Supplemental data

Basic residues of β-Sheet A contribute to heparin binding and activation of human serpinA12 (vaspin)*

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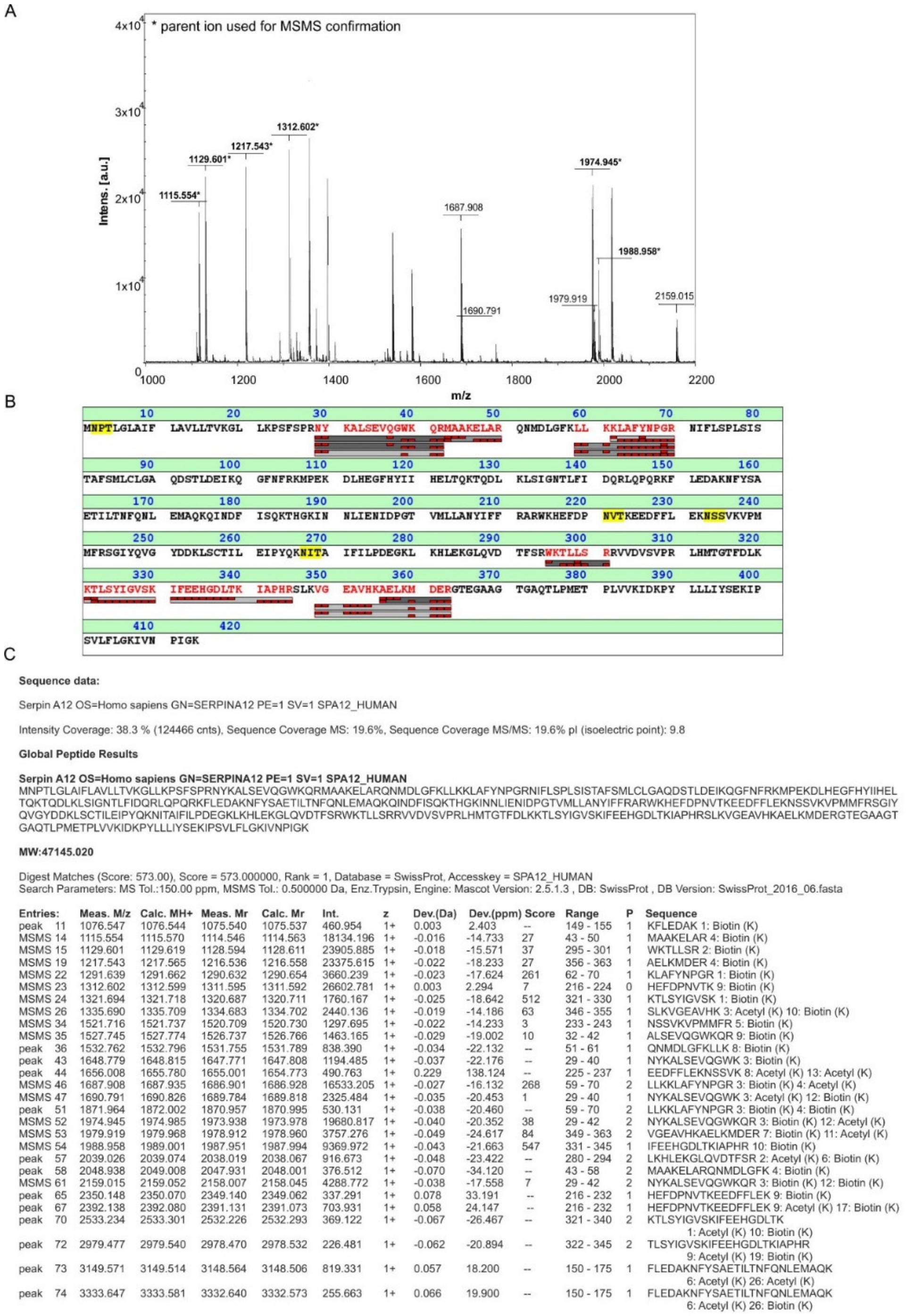
Supplemental Figure 1



MNPTLGLAIF LAVLLTVKGL LKPSFSPRNY KALSEVQGWK QRMAAKELAR QNMDLGFKLL KKLAFYNPGR NIFLSPLSIS
TAFSMLCLGA QDSTLDEIKQ GFNFRKMPEK DLHEGFHYII HELTQKTQDL KLSIGNTLFI DQRLQPQRKF LEDAKNFYSA
ETILTNFQNL EMAQKQINDF ISQKTHGKIN NLIENIDPGT VMLLANYIFF RARWKHEFDP NVTKEEDFFL EKNSSVKVPM
MFRSGIYQVG YDDKLSCTIL EIPYQKNITA IFILPDEGKL KHLEKGLQVD TFSRWKTLLS RRVVDVSVPR LHMTGTFDLK
KTLSYIGVSK IFEEHGDLTK IAPHRSLKVG EAVHKAELKM DERGTEGAAG TGAQTLPMET PLVVKIDKPY LLLIYSEKIP
SVLFLGKIVN PIGK

Sequence data:

Serpin A12 OS=Homo sapiens GN=SERPINA12 PE=1 SV=1 SPA12_HUMAN

Intensity Coverage: 38.3 % (124466 cnts), Sequence Coverage MS: 19.6%, Sequence Coverage MS/MS: 19.6% pI (isoelectric point): 9.8

Global Peptide Results

Serpin A12 OS=Homo sapiens GN=SERPINA12 PE=1 SV=1 SPA12_HUMAN
MNPTLGLAIFLAVLLTVKGLLKPSFSPRNYKALSEVQGWKQRMAAKELARQNMDLGFKLLKKLAFYNPGRNIFLSPLSISTAFSMLCLGAQDSTLDEIKQGFNFRKMPEKDLHEGFHYIIHEL
TQKTQDLKLSIGNTLFIDQRLQPQRKFLEDAKNFYSAETILTNFQNLEMAQKQINDFISQKTHGKINNLIENIDPGTVMLLANYIFFRARWKHEFDPNVTKEEDFFLEKNSSVKVPMMFRSGIY
QVGYDDKLSCTILEIPYQKNITAIFILPDEGKLKHLEKGLQVDTFSRWKTLLSRRVVDVSVPRLHMTGTFDLKKTLSYIGVSKIFEEHGDLTKIAPHRSLKVGEAVHKAELKMDERGTEGAAGT
GAQTLPMETPLVVKIDKPYLLLIYSEKIPSVLFLGKIVNPIGK

MW:47145.020

Digest Matches (Score: 573.00), Score = 573.000000, Rank = 1, Database = SwissProt, Accesskey = SPA12_HUMAN
Search Parameters: MS Tol.:150.00 ppm, MSMS Tol.: 0.500000 Da, Enz.Trypsin, Engine: Mascot Version: 2.5.1.3 , DB: SwissProt , DB Version: SwissProt_2016_06.fasta

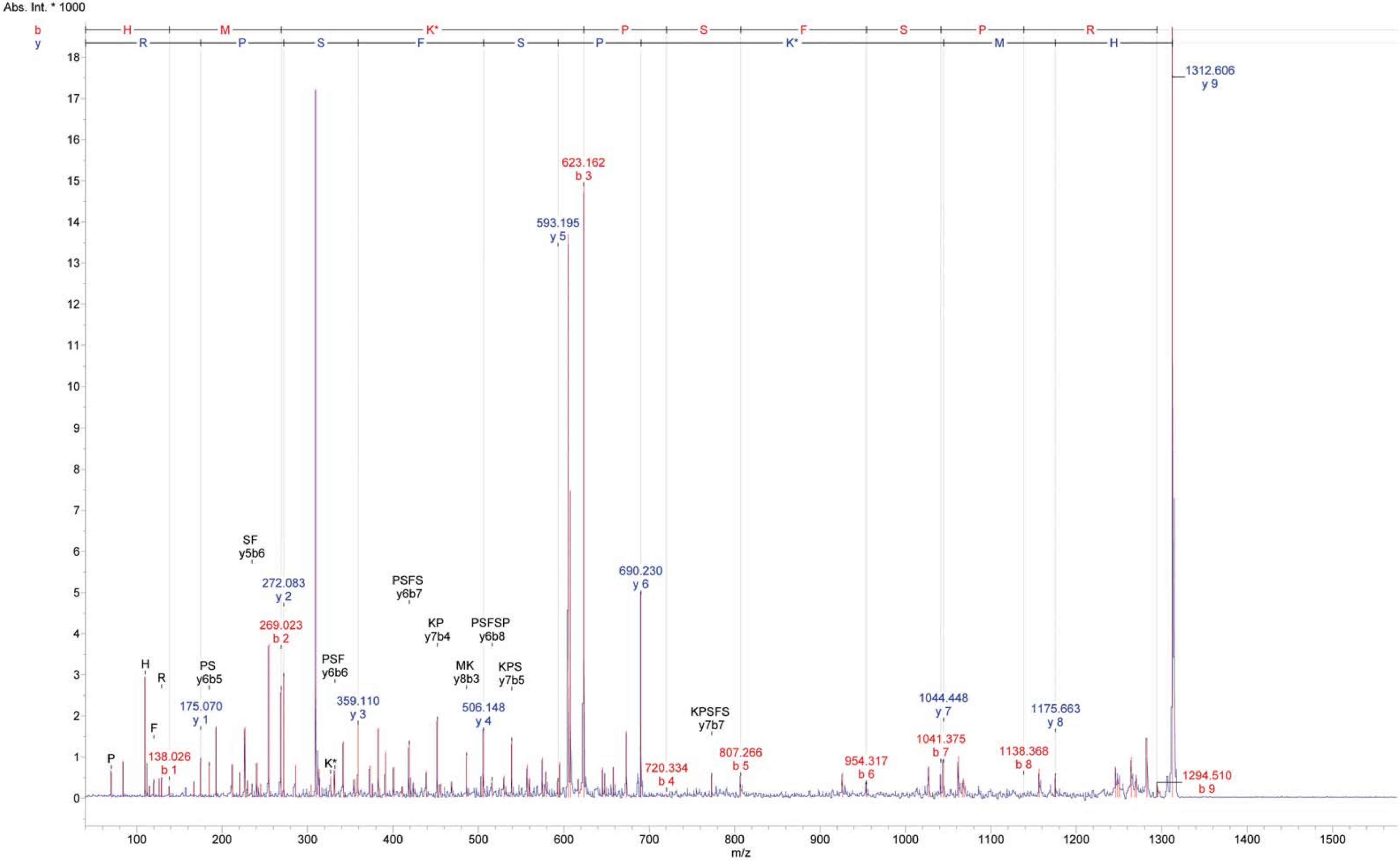
Entries:	Meas. M/z	Calc. MH+	Meas. Mr	Calc. Mr	Int.	z	Dev.(Da)	Dev.(ppm)	Score	Range	P	Sequence
peak 11	1076.547	1076.544	1075.540	1075.537	460.954	1+	0.003	2.403	--	149 - 155	1	KFLEDAK 1: Biotin (K)
MSMS 14	1115.554	1115.570	1114.546	1114.563	18134.196	1+	-0.016	-14.733	27	43 - 50	1	MAAKELAR 4: Biotin (K)
MSMS 15	1129.601	1129.619	1128.594	1128.611	23905.885	1+	-0.018	-15.571	37	295 - 301	1	WKTLLSR 2: Biotin (K)
MSMS 19	1217.543	1217.565	1216.536	1216.558	23375.615	1+	-0.022	-18.233	27	356 - 363	1	AELKMDER 4: Biotin (K)
MSMS 22	1291.639	1291.662	1290.632	1290.654	3660.239	1+	-0.023	-17.624	261	62 - 70	1	KLAFYNPGR 1: Biotin (K)
MSMS 23	1312.602	1312.599	1311.595	1311.592	26602.781	1+	0.003	2.294	7	216 - 224	0	HEFDPNVTK 9: Biotin (K)
MSMS 24	1321.694	1321.718	1320.687	1320.711	1760.167	1+	-0.025	-18.642	512	321 - 330	1	KTLSYIGVSK 1: Biotin (K)
MSMS 26	1335.690	1335.709	1334.683	1334.702	2440.136	1+	-0.019	-14.186	63	346 - 355	1	SLKVGEAVHK 3: Acetyl (K) 10: Biotin (K)
MSMS 34	1521.716	1521.737	1520.709	1520.730	1297.695	1+	-0.022	-14.233	3	233 - 243	1	NSSVKVPMMFR 5: Biotin (K)
MSMS 35	1527.745	1527.774	1526.737	1526.766	1463.165	1+	-0.029	-19.002	10	32 - 42	1	ALSEVQGWKQR 9: Biotin (K)
peak 36	1532.762	1532.796	1531.755	1531.789	838.390	1+	-0.034	-22.132	--	51 - 61	1	QNMDLGFKLLK 8: Biotin (K)
peak 43	1648.779	1648.815	1647.771	1647.808	1194.485	1+	-0.037	-22.176	--	29 - 40	1	NYKALSEVQGWK 3: Biotin (K)
peak 44	1656.008	1655.780	1655.001	1654.773	490.763	1+	0.229	138.124	--	225 - 237	1	EEDFFLEKNSSVK 8: Acetyl (K) 13: Acetyl (K)
MSMS 46	1687.908	1687.935	1686.901	1686.928	16533.205	1+	-0.027	-16.132	268	59 - 70	2	LLKKLAFYNPGR 3: Biotin (K) 4: Acetyl (K)
MSMS 47	1690.791	1690.826	1689.784	1689.818	2325.484	1+	-0.035	-20.453	1	29 - 40	1	NYKALSEVQGWK 3: Acetyl (K) 12: Biotin (K)
peak 51	1871.964	1872.002	1870.957	1870.995	530.131	1+	-0.038	-20.460	--	59 - 70	2	LLKKLAFYNPGR 3: Biotin (K) 4: Biotin (K)
MSMS 52	1974.945	1974.985	1973.938	1973.978	19680.817	1+	-0.040	-20.352	38	29 - 42	2	NYKALSEVQGWKQR 3: Biotin (K) 12: Acetyl (K)
MSMS 53	1979.919	1979.968	1978.912	1978.960	3757.276	1+	-0.049	-24.617	84	349 - 363	2	VGEAVHKAELKMDER 7: Biotin (K) 11: Acetyl (K)
MSMS 54	1988.958	1989.001	1987.951	1987.994	9369.972	1+	-0.043	-21.663	547	331 - 345	1	IFEEHGDLTKIAPHR 10: Biotin (K)
peak 57	2039.026	2039.074	2038.019	2038.067	916.673	1+	-0.048	-23.422	--	280 - 294	2	LKHLEKGLQVDTFSR 2: Acetyl (K) 6: Biotin (K)
peak 58	2048.938	2049.008	2047.931	2048.001	376.512	1+	-0.070	-34.120	--	43 - 58	2	MAAKELARQNMDLGFK 4: Biotin (K)
MSMS 61	2159.015	2159.052	2158.007	2158.045	4288.772	1+	-0.038	-17.558	7	29 - 42	2	NYKALSEVQGWKQR 3: Biotin (K) 12: Biotin (K)
peak 65	2350.148	2350.070	2349.140	2349.062	337.291	1+	0.078	33.191	--	216 - 232	1	HEFDPNVTKEEDFFLEK 9: Biotin (K)
peak 67	2392.138	2392.080	2391.131	2391.073	703.931	1+	0.058	24.147	--	216 - 232	1	HEFDPNVTKEEDFFLEK 9: Acetyl (K) 17: Biotin (K)
peak 70	2533.234	2533.301	2532.226	2532.293	369.122	1+	-0.067	-26.467	--	321 - 340	2	KTLSYIGVSKIFEEHGDLTK 1: Acetyl (K) 10: Biotin (K)
peak 72	2979.477	2979.540	2978.470	2978.532	226.481	1+	-0.062	-20.894	--	322 - 345	2	TLSYIGVSKIFEEHGDLTKIAPHR 9: Acetyl (K) 19: Biotin (K)
peak 73	3149.571	3149.514	3148.564	3148.506	819.331	1+	0.057	18.200	--	150 - 175	1	FLEDAKNFYSAETILTNFQNLEMAQK 6: Acetyl (K) 26: Acetyl (K)
peak 74	3333.647	3333.581	3332.640	3332.573	255.663	1+	0.066	19.900	--	150 - 175	1	FLEDAKNFYSAETILTNFQNLEMAQK 6: Acetyl (K) 26: Biotin (K)

Supplemental Figure 1. (A) A representative mass spectrum of the isolated biotinylated peptides after selective labelling and tryptic digestion. (B) Sequence of human vaspin and sequence coverage of peaks analyzed by MSMS. (C) Example of Mascot Server search result using combined MS and MSMS peaks.

Supplementary Spectrum S1

Spectrum Analysis Report

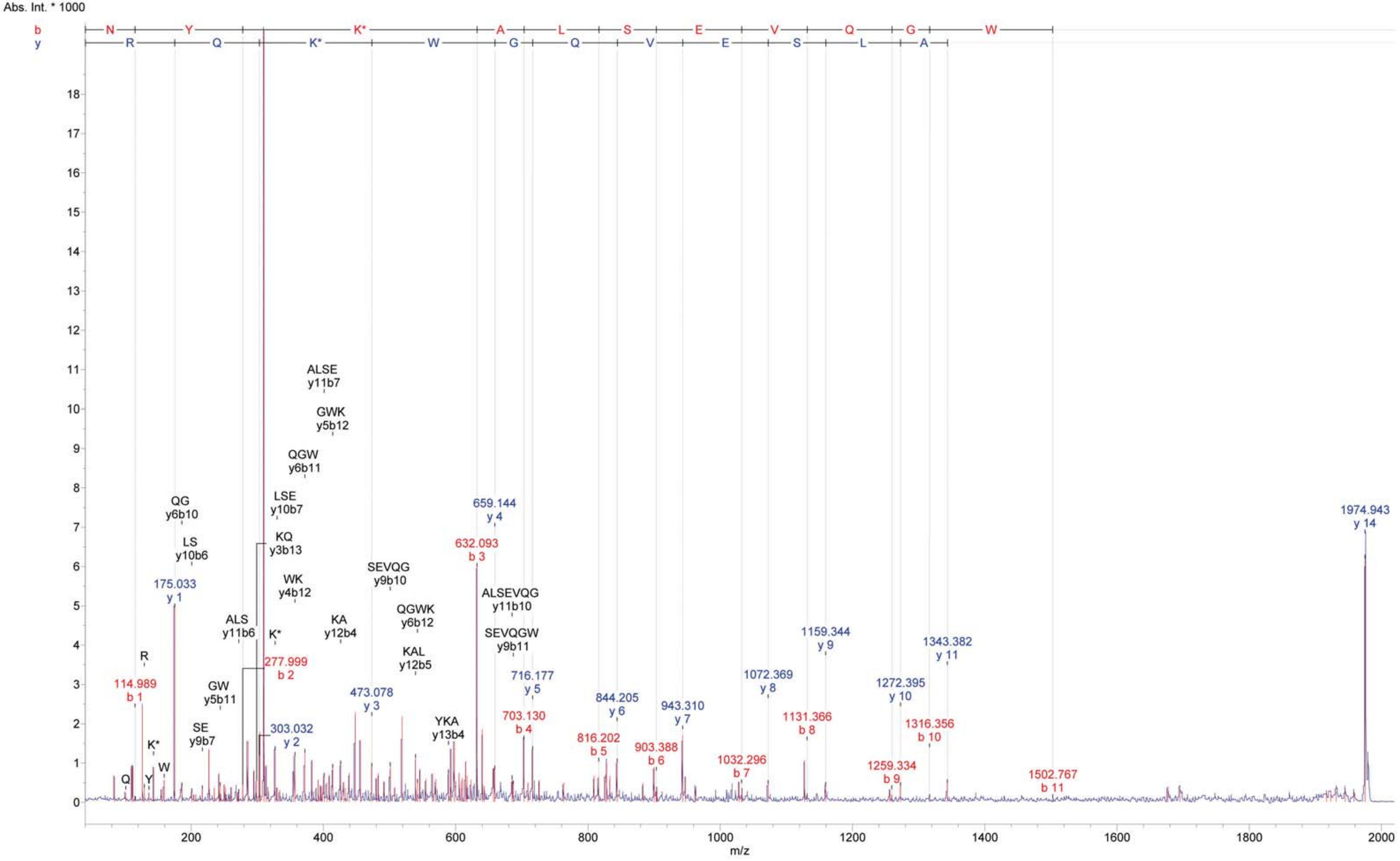
Sequence Name:		Parentmass:	1312.602	Mass Error:	-0.027	MH+ (mono):	1312.629
MH+ (avg):	1313.576	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	88
Above Threshold:	88	Assigned Peaks:	28	Not assigned Peaks:	60		



Spectrum Analysis Report

Supplementary Spectrum S2

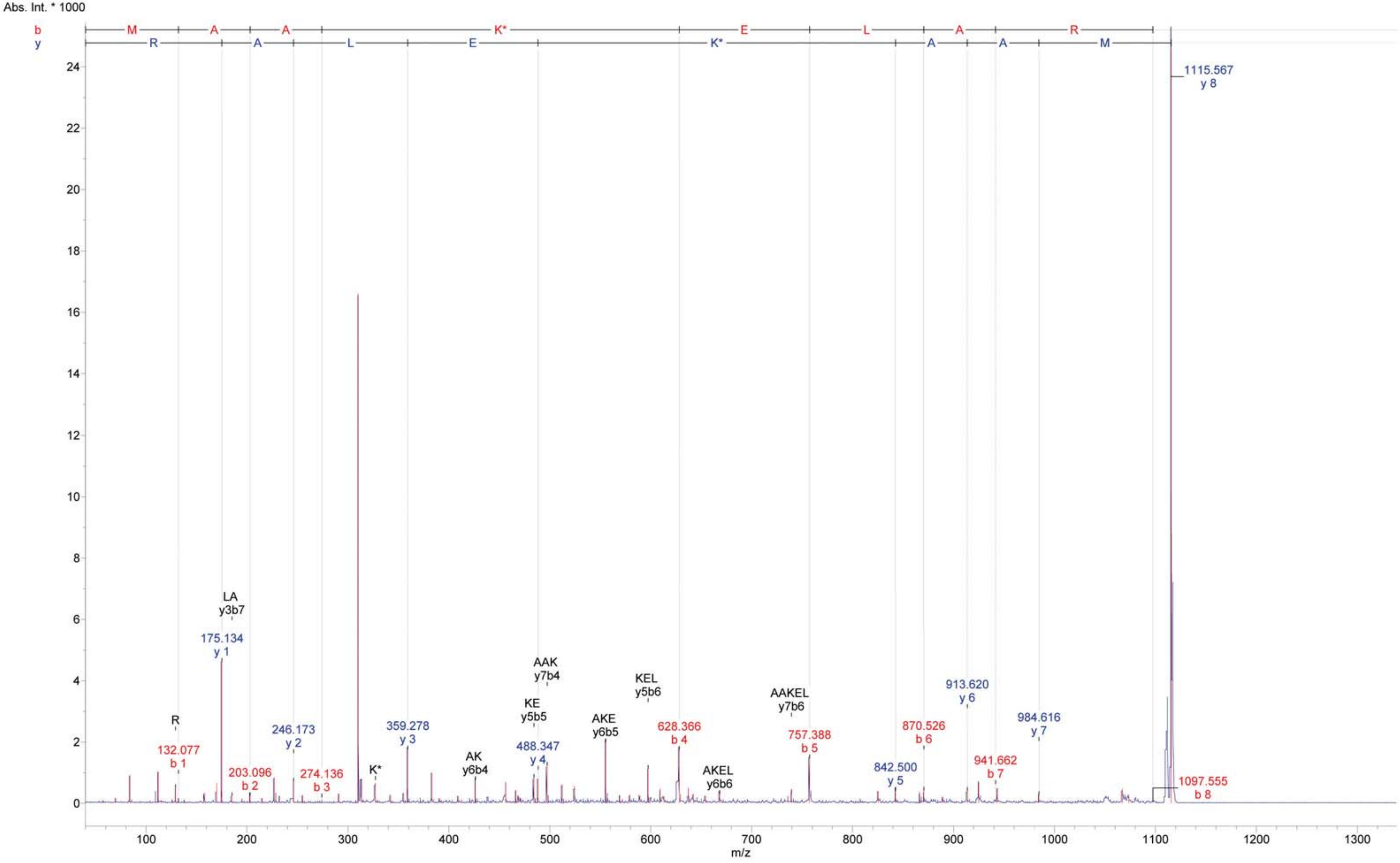
Sequence Name:		Parentmass:	1974.945	Mass Error:	-0.041	MH+ (mono):	1974.986
MH+ (avg):	1976.244	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	126
Above Threshold:	126	Assigned Peaks:	31	Not assigned Peaks:	95		



Spectrum Analysis Report

Supplementary Spectrum S3

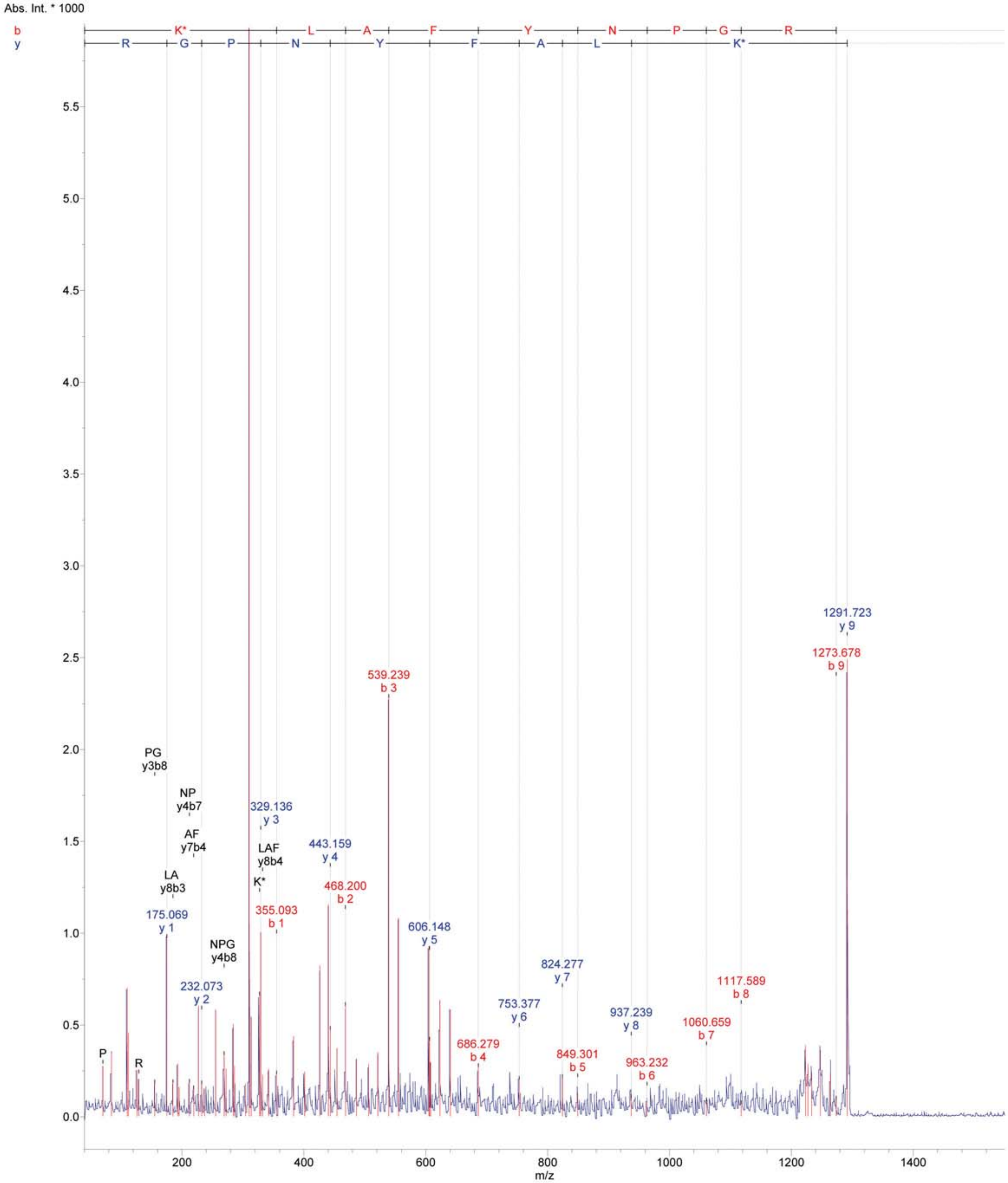
Sequence Name:		Parentmass:	1115.554	Mass Error:	-0.017	MH+ (mono):	1115.571
MH+ (avg):	1116.383	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	71
Above Threshold:	71	Assigned Peaks:	22	Not assigned Peaks:	49		



Spectrum Analysis Report

Supplementary Spectrum S4

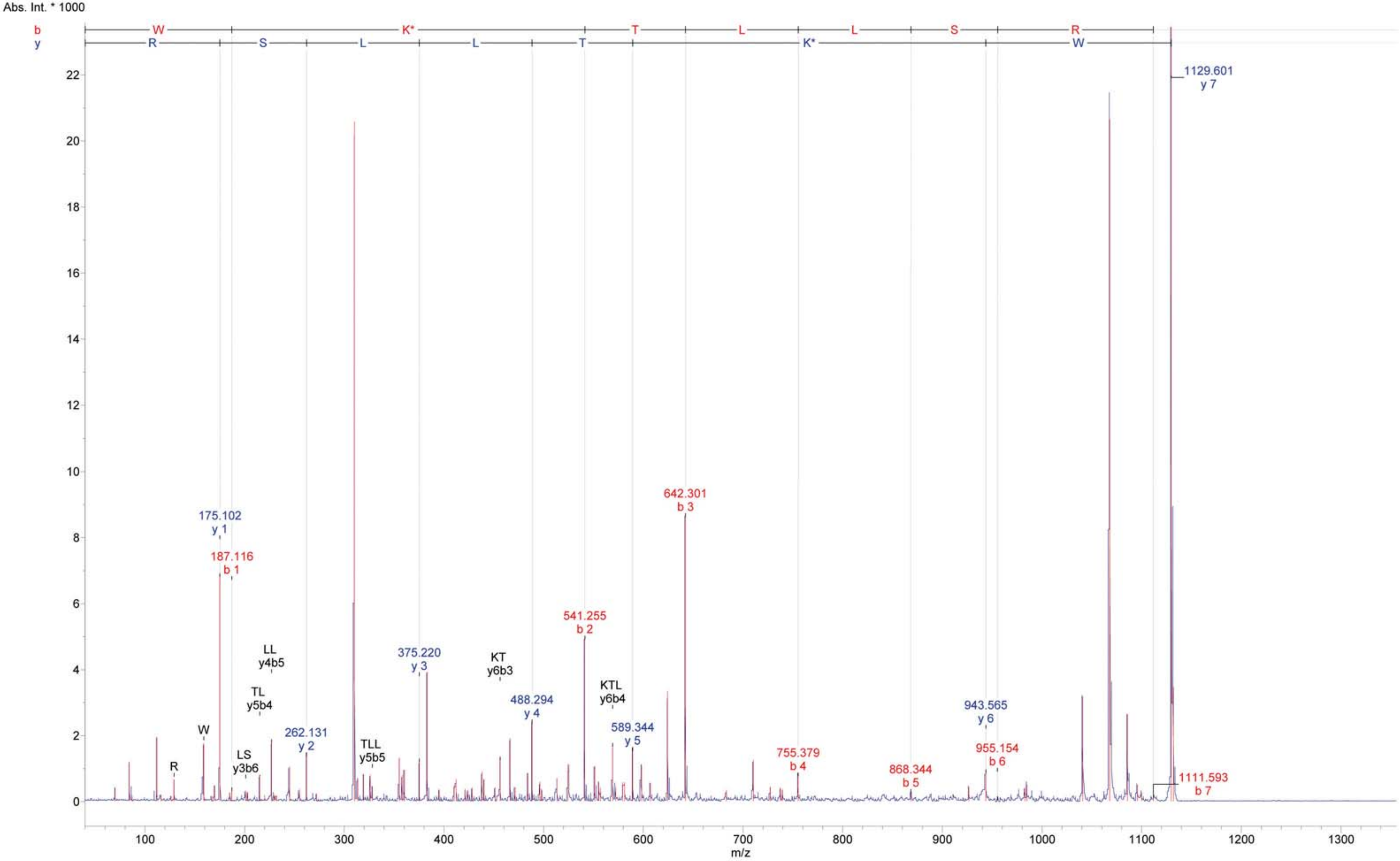
Sequence Name:		Parentmass:	1291.723	Mass Error:	0.061
MH+ (mono):	1291.662	MH+ (avg):	1292.532	Threshold (a.i.):	0.000
Tolerance (Da):	0.500	Number of Peaks:	61	Above Threshold:	61
Assigned Peaks:	23	Not assigned Peaks:	38		



Spectrum Analysis Report

Supplementary Spectrum S5

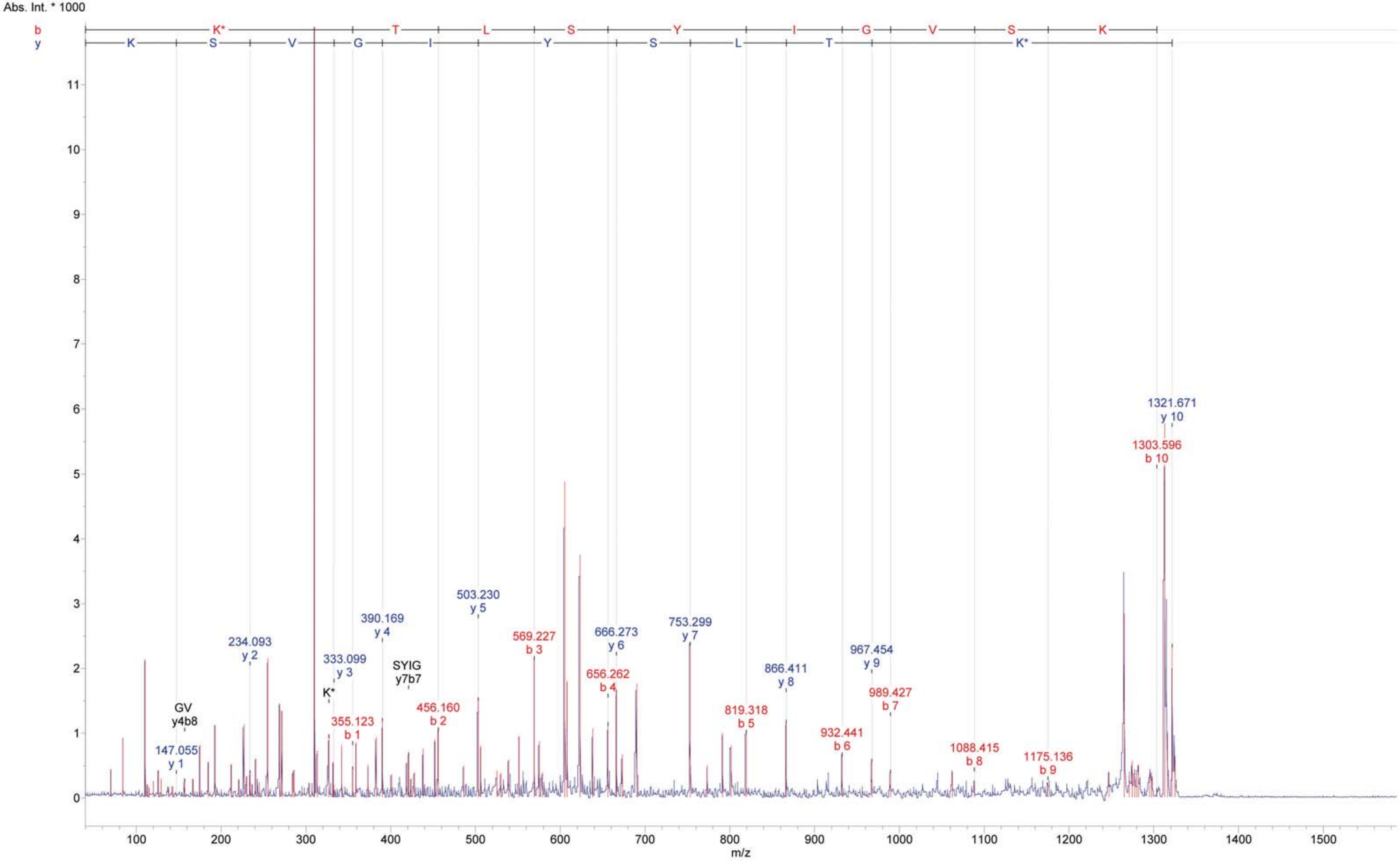
Sequence Name:		Parentmass:	1129.601	Mass Error:	-0.018	MH+ (mono):	1129.619
MH+ (avg):	1130.387	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	85
Above Threshold:	85	Assigned Peaks:	19	Not assigned Peaks:	66		



Spectrum Analysis Report

Supplementary Spectrum S6

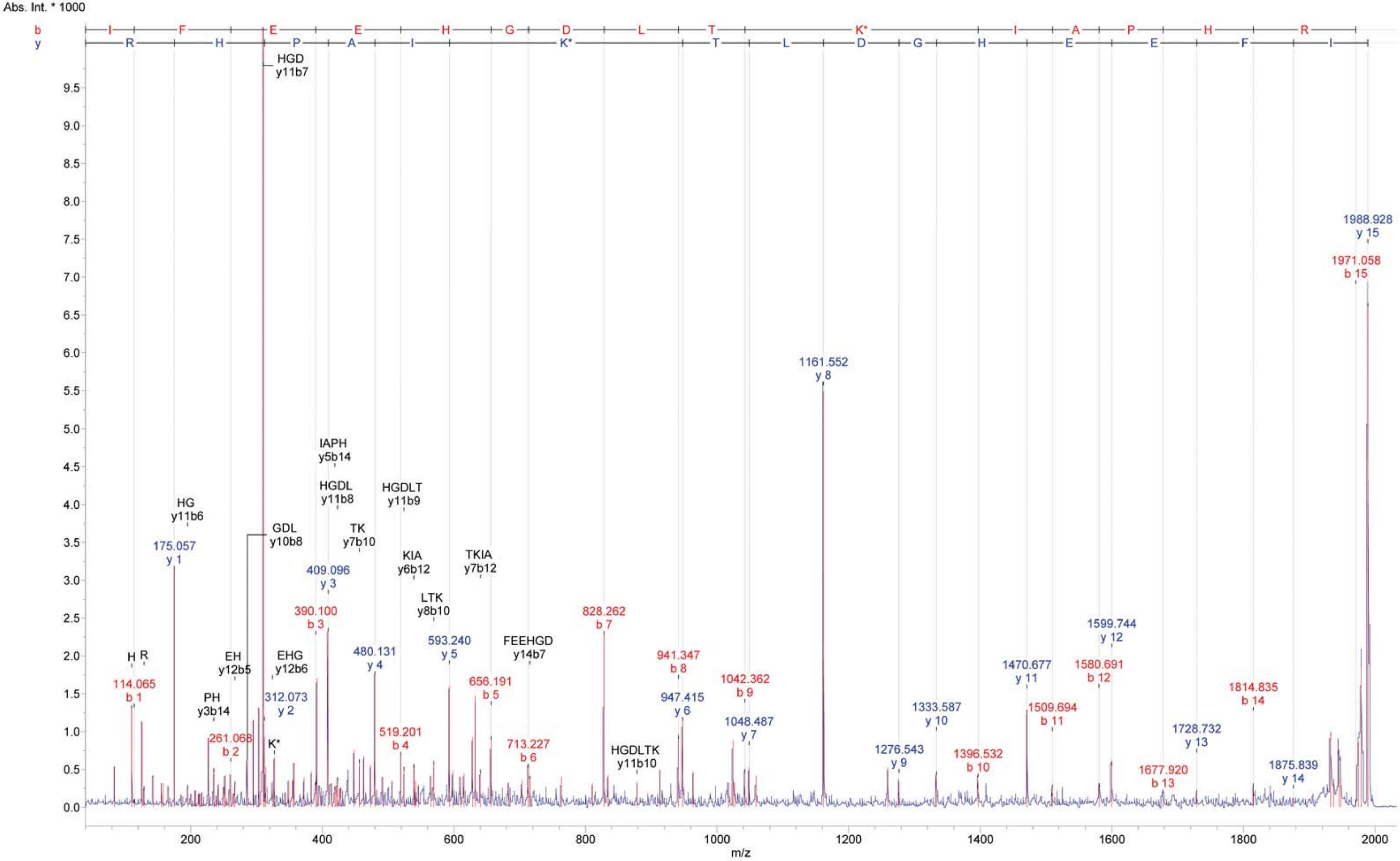
Sequence Name:		Parentmass:	1321.694	Mass Error:	-0.025	MH+ (mono):	1321.719
MH+ (avg):	1322.597	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	93
Above Threshold:	93	Assigned Peaks:	24	Not assigned Peaks:	69		



Spectrum Analysis Report

Supplementary Spectrum S7

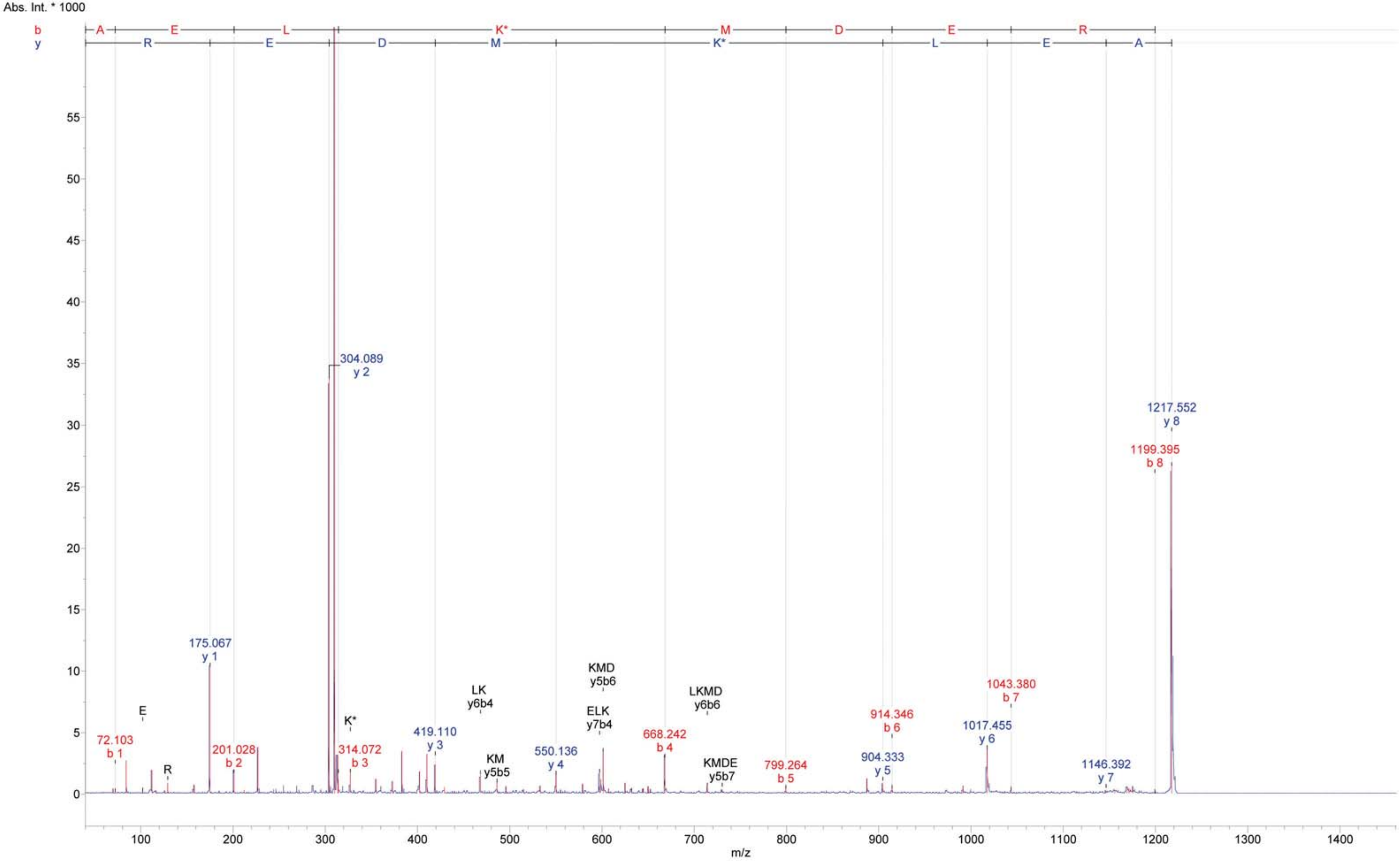
Sequence Name:		Parentmass:	1988.958	Mass Error:	-0.044	MH+ (mono):	1989.002
MH+ (avg):	1990.271	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	113
Above Threshold:	113	Assigned Peaks:	36	Not assigned Peaks:	77		



Spectrum Analysis Report

Supplementary Spectrum S8

Sequence Name:		Parentmass:	1217.543	Mass Error:	-0.023	MH+ (mono):	1217.566
MH+ (avg):	1218.428	Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	59
Above Threshold:	59	Assigned Peaks:	21	Not assigned Peaks:	38		



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