □ 2 ● 2	5.75
1434.584	1	1434.587	$z+1_{10}$ + □ 1 ● 1	-2.08
1582.652	1	1582.648	c_5 + □ 3 ● 3	2.72
1655.183	2	3309.366	M	-2.05
1729.742	1	1729.740	$z+1_{13}$ + □ 1 ● 1	1.05

B3 (28-30 min)

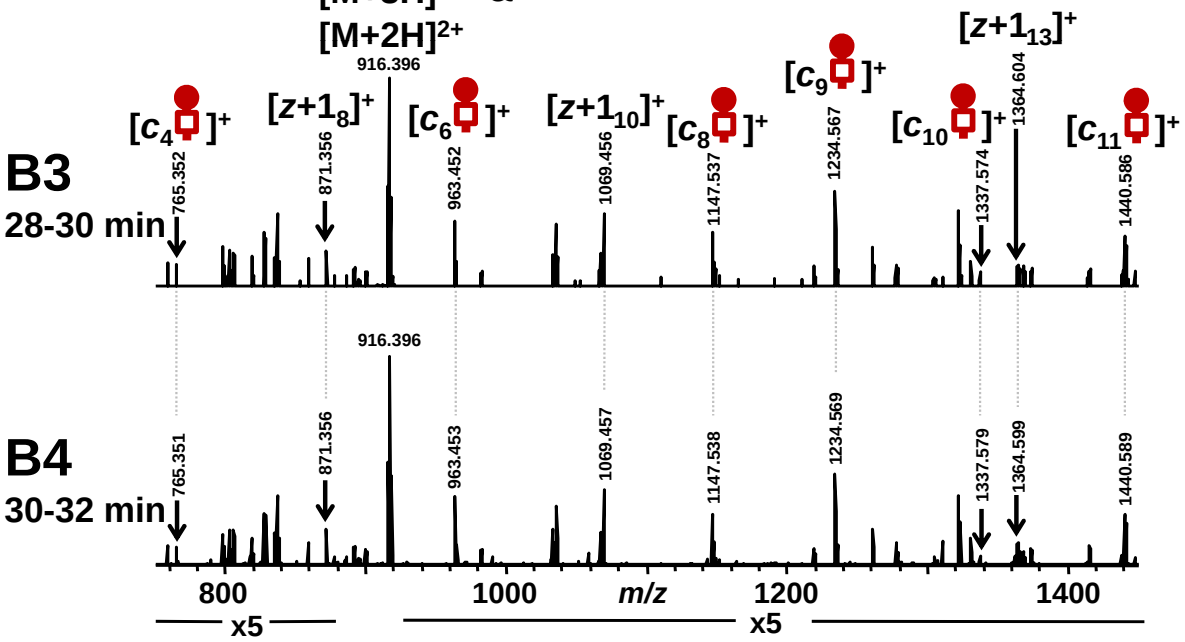
m/z	Charge	Theoretical MW	Assignment	Mass error
1069.459	1	1069.455	$z+1_{10}$	3.95
1103.793	3	3309.366	M	-0.32
1130.487	1	1130.484	c_4 + □ 2 ● 2	3.10
1434.587	1	1434.587	$z+1_{10}$ + □ 1 ● 1	0.01
1582.644	1	1582.648	c_5 + □ 3 ● 3	-2.34
1655.186	2	3309.366	M	-0.24
1729.741	1	1729.740	$z+1_{13}$ + □ 1 ● 1	0.47

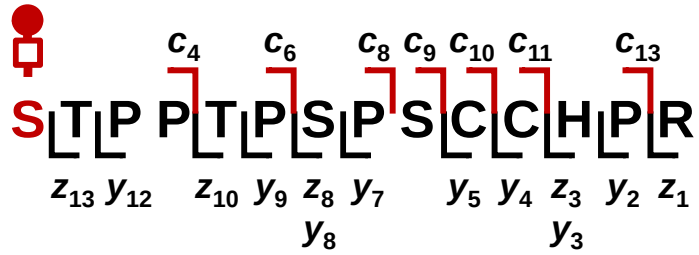
Normal human IgA1

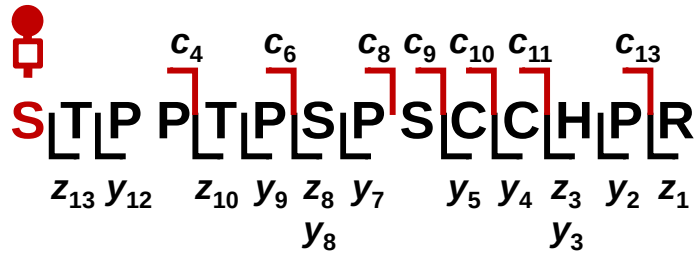
Ser^{232}-Arg^{245} + $GalNAc_1Gal_1$

AI-ECD FT-ICR MS/MS
(100 scans)

$[M+3H]^{2+}$•&
$[M+2H]^{2+}$



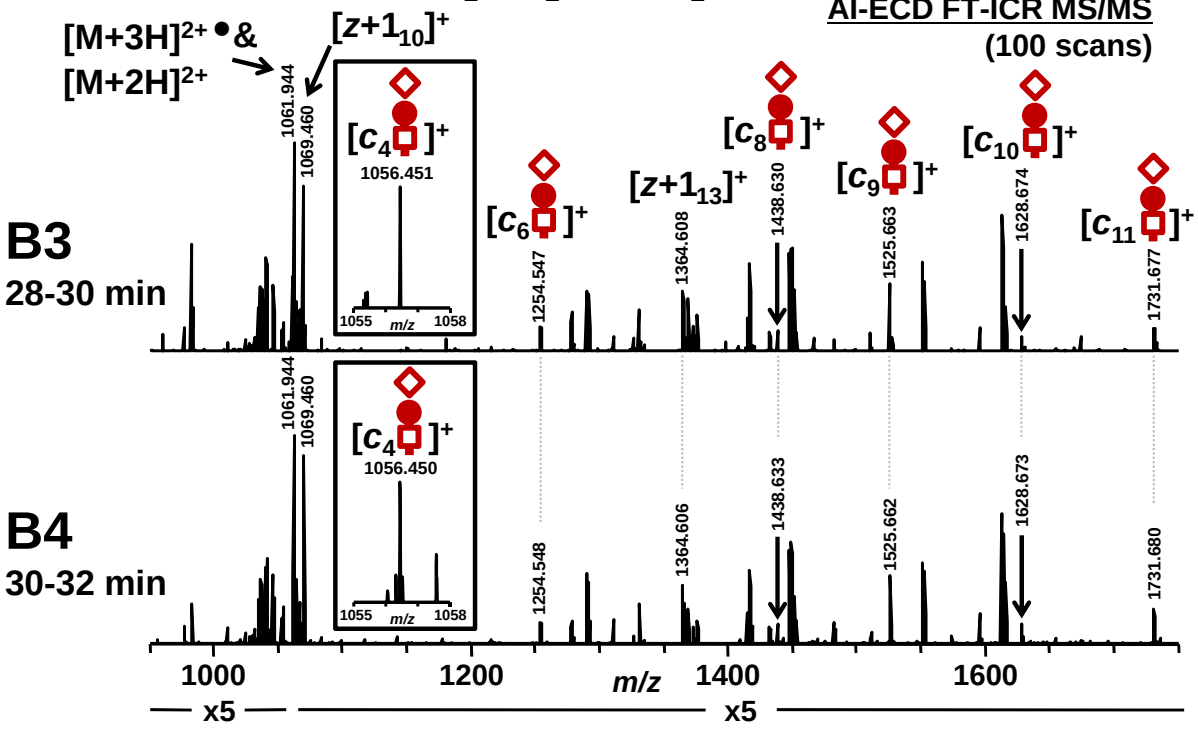


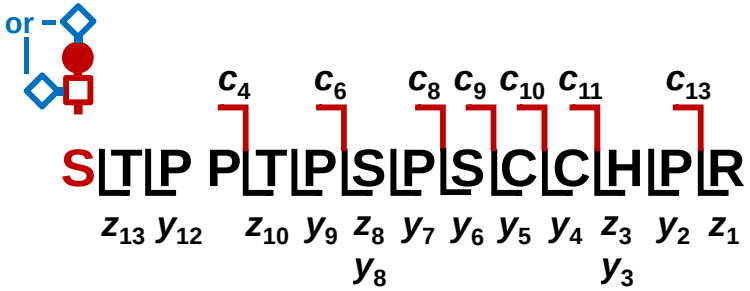


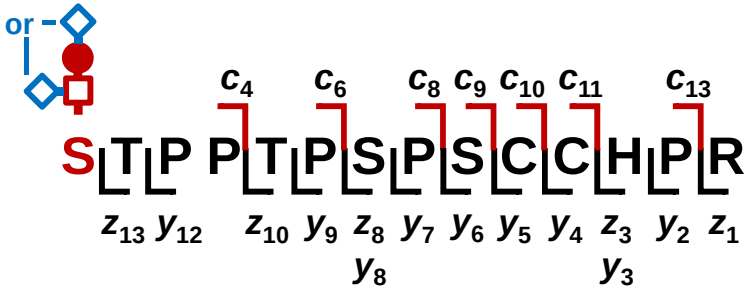
Ser^{232}-Arg^{245} + $GalNAc_1Gal_1NeuAc_1$

AI-ECD FT-ICR MS/MS
(100 scans)

$[M+3H]^{2+}$•&
$[M+2H]^{2+}$
$[z+1_{10}]^+$







Ser^{232}-Arg^{245} + $GalNAc_1Gal_1$

B3 (28-30 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
765.352	1	765.351	c_4	+ □ 1 ● 1	0.91
871.356	1	871.354	$z+1_8$		1.86
916.396	2	1831.784	M		0.56
963.452	1	963.452	c_6	+ □ 1 ● 1	0.31
1069.456	1	1069.455	$z+1_{10}$		1.14
1147.537	1	1147.537	c_8	+ □ 1 ● 1	0.44
1234.567	1	1234.569	c_9	+ □ 1 ● 1	-1.21
1337.574	1	1337.578	c_{10}	+ □ 1 ● 1	-2.77
1364.604	1	1364.608	$z+1_{13}$		-2.92
1440.586	1	1440.587	c_{11}	+ □ 1 ● 1	-0.62

B4 (30-32 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
765.351	1	765.351	c_4	+ □ 1 ● 1	-0.39
871.356	1	871.354	$z+1_8$		1.86
916.396	2	1831.784	M		0.56
963.453	1	963.452	c_6	+ □ 1 ● 1	1.35
1069.457	1	1069.455	$z+1_{10}$		2.08
1147.538	1	1147.537	c_8	+ □ 1 ● 1	1.31
1234.569	1	1234.569	c_9	+ □ 1 ● 1	0.40
1337.579	1	1337.578	c_{10}	+ □ 1 ● 1	0.97
1364.599	1	1364.608	$z+1_{13}$		-6.29
1440.589	1	1440.587	c_{11}	+ □ 1 ● 1	1.46

Ser^{232}-Arg^{245} + $GalNAc_1Gal_1NeuAc_1$

B3 (28-30 min)

m/z	Charge	Theoretical MW	Assignment		Mass error
1056.451	1	1056.447	c_4	+ □ 1 ● 1 ◇ 1	4.07
1061.944	2	2122.879	M		0.76
1069.460	1	1069.455	$z+1_{10}$		4.88
1254.547	1	1254.547	c_6	+ □ 1 ● 1 ◇ 1	-0.08
1364.608	1	1364.608	$z+1_{13}$		0.01
1438.630	1	1438.632	c_8	+ □ 1 ● 1 ◇ 1	-1.32
1525.663	1	1525.664	c_9	+ □ 1 ● 1 ◇ 1	-0.59
1628.674	1	1628.673	c_{10}	+ □ 1 ● 1 ◇ 1	0.55
1731.677	1	1731.682	c_{11}	+ □ 1 ● 1 ◇ 1	-3.06

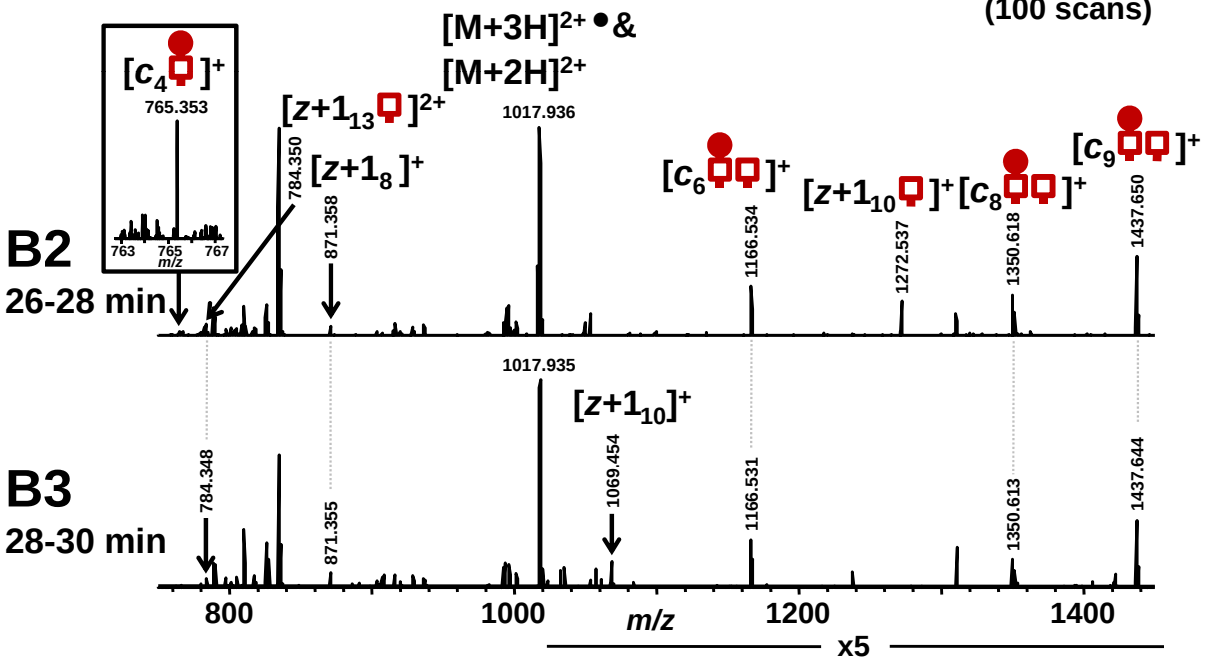
B4 (30-32 min)

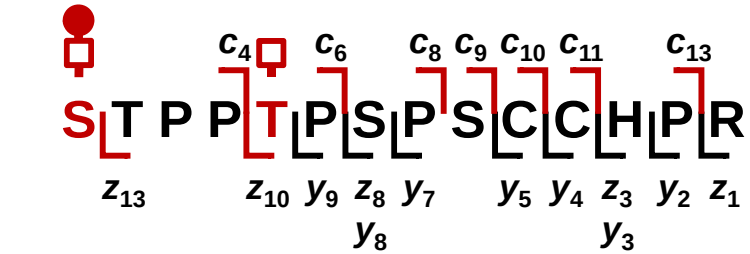
m/z	Charge	Theoretical MW	Assignment		Mass error
1056.450	1	1056.447	c_4	+ □ 1 ● 1 ◇ 1	3.12
1061.944	2	2122.879	M		0.76
1069.460	1	1069.455	$z+1_{10}$		4.88
1254.548	1	1254.547	c_6	+ □ 1 ● 1 ◇ 1	0.72
1364.606	1	1364.608	$z+1_{13}$		-1.45
1438.633	1	1438.632	c_8	+ □ 1 ● 1 ◇ 1	0.76
1525.662	1	1525.664	c_9	+ □ 1 ● 1 ◇ 1	-1.25
1628.673	1	1628.673	c_{10}	+ □ 1 ● 1 ◇ 1	-0.06
1731.680	1	1731.682	c_{11}	+ □ 1 ● 1 ◇ 1	-1.33

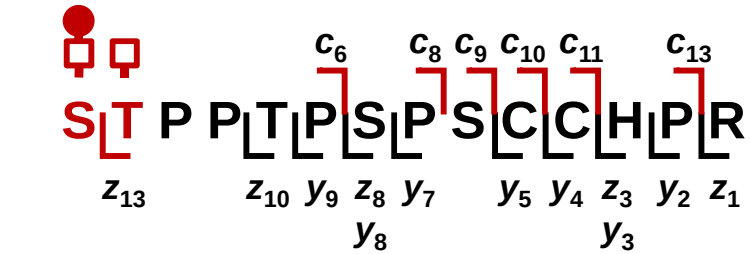
Normal human IgA1

Ser^{232}-Arg^{245} + $GalNAc_2Gal_1$

AI-ECD FT-ICR MS/MS
(100 scans)

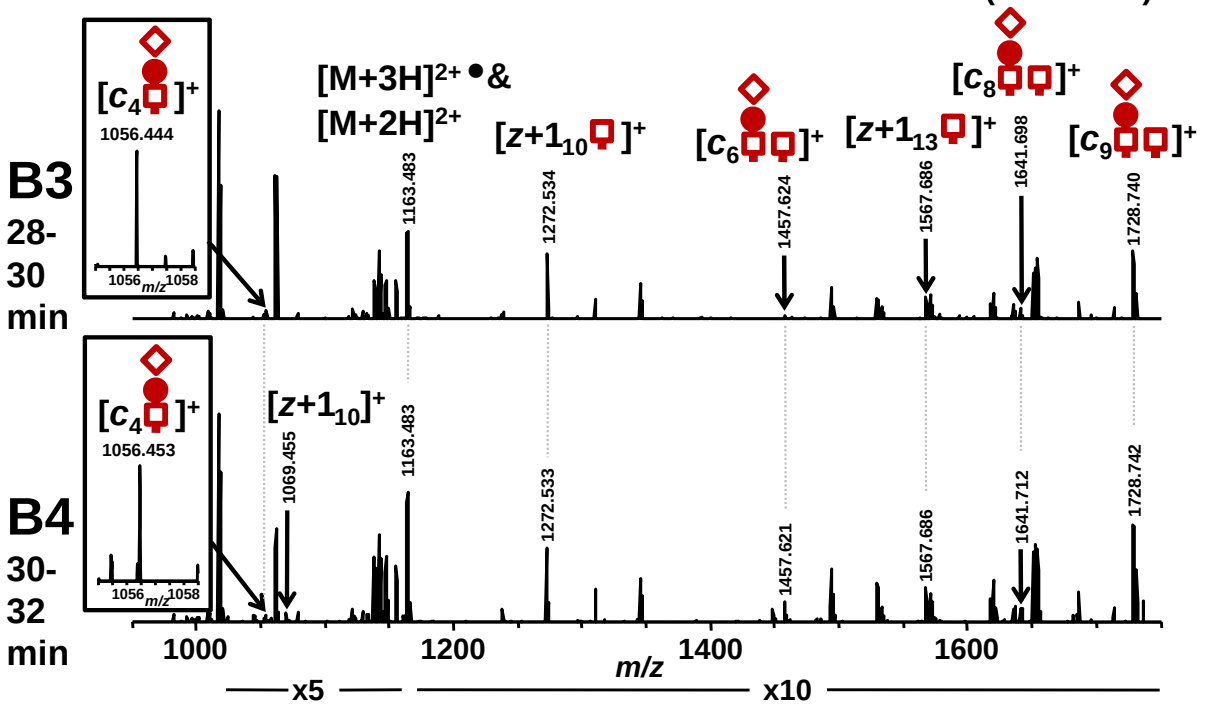


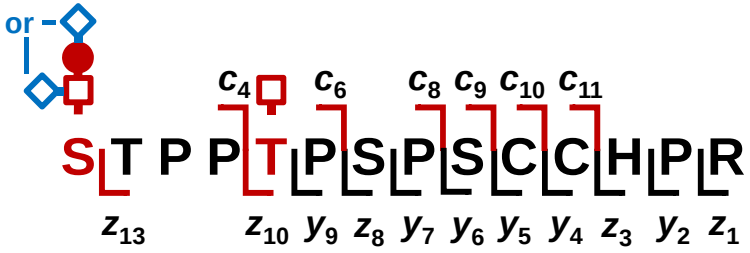


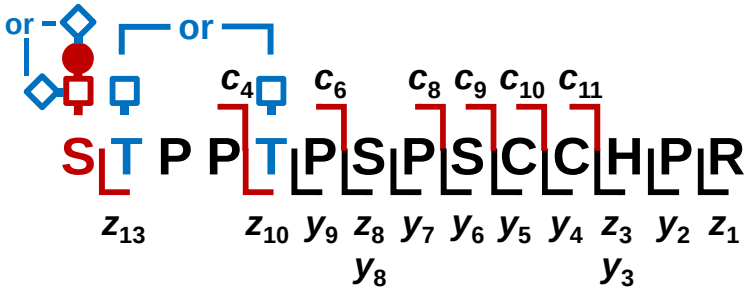


Ser^{232}-Arg^{245} + $GalNAc_2Gal_1NeuAc_1$

AI-ECD FT-ICR MS/MS
(100 scans)







Ser^{232}-Arg^{245} + $GalNAc_2Gal_1$

B2 (26-28 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
765.353	1	765.351	c_4	+ □ 1 ● 1	2.22
784.350	2	1567.687	$z+1_{13}$	+ □ 1	3.41
871.358	1	871.354	$z+1_8$		4.15
1017.936	2	2034.863	M		0.80
1166.534	1	1166.531	c_6	+ □ 2 ● 1	2.49
1272.537	1	1272.534	$z+1_{10}$	+ □ 1	2.22
1350.618	1	1350.616	c_8	+ □ 2 ● 1	1.55
1437.650	1	1437.648	c_9	+ □ 2 ● 1	1.46

B3 (28-30 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
784.348	2	1567.687	$z+1_{13}$	+ □ 1	0.85
871.355	1	871.354	$z+1_8$		0.71
1017.935	2	2034.863	M		-0.19
1069.454	1	1069.455	$z+1_{10}$		-0.73
1166.531	1	1166.531	c_6	+ □ 2 ● 1	-0.09
1350.613	1	1350.616	c_8	+ □ 2 ● 1	-2.15
1437.644	1	1437.648	c_9	+ □ 2 ● 1	-2.71

Ser^{232}-Arg^{245} + $GalNAc_2Gal_1NeuAc_1$

B3 (28-30 min)

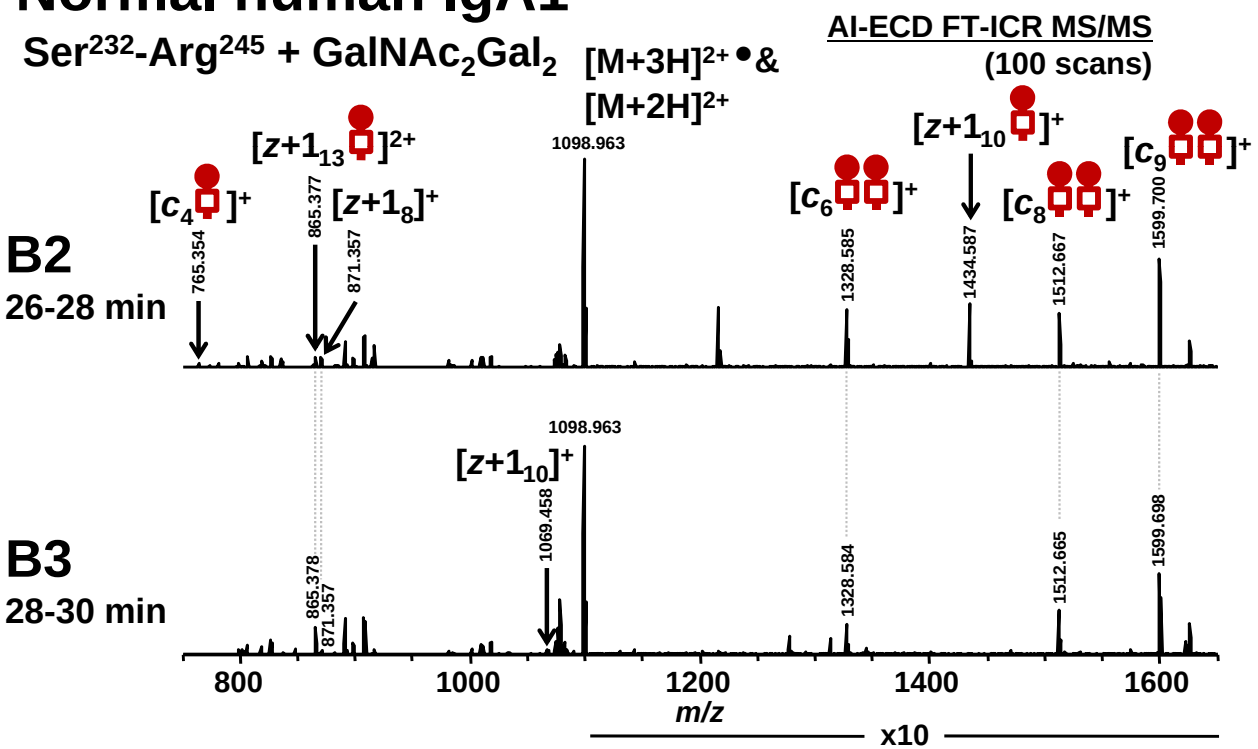
m/z	Charge	Theoretical MW		Assignment	Mass error
1056.444	1	1056.447	c_4	+ □ 1 ● 1 ◇ 1	-2.56
1163.483	2	2325.959	M		0.09
1272.534	1	1272.534	$z+1_{10}$	+ □ 1	-0.14
1457.624	1	1457.627	c_6	+ □ 2 ● 1 ◇ 1	-1.72
1567.686	1	1567.687	$z+1_{13}$	+ □ 1	-0.88
1641.698	1	1641.711	c_8	+ □ 2 ● 1 ◇ 1	-8.10
1728.740	1	1728.743	c_9	+ □ 2 ● 1 ◇ 1	-1.91

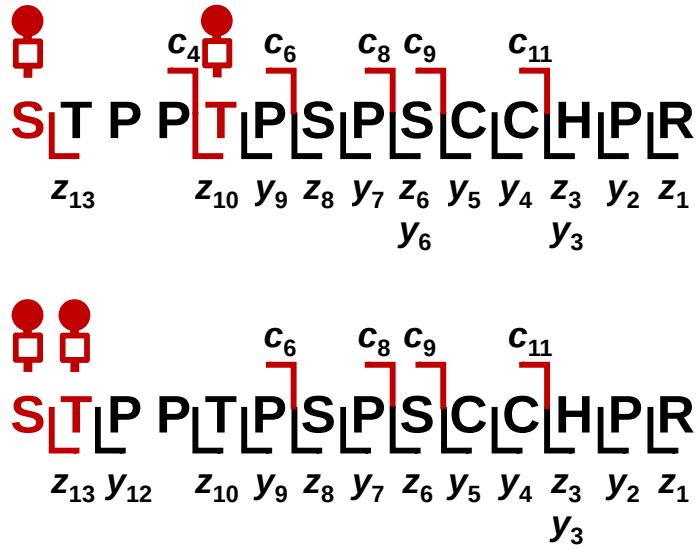
B4 (30-32 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
1056.453	1	1056.447	c_4	+ □ 1 ● 1 ◇ 1	5.96
1069.455	1	1069.455	$z+1_{10}$		0.21
1163.483	2	2325.959	M		0.09
1272.533	1	1272.534	$z+1_{10}$	+ □ 1	-0.93
1457.621	1	1457.627	c_6	+ □ 2 ● 1 ◇ 1	-3.77
1567.686	1	1567.687	$z+1_{13}$	+ □ 1	-0.88
1641.712	1	1641.711	c_8	+ □ 2 ● 1 ◇ 1	0.43
1728.742	1	1728.743	c_9	+ □ 2 ● 1 ◇ 1	-0.75

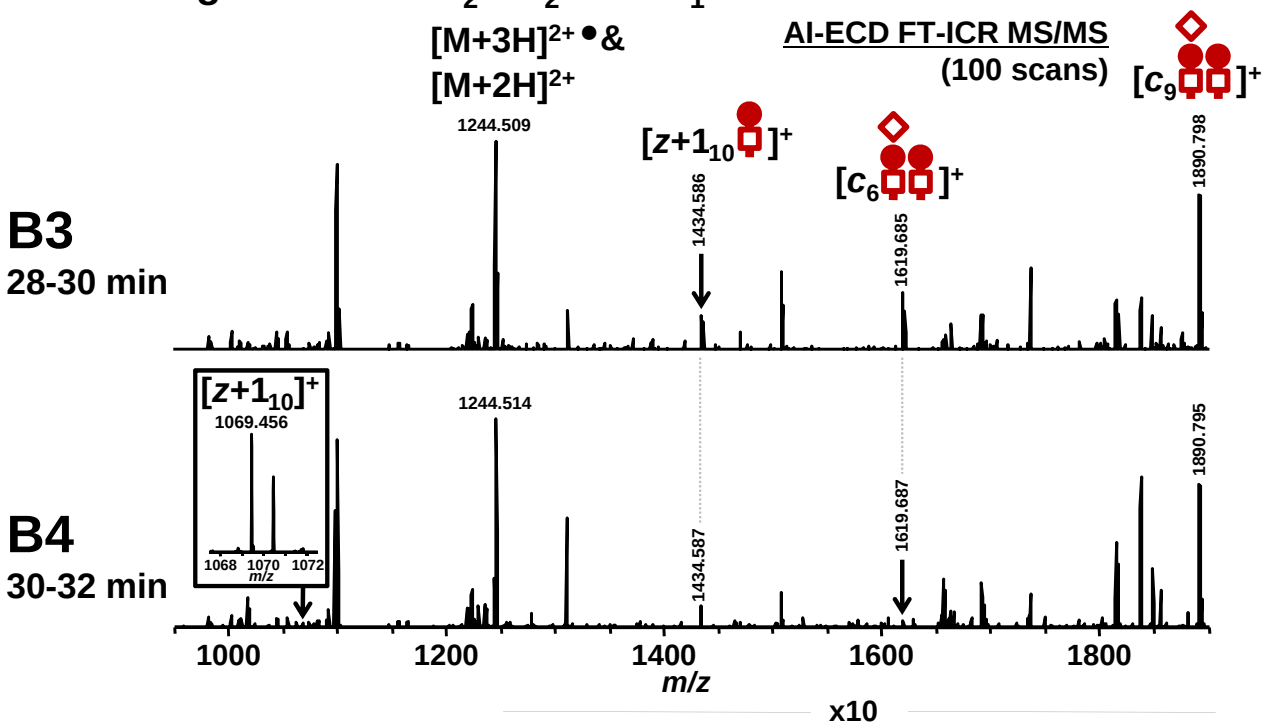
Normal human IgA1

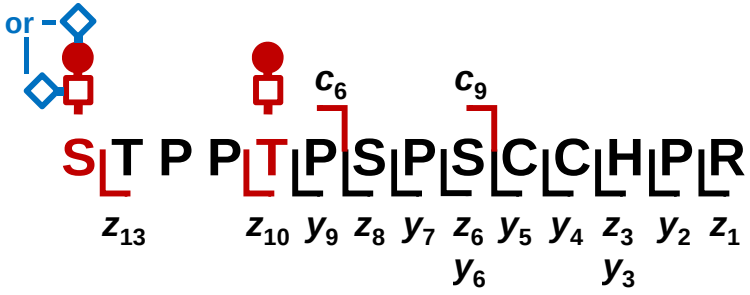
Ser^{232}-Arg^{245} + $GalNAc_2Gal_2$

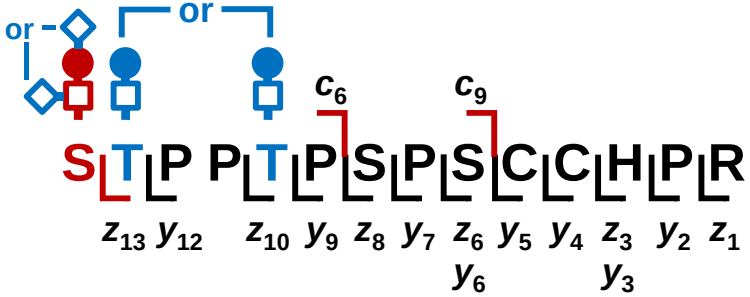




Ser^{232}-Arg^{245} + $GalNAc_2Gal_2NeuAc_1$







Ser^{232}-Arg^{245} + $GalNAc_2Gal_2$

B2 (26-28 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
765.354	1	765.351	c_4	+ □ 1 ● 1	3.53
865.377	2	1729.740	$z+1_{13}$	+ □ 1 ● 1	3.78
871.357	1	871.354	$z+1_8$		3.01
1098.963	2	2196.916	M		1.28
1328.585	1	1328.584	c_6	+ □ 2 ● 2	0.83
1434.587	1	1434.587	$z+1_{10}$	+ □ 1 ● 1	0.01
1512.667	1	1512.669	c_8	+ □ 2 ● 2	-1.12
1599.700	1	1599.701	c_9	+ □ 2 ● 2	-0.44

B3 (28-30 min)

m/z	Charge	Theoretical MW		Assignment	Mass error
865.378	2	1729.740	$z+1_{13}$	+ □ 1 ● 1	4.94
871.357	1	871.354	$z+1_8$		3.01
1069.458	1	1069.455	$z+1_{10}$		3.01
1098.963	2	2196.916	M		1.28
1328.584	1	1328.584	c_6	+ □ 2 ● 2	0.08
1512.665	1	1512.669	c_8	+ □ 2 ● 2	-2.45
1599.698	1	1599.701	c_9	+ □ 2 ● 2	-1.69

Ser^{232}-Arg^{245} + $GalNAc_2Gal_2NeuAc_1$

B3 (28-30 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
1244.509	2	2488.011	M	-0.23
1434.586	1	1434.587	$z+1_{10}$ + □ 1 ● 1	-0.68
1619.685	1	1619.679	c_6 + □ 2 ● 2 ◇ 1	3.52
1890.798	1	1890.796	c_9 + □ 2 ● 2 ◇ 1	1.00

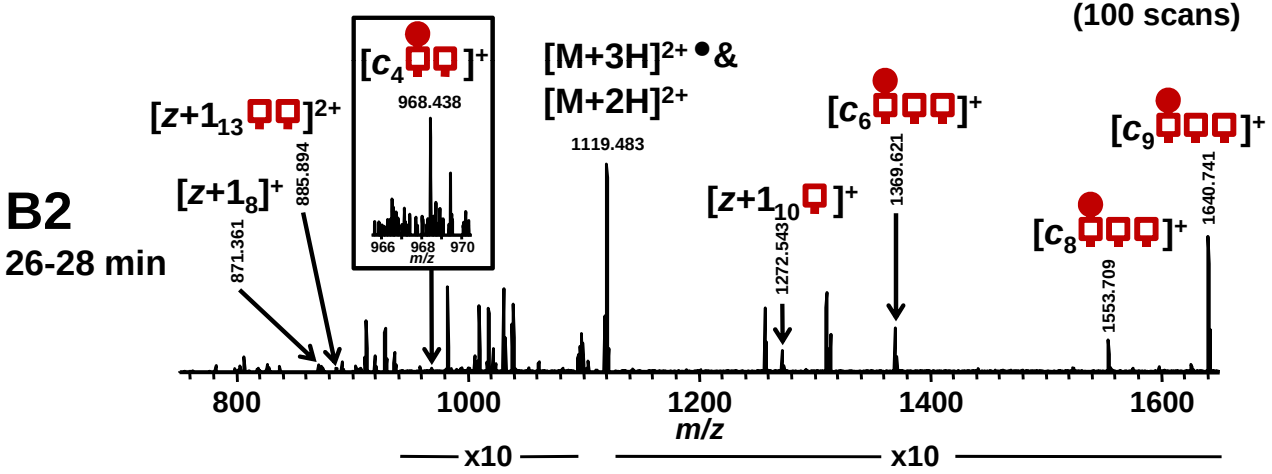
B4 (30-32 min)

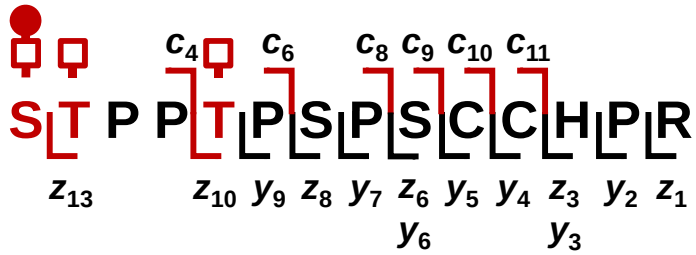
m/z	Charge	Theoretical MW	Assignment	Mass error
1069.456	1	1069.455	$z+1_{10}$	1.14
1244.514	2	2488.011	M	3.79
1434.587	1	1434.587	$z+1_{10}$ + □ 1 ● 1	0.01
1619.687	1	1619.679	c_6 + □ 2 ● 2 ◇ 1	4.75
1890.795	1	1890.796	c_9 + □ 2 ● 2 ◇ 1	-0.58

Normal human IgA1

Ser^{232}-Arg^{245} + $GalNAc_3Gal_1$

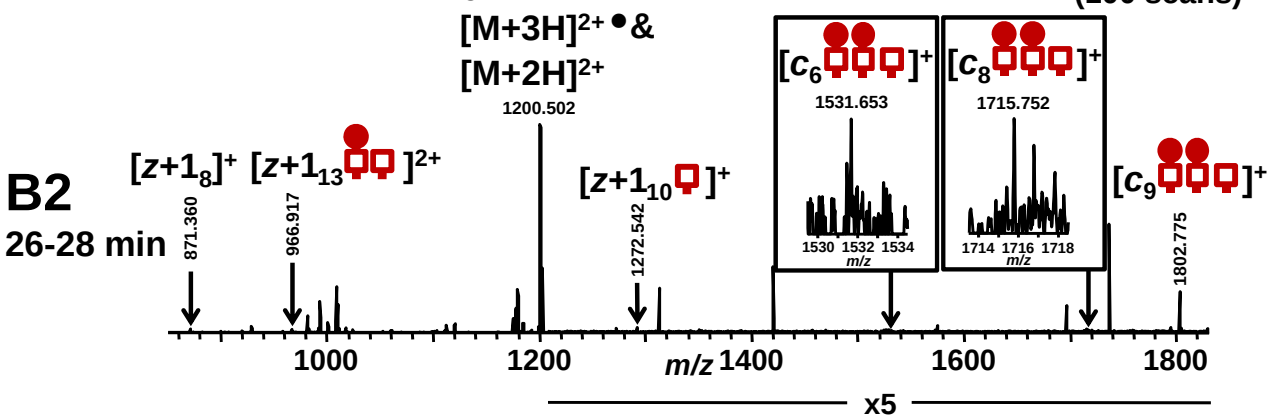
AI-ECD FT-ICR MS/MS
(100 scans)

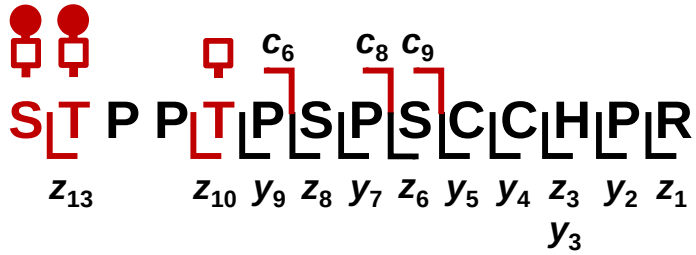




Ser^{232}-Arg^{245} + $GalNAc_3Gal_2$

AI-ECD FT-ICR MS/MS
(100 scans)





Ser^{232}-Arg^{245} + GalNAc$_3$Gal$_1$

B2 (26-28 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
871.361	1	871.354	$z+1_8$	7.60
885.894	2	1770.767	$z+1_{13}$ + □ 2	7.87
968.438	1	968.431	c_4 + □ 2 ● 1	7.54
1119.483	2	2237.943	M	7.25
1272.543	1	1272.534	$z+1_{10}$ + □ 1	6.93
1369.621	1	1369.611	c_6 + □ 3 ● 1	7.67
1553.709	1	1553.695	c_8 + □ 3 ● 1	8.82
1640.741	1	1640.727	c_9 + □ 3 ● 1	8.35

Ser^{232}-Arg^{245} + GalNAc$_3$Gal$_2$

B2 (26-28 min)

m/z	Charge	Theoretical MW	Assignment	Mass error
871.360	1	871.354	$z+1_8$	6.45
966.917	2	1932.820	$z+1_{13}$ + □ 2 ● 1	3.69
1200.502	2	2399.995	M	1.43
1272.542	1	1272.534	$z+1_{10}$ + □ 1	6.15
1531.653	1	1531.663	c_6 + □ 3 ● 2	-6.72
1715.752	1	1715.748	c_8 + □ 3 ● 2	2.27
1802.775	1	1802.780	c_9 + □ 3 ● 2	-2.83