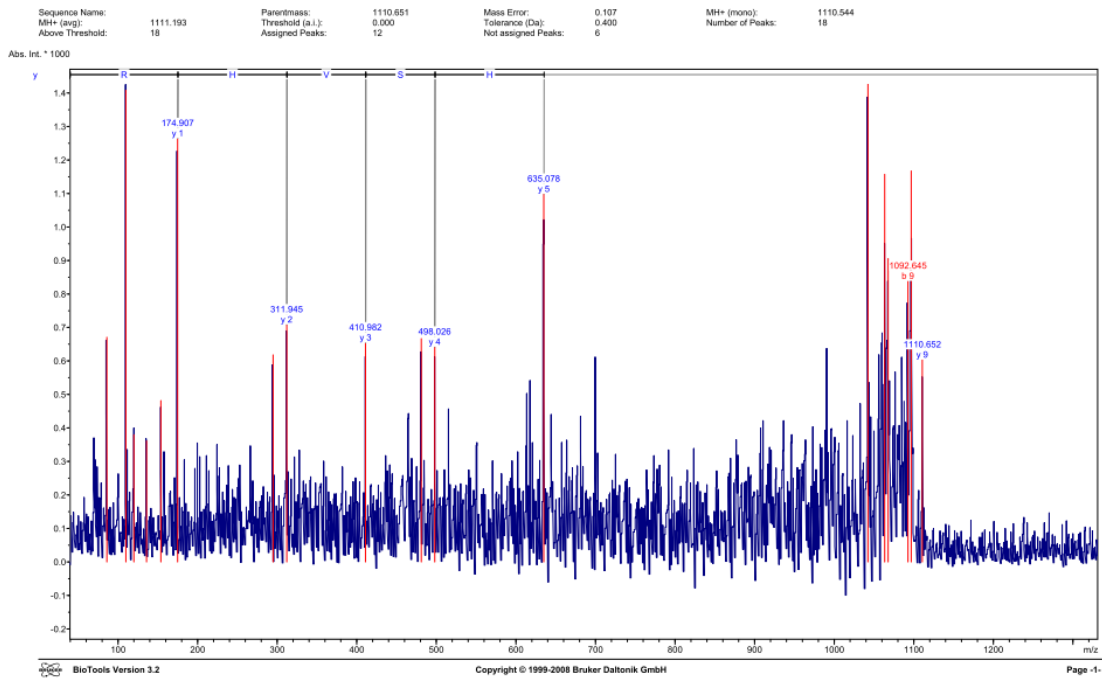


Supplementary Materials: Proteomic Analyses of *Agkistrodon contortrix contortrix* Venom Using 2D Electrophoresis and MS Techniques

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.



(A)

Display Parameter: Parentmass: 1110.651, Mass Error: 0.107, MH+ (mono): 1110.544, MH+ (avg): 1111.193, Threshold (a.i.): 0.000, Tolerance (Da): 0.400, Number of Peaks: 18, Above Threshold: 18, Assigned Peaks: 12, Not assigned Peaks: 6

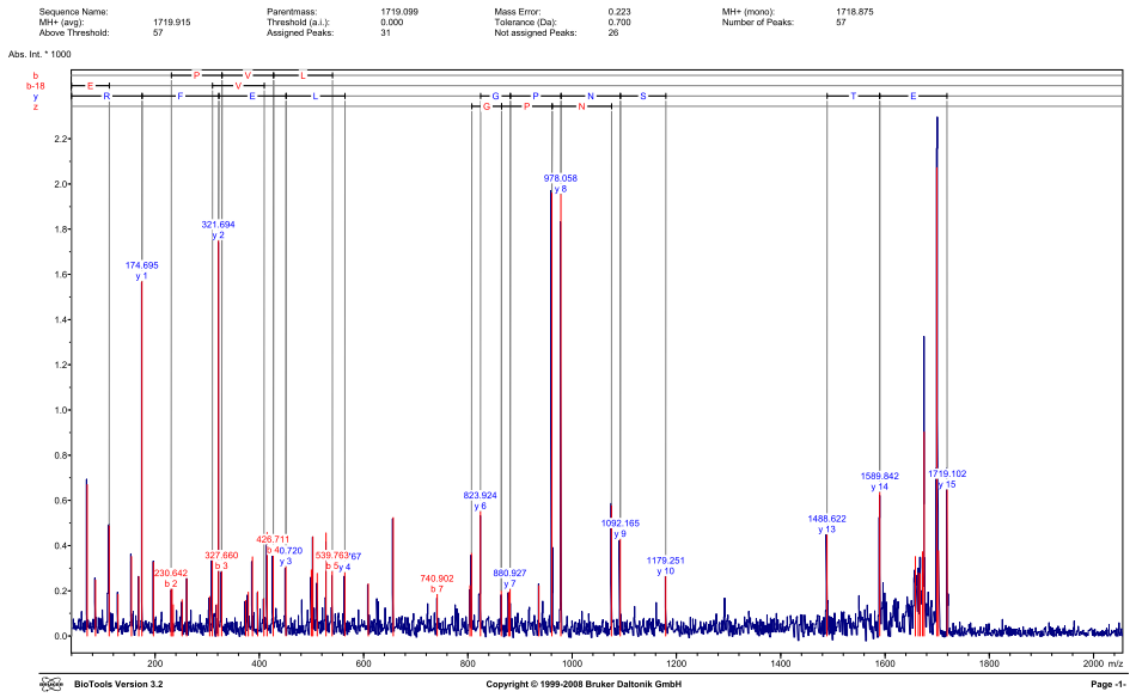
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	85.931	0.1	2	109.895	0.1	3	119.894	0.1	4	135.894	0.1	5	153.888	0.1
6	174.907	1.2	7	204.913	0.5	8	311.945	0.7	9	410.982	0.6	10	481.006	0.5
11	498.026	0.6	12	635.078	1.0	13	1042.283	0.5	14	1063.307	0.5	15	1067.793	0.5
16	1092.645	0.8	17	1092.645	0.8	18	1110.652	1.4						

Calculated Masses: QAFHSVHR

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	101.071	84.044	83.060	129.066	112.039	111.055	147.076	146.092	101.071	201.098	175.119	158.092	S	R
2	A	172.100	155.082	154.097	200.103	183.076	182.092	218.114	217.130	44.089	338.157	312.178	295.151	S	H
3	F	319.170	302.150	301.165	341.171	324.145	323.161	365.182	364.198	120.881	431.220	411.248	394.220	F	V
4	E	448.210	431.193	430.208	478.214	459.187	458.203	494.225	493.241	102.055	524.258	498.278	481.252	E	S
5	H	585.270	568.251	567.267	613.273	594.246	593.262	631.283	630.299	110.071	661.310	636.337	619.311	H	
6	S	672.310	655.293	654.299	700.305	683.278	682.294	719.315	717.331	40.344	750.359	724.380	717.353	S	A
7	V	773.370	754.352	753.368	799.375	782.347	781.363	817.384	816.400	72.081	837.427	811.448	804.422	V	
8	H	808.420	791.411	790.427	836.433	819.406	818.422	854.443	853.459	110.071	1029.461	1003.485	993.459	H	
9	R	1064.538	1047.512	1046.528	1092.533	1075.507	1074.523	1110.544	1109.560	129.113	1138.523	1110.544	1093.517	R	Q

(B)

Figure S1. Annotated MS/MS spectrum of ion 1110.651 m/z detected in area #1. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 1719.099 Mass Error: 0.223 MH+ (mono): 1718.875 MH+ (avg): 1719.915
 Threshold (a.l.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 57 Above Threshold: 57
 Assigned Peaks: 31 Not assigned Peaks: 26

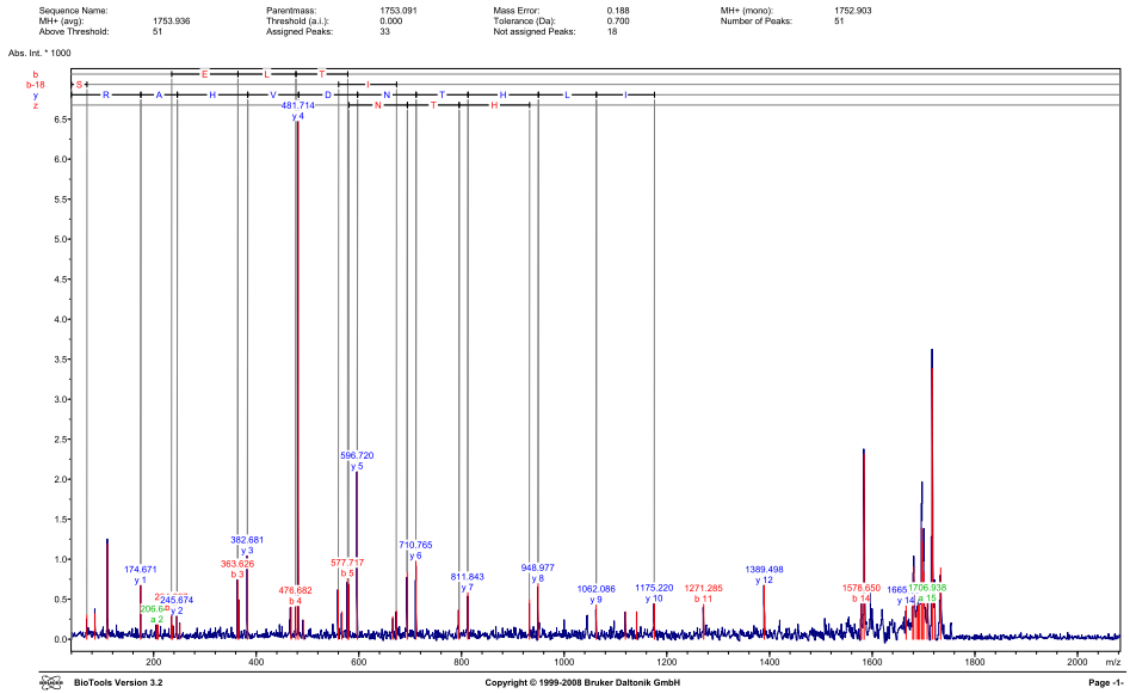
Peak#	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	89.765	669.717	2	85.752	247.859	3	111.729	485.472	4	128.737	384.337	5	154.879	351.681
6	168.738	262.876	7	174.695	1570.659	8	198.701	326.898	9	230.642	208.711	10	232.668	229.852
11	234.620	138.181	12	251.878	161.133	13	260.449	295.508	14	304.680	174.751	15	309.689	352.686
16	317.630	138.609	17	321.694	1751.162	18	327.660	288.010	19	373.711	157.517	20	378.720	194.354
21	386.704	349.862	22	396.732	196.104	23	408.713	167.135	24	414.694	457.456	25	426.711	358.421
26	450.720	368.492	27	469.766	292.536	28	502.731	438.030	29	510.739	276.664	30	527.751	438.034
31	539.753	288.031	32	563.767	259.876	33	608.795	231.049	34	656.798	523.770	35	740.802	185.291
39	803.895	222.896	37	806.896	307.889	38	823.924	552.701	39	863.920	201.520	40	877.902	192.451
41	880.927	268.891	42	936.961	222.741	43	961.021	1963.224	44	978.069	1956.364	45	1076.111	578.865
46	1092.165	420.696	47	1179.251	254.951	48	1488.622	448.788	49	1589.842	638.157	50	1658.138	351.306
51	1663.882	278.621	52	1667.335	275.526	53	1671.712	372.741	54	1676.135	902.221	55	1699.293	2072.240
56	1702.392	377.086	57	1719.102	648.185									

Calculated Masses:
 ETPVLSNFGPTLEFR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	f	x	y	z	C-Term	Ion
1	F	102.051	85.028	84.344	130.050	113.023	112.039	148.060	147.076	182.065	201.098	175.119	158.092	15	R
2	F	203.103	186.076	185.092	231.099	214.071	213.087	249.108	248.124	284.060	348.167	322.187	305.161	14	P
3	P	300.155	283.129	282.145	328.150	311.124	310.140	346.161	345.177	380.165	477.209	451.230	434.203	13	E
4	V	396.220	382.197	381.213	427.219	410.192	409.208	445.229	444.245	472.261	590.293	564.314	547.287	12	L
5	L	512.308	495.281	494.297	540.303	523.276	522.292	558.313	557.329	666.366	763.397	737.377	710.351	11	Y
6	S	599.340	582.313	581.329	627.335	610.308	609.324	645.345	644.361	804.444	850.499	824.430	807.404	10	P
7	N	713.381	696.356	695.372	741.378	724.351	723.367	759.388	758.404	877.455	897.431	881.452	864.425	9	G
8	P	810.438	793.409	792.425	838.431	821.404	820.420	856.441	855.457	70.865	1004.484	978.504	961.478	8	P
9	G	867.457	850.431	849.446	895.452	878.425	877.441	913.463	912.479	30.034	1118.527	1092.547	1075.521	7	N
10	P	964.510	947.483	946.499	992.505	975.478	974.494	1010.515	1009.531	70.865	1205.559	1179.579	1162.553	6	S
11	V	1127.573	1110.547	1109.563	1155.568	1138.542	1137.557	1173.579	1172.595	138.078	1318.643	1292.663	1276.637	5	L
12	L	1240.657	1223.631	1222.647	1268.652	1251.626	1250.642	1286.663	1285.679	86.996	1417.711	1391.732	1374.705	4	V
13	E	1369.700	1352.674	1351.689	1397.695	1380.669	1379.684	1415.705	1414.721	122.055	1514.764	1488.785	1471.758	3	P
14	F	1516.768	1499.742	1498.758	1544.763	1527.737	1526.753	1562.774	1561.790	120.081	1615.811	1589.832	1572.806	2	T
15	R	1672.869	1655.843	1654.859	1700.864	1683.838	1682.854	1718.875	1717.891	129.113	1744.854	1718.875	1701.848	1	E

(B)

Figure S2. Annotated MS/MS spectrum of ion 1719.099 m/z detected in area #1. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 1753.091; Mass Error: 0.188; MH+ (mono): 1752.903; MH+ (avg): 1753.936; Threshold (a.i.): 0.000; Tolerance (Da): 0.700; Number of Peaks: 51; Above Threshold: 51; Assigned Peaks: 33; Not assigned Peaks: 18

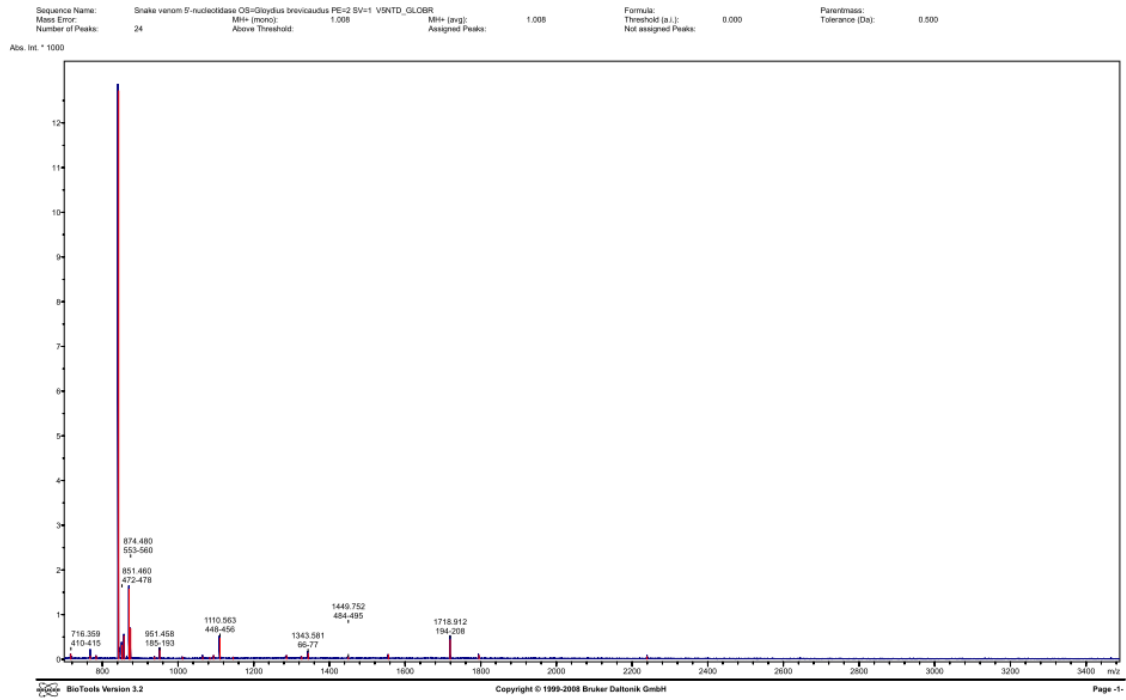
Peak#	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.750		2	85.728		3	109.704		4	1194.728		5	206.648	
6	206.671		7	234.627		8	236.654		9	245.674		10	250.663	
11	383.026		12	385.072		13	382.681		14	487.640		15	476.682	
16	487.714		17	491.623		18	556.713		19	568.689		20	577.711	
21	579.708		22	596.720		23	665.760		24	672.764		25	693.766	
26	710.765		27	754.823		28	811.843		29	831.930		30	946.977	
31	1062.086		32	1119.110		33	1141.063		34	1173.220		35	1271.285	
36	1389.498		37	1578.650		38	1583.607		39	1665.690		40	1678.639	
41	1680.650		42	1660.669		43	1669.670		44	1691.671		45	1695.670	
46	1697.684		47	1754.676		48	1736.658		49	1738.616		50	1741.676	
51	1753.024		52	891.910										

Calculated Masses: SFE...LH...TNDVHAR

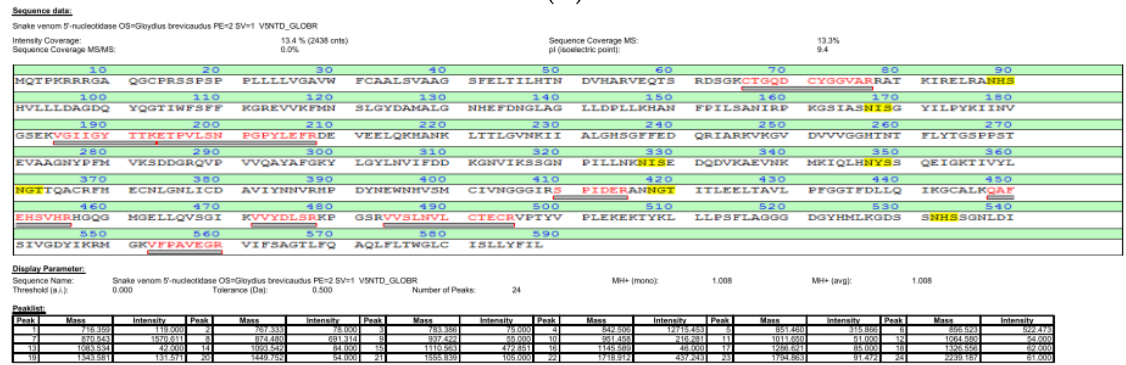
N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
1	S	60.044	43.018	42.034	85.039	71.013	70.029	106.050	105.066	60.044	201.098	175.119	158.092	15	R
2	F	207.113	180.086	169.102	235.168	218.081	217.097	253.118	252.134	120.081	272.135	246.156	229.139	14	A
3	E	336.155	319.129	318.145	344.190	327.124	326.140	382.161	381.177	102.055	409.194	383.219	366.188	13	H
4	L	449.239	432.213	431.229	477.234	460.208	459.224	495.245	494.261	88.096	508.263	482.283	465.257	12	V
5	T	550.287	533.261	532.277	578.282	561.256	560.271	596.293	595.309	74.050	623.290	607.310	589.284	11	D
6	I	663.371	646.345	645.361	691.366	674.340	673.356	709.377	708.393	88.096	737.333	711.353	694.327	10	N
7	L	776.455	759.429	758.445	804.450	787.424	786.440	822.461	821.477	88.096	838.380	812.401	795.374	9	T
8	H	873.514	856.488	855.504	901.509	884.483	883.499	919.520	918.536	110.071	915.439	889.460	872.433	8	H
9	T	1014.582	997.556	996.571	1042.577	1025.550	1024.566	1060.587	1059.603	74.050	1088.523	1062.544	1045.517	7	L
10	N	1128.605	1111.579	1110.594	1156.600	1139.573	1138.589	1174.610	1173.626	87.055	1201.607	1175.628	1158.601	6	I
11	D	1243.632	1226.605	1225.621	1271.627	1254.600	1253.616	1289.637	1288.653	88.099	1302.625	1276.645	1259.619	5	L
12	V	1342.700	1325.674	1324.690	1370.695	1353.669	1352.684	1388.705	1387.721	72.081	1415.709	1389.730	1372.703	4	L
13	H	1479.759	1462.733	1461.748	1507.754	1490.727	1489.743	1525.765	1524.781	110.071	1544.782	1518.802	1501.776	3	E
14	A	1550.789	1533.763	1532.778	1578.781	1561.755	1560.771	1596.792	1595.808	44.049	1611.850	1585.871	1568.844	2	F
15	R	1706.897	1689.871	1688.887	1734.892	1717.866	1716.882	1752.903	1751.919	129.113	1778.882	1752.903	1735.876	1	S

(B)

Figure S3. Annotated MS/MS spectrum of ion 1753.091 m/z detected in area #1. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.

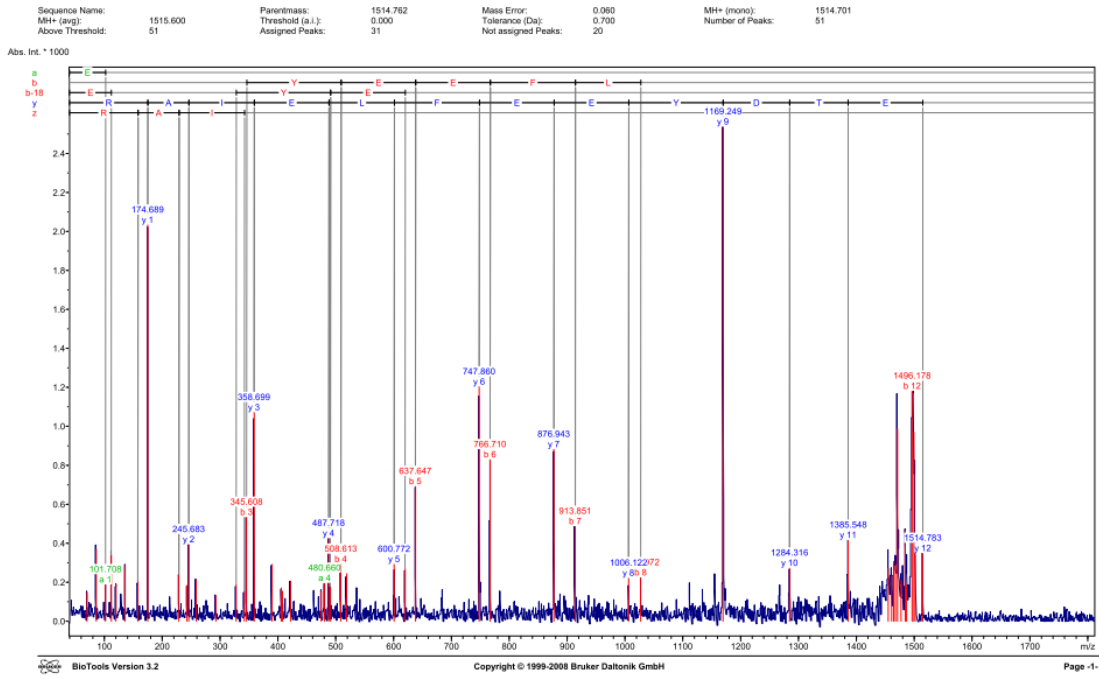


(A)



(B)

Figure S4. Annotated MS spectrum detected in area #1. (A) MS spectrum; (B) Peak list and sequence data.



(A)

Display Parameter:

Parentmass: 1514.762 Mass Error: 0.060 MH+ (mono): 1514.701 MH+ (avg): 1515.600
 Threshold (a.l.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 51 Above Threshold: 51
 Assigned Peaks: 31 Not assigned Peaks: 20

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.798	144.342	2	85.785	370.802	3	101.706	188.694	4	111.735	336.748	5	119.703	189.862
6	135.687	286.051	7	157.863	206.626	8	174.689	2034.276	9	228.669	241.341	10	242.679	183.162
11	245.693	394.207	12	258.634	211.891	13	292.632	132.922	14	327.606	186.866	15	341.647	153.274
18	345.630	534.592	17	358.699	1071.347	18	389.690	282.154	19	405.622	171.036	20	407.626	154.817
21	421.581	296.166	22	474.613	152.614	23	490.660	195.809	24	487.718	425.368	25	490.678	177.852
28	508.613	293.197	27	518.658	243.713	28	600.722	282.860	29	619.695	270.396	30	637.647	692.762
31	747.660	1263.182	32	766.710	830.132	33	876.843	882.512	34	813.851	487.623	35	1006.122	221.689
38	1169.912	224.338	37	1169.249	2537.812	38	1284.318	273.534	39	1385.548	417.008	40	1454.804	289.168
41	1460.778	251.452	42	1464.070	308.232	43	1487.354	282.247	44	1470.776	886.059	45	1477.052	207.887
46	1484.218	466.328	47	1486.673	187.193	48	1496.178	1182.011	49	1499.215	969.785	50	1501.447	354.050
51	1514.763	349.679												

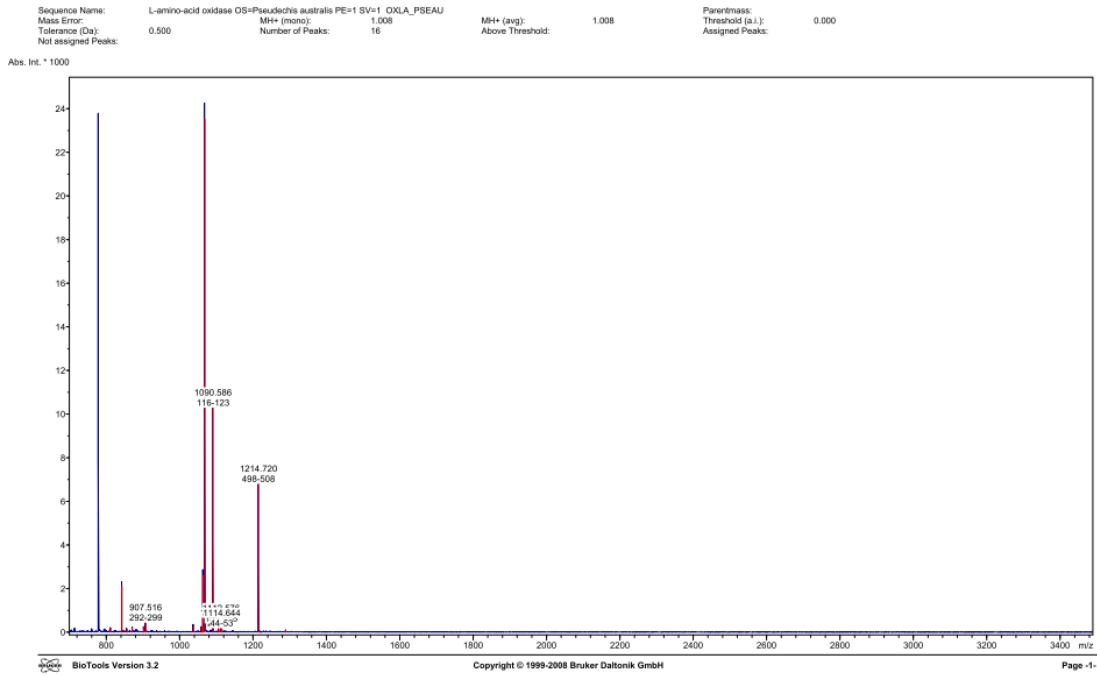
Calculated Masses:

ETDVEEFLLEIAR

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	x	y	z	C-Term	Ion
2	T	102.055	85.028	84.044	130.050	113.023	112.039	148.060	147.076	102.055	201.098	175.119	158.092	12	R
3	D	203.107	186.076	185.092	231.099	214.071	213.087	249.106	248.124	74.060	272.130	246.156	229.130	11	A
4	V	481.193	464.166	463.182	509.188	492.161	491.177	527.196	526.214	136.076	514.262	488.283	471.256	9	E
5	E	810.230	793.209	792.225	838.230	821.204	820.220	856.241	855.257	102.055	827.340	801.367	784.340	8	L
6	E	795.270	778.252	777.268	797.273	780.246	779.262	795.281	794.300	102.055	774.414	748.435	731.409	7	E
7	F	886.347	869.320	868.336	914.341	897.315	896.331	932.352	931.368	120.081	903.457	877.478	860.451	6	E
8	E	995.431	980.404	981.420	1022.423	1010.399	1009.415	1045.436	1044.452	86.986	1032.509	1006.530	989.504	5	E
9	E	1128.473	1111.447	1110.463	1152.466	1139.442	1138.458	1174.470	1173.486	102.055	1156.563	1169.584	1152.557	4	Y
10	I	1241.557	1224.531	1223.547	1269.552	1252.526	1251.542	1287.563	1286.579	86.996	1310.660	1284.611	1267.584	3	D
11	A	1312.599	1296.569	1294.584	1340.591	1323.563	1322.579	1359.600	1357.616	44.049	1411.639	1385.569	1368.612	2	E
12	R	1468.655	1451.629	1450.645	1496.650	1479.624	1478.640	1514.701	1513.717	129.113	1540.660	1514.701	1487.674	1	E

(B)

Figure S5. Annotated MS/MS spectrum of ion 1514.762 m/z detected in area #2. (A) MS/MS spectrum. (B) Peak list and amino acid sequence.



(A)

Sequence data:

L-amino-acid oxidase OS=Pseudechis australis PE=1 SV=1 OXLA_PSEAU

Intensity Coverage: 37.9 % (18125 conts)
 Sequence Coverage MS: 10.4%
 Sequence Coverage MS/MS: 0.0% pl (isoelectric point): 6.3

10	20	30	40	50	60	70	80	90	100	110	120	130	140
MDVFFRFSLL	FLAALGSCAD	DRRPLEECF	READYEEFLE	IARNGLQRTS	NFPRVVVQGA	GMAGLSAAYV	LAGAGHQVTL	LEASERVQGR	VNTYRNEKDG	UYVNLGPRRL	FERHRIREY	IRKFOLELNE	FIQENDNAVY
150	160	170	180	190	200	210	220	230	240	250	260	270	280
FIKIHRRVS	EVKKEPQVFR	IPVPRSEKGR	SASQLTRSL	QRVIEELKRT	NGNFIILNVD	TTSTKELIK	EGHLSGAVD	RIGDLNESD	STYLSFIESL	KSDDFSTEK	RFRIVGGFD	QLPKSNYQAI	AEKRVLNAGV
300	310	320	330	340	350	360	370	380	390	400	410	420	430
IKIQNAEDV	RVTYQTPAKT	LSVVIADYVI	VCSTRRAARR	IRFEPFLPK	KAKALRSIHY	RSSTKIFLTC	SGRFVADGI	HGGKSTDLF	SRFIYTNNS	FTSIOIVIVA	VTIADDTDF	QALDIETSD	IVINDLSLIR
430	440	450	460	470	480	490	500	510	520				
QLPKKIQAL	CYPSKIQRUS	LDEYFAGAIT	SFTPVQFQDF	FEIVAAPVGR	IYFAGEYTS	VRGWLDTIK	SGLTAARDVN	LASQKPSRI	IQ	LSDINNEL			

Display Parameter:

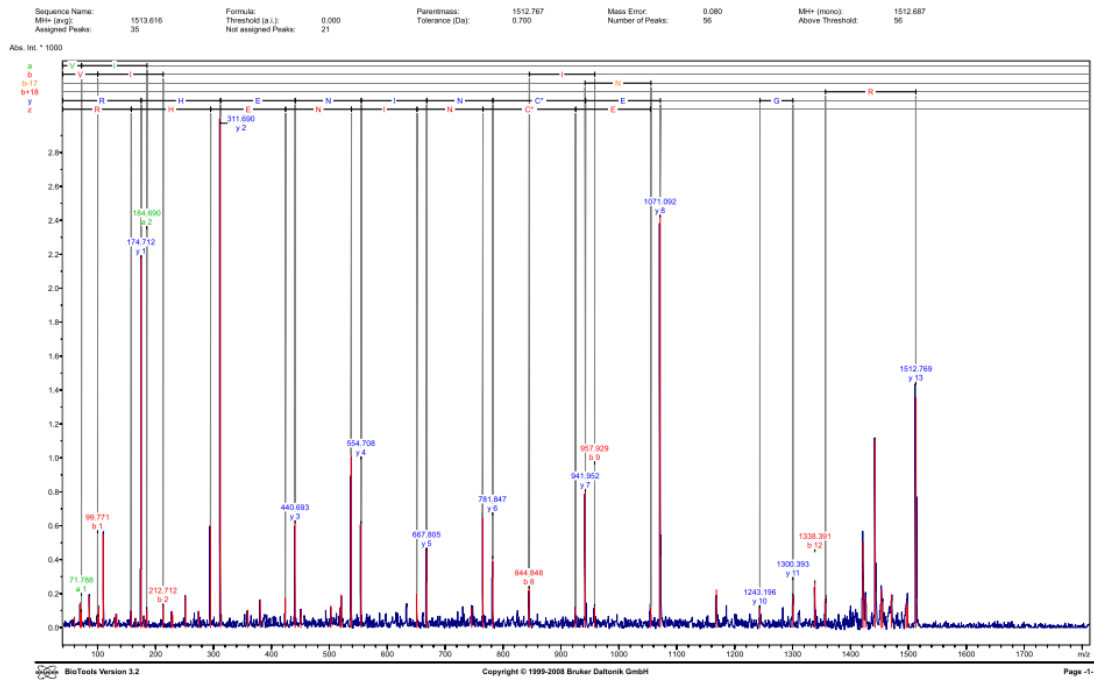
Sequence Name: L-amino-acid oxidase OS=Pseudechis australis PE=1 SV=1 OXLA_PSEAU
 MH+ (avg): 1.008 MH+ (mono): 1.008
 Threshold (a.i.): 0.000 Tolerance (Da): 0.500 Number of Peaks: 16

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
0	81.451	65.487	2	82.537	203.441	3	86.554	1.26473	4	87.571	165.672	8	102.434	2.9300
9	907.510	434.994	1	1037.598	289.464	6	1099.502	235.579	9	1063.592	2602.595	10	1065.604	23503.714
11	1090.586	10291.882	12	1106.586	202.855	13	1112.576	400.537	14	1114.644	189.146	15	1214.720	6794.976
16	1268.657	65.256												

(B)

Figure S6. Annotated MS spectrum detected in area #2. (A) MS spectrum; (B) Peak list and sequence data.



(A)

Display Parameter: Parentmass: 1512.767, Mass Error: 0.080, MH+ (mono): 1512.687, MH+ (avg): 1513.616, Threshold (a.l.): 0.000, Tolerance (Da): 0.700, Number of Peaks: 56, Above Threshold: 56, Assigned Peaks: 35, Not assigned Peaks: 21

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.723	69.896	4	62.937	151.217	3	71.768	39.262	4	82.777	142.971	5	92.711	31.979
2	109.733	449.747	3	129.723	81.453	8	132.642	77.964	10	187.733	102.007	11	192.630	94.735
13	139.674	69.506	14	144.660	138.384	15	174.724	137.300	16	222.685	69.449	17	228.620	79.333
18	214.691	82.694	20	264.679	592.619	21	311.630	3006.920	22	368.626	102.268	23	388.664	184.871
24	420.693	832.211	25	450.674	124.848	26	490.694	472.458	27	518.658	114.508	28	538.650	139.250
31	524.703	910.042	32	550.695	235.229	33	589.695	460.188	34	745.699	121.403	35	754.833	820.850
37	844.402	244.719	38	864.888	185.170	39	961.952	819.070	40	987.600	121.211	41	1036.000	194.194
42	1168.193	201.877	43	1241.185	170.462	45	1300.302	183.961	46	1338.301	261.130	47	1398.301	176.810
48	1426.697	178.507	50	1442.172	1188.940	51	1482.654	222.727	52	1484.267	142.701	53	1476.232	188.953
55	1488.697	121.056	59	1512.767	1360.914									

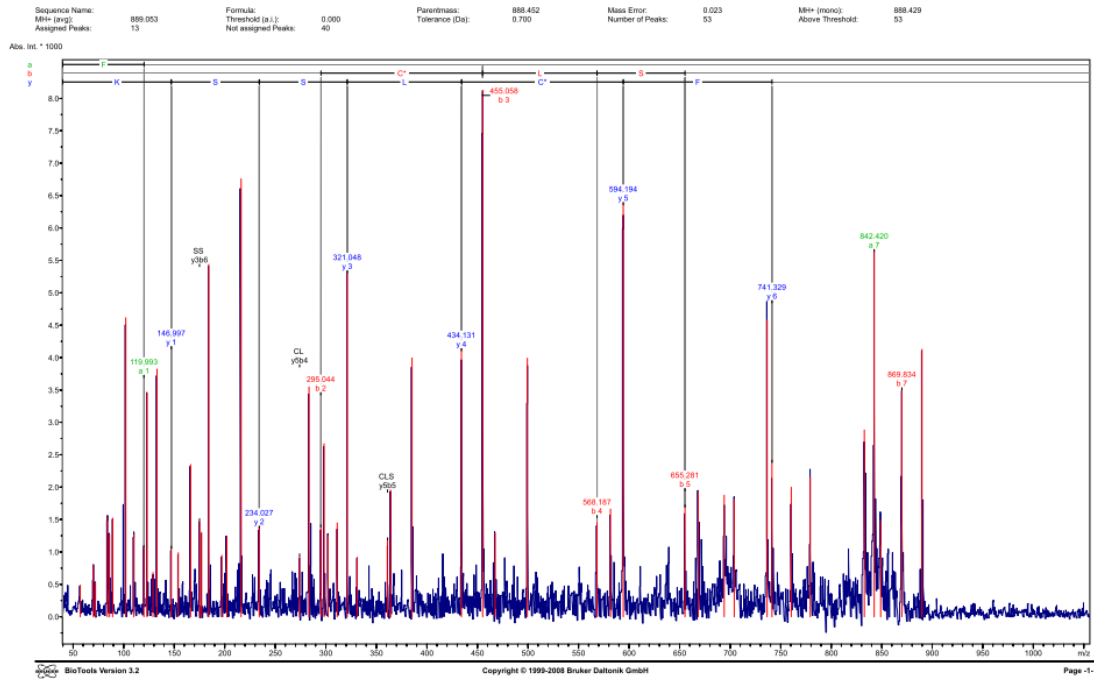
Calculated Masses: VDDGCKNRR7, Carbamidomethyl (C)

R-Yeem	Ion	a	a-17	a-19	b	b-17	b-19	b+18	c	l	x	y	z	C-Yeem	Ion
1	V	72.091	86.903	104.404	109.403	124.405	134.405	149.406	177.110	77.083	80.100	176.110	188.604	1	10
2	G	165.182	180.181	204.404	209.403	224.405	234.405	249.406	277.110	165.188	168.199	276.110	288.604	2	11
3	G	248.180	263.180	284.178	289.181	304.185	314.185	329.186	362.191	248.192	251.200	360.191	372.604	3	12
4	G	292.200	307.201	324.187	329.203	344.209	354.209	369.210	402.214	292.204	295.213	400.214	412.604	4	13
5	D	416.200	431.201	448.204	453.209	468.217	478.217	493.218	531.224	416.208	419.217	530.218	542.604	5	14
6	E	451.211	466.211	483.211	488.214	503.221	513.221	528.222	561.228	451.215	454.221	560.222	572.604	6	15
7	C'	701.301	686.301	685.297	711.303	718.299	717.292	748.311	748.310	133.043	168.200	842.421	822.384	7	16
8	N	812.287	802.281	799.280	828.283	835.279	834.272	865.285	865.284	167.085	197.242	1011.464	1004.427	8	17
9	I	820.431	814.430	812.424	842.428	841.423	840.419	870.430	870.429	86.096	1212.270	1138.091	1159.484	9	18
10	D	1044.470	1037.470	1036.464	1067.472	1066.468	1065.464	1096.476	1096.475	177.082	1408.411	1243.517	1264.604	10	19
11	E	1174.500	1167.500	1166.494	1197.496	1196.492	1195.488	1226.499	1226.498	167.082	1538.411	1373.517	1394.604	11	20
12	H	1310.570	1303.570	1302.564	1333.566	1332.562	1331.558	1362.569	1362.568	135.071	1438.602	1419.610	1440.604	12	21
13	R	1606.600	1600.601	1600.593	1631.595	1631.587	1631.580	1662.591	1662.590	133.113	1530.602	1512.604	1493.604	13	22

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(B)

Figure S7. Annotated MS/MS spectrum of ion 1512.767 *m/z* detected in area #3. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 888.452 Mass Error: 0.023 MH+ (mono): 888.429 MH+ (avg): 889.053 Threshold (a.l.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 53 Above Threshold: 53 Assigned Peaks: 13 Not assigned Peaks: 40

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
56	86.200	486.413	3	89.042	15.241	5	11.990	327.065	4	83.912	154.424	6	86.000	1081.000
13	102.000	4610.877	3	109.872	126.926	5	119.990	1061.951	10	120.000	349.474	11	126.000	263.436
19	128.000	106.192	11	133.064	650.926	15	150.992	2459.064	16	159.044	1919.919	17	174.000	1333.920
19	137.000	848.197	20	202.025	1231.880	21	215.052	8758.944	22	234.030	1480.228	23	274.917	1011.480
25	250.024	130.223	26	265.166	2628.163	27	302.138	1926.116	28	311.224	1449.621	29	321.920	3210.152
33	361.024	1179.068	33	384.048	1966.261	33	385.274	3926.044	34	434.131	4140.731	35	450.000	8439.911
36	409.284	1077.787	39	508.184	1466.480	39	511.420	1867.111	40	566.164	8295.061	41	655.281	689.817
43	684.000	1879.440	43	925.033	1820.420	45	710.480	2577.611	46	741.329	2376.620	47	799.400	2020.854
49	832.711	2692.154	50	842.420	5688.910	51	868.700	1387.450	52	869.834	3536.400	53	889.053	4127.817

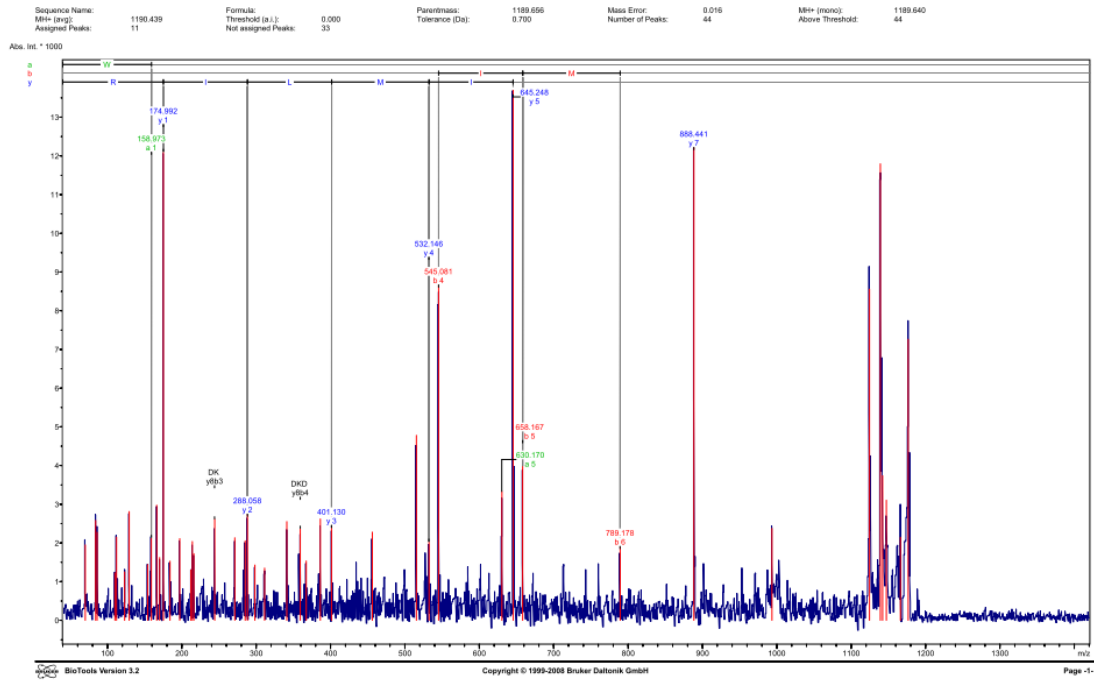
Calculated Masses:
 P1-C15S8-C, Carboxymethyl (C)

N-Term	Ion	a	b	y	C-Term	Ion
1	P	120.081	128.070	147.113	P	K
1	F	157.101	165.144	184.183	F	K
3	C+	427.150	435.173	521.177	S	S
4	S	466.205	474.209	524.204	S	S
4	S	677.205	685.201	684.204	S	S
5	S	714.205	722.203	741.200	S	F
7	K	842.251	810.211	810.211	K	

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(B)

Figure S8. Annotated MS/MS spectrum of ion 888.452 *m/z* detected in area #3. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 1189.656 Mass Error: 0.016 Mi+ (mono): 1189.640 Mi+ (avg): 1190.439 Threshold (a.i.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 44 Above Threshold: 44 Assigned Peaks: 11 Not assigned Peaks: 33

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
10	128.067	2811.318	1	131.062	1441.812	2	158.073	2138.266	10	186.071	2677.710	11	202.073	1621.452
11	183.069	3331.105	3	186.066	2111.681	4	219.068	3002.804	12	233.064	2033.250	13	249.066	1743.400
12	217.070	2138.240	20	288.059	2005.480	21	288.059	2748.330	22	288.051	1431.430	23	311.067	1382.430
20	332.074	2029.571	28	361.074	1536.131	24	330.070	2618.358	25	401.074	2253.251	26	425.070	2202.430
33	532.124	3032.650	33	545.081	8669.033	33	550.130	3330.533	34	645.245	1950.430	35	658.187	5683.054
34	686.441	12419.881	38	692.388	2211.680	36	1124.241	3369.140	38	1189.656	11298.400	41	1189.121	3749.304
43	1189.125	2148.961	44	1176.560	7383.730									

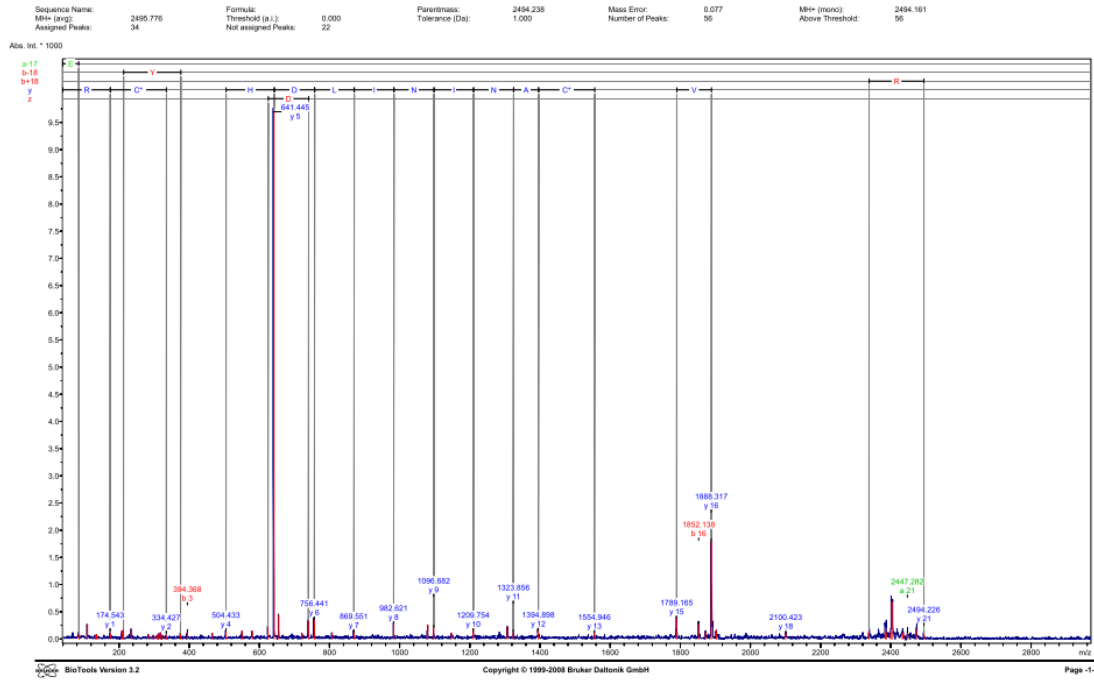
Calculated Masses:
 WQWDRMLR

Mi.Term	Ion	a	b	y	C.Term	Ion
1	W	159.092	197.057	178.111		
2	D	278.110	302.113	288.203	S	L
3	R	402.211	430.204	401.207		
4	D	617.241	645.233	632.238		
5	L	636.262	658.253	654.251		
6	M	751.262	789.259	752.252	L	D
7	L	874.441	874.441	884.443		
8	L	887.433	1016.428	1033.560		
9	R	1141.634	1171.620	1189.620		

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(B)

Figure S10. Annotated MS/MS spectrum of ion 1189.656 m/z detected in area #4. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 2494.238
 Tolerance (Da): 1.000
 Mass Error: 0.077
 Number of Peaks: 56
 MH+ (mono): 2494.161
 Above Threshold: 56
 MH+ (avg): 2495.776
 Assigned Peaks: 34
 Threshold (a.i.): 0.000
 Not assigned Peaks: 22

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
85	201	85	201	85	201	85	201	85	201	85	201	85	201	85
11	174.543	1.115	11	174.543	1.115	11	174.543	1.115	11	174.543	1.115	11	174.543	1.115
13	304.368	0.146	13	304.368	0.146	13	304.368	0.146	13	304.368	0.146	13	304.368	0.146
15	334.427	0.050	15	334.427	0.050	15	334.427	0.050	15	334.427	0.050	15	334.427	0.050
23	504.433	0.050	23	504.433	0.050	23	504.433	0.050	23	504.433	0.050	23	504.433	0.050
33	541.445	952.294	33	541.445	952.294	33	541.445	952.294	33	541.445	952.294	33	541.445	952.294
34	571.400	0.050	34	571.400	0.050	34	571.400	0.050	34	571.400	0.050	34	571.400	0.050
43	750.441	0.050	43	750.441	0.050	43	750.441	0.050	43	750.441	0.050	43	750.441	0.050
49	869.551	0.050	49	869.551	0.050	49	869.551	0.050	49	869.551	0.050	49	869.551	0.050
59	1096.652	0.050	59	1096.652	0.050	59	1096.652	0.050	59	1096.652	0.050	59	1096.652	0.050
69	1206.754	0.050	69	1206.754	0.050	69	1206.754	0.050	69	1206.754	0.050	69	1206.754	0.050
79	1323.856	0.050	79	1323.856	0.050	79	1323.856	0.050	79	1323.856	0.050	79	1323.856	0.050
89	1394.898	0.050	89	1394.898	0.050	89	1394.898	0.050	89	1394.898	0.050	89	1394.898	0.050
99	1554.946	0.050	99	1554.946	0.050	99	1554.946	0.050	99	1554.946	0.050	99	1554.946	0.050
109	1789.165	0.050	109	1789.165	0.050	109	1789.165	0.050	109	1789.165	0.050	109	1789.165	0.050
119	1866.317	0.050	119	1866.317	0.050	119	1866.317	0.050	119	1866.317	0.050	119	1866.317	0.050
129	1952.138	0.050	129	1952.138	0.050	129	1952.138	0.050	129	1952.138	0.050	129	1952.138	0.050
139	2100.423	0.050	139	2100.423	0.050	139	2100.423	0.050	139	2100.423	0.050	139	2100.423	0.050
149	2447.232	0.050	149	2447.232	0.050	149	2447.232	0.050	149	2447.232	0.050	149	2447.232	0.050
159	2494.238	0.050	159	2494.238	0.050	159	2494.238	0.050	159	2494.238	0.050	159	2494.238	0.050
169	2494.238	952.294	169	2494.238	952.294	169	2494.238	952.294	169	2494.238	952.294	169	2494.238	952.294

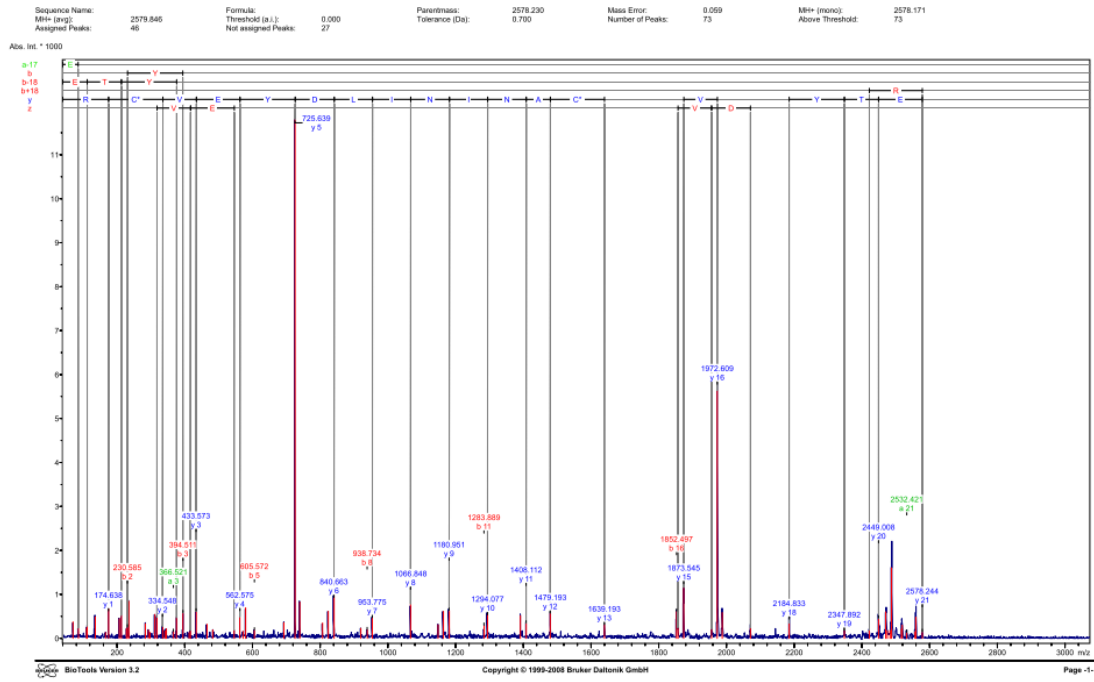
Calculated Masses:
 EYFDVPHCANLLDHAVCR: Carbamidothiyl (C) 20: Carbamidothiyl (C)

N-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	c	f	f	f	C-Term	Ion
1	F	102.050	18.000	18.000	133.050	117.050	149.050	147.070	192.050	191.000	171.119	191.062	21	F	
2	F	204.100	36.000	36.000	266.100	234.100	298.100	296.140	384.100	381.100	332.100	318.121	40	F	
3	F	306.150	54.000	54.000	399.150	348.150	447.150	445.180	576.150	573.150	498.119	474.179	59	F	
4	F	408.200	72.000	72.000	532.200	456.200	594.200	592.220	768.200	765.200	664.139	630.229	68	F	
5	F	510.250	90.000	90.000	665.250	570.250	744.250	742.260	972.250	969.250	832.159	788.259	77	F	
6	F	612.300	108.000	108.000	798.300	684.300	887.300	885.310	1188.300	1185.300	1016.179	962.279	86	F	
7	F	714.350	126.000	126.000	931.350	798.350	1090.350	1088.360	1440.350	1437.350	1240.199	1178.299	95	F	
8	F	816.400	144.000	144.000	1064.400	912.400	1281.400	1279.410	1728.400	1725.400	1472.219	1400.319	104	F	
9	F	918.450	162.000	162.000	1197.450	1026.450	1458.450	1456.460	1944.450	1941.450	1684.239	1602.339	113	F	
10	F	1020.500	180.000	180.000	1330.500	1140.500	1746.500	1744.510	2304.500	2301.500	1968.259	1876.359	122	F	
11	F	1122.550	198.000	198.000	1463.550	1254.550	1983.550	1981.560	2640.550	2637.550	2224.279	2122.379	131	F	
12	F	1224.600	216.000	216.000	1596.600	1362.600	2211.600	2209.610	2928.600	2925.600	2448.299	2336.399	140	F	
13	F	1326.650	234.000	234.000	1729.650	1491.650	2440.650	2438.660	3216.650	3213.650	2696.319	2574.419	149	F	
14	F	1428.700	252.000	252.000	1862.700	1620.700	2669.700	2667.710	3504.700	3501.700	2954.339	2822.439	158	F	
15	F	1530.750	270.000	270.000	1995.750	1749.750	2900.750	2898.760	3800.750	3797.750	3212.359	3080.459	167	F	
16	F	1632.800	288.000	288.000	2128.800	1878.800	3130.800	3128.810	4090.800	4087.800	3470.379	3338.479	176	F	
17	F	1734.850	306.000	306.000	2261.850	2007.850	3360.850	3358.860	4380.850	4377.850	3728.399	3586.499	185	F	
18	F	1836.900	324.000	324.000	2394.900	2136.900	3590.900	3588.910	4670.900	4667.900	3986.419	3834.519	194	F	
19	F	1938.950	342.000	342.000	2527.950	2265.950	3820.950	3818.960	4960.950	4957.950	4244.439	4082.539	203	F	
20	F	2041.000	360.000	360.000	2660.000	2395.000	4050.000	4048.010	5250.000	5247.000	4502.459	4328.559	212	F	
21	F	2143.050	378.000	378.000	2793.050	2524.050	4280.050	4278.060	5540.050	5537.050	4760.479	4564.579	221	F	
22	F	2245.100	396.000	396.000	2926.100	2653.100	4510.100	4508.110	5830.100	5827.100	5018.499	4802.599	230	F	

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(B)

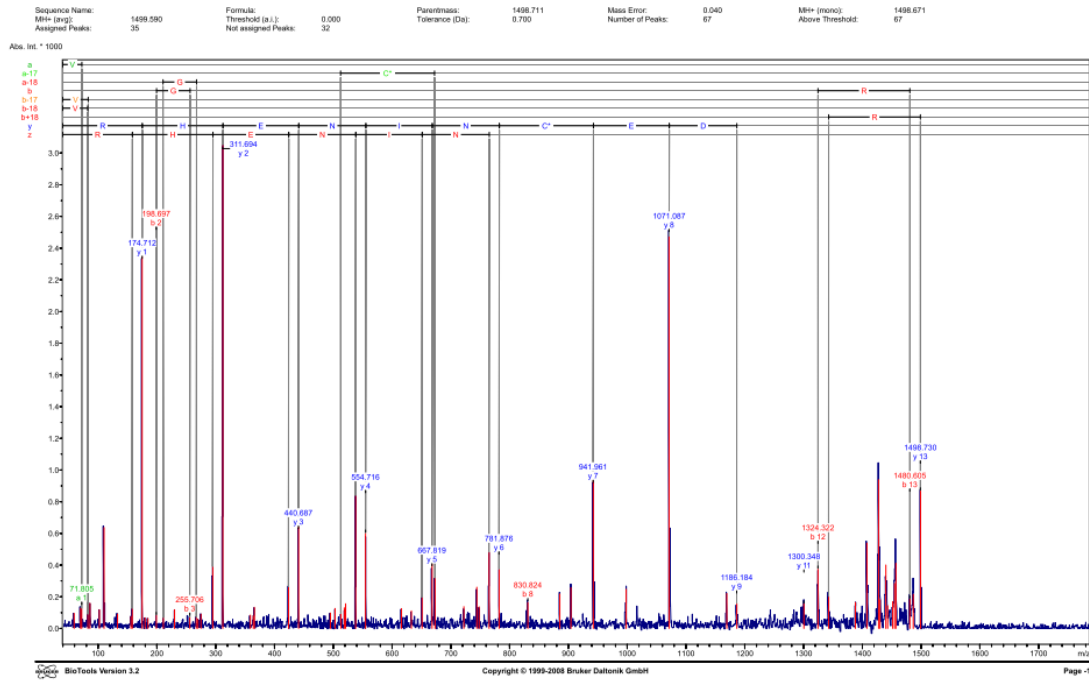
Figure S14. Annotated MS/MS spectrum of ion 2494.238 m/z detected in area #4. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 2578.230
 Tolerance (Da): 0.700
 Mass Error: 0.059
 Number of Peaks: 73
 Mi+ (mono): 2578.171
 Above Threshold: 73
 Mi+ (avg): 2578.846
 Assigned Peaks: 46
 Threshold (a.i.): 0.000
 Not assigned Peaks: 27

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
69	700	374.040	69	829	231.614	69	958	230.031	69	1117	229.548	69	1266	185.984
70	714	632	70	843	206.252	70	972	205.050	70	1131	204.010	70	1280	162.000
71	728	1133	71	857	202.436	71	996	191.000	71	1155	190.000	71	1304	154.400
72	742	341	72	871	181.595	72	1010	170.000	72	1169	169.000	72	1318	146.800
73	756	297	73	885	167.810	73	1024	156.000	73	1183	155.000	73	1332	139.200
74	770	253	74	909	154.025	74	1038	142.000	74	1197	141.000	74	1346	131.600
75	784	209	75	923	140.240	75	1052	128.000	75	1211	127.000	75	1360	124.000
76	798	165	76	937	126.455	76	1066	114.000	76	1225	113.000	76	1374	116.400
77	812	121	77	951	112.670	77	1080	100.000	77	1239	99.000	77	1388	108.800
78	826	77	78	965	98.885	78	1094	86.000	78	1253	85.000	78	1402	102.200
79	840	33	79	979	85.100	79	1108	72.000	79	1267	71.000	79	1416	94.600
80	854	19	80	993	71.315	80	1122	58.000	80	1281	57.000	80	1430	87.000
81	868	5	81	1007	57.530	81	1136	44.000	81	1295	43.000	81	1444	79.400
82	882	1	82	1021	43.745	82	1150	30.000	82	1309	29.000	82	1458	71.800
83	896	0	83	1035	29.960	83	1164	16.000	83	1323	15.000	83	1472	64.200
84	910	0	84	1049	16.175	84	1178	2.000	84	1337	1.000	84	1486	56.600
85	924	0	85	1063	1.390	85	1192	0.000	85	1351	0.000	85	1500	49.000
86	938	0	86	1077	0.705	86	1206	0.000	86	1365	0.000	86	1514	41.400
87	952	0	87	1091	0.020	87	1220	0.000	87	1379	0.000	87	1528	33.800
88	966	0	88	1105	0.000	88	1234	0.000	88	1393	0.000	88	1542	26.200
89	980	0	89	1119	0.000	89	1248	0.000	89	1407	0.000	89	1556	18.600
90	994	0	90	1133	0.000	90	1262	0.000	90	1421	0.000	90	1570	11.000
91	1008	0	91	1147	0.000	91	1276	0.000	91	1435	0.000	91	1584	3.400
92	1022	0	92	1161	0.000	92	1290	0.000	92	1449	0.000	92	1598	0.000
93	1036	0	93	1175	0.000	93	1304	0.000	93	1463	0.000	93	1612	0.000
94	1050	0	94	1189	0.000	94	1318	0.000	94	1477	0.000	94	1626	0.000
95	1064	0	95	1203	0.000	95	1332	0.000	95	1491	0.000	95	1640	0.000
96	1078	0	96	1217	0.000	96	1346	0.000	96	1505	0.000	96	1654	0.000
97	1092	0	97	1231	0.000	97	1360	0.000	97	1519	0.000	97	1668	0.000
98	1106	0	98	1245	0.000	98	1374	0.000	98	1533	0.000	98	1682	0.000
99	1120	0	99	1259	0.000	99	1388	0.000	99	1547	0.000	99	1696	0.000
100	1134	0	100	1273	0.000	100	1402	0.000	100	1561	0.000	100	1710	0.000
101	1148	0	101	1287	0.000	101	1416	0.000	101	1575	0.000	101	1724	0.000
102	1162	0	102	1301	0.000	102	1430	0.000	102	1589	0.000	102	1738	0.000
103	1176	0	103	1315	0.000	103	1444	0.000	103	1603	0.000	103	1752	0.000
104	1190	0	104	1329	0.000	104	1458	0.000	104	1617	0.000	104	1766	0.000
105	1204	0	105	1343	0.000	105	1472	0.000	105	1631	0.000	105	1780	0.000
106	1218	0	106	1357	0.000	106	1486	0.000	106	1645	0.000	106	1794	0.000
107	1232	0	107	1371	0.000	107	1500	0.000	107	1659	0.000	107	1808	0.000
108	1246	0	108	1385	0.000	108	1514	0.000	108	1673	0.000	108	1822	0.000
109	1260	0	109	1399	0.000	109	1528	0.000	109	1687	0.000	109	1836	0.000
110	1274	0	110	1413	0.000	110	1542	0.000	110	1701	0.000	110	1850	0.000
111	1288	0	111	1427	0.000	111	1556	0.000	111	1715	0.000	111	1864	0.000
112	1302	0	112	1441	0.000	112	1570	0.000	112	1729	0.000	112	1878	0.000
113	1316	0	113	1455	0.000	113	1584	0.000	113	1743	0.000	113	1892	0.000
114	1330	0	114	1469	0.000	114	1598	0.000	114	1757	0.000	114	1906	0.000
115	1344	0	115	1483	0.000	115	1612	0.000	115	1771	0.000	115	1920	0.000
116	1358	0	116	1497	0.000	116	1626	0.000	116	1785	0.000	116	1934	0.000
117	1372	0	117	1511	0.000	117	1640	0.000	117	1799	0.000	117	1948	0.000
118	1386	0	118	1525	0.000	118	1654	0.000	118	1813	0.000	118	1962	0.000
119	1400	0	119	1539	0.000	119	1668	0.000	119	1827	0.000	119	1976	0.000
120	1414	0	120	1553	0.000	120	1682	0.000	120	1841	0.000	120	1990	0.000
121	1428	0	121	1567	0.000	121	1696	0.000	121	1855	0.000	121	2004	0.000
122	1442	0	122	1581	0.000	122	1710	0.000	122	1869	0.000	122	2018	0.000
123	1456	0	123	1595	0.000	123	1724	0.000	123	1883	0.000	123	2032	0.000
124	1470	0	124	1609	0.000	124	1738	0.000	124	1897	0.000	124	2046	0.000
125	1484	0	125	1623	0.000	125	1752	0.000	125	1911	0.000	125	2060	0.000
126	1498	0	126	1637	0.000	126	1766	0.000	126	1925	0.000	126	2074	0.000
127	1512	0	127	1651	0.000	127	1780	0.000	127	1939	0.000	127	2088	0.000
128	1526	0	128	1665	0.000	128	1794	0.000	128	1953	0.000	128	2102	0.000
129	1540	0	129	1679	0.000	129	1808	0.000	129	1967	0.000	129	2116	0.000
130	1554	0	130	1693	0.000	130	1822	0.000	130	1981	0.000	130	2130	0.000
131	1568	0	131	1707	0.000	131	1836	0.000	131	1995	0.000	131	2144	0.000
132	1582	0	132	1721	0.000	132	1850	0.000	132	2009	0.000	132	2158	0.000
133	1596	0	133	1735	0.000	133	1864	0.000	133	2023	0.000	133	2172	0.000
134	1610	0	134	1749	0.000	134	1878	0.000	134	2037	0.000	134	2186	0.000
135	1624	0	135	1763	0.000	135	1892	0.000	135	2051	0.000	135	2200	0.000
136	1638	0	136	1777	0.000	136	1906	0.000	136	2065	0.000	136	2214	0.000
137	1652	0	137	1791	0.000	137	1920	0.000	137	2079	0.000	137	2228	0.000
138	1666	0	138	1805	0.000	138	1934	0.000	138	2093	0.000	138	2242	0.000
139	1680	0	139	1819	0.000	139	1948	0.000	139	2107	0.000	139	2256	0.000
140	1694	0	140	1833	0.000	140	1962	0.000	140	2121	0.000	140	2270	0.000
141	1708	0	141	1847	0.000	141	1976	0.000	141	2135	0.000	141	2284	0.000
142	1722	0	142	1861	0.000	142	1990	0.000	142	2149	0.000	142	2298	0.000
143	1736	0	143	1875	0.000	143	2004	0.000	143	2163	0.000	143	2312	0.000
144	1750	0	144	1889	0.000	144	2018	0.000	144	2177	0.000	144	2326	0.000
145	1764	0	145	1903	0.000	145	2032	0.000	145	2191	0.000	145	2340	0.000
146	1778	0	146	1917	0.000	146	2046	0.000	146	2205	0.000	146	2354	0.000
147	1792	0	147	1931	0.000	147	2060	0.000	147	2219	0.000	147	2368	0.000
148	1806	0	148	1945	0.000	148	2074	0.000	148	2233	0.000	148	2382	0.000
149	1820	0	149	1959	0.000	149	2088	0.000	149	2247	0.000	149	2396	0.000
150	1834	0	150	1973	0.000	150	2102	0.000	150	2261	0.000	150	2410	0.000
151	1848	0	151	1987	0.000	151	2116	0.000	151	2275	0.000	151	2424	0.000
152	1862	0	152	2001	0.000	152	2130	0.000	152	2289	0.000	152	2438	0.000
153	1876	0	153	2015	0.000	153	2144	0.000	153	2303	0.000	153	2452	0.000
154	1890	0	154	2029	0.000									



(A)

Display Parameter: Parentmass: 1498.711 Mass Error: 0.040 MH+ (mono): 1498.671 MH+ (avg): 1499.590 Threshold (a.i.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 67 Above Threshold: 67

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.812	0.056	2	69.767	0.031	3	119.055	1	82.311	0.899	4	101.180	119.462	
4	109.743	0.082	5	132.727	0.050	6	155.581	25.012	10	187.950	127.500	11	172.730	240.312
12	184.660	0.399	13	199.091	0.159	14	213.582	69.113	16	229.029	117.693	17	255.724	77.461
18	289.875	37.873	20	274.600	30.762	21	288.883	392.730	22	311.594	3081.575	23	338.840	81.954
25	350.604	133.442	26	347.655	259.178	27	400.977	140.749	28	424.705	67.430	29	370.702	170.930
31	318.930	130.010	32	325.877	165.200	33	337.801	840.743	34	364.745	650.420	35	411.750	124.930
36	650.495	109.326	37	669.816	609.180	38	612.833	118.874	39	347.851	167.594	41	618.864	280.350
43	764.824	481.483	44	781.820	317.458	45	530.843	163.807	46	584.950	217.633	47	631.920	297.446
48	668.669	264.824	49	107.084	4412.084	51	1189.184	229.555	52	1186.184	164.060	53	1207.489	157.650
54	1159.401	202.574	55	1387.987	84.180	57	1289.577	538.735	58	1429.981	930.000	59	1249.820	181.416
61	1482.850	181.980	62	1451.784	180.531	63	1462.780	284.760	64	1458.953	411.430	65	1486.000	189.430
67	1498.711	871.397												

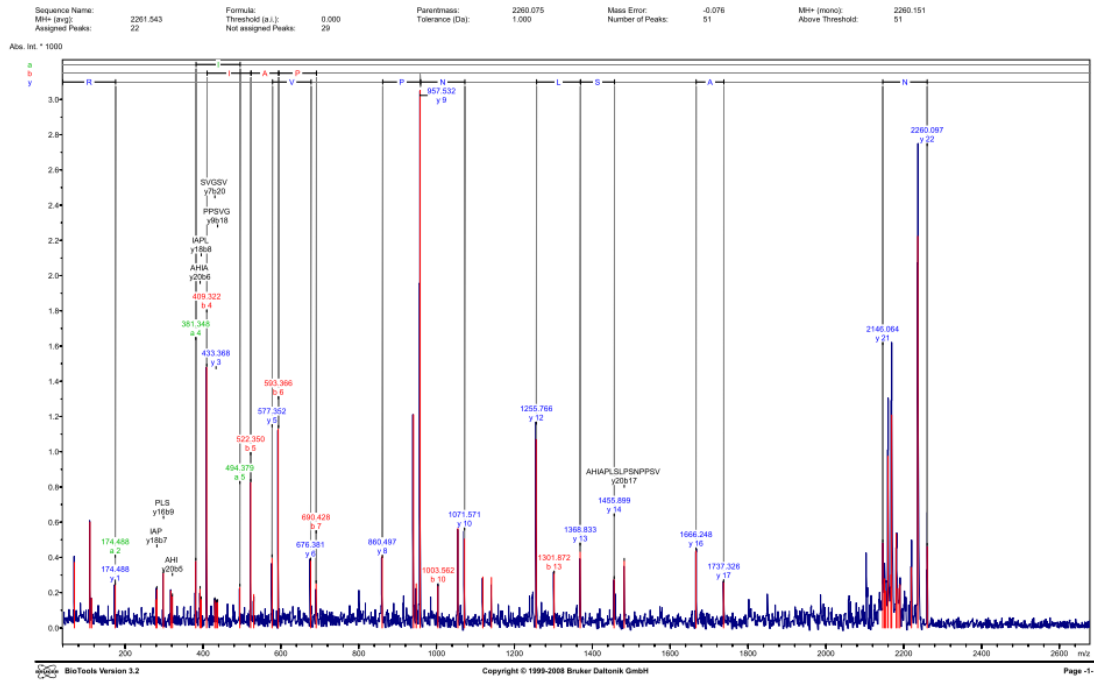
Calculated Masses: VGGDECNNEHR7: Carbamatoethyl (C)

IC-Term	len	a	a-17	a-18	b	b-17	b-18	b+18	c	y	z	z	z	C-Term	len
1	7	72.881	153.093	154.103	703.912	83.449	84.965	148.598	171.100	72.081	701.998	175.119	186.692	7	18
2	7	171.181	151.921	153.103	199.144	182.118	181.183	217.155	216.171	72.081	538.197	312.178	285.181	7	18
3	7	228.174	211.141	218.160	386.180	230.100	229.105	274.176	273.102	30.102	487.200	441.200	442.184	13	18
4	7	285.166	268.151	267.161	519.189	266.100	265.195	351.169	350.211	30.102	611.243	555.243	556.227	13	18
5	7	300.210	303.211	302.203	428.214	411.180	410.202	448.220	447.241	68.093	684.292	648.292	651.321	8	18
6	7	350.260	313.231	311.251	269.214	440.220	336.265	335.265	334.261	182.093	608.290	742.290	745.364	8	18
7	7	400.260	472.260	471.262	277.260	700.261	669.277	739.260	734.310	133.043	668.200	842.242	845.384	7	18
8	7	450.310	728.309	728.303	311.310	814.304	813.309	849.341	848.321	87.093	109.443	1271.464	1274.517	6	18
9	7	518.410	699.301	698.299	444.214	897.389	826.494	924.423	921.441	86.098	1412.290	1186.491	1189.464	6	18
10	7	678.506	1174.338	1174.334	1097.478	1041.411	1040.474	1076.456	1076.456	87.093	1669.411	1433.474	1436.498	6	18
11	7	1109.426	1749.470	1749.464	1197.200	1170.414	1169.480	1205.410	1204.520	102.095	1506.211	1300.433	1283.507	6	18
12	7	1286.856	1749.470	1749.464	1244.200	1207.200	1206.248	1244.260	1244.260	118.017	1420.260	1209.602	1282.674	2	18
13	7	1286.856	1244.261	1244.261	1480.602	1463.613	1462.625	1498.616	1497.621	134.111	1542.602	1488.616	1511.621	1	18

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(B)

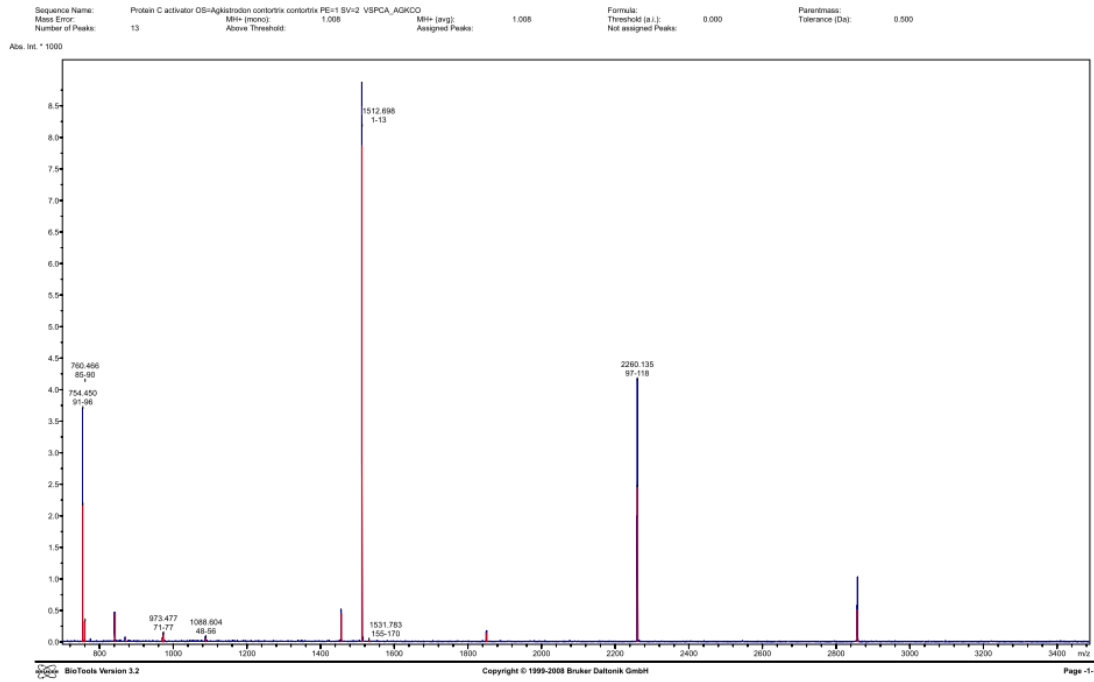
Figure S17. Annotated MS/MS spectrum of ion 1498.711 m/z detected in area #5. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 2260.075
 Tolerance (Da): 1.000
 Mass Error: -0.076
 Number of Peaks: 51
 MH+ (mono): 2260.151
 Above Threshold: 51
 MH+ (avg): 2261.543
 Assigned Peaks: 22
 Threshold (a.i.): 0.000
 Not assigned Peaks: 29

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
13	288.352	374.161	3	217.248	511.231	8	174.488	107.750	4	174.488	261.429	11	226.300	221.000
14	288.352	374.161	4	217.248	511.231	9	174.488	178.760	10	281.545	301.027	12	226.300	221.000
15	288.352	374.161	5	217.248	511.231	10	174.488	143.419	11	437.424	142.920	13	226.300	221.000
16	288.352	374.161	6	217.248	511.231	11	174.488	1134.330	22	676.381	339.140	23	880.420	253.950
17	288.352	374.161	7	217.248	511.231	12	174.488	1140.004	20	1003.358	239.370	24	1058.271	364.410
18	288.352	374.161	8	217.248	511.231	13	174.488	1079.311	21	1301.317	321.450	25	1369.833	234.444
19	288.352	374.161	9	217.248	511.231	14	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
20	288.352	374.161	10	217.248	511.231	15	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
21	288.352	374.161	11	217.248	511.231	16	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
22	288.352	374.161	12	217.248	511.231	17	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
23	288.352	374.161	13	217.248	511.231	18	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
24	288.352	374.161	14	217.248	511.231	19	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
25	288.352	374.161	15	217.248	511.231	20	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
26	288.352	374.161	16	217.248	511.231	21	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
27	288.352	374.161	17	217.248	511.231	22	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
28	288.352	374.161	18	217.248	511.231	23	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
29	288.352	374.161	19	217.248	511.231	24	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
30	288.352	374.161	20	217.248	511.231	25	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
31	288.352	374.161	21	217.248	511.231	26	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
32	288.352	374.161	22	217.248	511.231	27	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
33	288.352	374.161	23	217.248	511.231	28	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
34	288.352	374.161	24	217.248	511.231	29	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
35	288.352	374.161	25	217.248	511.231	30	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
36	288.352	374.161	26	217.248	511.231	31	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
37	288.352	374.161	27	217.248	511.231	32	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
38	288.352	374.161	28	217.248	511.231	33	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
39	288.352	374.161	29	217.248	511.231	34	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
40	288.352	374.161	30	217.248	511.231	35	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
41	288.352	374.161	31	217.248	511.231	36	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
42	288.352	374.161	32	217.248	511.231	37	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
43	288.352	374.161	33	217.248	511.231	38	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
44	288.352	374.161	34	217.248	511.231	39	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
45	288.352	374.161	35	217.248	511.231	40	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
46	288.352	374.161	36	217.248	511.231	41	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
47	288.352	374.161	37	217.248	511.231	42	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
48	288.352	374.161	38	217.248	511.231	43	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
49	288.352	374.161	39	217.248	511.231	44	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
50	288.352	374.161	40	217.248	511.231	45	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
51	288.352	374.161	41	217.248	511.231	46	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
52	288.352	374.161	42	217.248	511.231	47	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
53	288.352	374.161	43	217.248	511.231	48	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
54	288.352	374.161	44	217.248	511.231	49	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
55	288.352	374.161	45	217.248	511.231	50	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
56	288.352	374.161	46	217.248	511.231	51	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
57	288.352	374.161	47	217.248	511.231	52	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
58	288.352	374.161	48	217.248	511.231	53	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
59	288.352	374.161	49	217.248	511.231	54	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
60	288.352	374.161	50	217.248	511.231	55	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
61	288.352	374.161	51	217.248	511.231	56	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
62	288.352	374.161	52	217.248	511.231	57	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
63	288.352	374.161	53	217.248	511.231	58	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
64	288.352	374.161	54	217.248	511.231	59	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
65	288.352	374.161	55	217.248	511.231	60	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
66	288.352	374.161	56	217.248	511.231	61	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
67	288.352	374.161	57	217.248	511.231	62	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
68	288.352	374.161	58	217.248	511.231	63	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
69	288.352	374.161	59	217.248	511.231	64	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
70	288.352	374.161	60	217.248	511.231	65	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
71	288.352	374.161	61	217.248	511.231	66	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
72	288.352	374.161	62	217.248	511.231	67	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
73	288.352	374.161	63	217.248	511.231	68	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
74	288.352	374.161	64	217.248	511.231	69	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
75	288.352	374.161	65	217.248	511.231	70	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
76	288.352	374.161	66	217.248	511.231	71	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
77	288.352	374.161	67	217.248	511.231	72	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
78	288.352	374.161	68	217.248	511.231	73	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
79	288.352	374.161	69	217.248	511.231	74	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
80	288.352	374.161	70	217.248	511.231	75	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
81	288.352	374.161	71	217.248	511.231	76	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
82	288.352	374.161	72	217.248	511.231	77	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
83	288.352	374.161	73	217.248	511.231	78	174.488	1608.387	20	2146.064	483.391	41	2160.151	236.443
84	288.352	374.16												



(A)

Sequence data:
 Protein C activator OS=Aglkistrodon contortrix contortrix PE=1 SV=2 VSPCA_AGKCO
 Intensity Coverage: 88.1% (12970 ions) Sequence Coverage MS: 34.2%
 Sequence Coverage MS/MS: 0.0% pI (isoelectric point): 9.7

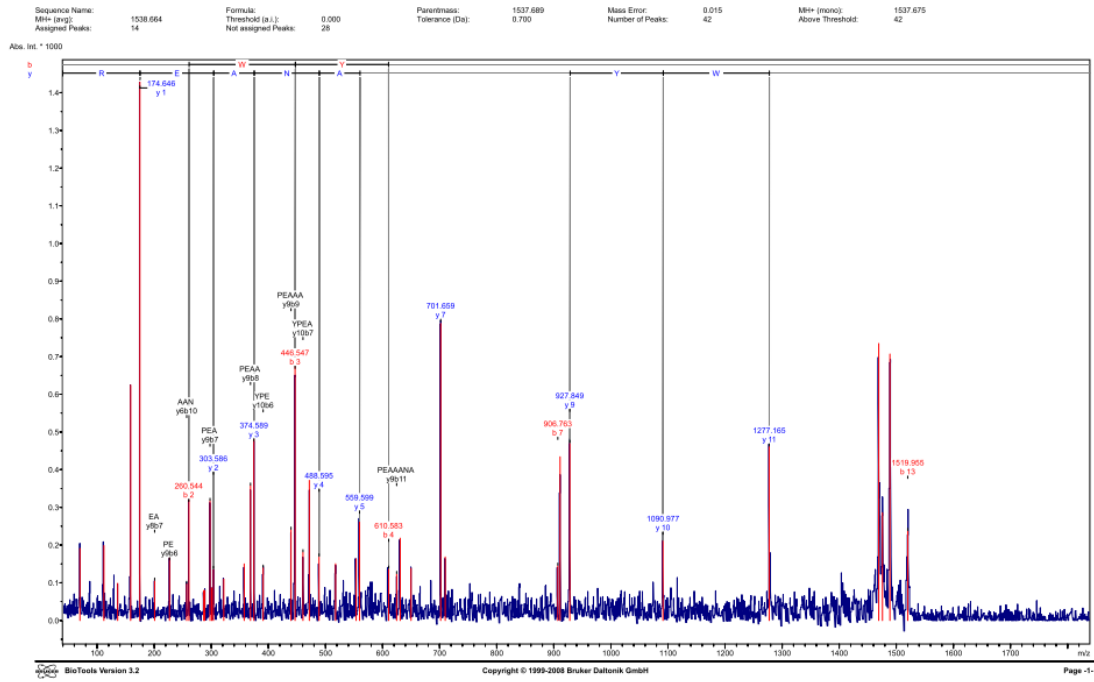
1-0	2-0	3-0	4-0	5-0	6-0	7-0	8-0	9-0	1-0-0	1-1-0		
VIGDECHEN	ENRFLALVYA	NQS	LCOOTLI	HQEWVLTARH	CDRGNHRIE	GMHNLK	VLSK	DALRRFPKKE	YFCLNTRNDG	IWDKDIHLIR	LNRFPVRSAN	IAPLPLPSNP
1-2-0	1-3-0	1-4-0	1-5-0	1-6-0	1-7-0	1-8-0	1-9-0	2-0-0	2-1-0	2-2-0		
PSVGSVCRIM	GWGITSPNA	ILPDVPRCAN	INILDYAVCQ	AAYKGLAAT	LCAGILEGK	DTCKGDSGGP	LICNGQFQGI	LSVGGNPCAQ	PRKPGIYIKV	FDYTDWIQSI		
2-3-0	2-4-0											
ISGNTDATCP	P											

Display Parameter:
 Sequence Name: Protein C activator OS=Aglkistrodon contortrix contortrix PE=1 SV=2 VSPCA_AGKCO
 Threshold (s.l.): 0.000 Tolerance (Da): 0.500 Number of Peaks: 13 M+ (mono): 1.008 M+ (avg): 1.008

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	754.450	2164.000	3	769.489	321.000	3	842.521	283.710	4	870.555	65.340	5	897.587	80.437
11	1088.604	78.928	8	1095.120	285.720	9	1512.868	2873.710	10	1531.783	27.000	11	1950.120	11.260
13	2280.135	810.887											2360.330	125.450

(B)

Figure S19. Annotated MS spectrum detected in area #5. (A) MS spectrum; (B) Peak list and sequence data.



(A)

Display Parameter: Parentmass: 1537.689 Mass Error: 0.015 MH+ (mono): 1537.675 MH+ (avg): 1538.664 Threshold (a.l.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 42 Above Threshold: 42 Assigned Peaks: 14 Not assigned Peaks: 26

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	89.793	117.061	1	117.072	10.247	3	55.955	37.715	4	165.934	64.831	5	4.641	134.816
2	226.055	160.811	3	252.213	37.210	5	250.544	321.451	10	286.951	75.900	11	258.527	80.455
13	350.959	66.700	11	303.995	136.544	15	311.959	119.154	16	327.914	159.954	17	326.954	174.449
19	380.974	140.414	20	439.963	24.103	21	446.947	574.705	22	460.911	181.083	23	471.963	373.813
25	517.951	121.916	24	551.945	153.320	27	559.959	962.805	28	610.933	137.952	29	624.924	114.450
31	656.939	133.430	32	703.929	783.320	33	709.940	169.742	34	806.783	143.267	35	810.770	434.372
38	1050.911	217.281	39	1217.789	468.720	39	1426.120	184.291	41	1416.955	268.271	41	1488.441	787.730
41	1537.689	1000.000												

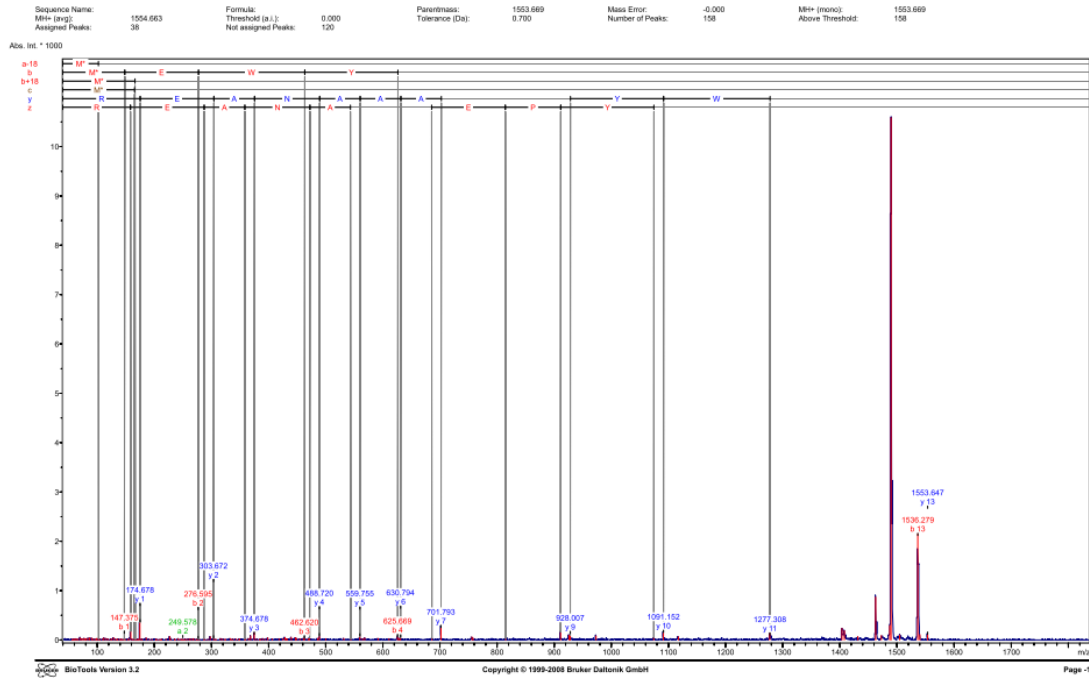
Calculated Masses: MEWVPEAAANAEER

No	Term	Ion	a	b	y	C-term	Ion
1	M	1542.050	139.440			12.8.113	R
2	E	239.059	261.090			3.4.163	R
3	W	416.176	447.170			37.5.159	A
4	Y	165.934	618.323			6.9.161	N
5	P	678.921	710.320			56.9.219	A
6	A	89.793	90.306			1.1.161	A
7	A	875.371	907.363			7.9.163	A
8	A	892.400	918.400			8.1.160	E
9	A	1074.451	1076.451			9.4.161	E
10	N	1126.450	1128.450			10.1.172	V
11	A	1208.920	1210.920			12.7.161	V
12	E	1338.920	1340.920			13.6.161	E
13	E	1497.650	1499.650			15.1.161	E

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(B)

Figure S21. Annotated MS/MS spectrum of ion 1537.689 m/z detected in area #7. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 1553.669 Mass Error: -0.000 M+ (mono): 1553.669 M+ (avg): 1554.663 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 158 Above Threshold: 158 Not assigned Peaks: 120

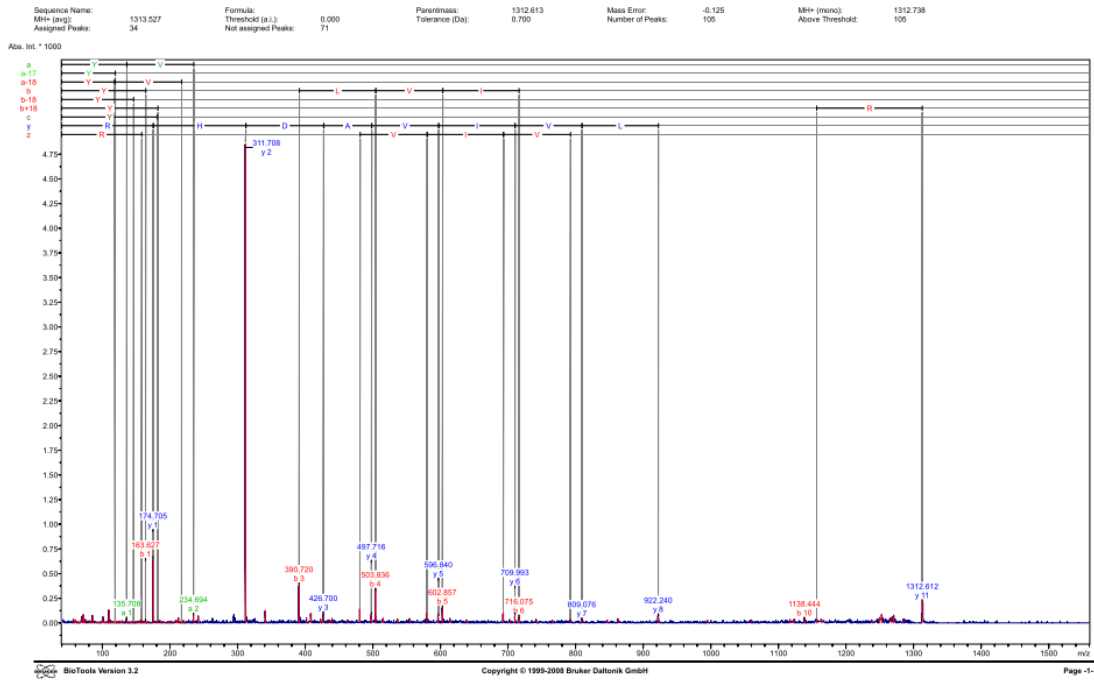
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
23	55.800	15.044	4	71.022	15.123	4	82.044	15.211	5	92.441	21.144	11	84.933	19.473
24	66.163	10.261	3	69.719	25.803	3	77.820	21.155	10	74.300	23.067	11	77.973	31.901
10	80.613	18.934	11	13.525	18.964	12	68.981	40.060	18	96.207	19.081	17	63.243	13.350
18	88.343	21.440	30	99.344	13.268	21	169.319	20.800	25	104.762	11.769	23	108.911	22.899
31	133.819	7.585	35	118.974	19.294	32	102.564	8.752	34	124.758	15.439	32	129.714	22.442
33	134.455	9.787	35	132.933	19.977	33	158.739	15.174	34	141.989	17.351	32	149.711	16.976
37	167.335	11.674	38	140.174	11.417	39	163.648	15.110	40	136.080	12.420	41	158.850	17.513
38	168.789	25.011	41	105.055	15.582	42	105.612	17.403	43	110.058	12.451	41	115.950	19.433
48	177.224	12.864	50	178.260	14.820	51	165.550	40.183	52	181.177	16.303	53	165.910	11.130
55	203.562	16.549	59	205.435	15.424	54	200.919	8.884	57	210.523	18.117	59	219.211	14.429
63	228.628	72.131	63	228.534	10.427	63	228.187	13.872	63	238.934	10.007	65	241.673	25.481
67	237.209	14.864	68	448.529	8.981	68	611.133	4.034	61	263.164	14.401	71	258.083	8.313
73	261.999	16.848	74	264.349	18.316	75	287.638	25.076	76	270.819	16.363	77	274.873	11.923
85	318.811	7.294	85	285.673	12.429	81	315.547	26.713	82	314.657	17.657	83	277.638	27.414
88	318.954	10.569	87	307.977	13.443	88	313.441	27.448	88	318.181	17.811	88	324.191	10.329
91	332.867	27.430	92	330.746	10.017	93	337.862	14.269	94	342.656	16.880	95	337.820	17.171
103	358.063	44.916	98	358.718	15.513	96	355.863	28.461	100	368.658	18.179	101	373.874	10.426
103	384.209	12.883	104	385.880	16.939	105	389.589	28.809	109	384.445	13.183	109	388.640	45.133
109	418.268	21.484	110	424.874	10.441	111	429.411	40.919	112	436.959	24.461	113	439.262	18.433
119	448.609	46.211	118	444.620	10.127	117	464.873	20.419	118	460.910	10.067	119	468.420	44.680
121	411.611	26.531	122	485.924	11.481	123	488.280	8.413	124	489.103	28.520	125	491.690	10.359
123	586.755	73.858	128	584.503	23.028	129	588.277	39.777	130	587.441	31.858	131	610.850	23.877
130	614.815	16.503	131	616.794	18.681	132	615.881	40.481	133	617.183	20.919	134	620.901	30.359
133	614.815	93.187	134	618.085	16.081	141	626.007	107.481	142	626.007	206.014	143	679.113	18.856
140	1081.152	136.306	136	1117.177	65.137	147	1277.268	146.020	148	1403.059	206.019	149	1407.960	188.140
151	1462.465	166.400	145	1474.633	65.967	153	1467.268	261.464	152	1488.814	1099.260	154	1504.217	130.452
153	1540.109	158.759	153	1553.647	109.809	153	1553.647	109.809	153	1553.647	109.809	153	1553.647	109.809

Calculated Masses: MSWVPEAAAKDSE1 Oxidation (M)

Residue	Mon	a	b	b+16	b	b+17	b+18	b+18	b+18	c	e	e	e	Chrom	Seq
1	W	170.048	170.021	192.037	148.043	131.019	132.032	166.053	165.069	120.048	201.058	175.119	158.092	13	W
2	E	240.090	240.063	277.085	200.095	229.074	226.091	261.110	262.092	151.113	284.101	261.125	281.125	11	E
3	W	170.048	170.021	192.037	148.043	131.019	132.032	166.053	165.069	120.048	201.058	175.119	158.092	13	W
4	Y	166.053	166.026	188.042	144.048	127.024	128.037	162.058	161.074	116.053	197.063	172.124	155.097	11	Y
5	F	166.053	166.026	188.042	144.048	127.024	128.037	162.058	161.074	116.053	197.063	172.124	155.097	11	F
6	A	84.026	84.000	106.016	62.032	45.008	46.021	80.041	79.057	34.026	63.035	48.096	33.070	6	A
7	A	84.026	84.000	106.016	62.032	45.008	46.021	80.041	79.057	34.026	63.035	48.096	33.070	6	A
8	R	99.040	99.014	121.030	77.046	60.022	61.035	95.048	94.064	49.040	64.049	49.099	34.073	8	R
9	A	84.026	84.000	106.016	62.032	45.008	46.021	80.041	79.057	34.026	63.035	48.096	33.070	6	A
10	S	115.043	115.017	137.033	93.049	76.023	77.036	111.049	110.065	41.043	56.052	41.111	26.085	10	S
11	D	133.030	133.004	155.020	111.036	94.010	95.023	129.036	128.052	59.030	74.039	59.107	44.081	11	D
12	S	115.043	115.017	137.033	93.049	76.023	77.036	111.049	110.065	41.043	56.052	41.111	26.085	10	S
13	R	107.061	107.035	129.051	85.067	68.041	69.054	103.067	102.083	37.061	52.070	37.128	22.092	13	R

(B)

Figure S22. Annotated MS/MS spectrum of ion 1553.669 m/z detected in area #7. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



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(A)

Display Parameter: Parentmass: 1312.613 Mass Error: -0.125 Mi+ (mono): 1312.738 Mi+ (avg): 1313.527 Threshold (a.i.): 0.000 Tolerance (Da): 0.700 Number of Peaks: 105 Above Threshold: 105 Not assigned Peaks: 71

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	67.055	1.000	2	99.760	1.000	3	81.307	19.103	4	85.311	7.951	5	97.915	7.784
6	71.702	82.261	7	74.986	13.307	8	80.640	23.450	9	82.977	13.111	10	85.760	10.430
11	80.859	6.536	12	84.903	10.200	13	89.662	10.000	14	93.333	6.922	15	96.780	6.000
16	106.897	9.481	17	109.744	125.703	18	112.252	19.800	19	114.293	14.711	20	116.851	10.151
21	114.663	13.730	22	122.223	17.929	23	128.818	19.044	24	126.747	15.201	25	129.921	11.350
31	139.622	16.711	32	142.749	17.639	33	154.269	14.136	34	146.555	12.113	35	152.250	14.300
36	157.693	26.511	37	162.995	8.711	38	161.589	9.709	39	163.929	13.204	40	169.691	8.780
41	174.703	849.691	42	178.073	12.303	43	180.301	17.432	44	181.623	30.123	45	185.739	24.473
46	197.693	16.516	47	198.964	12.289	48	197.489	19.163	49	198.911	20.897	50	200.291	20.824
51	216.859	14.177	52	219.985	13.544	53	224.713	16.814	54	224.994	30.759	55	241.691	39.686
56	250.752	120.694	57	260.721	485.468	58	261.990	37.950	59	268.693	22.417	60	267.720	36.350
61	285.744	29.511	62	293.691	10.000	63	293.691	10.000	64	293.691	10.000	65	293.691	10.000
71	314.700	48.120	72	338.719	39.837	73	354.815	35.951	74	349.338	107.914	75	356.840	30.156
81	414.611	39.201	82	438.717	31.067	83	459.904	113.169	84	469.543	25.160	85	479.951	16.810
86	492.023	30.960	87	502.960	26.521	88	511.087	36.711	89	500.700	57.350	90	487.017	21.480
91	622.201	24.181	92	656.119	21.061	93	650.311	26.353	94	619.700	31.941	95	629.941	31.859
96	1166.474	52.278	97	1164.021	39.308	98	1738.311	25.021	99	1249.600	37.660	100	1269.810	83.191
101	1210.969	72.929	102	1264.959	28.521	103	1372.811	29.084						

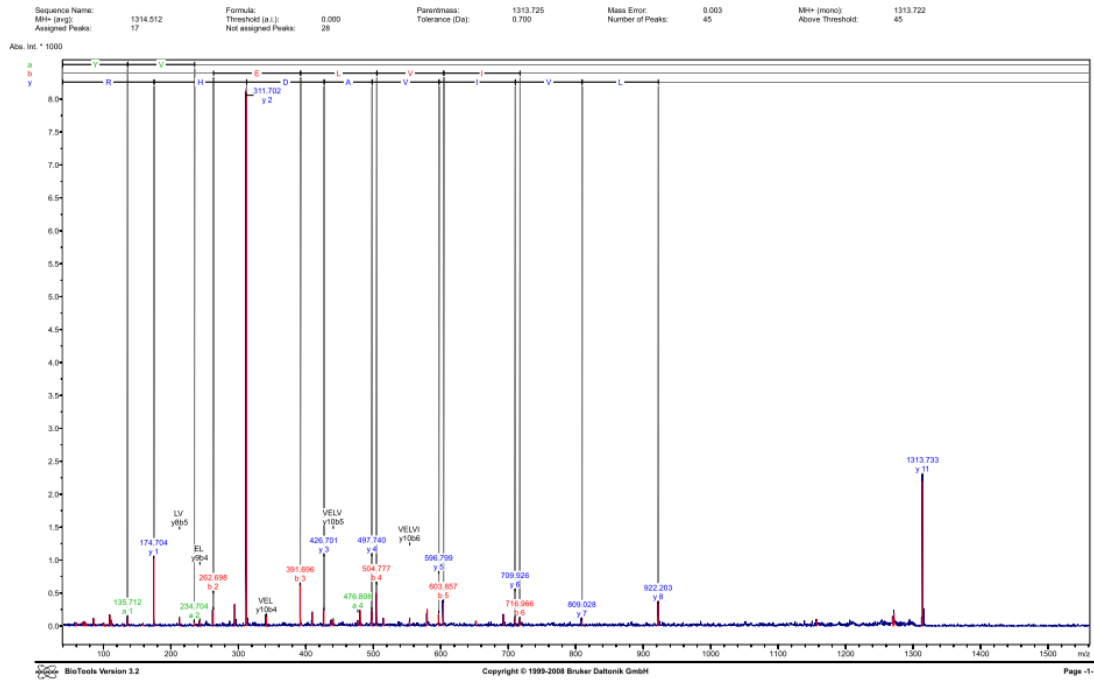
Calculated Masses: YIGLVVWVHRE

R-Term	Ion	a	a-17	a-16	b	b-17	b-16	b+16	c	l	x	y	z	C-Term	Ion
1	V	136.070	119.040	118.083	164.071	147.041	146.080	182.081	181.097	136.070	201.088	175.119	158.092	11	R
2	V	235.146	218.114	217.134	263.130	246.119	245.159	281.150	280.164	234.081	338.159	312.178	295.151	10	L
3	D	361.201	345.170	344.190	391.199	374.171	373.187	409.208	408.224	361.201	451.184	427.205	410.179	9	D
4	V	476.257	460.226	459.246	504.252	487.224	486.240	521.251	520.265	476.257	561.241	537.262	520.255	8	V
5	V	591.313	575.282	574.302	618.311	601.283	600.299	635.310	634.324	591.313	675.307	651.328	634.321	7	V
6	V	706.369	690.338	689.358	732.367	715.339	714.355	749.366	748.380	706.369	789.373	765.394	748.387	6	V
7	A	821.425	805.394	804.414	847.423	830.395	829.411	864.422	863.436	821.425	904.429	880.450	863.443	5	A
8	D	936.481	920.450	919.470	961.479	944.451	943.467	978.478	977.492	936.481	1018.485	994.506	977.499	4	D
9	H	1101.537	1085.506	1084.526	1126.535	1109.507	1108.523	1143.534	1142.548	1101.537	1181.541	1157.562	1140.555	3	H
10	H	1110.613	1094.582	1093.602	1134.611	1117.583	1116.599	1151.610	1150.624	1110.613	1190.617	1166.638	1155.631	2	H
11	R	1275.669	1259.638	1258.658	1300.667	1283.639	1282.655	1317.666	1316.680	1275.669	1355.683	1331.704	1320.697	1	R

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(B)

Figure S24. Annotated MS/MS spectrum of ion 1312.613 m/z detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: 1313.725 Mass Error: 0.003 M+ (mono): 1313.722 M+ (avg): 1314.512 Threshold (a.l.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 45 Above Threshold: 45 Assigned Peaks: 17 Not assigned Peaks: 28

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.071	35.277	4	66.913	4.811	3	69.711	30.242	4	71.800	67.261	5	74.201	27.244
2	89.724	40.187	3	107.744	25.009	6	109.764	163.000	10	111.700	67.887	11	128.740	35.930
10	138.213	35.891	14	174.905	1031.483	15	217.224	98.064	16	224.194	67.261	17	257.753	77.283
18	284.822	332.390	20	311.702	8116.486	21	341.740	182.061	22	381.890	456.763	23	408.887	219.189
24	437.893	36.141	25	481.724	27.779	26	483.569	24.024	28	509.710	230.000	29	537.756	236.152
30	574.700	117.380	31	523.642	30.027	33	539.800	253.986	34	588.789	100.140	35	603.821	58.140
37	622.923	188.171	38	709.026	115.282	39	715.980	104.510	40	809.020	122.810	41	822.203	27.182
43	1280.717	12.021	44	1271.825	100.262	45	1313.722	2160.929						

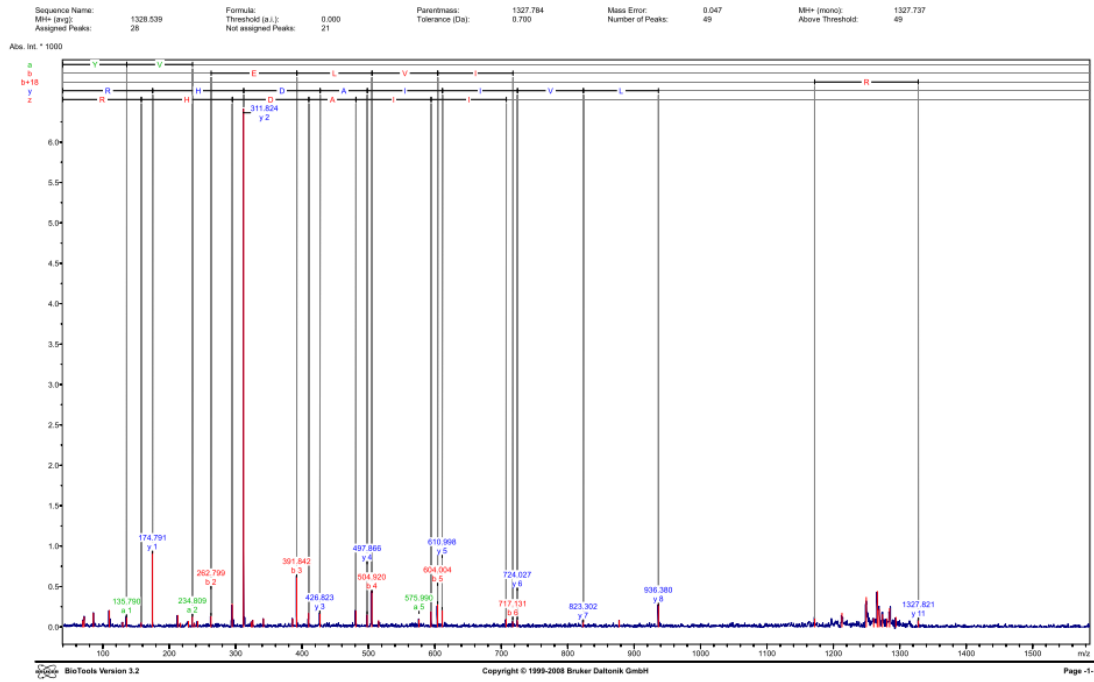
Calculated Masses:
 YVELVWACHR

Ion	Ion	a	b	y	Q-Term	Ion
1	V	238.070	282.090	Y4.113	10	R
2	V	235.144	281.139	Y12.193	10	R
3	L	269.191	302.189	Y2.162	3	A
4	V	276.330	304.334	Y9.310	7	V
5	L	292.490	312.431	Y10.384	6	L
6	V	328.490	318.430	Y9.483	5	V
7	A	335.020	319.624	Y2.474	4	L
8	D	374.500	309.351	Y10.180	3	L
9	R	413.810	320.391	Y10.093	3	L
11	R	420.710	320.711	Y13.721	1	V

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(B)

Figure S25. Annotated MS/MS spectrum of ion 1313.725 *m/z* detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parent mass: 1327.784
 Tolerance (Da): 0.700
 Mass Error: 0.047
 Number of Peaks: 49
 MH+ (mono): 1327.737
 Above Threshold: 49
 MH+ (avg): 1328.539
 Assigned Peaks: 26
 Threshold (s.l.): 0.000
 Not assigned Peaks: 21

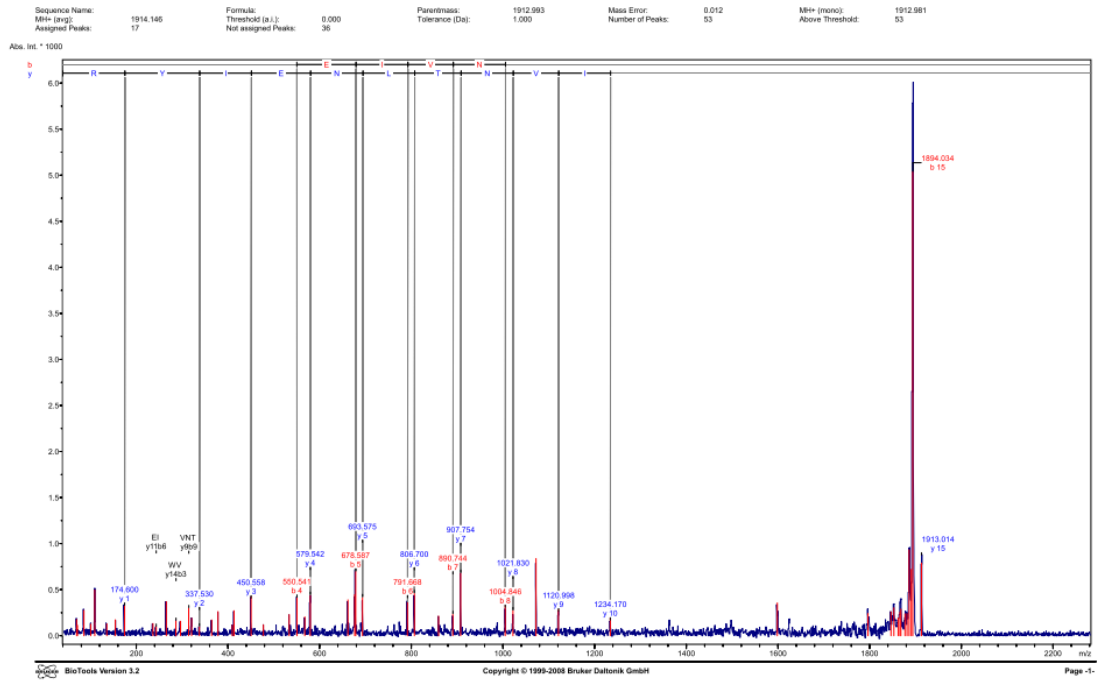
Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	89.055	77.853	1	71.064	103.011	1	85.838	109.149	1	109.800	254.142	1	29.854	35.990
2	107.700	50.174	2	174.791	328.260	2	232.826	142.780	10	216.250	26.620	11	228.820	65.116
3	139.499	43.093	3	224.874	45.323	3	259.292	137.165	11	269.104	293.950	12	311.824	34.367
10	328.874	32.731	20	341.840	181.439	21	385.833	39.009	22	381.842	448.345	23	409.815	137.233
20	430.864	206.363	24	497.856	139.814	25	534.820	45.114	26	616.328	79.261	27	739.897	91.352
30	694.034	261.449	33	819.988	229.061	34	787.024	107.243	35	747.131	91.150	36	724.027	89.774
38	817.816	30.385	39	828.309	283.181	39	1111.684	139.669	40	1029.814	111.284	41	1249.284	100.426
43	1265.825	441.319	44	1268.849	218.829	45	1273.839	183.291	46	1280.850	107.603	47	1324.831	229.372
49	1327.821	86.927												

Calculated Masses:
 YVELVQDRIH

b-Term	Ion	a	a-17	a-18	b	b-17	b-18	b+18	c	i	s	y	z	C-Term	Seq
1	V	136.076	118.040	118.069	184.074	147.044	146.060	182.081	181.097	186.078	201.098	175.119	168.092	11	R
2	V	233.146	215.110	214.134	283.130	246.100	245.116	283.135	282.151	287.161	324.181	319.174	288.151	10	L
3	E	324.181	306.145	305.169	352.183	315.153	314.171	418.192	409.208	402.055	453.184	427.205	410.179	9	D
4	V	419.217	401.181	400.205	458.219	421.189	420.205	525.216	516.232	508.089	562.218	536.242	481.218	8	L
5	V	475.338	457.302	456.326	504.334	467.304	466.320	559.332	550.348	541.201	597.335	571.358	544.338	7	L
6	I	609.420	591.384	590.408	617.413	580.383	579.399	699.435	690.451	748.440	68.088	750.380	724.410	6	L
7	V	636.461	618.425	617.449	630.454	593.424	592.440	675.451	674.467	683.094	740.469	724.418	695.458	5	L
8	A	874.543	856.507	855.531	891.535	854.505	853.521	919.550	918.566	944.083	897.514	936.563	912.537	4	L
9	V	969.579	951.543	950.567	1016.569	979.539	978.555	1048.574	1047.590	1078.099	1001.544	1048.599	1024.572	3	L
10	H	1126.630	1108.594	1107.618	1163.632	1126.602	1125.618	1197.637	1196.653	1188.071	1180.603	1164.674	1147.647	2	V
11	H	1281.713	1263.677	1262.701	1318.714	1281.684	1280.700	1352.723	1351.739	1384.113	1353.118	1387.723	1310.710	1	V

(B)

Figure S26. Annotated MS/MS spectrum of ion 1327.784 m/z detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 1912.993
 Tolerance (Da): 1.000
 Mass Error: 0.012
 Number of Peaks: 53
 M⁺ (mono): 1912.981
 Above Threshold: 53
 M⁺ (avg): 1914.146
 Assigned Peaks: 17
 Threshold (a.i.): 0.000
 Not assigned Peaks: 36

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	89.211	177.178	1	71.229	113.841	8	85.728	275.903	100	100.950	126.241	8	169.629	438.680
2	158.202	177.986	2	174.606	331.418	9	258.243	131.174	10	283.213	97.481	11	295.520	470.430
3	186.493	197.950	3	174.606	314.826	10	437.324	239.823	11	437.324	239.823	12	437.324	239.823
13	409.541	134.811	20	413.541	211.790	21	460.580	433.889	22	477.989	118.181	23	533.927	229.243
24	579.574	265.059	28	579.574	459.114	34	651.953	389.459	35	676.954	445.920	36	676.954	219.217
33	761.824	389.344	33	808.700	485.600	33	859.689	213.521	34	860.744	238.532	35	860.744	686.650
38	1041.839	219.344	38	1079.864	879.824	38	1100.989	264.384	39	1254.116	199.029	41	1254.116	368.888
43	1348.020	268.868	43	1352.879	333.774	45	1382.209	193.330	46	1505.800	204.931	47	1508.161	1879.845
48	1581.868	230.731	48	1608.749	323.689	51	1660.841	219.413	51	1664.054	3026.321	53	1912.981	188.774

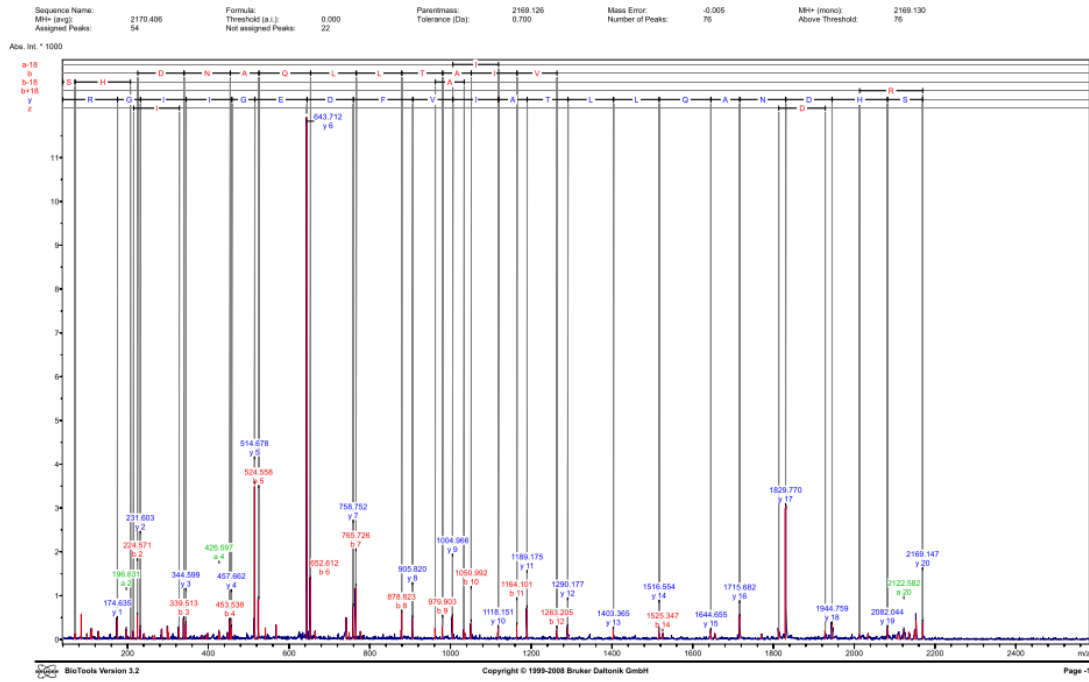
Calculated Masses:
 RYLIENLTYNIV

R1-term	Ion	a	b	y	C1-term	Ion
1	Y	72.850	102.050	178.119	16	R
2	W	269.130	289.130	338.182	16	Y
3	Y	389.200	389.200	481.289	19	L
4	Y	529.271	529.271	630.393	15	E
5	L	651.314	679.329	684.352	11	N
6	Y	749.388	749.388	817.429	10	L
7	Y	877.429	877.429	958.484	9	N
8	N	877.429	1005.504	1022.527	9	N
9	L	1074.495	1138.595	1174.595	9	Y
10	L	1192.611	1218.630	1234.673	6	L
11	N	1329.650	1333.674	1363.673	5	Y
12	E	1429.720	1489.720	1509.769	4	Y
13	L	1527.810	1533.809	1553.810	3	Y
14	Y	1719.879	1726.899	1811.933	2	W
15	R	1866.970	1924.970	1912.981	1	R

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(B)

Figure S28. Annotated MS/MS spectrum of ion 1912.993 m/z detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 2169.126
 Tolerance (Da): 0.700
 Mass Error: -0.005
 Number of Peaks: 76
 M⁺ (mono): 2169.130
 Above Threshold: 76
 M⁺ (avg): 2170.486
 Assigned Peaks: 54
 Threshold (a.i.): 0.000
 Not assigned Peaks: 22

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
8	89.711	142.108	7	71.250	183.930	3	85.943	585.238	4	99.703	126.702	5	169.702	188.885
13	138.859	177.808	11	174.835	477.474	10	185.911	292.858	11	207.858	39.011	17	212.909	358.874
15	201.803	258.894	14	247.862	355.354	15	259.831	75.988	16	287.830	152.959	18	292.917	437.850
18	301.803	190.809	20	327.807	288.803	21	339.813	473.800	22	344.805	201.900	23	384.827	31.933
24	388.869	131.801	26	426.897	305.832	27	438.862	135.868	28	448.839	133.859	29	458.833	222.858
31	514.878	3548.871	33	524.858	323.825	32	529.837	287.833	34	568.864	328.802	35	643.917	1202.813
37	624.869	205.850	38	641.874	409.814	39	658.876	163.818	40	688.874	793.864	41	763.924	1026.842
43	679.893	622.892	44	808.830	484.809	45	881.809	272.810	46	879.803	317.800	47	1003.860	812.837
49	1034.889	154.899	50	1056.896	307.878	51	1118.931	309.895	52	1164.911	333.833	53	1198.918	718.832
55	1280.177	281.868	56	1420.885	242.898	57	1518.924	228.839	58	1625.847	142.865	59	1644.865	418.898
61	1673.846	800.808	62	1759.864	106.819	63	1828.912	23.835	64	1854.878	189.844	65	1892.892	358.848
67	2012.899	139.897	68	2033.903	113.899	69	2080.944	79.888	70	2107.948	191.841	71	2140.970	114.858
73	2138.895	165.840	74	2148.875	188.822	75	2162.922	423.816	76	2169.126	394.962			

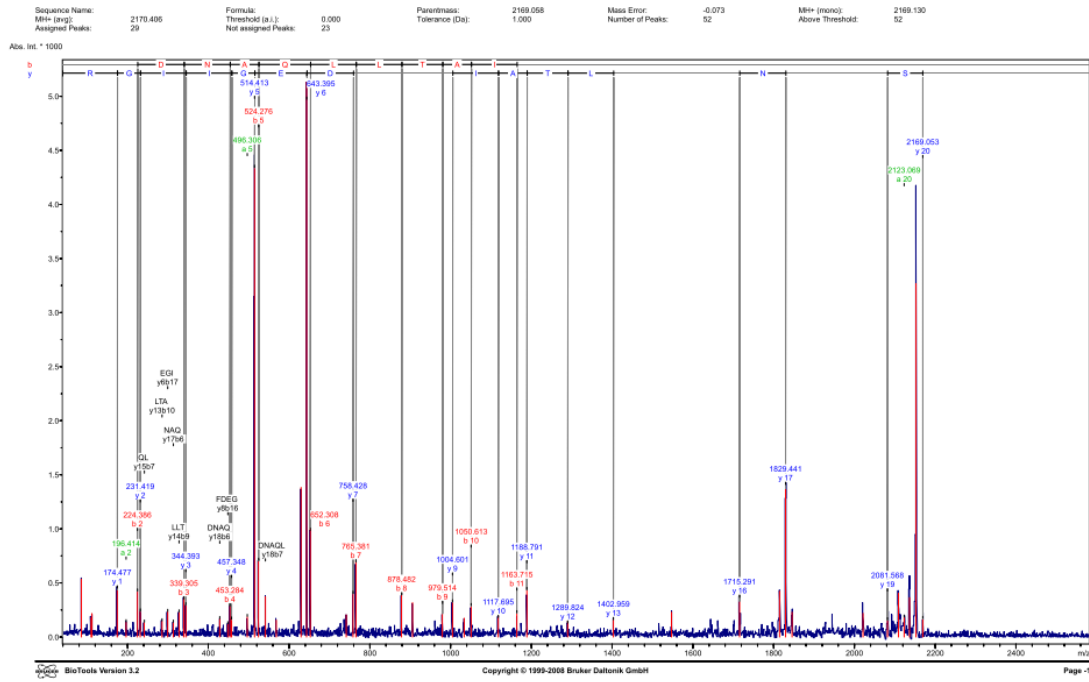
Calculated Masses:
 SENEQUALKTFEELGIGR

M.Yeem	Ion	a	a-17	a-15	b	b-17	b-15	c	x	y	z	O.Yeem	Ym	
1	S	89.711	28.111	48.004	88.803	71.253	79.822	106.002	155.002	160.014	201.008	175.113	158.002	26
2	H	127.127	97.027	119.005	225.803	208.823	217.888	244.108	293.128	318.071	368.106	292.145	215.116	29
3	D	174.154	144.054	166.032	272.830	255.850	264.915	291.135	340.155	365.109	415.144	339.183	262.188	32
4	N	221.181	191.081	213.059	320.857	303.877	312.942	339.162	388.182	397.247	447.282	371.321	314.324	35
5	A	268.208	238.108	260.086	368.884	351.904	360.969	387.189	436.209	445.274	495.309	419.348	357.351	38
6	Q	315.235	285.135	307.113	416.911	399.931	408.996	435.216	484.236	493.301	543.336	467.375	404.378	41
7	L	362.262	332.162	354.140	464.938	447.958	456.023	482.243	531.263	540.328	590.363	514.402	451.405	44
8	L	409.289	379.189	401.167	512.965	495.985	504.050	530.270	579.290	588.355	638.390	562.429	498.432	47
9	L	456.316	426.216	448.194	560.992	543.012	551.077	577.297	626.317	635.382	685.417	609.456	544.459	50
10	A	503.343	473.243	495.221	608.019	591.039	600.104	626.324	675.344	684.409	734.444	658.483	594.486	53
11	L	550.370	520.270	542.248	656.046	639.066	647.131	673.351	722.371	731.436	781.471	705.510	640.513	56
12	V	597.397	567.297	589.275	704.073	687.093	695.158	721.378	770.398	779.463	829.508	753.547	687.550	59
13	L	644.424	614.324	636.302	752.100	735.120	743.185	769.405	818.425	827.490	877.535	801.574	735.577	62
14	L	691.451	661.351	683.329	800.127	783.147	791.212	817.432	866.452	875.517	925.562	849.601	782.604	65
15	E	738.478	708.378	730.356	848.154	831.174	839.239	865.459	914.479	923.544	973.589	897.628	829.631	68
16	L	785.505	755.405	777.383	896.181	879.201	887.266	913.486	962.506	971.571	1021.616	945.655	876.658	71
17	I	832.532	802.432	824.410	944.208	927.228	935.293	961.513	1010.533	1019.598	1069.643	993.682	917.685	74
18	L	879.559	849.459	871.437	992.235	975.255	983.320	1009.540	1058.560	1067.625	1117.670	1041.709	965.712	77
19	L	926.586	896.486	918.464	1040.262	1023.282	1031.347	1057.567	1106.587	1115.652	1165.697	1089.736	1013.739	80
20	R	973.613	943.513	965.491	1088.289	1071.309	1079.374	1105.594	1154.614	1163.679	1213.724	1137.763	1061.766	83

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(B)

Figure S29. Annotated MS/MS spectrum of ion 2169.126 m/z detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 2169.058, Mass Error: -0.073, M+H (mono): 2169.130, M+H (avg): 2170.486, Threshold (a.i.): 0.000, Tolerance (Da): 1.000, Number of Peaks: 52, Above Threshold: 52, Assigned Peaks: 29, Not assigned Peaks: 23

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	85.090	936.295	1	109.560	17.281	1	11.530	210.265	1	174.477	45.644	1	224.386	224.386
2	231.419	237.341	2	241.407	134.020	2	285.292	145.981	10	289.364	232.820	11	313.320	334.413
3	339.309	374.199	3	344.393	439.189	3	359.289	187.184	11	449.465	113.339	12	489.402	489.402
10	496.393	187.189	20	514.413	439.189	21	524.276	305.359	22	541.335	373.419	23	568.372	597.736
20	653.414	329.781	24	656.306	1029.119	24	751.431	205.769	26	756.424	297.770	25	793.321	715.359
33	805.414	319.189	33	829.544	214.420	33	1004.601	191.040	34	1033.575	174.513	35	1059.613	106.188
36	1189.419	229.878	39	1189.561	405.084	39	1266.041	169.065	40	1282.069	169.284	41	1481.124	230.343
43	1514.702	429.540	44	1529.441	1373.295	45	1545.113	230.133	46	2081.492	419.077	47	2091.509	155.950
49	2123.069	181.984	50	2136.061	364.404	51	2162.408	209.669	52	2169.053	167.920			

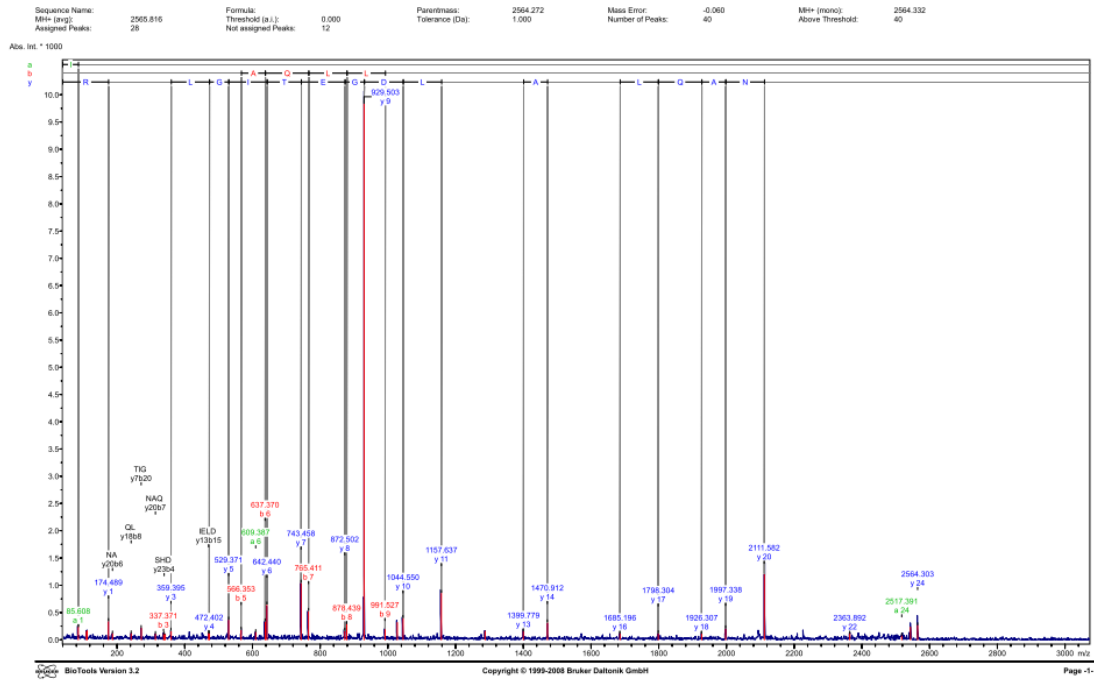
Calculated Masses: SPINAGLTAATFDGIGR

N-Term	Ion	a	b	y	C-Term	Ion
1	B	160.044	18.030	178.113	20	R
2	H	182.103	239.089	331.481	19	D
3	D	114.130	346.123	345.224	18	I
4	A	46.177	454.166	456.369	16	G
5	A	482.810	456.369	458.359	16	G
6	D	426.260	463.264	464.273	15	E
7	L	458.369	465.341	467.400	15	D
8	L	452.437	479.432	480.465	13	F
9	L	464.456	489.487	490.500	14	F
10	A	1023.322	1051.517	1118.620	11	I
11	I	1136.620	1168.661	1189.694	10	A
12	V	1238.672	1293.899	1296.723	9	I
13	R	147.174	147.174	147.174	9	L
14	D	482.770	1545.120	1487.899	9	L
15	E	1626.810	1654.807	1641.932	8	A
16	G	1619.836	1711.811	1715.969	8	A
17	I	1768.910	1824.913	1838.912	7	N
18	L	1819.926	1897.977	1924.979	7	N
19	G	1867.992	1956.110	2002.083	7	H
20	R	372.124	2111.113	2169.103		

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(B)

Figure S30. Annotated MS/MS spectrum of ion 2169.058 m/z detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 2564.272 Mass Error: -0.060 MH+ (mono): 2564.332 MH+ (avg): 2565.816 Threshold (a.l.): 0.000
 Tolerance (Da): 1.000 Number of Peaks: 40 Above Threshold: 40 Assigned Peaks: 28 Not assigned Peaks: 12

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	85.058	0.1	2	174.489	1.1	3	350.395	0.3	4	472.402	0.4	5	529.371	1.5	6	566.353	0.5
7	637.379	2.5	8	642.460	1.5	9	743.458	1.8	10	765.411	1.0	11	829.503	10.0	12	872.502	1.8
13	1044.550	1.0	14	1157.637	1.5	15	1399.779	0.5	16	1470.812	1.0	17	1605.195	0.5	18	1798.304	0.8
19	1926.307	0.5	20	1997.338	0.8	21	2111.582	1.5	22	2363.892	0.5	23	2517.391	0.5	24	2564.303	1.0

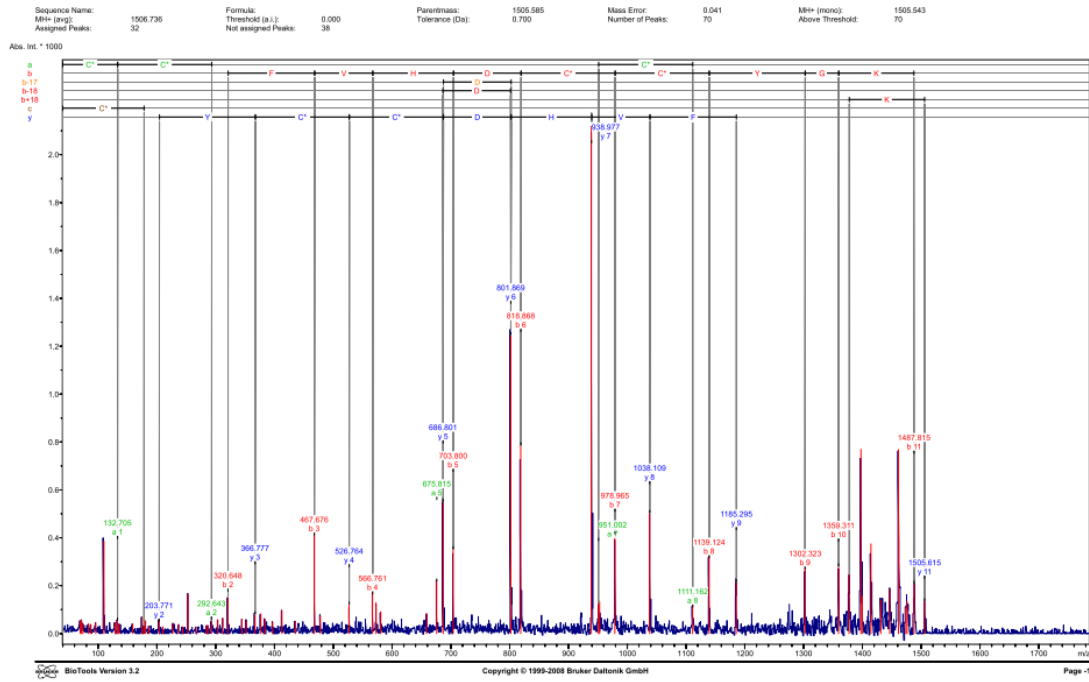
Calculated Masses:
 ISHDNAQLLTAELDDGETGLANR

b	Ion	a	b	y	C	Ion
1	L	85.058	114.020	175.139	2	R
2	L	174.489	211.971	259.159	3	R
3	H	310.181	338.182	365.191	22	A
4	N	420.710	453.321	473.321	7	L
5	N	529.371	567.352	583.352	20	G
6	L	612.256	632.256	633.256	18	L
7	L	725.323	765.343	744.458	18	L
8	L	829.503	872.452	872.452	17	L
9	L	829.503	872.458	872.458	18	L
10	L	1044.550	1043.201	1045.207	19	D
11	A	1157.637	1142.891	1158.611	14	L
12	L	1242.650	1277.650	1287.652	13	E
13	L	1379.733	1408.734	1409.728	12	L
14	L	1497.812	1519.813	1471.723	11	A
15	L	1605.195	1630.195	1572.709	10	L
16	L	1605.195	1631.201	1635.207	9	L
17	E	1707.430	1724.300	1718.391	8	L
18	L	1825.850	1821.850	1827.063	7	Q
19	L	2007.030	2035.031	1991.067	6	A
20	L	2095.051	2095.051	2125.302	5	L
21	A	2174.140	2205.140	2227.150	4	D
22	A	2248.150	2278.151	2284.153	3	L
23	N	2302.220	2330.220	2341.241	2	B
24	R	2518.320	2520.321	2544.331	1	L

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(B)

Figure S31. Annotated MS/MS spectrum of ion 2564.272 m/z detected in area #8. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 1505.585
 Tolerance (Da): 0.700
 Mass Error: 0.041
 Number of Peaks: 70
 M+ (mono): 1505.543
 Above Threshold: 70
 M+ (avg): 1506.736
 Assigned Peaks: 32
 Threshold (a.i.): 0.000
 Not assigned Peaks: 36

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	69.853	26.001	71	79.971	142.111	73	82.029	133.063	75	90.113	133.063	77	98.160	45.828
11	109.125	386.255	81	139.786	45.443	83	147.783	34.259	85	156.780	22.460	87	165.777	20.223
13	227.052	42.787	91	236.742	33.840	93	245.739	29.717	95	254.736	186.510	97	263.733	34.771
21	286.824	33.026	101	296.521	31.959	103	305.518	27.836	105	314.515	65.953	107	323.512	59.755
31	351.763	52.919	111	361.777	39.490	113	370.774	35.367	115	379.771	83.721	117	388.768	89.197
33	435.499	15.569	121	445.513	14.498	123	454.510	14.375	125	463.507	149.924	127	472.504	123.682
41	480.070	40.805	131	490.084	35.679	133	499.081	31.556	135	508.078	550.033	137	517.075	121.767
43	518.883	189.766	141	528.897	212.779	143	537.894	192.653	145	546.891	139.441	147	555.888	138.239
51	1111.162	120.133	151	1121.177	105.584	153	1130.174	116.538	155	1139.171	278.421	157	1148.168	248.339
53	1185.285	189.766	161	1195.190	175.229	163	1204.187	186.183	165	1213.184	142.460	167	1222.181	141.258
61	1287.413	703.311	171	1297.427	583.269	173	1306.424	503.223	175	1315.421	142.900	177	1324.418	708.871
63	1413.453	109.805	181	1423.467	117.661	183	1432.464	127.615	185	1441.461	137.569	187	1450.458	136.367

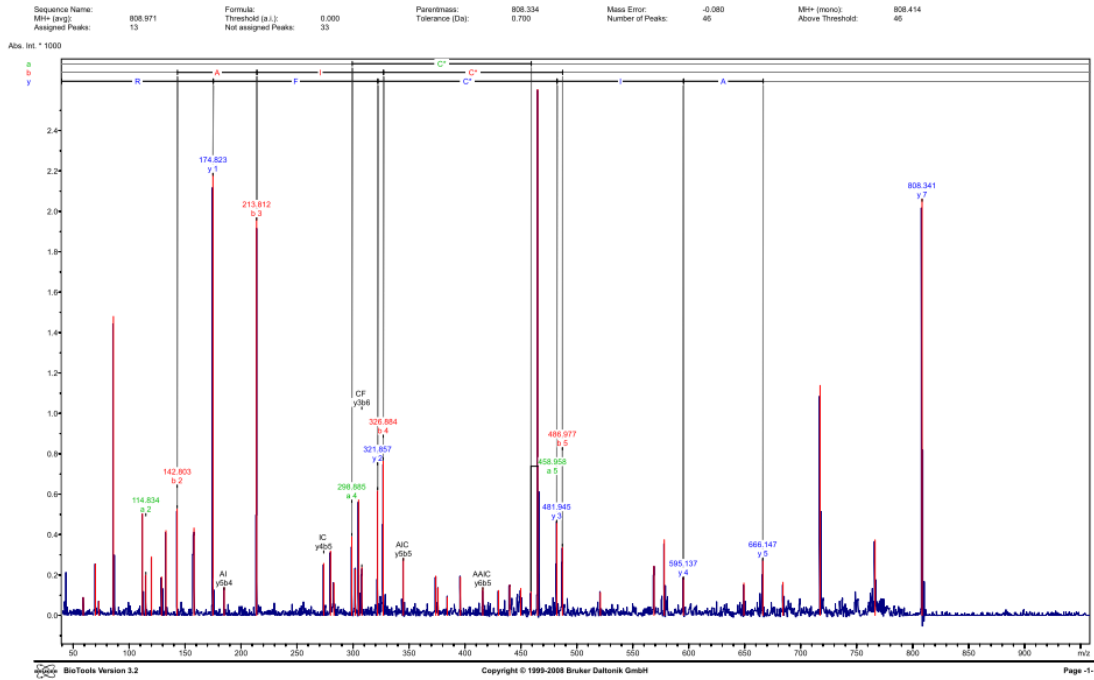
Calculated Masses:
 CDFWDCYGR: 1: Carbanisomethyl (C) 2: Carbanisomethyl (C) 3: Carbanisomethyl (C) 6: Carbanisomethyl (C)

16-Term	16m	a	a-17	a-18	b	b-17	b-18	b+18	c	y	z	C-term	16m	
1	C	132.042	116.110	115.063	517.333	142.111	175.324	132.042	133.063	133.063	133.063	133.063	11	69
2	C	253.074	236.942	235.063	324.555	324.555	324.555	324.555	324.555	324.555	324.555	324.555	12	81
3	C	485.170	468.138	466.189	588.374	588.374	588.374	588.374	588.374	588.374	588.374	588.374	13	93
4	V	678.265	661.233	659.284	779.311	779.311	779.311	779.311	779.311	779.311	779.311	779.311	14	105
5	H	871.360	854.328	852.379	963.338	963.338	963.338	963.338	963.338	963.338	963.338	963.338	15	117
6	D	1064.455	1047.423	1045.474	1159.351	1159.351	1159.351	1159.351	1159.351	1159.351	1159.351	1159.351	16	129
7	C	1257.550	1240.518	1238.569	1355.369	1355.369	1355.369	1355.369	1355.369	1355.369	1355.369	1355.369	17	141
8	V	1450.645	1433.613	1431.664	1551.382	1551.382	1551.382	1551.382	1551.382	1551.382	1551.382	1551.382	18	153
9	K	1643.740	1626.708	1624.759	1757.401	1757.401	1757.401	1757.401	1757.401	1757.401	1757.401	1757.401	19	165

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(B)

Figure S32. Annotated MS/MS spectrum of ion 1505.585 m/z detected in area #9. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 808.334
 Mass Error: -0.080
 M+ (mono): 808.414
 M+ (avg): 808.871
 Threshold (a.l.): 0.000
 Tolerance (Da): 0.700
 Number of Peaks: 46
 Above Threshold: 46
 Assigned Peaks: 13
 Not assigned Peaks: 33

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	58.800	89.748	1	66.834	251.261	3	72.820	89.701	1	82.807	449.021	3	111.822	519.219	11	114.834	299.201
2	118.801	280.811	3	132.834	181.112	19	152.772	419.814	10	182.803	530.372	11	197.810	432.288	12	174.823	2189.809
10	144.814	139.046	11	213.834	1699.424	15	273.823	297.885	14	298.885	119.820	17	299.890	781.452	18	298.885	389.124
18	307.885	235.046	20	304.880	841.924	21	387.784	238.890	22	347.889	821.000	23	368.880	787.380	24	344.842	284.309
25	318.819	124.524	28	378.808	163.024	31	383.820	89.110	30	395.851	193.241	32	413.814	138.332	33	430.840	173.258
31	438.814	157.620	32	448.811	143.823	33	458.808	139.811	34	464.821	2821.568	35	481.843	471.043	36	486.877	549.829
41	632.869	118.981	42	668.804	48.184	43	683.809	14.824	44	688.729	189.211	41	842.110	199.844	45	686.141	214.824
43	684.119	164.988	44	717.868	170.081	45	735.911	373.820	46	808.341	2051.750						

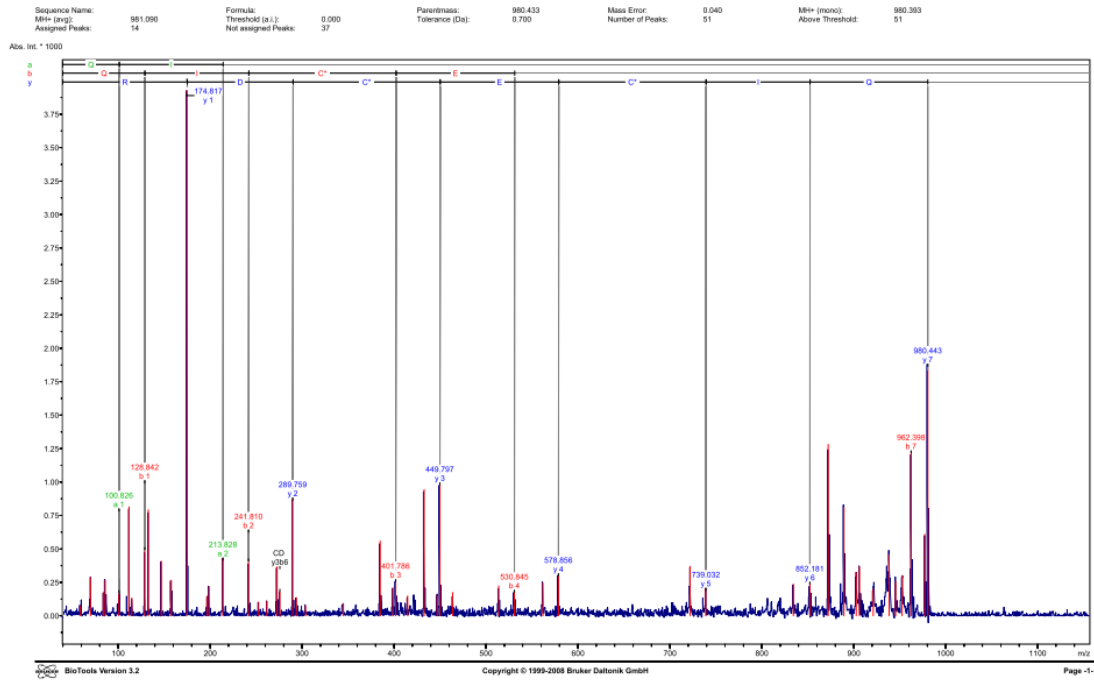
Calculated Masses:
 AAACFR S: Carbamidomethyl (C)

M.Term	Seq	a	b	y	C.Term	Seq
1	A	114.834	213.812	307.885	R	
2	A	118.837	142.803	322.187	F	
3	A	158.112	214.148	489.424	F	
4	I	229.220	337.223	588.302	F	
5	C	499.230	487.233	688.239	A	
6	F	498.224	638.224	817.803	A	
7	R	702.428	700.431	808.413	A	

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(B)

Figure S33. Annotated MS/MS spectrum of ion 808.334 *m/z* detected in area #9. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter:
 Parentmass: 980.433
 Tolerance (Da): 0.700

Mass Error: 0.040
 Number of Peaks: 51

MH+ (mono): 980.393
 Above Threshold: 51

MH+ (avg): 981.090
 Assigned Peaks: 14

Threshold (a.i.): 0.000
 Not assigned Peaks: 37

Peaks

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
68	68.025	72.191	7	69.049	285.199	3	63.040	172.123	4	85.000	207.856	5	100.826	189.793	13	111.840	814.469
11	11.829	1.32698	2	178.024	411.144	8	107.074	26.308	10	148.103	237.839	11	157.859	405.424	12	174.817	401.129
13	138.005	147.985	14	158.784	213.828	15	213.828	433.000	16	241.810	456.621	17	259.793	107.150	18	261.736	119.253
19	212.750	374.985	20	272.720	180.400	21	289.780	881.951	22	292.814	136.527	23	303.777	76.634	24	344.493	97.324
25	358.769	507.858	26	368.825	219.943	27	371.860	622.903	28	415.707	153.853	29	439.763	253.903	30	456.817	159.355
31	448.707	995.191	32	483.820	118.345	33	513.859	242.074	34	530.845	187.811	35	581.890	248.136	36	578.858	269.654
37	717.054	316.411	38	749.036	268.119	39	824.974	238.074	40	882.913	259.741	41	874.744	182.249	42	889.799	814.864
43	892.028	342.489	44	906.149	388.063	45	941.159	187.060	46	938.130	457.087	47	945.650	553.816	48	952.431	307.189
49	956.393	124.460	50	971.171	628.919	51	980.433	450.184									

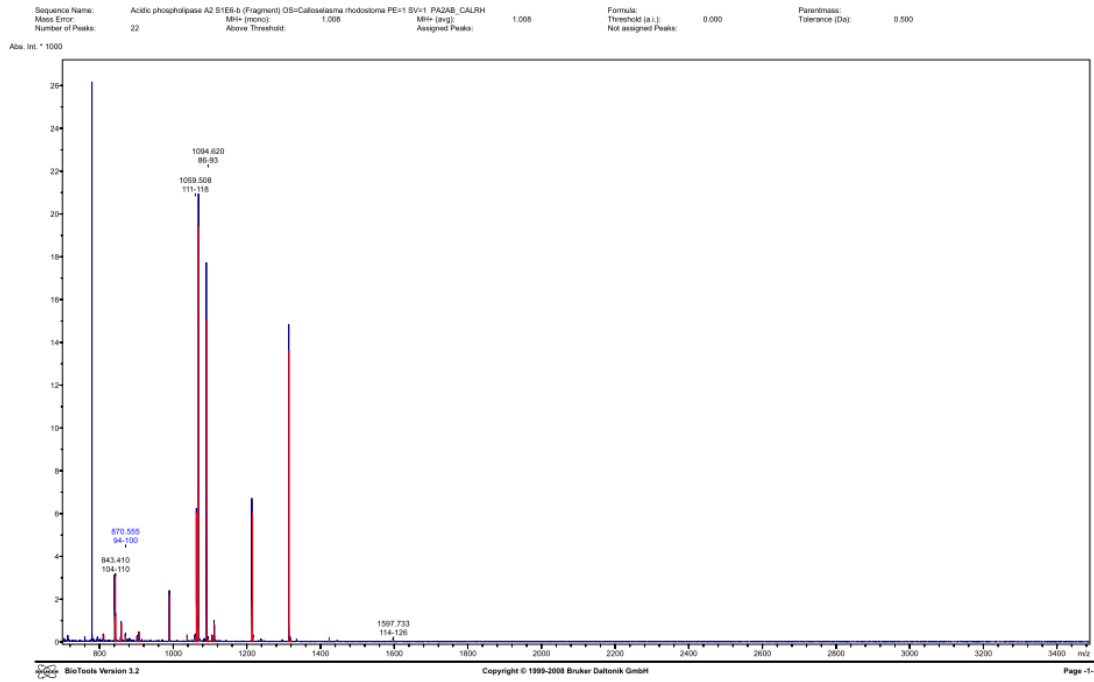
Calculated Masses
 ODCEDR3: Carbamidoethyl (C) 5: Carbamidoethyl (C)

Residue	Ion	a	b	y	C-Form	Ion
1	D	102.074	129.068	178.113	7	R
2	I	214.150	243.150	293.160	6	D
3	E	374.180	402.181	458.177	5	D'
4	E	533.201	557.201	612.211	4	E
5	C'	693.231	721.231	776.242	3	C'
6	R	753.260	782.261	837.274	2	R
7	R	913.287	942.282	998.282	1	D

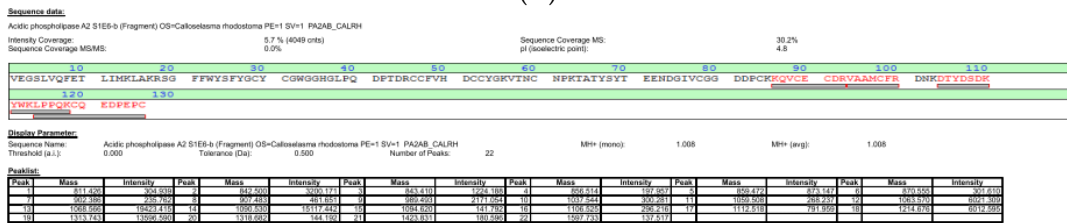
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(B)

Figure S34. Annotated MS/MS spectrum of ion 980.433 *m/z* detected in area #9. (A) MS/MS spectrum. (B) Peak list and amino acid sequence.



(A)



(B)

Figure S35. Annotated MS spectrum detected in area #9. (A) MS spectrum; (B) Peak list and sequence data.



(A)

Sequence data:
 Acidic phosphatase A2 A OS=Glycydus halys PE=1 SV=2 PAZAT_GLOHA
 Intensity Coverage: 90.0 % (25361 sites)
 Sequence Coverage MS: 25.8%
 Sequence Coverage MSMB: 0.0%
 pI (isoelectric point): 4.7

10	20	30	40	50	60	70	80	90
SLLQFETILM	KVARKSGMVW	YSNYGTCYCW	GGQGRPQDAT	DRCCFVHDC	YGRVIGCDPK	MDVYSFSEEN	GDIVCGGDDP	CKKEICECDR
100	110	120	130					
AAATCRDNL	NTYNDKFWA	FGAKNCPQEE	SEPC					

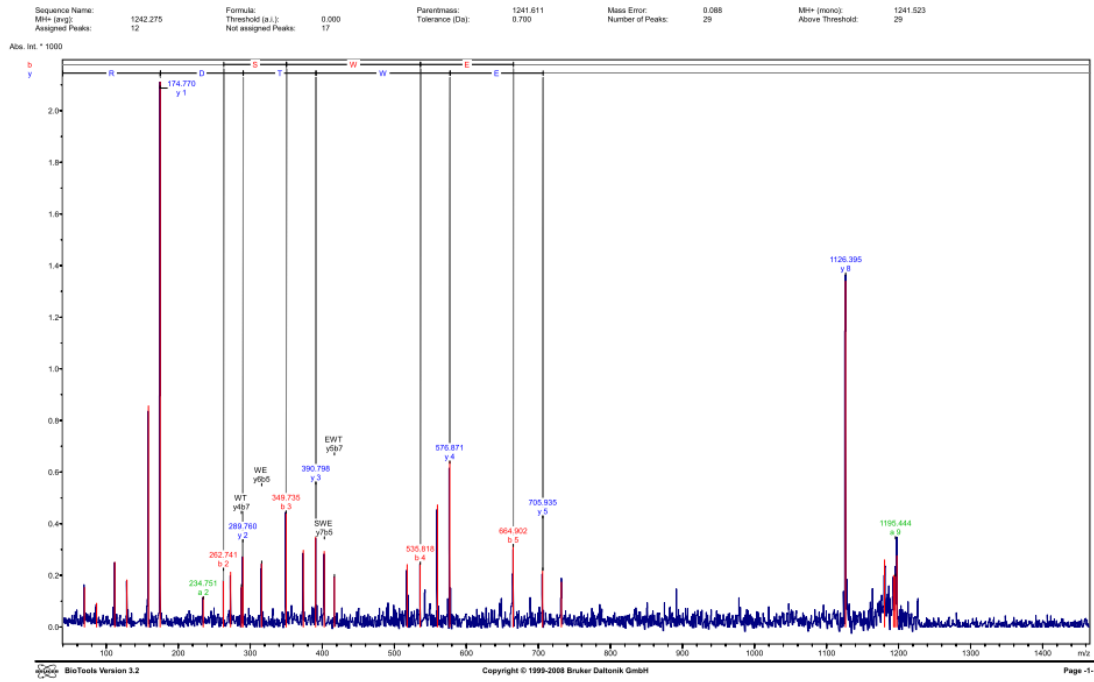
Display Parameter:
 Sequence Name: Acidic phosphatase A2 A OS=Glycydus halys PE=1 SV=2 PAZAT_GLOHA
 Threshold (a.i.): 0.000
 Tolerance (Da): 0.500
 Number of Peaks: 10
 MIt+ (mono): 1.008
 MIt+ (avg): 1.008

Peaklist:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	89.444	25.825	4	86.454	1341.00	0	497.592	9.08	10	806.023	99.861	4	807.522	100.000
	81.453	744.085	3	1157.087	411.830	0	1163.040	4.00	11	1506.617	15.530			

(B)

Figure S36. Annotated MS spectrum detected in area #9. (A) MS spectrum; (B) Peak list and sequence data.



(A)

Display Parameter: Parentmass: 1241.611 Mass Error: 0.088 MH+ (mono): 1241.523 MH+ (avg): 1242.275 Threshold (a.l.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 29 Above Threshold: 29 Assigned Peaks: 12 Not assigned Peaks: 17

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	89.204	151.143	1	89.204	151.143	1	117.300	250.511	4	126.777	152.471	1	141.700	258.400
2	214.751	117.462	3	262.741	135.331	5	272.720	212.564	10	287.750	154.430	11	289.780	271.393
13	289.780	441.060	14	374.729	227.222	15	390.786	349.761	16	409.747	253.150	17	418.744	363.440
18	338.818	251.947	20	569.830	47.810	21	664.911	643.911	22	664.902	320.332	23	706.535	218.936
25	1126.395	1357.920	24	1126.395	200.318	27	1126.395	200.318	28	1195.444	190.504	29	1195.444	276.100

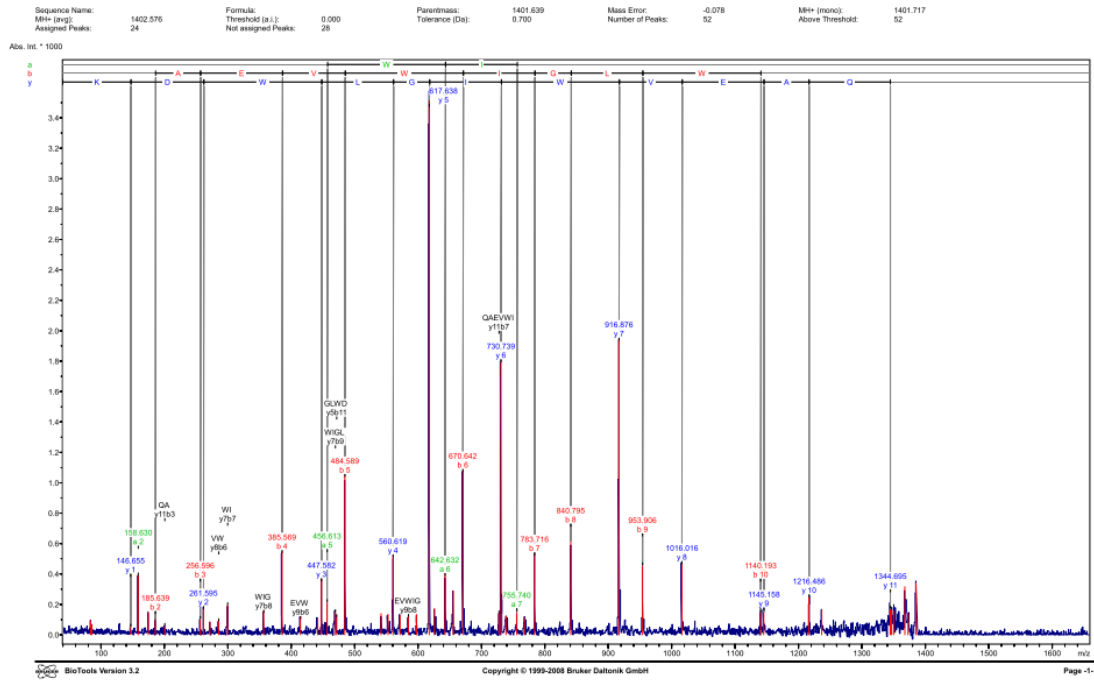
Calculated Masses:
 DFSEWYDQR

Id	Ion	a	b	y	C-Term	Ion
1	D	89.100	118.000	126.100	0	D
2	F	215.100	215.100	200.100	0	F
3	S	322.140	322.140	391.184	7	F
4	W	269.210	269.210	272.273	0	W
5	E	137.200	444.200	708.213	0	E
6	W	133.241	651.241	636.240	0	W
7	F	624.380	624.380	999.292	3	S
8	D	109.210	109.210	1126.459	2	D
9	D	1195.811	1195.811	161.160	2	D

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(B)

Figure S37. Annotated MS/MS spectrum of ion 1241.611 *m/z* detected in area #10. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 1401.639 Mass Error: -0.078 Mh+ (mono): 1401.717 Mh+ (avg): 1402.576 Threshold (a.i.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 52 Above Threshold: 52 Assigned Peaks: 24 Not assigned Peaks: 26

Peaks:

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity						
81	81.030	91.540	1	85.071	15.000	3	145.055	83.330	4	148.030	89.870	5	174.027	148.930	6	185.030	98.950						
13	103.059	28.523	2	105.058	15.300	8	117.054	108.112	9	121.050	86.180	11	125.050	20.250	12	129.050	102.510						
10	139.064	167.897	14	155.065	254.030	15	171.061	130.889	16	187.061	109.050	17	203.061	330.150	18	219.061	275.180						
12	155.064	140.267	20	171.060	118.810	21	187.056	1050.950	22	203.051	552.800	23	219.050	134.450	24	235.050	520.400						
25	251.057	103.810	30	267.052	151.611	34	283.048	140.700	35	299.043	317.051	36	315.038	113.900	37	331.033	255.330						
31	325.053	289.530	32	341.049	1045.920	33	357.044	141.030	38	373.039	1748.810	39	389.034	222.410	40	405.029	149.380						
39	409.050	111.024	39	425.045	800.051	40	441.040	818.059	41	457.035	1205.031	42	473.030	456.910	43	489.025	269.910						
43	1130.103	146.300	44	1146.098	190.377	45	1162.093	960.342	46	1178.088	148.260	47	1194.083	1341.660	48	1210.078	177.370	49	1226.073	1348.710	50	1242.068	667.830
50	1258.074	169.440	51	1274.069	337.950	52	1290.064	146.051	53	1306.059	339.870												

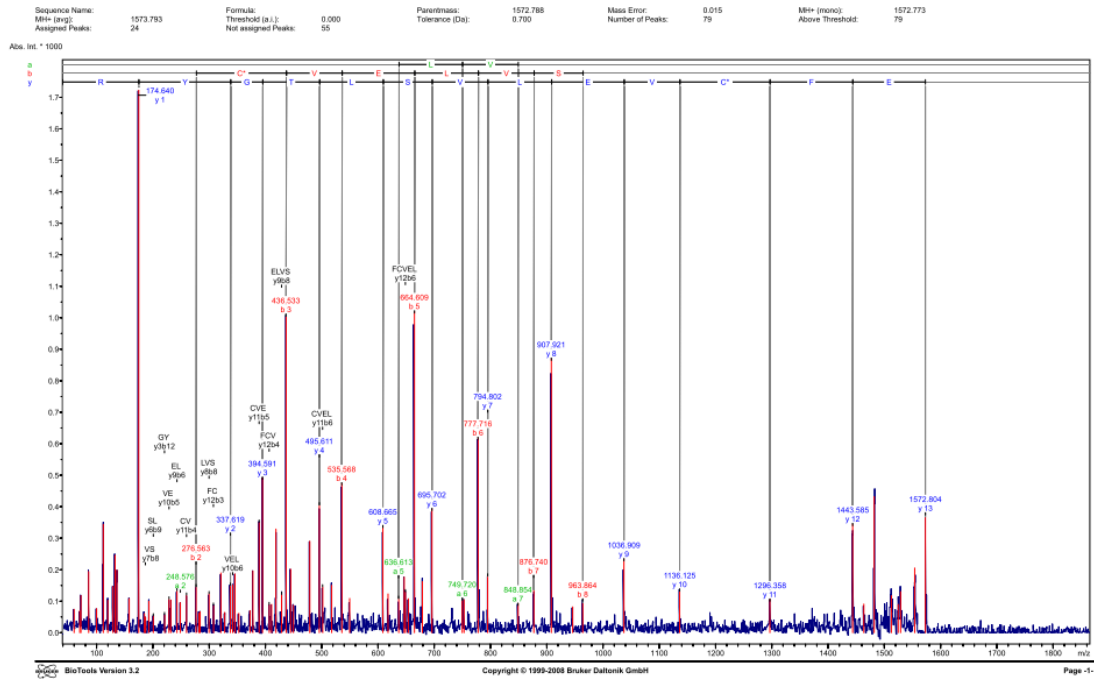
Calculated Masses:
 QKAEVWVWVGLWVQIYVWELQ

No	Term	Ion	a	b	y	Cx	Term	Ion
1	G	30.032	168.020	147.913	12	K		
2	D	158.026	168.020	792.400	11	D		
3	A	226.130	287.120	448.213	10	V		
4	E	355.174	385.164	611.303	9	E		
5	V	457.841	468.231	618.253	8	V		
6	I	44.230	413.211	711.400	7	I		
7	L	756.404	764.390	917.489	6	L		
8	Q	814.470	841.420	1016.569	5	Q		
9	W	105.050	854.951	1155.951	4	W		
10	V	1117.850	1148.881	1216.930	3	A		
11	D	1242.010	1270.811	1244.891	2	D		
12	K	1356.110	1383.700	1481.710	1	K		

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(B)

Figure S38. Annotated MS/MS spectrum of ion 1401.639 *m/z* detected in area #10. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.



(A)

Display Parameter: Parentmass: 1572.788 Mass Error: 0.015 M⁺ (mono): 1572.773 M⁺ (avg): 1573.793 Threshold (a.l.): 0.000
 Tolerance (Da): 0.700 Number of Peaks: 79 Above Threshold: 79 Assigned Peaks: 24 Not assigned Peaks: 55

Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity	Peak	Mass	Intensity
1	59.734	67.275	2	69.750	10.611	3	117.917	119.730	4	86.732	124.420	5	91.723	26.544
6	119.654	1.00001	7	129.714	127.113	8	132.280	236.900	10	136.560	128.020	11	157.424	103.610
12	184.692	61.891	13	169.269	33.442	14	172.832	99.804	15	209.990	149.491	16	220.250	169.910
18	231.818	103.539	20	242.588	159.330	21	248.576	86.585	22	269.593	118.327	23	276.583	148.193
25	278.019	66.541	26	296.820	193.320	27	307.834	96.333	28	320.714	199.741	29	327.531	84.114
31	341.817	151.944	32	349.560	166.267	33	352.200	61.511	34	377.493	31.251	35	377.570	198.380
36	384.801	68.820	37	426.569	18.261	38	431.261	89.165	39	418.455	28.820	41	448.684	121.837
43	444.690	207.320	44	449.557	87.173	45	478.327	290.942	46	485.611	434.627	47	501.931	144.450
48	502.669	474.729	49	474.516	108.660	51	498.664	248.664	52	497.454	141.430	53	496.916	108.154
54	528.755	129.580	55	544.647	101.250	56	554.200	1092.591	58	576.590	142.247	59	586.916	69.126
61	732.790	1.04834	62	777.716	611.200	63	782.900	178.900	65	848.854	38.130	66	878.740	130.160
68	848.844	81.659	69	863.664	34.826	70	1070.200	233.119	71	1138.124	119.820	72	1226.261	107.410
73	1483.472	30.960	74	1481.666	43.831	75	1512.281	117.407	76	1524.134	89.572	77	1528.841	130.674
78	1572.804	307.730												

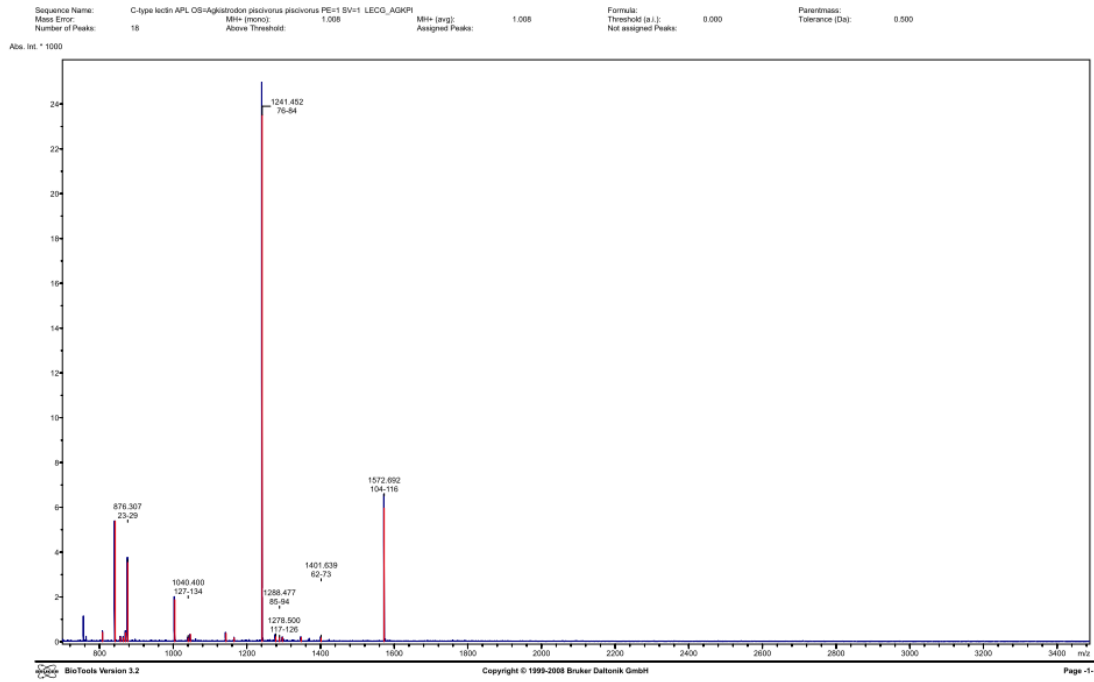
Calculated Masses:
 EFCVELSLTYGR 3: Carbamidomethyl (C)

R.T. (min)	Ion	a	b	y	C-Term	Ion
1	E	249.059	126.029	175.119	13	D
2	F	249.129	126.099	175.189	14	F
3	CV	406.150	203.070	305.261	11	G
4	V	406.220	203.140	305.331	10	G
5	E	437.261	218.131	339.333	9	L
6	L	437.331	218.201	339.403	8	L
7	V	469.411	234.211	375.424	7	V
8	L	469.481	234.281	375.494	6	L
9	L	1029.521	514.761	1237.561	2	L
10		1109.051	554.791	1138.831	4	V
11	G	1209.051	604.821	1206.861	3	C
12	V	1370.660	685.330	1449.790	2	F
13	R	1526.761	763.381	1572.771	1	E

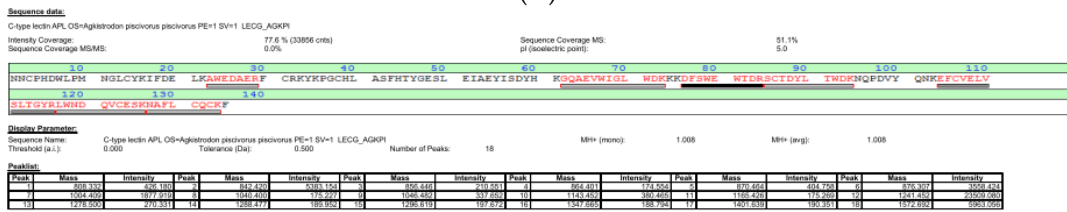
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(B)

Figure S39. Annotated MS/MS spectrum of ion 1572.788 *m/z* detected in area #10. (A) MS/MS spectrum; (B) Peak list and amino acid sequence.

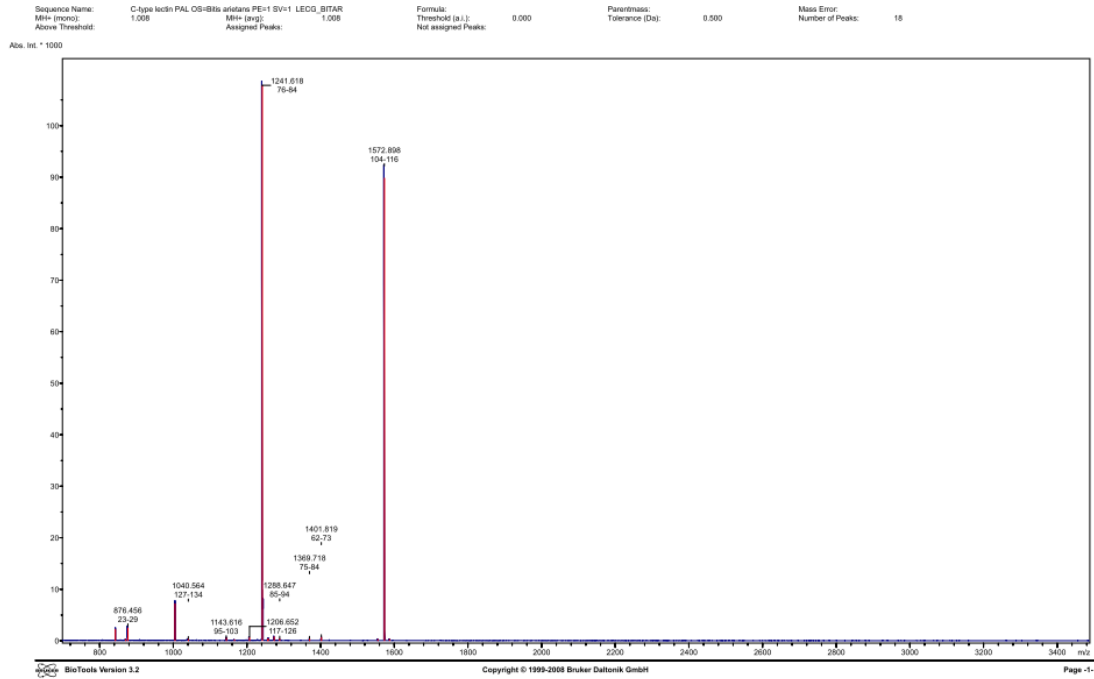


(A)

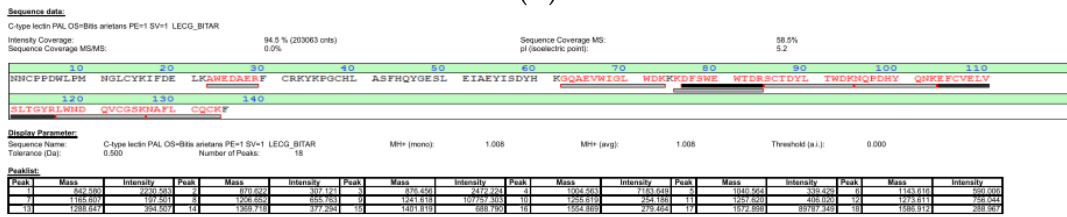


(B)

Figure S40. Annotated MS spectrum detected in area #10. (A) MS spectrum; (B) Peak list and sequence data.



(A)



(B)

Figure S41. Annotated MS spectrum detected in area #10. (A) MS spectrum; (B) Peak list and sequence data.