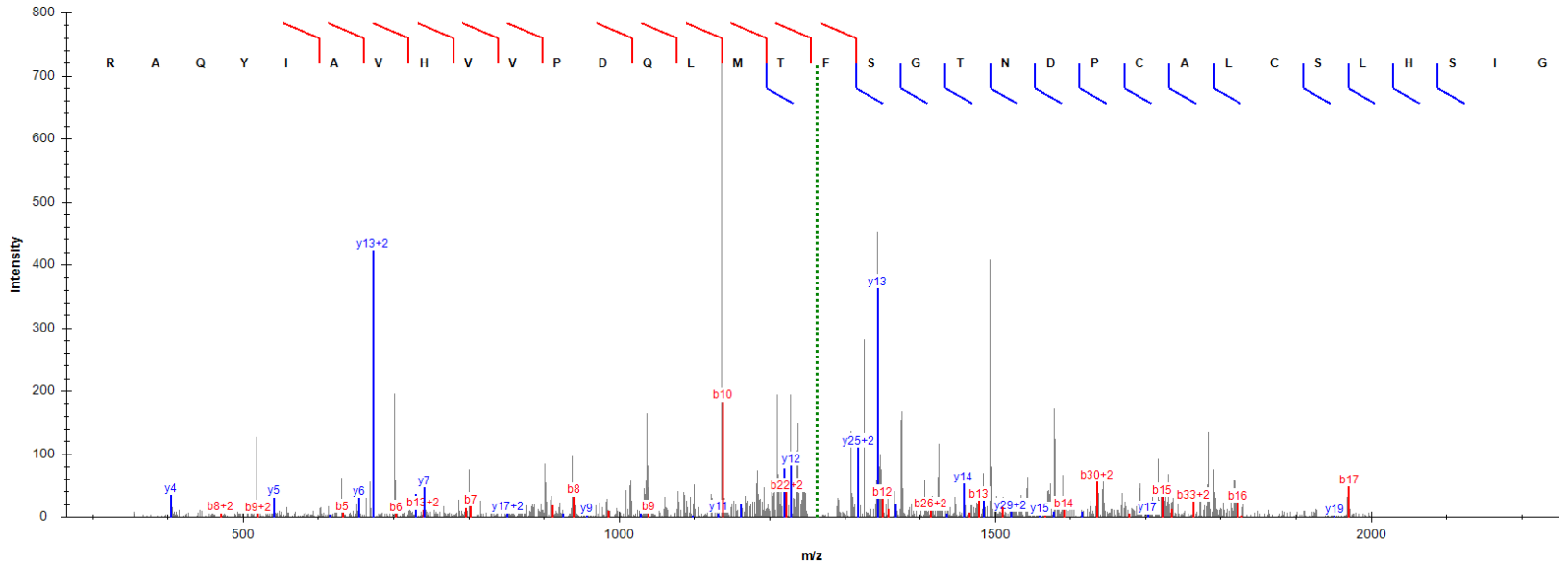
Saha et al. "Arginylation meets methylation: posttranslational modifications double up to regulate nuclear proteins and nuclear architecture in vivo"

Dataset S2

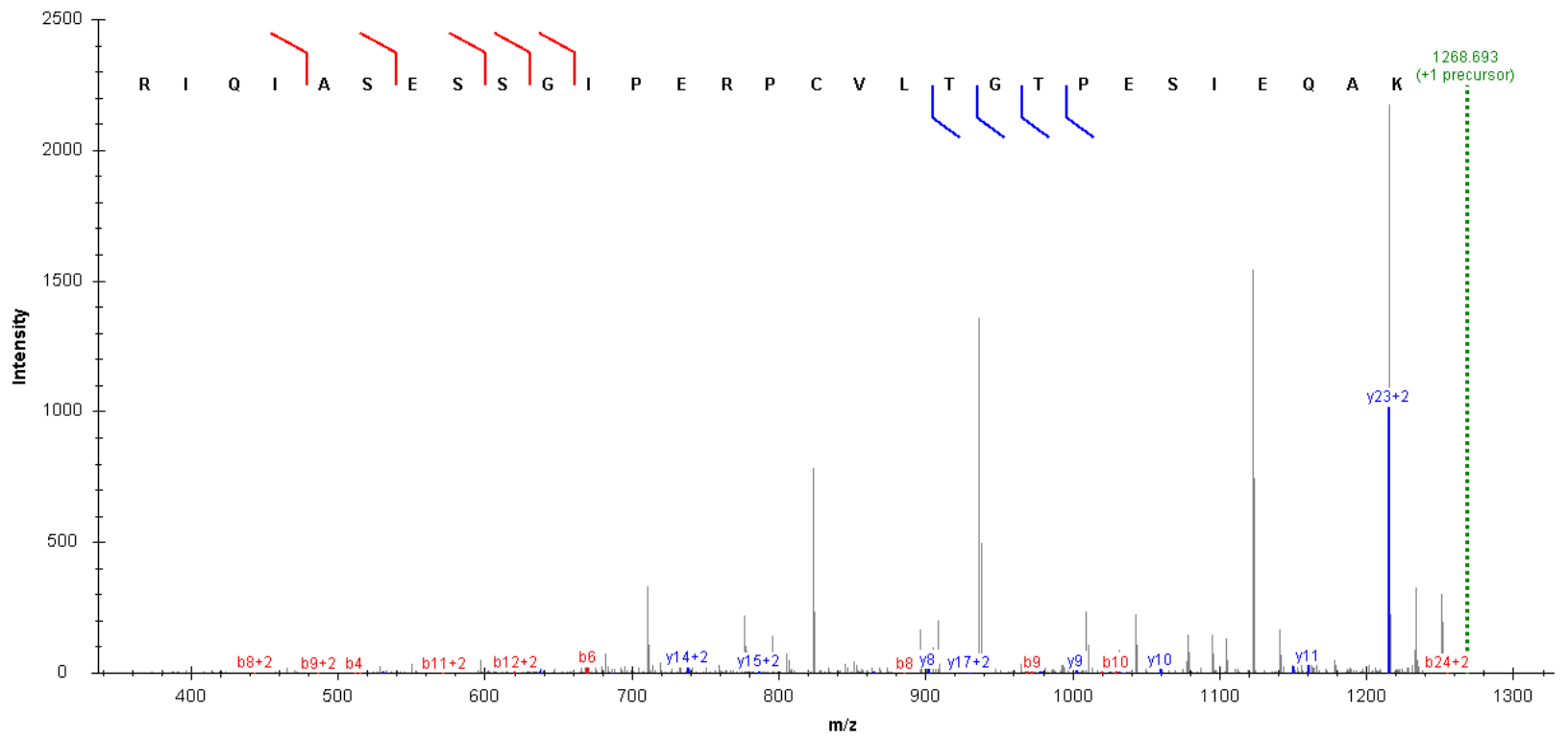
Mass spectra of arginylated peptides with detailed description of b and y ions

The following dataset contains the mass spectra of identified arginylated peptides. Each spectrum is followed by a table containing the expected and identified ions for the spectrum. The identified ions are highlighted in bold font in the tables. In the mass spectra b and y ions are marked in red and blue respectively. The complete sequence of the modified peptide is represented on top of each spectrum.



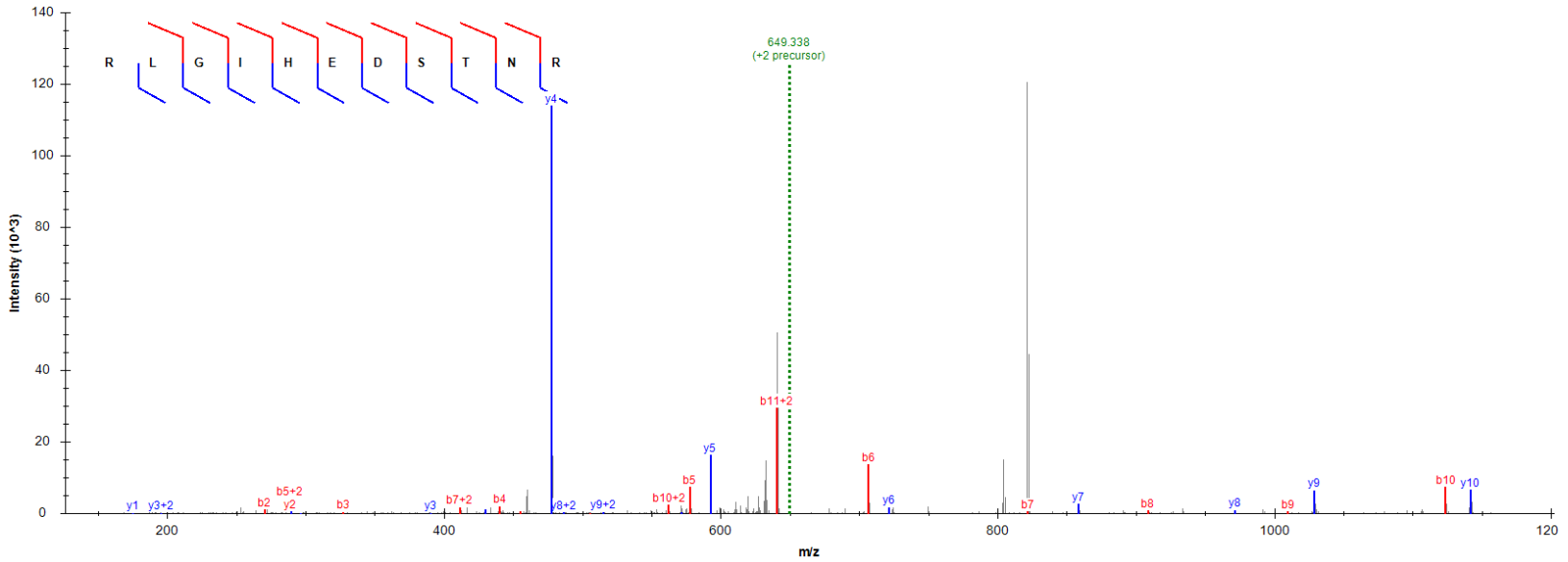
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	34	3671.813	1836.410
228.146	114.576	2	A	33	3515.712	1758.360
356.204	178.606	3	Q	32	3444.675	**1722.841**
519.267	260.137	4	Y	31	3316.616	1658.812
632.351	316.679	5	I	30	3153.553	**1577.280**
703.389	352.198	6	A	29	3040.469	**1520.738**
802.457	401.732	7	V	28	2969.432	**1485.220**
939.516	**470.262**	8	H	27	2870.363	**1435.685**
1038.584	**519.796**	9	V	26	2733.304	**1367.156**
1137.653	569.330	10	V	25	2634.236	**1317.622**
1234.706	617.856	11	P	24	2535.168	1268.087
1349.732	675.370	12	D	23	2438.115	**1219.561**
1477.791	**739.399**	13	Q	22	2323.088	**1162.048**
1590.875	**795.941**	14	L	21	2195.029	**1098.018**
1721.916	861.461	15	M	20	2081.945	1041.476
1822.963	**911.985**	16	T	19	**1950.905**	975.956
1970.032	**985.519**	17	F	18	1849.857	**925.432**
2057.064	1029.035	18	S	17	**1702.789**	**851.898**
2114.085	1057.546	19	G	16	**1615.757**	808.382
2215.133	1108.070	20	T	15	**1558.735**	779.871

2329.176	1165.092	21	N	14	**1457.688**	**729.347**
2444.203	**1222.605**	22	D	13	**1343.645**	**672.326**
2541.255	1271.131	23	P	12	**1228.618**	**614.812**
2644.265	1322.636	24	C	11	**1131.565**	566.286
2715.302	**1358.155**	25	A	10	**1028.556**	514.782
2828.386	**1414.697**	26	L	9	**957.519**	479.263
2931.395	**1466.201**	27	C	8	844.435	422.721
3018.427	**1509.717**	28	S	7	**741.425**	371.216
3131.511	**1566.259**	29	L	6	**654.393**	327.700
3268.570	**1634.789**	30	H	5	**541.309**	271.158
3355.602	**1678.305**	31	S	4	**404.250**	202.629
3468.686	**1734.847**	32	I	3	317.218	159.113
3525.708	**1763.357**	33	G	2	204.134	102.571
3653.803	**1827.405**	34	K	1	147.113	74.060

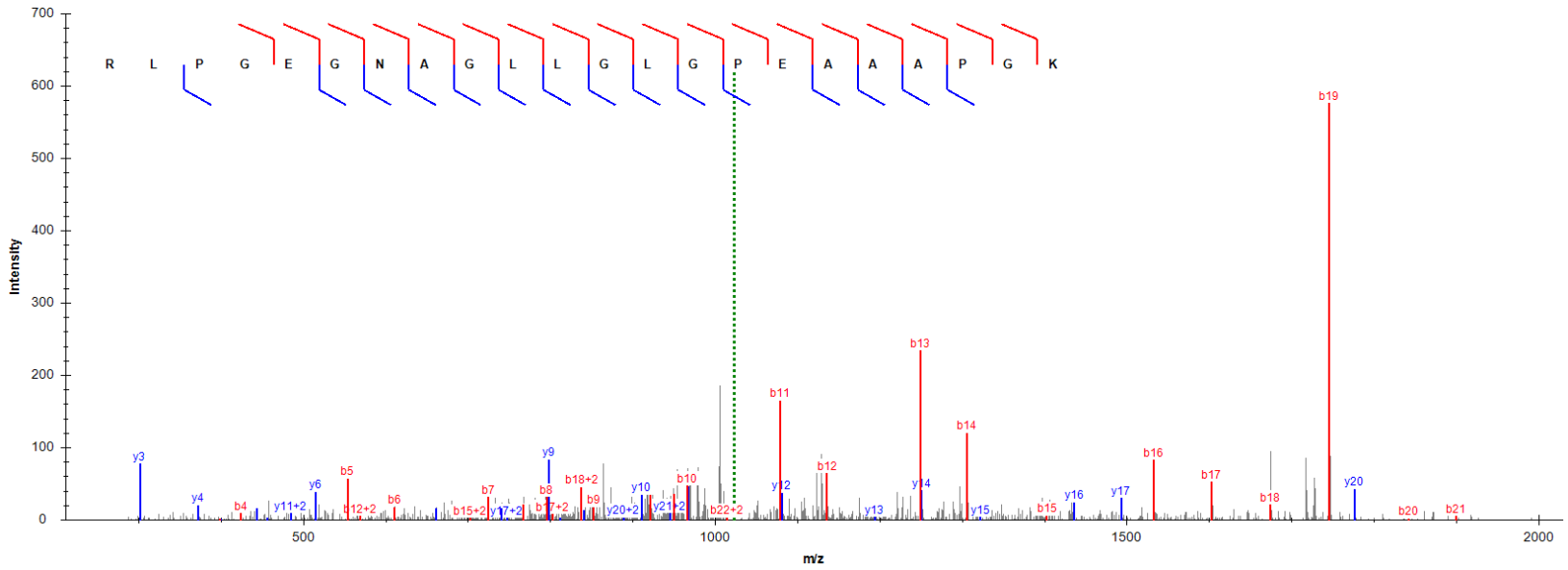


b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	29	3096.599	1548.803
270.192	135.600	2	I	28	2940.498	1470.753
398.251	199.629	3	Q	27	2827.414	1414.211
511.335	256.171	4	I	26	2699.356	1350.181
582.372	291.690	5	A	25	2586.272	1293.639
669.404	335.206	6	S	24	2515.234	1258.121
798.447	399.727	7	E	23	2428.202	**1214.605**
885.479	**443.243**	8	S	22	2299.160	**1150.084**
972.511	**486.759**	9	S	21	2212.128	1106.568
1029.532	**515.270**	10	G	20	2125.096	1063.052
1142.616	**571.812**	11	I	19	2068.074	**1034.541**
1239.669	**620.338**	12	P	18	1954.990	**977.999**
1368.712	684.860	13	E	17	1857.937	**929.472**
1524.813	762.910	14	R	16	1728.895	**864.951**
1621.866	811.436	15	P	15	1572.794	**786.901**
1724.875	862.941	16	C	14	1475.741	**738.374**
1823.943	912.475	17	V	13	1372.732	**686.870**
1937.027	**969.017**	18	L	12	1273.663	**637.335**
2038.075	**1019.541**	19	T	11	**1160.579**	580.793
2095.096	1048.052	20	G	10	**1059.532**	**530.269**
2196.144	1098.576	21	T	9	**1002.510**	501.759

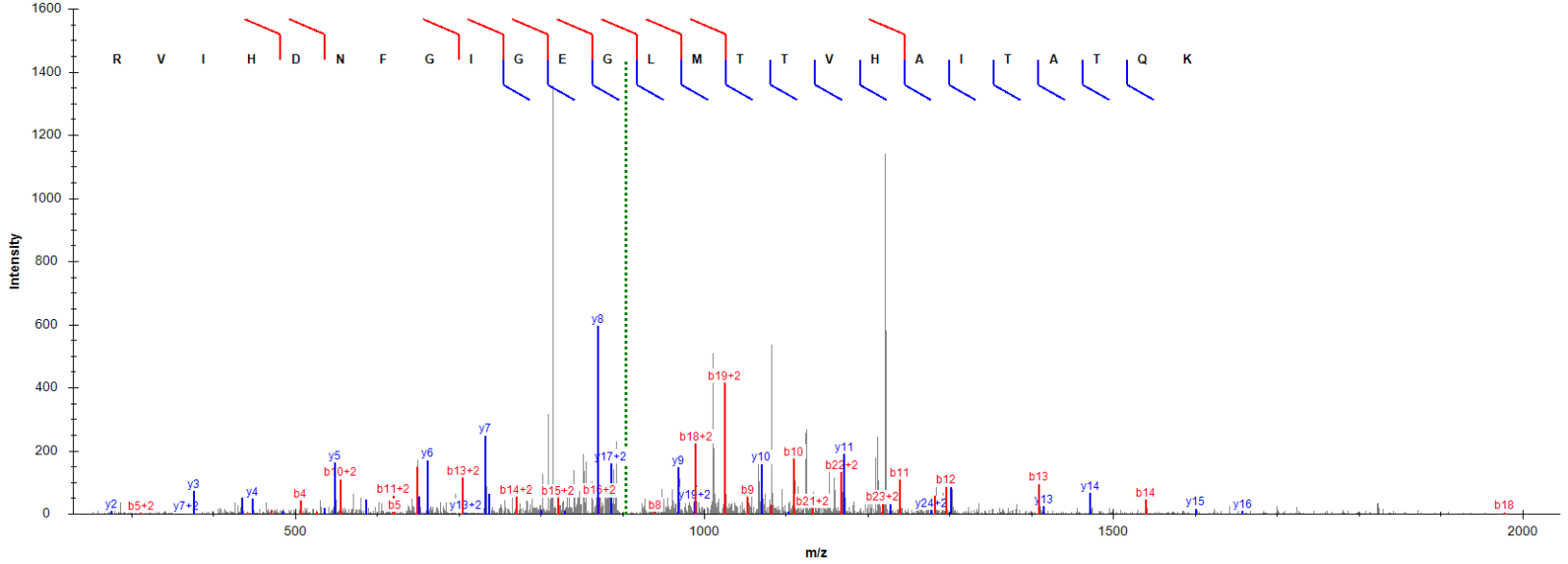
2293.197	1147.102	22	P	8	**901.463**	451.235
2422.239	1211.623	23	E	7	804.410	402.709
2509.272	**1255.139**	24	S	6	675.367	338.187
2622.356	1311.681	25	I	5	588.335	294.671
2751.398	1376.203	26	E	4	475.251	238.129
2879.457	1440.232	27	Q	3	346.208	173.608
2950.494	1475.751	28	A	2	218.150	109.579
3078.589	1539.798	29	K	1	147.113	74.060



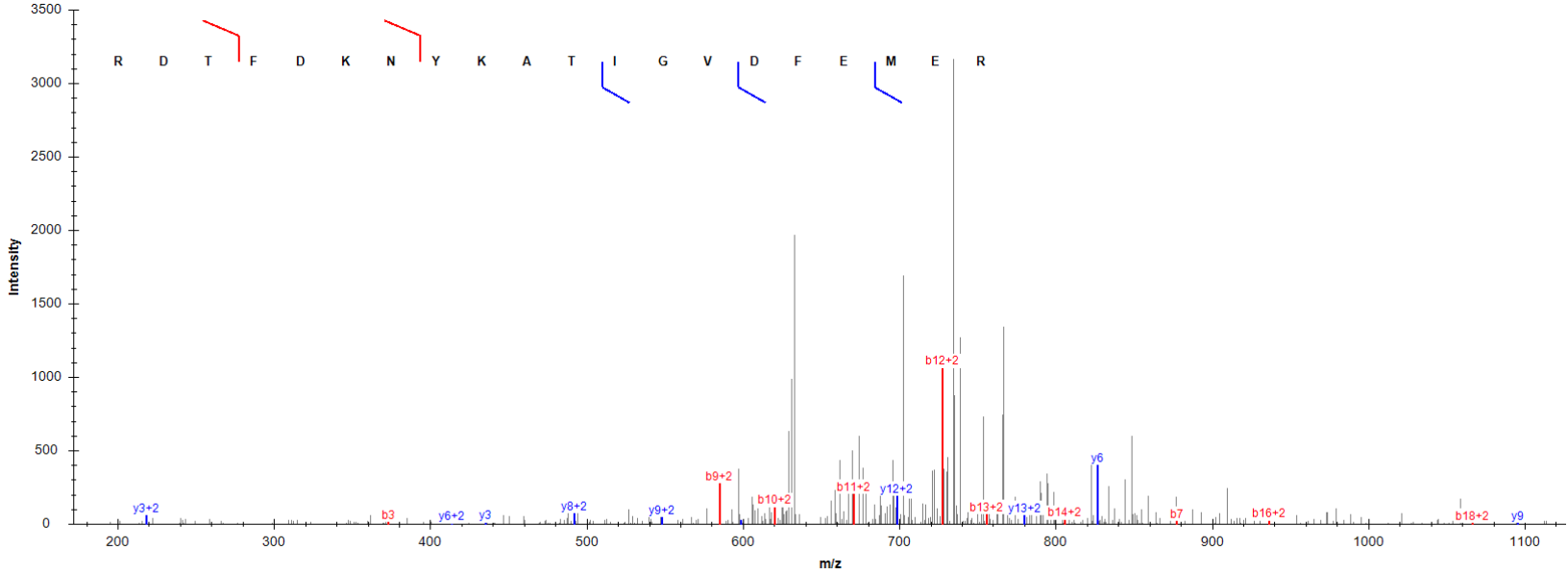
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	11	1297.661	649.334
270.192	135.600	2	L	10	**1141.560**	**571.283**
327.214	164.111	3	G	9	**1028.476**	**514.741**
440.298	220.653	4	I	8	**971.454**	**486.231**
577.357	**289.182**	5	H	7	**858.370**	**429.689**
706.399	353.703	6	E	6	**721.311**	361.159
821.426	**411.217**	7	D	5	**592.269**	**296.638**
908.458	**454.733**	8	S	4	**477.242**	239.124
1009.506	**505.257**	9	T	3	**390.210**	**195.608**
1123.549	**562.278**	10	N	2	**289.162**	145.085
1279.650	**640.329**	11	R	1	**175.119**	88.063



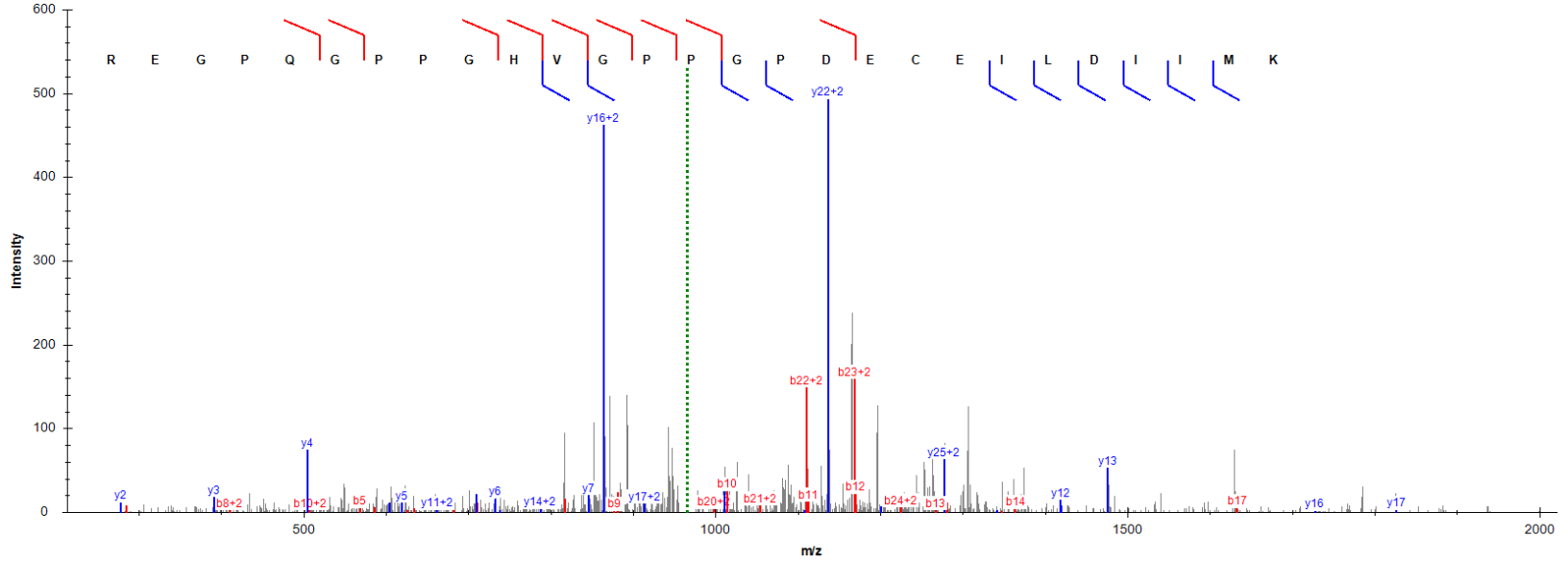
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	22	2045.114	1023.061
270.192	135.600	2	L	21	1889.013	**945.010**
367.245	184.126	3	P	20	**1775.929**	**888.468**
424.267	212.637	4	G	19	1678.876	**839.942**
553.309	277.158	5	E	18	1621.854	**811.431**
610.331	305.669	6	G	17	**1492.812**	**746.910**
724.374	362.690	7	N	16	**1435.790**	718.399
795.411	**398.209**	8	A	15	**1321.747**	**661.377**
852.432	426.720	9	G	14	**1250.710**	625.859
965.516	483.262	10	L	13	**1193.689**	597.348
1078.600	539.804	11	L	12	**1080.605**	540.806
1135.622	**568.315**	12	G	11	**967.521**	**484.264**
1248.706	624.857	13	L	10	**910.499**	**455.753**
1305.727	653.367	14	G	9	**797.415**	**399.211**
1402.780	**701.894**	15	P	8	**740.394**	370.701
1531.823	**766.415**	16	E	7	643.341	322.174
1602.860	**801.934**	17	A	6	**514.298**	257.653
1673.897	**837.452**	18	A	5	**443.261**	222.134
1744.934	872.971	19	A	4	**372.224**	186.616
1841.987	**921.497**	20	P	3	**301.187**	151.097
1899.008	**950.008**	21	G	2	204.134	102.571
2027.103	**1014.055**	22	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	25	2709.414	1355.211
256.177	128.592	2	V	24	2553.313	**1277.160**
369.261	185.134	3	I	23	2454.245	**1227.626**
506.320	253.664	4	H	22	2341.161	1171.084
621.347	**311.177**	5	D	21	2204.102	**1102.554**
735.390	368.198	6	N	20	2089.075	1045.041
882.458	**441.733**	7	F	19	1975.032	**988.020**
939.480	**470.243**	8	G	18	1827.963	914.485
1052.564	**526.785**	9	I	17	1770.942	**885.975**
1109.585	**555.296**	10	G	16	**1657.858**	**829.433**
1238.628	**619.817**	11	E	15	**1600.836**	**800.922**
1295.649	**648.328**	12	G	14	**1471.794**	**736.401**
1408.733	**704.870**	13	L	13	**1414.772**	**707.890**
1539.774	**770.390**	14	M	12	**1301.688**	**651.348**
1640.821	**820.914**	15	T	11	**1170.648**	**585.827**
1741.869	**871.438**	16	T	10	**1069.600**	**535.304**
1840.937	920.972	17	V	9	**968.552**	**484.780**
1977.996	**989.502**	18	H	8	**869.484**	**435.246**
2049.033	**1025.020**	19	A	7	**732.425**	**366.716**
2162.118	**1081.562**	20	I	6	**661.388**	331.198
2263.165	**1132.086**	21	T	5	**548.304**	**274.656**
2334.202	**1167.605**	22	A	4	**447.256**	224.132
2435.250	**1218.129**	23	T	3	**376.219**	188.613
2563.309	**1282.158**	24	Q	2	**275.171**	138.089
2691.404	1346.205	25	K	1	147.113	74.060

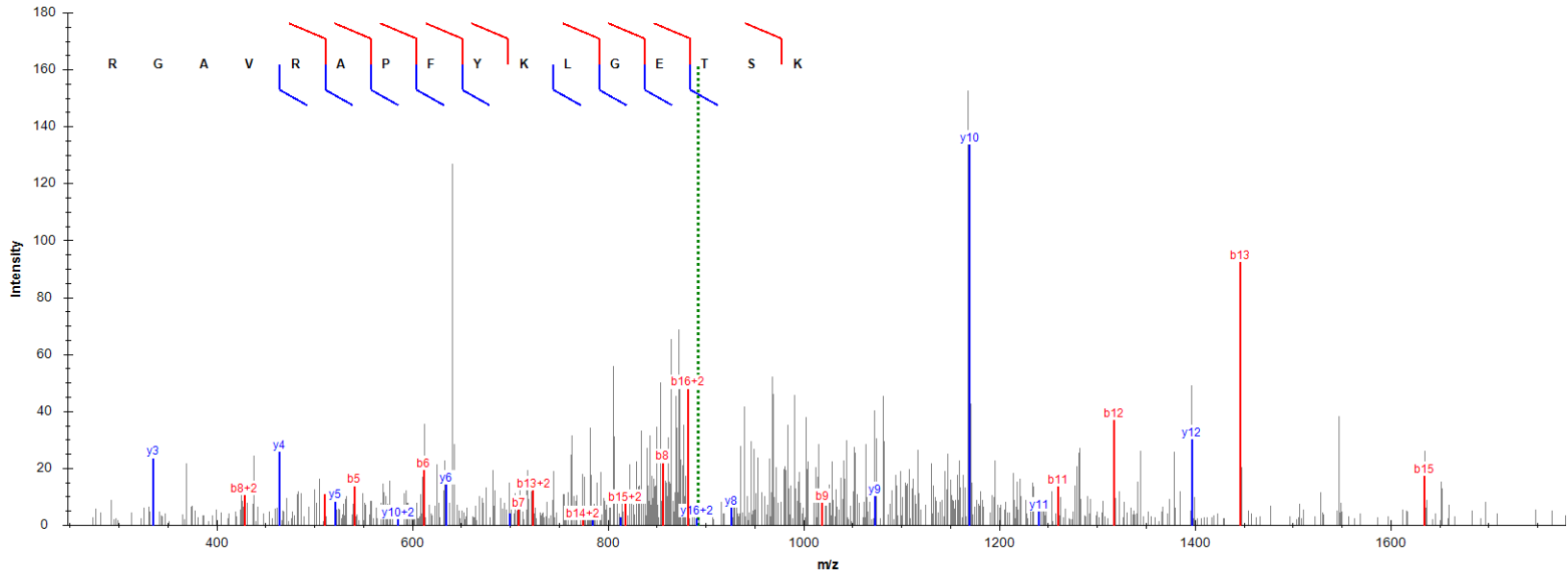


b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	20	2435.166	1218.087
272.135	136.571	2	D	19	2279.065	1140.036
373.183	187.095	3	T	18	2164.038	1082.523
520.251	260.629	4	F	17	2062.990	1031.999
635.278	318.143	5	D	16	1915.922	958.465
763.373	382.190	6	K	15	1800.895	900.951
877.416	439.212	7	N	14	1672.800	836.904
1040.480	520.743	8	Y	13	1558.757	**779.882**
1168.575	**584.791**	9	K	12	1395.694	**698.350**
1239.612	**620.309**	10	A	11	1267.599	634.303
1340.659	**670.833**	11	T	10	1196.562	**598.784**
1453.743	**727.375**	12	I	9	**1095.514**	**548.261**
1510.765	**755.886**	13	G	8	982.430	**491.719**
1609.833	**805.420**	14	V	7	925.408	463.208
1724.860	862.934	15	D	6	**826.340**	**413.674**
1871.929	**936.468**	16	F	5	711.313	356.160
2000.971	1000.989	17	E	4	564.245	282.626
2132.012	**1066.509**	18	M	3	**435.202**	**218.105**
2261.054	1131.031	19	E	2	304.162	152.584
2417.155	1209.081	20	R	1	175.119	88.063



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	27	2838.391	**1419.699**
286.151	143.579	2	E	26	2682.290	**1341.649**
343.172	172.090	3	G	25	2553.248	**1277.127**
440.225	220.616	4	P	24	2496.226	1248.617
568.284	**284.646**	5	Q	23	2399.173	**1200.090**
625.305	313.156	6	G	22	2271.115	**1136.061**
722.358	361.683	7	P	21	2214.093	**1107.550**
819.411	**410.209**	8	P	20	2117.041	1059.024
876.432	438.720	9	G	19	2019.988	**1010.498**
1013.491	**507.249**	10	H	18	1962.966	981.987
1112.560	556.783	11	V	17	**1825.907**	**913.457**
1169.581	**585.294**	12	G	16	**1726.839**	**863.923**
1266.634	**633.821**	13	P	15	1669.818	835.412
1363.687	**682.347**	14	P	14	1572.765	**786.886**
1420.708	**710.858**	15	G	13	**1475.712**	**738.360**
1517.761	759.384	16	P	12	**1418.691**	**709.849**
1632.788	**816.898**	17	D	11	1321.638	**661.323**
1761.830	**881.419**	18	E	10	1206.611	**603.809**
1864.840	932.923	19	C	9	1077.568	539.288
1993.882	**997.445**	20	E	8	974.559	487.783
2106.966	**1053.987**	21	I	7	**845.516**	423.262
2220.050	**1110.529**	22	L	6	**732.432**	366.720
2335.077	**1168.042**	23	D	5	**619.348**	310.178
2448.161	**1224.584**	24	I	4	**504.321**	252.664
2561.245	**1281.126**	25	I	3	**391.237**	196.122

2692.286	**1346.647**	26	M	2	**278.153**	139.580
2820.381	1410.694	27	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	16	1779.986	**890.497**
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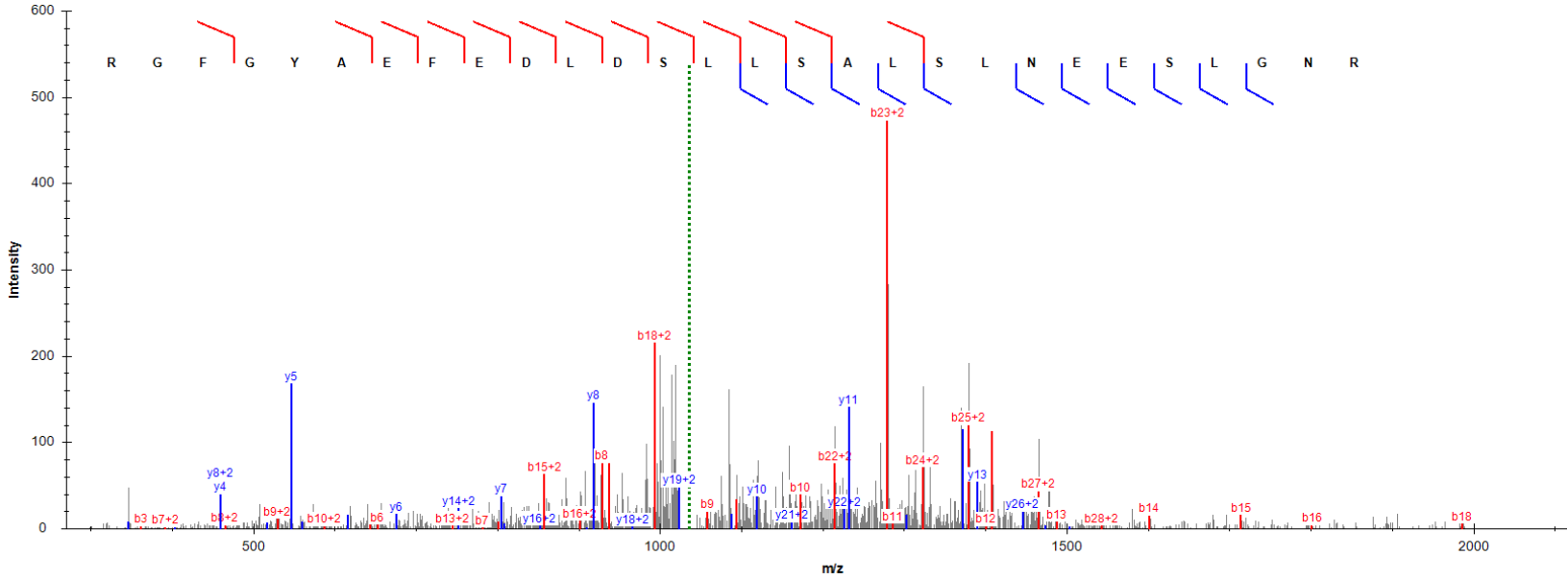
285.167	143.087	3	A	14	1566.864	**783.936**
384.235	192.621	4	V	13	1495.827	748.417
540.336	270.672	5	R	12	**1396.758**	**698.883**
611.374	306.190	6	A	11	**1240.657**	620.832
708.426	354.717	7	P	10	**1169.620**	**585.314**
855.495	**428.251**	8	F	9	**1072.567**	536.787
1018.558	**509.783**	9	Y	8	**925.499**	463.253
1146.653	573.830	10	K	7	762.436	381.721
1259.737	630.372	11	L	6	**634.341**	317.674
1316.759	658.883	12	G	5	**521.257**	261.132
1445.801	**723.404**	13	E	4	**464.235**	232.621
1546.849	**773.928**	14	T	3	**335.193**	168.100
1633.881	**817.444**	15	S	2	234.145	117.576
1761.976	**881.492**	16	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
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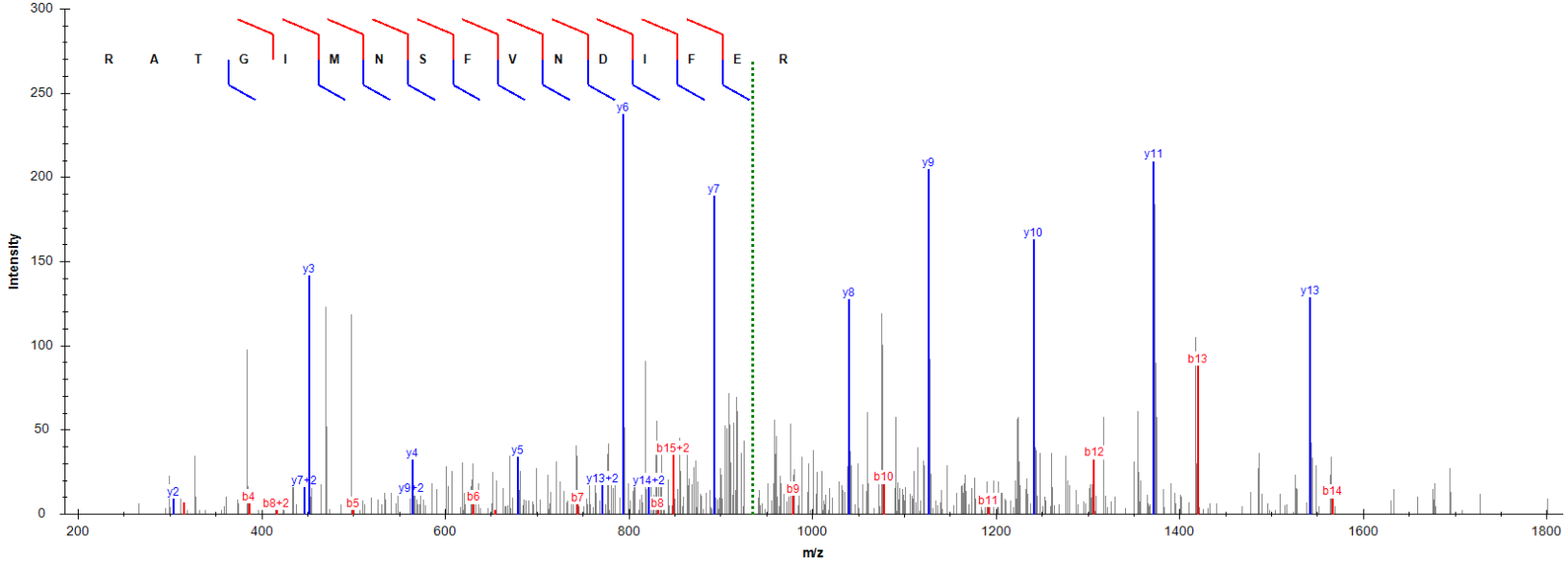
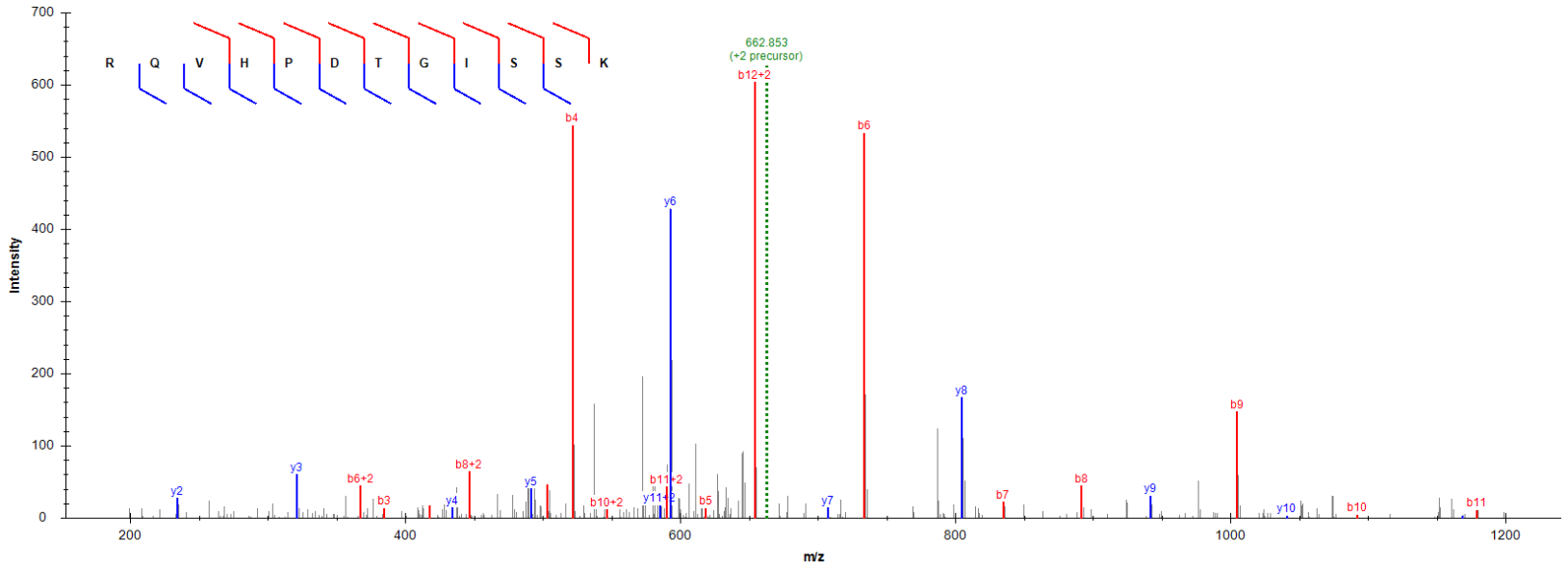
361.198	181.103	3	F	26	2889.379	**1445.193**
418.220	209.614	4	G	25	2742.310	**1371.659**
581.283	291.145	5	Y	24	2685.289	1343.148
652.320	326.664	6	A	23	2522.226	1261.616
781.363	**391.185**	7	E	22	2451.189	**1226.098**
928.431	**464.719**	8	F	21	2322.146	**1161.577**
1057.474	**529.241**	9	E	20	2175.078	**1088.042**
1172.501	**586.754**	10	D	19	2046.035	**1023.521**
1285.585	**643.296**	11	L	18	1931.008	**966.008**
1400.612	700.809	12	D	17	1817.924	**909.466**
1487.644	**744.326**	13	S	16	1702.897	**851.952**
1600.728	**800.868**	14	L	15	1615.865	**808.436**
1713.812	**857.410**	15	L	14	**1502.781**	**751.894**
1800.844	**900.926**	16	S	13	**1389.697**	695.352
1871.881	**936.444**	17	A	12	**1302.665**	651.836
1984.965	**992.986**	18	L	11	**1231.628**	**616.317**
2071.997	1036.502	19	S	10	**1118.544**	**559.775**
2185.081	**1093.044**	20	L	9	1031.512	**516.259**
2299.124	1150.066	21	N	8	**918.428**	**459.717**
2428.167	**1214.587**	22	E	7	**804.385**	**402.696**
2557.209	**1279.108**	23	E	6	**675.342**	338.175
2644.241	**1322.624**	24	S	5	**546.299**	273.653
2757.325	**1379.166**	25	L	4	**459.267**	230.137

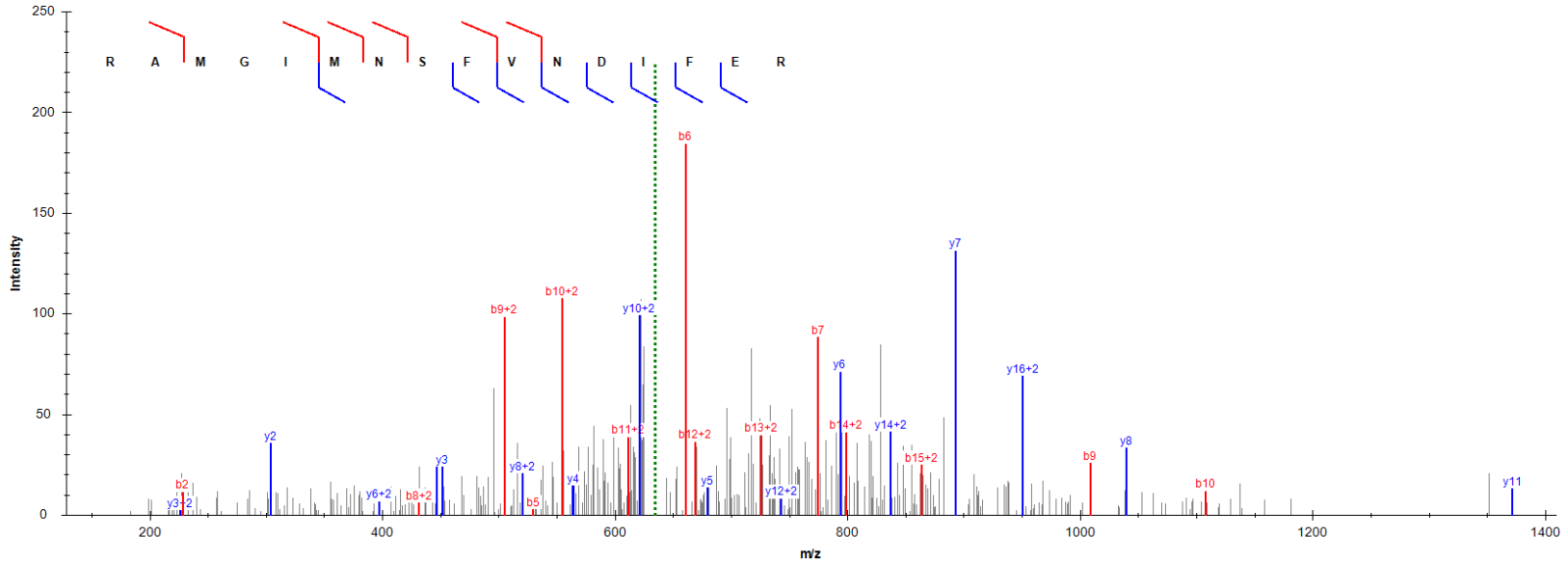
2814.347	**1407.677**	26	G	3	**346.183**	173.595
2928.390	**1464.699**	27	N	2	289.162	145.085
3084.491	**1542.749**	28	R	1	175.119	88.063



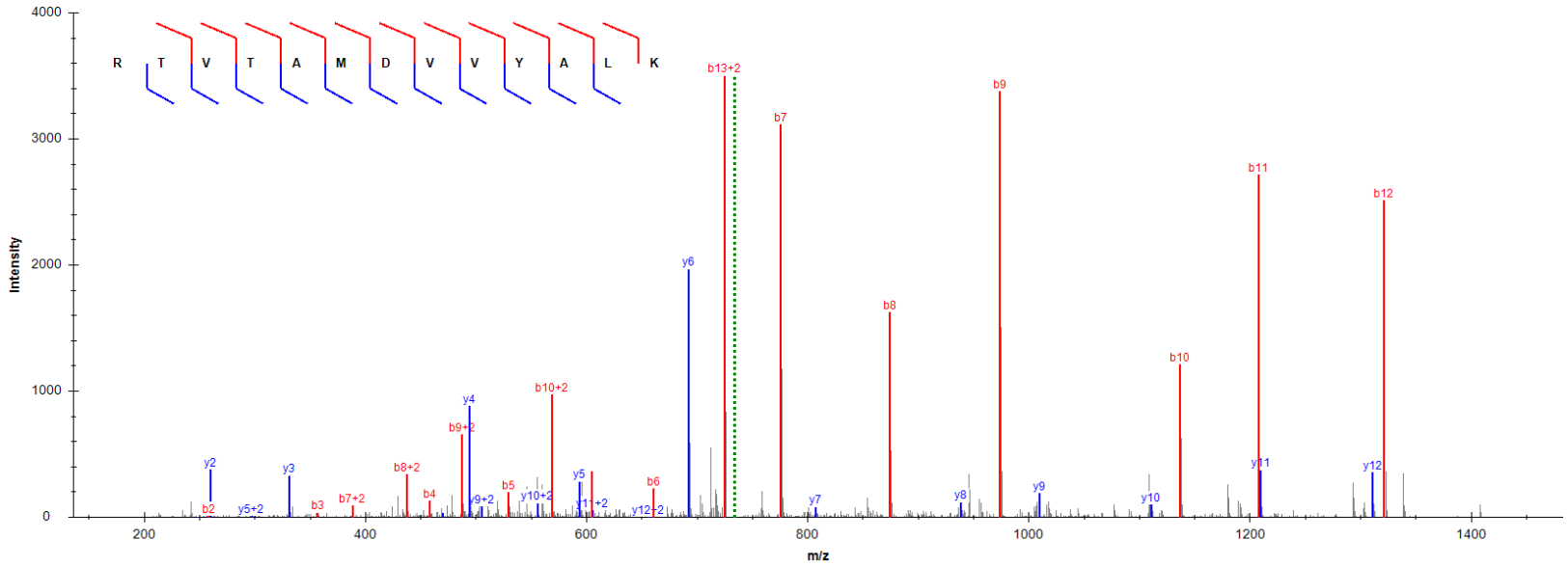
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	16	1869.928	935.467
228.146	114.576	2	A	15	1713.826	857.417
329.193	165.100	3	T	14	1642.789	**821.898**
386.215	193.611	4	G	13	**1541.742**	**771.374**
499.299	250.153	5	I	12	1484.720	742.864
630.339	**315.673**	6	M	11	**1371.636**	686.322
744.382	372.695	7	N	10	**1240.596**	620.801
831.414	**416.211**	8	S	9	**1126.553**	**563.780**
978.483	489.745	9	F	8	**1039.521**	520.264
1077.551	539.279	10	V	7	**892.452**	**446.730**
1191.594	596.301	11	N	6	**793.384**	397.196
1306.621	**653.814**	12	D	5	**679.341**	340.174
1419.705	710.356	13	I	4	**564.314**	282.661
1566.773	783.890	14	F	3	**451.230**	226.119
1695.816	**848.412**	15	E	2	**304.162**	152.584
1851.917	926.462	16	R	1	175.119	88.063



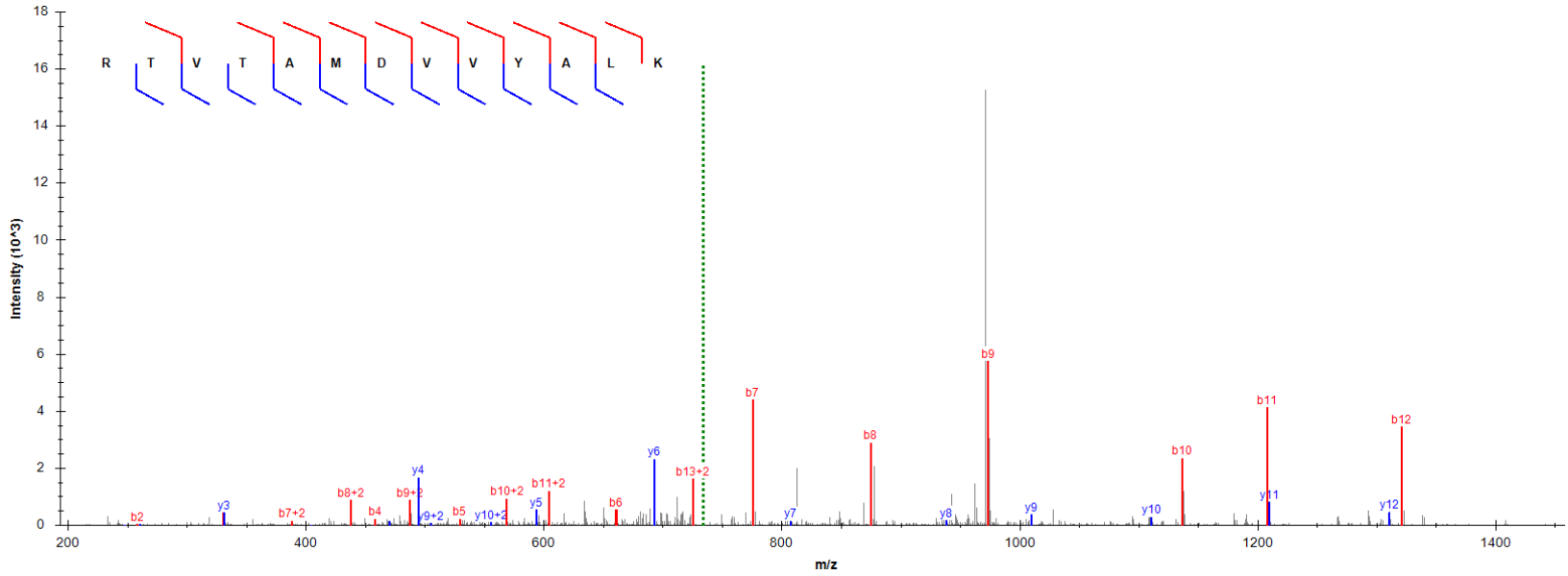
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	12	1324.697	662.852
285.167	143.087	2	Q	11	**1168.596**	**584.801**
384.235	192.621	3	V	10	**1040.537**	520.772
521.294	261.151	4	H	9	**941.469**	471.238
618.347	309.677	5	P	8	**804.410**	402.709
733.374	**367.191**	6	D	7	**707.357**	354.182
834.422	**417.714**	7	T	6	**592.330**	296.669
891.443	**446.225**	8	G	5	**491.282**	246.145
1004.527	**502.767**	9	I	4	**434.261**	217.634
1091.559	**546.283**	10	S	3	**321.177**	161.092
1178.591	**589.799**	11	S	2	**234.145**	117.576
1306.686	**653.847**	12	K	1	147.113	74.060



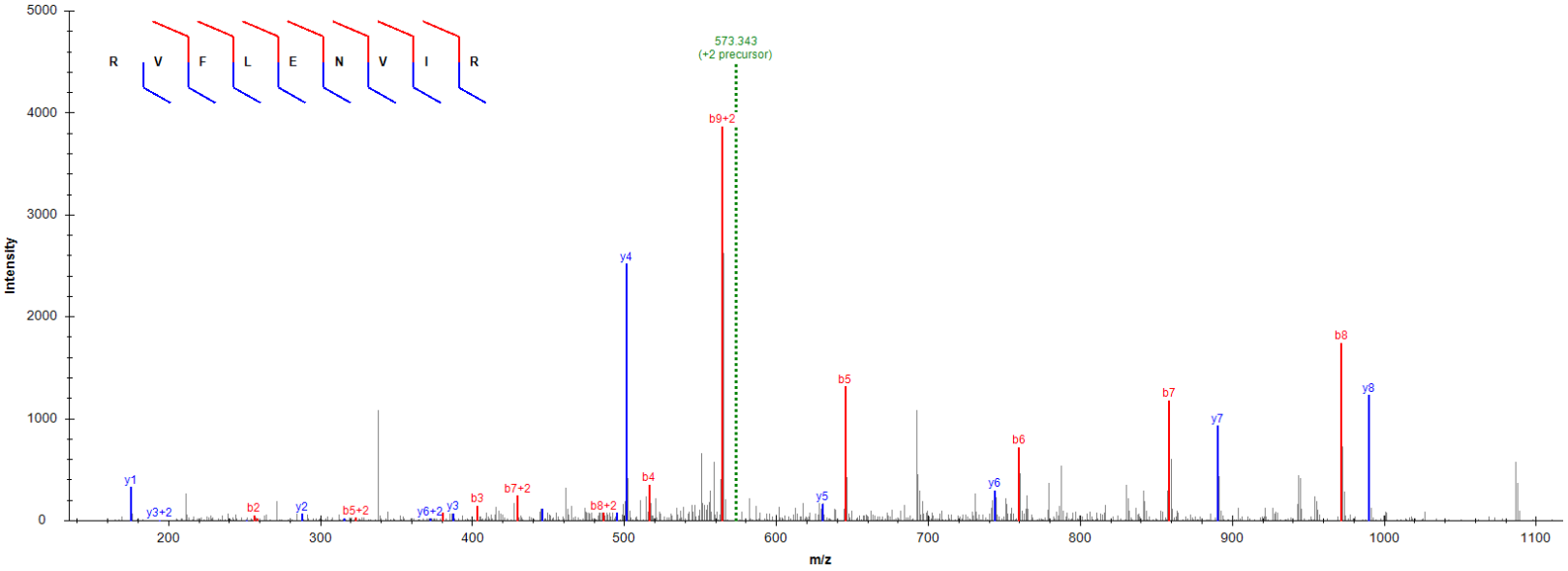
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	16	1899.920	**950.464**
228.146	114.576	2	A	15	1743.819	872.413
359.186	180.097	3	M	14	1672.782	**836.895**
416.207	208.607	4	G	13	1541.742	771.374
529.292	265.149	5	I	12	1484.720	**742.864**
660.332	330.670	6	M	11	**1371.636**	686.322
774.375	387.691	7	N	10	1240.596	**620.801**
861.407	**431.207**	8	S	9	1126.553	**563.780**
1008.475	**504.741**	9	F	8	**1039.521**	**520.264**
1107.544	**554.276**	10	V	7	**892.452**	**446.730**
1221.587	**611.297**	11	N	6	**793.384**	**397.196**
1336.614	**668.810**	12	D	5	**679.341**	340.174
1449.698	**725.352**	13	I	4	**564.314**	282.661
1596.766	**798.887**	14	F	3	**451.230**	**226.119**
1725.809	**863.408**	15	E	2	**304.162**	152.584
1881.910	941.459	16	R	1	175.119	88.063



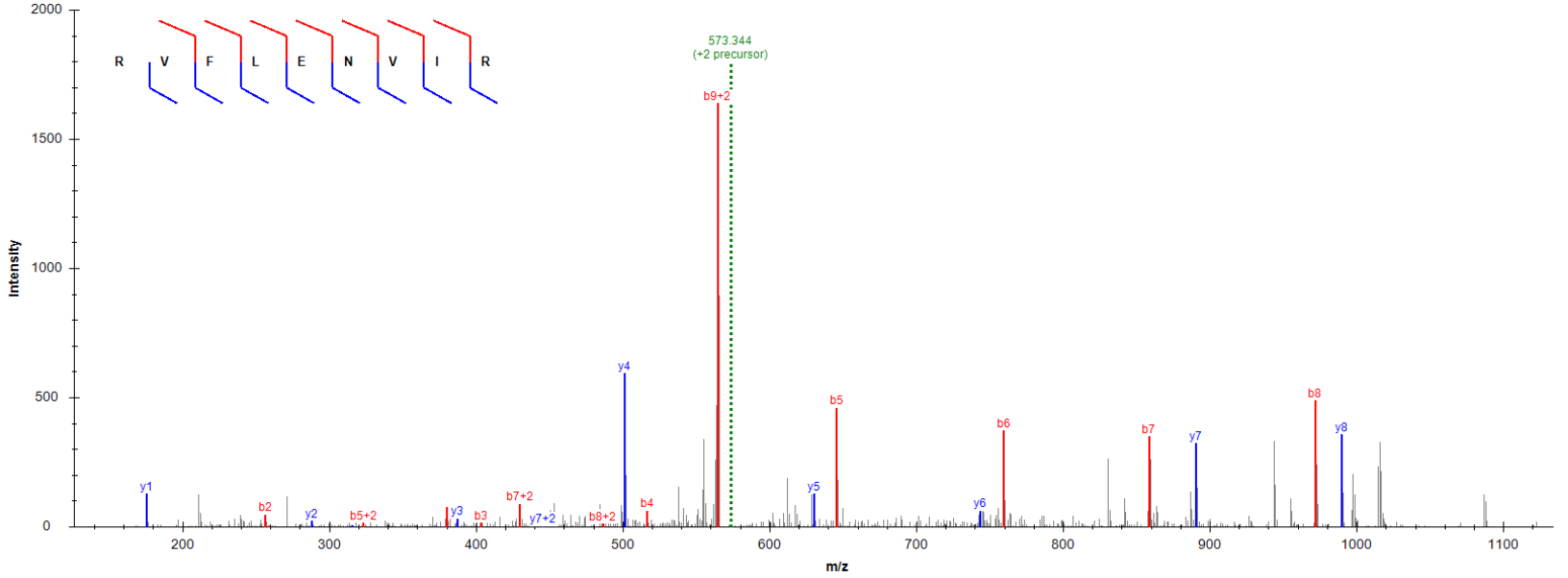
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	13	1466.804	733.905
258.156	129.582	2	T	12	**1310.702**	**655.855**
357.224	179.116	3	V	11	**1209.655**	**605.331**
458.272	229.640	4	T	10	**1110.586**	**555.797**
529.309	265.158	5	A	9	**1009.539**	**505.273**
660.350	330.679	6	M	8	**938.502**	**469.754**
775.377	**388.192**	7	D	7	**807.461**	404.234
874.445	**437.726**	8	V	6	**692.434**	346.721
973.514	**487.260**	9	V	5	**593.366**	**297.187**
1136.577	**568.792**	10	Y	4	**494.297**	**247.652**
1207.614	**604.311**	11	A	3	**331.234**	166.121
1320.698	**660.853**	12	L	2	**260.197**	130.602
1448.793	**724.900**	13	K	1	147.113	74.060



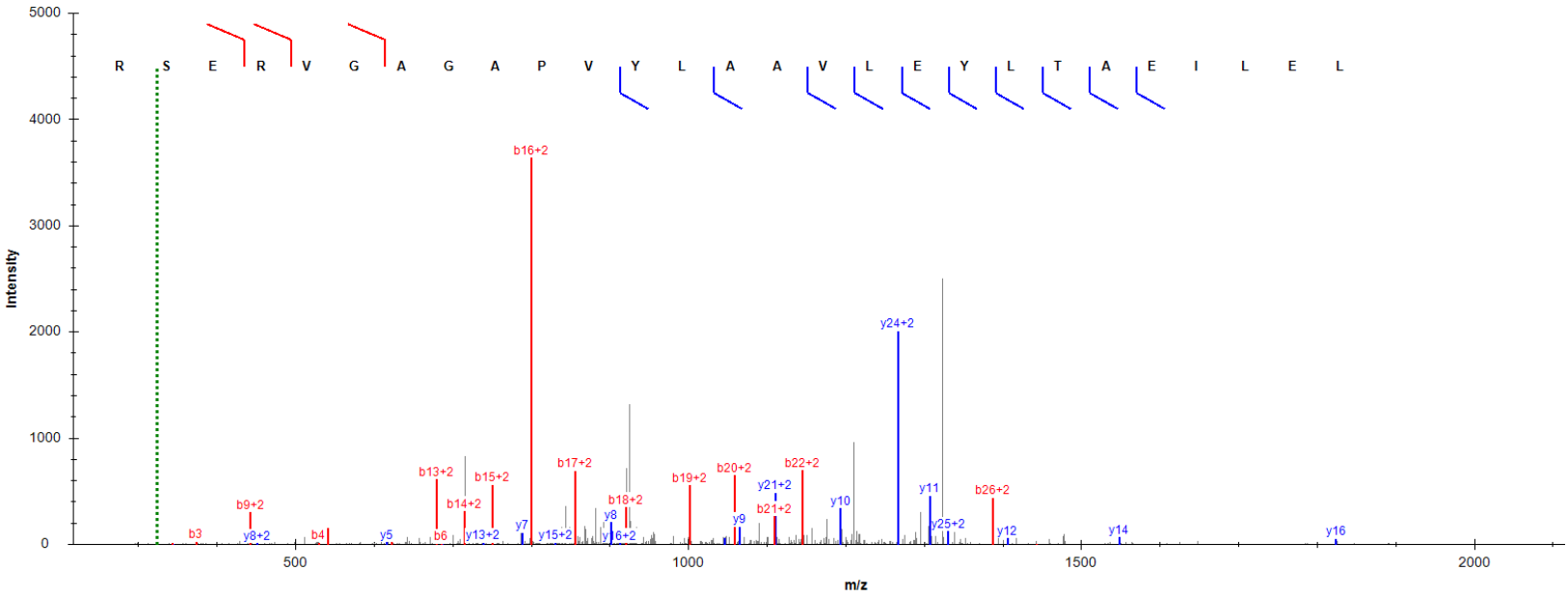
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	13	1466.804	733.905
258.156	129.582	2	T	12	**1310.702**	655.855
357.224	179.116	3	V	11	**1209.655**	605.331
458.272	229.640	4	T	10	**1110.586**	**555.797**
529.309	265.158	5	A	9	**1009.539**	**505.273**
660.350	**330.679**	6	M	8	**938.502**	**469.754**
775.377	**388.192**	7	D	7	**807.461**	**404.234**
874.445	**437.726**	8	V	6	**692.434**	346.721
973.514	**487.260**	9	V	5	**593.366**	297.187
1136.577	**568.792**	10	Y	4	**494.297**	**247.652**
1207.614	**604.311**	11	A	3	**331.234**	166.121
1320.698	**660.853**	12	L	2	**260.197**	130.602
1448.793	**724.900**	13	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	9	1145.679	573.343
256.177	128.592	2	V	8	**989.578**	**495.293**
403.245	202.126	3	F	7	**890.509**	**445.758**
516.329	**258.668**	4	L	6	**743.441**	**372.224**
645.372	**323.190**	5	E	5	**630.357**	**315.682**
759.415	**380.211**	6	N	4	**501.314**	**251.161**
858.483	**429.745**	7	V	3	**387.271**	**194.139**
971.567	**486.287**	8	I	2	**288.203**	144.605
1127.668	**564.338**	9	R	1	**175.119**	88.063

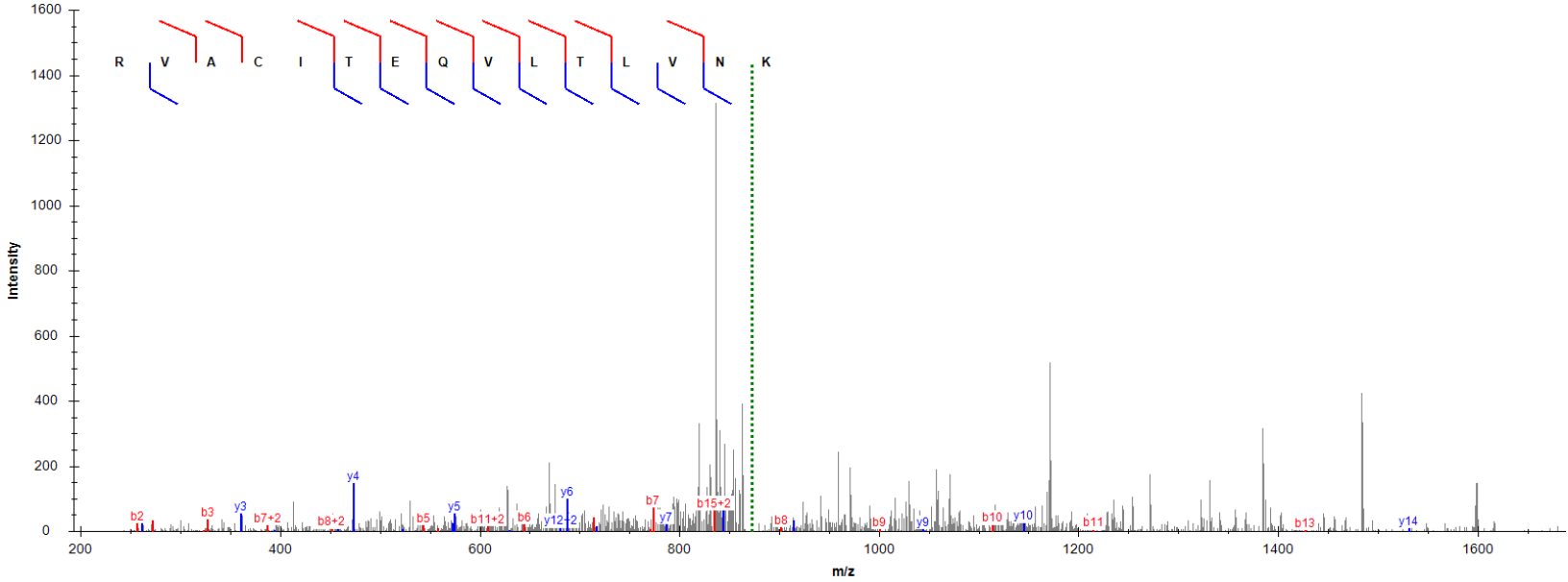


b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	9	1145.679	573.343
256.177	128.592	2	V	8	**989.578**	495.293
403.245	202.126	3	F	7	**890.509**	**445.758**
516.329	**258.668**	4	L	6	**743.441**	**372.224**
645.372	**323.190**	5	E	5	**630.357**	**315.682**
759.415	**380.211**	6	N	4	**501.314**	251.161
858.483	**429.745**	7	V	3	**387.271**	194.139
971.567	**486.287**	8	I	2	**288.203**	144.605
1127.668	**564.338**	9	R	1	**175.119**	88.063

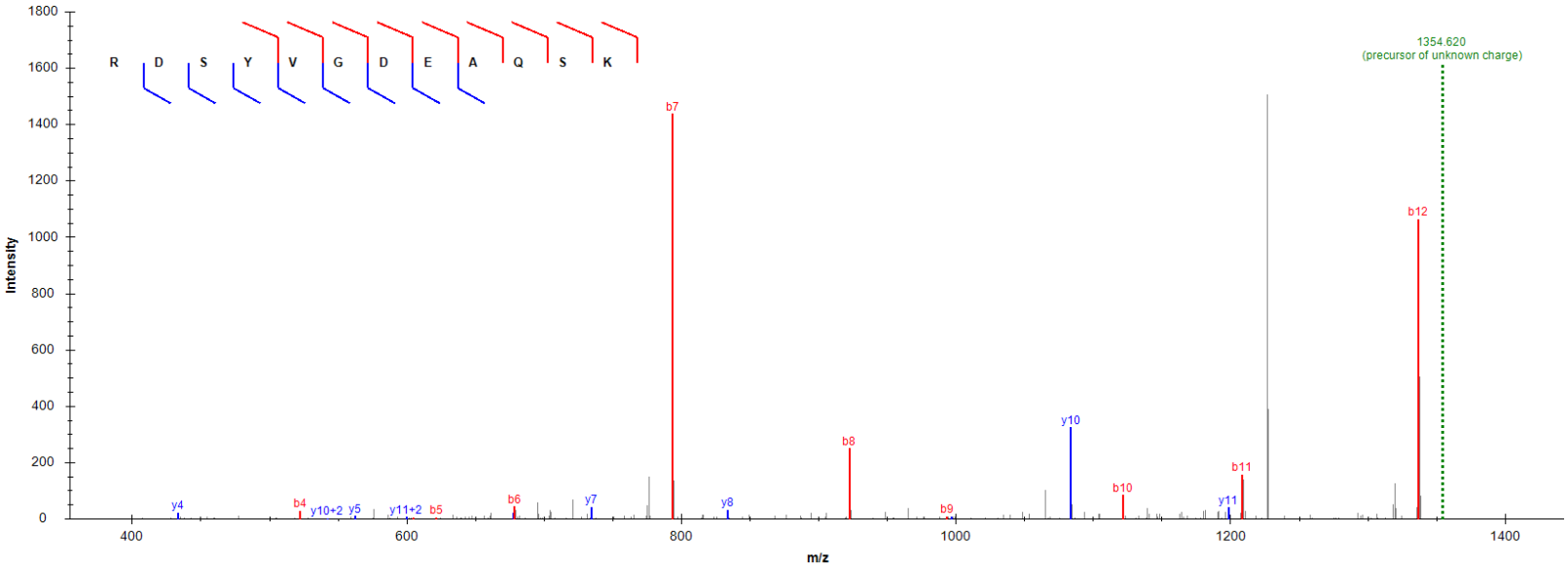


b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	27	2903.588	1452.297
244.140	122.574	2	S	26	2747.487	1374.247
373.183	187.095	3	E	25	2660.455	**1330.731**
529.284	265.146	4	R	24	2531.412	**1266.210**
628.353	314.680	5	V	23	2375.311	1188.159
685.374	**343.191**	6	G	22	2276.242	1138.625
756.411	378.709	7	A	21	2219.221	**1110.114**
813.433	407.220	8	G	20	2148.184	1074.596
884.470	**442.738**	9	A	19	2091.162	**1046.085**
981.522	491.265	10	P	18	2020.125	1010.566
1080.591	**540.799**	11	V	17	1923.073	962.040
1243.654	**622.331**	12	Y	16	**1824.004**	**912.506**
1356.738	**678.873**	13	L	15	1660.941	**830.974**
1427.775	**714.391**	14	A	14	**1547.857**	774.432
1498.812	**749.910**	15	A	13	1476.820	**738.913**
1597.881	**799.444**	16	V	12	**1405.782**	703.395
1710.965	**855.986**	17	L	11	**1306.714**	653.861
1840.008	**920.507**	18	E	10	**1193.630**	597.319
2003.071	**1002.039**	19	Y	9	**1064.587**	532.797
2116.155	**1058.581**	20	L	8	**901.524**	**451.266**
2217.203	**1109.105**	21	T	7	**788.440**	394.724

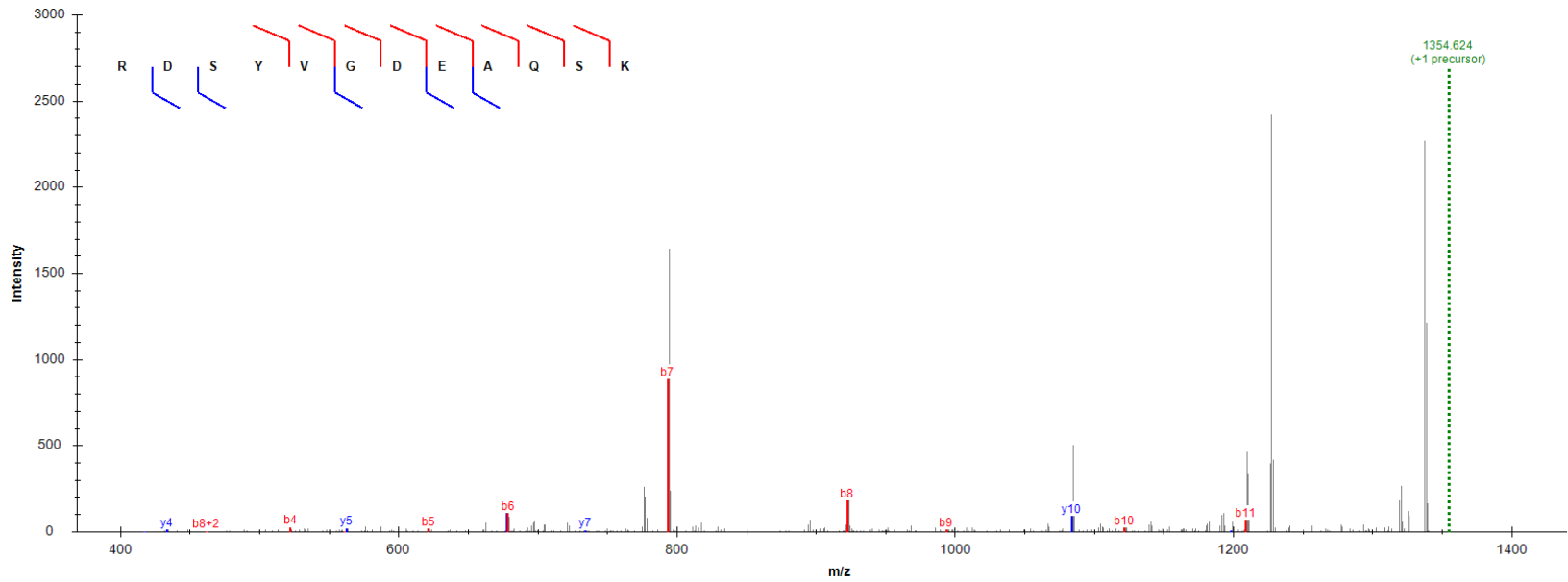
2288.240	**1144.624**	22	A	6	**687.392**	**344.200**
2417.282	1209.145	23	E	5	**616.355**	308.681
2530.366	1265.687	24	I	4	487.313	244.160
2643.450	1322.229	25	L	3	374.229	187.618
2772.493	**1386.750**	26	E	2	261.144	131.076
2885.577	**1443.292**	27	L	1	132.102	66.555



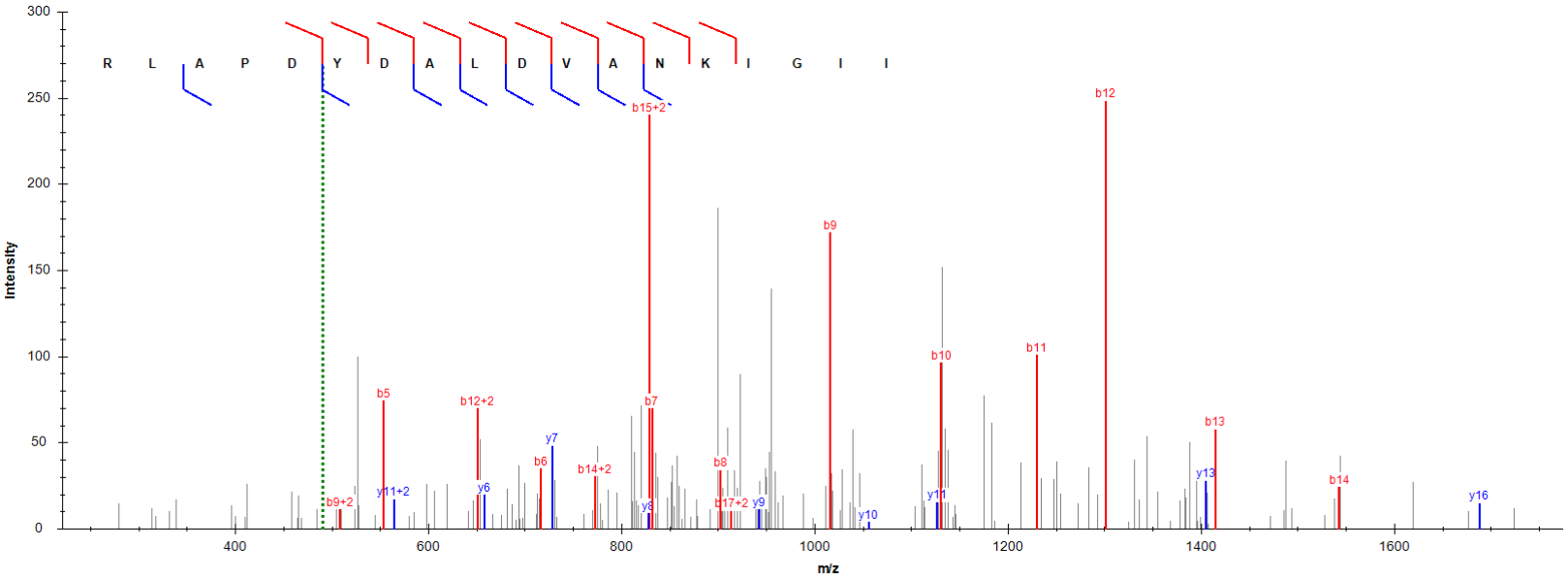
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	15	1686.957	**843.982**
256.177	128.592	2	V	14	**1530.856**	765.932
327.214	164.111	3	A	13	1431.788	**716.397**
430.223	215.615	4	C	12	1360.750	**680.879**
543.307	**272.157**	5	I	11	1257.741	**629.374**
644.355	**322.681**	6	T	10	**1144.657**	**572.832**
773.397	**387.202**	7	E	9	**1043.610**	**522.308**
901.456	**451.232**	8	Q	8	**914.567**	**457.787**
1000.524	500.766	9	V	7	**786.508**	**393.758**
1113.608	**557.308**	10	L	6	**687.440**	344.224
1214.656	**607.832**	11	T	5	**574.356**	287.682
1327.740	664.374	12	L	4	**473.308**	237.158
1426.809	**713.908**	13	V	3	**360.224**	180.616
1540.852	**770.929**	14	N	2	**261.156**	131.082
1668.947	**834.977**	15	K	1	147.113	74.060



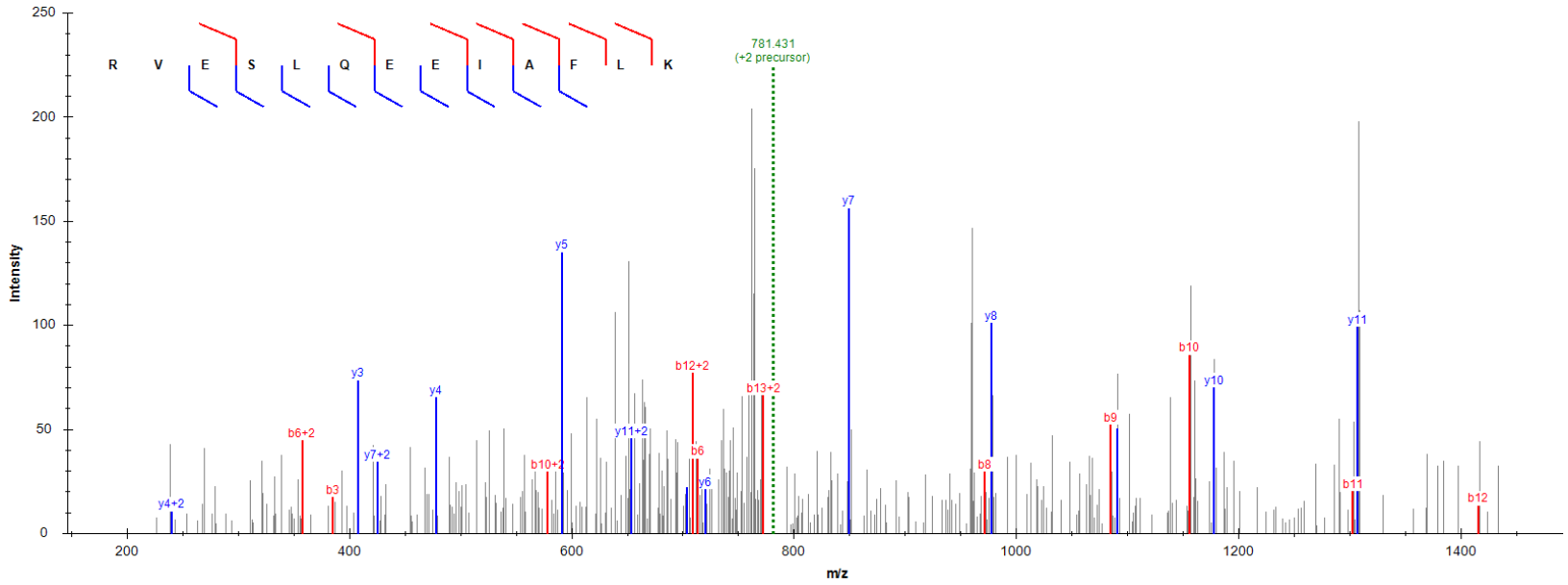
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	12	1354.623	**677.815**
272.135	136.571	2	D	11	**1198.522**	**599.765**
359.167	180.087	3	S	10	**1083.495**	**542.251**
522.231	261.619	4	Y	9	**996.463**	498.735
621.299	311.153	5	V	8	**833.400**	417.204
678.321	339.664	6	G	7	**734.332**	367.669
793.348	397.177	7	D	6	**677.310**	339.159
922.390	461.699	8	E	5	**562.283**	281.645
993.427	497.217	9	A	4	**433.241**	217.124
1121.486	561.247	10	Q	3	362.203	181.605
1208.518	**604.763**	11	S	2	234.145	117.576
1336.613	668.810	12	K	1	147.113	74.060



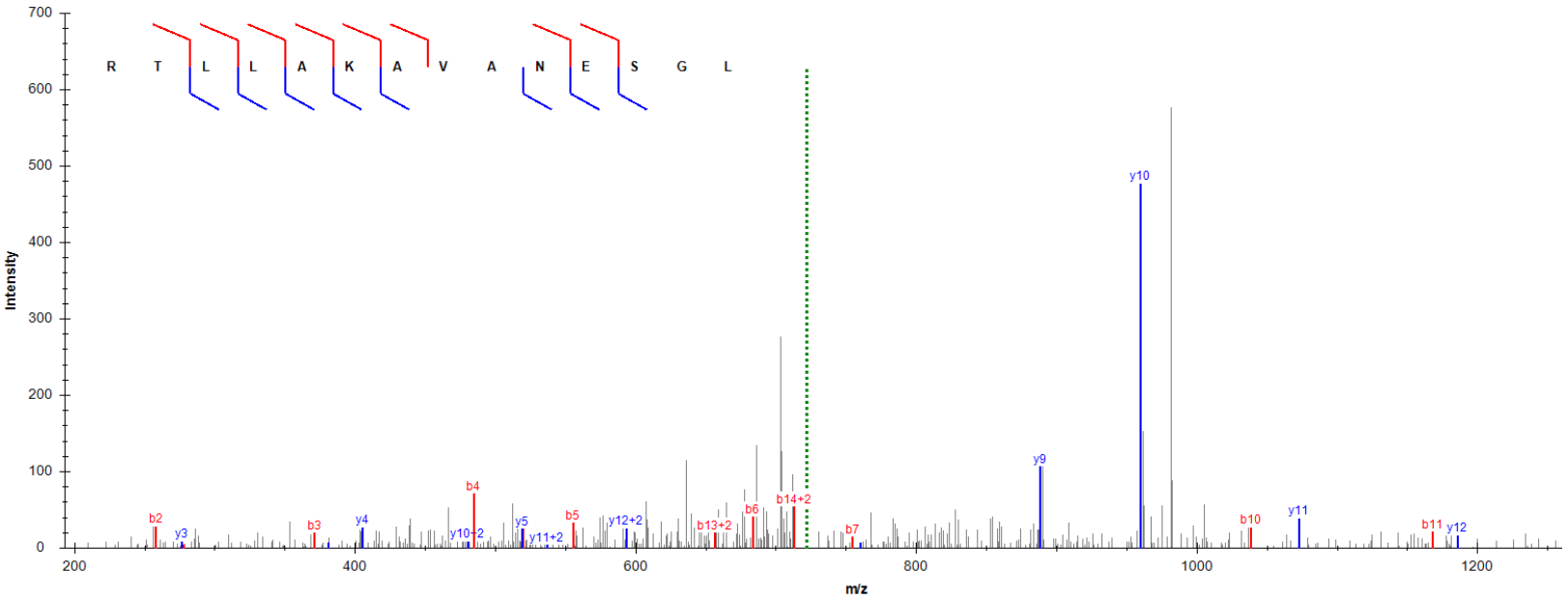
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	12	1354.623	**677.815**
272.135	136.571	2	D	11	**1198.522**	599.765
359.167	180.087	3	S	10	**1083.495**	542.251
522.231	261.619	4	Y	9	996.463	498.735
621.299	311.153	5	V	8	833.400	**417.204**
678.321	339.664	6	G	7	**734.332**	367.669
793.348	397.177	7	D	6	677.310	339.159
922.390	**461.699**	8	E	5	**562.283**	281.645
993.427	497.217	9	A	4	**433.241**	217.124
1121.486	**561.247**	10	Q	3	362.203	181.605
1208.518	604.763	11	S	2	234.145	117.576
1336.613	668.810	12	K	1	147.113	74.060



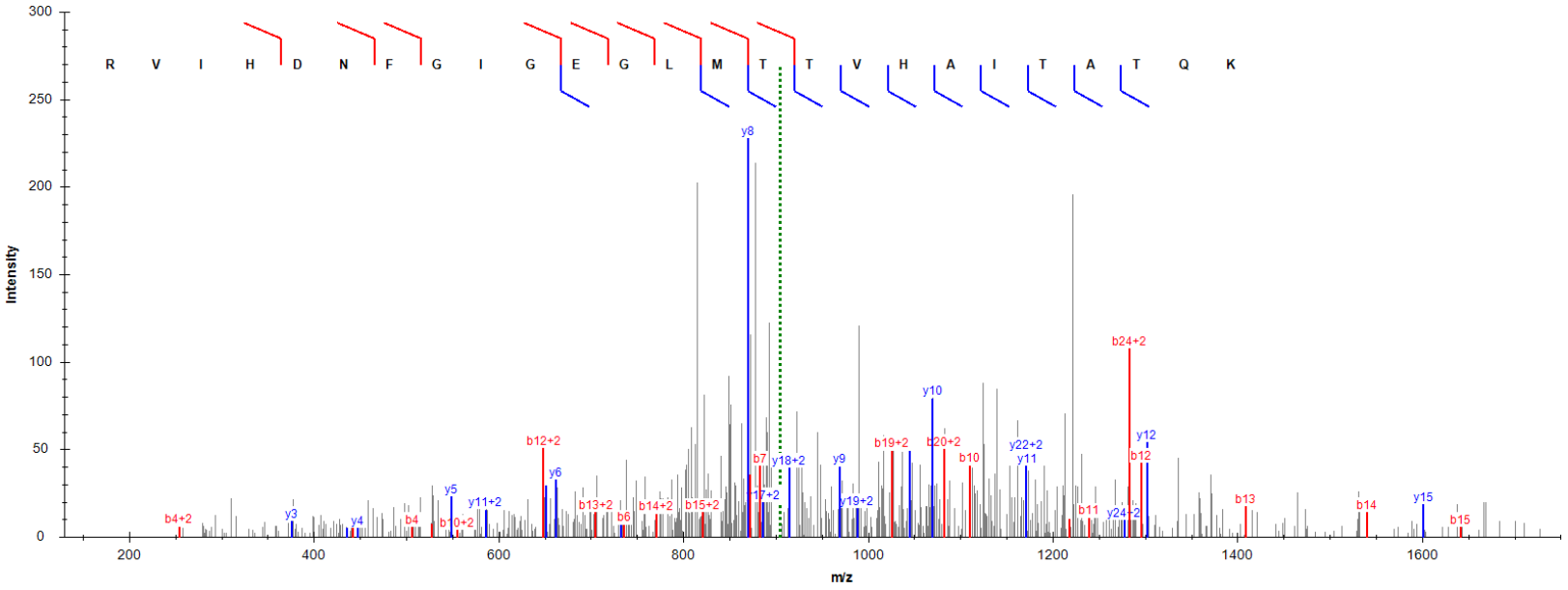
b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	18	1957.075	979.041
270.192	135.600	2	L	17	1800.974	900.991
341.230	171.118	3	A	16	**1687.890**	844.449
438.282	219.645	4	P	15	1616.853	808.930
553.309	277.158	5	D	14	1519.800	760.404
716.373	358.690	6	Y	13	**1404.773**	702.890
831.400	416.203	7	D	12	1241.710	621.359
902.437	451.722	8	A	11	**1126.683**	**563.845**
1015.521	**508.264**	9	L	10	**1055.646**	528.327
1130.548	565.777	10	D	9	**942.562**	471.785
1229.616	615.312	11	V	8	**827.535**	414.271
1300.653	**650.830**	12	A	7	**728.467**	364.737
1414.696	707.852	13	N	6	**657.429**	329.218
1542.791	**771.899**	14	K	5	543.386	272.197
1655.875	**828.441**	15	I	4	415.291	208.149
1712.897	856.952	16	G	3	302.207	151.607
1825.981	**913.494**	17	I	2	245.186	123.097
1939.065	970.036	18	I	1	132.102	66.555



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	13	1561.858	781.433
256.177	128.592	2	V	12	1405.757	**703.382**
385.219	193.113	3	E	11	**1306.689**	**653.848**
472.251	236.629	4	S	10	**1177.646**	589.327
585.335	293.171	5	L	9	**1090.614**	545.811
713.394	**357.201**	6	Q	8	**977.530**	489.269
842.437	421.722	7	E	7	**849.472**	**425.239**
971.479	486.243	8	E	6	**720.429**	360.718
1084.563	542.785	9	I	5	**591.386**	296.197
1155.600	**578.304**	10	A	4	**478.302**	**239.655**
1302.669	651.838	11	F	3	**407.265**	204.136
1415.753	**708.380**	12	L	2	260.197	130.602
1543.848	**772.428**	13	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	14	1442.833	721.920
258.156	129.582	2	T	13	1286.731	643.869
371.240	186.124	3	L	12	**1185.684**	**593.346**
484.324	242.666	4	L	11	**1072.600**	**536.803**
555.361	**278.184**	5	A	10	**959.516**	**480.261**
683.456	342.232	6	K	9	**888.479**	444.743
754.493	377.750	7	A	8	**760.384**	**380.695**
853.562	427.285	8	V	7	689.346	345.177
924.599	462.803	9	A	6	590.278	295.643
1038.642	**519.825**	10	N	5	**519.241**	260.124
1167.684	584.346	11	E	4	**405.198**	203.103
1254.716	627.862	12	S	3	**276.155**	138.581
1311.738	**656.373**	13	G	2	189.123	95.065
1424.822	**712.915**	14	L	1	132.102	66.555



b	b(+2)	#	seq	#	y	y(+2)
157.108	79.058	1	R	25	2709.414	1355.211
256.177	128.592	2	V	24	2553.313	**1277.160**
369.261	185.134	3	I	23	2454.245	1227.626
506.320	**253.664**	4	H	22	2341.161	**1171.084**
621.347	311.177	5	D	21	2204.102	1102.554
735.390	368.198	6	N	20	2089.075	**1045.041**
882.458	**441.733**	7	F	19	1975.032	**988.020**
939.480	470.243	8	G	18	1827.963	**914.485**
1052.564	**526.785**	9	I	17	1770.942	**885.975**
1109.585	**555.296**	10	G	16	1657.858	829.433
1238.628	619.817	11	E	15	**1600.836**	800.922
1295.649	**648.328**	12	G	14	1471.794	736.401
1408.733	**704.870**	13	L	13	1414.772	707.890
1539.774	**770.390**	14	M	12	**1301.688**	**651.348**
1640.821	**820.914**	15	T	11	**1170.648**	**585.827**
1741.869	**871.438**	16	T	10	**1069.600**	535.304
1840.937	920.972	17	V	9	**968.552**	484.780
1977.996	989.502	18	H	8	**869.484**	**435.246**
2049.033	**1025.020**	19	A	7	**732.425**	366.716
2162.118	**1081.562**	20	I	6	**661.388**	331.198
2263.165	1132.086	21	T	5	**548.304**	274.656
2334.202	1167.605	22	A	4	**447.256**	224.132

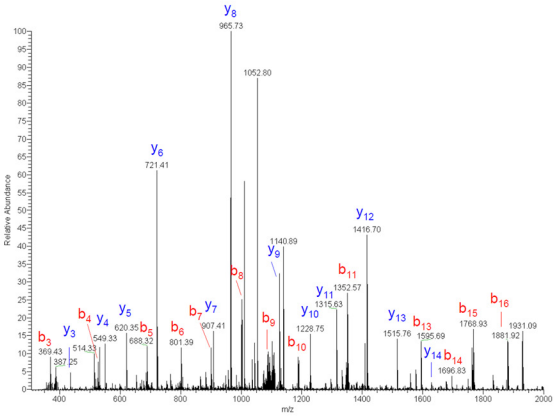
2435.250	**1218.129**	23	T	3	**376.219**	188.613
2563.309	**1282.158**	24	Q	2	275.171	138.089
2691.404	1346.205	25	K	1	147.113	74.060

Figure S1 to S5

Saha_et_al_Figure S1

Natural peptide

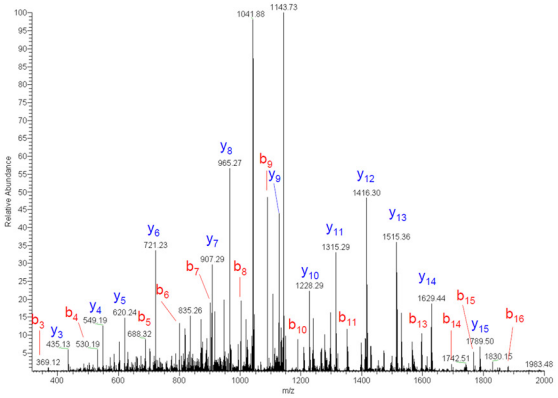
R** SPCCIVTSTYGWTANMER



b	b(+2)	#	seq	#	y	y(+2)
185.140	93.073	1	R	19	2203.009	**1102.008**
272.172	136.589	2	S	18	2018.877	**1009.942**
369.224	185.116	3	P	17	**1931.845**	**966.426**
472.234	236.620	4	C	16	**1834.792**	**917.900**
575.243	288.125	5	C	15	**1731.783**	**866.395**
688.327	344.667	6	I	14	**1628.774**	**814.890**
787.395	394.201	7	V	13	**1515.690**	**758.348**
888.443	**444.725**	8	T	12	**1416.621**	**708.814**
975.475	**488.241**	9	S	11	**1315.574**	**658.290**
1076.523	**538.765**	10	T	10	**1228.542**	**614.774**
1239.586	**620.297**	11	Y	9	**1127.494**	564.251
1296.608	**648.807**	12	G	8	**964.431**	**482.719**
1482.687	741.847	13	W	7	**907.409**	**454.208**
1583.734	792.371	14	T	6	**721.330**	361.169
1654.772	**827.889**	15	A	5	**620.282**	310.645
1768.815	**884.911**	16	N	4	**549.245**	275.126
1899.855	**950.431**	17	M	3	**435.202**	218.105
2028.898	**1014.952**	18	E	2	304.162	152.584
2184.999	**1093.003**	19	R	1	175.119	88.063

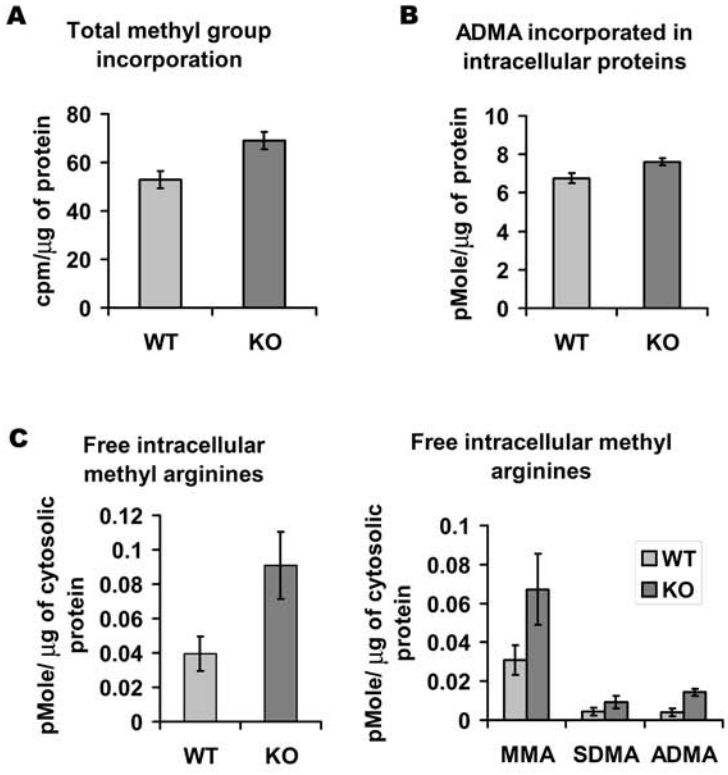
Synthetic peptide

R** SPCCIVTSTYGWTANMER

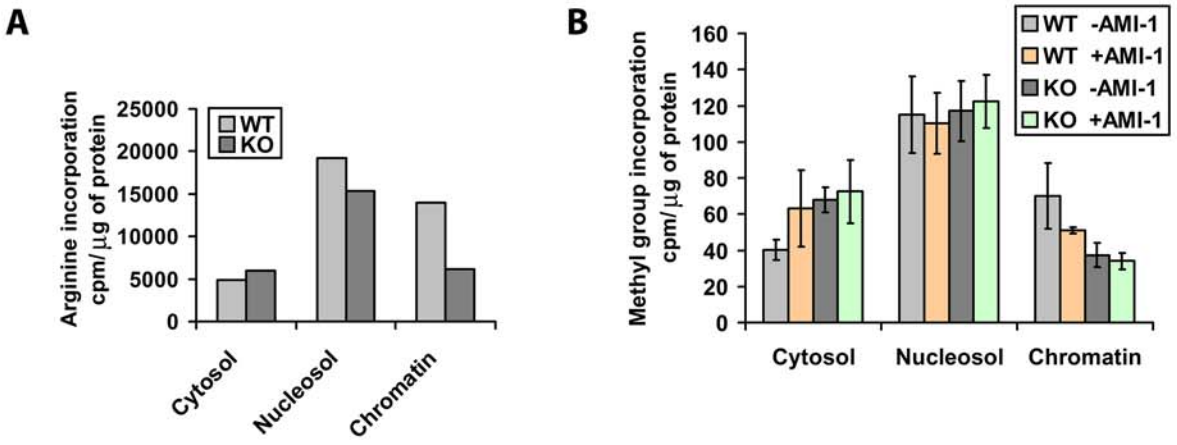


b	b(+2)	#	seq	#	y	y(+2)
185.140	93.073	1	R	19	2203.009	1102.008
272.172	136.589	2	S	18	2018.877	**1009.942**
369.224	185.116	3	P	17	**1931.845**	**966.426**
472.234	236.620	4	C	16	**1834.792**	**917.900**
575.243	288.125	5	C	15	**1731.783**	866.395
688.327	344.667	6	I	14	**1628.774**	**814.890**
787.395	394.201	7	V	13	**1515.690**	**758.348**
888.443	**444.725**	8	T	12	**1416.621**	**708.814**
975.475	**488.241**	9	S	11	**1315.574**	**658.290**
1076.523	538.765	10	T	10	**1228.542**	**614.774**
1239.586	**620.297**	11	Y	9	**1127.494**	**564.251**
1296.608	**648.807**	12	G	8	**964.431**	482.719
1482.687	**741.847**	13	W	7	**907.409**	**454.208**
1583.734	**792.371**	14	T	6	**721.330**	361.169
1654.772	**827.889**	15	A	5	**620.282**	310.645
1768.815	884.911	16	N	4	**549.245**	275.126
1899.855	**950.431**	17	M	3	**435.202**	218.105
2028.898	**1014.952**	18	E	2	304.162	152.584
2184.999	**1093.003**	19	R	1	175.119	88.063

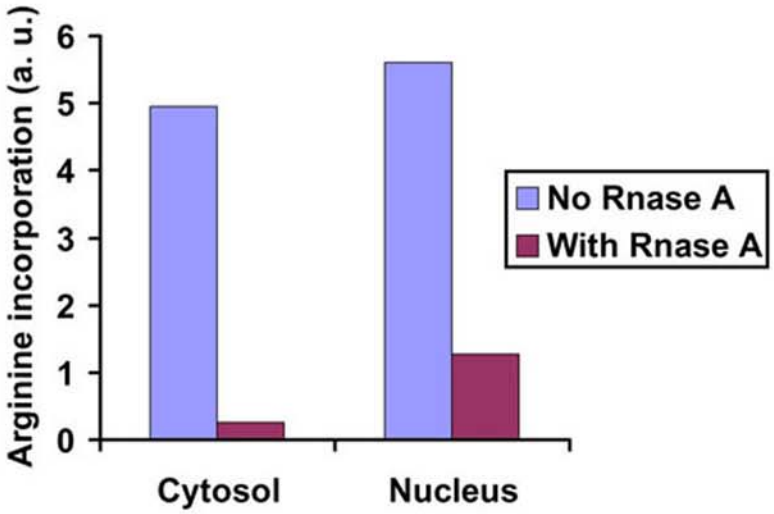
Saha_et_al_Figure S2



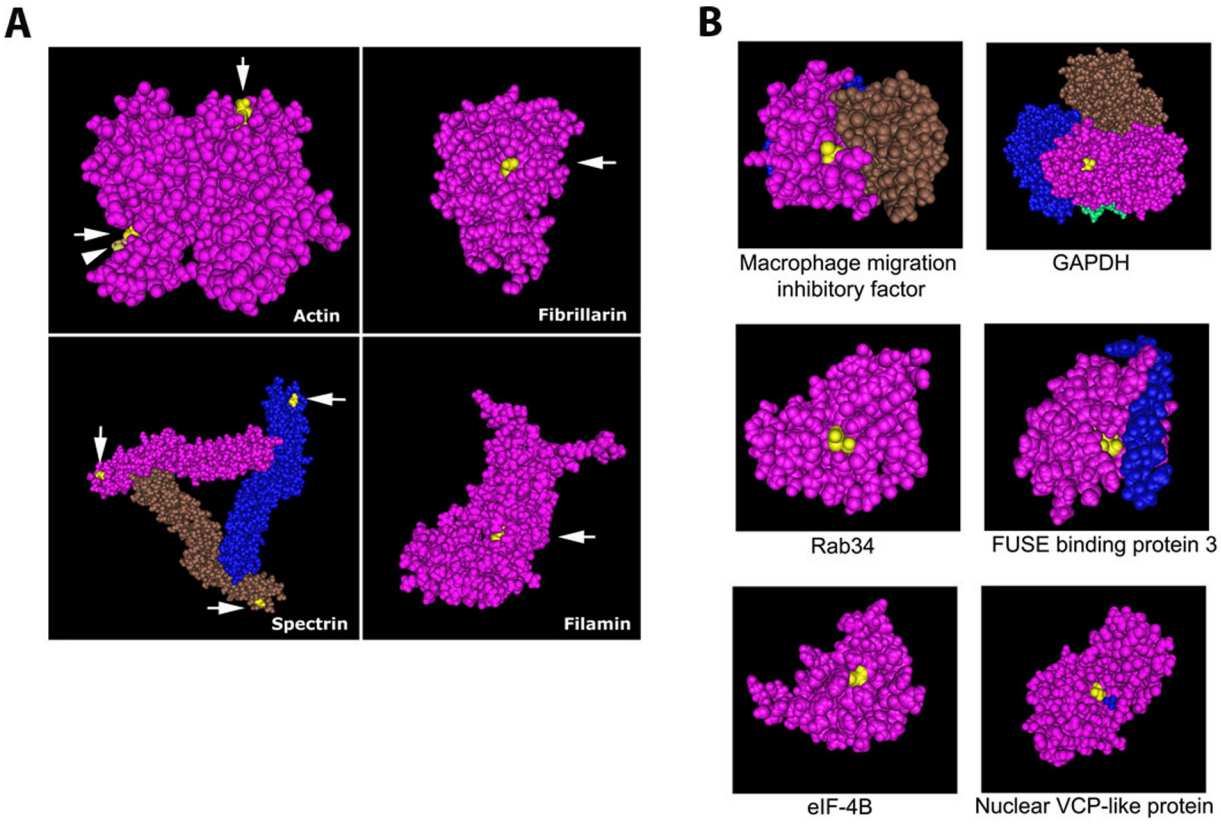
Saha_et_al_Figure S3



Saha_et_al_Figure S4



Saha_et_al_Figure S5

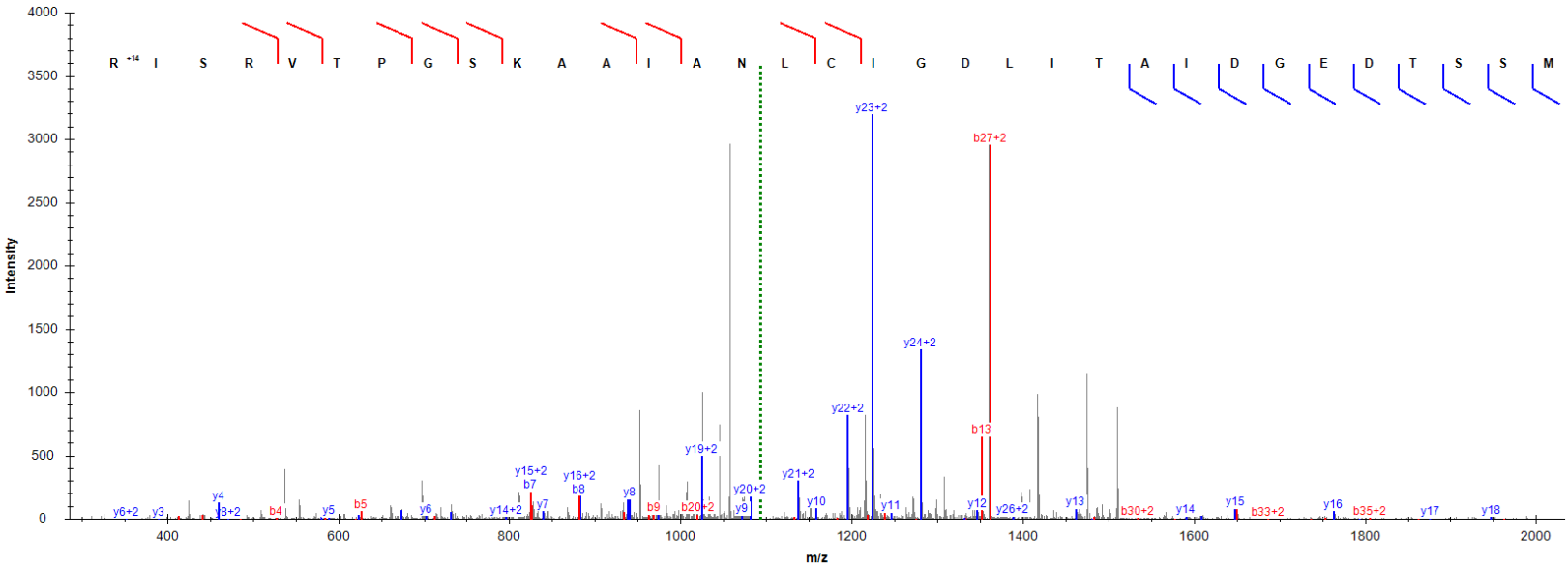


Saha et al. "Arginylation meets methylation: posttranslational modifications double up to regulate nuclear proteins and nuclear architecture in vivo"

Dataset S1

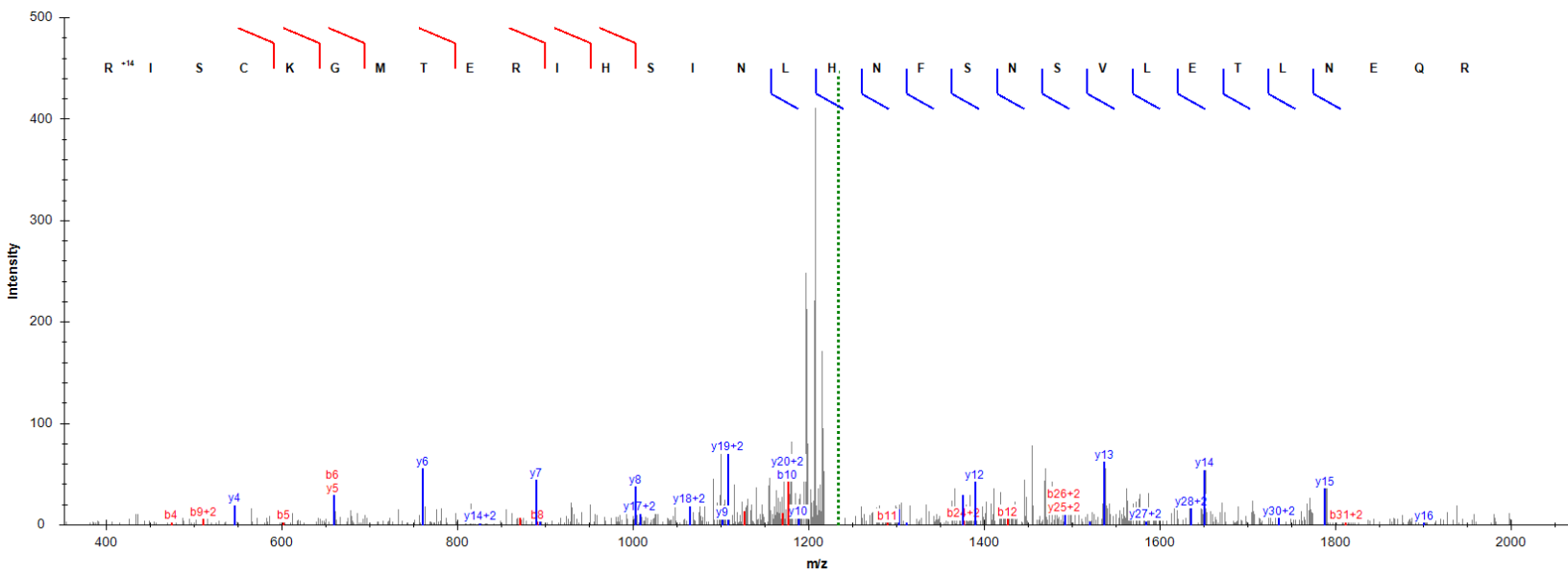
Mass spectra of arginylated/methylated peptides with detailed description of b and y ions

The following dataset contains the mass spectra of identified arginylated/methylated peptides. Each spectrum is followed by a table containing the expected and identified ions for the spectrum. The identified ions are highlighted in bold font in the tables. In the mass spectra b and y ions are marked in red and blue respectively. The complete sequence of the modified peptide is represented on top of each spectrum.



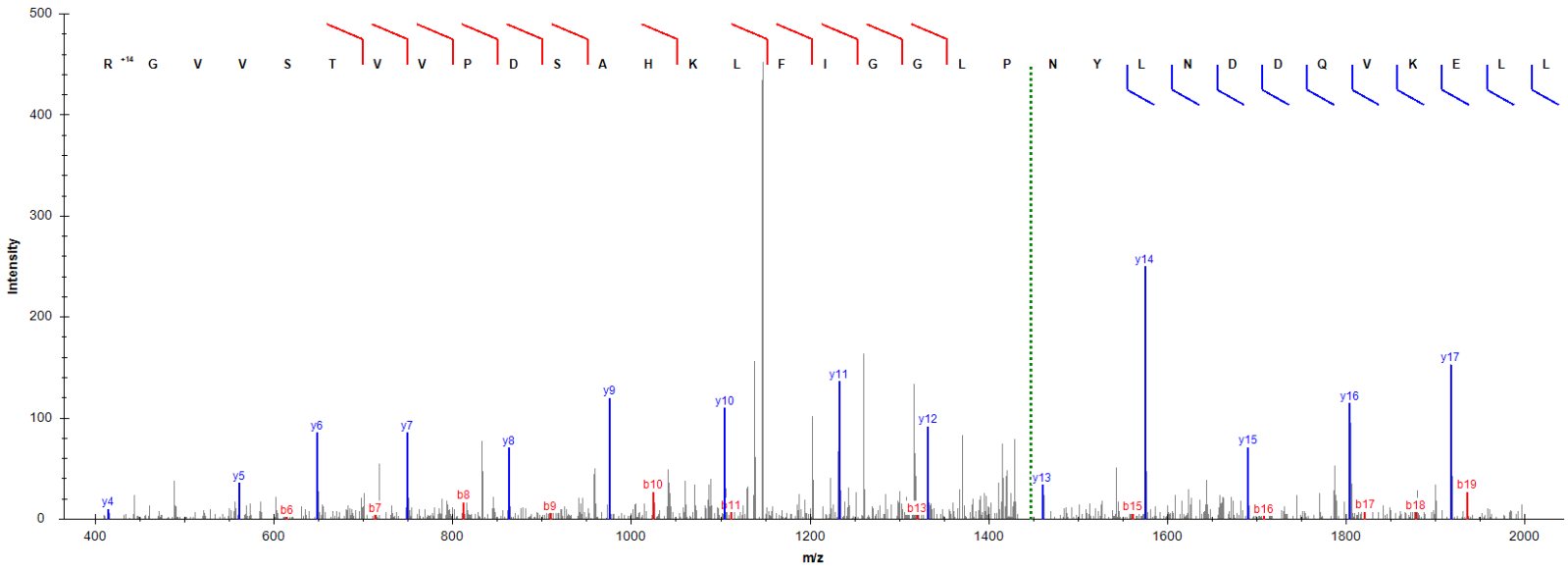
b	b(+2)	#	seq	#	y	y(+2)
171.124	86.066	1	R	41	4311.207	2156.107
284.208	142.608	2	I	40	4141.090	2071.049
371.240	186.124	3	S	39	4028.006	2014.507
527.341	264.174	4	R	38	3940.974	1970.991
626.410	313.708	5	V	37	3784.873	1892.940
727.457	364.232	6	T	36	3685.805	1843.406
824.510	**412.759**	7	P	35	3584.757	**1792.882**
881.532	**441.269**	8	G	34	3487.704	1744.356
968.564	**484.785**	9	S	33	3430.683	1715.845
1096.659	548.833	10	K	32	3343.651	1672.329
1167.696	**584.351**	11	A	31	3215.556	**1608.282**
1238.733	**619.870**	12	A	30	3144.519	1572.763
1351.817	676.412	13	I	29	3073.482	1537.244
1422.854	**711.931**	14	A	28	2960.398	**1480.702**
1536.897	768.952	15	N	27	2889.360	1445.184
1649.981	**825.494**	16	L	26	2775.318	**1388.162**
1752.990	876.999	17	C	25	2662.233	**1331.620**
1866.074	**933.541**	18	I	24	2559.224	**1280.116**
1923.096	**962.051**	19	G	23	2446.140	**1223.574**
2038.123	**1019.565**	20	D	22	2389.119	**1195.063**
2151.207	1076.107	21	L	21	2274.092	**1137.550**
2264.291	**1132.649**	22	I	20	2161.008	**1081.008**
2365.338	**1183.173**	23	T	19	2047.924	**1024.465**
2436.376	**1218.691**	24	A	18	**1946.876**	**973.942**

2549.460	**1275.233**	25	I	17	**1875.839**	**938.423**
2664.487	**1332.747**	26	D	16	**1762.755**	**881.881**
2721.508	**1361.258**	27	G	15	**1647.728**	**824.368**
2850.551	1425.779	28	E	14	**1590.706**	**795.857**
2965.578	**1483.292**	29	D	13	**1461.664**	**731.336**
3066.625	**1533.816**	30	T	12	**1346.637**	**673.822**
3153.657	**1577.332**	31	S	11	**1245.589**	**623.298**
3240.689	1620.848	32	S	10	**1158.557**	**579.782**
3371.730	**1686.369**	33	M	9	**1071.525**	536.266
3472.777	**1736.892**	34	T	8	**940.485**	**470.746**
3609.836	**1805.422**	35	H	7	**839.437**	420.222
3722.920	**1861.964**	36	L	6	**702.378**	**351.693**
3851.963	1926.485	37	E	5	**589.294**	295.151
3923.000	**1962.004**	38	A	4	**460.251**	230.629
4051.059	2026.033	39	Q	3	**389.214**	195.111
4165.102	2083.054	40	N	2	261.156	131.082
4293.197	2147.102	41	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
171.124	86.066	1	R	31	3640.844	1820.925
284.208	142.608	2	I	30	3470.727	**1735.867**
371.240	186.124	3	S	29	3357.643	1679.325
474.249	237.628	4	C	28	3270.611	**1635.809**
602.344	301.676	5	K	27	3167.601	**1584.304**
659.366	330.187	6	G	26	3039.506	**1520.257**
790.406	395.707	7	M	25	2982.485	**1491.746**
891.454	446.231	8	T	24	2851.445	**1426.226**
1020.497	**510.752**	9	E	23	2750.397	**1375.702**
1176.598	588.802	10	R	22	2621.354	**1311.181**
1289.682	645.344	11	I	21	2465.253	1233.130
1426.741	713.874	12	H	20	2352.169	**1176.588**
1513.773	757.390	13	S	19	2215.110	**1108.059**
1626.857	813.932	14	I	18	2128.078	**1064.543**
1740.900	**870.953**	15	N	17	2014.994	**1008.001**
1853.984	927.495	16	L	16	**1900.951**	950.979
1991.043	996.025	17	H	15	**1787.867**	**894.437**
2105.086	1053.046	18	N	14	**1650.808**	**825.908**
2252.154	**1126.581**	19	F	13	**1536.765**	768.886
2339.186	**1170.097**	20	S	12	**1389.697**	695.352
2453.229	1227.118	21	N	11	**1302.665**	651.836
2540.261	1270.634	22	S	10	**1188.622**	594.815
2639.329	1320.168	23	V	9	**1101.590**	551.299
2752.413	**1376.710**	24	L	8	**1002.521**	501.764

2881.456	1441.232	25	E	7	**889.437**	445.222
2982.504	**1491.755**	26	T	6	**760.395**	380.701
3095.588	1548.298	27	L	5	**659.347**	330.177
3209.631	1605.319	28	N	4	**546.263**	273.635
3338.673	1669.840	29	E	3	432.220	216.614
3466.732	1733.870	30	Q	2	303.178	152.092
3622.833	**1811.920**	31	R	1	175.119	88.063



b	#	seq	#	y
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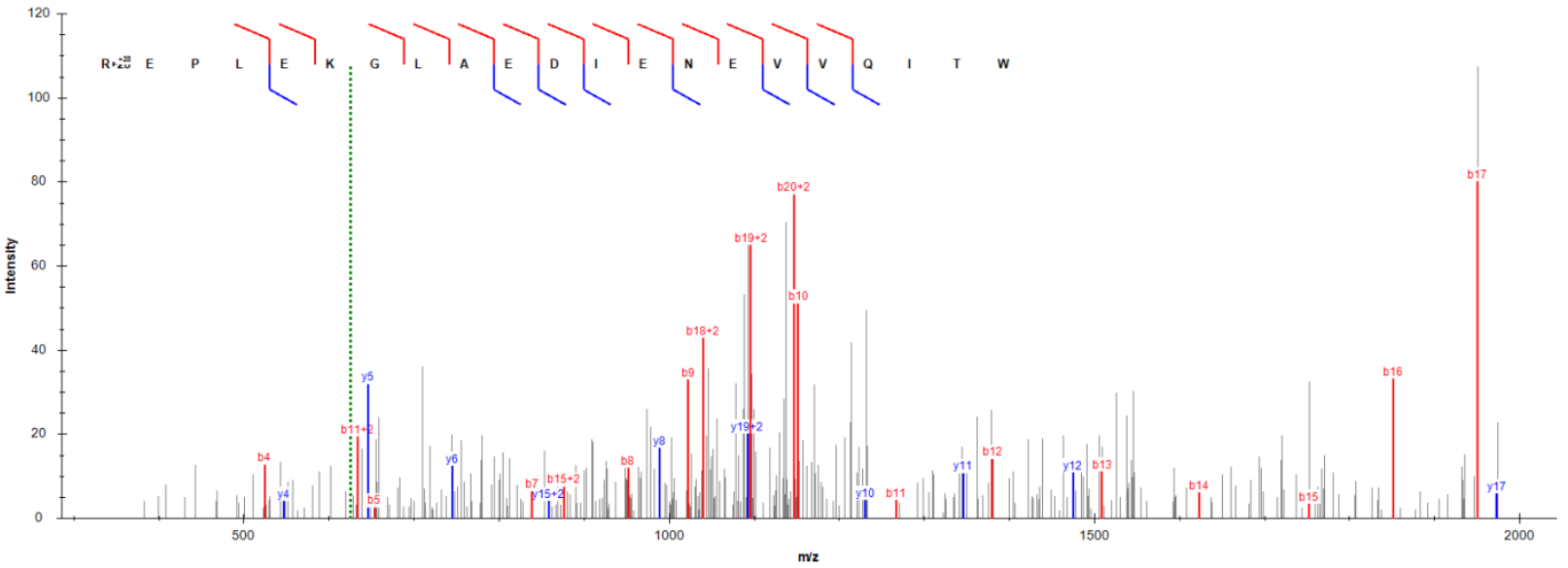
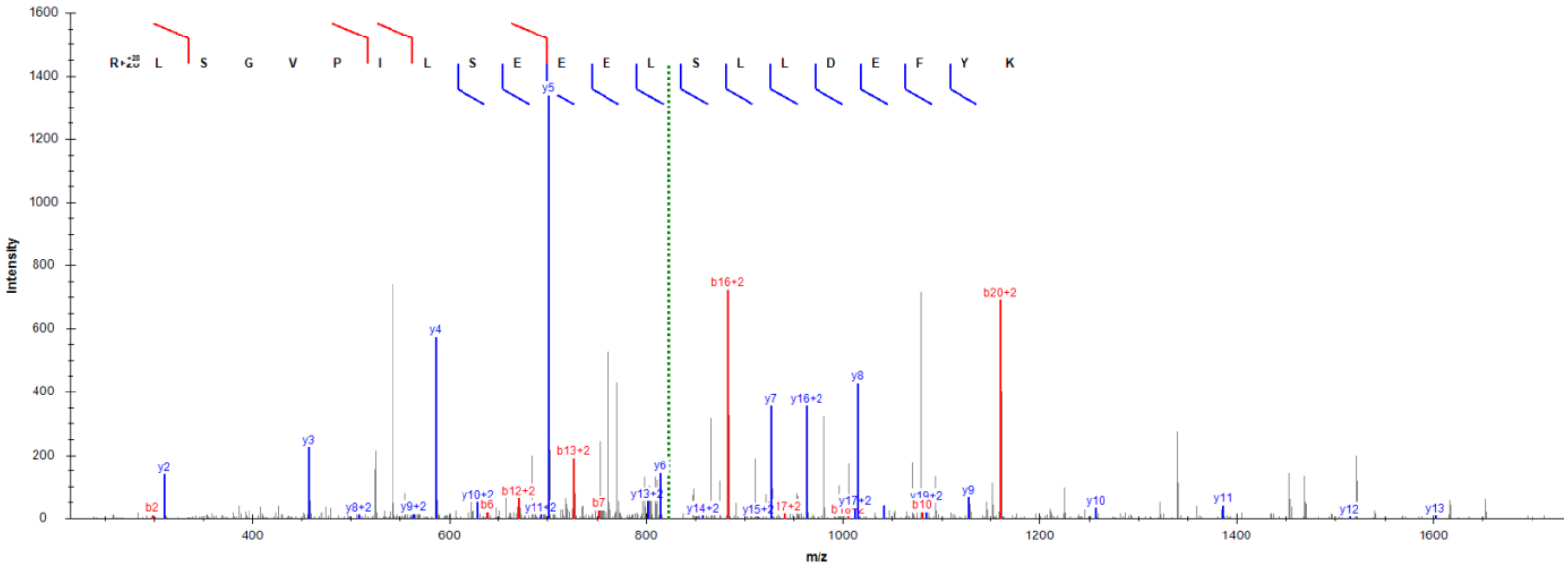
228.146	2	G	39	4168.233
327.214	3	V	38	4111.211
426.282	4	V	37	4012.143
513.314	5	S	36	3913.075
614.362	6	T	35	3826.043
713.430	7	V	34	3724.995
812.499	8	V	33	3625.926
909.552	9	P	32	3526.858
1024.579	10	D	31	3429.805
1111.611	11	S	30	3314.778
1182.648	12	A	29	3227.746
1319.707	13	H	28	3156.709
1447.802	14	K	27	3019.650
1560.886	15	L	26	2891.555
1707.954	16	F	25	2778.471
1821.038	17	I	24	2631.403
1878.060	18	G	23	2518.319
1935.081	19	G	22	2461.297
2048.165	20	L	21	2404.276
2145.218	21	P	20	2291.192

2259.261	22	N	19	2194.139
2422.324	23	Y	18	2080.096
2535.408	24	L	17	**1917.033**
2649.451	25	N	16	**1803.949**
2764.478	26	D	15	**1689.906**
2879.505	27	D	14	**1574.879**
3007.564	28	Q	13	**1459.852**
3106.632	29	V	12	**1331.793**
3234.727	30	K	11	**1232.725**
3363.770	31	E	10	**1104.630**
3476.854	32	L	9	**975.587**
3589.938	33	L	8	**862.503**
3690.985	34	T	7	**749.419**
3778.017	35	S	6	**648.372**
3925.086	36	F	5	**561.340**
3982.107	37	G	4	**414.271**
4079.160	38	P	3	357.250
4192.244	39	L	2	260.197
4320.339	40	K	1	147.113



b	b(+2)	#	seq	#	y	y(+2)
185.140	93.073	1	R	21	2496.298	1248.653
314.182	157.595	2	E	20	2312.166	1156.586
411.235	206.121	3	P	19	2183.123	**1092.065**
524.319	262.663	4	L	18	2086.070	1043.539
653.362	327.184	5	E	17	**1972.986**	986.997
781.457	391.232	6	K	16	1843.944	922.475
838.478	419.743	7	G	15	1715.849	**858.428**
951.562	476.285	8	L	14	1658.827	829.917
1022.599	511.803	9	A	13	1545.743	773.375
1151.642	576.325	10	E	12	**1474.706**	737.857
1266.669	**633.838**	11	D	11	**1345.663**	673.335
1379.753	690.380	12	I	10	**1230.636**	615.822
1508.795	754.901	13	E	9	1117.552	559.280
1622.838	811.923	14	N	8	**988.510**	494.759
1751.881	**876.444**	15	E	7	874.467	437.737
1850.949	925.978	16	V	6	**745.424**	373.216
1950.018	975.513	17	V	5	**646.356**	323.682
2078.076	**1039.542**	18	Q	4	**547.287**	274.147
2191.160	**1096.084**	19	I	3	419.229	210.118
2292.208	**1146.608**	20	T	2	306.145	153.576
2478.287	1239.647	21	W	1	205.097	103.052



b	b(+2)	#	seq	#	y	y(+2)
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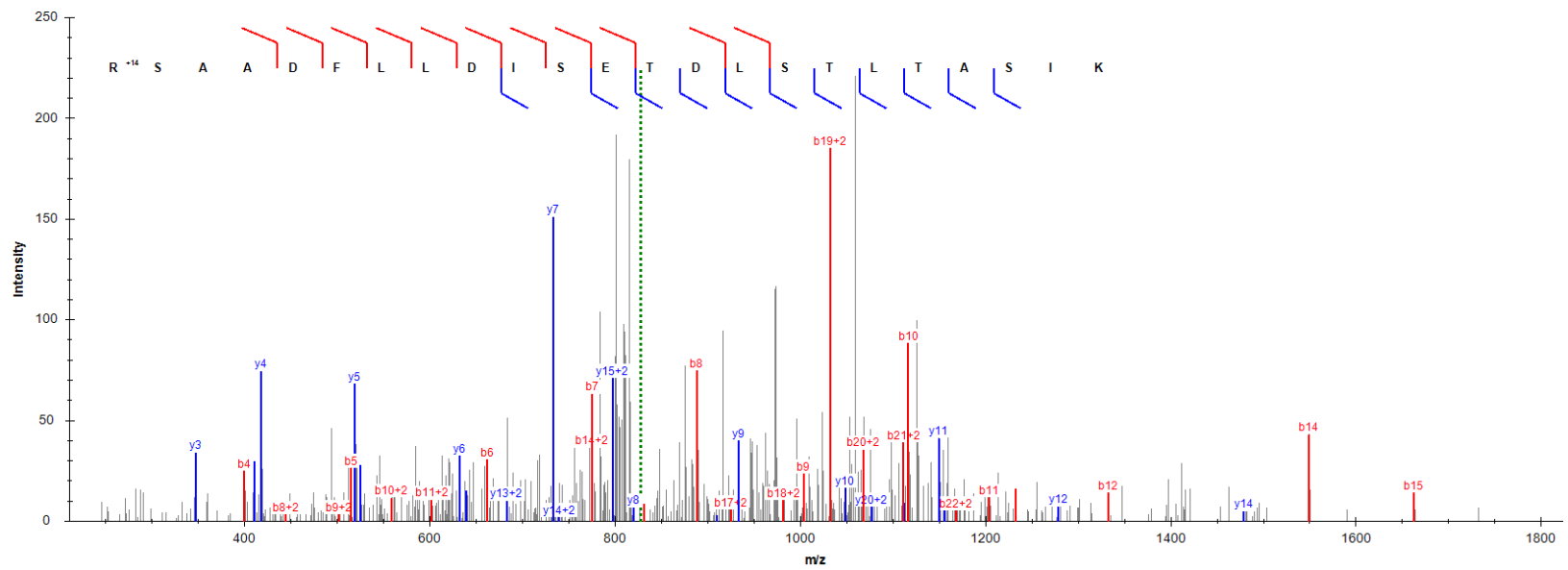
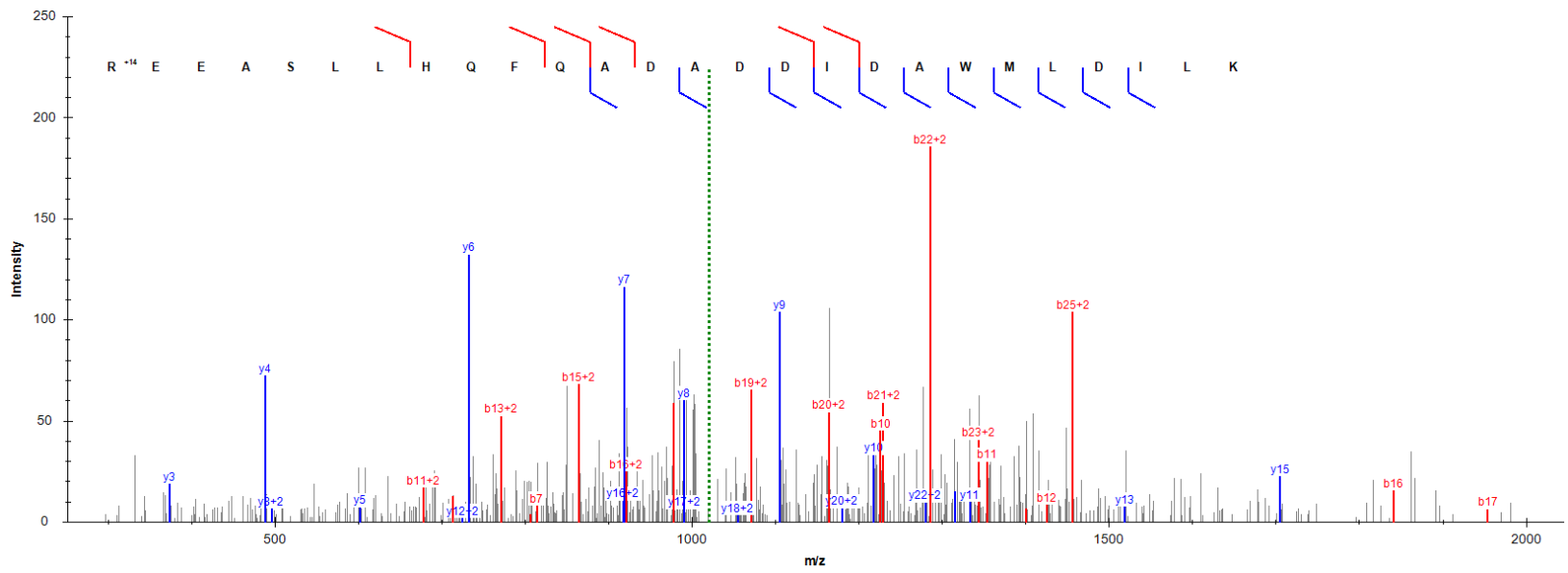
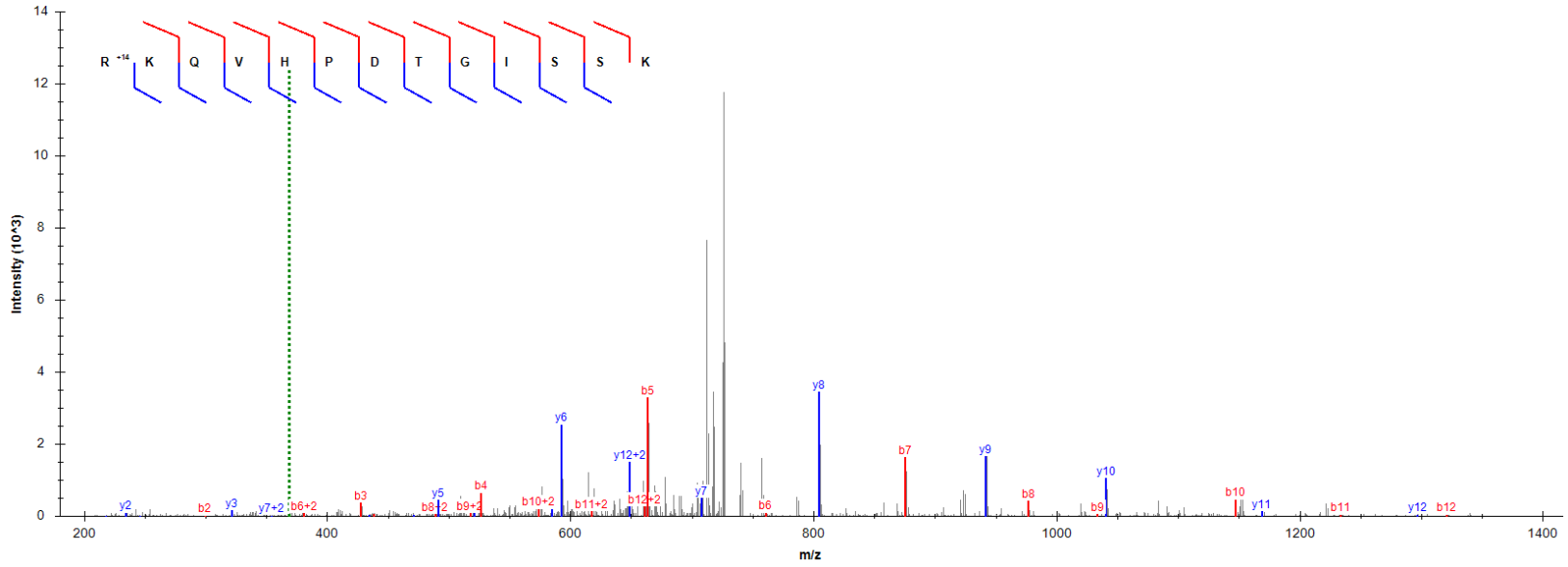
298.224	149.616	2	L	20	2281.185	1141.096
385.256	193.132	3	S	19	2168.101	**1084.554**
442.277	221.642	4	G	18	2081.069	**1041.038**
541.346	271.176	5	V	17	2024.047	**1012.527**
638.398	319.703	6	P	16	1924.979	**962.993**
751.482	376.245	7	I	15	1827.926	**914.467**
864.567	432.787	8	L	14	1714.842	**857.925**
951.599	476.303	9	S	13	**1601.758**	**801.383**
1080.641	540.824	10	E	12	**1514.726**	757.867
1209.684	605.346	11	E	11	**1385.683**	**693.345**
1338.726	**669.867**	12	E	10	**1256.641**	**628.824**
1451.810	**726.409**	13	L	9	**1127.598**	**564.303**
1538.842	769.925	14	S	8	**1014.514**	**507.761**
1651.927	826.467	15	L	7	**927.482**	464.245
1765.011	**883.009**	16	L	6	**814.398**	407.703
1880.038	**940.522**	17	D	5	**701.314**	351.161
2009.080	**1005.044**	18	E	4	**586.287**	293.647
2156.149	1078.578	19	F	3	**457.245**	229.126
2319.212	**1160.110**	20	Y	2	**310.176**	155.592
2447.307	1224.157	21	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
171.124	86.066	1	R	23	2481.308	1241.158
258.156	129.582	2	S	22	2311.192	**1156.099**
329.193	165.100	3	A	21	2224.159	**1112.583**
400.230	200.619	4	A	20	2153.122	**1077.065**
515.257	258.132	5	D	19	2082.085	1041.546
662.326	331.666	6	F	18	1967.058	984.033
775.410	388.209	7	L	17	1819.990	**910.499**
888.494	**444.751**	8	L	16	1706.906	853.957
1003.521	**502.264**	9	D	15	1593.822	**797.415**
1116.605	**558.806**	10	I	14	**1478.795**	**739.901**
1203.637	**602.322**	11	S	13	1365.711	**683.359**
1332.679	666.843	12	E	12	**1278.679**	**639.843**
1433.727	717.367	13	T	11	**1149.636**	575.322
1548.754	**774.881**	14	D	10	**1048.588**	**524.798**
1661.838	**831.423**	15	L	9	**933.562**	467.284
1748.870	874.939	16	S	8	**820.477**	**410.742**
1849.918	**925.463**	17	T	7	**733.445**	367.226
1963.002	**982.005**	18	L	6	**632.398**	316.703
2064.050	**1032.528**	19	T	5	**519.314**	260.160
2135.087	**1068.047**	20	A	4	**418.266**	209.637
2222.119	**1111.563**	21	S	3	**347.229**	174.118
2335.203	**1168.105**	22	I	2	260.197	130.602
2463.298	**1232.153**	23	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
171.124	86.066	1	R	26	3057.499	1529.253
300.167	150.587	2	E	25	2887.382	1444.195
429.209	215.108	3	E	24	2758.339	1379.673
500.246	250.627	4	A	23	2629.297	**1315.152**
587.278	294.143	5	S	22	2558.260	**1279.633**
700.362	350.685	6	L	21	2471.228	1236.117
813.447	407.227	7	L	20	2358.143	**1179.575**
950.505	475.756	8	H	19	2245.059	1123.033
1078.564	539.786	9	Q	18	2108.000	**1054.504**
1225.632	613.320	10	F	17	1979.942	**990.475**
1353.691	**677.349**	11	Q	16	1832.873	**916.940**
1424.728	**712.868**	12	A	15	**1704.815**	852.911
1539.755	**770.381**	13	D	14	1633.778	817.393
1610.792	**805.900**	14	A	13	**1518.751**	759.879
1725.819	**863.413**	15	D	12	1447.714	**724.361**
1840.846	**920.927**	16	D	11	**1332.687**	666.847
1953.930	**977.469**	17	I	10	**1217.660**	609.334
2068.957	1034.982	18	D	9	**1104.576**	552.792
2139.994	**1070.501**	19	A	8	**989.549**	**495.278**
2326.074	**1163.540**	20	W	7	**918.512**	459.760
2457.114	**1229.061**	21	M	6	**732.432**	366.720
2570.198	**1285.603**	22	L	5	**601.392**	301.200
2685.225	**1343.116**	23	D	4	**488.308**	244.658
2798.309	**1399.658**	24	I	3	**373.281**	187.144
2911.393	**1456.200**	25	L	2	260.197	130.602
3039.488	1520.248	26	K	1	147.113	74.060



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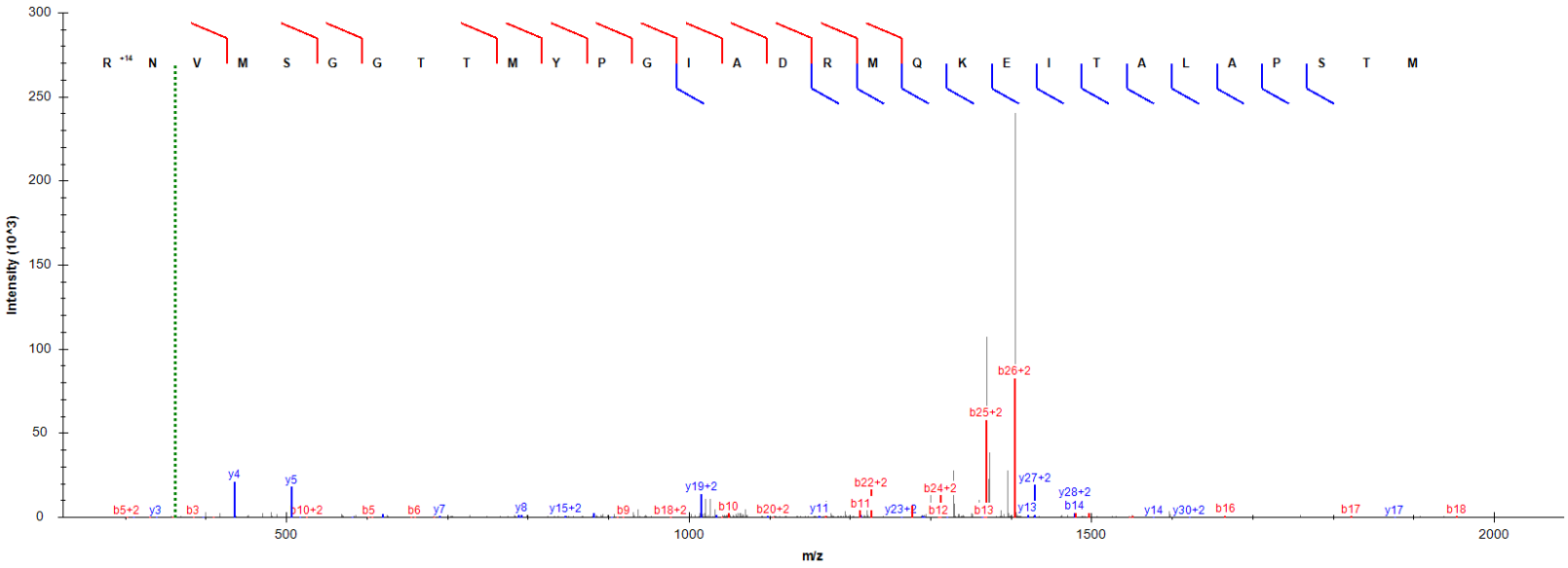
171.124	86.066	1	R	13	1466.807	733.907
299.219	150.113	2	K	12	**1296.691**	**648.849**
427.278	214.142	3	Q	11	**1168.596**	**584.801**
526.346	263.677	4	V	10	**1040.537**	**520.772**
663.405	332.206	5	H	9	**941.469**	**471.238**
760.458	**380.732**	6	P	8	**804.410**	402.709
875.485	**438.246**	7	D	7	**707.357**	**354.182**
976.532	**488.770**	8	T	6	**592.330**	296.669
1033.554	**517.281**	9	G	5	**491.282**	**246.145**
1146.638	**573.823**	10	I	4	**434.261**	**217.634**
1233.670	**617.339**	11	S	3	**321.177**	161.092
1320.702	**660.855**	12	S	2	**234.145**	117.576
1448.797	724.902	13	K	1	147.113	74.060



b	b(+2)	#	seq	#	y	y(+2)
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384.235	192.621	3	V	28	2957.424	**1479.216**
515.276	258.142	4	M	27	2858.356	**1429.681**
602.308	**301.658**	5	S	26	2727.315	**1364.161**
659.329	**330.168**	6	G	25	2640.283	**1320.645**
716.351	**358.679**	7	G	24	2583.262	**1292.134**
817.399	**409.203**	8	T	23	2526.240	**1263.624**
918.446	459.727	9	T	22	2425.192	**1213.100**
1049.487	**525.247**	10	M	21	2324.145	**1162.576**
1212.550	**606.779**	11	Y	20	2193.104	**1097.056**
1309.603	**655.305**	12	P	19	2030.041	**1015.524**
1366.624	**683.816**	13	G	18	1932.988	966.998
1479.708	740.358	14	I	17	**1875.967**	938.487
1550.745	775.876	15	A	16	1762.883	**881.945**
1665.772	833.390	16	D	15	1691.846	**846.426**
1821.873	**911.440**	17	R	14	**1576.819**	**788.913**
1952.914	**976.961**	18	M	13	**1420.717**	710.862
2080.973	**1040.990**	19	Q	12	**1289.677**	645.342
2209.068	**1105.037**	20	K	11	**1161.618**	**581.313**
2338.110	**1169.559**	21	E	10	**1033.523**	**517.265**
2451.194	**1226.101**	22	I	9	**904.481**	452.744
2552.242	**1276.625**	23	T	8	**791.397**	**396.202**
2623.279	**1312.143**	24	A	7	**690.349**	345.678

2736.363	**1368.685**	25	L	6	**619.312**	**310.160**
2807.400	**1404.204**	26	A	5	**506.228**	253.618
2904.453	1452.730	27	P	4	**435.191**	218.099
2991.485	**1496.246**	28	S	3	**338.138**	169.573
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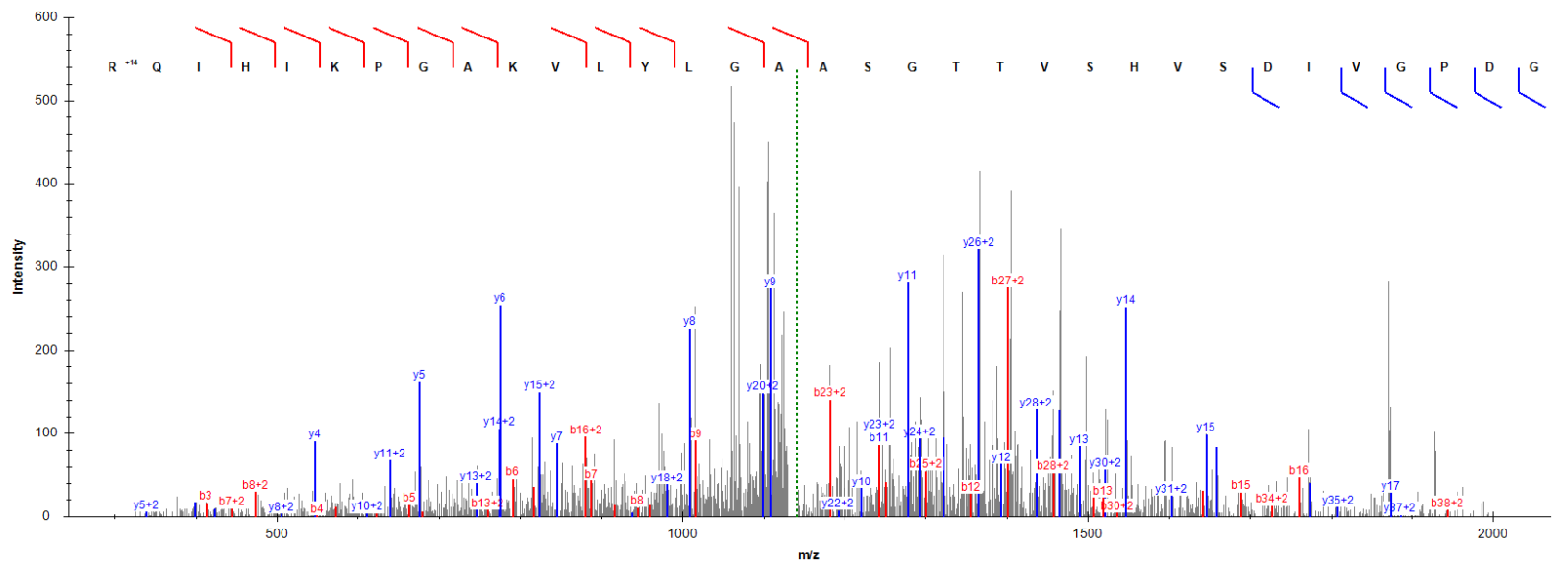

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549.326	275.166	4	H	40	4148.193	2074.600
662.410	331.708	5	I	39	4011.134	2006.071
790.505	395.756	6	K	38	3898.050	1949.529
887.557	**444.282**	7	P	37	3769.955	**1885.481**
944.579	**472.793**	8	G	36	3672.902	1836.955
1015.616	508.312	9	A	35	3615.881	**1808.444**
1143.711	**572.359**	10	K	34	3544.843	**1772.925**
1242.779	**621.893**	11	V	33	3416.748	1708.878
1355.863	**678.435**	12	L	32	3317.680	**1659.344**
1518.927	**759.967**	13	Y	31	3204.596	**1602.802**
1632.011	**816.509**	14	L	30	3041.533	**1521.270**
1689.032	845.020	15	G	29	2928.449	**1464.728**
1760.069	**880.538**	16	A	28	2871.427	**1436.217**
1831.107	**916.057**	17	A	27	2800.390	**1400.699**
1918.139	**959.573**	18	S	26	2729.353	**1365.180**
1975.160	988.084	19	G	25	2642.321	**1321.664**
2076.208	1038.607	20	T	24	2585.299	**1293.153**
2177.255	1089.131	21	T	23	2484.252	**1242.630**
2276.324	1138.666	22	V	22	2383.204	**1192.106**
2363.356	**1182.182**	23	S	21	2284.136	1142.571
2500.415	**1250.711**	24	H	20	2197.104	**1099.055**
2599.483	**1300.245**	25	V	19	2060.045	1030.526

2686.515	1343.761	26	S	18	1960.976	**980.992**
2801.542	**1401.275**	27	D	17	**1873.944**	**937.476**
2914.626	**1457.817**	28	I	16	1758.917	**879.962**
3013.695	**1507.351**	29	V	15	**1645.833**	**823.420**
3070.716	**1535.862**	30	G	14	**1546.765**	**773.886**
3167.769	1584.388	31	P	13	**1489.743**	**745.375**
3282.796	**1641.902**	32	D	12	**1392.691**	696.849
3339.817	1670.412	33	G	11	**1277.664**	**639.335**
3452.901	**1726.954**	34	L	10	**1220.642**	**610.825**
3551.970	1776.488	35	V	9	**1107.558**	554.283
3715.033	1858.020	36	Y	8	**1008.490**	**504.749**
3786.070	1893.539	37	A	7	**845.426**	**423.217**
3885.139	**1943.073**	38	V	6	**774.389**	387.698
4014.181	2007.594	39	E	5	**675.321**	**338.164**
4161.250	2081.128	40	F	4	**546.278**	273.643
4248.282	2124.644	41	S	3	**399.210**	200.109
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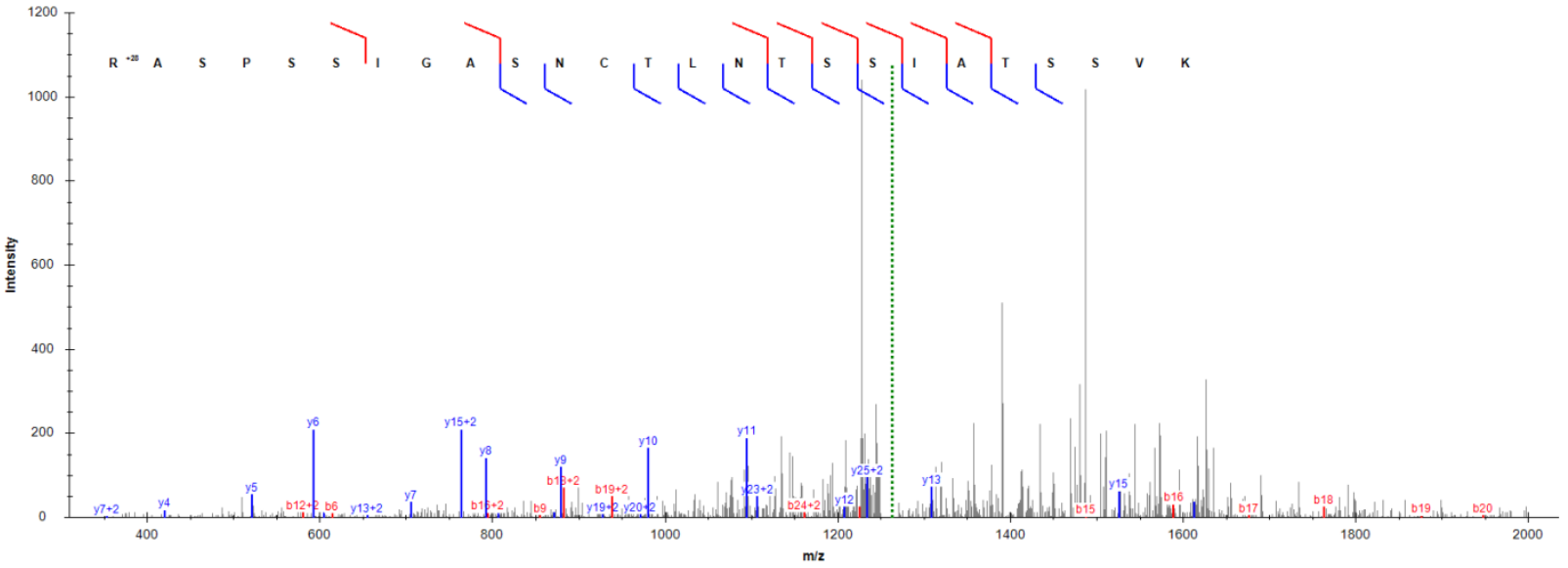

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440.262	220.634	4	P	22	2125.044	1063.026
527.294	264.150	5	S	21	2027.991	1014.499
614.326	307.666	6	S	20	1940.959	**970.983**
727.410	364.208	7	I	19	1853.927	**927.467**
784.431	392.719	8	G	18	1740.843	**870.925**
855.468	428.238	9	A	17	1683.822	842.415
942.500	471.754	10	S	16	**1612.785**	**806.896**
1056.543	528.775	11	N	15	**1525.753**	**763.380**
1159.552	**580.280**	12	C	14	1411.710	706.358
1260.600	630.804	13	T	13	**1308.701**	**654.854**
1373.684	687.346	14	L	12	**1207.653**	**604.330**
1487.727	744.367	15	N	11	**1094.569**	547.788
1588.775	**794.891**	16	T	10	**980.526**	490.767
1675.807	838.407	17	S	9	**879.478**	440.243
1762.839	**881.923**	18	S	8	**792.446**	396.727
1875.923	**938.465**	19	I	7	**705.414**	**353.211**
1946.960	973.984	20	A	6	**592.330**	296.669
2048.008	1024.507	21	T	5	**521.293**	261.150
2135.040	1068.023	22	S	4	**420.245**	210.626
2222.072	1111.540	23	S	3	333.213	167.110
2321.140	**1161.074**	24	V	2	246.181	123.594
2449.235	**1225.121**	25	K	1	147.113	74.060

Saha et al. "Arginylation and methylation double up to regulate nuclear proteins and nuclear architecture in vivo": Supplemental Information.

Inventory of Supplemental Information

Supplemental Table S1: Related to Figures 1 and S1 and Table 1

Supplemental Table S2: Related to Figures 4 and S5, Tables 1 and 2 and Datasets 1 and 2

Supplemental Table S3: Related to Tables 1 and 2 and Datasets 1 and 2

Supplemental Table S4: Related to Tables 1 and 2 and Datasets 1 and 2

Figure S1: Related to Figure 1 and Table 1.

Figure S2: Related to Figure 2.

Figure S3: Related to Figure 2.

Figure S4: Related to Figure 3.

Figure S5: Related to Figure 4 and Tables 1 and 2.

Dataset S1: Related to Figure 4 and Table 1.

Dataset S2: Related to Figure 4 and Table 2.

Supplemental Figure and Table Legends and Experimental Procedures.

Supplemental Table Legends:

Supplemental Table S1. Accession numbers, peptide sequences, and database search parameters used for the identification of the arginylated/methylated peptides in the cytosolic samples from heart and fibroblasts and the analysis of the peptide standards shown in Fig. 1 and S1. See Experimental Procedures for method description.

Supplemental Table S2. Accession numbers, peptide sequences, and database search parameters used for the identification of the arginylated and arginylated/methylated peptides in nuclear subfractions shown in Tables 1 and 2 and Supplemental Datasets S1 and S2. See Experimental Procedures for method description.

Supplemental Table S3. Mass ambiguities considered during the validation of monomethyl-arginylated peptides, listing the identity of residues in the positions preceding the arginylation site (denoted as -1 and -2 for the two residues found N-terminally of the arginylation site in the protein sequence).

Supplemental Table S4. Mass ambiguities considered during the validation of dimethyl-arginylated peptides, listing the identity of residues in the positions preceding the arginylation site (denoted as -1 and -2 for the two residues found N-terminally of the arginylation site in the protein sequence).

Supplemental Figure Legends:

Figure S1. MS/MS spectra of the experimentally identified dimethyl-arginylated HSP90/HSP84b peptide (AAA37866) (left, natural peptide) and synthetic standard peptide containing N-terminal dimethylated Arg (right, dimethyl groups in both are denoted with double stars). Peptide sequences and b and y ion masses are shown on the top right for each spectrum and in the tables underneath. See Supplemental Table S1 for the search parameters.

Figure S2. Estimation of intracellular methylated Arg derivatives. A. In vivo total methyl group incorporation in the presence of translation inhibitors, using ^{3}H-Met as methyl donor (derived by dividing the total cpm of ^{3}H-Met incorporation by the total protein amount in the cytosolic and nuclear fractions, from the same data as that shown in Fig 2B of the main text) presented as cpm. per μg of protein. Ate1 KO cells have overall higher methylation. B. Estimation of methylated Arg concentration in TCA-precipitated total intracellular protein by amino acid hydrolysis followed by HPLC. Out of the three types of methyl-Arg derivatives analysed, only asymmetric dimethyl Arg (ADMA) was detected during the analysis. Error bars +/- SEM, n = 3, p value is 0.06. Overall, levels of protein-incorporated methylated Arg are higher in Ate KO cells. C. Estimation of free intracellular methylated Arg derivatives monomethyl-Arg (MMA), symmetric dimethyl-Arg (SDMA), and asymmetric dimethyl-Arg (ADMA) in WT and Ate1 KO cell cytosol (100,000 x g supernatant) shown as a total (left) and by individual derivatives (right). The free amino acid concentrations were normalized per μg of cytosolic protein present in the two cell types. Error bars +/- SEM, n = 6. Left panel, p values are 0.04. Right panel, p values are MMA: 0.09; SDMA: 0.2; ADMA: 0.003. Consistent with the results shown in A and B, methyl-Arg levels are higher in Ate1 knockout cells.

Figure S3. Control experiments for *in vivo* incorporation of arginine and methyl groups. A. In vivo incorporation of ^{3}H-Arg into different subcellular fractions of wild type (WT) and Ate1 knockout (KO) cells in the absence of protein synthesis inhibitors, presented as cpm per μg of protein. **B.** *In vivo* incorporation of ^{3}H-Met into different subcellular fractions of cycloheximide/chloramphenicol-treated wild type (WT) and Ate1 knockout (KO) cells in the presence and absence of protein arginine methyl transferase inhibitor AMI-1, presented as cpm per μg of protein.

Figure S4. *In vitro* Arg incorporation by endogenous ATE1 is Arg-tRNA dependent. ^{3}H-Arg incorporation by endogenous ATE1 into cellular proteins in the cytosolic and nuclear extract at the 30 min time point (similarly to that shown in Fig. 3A of the main text) in the presence and absence of RNase A. RNase A abolishes the majority of arginine incorporation activity in both cytosol and nuclear extracts.

Figure S5. Location of modified residues in tertiary structures of identified proteins. A. Structures of some of the arginylated/methylated proteins identified in this study. Modified residues are marked with yellow highlight and arrowheads (arginylated) or arrows (methylated/arginylated). PDB identifiers for the shown structures: actin, 1J6Z (modified sites are located on the actin subunit interface (top) and outer surface (left); neighboring residues are highlighted for visibility of the arginylation/methylation sites); fibrillarin, 1G8A (modified site is located on the molecule surface); filamin fragment: 2K7Q; spectrin fragment: 1CUN (modified sites are located on the surfaces exposed to the molecular interactions in a folded protein). B. Structures of some of the arginylated proteins identified in this study. The

arginylated residues are marked in yellow. Macrophage migration inhibitory factor; PDB identifier: 1MFI; the image shows a trimer of the protein. GAPDH; PDB identifier: 1U8F; the image shows a tetramer of the protein. Rab 34; PDB identifier: 2FOL; the arginylation site is in the GTP and Mg binding site. FUSE binding protein 3; PDB identifier: 1X4N; the blue molecule represents an RNA molecule bound to the protein and the arginylated residue is one of the nucleotide binding residue. eIF-4B; PDB identifier: 2J76; the arginylation site is on the RNA recognition motif and RNA-binding site. Nuclear VCP-like protein; PDB identifier: 2X8A; the arginylation site is in the ATP binding pocket/ Walker A motif. The blue molecule represents a phosphate ion.

Supplemental Dataset Legends:

Dataset S1. Related to Table 1. Mass spectra and ion mass tables of arginylated/methylated peptides. Each spectrum is followed by the corresponding ion mass table.

Dataset S2. Related to Table 2. Mass spectra and ion mass tables of arginylated peptides. Each spectrum is followed by the corresponding ion mass table.

Supplemental Experimental Procedures:

Nuclear fractionation and nuclear protein isolation for mass spectrometry. Cells were lysed in the lysis buffer (0.3 M sucrose, 4 mM Mg acetate, 12.5 mM KCl, 50 mM Tris pH: 8.0, 0.5 mM arginine, 1 mM DTT, 0.2 mM PMSF, protease inhibitor cocktail). Nucleus and cytosol were separated by spinning for 5 min at 2000 x g, 4^{o}C. The nuclei-containing pellet was resuspended in buffer B (50 mM Tris pH:7.5, 25 mM KCl, 5 mM $MgCl_2$ 0.5% NP 40, 1 mM DTT, 0.2 mM PMSF, protease inhibitor cocktail) and further purified by two extractions with buffer B followed by spinning for 5 min at 2000 x g, 4^{o}C through 0.88 M sucrose in buffer B. Pure nuclei were lysed by resuspending in the hypertonic nuclear lysis buffer (50 mM Tris pH: 8.0, 100 mM KCl, 400 mM NaCl, 0.5 mM arginine, 4% Triton X 100, 1 mM DTT, 0.2 mM PMSF, protease inhibitor cocktail) and incubating on ice for 30 min with occasional mixing. The lysate was fractionated by spinning for 10 min at 16,000 x g at 4°C. The supernatant was collected as 'nucleosol' and the chromatin pellet was further extracted with histone extraction buffer (same as nuclear lysis buffer except NaCl concentration was 2 M and the buffer had no Triton X 100). The pellet was resuspended by pipetting and incubated on ice for 30 min. The suspension was centrifuged at 100,000 x g for 30 min at 4°C and the supernatant was collected as 'chromatin associated proteins'. The pellet was further extracted by re-suspending in buffer C (10 mM Tris pH: 7.5, 2.5 mM MgCl2, 0.5 mM CaCl2) and DNase I treatment at 25°C for 20 min. The mix was centrifuged at 100,000 x g for 30 min at 4°C and the supernatant was collected as 'chromatin integrated proteins'. Proteins from each fraction were precipitated by 20% TCA and the pellets were analyzed by mass spectrometry.

Estimation of intracellular methyl-Arg concentrations in the protein and free metabolite pools. For estimation of protein-integrated methyl arginine concentrations cell pellet was re-suspended in buffer D (10 mM Tris pH: 7.5, 25 mM KCl, 1 mM DTT, 0.2 mM PMSF, protease inhibitor cocktail) and lysed by sonication. The whole cell lysate was precipitated by 10% TCA and the TCA pellet was analyzed by dissolving in 70% formic acid for hydrolysis and subsequent HPLC analysis. For estimation of free methyl arginine concentrations cells were lysed in buffer E (10 mM Tris pH: 7.5 and 25mM KCl) in the same way as mentioned above and the whole cell lysate was spun at 100,000 x g for 45 min at 4°C and the supernatant was collected as cytosol. The proteins present in cytosol are precipitated by 10% TCA and the supernatant was analyzed by HPLC without acid hydrolysis. The pure methyl arginines (MMA, SDMA, and ADMA) were used as the standards in HPLC analysis. The amounts of methy arginines injected as standrads were: MMA: 1.05 nMole; ADMA: 0.91 nMole; SDMA: 0.91 nMole. HPLC, amino acid hydrolysis, and Arg determination was performed by the W.M. Keck Foundation Biotechnology Resource Laboratory at Yale University.

In vitro arginylation assay to estimate endogenous ATE1 activity in cellular fractions. Prior to the assay, L-[^{3}H] Arginine (Perkin Elmer) was charged to the $tRNA^{Arg}$ using arginyl-tRNA synthetase (RRS) in a reaction mix containing 50 mM Hepes, pH 7.5, 25 mM KCl, 15 mM $MgCl_2$, 0.1 mM DTT, 2.5 mM ATP, 12.5 μM L-[^{3}H]-Arginine, 40 μM $tRNA^{Arg}$, 0.6 μM RRS, at 37°C for 1 hr. The charged tRNA was purified by chloroform extraction, 80% ethanol wash, and re-suspension in water. This purified charged tRNA was used for the final arginylation assay. For the in vitro arginylation assay cells were lysed using buffer A (50 mM Tris pH: 8, 0.3 M Sucrose, 4 mM Mg-acetate, 12.5 mM KCl, 10 mM β-ME, 0.5% NP 40, 1 mM DTT, 0.2 mM

PMSF, protease inhibitor cocktail). Nucleus and cytosol were separated by spinning at 4^{o}C for 5 min at 2000 x g. The supernatant was collected as cytosol and the nuclear pellet was re-suspended in buffer B (50 mM Tris pH: 7.5, 25 mM KCl, 5 mM $MgCl_2$ 0.5% NP 40, 1 mM DTT, 0.2 mM PMSF, protease inhibitor cocktail) and layered on equal volume of 0.88 M sucrose in buffer B and spun at 4^{o}C for 5 min at 2000 x g. The pellet was collected as pure nuclei and lysed in nuclear lysis buffer C (50 mM Tris pH:8.0, 25 mM KCl, 1 mM DTT, 0.2 mM PMSF, protease inhibitor cocktail) by sonication, followed by centrifugation at 4^{o}C for 10 min at 16000 x g. The supernatant was collected as the soluble nuclear fraction for the assay. Protein concentration in the cytosolic and nuclear fraction were estimated by the Bradford assay. To estimate the endogenous ATE1 activity in the cytosolic and nuclear fractions, specific amount of the cytosolic and nuclear proteins were diluted in the ATE1 assay buffer (final concentration, 50 mM Hepes, pH 7.5, 25 mM KCl, 15 mM $MgCl_2$, 0.1 mM DTT, 2.5 mM ATP, 400 μg/ml cycloheximide) and incubated with 60 uM L-[^{3}H]-Arginine-charged $tRNA^{Arg}$ at 37°C for different time points. For the RNase A control assays, 3μg of RNase A/10μl reaction mix was added before transferring the reaction mix to 37°C. 10 μl of the reaction at each time point was immediately quenched into 40 μl of 20% Trichloroacetic acid (TCA) containing 1 mM of unlabeled Arg, and kept at room temperature for at least 10 min, followed by heating at 95^{o}C for 15 min (to destroy the excess of the labeled Arg-tRNA), cooling down on ice for 20 min, and spinning at 16,000 x g for 30 min at 4°C to collect the pellets containing precipitated proteins. Pellets were washed 3x with 10% cold TCA and once with cold acetone, air dried, and counted in a liquid scintillation counter.

In vitro methyl-Arg incorporation assay. This assay was performed as a single step reaction (synthesis of methyl arginine charged tRNA coupled to the transfer of methyarginine onto the substrate) using purified RRS and ATE1-1 enzyme system and using a natural actin N-terminal peptide (DDIAALVVDNGSGMCK) as a substrate. The reaction mix (50 μM peptide, 50 mM Hepes pH 7.5, 25 mM KCl, 15 mM $MgCl_2$, 0.1 mM DTT, 2.5 mM ATP, 4 mM methyarginine, 50 μM $tRNA^{Arg}$, 0.6 μM RRS, and 3.4 μM Ate1-1) was prepared with either of the three different methylarginine species MMA, SDMA and ADMA and incubated at 37°C for 1 hr. The peptides were purified using C18 columns and analyzed by MALDI-TOF mass spectrometry.