Photobinding of Triflusal to Human Serum Albumin Investigated by Fluorescence, Proteomic Analysis and Computational Studies.

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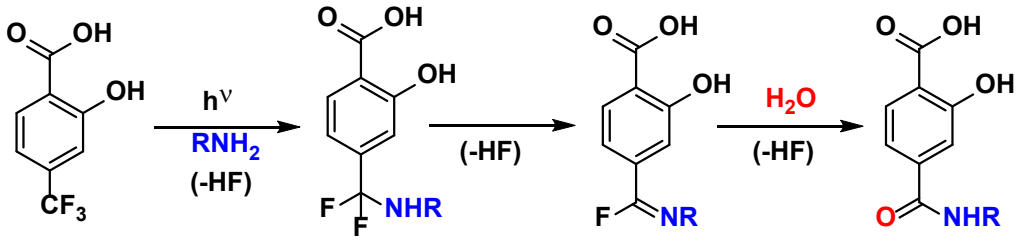
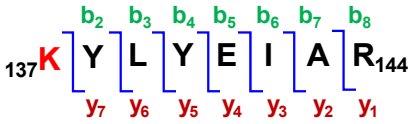
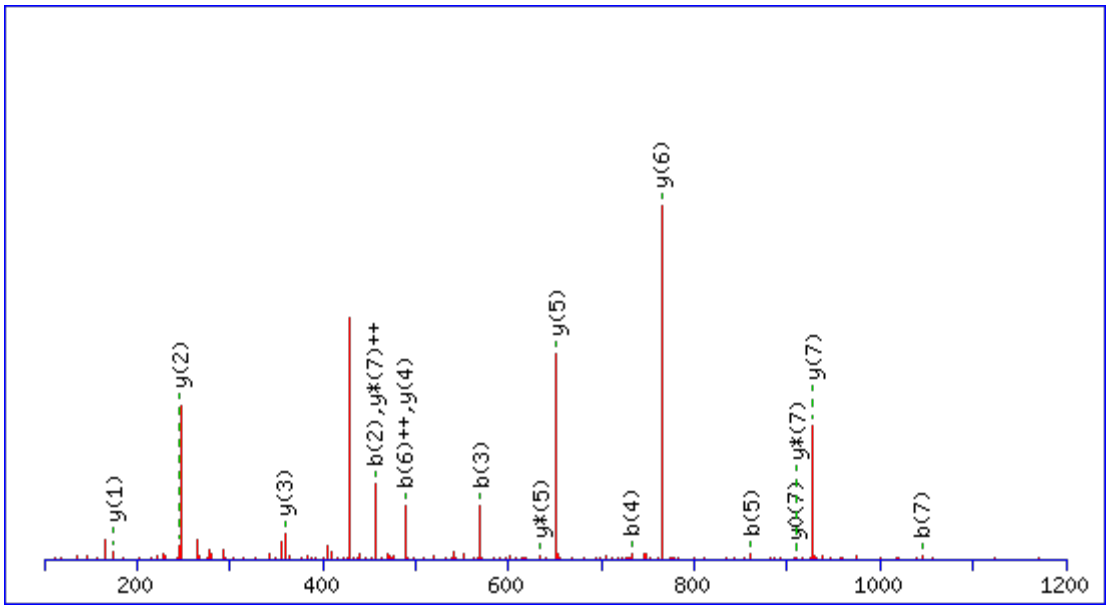
Scheme S1. A plausible mechanism for the photochemical reaction between Lys and HTB.

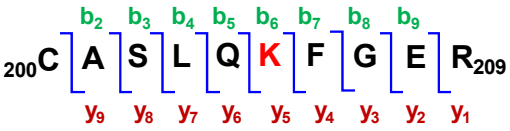


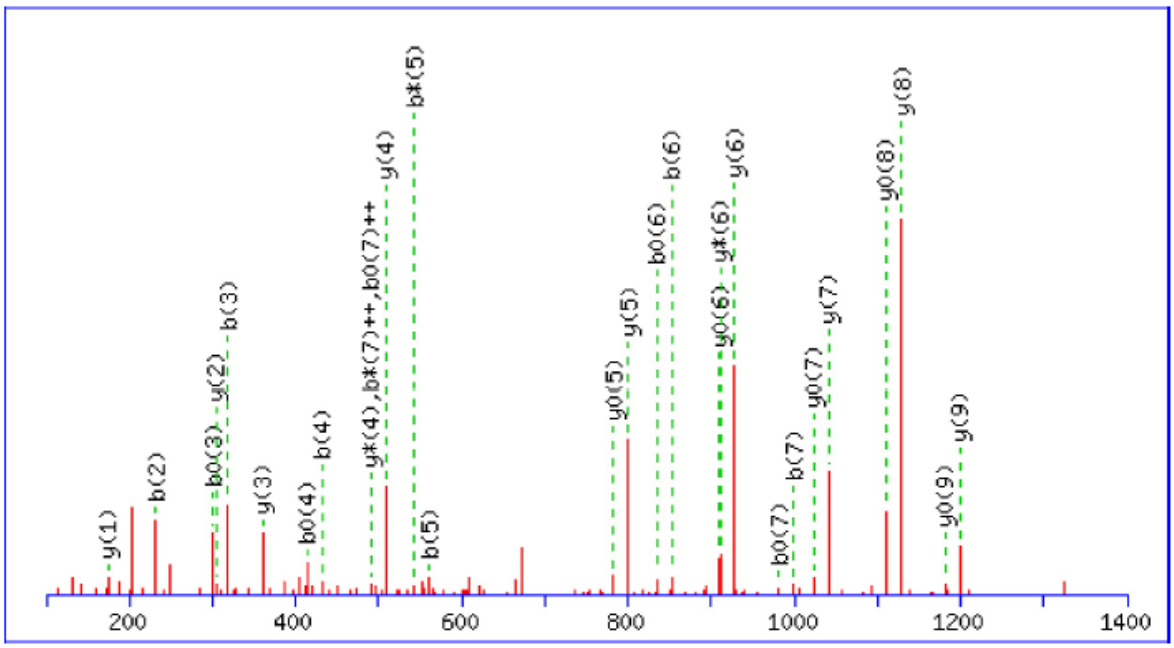




#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	293.1132	147.0602	276.0866	138.5470			K							8
2	**456.1765**	228.5919	439.1500	220.0786			Y	***927.4934***	464.2504	910.4669	455.7371	909.4829	455.2451	7
3	**569.2606**	285.1339	552.2340	276.6207			L	***764.4301***	382.7187	747.4036	374.2054	746.4196	373.7134	6
4	**732.3239**	366.6656	715.2974	358.1523			Y	***651.3461***	326.1767	634.3195	317.6634	633.3355	317.1714	5
5	**861.3665**	431.1869	844.3400	422.6736	843.3559	422.1816	E	***488.2827***	244.6450	471.2562	236.1317	470.2722	235.6397	4
6	974.4506	487.7289	957.4240	479.2157	956.4400	478.7236	I	***359.2401***	180.1237	342.2136	171.6104			3
7	**1045.4877**	523.2475	1028.4611	514.7342	1027.4771	514.2422	A	***246.1561***	123.5817	229.1295	115.0684			2
8							R	***175.1190***	88.0631	158.0924	79.5498			1

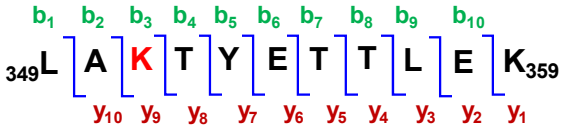
Figure S1. Modified peptide and ESI-MS/MS assigned spectrum of $_{137}$KYLYEIAR$_{144}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.

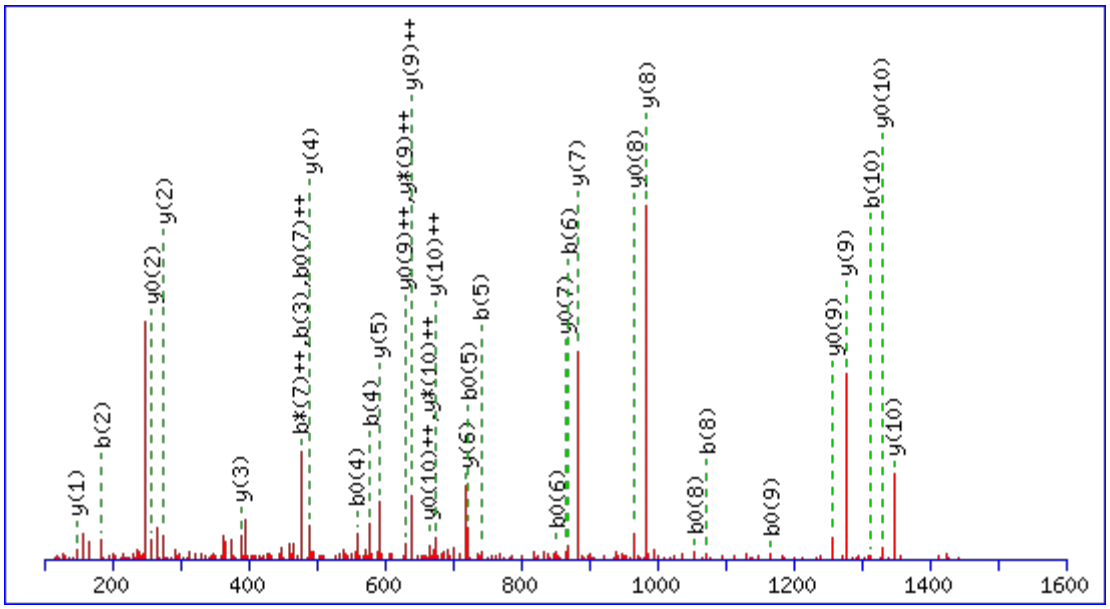




#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	161.0379	81.0226					C							10
2	232.0750	116.5412					A	1199.5691	600.2882	1182.5426	591.7749	1181.5586	591.2829	9
3	319.1071	160.0572			301.0965	151.0519	S	1128.5320	564.7696	1111.5055	556.2564	1110.5215	555.7644	8
4	432.1911	216.5992			414.1806	207.5939	L	1041.5000	521.2536	1024.4734	512.7404	1023.4894	512.2483	7
5	560.2497	280.6285	543.2232	272.1152	542.2391	271.6232	Q	928.4159	464.7116	911.3894	456.1983	910.4054	455.7063	6
6	852.3556	426.6815	835.3291	418.1682	834.3451	417.6762	K	800.3573	400.6823	783.3308	392.1690	782.3468	391.6770	5
7	999.4240	500.2157	982.3975	491.7024	981.4135	491.2104	F	508.2514	254.6293	491.2249	246.1161	490.2409	245.6241	4
8	1056.4455	528.7264	1039.4190	520.2131	1038.4349	519.7211	G	361.1830	181.0951	344.1565	172.5819	343.1724	172.0899	3
9	1185.4881	593.2477	1168.4616	584.7344	1167.4775	584.2424	E	304.1615	152.5844	287.1350	144.0711	286.1510	143.5791	2
10							R	175.1190	88.0631	158.0924	79.5498			1

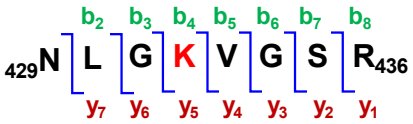
Figure S2. Modified peptide and ESI-MS/MS assigned spectrum of $_{200}$CASLQKFGER$_{209}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.

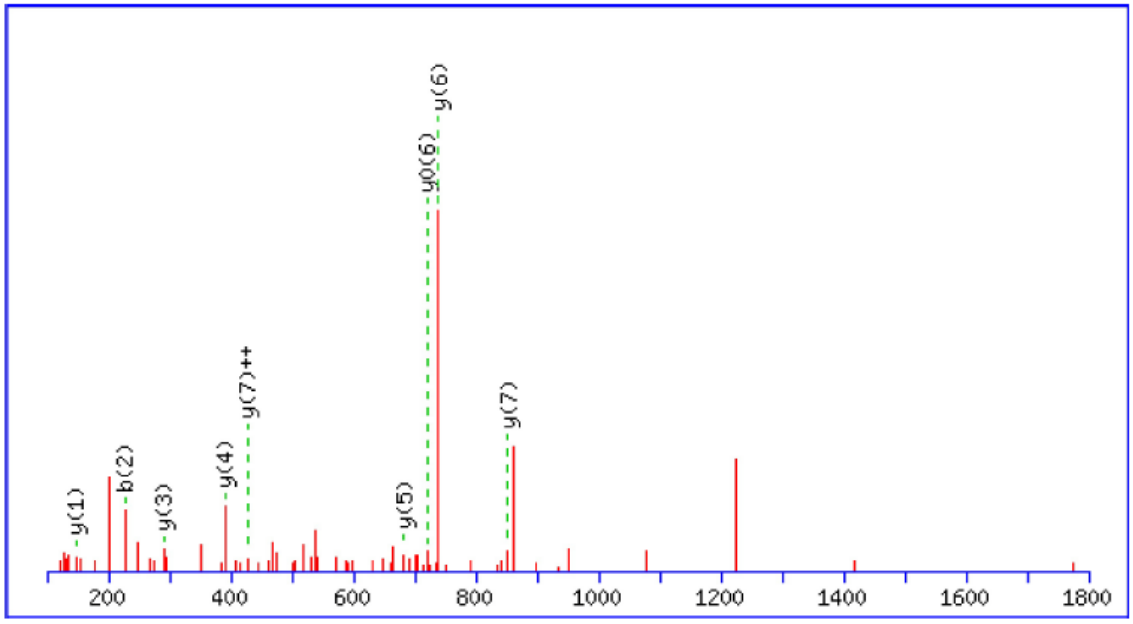




#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	114.0913	57.5493					L							11
2	**185.1285**	93.0679					A	***1347.6315***	674.3194	1330.6049	665.8061	1329.6209	665.3141	10
3	**477.2344**	239.1208	460.2078	230.6076			K	***1276.5943***	638.8008	1259.5678	630.2875	1258.5838	629.7955	9
4	**578.2821**	289.6447	561.2555	281.1314	560.2715	280.6394	T	***984.4884***	492.7478	967.4619	484.2346	966.4779	483.7426	8
5	**741.3454**	371.1763	724.3188	362.6631	723.3348	362.1710	Y	***883.4407***	442.2240	866.4142	433.7107	865.4302	433.2187	7
6	**870.3880**	435.6976	853.3614	427.1844	852.3774	426.6923	E	***720.3774***	360.6923	703.3509	352.1791	702.3668	351.6871	6
7	971.4357	486.2215	954.4091	477.7082	953.4251	477.2162	T	***591.3348***	296.1710	574.3083	287.6578	573.3243	287.1658	5
8	**1072.4833**	536.7453	1055.4568	528.2320	1054.4728	527.7400	T	***490.2871***	245.6472	473.2606	237.1339	472.2766	236.6419	4
9	1185.5674	593.2873	1168.5408	584.7741	1167.5568	584.2821	L	***389.2395***	195.1234	372.2129	186.6101	371.2289	186.1181	3
10	**1314.6100**	657.8086	1297.5834	649.2954	1296.5994	648.8034	E	***276.1554***	138.5813	259.1288	130.0681	258.1448	129.5761	2
11							K	***147.1128***	74.0600	130.0863	65.5468			1

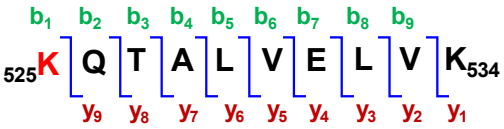
Figure S3. Modified peptide and ESI-MS/MS assigned spectrum of $_{349}$LAKTYETTLEK$_{359}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.

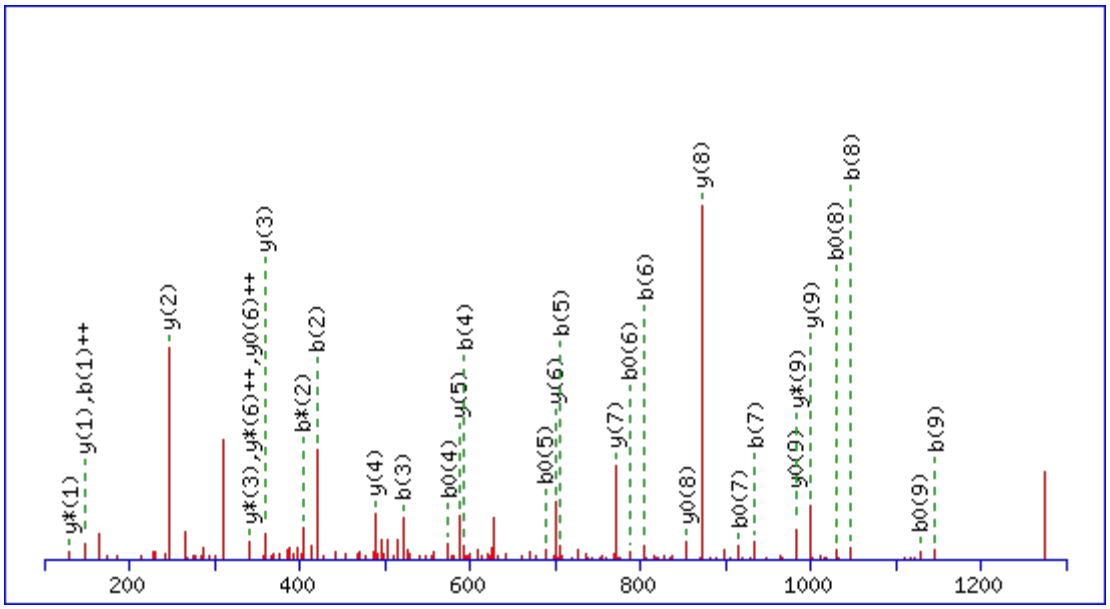




#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	115.0502	58.0287	98.0237	49.5155			N							8
2	228.1343	114.5708	211.1077	106.0575			L	*852.4462*	426.7267	835.4196	418.2134	834.4356	417.7214	7
3	285.1557	143.0815	268.1292	134.5682			G	*739.3621*	370.1847	722.3355	361.6714	721.3515	361.1794	6
4	577.2617	289.1345	560.2351	280.6212			K	*682.3406*	341.6740	665.3141	333.1607	664.3301	332.6687	5
5	676.3301	338.6687	659.3035	330.1554			V	*390.2347*	195.6210	373.2082	187.1077	372.2241	186.6157	4
6	733.3515	367.1794	716.3250	358.6661			G	*291.1663*	146.0868	274.1397	137.5735	273.1557	137.0815	3
7	820.3836	410.6954	803.3570	402.1821	802.3730	401.6901	S	234.1448	117.5761	217.1183	109.0628	216.1343	108.5708	2
8							K	*147.1128*	74.0600	130.0863	65.5468			1

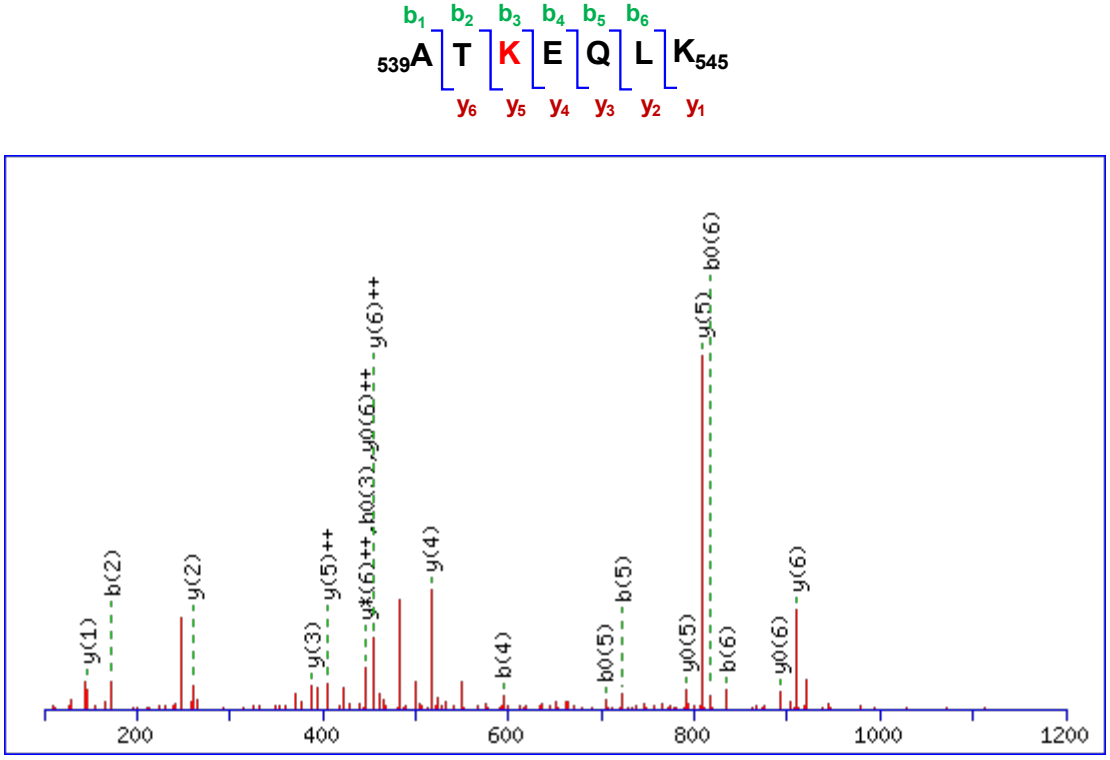
Figure S4. Modified peptide and ESI-MS/MS assigned spectrum of $_{429}$NLGKVGSR$_{436}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.





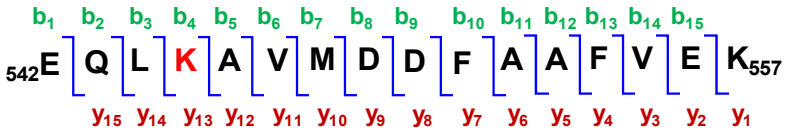
#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	293.1132	147.0602	276.0866	138.5470			K							10
2	**421.1718**	211.0895	404.1452	202.5763			Q	***1000.6037***	500.8055	983.5772	492.2922	982.5932	491.8002	9
3	**522.2195**	261.6134	505.1929	253.1001	504.2089	252.6081	T	***872.5451***	436.7762	855.5186	428.2629	854.5346	427.7709	8
4	**593.2566**	297.1319	576.2300	288.6186	575.2460	288.1266	A	***771.4975***	386.2524	754.4709	377.7391	753.4869	377.2471	7
5	**706.3406**	353.6740	689.3141	345.1607	688.3301	344.6687	L	***700.4604***	350.7338	683.4338	342.2205	682.4498	341.7285	6
6	**805.4090**	403.2082	788.3825	394.6949	787.3985	394.2029	V	***587.3763***	294.1918	570.3497	285.6785	569.3657	285.1865	5
7	**934.4516**	467.7295	917.4251	459.2162	916.4411	458.7242	E	***488.3079***	244.6576	471.2813	236.1443	470.2973	235.6523	4
8	**1047.5357**	524.2715	1030.5092	515.7582	1029.5251	515.2662	L	***359.2653***	180.1363	342.2387	171.6230			3
9	**1146.6041**	573.8057	1129.5776	565.2924	1128.5936	564.8004	V	***246.1812***	123.5942	229.1547	115.0810			2
10							K	***147.1128***	74.0600	130.0863	65.5468			1

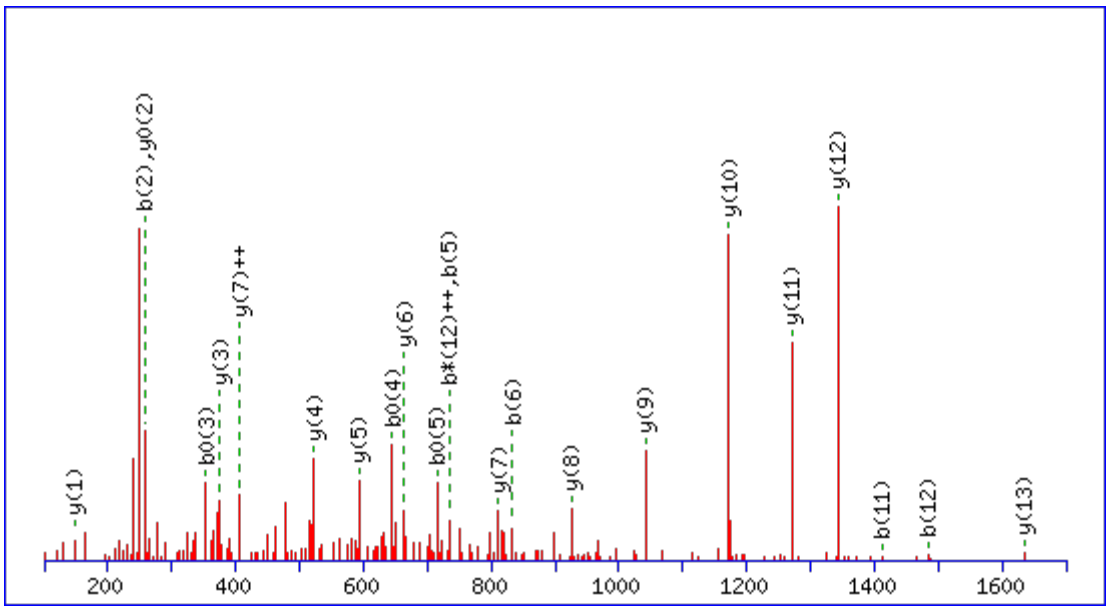
Figure S5. Modified peptide and ESI-MS/MS assigned spectrum of $_{525}$KQTALVELVK$_{534}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.



#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	72.0444	36.5258					A							7
2	**173.0921**	87.0497			155.0815	78.0444	T	***910.4516***	455.7295	893.4251	447.2162	892.4411	446.7242	6
3	465.1980	233.1026	448.1714	224.5894	447.1874	224.0974	K	***809.4040***	405.2056	792.3774	396.6923	791.3934	396.2003	5
4	**594.2406**	297.6239	577.2140	289.1107	576.2300	288.6186	E	***517.2980***	259.1527	500.2715	250.6394	499.2875	250.1474	4
5	**722.2992**	361.6532	705.2726	353.1399	704.2886	352.6479	Q	***388.2554***	194.6314	371.2289	186.1181			3
6	**835.3832**	418.1953	818.3567	409.6820	817.3727	409.1900	L	***260.1969***	130.6021	243.1703	122.0888			2
7							K	***147.1128***	74.0600	130.0863	65.5468			1

Figure S6. Modified peptide and ESI-MS/MS assigned spectrum of $_{539}$ATKEQLK$_{545}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.





#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	130.0499	65.5286			112.0393	56.5233	E							16
2	**258.1084**	129.5579	241.0819	121.0446	240.0979	120.5526	Q	1875.8833	938.4453	1858.8568	929.9320	1857.8728	929.4400	15
3	371.1925	186.0999	354.1660	177.5866	353.1819	177.0946	L	1747.8248	874.4160	1730.7982	865.9027	1729.8142	865.4107	14
4	663.2984	332.1529	646.2719	323.6396	645.2879	323.1476	K	***1634.7407***	817.8740	1617.7141	809.3607	1616.7301	808.8687	13
5	**734.3355**	367.6714	717.3090	359.1581	716.3250	358.6661	A	***1342.6348***	671.8210	1325.6082	663.3077	1324.6242	662.8157	12
6	**833.4040**	417.2056	816.3774	408.6923	815.3934	408.2003	V	***1271.5977***	636.3025	1254.5711	627.7892	1253.5871	627.2972	11
7	964.4444	482.7259	947.4179	474.2126	946.4339	473.7206	M	***1172.5292***	586.7683	1155.5027	578.2550	1154.5187	577.7630	10
8	1079.4714	540.2393	1062.4448	531.7261	1061.4608	531.2341	D	***1041.4888***	521.2480	1024.4622	512.7347	1023.4782	512.2427	9
9	1194.4983	597.7528	1177.4718	589.2395	1176.4878	588.7475	D	***926.4618***	463.7345	909.4353	455.2213	908.4512	454.7293	8
10	1341.5667	671.2870	1324.5402	662.7737	1323.5562	662.2817	F	***811.4349***	406.2211	794.4083	397.7078	793.4243	397.2158	7
11	**1412.6039**	706.8056	1395.5773	698.2923	1394.5933	697.8003	A	***664.3665***	332.6869	647.3399	324.1736	646.3559	323.6816	6
12	**1483.6410**	742.3241	1466.6144	733.8109	1465.6304	733.3188	A	***593.3293***	297.1683	576.3028	288.6550	575.3188	288.1630	5
13	1630.7094	815.8583	1613.6828	807.3451	1612.6988	806.8530	F	***522.2922***	261.6498	505.2657	253.1365	504.2817	252.6445	4
14	1729.7778	865.3925	1712.7513	856.8793	1711.7672	856.3873	V	***375.2238***	188.1155	358.1973	179.6023	357.2132	179.1103	3
15	1858.8204	929.9138	1841.7938	921.4006	1840.8098	920.9086	E	276.1554	138.5813	259.1288	130.0681	258.1448	129.5761	2
16							K	***147.1128***	74.0600	130.0863	65.5468			1

Figure S7. Modified peptide and ESI-MS/MS assigned spectrum of $_{542}$EQLKAVMDDFAAFVEK$_{557}$. For clarity, the amino acid numbering used corresponds to the provided in PDB structures as the first 24 amino acids are usually not observed.

$_{198}$L**K**CASLQK$_{205}$

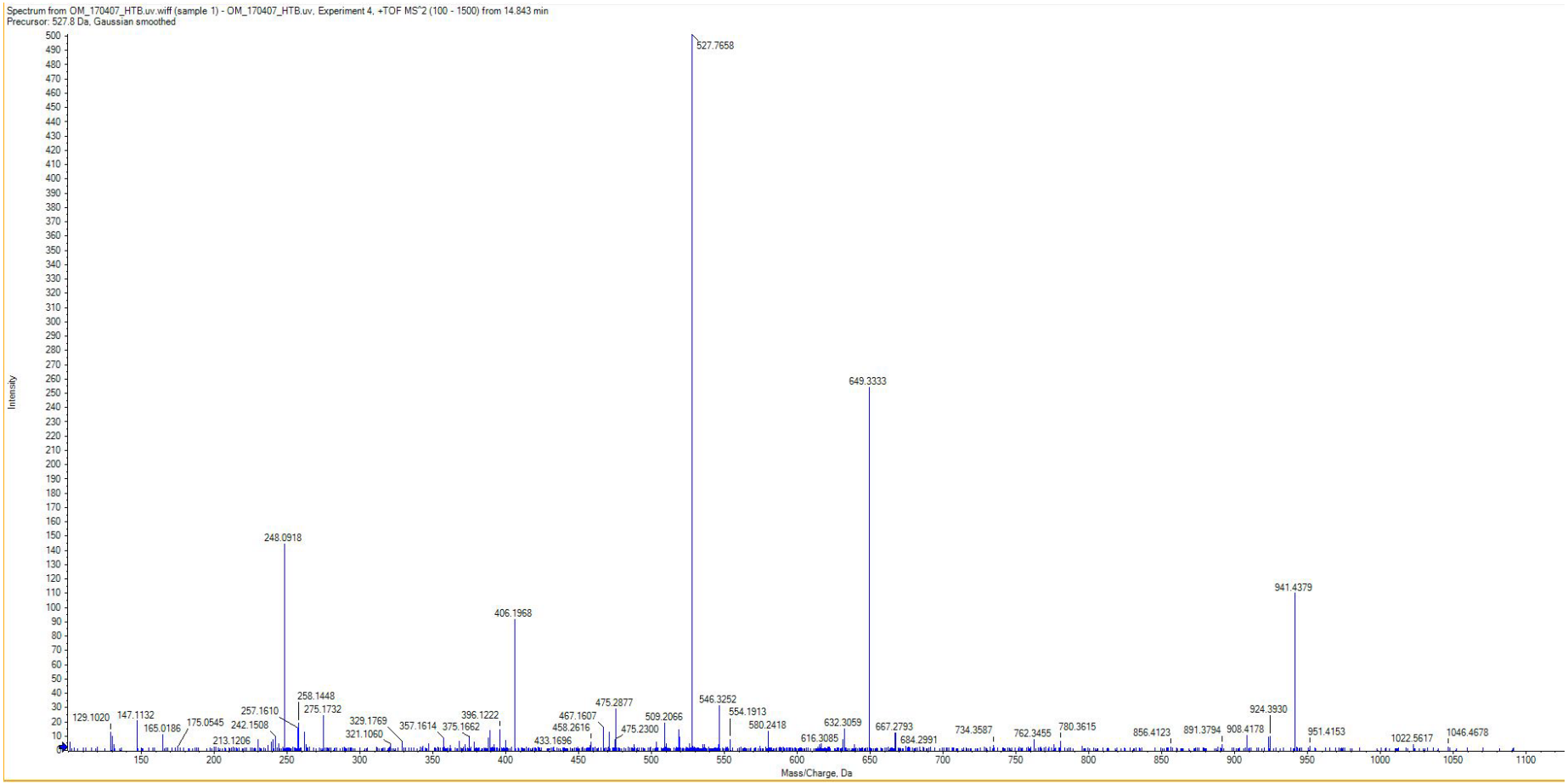


Figure S8. Original ESI-HRMS/MS spectrum of the modified peptide $_{198}$L**K**CASLQK$_{205}$

$_{137}$**K**YLYEIAR$_{144}$

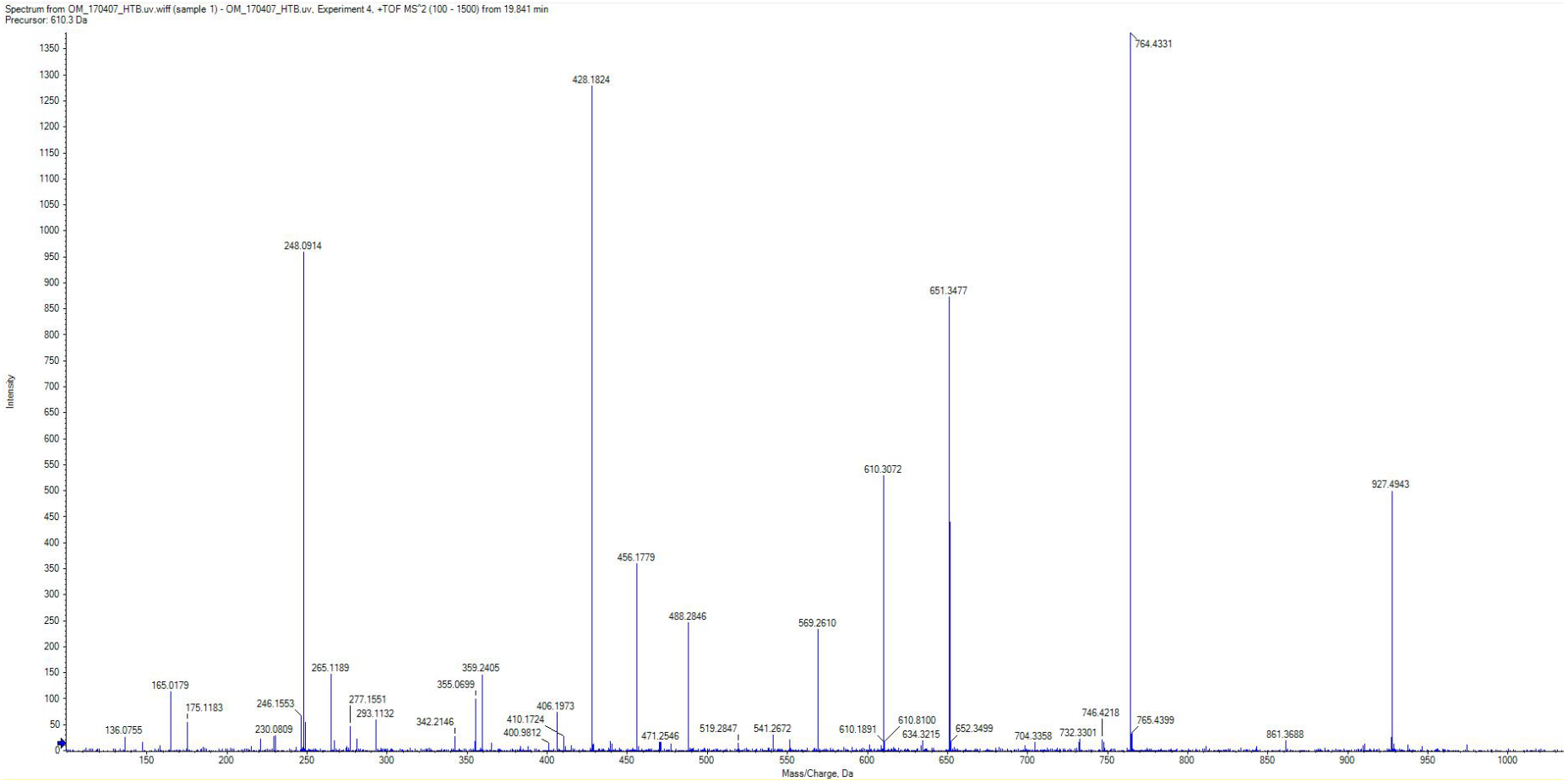


Figure S9. Original ESI-HRMS/MS spectrum of the modified peptide $_{137}$**K**YLYEIAR$_{144}$

$_{200}$CASLQ**K**FGER$_{209}$

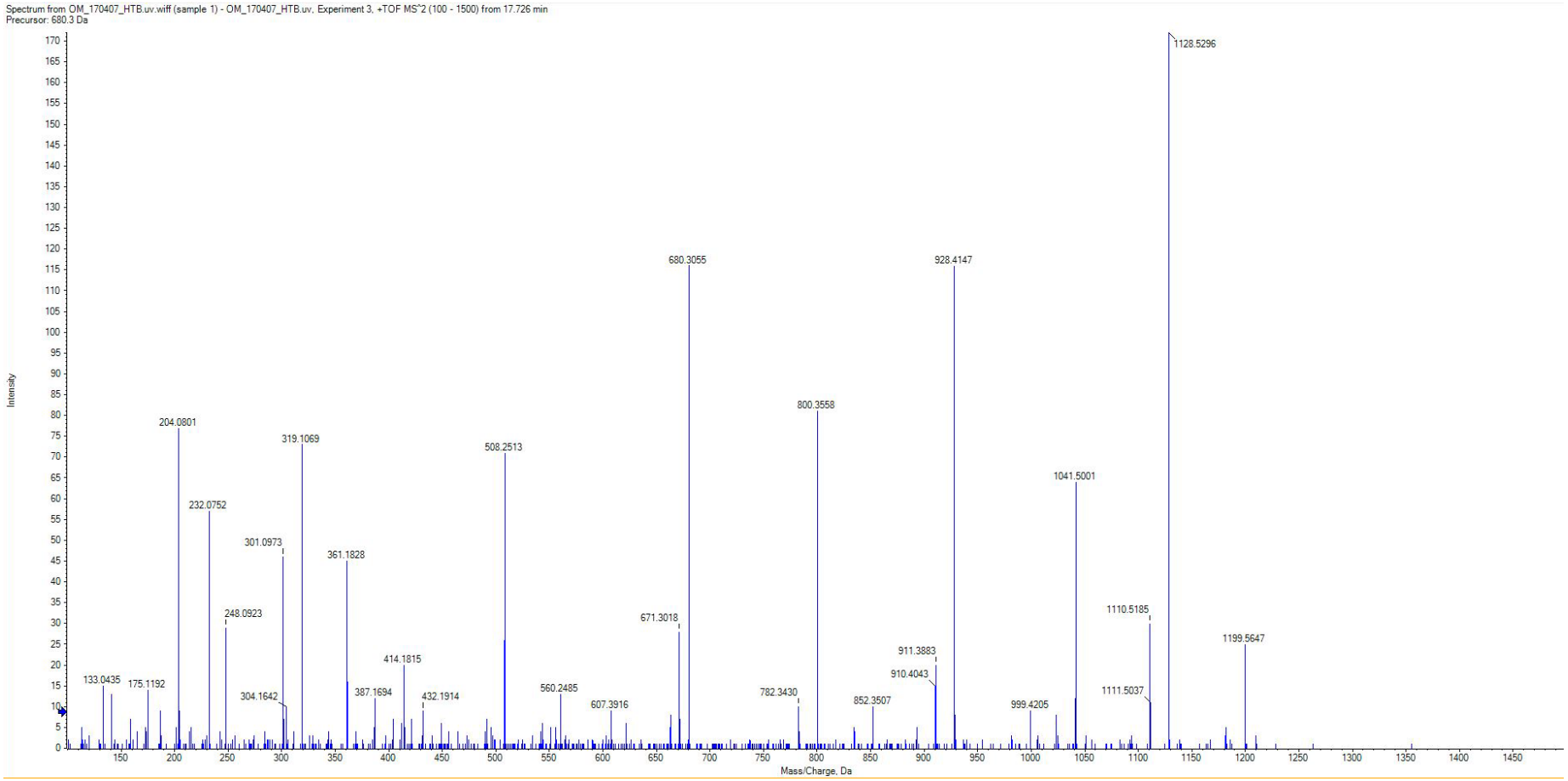


Figure S10. Original ESI-HRMS/MS spectrum of the modified peptide $_{200}$CASLQ**K**FGER$_{209}$

$_{349}$LA**K**TYETTLEK$_{359}$

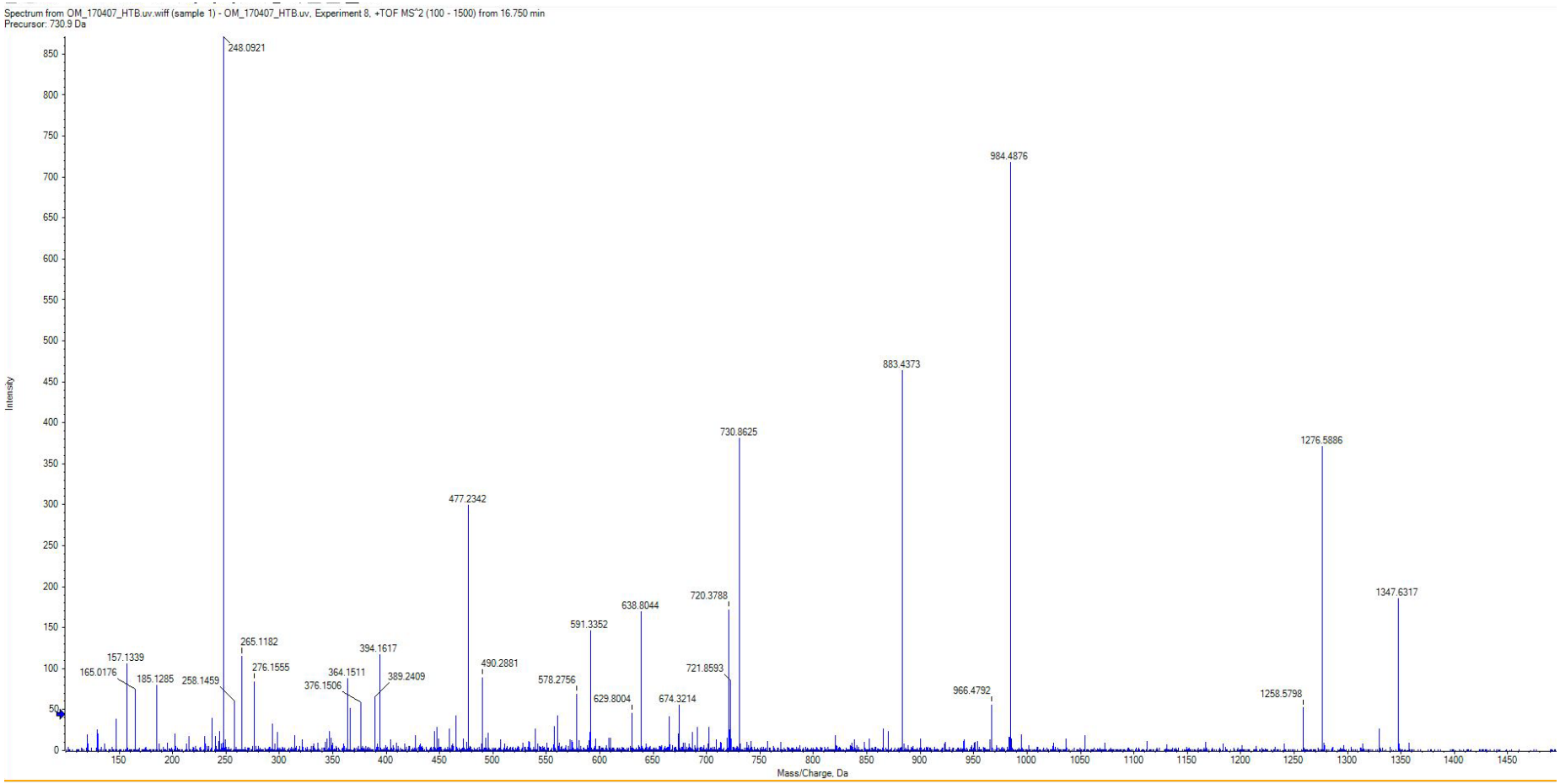


Figure S11. Original ESI-HRMS/MS spectrum of the modified peptide $_{349}$LA**K**TYETTLEK$_{359}$

$_{429}$NLG**K**VGSR$_{436}$

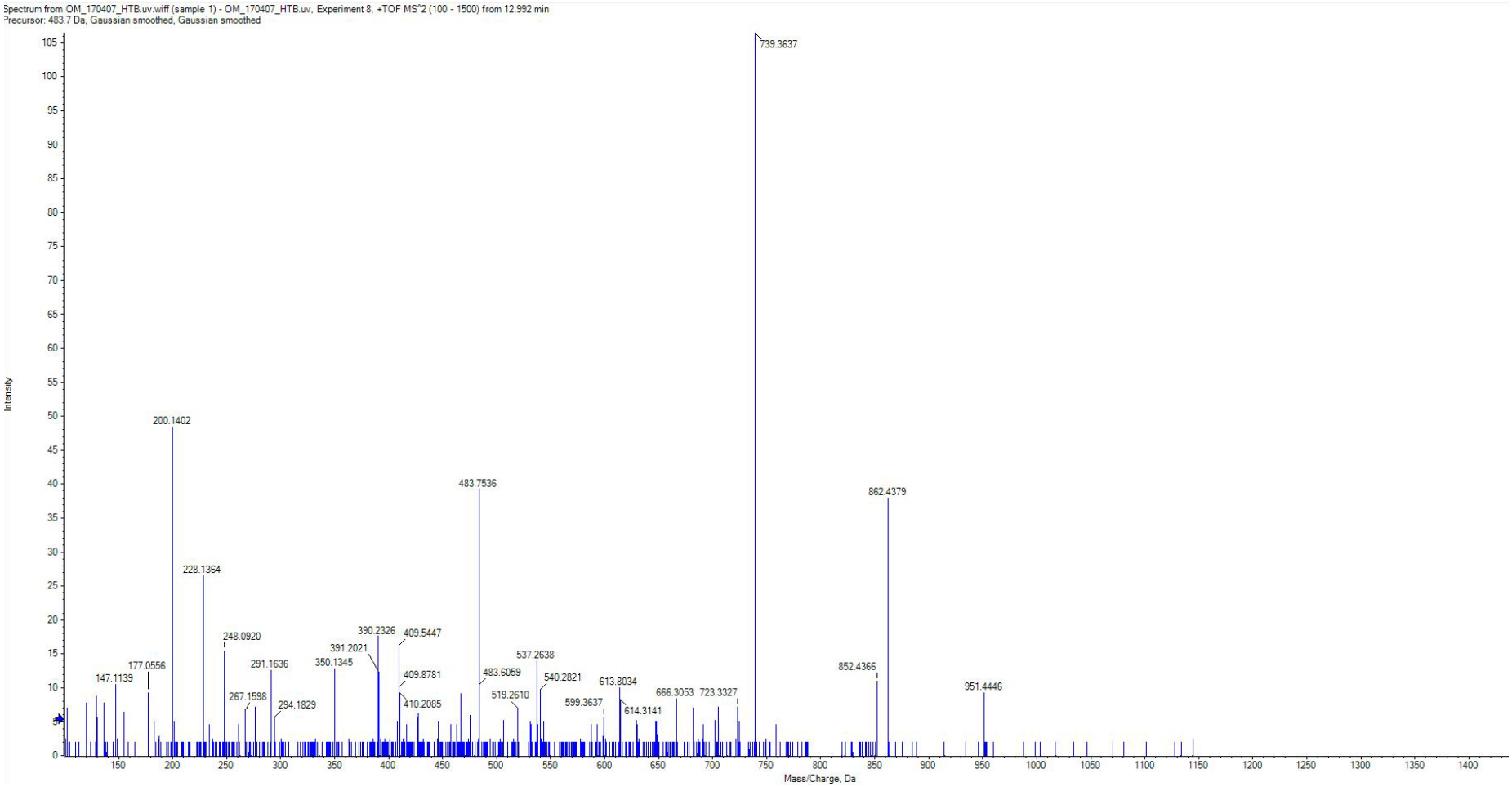


Figure S12. Original ESI-HRMS/MS spectrum of the modified peptide $_{429}$NLG**K**VGSR$_{436}$

$_{525}$**K**QTALVELVK$_{534}$

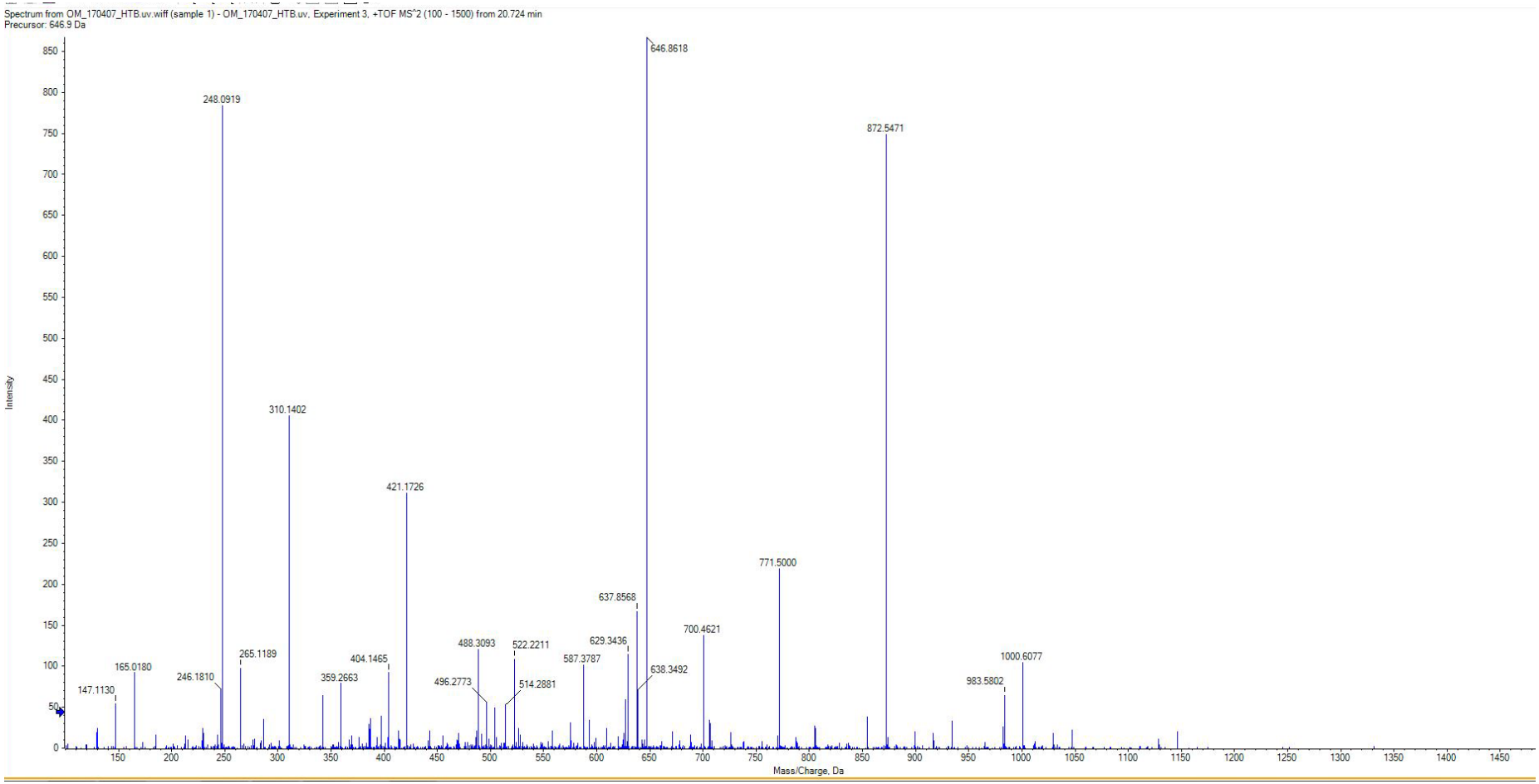


Figure S13. Original ESI-HRMS/MS spectrum of the modified peptide $_{525}$**K**QTALVELVK$_{534}$

$_{539}$AT**K**EQLK$_{545}$

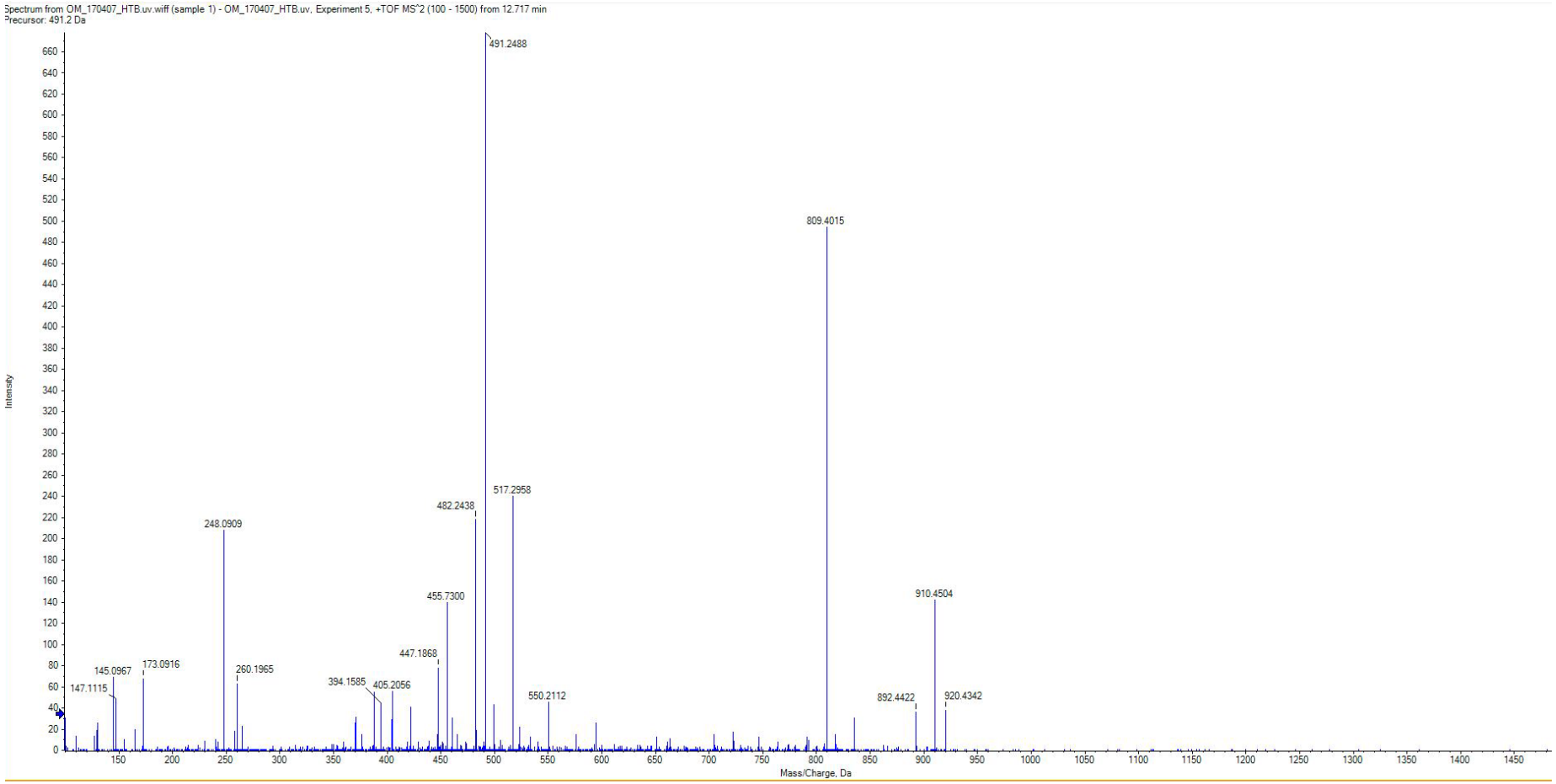


Figure S14. Original ESI-HRMS/MS spectrum of the modified peptide $_{539}$AT**K**EQLK$_{545}$

$_{542}$EQL**K**AVMDDFAAFVEK$_{557}$

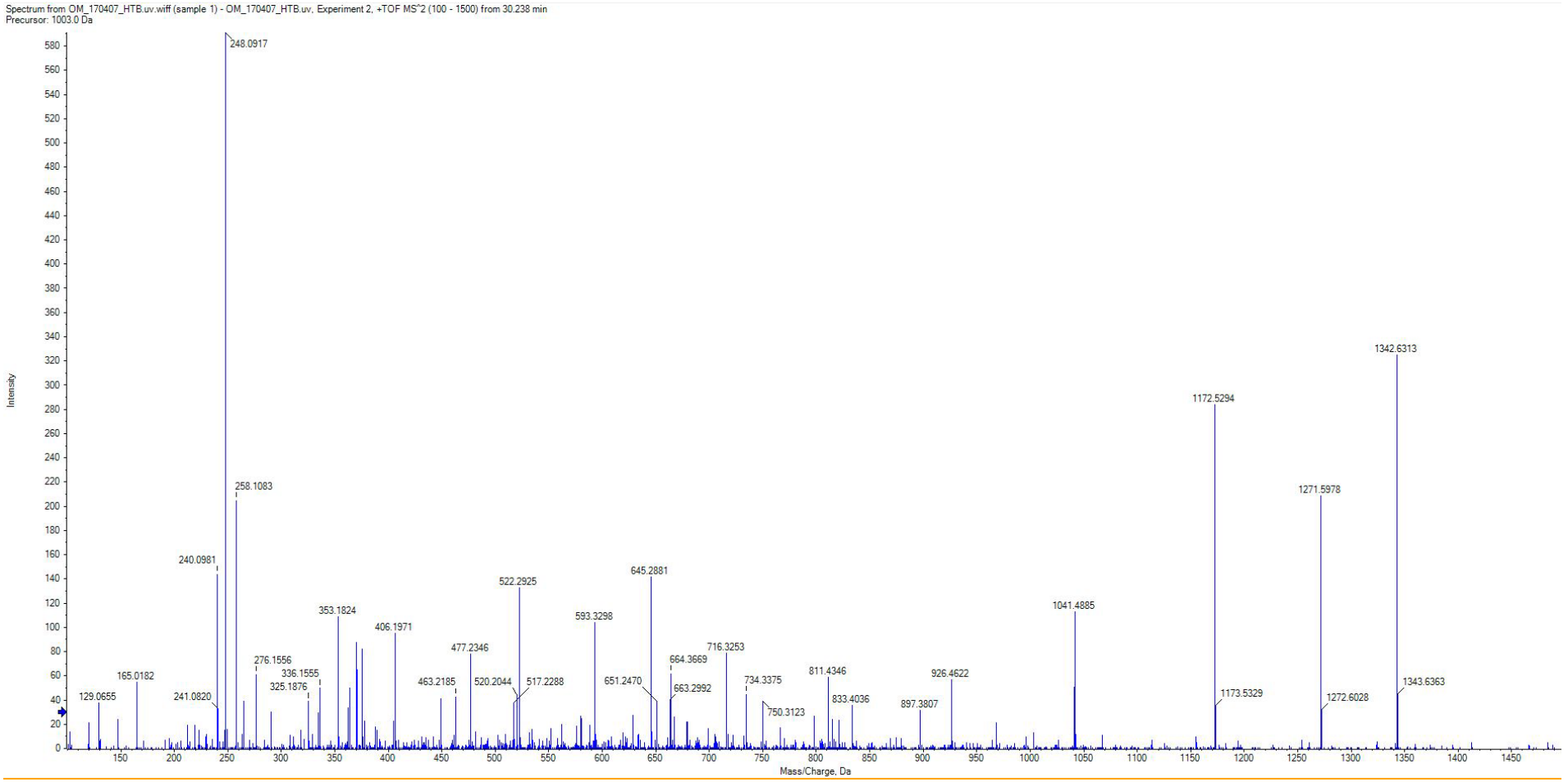


Figure S15. Original ESI-HRMS/MS spectrum of the modified peptide $_{542}$EQL**K**AVMDDFAAFVEK$_{557}$

Table S1. List of ions detected for $_{198}$L**K**CASLQK$_{205}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
101.06819	0.02909	5.80116	0.01986	0.00402	25159.08309	0	Yes	*100.0604	*101.0682
120.07944	0.00941	2.39365	0.02474	0.00358	33574.84884	0	Yes	*119.0716	*120.0794
129.06402	0.00976	2.39365	0.02244	0.00371	34808.29306	0	Yes	*128.0562	*129.0640
129.10202	0.14311	12.68534	0.0513	0.01182	10925.78652	0	Yes	*128.0942	*129.1020
130.08519	0.09468	10.11586	0.06115	0.00761	17084.01505	0	Yes	*129.0774	*130.0852
131.11923	0.02295	3.98942	0.03555	0.00374	35081.85473	2	Yes	*260.2228 (2)	*131.1192 (2)
147.11318	0.22568	20.68788	0.0445	0.00975	15091.14779	0	Yes	*146.1053	*147.1132
165.01861	0.16915	11.19782	0.058	0.01519	10862.73496	0	Yes	*164.0108	*165.0186
173.09121	0.0226	2.0277	0.04084	0.01114	15536.71578	0	Yes	*172.0834	*173.0912
175.05453	0.03409	2.61015	0.04481	0.01785	9804.35467	0	Yes	*174.0467	*175.0545
200.13577	0.01215	2.39365	0.03194	0.00462	43345.56014	0	Yes	*199.1279	*200.1358
201.12707	0.02436	2.39446	0.04002	0.01263	15921.18608	0	Yes	*200.1192	*201.1271
203.10497	0.02448	2.0277	0.04022	0.01207	16829.92656	0	Yes	*202.0971	*203.1050
213.12058	0.0209	2.60962	0.03296	0.00796	26774.82789	0	Yes	*212.1128	*213.1206
222.1298	0.03413	2.0277	0.05047	0.0207	10729.39564	0	Yes	*221.1220	*222.1298
230.0839	0.09118	7.72141	0.06849	0.00714	32213.75175	1	Yes	*229.0761 (1)	*230.0839 (1)
231.09234	0.04352	2.0277	0.06864	0.03794	6091.08489	1	No	230.0845 (1)	231.0923 (1)
237.13324	0.03086	3.98996	0.04346	0.00519	45659.45915	0	Yes	*236.1254	*237.1332
239.14758	0.09739	6.1259	0.08292	0.0128	18677.13642	0	Yes	*238.1398	*239.1476
240.13435	0.10203	7.93737	0.05248	0.00986	24352.59644	0	Yes	*239.1265	*240.1343
242.15083	0.13809	9.59911	0.05709	0.01186	20417.73659	0	Yes	*241.1430	*242.1508
244.07548	0.07603	4.63785	0.07495	0.01348	18112.82206	1	Yes	*243.0677 (1)	*244.0755 (1)
247.31324	0.02701	2.39365	0.04882	0.01845	13407.10701	1	Yes	*246.3054 (1)	*247.3132 (1)
248.09177	2.5475	144.89318	0.09779	0.01547	16041.77856	0	Yes	*247.0839	*248.0918
254.14667	0.04107	2.39365	0.05849	0.02683	9472.15496	1	Yes	*253.1388 (1)	*254.1467 (1)
257.16099	0.27084	15.94339	0.06336	0.01645	15635.32342	0	Yes	*256.1532	*257.1610
258.14482	0.30355	19.17827	0.06348	0.01457	17717.36058	1	Yes	*257.1370 (1)	*258.1448 (1)
262.0864	0.18537	12.684	0.05939	0.01085	24158.4675	1	Yes	*261.0786 (1)	*262.0864 (1)
263.09995	0.05572	4.20592	0.05493	0.0194	13560.06387	1	No	262.0921 (1)	263.1000 (1)
265.1173	0.06525	2.82638	0.05514	0.03008	8812.29556	0	Yes	*264.1095	*265.1173
272.16395	0.06612	2.02823	0.07914	0.04619	5892.19234	0	Yes	*271.1561	*272.1639
275.17323	0.45111	24.78823	0.09831	0.0132	20848.75392	1	Yes	*274.1654 (1)	*275.1732 (1)
289.19774	0.02434	2.60962	0.04319	0.00927	31189.679	0	Yes	*288.1899	*289.1977
293.11066	0.04901	2.02823	0.06281	0.02861	10244.61579	2	Yes	*584.2057 (2)	*293.1107 (2)
311.17782	0.04545	2.60962	0.0896	0.05865	5305.79187	1	Yes	*310.1700 (1)	*311.1778 (1)
312.15325	0.04046	2.0277	0.05983	0.02454	12719.178	1	No	311.1454 (1)	312.1532 (1)
320.17078	0.02561	2.39419	0.05049	0.01448	22111.40542	0	Yes	*319.1629	*320.1708
321.10597	0.08207	4.5304	0.06574	0.01535	20920.3068	0	Yes	*320.0981	*321.1060
329.17693	0.19736	6.12724	0.1024	0.03933	8370.39219	1	Yes	*328.1691 (1)	*329.1769 (1)
341.17571	0.01586	2.39365	0.0417	0.00603	56594.38526	0	Yes	*340.1679	*341.1757
343.16718	0.03182	2.7176	0.04705	0.01116	30736.11606	0	Yes	*342.1594	*343.1672
347.17483	0.10667	4.85328	0.08413	0.01446	24009.07958	0	Yes	*346.1670	*347.1748
353.2236	0.04842	2.61069	0.06364	0.02402	14705.92523	1	Yes	*352.2158 (1)	*353.2236 (1)
357.16137	0.28673	9.12731	0.08533	0.02379	15015.97428	1	Yes	*356.1535 (1)	*357.1614 (1)
358.17172	0.01625	2.39365	0.04273	0.00618	57986.92779	1	No	357.1639 (1)	358.1717 (1)
362.12899	0.04903	3.98996	0.06444	0.00642	56424.10274	0	Yes	*361.1212	*362.1290
368.13326	0.13182	6.12644	0.08663	0.02459	14972.0563	1	Yes	*367.1254 (1)	*368.1333 (1)
371.21694	0.02758	2.39419	0.05437	0.01559	23808.79781	3	No	1110.6273 (3)	371.2169 (3)
372.12129	0.03865	3.98942	0.07077	0.0063	59106.20454	0	Yes	*371.1135	*372.1213
375.16623	0.27169	9.4938	0.09839	0.02522	14875.76579	1	Yes	*374.1584 (1)	*375.1662 (1)
376.19414	0.02776	2.39365	0.06021	0.02117	17771.81955	1	No	375.1863 (1)	376.1941 (1)
378.2049	0.13361	6.12644	0.08232	0.02162	17496.6941	0	Yes	*377.1971	*378.2049

388.25705	0.31587	8.91242	0.10009	0.033	11765.25397	1	Yes	*387.2492 (1)	*388.2570 (1)
389.1719	0.37836	14.24097	0.08907	0.02619	14859.65088	1	Yes	*388.1641 (1)	*389.1719 (1)
390.14663	0.03392	2.0277	0.04459	0.01673	23325.80711	2	Yes	*778.2776 (2)	*390.1466 (2)
390.6875	0.01697	2.39365	0.04462	0.00645	60561.89932	0	Yes	*389.6797	*390.6875
392.19726	0.08504	4.3139	0.07265	0.02119	18511.80967	2	Yes	*782.3789 (2)	*392.1973 (2)
396.12224	0.31335	14.66996	0.08425	0.01837	21558.61604	1	Yes	*395.1144 (1)	*396.1222 (1)
400.22173	0.06299	7.18096	0.07339	0.00653	61297.27889	0	Yes	*399.2139	*400.2217
404.15295	0.02877	2.60962	0.05106	0.01096	36871.29263	0	Yes	*403.1451	*404.1529
406.0942	0.02884	2.60962	0.05118	0.01099	36959.62189	0	Yes	*405.0864	*406.0942
406.1968	2.1289	91.58046	0.10238	0.02016	20149.18765	0	Yes	*405.1890	*406.1968
414.17872	0.01748	2.39365	0.04595	0.00664	62356.0786	0	Yes	*413.1709	*414.1787
422.23497	0.01765	2.39365	0.04639	0.00671	62959.61458	3	Yes	*1263.6814 (3)	*422.2350 (3)
424.13038	0.04716	2.02823	0.06393	0.02325	18242.94615	0	Yes	*423.1225	*424.1304
433.1696	0.05362	2.61015	0.07635	0.03247	13339.87893	0	Yes	*432.1618	*433.1696
449.15263	0.0546	2.60962	0.10765	0.06448	6965.58672	1	Yes	*448.1448 (1)	*449.1526 (1)
452.69859	0.01827	2.39365	0.04803	0.00694	65191.31421	0	Yes	*451.6908	*452.6986
457.22361	0.04897	2.0277	0.08448	0.04177	10946.50148	0	Yes	*456.2158	*457.2236
458.20314	0.03064	3.98942	0.04228	0.00699	65586.46599	0	Yes	*457.1953	*458.2031
458.2616	0.11643	6.1259	0.08458	0.01159	39531.27793	0	Yes	*457.2538	*458.2616
461.1823	0.03074	2.60962	0.05454	0.01171	39386.79691	0	Yes	*460.1745	*461.1823
467.16067	0.4331	15.94366	0.10369	0.0269	17364.97708	1	Yes	*466.1528 (1)	*467.1607 (1)
470.25848	0.03104	2.39419	0.05508	0.01755	26797.44286	0	Yes	*469.2506	*470.2585
471.22806	0.31692	13.0521	0.08576	0.02461	19149.48634	0	Yes	*470.2202	*471.2281
474.2622	0.04987	2.0277	0.07375	0.03025	15677.69125	2	No	946.5087 (2)	474.2622 (2)
475.22999	0.16369	7.93898	0.06152	0.01714	27719.92024	0	Yes	*474.2222	*475.2300
475.28775	0.84417	29.17265	0.10459	0.02804	16948.00144	0	Yes	*474.2799	*475.2877
484.24806	0.0189	2.39365	0.04968	0.00718	67424.74317	0	Yes	*483.2402	*484.2481
487.75936	0.05058	2.0277	0.07479	0.03068	15899.29646	2	Yes	*973.5031 (2)	*487.7594 (2)
488.25558	0.0759	4.3139	0.06859	0.01484	32899.82541	2	No	974.4955 (2)	488.2556 (2)
499.28509	0.08315	2.61042	0.08828	0.04475	11157.009	0	Yes	*498.2773	*499.2851
503.22901	0.19907	5.91074	0.12661	0.02703	18617.35917	1	Yes	*502.2212 (1)	*503.2290 (1)
509.20662	0.68472	19.50383	0.12736	0.02836	17956.04086	1	Yes	*508.1988 (1)	*509.2066 (1)
509.85887	0.01939	2.39365	0.05098	0.00737	69184.76821	0	Yes	*508.8510	*509.8589
510.26548	0.0776	4.52933	0.07012	0.01404	36330.98939	0	Yes	*509.2577	*510.2655
517.22122	0.03255	2.39419	0.06418	0.0184	28103.72456	1	Yes	*516.2134 (1)	*517.2212 (1)
518.76032	0.2608	14.86169	0.10927	0.01291	40192.90798	2	Yes	*1035.5050 (2)	*518.7603 (2)
519.25473	0.19569	9.27597	0.07717	0.01978	26251.35034	2	No	1036.4938 (2)	519.2547 (2)
523.78651	0.01965	2.39365	0.05167	0.00747	70123.36176	0	Yes	*522.7787	*523.7865
526.08305	0.09262	4.42215	0.07767	0.0236	22289.26949	3	Yes	*1575.2257 (3)	*526.0831 (3)
526.19304	0.0598	2.60962	0.10358	0.05685	9255.96644	3	Yes	*1575.5556 (3)	*526.1930 (3)
527.51722	0.11835	2.39365	0.12315	0.08403	6278.01679	2	No	1053.0188 (2)	527.5172 (2)
527.61446	0.05988	3.98996	0.07779	0.00775	68107.30461	3	Yes	*1579.8199 (3)	*527.6145 (3)
527.70035	0.03288	2.60962	0.03241	0.01287	41014.03469	0	Yes	*526.6925	*527.7003
527.76584	15.42373	500.92914	0.17505	0.02848	18532.42412	0	Yes	*526.7580	*527.7658
527.94512	0.07893	2.60962	0.11023	0.05694	9271.44544	3	No	1580.8119 (3)	527.9451 (3)
528.28357	0.13159	2.82612	0.12324	0.07651	6904.97308	3	No	1581.8272 (3)	528.2836 (3)
529.30096	0.08562	2.39419	0.11037	0.06281	8426.62497	1	Yes	*528.2931 (1)	*529.3010 (1)
535.22379	0.0596	4.20539	0.07182	0.0104	51449.40926	0	Yes	*534.2160	*535.2238
536.1767	0.14512	4.31417	0.09148	0.03794	14132.00261	1	Yes	*535.1689 (1)	*536.1767 (1)
539.27213	0.03324	2.39365	0.07864	0.0319	16906.489	0	Yes	*538.2643	*539.2721
546.26522	0.05352	4.20592	0.03957	0.01547	35319.10798	0	Yes	*545.2574	*546.2652
546.32523	1.24523	31.69825	0.10554	0.03527	15490.22071	0	Yes	*545.3174	*546.3252
551.20895	0.0336	2.39365	0.08613	0.03887	14179.43346	2	No	1100.4022 (2)	551.2090 (2)
552.25612	0.03364	2.39419	0.06632	0.01902	29039.84988	2	No	1102.4966 (2)	552.2561 (2)
554.19131	0.16173	8.04615	0.07972	0.02084	26589.76787	0	Yes	*553.1835	*554.1913

561.18356	0.04747	2.39419	0.07354	0.0265	21179.30398	0	Yes	*560.1757	*561.1836
574.20389	0.04116	2.0277	0.06086	0.02029	28298.02842	0	Yes	*573.1961	*574.2039
574.27331	0.08232	2.93356	0.1082	0.05827	9855.38576	0	Yes	*573.2655	*574.2733
578.23733	0.10325	2.60962	0.1425	0.09322	6203.08167	2	Yes	*1154.4590 (2)	*578.2373 (2)
580.2418	0.48268	13.27048	0.12916	0.04011	14466.21783	1	Yes	*579.2340 (1)	*580.2418 (1)
588.31656	0.10415	2.60962	0.12321	0.07453	7893.4683	1	Yes	*587.3087 (1)	*588.3166 (1)
590.30107	0.02087	2.39365	0.05485	0.00793	74442.79435	0	Yes	*589.2932	*590.3011
596.36042	0.05592	2.02823	0.07581	0.02757	21632.16188	1	Yes	*595.3526 (1)	*596.3604 (1)
614.30044	0.05676	2.60962	0.09093	0.04118	14918.44699	0	Yes	*613.2926	*614.3004
615.27566	0.07101	3.99076	0.091	0.01967	31282.83047	1	Yes	*614.2678 (1)	*615.2757 (1)
616.30849	0.09239	4.52933	0.09808	0.01496	41190.60892	1	Yes	*615.3007 (1)	*616.3085 (1)
621.27718	0.09989	2.61015	0.11254	0.06221	9987.40146	1	Yes	*620.2694 (1)	*621.2772 (1)
622.24613	0.06427	2.39365	0.13375	0.08354	7448.3898	1	No	621.2383 (1)	622.2461 (1)
631.2495	0.03481	2.39419	0.04963	0.02033	31047.46574	2	No	1260.4833 (2)	631.2495 (2)
631.3197	0.24455	7.72301	0.10636	0.03947	15996.55604	0	Yes	*630.3119	*631.3197
632.30589	0.47508	15.18591	0.15612	0.0347	18219.87811	1	Yes	*631.2981 (1)	*632.3059 (1)
639.2877	0.13752	4.42215	0.10703	0.04293	14892.66417	1	Yes	*638.2799 (1)	*639.2877 (1)
648.31486	0.07289	2.0277	0.1006	0.04974	13034.15296	0	Yes	*647.3070	*648.3149
649.33326	11.0365	254.40488	0.2373	0.03631	17882.38637	0	Yes	*648.3254	*649.3333
662.32181	0.0221	2.39365	0.0581	0.0084	78853.44907	0	Yes	*661.3140	*662.3218
667.27932	0.43628	12.57816	0.15308	0.02991	22311.23414	0	Yes	*666.2715	*667.2793
674.28536	0.07433	2.71813	0.10259	0.04938	13653.8293	1	Yes	*673.2775 (1)	*674.2854 (1)
675.8605	0.06698	2.39365	0.10271	0.05038	13414.09332	2	Yes	*1349.7053 (2)	*675.8605 (2)
676.36139	0.05211	2.39472	0.08807	0.0336	20129.21222	2	No	1350.7071 (2)	676.3614 (2)
676.88257	0.02234	2.39365	0.05874	0.00849	79715.51979	2	No	1351.7495 (2)	676.8826 (2)
684.29911	0.06739	2.82612	0.0812	0.02619	26126.29007	0	Yes	*683.2913	*684.2991
686.27597	0.0225	2.39365	0.05914	0.00855	80266.74355	2	Yes	*1370.5363 (2)	*686.2760 (2)
691.30988	0.09785	2.7184	0.11872	0.06484	10661.18092	0	Yes	*690.3020	*691.3099
728.36271	0.05408	2.60962	0.09139	0.04403	16540.63078	1	Yes	*727.3549 (1)	*728.3627 (1)
732.28821	0.02324	2.39365	0.06109	0.00883	82913.91458	0	Yes	*731.2804	*732.2882
734.35868	0.1086	3.98942	0.15295	0.04431	16574.47687	0	Yes	*733.3509	*734.3587
752.3799	0.09422	2.61015	0.10837	0.05297	14202.71797	1	Yes	*751.3721 (1)	*752.3799 (1)
758.45935	0.02365	2.39365	0.06217	0.00899	84382.5476	0	Yes	*757.4515	*758.4594
760.29163	0.03947	2.60962	0.07003	0.01503	50571.54274	0	Yes	*759.2838	*760.2916
762.34552	0.30035	7.72328	0.15584	0.03917	19461.0776	1	Yes	*761.3377 (1)	*762.3455 (1)
767.24349	0.02379	2.39365	0.05472	0.00904	84869.78617	0	Yes	*766.2357	*767.2435
770.23237	0.02383	2.39365	0.06266	0.00906	85034.93713	0	Yes	*769.2245	*770.2324
772.40334	0.02387	2.39365	0.06274	0.00907	85154.69319	0	Yes	*771.3955	*772.4033
775.92097	0.07176	4.42135	0.06289	0.01521	51016.31905	2	Yes	*1549.8263 (2)	*775.9210 (2)
780.36145	0.27189	6.66715	0.13402	0.03548	21993.34887	0	Yes	*779.3536	*780.3615
795.34417	0.20182	3.04315	0.15121	0.08984	8853.12978	1	Yes	*794.3363 (1)	*795.3442 (1)
856.41231	0.02513	2.39365	0.06607	0.00955	89666.08135	0	Yes	*855.4045	*856.4123
888.39289	0.07679	2.39419	0.11776	0.05614	15824.02961	0	Yes	*887.3851	*888.3929
891.37936	0.05983	4.20539	0.07583	0.0134	66500.37994	1	No	890.3715 (1)	891.3794 (1)
908.4178	0.43139	10.33504	0.17861	0.0426	21323.91458	1	Yes	*907.4100 (1)	*908.4178 (1)
923.42823	0.33056	9.49193	0.15436	0.02682	34424.76669	0	Yes	*922.4204	*923.4282
924.39301	0.23499	9.79192	0.11154	0.01143	80904.33272	0	Yes	*923.3852	*924.3930
941.43792	6.28003	109.98362	0.30306	0.05313	17718.18592	0	Yes	*940.4301	*941.4379
942.46625	0.04394	2.39419	0.08663	0.02484	37936.52668	0	Yes	*941.4584	*942.4663
951.4153	0.20308	3.04262	0.1915	0.12392	7677.60567	1	No	950.4075 (1)	951.4153 (1)
1022.56167	0.06408	3.98942	0.09926	0.01044	97971.77345	0	Yes	*1021.5538	*1022.5617
1046.46782	0.07408	2.60962	0.10955	0.04653	22489.62511	0	Yes	*1045.4600	*1046.4678

Table S2. List of ions detected for $_{137}$**K**YLYEIAR$_{144}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
136.07549	0.27488	27	0.01975	0.0102	13334.26761	0	Yes	*135.0677	*136.0755
147.00714	0.17108	17	0.02737	0.008	18366.55549	0	Yes	*145.9993	*147.0071
165.01788	1.52074	114	0.03625	0.01208	13656.14822	0	Yes	*164.0101	*165.0179
175.11828	0.67967	55	0.04108	0.01188	14746.45727	0	Yes	*174.1105	*175.1183
221.08497	0.29792	23	0.03357	0.0111	19913.94257	0	Yes	*220.0771	*221.0850
229.12871	0.42717	28	0.0299	0.01417	16165.17915	0	Yes	*228.1209	*229.1287
230.08089	0.31676	29	0.03424	0.00999	23035.88515	0	Yes	*229.0731	*230.0809
246.1553	1.29727	68	0.07527	0.01541	15978.57383	0	Yes	*245.1475	*246.1553
248.09138	14.74161	959	0.10223	0.01365	18179.9512	0	Yes	*247.0836	*248.0914
249.15997	0.95994	55	0.04455	0.01525	16339.87726	0	Yes	*248.1521	*249.1600
265.11888	2.10908	148	0.05054	0.01207	21960.74696	0	Yes	*264.1110	*265.1189
266.99851	0.25823	19	0.0415	0.01057	25248.80119	0	Yes	*265.9907	*266.9985
277.15509	1.01948	47	0.06577	0.02089	13269.38544	0	Yes	*276.1473	*277.1551
281.05136	0.38321	22	0.04258	0.0163	17237.13422	0	Yes	*280.0435	*281.0514
293.11323	1.03634	60	0.05315	0.0141	20792.7927	0	Yes	*292.1054	*293.1132
342.21455	0.54815	27	0.05742	0.01887	18137.1262	0	Yes	*341.2067	*342.2146
355.06992	2.18554	100	0.07976	0.01882	18865.62466	0	Yes	*354.0621	*355.0699
359.2405	3.13971	147	0.13371	0.01845	19475.31476	0	Yes	*358.2327	*359.2405
365.15019	0.36669	15	0.05932	0.02244	16272.99998	0	Yes	*364.1424	*365.1502
400.98118	0.24864	15	0.05651	0.01589	25229.57512	0	Yes	*399.9733	*400.9812
406.19728	1.8314	74	0.091	0.02292	17724.27141	0	Yes	*405.1894	*406.1973
410.17239	0.69441	28	0.06858	0.02072	19797.7703	0	Yes	*409.1646	*410.1724
428.18243	33.45141	1279	0.1635	0.02357	18165.61814	0	Yes	*427.1746	*428.1824
429.1847	0.46478	14	0.08185	0.02874	14931.11343	0	Yes	*428.1769	*429.1847
439.15088	0.49676	18	0.06505	0.02996	14656.36907	1	Yes	*438.1430 (1)	*439.1509 (1)
440.21961	0.24868	14	0.06513	0.00791	55635.46697	1	Yes	*439.2118 (1)	*440.2196 (1)
456.17795	10.70758	360	0.13863	0.02649	17218.86276	0	Yes	*455.1701	*456.1779
470.27347	0.62728	17	0.05508	0.03679	12782.18807	1	Yes	*469.2656 (1)	*470.2735 (1)
471.2546	0.4564	17	0.07351	0.03814	12357.42731	1	No	470.2468 (1)	471.2546 (1)
488.28458	7.63268	246	0.11848	0.02805	17409.43707	0	Yes	*487.2768	*488.2846
519.28474	0.3344	15	0.05788	0.01833	28333.45065	2	Yes	*1036.5538 (2)	*519.2847 (2)
541.26723	0.97826	31	0.07879	0.03429	15785.7787	1	Yes	*540.2594 (1)	*541.2672 (1)
551.24802	0.76196	22	0.08613	0.03423	16102.92951	1	Yes	*550.2402 (1)	*551.2480 (1)
569.26102	8.40964	234	0.1414	0.03163	17999.70228	0	Yes	*568.2532	*569.2610
610.18913	0.71452	18	0.12547	0.03547	17200.89644	0	Yes	*609.1813	*610.1891
610.30725	18.66998	530	0.16732	0.0328	18607.90804	0	Yes	*609.2994	*610.3072
610.80999	0.54401	18	0.06277	0.03036	20116.54054	0	Yes	*609.8022	*610.8100
634.32152	0.65744	19	0.10661	0.03258	19472.18725	0	Yes	*633.3137	*634.3215
651.34767	35.14677	874	0.21607	0.03595	18120.47984	0	Yes	*650.3398	*651.3477
652.34995	0.66311	19	0.07929	0.04114	15855.16858	0	Yes	*651.3421	*652.3499
704.33584	0.65907	17	0.09736	0.05029	14006.48509	0	Yes	*703.3280	*704.3358
732.33007	0.96606	23	0.09928	0.03899	18784.87514	0	Yes	*731.3222	*732.3301
746.42182	0.78641	22	0.08481	0.0302	24718.17289	1	Yes	*745.4140 (1)	*746.4218 (1)
747.41157	0.82937	17	0.10029	0.05915	12636.17235	1	No	746.4037 (1)	747.4116 (1)
764.43313	65.21644	1381	0.19506	0.04345	17594.67408	0	Yes	*763.4253	*764.4331
765.43994	1.58883	36	0.17176	0.0387	19778.40535	0	Yes	*764.4321	*765.4399
861.36881	1.04358	19	0.14908	0.05913	14568.16973	1	Yes	*860.3610 (1)	*861.3688 (1)
927.4943	28.3271	500	0.24065	0.05487	16902.93447	0	Yes	*926.4865	*927.4943

Table S3. List of ions detected for $_{200}$CASLQ**K**FGER$_{209}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
133.04354	0.15624	15	0.01953	0.00929	14320.66201	0	Yes	*132.0357	*133.0435
141.06564	0.09385	13	0.01676	0.00584	24173.48263	0	Yes	*140.0578	*141.0656
175.11917	0.17178	14	0.02241	0.01162	15072.90963	0	Yes	*174.1113	*175.1192
187.05333	0.13894	9	0.04246	0.01168	16021.47752	0	Yes	*186.0455	*187.0533
204.08007	1.09453	77	0.04031	0.01303	15659.91292	1	Yes	*203.0722 (1)	*204.0801 (1)
232.07521	0.96513	57	0.03869	0.01499	15486.72469	0	Yes	*231.0674	*232.0752
248.09226	0.39115	29	0.03556	0.01131	21942.44202	0	Yes	*247.0844	*248.0923
301.09729	0.89855	46	0.06366	0.01632	18446.71425	0	Yes	*300.0895	*301.0973
304.16418	0.14765	10	0.02953	0.01476	20600.49414	0	Yes	*303.1564	*304.1642
319.10687	1.3989	73	0.07058	0.01721	18540.12378	0	Yes	*318.0990	*319.1069
361.18279	1.019	45	0.06436	0.02099	17211.46781	0	Yes	*360.1750	*361.1828
387.16936	0.19157	12	0.04442	0.01629	23770.2292	0	Yes	*386.1615	*387.1694
414.18148	0.49391	20	0.05169	0.02355	17589.58773	1	Yes	*413.1736 (1)	*414.1815 (1)
432.19139	0.20533	9	0.04107	0.02141	20183.17094	0	Yes	*431.1836	*432.1914
508.25128	2.22353	71	0.11452	0.02752	18471.0791	0	Yes	*507.2435	*508.2513
560.2485	0.32396	13	0.05344	0.0268	20906.57881	1	Yes	*559.2407 (1)	*560.2485 (1)
607.39155	0.35818	9	0.09041	0.03941	15411.74203	0	Yes	*606.3837	*607.3916
671.30184	1.09674	28	0.10967	0.03789	17718.2535	0	Yes	*670.2940	*671.3018
680.30545	4.57456	116	0.19137	0.03613	18830.5163	0	Yes	*679.2976	*680.3055
782.34297	0.35914	10	0.09472	0.03881	20159.16969	1	Yes	*781.3351 (1)	*782.3430 (1)
800.35577	3.99179	81	0.13572	0.04386	18249.45758	0	Yes	*799.3479	*800.3558
852.35066	0.41606	10	0.11534	0.03419	24929.04235	0	Yes	*851.3428	*852.3507
910.40426	0.85148	15	0.12772	0.05393	16882.18082	1	Yes	*909.3964 (1)	*910.4043 (1)
911.38825	1.10326	20	0.12779	0.04686	19450.64863	1	No	910.3804 (1)	911.3883 (1)
928.41472	6.43174	116	0.18917	0.05107	18179.12411	0	Yes	*927.4069	*928.4147
999.42048	0.33901	9	0.14274	0.02007	49789.3411	0	Yes	*998.4126	*999.4205
1041.50012	3.70208	64	0.17304	0.0545	19110.28662	0	Yes	*1040.4923	*1041.5001
1110.51852	2.00778	30	0.18808	0.06903	16086.34676	1	Yes	*1109.5107 (1)	*1110.5185 (1)
1111.50371	0.59272	11	0.14112	0.04032	27566.26238	1	No	1110.4959 (1)	1111.5037 (1)
1128.52962	12.08712	172	0.24648	0.06463	17461.38954	0	Yes	*1127.5218	*1128.5296
1199.56473	1.51495	25	0.12706	0.0657	18259.29392	0	Yes	*1198.5569	*1199.5647

Table S4. List of ions detected for $_{349}$LA**K**TYETTLEK$_{359}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
157.13393	1.16029	106	0.03537	0.01028	15280.26132	0	Yes	*156.1261	*157.1339
165.01756	0.85372	75	0.03263	0.01013	16288.08549	0	Yes	*164.0097	*165.0176
185.12855	1.00484	79.8	0.05376	0.01198	15459.07735	0	Yes	*184.1207	*185.1285
248.09215	14.45486	871	0.10223	0.01485	16702.48719	0	Yes	*247.0843	*248.0921
258.14586	1.07004	60	0.06801	0.01608	16056.44684	0	Yes	*257.1380	*258.1459
265.11816	1.9896	115	0.06433	0.01432	18519.37237	0	Yes	*264.1103	*265.1182
276.15553	1.57336	84	0.07034	0.01512	18261.74633	0	Yes	*275.1477	*276.1555
364.15115	1.72325	88	0.09155	0.01695	21487.15174	0	Yes	*363.1433	*364.1511
366.16709	1.30681	52	0.0756	0.02239	16355.76254	0	Yes	*365.1593	*366.1671
376.1506	1.46681	59	0.08757	0.02208	17036.13469	1	Yes	*375.1428 (1)	*376.1506 (1)
389.24088	1.7009	65	0.06681	0.02517	15464.43229	0	Yes	*388.2330	*389.2409
394.16172	2.96381	117	0.10085	0.02234	17645.34144	0	Yes	*393.1539	*394.1617
477.23424	9.77743	300	0.14796	0.02735	17447.02916	0	Yes	*476.2264	*477.2342
490.28806	2.79625	89	0.09998	0.02611	18777.64775	0	Yes	*489.2802	*490.2881
578.27564	3.27432	69	0.14251	0.05702	10141.20164	0	Yes	*577.2678	*578.2756
591.33519	5.37667	146	0.13038	0.03431	17234.16819	0	Yes	*590.3274	*591.3352
629.80041	1.55097	46	0.12748	0.03364	18721.91493	0	Yes	*628.7926	*629.8004
638.80444	6.14107	170	0.12839	0.03287	19434.42978	0	Yes	*637.7966	*638.8044
674.32144	2.05553	56	0.08794	0.03235	20846.38229	0	Yes	*673.3136	*674.3214
720.37883	7.77871	172	0.16663	0.04117	17496.35371	0	Yes	*719.3710	*720.3788
721.85927	3.19202	86	0.09857	0.03342	21601.59571	0	Yes	*720.8514	*721.8593
730.86253	15.47952	381	0.16021	0.03727	19611.33812	0	Yes	*729.8547	*730.8625
883.43728	24.42514	464	0.2097	0.05142	17182.24365	0	Yes	*882.4295	*883.4373
966.47924	3.16709	56	0.19301	0.05571	17348.66472	0	Yes	*965.4714	*966.4792
984.48764	44.60438	718	0.25678	0.05777	17040.75356	0	Yes	*983.4798	*984.4876
1258.57983	3.03348	52	0.20023	0.06638	18959.42999	0	Yes	*1257.5720	*1258.5798
1276.5886	26.96154	371	0.28232	0.07131	17902.90394	0	Yes	*1275.5808	*1276.5886
1347.63171	13.11524	186	0.30043	0.06509	20703.24629	0	Yes	*1346.6239	*1347.6317

Table S5. List of ions detected for $_{429}$NLG**K**VGSR$_{436}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
102.05596	0.03814	7.11652	0.04846	0.00488	20914.11897	0	Yes	*101.0481	*102.0560
120.07821	0.05409	7.80601	0.05257	0.00661	18168.12681	0	Yes	*119.0704	*120.0782
129.10197	0.08578	8.84024	0.06413	0.00797	16196.21817	2	Yes	*256.1883 (2)	*129.1020 (2)
130.08333	0.06293	5.69007	0.07403	0.00939	13856.34784	0	Yes	*129.0755	*130.0833
136.07485	0.07791	7.84244	0.06255	0.00862	15787.01938	1	Yes	*135.0670 (1)	*136.0749 (1)
147.11389	0.08453	10.48203	0.06503	0.00691	21291.61815	0	Yes	*146.1061	*147.1139
155.11489	0.07233	6.37956	0.06678	0.01076	14417.96446	0	Yes	*154.1071	*155.1149
177.05564	0.06569	9.27542	0.06759	0.00528	33517.82637	0	Yes	*176.0478	*177.0556
200.14015	0.6162	48.51666	0.08384	0.01098	18226.47769	0	Yes	*199.1323	*200.1402
228.13636	0.44736	26.56152	0.08951	0.0183	12465.198	1	Yes	*227.1285 (1)	*228.1364 (1)
248.09202	0.21039	15.47631	0.09334	0.01029	24104.50875	0	Yes	*247.0842	*248.0920
267.15978	0.08069	6.68401	0.08303	0.01416	18868.82569	0	Yes	*266.1519	*267.1598
276.17037	0.07721	7.15278	0.08441	0.00968	28515.36765	0	Yes	*275.1625	*276.1704
291.16356	0.18333	12.54646	0.10594	0.01415	20577.30743	0	Yes	*290.1557	*291.1636
294.18289	0.09463	5.69025	0.09681	0.01739	16915.92659	1	Yes	*293.1751 (1)	*294.1829 (1)
350.13454	0.23908	12.89524	0.11617	0.01525	22959.12722	0	Yes	*349.1267	*350.1345
390.23257	0.48758	17.59055	0.12822	0.02756	14157.68821	0	Yes	*389.2247	*390.2326
391.20207	0.16656	12.25339	0.13954	0.00938	41691.1794	0	Yes	*390.1942	*391.2021
409.54466	0.38784	16.25075	0.13706	0.02387	17160.52583	3	Yes	*1225.6105 (3)	*409.5447 (3)
409.8781	0.23515	10.13163	0.11998	0.02188	18729.12273	3	No	1226.6108 (3)	409.8781 (3)
410.20852	0.08234	9.23916	0.06859	0.00774	53023.68704	3	No	1227.6021 (3)	410.2085 (3)
426.72779	0.11397	5.69025	0.11659	0.02095	20373.35875	0	Yes	*425.7200	*426.7278
427.18728	0.12003	6.3433	0.12249	0.01534	27841.54993	3	Yes	*1278.5384 (3)	*427.1873 (3)
466.72409	0.31366	9.13366	0.15242	0.03735	12495.4894	0	Yes	*465.7163	*466.7241
475.23531	0.17092	5.91114	0.11074	0.02957	16071.96543	0	Yes	*474.2275	*475.2353
483.60586	0.15509	10.48203	0.06826	0.0137	35310.2622	0	Yes	*482.5980	*483.6059
483.75364	1.29649	39.27639	0.11793	0.02919	16573.98214	0	Yes	*482.7458	*483.7536
519.26105	0.25144	7.11798	0.13504	0.03948	13152.80964	1	Yes	*518.2532 (1)	*519.2610 (1)
537.26384	0.37692	13.92198	0.15699	0.02292	23441.98202	1	Yes	*536.2560 (1)	*537.2638 (1)
540.28214	0.16199	9.75668	0.12463	0.01044	51747.52459	2	Yes	*1078.5486 (2)	*540.2821 (2)
599.3637	0.11374	5.69007	0.13127	0.02015	29742.96951	1	Yes	*598.3559 (1)	*599.3637 (1)
613.80338	0.33812	10.01028	0.17479	0.03493	17571.72751	2	Yes	*1225.5911 (2)	*613.8034 (2)
614.31407	0.20871	8.3233	0.16786	0.01689	36371.85853	2	No	1226.6125 (2)	614.3141 (2)
666.30526	0.27733	8.4444	0.11655	0.04175	15959.31561	0	Yes	*665.2974	*666.3053
682.34742	0.19721	7.11669	0.17692	0.03737	18258.55757	0	Yes	*681.3396	*682.3474
705.349	0.10026	7.11652	0.12741	0.01283	54981.94365	0	Yes	*704.3412	*705.3490
723.33272	0.14838	7.15295	0.15179	0.01351	53526.28684	1	Yes	*722.3249 (1)	*723.3327 (1)
739.36365	5.31381	106.45715	0.24555	0.04788	15442.45872	0	Yes	*738.3558	*739.3637
852.43659	0.27978	10.96306	0.17303	0.01805	47228.13062	0	Yes	*851.4288	*852.4366
862.43795	1.99545	37.9659	0.25691	0.04756	18135.37004	0	Yes	*861.4301	*862.4379
951.44465	0.27766	9.32377	0.1828	0.04308	22083.1908	1	Yes	*950.4368 (1)	*951.4446 (1)

Table S6. List of ions detected for $_{525}$**K**QTALVELVK$_{534}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
147.11301	0.60584	54	0.02738	0.0104	14148.09714	0	Yes	*146.1052	147.11301
165.01799	1.13829	92	0.03625	0.01111	14854.74431	0	Yes	*164.0102	165.01799
246.18096	1.17336	72	0.06199	0.01458	16884.21078	0	Yes	*245.1731	246.18096
248.0919	12.45688	784	0.11557	0.01426	17400.56096	0	Yes	*247.0841	248.0919
265.11894	1.70701	98	0.06433	0.01536	17262.13704	0	Yes	*264.1111	265.11894
310.14015	7.8597	406	0.0994	0.01732	17902.27254	0	Yes	*309.1323	310.14015
342.20318	1.2555	64	0.06787	0.0173	19783.87993	0	Yes	*341.1954	342.20318
359.26626	1.79455	79	0.11767	0.0188	19109.09643	0	Yes	*358.2584	359.26626
404.14654	2.40543	92	0.0851	0.02344	17241.96099	0	Yes	*403.1387	404.14654
421.17263	8.49896	311	0.09846	0.02404	17516.27187	0	Yes	*420.1648	421.17263
488.30928	3.71665	121	0.11225	0.0277	17626.90163	0	Yes	*487.3014	488.30928
496.27727	1.67854	56	0.10059	0.02969	16716.99639	0	Yes	*495.2694	496.27727
504.21008	1.22615	49	0.06337	0.02371	21265.87244	1	Yes	*503.2022 (1)	504.21008
514.28809	1.65113	53	0.0832	0.02934	17531.22807	0	Yes	*513.2803	514.28809
522.22106	3.63073	109	0.14833	0.02999	17414.16532	0	Yes	*521.2132	522.22106
587.37871	4.03523	102	0.13679	0.03581	16400.45151	0	Yes	*586.3709	587.37871
627.37199	2.29016	60	0.1343	0.03534	17751.50229	0	Yes	*626.3642	627.37199
629.34363	3.84416	114	0.12743	0.03263	19284.51213	0	Yes	*628.3358	629.34363
637.85684	5.65187	167	0.10691	0.03022	21109.66511	2	Yes	*1273.6980 (2)	637.85684
638.3492	2.55252	71	0.09982	0.03418	18673.99521	2	No	1274.6827 (2)	638.3492
646.86185	31.71881	866.2	0.20815	0.03397	19042.82204	0	Yes	*645.8540	646.86185
700.46207	5.93022	138	0.13444	0.03952	17723.22558	0	Yes	*699.4542	700.46207
771.50001	10.16637	219	0.2038	0.03983	19370.71209	0	Yes	*770.4922	771.50001
872.54706	41.52942	749	0.30843	0.04964	17578.01607	0	Yes	*871.5392	872.54706
983.58016	3.69946	65	0.18586	0.05244	18756.14167	1	No	982.5723 (1)	983.58016
1000.60773	6.73517	105	0.21424	0.06069	16486.27723	0	Yes	*999.5999	1000.60773
147.11301	0.60584	54	0.02738	0.0104	14148.09714	0	Yes	*146.1052	147.11301
165.01799	1.13829	92	0.03625	0.01111	14854.74431	0	Yes	*164.0102	165.01799

Table S7. List of ions detected for $_{539}$AT**K**EQLK$_{545}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
145.0967	0.76653	69	0.03059	0.00953	15232.62123	0	Yes	*144.0889	145.0967
147.11154	0.59214	49	0.03081	0.01007	14601.84157	0	Yes	*146.1037	147.11154
173.09161	0.8595	68	0.03341	0.01189	14551.76868	0	Yes	*172.0838	173.09161
248.09087	3.54258	208	0.07556	0.01551	15994.44396	0	Yes	*247.0830	248.09087
260.19648	0.95593	63	0.05918	0.01317	19756.15222	0	Yes	*259.1886	260.19648
388.25478	1.16771	55	0.09453	0.01959	19814.78257	0	Yes	*387.2470	388.25478
394.15852	1.09251	45	0.10645	0.02056	19175.55258	0	Yes	*393.1507	394.15852
405.20558	1.21565	56	0.06817	0.01976	20503.26894	0	Yes	*404.1978	405.20558
422.15433	1.04657	41	0.06958	0.02411	17510.77151	0	Yes	*421.1465	422.15433
447.18679	2.30947	78	0.11935	0.02493	17935.07903	0	Yes	*446.1790	447.18679
455.73	3.72908	140	0.12049	0.02277	20015.82437	0	Yes	*454.7222	455.73
482.24381	6.0484	218	0.13014	0.02709	17799.87665	0	Yes	*481.2360	482.24381
491.24877	19.87122	678	0.1376	0.02656	18495.00179	0	Yes	*490.2409	491.24877
499.28698	1.43454	43	0.1072	0.03018	16546.1002	1	Yes	*498.2791 (1)	499.28698
517.29577	6.82596	240	0.15404	0.02566	20157.50228	0	Yes	*516.2879	517.29577
550.21116	1.57543	46	0.10591	0.02606	21110.00955	0	Yes	*549.2033	550.21116
809.40151	25.90019	495	0.21677	0.05043	16049.69837	0	Yes	*808.3937	809.40151
892.44219	1.28984	36	0.10959	0.03398	26266.08966	0	Yes	*891.4344	892.44219
910.45042	7.85083	142	0.17881	0.05496	16564.65681	0	Yes	*909.4426	910.45042
920.43421	2.15752	38	0.12842	0.0585	15732.84321	0	Yes	*919.4264	920.43421

Table S8. List of ions detected for $_{542}$EQL**K**AVMDDFAAFVEK$_{557}$

Mass/Charge	Area	Height	Width	Width at 50%	Resolution	Charge	Monoisotopic	Mass(charge)	Mass/charge (charge)
129.06547	0.36869	38	0.02244	0.0087	14829.47043	0	Yes	*128.0576	*129.0655
165.01824	0.6779	55	0.03625	0.01141	14459.14734	0	Yes	*164.0104	*165.0182
240.09813	2.29349	144	0.0481	0.01466	16376.14994	0	Yes	*239.0903	*240.0981
241.08198	0.62658	33	0.07887	0.01587	15189.76843	1	Yes	*240.0742 (1)	*241.0820 (1)
248.09171	10.19662	591	0.07556	0.01575	15754.58453	0	Yes	*247.0839	*248.0917
258.10834	3.42978	205	0.05894	0.01522	16953.90712	0	Yes	*257.1005	*258.1083
258.14407	0.91362	61	0.04081	0.01527	16905.95181	0	Yes	*257.1362	*258.1441
265.11849	0.65248	39	0.05974	0.01407	18840.29509	0	Yes	*264.1107	*265.1185
276.15558	1.13957	61	0.05159	0.01706	16182.72846	0	Yes	*275.1477	*276.1556
290.15001	0.58645	30	0.07691	0.0172	16870.34778	0	Yes	*289.1422	*290.1500
325.18761	0.75316	39	0.05598	0.0173	18794.54618	1	Yes	*324.1798 (1)	*325.1876 (1)
334.13997	0.57259	30	0.06706	0.01782	18750.65874	0	Yes	*333.1321	*334.1400
336.15547	0.95719	50	0.06209	0.01791	18769.14956	0	Yes	*335.1476	*336.1555
353.18237	2.42897	109	0.07955	0.01927	18327.0112	1	Yes	*352.1745 (1)	*353.1824 (1)
362.10218	0.71958	34	0.06981	0.01805	20062.10749	0	Yes	*361.0943	*362.1022
364.1506	1.14704	50	0.07001	0.02116	17205.80931	1	Yes	*363.1428 (1)	*364.1506 (1)
370.20875	1.95471	88	0.09773	0.01925	19230.69749	1	Yes	*369.2009 (1)	*370.2087 (1)
371.19327	1.54682	65	0.08699	0.02137	17371.18341	1	No	370.1854 (1)	371.1933 (1)
375.22431	1.90778	82	0.07653	0.0207	18124.23256	0	Yes	*374.2165	*375.2243
406.19708	2.58215	95	0.10806	0.02427	16736.63665	1	Yes	*405.1893 (1)	*406.1971 (1)
449.16722	1.09748	41	0.10168	0.02313	19422.76772	1	Yes	*448.1594 (1)	*449.1672 (1)
463.21854	1.33316	43	0.12755	0.02605	17782.46348	0	Yes	*462.2107	*463.2185
477.23464	2.47827	78	0.14179	0.02866	16650.66836	1	Yes	*476.2268 (1)	*477.2346 (1)
517.22877	1.34136	38	0.1091	0.03129	16531.40842	1	Yes	*516.2209 (1)	*517.2288 (1)
520.20439	1.59624	44	0.12873	0.03043	17096.99838	1	Yes	*519.1966 (1)	*520.2044 (1)
522.29251	4.4984	133	0.14833	0.03071	17007.6214	1	Yes	*521.2847 (1)	*522.2925 (1)
593.32983	3.78753	104	0.15123	0.03246	18278.69588	0	Yes	*592.3220	*593.3298
645.28812	5.82806	142	0.17205	0.03797	16993.76216	1	Yes	*644.2803 (1)	*645.2881 (1)
651.24699	2.26853	39	0.21606	0.04226	15410.3624	1	Yes	*650.2392 (1)	*651.2470 (1)
663.29917	1.76611	40	0.14536	0.04023	16486.35051	0	Yes	*662.2913	*663.2992
664.36687	2.61856	62	0.21093	0.03546	18735.81696	1	Yes	*663.3590 (1)	*664.3669 (1)
716.32529	3.19109	79	0.11329	0.03711	19304.24519	1	Yes	*715.3175 (1)	*716.3253 (1)
734.33751	2.03417	45	0.13	0.04079	18004.97521	1	Yes	*733.3297 (1)	*734.3375 (1)
750.31229	1.70832	39	0.1546	0.03981	18847.63465	1	Yes	*749.3045 (1)	*750.3123 (1)
811.43462	2.92607	59	0.16881	0.04604	17624.71967	1	Yes	*810.4268 (1)	*811.4346 (1)
833.40363	1.75563	36	0.13849	0.04592	18149.79498	1	Yes	*832.3958 (1)	*833.4036 (1)
897.38068	1.67383	32	0.14371	0.04903	18302.21633	0	Yes	*896.3728	*897.3807
926.46218	3.19531	57	0.20615	0.04993	18556.41439	0	Yes	*925.4543	*926.4622
1041.48855	7.222	113	0.20946	0.05794	17974.211	0	Yes	*1040.4807	*1041.4885
1172.5294	20.72746	284	0.34787	0.06645	17644.63471	0	Yes	*1171.5216	*1172.5294
1173.53291	2.67784	36	0.23202	0.06815	17218.75772	0	Yes	*1172.5251	*1173.5329
1271.59781	16.08084	209	0.3019	0.07049	18038.14244	0	Yes	*1270.5900	*1271.5978
1272.60276	2.26509	32	0.20134	0.07047	18058.92186	0	Yes	*1271.5949	*1272.6028
1342.63133	25.54068	325	0.35158	0.0737	18218.68666	0	Yes	*1341.6235	*1342.6313
1343.63631	3.63082	45	0.20689	0.07343	18299.32938	0	Yes	*1342.6285	*1343.6363

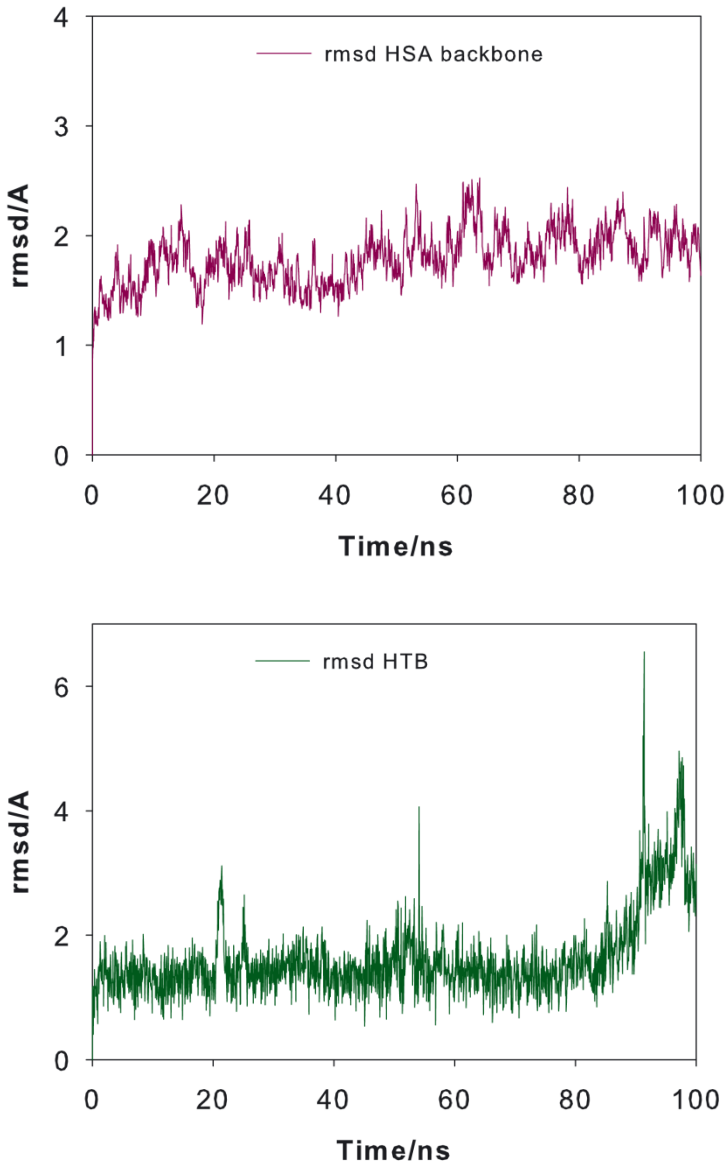


Figure S16. The rmsd plots for the protein backbone (Cα, C, N and O atoms) (up) and ligand (down) calculated for the binary HTB@HSA complex obtained from MD simulation studies.