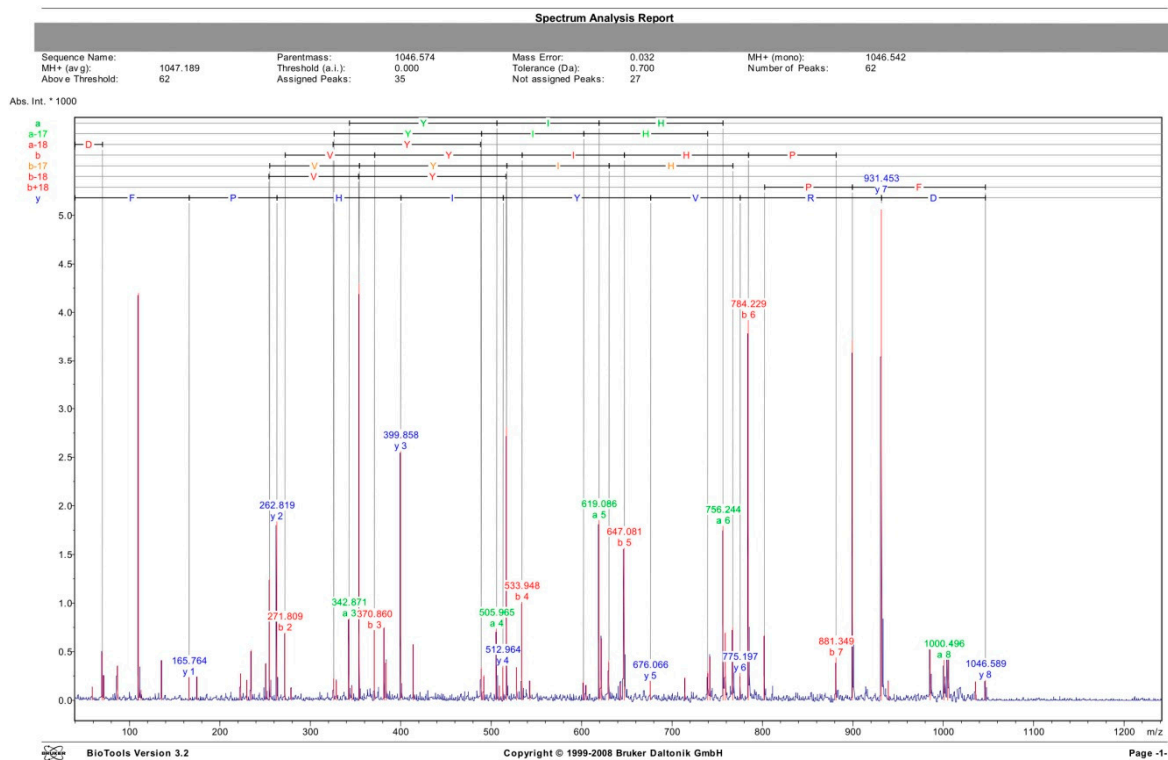


Supplementary Materials: Proteome and Peptidome of *Vipera berus berus* Venom

Aleksandra Bocian, Małgorzata Urbanik, Konrad Hus, Andrzej Łyskowski,
Vladimír Petrilla, Zuzana Andrejčáková, Monika Petrillová and Jaroslav Legath

Selected MS and MS/MS Annotated Spectra used for Protein and Peptide Identification

Area 1. Annotated MS/MS spectrum of ion 1046.574 m/z.



Spectrum Analysis Report

Display Parameter:	Parentmass:	1046.574	Mass Error:	0.032	MH+ (mono):	1046.542	MH+ (avg):	1047.189
Threshold (a.l.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	62	Above Threshold:	62	
Assigned Peaks:	35	Not assigned Peaks:	27					

Peaklist:

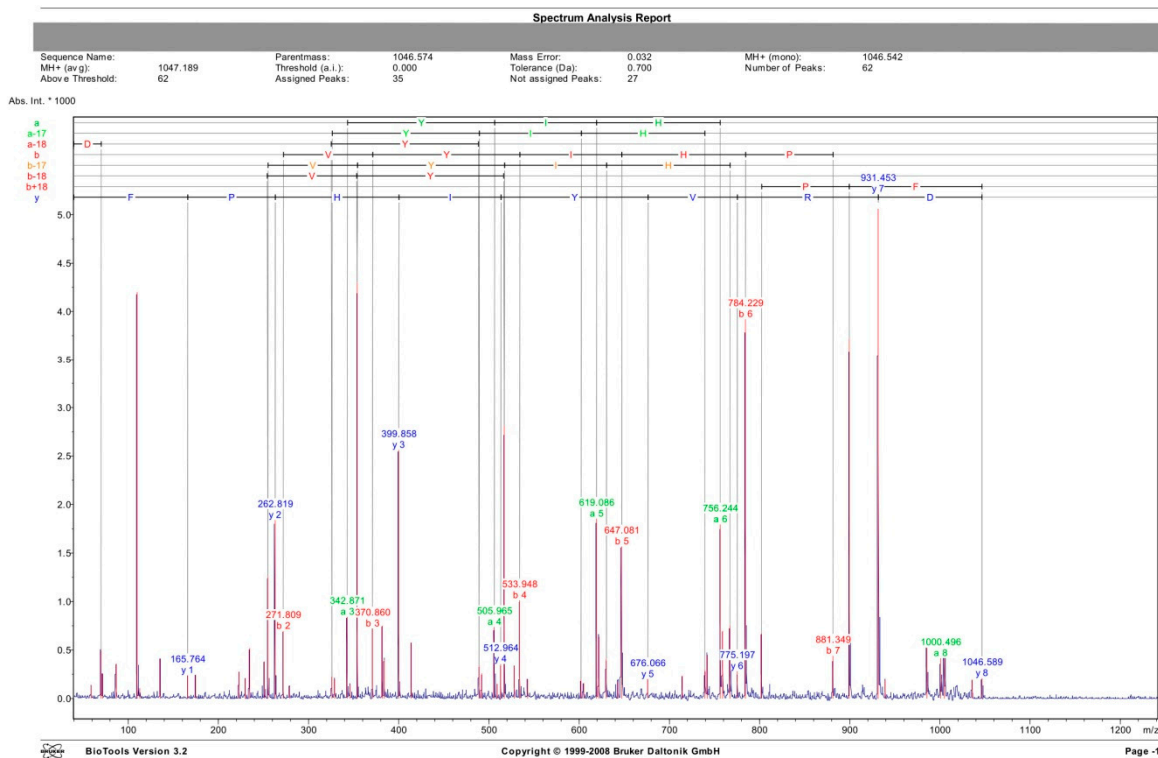
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.841	132.159	2	69.865	498.245	3	71.869	256.271	4	86.850	380.129	5	109.818	4202.408
6	112.824	108.794	7	135.809	411.972	8	165.764	240.044	9	174.821	244.590	10	222.849	276.943
11	229.802	212.178	12	234.807	520.571	13	250.827	384.116	14	254.783	1256.001	15	262.819	1839.622
16	271.809	696.719	17	279.016	127.240	18	325.866	228.955	19	328.915	201.144	20	342.871	843.072
21	346.113	142.528	22	353.853	4297.906	23	370.860	720.896	24	381.850	752.246	25	383.953	400.974
26	399.858	2861.915	27	413.864	577.251	28	488.958	343.859	29	491.980	280.729	30	506.965	738.269
31	509.054	147.996	32	512.964	356.662	33	516.943	2808.390	34	528.238	341.272	35	533.948	1013.366
36	542.879	201.688	37	602.070	197.489	38	605.023	158.256	39	619.086	1853.371	40	622.068	637.158
41	630.088	412.111	42	643.303	172.112	43	647.081	1568.024	44	678.066	199.785	45	714.197	238.801
46	739.214	298.317	47	742.097	451.583	48	756.244	1794.773	49	758.970	700.023	50	767.182	754.570
51	775.197	282.431	52	784.229	3821.564	53	802.274	670.928	54	881.349	441.579	55	899.393	3717.282
56	931.453	5215.078	57	939.297	180.885	58	985.526	528.154	59	1000.496	416.983	60	1004.628	553.061
61	1035.696	191.849	62	1046.589	210.618									

Calculated Masses:
DRVYHPPF

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term.	Ion
1	D	68.039	71.013	70.029	116.034	99.008	98.024	134.045	133.061	88.039	192.066	166.086	149.080	8	F
2	R	244.140	227.114	226.130	272.135	255.199	254.125	290.146	289.162	129.113	289.116	263.139	246.112	7	P
3	V	343.209	326.182	325.198	371.204	354.177	353.193	389.214	388.230	72.081	406.177	400.198	383.171	6	H
4	Y	506.272	489.246	488.262	534.267	517.241	516.257	552.278	551.294	136.076	539.261	513.282	496.255	5	I
5	I	619.356	602.330	601.346	647.351	630.325	629.341	665.362	664.378	86.095	702.325	676.345	659.319	4	V
6	H	756.415	739.389	738.405	784.410	767.383	766.399	802.421	801.437	110.071	801.383	775.414	758.387	3	V
7	P	853.468	836.441	835.457	881.463	864.436	863.452	899.473	898.489	70.065	957.494	931.515	914.488	2	R
8	F	1000.536	983.510	982.526	1028.531	1011.505	1010.521	1046.542	1045.558	120.081	1072.521	1046.542	1029.515	1	D

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Area 1. Annotated MS/MS spectrum of ion 1046.574 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1046.574	Mass Error:	0.032	MH+ (mono):	1046.542	MH+ (avg):	1047.189
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	62	Above Threshold:	62
Assigned Peaks:	35	Not assigned Peaks:	27				

Peaklist:

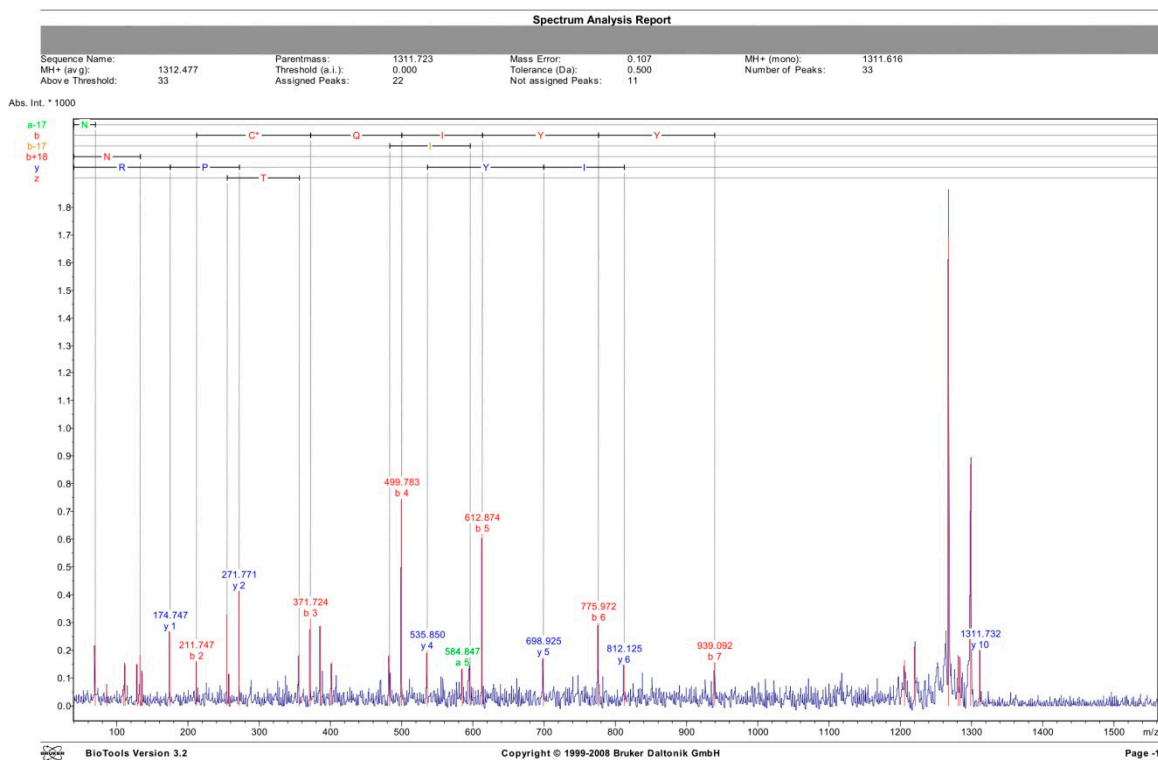
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.841	132.159	2	69.865	498.245	3	71.869	256.271	4	86.850	360.129	5	109.818	4202.408
6	112.824	108.794	7	135.809	411.972	8	165.764	240.044	9	174.821	244.590	10	222.849	278.943
11	229.802	212.178	12	234.807	520.571	13	250.827	384.118	14	254.793	1256.001	15	262.819	1839.622
16	271.809	696.719	17	279.016	127.240	18	325.866	228.955	19	328.915	201.144	20	342.871	843.072
21	348.113	142.528	22	353.853	4291.906	23	370.860	720.696	24	381.850	732.246	25	383.953	400.374
26	399.858	2561.915	27	413.884	577.251	28	488.958	343.859	29	491.980	260.729	30	505.965	738.269
31	509.054	147.996	32	512.964	356.662	33	516.943	2808.390	34	528.238	341.272	35	533.948	1013.366
36	542.879	201.688	37	602.070	197.489	38	605.023	158.256	39	610.086	1853.371	40	622.068	637.158
41	630.068	412.111	42	643.303	172.112	43	647.061	1568.024	44	676.066	199.785	45	714.197	238.801
46	739.214	298.317	47	742.097	451.583	48	756.244	1794.773	49	758.970	700.023	50	767.182	754.870
51	775.197	282.431	52	784.229	3921.564	53	802.274	670.928	54	861.349	441.576	55	899.393	3712.292
56	931.453	5215.078	57	939.297	190.885	58	985.525	525.154	59	1000.496	416.983	60	1004.629	553.061
61	1035.696	191.849	62	1046.589	210.618									

Calculated Masses:
DRVYHFP

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	D	88.039	71.013	70.029	116.034	99.008	98.024	134.045	133.061	88.039	192.066	166.086	149.060	8	F
2	R	244.140	227.114	225.130	272.135	255.109	254.125	290.148	289.162	129.113	289.118	283.139	245.112	7	P
3	V	343.209	326.182	325.198	371.204	354.177	353.193	389.214	388.230	72.081	426.177	400.198	383.171	6	H
4	Y	506.272	489.246	488.262	534.267	517.241	516.257	552.278	551.294	136.076	539.261	513.282	496.255	5	I
5	I	619.356	602.330	601.346	647.351	630.325	629.341	665.362	664.378	85.061	702.325	678.345	659.319	4	V
6	H	756.415	739.389	738.405	784.410	767.383	766.399	802.421	801.437	110.071	801.393	775.414	758.387	3	V
7	P	853.468	836.441	835.457	881.463	864.436	863.452	899.473	898.489	70.065	957.494	931.515	914.488	2	R
8	F	1000.536	983.510	982.526	1028.531	1011.505	1010.521	1046.542	1045.558	120.051	1072.521	1046.542	1029.515	1	D

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Area 2. Annotated MS/MS spectrum of ion 1311.723 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1311.723	Mass Error:	0.107	MH+ (mono):	1311.616	MH+ (avg):	1312.477
Threshold (a.i.):	0.000	Tolerance (Da):	0.500	Number of Peaks:	33	Above Threshold:	33
Assigned Peaks:	22	Not assigned Peaks:	11				

Peaklist:

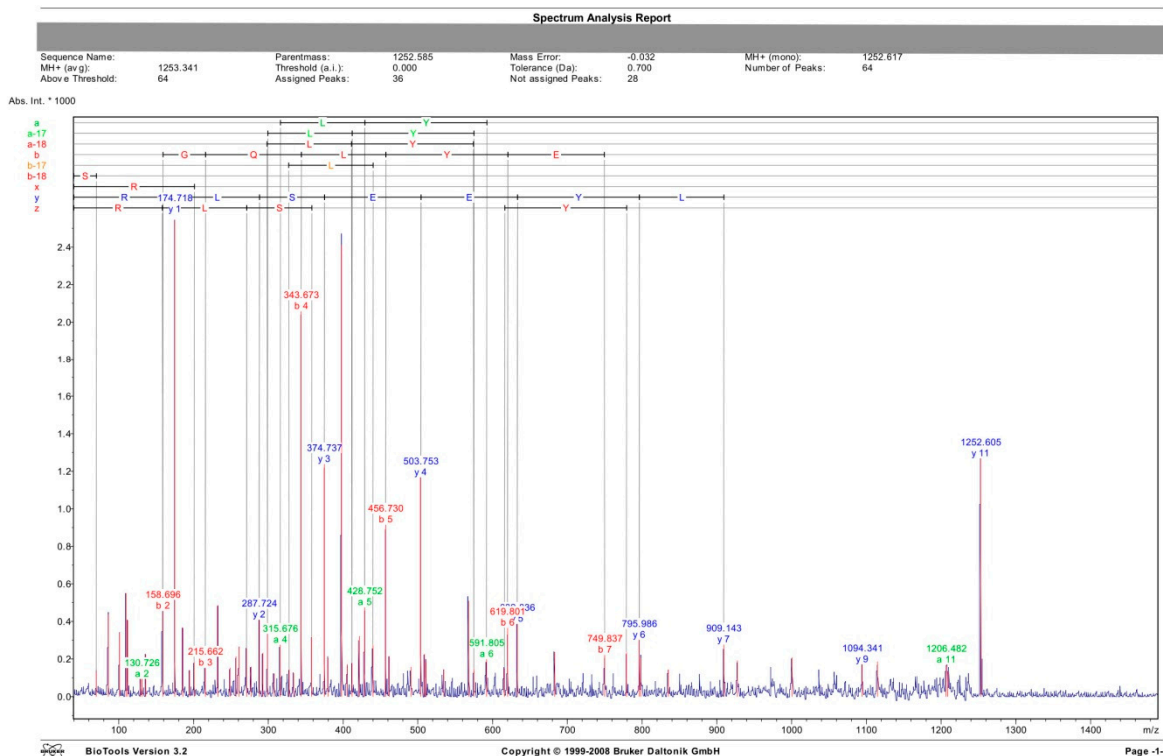
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.928	221.927	2	85.806	79.441	3	109.711	75.361	4	111.788	149.492	5	126.783	150.830
6	132.713	179.870	7	135.737	119.601	8	174.747	267.735	9	211.747	150.403	10	254.741	331.830
11	257.697	115.933	12	271.771	414.368	13	355.763	188.594	14	371.724	314.998	15	385.741	289.759
16	401.811	157.259	17	482.749	186.716	18	499.783	747.129	19	535.850	198.157	20	584.847	137.353
21	595.894	136.118	22	612.874	618.606	23	698.925	175.176	24	775.972	239.355	25	812.125	147.509
26	939.092	158.080	27	1205.820	164.722	28	1220.642	208.929	29	1267.723	1694.006	30	1281.290	178.477
31	1283.834	165.243	32	1298.428	870.607	33	1311.732	200.803						

Calculated Masses:
NPCQIYYTPR 3: Carbamidomethyl (C)

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term.	Ion
1	N	87.055	70.029	69.045	115.050	98.024	97.040	133.061	132.077	87.055	201.098	175.119	158.092	10	R
2	P	154.108	167.082	166.097	212.103	195.078	194.092	230.114	229.130	70.065	298.151	272.112	255.145	9	P
3	C*	344.139	327.112	326.128	372.134	355.107	354.123	390.144	389.160	133.043	399.199	373.219	356.193	8	T
4	Q	472.197	455.171	454.187	500.192	483.166	482.182	518.203	517.219	101.071	562.262	536.283	519.256	7	Y
5	I	585.281	568.255	567.271	613.278	596.250	595.266	631.287	630.303	86.096	725.325	699.346	682.320	6	V
6	V	748.345	731.318	730.334	776.340	759.313	758.329	794.350	793.366	136.076	838.409	812.430	795.404	5	I
7	Y	911.408	894.381	893.397	939.403	922.376	921.392	957.413	956.429	136.076	966.468	940.489	923.462	4	Q
8	T	1072.456	985.429	984.445	1040.451	1023.424	1022.440	1058.461	1057.477	74.060	1128.499	1100.519	1083.493	3	C*
9	P	1109.508	1092.482	1091.498	1137.503	1120.477	1119.493	1155.514	1154.530	70.065	1223.551	1197.572	1180.546	2	P
10	R	1265.610	1248.583	1247.599	1293.604	1276.578	1275.594	1311.615	1310.631	129.113	1337.594	1311.615	1294.588	1	N

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Area 3. Annotated MS/MS spectrum of ion 1252.585 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1252.585	Mass Error:	-0.032	MH+ (mono):	1252.617	MH+ (avg):	1253.341
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	64	Above Threshold:	64
Assigned Peaks:	36	Not assigned Peaks:	28				

Peaklist:

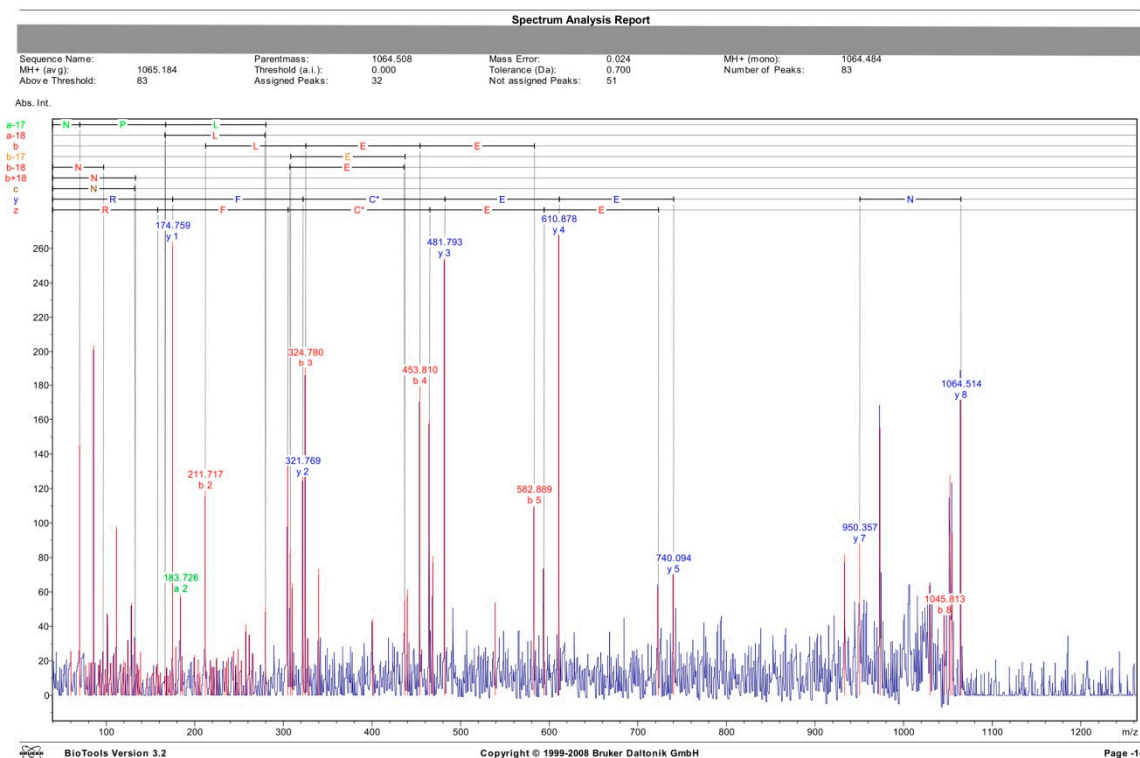
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.793	135.494	2	85.803	438.962	3	100.752	338.743	4	109.733	551.573	5	111.746	406.852
6	126.762	146.589	7	130.726	93.744	8	135.722	225.852	9	158.696	456.966	10	174.718	293.821
11	185.678	366.654	12	194.656	141.682	13	200.702	184.725	14	215.662	153.937	15	232.689	487.120
16	248.676	154.192	17	256.686	214.025	18	260.701	267.899	19	270.728	257.021	20	276.706	160.398
21	287.724	409.669	22	292.652	234.192	23	298.708	398.223	24	307.695	123.763	25	315.676	278.524
26	327.670	145.902	27	333.704	124.761	28	343.673	2058.408	29	357.737	317.547	30	374.737	1238.367
31	379.718	207.077	32	397.713	2414.096	33	406.704	173.086	34	411.765	180.553	35	421.679	322.944
36	428.752	475.771	37	439.745	274.262	38	456.730	915.905	39	461.749	215.266	40	480.681	159.437
41	503.753	1167.013	42	508.712	227.421	43	510.749	186.775	44	534.723	142.266	45	567.820	511.059
46	574.803	148.092	47	591.805	199.786	48	616.795	152.153	49	619.801	366.533	50	632.836	387.671
51	692.823	238.330	52	749.837	222.777	53	778.801	236.575	54	795.986	302.993	55	798.106	297.631
56	834.961	144.367	57	909.143	277.815	58	927.356	192.851	59	1000.338	209.194	60	1094.341	171.618
61	1114.832	187.700	62	1206.482	169.273	63	1208.635	137.338	64	1252.605	1268.629			

Calculated Masses:
SAGOLYEESLR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	S	60.044	43.018	42.034	88.039	71.013	70.029	106.050	105.068	60.044	201.098	175.119	158.092	11	R
2	A	131.682	114.055	113.071	159.078	142.050	141.068	177.087	176.103	44.049	314.182	288.263	271.176	10	L
3	G	188.103	171.076	170.092	216.098	199.071	198.087	234.108	233.124	30.034	401.214	375.235	358.208	9	S
4	Q	316.162	298.135	296.151	344.156	327.130	326.146	362.167	361.183	101.071	530.257	504.278	487.251	8	E
5	L	429.246	412.219	411.235	457.241	440.214	439.230	475.251	474.267	85.096	659.299	633.320	616.294	7	E
6	Y	592.309	575.282	574.298	620.304	603.277	602.293	638.314	637.330	136.076	822.363	796.384	779.357	6	Y
7	E	721.352	704.325	703.341	749.346	732.320	731.336	767.357	766.373	102.055	935.447	909.468	892.441	5	L
8	E	850.394	833.368	832.384	878.389	861.362	860.378	896.400	895.416	102.055	1063.505	1037.526	1020.500	4	Q
9	S	937.426	920.400	919.416	965.421	948.395	947.411	983.432	982.448	60.044	1120.527	1094.548	1077.521	3	G
10	L	1050.510	1033.484	1032.500	1078.505	1061.479	1060.495	1096.516	1095.532	86.096	1191.564	1165.585	1148.558	2	A
11	R	1206.611	1189.585	1188.601	1234.606	1217.580	1216.596	1252.617	1251.633	129.113	1278.596	1252.617	1235.590	1	S

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Area 3. Annotated MS/MS spectrum of ion 1064.508 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1064.508 Mass Error: 0.024 MH+ (mono): 1064.484 MH+ (avg): 1065.184
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 83 Above Threshold: 83
 Assigned Peaks: 32 Not assigned Peaks: 51

Peaklist:

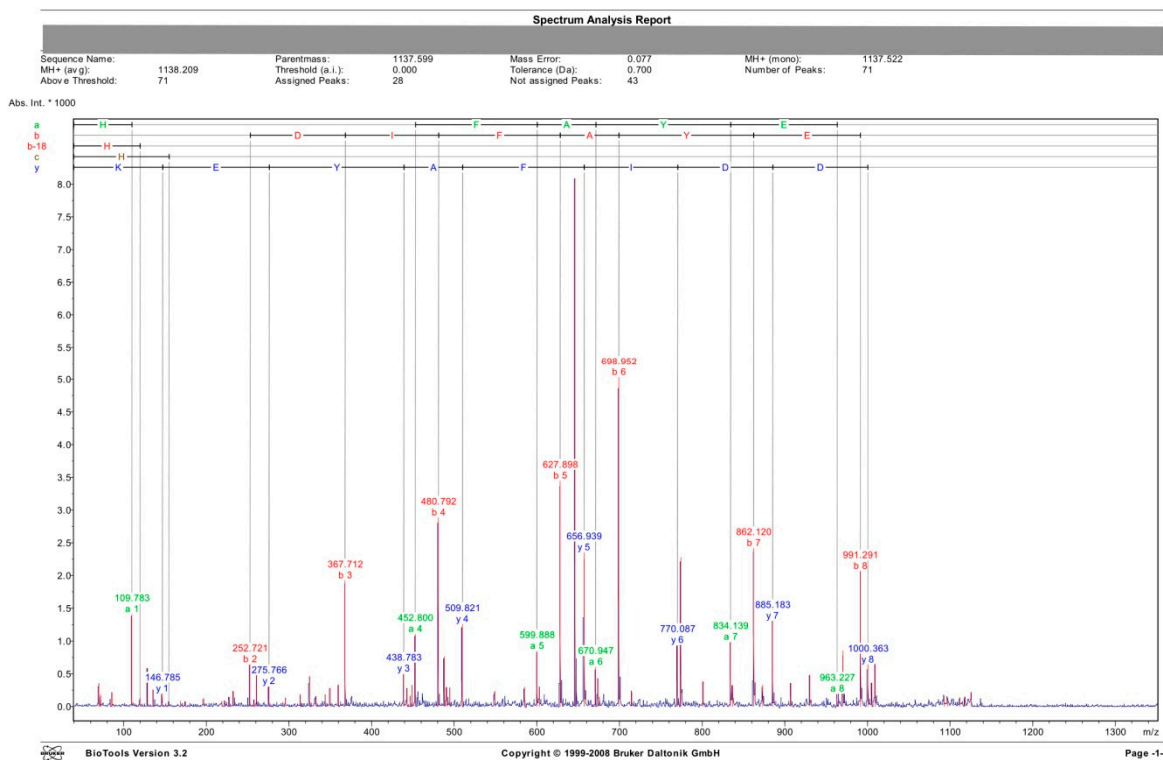
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	60.244	25.829	2	69.831	146.353	3	76.808	17.785	4	80.478	19.302	5	83.242	19.259
6	85.843	203.847	7	92.069	17.536	8	93.560	20.800	9	96.481	26.940	10	99.095	13.705
11	101.773	46.706	12	105.260	18.978	13	108.103	23.720	14	111.774	98.051	15	116.275	17.429
16	119.758	20.607	17	121.422	19.005	18	124.745	32.325	19	128.781	53.917	20	132.729	31.032
21	135.837	17.423	22	138.896	16.450	23	138.787	28.555	24	148.706	13.223	25	152.650	13.314
26	156.336	16.739	27	157.744	18.637	28	161.242	12.627	29	168.403	11.393	30	168.359	16.344
31	169.859	11.886	32	172.148	13.538	33	174.759	264.002	34	178.747	28.279	35	183.726	58.898
36	186.071	14.588	37	189.770	23.572	38	203.843	20.876	39	205.622	13.133	40	211.717	118.753
41	217.731	20.555	42	219.858	16.293	43	222.124	16.535	44	224.745	22.043	45	233.432	16.590
46	235.771	20.259	47	237.850	22.170	48	243.706	25.953	49	246.428	18.179	50	248.732	27.237
51	252.810	20.279	52	257.655	41.150	53	261.741	35.557	54	263.778	23.887	55	279.713	51.611
56	304.734	138.202	57	307.737	85.650	58	309.800	65.216	59	321.769	126.729	60	324.780	190.096
61	327.729	33.494	62	339.747	73.822	63	400.719	44.322	64	436.799	55.904	65	439.775	61.426
66	453.810	179.437	67	464.758	160.465	68	468.796	80.861	69	481.793	254.271	70	538.869	54.192
71	582.889	110.102	72	593.890	72.511	73	610.878	267.784	74	722.907	62.891	75	740.094	70.207
76	933.296	81.916	77	950.357	87.996	78	973.299	155.280	79	1029.648	65.588	80	1045.813	46.454
81	1052.186	127.770	82	1054.765	94.357	83	1064.514	171.377						

Calculated Masses:
 NPLEEFR b. Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-16	b	b-17	b-16	b-15	b-14	c	i	x	y	z	C-Term	Ion
1	N	87.055	78.029	69.045	115.050	98.024	97.040	133.061	132.077	87.055	201.098	348.167	175.119	158.092	6	R
2	P	184.108	167.082	166.097	212.103	195.076	194.092	230.114	229.130	70.065	348.167	322.187	305.161	7	F	
3	L	297.192	280.166	279.182	325.187	308.160	307.176	343.198	342.214	86.096	508.197	482.218	465.191	8	C*	
4	E	428.235	409.208	408.224	454.230	437.203	436.219	472.240	471.256	102.055	637.240	611.261	594.234	9	E	
5	E	555.277	538.251	537.267	583.272	566.246	565.262	601.283	600.299	102.055	786.282	740.303	723.277	4	E	
6	C*	715.308	696.281	695.297	743.303	726.276	725.292	761.313	760.329	133.043	879.367	853.387	836.361	3	L	
7	F	862.376	845.350	844.366	890.371	873.345	872.361	908.382	907.398	120.051	976.419	950.440	933.413	2	P	
8	R	1018.477	1001.451	1000.467	1046.472	1029.446	1028.462	1064.483	1063.499	129.113	1090.462	1064.483	1047.456	1	N	

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Area 3. Annotated MS/MS spectrum of ion 1137.599 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1137.599	Mass Error:	0.077	MH+ (mono):	1137.522	MH+ (avg):	1138.209
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	71	Above Threshold:	71
Assigned Peaks:	28	Not assigned Peaks:	43				

Peaklist:

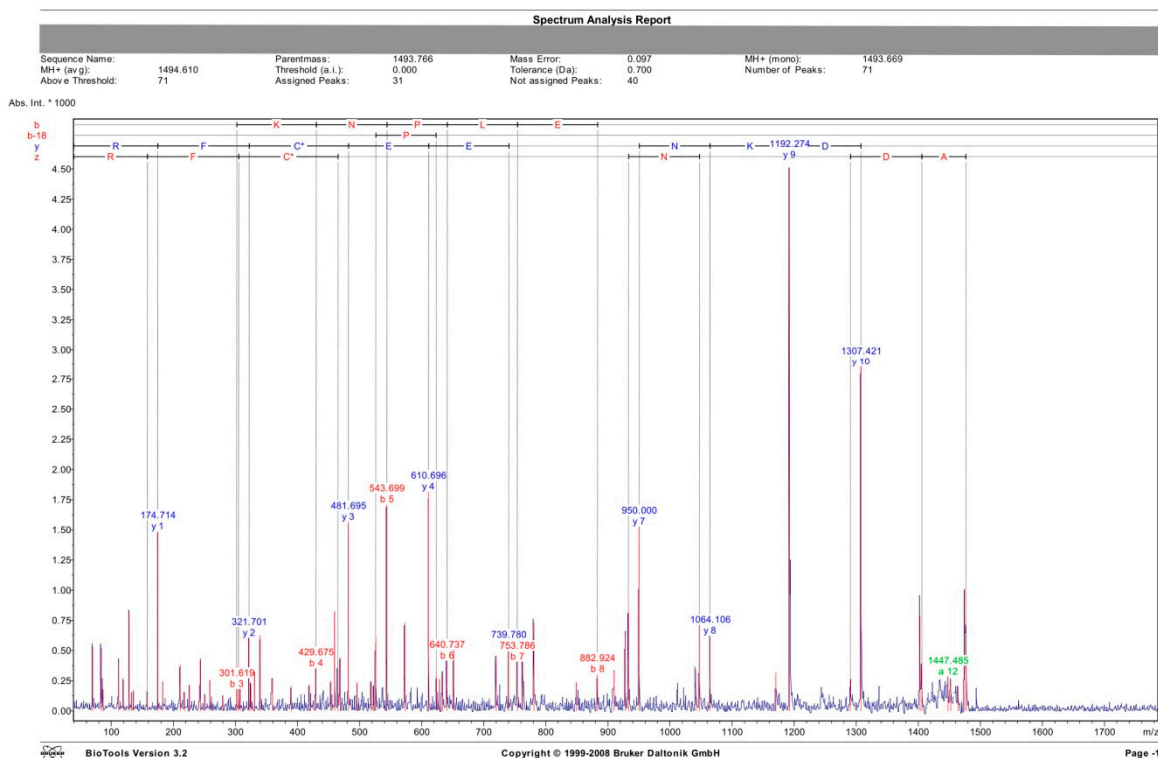
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.816	343.836	2	71.826	189.351	3	83.828	113.505	4	85.829	216.619	5	109.783	1410.460
6	119.786	127.164	7	128.786	588.410	8	135.784	256.266	9	146.785	196.534	10	154.743	80.691
11	168.819	82.002	12	174.764	77.173	13	196.786	131.240	14	218.746	83.513	15	222.754	93.353
16	227.822	147.788	17	232.785	238.738	18	252.721	645.376	19	257.774	107.832	20	260.760	643.451
21	275.766	311.945	22	285.766	137.382	23	313.777	193.026	24	324.846	446.919	25	332.818	161.681
26	343.741	187.793	27	349.788	284.947	28	359.808	334.088	29	367.712	1927.375	30	438.783	501.639
31	442.828	285.223	32	446.796	167.186	33	448.823	318.048	34	452.800	1107.542	35	480.792	2886.692
36	487.839	769.128	37	490.794	299.923	38	494.721	291.238	39	509.821	1258.117	40	548.937	238.976
41	584.968	301.358	42	599.888	846.409	43	602.952	307.497	44	627.898	3449.228	45	646.015	8251.069
46	656.939	2354.501	47	670.947	604.765	48	673.901	426.309	49	698.952	5032.405	50	714.705	219.482
51	770.087	938.651	52	774.153	2281.561	53	801.863	384.730	54	834.139	686.599	55	836.802	323.125
56	862.120	2420.739	57	873.230	335.233	58	885.183	1308.410	59	907.301	361.966	60	930.213	489.515
61	963.227	193.910	62	970.304	857.672	63	991.291	2068.049	64	1000.363	639.914	65	1005.259	363.334
66	1009.321	659.582	67	1082.536	172.839	68	1097.087	136.056	69	1111.640	131.236	70	1117.472	157.670
71	1125.811	210.636												

Calculated Masses:
HDDIFAYEK

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	H	110.071	93.045	92.061	138.066	121.040	120.056	156.077	155.093	110.071	173.092	147.113	130.086	9	K
2	D	225.098	208.072	207.088	253.093	236.067	235.083	271.104	270.120	88.039	302.135	276.155	259.129	8	E
3	D	340.125	323.099	322.115	368.120	351.094	350.110	386.131	385.147	83.059	465.198	439.219	422.192	7	Y
4	I	453.209	436.183	435.199	481.204	464.178	463.194	499.215	498.231	86.096	536.235	510.256	493.229	6	A
5	F	600.278	583.251	582.267	628.273	611.246	610.262	646.283	645.299	120.081	683.304	657.324	640.298	5	F
6	A	671.315	654.289	653.304	699.310	682.283	681.299	717.320	716.336	44.049	796.388	770.408	753.382	4	I
7	Y	834.378	817.352	816.368	862.373	845.346	844.362	880.384	879.400	136.076	911.415	885.435	868.409	3	D
8	E	963.421	946.394	945.410	991.416	974.389	973.405	1009.426	1008.442	102.055	1028.441	1000.462	983.436	2	D
9	K	1091.516	1074.489	1073.505	1119.511	1102.484	1101.500	1137.521	1136.537	101.107	1163.500	1137.521	1120.495	1	H

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Area 3. Annotated MS/MS spectrum of ion 1493.766 m/z.



Spectrum Analysis Report

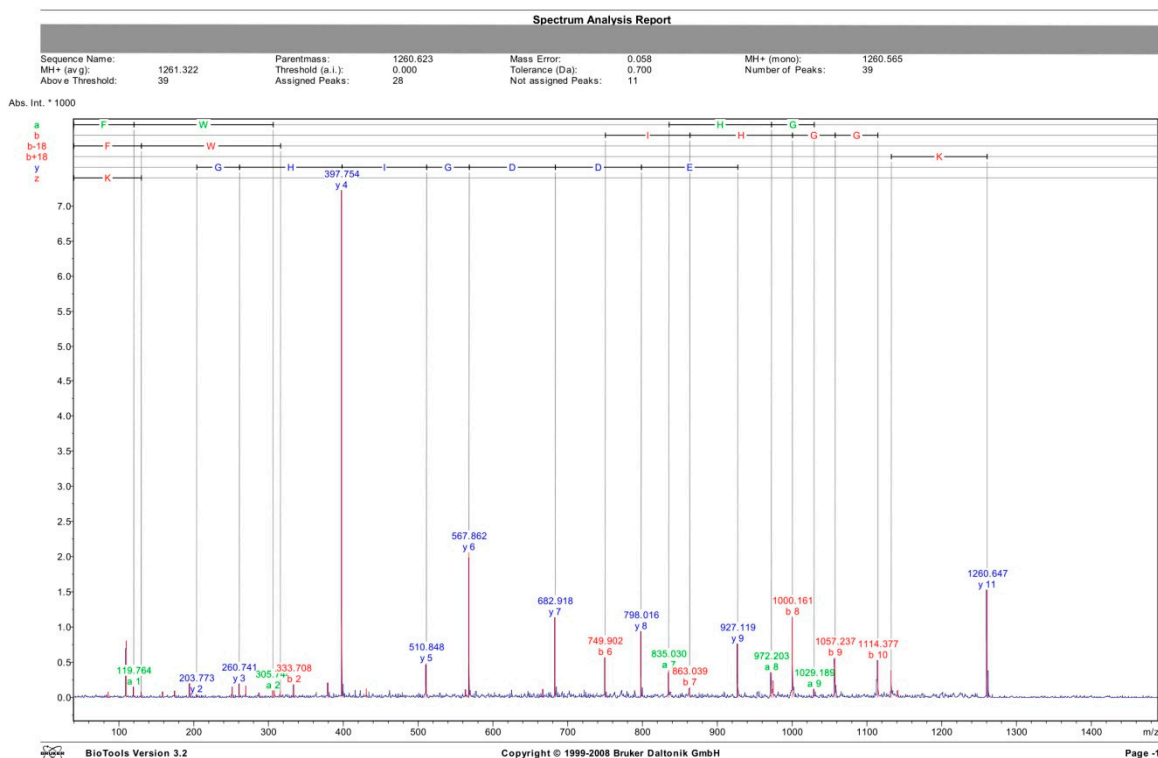
Display Parameter: Parentmass: 1493.766 Mass Error: 0.097 MH+ (mono): 1493.669 MH+ (avg): 1494.610
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 71
 Assigned Peaks: 31 Not assigned Peaks: 40 Above Threshold: 71

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.786	535.000	2	83.780	522.353	3	86.759	179.815	4	111.736	404.479	5	119.744	252.616
6	126.742	814.149	7	132.718	147.264	8	135.679	158.545	9	157.700	157.081	10	174.714	1487.122
11	182.743	245.937	12	210.719	383.533	13	217.698	158.171	14	225.698	215.399	15	243.679	433.203
16	250.686	137.867	17	258.613	259.311	18	279.669	122.667	19	301.619	179.997	20	304.683	379.614
21	307.668	225.272	22	321.701	603.562	23	324.723	223.328	24	330.746	321.783	25	338.707	625.370
26	359.608	270.042	27	389.695	206.157	28	418.643	220.812	29	429.675	352.456	30	453.716	251.210
31	459.744	828.781	32	464.678	349.062	33	466.696	441.304	34	481.695	1565.615	35	495.677	238.176
36	518.698	248.053	37	522.642	214.592	38	525.687	616.799	39	543.699	1710.060	40	572.607	731.432
41	610.696	1816.242	42	623.742	299.958	43	628.750	265.302	44	633.667	331.401	45	640.737	414.690
46	651.638	951.091	47	719.840	457.348	48	739.780	497.298	49	753.786	406.528	50	762.730	503.373
51	780.748	735.241	52	848.942	238.046	53	882.024	303.847	54	909.848	324.258	55	927.860	628.996
56	932.935	832.334	57	950.000	1527.053	58	1041.118	341.143	59	1047.057	738.955	60	1064.106	622.161
61	1170.363	319.204	62	1192.274	4574.991	63	1290.335	265.616	64	1307.421	2854.830	65	1402.620	791.963
66	1405.563	368.177	67	1447.485	262.744	68	1452.054	245.644	69	1463.647	204.076	70	1474.443	1016.820
71	1477.958	407.507												

Calculated Masses:
 ADDKNPLEECFR 10: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	A	44.049	27.023	26.039	72.044	55.018	54.034	90.055	89.071	44.049	201.088	175.119	158.092	12	R
2	D	159.076	142.050	141.066	187.071	170.045	169.061	205.082	204.098	88.039	348.167	322.187	305.161	11	F
3	D	214.103	257.077	256.093	302.098	285.072	284.088	320.109	319.125	88.039	508.197	482.216	465.191	10	C*
4	K	402.198	385.172	384.188	430.193	413.167	412.183	448.204	447.220	101.107	637.240	611.261	594.234	9	E
5	N	516.241	499.215	498.231	544.236	527.210	526.226	562.247	561.263	87.055	766.282	740.303	723.277	8	E
6	P	613.294	596.267	595.283	641.289	624.262	623.278	659.299	658.315	70.065	879.307	853.327	836.301	7	L
7	L	726.378	709.352	708.368	754.373	737.346	736.362	772.384	771.400	86.096	976.419	950.440	933.413	6	P
8	E	855.421	838.394	837.410	883.416	866.389	865.405	901.426	900.442	102.055	1090.462	1064.483	1047.456	5	N
9	E	984.463	967.437	966.453	1012.458	995.432	994.448	1030.469	1029.485	102.055	1218.537	1192.578	1175.551	4	K
10	C*	1144.494	1127.467	1126.483	1172.489	1155.462	1154.478	1190.499	1189.515	133.043	1333.584	1307.605	1290.578	3	D
11	F	1291.562	1274.536	1273.552	1319.557	1302.531	1301.547	1337.568	1336.584	120.081	1448.611	1422.632	1405.605	2	D
12	R	1447.663	1430.637	1429.653	1475.658	1458.632	1457.648	1493.669	1492.685	129.113	1519.648	1493.669	1476.642	1	A

Area 3. Annotated MS/MS spectrum of ion 1260.623 m/z.



Spectrum Analysis Report

Display Parameter:		Parentmass:	1260.623	Mass Error:	0.058	MH+ (mono):	1260.565	MH+ (avg):	1261.322
		Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	39	Above Threshold:	39
		Assigned Peaks:	28	Not assigned Peaks:	11				

Peaklist:

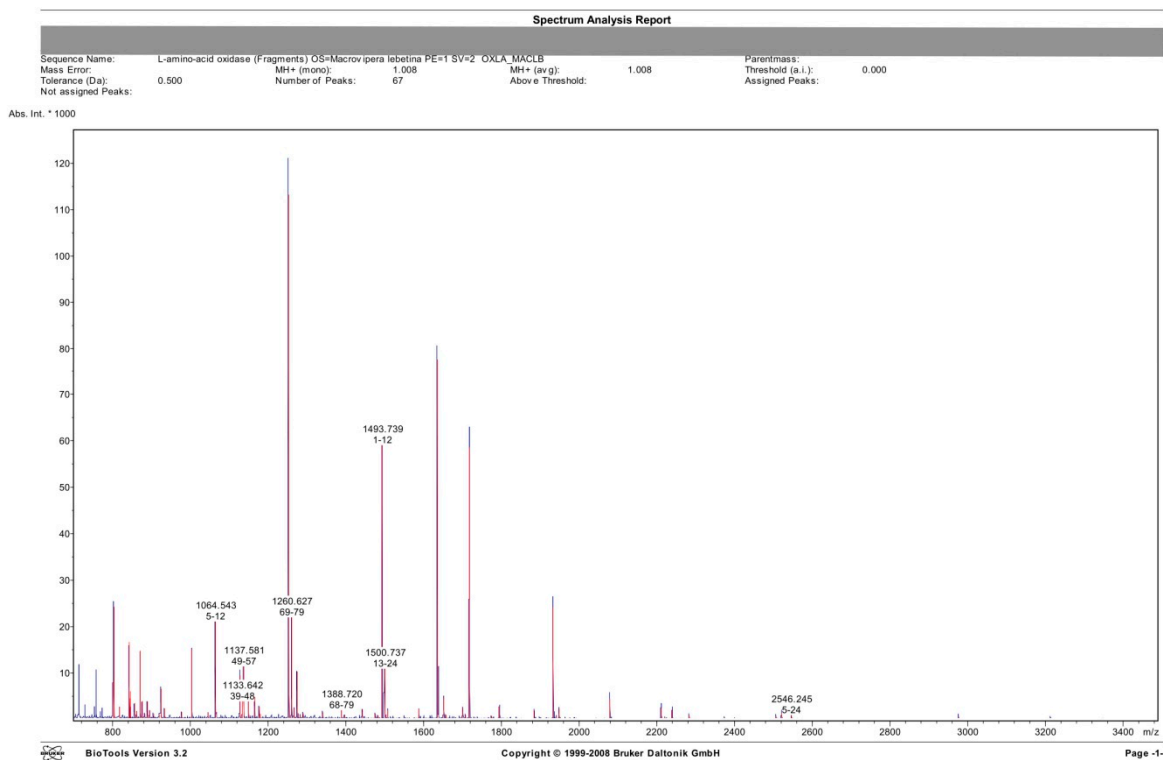
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	83.763	41.274	2	85.811	76.589	3	109.761	809.766	4	119.764	153.613	5	129.722	78.582
6	158.744	83.771	7	174.703	97.548	8	194.716	242.710	9	203.773	44.434	10	251.676	152.532
11	260.741	197.775	12	269.701	167.081	13	287.677	67.138	14	305.744	97.987	15	307.727	139.552
16	315.684	94.405	17	333.708	187.865	18	379.733	216.777	19	397.754	7226.385	20	430.733	127.606
21	510.848	484.471	22	563.788	114.094	23	567.862	2363.657	24	666.890	121.382	25	862.918	1142.320
26	749.902	573.819	27	798.016	940.423	28	835.030	389.138	29	863.039	142.839	30	927.119	765.625
31	972.203	358.851	32	974.751	206.653	33	1000.161	1145.100	34	1029.189	120.803	35	1057.237	567.054
38	1114.377	529.165	37	1132.371	380.499	38	1141.247	108.700	39	1260.647	1530.961			

Calculated Masses:
FWDDGHHGK

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	F	120.081	103.054	102.070	148.076	131.049	130.065	166.086	165.102	120.081	173.092	147.113	130.086	11	K
2	W	306.160	289.134	288.150	334.155	317.128	316.144	352.166	351.182	199.092	230.114	204.134	187.108	10	G
3	E	435.203	418.176	417.192	463.198	446.171	445.187	481.208	480.224	102.055	287.135	261.156	244.129	9	G
4	D	550.230	533.203	532.219	578.225	561.198	560.214	596.235	595.251	88.039	424.194	398.215	381.188	8	H
5	D	665.257	648.230	647.246	693.251	676.225	675.241	711.262	710.278	88.039	537.278	511.299	494.272	7	I
6	G	722.278	705.251	704.267	750.273	733.246	732.262	768.284	767.299	30.034	594.299	568.320	551.294	6	G
7	I	835.302	818.275	817.292	863.307	846.280	845.296	881.308	880.324	88.096	709.326	683.347	666.321	5	D
8	H	972.421	955.394	954.410	1000.416	983.389	982.405	1018.426	1017.442	110.071	824.353	798.374	781.348	4	D
9	G	1029.442	1012.415	1011.432	1057.437	1040.411	1039.427	1075.448	1074.464	30.034	953.396	927.417	910.390	3	E
10	G	1086.454	1069.427	1068.443	1114.459	1097.432	1096.448	1132.469	1131.485	30.034	1139.475	1113.496	1096.469	2	W
11	K	1214.559	1197.532	1196.548	1242.554	1225.527	1224.543	1260.564	1259.580	101.107	1286.544	1260.564	1243.538	1	F

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Area 3. Annotated MS spectrum 1.



Spectrum Analysis Report

Sequence data:
 L-amino-acid oxidase (Fragments) OS=Macrospira lebetina PE=1 SV=2 OXLA_MACLB
 Intensity Coverage: 21.5 % (131184 cnts) Sequence Coverage MS: 51.4%
 Sequence Coverage MS/MS: 0.0% pl (isoelectric point): 4.4

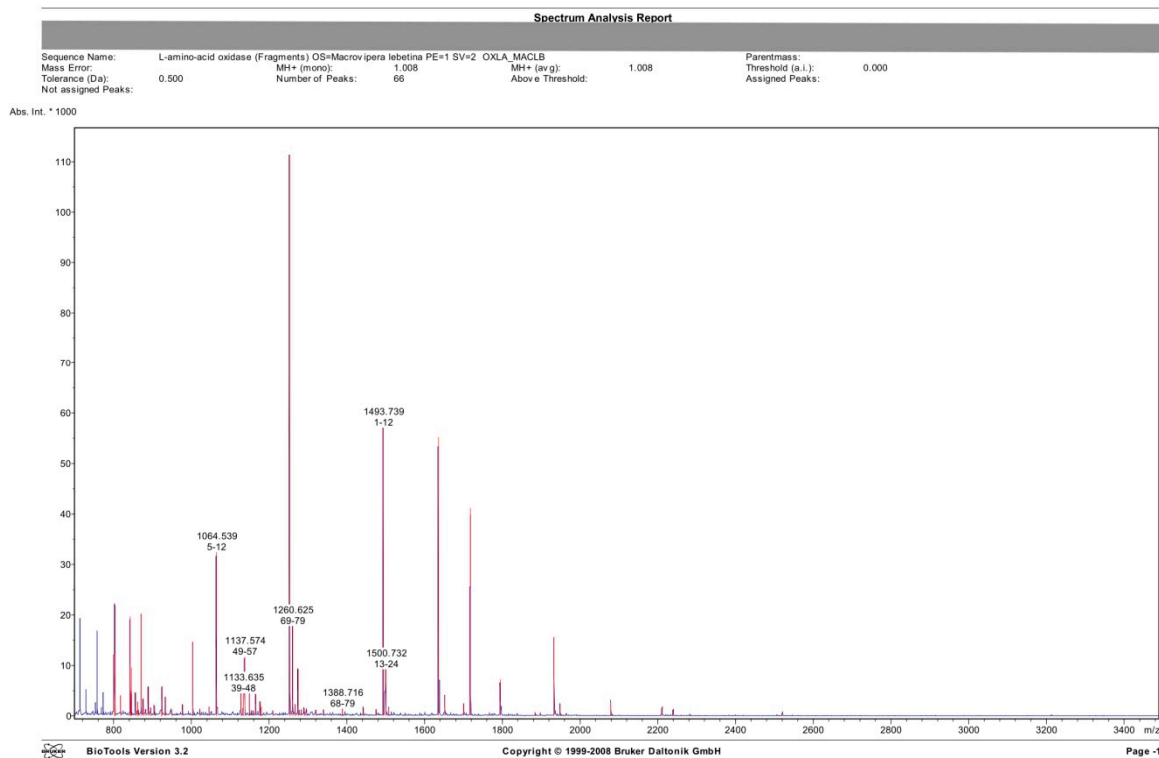
10	20	30	40	50	60	70	80	90	100	110
A D D P N P L E E C F R E D D T E F L E I A N G L E G W Y A N L G P N R Y V R P E E G E H D D I F A Y E F D E I V G H D K K F W E D D I H O O R E T F C Y S P M I Q K P Y Q P H F S E A L T A P V G R										

Display Parameter:
 Sequence Name: L-amino-acid oxidase (Fragments) OS=Macrospira lebetina PE=1 SV=2 OXLA_MACLB
 MH+ (avg): 1.008 Threshold (a.l.): 0.000 Tolerance (Da): 0.500 MH+ (mono): 1.008
 Number of Peaks: 67

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	801.544	3154.699	2	803.477	24198.183	3	817.521	2388.171	4	842.562	16942.805	5	844.535	4548.800
6	845.570	6055.236	7	856.578	3534.049	8	861.549	1715.237	9	870.597	14836.669	10	876.492	3665.253
11	882.522	1181.345	12	889.600	3842.561	13	895.526	1919.414	14	905.572	1229.809	15	918.540	1147.030
16	924.576	6562.769	17	933.630	2404.758	18	977.659	1574.993	19	1003.602	12566.076	20	1045.620	1523.909
21	1064.543	21060.262	22	1127.640	9495.382	23	1133.642	3880.082	24	1137.581	11422.342	25	1149.583	6874.682
26	1165.761	4850.660	27	1177.647	2751.347	28	1179.667	1220.383	29	1252.681	113235.987	30	1260.627	21960.865
31	1266.694	2382.128	32	1274.651	10294.676	33	1282.612	925.895	34	1290.638	1527.183	35	1340.685	1537.644
36	1388.720	1981.743	37	1396.814	878.548	38	1442.764	2144.462	39	1475.749	1213.376	40	1482.748	829.603
41	1493.739	59010.808	42	1500.737	10912.461	43	1507.750	1951.552	44	1587.834	2225.570	45	1636.834	77655.189
46	1651.825	4656.694	47	1657.845	380.359	48	1700.863	2457.596	49	1707.851	680.602	50	1717.908	36538.424
51	1774.922	757.596	52	1784.888	2825.612	53	1884.888	1898.947	54	1932.977	24085.264	55	1941.005	663.420
56	1948.969	2276.209	57	2079.979	4356.947	58	2211.188	2466.645	59	2221.206	423.256	60	2238.218	2044.002
61	2293.256	843.197	62	2313.263	402.427	63	2506.283	679.562	64	2521.318	1335.951	65	2546.245	935.866
66	2975.413	620.349	67	3212.642	295.400									

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Area 3. Annotated MS spectrum 2.



Spectrum Analysis Report

Sequence data:
 L-amino-acid oxidase (Fragments) OS=Macropira lebetina PE=1 SV=2 OXLA_MACLB
 Intensity Coverage: 23.1 % (134117 cnts) Sequence Coverage MS: 51.4%
 Sequence Coverage MS/MS: 0.0% pl (isoelectric point): 4.4

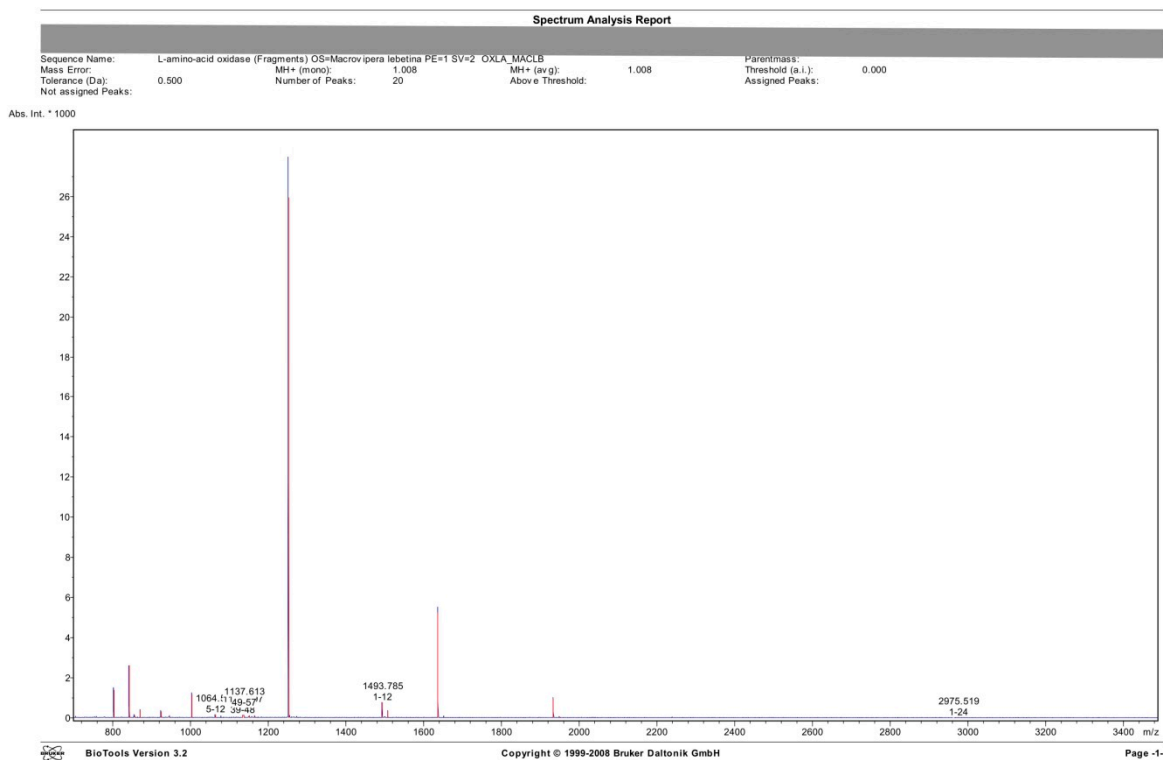
10	20	30	40	50	60	70	80	90	100	110
ADDYMPLEEC FREDDEYFL KIAENGLGV YANLGNRP VPRSEGGND DIFAYEYDE IVGGHDKRYV EDDGIHQRE TFCYSPMIQR FYQGFHSEA LTAIPVGR										

Display Parameter:
 Sequence Name: L-amino-acid oxidase (Fragments) OS=Macropira lebetina PE=1 SV=2 OXLA_MACLB MH+ (mono): 1.008
 MH+ (avg): 1.008 Threshold (a.i.): 0.000 Tolerance (Da): 0.500 MH+ (mono): 1.008
 Number of Peaks: 66

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	801.539	12485.222	2	803.469	21929.975	3	817.517	4051.369	4	842.557	19704.285	5	844.522	5000.734
6	845.566	9625.394	7	856.572	4644.810	8	861.541	2813.328	9	864.542	1327.577	10	870.594	20315.984
11	876.490	3599.005	12	882.611	1308.186	13	889.601	5601.339	14	895.521	1628.658	15	906.568	2017.214
16	922.570	1153.900	17	924.571	5911.921	18	933.628	3829.197	19	949.597	1224.110	20	977.656	2239.856
21	1003.599	14751.471	22	1021.685	1323.635	23	1045.676	1803.749	24	1064.539	32428.353	25	1127.635	8299.172
26	1133.635	4451.103	27	1137.574	11719.966	28	1145.577	4776.456	29	1159.568	685.724	30	1165.756	4264.772
31	1177.641	2892.538	32	1179.655	1865.111	33	1209.678	983.587	34	1252.676	114487.674	35	1260.625	17794.880
36	1266.689	2196.371	37	1274.646	9249.011	38	1282.609	1237.011	39	1290.634	1577.765	40	1296.629	1263.277
41	1320.650	1198.349	42	1340.676	1103.543	43	1389.716	1416.180	44	1442.767	1607.002	45	1475.763	1394.902
46	1493.739	57068.551	47	1500.732	9239.986	48	1507.746	1641.049	49	1635.830	55216.924	50	1657.823	3967.873
51	1700.875	2502.849	52	1717.907	41154.163	53	1766.840	601.329	54	1794.882	7257.849	55	1884.971	544.302
56	1897.770	666.198	57	1932.976	15665.156	58	1948.968	2344.735	59	1964.968	456.660	60	2079.079	2622.723
61	2211.181	1551.388	62	2239.215	1123.448	63	2283.240	333.280	64	2506.269	191.921	65	2521.315	644.461
66	3212.620	96.315												

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Area 3. Annotated MS spectrum 3.



Spectrum Analysis Report

Sequence data:
 L-amino-acid oxidase (Fragments) OS=Macropipera lebetina PE=1 SV=2 OXLA_MACLB
 Intensity Coverage: 4.1% (1659 cnts) Sequence Coverage MS: 40.2%
 Sequence Coverage MS/MS: 0.0% pI (isoelectric point): 4.4

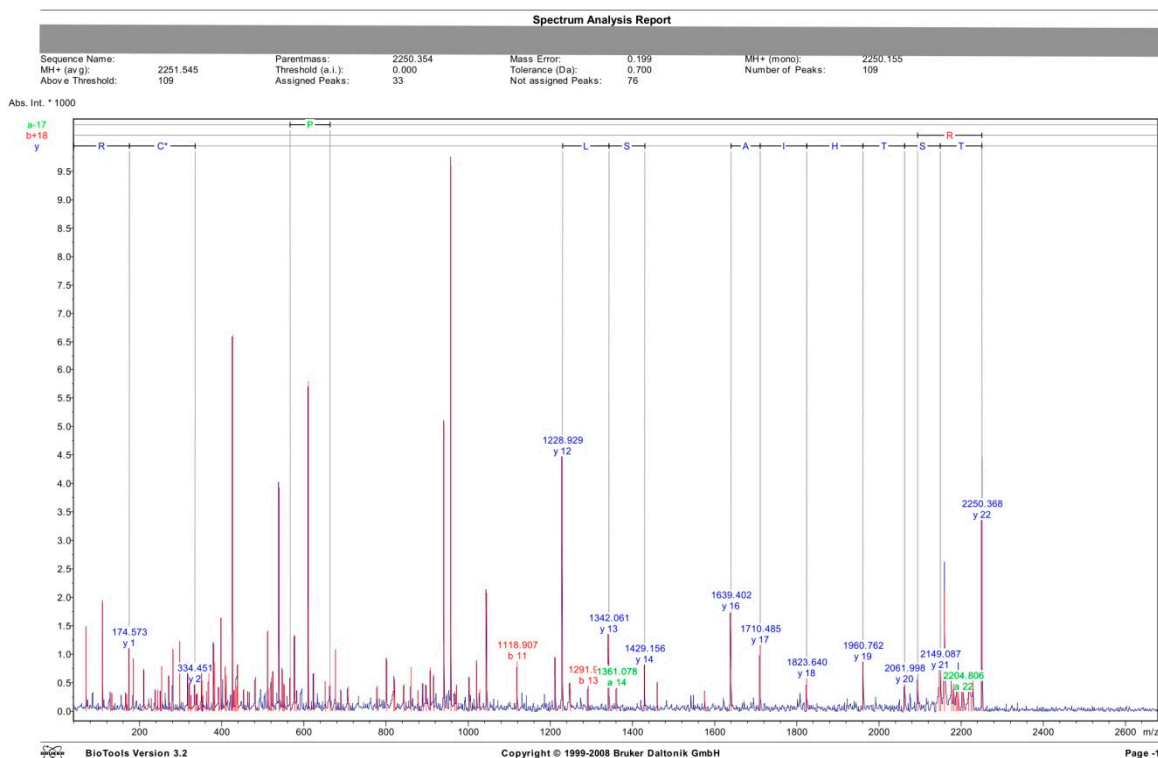
10	20	30	40	50	60	70	80	90	100	110	
ADDNPLEEC	FREDDYEEFL	KIANKLEGW	YANLGNRYP	VKPEEGEHD	DIFAYE	FDE	IVGGNDKFW	EDDGIROGKE	TFCYSPMIQR	PYQGFHSEA	LTAIPVGR

Display Parameter:
 Sequence Name: L-amino-acid oxidase (Fragments) OS=Macropipera lebetina PE=1 SV=2 OXLA_MACLB
 MH+ (avg): 1.008 Threshold (a.l.): 0.000 Tolerance (Da): 0.500 MH+ (mono): 1.008
 Number of Peaks: 20

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	803.479	1395.612	2	842.578	2929.728	3	856.593	140.920	4	870.614	388.020	5	924.593	337.792
6	946.556	64.000	7	1003.629	1171.226	8	1064.576	177.243	9	1078.378	22.000	10	1133.697	143.000
11	1137.613	518.253	12	1151.685	118.000	13	1165.750	86.000	14	1252.718	25956.205	15	1493.785	784.806
16	1507.802	341.611	17	1635.673	5246.347	18	1933.017	965.499	19	1948.993	69.000	20	2975.519	36.000

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Area 4. Annotated MS/MS spectrum of ion 2250.354 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 2250.354 Mass Error: 0.199 MH+ (mono): 2250.155 MH+ (avg): 2251.545
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 109 Above Threshold: 109
 Assigned Peaks: 33 Not assigned Peaks: 76

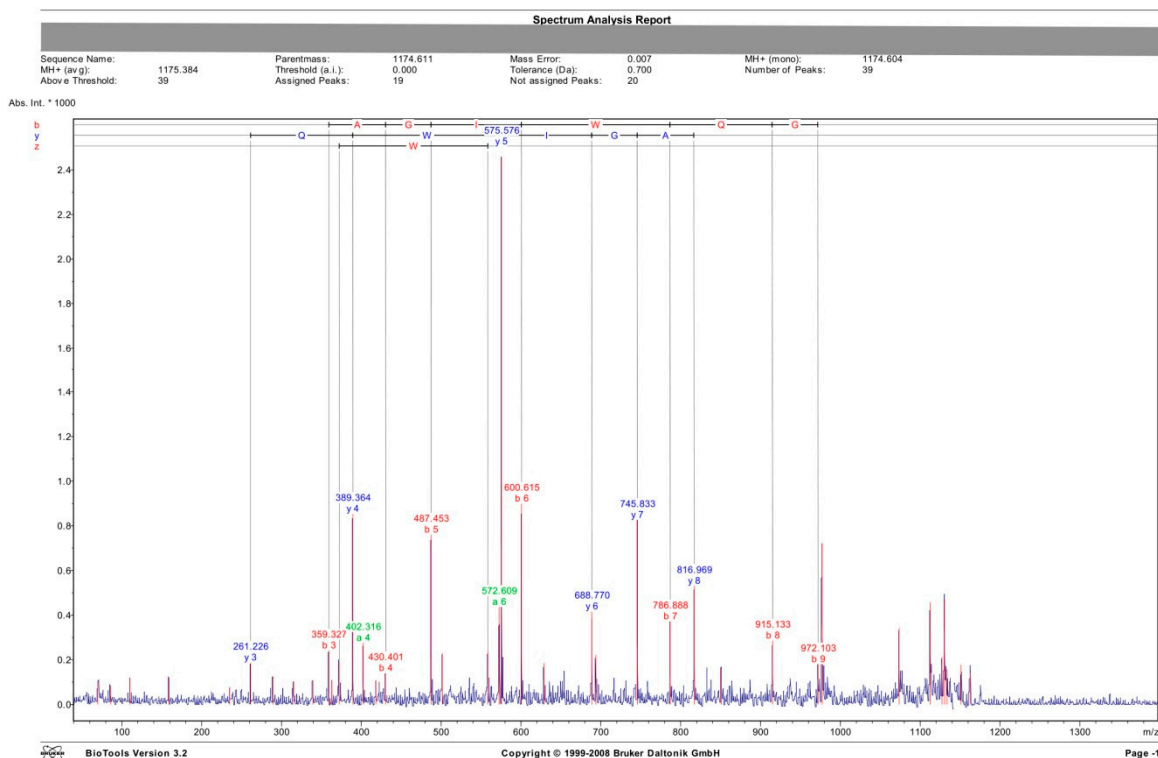
Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.704	1402.245	2	109.631	1899.934	3	126.623	318.672	4	132.588	298.546	5	166.582	310.720
6	168.570	304.675	7	174.573	1104.464	8	184.542	688.851	9	210.651	714.933	10	228.538	231.631
11	238.497	359.046	12	243.499	367.326	13	290.529	357.402	14	253.493	770.492	15	271.469	616.343
16	281.494	1070.004	17	297.502	1214.483	18	317.452	853.382	19	321.498	496.208	20	325.486	286.637
21	334.451	474.168	22	338.473	283.125	23	340.486	305.825	24	350.487	724.860	25	352.513	541.741
26	362.469	341.713	27	368.486	755.814	28	380.486	1186.028	29	382.476	857.763	30	392.518	427.618
31	398.473	1643.776	32	408.472	792.260	33	410.581	627.543	34	422.484	291.014	35	426.458	6622.632
36	430.504	367.853	37	433.460	560.535	38	435.601	448.353	39	438.469	822.118	40	453.548	388.854
41	467.504	341.025	42	481.546	598.301	43	511.514	1417.175	44	514.999	395.773	45	520.466	592.171
46	524.506	707.346	47	539.502	3926.901	48	547.595	728.977	49	550.518	487.312	50	552.496	457.340
51	586.521	811.199	52	577.487	1334.752	53	582.529	370.241	54	610.534	5796.174	55	623.550	660.622
56	651.535	528.745	57	663.625	455.657	58	676.547	1091.556	59	690.638	359.435	60	707.580	437.191
61	778.621	456.505	62	801.590	903.004	63	816.688	410.378	64	820.695	564.197	65	843.633	477.132
66	880.668	767.027	67	877.687	367.342	68	889.713	483.388	69	897.664	450.252	70	907.726	771.392
71	915.692	655.178	72	940.699	5027.423	73	957.700	9601.370	74	966.892	348.471	75	971.672	469.104
76	1002.803	592.671	77	1020.775	819.767	78	1027.733	378.584	79	1044.746	2082.606	80	1118.907	877.623
81	1211.878	945.787	82	1228.929	4471.034	83	1247.898	502.335	84	1291.986	447.530	85	1342.061	1353.576
86	1361.078	414.893	87	1429.156	819.754	88	1460.105	519.880	89	1575.079	346.818	90	1638.402	1755.679
91	1710.485	1163.936	92	1823.640	576.833	93	1960.762	870.423	94	2061.998	472.485	95	2093.930	546.367
96	2146.371	509.175	97	2149.087	720.897	98	2159.272	2115.605	99	2176.358	472.940	100	2181.962	455.090
101	2187.216	287.295	102	2190.309	559.340	103	2192.759	395.250	104	2202.682	337.659	105	2204.806	339.764
106	2218.044	620.860	107	2223.850	242.034	108	2229.079	541.812	109	2250.368	3356.849			

Calculated Masses:
 TSTHIAFLSLPSSPPSVGSVCR 21: Carbamidomethyl (C)

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term.	Ion
1	T	74.060	57.033	56.049	102.055	85.028	84.044	120.066	119.082	74.060	201.098	175.119	158.092	22	R
2	S	161.092	144.066	143.082	189.087	172.060	171.076	207.098	206.114	60.044	361.129	335.150	318.133	21	C*
3	T	262.140	245.113	244.129	290.135	273.108	272.124	308.145	307.161	74.060	460.197	434.218	417.191	20	V
4	H	399.199	382.172	381.188	427.194	410.167	409.183	445.204	444.220	110.071	547.229	521.250	504.223	19	S
5	I	512.263	495.236	494.252	540.278	523.251	522.267	558.288	557.304	86.096	694.251	678.272	661.245	18	G
6	A	583.320	566.293	565.309	611.315	594.288	593.304	629.325	628.341	44.040	703.319	677.340	660.313	17	V
7	P	680.373	663.346	662.362	708.368	691.341	690.357	726.378	725.394	70.065	790.351	764.372	747.345	16	S
8	L	793.457	776.430	775.446	821.452	804.425	803.441	839.462	838.478	86.096	887.404	861.425	844.398	15	P
9	S	880.489	863.462	862.478	908.484	891.457	890.473	926.494	925.510	60.044	984.457	958.477	941.451	14	P
10	L	993.573	976.546	975.562	1021.568	1004.541	1003.557	1039.578	1038.594	86.096	1071.489	1045.510	1028.483	13	S
11	P	1060.626	1043.599	1042.615	1116.620	1101.594	1100.610	1136.631	1135.647	70.065	1158.621	1132.642	1115.615	12	S
12	S	1174.688	1160.631	1159.647	1205.652	1189.626	1187.642	1223.663	1222.679	60.044	1255.674	1229.694	1212.668	11	P
13	S	1264.690	1247.663	1246.679	1292.684	1275.658	1274.674	1310.695	1309.711	60.044	1368.658	1342.678	1325.652	10	L
14	P	1361.742	1344.716	1343.732	1389.737	1372.711	1371.727	1407.748	1406.764	70.065	1455.690	1429.710	1412.684	9	S
15	P	1458.795	1441.769	1440.785	1486.790	1469.763	1468.779	1504.791	1503.807	70.065	1568.774	1542.794	1525.768	8	L
16	S	1545.827	1528.801	1527.817	1573.822	1556.795	1555.811	1591.833	1590.849	60.044	1665.826	1639.847	1622.821	7	P
17	V	1644.896	1627.869	1626.885	1672.890	1655.864	1654.880	1690.901	1689.917	72.081	1736.864	1710.884	1693.858	6	A
18	G	1701.917	1684.890	1683.906	1729.912	1712.885	1711.901	1747.922	1746.938	30.034	1849.848	1823.868	1806.842	5	I
19	S	1788.949	1771.922	1770.938	1816.944	1799.917	1798.933	1834.955	1833.971	60.044	1987.007	1961.027	1944.001	4	H
20	V	1888.017	1871.991	1870.007	1916.012	1898.986	1898.002	1934.023	1933.039	72.081	2098.054	2062.074	2045.048	3	T
21	C*	2048.048	2031.022	2030.038	2076.043	2059.016	2058.032	2094.054	2093.070	133.043	2113.086	2109.107	2102.080	2	S
22	R	2204.149	2187.123	2186.139	2232.144	2215.118	2214.134	2250.155	2249.171	129.113	2276.134	2250.155	2233.128	1	T

Area 4. Annotated MS/MS spectrum of ion 1174.611 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1174.611	Mass Error:	0.007	MH+ (mono):	1174.604	MH+ (avg):	1175.384
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	39	Above Threshold:	39
Assigned Peaks:	19	Not assigned Peaks:	20				

Peaklist:

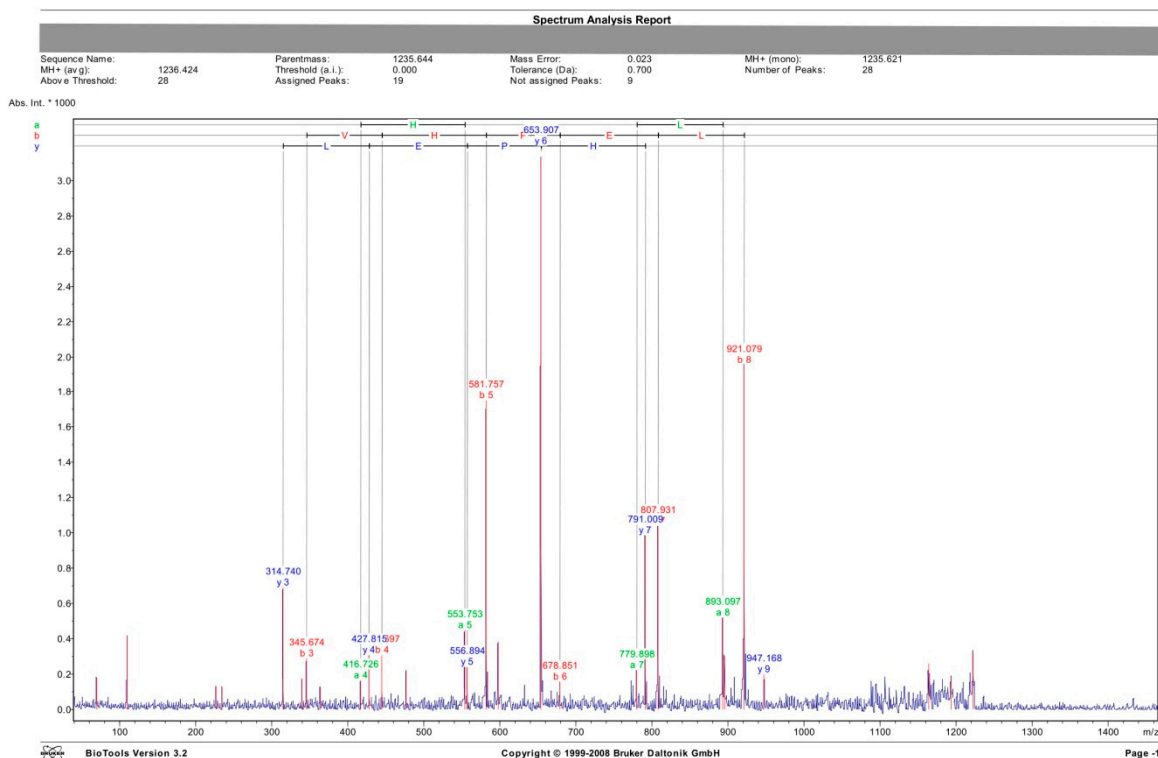
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	70.050	101.997	2	86.072	85.428	3	110.052	115.615	4	159.122	120.026	5	235.150	77.562
6	261.226	187.337	7	289.217	127.517	8	315.294	103.203	9	339.324	109.214	10	366.327	241.524
11	363.316	106.219	12	372.354	192.287	13	389.364	853.476	14	402.316	275.784	15	418.353	109.686
16	430.401	140.629	17	487.453	780.209	18	501.477	229.955	19	558.522	241.919	20	572.609	436.554
21	575.576	2504.424	22	600.615	899.837	23	628.666	185.865	24	688.770	416.275	25	693.785	222.439
26	745.833	825.995	27	786.888	372.179	28	816.969	530.552	29	851.051	166.463	30	915.133	286.600
31	972.103	180.034	32	977.216	722.841	33	1073.466	342.881	34	1112.526	457.598	35	1127.186	213.070
36	1130.557	470.899	37	1133.770	158.144	38	1151.241	177.595	39	1162.446	142.045			

Calculated Masses:
VVCAGINWGGK 3: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	V	72.081	55.054	54.070	100.076	83.049	82.065	118.086	117.102	72.081	173.092	147.113	130.086	11	K
2	V	171.149	154.123	153.139	199.144	182.118	181.134	217.155	216.171	72.081	230.114	204.134	187.108	10	G
3	C+	331.180	314.153	313.169	359.175	342.148	341.164	377.185	376.201	133.043	287.135	261.156	244.129	9	G
4	A	482.217	385.190	384.206	430.212	413.185	412.201	448.222	447.238	44.049	415.194	389.214	372.188	8	Q
5	G	459.238	442.212	441.228	487.233	470.207	469.223	505.244	504.260	30.034	601.273	575.294	558.267	7	W
6	I	572.322	555.296	554.312	600.317	583.291	582.307	618.328	617.344	86.096	714.357	688.378	671.351	6	I
7	W	758.402	741.375	740.391	786.397	769.370	768.386	804.407	803.423	159.092	771.376	745.399	728.373	5	G
8	Q	896.460	869.434	868.450	914.455	897.429	896.445	932.466	931.482	101.071	842.416	816.436	799.410	4	A
9	G	943.482	926.455	925.471	971.477	954.450	953.466	989.487	988.503	30.034	1002.446	976.467	959.440	3	C+
10	G	1000.503	983.477	982.493	1028.498	1011.472	1010.488	1046.509	1045.525	30.034	1101.515	1075.535	1058.508	2	V
11	K	1128.588	1111.572	1110.588	1156.593	1139.567	1138.583	1174.604	1173.620	101.107	1200.583	1174.604	1157.577	1	V

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Area 4. Annotated MS/MS spectrum of ion 1235.644 m/z.



Spectrum Analysis Report

Display Parameter:		Parentmass:	1235.644	Mass Error:	0.023	MH+ (mono):	1235.621	MH+ (avg):	1236.424
		Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	28	Above Threshold:	28
		Assigned Peaks:	19	Not assigned Peaks:	9				

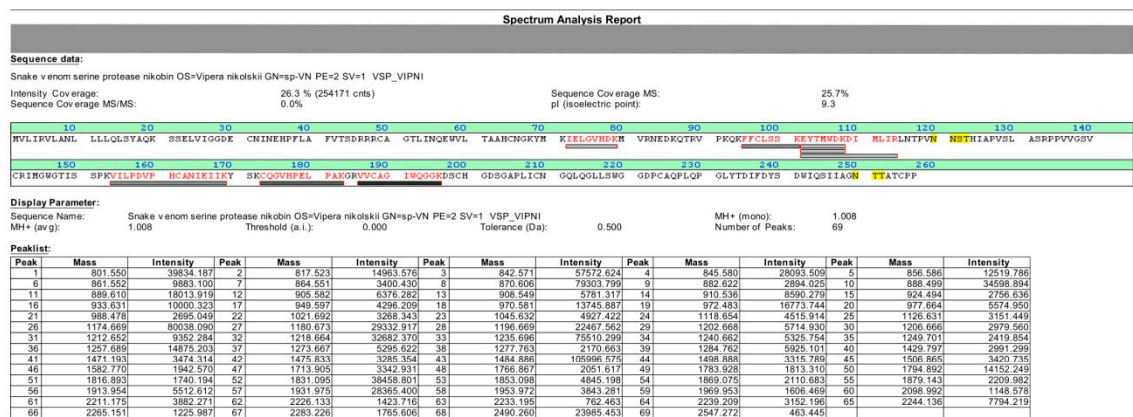
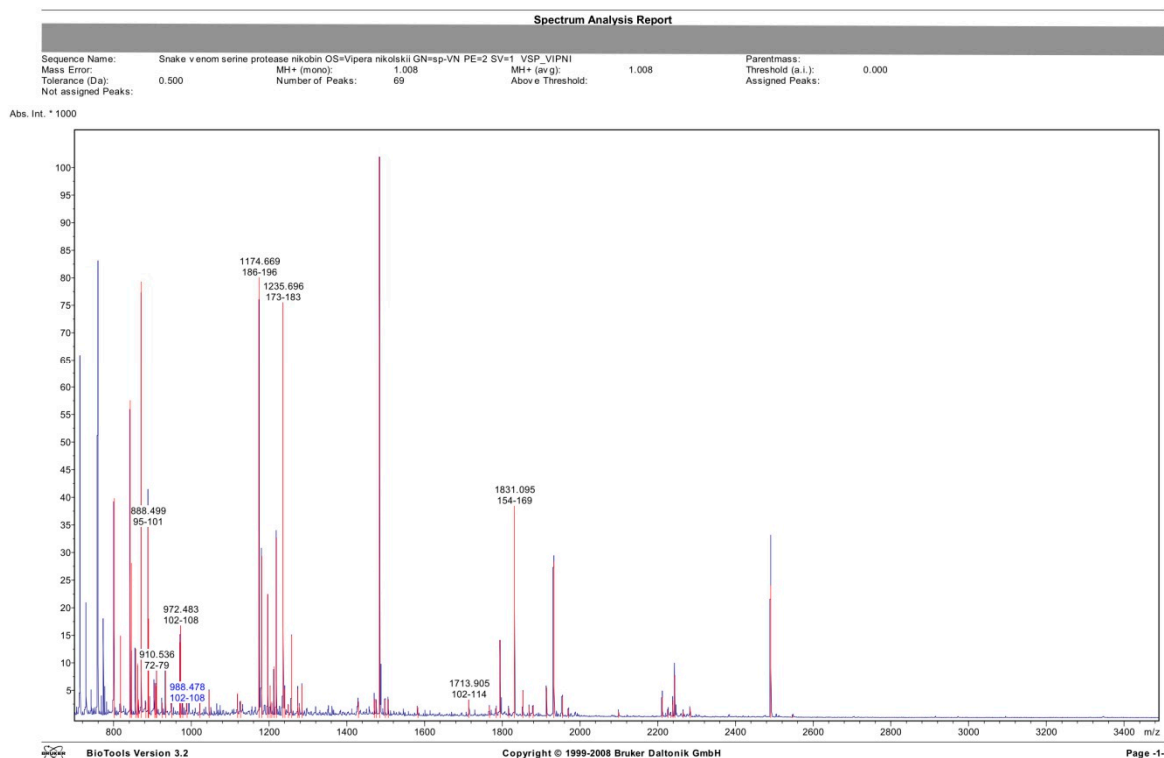
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.801	161.133	2	109.748	418.087	3	226.681	132.129	4	234.701	128.984	5	314.740	690.275
6	339.725	177.557	7	345.674	288.488	8	363.688	129.053	9	416.726	164.709	10	427.815	308.084
11	444.697	307.910	12	476.743	225.134	13	553.753	448.557	14	556.894	241.612	15	581.757	1749.883
16	597.762	385.589	17	653.907	3196.813	18	678.851	157.215	19	779.898	223.123	20	791.009	986.103
21	807.931	1038.627	22	893.097	518.896	23	896.815	301.869	24	921.079	1955.864	25	947.168	199.627
26	1163.943	259.224	27	1193.662	184.929	28	1222.296	321.576						

Calculated Masses:
CQGVHPELPAK 1: Carbamidomethyl (C)

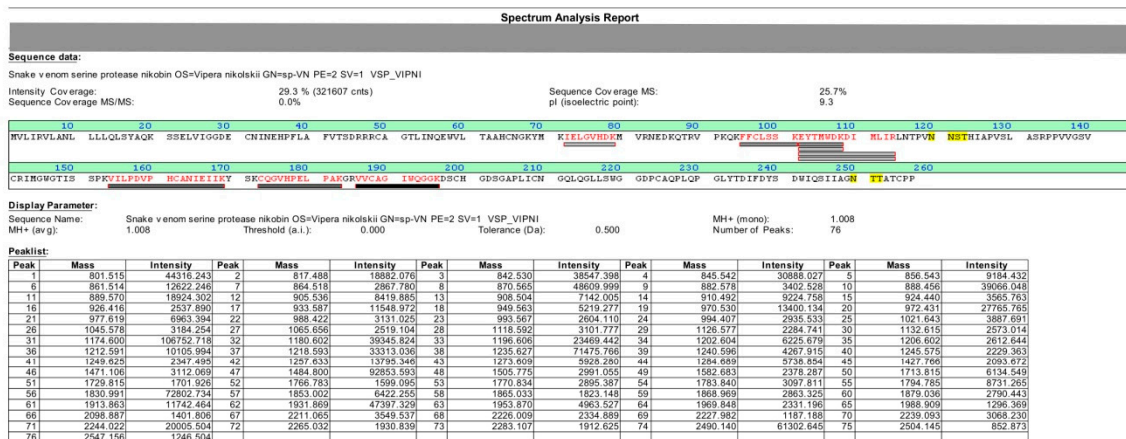
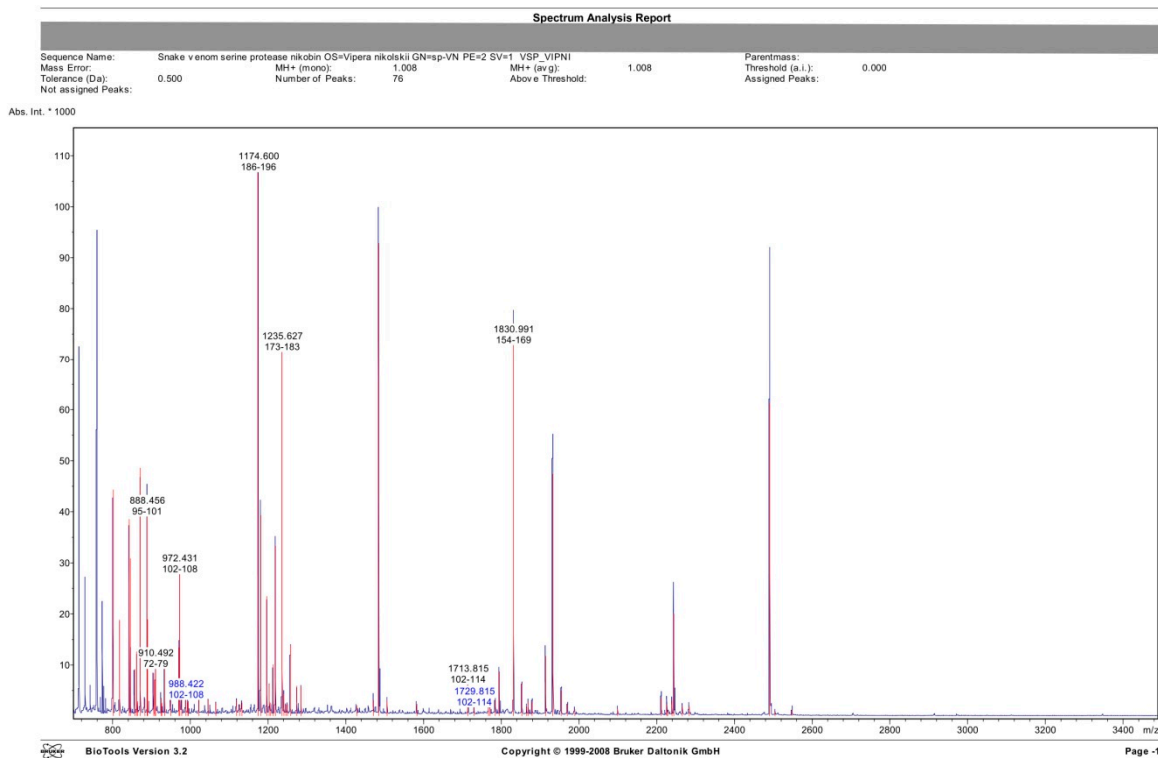
N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	C*	133.043	116.016	115.032	161.038	144.011	143.027	179.048	178.064	133.043	173.092	147.113	130.086	11	K
2	Q	261.102	244.075	243.091	289.097	272.070	271.086	307.107	306.123	101.071	244.129	218.150	201.123	10	A
3	G	318.123	301.097	300.112	346.118	329.091	328.107	364.129	363.145	30.034	341.182	315.203	298.176	9	P
4	V	417.191	400.165	399.181	445.186	428.160	427.176	463.197	462.213	72.081	454.266	428.287	411.260	8	L
5	H	554.250	537.224	536.240	582.245	565.219	564.235	600.256	599.272	110.071	583.309	557.329	540.303	7	E
6	P	651.303	634.277	633.293	679.298	662.272	661.287	697.309	696.325	70.065	680.361	654.382	637.356	6	P
7	E	780.346	763.319	762.335	808.341	791.314	790.330	826.351	825.367	102.055	817.420	791.441	774.414	5	H
8	L	893.430	876.403	875.419	921.425	904.398	903.414	939.435	938.451	86.096	916.489	890.509	873.483	4	V
9	P	990.463	973.436	972.452	1018.477	1001.451	1000.467	1036.488	1035.504	70.065	973.510	947.531	930.504	3	G
10	A	1081.520	1064.493	1063.509	1089.515	1072.488	1071.504	1107.525	1106.541	44.049	1101.569	1075.589	1058.563	2	Q
11	K	1189.615	1172.588	1171.604	1217.610	1200.583	1199.599	1235.620	1234.636	101.107	1261.599	1235.620	1218.594	1	C*

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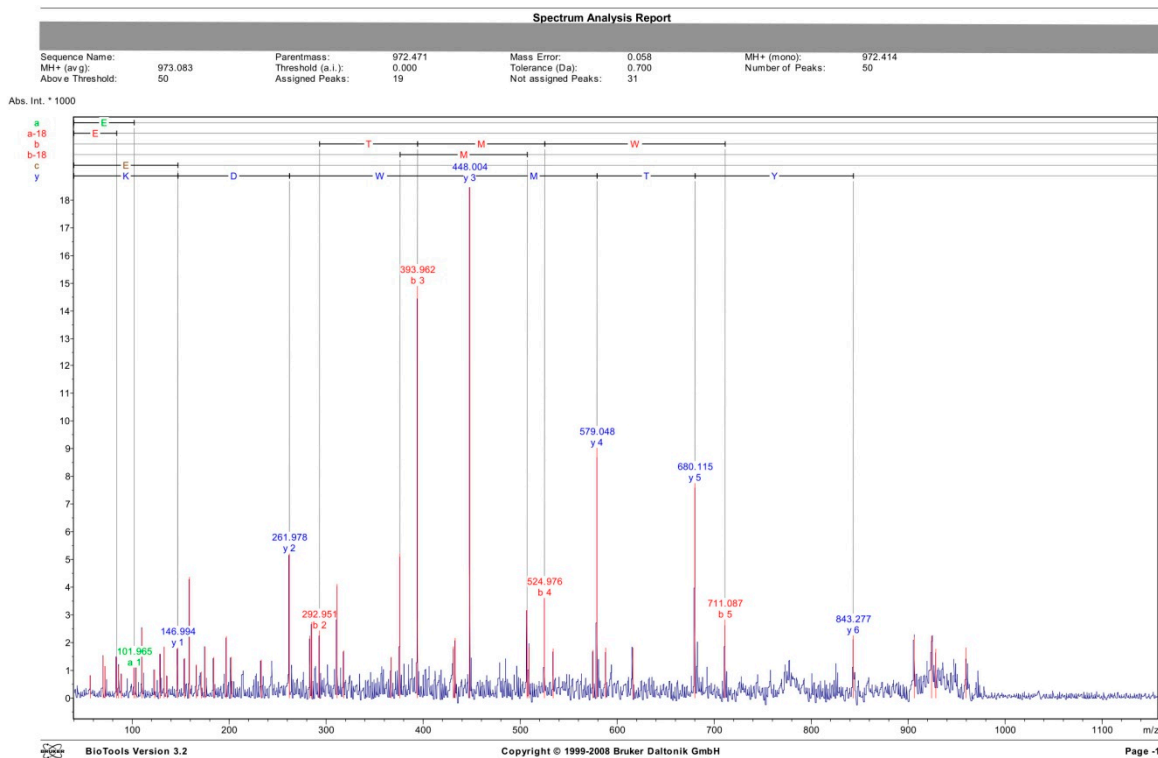
Area 4. Annotated MS spectrum 1.



Area 4. Annotated MS spectrum 2.



Area 4. Annotated MS/MS spectrum of ion 972.471 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	972.471	Mass Error:	0.058	MH+ (mono):	972.414	MH+ (avg):	973.083
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	50	Above Threshold:	50
Assigned Peaks:	19	Not assigned Peaks:	31				

Peaklist:

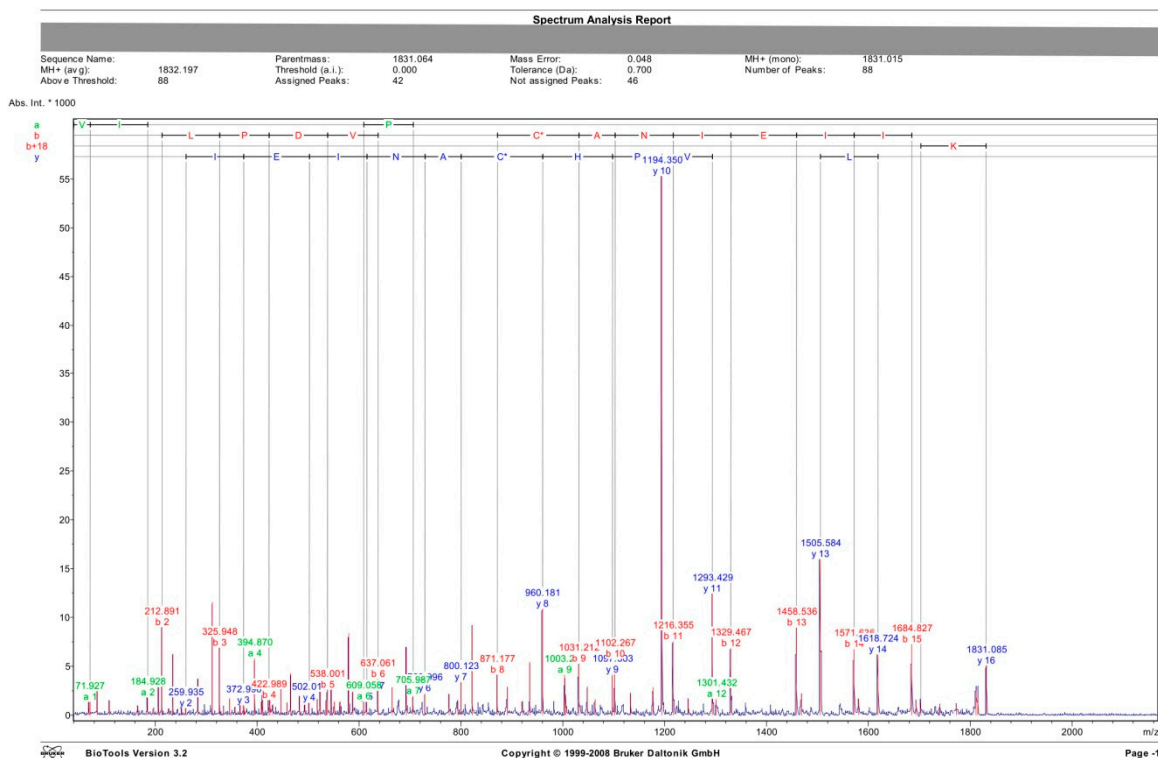
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	56.973	829.496	2	69.981	1503.596	3	72.001	1155.524	4	83.980	1474.844	5	85.981	1169.402
6	88.982	888.984	7	101.985	1101.256	8	103.970	1549.259	9	109.983	2518.579	10	122.984	1031.981
11	128.998	1603.410	12	132.964	1862.959	13	135.971	802.770	14	148.994	1819.768	15	153.972	1441.114
16	158.975	4372.663	17	165.994	1217.130	18	170.963	961.834	19	174.975	1856.325	20	183.976	1486.099
21	198.994	2240.548	22	201.989	1494.273	23	232.968	1395.919	24	261.978	5217.831	25	283.982	2258.590
26	285.023	2745.510	27	292.951	2443.301	28	311.134	4119.538	29	317.993	1721.690	30	367.039	1492.483
31	375.980	5222.764	32	393.962	14905.571	33	431.000	1866.568	34	432.954	2174.708	35	448.004	18619.124
36	506.989	3104.571	37	508.993	1839.848	38	524.976	3821.844	39	533.975	1799.542	40	575.058	1741.696
41	579.048	9031.054	42	588.027	1820.581	43	616.031	1820.650	44	680.115	7760.318	45	711.087	2834.050
46	843.277	2264.893	47	906.090	2202.201	48	923.995	2249.990	49	928.423	1777.919	50	959.645	1828.821

Calculated Masses:
EYTMWDK

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	E	162.055	85.028	84.044	130.050	113.023	112.039	148.060	147.076	102.055	173.092	147.113	130.086	7	K
2	Y	285.118	248.082	247.108	393.113	278.087	275.103	311.124	310.140	106.076	288.119	282.140	245.113	6	D
3	Y	386.166	349.139	348.155	394.161	377.134	376.150	412.171	411.187	74.060	474.198	448.219	431.193	5	W
4	M	497.206	480.180	479.196	525.201	508.175	507.191	543.212	542.228	104.053	605.239	578.260	562.233	4	M
5	W	683.286	666.259	665.275	711.281	694.254	693.270	729.291	728.307	159.092	796.286	680.307	663.281	3	Y
6	D	798.313	781.286	780.302	826.308	809.281	808.297	844.318	843.334	88.039	889.350	843.371	826.344	2	Y
7	K	926.408	909.381	908.397	954.403	937.376	936.392	972.413	971.429	101.107	998.392	972.413	955.387	1	E

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Area 4. Annotated MS/MS spectrum of ion 1831.064 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1831.064 Mass Error: 0.048 MH+ (mono): 1831.015 MH+ (avg): 1832.197
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 88 Above Threshold: 88
 Assigned Peaks: 42 Not assigned Peaks: 46

Peaklist:

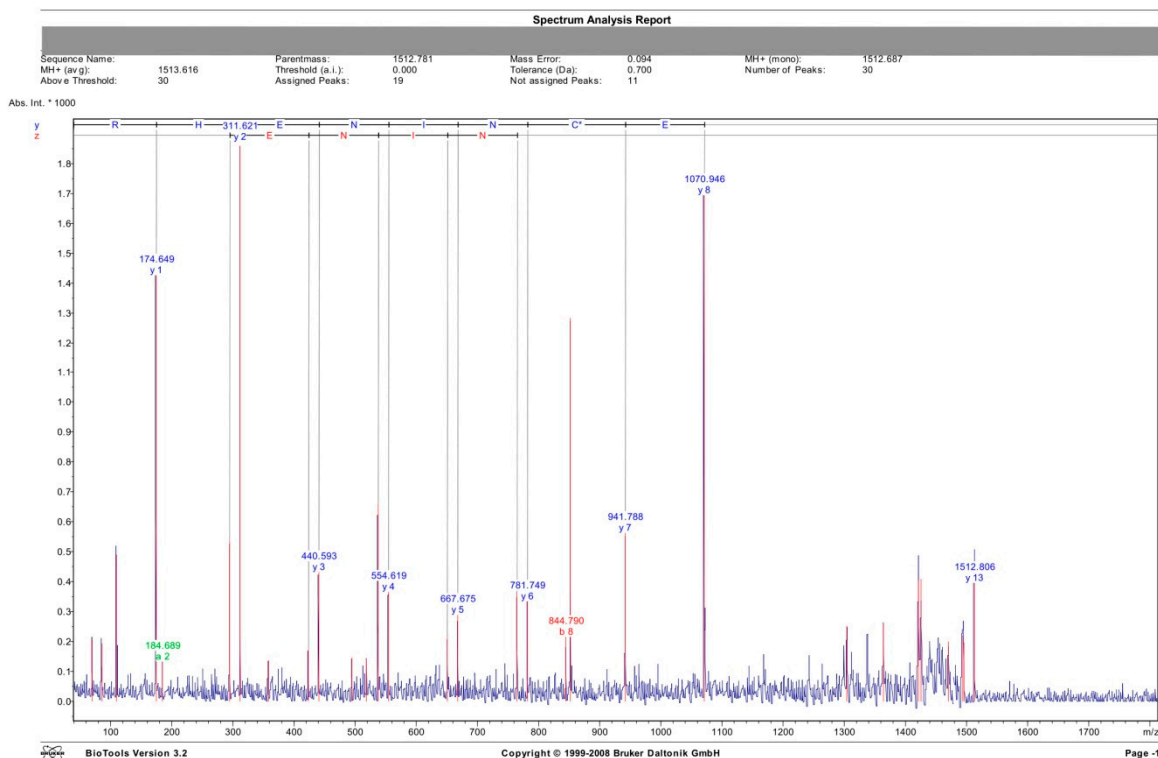
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	
1	69.907	1966.970	2	71.927	1351.950	3	85.934	3142.713	4	109.870	1481.515	5	166.834	960.110	
6	184.926	1810.875	7	198.895	806.856	8	206.876	2861.971	9	212.891	8969.850	10	226.920	684.187	
11	234.872	6288.193	12	251.891	1148.003	13	259.935	714.319	14	283.905	3763.893	15	311.868	11589.454	
16	325.948	6902.517	17	333.911	912.807	18	345.849	1737.566	19	356.928	875.041	20	366.879	1967.455	
21	372.966	1074.525	22	374.914	887.414	23	384.870	6798.055	24	408.927	1441.182	25	410.927	2142.645	
26	422.989	1542.229	27	424.952	2625.377	28	430.896	1107.935	29	448.967	3578.328	30	458.881	1312.167	
31	465.890	4306.174	32	462.906	1999.816	33	493.954	1093.310	34	502.019	1279.171	35	517.981	1675.845	
36	523.997	3056.916	37	538.923	1475.297	38	538.001	2600.792	39	545.950	3315.117	40	551.930	1409.807	
41	562.927	1410.641	42	579.907	8401.381	43	587.942	2445.924	44	609.058	1418.051	45	615.067	1363.506	
46	637.061	3697.697	47	664.999	2908.010	48	692.992	6947.665	49	705.987	1966.974	50	729.996	2237.539	
51	777.044	2149.433	52	794.060	1416.023	53	800.123	3384.932	54	822.032	9137.087	55	871.177	4135.491	
56	891.061	2927.755	57	921.092	1470.341	58	935.112	5451.750	59	960.181	10875.962	60	1003.246	4128.474	
61	1006.231	2143.709	62	1031.212	5278.714	63	1046.211	2974.510	64	1063.335	1603.712	65	1097.303	4151.842	
66	1102.267	5750.599	67	1133.266	2166.408	68	1177.307	2883.056	69	1194.350	55309.862	70	1216.355	7562.069	
71	1246.337	1641.877	72	1293.429	12425.309	73	1301.432	1656.863	74	1329.467	6849.995	75	1458.536	8963.918	
76	1468.873	2235.222	77	1505.584	15980.754	78	1571.636	6769.149	79	1581.118	1655.940	80	1618.724	6205.549	
81	1684.827	7240.957	82	1693.399	1482.703	83	1702.832	1381.715	84	1740.200	961.052	85	1772.879	956.534	
86	1811.148	2635.460	87	1814.570	1710.355	88	1831.085	5062.948							

Calculated Masses:
 VILPDPVHCANIELIK 9: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	I	72.081	55.054	54.070	100.076	83.049	82.065	118.086	117.102	72.081	173.092	147.113	130.086	16	K
2	I	185.165	168.138	167.154	213.160	196.133	195.149	231.170	230.186	86.096	286.176	260.197	243.170	15	I
3	L	238.249	281.222	280.238	326.244	309.217	308.233	344.254	343.270	86.096	399.260	373.281	356.254	14	I
4	P	395.302	378.275	377.291	423.297	406.270	405.286	441.307	440.323	70.065	528.303	502.324	485.297	13	E
5	D	510.329	493.302	492.318	538.324	521.297	520.313	556.334	555.350	88.039	641.367	615.408	598.381	12	I
6	V	609.397	592.370	591.386	637.392	620.365	619.381	655.403	654.418	72.081	755.430	729.451	712.424	11	N
7	P	706.450	689.423	688.439	734.445	717.418	716.434	752.455	751.471	70.065	826.467	800.488	783.461	10	A
8	H	843.509	826.482	825.498	871.504	854.477	853.493	889.514	888.530	110.071	996.498	960.518	943.492	9	C*
9	C*	1003.539	986.513	985.529	1031.534	1014.508	1013.524	1049.545	1048.561	133.043	1123.556	1097.577	1080.551	8	H
10	A	1074.576	1057.550	1056.566	1102.571	1085.545	1084.561	1120.582	1119.598	44.040	1220.609	1194.630	1177.603	7	P
11	N	1188.619	1171.593	1170.609	1216.614	1199.588	1198.604	1234.625	1233.641	87.055	1319.678	1293.698	1276.672	6	V
12	I	1301.703	1284.677	1283.693	1329.698	1312.672	1311.688	1347.709	1346.725	86.096	1434.705	1408.725	1391.699	5	D
13	E	1430.748	1413.719	1412.735	1458.741	1441.714	1440.730	1476.752	1475.768	102.055	1531.757	1505.778	1488.752	4	P
14	I	1543.830	1526.804	1525.820	1571.825	1554.798	1553.814	1589.836	1588.852	86.096	1644.841	1618.862	1601.836	3	L
15	I	1658.914	1639.888	1638.904	1684.909	1667.883	1666.899	1702.920	1701.936	86.096	1757.925	1731.946	1714.920	2	I
16	K	1785.009	1767.983	1766.999	1813.004	1796.978	1794.993	1831.015	1830.031	101.107	1886.994	1831.015	1813.988	1	V

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Area 5. Annotated MS/MS spectrum of ion 1512.781 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1512.781	Mass Error:	0.094	MH+ (mono):	1512.687	MH+ (avg):	1513.616
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	30	Above Threshold:	30
Assigned Peaks:	19	Not assigned Peaks:	11				

Peaklist:

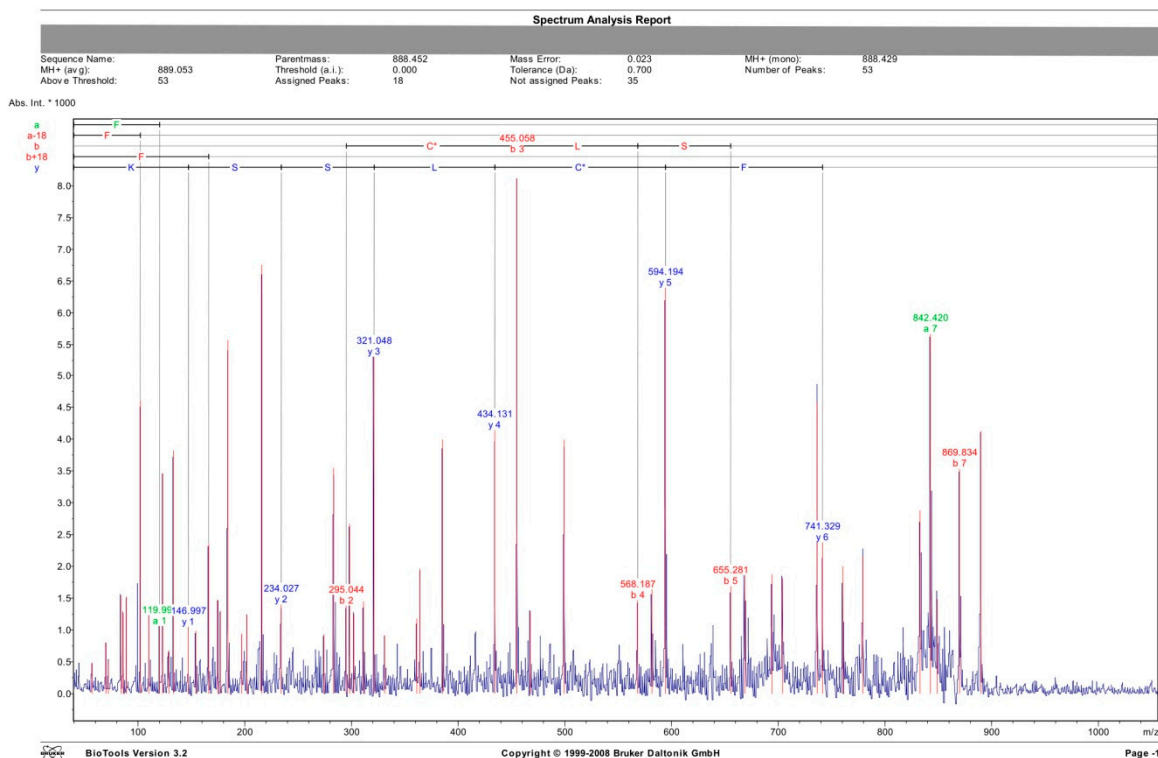
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.682	206.384	2	85.747	194.033	3	109.699	490.776	4	174.649	1426.767	5	184.689	132.349
6	294.810	535.696	7	311.621	1972.651	8	358.525	136.448	9	423.598	112.522	10	440.593	431.651
11	494.607	146.687	12	518.534	140.528	13	537.562	658.944	14	554.619	365.902	15	650.650	214.409
16	667.675	288.698	17	764.743	366.633	18	781.749	333.828	19	844.790	215.131	20	851.799	1284.091
21	941.788	562.711	22	1070.946	1694.398	23	1303.876	252.813	24	1364.220	258.583	25	1421.415	484.718
26	1425.493	408.885	27	1470.553	200.507	28	1493.692	221.755	29	1495.691	196.822	30	1512.806	395.537

Calculated Masses:
VIGDGCNINEHR 7: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	V	72.081	55.054	54.070	100.076	83.049	82.065	118.086	117.102	72.081	201.098	175.119	158.092	13	R
2	I	185.165	168.138	167.154	213.160	196.133	195.149	231.170	230.186	86.096	338.157	312.178	295.151	12	H
3	G	242.186	225.160	224.176	270.181	253.155	252.171	288.192	287.208	30.034	487.200	441.220	424.194	11	E
4	G	299.208	282.181	281.197	327.203	310.176	309.192	345.213	344.229	30.034	581.243	555.263	538.237	10	N
5	D	414.235	397.208	396.224	442.230	425.203	424.219	460.240	459.256	88.039	694.327	668.347	651.321	9	I
6	E	543.277	526.251	525.267	571.272	554.246	553.262	589.283	588.299	102.055	898.370	872.390	855.364	8	N
7	C*	703.308	686.281	685.297	731.303	714.276	713.292	749.313	748.329	133.043	988.400	942.421	925.394	7	C*
8	N	817.351	800.324	799.340	845.346	828.319	827.335	863.356	862.372	87.055	1097.443	1071.464	1054.437	6	E
9	I	930.435	913.408	912.424	958.430	941.403	940.419	976.440	975.456	86.096	1212.470	1186.491	1169.464	5	D
10	N	1044.478	1027.451	1026.467	1072.473	1055.446	1054.462	1090.483	1089.499	87.055	1269.491	1243.512	1226.485	4	G
11	E	1173.520	1156.494	1155.510	1201.515	1184.489	1183.505	1219.526	1218.542	102.055	1326.513	1300.533	1283.507	3	G
12	H	1310.579	1293.553	1292.569	1338.574	1321.548	1320.564	1356.585	1355.601	110.071	1439.597	1413.618	1396.591	2	I
13	R	1466.680	1449.654	1448.670	1494.675	1477.649	1476.665	1512.686	1511.702	129.113	1538.665	1512.686	1495.659	1	V

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Area 5. Annotated MS/MS spectrum of ion 888.452 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 888.452 Mass Error: 0.023 MH+ (mono): 888.429 MH+ (avg): 889.053
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 53 Above Threshold: 53
 Assigned Peaks: 18 Not assigned Peaks: 35

Peaklist:

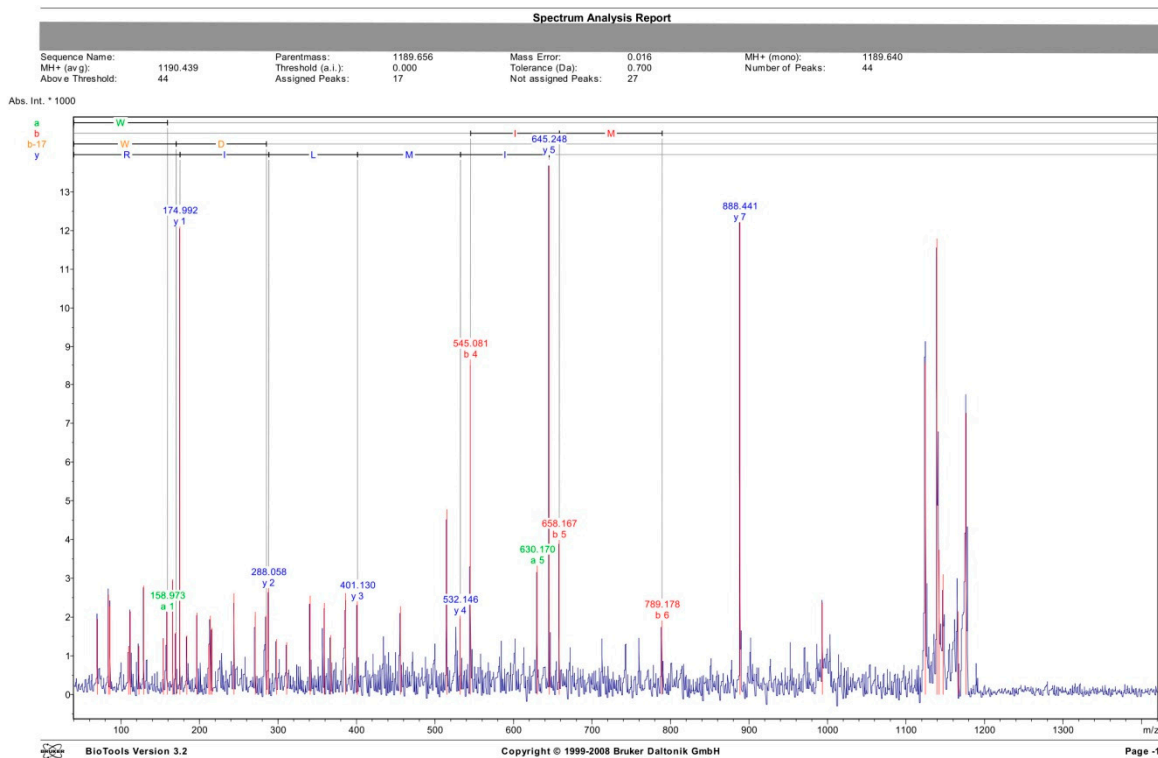
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	56.902	486.413	2	69.942	795.242	3	71.986	526.068	4	83.972	1544.545	5	86.009	1261.505
6	88.965	325.353	7	102.000	4615.877	8	109.973	1269.961	9	119.993	1061.291	10	123.020	3459.474
11	129.000	683.436	12	132.973	3822.179	13	146.997	1048.126	14	153.984	990.236	15	166.055	2349.984
16	175.014	1473.619	17	177.026	1303.520	18	184.083	5571.883	19	197.007	948.157	20	202.025	1231.880
21	218.052	6768.664	22	234.027	1400.228	23	274.017	531.482	24	283.296	3548.925	25	295.044	1380.273
26	298.168	2668.943	27	302.138	1255.318	28	311.227	1448.461	29	321.048	5308.246	30	331.043	918.732
31	361.047	1179.058	32	364.046	1966.261	33	385.274	3995.934	34	434.131	4140.731	35	455.058	8495.811
36	497.361	1294.450	37	499.343	3391.767	38	568.187	1466.639	39	581.456	1861.112	40	594.194	6395.061
41	655.281	1687.851	42	668.454	1931.467	43	694.094	1876.648	44	704.033	1820.428	45	736.480	4577.611
46	741.329	2376.846	47	760.405	2000.854	48	779.201	2152.524	49	832.711	2882.154	50	842.420	5668.875
51	848.794	1467.540	52	869.834	3536.499	53	889.653	4127.877						

Calculated Masses:
 FFCLSSK 3: Carbamidomethyl I (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	F	120.081	103.054	102.070	148.076	131.049	130.065	166.086	165.102	120.081	173.092	147.113	130.086	7	K
2	F	267.149	250.123	249.139	295.144	278.118	277.134	313.155	312.171	120.081	260.124	234.145	217.118	6	S
3	C*	427.180	410.153	409.169	455.175	438.148	437.164	473.185	472.201	133.043	347.156	321.177	304.150	5	S
4	L	540.264	523.237	522.253	568.259	551.232	550.248	586.269	585.285	86.096	460.240	434.261	417.234	4	L
5	S	627.296	610.269	609.285	655.291	638.264	637.280	673.301	672.317	60.044	620.271	594.292	577.265	3	C*
6	S	714.328	697.301	696.317	742.323	725.296	724.312	760.333	759.349	60.044	767.339	741.360	724.333	2	F
7	K	842.423	825.396	824.412	870.418	853.391	852.407	888.428	887.444	101.107	914.408	888.428	871.402	1	F

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Area 5. Annotated MS/MS spectrum of ion 1189.656 m/z.



Spectrum Analysis Report

Display Parameter:	Parentmass:	1189.656	Mass Error:	0.018	MH+ (mono):	1189.640	MH+ (avg):	1190.439
	Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	44	Above Threshold:	44
	Assigned Peaks:	17	Not assigned Peaks:	27				

Peaklist:

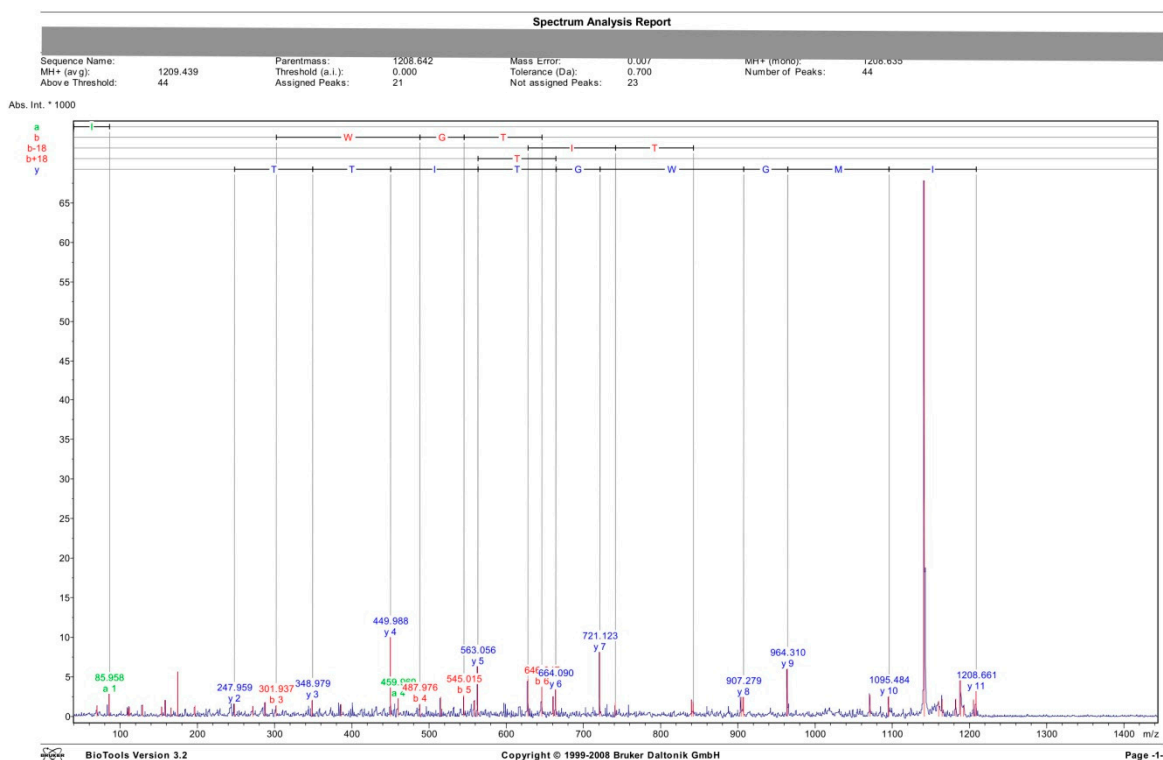
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.988	1951.459	2	83.975	2581.839	3	86.009	2275.108	4	109.939	1227.294	5	111.972	2149.867
6	122.999	1256.430	7	128.997	2913.319	8	153.982	1444.512	9	158.973	2136.322	10	166.011	2977.716
11	169.931	1621.322	12	174.992	12107.406	13	183.988	1531.105	14	198.992	2114.026	15	211.998	1302.597
16	213.998	2036.555	17	215.989	1723.260	18	243.996	2613.610	19	271.030	2135.326	20	285.019	2055.698
21	288.058	2748.332	22	298.051	1431.458	23	311.087	1352.428	24	341.019	2551.690	25	368.018	2369.847
26	367.077	1536.193	27	386.099	2618.908	28	401.130	2404.588	29	456.090	2280.326	30	515.140	4780.260
31	532.146	2035.626	32	545.081	8669.033	33	630.170	3330.533	34	645.248	13950.409	35	658.167	3993.054
36	789.178	1912.414	37	888.441	12218.851	38	993.368	2377.892	39	1124.561	8559.726	40	1139.183	11795.402
41	1142.121	3739.024	42	1147.181	3103.887	43	1166.125	2145.961	44	1176.590	7263.730			

Calculated Masses:
WDKDMLIR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	199.092	x	y	z	C-Term	Ion
1	W	159.092	142.065	141.081	167.087	170.060	169.078	205.097	204.113	199.092	201.098	175.119	158.092	9	R	
2	D	274.119	287.092	296.108	302.114	285.087	284.103	320.124	319.140	88.039	314.162	288.203	271.176	8	I	
3	K	402.214	385.187	384.203	430.208	413.182	412.198	448.219	447.235	101.107	427.256	401.287	384.261	7	L	
4	D	517.241	500.214	499.230	545.235	528.209	527.225	563.246	562.262	88.039	558.307	532.328	515.301	6	M	
5	I	630.325	613.298	612.314	658.320	641.293	640.309	676.330	675.345	86.096	671.391	645.412	628.385	5	I	
6	M	761.365	744.339	743.355	789.360	772.333	771.349	807.371	806.387	104.053	788.418	760.439	743.412	4	D	
7	L	874.449	857.423	856.439	902.444	885.418	884.433	920.455	919.471	86.096	914.513	888.534	871.507	3	K	
8	I	987.533	970.507	969.523	1015.528	998.502	997.518	1033.539	1032.555	86.096	1029.540	1003.560	986.534	2	D	
9	K	1143.634	1126.608	1125.624	1171.629	1154.603	1153.619	1189.640	1188.656	129.113	1215.619	1189.640	1172.613	1	W	

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Area 5. Annotated MS/MS spectrum of ion 1208.642 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1208.642	Mass Error:	0.007	MH+ (mono):	1208.635	MH+ (avg):	1209.439
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	44	Above Threshold:	44
Assigned Peaks:	21	Not assigned Peaks:	23				

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.939	1316.609	2	85.958	2855.790	3	109.899	1052.899	4	111.923	1210.909	5	128.942	1475.463
6	153.922	1205.242	7	158.929	2085.436	8	165.920	1144.857	9	174.930	5682.127	10	196.926	1382.436
11	247.959	1617.452	12	271.949	1329.827	13	287.966	1853.963	14	301.937	1448.276	15	348.979	2118.559
16	386.012	1974.154	17	449.988	10023.731	18	459.969	2304.335	19	487.976	1613.690	20	514.987	2503.822
21	545.015	2712.625	22	559.011	2089.724	23	563.056	6343.080	24	628.031	4711.806	25	646.047	3759.679
26	661.148	2584.398	27	664.090	3454.761	28	721.123	8140.831	29	741.100	1749.907	30	840.291	2163.035
31	842.167	1881.462	32	904.269	2606.545	33	907.279	2469.624	34	964.310	6035.407	35	1071.298	2751.792
36	1095.484	2585.529	37	1141.387	68295.724	38	1160.236	1999.814	39	1164.598	2224.776	40	1182.292	2274.138
41	1188.286	5800.729	42	1192.227	1383.739	43	1205.334	2192.811	44	1208.661	3180.918			

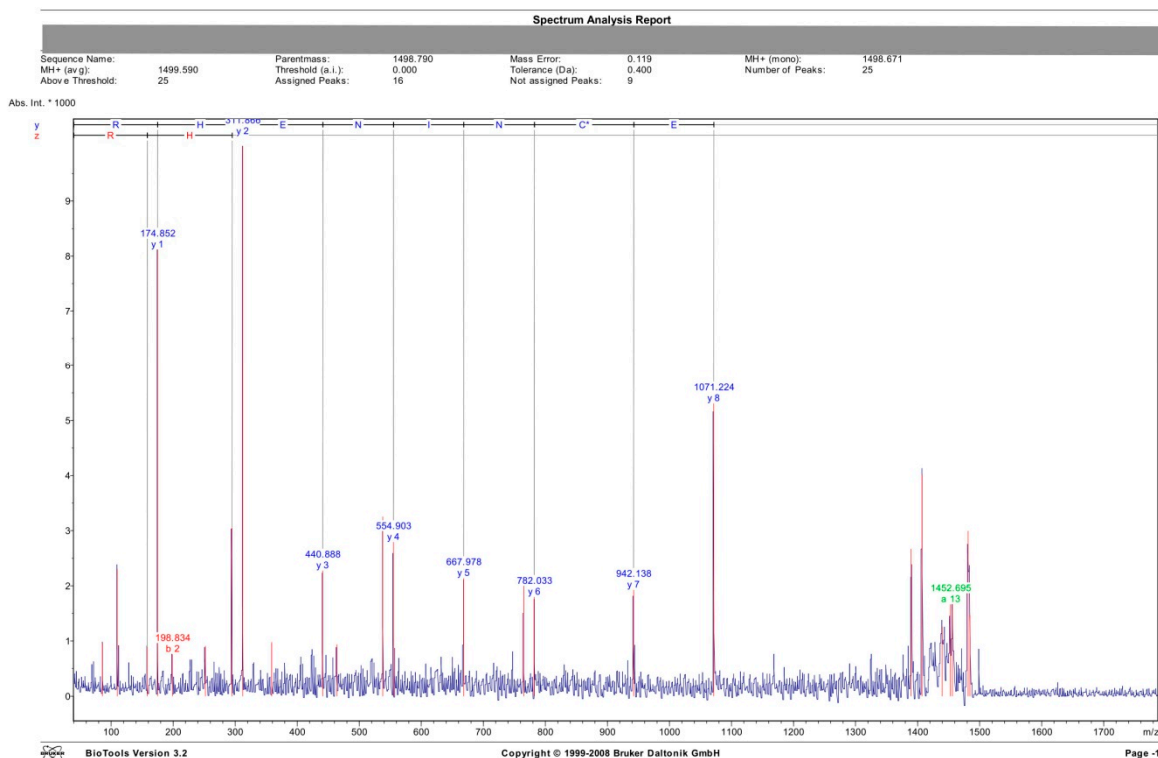
Calculated Masses:

IMGWGTTTTK

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	I	86.096	69.070	68.086	114.091	97.065	96.081	132.102	131.118	86.096	173.092	147.113	130.086	11	K
2	M	217.137	200.110	199.126	245.132	228.105	227.121	263.142	262.158	104.053	274.140	248.160	231.134	10	T
3	G	274.158	257.132	256.148	302.153	285.127	284.143	320.164	319.180	30.034	378.187	349.200	332.182	9	T
4	W	460.238	443.211	442.227	488.233	471.206	470.222	506.243	505.259	199.092	476.235	450.256	433.229	8	Y
5	G	517.259	500.233	499.249	545.254	528.228	527.243	563.265	562.281	30.034	589.319	563.340	546.313	7	I
6	T	618.307	601.280	600.296	646.302	629.275	628.291	664.312	663.328	74.060	690.367	664.388	647.361	6	T
7	I	731.391	714.364	713.380	759.386	742.359	741.375	777.396	776.412	86.096	747.388	721.409	704.382	5	G
8	T	832.439	815.412	814.428	860.433	843.407	842.423	878.444	877.460	74.060	933.468	907.488	890.462	4	W
9	T	933.486	916.460	915.476	961.481	944.455	943.471	979.492	978.508	74.060	990.499	964.510	947.483	3	G
10	T	1034.534	1017.507	1016.523	1062.529	1045.502	1044.518	1080.539	1079.555	74.060	1121.530	1095.550	1078.524	2	M
11	K	1162.629	1145.602	1144.618	1190.624	1173.597	1172.613	1208.634	1207.650	101.107	1234.614	1208.634	1191.608	1	I

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Area 5. Annotated MS/MS spectrum of ion 1498.790 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1498.790	Mass Error:	0.119	MH+ (mono):	1498.671	MH+ (avg):	1499.590
Threshold (a.i.):	0.000	Tolerance (Da):	0.400	Number of Peaks:	25	Above Threshold:	25
Assigned Peaks:	16	Not assigned Peaks:	9				

Peaklist:

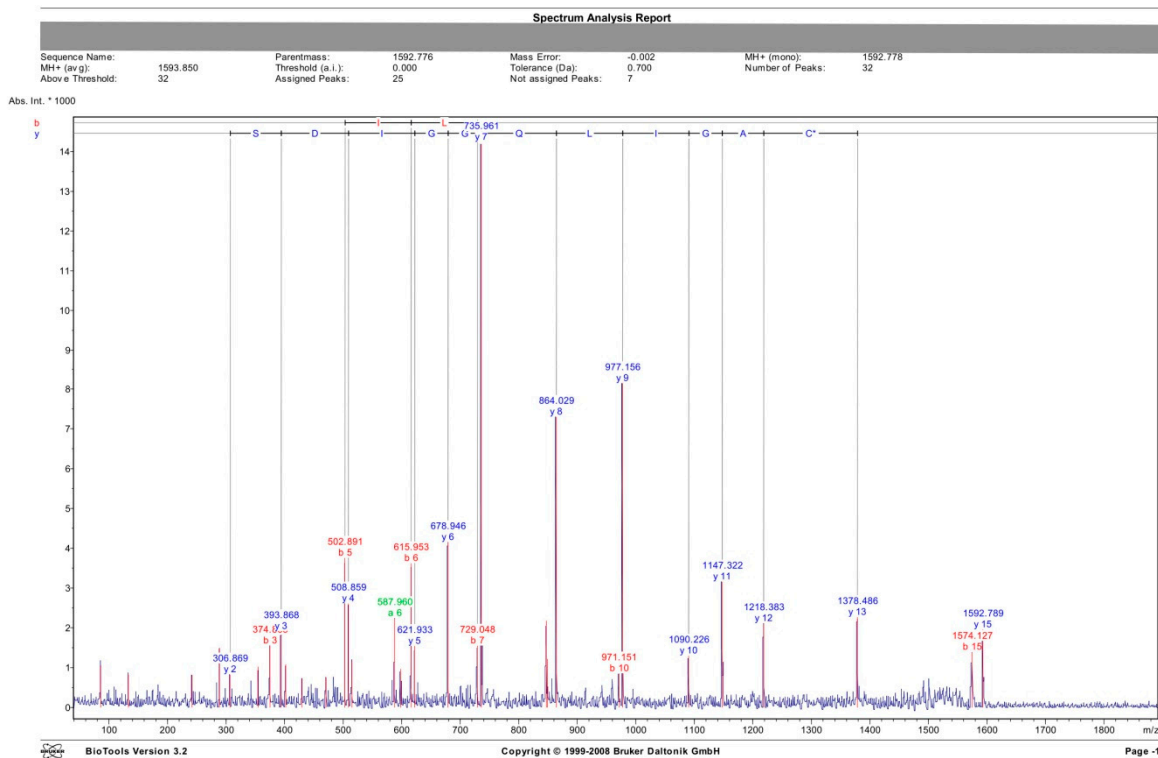
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	85.886	865.286	2	109.840	2304.396	3	157.837	889.073	4	174.852	8119.756	5	196.834	763.869
6	251.835	911.903	7	294.851	3065.086	8	311.866	10175.752	9	358.812	686.094	10	440.888	2278.247
11	463.914	942.031	12	537.869	3256.406	13	554.903	2794.946	14	667.978	2140.914	15	764.989	2011.967
16	782.033	1800.155	17	942.138	1928.426	18	1071.224	5308.886	19	1389.488	2674.597	20	1407.110	4024.491
21	1439.812	1259.628	22	1452.695	1967.502	23	1455.973	1774.842	24	1481.239	2988.493	25	1484.227	1471.720

Calculated Masses:
VVGDECNINEHR 7: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	V	72.081	55.054	54.070	100.076	83.049	82.065	118.086	117.102	72.081	201.098	175.119	158.092	13	R
2	V	171.149	154.123	153.139	199.144	182.118	181.134	217.155	216.171	72.081	338.157	312.178	295.151	12	H
3	G	228.171	211.144	210.160	256.166	239.139	238.155	274.176	273.192	30.034	467.200	441.220	424.194	11	E
4	G	285.192	268.166	267.182	313.187	296.160	295.176	331.198	330.214	30.034	551.243	555.263	538.237	10	N
5	D	400.219	383.193	382.208	428.214	411.187	410.203	446.225	445.241	88.039	694.327	668.347	651.321	9	I
6	E	529.262	512.235	511.251	557.257	540.230	539.246	575.267	574.283	102.055	808.370	782.390	765.364	8	N
7	C*	689.292	672.266	671.282	717.287	700.261	699.277	735.298	734.314	133.043	968.400	942.421	925.394	7	C*
8	N	803.335	786.309	785.325	831.330	814.304	813.320	849.341	848.357	87.055	1097.443	1071.464	1054.437	6	E
9	I	916.419	899.393	898.409	944.414	927.388	926.404	962.425	961.441	86.096	1212.470	1186.491	1169.464	5	D
10	N	1030.462	1013.436	1012.452	1058.457	1041.431	1040.447	1076.468	1075.484	87.055	1289.491	1263.512	1246.485	4	G
11	E	1159.505	1142.479	1141.494	1187.500	1170.473	1169.489	1205.510	1204.526	102.055	1326.513	1300.533	1283.507	3	G
12	H	1296.564	1279.537	1278.553	1324.559	1307.532	1306.548	1342.569	1341.585	110.071	1425.581	1399.602	1382.575	2	V
13	R	1452.665	1435.638	1434.654	1480.660	1463.633	1462.649	1498.670	1497.686	129.113	1524.650	1498.670	1481.644	1	V

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Area 5. Annotated MS/MS spectrum of ion 1592.776 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1592.776	Mass Error:	-0.002	MH+ (mono):	1592.776	MH+ (avg):	1593.850
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	32	Above Threshold:	32
Assigned Peaks:	25	Not assigned Peaks:	7				

Peaklist:

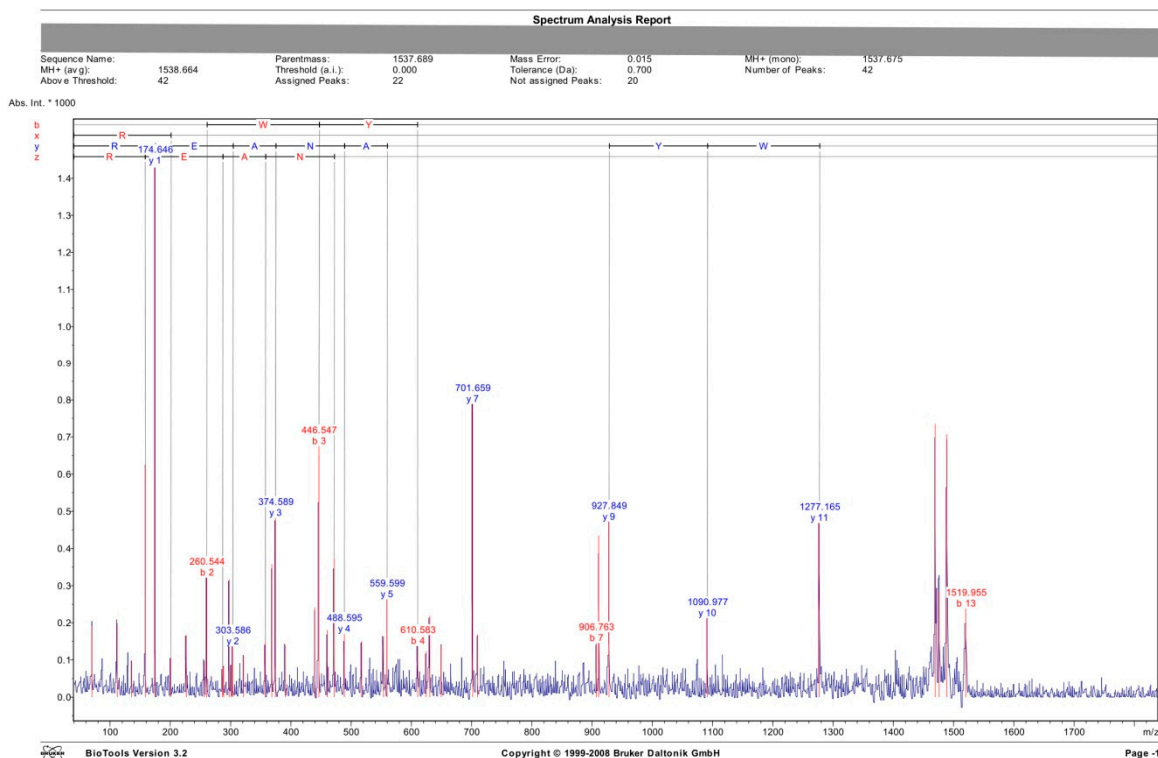
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	85.905	1063.412	2	132.847	830.626	3	241.891	617.863	4	288.827	1496.918	5	306.869	629.366
6	354.904	1029.565	7	374.863	1551.329	8	393.868	1915.657	9	401.873	1086.438	10	429.880	743.303
11	470.889	757.054	12	502.891	3759.363	13	508.859	2611.117	14	514.891	1165.983	15	587.960	2245.748
16	597.986	869.469	17	615.953	3623.859	18	621.933	1545.009	19	678.946	4151.695	20	729.048	1564.907
21	735.961	14240.065	22	847.039	2181.152	23	848.966	1222.166	24	864.029	7304.431	25	971.151	855.766
26	977.156	8147.261	27	1090.226	1301.177	28	1147.322	3160.719	29	1218.383	2116.883	30	1378.486	2272.304
31	1574.127	1396.536	32	1592.789	1961.810									

Calculated Masses:
 TLAGILGGIDSK 3: Carbamidomethyl (C) 14: Carbamidomethyl (C)

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term.	Ion
1	T	74.060	57.033	56.049	102.055	85.028	84.044	120.066	119.082	74.060	173.092	147.113	130.086	15	K
2	L	187.144	170.118	169.134	215.139	198.112	197.128	233.150	232.166	86.096	333.123	387.143	290.117	14	C*
3	C*	347.175	330.148	329.164	375.170	358.143	357.159	393.180	392.196	133.043	420.155	394.175	377.149	13	S
4	A	418.212	401.185	400.201	446.207	429.180	428.196	464.217	463.233	44.049	535.182	509.202	492.176	12	D
5	G	475.233	458.207	457.223	503.228	486.202	485.218	521.239	520.255	30.034	648.266	622.246	605.260	11	I
6	I	588.317	571.291	570.307	616.312	599.286	598.302	634.323	633.339	86.096	705.287	679.308	662.281	10	G
7	L	701.401	684.375	683.391	729.396	712.370	711.386	747.407	746.423	86.096	762.309	736.329	719.303	9	G
8	Q	829.460	812.433	811.449	857.455	840.428	839.444	875.466	874.481	101.071	890.387	864.368	847.361	8	Q
9	G	886.481	869.455	868.471	914.476	897.450	896.466	932.487	931.503	30.034	1003.451	977.472	960.446	7	L
10	G	943.503	926.476	925.492	971.498	954.471	953.487	989.508	988.524	30.034	1116.535	1090.556	1073.530	6	I
11	I	1056.587	1039.560	1038.576	1084.582	1067.555	1066.571	1102.593	1101.608	86.096	1173.557	1147.576	1130.551	5	G
12	D	1171.614	1154.587	1153.603	1199.609	1182.582	1181.598	1217.619	1216.635	88.039	1244.594	1218.615	1201.588	4	A
13	S	1258.646	1241.619	1240.635	1286.641	1269.614	1268.630	1304.651	1303.667	80.044	1404.625	1378.645	1361.619	3	C*
14	C*	1418.677	1401.650	1400.666	1446.672	1429.645	1428.661	1464.682	1463.698	133.043	1517.709	1491.729	1474.703	2	L
15	K	1546.772	1529.745	1528.761	1574.767	1557.740	1556.756	1592.777	1591.793	101.107	1618.756	1592.777	1575.751	1	T

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Area 6. Annotated MS/MS spectrum of ion 1537.689 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1537.689	Mass Error:	0.015	MH+ (mono):	1537.675	MH+ (avg):	1538.664
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	42	Above Threshold:	42
Assigned Peaks:	22	Not assigned Peaks:	20				

Peaklist:

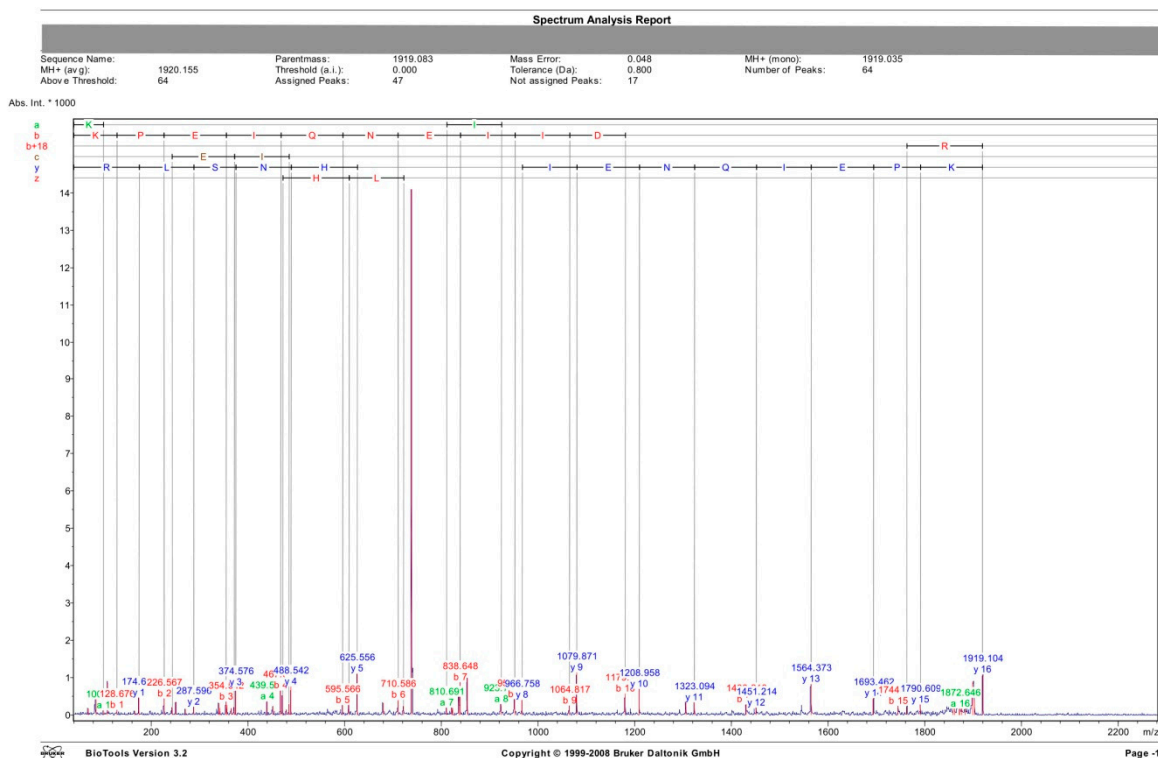
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.736	191.706	2	111.712	199.027	3	135.665	98.715	4	156.634	624.835	5	174.646	1434.016
6	200.552	108.650	7	226.596	166.861	8	256.613	97.210	9	260.544	321.451	10	286.561	79.806
11	288.547	80.255	12	297.570	317.376	13	300.565	86.750	14	303.586	136.642	15	321.596	110.425
16	357.551	150.069	17	368.564	357.901	18	374.589	481.942	19	390.577	140.414	20	439.563	241.021
21	446.547	874.708	22	460.571	181.064	23	471.583	373.817	24	488.595	169.567	25	517.540	150.616
26	553.548	163.703	27	559.599	282.805	28	610.583	137.552	29	624.608	123.420	30	630.607	218.757
31	649.632	136.638	32	701.659	788.346	33	709.640	168.762	34	906.763	145.267	35	910.778	434.375
36	927.849	471.358	37	1090.977	212.267	38	1277.165	468.729	39	1469.146	734.927	40	1475.690	286.271
41	1488.484	707.030	42	1519.955	237.926									

Calculated Masses:
MEWYPEAANAER

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	M	104.053	87.026	86.042	132.048	115.021	114.037	150.058	149.074	104.053	201.098	175.119	158.092	13	R
2	E	233.095	216.069	215.085	261.090	244.064	243.080	279.101	278.117	102.055	330.141	304.162	287.135	12	E
3	W	419.175	402.148	401.164	447.170	430.143	429.159	465.180	464.196	159.092	401.178	375.199	358.172	11	A
4	Y	582.238	565.212	564.228	610.233	593.206	592.222	628.244	627.260	136.076	515.221	489.242	472.215	10	N
5	P	679.291	662.264	661.280	707.286	690.259	689.275	725.296	724.312	70.065	586.258	560.279	543.252	9	A
6	E	898.333	791.307	790.323	836.328	819.302	818.318	854.339	853.355	102.055	657.295	631.316	614.299	8	A
7	A	879.371	862.344	861.360	907.365	890.339	889.355	925.376	924.392	44.049	728.332	702.353	685.326	7	A
8	A	950.408	933.381	932.397	978.403	961.376	960.392	996.413	995.429	44.049	857.375	831.396	814.369	6	E
9	A	1021.445	1004.418	1003.434	1049.440	1032.413	1031.429	1067.450	1066.466	44.049	954.428	928.448	911.422	5	P
10	N	1135.488	1118.461	1117.477	1163.483	1146.456	1145.472	1181.493	1180.509	87.055	1117.491	1091.512	1074.485	4	Y
11	A	1206.525	1189.498	1188.514	1234.520	1217.493	1216.509	1252.530	1251.546	44.049	1303.570	1277.591	1260.564	3	W
12	E	1335.567	1318.541	1317.557	1363.562	1346.536	1345.552	1381.573	1380.589	102.055	1432.613	1406.634	1389.607	2	E
13	R	1491.609	1474.642	1473.658	1519.663	1502.637	1501.653	1537.674	1536.690	129.113	1563.653	1537.674	1520.647	1	M

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Area 6. Annotated MS/MS spectrum of ion 1919.083 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1919.083	Mass Error:	0.048	MH+ (mono):	1919.035	MH+ (avg):	1920.155
Threshold (a.i.):	0.000	Tolerance (Da):	0.800	Number of Peaks:	64	Above Threshold:	64
Assigned Peaks:	47	Not assigned Peaks:	17				

Peaklist:

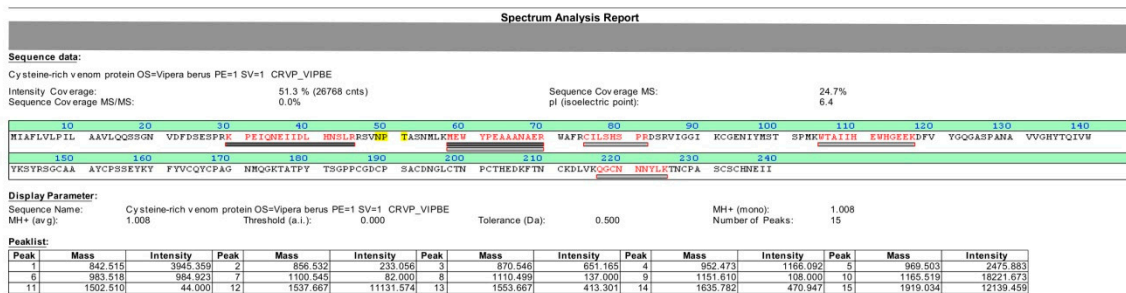
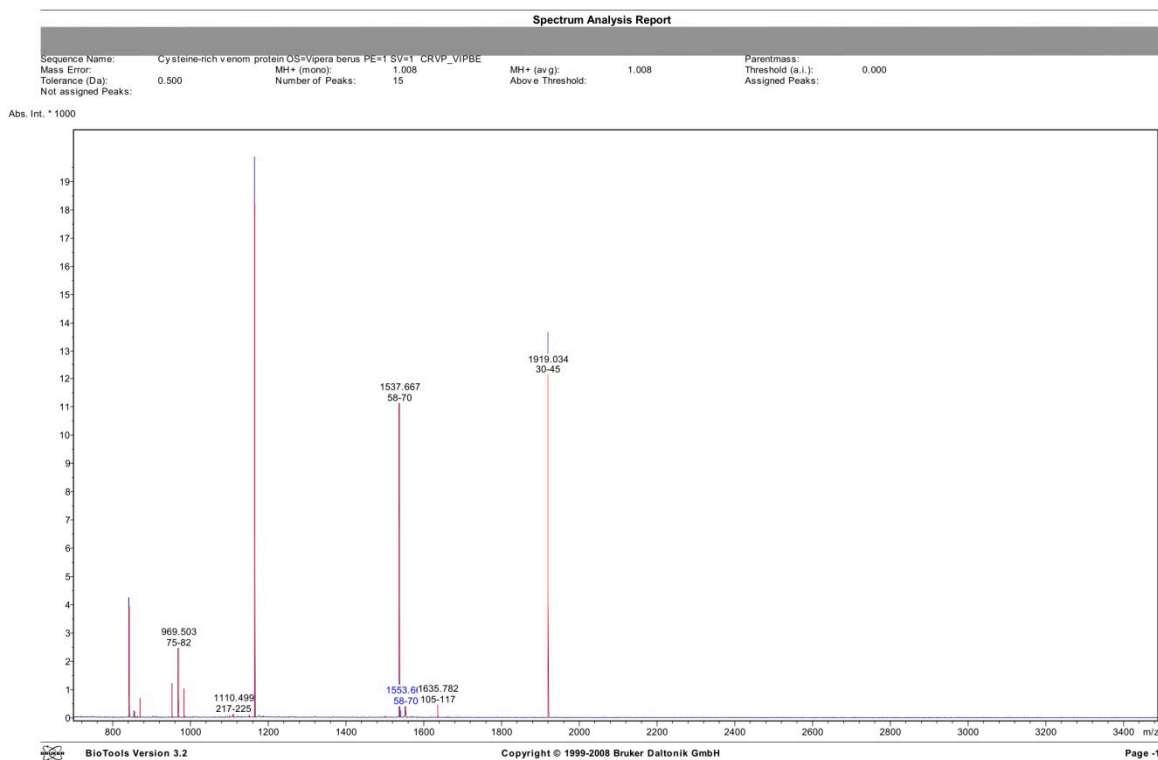
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.743	183.296	2	85.737	547.237	3	100.669	124.960	4	109.657	862.611	5	126.676	133.026
6	165.593	113.922	7	174.630	481.209	8	226.567	439.126	9	243.539	204.624	10	250.162	350.474
11	270.587	163.836	12	287.596	219.746	13	339.556	321.415	14	341.565	191.932	15	354.542	357.949
16	356.539	271.400	17	365.528	184.930	18	371.485	216.771	19	374.576	741.663	20	439.571	366.190
21	451.549	247.241	22	467.541	659.776	23	471.535	537.121	24	479.497	150.776	25	484.530	303.255
26	488.542	760.584	27	595.566	264.610	28	608.550	451.697	29	625.556	1111.603	30	679.580	331.562
31	710.586	408.518	32	721.596	246.278	33	738.618	14315.169	34	810.691	193.603	35	821.572	195.225
36	823.631	189.622	37	838.619	729.155	38	838.648	676.129	39	853.648	994.284	40	923.726	292.645
41	951.750	422.505	42	966.758	404.363	43	1064.817	250.717	44	1079.871	1141.066	45	1179.903	573.248
46	1208.958	696.111	47	1306.034	356.315	48	1323.094	335.478	49	1430.218	286.163	50	1451.214	193.102
51	1564.373	830.713	52	1693.462	453.762	53	1744.548	238.599	54	1762.588	205.268	55	1790.609	276.629
56	1858.073	273.107	57	1861.462	162.332	58	1870.262	168.108	59	1872.646	167.528	60	1876.000	187.942
61	1883.316	162.279	62	1899.004	898.076	63	1902.249	410.830	64	1919.104	1082.336			

Calculated Masses:
KPEIQNEIIDLHNSLR

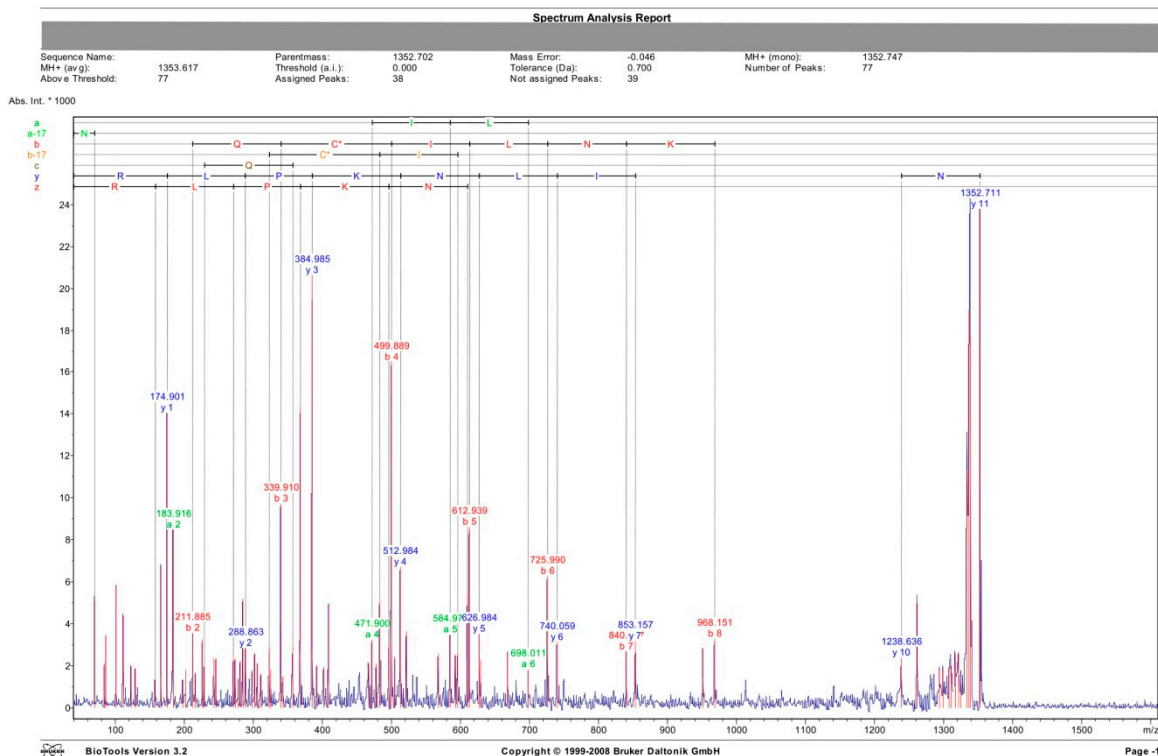
N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	K	161.107	84.081	83.097	129.102	112.076	111.092	147.113	146.129	101.107	201.098	175.119	158.092	16	R
2	P	198.160	181.134	180.150	226.155	209.129	208.144	244.166	243.182	70.965	314.192	288.203	271.176	15	L
3	E	327.203	310.176	309.192	355.198	338.171	337.187	373.208	372.224	102.055	401.214	375.235	358.208	14	S
4	I	446.287	423.260	422.276	468.282	451.255	450.271	486.292	485.308	86.096	515.257	489.278	472.251	13	N
5	Q	568.345	551.319	550.335	596.340	579.314	578.330	614.351	613.367	101.071	652.316	626.337	609.310	12	H
6	N	682.388	665.362	664.378	710.383	693.357	692.373	728.394	727.410	87.055	765.400	739.421	722.394	11	L
7	E	811.431	794.404	793.420	839.426	822.399	821.415	857.436	856.452	102.055	880.427	854.448	837.421	10	D
8	I	924.515	907.488	906.504	952.510	935.483	934.499	970.520	969.536	86.096	993.511	967.532	950.505	9	I
9	I	1037.599	1020.572	1019.588	1065.594	1048.567	1047.583	1083.604	1082.620	86.096	1106.595	1080.616	1063.589	8	I
10	D	1152.626	1135.599	1134.615	1180.621	1163.594	1162.610	1198.631	1197.647	88.039	1235.638	1209.659	1192.632	7	E
11	L	1265.710	1248.683	1247.699	1293.705	1276.678	1275.694	1311.715	1310.731	86.096	1349.681	1323.702	1306.675	6	N
12	H	1402.769	1385.742	1384.758	1430.764	1413.737	1412.753	1448.774	1447.790	110.071	1477.739	1451.760	1434.734	5	Q
13	N	1516.812	1499.785	1498.801	1544.807	1527.780	1526.796	1562.817	1561.833	87.055	1590.823	1564.844	1547.818	4	I
14	S	1603.844	1586.817	1585.833	1631.839	1614.812	1613.828	1649.849	1648.865	60.044	1719.866	1693.887	1676.860	3	E
15	L	1716.928	1699.901	1698.917	1744.923	1727.896	1726.912	1762.933	1761.949	86.096	1816.919	1790.940	1773.913	2	P
16	R	1873.029	1856.002	1855.018	1901.024	1883.997	1883.013	1919.034	1918.050	129.113	1945.014	1919.034	1902.008	1	K

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Area 6. Annotated MS spectrum.



Area 7. Annotated MS/MS spectrum of ion 1352.702 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1352.702 Mass Error: -0.046 MH+ (mono): 1352.747 MH+ (avg): 1353.617
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 77 Above Threshold: 77
 Assigned Peaks: 38 Not assigned Peaks: 39

Peaklist:

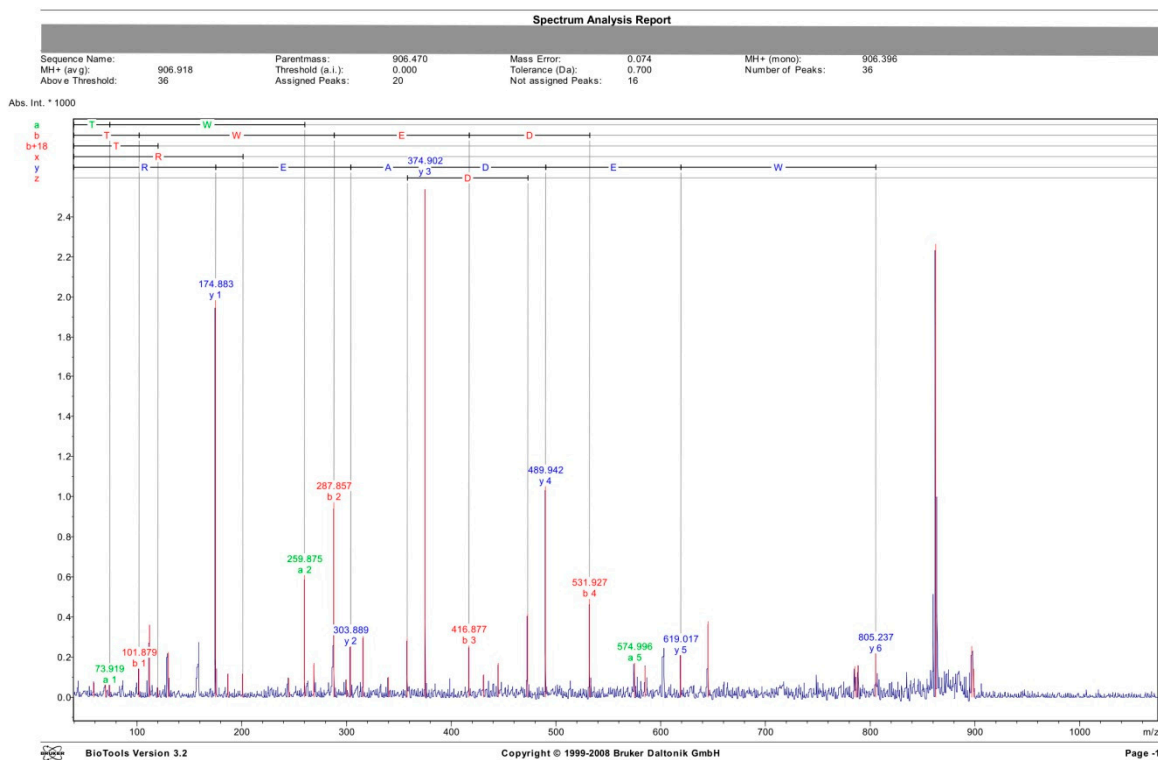
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.910	5065.252	2	83.872	2102.419	3	85.917	3457.762	4	100.895	5758.177	5	111.885	4371.352
6	122.876	1974.106	7	128.902	1851.665	8	157.876	1329.482	9	165.920	6765.764	10	174.901	14039.176
11	183.916	8476.028	12	197.881	1342.141	13	201.866	1805.846	14	211.885	3567.100	15	215.872	1576.102
16	225.896	3247.634	17	228.897	2012.625	18	242.878	2379.322	19	245.892	2348.402	20	270.923	2374.222
21	273.887	2327.583	22	277.870	1402.269	23	280.901	2241.263	24	284.930	5205.458	25	288.883	2848.883
26	297.926	1804.046	27	301.948	2619.556	28	305.888	2137.419	29	310.960	1628.405	30	322.888	2925.059
31	324.958	1829.386	32	339.910	9718.122	33	342.921	1495.028	34	356.924	2905.438	35	367.966	14354.929
36	384.985	29649.534	37	391.896	2055.676	38	401.915	1955.561	39	408.913	4974.402	40	487.060	2059.741
41	471.900	3247.470	42	477.964	2110.729	43	482.893	5106.122	44	495.973	3065.326	45	499.889	16508.671
46	504.931	2442.597	47	512.984	6708.245	48	521.951	3648.397	49	567.992	2979.260	50	584.971	3495.130
51	592.968	2351.508	52	598.918	2929.541	53	609.987	5385.368	54	612.939	8611.992	55	626.984	3522.573
56	628.961	2267.172	57	668.150	2673.040	58	698.011	1835.941	59	725.990	6273.565	60	740.059	3126.003
61	840.047	2679.019	62	853.157	3181.052	63	951.198	2795.373	64	968.151	3284.891	65	1238.636	2388.804
66	1281.876	4979.990	67	1293.812	1808.184	68	1298.874	1837.302	69	1307.571	1851.768	70	1310.845	2023.643
71	1316.960	2578.750	72	1321.573	2655.980	73	1324.876	1475.611	74	1333.454	11352.822	75	1336.458	19014.176
76	1338.504	17785.474	77	1352.711	23800.547									

Calculated Masses:
 NPQCLLNKPLR 4: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term	Ion
1	N	87.055	76.029	69.045	115.050	98.024	97.040	133.081	132.077	87.055	201.098	175.119	158.092	11	R
2	P	184.108	167.082	166.097	212.103	195.076	194.092	230.114	229.130	70.065	314.182	288.203	271.176	10	L
3	Q	312.167	295.140	294.156	340.162	323.135	322.151	358.172	357.188	101.071	411.235	385.256	368.229	9	P
4	C*	472.197	455.171	454.187	500.192	483.166	482.182	518.203	517.219	133.043	539.330	513.351	496.324	8	K
5	I	585.211	568.255	567.271	613.276	596.250	595.266	631.287	630.303	86.096	653.373	627.394	610.367	7	N
6	L	698.365	681.339	680.355	726.360	709.334	708.350	744.371	743.387	86.096	796.457	740.478	723.451	6	L
7	N	812.408	795.382	794.398	840.403	823.377	822.393	858.414	857.430	87.055	879.541	853.562	836.535	5	I
8	K	940.503	923.477	922.493	968.498	951.472	950.488	996.509	995.525	101.107	1039.572	1013.552	996.566	4	C*
9	P	1037.556	1020.530	1019.545	1065.551	1048.524	1047.540	1083.562	1082.578	70.065	1167.630	1141.651	1124.624	3	Q
10	L	1150.640	1133.614	1132.630	1178.635	1161.608	1160.624	1196.646	1195.662	86.096	1264.683	1238.704	1221.677	2	P
11	R	1306.741	1289.715	1288.731	1334.736	1317.710	1316.726	1352.747	1351.763	129.113	1378.726	1352.747	1335.720	1	N

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Area 8. Annotated MS/MS spectrum of ion 906.470 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	906.470	Mass Error:	0.074	MH+ (mono):	906.396	MH+ (avg):	906.918
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	36	Above Threshold:	36
Assigned Peaks:	20	Not assigned Peaks:	16				

Peaklist:

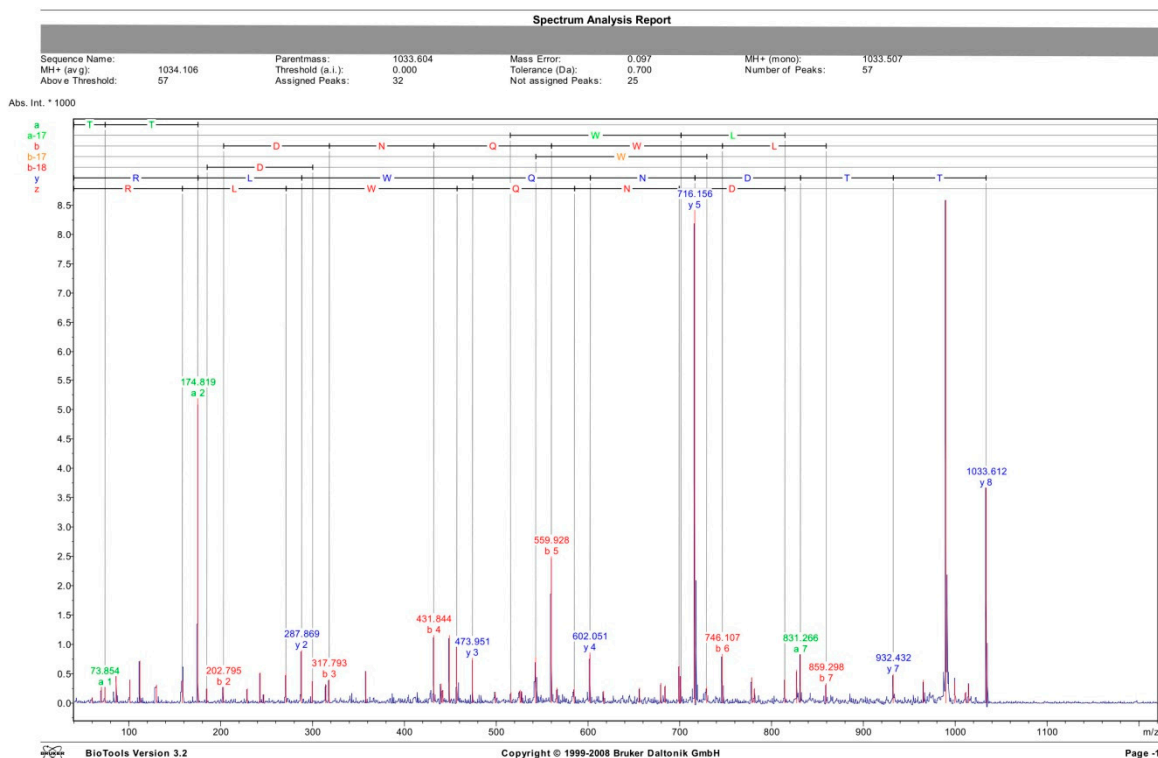
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.919	73.528	2	69.922	119.166	3	73.919	61.187	4	101.879	143.001	5	111.903	362.691
6	119.914	48.501	7	129.895	225.340	8	174.883	1984.574	9	188.853	117.581	10	200.847	119.080
11	244.825	96.662	12	259.875	608.640	13	268.851	171.612	14	287.857	972.167	15	299.856	89.139
16	303.889	254.334	17	315.845	304.714	18	339.896	101.396	19	357.875	293.583	20	374.902	2600.803
21	416.877	297.521	22	430.899	114.263	23	444.879	171.333	24	472.912	417.532	25	489.942	1051.690
26	531.927	490.850	27	574.996	172.049	28	585.032	152.353	29	619.017	209.573	30	645.034	378.852
31	785.239	153.821	32	788.156	160.231	33	805.237	217.994	34	862.402	2265.972	35	896.831	255.080
36	898.793	143.110												

Calculated Masses:
TWEDAER

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	T	74.060	57.033	58.049	102.055	85.028	84.044	120.066	119.082	74.060	291.098	175.119	158.092	7	R
2	W	260.139	243.113	242.129	288.134	271.108	270.124	306.145	305.161	159.092	330.141	304.162	287.135	6	E
3	E	389.182	372.155	371.171	417.177	400.150	399.166	435.187	434.203	102.055	401.178	375.199	358.172	5	A
4	D	594.209	487.182	486.198	532.204	515.177	514.193	550.214	549.230	88.039	518.205	490.226	473.199	4	D
5	A	575.246	558.219	557.235	603.241	586.214	585.230	621.251	620.267	44.040	645.247	619.268	602.242	3	E
6	E	704.289	687.262	686.278	732.284	715.257	714.273	750.294	749.310	102.055	831.327	805.348	788.321	2	W
7	R	860.390	843.363	842.379	888.385	871.358	870.374	906.395	905.411	129.113	932.374	906.395	889.369	1	T

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Area 8. Annotated MS/MS spectrum of ion 1033.604 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1033.604	Mass Error:	0.097	MH+ (mono):	1033.507	MH+ (avg):	1034.106
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	57	Above Threshold:	57
Assigned Peaks:	32	Not assigned Peaks:	25				

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	59.840	101.370	2	69.846	437.583	3	73.854	274.026	4	85.863	528.492	5	100.833	399.318
6	111.833	725.201	7	129.803	308.694	8	157.791	393.084	9	174.819	5189.708	10	184.781	253.816
11	202.795	278.433	12	228.818	253.908	13	242.789	524.628	14	246.775	150.569	15	270.846	513.006
16	287.869	905.603	17	299.828	378.465	18	313.856	325.729	19	317.793	404.945	20	357.802	541.391
21	431.844	1168.222	22	439.870	335.817	23	441.825	220.350	24	448.872	1159.970	25	456.913	1100.983
26	473.951	772.124	27	498.911	195.145	28	515.874	188.803	29	525.890	226.461	30	527.933	198.167
31	542.889	786.334	32	569.928	2498.327	33	565.996	266.541	34	584.994	254.202	35	602.051	864.990
36	616.989	209.650	37	658.068	265.087	38	679.103	348.157	39	684.045	303.659	40	698.106	637.395
41	701.044	458.358	42	716.156	8417.641	43	729.063	283.549	44	746.107	840.568	45	778.231	440.221
46	781.265	257.797	47	814.238	403.801	48	827.212	671.534	49	831.266	834.490	50	859.298	337.601
51	932.432	495.990	52	965.330	398.028	53	989.548	8714.517	54	999.542	363.953	55	1011.521	194.321
56	1014.629	322.874	57	1033.612	3667.912									

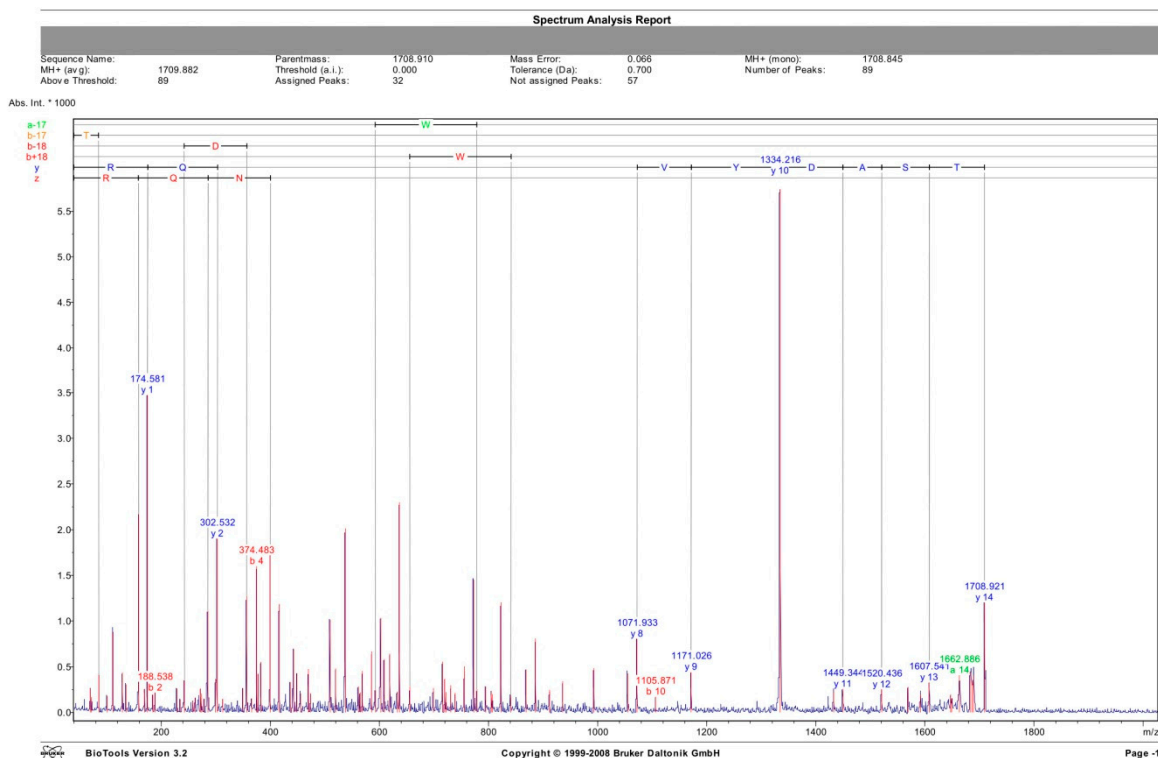
Calculated Masses:

TTDNGWLR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	j	x	y	z	C-Term	Ion
1	T	74.060	57.033	56.049	102.055	85.028	84.044	120.066	119.082	74.060	201.088	175.119	158.092	5	R	
2	T	175.168	158.081	157.097	203.103	186.076	185.092	221.113	220.129	74.060	314.182	288.203	271.176	7	L	
3	D	290.135	273.108	272.124	318.130	301.103	300.119	336.140	335.156	88.039	500.202	474.282	457.256	6	W	
4	N	404.178	387.151	386.167	432.173	415.146	414.162	450.183	449.199	87.055	628.320	602.341	585.314	5	Q	
5	Q	532.236	515.210	514.226	560.231	543.205	542.221	578.242	577.258	101.071	742.363	716.384	699.357	4	N	
6	W	718.315	701.289	700.305	746.310	729.284	728.300	764.321	763.337	159.092	857.390	831.411	814.384	3	D	
7	L	831.400	814.373	813.389	859.394	842.368	841.384	877.405	876.421	86.096	958.438	932.458	915.432	2	T	
8	R	987.501	970.474	969.490	1015.495	998.469	997.485	1033.506	1032.522	129.113	1059.485	1033.506	1016.480	1	T	

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Area 8. Annotated MS/MS spectrum of ion 1708.910 m/z.



Spectrum Analysis Report

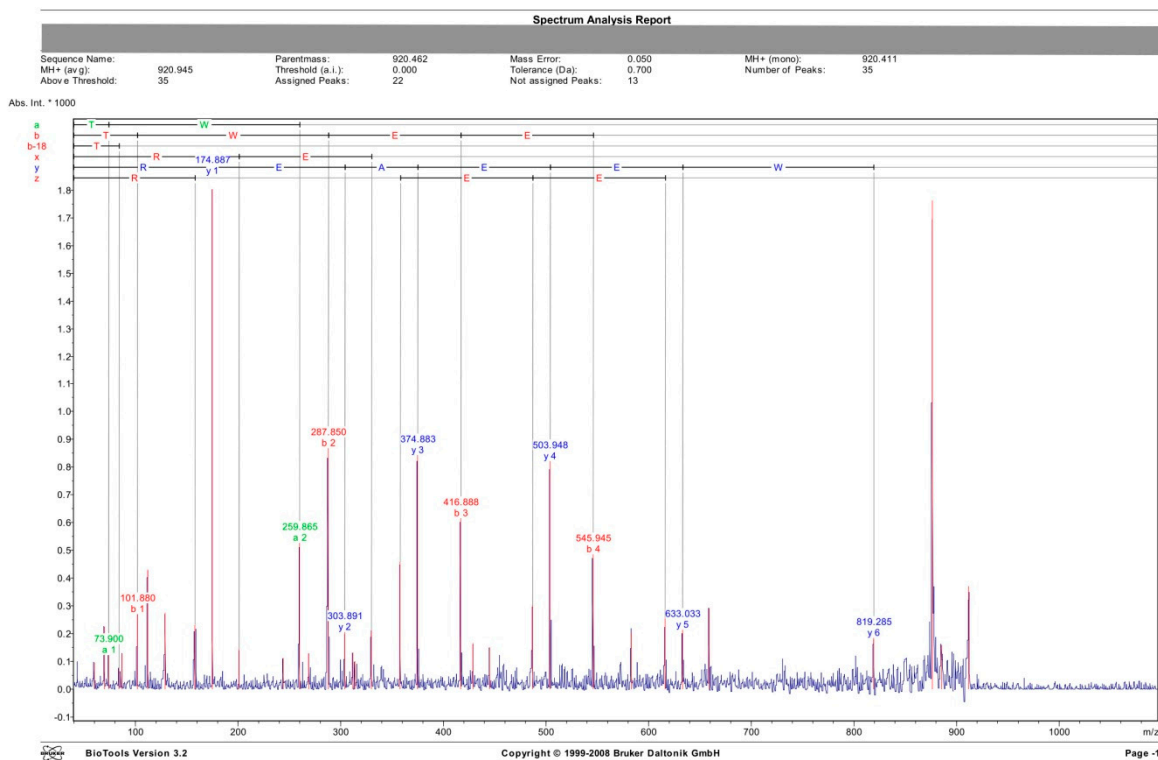
Display Parameter: Parentmass: 1708.910 Mass Error: 0.068 MH+ (mono): 1708.845 MH+ (avg): 1709.882
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 89 Above Threshold: 89
 Assigned Peaks: 32 Not assigned Peaks: 57

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.693	264.716	2	71.760	168.365	3	85.680	405.676	4	100.650	181.989	5	111.640	892.285
6	128.832	430.026	7	135.684	308.408	8	158.585	2163.922	9	169.530	236.952	10	174.581	3475.044
11	184.535	193.875	12	188.538	215.046	13	228.543	262.439	14	234.530	143.860	15	242.509	351.518
16	257.549	131.234	17	262.534	183.152	18	271.557	263.750	19	273.472	207.729	20	278.489	150.691
21	298.521	1112.268	22	299.533	368.081	23	302.532	1901.775	24	312.520	148.129	25	348.474	298.497
26	356.512	1276.036	27	365.487	154.426	28	374.483	1600.544	29	377.472	426.950	30	382.493	555.788
31	399.512	1783.981	32	416.517	1188.761	33	436.448	333.033	34	442.485	693.721	35	448.497	428.419
36	455.526	209.125	37	489.541	475.858	38	473.507	212.889	39	509.489	1015.786	40	519.488	482.350
41	537.477	2014.807	42	561.500	286.127	43	564.494	218.821	44	568.521	454.901	45	585.518	698.474
46	592.509	245.185	47	602.549	1035.823	48	608.557	584.374	49	618.534	643.592	50	632.536	229.486
51	636.534	2300.353	52	658.594	281.546	53	698.553	287.778	54	715.620	556.423	55	719.556	369.977
56	721.553	224.098	57	730.609	299.273	58	738.594	215.727	59	755.607	506.658	60	772.647	1454.402
61	778.573	253.699	62	794.591	285.718	63	804.637	232.461	64	806.632	200.703	65	822.624	1204.604
66	840.688	189.552	67	868.720	470.236	68	885.748	811.804	69	911.696	247.492	70	935.725	342.734
71	992.750	485.733	72	1054.857	427.905	73	1071.933	806.260	74	1105.871	172.301	75	1171.026	442.651
76	1334.216	5888.905	77	1432.326	228.242	78	1449.344	256.885	79	1520.436	251.054	80	1569.133	279.825
81	1591.428	196.577	82	1607.541	328.454	83	1646.898	198.769	84	1648.764	154.734	85	1662.886	408.585
86	1682.764	449.988	87	1685.724	337.695	88	1688.633	405.012	89	1708.921	1202.921			

Calculated Masses:
 TSADYVWGLWNGR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	T	74.060	57.033	56.049	102.055	85.028	84.044	120.066	119.082	74.060	201.098	175.119	158.092	14	R
2	S	161.092	144.066	143.082	189.087	172.060	171.076	207.098	206.114	60.044	329.157	303.178	286.151	13	Q
3	A	232.129	215.103	214.119	260.124	243.098	242.114	278.135	277.151	44.049	443.200	417.220	400.194	12	N
4	D	347.156	330.130	329.146	375.151	358.124	357.140	393.162	392.178	88.039	629.279	603.300	586.273	11	W
5	Y	510.219	493.193	492.209	538.214	521.188	520.204	556.225	555.241	136.076	742.363	716.384	699.357	10	L
6	V	609.288	592.261	591.277	637.283	620.256	619.272	655.293	654.309	72.081	799.385	773.405	756.379	9	G
7	W	795.367	778.341	777.357	823.362	806.336	805.352	841.373	840.389	159.092	912.469	886.489	869.463	8	I
8	I	908.451	891.425	890.441	936.446	919.420	918.436	954.457	953.473	86.096	1098.548	1072.569	1055.542	7	W
9	G	985.473	948.446	947.462	993.468	976.441	975.457	1011.478	1010.494	30.034	1197.616	1171.637	1154.611	6	V
10	L	1078.557	1061.530	1060.546	1106.552	1089.525	1088.541	1124.562	1123.578	86.096	1360.680	1334.700	1317.674	5	Y
11	W	1264.636	1247.610	1246.626	1292.631	1275.604	1274.620	1310.642	1309.658	159.092	1475.707	1449.727	1432.701	4	D
12	N	1378.678	1361.652	1360.668	1406.674	1389.647	1388.663	1424.684	1423.700	87.055	1546.744	1520.764	1503.738	3	A
13	Q	1506.798	1489.771	1488.787	1534.793	1517.766	1516.782	1552.743	1551.759	101.071	1633.776	1607.797	1590.770	2	S
14	R	1662.839	1645.812	1644.828	1690.834	1673.807	1672.823	1708.844	1707.860	129.113	1734.823	1708.844	1691.818	1	T

Area 8. Annotated MS/MS spectrum of ion 920.462 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	920.462	Mass Error:	0.050	MH+ (mono):	920.411	MH+ (avg):	920.945
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	35	Above Threshold:	35
Assigned Peaks:	22	Not assigned Peaks:	13				

Peaklist:

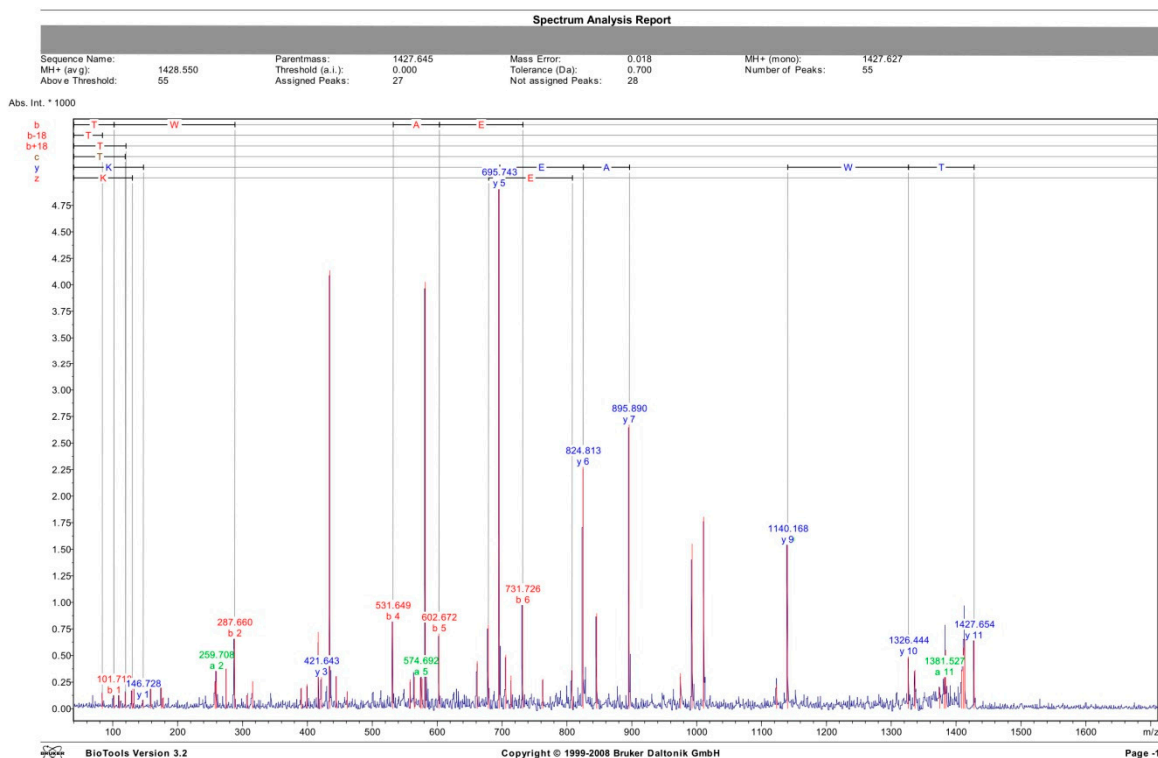
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	59.892	96.345	2	69.900	225.016	3	73.900	123.150	4	83.947	74.618	5	86.919	127.255
6	101.880	270.253	7	111.901	431.080	8	128.897	274.830	9	157.872	230.725	10	174.887	185.706
11	200.840	143.767	12	243.862	112.382	13	289.865	526.660	14	268.850	129.909	15	287.850	867.312
16	303.891	205.426	17	311.832	131.390	18	318.858	100.588	19	329.831	210.146	20	357.859	458.432
21	374.883	842.048	22	418.888	815.411	23	428.870	165.408	24	448.870	150.327	25	486.878	301.315
26	503.948	820.205	27	545.945	485.607	28	583.036	205.010	29	615.987	254.610	30	633.033	213.817
31	659.039	291.379	32	819.285	184.862	33	876.392	1763.633	34	885.407	159.648	35	911.749	370.751

Calculated Masses:
TWEEAER

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term	Ion
1	T	74.060	57.033	56.049	102.055	85.028	84.044	120.066	119.082	74.060	201.098	175.119	158.092	7	R
2	W	260.139	243.113	242.139	288.134	271.108	270.124	306.145	305.161	159.051	330.141	304.162	287.135	6	E
3	E	389.182	372.155	371.171	417.177	400.150	399.166	435.187	434.203	102.055	401.178	375.199	358.172	5	A
4	E	518.225	501.198	500.214	546.219	529.193	528.209	564.230	563.246	102.055	530.221	504.241	487.215	4	E
5	A	589.262	572.235	571.251	617.257	600.230	599.246	635.267	634.283	44.049	659.283	633.284	616.257	3	E
6	E	718.304	701.278	700.294	746.299	729.273	728.289	764.310	763.326	102.055	845.342	819.363	802.337	2	W
7	R	874.405	857.379	856.395	902.400	885.374	884.390	920.411	919.427	129.113	946.390	920.411	903.384	1	T

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Area 8. Annotated MS/MS spectrum of ion 1427.645 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1427.645
 Threshold (a.i.): 0.000
 Assigned Peaks: 27
 Mass Error: 0.018
 Tolerance (Da): 0.700
 Not assigned Peaks: 28
 MH+ (mono): 1427.627
 Number of Peaks: 55
 MH+ (avg): 1428.550
 Above Threshold: 55

Peaklist:

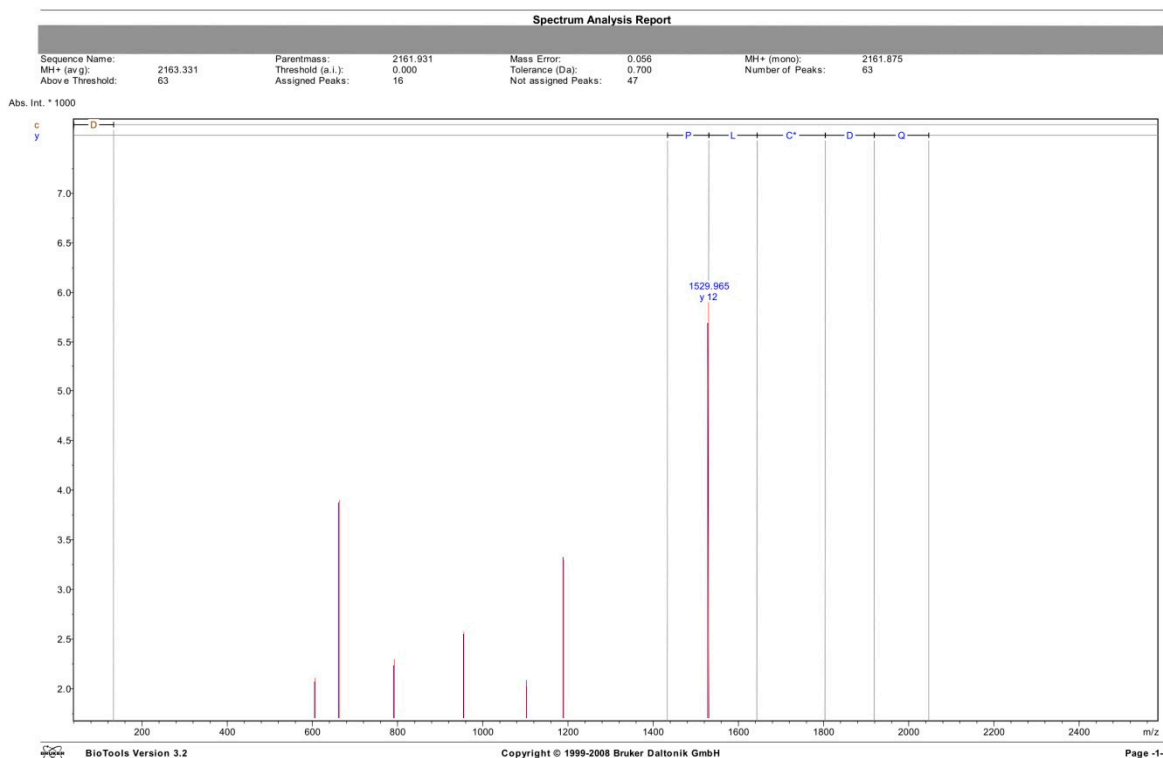
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	83.770	144.580	2	101.718	125.030	3	109.708	136.340	4	119.712	151.598	5	129.709	170.773
6	132.861	242.407	7	146.129	83.109	8	158.890	238.530	9	174.694	198.569	10	177.668	103.013
11	257.694	256.620	12	259.708	354.628	13	274.702	378.302	14	287.660	659.658	15	307.634	136.978
16	315.641	258.347	17	390.651	196.284	18	399.664	231.286	19	416.652	721.904	20	421.643	297.300
21	434.672	4137.888	22	444.634	307.552	23	461.648	166.272	24	531.649	819.787	25	568.657	278.134
26	564.686	334.246	27	574.692	298.139	28	576.662	286.335	29	581.699	4029.075	30	602.672	707.719
31	661.697	447.624	32	678.712	789.238	33	695.743	4911.063	34	705.731	508.412	35	713.737	311.937
36	731.726	974.290	37	762.681	278.438	38	807.611	367.857	39	824.813	2277.068	40	845.795	698.486
41	895.890	2673.718	42	974.936	333.997	43	992.979	1552.715	44	1010.988	1807.045	45	1123.207	226.778
46	1140.168	1541.822	47	1326.444	491.706	48	1336.487	364.776	49	1374.892	199.717	50	1381.527	295.139
51	1383.731	553.662	52	1408.327	369.054	53	1411.200	973.370	54	1413.246	654.026	55	1427.654	641.563

Calculated Masses:
 TWDEAEKFCNK 9: Carbamidomethyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b-18.044	b+18	c	i	x	y	z	C-Term	Ion
1	T	74.060	57.033	58.049	102.055	85.028	84.044	120.866	119.082	74.060	173.092	147.113	130.086	11	K	
2	W	260.139	243.113	242.129	288.134	271.108	270.124	306.145	305.161	199.092	287.135	261.156	244.129	10	N	
3	D	375.166	358.140	357.156	403.161	386.135	385.151	421.172	420.188	88.039	447.166	421.186	404.160	9	C*	
4	E	594.209	487.182	486.198	532.204	515.177	514.193	550.214	549.230	102.055	594.234	568.255	551.238	8	F	
5	A	575.246	558.219	557.235	603.241	586.214	585.230	621.251	620.267	44.040	722.329	696.350	679.323	7	K	
6	E	704.289	687.262	686.278	732.284	715.257	714.273	750.294	749.310	102.055	851.372	825.392	806.366	6	E	
7	K	832.384	815.357	814.373	860.378	843.352	842.368	878.389	877.405	101.107	922.409	896.429	879.403	5	A	
8	F	979.452	962.425	961.441	1007.447	990.420	989.436	1025.457	1024.473	120.081	1051.451	1025.472	1008.446	4	E	
9	C*	1139.483	1122.456	1121.472	1167.478	1150.451	1149.467	1185.488	1184.504	133.043	1166.478	1140.499	1123.472	3	D	
10	N	1253.526	1236.499	1235.515	1281.520	1264.494	1263.510	1299.531	1298.547	87.055	1352.558	1326.578	1309.552	2	W	
11	K	1381.621	1364.594	1363.610	1409.615	1392.589	1391.605	1427.626	1426.642	101.107	1453.605	1427.626	1410.599	1	T	

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Area 8. Annotated MS/MS spectrum of ion 2161.931 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 2161.931 Mass Error: 0.058 MH+ (mono): 2161.875 MH+ (avg): 2163.331
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 63 Above Threshold: 63
 Assigned Peaks: 16 Not assigned Peaks: 47

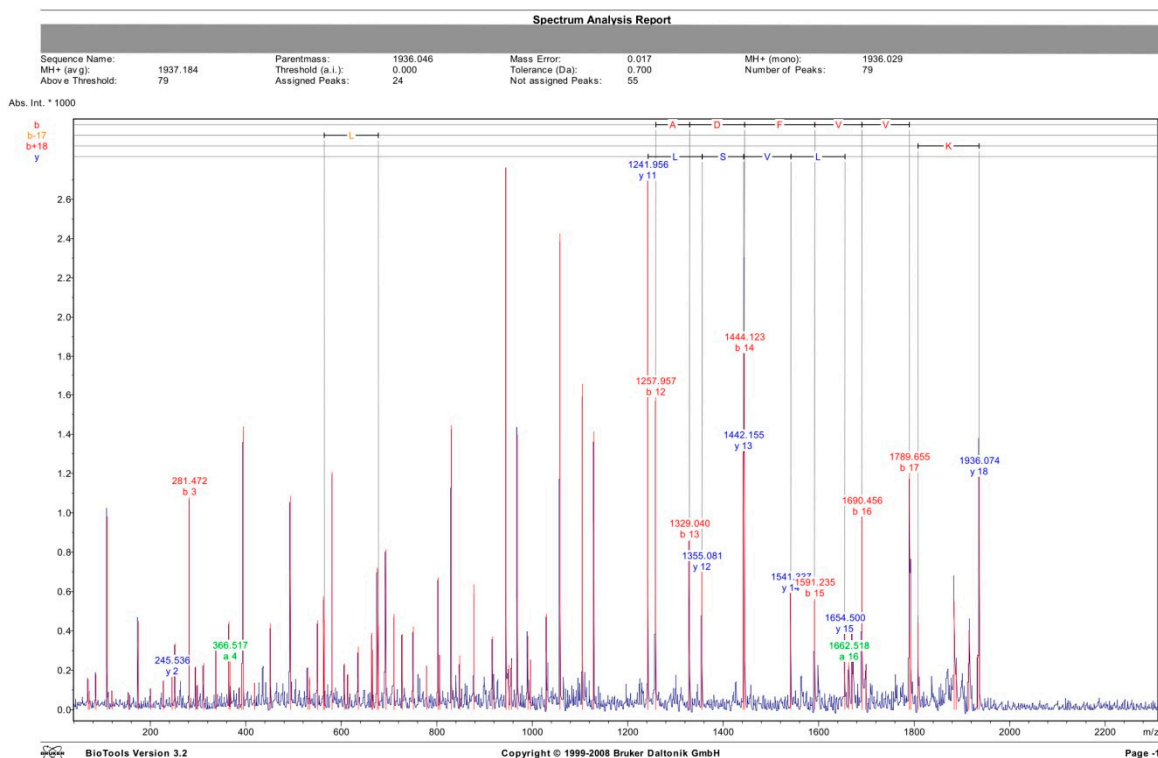
Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	109.605	626.436	2	132.536	137.798	3	135.542	162.113	4	158.539	221.837	5	174.501	135.132
6	194.497	198.137	7	243.407	320.094	8	273.397	147.820	9	275.369	188.177	10	295.390	228.011
11	297.356	392.571	12	312.420	309.383	13	323.400	198.923	14	340.391	376.965	15	354.334	376.134
16	358.345	471.687	17	370.350	151.504	18	375.353	151.838	19	409.388	244.396	20	427.353	770.350
21	455.335	186.501	22	469.354	994.361	23	483.342	227.173	24	518.281	733.369	25	540.350	455.766
26	544.396	1103.196	27	556.375	255.489	28	574.355	268.653	29	606.357	2110.621	30	628.358	248.575
31	631.331	544.615	32	646.323	330.303	33	663.366	3900.165	34	692.399	276.235	35	709.410	258.500
36	720.385	221.843	37	737.390	315.773	38	774.366	328.726	39	792.382	2295.266	40	866.429	492.133
41	923.499	345.449	42	955.478	2576.076	43	971.449	293.864	44	1032.610	481.495	45	1060.534	652.296
46	1102.586	2022.853	47	1171.870	247.966	48	1189.634	3295.237	49	1220.682	250.039	50	1375.803	733.720
51	1432.915	646.540	52	1511.970	374.945	53	1529.965	6902.089	54	1643.089	534.352	55	1692.100	424.519
56	1803.202	776.980	57	1918.457	325.597	58	2028.536	261.291	59	2033.605	398.088	60	2046.688	623.408
61	2056.964	222.040	62	2070.386	445.106	63	2101.251	258.569						

Calculated Masses:
 DODCLPGWSPYEGHCYK 4: Carbamidomethyl (C) 15: Carbamidomethyl (C)

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term.	Ion
1	D	88.039	71.013	70.029	116.034	99.008	98.024	134.045	133.061	88.039	173.092	147.113	130.086	17	K
2	Q	216.098	199.071	198.087	244.093	227.066	226.082	262.103	261.119	101.071	336.155	310.176	293.150	16	Y
3	D	331.125	314.098	313.114	358.120	342.093	341.109	377.130	376.146	88.039	496.186	470.207	453.180	15	C*
4	C*	491.155	474.129	473.145	519.150	502.124	501.140	537.161	536.177	133.043	633.245	607.266	590.239	14	H
5	L	694.240	687.213	686.229	832.234	815.208	814.224	850.245	849.261	88.066	690.266	664.287	647.261	13	G
6	P	701.292	684.266	683.282	729.287	712.261	711.277	747.298	746.314	70.065	819.309	793.330	776.303	12	E
7	G	758.314	741.287	740.303	786.309	769.282	768.298	804.319	803.335	30.034	982.372	956.393	939.367	11	Y
8	W	944.393	927.367	926.383	972.388	955.361	954.377	990.399	989.415	159.092	1129.441	1103.461	1086.435	10	F
9	S	1031.425	1014.399	1013.415	1059.420	1042.393	1041.409	1077.431	1076.447	60.044	1216.473	1190.494	1173.467	9	S
10	F	1178.494	1161.467	1160.483	1206.488	1189.462	1188.478	1224.499	1223.515	120.081	1402.552	1376.573	1359.546	8	W
11	Y	1361.557	1344.530	1343.546	1389.552	1372.525	1371.541	1407.562	1406.578	136.076	1459.574	1433.594	1416.568	7	G
12	E	1470.599	1453.573	1452.589	1498.594	1481.568	1480.584	1516.605	1515.621	102.055	1556.626	1530.647	1513.621	6	P
13	G	1527.621	1510.594	1509.610	1555.616	1538.589	1537.605	1573.626	1572.642	30.034	1669.710	1643.731	1626.705	5	L
14	H	1664.680	1647.653	1646.669	1692.675	1675.648	1674.664	1710.685	1709.701	110.071	1829.741	1803.762	1786.735	4	C*
15	C*	1824.710	1807.684	1806.700	1852.705	1835.679	1834.695	1870.716	1869.732	133.043	1944.768	1918.789	1901.762	3	D
16	Y	1987.774	1970.747	1969.763	2015.769	1998.742	1997.758	2033.779	2032.795	136.076	2072.827	2046.847	2029.821	2	Q
17	K	2115.869	2098.842	2097.858	2143.864	2126.837	2125.853	2161.874	2160.890	101.107	2187.853	2161.874	2144.848	1	D

Area 8. Annotated MS/MS spectrum of ion 1936.046 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1936.046 Mass Error: 0.017 MH+ (mono): 1936.029 MH+ (avg): 1937.184
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 79 Above Threshold: 79
 Assigned Peaks: 24 Not assigned Peaks: 55

Peaklist:

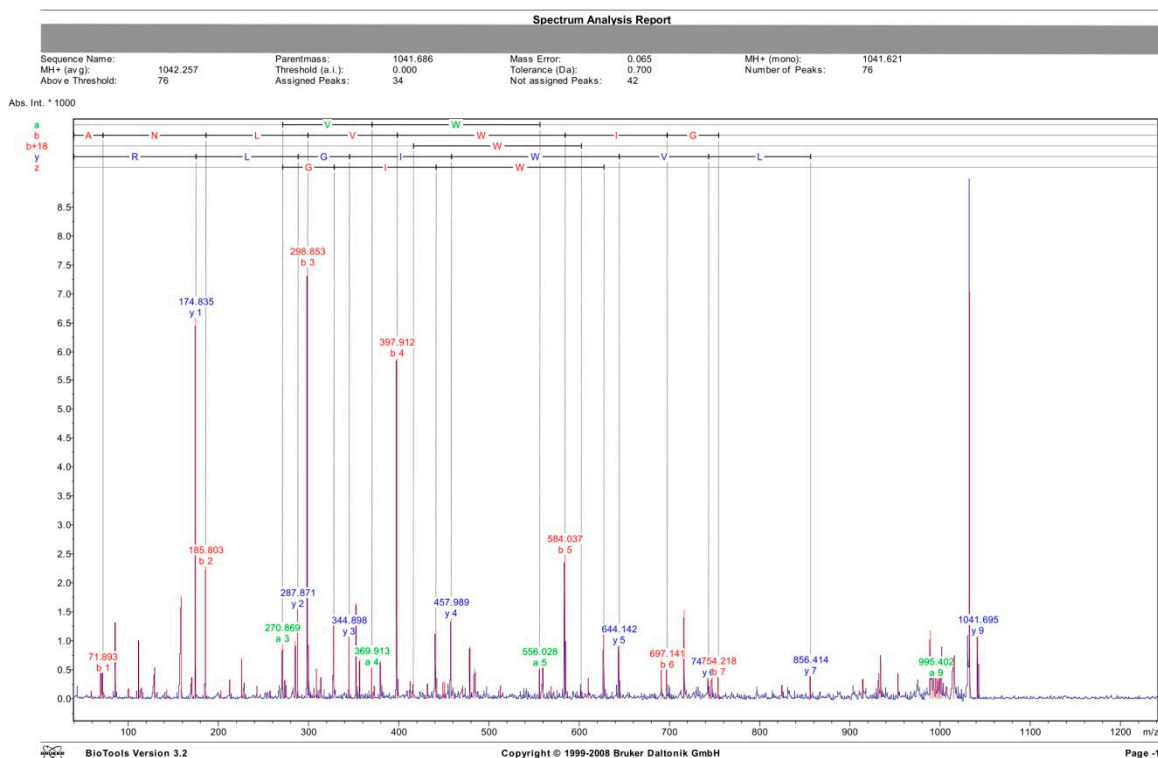
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.677	154.820	2	71.696	95.671	3	85.696	176.250	4	109.621	981.962	5	119.626	94.850
6	154.564	87.186	7	174.657	456.011	8	200.504	194.328	9	227.550	148.959	10	245.536	167.856
11	251.501	336.381	12	281.472	1079.343	13	294.503	220.273	14	298.508	128.641	15	311.509	236.902
16	337.491	346.021	17	364.498	449.146	18	366.517	244.381	19	386.449	114.669	20	391.436	238.572
21	394.476	1439.606	22	418.481	134.276	23	451.474	439.732	24	483.500	1088.976	25	525.477	214.937
26	533.453	166.081	27	550.468	454.705	28	562.496	575.208	29	564.520	458.787	30	580.527	1209.039
31	606.470	235.204	32	613.460	181.354	33	635.528	319.868	34	663.529	390.557	35	666.576	303.880
36	675.578	721.667	37	677.590	428.300	38	693.568	816.350	39	710.521	487.196	40	727.544	384.830
41	750.530	423.310	42	778.512	212.332	43	802.534	671.223	44	805.857	278.654	45	830.626	1446.311
46	847.608	275.154	47	877.606	637.773	48	916.645	372.187	49	944.675	2861.350	50	950.678	228.988
51	956.615	248.936	52	968.699	1398.132	53	990.717	375.153	54	996.671	245.445	55	1029.621	488.316
56	1057.775	2428.612	57	1104.814	1655.506	58	1128.838	1413.678	59	1241.956	2694.034	60	1257.957	1586.885
61	1329.040	863.602	62	1355.081	699.442	63	1442.155	1313.748	64	1444.123	1816.136	65	1541.937	592.159
66	1591.235	564.368	67	1654.500	384.251	68	1662.518	242.214	69	1670.253	462.234	70	1690.456	979.883
71	1698.367	228.307	72	1789.655	1202.330	73	1792.824	389.558	74	1807.777	440.482	75	1883.748	549.109
76	1887.964	230.638	77	1914.725	403.868	78	1932.518	280.131	79	1936.074	1183.048			

Calculated Masses:
 GSHLVSLHNAEADFVVK

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	G	30.034	13.067	12.023	58.029	41.002	40.018	76.039	75.055	30.034	173.092	147.113	130.086	18	K
2	S	117.066	100.039	99.055	145.061	128.034	127.050	183.071	182.087	80.044	272.160	246.181	228.155	17	V
3	H	254.125	237.098	236.114	282.120	265.093	264.109	300.130	299.146	110.071	371.229	345.250	328.223	16	V
4	L	367.209	350.182	349.198	395.204	378.177	377.193	413.214	412.230	86.096	518.297	492.318	475.291	15	F
5	V	466.277	449.251	448.267	494.272	477.246	476.262	512.283	511.299	72.081	633.324	607.345	590.318	14	D
6	S	553.309	536.283	535.299	581.304	564.278	563.294	599.315	598.331	60.044	704.361	678.382	661.356	13	A
7	L	666.393	649.367	648.383	694.398	677.362	676.378	712.399	711.415	86.096	833.404	807.425	790.398	12	E
8	H	803.452	786.426	785.442	831.447	814.421	813.437	849.458	848.474	110.071	904.441	878.462	861.435	11	A
9	N	917.495	900.469	899.485	945.490	928.464	927.480	963.501	962.517	87.055	1017.525	991.546	974.519	10	I
10	I	1030.579	1013.553	1012.569	1058.574	1041.548	1040.564	1076.585	1075.601	86.096	1131.568	1105.589	1088.562	9	N
11	A	1101.616	1084.590	1083.606	1129.611	1112.585	1111.601	1147.622	1146.638	44.049	1268.627	1242.648	1225.621	8	H
12	E	1230.659	1213.632	1212.648	1258.654	1241.627	1240.643	1276.664	1275.680	102.055	1381.711	1355.732	1338.705	7	L
13	A	1301.696	1284.670	1283.685	1329.691	1312.664	1311.680	1347.702	1346.718	44.049	1468.743	1442.764	1425.737	6	S
14	D	1416.723	1399.696	1398.712	1444.718	1427.691	1426.707	1462.728	1461.744	86.039	1567.811	1541.832	1524.806	5	V
15	F	1563.791	1546.765	1545.781	1591.786	1574.760	1573.776	1609.797	1608.813	120.081	1690.896	1664.916	1647.890	4	L
16	V	1662.860	1645.833	1644.849	1690.855	1673.828	1672.844	1708.865	1707.881	72.081	1817.954	1791.975	1774.949	3	H
17	V	1761.828	1744.802	1743.818	1789.823	1772.797	1771.813	1807.834	1806.850	72.081	1904.986	1879.007	1861.981	2	S
18	K	1880.823	1872.807	1872.813	1918.818	1900.802	1900.808	1936.829	1935.845	101.107	1962.908	1936.929	1919.902	1	G

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Area 8. Annotated MS/MS spectrum of ion 1041.686 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1041.686	Mass Error:	0.065	MH+ (mono):	1041.621	MH+ (av g):	1042.257
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	76	Above Threshold:	76
Assigned Peaks:	34	Not assigned Peaks:	42				

Peaklist:

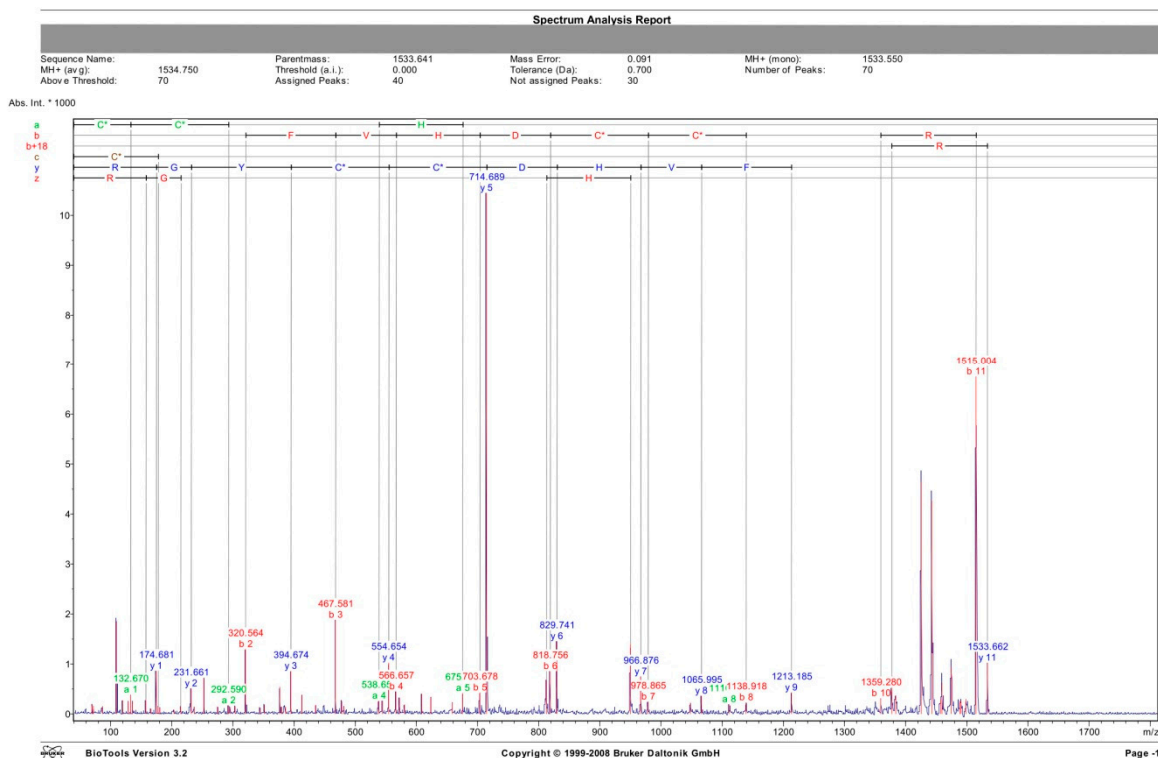
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.851	137.124	2	69.861	772.296	3	71.893	440.719	4	85.881	1314.254	5	100.829	181.268
6	111.846	1013.434	7	114.836	187.135	8	128.850	420.826	9	142.840	151.888	10	156.818	1771.833
11	170.830	373.724	12	174.835	6585.556	13	185.803	2284.423	14	202.809	145.292	15	212.827	333.168
16	225.844	700.579	17	228.836	286.895	18	242.816	220.258	19	257.856	135.627	20	270.869	944.086
21	274.096	327.064	22	284.887	1001.860	23	287.871	1548.303	24	298.853	7453.891	25	306.078	181.800
26	308.778	522.573	27	313.841	374.249	28	327.869	1353.794	29	344.898	1072.731	30	352.820	1651.589
31	356.873	694.235	32	369.913	544.382	33	373.154	210.924	34	379.870	657.014	35	397.912	5886.700
36	412.882	310.080	37	415.974	243.411	38	431.939	262.689	39	440.956	1193.208	40	448.940	297.970
41	450.948	287.952	42	457.989	1385.009	43	470.898	229.754	44	478.936	896.981	45	483.993	517.410
46	512.975	239.338	47	556.028	532.459	48	560.066	632.899	49	568.959	222.856	50	584.037	2475.207
51	602.110	267.289	52	610.055	369.013	53	627.061	1335.037	54	644.142	621.254	55	691.127	778.181
56	697.141	498.976	57	716.264	1532.698	58	743.293	361.975	59	747.243	430.272	60	754.218	370.382
61	825.240	239.468	62	856.414	390.818	63	914.701	350.344	64	932.336	410.942	65	934.262	662.807
66	953.572	449.540	67	989.090	1177.005	68	992.262	417.785	69	995.402	355.885	70	997.639	398.464
71	999.877	505.286	72	1001.870	754.990	73	1006.633	223.915	74	1015.057	720.047	75	1032.799	7038.152
76	1041.695	1083.408												

Calculated Masses:
ANLVWIGLR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term	Ion
1	A	44.049	27.023	26.039	72.044	55.018	54.034	90.055	89.071	44.049	201.098	175.119	158.092	9	R
2	N	158.092	141.066	140.082	186.087	169.061	168.077	204.098	203.114	87.051	314.182	288.203	271.176	8	L
3	L	271.176	254.150	253.166	299.171	282.145	281.161	317.182	316.198	86.096	371.204	345.224	328.198	7	G
4	V	370.245	353.218	352.234	398.240	381.213	380.229	416.250	415.266	72.081	484.288	458.309	441.282	6	I
5	W	586.224	539.298	538.314	594.319	567.293	566.309	602.338	601.346	159.092	670.387	644.388	627.361	5	W
6	I	689.408	652.382	651.398	697.403	680.377	679.393	715.414	714.430	86.096	769.436	743.456	726.430	4	V
7	G	726.430	709.403	708.419	754.425	737.398	736.414	772.435	771.451	30.034	862.520	856.540	839.514	3	L
8	L	839.514	822.487	821.503	867.509	850.482	849.498	885.519	884.535	86.096	996.563	970.553	953.557	2	N
9	R	995.615	978.588	977.604	1023.610	1006.583	1005.599	1041.620	1040.636	129.113	1067.600	1041.620	1024.594	1	A

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Area 9. Annotated MS/MS spectrum of ion 1533.641m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1533.641 Mass Error: 0.091 MH+ (mono): 1533.550 MH+ (avg): 1534.750
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 70 Above Threshold: 70
 Assigned Peaks: 40 Not assigned Peaks: 30

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.759	184.457	2	71.774	164.499	3	86.754	159.733	4	109.711	1858.705	5	119.744	276.796
6	129.796	292.970	7	132.670	388.055	8	135.700	245.413	9	157.693	274.324	10	165.643	109.625
11	174.681	864.403	12	177.634	157.492	13	180.709	122.772	14	203.612	80.306	15	214.661	153.981
16	231.661	513.149	17	236.643	146.864	18	252.626	719.782	19	275.587	141.123	20	292.590	172.229
21	295.631	142.503	22	303.579	158.836	23	320.564	1295.980	24	344.613	126.182	25	351.674	186.977
26	376.598	546.027	27	379.650	147.150	28	386.017	149.093	29	394.674	858.297	30	412.566	382.739
31	435.544	182.326	32	467.581	1883.469	33	477.993	259.981	34	481.574	145.291	35	536.656	262.590
36	544.640	442.969	37	554.654	1029.054	38	566.667	450.838	39	572.633	327.638	40	580.528	191.364
41	608.649	407.815	42	623.664	343.345	43	658.690	229.026	44	675.676	420.223	45	703.678	429.796
46	714.689	10450.668	47	812.732	682.540	48	818.756	855.050	49	829.741	1455.148	50	948.835	1402.541
51	966.876	750.879	52	978.865	245.201	53	1047.807	229.734	54	1065.695	354.157	55	1110.971	138.414
56	1138.918	233.732	57	1213.185	430.765	58	1359.280	317.139	59	1377.288	526.091	60	1383.776	375.366
61	1425.305	4653.307	62	1442.458	4263.258	63	1487.065	280.733	64	1459.323	625.393	65	1474.514	952.622
66	1486.745	262.311	67	1490.638	257.867	68	1496.523	300.063	69	1515.004	6752.401	70	1533.662	1023.673

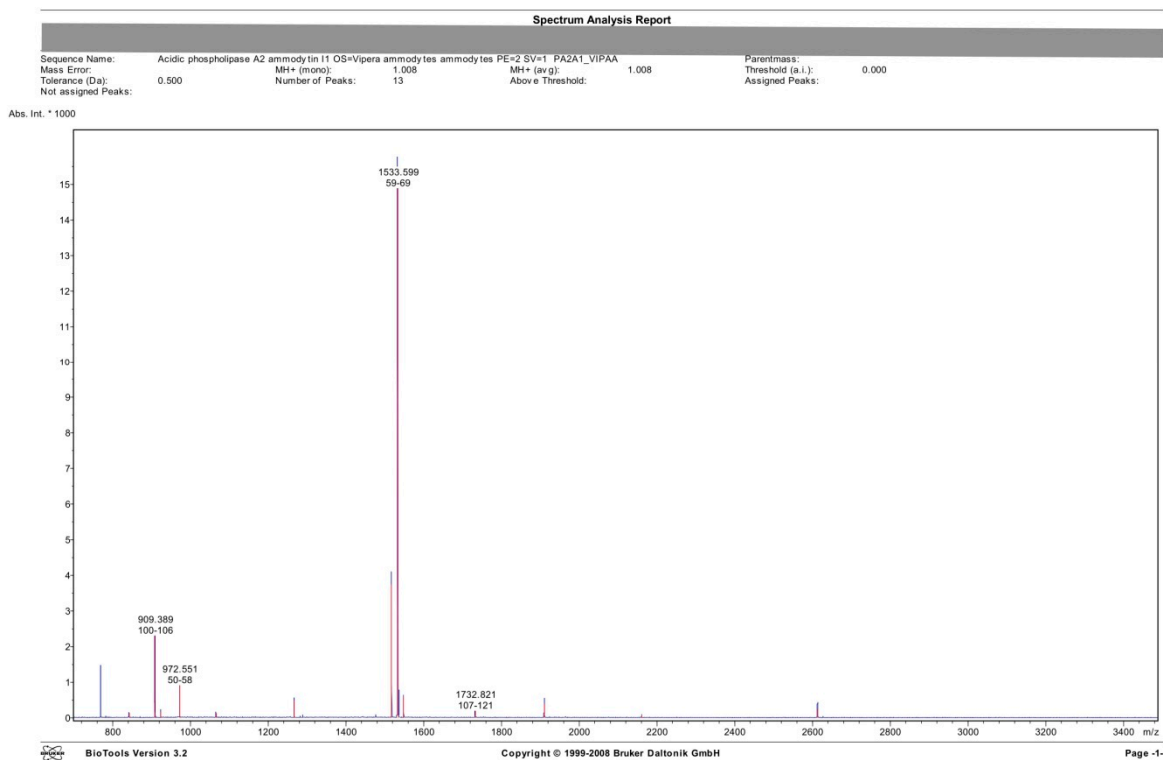
Calculated Masses:
 GCFVHDCYGR 1: Carbamidomethyl (C) 2: Carbamidomethyl (C) 7: Carbamidomethyl (C) 8: Carbamidomethyl (C)

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term.	Ion
1	C*	133.043	116.016	115.032	161.038	144.011	143.027	179.048	178.064	133.043	201.088	175.119	158.092	11	R
2	C*	293.074	276.047	275.063	321.069	304.042	303.058	339.079	338.095	133.043	258.120	232.140	215.114	10	G
3	F	440.142	423.116	422.132	468.137	451.110	450.126	486.148	485.164	120.081	421.183	395.204	378.177	9	Y
4	V	539.210	522.184	521.200	567.205	550.179	549.195	585.216	584.232	72.081	581.214	555.234	538.208	8	C*
5	H	676.269	659.243	658.259	704.264	687.238	686.254	722.275	721.291	110.071	741.244	715.265	698.239	7	C*
6	D	791.296	774.270	773.286	819.291	802.265	801.281	837.302	836.318	88.039	856.271	830.292	813.265	6	D
7	C*	951.327	934.300	933.316	979.322	962.295	961.311	997.332	996.348	133.043	993.330	967.351	950.324	5	H
8	C*	1111.358	1094.331	1093.347	1139.353	1122.326	1121.342	1157.363	1156.379	133.043	1092.399	1066.419	1049.393	4	V
9	Y	1274.421	1257.394	1256.410	1302.416	1285.389	1284.405	1320.426	1319.442	136.076	1239.467	1213.488	1196.461	3	F
10	G	1331.442	1314.416	1313.432	1359.437	1342.411	1341.427	1377.448	1376.464	30.034	1399.496	1373.518	1356.492	2	C*
11	R	1487.544	1470.517	1469.533	1515.538	1498.512	1497.528	1533.549	1532.565	129.113	1559.528	1533.549	1516.522	1	C*

bioRxiv

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Area 9. Annotated MS spectrum.



Spectrum Analysis Report

Sequence data:
 Acidic phospholipase A2 ammodytin I1 OS=Vipera ammodyt tes ammodyt tes PE=2 SV=1 PAZA1_VIPAA
 Intensity Coverage: 75.4 % (18321 cnts) Sequence Coverage MS: 30.4%
 Sequence Coverage MS/MS: 0.0% pl (isoelectric point): 4.9

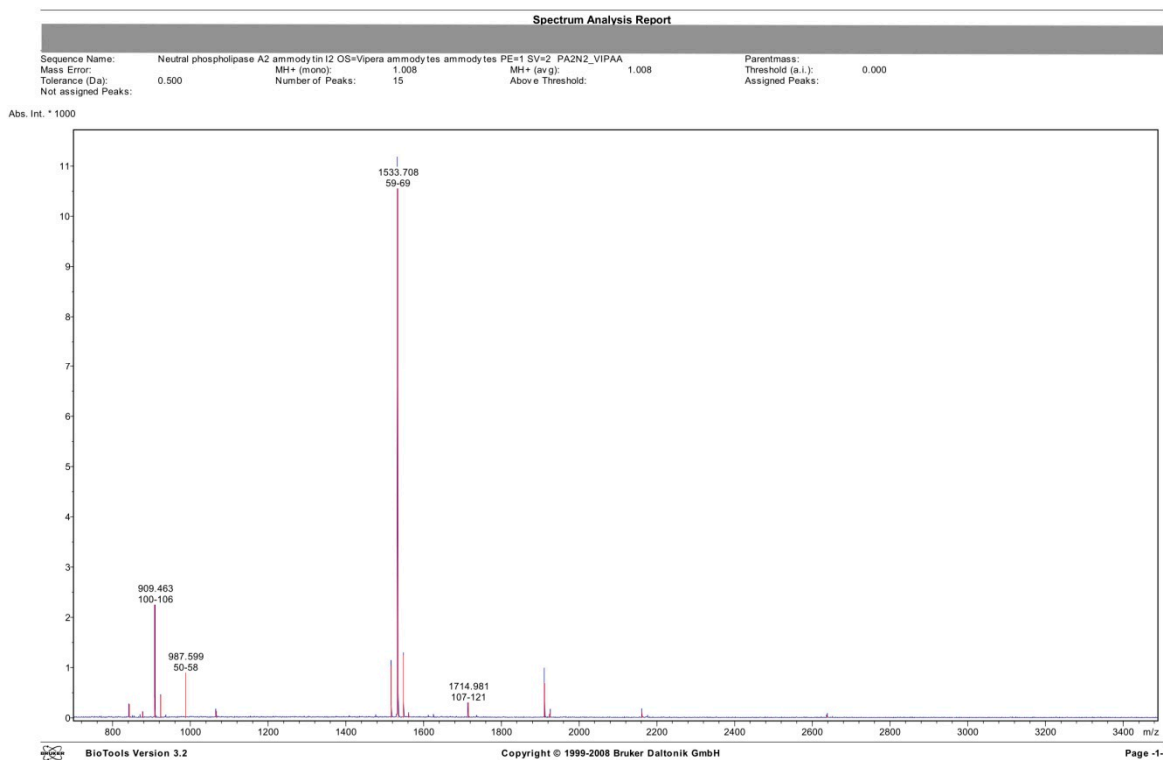
10	20	30	40	50	60	70	80	90	100	110	120	130	140
MRILWIVAVC	LIGAECHLSQ	FGRINRKTG	IFGIRSYIYY	GTCYGRGGG	RPLDATERCC	FVMDCCYGRV	NGCDPKRQTY	SYSPFRGDIIV	CGGDDPCLRA	VCECPVVAAL	CFGENRNTYD	EKYRLTSLFD	CRKESEQC

Display Parameter:
 Sequence Name: Acidic phospholipase A2 ammodytin I1 OS=Vipera ammodyt tes ammodyt tes PE=2 SV=1 PAZA1_VIPAA MH+ (mono): 1.008
 MH+ (avg): 1.008 Threshold (a.i.): 0.000 Tolerance (Da): 0.500 Number of Peaks: 13

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	842.539	140.884	2	909.389	2308.851	3	923.402	173.497	4	972.551	916.339	5	1066.457	139.805
6	1298.868	498.588	7	1518.890	3745.876	8	1533.599	14892.768	9	1547.618	583.526	10	1732.821	262.740
11	1909.862	393.958	12	2159.941	63.167	13	2613.122	255.339						

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Area 10. Annotated MS spectrum.



Spectrum Analysis Report

Sequence data:
 Neutral phospholipase A2 ammodytin I2 OS=Vipera ammodytes ammodytes PE=1 SV=2 PA2N2_VIPAA
 Intensity Coverage: 76.5 % (14018 cnts) Sequence Coverage MS: 30.7%
 Sequence Coverage MS/MS: 0.0% pl (isoelectric point): 6.1

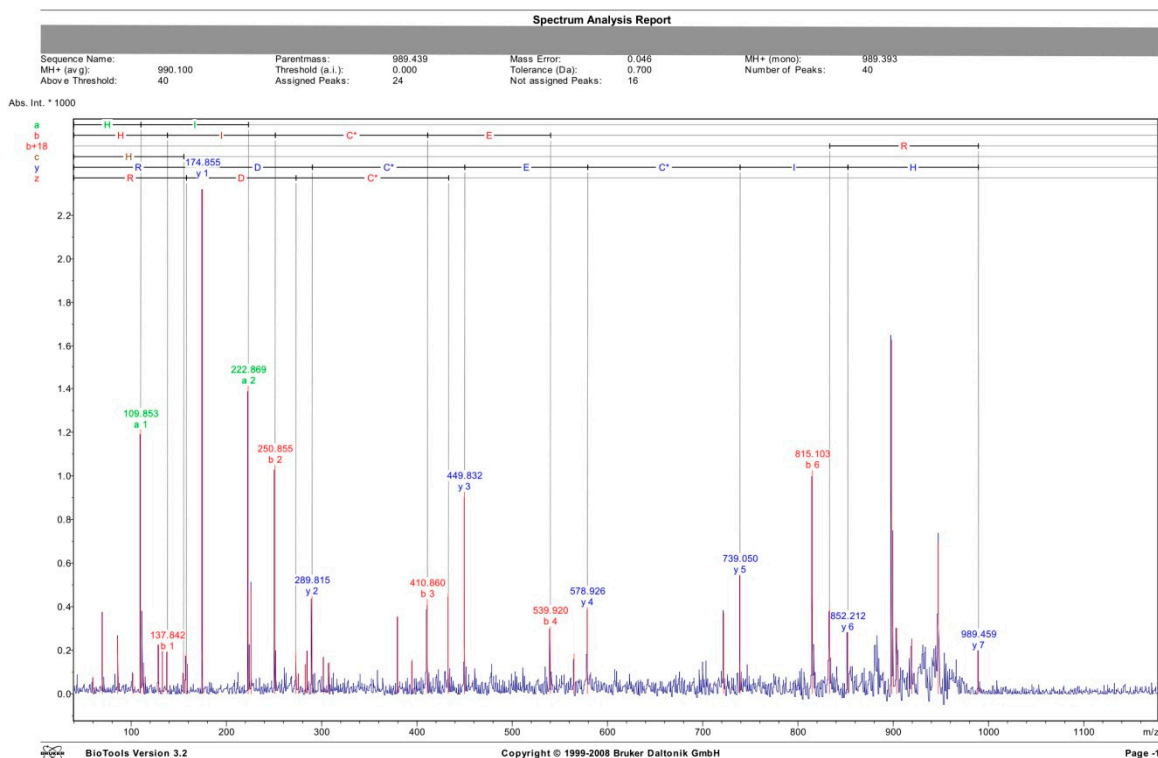
10	20	30	40	50	60	70	80	90	100	110	120	130	140
MRTLVIVAVC	LIGVEGNLYQ	FGNIFKMTK	KSALLSYSNY	GTCYGRGGG	KPQDATERCC	FVMDCCYGRV	NGCDPLSIY	SYSFENGIV	CGGDDPCLRA	VCECPVAAL	CFGELNLYD	EKYKNTPSH	CTETECC

Display Parameter:
 Sequence Name: Neutral phospholipase A2 ammodytin I2 OS=Vipera ammodytes ammodytes PE=1 SV=2 PA2N2_VIPAA MH+ (mono): 1.008
 MH+ (avg): 1.008 Threshold (a.i.): 0.000 Tolerance (Da): 0.500 Number of Peaks: 15

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	842.605	275.797	2	877.480	118.239	3	908.463	2253.037	4	923.479	438.802	5	987.599	901.986
6	1066.549	137.022	7	1518.673	1039.958	8	1533.708	10554.174	9	1547.728	1249.471	10	1561.741	84.402
11	1714.981	308.068	12	1910.983	693.719	13	1924.992	111.181	14	2161.090	108.325	15	2637.441	54.449

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Area 11. Annotated MS/MS spectrum of ion 989.439 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	989.439	Mass Error:	0.048	MH+ (mono):	989.393	MH+ (avg):	990.100
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	40	Above Threshold:	40
Assigned Peaks:	24	Not assigned Peaks:	16				

Peaklist:

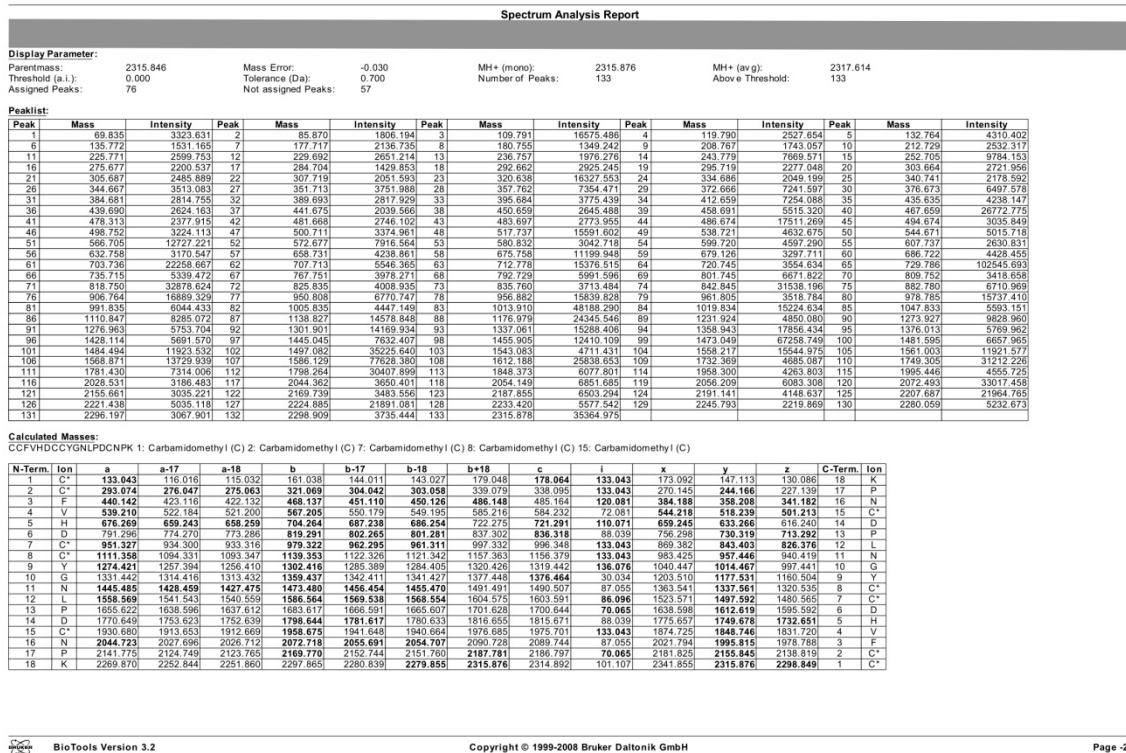
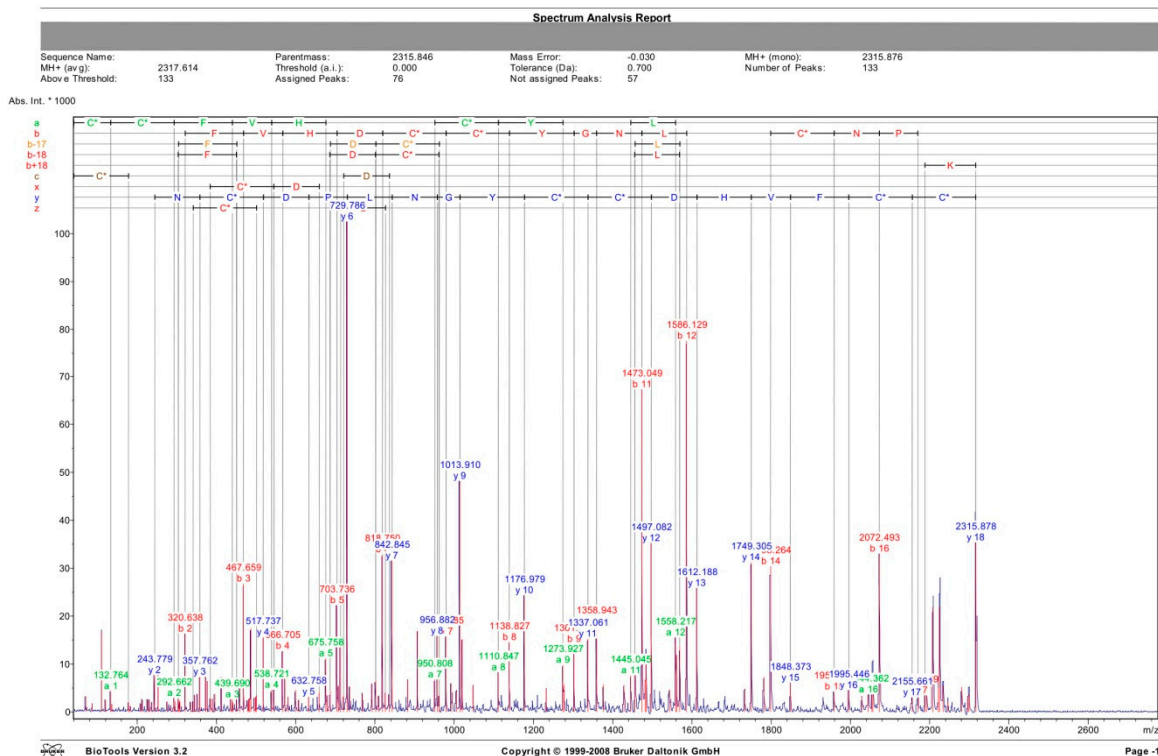
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	59.899	77.496	2	69.899	370.617	3	85.903	280.132	4	101.839	94.743	5	109.853	1211.232
6	112.854	141.094	7	128.879	223.549	8	132.813	244.789	9	137.842	195.090	10	154.805	63.803
11	157.852	185.799	12	174.855	2369.797	13	222.869	1413.132	14	225.896	477.811	15	250.855	1050.164
16	272.809	198.924	17	275.785	93.526	18	282.863	137.328	19	284.859	198.474	20	289.815	448.011
21	301.866	171.788	22	307.820	146.634	23	379.859	396.316	24	394.897	157.520	25	410.860	434.687
26	432.836	464.084	27	449.832	926.776	28	539.920	308.317	29	564.891	184.573	30	578.926	397.446
31	722.010	371.777	32	739.050	548.438	33	815.103	1026.358	34	833.154	390.114	35	852.212	283.284
36	898.294	1628.348	37	903.826	302.778	38	919.449	247.021	39	947.485	692.258	40	989.459	199.990

Calculated Masses:
HICECDR 3: Carbamidomethyl (C) 5: Carbamidomethyl (C)

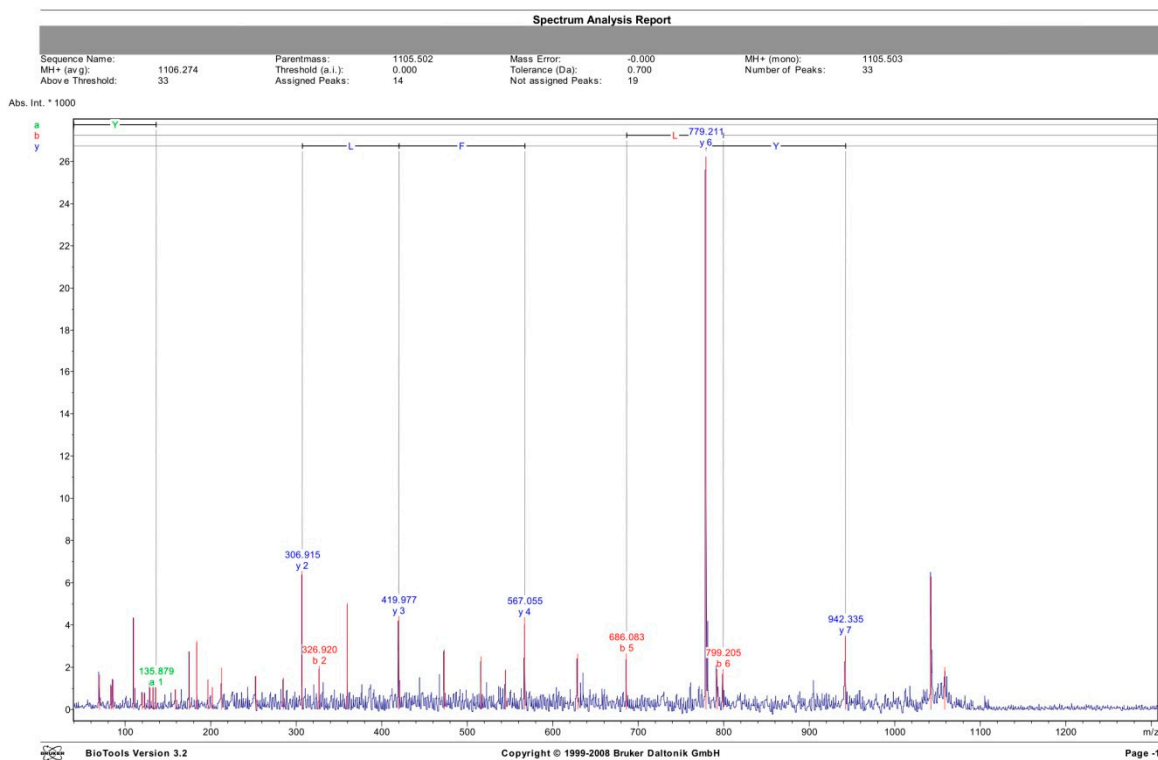
N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	H	110.071	93.045	92.061	138.066	121.040	120.056	156.077	155.093	110.071	201.098	175.119	158.092	7	R	
2	I	223.155	206.129	205.145	251.150	234.124	233.140	269.161	268.177	86.096	316.125	290.146	273.119	6	D	
3	C*	383.186	366.159	365.175	411.181	394.154	393.170	429.191	428.207	133.043	476.156	450.177	433.150	5	C*	
4	E	512.229	495.202	494.218	540.223	523.197	522.213	558.234	557.250	102.055	605.198	579.219	562.193	4	E	
5	C*	672.259	655.233	654.249	700.254	683.228	682.244	718.265	717.281	133.043	765.229	739.250	722.223	3	C*	
6	D	787.286	770.260	769.276	815.281	798.255	797.271	833.292	832.308	88.039	878.313	852.334	835.307	2	I	
7	R	943.387	926.361	925.377	971.382	954.356	953.372	989.393	988.408	129.113	1015.372	989.393	972.366	1	H	

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Area 11. Annotated MS/MS spectrum of ion 2315.846 m/z.



Area 11. Annotated MS/MS spectrum of ion 1105.502 m/z.



Spectrum Analysis Report

Display Parameter:

Parentmass:	1105.502	Mass Error:	-0.000	MH+ (mono):	1105.503	MH+ (avg):	1106.274
Threshold (a.i.):	0.000	Tolerance (Da):	0.700	Number of Peaks:	33	Above Threshold:	33
Assigned Peaks:	14	Not assigned Peaks:	19				

Peaklist:

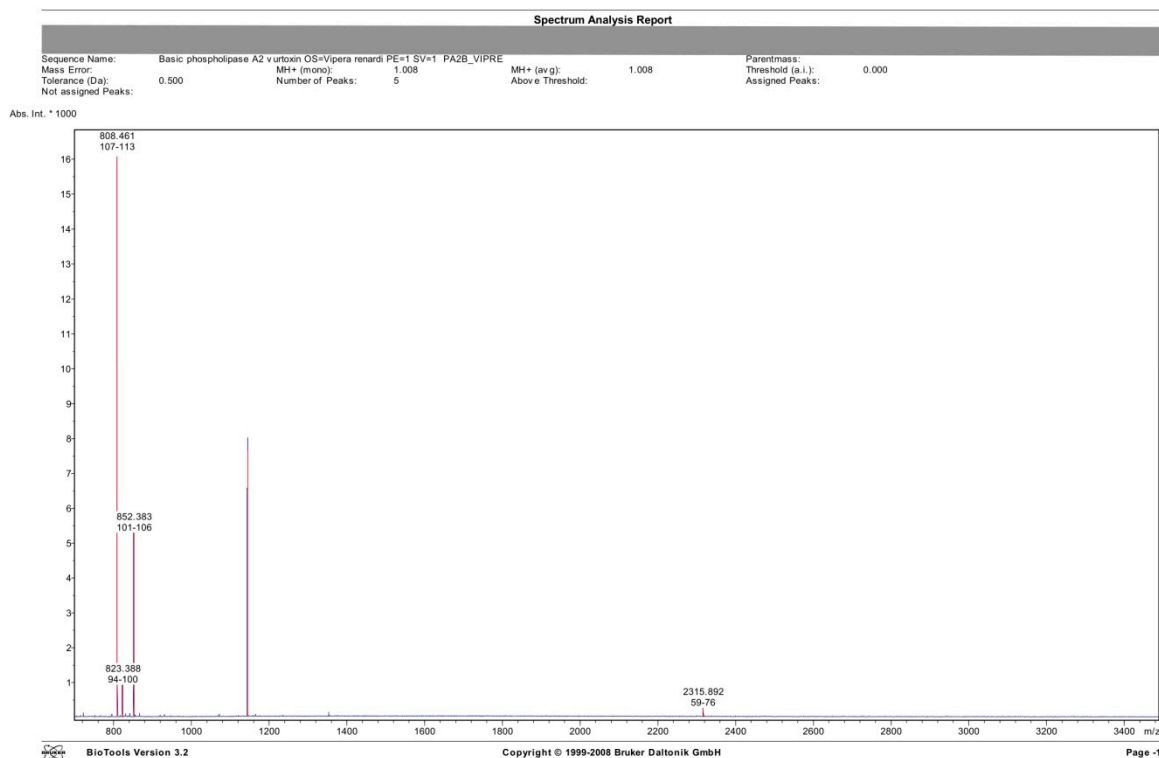
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.919	1652.840	2	83.910	1114.795	3	85.932	1406.645	4	109.890	4332.886	5	119.884	779.261
6	122.919	745.767	7	128.922	1318.721	8	132.873	1182.715	9	135.879	1052.849	10	158.889	967.837
11	174.916	2729.286	12	183.875	3255.213	13	196.916	1427.052	14	201.900	1054.820	15	212.877	1986.217
16	252.877	1604.988	17	284.948	1512.895	18	306.915	6554.001	19	326.920	2064.297	20	359.920	5037.013
21	419.977	4422.943	22	472.994	2947.974	23	518.006	2514.886	24	544.925	1804.235	25	567.055	4311.380
26	629.067	2639.973	27	686.083	2662.096	28	779.211	26648.386	29	792.151	2127.911	30	799.205	1922.823
31	942.335	3508.690	32	1042.608	6290.131	33	1058.448	2020.588						

Calculated Masses:
 YYPDFLCK 7: Carbamidomethyl (C)

N-Term.	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term.	Ion
1	Y	136.076	119.049	118.065	164.071	147.044	146.060	182.081	181.097	136.076	173.092	147.113	130.086	8	K
2	Y	259.139	282.112	281.128	327.134	310.107	309.123	345.144	344.160	136.076	333.123	387.143	290.117	7	C*
3	P	396.192	379.165	378.181	424.187	407.160	406.176	442.197	441.213	70.065	446.207	426.228	403.201	6	L
4	D	511.219	494.192	493.208	539.214	522.187	521.203	557.224	556.240	88.039	593.275	567.296	550.269	5	F
5	F	658.287	641.261	640.277	686.282	669.256	668.271	704.293	703.309	120.081	738.302	682.323	665.296	4	D
6	L	771.371	754.345	753.361	799.366	782.340	781.356	817.377	816.393	86.096	805.355	779.376	762.349	3	P
7	C*	931.402	914.375	913.391	959.397	942.370	941.386	977.407	976.423	133.043	968.418	942.439	925.412	2	Y
8	K	1059.497	1042.470	1041.486	1087.492	1070.465	1069.481	1105.502	1104.518	101.107	1131.482	1105.502	1088.476	1	Y

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Area 11. Annotated MS spectrum 1.



Spectrum Analysis Report

Sequence data:
 Basic phospholipase A2 v urtoxin OS=Vipera renardi PE=1 SV=1 PA2B_VIPRE
 Intensity Coverage: 74.9 % (22721 cnts) Sequence Coverage MS: 27.5%
 Sequence Coverage MS/MS: 0.0% pl (isoelectric point): 9.7

10	20	30	40	50	60	70	80	90	100	110	120	130	140
MRTLWIVAVC	LIVGEGSLLLE	FORHILEETG	RNPLTSYSFY	GTCYGVGGEG	TPKDATDRCC	FVMDCCYGNL	PBCNPKIDRY	KYHRKGAIV	CGRQTSCENR	ICECPAAAL	CFRKNLRTYN	HIKYYPDFL	CKKESEKC

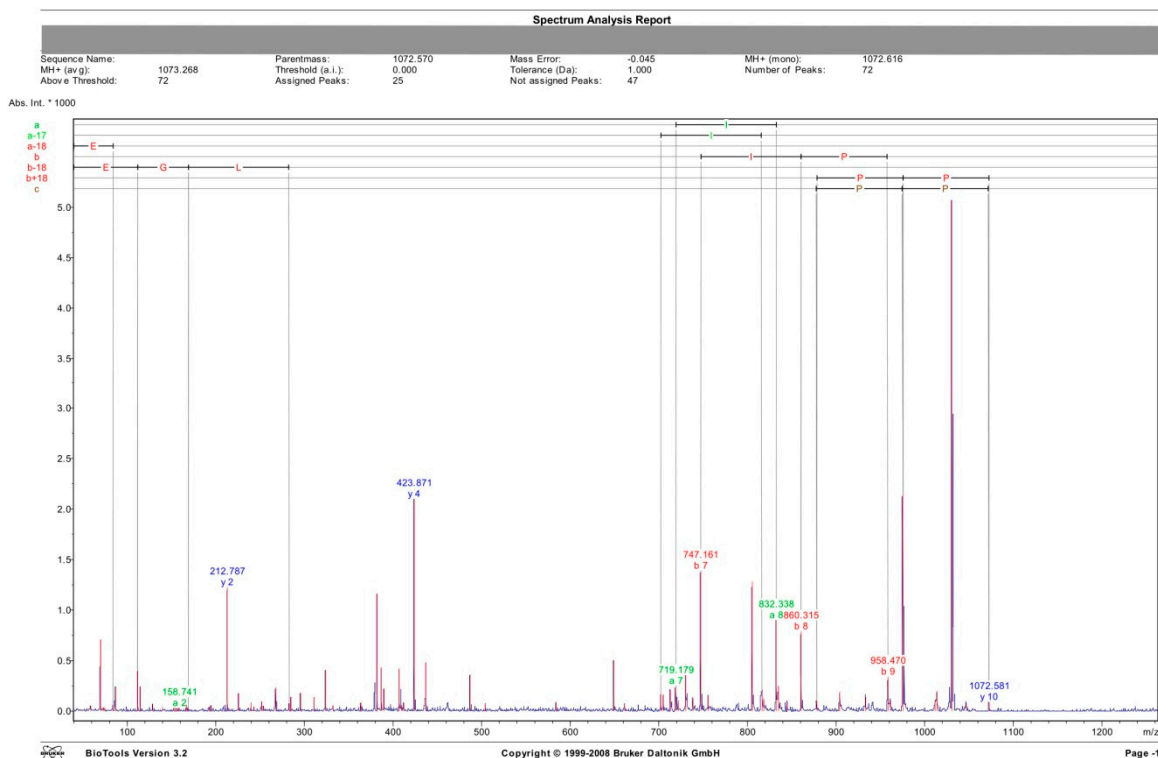
Display Parameter:
 Sequence Name: Basic phospholipase A2 v urtoxin OS=Vipera renardi PE=1 SV=1 PA2B_VIPRE MH+ (mono): 1.008
 MH+ (avg): 1.008 Threshold (a.i.): 0.000 Tolerance (Da): 0.500 MH+ (mono): 1.008
 Number of Peaks: 5

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	808.461	16204.710	2	823.388	942.130	3	852.383	5297.561	4	1144.657	7632.483	5	2315.892	276.539

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Annotated MS/MS spectrum of peptide 1072.570 m/z.



Spectrum Analysis Report

Display Parameter:	Parentmass:	1072.570	Mass Error:	-0.045	MH+ (mono):	1072.616	MH+ (avg):	1073.268
	Threshold (a.i.):	0.000	Tolerance (Da):	1.000	Number of Peaks:	72	Above Threshold:	72
	Assigned Peaks:	25	Not assigned Peaks:	47				

Peaklist:

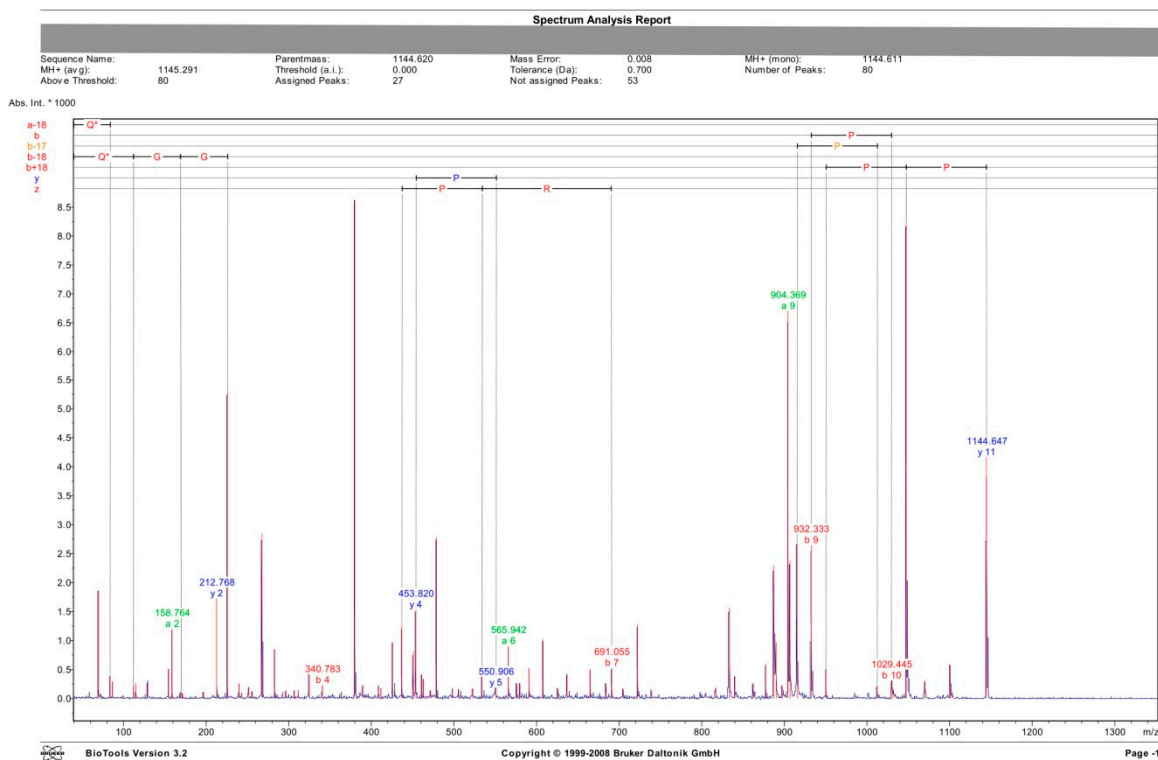
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.804	54.030	2	69.839	706.327	3	72.860	36.175	4	74.464	36.691	5	83.811	57.810
6	86.841	244.965	7	111.814	400.346	8	114.805	244.389	9	128.812	70.708	10	138.787	38.876
11	152.753	31.544	12	154.738	39.733	13	156.788	27.874	14	158.741	30.524	15	166.817	63.399
16	168.807	36.753	17	192.772	41.137	18	194.798	57.016	19	212.787	1224.182	20	225.804	177.360
21	239.782	84.221	22	242.871	41.094	23	251.784	98.501	24	253.788	50.710	25	267.788	235.839
26	282.844	77.055	27	284.803	140.101	28	295.811	182.333	29	310.831	141.388	30	323.800	407.748
31	332.556	57.669	32	363.875	90.283	33	381.859	1180.679	34	386.577	433.045	35	388.830	220.190
36	406.855	428.061	37	409.834	81.784	38	412.115	81.432	39	423.871	2098.975	40	436.890	488.695
41	486.911	363.486	42	503.899	79.299	43	584.014	92.371	44	649.080	504.030	45	661.140	78.668
46	702.173	174.050	47	705.057	166.669	48	713.174	211.742	49	719.179	249.012	50	721.982	107.020
51	730.159	486.318	52	738.556	129.187	53	747.161	1389.334	54	755.542	161.062	55	805.274	1281.351
56	816.301	192.431	57	818.061	125.222	58	832.338	899.077	59	834.916	240.836	60	844.849	99.838
61	860.315	788.382	62	878.328	101.207	63	903.880	192.609	64	933.449	141.219	65	958.470	340.228
66	981.521	108.111	67	975.477	2152.227	68	1011.579	115.466	69	1013.666	201.953	70	1030.623	5318.954
71	1046.841	77.855	72	1072.581	90.239									

Calculated Masses:
EGLPPRPPIP

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	E	102.055	85.028	84.044	130.050	113.023	112.039	148.060	147.076	102.055	142.050	116.071	99.044	0	P
2	G	189.076	142.050	141.066	187.071	170.045	169.061	205.082	204.098	30.034	239.103	213.123	196.097	9	P
3	L	272.150	255.134	254.150	300.155	283.129	282.145	318.166	317.182	86.096	352.187	328.207	309.181	8	I
4	P	369.213	352.187	351.203	397.208	380.182	379.198	415.219	414.235	70.065	449.239	423.260	406.234	7	P
5	P	466.266	449.239	448.255	494.261	477.234	476.250	512.271	511.287	70.065	605.341	579.361	562.335	6	R
6	R	622.307	605.341	604.357	650.382	633.355	632.351	668.373	667.389	129.113	702.393	676.414	659.388	5	P
7	P	719.420	702.393	701.409	747.415	730.388	729.404	765.425	764.441	70.065	799.446	773.467	756.440	4	P
8	I	832.564	815.477	814.493	860.499	843.472	842.488	878.509	877.525	86.096	912.530	886.551	869.524	3	L
9	P	929.537	912.530	911.546	957.552	940.525	939.541	975.562	974.578	70.065	989.552	943.572	925.546	2	G
10	P	1026.609	1009.583	1008.599	1054.604	1037.578	1036.594	1072.615	1071.631	70.065	1098.594	1072.615	1055.588	1	E

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Annotated MS/MS spectrum of peptide 1144.620 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1144.620 Mass Error: 0.008 MH+ (mono): 1144.611 MH+ (avg): 1145.291
 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 80
 Assigned Peaks: 27 Not assigned Peaks: 53 Above Threshold: 80

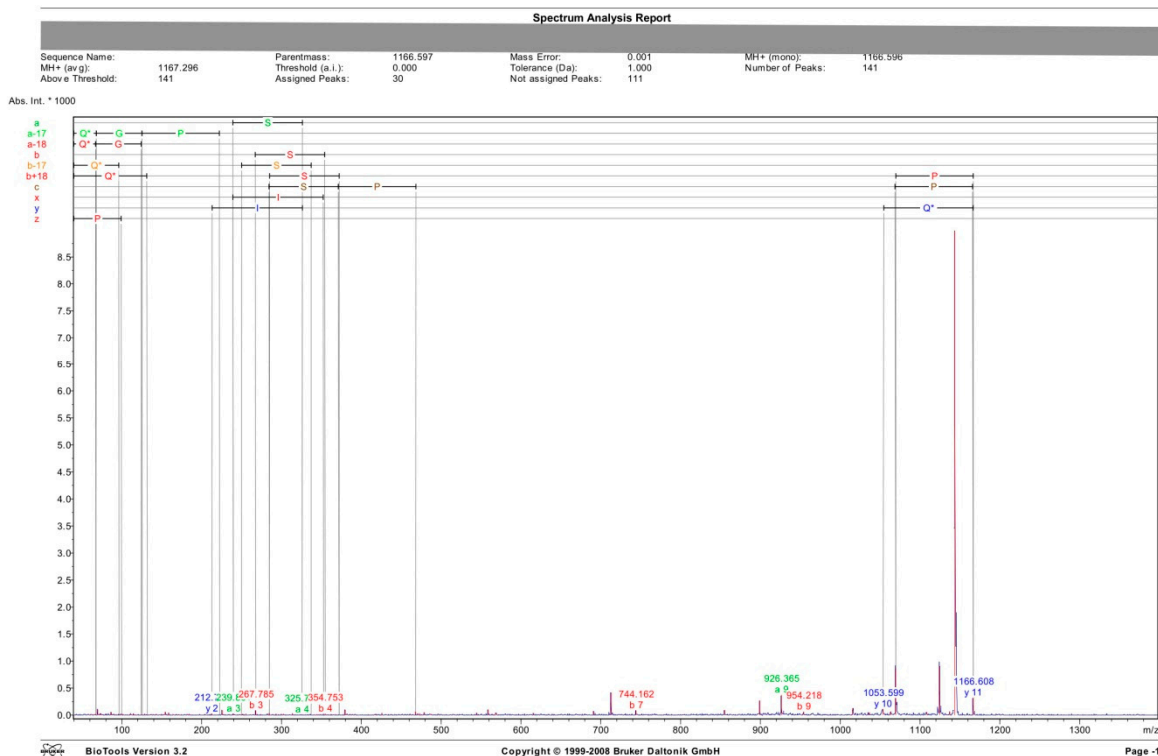
Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.791	103.476	2	69.819	1860.238	3	72.822	80.027	4	83.814	381.228	5	86.826	291.511
6	99.817	51.066	7	111.799	209.413	8	114.788	260.626	9	128.786	258.306	10	154.750	658.488
11	158.764	1197.544	12	169.747	105.671	13	171.767	88.021	14	196.780	113.379	15	212.768	1724.577
16	225.796	5302.895	17	239.767	283.537	18	243.028	100.978	19	251.772	203.776	20	256.796	119.537
21	287.766	2850.168	22	282.788	855.307	23	292.807	109.182	24	296.844	138.884	25	306.823	137.075
26	311.801	140.826	27	324.824	431.749	28	340.783	228.519	29	363.855	114.328	30	379.843	8676.980
31	389.894	222.945	32	408.803	229.889	33	411.823	164.109	34	425.847	973.333	35	436.812	1254.270
36	450.939	821.932	37	453.820	1531.078	38	460.908	426.047	39	463.024	324.146	40	471.818	144.241
41	478.916	2779.339	42	498.421	175.671	43	505.906	158.235	44	522.949	182.777	45	533.891	444.683
46	550.908	185.526	47	565.942	903.974	48	576.008	263.444	49	579.968	260.246	50	590.905	526.665
51	607.946	1022.627	52	625.970	183.899	53	637.056	417.223	54	665.045	511.490	55	684.305	252.554
56	691.055	526.389	57	705.090	169.210	58	722.107	1279.763	59	739.311	138.043	60	817.205	187.382
61	833.234	1565.577	62	840.072	387.379	63	862.288	261.169	64	877.262	596.878	65	887.318	2302.499
66	889.968	975.334	67	897.289	234.537	68	904.369	6705.468	69	908.895	2382.668	70	915.286	2672.872
71	932.333	2644.201	72	950.359	496.575	73	1012.407	220.651	74	1029.445	309.359	75	1031.628	195.551
76	1047.507	8209.386	77	1070.114	309.290	78	1100.624	578.195	79	1103.675	103.328	80	1144.647	4160.337

Calculated Masses:
 OGGPPRPQIPP 1: Deamidated (NQ)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	G ⁺	102.055	85.028	84.044	130.050	113.023	112.039	148.060	147.078	102.055	142.050	116.071	99.044	11	P ⁻
2	G	158.676	142.050	141.068	187.071	178.045	169.061	205.082	204.098	30.034	239.183	213.123	196.097	10	P
3	G	216.098	199.071	198.087	244.093	227.066	226.082	262.103	261.119	30.034	352.187	326.207	309.181	9	I
4	P	313.151	296.124	295.140	341.146	324.119	323.135	359.156	358.172	70.065	480.245	454.266	437.239	8	Q
5	P	410.203	393.177	392.193	438.198	421.172	420.188	456.209	455.225	70.065	577.298	551.319	534.292	7	P
6	R	566.305	549.278	548.294	594.299	577.273	576.289	612.310	611.326	129.113	733.399	707.420	690.393	6	R
7	P	663.357	646.331	645.347	691.352	674.326	673.342	709.363	708.379	70.065	830.452	804.473	787.446	5	P
8	Q	751.416	734.390	733.405	819.411	802.384	801.400	837.421	836.437	101.071	927.505	901.526	884.499	4	P
9	I	904.500	887.473	886.489	932.495	915.468	914.484	950.505	949.521	86.096	984.526	958.547	941.520	3	G
10	P	1001.553	984.526	983.542	1029.548	1012.521	1011.537	1047.558	1046.574	70.065	1041.548	1015.568	998.542	2	G
11	P	1098.605	1081.579	1080.595	1126.600	1109.574	1108.590	1144.611	1143.627	70.065	1170.590	1144.611	1127.584	1	Q ⁺

Annotated MS/MS spectrum of peptide 1166.597 m/z.



Spectrum Analysis Report

Display Parameter: Parentmass: 1166.597 Mass Error: 0.001 MH+ (mono): 1166.596 MH+ (avg): 1167.296
 Threshold (a.i.): 0.000 Tolerance (Da): 1.000 Number of Peaks: 141 Above Threshold: 141
 Assigned Peaks: 30 Not assigned Peaks: 111

Peaklist:

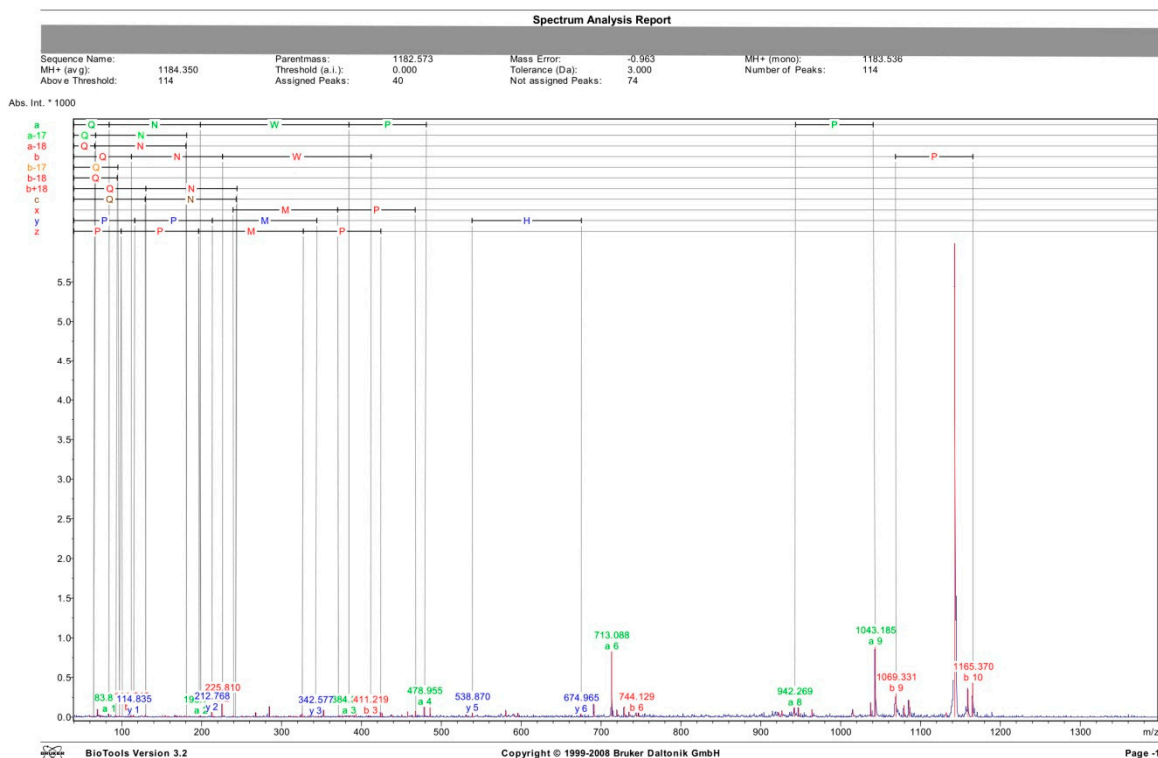
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	59.306	9.477	2	60.819	12.672	3	63.192	13.250	4	65.591	10.865	5	67.492	14.744
6	69.794	107.891	7	72.735	14.595	8	74.072	31.349	9	80.464	23.295	10	86.752	65.381
11	89.890	19.272	12	93.690	12.222	13	96.577	21.788	14	99.775	23.860	15	101.639	16.087
16	104.836	6.643	17	107.141	8.810	18	110.296	14.562	19	111.579	22.022	20	114.775	26.071
21	119.736	9.138	22	121.276	10.065	23	123.918	8.984	24	125.231	7.220	25	128.773	23.393
26	131.859	10.166	27	137.308	11.730	28	138.874	12.022	29	140.924	10.460	30	143.727	14.871
31	146.646	4.862	32	147.852	7.474	33	150.586	18.429	34	154.751	58.099	35	158.793	42.149
36	163.839	14.872	37	168.092	12.050	38	168.616	16.150	39	171.840	9.737	40	174.796	12.252
41	178.788	10.726	42	182.080	16.000	43	184.415	21.672	44	191.968	3.602	45	194.752	5.752
46	197.799	15.471	47	204.293	16.232	48	210.766	14.742	49	212.778	26.646	50	217.278	3.860
51	222.439	7.715	52	225.803	93.920	53	229.525	10.306	54	234.758	12.763	55	239.801	27.276
56	243.095	8.438	57	244.869	9.338	58	247.779	10.010	59	249.514	11.025	60	251.893	17.873
61	255.449	24.211	62	259.659	4.572	63	261.147	7.694	64	264.568	9.143	65	267.785	88.442
66	271.496	8.291	67	274.164	15.231	68	282.755	25.038	69	284.817	35.509	70	289.182	10.270
71	290.786	10.666	72	293.353	20.017	73	296.826	11.260	74	300.105	18.600	75	301.579	10.885
76	302.979	15.553	77	305.759	9.271	78	313.820	30.259	79	317.909	16.344	80	325.769	11.124
81	329.291	6.289	82	333.557	11.213	83	337.154	5.382	84	341.743	9.032	85	343.940	12.481
86	345.709	12.821	87	348.057	14.205	88	350.480	11.895	89	352.783	15.326	90	354.753	28.913
91	357.907	6.745	92	359.711	8.221	93	362.807	15.377	94	365.359	6.978	95	367.499	12.685
96	369.749	7.658	97	372.150	10.255	98	377.259	13.995	99	379.863	100.028	100	382.451	21.046
101	386.128	17.533	102	393.005	14.002	103	406.667	9.814	104	413.921	9.633	105	416.950	9.496
106	418.841	19.720	107	425.878	38.938	108	431.922	12.020	109	441.857	14.626	110	461.885	17.502
111	467.923	68.734	112	470.973	26.134	113	473.070	26.235	114	473.000	52.465	115	496.868	17.069
116	488.073	17.149	117	496.675	22.120	118	515.991	15.538	119	544.879	43.826	120	558.947	102.705
121	564.157	19.419	122	568.011	45.699	123	566.942	19.333	124	616.065	35.577	125	691.245	71.120
128	713.091	418.548	129	744.162	87.912	130	855.207	98.162	131	889.272	273.492	132	926.365	378.152
131	954.218	66.567	132	1015.370	129.188	133	1035.437	54.592	134	1053.599	114.444	135	1063.265	68.583
136	1069.531	860.630	137	1108.719	51.857	138	1124.650	909.722	139	1137.283	62.850	140	1143.502	9274.172
141	1166.608	324.549												

Calculated Masses:
 GQSPRRHPIPP N-Term: Gln->pyro-Glu (N-term Q) 1: Deamidated (NQ)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	Q'	85.028	68.002	67.018	113.023	95.997	95.013	131.034	130.050	85.028	142.050	116.071	99.044	11	P
2	G	142.050	125.023	124.039	170.045	153.018	152.034	188.055	187.071	30.034	239.103	213.123	196.097	10	P
3	P	239.103	222.076	221.092	267.098	250.071	249.087	285.108	284.124	70.065	352.187	326.207	309.181	9	I
4	S	326.135	309.108	308.124	354.130	337.103	336.119	372.140	371.156	60.044	449.239	423.260	406.234	8	P
5	P	423.167	406.141	405.157	451.162	434.136	433.152	469.169	468.185	70.065	536.268	510.289	493.263	7	H
6	R	579.289	562.262	561.278	607.283	590.257	589.273	625.294	624.310	129.113	742.399	716.420	699.394	6	R
7	H	716.347	699.321	698.337	744.342	727.316	726.332	762.353	761.369	110.071	839.452	813.473	796.446	5	P
8	P	813.400	796.374	795.390	841.395	824.369	823.385	859.406	858.422	70.065	928.484	902.505	885.478	4	S
9	I	926.484	909.458	908.474	954.479	937.453	936.469	972.490	971.506	86.096	1023.537	997.558	980.531	3	P
10	P	1023.537	1006.510	1005.526	1051.532	1034.505	1033.521	1069.543	1068.559	70.065	1080.559	1054.579	1037.553	2	G
11	P	1120.590	1103.563	1102.579	1148.585	1131.558	1130.574	1166.596	1165.611	70.065	1192.575	1166.595	1149.569	1	Q'

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Annotated MS/MS spectrum of peptide 1182.573 m/z.



Spectrum Analysis Report

Display Parameter:	1182.573	Mass Error:	-0.963	MH+ (mono):	1183.536	MH+ (avg):	1184.350
Parentmass:	1182.573	Threshold (a.i.):	0.000	Tolerance (Da):	3.000	Number of Peaks:	114
Assigned Peaks:	40	Not assigned Peaks:	74	Above Threshold:	114		

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	59.738	21.980	2	64.404	16.865	3	69.812	97.501	4	72.703	25.033	5	76.280	18.907
6	83.811	41.387	7	92.307	24.307	8	96.871	22.822	9	100.545	15.285	10	106.858	14.858
11	109.394	13.614	12	111.812	63.484	13	114.835	25.033	14	124.833	16.267	15	129.757	27.579
16	150.834	25.776	17	154.739	21.785	18	157.421	13.107	19	158.703	12.724	20	166.723	24.038
21	189.747	18.031	22	172.653	16.502	23	178.184	7.771	24	178.743	16.026	25	180.986	10.892
26	182.831	9.146	27	184.791	10.458	28	191.772	9.801	29	194.649	7.196	30	196.760	10.018
31	198.755	18.971	32	203.255	9.517	33	212.788	62.957	34	215.064	11.132	35	216.774	9.273
36	220.819	8.188	37	225.810	169.455	38	239.813	18.922	39	242.339	8.540	40	250.796	17.038
41	256.062	11.499	42	260.091	11.694	43	261.330	7.446	44	262.802	8.699	45	267.788	59.656
46	273.543	10.665	47	277.796	19.836	48	284.825	136.202	49	289.781	15.045	50	293.566	16.500
51	295.860	10.991	52	303.815	11.872	53	309.787	18.137	54	311.819	16.756	55	315.431	13.160
56	318.123	14.283	57	319.546	13.868	58	323.850	27.902	59	325.839	40.297	60	329.232	12.764
61	332.837	16.472	62	335.803	25.663	63	339.318	18.929	64	342.577	15.475	65	346.276	20.762
66	349.781	17.153	67	352.824	91.071	68	371.238	15.884	69	373.339	18.414	70	376.311	33.532
71	379.879	115.441	72	384.336	18.710	73	386.670	33.673	74	389.739	48.834	75	393.272	40.403
76	408.888	24.178	77	411.219	18.903	78	423.859	58.021	79	425.818	52.234	80	437.816	31.965
81	450.851	31.421	82	457.859	71.444	83	463.975	26.964	84	467.840	79.866	85	478.955	130.080
86	485.876	126.566	87	531.686	29.667	88	538.870	54.170	89	580.896	79.638	90	591.075	39.147
91	596.019	53.026	92	674.965	40.964	93	691.134	159.833	94	713.088	829.701	95	719.963	84.034
96	729.025	134.443	97	735.094	66.562	98	744.129	54.103	99	747.049	56.575	100	822.263	67.406
101	926.563	80.644	102	942.269	121.769	103	947.260	123.777	104	964.168	98.663	105	1015.269	95.083
106	1037.379	181.966	107	1043.185	891.816	108	1069.331	300.911	109	1079.170	148.409	110	1085.424	215.995
111	1132.158	60.423	112	1142.852	6034.370	113	1159.254	346.867	114	1165.370	433.160			

Calculated Masses:
GNWPHPPMPP N-Term: Gln-pyro-Glu (N-term Q)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	l	x	y	z	C-Term	Ion
1	Q	84.044	67.018	66.034	112.039	95.013	94.029	139.050	129.066	84.044	142.050	116.071	99.044	10	P
2	N	198.087	181.061	180.077	226.082	209.056	208.072	244.093	243.109	87.055	239.103	213.123	196.097	9	P
3	W	384.167	367.140	366.156	412.162	395.135	394.151	430.172	429.188	159.092	370.143	344.164	327.137	8	M
4	P	481.219	464.193	463.209	509.214	492.188	491.204	527.225	526.241	70.065	487.196	441.217	424.190	7	P
5	H	618.278	601.252	600.268	646.273	629.247	628.263	664.284	663.300	110.071	564.249	538.269	521.243	6	P
6	P	715.331	698.305	697.321	743.326	726.299	725.315	761.337	760.353	70.065	701.308	675.328	658.302	5	H
7	P	812.384	795.357	794.373	840.379	823.352	822.368	858.389	857.405	70.065	798.360	772.381	755.355	4	P
8	M	943.424	926.398	925.414	971.419	954.393	953.409	989.430	988.446	104.093	984.440	958.460	941.434	3	W
9	P	1040.477	1023.451	1022.467	1068.472	1051.445	1050.461	1086.483	1085.499	70.065	1098.483	1072.503	1055.477	2	N
10	P	1137.530	1120.503	1119.519	1165.525	1148.498	1147.514	1183.535	1182.551	70.065	1209.515	1183.535	1166.509	1	Q

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