Supplemental Spectra S2

Tandem mass spectra of peptides derived from human recombinant pro-alpha 1(V) collagen. Each spectrum is accompanied by a table of sequence-specific product ions identified from the spectrum along with product ion mass errors. Localized modifications are indicated above the table and are identified as bold letters in the peptide sequence. Unlocalized and pseudolocalized sites of modification are also given. Note: each product ion in the table met the requirements of having < 10 ppm mass error and a signal-to-noise ratio > 3.

Human

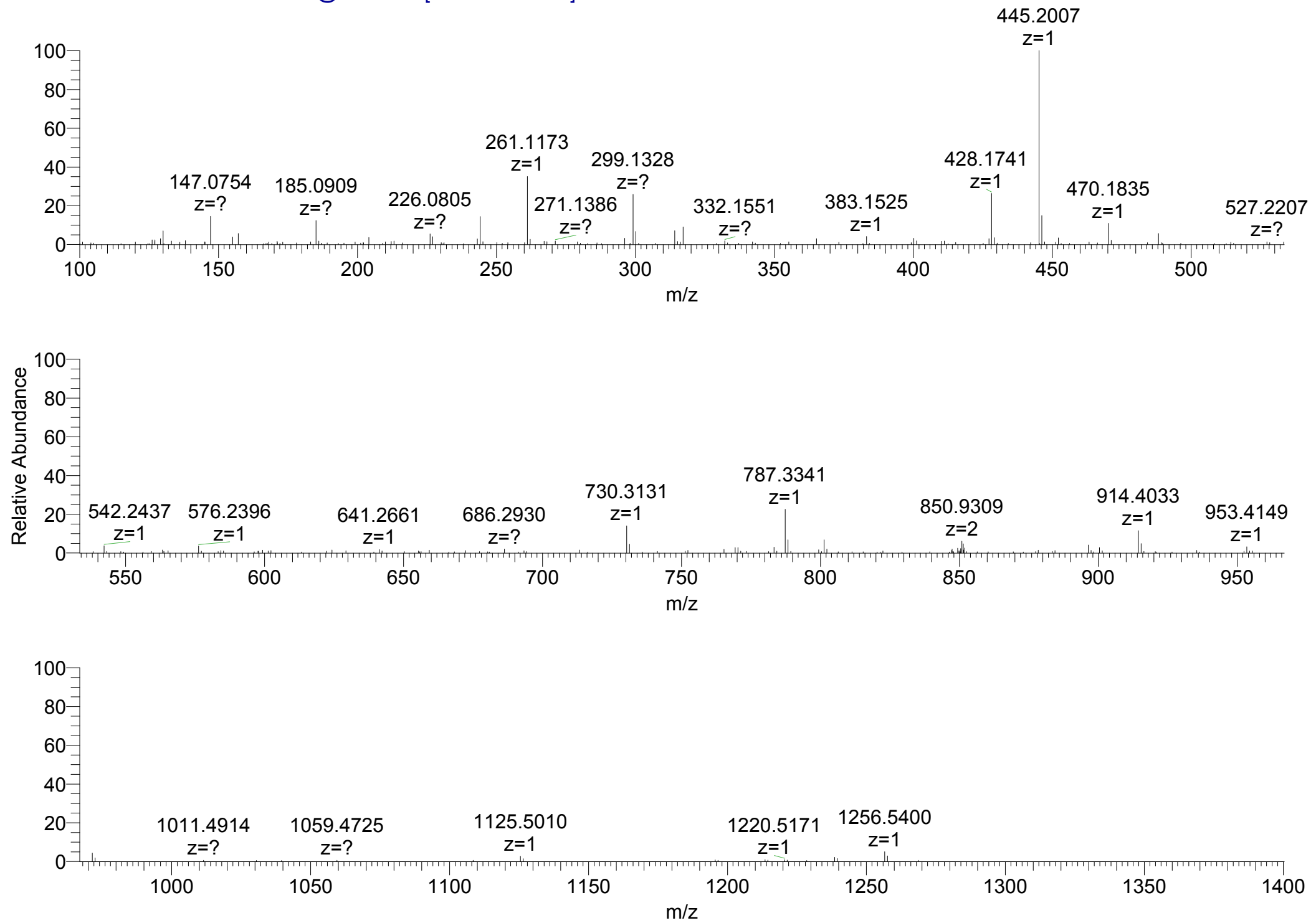
1.

P435-OH

#422-438: DPTSSPSEIGPGM**P**ANQ

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+OH	2	850.8750	850.8673	-0.0154	-9.1
y1/SS-28	1	147.0764	147.0754	-0.0010	-6.8
a2/PS/PA-OH	1	185.0921	185.0909	-0.0012	-6.5
y2-NH3	1	244.0928	244.0911	-0.0017	-7.0
y2	1	261.1193	261.1173	-0.0020	-7.7
PAN+OH	1	299.1350	299.1328	-0.0022	-7.4
y4-NH3+OH	1	428.1776	428.1741	-0.0035	-8.2
y4+OH	1	445.2041	445.2007	-0.0034	-7.7
b5-H2O/ SSPSE-H2O	1	470.1882	470.1835	-0.0047	-10.0
y5+OH	1	576.2446	576.2396	-0.0050	-8.7
y7+OH	1	730.3189	730.3131	-0.0058	-8.0
y8+OH	1	787.3403	787.3341	-0.0062	-7.9
b9	1	914.4102	914.4033	-0.0069	-7.6
b10	1	971.4316	971.4238	-0.0078	-8.0
b12	1	1125.5059	1125.5010	-0.0049	-4.4
b13	1	1256.5463	1256.5400	-0.0063	-5.0

12_9_2011Col5a1_AspNGluC_1 #2777 RT: 24.72 AV: 1 NL: 8.38E4
T: FTMS + c NSI d Full ms2 850.87@hcd30.00 [100.00-1715.00]



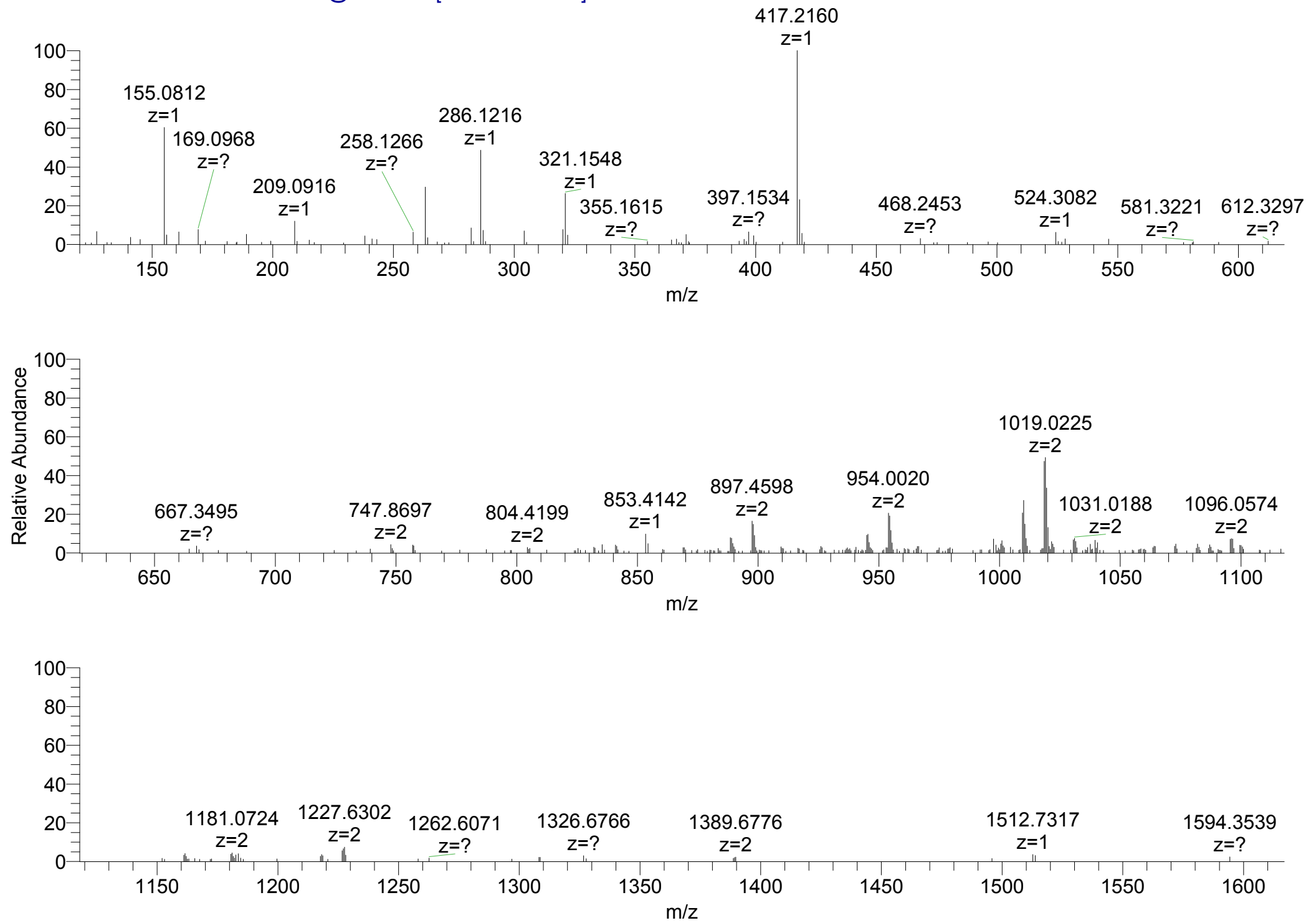
2.

K452-OH.Gal.Glc, K455-OH.Gal.Glc

#443-466: EGIGGPRGE**K**GQ**K**GEPAIIEPGML

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+2Gal.Glc	3	1034.1586	1034.1625	0.0117	3.8
GP	1	155.0815	155.0812	-0.0003	-1.9
EP-H2O	1	209.0921	209.0916	-0.0005	-2.4
y2	1	263.1424	263.1419	-0.0005	-1.9
PGM	1	286.1220	286.1216	-0.0004	-1.4
y4	1	417.2166	417.2160	-0.0006	-1.4
b7	1	667.3522	667.3495	-0.0027	-4.1
b9	1	853.4163	853.4142	-0.0021	-2.5
b18+2OH	2	897.4607	897.4598	-0.0018	-1.0
b19+2OH	1	954.0027	954.0020	-0.0007	-0.7
b20+2OH	2	1018.5240	1018.5233	-0.0014	-0.7
b22+2OH	2	1095.5611	1095.5616	0.0010	0.5
[M+2H]+2OH	2	1226.6287	1226.6240	-0.0094	-3.8
b15+2OH	1	1512.7401	1512.7317	-0.0084	-5.6

10_18_2011Collagen_Chromtrypsin_HCD #3285 RT: 25.63 AV: 1 NL: 1.30E5
T: FTMS + c NSI d Full ms2 1034.50@hcd30.00 [120.00-2000.00]



Human

3.

P501-OH, P504-OH, P507-OH, P513-OH, P515-OH, P516-OH

#499-525: GP**P**GR**P**GL**P**GADGL**P**GPPGTMLMLPFR

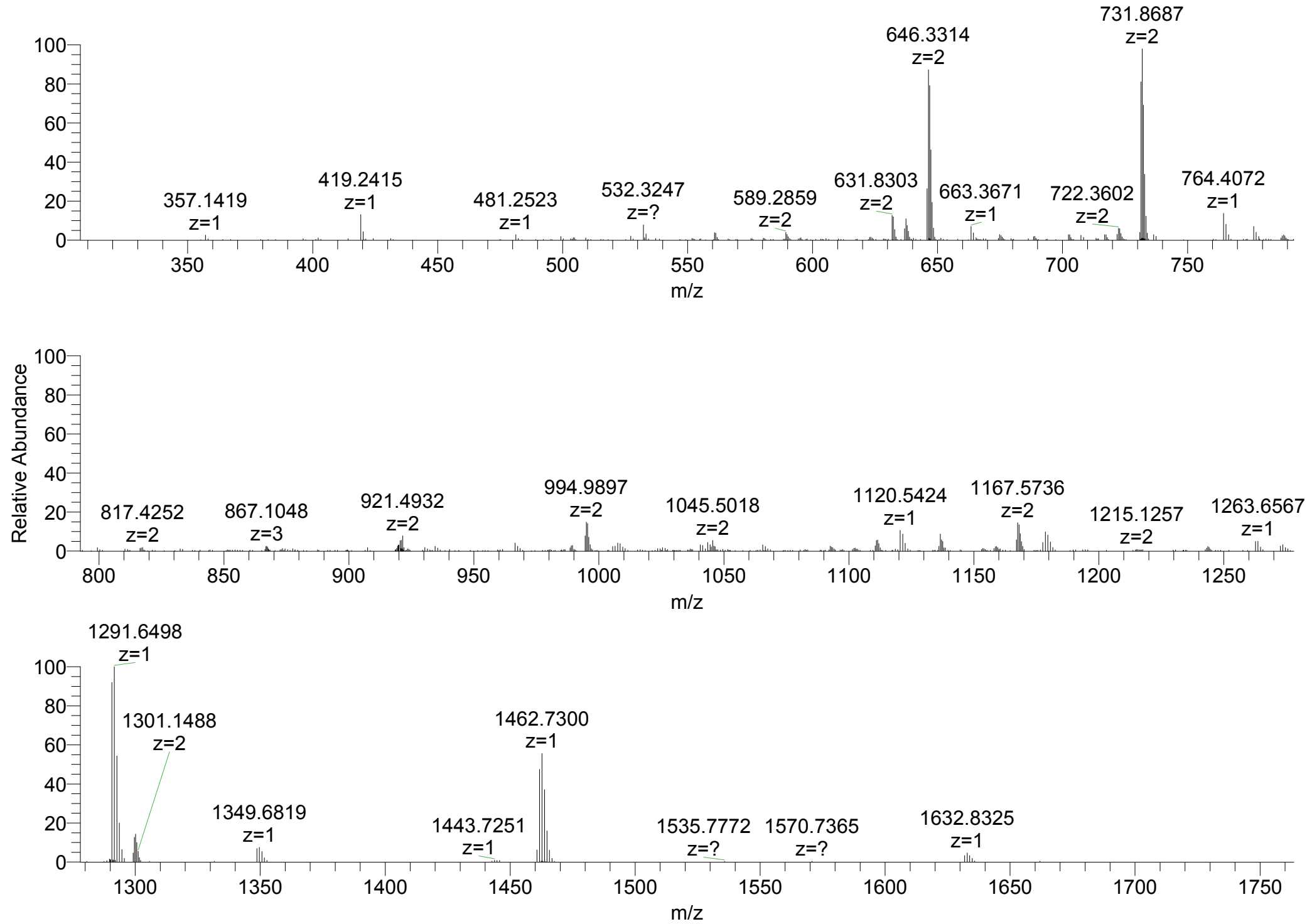
MS^2: GP**P**GR**P**GL**P**GADGL**P**GPPGTMLMLPFR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+6OH	3	917.7913	917.7928	0.0045	1.6
y3	1	419.2401	419.2401	0.0000	0.0
y11+2OH	2	646.3305	646.3314	0.0018	1.4
y13+3OH (MS^3)	3	731.3651	731.3670	0.0057	2.6
b8+2OH	1	764.4050	764.4072	0.0022	2.9
y19+4OH	2	994.4844	994.4891	0.0094	4.7
b24+6OH	2	1167.0669	1167.0731	0.0124	5.3
y11+2OH	1	1290.6437	1290.6490	0.0053	4.1
y25+6OH	2	1299.1462	1299.1527	0.0130	5.0
y12+2OH	1	1348.6752	1348.6769	0.0017	1.3
y13+3OH	1	1461.7229	1461.7268	0.0039	2.7
y15+3OH	1	1631.8284	1631.8324	0.0040	2.5

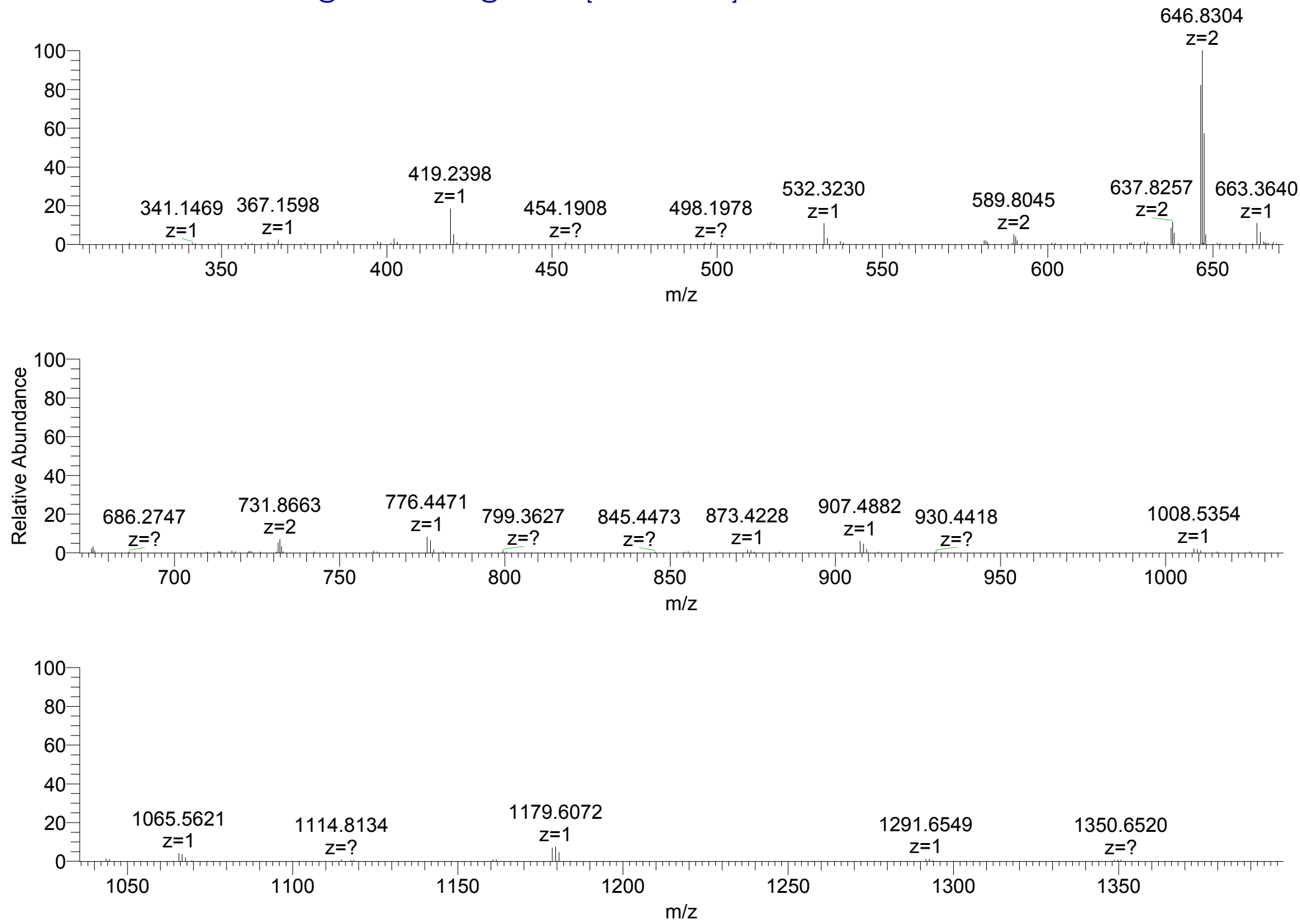
MS^3: **P**G**PP**GTMLMLPFR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
b2/PG+OH	1	171.0764	171.0762	-0.0002	-1.2
b3+OH/GPP+2OH	1	284.1241	284.1239	-0.0002	-0.7
y3	1	419.2401	419.2398	-0.0003	-0.7
y4	1	532.3242	532.3230	-0.0012	-2.3
y10+2OH	2	589.8067	589.8045	-0.0044	-3.7
y11+2OH	2	646.3305	646.3298	-0.0014	-1.1
y5+OH	1	663.3647	663.3640	-0.0007	-1.1
y6	1	776.4487	776.4471	-0.0016	-2.1
y7	1	907.4892	907.4882	-0.0010	-1.1
y9	1	1065.5584	1065.5621	0.0037	3.5
y10+OH	1	1178.6060	1178.6029	-0.0031	-2.6
y11+2OH	1	1291.6537	1291.6549	0.0012	0.9

10_7_2011Collagen_Trypsin_MS3_CIDandHCD #5480 RT: 46.89 AV: 1 NL: 1.04E5
T: FTMS + c NSI d Full ms2 918.13@cid35.00 [240.00-2000.00]



10_7_2011Collagen_Trypsin_MS3_CIDandHCD #5481 RT: 46.90 AV: 1 NL: 8.68E4
T: FTMS + c NSI d Full ms3 918.13@cid35.00 731.87@hcd30.00 [110.00-1475.00]



Human

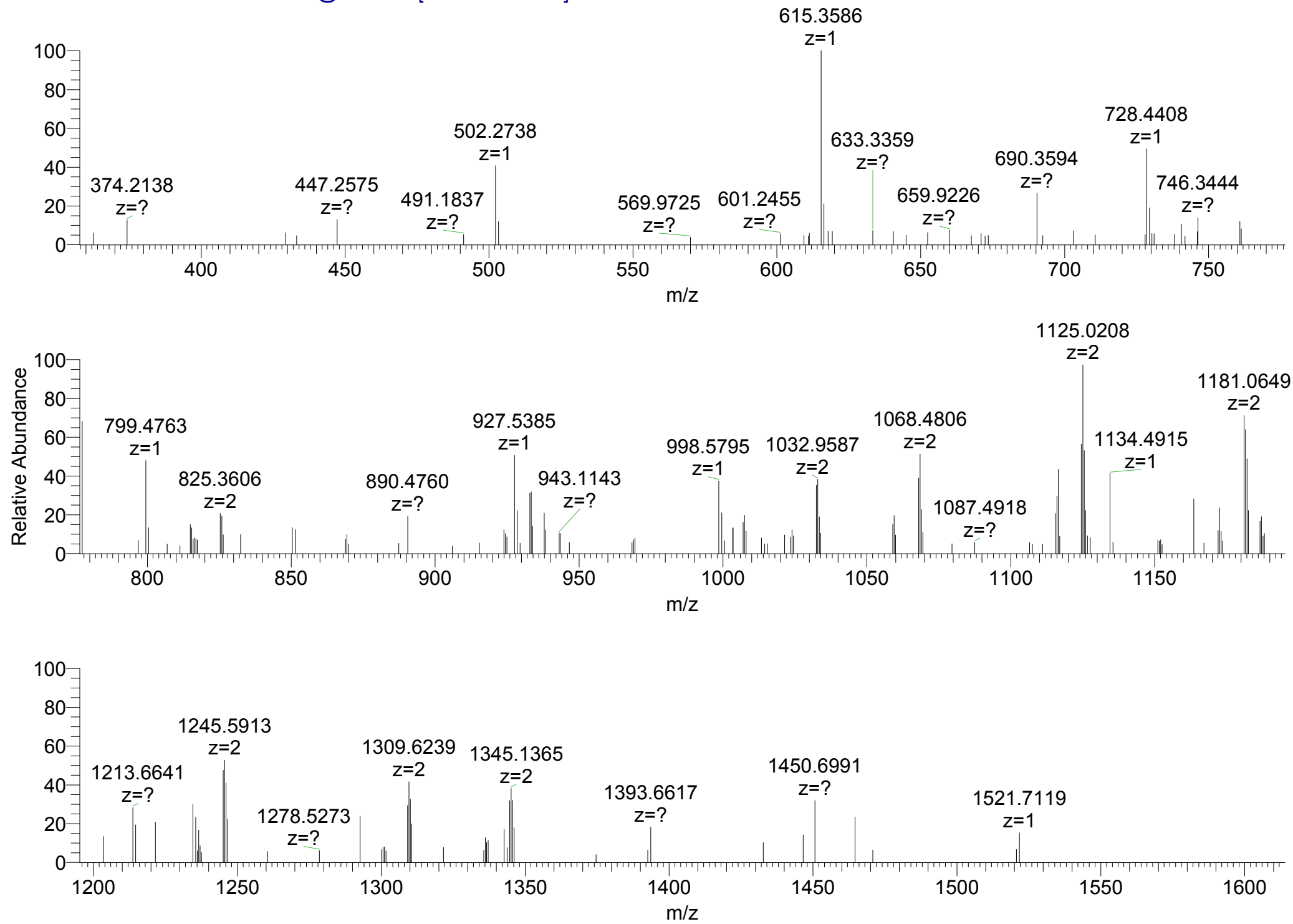
4.

K535-OH

#526-554: FGGGGDAGS**K**GPMVSAQESQAQAILQQAR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+OH	3	954.7981	954.7964	-0.0051	-1.8
y4	1	502.2732	502.2738	0.0006	1.2
y5	1	615.3573	615.3586	0.0013	2.1
y6	1	728.4413	728.4408	-0.0005	-0.7
y7	1	799.4785	799.4763	-0.0022	-2.8
b18+OH	2	825.3648	825.3606	-0.0084	-5.1
b10+OH	1	850.3690	850.3683	-0.0007	-0.8
y8	1	927.5370	927.5385	0.0015	1.6
y9	1	998.5742	998.5795	0.0053	5.3
b22+OH	2	1032.4580	1032.4568	-0.0024	-1.2
b23+OH	2	1067.9765	1067.9731	-0.0068	-3.2
b24+OH	2	1124.5186	1124.5168	-0.0036	-1.6
b25+OH	2	1181.0606	1181.0649	0.0086	3.6
y11	1	1213.6648	1213.6641	-0.0007	-0.6
b26+OH	2	1245.0899	1245.0878	-0.0042	-1.7
b27+OH	2	1309.1192	1309.1256	0.0128	4.9
b28+OH	2	1344.6377	1344.6343	-0.0068	-2.5

11_9_2011Col5a1_Trypsin_MS3_CIDandHCD_micro4 #4879 RT: 63.94 AV: 1 NL: 5.05E6
T: FTMS + c NSI d Full ms2 955.13@cid35.00 [250.00-2000.00]



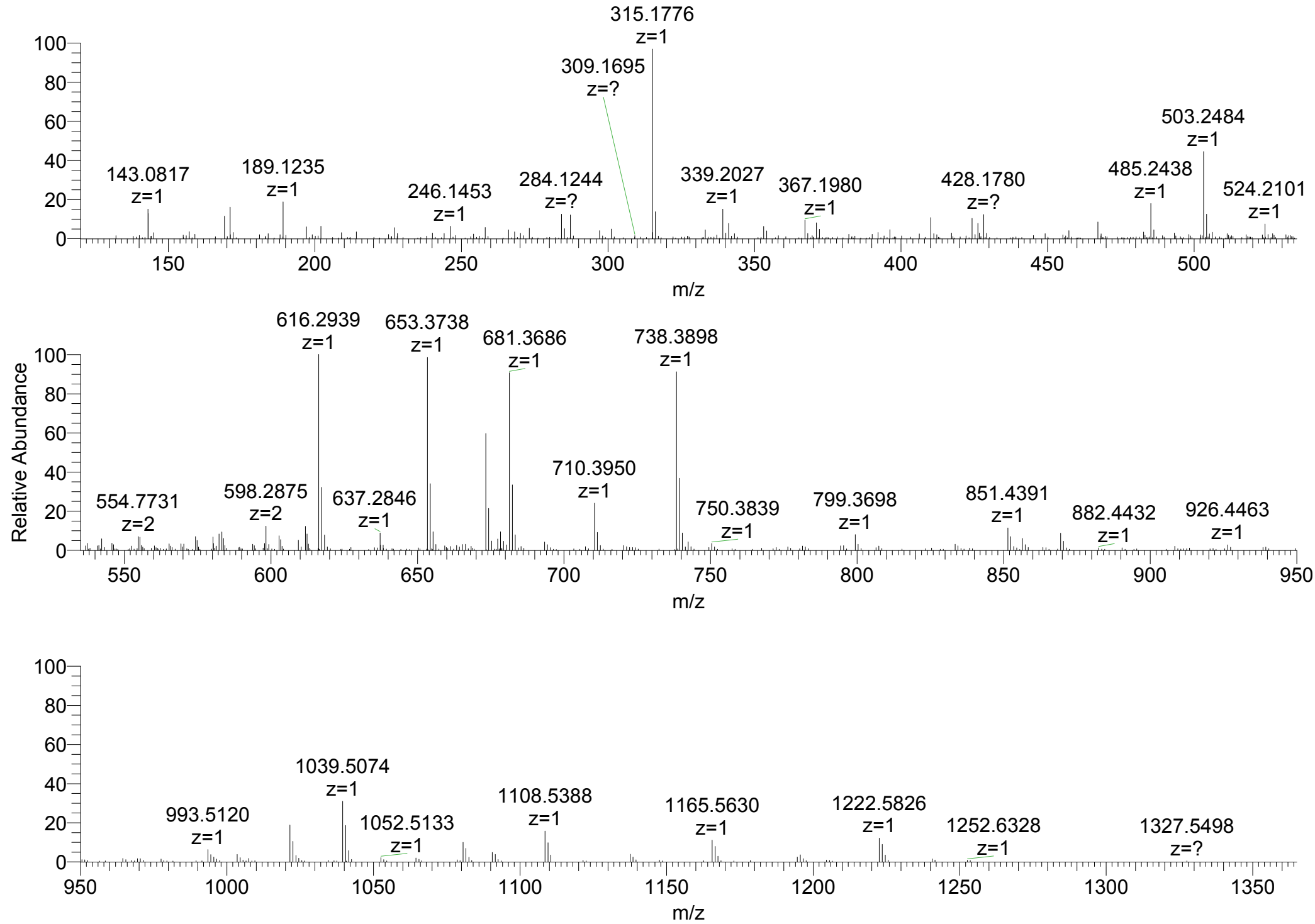
5.

P570-OH, P575-OH, P576-OH

#567-581: TGR**P**GPVG**PP**GSGGL

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+3OH	2	677.3415	677.3419	0.0008	0.6
PG-28+OH	1	143.0815	143.0817	0.0002	1.4
y2	1	189.1234	189.1235	0.0001	0.5
b3	1	315.1775	315.1776	0.0001	0.3
y6+OH	1	503.2460	503.2484	0.0024	4.8
GPPGSGG-H2O+2OH	1	524.2100	524.2101	0.0001	0.2
b12+3OH	2	554.7727	554.7731	0.0008	0.7
y7+2OH	1	616.2937	616.2939	0.0002	0.3
a7+OH	1	653.3729	653.3738	0.0009	1.4
y8+2OH	1	673.3151	673.3154	0.0003	0.4
b7+OH	1	681.3678	681.3686	0.0008	1.2
a8+OH	1	710.3944	710.3950	0.0006	0.8
b8+OH	1	738.3893	738.3898	0.0005	0.7
b9+2OH	1	851.4370	851.4391	0.0021	2.5
y10+2OH	1	869.4363	869.4376	0.0013	1.5
a11+3OH	1	993.5112	993.5120	0.0008	0.8
b11+3OH	1	1021.5061	1021.5068	0.0007	0.7
y12+3OH	1	1039.5055	1039.5074	0.0019	1.8
b12+3OH	1	1108.5382	1108.5388	0.0006	0.5
b13+3OH	1	1165.5596	1165.5630	0.0034	2.9
b14+3OH	1	1222.5811	1222.5826	0.0015	1.2

10_18_2011Collagen_Chromtrypsin_HCD #1383 RT: 12.03 AV: 1 NL: 2.46E5
T: FTMS + c NSI d Full ms2 677.34@hcd30.00 [120.00-1365.00]



6.

P576-OH, K582-OH.Gal.Glc, P585-OH

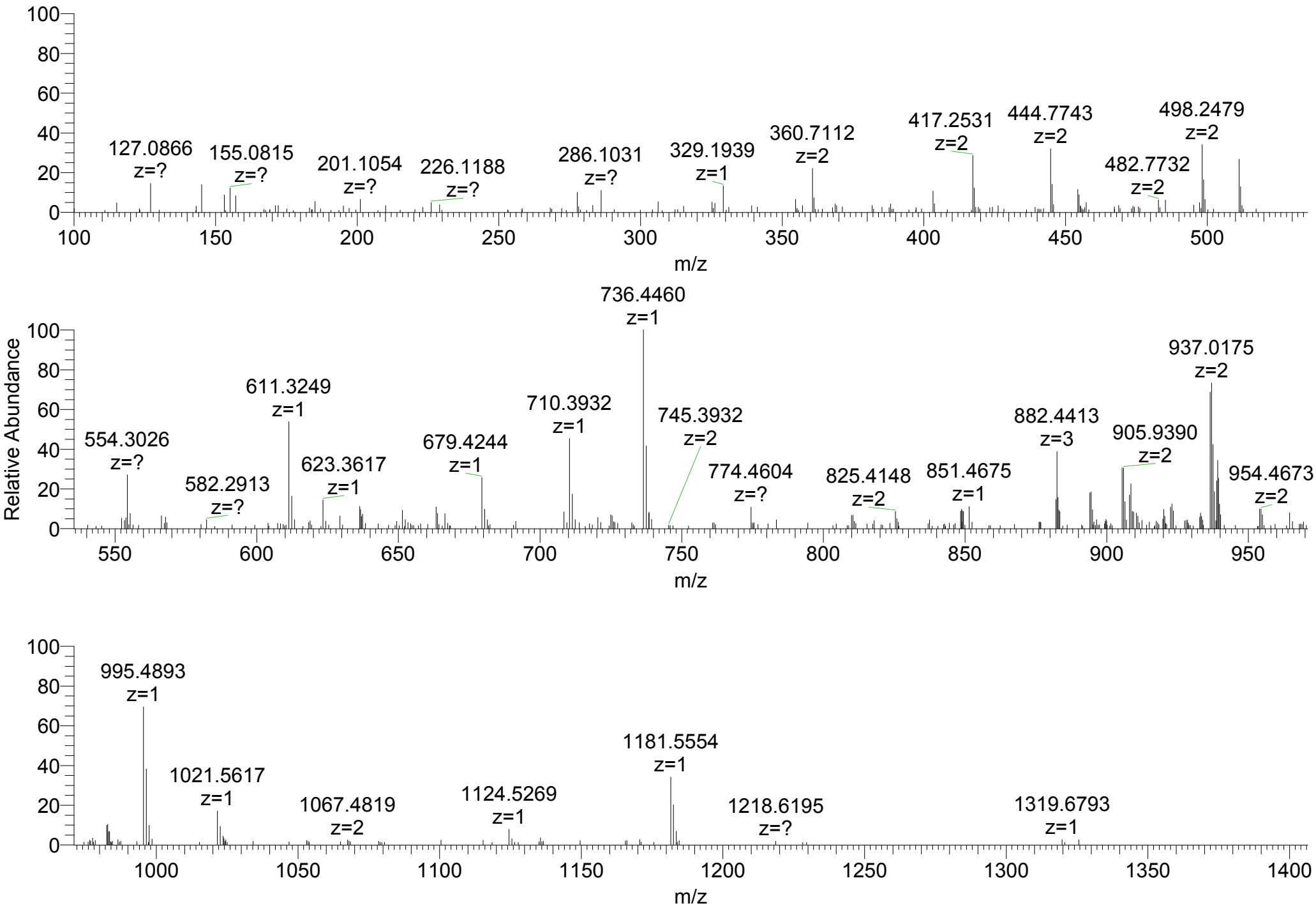
#555-594: LALRGPAGPMGLTGRPGPVGP**P**GSGGL**K**GE**P**GDVGPQGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+5H]+4OH+Gal.Glc	5	821.2160	821.2167	0.0035	0.9
b9	2	417.2532	417.2531	-0.0002	-0.2
y10+OH	2	498.2489	498.2479	-0.0020	-2.0
b11	2	511.2842	511.2849	0.0014	1.4
y5/TGRPGP-28+OH	1	554.3045	554.3026	-0.0019	-3.4
y6	1	611.3260	611.3249	-0.0011	-1.8
b7	1	679.4250	679.4244	-0.0006	-0.9
y7	1	710.3944	710.3932	-0.0012	-1.7
b8	1	736.4464	736.4460	-0.0004	-0.5
y28+4OH	3	882.1073	882.1072	-0.0003	-0.1
a19+OH	2	894.0091	894.0094	0.0006	0.3
y19+OH	2	905.4399	905.4405	0.0012	0.7
b19+OH	2	908.0065	908.0052	-0.0026	-1.4
b20+OH	2	936.5173	936.5183	0.0020	1.1
y30+4OH	3	938.8092	938.8063	-0.0087	-3.1
y20+3OH	2	953.9663	953.9629	-0.0068	-3.6
y10+OH	1	995.4905	995.4893	-0.0012	-1.2
b11/ALRGPAGPMGL	1	1021.5611	1021.5617	0.0006	0.6
y11+OH	1	1124.5331	1124.5269	-0.0062	-5.5
y12+OH	1	1181.5545	1181.5554	0.0009	0.8

***Unlocalized sites: P570-OH?, P572-OH?**

Pseudolocalized sites: P570-OH

10_7_2011Collagen_Trypsin_HCDandETD_111009033323 #4763 RT: 31.93 AV: 1 NL: 5.55E6
T: FTMS + c NSI d Full ms2 821.62@hcd35.00 [100.00-2000.00]



7.

P599-OH, P600-OH, P606-OH

#595-608: GVQG**PP**GPAGK**P**GR

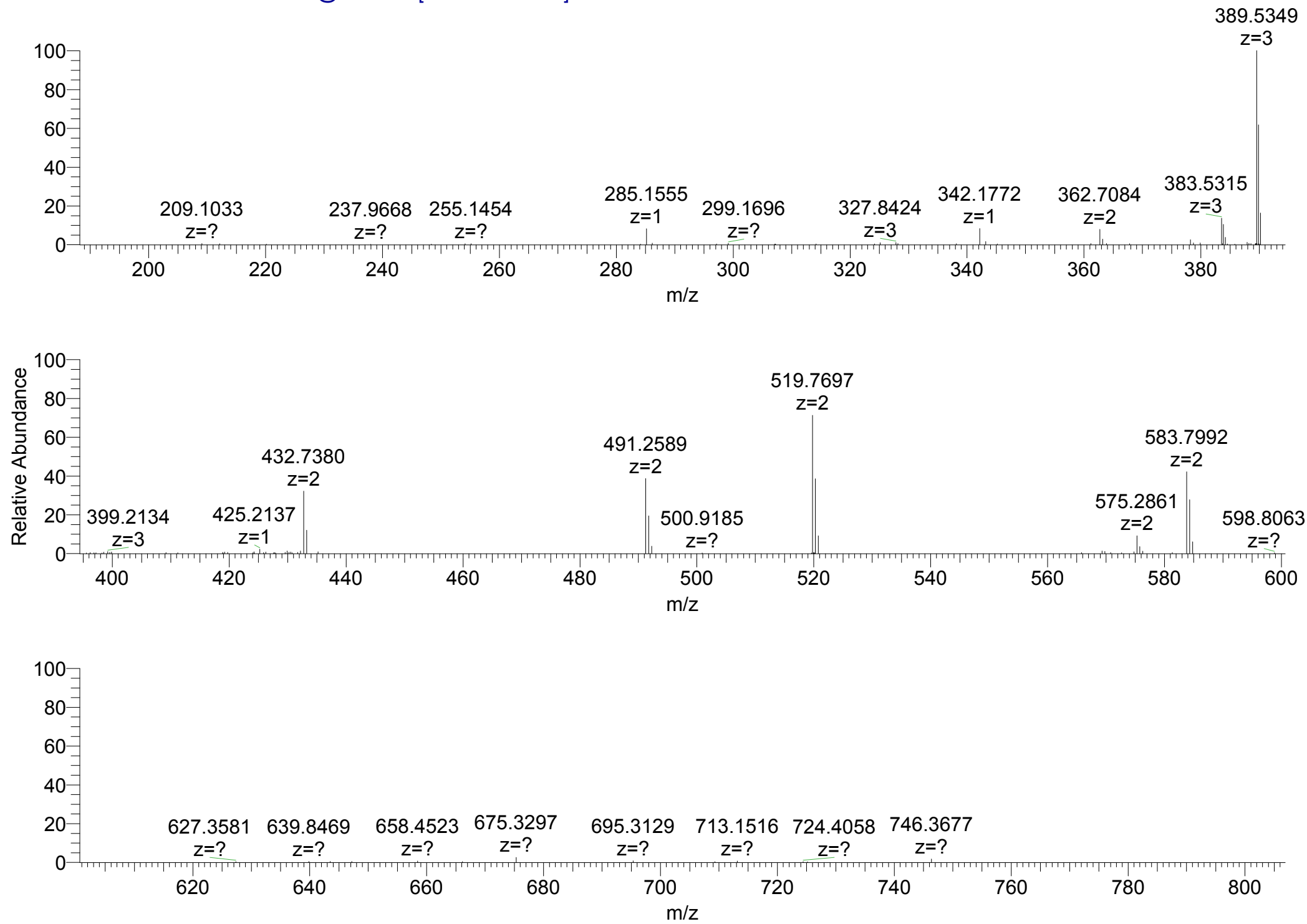
MS^2: GVQGPPGPAGKPGR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+3OH	3	441.5652	441.5652	0.0000	0.0
b3/VQG	1	285.1557	285.1555	-0.0002	-0.7
b13+3OH	3	383.5280	383.5315	0.0105	9.1
y12+3OH(MS^3)	3	389.5353	389.5349	-0.0012	-1.0
y10+3OH	1	491.2567	491.2589	0.0022	4.5
y11+3OH	1	519.7700	519.7697	-0.0003	-0.6
y12+3OH	1	583.7993	583.7992	-0.0001	-0.2

MS^3: QG**PP**GPAGK**P**GR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
K	1	129.1022	129.1021	-0.0001	-0.8
y10+3OH	3	327.8419	327.8415	-0.0012	-1.2
y3	1	345.1881	345.1877	-0.0004	-1.2
y7+OH	2	349.7008	349.7005	-0.0006	-0.9
y8+OH	2	378.2116	378.2113	-0.0006	-0.8
y9+2OH	2	434.7354	434.7343	-0.0022	-2.5
y4	1	473.2831	473.2828	-0.0003	-0.6
y10+3OH	2	491.2592	491.2589	-0.0006	-0.6
GPPGPA+2OH	1	509.2354	509.2339	-0.0015	-3.0
y5+OH	1	530.3045	530.3033	-0.0012	-2.3
y6+OH	1	601.3416	601.3408	-0.0008	-1.3
y7+OH	1	698.3944	698.3996	0.0052	7.5

10_7_2011Collagen_Trypsin_MS3_CIDandHCD #1096 RT: 12.14 AV: 1 NL: 5.91E4
T: FTMS + c NSI d Full ms2 441.57@cid35.00 [110.00-1335.00]



10_7_2011Collagen_Trypsin_MS3_CIDandHCD #1097 RT: 12.15 AV: 1 NL: 9.64E3
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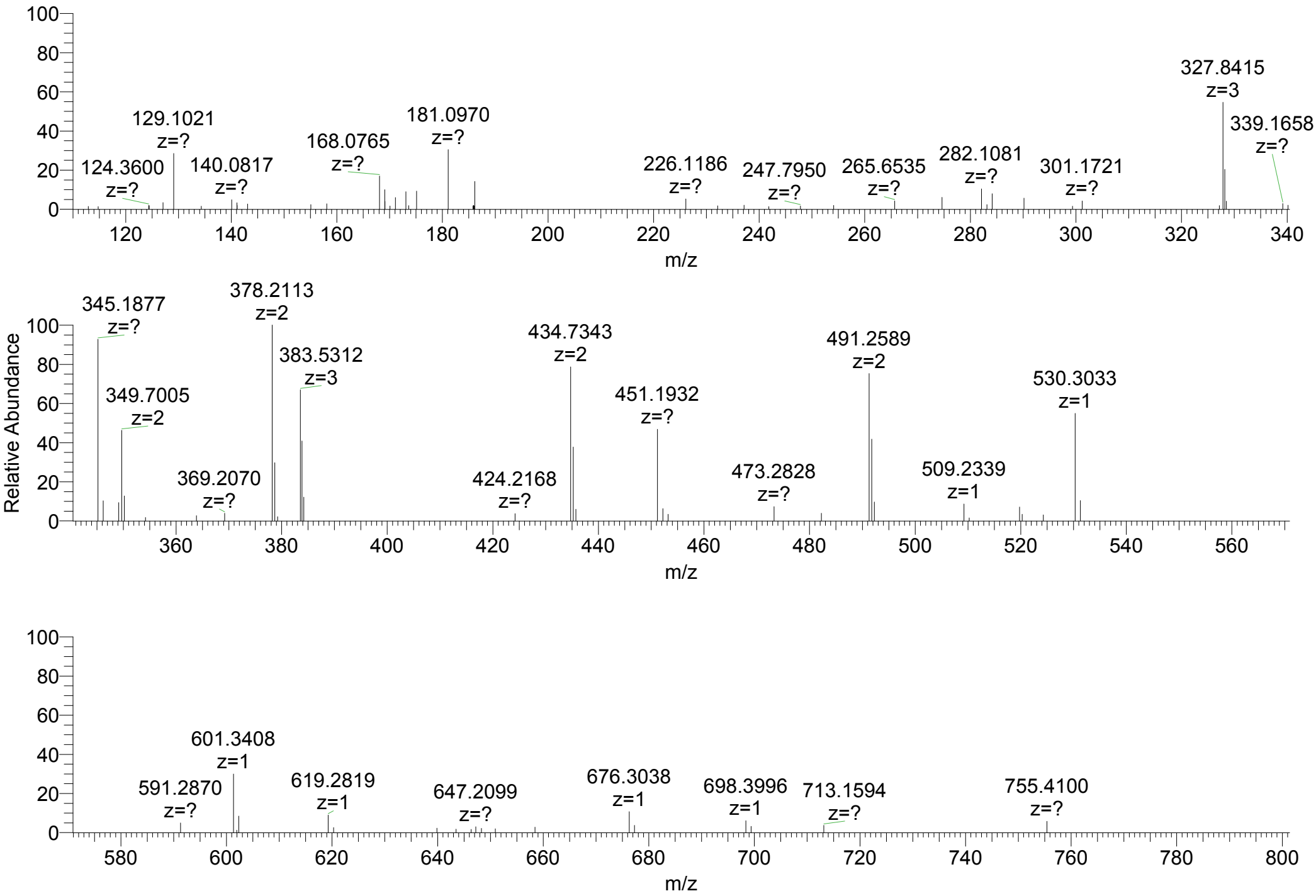


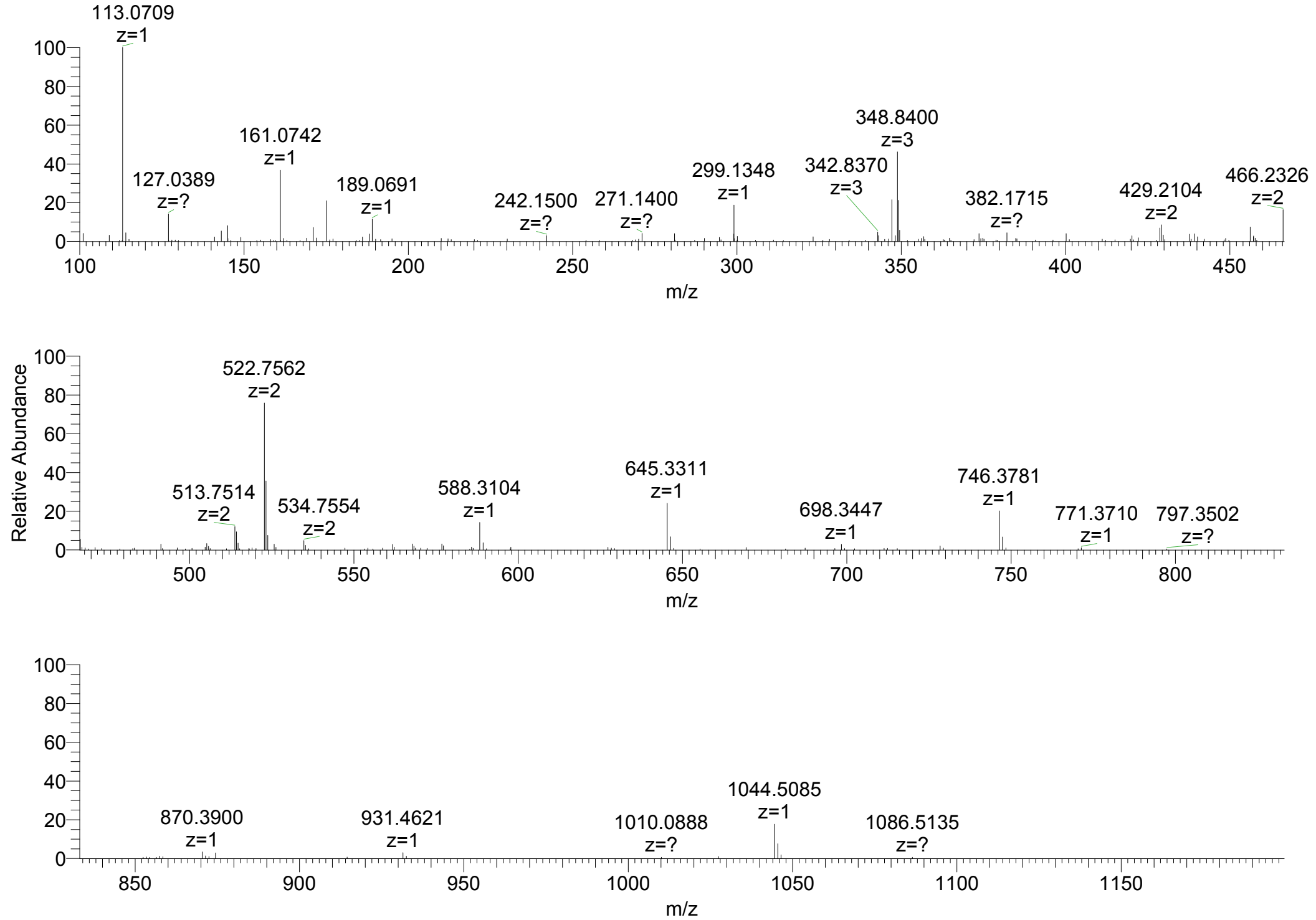
8.

P621-OH, K627-OH.Gal.Glc

#619-630: GM**P**GQTGP**K**GDR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+Gal.Glc	3	519.5630	519.5618	-0.0036	-2.3
a2	1	161.0743	161.0742	-0.0001	-0.6
y1	1	175.1190	175.1188	-0.0002	-1.1
b2	1	189.0692	189.0691	-0.0001	-0.5
GKP-H2O+OH/PGQ+OH	1	299.1350	299.1348	-0.0002	-0.7
y10+OH	3	348.8405	348.8400	-0.0015	-1.4
y9+OH	2	466.2332	466.2326	-0.0012	-1.3
y10-H2O+2OH	2	513.7518	513.7514	-0.0008	-0.8
y10+2OH	2	522.7571	522.7562	-0.0018	-1.7
y5+OH	1	588.3100	588.3104	0.0004	0.7
y6+OH	1	645.3315	645.3311	-0.0004	-0.6
y7+OH	1	746.3791	746.3781	-0.0010	-1.3
y10+2OH	1	1044.5069	1044.5085	0.0016	1.5

11_7_2011Collagen_nonDenatured #577 RT: 7.79 AV: 1 NL: 6.57E4
T: FTMS + c NSI d Full ms2 519.56@hcd35.00 [100.00-1570.00]



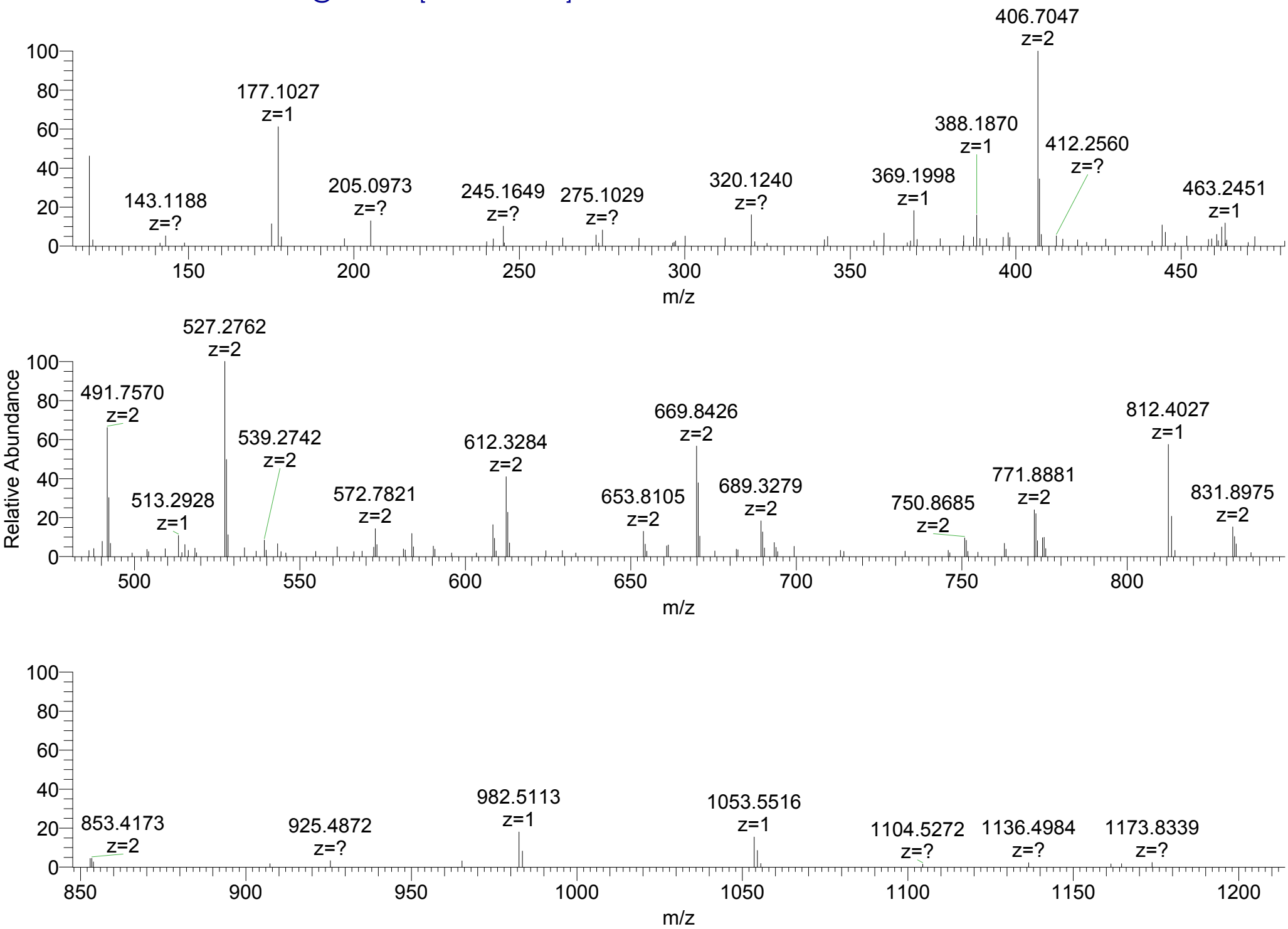
9.

P639-OH, K642-OH.Gal.Glc

#631-645: GFDGLAGL**P**GE**K**GHR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+Gal.Glc	3	622.9620	622.9612	-0.0024	-1.3
a2	1	177.1022	177.1027	0.0005	2.8
b2	1	205.0972	205.0973	0.0001	0.4
b3/FDG	1	320.1241	320.1240	-0.0001	-0.3
y3	1	369.1993	369.1998	0.0005	1.4
y7+2OH	2	406.7041	406.7047	0.0012	1.5
y9+2OH	2	491.7569	491.7570	0.0002	0.2
y10+2OH	2	527.2754	527.2762	0.0016	1.5
y10+2OH+Gal	2	608.3018	608.3047	0.0058	4.8
y12+2OH	2	612.3282	612.3284	0.0004	0.3
y9+2OH+Gal.Glc	2	653.8097	653.8105	0.0016	1.2
y13+2OH	2	669.8417	669.8426	0.0018	1.3
y13+2OH+Gal	2	750.8681	750.8685	0.0008	0.5
[M+2H]+2OH	2	771.8866	771.8881	0.0030	1.9
y7+2OH	1	812.4009	812.4027	0.0018	2.2
y13+2OH+Gal.Glc	2	831.8945	831.8975	0.0060	3.6
y9+2OH	1	982.5065	982.5113	0.0048	4.9
y10+2OH	1	1053.5436	1053.5516	0.0080	7.6

9_22_2011CollagenTrypsin_HCD_1 #2368 RT: 21.73 AV: 1 NL: 4.36E5
T: FTMS + c NSI d Full ms2 622.96@hcd30.00 [115.00-1880.00]



10.

P639-OH, K642-OH.Gal, P657-OH

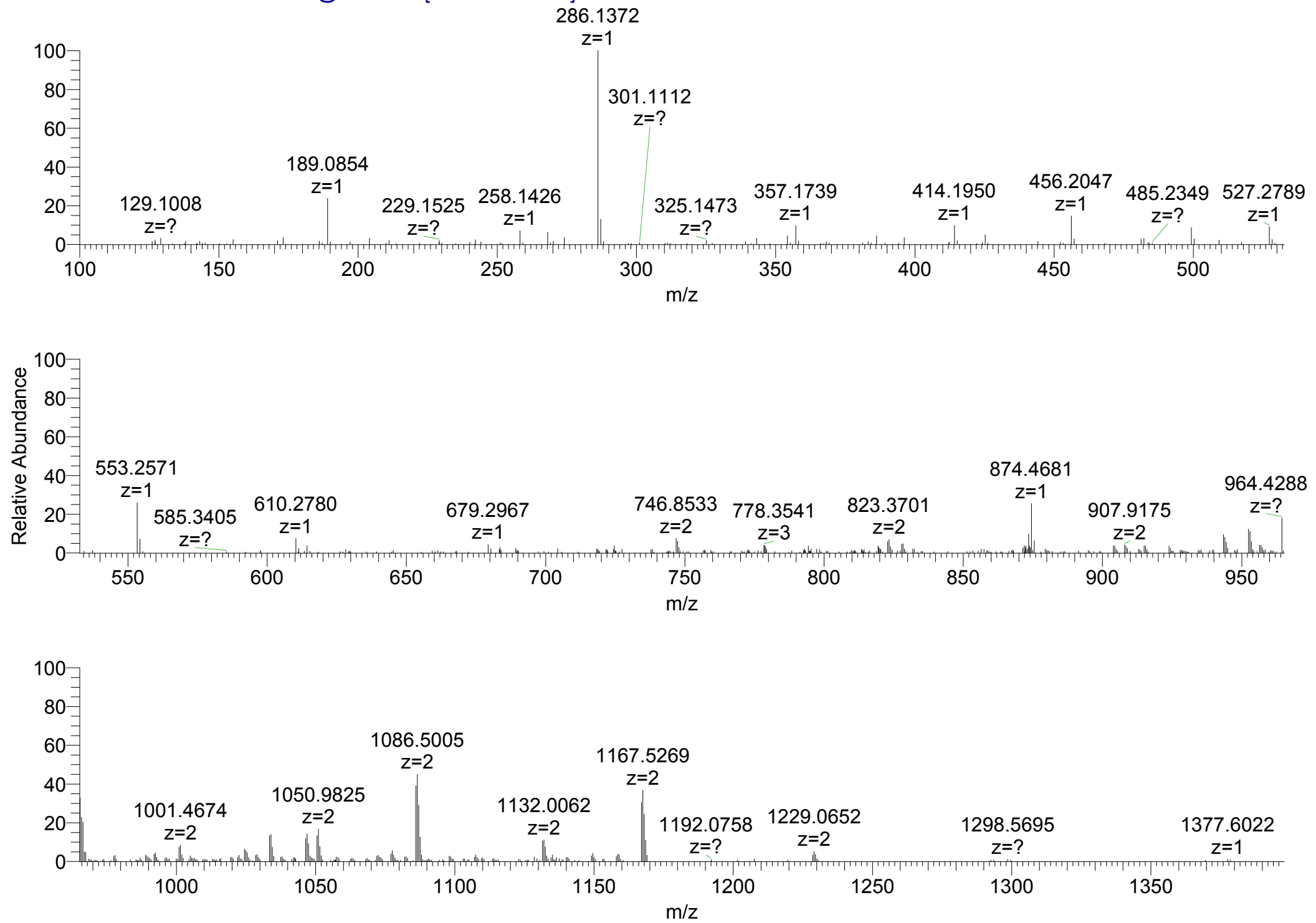
#633-658: DGLAGL**P**GE**K**GHRGDPGPSGPPGP**P**G

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+5OH+Gal	3	873.4037	873.3955	-0.0246	-9.4
y2+OH	1	189.0870	189.0854	-0.0016	-8.5
a3	1	258.1448	258.1426	-0.0022	-8.6
b3	1	286.1397	286.1372	-0.0025	-8.8
b4	1	357.1769	357.1739	-0.0030	-8.4
b5	1	414.1983	414.1950	-0.0033	-8.0
y5+2OH	1	456.2089	456.2047	-0.0042	-9.2
b6	1	527.2824	527.2789	-0.0035	-6.7
y6+2OH	1	553.2617	553.2571	-0.0046	-8.3
y7+2OH	1	610.2831	610.2780	-0.0051	-8.4
y8-H2O+2OH	1	679.3046	679.2967	-0.0079	-11.6
b15+2OH+Gal	2	746.8606	746.8533	-0.0146	-9.8
b20+3OH+Gal	2	952.4483	952.4392	-0.0182	-9.6
y20+5OH	2	965.4379	965.4297	-0.0164	-8.5
b21+3OH	2	1000.9747	1000.9637	-0.0220	-11.0
y22+5OH	2	1050.4907	1050.4823	-0.0168	-8.0
y23+5OH	2	1086.0092	1086.0010	-0.0164	-7.6
y22+5OH+Gal	2	1131.5171	1131.5063	-0.0216	-9.6
y23+5OH+Gal	2	1167.0356	1167.0267	-0.0178	-7.6
[M+2H]+5OH	2	1228.5755	1228.5625	-0.0260	-10.6

***Unlocalized sites: P648-OH?, P650-OH?, P654-OH?, P656-OH?**

Pseudolocalized sites: P648-OH, P654-OH

12_9_2011Col5a1_AspNGluC_3 #2030 RT: 18.48 AV: 1 NL: 7.99E4
T: FTMS + c NSI d Full ms2 873.73@hcd30.00 [100.00-2000.00]



Human

11.

P648-OH, P653-OH, P654-OH, P656-OH, P657-OH

#646-672: GD**P**GPSG**PP**G**PP**GDDGERGDDGEVGPR

MS^2: GD**P**GPSGP**P**GPPGDDGERGDDGEVGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
MH+4OH	3	869.6990	869.6970	-0.0060	-2.3
y4	1	428.2616	428.2623	0.0007	1.6
y12	2	622.2867	622.2885	0.0036	2.9
y20+3OH	3	675.2911	675.2936	0.0075	3.7
y13	2	679.8002	679.8024	0.0044	3.2
y7	1	729.3526	729.3558	0.0032	4.4
y23+3OH	3	755.6599	755.6622	0.0069	3.0
y25+4OH(MS^3)	3	812.3496	812.3511	0.0045	1.8
y18+OH	2	899.3854	899.3877	0.0046	2.6
y19+2OH	2	955.9092	955.9120	0.0056	2.9
y19+3OH	2	963.9066	963.9094	0.0056	2.9
y20+3OH	2	1012.4330	1012.4366	0.0072	3.6
y21+3OH	2	1040.9438	1040.9456	0.0036	1.7
y23+3OH	2	1132.9862	1132.9895	0.0066	2.9

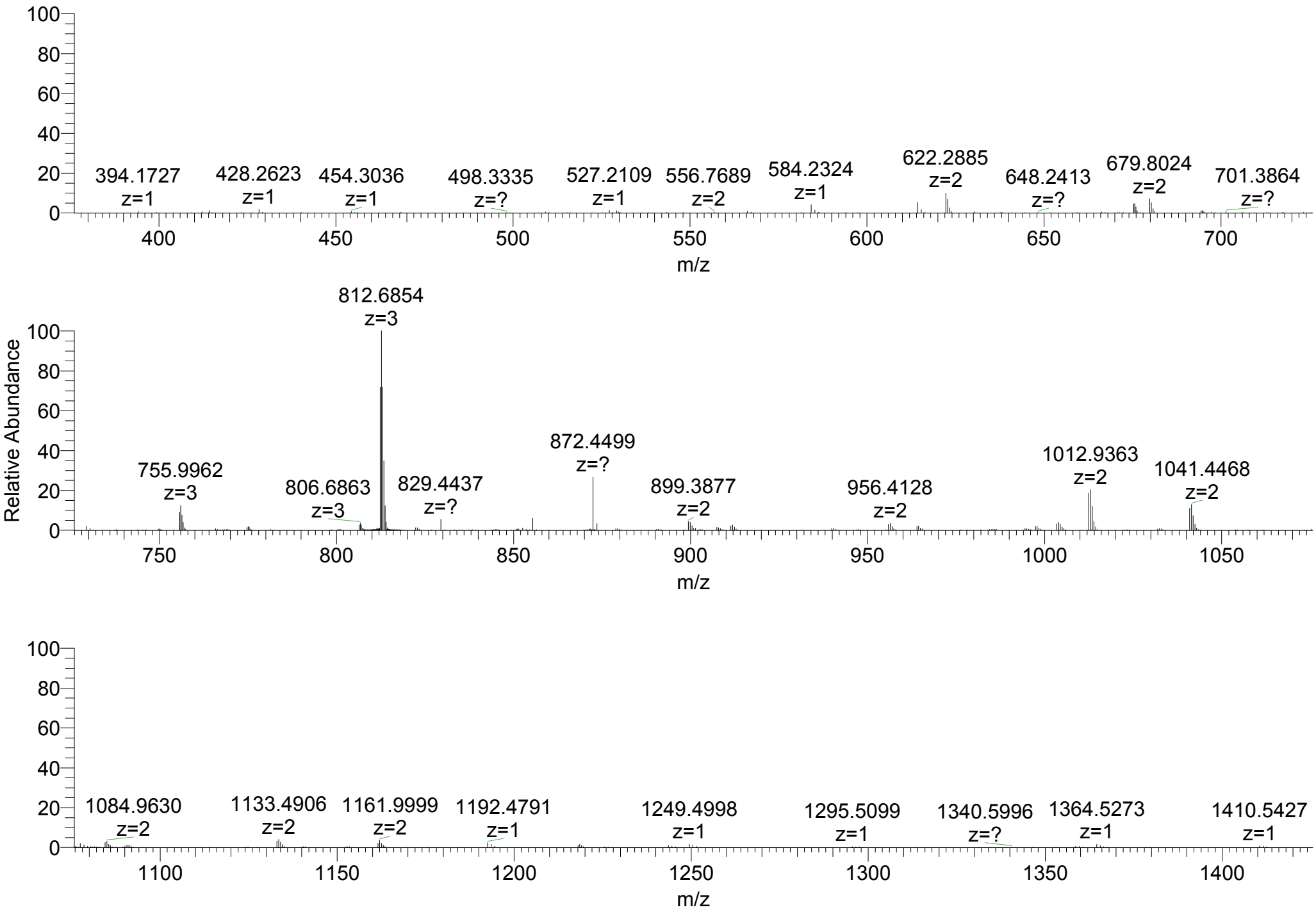
MS^3: **P**GPSGP**P**G**PP**GDDGERGDDGEVGPR or **P**GPSG**PP**GPPGDDGERGDDGEVGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
MH+4OH	3	812.3496	812.3511	0.0045	1.8
b4-H2O+OH	1	337.1506	337.1500	-0.0006	-1.8
b5-H2O+OH	1	394.1721	394.1717	-0.0004	-1.0
b5+OH	1	412.1827	412.1824	-0.0003	-0.7
y4	1	428.2616	428.2607	-0.0009	-2.1
y10	2	529.2547	529.2556	0.0018	1.7
y6	1	614.3257	614.3246	-0.0011	-1.8
y12	2	622.2867	622.2862	-0.0010	-0.8
y20+3OH	3	675.2911	675.2908	-0.0009	-0.4
y13	2	679.8002	679.7995	-0.0014	-1.0
y23+3OH	3	755.6599	755.6584	-0.0045	-2.0
y24+3OH	3	774.6670	774.6658	-0.0036	-1.6
MH-H2O+4OH	3	806.3461	806.3450	-0.0033	-1.4
MH+4OH	3	812.3496	812.3422	-0.0222	-9.1
y18+OH	2	899.3854	899.3850	-0.0008	-0.4
y18+2OH	2	907.3828	907.3815	-0.0026	-1.4
b19+4OH	2	911.3615	911.3618	0.0006	0.3

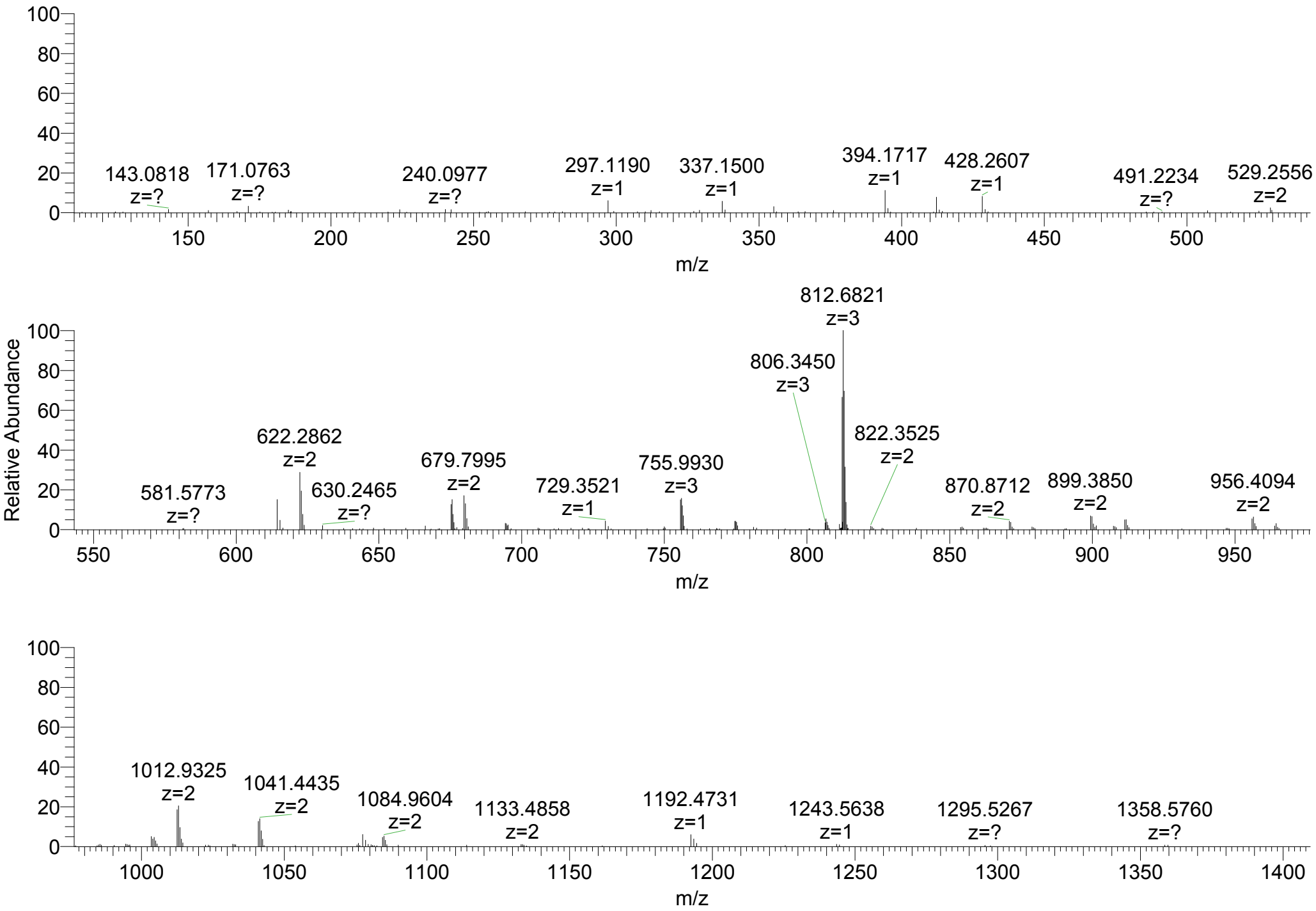
Human

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
y19+3OH	2	963.9066	963.9030	-0.0072	-3.7
y19+2OH	2	955.9092	955.9072	-0.0040	-2.1
y20+3OH	2	1012.4330	1012.4333	0.0006	0.3
y21+3OH	2	1040.9438	1040.9413	-0.0050	-2.4

10_7_2011Collagen_Trypsin_MS3_CIDandHCD #1990 RT: 18.60 AV: 1 NL: 5.18E5
T: FTMS + c NSI d Full ms2 870.03@cid35.00 [225.00-2000.00]



10_7_2011Collagen_Trypsin_MS3_CIDandHCD #1991 RT: 18.61 AV: 1 NL: 1.28E5
T: FTMS + c NSI d Full ms3 870.03@cid35.00 812.69@hcd30.00 [110.00-2000.00]



12.

P675-OH, P678-OH

#673-681: GL**P**GE**P**GPR

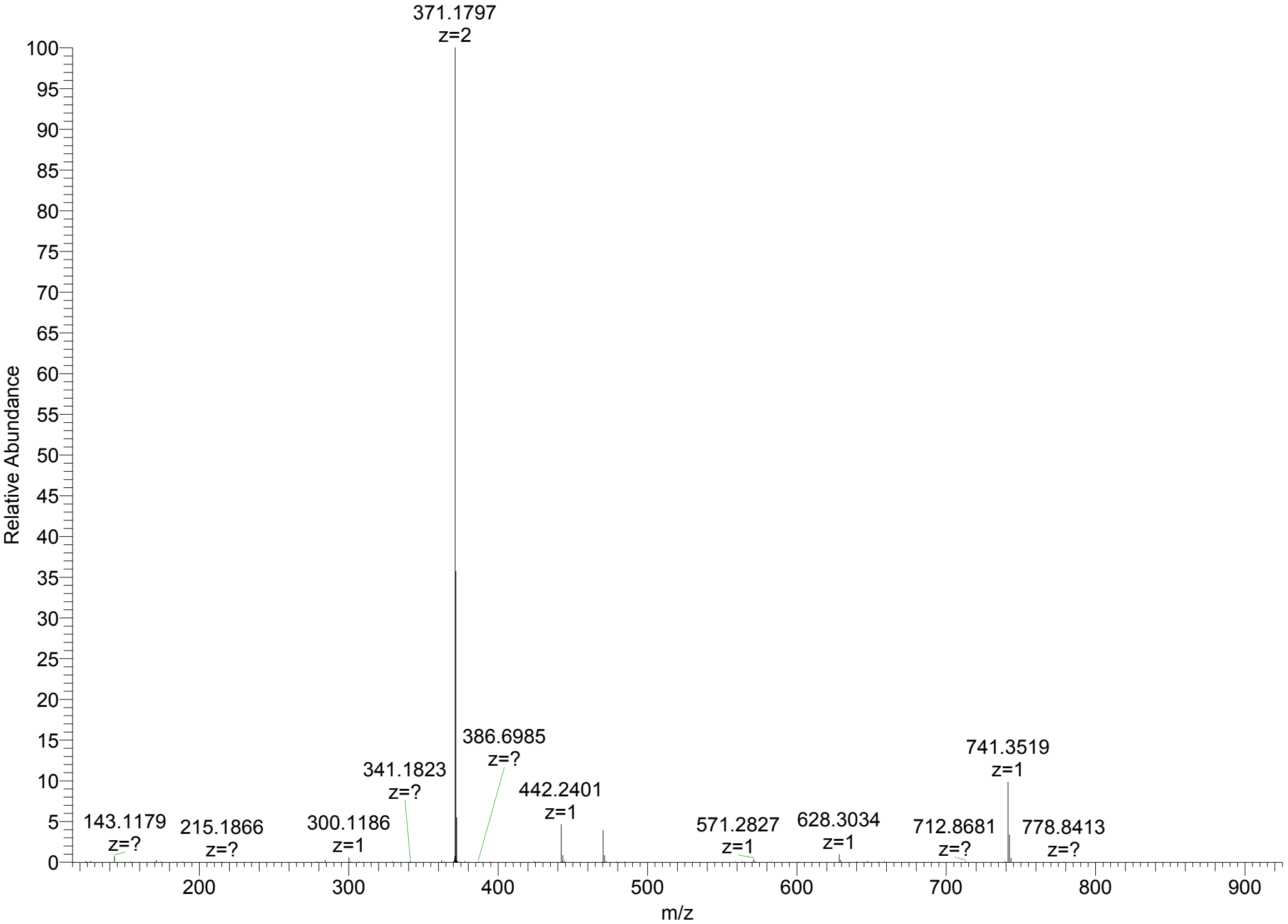
MS^2: GL**P**GEPGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+2OH	2	456.2327	456.2319	-0.0016	-1.8
y7+2OH(MS^3)	2	371.1799	371.1797	-0.0004	-0.5
y4+OH	1	442.2409	442.2401	-0.0008	-1.8
b5+OH	1	470.2245	470.2240	-0.0005	-1.1
y7+2OH	1	741.3526	741.3519	-0.0007	-0.9

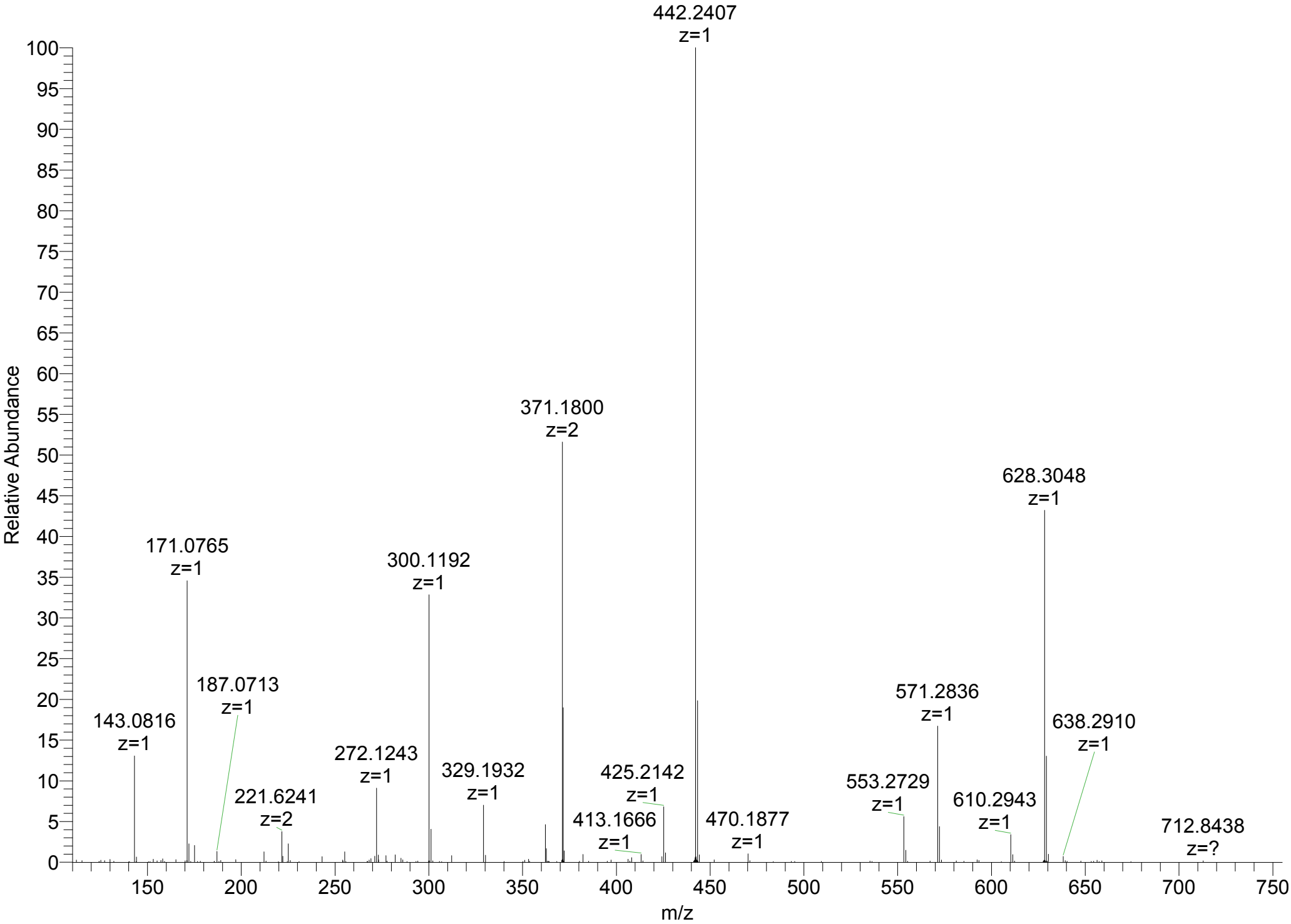
MS^3: **P**GE**P**GPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
PG-28+OH/ a2+OH	1	143.0815	143.0816	0.0001	0.7
PG+OH/b2+OH	1	171.0764	171.0765	0.0001	0.6
y4+OH	2	221.6241	221.6241	0.0000	0.0
GEP-28+OH/a3	1	272.1241	272.1243	0.0002	0.7
EPG+OH/b3	1	300.1190	300.1192	0.0002	0.7
y3	1	329.1932	329.1932	0.0000	0.0
[M+2H]+2OH	2	371.1799	371.1800	0.0002	0.3
y4+OH	1	442.2409	442.2407	-0.0002	-0.5
b5+2OH	1	470.1882	470.1877	-0.0005	-1.1
y5-H2O+OH	1	553.2729	553.2729	0.0000	0.0
y5+OH	1	571.2835	571.2836	0.0001	0.2
y6-H2O+OH	1	610.2944	610.2943	-0.0001	-0.2
y6+OH	1	628.3049	628.3048	-0.0001	-0.2

10_7_2011Collagen_Trypsin_MS3_CIDandHCD #1382 RT: 14.52 AV: 1 NL: 4.69E7
T: FTMS + c NSI d Full ms2 456.73@cid35.00 [115.00-925.00]



10_7_2011Collagen_Trypsin_MS3_CIDandHCD #1383 RT: 14.52 AV: 1 NL: 2.66E7
T: FTMS + c NSI d Full ms3 456.73@cid35.00 371.18@hcd30.00 [110.00-755.00]



13.

P690-OH, P693-OH, P696-OH, P705-OH

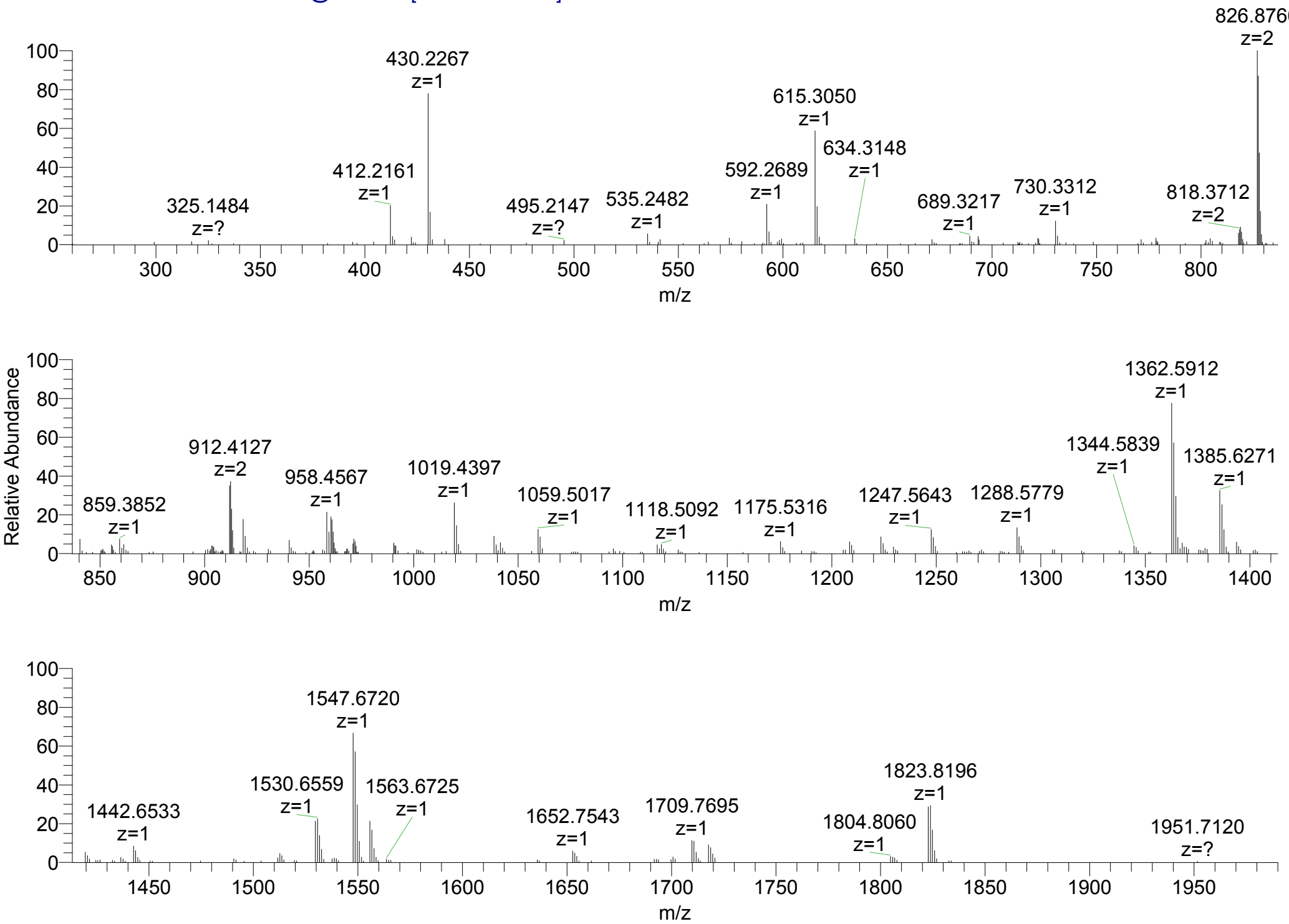
#688-708: GP**P**GP**P**GP**P**GVTGMDGQ**P**GPK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+5OH	2	988.9546	988.9441	-0.0210	-10.6
y4+2OH	1	430.2296	430.2267	-0.0029	-6.8
b6+2OH	1	535.2511	535.2482	-0.0029	-5.4
b7+2OH	1	592.2726	592.2689	-0.0037	-6.3
y6+2OH	1	615.3097	615.3050	-0.0047	-7.7
b8+2OH	1	689.3253	689.3217	-0.0036	-5.2
y7+2OH	1	730.3366	730.3312	-0.0054	-7.4
y16+4OH	2	778.3565	778.3506	-0.0118	-7.6
y17+4OH	2	826.8829	826.8766	-0.0126	-7.6
b10+3OH	1	859.3945	859.3852	-0.0093	-10.8
y19+5OH	2	911.9174	911.9111	-0.0126	-6.9
y9+2OH	1	918.3986	918.3918	-0.0068	-7.4
b11+3OH	1	958.4629	958.4567	-0.0062	-6.5
y10+2OH	1	1019.4462	1019.4397	-0.0065	-6.4
b12+3OH	1	1059.5106	1059.5017	-0.0089	-8.4
y12+2OH	1	1175.5361	1175.5316	-0.0045	-3.8
b14+3OH	1	1247.5725	1247.5643	-0.0082	-6.6
y13+3OH	1	1288.5838	1288.5779	-0.0059	-4.6
b15-H2O+3OH	1	1344.5889	1344.5839	-0.0050	-3.7
b15+3OH	1	1362.5994	1362.5912	-0.0082	-6.0
y14+3OH	1	1385.6366	1385.6271	-0.0095	-6.9
y15+3OH	1	1442.6580	1442.6533	-0.0047	-3.3
b17-H2O+3OH	1	1529.6689	1529.6578	-0.0111	-7.3
b17+3OH	1	1547.6795	1547.6720	-0.0075	-4.8
y16+4OH	1	1555.7057	1555.6970	-0.0087	-5.6
y17+4OH	1	1652.7582	1652.7543	-0.0039	-2.4
y18+4OH	1	1709.7799	1709.7695	-0.0104	-6.1
b19+4OH	1	1717.7486	1717.7375	-0.0111	-6.5
y19+5OH	1	1822.8276	1822.8176	-0.0100	-5.5

***Unlocalized sites: P707-OH?, K708-OH?**

Pseudolocalized sites: K708-OH

12_9_2011Col5a1_Trypsin_target_MS3 #1594 RT: 20.70 AV: 1 NL: 9.31E4
T: FTMS + c NSI d Full ms2 988.94@cid35.00 [260.00-1990.00]



14.

K708-OH.Gal.Glc

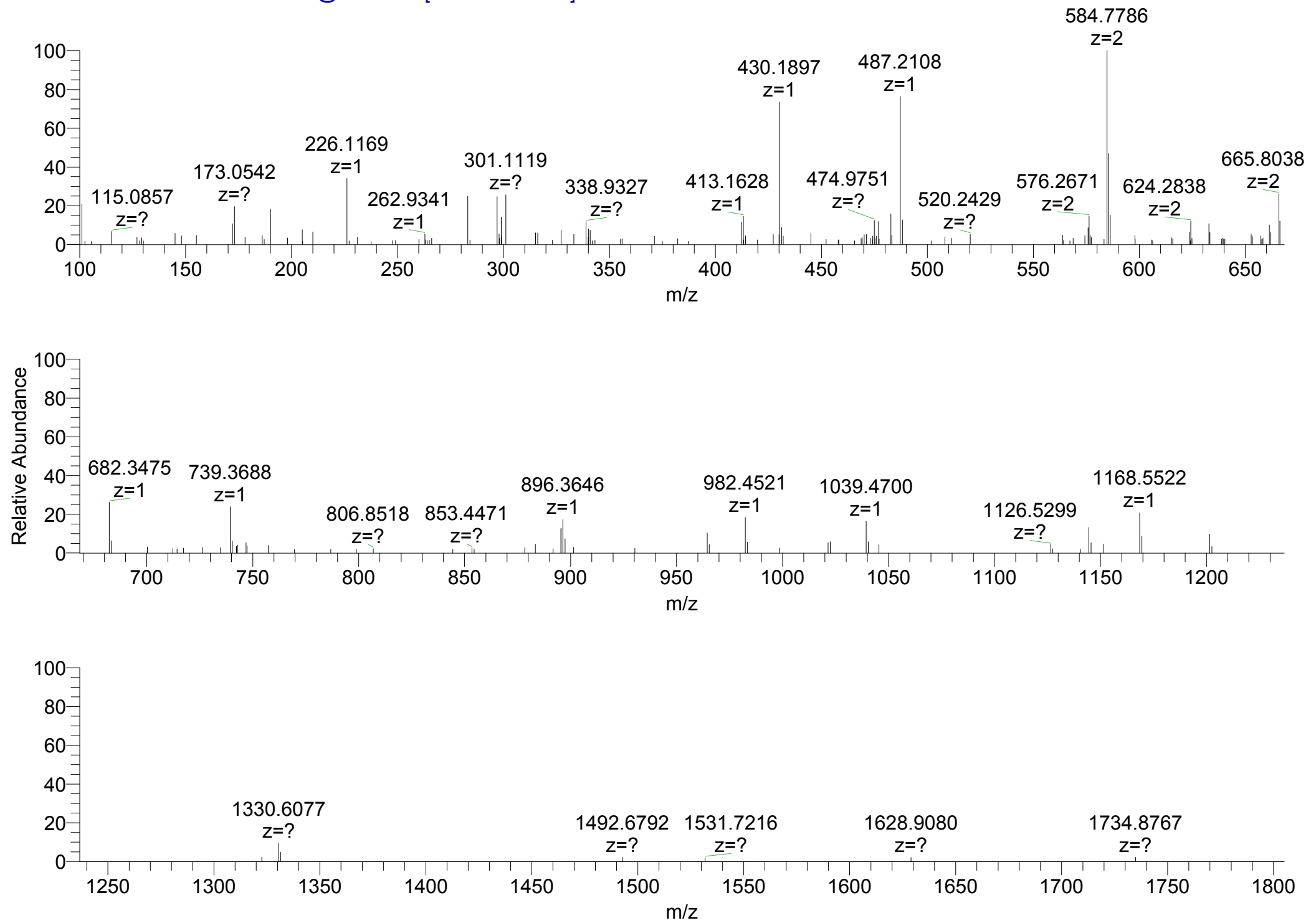
#702-716: DGQPGP**K**GNVGPQGE

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+2OH+Gal.Glc	2	896.8896	896.8809	-0.0174	-9.7
b2	1	173.0557	173.0542	-0.0015	-8.7
PQ	1	226.1186	226.1169	-0.0017	-7.6
b3	1	301.1143	301.1119	-0.0024	-8.0
y4-NH3	1	413.1667	413.1628	-0.0039	-9.5
y4	1	430.1932	430.1897	-0.0035	-8.2
y5	1	487.2147	487.2108	-0.0039	-8.0
y12+2OH	2	584.7833	584.7786	-0.0094	-8.1
b13-NH3+2OH	2	624.2862	624.2838	-0.0048	-3.9
y12+2OH+Gal	2	665.8097	665.8083	-0.0028	-2.1
PGPKGNV+2OH	1	682.3519	682.3475	-0.0044	-6.5
PGPKGNVG+2OH	1	739.3733	739.3688	-0.0045	-6.1
b10+2OH	1	982.4588	982.4521	-0.0067	-6.8
b11+2OH	1	1039.4803	1039.4700	-0.0103	-9.9
y12+2OH	1	1168.5593	1168.5522	-0.0071	-6.1
y12+2OH+Gal	1	1330.6121	1330.6077	-0.0044	-3.3

***Unlocalized sites: P705-OH?, P707-OH?**

Pseudolocalized sites: P705-OH

12_9_2011Col5a1_AspNGluC_1 #1065 RT: 10.73 AV: 1 NL: 1.97E4
T: FTMS + c NSI d Full ms2 896.88@hcd30.00 [100.00-1805.00]



15.

P717-OH, P726-OH, P732-OH, P741-OH, K744-OH

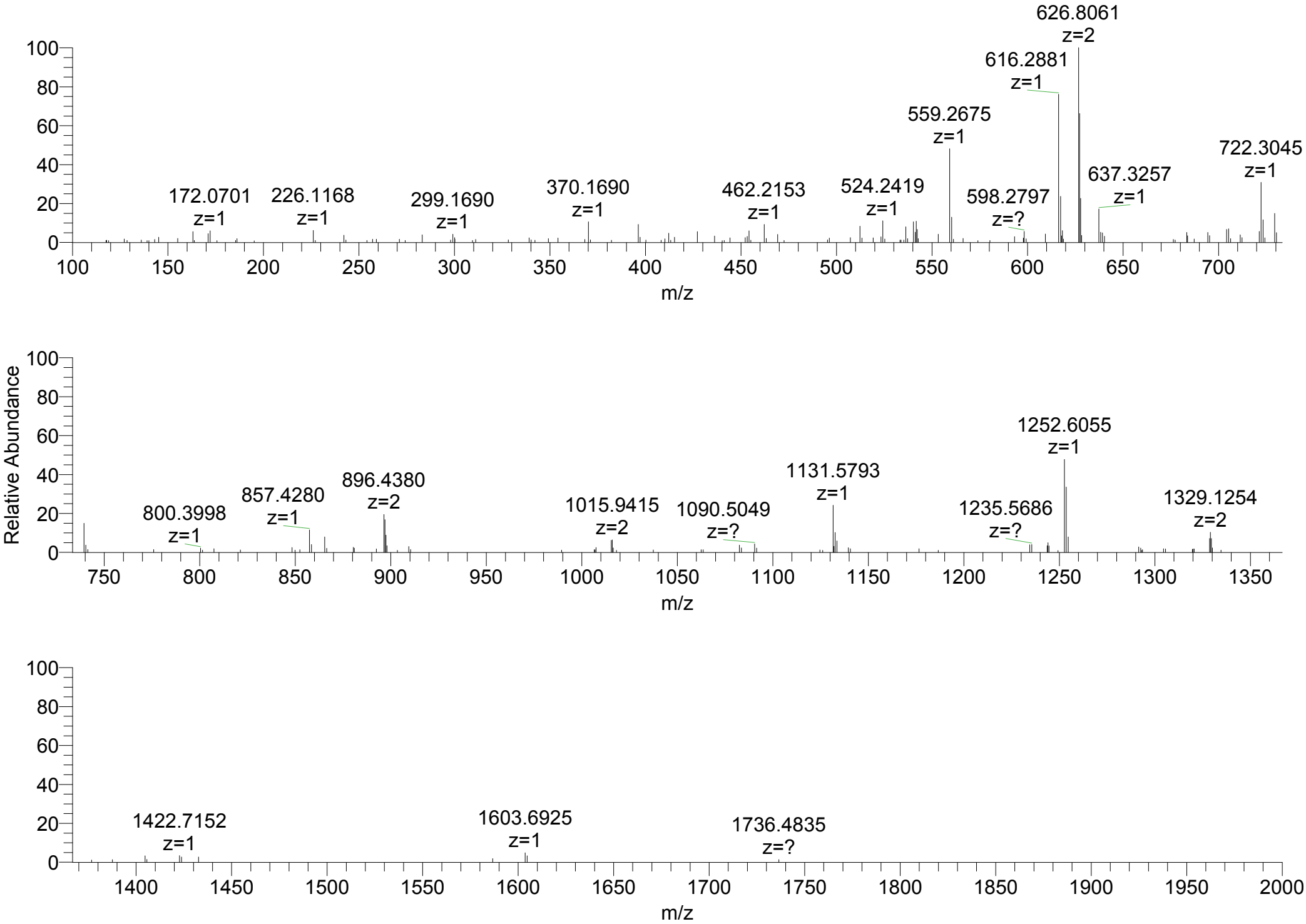
#709-744: GNVGPQGE**P**GPPGQQGN**P**GAQGL**P**GPQGAIGP**P**GE**K**

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+6OH	3	1132.2013	1132.1937	-0.0228	-6.7
y4+2OH	1	462.2195	462.2153	-0.0042	-9.1
y5+2OH	1	559.2722	559.2675	-0.0047	-8.4
y6+2OH	1	616.2937	616.2881	-0.0056	-9.1
y13+3OH	2	626.8120	626.8061	-0.0118	-9.4
b8-NH3	1	722.3104	722.3045	-0.0059	-8.2
y7+2OH	1	729.3717	729.3708	-0.0009	-1.2
b8	1	739.3369	739.3306	-0.0063	-8.5
y9+2OH	1	857.4363	857.4280	-0.0083	-9.7
y19+4OH	2	896.4472	896.4380	-0.0184	-10.3
b10+OH	1	909.4061	909.3950	-0.0111	-12.2
y11+2OH	1	1082.5477	1082.5372	-0.0105	-9.7
y13+3OH	1	1252.6168	1252.6055	-0.0113	-9.0
b17+2OH	1	1603.7095	1603.6925	-0.0170	-10.6

***Unlocalized sites: P719-OH?, P720-OH?**

Pseudolocalized sites: P720-OH

12_9_2011Col5a1_Trypsin_CE30_nontrapping #5713 RT: 55.69 AV: 1 NL: 3.61E4
T: FTMS + c NSI d Full ms2 1132.86@hcd30.00 [100.00-2000.00]



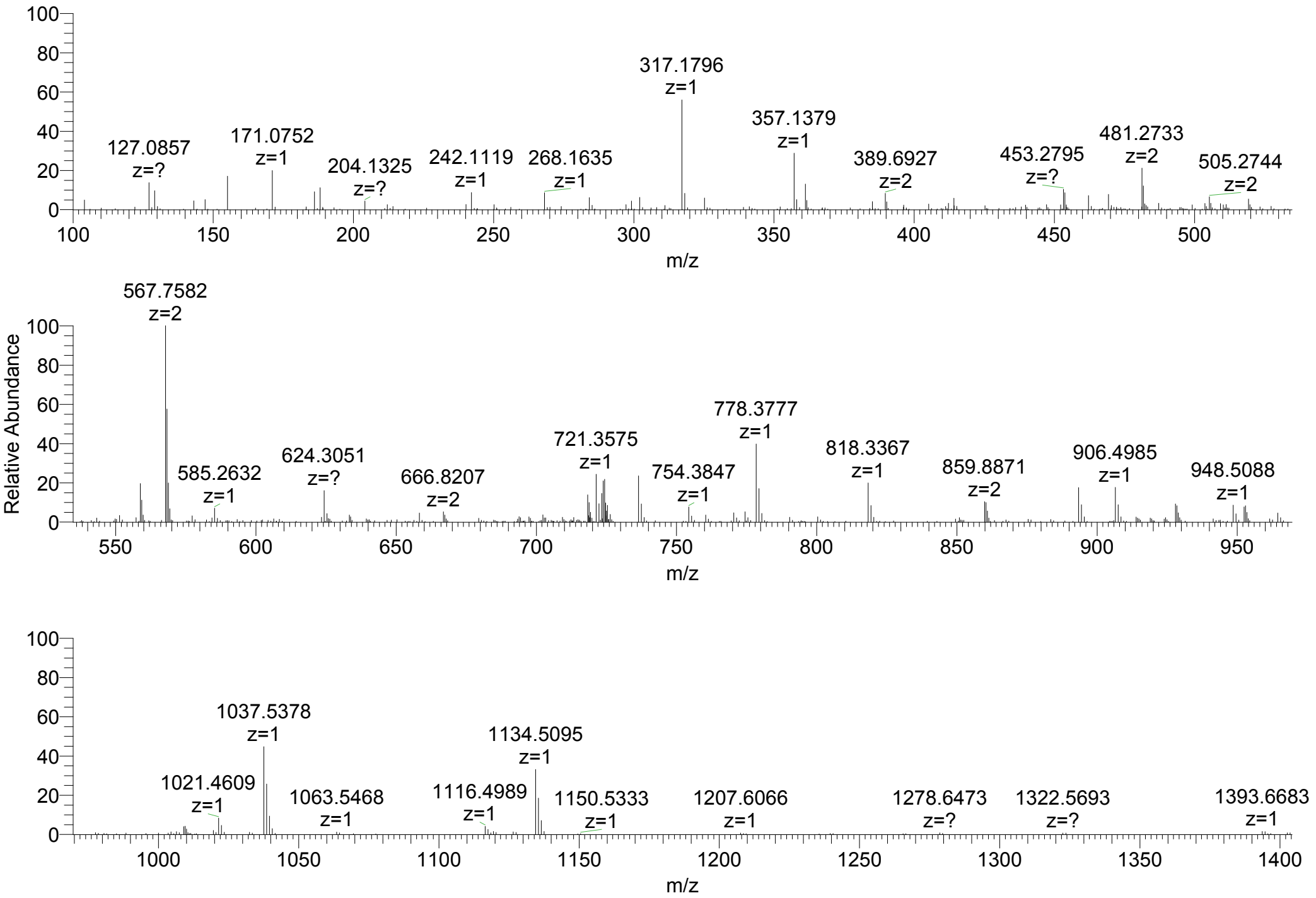
16.

P750-OH, P753-OH, P756-OH, P762-OH, P765-OH

#745-767: GPLGK**P**GL**P**GM**P**GADGP**P**GH**P**GK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+5OH	3	724.3565	724.3506	-0.0177	-8.2
y2	1	204.1343	204.1325	-0.0018	-8.9
b3/PLG	1	268.1656	268.1635	-0.0021	-7.9
y3+OH	1	317.1819	317.1796	-0.0023	-7.3
PGAD+OH	1	357.1405	357.1379	-0.0026	-7.3
y7+2OH	2	361.1850	361.1826	-0.0048	-6.7
y8+2OH	2	389.6958	389.6927	-0.0062	-8.0
y12-H2O+3OH	2	558.7570	558.7531	-0.0078	-7.0
y12+3OH	2	567.7624	567.7582	-0.0084	-7.4
y6+2OH	1	624.3100	624.3051	-0.0049	-7.9
y7+2OH	1	721.3628	721.3575	-0.0053	-7.4
b8+OH	1	736.4352	736.4299	-0.0053	-7.2
y8+2OH	1	778.3842	778.3777	-0.0065	-8.4
y18+5OH	2	859.8938	859.8871	-0.0134	-7.8
b10+2OH	1	906.5043	906.4985	-0.0058	-6.4
y11+2OH	1	1021.4697	1021.4609	-0.0088	-8.6
b11+2OH	1	1037.5448	1037.5378	-0.0070	-6.8
y12+3OH	1	1134.5174	1134.5095	-0.0079	-7.0

12_9_2011Col5a1_Trypsin_CE30_nontrapping #5040 RT: 49.85 AV: 1 NL: 1.73E5
T: FTMS + c NSI d Full ms2 724.68@hcd30.00 [100.00-2000.00]



17.

K774-OH.Gal.Glc, P780-OH, P789-OH

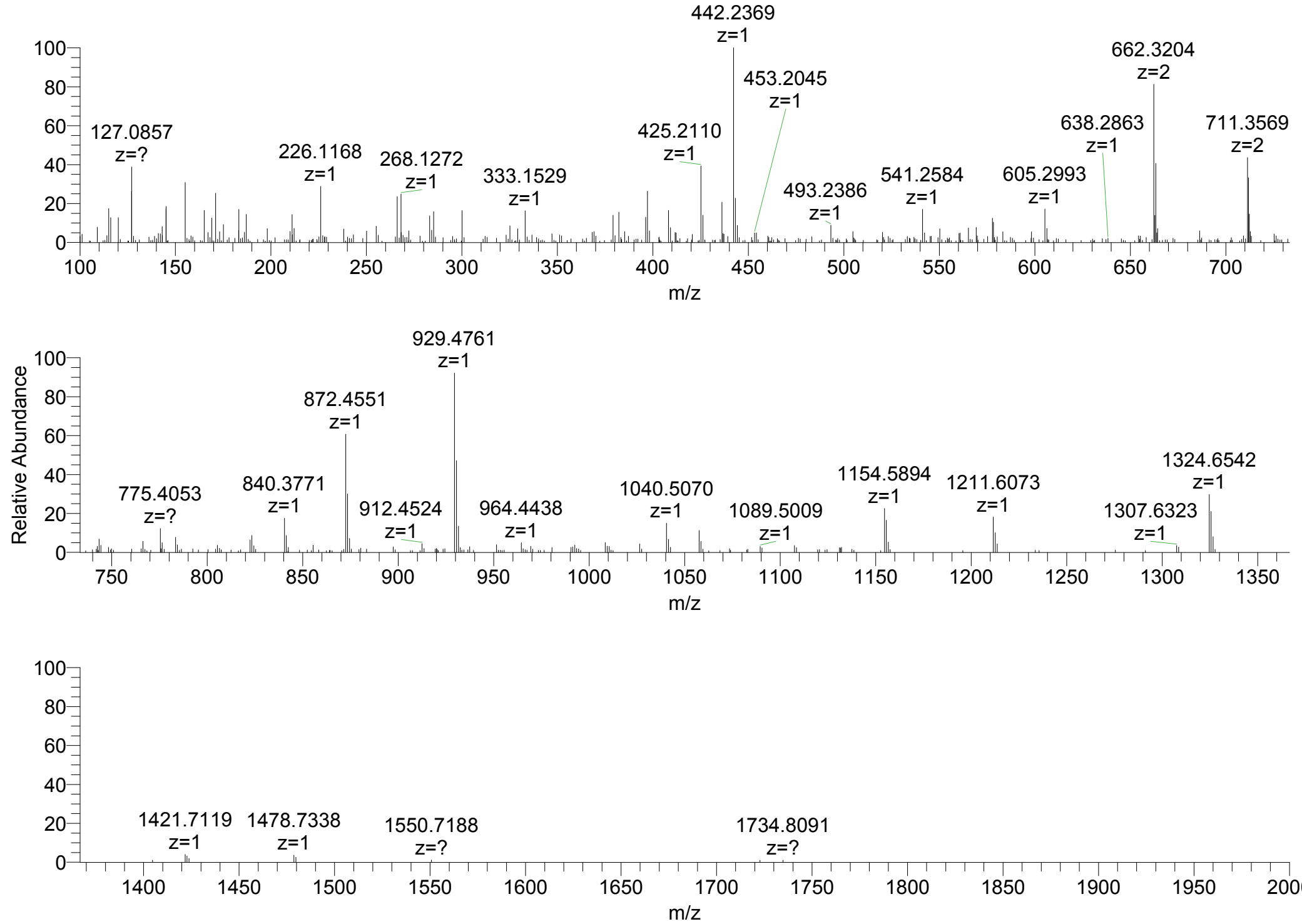
#768-792: EGPPGE**K**GGQGP**P**GPQGPIGY**P**GPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+4OH+Gal.Glc	3	924.4263	924.4192	-0.0213	-7.7
GP-28	1	127.0866	127.0857	-0.0009	-7.1
PQ	1	226.1186	226.1168	-0.0018	-8.0
PGP+OH	1	268.1292	268.1272	-0.0020	-7.5
y2	1	272.1717	272.1700	-0.0017	-6.3
GQGPP-28+OH/ y4-NH3+OH	1	425.2143	425.2110	-0.0033	-7.8
y4+OH	1	442.2409	442.2369	-0.0040	-9.1
PPGPQ+OH	1	493.2405	493.2385	-0.0020	-4.1
PPGEK+2OH	1	541.2617	541.2584	-0.0033	-6.1
y5+OH	1	605.3042	605.2993	-0.0049	-8.1
y6+OH	1	662.3257	662.3204	-0.0053	-8.0
y13+2OH	2	662.8359	662.8297	-0.0124	-9.4
y14+2OH	2	711.3622	711.3569	-0.0106	-7.5
y7+OH	1	775.4097	775.4053	-0.0044	-5.7
y8+OH	1	872.4625	872.4551	-0.0074	-8.5
y9+OH	1	929.4839	929.4761	-0.0078	-8.4
y10-NH3+OH	1	1040.5160	1040.5070	-0.0090	-8.7
y10+OH	1	1057.5425	1057.5356	-0.0069	-6.5
y11+OH	1	1154.5953	1154.5894	-0.0059	-5.1
y12+OH	1	1211.6167	1211.6073	-0.0094	-7.8
y13+2OH	1	1324.6644	1324.6542	-0.0102	-7.7
y14+2OH	1	1421.7172	1421.7119	-0.0053	-3.7
y15+2OH	1	1478.7387	1478.7338	-0.0049	-3.3

***Unlocalized sites: P770-OH?, P771-OH?**

Pseudolocalized sites: P771-OH

12_9_2011Col5a1_Trypsin_CE40 #2176 RT: 20.69 AV: 1 NL: 6.20E4
T: FTMS + c NSI d Full ms2 924.75@hcd40.00 [100.00-2000.00]



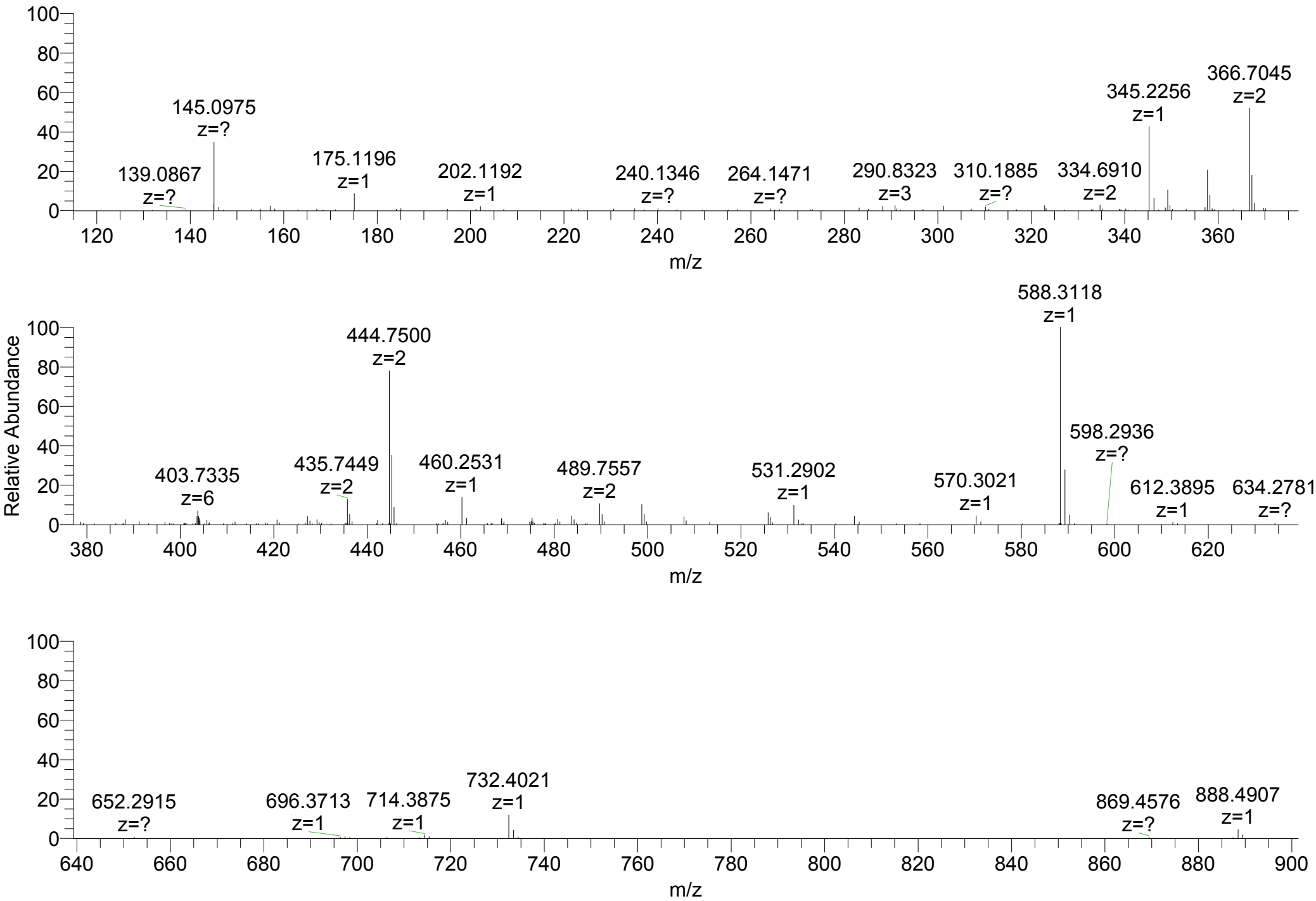
18.

K795-OH.Gal.Glc

#793-801: GV**K**GADGIR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+OH+Gal.Glc	3	404.8700	404.8701	0.0003	0.2
y1	1	175.1190	175.1196	0.0006	3.4
y3	1	345.2245	345.2256	0.0011	3.2
y7+OH	2	366.7036	366.7045	0.0018	2.5
[M+2H]-H2O+OH	2	435.7432	435.7449	0.0034	3.9
[M+2H]+OH	2	444.7485	444.7500	0.0030	3.4
y4	1	460.2514	460.2531	0.0017	3.7
y5	1	531.2885	531.2902	0.0017	3.2
y6-H2O	1	570.2994	570.3021	0.0027	4.7
y6	1	588.3100	588.3118	0.0018	3.1
y7+OH	1	732.3999	732.4021	0.0022	3.0
[M+H]+OH	1	888.4898	888.4907	0.0009	1.0

9_22_2011CollagenTrypsin_HCD_1 #522 RT: 7.17 AV: 1 NL: 5.84E4
T: FTMS + c NSI d Full ms2 404.87@hcd30.00 [115.00-1225.00]



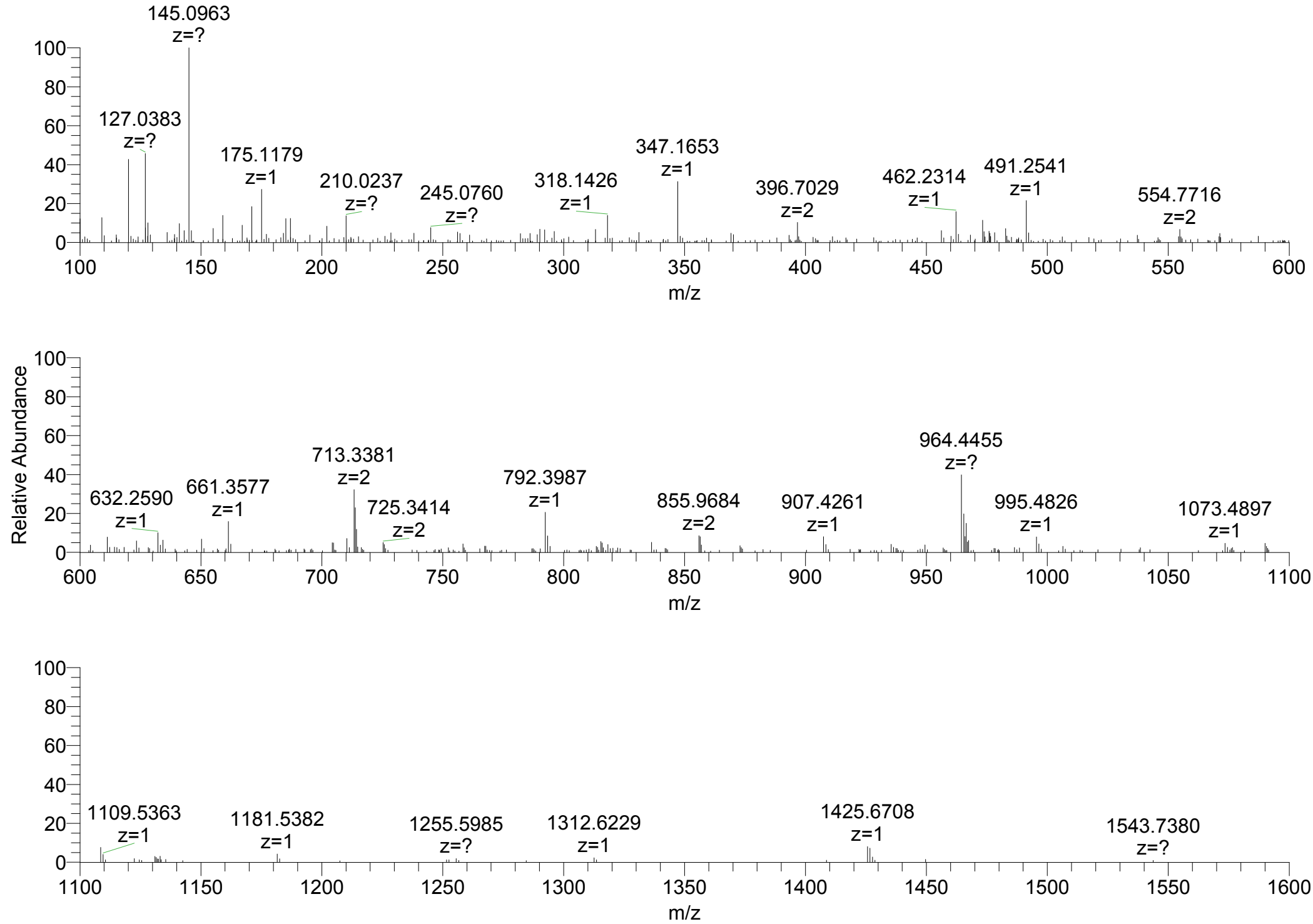
19.

K810-OH.Gal.Glc, P816-OH, K819-OH.Gal.Glc, K825-OH.Gal.Glc

#808-828: GE**K**GEDGF**P**GF**K**GDMGI**K**GDR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+4OH+3Gal.Glc	4	809.0882	809.0820	-0.0248	-7.7
y1	1	175.1190	175.1179	-0.0011	-6.3
y3	1	347.1674	347.1653	-0.0021	-6.1
y7+OH	2	396.7053	396.7029	-0.0048	-6.1
y4+OH	1	491.2572	491.2541	-0.0031	-6.3
y10+2OH	1	554.7744	554.7716	-0.0028	-5.1
y6+OH	1	661.3628	661.3577	-0.0051	-7.7
y13+3OH	2	713.3432	713.3381	-0.0102	-7.2
y7+OH	1	792.4032	792.3981	-0.0051	-6.4
y8+OH	1	907.4302	907.4261	-0.0041	-4.5
y9+OH	1	964.4517	964.4455	-0.0062	-6.4
y10+2OH	1	1108.5415	1108.5354	-0.0061	-5.5
y13+3OH	1	1425.6791	1425.6708	-0.0083	-5.8

12_9_2011Col5a1_Trypsin_CE40 #2314 RT: 21.86 AV: 1 NL: 5.57E4
T: FTMS + c NSI d Full ms2 809.08@hcd40.00 [100.00-2000.00]



20.

P833-OH, P834-OH, K846-OH.Gal.Glc

#829-848: GEIG**PP**GPRGEDGPEGP**K**GR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+3OH+Gal.Glc	4	583.5200	583.5144	-0.0224	-9.6
GE-28	1	159.0764	159.0756	-0.0008	-5.1
GE/b2	1	187.0713	187.0703	-0.0010	-5.4
b4	1	357.1769	357.1744	-0.0025	-7.0
y8+OH	2	407.2143	407.2123	-0.0040	-4.9
y16+3OH	3	550.9325	550.9297	-0.0084	-5.1
y17+3OH	3	569.9397	569.9368	-0.0087	-5.1
y18+3OH	3	607.6344	607.6310	-0.0102	-5.6
y14+OH	2	712.8475	712.8446	-0.0058	-4.1
y15+2OH	2	769.3713	769.3658	-0.0110	-7.2
y8+OH	1	813.4213	813.4161	-0.0052	-6.4
y16+3OH	2	825.8952	825.8911	-0.0082	-5.0
y17+3OH	2	854.4059	854.4008	-0.0102	-6.0
y18+3OH	2	910.9479	910.9422	-0.0114	-6.3
y17+3OH+Gal	2	935.4323	935.4269	-0.0108	-5.8
y18+3OH+Gal	2	991.9743	991.9700	-0.0086	-4.3

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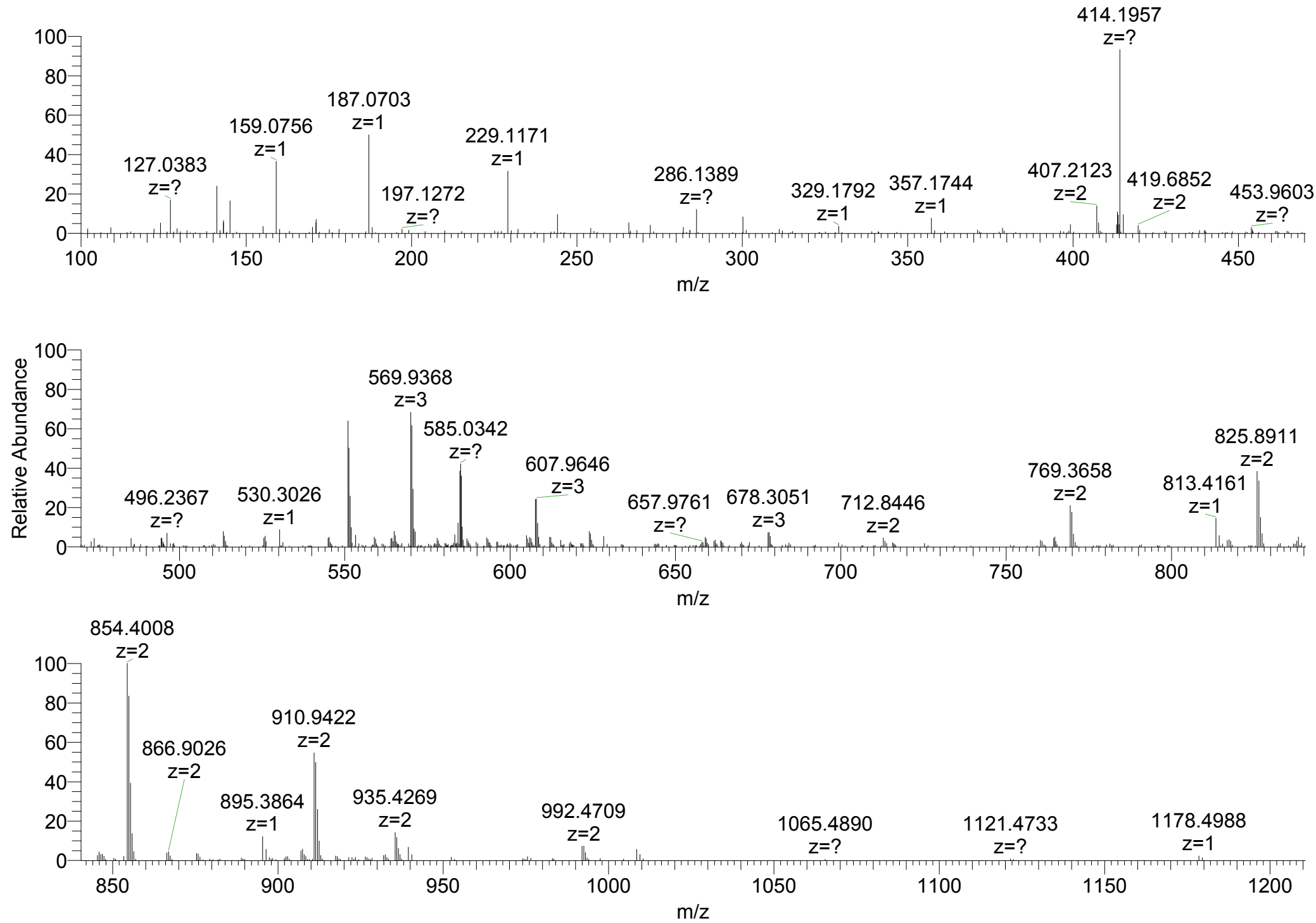
12_9_2011Col5a1_ArgC_3 #1260 RT: 12.67 AV: 1 NL: 1.60E5
T: FTMS + c NSI d Full ms2 583.77@hcd30.00 [100.00-2000.00]



21.

P855-OH

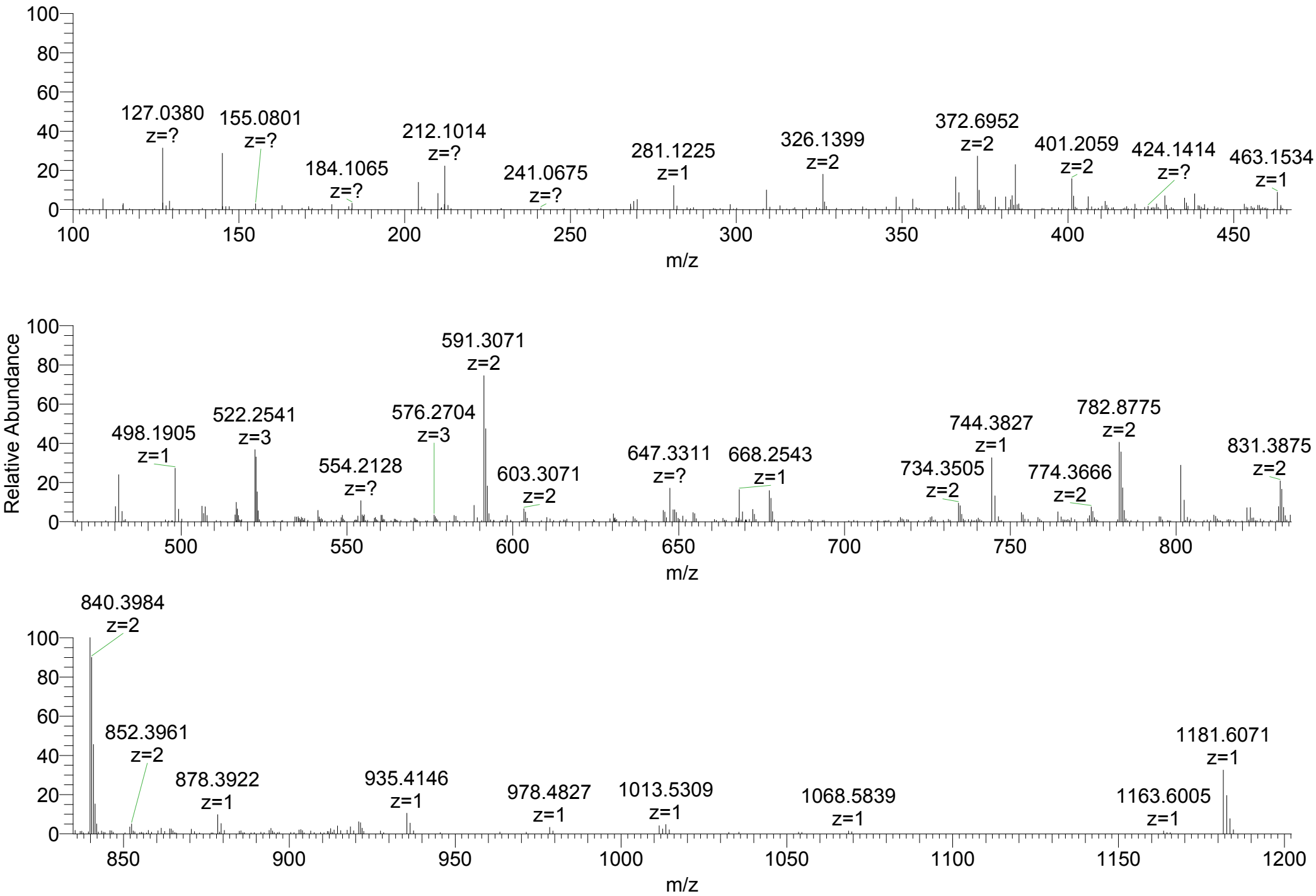
#849-866: GGPNGD**P**GPLGPPGEKGK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+3OH+Gal.Glc	3	668.3078	668.3015	-0.0189	-9.4
b3/PN	1	212.1030	212.1014	-0.0016	-7.6
a4-NH3	1	281.1244	281.1225	-0.0019	-6.8
b4-NH3	1	309.1193	309.1168	-0.0025	-8.1
b4/GPNG	1	326.1459	326.1399	-0.0060	-18.5
y7+2OH	2	372.6980	372.6952	-0.0056	-7.5
y8+2OH	2	401.2087	401.2059	-0.0056	-7.0
b6-H2O-NH3	1	463.1572	463.1534	-0.0038	-8.2
b6	1	498.1943	498.1905	-0.0038	-7.6
y10+2OH	2	506.2771	506.2725	-0.0092	-9.1
y16+3OH	3	522.2582	522.2541	-0.0123	-7.9
y12+3OH	2	591.3117	591.3071	-0.0092	-7.8
y6+2OH	1	647.3359	647.3311	-0.0048	-7.4
b8+OH	1	668.2634	668.2543	-0.0091	-13.6
y14+3OH	2	677.3359	677.3304	-0.0110	-8.1
y15+3OH	2	734.3573	734.3505	-0.0136	-9.3
y7+2OH	1	744.3886	744.3827	-0.0059	-7.9
y16+3OH	2	782.8837	782.8775	-0.0124	-7.9
y8+2OH	1	801.4101	801.4042	-0.0059	-7.4
[M+2H]+3OH	2	839.9052	839.8974	-0.0156	-9.3
b10+OH	1	878.4003	878.3922	-0.0081	-9.2
b11+OH	1	935.4217	935.4146	-0.0071	-7.6
y12+3OH	1	1181.6161	1181.6071	-0.0090	-7.6

***Unlocalized sites: P861-OH?, K864-OH.Gal.Glc?, K866-OH.Gal.Glc**

Pseudolocalized sites: P861-OH, K864-OH.Gal.Glc

12_9_2011Col5a1_Trypsin_CE30 #1129 RT: 12.00 AV: 1 NL: 1.41E5
T: FTMS + c NSI d Full ms2 669.30@hcd30.00 [100.00-2000.00]



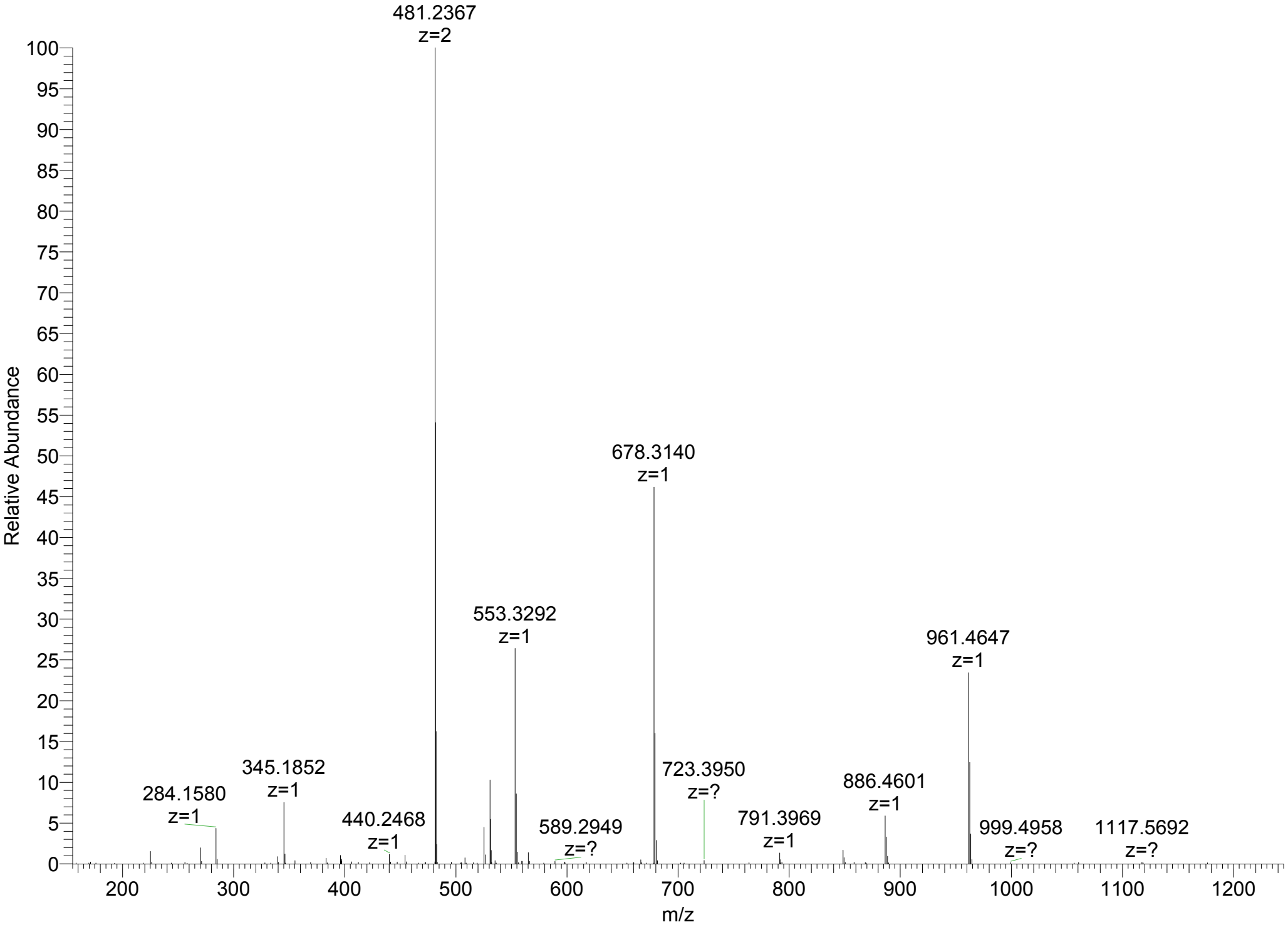
22.

P870-OH, P873-OH, P876-OH

#867-878: LGV**P**GL**P**GY**P**GR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+3OH	2	615.8275	615.8218	-0.0114	-9.3
y3+OH	1	345.1881	345.1852	-0.0029	-8.4
b5+OH/GVPGL+OH	1	440.2504	440.2468	-0.0036	-8.2
y9+3OH	2	481.2405	481.2367	-0.0076	-7.9
y10+3OH	2	530.7747	530.7693	-0.0108	-10.2
b6+OH	1	553.3344	553.3292	-0.0052	-9.4
y6+2OH	1	678.3206	678.3140	-0.0066	-9.7
y7+2OH	1	791.4046	791.3969	-0.0077	-9.7
b9+2OH	1	886.4669	886.4601	-0.0068	-7.7
y9+3OH	1	961.4738	961.4647	-0.0091	-9.5

12_9_2011Col5a1_Trypsin_target_MS3 #2575 RT: 31.83 AV: 1 NL: 1.27E6
T: FTMS + c NSI d Full ms2 615.82@cid35.00 [155.00-1245.00]



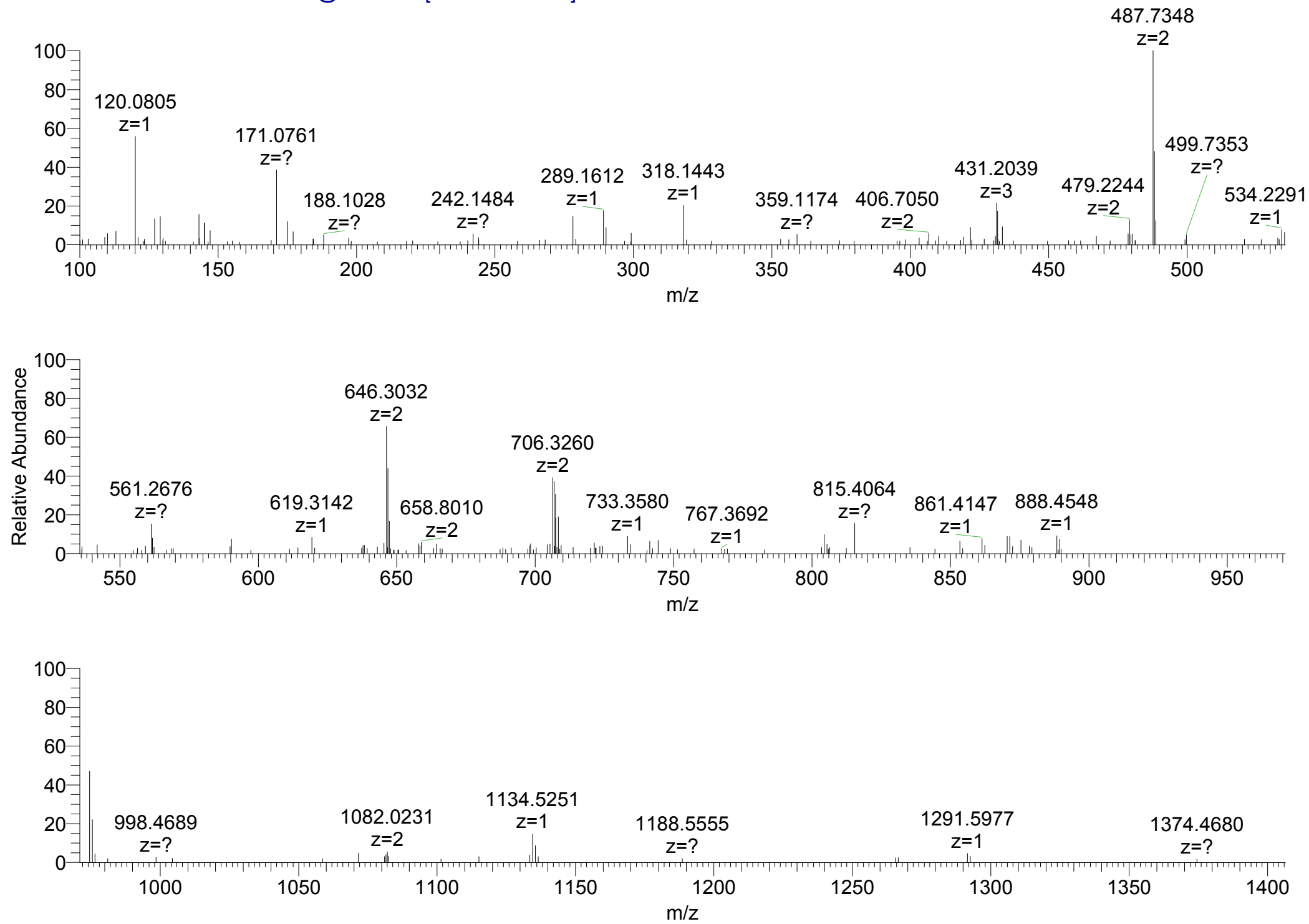
23.

K882-OH.Gal.Glc, P888-OH, P891-OH, K897-OH.Gal.Glc

#879-900: QGP**K**GSIGF**P**GF**P**GANGE**K**GGR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+4OH+2Gal.Glc	4	707.5714	707.5703	-0.0044	-1.6
F	1	120.0808	120.0805	-0.0003	-2.5
PG+OH	1	171.0764	171.0761	-0.0003	-1.8
PGF+OH/GFP+OH	1	318.1448	318.1443	-0.0005	-1.6
y13+3OH	3	431.2057	431.2039	-0.0054	-4.2
y10-NH3+2OH	2	479.2229	479.2244	0.0030	3.1
y10+2OH	2	487.7361	487.7348	-0.0026	-2.7
y6+OH	1	619.3158	619.3142	-0.0016	-2.6
y13+3OH	2	646.3049	646.3032	-0.0034	-2.6
y7+OH	1	733.3587	733.3580	-0.0007	-1.0
b9+OH	1	888.4574	888.4548	-0.0026	-2.9
y10+2OH	1	974.4650	974.4625	-0.0025	-2.6
y13	1	1291.6062	1291.5977	-0.0085	-6.6

10_7_2011Collagen_Trypsin_HCDandETD_111009033323 #3471 RT: 24.64 AV: 1 NL: 3.79E4
T: FTMS + c NSI d Full ms2 707.82@hcd35.00 [100.00-2000.00]



24.

P903-OH

#901-909: GT**P**GKPGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+2OH	2	499.7407	499.7373	-0.0068	-6.8
K	1	129.1022	129.1012	-0.0010	-7.8
b2	1	159.0764	159.0757	-0.0007	-4.4
PGK+OH/GKP+OH/ KPG+OH	1	299.1714	299.1692	-0.0022	-7.4
y7+2OH	2	370.7061	370.7034	-0.0054	-7.3
y4+OH	1	442.2409	442.2369	-0.0040	-9.1
y6+OH	1	627.3573	627.3539	-0.0034	-5.4
y7+2OH	1	740.4050	740.3983	-0.0067	-9.1

***Unlocalized sites: P906-OH?, P908-OH?**

Pseudolocalized sites: P906-OH

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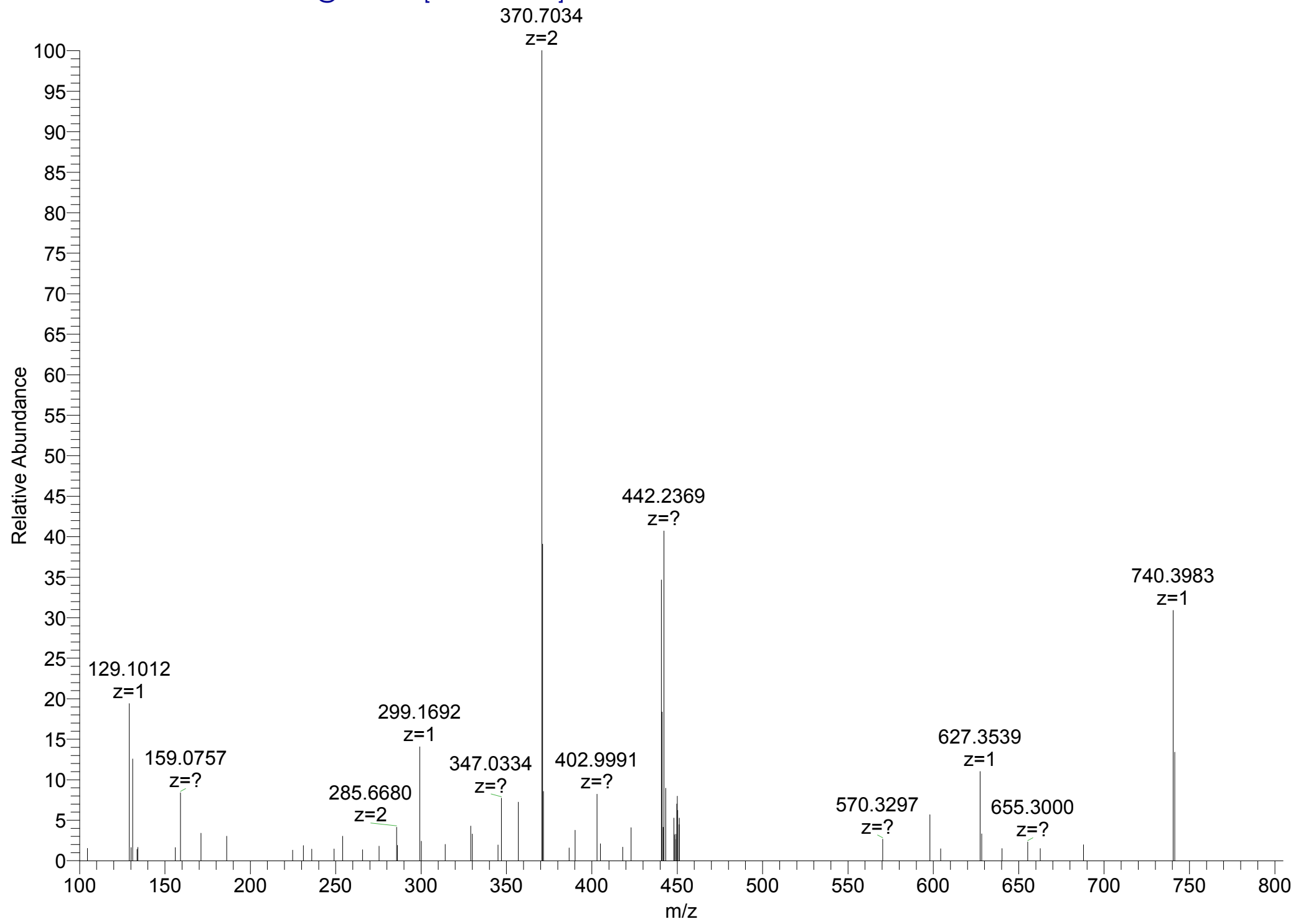
12_9_2011Col5a1_ArgC_3 #199 RT: 3.04 AV: 1 NL: 2.23E4
T: FTMS + c NSI d Full ms2 449.74@hcd30.00 [100.00-910.00]



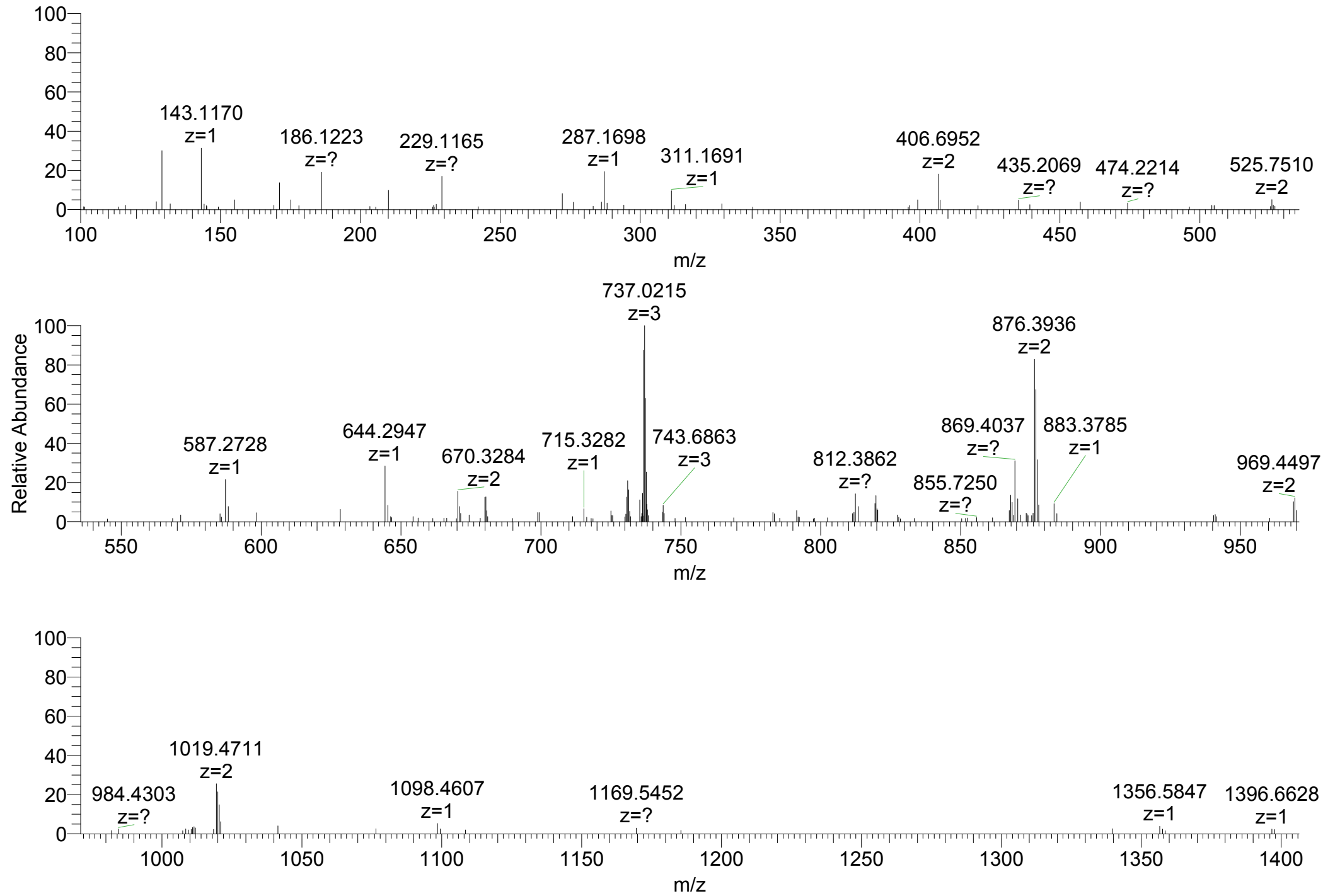
25.

P930-OH, P944-OH, P945-OH

#925-948: GITGK**P**GPKGNSGGDGPAG**PP**GER

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+3OH	3	736.6928	736.6862	-0.0198	-9.0
y8+2OH	2	406.6985	406.6952	-0.0066	-8.1
y5+2OH	1	587.2784	587.2728	-0.0056	-9.6
y6+2OH	1	644.2998	644.2947	-0.0051	-7.9
b15+OH	2	670.3337	670.3284	-0.0106	-7.9
y7+2OH	1	715.3369	715.3282	-0.0087	-12.2
[M+3H]+3OH	3	736.6928	736.6868	-0.0180	-8.2
y17+2OH	2	791.3662	791.3610	-0.0104	-6.6
y8+2OH	1	812.3897	812.3862	-0.0035	-4.3
y19+3OH	2	876.4008	876.3936	-0.0144	-8.2
y21+3OH	2	968.9590	968.9550	-0.0080	-4.1
y22+3OH	2	1019.4829	1019.4711	-0.0236	-11.6
y12+3OH	1	1098.4810	1098.4607	-0.0203	-18.5
y15+2OH	1	1356.5775	1356.5847	0.0072	5.3

12_9_2011Col5a1_ArgC_3 #981 RT: 10.28 AV: 1 NL: 2.59E4
T: FTMS + c NSI d Full ms2 737.02@hcd30.00 [100.00-2000.00]



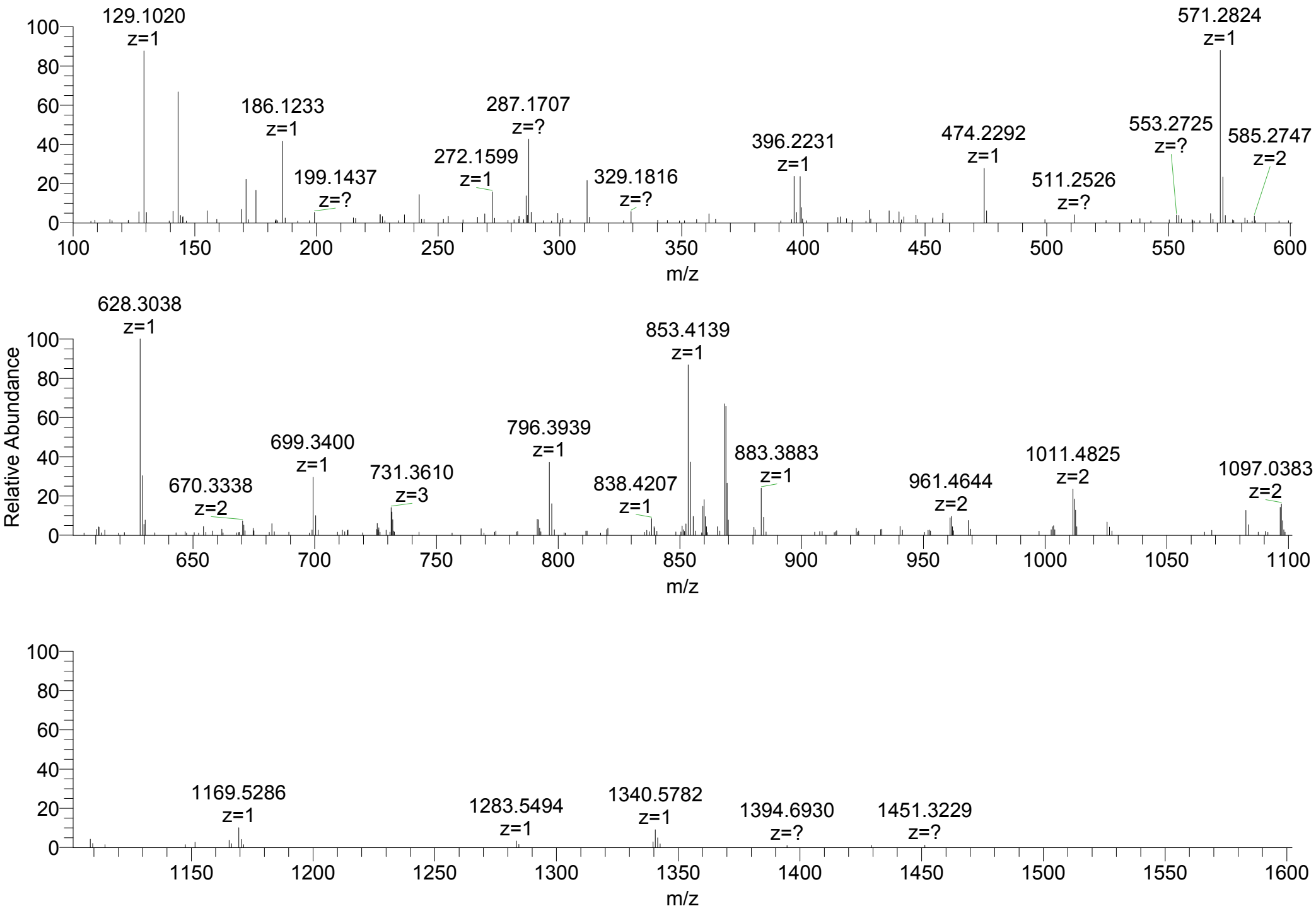
26.

K933-OH.Gal.Glc, P945-OH

#925-948: GITGKPGP**K**GNSGGDGPAGP**P**GER

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+Gal.Glc	3	839.3964	839.3944	-0.0060	-2.4
K	1	129.1022	129.1020	-0.0002	-1.6
a2	1	143.1179	143.1177	-0.0002	-1.4
GK	1	186.1237	186.1233	-0.0004	-2.2
ITG/b3/PRG	1	272.1605	272.1599	-0.0006	-2.2
TGK	1	287.1714	287.1707	-0.0007	-2.4
b4-H2O/ AGPP-28+OH	1	311.1714	311.1709	-0.0005	-1.6
PGPK+OH	1	396.2241	396.2231	-0.0010	-2.5
y9+OH	2	427.2118	427.2114	-0.0008	-0.9
y4+OH	1	474.2307	474.2293	-0.0014	-3.0
y5+OH	1	571.2835	571.2824	-0.0011	-1.9
y6+OH	1	628.3049	628.3038	-0.0011	-1.8
b15+OH	2	670.3337	670.3338	0.0002	0.1
y7+OH	1	699.3420	699.3400	-0.0020	-2.9
[M+3H]+2OH	3	731.3612	731.3610	-0.0006	-0.3
y8+OH	1	796.3948	796.3939	-0.0009	-1.1
y9+OH	1	853.4163	853.4139	-0.0024	-2.8
y19+2OH	2	868.4033	868.4013	-0.0040	-2.3
y21+2OH	2	960.9616	960.9589	-0.0054	-2.8
y22+2OH	2	1011.4854	1011.4825	-0.0058	-2.9
y13+OH	1	1169.5182	1169.5286	0.0104	8.9
y14+OH	1	1283.5611	1283.5494	-0.0117	-9.1
y15+OH	1	1340.5825	1340.5782	-0.0043	-3.2

10_7_2011Collagen_Trypsin_HCDandETD_111009033323 #1625 RT: 14.37 AV: 1 NL: 1.49E5
T: FTMS + c NSI d Full ms2 839.73@hcd35.00 [100.00-2000.00]



27.

P960-OH

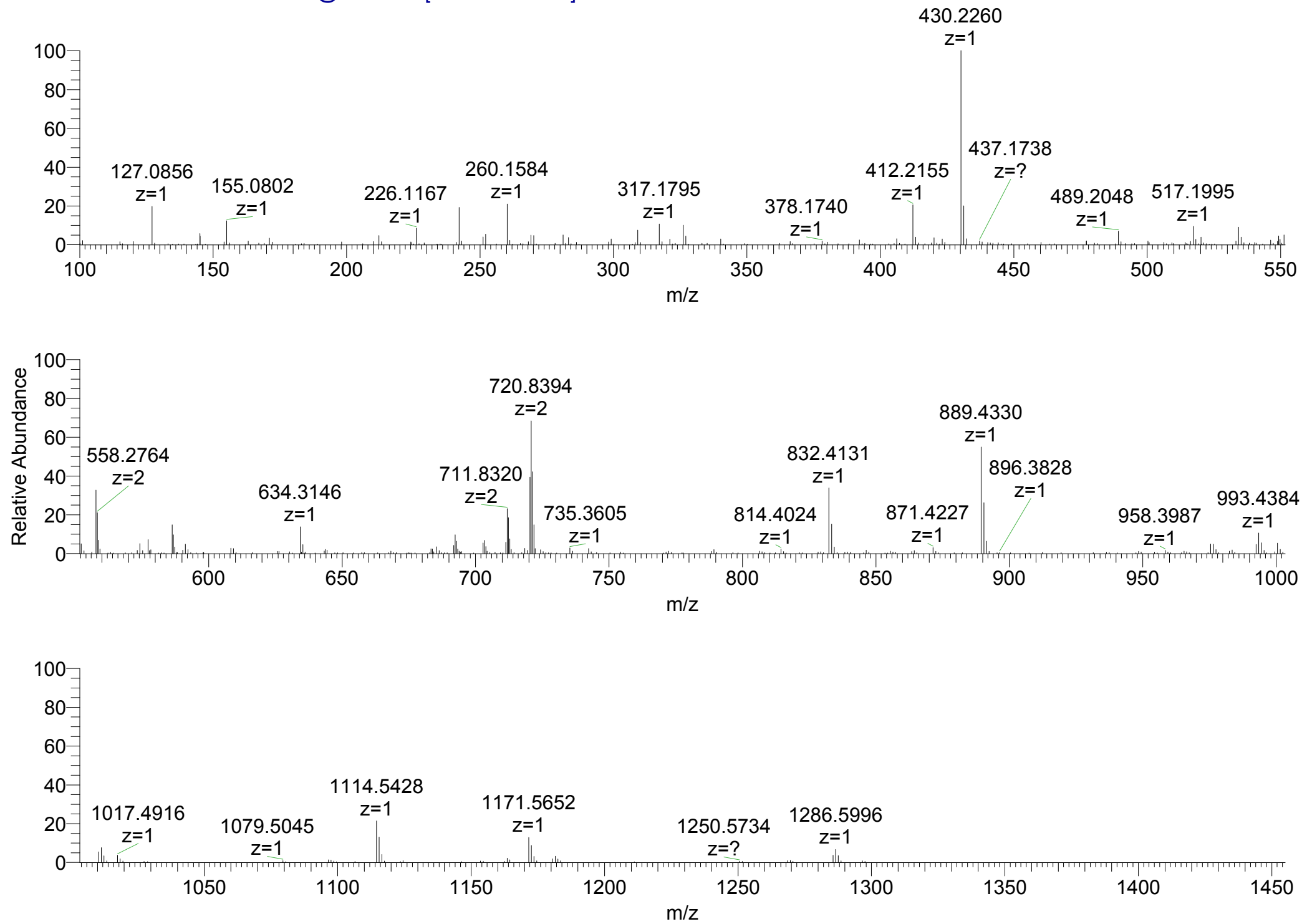
#949-963: GPNGPQGPTGF**P**GPK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+2OH	2	720.3493	720.3426	-0.0134	-9.3
b2/GP	1	155.0815	155.0802	-0.0013	-8.4
y2+OH	1	260.1605	260.1584	-0.0021	-8.1
y3+OH	1	317.1819	317.1795	-0.0024	-7.6
y4+2OH	1	430.2296	430.2296	0.0000	0.0
b6-2NH3	1	517.2041	517.1995	-0.0046	-8.9
y11+2OH	2	557.7800	557.7754	-0.0092	-8.3
y12+2OH	2	586.2907	586.2853	-0.0108	-9.2
y6+2OH	1	634.3195	634.3146	-0.0049	-7.7
[M+2H]-H2O+2OH	2	711.3440	711.3383	-0.0114	-8.0
[M+2H]+2OH	2	720.3493	720.3416	-0.0154	-10.7
y7+2OH	1	735.3672	735.3605	-0.0067	-9.1
y8+2OH	1	832.4199	832.4131	-0.0068	-8.2
y9+2OH	1	889.4414	889.4330	-0.0084	-9.5
y11+2OH	1	1114.5527	1114.5428	-0.0099	-8.9
y12+2OH	1	1171.5742	1171.5652	-0.0090	-7.7

***Unlocalized sites: P962-OH?, K963-OH?**

Pseudolocalized sites: K963-OH

12_9_2011Col5a1_Trypsin_CE30 #2101 RT: 20.27 AV: 1 NL: 1.27E6
T: FTMS + c NSI d Full ms2 720.34@hcd30.00 [100.00-1455.00]



28.

P966-OH, P969-OH, P975-OH, P978-OH

#964-981: GP**P**GP**P**GKDGL**P**GH**P**GQR

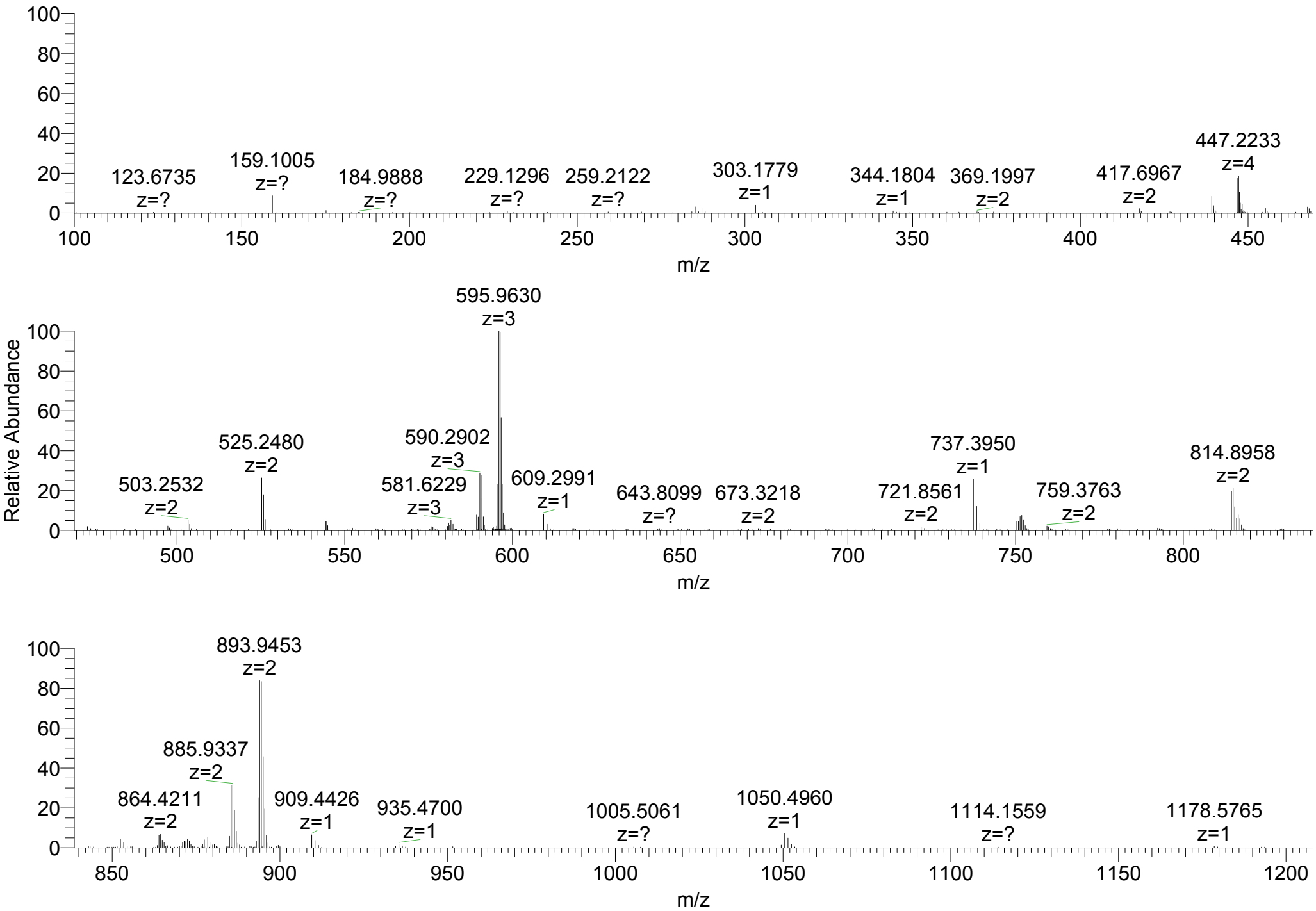
MS^2: GPPGPPGKDGL**P**GH**P**GQR (ETD)

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+4OH	4	446.9723	446.9725	0.0008	0.4
z1	1	159.1002	159.1005	0.0003	1.9
z8+2OH	2	439.2237	439.2238	0.0002	0.2
[M+4H]+4OH	4	446.9723	446.9724	0.0004	0.2
z10+2OH	2	525.2479	525.2480	0.0002	0.2
[M+3H]+4OH(MS^3)	3	595.6273	595.6260	-0.0039	-2.2
c7+2OH	1	609.2991	609.2991	0.0000	0.0
c8+2OH	1	737.3941	737.3950	0.0009	1.2
c17+4OH	2	814.3948	814.3951	0.0006	0.4
c10+2OH	1	909.4425	909.4426	0.0001	0.1

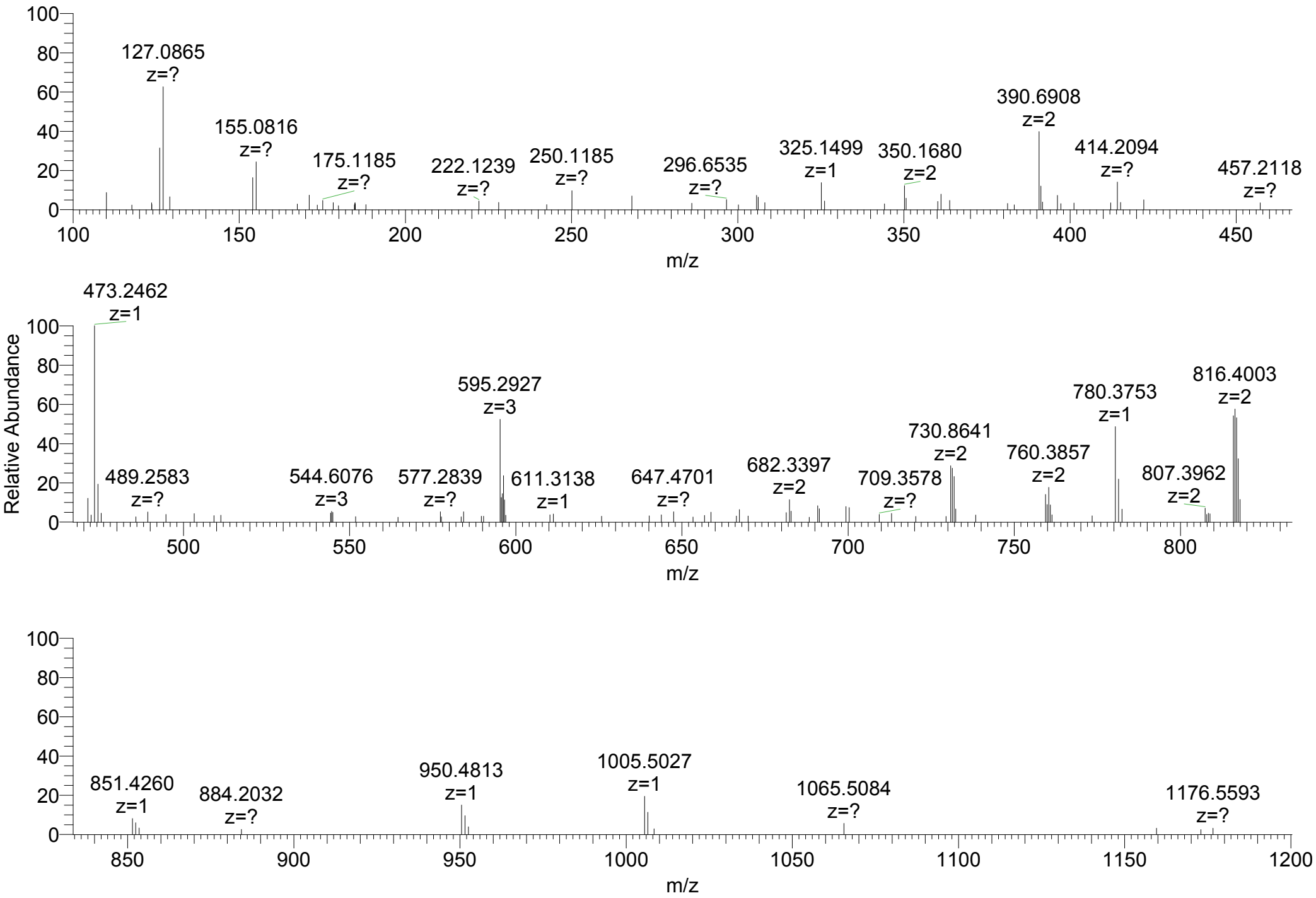
MS^3: GP**P**GP**P**GKDGL**P**GH**P**GQR (HCD)

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
a2	1	127.0866	127.0865	-0.0001	-0.8
b2/GP	1	155.0815	155.0815	0.0000	0.0
GPPG+OH/b4+OH	1	325.1506	325.1499	-0.0007	-2.2
y7+2OH	2	390.6910	390.6908	-0.0004	-0.5
y4+OH	1	473.2467	473.2462	-0.0005	-1.1
y16+4OH	3	544.2693	544.2690	-0.0009	-0.6
y13+3OH	2	682.3393	682.3397	0.0008	0.6
y14+3OH	2	730.8657	730.8641	-0.0032	-2.2
y15+3OH	2	759.3764	759.3748	-0.0032	-2.1
y7+2OH	1	780.3747	780.3753	0.0006	0.8
y16+4OH	2	815.9002	815.8990	-0.0024	-1.5
y9+2OH	1	950.4803	950.4813	0.0010	1.1
b11+2OH	1	1005.5000	1005.5027	0.0027	2.7

10_7_2011Collagen_Trypsin_MS3_ETDandHCD #1143 RT: 13.31 AV: 1 NL: 1.80E5
T: FTMS + c NSI d Full ms2 447.22@etd27.50 [100.00-1800.00]



10_7_2011Collagen_Trypsin_MS3_ETDandHCD #1144 RT: 13.32 AV: 1 NL: 1.37E4
T: FTMS + c NSI d Full ms3 447.22@etd36.67 595.96@hcd30.00 [100.00-1800.00]



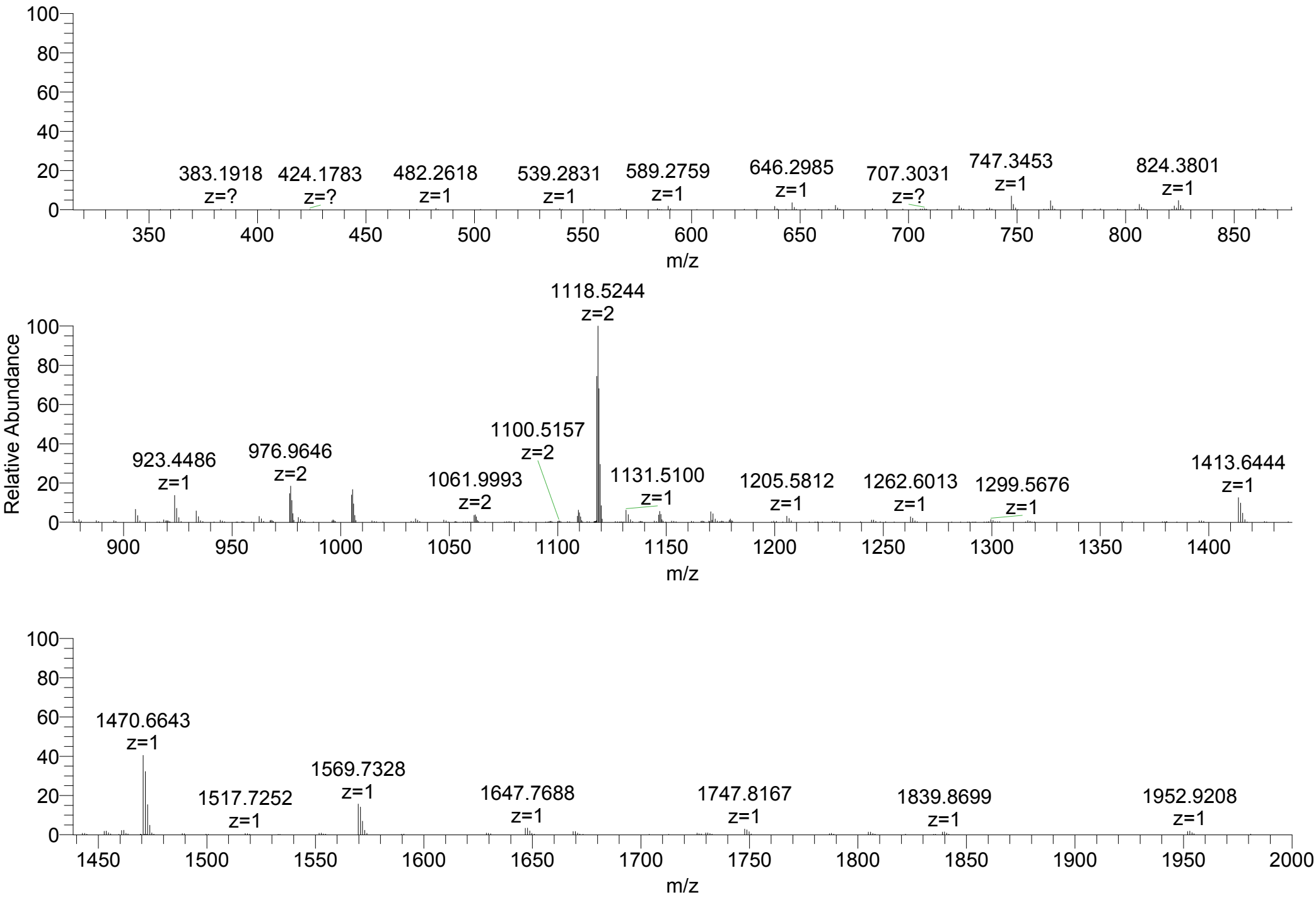
29.

P992-OH, P993-OH, P995-OH, P996-OH

#990-1014: TG**PP**G**PP**GVVGPQGPTGETGPMGER

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+4OH	2	1197.0555	1197.0542	-0.0026	-1.1
y5	1	589.2763	589.2759	-0.0004	-0.7
y6	1	646.2977	646.2985	0.0008	1.2
y7	1	747.3454	747.3453	-0.0001	-0.1
b9+4OH	1	824.3785	824.3801	0.0016	1.9
b10+4OH	1	923.4469	923.4486	0.0017	1.8
y20+2OH	2	976.4625	976.4645	0.0040	2.1
y21+2OH	2	1004.9733	1004.9761	0.0056	2.8
y22+3OH	2	1061.4971	1061.4967	-0.0008	-0.4
y23+4OH	2	1118.0210	1118.0247	0.0074	3.3
y11	1	1131.5099	1131.5100	0.0001	0.1
b13+4OH	1	1205.5797	1205.5813	0.0016	1.3
b14+4OH	1	1262.6012	1262.6013	0.0001	0.1
y14	1	1413.6427	1413.6444	0.0017	1.2
y15	1	1470.6642	1470.6643	0.0001	0.1
y16	1	1569.7326	1569.7328	0.0002	0.1
b18+4OH	1	1646.7657	1646.7671	0.0014	0.9
b19+4OH	1	1747.8133	1747.8167	0.0034	1.9

10_7_2011Collagen_Trypsin_MS3_CIDandHCD #3097 RT: 26.41 AV: 1 NL: 8.43E5
T: FTMS + c NSI d Full ms2 1197.56@cid35.00 [315.00-2000.00]



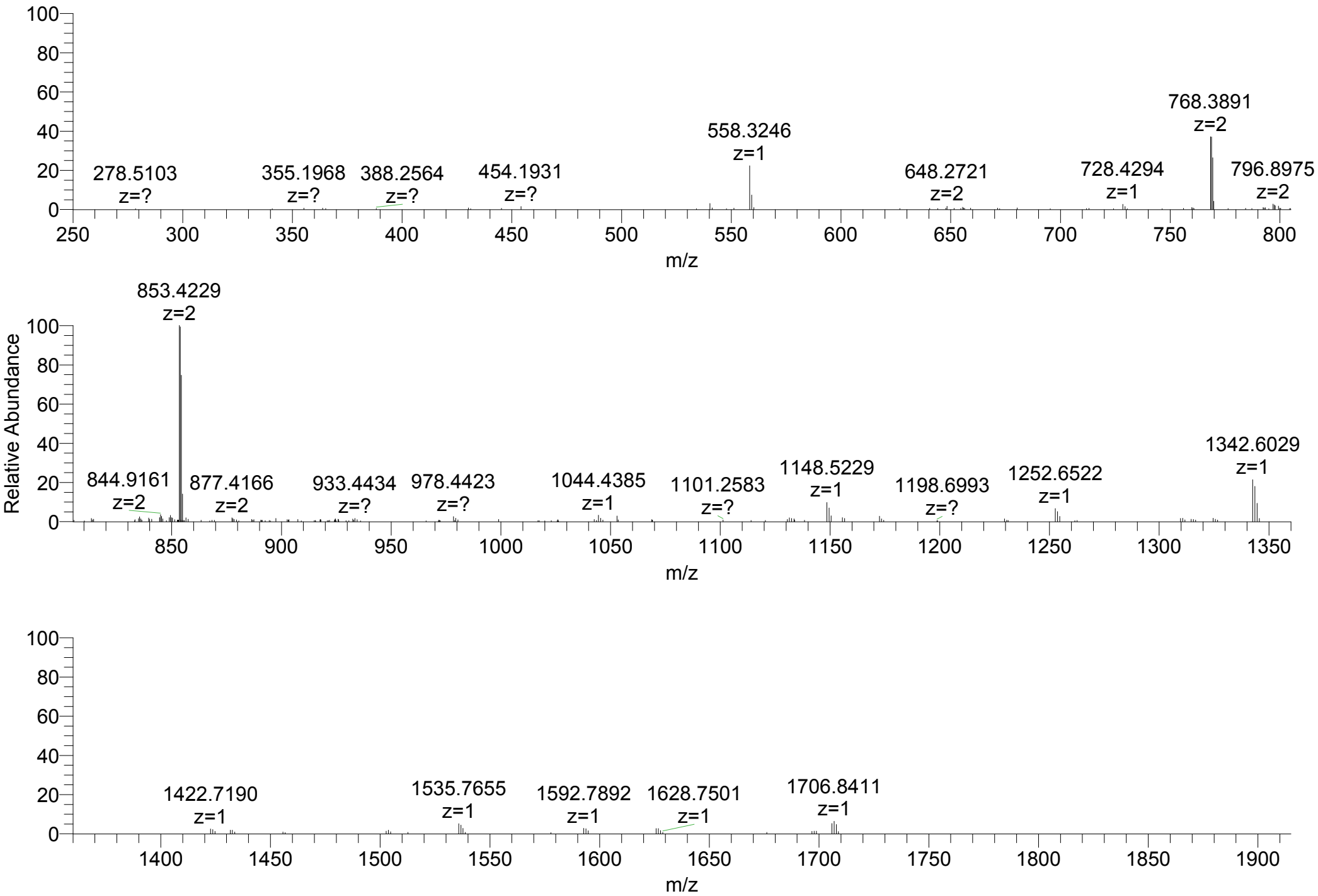
30.

P1017-OH, P1019-OH, P1020-OH, P1023-OH, P1029-OH

#1015-1034: GH**P**G**PP**GP**P**GEQGL**P**GLAGK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+5OH	2	950.4634	950.4630	-0.0008	-0.4
y6+OH	1	558.3246	558.3246	0.0000	0.0
y8+OH	1	728.4301	728.4294	-0.0007	-1.0
y16+4OH	2	768.3886	768.3891	0.0010	0.7
y17+4OH	2	796.8994	796.8975	-0.0038	-2.4
y18+5OH	2	853.4232	853.4229	-0.0006	-0.4
b11+4OH	1	1044.4381	1044.4385	0.0004	0.4
y12+2OH	1	1155.6004	1155.6088	0.0084	7.3
y13+2OH	1	1252.6532	1252.6522	-0.0010	-0.8
b14+4OH	1	1342.6022	1342.6029	0.0007	0.5
y15+3OH	1	1422.7223	1422.7190	-0.0033	-2.3
y16+4OH	1	1535.7700	1535.7655	-0.0045	-2.9
y17+4OH	1	1592.7915	1592.7892	-0.0023	-1.4
b17+5OH	1	1625.7554	1625.7533	-0.0021	-1.3
y18+5OH	1	1705.8392	1705.8480	0.0088	5.2

10_7_2011Collagen_Trypsin_MS3_CIDandHCD #2507 RT: 22.17 AV: 1 NL: 4.74E5
T: FTMS + c NSI d Full ms2 950.46@cid35.00 [250.00-1915.00]



Human

31.

K1038-OH, P1041-OH, P1047-OH

#1035-1049: EGT**K**GD**P**GPAGL**P**GK

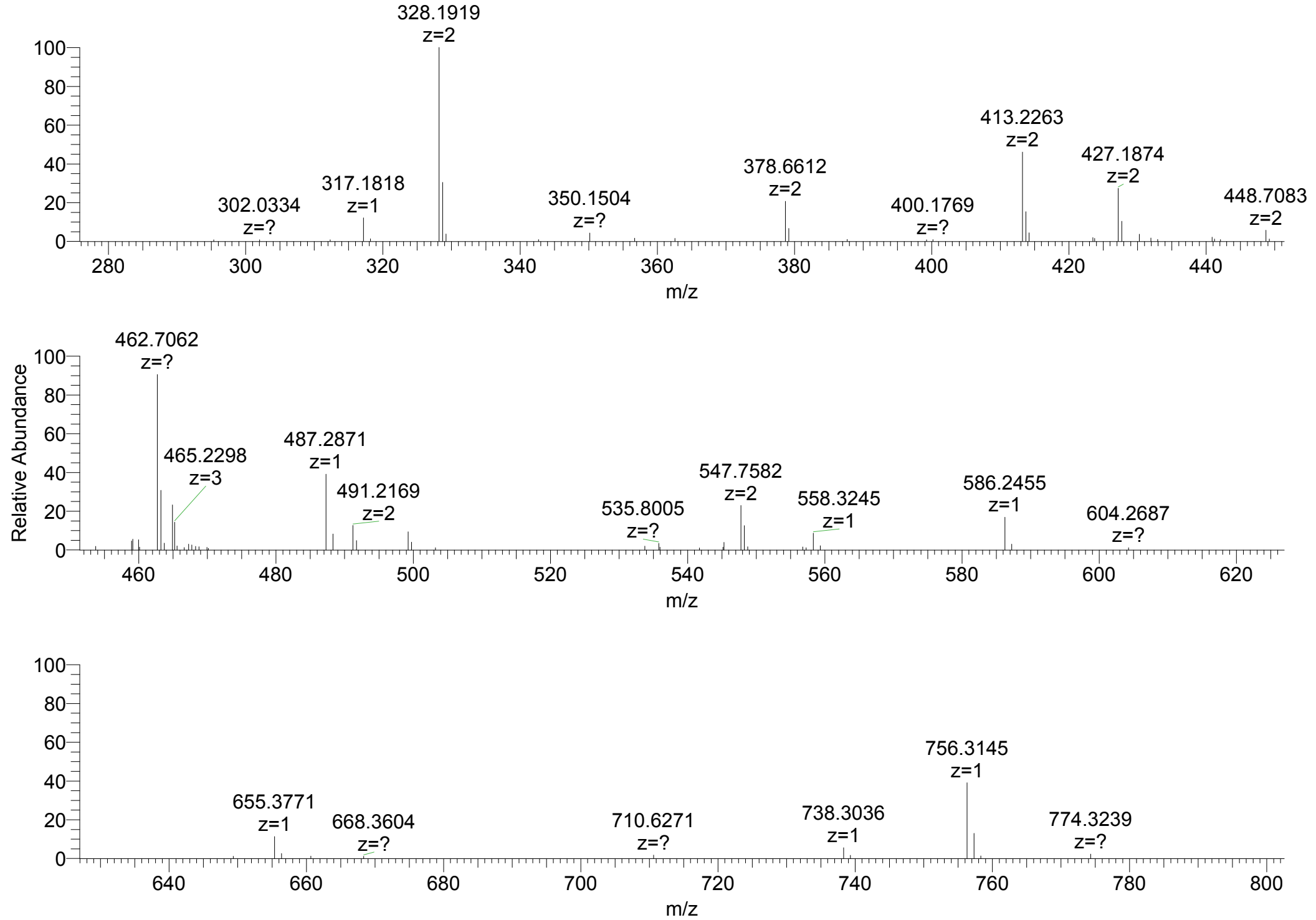
MS^2: EGT**K**GD**P**GPAGLPGK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
MH+3OH	3	476.9037	476.9025	-0.0036	-2.5
y3+OH	1	317.1819	317.1818	-0.0001	-0.3
y7+OH(MS^3)	2	328.1923	328.1919	-0.0008	-1.2
b8-H2O+2OH	2	378.6616	378.6612	-0.0008	-1.1
y9+2OH	2	413.2269	413.2263	-0.0012	-1.5
b9-H2O+2OH	2	427.1880	427.1874	-0.0012	-1.4
b10-H2O+2OH	2	462.7065	462.7062	-0.0006	-0.6
y5+OH	1	487.2875	487.2871	-0.0004	-0.8
y11+2OH	2	499.2511	499.2506	-0.0010	-1.0
b12-H2O+2OH	2	547.7593	547.7582	-0.0022	-2.0
y6+OH	1	558.3246	558.3245	-0.0001	-0.2
b6-H2O+OH	1	586.2467	586.2455	-0.0012	-2.1
y7+OH	1	655.3774	655.3771	-0.0003	-0.5
b8-2H2O+2OH	1	738.3053	738.3036	-0.0017	-2.3
b8-H2O+2OH	1	756.3159	756.3145	-0.0014	-1.9

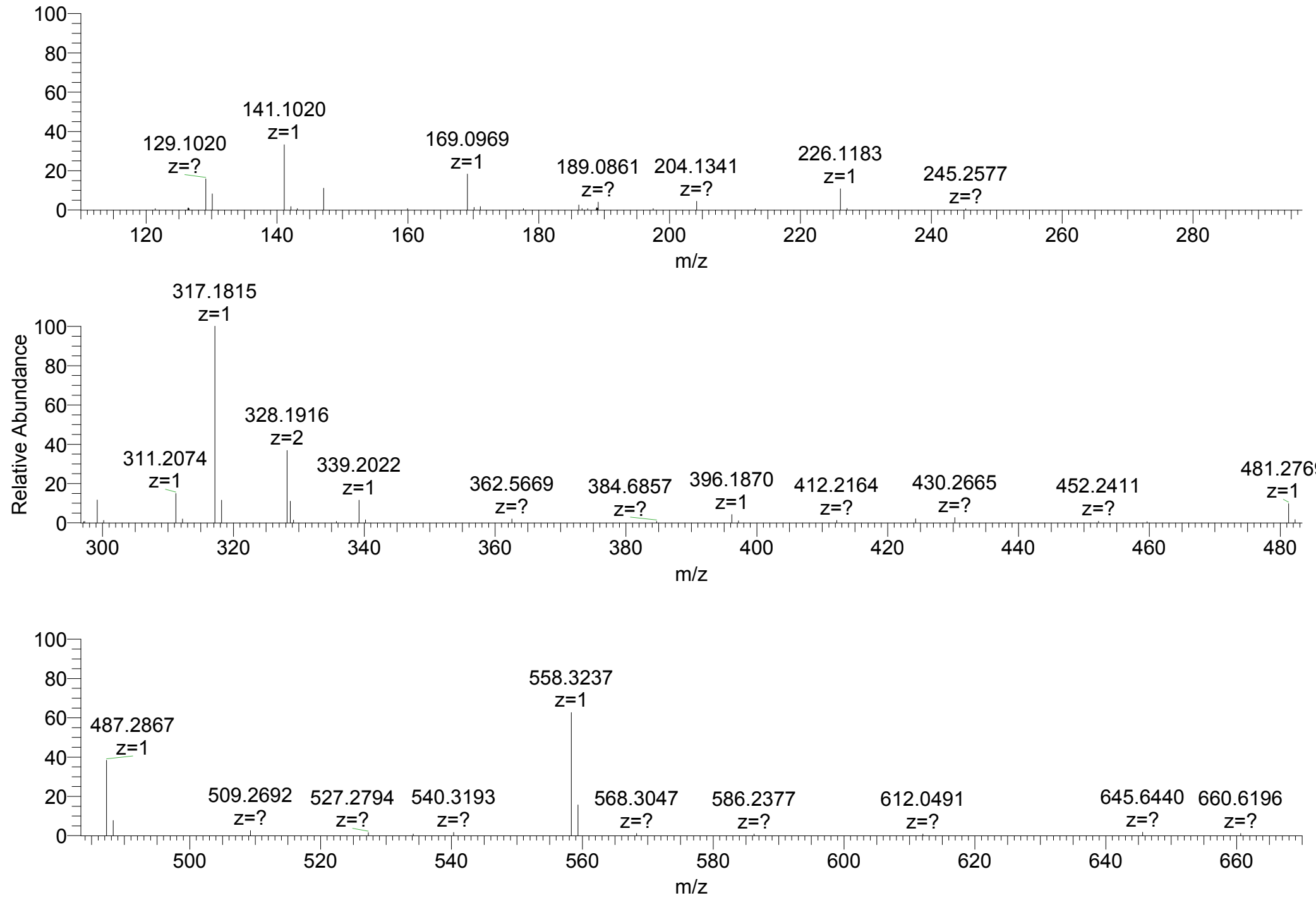
MS^3: PAGL**P**GK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
y1	1	147.1128	147.1125	-0.0003	-2.1
b2	1	169.0972	169.0969	-0.0003	-1.8
b3	1	226.1186	226.1183	-0.0003	-1.3
y3+OH	1	317.1815	317.1819	0.0004	1.3
[M+2H]+OH	2	328.1923	328.1916	-0.0014	-2.1
y5+OH	1	487.2875	487.2867	-0.0008	-1.6
y6+OH	1	558.3246	558.3237	-0.0009	-1.6

11_9_2011Col5a1_Trypsin_MS3_CIDandHCD_micro4 #591 RT: 10.04 AV: 1 NL: 4.50E5
T: FTMS + c NSI d Full ms2 476.90@cid35.00 [120.00-1445.00]



11_9_2011Col5a1_Trypsin_MS3_CIDandHCD_micro4 #592 RT: 10.05 AV: 1 NL: 1.69E5
T: FTMS + c NSI d Full ms3 476.90@cid35.00 328.19@hcd30.00 [110.00-670.00]



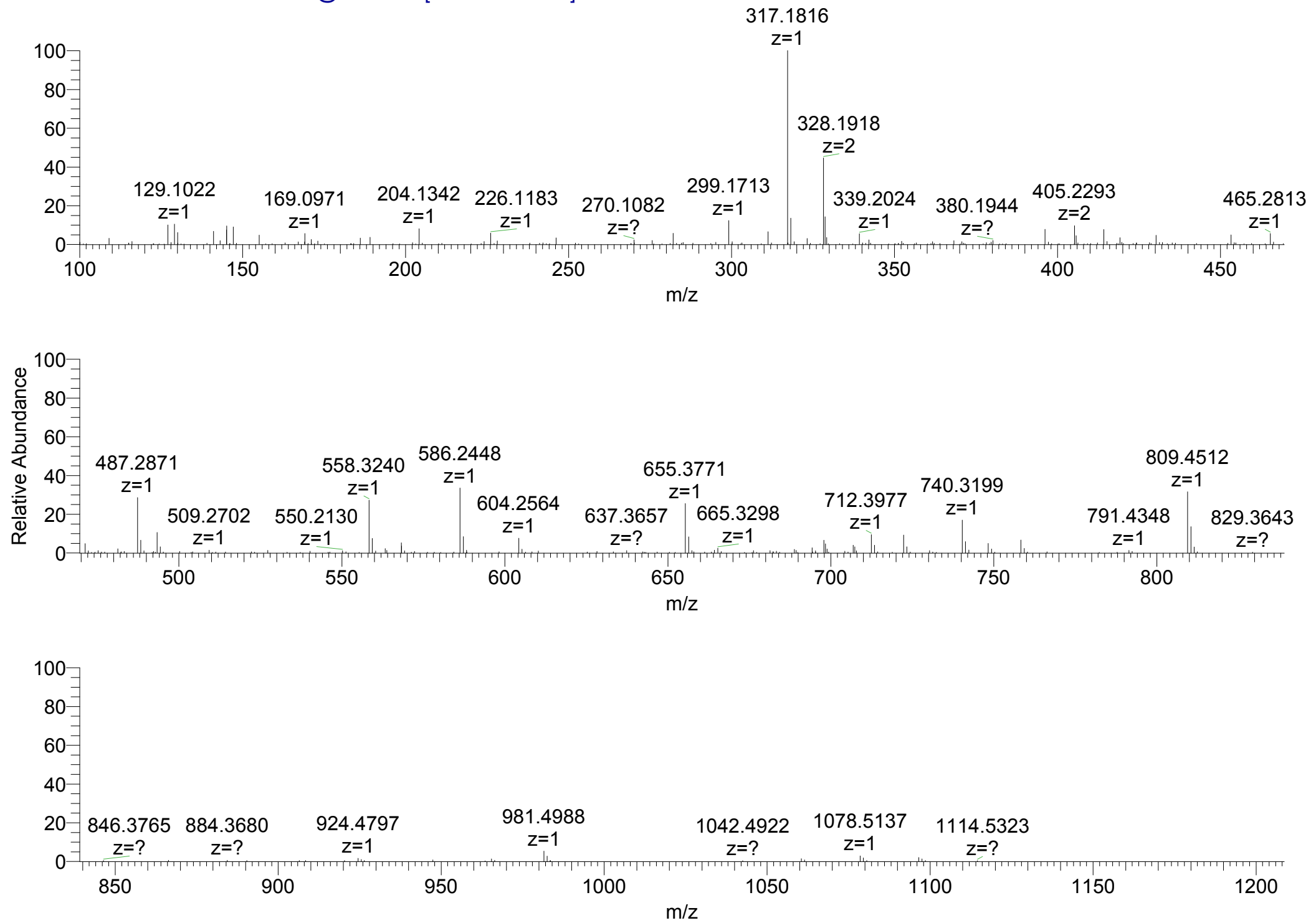
32.

K1038-OH.Gal.Glc, P1047-OH

#1035-1049: EGT**K**GDPGPAGL**P**GK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+Gal.Glc	3	579.6073	579.6051	-0.0066	-3.8
K	1	129.1022	129.1022	0.0000	0.0
y2	1	204.1343	204.1342	-0.0001	-0.5
PAG	1	226.1186	226.1183	-0.0003	-1.3
y3+OH	1	317.1819	317.1816	-0.0003	-0.9
y7+OH	2	328.1923	328.1918	-0.0010	-1.5
y9+OH	2	405.2294	405.2293	-0.0002	-0.2
y5+OH	1	487.2875	487.2871	-0.0004	-0.8
y6+OH	1	558.3246	558.3240	-0.0006	-1.1
b6-H2O+OH	1	586.2467	586.2448	-0.0019	-3.2
b6+OH	1	604.2573	604.2564	-0.0009	-1.5
y7+OH	1	655.3774	655.3771	-0.0003	-0.5
y8+OH	1	712.3988	712.3977	-0.0011	-1.5
b8-H2O+OH	1	740.3210	740.3199	-0.0011	-1.5
b8+OH	1	758.3315	758.3307	-0.0008	-1.1
y9+OH	1	809.4516	809.4512	-0.0004	-0.5
y11+OH	1	981.5000	981.4988	-0.0012	-1.2
b12-H2O+OH	1	1078.5164	1078.5137	-0.0027	-2.5

10_7_2011Collagen_Trypsin_HCDandETD_111009033323 #1654 RT: 14.54 AV: 1 NL: 4.14E6
T: FTMS + c NSI d Full ms2 579.61@hcd35.00 [100.00-1750.00]



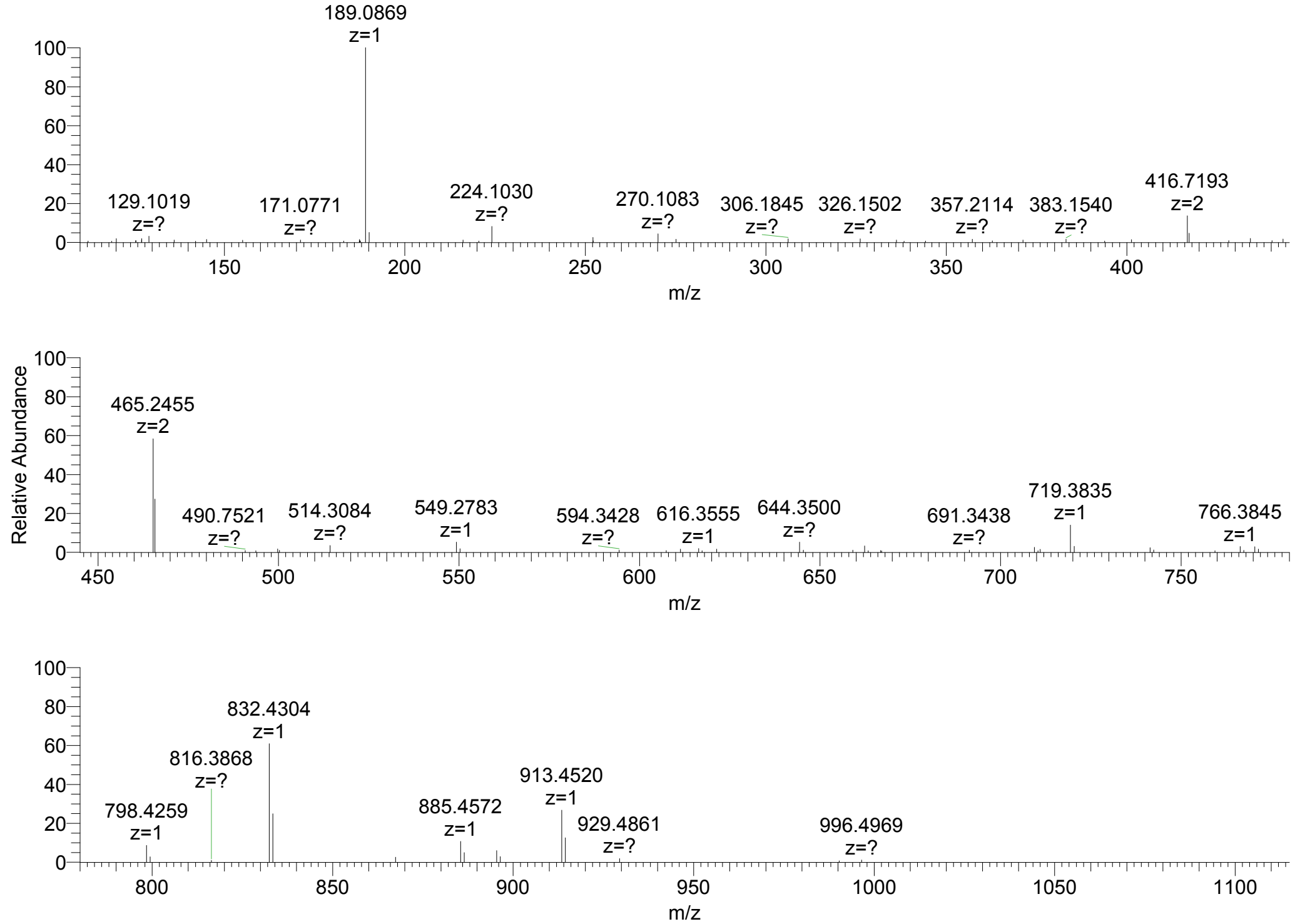
33.

P1053-OH, P1059-OH

#1050-1060: DGP**P**GLRGF**P**G

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+2OH	2	551.2698	551.2687	-0.0022	-2.0
y2+OH	1	189.0870	189.0869	-0.0001	-0.5
b3	1	270.1084	270.1083	-0.0001	-0.4
y8+2OH	2	416.7192	416.7193	0.0002	0.2
y9+2OH	2	465.2456	465.2455	-0.0002	-0.2
y5+OH	1	549.2780	549.2783	0.0003	0.5
GLRGFP+OH	1	644.3515	644.3500	-0.0015	-2.3
y7+OH	1	719.3835	719.3835	0.0000	0.0
GPPGLRGF+OH	1	798.4257	798.4259	0.0002	0.3
y8+2OH	1	832.4312	832.4304	-0.0008	-1.0
a9+OH	1	885.4577	885.4572	-0.0005	-0.6
b9+OH	1	913.4526	913.4520	-0.0006	-0.7

11_9_2011Col5a1_AspN_HCD1 #4606 RT: 27.66 AV: 1 NL: 1.35E7
T: FTMS + c NSI d Full ms2 551.27@hcd30.00 [110.00-1115.00]



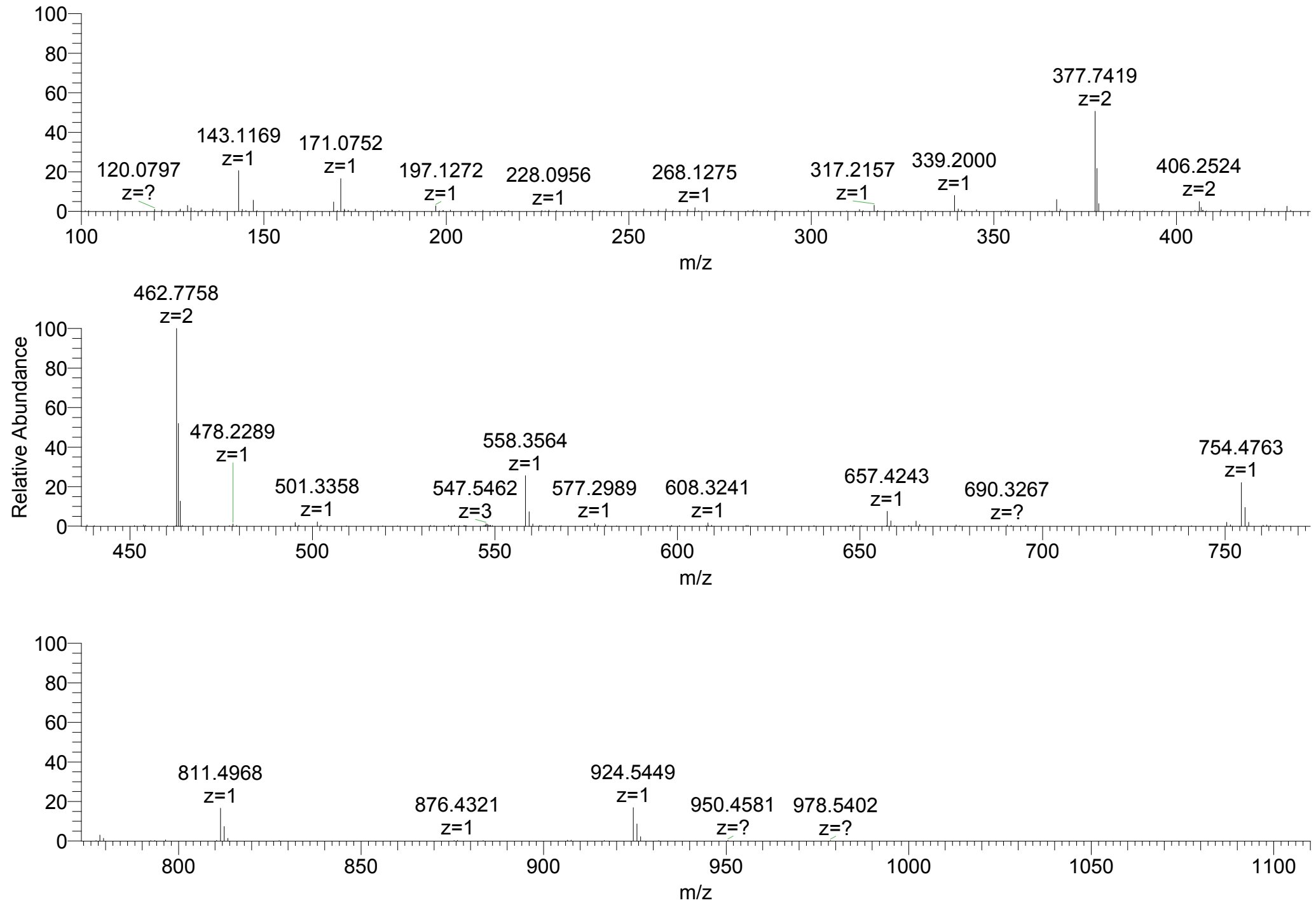
34.

P1065-OH

#1063-1074: GL**P**GPVGALGLK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+OH	2	547.8320	547.8282	-0.0076	-6.9
PG+OH	1	171.0764	171.0752	-0.0012	-7.1
y3	1	317.2183	317.2157	-0.0026	-8.2
PGPV-28+OH	1	339.2027	339.2000	-0.0027	-8.0
PGPV+OH	1	367.1976	367.1948	-0.0028	-7.6
y8	2	377.7447	377.7419	-0.0056	-7.4
y9	2	406.2554	406.2524	-0.0060	-7.4
y10+OH	2	462.7793	462.7758	-0.0070	-7.6
y5	1	501.3395	501.3358	-0.0037	-7.4
y6	1	558.3610	558.3564	-0.0046	-8.3
y7	1	657.4294	657.4243	-0.0051	-7.8
y8	1	754.4822	754.4763	-0.0059	-7.8
y9	1	811.5036	811.4968	-0.0068	-8.4
y10+OH	1	924.5513	924.5449	-0.0064	-6.9

12_9_2011Col5a1_Trypsin_CE30_nontrapping #7247 RT: 69.04 AV: 1 NL: 2.44E5
T: FTMS + c NSI d Full ms2 547.83@hcd30.00 [100.00-1110.00]



35.

K1074-OH.Gal.Glc, P1083-OH, P1089-OH

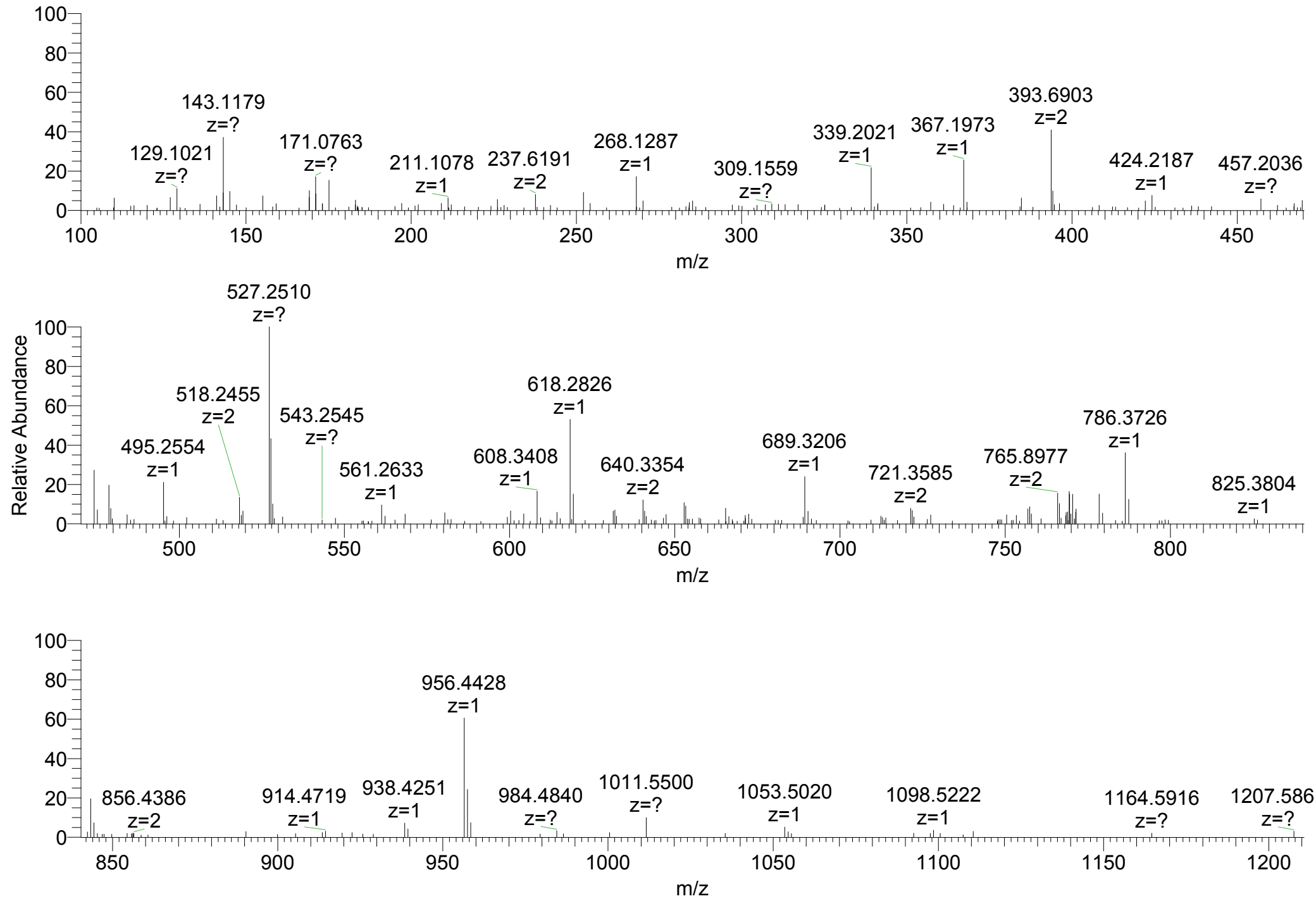
#1063-1092: GLPGPVGALGL**K**GNEGPPGP**P**GPAGS**P**GER

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+4OH+Gal.Glc	4	770.1282	770.1282	0.0000	0.0
a2/GL-28	1	143.1179	143.1179	0.0000	0.0
y4+OH	2	237.6190	237.6191	0.0002	0.4
GPP+OH	1	268.1292	268.1287	-0.0005	-1.9
PGPV+OH	1	367.1976	367.1973	-0.0003	-0.8
y8+OH	2	393.6907	393.6903	-0.0008	-1.0
y4+OH	1	474.2307	474.2300	-0.0007	-1.5
y10+2OH	2	478.7252	478.7253	0.0002	0.2
PGPVGA+OH	1	495.2562	495.2554	-0.0008	-1.6
y11+2OH	2	527.2516	527.2510	-0.0012	-1.1
y5+OH	1	561.2627	561.2633	0.0006	1.1
y6+OH	1	618.2842	618.2826	-0.0016	-2.6
y14+2OH	2	652.8151	652.8134	-0.0034	-2.6
y7+OH	1	689.3213	689.3206	-0.0007	-1.0
b9+OH	1	778.4458	778.4451	-0.0007	-0.9
y8+OH	1	786.3741	786.3726	-0.0015	-1.9
y9+OH	1	843.3955	843.3960	0.0005	0.6
y10+OH	1	956.4432	956.4428	-0.0004	-0.4
y11+2OH	1	1053.4960	1053.5020	0.0060	5.7

***Unlocalized sites: P1065-OH?, P1067-OH?**

Pseudolocalized sites: P1065-OH

10_7_2011Collagen_Trypsin_HCDandETD_111009033323 #4987 RT: 33.34 AV: 1 NL: 1.77E4
T: FTMS + c NSI d Full ms2 770.38@hcd35.00 [100.00-2000.00]



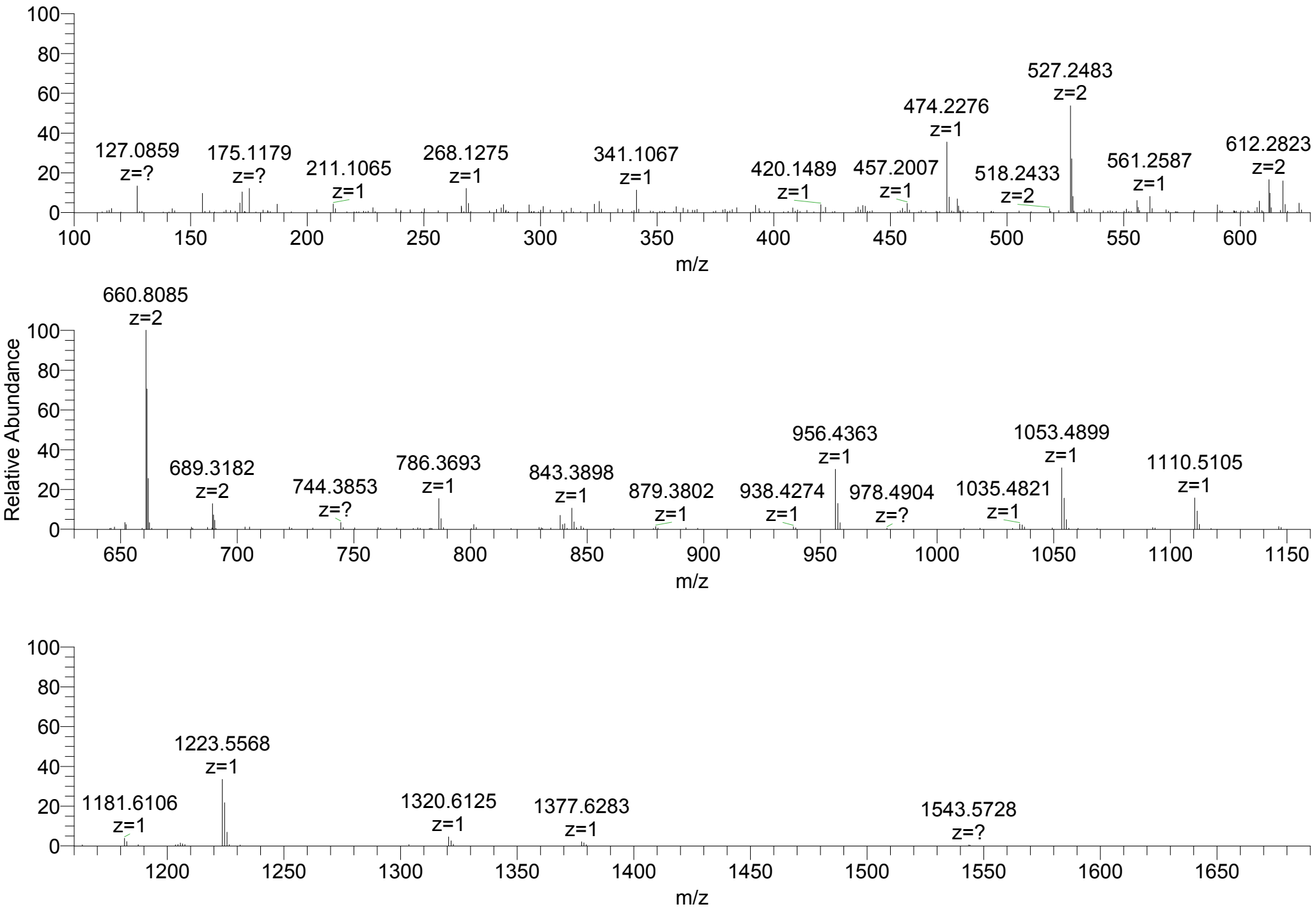
36.

P1080-OH, P1083-OH, P1089-OH

#1075-1092: GNEGP**P**GP**P**GPAGS**P**GER

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+3OH	2	839.3768	839.3705	-0.0126	-7.5
y1	1	175.1190	175.1179	-0.0011	-6.3
b4-NH3	1	341.1092	341.1067	-0.0025	-7.4
y4+OH	1	474.2307	474.2276	-0.0031	-6.6
y11+2OH	2	527.2516	527.2483	-0.0066	-6.3
y5+OH	1	561.2627	561.2587	-0.0040	-7.1
y13+3OH	2	612.2862	612.2823	-0.0078	-6.4
y6+OH	1	618.2842	618.2802	-0.0040	-6.5
y14+3OH	2	660.8126	660.8085	-0.0082	-6.2
y15+3OH	2	689.3233	689.3182	-0.0102	-7.4
y8+OH	1	786.3741	786.3693	-0.0048	-6.1
y9+OH	1	843.3955	843.3898	-0.0057	-6.8
y10+2OH	1	956.4432	956.4363	-0.0069	-7.2
y11+2OH	1	1053.4960	1053.4899	-0.0061	-5.8
y12+2OH	1	1110.5174	1110.5105	-0.0069	-6.2
y13+3OH	1	1223.5651	1223.5568	-0.0083	-6.8
y14+3OH	1	1320.6179	1320.6125	-0.0054	-4.1

12_9_2011Col5a1_Trypsin_CE35 #1362 RT: 13.25 AV: 1 NL: 1.10E5
T: FTMS + c NSI d Full ms2 839.37@hcd35.00 [100.00-1690.00]



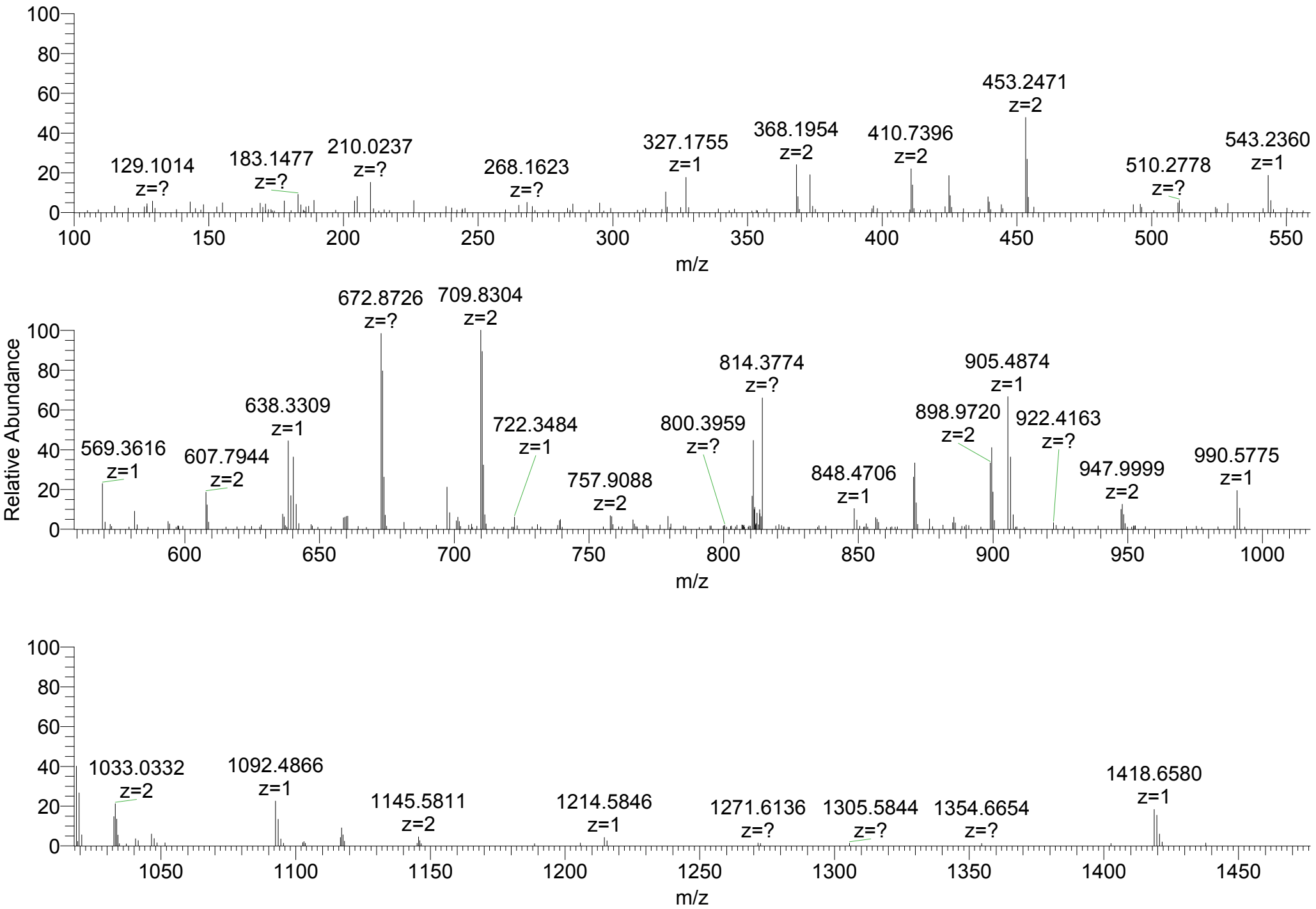
37.

P1104-OH, P1107-OH, P1113-OH

#1092-1118: RGPAGAAGPIGI**P**GR**P**GPQGP**P**GPAGE

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+3OH	3	812.7508	812.7436	-0.0216	-8.9
b9	2	368.1985	368.1954	-0.0062	-8.4
y4	1	373.1718	373.1685	-0.0033	-8.9
a10	2	410.7430	410.7396	-0.0068	-8.3
b10	2	424.7405	424.7370	-0.0070	-8.3
b11	2	453.2512	453.2471	-0.0082	-9.1
y6+OH	1	543.2409	543.2360	-0.0049	-9.0
b8	1	638.3369	638.3309	-0.0060	-9.4
b15+OH	2	672.8784	672.8726	-0.0116	-8.6
y8+OH	1	697.3151	697.3076	-0.0075	-10.8
y15+3OH	2	709.8366	709.8304	-0.0124	-8.7
b17+2OH	2	757.9130	757.9088	-0.0084	-5.5
b10	1	848.4737	848.4706	-0.0031	-3.7
b19+2OH	2	870.4686	870.4597	-0.0178	-10.2
b20+2OH	2	898.9794	898.9720	-0.0148	-8.2
b11	1	905.4952	905.4874	-0.0078	-8.6
b21+2OH	2	947.5057	947.5020	-0.0074	-3.9
a12	1	990.5842	990.5775	-0.0067	-6.8
b12	1	1018.5792	1018.5719	-0.0073	-7.2
b23+3OH	2	1032.5403	1032.5320	-0.0166	-8.0
y12+2OH	1	1092.4956	1092.4866	-0.0090	-8.2
y15+3OH	1	1418.6659	1418.6580	-0.0079	-5.6

12_9_2011Col5a1_AspNGluC_1 #2791 RT: 24.84 AV: 1 NL: 3.94E4
T: FTMS + c NSI d Full ms2 812.74@hcd30.00 [100.00-2000.00]



38.

K1119-OH.Gal.Glc

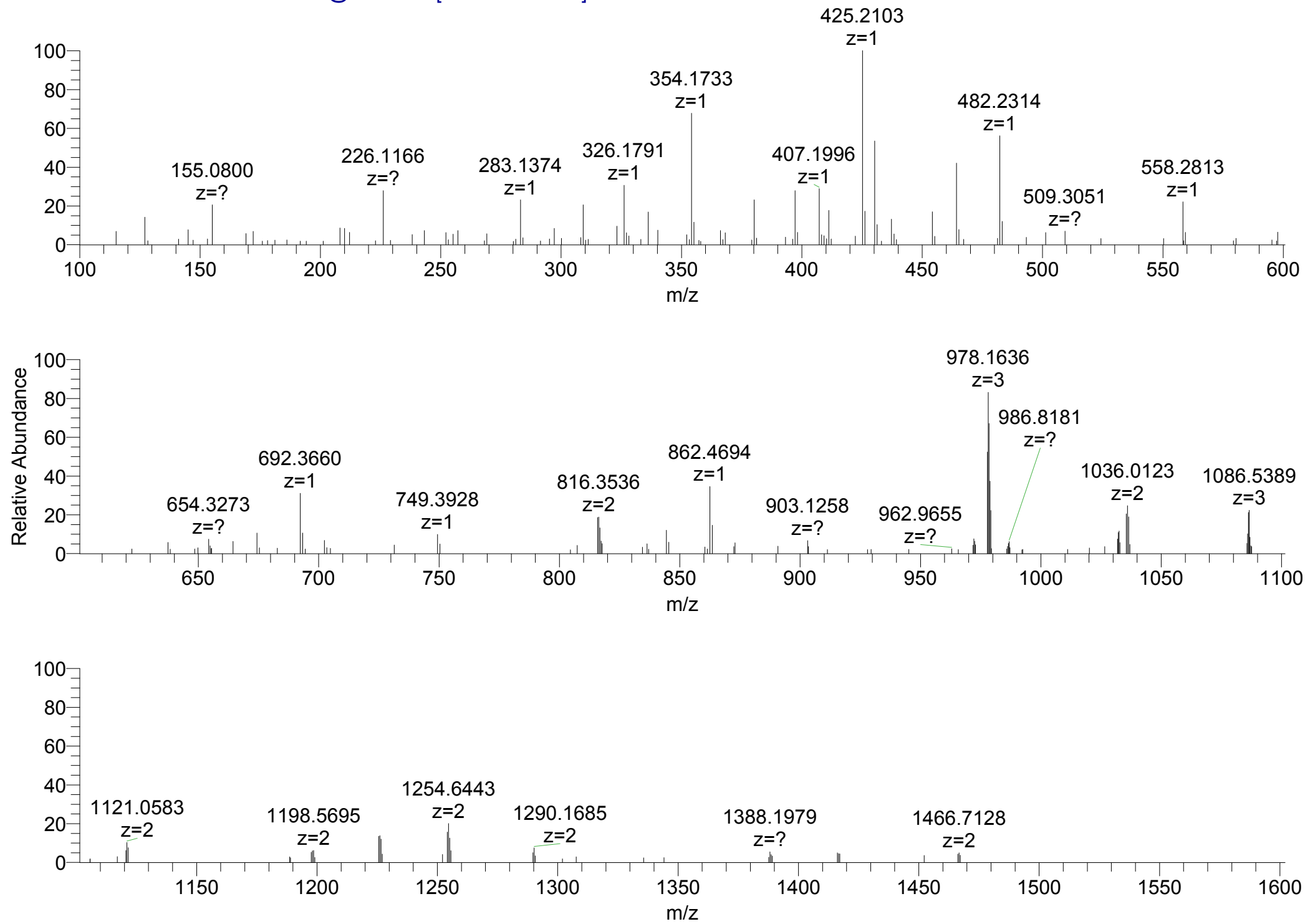
#1093-1125: GPAGAAGPIGIPGRPGPQGPPGPAGE**K**GAPGEK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+Gal.Glc	3	1085.8758	1085.8657	-0.0303	-9.3
b2/GP	1	155.0815	155.0800	-0.0015	-9.7
GPA/APG	1	226.1186	226.1166	-0.0020	-8.9
b4/GAPG	1	283.1401	283.1374	-0.0027	-9.6
a5	1	326.1823	326.1791	-0.0032	-9.8
b6/AGAAGP	1	425.2143	425.2103	-0.0040	-9.4
y4	1	430.2296	430.2251	-0.0045	-10.5
b7	1	482.2358	482.2314	-0.0044	-9.1
y6	1	558.2882	558.2813	-0.0069	-12.4
b9/PAGAAGPIG	1	692.3726	692.3660	-0.0066	-9.5
b10	1	749.3941	749.3928	-0.0013	-1.7
b11/AGAAGPIGIPG	1	862.4781	862.4694	-0.0087	-10.1
[M+3H]+2OH	3	977.8406	977.8304	-0.0306	-10.4
y22+2OH	2	1035.5218	1035.5109	-0.0218	-10.5
[M+3H]+2OH+Gal.Glc	3	1085.8758	1085.8650	-0.0324	-10.0
y24+2OH	2	1120.5745	1120.5687	-0.0116	-5.2
y26+2OH	2	1225.6430	1225.6295	-0.0270	-11.0
y27+2OH	2	1254.1537	1254.1458	-0.0158	-6.3
y28+2OH	2	1289.6723	1289.6715	-0.0016	-0.6

***Unlocalized sites: P1104-OH?, P1107-OH?, P1109-OH?, P1112-OH?, P1113-OH?, P1115-OH?**

Pseudolocalized sites: P1104-OH or P1107-OH or P1113-OH

12_9_2011Col5a1_Trypsin_target #2605 RT: 23.70 AV: 1 NL: 1.80E4
T: FTMS + c NSI d Full ms2 1086.20@hcd30.00 [100.00-2000.00]



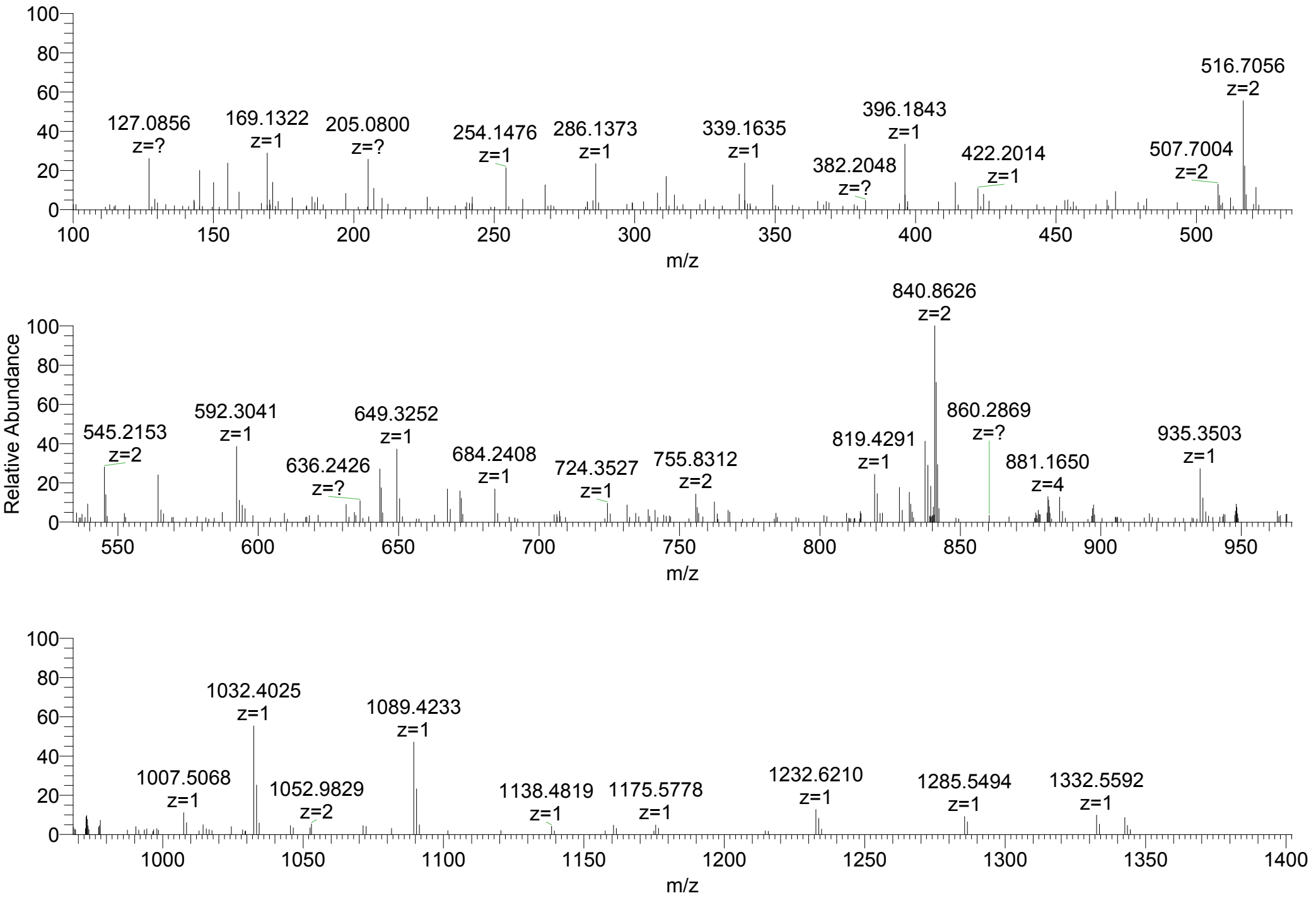
39.

P1143-OH, P1152-OH, K1158-OH

#1134-1160: DGLQGPVGL**P**GPAGPVGP**P**GEDGD**K**GE

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+3OH	3	839.7295	839.7222	-0.0219	-8.7
GP-28	1	127.0866	127.0856	-0.0010	-7.9
PV-28	1	169.1335	169.1322	-0.0013	-7.7
y2	1	205.0819	205.0800	-0.0019	-9.3
PVG/VGP/GPV	1	254.1499	254.1476	-0.0023	-9.1
b3	1	286.1397	286.1373	-0.0024	-8.4
GLQG-NH3/PGPA+OH	1	339.1663	339.1635	-0.0028	-8.3
y3+OH	1	349.1718	349.1685	-0.0033	-9.5
PGPAG+OH/b4-H2O	1	396.1878	396.1843	-0.0035	-8.9
b4	1	414.1983	414.1935	-0.0048	-11.6
y10-H2O+2OH	2	507.7042	507.7004	-0.0076	-7.5
y10+2OH	2	516.7056	516.7095	0.0078	7.6
y11+2OH	2	545.2153	545.2202	0.0098	9.0
PGPAGPV+OH/ AGPVGPP+OH	1	592.3089	592.3041	-0.0048	-8.1
y13+2OH	2	643.2808	643.2759	-0.0098	-7.6
AGPVGPPG+OH/ PGPAGPVG+OH/ b7-H2O	1	649.3304	649.3252	-0.0052	-8.0
b7	1	667.3410	667.3348	-0.0062	-9.3
y14+2OH	2	671.7915	671.7862	-0.0106	-7.9
y16+2OH	2	755.8364	755.8312	-0.0104	-6.9
b9	1	837.4465	837.4465	0.0000	0.0
y18+3OH	1	840.8710	840.8626	-0.0084	-10.0
y9+2OH	1	935.3589	935.3503	-0.0086	-9.2
y10+2OH	1	1032.4116	1032.4025	-0.0091	-8.8
y11+2OH	1	1089.4331	1089.4233	-0.0098	-9.0
b14+OH	1	1232.6270	1232.6210	-0.0060	-4.9
y13+2OH	1	1285.5543	1285.5494	-0.0049	-3.8

12_9_2011Col5a1_AspNGluC_1 #4148 RT: 36.20 AV: 1 NL: 2.52E4
T: FTMS + c NSI d Full ms2 840.06@hcd30.00 [100.00-2000.00]



40.

P1143-OH, P1164-OH, K1167-OH

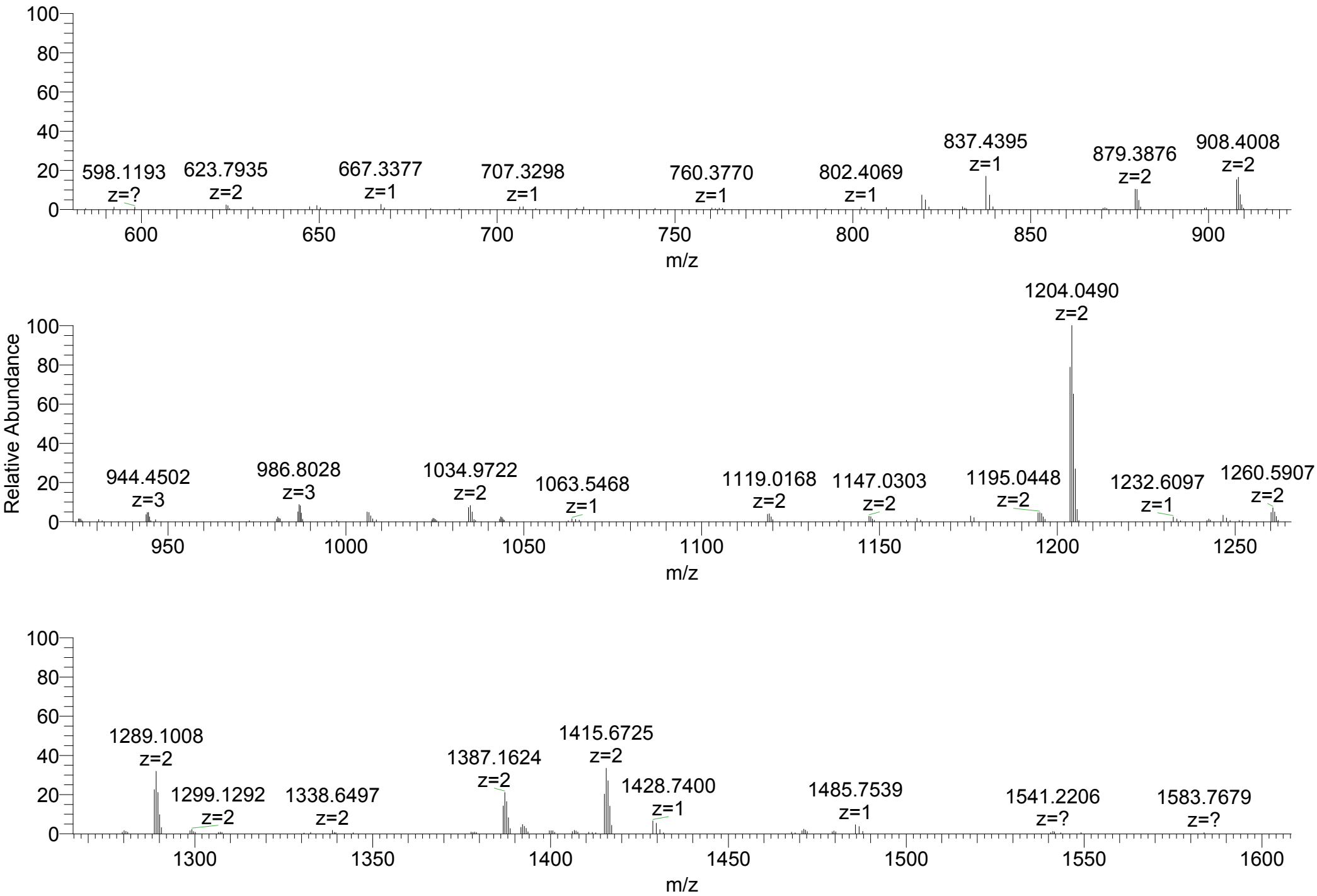
#1134-1167: DGLQGPVGL**P**GPAGPVGPPGEDGDKGEIGE**P**GQ**K**

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+4OH	3	1081.5198	1081.5090	-0.0324	-10.0
y12+2OH	2	623.7991	623.7935	-0.0112	-9.0
b7	1	667.3410	667.3377	-0.0033	-5.0
b9-H2O	1	819.4359	819.4290	-0.0069	-8.4
b9	1	837.4465	837.4395	-0.0070	-8.4
y17+2OH	2	879.3949	879.3876	-0.0146	-8.3
y18+2OH	2	907.9056	907.8998	-0.0116	-6.4
y30+4OH	3	943.7894	943.7801	-0.0279	-9.9
y31+4OH	3	986.4756	986.4702	-0.0162	-5.5
y20+3OH	2	1005.9662	1005.9584	-0.0156	-7.8
y21+3OH	2	1034.4769	1034.4695	-0.0148	-7.2
y23+3OH	2	1118.5218	1118.5144	-0.0148	-6.6
y25+4OH	2	1203.5564	1203.5486	-0.0156	-6.5
y26+4OH	2	1260.0984	1260.0901	-0.0166	-6.6
y27+4OH	2	1288.6092	1288.6005	-0.0174	-6.8
b28+2OH	2	1298.6299	1298.6261	-0.0076	-2.9
y29+4OH	2	1386.6698	1386.6604	-0.0188	-6.8
b30+2OH	2	1391.6619	1391.6538	-0.0162	-5.8
y30+4OH	2	1415.1805	1415.1715	-0.0180	-6.4
b16+OH	1	1428.7482	1428.7400	-0.0082	-5.7
b17+OH	1	1485.7696	1485.7539	-0.0157	-10.6

***Unlocalized sites: P1151-OH?, P1152-OH?**

Pseudolocalized sites: P1152-OH

12_9_2011Col5a1_Trypsin_target_MS3 #2877 RT: 35.35 AV: 1 NL: 1.04E5
T: FTMS + c NSI d Full ms2 1081.84@cid35.00 [285.00-2000.00]



41.

K1173-OH.Gal.Glc, P1179-OH, P1191-OH

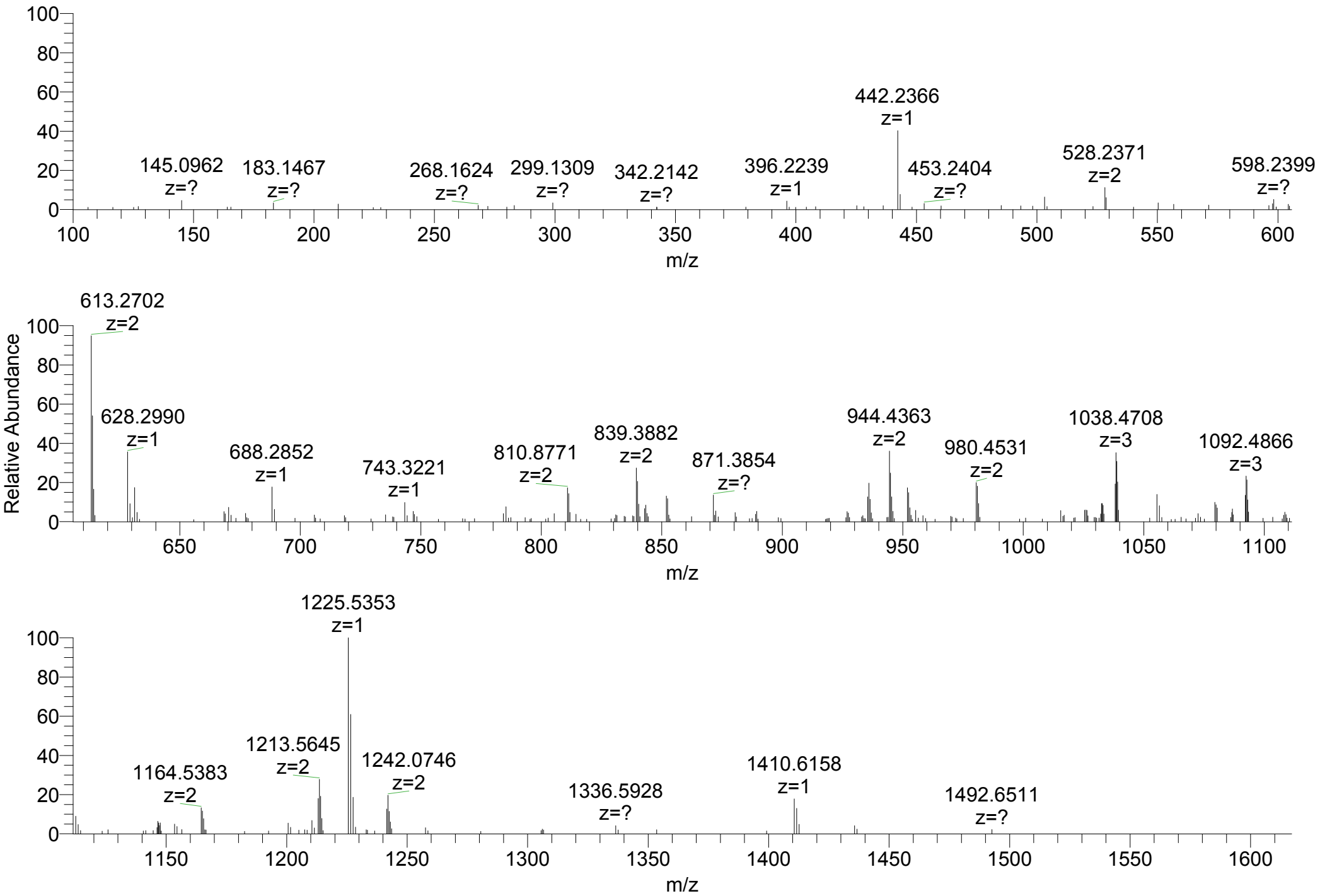
#1171-1203: GD**K**GEQGP**P**GPTGPQGPIGQ**P**GPSGADGEPGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+4OH+Gal.Glc	3	1146.1801	1146.1702	-0.0297	-8.6
y4+OH	1	442.2409	442.2366	-0.0043	-9.7
b5+OH	1	503.2096	503.2056	-0.0040	-8.0
y11+OH	1	528.2413	528.2371	-0.0042	-8.0
y13+2OH	2	613.2758	613.2702	-0.0112	-9.1
y6+OH	1	628.3049	628.2990	-0.0059	-9.4
b7+OH	1	688.2897	688.2852	-0.0045	-6.5
y7+OH	1	743.3319	743.3221	-0.0098	-13.2
b8+OH	1	785.3424	785.3345	-0.0079	-10.1
y17+2OH	2	810.8843	810.8771	-0.0144	-8.9
y18+2OH	2	839.3950	839.3882	-0.0136	-8.1
b18+2OH	2	851.9052	851.8987	-0.0130	-7.6
y9+OH	1	871.3904	871.3854	-0.0050	-5.7
b20+2OH	2	944.4452	944.4362	-0.0180	-9.5
y20+2OH	2	951.9507	951.9408	-0.0198	-10.4
y21+2OH	2	980.4614	980.4531	-0.0166	-8.5
[M+3H]+4OH	3	1038.1449	1038.1359	-0.0270	-8.7
y11+OH	1	1055.4752	1055.4668	-0.0084	-8.0
y23+2OH	2	1079.5116	1079.5020	-0.0192	-8.9
[M+3H]+4OH+Gal	1	1092.1625	1092.1552	-0.0073	-6.7
y25+3OH	2	1164.5462	1164.5383	-0.0158	-6.8
b25-2H2O+Gal+3OH	2	1213.0488	1213.0587	0.0198	8.2
y13+2OH	1	1225.5444	1225.5353	-0.0091	-7.4
y27+3OH	2	1241.5833	1241.5734	-0.0198	-8.0
y15+2OH	1	1410.6244	1410.6158	-0.0086	-6.1

***Unlocalized sites: P1200-OH?, P1202-OH?**

Pseudolocalized sites: P1200-OH

12_9_2011Col5a1_Trypsin_CE30 #2007 RT: 19.49 AV: 1 NL: 3.06E4
T: FTMS + c NSI d Full ms2 1146.17@hcd30.00 [100.00-2000.00]



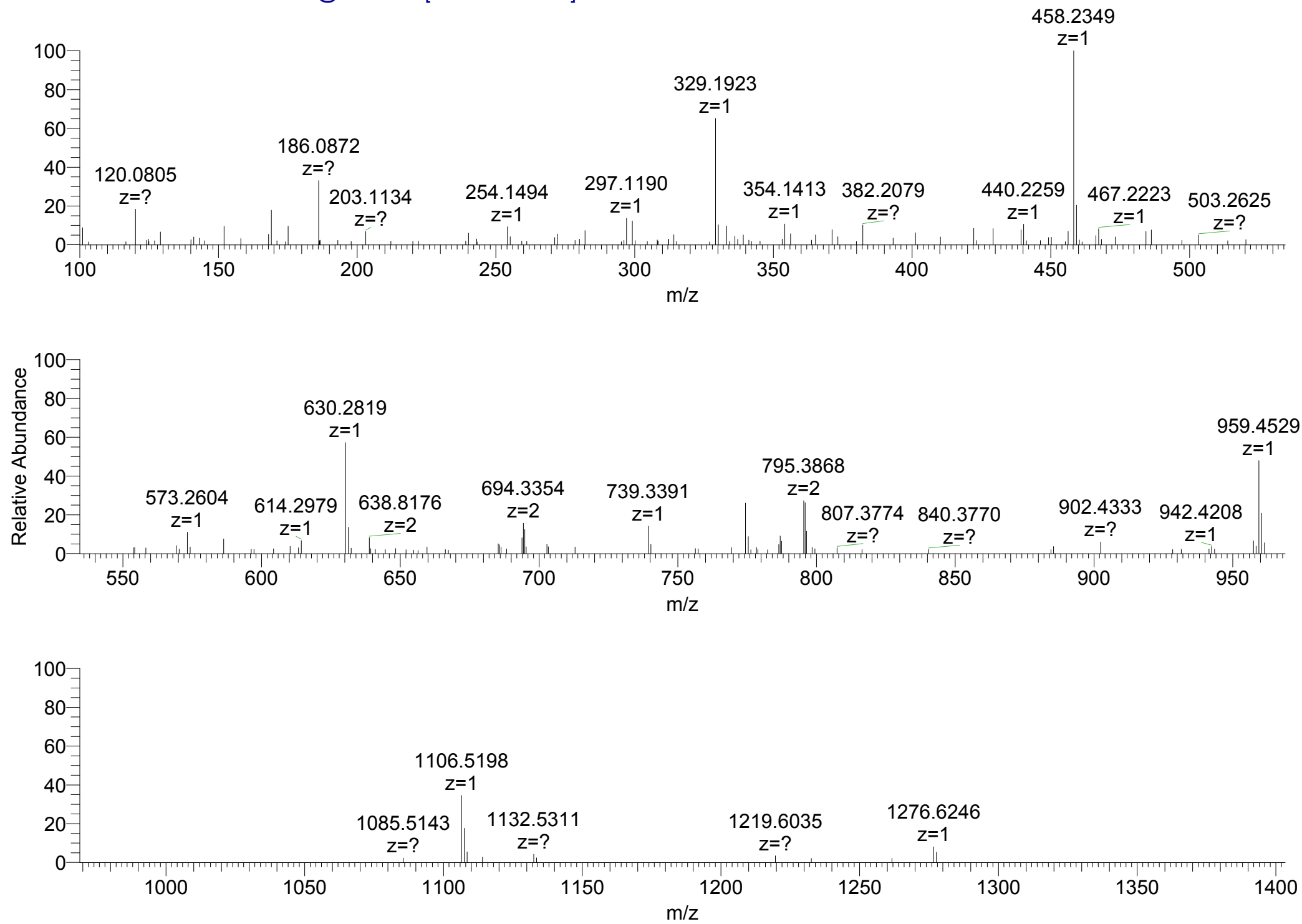
42.

K1212-OH.Gal.Glc

#1204-1218: GQQGLFGQ**K**GDEGPR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+OH+Gal.Glc	2	957.4398	957.4384	-0.0028	-1.5
F	1	120.0808	120.0805	-0.0003	-2.5
QG/b2	1	186.0873	186.0872	-0.0001	-0.5
y3	1	329.1932	329.1923	-0.0009	-2.7
b4-NH3	1	354.1408	354.1413	0.0005	1.4
y4	1	458.2358	458.2349	-0.0009	-2.0
y5	1	573.2627	573.2604	-0.0023	-4.0
y6	1	630.2842	630.2819	-0.0023	-3.7
y7+OH	1	774.3741	774.3729	-0.0012	-1.6
[M+2H]+OH	2	795.3870	795.3868	-0.0004	-0.3
y9+OH	1	959.4541	959.4529	-0.0012	-1.3
y10+OH	1	1106.5225	1106.5198	-0.0027	-2.4
y12+OH	1	1276.6280	1276.6246	-0.0034	-2.7

10_7_2011Collagen_Trypsin_HCDandETD #2357 RT: 18.30 AV: 1 NL: 9.15E5
T: FTMS + c NSI d Full ms2 957.94@hcd35.00 [100.00-1930.00]



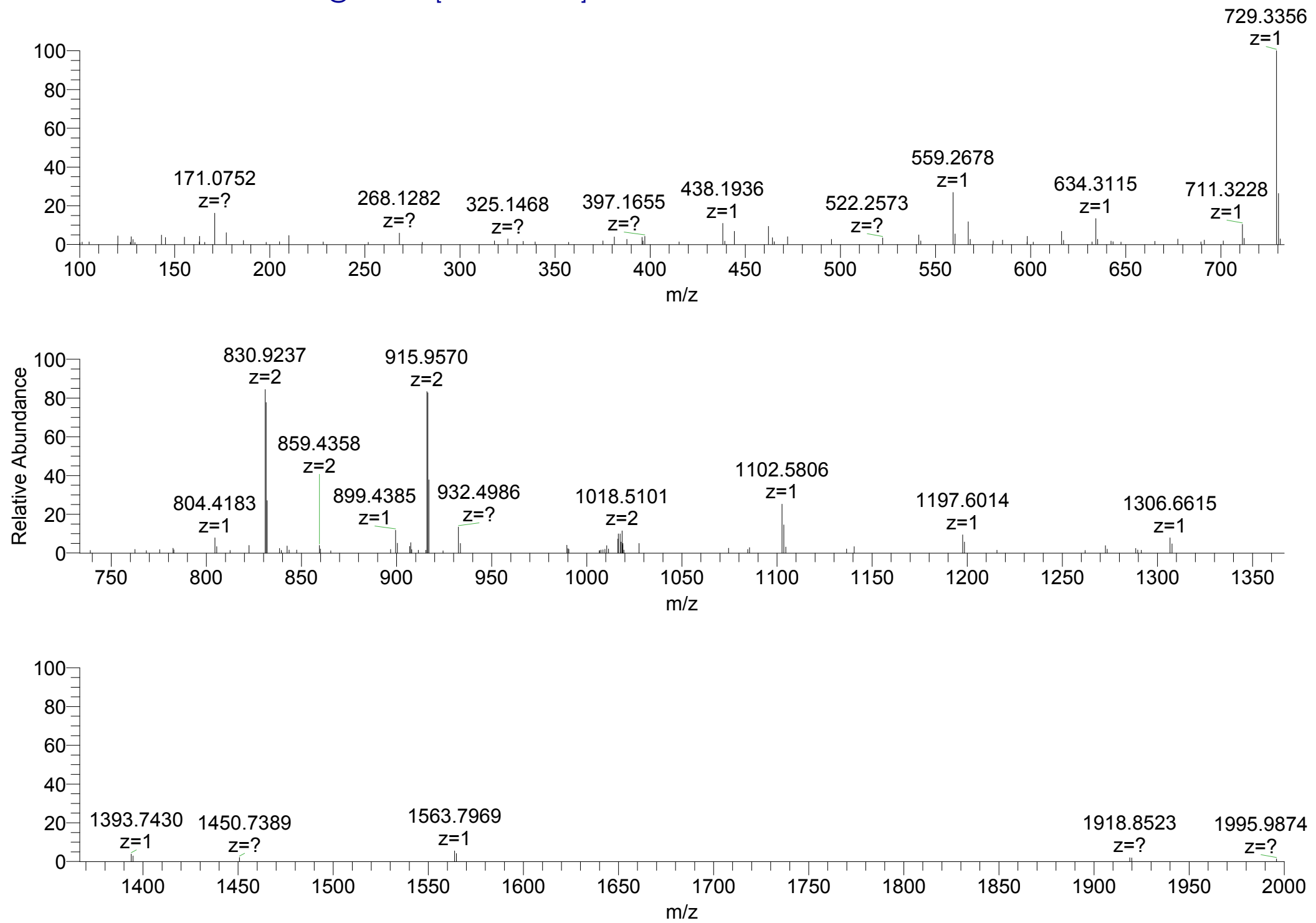
43.

P1221-OH, P1224-OH, P1233-OH, P1236-OH, K1239-OH

#1219-1239: GF**P**GP**P**GPVGLQGL**P**GP**P**GE**K**

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+5OH	2	1018.0102	1018.0025	-0.0154	-7.6
y4+2OH	1	462.2195	462.2156	-0.0039	-8.5
y5+2OH	1	559.2722	559.2678	-0.0044	-7.9
y7+3OH	1	729.3414	729.3356	-0.0058	-8.0
y17+4OH	2	830.9307	830.9237	-0.0140	-8.4
y18+4OH	2	859.4414	859.4358	-0.0112	-6.5
y9+3OH	1	899.4469	899.4385	-0.0084	-9.3
y19+5OH	2	915.9652	915.9570	-0.0164	-9.0
y12+3OH	1	1197.6110	1197.6014	-0.0096	-8.0
y14+3OH	1	1393.7322	1393.7430	0.0108	7.8
y16+4OH	1	1563.8013	1563.7969	-0.0044	-2.8

12_9_2011Col5a1_Trypsin_CE30 #4225 RT: 38.27 AV: 1 NL: 2.97E4
T: FTMS + c NSI d Full ms2 1018.00@hcd30.00 [100.00-2000.00]



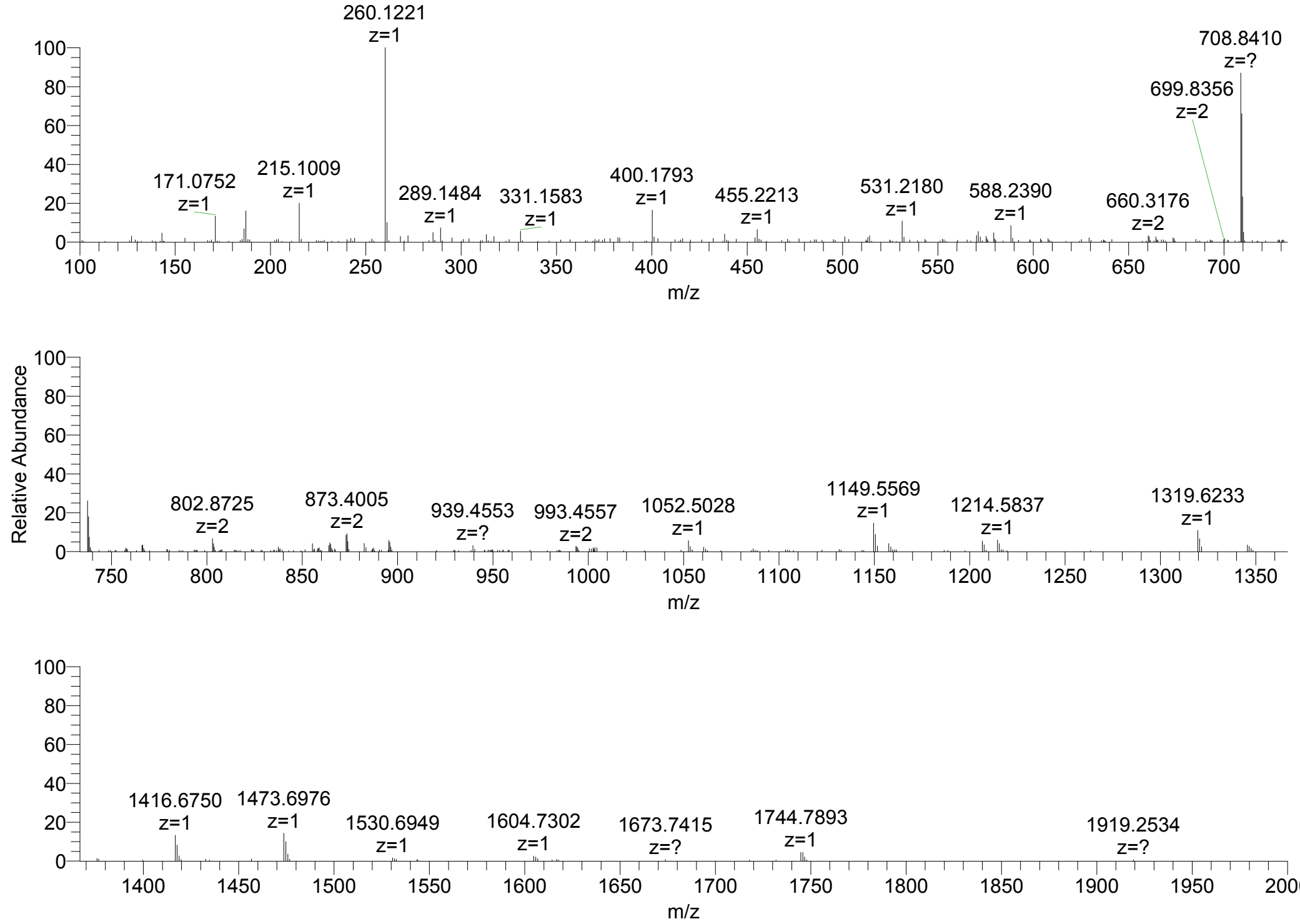
44.

P1251-OH, P1254-OH, P1263-OH

#1244-1265: DVGQMGP**P**GP**P**GPRGPSGA**P**GA

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+3OH	2	1002.4656	1002.4570	-0.0172	-8.6
b2	1	215.1026	215.1009	-0.0017	-7.9
y3+OH	1	260.1241	260.1221	-0.0020	-7.7
y4+OH	1	331.1612	331.1583	-0.0029	-8.8
b4	1	400.1827	400.1793	-0.0034	-8.5
b5	1	531.2232	531.2180	-0.0052	-9.8
b6	1	588.2446	588.2390	-0.0056	-9.5
y15+3OH	2	660.3206	660.3176	-0.0060	-4.6
y16+3OH	2	708.8469	708.8410	-0.0118	-8.3
y17+3OH	2	737.3577	737.3521	-0.0112	-7.6
y18+3OH	2	802.8779	802.8725	-0.0108	-6.7
y11+OH	1	939.4643	939.4553	-0.0090	-9.6
y12+2OH	1	1052.5119	1052.5028	-0.0091	-8.7
y13+2OH	1	1149.5647	1149.5569	-0.0078	-6.8
y15+3OH	1	1319.6339	1319.6233	-0.0106	-8.0
y16+3OH	1	1416.6866	1416.6750	-0.0116	-8.2
y17+3OH	1	1473.7081	1473.6976	-0.0105	-7.1

12_9_2011Col5a1_AspNGluC_1 #2370 RT: 21.30 AV: 1 NL: 8.97E4
T: FTMS + c NSI d Full ms2 1002.46@hcd30.00 [100.00-2000.00]



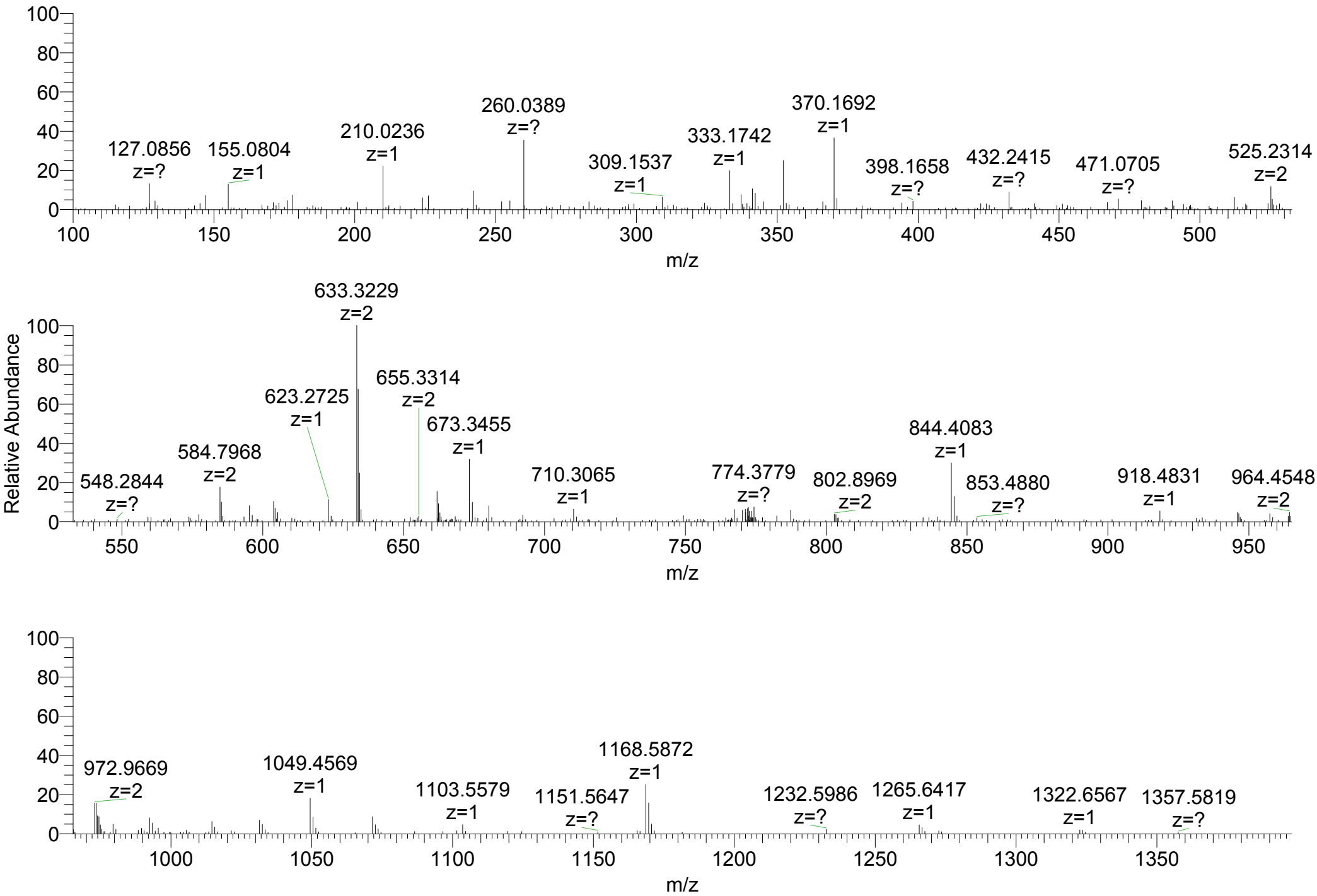
45.

P1278-OH

#1258-1284: GPSGAPGADGPQGPPGGIGN**P**GAVGEK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+OH	3	772.0401	772.0329	-0.0216	-9.3
GP/b2	1	155.0815	155.0804	-0.0011	-7.1
y3	1	333.1769	333.1742	-0.0027	-8.1
b5	1	370.1721	370.1692	-0.0029	-7.9
y4	1	432.2453	432.2415	-0.0038	-8.8
y13+OH	2	584.8015	584.7968	-0.0094	-8.1
y14+OH	2	633.3279	633.3299	0.0040	3.2
y7+OH	1	673.3515	673.3455	-0.0060	-8.9
b9	1	710.3104	710.3065	-0.0039	-5.5
y18+OH	2	802.9050	802.8969	-0.0162	-10.1
y9+OH	1	844.4159	844.4083	-0.0076	-9.0
b13	1	1049.4647	1049.4569	-0.0078	-7.4
y12+OH	1	1071.5429	1071.5326	-0.0103	-9.6
y13+OH	1	1168.5957	1168.5872	-0.0085	-7.3
y14+OH	1	1265.6484	1265.6417	-0.0067	-5.3
y15+OH	1	1322.6699	1322.6567	-0.0132	-10.0

12_9_2011Col5a1_Trypsin_CE30 #2421 RT: 22.90 AV: 1 NL: 7.63E4
T: FTMS + c NSI d Full ms2 772.37@hcd30.00 [100.00-2000.00]



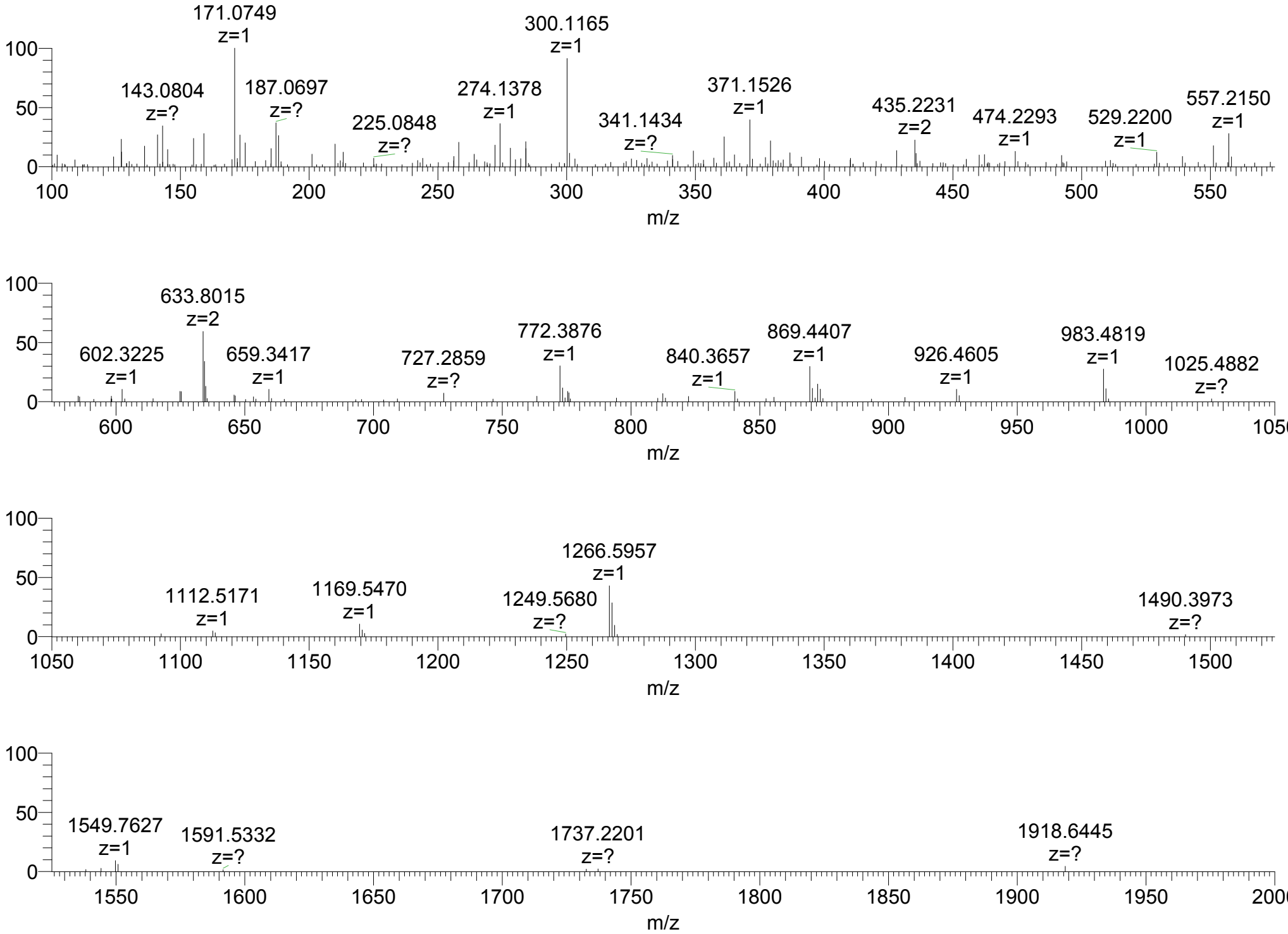
46.

P1287-OH, P1293-OH, P1302-OH, K1305-OH.Gal.Glc

#1285-1308: GE**P**GEAGE**P**GLPGEGGP**P**GP**K**GER

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+4OH+Gal.Glc	3	872.7192	872.7123	-0.0207	-7.9
PG-28+OH	1	143.0815	143.0804	-0.0011	-7.7
PG+OH	1	171.0764	171.0749	-0.0015	-8.8
EG/b2/GE	1	187.0713	187.0697	-0.0016	-8.6
b3/PGE+OH/EPG+OH	1	300.1190	300.1165	-0.0025	-8.4
AGEP+OH/PGEA+OH	1	371.1561	371.1526	-0.0035	-9.5
y8+2OH	2	435.2274	435.2231	-0.0086	-9.9
b6/EPGEAG+OH	1	557.2202	557.2150	-0.0052	-9.3
y13+2OH	2	633.8073	633.8015	-0.0116	-9.2
y6+OH	1	659.3471	659.3417	-0.0054	-8.2
y7+2OH	1	772.3948	772.3876	-0.0072	-9.3
y8+2OH	1	869.4476	869.4407	-0.0069	-7.9
y9+2OH	1	926.4690	926.4605	-0.0085	-9.2
y10+2OH	1	983.4905	983.4819	-0.0086	-8.8
y12+2OH	1	1169.5545	1169.5470	-0.0075	-6.4
y13+2OH	1	1266.6073	1266.5957	-0.0116	-9.2
y16+3OH	1	1549.7605	1549.7627	0.0022	1.4

12_9_2011Col5a1_Trypsin_CE40 #1771 RT: 17.23 AV: 1 NL: 2.18E4
T: FTMS + c NSI d Full ms2 873.38@hcd40.00 [100.00-2000.00]



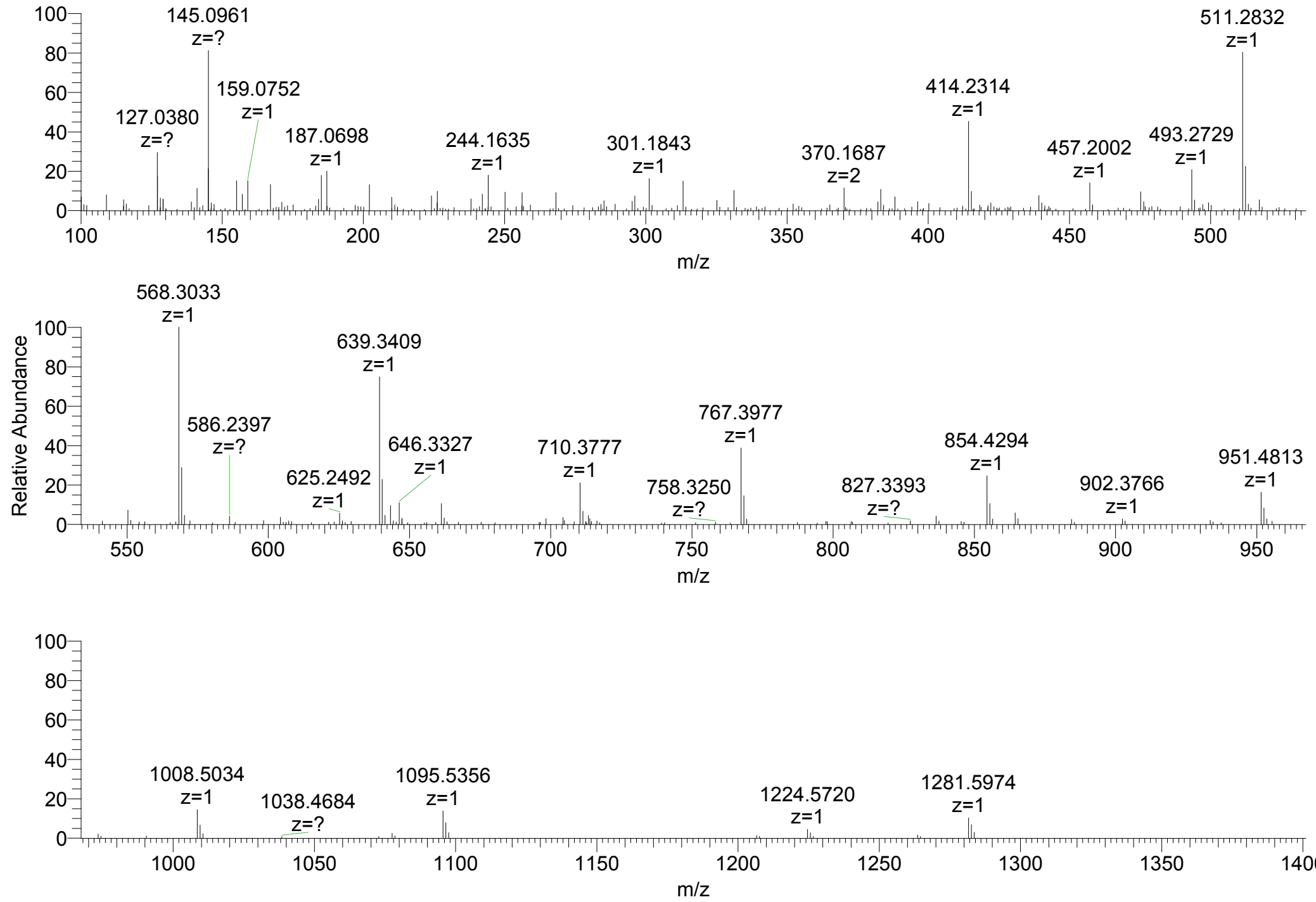
47.

K1311-OH.Gal.Glc, P1323-OH

#1309-1326: GE**K**GESGPSGAAGP**P**GPK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH+Gal.Glc	3	645.9604	645.9532	-0.0216	-11.2
b2/GE	1	187.0713	187.0698	-0.0015	-8.1
y2	1	244.1656	244.1635	-0.0021	-8.6
y3	1	301.1870	301.1843	-0.0027	-9.0
y4+OH	1	414.2347	414.2314	-0.0033	-8.0
y5+OH	1	511.2875	511.2832	-0.0043	-8.4
y6+OH	1	568.3089	568.3033	-0.0056	-9.9
y7+OH	1	639.3461	639.3409	-0.0052	-8.1
b7+OH	1	661.2788	661.2729	-0.0059	-8.9
y8+OH	1	710.3832	710.3777	-0.0055	-7.8
y9+OH	1	767.4046	767.3977	-0.0069	-9.0
y10+OH	1	854.4367	854.4294	-0.0073	-8.6
y11+OH	1	951.4894	951.4813	-0.0081	-8.5
y12+OH	1	1008.5109	1008.5034	-0.0075	-7.4
y13+OH	1	1095.5429	1095.5356	-0.0073	-6.7
y14+OH	1	1224.5855	1224.5720	-0.0135	-11.0
y15+OH	1	1281.6070	1281.5974	-0.0096	-7.5

12_9_2011Col5a1_Trypsin_CE40 #848 RT: 9.16 AV: 1 NL: 5.59E4
T: FTMS + c NSI d Full ms2 646.29@hcd40.00 [100.00-1950.00]



48.

P1338-OH, P1344-OH, P1347-OH, P1353-OH

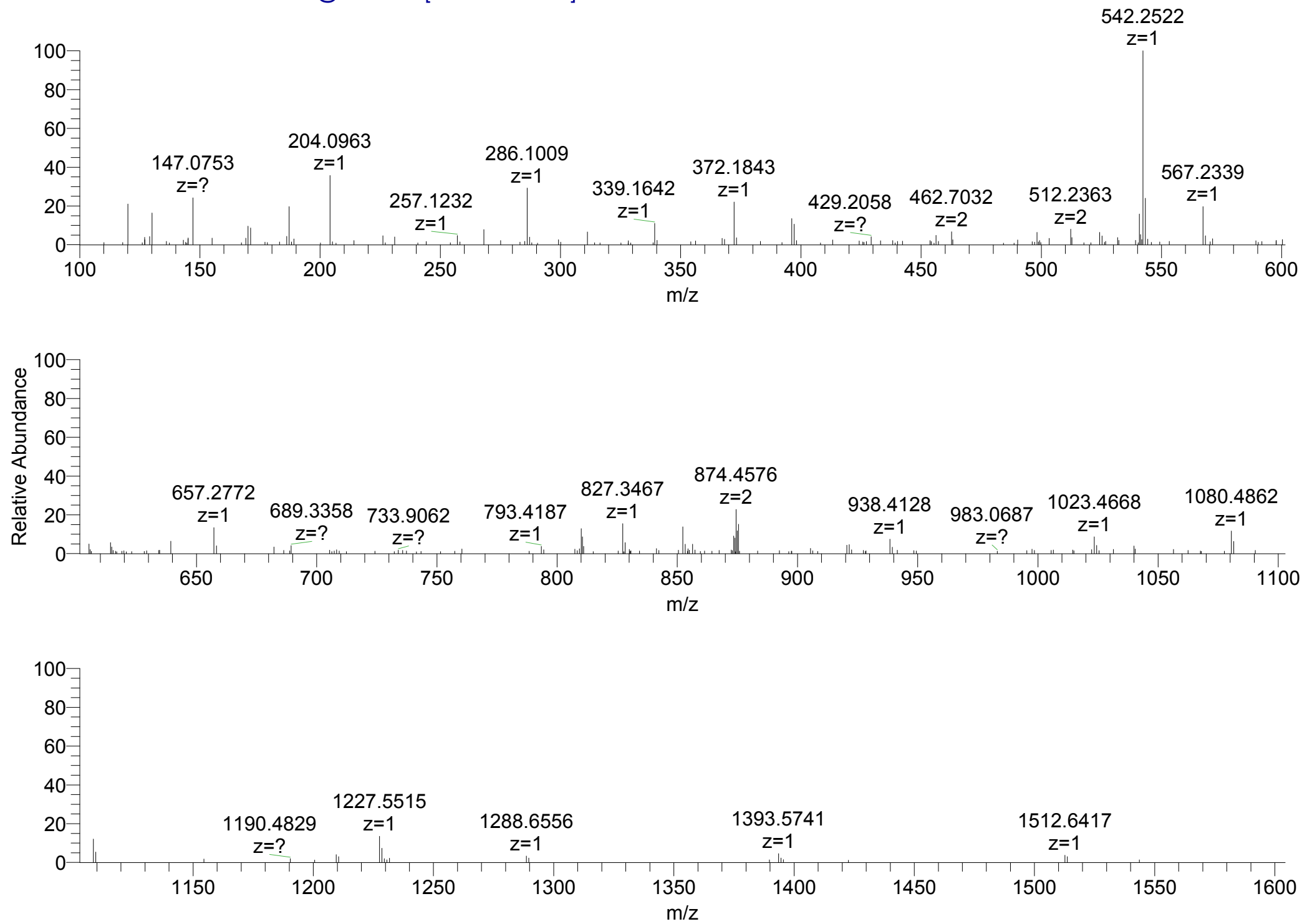
#1331-1358: DDGPKGS**P**GPVGF**P**GD**P**GPPGE**P**GPAGQ

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+5OH	3	874.0526	874.0450	-0.0228	-8.7
y1	1	147.0764	147.0753	-0.0011	-7.5
y2	1	204.0979	204.0963	-0.0016	-7.9
y4	1	372.1878	372.1843	-0.0035	-9.4
b10+OH	2	462.7065	462.7032	-0.0066	-7.1
b11+OH	2	512.2407	512.2363	-0.0088	-8.6
y6+OH	1	542.2569	542.2522	-0.0047	-8.7
b7	1	657.2838	657.2772	-0.0066	-10.1
b9+OH	1	827.3530	827.3467	-0.0063	-7.6
y10+2OH	1	938.4214	938.4128	-0.0086	-9.2
b11+OH	1	1023.4742	1023.4668	-0.0074	-7.2
b12+OH	1	1080.4956	1080.4862	-0.0094	-8.7
y12+3OH	1	1108.4905	1108.4823	-0.0082	-7.4
b13+OH	1	1227.5640	1227.5515	-0.0125	-10.2
y15+4OH	1	1393.5866	1393.5741	-0.0125	-9.0

***Unlocalized sites: P1349-OH?, P1350-OH?**

Pseudolocalized sites: P1350-OH

12_9_2011Col5a1_AspNGluC_3 #2874 RT: 25.56 AV: 1 NL: 3.85E4
T: FTMS + c NSI d Full ms2 874.38@hcd30.00 [100.00-2000.00]



49.

P1350-OH, P1353-OH

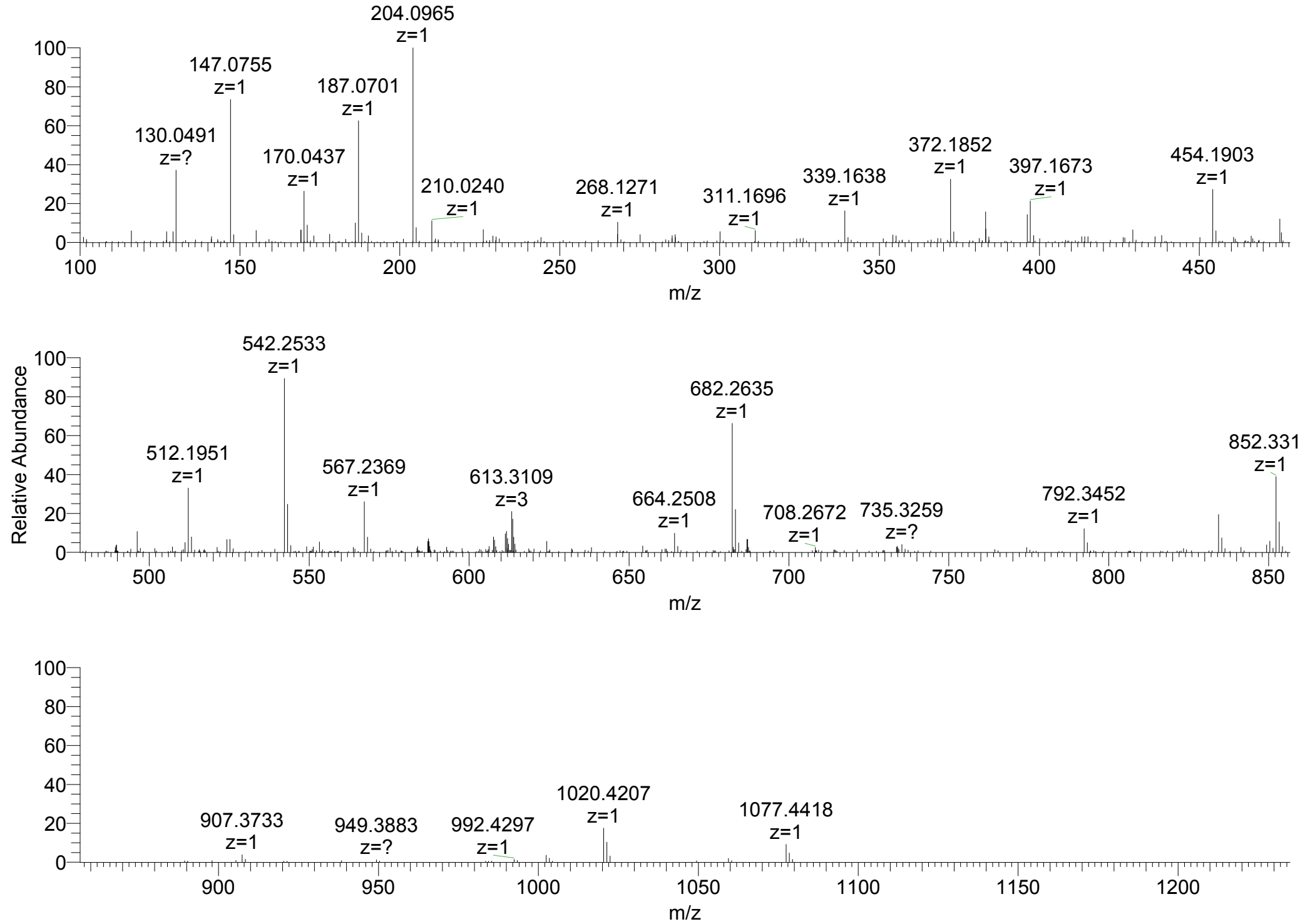
#1346-1358: DPGP**P**GE**P**GPAGQ

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+3OH	2	612.2624	612.2568	-0.0112	-9.2
y1	1	147.0764	147.0755	-0.0009	-6.2
y2-NH3	1	187.0713	187.0701	-0.0012	-6.4
y2	1	204.0979	204.0965	-0.0014	-6.9
y4	1	372.1878	372.1852	-0.0026	-7.0
b4+OH	1	383.1561	383.1535	-0.0026	-6.8
y5	1	429.2029	429.2065	0.0036	8.4
y6+OH	1	542.2569	542.2533	-0.0036	-6.7
b7+2OH	1	682.2679	682.2635	-0.0044	-6.5
b9+3OH	1	862.3370	862.3315	-0.0055	-6.4
b11+3OH	1	1020.4269	1020.4207	-0.0062	-6.1
b12+3OH	1	1077.4483	1077.4418	-0.0065	-6.0

***Unlocalized sites: P1347-OH?, P1349-OH?**

Pseudolocalized sites: P1347-OH

12_9_2011Col5a1_AspNGluC_1 #1103 RT: 11.04 AV: 1 NL: 1.06E5
T: FTMS + c NSI d Full ms2 612.26@hcd30.00 [100.00-1235.00]



50.

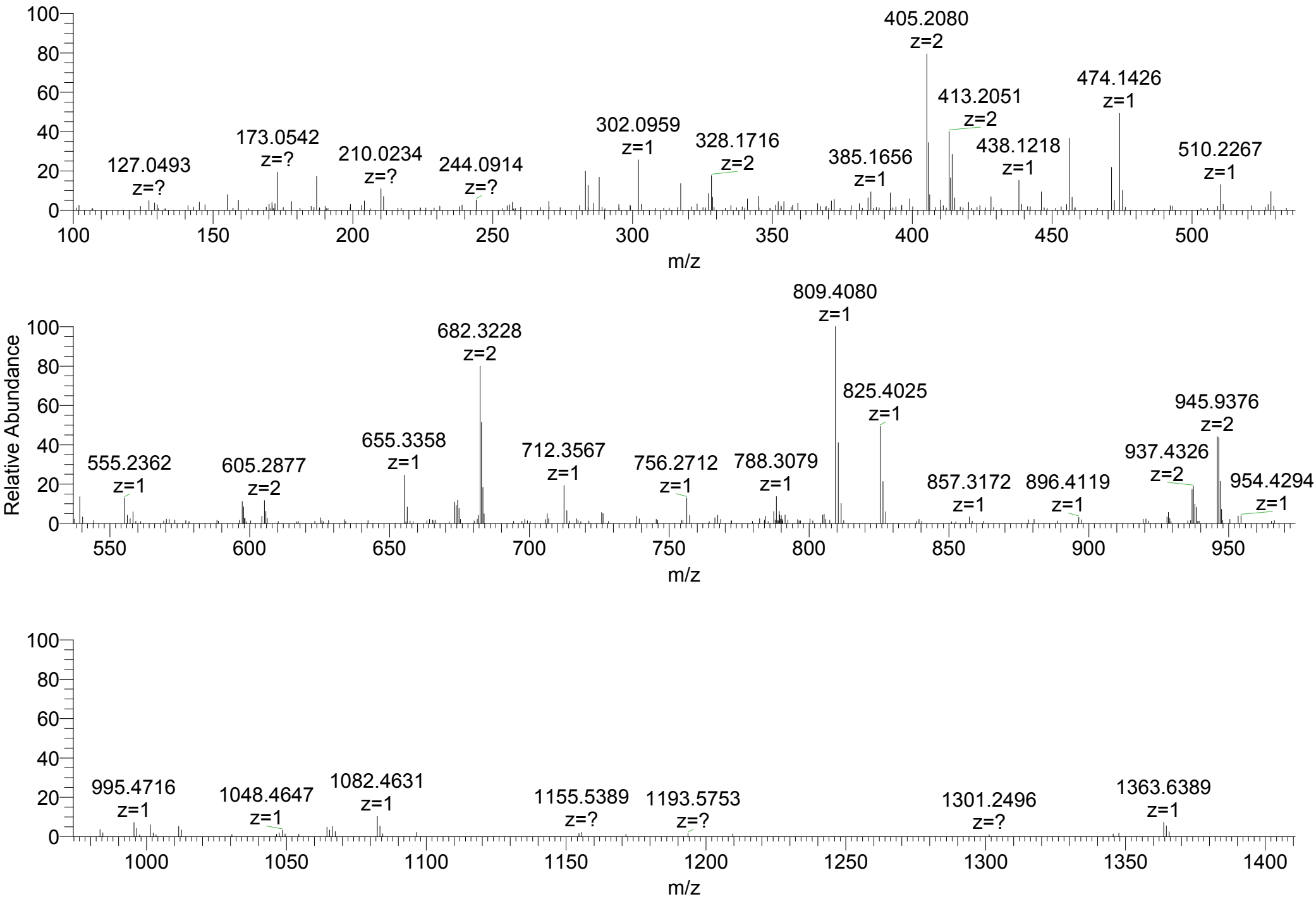
P1377-OH, P1383-OH, P1389-OH

#1366-1391: GDDGEPGQTGS**P**GPTGEPGPSGP**P**GK and

GDDGEPGQTGSPGPTGE**P**GPSGP**P**GK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH	3	788.6789	788.6719	-0.0210	-8.9
b2	1	173.0557	173.0542	-0.0015	-8.7
y2	1	204.1343	204.1326	-0.0017	-8.4
y3+OH	1	317.1819	317.1796	-0.0023	-7.3
y7+OH	2	328.1741	328.1716	-0.0050	-7.6
y9+OH	2	405.2112	405.2080	-0.0064	-7.9
y9+2OH	2	413.2087	413.2051	-0.0072	-8.7
b5-2H2O	1	438.1256	438.1218	-0.0038	-8.7
b5-H2O	1	456.1361	456.1326	-0.0035	-7.7
b5	1	474.1467	474.1426	-0.0041	-8.7
y13+OH	2	597.2935	597.2875	-0.0120	-10.1
y13+2OH	2	605.2909	605.2877	-0.0064	-5.3
y7+OH	1	655.3410	655.3358	-0.0052	-7.9
y15+2OH	2	682.3281	682.3228	-0.0106	-7.8
y8+OH	1	712.3624	712.3567	-0.0057	-8.0
b8	1	756.2795	756.2712	-0.0083	-11.0
y9+OH	1	809.4152	809.4080	-0.0072	-8.9
y9+2OH	1	825.4101	825.4025	-0.0076	-9.2
y21-H2O+2OH	2	936.9398	936.9329	-0.0138	-7.4
y21+2OH	2	945.9450	945.9376	-0.0148	-7.8
y11+OH	1	995.4793	995.4716	-0.0077	-7.7
y11+2OH	1	1011.4742	1011.4652	-0.0090	-8.9
y15+2OH	1	1363.6488	1363.6389	-0.0099	-7.3

12_9_2011Col5a1_Trypsin_CE30 #1508 RT: 15.28 AV: 1 NL: 4.39E4
T: FTMS + c NSI d Full ms2 789.01@hcd30.00 [100.00-2000.00]



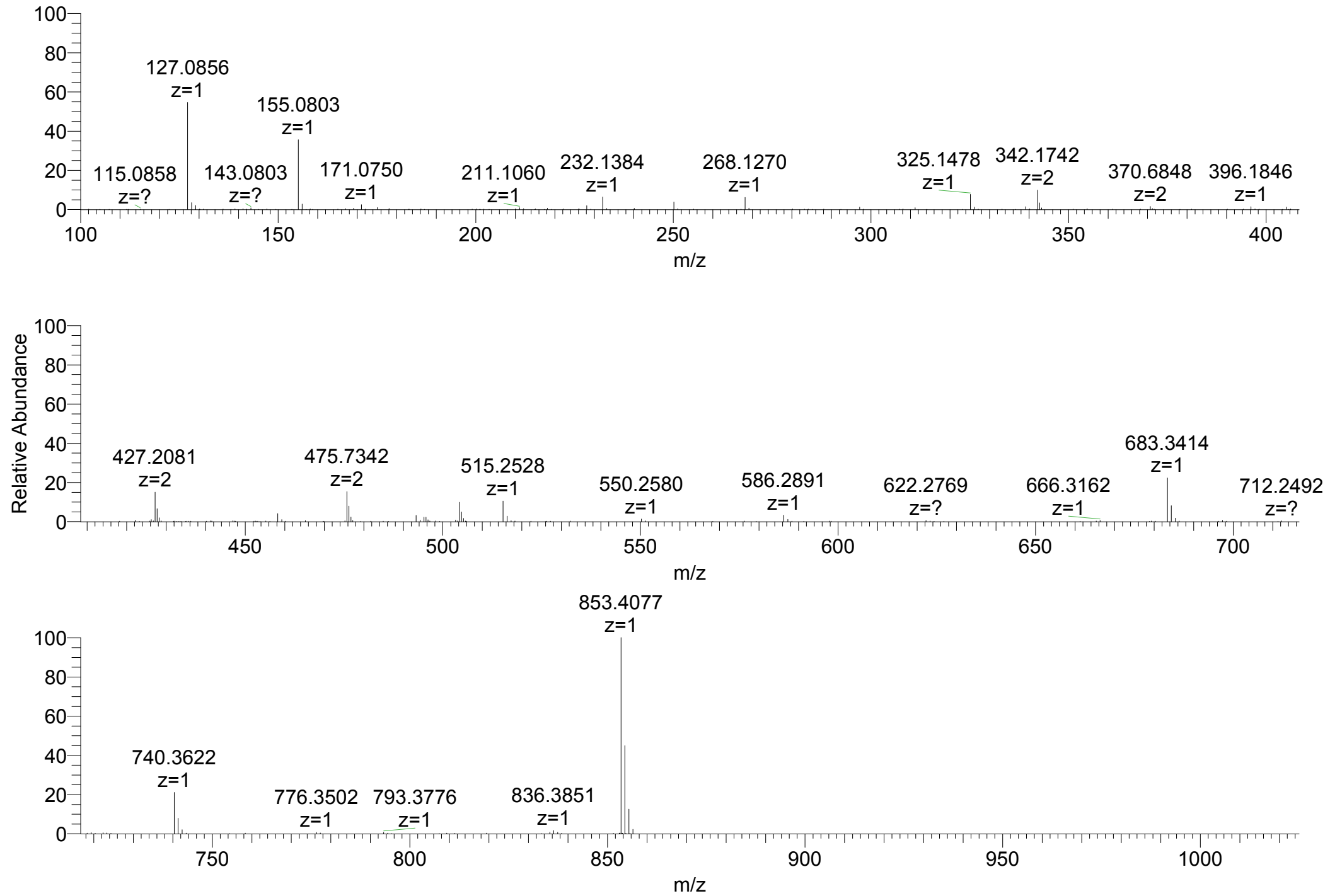
51.

P1395-OH

#1393-1403: GP**P**GPAGPEGR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+OH	2	504.2489	504.2444	-0.0090	-8.9
b2/GP	1	155.0815	155.0803	-0.0012	-7.8
y2	1	232.1404	232.1384	-0.0020	-8.7
b3+OH	1	268.1292	268.1270	-0.0022	-8.2
y7	2	342.1772	342.1742	-0.0060	-8.8
y9+OH	2	427.2118	427.2081	-0.0074	-8.7
y10+OH	2	475.7381	475.7342	-0.0078	-8.2
y5	1	515.2572	515.2528	-0.0044	-8.6
b7+OH	1	550.2620	550.2580	-0.0040	-7.3
y6	1	586.2944	586.2891	-0.0053	-9.1
y7	1	683.3471	683.3414	-0.0057	-8.4
y8	1	740.3686	740.3622	-0.0064	-8.7
y9+OH	1	853.4163	853.4077	-0.0086	-10.1

12_9_2011Col5a1_ArgC_3 #1001 RT: 10.46 AV: 1 NL: 1.58E6
T: FTMS + c NSI d Full ms2 505.25@hcd30.00 [100.00-1025.00]



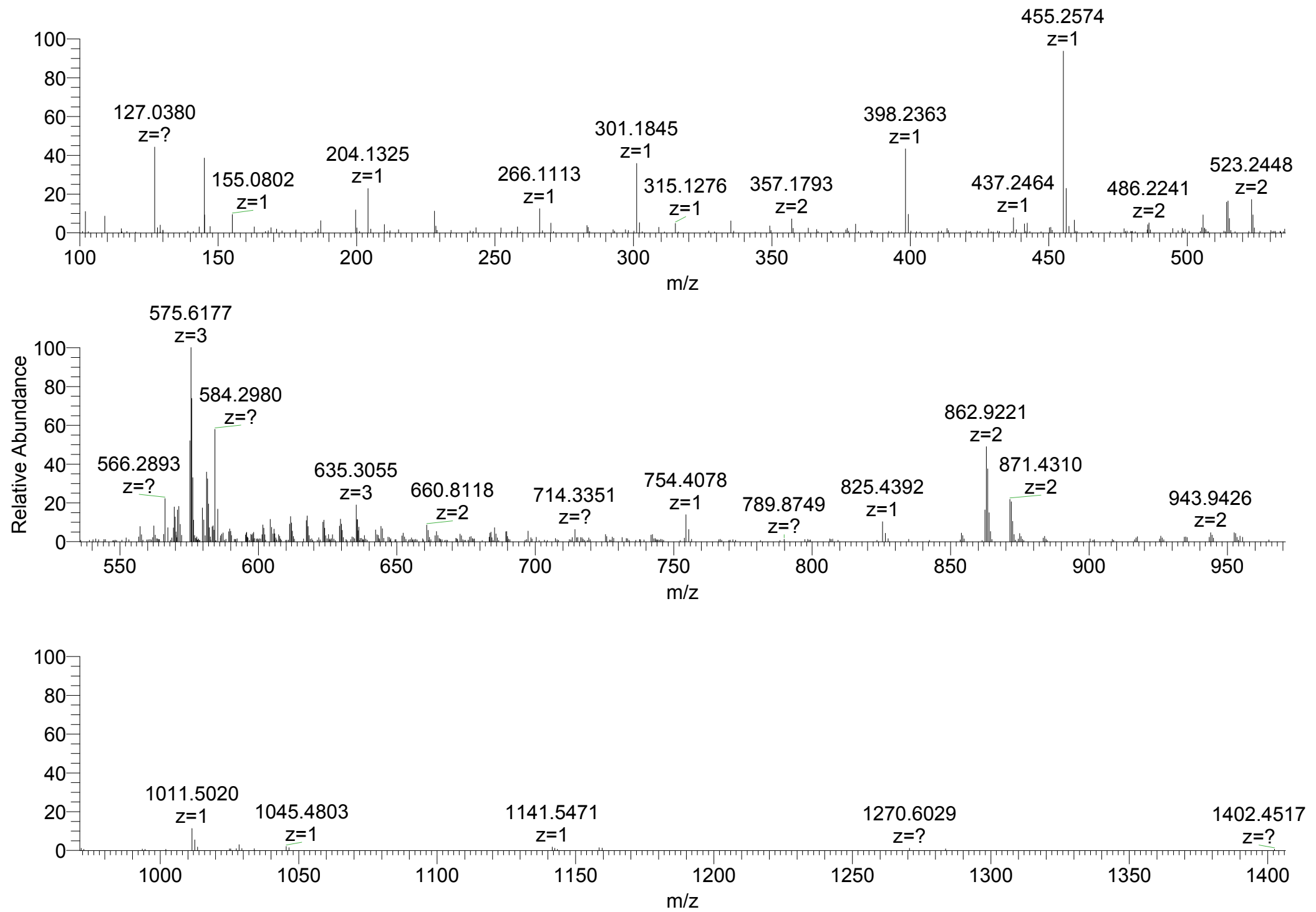
52.

K1407-OH.Gal.Glc, K1410-OH.Gal.Glc

#1404-1421: QGE**K**GA**K**GEAGLEGPPGK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+2OH+2Gal.Glc	4	598.2762	598.2699	-0.0252	-10.5
y2	1	204.1343	204.1325	-0.0018	-8.9
y5	2	228.1343	228.1323	-0.0040	-8.8
EGP-H2O	1	266.1135	266.1113	-0.0022	-8.3
y3	1	301.1870	301.1845	-0.0025	-8.3
y4	1	398.2398	398.2363	-0.0035	-8.8
y5	1	455.2613	455.2574	-0.0039	-8.6
b11-H2O+2OH	2	514.2438	514.2393	-0.0090	-8.8
b11+2OH	2	523.2491	523.2448	-0.0086	-8.2
[M+3H]-H2O+2OH	3	575.2918	575.2870	-0.0144	-8.4
b12+2OH	2	579.7911	579.7867	-0.0088	-7.6
[M+3H]+2OH	3	581.2954	581.2903	-0.0153	-8.8
y8	1	754.4094	754.4078	-0.0016	-2.1
y9	1	825.4465	825.4392	-0.0073	-8.9
[M+2H]-H2O+2OH	1	862.4341	862.4271	-0.0070	-8.1
[M+2H]+2OH	2	871.4394	871.4310	-0.0168	-9.7
y11	1	1011.5106	1011.5020	-0.0086	-8.5

12_9_2011Col5a1_Trypsin_CE30 #925 RT: 10.21 AV: 1 NL: 7.42E4
T: FTMS + c NSI d Full ms2 598.27@hcd30.00 [100.00-2000.00]



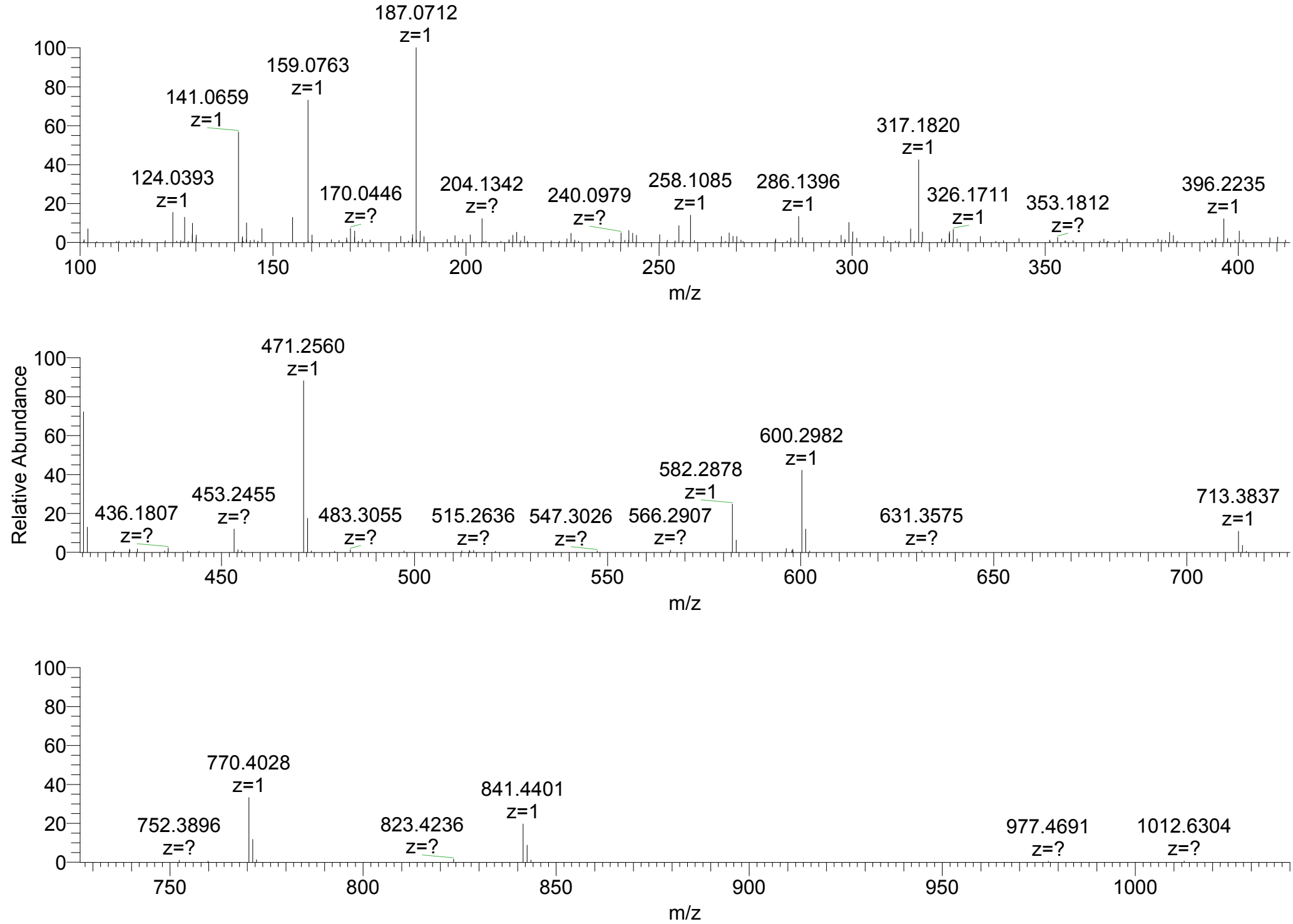
53.

P1419-OH

#1411-1421: GEAGLEGP**P**GK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+OH	2	514.2564	514.2542	-0.0044	-4.3
EG-28/a2	1	159.0764	159.0763	-0.0001	-0.6
b2/EG	1	187.0713	187.0712	-0.0001	-0.5
y2	1	204.1343	204.1342	-0.0001	-0.5
b3/EAG	1	258.1084	258.1085	0.0001	0.4
y3+OH	1	317.1819	317.1820	0.0001	0.3
y4+OH	1	414.2347	414.2346	-0.0001	-0.2
y5+OH	1	471.2562	471.2560	-0.0002	-0.4
y6-H2O+OH	1	582.2882	582.2878	-0.0004	-0.7
y6+OH	1	600.2988	600.2982	-0.0006	-1.0
y7+OH	1	713.3828	713.3837	0.0009	1.3
y8+OH	1	770.4043	770.4028	-0.0015	-1.9
y9+OH	1	841.4414	841.4401	-0.0013	-1.5

11_7_2011Collagen_Denatured #1195 RT: 14.31 AV: 1 NL: 3.55E4
T: FTMS + c NSI d Full ms2 514.25@hcd35.00 [100.00-1040.00]



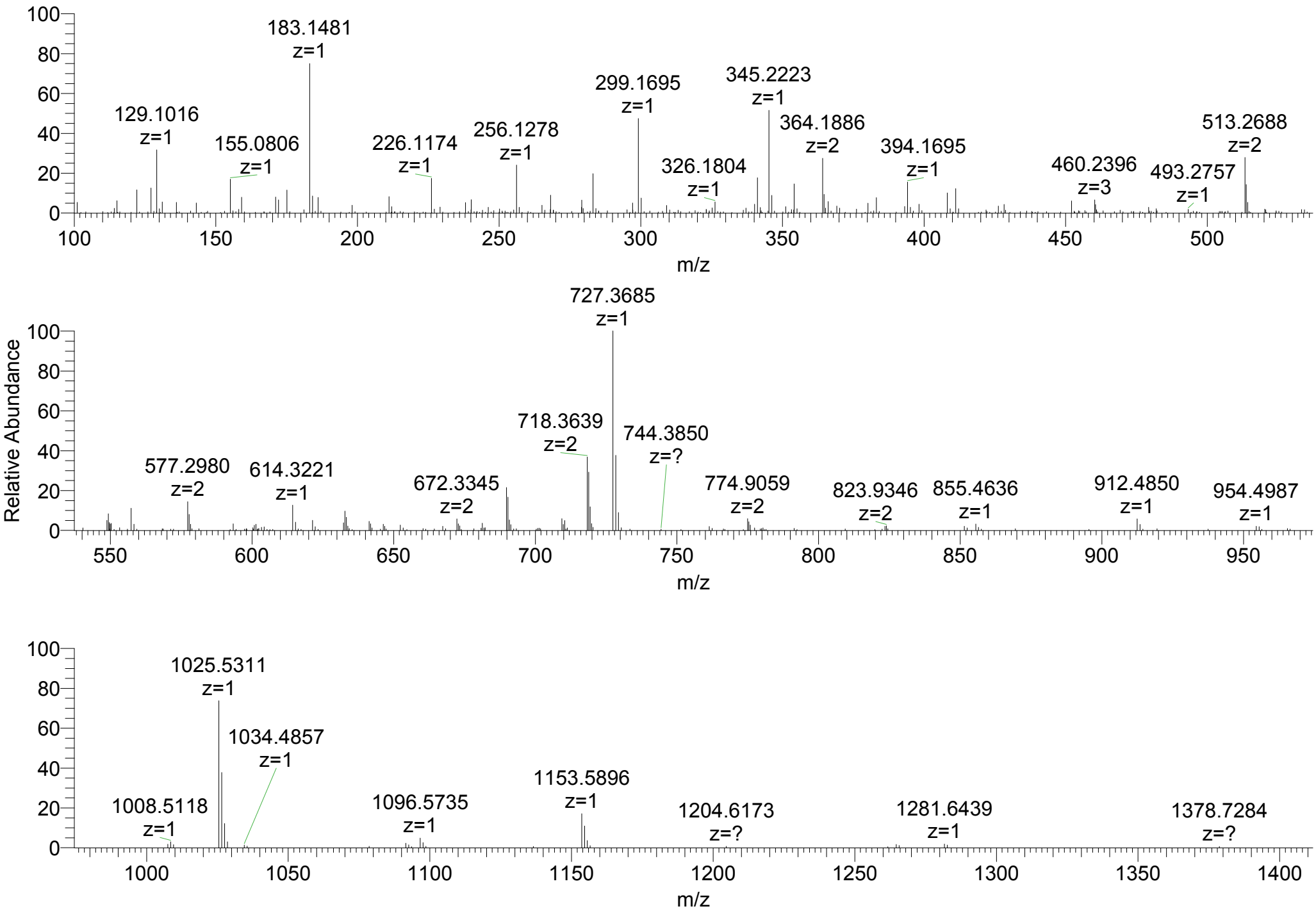
54.

P1431-OH, P1434-OH

#1422-1440: TGPIGPQGA**P**GK**P**GPDGLR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+2OH	3	601.9831	601.9777	-0.0162	-9.0
K	1	129.1022	129.1016	-0.0006	-4.7
GP	1	155.0815	155.0806	-0.0009	-5.8
PI-28	1	183.1492	183.1481	-0.0011	-6.0
PQ	1	226.1186	226.1174	-0.0012	-5.3
b3	1	256.1292	256.1278	-0.0014	-5.5
PGK+OH/GKP+OH/ KPG+OH	1	299.1714	299.1695	-0.0019	-6.4
y3	1	345.2245	345.2223	-0.0022	-6.4
y7+OH	2	364.1903	364.1886	-0.0034	-4.7
GPQGA-NH3	1	394.1721	394.1695	-0.0026	-6.6
y14+2OH	3	460.2406	460.2396	-0.0030	-2.2
y10+2OH	2	513.2724	513.2688	-0.0072	-7.0
y5	1	557.3042	557.3007	-0.0035	-6.3
y12+2OH	2	577.3016	577.2980	-0.0072	-6.2
y6	1	614.3257	614.3221	-0.0036	-5.9
y14+2OH	2	689.8573	689.8529	-0.0088	-6.4
y15+2OH	2	718.3680	718.3639	-0.0082	-5.7
y7+OH	1	727.3733	727.3685	-0.0048	-6.6
y16+2OH	2	774.9101	774.9059	-0.0084	-5.4
y8+OH	1	855.4683	855.4636	-0.0047	-5.5
y9+OH	1	912.4898	912.4898	0.0000	0.0
y10+2OH	1	1025.5374	1025.5311	-0.0063	-6.1
y12+2OH	1	1153.5960	1153.5896	-0.0064	-5.6

12_9_2011Col5a1_Trypsin_CE35 #2032 RT: 19.05 AV: 1 NL: 1.07E5
T: FTMS + c NSI d Full ms2 602.31@hcd35.00 [100.00-1820.00]



55.

P1452-OH, P1470-OH, K1473-OH

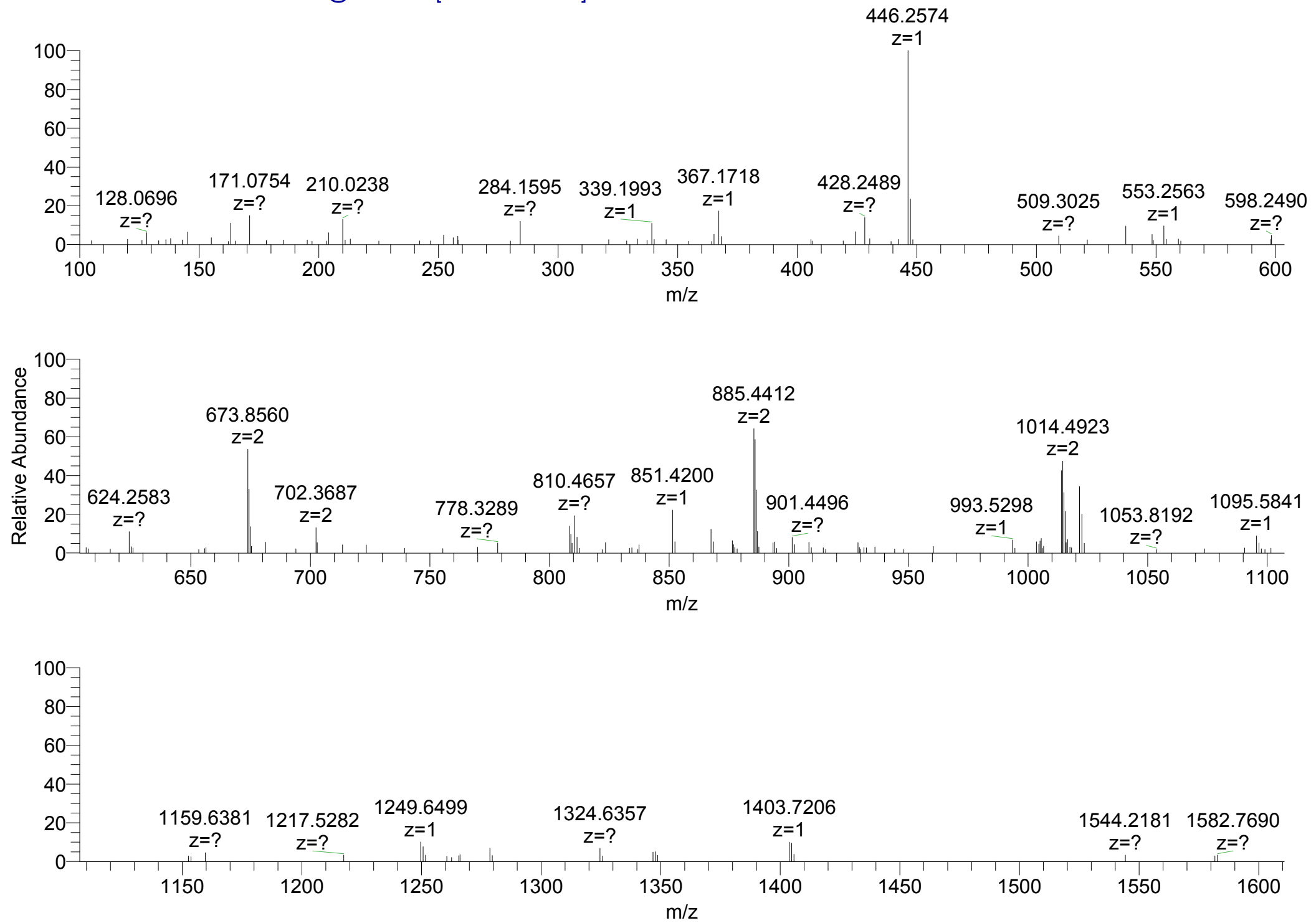
#1441-1473: GIPGPVGEQGL**P**GSPGPDGPPGPMGPPGL**P**GL**K**

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+4OH	3	1016.5096	1016.5016	-0.0240	-7.9
y4+2OH	1	446.2609	446.2574	-0.0035	-7.9
b6+OH	1	537.3031	537.2996	-0.0035	-6.5
y14+2OH	2	673.8605	673.8560	-0.0090	-6.7
y15+2OH	2	702.3712	702.3687	-0.0050	-3.6
y8+2OH	1	810.4720	810.4657	-0.0063	-7.8
b9+OH	1	851.4258	851.4200	-0.0058	-6.8
y19+2OH	2	885.4482	885.4412	-0.0140	-7.9
y22+3OH	2	1013.9988	1013.9922	-0.0132	-6.5
b11+OH	1	1021.5313	1021.5255	-0.0058	-5.7
y11+2OH	1	1095.5867	1095.5841	-0.0026	-2.4
y13+2OH	1	1249.6609	1249.6499	-0.0110	-8.8

***Unlocalized sites: P1443-OH?, P1445-OH?**

Pseudolocalized sites: P1443-OH

12_9_2011Col5a1_Trypsin_CE30 #5401 RT: 48.39 AV: 1 NL: 2.09E4
T: FTMS + c NSI d Full ms2 1017.17@hcd30.00 [100.00-2000.00]



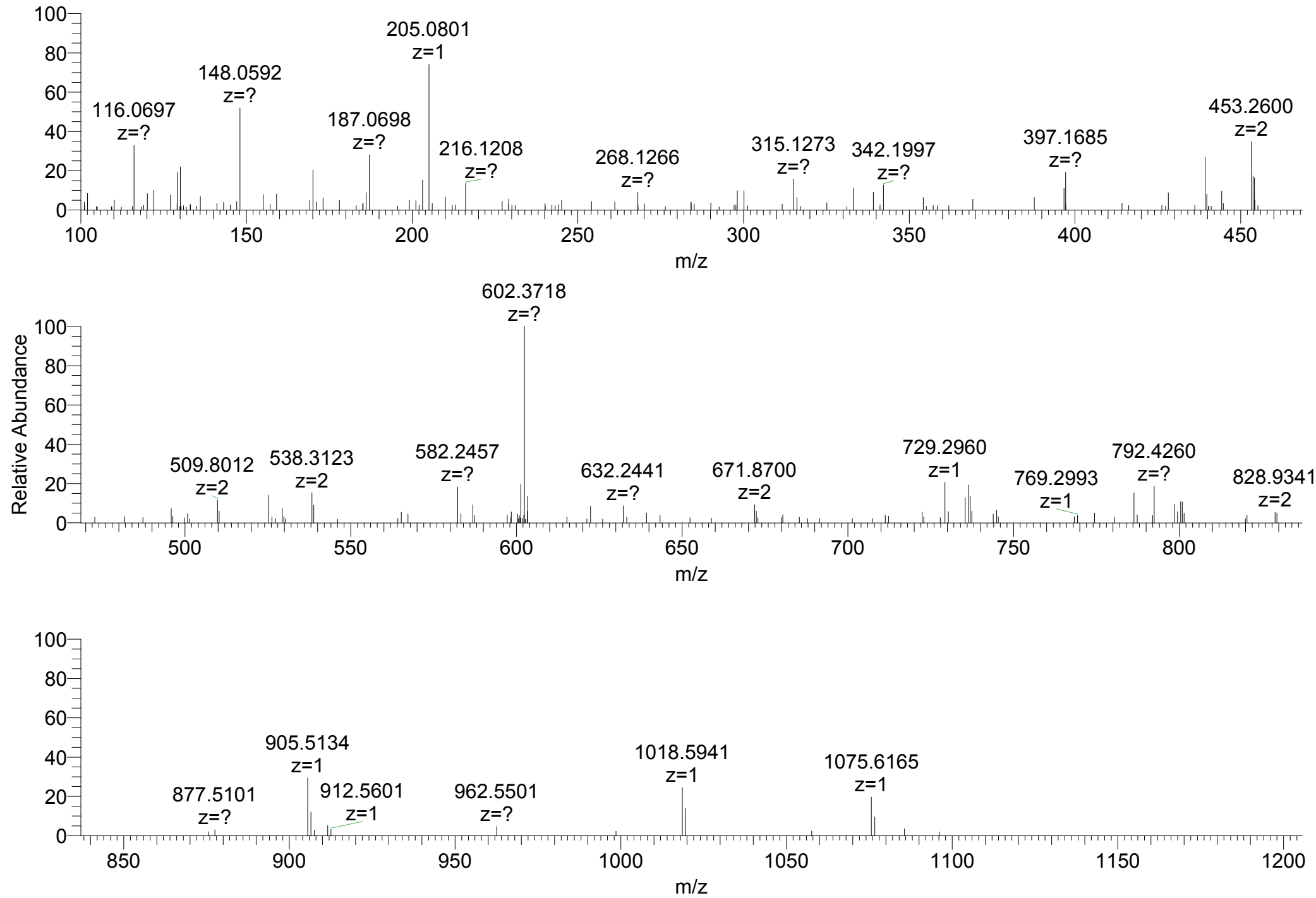
56.

K1482-OH, P1485-OH, P1494-OH

#1482-1499: **K**GH**P**GLIGLIGP**P**GEQGE

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+3H]+3OH	3	601.9794	601.9736	-0.0174	-9.7
y1	1	148.0604	148.0592	-0.0012	-8.2
GE/y2-H2O	1	187.0713	187.0698	-0.0015	-8.1
y2	1	205.0819	205.0801	-0.0018	-8.8
y3-H2O/GEQ/EQG	1	315.1299	315.1273	-0.0026	-8.3
b9+2OH	2	453.2638	453.2600	-0.0076	-8.4
b10+2OH	2	509.8058	509.8012	-0.0092	-9.0
b11+2OH	2	538.3166	538.3123	-0.0086	-8.0
b12+2OH	2	586.8429	586.8370	-0.0118	-10.1
y6+OH	1	632.2522	632.2441	-0.0081	-12.8
b14+3OH	2	671.8775	671.8700	-0.0150	-11.2
y7+OH	1	729.2960	729.2960	0.0000	0.0
b15+3OH	2	736.3988	736.3949	-0.0078	-5.3
y8+OH	1	786.3264	786.3234	-0.0030	-3.8
b8+2OH	1	792.4363	792.4260	-0.0103	-13.0
b17+3OH	2	828.9388	828.9341	-0.0094	-5.7
b9+2OH	1	905.5203	905.5134	-0.0069	-7.6
b10+2OH	1	1018.6044	1018.5941	-0.0103	-10.1
b11+2OH	1	1075.6259	1075.6165	-0.0094	-8.7

12_9_2011Col5a1_AspNGluC_2 #4067 RT: 36.04 AV: 1 NL: 1.98E4
T: FTMS + c NSI d Full ms2 602.31@hcd30.00 [100.00-1820.00]



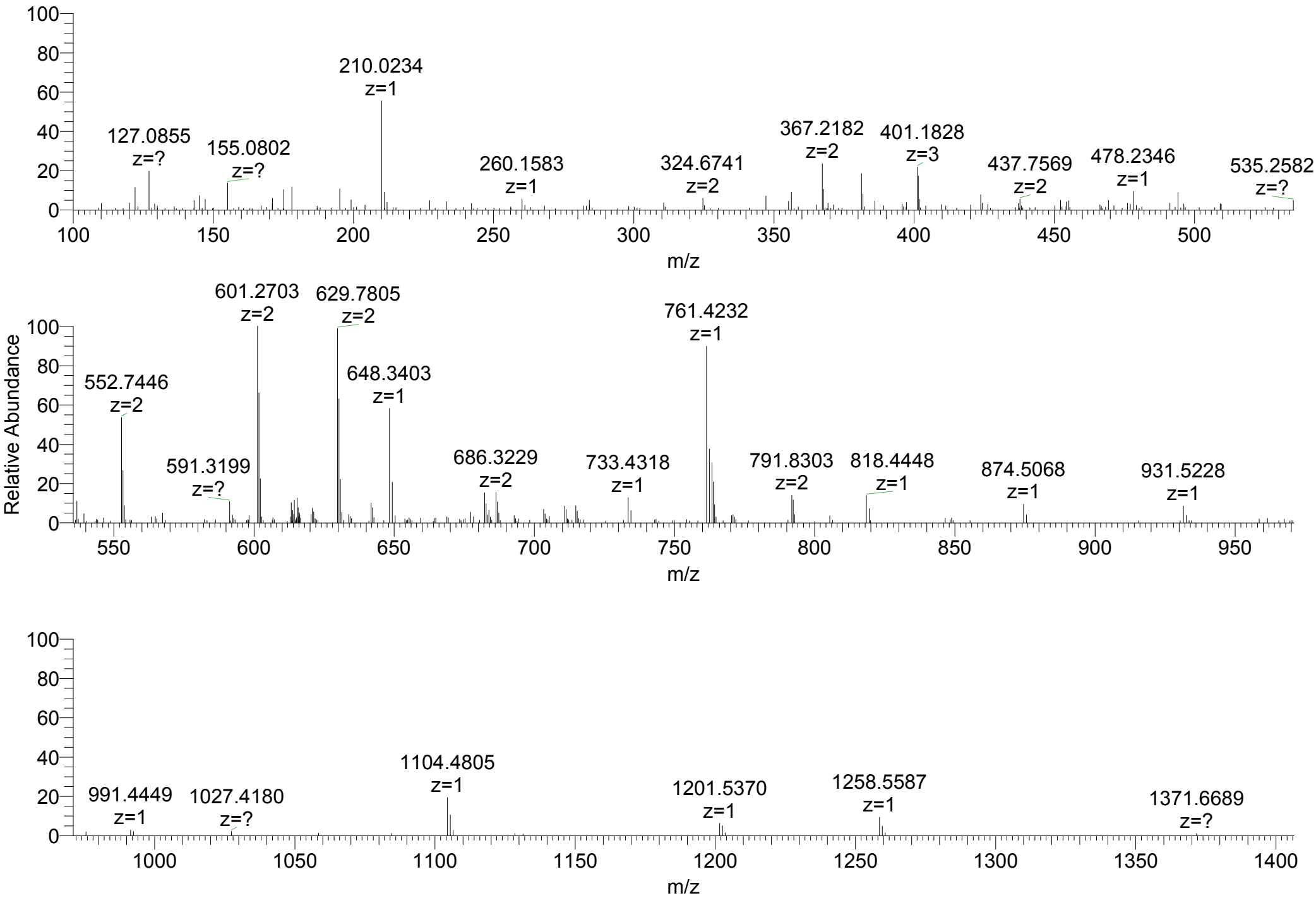
57.

P1485-OH, P1494-OH, K1500-OH.Gal.Glc

#1483-1503: GH**P**GLIGLIGP**P**GEQGE**K**GDR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+3OH+Gal.Glc	4	614.8001	614.7947	-0.0216	-8.8
GP-28	1	127.0866	127.0855	-0.0011	-8.7
GP	1	155.0815	155.0802	-0.0013	-8.4
b7+OH	2	324.6768	324.6741	-0.0054	-8.3
a8+OH	2	367.2214	367.2182	-0.0064	-8.7
b8+OH	2	381.2189	381.2153	-0.0072	-9.5
y11+2OH	3	401.1863	401.1828	-0.0105	-8.7
y10+2OH	2	552.7494	552.7446	-0.0096	-8.7
y11+2OH	2	601.2758	601.2703	-0.0110	-9.2
y12+2OH	2	629.7866	629.7805	-0.0122	-9.7
b7+OH	1	648.3464	648.3403	-0.0061	-9.4
y13+2OH	2	686.3286	686.3229	-0.0114	-8.3
a8+OH	1	733.4355	733.4318	-0.0037	-5.1
b8+OH	1	761.4304	761.4232	-0.0072	-9.5
y12+2OH+Gal.Glc	2	791.8394	791.8303	-0.0182	-11.5
b9+OH	1	874.5145	874.5068	-0.0077	-8.8
y10+2OH	1	1104.4916	1104.4805	-0.0111	-10.1
y11+2OH	1	1201.5444	1201.5370	-0.0074	-6.2
y12+2OH	1	1258.5658	1258.5587	-0.0071	-5.6

12_9_2011Col5a1_Trypsin_CE30 #3027 RT: 28.03 AV: 1 NL: 4.70E4
T: FTMS + c NSI d Full ms2 615.05@hcd30.00 [100.00-2000.00]



58.

P1506-OH

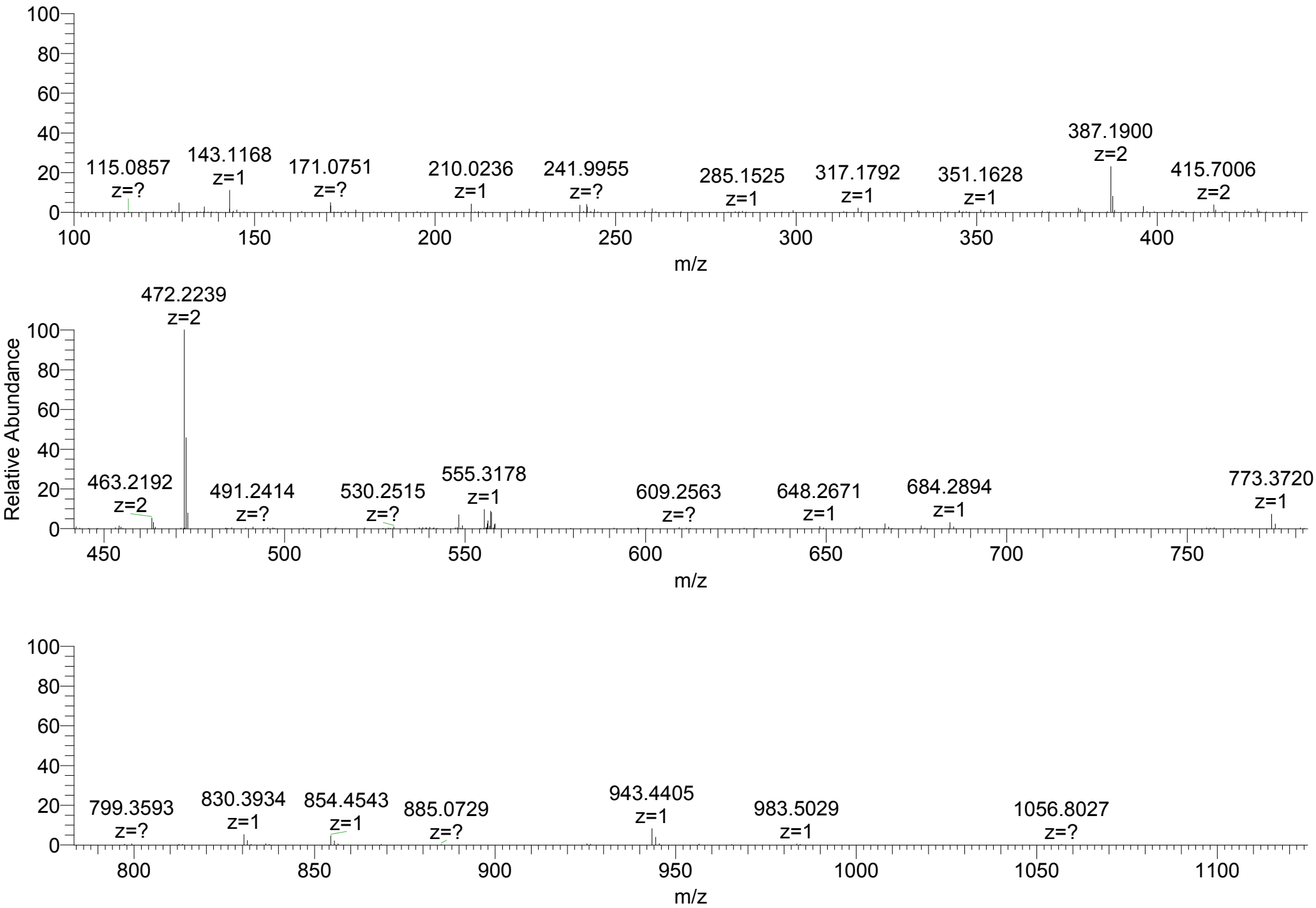
#1504-1515: GL**P**GPQGSSGPK

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+2OH	2	557.2804	557.2748	-0.0112	-10.1
y3+OH	1	317.1819	317.1792	-0.0027	-8.5
y4-NH3	1	387.1874	387.1900	0.0026	6.7
y9+OH	2	415.7038	415.7006	-0.0064	-7.7
y10+2OH	2	472.2276	472.2239	-0.0074	-7.9
y8+OH	1	773.3788	773.3720	-0.0068	-8.8
y9+OH	1	830.4003	830.3934	-0.0069	-8.3
y10+2OH	1	943.4480	943.4405	-0.0075	-8.0

***Unlocalized sites: P1514-OH?, K1515-OH?**

Pseudolocalized sites: K1515-OH

12_9_2011Col5a1_Trypsin_CE30 #1171 RT: 12.37 AV: 1 NL: 2.70E5
T: FTMS + c NSI d Full ms2 557.27@hcd30.00 [100.00-1125.00]



59.

K1554-OH.Gal

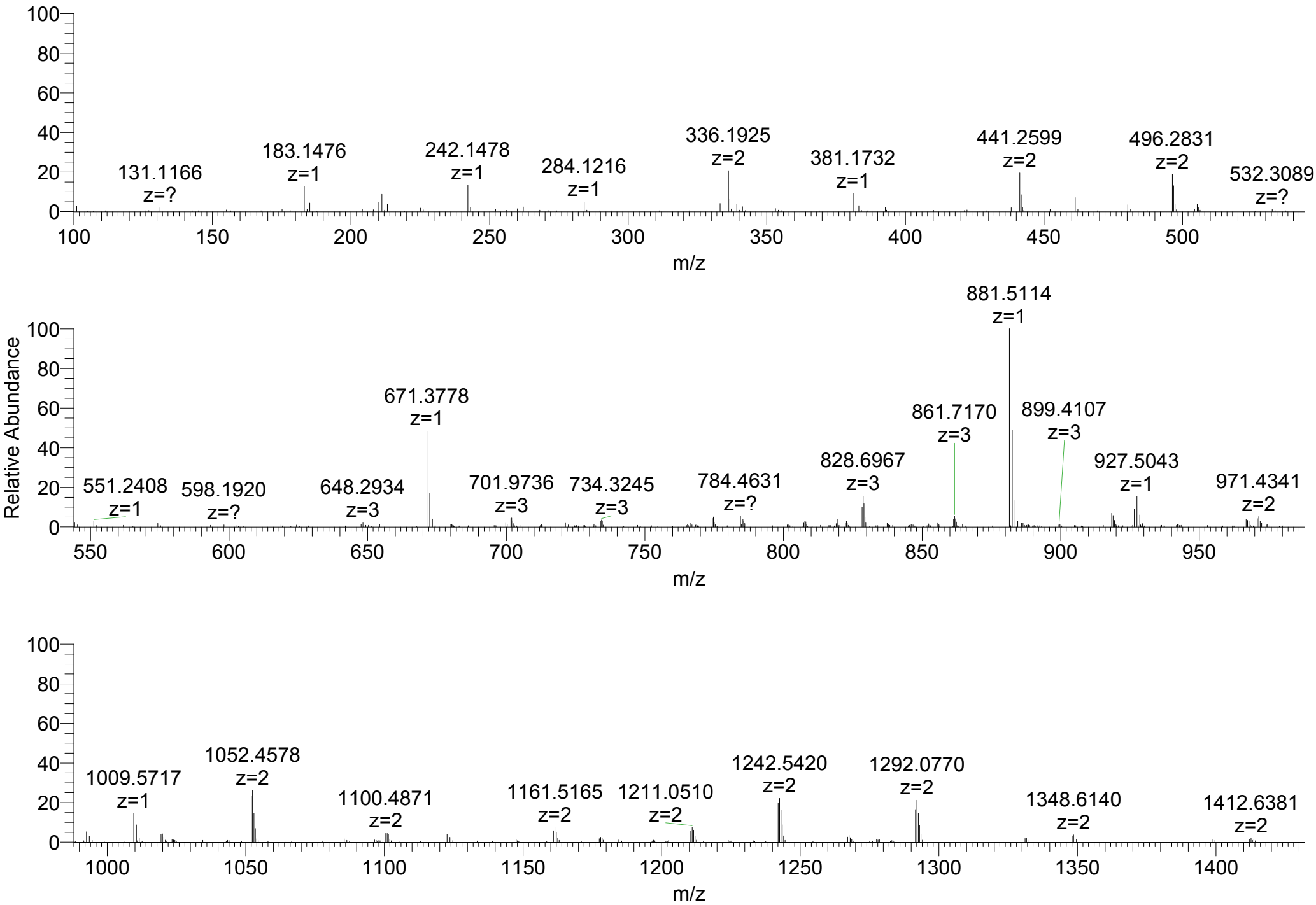
#1546-1582: GSSGPTGP**K**GEAGHPGPPGPPGPPGEVIQPLPIQASR

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+4H]+4OH+Gal	4	926.7104	926.7028	-0.0304	-8.2
PI-28/PL-28/LP-28	1	183.1492	183.1476	-0.0016	-8.8
IQ/PK+OH	1	242.1499	242.1478	-0.0021	-8.7
PGE	1	284.1241	284.1216	-0.0025	-8.8
y6	2	336.1954	336.1925	-0.0058	-8.7
PPGE/PGPP+2OH	1	381.1769	381.1732	-0.0037	-9.7
y8	2	441.2638	441.2599	-0.0078	-8.9
y4	1	461.2467	461.2428	-0.0039	-8.5
y9-H2O	2	496.2878	496.2831	-0.0094	-9.5
y10-H2O-NH3	2	544.3166	544.3124	-0.0084	-7.7
y6	1	671.3835	671.3778	-0.0057	-8.5
b26+4OH+Gal	3	828.3701	828.3644	-0.0171	-6.9
y8	1	881.5203	881.5114	-0.0089	-10.1
y9	1	1009.5789	1009.5717	-0.0072	-7.1
b22+4OH+Gal	2	1051.9677	1051.9567	-0.0220	-10.5
b23+4OH+Gal	2	1100.4931	1100.4871	-0.0120	-5.5
b26+4OH	2	1161.0251	1161.0183	-0.0136	-5.9
b27+4OH	2	1210.5593	1210.5513	-0.0160	-6.6
b26+4OH+Gal	2	1242.0515	1242.0410	-0.0210	-8.5
b27+4OH+Gal	2	1291.5857	1291.5769	-0.0176	-6.8
b28+4OH+Gal	2	1348.1277	1348.1147	-0.0260	-9.7

***Unlocalized sites: P1550-OH?, P1553-OH?, P1560-OH?, P1562-OH?, P1563-OH?, P1565-OH?, P1566-OH?**

Pseudolocalized sites: P1560-OH, P1562-OH, P1566-OH

12_9_2011Col5a1_Trypsin_CE30 #3564 RT: 32.62 AV: 1 NL: 1.23E5
T: FTMS + c NSI d Full ms2 927.20@hcd30.00 [100.00-2000.00]



60.

P1560-OH, P1563-OH, P1566-OH, P1569-OH

#1557-1571: AGH**P**GP**P**GP**P**GP**P**GE

Ion	charge state	Theoretical m/z (mono)	Experimental m/z (mono)	Mass error (Da)	Mass error (PPM)
[M+2H]+4OH	2	692.8100	692.8033	-0.0134	-9.7
b3	1	266.1248	266.1228	-0.0020	-7.5
y3+OH	1	318.1296	318.1272	-0.0024	-7.6
b9+2OH	2	400.6879	400.6841	-0.0076	-9.5
y4+OH	1	415.1823	415.1789	-0.0034	-8.2
b11+3OH	2	485.7225	485.7188	-0.0074	-7.6
b12+3OH	2	534.2489	534.2441	-0.0096	-9.0
y6+2OH	1	585.2515	585.2465	-0.0050	-8.6
b14+4OH	2	619.2835	619.2796	-0.0078	-6.3
y7+2OH	1	682.3042	682.2980	-0.0062	-9.1
b8+2OH	1	703.3158	703.3094	-0.0064	-9.1
y8+2OH	1	739.3257	739.3168	-0.0089	-12.1
b9+2OH	1	800.3686	800.3616	-0.0070	-8.8
y9+3OH	1	852.3734	852.3616	-0.0118	-13.9
b10+3OH	1	913.4163	913.4089	-0.0074	-8.1
y10+3OH	1	949.4262	949.4210	-0.0052	-5.5
b11+3OH	1	970.4377	970.4299	-0.0078	-8.0
b12+3OH	1	1067.4905	1067.4817	-0.0088	-8.3
y12+4OH	1	1119.4953	1119.4893	-0.0060	-5.4

12_9_2011Col5a1_AspNGluC_2 #1327 RT: 13.05 AV: 1 NL: 3.31E4
T: FTMS + c NSI d Full ms2 692.80@hcd30.00 [100.00-1400.00]