

Table 1

Position	Exp. Peak (In.)	Charge State	M+H(In.)	Theo. Mass	Error(ppm)
1-16(1Met-Ox)	541.9650	3	1623.8794	1623.8780	-0.83
1-16(1Met-Ox)	812.4440	2	1623.8802	1623.8780	-1.34
1-16(1Met-Ox,1Nit)	834.9350	2	1668.8622	1668.8631	0.55
6-16	478.3010	2	955.5942	955.5940	-0.18
6-16	955.5930	1	955.5930	955.5940	1.05
17-41	990.1520	3	2968.4404	2968.4406	0.07
17-42	774.6400	4	3095.5365	3095.5326	-1.27
17-42	1032.5170	3	3095.5354	3095.5326	-0.89
17-42(1Nit)	1047.5090	3	3140.5114	3140.5176	1.99
43-73(2Met-Ox)	899.4150	4	3594.6365	3594.6402	1.02
74-88	538.6060	3	1613.8024	1613.7998	-1.58
74-88	807.4040	2	1613.8002	1613.7998	-0.23
74-102	1148.5759	3	3443.7121	3443.7170	1.44
89-97	597.7820	2	1194.5562	1194.5544	-1.49
89-101	564.9510	3	1692.8374	1692.8346	-1.62
89-102	462.9900	4	1848.9365	1848.9357	-0.45
89-102	616.9830	3	1848.9334	1848.9357	1.27
89-102	924.9720	2	1848.9362	1848.9357	-0.26
89-102(1Nit)	631.9800	3	1893.9244	1893.9207	-1.93
102-123(1Met-Ox)	806.4150	3	2417.2294	2417.2281	-0.52
102-123(1Met-Ox,1CysO3)	822.4110	3	2465.2174	2465.2128	-1.85
103-117(1Met-Ox)	544.6170	3	1631.8354	1631.8314	-2.42
103-123	749.0510	3	2245.1374	2245.1321	-2.34
103-123	1123.0700	2	2245.1322	2245.1321	-0.03
103-123(1Met-Ox)	566.0380	4	2261.1285	2261.1270	-0.67
103-123(1Met-Ox)	754.3790	3	2261.1214	2261.1270	2.50
103-123(1Met-Ox)	1131.0670	2	2261.1262	2261.1270	0.36
103-123(1Met-Ox,1CysO)	759.7140	3	2277.1264	2277.1219	-1.95
103-123(1Met-Ox, 1Cys(NO))	764.3770	3	2291.1154	2291.1200	2.02
103-123(1Met-Ox,1CysO2)	765.0450	3	2293.1194	2293.1168	-1.11
103-123(1Met-Ox,1CysO3)	578.0340	4	2309.1125	2309.1117	-0.36
103-123(1Met-Ox,1CysO3)	770.3745	3	2309.1079	2309.1117	1.67
103-123(1Met-Ox,1CysO3)	1155.0620	2	2309.1162	2309.1117	-1.94
103-117(1Met-Ox)	816.4200	2	1631.8322	1631.8314	-0.47
103-128(1Met-Ox)	709.1110	4	2833.4205	2833.4188	-0.61
103-128(1Met-Ox)	945.1450	3	2833.4194	2833.4188	-0.19
105-123	673.3270	3	2017.9654	2017.9687	1.66
105-123(1Met-Ox)	678.6610	3	2033.9674	2033.9636	-1.84
105-123(1Met-Ox)	1017.4840	2	2033.9602	2033.9636	1.68
129-135	401.2150	2	801.4222	801.4219	-0.34
129-135	801.4230	1	801.4230	801.4219	-1.37
136-147	664.8410	2	1328.6742	1328.6738	-0.28
136-147(1Nit)	687.3350	2	1373.6622	1373.6589	-2.38
148-161	552.2905	3	1654.8559	1654.8553	-0.33
148-161	827.9320	2	1654.8562	1654.8553	-0.53
148-161(1Nit)	850.4240	2	1699.8402	1699.8404	0.13
150-161	466.5740	3	1397.7064	1397.7065	0.11
150-161	699.3560	2	1397.7042	1397.7065	1.66
150-161	1397.7030	1	1397.7030	1397.7065	2.50
150-161(1Nit)	721.8510	2	1442.6942	1442.6916	-1.78
162-169	540.3260	2	1079.6442	1079.6438	-0.35
170-185(1Met-Ox)	560.2475	3	1678.7269	1678.7239	-1.76
170-185(1Met-Ox)	839.8670	2	1678.7262	1678.7239	-1.36
170-189	688.9800	3	2064.9244	2064.9227	-0.80
170-189(1Met-Ox)	694.3110	3	2080.9174	2080.9176	0.12
170-189(1Met-Ox)	1040.9630	2	2080.9182	2080.9176	-0.28
170-189(1Met-Ox,1CysO3)	710.3070	3	2128.9054	2128.9023	-1.43
170-189(1Met-Ox,1CysO3)	1064.9570	2	2128.9062	2128.9023	-1.82
170-189(1Met-Ox,2CysO3)	1088.9490	2	2176.8902	2176.8870	-1.46
170-189(1Met-Ox,3CysO3)	1112.9400	2	2224.8722	2224.8717	-0.21
171-185(1Met-Ox)	775.8190	2	1550.6302	1550.6289	-0.82
171-189(1Met-Ox)	976.9160	2	1952.8242	1952.8226	-0.81
171-189(1Met-Ox,1CysO3)	1000.9070	2	2000.8062	2000.8073	0.56

Error
Average =1.09
 $\sigma = 0.74$

Table 2 (Supplemental data)

Position	CAD			Position	ECD		
	M+H	Theo. Mass	Error(ppm)		M+H	Theo. Mass	Error(ppm)
				c2	245.198	245.198	0.00
				c3	360.225	360.225	0.00
				c4	447.257	447.257	0.00
				c5	562.284	562.284	0.00
b6	660.285	660.284	-1.51	c6	677.311	677.311	0.00
b7	759.353	759.352	-1.32				
				c8	873.432	873.432	0.00
b9	1003.440	1003.441	1.00	c9	1020.468	1020.467	-0.98
b10	1102.508	1102.508	0.00	c10	1119.536	1119.536	0.00
b11	1215.594	1215.593	-0.82	c11	1232.620	1232.620	0.00
b12	1314.662	1314.662	0.00	c12	1330.680	1330.680	0.00
b13	1371.683	1371.683	0.00	c13	1388.708	1388.710	1.44
				c14	1502.750	1502.752	1.33
				c15	1630.846	1630.847	0.61
				c16	1781.836	1781.841	2.81
b17	1879.840	1879.842		c17	1896.865	1896.868	1.58
b18	1992.928	1992.926		c18	2009.950	2009.952	1.00
b19	2063.964	2063.963		c19	2080.990	2080.989	-0.48
b20	2134.998	2135.000		c20	2152.028	2152.027	-0.46
				z2	230.138	230.138	0.00
y3	317.194	317.194		z3	301.175	301.175	0.00
y4	430.279	430.278	-2.32	z4	414.259	414.259	0.00
y5	545.305	545.305	0.00	z5	529.286	529.286	0.00
y7	824.395	824.394	-1.21	z7	808.374	808.375	1.24
y8	938.436	938.437	1.07	z8	922.419	922.418	-1.08
y9	995.458	995.458	0.00	z9	979.438	979.439	1.02
y10	1094.526	1094.526	0.00	z10	1078.510	1078.508	-1.85
y11	1207.609	1207.610	0.83	z11	1191.594	1191.592	-1.68
				z12	1290.658	1290.660	1.55
				z13	1437.700	1437.696	-2.78
y14	1550.768	1550.767					
y15	1649.836	1649.835	-0.61	z16	1748.843	1748.844	0.57
				z17	1863.876	1863.871	-2.68
				z18	1950.900	1950.903	1.54
y19	2081.946	2081.948	0.96				

Table 3 (Supplemental data)

CAD				ECD			
Position	M+H	Theo. Mass	Error(ppm)	Position	M+H	Theo. Mass	Error(ppm)
				c2	245.198	245.198	0.00
				c3	360.225	360.225	0.00
				c4	447.257	447.257	0.00
b5	545.257	545.257	0.00	c5	562.283	562.284	1.78
b6	660.284	660.284	0.00	c6	677.311	677.311	0.00
b7	759.352	759.352	0.00				
b8	856.404	856.405	1.17	c8	873.431	873.432	1.14
b9	987.444	987.446	2.03	c9	1004.473	1004.472	-1.00
b10	1086.513	1086.514	0.92	c10	1103.541	1103.541	0.00
b11	1199.600	1199.598	-1.67	c11	1216.625	1216.625	0.00
b12	1298.665	1298.667	1.54	c12	1315.693	1315.693	0.00
				c13	1372.714	1372.715	0.73
				c14	1486.756	1486.758	1.35
				c16	2022.93	2022.930	0.00
				c17	2137.96	2137.957	-1.40
				c18	2251.040	2251.041	0.44
				c19	2322.086	2322.078	-3.45
				c20	2393.112	2393.115	1.25
				z2	230.138	230.138	0.00
				z3	301.175	301.175	0.00
y4	430.278	430.278	0.00	z4	414.259	414.259	0.00
y5	545.305	545.305	0.00	z5	529.286	529.286	0.00
y6	953.381	953.382	1.05				
y7	1081.478	1081.477	-0.92				
y8	1195.518	1195.520	1.67	z8	1178.500	1178.501	0.85
y9	1252.538	1252.541	2.40				
y10	1351.607	1351.610	2.22				
y11	1464.694	1464.694	0.00	z11	1448.674	1448.675	0.69
y12	1563.762	1563.762	0.00	z12	1547.744	1547.744	0.00
				z13	1678.784	1678.784	0.00
y14	1791.854	1791.856	1.12				
y15	1890.922	1890.924	1.06	z15	1874.908	1874.905	-1.60
y16	2005.952	2005.951	-0.50	z16	1989.934	1989.932	-1.01
y17	2120.978	2120.978	0.00	z17	2104.966	2104.959	-3.33
y18	2208.006	2208.010	1.81	z18	2191.992	2191.991	-0.46
				z19	2307.016	2307.018	0.87
y20	2451.126	2451.132	2.45				