

Supplementary material.

Figures

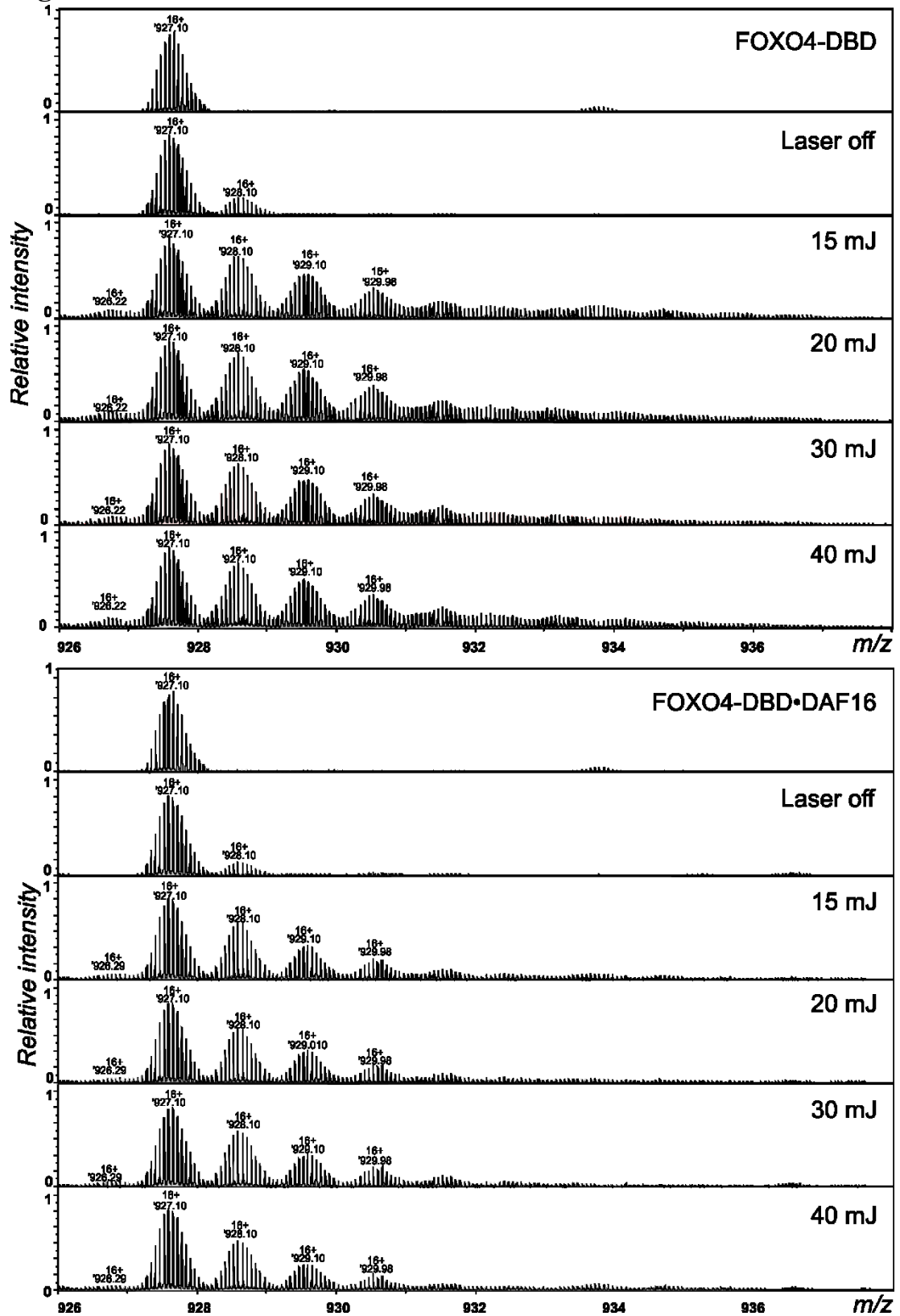


Fig. S1 | Mass spectra of both, FOXO4-DBD and FOXO4-DBD•DAF16 submitted FPOP experiment at frequency of 15 Hz.

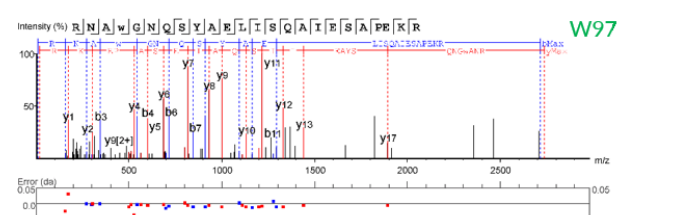
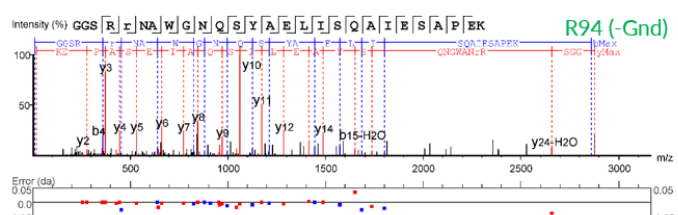
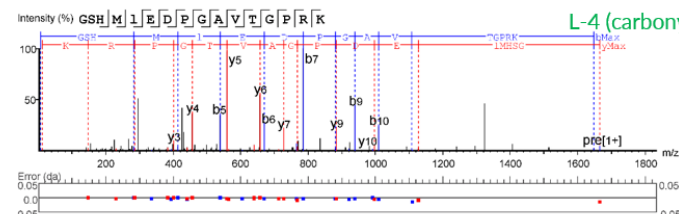
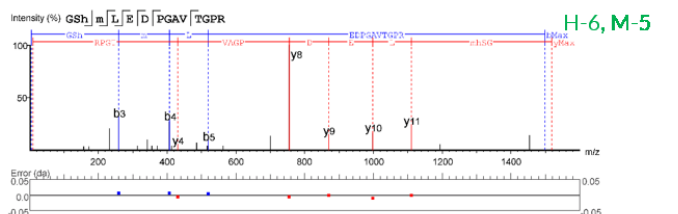
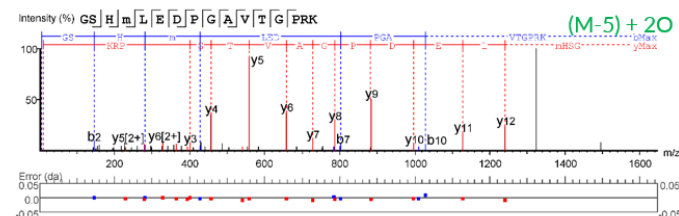
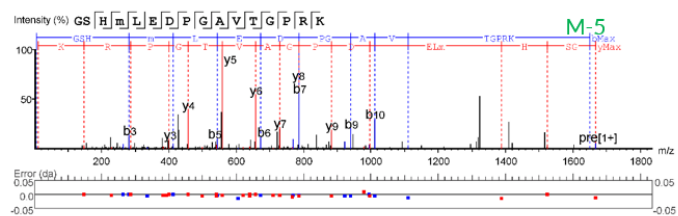
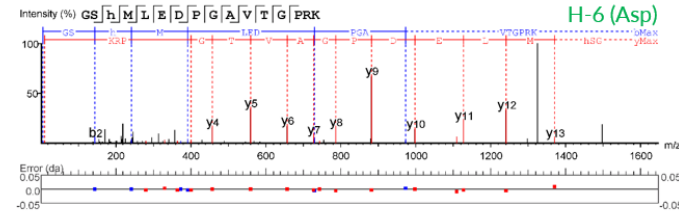
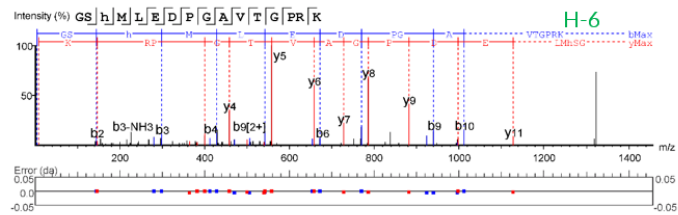


Fig S2 | Collision spectra of individual identified modifications during LC-MS/MS analysis. Exported from Peaks® X+ software (Bioinformatics Solution Inc., Canada)

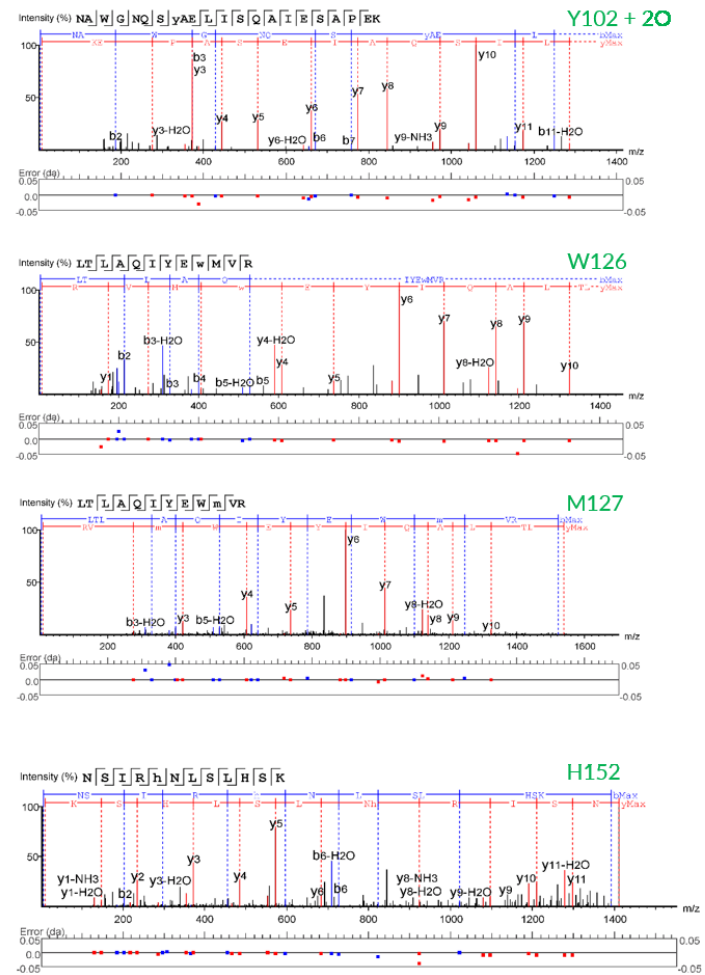
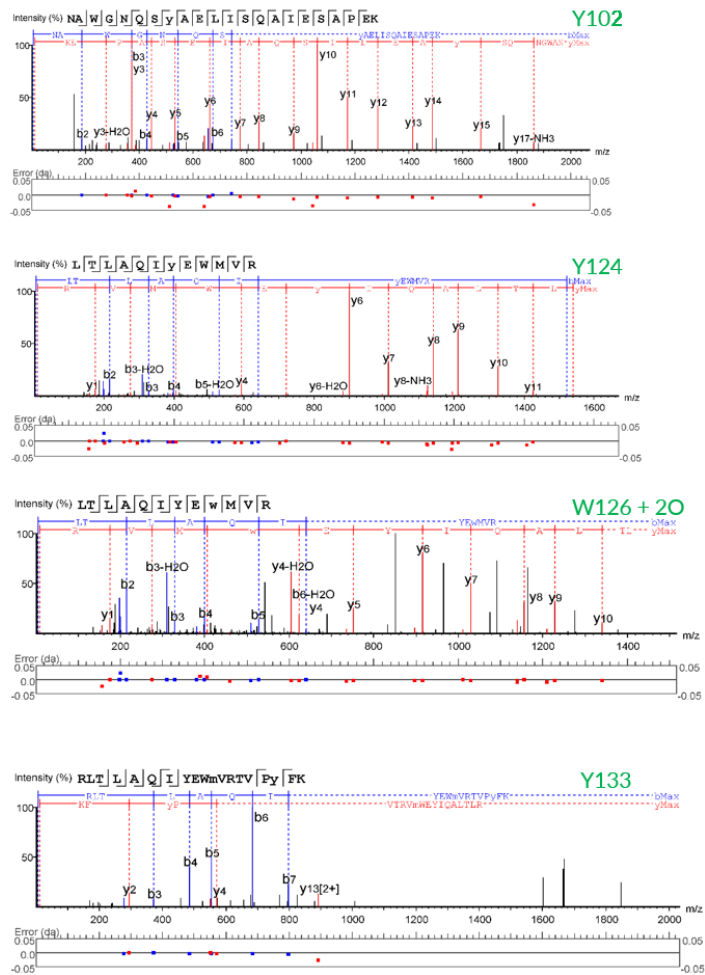


Fig S3 | Collision spectra of individual identified modifications during LC-MS/MS analysis. Exported from Peaks[®] X+ software (Bioinformatics Solution Inc., Canada)

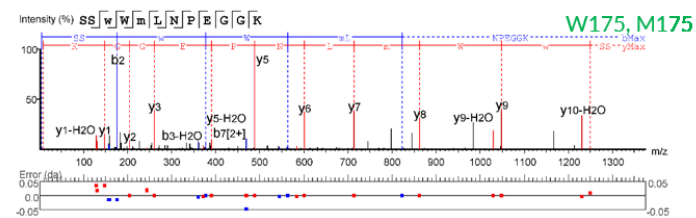
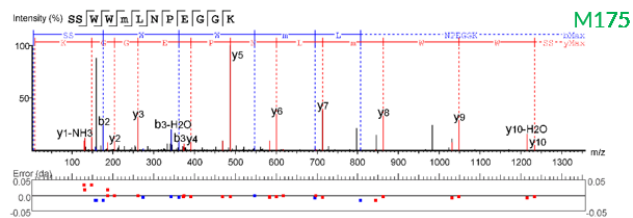
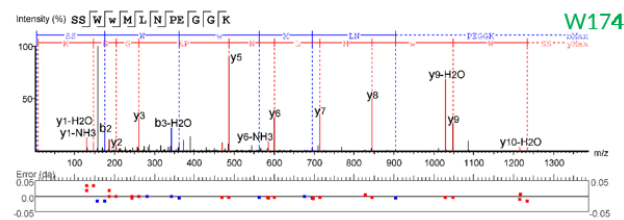
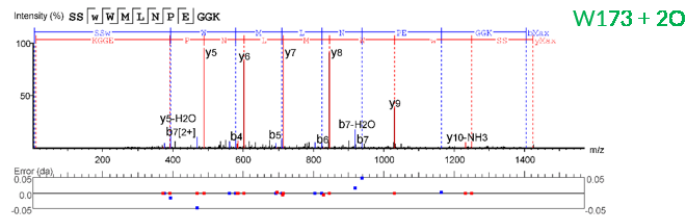
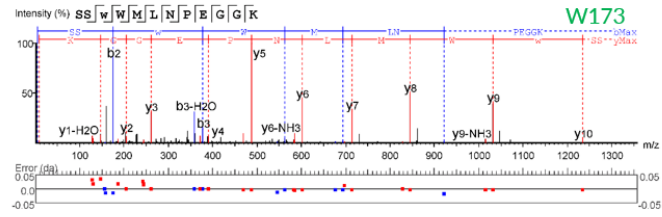
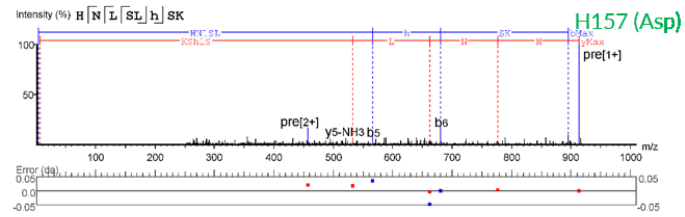
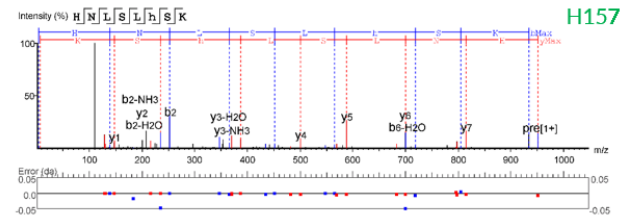
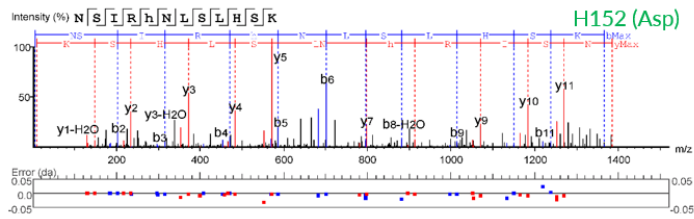


Fig S4 | Collision spectra of individual identified modifications during LC-MS/MS analysis. Exported from Peaks[®] X+ software (Bioinformatics Solution Inc., Canada)

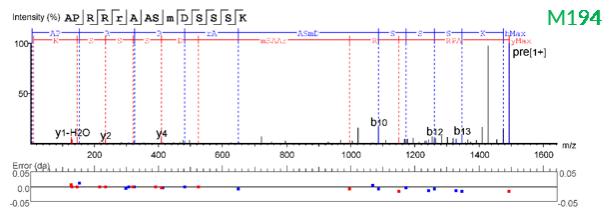
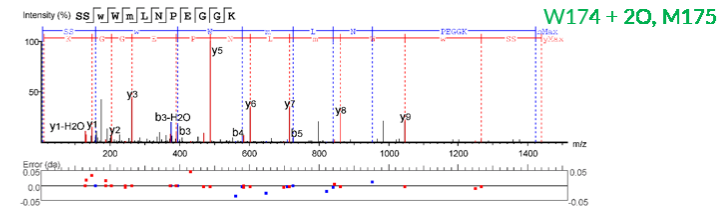
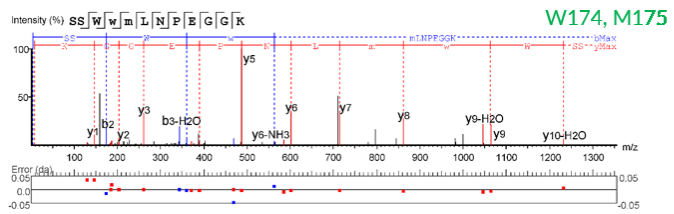


Fig S5 | Collision spectra of individual identified modifications during LC-MS/MS analysis. Exported from Peaks[®] X+ software (Bioinformatics Solution Inc., Canada)

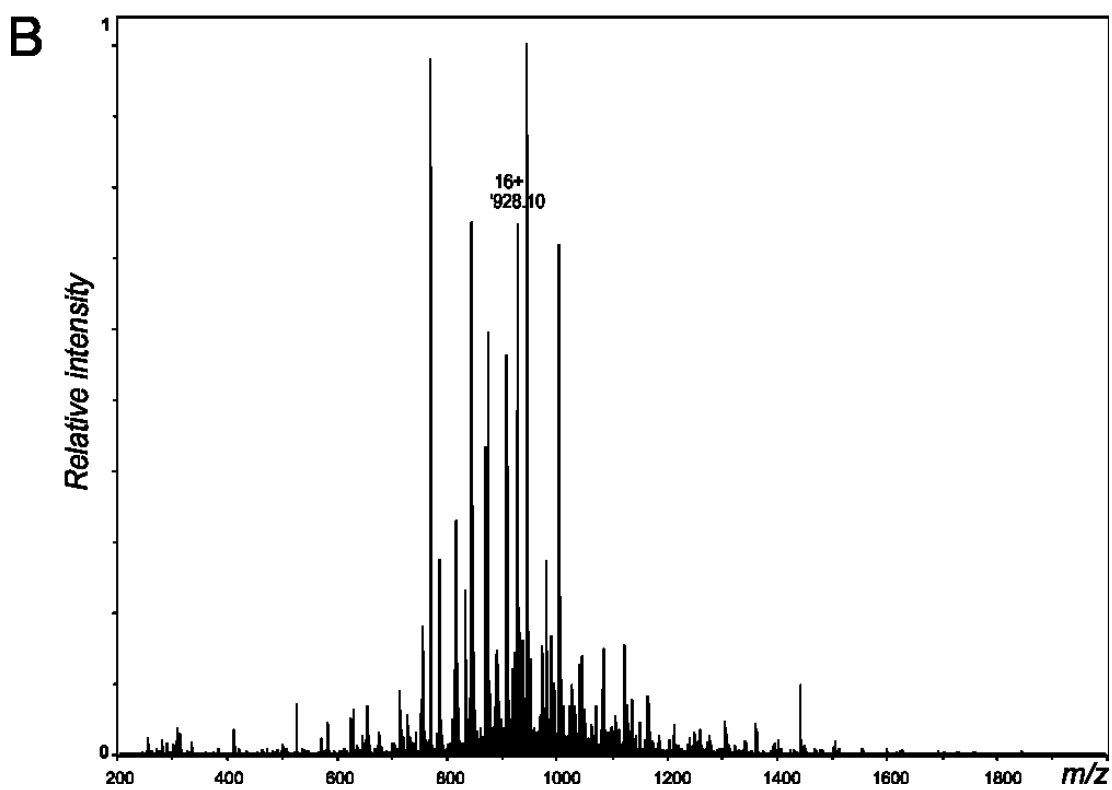
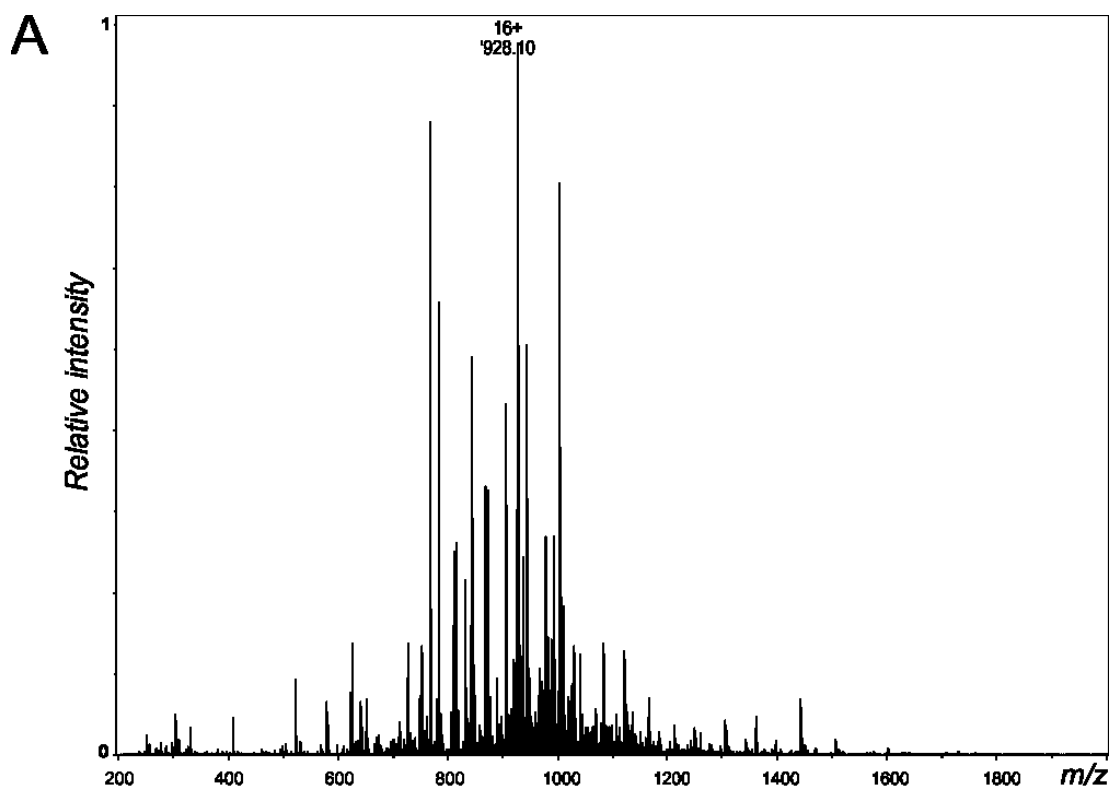


Fig. S6 | Raw CID fragmented spectra of singly oxidized +16 ion for both, apo (A) and holo (B) form, respectively. Closer view with range m/z 200-2000.

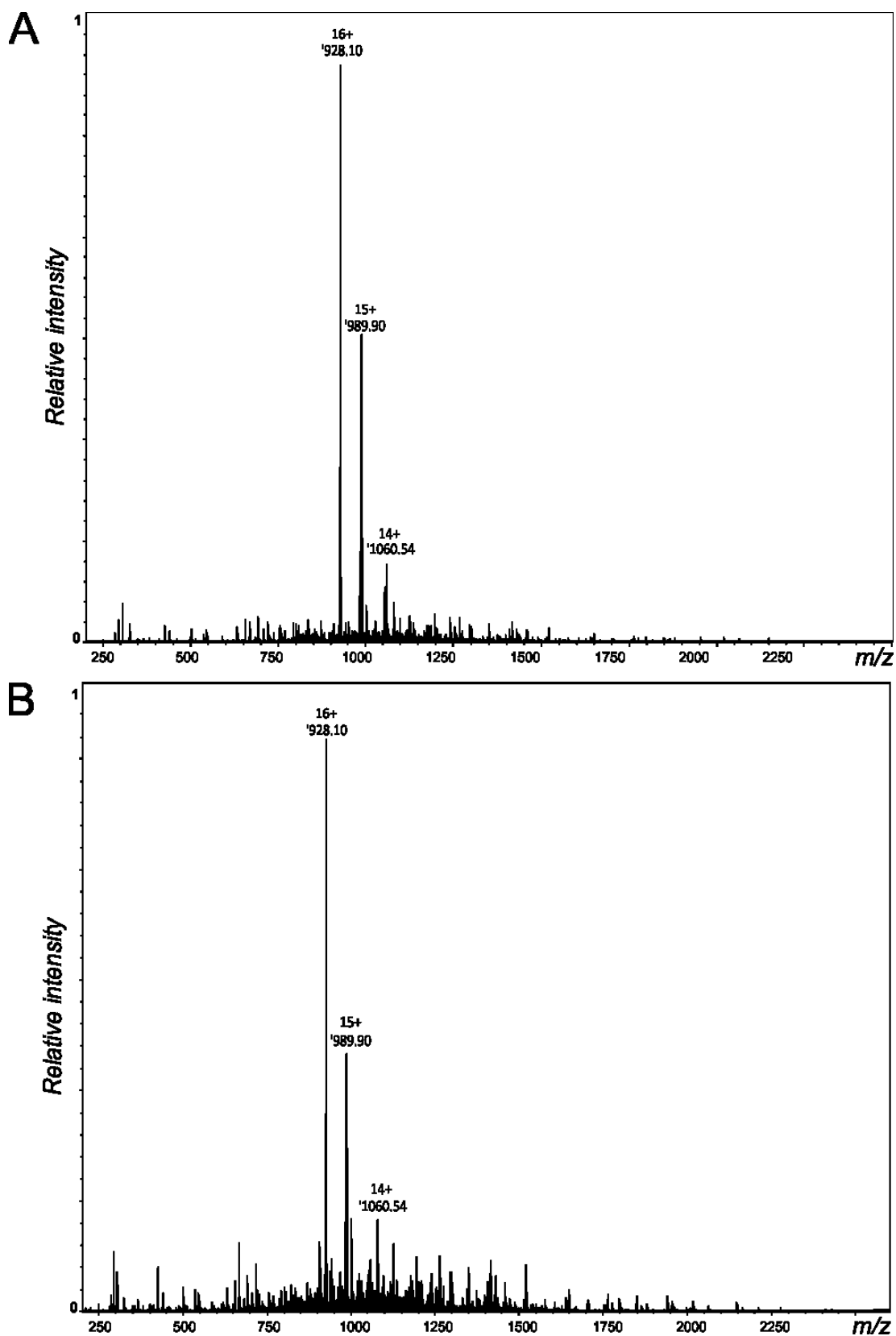


Fig. S7 | Raw CECD fragmented spectra of singly oxidized +16 ion for both, apo (A) and holo (B) form, respectively.

Tables

Table 1 | List of deconvoluted ions of intact +16 unmodified ion obtained by CID fragmentation.

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
282.12	282.1202	0.8	b3	10899607
413.1604	413.1607	0.7	b4	37840196
526.2447	526.2448	0.2	b5	82471656
655.2884	655.2874	1.5	b6	61136096
770.3143	770.3143	0.1	b7	358584928
995.4257	995.4257	0	b10	2765052
1094.4944	1094.4941	0.2	b11	1704808
3138.5051	3138.5042	0.3	b30	14644717
3267.5479	3267.5469	0.3	b31	158089232
3380.6311	3380.6309	0.1	b32	301879104
3493.7151	3493.7148	0.1	b33	135449344
3580.7476	3580.7468	0.2	b34	25425692
3708.8054	3708.8054	0	b35	52849440
3779.8423	3779.8425	0.1	b36	192320816
3892.9241	3892.9268	0.7	b37	14716519
4021.9712	4021.9692	0.5	b38	10694985
4180.0371	4180.0381	0.2	b40	7547580
5621.8223	5621.8311	1.6	b52	3826092
6295.1851	6295.168	2.7	b57	1573781
6394.2295	6394.2368	1.1	b58	1478216
7044.5327	7044.543	1.5	b63	2573054
7172.6421	7172.6382	0.5	b64	5613673
11133.6123	11133.6113	0.1	b100	1659715
11450.752	11450.7314	1.8	b102	3464425
11563.8105	11563.8154	0.4	b103	8121213
11677.8536	11677.85859	0.1	b104	18935182
14800.5498	14800.5537	0.3	b134	61758132
518.3051	518.305	0.2	y5	6065825
1289.765	1289.7654	0.3	y12	75326240
1764.9402	1764.9391	0.6	y17	12817400
1921.0391	1921.0402	0.6	y18	21681480
2077.1426	2077.1414	0.6	y19	7655432
2401.3325	2401.3323	0.1	y22	1452486
2401.3391	2401.3323	2.8	y22	1161747
2673.4761	2673.4807	1.7	y25	12948997
2801.5771	2801.5757	0.5	y26	1165189
2915.6204	2915.6187	0.6	y28	111344664
3044.6619	3044.6614	0.2	y29	11143255

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
3141.7151	3141.7141	0.3	y30	468265024
3255.759	3255.7571	0.6	y31	91243656
3368.842	3368.8411	0.3	y32	121003712
3685.9604	3685.9609	0.1	y34	75221216
3872.0398	3872.0403	0.1	y35	17781560
3959.0781	3959.0723	1.5	y36	20226908
4046.104	4046.1042	0.1	y37	53614748
4231.2236	4231.2207	0.7	y39	9792836
4332.269	4332.2686	0.1	y40	5754098
4403.3071	4403.3057	0.3	y41	28005192
4532.3467	4532.3481	0.3	y42	9171201
4646.3906	4646.3911	0.1	y43	21922360
4783.4502	4783.4497	0.1	y44	28165002
4882.5176	4882.5186	0.2	y45	19548780
5010.6123	5010.6133	0.2	y46	3185547
5123.6948	5123.6973	0.5	y47	1353647
5270.7651	5270.7656	0.1	y48	40941472
5485.8945	5485.8926	0.4	y50	17708978
5622.9497	5622.9517	0.3	y51	3163396
7028.7109	7028.7095	0.2	y63	2057172
7099.7422	7099.7466	0.6	y64	2573322
7273.7969	7273.8105	1.9	y66	3943140
7474.8843	7474.8857	0.2	y68	31755186
7589.9175	7589.9126	0.6	y69	2413538
7646.9326	7646.9341	0.2	y70	63132224
7775.0288	7775.0293	0.1	y71	50707840
7890.0557	7890.0562	0.1	y72	38551412
8018.1499	8018.1509	0.1	y73	931599
8425.332	8425.3359	0.5	y76	28977522
9197.7412	9197.7412	0	y82	31789050
9489.8623	9489.8467	1.6	y84	7609394
9602.9229	9602.9307	0.8	y85	4130738
10413.4365	10413.4385	0.2	y92	54484624
10639.5342	10639.5342	0	y94	98041680
10797.6035	10797.6035	0	y96	127520960
10926.6455	10926.6455	0	y97	153706208
11039.7285	11039.7295	0.1	y98	248313392
11110.7676	11110.7666	0.1	y99	110942192
11238.8281	11238.8252	0.3	y100	18581026
11325.8574	11325.8574	0	y101	133334616
11438.957	11438.9414	1.4	y102	12462050
14049.2627	14049.2578	0.3	y127	88021592
14293.3213	14293.3281	0.5	y129	9638123
14406.4111	14406.4121	0.1	y130	13299672

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
426.2349	426.2353	0.9	b(8-12)	829831
1377.7831	1377.7828	0.2	b(8-21)	2145392
2048.0669	2048.0652	0.8	b(8-27)	1309430
2298.1624	2298.1604	0.8	b(8-29)	8157237
2369.1978	2369.1975	0.1	b(8-30)	22482396
2498.2388	2498.2402	0.6	b(8-31)	194147520
2611.3245	2611.3242	0.1	b(8-32)	282332384
2724.4084	2724.4084	0	b(8-33)	220132976
2811.4409	2811.4404	0.2	b(8-34)	10885295
2939.4971	2939.499	0.7	b(8-35)	2762266
2939.4985	2939.499	0.2	b(8-35)	97383016
2939.5002	2939.499	0.4	b(8-35)	8770775
3010.5359	3010.5361	0.1	b(8-36)	257340896
3123.6187	3123.6201	0.5	b(8-37)	579116
3123.6194	3123.6201	0.2	b(8-37)	39177240
3252.6611	3252.6628	0.5	b(8-38)	60032284
3339.6914	3339.6948	1	b(8-39)	9575493
3410.7288	3410.7319	0.9	b(8-40)	14785669
3410.7307	3410.7319	0.4	b(8-40)	2062097
3636.8232	3636.8274	1.1	b(8-42)	12302053
3764.9202	3764.9224	0.6	b(8-43)	810316
4852.5249	4852.5244	0.1	b(8-52)	10182534
5624.9316	5624.9302	0.3	b(8-58)	2369847
6275.2319	6275.2363	0.7	b(8-63)	12481910
6403.332	6403.3315	0.1	b(8-64)	8813757
3551.8379	3551.8362	0.5	b(34-63)	7994500
3265.71	3265.7085	0.4	b(37-63)	14171783
3565.8535	3565.8518	0.5	b(37-66)	9451238
3152.6216	3152.6245	0.9	b(38-63)	1241812
3452.7656	3452.7678	0.6	b(38-66)	5849134
3023.5815	3023.5818	0.1	b(39-63)	4175081
838.5153	838.5151	0.3	b(41-47)	970121
909.5518	909.5522	0.5	b(41-48)	8000004
1150.6945	1150.6948	0.3	b(41-50)	11804504
1442.7968	1442.8008	2.8	b(41-52)	27989162
2215.2061	2215.2063	0.1	b(41-58)	9165868
2622.3889	2622.3909	0.7	b(41-61)	4133971
2750.4858	2750.4858	0	b(41-62)	3551170
2865.5132	2865.5127	0.2	b(41-63)	10378557
2993.6118	2993.6077	1.4	b(41-64)	8502985
5369.7793	5369.7759	0.6	b(41-86)	4152806
6594.4453	6594.4375	1.2	b(41-97)	3310968
2939.5688	2939.5608	2.7	b(43-66)	3991248
408.1921	408.1923	0.4	b(59-61)	5188898

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
651.314	651.3143	0.4	b(59-63)	5735446
779.4086	779.4092	0.8	b(59-64)	13809855
1326.594	1326.5967	2	b(59-70)	1682531
1397.632	1397.6338	1.3	b(59-71)	2128399
1454.653	1454.6553	1.6	b(59-72)	659362
3642.8979	3642.8936	1.2	b(59-90)	960488
691.3415	691.3416	0.1	b(61-66)	1194278
7140.6548	7140.6602	0.8	b(41-101)	2063072
7384.7773	7384.7847	1	b(41-103)	5506867
7724.9141	7724.9229	1.1	b(41-106)	1009380
5898.0044	5898.021	2.8	b(70-122)	4276767
1377.7831	1377.7828	0.2	b(105-117)	2145392
1852.9524	1852.9565	2.2	b(105-122)	9968698
3052.6677	3052.6665	0.4	b(105-133)	47690604
3123.7036	3123.7036	0	b(105-134)	5795855
3123.7065	3123.7036	0.9	b(105-134)	59989676
1384.7274	1384.7233	3	b(110-122)	778352

Table 2 | List of deconvoluted ions of intact +16 unmodified ion obtained by ECD fragmentation.

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
430.1873	430.1872	0.1	c4	26874766
1012.4531	1012.4522	0.8	c10	4909611
1212.5682	1212.5682	0	c12	30907316
1366.6417	1366.6426	0.6	c14	5981035
1522.744	1522.7437	0.2	c15	47457056
1650.839	1650.8386	0.2	c16	44541128
1707.8593	1707.8601	0.5	c17	14826204
1764.8793	1764.8816	1.3	c18	7834784
1851.9122	1851.9136	0.7	c19	53969080
2008.0155	2008.0148	0.4	c20	90411224
2164.1174	2164.1157	0.8	c21	155572352
2278.1597	2278.1587	0.4	c22	19479826
2349.1936	2349.1958	0.9	c23	6761845
2535.2747	2535.2751	0.2	c24	31289270
2592.2974	2592.2966	0.3	c25	43335900
2706.3403	2706.3394	0.4	c26	72057632
2834.3989	2834.3979	0.3	c27	85566592
2921.4304	2921.4302	0.1	c28	41391068
3084.4949	3084.4934	0.5	c29	21998326
3155.5317	3155.5305	0.4	c30	55205408
3284.574	3284.5732	0.2	c31	28026324
3597.7717	3597.7732	0.4	c34	14062952
3796.8623	3796.8689	1.7	c36	2571801
3909.9531	3909.9531	0	c37	104915056
4038.9946	4038.9956	0.2	c38	18668636
4126.0278	4126.0278	0	c39	73649952
4294.1157	4294.1177	0.5	c41	9351929
4551.2554	4551.2554	0	c43	4168611
4707.3564	4707.3564	0	c44	6925152
4820.4419	4820.4404	0.3	c45	57903232
4921.4839	4921.4883	0.9	c46	12507476
5034.5767	5034.5723	0.9	c47	4474374
5105.6104	5105.6094	0.2	c48	65483400
5233.6694	5233.668	0.3	c49	20347270
5346.7544	5346.752	0.5	c50	9173756
5509.8159	5509.8154	0.1	c51	22893330
5638.8594	5638.8579	0.3	c52	134180336
5824.9375	5824.9375	0	c53	58400276
6055.0464	6055.0464	0	c55	22360410
6211.1499	6211.1475	0.4	c56	20470660
6312.1934	6312.1948	0.2	c57	10497595

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
6508.3184	6508.3164	0.3	c59	48456948
6671.3823	6671.3794	0.4	c60	108443680
6818.4502	6818.4478	0.4	c61	89722576
6946.5483	6946.543	0.8	c62	65290116
7061.5718	7061.5698	0.3	c63	81113096
7189.6675	7189.665	0.3	c64	74129064
7189.668	7189.665	0.4	c64	66581376
7189.6694	7189.665	0.6	c64	15663888
7361.7163	7361.7134	0.4	c66	4852251
7448.749	7448.7451	0.5	c67	83141704
7562.7905	7562.7881	0.3	c68	11492163
7649.8232	7649.8203	0.4	c69	30906580
7736.8545	7736.8525	0.3	c70	53088360
7807.8921	7807.8896	0.3	c71	46102700
7864.9194	7864.9111	1.1	c72	55946444
8050.9946	8050.9902	0.5	c73	60817740
8179.0874	8179.085	0.3	c74	47183532
8293.1318	8293.1279	0.5	c75	47705576
8493.248	8493.2441	0.5	c77	9864620
8649.3486	8649.3447	0.5	c78	49239456
8786.4072	8786.4033	0.4	c79	34406012
8900.4512	8900.4463	0.5	c80	45796072
9100.5703	9100.5625	0.9	c82	32110374
9213.6504	9213.6465	0.4	c83	48792228
9350.7119	9350.7061	0.6	c84	40304592
9437.7441	9437.7383	0.6	c85	111098680
9825.9912	9825.9854	0.6	c88	20578652
9954.0879	9954.0801	0.8	c89	23781204
10053.1563	10053.1484	0.8	c90	55873696
10190.2158	10190.208	0.8	c91	42992764
10304.2578	10304.251	0.7	c92	62488140
10433.2998	10433.293	0.7	c93	23404396
10605.3779	10605.3779	0	c95	6410492
10662.4072	10662.3994	0.7	c96	100727000
10790.501	10790.4941	0.6	c97	78110096
10877.5391	10877.5264	1.2	c98	28476460
11580.8496	11580.8418	0.7	c103	14711917
11791.9453	11791.9375	0.7	c105	52343852
11920.9873	11920.9795	0.7	c106	62065916
11978.0127	11978.001	1	c107	28146444
12035.0293	12035.0225	0.6	c108	32242368
12307.1797	12307.1709	0.7	c111	12099612
12435.2764	12435.2666	0.8	c112	17071284
12603.3652	12603.3564	0.7	c114	13891335

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
12759.4717	12759.457	1.1	c115	27407184
12915.5654	12915.5586	0.5	c116	36997736
13071.6699	13071.6592	0.8	c117	33894788
13213.7461	13213.7334	1	c119	11050336
13431.8193	13431.8066	0.9	c121	26755034
13546.8438	13546.833	0.8	c122	19149400
13720.9102	13720.8975	0.9	c124	20238820
13807.9404	13807.9297	0.8	c125	27690866
14049.1123	14049.1084	0.3	c127	17954342
14162.2012	14162.1924	0.6	c128	17537974
14375.3213	14375.3154	0.4	c130	26412550
445.2648	445.2649	0.3	z4	16514548
658.3873	658.3875	0.3	z6	19640030
771.4719	771.4716	0.4	z7	12272052
884.5556	884.5557	0.1	z8	7551687
1012.6508	1012.6506	0.2	z9	11821671
1099.6831	1099.6827	0.3	z10	28210386
1186.7153	1186.7147	0.5	z11	13536819
1273.7473	1273.7468	0.4	z12	29498770
1388.7747	1388.7737	0.7	z13	33701520
1519.8152	1519.8142	0.6	z14	16949464
1748.9224	1748.9205	1	z17	22201894
1905.0232	1905.0216	0.8	z18	40174792
2061.1238	2061.1228	0.5	z19	14199253
2217.2251	2217.2239	0.6	z20	24907506
2385.3154	2385.3137	0.7	z22	29824236
2513.4102	2513.4087	0.6	z23	24831852
2570.4336	2570.4302	1.3	z24	14126365
2657.4646	2657.4622	0.9	z25	4480117
2785.5593	2785.5571	0.8	z26	62383368
2842.5811	2842.5786	0.9	z27	38019384
2899.6023	2899.6001	0.8	z28	54136476
3028.645	3028.6428	0.7	z29	50296468
3943.0571	3943.0537	0.9	z36	46804520
4030.0881	4030.0857	0.6	z37	38934572
4158.1836	4158.1807	0.7	z38	108314736
4387.29	4387.2871	0.7	z41	21055616
4516.3315	4516.3296	0.4	z42	42625132
4630.375	4630.3726	0.5	z43	7462942
4767.4336	4767.4312	0.5	z44	36805824
4866.5015	4866.5	0.3	z45	10672139
4994.5977	4994.5947	0.6	z46	29150586
5254.75	5254.7471	0.6	z48	18816876
5382.8452	5382.8423	0.5	z49	85550648

[M+H] ⁺ observed	[M+H] ⁺ calculate	Error (ppm)	Ion	Intensity
5469.8765	5469.874	0.4	z50	11319370
5606.9365	5606.9331	0.6	z51	37293056
5720.02	5720.0171	0.5	z52	11643395
5920.1367	5920.1333	0.6	z54	20508712
6034.1797	6034.1763	0.6	z55	14382410
6327.3408	6327.3364	0.7	z57	25984502
6527.4561	6527.4521	0.6	z59	29020234
6641.5	6641.4951	0.7	z60	20550864
6769.5952	6769.5903	0.7	z61	32611010
6955.6738	6955.6694	0.6	z62	47096136
7012.6938	7012.6909	0.4	z63	9658138
7083.7324	7083.728	0.6	z64	56601132
7170.7646	7170.7603	0.6	z65	20311870
7371.8403	7371.835	0.7	z67	26595890
7458.8721	7458.8672	0.7	z68	16542284
7573.8999	7573.894	0.8	z69	37299796
7630.9214	7630.9155	0.8	z70	76876296
7759.0166	7759.0107	0.8	z71	31694672
7874.042	7874.0376	0.6	z72	33641328
8002.1382	8002.1323	0.7	z73	58843028
8149.2065	8149.2007	0.7	z74	68750992
8312.2705	8312.2646	0.7	z75	15590688
8609.4375	8609.4336	0.5	z78	23876540
8995.6484	8995.6436	0.5	z81	14612019
9181.7275	9181.7227	0.5	z82	18275530
9714.9795	9714.9707	0.9	z86	36609460
9786.0166	9786.0078	0.9	z87	8666547
10000.1465	10000.1396	0.7	z89	11892753
11094.7568	11094.748	0.8	z99	7428167
11986.1885	11986.1826	0.5	z107	47653792
12285.3145	12285.3047	0.8	z110	8374234
12656.4736	12656.4648	0.7	z113	92800448
13055.7139	13055.6992	1.1	z116	13661956
14802.5576	14802.5459	0.8	z134	248860384
1115.7018	1115.7013	0.4	y10	2507047
1202.7339	1202.7333	0.5	y11	8575645
2801.5774	2801.5757	0.6	y26	9452834
2858.5994	2858.5972	0.8	y27	5542910
9197.749	9197.7412	0.8	y82	23974692

Svoluji k zapůjčení této práce pro studijní účely a prosím, aby byla řádně vedena evidence vypůjčovateli.

Jméno a příjmení s adresou	Číslo OP	Datum vypůjčení	Poznámka
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